



## Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 04:42 PM JST

PDB ID : 8Z9D  
EMDB ID : EMD-39860  
Title : cryo-EM structure of PSII-LHCII megacomplex from spinach  
Authors : Shan, J.Y.; Liu, Z.F.  
Deposited on : 2024-04-23  
Resolution : 3.22 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

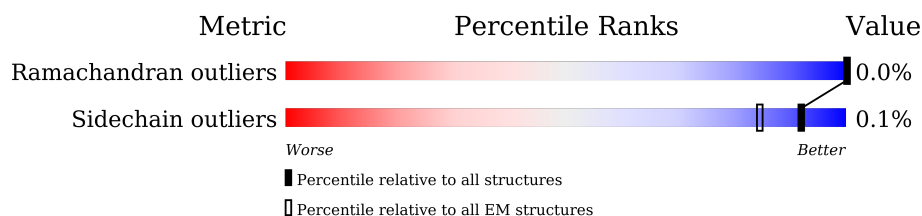
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

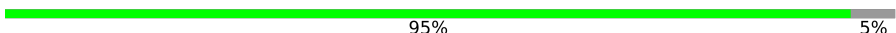
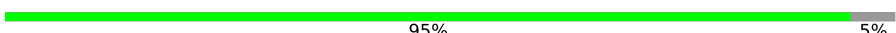
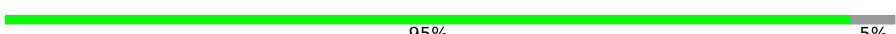
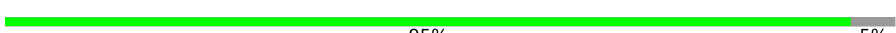






The reported resolution of this entry is 3.22 Å.

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	207382	16835
Sidechain outliers	206894	16415











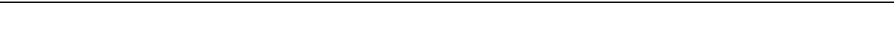

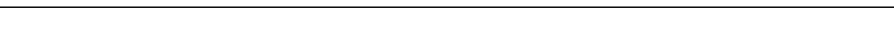
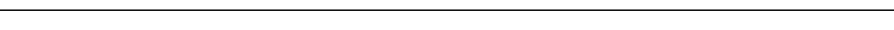











The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	351	 95% 5%
1	AA	351	 95% 5%
1	Aa	351	 95% 5%
1	a	351	 95% 5%
2	O	332	 71% 29%
2	OO	332	 71% 29%
2	Oo	332	 70% 30%
2	o	332	 70% 30%
3	R	286	 79% 21%
3	RR	286	 79% 21%

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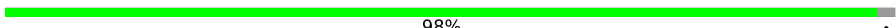
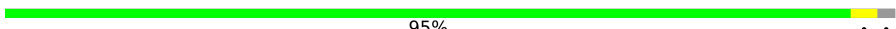
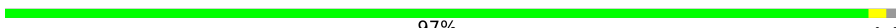
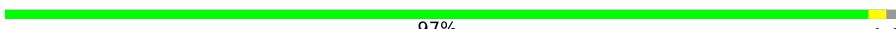














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Mol	Chain	Length	Quality of chain	
3	Rr	286		80% 20%
3	r	286		80% 20%
4	S	295		75% 25%
4	SS	295		75% 25%
4	Ss	295		72% 28%
4	s	295		72% 28%
5	T	33		91% 9%
5	TT	33		91% 9%
5	Tt	33		91% 9%
5	t	33		91% 9%
6	U	99		27% 73%
6	UU	99		27% 73%
6	Uu	99		26% 74%
6	u	99		26% 74%
7	W	137		39% 61%
7	WW	137		39% 61%
7	Ww	137		39% 61%
7	w	137		39% 61%
8	X	117		39% 61%
8	XX	117		41% 59%
8	Xx	117		29% 71%
8	x	117		29% 71%
9	G	267		80% 19%
9	GG	267		81% 19%
9	Gg	267		81% 19%

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Mol	Chain	Length	Quality of chain
9	N	267	 81% 19%
9	NN	267	 82% 18%
9	Nn	267	 82% 18%
9	Y	267	 82% 18%
9	YY	267	 81% 18%
9	Yy	267	 82% 18%
9	g	267	 81% 19%
9	n	267	 81% 18%
9	y	267	 82% 18%
10	Z	62	 98%
10	ZZ	62	 95%
10	Zz	62	 97%
10	z	62	 97%
11	4	259	 71% 28%
11	44	259	 71% 28%
12	P	267	 69% 30%
12	PP	267	 70% 30%
12	Pp	267	 70% 30%
12	p	267	 70% 30%
13	Q	232	 63% 37%
13	QQ	232	 63% 37%
13	Qq	232	 63% 37%
13	q	232	 63% 37%
14	1	267	 77% 22%
14	11	267	 76% 23%




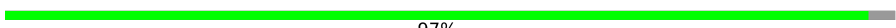
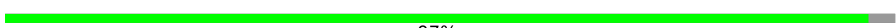








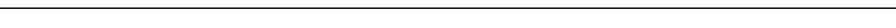


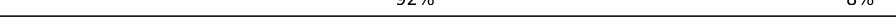
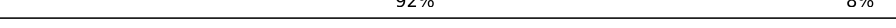
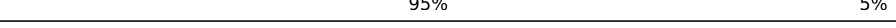
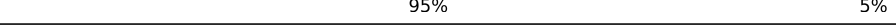
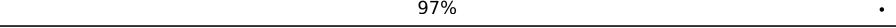
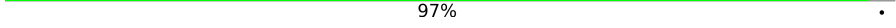
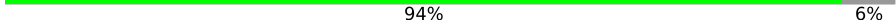
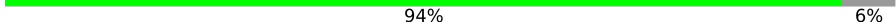
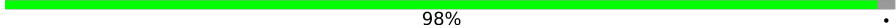
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Mol	Chain	Length	Quality of chain	
14	2	267	<div><div></div></div>	82% 18%
14	22	267	<div><div></div></div>	82% 18%
15	3	264	<div><div></div></div>	79% 21%
15	33	264	<div><div></div></div>	78% 22%
16	0	140	<div><div></div></div>	71% 29%
16	00	140	<div><div></div></div>	71% 29%
17	5	199	<div><div></div></div>	20% 80%
17	55	199	<div><div></div></div>	20% 80%
18	C	473	<div><div></div></div>	95% 5%
18	CC	473	<div><div></div></div>	95% 5%
18	Cc	473	<div><div></div></div>	95% 5%
18	c	473	<div><div></div></div>	95% 5%
19	D	352	<div><div></div></div>	96% .
19	DD	352	<div><div></div></div>	96% .
19	Dd	352	<div><div></div></div>	97% .
19	d	352	<div><div></div></div>	97% .
20	E	83	<div><div></div></div>	96% .
20	EE	83	<div><div></div></div>	96% .
20	Ee	83	<div><div></div></div>	90% 10%
20	e	83	<div><div></div></div>	90% 10%
21	F	39	<div><div></div></div>	87% 13%
21	FF	39	<div><div></div></div>	87% 13%
21	Ff	39	<div><div></div></div>	79% 21%
21	f	39	<div><div></div></div>	79% 21%
22	H	73	<div><div></div></div>	81% 19%

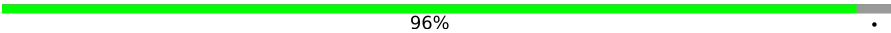
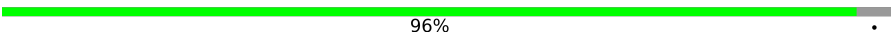
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Mol	Chain	Length	Quality of chain
22	HH	73	 81% 19%
22	Hh	73	 81% 19%
22	h	73	 81% 19%
23	I	36	 97% .
23	II	36	 97% .
23	Ii	36	 92% 8%
23	i	36	 92% 8%
24	J	40	 92% 8%
24	JJ	40	 92% 8%
24	Jj	40	 85% 15%
24	j	40	 85% 15%
25	K	59	 63% 37%
25	KK	59	 63% 37%
25	Kk	59	 63% 37%
25	k	59	 63% 37%
26	L	38	 92% 8%
26	LL	38	 92% 8%
26	Ll	38	 95% 5%
26	l	38	 95% 5%
27	M	34	 97% .
27	MM	34	 97% .
27	Mm	34	 94% 6%
27	m	34	 94% 6%
28	B	508	 98% .
28	BB	508	 98% .

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Mol	Chain	Length	Quality of chain
28	Bb	508	 96%
28	b	508	 96%

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
32	CLA	1	602	X	-	-	-
32	CLA	1	603	X	-	-	-
32	CLA	1	604	X	-	-	-
32	CLA	1	609	X	-	-	-
32	CLA	1	610	X	-	-	-
32	CLA	1	611	X	-	-	-
32	CLA	1	612	X	-	-	-
32	CLA	1	613	X	-	-	-
32	CLA	11	602	X	-	-	-
32	CLA	11	603	X	-	-	-
32	CLA	11	604	X	-	-	-
32	CLA	11	609	X	-	-	-
32	CLA	11	610	X	-	-	-
32	CLA	11	611	X	-	-	-
32	CLA	11	612	X	-	-	-
32	CLA	11	613	X	-	-	-
32	CLA	2	602	X	-	-	-
32	CLA	2	603	X	-	-	-
32	CLA	2	604	X	-	-	-
32	CLA	2	609	X	-	-	-
32	CLA	2	610	X	-	-	-
32	CLA	2	611	X	-	-	-
32	CLA	2	612	X	-	-	-
32	CLA	2	613	X	-	-	-
32	CLA	22	602	X	-	-	-
32	CLA	22	603	X	-	-	-
32	CLA	22	604	X	-	-	-
32	CLA	22	609	X	-	-	-
32	CLA	22	610	X	-	-	-
32	CLA	22	611	X	-	-	-
32	CLA	22	612	X	-	-	-
32	CLA	22	613	X	-	-	-
32	CLA	3	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	3	603	X	-	-	-
32	CLA	3	604	X	-	-	-
32	CLA	3	609	X	-	-	-
32	CLA	3	610	X	-	-	-
32	CLA	3	611	X	-	-	-
32	CLA	3	612	X	-	-	-
32	CLA	3	613	X	-	-	-
32	CLA	33	602	X	-	-	-
32	CLA	33	603	X	-	-	-
32	CLA	33	604	X	-	-	-
32	CLA	33	609	X	-	-	-
32	CLA	33	610	X	-	-	-
32	CLA	33	611	X	-	-	-
32	CLA	33	612	X	-	-	-
32	CLA	33	613	X	-	-	-
32	CLA	4	303	X	-	-	-
32	CLA	4	304	X	-	-	-
32	CLA	4	305	X	-	-	-
32	CLA	4	310	X	-	-	-
32	CLA	4	311	X	-	-	-
32	CLA	4	312	X	-	-	-
32	CLA	44	602	X	-	-	-
32	CLA	44	603	X	-	-	-
32	CLA	44	604	X	-	-	-
32	CLA	44	609	X	-	-	-
32	CLA	44	610	X	-	-	-
32	CLA	44	611	X	-	-	-
32	CLA	44	615	X	-	-	-
32	CLA	A	405	X	-	-	-
32	CLA	A	406	X	-	-	-
32	CLA	A	408	X	-	-	-
32	CLA	AA	405	X	-	-	-
32	CLA	AA	406	X	-	-	-
32	CLA	AA	408	X	-	-	-
32	CLA	Aa	405	X	-	-	-
32	CLA	Aa	406	X	-	-	-
32	CLA	Aa	407	X	-	-	-
32	CLA	Aa	410	X	-	-	-
32	CLA	B	604	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	B	609	X	-	-	-
32	CLA	B	610	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	618	X	-	-	-
32	CLA	B	619	X	-	-	-
32	CLA	B	620	X	-	-	-
32	CLA	B	621	X	-	-	-
32	CLA	B	622	X	-	-	-
32	CLA	B	623	X	-	-	-
32	CLA	B	624	X	-	-	-
32	CLA	BB	601	X	-	-	-
32	CLA	BB	602	X	-	-	-
32	CLA	BB	603	X	-	-	-
32	CLA	BB	604	X	-	-	-
32	CLA	BB	605	X	-	-	-
32	CLA	BB	606	X	-	-	-
32	CLA	BB	607	X	-	-	-
32	CLA	BB	608	X	-	-	-
32	CLA	BB	610	X	-	-	-
32	CLA	BB	611	X	-	-	-
32	CLA	BB	612	X	-	-	-
32	CLA	BB	613	X	-	-	-
32	CLA	BB	614	X	-	-	-
32	CLA	BB	615	X	-	-	-
32	CLA	Bb	601	X	-	-	-
32	CLA	Bb	602	X	-	-	-
32	CLA	Bb	603	X	-	-	-
32	CLA	Bb	604	X	-	-	-
32	CLA	Bb	605	X	-	-	-
32	CLA	Bb	606	X	-	-	-
32	CLA	Bb	607	X	-	-	-
32	CLA	Bb	608	X	-	-	-
32	CLA	Bb	609	X	-	-	-
32	CLA	Bb	610	X	-	-	-
32	CLA	Bb	611	X	-	-	-
32	CLA	Bb	612	X	-	-	-
32	CLA	Bb	613	X	-	-	-
32	CLA	Bb	614	X	-	-	-
32	CLA	Bb	615	X	-	-	-
32	CLA	Bb	616	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	C	506	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	511	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	C	514	X	-	-	-
32	CLA	C	515	X	-	-	-
32	CLA	CC	502	X	-	-	-
32	CLA	CC	504	X	-	-	-
32	CLA	CC	505	X	-	-	-
32	CLA	CC	506	X	-	-	-
32	CLA	CC	507	X	-	-	-
32	CLA	CC	508	X	-	-	-
32	CLA	CC	509	X	-	-	-
32	CLA	CC	510	X	-	-	-
32	CLA	CC	511	X	-	-	-
32	CLA	CC	512	X	-	-	-
32	CLA	CC	513	X	-	-	-
32	CLA	CC	514	X	-	-	-
32	CLA	Cc	503	X	-	-	-
32	CLA	Cc	505	X	-	-	-
32	CLA	Cc	506	X	-	-	-
32	CLA	Cc	507	X	-	-	-
32	CLA	Cc	508	X	-	-	-
32	CLA	Cc	509	X	-	-	-
32	CLA	Cc	510	X	-	-	-
32	CLA	Cc	511	X	-	-	-
32	CLA	Cc	512	X	-	-	-
32	CLA	Cc	513	X	-	-	-
32	CLA	Cc	514	X	-	-	-
32	CLA	Cc	515	X	-	-	-
32	CLA	D	401	X	-	-	-
32	CLA	D	404	X	-	-	-
32	CLA	D	405	X	-	-	-
32	CLA	DD	401	X	-	-	-
32	CLA	DD	403	X	-	-	-
32	CLA	DD	404	X	-	-	-
32	CLA	Dd	402	X	-	-	-
32	CLA	G	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	G	603	X	-	-	-
32	CLA	G	604	X	-	-	-
32	CLA	G	610	X	-	-	-
32	CLA	G	611	X	-	-	-
32	CLA	G	612	X	-	-	-
32	CLA	G	613	X	-	-	-
32	CLA	G	614	X	-	-	-
32	CLA	GG	602	X	-	-	-
32	CLA	GG	603	X	-	-	-
32	CLA	GG	604	X	-	-	-
32	CLA	GG	610	X	-	-	-
32	CLA	GG	611	X	-	-	-
32	CLA	GG	612	X	-	-	-
32	CLA	GG	613	X	-	-	-
32	CLA	GG	614	X	-	-	-
32	CLA	Gg	304	X	-	-	-
32	CLA	Gg	305	X	-	-	-
32	CLA	Gg	311	X	-	-	-
32	CLA	Gg	312	X	-	-	-
32	CLA	Gg	313	X	-	-	-
32	CLA	Gg	314	X	-	-	-
32	CLA	Gg	315	X	-	-	-
32	CLA	N	602	X	-	-	-
32	CLA	N	603	X	-	-	-
32	CLA	N	604	X	-	-	-
32	CLA	N	610	X	-	-	-
32	CLA	N	611	X	-	-	-
32	CLA	N	612	X	-	-	-
32	CLA	N	613	X	-	-	-
32	CLA	N	614	X	-	-	-
32	CLA	NN	602	X	-	-	-
32	CLA	NN	603	X	-	-	-
32	CLA	NN	604	X	-	-	-
32	CLA	NN	610	X	-	-	-
32	CLA	NN	611	X	-	-	-
32	CLA	NN	612	X	-	-	-
32	CLA	NN	613	X	-	-	-
32	CLA	NN	614	X	-	-	-
32	CLA	Nn	301	X	-	-	-
32	CLA	Nn	302	X	-	-	-
32	CLA	Nn	303	X	-	-	-
32	CLA	Nn	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	Nn	312	X	-	-	-
32	CLA	Nn	313	X	-	-	-
32	CLA	Nn	314	X	-	-	-
32	CLA	R	601	X	-	-	-
32	CLA	R	602	X	-	-	-
32	CLA	R	603	X	-	-	-
32	CLA	R	604	X	-	-	-
32	CLA	R	608	X	-	-	-
32	CLA	R	609	X	-	-	-
32	CLA	R	610	X	-	-	-
32	CLA	R	611	X	-	-	-
32	CLA	R	612	X	-	-	-
32	CLA	R	613	X	-	-	-
32	CLA	RR	302	X	-	-	-
32	CLA	RR	303	X	-	-	-
32	CLA	RR	304	X	-	-	-
32	CLA	RR	308	X	-	-	-
32	CLA	RR	309	X	-	-	-
32	CLA	RR	310	X	-	-	-
32	CLA	RR	311	X	-	-	-
32	CLA	RR	312	X	-	-	-
32	CLA	RR	313	X	-	-	-
32	CLA	Rr	601	X	-	-	-
32	CLA	Rr	602	X	-	-	-
32	CLA	Rr	603	X	-	-	-
32	CLA	Rr	604	X	-	-	-
32	CLA	Rr	608	X	-	-	-
32	CLA	Rr	609	X	-	-	-
32	CLA	Rr	610	X	-	-	-
32	CLA	Rr	611	X	-	-	-
32	CLA	Rr	612	X	-	-	-
32	CLA	Rr	613	X	-	-	-
32	CLA	S	602	X	-	-	-
32	CLA	S	603	X	-	-	-
32	CLA	S	604	X	-	-	-
32	CLA	S	608	X	-	-	-
32	CLA	S	609	X	-	-	-
32	CLA	S	610	X	-	-	-
32	CLA	S	611	X	-	-	-
32	CLA	S	612	X	-	-	-
32	CLA	S	613	X	-	-	-
32	CLA	SS	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	SS	304	X	-	-	-
32	CLA	SS	305	X	-	-	-
32	CLA	SS	309	X	-	-	-
32	CLA	SS	310	X	-	-	-
32	CLA	SS	311	X	-	-	-
32	CLA	SS	312	X	-	-	-
32	CLA	SS	313	X	-	-	-
32	CLA	SS	314	X	-	-	-
32	CLA	Ss	602	X	-	-	-
32	CLA	Ss	603	X	-	-	-
32	CLA	Ss	604	X	-	-	-
32	CLA	Ss	608	X	-	-	-
32	CLA	Ss	609	X	-	-	-
32	CLA	Ss	610	X	-	-	-
32	CLA	Ss	611	X	-	-	-
32	CLA	Ss	612	X	-	-	-
32	CLA	Ss	613	X	-	-	-
32	CLA	X	201	X	-	-	-
32	CLA	XX	201	X	-	-	-
32	CLA	Y	602	X	-	-	-
32	CLA	Y	603	X	-	-	-
32	CLA	Y	610	X	-	-	-
32	CLA	Y	611	X	-	-	-
32	CLA	Y	612	X	-	-	-
32	CLA	Y	613	X	-	-	-
32	CLA	Y	614	X	-	-	-
32	CLA	YY	602	X	-	-	-
32	CLA	YY	603	X	-	-	-
32	CLA	YY	610	X	-	-	-
32	CLA	YY	611	X	-	-	-
32	CLA	YY	612	X	-	-	-
32	CLA	YY	613	X	-	-	-
32	CLA	YY	614	X	-	-	-
32	CLA	Yy	602	X	-	-	-
32	CLA	Yy	603	X	-	-	-
32	CLA	Yy	604	X	-	-	-
32	CLA	Yy	610	X	-	-	-
32	CLA	Yy	611	X	-	-	-
32	CLA	Yy	612	X	-	-	-
32	CLA	Yy	613	X	-	-	-
32	CLA	Yy	614	X	-	-	-
32	CLA	a	405	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	a	406	X	-	-	-
32	CLA	a	407	X	-	-	-
32	CLA	a	410	X	-	-	-
32	CLA	b	601	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	604	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	610	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-
32	CLA	b	616	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	502	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	505	X	-	-	-
32	CLA	c	506	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	511	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-
32	CLA	d	402	X	-	-	-
32	CLA	g	603	X	-	-	-
32	CLA	g	604	X	-	-	-
32	CLA	g	610	X	-	-	-
32	CLA	g	611	X	-	-	-
32	CLA	g	612	X	-	-	-
32	CLA	g	613	X	-	-	-
32	CLA	g	614	X	-	-	-
32	CLA	n	602	X	-	-	-
32	CLA	n	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	n	604	X	-	-	-
32	CLA	n	610	X	-	-	-
32	CLA	n	611	X	-	-	-
32	CLA	n	612	X	-	-	-
32	CLA	n	613	X	-	-	-
32	CLA	n	614	X	-	-	-
32	CLA	r	601	X	-	-	-
32	CLA	r	602	X	-	-	-
32	CLA	r	603	X	-	-	-
32	CLA	r	604	X	-	-	-
32	CLA	r	608	X	-	-	-
32	CLA	r	609	X	-	-	-
32	CLA	r	610	X	-	-	-
32	CLA	r	611	X	-	-	-
32	CLA	r	612	X	-	-	-
32	CLA	r	613	X	-	-	-
32	CLA	s	602	X	-	-	-
32	CLA	s	603	X	-	-	-
32	CLA	s	604	X	-	-	-
32	CLA	s	608	X	-	-	-
32	CLA	s	609	X	-	-	-
32	CLA	s	610	X	-	-	-
32	CLA	s	611	X	-	-	-
32	CLA	s	612	X	-	-	-
32	CLA	s	613	X	-	-	-
32	CLA	y	304	X	-	-	-
32	CLA	y	305	X	-	-	-
32	CLA	y	306	X	-	-	-
32	CLA	y	312	X	-	-	-
32	CLA	y	313	X	-	-	-
32	CLA	y	314	X	-	-	-
32	CLA	y	315	X	-	-	-
32	CLA	y	316	X	-	-	-
35	PL9	A	410	-	X	-	-
35	PL9	AA	410	-	X	-	-
35	PL9	D	407	-	X	-	-
35	PL9	DD	406	-	X	-	-
35	PL9	Dd	404	-	X	-	-
35	PL9	d	404	-	X	-	-
39	CHL	1	601	X	-	-	-
39	CHL	1	605	X	-	-	-
39	CHL	1	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	1	607	X	-	-	-
39	CHL	1	608	X	-	-	-
39	CHL	11	601	X	-	-	-
39	CHL	11	605	X	-	-	-
39	CHL	11	606	X	-	-	-
39	CHL	11	607	X	-	-	-
39	CHL	11	608	X	-	-	-
39	CHL	2	601	X	-	-	-
39	CHL	2	605	X	-	-	-
39	CHL	2	606	X	-	-	-
39	CHL	2	607	X	-	-	-
39	CHL	2	608	X	-	-	-
39	CHL	22	601	X	-	-	-
39	CHL	22	605	X	-	-	-
39	CHL	22	606	X	-	-	-
39	CHL	22	607	X	-	-	-
39	CHL	22	608	X	-	-	-
39	CHL	3	601	X	-	-	-
39	CHL	3	605	X	-	-	-
39	CHL	3	606	X	-	-	-
39	CHL	3	607	X	-	-	-
39	CHL	3	608	X	-	-	-
39	CHL	33	601	X	-	-	-
39	CHL	33	605	X	-	-	-
39	CHL	33	606	X	-	-	-
39	CHL	33	607	X	-	-	-
39	CHL	33	608	X	-	-	-
39	CHL	4	302	X	-	-	-
39	CHL	4	306	X	-	-	-
39	CHL	4	307	X	-	-	-
39	CHL	4	308	X	-	-	-
39	CHL	4	309	X	-	-	-
39	CHL	44	601	X	-	-	-
39	CHL	44	605	X	-	-	-
39	CHL	44	606	X	-	-	-
39	CHL	44	607	X	-	-	-
39	CHL	44	608	X	-	-	-
39	CHL	G	601	X	-	-	-
39	CHL	G	605	X	-	-	-
39	CHL	G	606	X	-	-	-
39	CHL	G	607	X	-	-	-
39	CHL	G	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	G	609	X	-	-	-
39	CHL	GG	601	X	-	-	-
39	CHL	GG	605	X	-	-	-
39	CHL	GG	606	X	-	-	-
39	CHL	GG	607	X	-	-	-
39	CHL	GG	608	X	-	-	-
39	CHL	GG	609	X	-	-	-
39	CHL	Gg	302	X	-	-	-
39	CHL	Gg	306	X	-	-	-
39	CHL	Gg	307	X	-	-	-
39	CHL	Gg	308	X	-	-	-
39	CHL	Gg	309	X	-	-	-
39	CHL	Gg	310	X	-	-	-
39	CHL	N	601	X	-	-	-
39	CHL	N	605	X	-	-	-
39	CHL	N	606	X	-	-	-
39	CHL	N	607	X	-	-	-
39	CHL	N	608	X	-	-	-
39	CHL	N	609	X	-	-	-
39	CHL	NN	601	X	-	-	-
39	CHL	NN	605	X	-	-	-
39	CHL	NN	606	X	-	-	-
39	CHL	NN	607	X	-	-	-
39	CHL	NN	608	X	-	-	-
39	CHL	NN	609	X	-	-	-
39	CHL	Nn	311	X	-	-	-
39	CHL	Nn	315	X	-	-	-
39	CHL	Nn	316	X	-	-	-
39	CHL	Nn	317	X	-	-	-
39	CHL	Nn	318	X	-	-	-
39	CHL	Nn	319	X	-	-	-
39	CHL	R	605	X	-	-	-
39	CHL	R	606	X	-	-	-
39	CHL	R	607	X	-	-	-
39	CHL	RR	305	X	-	-	-
39	CHL	RR	306	X	-	-	-
39	CHL	RR	307	X	-	-	-
39	CHL	Rr	605	X	-	-	-
39	CHL	Rr	606	X	-	-	-
39	CHL	Rr	607	X	-	-	-
39	CHL	S	601	X	-	-	-
39	CHL	S	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	S	606	X	-	-	-
39	CHL	S	607	X	-	-	-
39	CHL	SS	302	X	-	-	-
39	CHL	SS	306	X	-	-	-
39	CHL	SS	307	X	-	-	-
39	CHL	SS	308	X	-	-	-
39	CHL	Ss	601	X	-	-	-
39	CHL	Ss	605	X	-	-	-
39	CHL	Ss	606	X	-	-	-
39	CHL	Ss	607	X	-	-	-
39	CHL	Y	601	X	-	-	-
39	CHL	Y	605	X	-	-	-
39	CHL	Y	606	X	-	-	-
39	CHL	Y	607	X	-	-	-
39	CHL	Y	608	X	-	-	-
39	CHL	Y	609	X	-	-	-
39	CHL	YY	601	X	-	-	-
39	CHL	YY	605	X	-	-	-
39	CHL	YY	606	X	-	-	-
39	CHL	YY	607	X	-	-	-
39	CHL	YY	608	X	-	-	-
39	CHL	YY	609	X	-	-	-
39	CHL	Yy	601	X	-	-	-
39	CHL	Yy	605	X	-	-	-
39	CHL	Yy	606	X	-	-	-
39	CHL	Yy	607	X	-	-	-
39	CHL	Yy	608	X	-	-	-
39	CHL	Yy	609	X	-	-	-
39	CHL	g	601	X	-	-	-
39	CHL	g	605	X	-	-	-
39	CHL	g	606	X	-	-	-
39	CHL	g	607	X	-	-	-
39	CHL	g	608	X	-	-	-
39	CHL	g	609	X	-	-	-
39	CHL	n	601	X	-	-	-
39	CHL	n	605	X	-	-	-
39	CHL	n	606	X	-	-	-
39	CHL	n	607	X	-	-	-
39	CHL	n	608	X	-	-	-
39	CHL	n	609	X	-	-	-
39	CHL	r	605	X	-	-	-
39	CHL	r	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	r	607	X	-	-	-
39	CHL	s	601	X	-	-	-
39	CHL	s	605	X	-	-	-
39	CHL	s	606	X	-	-	-
39	CHL	s	607	X	-	-	-
39	CHL	y	303	X	-	-	-
39	CHL	y	307	X	-	-	-
39	CHL	y	308	X	-	-	-
39	CHL	y	309	X	-	-	-
39	CHL	y	310	X	-	-	-
39	CHL	y	311	X	-	-	-

## 2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 339330 atoms, of which 168031 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0
			5145	1710	2526	431	465	13		
1	a	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		
1	AA	335	Total	C	H	N	O	S	0	0
			5146	1710	2527	431	465	13		
1	Aa	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		

- Molecule 2 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Oo	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	O	236	Total	C	H	N	O	S	0	0
			3559	1136	1765	292	363	3		
2	o	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	OO	236	Total	C	H	N	O	S	0	0
			3561	1136	1767	292	363	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Rr	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	R	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		
3	r	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	RR	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ss	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	S	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		
4	s	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	SS	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Tt	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	T	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	t	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	TT	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		

- Molecule 6 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Uu	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	U	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		
6	u	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	UU	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		

- Molecule 7 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ww	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	W	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	w	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	WW	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

- Molecule 8 is a protein called Photosystem II reaction center X protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Xx	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	X	46	Total	C	H	N	O		0	0
			667	213	341	53	60			
8	x	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	XX	48	Total	C	H	N	O	S	0	0
			701	223	359	55	62	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Xx	45	GLY	SER	conflict	UNP A0A9R0JQ89
X	45	GLY	SER	conflict	UNP A0A9R0JQ89
x	45	GLY	SER	conflict	UNP A0A9R0JQ89
XX	45	GLY	SER	conflict	UNP A0A9R0JQ89

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Yy	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	G	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	N	217	Total	C	H	N	O	S	0	0
			3245	1077	1589	269	303	7		
9	Y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	g	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	n	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	GG	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	NN	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	YY	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	Gg	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	Nn	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Zz	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	Z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	ZZ	61	Total	C	H	N	O	0	0
			933	306	479	68	80		

- Molecule 11 is a protein called Chlorophyll a-b binding protein CP24, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	44	186	Total 2847	C 952	H 1395	N 234	O 262	S 4	0	0
11	4	186	Total 2847	C 952	H 1395	N 234	O 262	S 4	0	0

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Pp	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	p	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	P	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	PP	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Qq	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	Q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	QQ	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	11	206	Total	C	H	N	O	S	0	0
			3075	1021	1505	254	288	7		
14	22	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		
14	1	207	Total	C	H	N	O	S	0	0
			3086	1024	1510	255	290	7		
14	2	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	33	207	Total	C	H	N	O	S	0	0
			3189	1061	1575	258	290	5		
15	3	209	Total	C	H	N	O	S	0	0
			3195	1063	1573	260	294	5		

- Molecule 16 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	0	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		
16	00	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		

- Molecule 17 is a protein called Photosystem II reaction center proteins PsbY, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
17	55	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	C	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	c	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		
18	CC	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	Cc	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		

- Molecule 19 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D	339	Total	C	H	N	O	S	0	0
			5274	1780	2580	441	461	12		
19	d	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		
19	DD	339	Total	C	H	N	O	S	0	0
			5275	1780	2581	441	461	12		
19	Dd	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		

- Molecule 20 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	e	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		
20	EE	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	Ee	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		

- Molecule 21 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	f	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0
21	FF	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	Ff	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	h	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	HH	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	Hh	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	i	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0
23	II	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	Ii	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	37	Total	C	H	N	O		
			552	182	283	41	46	0	0
24	j	34	Total	C	H	N	O		
			505	168	258	38	41	0	0
24	JJ	37	Total	C	H	N	O		
			552	182	283	41	46	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	Jj	34	Total	C	H	N	O	0	0
			505	168	258	38	41		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	k	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	KK	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	Kk	37	Total 616	C 217	H 310	N 43	O 45	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	l	36	Total 596	C 201	H 292	N 48	O 55	0	0
26	LL	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	Ll	36	Total 596	C 201	H 292	N 48	O 55	0	0

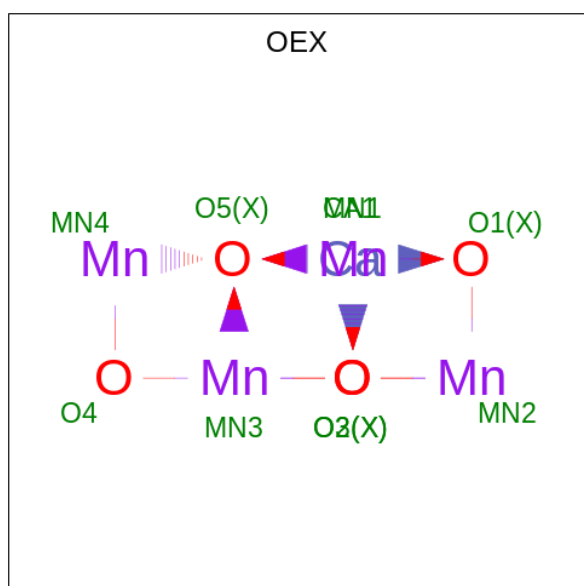
- Molecule 27 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	M	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	m	32	Total 523	C 172	H 273	N 36	O 42		0	0
27	MM	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	Mm	32	Total 523	C 172	H 273	N 36	O 42		0	0

- Molecule 28 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		
28	BB	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	B	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	Bb	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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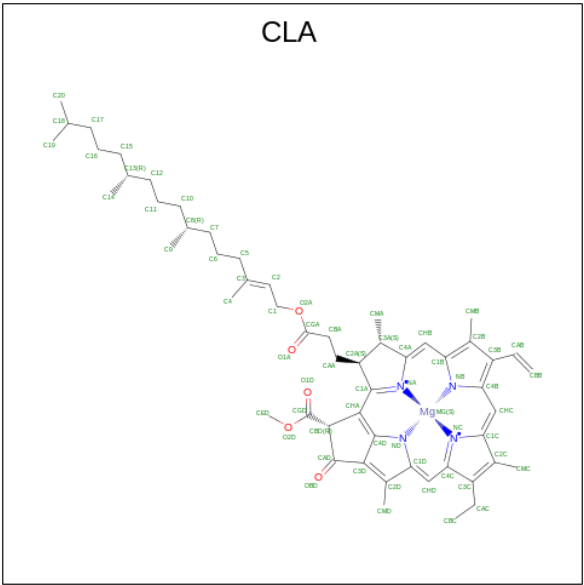
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Mol	Chain	Residues	Atoms		AltConf
30	AA	1	Total	Fe	0
			1	1	
30	Aa	1	Total	Fe	0
			1	1	

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Cl	0
			2	2	
31	a	2	Total	Cl	0
			2	2	
31	AA	2	Total	Cl	0
			2	2	
31	Aa	2	Total	Cl	0
			2	2	

- Molecule 32 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms						AltConf
32	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms						AltConf
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	G	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	X	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	c	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
32	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	r	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	s	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	CC	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	SS	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	XX	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	YY	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	YY	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	YY	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Aa	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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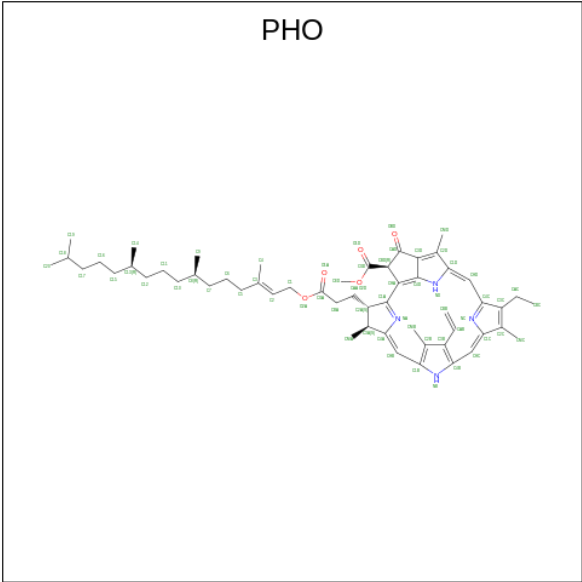
Mol	Chain	Residues	Atoms						AltConf
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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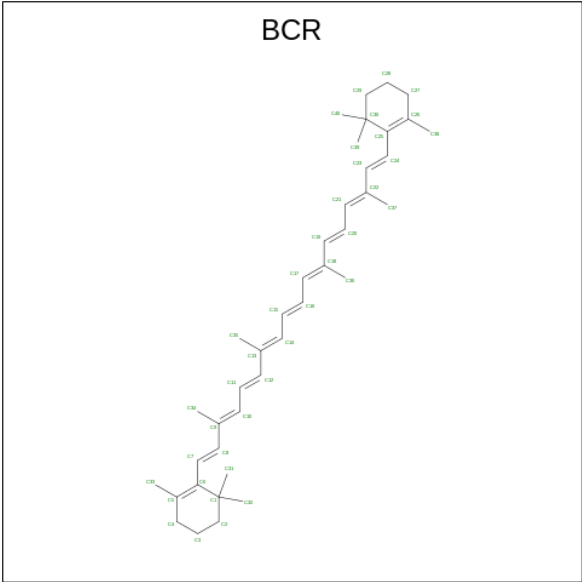
Mol	Chain	Residues	Atoms						AltConf
32	Gg	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	D	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	AA	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	DD	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 34 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	D	1	Total	C	H	0
			96	40	56	
34	H	1	Total	C	H	0
			96	40	56	
34	K	1	Total	C	H	0
			96	40	56	
34	T	1	Total	C	H	0
			96	40	56	
34	a	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	

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Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total 96	C 40	H 56	0
34	d	1	Total 96	C 40	H 56	0
34	h	1	Total 96	C 40	H 56	0
34	k	1	Total 96	C 40	H 56	0
34	AA	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	DD	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	KK	1	Total 96	C 40	H 56	0
34	TT	1	Total 96	C 40	H 56	0
34	XX	1	Total 96	C 40	H 56	0
34	Aa	1	Total 96	C 40	H 56	0

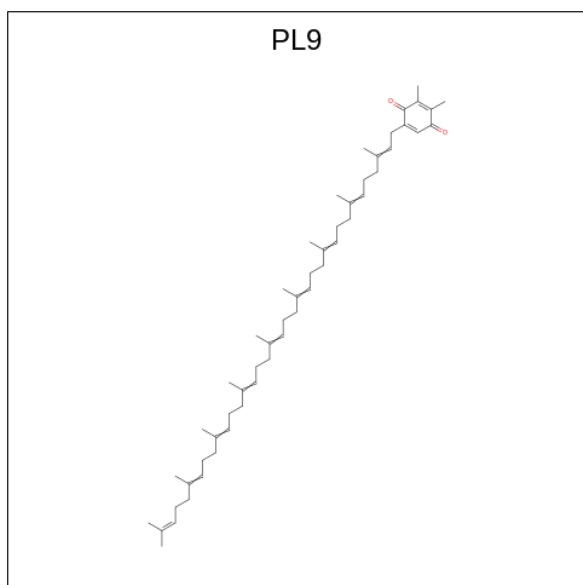
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Mol	Chain	Residues	Atoms			AltConf
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Dd	1	Total	C	H	0
			96	40	56	
34	Hh	1	Total	C	H	0
			96	40	56	
34	Kk	1	Total	C	H	0
			96	40	56	

- Molecule 35 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:  $C_{53}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



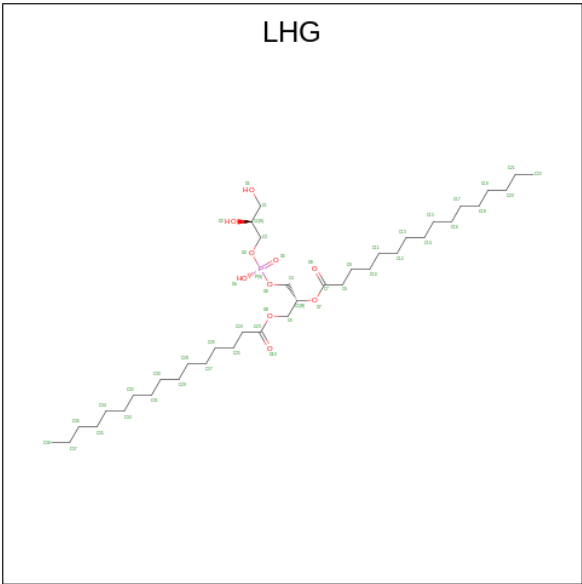
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms			AltConf
35	D	1	Total	C	O	0
			55	53	2	
35	d	1	Total	C	O	0
			55	53	2	
35	AA	1	Total	C	O	0
			55	53	2	
35	DD	1	Total	C	O	0
			55	53	2	
35	Dd	1	Total	C	O	0
			55	53	2	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	A	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	A	1	Total	C	H	O	P	0
			108	34	63	10	1	
36	Rr	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Ss	1	Total	C	H	O	P	0
			117	37	69	10	1	
36	Yy	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
36	44	1	Total 33	C 10	H 12	O 10	P 1	0
36	44	1	Total 31	C 8	H 12	O 10	P 1	0
36	11	1	Total 72	C 23	H 38	O 10	P 1	0
36	22	1	Total 72	C 23	H 38	O 10	P 1	0
36	33	1	Total 72	C 23	H 38	O 10	P 1	0
36	1	1	Total 60	C 19	H 30	O 10	P 1	0
36	3	1	Total 72	C 23	H 38	O 10	P 1	0
36	0	1	Total 114	C 36	H 67	O 10	P 1	0
36	C	1	Total 63	C 20	H 32	O 10	P 1	0
36	D	1	Total 102	C 32	H 59	O 10	P 1	0
36	D	1	Total 123	C 38	H 74	O 10	P 1	0
36	D	1	Total 72	C 23	H 38	O 10	P 1	0
36	G	1	Total 72	C 23	H 38	O 10	P 1	0
36	J	1	Total 51	C 16	H 24	O 10	P 1	0
36	K	1	Total 72	C 23	H 38	O 10	P 1	0
36	N	1	Total 84	C 27	H 46	O 10	P 1	0
36	Y	1	Total 123	C 38	H 74	O 10	P 1	0
36	a	1	Total 81	C 26	H 44	O 10	P 1	0
36	d	1	Total 102	C 32	H 59	O 10	P 1	0
36	d	1	Total 123	C 38	H 74	O 10	P 1	0
36	g	1	Total 72	C 23	H 38	O 10	P 1	0

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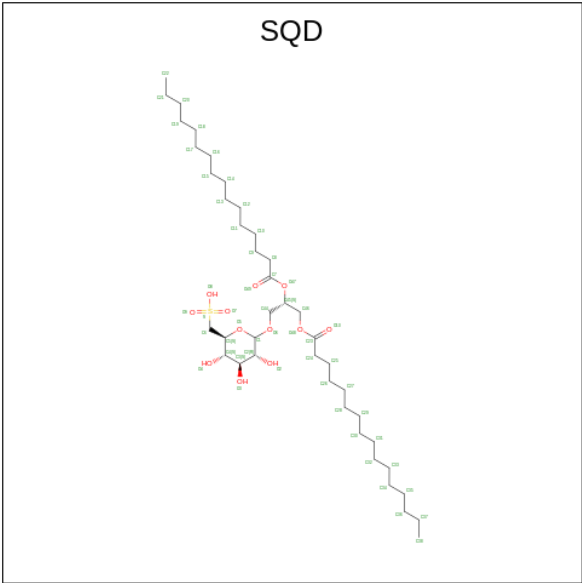
Mol	Chain	Residues	Atoms					AltConf
36	l	1	Total 123	C 38	H 74	O 10	P 1	0
36	n	1	Total 123	C 38	H 74	O 10	P 1	0
36	r	1	Total 123	C 38	H 74	O 10	P 1	0
36	s	1	Total 117	C 37	H 69	O 10	P 1	0
36	y	1	Total 123	C 38	H 74	O 10	P 1	0
36	4	1	Total 31	C 8	H 12	O 10	P 1	0
36	4	1	Total 33	C 10	H 12	O 10	P 1	0
36	AA	1	Total 72	C 23	H 38	O 10	P 1	0
36	AA	1	Total 108	C 34	H 63	O 10	P 1	0
36	BB	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 81	C 26	H 44	O 10	P 1	0
36	DD	1	Total 102	C 32	H 59	O 10	P 1	0
36	DD	1	Total 123	C 38	H 74	O 10	P 1	0
36	EE	1	Total 93	C 29	H 53	O 10	P 1	0
36	GG	1	Total 72	C 23	H 38	O 10	P 1	0
36	II	1	Total 72	C 23	H 38	O 10	P 1	0
36	JJ	1	Total 69	C 22	H 36	O 10	P 1	0
36	KK	1	Total 72	C 23	H 38	O 10	P 1	0
36	NN	1	Total 84	C 27	H 46	O 10	P 1	0
36	SS	1	Total 48	C 15	H 22	O 10	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
36	YY	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	Dd	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	Gg	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	Ll	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Nn	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



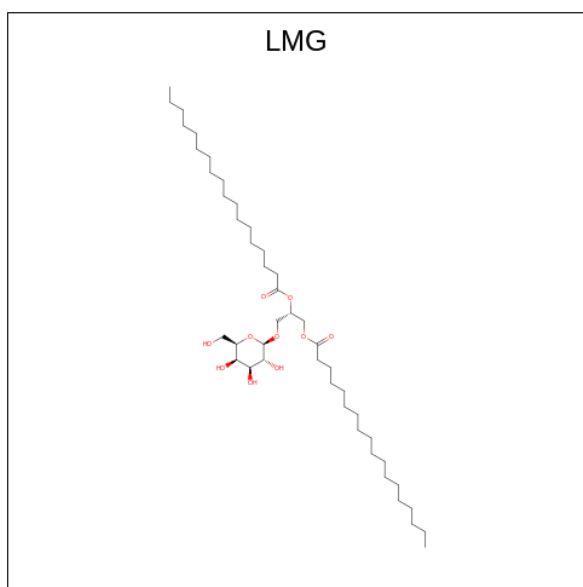
Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	C	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			72	23	36	12	1	

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Mol	Chain	Residues	Atoms					AltConf
37	l	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	AA	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	BB	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	CC	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	B	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	B	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	Aa	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	Ll	1	Total	C	H	O	S	0
			132	41	78	12	1	

- Molecule 38 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



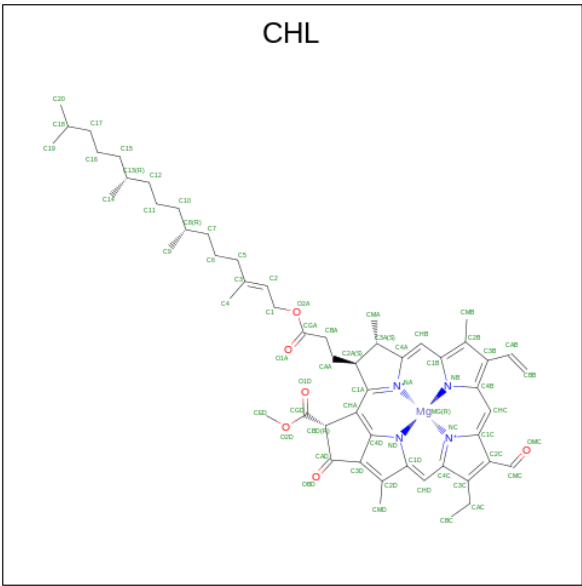
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	H	O	0
			78	26	42	10	

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Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total 123	C 41	H 72	O 10	0
38	F	1	Total 108	C 36	H 62	O 10	0
38	W	1	Total 114	C 38	H 66	O 10	0
38	a	1	Total 97	C 33	H 54	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	c	1	Total 72	C 24	H 38	O 10	0
38	j	1	Total 108	C 36	H 62	O 10	0
38	m	1	Total 123	C 41	H 72	O 10	0
38	AA	1	Total 78	C 26	H 42	O 10	0
38	BB	1	Total 105	C 35	H 60	O 10	0
38	CC	1	Total 87	C 29	H 48	O 10	0
38	DD	1	Total 108	C 36	H 62	O 10	0
38	B	1	Total 105	C 35	H 60	O 10	0
38	WW	1	Total 114	C 38	H 66	O 10	0
38	Aa	1	Total 97	C 33	H 54	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Cc	1	Total 72	C 24	H 38	O 10	0
38	Dd	1	Total 108	C 36	H 62	O 10	0
38	Mm	1	Total 123	C 41	H 72	O 10	0

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms						AltConf
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	44	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	2	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	3	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	G	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	G	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	N	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	N	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	R	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	S	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	S	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	S	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	S	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Y	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	g	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	g	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	g	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	n	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	r	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	s	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	y	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	y	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			86	39	36	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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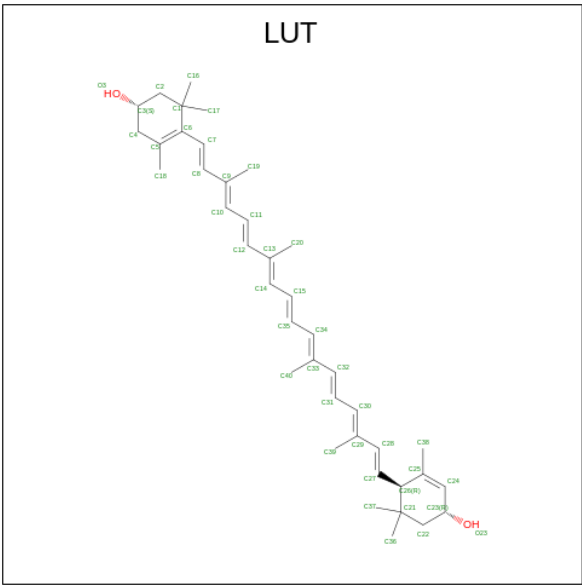
Mol	Chain	Residues	Atoms						AltConf
39	SS	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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



Mol	Chain	Residues	Atoms				AltConf
40	Rr	1	Total	C	H	O	0
			98	40	56	2	
40	Ss	1	Total	C	H	O	0
			98	40	56	2	
40	Ss	1	Total	C	H	O	0
			98	40	56	2	
40	Yy	1	Total	C	H	O	0
			98	40	56	2	
40	Yy	1	Total	C	H	O	0
			98	40	56	2	
40	44	1	Total	C	H	O	0
			98	40	56	2	
40	22	1	Total	C	H	O	0
			98	40	56	2	
40	2	1	Total	C	H	O	0
			98	40	56	2	
40	G	1	Total	C	H	O	0
			98	40	56	2	
40	G	1	Total	C	H	O	0
			98	40	56	2	

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Mol	Chain	Residues	Atoms				AltConf
40	N	1	Total 98	C 40	H 56	O 2	0
40	N	1	Total 98	C 40	H 56	O 2	0
40	R	1	Total 98	C 40	H 56	O 2	0
40	S	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	r	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	4	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	RR	1	Total 98	C 40	H 56	O 2	0

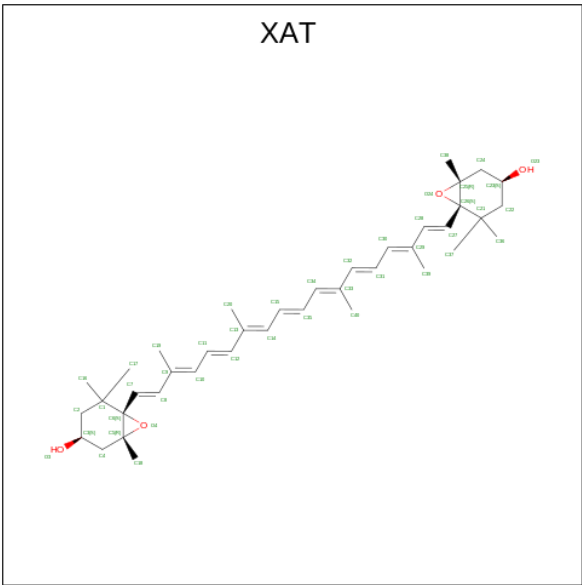
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Mol	Chain	Residues	Atoms				AltConf
40	SS	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



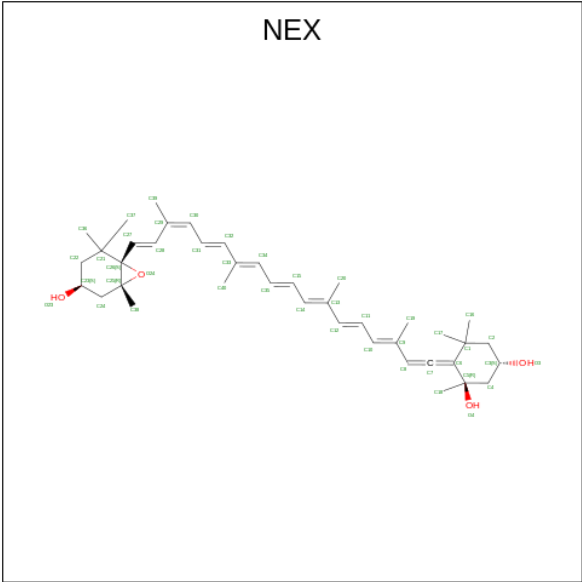
Mol	Chain	Residues	Atoms				AltConf
41	Rr	1	Total	C	H	O	0
			100	40	56	4	
41	Yy	1	Total	C	H	O	0
			100	40	56	4	
41	44	1	Total	C	H	O	0
			100	40	56	4	
41	G	1	Total	C	H	O	0
			100	40	56	4	

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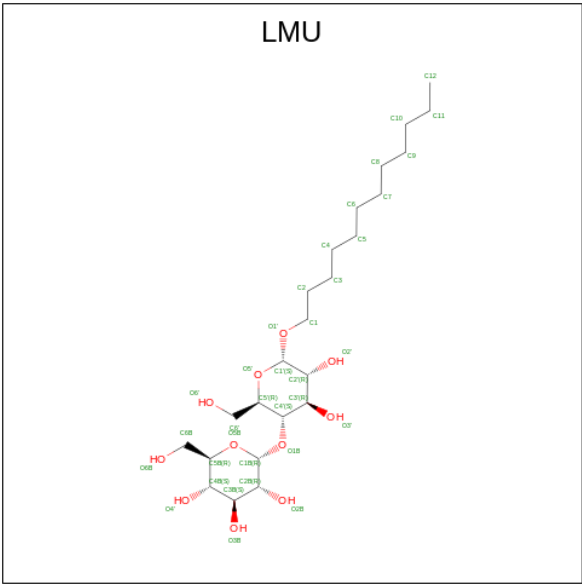
Mol	Chain	Residues	Atoms				AltConf
41	G	1	Total	C	H	O	0
			100	40	56	4	
41	N	1	Total	C	H	O	0
			100	40	56	4	
41	R	1	Total	C	H	O	0
			100	40	56	4	
41	g	1	Total	C	H	O	0
			100	40	56	4	
41	r	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	y	1	Total	C	H	O	0
			100	40	56	4	
41	4	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	GG	1	Total	C	H	O	0
			100	40	56	4	
41	NN	1	Total	C	H	O	0
			100	40	56	4	
41	RR	1	Total	C	H	O	0
			100	40	56	4	
41	Gg	1	Total	C	H	O	0
			100	40	56	4	
41	Nn	1	Total	C	H	O	0
			100	40	56	4	

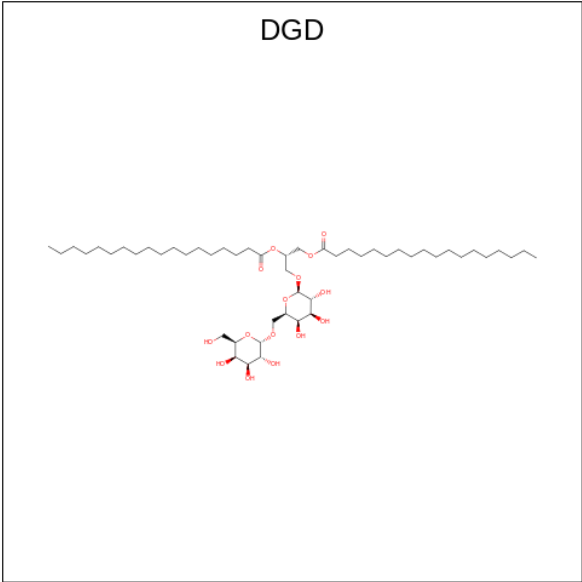
- Molecule 42 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
42	Rr	1	Total	C	H	O	0
			100	40	56	4	
42	Yy	1	Total	C	H	O	0
			100	40	56	4	
42	N	1	Total	C	H	O	0
			100	40	56	4	
42	R	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	g	1	Total	C	H	O	0
			100	40	56	4	
42	n	1	Total	C	H	O	0
			100	40	56	4	
42	y	1	Total	C	H	O	0
			100	40	56	4	
42	NN	1	Total	C	H	O	0
			100	40	56	4	
42	RR	1	Total	C	H	O	0
			100	40	56	4	
42	YY	1	Total	C	H	O	0
			100	40	56	4	
42	Gg	1	Total	C	H	O	0
			100	40	56	4	
42	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).





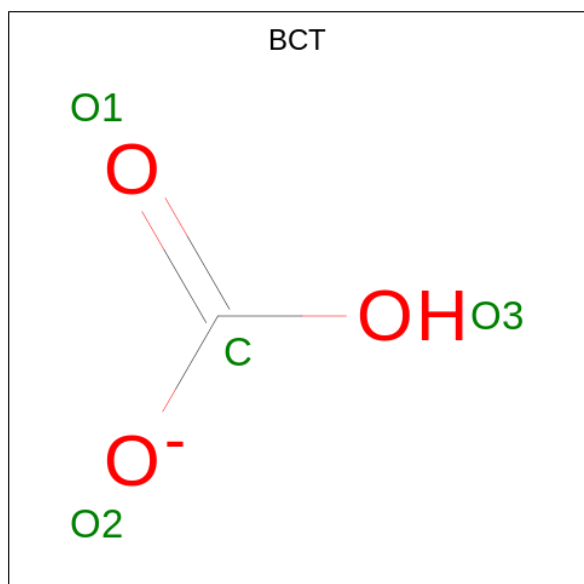
Mol	Chain	Residues	Atoms				AltConf
44	C	1	Total	C	H	O	0
			117	40	62	15	
44	C	1	Total	C	H	O	0
			132	47	70	15	
44	C	1	Total	C	H	O	0
			110	37	58	15	
44	D	1	Total	C	H	O	0
			132	47	70	15	
44	a	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			108	37	56	15	
44	h	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			117	40	62	15	
44	BB	1	Total	C	H	O	0
			121	42	64	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	
44	CC	1	Total	C	H	O	0
			132	47	70	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	

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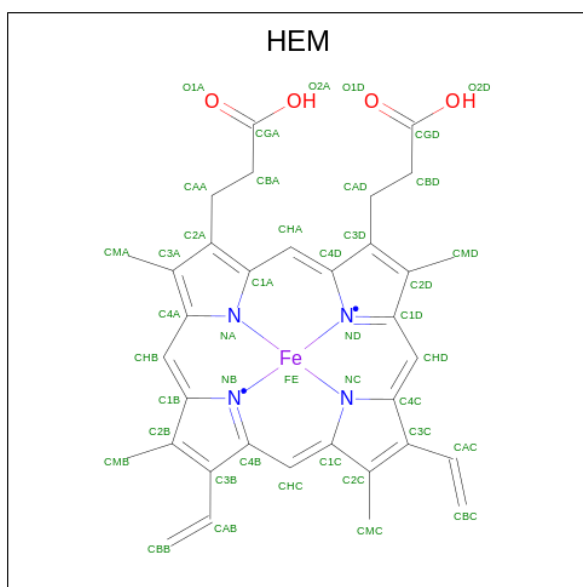
Mol	Chain	Residues	Atoms				AltConf
44	B	1	Total	C	H	O	0
			117	40	62	15	
44	B	1	Total	C	H	O	0
			121	42	64	15	
44	Aa	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			108	37	56	15	
44	Hh	1	Total	C	H	O	0
			132	47	70	15	

- Molecule 45 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				AltConf
45	D	1	Total	C	O		0
			4	1	3		
45	a	1	Total	C	H	O	0
			5	1	1	3	
45	AA	1	Total	C	O		0
			4	1	3		
45	Aa	1	Total	C	H	O	0
			5	1	1	3	

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms						AltConf
46	E	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	e	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	EE	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
46	Ee	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

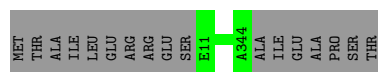
- Molecule 1: Photosystem II protein D1

Chain A: 



- Molecule 1: Photosystem II protein D1

Chain a: 



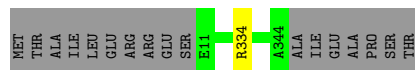
- Molecule 1: Photosystem II protein D1

Chain AA: 



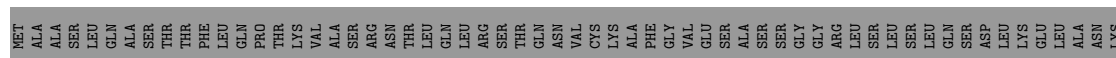
- Molecule 1: Photosystem II protein D1

Chain Aa: 



- Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic

Chain Oo: 



- Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic

- Molecule 2: Oxygen-evolving enhancer protein 1, chloroplastic

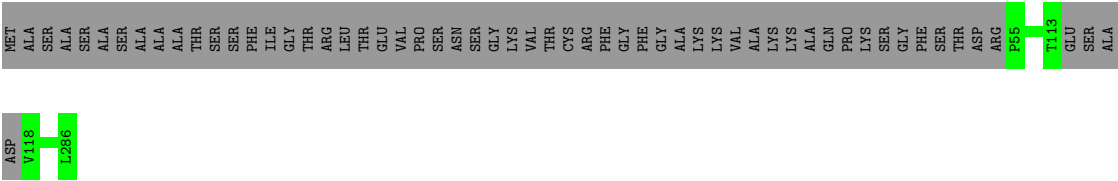
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

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

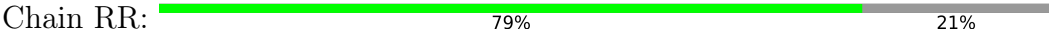
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



WORLD WIDE  
PDB  
PROTEIN DATA BANK



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



● Molecule 4: Chlorophyll a-b binding protein, chloroplastic



● Molecule 4: Chlorophyll a-b binding protein, chloroplastic



● Molecule 4: Chlorophyll a-b binding protein, chloroplastic



● Molecule 4: Chlorophyll a-b binding protein, chloroplastic



MET ALA SER VAL ALA SER THR ALA ALA CYS LEU GLY LYS SER SER GLU LEU LEU GLY ASN SER SER LEU LEU ARG SER SER ALA THR SER ALA PRO CYS CYS THR PRO SER VAL GLY CYS CYS THR VAL GLY PHE PHE GLY LYS LYS ALA ALA THR PRO PRO ALA LYS SER

LYS ALA LYS VAL ALA VAL ALA SER THR ALA ALA ASP ASP GLU L74 L100 L295

- Molecule 5: Photosystem II reaction center protein T

Chain Tt: 91% 9%

H1 S30 THR LYS LYS

- Molecule 5: Photosystem II reaction center protein T

Chain T: 91% 9%

H1 S30 THR LYS LYS

- Molecule 5: Photosystem II reaction center protein T

Chain t: 91% 9%

H1 S30 THR LYS LYS

- Molecule 5: Photosystem II reaction center protein T

Chain TT: 91% 9%

H1 S30 THR LYS LYS

- Molecule 6: Photosystem II 5 kDa protein, chloroplastic

Chain Uu: 26% 74%

MET ALA SER ILE THR MET THR ALA SER PHE LEU GLY THR THR VAL SER SER GLN PRO PRO THR HIS HIS LEU ARG ARG GLY VAL VAL MET MET ALA LYS ALA MET PRO GLU THR THR THR THR THR LYS LYS GLU GLU THR THR SER SER LYS ARG ARG ASP VAL PHE PHE VAL ALA ALA ALA ALA ALA

ALA CYS SER VAL ALA ARG ILE ALA MET SER PHE LEU GLU GLU PRO K3 K28


- Molecule 6: Photosystem II 5 kDa protein, chloroplastic

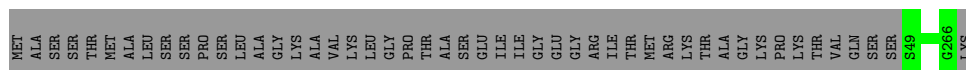
Chain U: 27% 73%

MET ALA SER ILE THR MET THR ALA SER PHE LEU GLY THR THR VAL SER SER GLN PRO PRO THR HIS HIS LEU ARG ARG GLY VAL VAL MET MET ALA LYS ALA MET PRO GLU THR THR THR THR THR LYS LYS GLU GLU THR THR SER SER LYS ARG ARG ASP VAL PHE PHE VAL ALA ALA ALA ALA ALA




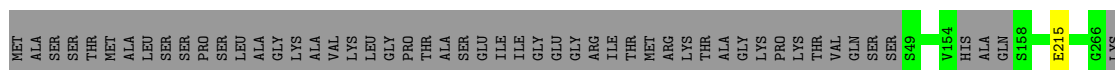


Chain Yy:  82% 18%




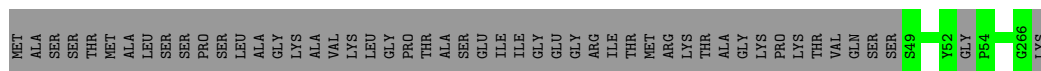
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain G:  80% 19%




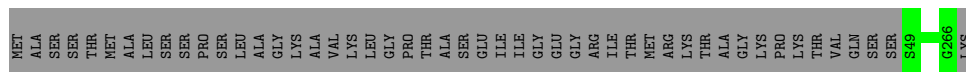
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain N:  81% 19%




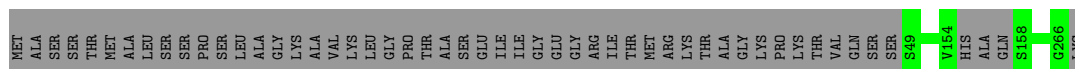
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain Y:  82% 18%




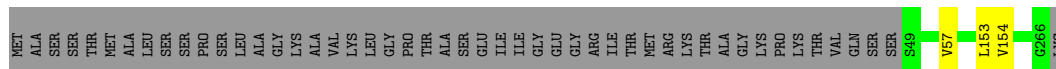
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain g:  81% 19%




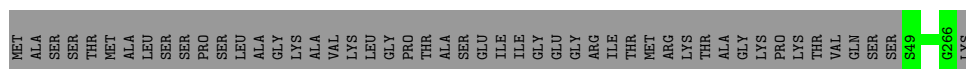
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain n:  81% 18%

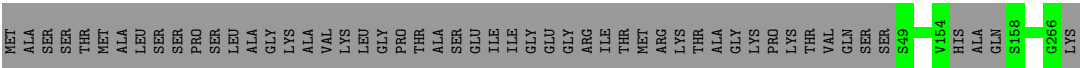
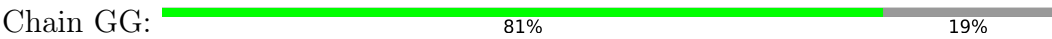


- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

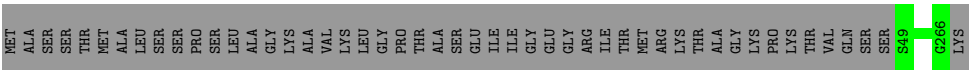
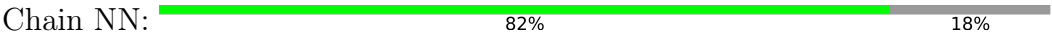
Chain y:  82% 18%



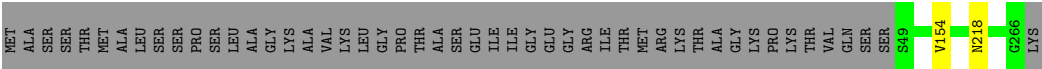
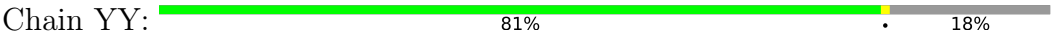
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic



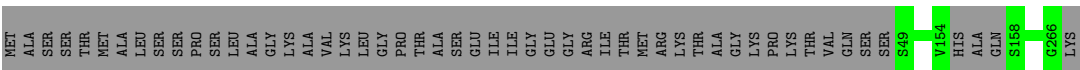
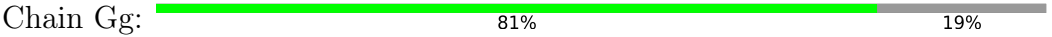
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic



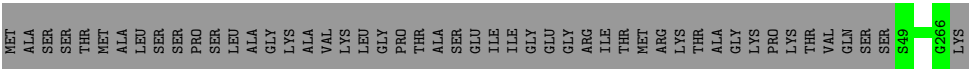
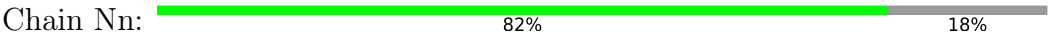
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic



- Molecule 9: Chlorophyll a-b binding protein, chloroplastic



- Molecule 9: Chlorophyll a-b binding protein, chloroplastic



- Molecule 10: Photosystem II reaction center protein Z



- Molecule 10: Photosystem II reaction center protein Z



- Molecule 10: Photosystem II reaction center protein Z

MET T2 L46 S62

- 

- [illegible]

ILE  
PRO  
ALA  
VAL  
LYS  
GLY  
GLY  
GLY  
ASN  
PHE  
LEU  
ASP  
PRO  
E74  
D83  
D171  
L259

- [illegible]

ILE	PRO	ALA	VAL	LYS	GLY	GLY	GLY	ASN	PHE	LEU	ASP	PRO	E74	Q152	L153	L259
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | SER | THR | ALA | CYS | PHE | LEU | HIS | HIS | HIS | ALA | ALA | ALA | ILE | SER | SER | PRO | ALA | ALA | ALA | GLN | ARG | GLY | GLY | SER | ALA | ALA | ALA | GLN | ARG | ARG | TYR | GLN | ALA | ALA | VAL | VAL | ASN | ASN | GLN | GLN | ILE | ILE | VAL | VAL | CYS | CYS | LYS | LYS | ALA | ALA | GLN | GLY | ASN | ASN | VAL | VAL | GLY | GLY | ASN | ASN | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

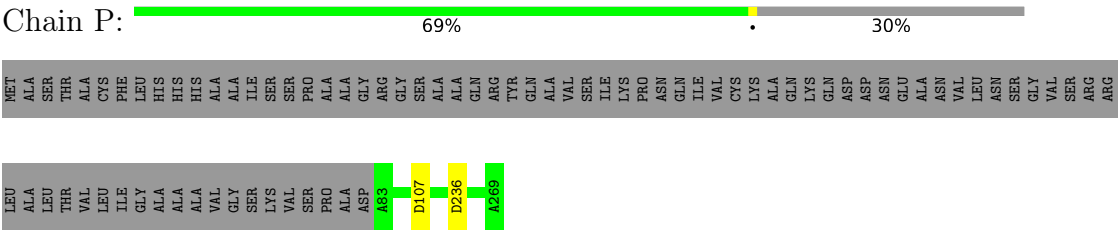
LEU  
ALA  
LEU  
THR  
VAL  
LEU  
ILE  
GLY  
ALA  
ALA  
ALA  
VAL  
GLY  
SER  
LYS  
VAL  
SER  
PRO  
ALA  
ASP  
A83  
K121  
A269

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | SER | THR | ALA | CYS | PHE | LEU | HIS | HIS | HIS | ALA | ALA | ALA | SER | SER | PRO | ALA | ALA | ALA | GLN | ARG | GLY | GLY | SER | SER | ALA | ALA | ALA | GLN | ARG | TYR | GLN | ALA | VAL | ASN | GLN | ILE | ILE | VAL | CYS | LYS | PRO | ASP | ASP | ASN | GLU | ALA | ALA | ASN | VAL | VAL | GLY | VAL | SER | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

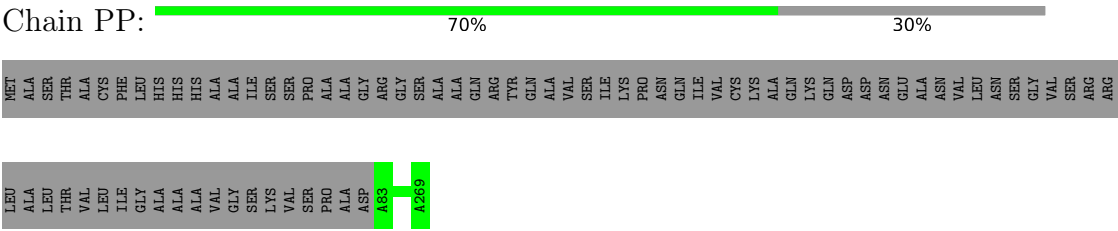
LEU	ALA	LEU	THR	VAL	LEU	ILE	GLY	ALA	ALA	ALA	VAL	GLY	SER	LYS	VAL	SER	PRO	ALA	ASP	A83	A269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------



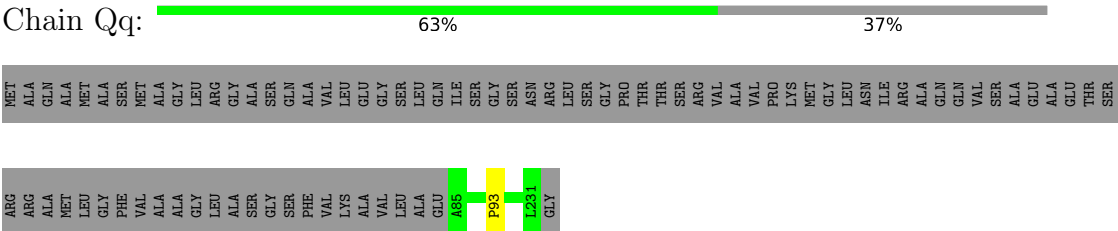
• Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



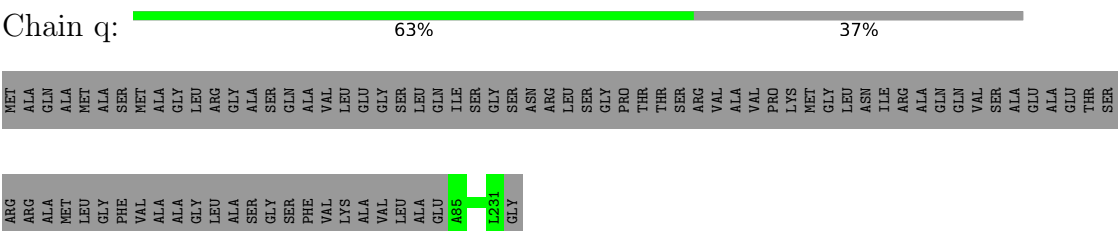
• Molecule 12: Oxygen-evolving enhancer protein 2, chloroplastic



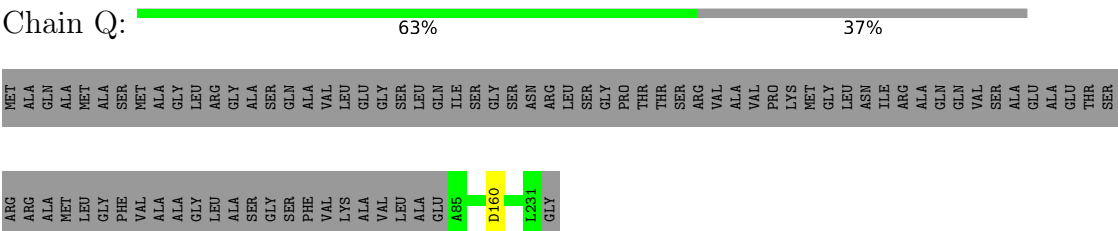
• Molecule 13: Oxygen-evolving enhancer protein 3, chloroplastic



• Molecule 13: Oxygen-evolving enhancer protein 3, chloroplastic



• Molecule 13: Oxygen-evolving enhancer protein 3, chloroplastic



• Molecule 13: Oxygen-evolving enhancer protein 3, chloroplastic

[illegible]

- Chain 11:  76% 23%

V154	L190	Tyr	Pro	Gly	Ser	F196	Q232	G266	Asn																																															
MET	ALA	SER	THR	MET	ALA	LEU	SER	PRO	ALA	PHE	GLY	LYS	VAL	LYS	LEU	ASN	PRO	SER	THR	SER	ASP	MET	ILE	ILE	GLY	GLU	GLY	ARG	ILE	SER	MET	ARG	LYS	LYS	ALA	GLY	LYS	PRO	LYS	ASN	VAL	SER	SER	SER	GLY	S49	P50	#51	TYR	GLY	PRO	ASP	ARG	VAL	LYS	YS69

- Chain 22:  82% 18%

MET	ALA	SER	SER	THR	MET	ALA	LEU	SER	SER	PRO	PHI	GLY	GLY	LYS	VAL	LYS	LEU	ASN	PRO	SER	THR	SER	ASP	MET	ILE	GLY	GLU	GLY	ARG	ILE	SER	MET	ARG	LYS	SER	ALA	GLY	LYS	PRO	ASN	VAL	SER	SER	GLY	\$49	G266	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----

- Chain 1:  77% 22%

[illegible]

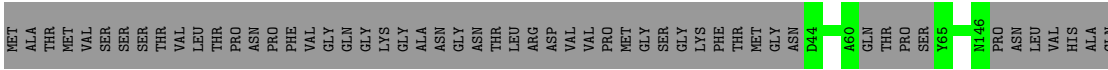
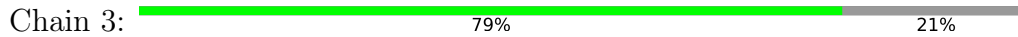
- Chain 2:  82% 18%

MET	ALA	SER	SER	THR	MET	ALA	LEU	SER	SER	PRO	ALA	PRO	PHE	GLY	GLY	GLY	ALA	ALA	VAL	LYS	LEU	LEU	ASN	PRO	SER	THR	SER	ASP	MET	ILE	GLY	GLY	GLY	GLY	GLU	GLY	ARG	ARG	ILE	SER	MET	ARG	LYS	SER	ALA	ALA	GLY	GLY	PRO	LYS	LYS	ASN	VAL	SER	SER	SER	GLY	S49	C266
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

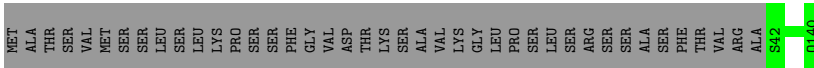
- Chain 33:  78% 22%

[illegible]

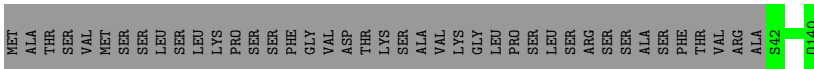
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



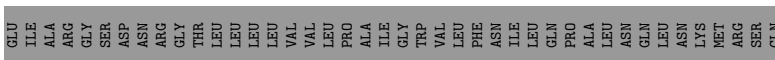
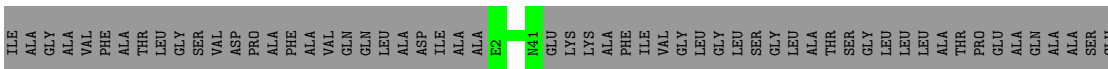
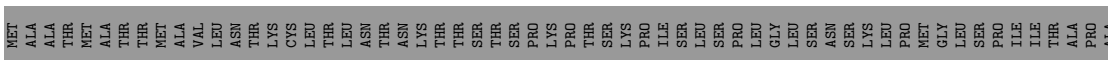
- Molecule 16: Photosystem II 10 kDa polypeptide, chloroplastic



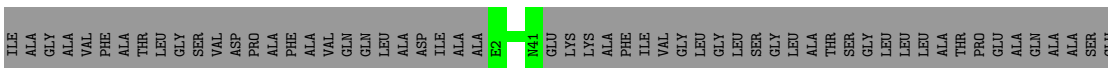
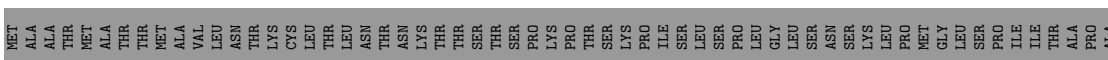
- Molecule 16: Photosystem II 10 kDa polypeptide, chloroplastic



- Molecule 17: Photosystem II reaction center proteins PsbY, chloroplastic



- Molecule 17: Photosystem II reaction center proteins PsbY, chloroplatic



GLU  
ILE  
ALA  
ARG  
GLY  
SER  
ASP  
ASN  
ARG  
GLY  
THR  
LEU  
LEU  
LEU  
VAL  
VAL  
ASN  
PRO  
ALA  
ILE  
GLY  
TRP  
LEU  
VAL  
LEU  
PHE  
ASN  
ILE  
LEU  
GLN  
PRO  
ALA  
LEU  
ASN  
GLN  
LEU  
ASN  
LYS  
MET  
ARG  
SER  
GLN

- Molecule 18: Photosystem II CP43 reaction center protein

Chain C:  95% 5%

MET  
LYS  
THR  
LEU  
LEU  
TYR  
SER  
LEU  
ARG  
ARG  
PHE  
TYR  
PRO  
VAL  
GLU  
THR  
LEU  
PHE  
ASN  
GLY  
THR  
LEU  
THR  
LEU  
A24  
V417  
L472  
ASN

- Molecule 18: Photosystem II CP43 reaction center protein

Chain c:  95% 5%

MET  
LYS  
THR  
LEU  
TYR  
SER  
LEU  
ARG  
ARG  
PHE  
TYR  
PRO  
VAL  
GLU  
THR  
LEU  
PHE  
ASN  
GLY  
THR  
LEU  
THR  
LEU  
A24  
L472  
ASN

- Molecule 18: Photosystem II CP43 reaction center protein

Chain CC:  95% 5%

MET  
LYS  
THR  
LEU  
TYR  
SER  
LEU  
ARG  
ARG  
PHE  
TYR  
PRO  
VAL  
GLU  
THR  
LEU  
PHE  
ASN  
GLY  
THR  
LEU  
THR  
LEU  
A24  
L472  
ASN

- Molecule 18: Photosystem II CP43 reaction center protein

Chain Cc:  95% 5%

MET  
LYS  
THR  
LEU  
TYR  
SER  
LEU  
ARG  
ARG  
PHE  
TYR  
PRO  
VAL  
GLU  
THR  
LEU  
PHE  
ASN  
GLY  
THR  
LEU  
THR  
LEU  
A24  
N68  
L472  
ASN

- Molecule 19: Photosystem II D2 protein

Chain D:  96% .

MET  
THR  
ILE  
ALA  
VAL  
GLY  
LYS  
PHE  
THR  
LYS  
ASP  
GLU  
LYS  
D13  
A351

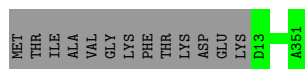
- Molecule 19: Photosystem II D2 protein

Chain d:  97% .

MET  
THR  
ILE  
ALA  
VAL  
GLY  
LYS  
PHE  
THR  
LYS  
ASP  
GLU  
K12  
A351

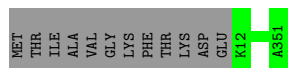
- Molecule 19: Photosystem II D2 protein

Chain DD:  96% .



- Molecule 19: Photosystem II D2 protein

Chain Dd: 97%



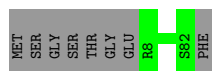
- Molecule 20: Cytochrome b559 subunit alpha

Chain E: 96%



- Molecule 20: Cytochrome b559 subunit alpha

Chain e: 90%



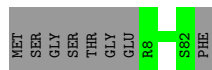
- Molecule 20: Cytochrome b559 subunit alpha

Chain EE: 96%



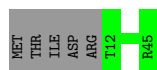
- Molecule 20: Cytochrome b559 subunit alpha

Chain Ee: 90%



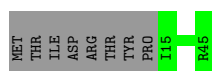
- Molecule 21: Cytochrome b559 subunit beta

Chain F: 87%



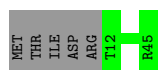
- Molecule 21: Cytochrome b559 subunit beta

Chain f: 79%



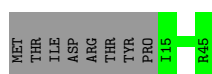
- Molecule 21: Cytochrome b559 subunit beta

Chain FF: 87% 13%



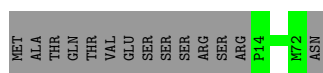
- Molecule 21: Cytochrome b559 subunit beta

Chain Ff: 79% 21%



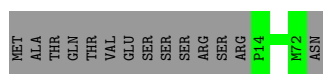
- Molecule 22: Photosystem II reaction center protein H

Chain H: 81% 19%



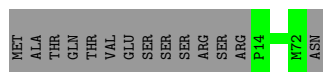
- Molecule 22: Photosystem II reaction center protein H

Chain h: 81% 19%



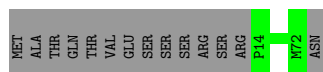
- Molecule 22: Photosystem II reaction center protein H

Chain HH: 81% 19%



- Molecule 22: Photosystem II reaction center protein H

Chain Hh: 81% 19%

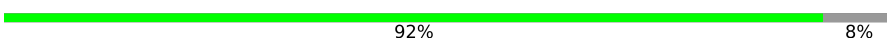


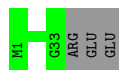
- Molecule 23: Photosystem II reaction center protein I

Chain I: 97% 3%



- Molecule 23: Photosystem II reaction center protein I

Chain i:  92% 8%



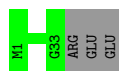
- Molecule 23: Photosystem II reaction center protein I

Chain II:  97% .

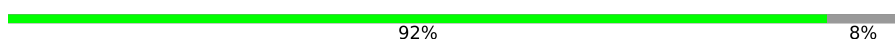


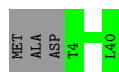
- Molecule 23: Photosystem II reaction center protein I

Chain Ii:  92% 8%




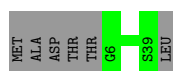
- Molecule 24: Photosystem II reaction center protein J

Chain J:  92% 8%



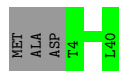
- Molecule 24: Photosystem II reaction center protein J

Chain j:  85% 15%




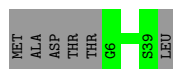
- Molecule 24: Photosystem II reaction center protein J

Chain JJ:  92% 8%



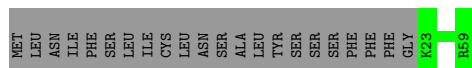
- Molecule 24: Photosystem II reaction center protein J

Chain Jj:  85% 15%



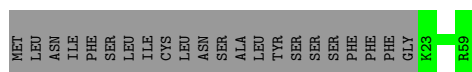
- Molecule 25: Photosystem II reaction center protein K

Chain K: 63% 37%



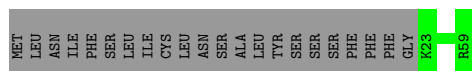
- Molecule 25: Photosystem II reaction center protein K

Chain k: 63% 37%



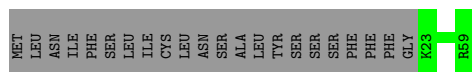
- Molecule 25: Photosystem II reaction center protein K

Chain KK: 63% 37%



- Molecule 25: Photosystem II reaction center protein K

Chain Kk: 63% 37%



- Molecule 26: Photosystem II reaction center protein L

Chain L: 92% 8%



- Molecule 26: Photosystem II reaction center protein L

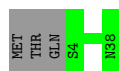
Chain l: 95% 5%



- Molecule 26: Photosystem II reaction center protein L

Chain LL: 92% 8%





- Molecule 26: Photosystem II reaction center protein L

Chain Ll: 95% 5%



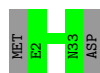
- Molecule 27: Photosystem II reaction center protein M

Chain M: 97% .



- Molecule 27: Photosystem II reaction center protein M

Chain m: 94% 6%



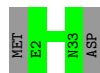
- Molecule 27: Photosystem II reaction center protein M

Chain MM: 97% .



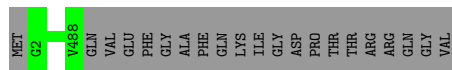
- Molecule 27: Photosystem II reaction center protein M

Chain Mm: 94% 6%



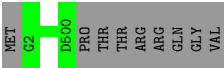
- Molecule 28: Photosystem II CP47 reaction center protein

Chain b: 96% .

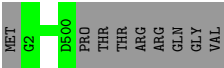


- Molecule 28: Photosystem II CP47 reaction center protein

Chain BB: 98% .



- Molecule 28: Photosystem II CP47 reaction center protein



- Molecule 28: Photosystem II CP47 reaction center protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93684	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/2700	0.55	0/3682
1	AA	0.30	0/2700	0.53	0/3682
1	Aa	0.29	0/2694	0.54	0/3674
1	a	0.30	0/2694	0.54	0/3674
2	O	0.28	0/1829	0.55	0/2471
2	OO	0.28	0/1829	0.54	0/2471
2	Oo	0.28	0/1811	0.54	0/2448
2	o	0.28	0/1811	0.55	0/2448
3	R	0.27	0/1819	0.55	0/2475
3	RR	0.28	0/1819	0.56	0/2475
3	Rr	0.28	0/1824	0.55	0/2481
3	r	0.27	0/1824	0.54	0/2481
4	S	0.29	0/1760	0.57	0/2393
4	SS	0.29	0/1760	0.57	1/2393 (0.0%)
4	Ss	0.28	0/1696	0.53	0/2305
4	s	0.28	0/1696	0.53	0/2305
5	T	0.35	0/252	0.51	0/341
5	TT	0.34	0/252	0.48	0/341
5	Tt	0.32	0/252	0.47	0/341
5	t	0.33	0/252	0.49	0/341
6	U	0.34	0/214	0.67	0/286
6	UU	0.31	0/214	0.57	0/286
6	Uu	0.34	0/206	0.70	0/275
6	u	0.32	0/206	0.73	0/275
7	W	0.31	0/429	0.59	0/582
7	WW	0.32	0/429	0.55	0/582
7	Ww	0.31	0/429	0.52	0/582
7	w	0.31	0/429	0.58	0/582
8	X	0.28	0/331	0.49	0/453
8	XX	0.27	0/347	0.54	0/473
8	Xx	0.25	0/241	0.44	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	x	0.29	0/241	0.48	0/330
9	G	0.33	0/1686	0.62	1/2295 (0.0%)
9	GG	0.29	0/1686	0.55	0/2295
9	Gg	0.29	0/1686	0.54	0/2295
9	N	0.30	0/1707	0.55	0/2323
9	NN	0.29	0/1712	0.53	0/2332
9	Nn	0.30	0/1712	0.55	0/2332
9	Y	0.30	0/1712	0.53	0/2332
9	YY	0.28	0/1712	0.51	0/2332
9	Yy	0.29	0/1712	0.52	0/2332
9	g	0.31	0/1686	0.55	0/2295
9	n	0.32	0/1712	0.58	0/2332
9	y	0.31	0/1712	0.54	0/2332
10	Z	0.27	0/464	0.46	0/636
10	ZZ	0.25	0/464	0.47	0/636
10	Zz	0.25	0/464	0.49	0/636
10	z	0.29	0/464	0.60	1/636 (0.2%)
11	4	0.30	0/1501	0.61	3/2043 (0.1%)
11	44	0.28	0/1501	0.54	0/2043
12	P	0.31	0/1465	0.61	2/1978 (0.1%)
12	PP	0.28	0/1465	0.54	0/1978
12	Pp	0.28	0/1465	0.53	0/1978
12	p	0.28	0/1465	0.53	0/1978
13	Q	0.31	0/1177	0.62	1/1597 (0.1%)
13	QQ	0.28	0/1177	0.55	0/1597
13	Qq	0.29	0/1177	0.62	1/1597 (0.1%)
13	q	0.29	0/1177	0.61	0/1597
14	1	0.30	0/1622	0.53	0/2206
14	11	0.29	0/1616	0.56	0/2198
14	2	0.28	0/1713	0.52	0/2333
14	22	0.28	0/1713	0.51	0/2333
15	3	0.29	0/1668	0.58	0/2265
15	33	0.27	0/1661	0.52	0/2257
16	0	0.30	0/736	0.57	0/997
16	00	0.29	0/736	0.54	0/997
17	5	0.29	0/313	0.60	0/426
17	55	0.26	0/313	0.62	0/426
18	C	0.30	0/3589	0.55	0/4891
18	CC	0.29	0/3589	0.52	0/4891
18	Cc	0.28	0/3589	0.54	0/4891
18	c	0.29	0/3589	0.55	0/4891
19	D	0.32	0/2787	0.55	0/3800
19	DD	0.30	0/2787	0.54	0/3800

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	Dd	0.28	0/2796	0.52	0/3811
19	d	0.30	0/2796	0.53	0/3811
20	E	0.32	0/658	0.59	0/894
20	EE	0.29	0/658	0.55	0/894
20	Ee	0.27	0/628	0.57	0/854
20	e	0.30	0/628	0.60	0/854
21	F	0.28	0/285	0.57	0/387
21	FF	0.27	0/285	0.56	0/387
21	Ff	0.26	0/257	0.64	0/347
21	f	0.27	0/257	0.65	0/347
22	H	0.28	0/444	0.52	0/605
22	HH	0.27	0/444	0.50	0/605
22	Hh	0.27	0/444	0.50	0/605
22	h	0.28	0/444	0.55	0/605
23	I	0.35	0/294	0.57	0/397
23	II	0.33	0/294	0.53	0/397
23	Ii	0.31	0/274	0.50	0/371
23	i	0.36	0/274	0.56	0/371
24	J	0.28	0/275	0.61	0/374
24	JJ	0.30	0/275	0.57	0/374
24	Jj	0.26	0/253	0.57	0/343
24	j	0.28	0/253	0.55	0/343
25	K	0.33	0/320	0.56	0/436
25	KK	0.31	0/320	0.49	0/436
25	Kk	0.29	0/319	0.55	0/436
25	k	0.30	0/320	0.56	0/436
26	L	0.35	0/303	0.54	0/412
26	LL	0.32	0/303	0.49	0/412
26	Ll	0.31	0/312	0.49	0/424
26	l	0.32	0/312	0.50	0/424
27	M	0.31	0/262	0.45	0/358
27	MM	0.29	0/262	0.45	0/358
27	Mm	0.32	0/254	0.46	0/348
27	m	0.35	0/254	0.50	0/348
28	B	0.30	0/4047	0.56	0/5507
28	BB	0.30	0/4047	0.55	0/5507
28	Bb	0.29	0/3951	0.55	0/5379
28	b	0.30	0/3951	0.57	0/5379
All	All	0.29	0/137625	0.55	10/187193 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
2	OO	0	1
9	YY	0	2
9	n	0	2
14	11	0	2
All	All	0	8

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	160	ASP	CB-CG-OD2	6.96	124.56	118.30
13	Qq	93	PRO	CA-N-CD	-6.81	101.97	111.50
4	SS	100	LEU	CA-CB-CG	6.47	130.19	115.30
9	G	215	GLU	OE1-CD-OE2	-6.16	115.91	123.30
12	P	236	ASP	CB-CG-OD2	5.95	123.66	118.30
11	4	152	GLN	CA-CB-CG	5.89	126.36	113.40
11	4	153	LEU	CA-CB-CG	5.84	128.74	115.30
10	z	46	LEU	CA-CB-CG	5.28	127.45	115.30
12	P	107	ASP	CB-CG-OD1	5.09	122.88	118.30
11	4	153	LEU	CB-CG-CD1	5.03	119.55	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	11	154	VAL	Peptide
14	11	232	GLN	Peptide
2	O	266	GLU	Peptide
2	OO	266	GLU	Peptide
9	YY	154	VAL	Peptide
9	YY	218	ASN	Peptide
9	n	153	LEU	Peptide
9	n	154	VAL	Peptide

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

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/351 (95%)	313 (94%)	20 (6%)	0	100	100
1	AA	333/351 (95%)	305 (92%)	28 (8%)	0	100	100
1	Aa	332/351 (95%)	317 (96%)	14 (4%)	1 (0%)	37	68
1	a	332/351 (95%)	318 (96%)	14 (4%)	0	100	100
2	O	232/332 (70%)	219 (94%)	13 (6%)	0	100	100
2	OO	232/332 (70%)	216 (93%)	16 (7%)	0	100	100
2	Oo	230/332 (69%)	206 (90%)	24 (10%)	0	100	100
2	o	230/332 (69%)	210 (91%)	20 (9%)	0	100	100
3	R	223/286 (78%)	215 (96%)	8 (4%)	0	100	100
3	RR	223/286 (78%)	212 (95%)	10 (4%)	1 (0%)	30	63
3	Rr	224/286 (78%)	216 (96%)	8 (4%)	0	100	100
3	r	224/286 (78%)	216 (96%)	8 (4%)	0	100	100
4	S	220/295 (75%)	205 (93%)	14 (6%)	1 (0%)	25	59
4	SS	220/295 (75%)	201 (91%)	19 (9%)	0	100	100
4	Ss	211/295 (72%)	196 (93%)	15 (7%)	0	100	100
4	s	211/295 (72%)	199 (94%)	12 (6%)	0	100	100
5	T	28/33 (85%)	28 (100%)	0	0	100	100
5	TT	28/33 (85%)	28 (100%)	0	0	100	100
5	Tt	28/33 (85%)	28 (100%)	0	0	100	100
5	t	28/33 (85%)	28 (100%)	0	0	100	100
6	U	25/99 (25%)	25 (100%)	0	0	100	100
6	UU	25/99 (25%)	24 (96%)	1 (4%)	0	100	100
6	Uu	24/99 (24%)	22 (92%)	2 (8%)	0	100	100
6	u	24/99 (24%)	24 (100%)	0	0	100	100
7	W	52/137 (38%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	WW	52/137 (38%)	52 (100%)	0	0	100	100
7	Ww	52/137 (38%)	50 (96%)	2 (4%)	0	100	100
7	w	52/137 (38%)	48 (92%)	4 (8%)	0	100	100
8	X	44/117 (38%)	43 (98%)	1 (2%)	0	100	100
8	XX	46/117 (39%)	46 (100%)	0	0	100	100
8	Xx	32/117 (27%)	32 (100%)	0	0	100	100
8	x	32/117 (27%)	32 (100%)	0	0	100	100
9	G	211/267 (79%)	198 (94%)	13 (6%)	0	100	100
9	GG	211/267 (79%)	200 (95%)	11 (5%)	0	100	100
9	Gg	211/267 (79%)	197 (93%)	14 (7%)	0	100	100
9	N	213/267 (80%)	196 (92%)	17 (8%)	0	100	100
9	NN	216/267 (81%)	203 (94%)	13 (6%)	0	100	100
9	Nn	216/267 (81%)	195 (90%)	21 (10%)	0	100	100
9	Y	216/267 (81%)	207 (96%)	9 (4%)	0	100	100
9	YY	216/267 (81%)	205 (95%)	11 (5%)	0	100	100
9	Yy	216/267 (81%)	204 (94%)	12 (6%)	0	100	100
9	g	211/267 (79%)	197 (93%)	14 (7%)	0	100	100
9	n	216/267 (81%)	195 (90%)	20 (9%)	1 (0%)	25	59
9	y	216/267 (81%)	206 (95%)	10 (5%)	0	100	100
10	Z	59/62 (95%)	59 (100%)	0	0	100	100
10	ZZ	59/62 (95%)	59 (100%)	0	0	100	100
10	Zz	59/62 (95%)	59 (100%)	0	0	100	100
10	z	59/62 (95%)	59 (100%)	0	0	100	100
11	4	184/259 (71%)	172 (94%)	12 (6%)	0	100	100
11	44	184/259 (71%)	174 (95%)	8 (4%)	2 (1%)	12	43
12	P	185/267 (69%)	169 (91%)	16 (9%)	0	100	100
12	PP	185/267 (69%)	171 (92%)	14 (8%)	0	100	100
12	Pp	185/267 (69%)	176 (95%)	9 (5%)	0	100	100
12	p	185/267 (69%)	178 (96%)	7 (4%)	0	100	100
13	Q	145/232 (62%)	135 (93%)	10 (7%)	0	100	100
13	QQ	145/232 (62%)	134 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Qq	145/232 (62%)	138 (95%)	7 (5%)	0	100	100
13	q	145/232 (62%)	141 (97%)	4 (3%)	0	100	100
14	1	201/267 (75%)	191 (95%)	9 (4%)	1 (0%)	25	59
14	11	200/267 (75%)	189 (94%)	11 (6%)	0	100	100
14	2	216/267 (81%)	203 (94%)	13 (6%)	0	100	100
14	22	216/267 (81%)	206 (95%)	10 (5%)	0	100	100
15	3	203/264 (77%)	195 (96%)	8 (4%)	0	100	100
15	33	201/264 (76%)	190 (94%)	11 (6%)	0	100	100
16	0	97/140 (69%)	90 (93%)	7 (7%)	0	100	100
16	00	97/140 (69%)	90 (93%)	7 (7%)	0	100	100
17	5	38/199 (19%)	38 (100%)	0	0	100	100
17	55	38/199 (19%)	36 (95%)	2 (5%)	0	100	100
18	C	447/473 (94%)	429 (96%)	17 (4%)	1 (0%)	44	74
18	CC	447/473 (94%)	433 (97%)	14 (3%)	0	100	100
18	Cc	447/473 (94%)	423 (95%)	24 (5%)	0	100	100
18	c	447/473 (94%)	421 (94%)	26 (6%)	0	100	100
19	D	337/352 (96%)	322 (96%)	15 (4%)	0	100	100
19	DD	337/352 (96%)	323 (96%)	14 (4%)	0	100	100
19	Dd	338/352 (96%)	328 (97%)	10 (3%)	0	100	100
19	d	338/352 (96%)	328 (97%)	10 (3%)	0	100	100
20	E	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
20	EE	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
20	Ee	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
20	e	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
21	F	32/39 (82%)	31 (97%)	1 (3%)	0	100	100
21	FF	32/39 (82%)	30 (94%)	2 (6%)	0	100	100
21	Ff	29/39 (74%)	29 (100%)	0	0	100	100
21	f	29/39 (74%)	29 (100%)	0	0	100	100
22	H	57/73 (78%)	54 (95%)	3 (5%)	0	100	100
22	HH	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
22	Hh	57/73 (78%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
23	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
23	II	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
23	Ii	31/36 (86%)	31 (100%)	0	0	100	100
23	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
24	J	35/40 (88%)	35 (100%)	0	0	100	100
24	JJ	35/40 (88%)	35 (100%)	0	0	100	100
24	Jj	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
24	j	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
25	K	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
25	KK	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
25	Kk	35/59 (59%)	31 (89%)	4 (11%)	0	100	100
25	k	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
26	L	33/38 (87%)	33 (100%)	0	0	100	100
26	LL	33/38 (87%)	33 (100%)	0	0	100	100
26	Ll	34/38 (90%)	34 (100%)	0	0	100	100
26	l	34/38 (90%)	34 (100%)	0	0	100	100
27	M	31/34 (91%)	31 (100%)	0	0	100	100
27	MM	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
27	Mm	30/34 (88%)	30 (100%)	0	0	100	100
27	m	30/34 (88%)	30 (100%)	0	0	100	100
28	B	497/508 (98%)	472 (95%)	25 (5%)	0	100	100
28	BB	497/508 (98%)	477 (96%)	20 (4%)	0	100	100
28	Bb	485/508 (96%)	471 (97%)	14 (3%)	0	100	100
28	b	485/508 (96%)	471 (97%)	14 (3%)	0	100	100
All	All	16994/21780 (78%)	16158 (95%)	828 (5%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	44	171	ASP
14	1	147	TYR
9	n	57	VAL

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Mol	Chain	Res	Type
3	RR	58	TYR
1	Aa	334	ARG
18	C	417	VAL
11	44	83	ASP
4	S	87	PRO

### 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	A	271/284 (95%)	271 (100%)	0	100	100
1	AA	271/284 (95%)	271 (100%)	0	100	100
1	Aa	270/284 (95%)	270 (100%)	0	100	100
1	a	270/284 (95%)	270 (100%)	0	100	100
2	O	196/269 (73%)	196 (100%)	0	100	100
2	OO	196/269 (73%)	196 (100%)	0	100	100
2	Oo	194/269 (72%)	194 (100%)	0	100	100
2	o	194/269 (72%)	194 (100%)	0	100	100
3	R	185/229 (81%)	185 (100%)	0	100	100
3	RR	185/229 (81%)	185 (100%)	0	100	100
3	Rr	186/229 (81%)	186 (100%)	0	100	100
3	r	186/229 (81%)	186 (100%)	0	100	100
4	S	173/226 (76%)	173 (100%)	0	100	100
4	SS	173/226 (76%)	173 (100%)	0	100	100
4	Ss	167/226 (74%)	166 (99%)	1 (1%)	84	91
4	s	167/226 (74%)	167 (100%)	0	100	100
5	T	27/30 (90%)	27 (100%)	0	100	100
5	TT	27/30 (90%)	27 (100%)	0	100	100
5	Tt	27/30 (90%)	27 (100%)	0	100	100
5	t	27/30 (90%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	U	23/80 (29%)	23 (100%)	0	100	100
6	UU	23/80 (29%)	23 (100%)	0	100	100
6	Uu	22/80 (28%)	22 (100%)	0	100	100
6	u	22/80 (28%)	22 (100%)	0	100	100
7	W	44/110 (40%)	44 (100%)	0	100	100
7	WW	44/110 (40%)	44 (100%)	0	100	100
7	Ww	44/110 (40%)	44 (100%)	0	100	100
7	w	44/110 (40%)	44 (100%)	0	100	100
8	X	34/90 (38%)	34 (100%)	0	100	100
8	XX	36/90 (40%)	36 (100%)	0	100	100
8	Xx	25/90 (28%)	25 (100%)	0	100	100
8	x	25/90 (28%)	25 (100%)	0	100	100
9	G	165/205 (80%)	165 (100%)	0	100	100
9	GG	165/205 (80%)	165 (100%)	0	100	100
9	Gg	165/205 (80%)	165 (100%)	0	100	100
9	N	167/205 (82%)	167 (100%)	0	100	100
9	NN	167/205 (82%)	167 (100%)	0	100	100
9	Nn	167/205 (82%)	167 (100%)	0	100	100
9	Y	167/205 (82%)	167 (100%)	0	100	100
9	YY	167/205 (82%)	167 (100%)	0	100	100
9	Yy	167/205 (82%)	167 (100%)	0	100	100
9	g	165/205 (80%)	165 (100%)	0	100	100
9	n	167/205 (82%)	167 (100%)	0	100	100
9	y	167/205 (82%)	167 (100%)	0	100	100
10	Z	52/53 (98%)	52 (100%)	0	100	100
10	ZZ	52/53 (98%)	50 (96%)	2 (4%)	28	59
10	Zz	52/53 (98%)	51 (98%)	1 (2%)	52	74
10	z	52/53 (98%)	52 (100%)	0	100	100
11	4	145/198 (73%)	145 (100%)	0	100	100
11	44	145/198 (73%)	145 (100%)	0	100	100
12	P	153/212 (72%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	PP	153/212 (72%)	153 (100%)	0	100	100
12	Pp	153/212 (72%)	152 (99%)	1 (1%)	81	90
12	p	153/212 (72%)	153 (100%)	0	100	100
13	Q	128/187 (68%)	128 (100%)	0	100	100
13	QQ	128/187 (68%)	128 (100%)	0	100	100
13	Qq	128/187 (68%)	128 (100%)	0	100	100
13	q	128/187 (68%)	128 (100%)	0	100	100
14	1	160/206 (78%)	160 (100%)	0	100	100
14	11	159/206 (77%)	158 (99%)	1 (1%)	84	91
14	2	168/206 (82%)	168 (100%)	0	100	100
14	22	168/206 (82%)	168 (100%)	0	100	100
15	3	164/209 (78%)	164 (100%)	0	100	100
15	33	164/209 (78%)	164 (100%)	0	100	100
16	0	72/107 (67%)	72 (100%)	0	100	100
16	00	72/107 (67%)	72 (100%)	0	100	100
17	5	33/158 (21%)	33 (100%)	0	100	100
17	55	33/158 (21%)	33 (100%)	0	100	100
18	C	351/374 (94%)	351 (100%)	0	100	100
18	CC	351/374 (94%)	351 (100%)	0	100	100
18	Cc	351/374 (94%)	350 (100%)	1 (0%)	91	95
18	c	351/374 (94%)	351 (100%)	0	100	100
19	D	271/282 (96%)	271 (100%)	0	100	100
19	DD	271/282 (96%)	271 (100%)	0	100	100
19	Dd	272/282 (96%)	272 (100%)	0	100	100
19	d	272/282 (96%)	272 (100%)	0	100	100
20	E	70/73 (96%)	70 (100%)	0	100	100
20	EE	70/73 (96%)	70 (100%)	0	100	100
20	Ee	67/73 (92%)	67 (100%)	0	100	100
20	e	67/73 (92%)	67 (100%)	0	100	100
21	F	29/34 (85%)	29 (100%)	0	100	100
21	FF	29/34 (85%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Ff	26/34 (76%)	26 (100%)	0	100	100
21	f	26/34 (76%)	26 (100%)	0	100	100
22	H	48/61 (79%)	48 (100%)	0	100	100
22	HH	48/61 (79%)	48 (100%)	0	100	100
22	Hh	48/61 (79%)	48 (100%)	0	100	100
22	h	48/61 (79%)	48 (100%)	0	100	100
23	I	32/33 (97%)	32 (100%)	0	100	100
23	II	32/33 (97%)	32 (100%)	0	100	100
23	Ii	30/33 (91%)	30 (100%)	0	100	100
23	i	30/33 (91%)	30 (100%)	0	100	100
24	J	28/30 (93%)	28 (100%)	0	100	100
24	JJ	28/30 (93%)	28 (100%)	0	100	100
24	Jj	25/30 (83%)	25 (100%)	0	100	100
24	j	25/30 (83%)	25 (100%)	0	100	100
25	K	32/52 (62%)	32 (100%)	0	100	100
25	KK	32/52 (62%)	32 (100%)	0	100	100
25	Kk	32/52 (62%)	32 (100%)	0	100	100
25	k	32/52 (62%)	32 (100%)	0	100	100
26	L	33/36 (92%)	33 (100%)	0	100	100
26	LL	33/36 (92%)	33 (100%)	0	100	100
26	Ll	34/36 (94%)	34 (100%)	0	100	100
26	l	34/36 (94%)	34 (100%)	0	100	100
27	M	29/30 (97%)	29 (100%)	0	100	100
27	MM	29/30 (97%)	29 (100%)	0	100	100
27	Mm	28/30 (93%)	28 (100%)	0	100	100
27	m	28/30 (93%)	28 (100%)	0	100	100
28	B	398/406 (98%)	398 (100%)	0	100	100
28	BB	398/406 (98%)	398 (100%)	0	100	100
28	Bb	389/406 (96%)	389 (100%)	0	100	100
28	b	389/406 (96%)	389 (100%)	0	100	100
All	All	13835/17352 (80%)	13828 (100%)	7 (0%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Ss	83	ARG
10	Zz	58	ASN
12	Pp	121	LYS
14	11	232	GLN
10	ZZ	37	LYS
10	ZZ	58	ASN
18	Cc	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
14	2	247	HIS
1	a	190	HIS
11	4	152	GLN
28	B	343	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 781 ligands modelled in this entry, 12 are monoatomic - leaving 769 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
46	HEM	Ee	101	20,21	41,50,50	1.48	3 (7%)	45,82,82	1.42	7 (15%)
39	CHL	11	608	14	40,49,74	1.87	5 (12%)	42,83,114	1.63	7 (16%)
32	CLA	Gg	314	9	39,48,73	1.92	7 (17%)	45,82,113	1.43	6 (13%)
39	CHL	22	608	14	40,49,74	1.94	5 (12%)	42,83,114	1.39	6 (14%)
32	CLA	C	509	-	65,73,73	1.47	9 (13%)	76,113,113	1.34	8 (10%)
32	CLA	B	619	-	65,73,73	1.50	8 (12%)	76,113,113	1.20	9 (11%)
44	DGD	Hh	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.92	2 (2%)
44	DGD	h	102	-	63,63,67	0.90	2 (3%)	77,77,81	0.80	2 (2%)
32	CLA	GG	610	9	49,57,73	1.76	9 (18%)	55,93,113	1.24	6 (10%)
32	CLA	b	601	-	65,73,73	1.52	7 (10%)	76,113,113	1.28	10 (13%)
34	BCR	Kk	101	-	41,41,41	0.85	0	56,56,56	1.98	13 (23%)
34	BCR	T	101	-	41,41,41	0.97	1 (2%)	56,56,56	2.06	19 (33%)
34	BCR	DD	405	-	41,41,41	0.83	0	56,56,56	1.91	15 (26%)
39	CHL	4	306	-	46,54,74	1.81	4 (8%)	49,90,114	1.71	6 (12%)
32	CLA	N	602	9	65,73,73	1.49	8 (12%)	76,113,113	1.25	9 (11%)
32	CLA	b	609	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	8 (10%)
32	CLA	y	315	9	59,67,73	1.61	7 (11%)	68,105,113	1.26	6 (8%)
32	CLA	AA	406	-	49,57,73	1.72	8 (16%)	55,93,113	1.39	9 (16%)
44	DGD	CC	522	-	56,56,67	0.92	3 (5%)	70,70,81	1.11	5 (7%)
32	CLA	11	603	-	39,48,73	1.97	7 (17%)	45,82,113	1.41	7 (15%)
39	CHL	r	606	-	50,58,74	1.72	4 (8%)	52,94,114	1.50	7 (13%)
32	CLA	22	613	-	39,48,73	1.97	5 (12%)	45,82,113	1.47	7 (15%)
32	CLA	B	605	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	12 (15%)
43	LMU	C	502	-	28,28,36	0.77	0	39,39,47	0.95	1 (2%)
39	CHL	s	607	-	49,57,74	1.76	5 (10%)	52,93,114	1.23	6 (11%)
32	CLA	Yy	602	9	65,73,73	1.49	7 (10%)	76,113,113	1.21	7 (9%)
32	CLA	BB	607	-	65,73,73	1.47	9 (13%)	76,113,113	1.33	9 (11%)
32	CLA	Bb	607	-	65,73,73	1.52	8 (12%)	76,113,113	1.13	6 (7%)
32	CLA	11	609	14	39,48,73	1.96	7 (17%)	45,82,113	1.45	7 (15%)
32	CLA	N	613	9	49,57,73	1.75	7 (14%)	55,93,113	1.43	7 (12%)
39	CHL	33	606	-	40,49,74	1.94	5 (12%)	42,83,114	1.41	7 (16%)
39	CHL	Yy	608	-	50,58,74	1.68	6 (12%)	52,94,114	1.27	6 (11%)
38	LMG	A	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.11	3 (6%)
42	NEX	g	617	32	38,46,46	1.09	3 (7%)	50,70,70	2.61	16 (32%)
43	LMU	R	618	-	28,28,36	0.79	0	39,39,47	0.98	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	N	603	-	42,50,73	1.82	7 (16%)	48,85,113	1.48	8 (16%)
36	LHG	0	201	-	46,46,48	0.97	2 (4%)	49,52,54	0.84	2 (4%)
37	SQD	LL	102	-	53,54,54	1.19	4 (7%)	62,65,65	1.10	6 (9%)
39	CHL	SS	308	4	49,57,74	1.77	5 (10%)	52,93,114	1.25	5 (9%)
32	CLA	Yy	613	9	59,67,73	1.61	7 (11%)	68,105,113	1.30	7 (10%)
34	BCR	h	101	-	41,41,41	1.04	3 (7%)	56,56,56	2.51	23 (41%)
32	CLA	B	608	-	65,73,73	1.47	6 (9%)	76,113,113	1.17	6 (7%)
39	CHL	N	605	9	42,50,74	1.86	5 (11%)	44,85,114	1.56	6 (13%)
32	CLA	1	611	14	39,48,73	1.97	8 (20%)	45,82,113	1.35	5 (11%)
32	CLA	y	305	-	49,57,73	1.71	8 (16%)	55,93,113	1.36	6 (10%)
32	CLA	AA	408	-	60,68,73	1.57	8 (13%)	70,107,113	1.20	9 (12%)
32	CLA	B	609	-	60,68,73	1.52	6 (10%)	70,107,113	1.31	9 (12%)
36	LHG	CC	523	-	36,36,48	1.05	2 (5%)	39,42,54	1.03	3 (7%)
32	CLA	B	611	-	41,49,73	1.82	6 (14%)	47,84,113	1.47	8 (17%)
32	CLA	g	610	9	49,57,73	1.77	8 (16%)	55,93,113	1.22	7 (12%)
32	CLA	3	611	15	39,48,73	1.94	6 (15%)	45,82,113	1.42	8 (17%)
39	CHL	1	606	-	40,49,74	1.94	5 (12%)	42,83,114	1.41	5 (11%)
32	CLA	N	604	-	41,49,73	1.86	6 (14%)	47,84,113	1.38	8 (17%)
36	LHG	22	615	32	33,33,48	1.13	2 (6%)	36,39,54	0.94	2 (5%)
40	LUT	Gg	316	-	42,43,43	0.94	0	51,60,60	1.41	6 (11%)
32	CLA	b	603	-	65,73,73	1.52	8 (12%)	76,113,113	1.15	8 (10%)
32	CLA	22	602	14	39,48,73	1.95	6 (15%)	45,82,113	1.42	8 (17%)
39	CHL	3	606	-	40,49,74	1.92	5 (12%)	42,83,114	1.43	7 (16%)
32	CLA	44	615	3	49,57,73	1.73	6 (12%)	55,93,113	1.42	6 (10%)
32	CLA	n	611	36	49,57,73	1.72	6 (12%)	55,93,113	1.39	7 (12%)
40	LUT	Nn	306	-	42,43,43	0.97	0	51,60,60	1.30	5 (9%)
32	CLA	R	601	3	49,57,73	1.76	7 (14%)	55,93,113	1.46	5 (9%)
32	CLA	B	621	-	65,73,73	1.51	7 (10%)	76,113,113	1.19	9 (11%)
39	CHL	Rr	606	-	50,58,74	1.71	4 (8%)	52,94,114	1.26	5 (9%)
40	LUT	SS	315	-	42,43,43	1.00	1 (2%)	51,60,60	1.31	7 (13%)
35	PL9	D	407	-	55,55,55	4.24	19 (34%)	68,69,69	3.87	37 (54%)
37	SQD	A	412	-	34,35,54	1.47	4 (11%)	43,46,65	1.16	4 (9%)
39	CHL	1	607	-	40,49,74	1.93	4 (10%)	42,83,114	1.62	7 (16%)
36	LHG	y	320	32	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
39	CHL	RR	306	-	50,58,74	1.61	7 (14%)	52,94,114	1.58	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Nn	305	-	49,57,73	1.72	5 (10%)	55,93,113	1.30	8 (14%)
32	CLA	G	614	-	41,49,73	1.86	6 (14%)	47,84,113	1.32	7 (14%)
44	DGD	C	519	-	56,56,67	0.94	2 (3%)	70,70,81	0.94	3 (4%)
39	CHL	GG	609	9	43,51,74	1.86	5 (11%)	45,86,114	1.63	7 (15%)
32	CLA	YY	603	-	49,57,73	1.70	7 (14%)	55,93,113	1.45	7 (12%)
32	CLA	33	609	15	39,48,73	1.94	6 (15%)	45,82,113	1.44	7 (15%)
32	CLA	C	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	8 (10%)
39	CHL	11	606	-	40,49,74	1.94	5 (12%)	42,83,114	1.38	5 (11%)
40	LUT	Nn	307	-	42,43,43	0.99	0	51,60,60	1.52	7 (13%)
32	CLA	Ss	609	4	49,57,73	1.72	6 (12%)	55,93,113	1.33	8 (14%)
32	CLA	22	603	-	39,48,73	1.93	6 (15%)	45,82,113	1.41	8 (17%)
41	XAT	NN	617	-	39,47,47	1.15	4 (10%)	54,74,74	2.50	13 (24%)
40	LUT	G	615	-	42,43,43	0.94	0	51,60,60	1.49	6 (11%)
32	CLA	r	613	3	49,57,73	1.74	7 (14%)	55,93,113	1.37	7 (12%)
32	CLA	BB	611	-	65,73,73	1.47	7 (10%)	76,113,113	1.24	7 (9%)
36	LHG	A	413	-	36,36,48	1.07	2 (5%)	39,42,54	1.01	3 (7%)
32	CLA	Cc	507	-	65,73,73	1.49	7 (10%)	76,113,113	1.17	7 (9%)
39	CHL	r	607	-	50,58,74	1.72	5 (10%)	52,94,114	1.45	7 (13%)
32	CLA	CC	507	-	65,73,73	1.49	8 (12%)	76,113,113	1.41	8 (10%)
39	CHL	GG	606	-	43,51,74	1.82	6 (13%)	45,86,114	1.29	6 (13%)
32	CLA	BB	615	-	41,49,73	1.84	6 (14%)	47,84,113	1.53	9 (19%)
32	CLA	2	602	14	39,48,73	1.97	6 (15%)	45,82,113	1.44	7 (15%)
32	CLA	A	406	-	49,57,73	1.72	8 (16%)	55,93,113	1.37	8 (14%)
32	CLA	c	508	-	60,68,73	1.55	7 (11%)	70,107,113	1.24	8 (11%)
32	CLA	YY	610	9	65,73,73	1.52	8 (12%)	76,113,113	1.17	7 (9%)
39	CHL	YY	601	9	66,74,74	1.48	6 (9%)	73,114,114	1.15	4 (5%)
40	LUT	g	615	-	42,43,43	0.94	1 (2%)	51,60,60	1.45	5 (9%)
32	CLA	C	512	-	65,73,73	1.50	8 (12%)	76,113,113	1.26	7 (9%)
33	PHO	Aa	408	-	51,69,69	1.04	5 (9%)	47,99,99	1.09	5 (10%)
32	CLA	4	310	-	45,53,73	1.82	7 (15%)	52,89,113	1.35	6 (11%)
41	XAT	Gg	301	-	39,47,47	1.22	4 (10%)	54,74,74	2.84	11 (20%)
32	CLA	r	604	-	49,57,73	1.72	7 (14%)	55,93,113	1.28	6 (10%)
32	CLA	1	613	-	39,48,73	1.94	5 (12%)	45,82,113	1.46	7 (15%)
39	CHL	3	605	-	40,49,74	1.94	5 (12%)	42,83,114	1.42	7 (16%)
32	CLA	C	510	-	65,73,73	1.48	7 (10%)	76,113,113	1.30	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	4	311	36	45,53,73	1.82	6 (13%)	52,89,113	1.34	7 (13%)
39	CHL	Yy	601	9	66,74,74	1.50	6 (9%)	73,114,114	1.11	5 (6%)
32	CLA	r	602	3	65,73,73	1.51	7 (10%)	76,113,113	1.20	9 (11%)
32	CLA	s	604	-	49,57,73	1.76	7 (14%)	55,93,113	1.29	6 (10%)
32	CLA	c	509	-	65,73,73	1.50	8 (12%)	76,113,113	1.17	7 (9%)
34	BCR	a	411	-	41,41,41	0.99	3 (7%)	56,56,56	1.64	10 (17%)
39	CHL	R	606	-	50,58,74	1.67	6 (12%)	52,94,114	1.49	10 (19%)
39	CHL	RR	307	-	50,58,74	1.70	5 (10%)	52,94,114	1.44	6 (11%)
35	PL9	Dd	404	-	55,55,55	4.25	19 (34%)	68,69,69	3.86	37 (54%)
38	LMG	Bb	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.95	2 (4%)
32	CLA	Aa	405	-	65,73,73	1.49	8 (12%)	76,113,113	1.26	7 (9%)
44	DGD	B	601	-	56,56,67	0.92	2 (3%)	70,70,81	0.97	4 (5%)
32	CLA	s	610	36	49,57,73	1.73	7 (14%)	55,93,113	1.42	7 (12%)
39	CHL	4	309	11	46,54,74	1.83	5 (10%)	49,90,114	1.67	8 (16%)
32	CLA	D	405	-	65,73,73	1.52	7 (10%)	76,113,113	1.14	6 (7%)
36	LHG	J	101	-	26,26,48	1.33	2 (7%)	29,32,54	1.36	3 (10%)
32	CLA	GG	612	9	49,57,73	1.75	6 (12%)	55,93,113	1.45	8 (14%)
46	HEM	e	101	20,21	41,50,50	1.47	3 (7%)	45,82,82	1.41	7 (15%)
41	XAT	Rr	615	-	39,47,47	1.03	1 (2%)	54,74,74	2.46	21 (38%)
32	CLA	C	513	18	65,73,73	1.50	8 (12%)	76,113,113	1.25	6 (7%)
32	CLA	B	610	-	65,73,73	1.49	7 (10%)	76,113,113	1.25	9 (11%)
40	LUT	S	614	-	42,43,43	0.89	0	51,60,60	1.51	8 (15%)
46	HEM	E	101	20,21	41,50,50	1.49	3 (7%)	45,82,82	1.25	4 (8%)
32	CLA	r	603	-	49,57,73	1.75	7 (14%)	55,93,113	1.44	6 (10%)
32	CLA	Cc	510	-	60,68,73	1.55	7 (11%)	70,107,113	1.19	7 (10%)
41	XAT	g	619	-	39,47,47	1.22	4 (10%)	54,74,74	2.84	11 (20%)
32	CLA	RR	313	-	41,49,73	1.88	7 (17%)	47,84,113	1.44	8 (17%)
39	CHL	n	609	9	50,58,74	1.65	6 (12%)	52,94,114	1.54	9 (17%)
37	SQD	LL	101	-	35,36,54	1.45	4 (11%)	44,47,65	1.15	5 (11%)
36	LHG	D	408	-	42,42,48	1.00	2 (4%)	45,48,54	1.02	2 (4%)
39	CHL	Ss	601	4	52,60,74	1.69	5 (9%)	56,97,114	1.23	6 (10%)
32	CLA	Rr	602	3	65,73,73	1.54	7 (10%)	76,113,113	1.22	8 (10%)
32	CLA	r	608	3	49,57,73	1.74	6 (12%)	55,93,113	1.36	6 (10%)
32	CLA	22	609	14	39,48,73	1.95	7 (17%)	45,82,113	1.55	7 (15%)
44	DGD	D	411	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	r	611	-	49,57,73	1.79	7 (14%)	55,93,113	1.31	7 (12%)
36	LHG	YY	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
32	CLA	A	405	-	65,73,73	1.49	7 (10%)	76,113,113	1.17	6 (7%)
32	CLA	Bb	611	-	65,73,73	1.48	7 (10%)	76,113,113	1.20	7 (9%)
36	LHG	Y	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.85	2 (3%)
36	LHG	KK	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.10	3 (8%)
39	CHL	Yy	607	-	43,51,74	1.80	5 (11%)	45,86,114	1.46	6 (13%)
39	CHL	N	607	-	66,74,74	1.48	5 (7%)	73,114,114	1.17	6 (8%)
32	CLA	1	610	36	39,48,73	1.95	5 (12%)	45,82,113	1.45	7 (15%)
39	CHL	NN	606	-	42,50,74	1.84	5 (11%)	44,85,114	1.35	4 (9%)
32	CLA	33	604	-	39,48,73	1.96	5 (12%)	45,82,113	1.50	8 (17%)
32	CLA	s	608	4	49,57,73	1.72	6 (12%)	55,93,113	1.42	8 (14%)
42	NEX	Yy	617	-	38,46,46	1.07	1 (2%)	50,70,70	2.02	13 (26%)
32	CLA	33	611	15	39,48,73	1.93	6 (15%)	45,82,113	1.49	8 (17%)
32	CLA	B	618	-	65,73,73	1.48	8 (12%)	76,113,113	1.16	9 (11%)
32	CLA	N	611	36	49,57,73	1.74	5 (10%)	55,93,113	1.42	9 (16%)
32	CLA	Aa	406	1	65,73,73	1.56	9 (13%)	76,113,113	1.24	10 (13%)
38	LMG	DD	409	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	1 (1%)
39	CHL	2	606	-	40,49,74	1.95	4 (10%)	42,83,114	1.61	7 (16%)
32	CLA	GG	604	-	42,50,73	1.85	7 (16%)	48,85,113	1.33	6 (12%)
38	LMG	a	412	-	42,42,55	1.03	2 (4%)	50,50,63	1.10	4 (8%)
32	CLA	CC	505	-	65,73,73	1.50	8 (12%)	76,113,113	1.23	9 (11%)
32	CLA	Ss	613	-	49,57,73	1.72	6 (12%)	55,93,113	1.31	8 (14%)
32	CLA	Cc	504	-	65,73,73	1.48	7 (10%)	76,113,113	1.27	9 (11%)
39	CHL	g	609	9	43,51,74	1.81	5 (11%)	45,86,114	1.57	7 (15%)
32	CLA	Dd	401	-	65,73,73	1.52	8 (12%)	76,113,113	1.28	7 (9%)
32	CLA	Yy	612	9	65,73,73	1.49	8 (12%)	76,113,113	1.25	8 (10%)
34	BCR	Cc	518	-	41,41,41	0.89	1 (2%)	56,56,56	1.90	11 (19%)
39	CHL	YY	609	9	66,74,74	1.51	7 (10%)	73,114,114	1.14	8 (10%)
39	CHL	2	607	-	40,49,74	1.93	5 (12%)	42,83,114	1.40	6 (14%)
32	CLA	B	623	-	65,73,73	1.50	7 (10%)	76,113,113	1.14	7 (9%)
44	DGD	BB	623	-	63,63,67	0.89	3 (4%)	77,77,81	0.93	2 (2%)
32	CLA	Ss	608	4	49,57,73	1.71	6 (12%)	55,93,113	1.42	9 (16%)
32	CLA	y	314	9	65,73,73	1.49	8 (12%)	76,113,113	1.21	8 (10%)
29	OEX	Cc	502	18,1	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	LHG	AA	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.89	2 (4%)
38	LMG	Dd	408	-	46,46,55	0.97	2 (4%)	54,54,63	1.02	3 (5%)
32	CLA	BB	613	-	60,68,73	1.53	6 (10%)	70,107,113	1.28	9 (12%)
41	XAT	GG	617	-	39,47,47	1.07	2 (5%)	54,74,74	2.51	16 (29%)
32	CLA	Rr	611	-	49,57,73	1.74	6 (12%)	55,93,113	1.34	6 (10%)
32	CLA	S	613	-	45,53,73	1.80	6 (13%)	52,89,113	1.33	7 (13%)
39	CHL	g	606	-	43,51,74	1.82	5 (11%)	45,86,114	1.32	4 (8%)
39	CHL	NN	608	-	42,50,74	1.87	6 (14%)	44,85,114	1.31	5 (11%)
32	CLA	YY	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.34	8 (14%)
34	BCR	BB	616	-	41,41,41	0.95	1 (2%)	56,56,56	1.89	13 (23%)
39	CHL	Y	608	-	50,58,74	1.68	6 (12%)	52,94,114	1.30	6 (11%)
32	CLA	Cc	508	-	65,73,73	1.47	6 (9%)	76,113,113	1.29	10 (13%)
32	CLA	Bb	601	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	9 (11%)
32	CLA	Nn	314	-	49,57,73	1.72	7 (14%)	55,93,113	1.30	8 (14%)
36	LHG	1	614	32	29,29,48	1.21	2 (6%)	32,35,54	1.12	2 (6%)
32	CLA	GG	603	-	65,73,73	1.51	8 (12%)	76,113,113	1.17	7 (9%)
39	CHL	1	608	14	40,49,74	1.85	5 (12%)	42,83,114	1.75	8 (19%)
32	CLA	C	514	-	65,73,73	1.50	8 (12%)	76,113,113	1.30	7 (9%)
32	CLA	Ss	602	4	49,57,73	1.73	7 (14%)	55,93,113	1.37	8 (14%)
39	CHL	2	601	14	40,49,74	1.94	6 (15%)	42,83,114	1.42	5 (11%)
34	BCR	d	403	-	41,41,41	0.87	0	56,56,56	2.03	18 (32%)
39	CHL	Y	607	-	43,51,74	1.84	5 (11%)	45,86,114	1.56	8 (17%)
43	LMU	RR	301	-	28,28,36	0.76	0	39,39,47	0.75	0
39	CHL	Nn	316	-	50,58,74	1.71	5 (10%)	52,94,114	1.33	5 (9%)
39	CHL	Y	606	-	44,52,74	1.83	6 (13%)	46,87,114	1.23	5 (10%)
32	CLA	Gg	303	9	49,57,73	1.77	7 (14%)	55,93,113	1.57	6 (10%)
32	CLA	33	613	-	39,48,73	1.94	6 (15%)	45,82,113	1.48	9 (20%)
36	LHG	Dd	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
32	CLA	a	405	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	6 (7%)
36	LHG	n	618	32	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
42	NEX	RR	317	-	38,46,46	1.08	2 (5%)	50,70,70	2.03	13 (26%)
35	PL9	A	410	-	55,55,55	4.31	22 (40%)	68,69,69	3.77	38 (55%)
32	CLA	4	303	11	45,53,73	1.81	7 (15%)	52,89,113	1.38	8 (15%)
32	CLA	N	612	9	42,50,73	1.85	7 (16%)	48,85,113	1.41	8 (16%)
39	CHL	1	605	14	40,49,74	1.92	5 (12%)	42,83,114	1.61	7 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	R	605	-	50,58,74	1.66	5 (10%)	52,94,114	1.75	12 (23%)
32	CLA	Aa	407	-	49,57,73	1.72	8 (16%)	55,93,113	1.45	9 (16%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
32	CLA	BB	608	-	65,73,73	1.51	7 (10%)	76,113,113	1.20	8 (10%)
40	LUT	Rr	614	-	42,43,43	0.92	0	51,60,60	1.38	8 (15%)
32	CLA	22	610	36	42,50,73	1.89	5 (11%)	48,85,113	1.40	7 (14%)
32	CLA	22	612	14	39,48,73	1.93	6 (15%)	45,82,113	1.49	7 (15%)
41	XAT	y	301	-	39,47,47	1.06	3 (7%)	54,74,74	2.48	19 (35%)
32	CLA	SS	303	4	49,57,73	1.72	7 (14%)	55,93,113	1.37	9 (16%)
34	BCR	Bb	619	-	41,41,41	0.90	1 (2%)	56,56,56	2.04	15 (26%)
40	LUT	Y	616	-	42,43,43	0.99	0	51,60,60	1.57	11 (21%)
32	CLA	c	504	-	55,63,73	1.61	7 (12%)	64,101,113	1.22	6 (9%)
33	PHO	a	409	-	51,69,69	1.02	3 (5%)	47,99,99	1.05	4 (8%)
44	DGD	CC	518	-	56,56,67	0.92	2 (3%)	70,70,81	0.95	4 (5%)
39	CHL	Gg	307	-	43,51,74	1.83	5 (11%)	45,86,114	1.31	4 (8%)
32	CLA	G	604	-	42,50,73	1.84	6 (14%)	48,85,113	1.29	5 (10%)
32	CLA	R	608	3	49,57,73	1.71	7 (14%)	55,93,113	1.46	7 (12%)
36	LHG	G	618	32	33,33,48	1.12	2 (6%)	36,39,54	1.14	3 (8%)
40	LUT	Ss	615	-	42,43,43	0.99	1 (2%)	51,60,60	1.69	13 (25%)
32	CLA	Gg	305	-	42,50,73	1.86	6 (14%)	48,85,113	1.30	5 (10%)
44	DGD	c	517	-	56,56,67	0.91	2 (3%)	70,70,81	1.11	6 (8%)
40	LUT	YY	615	-	42,43,43	0.96	1 (2%)	51,60,60	1.78	9 (17%)
32	CLA	c	511	18	65,73,73	1.54	7 (10%)	76,113,113	1.15	5 (6%)
39	CHL	3	608	15	40,49,74	1.93	5 (12%)	42,83,114	1.36	6 (14%)
32	CLA	Yy	610	9	65,73,73	1.52	9 (13%)	76,113,113	1.14	6 (7%)
32	CLA	33	603	-	39,48,73	1.95	5 (12%)	45,82,113	1.48	8 (17%)
32	CLA	G	602	9	49,57,73	1.77	7 (14%)	55,93,113	1.32	5 (9%)
42	NEX	NN	618	-	38,46,46	1.12	2 (5%)	50,70,70	2.22	14 (28%)
34	BCR	Dd	403	-	41,41,41	0.86	0	56,56,56	2.03	18 (32%)
32	CLA	1	604	-	39,48,73	1.96	6 (15%)	45,82,113	1.50	8 (17%)
40	LUT	r	614	-	42,43,43	0.94	1 (2%)	51,60,60	1.38	7 (13%)
39	CHL	g	607	-	50,58,74	1.70	6 (12%)	52,94,114	1.25	5 (9%)
36	LHG	g	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
34	BCR	C	518	-	41,41,41	0.88	0	56,56,56	2.07	17 (30%)
39	CHL	Gg	310	9	43,51,74	1.81	5 (11%)	45,86,114	1.63	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	R	602	3	65,73,73	1.52	8 (12%)	76,113,113	1.25	9 (11%)
34	BCR	Cc	516	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
39	CHL	22	605	-	40,49,74	1.93	4 (10%)	42,83,114	1.63	8 (19%)
42	NEX	Y	617	-	38,46,46	1.08	2 (5%)	50,70,70	2.12	13 (26%)
39	CHL	22	601	14	40,49,74	1.95	5 (12%)	42,83,114	1.41	6 (14%)
32	CLA	2	610	-	39,48,73	1.91	6 (15%)	45,82,113	1.42	8 (17%)
32	CLA	G	603	-	65,73,73	1.52	8 (12%)	76,113,113	1.17	8 (10%)
32	CLA	b	602	-	65,73,73	1.50	7 (10%)	76,113,113	1.19	9 (11%)
39	CHL	G	609	9	43,51,74	1.85	5 (11%)	45,86,114	1.53	6 (13%)
32	CLA	Dd	402	-	65,73,73	1.50	7 (10%)	76,113,113	1.19	7 (9%)
39	CHL	33	601	15	40,49,74	1.92	5 (12%)	42,83,114	1.39	5 (11%)
32	CLA	Cc	515	-	43,51,73	1.80	7 (16%)	49,86,113	1.43	7 (14%)
32	CLA	1	603	-	39,48,73	1.92	7 (17%)	45,82,113	1.36	5 (11%)
32	CLA	y	313	36	42,50,73	1.85	7 (16%)	48,85,113	1.41	6 (12%)
32	CLA	Bb	616	-	65,73,73	1.48	7 (10%)	76,113,113	1.20	7 (9%)
32	CLA	Rr	613	3	49,57,73	1.74	7 (14%)	55,93,113	1.37	7 (12%)
36	LHG	d	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.97	2 (4%)
39	CHL	G	607	-	46,54,74	1.77	5 (10%)	49,90,114	1.34	5 (10%)
32	CLA	b	613	-	65,73,73	1.49	8 (12%)	76,113,113	1.37	9 (11%)
39	CHL	2	605	-	40,49,74	1.95	4 (10%)	42,83,114	1.62	7 (16%)
40	LUT	2	614	-	42,43,43	1.08	4 (9%)	51,60,60	1.84	12 (23%)
32	CLA	CC	509	-	65,73,73	1.48	7 (10%)	76,113,113	1.29	8 (10%)
39	CHL	N	608	-	42,50,74	1.87	7 (16%)	44,85,114	1.31	5 (11%)
41	XAT	RR	316	-	39,47,47	1.01	2 (5%)	54,74,74	2.30	16 (29%)
40	LUT	NN	616	-	42,43,43	0.94	1 (2%)	51,60,60	1.67	10 (19%)
40	LUT	Gg	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.64	10 (19%)
40	LUT	n	616	-	42,43,43	0.99	0	51,60,60	1.50	8 (15%)
32	CLA	a	407	-	49,57,73	1.73	8 (16%)	55,93,113	1.42	8 (14%)
32	CLA	Gg	304	-	65,73,73	1.51	8 (12%)	76,113,113	1.15	8 (10%)
40	LUT	R	615	-	42,43,43	0.89	0	51,60,60	1.57	12 (23%)
39	CHL	GG	608	-	42,50,74	1.84	6 (14%)	44,85,114	1.35	6 (13%)
32	CLA	DD	403	-	65,73,73	1.49	8 (12%)	76,113,113	1.31	7 (9%)
42	NEX	YY	617	-	38,46,46	1.08	2 (5%)	50,70,70	2.07	13 (26%)
32	CLA	BB	612	-	65,73,73	1.47	6 (9%)	76,113,113	1.16	6 (7%)
36	LHG	CC	521	-	33,33,48	1.12	2 (6%)	36,39,54	1.03	2 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	2	608	14	40,49,74	1.95	6 (15%)	42,83,114	1.37	6 (14%)
45	BCT	AA	413	30	2,3,3	1.26	0	2,3,3	4.14	2 (100%)
32	CLA	S	612	4	49,57,73	1.74	7 (14%)	55,93,113	1.25	6 (10%)
32	CLA	Bb	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	9 (11%)
32	CLA	11	613	-	39,48,73	1.96	5 (12%)	45,82,113	1.44	7 (15%)
32	CLA	Gg	313	9	49,57,73	1.72	8 (16%)	55,93,113	1.37	8 (14%)
40	LUT	s	614	-	42,43,43	1.05	2 (4%)	51,60,60	1.49	8 (15%)
32	CLA	b	607	-	65,73,73	1.52	8 (12%)	76,113,113	1.14	8 (10%)
38	LMG	Aa	412	-	42,42,55	1.05	3 (7%)	50,50,63	1.09	4 (8%)
36	LHG	DD	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.92	2 (3%)
38	LMG	AA	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.13	3 (6%)
36	LHG	AA	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.22	4 (11%)
32	CLA	CC	512	18	65,73,73	1.50	9 (13%)	76,113,113	1.22	7 (9%)
39	CHL	Gg	302	9	66,74,74	1.51	6 (9%)	73,114,114	1.11	4 (5%)
36	LHG	Nn	310	32	48,48,48	0.95	2 (4%)	51,54,54	1.05	2 (3%)
37	SQD	L	102	-	35,36,54	1.45	4 (11%)	44,47,65	1.23	5 (11%)
39	CHL	SS	302	4	52,60,74	1.68	5 (9%)	56,97,114	1.21	5 (8%)
39	CHL	Gg	306	9	43,51,74	1.86	6 (13%)	45,86,114	1.33	6 (13%)
38	LMG	WW	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
36	LHG	Dd	407	-	36,36,48	1.07	2 (5%)	39,42,54	0.91	2 (5%)
32	CLA	4	312	-	45,53,73	1.80	6 (13%)	52,89,113	1.41	6 (11%)
32	CLA	Gg	311	9	49,57,73	1.70	6 (12%)	55,93,113	1.39	8 (14%)
34	BCR	B	613	-	41,41,41	0.98	3 (7%)	56,56,56	1.78	12 (21%)
36	LHG	33	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.10	2 (5%)
39	CHL	44	601	-	44,53,74	1.83	5 (11%)	46,89,114	1.29	5 (10%)
38	LMG	Mm	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.83	2 (3%)
40	LUT	g	616	-	42,43,43	0.87	1 (2%)	51,60,60	1.59	9 (17%)
38	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.01	3 (5%)
32	CLA	RR	309	3	65,73,73	1.52	8 (12%)	76,113,113	1.16	8 (10%)
36	LHG	C	522	-	30,30,48	1.16	2 (6%)	33,36,54	1.06	2 (6%)
32	CLA	y	306	-	49,57,73	1.69	7 (14%)	55,93,113	1.32	7 (12%)
41	XAT	44	613	-	39,47,47	0.97	2 (5%)	54,74,74	2.56	12 (22%)
32	CLA	3	613	-	39,48,73	1.94	6 (15%)	45,82,113	1.45	8 (17%)
32	CLA	2	613	-	39,48,73	1.91	7 (17%)	45,82,113	1.38	7 (15%)
32	CLA	c	513	-	43,51,73	1.79	6 (13%)	49,86,113	1.43	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	11	602	14	39,48,73	1.93	5 (12%)	45,82,113	1.47	8 (17%)
32	CLA	g	612	9	49,57,73	1.74	7 (14%)	55,93,113	1.40	9 (16%)
32	CLA	NN	611	36	49,57,73	1.72	6 (12%)	55,93,113	1.44	9 (16%)
32	CLA	Bb	603	-	65,73,73	1.51	9 (13%)	76,113,113	1.18	8 (10%)
39	CHL	Gg	309	-	42,50,74	1.84	6 (14%)	44,85,114	1.29	5 (11%)
32	CLA	C	515	-	49,57,73	1.70	7 (14%)	55,93,113	1.42	8 (14%)
39	CHL	NN	605	9	42,50,74	1.84	5 (11%)	44,85,114	1.63	7 (15%)
32	CLA	C	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	8 (10%)
32	CLA	B	622	-	65,73,73	1.50	8 (12%)	76,113,113	1.27	10 (13%)
32	CLA	S	604	-	49,57,73	1.73	7 (14%)	55,93,113	1.40	8 (14%)
32	CLA	CC	513	-	65,73,73	1.48	8 (12%)	76,113,113	1.28	6 (7%)
34	BCR	H	101	-	41,41,41	0.99	2 (4%)	56,56,56	2.17	21 (37%)
32	CLA	b	614	-	65,73,73	1.47	6 (9%)	76,113,113	1.24	7 (9%)
32	CLA	RR	308	3	49,57,73	1.71	7 (14%)	55,93,113	1.46	7 (12%)
39	CHL	22	606	-	40,49,74	1.95	4 (10%)	42,83,114	1.68	7 (16%)
42	NEX	R	617	-	38,46,46	1.09	2 (5%)	50,70,70	2.01	13 (26%)
32	CLA	2	604	-	39,48,73	1.95	6 (15%)	45,82,113	1.53	8 (17%)
39	CHL	n	607	-	66,74,74	1.48	5 (7%)	73,114,114	1.21	6 (8%)
32	CLA	Nn	312	9	65,73,73	1.47	8 (12%)	76,113,113	1.29	10 (13%)
36	LHG	EE	101	-	39,39,48	1.05	2 (5%)	42,45,54	0.90	2 (4%)
39	CHL	S	601	4	52,60,74	1.69	5 (9%)	56,97,114	1.20	5 (8%)
39	CHL	Nn	319	9	50,58,74	1.64	6 (12%)	52,94,114	1.50	8 (15%)
39	CHL	33	605	-	40,49,74	1.95	5 (12%)	42,83,114	1.41	7 (16%)
34	BCR	KK	103	-	41,41,41	0.82	0	56,56,56	2.18	19 (33%)
32	CLA	RR	314	3	49,57,73	1.81	7 (14%)	55,93,113	1.37	9 (16%)
39	CHL	44	605	-	46,54,74	1.83	4 (8%)	49,90,114	1.58	6 (12%)
37	SQD	C	501	-	53,54,54	1.17	4 (7%)	62,65,65	1.07	5 (8%)
32	CLA	Y	603	-	49,57,73	1.71	7 (14%)	55,93,113	1.40	7 (12%)
32	CLA	s	613	-	49,57,73	1.73	6 (12%)	55,93,113	1.32	7 (12%)
38	LMG	F	101	-	46,46,55	0.98	2 (4%)	54,54,63	0.90	2 (3%)
39	CHL	R	607	-	50,58,74	1.69	5 (10%)	52,94,114	1.44	6 (11%)
32	CLA	S	602	4	49,57,73	1.72	7 (14%)	55,93,113	1.35	9 (16%)
32	CLA	SS	314	-	49,57,73	1.73	7 (14%)	55,93,113	1.29	8 (14%)
39	CHL	s	606	-	50,58,74	1.72	4 (8%)	52,94,114	1.54	7 (13%)
32	CLA	C	507	-	65,73,73	1.48	7 (10%)	76,113,113	1.20	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	D	404	-	65,73,73	1.48	8 (12%)	76,113,113	1.32	8 (10%)
32	CLA	R	612	3	42,50,73	1.85	7 (16%)	48,85,113	1.34	7 (14%)
32	CLA	BB	606	-	65,73,73	1.50	7 (10%)	76,113,113	1.15	7 (9%)
32	CLA	RR	312	3	42,50,73	1.86	7 (16%)	48,85,113	1.30	5 (10%)
32	CLA	Bb	602	-	65,73,73	1.50	9 (13%)	76,113,113	1.17	8 (10%)
32	CLA	Bb	614	-	65,73,73	1.45	6 (9%)	76,113,113	1.23	7 (9%)
32	CLA	b	616	-	65,73,73	1.48	7 (10%)	76,113,113	1.19	7 (9%)
39	CHL	Yy	606	-	44,52,74	1.80	4 (9%)	46,87,114	1.34	5 (10%)
32	CLA	GG	613	9	39,48,73	1.92	8 (20%)	45,82,113	1.58	9 (20%)
32	CLA	d	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.15	8 (10%)
41	XAT	G	619	-	39,47,47	1.19	2 (5%)	54,74,74	2.93	13 (24%)
32	CLA	B	624	-	65,73,73	1.49	9 (13%)	76,113,113	1.29	9 (11%)
32	CLA	c	502	-	65,73,73	1.49	7 (10%)	76,113,113	1.28	11 (14%)
32	CLA	g	604	42	42,50,73	1.88	7 (16%)	48,85,113	1.27	5 (10%)
33	PHO	a	408	-	51,69,69	1.03	5 (9%)	47,99,99	1.09	5 (10%)
32	CLA	33	602	15	39,48,73	1.94	5 (12%)	45,82,113	1.46	8 (17%)
39	CHL	GG	601	9	66,74,74	1.51	5 (7%)	73,114,114	1.10	6 (8%)
32	CLA	g	611	36	65,73,73	1.51	6 (9%)	76,113,113	1.39	10 (13%)
39	CHL	y	310	-	50,58,74	1.69	6 (12%)	52,94,114	1.25	6 (11%)
32	CLA	G	611	36	52,60,73	1.70	6 (11%)	60,97,113	1.26	5 (8%)
32	CLA	Y	611	36	42,50,73	1.84	7 (16%)	48,85,113	1.37	5 (10%)
32	CLA	AA	405	-	65,73,73	1.49	7 (10%)	76,113,113	1.19	6 (7%)
32	CLA	CC	506	-	65,73,73	1.48	7 (10%)	76,113,113	1.23	8 (10%)
39	CHL	Nn	311	9	50,58,74	1.70	5 (10%)	52,94,114	1.27	4 (7%)
34	BCR	Bb	617	-	41,41,41	1.05	2 (4%)	56,56,56	2.11	16 (28%)
39	CHL	G	605	9	43,51,74	1.88	5 (11%)	45,86,114	1.21	4 (8%)
39	CHL	G	606	-	43,51,74	1.83	6 (13%)	45,86,114	1.30	6 (13%)
40	LUT	GG	616	-	42,43,43	0.95	1 (2%)	51,60,60	1.54	8 (15%)
32	CLA	Ss	604	-	49,57,73	1.75	6 (12%)	55,93,113	1.36	8 (14%)
32	CLA	44	602	11	45,53,73	1.81	7 (15%)	52,89,113	1.38	9 (17%)
40	LUT	N	616	-	42,43,43	0.97	1 (2%)	51,60,60	1.64	10 (19%)
32	CLA	3	604	-	39,48,73	1.98	5 (12%)	45,82,113	1.46	7 (15%)
32	CLA	RR	304	-	49,57,73	1.75	7 (14%)	55,93,113	1.43	9 (16%)
32	CLA	R	614	3	49,57,73	1.83	8 (16%)	55,93,113	1.38	8 (14%)
40	LUT	Yy	615	-	42,43,43	0.98	1 (2%)	51,60,60	2.06	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Rr	608	3	49,57,73	1.73	6 (12%)	55,93,113	1.36	8 (14%)
32	CLA	SS	304	-	45,53,73	1.80	6 (13%)	52,89,113	1.42	8 (15%)
32	CLA	3	602	15	39,48,73	1.93	6 (15%)	45,82,113	1.47	8 (17%)
34	BCR	c	514	-	41,41,41	0.93	2 (4%)	56,56,56	2.15	18 (32%)
33	PHO	D	402	-	51,69,69	1.02	4 (7%)	47,99,99	1.11	6 (12%)
32	CLA	y	316	-	49,57,73	1.72	7 (14%)	55,93,113	1.38	9 (16%)
36	LHG	SS	301	-	25,25,48	1.30	2 (8%)	28,31,54	1.09	2 (7%)
39	CHL	Nn	317	-	66,74,74	1.47	5 (7%)	73,114,114	1.25	7 (9%)
37	SQD	L	101	-	53,54,54	1.19	4 (7%)	62,65,65	1.10	6 (9%)
32	CLA	g	613	9	39,48,73	1.97	10 (25%)	45,82,113	1.41	7 (15%)
34	BCR	BB	617	-	41,41,41	0.97	2 (4%)	56,56,56	1.75	12 (21%)
32	CLA	CC	510	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	8 (10%)
32	CLA	2	612	14	39,48,73	1.93	5 (12%)	45,82,113	1.51	8 (17%)
46	HEM	EE	102	20,21	41,50,50	1.48	3 (7%)	45,82,82	1.23	5 (11%)
32	CLA	3	603	-	39,48,73	1.96	5 (12%)	45,82,113	1.44	8 (17%)
41	XAT	Nn	308	-	39,47,47	1.16	3 (7%)	54,74,74	2.78	16 (29%)
32	CLA	Ss	610	36	49,57,73	1.72	7 (14%)	55,93,113	1.42	7 (12%)
39	CHL	22	607	-	40,49,74	1.95	5 (12%)	42,83,114	1.40	6 (14%)
32	CLA	RR	311	-	49,57,73	1.73	7 (14%)	55,93,113	1.34	6 (10%)
32	CLA	GG	611	36	52,60,73	1.68	6 (11%)	60,97,113	1.28	6 (10%)
32	CLA	RR	303	-	49,57,73	1.70	7 (14%)	55,93,113	1.43	6 (10%)
37	SQD	B	617	-	35,36,54	1.48	4 (11%)	44,47,65	4.31	10 (22%)
39	CHL	g	605	9	43,51,74	1.87	6 (13%)	45,86,114	1.31	6 (13%)
32	CLA	n	614	-	49,57,73	1.72	6 (12%)	55,93,113	1.26	7 (12%)
32	CLA	11	612	-	39,48,73	1.98	11 (28%)	45,82,113	1.73	10 (22%)
32	CLA	s	611	4	49,57,73	1.72	7 (14%)	55,93,113	1.40	9 (16%)
32	CLA	B	620	-	65,73,73	1.48	9 (13%)	76,113,113	1.26	8 (10%)
39	CHL	Ss	607	-	49,57,74	1.75	5 (10%)	52,93,114	1.24	6 (11%)
32	CLA	S	603	-	45,53,73	1.82	6 (13%)	52,89,113	1.43	7 (13%)
32	CLA	G	613	9	39,48,73	1.93	7 (17%)	45,82,113	1.47	9 (20%)
32	CLA	33	612	15	39,48,73	1.95	7 (17%)	45,82,113	1.41	7 (15%)
32	CLA	b	605	-	65,73,73	1.48	7 (10%)	76,113,113	1.19	7 (9%)
39	CHL	s	605	-	50,58,74	1.73	4 (8%)	52,94,114	1.45	6 (11%)
34	BCR	CC	516	-	41,41,41	0.95	1 (2%)	56,56,56	1.89	13 (23%)
40	LUT	RR	315	-	42,43,43	0.88	1 (2%)	51,60,60	1.54	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Bb	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.21	9 (11%)
39	CHL	Ss	605	-	50,58,74	1.72	5 (10%)	52,94,114	1.43	6 (11%)
36	LHG	4	315	32	20,20,48	1.35	2 (10%)	23,26,54	1.40	2 (8%)
32	CLA	g	602	9	49,57,73	1.77	7 (14%)	55,93,113	1.91	9 (16%)
32	CLA	d	401	-	65,73,73	1.52	8 (12%)	76,113,113	1.33	9 (11%)
44	DGD	a	415	-	56,56,67	0.97	2 (3%)	70,70,81	0.91	3 (4%)
32	CLA	n	610	9	65,73,73	1.52	8 (12%)	76,113,113	1.13	10 (13%)
32	CLA	R	604	-	49,57,73	1.74	7 (14%)	55,93,113	1.45	8 (14%)
39	CHL	g	608	-	42,50,74	1.84	6 (14%)	44,85,114	1.30	5 (11%)
32	CLA	c	512	-	65,73,73	1.47	7 (10%)	76,113,113	1.23	8 (10%)
39	CHL	NN	601	9	44,52,74	1.83	5 (11%)	46,87,114	1.51	8 (17%)
32	CLA	s	602	4	49,57,73	1.74	7 (14%)	55,93,113	1.36	8 (14%)
32	CLA	3	609	15	39,48,73	1.96	5 (12%)	45,82,113	1.47	8 (17%)
39	CHL	RR	305	-	50,58,74	1.65	4 (8%)	52,94,114	1.75	13 (25%)
34	BCR	CC	515	-	41,41,41	0.97	1 (2%)	56,56,56	2.02	17 (30%)
34	BCR	CC	517	-	41,41,41	0.91	1 (2%)	56,56,56	2.00	14 (25%)
32	CLA	s	603	-	49,57,73	1.76	6 (12%)	55,93,113	1.31	7 (12%)
32	CLA	4	304	-	45,53,73	1.82	7 (15%)	52,89,113	1.51	8 (15%)
39	CHL	44	606	-	46,54,74	1.79	6 (13%)	49,90,114	1.29	5 (10%)
32	CLA	2	611	14	39,48,73	1.94	5 (12%)	45,82,113	1.45	8 (17%)
32	CLA	B	607	-	65,73,73	1.48	8 (12%)	76,113,113	1.23	6 (7%)
39	CHL	Y	609	9	66,74,74	1.51	6 (9%)	73,114,114	1.20	8 (10%)
32	CLA	g	603	-	65,73,73	1.52	8 (12%)	76,113,113	1.13	8 (10%)
32	CLA	y	304	9	65,73,73	1.50	8 (12%)	76,113,113	1.19	6 (7%)
40	LUT	4	313	-	42,43,43	0.93	0	51,60,60	1.38	6 (11%)
32	CLA	c	510	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	8 (10%)
39	CHL	44	607	-	46,54,74	1.77	7 (15%)	49,90,114	1.30	5 (10%)
40	LUT	y	317	-	42,43,43	0.96	1 (2%)	51,60,60	2.02	11 (21%)
34	BCR	K	102	-	41,41,41	0.81	0	56,56,56	2.18	18 (32%)
32	CLA	BB	610	-	65,73,73	1.49	7 (10%)	76,113,113	1.33	9 (11%)
32	CLA	SS	313	4	49,57,73	1.73	7 (14%)	55,93,113	1.25	6 (10%)
32	CLA	r	601	3	49,57,73	1.75	5 (10%)	55,93,113	1.32	7 (12%)
39	CHL	y	307	9	48,56,74	1.73	5 (10%)	51,92,114	1.31	7 (13%)
32	CLA	11	604	-	39,48,73	1.95	5 (12%)	45,82,113	1.64	9 (20%)
32	CLA	y	312	9	65,73,73	1.51	8 (12%)	76,113,113	1.12	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	CC	514	-	49,57,73	1.68	6 (12%)	55,93,113	1.40	8 (14%)
34	BCR	c	516	-	41,41,41	0.89	1 (2%)	56,56,56	2.02	15 (26%)
40	LUT	YY	616	-	42,43,43	0.94	0	51,60,60	1.46	8 (15%)
41	XAT	y	302	-	39,47,47	1.17	3 (7%)	54,74,74	2.73	17 (31%)
34	BCR	Aa	411	-	41,41,41	1.00	3 (7%)	56,56,56	1.60	10 (17%)
32	CLA	c	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.32	8 (10%)
32	CLA	Y	613	9	59,67,73	1.59	8 (13%)	68,105,113	1.23	7 (10%)
36	LHG	K	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.08	2 (5%)
39	CHL	Rr	607	-	50,58,74	1.71	5 (10%)	52,94,114	1.46	7 (13%)
34	BCR	b	617	-	41,41,41	1.00	2 (4%)	56,56,56	2.10	16 (28%)
32	CLA	n	604	-	49,57,73	1.72	7 (14%)	55,93,113	1.25	6 (10%)
32	CLA	Bb	605	-	65,73,73	1.48	7 (10%)	76,113,113	1.20	8 (10%)
36	LHG	DD	407	-	42,42,48	0.99	2 (4%)	45,48,54	1.02	2 (4%)
32	CLA	N	614	-	41,49,73	1.88	6 (14%)	47,84,113	1.38	7 (14%)
32	CLA	SS	311	-	49,57,73	1.72	7 (14%)	55,93,113	1.45	7 (12%)
32	CLA	Bb	612	-	65,73,73	1.47	7 (10%)	76,113,113	1.30	6 (7%)
38	LMG	CC	520	-	39,39,55	1.06	2 (5%)	47,47,63	0.95	2 (4%)
40	LUT	y	318	-	42,43,43	0.91	0	51,60,60	1.55	10 (19%)
32	CLA	Gg	312	36	65,73,73	1.50	6 (9%)	76,113,113	1.35	10 (13%)
40	LUT	44	612	-	42,43,43	0.91	0	51,60,60	1.38	6 (11%)
32	CLA	s	609	4	49,57,73	1.71	6 (12%)	55,93,113	1.37	9 (16%)
32	CLA	Gg	315	-	49,57,73	1.73	7 (14%)	55,93,113	1.29	8 (14%)
32	CLA	A	408	-	60,68,73	1.57	7 (11%)	70,107,113	1.19	8 (11%)
32	CLA	NN	604	-	41,49,73	1.85	6 (14%)	47,84,113	1.38	8 (17%)
36	LHG	A	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.22	3 (8%)
32	CLA	Yy	614	-	49,57,73	1.71	7 (14%)	55,93,113	1.39	8 (14%)
39	CHL	Ss	606	-	50,58,74	1.72	4 (8%)	52,94,114	1.56	7 (13%)
39	CHL	n	601	9	50,58,74	1.71	5 (10%)	52,94,114	1.30	4 (7%)
42	NEX	Nn	309	-	38,46,46	1.06	1 (2%)	50,70,70	2.10	12 (24%)
29	OEX	A	401	18,1	0,15,15	-	-	-	-	-
32	CLA	b	608	-	65,73,73	1.51	8 (12%)	76,113,113	1.23	8 (10%)
32	CLA	Aa	410	-	60,68,73	1.57	8 (13%)	70,107,113	1.23	9 (12%)
38	LMG	b	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.11	4 (9%)
39	CHL	S	607	-	43,51,74	1.89	5 (11%)	45,86,114	1.26	5 (11%)
39	CHL	SS	306	4	42,50,74	1.80	5 (11%)	44,85,114	1.67	6 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Rr	601	3	49,57,73	1.75	5 (10%)	55,93,113	1.31	8 (14%)
32	CLA	C	504	-	65,73,73	1.46	7 (10%)	76,113,113	1.32	8 (10%)
39	CHL	YY	606	-	44,52,74	1.80	6 (13%)	46,87,114	1.29	5 (10%)
34	BCR	b	619	-	41,41,41	0.89	1 (2%)	56,56,56	1.93	12 (21%)
42	NEX	N	618	-	38,46,46	1.13	2 (5%)	50,70,70	2.22	15 (30%)
39	CHL	3	601	15	40,49,74	1.92	5 (12%)	42,83,114	1.44	4 (9%)
32	CLA	NN	602	9	65,73,73	1.50	8 (12%)	76,113,113	1.26	10 (13%)
44	DGD	BB	625	-	57,57,67	0.91	2 (3%)	70,70,81	0.94	3 (4%)
34	BCR	XX	202	-	41,41,41	0.92	1 (2%)	56,56,56	2.14	16 (28%)
34	BCR	D	406	-	41,41,41	0.83	0	56,56,56	1.92	16 (28%)
44	DGD	Aa	401	-	56,56,67	0.96	2 (3%)	70,70,81	0.90	3 (4%)
32	CLA	YY	611	36	42,50,73	1.83	7 (16%)	48,85,113	1.37	7 (14%)
35	PL9	AA	410	-	55,55,55	4.33	23 (41%)	68,69,69	3.71	38 (55%)
32	CLA	22	611	14	39,48,73	1.94	6 (15%)	45,82,113	1.49	8 (17%)
36	LHG	D	409	-	48,48,48	0.90	2 (4%)	51,54,54	0.91	2 (3%)
39	CHL	G	608	-	42,50,74	1.84	5 (11%)	44,85,114	1.39	7 (15%)
39	CHL	NN	609	9	50,58,74	1.67	6 (12%)	52,94,114	1.48	10 (19%)
37	SQD	Ll	101	-	53,54,54	1.18	4 (7%)	62,65,65	1.02	4 (6%)
41	XAT	r	615	-	39,47,47	1.02	1 (2%)	54,74,74	2.49	14 (25%)
39	CHL	4	308	-	46,54,74	1.76	5 (10%)	49,90,114	1.55	8 (16%)
36	LHG	Yy	618	32	48,48,48	0.91	2 (4%)	51,54,54	0.99	4 (7%)
32	CLA	R	603	-	49,57,73	1.72	7 (14%)	55,93,113	1.41	7 (12%)
32	CLA	r	610	36	49,57,73	1.75	6 (12%)	55,93,113	1.38	7 (12%)
45	BCT	a	413	30	2,3,3	1.28	0	2,3,3	3.84	2 (100%)
32	CLA	Nn	303	9	49,57,73	1.73	6 (12%)	55,93,113	1.40	8 (14%)
32	CLA	DD	401	-	65,73,73	1.50	8 (12%)	76,113,113	1.26	9 (11%)
32	CLA	Bb	610	-	65,73,73	1.52	8 (12%)	76,113,113	1.23	9 (11%)
44	DGD	c	518	-	53,53,67	0.95	2 (3%)	67,67,81	0.89	2 (2%)
39	CHL	Nn	318	-	50,58,74	1.71	6 (12%)	52,94,114	1.29	5 (9%)
40	LUT	n	615	-	42,43,43	0.97	0	51,60,60	1.30	5 (9%)
32	CLA	c	506	-	65,73,73	1.47	6 (9%)	76,113,113	1.26	10 (13%)
37	SQD	l	102	-	53,54,54	1.18	4 (7%)	62,65,65	1.03	4 (6%)
32	CLA	D	401	-	65,73,73	1.49	8 (12%)	76,113,113	1.26	9 (11%)
32	CLA	r	609	3	65,73,73	1.50	7 (10%)	76,113,113	1.19	6 (7%)
39	CHL	s	601	4	52,60,74	1.70	5 (9%)	56,97,114	1.45	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	22	604	-	39,48,73	1.95	6 (15%)	45,82,113	1.49	8 (17%)
32	CLA	N	610	9	65,73,73	1.53	8 (12%)	76,113,113	1.12	8 (10%)
32	CLA	BB	603	-	65,73,73	1.48	9 (13%)	76,113,113	1.26	8 (10%)
39	CHL	Yy	605	9	48,56,74	1.75	6 (12%)	51,92,114	1.29	7 (13%)
36	LHG	N	619	32	37,37,48	1.07	2 (5%)	40,43,54	1.06	3 (7%)
32	CLA	Yy	604	-	49,57,73	1.70	7 (14%)	55,93,113	1.31	6 (10%)
37	SQD	B	602	-	46,47,54	1.28	4 (8%)	55,58,65	1.05	5 (9%)
32	CLA	r	612	3	49,57,73	1.74	7 (14%)	55,93,113	1.36	7 (12%)
39	CHL	SS	307	-	42,50,74	1.85	5 (11%)	44,85,114	1.34	4 (9%)
32	CLA	R	611	-	49,57,73	1.72	7 (14%)	55,93,113	1.35	6 (10%)
32	CLA	NN	612	9	42,50,73	1.84	6 (14%)	48,85,113	1.42	8 (16%)
34	BCR	BB	620	-	41,41,41	0.83	0	56,56,56	1.99	18 (32%)
36	LHG	NN	619	32	37,37,48	1.08	2 (5%)	40,43,54	1.03	2 (5%)
33	PHO	Aa	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.07	5 (10%)
42	NEX	Y	619	-	38,46,46	1.08	1 (2%)	50,70,70	2.23	15 (30%)
32	CLA	BB	609	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	12 (15%)
42	NEX	Rr	616	-	38,46,46	1.07	1 (2%)	50,70,70	2.22	16 (32%)
34	BCR	AA	409	-	41,41,41	1.01	3 (7%)	56,56,56	1.97	14 (25%)
32	CLA	S	608	4	41,49,73	1.90	7 (17%)	47,84,113	1.36	7 (14%)
39	CHL	Yy	609	9	66,74,74	1.48	6 (9%)	73,114,114	1.52	8 (10%)
39	CHL	N	609	9	50,58,74	1.65	6 (12%)	52,94,114	1.57	11 (21%)
32	CLA	Bb	613	-	65,73,73	1.49	8 (12%)	76,113,113	1.38	9 (11%)
44	DGD	C	523	-	53,53,67	0.93	2 (3%)	67,67,81	0.93	2 (2%)
32	CLA	3	610	36	39,48,73	1.90	5 (12%)	45,82,113	1.58	9 (20%)
34	BCR	k	101	-	41,41,41	0.88	0	56,56,56	1.92	15 (26%)
32	CLA	n	603	-	49,57,73	1.70	7 (14%)	55,93,113	1.40	8 (14%)
32	CLA	Rr	610	36	49,57,73	1.80	6 (12%)	55,93,113	1.42	6 (10%)
39	CHL	YY	605	9	48,56,74	1.76	5 (10%)	51,92,114	1.22	5 (9%)
34	BCR	TT	101	-	41,41,41	0.98	1 (2%)	56,56,56	2.04	18 (32%)
32	CLA	Bb	615	-	65,73,73	1.50	8 (12%)	76,113,113	1.21	7 (9%)
32	CLA	YY	613	9	59,67,73	1.57	7 (11%)	68,105,113	1.23	8 (11%)
34	BCR	Cc	517	-	41,41,41	1.03	2 (4%)	56,56,56	1.79	14 (25%)
39	CHL	n	606	-	50,58,74	1.71	5 (10%)	52,94,114	1.36	5 (9%)
32	CLA	4	305	-	45,53,73	1.78	6 (13%)	52,89,113	1.44	8 (15%)
32	CLA	YY	604	-	49,57,73	1.72	7 (14%)	55,93,113	1.39	8 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Yy	603	-	49,57,73	1.69	7 (14%)	55,93,113	1.44	8 (14%)
41	XAT	Yy	619	-	39,47,47	1.05	2 (5%)	54,74,74	2.45	19 (35%)
32	CLA	b	612	-	65,73,73	1.47	7 (10%)	76,113,113	1.29	7 (9%)
32	CLA	XX	201	-	41,49,73	1.90	7 (17%)	47,84,113	1.31	5 (10%)
44	DGD	Cc	520	-	53,53,67	0.95	2 (3%)	67,67,81	0.88	1 (1%)
32	CLA	Rr	612	3	49,57,73	1.73	7 (14%)	55,93,113	1.32	6 (10%)
36	LHG	Ss	616	32	47,47,48	0.94	2 (4%)	50,53,54	0.89	2 (4%)
32	CLA	CC	502	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	9 (11%)
34	BCR	C	516	-	41,41,41	0.95	1 (2%)	56,56,56	2.07	17 (30%)
36	LHG	GG	618	32	33,33,48	1.12	2 (6%)	36,39,54	1.14	3 (8%)
40	LUT	NN	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.34	8 (15%)
39	CHL	44	608	11	46,54,74	1.82	4 (8%)	49,90,114	1.58	7 (14%)
37	SQD	BB	621	-	35,36,54	1.48	5 (14%)	44,47,65	4.32	10 (22%)
32	CLA	2	603	-	39,48,73	1.94	6 (15%)	45,82,113	1.45	8 (17%)
39	CHL	4	302	-	44,53,74	1.84	6 (13%)	46,89,114	1.28	5 (10%)
36	LHG	II	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.01	2 (5%)
36	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	3 (5%)
32	CLA	44	610	36	45,53,73	1.82	6 (13%)	52,89,113	1.34	7 (13%)
42	NEX	n	617	-	38,46,46	1.08	1 (2%)	50,70,70	2.13	13 (26%)
32	CLA	Y	602	9	65,73,73	1.50	6 (9%)	76,113,113	1.20	9 (11%)
32	CLA	Y	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.32	8 (14%)
44	DGD	CC	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.93	3 (3%)
32	CLA	Cc	513	18	65,73,73	1.52	7 (10%)	76,113,113	1.21	8 (10%)
39	CHL	n	608	-	50,58,74	1.72	6 (12%)	52,94,114	1.29	6 (11%)
32	CLA	BB	601	-	65,73,73	1.49	7 (10%)	76,113,113	1.17	9 (11%)
32	CLA	Cc	511	-	65,73,73	1.50	7 (10%)	76,113,113	1.17	8 (10%)
32	CLA	CC	511	-	65,73,73	1.50	8 (12%)	76,113,113	1.25	7 (9%)
32	CLA	a	410	-	60,68,73	1.57	7 (11%)	70,107,113	1.23	8 (11%)
40	LUT	G	616	-	42,43,43	0.93	0	51,60,60	1.59	9 (17%)
40	LUT	N	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.48	8 (15%)
34	BCR	Hh	101	-	41,41,41	1.06	4 (9%)	56,56,56	2.42	22 (39%)
36	LHG	4	301	32	18,18,48	1.77	3 (16%)	17,22,54	1.48	1 (5%)
32	CLA	Cc	512	-	65,73,73	1.50	7 (10%)	76,113,113	1.25	8 (10%)
36	LHG	Gg	319	32	33,33,48	1.12	2 (6%)	36,39,54	1.17	3 (8%)
44	DGD	B	603	-	57,57,67	0.92	2 (3%)	70,70,81	0.93	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	S	611	4	49,57,73	1.72	6 (12%)	55,93,113	1.45	7 (12%)
32	CLA	Bb	608	-	65,73,73	1.48	9 (13%)	76,113,113	1.22	8 (10%)
32	CLA	Bb	609	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	9 (11%)
39	CHL	4	307	-	46,54,74	1.79	6 (13%)	49,90,114	1.31	5 (10%)
39	CHL	S	605	-	42,50,74	1.88	4 (9%)	44,85,114	1.64	6 (13%)
32	CLA	Cc	506	-	55,63,73	1.60	7 (12%)	64,101,113	1.27	8 (12%)
41	XAT	4	314	-	39,47,47	1.00	0	54,74,74	2.62	15 (27%)
32	CLA	BB	614	-	65,73,73	1.49	7 (10%)	76,113,113	1.28	10 (13%)
39	CHL	r	605	3	50,58,74	1.71	5 (10%)	52,94,114	1.35	6 (11%)
32	CLA	11	611	14	39,48,73	1.93	5 (12%)	45,82,113	1.53	8 (17%)
39	CHL	33	607	-	40,49,74	1.93	5 (12%)	42,83,114	1.64	7 (16%)
38	LMG	W	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.05	2 (3%)
32	CLA	S	610	-	49,57,73	1.71	7 (14%)	55,93,113	1.42	6 (10%)
32	CLA	a	406	1	65,73,73	1.59	9 (13%)	76,113,113	1.24	9 (11%)
40	LUT	GG	615	-	42,43,43	0.93	0	51,60,60	1.45	7 (13%)
37	SQD	CC	501	-	53,54,54	1.16	5 (9%)	62,65,65	1.23	5 (8%)
34	BCR	A	409	-	41,41,41	1.00	3 (7%)	56,56,56	1.98	14 (25%)
40	LUT	s	615	-	42,43,43	0.92	0	51,60,60	1.59	12 (23%)
44	DGD	BB	624	-	56,56,67	0.92	2 (3%)	70,70,81	0.98	4 (5%)
32	CLA	R	609	3	65,73,73	1.52	8 (12%)	76,113,113	1.17	8 (10%)
32	CLA	Rr	603	-	49,57,73	1.74	7 (14%)	55,93,113	1.40	6 (10%)
39	CHL	g	601	9	66,74,74	1.49	5 (7%)	73,114,114	1.12	6 (8%)
34	BCR	B	614	-	41,41,41	0.96	2 (4%)	56,56,56	1.85	13 (23%)
32	CLA	44	604	-	45,53,73	1.78	7 (15%)	52,89,113	1.38	7 (13%)
44	DGD	C	520	-	63,63,67	0.86	2 (3%)	77,77,81	0.86	2 (2%)
38	LMG	b	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.95	2 (4%)
45	BCT	Aa	414	30	2,3,3	1.27	0	2,3,3	3.93	2 (100%)
40	LUT	Yy	616	-	42,43,43	0.91	0	51,60,60	1.55	10 (19%)
34	BCR	C	517	-	41,41,41	0.93	1 (2%)	56,56,56	1.88	12 (21%)
32	CLA	YY	612	9	58,66,73	1.66	6 (10%)	67,104,113	1.49	15 (22%)
32	CLA	Rr	609	3	65,73,73	1.49	6 (9%)	76,113,113	1.25	7 (9%)
32	CLA	Y	604	-	49,57,73	1.71	7 (14%)	55,93,113	1.33	8 (14%)
38	LMG	j	101	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
32	CLA	X	201	-	41,49,73	1.88	7 (17%)	47,84,113	1.43	7 (14%)
34	BCR	b	618	-	41,41,41	0.90	1 (2%)	56,56,56	1.92	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	GG	602	9	49,57,73	1.75	7 (14%)	55,93,113	1.40	6 (10%)
32	CLA	Cc	503	-	65,73,73	1.49	7 (10%)	76,113,113	1.30	7 (9%)
32	CLA	Y	612	9	65,73,73	1.54	7 (10%)	76,113,113	1.21	10 (13%)
34	BCR	BB	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.87	13 (23%)
32	CLA	1	609	14	39,48,73	1.97	8 (20%)	45,82,113	1.52	6 (13%)
39	CHL	Rr	605	3	50,58,74	1.70	5 (10%)	52,94,114	1.48	6 (11%)
32	CLA	SS	312	4	49,57,73	1.72	6 (12%)	55,93,113	1.41	7 (12%)
32	CLA	33	610	36	39,48,73	1.92	5 (12%)	45,82,113	1.49	8 (17%)
32	CLA	C	506	-	65,73,73	1.50	8 (12%)	76,113,113	1.23	7 (9%)
36	LHG	D	410	-	33,33,48	1.12	2 (6%)	36,39,54	1.11	3 (8%)
42	NEX	y	319	-	38,46,46	1.07	1 (2%)	50,70,70	2.01	11 (22%)
32	CLA	RR	310	36	49,57,73	1.75	6 (12%)	55,93,113	1.29	7 (12%)
38	LMG	BB	619	-	45,45,55	0.98	2 (4%)	53,53,63	0.93	2 (3%)
36	LHG	a	414	-	36,36,48	1.07	2 (5%)	39,42,54	0.92	2 (5%)
39	CHL	y	308	-	44,52,74	1.81	5 (11%)	46,87,114	1.32	5 (10%)
43	LMU	KK	102	-	28,28,36	0.76	0	39,39,47	0.88	1 (2%)
32	CLA	SS	310	4	41,49,73	1.92	6 (14%)	47,84,113	1.37	6 (12%)
39	CHL	11	607	-	40,49,74	1.91	4 (10%)	42,83,114	1.71	10 (23%)
32	CLA	Cc	514	-	65,73,73	1.47	7 (10%)	76,113,113	1.25	8 (10%)
34	BCR	B	616	-	41,41,41	0.85	0	56,56,56	1.97	19 (33%)
29	OEX	AA	401	18,1	0,15,15	-	-	-	-	-
39	CHL	YY	607	-	43,51,74	1.85	5 (11%)	45,86,114	1.54	8 (17%)
39	CHL	N	606	-	42,50,74	1.85	6 (14%)	44,85,114	1.35	5 (11%)
41	XAT	G	617	-	39,47,47	1.10	2 (5%)	54,74,74	2.50	14 (25%)
36	LHG	Dd	405	-	42,42,48	0.98	2 (4%)	45,48,54	0.95	2 (4%)
41	XAT	R	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.29	16 (29%)
32	CLA	44	603	-	45,53,73	1.80	7 (15%)	52,89,113	1.44	6 (11%)
32	CLA	S	609	4	41,49,73	1.89	6 (14%)	47,84,113	1.44	6 (12%)
33	PHO	DD	402	-	51,69,69	1.03	5 (9%)	47,99,99	1.10	5 (10%)
32	CLA	BB	604	-	65,73,73	1.52	7 (10%)	76,113,113	1.15	9 (11%)
29	OEX	a	401	18,1	0,15,15	-	-	-	-	-
32	CLA	b	615	-	65,73,73	1.51	8 (12%)	76,113,113	1.20	7 (9%)
32	CLA	1	612	14	39,48,73	1.94	5 (12%)	45,82,113	1.56	7 (15%)
32	CLA	Cc	505	-	65,73,73	1.50	7 (10%)	76,113,113	1.21	7 (9%)
36	LHG	s	616	32	47,47,48	0.95	2 (4%)	50,53,54	0.90	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	SQD	Aa	413	-	46,47,54	1.27	4 (8%)	55,58,65	1.04	5 (9%)
39	CHL	y	309	-	43,51,74	1.81	5 (11%)	45,86,114	1.52	7 (15%)
39	CHL	GG	605	9	43,51,74	1.87	5 (11%)	45,86,114	1.24	5 (11%)
32	CLA	DD	404	-	65,73,73	1.50	7 (10%)	76,113,113	1.15	6 (7%)
32	CLA	b	606	-	65,73,73	1.50	8 (12%)	76,113,113	1.21	9 (11%)
32	CLA	Ss	612	4	49,57,73	1.74	6 (12%)	55,93,113	1.34	7 (12%)
32	CLA	BB	605	-	65,73,73	1.49	8 (12%)	76,113,113	1.26	9 (11%)
32	CLA	NN	614	-	41,49,73	1.88	6 (14%)	47,84,113	1.38	7 (14%)
39	CHL	Gg	308	-	50,58,74	1.69	5 (10%)	52,94,114	1.24	5 (9%)
33	PHO	A	407	-	51,69,69	1.03	4 (7%)	47,99,99	1.22	8 (17%)
32	CLA	C	508	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
32	CLA	c	501	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	10 (13%)
32	CLA	CC	508	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	10 (13%)
36	LHG	BB	622	-	33,33,48	1.12	2 (6%)	36,39,54	1.01	2 (5%)
39	CHL	y	311	9	66,74,74	1.50	6 (9%)	73,114,114	1.14	7 (9%)
39	CHL	33	608	15	40,49,74	1.92	5 (12%)	42,83,114	1.69	8 (19%)
36	LHG	Rr	617	32	48,48,48	0.98	2 (4%)	51,54,54	0.97	2 (3%)
36	LHG	JJ	101	-	32,32,48	1.13	2 (6%)	35,38,54	1.13	3 (8%)
41	XAT	N	617	-	39,47,47	1.13	3 (7%)	54,74,74	2.50	14 (25%)
32	CLA	B	604	-	65,73,73	1.54	7 (10%)	76,113,113	1.21	7 (9%)
39	CHL	N	601	9	44,52,74	1.85	6 (13%)	46,87,114	1.34	7 (15%)
39	CHL	YY	608	-	50,58,74	1.69	6 (12%)	52,94,114	1.28	6 (11%)
39	CHL	Nn	315	9	48,56,74	1.74	5 (10%)	51,92,114	1.60	8 (15%)
40	LUT	Ss	614	-	42,43,43	1.08	2 (4%)	51,60,60	1.46	10 (19%)
38	LMG	m	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.82	2 (3%)
34	BCR	c	515	-	41,41,41	1.01	3 (7%)	56,56,56	1.69	12 (21%)
39	CHL	l	601	14	40,49,74	1.94	6 (15%)	42,83,114	1.41	5 (11%)
32	CLA	n	612	9	49,57,73	1.72	8 (16%)	55,93,113	1.34	7 (12%)
32	CLA	Nn	313	-	49,57,73	1.71	7 (14%)	55,93,113	1.42	8 (14%)
36	LHG	44	614	32	20,20,48	1.30	2 (10%)	23,26,54	1.50	2 (8%)
32	CLA	B	606	-	65,73,73	1.50	7 (10%)	76,113,113	1.29	8 (10%)
32	CLA	NN	610	9	65,73,73	1.52	8 (12%)	76,113,113	1.16	9 (11%)
40	LUT	22	614	-	42,43,43	1.12	4 (9%)	51,60,60	1.77	11 (21%)
41	XAT	GG	619	-	39,47,47	1.19	3 (7%)	54,74,74	2.94	12 (22%)
32	CLA	R	610	36	49,57,73	1.77	7 (14%)	55,93,113	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	g	614	-	49,57,73	1.73	7 (14%)	55,93,113	1.29	8 (14%)
38	LMG	Cc	501	-	34,34,55	1.14	3 (8%)	42,42,63	1.27	6 (14%)
32	CLA	Nn	301	9	65,73,73	1.52	8 (12%)	76,113,113	1.18	10 (13%)
32	CLA	G	612	9	49,57,73	1.75	7 (14%)	55,93,113	1.38	8 (14%)
32	CLA	YY	602	9	65,73,73	1.51	7 (10%)	76,113,113	1.18	8 (10%)
39	CHL	11	601	14	40,49,74	1.95	6 (15%)	42,83,114	1.42	6 (14%)
32	CLA	n	613	9	49,57,73	1.76	8 (16%)	55,93,113	1.36	7 (12%)
39	CHL	NN	607	-	66,74,74	1.48	5 (7%)	73,114,114	1.17	5 (6%)
33	PHO	AA	407	-	51,69,69	1.05	5 (9%)	47,99,99	1.22	7 (14%)
32	CLA	44	611	-	45,53,73	1.79	6 (13%)	52,89,113	1.41	6 (11%)
32	CLA	Ss	603	-	49,57,73	1.76	6 (12%)	55,93,113	1.31	7 (12%)
32	CLA	R	613	-	41,49,73	1.90	7 (17%)	47,84,113	1.44	8 (17%)
32	CLA	Nn	302	36	49,57,73	1.73	6 (12%)	55,93,113	1.37	7 (12%)
36	LHG	A	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.89	2 (4%)
40	LUT	Y	615	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	12 (23%)
32	CLA	c	505	-	65,73,73	1.48	8 (12%)	76,113,113	1.11	7 (9%)
35	PL9	d	404	-	55,55,55	4.25	19 (34%)	68,69,69	3.83	37 (54%)
32	CLA	11	610	36	39,48,73	1.95	5 (12%)	45,82,113	1.46	8 (17%)
32	CLA	Nn	304	9	49,57,73	1.76	7 (14%)	55,93,113	1.36	8 (14%)
39	CHL	n	605	9	48,56,74	1.76	6 (12%)	51,92,114	1.37	7 (13%)
32	CLA	C	505	-	65,73,73	1.50	7 (10%)	76,113,113	1.26	10 (13%)
34	BCR	B	612	-	41,41,41	0.95	0	56,56,56	1.75	13 (23%)
39	CHL	S	606	-	42,50,74	1.86	5 (11%)	44,85,114	1.35	4 (9%)
32	CLA	s	612	4	49,57,73	1.73	6 (12%)	55,93,113	1.34	7 (12%)
32	CLA	2	609	14	39,48,73	1.95	6 (15%)	45,82,113	1.48	7 (15%)
32	CLA	G	610	9	49,57,73	1.80	8 (16%)	55,93,113	1.52	7 (12%)
32	CLA	Y	610	9	65,73,73	1.50	7 (10%)	76,113,113	1.25	9 (11%)
39	CHL	Y	601	9	66,74,74	1.50	6 (9%)	73,114,114	1.16	5 (6%)
32	CLA	CC	503	-	65,73,73	1.46	7 (10%)	76,113,113	1.31	9 (11%)
32	CLA	Ss	611	4	49,57,73	1.73	7 (14%)	55,93,113	1.41	9 (16%)
32	CLA	n	602	9	65,73,73	1.50	9 (13%)	76,113,113	1.28	12 (15%)
32	CLA	NN	603	-	42,50,73	1.80	7 (16%)	48,85,113	1.49	8 (16%)
32	CLA	b	611	-	65,73,73	1.49	7 (10%)	76,113,113	1.19	8 (10%)
38	LMG	Bb	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.10	5 (11%)
32	CLA	CC	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.20	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	CLA	Rr	604	-	49,57,73	1.74	7 (14%)	55,93,113	1.26	7 (12%)
32	CLA	44	609	11	45,53,73	1.79	6 (13%)	52,89,113	1.36	6 (11%)
36	LHG	3	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.14	3 (8%)
36	LHG	r	616	32	48,48,48	0.97	2 (4%)	51,54,54	0.92	2 (3%)
32	CLA	b	604	-	65,73,73	1.48	7 (10%)	76,113,113	1.30	9 (11%)
32	CLA	RR	302	3	65,73,73	1.51	8 (12%)	76,113,113	1.29	10 (13%)
42	NEX	Gg	318	-	38,46,46	1.10	3 (7%)	50,70,70	2.44	14 (28%)
34	BCR	Bb	618	-	41,41,41	0.89	1 (2%)	56,56,56	1.94	12 (21%)
32	CLA	3	612	15	39,48,73	1.96	7 (17%)	45,82,113	1.41	7 (15%)
36	LHG	44	616	32	18,18,48	1.77	3 (16%)	17,22,54	1.42	1 (5%)
32	CLA	b	610	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	7 (9%)
39	CHL	G	601	9	66,74,74	1.50	4 (6%)	73,114,114	1.07	5 (6%)
37	SQD	AA	412	-	34,35,54	1.46	4 (11%)	43,46,65	1.16	4 (9%)
39	CHL	GG	607	-	46,54,74	1.77	5 (10%)	49,90,114	1.31	4 (8%)
39	CHL	11	605	14	40,49,74	1.97	5 (12%)	42,83,114	1.43	6 (14%)
39	CHL	y	303	9	66,74,74	1.51	6 (9%)	73,114,114	1.11	5 (6%)
45	BCT	D	403	30	2,3,3	1.26	0	2,3,3	4.02	2 (100%)
32	CLA	GG	614	-	41,49,73	1.86	6 (14%)	47,84,113	1.33	7 (14%)
32	CLA	SS	305	-	49,57,73	1.74	7 (14%)	55,93,113	1.42	8 (14%)
36	LHG	11	614	32	33,33,48	1.14	2 (6%)	36,39,54	1.11	3 (8%)
36	LHG	Ll	102	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
32	CLA	BB	602	-	65,73,73	1.50	8 (12%)	76,113,113	1.21	9 (11%)
32	CLA	1	602	14	39,48,73	1.92	5 (12%)	45,82,113	1.52	8 (17%)
32	CLA	NN	613	9	49,57,73	1.75	8 (16%)	55,93,113	1.30	5 (9%)
44	DGD	Cc	519	-	56,56,67	0.91	2 (3%)	70,70,81	1.11	7 (10%)
39	CHL	Y	605	9	48,56,74	1.74	6 (12%)	51,92,114	1.29	6 (11%)
38	LMG	B	615	-	45,45,55	0.98	2 (4%)	53,53,63	0.93	2 (3%)
32	CLA	c	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.15	7 (9%)
32	CLA	Cc	509	-	65,73,73	1.48	7 (10%)	76,113,113	1.30	7 (9%)
32	CLA	Yy	611	36	42,50,73	1.84	7 (16%)	48,85,113	1.44	6 (12%)
39	CHL	3	607	-	40,49,74	1.93	4 (10%)	42,83,114	1.61	7 (16%)
32	CLA	SS	309	4	41,49,73	1.88	6 (14%)	47,84,113	1.40	7 (14%)
38	LMG	c	519	-	34,34,55	1.14	3 (8%)	42,42,63	1.20	6 (14%)
35	PL9	DD	406	-	55,55,55	4.25	19 (34%)	68,69,69	3.82	37 (54%)



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
46	HEM	Ee	101	20,21	-	6/12/54/54	-
39	CHL	11	608	14	3/3/19/26	2/10/104/137	-
32	CLA	Gg	314	9	1/1/13/20	2/8/82/115	-
39	CHL	22	608	14	3/3/19/26	2/10/104/137	-
32	CLA	C	509	-	1/1/20/20	10/37/115/115	-
32	CLA	B	619	-	1/1/20/20	21/37/115/115	-
44	DGD	Hh	102	-	-	12/51/91/95	0/2/2/2
44	DGD	h	102	-	-	8/51/91/95	0/2/2/2
32	CLA	GG	610	9	1/1/16/20	7/18/96/115	-
32	CLA	b	601	-	1/1/20/20	16/37/115/115	-
34	BCR	Kk	101	-	-	4/29/63/63	0/2/2/2
34	BCR	T	101	-	-	3/29/63/63	0/2/2/2
34	BCR	DD	405	-	-	2/29/63/63	0/2/2/2
39	CHL	4	306	-	3/3/21/26	5/15/113/137	-
32	CLA	N	602	9	1/1/20/20	14/37/115/115	-
32	CLA	b	609	-	1/1/20/20	17/37/115/115	-
32	CLA	y	315	9	1/1/18/20	11/30/108/115	-
32	CLA	AA	406	-	1/1/16/20	7/18/96/115	-
44	DGD	CC	522	-	-	11/44/84/95	0/2/2/2
32	CLA	11	603	-	1/1/13/20	5/8/82/115	-
39	CHL	r	606	-	3/3/22/26	4/20/118/137	-
32	CLA	22	613	-	1/1/13/20	4/8/82/115	-
32	CLA	B	605	-	-	15/37/115/115	-
43	LMU	C	502	-	-	4/13/53/61	0/2/2/2
39	CHL	s	607	-	3/3/22/26	7/19/117/137	-
32	CLA	Yy	602	9	1/1/20/20	15/37/115/115	-
32	CLA	BB	607	-	1/1/20/20	12/37/115/115	-
32	CLA	Bb	607	-	1/1/20/20	11/37/115/115	-
32	CLA	11	609	14	1/1/13/20	2/8/82/115	-
32	CLA	N	613	9	1/1/16/20	8/18/96/115	-
39	CHL	33	606	-	3/3/19/26	4/10/104/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Yy	608	-	3/3/22/26	6/20/118/137	-
38	LMG	A	415	-	-	4/31/51/70	0/1/1/1
42	NEX	g	617	32	-	3/27/83/83	0/3/3/3
43	LMU	R	618	-	-	5/13/53/61	0/2/2/2
32	CLA	N	603	-	1/1/14/20	6/10/88/115	-
36	LHG	0	201	-	-	11/51/51/53	-
37	SQD	LL	102	-	-	16/49/69/69	0/1/1/1
39	CHL	SS	308	4	3/3/22/26	5/19/117/137	-
32	CLA	Yy	613	9	1/1/18/20	9/30/108/115	-
39	CHL	N	605	9	3/3/20/26	4/10/108/137	-
32	CLA	B	608	-	1/1/20/20	14/37/115/115	-
34	BCR	h	101	-	-	7/29/63/63	0/2/2/2
32	CLA	1	611	14	1/1/13/20	2/8/82/115	-
32	CLA	y	305	-	1/1/16/20	5/18/96/115	-
32	CLA	AA	408	-	1/1/19/20	8/31/109/115	-
32	CLA	B	609	-	1/1/19/20	7/31/109/115	-
36	LHG	CC	523	-	-	10/41/41/53	-
32	CLA	B	611	-	1/1/14/20	3/8/86/115	-
32	CLA	g	610	9	1/1/16/20	6/18/96/115	-
32	CLA	3	611	15	1/1/13/20	4/8/82/115	-
39	CHL	1	606	-	3/3/19/26	4/10/104/137	-
32	CLA	N	604	-	1/1/14/20	5/8/86/115	-
36	LHG	22	615	32	-	9/38/38/53	-
40	LUT	Gg	316	-	-	2/29/67/67	0/2/2/2
32	CLA	b	603	-	1/1/20/20	16/37/115/115	-
32	CLA	22	602	14	1/1/13/20	2/8/82/115	-
39	CHL	3	606	-	3/3/19/26	4/10/104/137	-
32	CLA	44	615	3	1/1/16/20	9/18/96/115	-
32	CLA	n	611	36	1/1/16/20	5/18/96/115	-
40	LUT	Nn	306	-	-	1/29/67/67	0/2/2/2
32	CLA	R	601	3	1/1/16/20	8/18/96/115	-
32	CLA	B	621	-	1/1/20/20	12/37/115/115	-
39	CHL	Rr	606	-	3/3/22/26	6/20/118/137	-
40	LUT	SS	315	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PL9	D	407	-	-	28/53/73/73	0/1/1/1
37	SQD	A	412	-	-	6/30/50/69	0/1/1/1
39	CHL	1	607	-	3/3/19/26	2/10/104/137	-
36	LHG	y	320	32	-	23/53/53/53	-
39	CHL	RR	306	-	3/3/21/26	11/20/118/137	-
32	CLA	Nn	305	-	-	7/18/96/115	-
32	CLA	G	614	-	1/1/14/20	2/8/86/115	-
44	DGD	C	519	-	-	9/44/84/95	0/2/2/2
39	CHL	GG	609	9	3/3/20/26	4/12/110/137	-
32	CLA	YY	603	-	1/1/16/20	7/18/96/115	-
32	CLA	33	609	15	1/1/13/20	1/8/82/115	-
32	CLA	C	511	-	1/1/20/20	12/37/115/115	-
39	CHL	11	606	-	3/3/19/26	4/10/104/137	-
40	LUT	Nn	307	-	-	2/29/67/67	0/2/2/2
32	CLA	Ss	609	4	1/1/16/20	10/18/96/115	-
32	CLA	22	603	-	1/1/13/20	2/8/82/115	-
41	XAT	NN	617	-	-	0/31/93/93	0/4/4/4
40	LUT	G	615	-	-	2/29/67/67	0/2/2/2
32	CLA	r	613	3	1/1/16/20	9/18/96/115	-
32	CLA	BB	611	-	1/1/20/20	6/37/115/115	-
36	LHG	A	413	-	-	11/41/41/53	-
32	CLA	Cc	507	-	1/1/20/20	12/37/115/115	-
39	CHL	r	607	-	3/3/22/26	8/20/118/137	-
32	CLA	CC	507	-	1/1/20/20	13/37/115/115	-
39	CHL	GG	606	-	3/3/20/26	5/12/110/137	-
32	CLA	BB	615	-	1/1/14/20	3/8/86/115	-
32	CLA	2	602	14	1/1/13/20	4/8/82/115	-
32	CLA	A	406	-	1/1/16/20	9/18/96/115	-
32	CLA	c	508	-	1/1/19/20	11/31/109/115	-
32	CLA	YY	610	9	1/1/20/20	15/37/115/115	-
39	CHL	YY	601	9	3/3/26/26	14/39/137/137	-
40	LUT	g	615	-	-	1/29/67/67	0/2/2/2
32	CLA	C	512	-	1/1/20/20	10/37/115/115	-
33	PHO	Aa	408	-	-	7/37/103/103	0/5/6/6
32	CLA	4	310	-	1/1/15/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	Gg	301	-	-	1/31/93/93	0/4/4/4
32	CLA	r	604	-	1/1/16/20	14/18/96/115	-
32	CLA	1	613	-	1/1/13/20	2/8/82/115	-
39	CHL	3	605	-	3/3/19/26	5/10/104/137	-
32	CLA	C	510	-	1/1/20/20	13/37/115/115	-
32	CLA	4	311	36	1/1/15/20	6/13/91/115	-
39	CHL	Yy	601	9	3/3/26/26	14/39/137/137	-
32	CLA	r	602	3	1/1/20/20	14/37/115/115	-
32	CLA	s	604	-	1/1/16/20	9/18/96/115	-
32	CLA	c	509	-	1/1/20/20	12/37/115/115	-
39	CHL	R	606	-	3/3/22/26	8/20/118/137	-
39	CHL	RR	307	-	3/3/22/26	8/20/118/137	-
34	BCR	a	411	-	-	4/29/63/63	0/2/2/2
35	PL9	Dd	404	-	-	28/53/73/73	0/1/1/1
38	LMG	Bb	620	-	-	4/31/51/70	0/1/1/1
32	CLA	Aa	405	-	1/1/20/20	14/37/115/115	-
44	DGD	B	601	-	-	6/44/84/95	0/2/2/2
32	CLA	s	610	36	1/1/16/20	8/18/96/115	-
39	CHL	4	309	11	3/3/21/26	7/15/113/137	-
32	CLA	D	405	-	1/1/20/20	6/37/115/115	-
36	LHG	J	101	-	-	10/30/30/53	-
32	CLA	GG	612	9	1/1/16/20	8/18/96/115	-
46	HEM	e	101	20,21	-	3/12/54/54	-
41	XAT	Rr	615	-	-	2/31/93/93	0/4/4/4
32	CLA	C	513	18	1/1/20/20	18/37/115/115	-
32	CLA	B	610	-	1/1/20/20	9/37/115/115	-
40	LUT	S	614	-	-	2/29/67/67	0/2/2/2
46	HEM	E	101	20,21	-	0/12/54/54	-
32	CLA	r	603	-	1/1/16/20	7/18/96/115	-
32	CLA	Cc	510	-	1/1/19/20	8/31/109/115	-
41	XAT	g	619	-	-	1/31/93/93	0/4/4/4
32	CLA	RR	313	-	1/1/14/20	4/8/86/115	-
39	CHL	n	609	9	3/3/22/26	6/20/118/137	-
37	SQD	LL	101	-	-	9/31/51/69	0/1/1/1
39	CHL	Ss	601	4	3/3/23/26	7/23/121/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	D	408	-	-	13/47/47/53	-
32	CLA	Rr	602	3	1/1/20/20	12/37/115/115	-
32	CLA	r	608	3	1/1/16/20	11/18/96/115	-
32	CLA	22	609	14	1/1/13/20	5/8/82/115	-
44	DGD	D	411	-	-	7/51/91/95	0/2/2/2
32	CLA	r	611	-	1/1/16/20	11/18/96/115	-
36	LHG	YY	618	32	-	19/53/53/53	-
32	CLA	A	405	-	1/1/20/20	16/37/115/115	-
32	CLA	Bb	611	-	1/1/20/20	7/37/115/115	-
39	CHL	Yy	607	-	3/3/20/26	3/12/110/137	-
39	CHL	N	607	-	3/3/26/26	12/39/137/137	-
39	CHL	NN	606	-	3/3/20/26	3/10/108/137	-
36	LHG	Y	618	32	-	18/53/53/53	-
32	CLA	1	610	36	1/1/13/20	6/8/82/115	-
36	LHG	KK	101	-	-	8/38/38/53	-
32	CLA	33	604	-	1/1/13/20	3/8/82/115	-
32	CLA	s	608	4	1/1/16/20	9/18/96/115	-
42	NEX	Yy	617	-	-	3/27/83/83	0/3/3/3
32	CLA	33	611	15	1/1/13/20	4/8/82/115	-
32	CLA	B	618	-	1/1/20/20	10/37/115/115	-
32	CLA	N	611	36	1/1/16/20	9/18/96/115	-
32	CLA	Aa	406	1	1/1/20/20	11/37/115/115	-
38	LMG	DD	409	-	-	4/41/61/70	0/1/1/1
39	CHL	2	606	-	3/3/19/26	2/10/104/137	-
32	CLA	GG	604	-	1/1/14/20	5/10/88/115	-
38	LMG	a	412	-	-	10/37/57/70	0/1/1/1
32	CLA	CC	505	-	1/1/20/20	7/37/115/115	-
32	CLA	Ss	613	-	1/1/16/20	7/18/96/115	-
39	CHL	g	609	9	3/3/20/26	6/12/110/137	-
32	CLA	Cc	504	-	-	14/37/115/115	-
32	CLA	Dd	401	-	-	12/37/115/115	-
32	CLA	Yy	612	9	1/1/20/20	8/37/115/115	-
34	BCR	Cc	518	-	-	3/29/63/63	0/2/2/2
39	CHL	YY	609	9	3/3/26/26	10/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	2	607	-	3/3/19/26	4/10/104/137	-
32	CLA	B	623	-	1/1/20/20	11/37/115/115	-
44	DGD	BB	623	-	-	8/51/91/95	0/2/2/2
32	CLA	Ss	608	4	1/1/16/20	9/18/96/115	-
32	CLA	y	314	9	1/1/20/20	11/37/115/115	-
36	LHG	AA	414	-	-	10/49/49/53	-
38	LMG	Dd	408	-	-	6/41/61/70	0/1/1/1
32	CLA	BB	613	-	1/1/19/20	8/31/109/115	-
41	XAT	GG	617	-	-	2/31/93/93	0/4/4/4
32	CLA	Rr	611	-	1/1/16/20	11/18/96/115	-
32	CLA	S	613	-	1/1/15/20	4/13/91/115	-
39	CHL	g	606	-	3/3/20/26	6/12/110/137	-
39	CHL	NN	608	-	3/3/20/26	3/10/108/137	-
32	CLA	YY	614	-	1/1/16/20	11/18/96/115	-
34	BCR	BB	616	-	-	4/29/63/63	0/2/2/2
39	CHL	Y	608	-	3/3/22/26	6/20/118/137	-
32	CLA	Cc	508	-	1/1/20/20	18/37/115/115	-
32	CLA	Bb	601	-	1/1/20/20	14/37/115/115	-
32	CLA	Nn	314	-	1/1/16/20	4/18/96/115	-
36	LHG	1	614	32	-	8/34/34/53	-
32	CLA	GG	603	-	1/1/20/20	10/37/115/115	-
39	CHL	1	608	14	3/3/19/26	3/10/104/137	-
32	CLA	C	514	-	1/1/20/20	8/37/115/115	-
32	CLA	Ss	602	4	1/1/16/20	11/18/96/115	-
39	CHL	2	601	14	3/3/19/26	2/10/104/137	-
39	CHL	Y	607	-	3/3/20/26	2/12/110/137	-
34	BCR	d	403	-	-	4/29/63/63	0/2/2/2
43	LMU	RR	301	-	-	3/13/53/61	0/2/2/2
39	CHL	Nn	316	-	3/3/22/26	1/20/118/137	-
39	CHL	Y	606	-	3/3/20/26	4/13/111/137	-
32	CLA	Gg	303	9	-	10/18/96/115	-
32	CLA	33	613	-	1/1/13/20	4/8/82/115	-
36	LHG	Dd	406	-	-	10/53/53/53	-
32	CLA	a	405	-	1/1/20/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	n	618	32	-	12/53/53/53	-
42	NEX	RR	317	-	-	3/27/83/83	0/3/3/3
35	PL9	A	410	-	-	24/53/73/73	0/1/1/1
32	CLA	4	303	11	1/1/15/20	8/13/91/115	-
32	CLA	N	612	9	1/1/14/20	3/10/88/115	-
39	CHL	1	605	14	3/3/19/26	4/10/104/137	-
39	CHL	R	605	-	3/3/22/26	7/20/118/137	-
32	CLA	Aa	407	-	1/1/16/20	8/18/96/115	-
36	LHG	d	406	-	-	10/53/53/53	-
32	CLA	BB	608	-	1/1/20/20	13/37/115/115	-
40	LUT	Rr	614	-	-	2/29/67/67	0/2/2/2
32	CLA	22	610	36	1/1/14/20	6/10/88/115	-
32	CLA	22	612	14	1/1/13/20	3/8/82/115	-
41	XAT	y	301	-	-	3/31/93/93	0/4/4/4
32	CLA	SS	303	4	1/1/16/20	10/18/96/115	-
34	BCR	Bb	619	-	-	2/29/63/63	0/2/2/2
40	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
32	CLA	c	504	-	1/1/18/20	4/25/103/115	-
33	PHO	a	409	-	-	16/37/103/103	0/5/6/6
44	DGD	CC	518	-	-	11/44/84/95	0/2/2/2
39	CHL	Gg	307	-	3/3/20/26	6/12/110/137	-
32	CLA	G	604	-	1/1/14/20	6/10/88/115	-
32	CLA	R	608	3	1/1/16/20	9/18/96/115	-
36	LHG	G	618	32	-	7/38/38/53	-
40	LUT	Ss	615	-	-	0/29/67/67	0/2/2/2
32	CLA	Gg	305	-	1/1/14/20	6/10/88/115	-
44	DGD	c	517	-	-	5/44/84/95	0/2/2/2
40	LUT	YY	615	-	-	4/29/67/67	0/2/2/2
32	CLA	c	511	18	1/1/20/20	10/37/115/115	-
39	CHL	3	608	15	3/3/19/26	3/10/104/137	-
32	CLA	Yy	610	9	1/1/20/20	10/37/115/115	-
32	CLA	33	603	-	1/1/13/20	4/8/82/115	-
32	CLA	G	602	9	1/1/16/20	8/18/96/115	-
42	NEX	NN	618	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	Dd	403	-	-	4/29/63/63	0/2/2/2
32	CLA	1	604	-	1/1/13/20	3/8/82/115	-
40	LUT	r	614	-	-	2/29/67/67	0/2/2/2
39	CHL	g	607	-	3/3/22/26	5/20/118/137	-
36	LHG	g	618	32	-	9/38/38/53	-
34	BCR	C	518	-	-	2/29/63/63	0/2/2/2
39	CHL	Gg	310	9	3/3/20/26	6/12/110/137	-
32	CLA	R	602	3	1/1/20/20	18/37/115/115	-
34	BCR	Cc	516	-	-	4/29/63/63	0/2/2/2
39	CHL	22	605	-	3/3/19/26	2/10/104/137	-
42	NEX	Y	617	-	-	2/27/83/83	0/3/3/3
39	CHL	22	601	14	3/3/19/26	3/10/104/137	-
32	CLA	2	610	-	1/1/13/20	3/8/82/115	-
32	CLA	G	603	-	1/1/20/20	11/37/115/115	-
32	CLA	b	602	-	1/1/20/20	14/37/115/115	-
39	CHL	G	609	9	3/3/20/26	3/12/110/137	-
32	CLA	Dd	402	-	1/1/20/20	14/37/115/115	-
39	CHL	33	601	15	3/3/19/26	5/10/104/137	-
32	CLA	Cc	515	-	1/1/14/20	9/11/89/115	-
32	CLA	1	603	-	1/1/13/20	5/8/82/115	-
32	CLA	y	313	36	1/1/14/20	3/10/88/115	-
32	CLA	Bb	616	-	1/1/20/20	12/37/115/115	-
32	CLA	Rr	613	3	1/1/16/20	8/18/96/115	-
39	CHL	G	607	-	3/3/21/26	6/15/113/137	-
36	LHG	d	405	-	-	9/47/47/53	-
32	CLA	b	613	-	1/1/20/20	14/37/115/115	-
39	CHL	2	605	-	3/3/19/26	2/10/104/137	-
40	LUT	2	614	-	-	4/29/67/67	0/2/2/2
32	CLA	CC	509	-	1/1/20/20	16/37/115/115	-
39	CHL	N	608	-	3/3/20/26	3/10/108/137	-
41	XAT	RR	316	-	-	0/31/93/93	0/4/4/4
40	LUT	NN	616	-	-	2/29/67/67	0/2/2/2
40	LUT	Gg	317	-	-	1/29/67/67	0/2/2/2
40	LUT	n	616	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	407	-	1/1/16/20	6/18/96/115	-
32	CLA	Gg	304	-	1/1/20/20	13/37/115/115	-
40	LUT	R	615	-	-	0/29/67/67	0/2/2/2
39	CHL	GG	608	-	3/3/20/26	6/10/108/137	-
32	CLA	DD	403	-	1/1/20/20	13/37/115/115	-
42	NEX	YY	617	-	-	2/27/83/83	0/3/3/3
32	CLA	BB	612	-	1/1/20/20	14/37/115/115	-
39	CHL	2	608	14	3/3/19/26	3/10/104/137	-
36	LHG	CC	521	-	-	7/38/38/53	-
32	CLA	S	612	4	1/1/16/20	6/18/96/115	-
32	CLA	Bb	604	-	1/1/20/20	9/37/115/115	-
32	CLA	11	613	-	1/1/13/20	2/8/82/115	-
32	CLA	Gg	313	9	1/1/16/20	12/18/96/115	-
40	LUT	s	614	-	-	2/29/67/67	0/2/2/2
32	CLA	b	607	-	1/1/20/20	11/37/115/115	-
38	LMG	Aa	412	-	-	7/37/57/70	0/1/1/1
36	LHG	DD	408	-	-	10/53/53/53	-
38	LMG	AA	415	-	-	4/31/51/70	0/1/1/1
36	LHG	AA	411	-	-	13/38/38/53	-
32	CLA	CC	512	18	1/1/20/20	16/37/115/115	-
39	CHL	Gg	302	9	3/3/26/26	12/39/137/137	-
36	LHG	Nn	310	32	-	16/53/53/53	-
37	SQD	L	102	-	-	10/31/51/69	0/1/1/1
39	CHL	SS	302	4	3/3/23/26	8/23/121/137	-
39	CHL	Gg	306	9	3/3/20/26	6/12/110/137	-
38	LMG	WW	201	-	-	8/43/63/70	0/1/1/1
36	LHG	Dd	407	-	-	5/41/41/53	-
32	CLA	4	312	-	1/1/15/20	7/13/91/115	-
32	CLA	Gg	311	9	1/1/16/20	9/18/96/115	-
34	BCR	B	613	-	-	4/29/63/63	0/2/2/2
36	LHG	33	614	32	-	11/38/38/53	-
39	CHL	44	601	-	3/3/21/26	2/13/111/137	-
38	LMG	Mm	101	-	-	10/46/66/70	0/1/1/1
40	LUT	g	616	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMG	C	521	-	-	10/46/66/70	0/1/1/1
32	CLA	RR	309	3	1/1/20/20	10/37/115/115	-
36	LHG	C	522	-	-	9/35/35/53	-
32	CLA	y	306	-	1/1/16/20	8/18/96/115	-
41	XAT	44	613	-	-	0/31/93/93	0/4/4/4
32	CLA	3	613	-	1/1/13/20	4/8/82/115	-
32	CLA	2	613	-	1/1/13/20	2/8/82/115	-
32	CLA	c	513	-	1/1/14/20	9/11/89/115	-
32	CLA	11	602	14	1/1/13/20	2/8/82/115	-
32	CLA	g	612	9	1/1/16/20	12/18/96/115	-
32	CLA	NN	611	36	1/1/16/20	12/18/96/115	-
32	CLA	Bb	603	-	1/1/20/20	17/37/115/115	-
39	CHL	Gg	309	-	3/3/20/26	3/10/108/137	-
32	CLA	C	515	-	1/1/16/20	8/18/96/115	-
39	CHL	NN	605	9	3/3/20/26	5/10/108/137	-
32	CLA	C	503	-	1/1/20/20	13/37/115/115	-
32	CLA	B	622	-	1/1/20/20	19/37/115/115	-
32	CLA	S	604	-	1/1/16/20	7/18/96/115	-
32	CLA	CC	513	-	1/1/20/20	8/37/115/115	-
34	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	CLA	b	614	-	1/1/20/20	7/37/115/115	-
32	CLA	RR	308	3	1/1/16/20	8/18/96/115	-
39	CHL	22	606	-	3/3/19/26	2/10/104/137	-
42	NEX	R	617	-	-	2/27/83/83	0/3/3/3
32	CLA	2	604	-	1/1/13/20	3/8/82/115	-
39	CHL	n	607	-	3/3/26/26	17/39/137/137	-
32	CLA	Nn	312	9	1/1/20/20	13/37/115/115	-
39	CHL	Nn	319	9	3/3/22/26	7/20/118/137	-
39	CHL	S	601	4	3/3/23/26	8/23/121/137	-
36	LHG	EE	101	-	-	9/44/44/53	-
39	CHL	33	605	-	3/3/19/26	3/10/104/137	-
34	BCR	KK	103	-	-	4/29/63/63	0/2/2/2
39	CHL	44	605	-	3/3/21/26	5/15/113/137	-
32	CLA	RR	314	3	-	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SQD	C	501	-	-	16/49/69/69	0/1/1/1
32	CLA	Y	603	-	1/1/16/20	8/18/96/115	-
32	CLA	s	613	-	1/1/16/20	4/18/96/115	-
38	LMG	F	101	-	-	3/41/61/70	0/1/1/1
39	CHL	R	607	-	3/3/22/26	8/20/118/137	-
32	CLA	S	602	4	1/1/16/20	9/18/96/115	-
32	CLA	SS	314	-	1/1/16/20	7/18/96/115	-
39	CHL	s	606	-	3/3/22/26	11/20/118/137	-
32	CLA	C	507	-	1/1/20/20	13/37/115/115	-
32	CLA	D	404	-	1/1/20/20	16/37/115/115	-
32	CLA	R	612	3	1/1/14/20	1/10/88/115	-
32	CLA	BB	606	-	1/1/20/20	12/37/115/115	-
32	CLA	RR	312	3	1/1/14/20	2/10/88/115	-
32	CLA	Bb	602	-	1/1/20/20	11/37/115/115	-
32	CLA	Bb	614	-	1/1/20/20	8/37/115/115	-
32	CLA	b	616	-	1/1/20/20	12/37/115/115	-
39	CHL	Yy	606	-	3/3/20/26	3/13/111/137	-
32	CLA	GG	613	9	1/1/13/20	4/8/82/115	-
32	CLA	d	402	-	1/1/20/20	10/37/115/115	-
41	XAT	G	619	-	-	1/31/93/93	0/4/4/4
32	CLA	B	624	-	1/1/20/20	11/37/115/115	-
32	CLA	c	502	-	1/1/20/20	9/37/115/115	-
32	CLA	g	604	42	1/1/14/20	6/10/88/115	-
33	PHO	a	408	-	-	8/37/103/103	0/5/6/6
32	CLA	33	602	15	1/1/13/20	2/8/82/115	-
39	CHL	GG	601	9	3/3/26/26	11/39/137/137	-
32	CLA	g	611	36	1/1/20/20	17/37/115/115	-
39	CHL	y	310	-	3/3/22/26	6/20/118/137	-
32	CLA	G	611	36	1/1/17/20	8/22/100/115	-
32	CLA	Y	611	36	1/1/14/20	3/10/88/115	-
32	CLA	AA	405	-	1/1/20/20	14/37/115/115	-
32	CLA	CC	506	-	1/1/20/20	17/37/115/115	-
39	CHL	Nn	311	9	3/3/22/26	6/20/118/137	-
34	BCR	Bb	617	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	G	605	9	3/3/20/26	4/12/110/137	-
39	CHL	G	606	-	3/3/20/26	5/12/110/137	-
40	LUT	GG	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Ss	604	-	1/1/16/20	10/18/96/115	-
32	CLA	44	602	11	1/1/15/20	8/13/91/115	-
40	LUT	N	616	-	-	3/29/67/67	0/2/2/2
32	CLA	3	604	-	1/1/13/20	3/8/82/115	-
32	CLA	RR	304	-	1/1/16/20	5/18/96/115	-
32	CLA	R	614	3	-	8/18/96/115	-
40	LUT	Yy	615	-	-	3/29/67/67	0/2/2/2
32	CLA	Rr	608	3	1/1/16/20	12/18/96/115	-
32	CLA	SS	304	-	1/1/15/20	3/13/91/115	-
32	CLA	3	602	15	1/1/13/20	2/8/82/115	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
33	PHO	D	402	-	-	9/37/103/103	0/5/6/6
32	CLA	y	316	-	1/1/16/20	8/18/96/115	-
36	LHG	SS	301	-	-	4/30/30/53	-
39	CHL	Nn	317	-	3/3/26/26	14/39/137/137	-
37	SQD	L	101	-	-	16/49/69/69	0/1/1/1
32	CLA	g	613	9	1/1/13/20	6/8/82/115	-
34	BCR	BB	617	-	-	4/29/63/63	0/2/2/2
32	CLA	CC	510	-	1/1/20/20	13/37/115/115	-
32	CLA	2	612	14	1/1/13/20	2/8/82/115	-
46	HEM	EE	102	20,21	-	0/12/54/54	-
32	CLA	3	603	-	1/1/13/20	3/8/82/115	-
41	XAT	Nn	308	-	-	1/31/93/93	0/4/4/4
32	CLA	Ss	610	36	1/1/16/20	8/18/96/115	-
39	CHL	22	607	-	3/3/19/26	3/10/104/137	-
32	CLA	RR	311	-	1/1/16/20	6/18/96/115	-
32	CLA	GG	611	36	1/1/17/20	8/22/100/115	-
32	CLA	RR	303	-	1/1/16/20	3/18/96/115	-
37	SQD	B	617	-	-	5/31/51/69	0/1/1/1
39	CHL	g	605	9	3/3/20/26	6/12/110/137	-
32	CLA	n	614	-	1/1/16/20	8/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	11	612	-	1/1/13/20	3/8/82/115	-
32	CLA	s	611	4	1/1/16/20	10/18/96/115	-
32	CLA	B	620	-	1/1/20/20	10/37/115/115	-
39	CHL	Ss	607	-	3/3/22/26	6/19/117/137	-
32	CLA	S	603	-	1/1/15/20	4/13/91/115	-
32	CLA	G	613	9	1/1/13/20	5/8/82/115	-
32	CLA	33	612	15	1/1/13/20	5/8/82/115	-
32	CLA	b	605	-	1/1/20/20	11/37/115/115	-
39	CHL	s	605	-	3/3/22/26	9/20/118/137	-
34	BCR	CC	516	-	-	5/29/63/63	0/2/2/2
40	LUT	RR	315	-	-	2/29/67/67	0/2/2/2
32	CLA	Bb	606	-	1/1/20/20	7/37/115/115	-
39	CHL	Ss	605	-	3/3/22/26	12/20/118/137	-
36	LHG	4	315	32	-	8/23/23/53	-
32	CLA	g	602	9	-	7/18/96/115	-
32	CLA	d	401	-	-	11/37/115/115	-
44	DGD	a	415	-	-	9/44/84/95	0/2/2/2
32	CLA	n	610	9	1/1/20/20	12/37/115/115	-
32	CLA	R	604	-	1/1/16/20	5/18/96/115	-
39	CHL	g	608	-	3/3/20/26	2/10/108/137	-
32	CLA	c	512	-	1/1/20/20	8/37/115/115	-
39	CHL	NN	601	9	3/3/20/26	3/13/111/137	-
32	CLA	s	602	4	1/1/16/20	11/18/96/115	-
32	CLA	3	609	15	1/1/13/20	3/8/82/115	-
39	CHL	RR	305	-	3/3/22/26	8/20/118/137	-
34	BCR	CC	515	-	-	6/29/63/63	0/2/2/2
34	BCR	CC	517	-	-	2/29/63/63	0/2/2/2
32	CLA	s	603	-	1/1/16/20	9/18/96/115	-
32	CLA	4	304	-	1/1/15/20	5/13/91/115	-
39	CHL	44	606	-	3/3/21/26	4/15/113/137	-
32	CLA	2	611	14	1/1/13/20	3/8/82/115	-
32	CLA	B	607	-	1/1/20/20	8/37/115/115	-
39	CHL	Y	609	9	3/3/26/26	10/39/137/137	-
32	CLA	g	603	-	1/1/20/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	y	304	9	1/1/20/20	13/37/115/115	-
40	LUT	4	313	-	-	2/29/67/67	0/2/2/2
32	CLA	c	510	-	1/1/20/20	17/37/115/115	-
39	CHL	44	607	-	3/3/21/26	7/15/113/137	-
40	LUT	y	317	-	-	3/29/67/67	0/2/2/2
34	BCR	K	102	-	-	5/29/63/63	0/2/2/2
32	CLA	BB	610	-	1/1/20/20	15/37/115/115	-
32	CLA	SS	313	4	1/1/16/20	8/18/96/115	-
32	CLA	r	601	3	1/1/16/20	10/18/96/115	-
39	CHL	y	307	9	3/3/21/26	8/18/116/137	-
32	CLA	11	604	-	1/1/13/20	4/8/82/115	-
32	CLA	y	312	9	1/1/20/20	12/37/115/115	-
32	CLA	CC	514	-	1/1/16/20	8/18/96/115	-
34	BCR	c	516	-	-	4/29/63/63	0/2/2/2
40	LUT	YY	616	-	-	2/29/67/67	0/2/2/2
41	XAT	y	302	-	-	1/31/93/93	0/4/4/4
34	BCR	Aa	411	-	-	4/29/63/63	0/2/2/2
32	CLA	c	507	-	1/1/20/20	10/37/115/115	-
32	CLA	Y	613	9	1/1/18/20	13/30/108/115	-
36	LHG	K	101	-	-	11/38/38/53	-
39	CHL	Rr	607	-	3/3/22/26	8/20/118/137	-
34	BCR	b	617	-	-	4/29/63/63	0/2/2/2
32	CLA	n	604	-	1/1/16/20	6/18/96/115	-
32	CLA	Bb	605	-	1/1/20/20	13/37/115/115	-
36	LHG	DD	407	-	-	14/47/47/53	-
32	CLA	N	614	-	1/1/14/20	3/8/86/115	-
32	CLA	SS	311	-	1/1/16/20	6/18/96/115	-
32	CLA	Bb	612	-	1/1/20/20	15/37/115/115	-
38	LMG	CC	520	-	-	3/34/54/70	0/1/1/1
40	LUT	y	318	-	-	2/29/67/67	0/2/2/2
32	CLA	Gg	312	36	1/1/20/20	17/37/115/115	-
40	LUT	44	612	-	-	2/29/67/67	0/2/2/2
32	CLA	s	609	4	1/1/16/20	8/18/96/115	-
32	CLA	Gg	315	-	1/1/16/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	A	408	-	1/1/19/20	8/31/109/115	-
32	CLA	NN	604	-	1/1/14/20	5/8/86/115	-
36	LHG	A	411	-	-	12/38/38/53	-
32	CLA	Yy	614	-	1/1/16/20	8/18/96/115	-
39	CHL	Ss	606	-	3/3/22/26	11/20/118/137	-
39	CHL	n	601	9	3/3/22/26	6/20/118/137	-
42	NEX	Nn	309	-	-	2/27/83/83	0/3/3/3
32	CLA	b	608	-	1/1/20/20	8/37/115/115	-
39	CHL	S	607	-	3/3/20/26	2/12/110/137	-
32	CLA	Aa	410	-	1/1/19/20	10/31/109/115	-
39	CHL	SS	306	4	3/3/20/26	3/10/108/137	-
39	CHL	YY	606	-	3/3/20/26	5/13/111/137	-
38	LMG	b	621	-	-	9/31/51/70	0/1/1/1
32	CLA	Rr	601	3	1/1/16/20	11/18/96/115	-
32	CLA	C	504	-	-	14/37/115/115	-
34	BCR	b	619	-	-	4/29/63/63	0/2/2/2
42	NEX	N	618	-	-	2/27/83/83	0/3/3/3
39	CHL	3	601	15	3/3/19/26	5/10/104/137	-
32	CLA	NN	602	9	1/1/20/20	14/37/115/115	-
44	DGD	BB	625	-	-	3/43/83/95	0/2/2/2
34	BCR	XX	202	-	-	6/29/63/63	0/2/2/2
34	BCR	D	406	-	-	2/29/63/63	0/2/2/2
44	DGD	Aa	401	-	-	9/44/84/95	0/2/2/2
32	CLA	YY	611	36	1/1/14/20	2/10/88/115	-
39	CHL	G	608	-	3/3/20/26	6/10/108/137	-
32	CLA	22	611	14	1/1/13/20	2/8/82/115	-
35	PL9	AA	410	-	-	27/53/73/73	0/1/1/1
39	CHL	NN	609	9	3/3/22/26	6/20/118/137	-
36	LHG	D	409	-	-	7/53/53/53	-
37	SQD	Ll	101	-	-	9/49/69/69	0/1/1/1
41	XAT	r	615	-	-	1/31/93/93	0/4/4/4
39	CHL	4	308	-	3/3/21/26	6/15/113/137	-
36	LHG	Yy	618	32	-	19/53/53/53	-
32	CLA	R	603	-	1/1/16/20	3/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	r	610	36	1/1/16/20	10/18/96/115	-
32	CLA	Nn	303	9	1/1/16/20	6/18/96/115	-
32	CLA	DD	401	-	1/1/20/20	6/37/115/115	-
32	CLA	Bb	610	-	1/1/20/20	14/37/115/115	-
44	DGD	c	518	-	-	6/41/81/95	0/2/2/2
39	CHL	Nn	318	-	3/3/22/26	7/20/118/137	-
40	LUT	n	615	-	-	2/29/67/67	0/2/2/2
32	CLA	c	506	-	1/1/20/20	18/37/115/115	-
37	SQD	l	102	-	-	10/49/69/69	0/1/1/1
32	CLA	D	401	-	1/1/20/20	8/37/115/115	-
32	CLA	r	609	3	1/1/20/20	13/37/115/115	-
39	CHL	s	601	4	3/3/23/26	10/23/121/137	-
32	CLA	22	604	-	1/1/13/20	2/8/82/115	-
32	CLA	N	610	9	1/1/20/20	13/37/115/115	-
32	CLA	BB	603	-	1/1/20/20	13/37/115/115	-
39	CHL	Yy	605	9	3/3/21/26	9/18/116/137	-
36	LHG	N	619	32	-	11/42/42/53	-
32	CLA	Yy	604	-	1/1/16/20	10/18/96/115	-
37	SQD	B	602	-	-	10/42/62/69	0/1/1/1
32	CLA	r	612	3	1/1/16/20	4/18/96/115	-
39	CHL	SS	307	-	3/3/20/26	1/10/108/137	-
32	CLA	R	611	-	1/1/16/20	6/18/96/115	-
32	CLA	NN	612	9	1/1/14/20	4/10/88/115	-
34	BCR	BB	620	-	-	5/29/63/63	0/2/2/2
36	LHG	NN	619	32	-	10/42/42/53	-
33	PHO	Aa	409	-	-	16/37/103/103	0/5/6/6
42	NEX	Y	619	-	-	3/27/83/83	0/3/3/3
32	CLA	BB	609	-	-	13/37/115/115	-
42	NEX	Rr	616	-	-	3/27/83/83	0/3/3/3
34	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
32	CLA	S	608	4	1/1/14/20	6/8/86/115	-
39	CHL	Yy	609	9	3/3/26/26	11/39/137/137	-
39	CHL	N	609	9	3/3/22/26	6/20/118/137	-
32	CLA	Bb	613	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	C	523	-	-	9/41/81/95	0/2/2/2
32	CLA	3	610	36	1/1/13/20	6/8/82/115	-
34	BCR	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	n	603	-	1/1/16/20	10/18/96/115	-
32	CLA	Rr	610	36	1/1/16/20	11/18/96/115	-
39	CHL	YY	605	9	3/3/21/26	6/18/116/137	-
34	BCR	TT	101	-	-	5/29/63/63	0/2/2/2
32	CLA	Bb	615	-	1/1/20/20	14/37/115/115	-
32	CLA	YY	613	9	1/1/18/20	9/30/108/115	-
39	CHL	n	606	-	3/3/22/26	1/20/118/137	-
34	BCR	Cc	517	-	-	5/29/63/63	0/2/2/2
32	CLA	4	305	-	1/1/15/20	6/13/91/115	-
32	CLA	YY	604	-	-	11/18/96/115	-
32	CLA	Yy	603	-	1/1/16/20	6/18/96/115	-
41	XAT	Yy	619	-	-	3/31/93/93	0/4/4/4
32	CLA	b	612	-	1/1/20/20	13/37/115/115	-
32	CLA	XX	201	-	1/1/14/20	2/8/86/115	-
44	DGD	Cc	520	-	-	7/41/81/95	0/2/2/2
32	CLA	Rr	612	3	1/1/16/20	7/18/96/115	-
36	LHG	Ss	616	32	-	9/52/52/53	-
32	CLA	CC	502	-	1/1/20/20	15/37/115/115	-
34	BCR	C	516	-	-	6/29/63/63	0/2/2/2
36	LHG	GG	618	32	-	7/38/38/53	-
40	LUT	NN	615	-	-	2/29/67/67	0/2/2/2
39	CHL	44	608	11	3/3/21/26	4/15/113/137	-
37	SQD	BB	621	-	-	5/31/51/69	0/1/1/1
32	CLA	2	603	-	1/1/13/20	3/8/82/115	-
39	CHL	4	302	-	3/3/21/26	2/13/111/137	-
36	LHG	II	101	-	-	11/38/38/53	-
36	LHG	l	101	-	-	13/53/53/53	-
32	CLA	44	610	36	1/1/15/20	6/13/91/115	-
42	NEX	n	617	-	-	3/27/83/83	0/3/3/3
32	CLA	Y	602	9	1/1/20/20	18/37/115/115	-
32	CLA	Y	614	-	1/1/16/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	CC	519	-	-	5/51/91/95	0/2/2/2
32	CLA	Cc	513	18	1/1/20/20	9/37/115/115	-
39	CHL	n	608	-	3/3/22/26	9/20/118/137	-
32	CLA	BB	601	-	1/1/20/20	10/37/115/115	-
32	CLA	Cc	511	-	1/1/20/20	16/37/115/115	-
32	CLA	CC	511	-	1/1/20/20	8/37/115/115	-
32	CLA	a	410	-	1/1/19/20	9/31/109/115	-
40	LUT	G	616	-	-	2/29/67/67	0/2/2/2
40	LUT	N	615	-	-	1/29/67/67	0/2/2/2
34	BCR	Hh	101	-	-	8/29/63/63	0/2/2/2
36	LHG	4	301	32	-	9/21/21/53	-
32	CLA	Cc	512	-	1/1/20/20	15/37/115/115	-
36	LHG	Gg	319	32	-	7/38/38/53	-
44	DGD	B	603	-	-	6/43/83/95	0/2/2/2
32	CLA	S	611	4	1/1/16/20	9/18/96/115	-
32	CLA	Bb	608	-	1/1/20/20	9/37/115/115	-
32	CLA	Bb	609	-	1/1/20/20	17/37/115/115	-
39	CHL	4	307	-	3/3/21/26	4/15/113/137	-
39	CHL	S	605	-	3/3/20/26	3/10/108/137	-
32	CLA	Cc	506	-	1/1/18/20	7/25/103/115	-
41	XAT	4	314	-	-	0/31/93/93	0/4/4/4
32	CLA	BB	614	-	1/1/20/20	8/37/115/115	-
39	CHL	r	605	3	3/3/22/26	8/20/118/137	-
32	CLA	11	611	14	1/1/13/20	2/8/82/115	-
39	CHL	33	607	-	3/3/19/26	3/10/104/137	-
38	LMG	W	201	-	-	6/43/63/70	0/1/1/1
32	CLA	S	610	-	1/1/16/20	7/18/96/115	-
32	CLA	a	406	1	1/1/20/20	11/37/115/115	-
40	LUT	GG	615	-	-	2/29/67/67	0/2/2/2
37	SQD	CC	501	-	-	11/49/69/69	0/1/1/1
34	BCR	A	409	-	-	5/29/63/63	0/2/2/2
40	LUT	s	615	-	-	2/29/67/67	0/2/2/2
44	DGD	BB	624	-	-	9/44/84/95	0/2/2/2
32	CLA	R	609	3	1/1/20/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Rr	603	-	1/1/16/20	6/18/96/115	-
39	CHL	g	601	9	3/3/26/26	12/39/137/137	-
34	BCR	B	614	-	-	4/29/63/63	0/2/2/2
32	CLA	44	604	-	1/1/15/20	6/13/91/115	-
44	DGD	C	520	-	-	4/51/91/95	0/2/2/2
38	LMG	b	620	-	-	4/31/51/70	0/1/1/1
40	LUT	Yy	616	-	-	3/29/67/67	0/2/2/2
34	BCR	C	517	-	-	5/29/63/63	0/2/2/2
32	CLA	YY	612	9	1/1/18/20	12/29/107/115	-
32	CLA	Rr	609	3	1/1/20/20	13/37/115/115	-
32	CLA	Y	604	-	-	11/18/96/115	-
38	LMG	j	101	-	-	3/41/61/70	0/1/1/1
32	CLA	X	201	-	1/1/14/20	3/8/86/115	-
34	BCR	b	618	-	-	4/29/63/63	0/2/2/2
32	CLA	GG	602	9	1/1/16/20	7/18/96/115	-
32	CLA	Cc	503	-	1/1/20/20	16/37/115/115	-
32	CLA	Y	612	9	1/1/20/20	11/37/115/115	-
34	BCR	BB	618	-	-	4/29/63/63	0/2/2/2
32	CLA	1	609	14	1/1/13/20	2/8/82/115	-
39	CHL	Rr	605	3	3/3/22/26	8/20/118/137	-
32	CLA	SS	312	4	1/1/16/20	8/18/96/115	-
32	CLA	33	610	36	1/1/13/20	5/8/82/115	-
32	CLA	C	506	-	1/1/20/20	7/37/115/115	-
36	LHG	D	410	-	-	10/38/38/53	-
42	NEX	y	319	-	-	3/27/83/83	0/3/3/3
32	CLA	RR	310	36	1/1/16/20	11/18/96/115	-
38	LMG	BB	619	-	-	10/40/60/70	0/1/1/1
36	LHG	a	414	-	-	5/41/41/53	-
39	CHL	y	308	-	3/3/20/26	2/13/111/137	-
43	LMU	KK	102	-	-	5/13/53/61	0/2/2/2
32	CLA	SS	310	4	1/1/14/20	3/8/86/115	-
39	CHL	11	607	-	3/3/19/26	2/10/104/137	-
32	CLA	Cc	514	-	1/1/20/20	8/37/115/115	-
34	BCR	B	616	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	YY	607	-	3/3/20/26	2/12/110/137	-
39	CHL	N	606	-	3/3/20/26	1/10/108/137	-
41	XAT	G	617	-	-	2/31/93/93	0/4/4/4
36	LHG	Dd	405	-	-	9/47/47/53	-
41	XAT	R	616	-	-	0/31/93/93	0/4/4/4
32	CLA	44	603	-	1/1/15/20	8/13/91/115	-
32	CLA	S	609	4	1/1/14/20	2/8/86/115	-
33	PHO	DD	402	-	-	11/37/103/103	0/5/6/6
32	CLA	BB	604	-	1/1/20/20	13/37/115/115	-
32	CLA	b	615	-	1/1/20/20	14/37/115/115	-
32	CLA	l	612	14	1/1/13/20	1/8/82/115	-
32	CLA	Cc	505	-	1/1/20/20	13/37/115/115	-
36	LHG	s	616	32	-	9/52/52/53	-
37	SQD	Aa	413	-	-	10/42/62/69	0/1/1/1
39	CHL	y	309	-	3/3/20/26	4/12/110/137	-
39	CHL	GG	605	9	3/3/20/26	3/12/110/137	-
32	CLA	DD	404	-	1/1/20/20	8/37/115/115	-
32	CLA	b	606	-	1/1/20/20	8/37/115/115	-
32	CLA	Ss	612	4	1/1/16/20	9/18/96/115	-
32	CLA	BB	605	-	1/1/20/20	16/37/115/115	-
32	CLA	NN	614	-	1/1/14/20	3/8/86/115	-
39	CHL	Gg	308	-	3/3/22/26	6/20/118/137	-
39	CHL	y	311	9	3/3/26/26	12/39/137/137	-
32	CLA	C	508	-	1/1/20/20	13/37/115/115	-
32	CLA	c	501	-	1/1/20/20	18/37/115/115	-
32	CLA	CC	508	-	1/1/20/20	10/37/115/115	-
33	PHO	A	407	-	-	11/37/103/103	0/5/6/6
36	LHG	BB	622	-	-	9/38/38/53	-
39	CHL	33	608	15	3/3/19/26	3/10/104/137	-
36	LHG	Rr	617	32	-	11/53/53/53	-
36	LHG	JJ	101	-	-	9/37/37/53	-
41	XAT	N	617	-	-	0/31/93/93	0/4/4/4
32	CLA	B	604	-	1/1/20/20	11/37/115/115	-
39	CHL	N	601	9	3/3/20/26	3/13/111/137	-
39	CHL	YY	608	-	3/3/22/26	6/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Nn	315	9	3/3/21/26	6/18/116/137	-
40	LUT	Ss	614	-	-	2/29/67/67	0/2/2/2
38	LMG	m	101	-	-	13/46/66/70	0/1/1/1
34	BCR	c	515	-	-	5/29/63/63	0/2/2/2
39	CHL	l	601	14	3/3/19/26	4/10/104/137	-
32	CLA	n	612	9	1/1/16/20	7/18/96/115	-
32	CLA	Nn	313	-	1/1/16/20	10/18/96/115	-
36	LHG	44	614	32	-	7/23/23/53	-
32	CLA	B	606	-	1/1/20/20	16/37/115/115	-
32	CLA	NN	610	9	1/1/20/20	12/37/115/115	-
40	LUT	22	614	-	-	4/29/67/67	0/2/2/2
41	XAT	GG	619	-	-	1/31/93/93	0/4/4/4
32	CLA	R	610	36	1/1/16/20	11/18/96/115	-
32	CLA	g	614	-	1/1/16/20	9/18/96/115	-
38	LMG	Cc	501	-	-	7/29/49/70	0/1/1/1
32	CLA	Nn	301	9	1/1/20/20	12/37/115/115	-
32	CLA	G	612	9	1/1/16/20	8/18/96/115	-
32	CLA	YY	602	9	1/1/20/20	15/37/115/115	-
39	CHL	11	601	14	3/3/19/26	3/10/104/137	-
32	CLA	n	613	9	1/1/16/20	10/18/96/115	-
39	CHL	NN	607	-	3/3/26/26	12/39/137/137	-
33	PHO	AA	407	-	-	7/37/103/103	0/5/6/6
32	CLA	44	611	-	1/1/15/20	5/13/91/115	-
32	CLA	Ss	603	-	1/1/16/20	9/18/96/115	-
32	CLA	R	613	-	1/1/14/20	6/8/86/115	-
32	CLA	Nn	302	36	1/1/16/20	3/18/96/115	-
36	LHG	A	414	-	-	10/49/49/53	-
40	LUT	Y	615	-	-	4/29/67/67	0/2/2/2
32	CLA	c	505	-	1/1/20/20	12/37/115/115	-
35	PL9	d	404	-	-	28/53/73/73	0/1/1/1
32	CLA	11	610	36	1/1/13/20	3/8/82/115	-
32	CLA	Nn	304	9	1/1/16/20	9/18/96/115	-
39	CHL	n	605	9	3/3/21/26	8/18/116/137	-
32	CLA	C	505	-	1/1/20/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	B	612	-	-	4/29/63/63	0/2/2/2
39	CHL	S	606	-	3/3/20/26	1/10/108/137	-
32	CLA	s	612	4	1/1/16/20	9/18/96/115	-
32	CLA	2	609	14	1/1/13/20	2/8/82/115	-
32	CLA	G	610	9	1/1/16/20	7/18/96/115	-
32	CLA	Y	610	9	1/1/20/20	17/37/115/115	-
39	CHL	Y	601	9	3/3/26/26	14/39/137/137	-
32	CLA	CC	503	-	-	15/37/115/115	-
32	CLA	Ss	611	4	1/1/16/20	10/18/96/115	-
32	CLA	n	602	9	1/1/20/20	13/37/115/115	-
32	CLA	NN	603	-	1/1/14/20	6/10/88/115	-
32	CLA	b	611	-	1/1/20/20	7/37/115/115	-
38	LMG	Bb	621	-	-	8/31/51/70	0/1/1/1
32	CLA	CC	504	-	1/1/20/20	14/37/115/115	-
32	CLA	Rr	604	-	1/1/16/20	11/18/96/115	-
32	CLA	44	609	11	1/1/15/20	5/13/91/115	-
36	LHG	3	614	32	-	11/38/38/53	-
36	LHG	r	616	32	-	13/53/53/53	-
32	CLA	b	604	-	1/1/20/20	11/37/115/115	-
32	CLA	RR	302	3	1/1/20/20	17/37/115/115	-
42	NEX	Gg	318	-	-	3/27/83/83	0/3/3/3
34	BCR	Bb	618	-	-	4/29/63/63	0/2/2/2
32	CLA	3	612	15	1/1/13/20	4/8/82/115	-
36	LHG	44	616	32	-	8/21/21/53	-
32	CLA	b	610	-	1/1/20/20	9/37/115/115	-
39	CHL	G	601	9	3/3/26/26	14/39/137/137	-
37	SQD	AA	412	-	-	7/30/50/69	0/1/1/1
39	CHL	GG	607	-	3/3/21/26	6/15/113/137	-
39	CHL	11	605	14	3/3/19/26	4/10/104/137	-
39	CHL	y	303	9	3/3/26/26	14/39/137/137	-
32	CLA	GG	614	-	1/1/14/20	3/8/86/115	-
32	CLA	SS	305	-	1/1/16/20	8/18/96/115	-
36	LHG	11	614	32	-	16/38/38/53	-
36	LHG	Ll	102	-	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	BB	602	-	1/1/20/20	21/37/115/115	-
32	CLA	1	602	14	1/1/13/20	3/8/82/115	-
32	CLA	NN	613	9	1/1/16/20	9/18/96/115	-
44	DGD	Cc	519	-	-	8/44/84/95	0/2/2/2
39	CHL	Y	605	9	3/3/21/26	6/18/116/137	-
38	LMG	B	615	-	-	8/40/60/70	0/1/1/1
32	CLA	c	503	-	1/1/20/20	9/37/115/115	-
32	CLA	Cc	509	-	1/1/20/20	12/37/115/115	-
32	CLA	Yy	611	36	1/1/14/20	3/10/88/115	-
39	CHL	3	607	-	3/3/19/26	2/10/104/137	-
32	CLA	SS	309	4	1/1/14/20	5/8/86/115	-
38	LMG	c	519	-	-	7/29/49/70	0/1/1/1
35	PL9	DD	406	-	-	27/53/73/73	0/1/1/1

All (3906) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	AA	410	PL9	C23-C24	10.46	1.58	1.33
35	A	410	PL9	C23-C24	10.36	1.57	1.33
35	d	404	PL9	C23-C24	10.20	1.57	1.33
35	Dd	404	PL9	C23-C24	10.20	1.57	1.33
35	DD	406	PL9	C23-C24	10.17	1.57	1.33
35	A	410	PL9	C38-C39	10.14	1.57	1.33
35	AA	410	PL9	C38-C39	10.14	1.57	1.33
35	D	407	PL9	C23-C24	10.14	1.57	1.33
35	DD	406	PL9	C38-C39	9.97	1.56	1.33
35	d	404	PL9	C38-C39	9.97	1.56	1.33
35	D	407	PL9	C38-C39	9.95	1.56	1.33
35	Dd	404	PL9	C38-C39	9.92	1.56	1.33
35	AA	410	PL9	C18-C19	9.83	1.56	1.33
35	A	410	PL9	C18-C19	9.75	1.56	1.33
35	Dd	404	PL9	C18-C19	9.66	1.56	1.33
35	d	404	PL9	C18-C19	9.63	1.56	1.33
35	DD	406	PL9	C18-C19	9.61	1.56	1.33
35	D	407	PL9	C18-C19	9.60	1.56	1.33
35	AA	410	PL9	C28-C29	9.54	1.55	1.33
35	A	410	PL9	C28-C29	9.47	1.55	1.33
35	Dd	404	PL9	C28-C29	9.33	1.55	1.33
35	D	407	PL9	C28-C29	9.31	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	404	PL9	C28-C29	9.31	1.55	1.33
35	DD	406	PL9	C28-C29	9.29	1.55	1.33
35	DD	406	PL9	C33-C34	9.07	1.54	1.33
35	AA	410	PL9	C33-C34	9.07	1.54	1.33
35	A	410	PL9	C33-C34	9.05	1.54	1.33
35	Dd	404	PL9	C33-C34	9.00	1.54	1.33
35	d	404	PL9	C33-C34	9.00	1.54	1.33
35	D	407	PL9	C33-C34	8.94	1.54	1.33
35	A	410	PL9	C43-C44	8.88	1.54	1.33
35	AA	410	PL9	C43-C44	8.87	1.54	1.33
35	A	410	PL9	C8-C9	8.85	1.54	1.33
35	AA	410	PL9	C8-C9	8.85	1.54	1.33
35	Dd	404	PL9	C8-C9	8.83	1.54	1.33
35	DD	406	PL9	C8-C9	8.80	1.54	1.33
35	D	407	PL9	C8-C9	8.77	1.54	1.33
35	D	407	PL9	C43-C44	8.75	1.54	1.33
35	d	404	PL9	C43-C44	8.72	1.53	1.33
35	DD	406	PL9	C43-C44	8.72	1.53	1.33
35	d	404	PL9	C8-C9	8.71	1.53	1.33
35	Dd	404	PL9	C43-C44	8.65	1.53	1.33
39	2	606	CHL	C4B-NB	8.63	1.42	1.35
39	S	605	CHL	C4B-NB	8.56	1.42	1.35
39	2	605	CHL	C4B-NB	8.54	1.42	1.35
39	N	601	CHL	C4B-NB	8.54	1.42	1.35
39	22	606	CHL	C4B-NB	8.53	1.42	1.35
39	4	309	CHL	C4B-NB	8.51	1.42	1.35
39	33	607	CHL	C4B-NB	8.51	1.42	1.35
39	3	607	CHL	C4B-NB	8.50	1.42	1.35
39	44	605	CHL	C4B-NB	8.49	1.42	1.35
39	11	605	CHL	C4B-NB	8.47	1.42	1.35
39	s	601	CHL	C4B-NB	8.47	1.42	1.35
39	33	608	CHL	C4B-NB	8.47	1.42	1.35
39	22	601	CHL	C4B-NB	8.46	1.42	1.35
39	1	607	CHL	C4B-NB	8.46	1.42	1.35
39	s	605	CHL	C4B-NB	8.46	1.42	1.35
39	22	605	CHL	C4B-NB	8.46	1.42	1.35
39	G	605	CHL	C4B-NB	8.44	1.42	1.35
39	11	607	CHL	C4B-NB	8.43	1.42	1.35
39	S	607	CHL	C4B-NB	8.42	1.42	1.35
39	GG	609	CHL	C4B-NB	8.42	1.42	1.35
39	n	605	CHL	C4B-NB	8.42	1.42	1.35
39	2	608	CHL	C4B-NB	8.41	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	605	CHL	C4B-NB	8.41	1.42	1.35
39	GG	605	CHL	C4B-NB	8.41	1.42	1.35
39	2	601	CHL	C4B-NB	8.40	1.42	1.35
39	33	605	CHL	C4B-NB	8.40	1.42	1.35
39	22	607	CHL	C4B-NB	8.39	1.42	1.35
39	44	608	CHL	C4B-NB	8.39	1.42	1.35
39	Nn	315	CHL	C4B-NB	8.39	1.42	1.35
39	11	601	CHL	C4B-NB	8.38	1.42	1.35
39	G	609	CHL	C4B-NB	8.38	1.42	1.35
39	33	606	CHL	C4B-NB	8.38	1.42	1.35
39	1	601	CHL	C4B-NB	8.38	1.42	1.35
39	22	608	CHL	C4B-NB	8.37	1.42	1.35
39	YY	607	CHL	C4B-NB	8.37	1.42	1.35
39	11	606	CHL	C4B-NB	8.36	1.42	1.35
39	3	608	CHL	C4B-NB	8.35	1.42	1.35
39	g	605	CHL	C4B-NB	8.34	1.42	1.35
39	3	605	CHL	C4B-NB	8.34	1.42	1.35
39	Ss	606	CHL	C4B-NB	8.33	1.42	1.35
39	3	606	CHL	C4B-NB	8.33	1.42	1.35
39	NN	601	CHL	C4B-NB	8.32	1.42	1.35
39	Ss	605	CHL	C4B-NB	8.31	1.42	1.35
39	1	606	CHL	C4B-NB	8.30	1.42	1.35
39	NN	605	CHL	C4B-NB	8.30	1.42	1.35
39	y	308	CHL	C4B-NB	8.29	1.42	1.35
39	YY	605	CHL	C4B-NB	8.29	1.42	1.35
39	SS	308	CHL	C4B-NB	8.28	1.42	1.35
39	2	607	CHL	C4B-NB	8.28	1.42	1.35
39	1	605	CHL	C4B-NB	8.27	1.42	1.35
39	Ss	607	CHL	C4B-NB	8.27	1.42	1.35
39	Y	607	CHL	C4B-NB	8.27	1.42	1.35
39	s	606	CHL	C4B-NB	8.27	1.42	1.35
39	NN	608	CHL	C4B-NB	8.27	1.42	1.35
39	4	306	CHL	C4B-NB	8.27	1.42	1.35
39	Gg	306	CHL	C4B-NB	8.26	1.42	1.35
32	R	614	CLA	C4B-NB	8.25	1.42	1.35
39	N	608	CHL	C4B-NB	8.25	1.42	1.35
39	s	607	CHL	C4B-NB	8.24	1.42	1.35
39	Rr	607	CHL	C4B-NB	8.24	1.42	1.35
39	y	303	CHL	C4B-NB	8.24	1.42	1.35
39	r	607	CHL	C4B-NB	8.23	1.42	1.35
39	y	309	CHL	C4B-NB	8.22	1.42	1.35
39	Y	601	CHL	C4B-NB	8.22	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	GG	601	CHL	C4B-NB	8.21	1.42	1.35
39	Gg	302	CHL	C4B-NB	8.20	1.42	1.35
39	r	605	CHL	C4B-NB	8.20	1.42	1.35
39	Yy	606	CHL	C4B-NB	8.18	1.42	1.35
39	G	601	CHL	C4B-NB	8.18	1.42	1.35
39	Y	606	CHL	C4B-NB	8.18	1.42	1.35
39	4	302	CHL	C4B-NB	8.18	1.42	1.35
39	n	601	CHL	C4B-NB	8.17	1.42	1.35
32	Rr	610	CLA	C4B-NB	8.16	1.42	1.35
39	RR	307	CHL	C4B-NB	8.16	1.42	1.35
39	44	601	CHL	C4B-NB	8.15	1.42	1.35
39	r	606	CHL	C4B-NB	8.14	1.42	1.35
39	n	608	CHL	C4B-NB	8.14	1.42	1.35
39	S	606	CHL	C4B-NB	8.13	1.42	1.35
32	RR	314	CLA	C4B-NB	8.13	1.42	1.35
32	r	611	CLA	C4B-NB	8.13	1.42	1.35
39	Yy	605	CHL	C4B-NB	8.13	1.42	1.35
32	G	610	CLA	C4B-NB	8.13	1.42	1.35
39	Yy	601	CHL	C4B-NB	8.13	1.42	1.35
39	n	606	CHL	C4B-NB	8.13	1.42	1.35
32	3	609	CLA	C4B-NB	8.12	1.42	1.35
39	Y	605	CHL	C4B-NB	8.12	1.42	1.35
39	YY	601	CHL	C4B-NB	8.12	1.42	1.35
39	Gg	310	CHL	C4B-NB	8.12	1.42	1.35
39	YY	609	CHL	C4B-NB	8.11	1.42	1.35
39	Y	609	CHL	C4B-NB	8.11	1.42	1.35
39	g	609	CHL	C4B-NB	8.11	1.42	1.35
32	3	604	CLA	C4B-NB	8.10	1.42	1.35
39	S	601	CHL	C4B-NB	8.10	1.42	1.35
39	Rr	605	CHL	C4B-NB	8.08	1.42	1.35
32	SS	310	CLA	C4B-NB	8.08	1.42	1.35
39	R	607	CHL	C4B-NB	8.08	1.42	1.35
39	Nn	316	CHL	C4B-NB	8.08	1.42	1.35
32	22	613	CLA	C4B-NB	8.07	1.42	1.35
39	G	608	CHL	C4B-NB	8.06	1.42	1.35
39	y	307	CHL	C4B-NB	8.06	1.42	1.35
39	y	311	CHL	C4B-NB	8.06	1.42	1.35
39	g	601	CHL	C4B-NB	8.06	1.42	1.35
39	4	308	CHL	C4B-NB	8.05	1.42	1.35
39	SS	307	CHL	C4B-NB	8.05	1.42	1.35
35	A	410	PL9	C13-C14	8.05	1.52	1.33
35	AA	410	PL9	C13-C14	8.05	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	YY	606	CHL	C4B-NB	8.04	1.42	1.35
39	Ss	601	CHL	C4B-NB	8.03	1.42	1.35
39	g	608	CHL	C4B-NB	8.03	1.42	1.35
39	Gg	307	CHL	C4B-NB	8.03	1.42	1.35
39	g	606	CHL	C4B-NB	8.03	1.42	1.35
39	Rr	606	CHL	C4B-NB	8.02	1.42	1.35
39	33	601	CHL	C4B-NB	8.02	1.42	1.35
39	Nn	311	CHL	C4B-NB	8.02	1.42	1.35
39	GG	608	CHL	C4B-NB	8.02	1.42	1.35
39	4	307	CHL	C4B-NB	8.02	1.42	1.35
32	11	610	CLA	C4B-NB	8.02	1.42	1.35
32	RR	304	CLA	C4B-NB	8.02	1.42	1.35
39	SS	302	CHL	C4B-NB	8.01	1.42	1.35
39	44	607	CHL	C4B-NB	8.01	1.42	1.35
32	11	603	CLA	C4B-NB	8.00	1.42	1.35
39	RR	305	CHL	C4B-NB	8.00	1.42	1.35
39	Gg	309	CHL	C4B-NB	8.00	1.42	1.35
39	11	608	CHL	C4B-NB	8.00	1.42	1.35
39	G	606	CHL	C4B-NB	8.00	1.42	1.35
39	N	606	CHL	C4B-NB	8.00	1.42	1.35
39	Yy	609	CHL	C4B-NB	7.99	1.42	1.35
35	Dd	404	PL9	C13-C14	7.99	1.52	1.33
39	R	605	CHL	C4B-NB	7.99	1.42	1.35
39	Y	608	CHL	C4B-NB	7.97	1.42	1.35
39	NN	606	CHL	C4B-NB	7.97	1.42	1.35
32	1	609	CLA	C4B-NB	7.97	1.42	1.35
39	Yy	607	CHL	C4B-NB	7.96	1.42	1.35
39	44	606	CHL	C4B-NB	7.96	1.42	1.35
39	YY	608	CHL	C4B-NB	7.94	1.42	1.35
39	Nn	318	CHL	C4B-NB	7.94	1.42	1.35
32	1	610	CLA	C4B-NB	7.94	1.42	1.35
32	YY	612	CLA	C4B-NB	7.94	1.42	1.35
32	s	603	CLA	C4B-NB	7.93	1.42	1.35
32	11	604	CLA	C4B-NB	7.93	1.42	1.35
32	3	603	CLA	C4B-NB	7.93	1.42	1.35
32	11	609	CLA	C4B-NB	7.93	1.42	1.35
32	Ss	603	CLA	C4B-NB	7.92	1.42	1.35
32	33	604	CLA	C4B-NB	7.92	1.42	1.35
39	GG	606	CHL	C4B-NB	7.92	1.42	1.35
35	d	404	PL9	C13-C14	7.92	1.52	1.33
39	3	601	CHL	C4B-NB	7.91	1.42	1.35
39	NN	607	CHL	C4B-NB	7.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	607	CHL	C4B-NB	7.91	1.42	1.35
32	22	610	CLA	C4B-NB	7.90	1.42	1.35
32	1	604	CLA	C4B-NB	7.90	1.42	1.35
32	2	602	CLA	C4B-NB	7.90	1.42	1.35
32	R	610	CLA	C4B-NB	7.89	1.42	1.35
35	D	407	PL9	C13-C14	7.87	1.51	1.33
39	g	607	CHL	C4B-NB	7.87	1.42	1.35
35	DD	406	PL9	C13-C14	7.87	1.51	1.33
32	1	611	CLA	C4B-NB	7.87	1.42	1.35
32	g	610	CLA	C4B-NB	7.87	1.42	1.35
32	11	613	CLA	C4B-NB	7.87	1.42	1.35
32	2	609	CLA	C4B-NB	7.87	1.42	1.35
32	Rr	602	CLA	C4B-NB	7.86	1.42	1.35
32	R	604	CLA	C4B-NB	7.86	1.42	1.35
39	Yy	608	CHL	C4B-NB	7.86	1.42	1.35
32	3	612	CLA	C4B-NB	7.86	1.42	1.35
32	22	604	CLA	C4B-NB	7.85	1.42	1.35
39	1	608	CHL	C4B-NB	7.85	1.42	1.35
39	y	310	CHL	C4B-NB	7.84	1.42	1.35
39	N	607	CHL	C4B-NB	7.84	1.42	1.35
32	B	604	CLA	C4B-NB	7.83	1.42	1.35
32	33	609	CLA	C4B-NB	7.83	1.42	1.35
32	33	603	CLA	C4B-NB	7.83	1.42	1.35
32	22	609	CLA	C4B-NB	7.83	1.42	1.35
39	Gg	308	CHL	C4B-NB	7.81	1.42	1.35
32	1	612	CLA	C4B-NB	7.81	1.42	1.35
39	GG	607	CHL	C4B-NB	7.81	1.42	1.35
32	Ss	612	CLA	C4B-NB	7.80	1.42	1.35
32	s	604	CLA	C4B-NB	7.80	1.42	1.35
32	XX	201	CLA	C4B-NB	7.80	1.42	1.35
39	n	607	CHL	C4B-NB	7.80	1.42	1.35
32	33	602	CLA	C4B-NB	7.79	1.42	1.35
39	SS	306	CHL	C4B-NB	7.78	1.42	1.35
32	2	604	CLA	C4B-NB	7.77	1.42	1.35
32	y	315	CLA	C4B-NB	7.77	1.42	1.35
32	2	611	CLA	C4B-NB	7.77	1.42	1.35
32	N	611	CLA	C4B-NB	7.77	1.42	1.35
32	r	603	CLA	C4B-NB	7.77	1.42	1.35
32	3	611	CLA	C4B-NB	7.76	1.42	1.35
32	r	608	CLA	C4B-NB	7.76	1.42	1.35
32	33	612	CLA	C4B-NB	7.76	1.42	1.35
39	R	606	CHL	C4B-NB	7.76	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	604	CLA	C4B-NB	7.75	1.42	1.35
32	3	613	CLA	C4B-NB	7.75	1.42	1.35
32	S	608	CLA	C4B-NB	7.75	1.42	1.35
39	NN	609	CHL	C4B-NB	7.74	1.42	1.35
32	Ss	604	CLA	C4B-NB	7.74	1.42	1.35
32	s	602	CLA	C4B-NB	7.74	1.42	1.35
32	Nn	302	CLA	C4B-NB	7.73	1.42	1.35
32	r	601	CLA	C4B-NB	7.73	1.42	1.35
32	11	611	CLA	C4B-NB	7.72	1.42	1.35
32	22	611	CLA	C4B-NB	7.72	1.42	1.35
35	A	410	PL9	C48-C49	7.72	1.54	1.32
32	Rr	611	CLA	C4B-NB	7.72	1.42	1.35
32	1	613	CLA	C4B-NB	7.72	1.42	1.35
32	Gg	305	CLA	C4B-NB	7.71	1.42	1.35
32	2	603	CLA	C4B-NB	7.71	1.42	1.35
32	33	613	CLA	C4B-NB	7.71	1.42	1.35
32	a	406	CLA	C4B-NB	7.70	1.42	1.35
32	SS	309	CLA	C4B-NB	7.70	1.42	1.35
32	22	602	CLA	C4B-NB	7.70	1.42	1.35
32	g	602	CLA	C4B-NB	7.70	1.42	1.35
32	R	601	CLA	C4B-NB	7.70	1.42	1.35
39	N	609	CHL	C4B-NB	7.70	1.42	1.35
32	S	604	CLA	C4B-NB	7.70	1.42	1.35
32	RR	310	CLA	C4B-NB	7.70	1.42	1.35
32	1	602	CLA	C4B-NB	7.69	1.42	1.35
35	AA	410	PL9	C48-C49	7.69	1.54	1.32
32	s	612	CLA	C4B-NB	7.69	1.42	1.35
32	44	615	CLA	C4B-NB	7.68	1.42	1.35
32	s	611	CLA	C4B-NB	7.68	1.42	1.35
32	Rr	603	CLA	C4B-NB	7.68	1.42	1.35
39	Nn	317	CHL	C4B-NB	7.68	1.42	1.35
32	GG	602	CLA	C4B-NB	7.67	1.42	1.35
32	S	603	CLA	C4B-NB	7.67	1.42	1.35
32	Nn	303	CLA	C4B-NB	7.67	1.42	1.35
32	NN	611	CLA	C4B-NB	7.66	1.42	1.35
32	d	402	CLA	C4B-NB	7.66	1.42	1.35
32	Ss	611	CLA	C4B-NB	7.66	1.42	1.35
32	g	613	CLA	C4B-NB	7.66	1.42	1.35
32	3	602	CLA	C4B-NB	7.66	1.42	1.35
32	N	613	CLA	C4B-NB	7.66	1.42	1.35
32	r	613	CLA	C4B-NB	7.66	1.42	1.35
32	Rr	608	CLA	C4B-NB	7.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	33	611	CLA	C4B-NB	7.66	1.42	1.35
32	2	612	CLA	C4B-NB	7.65	1.42	1.35
32	R	602	CLA	C4B-NB	7.65	1.42	1.35
32	b	610	CLA	C4B-NB	7.65	1.42	1.35
32	G	602	CLA	C4B-NB	7.65	1.42	1.35
32	X	201	CLA	C4B-NB	7.64	1.42	1.35
32	r	610	CLA	C4B-NB	7.64	1.42	1.35
32	Yy	613	CLA	C4B-NB	7.64	1.42	1.35
32	SS	305	CLA	C4B-NB	7.64	1.42	1.35
32	N	612	CLA	C4B-NB	7.64	1.42	1.35
32	GG	604	CLA	C4B-NB	7.64	1.42	1.35
32	YY	604	CLA	C4B-NB	7.64	1.42	1.35
32	4	304	CLA	C4B-NB	7.63	1.42	1.35
32	Gg	314	CLA	C4B-NB	7.63	1.42	1.35
32	22	612	CLA	C4B-NB	7.63	1.42	1.35
32	Nn	304	CLA	C4B-NB	7.63	1.42	1.35
35	D	407	PL9	C48-C49	7.62	1.54	1.32
32	Rr	601	CLA	C4B-NB	7.62	1.42	1.35
32	11	602	CLA	C4B-NB	7.62	1.42	1.35
32	RR	302	CLA	C4B-NB	7.62	1.42	1.35
32	n	612	CLA	C4B-NB	7.62	1.42	1.35
32	NN	614	CLA	C4B-NB	7.61	1.42	1.35
32	33	610	CLA	C4B-NB	7.61	1.42	1.35
32	SS	304	CLA	C4B-NB	7.61	1.42	1.35
32	D	405	CLA	C4B-NB	7.61	1.42	1.35
32	Ss	602	CLA	C4B-NB	7.61	1.42	1.35
32	Bb	607	CLA	C4B-NB	7.61	1.42	1.35
32	SS	311	CLA	C4B-NB	7.60	1.42	1.35
32	y	313	CLA	C4B-NB	7.60	1.42	1.35
32	n	613	CLA	C4B-NB	7.60	1.42	1.35
32	G	612	CLA	C4B-NB	7.60	1.42	1.35
32	y	316	CLA	C4B-NB	7.60	1.42	1.35
32	n	611	CLA	C4B-NB	7.59	1.42	1.35
32	44	610	CLA	C4B-NB	7.59	1.42	1.35
32	d	401	CLA	C4B-NB	7.59	1.42	1.35
32	NN	612	CLA	C4B-NB	7.59	1.42	1.35
32	4	303	CLA	C4B-NB	7.59	1.42	1.35
32	Rr	613	CLA	C4B-NB	7.59	1.42	1.35
32	S	609	CLA	C4B-NB	7.59	1.42	1.35
32	4	310	CLA	C4B-NB	7.59	1.42	1.35
35	d	404	PL9	C48-C49	7.59	1.54	1.32
32	GG	610	CLA	C4B-NB	7.59	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	GG	611	CLA	C4B-NB	7.58	1.42	1.35
32	Gg	303	CLA	C4B-NB	7.58	1.42	1.35
32	44	602	CLA	C4B-NB	7.58	1.42	1.35
32	4	311	CLA	C4B-NB	7.58	1.42	1.35
32	G	611	CLA	C4B-NB	7.58	1.42	1.35
35	DD	406	PL9	C48-C49	7.58	1.54	1.32
32	S	611	CLA	C4B-NB	7.57	1.42	1.35
32	GG	612	CLA	C4B-NB	7.57	1.42	1.35
32	BB	604	CLA	C4B-NB	7.57	1.42	1.35
32	Nn	301	CLA	C4B-NB	7.57	1.42	1.35
35	Dd	404	PL9	C48-C49	7.57	1.54	1.32
32	22	603	CLA	C4B-NB	7.57	1.42	1.35
32	Y	610	CLA	C4B-NB	7.57	1.42	1.35
32	R	613	CLA	C4B-NB	7.57	1.42	1.35
32	s	608	CLA	C4B-NB	7.57	1.42	1.35
32	Bb	610	CLA	C4B-NB	7.57	1.42	1.35
32	GG	613	CLA	C4B-NB	7.56	1.42	1.35
32	N	614	CLA	C4B-NB	7.56	1.42	1.35
32	Rr	612	CLA	C4B-NB	7.56	1.42	1.35
32	c	511	CLA	C4B-NB	7.56	1.42	1.35
32	b	607	CLA	C4B-NB	7.56	1.41	1.35
32	c	510	CLA	C4B-NB	7.56	1.41	1.35
32	BB	608	CLA	C4B-NB	7.56	1.41	1.35
32	N	604	CLA	C4B-NB	7.55	1.41	1.35
32	Y	612	CLA	C4B-NB	7.55	1.41	1.35
32	Nn	313	CLA	C4B-NB	7.55	1.41	1.35
32	44	609	CLA	C4B-NB	7.55	1.41	1.35
32	YY	610	CLA	C4B-NB	7.55	1.41	1.35
32	r	612	CLA	C4B-NB	7.55	1.41	1.35
32	Gg	315	CLA	C4B-NB	7.55	1.41	1.35
32	RR	311	CLA	C4B-NB	7.55	1.41	1.35
32	S	612	CLA	C4B-NB	7.55	1.41	1.35
32	b	601	CLA	C4B-NB	7.55	1.41	1.35
32	b	615	CLA	C4B-NB	7.55	1.41	1.35
32	Dd	401	CLA	C4B-NB	7.55	1.41	1.35
35	A	410	PL9	O1-C4	7.54	1.39	1.23
32	G	604	CLA	C4B-NB	7.54	1.41	1.35
32	R	609	CLA	C4B-NB	7.54	1.41	1.35
32	2	610	CLA	C4B-NB	7.54	1.41	1.35
32	Bb	601	CLA	C4B-NB	7.54	1.41	1.35
32	S	602	CLA	C4B-NB	7.53	1.41	1.35
32	r	602	CLA	C4B-NB	7.53	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Gg	312	CLA	C4B-NB	7.53	1.41	1.35
32	Y	614	CLA	C4B-NB	7.53	1.41	1.35
32	RR	313	CLA	C4B-NB	7.53	1.41	1.35
32	Y	602	CLA	C4B-NB	7.52	1.41	1.35
32	G	613	CLA	C4B-NB	7.52	1.41	1.35
32	NN	604	CLA	C4B-NB	7.52	1.41	1.35
32	N	610	CLA	C4B-NB	7.52	1.41	1.35
32	4	312	CLA	C4B-NB	7.52	1.41	1.35
32	Dd	402	CLA	C4B-NB	7.52	1.41	1.35
39	n	609	CHL	C4B-NB	7.52	1.41	1.35
32	RR	309	CLA	C4B-NB	7.52	1.41	1.35
32	B	606	CLA	C4B-NB	7.51	1.41	1.35
32	Y	611	CLA	C4B-NB	7.51	1.41	1.35
32	NN	613	CLA	C4B-NB	7.51	1.41	1.35
32	2	613	CLA	C4B-NB	7.51	1.41	1.35
32	Y	604	CLA	C4B-NB	7.51	1.41	1.35
32	g	614	CLA	C4B-NB	7.51	1.41	1.35
32	NN	610	CLA	C4B-NB	7.51	1.41	1.35
32	GG	614	CLA	C4B-NB	7.51	1.41	1.35
32	Ss	608	CLA	C4B-NB	7.51	1.41	1.35
35	Dd	404	PL9	O1-C4	7.50	1.39	1.23
32	G	614	CLA	C4B-NB	7.50	1.41	1.35
32	SS	313	CLA	C4B-NB	7.50	1.41	1.35
32	BB	615	CLA	C4B-NB	7.50	1.41	1.35
32	R	603	CLA	C4B-NB	7.50	1.41	1.35
35	AA	410	PL9	O1-C4	7.50	1.39	1.23
32	Ss	613	CLA	C4B-NB	7.50	1.41	1.35
32	Ss	610	CLA	C4B-NB	7.50	1.41	1.35
32	Cc	513	CLA	C4B-NB	7.50	1.41	1.35
32	Rr	604	CLA	C4B-NB	7.50	1.41	1.35
32	RR	312	CLA	C4B-NB	7.50	1.41	1.35
32	S	610	CLA	C4B-NB	7.49	1.41	1.35
32	A	408	CLA	C4B-NB	7.49	1.41	1.35
32	n	610	CLA	C4B-NB	7.49	1.41	1.35
32	Cc	511	CLA	C4B-NB	7.49	1.41	1.35
32	CC	510	CLA	C4B-NB	7.48	1.41	1.35
32	YY	602	CLA	C4B-NB	7.48	1.41	1.35
32	1	603	CLA	C4B-NB	7.48	1.41	1.35
32	DD	404	CLA	C4B-NB	7.48	1.41	1.35
32	s	610	CLA	C4B-NB	7.48	1.41	1.35
32	r	609	CLA	C4B-NB	7.47	1.41	1.35
32	SS	312	CLA	C4B-NB	7.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	YY	603	CLA	C4B-NB	7.47	1.41	1.35
32	a	407	CLA	C4B-NB	7.47	1.41	1.35
32	b	603	CLA	C4B-NB	7.47	1.41	1.35
32	Yy	610	CLA	C4B-NB	7.46	1.41	1.35
32	Nn	305	CLA	C4B-NB	7.46	1.41	1.35
32	C	506	CLA	C4B-NB	7.46	1.41	1.35
32	Y	613	CLA	C4B-NB	7.46	1.41	1.35
32	4	305	CLA	C4B-NB	7.46	1.41	1.35
32	Yy	614	CLA	C4B-NB	7.46	1.41	1.35
32	b	602	CLA	C4B-NB	7.46	1.41	1.35
32	BB	606	CLA	C4B-NB	7.46	1.41	1.35
32	Rr	609	CLA	C4B-NB	7.46	1.41	1.35
32	a	410	CLA	C4B-NB	7.46	1.41	1.35
32	g	612	CLA	C4B-NB	7.46	1.41	1.35
32	SS	303	CLA	C4B-NB	7.46	1.41	1.35
32	R	612	CLA	C4B-NB	7.46	1.41	1.35
32	n	604	CLA	C4B-NB	7.45	1.41	1.35
32	Aa	407	CLA	C4B-NB	7.45	1.41	1.35
32	n	614	CLA	C4B-NB	7.45	1.41	1.35
32	Cc	505	CLA	C4B-NB	7.45	1.41	1.35
32	R	608	CLA	C4B-NB	7.45	1.41	1.35
32	YY	614	CLA	C4B-NB	7.45	1.41	1.35
32	N	603	CLA	C4B-NB	7.45	1.41	1.35
32	c	508	CLA	C4B-NB	7.45	1.41	1.35
32	3	610	CLA	C4B-NB	7.44	1.41	1.35
32	C	503	CLA	C4B-NB	7.44	1.41	1.35
32	B	621	CLA	C4B-NB	7.44	1.41	1.35
32	s	613	CLA	C4B-NB	7.43	1.41	1.35
32	B	611	CLA	C4B-NB	7.43	1.41	1.35
35	d	404	PL9	O1-C4	7.43	1.39	1.23
32	44	603	CLA	C4B-NB	7.43	1.41	1.35
32	C	511	CLA	C4B-NB	7.43	1.41	1.35
32	Cc	512	CLA	C4B-NB	7.43	1.41	1.35
32	44	611	CLA	C4B-NB	7.42	1.41	1.35
32	B	610	CLA	C4B-NB	7.42	1.41	1.35
32	Cc	507	CLA	C4B-NB	7.42	1.41	1.35
32	AA	408	CLA	C4B-NB	7.42	1.41	1.35
32	Bb	602	CLA	C4B-NB	7.42	1.41	1.35
32	RR	303	CLA	C4B-NB	7.42	1.41	1.35
32	C	513	CLA	C4B-NB	7.42	1.41	1.35
39	Nn	319	CHL	C4B-NB	7.42	1.41	1.35
32	R	611	CLA	C4B-NB	7.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	509	CLA	C4B-NB	7.41	1.41	1.35
32	NN	602	CLA	C4B-NB	7.41	1.41	1.35
32	Yy	611	CLA	C4B-NB	7.41	1.41	1.35
32	n	603	CLA	C4B-NB	7.41	1.41	1.35
32	y	304	CLA	C4B-NB	7.40	1.41	1.35
32	Bb	604	CLA	C4B-NB	7.40	1.41	1.35
32	Ss	609	CLA	C4B-NB	7.40	1.41	1.35
32	BB	610	CLA	C4B-NB	7.40	1.41	1.35
32	b	608	CLA	C4B-NB	7.40	1.41	1.35
32	CC	505	CLA	C4B-NB	7.40	1.41	1.35
32	RR	308	CLA	C4B-NB	7.40	1.41	1.35
32	g	611	CLA	C4B-NB	7.39	1.41	1.35
32	s	609	CLA	C4B-NB	7.39	1.41	1.35
32	b	611	CLA	C4B-NB	7.39	1.41	1.35
32	n	602	CLA	C4B-NB	7.39	1.41	1.35
32	Cc	510	CLA	C4B-NB	7.39	1.41	1.35
32	CC	509	CLA	C4B-NB	7.38	1.41	1.35
32	B	623	CLA	C4B-NB	7.38	1.41	1.35
32	BB	614	CLA	C4B-NB	7.38	1.41	1.35
32	Y	603	CLA	C4B-NB	7.38	1.41	1.35
32	C	514	CLA	C4B-NB	7.37	1.41	1.35
32	Bb	615	CLA	C4B-NB	7.37	1.41	1.35
32	y	312	CLA	C4B-NB	7.37	1.41	1.35
32	SS	314	CLA	C4B-NB	7.37	1.41	1.35
32	Aa	410	CLA	C4B-NB	7.37	1.41	1.35
32	N	602	CLA	C4B-NB	7.37	1.41	1.35
32	b	614	CLA	C4B-NB	7.37	1.41	1.35
32	c	505	CLA	C4B-NB	7.37	1.41	1.35
32	A	406	CLA	C4B-NB	7.36	1.41	1.35
32	G	603	CLA	C4B-NB	7.36	1.41	1.35
32	Gg	311	CLA	C4B-NB	7.36	1.41	1.35
32	b	606	CLA	C4B-NB	7.36	1.41	1.35
32	Aa	406	CLA	C4B-NB	7.36	1.41	1.35
35	DD	406	PL9	O1-C4	7.35	1.39	1.23
32	Cc	515	CLA	C4B-NB	7.35	1.41	1.35
32	C	510	CLA	C4B-NB	7.35	1.41	1.35
32	YY	613	CLA	C4B-NB	7.34	1.41	1.35
32	GG	603	CLA	C4B-NB	7.34	1.41	1.35
32	b	604	CLA	C4B-NB	7.34	1.41	1.35
32	Bb	603	CLA	C4B-NB	7.33	1.41	1.35
32	S	613	CLA	C4B-NB	7.33	1.41	1.35
32	CC	512	CLA	C4B-NB	7.33	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	D	407	PL9	O1-C4	7.33	1.39	1.23
32	Yy	602	CLA	C4B-NB	7.33	1.41	1.35
32	BB	613	CLA	C4B-NB	7.33	1.41	1.35
32	Gg	304	CLA	C4B-NB	7.32	1.41	1.35
32	Nn	314	CLA	C4B-NB	7.32	1.41	1.35
32	C	507	CLA	C4B-NB	7.32	1.41	1.35
32	44	604	CLA	C4B-NB	7.32	1.41	1.35
32	C	505	CLA	C4B-NB	7.32	1.41	1.35
32	c	503	CLA	C4B-NB	7.32	1.41	1.35
32	AA	406	CLA	C4B-NB	7.32	1.41	1.35
32	BB	602	CLA	C4B-NB	7.32	1.41	1.35
32	BB	601	CLA	C4B-NB	7.31	1.41	1.35
32	B	622	CLA	C4B-NB	7.31	1.41	1.35
32	g	603	CLA	C4B-NB	7.31	1.41	1.35
32	Gg	313	CLA	C4B-NB	7.31	1.41	1.35
32	CC	506	CLA	C4B-NB	7.30	1.41	1.35
32	r	604	CLA	C4B-NB	7.30	1.41	1.35
32	CC	513	CLA	C4B-NB	7.30	1.41	1.35
32	BB	612	CLA	C4B-NB	7.29	1.41	1.35
32	Yy	604	CLA	C4B-NB	7.29	1.41	1.35
32	c	504	CLA	C4B-NB	7.28	1.41	1.35
32	C	515	CLA	C4B-NB	7.28	1.41	1.35
32	c	502	CLA	C4B-NB	7.27	1.41	1.35
32	Bb	616	CLA	C4B-NB	7.27	1.41	1.35
32	B	619	CLA	C4B-NB	7.26	1.41	1.35
32	Bb	611	CLA	C4B-NB	7.26	1.41	1.35
32	NN	603	CLA	C4B-NB	7.26	1.41	1.35
32	YY	611	CLA	C4B-NB	7.26	1.41	1.35
32	C	512	CLA	C4B-NB	7.26	1.41	1.35
32	Cc	503	CLA	C4B-NB	7.25	1.41	1.35
32	b	616	CLA	C4B-NB	7.25	1.41	1.35
32	C	508	CLA	C4B-NB	7.24	1.41	1.35
32	B	607	CLA	C4B-NB	7.24	1.41	1.35
32	b	605	CLA	C4B-NB	7.24	1.41	1.35
32	B	620	CLA	C4B-NB	7.24	1.41	1.35
32	c	501	CLA	C4B-NB	7.24	1.41	1.35
32	b	612	CLA	C4B-NB	7.24	1.41	1.35
32	CC	504	CLA	C4B-NB	7.24	1.41	1.35
32	c	513	CLA	C4B-NB	7.24	1.41	1.35
32	B	609	CLA	C4B-NB	7.23	1.41	1.35
32	c	506	CLA	C4B-NB	7.23	1.41	1.35
32	AA	405	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	605	CLA	C4B-NB	7.22	1.41	1.35
32	A	405	CLA	C4B-NB	7.22	1.41	1.35
32	Cc	508	CLA	C4B-NB	7.22	1.41	1.35
32	y	306	CLA	C4B-NB	7.21	1.41	1.35
32	Bb	614	CLA	C4B-NB	7.21	1.41	1.35
32	B	618	CLA	C4B-NB	7.21	1.41	1.35
32	B	624	CLA	C4B-NB	7.21	1.41	1.35
32	CC	507	CLA	C4B-NB	7.21	1.41	1.35
32	Bb	605	CLA	C4B-NB	7.21	1.41	1.35
32	D	401	CLA	C4B-NB	7.20	1.41	1.35
32	Bb	606	CLA	C4B-NB	7.20	1.41	1.35
32	CC	502	CLA	C4B-NB	7.20	1.41	1.35
32	DD	401	CLA	C4B-NB	7.20	1.41	1.35
32	Cc	504	CLA	C4B-NB	7.20	1.41	1.35
32	b	613	CLA	C4B-NB	7.19	1.41	1.35
32	Cc	514	CLA	C4B-NB	7.19	1.41	1.35
32	a	405	CLA	C4B-NB	7.18	1.41	1.35
32	Aa	405	CLA	C4B-NB	7.17	1.41	1.35
32	Bb	612	CLA	C4B-NB	7.17	1.41	1.35
32	CC	511	CLA	C4B-NB	7.17	1.41	1.35
32	BB	609	CLA	C4B-NB	7.17	1.41	1.35
32	B	605	CLA	C4B-NB	7.16	1.41	1.35
32	B	608	CLA	C4B-NB	7.16	1.41	1.35
32	DD	403	CLA	C4B-NB	7.15	1.41	1.35
32	c	512	CLA	C4B-NB	7.15	1.41	1.35
32	Cc	509	CLA	C4B-NB	7.14	1.41	1.35
32	Bb	613	CLA	C4B-NB	7.14	1.41	1.35
32	Bb	608	CLA	C4B-NB	7.13	1.41	1.35
32	BB	603	CLA	C4B-NB	7.12	1.41	1.35
32	Yy	603	CLA	C4B-NB	7.12	1.41	1.35
32	y	305	CLA	C4B-NB	7.11	1.41	1.35
32	c	507	CLA	C4B-NB	7.11	1.41	1.35
32	C	509	CLA	C4B-NB	7.10	1.41	1.35
32	CC	514	CLA	C4B-NB	7.10	1.41	1.35
32	11	612	CLA	C4B-NB	7.09	1.41	1.35
32	BB	611	CLA	C4B-NB	7.09	1.41	1.35
32	D	404	CLA	C4B-NB	7.08	1.41	1.35
32	BB	607	CLA	C4B-NB	7.07	1.41	1.35
32	Cc	506	CLA	C4B-NB	7.04	1.41	1.35
32	Yy	612	CLA	C4B-NB	7.02	1.41	1.35
32	CC	503	CLA	C4B-NB	6.99	1.41	1.35
32	C	504	CLA	C4B-NB	6.98	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	314	CLA	C4B-NB	6.98	1.41	1.35
32	Nn	312	CLA	C4B-NB	6.94	1.41	1.35
32	b	609	CLA	C4B-NB	6.87	1.41	1.35
39	RR	306	CHL	C4B-NB	6.86	1.41	1.35
32	CC	508	CLA	C4B-NB	6.82	1.41	1.35
32	Bb	609	CLA	C4B-NB	6.79	1.41	1.35
35	DD	406	PL9	C3-C4	-6.47	1.38	1.49
35	D	407	PL9	C3-C4	-6.41	1.39	1.49
35	d	404	PL9	C3-C4	-6.36	1.39	1.49
35	Dd	404	PL9	C3-C4	-6.31	1.39	1.49
35	A	410	PL9	C3-C4	-5.98	1.39	1.49
35	AA	410	PL9	C3-C4	-5.94	1.39	1.49
35	A	410	PL9	O2-C1	5.78	1.39	1.24
35	Dd	404	PL9	C6-C1	-5.76	1.38	1.48
35	AA	410	PL9	O2-C1	5.76	1.39	1.24
35	DD	406	PL9	C6-C1	-5.71	1.38	1.48
35	D	407	PL9	C6-C1	-5.70	1.38	1.48
35	d	404	PL9	C6-C1	-5.70	1.38	1.48
35	Dd	404	PL9	O2-C1	5.65	1.39	1.24
35	d	404	PL9	O2-C1	5.64	1.39	1.24
36	44	616	LHG	O7-C7	5.63	1.45	1.33
35	DD	406	PL9	O2-C1	5.61	1.39	1.24
35	D	407	PL9	O2-C1	5.59	1.39	1.24
36	4	301	LHG	O7-C7	5.59	1.45	1.33
35	AA	410	PL9	C6-C1	-5.36	1.39	1.48
35	A	410	PL9	C6-C1	-5.36	1.39	1.48
37	BB	621	SQD	O8-S	5.01	1.65	1.47
37	B	617	SQD	O8-S	5.00	1.65	1.47
36	4	315	LHG	O7-C7	4.79	1.46	1.35
36	J	101	LHG	O7-C7	4.72	1.45	1.35
46	E	101	HEM	C3C-C2C	-4.67	1.33	1.40
37	l	102	SQD	O8-S	4.63	1.64	1.47
37	Ll	101	SQD	O8-S	4.62	1.64	1.47
37	Aa	413	SQD	O8-S	4.61	1.63	1.47
37	B	602	SQD	O8-S	4.61	1.63	1.47
37	L	102	SQD	O8-S	4.60	1.63	1.47
37	LL	101	SQD	O8-S	4.59	1.63	1.47
37	L	101	SQD	O8-S	4.59	1.63	1.47
37	LL	102	SQD	O8-S	4.59	1.63	1.47
37	A	412	SQD	O8-S	4.58	1.63	1.47
37	C	501	SQD	O8-S	4.54	1.63	1.47
46	EE	102	HEM	C3C-C2C	-4.50	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	410	PL9	C7-C3	4.48	1.55	1.51
36	44	614	LHG	O7-C7	4.48	1.45	1.35
37	AA	412	SQD	O8-S	4.47	1.63	1.47
35	AA	410	PL9	C7-C3	4.47	1.55	1.51
37	CC	501	SQD	O8-S	4.45	1.63	1.47
36	Rr	617	LHG	O7-C7	4.44	1.46	1.34
36	r	616	LHG	O7-C7	4.38	1.46	1.34
44	a	415	DGD	O1G-C1A	4.38	1.46	1.33
36	Rr	617	LHG	O8-C23	4.37	1.46	1.33
36	r	616	LHG	O8-C23	4.36	1.46	1.33
44	Aa	401	DGD	O1G-C1A	4.36	1.46	1.33
37	B	602	SQD	O48-C23	4.35	1.46	1.33
44	a	415	DGD	O2G-C1B	4.34	1.46	1.34
37	Aa	413	SQD	O48-C23	4.34	1.46	1.33
37	L	101	SQD	O48-C23	4.33	1.46	1.33
38	W	201	LMG	O7-C10	4.33	1.46	1.34
38	WW	201	LMG	O7-C10	4.33	1.46	1.34
37	LL	102	SQD	O48-C23	4.32	1.46	1.33
36	l	614	LHG	O8-C23	4.32	1.46	1.33
44	Hh	102	DGD	O2G-C1B	4.32	1.46	1.34
44	C	519	DGD	O1G-C1A	4.31	1.45	1.33
37	BB	621	SQD	O48-C23	4.31	1.45	1.33
36	11	614	LHG	O8-C23	4.31	1.45	1.33
44	CC	518	DGD	O1G-C1A	4.31	1.45	1.33
44	Aa	401	DGD	O2G-C1B	4.31	1.46	1.34
36	EE	101	LHG	O7-C7	4.30	1.46	1.34
44	B	603	DGD	O1G-C1A	4.30	1.45	1.33
38	j	101	LMG	O8-C28	4.30	1.45	1.33
38	BB	619	LMG	O8-C28	4.29	1.45	1.33
36	Nn	310	LHG	O7-C7	4.29	1.46	1.34
36	SS	301	LHG	O8-C23	4.29	1.45	1.33
37	B	617	SQD	O48-C23	4.28	1.45	1.33
44	Cc	520	DGD	O1G-C1A	4.28	1.45	1.33
36	0	201	LHG	O7-C7	4.28	1.46	1.34
37	A	412	SQD	O48-C23	4.28	1.45	1.33
44	h	102	DGD	O1G-C1A	4.28	1.45	1.33
44	h	102	DGD	O2G-C1B	4.28	1.46	1.34
38	CC	520	LMG	O8-C28	4.28	1.45	1.33
36	n	618	LHG	O7-C7	4.28	1.46	1.34
38	Aa	412	LMG	O8-C28	4.27	1.45	1.33
38	Bb	621	LMG	O8-C28	4.27	1.45	1.33
36	g	618	LHG	O8-C23	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Gg	319	LHG	O8-C23	4.27	1.45	1.33
38	B	615	LMG	O8-C28	4.26	1.45	1.33
44	c	518	DGD	O1G-C1A	4.26	1.45	1.33
38	Dd	408	LMG	O8-C28	4.26	1.45	1.33
38	b	621	LMG	O8-C28	4.26	1.45	1.33
44	BB	625	DGD	O1G-C1A	4.26	1.45	1.33
44	C	519	DGD	O2G-C1B	4.26	1.46	1.34
38	m	101	LMG	O7-C10	4.26	1.46	1.34
36	3	614	LHG	O8-C23	4.26	1.45	1.33
36	n	618	LHG	O8-C23	4.25	1.45	1.33
36	NN	619	LHG	O8-C23	4.25	1.45	1.33
36	Ll	102	LHG	O8-C23	4.25	1.45	1.33
37	L	102	SQD	O48-C23	4.25	1.45	1.33
36	G	618	LHG	O8-C23	4.25	1.45	1.33
37	LL	101	SQD	O48-C23	4.25	1.45	1.33
44	BB	624	DGD	O1G-C1A	4.25	1.45	1.33
36	D	410	LHG	O8-C23	4.25	1.45	1.33
36	22	615	LHG	O8-C23	4.25	1.45	1.33
37	AA	412	SQD	O48-C23	4.24	1.45	1.33
36	GG	618	LHG	O8-C23	4.24	1.45	1.33
44	B	601	DGD	O1G-C1A	4.24	1.45	1.33
36	22	615	LHG	O7-C7	4.24	1.46	1.34
38	A	415	LMG	O8-C28	4.24	1.45	1.33
36	s	616	LHG	O8-C23	4.24	1.45	1.33
37	Ll	101	SQD	O48-C23	4.24	1.45	1.33
36	NN	619	LHG	O7-C7	4.23	1.46	1.34
38	W	201	LMG	O8-C28	4.23	1.45	1.33
36	BB	622	LHG	O7-C7	4.23	1.46	1.34
38	Mm	101	LMG	O7-C10	4.23	1.46	1.34
37	l	102	SQD	O48-C23	4.23	1.45	1.33
38	AA	415	LMG	O8-C28	4.23	1.45	1.33
38	b	620	LMG	O8-C28	4.22	1.45	1.33
36	N	619	LHG	O7-C7	4.22	1.46	1.34
36	Nn	310	LHG	O8-C23	4.22	1.45	1.33
36	AA	414	LHG	O7-C7	4.22	1.46	1.34
38	F	101	LMG	O8-C28	4.22	1.45	1.33
36	KK	101	LHG	O8-C23	4.22	1.45	1.33
36	A	414	LHG	O7-C7	4.22	1.46	1.34
36	33	614	LHG	O8-C23	4.22	1.45	1.33
38	DD	409	LMG	O8-C28	4.22	1.45	1.33
44	D	411	DGD	O1G-C1A	4.21	1.45	1.33
38	a	412	LMG	O8-C28	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	BB	623	DGD	O2G-C1B	4.21	1.46	1.34
38	Bb	620	LMG	O7-C10	4.21	1.46	1.34
36	II	101	LHG	O8-C23	4.20	1.45	1.33
38	WW	201	LMG	O8-C28	4.20	1.45	1.33
36	11	614	LHG	O7-C7	4.20	1.46	1.34
36	D	408	LHG	O8-C23	4.20	1.45	1.33
38	Bb	620	LMG	O8-C28	4.20	1.45	1.33
36	EE	101	LHG	O8-C23	4.20	1.45	1.33
36	K	101	LHG	O8-C23	4.19	1.45	1.33
38	c	519	LMG	O8-C28	4.19	1.45	1.33
35	d	404	PL9	C7-C3	4.19	1.55	1.51
36	33	614	LHG	O7-C7	4.19	1.46	1.34
36	1	614	LHG	O7-C7	4.19	1.46	1.34
44	Hh	102	DGD	O1G-C1A	4.19	1.45	1.33
36	0	201	LHG	O8-C23	4.18	1.45	1.33
36	SS	301	LHG	O7-C7	4.18	1.46	1.34
36	CC	521	LHG	O8-C23	4.18	1.45	1.33
38	DD	409	LMG	O7-C10	4.18	1.46	1.34
36	DD	407	LHG	O8-C23	4.18	1.45	1.33
36	A	411	LHG	O7-C7	4.18	1.46	1.34
36	a	414	LHG	O7-C7	4.18	1.46	1.34
44	C	523	DGD	O1G-C1A	4.18	1.45	1.33
38	Mm	101	LMG	O8-C28	4.17	1.45	1.33
38	F	101	LMG	O7-C10	4.17	1.46	1.34
38	b	620	LMG	O7-C10	4.17	1.46	1.34
36	K	101	LHG	O7-C7	4.17	1.46	1.34
36	N	619	LHG	O8-C23	4.17	1.45	1.33
36	Dd	407	LHG	O7-C7	4.16	1.46	1.34
36	l	101	LHG	O8-C23	4.16	1.45	1.33
36	d	405	LHG	O8-C23	4.16	1.45	1.33
36	A	411	LHG	O8-C23	4.16	1.45	1.33
44	CC	522	DGD	O1G-C1A	4.16	1.45	1.33
38	Cc	501	LMG	O8-C28	4.16	1.45	1.33
36	s	616	LHG	O7-C7	4.16	1.46	1.34
38	m	101	LMG	O8-C28	4.16	1.45	1.33
35	DD	406	PL9	C7-C3	4.16	1.55	1.51
36	BB	622	LHG	O8-C23	4.16	1.45	1.33
36	II	101	LHG	O7-C7	4.15	1.46	1.34
38	C	521	LMG	O8-C28	4.15	1.45	1.33
44	BB	623	DGD	O1G-C1A	4.15	1.45	1.33
36	C	522	LHG	O8-C23	4.15	1.45	1.33
38	AA	415	LMG	O7-C10	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	520	DGD	O1G-C1A	4.14	1.45	1.33
36	AA	411	LHG	O7-C7	4.14	1.46	1.34
36	AA	411	LHG	O8-C23	4.14	1.45	1.33
37	Ll	101	SQD	O47-C7	4.14	1.46	1.34
44	CC	518	DGD	O2G-C1B	4.14	1.46	1.34
36	A	413	LHG	O7-C7	4.14	1.46	1.34
36	JJ	101	LHG	O7-C7	4.14	1.46	1.34
35	D	407	PL9	C7-C3	4.14	1.55	1.51
38	A	415	LMG	O7-C10	4.14	1.46	1.34
37	l	102	SQD	O47-C7	4.13	1.46	1.34
38	Aa	412	LMG	O7-C10	4.13	1.46	1.34
44	C	520	DGD	O2G-C1B	4.13	1.45	1.34
38	CC	520	LMG	O7-C10	4.13	1.45	1.34
35	Dd	404	PL9	C7-C3	4.13	1.55	1.51
36	J	101	LHG	O8-C23	4.13	1.45	1.33
36	GG	618	LHG	O7-C7	4.12	1.45	1.34
36	Dd	405	LHG	O8-C23	4.12	1.45	1.33
36	d	406	LHG	O8-C23	4.12	1.45	1.33
44	Cc	519	DGD	O1G-C1A	4.12	1.45	1.33
36	AA	414	LHG	O8-C23	4.12	1.45	1.33
36	KK	101	LHG	O7-C7	4.12	1.45	1.34
36	A	413	LHG	O8-C23	4.12	1.45	1.33
36	Ss	616	LHG	O8-C23	4.12	1.45	1.33
36	D	408	LHG	O7-C7	4.12	1.45	1.34
36	Y	618	LHG	O7-C7	4.12	1.45	1.34
32	g	612	CLA	C1D-ND	4.12	1.42	1.37
36	JJ	101	LHG	O8-C23	4.11	1.45	1.33
32	GG	612	CLA	C1D-ND	4.11	1.42	1.37
36	y	320	LHG	O8-C23	4.11	1.45	1.33
44	c	517	DGD	O1G-C1A	4.11	1.45	1.33
36	A	414	LHG	O8-C23	4.10	1.45	1.33
36	g	618	LHG	O7-C7	4.10	1.45	1.34
44	D	411	DGD	O2G-C1B	4.10	1.45	1.34
36	YY	618	LHG	O8-C23	4.10	1.45	1.33
44	B	603	DGD	O2G-C1B	4.10	1.45	1.34
36	Ss	616	LHG	O7-C7	4.10	1.45	1.34
36	G	618	LHG	O7-C7	4.10	1.45	1.34
36	a	414	LHG	O8-C23	4.09	1.45	1.33
44	CC	519	DGD	O1G-C1A	4.09	1.45	1.33
44	CC	519	DGD	O2G-C1B	4.09	1.45	1.34
36	CC	521	LHG	O7-C7	4.09	1.45	1.34
36	DD	407	LHG	O7-C7	4.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	618	LHG	O8-C23	4.09	1.45	1.33
32	1	609	CLA	C1D-ND	4.09	1.42	1.37
36	Dd	406	LHG	O8-C23	4.09	1.45	1.33
38	a	412	LMG	O7-C10	4.08	1.45	1.34
36	Dd	407	LHG	O8-C23	4.08	1.45	1.33
37	B	617	SQD	O47-C7	4.08	1.45	1.34
36	3	614	LHG	O7-C7	4.08	1.45	1.34
32	r	610	CLA	C1D-ND	4.08	1.42	1.37
36	YY	618	LHG	O7-C7	4.08	1.45	1.34
36	Gg	319	LHG	O7-C7	4.08	1.45	1.34
36	CC	523	LHG	O7-C7	4.08	1.45	1.34
36	Yy	618	LHG	O8-C23	4.08	1.45	1.33
37	BB	621	SQD	O47-C7	4.07	1.45	1.34
36	d	406	LHG	O7-C7	4.07	1.45	1.34
44	Cc	520	DGD	O2G-C1B	4.07	1.45	1.34
36	d	405	LHG	O7-C7	4.07	1.45	1.34
37	C	501	SQD	O47-C7	4.06	1.45	1.34
36	C	522	LHG	O7-C7	4.06	1.45	1.34
37	AA	412	SQD	O47-C7	4.06	1.45	1.34
38	Dd	408	LMG	O7-C10	4.06	1.45	1.34
44	c	518	DGD	O2G-C1B	4.06	1.45	1.34
44	BB	625	DGD	O2G-C1B	4.05	1.45	1.34
38	B	615	LMG	O7-C10	4.05	1.45	1.34
38	j	101	LMG	O7-C10	4.05	1.45	1.34
36	Dd	405	LHG	O7-C7	4.05	1.45	1.34
37	B	602	SQD	O47-C7	4.05	1.45	1.34
44	C	523	DGD	O2G-C1B	4.04	1.45	1.34
36	D	409	LHG	O7-C7	4.04	1.45	1.34
37	L	102	SQD	O47-C7	4.04	1.45	1.34
36	l	101	LHG	O7-C7	4.04	1.45	1.34
32	r	601	CLA	C1D-ND	4.04	1.42	1.37
32	G	612	CLA	C1D-ND	4.04	1.42	1.37
37	LL	101	SQD	O47-C7	4.04	1.45	1.34
36	Dd	406	LHG	O7-C7	4.04	1.45	1.34
36	CC	523	LHG	O8-C23	4.04	1.45	1.33
36	D	410	LHG	O7-C7	4.03	1.45	1.34
37	L	101	SQD	O47-C7	4.03	1.45	1.34
32	S	608	CLA	C1D-ND	4.03	1.42	1.37
32	G	610	CLA	C1D-ND	4.03	1.42	1.37
38	c	519	LMG	O7-C10	4.02	1.45	1.34
37	Aa	413	SQD	O47-C7	4.02	1.45	1.34
37	LL	102	SQD	O47-C7	4.02	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Bb	621	LMG	O7-C10	4.02	1.45	1.34
37	CC	501	SQD	O47-C7	4.02	1.45	1.34
37	A	412	SQD	O47-C7	4.02	1.45	1.34
38	BB	619	LMG	O7-C10	4.02	1.45	1.34
38	Cc	501	LMG	O7-C10	4.01	1.45	1.34
39	4	306	CHL	C1D-ND	4.01	1.42	1.37
38	b	621	LMG	O7-C10	4.01	1.45	1.34
44	c	517	DGD	O2G-C1B	4.01	1.45	1.34
36	Ll	102	LHG	O7-C7	4.01	1.45	1.34
32	3	609	CLA	C1D-ND	4.01	1.42	1.37
32	Rr	601	CLA	C1D-ND	4.00	1.42	1.37
37	C	501	SQD	O48-C23	4.00	1.45	1.33
32	1	612	CLA	C1D-ND	4.00	1.42	1.37
36	DD	408	LHG	O8-C23	4.00	1.45	1.33
36	DD	408	LHG	O7-C7	4.00	1.45	1.34
32	YY	612	CLA	C1D-ND	3.99	1.42	1.37
32	Aa	406	CLA	C1D-ND	3.99	1.42	1.37
46	Ee	101	HEM	C3C-C2C	-3.99	1.34	1.40
37	CC	501	SQD	O48-C23	3.99	1.45	1.33
44	Cc	519	DGD	O2G-C1B	3.99	1.45	1.34
44	BB	624	DGD	O2G-C1B	3.99	1.45	1.34
36	D	409	LHG	O8-C23	3.98	1.45	1.33
32	G	611	CLA	C1D-ND	3.98	1.42	1.37
32	d	401	CLA	C1D-ND	3.98	1.42	1.37
38	C	521	LMG	O7-C10	3.97	1.45	1.34
32	Rr	602	CLA	C1D-ND	3.96	1.42	1.37
32	3	610	CLA	C1D-ND	3.96	1.42	1.37
44	B	601	DGD	O2G-C1B	3.96	1.45	1.34
32	33	609	CLA	C1D-ND	3.95	1.42	1.37
32	1	611	CLA	C1D-ND	3.95	1.42	1.37
32	11	604	CLA	C1D-ND	3.94	1.42	1.37
32	11	613	CLA	C1D-ND	3.94	1.42	1.37
32	1	603	CLA	C1D-ND	3.94	1.42	1.37
32	r	612	CLA	C1D-ND	3.94	1.42	1.37
32	R	614	CLA	C1D-ND	3.93	1.42	1.37
32	S	609	CLA	C1D-ND	3.92	1.42	1.37
32	22	610	CLA	C1D-ND	3.92	1.42	1.37
32	RR	312	CLA	C1D-ND	3.92	1.42	1.37
36	y	320	LHG	O7-C7	3.92	1.45	1.34
32	11	609	CLA	C1D-ND	3.91	1.42	1.37
32	Rr	610	CLA	C1D-ND	3.90	1.42	1.37
36	Yy	618	LHG	O7-C7	3.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	33	604	CLA	C1D-ND	3.90	1.42	1.37
32	3	604	CLA	C1D-ND	3.90	1.42	1.37
46	e	101	HEM	C3C-C2C	-3.88	1.35	1.40
32	S	603	CLA	C1D-ND	3.88	1.42	1.37
32	44	615	CLA	C1D-ND	3.88	1.42	1.37
32	g	611	CLA	C1D-ND	3.87	1.42	1.37
32	s	613	CLA	C1D-ND	3.87	1.42	1.37
32	22	602	CLA	C1D-ND	3.87	1.42	1.37
32	s	610	CLA	C1D-ND	3.87	1.42	1.37
32	2	610	CLA	C1D-ND	3.87	1.42	1.37
32	33	610	CLA	C1D-ND	3.87	1.42	1.37
32	GG	613	CLA	C1D-ND	3.86	1.42	1.37
32	2	612	CLA	C1D-ND	3.86	1.42	1.37
32	Ss	611	CLA	C1D-ND	3.86	1.42	1.37
32	3	612	CLA	C1D-ND	3.86	1.42	1.37
39	SS	306	CHL	C1D-ND	3.86	1.42	1.37
32	Gg	303	CLA	C4D-ND	-3.86	1.32	1.37
32	11	602	CLA	C1D-ND	3.86	1.42	1.37
39	2	608	CHL	C1D-ND	3.86	1.42	1.37
32	3	611	CLA	C1D-ND	3.86	1.42	1.37
32	Gg	314	CLA	C1D-ND	3.85	1.42	1.37
32	1	604	CLA	C1D-ND	3.85	1.42	1.37
32	1	613	CLA	C1D-ND	3.85	1.42	1.37
32	SS	309	CLA	C1D-ND	3.85	1.42	1.37
32	Ss	613	CLA	C1D-ND	3.85	1.42	1.37
32	Dd	401	CLA	C1D-ND	3.85	1.42	1.37
32	SS	310	CLA	C1D-ND	3.85	1.42	1.37
32	r	611	CLA	C1D-ND	3.84	1.42	1.37
32	r	609	CLA	C1D-ND	3.84	1.42	1.37
39	22	605	CHL	C1D-ND	3.84	1.42	1.37
39	1	605	CHL	C1D-ND	3.84	1.42	1.37
32	Ss	610	CLA	C1D-ND	3.83	1.42	1.37
32	n	610	CLA	C1D-ND	3.83	1.42	1.37
32	22	611	CLA	C1D-ND	3.83	1.42	1.37
32	2	611	CLA	C1D-ND	3.83	1.42	1.37
32	Rr	611	CLA	C1D-ND	3.82	1.42	1.37
32	11	611	CLA	C1D-ND	3.82	1.42	1.37
39	44	605	CHL	C1D-ND	3.82	1.42	1.37
39	Nn	319	CHL	C1D-ND	3.82	1.42	1.37
32	2	604	CLA	C1D-ND	3.82	1.42	1.37
32	Ss	603	CLA	C1D-ND	3.82	1.42	1.37
32	2	609	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	603	CLA	C1D-ND	3.81	1.42	1.37
32	33	611	CLA	C1D-ND	3.81	1.42	1.37
32	SS	313	CLA	C1D-ND	3.81	1.42	1.37
32	33	613	CLA	C1D-ND	3.80	1.42	1.37
32	3	602	CLA	C1D-ND	3.80	1.42	1.37
32	S	612	CLA	C1D-ND	3.80	1.42	1.37
32	c	511	CLA	C1D-ND	3.80	1.42	1.37
39	22	607	CHL	C1D-ND	3.80	1.42	1.37
32	Aa	410	CLA	C1D-ND	3.80	1.42	1.37
46	EE	102	HEM	C3C-CAC	3.80	1.55	1.47
32	44	610	CLA	C1D-ND	3.79	1.42	1.37
44	CC	522	DGD	O2G-C1B	3.79	1.45	1.34
32	3	603	CLA	C1D-ND	3.79	1.42	1.37
32	Ss	604	CLA	C1D-ND	3.79	1.42	1.37
32	Nn	303	CLA	C1D-ND	3.79	1.42	1.37
32	3	613	CLA	C1D-ND	3.79	1.42	1.37
32	33	612	CLA	C1D-ND	3.79	1.42	1.37
32	a	410	CLA	C1D-ND	3.79	1.42	1.37
39	22	608	CHL	C1D-ND	3.79	1.42	1.37
39	RR	306	CHL	C1D-ND	3.79	1.42	1.37
32	11	603	CLA	C1D-ND	3.78	1.42	1.37
32	2	602	CLA	C1D-ND	3.78	1.42	1.37
32	n	612	CLA	C1D-ND	3.78	1.42	1.37
32	R	613	CLA	C1D-ND	3.78	1.42	1.37
32	r	603	CLA	C1D-ND	3.78	1.42	1.37
32	R	612	CLA	C1D-ND	3.78	1.42	1.37
32	22	604	CLA	C1D-ND	3.78	1.42	1.37
32	R	601	CLA	C1D-ND	3.78	1.42	1.37
32	N	614	CLA	C1D-ND	3.78	1.42	1.37
39	2	601	CHL	C1D-ND	3.78	1.42	1.37
32	22	613	CLA	C1D-ND	3.77	1.42	1.37
32	33	603	CLA	C1D-ND	3.77	1.42	1.37
39	3	607	CHL	C1D-ND	3.77	1.42	1.37
32	22	609	CLA	C1D-ND	3.77	1.42	1.37
32	Cc	506	CLA	C1D-ND	3.77	1.42	1.37
32	1	610	CLA	C1D-ND	3.77	1.42	1.37
32	s	611	CLA	C1D-ND	3.77	1.42	1.37
32	Bb	615	CLA	C1D-ND	3.77	1.42	1.37
39	n	609	CHL	C1D-ND	3.77	1.42	1.37
32	RR	311	CLA	C1D-ND	3.77	1.42	1.37
46	e	101	HEM	C3C-CAC	3.77	1.55	1.47
39	2	605	CHL	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Rr	613	CLA	C1D-ND	3.76	1.42	1.37
32	YY	604	CLA	C1D-ND	3.76	1.42	1.37
39	G	609	CHL	C1D-ND	3.76	1.42	1.37
32	S	611	CLA	C1D-ND	3.76	1.42	1.37
46	Ee	101	HEM	C3C-CAC	3.76	1.55	1.47
32	Rr	612	CLA	C1D-ND	3.76	1.42	1.37
32	b	613	CLA	C1D-ND	3.76	1.42	1.37
32	r	602	CLA	C1D-ND	3.75	1.42	1.37
32	RR	308	CLA	C1D-ND	3.75	1.42	1.37
32	33	602	CLA	C1D-ND	3.75	1.42	1.37
32	s	604	CLA	C1D-ND	3.75	1.42	1.37
39	33	606	CHL	C1D-ND	3.75	1.42	1.37
32	N	612	CLA	C1D-ND	3.75	1.42	1.37
32	r	604	CLA	C1D-ND	3.75	1.42	1.37
32	SS	312	CLA	C1D-ND	3.75	1.42	1.37
32	Bb	613	CLA	C1D-ND	3.75	1.42	1.37
32	g	614	CLA	C1D-ND	3.74	1.42	1.37
32	RR	310	CLA	C1D-ND	3.74	1.42	1.37
39	22	606	CHL	C1D-ND	3.74	1.42	1.37
32	22	603	CLA	C1D-ND	3.74	1.42	1.37
42	NN	618	NEX	C7-C8	-3.74	1.25	1.32
32	R	610	CLA	C1D-ND	3.74	1.42	1.37
32	NN	614	CLA	C1D-ND	3.74	1.42	1.37
32	CC	505	CLA	C1D-ND	3.74	1.42	1.37
32	GG	610	CLA	C1D-ND	3.74	1.42	1.37
32	1	602	CLA	C1D-ND	3.74	1.42	1.37
32	Rr	604	CLA	C1D-ND	3.73	1.42	1.37
32	Gg	313	CLA	C1D-ND	3.73	1.42	1.37
32	R	608	CLA	C1D-ND	3.73	1.42	1.37
39	2	607	CHL	C1D-ND	3.73	1.42	1.37
32	Nn	305	CLA	C1D-ND	3.73	1.42	1.37
32	Y	604	CLA	C1D-ND	3.73	1.42	1.37
39	11	606	CHL	C1D-ND	3.73	1.42	1.37
32	b	615	CLA	C1D-ND	3.73	1.42	1.37
39	11	601	CHL	C1D-ND	3.72	1.42	1.37
39	1	606	CHL	C1D-ND	3.72	1.42	1.37
32	44	603	CLA	C1D-ND	3.72	1.42	1.37
39	Y	609	CHL	C1D-ND	3.72	1.42	1.37
39	s	607	CHL	C1D-ND	3.72	1.42	1.37
32	s	603	CLA	C1D-ND	3.72	1.42	1.37
32	RR	302	CLA	C1D-ND	3.72	1.42	1.37
32	Cc	513	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	605	CHL	C1D-ND	3.72	1.42	1.37
32	R	611	CLA	C1D-ND	3.72	1.42	1.37
32	a	407	CLA	C1D-ND	3.72	1.42	1.37
32	N	610	CLA	C1D-ND	3.72	1.42	1.37
32	SS	311	CLA	C1D-ND	3.72	1.42	1.37
32	C	511	CLA	C1D-ND	3.71	1.42	1.37
32	b	601	CLA	C1D-ND	3.71	1.42	1.37
32	Rr	603	CLA	C1D-ND	3.71	1.42	1.37
32	g	603	CLA	C1D-ND	3.71	1.42	1.37
32	r	608	CLA	C1D-ND	3.71	1.42	1.37
39	Ss	605	CHL	C1D-ND	3.71	1.42	1.37
32	4	304	CLA	C1D-ND	3.71	1.42	1.37
32	S	613	CLA	C1D-ND	3.71	1.42	1.37
32	n	614	CLA	C1D-ND	3.71	1.42	1.37
32	RR	313	CLA	C1D-ND	3.71	1.42	1.37
32	g	602	CLA	C1D-ND	3.71	1.42	1.37
32	RR	314	CLA	C1D-ND	3.71	1.42	1.37
32	Aa	405	CLA	C1D-ND	3.71	1.42	1.37
46	E	101	HEM	C3C-CAC	3.71	1.55	1.47
32	Rr	609	CLA	C1D-ND	3.71	1.42	1.37
32	n	604	CLA	C1D-ND	3.71	1.42	1.37
39	11	607	CHL	C1D-ND	3.71	1.42	1.37
39	22	601	CHL	C1D-ND	3.71	1.42	1.37
32	b	606	CLA	C1D-ND	3.70	1.42	1.37
39	1	607	CHL	C1D-ND	3.70	1.42	1.37
39	n	607	CHL	C1D-ND	3.70	1.42	1.37
32	44	611	CLA	C1D-ND	3.70	1.42	1.37
32	2	613	CLA	C1D-ND	3.70	1.42	1.37
32	Bb	603	CLA	C1D-ND	3.70	1.42	1.37
39	SS	306	CHL	CHC-C1C	3.70	1.44	1.35
32	Nn	302	CLA	C1D-ND	3.70	1.42	1.37
42	N	618	NEX	C7-C8	-3.70	1.25	1.32
32	Ss	602	CLA	C1D-ND	3.70	1.42	1.37
39	2	606	CHL	C1D-ND	3.70	1.42	1.37
32	G	603	CLA	C1D-ND	3.70	1.42	1.37
32	Gg	315	CLA	C1D-ND	3.70	1.42	1.37
39	33	607	CHL	C1D-ND	3.70	1.42	1.37
32	c	510	CLA	C1D-ND	3.70	1.42	1.37
32	Cc	512	CLA	C1D-ND	3.70	1.42	1.37
32	B	604	CLA	C1D-ND	3.69	1.42	1.37
39	3	606	CHL	C1D-ND	3.69	1.42	1.37
39	S	607	CHL	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	613	CLA	C1D-ND	3.69	1.42	1.37
39	SS	308	CHL	C1D-ND	3.69	1.42	1.37
32	G	614	CLA	C1D-ND	3.69	1.42	1.37
32	GG	614	CLA	C1D-ND	3.69	1.42	1.37
32	BB	608	CLA	C1D-ND	3.69	1.42	1.37
32	22	612	CLA	C1D-ND	3.69	1.42	1.37
32	C	508	CLA	C1D-ND	3.69	1.42	1.37
39	Ss	607	CHL	C1D-ND	3.69	1.42	1.37
32	11	610	CLA	C1D-ND	3.69	1.42	1.37
32	BB	612	CLA	C1D-ND	3.69	1.42	1.37
32	A	408	CLA	C1D-ND	3.69	1.42	1.37
32	C	515	CLA	C1D-ND	3.69	1.42	1.37
32	y	304	CLA	C1D-ND	3.69	1.42	1.37
32	Cc	510	CLA	C1D-ND	3.68	1.42	1.37
32	S	604	CLA	C1D-ND	3.68	1.42	1.37
32	s	608	CLA	C1D-ND	3.68	1.42	1.37
32	NN	612	CLA	C1D-ND	3.68	1.42	1.37
32	SS	304	CLA	C1D-ND	3.68	1.42	1.37
32	g	604	CLA	C1D-ND	3.68	1.42	1.37
32	SS	314	CLA	C1D-ND	3.68	1.42	1.37
32	4	311	CLA	C1D-ND	3.68	1.42	1.37
39	S	605	CHL	C1D-ND	3.68	1.42	1.37
32	SS	305	CLA	C1D-ND	3.68	1.42	1.37
32	Gg	304	CLA	C1D-ND	3.68	1.42	1.37
32	C	509	CLA	C1D-ND	3.68	1.42	1.37
32	y	305	CLA	C1D-ND	3.67	1.42	1.37
32	4	312	CLA	C1D-ND	3.67	1.42	1.37
32	CC	514	CLA	C1D-ND	3.67	1.42	1.37
32	Gg	312	CLA	C1D-ND	3.67	1.42	1.37
32	n	611	CLA	C1D-ND	3.67	1.42	1.37
32	Bb	604	CLA	C1D-ND	3.67	1.42	1.37
32	Bb	601	CLA	C1D-ND	3.67	1.42	1.37
32	B	609	CLA	C1D-ND	3.66	1.42	1.37
39	33	605	CHL	C1D-ND	3.66	1.42	1.37
39	Ss	606	CHL	C1D-ND	3.66	1.42	1.37
32	c	513	CLA	C1D-ND	3.66	1.42	1.37
32	BB	609	CLA	C1D-ND	3.66	1.42	1.37
32	C	506	CLA	C1D-ND	3.66	1.42	1.37
32	b	603	CLA	C1D-ND	3.66	1.42	1.37
32	N	602	CLA	C1D-ND	3.66	1.42	1.37
32	g	610	CLA	C1D-ND	3.66	1.42	1.37
32	Gg	311	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Rr	608	CLA	C1D-ND	3.66	1.42	1.37
32	YY	602	CLA	C1D-ND	3.66	1.42	1.37
32	G	602	CLA	C1D-ND	3.66	1.42	1.37
32	Y	614	CLA	C1D-ND	3.65	1.42	1.37
39	11	605	CHL	C1D-ND	3.65	1.42	1.37
32	B	608	CLA	C1D-ND	3.65	1.42	1.37
39	s	606	CHL	C1D-ND	3.65	1.42	1.37
32	G	613	CLA	C1D-ND	3.65	1.42	1.37
32	C	512	CLA	C1D-ND	3.65	1.42	1.37
32	CC	508	CLA	C1D-ND	3.65	1.42	1.37
32	CC	510	CLA	C1D-ND	3.65	1.42	1.37
32	GG	604	CLA	C1D-ND	3.65	1.42	1.37
32	Nn	312	CLA	C1D-ND	3.65	1.42	1.37
39	g	607	CHL	C1D-ND	3.65	1.42	1.37
32	4	310	CLA	C1D-ND	3.64	1.42	1.37
32	B	623	CLA	C1D-ND	3.64	1.42	1.37
32	Bb	606	CLA	C1D-ND	3.64	1.42	1.37
32	a	406	CLA	C1D-ND	3.64	1.42	1.37
32	c	508	CLA	C1D-ND	3.64	1.42	1.37
32	NN	610	CLA	C1D-ND	3.64	1.42	1.37
39	R	607	CHL	C1D-ND	3.64	1.42	1.37
32	Cc	515	CLA	C1D-ND	3.64	1.42	1.37
32	Yy	602	CLA	C1D-ND	3.64	1.42	1.37
39	3	601	CHL	C1D-ND	3.64	1.42	1.37
32	Bb	616	CLA	C1D-ND	3.64	1.42	1.37
32	Cc	504	CLA	C1D-ND	3.64	1.42	1.37
32	Ss	609	CLA	C1D-ND	3.64	1.42	1.37
32	s	609	CLA	C1D-ND	3.64	1.42	1.37
32	CC	507	CLA	C1D-ND	3.64	1.42	1.37
32	c	504	CLA	C1D-ND	3.64	1.42	1.37
32	Yy	603	CLA	C1D-ND	3.64	1.42	1.37
32	C	510	CLA	C1D-ND	3.64	1.42	1.37
32	RR	303	CLA	C1D-ND	3.64	1.42	1.37
32	Bb	607	CLA	C1D-ND	3.63	1.42	1.37
39	G	608	CHL	C1D-ND	3.63	1.42	1.37
39	1	601	CHL	C1D-ND	3.63	1.42	1.37
32	Ss	608	CLA	C1D-ND	3.63	1.42	1.37
32	c	512	CLA	C1D-ND	3.63	1.42	1.37
32	4	305	CLA	C1D-ND	3.63	1.42	1.37
32	c	501	CLA	C1D-ND	3.62	1.42	1.37
32	c	503	CLA	C1D-ND	3.62	1.42	1.37
39	r	606	CHL	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	610	CLA	C1D-ND	3.62	1.42	1.37
32	Y	612	CLA	C1D-ND	3.62	1.42	1.37
39	1	608	CHL	C1D-ND	3.62	1.42	1.37
39	3	608	CHL	C1D-ND	3.62	1.42	1.37
32	4	303	CLA	C1D-ND	3.62	1.42	1.37
32	BB	601	CLA	C1D-ND	3.62	1.42	1.37
32	CC	511	CLA	C1D-ND	3.62	1.42	1.37
42	YY	617	NEX	C7-C8	-3.62	1.25	1.32
32	CC	512	CLA	C1D-ND	3.62	1.42	1.37
32	a	405	CLA	C1D-ND	3.61	1.42	1.37
32	b	611	CLA	C1D-ND	3.61	1.42	1.37
32	AA	408	CLA	C1D-ND	3.61	1.42	1.37
32	S	602	CLA	C1D-ND	3.61	1.42	1.37
39	G	605	CHL	C1D-ND	3.61	1.42	1.37
32	YY	612	CLA	C4D-ND	-3.61	1.32	1.37
32	C	514	CLA	C1D-ND	3.61	1.42	1.37
32	GG	603	CLA	C1D-ND	3.61	1.42	1.37
32	NN	604	CLA	C1D-ND	3.61	1.42	1.37
42	Y	617	NEX	C7-C8	-3.61	1.26	1.32
32	B	618	CLA	C1D-ND	3.61	1.42	1.37
32	g	613	CLA	C1D-ND	3.61	1.42	1.37
32	d	402	CLA	C1D-ND	3.61	1.42	1.37
39	S	606	CHL	C1D-ND	3.61	1.42	1.37
39	4	302	CHL	C1D-ND	3.61	1.42	1.37
32	Y	603	CLA	C1D-ND	3.60	1.42	1.37
32	c	502	CLA	C1D-ND	3.60	1.42	1.37
32	YY	614	CLA	C1D-ND	3.60	1.42	1.37
39	11	608	CHL	C1D-ND	3.60	1.42	1.37
39	GG	607	CHL	C1D-ND	3.60	1.42	1.37
32	D	405	CLA	C1D-ND	3.60	1.42	1.37
39	44	601	CHL	C1D-ND	3.60	1.42	1.37
32	b	616	CLA	C1D-ND	3.60	1.42	1.37
32	Nn	314	CLA	C1D-ND	3.60	1.42	1.37
39	GG	609	CHL	C1D-ND	3.60	1.42	1.37
32	Yy	612	CLA	C1D-ND	3.60	1.42	1.37
32	R	609	CLA	C1D-ND	3.60	1.42	1.37
32	44	609	CLA	C1D-ND	3.60	1.42	1.37
32	b	607	CLA	C1D-ND	3.60	1.42	1.37
32	s	612	CLA	C1D-ND	3.60	1.42	1.37
32	CC	509	CLA	C1D-ND	3.60	1.42	1.37
32	Cc	509	CLA	C1D-ND	3.60	1.42	1.37
39	r	607	CHL	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	610	CLA	C1D-ND	3.60	1.42	1.37
39	33	601	CHL	C1D-ND	3.59	1.42	1.37
32	BB	613	CLA	C1D-ND	3.59	1.42	1.37
32	Cc	503	CLA	C1D-ND	3.59	1.42	1.37
32	D	404	CLA	C1D-ND	3.59	1.42	1.37
32	b	614	CLA	C1D-ND	3.59	1.42	1.37
39	s	605	CHL	C1D-ND	3.59	1.42	1.37
32	N	604	CLA	C1D-ND	3.59	1.42	1.37
39	N	605	CHL	C1D-ND	3.59	1.42	1.37
39	RR	307	CHL	C1D-ND	3.59	1.42	1.37
39	y	311	CHL	C1D-ND	3.59	1.42	1.37
32	Yy	614	CLA	C1D-ND	3.59	1.42	1.37
32	Bb	614	CLA	C1D-ND	3.59	1.42	1.37
39	n	605	CHL	C1D-ND	3.59	1.42	1.37
39	Y	605	CHL	C1D-ND	3.59	1.42	1.37
39	Yy	605	CHL	C1D-ND	3.59	1.42	1.37
39	GG	608	CHL	C1D-ND	3.59	1.42	1.37
32	s	602	CLA	C1D-ND	3.58	1.42	1.37
32	RR	304	CLA	C1D-ND	3.58	1.42	1.37
32	X	201	CLA	C1D-ND	3.58	1.42	1.37
32	R	603	CLA	C1D-ND	3.58	1.42	1.37
32	Cc	511	CLA	C1D-ND	3.58	1.42	1.37
39	n	606	CHL	C1D-ND	3.58	1.42	1.37
32	Cc	514	CLA	C1D-ND	3.58	1.42	1.37
32	S	610	CLA	C1D-ND	3.58	1.42	1.37
32	y	312	CLA	C1D-ND	3.58	1.42	1.37
32	B	605	CLA	C1D-ND	3.58	1.42	1.37
32	y	314	CLA	C1D-ND	3.58	1.42	1.37
39	4	309	CHL	CHC-C1C	3.58	1.44	1.35
32	R	604	CLA	C1D-ND	3.58	1.42	1.37
32	c	506	CLA	C1D-ND	3.58	1.42	1.37
32	Aa	407	CLA	C1D-ND	3.58	1.42	1.37
39	Gg	308	CHL	C1D-ND	3.58	1.42	1.37
32	b	610	CLA	C1D-ND	3.57	1.42	1.37
39	Ss	601	CHL	C1D-ND	3.57	1.42	1.37
39	GG	605	CHL	C1D-ND	3.57	1.42	1.37
32	XX	201	CLA	C1D-ND	3.57	1.42	1.37
39	33	608	CHL	C1D-ND	3.57	1.42	1.37
39	G	607	CHL	C1D-ND	3.57	1.42	1.37
32	R	602	CLA	C1D-ND	3.57	1.42	1.37
32	RR	309	CLA	C1D-ND	3.57	1.42	1.37
39	YY	609	CHL	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Nn	311	CHL	C1D-ND	3.57	1.42	1.37
32	Bb	611	CLA	C1D-ND	3.57	1.42	1.37
39	44	608	CHL	C1D-ND	3.57	1.42	1.37
39	Y	607	CHL	C1D-ND	3.57	1.42	1.37
39	r	605	CHL	C1D-ND	3.57	1.42	1.37
39	s	607	CHL	CHC-C1C	3.57	1.44	1.35
32	G	604	CLA	C1D-ND	3.57	1.42	1.37
32	N	611	CLA	C1D-ND	3.57	1.42	1.37
39	Yy	607	CHL	C1D-ND	3.57	1.42	1.37
39	SS	307	CHL	C1D-ND	3.57	1.42	1.37
42	Y	619	NEX	C7-C8	-3.57	1.26	1.32
32	Ss	612	CLA	C1D-ND	3.57	1.42	1.37
32	y	316	CLA	C1D-ND	3.57	1.42	1.37
32	CC	504	CLA	C1D-ND	3.56	1.42	1.37
32	Gg	303	CLA	C1D-ND	3.56	1.42	1.37
32	YY	610	CLA	C1D-ND	3.56	1.42	1.37
32	Gg	305	CLA	C1D-ND	3.56	1.42	1.37
32	c	509	CLA	C1D-ND	3.56	1.42	1.37
32	Bb	609	CLA	C1D-ND	3.56	1.42	1.37
39	s	601	CHL	C1D-ND	3.56	1.42	1.37
32	b	605	CLA	C1D-ND	3.56	1.42	1.37
39	N	607	CHL	C1D-ND	3.56	1.42	1.37
39	Nn	317	CHL	C1D-ND	3.56	1.42	1.37
39	Nn	318	CHL	C1D-ND	3.56	1.42	1.37
32	BB	606	CLA	C1D-ND	3.55	1.42	1.37
39	Rr	606	CHL	C1D-ND	3.55	1.42	1.37
39	Gg	306	CHL	C1D-ND	3.55	1.42	1.37
39	Nn	315	CHL	C1D-ND	3.55	1.42	1.37
32	44	604	CLA	C1D-ND	3.55	1.42	1.37
32	Dd	402	CLA	C1D-ND	3.55	1.42	1.37
39	S	601	CHL	C1D-ND	3.55	1.42	1.37
32	C	505	CLA	C1D-ND	3.55	1.42	1.37
32	y	306	CLA	C1D-ND	3.55	1.42	1.37
39	YY	605	CHL	C1D-ND	3.55	1.42	1.37
32	YY	603	CLA	C1D-ND	3.55	1.42	1.37
39	GG	606	CHL	C1D-ND	3.55	1.42	1.37
32	Nn	301	CLA	C1D-ND	3.55	1.42	1.37
32	a	406	CLA	C4D-ND	-3.54	1.32	1.37
39	Ss	606	CHL	CHC-C1C	3.54	1.44	1.35
32	B	606	CLA	C1D-ND	3.54	1.42	1.37
32	Bb	605	CLA	C1D-ND	3.54	1.42	1.37
39	g	608	CHL	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	SS	303	CLA	C1D-ND	3.54	1.42	1.37
42	g	617	NEX	C7-C8	-3.54	1.26	1.32
32	BB	615	CLA	C1D-ND	3.54	1.42	1.37
39	Nn	316	CHL	C1D-ND	3.54	1.42	1.37
32	B	619	CLA	C1D-ND	3.54	1.42	1.37
32	C	513	CLA	C1D-ND	3.54	1.42	1.37
42	Nn	309	NEX	C7-C8	-3.54	1.26	1.32
39	Gg	307	CHL	C1D-ND	3.53	1.42	1.37
42	n	617	NEX	C7-C8	-3.53	1.26	1.32
32	Bb	610	CLA	C1D-ND	3.53	1.42	1.37
32	Bb	612	CLA	C1D-ND	3.53	1.42	1.37
39	r	606	CHL	CHC-C1C	3.53	1.44	1.35
32	BB	605	CLA	C1D-ND	3.53	1.42	1.37
32	GG	602	CLA	C1D-ND	3.53	1.42	1.37
39	SS	302	CHL	C1D-ND	3.53	1.42	1.37
32	Yy	610	CLA	C1D-ND	3.53	1.42	1.37
32	CC	513	CLA	C1D-ND	3.53	1.42	1.37
32	c	507	CLA	C1D-ND	3.53	1.42	1.37
39	G	606	CHL	C1D-ND	3.52	1.42	1.37
39	g	605	CHL	CHC-C1C	3.52	1.44	1.35
32	C	504	CLA	C1D-ND	3.52	1.42	1.37
32	C	503	CLA	C1D-ND	3.52	1.42	1.37
32	Yy	604	CLA	C1D-ND	3.52	1.42	1.37
39	Gg	309	CHL	C1D-ND	3.52	1.42	1.37
39	G	601	CHL	C1D-ND	3.52	1.42	1.37
32	n	602	CLA	C1D-ND	3.52	1.42	1.37
32	Cc	508	CLA	C1D-ND	3.52	1.42	1.37
32	Cc	507	CLA	C1D-ND	3.52	1.42	1.37
32	NN	602	CLA	C1D-ND	3.52	1.42	1.37
32	Y	602	CLA	C1D-ND	3.52	1.42	1.37
39	GG	601	CHL	C1D-ND	3.52	1.42	1.37
39	Rr	605	CHL	CHC-C1C	3.52	1.44	1.35
32	n	603	CLA	C1D-ND	3.51	1.42	1.37
39	N	606	CHL	CHC-C1C	3.51	1.44	1.35
39	Gg	306	CHL	CHC-C1C	3.51	1.44	1.35
32	44	602	CLA	C1D-ND	3.51	1.42	1.37
39	NN	607	CHL	C1D-ND	3.51	1.42	1.37
39	n	608	CHL	C1D-ND	3.51	1.42	1.37
39	G	605	CHL	CHC-C1C	3.51	1.44	1.35
32	CC	502	CLA	C1D-ND	3.51	1.42	1.37
39	44	606	CHL	C1D-ND	3.51	1.42	1.37
39	g	609	CHL	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	401	CLA	C1D-ND	3.51	1.42	1.37
39	g	601	CHL	C1D-ND	3.51	1.42	1.37
32	b	609	CLA	C1D-ND	3.51	1.42	1.37
42	RR	317	NEX	C7-C8	-3.51	1.26	1.32
39	4	308	CHL	C1D-ND	3.50	1.42	1.37
39	y	309	CHL	C1D-ND	3.50	1.42	1.37
32	DD	403	CLA	C1D-ND	3.50	1.42	1.37
39	N	601	CHL	C1D-ND	3.50	1.42	1.37
39	Rr	607	CHL	C1D-ND	3.50	1.42	1.37
39	YY	607	CHL	C1D-ND	3.50	1.42	1.37
39	s	606	CHL	CHC-C1C	3.50	1.43	1.35
39	y	307	CHL	C1D-ND	3.50	1.42	1.37
32	NN	611	CLA	C1D-ND	3.50	1.42	1.37
32	g	602	CLA	C4D-ND	-3.50	1.32	1.37
32	B	620	CLA	C1D-ND	3.49	1.42	1.37
39	SS	308	CHL	CHC-C1C	3.49	1.43	1.35
32	b	604	CLA	C1D-ND	3.49	1.42	1.37
39	4	307	CHL	C1D-ND	3.49	1.42	1.37
39	4	307	CHL	CHC-C1C	3.49	1.43	1.35
32	B	611	CLA	C1D-ND	3.49	1.42	1.37
32	Nn	304	CLA	C1D-ND	3.49	1.42	1.37
39	Yy	609	CHL	C1D-ND	3.49	1.42	1.37
32	Nn	313	CLA	C1D-ND	3.49	1.42	1.37
39	g	605	CHL	C1D-ND	3.49	1.42	1.37
32	Cc	505	CLA	C1D-ND	3.49	1.42	1.37
39	2	605	CHL	CHC-C1C	3.49	1.43	1.35
32	DD	404	CLA	C1D-ND	3.48	1.42	1.37
32	B	622	CLA	C1D-ND	3.48	1.42	1.37
32	NN	613	CLA	C1D-ND	3.48	1.42	1.37
39	22	605	CHL	CHC-C1C	3.48	1.43	1.35
39	33	607	CHL	CHC-C1C	3.48	1.43	1.35
32	BB	614	CLA	C1D-ND	3.48	1.42	1.37
39	Ss	607	CHL	CHC-C1C	3.48	1.43	1.35
32	n	613	CLA	C1D-ND	3.48	1.42	1.37
32	BB	603	CLA	C1D-ND	3.48	1.42	1.37
42	Rr	616	NEX	C7-C8	-3.48	1.26	1.32
39	NN	606	CHL	CHC-C1C	3.48	1.43	1.35
39	YY	606	CHL	CHC-C1C	3.48	1.43	1.35
32	B	610	CLA	C1D-ND	3.47	1.42	1.37
39	g	606	CHL	C1D-ND	3.47	1.42	1.37
39	N	606	CHL	C1D-ND	3.47	1.42	1.37
39	Gg	310	CHL	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	310	CHL	C1D-ND	3.47	1.42	1.37
32	Y	611	CLA	C1D-ND	3.47	1.42	1.37
42	y	319	NEX	C7-C8	-3.47	1.26	1.32
32	A	406	CLA	C1D-ND	3.47	1.42	1.37
32	y	315	CLA	C1D-ND	3.47	1.42	1.37
39	R	606	CHL	C1D-ND	3.47	1.42	1.37
39	Rr	606	CHL	CHC-C1C	3.47	1.43	1.35
39	44	608	CHL	CHC-C1C	3.47	1.43	1.35
39	GG	608	CHL	CHC-C1C	3.47	1.43	1.35
39	44	606	CHL	CHC-C1C	3.47	1.43	1.35
32	b	612	CLA	C1D-ND	3.47	1.42	1.37
32	DD	401	CLA	C1D-ND	3.47	1.42	1.37
32	AA	405	CLA	C1D-ND	3.46	1.42	1.37
39	N	608	CHL	C1D-ND	3.46	1.42	1.37
39	33	601	CHL	CHC-C1C	3.46	1.43	1.35
42	R	617	NEX	C7-C8	-3.46	1.26	1.32
32	c	505	CLA	C1D-ND	3.46	1.42	1.37
39	Nn	318	CHL	CHC-C1C	3.46	1.43	1.35
39	Y	606	CHL	C1D-ND	3.46	1.42	1.37
39	NN	601	CHL	C1D-ND	3.46	1.42	1.37
32	B	624	CLA	C1D-ND	3.46	1.42	1.37
32	Aa	406	CLA	C4D-ND	-3.46	1.32	1.37
32	A	405	CLA	C1D-ND	3.46	1.42	1.37
32	C	507	CLA	C1D-ND	3.46	1.42	1.37
39	YY	606	CHL	C1D-ND	3.46	1.42	1.37
39	G	608	CHL	CHC-C1C	3.46	1.43	1.35
39	Yy	608	CHL	C1D-ND	3.45	1.42	1.37
32	BB	602	CLA	C1D-ND	3.45	1.42	1.37
32	Y	613	CLA	C4D-ND	-3.45	1.33	1.37
39	1	606	CHL	CHC-C1C	3.45	1.43	1.35
39	SS	302	CHL	CHC-C1C	3.45	1.43	1.35
39	NN	608	CHL	C1D-ND	3.45	1.42	1.37
39	S	607	CHL	CHC-C1C	3.45	1.43	1.35
32	Yy	611	CLA	C1D-ND	3.44	1.42	1.37
39	4	302	CHL	CHC-C1C	3.44	1.43	1.35
32	Yy	613	CLA	C1D-ND	3.44	1.42	1.37
39	G	606	CHL	CHC-C1C	3.44	1.43	1.35
39	Nn	316	CHL	CHC-C1C	3.44	1.43	1.35
39	44	601	CHL	CHC-C1C	3.44	1.43	1.35
39	11	607	CHL	CHC-C1C	3.44	1.43	1.35
39	S	601	CHL	CHC-C1C	3.44	1.43	1.35
32	11	612	CLA	C1D-ND	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	11	606	CHL	CHC-C1C	3.44	1.43	1.35
32	y	313	CLA	C1D-ND	3.44	1.42	1.37
32	Yy	613	CLA	C4D-ND	-3.43	1.33	1.37
39	3	601	CHL	CHC-C1C	3.43	1.43	1.35
39	NN	605	CHL	C1D-ND	3.43	1.42	1.37
32	N	613	CLA	C4D-ND	-3.43	1.33	1.37
39	YY	608	CHL	C1D-ND	3.43	1.42	1.37
32	BB	604	CLA	C1D-ND	3.43	1.42	1.37
39	r	605	CHL	CHC-C1C	3.43	1.43	1.35
39	n	608	CHL	CHC-C1C	3.43	1.43	1.35
39	44	605	CHL	CHC-C1C	3.43	1.43	1.35
39	g	607	CHL	CHC-C1C	3.43	1.43	1.35
32	NN	613	CLA	C4D-ND	-3.42	1.33	1.37
39	44	607	CHL	CHC-C1C	3.42	1.43	1.35
39	3	607	CHL	CHC-C1C	3.42	1.43	1.35
39	SS	307	CHL	CHC-C1C	3.42	1.43	1.35
39	4	308	CHL	CHC-C1C	3.42	1.43	1.35
39	NN	609	CHL	CHC-C1C	3.42	1.43	1.35
39	Y	606	CHL	CHC-C1C	3.42	1.43	1.35
32	CC	503	CLA	C1D-ND	3.42	1.42	1.37
39	NN	608	CHL	CHC-C1C	3.42	1.43	1.35
39	Yy	601	CHL	C1D-ND	3.42	1.42	1.37
39	y	308	CHL	C1D-ND	3.42	1.42	1.37
39	R	606	CHL	CHC-C1C	3.42	1.43	1.35
39	3	605	CHL	CHC-C1C	3.42	1.43	1.35
39	44	607	CHL	C1D-ND	3.42	1.42	1.37
32	b	602	CLA	C1D-ND	3.42	1.42	1.37
39	22	608	CHL	CHC-C1C	3.42	1.43	1.35
32	Bb	602	CLA	C1D-ND	3.42	1.42	1.37
39	YY	607	CHL	CHC-C1C	3.42	1.43	1.35
39	1	607	CHL	CHC-C1C	3.41	1.43	1.35
32	BB	607	CLA	C1D-ND	3.41	1.42	1.37
39	N	608	CHL	CHC-C1C	3.41	1.43	1.35
39	GG	605	CHL	CHC-C1C	3.41	1.43	1.35
39	R	605	CHL	CHC-C1C	3.40	1.43	1.35
39	33	605	CHL	CHC-C1C	3.40	1.43	1.35
39	Y	608	CHL	C1D-ND	3.40	1.42	1.37
39	N	609	CHL	CHC-C1C	3.40	1.43	1.35
32	Y	613	CLA	C1D-ND	3.40	1.42	1.37
39	Ss	601	CHL	CHC-C1C	3.40	1.43	1.35
39	Rr	607	CHL	CHC-C1C	3.40	1.43	1.35
39	GG	606	CHL	CHC-C1C	3.40	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AA	406	CLA	C1D-ND	3.40	1.42	1.37
32	BB	611	CLA	C1D-ND	3.40	1.42	1.37
39	22	606	CHL	CHC-C1C	3.40	1.43	1.35
39	2	606	CHL	CHC-C1C	3.40	1.43	1.35
39	Y	608	CHL	CHC-C1C	3.40	1.43	1.35
39	g	609	CHL	CHC-C1C	3.39	1.43	1.35
39	4	309	CHL	C1D-ND	3.39	1.42	1.37
32	Bb	608	CLA	C1D-ND	3.39	1.42	1.37
39	2	607	CHL	CHC-C1C	3.39	1.43	1.35
32	YY	613	CLA	C1D-ND	3.39	1.42	1.37
32	B	621	CLA	C1D-ND	3.39	1.41	1.37
42	Yy	617	NEX	C7-C8	-3.39	1.26	1.32
32	N	613	CLA	C1D-ND	3.39	1.41	1.37
32	G	602	CLA	C4D-ND	-3.39	1.33	1.37
39	s	601	CHL	CHC-C1C	3.39	1.43	1.35
32	AA	406	CLA	C4D-ND	-3.38	1.33	1.37
39	g	606	CHL	CHC-C1C	3.38	1.43	1.35
39	r	607	CHL	CHC-C1C	3.38	1.43	1.35
36	4	301	LHG	O7-C5	-3.38	1.42	1.46
39	R	607	CHL	CHC-C1C	3.38	1.43	1.35
39	Gg	302	CHL	CHC-C1C	3.38	1.43	1.35
39	RR	305	CHL	CHC-C1C	3.38	1.43	1.35
39	Gg	307	CHL	CHC-C1C	3.38	1.43	1.35
39	Rr	605	CHL	C1D-ND	3.38	1.41	1.37
39	Y	607	CHL	CHC-C1C	3.38	1.43	1.35
39	NN	609	CHL	C1D-ND	3.37	1.41	1.37
39	y	308	CHL	CHC-C1C	3.37	1.43	1.35
32	DD	401	CLA	C4D-ND	-3.37	1.33	1.37
39	S	605	CHL	CHC-C1C	3.37	1.43	1.35
39	NN	606	CHL	C1D-ND	3.37	1.41	1.37
39	33	608	CHL	CHC-C1C	3.37	1.43	1.35
39	Gg	309	CHL	CHC-C1C	3.37	1.43	1.35
39	S	606	CHL	CHC-C1C	3.36	1.43	1.35
39	Yy	609	CHL	CHC-C1C	3.36	1.43	1.35
36	44	616	LHG	O7-C5	-3.36	1.42	1.46
32	CC	506	CLA	C1D-ND	3.36	1.41	1.37
39	YY	608	CHL	CHC-C1C	3.36	1.43	1.35
39	Nn	315	CHL	CHC-C1C	3.36	1.43	1.35
32	YY	613	CLA	C4D-ND	-3.36	1.33	1.37
39	Gg	308	CHL	CHC-C1C	3.36	1.43	1.35
32	b	608	CLA	C1D-ND	3.36	1.41	1.37
32	Ss	609	CLA	C4D-ND	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	22	601	CHL	CHC-C1C	3.36	1.43	1.35
39	y	303	CHL	C1D-ND	3.36	1.41	1.37
39	n	606	CHL	CHC-C1C	3.35	1.43	1.35
32	y	315	CLA	C4D-ND	-3.35	1.33	1.37
39	3	606	CHL	CHC-C1C	3.35	1.43	1.35
39	Y	601	CHL	C1D-ND	3.35	1.41	1.37
32	s	609	CLA	C4D-ND	-3.35	1.33	1.37
39	Gg	310	CHL	CHC-C1C	3.35	1.43	1.35
39	Yy	608	CHL	CHC-C1C	3.35	1.43	1.35
32	A	406	CLA	C4D-ND	-3.35	1.33	1.37
39	1	601	CHL	CHC-C1C	3.35	1.43	1.35
39	g	608	CHL	CHC-C1C	3.35	1.43	1.35
39	Y	605	CHL	CHC-C1C	3.35	1.43	1.35
32	BB	607	CLA	C4D-ND	-3.35	1.33	1.37
39	y	309	CHL	CHC-C1C	3.34	1.43	1.35
32	b	601	CLA	C4D-ND	-3.34	1.33	1.37
39	3	601	CHL	C4D-ND	-3.34	1.33	1.37
39	2	608	CHL	CHC-C1C	3.34	1.43	1.35
39	22	607	CHL	CHC-C1C	3.34	1.43	1.35
39	RR	307	CHL	CHC-C1C	3.34	1.43	1.35
39	11	601	CHL	CHC-C1C	3.34	1.43	1.35
39	N	609	CHL	C1D-ND	3.34	1.41	1.37
39	NN	605	CHL	CHC-C1C	3.34	1.43	1.35
39	s	605	CHL	CHC-C1C	3.33	1.43	1.35
39	n	609	CHL	CHC-C1C	3.33	1.43	1.35
39	G	607	CHL	CHC-C1C	3.33	1.43	1.35
39	Nn	311	CHL	CHC-C1C	3.33	1.43	1.35
32	GG	611	CLA	C1D-ND	3.33	1.41	1.37
39	33	606	CHL	CHC-C1C	3.33	1.43	1.35
32	CC	504	CLA	C4D-ND	-3.33	1.33	1.37
39	y	310	CHL	CHC-C1C	3.32	1.43	1.35
32	C	505	CLA	C4D-ND	-3.32	1.33	1.37
39	4	306	CHL	CHC-C1C	3.32	1.43	1.35
39	Yy	606	CHL	C1D-ND	3.32	1.41	1.37
39	2	601	CHL	CHC-C1C	3.32	1.43	1.35
39	N	605	CHL	CHC-C1C	3.31	1.43	1.35
39	y	307	CHL	CHC-C1C	3.31	1.43	1.35
39	YY	601	CHL	C1D-ND	3.31	1.41	1.37
32	D	401	CLA	C4D-ND	-3.31	1.33	1.37
32	CC	503	CLA	C4D-ND	-3.30	1.33	1.37
32	B	618	CLA	C4D-ND	-3.30	1.33	1.37
32	DD	404	CLA	C4D-ND	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Yy	606	CHL	CHC-C1C	3.30	1.43	1.35
39	l	605	CHL	CHC-C1C	3.30	1.43	1.35
39	n	601	CHL	C1D-ND	3.30	1.41	1.37
39	g	601	CHL	CHC-C1C	3.30	1.43	1.35
32	Cc	512	CLA	C4D-ND	-3.29	1.33	1.37
36	4	301	LHG	O8-C23	3.29	1.46	1.33
39	Gg	302	CHL	C1D-ND	3.28	1.41	1.37
39	Nn	319	CHL	CHC-C1C	3.28	1.43	1.35
32	R	613	CLA	C4D-ND	-3.28	1.33	1.37
32	n	602	CLA	CHC-C1C	3.28	1.43	1.35
32	Gg	304	CLA	C4D-ND	-3.27	1.33	1.37
39	n	601	CHL	CHC-C1C	3.27	1.43	1.35
39	GG	607	CHL	CHC-C1C	3.27	1.43	1.35
32	D	405	CLA	C4D-ND	-3.27	1.33	1.37
39	G	601	CHL	CHC-C1C	3.27	1.43	1.35
32	NN	603	CLA	C1D-ND	3.26	1.41	1.37
32	B	624	CLA	C4D-ND	-3.26	1.33	1.37
39	Yy	605	CHL	CHC-C1C	3.26	1.43	1.35
36	44	616	LHG	O8-C23	3.26	1.45	1.33
32	R	612	CLA	C4D-ND	-3.26	1.33	1.37
39	GG	609	CHL	CHC-C1C	3.26	1.43	1.35
32	Bb	602	CLA	C4D-ND	-3.26	1.33	1.37
39	YY	605	CHL	CHC-C1C	3.26	1.43	1.35
32	c	510	CLA	C4D-ND	-3.25	1.33	1.37
39	NN	607	CHL	CHC-C1C	3.25	1.43	1.35
32	B	621	CLA	C4D-ND	-3.25	1.33	1.37
32	y	305	CLA	C4D-ND	-3.25	1.33	1.37
32	N	603	CLA	C1D-ND	3.25	1.41	1.37
32	Nn	314	CLA	C4D-ND	-3.25	1.33	1.37
39	Yy	601	CHL	CHC-C1C	3.25	1.43	1.35
39	n	605	CHL	CHC-C1C	3.25	1.43	1.35
32	RR	312	CLA	C4D-ND	-3.25	1.33	1.37
39	N	607	CHL	CHC-C1C	3.24	1.43	1.35
32	B	604	CLA	CHC-C1C	3.24	1.43	1.35
39	GG	601	CHL	CHC-C1C	3.24	1.43	1.35
39	3	608	CHL	CHC-C1C	3.24	1.43	1.35
39	11	605	CHL	CHC-C1C	3.24	1.43	1.35
32	c	511	CLA	C4D-ND	-3.24	1.33	1.37
32	BB	604	CLA	C4D-ND	-3.23	1.33	1.37
32	Yy	603	CLA	C4D-ND	-3.23	1.33	1.37
39	Ss	605	CHL	CHC-C1C	3.23	1.43	1.35
39	G	609	CHL	CHC-C1C	3.23	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	601	CLA	C4D-ND	-3.23	1.33	1.37
39	y	303	CHL	CHC-C1C	3.23	1.43	1.35
32	n	614	CLA	C4D-ND	-3.23	1.33	1.37
32	CC	511	CLA	C4D-ND	-3.23	1.33	1.37
32	Bb	603	CLA	C4D-ND	-3.23	1.33	1.37
32	B	622	CLA	C4D-ND	-3.23	1.33	1.37
32	a	407	CLA	C4D-ND	-3.22	1.33	1.37
39	Nn	317	CHL	CHC-C1C	3.22	1.43	1.35
32	BB	601	CLA	C4D-ND	-3.22	1.33	1.37
39	y	311	CHL	CHC-C1C	3.22	1.43	1.35
39	Y	601	CHL	CHC-C1C	3.22	1.43	1.35
32	y	313	CLA	C4D-ND	-3.22	1.33	1.37
32	GG	611	CLA	C4D-ND	-3.22	1.33	1.37
32	Yy	611	CLA	C4D-ND	-3.22	1.33	1.37
32	YY	611	CLA	CMD-C2D	-3.22	1.44	1.50
32	Nn	305	CLA	C4D-ND	-3.21	1.33	1.37
32	Bb	607	CLA	C4D-ND	-3.21	1.33	1.37
32	Gg	311	CLA	CHC-C1C	3.21	1.43	1.35
32	g	610	CLA	CHC-C1C	3.21	1.43	1.35
39	R	605	CHL	C1D-ND	3.21	1.41	1.37
32	b	609	CLA	CHC-C1C	3.20	1.43	1.35
32	GG	613	CLA	C4D-ND	-3.20	1.33	1.37
32	A	405	CLA	C4D-ND	-3.20	1.33	1.37
32	g	603	CLA	C4D-ND	-3.20	1.33	1.37
39	YY	601	CHL	CHC-C1C	3.19	1.43	1.35
32	Cc	513	CLA	C4D-ND	-3.19	1.33	1.37
32	c	513	CLA	C4D-ND	-3.19	1.33	1.37
32	C	503	CLA	C4D-ND	-3.19	1.33	1.37
32	CC	514	CLA	C4D-ND	-3.19	1.33	1.37
39	n	607	CHL	CHC-C1C	3.19	1.43	1.35
32	GG	610	CLA	CHC-C1C	3.19	1.43	1.35
32	Nn	301	CLA	C4D-ND	-3.19	1.33	1.37
42	Gg	318	NEX	C7-C8	-3.19	1.26	1.32
32	b	611	CLA	C4D-ND	-3.19	1.33	1.37
32	Cc	515	CLA	C4D-ND	-3.18	1.33	1.37
32	Cc	504	CLA	C4D-ND	-3.18	1.33	1.37
39	11	608	CHL	CHC-C1C	3.18	1.43	1.35
32	B	607	CLA	C1D-ND	3.18	1.41	1.37
32	44	609	CLA	CHC-C1C	3.18	1.43	1.35
32	SS	310	CLA	CHC-C1C	3.17	1.43	1.35
32	G	613	CLA	C4D-ND	-3.17	1.33	1.37
32	Nn	304	CLA	C4D-ND	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	316	CLA	C4D-ND	-3.17	1.33	1.37
32	YY	611	CLA	C4D-ND	-3.17	1.33	1.37
32	Yy	610	CLA	CHC-C1C	3.17	1.43	1.35
39	YY	609	CHL	CHC-C1C	3.17	1.43	1.35
32	C	512	CLA	C4D-ND	-3.17	1.33	1.37
32	C	515	CLA	C4D-ND	-3.17	1.33	1.37
32	B	619	CLA	C4D-ND	-3.17	1.33	1.37
32	N	604	CLA	C4D-ND	-3.17	1.33	1.37
32	Cc	509	CLA	C4D-ND	-3.17	1.33	1.37
39	Yy	607	CHL	CHC-C1C	3.17	1.43	1.35
32	B	605	CLA	C4D-ND	-3.17	1.33	1.37
32	Bb	611	CLA	C4D-ND	-3.16	1.33	1.37
32	R	609	CLA	CHC-C1C	3.16	1.43	1.35
32	N	611	CLA	C4D-ND	-3.16	1.33	1.37
32	y	312	CLA	CHC-C1C	3.16	1.43	1.35
32	44	602	CLA	C4D-ND	-3.16	1.33	1.37
32	4	311	CLA	C4D-ND	-3.16	1.33	1.37
32	Y	611	CLA	C4D-ND	-3.16	1.33	1.37
39	N	601	CHL	CHC-C1C	3.16	1.43	1.35
32	n	611	CLA	C4D-ND	-3.16	1.33	1.37
32	n	604	CLA	C4D-ND	-3.16	1.33	1.37
32	N	610	CLA	CHC-C1C	3.16	1.43	1.35
32	Bb	609	CLA	CHC-C1C	3.15	1.43	1.35
32	n	613	CLA	C4D-ND	-3.15	1.33	1.37
32	BB	609	CLA	C4D-ND	-3.15	1.33	1.37
32	n	603	CLA	C4D-ND	-3.15	1.33	1.37
32	NN	611	CLA	C4D-ND	-3.15	1.33	1.37
32	RR	309	CLA	CHC-C1C	3.15	1.43	1.35
32	b	607	CLA	C4D-ND	-3.15	1.33	1.37
32	b	602	CLA	C4D-ND	-3.15	1.33	1.37
32	r	611	CLA	C4D-ND	-3.15	1.33	1.37
32	b	608	CLA	C4D-ND	-3.14	1.33	1.37
32	11	612	CLA	CHC-C1C	3.14	1.43	1.35
32	Bb	610	CLA	C4D-ND	-3.14	1.33	1.37
32	NN	602	CLA	CHC-C1C	3.14	1.43	1.35
32	11	612	CLA	CMD-C2D	-3.14	1.44	1.50
39	Y	609	CHL	CHC-C1C	3.14	1.43	1.35
32	44	610	CLA	C4D-ND	-3.14	1.33	1.37
32	BB	602	CLA	C4D-ND	-3.14	1.33	1.37
32	DD	403	CLA	C4D-ND	-3.14	1.33	1.37
39	RR	305	CHL	C1D-ND	3.14	1.41	1.37
32	Ss	612	CLA	C4D-ND	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	GG	603	CLA	C4D-ND	-3.14	1.33	1.37
39	33	601	CHL	C4D-ND	-3.14	1.33	1.37
32	G	611	CLA	C4D-ND	-3.13	1.33	1.37
32	NN	614	CLA	C4D-ND	-3.13	1.33	1.37
32	C	504	CLA	C4D-ND	-3.13	1.33	1.37
32	BB	605	CLA	C4D-ND	-3.13	1.33	1.37
32	C	513	CLA	C4D-ND	-3.13	1.33	1.37
32	c	509	CLA	C4D-ND	-3.13	1.33	1.37
32	AA	405	CLA	C4D-ND	-3.13	1.33	1.37
32	B	606	CLA	C4D-ND	-3.13	1.33	1.37
32	Bb	609	CLA	C4D-ND	-3.13	1.33	1.37
32	Nn	313	CLA	C4D-ND	-3.13	1.33	1.37
32	R	602	CLA	C4D-ND	-3.13	1.33	1.37
32	X	201	CLA	C4D-ND	-3.13	1.33	1.37
32	c	503	CLA	C4D-ND	-3.13	1.33	1.37
32	NN	610	CLA	CHC-C1C	3.12	1.43	1.35
32	b	610	CLA	C4D-ND	-3.12	1.33	1.37
32	Y	614	CLA	C4D-ND	-3.12	1.33	1.37
32	c	502	CLA	C4D-ND	-3.12	1.33	1.37
32	c	504	CLA	C4D-ND	-3.12	1.33	1.37
32	2	602	CLA	CHC-C1C	3.12	1.43	1.35
32	NN	604	CLA	C4D-ND	-3.12	1.33	1.37
32	Dd	402	CLA	C4D-ND	-3.12	1.33	1.37
32	YY	614	CLA	C4D-ND	-3.12	1.33	1.37
32	b	605	CLA	C4D-ND	-3.11	1.33	1.37
32	N	603	CLA	C4D-ND	-3.11	1.33	1.37
32	BB	608	CLA	C4D-ND	-3.11	1.33	1.37
32	Aa	407	CLA	C4D-ND	-3.11	1.33	1.37
32	Cc	510	CLA	C4D-ND	-3.11	1.33	1.37
32	Rr	608	CLA	C4D-ND	-3.11	1.33	1.37
32	N	614	CLA	C4D-ND	-3.11	1.33	1.37
32	BB	612	CLA	C4D-ND	-3.11	1.33	1.37
32	22	602	CLA	CHC-C1C	3.11	1.42	1.35
32	Bb	605	CLA	C4D-ND	-3.11	1.33	1.37
32	A	408	CLA	C4D-ND	-3.11	1.33	1.37
32	22	603	CLA	C4D-ND	-3.11	1.33	1.37
32	CC	512	CLA	C4D-ND	-3.11	1.33	1.37
32	BB	603	CLA	C4D-ND	-3.11	1.33	1.37
32	SS	303	CLA	C4D-ND	-3.11	1.33	1.37
32	a	410	CLA	C4D-ND	-3.10	1.33	1.37
32	b	603	CLA	C4D-ND	-3.10	1.33	1.37
32	Bb	608	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	608	CLA	C4D-ND	-3.10	1.33	1.37
32	XX	201	CLA	C4D-ND	-3.10	1.33	1.37
32	Cc	511	CLA	C4D-ND	-3.10	1.33	1.37
32	2	603	CLA	C4D-ND	-3.10	1.33	1.37
32	n	610	CLA	CHC-C1C	3.10	1.42	1.35
32	3	609	CLA	CHC-C1C	3.10	1.42	1.35
32	Nn	302	CLA	C4D-ND	-3.10	1.33	1.37
32	a	406	CLA	C3B-C2B	-3.10	1.36	1.40
32	GG	602	CLA	C4D-ND	-3.10	1.33	1.37
32	Yy	614	CLA	C4D-ND	-3.10	1.33	1.37
32	YY	610	CLA	CHC-C1C	3.10	1.42	1.35
32	AA	408	CLA	C4D-ND	-3.10	1.33	1.37
32	NN	603	CLA	C4D-ND	-3.10	1.33	1.37
32	Bb	612	CLA	C4D-ND	-3.10	1.33	1.37
32	Cc	505	CLA	C4D-ND	-3.10	1.33	1.37
32	B	608	CLA	C4D-ND	-3.10	1.33	1.37
32	4	310	CLA	CHC-C1C	3.10	1.42	1.35
39	NN	601	CHL	CHC-C1C	3.09	1.42	1.35
32	R	609	CLA	C4D-ND	-3.09	1.33	1.37
32	R	610	CLA	C4D-ND	-3.09	1.33	1.37
32	b	604	CLA	C4D-ND	-3.09	1.33	1.37
32	C	506	CLA	C4D-ND	-3.09	1.33	1.37
32	33	609	CLA	CHC-C1C	3.09	1.42	1.35
32	B	620	CLA	C4D-ND	-3.09	1.33	1.37
32	Cc	503	CLA	C4D-ND	-3.09	1.33	1.37
32	b	614	CLA	C4D-ND	-3.09	1.33	1.37
32	Y	610	CLA	CHC-C1C	3.09	1.42	1.35
32	Rr	604	CLA	C4D-ND	-3.09	1.33	1.37
32	SS	313	CLA	C4D-ND	-3.09	1.33	1.37
32	r	602	CLA	CHC-C1C	3.09	1.42	1.35
39	1	608	CHL	CHC-C1C	3.08	1.42	1.35
32	3	604	CLA	C4D-ND	-3.08	1.33	1.37
32	CC	511	CLA	CHC-C1C	3.08	1.42	1.35
32	r	612	CLA	C4D-ND	-3.08	1.33	1.37
32	BB	606	CLA	C4D-ND	-3.08	1.33	1.37
32	Gg	305	CLA	C4D-ND	-3.08	1.33	1.37
32	Yy	612	CLA	C4D-ND	-3.08	1.33	1.37
32	c	507	CLA	C4D-ND	-3.08	1.33	1.37
32	CC	509	CLA	C4D-ND	-3.08	1.33	1.37
32	Gg	312	CLA	C4D-ND	-3.08	1.33	1.37
32	R	602	CLA	CHC-C1C	3.08	1.42	1.35
32	b	612	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	602	CLA	CHC-C1C	3.08	1.42	1.35
32	SS	314	CLA	C4D-ND	-3.08	1.33	1.37
32	c	508	CLA	C4D-ND	-3.07	1.33	1.37
32	b	603	CLA	CHC-C1C	3.07	1.42	1.35
32	YY	602	CLA	CHC-C1C	3.07	1.42	1.35
32	RR	309	CLA	C4D-ND	-3.07	1.33	1.37
32	C	509	CLA	C4D-ND	-3.07	1.33	1.37
32	Gg	312	CLA	CHC-C1C	3.07	1.42	1.35
32	R	601	CLA	C4D-ND	-3.07	1.33	1.37
32	y	304	CLA	CHC-C1C	3.07	1.42	1.35
32	22	602	CLA	C4D-ND	-3.07	1.33	1.37
32	d	402	CLA	C4D-ND	-3.07	1.33	1.37
32	B	609	CLA	C4D-ND	-3.07	1.33	1.37
32	G	603	CLA	C4D-ND	-3.07	1.33	1.37
32	Gg	314	CLA	C4D-ND	-3.07	1.33	1.37
32	N	602	CLA	CHC-C1C	3.07	1.42	1.35
32	BB	610	CLA	C4D-ND	-3.07	1.33	1.37
32	Yy	610	CLA	C4D-ND	-3.07	1.33	1.37
32	S	613	CLA	C4D-ND	-3.07	1.33	1.37
32	c	506	CLA	C4D-ND	-3.07	1.33	1.37
32	Bb	604	CLA	C4D-ND	-3.07	1.33	1.37
32	11	604	CLA	CHC-C1C	3.06	1.42	1.35
39	RR	306	CHL	CHC-C1C	3.06	1.42	1.35
39	Rr	606	CHL	C4D-ND	-3.06	1.33	1.37
32	BB	613	CLA	C4D-ND	-3.06	1.33	1.37
32	S	608	CLA	CHC-C1C	3.06	1.42	1.35
32	s	608	CLA	CHC-C1C	3.06	1.42	1.35
32	Rr	613	CLA	C4D-ND	-3.06	1.33	1.37
32	Aa	410	CLA	C4D-ND	-3.06	1.33	1.37
32	r	604	CLA	C4D-ND	-3.06	1.33	1.37
39	r	606	CHL	C4D-ND	-3.06	1.33	1.37
32	Bb	614	CLA	C4D-ND	-3.06	1.33	1.37
32	1	604	CLA	CHC-C1C	3.06	1.42	1.35
32	S	609	CLA	CHC-C1C	3.06	1.42	1.35
32	Ss	604	CLA	C4D-ND	-3.05	1.33	1.37
32	s	604	CLA	C4D-ND	-3.05	1.33	1.37
32	s	602	CLA	C4D-ND	-3.05	1.33	1.37
32	B	610	CLA	C4D-ND	-3.05	1.33	1.37
32	Nn	301	CLA	CHC-C1C	3.05	1.42	1.35
46	Ee	101	HEM	CAB-C3B	3.05	1.55	1.47
32	Y	603	CLA	C4D-ND	-3.05	1.33	1.37
32	g	611	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	613	CLA	C4D-ND	-3.05	1.33	1.37
32	Yy	604	CLA	C4D-ND	-3.05	1.33	1.37
32	s	603	CLA	C4D-ND	-3.05	1.33	1.37
32	N	612	CLA	C4D-ND	-3.05	1.33	1.37
32	XX	201	CLA	CHC-C1C	3.05	1.42	1.35
32	S	612	CLA	C4D-ND	-3.04	1.33	1.37
32	RR	310	CLA	C4D-ND	-3.04	1.33	1.37
32	Ss	609	CLA	CHC-C1C	3.04	1.42	1.35
32	Y	602	CLA	C4D-ND	-3.04	1.33	1.37
32	C	510	CLA	C4D-ND	-3.04	1.33	1.37
32	Cc	504	CLA	CHC-C1C	3.04	1.42	1.35
32	RR	313	CLA	C4D-ND	-3.04	1.33	1.37
32	Cc	507	CLA	C4D-ND	-3.04	1.33	1.37
32	BB	614	CLA	C4D-ND	-3.04	1.33	1.37
32	Yy	602	CLA	CHC-C1C	3.04	1.42	1.35
32	NN	611	CLA	CHC-C1C	3.04	1.42	1.35
37	CC	501	SQD	C6-S	-3.04	1.66	1.77
32	Cc	514	CLA	C4D-ND	-3.04	1.33	1.37
37	C	501	SQD	C6-S	-3.04	1.66	1.77
32	s	609	CLA	CHC-C1C	3.04	1.42	1.35
32	b	609	CLA	C4D-ND	-3.04	1.33	1.37
32	C	504	CLA	CHC-C1C	3.03	1.42	1.35
39	Yy	609	CHL	C4D-ND	-3.03	1.33	1.37
32	4	305	CLA	C4D-ND	-3.03	1.33	1.37
32	N	611	CLA	CHC-C1C	3.03	1.42	1.35
32	SS	309	CLA	CHC-C1C	3.03	1.42	1.35
32	44	604	CLA	C4D-ND	-3.03	1.33	1.37
32	Nn	302	CLA	CHC-C1C	3.03	1.42	1.35
32	CC	503	CLA	CHC-C1C	3.03	1.42	1.35
32	Nn	314	CLA	CHC-C1C	3.03	1.42	1.35
32	X	201	CLA	CHC-C1C	3.03	1.42	1.35
32	RR	302	CLA	C4D-ND	-3.03	1.33	1.37
32	B	623	CLA	C4D-ND	-3.03	1.33	1.37
37	AA	412	SQD	C6-S	-3.03	1.66	1.77
32	C	512	CLA	CHC-C1C	3.03	1.42	1.35
32	CC	507	CLA	CHC-C1C	3.03	1.42	1.35
32	R	608	CLA	CHC-C1C	3.03	1.42	1.35
32	y	306	CLA	C4D-ND	-3.03	1.33	1.37
32	S	602	CLA	C4D-ND	-3.02	1.33	1.37
32	CC	513	CLA	C4D-ND	-3.02	1.33	1.37
32	r	613	CLA	C4D-ND	-3.02	1.33	1.37
32	C	508	CLA	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	GG	610	CLA	C4D-ND	-3.02	1.33	1.37
32	GG	614	CLA	C4D-ND	-3.02	1.33	1.37
32	YY	602	CLA	C4D-ND	-3.02	1.33	1.37
32	Y	612	CLA	C4D-ND	-3.02	1.33	1.37
32	s	613	CLA	C4D-ND	-3.02	1.33	1.37
32	n	604	CLA	CHC-C1C	3.02	1.42	1.35
32	R	603	CLA	C4D-ND	-3.02	1.33	1.37
32	NN	602	CLA	C4D-ND	-3.02	1.33	1.37
32	Bb	606	CLA	C4D-ND	-3.02	1.33	1.37
32	BB	615	CLA	C4D-ND	-3.02	1.33	1.37
32	Rr	602	CLA	CHC-C1C	3.02	1.42	1.35
32	Cc	508	CLA	C4D-ND	-3.02	1.33	1.37
32	BB	608	CLA	CHC-C1C	3.02	1.42	1.35
32	C	514	CLA	C4D-ND	-3.02	1.33	1.37
32	c	501	CLA	C4D-ND	-3.02	1.33	1.37
32	CC	508	CLA	C4D-ND	-3.02	1.33	1.37
39	Y	606	CHL	C4D-ND	-3.02	1.33	1.37
32	3	612	CLA	C4D-ND	-3.01	1.33	1.37
32	4	312	CLA	C4D-ND	-3.01	1.33	1.37
32	c	506	CLA	CHC-C1C	3.01	1.42	1.35
32	GG	611	CLA	CHC-C1C	3.01	1.42	1.35
46	e	101	HEM	CAB-C3B	3.01	1.55	1.47
32	Cc	515	CLA	CHC-C1C	3.01	1.42	1.35
32	1	604	CLA	C4D-ND	-3.01	1.33	1.37
32	Ss	613	CLA	C4D-ND	-3.01	1.33	1.37
32	SS	314	CLA	CHC-C1C	3.01	1.42	1.35
39	Yy	606	CHL	C4D-ND	-3.01	1.33	1.37
32	Ss	613	CLA	CHC-C1C	3.01	1.42	1.35
32	Ss	602	CLA	C4D-ND	-3.01	1.33	1.37
32	s	612	CLA	C4D-ND	-3.01	1.33	1.37
32	NN	610	CLA	C4D-ND	-3.01	1.33	1.37
32	11	613	CLA	CHC-C1C	3.01	1.42	1.35
32	c	513	CLA	CHC-C1C	3.01	1.42	1.35
32	D	404	CLA	CHC-C1C	3.01	1.42	1.35
32	2	602	CLA	C4D-ND	-3.01	1.33	1.37
32	b	601	CLA	CHC-C1C	3.01	1.42	1.35
32	DD	403	CLA	CHC-C1C	3.01	1.42	1.35
32	Cc	506	CLA	C4D-ND	-3.01	1.33	1.37
39	Nn	318	CHL	C4D-ND	-3.00	1.33	1.37
32	2	610	CLA	CHC-C1C	3.00	1.42	1.35
32	c	502	CLA	CHC-C1C	3.00	1.42	1.35
32	1	613	CLA	CHC-C1C	3.00	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	510	CLA	CHC-C1C	3.00	1.42	1.35
32	s	610	CLA	C4D-ND	-3.00	1.33	1.37
32	22	610	CLA	CHC-C1C	3.00	1.42	1.35
32	4	303	CLA	C4D-ND	-3.00	1.33	1.37
32	s	602	CLA	CHC-C1C	3.00	1.42	1.35
32	Bb	603	CLA	CHC-C1C	3.00	1.42	1.35
32	33	603	CLA	C4D-ND	-3.00	1.33	1.37
32	2	609	CLA	C4D-ND	-3.00	1.33	1.37
32	2	613	CLA	CHC-C1C	3.00	1.42	1.35
32	NN	614	CLA	CHC-C1C	3.00	1.42	1.35
32	11	602	CLA	C4D-ND	-3.00	1.33	1.37
32	Nn	312	CLA	CHC-C1C	3.00	1.42	1.35
32	SS	305	CLA	C4D-ND	-3.00	1.33	1.37
32	c	512	CLA	C4D-ND	-3.00	1.33	1.37
32	g	614	CLA	C4D-ND	-3.00	1.33	1.37
32	n	611	CLA	CHC-C1C	3.00	1.42	1.35
32	Bb	601	CLA	CHC-C1C	3.00	1.42	1.35
32	11	603	CLA	CHC-C1C	3.00	1.42	1.35
32	C	511	CLA	CHC-C1C	2.99	1.42	1.35
32	2	611	CLA	CHC-C1C	2.99	1.42	1.35
32	RR	308	CLA	CHC-C1C	2.99	1.42	1.35
32	3	603	CLA	C4D-ND	-2.99	1.33	1.37
32	G	614	CLA	C4D-ND	-2.99	1.33	1.37
32	Ss	602	CLA	CHC-C1C	2.99	1.42	1.35
32	YY	611	CLA	CHC-C1C	2.99	1.42	1.35
32	Aa	406	CLA	CHC-C1C	2.99	1.42	1.35
32	4	311	CLA	CHC-C1C	2.99	1.42	1.35
32	33	612	CLA	C4D-ND	-2.99	1.33	1.37
32	Cc	508	CLA	CHC-C1C	2.99	1.42	1.35
32	33	612	CLA	CHC-C1C	2.99	1.42	1.35
39	4	309	CHL	C4D-ND	-2.99	1.33	1.37
32	D	404	CLA	C4D-ND	-2.99	1.33	1.37
32	11	611	CLA	CHC-C1C	2.99	1.42	1.35
32	3	611	CLA	C4D-ND	-2.99	1.33	1.37
32	AA	406	CLA	CHC-C1C	2.99	1.42	1.35
32	CC	507	CLA	C4D-ND	-2.99	1.33	1.37
32	Rr	609	CLA	CHC-C1C	2.99	1.42	1.35
32	G	604	CLA	C4D-ND	-2.98	1.33	1.37
32	44	602	CLA	CHC-C1C	2.98	1.42	1.35
32	G	611	CLA	CHC-C1C	2.98	1.42	1.35
32	22	613	CLA	C4D-ND	-2.98	1.33	1.37
32	b	606	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	611	CLA	C4D-ND	-2.98	1.33	1.37
32	Rr	601	CLA	CHC-C1C	2.98	1.42	1.35
32	RR	304	CLA	CHC-C1C	2.98	1.42	1.35
32	s	613	CLA	CHC-C1C	2.98	1.42	1.35
32	B	604	CLA	C4D-ND	-2.98	1.33	1.37
32	GG	604	CLA	C4D-ND	-2.98	1.33	1.37
32	YY	610	CLA	C4D-ND	-2.98	1.33	1.37
32	Dd	401	CLA	C4D-ND	-2.98	1.33	1.37
32	3	604	CLA	CHC-C1C	2.98	1.42	1.35
32	Ss	608	CLA	CHC-C1C	2.98	1.42	1.35
32	r	609	CLA	CHC-C1C	2.98	1.42	1.35
32	Y	604	CLA	C4D-ND	-2.98	1.33	1.37
32	4	304	CLA	C4D-ND	-2.98	1.33	1.37
32	11	602	CLA	CHC-C1C	2.98	1.42	1.35
32	22	611	CLA	CHC-C1C	2.98	1.42	1.35
32	Gg	305	CLA	CHC-C1C	2.98	1.42	1.35
39	N	606	CHL	C4D-ND	-2.98	1.33	1.37
39	Gg	307	CHL	C4D-ND	-2.98	1.33	1.37
32	44	609	CLA	C4D-ND	-2.98	1.33	1.37
32	Yy	611	CLA	CHC-C1C	2.98	1.42	1.35
32	22	612	CLA	C4D-ND	-2.98	1.33	1.37
32	1	602	CLA	CHC-C1C	2.98	1.42	1.35
32	RR	302	CLA	CHC-C1C	2.98	1.42	1.35
32	44	611	CLA	C4D-ND	-2.98	1.33	1.37
32	2	604	CLA	C4D-ND	-2.98	1.33	1.37
32	C	508	CLA	C4D-ND	-2.98	1.33	1.37
32	CC	505	CLA	C4D-ND	-2.98	1.33	1.37
32	Nn	312	CLA	C4D-ND	-2.98	1.33	1.37
32	s	611	CLA	CHC-C1C	2.98	1.42	1.35
32	33	604	CLA	C4D-ND	-2.98	1.33	1.37
32	Bb	613	CLA	C4D-ND	-2.98	1.33	1.37
32	R	610	CLA	CHC-C1C	2.98	1.42	1.35
32	N	602	CLA	C4D-ND	-2.98	1.33	1.37
32	N	614	CLA	CHC-C1C	2.98	1.42	1.35
32	r	601	CLA	CHC-C1C	2.98	1.42	1.35
32	y	314	CLA	C4D-ND	-2.98	1.33	1.37
32	1	602	CLA	C4D-ND	-2.97	1.33	1.37
32	y	312	CLA	C4D-ND	-2.97	1.33	1.37
32	G	604	CLA	CHC-C1C	2.97	1.42	1.35
32	DD	401	CLA	CHC-C1C	2.97	1.42	1.35
32	3	602	CLA	C4D-ND	-2.97	1.33	1.37
32	Yy	602	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	610	CLA	C4D-ND	-2.97	1.33	1.37
32	S	609	CLA	C4D-ND	-2.97	1.33	1.37
32	33	613	CLA	CHC-C1C	2.97	1.42	1.35
32	22	612	CLA	CHC-C1C	2.97	1.42	1.35
32	g	611	CLA	C4D-ND	-2.97	1.33	1.37
32	2	603	CLA	CHC-C1C	2.97	1.42	1.35
32	a	410	CLA	CHC-C1C	2.97	1.42	1.35
32	n	602	CLA	C4D-ND	-2.97	1.33	1.37
32	33	604	CLA	CHC-C1C	2.97	1.42	1.35
32	33	610	CLA	C4D-ND	-2.97	1.33	1.37
32	CC	502	CLA	CHC-C1C	2.97	1.42	1.35
32	Ss	608	CLA	C4D-ND	-2.97	1.33	1.37
32	2	611	CLA	C4D-ND	-2.97	1.33	1.37
32	S	613	CLA	CHC-C1C	2.97	1.42	1.35
37	Ll	101	SQD	C6-S	-2.97	1.66	1.77
37	B	602	SQD	C6-S	-2.97	1.66	1.77
32	Rr	611	CLA	C4D-ND	-2.97	1.33	1.37
32	Aa	407	CLA	CHC-C1C	2.97	1.42	1.35
32	NN	612	CLA	C4D-ND	-2.97	1.33	1.37
39	11	605	CHL	C4D-ND	-2.97	1.33	1.37
39	44	608	CHL	C4D-ND	-2.97	1.33	1.37
39	NN	606	CHL	C4D-ND	-2.97	1.33	1.37
32	c	509	CLA	CHC-C1C	2.96	1.42	1.35
32	Rr	611	CLA	CHC-C1C	2.96	1.42	1.35
32	y	313	CLA	CHC-C1C	2.96	1.42	1.35
32	RR	313	CLA	CHC-C1C	2.96	1.42	1.35
32	r	613	CLA	CHC-C1C	2.96	1.42	1.35
32	Ss	604	CLA	CHC-C1C	2.96	1.42	1.35
33	AA	407	PHO	CAC-C3C	-2.96	1.47	1.52
32	BB	601	CLA	CHC-C1C	2.96	1.42	1.35
32	33	602	CLA	CHC-C1C	2.96	1.42	1.35
32	3	612	CLA	CHC-C1C	2.96	1.42	1.35
32	44	610	CLA	CHC-C1C	2.96	1.42	1.35
32	a	407	CLA	CHC-C1C	2.96	1.42	1.35
32	33	611	CLA	C4D-ND	-2.96	1.33	1.37
32	33	603	CLA	CHC-C1C	2.96	1.42	1.35
37	Aa	413	SQD	C6-S	-2.96	1.66	1.77
32	YY	614	CLA	CHC-C1C	2.96	1.42	1.35
32	Aa	410	CLA	CHC-C1C	2.96	1.42	1.35
32	b	610	CLA	CHC-C1C	2.96	1.42	1.35
32	RR	303	CLA	C4D-ND	-2.96	1.33	1.37
32	S	603	CLA	CHC-C1C	2.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	611	CLA	CHC-C1C	2.96	1.42	1.35
32	2	609	CLA	CHC-C1C	2.96	1.42	1.35
32	44	604	CLA	CHC-C1C	2.96	1.42	1.35
32	SS	305	CLA	CHC-C1C	2.96	1.42	1.35
32	B	607	CLA	C4D-ND	-2.95	1.33	1.37
32	Gg	311	CLA	C4D-ND	-2.95	1.33	1.37
39	Yy	605	CHL	C4D-ND	-2.95	1.33	1.37
32	b	613	CLA	C4D-ND	-2.95	1.33	1.37
32	R	604	CLA	CHC-C1C	2.95	1.42	1.35
32	11	610	CLA	CHC-C1C	2.95	1.42	1.35
37	A	412	SQD	C6-S	-2.95	1.66	1.77
32	3	603	CLA	CHC-C1C	2.95	1.42	1.35
39	n	601	CHL	C4D-ND	-2.95	1.33	1.37
32	3	611	CLA	CHC-C1C	2.95	1.42	1.35
32	Cc	505	CLA	CHC-C1C	2.95	1.42	1.35
32	4	305	CLA	CHC-C1C	2.95	1.42	1.35
32	22	611	CLA	C4D-ND	-2.95	1.33	1.37
32	R	613	CLA	CHC-C1C	2.95	1.42	1.35
32	r	603	CLA	CHC-C1C	2.95	1.42	1.35
32	d	401	CLA	C4D-ND	-2.95	1.33	1.37
37	LL	102	SQD	C6-S	-2.95	1.66	1.77
32	33	610	CLA	CHC-C1C	2.95	1.42	1.35
32	R	611	CLA	C4D-ND	-2.95	1.33	1.37
37	l	102	SQD	C6-S	-2.95	1.66	1.77
32	c	508	CLA	CHC-C1C	2.95	1.42	1.35
32	22	609	CLA	C4D-ND	-2.95	1.33	1.37
32	3	613	CLA	C4D-ND	-2.95	1.33	1.37
32	s	608	CLA	C4D-ND	-2.95	1.33	1.37
32	Bb	613	CLA	CHC-C1C	2.95	1.42	1.35
32	Rr	601	CLA	C4D-ND	-2.95	1.33	1.37
32	Ss	610	CLA	C4D-ND	-2.95	1.33	1.37
39	G	601	CHL	C4D-ND	-2.95	1.33	1.37
32	22	603	CLA	CHC-C1C	2.94	1.42	1.35
32	3	613	CLA	CHC-C1C	2.94	1.42	1.35
32	RR	311	CLA	CHC-C1C	2.94	1.42	1.35
32	S	602	CLA	CHC-C1C	2.94	1.42	1.35
32	S	611	CLA	C4D-ND	-2.94	1.33	1.37
32	Aa	406	CLA	C3B-C2B	-2.94	1.36	1.40
32	44	615	CLA	CHC-C1C	2.94	1.42	1.35
32	Cc	512	CLA	CHC-C1C	2.94	1.42	1.35
32	S	604	CLA	CHC-C1C	2.94	1.42	1.35
32	RR	304	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	505	CLA	CHC-C1C	2.94	1.42	1.35
32	2	612	CLA	CHC-C1C	2.94	1.42	1.35
32	Bb	607	CLA	CHC-C1C	2.94	1.42	1.35
32	33	602	CLA	C4D-ND	-2.94	1.33	1.37
32	Ss	611	CLA	CHC-C1C	2.94	1.42	1.35
37	L	101	SQD	C6-S	-2.94	1.66	1.77
32	22	609	CLA	CHC-C1C	2.94	1.42	1.35
32	g	604	CLA	C4D-ND	-2.94	1.33	1.37
32	r	608	CLA	CHC-C1C	2.94	1.42	1.35
32	Dd	402	CLA	CHC-C1C	2.94	1.42	1.35
32	Rr	603	CLA	CHC-C1C	2.94	1.42	1.35
32	Y	604	CLA	CHC-C1C	2.94	1.42	1.35
32	g	614	CLA	CHC-C1C	2.94	1.42	1.35
32	S	604	CLA	C4D-ND	-2.94	1.33	1.37
32	d	401	CLA	CHC-C1C	2.94	1.42	1.35
32	g	610	CLA	C4D-ND	-2.94	1.33	1.37
32	11	609	CLA	CHC-C1C	2.94	1.42	1.35
32	G	614	CLA	CHC-C1C	2.94	1.42	1.35
32	NN	604	CLA	CHC-C1C	2.94	1.42	1.35
32	b	616	CLA	C4D-ND	-2.94	1.33	1.37
32	SS	309	CLA	C4D-ND	-2.94	1.33	1.37
32	Gg	315	CLA	CHC-C1C	2.93	1.42	1.35
32	1	612	CLA	CHC-C1C	2.93	1.42	1.35
32	RR	310	CLA	CHC-C1C	2.93	1.42	1.35
32	Ss	611	CLA	C4D-ND	-2.93	1.33	1.37
32	Bb	616	CLA	C4D-ND	-2.93	1.33	1.37
32	1	612	CLA	C4D-ND	-2.93	1.33	1.37
32	SS	303	CLA	CHC-C1C	2.93	1.42	1.35
32	C	506	CLA	CHC-C1C	2.93	1.42	1.35
32	c	510	CLA	CHC-C1C	2.93	1.42	1.35
32	B	618	CLA	CHC-C1C	2.93	1.42	1.35
32	22	604	CLA	C4D-ND	-2.93	1.33	1.37
32	a	405	CLA	C4D-ND	-2.93	1.33	1.37
39	g	606	CHL	C4D-ND	-2.93	1.33	1.37
32	4	312	CLA	CHC-C1C	2.93	1.42	1.35
32	11	603	CLA	C4D-ND	-2.93	1.33	1.37
32	Rr	613	CLA	CHC-C1C	2.93	1.42	1.35
32	b	607	CLA	CHC-C1C	2.93	1.42	1.35
32	CC	502	CLA	C4D-ND	-2.93	1.33	1.37
32	N	610	CLA	C4D-ND	-2.93	1.33	1.37
32	33	611	CLA	CHC-C1C	2.93	1.42	1.35
32	R	604	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	310	CLA	C4D-ND	-2.93	1.33	1.37
32	Gg	315	CLA	C4D-ND	-2.93	1.33	1.37
32	2	604	CLA	CHC-C1C	2.93	1.42	1.35
37	L	102	SQD	C6-S	-2.93	1.66	1.77
32	c	505	CLA	C4D-ND	-2.93	1.33	1.37
32	Bb	604	CLA	CHC-C1C	2.93	1.42	1.35
32	Rr	612	CLA	C4D-ND	-2.92	1.33	1.37
32	S	610	CLA	C4D-ND	-2.92	1.33	1.37
32	BB	602	CLA	CHC-C1C	2.92	1.42	1.35
32	YY	603	CLA	C4D-ND	-2.92	1.33	1.37
32	g	612	CLA	C4D-ND	-2.92	1.33	1.37
32	s	604	CLA	CHC-C1C	2.92	1.42	1.35
32	4	303	CLA	CHC-C1C	2.92	1.42	1.35
32	Rr	608	CLA	CHC-C1C	2.92	1.42	1.35
32	RR	312	CLA	CHC-C1C	2.92	1.42	1.35
32	SS	312	CLA	CHC-C1C	2.92	1.42	1.35
32	Cc	510	CLA	CHC-C1C	2.92	1.42	1.35
32	44	603	CLA	C4D-ND	-2.92	1.33	1.37
32	C	511	CLA	C4D-ND	-2.92	1.33	1.37
32	b	616	CLA	CHC-C1C	2.92	1.42	1.35
32	g	604	CLA	CHC-C1C	2.92	1.42	1.35
32	B	622	CLA	CHC-C1C	2.92	1.42	1.35
39	GG	609	CHL	C4D-ND	-2.92	1.33	1.37
32	1	610	CLA	CHC-C1C	2.92	1.42	1.35
32	BB	611	CLA	C4D-ND	-2.92	1.33	1.37
37	LL	101	SQD	C6-S	-2.92	1.66	1.77
46	E	101	HEM	CAB-C3B	2.92	1.55	1.47
32	22	613	CLA	CHC-C1C	2.92	1.42	1.35
32	s	612	CLA	CHC-C1C	2.92	1.42	1.35
32	AA	408	CLA	CHC-C1C	2.92	1.42	1.35
32	1	603	CLA	C4D-ND	-2.92	1.33	1.37
32	2	610	CLA	C4D-ND	-2.92	1.33	1.37
32	n	614	CLA	CHC-C1C	2.92	1.42	1.35
32	Bb	616	CLA	CHC-C1C	2.92	1.42	1.35
32	y	316	CLA	CHC-C1C	2.91	1.42	1.35
32	R	611	CLA	CHC-C1C	2.91	1.42	1.35
32	BB	615	CLA	CHC-C1C	2.91	1.42	1.35
39	GG	606	CHL	C4D-ND	-2.91	1.33	1.37
39	RR	305	CHL	C4D-ND	-2.91	1.33	1.37
32	b	615	CLA	CHC-C1C	2.91	1.42	1.35
32	c	503	CLA	CHC-C1C	2.91	1.42	1.35
32	YY	604	CLA	CHC-C1C	2.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	610	CLA	CHC-C1C	2.91	1.42	1.35
32	22	604	CLA	CHC-C1C	2.91	1.42	1.35
32	GG	614	CLA	CHC-C1C	2.91	1.42	1.35
32	r	611	CLA	CHC-C1C	2.91	1.42	1.35
32	2	612	CLA	C4D-ND	-2.91	1.33	1.37
32	D	401	CLA	CHC-C1C	2.91	1.42	1.35
32	RR	311	CLA	C4D-ND	-2.91	1.33	1.37
32	Ss	603	CLA	C4D-ND	-2.91	1.33	1.37
32	C	507	CLA	C4D-ND	-2.91	1.33	1.37
32	SS	313	CLA	CHC-C1C	2.91	1.42	1.35
32	SS	311	CLA	CHC-C1C	2.91	1.42	1.35
32	S	611	CLA	CHC-C1C	2.91	1.42	1.35
32	DD	404	CLA	CHC-C1C	2.91	1.42	1.35
32	Y	612	CLA	CHC-C1C	2.91	1.42	1.35
32	B	619	CLA	CHC-C1C	2.91	1.42	1.35
32	3	602	CLA	CHC-C1C	2.91	1.42	1.35
32	N	603	CLA	CHC-C1C	2.91	1.42	1.35
32	b	615	CLA	C4D-ND	-2.91	1.33	1.37
32	Cc	511	CLA	CHC-C1C	2.91	1.42	1.35
32	SS	312	CLA	C4D-ND	-2.91	1.33	1.37
32	44	611	CLA	CHC-C1C	2.90	1.42	1.35
32	B	611	CLA	CHC-C1C	2.90	1.42	1.35
33	Aa	408	PHO	CAC-C3C	-2.90	1.47	1.52
32	S	603	CLA	C4D-ND	-2.90	1.33	1.37
32	r	602	CLA	C4D-ND	-2.90	1.33	1.37
39	YY	609	CHL	C4D-ND	-2.90	1.33	1.37
32	NN	612	CLA	CHC-C1C	2.90	1.42	1.35
32	YY	604	CLA	C4D-ND	-2.90	1.33	1.37
39	1	608	CHL	C4D-ND	-2.90	1.33	1.37
32	SS	304	CLA	C4D-ND	-2.90	1.33	1.37
39	y	308	CHL	C4D-ND	-2.90	1.33	1.37
39	4	307	CHL	C4D-ND	-2.90	1.33	1.37
32	Rr	610	CLA	CHC-C1C	2.90	1.42	1.35
32	SS	304	CLA	CHC-C1C	2.90	1.42	1.35
32	Bb	610	CLA	CHC-C1C	2.90	1.42	1.35
32	b	613	CLA	CHC-C1C	2.90	1.42	1.35
32	d	402	CLA	CHC-C1C	2.90	1.42	1.35
32	Nn	305	CLA	CHC-C1C	2.90	1.42	1.35
32	C	505	CLA	CHC-C1C	2.90	1.42	1.35
39	Y	607	CHL	C4D-ND	-2.90	1.33	1.37
32	CC	506	CLA	CHC-C1C	2.90	1.42	1.35
32	Rr	609	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	506	CLA	C4D-ND	-2.90	1.33	1.37
32	N	604	CLA	CHC-C1C	2.90	1.42	1.35
32	r	612	CLA	CHC-C1C	2.90	1.42	1.35
32	BB	613	CLA	CHC-C1C	2.90	1.42	1.35
32	33	613	CLA	C4D-ND	-2.90	1.33	1.37
32	Bb	615	CLA	C4D-ND	-2.90	1.33	1.37
32	BB	605	CLA	CHC-C1C	2.90	1.42	1.35
32	B	607	CLA	CHC-C1C	2.90	1.42	1.35
32	Bb	602	CLA	CHC-C1C	2.90	1.42	1.35
46	EE	102	HEM	CAB-C3B	2.89	1.55	1.47
32	Yy	614	CLA	CHC-C1C	2.89	1.42	1.35
32	Bb	615	CLA	CHC-C1C	2.89	1.42	1.35
39	GG	607	CHL	C4D-ND	-2.89	1.33	1.37
32	b	606	CLA	CHC-C1C	2.89	1.42	1.35
32	3	610	CLA	CHC-C1C	2.89	1.42	1.35
32	RR	308	CLA	C4D-ND	-2.89	1.33	1.37
39	YY	608	CHL	C4D-ND	-2.89	1.33	1.37
32	S	612	CLA	CHC-C1C	2.89	1.42	1.35
32	1	611	CLA	C4D-ND	-2.89	1.33	1.37
32	G	610	CLA	C4D-ND	-2.89	1.33	1.37
32	b	611	CLA	CHC-C1C	2.89	1.42	1.35
32	BB	609	CLA	CHC-C1C	2.89	1.42	1.35
32	RR	314	CLA	CHC-C1C	2.89	1.42	1.35
32	CC	510	CLA	C4D-ND	-2.89	1.33	1.37
32	SS	311	CLA	C4D-ND	-2.89	1.33	1.37
39	N	608	CHL	C4D-ND	-2.89	1.33	1.37
32	Ss	603	CLA	CHC-C1C	2.89	1.42	1.35
32	Y	614	CLA	CHC-C1C	2.89	1.42	1.35
32	BB	610	CLA	CHC-C1C	2.89	1.42	1.35
32	y	304	CLA	C4D-ND	-2.89	1.33	1.37
39	YY	606	CHL	C4D-ND	-2.89	1.33	1.37
32	Ss	612	CLA	CHC-C1C	2.89	1.42	1.35
32	GG	604	CLA	CHC-C1C	2.89	1.42	1.35
32	C	507	CLA	CHC-C1C	2.89	1.42	1.35
32	N	612	CLA	CHC-C1C	2.89	1.42	1.35
32	11	611	CLA	C4D-ND	-2.89	1.33	1.37
39	11	608	CHL	C4D-ND	-2.88	1.33	1.37
32	Dd	401	CLA	CHC-C1C	2.88	1.42	1.35
32	11	610	CLA	C4D-ND	-2.88	1.33	1.37
32	3	610	CLA	C4D-ND	-2.88	1.33	1.37
32	r	609	CLA	C4D-ND	-2.88	1.33	1.37
32	C	515	CLA	CHC-C1C	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	613	CLA	CHC-C1C	2.88	1.42	1.35
39	Ss	605	CHL	C4D-ND	-2.88	1.33	1.37
39	Y	608	CHL	C4D-ND	-2.88	1.33	1.37
32	R	612	CLA	CHC-C1C	2.88	1.42	1.35
32	C	503	CLA	CHC-C1C	2.88	1.42	1.35
32	b	614	CLA	CHC-C1C	2.88	1.42	1.35
32	Ss	610	CLA	CHC-C1C	2.88	1.42	1.35
32	Bb	611	CLA	CHC-C1C	2.88	1.42	1.35
39	Yy	601	CHL	C4D-ND	-2.88	1.33	1.37
39	Nn	317	CHL	C4D-ND	-2.88	1.33	1.37
32	A	406	CLA	CHC-C1C	2.88	1.42	1.35
39	G	607	CHL	C4D-ND	-2.88	1.33	1.37
32	b	604	CLA	CHC-C1C	2.88	1.42	1.35
32	22	610	CLA	C4D-ND	-2.88	1.33	1.37
32	Rr	612	CLA	CHC-C1C	2.88	1.42	1.35
32	R	603	CLA	CHC-C1C	2.87	1.42	1.35
32	Cc	506	CLA	CHC-C1C	2.87	1.42	1.35
32	Nn	303	CLA	C4D-ND	-2.87	1.33	1.37
32	R	614	CLA	CHC-C1C	2.87	1.42	1.35
39	RR	307	CHL	C4D-ND	-2.87	1.33	1.37
32	BB	614	CLA	CHC-C1C	2.87	1.42	1.35
32	r	601	CLA	C4D-ND	-2.87	1.33	1.37
39	YY	601	CHL	C4D-ND	-2.87	1.33	1.37
32	c	507	CLA	CHC-C1C	2.87	1.42	1.35
32	n	612	CLA	CHC-C1C	2.87	1.42	1.35
32	Y	603	CLA	CHC-C1C	2.87	1.42	1.35
32	44	603	CLA	CHC-C1C	2.87	1.42	1.35
39	Y	609	CHL	C4D-ND	-2.87	1.33	1.37
32	Cc	507	CLA	CHC-C1C	2.87	1.42	1.35
32	s	611	CLA	C4D-ND	-2.87	1.33	1.37
39	n	606	CHL	C4D-ND	-2.87	1.33	1.37
39	NN	609	CHL	C4D-ND	-2.87	1.33	1.37
32	Bb	614	CLA	CHC-C1C	2.87	1.42	1.35
32	c	511	CLA	CHC-C1C	2.87	1.42	1.35
39	y	311	CHL	C4D-ND	-2.86	1.33	1.37
32	B	610	CLA	CHC-C1C	2.86	1.42	1.35
32	Gg	303	CLA	CHC-C1C	2.86	1.42	1.35
33	A	407	PHO	CAC-C3C	-2.86	1.47	1.52
32	NN	603	CLA	CHC-C1C	2.86	1.42	1.35
32	Bb	606	CLA	CHC-C1C	2.86	1.42	1.35
39	y	303	CHL	C4D-ND	-2.86	1.33	1.37
39	YY	607	CHL	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	505	CLA	CHC-C1C	2.86	1.42	1.35
32	11	609	CLA	C4D-ND	-2.86	1.33	1.37
39	SS	308	CHL	C4D-ND	-2.86	1.33	1.37
32	Cc	513	CLA	CHC-C1C	2.86	1.42	1.35
32	44	615	CLA	C4D-ND	-2.86	1.33	1.37
39	Gg	302	CHL	C4D-ND	-2.86	1.33	1.37
32	r	610	CLA	C4D-ND	-2.86	1.33	1.37
39	r	607	CHL	C4D-ND	-2.86	1.33	1.37
32	RR	303	CLA	CHC-C1C	2.86	1.42	1.35
32	Bb	608	CLA	CHC-C1C	2.86	1.42	1.35
39	GG	601	CHL	C4D-ND	-2.86	1.33	1.37
32	r	610	CLA	CHC-C1C	2.86	1.42	1.35
32	r	603	CLA	C4D-ND	-2.86	1.33	1.37
39	s	605	CHL	C4D-ND	-2.86	1.33	1.37
32	s	610	CLA	CHC-C1C	2.86	1.42	1.35
32	y	306	CLA	CHC-C1C	2.85	1.42	1.35
39	y	310	CHL	C4D-ND	-2.85	1.33	1.37
39	Gg	309	CHL	C4D-ND	-2.85	1.33	1.37
32	g	603	CLA	CHC-C1C	2.85	1.42	1.35
39	NN	607	CHL	C4D-ND	-2.85	1.33	1.37
32	b	608	CLA	CHC-C1C	2.85	1.42	1.35
32	BB	606	CLA	CHC-C1C	2.85	1.42	1.35
32	11	604	CLA	C4D-ND	-2.85	1.33	1.37
32	GG	612	CLA	C4D-ND	-2.85	1.33	1.37
32	Cc	509	CLA	CHC-C1C	2.85	1.42	1.35
39	g	608	CHL	C4D-ND	-2.85	1.33	1.37
32	r	604	CLA	CHC-C1C	2.85	1.42	1.35
32	BB	612	CLA	CHC-C1C	2.85	1.42	1.35
39	44	606	CHL	C4D-ND	-2.85	1.33	1.37
32	B	621	CLA	CHC-C1C	2.85	1.42	1.35
32	CC	514	CLA	CHC-C1C	2.85	1.42	1.35
32	R	608	CLA	C4D-ND	-2.85	1.33	1.37
32	CC	512	CLA	CHC-C1C	2.85	1.42	1.35
32	33	609	CLA	C4D-ND	-2.85	1.33	1.37
32	Bb	612	CLA	CHC-C1C	2.85	1.42	1.35
39	R	605	CHL	C4D-ND	-2.85	1.33	1.37
32	B	608	CLA	CHC-C1C	2.85	1.42	1.35
39	n	609	CHL	C4D-ND	-2.85	1.33	1.37
32	B	606	CLA	CHC-C1C	2.84	1.42	1.35
39	S	607	CHL	C4D-ND	-2.84	1.33	1.37
32	C	510	CLA	CHC-C1C	2.84	1.42	1.35
32	GG	612	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	612	CLA	C4D-ND	-2.84	1.33	1.37
32	B	605	CLA	CHC-C1C	2.84	1.42	1.35
32	Aa	405	CLA	C4D-ND	-2.84	1.33	1.37
39	Nn	319	CHL	C4D-ND	-2.84	1.33	1.37
32	l	611	CLA	CHC-C1C	2.84	1.42	1.35
39	NN	608	CHL	C4D-ND	-2.84	1.33	1.37
35	A	410	PL9	C36-C34	2.84	1.57	1.51
39	N	609	CHL	C4D-ND	-2.84	1.33	1.37
32	YY	603	CLA	CHC-C1C	2.84	1.42	1.35
32	G	603	CLA	CHC-C1C	2.84	1.42	1.35
32	B	623	CLA	CHC-C1C	2.84	1.42	1.35
32	Y	610	CLA	C4D-ND	-2.84	1.33	1.37
39	RR	306	CHL	C4D-ND	-2.84	1.33	1.37
32	Rr	602	CLA	C4D-ND	-2.83	1.33	1.37
39	n	608	CHL	C4D-ND	-2.83	1.33	1.37
32	C	513	CLA	CHC-C1C	2.83	1.42	1.35
32	B	609	CLA	CHC-C1C	2.83	1.42	1.35
32	b	608	CLA	CMB-C2B	-2.83	1.45	1.51
32	Nn	304	CLA	CHC-C1C	2.83	1.42	1.35
39	Y	601	CHL	C4D-ND	-2.83	1.33	1.37
33	a	408	PHO	CAC-C3C	-2.83	1.47	1.52
32	b	612	CLA	CHC-C1C	2.83	1.42	1.35
32	n	610	CLA	C4D-ND	-2.83	1.33	1.37
32	CC	509	CLA	CHC-C1C	2.83	1.42	1.35
39	l1	601	CHL	C4D-ND	-2.83	1.33	1.37
32	Yy	604	CLA	CHC-C1C	2.83	1.42	1.35
32	BB	603	CLA	CHC-C1C	2.83	1.42	1.35
32	A	408	CLA	CHC-C1C	2.83	1.42	1.35
32	BB	611	CLA	CHC-C1C	2.83	1.42	1.35
32	Rr	603	CLA	C4D-ND	-2.82	1.33	1.37
39	g	609	CHL	C4D-ND	-2.82	1.33	1.37
39	N	605	CHL	C4D-ND	-2.82	1.33	1.37
39	NN	601	CHL	C4D-ND	-2.82	1.33	1.37
32	Rr	610	CLA	C4D-ND	-2.82	1.33	1.37
39	Rr	607	CHL	C4D-ND	-2.82	1.33	1.37
32	G	612	CLA	CHC-C1C	2.82	1.42	1.35
32	AA	405	CLA	CHC-C1C	2.82	1.42	1.35
32	c	504	CLA	CHC-C1C	2.82	1.42	1.35
32	Cc	514	CLA	CHC-C1C	2.82	1.42	1.35
32	B	620	CLA	CHC-C1C	2.82	1.42	1.35
39	G	606	CHL	C4D-ND	-2.82	1.33	1.37
39	Gg	308	CHL	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	44	605	CHL	C4D-ND	-2.82	1.33	1.37
32	SS	310	CLA	C4D-ND	-2.82	1.33	1.37
32	YY	613	CLA	CHC-C1C	2.82	1.42	1.35
32	Bb	605	CLA	CHC-C1C	2.82	1.42	1.35
39	YY	605	CHL	C4D-ND	-2.81	1.33	1.37
32	C	509	CLA	CHC-C1C	2.81	1.42	1.35
32	CC	504	CLA	CHC-C1C	2.81	1.42	1.35
39	n	607	CHL	C4D-ND	-2.81	1.33	1.37
32	s	603	CLA	CHC-C1C	2.81	1.42	1.35
32	b	602	CLA	CHC-C1C	2.81	1.42	1.35
32	c	512	CLA	CHC-C1C	2.81	1.42	1.35
39	33	608	CHL	C4D-ND	-2.81	1.33	1.37
39	G	609	CHL	C4D-ND	-2.81	1.33	1.37
39	g	601	CHL	C4D-ND	-2.81	1.33	1.37
39	g	607	CHL	C4D-ND	-2.81	1.33	1.37
39	y	309	CHL	C4D-ND	-2.81	1.33	1.37
32	A	405	CLA	CHC-C1C	2.81	1.42	1.35
32	D	405	CLA	CHC-C1C	2.81	1.42	1.35
32	CC	508	CLA	CHC-C1C	2.81	1.42	1.35
32	C	514	CLA	CHC-C1C	2.81	1.42	1.35
32	c	511	CLA	C3B-C2B	-2.80	1.36	1.40
32	CC	513	CLA	CHC-C1C	2.80	1.42	1.35
39	Rr	605	CHL	C4D-ND	-2.80	1.33	1.37
39	Gg	310	CHL	C4D-ND	-2.80	1.33	1.37
39	S	605	CHL	C4D-ND	-2.80	1.33	1.37
35	AA	410	PL9	C36-C34	2.80	1.57	1.51
32	Gg	313	CLA	C4D-ND	-2.80	1.33	1.37
32	Rr	604	CLA	CHC-C1C	2.80	1.42	1.35
39	Nn	316	CHL	C4D-ND	-2.80	1.33	1.37
32	Gg	304	CLA	CHC-C1C	2.79	1.42	1.35
39	R	607	CHL	C4D-ND	-2.79	1.33	1.37
32	a	406	CLA	CHC-C1C	2.79	1.42	1.35
32	Gg	313	CLA	CHC-C1C	2.79	1.42	1.35
32	S	608	CLA	C4D-ND	-2.79	1.33	1.37
39	Yy	608	CHL	C4D-ND	-2.79	1.33	1.37
39	1	601	CHL	C4D-ND	-2.79	1.33	1.37
32	BB	604	CLA	CHC-C1C	2.79	1.42	1.35
32	Nn	303	CLA	CHC-C1C	2.79	1.42	1.35
32	N	613	CLA	CHC-C1C	2.79	1.42	1.35
32	Nn	313	CLA	CHC-C1C	2.78	1.42	1.35
32	Cc	503	CLA	CHC-C1C	2.78	1.42	1.35
32	c	511	CLA	CMB-C2B	-2.78	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DD	402	PHO	CAC-C3C	-2.78	1.47	1.52
39	R	606	CHL	C4D-ND	-2.78	1.33	1.37
32	a	405	CLA	CHC-C1C	2.78	1.42	1.35
32	Gg	314	CLA	CHC-C1C	2.78	1.42	1.35
32	Y	613	CLA	CHC-C1C	2.78	1.42	1.35
32	G	610	CLA	CHC-C1C	2.78	1.42	1.35
32	g	602	CLA	CMB-C2B	-2.78	1.45	1.51
32	2	613	CLA	C4D-ND	-2.78	1.33	1.37
32	b	605	CLA	CHC-C1C	2.77	1.42	1.35
39	22	606	CHL	C4D-ND	-2.77	1.33	1.37
39	N	601	CHL	C4D-ND	-2.77	1.33	1.37
32	BB	607	CLA	CHC-C1C	2.77	1.42	1.35
32	1	603	CLA	CHC-C1C	2.77	1.42	1.35
39	s	601	CHL	C4D-ND	-2.77	1.33	1.37
39	y	307	CHL	C4D-ND	-2.77	1.33	1.37
39	Ss	601	CHL	C4D-ND	-2.77	1.33	1.37
39	3	608	CHL	C4D-ND	-2.77	1.33	1.37
39	S	606	CHL	C4D-ND	-2.77	1.33	1.37
32	R	601	CLA	CHC-C1C	2.77	1.42	1.35
32	11	613	CLA	C4D-ND	-2.77	1.33	1.37
39	33	607	CHL	C4D-ND	-2.76	1.33	1.37
32	1	609	CLA	CHC-C1C	2.76	1.42	1.35
39	1	607	CHL	C4D-ND	-2.76	1.33	1.37
39	22	608	CHL	C4D-ND	-2.76	1.33	1.37
32	n	613	CLA	CMB-C2B	-2.76	1.45	1.51
32	GG	602	CLA	CHC-C1C	2.76	1.42	1.35
32	Aa	405	CLA	CHC-C1C	2.76	1.42	1.35
32	g	612	CLA	CHC-C1C	2.75	1.42	1.35
32	c	501	CLA	CHC-C1C	2.75	1.42	1.35
33	D	402	PHO	CAC-C3C	-2.75	1.47	1.52
32	y	305	CLA	CHC-C1C	2.75	1.42	1.35
35	d	404	PL9	C36-C34	2.75	1.57	1.51
32	Yy	603	CLA	CHC-C1C	2.75	1.42	1.35
39	Gg	306	CHL	C4D-ND	-2.75	1.33	1.37
39	N	607	CHL	C4D-ND	-2.75	1.33	1.37
39	4	306	CHL	C4D-ND	-2.75	1.33	1.37
39	Nn	315	CHL	C4D-ND	-2.75	1.33	1.37
32	n	613	CLA	CHC-C1C	2.75	1.42	1.35
39	4	308	CHL	C4D-ND	-2.74	1.33	1.37
32	DD	401	CLA	CMB-C2B	-2.74	1.45	1.51
32	g	613	CLA	CHC-C1C	2.74	1.42	1.35
39	2	605	CHL	C4D-ND	-2.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	SS	307	CHL	C4D-ND	-2.74	1.33	1.37
35	DD	406	PL9	C36-C34	2.74	1.57	1.51
39	44	607	CHL	C4D-ND	-2.74	1.33	1.37
39	3	607	CHL	C4D-ND	-2.74	1.33	1.37
32	GG	603	CLA	CHC-C1C	2.74	1.42	1.35
39	22	607	CHL	C4D-ND	-2.73	1.33	1.37
39	2	606	CHL	C4D-ND	-2.73	1.33	1.37
32	NN	613	CLA	CHC-C1C	2.73	1.42	1.35
32	N	613	CLA	CMB-C2B	-2.73	1.46	1.51
32	4	304	CLA	CHC-C1C	2.73	1.42	1.35
32	B	624	CLA	CHC-C1C	2.73	1.42	1.35
32	G	612	CLA	C4D-ND	-2.73	1.33	1.37
39	1	606	CHL	C4D-ND	-2.73	1.33	1.37
32	y	315	CLA	CHC-C1C	2.72	1.42	1.35
35	D	407	PL9	C36-C34	2.72	1.57	1.51
39	33	605	CHL	C4D-ND	-2.72	1.33	1.37
35	Dd	404	PL9	C36-C34	2.72	1.57	1.51
39	NN	605	CHL	C4D-ND	-2.72	1.33	1.37
39	S	601	CHL	C4D-ND	-2.72	1.33	1.37
32	B	607	CLA	CMB-C2B	-2.72	1.46	1.51
39	GG	608	CHL	C4D-ND	-2.72	1.33	1.37
32	Yy	613	CLA	CHC-C1C	2.72	1.41	1.35
32	G	602	CLA	CHC-C1C	2.71	1.41	1.35
35	AA	410	PL9	C21-C19	2.71	1.56	1.51
39	11	606	CHL	C4D-ND	-2.71	1.34	1.37
39	SS	302	CHL	C4D-ND	-2.71	1.34	1.37
39	r	605	CHL	C4D-ND	-2.71	1.34	1.37
39	33	606	CHL	C4D-ND	-2.71	1.34	1.37
39	g	605	CHL	C4D-ND	-2.71	1.34	1.37
39	2	607	CHL	C4D-ND	-2.70	1.34	1.37
32	GG	613	CLA	CHC-C1C	2.70	1.41	1.35
32	Yy	612	CLA	CHC-C1C	2.70	1.41	1.35
39	4	302	CHL	C4D-ND	-2.70	1.34	1.37
32	3	609	CLA	C4D-ND	-2.70	1.34	1.37
39	3	605	CHL	C4D-ND	-2.70	1.34	1.37
32	D	401	CLA	CMB-C2B	-2.69	1.46	1.51
39	3	606	CHL	C4D-ND	-2.69	1.34	1.37
32	y	314	CLA	CHC-C1C	2.69	1.41	1.35
32	n	603	CLA	CHC-C1C	2.69	1.41	1.35
39	2	608	CHL	C4D-ND	-2.69	1.34	1.37
39	G	605	CHL	C4D-ND	-2.69	1.34	1.37
32	g	602	CLA	CHC-C1C	2.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	602	CLA	C3B-C2B	-2.69	1.36	1.40
32	1	613	CLA	C4D-ND	-2.69	1.34	1.37
39	11	607	CHL	C4D-ND	-2.69	1.34	1.37
32	BB	611	CLA	CMD-C2D	-2.68	1.45	1.50
39	Nn	311	CHL	C4D-ND	-2.68	1.34	1.37
32	Nn	304	CLA	CMB-C2B	-2.68	1.46	1.51
32	R	601	CLA	CMB-C2B	-2.68	1.46	1.51
32	YY	611	CLA	C1D-ND	2.68	1.41	1.37
32	BB	602	CLA	CMB-C2B	-2.67	1.46	1.51
39	2	601	CHL	C4D-ND	-2.67	1.34	1.37
32	Bb	610	CLA	CMB-C2B	-2.67	1.46	1.51
39	44	601	CHL	C4D-ND	-2.67	1.34	1.37
39	Y	605	CHL	C4D-ND	-2.67	1.34	1.37
33	a	409	PHO	CAC-C3C	-2.67	1.47	1.52
39	Ss	607	CHL	C4D-ND	-2.67	1.34	1.37
39	GG	605	CHL	C4D-ND	-2.66	1.34	1.37
39	1	605	CHL	C4D-ND	-2.66	1.34	1.37
39	G	608	CHL	C4D-ND	-2.66	1.34	1.37
32	B	607	CLA	CMD-C2D	-2.66	1.45	1.50
32	BB	604	CLA	CMB-C2B	-2.66	1.46	1.51
39	s	606	CHL	C4D-ND	-2.66	1.34	1.37
40	22	614	LUT	C32-C33	2.66	1.51	1.45
32	N	610	CLA	C3B-C2B	-2.65	1.36	1.40
32	BB	604	CLA	C3B-C2B	-2.65	1.36	1.40
39	22	605	CHL	C4D-ND	-2.65	1.34	1.37
32	RR	302	CLA	CMB-C2B	-2.65	1.46	1.51
32	BB	611	CLA	CMB-C2B	-2.65	1.46	1.51
32	Bb	608	CLA	CMB-C2B	-2.64	1.46	1.51
32	11	612	CLA	C3B-CAB	-2.64	1.42	1.47
39	Ss	606	CHL	C4D-ND	-2.64	1.34	1.37
35	AA	410	PL9	C7-C8	2.64	1.54	1.50
32	B	621	CLA	CMB-C2B	-2.64	1.46	1.51
39	Yy	607	CHL	C4D-ND	-2.64	1.34	1.37
32	B	606	CLA	CMB-C2B	-2.64	1.46	1.51
39	SS	306	CHL	C4D-ND	-2.64	1.34	1.37
32	g	613	CLA	C3B-C2B	-2.63	1.36	1.40
32	B	624	CLA	CMB-C2B	-2.63	1.46	1.51
39	22	601	CHL	C4D-ND	-2.62	1.34	1.37
32	Rr	610	CLA	CMB-C2B	-2.62	1.46	1.51
39	11	605	CHL	C1B-NB	2.62	1.37	1.35
32	GG	602	CLA	CMB-C2B	-2.61	1.46	1.51
32	Bb	612	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	RR	314	CLA	C4D-ND	-2.61	1.34	1.37
32	C	508	CLA	CMB-C2B	-2.61	1.46	1.51
32	b	612	CLA	CMB-C2B	-2.61	1.46	1.51
32	g	610	CLA	C3B-C2B	-2.61	1.36	1.40
32	CC	502	CLA	CMB-C2B	-2.60	1.46	1.51
32	11	612	CLA	CMB-C2B	-2.60	1.46	1.51
32	1	609	CLA	C4D-ND	-2.60	1.34	1.37
32	g	610	CLA	CMB-C2B	-2.60	1.46	1.51
32	b	610	CLA	CMB-C2B	-2.59	1.46	1.51
32	BB	610	CLA	CMB-C2B	-2.59	1.46	1.51
42	g	617	NEX	C28-C29	2.59	1.51	1.45
32	G	610	CLA	CMB-C2B	-2.59	1.46	1.51
39	s	607	CHL	C4D-ND	-2.59	1.34	1.37
33	Aa	409	PHO	CAC-C3C	-2.59	1.47	1.52
32	G	602	CLA	CMB-C2B	-2.58	1.46	1.51
32	X	201	CLA	CMB-C2B	-2.58	1.46	1.51
32	C	506	CLA	CMB-C2B	-2.58	1.46	1.51
32	C	503	CLA	CMB-C2B	-2.58	1.46	1.51
32	B	622	CLA	CMB-C2B	-2.58	1.46	1.51
32	11	612	CLA	MG-NC	2.57	2.12	2.06
32	Cc	513	CLA	CMB-C2B	-2.57	1.46	1.51
32	Bb	603	CLA	CMB-C2B	-2.57	1.46	1.51
32	B	619	CLA	CMB-C2B	-2.57	1.46	1.51
32	Aa	406	CLA	CMB-C2B	-2.57	1.46	1.51
32	BB	605	CLA	CMB-C2B	-2.57	1.46	1.51
32	d	402	CLA	CMB-C2B	-2.57	1.46	1.51
32	CC	508	CLA	CMB-C2B	-2.56	1.46	1.51
32	YY	612	CLA	C3B-C2B	-2.56	1.36	1.40
32	a	406	CLA	CMB-C2B	-2.56	1.46	1.51
32	C	509	CLA	CMB-C2B	-2.56	1.46	1.51
32	11	612	CLA	C4D-ND	-2.55	1.34	1.37
32	y	305	CLA	CMB-C2B	-2.55	1.46	1.51
41	Gg	301	XAT	C32-C33	2.55	1.51	1.45
35	A	410	PL9	C21-C19	2.55	1.56	1.51
32	NN	603	CLA	CMB-C2B	-2.55	1.46	1.51
32	g	611	CLA	CMB-C2B	-2.55	1.46	1.51
32	B	621	CLA	C3B-C2B	-2.55	1.36	1.40
32	Yy	603	CLA	CMB-C2B	-2.54	1.46	1.51
32	g	603	CLA	C3B-C2B	-2.54	1.36	1.40
32	Cc	503	CLA	C3B-C2B	-2.54	1.36	1.40
35	A	410	PL9	C7-C8	2.54	1.54	1.50
32	AA	408	CLA	C3B-C2B	-2.54	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CC	507	CLA	CMB-C2B	-2.54	1.46	1.51
32	R	614	CLA	C4D-ND	-2.53	1.34	1.37
32	Yy	604	CLA	CMB-C2B	-2.53	1.46	1.51
32	AA	405	CLA	CMB-C2B	-2.53	1.46	1.51
32	Aa	407	CLA	CMB-C2B	-2.53	1.46	1.51
32	b	613	CLA	CMB-C2B	-2.53	1.46	1.51
32	DD	403	CLA	CMB-C2B	-2.53	1.46	1.51
32	Dd	402	CLA	CMB-C2B	-2.53	1.46	1.51
32	Rr	613	CLA	CMB-C2B	-2.53	1.46	1.51
32	a	407	CLA	CMB-C2B	-2.53	1.46	1.51
32	Bb	613	CLA	CMB-C2B	-2.53	1.46	1.51
36	4	315	LHG	O8-C23	2.53	1.45	1.33
32	11	612	CLA	C3B-C2B	-2.53	1.36	1.40
32	C	513	CLA	CMB-C2B	-2.53	1.46	1.51
32	b	604	CLA	CMB-C2B	-2.53	1.46	1.51
32	CC	505	CLA	CMB-C2B	-2.53	1.46	1.51
32	RR	309	CLA	C3B-C2B	-2.53	1.36	1.40
32	CC	509	CLA	CMB-C2B	-2.53	1.46	1.51
32	y	312	CLA	C3B-C2B	-2.53	1.36	1.40
41	g	619	XAT	C32-C33	2.53	1.51	1.45
32	N	603	CLA	CMB-C2B	-2.53	1.46	1.51
32	RR	314	CLA	C3B-C2B	-2.52	1.36	1.40
32	Aa	410	CLA	C3B-C2B	-2.52	1.36	1.40
32	BB	607	CLA	CMB-C2B	-2.52	1.46	1.51
32	AA	406	CLA	CMB-C2B	-2.52	1.46	1.51
35	A	410	PL9	C41-C39	2.52	1.56	1.51
32	b	606	CLA	CMB-C2B	-2.52	1.46	1.51
32	c	501	CLA	C3B-C2B	-2.52	1.36	1.40
32	C	510	CLA	CMB-C2B	-2.52	1.46	1.51
32	a	405	CLA	CMB-C2B	-2.52	1.46	1.51
32	BB	603	CLA	CMB-C2B	-2.51	1.46	1.51
32	GG	602	CLA	C3B-C2B	-2.51	1.36	1.40
32	CC	512	CLA	C3B-C2B	-2.51	1.36	1.40
32	RR	308	CLA	CMB-C2B	-2.51	1.46	1.51
32	SS	311	CLA	CMB-C2B	-2.51	1.46	1.51
32	C	511	CLA	CMB-C2B	-2.51	1.46	1.51
32	Ss	604	CLA	CMB-C2B	-2.51	1.46	1.51
32	YY	611	CLA	MG-ND	-2.51	2.00	2.05
32	2	604	CLA	CMB-C2B	-2.51	1.46	1.51
32	C	512	CLA	CMB-C2B	-2.50	1.46	1.51
32	CC	512	CLA	CMB-C2B	-2.50	1.46	1.51
32	A	408	CLA	C3B-C2B	-2.50	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Rr	602	CLA	CMB-C2B	-2.50	1.46	1.51
32	RR	304	CLA	CMB-C2B	-2.50	1.46	1.51
32	YY	612	CLA	CHC-C1C	2.50	1.41	1.35
32	22	609	CLA	CMB-C2B	-2.50	1.46	1.51
32	Rr	603	CLA	CMB-C2B	-2.50	1.46	1.51
32	G	602	CLA	C3B-C2B	-2.50	1.36	1.40
32	C	515	CLA	CMB-C2B	-2.50	1.46	1.51
32	R	608	CLA	CMB-C2B	-2.50	1.46	1.51
32	Bb	604	CLA	CMB-C2B	-2.50	1.46	1.51
32	b	602	CLA	CMB-C2B	-2.50	1.46	1.51
32	Bb	606	CLA	CMB-C2B	-2.49	1.46	1.51
32	Y	603	CLA	CMB-C2B	-2.49	1.46	1.51
32	S	610	CLA	CMB-C2B	-2.49	1.46	1.51
32	GG	612	CLA	CMB-C2B	-2.49	1.46	1.51
32	Bb	605	CLA	CMB-C2B	-2.49	1.46	1.51
37	BB	621	SQD	C6-S	-2.49	1.68	1.77
32	B	620	CLA	CMB-C2B	-2.49	1.46	1.51
36	44	614	LHG	O8-C23	2.49	1.45	1.33
32	BB	609	CLA	CMB-C2B	-2.49	1.46	1.51
32	B	605	CLA	CMB-C2B	-2.49	1.46	1.51
32	Nn	312	CLA	CMB-C2B	-2.49	1.46	1.51
32	B	619	CLA	C3B-C2B	-2.49	1.36	1.40
32	CC	510	CLA	CMB-C2B	-2.49	1.46	1.51
32	Cc	504	CLA	CMB-C2B	-2.49	1.46	1.51
35	AA	410	PL9	C41-C39	2.48	1.56	1.51
32	y	306	CLA	CMB-C2B	-2.48	1.46	1.51
32	A	406	CLA	CMB-C2B	-2.48	1.46	1.51
32	s	604	CLA	CMB-C2B	-2.48	1.46	1.51
42	Gg	318	NEX	C28-C29	2.48	1.51	1.45
32	YY	614	CLA	CMB-C2B	-2.48	1.46	1.51
32	c	512	CLA	CMB-C2B	-2.48	1.46	1.51
32	Cc	511	CLA	CMB-C2B	-2.48	1.46	1.51
32	CC	510	CLA	C3B-C2B	-2.48	1.36	1.40
32	44	602	CLA	CMB-C2B	-2.48	1.46	1.51
32	Gg	312	CLA	CMB-C2B	-2.48	1.46	1.51
32	y	304	CLA	CMB-C2B	-2.48	1.46	1.51
32	RR	309	CLA	CMB-C2B	-2.48	1.46	1.51
32	y	314	CLA	C3B-C2B	-2.48	1.36	1.40
32	r	603	CLA	CMB-C2B	-2.48	1.46	1.51
32	SS	314	CLA	CMB-C2B	-2.48	1.46	1.51
37	B	617	SQD	C6-S	-2.48	1.68	1.77
32	Cc	507	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Yy	613	CLA	C3B-C2B	-2.47	1.36	1.40
32	Aa	405	CLA	CMB-C2B	-2.47	1.46	1.51
32	NN	613	CLA	CMB-C2B	-2.47	1.46	1.51
32	CC	505	CLA	C3B-C2B	-2.47	1.36	1.40
32	Cc	513	CLA	C3B-C2B	-2.47	1.36	1.40
32	r	613	CLA	CMB-C2B	-2.47	1.46	1.51
32	c	503	CLA	CMB-C2B	-2.47	1.46	1.51
32	CC	511	CLA	C3B-C2B	-2.47	1.36	1.40
32	A	405	CLA	CMB-C2B	-2.47	1.46	1.51
32	C	514	CLA	CMB-C2B	-2.47	1.46	1.51
32	DD	404	CLA	CMB-C2B	-2.47	1.46	1.51
35	Dd	404	PL9	C7-C8	2.47	1.54	1.50
32	a	410	CLA	C3B-C2B	-2.47	1.36	1.40
32	g	604	CLA	CMB-C2B	-2.47	1.46	1.51
32	D	405	CLA	CMB-C2B	-2.47	1.46	1.51
32	Y	614	CLA	CMB-C2B	-2.47	1.46	1.51
39	g	605	CHL	C1B-NB	2.47	1.37	1.35
32	Cc	510	CLA	CMB-C2B	-2.46	1.46	1.51
32	c	509	CLA	CMB-C2B	-2.46	1.46	1.51
32	BB	608	CLA	CMB-C2B	-2.46	1.46	1.51
32	Yy	602	CLA	CMB-C2B	-2.46	1.46	1.51
32	G	612	CLA	CMB-C2B	-2.46	1.46	1.51
32	b	601	CLA	CMB-C2B	-2.46	1.46	1.51
32	CC	504	CLA	CMB-C2B	-2.46	1.46	1.51
32	n	602	CLA	CMB-C2B	-2.46	1.46	1.51
32	YY	603	CLA	CMB-C2B	-2.46	1.46	1.51
32	2	603	CLA	CMB-C2B	-2.46	1.46	1.51
32	SS	303	CLA	CMB-C2B	-2.46	1.46	1.51
32	Y	602	CLA	CMB-C2B	-2.46	1.46	1.51
32	c	501	CLA	CMB-C2B	-2.46	1.46	1.51
32	a	410	CLA	CMB-C2B	-2.46	1.46	1.51
32	R	604	CLA	CMB-C2B	-2.46	1.46	1.51
32	Aa	410	CLA	CMB-C2B	-2.46	1.46	1.51
32	R	602	CLA	CMB-C2B	-2.46	1.46	1.51
32	BB	602	CLA	C3B-C2B	-2.46	1.37	1.40
32	Bb	601	CLA	CMB-C2B	-2.45	1.46	1.51
32	Y	612	CLA	CMB-C2B	-2.45	1.46	1.51
32	GG	604	CLA	CMB-C2B	-2.45	1.46	1.51
32	Gg	315	CLA	CMB-C2B	-2.45	1.46	1.51
32	NN	610	CLA	C3B-C2B	-2.45	1.37	1.40
32	R	614	CLA	C3B-C2B	-2.45	1.37	1.40
32	b	603	CLA	C3B-C2B	-2.45	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Yy	610	CLA	CMB-C2B	-2.45	1.46	1.51
32	b	605	CLA	CMB-C2B	-2.45	1.46	1.51
32	AA	408	CLA	CMB-C2B	-2.45	1.46	1.51
32	Dd	401	CLA	CMB-C2B	-2.45	1.46	1.51
32	CC	506	CLA	CMB-C2B	-2.45	1.46	1.51
32	Yy	610	CLA	C3B-C2B	-2.45	1.37	1.40
34	Hh	101	BCR	C19-C18	2.44	1.51	1.45
32	1	612	CLA	CMB-C2B	-2.44	1.46	1.51
32	B	604	CLA	CMB-C2B	-2.44	1.46	1.51
32	Cc	505	CLA	CMB-C2B	-2.44	1.46	1.51
39	y	310	CHL	CMB-C2B	-2.44	1.46	1.51
32	33	604	CLA	CMB-C2B	-2.44	1.46	1.51
32	g	612	CLA	CMB-C2B	-2.44	1.46	1.51
32	y	313	CLA	CMB-C2B	-2.44	1.46	1.51
32	R	611	CLA	CMB-C2B	-2.44	1.46	1.51
32	Nn	314	CLA	CMB-C2B	-2.44	1.46	1.51
32	RR	311	CLA	CMB-C2B	-2.44	1.46	1.51
32	C	511	CLA	C3B-C2B	-2.44	1.37	1.40
32	Y	612	CLA	C3B-C2B	-2.44	1.37	1.40
35	DD	406	PL9	C7-C8	2.44	1.54	1.50
32	44	604	CLA	CMB-C2B	-2.44	1.46	1.51
32	CC	511	CLA	CMB-C2B	-2.44	1.46	1.51
40	2	614	LUT	C32-C33	2.44	1.51	1.45
32	CC	514	CLA	CMB-C2B	-2.44	1.46	1.51
32	Yy	611	CLA	CMB-C2B	-2.44	1.46	1.51
32	4	305	CLA	CMB-C2B	-2.44	1.46	1.51
32	Bb	616	CLA	CMB-C2B	-2.44	1.46	1.51
32	Bb	607	CLA	CMB-C2B	-2.44	1.46	1.51
32	Yy	612	CLA	CMB-C2B	-2.44	1.46	1.51
32	b	607	CLA	CMB-C2B	-2.44	1.46	1.51
32	Rr	604	CLA	C3B-C2B	-2.44	1.37	1.40
39	G	605	CHL	C1B-NB	2.43	1.37	1.35
32	S	613	CLA	CMB-C2B	-2.43	1.46	1.51
32	Bb	611	CLA	CMB-C2B	-2.43	1.46	1.51
32	Y	613	CLA	C3B-C2B	-2.43	1.37	1.40
32	Rr	612	CLA	CMB-C2B	-2.43	1.46	1.51
32	c	505	CLA	CMB-C2B	-2.43	1.46	1.51
32	BB	615	CLA	CMB-C2B	-2.43	1.46	1.51
32	Gg	304	CLA	C3B-C2B	-2.43	1.37	1.40
35	DD	406	PL9	C21-C19	2.43	1.56	1.51
32	b	603	CLA	CMB-C2B	-2.43	1.46	1.51
32	c	510	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	609	CLA	CMB-C2B	-2.43	1.46	1.51
32	Cc	515	CLA	CMB-C2B	-2.43	1.46	1.51
32	DD	401	CLA	C3B-C2B	-2.43	1.37	1.40
32	2	609	CLA	CMB-C2B	-2.43	1.46	1.51
32	Cc	509	CLA	CMB-C2B	-2.43	1.46	1.51
32	33	602	CLA	CMB-C2B	-2.43	1.46	1.51
32	s	612	CLA	CMB-C2B	-2.43	1.46	1.51
32	RR	313	CLA	CMB-C2B	-2.43	1.46	1.51
32	N	602	CLA	CMB-C2B	-2.43	1.46	1.51
32	NN	602	CLA	CMB-C2B	-2.43	1.46	1.51
32	R	613	CLA	CMB-C2B	-2.43	1.46	1.51
32	b	609	CLA	CMB-C2B	-2.43	1.46	1.51
32	R	609	CLA	CMB-C2B	-2.43	1.46	1.51
32	Y	610	CLA	CMB-C2B	-2.43	1.46	1.51
32	b	611	CLA	CMB-C2B	-2.42	1.46	1.51
32	n	613	CLA	C3B-C2B	-2.42	1.37	1.40
34	h	101	BCR	C19-C18	2.42	1.51	1.45
32	4	304	CLA	CMB-C2B	-2.42	1.46	1.51
32	Cc	514	CLA	CMB-C2B	-2.42	1.46	1.51
32	1	609	CLA	C3B-C2B	-2.42	1.37	1.40
32	CC	503	CLA	CMB-C2B	-2.42	1.46	1.51
32	33	611	CLA	CMB-C2B	-2.42	1.46	1.51
32	c	508	CLA	CMB-C2B	-2.42	1.46	1.51
32	YY	602	CLA	CMB-C2B	-2.42	1.46	1.51
39	Gg	306	CHL	C1B-NB	2.42	1.37	1.35
32	Cc	512	CLA	CMB-C2B	-2.42	1.46	1.51
32	11	604	CLA	CMB-C2B	-2.42	1.46	1.51
32	C	505	CLA	CMB-C2B	-2.42	1.46	1.51
32	Gg	313	CLA	CMB-C2B	-2.42	1.46	1.51
32	c	507	CLA	CMB-C2B	-2.42	1.46	1.51
34	H	101	BCR	C8-C9	2.42	1.51	1.45
32	YY	613	CLA	CMB-C2B	-2.42	1.46	1.51
32	y	306	CLA	C3B-C2B	-2.42	1.37	1.40
32	B	609	CLA	CMB-C2B	-2.42	1.46	1.51
32	Gg	305	CLA	CMB-C2B	-2.42	1.46	1.51
32	Yy	614	CLA	CMB-C2B	-2.41	1.46	1.51
32	s	610	CLA	CMB-C2B	-2.41	1.46	1.51
32	Rr	611	CLA	CMB-C2B	-2.41	1.46	1.51
32	C	507	CLA	CMB-C2B	-2.41	1.46	1.51
32	4	312	CLA	CMB-C2B	-2.41	1.46	1.51
39	33	601	CHL	C1B-NB	2.41	1.37	1.35
32	y	315	CLA	C3B-C2B	-2.41	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	506	CLA	C3B-C2B	-2.41	1.37	1.40
32	y	316	CLA	CMB-C2B	-2.41	1.46	1.51
32	YY	610	CLA	CMB-C2B	-2.41	1.46	1.51
32	GG	611	CLA	CMB-C2B	-2.41	1.46	1.51
32	Bb	602	CLA	CMB-C2B	-2.41	1.46	1.51
32	Gg	303	CLA	CMB-C2B	-2.41	1.46	1.51
32	l	604	CLA	CMB-C2B	-2.41	1.46	1.51
32	C	513	CLA	C3B-C2B	-2.41	1.37	1.40
32	g	614	CLA	CMB-C2B	-2.41	1.46	1.51
32	Ss	609	CLA	CMB-C2B	-2.41	1.46	1.51
32	C	504	CLA	CMB-C2B	-2.41	1.46	1.51
32	Rr	609	CLA	CMB-C2B	-2.41	1.46	1.51
41	G	619	XAT	C32-C33	2.41	1.51	1.45
35	d	404	PL9	C7-C8	2.41	1.54	1.50
32	BB	614	CLA	CMB-C2B	-2.41	1.46	1.51
39	3	608	CHL	C1B-NB	2.40	1.37	1.35
32	A	408	CLA	CMB-C2B	-2.40	1.46	1.51
32	S	609	CLA	CMB-C2B	-2.40	1.46	1.51
32	B	623	CLA	CMB-C2B	-2.40	1.46	1.51
32	Aa	405	CLA	C3B-C2B	-2.40	1.37	1.40
32	Cc	506	CLA	CMB-C2B	-2.40	1.46	1.51
32	y	312	CLA	CMB-C2B	-2.40	1.46	1.51
32	Nn	302	CLA	CMB-C2B	-2.40	1.46	1.51
32	SS	305	CLA	CMB-C2B	-2.40	1.46	1.51
32	c	502	CLA	CMB-C2B	-2.40	1.46	1.51
32	3	602	CLA	CMB-C2B	-2.40	1.46	1.51
32	Cc	508	CLA	CMB-C2B	-2.40	1.46	1.51
32	B	618	CLA	CMB-C2B	-2.40	1.46	1.51
32	g	604	CLA	C3B-C2B	-2.40	1.37	1.40
32	N	604	CLA	CMB-C2B	-2.40	1.46	1.51
32	c	513	CLA	CMB-C2B	-2.40	1.46	1.51
32	Rr	608	CLA	CMB-C2B	-2.40	1.46	1.51
32	Yy	604	CLA	C3B-C2B	-2.40	1.37	1.40
32	g	603	CLA	CMB-C2B	-2.40	1.46	1.51
32	N	614	CLA	CMB-C2B	-2.40	1.46	1.51
32	Yy	613	CLA	CMB-C2B	-2.40	1.46	1.51
32	R	612	CLA	CMB-C2B	-2.40	1.46	1.51
32	y	314	CLA	CMB-C2B	-2.40	1.46	1.51
32	YY	611	CLA	CMB-C2B	-2.40	1.46	1.51
35	D	407	PL9	C7-C8	2.39	1.54	1.50
32	3	604	CLA	CMB-C2B	-2.39	1.46	1.51
32	CC	513	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	611	CLA	CMB-C2B	-2.39	1.46	1.51
32	RR	314	CLA	CMB-C2B	-2.39	1.46	1.51
32	b	616	CLA	CMB-C2B	-2.39	1.46	1.51
32	r	608	CLA	CMB-C2B	-2.39	1.46	1.51
32	4	310	CLA	C3B-C2B	-2.39	1.37	1.40
32	B	623	CLA	C3B-C2B	-2.39	1.37	1.40
32	22	604	CLA	CMB-C2B	-2.39	1.46	1.51
32	GG	614	CLA	CMB-C2B	-2.39	1.46	1.51
32	11	611	CLA	CMB-C2B	-2.39	1.46	1.51
32	BB	601	CLA	CMB-C2B	-2.39	1.46	1.51
39	n	605	CHL	C4D-ND	-2.39	1.34	1.37
32	r	610	CLA	CMB-C2B	-2.39	1.46	1.51
32	Bb	606	CLA	C3B-C2B	-2.39	1.37	1.40
32	33	609	CLA	CMB-C2B	-2.39	1.46	1.51
32	4	303	CLA	CMB-C2B	-2.38	1.46	1.51
32	YY	612	CLA	CMB-C2B	-2.38	1.46	1.51
32	Nn	313	CLA	CMB-C2B	-2.38	1.46	1.51
32	YY	610	CLA	C3B-C2B	-2.38	1.37	1.40
32	Bb	603	CLA	C3B-C2B	-2.38	1.37	1.40
32	Rr	604	CLA	CMB-C2B	-2.38	1.46	1.51
32	R	614	CLA	CMB-C2B	-2.38	1.46	1.51
32	b	615	CLA	CMB-C2B	-2.38	1.46	1.51
32	n	603	CLA	CMB-C2B	-2.38	1.46	1.51
32	BB	606	CLA	CMB-C2B	-2.38	1.46	1.51
32	Ss	602	CLA	CMB-C2B	-2.38	1.46	1.51
32	r	604	CLA	C3B-C2B	-2.38	1.37	1.40
32	a	406	CLA	MG-NA	2.38	2.11	2.06
32	NN	614	CLA	CMB-C2B	-2.38	1.46	1.51
32	44	611	CLA	CMB-C2B	-2.38	1.46	1.51
32	n	602	CLA	C3B-C2B	-2.38	1.37	1.40
32	Gg	304	CLA	CMB-C2B	-2.38	1.46	1.51
39	33	605	CHL	C1B-NB	2.38	1.37	1.35
32	Ss	610	CLA	CMB-C2B	-2.38	1.46	1.51
32	a	405	CLA	C3B-C2B	-2.38	1.37	1.40
32	XX	201	CLA	C3B-C2B	-2.38	1.37	1.40
32	22	610	CLA	CMB-C2B	-2.38	1.46	1.51
32	r	609	CLA	CMB-C2B	-2.38	1.46	1.51
32	SS	313	CLA	CMB-C2B	-2.38	1.46	1.51
32	Ss	612	CLA	CMB-C2B	-2.38	1.46	1.51
32	22	612	CLA	CMB-C2B	-2.38	1.46	1.51
32	b	608	CLA	C3B-C2B	-2.38	1.37	1.40
32	44	603	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	R	609	CLA	C3B-C2B	-2.38	1.37	1.40
32	33	603	CLA	CMB-C2B	-2.38	1.46	1.51
32	11	603	CLA	CMB-C2B	-2.37	1.46	1.51
32	4	311	CLA	CMB-C2B	-2.37	1.46	1.51
35	D	407	PL9	C21-C19	2.37	1.56	1.51
32	D	404	CLA	CMB-C2B	-2.37	1.46	1.51
32	11	613	CLA	CMB-C2B	-2.37	1.46	1.51
32	NN	604	CLA	CMB-C2B	-2.37	1.46	1.51
32	G	603	CLA	CMB-C2B	-2.37	1.46	1.51
32	Gg	311	CLA	CMB-C2B	-2.37	1.46	1.51
32	G	603	CLA	C3B-C2B	-2.37	1.37	1.40
32	b	607	CLA	C3B-C2B	-2.37	1.37	1.40
32	r	602	CLA	CMB-C2B	-2.37	1.46	1.51
32	44	610	CLA	CMB-C2B	-2.37	1.46	1.51
32	BB	613	CLA	CMB-C2B	-2.37	1.46	1.51
32	S	608	CLA	CMB-C2B	-2.37	1.46	1.51
32	r	601	CLA	CMB-C2B	-2.36	1.46	1.51
32	s	613	CLA	CMB-C2B	-2.36	1.46	1.51
32	4	310	CLA	CMB-C2B	-2.36	1.46	1.51
32	r	611	CLA	CMB-C2B	-2.36	1.46	1.51
32	c	504	CLA	C3B-C2B	-2.36	1.37	1.40
32	Cc	503	CLA	CMB-C2B	-2.36	1.46	1.51
32	Ss	603	CLA	CMB-C2B	-2.36	1.46	1.51
32	n	611	CLA	CMB-C2B	-2.36	1.46	1.51
32	R	603	CLA	CMB-C2B	-2.36	1.46	1.51
32	GG	603	CLA	CMB-C2B	-2.36	1.46	1.51
32	NN	610	CLA	CMB-C2B	-2.36	1.46	1.51
32	11	609	CLA	CMB-C2B	-2.36	1.46	1.51
32	22	603	CLA	CMB-C2B	-2.36	1.46	1.51
32	3	603	CLA	CMB-C2B	-2.36	1.46	1.51
32	B	610	CLA	CMB-C2B	-2.36	1.46	1.51
32	CC	508	CLA	C3B-C2B	-2.36	1.37	1.40
32	Bb	615	CLA	CMB-C2B	-2.35	1.46	1.51
32	n	614	CLA	CMB-C2B	-2.35	1.46	1.51
32	Y	613	CLA	CMB-C2B	-2.35	1.46	1.51
32	Nn	301	CLA	CMB-C2B	-2.35	1.46	1.51
32	A	406	CLA	C3B-C2B	-2.35	1.37	1.40
32	S	604	CLA	CMB-C2B	-2.35	1.46	1.51
32	d	401	CLA	CMB-C2B	-2.35	1.46	1.51
32	Yy	602	CLA	C3B-C2B	-2.35	1.37	1.40
32	b	614	CLA	CMB-C2B	-2.35	1.46	1.51
32	AA	406	CLA	C3B-C2B	-2.35	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Gg	314	CLA	CMB-C2B	-2.35	1.46	1.51
32	Gg	313	CLA	C3B-C2B	-2.35	1.37	1.40
32	22	611	CLA	CMB-C2B	-2.35	1.46	1.51
32	c	506	CLA	CMB-C2B	-2.35	1.46	1.51
32	Bb	607	CLA	C3B-C2B	-2.35	1.37	1.40
32	B	608	CLA	CMB-C2B	-2.35	1.46	1.51
32	c	509	CLA	C3B-C2B	-2.35	1.37	1.40
32	4	304	CLA	C3B-C2B	-2.34	1.37	1.40
32	NN	611	CLA	CMB-C2B	-2.34	1.46	1.51
32	Cc	511	CLA	C3B-C2B	-2.34	1.37	1.40
32	SS	312	CLA	CMB-C2B	-2.34	1.46	1.51
32	B	622	CLA	C3B-C2B	-2.34	1.37	1.40
32	RR	310	CLA	C3B-C2B	-2.34	1.37	1.40
32	r	612	CLA	CMB-C2B	-2.34	1.46	1.51
32	RR	312	CLA	CMB-C2B	-2.34	1.46	1.51
32	b	605	CLA	C3B-C2B	-2.34	1.37	1.40
32	Bb	610	CLA	C3B-C2B	-2.34	1.37	1.40
32	G	613	CLA	CMB-C2B	-2.34	1.46	1.51
32	S	602	CLA	CMB-C2B	-2.34	1.46	1.51
32	1	613	CLA	CMB-C2B	-2.33	1.46	1.51
35	Dd	404	PL9	C21-C19	2.33	1.56	1.51
41	GG	619	XAT	C32-C33	2.33	1.51	1.45
32	G	610	CLA	C3B-C2B	-2.33	1.37	1.40
39	Yy	608	CHL	CMB-C2B	-2.33	1.46	1.51
32	S	612	CLA	CMB-C2B	-2.33	1.46	1.51
35	d	404	PL9	C21-C19	2.33	1.56	1.51
32	N	613	CLA	C3B-C2B	-2.33	1.37	1.40
32	r	604	CLA	CMB-C2B	-2.33	1.46	1.51
32	C	512	CLA	C3B-C2B	-2.33	1.37	1.40
32	33	612	CLA	CMB-C2B	-2.33	1.46	1.51
32	SS	309	CLA	CMB-C2B	-2.33	1.46	1.51
32	2	612	CLA	CMB-C2B	-2.33	1.46	1.51
32	N	612	CLA	CMB-C2B	-2.33	1.46	1.51
39	Gg	302	CHL	CMD-C2D	-2.33	1.45	1.50
32	Yy	612	CLA	C3B-C2B	-2.33	1.37	1.40
34	Bb	617	BCR	C12-C13	2.33	1.50	1.45
32	G	613	CLA	C3B-C2B	-2.33	1.37	1.40
32	Rr	601	CLA	CMB-C2B	-2.33	1.46	1.51
32	11	610	CLA	CMB-C2B	-2.33	1.46	1.51
32	R	610	CLA	CMB-C2B	-2.32	1.46	1.51
32	2	602	CLA	CMB-C2B	-2.32	1.46	1.51
32	Nn	304	CLA	C3B-C2B	-2.32	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	401	CLA	C3B-C2B	-2.32	1.37	1.40
32	s	603	CLA	CMB-C2B	-2.32	1.46	1.51
32	1	602	CLA	CMB-C2B	-2.32	1.46	1.51
32	D	404	CLA	CMD-C2D	-2.32	1.45	1.50
32	Bb	605	CLA	C3B-C2B	-2.32	1.37	1.40
32	y	315	CLA	CMB-C2B	-2.32	1.46	1.51
32	s	602	CLA	CMB-C2B	-2.32	1.46	1.51
32	RR	303	CLA	CMB-C2B	-2.32	1.46	1.51
32	RR	310	CLA	CMB-C2B	-2.32	1.46	1.51
32	c	502	CLA	CMD-C2D	-2.32	1.45	1.50
32	b	612	CLA	CMD-C2D	-2.32	1.45	1.50
32	1	610	CLA	CMB-C2B	-2.32	1.46	1.51
32	N	610	CLA	CMB-C2B	-2.32	1.46	1.51
32	S	603	CLA	CMB-C2B	-2.32	1.46	1.51
32	c	504	CLA	CMB-C2B	-2.32	1.46	1.51
32	Rr	602	CLA	C3B-C2B	-2.32	1.37	1.40
32	B	624	CLA	C3B-C2B	-2.32	1.37	1.40
32	NN	613	CLA	C3B-C2B	-2.32	1.37	1.40
40	Y	615	LUT	C22-C21	-2.31	1.51	1.54
32	R	602	CLA	C3B-C2B	-2.31	1.37	1.40
32	Nn	305	CLA	CMB-C2B	-2.31	1.46	1.51
35	DD	406	PL9	C41-C39	2.31	1.56	1.51
32	Ss	613	CLA	CMB-C2B	-2.31	1.46	1.51
32	GG	613	CLA	CMB-C2B	-2.31	1.46	1.51
32	N	610	CLA	C3B-CAB	-2.31	1.43	1.47
39	GG	605	CHL	C1B-NB	2.31	1.37	1.35
32	1	609	CLA	CMB-C2B	-2.31	1.46	1.51
35	D	407	PL9	C41-C39	2.31	1.56	1.51
32	G	614	CLA	CMB-C2B	-2.31	1.46	1.51
32	Bb	614	CLA	CMB-C2B	-2.31	1.46	1.51
32	B	605	CLA	C3B-C2B	-2.31	1.37	1.40
32	3	611	CLA	CMB-C2B	-2.31	1.46	1.51
32	SS	304	CLA	CMB-C2B	-2.31	1.46	1.51
32	R	610	CLA	C3B-C2B	-2.31	1.37	1.40
32	CC	506	CLA	CMD-C2D	-2.31	1.45	1.50
32	22	613	CLA	CMB-C2B	-2.31	1.46	1.51
32	3	610	CLA	CMB-C2B	-2.31	1.46	1.51
32	R	614	CLA	CMD-C2D	-2.31	1.45	1.50
32	X	201	CLA	C3B-C2B	-2.31	1.37	1.40
32	Ss	608	CLA	CMB-C2B	-2.30	1.46	1.51
39	S	607	CHL	C1B-NB	2.30	1.37	1.35
32	2	611	CLA	CMB-C2B	-2.30	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	NN	606	CHL	CMD-C2D	-2.30	1.45	1.50
39	22	608	CHL	C1B-NB	2.30	1.37	1.35
32	RR	302	CLA	C3B-C2B	-2.30	1.37	1.40
32	B	611	CLA	CMB-C2B	-2.30	1.46	1.51
32	s	609	CLA	CMB-C2B	-2.30	1.46	1.51
32	Y	604	CLA	CMB-C2B	-2.30	1.46	1.51
32	YY	604	CLA	CMB-C2B	-2.30	1.46	1.51
32	n	610	CLA	CMB-C2B	-2.30	1.46	1.51
40	22	614	LUT	C12-C13	2.30	1.50	1.45
39	Y	609	CHL	CMB-C2B	-2.30	1.46	1.51
32	b	610	CLA	C3B-C2B	-2.30	1.37	1.40
32	AA	405	CLA	C3B-C2B	-2.30	1.37	1.40
32	C	505	CLA	C3B-C2B	-2.30	1.37	1.40
32	Y	603	CLA	C3B-C2B	-2.30	1.37	1.40
32	S	611	CLA	CMB-C2B	-2.30	1.46	1.51
32	BB	605	CLA	C3B-C2B	-2.30	1.37	1.40
32	YY	613	CLA	C3B-C2B	-2.30	1.37	1.40
32	g	613	CLA	CMB-C2B	-2.29	1.46	1.51
32	XX	201	CLA	CMB-C2B	-2.29	1.46	1.51
32	GG	610	CLA	CMB-C2B	-2.29	1.46	1.51
32	D	405	CLA	C3B-C2B	-2.29	1.37	1.40
39	3	605	CHL	C1B-NB	2.29	1.37	1.35
32	b	606	CLA	C3B-C2B	-2.29	1.37	1.40
41	Nn	308	XAT	O24-C25	-2.29	1.42	1.46
32	Bb	615	CLA	C3B-C2B	-2.29	1.37	1.40
32	CC	504	CLA	C3B-C2B	-2.29	1.37	1.40
32	Cc	506	CLA	C3B-C2B	-2.29	1.37	1.40
32	11	602	CLA	CMB-C2B	-2.29	1.46	1.51
32	s	608	CLA	CMB-C2B	-2.29	1.46	1.51
40	Ss	614	LUT	C32-C33	2.29	1.50	1.45
32	BB	603	CLA	C3B-C2B	-2.29	1.37	1.40
32	Y	611	CLA	CMB-C2B	-2.29	1.46	1.51
32	y	314	CLA	CMD-C2D	-2.28	1.46	1.50
40	Ss	614	LUT	C8-C9	2.28	1.50	1.45
34	AA	409	BCR	C8-C9	2.28	1.50	1.45
32	A	405	CLA	C3B-C2B	-2.28	1.37	1.40
32	44	603	CLA	C3B-C2B	-2.28	1.37	1.40
32	GG	610	CLA	C3B-C2B	-2.28	1.37	1.40
32	1	611	CLA	C3B-C2B	-2.28	1.37	1.40
32	Gg	305	CLA	C3B-C2B	-2.28	1.37	1.40
32	BB	609	CLA	C3B-C2B	-2.28	1.37	1.40
39	22	601	CHL	C1B-NB	2.28	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Bb	608	CLA	C3B-C2B	-2.28	1.37	1.40
32	RR	304	CLA	C3B-C2B	-2.27	1.37	1.40
42	g	617	NEX	O24-C25	-2.27	1.43	1.46
40	Ss	615	LUT	C8-C9	2.27	1.50	1.45
32	CC	511	CLA	C3B-CAB	-2.27	1.43	1.47
32	n	610	CLA	C3B-C2B	-2.27	1.37	1.40
32	GG	603	CLA	C3B-C2B	-2.27	1.37	1.40
32	Nn	312	CLA	C3B-C2B	-2.27	1.37	1.40
32	44	615	CLA	CMB-C2B	-2.27	1.46	1.51
32	NN	610	CLA	C3B-CAB	-2.27	1.43	1.47
39	22	607	CHL	C1B-NB	2.26	1.37	1.35
32	Nn	303	CLA	CMB-C2B	-2.26	1.46	1.51
32	C	507	CLA	CMD-C2D	-2.26	1.46	1.50
32	NN	602	CLA	C3B-C2B	-2.26	1.37	1.40
32	R	604	CLA	C3B-C2B	-2.26	1.37	1.40
32	C	503	CLA	CMD-C2D	-2.26	1.46	1.50
39	y	311	CHL	CMB-C2B	-2.26	1.46	1.51
35	d	404	PL9	C41-C39	2.25	1.56	1.51
39	NN	609	CHL	CMB-C2B	-2.25	1.47	1.51
32	b	615	CLA	C3B-C2B	-2.25	1.37	1.40
32	Aa	406	CLA	MG-NA	2.25	2.11	2.06
32	Gg	303	CLA	C3B-C2B	-2.25	1.37	1.40
32	Gg	314	CLA	C3B-C2B	-2.25	1.37	1.40
34	BB	617	BCR	C23-C22	2.25	1.50	1.45
32	G	612	CLA	C3B-C2B	-2.25	1.37	1.40
32	Ss	609	CLA	CMC-C2C	-2.25	1.46	1.50
44	CC	522	DGD	O3G-C1D	2.25	1.44	1.40
32	B	607	CLA	C3B-C2B	-2.25	1.37	1.40
32	c	501	CLA	CMD-C2D	-2.25	1.46	1.50
32	3	612	CLA	CMB-C2B	-2.25	1.47	1.51
32	RR	314	CLA	CMD-C2D	-2.25	1.46	1.50
32	G	611	CLA	CMB-C2B	-2.25	1.47	1.51
40	s	614	LUT	C8-C9	2.25	1.50	1.45
32	CC	503	CLA	CMD-C2D	-2.24	1.46	1.50
32	BB	606	CLA	C3B-C2B	-2.24	1.37	1.40
32	BB	602	CLA	CMD-C2D	-2.24	1.46	1.50
32	G	604	CLA	CMB-C2B	-2.24	1.47	1.51
32	n	604	CLA	CMB-C2B	-2.24	1.47	1.51
32	NN	612	CLA	CMB-C2B	-2.24	1.47	1.51
32	BB	614	CLA	C3B-C2B	-2.23	1.37	1.40
32	SS	310	CLA	CMB-C2B	-2.23	1.47	1.51
34	AA	409	BCR	C12-C13	2.23	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	DD	406	PL9	C5-C4	-2.23	1.39	1.47
32	B	608	CLA	CMD-C2D	-2.23	1.46	1.50
32	Bb	616	CLA	C3B-C2B	-2.23	1.37	1.40
34	H	101	BCR	C19-C18	2.23	1.50	1.45
34	A	409	BCR	C8-C9	2.23	1.50	1.45
32	Y	610	CLA	C3B-C2B	-2.23	1.37	1.40
32	3	613	CLA	CMB-C2B	-2.23	1.47	1.51
32	y	304	CLA	C3B-C2B	-2.23	1.37	1.40
32	44	609	CLA	CMB-C2B	-2.23	1.47	1.51
32	B	619	CLA	CMD-C2D	-2.23	1.46	1.50
32	Cc	507	CLA	CMD-C2D	-2.23	1.46	1.50
32	b	601	CLA	CMC-C2C	-2.22	1.46	1.50
39	2	607	CHL	C1B-NB	2.22	1.37	1.35
32	C	504	CLA	C3B-C2B	-2.22	1.37	1.40
32	a	407	CLA	C3B-C2B	-2.22	1.37	1.40
32	BB	612	CLA	CMD-C2D	-2.22	1.46	1.50
32	y	305	CLA	C3B-C2B	-2.22	1.37	1.40
32	S	610	CLA	CMD-C2D	-2.22	1.46	1.50
32	1	611	CLA	CMB-C2B	-2.22	1.47	1.51
34	c	515	BCR	C12-C13	2.22	1.50	1.45
32	Aa	407	CLA	C3B-C2B	-2.22	1.37	1.40
32	Y	613	CLA	CMD-C2D	-2.22	1.46	1.50
32	Y	612	CLA	CMD-C2D	-2.22	1.46	1.50
32	a	406	CLA	CMD-C2D	-2.22	1.46	1.50
40	2	614	LUT	C12-C13	2.22	1.50	1.45
39	1	601	CHL	C1B-NB	2.22	1.37	1.35
32	y	305	CLA	CMD-C2D	-2.22	1.46	1.50
32	s	611	CLA	CMB-C2B	-2.22	1.47	1.51
39	Yy	609	CHL	CMB-C2B	-2.22	1.47	1.51
32	CC	512	CLA	C3B-CAB	-2.22	1.43	1.47
32	a	405	CLA	CMD-C2D	-2.22	1.46	1.50
32	GG	604	CLA	C3B-C2B	-2.22	1.37	1.40
39	2	608	CHL	C1B-NB	2.22	1.37	1.35
32	d	402	CLA	C3B-C2B	-2.22	1.37	1.40
39	2	601	CHL	C1B-NB	2.22	1.37	1.35
32	Cc	505	CLA	CMD-C2D	-2.22	1.46	1.50
32	b	616	CLA	C3B-C2B	-2.21	1.37	1.40
34	Aa	411	BCR	C12-C13	2.21	1.50	1.45
39	3	601	CHL	C1B-NB	2.21	1.37	1.35
32	Ss	611	CLA	CMB-C2B	-2.21	1.47	1.51
32	CC	502	CLA	CMD-C2D	-2.21	1.46	1.50
32	Bb	601	CLA	CMC-C2C	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	401	CLA	CMD-C2D	-2.21	1.46	1.50
32	GG	611	CLA	CMD-C2D	-2.21	1.46	1.50
39	N	606	CHL	CMD-C2D	-2.21	1.46	1.50
34	Hh	101	BCR	C23-C22	2.21	1.50	1.45
32	SS	312	CLA	CMD-C2D	-2.21	1.46	1.50
32	r	611	CLA	C3B-C2B	-2.21	1.37	1.40
32	n	612	CLA	CMB-C2B	-2.21	1.47	1.51
34	B	613	BCR	C23-C22	2.21	1.50	1.45
32	BB	606	CLA	CMD-C2D	-2.21	1.46	1.50
32	Bb	602	CLA	C3B-C2B	-2.21	1.37	1.40
34	Cc	517	BCR	C12-C13	2.21	1.50	1.45
32	Bb	607	CLA	CMD-C2D	-2.21	1.46	1.50
32	44	602	CLA	C3B-C2B	-2.21	1.37	1.40
32	3	609	CLA	CMB-C2B	-2.21	1.47	1.51
32	r	602	CLA	C3B-C2B	-2.21	1.37	1.40
32	Bb	612	CLA	CMD-C2D	-2.21	1.46	1.50
32	RR	312	CLA	C3B-C2B	-2.21	1.37	1.40
32	BB	612	CLA	CMB-C2B	-2.21	1.47	1.51
32	2	613	CLA	CMB-C2B	-2.21	1.47	1.51
32	S	611	CLA	CMD-C2D	-2.21	1.46	1.50
40	s	614	LUT	C32-C33	2.21	1.50	1.45
35	D	407	PL9	C5-C4	-2.20	1.39	1.47
41	G	617	XAT	C32-C33	2.20	1.50	1.45
32	D	404	CLA	CMC-C2C	-2.20	1.46	1.50
40	2	614	LUT	C8-C9	2.20	1.50	1.45
39	Ss	607	CHL	C1B-NB	2.20	1.37	1.35
32	b	602	CLA	C3B-C2B	-2.20	1.37	1.40
32	s	604	CLA	C3B-C2B	-2.20	1.37	1.40
32	B	620	CLA	C3B-C2B	-2.20	1.37	1.40
32	Dd	402	CLA	C3B-C2B	-2.20	1.37	1.40
32	Bb	603	CLA	CMD-C2D	-2.20	1.46	1.50
32	1	603	CLA	CMB-C2B	-2.20	1.47	1.51
41	y	302	XAT	O4-C5	-2.20	1.43	1.46
32	c	507	CLA	CMD-C2D	-2.20	1.46	1.50
39	Rr	605	CHL	CMD-C2D	-2.20	1.46	1.50
32	SS	314	CLA	C3B-C2B	-2.20	1.37	1.40
32	c	513	CLA	CMD-C2D	-2.20	1.46	1.50
35	Dd	404	PL9	C5-C4	-2.20	1.39	1.47
32	DD	403	CLA	CMD-C2D	-2.20	1.46	1.50
32	YY	613	CLA	CMD-C2D	-2.20	1.46	1.50
32	Cc	505	CLA	C3B-C2B	-2.20	1.37	1.40
32	BB	614	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	33	606	CHL	C1B-NB	2.19	1.37	1.35
32	BB	608	CLA	CMD-C2D	-2.19	1.46	1.50
34	b	617	BCR	C12-C13	2.19	1.50	1.45
32	b	613	CLA	C3B-C2B	-2.19	1.37	1.40
32	CC	513	CLA	CMD-C2D	-2.19	1.46	1.50
32	BB	611	CLA	C3B-C2B	-2.19	1.37	1.40
32	AA	405	CLA	CMD-C2D	-2.19	1.46	1.50
41	Nn	308	XAT	O4-C5	-2.19	1.43	1.46
39	G	608	CHL	C1B-NB	2.19	1.37	1.35
32	DD	403	CLA	C3B-C2B	-2.19	1.37	1.40
32	Aa	405	CLA	CMD-C2D	-2.19	1.46	1.50
35	d	404	PL9	C5-C4	-2.19	1.39	1.47
34	Aa	411	BCR	C8-C9	2.19	1.50	1.45
32	a	406	CLA	C4B-CHC	-2.19	1.34	1.41
32	g	613	CLA	C1B-NB	2.19	1.37	1.35
39	SS	308	CHL	C1B-NB	2.19	1.37	1.35
32	Bb	613	CLA	C3B-C2B	-2.19	1.37	1.40
32	Bb	608	CLA	C3B-CAB	-2.19	1.43	1.47
40	y	317	LUT	C22-C21	-2.19	1.52	1.54
32	B	623	CLA	CMD-C2D	-2.19	1.46	1.50
33	D	402	PHO	CMD-C2D	-2.19	1.46	1.51
32	Yy	612	CLA	CMD-C2D	-2.19	1.46	1.50
32	b	603	CLA	CMD-C2D	-2.19	1.46	1.50
34	Bb	619	BCR	C23-C22	2.19	1.50	1.45
32	22	609	CLA	C3B-C2B	-2.19	1.37	1.40
33	A	407	PHO	CMD-C2D	-2.19	1.46	1.51
33	AA	407	PHO	CMD-C2D	-2.19	1.46	1.51
32	N	602	CLA	C3B-C2B	-2.19	1.37	1.40
39	11	601	CHL	C1B-NB	2.18	1.37	1.35
32	Yy	603	CLA	C3B-C2B	-2.18	1.37	1.40
32	33	613	CLA	CMB-C2B	-2.18	1.47	1.51
32	Rr	613	CLA	CMD-C2D	-2.18	1.46	1.50
32	s	602	CLA	C3B-C2B	-2.18	1.37	1.40
32	22	602	CLA	CMB-C2B	-2.18	1.47	1.51
35	Dd	404	PL9	C41-C39	2.18	1.55	1.51
32	BB	610	CLA	CMD-C2D	-2.18	1.46	1.50
34	A	409	BCR	C12-C13	2.18	1.50	1.45
35	AA	410	PL9	C5-C4	-2.18	1.39	1.47
32	R	603	CLA	C3B-C2B	-2.18	1.37	1.40
32	R	603	CLA	CMD-C2D	-2.18	1.46	1.50
32	GG	603	CLA	C3B-CAB	-2.18	1.43	1.47
42	Gg	318	NEX	O24-C25	-2.18	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	NN	601	CHL	CMD-C2D	-2.18	1.46	1.50
32	Nn	314	CLA	C3B-C2B	-2.18	1.37	1.40
32	Dd	401	CLA	CMD-C2D	-2.18	1.46	1.50
39	1	608	CHL	CMD-C2D	-2.18	1.46	1.50
32	Rr	610	CLA	C3B-C2B	-2.18	1.37	1.40
32	G	603	CLA	C3B-CAB	-2.18	1.43	1.47
33	AA	407	PHO	CMB-C2B	-2.18	1.46	1.51
39	Gg	309	CHL	CMB-C2B	-2.18	1.47	1.51
32	YY	614	CLA	CMD-C2D	-2.18	1.46	1.50
41	y	302	XAT	O24-C25	-2.18	1.43	1.46
40	Yy	615	LUT	C22-C21	-2.18	1.52	1.54
32	33	612	CLA	C3B-C2B	-2.18	1.37	1.40
32	C	507	CLA	C3B-C2B	-2.18	1.37	1.40
32	Dd	401	CLA	C3B-C2B	-2.18	1.37	1.40
32	CC	508	CLA	CMD-C2D	-2.18	1.46	1.50
41	Rr	615	XAT	O24-C25	-2.17	1.43	1.46
34	a	411	BCR	C8-C9	2.17	1.50	1.45
32	Cc	503	CLA	CMD-C2D	-2.17	1.46	1.50
39	g	608	CHL	CMB-C2B	-2.17	1.47	1.51
32	d	401	CLA	CMC-C2C	-2.17	1.46	1.50
32	C	514	CLA	CMD-C2D	-2.17	1.46	1.50
32	CC	507	CLA	CMD-C2D	-2.17	1.46	1.50
32	Bb	614	CLA	CMD-C2D	-2.17	1.46	1.50
32	C	512	CLA	C3B-CAB	-2.17	1.43	1.47
32	r	613	CLA	CMD-C2D	-2.17	1.46	1.50
32	RR	304	CLA	CMD-C2D	-2.17	1.46	1.50
32	R	608	CLA	C3B-C2B	-2.17	1.37	1.40
32	y	312	CLA	C3B-CAB	-2.17	1.43	1.47
32	Gg	315	CLA	C3B-C2B	-2.17	1.37	1.40
32	BB	605	CLA	CMD-C2D	-2.17	1.46	1.50
32	g	612	CLA	C3B-C2B	-2.17	1.37	1.40
32	Bb	611	CLA	C3B-C2B	-2.17	1.37	1.40
32	Cc	510	CLA	C3B-C2B	-2.17	1.37	1.40
32	Nn	301	CLA	C3B-C2B	-2.17	1.37	1.40
32	y	314	CLA	C3B-CAB	-2.17	1.43	1.47
40	22	614	LUT	C8-C9	2.17	1.50	1.45
32	Yy	613	CLA	CMD-C2D	-2.17	1.46	1.50
32	B	604	CLA	CMD-C2D	-2.16	1.46	1.50
39	R	605	CHL	CMD-C2D	-2.16	1.46	1.50
32	Bb	613	CLA	CMD-C2D	-2.16	1.46	1.50
32	R	612	CLA	C3B-C2B	-2.16	1.37	1.40
32	b	614	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	GG	608	CHL	C1B-NB	2.16	1.37	1.35
32	C	510	CLA	CMD-C2D	-2.16	1.46	1.50
32	2	602	CLA	C3B-C2B	-2.16	1.37	1.40
32	B	610	CLA	C3B-C2B	-2.16	1.37	1.40
32	Gg	312	CLA	C3B-C2B	-2.16	1.37	1.40
32	DD	404	CLA	C3B-C2B	-2.16	1.37	1.40
32	S	612	CLA	C3B-C2B	-2.16	1.37	1.40
32	CC	509	CLA	CMD-C2D	-2.16	1.46	1.50
32	C	509	CLA	CMD-C2D	-2.16	1.46	1.50
32	Cc	509	CLA	CMD-C2D	-2.16	1.46	1.50
32	Yy	610	CLA	C3B-CAB	-2.16	1.43	1.47
32	B	618	CLA	CMD-C2D	-2.16	1.46	1.50
32	r	609	CLA	C3B-C2B	-2.16	1.37	1.40
32	BB	603	CLA	CMD-C2D	-2.16	1.46	1.50
32	B	610	CLA	CMD-C2D	-2.16	1.46	1.50
32	Bb	611	CLA	CMD-C2D	-2.16	1.46	1.50
33	a	408	PHO	CMD-C2D	-2.16	1.46	1.51
32	Y	614	CLA	CMD-C2D	-2.16	1.46	1.50
32	y	315	CLA	CMD-C2D	-2.16	1.46	1.50
39	Nn	316	CHL	CMD-C2D	-2.16	1.46	1.50
34	h	101	BCR	C8-C9	2.16	1.50	1.45
34	B	614	BCR	C23-C22	2.16	1.50	1.45
32	BB	604	CLA	CMD-C2D	-2.16	1.46	1.50
32	CC	506	CLA	C3B-C2B	-2.16	1.37	1.40
32	B	604	CLA	C3B-C2B	-2.15	1.37	1.40
32	DD	401	CLA	C3B-CAB	-2.15	1.43	1.47
32	DD	401	CLA	CMD-C2D	-2.15	1.46	1.50
32	Bb	615	CLA	CMD-C2D	-2.15	1.46	1.50
32	g	603	CLA	C3B-CAB	-2.15	1.43	1.47
32	Aa	410	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	503	CLA	C3B-C2B	-2.15	1.37	1.40
44	BB	623	DGD	O3G-C1D	2.15	1.43	1.40
39	s	607	CHL	C1B-NB	2.15	1.37	1.35
32	2	610	CLA	CMB-C2B	-2.15	1.47	1.51
32	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
32	C	514	CLA	C3B-C2B	-2.15	1.37	1.40
32	C	509	CLA	C3B-C2B	-2.15	1.37	1.40
32	D	401	CLA	CMD-C2D	-2.15	1.46	1.50
34	h	101	BCR	C23-C22	2.15	1.50	1.45
32	C	513	CLA	CMD-C2D	-2.15	1.46	1.50
32	Rr	613	CLA	C3B-C2B	-2.15	1.37	1.40
32	C	505	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	XX	201	CLA	CMD-C2D	-2.15	1.46	1.50
39	y	303	CHL	CMD-C2D	-2.15	1.46	1.50
32	r	603	CLA	CMD-C2D	-2.15	1.46	1.50
32	b	613	CLA	CMD-C2D	-2.15	1.46	1.50
32	YY	603	CLA	CMD-C2D	-2.15	1.46	1.50
32	33	610	CLA	CMB-C2B	-2.15	1.47	1.51
32	B	609	CLA	CMD-C2D	-2.15	1.46	1.50
32	B	622	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	505	CLA	CMD-C2D	-2.15	1.46	1.50
35	A	410	PL9	C5-C4	-2.15	1.39	1.47
32	y	304	CLA	CMD-C2D	-2.15	1.46	1.50
39	n	609	CHL	CMB-C2B	-2.15	1.47	1.51
32	Aa	407	CLA	CMD-C2D	-2.14	1.46	1.50
33	DD	402	PHO	CMD-C2D	-2.14	1.46	1.51
33	AA	407	PHO	CMC-C2C	-2.14	1.46	1.51
32	Yy	614	CLA	C3B-C2B	-2.14	1.37	1.40
32	G	611	CLA	C3B-C2B	-2.14	1.37	1.40
32	NN	603	CLA	C3B-C2B	-2.14	1.37	1.40
32	GG	602	CLA	CMD-C2D	-2.14	1.46	1.50
32	Nn	301	CLA	CMC-C2C	-2.14	1.46	1.50
32	YY	602	CLA	C3B-C2B	-2.14	1.37	1.40
32	Yy	611	CLA	C3B-C2B	-2.14	1.37	1.40
32	4	303	CLA	C3B-C2B	-2.14	1.37	1.40
32	B	611	CLA	CMD-C2D	-2.14	1.46	1.50
32	SS	304	CLA	CMD-C2D	-2.14	1.46	1.50
32	Aa	406	CLA	CMD-C2D	-2.14	1.46	1.50
32	Yy	603	CLA	CMD-C2D	-2.14	1.46	1.50
32	N	610	CLA	CMD-C2D	-2.14	1.46	1.50
32	n	610	CLA	CMD-C2D	-2.14	1.46	1.50
33	a	409	PHO	CMD-C2D	-2.14	1.46	1.51
41	RR	316	XAT	O4-C5	-2.14	1.43	1.46
32	GG	610	CLA	C1B-NB	2.14	1.37	1.35
32	BB	613	CLA	CMD-C2D	-2.14	1.46	1.50
32	b	604	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	503	CLA	CMD-C2D	-2.14	1.46	1.50
32	RR	303	CLA	CMD-C2D	-2.14	1.46	1.50
32	A	405	CLA	CMD-C2D	-2.13	1.46	1.50
32	Bb	604	CLA	CMD-C2D	-2.13	1.46	1.50
41	GG	617	XAT	C32-C33	2.13	1.50	1.45
39	N	609	CHL	CMB-C2B	-2.13	1.47	1.51
32	YY	603	CLA	C3B-C2B	-2.13	1.37	1.40
32	BB	601	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	609	CHL	CMD-C2D	-2.13	1.46	1.50
39	n	605	CHL	C1B-NB	2.13	1.37	1.35
32	CC	510	CLA	CMD-C2D	-2.13	1.46	1.50
32	G	610	CLA	MG-NC	2.13	2.11	2.06
39	44	607	CHL	CMD-C2D	-2.13	1.46	1.50
32	R	604	CLA	CMD-C2D	-2.13	1.46	1.50
39	11	606	CHL	C1B-NB	2.13	1.37	1.35
41	NN	617	XAT	O4-C5	-2.13	1.43	1.46
39	4	302	CHL	C1B-NB	2.13	1.37	1.35
33	AA	407	PHO	C3B-C2B	-2.13	1.37	1.40
33	A	407	PHO	CMC-C2C	-2.13	1.46	1.51
35	AA	410	PL9	C26-C24	2.13	1.55	1.51
32	Rr	611	CLA	CMD-C2D	-2.13	1.46	1.50
32	g	613	CLA	CMD-C2D	-2.13	1.46	1.50
32	B	606	CLA	CMD-C2D	-2.13	1.46	1.50
33	Aa	409	PHO	CMC-C2C	-2.13	1.46	1.51
32	GG	612	CLA	C3B-C2B	-2.13	1.37	1.40
32	D	401	CLA	C3B-CAB	-2.13	1.43	1.47
32	DD	403	CLA	CMC-C2C	-2.13	1.46	1.50
37	CC	501	SQD	O6-C1	2.13	1.43	1.40
32	BB	607	CLA	CMD-C2D	-2.13	1.46	1.50
32	B	606	CLA	C3B-C2B	-2.12	1.37	1.40
39	n	607	CHL	CMD-C2D	-2.12	1.46	1.50
39	NN	609	CHL	CMD-C2D	-2.12	1.46	1.50
32	RR	308	CLA	C3B-C2B	-2.12	1.37	1.40
33	A	407	PHO	CMB-C2B	-2.12	1.46	1.51
32	b	607	CLA	CMD-C2D	-2.12	1.46	1.50
32	SS	305	CLA	C3B-C2B	-2.12	1.37	1.40
32	C	511	CLA	C3B-CAB	-2.12	1.43	1.47
32	b	611	CLA	CMD-C2D	-2.12	1.46	1.50
33	Aa	409	PHO	CMD-C2D	-2.12	1.46	1.51
32	b	611	CLA	C3B-C2B	-2.12	1.37	1.40
33	a	408	PHO	CMC-C2C	-2.12	1.46	1.51
32	BB	615	CLA	CMD-C2D	-2.12	1.46	1.50
32	C	508	CLA	CMD-C2D	-2.12	1.46	1.50
32	Yy	602	CLA	CMD-C2D	-2.12	1.46	1.50
40	NN	615	LUT	C22-C21	-2.12	1.52	1.54
32	CC	510	CLA	C3B-CAB	-2.12	1.43	1.47
32	Ss	604	CLA	C3B-C2B	-2.12	1.37	1.40
32	c	510	CLA	CMD-C2D	-2.12	1.46	1.50
32	Cc	513	CLA	C3B-CAB	-2.12	1.43	1.47
33	Aa	408	PHO	CMB-C2B	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	610	CLA	C3B-C2B	-2.12	1.37	1.40
32	Nn	312	CLA	CMD-C2D	-2.12	1.46	1.50
32	b	616	CLA	CMD-C2D	-2.12	1.46	1.50
32	DD	404	CLA	CMD-C2D	-2.12	1.46	1.50
32	X	201	CLA	CMD-C2D	-2.11	1.46	1.50
32	CC	504	CLA	CMD-C2D	-2.11	1.46	1.50
39	RR	307	CHL	CMD-C2D	-2.11	1.46	1.50
33	DD	402	PHO	CMC-C2C	-2.11	1.46	1.51
32	C	511	CLA	CMD-C2D	-2.11	1.46	1.50
32	Cc	504	CLA	CMD-C2D	-2.11	1.46	1.50
39	G	606	CHL	C1B-NB	2.11	1.37	1.35
39	y	303	CHL	CMB-C2B	-2.11	1.47	1.51
32	BB	607	CLA	C3B-C2B	-2.11	1.37	1.40
32	Bb	616	CLA	CMD-C2D	-2.11	1.46	1.50
41	N	617	XAT	O4-C5	-2.11	1.43	1.46
32	SS	313	CLA	C3B-C2B	-2.11	1.37	1.40
32	YY	604	CLA	C3B-C2B	-2.11	1.37	1.40
33	DD	402	PHO	CMB-C2B	-2.11	1.46	1.51
32	Cc	512	CLA	CMD-C2D	-2.11	1.46	1.50
41	R	616	XAT	O24-C25	-2.11	1.43	1.46
39	RR	306	CHL	CMD-C2D	-2.11	1.46	1.50
32	B	620	CLA	CMD-C2D	-2.11	1.46	1.50
32	C	503	CLA	C3B-C2B	-2.11	1.37	1.40
32	Yy	614	CLA	CMD-C2D	-2.11	1.46	1.50
38	WW	201	LMG	O1-C1	2.11	1.43	1.40
32	b	603	CLA	C3B-CAB	-2.11	1.43	1.47
41	GG	619	XAT	C12-C13	2.11	1.50	1.45
32	b	615	CLA	CMD-C2D	-2.11	1.46	1.50
32	S	613	CLA	C3B-C2B	-2.11	1.37	1.40
32	Cc	509	CLA	C3B-C2B	-2.11	1.37	1.40
32	Rr	603	CLA	C3B-C2B	-2.11	1.37	1.40
34	BB	616	BCR	C30-C25	-2.11	1.50	1.53
34	C	516	BCR	C12-C13	2.11	1.50	1.45
32	SS	303	CLA	C3B-C2B	-2.11	1.37	1.40
32	Cc	512	CLA	C3B-C2B	-2.11	1.37	1.40
32	c	511	CLA	C3B-CAB	-2.10	1.43	1.47
41	NN	617	XAT	C32-C33	2.10	1.50	1.45
33	a	408	PHO	CMB-C2B	-2.10	1.46	1.51
33	Aa	408	PHO	CMC-C2C	-2.10	1.46	1.51
32	l	609	CLA	C3B-CAB	-2.10	1.43	1.47
32	R	608	CLA	CMD-C2D	-2.10	1.46	1.50
32	CC	503	CLA	C3B-C2B	-2.10	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Cc	501	LMG	O1-C1	2.10	1.43	1.40
32	g	613	CLA	C3B-CAB	-2.10	1.43	1.47
32	CC	512	CLA	CMD-C2D	-2.10	1.46	1.50
32	Y	602	CLA	C3B-C2B	-2.10	1.37	1.40
32	BB	602	CLA	C3B-CAB	-2.10	1.43	1.47
33	Aa	408	PHO	CMD-C2D	-2.10	1.46	1.51
39	YY	609	CHL	CMB-C2B	-2.10	1.47	1.51
32	G	604	CLA	C3B-C2B	-2.10	1.37	1.40
32	Cc	508	CLA	CMD-C2D	-2.10	1.46	1.50
38	c	519	LMG	O1-C1	2.10	1.43	1.40
39	Nn	319	CHL	CMB-C2B	-2.10	1.47	1.51
32	RR	308	CLA	CMD-C2D	-2.10	1.46	1.50
32	n	614	CLA	C3B-C2B	-2.10	1.37	1.40
32	r	613	CLA	C3B-C2B	-2.10	1.37	1.40
41	Gg	301	XAT	O4-C5	-2.10	1.43	1.46
32	R	602	CLA	CMD-C2D	-2.10	1.46	1.50
32	Y	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	Yy	611	CLA	CMD-C2D	-2.10	1.46	1.50
32	Rr	612	CLA	C3B-C2B	-2.10	1.37	1.40
32	G	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	b	613	CLA	C3B-CAB	-2.10	1.43	1.47
32	Bb	603	CLA	C3B-CAB	-2.10	1.43	1.47
39	r	605	CHL	CMD-C2D	-2.10	1.46	1.50
32	Bb	609	CLA	CMD-C2D	-2.10	1.46	1.50
32	CC	514	CLA	CMD-C2D	-2.10	1.46	1.50
32	n	602	CLA	CMD-C2D	-2.10	1.46	1.50
32	n	611	CLA	CMD-C2D	-2.10	1.46	1.50
32	Gg	314	CLA	CMD-C2D	-2.10	1.46	1.50
41	y	301	XAT	C28-C29	2.10	1.50	1.45
32	44	604	CLA	C3B-C2B	-2.10	1.37	1.40
32	AA	408	CLA	CMD-C2D	-2.10	1.46	1.50
32	Cc	510	CLA	CMD-C2D	-2.10	1.46	1.50
32	n	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	Bb	606	CLA	CMD-C2D	-2.10	1.46	1.50
32	l	611	CLA	C1B-NB	2.10	1.37	1.35
41	RR	316	XAT	O24-C25	-2.10	1.43	1.46
32	c	505	CLA	C3B-C2B	-2.09	1.37	1.40
40	N	616	LUT	C26-C27	2.09	1.53	1.50
34	Bb	617	BCR	C19-C18	2.09	1.50	1.45
32	y	316	CLA	CMD-C2D	-2.09	1.46	1.50
39	RR	306	CHL	CMB-C2B	-2.09	1.47	1.51
32	11	612	CLA	C1B-NB	2.09	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	NN	608	CHL	C1B-NB	2.09	1.37	1.35
32	Bb	610	CLA	CMD-C2D	-2.09	1.46	1.50
41	y	302	XAT	C12-C13	2.09	1.50	1.45
41	R	616	XAT	O4-C5	-2.09	1.43	1.46
32	R	610	CLA	CMD-C2D	-2.09	1.46	1.50
32	C	512	CLA	CMD-C2D	-2.09	1.46	1.50
32	b	605	CLA	CMD-C2D	-2.09	1.46	1.50
39	YY	609	CHL	CMD-C2D	-2.09	1.46	1.50
32	Aa	407	CLA	C3B-CAB	-2.09	1.43	1.47
32	Aa	410	CLA	C3B-CAB	-2.09	1.43	1.47
32	Bb	605	CLA	CMD-C2D	-2.09	1.46	1.50
32	CC	508	CLA	C3B-CAB	-2.09	1.43	1.47
32	Nn	303	CLA	CMD-C2D	-2.09	1.46	1.50
33	D	402	PHO	CMC-C2C	-2.09	1.46	1.51
32	Yy	612	CLA	C3B-CAB	-2.09	1.43	1.47
32	2	604	CLA	CMD-C2D	-2.09	1.46	1.50
32	s	613	CLA	CMD-C2D	-2.09	1.46	1.50
32	Cc	511	CLA	CMD-C2D	-2.09	1.46	1.50
32	r	603	CLA	C3B-C2B	-2.09	1.37	1.40
39	NN	605	CHL	CMD-C2D	-2.09	1.46	1.50
32	CC	505	CLA	C3B-CAB	-2.09	1.43	1.47
32	BB	608	CLA	C3B-C2B	-2.09	1.37	1.40
32	NN	602	CLA	C3B-CAB	-2.09	1.43	1.47
39	1	601	CHL	CMD-C2D	-2.09	1.46	1.50
32	BB	603	CLA	C3B-CAB	-2.09	1.43	1.47
39	Yy	601	CHL	CMB-C2B	-2.09	1.47	1.51
39	3	606	CHL	C1B-NB	2.09	1.37	1.35
39	YY	606	CHL	C1B-NB	2.09	1.37	1.35
32	B	624	CLA	CMD-C2D	-2.09	1.46	1.50
32	SS	313	CLA	CMD-C2D	-2.09	1.46	1.50
32	r	612	CLA	C3B-C2B	-2.09	1.37	1.40
34	B	613	BCR	C19-C18	2.09	1.50	1.45
32	N	612	CLA	CMD-C2D	-2.09	1.46	1.50
32	r	604	CLA	CMD-C2D	-2.09	1.46	1.50
32	S	602	CLA	C3B-C2B	-2.09	1.37	1.40
32	y	316	CLA	C3B-C2B	-2.09	1.37	1.40
32	c	512	CLA	CMD-C2D	-2.09	1.46	1.50
32	NN	610	CLA	CMD-C2D	-2.09	1.46	1.50
32	11	609	CLA	C3B-C2B	-2.09	1.37	1.40
32	y	312	CLA	CMD-C2D	-2.09	1.46	1.50
39	1	606	CHL	C1B-NB	2.09	1.37	1.35
34	b	618	BCR	C23-C22	2.08	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	Rr	608	CLA	CMD-C2D	-2.08	1.46	1.50
32	CC	509	CLA	C3B-C2B	-2.08	1.37	1.40
32	NN	613	CLA	CMD-C2D	-2.08	1.46	1.50
32	SS	309	CLA	CMD-C2D	-2.08	1.46	1.50
32	g	611	CLA	C3B-C2B	-2.08	1.37	1.40
32	R	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	R	612	CLA	CMD-C2D	-2.08	1.46	1.50
32	CC	505	CLA	CMD-C2D	-2.08	1.46	1.50
32	C	513	CLA	C3B-CAB	-2.08	1.43	1.47
32	Y	614	CLA	C3B-C2B	-2.08	1.37	1.40
32	YY	614	CLA	C3B-C2B	-2.08	1.37	1.40
32	Gg	304	CLA	C3B-CAB	-2.08	1.43	1.47
32	Nn	312	CLA	C3B-CAB	-2.08	1.43	1.47
32	Rr	603	CLA	CMD-C2D	-2.08	1.46	1.50
32	c	508	CLA	CMD-C2D	-2.08	1.46	1.50
32	g	614	CLA	CMD-C2D	-2.08	1.46	1.50
39	Y	609	CHL	CMD-C2D	-2.08	1.46	1.50
41	N	617	XAT	C12-C13	2.08	1.50	1.45
32	4	303	CLA	CMD-C2D	-2.08	1.46	1.50
41	r	615	XAT	O24-C25	-2.08	1.43	1.46
32	CC	513	CLA	C3B-C2B	-2.08	1.37	1.40
33	a	409	PHO	CMC-C2C	-2.08	1.46	1.51
32	g	610	CLA	C3B-CAB	-2.08	1.43	1.47
40	SS	315	LUT	C32-C33	2.08	1.50	1.45
32	A	406	CLA	CMD-C2D	-2.08	1.46	1.50
32	RR	309	CLA	CMD-C2D	-2.08	1.46	1.50
41	NN	617	XAT	C12-C13	2.08	1.50	1.45
32	a	410	CLA	CMD-C2D	-2.08	1.46	1.50
32	s	611	CLA	CMD-C2D	-2.08	1.46	1.50
39	Yy	609	CHL	CMD-C2D	-2.08	1.46	1.50
40	g	616	LUT	C8-C9	2.08	1.50	1.45
32	g	602	CLA	CMD-C2D	-2.08	1.46	1.50
32	a	407	CLA	C3B-CAB	-2.08	1.43	1.47
32	AA	406	CLA	C3B-CAB	-2.08	1.43	1.47
32	Ss	602	CLA	CMD-C2D	-2.08	1.46	1.50
32	n	604	CLA	CMD-C2D	-2.08	1.46	1.50
32	A	408	CLA	CMD-C2D	-2.08	1.46	1.50
32	GG	603	CLA	CMD-C2D	-2.08	1.46	1.50
32	Gg	313	CLA	CMD-C2D	-2.08	1.46	1.50
32	Ss	611	CLA	CMD-C2D	-2.08	1.46	1.50
39	N	601	CHL	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	44	601	CHL	C1B-NB	2.08	1.37	1.35
32	N	603	CLA	C3B-C2B	-2.08	1.37	1.40
32	Nn	314	CLA	CMD-C2D	-2.08	1.46	1.50
39	N	606	CHL	C1B-NB	2.08	1.37	1.35
32	GG	613	CLA	CMD-C2D	-2.08	1.46	1.50
39	11	608	CHL	CMD-C2D	-2.08	1.46	1.50
39	Nn	317	CHL	CMD-C2D	-2.08	1.46	1.50
34	TT	101	BCR	C12-C13	2.08	1.50	1.45
32	44	611	CLA	CMD-C2D	-2.08	1.46	1.50
32	N	604	CLA	CMD-C2D	-2.08	1.46	1.50
32	Nn	301	CLA	CMD-C2D	-2.08	1.46	1.50
32	2	613	CLA	CMD-C2D	-2.07	1.46	1.50
32	RR	312	CLA	CMD-C2D	-2.07	1.46	1.50
32	NN	614	CLA	C3B-C2B	-2.07	1.37	1.40
32	44	609	CLA	CMD-C2D	-2.07	1.46	1.50
32	AA	406	CLA	CMD-C2D	-2.07	1.46	1.50
39	Nn	319	CHL	CMD-C2D	-2.07	1.46	1.50
32	r	611	CLA	CMD-C2D	-2.07	1.46	1.50
32	c	506	CLA	CMD-C2D	-2.07	1.46	1.50
32	Gg	304	CLA	CMD-C2D	-2.07	1.46	1.50
39	g	606	CHL	CMD-C2D	-2.07	1.46	1.50
32	RR	302	CLA	CMD-C2D	-2.07	1.46	1.50
32	n	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	b	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	C	506	CLA	C3B-CAB	-2.07	1.43	1.47
32	Bb	613	CLA	C3B-CAB	-2.07	1.43	1.47
32	S	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	D	404	CLA	C3B-C2B	-2.07	1.37	1.40
40	NN	615	LUT	C12-C13	2.07	1.50	1.45
32	y	313	CLA	C3B-C2B	-2.07	1.37	1.40
32	Rr	609	CLA	CMD-C2D	-2.07	1.46	1.50
32	Ss	608	CLA	CMD-C2D	-2.07	1.46	1.50
32	G	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	22	602	CLA	C3B-C2B	-2.07	1.37	1.40
32	b	606	CLA	C3B-CAB	-2.07	1.43	1.47
32	b	606	CLA	CMD-C2D	-2.07	1.46	1.50
41	Nn	308	XAT	C12-C13	2.07	1.50	1.45
32	Bb	612	CLA	C3B-C2B	-2.07	1.37	1.40
32	BB	603	CLA	CMC-C2C	-2.07	1.46	1.50
32	Bb	606	CLA	C3B-CAB	-2.07	1.43	1.47
32	R	613	CLA	C3B-C2B	-2.07	1.37	1.40
32	s	610	CLA	C3B-C2B	-2.07	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	NN	612	CLA	CMD-C2D	-2.07	1.46	1.50
32	d	401	CLA	C3B-C2B	-2.07	1.37	1.40
39	N	607	CHL	CMD-C2D	-2.07	1.46	1.50
39	y	310	CHL	CMD-C2D	-2.07	1.46	1.50
34	BB	618	BCR	C23-C22	2.07	1.50	1.45
39	GG	606	CHL	C1B-NB	2.07	1.37	1.35
32	c	509	CLA	C3B-CAB	-2.07	1.43	1.47
32	n	610	CLA	C3B-CAB	-2.07	1.43	1.47
32	D	405	CLA	CMD-C2D	-2.07	1.46	1.50
39	Yy	607	CHL	CMD-C2D	-2.07	1.46	1.50
32	11	612	CLA	MG-NA	2.07	2.11	2.06
32	C	508	CLA	C3B-C2B	-2.07	1.37	1.40
32	Cc	504	CLA	C3B-C2B	-2.07	1.37	1.40
33	DD	402	PHO	C3B-C2B	-2.07	1.37	1.40
32	Yy	610	CLA	CMD-C2D	-2.07	1.46	1.50
32	2	609	CLA	C3B-C2B	-2.07	1.37	1.40
32	c	508	CLA	C3B-C2B	-2.07	1.37	1.40
39	Gg	302	CHL	C1B-NB	2.07	1.37	1.35
32	CC	511	CLA	CMD-C2D	-2.07	1.46	1.50
32	NN	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	Cc	514	CLA	CMD-C2D	-2.07	1.46	1.50
33	Aa	408	PHO	C3B-C2B	-2.07	1.37	1.40
39	Nn	311	CHL	CMD-C2D	-2.07	1.46	1.50
39	N	608	CHL	CMB-C2B	-2.07	1.47	1.51
32	Bb	615	CLA	C3B-CAB	-2.06	1.43	1.47
32	44	602	CLA	CMD-C2D	-2.06	1.46	1.50
39	Rr	607	CHL	CMD-C2D	-2.06	1.46	1.50
39	Yy	608	CHL	CMD-C2D	-2.06	1.46	1.50
32	Rr	604	CLA	CMD-C2D	-2.06	1.46	1.50
32	r	612	CLA	CMD-C2D	-2.06	1.46	1.50
41	G	619	XAT	C12-C13	2.06	1.50	1.45
34	T	101	BCR	C12-C13	2.06	1.50	1.45
32	s	608	CLA	CMD-C2D	-2.06	1.46	1.50
32	y	313	CLA	CMD-C2D	-2.06	1.46	1.50
40	RR	315	LUT	C22-C21	-2.06	1.52	1.54
32	Bb	603	CLA	CMC-C2C	-2.06	1.46	1.50
32	Gg	303	CLA	CMD-C2D	-2.06	1.46	1.50
34	c	516	BCR	C23-C22	2.06	1.50	1.45
34	Cc	517	BCR	C8-C9	2.06	1.50	1.45
40	N	615	LUT	C22-C21	-2.06	1.52	1.54
32	RR	303	CLA	C3B-C2B	-2.06	1.37	1.40
32	3	613	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	604	CLA	CMD-C2D	-2.06	1.46	1.50
37	BB	621	SQD	O6-C1	2.06	1.43	1.40
32	b	604	CLA	C3B-C2B	-2.06	1.37	1.40
32	Cc	506	CLA	CMD-C2D	-2.06	1.46	1.50
34	Cc	518	BCR	C23-C22	2.06	1.50	1.45
32	C	506	CLA	CMD-C2D	-2.06	1.46	1.50
32	g	603	CLA	CMD-C2D	-2.06	1.46	1.50
39	S	601	CHL	CMD-C2D	-2.06	1.46	1.50
32	c	512	CLA	C3B-C2B	-2.06	1.37	1.40
32	g	610	CLA	CMD-C2D	-2.06	1.46	1.50
32	B	620	CLA	CMC-C2C	-2.06	1.46	1.50
39	Y	606	CHL	CMD-C2D	-2.06	1.46	1.50
39	y	307	CHL	CMD-C2D	-2.06	1.46	1.50
32	S	602	CLA	CMD-C2D	-2.06	1.46	1.50
32	SS	303	CLA	CMD-C2D	-2.06	1.46	1.50
39	4	307	CHL	CMD-C2D	-2.06	1.46	1.50
40	NN	616	LUT	C8-C9	2.06	1.50	1.45
32	n	602	CLA	C3B-CAB	-2.06	1.43	1.47
32	c	509	CLA	CMD-C2D	-2.06	1.46	1.50
35	A	410	PL9	C31-C29	2.06	1.55	1.51
32	Cc	515	CLA	CMD-C2D	-2.06	1.46	1.50
39	y	309	CHL	CMD-C2D	-2.06	1.46	1.50
32	R	601	CLA	C3B-C2B	-2.06	1.37	1.40
32	22	603	CLA	CMD-C2D	-2.06	1.46	1.50
32	44	610	CLA	CMD-C2D	-2.06	1.46	1.50
39	g	609	CHL	CMD-C2D	-2.06	1.46	1.50
32	CC	507	CLA	C3B-C2B	-2.06	1.37	1.40
32	NN	604	CLA	CMD-C2D	-2.06	1.46	1.50
39	YY	606	CHL	CMD-C2D	-2.06	1.46	1.50
32	B	619	CLA	C3B-CAB	-2.06	1.43	1.47
39	Nn	318	CHL	CMB-C2B	-2.05	1.47	1.51
33	D	402	PHO	CMB-C2B	-2.05	1.46	1.51
32	4	304	CLA	CMD-C2D	-2.05	1.46	1.50
32	Bb	602	CLA	CMD-C2D	-2.05	1.46	1.50
32	Y	604	CLA	C3B-C2B	-2.05	1.37	1.40
32	GG	613	CLA	C3B-C2B	-2.05	1.37	1.40
41	g	619	XAT	O24-C25	-2.05	1.43	1.46
32	2	603	CLA	CMD-C2D	-2.05	1.46	1.50
39	N	605	CHL	CMD-C2D	-2.05	1.46	1.50
32	Cc	507	CLA	C3B-C2B	-2.05	1.37	1.40
32	Y	610	CLA	CMD-C2D	-2.05	1.46	1.50
32	a	407	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	602	CLA	CMD-C2D	-2.05	1.46	1.50
34	CC	516	BCR	C12-C13	2.05	1.50	1.45
32	4	312	CLA	CMD-C2D	-2.05	1.46	1.50
39	Y	608	CHL	CMB-C2B	-2.05	1.47	1.51
32	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
32	Cc	514	CLA	C3B-C2B	-2.05	1.37	1.40
32	C	509	CLA	C3B-CAB	-2.05	1.43	1.47
32	YY	610	CLA	CMD-C2D	-2.05	1.46	1.50
32	Bb	607	CLA	C3B-CAB	-2.05	1.43	1.47
32	B	624	CLA	CMC-C2C	-2.05	1.46	1.50
39	N	608	CHL	CMD-C2D	-2.05	1.46	1.50
32	C	514	CLA	C3B-CAB	-2.05	1.43	1.47
39	YY	608	CHL	CMB-C2B	-2.05	1.47	1.51
32	33	613	CLA	CMD-C2D	-2.05	1.46	1.50
32	C	515	CLA	CMD-C2D	-2.05	1.46	1.50
39	n	605	CHL	CMD-C2D	-2.05	1.46	1.50
32	11	603	CLA	C3B-C2B	-2.05	1.37	1.40
32	r	608	CLA	CMD-C2D	-2.05	1.46	1.50
39	Nn	318	CHL	CMD-C2D	-2.05	1.46	1.50
32	n	612	CLA	CMC-C2C	-2.05	1.46	1.50
32	B	621	CLA	CMD-C2D	-2.05	1.46	1.50
32	RR	313	CLA	C3B-C2B	-2.05	1.37	1.40
32	R	609	CLA	C3B-CAB	-2.05	1.43	1.47
32	C	510	CLA	C3B-C2B	-2.05	1.37	1.40
32	44	603	CLA	CMD-C2D	-2.05	1.46	1.50
39	YY	601	CHL	CMD-C2D	-2.05	1.46	1.50
34	AA	409	BCR	C19-C18	2.05	1.50	1.45
32	Y	611	CLA	C3B-C2B	-2.05	1.37	1.40
32	Rr	602	CLA	CMD-C2D	-2.05	1.46	1.50
32	Y	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	BB	607	CLA	C3B-CAB	-2.05	1.43	1.47
32	22	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	b	608	CLA	CMD-C2D	-2.05	1.46	1.50
32	4	311	CLA	CMD-C2D	-2.05	1.46	1.50
32	Bb	601	CLA	CMD-C2D	-2.04	1.46	1.50
32	Gg	315	CLA	CMD-C2D	-2.04	1.46	1.50
39	s	601	CHL	CMD-C2D	-2.04	1.46	1.50
39	y	311	CHL	CMD-C2D	-2.04	1.46	1.50
32	SS	311	CLA	CMD-C2D	-2.04	1.46	1.50
32	RR	309	CLA	C3B-CAB	-2.04	1.43	1.47
32	BB	605	CLA	C3B-CAB	-2.04	1.43	1.47
32	Dd	402	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Nh	315	CHL	CMD-C2D	-2.04	1.46	1.50
39	Gg	309	CHL	CMD-C2D	-2.04	1.46	1.50
32	3	612	CLA	C3B-C2B	-2.04	1.37	1.40
32	b	608	CLA	C3B-CAB	-2.04	1.43	1.47
39	44	606	CHL	CMD-C2D	-2.04	1.46	1.50
39	n	609	CHL	CMD-C2D	-2.04	1.46	1.50
39	R	607	CHL	CMD-C2D	-2.04	1.46	1.50
32	n	612	CLA	MG-NA	2.04	2.11	2.06
32	44	615	CLA	CMD-C2D	-2.04	1.46	1.50
32	BB	609	CLA	CMD-C2D	-2.04	1.46	1.50
32	N	613	CLA	MG-ND	-2.04	2.01	2.05
32	Ss	602	CLA	C3B-C2B	-2.04	1.37	1.40
32	22	612	CLA	C3B-C2B	-2.04	1.37	1.40
32	RR	311	CLA	CMD-C2D	-2.04	1.46	1.50
34	a	411	BCR	C12-C13	2.04	1.50	1.45
34	c	515	BCR	C8-C9	2.04	1.50	1.45
32	N	603	CLA	CMD-C2D	-2.04	1.46	1.50
39	g	608	CHL	CMD-C2D	-2.04	1.46	1.50
39	GG	601	CHL	CMD-C2D	-2.04	1.46	1.50
40	N	615	LUT	C12-C13	2.04	1.50	1.45
39	RR	306	CHL	C1B-NB	2.04	1.37	1.35
41	y	301	XAT	C12-C13	2.04	1.50	1.45
32	S	604	CLA	C3B-C2B	-2.04	1.37	1.40
39	Y	601	CHL	CMD-C2D	-2.04	1.46	1.50
39	n	606	CHL	CMD-C2D	-2.04	1.46	1.50
39	Y	605	CHL	CMD-C2D	-2.04	1.46	1.50
39	GG	607	CHL	CMD-C2D	-2.04	1.46	1.50
39	SS	307	CHL	CMD-C2D	-2.04	1.46	1.50
32	CC	504	CLA	C3B-CAB	-2.04	1.43	1.47
32	S	609	CLA	CMD-C2D	-2.04	1.46	1.50
39	G	607	CHL	CMD-C2D	-2.04	1.46	1.50
32	c	504	CLA	CMD-C2D	-2.04	1.46	1.50
39	Yy	605	CHL	CMD-C2D	-2.04	1.46	1.50
41	Gg	301	XAT	O24-C25	-2.04	1.43	1.46
32	G	612	CLA	CMD-C2D	-2.04	1.46	1.50
32	Y	604	CLA	CMD-C2D	-2.04	1.46	1.50
34	a	411	BCR	C23-C22	2.04	1.50	1.45
40	g	615	LUT	C12-C13	2.04	1.50	1.45
32	Y	613	CLA	C4B-CHC	-2.04	1.35	1.41
32	c	507	CLA	C3B-C2B	-2.04	1.37	1.40
32	n	603	CLA	C3B-C2B	-2.04	1.37	1.40
39	YY	605	CHL	C1B-NB	2.04	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	607	CHL	CMD-C2D	-2.04	1.46	1.50
32	CC	507	CLA	C3B-CAB	-2.04	1.43	1.47
32	G	613	CLA	CMD-C2D	-2.04	1.46	1.50
39	Y	607	CHL	CMD-C2D	-2.04	1.46	1.50
32	Ss	610	CLA	C3B-C2B	-2.04	1.37	1.40
41	GG	617	XAT	O4-C5	-2.03	1.43	1.46
32	NN	602	CLA	CMD-C2D	-2.03	1.46	1.50
39	Ss	601	CHL	CMD-C2D	-2.03	1.46	1.50
32	R	611	CLA	CMD-C2D	-2.03	1.46	1.50
32	CC	502	CLA	C3B-C2B	-2.03	1.37	1.40
32	RR	313	CLA	CMD-C2D	-2.03	1.46	1.50
32	Nn	313	CLA	CMD-C2D	-2.03	1.46	1.50
34	CC	515	BCR	C12-C13	2.03	1.50	1.45
32	33	609	CLA	C3B-C2B	-2.03	1.37	1.40
32	N	614	CLA	C3B-C2B	-2.03	1.37	1.40
32	R	602	CLA	CMC-C2C	-2.03	1.46	1.50
32	g	612	CLA	CMD-C2D	-2.03	1.46	1.50
32	4	305	CLA	CMD-C2D	-2.03	1.46	1.50
39	Ss	605	CHL	CMD-C2D	-2.03	1.46	1.50
39	y	308	CHL	CMD-C2D	-2.03	1.46	1.50
42	NN	618	NEX	O24-C25	-2.03	1.43	1.46
32	22	609	CLA	CMD-C2D	-2.03	1.46	1.50
32	YY	604	CLA	CMD-C2D	-2.03	1.46	1.50
39	Gg	307	CHL	CMD-C2D	-2.03	1.46	1.50
32	NN	613	CLA	MG-ND	-2.03	2.01	2.05
32	Bb	602	CLA	C3B-CAB	-2.03	1.43	1.47
32	b	612	CLA	C3B-C2B	-2.03	1.37	1.40
32	1	604	CLA	CMD-C2D	-2.03	1.46	1.50
32	1	611	CLA	CMD-C2D	-2.03	1.46	1.50
32	GG	613	CLA	C4B-CHC	-2.03	1.35	1.41
39	Y	601	CHL	CMB-C2B	-2.03	1.47	1.51
39	SS	302	CHL	CMD-C2D	-2.03	1.46	1.50
41	G	617	XAT	O4-C5	-2.03	1.43	1.46
39	NN	607	CHL	CMD-C2D	-2.03	1.46	1.50
38	Aa	412	LMG	O1-C1	2.03	1.43	1.40
32	Ss	613	CLA	CMD-C2D	-2.03	1.46	1.50
32	B	605	CLA	CMC-C2C	-2.03	1.46	1.50
32	g	613	CLA	C4B-CHC	-2.03	1.35	1.41
32	Ss	611	CLA	C3B-C2B	-2.03	1.37	1.40
32	2	610	CLA	CMD-C2D	-2.03	1.46	1.50
41	g	619	XAT	O4-C5	-2.03	1.43	1.46
32	1	609	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	307	CHL	CMB-C2B	-2.03	1.47	1.51
39	G	609	CHL	CMD-C2D	-2.03	1.46	1.50
39	NN	608	CHL	CMD-C2D	-2.03	1.46	1.50
32	RR	302	CLA	C3B-CAB	-2.03	1.43	1.47
32	R	613	CLA	CMD-C2D	-2.03	1.46	1.50
39	R	606	CHL	CMD-C2D	-2.03	1.46	1.50
41	y	301	XAT	O4-C5	-2.03	1.43	1.46
32	B	620	CLA	C3B-CAB	-2.03	1.43	1.47
34	Cc	516	BCR	C23-C22	2.03	1.50	1.45
39	n	608	CHL	CMB-C2B	-2.03	1.47	1.51
32	AA	408	CLA	C3B-CAB	-2.03	1.43	1.47
32	G	610	CLA	CMD-C2D	-2.03	1.46	1.50
32	N	602	CLA	CMD-C2D	-2.03	1.46	1.50
34	c	514	BCR	C23-C22	2.03	1.50	1.45
32	s	602	CLA	CMD-C2D	-2.03	1.46	1.50
41	Yy	619	XAT	C12-C13	2.03	1.50	1.45
41	Yy	619	XAT	O4-C5	-2.03	1.43	1.46
35	A	410	PL9	C26-C24	2.03	1.55	1.51
32	d	402	CLA	CMD-C2D	-2.03	1.46	1.50
32	GG	604	CLA	CMD-C2D	-2.03	1.46	1.50
39	Yy	601	CHL	CMD-C2D	-2.03	1.46	1.50
39	S	606	CHL	CMD-C2D	-2.03	1.46	1.50
39	2	601	CHL	CMB-C2B	-2.03	1.47	1.51
32	y	305	CLA	C3B-CAB	-2.03	1.43	1.47
39	Gg	310	CHL	CMD-C2D	-2.03	1.46	1.50
41	NN	617	XAT	C28-C29	2.03	1.50	1.45
32	n	613	CLA	C4B-CHC	-2.03	1.35	1.41
32	S	608	CLA	C3B-C2B	-2.03	1.37	1.40
32	33	612	CLA	CMD-C2D	-2.02	1.46	1.50
32	b	601	CLA	CMD-C2D	-2.02	1.46	1.50
39	N	601	CHL	C1B-NB	2.02	1.37	1.35
32	y	304	CLA	CMC-C2C	-2.02	1.46	1.50
35	AA	410	PL9	C37-C38	2.02	1.57	1.50
32	Yy	610	CLA	CMC-C2C	-2.02	1.46	1.50
39	4	308	CHL	CMD-C2D	-2.02	1.46	1.50
32	b	615	CLA	C3B-CAB	-2.02	1.43	1.47
41	44	613	XAT	O24-C25	-2.02	1.43	1.46
32	R	611	CLA	C3B-C2B	-2.02	1.37	1.40
42	Y	617	NEX	O24-C25	-2.02	1.43	1.46
39	YY	608	CHL	CMD-C2D	-2.02	1.46	1.50
32	S	610	CLA	C3B-C2B	-2.02	1.37	1.40
32	Cc	515	CLA	C3B-C2B	-2.02	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Aa	409	PHO	C3B-C2B	-2.02	1.37	1.40
40	r	614	LUT	C22-C21	-2.02	1.52	1.54
39	YY	609	CHL	C1B-NB	2.02	1.37	1.35
39	2	608	CHL	CMB-C2B	-2.02	1.47	1.51
34	BB	617	BCR	C19-C18	2.02	1.50	1.45
32	n	613	CLA	CMD-C2D	-2.02	1.46	1.50
32	3	611	CLA	CMD-C2D	-2.02	1.46	1.50
32	S	604	CLA	CMD-C2D	-2.02	1.46	1.50
32	s	610	CLA	CMD-C2D	-2.02	1.46	1.50
35	AA	410	PL9	C31-C29	2.02	1.55	1.51
32	Aa	406	CLA	C4B-CHC	-2.02	1.35	1.41
32	N	602	CLA	C3B-CAB	-2.02	1.43	1.47
34	b	619	BCR	C23-C22	2.02	1.50	1.45
32	c	505	CLA	CMC-C2C	-2.02	1.46	1.50
32	r	609	CLA	CMD-C2D	-2.02	1.46	1.50
39	33	608	CHL	CMD-C2D	-2.02	1.46	1.50
32	YY	610	CLA	C3B-CAB	-2.02	1.43	1.47
32	s	609	CLA	CMC-C2C	-2.02	1.46	1.50
40	YY	615	LUT	C22-C21	-2.02	1.52	1.54
41	N	617	XAT	C28-C29	2.02	1.50	1.45
32	Gg	311	CLA	CMD-C2D	-2.02	1.46	1.50
42	N	618	NEX	O24-C25	-2.02	1.43	1.46
39	N	608	CHL	C1B-NB	2.02	1.37	1.35
32	Ss	612	CLA	CMD-C2D	-2.02	1.46	1.50
32	R	601	CLA	CMD-C2D	-2.02	1.46	1.50
32	SS	314	CLA	CMD-C2D	-2.02	1.46	1.50
39	n	608	CHL	CMD-C2D	-2.02	1.46	1.50
39	GG	609	CHL	CMD-C2D	-2.02	1.46	1.50
32	BB	601	CLA	C3B-C2B	-2.02	1.37	1.40
32	Bb	604	CLA	C3B-C2B	-2.02	1.37	1.40
34	A	409	BCR	C19-C18	2.02	1.50	1.45
32	BB	607	CLA	CMC-C2C	-2.02	1.46	1.50
34	c	514	BCR	C12-C13	2.02	1.50	1.45
32	R	614	CLA	C1B-NB	2.02	1.37	1.35
32	Ss	603	CLA	CMD-C2D	-2.02	1.46	1.50
32	GG	610	CLA	CMD-C2D	-2.02	1.46	1.50
32	YY	602	CLA	CMD-C2D	-2.02	1.46	1.50
32	Nn	302	CLA	CMD-C2D	-2.02	1.46	1.50
33	a	408	PHO	C3B-C2B	-2.02	1.37	1.40
41	g	619	XAT	C28-C29	2.02	1.50	1.45
39	44	607	CHL	C1B-NB	2.02	1.37	1.35
32	A	406	CLA	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	XX	202	BCR	C23-C22	2.02	1.50	1.45
39	Yy	605	CHL	CMB-C2B	-2.02	1.47	1.51
32	Ss	610	CLA	CMD-C2D	-2.02	1.46	1.50
32	1	603	CLA	CMD-C2D	-2.02	1.46	1.50
32	n	604	CLA	C3B-C2B	-2.02	1.37	1.40
32	NN	611	CLA	CMD-C2D	-2.02	1.46	1.50
32	C	515	CLA	C3B-C2B	-2.02	1.37	1.40
32	s	611	CLA	C3B-C2B	-2.02	1.37	1.40
32	B	618	CLA	C3B-C2B	-2.02	1.37	1.40
40	Gg	317	LUT	C8-C9	2.02	1.50	1.45
35	A	410	PL9	C37-C38	2.01	1.57	1.50
39	Y	608	CHL	CMD-C2D	-2.01	1.46	1.50
39	Y	606	CHL	C1B-NB	2.01	1.37	1.35
32	RR	311	CLA	C3B-C2B	-2.01	1.37	1.40
32	s	603	CLA	CMD-C2D	-2.01	1.46	1.50
32	Dd	401	CLA	CMC-C2C	-2.01	1.46	1.50
38	W	201	LMG	O1-C1	2.01	1.43	1.40
32	Yy	604	CLA	CMD-C2D	-2.01	1.46	1.50
32	s	612	CLA	CMD-C2D	-2.01	1.46	1.50
39	YY	601	CHL	CMB-C2B	-2.01	1.47	1.51
39	g	605	CHL	CMD-C2D	-2.01	1.46	1.50
34	Hh	101	BCR	C8-C9	2.01	1.50	1.45
32	Nn	304	CLA	CMD-C2D	-2.01	1.46	1.50
41	44	613	XAT	O4-C5	-2.01	1.43	1.46
34	Bb	618	BCR	C23-C22	2.01	1.50	1.45
32	S	608	CLA	CMD-C2D	-2.01	1.46	1.50
32	BB	609	CLA	CMC-C2C	-2.01	1.46	1.50
32	Bb	608	CLA	CMD-C2D	-2.01	1.46	1.50
39	Gg	308	CHL	C1B-NB	2.01	1.37	1.35
32	Rr	612	CLA	CMD-C2D	-2.01	1.46	1.50
32	11	609	CLA	CMD-C2D	-2.01	1.46	1.50
32	n	602	CLA	CMC-C2C	-2.01	1.46	1.50
32	GG	614	CLA	CMD-C2D	-2.01	1.46	1.50
39	SS	306	CHL	CMD-C2D	-2.01	1.46	1.50
32	c	502	CLA	C3B-C2B	-2.01	1.37	1.40
34	c	515	BCR	C19-C18	2.01	1.50	1.45
39	g	607	CHL	CMD-C2D	-2.01	1.46	1.50
32	CC	513	CLA	C3B-CAB	-2.01	1.43	1.47
40	GG	616	LUT	C8-C9	2.01	1.50	1.45
32	y	306	CLA	CMD-C2D	-2.01	1.46	1.50
32	3	602	CLA	C3B-C2B	-2.01	1.37	1.40
32	SS	311	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	614	BCR	C19-C18	2.01	1.50	1.45
32	3	612	CLA	CMD-C2D	-2.01	1.46	1.50
32	C	509	CLA	CMC-C2C	-2.01	1.46	1.50
32	Bb	610	CLA	CMC-C2C	-2.01	1.46	1.50
34	b	617	BCR	C19-C18	2.01	1.50	1.45
32	S	603	CLA	CMD-C2D	-2.01	1.46	1.50
39	44	606	CHL	CMB-C2B	-2.01	1.47	1.51
41	Gg	301	XAT	C28-C29	2.01	1.50	1.45
34	Aa	411	BCR	C23-C22	2.01	1.50	1.45
32	1	603	CLA	C3B-C2B	-2.01	1.37	1.40
32	2	613	CLA	C3B-C2B	-2.01	1.37	1.40
39	g	607	CHL	C1B-NB	2.01	1.37	1.35
32	SS	310	CLA	CMD-C2D	-2.01	1.46	1.50
39	Y	605	CHL	CMB-C2B	-2.01	1.47	1.51
32	r	610	CLA	C3B-C2B	-2.01	1.37	1.40
32	B	624	CLA	C3B-CAB	-2.01	1.43	1.47
32	44	604	CLA	CMD-C2D	-2.01	1.46	1.50
32	CC	512	CLA	CMC-C2C	-2.01	1.46	1.50
32	B	618	CLA	CMC-C2C	-2.01	1.46	1.50
39	Gg	306	CHL	CMD-C2D	-2.01	1.46	1.50
34	B	613	BCR	C12-C13	2.01	1.50	1.45
32	Gg	313	CLA	C4B-CHC	-2.01	1.35	1.41
32	22	604	CLA	CMD-C2D	-2.00	1.46	1.50
39	33	607	CHL	CMD-C2D	-2.00	1.46	1.50
39	g	601	CHL	CMD-C2D	-2.00	1.46	1.50
39	YY	607	CHL	CMD-C2D	-2.00	1.46	1.50
32	B	622	CLA	C3B-CAB	-2.00	1.43	1.47
32	Aa	405	CLA	C4B-CHC	-2.00	1.35	1.41
32	Bb	608	CLA	CMC-C2C	-2.00	1.46	1.50
39	4	309	CHL	CMD-C2D	-2.00	1.46	1.50
32	g	614	CLA	C3B-C2B	-2.00	1.37	1.40
32	Nn	313	CLA	C3B-C2B	-2.00	1.37	1.40
39	4	302	CHL	CMB-C2B	-2.00	1.47	1.51
40	2	614	LUT	C28-C29	2.00	1.50	1.45
42	YY	617	NEX	O24-C25	-2.00	1.43	1.46
39	G	606	CHL	CMD-C2D	-2.00	1.46	1.50
39	GG	606	CHL	CMD-C2D	-2.00	1.46	1.50
34	C	517	BCR	C12-C13	2.00	1.50	1.45
32	b	607	CLA	C3B-CAB	-2.00	1.43	1.47
32	GG	610	CLA	C3B-CAB	-2.00	1.43	1.47
32	s	604	CLA	CMD-C2D	-2.00	1.46	1.50
32	SS	305	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	601	CHL	CMD-C2D	-2.00	1.46	1.50
35	AA	410	PL9	C42-C43	2.00	1.56	1.50
34	CC	517	BCR	C19-C18	2.00	1.50	1.45
39	GG	608	CHL	CMD-C2D	-2.00	1.46	1.50
39	1	605	CHL	C1B-NB	2.00	1.37	1.35
39	44	607	CHL	CMB-C2B	-2.00	1.47	1.51
32	N	612	CLA	C3B-C2B	-2.00	1.37	1.40
32	B	607	CLA	CMC-C2C	-2.00	1.46	1.50
39	11	601	CHL	CMD-C2D	-2.00	1.46	1.50
32	33	611	CLA	CMD-C2D	-2.00	1.46	1.50
32	G	614	CLA	CMD-C2D	-2.00	1.46	1.50
32	Bb	602	CLA	CMC-C2C	-2.00	1.46	1.50
42	R	617	NEX	C12-C13	2.00	1.50	1.45
42	RR	317	NEX	C12-C13	2.00	1.50	1.45
39	R	606	CHL	CMB-C2B	-2.00	1.47	1.51
34	Hh	101	BCR	C7-C6	2.00	1.52	1.45
32	11	603	CLA	CMD-C2D	-2.00	1.46	1.50
40	22	614	LUT	C28-C29	2.00	1.50	1.45
41	GG	619	XAT	O4-C5	-2.00	1.43	1.46
32	c	501	CLA	C3B-CAB	-2.00	1.43	1.47

All (5850) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BB	621	SQD	O9-S-C6	-19.31	83.99	106.94
37	B	617	SQD	O9-S-C6	-19.24	84.07	106.94
41	G	619	XAT	O24-C25-C24	14.32	124.14	113.38
41	GG	619	XAT	O24-C25-C24	14.28	124.11	113.38
41	g	619	XAT	O24-C25-C24	13.93	123.85	113.38
41	Gg	301	XAT	O24-C25-C24	13.73	123.69	113.38
41	Nn	308	XAT	O24-C25-C24	13.07	123.20	113.38
41	y	302	XAT	O24-C25-C24	11.66	122.14	113.38
37	BB	621	SQD	O8-S-O9	-11.53	83.10	111.27
37	B	617	SQD	O8-S-O9	-11.52	83.12	111.27
41	GG	619	XAT	O4-C5-C4	11.16	121.77	113.38
41	NN	617	XAT	O24-C25-C24	10.98	121.63	113.38
41	G	619	XAT	O4-C5-C4	10.71	121.43	113.38
41	Gg	301	XAT	O4-C5-C4	10.69	121.41	113.38
41	44	613	XAT	O4-C5-C4	10.68	121.41	113.38
41	g	619	XAT	O4-C5-C4	10.52	121.28	113.38
41	N	617	XAT	O24-C25-C24	10.36	121.17	113.38
41	44	613	XAT	O24-C25-C24	10.11	120.98	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	4	314	XAT	O24-C25-C24	10.07	120.94	113.38
37	B	617	SQD	O7-S-C6	9.92	118.73	106.94
37	BB	621	SQD	O7-S-C6	9.90	118.70	106.94
35	Dd	404	PL9	C7-C8-C9	-9.86	110.38	126.79
42	Gg	318	NEX	O24-C25-C24	9.83	120.77	113.38
35	d	404	PL9	C7-C8-C9	-9.60	110.81	126.79
35	D	407	PL9	C7-C8-C9	-9.42	111.11	126.79
41	GG	617	XAT	O24-C25-C24	9.37	120.42	113.38
35	DD	406	PL9	C7-C8-C9	-9.36	111.21	126.79
41	4	314	XAT	O4-C5-C4	9.33	120.39	113.38
41	G	617	XAT	O24-C25-C24	9.30	120.37	113.38
42	g	617	NEX	O24-C25-C24	9.25	120.33	113.38
37	B	617	SQD	O9-S-O7	-9.12	82.39	113.95
41	r	615	XAT	O4-C5-C4	9.11	120.22	113.38
37	BB	621	SQD	O9-S-O7	-9.10	82.47	113.95
35	AA	410	PL9	C7-C8-C9	-8.89	112.00	126.79
41	G	617	XAT	O4-C5-C4	8.86	120.03	113.38
35	A	410	PL9	C7-C8-C9	-8.83	112.08	126.79
41	GG	617	XAT	O4-C5-C4	8.82	120.00	113.38
42	Y	617	NEX	O24-C25-C24	8.82	120.00	113.38
40	Yy	615	LUT	C1-C6-C5	-8.77	110.26	122.61
42	Rr	616	NEX	O24-C25-C24	8.62	119.86	113.38
42	Y	619	NEX	O24-C25-C24	8.61	119.85	113.38
42	N	618	NEX	O24-C25-C24	8.17	119.52	113.38
42	YY	617	NEX	O24-C25-C24	8.14	119.50	113.38
41	y	301	XAT	O24-C25-C38	8.13	124.79	115.06
42	g	617	NEX	C39-C29-C30	-8.02	111.68	122.92
42	NN	618	NEX	O24-C25-C24	8.00	119.39	113.38
37	B	617	SQD	O8-S-C6	8.00	118.48	105.74
37	BB	621	SQD	O8-S-C6	7.94	118.39	105.74
41	y	301	XAT	O4-C5-C4	7.81	119.25	113.38
41	Nn	308	XAT	O4-C5-C4	7.78	119.23	113.38
41	Yy	619	XAT	O24-C25-C24	7.71	119.17	113.38
41	r	615	XAT	O24-C25-C24	7.70	119.17	113.38
42	n	617	NEX	O24-C25-C24	7.68	119.15	113.38
41	N	617	XAT	O4-C5-C4	7.58	119.08	113.38
41	NN	617	XAT	O4-C5-C4	7.48	119.00	113.38
32	g	602	CLA	C4A-NA-C1A	7.43	110.05	106.71
41	Rr	615	XAT	O24-C25-C24	7.27	118.84	113.38
40	y	317	LUT	C1-C6-C5	-7.26	112.39	122.61
42	Nn	309	NEX	O24-C25-C24	7.21	118.80	113.38
41	y	302	XAT	O4-C5-C4	7.15	118.76	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	R	617	NEX	O24-C25-C24	7.00	118.64	113.38
39	Yy	609	CHL	CMB-C2B-C1B	-6.96	117.76	128.46
41	Yy	619	XAT	O4-C5-C4	6.94	118.59	113.38
35	Dd	404	PL9	C37-C38-C39	-6.91	111.01	127.66
42	RR	317	NEX	O24-C25-C24	6.89	118.56	113.38
41	Rr	615	XAT	O4-C5-C4	6.89	118.56	113.38
35	D	407	PL9	C37-C38-C39	-6.86	111.14	127.66
34	h	101	BCR	C32-C1-C6	6.85	121.41	110.30
35	d	404	PL9	C37-C38-C39	-6.84	111.19	127.66
34	Hh	101	BCR	C32-C1-C6	6.82	121.36	110.30
35	d	404	PL9	C22-C23-C24	-6.79	111.31	127.66
35	DD	406	PL9	C37-C38-C39	-6.79	111.32	127.66
32	CC	507	CLA	C4A-NA-C1A	6.78	109.75	106.71
34	b	617	BCR	C28-C27-C26	-6.77	101.99	114.08
35	Dd	404	PL9	C22-C23-C24	-6.76	111.39	127.66
35	d	404	PL9	C12-C13-C14	-6.75	111.39	127.66
35	A	410	PL9	C22-C23-C24	-6.75	111.41	127.66
34	XX	202	BCR	C1-C6-C5	-6.75	113.11	122.61
35	Dd	404	PL9	C42-C43-C44	-6.68	111.56	127.66
34	KK	103	BCR	C30-C25-C26	-6.68	113.20	122.61
34	c	514	BCR	C3-C4-C5	-6.67	102.16	114.08
35	D	407	PL9	C32-C33-C34	-6.63	111.70	127.66
34	K	102	BCR	C30-C25-C26	-6.61	113.30	122.61
35	Dd	404	PL9	C12-C13-C14	-6.61	111.74	127.66
35	D	407	PL9	C17-C18-C19	-6.60	111.76	127.66
32	C	508	CLA	C4A-NA-C1A	6.58	109.67	106.71
35	d	404	PL9	C42-C43-C44	-6.58	111.81	127.66
41	R	616	XAT	O24-C25-C24	6.57	118.32	113.38
34	C	518	BCR	C3-C4-C5	-6.57	102.34	114.08
35	d	404	PL9	C27-C28-C29	-6.54	111.90	127.66
35	Dd	404	PL9	C27-C28-C29	-6.52	111.97	127.66
35	d	404	PL9	C17-C18-C19	-6.51	111.98	127.66
35	A	410	PL9	C17-C18-C19	-6.50	112.01	127.66
35	D	407	PL9	C27-C28-C29	-6.50	112.02	127.66
35	AA	410	PL9	C32-C33-C34	-6.49	112.04	127.66
35	DD	406	PL9	C32-C33-C34	-6.47	112.08	127.66
35	DD	406	PL9	C17-C18-C19	-6.47	112.08	127.66
35	D	407	PL9	C22-C23-C24	-6.47	112.09	127.66
34	Cc	516	BCR	C28-C27-C26	-6.46	102.55	114.08
32	GG	602	CLA	C4A-NA-C1A	6.42	109.59	106.71
35	D	407	PL9	C12-C13-C14	-6.41	112.21	127.66
35	DD	406	PL9	C22-C23-C24	-6.41	112.23	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	410	PL9	C32-C33-C34	-6.41	112.24	127.66
35	A	410	PL9	C27-C28-C29	-6.39	112.27	127.66
35	Dd	404	PL9	C17-C18-C19	-6.38	112.29	127.66
35	AA	410	PL9	C12-C13-C14	-6.38	112.30	127.66
35	D	407	PL9	C42-C43-C44	-6.37	112.32	127.66
35	DD	406	PL9	C12-C13-C14	-6.37	112.33	127.66
35	A	410	PL9	C12-C13-C14	-6.35	112.37	127.66
34	c	514	BCR	C28-C27-C26	-6.34	102.75	114.08
35	DD	406	PL9	C27-C28-C29	-6.34	112.41	127.66
34	CC	517	BCR	C3-C4-C5	-6.32	102.79	114.08
32	CC	502	CLA	C4A-NA-C1A	6.32	109.55	106.71
32	R	608	CLA	C4A-NA-C1A	6.29	109.53	106.71
35	DD	406	PL9	C42-C43-C44	-6.28	112.54	127.66
34	b	619	BCR	C3-C4-C5	-6.27	102.89	114.08
41	RR	316	XAT	O24-C25-C24	6.27	118.09	113.38
42	Gg	318	NEX	C39-C29-C30	-6.26	114.15	122.92
35	A	410	PL9	C42-C43-C44	-6.25	112.61	127.66
34	c	516	BCR	C3-C4-C5	-6.23	102.95	114.08
34	AA	409	BCR	C28-C27-C26	-6.22	102.96	114.08
35	AA	410	PL9	C37-C38-C39	-6.21	112.71	127.66
35	A	410	PL9	C37-C38-C39	-6.21	112.72	127.66
34	Bb	617	BCR	C28-C27-C26	-6.18	103.05	114.08
35	AA	410	PL9	C42-C43-C44	-6.17	112.80	127.66
34	C	517	BCR	C3-C4-C5	-6.16	103.07	114.08
32	b	609	CLA	C4A-NA-C1A	6.15	109.47	106.71
34	A	409	BCR	C28-C27-C26	-6.14	103.12	114.08
35	AA	410	PL9	C22-C23-C24	-6.13	112.91	127.66
35	AA	410	PL9	C17-C18-C19	-6.12	112.92	127.66
34	Kk	101	BCR	C1-C6-C5	-6.12	113.99	122.61
34	h	101	BCR	C28-C27-C26	-6.11	103.16	114.08
35	d	404	PL9	C32-C33-C34	-6.10	112.97	127.66
34	Bb	619	BCR	C3-C4-C5	-6.09	103.19	114.08
41	RR	316	XAT	O4-C5-C4	6.09	117.95	113.38
41	R	616	XAT	O4-C5-C4	6.08	117.95	113.38
41	Rr	615	XAT	O4-C5-C18	6.08	122.34	115.06
32	RR	308	CLA	C4A-NA-C1A	6.05	109.43	106.71
34	DD	405	BCR	C28-C27-C26	-6.04	103.29	114.08
35	DD	406	PL9	C16-C14-C13	-6.01	108.96	121.12
35	D	407	PL9	C16-C14-C13	-5.99	108.99	121.12
34	TT	101	BCR	C28-C27-C26	-5.99	103.38	114.08
34	D	406	BCR	C28-C27-C26	-5.94	103.47	114.08
34	Hh	101	BCR	C28-C27-C26	-5.93	103.48	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	AA	410	PL9	C27-C28-C29	-5.93	113.39	127.66
35	Dd	404	PL9	C46-C44-C43	-5.92	109.13	121.12
35	Dd	404	PL9	C32-C33-C34	-5.89	113.48	127.66
35	d	404	PL9	C46-C44-C43	-5.88	109.21	121.12
42	Yy	617	NEX	O24-C25-C24	5.88	117.80	113.38
32	C	504	CLA	C4A-NA-C1A	5.86	109.34	106.71
42	y	319	NEX	O24-C25-C24	5.86	117.78	113.38
35	D	407	PL9	C46-C44-C43	-5.85	109.27	121.12
35	d	404	PL9	C11-C9-C8	-5.85	109.27	121.12
34	Bb	618	BCR	C28-C27-C26	-5.83	103.67	114.08
35	D	407	PL9	C11-C9-C8	-5.82	109.34	121.12
34	C	518	BCR	C28-C27-C26	-5.82	103.69	114.08
34	b	618	BCR	C28-C27-C26	-5.82	103.69	114.08
39	l	608	CHL	CMB-C2B-C1B	-5.82	119.53	128.46
35	A	410	PL9	C11-C9-C8	-5.81	109.36	121.12
35	DD	406	PL9	C11-C9-C8	-5.80	109.39	121.12
35	DD	406	PL9	C46-C44-C43	-5.77	109.44	121.12
34	h	101	BCR	C1-C6-C5	-5.76	114.50	122.61
34	CC	516	BCR	C3-C4-C5	-5.76	103.79	114.08
41	Yy	619	XAT	O24-C25-C38	5.75	121.94	115.06
32	RR	304	CLA	C4A-NA-C1A	5.75	109.29	106.71
35	AA	410	PL9	C10-C9-C8	-5.74	108.94	123.68
35	AA	410	PL9	C15-C14-C13	-5.71	109.04	123.68
34	K	102	BCR	C3-C4-C5	-5.70	103.90	114.08
35	d	404	PL9	C45-C44-C43	-5.70	109.06	123.68
35	A	410	PL9	C16-C14-C13	-5.69	109.61	121.12
34	Cc	518	BCR	C30-C25-C26	-5.68	114.61	122.61
35	Dd	404	PL9	C10-C9-C8	-5.67	109.12	123.68
34	Cc	516	BCR	C3-C4-C5	-5.67	103.95	114.08
35	A	410	PL9	C46-C44-C43	-5.67	109.65	121.12
35	A	410	PL9	C10-C9-C8	-5.66	109.16	123.68
35	AA	410	PL9	C46-C44-C43	-5.66	109.67	121.12
32	R	604	CLA	C4A-NA-C1A	5.66	109.25	106.71
35	d	404	PL9	C10-C9-C8	-5.65	109.18	123.68
35	A	410	PL9	C45-C44-C43	-5.65	109.19	123.68
34	BB	620	BCR	C28-C27-C26	-5.65	103.99	114.08
35	AA	410	PL9	C16-C14-C13	-5.64	109.70	121.12
35	DD	406	PL9	C15-C14-C13	-5.64	109.21	123.68
35	D	407	PL9	C15-C14-C13	-5.64	109.22	123.68
35	Dd	404	PL9	C45-C44-C43	-5.64	109.22	123.68
35	Dd	404	PL9	C15-C14-C13	-5.63	109.23	123.68
35	Dd	404	PL9	C16-C14-C13	-5.63	109.72	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	407	PL9	C10-C9-C8	-5.63	109.24	123.68
36	4	301	LHG	O7-C7-O9	-5.63	118.41	125.57
35	D	407	PL9	C45-C44-C43	-5.62	109.27	123.68
32	S	611	CLA	C4A-NA-C1A	5.61	109.23	106.71
35	AA	410	PL9	C45-C44-C43	-5.61	109.29	123.68
34	CC	516	BCR	C30-C25-C26	-5.60	114.72	122.61
32	Gg	303	CLA	C4A-NA-C1A	5.60	109.22	106.71
34	T	101	BCR	C28-C27-C26	-5.59	104.09	114.08
35	d	404	PL9	C15-C14-C13	-5.59	109.35	123.68
32	Bb	609	CLA	C4A-NA-C1A	5.59	109.22	106.71
35	DD	406	PL9	C45-C44-C43	-5.58	109.37	123.68
39	GG	609	CHL	CMB-C2B-C1B	-5.58	119.89	128.46
32	n	611	CLA	C4A-NA-C1A	5.57	109.21	106.71
39	4	306	CHL	CMB-C2B-C1B	-5.57	119.91	128.46
35	Dd	404	PL9	C36-C34-C33	-5.55	109.88	121.12
32	C	509	CLA	C4A-NA-C1A	5.55	109.20	106.71
32	g	602	CLA	CGD-CBD-CAD	-5.54	92.79	110.73
39	22	606	CHL	CMB-C2B-C1B	-5.53	119.96	128.46
34	CC	517	BCR	C28-C27-C26	-5.53	104.21	114.08
32	S	610	CLA	C4A-NA-C1A	5.53	109.19	106.71
32	Ss	610	CLA	C4A-NA-C1A	5.52	109.19	106.71
36	44	616	LHG	O7-C7-O9	-5.50	118.57	125.57
34	C	517	BCR	C30-C25-C26	-5.49	114.89	122.61
34	B	616	BCR	C28-C27-C26	-5.48	104.29	114.08
35	D	407	PL9	C36-C34-C33	-5.48	110.04	121.12
34	XX	202	BCR	C28-C27-C26	-5.47	104.30	114.08
34	b	619	BCR	C28-C27-C26	-5.47	104.31	114.08
35	A	410	PL9	C15-C14-C13	-5.47	109.65	123.68
32	R	603	CLA	C4A-NA-C1A	5.47	109.16	106.71
32	B	605	CLA	C4A-NA-C1A	5.46	109.16	106.71
35	AA	410	PL9	C11-C9-C8	-5.46	110.07	121.12
35	DD	406	PL9	C10-C9-C8	-5.45	109.69	123.68
35	Dd	404	PL9	C11-C9-C8	-5.44	110.11	121.12
32	CC	508	CLA	C4A-NA-C1A	5.44	109.15	106.71
39	33	608	CHL	CMB-C2B-C1B	-5.44	120.11	128.46
34	KK	103	BCR	C3-C4-C5	-5.43	104.38	114.08
35	D	407	PL9	C21-C19-C18	-5.42	110.14	121.12
45	AA	413	BCT	O2-C-O1	5.42	133.61	119.55
34	CC	515	BCR	C30-C25-C26	-5.41	114.99	122.61
34	BB	616	BCR	C3-C4-C5	-5.41	104.42	114.08
32	s	610	CLA	C4A-NA-C1A	5.41	109.14	106.71
34	KK	103	BCR	C28-C27-C26	-5.41	104.42	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	k	101	BCR	C33-C5-C6	-5.40	118.46	124.53
35	Dd	404	PL9	C31-C29-C28	-5.39	110.20	121.12
32	Cc	503	CLA	C4A-NA-C1A	5.39	109.13	106.71
34	Aa	411	BCR	C3-C4-C5	-5.39	104.45	114.08
32	Bb	612	CLA	C4A-NA-C1A	5.38	109.13	106.71
35	DD	406	PL9	C21-C19-C18	-5.38	110.22	121.12
35	D	407	PL9	C35-C34-C33	-5.38	109.88	123.68
32	RR	303	CLA	C4A-NA-C1A	5.37	109.12	106.71
32	Cc	509	CLA	C4A-NA-C1A	5.37	109.12	106.71
39	4	309	CHL	CMB-C2B-C1B	-5.36	120.22	128.46
34	Hh	101	BCR	C1-C6-C5	-5.36	115.06	122.61
35	d	404	PL9	C16-C14-C13	-5.36	110.26	121.12
34	a	411	BCR	C3-C4-C5	-5.36	104.51	114.08
32	c	507	CLA	C4A-NA-C1A	5.36	109.11	106.71
34	A	409	BCR	C3-C4-C5	-5.36	104.51	114.08
40	Y	616	LUT	C1-C6-C5	-5.35	115.08	122.61
32	SS	311	CLA	C4A-NA-C1A	5.33	109.10	106.71
32	NN	611	CLA	C4A-NA-C1A	5.32	109.10	106.71
39	G	609	CHL	CMB-C2B-C1B	-5.32	120.29	128.46
34	c	516	BCR	C30-C25-C26	-5.30	115.14	122.61
34	Dd	403	BCR	C30-C25-C26	-5.30	115.14	122.61
32	G	610	CLA	C4A-NA-C1A	5.30	109.09	106.71
32	11	612	CLA	CBD-CHA-C1A	5.30	134.74	128.50
32	Bb	601	CLA	C4A-NA-C1A	5.29	109.08	106.71
42	g	617	NEX	C27-C28-C29	5.27	133.71	125.53
34	H	101	BCR	C28-C27-C26	-5.26	104.69	114.08
35	d	404	PL9	C36-C34-C33	-5.26	110.48	121.12
35	D	407	PL9	C40-C39-C38	-5.25	110.20	123.68
34	d	403	BCR	C30-C25-C26	-5.25	115.22	122.61
34	C	516	BCR	C30-C25-C26	-5.25	115.22	122.61
35	DD	406	PL9	C30-C29-C28	-5.25	110.22	123.68
32	4	304	CLA	C4A-NA-C1A	5.24	109.06	106.71
32	BB	609	CLA	C4A-NA-C1A	5.24	109.06	106.71
34	b	618	BCR	C3-C4-C5	-5.24	104.72	114.08
40	2	614	LUT	C3-C4-C5	-5.23	101.43	111.85
39	44	605	CHL	CMB-C2B-C1B	-5.23	120.43	128.46
32	Nn	302	CLA	C4A-NA-C1A	5.22	109.06	106.71
35	Dd	404	PL9	C40-C39-C38	-5.22	110.28	123.68
35	d	404	PL9	C31-C29-C28	-5.22	110.55	121.12
39	Gg	310	CHL	CMB-C2B-C1B	-5.22	120.44	128.46
32	CC	503	CLA	C4A-NA-C1A	5.21	109.05	106.71
32	y	313	CLA	C4A-NA-C1A	5.21	109.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	617	BCR	C3-C4-C5	-5.21	104.77	114.08
34	AA	409	BCR	C3-C4-C5	-5.21	104.78	114.08
32	Gg	312	CLA	C4A-NA-C1A	5.20	109.04	106.71
34	B	613	BCR	C3-C4-C5	-5.19	104.81	114.08
45	D	403	BCT	O2-C-O1	5.19	133.01	119.55
39	44	608	CHL	CMB-C2B-C1B	-5.19	120.49	128.46
34	Dd	403	BCR	C1-C6-C5	-5.18	115.31	122.61
35	AA	410	PL9	C35-C34-C33	-5.18	110.38	123.68
35	DD	406	PL9	C40-C39-C38	-5.18	110.38	123.68
34	b	617	BCR	C36-C18-C19	5.17	126.23	118.08
32	YY	604	CLA	C4A-NA-C1A	5.17	109.03	106.71
34	Bb	618	BCR	C3-C4-C5	-5.17	104.84	114.08
32	r	610	CLA	C4A-NA-C1A	5.17	109.03	106.71
35	d	404	PL9	C40-C39-C38	-5.16	110.44	123.68
39	r	606	CHL	CMB-C2B-C1B	-5.16	120.54	128.46
32	N	611	CLA	C4A-NA-C1A	5.15	109.02	106.71
40	Gg	317	LUT	C3-C4-C5	-5.15	101.60	111.85
32	YY	611	CLA	C4A-NA-C1A	5.15	109.02	106.71
45	Aa	414	BCT	O2-C-O1	5.14	132.89	119.55
32	Bb	604	CLA	C4A-NA-C1A	5.14	109.02	106.71
32	Yy	611	CLA	C4A-NA-C1A	5.13	109.01	106.71
32	r	612	CLA	C4A-NA-C1A	5.13	109.01	106.71
39	11	608	CHL	CMB-C2B-C1B	-5.13	120.58	128.46
35	DD	406	PL9	C35-C34-C33	-5.12	110.54	123.68
35	Dd	404	PL9	C21-C19-C18	-5.11	110.77	121.12
39	R	605	CHL	CMB-C2B-C1B	-5.11	120.61	128.46
39	NN	605	CHL	CMB-C2B-C1B	-5.11	120.61	128.46
34	Bb	617	BCR	C36-C18-C19	5.11	126.12	118.08
35	d	404	PL9	C21-C19-C18	-5.11	110.78	121.12
39	Yy	609	CHL	CMB-C2B-C3B	5.10	134.22	124.68
35	AA	410	PL9	C36-C34-C33	-5.10	110.80	121.12
34	Bb	617	BCR	C30-C25-C26	-5.09	115.44	122.61
32	Rr	610	CLA	C4A-NA-C1A	5.09	109.00	106.71
35	A	410	PL9	C25-C24-C23	-5.09	110.63	123.68
39	2	606	CHL	CMB-C2B-C1B	-5.09	120.65	128.46
32	b	612	CLA	C4A-NA-C1A	5.08	108.99	106.71
35	Dd	404	PL9	C35-C34-C33	-5.08	110.64	123.68
39	Ss	606	CHL	CMB-C2B-C1B	-5.08	120.66	128.46
35	DD	406	PL9	C31-C29-C28	-5.08	110.84	121.12
35	d	404	PL9	C35-C34-C33	-5.08	110.65	123.68
32	g	611	CLA	C4A-NA-C1A	5.08	108.99	106.71
39	Rr	607	CHL	CMB-C2B-C1B	-5.07	120.67	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	612	BCR	C3-C4-C5	-5.07	105.03	114.08
35	D	407	PL9	C20-C19-C18	-5.07	110.68	123.68
35	D	407	PL9	C30-C29-C28	-5.07	110.68	123.68
35	DD	406	PL9	C20-C19-C18	-5.06	110.69	123.68
34	XX	202	BCR	C3-C4-C5	-5.06	105.05	114.08
32	YY	603	CLA	C4A-NA-C1A	5.06	108.98	106.71
35	A	410	PL9	C41-C39-C38	-5.05	110.89	121.12
32	b	601	CLA	C4A-NA-C1A	5.05	108.98	106.71
35	D	407	PL9	C41-C39-C38	-5.05	110.90	121.12
35	D	407	PL9	C25-C24-C23	-5.05	110.73	123.68
32	G	602	CLA	C4A-NA-C1A	5.04	108.97	106.71
39	Rr	605	CHL	CMB-C2B-C1B	-5.03	120.73	128.46
32	Ss	602	CLA	C4A-NA-C1A	5.03	108.97	106.71
32	r	603	CLA	C4A-NA-C1A	5.03	108.97	106.71
39	SS	306	CHL	CMB-C2B-C1B	-5.03	120.74	128.46
35	d	404	PL9	C20-C19-C18	-5.03	110.79	123.68
35	A	410	PL9	C35-C34-C33	-5.02	110.79	123.68
35	AA	410	PL9	C41-C39-C38	-5.02	110.96	121.12
35	A	410	PL9	C26-C24-C23	-5.02	110.96	121.12
35	DD	406	PL9	C25-C24-C23	-5.02	110.81	123.68
39	s	606	CHL	CMB-C2B-C1B	-5.01	120.76	128.46
32	Yy	603	CLA	C4A-NA-C1A	5.01	108.96	106.71
32	GG	613	CLA	C4A-NA-C1A	5.01	108.96	106.71
34	k	101	BCR	C1-C6-C5	-5.00	115.57	122.61
39	r	607	CHL	CMB-C2B-C1B	-4.99	120.79	128.46
40	Nn	307	LUT	C1-C6-C5	-4.98	115.59	122.61
34	d	403	BCR	C1-C6-C5	-4.98	115.60	122.61
32	C	512	CLA	C4A-NA-C1A	4.98	108.94	106.71
35	A	410	PL9	C20-C19-C18	-4.98	110.91	123.68
32	b	604	CLA	C4A-NA-C1A	4.97	108.94	106.71
32	B	609	CLA	C4A-NA-C1A	4.97	108.94	106.71
32	Aa	407	CLA	C4A-NA-C1A	4.97	108.94	106.71
35	D	407	PL9	C26-C24-C23	-4.97	111.06	121.12
40	s	615	LUT	C3-C4-C5	-4.96	101.96	111.85
35	A	410	PL9	C30-C29-C28	-4.96	110.95	123.68
32	Y	611	CLA	C4A-NA-C1A	4.96	108.94	106.71
35	A	410	PL9	C21-C19-C18	-4.96	111.08	121.12
34	d	403	BCR	C3-C4-C5	-4.96	105.22	114.08
32	BB	613	CLA	C4A-NA-C1A	4.96	108.94	106.71
32	CC	509	CLA	C4A-NA-C1A	4.96	108.93	106.71
39	Nn	315	CHL	CMB-C2B-C1B	-4.95	120.85	128.46
45	a	413	BCT	O2-C-O1	4.95	132.39	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	102	BCR	C28-C27-C26	-4.95	105.24	114.08
35	D	407	PL9	C31-C29-C28	-4.95	111.11	121.12
35	A	410	PL9	C36-C34-C33	-4.95	111.11	121.12
32	c	510	CLA	C4A-NA-C1A	4.94	108.93	106.71
35	Dd	404	PL9	C20-C19-C18	-4.94	111.00	123.68
40	y	317	LUT	C18-C5-C6	4.94	130.08	124.53
35	AA	410	PL9	C40-C39-C38	-4.94	111.02	123.68
39	S	605	CHL	CMB-C2B-C1B	-4.93	120.88	128.46
39	33	607	CHL	CMB-C2B-C1B	-4.93	120.88	128.46
32	GG	611	CLA	C4A-NA-C1A	4.93	108.92	106.71
39	Y	607	CHL	CMB-C2B-C1B	-4.93	120.88	128.46
39	Ss	605	CHL	CMB-C2B-C1B	-4.93	120.88	128.46
39	s	605	CHL	CMB-C2B-C1B	-4.93	120.89	128.46
34	Bb	619	BCR	C30-C25-C26	-4.93	115.67	122.61
39	n	609	CHL	CMB-C2B-C1B	-4.93	120.89	128.46
39	YY	607	CHL	CMB-C2B-C1B	-4.93	120.89	128.46
32	S	604	CLA	C4A-NA-C1A	4.93	108.92	106.71
35	Dd	404	PL9	C25-C24-C23	-4.92	111.06	123.68
32	y	315	CLA	C4A-NA-C1A	4.92	108.92	106.71
35	AA	410	PL9	C20-C19-C18	-4.91	111.07	123.68
35	DD	406	PL9	C36-C34-C33	-4.90	111.20	121.12
32	Bb	610	CLA	C4A-NA-C1A	4.90	108.91	106.71
39	11	607	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
32	B	607	CLA	C4A-NA-C1A	4.90	108.91	106.71
34	Dd	403	BCR	C3-C4-C5	-4.90	105.33	114.08
39	s	601	CHL	CMB-C2B-C1B	-4.90	120.94	128.46
40	NN	616	LUT	C3-C4-C5	-4.90	102.10	111.85
35	A	410	PL9	C40-C39-C38	-4.89	111.14	123.68
32	y	306	CLA	C4A-NA-C1A	4.88	108.90	106.71
35	d	404	PL9	C25-C24-C23	-4.88	111.15	123.68
32	B	611	CLA	C4A-NA-C1A	4.88	108.90	106.71
35	Dd	404	PL9	C26-C24-C23	-4.87	111.25	121.12
35	d	404	PL9	C26-C24-C23	-4.87	111.26	121.12
32	B	608	CLA	C4A-NA-C1A	4.87	108.89	106.71
32	DD	404	CLA	C4A-NA-C1A	4.86	108.89	106.71
39	N	605	CHL	CMB-C2B-C1B	-4.86	121.00	128.46
32	G	611	CLA	C4A-NA-C1A	4.85	108.89	106.71
35	DD	406	PL9	C41-C39-C38	-4.85	111.30	121.12
32	44	603	CLA	C4A-NA-C1A	4.85	108.89	106.71
36	4	315	LHG	O7-C7-C8	4.84	120.00	111.09
34	Cc	518	BCR	C3-C4-C5	-4.84	105.43	114.08
32	BB	612	CLA	C4A-NA-C1A	4.84	108.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	RR	305	CHL	CMB-C2B-C1B	-4.84	121.02	128.46
39	g	609	CHL	CMB-C2B-C1B	-4.84	121.03	128.46
41	RR	316	XAT	C18-C5-C6	-4.84	114.15	122.26
32	2	604	CLA	C4A-NA-C1A	4.84	108.88	106.71
44	Hh	102	DGD	O2G-C1B-C2B	4.84	121.93	111.50
35	AA	410	PL9	C30-C29-C28	-4.84	111.27	123.68
35	AA	410	PL9	C25-C24-C23	-4.83	111.29	123.68
32	Yy	613	CLA	C4A-NA-C1A	4.83	108.88	106.71
32	C	511	CLA	C4A-NA-C1A	4.83	108.88	106.71
39	y	309	CHL	CMB-C2B-C1B	-4.82	121.05	128.46
32	CC	505	CLA	C4A-NA-C1A	4.82	108.87	106.71
32	CC	510	CLA	C4A-NA-C1A	4.82	108.87	106.71
32	S	603	CLA	C4A-NA-C1A	4.82	108.87	106.71
34	Bb	619	BCR	C28-C27-C26	-4.82	105.48	114.08
32	22	612	CLA	C4A-NA-C1A	4.81	108.87	106.71
32	Bb	613	CLA	C4A-NA-C1A	4.81	108.87	106.71
32	X	201	CLA	C4A-NA-C1A	4.81	108.87	106.71
32	d	401	CLA	C4A-NA-C1A	4.81	108.87	106.71
35	d	404	PL9	C41-C39-C38	-4.81	111.39	121.12
32	C	510	CLA	C4A-NA-C1A	4.80	108.86	106.71
32	Nn	313	CLA	C4A-NA-C1A	4.80	108.86	106.71
35	Dd	404	PL9	C30-C29-C28	-4.80	111.37	123.68
40	Ss	615	LUT	C1-C6-C5	-4.80	115.86	122.61
35	DD	406	PL9	C26-C24-C23	-4.80	111.41	121.12
35	Dd	404	PL9	C41-C39-C38	-4.79	111.42	121.12
32	C	506	CLA	C4A-NA-C1A	4.79	108.86	106.71
32	Cc	504	CLA	C4A-NA-C1A	4.79	108.86	106.71
35	d	404	PL9	C30-C29-C28	-4.79	111.40	123.68
32	b	613	CLA	C4A-NA-C1A	4.79	108.86	106.71
39	3	607	CHL	CMB-C2B-C1B	-4.78	121.11	128.46
34	h	101	BCR	C31-C1-C6	-4.77	102.56	110.30
36	J	101	LHG	O7-C7-C8	4.77	119.86	111.09
32	Bb	611	CLA	C4A-NA-C1A	4.77	108.85	106.71
41	R	616	XAT	C18-C5-C6	-4.77	114.27	122.26
32	44	615	CLA	C4A-NA-C1A	4.76	108.85	106.71
32	Cc	511	CLA	C4A-NA-C1A	4.76	108.85	106.71
39	2	605	CHL	CMB-C2B-C1B	-4.76	121.14	128.46
32	BB	611	CLA	C4A-NA-C1A	4.76	108.85	106.71
35	A	410	PL9	C31-C29-C28	-4.76	111.49	121.12
32	g	604	CLA	C4A-NA-C1A	4.75	108.84	106.71
34	BB	616	BCR	C30-C25-C26	-4.75	115.92	122.61
39	22	605	CHL	CMB-C2B-C1B	-4.75	121.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	607	CHL	CMB-C2B-C1B	-4.74	121.18	128.46
32	Dd	401	CLA	C4A-NA-C1A	4.74	108.83	106.71
40	G	616	LUT	C1-C6-C5	-4.73	115.95	122.61
39	4	308	CHL	CMB-C2B-C1B	-4.72	121.22	128.46
32	c	501	CLA	C4A-NA-C1A	4.71	108.82	106.71
36	44	614	LHG	O7-C7-C8	4.71	119.75	111.09
40	G	615	LUT	C1-C6-C5	-4.70	115.99	122.61
35	AA	410	PL9	C31-C29-C28	-4.70	111.61	121.12
32	D	405	CLA	C4A-NA-C1A	4.70	108.82	106.71
32	Y	604	CLA	C4A-NA-C1A	4.69	108.81	106.71
41	Rr	615	XAT	O24-C25-C38	4.69	120.67	115.06
41	RR	316	XAT	O24-C25-C38	4.69	120.67	115.06
35	AA	410	PL9	C26-C24-C23	-4.69	111.64	121.12
34	H	101	BCR	C34-C9-C8	4.68	125.45	118.08
34	Cc	517	BCR	C30-C25-C26	-4.68	116.03	122.61
32	S	612	CLA	C4A-NA-C1A	4.68	108.81	106.71
32	BB	610	CLA	C4A-NA-C1A	4.68	108.81	106.71
34	B	614	BCR	C1-C6-C5	-4.67	116.04	122.61
32	SS	305	CLA	C4A-NA-C1A	4.67	108.80	106.71
32	22	604	CLA	C4A-NA-C1A	4.66	108.80	106.71
32	g	602	CLA	O2D-CGD-CBD	4.66	119.54	111.27
35	AA	410	PL9	C21-C19-C18	-4.66	111.69	121.12
32	XX	201	CLA	C4A-NA-C1A	4.66	108.80	106.71
39	4	306	CHL	C4A-NA-C1A	4.66	108.80	106.71
41	Yy	619	XAT	O4-C5-C18	4.65	120.63	115.06
32	C	514	CLA	C4A-NA-C1A	4.65	108.80	106.71
39	RR	307	CHL	CMB-C2B-C1B	-4.65	121.31	128.46
32	c	513	CLA	C4A-NA-C1A	4.65	108.80	106.71
32	s	602	CLA	C4A-NA-C1A	4.65	108.80	106.71
39	SS	306	CHL	C4A-NA-C1A	4.65	108.80	106.71
32	a	407	CLA	C4A-NA-C1A	4.64	108.79	106.71
32	SS	312	CLA	C4A-NA-C1A	4.64	108.79	106.71
39	Nn	319	CHL	CMB-C2B-C1B	-4.64	121.33	128.46
32	GG	612	CLA	C4A-NA-C1A	4.62	108.78	106.71
34	b	617	BCR	C30-C25-C26	-4.62	116.10	122.61
32	b	610	CLA	C4A-NA-C1A	4.62	108.78	106.71
32	CC	513	CLA	C4A-NA-C1A	4.62	108.78	106.71
42	y	319	NEX	O24-C25-C38	4.62	120.59	115.06
32	Gg	305	CLA	C4A-NA-C1A	4.61	108.78	106.71
32	YY	612	CLA	C1B-CHB-C4A	-4.61	120.98	130.12
39	1	605	CHL	C4A-NA-C1A	4.61	108.78	106.71
32	c	511	CLA	C4A-NA-C1A	4.61	108.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Cc	513	CLA	C4A-NA-C1A	4.61	108.78	106.71
34	h	101	BCR	C1-C6-C7	4.60	128.80	115.78
40	22	614	LUT	C20-C13-C14	-4.60	116.48	122.92
32	SS	304	CLA	C4A-NA-C1A	4.60	108.77	106.71
41	N	617	XAT	C40-C33-C32	4.60	125.32	118.08
32	BB	603	CLA	C4A-NA-C1A	4.59	108.77	106.71
42	Gg	318	NEX	C16-C1-C6	4.59	114.58	110.47
40	n	616	LUT	C1-C6-C5	-4.59	116.15	122.61
32	2	612	CLA	C4A-NA-C1A	4.59	108.77	106.71
32	BB	615	CLA	C4A-NA-C1A	4.59	108.77	106.71
40	Y	615	LUT	C1-C6-C5	-4.59	116.15	122.61
32	22	610	CLA	C4A-NA-C1A	4.58	108.77	106.71
32	Y	603	CLA	C4A-NA-C1A	4.58	108.77	106.71
32	GG	604	CLA	C4A-NA-C1A	4.58	108.77	106.71
39	Nn	318	CHL	C4A-NA-C1A	4.58	108.77	106.71
41	r	615	XAT	O4-C5-C18	4.58	120.54	115.06
34	H	101	BCR	C3-C4-C5	-4.57	105.91	114.08
32	Yy	604	CLA	C4A-NA-C1A	4.57	108.76	106.71
32	r	613	CLA	C4A-NA-C1A	4.57	108.76	106.71
39	Nn	316	CHL	C4A-NA-C1A	4.57	108.76	106.71
32	11	604	CLA	C4A-NA-C1A	4.56	108.76	106.71
36	AA	411	LHG	O7-C7-C8	4.55	121.31	111.50
32	n	603	CLA	C4A-NA-C1A	4.55	108.75	106.71
32	Bb	616	CLA	C4A-NA-C1A	4.54	108.75	106.71
39	R	607	CHL	CMB-C2B-C1B	-4.54	121.48	128.46
32	c	506	CLA	C4A-NA-C1A	4.54	108.75	106.71
34	B	614	BCR	C33-C5-C6	-4.53	119.44	124.53
36	A	411	LHG	O7-C7-C8	4.53	121.26	111.50
32	Ss	608	CLA	C4A-NA-C1A	4.52	108.74	106.71
32	1	604	CLA	C4A-NA-C1A	4.51	108.73	106.71
32	Bb	615	CLA	C4A-NA-C1A	4.51	108.73	106.71
40	Y	615	LUT	C18-C5-C6	-4.51	119.47	124.53
32	b	616	CLA	C4A-NA-C1A	4.50	108.73	106.71
34	Kk	101	BCR	C4-C5-C6	-4.50	116.20	122.73
32	s	604	CLA	C4A-NA-C1A	4.50	108.73	106.71
32	Cc	508	CLA	C4A-NA-C1A	4.50	108.73	106.71
41	r	615	XAT	O24-C25-C38	4.49	120.44	115.06
34	BB	617	BCR	C36-C18-C19	4.49	125.16	118.08
32	SS	313	CLA	C4A-NA-C1A	4.49	108.72	106.71
34	BB	618	BCR	C1-C6-C5	-4.49	116.29	122.61
39	1	608	CHL	CMB-C2B-C3B	4.49	133.07	124.68
35	AA	410	PL9	C47-C48-C49	-4.48	112.44	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Kk	101	BCR	C34-C9-C8	4.48	125.13	118.08
32	3	610	CLA	C4A-NA-C1A	4.48	108.72	106.71
32	CC	511	CLA	C4A-NA-C1A	4.47	108.72	106.71
40	Yy	616	LUT	C1-C6-C5	-4.46	116.33	122.61
40	YY	615	LUT	C3-C4-C5	-4.46	102.96	111.85
34	Hh	101	BCR	C1-C6-C7	4.46	128.40	115.78
32	BB	605	CLA	C4A-NA-C1A	4.46	108.71	106.71
41	G	619	XAT	C20-C13-C12	4.46	125.11	118.08
35	A	410	PL9	C47-C48-C49	-4.46	112.50	127.75
40	22	614	LUT	C1-C6-C5	-4.46	116.33	122.61
41	Nn	308	XAT	C40-C33-C32	4.46	125.10	118.08
32	Cc	505	CLA	C4A-NA-C1A	4.46	108.71	106.71
32	Rr	613	CLA	C4A-NA-C1A	4.45	108.71	106.71
42	Yy	617	NEX	C38-C25-C26	-4.45	114.80	122.26
34	B	613	BCR	C36-C18-C19	4.45	125.09	118.08
34	BB	618	BCR	C28-C27-C26	-4.45	106.14	114.08
34	BB	618	BCR	C33-C5-C6	-4.45	119.53	124.53
32	4	312	CLA	C4A-NA-C1A	4.45	108.70	106.71
32	c	509	CLA	C4A-NA-C1A	4.44	108.70	106.71
32	b	605	CLA	C4A-NA-C1A	4.44	108.70	106.71
44	BB	623	DGD	O2G-C1B-C2B	4.43	121.06	111.50
32	Nn	314	CLA	C4A-NA-C1A	4.42	108.69	106.71
41	R	616	XAT	O24-C25-C38	4.42	120.36	115.06
40	2	614	LUT	C20-C13-C14	-4.42	116.73	122.92
40	g	616	LUT	C3-C4-C5	-4.42	103.06	111.85
32	B	606	CLA	C4A-NA-C1A	4.42	108.69	106.71
32	BB	614	CLA	C4A-NA-C1A	4.41	108.69	106.71
32	3	602	CLA	C4A-NA-C1A	4.40	108.69	106.71
32	Bb	605	CLA	C4A-NA-C1A	4.40	108.69	106.71
42	Yy	617	NEX	O24-C25-C38	4.40	120.33	115.06
34	Cc	518	BCR	C28-C27-C26	-4.40	106.22	114.08
35	DD	406	PL9	C47-C48-C49	-4.40	112.73	127.75
32	b	611	CLA	C4A-NA-C1A	4.40	108.68	106.71
32	44	604	CLA	C4A-NA-C1A	4.39	108.68	106.71
32	C	513	CLA	C4A-NA-C1A	4.39	108.68	106.71
32	Aa	405	CLA	C4A-NA-C1A	4.39	108.68	106.71
34	TT	101	BCR	C36-C18-C19	4.39	125.00	118.08
41	N	617	XAT	O4-C5-C18	4.39	120.31	115.06
39	G	607	CHL	C4A-NA-C1A	4.39	108.68	106.71
32	S	609	CLA	C4A-NA-C1A	4.39	108.68	106.71
42	NN	618	NEX	C40-C33-C32	4.39	124.99	118.08
36	Nn	310	LHG	O7-C7-C8	4.38	120.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	611	CLA	C4A-NA-C1A	4.38	108.68	106.71
41	R	616	XAT	C38-C25-C26	-4.38	114.92	122.26
32	A	406	CLA	C4A-NA-C1A	4.38	108.67	106.71
35	D	407	PL9	C47-C48-C49	-4.37	112.80	127.75
41	NN	617	XAT	O4-C5-C18	4.37	120.30	115.06
40	Gg	316	LUT	C3-C4-C5	-4.37	103.15	111.85
39	S	605	CHL	C4A-NA-C1A	4.37	108.67	106.71
41	RR	316	XAT	C38-C25-C26	-4.37	114.94	122.26
40	YY	615	LUT	C18-C5-C6	-4.37	119.63	124.53
39	n	608	CHL	C4A-NA-C1A	4.36	108.67	106.71
34	c	516	BCR	C28-C27-C26	-4.36	106.29	114.08
32	4	305	CLA	C4A-NA-C1A	4.36	108.67	106.71
32	B	622	CLA	C4A-NA-C1A	4.36	108.67	106.71
39	RR	306	CHL	C2A-C1A-CHA	4.35	131.47	123.86
42	Gg	318	NEX	C20-C13-C12	4.35	124.94	118.08
42	y	319	NEX	C38-C25-C26	-4.35	114.97	122.26
32	Cc	506	CLA	C4A-NA-C1A	4.35	108.66	106.71
32	Nn	303	CLA	C4A-NA-C1A	4.35	108.66	106.71
41	NN	617	XAT	C18-C5-C6	-4.35	114.97	122.26
34	CC	517	BCR	C1-C6-C5	-4.35	116.49	122.61
41	RR	316	XAT	O4-C5-C18	4.35	120.27	115.06
32	N	613	CLA	C4A-NA-C1A	4.34	108.66	106.71
35	Dd	404	PL9	C47-C48-C49	-4.34	112.91	127.75
41	G	617	XAT	C26-C27-C28	-4.34	116.82	125.99
40	GG	616	LUT	C1-C6-C5	-4.33	116.51	122.61
41	N	617	XAT	C18-C5-C6	-4.33	115.00	122.26
32	44	611	CLA	C4A-NA-C1A	4.33	108.65	106.71
39	Yy	607	CHL	C4A-NA-C1A	4.33	108.65	106.71
39	n	606	CHL	C4A-NA-C1A	4.33	108.65	106.71
41	y	302	XAT	C40-C33-C32	4.33	124.89	118.08
32	3	612	CLA	C4A-NA-C1A	4.33	108.65	106.71
32	a	405	CLA	C4A-NA-C1A	4.32	108.65	106.71
41	y	302	XAT	C18-C5-C6	-4.32	115.02	122.26
34	DD	405	BCR	C1-C6-C5	-4.32	116.53	122.61
32	s	612	CLA	C4A-NA-C1A	4.32	108.65	106.71
34	T	101	BCR	C36-C18-C19	4.32	124.88	118.08
42	Y	617	NEX	C39-C29-C30	-4.32	116.88	122.92
42	Gg	318	NEX	C27-C28-C29	4.31	132.22	125.53
32	Rr	603	CLA	C4A-NA-C1A	4.31	108.64	106.71
42	N	618	NEX	C40-C33-C32	4.31	124.87	118.08
38	Cc	501	LMG	O7-C10-C11	4.31	120.79	111.50
34	B	614	BCR	C28-C27-C26	-4.31	106.38	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	616	LUT	C1-C6-C5	-4.31	116.55	122.61
42	Yy	617	NEX	C26-C27-C28	-4.31	116.89	125.99
32	Rr	612	CLA	C4A-NA-C1A	4.31	108.64	106.71
35	d	404	PL9	C47-C48-C49	-4.31	113.03	127.75
32	Ss	612	CLA	C4A-NA-C1A	4.30	108.64	106.71
32	R	612	CLA	C4A-NA-C1A	4.30	108.64	106.71
32	Gg	314	CLA	C4A-NA-C1A	4.30	108.64	106.71
36	Yy	618	LHG	O7-C7-C8	4.29	120.75	111.50
42	YY	617	NEX	C39-C29-C30	-4.29	116.91	122.92
38	c	519	LMG	O7-C10-C11	4.29	120.75	111.50
32	Bb	614	CLA	C4A-NA-C1A	4.29	108.63	106.71
39	n	609	CHL	C4A-NA-C1A	4.29	108.63	106.71
42	RR	317	NEX	C38-C25-C26	-4.29	115.08	122.26
32	33	610	CLA	C4A-NA-C1A	4.29	108.63	106.71
32	NN	603	CLA	C4A-NA-C1A	4.29	108.63	106.71
44	c	517	DGD	O2G-C1B-C2B	4.28	120.73	111.50
34	D	406	BCR	C1-C6-C5	-4.28	116.58	122.61
32	R	601	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
41	GG	619	XAT	C20-C13-C12	4.28	124.82	118.08
40	YY	616	LUT	C1-C6-C5	-4.28	116.59	122.61
32	RR	312	CLA	C4A-NA-C1A	4.28	108.63	106.71
41	GG	617	XAT	C26-C27-C28	-4.27	116.97	125.99
32	SS	309	CLA	C4A-NA-C1A	4.27	108.62	106.71
34	T	101	BCR	C1-C6-C5	-4.27	116.60	122.61
34	B	612	BCR	C30-C25-C26	-4.26	116.61	122.61
32	2	609	CLA	C4A-NA-C1A	4.26	108.62	106.71
32	D	401	CLA	C4A-NA-C1A	4.25	108.62	106.71
32	B	610	CLA	C4A-NA-C1A	4.25	108.62	106.71
42	RR	317	NEX	C39-C29-C30	-4.24	116.98	122.92
32	b	607	CLA	C4A-NA-C1A	4.24	108.61	106.71
32	AA	405	CLA	C4A-NA-C1A	4.24	108.61	106.71
32	SS	303	CLA	C4A-NA-C1A	4.24	108.61	106.71
32	RR	302	CLA	C4A-NA-C1A	4.24	108.61	106.71
42	NN	618	NEX	C39-C29-C30	-4.24	116.99	122.92
32	Ss	613	CLA	C4A-NA-C1A	4.24	108.61	106.71
32	1	602	CLA	C4A-NA-C1A	4.24	108.61	106.71
32	y	305	CLA	C4A-NA-C1A	4.24	108.61	106.71
34	Bb	619	BCR	C36-C18-C19	4.23	124.75	118.08
36	g	618	LHG	O7-C7-C8	4.23	120.61	111.50
32	Ss	604	CLA	C4A-NA-C1A	4.22	108.61	106.71
32	Cc	512	CLA	C4A-NA-C1A	4.22	108.61	106.71
32	b	614	CLA	C4A-NA-C1A	4.22	108.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	g	617	NEX	C39-C29-C28	4.22	124.72	118.08
41	G	617	XAT	C38-C25-C26	-4.22	115.19	122.26
42	Nn	309	NEX	C38-C25-C26	-4.22	115.20	122.26
32	A	405	CLA	C4A-NA-C1A	4.22	108.60	106.71
39	g	606	CHL	C4A-NA-C1A	4.21	108.60	106.71
34	Hh	101	BCR	C31-C1-C6	-4.21	103.47	110.30
34	BB	620	BCR	C33-C5-C6	-4.21	119.80	124.53
32	s	608	CLA	C4A-NA-C1A	4.21	108.60	106.71
41	Rr	615	XAT	C38-C25-C26	-4.21	115.21	122.26
34	H	101	BCR	C8-C7-C6	-4.21	115.39	127.20
32	22	602	CLA	C4A-NA-C1A	4.21	108.60	106.71
44	CC	522	DGD	O2G-C1B-C2B	4.20	120.56	111.50
42	n	617	NEX	C40-C33-C32	4.20	124.70	118.08
32	Bb	607	CLA	C4A-NA-C1A	4.20	108.59	106.71
36	Gg	319	LHG	O7-C7-C8	4.20	120.56	111.50
42	R	617	NEX	C38-C25-C26	-4.20	115.22	122.26
39	Y	608	CHL	C4A-NA-C1A	4.20	108.59	106.71
40	N	616	LUT	C1-C6-C5	-4.20	116.70	122.61
40	NN	616	LUT	C1-C6-C5	-4.19	116.70	122.61
41	R	616	XAT	O4-C5-C18	4.19	120.08	115.06
32	CC	514	CLA	C4A-NA-C1A	4.19	108.59	106.71
32	A	408	CLA	C4A-NA-C1A	4.19	108.59	106.71
34	C	518	BCR	C1-C6-C5	-4.19	116.71	122.61
32	l	612	CLA	C4A-NA-C1A	4.18	108.59	106.71
32	n	614	CLA	C4A-NA-C1A	4.18	108.59	106.71
40	YY	615	LUT	C1-C6-C5	-4.18	116.72	122.61
42	n	617	NEX	C26-C27-C28	-4.18	117.16	125.99
32	AA	406	CLA	C4A-NA-C1A	4.18	108.58	106.71
32	RR	313	CLA	C4A-NA-C1A	4.18	108.58	106.71
42	Y	619	NEX	C20-C13-C12	4.17	124.65	118.08
40	44	612	LUT	C3-C4-C5	-4.17	103.54	111.85
42	y	319	NEX	C26-C27-C28	-4.17	117.18	125.99
34	Cc	517	BCR	C33-C5-C6	-4.17	119.85	124.53
40	g	615	LUT	C1-C6-C5	-4.16	116.75	122.61
32	NN	613	CLA	C4A-NA-C1A	4.16	108.58	106.71
32	n	604	CLA	C4A-NA-C1A	4.15	108.57	106.71
42	N	618	NEX	C39-C29-C30	-4.15	117.11	122.92
41	4	314	XAT	C40-C33-C32	4.15	124.62	118.08
36	n	618	LHG	O7-C7-C8	4.15	120.45	111.50
39	YY	608	CHL	C4A-NA-C1A	4.15	108.57	106.71
42	Y	619	NEX	C39-C29-C30	-4.15	117.11	122.92
41	GG	617	XAT	C38-C25-C26	-4.15	115.31	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	619	BCR	C36-C18-C19	4.15	124.61	118.08
32	Dd	402	CLA	C4A-NA-C1A	4.14	108.57	106.71
32	NN	612	CLA	C4A-NA-C1A	4.14	108.57	106.71
35	Dd	404	PL9	C51-C49-C48	-4.14	110.68	122.65
42	Rr	616	NEX	C20-C13-C12	4.14	124.60	118.08
32	YY	602	CLA	C4A-NA-C1A	4.14	108.57	106.71
40	GG	615	LUT	C1-C6-C5	-4.14	116.79	122.61
42	Nn	309	NEX	C26-C27-C28	-4.14	117.25	125.99
41	4	314	XAT	C18-C5-C6	-4.13	115.33	122.26
41	y	301	XAT	O4-C5-C18	4.13	120.01	115.06
41	Yy	619	XAT	C18-C5-C6	-4.13	115.33	122.26
41	y	302	XAT	O4-C5-C18	4.13	120.00	115.06
40	2	614	LUT	C1-C6-C5	-4.13	116.80	122.61
34	c	515	BCR	C38-C26-C25	-4.13	119.89	124.53
32	Yy	602	CLA	C4A-NA-C1A	4.13	108.56	106.71
32	11	613	CLA	C4A-NA-C1A	4.13	108.56	106.71
34	A	409	BCR	C30-C25-C26	-4.13	116.80	122.61
32	D	404	CLA	C4A-NA-C1A	4.12	108.56	106.71
39	R	607	CHL	C4A-NA-C1A	4.12	108.56	106.71
39	N	609	CHL	CMB-C2B-C1B	-4.12	122.13	128.46
32	4	311	CLA	C4A-NA-C1A	4.12	108.56	106.71
32	Rr	611	CLA	C4A-NA-C1A	4.12	108.56	106.71
32	G	604	CLA	C4A-NA-C1A	4.12	108.56	106.71
41	Nn	308	XAT	C18-C5-C6	-4.12	115.36	122.26
32	s	613	CLA	C4A-NA-C1A	4.11	108.56	106.71
32	AA	408	CLA	C4A-NA-C1A	4.11	108.56	106.71
35	d	404	PL9	C51-C49-C48	-4.11	110.77	122.65
42	R	617	NEX	O24-C25-C38	4.11	119.98	115.06
40	Y	615	LUT	C36-C21-C26	4.11	115.77	109.55
32	RR	311	CLA	C4A-NA-C1A	4.11	108.55	106.71
32	c	503	CLA	C4A-NA-C1A	4.10	108.55	106.71
32	CC	512	CLA	C4A-NA-C1A	4.10	108.55	106.71
35	D	407	PL9	C51-C49-C48	-4.10	110.80	122.65
40	Yy	615	LUT	C3-C4-C5	-4.10	103.69	111.85
40	N	616	LUT	C3-C4-C5	-4.09	103.70	111.85
32	33	602	CLA	C4A-NA-C1A	4.09	108.55	106.71
32	2	611	CLA	C4A-NA-C1A	4.09	108.55	106.71
32	44	602	CLA	C4A-NA-C1A	4.09	108.55	106.71
32	c	502	CLA	C4A-NA-C1A	4.09	108.55	106.71
32	DD	401	CLA	C4A-NA-C1A	4.09	108.55	106.71
36	Ll	102	LHG	O7-C7-C8	4.09	120.32	111.50
32	NN	604	CLA	C4A-NA-C1A	4.09	108.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	RR	310	CLA	C4A-NA-C1A	4.09	108.54	106.71
40	Y	615	LUT	C3-C4-C5	-4.08	103.72	111.85
32	B	620	CLA	C4A-NA-C1A	4.08	108.54	106.71
36	D	408	LHG	O7-C7-C8	4.08	120.30	111.50
44	Cc	519	DGD	O2G-C1B-C2B	4.08	120.29	111.50
35	AA	410	PL9	C7-C3-C4	4.08	120.19	116.88
32	11	602	CLA	C4A-NA-C1A	4.08	108.54	106.71
32	N	602	CLA	C4A-NA-C1A	4.08	108.54	106.71
32	c	504	CLA	C4A-NA-C1A	4.08	108.54	106.71
42	Nn	309	NEX	C39-C29-C30	-4.08	117.21	122.92
32	CC	507	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
41	y	301	XAT	O24-C25-C24	4.08	116.44	113.38
42	RR	317	NEX	O24-C25-C38	4.07	119.94	115.06
34	h	101	BCR	C8-C9-C10	4.07	125.19	118.94
32	33	612	CLA	C4A-NA-C1A	4.07	108.54	106.71
42	Yy	617	NEX	C39-C29-C30	-4.07	117.22	122.92
32	C	515	CLA	C4A-NA-C1A	4.07	108.53	106.71
36	y	320	LHG	O7-C7-C8	4.07	120.27	111.50
32	G	613	CLA	C4A-NA-C1A	4.07	108.53	106.71
39	S	606	CHL	C4A-NA-C1A	4.07	108.53	106.71
35	DD	406	PL9	C51-C49-C48	-4.07	110.90	122.65
40	4	313	LUT	C3-C4-C5	-4.06	103.76	111.85
36	DD	407	LHG	O7-C7-C8	4.06	120.26	111.50
41	4	314	XAT	C38-C25-C26	-4.06	115.45	122.26
34	Hh	101	BCR	C3-C4-C5	-4.06	106.83	114.08
42	g	617	NEX	C20-C13-C12	4.06	124.47	118.08
39	4	306	CHL	CMB-C2B-C3B	4.06	132.27	124.68
32	1	613	CLA	C4A-NA-C1A	4.06	108.53	106.71
41	y	301	XAT	C18-C5-C6	-4.06	115.46	122.26
34	C	516	BCR	C1-C6-C5	-4.06	116.90	122.61
32	N	604	CLA	C4A-NA-C1A	4.05	108.53	106.71
42	NN	618	NEX	C38-C25-C26	-4.05	115.47	122.26
40	22	614	LUT	C12-C13-C14	4.05	125.16	118.94
34	CC	515	BCR	C8-C9-C10	4.05	125.15	118.94
35	DD	406	PL9	C50-C49-C48	-4.05	110.95	122.65
32	2	610	CLA	C4A-NA-C1A	4.05	108.53	106.71
39	Y	609	CHL	C4A-NA-C1A	4.05	108.53	106.71
38	W	201	LMG	O7-C10-C11	4.05	120.22	111.50
42	n	617	NEX	C38-C25-C26	-4.05	115.48	122.26
36	GG	618	LHG	O7-C7-C8	4.04	120.21	111.50
32	N	603	CLA	C4A-NA-C1A	4.04	108.52	106.71
39	RR	307	CHL	C4A-NA-C1A	4.04	108.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	407	PL9	C50-C49-C48	-4.04	110.97	122.65
37	CC	501	SQD	O9-S-C6	4.04	111.74	106.94
41	N	617	XAT	C38-C25-C26	-4.04	115.49	122.26
41	Yy	619	XAT	C40-C33-C32	4.04	124.44	118.08
32	y	304	CLA	C4A-NA-C1A	4.04	108.52	106.71
39	22	606	CHL	CMB-C2B-C3B	4.04	132.23	124.68
44	D	411	DGD	O2G-C1B-C2B	4.03	120.19	111.50
32	22	611	CLA	C4A-NA-C1A	4.03	108.52	106.71
41	44	613	XAT	C6-C7-C8	-4.03	117.47	125.99
37	CC	501	SQD	O47-C7-C8	4.03	120.18	111.50
32	BB	607	CLA	C4A-NA-C1A	4.02	108.52	106.71
34	Bb	618	BCR	C36-C18-C19	4.02	124.42	118.08
39	NN	601	CHL	CMB-C2B-C1B	-4.02	122.28	128.46
36	KK	101	LHG	O7-C7-C8	4.02	120.17	111.50
41	G	617	XAT	C18-C5-C6	-4.02	115.52	122.26
42	R	617	NEX	C39-C29-C30	-4.02	117.29	122.92
39	RR	306	CHL	C3A-C2A-C1A	-4.02	95.32	101.34
42	Rr	616	NEX	C39-C29-C30	-4.01	117.30	122.92
34	c	515	BCR	C33-C5-C6	-4.01	120.02	124.53
41	R	616	XAT	C6-C7-C8	-4.01	117.51	125.99
42	y	319	NEX	C39-C29-C30	-4.01	117.30	122.92
36	11	614	LHG	O7-C7-C8	4.01	120.14	111.50
32	Bb	608	CLA	C4A-NA-C1A	4.01	108.51	106.71
32	Cc	514	CLA	C4A-NA-C1A	4.01	108.51	106.71
42	YY	617	NEX	C38-C25-C26	-4.01	115.55	122.26
38	AA	415	LMG	O7-C10-C11	4.00	120.13	111.50
36	N	619	LHG	O7-C7-C8	4.00	120.13	111.50
38	Dd	408	LMG	O7-C10-C11	4.00	120.12	111.50
34	B	616	BCR	C33-C5-C6	-4.00	120.04	124.53
32	B	604	CLA	C4A-NA-C1A	4.00	108.50	106.71
34	TT	101	BCR	C1-C6-C5	-4.00	116.99	122.61
36	NN	619	LHG	O7-C7-C8	4.00	120.11	111.50
40	GG	616	LUT	C3-C4-C5	-3.99	103.90	111.85
34	Cc	516	BCR	C36-C18-C19	3.99	124.37	118.08
40	S	614	LUT	C18-C5-C6	-3.99	120.04	124.53
37	BB	621	SQD	O47-C7-C8	3.99	120.09	111.50
34	C	516	BCR	C8-C9-C10	3.99	125.06	118.94
32	G	610	CLA	C1D-ND-C4D	-3.99	103.50	106.33
32	b	613	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
32	d	401	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
35	Dd	404	PL9	C50-C49-C48	-3.98	111.15	122.65
34	AA	409	BCR	C23-C22-C21	3.98	125.04	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	415	LMG	O7-C10-C11	3.98	120.07	111.50
42	N	618	NEX	C38-C25-C26	-3.98	115.60	122.26
42	Y	617	NEX	C38-C25-C26	-3.98	115.60	122.26
40	y	318	LUT	C1-C6-C5	-3.98	117.01	122.61
41	GG	617	XAT	C18-C5-C6	-3.97	115.60	122.26
35	d	404	PL9	C50-C49-C48	-3.97	111.16	122.65
32	S	602	CLA	C4A-NA-C1A	3.97	108.49	106.71
32	b	606	CLA	C4A-NA-C1A	3.97	108.49	106.71
44	BB	625	DGD	O2G-C1B-C2B	3.97	120.06	111.50
40	G	616	LUT	C3-C4-C5	-3.97	103.94	111.85
32	Bb	613	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
32	C	508	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
34	A	409	BCR	C23-C22-C21	3.97	125.03	118.94
38	WW	201	LMG	O7-C10-C11	3.97	120.05	111.50
41	y	301	XAT	C39-C29-C28	3.97	124.33	118.08
34	Hh	101	BCR	C8-C9-C10	3.97	125.03	118.94
34	AA	409	BCR	C30-C25-C26	-3.96	117.03	122.61
40	RR	315	LUT	C1-C6-C5	-3.96	117.03	122.61
32	b	615	CLA	C4A-NA-C1A	3.96	108.49	106.71
34	D	406	BCR	C1-C6-C7	3.96	126.98	115.78
38	C	521	LMG	O7-C10-C11	3.96	120.03	111.50
41	Nn	308	XAT	O4-C5-C18	3.96	119.80	115.06
32	R	613	CLA	C4A-NA-C1A	3.95	108.48	106.71
32	g	602	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
39	SS	307	CHL	C4A-NA-C1A	3.95	108.48	106.71
35	AA	410	PL9	C51-C49-C48	-3.95	111.24	122.65
38	j	101	LMG	O7-C10-C11	3.95	120.01	111.50
34	DD	405	BCR	C1-C6-C7	3.94	126.94	115.78
36	33	614	LHG	O7-C7-C8	3.94	120.00	111.50
40	N	615	LUT	C3-C4-C5	-3.94	104.00	111.85
32	B	623	CLA	C4A-NA-C1A	3.94	108.48	106.71
32	1	609	CLA	CBD-CHA-C1A	3.94	133.15	128.50
34	D	406	BCR	C30-C25-C26	-3.94	117.06	122.61
34	CC	517	BCR	C1-C6-C7	3.94	126.93	115.78
42	Y	619	NEX	C38-C25-C26	-3.94	115.66	122.26
41	NN	617	XAT	C38-C25-C26	-3.94	115.66	122.26
44	B	603	DGD	O2G-C1B-C2B	3.94	119.98	111.50
39	GG	607	CHL	C4A-NA-C1A	3.93	108.47	106.71
34	c	515	BCR	C1-C6-C5	-3.93	117.07	122.61
32	33	604	CLA	C4A-NA-C1A	3.93	108.47	106.71
39	Nn	315	CHL	C4A-NA-C1A	3.93	108.47	106.71
36	D	410	LHG	O7-C7-C8	3.93	119.97	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	410	PL9	C50-C49-C48	-3.93	111.29	122.65
32	YY	613	CLA	C4A-NA-C1A	3.93	108.47	106.71
34	BB	620	BCR	C1-C6-C5	-3.93	117.08	122.61
41	r	615	XAT	C38-C25-C26	-3.93	115.68	122.26
42	Rr	616	NEX	C38-C25-C26	-3.93	115.68	122.26
39	Yy	605	CHL	C4A-NA-C1A	3.92	108.47	106.71
32	DD	403	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
34	T	101	BCR	C15-C16-C17	-3.92	115.44	123.47
39	33	608	CHL	CMB-C2B-C3B	3.92	132.01	124.68
36	G	618	LHG	O7-C7-C8	3.92	119.94	111.50
32	44	609	CLA	C4A-NA-C1A	3.92	108.47	106.71
37	B	617	SQD	O47-C7-C8	3.92	119.94	111.50
42	Nn	309	NEX	C20-C13-C12	3.92	124.25	118.08
34	T	101	BCR	C33-C5-C6	-3.92	120.13	124.53
34	B	616	BCR	C1-C6-C5	-3.92	117.10	122.61
34	TT	101	BCR	C15-C16-C17	-3.91	115.45	123.47
32	Cc	515	CLA	C4A-NA-C1A	3.91	108.46	106.71
34	C	518	BCR	C1-C6-C7	3.91	126.84	115.78
32	C	510	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
34	a	411	BCR	C1-C6-C5	-3.90	117.11	122.61
32	Y	613	CLA	C4A-NA-C1A	3.90	108.46	106.71
32	CC	504	CLA	C4A-NA-C1A	3.90	108.46	106.71
32	N	603	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
34	b	618	BCR	C36-C18-C19	3.90	124.22	118.08
42	Nn	309	NEX	O24-C25-C38	3.90	119.73	115.06
34	XX	202	BCR	C36-C18-C19	3.90	124.22	118.08
36	Rr	617	LHG	O7-C7-C8	3.90	119.91	111.50
41	Rr	615	XAT	C20-C13-C12	3.90	124.22	118.08
32	33	603	CLA	C4A-NA-C1A	3.90	108.46	106.71
32	Aa	410	CLA	C4A-NA-C1A	3.89	108.46	106.71
37	LL	102	SQD	O47-C7-C8	3.89	119.89	111.50
32	R	614	CLA	C4A-NA-C1A	3.89	108.45	106.71
35	A	410	PL9	C15-C14-C16	-3.89	108.73	115.27
32	RR	314	CLA	C4A-NA-C1A	3.89	108.45	106.71
35	A	410	PL9	C51-C49-C48	-3.89	111.42	122.65
35	AA	410	PL9	C50-C49-C48	-3.89	111.42	122.65
34	Cc	516	BCR	C8-C9-C10	3.88	124.90	118.94
39	1	605	CHL	CBD-CHA-C1A	3.88	133.08	128.50
34	DD	405	BCR	C30-C25-C26	-3.88	117.15	122.61
32	BB	606	CLA	C4A-NA-C1A	3.88	108.45	106.71
39	y	308	CHL	C4A-NA-C1A	3.88	108.45	106.71
42	n	617	NEX	C20-C13-C12	3.88	124.19	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	N	618	NEX	C16-C1-C6	3.88	113.94	110.47
36	D	409	LHG	O7-C7-C8	3.87	119.85	111.50
32	C	505	CLA	C4A-NA-C1A	3.87	108.45	106.71
35	Dd	404	PL9	C15-C14-C16	-3.87	108.75	115.27
44	CC	519	DGD	O2G-C1B-C2B	3.87	119.85	111.50
32	c	508	CLA	C4A-NA-C1A	3.87	108.45	106.71
42	g	617	NEX	C16-C1-C6	3.87	113.93	110.47
32	22	609	CLA	C4A-NA-C1A	3.87	108.44	106.71
40	S	614	LUT	C3-C4-C5	-3.87	104.15	111.85
34	H	101	BCR	C34-C9-C10	-3.87	117.51	122.92
42	YY	617	NEX	C20-C13-C12	3.87	124.17	118.08
41	N	617	XAT	C40-C33-C34	-3.86	117.51	122.92
32	11	611	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
37	l	102	SQD	O47-C7-C8	3.86	119.83	111.50
34	B	612	BCR	C36-C18-C19	3.86	124.16	118.08
41	44	613	XAT	C18-C5-C6	-3.86	115.79	122.26
36	K	101	LHG	O7-C7-C8	3.86	119.82	111.50
32	s	611	CLA	C4A-NA-C1A	3.86	108.44	106.71
32	Gg	313	CLA	C4A-NA-C1A	3.86	108.44	106.71
36	r	616	LHG	O7-C7-C8	3.86	119.81	111.50
36	44	614	LHG	C5-O7-C7	-3.85	110.71	117.90
40	Ss	615	LUT	C16-C1-C6	3.85	116.55	110.30
32	b	608	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
32	BB	610	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
42	n	617	NEX	C39-C29-C30	-3.85	117.53	122.92
44	BB	624	DGD	O2G-C1B-C2B	3.85	119.80	111.50
32	r	608	CLA	C4A-NA-C1A	3.85	108.44	106.71
32	r	611	CLA	C4A-NA-C1A	3.85	108.44	106.71
34	CC	515	BCR	C1-C6-C5	-3.84	117.20	122.61
37	L	101	SQD	O47-C7-C8	3.84	119.78	111.50
32	22	603	CLA	C4A-NA-C1A	3.84	108.43	106.71
38	Bb	621	LMG	O7-C10-C11	3.84	119.78	111.50
42	Y	617	NEX	C20-C13-C12	3.84	124.13	118.08
32	Nn	305	CLA	C4A-NA-C1A	3.84	108.43	106.71
42	Nn	309	NEX	C40-C33-C32	3.84	124.12	118.08
34	Cc	517	BCR	C1-C6-C5	-3.83	117.21	122.61
39	Yy	608	CHL	C4A-NA-C1A	3.83	108.43	106.71
38	b	621	LMG	O7-C10-C11	3.83	119.77	111.50
39	Yy	607	CHL	O2D-CGD-O1D	-3.83	116.34	123.84
32	c	510	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
36	DD	408	LHG	O7-C7-C8	3.83	119.76	111.50
39	Y	607	CHL	C4A-NA-C1A	3.83	108.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Nn	319	CHL	C4A-NA-C1A	3.83	108.43	106.71
32	Gg	303	CLA	CHD-C1D-ND	-3.83	120.94	124.45
34	BB	616	BCR	C1-C6-C5	-3.82	117.23	122.61
44	B	601	DGD	O2G-C1B-C2B	3.82	119.74	111.50
32	a	410	CLA	C4A-NA-C1A	3.82	108.42	106.71
34	B	613	BCR	C1-C6-C5	-3.82	117.23	122.61
40	y	317	LUT	C4-C5-C6	-3.82	112.34	120.85
32	4	305	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
39	GG	609	CHL	CMB-C2B-C3B	3.81	131.81	124.68
32	B	621	CLA	C4A-NA-C1A	3.81	108.42	106.71
36	1	614	LHG	O7-C7-C8	3.81	119.71	111.50
32	Ss	609	CLA	C4A-NA-C1A	3.80	108.42	106.71
32	C	515	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
35	DD	406	PL9	C10-C9-C11	-3.80	108.88	115.27
34	Bb	617	BCR	C37-C22-C21	-3.80	117.60	122.92
34	BB	616	BCR	C27-C26-C25	-3.80	117.22	122.73
32	R	610	CLA	C4A-NA-C1A	3.80	108.41	106.71
40	s	615	LUT	C1-C6-C5	-3.80	117.27	122.61
39	44	605	CHL	CMB-C2B-C3B	3.79	131.78	124.68
32	NN	614	CLA	C4A-NA-C1A	3.79	108.41	106.71
32	d	402	CLA	C4A-NA-C1A	3.79	108.41	106.71
32	Rr	601	CLA	C4A-NA-C1A	3.79	108.41	106.71
32	Rr	609	CLA	C4A-NA-C1A	3.79	108.41	106.71
40	G	615	LUT	C3-C4-C5	-3.79	104.31	111.85
36	JJ	101	LHG	O7-C7-C8	3.78	119.66	111.50
34	BB	616	BCR	C36-C18-C19	3.78	124.04	118.08
41	R	616	XAT	C39-C29-C28	3.78	124.04	118.08
34	c	514	BCR	C30-C25-C26	-3.78	117.28	122.61
40	g	615	LUT	C3-C4-C5	-3.78	104.32	111.85
36	3	614	LHG	O7-C7-C8	3.78	119.64	111.50
32	Y	602	CLA	C4A-NA-C1A	3.78	108.40	106.71
37	Ll	101	SQD	O47-C7-C8	3.77	119.64	111.50
41	RR	316	XAT	C6-C7-C8	-3.77	118.02	125.99
39	n	607	CHL	C4A-NA-C1A	3.77	108.40	106.71
39	NN	607	CHL	C4A-NA-C1A	3.77	108.40	106.71
42	g	617	NEX	C26-C27-C28	3.77	133.96	125.99
34	k	101	BCR	C3-C4-C5	-3.77	107.35	114.08
44	C	520	DGD	O2G-C1B-C2B	3.76	119.61	111.50
32	11	604	CLA	CBD-CHA-C1A	3.76	132.94	128.50
32	3	604	CLA	C4A-NA-C1A	3.76	108.40	106.71
40	2	614	LUT	C12-C13-C14	3.76	124.71	118.94
32	s	603	CLA	C4A-NA-C1A	3.76	108.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	4	314	XAT	C39-C29-C28	3.76	124.00	118.08
34	KK	103	BCR	C34-C9-C8	3.76	124.00	118.08
34	Hh	101	BCR	C2-C1-C6	3.76	116.27	110.48
32	33	613	CLA	C4A-NA-C1A	3.76	108.40	106.71
44	C	519	DGD	O2G-C1B-C2B	3.76	119.60	111.50
32	2	603	CLA	C4A-NA-C1A	3.76	108.39	106.71
32	Bb	606	CLA	C4A-NA-C1A	3.76	108.39	106.71
41	G	619	XAT	C18-C5-C6	-3.76	115.97	122.26
32	c	512	CLA	C4A-NA-C1A	3.75	108.39	106.71
40	N	616	LUT	C36-C21-C26	3.75	115.23	109.55
38	Aa	412	LMG	O7-C10-C11	3.75	119.58	111.50
32	CC	514	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
32	Ss	611	CLA	C4A-NA-C1A	3.75	108.39	106.71
39	Yy	606	CHL	C4A-NA-C1A	3.74	108.39	106.71
32	C	503	CLA	C4A-NA-C1A	3.74	108.39	106.71
34	K	102	BCR	C37-C22-C23	3.74	123.97	118.08
39	4	309	CHL	CMB-C2B-C3B	3.73	131.66	124.68
39	11	608	CHL	CMB-C2B-C3B	3.73	131.66	124.68
32	BB	607	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
39	4	307	CHL	C4A-NA-C1A	3.73	108.38	106.71
39	Gg	307	CHL	C4A-NA-C1A	3.73	108.38	106.71
41	NN	617	XAT	C40-C33-C32	3.72	123.94	118.08
32	g	613	CLA	C4A-NA-C1A	3.72	108.38	106.71
34	BB	618	BCR	C36-C18-C19	3.72	123.93	118.08
32	Rr	608	CLA	C4A-NA-C1A	3.72	108.38	106.71
32	SS	314	CLA	C4A-NA-C1A	3.71	108.38	106.71
36	Dd	406	LHG	O7-C7-C8	3.71	119.50	111.50
42	Yy	617	NEX	C20-C13-C12	3.71	123.92	118.08
32	4	303	CLA	C4A-NA-C1A	3.71	108.37	106.71
34	C	516	BCR	C33-C5-C6	-3.71	120.36	124.53
41	y	302	XAT	C20-C13-C12	3.71	123.92	118.08
34	Cc	516	BCR	C30-C25-C26	-3.71	117.39	122.61
32	NN	602	CLA	C4A-NA-C1A	3.71	108.37	106.71
41	GG	619	XAT	C18-C5-C6	-3.70	116.05	122.26
35	DD	406	PL9	C45-C44-C46	-3.70	109.04	115.27
39	R	606	CHL	C2A-C1A-CHA	3.70	130.33	123.86
39	Gg	310	CHL	CMB-C2B-C3B	3.70	131.60	124.68
35	A	410	PL9	C7-C3-C4	3.70	119.88	116.88
34	BB	618	BCR	C30-C25-C26	-3.70	117.40	122.61
36	C	522	LHG	O7-C7-C8	3.70	119.47	111.50
34	B	614	BCR	C36-C18-C19	3.70	123.90	118.08
39	Gg	310	CHL	C4A-NA-C1A	3.70	108.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	403	BCR	C38-C26-C25	-3.70	120.38	124.53
34	b	617	BCR	C1-C6-C5	-3.70	117.41	122.61
34	BB	617	BCR	C1-C6-C5	-3.70	117.41	122.61
32	b	609	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
39	2	606	CHL	CMB-C2B-C3B	3.69	131.59	124.68
34	h	101	BCR	C3-C4-C5	-3.69	107.48	114.08
32	CC	509	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
32	S	613	CLA	C4A-NA-C1A	3.69	108.36	106.71
32	CC	506	CLA	C4A-NA-C1A	3.69	108.36	106.71
34	A	409	BCR	C29-C30-C25	3.69	116.16	110.48
40	Y	615	LUT	C1-C6-C7	3.69	126.21	115.78
39	11	601	CHL	C4A-NA-C1A	3.69	108.36	106.71
34	TT	101	BCR	C33-C5-C6	-3.69	120.39	124.53
32	11	611	CLA	C4A-NA-C1A	3.69	108.36	106.71
39	n	609	CHL	CMB-C2B-C3B	3.68	131.57	124.68
32	B	604	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
36	l	101	LHG	O7-C7-C8	3.68	119.44	111.50
40	YY	615	LUT	C1-C6-C7	3.68	126.19	115.78
32	3	603	CLA	C4A-NA-C1A	3.68	108.36	106.71
39	s	605	CHL	C4A-NA-C1A	3.68	108.36	106.71
34	Bb	617	BCR	C33-C5-C6	-3.68	120.40	124.53
32	b	614	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
39	NN	605	CHL	CMB-C2B-C3B	3.67	131.55	124.68
40	Rr	614	LUT	C3-C4-C5	-3.67	104.54	111.85
36	d	406	LHG	O7-C7-C8	3.67	119.40	111.50
32	r	609	CLA	C4A-NA-C1A	3.66	108.35	106.71
39	R	605	CHL	CMB-C2B-C3B	3.66	131.53	124.68
40	y	317	LUT	C3-C4-C5	-3.66	104.56	111.85
35	Dd	404	PL9	C45-C44-C46	-3.66	109.11	115.27
39	N	605	CHL	C4A-NA-C1A	3.66	108.35	106.71
32	NN	603	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
34	C	518	BCR	C36-C18-C19	3.66	123.84	118.08
36	CC	523	LHG	O7-C7-C8	3.66	119.38	111.50
32	BB	608	CLA	C4A-NA-C1A	3.66	108.35	106.71
32	Bb	609	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
32	Cc	515	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
32	a	406	CLA	C1B-CHB-C4A	-3.66	122.88	130.12
32	Ss	611	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
34	b	617	BCR	C36-C18-C17	-3.65	117.80	122.92
34	CC	515	BCR	C3-C4-C5	-3.65	107.55	114.08
32	l	612	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
32	Ss	603	CLA	C4A-NA-C1A	3.65	108.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Cc	504	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
41	44	613	XAT	C38-C25-C26	-3.65	116.14	122.26
32	YY	612	CLA	C4A-NA-C1A	3.65	108.35	106.71
39	n	601	CHL	C4A-NA-C1A	3.65	108.34	106.71
39	y	309	CHL	C4A-NA-C1A	3.65	108.34	106.71
41	g	619	XAT	C18-C5-C6	-3.64	116.15	122.26
35	D	407	PL9	C15-C14-C16	-3.64	109.14	115.27
39	Nn	311	CHL	C4A-NA-C1A	3.64	108.34	106.71
39	44	608	CHL	CMB-C2B-C3B	3.64	131.49	124.68
39	3	601	CHL	C4A-NA-C1A	3.64	108.34	106.71
39	y	310	CHL	C4A-NA-C1A	3.64	108.34	106.71
34	Bb	617	BCR	C1-C6-C5	-3.64	117.49	122.61
44	CC	518	DGD	O2G-C1B-C2B	3.64	119.34	111.50
37	C	501	SQD	O47-C7-C8	3.64	119.34	111.50
35	D	407	PL9	C45-C44-C46	-3.64	109.15	115.27
34	c	514	BCR	C8-C9-C10	3.64	124.52	118.94
32	Bb	613	CLA	CMB-C2B-C3B	3.64	131.48	124.68
32	R	601	CLA	CMB-C2B-C3B	3.64	131.48	124.68
39	Rr	605	CHL	CMB-C2B-C3B	3.64	131.48	124.68
32	b	613	CLA	CMB-C2B-C3B	3.63	131.47	124.68
32	Nn	304	CLA	C4A-NA-C1A	3.63	108.34	106.71
41	GG	619	XAT	C35-C15-C14	-3.63	116.04	123.47
34	Bb	617	BCR	C36-C18-C17	-3.63	117.84	122.92
39	Nn	317	CHL	C4A-NA-C1A	3.63	108.34	106.71
32	22	609	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
39	r	606	CHL	CMB-C2B-C3B	3.62	131.46	124.68
41	G	619	XAT	C35-C15-C14	-3.62	116.05	123.47
32	Bb	608	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
40	Gg	317	LUT	C1-C6-C5	-3.62	117.51	122.61
34	b	618	BCR	C37-C22-C23	3.62	123.78	118.08
34	Dd	403	BCR	C38-C26-C25	-3.62	120.46	124.53
39	NN	608	CHL	C4A-NA-C1A	3.62	108.33	106.71
34	Bb	618	BCR	C1-C6-C5	-3.62	117.52	122.61
44	c	518	DGD	O2G-C1B-C2B	3.62	119.30	111.50
34	C	516	BCR	C1-C6-C7	3.62	126.01	115.78
32	B	606	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
34	b	618	BCR	C30-C25-C26	-3.62	117.52	122.61
36	A	413	LHG	O7-C7-C8	3.62	119.29	111.50
42	NN	618	NEX	C20-C13-C12	3.61	123.77	118.08
32	Rr	610	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
34	c	514	BCR	C36-C18-C19	3.61	123.77	118.08
39	R	606	CHL	C3A-C2A-C1A	-3.61	95.93	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	22	613	CLA	C4A-NA-C1A	3.61	108.33	106.71
39	y	307	CHL	C4A-NA-C1A	3.61	108.33	106.71
34	Bb	618	BCR	C37-C22-C23	3.61	123.76	118.08
34	b	617	BCR	C37-C22-C21	-3.61	117.87	122.92
39	s	605	CHL	CMB-C2B-C3B	3.61	131.42	124.68
42	n	617	NEX	O24-C25-C38	3.60	119.37	115.06
34	Cc	517	BCR	C36-C18-C19	3.60	123.75	118.08
32	DD	403	CLA	C4A-NA-C1A	3.60	108.33	106.71
39	Ss	606	CHL	CMB-C2B-C3B	3.60	131.41	124.68
39	r	607	CHL	CMB-C2B-C3B	3.60	131.41	124.68
34	Cc	516	BCR	C30-C25-C24	3.60	125.96	115.78
32	D	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
39	Rr	607	CHL	CMB-C2B-C3B	3.60	131.41	124.68
32	BB	602	CLA	C4A-NA-C1A	3.59	108.32	106.71
32	s	608	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
41	G	617	XAT	C28-C29-C30	3.59	124.45	118.94
39	N	607	CHL	C4A-NA-C1A	3.59	108.32	106.71
34	Dd	403	BCR	C36-C18-C19	3.59	123.73	118.08
34	Aa	411	BCR	C1-C6-C5	-3.59	117.56	122.61
32	C	514	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
32	GG	614	CLA	C4A-NA-C1A	3.59	108.32	106.71
35	d	404	PL9	C45-C44-C46	-3.59	109.24	115.27
37	LL	101	SQD	O47-C7-C8	3.59	119.23	111.50
34	AA	409	BCR	C29-C30-C25	3.59	116.00	110.48
40	r	614	LUT	C3-C4-C5	-3.59	104.71	111.85
35	Dd	404	PL9	C10-C9-C11	-3.59	109.24	115.27
32	Dd	401	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
32	YY	614	CLA	C4A-NA-C1A	3.58	108.32	106.71
39	Ss	605	CHL	CMB-C2B-C3B	3.58	131.38	124.68
34	h	101	BCR	C2-C1-C6	3.58	116.00	110.48
35	d	404	PL9	C15-C14-C16	-3.58	109.25	115.27
41	4	314	XAT	C6-C7-C8	-3.58	118.42	125.99
32	Rr	609	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
36	CC	521	LHG	O7-C7-C8	3.57	119.20	111.50
34	d	403	BCR	C36-C18-C19	3.57	123.71	118.08
34	Kk	101	BCR	C30-C25-C26	-3.57	117.58	122.61
32	Aa	406	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
39	Y	605	CHL	C4A-NA-C1A	3.57	108.31	106.71
32	B	609	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
32	B	624	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
34	c	515	BCR	C30-C25-C26	-3.57	117.59	122.61
35	DD	406	PL9	C15-C14-C16	-3.57	109.27	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	514	BCR	C30-C25-C24	3.57	125.86	115.78
38	CC	520	LMG	O7-C10-C11	3.57	119.19	111.50
39	SS	306	CHL	CMB-C2B-C3B	3.56	131.34	124.68
32	Cc	507	CLA	C4A-NA-C1A	3.56	108.31	106.71
36	II	101	LHG	O7-C7-C8	3.56	119.17	111.50
32	Cc	512	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
34	B	614	BCR	C37-C22-C23	3.56	123.68	118.08
39	1	608	CHL	C1B-CHB-C4A	-3.56	123.08	130.12
32	44	610	CLA	C4A-NA-C1A	3.55	108.30	106.71
32	B	624	CLA	C4A-NA-C1A	3.55	108.30	106.71
34	c	514	BCR	C37-C22-C23	3.55	123.67	118.08
36	Y	618	LHG	O7-C7-C8	3.55	119.15	111.50
34	H	101	BCR	C38-C26-C25	-3.55	120.54	124.53
32	r	601	CLA	C4A-NA-C1A	3.55	108.30	106.71
41	y	302	XAT	C40-C33-C34	-3.55	117.95	122.92
39	4	309	CHL	C1B-CHB-C4A	-3.55	123.09	130.12
39	NN	606	CHL	C4A-NA-C1A	3.55	108.30	106.71
38	Mm	101	LMG	O7-C10-C11	3.55	119.14	111.50
32	44	615	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
39	G	609	CHL	CMB-C2B-C3B	3.55	131.31	124.68
41	Gg	301	XAT	C18-C5-C6	-3.54	116.32	122.26
39	YY	607	CHL	C4A-NA-C1A	3.54	108.30	106.71
40	YY	615	LUT	C36-C21-C26	3.54	114.91	109.55
44	h	102	DGD	O2G-C1B-C2B	3.54	119.13	111.50
34	c	515	BCR	C36-C18-C19	3.54	123.65	118.08
32	c	512	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
32	n	613	CLA	C4A-NA-C1A	3.54	108.30	106.71
35	AA	410	PL9	C10-C9-C11	-3.53	109.33	115.27
34	Cc	517	BCR	C38-C26-C25	-3.53	120.56	124.53
32	DD	403	CLA	CMB-C2B-C3B	3.53	131.29	124.68
32	d	401	CLA	CMB-C2B-C3B	3.53	131.29	124.68
37	L	102	SQD	O47-C7-C8	3.53	119.11	111.50
38	Bb	620	LMG	O7-C10-C11	3.53	119.11	111.50
32	Cc	510	CLA	C4A-NA-C1A	3.53	108.29	106.71
32	Aa	407	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
38	b	620	LMG	O7-C10-C11	3.53	119.11	111.50
39	Nn	315	CHL	CMB-C2B-C3B	3.53	131.28	124.68
34	Bb	618	BCR	C30-C25-C26	-3.53	117.65	122.61
44	Cc	520	DGD	O2G-C1B-C2B	3.53	119.10	111.50
32	1	609	CLA	C1D-ND-C4D	-3.52	103.83	106.33
41	r	615	XAT	C20-C13-C12	3.52	123.63	118.08
34	KK	103	BCR	C1-C6-C5	-3.52	117.66	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	617	BCR	C33-C5-C6	-3.52	120.58	124.53
38	F	101	LMG	O7-C10-C11	3.52	119.09	111.50
41	Yy	619	XAT	C39-C29-C28	3.52	123.62	118.08
32	11	610	CLA	C4A-NA-C1A	3.52	108.29	106.71
41	g	619	XAT	C35-C15-C14	-3.52	116.27	123.47
42	g	617	NEX	C35-C15-C14	-3.52	116.27	123.47
34	Cc	516	BCR	C37-C22-C23	3.52	123.62	118.08
41	y	301	XAT	C40-C33-C32	3.51	123.61	118.08
32	YY	603	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
34	c	516	BCR	C33-C5-C6	-3.51	120.58	124.53
32	3	613	CLA	C4A-NA-C1A	3.51	108.28	106.71
32	Y	610	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
34	T	101	BCR	C33-C5-C4	3.51	120.36	113.62
39	YY	607	CHL	CMB-C2B-C3B	3.51	131.24	124.68
39	Nn	319	CHL	CMB-C2B-C3B	3.51	131.24	124.68
32	Aa	410	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
34	k	101	BCR	C37-C22-C23	3.51	123.60	118.08
41	GG	617	XAT	O4-C5-C18	3.51	119.26	115.06
32	N	614	CLA	C4A-NA-C1A	3.51	108.28	106.71
32	Cc	508	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
34	CC	517	BCR	C36-C18-C19	3.51	123.60	118.08
39	Nn	315	CHL	O2D-CGD-O1D	-3.51	116.98	123.84
32	11	612	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
32	Yy	603	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
39	s	606	CHL	CMB-C2B-C3B	3.50	131.23	124.68
34	KK	103	BCR	C37-C22-C23	3.50	123.59	118.08
32	1	602	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
32	g	611	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
32	CC	507	CLA	CMB-C2B-C3B	3.50	131.23	124.68
32	s	611	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
35	D	407	PL9	C10-C9-C11	-3.50	109.39	115.27
32	G	612	CLA	C4A-NA-C1A	3.50	108.28	106.71
42	y	319	NEX	C40-C33-C32	3.50	123.59	118.08
32	11	604	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
39	g	609	CHL	CMB-C2B-C3B	3.50	131.22	124.68
34	KK	103	BCR	C27-C26-C25	-3.49	117.66	122.73
41	Gg	301	XAT	C35-C15-C14	-3.49	116.32	123.47
34	H	101	BCR	C23-C22-C21	3.49	124.30	118.94
39	Y	607	CHL	CMB-C2B-C3B	3.49	131.21	124.68
34	k	101	BCR	C33-C5-C4	3.49	120.32	113.62
39	33	607	CHL	CMB-C2B-C3B	3.49	131.21	124.68
35	A	410	PL9	C45-C44-C46	-3.49	109.41	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	502	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
38	m	101	LMG	O7-C10-C11	3.48	119.01	111.50
32	33	604	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
32	3	609	CLA	C4A-NA-C1A	3.48	108.27	106.71
39	S	605	CHL	CMB-C2B-C3B	3.48	131.18	124.68
39	Ss	607	CHL	C4A-NA-C1A	3.48	108.27	106.71
39	4	306	CHL	CHB-C4A-NA	3.48	129.32	124.51
41	G	617	XAT	O4-C5-C18	3.48	119.22	115.06
39	s	601	CHL	C4A-NA-C1A	3.47	108.27	106.71
32	CC	508	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
42	NN	618	NEX	C16-C1-C6	3.47	113.58	110.47
44	C	523	DGD	O2G-C1B-C2B	3.47	118.98	111.50
41	y	302	XAT	C38-C25-C26	-3.47	116.44	122.26
34	BB	618	BCR	C37-C22-C23	3.47	123.55	118.08
41	GG	617	XAT	C28-C29-C30	3.47	124.27	118.94
34	C	517	BCR	C36-C18-C19	3.47	123.54	118.08
42	YY	617	NEX	O24-C25-C38	3.47	119.21	115.06
32	B	607	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
32	N	612	CLA	C4A-NA-C1A	3.47	108.27	106.71
32	c	513	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
40	Ss	614	LUT	C1-C6-C5	-3.46	117.73	122.61
38	a	412	LMG	O7-C10-C11	3.46	118.97	111.50
32	Y	612	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
38	DD	409	LMG	O7-C10-C11	3.46	118.96	111.50
32	11	609	CLA	C4A-NA-C1A	3.46	108.26	106.71
32	Gg	311	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
37	Aa	413	SQD	O47-C7-C8	3.46	118.95	111.50
32	Gg	311	CLA	C4A-NA-C1A	3.46	108.26	106.71
34	H	101	BCR	C30-C25-C26	-3.46	117.75	122.61
42	NN	618	NEX	C26-C27-C28	-3.45	118.69	125.99
32	33	611	CLA	C4A-NA-C1A	3.45	108.26	106.71
32	C	508	CLA	CMB-C2B-C3B	3.45	131.14	124.68
34	CC	516	BCR	C36-C18-C19	3.45	123.52	118.08
32	B	618	CLA	C4A-NA-C1A	3.45	108.26	106.71
39	NN	609	CHL	CMB-C2B-C1B	-3.45	123.16	128.46
34	H	101	BCR	C1-C6-C5	-3.45	117.75	122.61
39	N	608	CHL	C4A-NA-C1A	3.45	108.26	106.71
39	11	605	CHL	O2D-CGD-O1D	-3.45	117.09	123.84
42	Rr	616	NEX	O24-C25-C38	3.45	119.19	115.06
34	CC	515	BCR	C1-C6-C7	3.45	125.53	115.78
34	b	618	BCR	C1-C6-C5	-3.45	117.76	122.61
32	Cc	514	CLA	CMB-C2B-C1B	-3.45	123.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	NN	615	LUT	C3-C4-C5	-3.44	104.99	111.85
38	B	615	LMG	O7-C10-C11	3.44	118.92	111.50
36	Ss	616	LHG	O7-C7-C8	3.44	118.92	111.50
32	Yy	610	CLA	C1B-CHB-C4A	-3.44	123.30	130.12
32	Bb	614	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
40	YY	616	LUT	C3-C4-C5	-3.44	105.00	111.85
39	r	605	CHL	O2D-CGD-O1D	-3.44	117.11	123.84
35	A	410	PL9	C10-C9-C11	-3.44	109.49	115.27
39	RR	305	CHL	C2A-C3A-C4A	-3.44	96.32	101.87
39	RR	305	CHL	CMB-C2B-C3B	3.44	131.11	124.68
39	11	607	CHL	CMB-C2B-C3B	3.44	131.10	124.68
39	4	308	CHL	CMB-C2B-C3B	3.44	131.10	124.68
40	Yy	615	LUT	C4-C5-C6	-3.44	113.19	120.85
34	c	516	BCR	C36-C18-C19	3.43	123.49	118.08
34	BB	620	BCR	C36-C18-C19	3.43	123.49	118.08
42	y	319	NEX	C20-C13-C12	3.43	123.49	118.08
32	c	510	CLA	CMB-C2B-C3B	3.43	131.10	124.68
32	R	602	CLA	C4A-NA-C1A	3.43	108.25	106.71
39	NN	605	CHL	C4A-NA-C1A	3.43	108.25	106.71
36	s	616	LHG	O7-C7-C8	3.43	118.89	111.50
32	BB	611	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
40	Ss	615	LUT	C19-C9-C8	3.43	123.48	118.08
35	d	404	PL9	C10-C9-C11	-3.43	109.50	115.27
42	Y	619	NEX	O24-C25-C38	3.42	119.16	115.06
32	g	612	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
32	Nn	312	CLA	C4A-NA-C1A	3.42	108.25	106.71
39	g	608	CHL	C4A-NA-C1A	3.42	108.25	106.71
32	R	609	CLA	C4A-NA-C1A	3.42	108.24	106.71
35	AA	410	PL9	C45-C44-C46	-3.42	109.52	115.27
32	R	601	CLA	C4A-NA-C1A	3.42	108.24	106.71
32	Rr	603	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
32	r	608	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
32	C	506	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
34	C	516	BCR	C3-C4-C5	-3.42	107.97	114.08
42	N	618	NEX	C26-C27-C28	-3.42	118.77	125.99
44	Aa	401	DGD	O2G-C1B-C2B	3.41	118.86	111.50
39	N	607	CHL	CHB-C4A-NA	3.41	129.23	124.51
32	a	407	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
39	Yy	609	CHL	C4A-NA-C1A	3.41	108.24	106.71
34	BB	620	BCR	C30-C25-C26	-3.41	117.81	122.61
40	N	615	LUT	C1-C6-C5	-3.41	117.81	122.61
39	N	605	CHL	CMB-C2B-C3B	3.41	131.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	3	609	CLA	CBD-CHA-C1A	3.41	132.52	128.50
39	s	601	CHL	CMB-C2B-C3B	3.41	131.06	124.68
34	BB	617	BCR	C37-C22-C23	3.41	123.45	118.08
32	R	614	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
39	R	605	CHL	C1B-CHB-C4A	-3.41	123.37	130.12
34	B	616	BCR	C30-C25-C26	-3.41	117.81	122.61
39	Ss	605	CHL	C4A-NA-C1A	3.41	108.24	106.71
32	C	515	CLA	CMB-C2B-C3B	3.41	131.05	124.68
44	a	415	DGD	O2G-C1B-C2B	3.41	118.84	111.50
34	h	101	BCR	C30-C25-C26	-3.41	117.82	122.61
32	Nn	312	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
32	C	509	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
41	y	302	XAT	C19-C9-C8	3.40	123.44	118.08
39	Rr	607	CHL	C4A-NA-C1A	3.40	108.23	106.71
41	Nn	308	XAT	C40-C33-C34	-3.40	118.16	122.92
32	D	401	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
32	DD	401	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
32	l	611	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
40	y	317	LUT	C17-C1-C6	-3.40	104.78	110.30
34	BB	620	BCR	C3-C4-C5	-3.40	108.01	114.08
41	RR	316	XAT	C39-C29-C28	3.40	123.43	118.08
42	N	618	NEX	C20-C13-C12	3.40	123.43	118.08
32	BB	615	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
32	Yy	614	CLA	C4A-NA-C1A	3.39	108.23	106.71
32	Ss	604	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
32	s	609	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
36	a	414	LHG	O7-C7-C8	3.39	118.82	111.50
38	BB	619	LMG	O7-C10-C11	3.39	118.81	111.50
37	B	602	SQD	O47-C7-C8	3.39	118.81	111.50
39	n	607	CHL	CHB-C4A-NA	3.39	129.20	124.51
39	SS	308	CHL	C4A-NA-C1A	3.39	108.23	106.71
32	r	603	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
32	s	609	CLA	C4A-NA-C1A	3.39	108.23	106.71
34	CC	516	BCR	C1-C6-C5	-3.39	117.84	122.61
32	B	619	CLA	C4A-NA-C1A	3.39	108.23	106.71
34	C	516	BCR	C36-C18-C19	3.39	123.41	118.08
32	33	603	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
39	N	609	CHL	C4A-NA-C1A	3.38	108.23	106.71
32	N	602	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
32	33	609	CLA	C4A-NA-C1A	3.38	108.23	106.71
34	d	403	BCR	C38-C26-C27	3.38	120.11	113.62
34	XX	202	BCR	C4-C5-C6	-3.38	117.83	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Bb	612	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
39	1	601	CHL	C4A-NA-C1A	3.37	108.22	106.71
34	B	613	BCR	C37-C22-C23	3.37	123.39	118.08
39	44	605	CHL	C4A-NA-C1A	3.37	108.22	106.71
34	B	616	BCR	C29-C30-C25	3.37	115.67	110.48
39	y	309	CHL	CMB-C2B-C3B	3.37	130.98	124.68
39	g	609	CHL	C4A-NA-C1A	3.36	108.22	106.71
32	Bb	613	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
32	2	609	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
32	Nn	313	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
32	a	410	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
34	Dd	403	BCR	C38-C26-C27	3.36	120.07	113.62
39	1	605	CHL	O2D-CGD-O1D	-3.36	117.27	123.84
39	2	605	CHL	CMB-C2B-C3B	3.36	130.96	124.68
39	n	605	CHL	O2D-CGD-O1D	-3.36	117.28	123.84
41	Rr	615	XAT	C19-C9-C8	3.36	123.36	118.08
40	s	614	LUT	C1-C6-C5	-3.35	117.89	122.61
32	C	510	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
32	1	612	CLA	CBD-CHA-C1A	3.35	132.45	128.50
32	n	602	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
32	CC	513	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
39	N	606	CHL	C4A-NA-C1A	3.35	108.21	106.71
39	s	606	CHL	C4A-NA-C1A	3.35	108.21	106.71
34	Cc	518	BCR	C33-C5-C6	-3.35	120.77	124.53
34	h	101	BCR	C36-C18-C17	-3.35	118.23	122.92
41	RR	316	XAT	C40-C33-C32	3.35	123.35	118.08
32	2	602	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
32	1	610	CLA	C4A-NA-C1A	3.35	108.21	106.71
34	Cc	518	BCR	C37-C22-C23	3.35	123.35	118.08
32	y	314	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
32	Bb	603	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
34	Bb	619	BCR	C36-C18-C17	-3.35	118.24	122.92
40	R	615	LUT	C1-C6-C5	-3.35	117.90	122.61
39	y	307	CHL	O2D-CGD-O1D	-3.35	117.30	123.84
39	3	607	CHL	CMB-C2B-C3B	3.35	130.94	124.68
42	RR	317	NEX	C20-C13-C12	3.34	123.35	118.08
32	DD	403	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
35	AA	410	PL9	C15-C14-C16	-3.34	109.65	115.27
39	Ss	601	CHL	C4A-NA-C1A	3.34	108.21	106.71
39	SS	302	CHL	C4A-NA-C1A	3.34	108.21	106.71
39	22	605	CHL	CMB-C2B-C3B	3.34	130.93	124.68
32	BB	614	CLA	CMB-C2B-C1B	-3.34	123.33	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	312	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
32	N	613	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
34	CC	515	BCR	C38-C26-C27	3.34	120.03	113.62
32	NN	602	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
41	y	301	XAT	C38-C25-C26	-3.34	116.67	122.26
32	33	611	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
42	Rr	616	NEX	C28-C29-C30	3.33	124.06	118.94
32	CC	509	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
34	Cc	518	BCR	C36-C18-C19	3.33	123.32	118.08
34	B	612	BCR	C1-C6-C5	-3.33	117.92	122.61
36	BB	622	LHG	O7-C7-C8	3.33	118.67	111.50
32	RR	309	CLA	C4A-NA-C1A	3.33	108.20	106.71
42	NN	618	NEX	O24-C25-C38	3.33	119.04	115.06
32	N	603	CLA	CMB-C2B-C3B	3.33	130.90	124.68
32	3	604	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
37	AA	412	SQD	O48-C23-C24	3.32	120.10	111.38
32	11	611	CLA	CMB-C2B-C3B	3.32	130.89	124.68
32	BB	601	CLA	C4A-NA-C1A	3.32	108.20	106.71
39	1	607	CHL	CMB-C2B-C3B	3.32	130.89	124.68
32	Rr	611	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
32	2	604	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
34	h	101	BCR	C36-C18-C19	3.32	123.30	118.08
34	d	403	BCR	C37-C22-C23	3.32	123.30	118.08
32	SS	311	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
32	CC	505	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
39	1	606	CHL	C4A-NA-C1A	3.31	108.20	106.71
41	G	617	XAT	O24-C25-C38	3.31	119.03	115.06
37	AA	412	SQD	O47-C7-C8	3.31	118.64	111.50
32	Cc	507	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
32	DD	403	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
34	A	409	BCR	C1-C6-C5	-3.31	117.95	122.61
34	B	613	BCR	C30-C25-C26	-3.31	117.95	122.61
36	YY	618	LHG	O7-C7-C8	3.31	118.63	111.50
39	Ss	606	CHL	C1B-CHB-C4A	-3.31	123.57	130.12
32	D	404	CLA	CMB-C2B-C3B	3.31	130.87	124.68
34	B	614	BCR	C30-C25-C26	-3.31	117.96	122.61
32	Bb	601	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
34	K	102	BCR	C34-C9-C8	3.30	123.28	118.08
32	C	505	CLA	C4-C3-C5	3.30	120.83	115.27
39	NN	607	CHL	CHB-C4A-NA	3.30	129.08	124.51
32	b	613	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
32	CC	514	CLA	CMB-C2B-C3B	3.30	130.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Cc	515	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
32	n	602	CLA	C4A-NA-C1A	3.30	108.19	106.71
34	Bb	619	BCR	C37-C22-C23	3.30	123.28	118.08
32	BB	605	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
34	Kk	101	BCR	C38-C26-C25	-3.30	120.82	124.53
36	d	405	LHG	O7-C7-C8	3.30	118.61	111.50
34	k	101	BCR	C38-C26-C25	-3.30	120.83	124.53
32	33	609	CLA	CBD-CHA-C1A	3.30	132.39	128.50
32	C	510	CLA	CMB-C2B-C3B	3.30	130.85	124.68
40	n	616	LUT	C3-C4-C5	-3.29	105.29	111.85
34	B	616	BCR	C36-C18-C19	3.29	123.27	118.08
32	Yy	612	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
32	BB	607	CLA	CMB-C2B-C3B	3.29	130.84	124.68
32	1	609	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
39	Nn	317	CHL	CHB-C4A-NA	3.29	129.07	124.51
32	S	603	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
32	Cc	512	CLA	CMB-C2B-C3B	3.29	130.84	124.68
39	3	606	CHL	C4A-NA-C1A	3.29	108.19	106.71
39	y	311	CHL	C4A-NA-C1A	3.29	108.19	106.71
42	Y	617	NEX	O24-C25-C38	3.29	119.00	115.06
32	AA	406	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
39	RR	305	CHL	C1B-CHB-C4A	-3.29	123.60	130.12
32	2	603	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
39	GG	609	CHL	C4A-NA-C1A	3.29	108.18	106.71
39	4	309	CHL	C4A-NA-C1A	3.29	108.18	106.71
42	N	618	NEX	O24-C25-C38	3.28	118.99	115.06
32	Cc	515	CLA	CMB-C2B-C3B	3.28	130.82	124.68
39	44	608	CHL	C1B-CHB-C4A	-3.28	123.62	130.12
32	RR	314	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
34	Kk	101	BCR	C37-C22-C23	3.28	123.25	118.08
32	G	614	CLA	C4A-NA-C1A	3.28	108.18	106.71
32	SS	310	CLA	C4A-NA-C1A	3.28	108.18	106.71
32	11	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
39	s	606	CHL	C1B-CHB-C4A	-3.28	123.63	130.12
39	RR	307	CHL	CMB-C2B-C3B	3.27	130.81	124.68
32	Rr	608	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
34	TT	101	BCR	C33-C5-C4	3.27	119.91	113.62
40	GG	615	LUT	C3-C4-C5	-3.27	105.33	111.85
32	YY	604	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
34	K	102	BCR	C1-C6-C5	-3.27	118.00	122.61
32	BB	610	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
32	Nn	301	CLA	C1B-CHB-C4A	-3.27	123.64	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	507	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
32	BB	610	CLA	CMB-C2B-C3B	3.27	130.79	124.68
32	SS	305	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
32	RR	309	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
32	b	602	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
34	C	516	BCR	C38-C26-C27	3.27	119.89	113.62
40	NN	616	LUT	C36-C21-C26	3.27	114.49	109.55
40	s	614	LUT	C1-C6-C7	3.27	125.02	115.78
32	Gg	303	CLA	C1D-ND-C4D	-3.27	104.02	106.33
36	Dd	407	LHG	O7-C7-C8	3.26	118.54	111.50
41	y	302	XAT	C39-C29-C28	3.26	123.21	118.08
32	Nn	301	CLA	C4A-NA-C1A	3.26	108.17	106.71
32	a	406	CLA	CHD-C1D-ND	-3.26	121.46	124.45
34	Aa	411	BCR	C36-C18-C19	3.25	123.20	118.08
39	Yy	607	CHL	CHB-C4A-NA	3.25	129.01	124.51
32	2	612	CLA	CBD-CHA-C1A	3.25	132.33	128.50
39	44	606	CHL	C4A-NA-C1A	3.25	108.17	106.71
39	r	605	CHL	C4A-NA-C1A	3.25	108.17	106.71
39	Gg	309	CHL	C4A-NA-C1A	3.25	108.17	106.71
34	Cc	517	BCR	C38-C26-C27	3.25	119.86	113.62
34	CC	515	BCR	C36-C18-C19	3.25	123.20	118.08
32	Yy	614	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
34	b	617	BCR	C37-C22-C23	3.25	123.20	118.08
42	Gg	318	NEX	C35-C15-C14	-3.25	116.82	123.47
32	22	609	CLA	CMB-C2B-C3B	3.25	130.75	124.68
34	B	616	BCR	C37-C22-C23	3.25	123.19	118.08
32	BB	613	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
32	Cc	509	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
34	BB	620	BCR	C29-C30-C25	3.24	115.47	110.48
32	n	603	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
32	B	622	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
32	Ss	611	CLA	CMB-C2B-C3B	3.24	130.75	124.68
40	R	615	LUT	C3-C4-C5	-3.24	105.40	111.85
32	22	610	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
32	y	314	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
32	A	406	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
40	Yy	615	LUT	C18-C5-C4	3.24	120.35	114.36
32	Gg	304	CLA	C4A-NA-C1A	3.24	108.16	106.71
39	G	609	CHL	C4A-NA-C1A	3.24	108.16	106.71
34	Kk	101	BCR	C3-C4-C5	-3.24	108.30	114.08
41	GG	617	XAT	O24-C25-C38	3.23	118.93	115.06
32	Bb	604	CLA	CMB-C2B-C1B	-3.23	123.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	605	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
34	Hh	101	BCR	C30-C25-C26	-3.23	118.06	122.61
44	CC	522	DGD	C2G-O2G-C1B	-3.23	109.84	117.79
32	Gg	315	CLA	C4A-NA-C1A	3.23	108.16	106.71
34	Dd	403	BCR	C37-C22-C23	3.23	123.16	118.08
32	X	201	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
32	BB	609	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
42	YY	617	NEX	C26-C27-C28	-3.23	119.17	125.99
34	BB	617	BCR	C30-C25-C26	-3.22	118.07	122.61
40	4	313	LUT	C1-C6-C5	-3.22	118.07	122.61
32	NN	610	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
32	b	612	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
39	1	607	CHL	C4A-NA-C1A	3.22	108.16	106.71
32	Bb	609	CLA	CMB-C2B-C3B	3.22	130.71	124.68
32	y	305	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
32	BB	607	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
32	Yy	612	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
32	4	305	CLA	CMB-C2B-C3B	3.22	130.70	124.68
32	n	610	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
34	b	619	BCR	C36-C18-C17	-3.21	118.42	122.92
32	BB	601	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
37	A	412	SQD	O48-C23-C24	3.21	119.80	111.38
32	SS	304	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
32	Yy	612	CLA	C4A-NA-C1A	3.21	108.15	106.71
34	AA	409	BCR	C1-C6-C5	-3.21	118.09	122.61
32	NN	603	CLA	CMB-C2B-C3B	3.21	130.68	124.68
32	n	613	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
32	GG	610	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
42	R	617	NEX	C28-C29-C30	3.20	123.86	118.94
32	A	408	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
42	Y	619	NEX	C2-C1-C6	3.20	112.33	109.21
32	GG	612	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
32	y	316	CLA	C4A-NA-C1A	3.20	108.15	106.71
32	B	618	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
39	n	601	CHL	CHB-C4A-NA	3.20	128.94	124.51
32	g	612	CLA	C4A-NA-C1A	3.20	108.14	106.71
39	R	607	CHL	CMB-C2B-C3B	3.20	130.67	124.68
40	Ss	614	LUT	C35-C15-C14	-3.20	116.92	123.47
32	Bb	610	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
41	Nn	308	XAT	C39-C29-C28	3.20	123.12	118.08
32	SS	310	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
32	44	615	CLA	CMB-C2B-C3B	3.20	130.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	610	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
32	Y	610	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
34	BB	620	BCR	C37-C22-C23	3.20	123.11	118.08
34	C	517	BCR	C1-C6-C5	-3.20	118.11	122.61
40	s	614	LUT	C35-C15-C14	-3.20	116.93	123.47
39	n	605	CHL	C1B-CHB-C4A	-3.19	123.79	130.12
42	YY	617	NEX	C28-C29-C30	3.19	123.84	118.94
32	AA	408	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
32	s	608	CLA	CMB-C2B-C3B	3.19	130.65	124.68
40	22	614	LUT	C3-C4-C5	-3.19	105.50	111.85
32	S	608	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
32	C	514	CLA	CMB-C2B-C3B	3.19	130.65	124.68
39	11	606	CHL	C4A-NA-C1A	3.19	108.14	106.71
42	R	617	NEX	C20-C13-C12	3.19	123.10	118.08
32	Y	603	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
39	GG	601	CHL	C4A-NA-C1A	3.19	108.14	106.71
39	Nn	317	CHL	C1-C2-C3	-3.19	120.53	126.04
32	B	624	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
39	S	607	CHL	C4A-NA-C1A	3.19	108.14	106.71
34	a	411	BCR	C36-C18-C19	3.19	123.10	118.08
36	Dd	405	LHG	O7-C7-C8	3.19	118.37	111.50
32	D	404	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
32	d	402	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
34	BB	617	BCR	C36-C18-C17	-3.18	118.47	122.92
32	Aa	406	CLA	CHD-C1D-ND	-3.18	121.53	124.45
32	Ss	608	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
32	Dd	402	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
32	b	610	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
39	r	606	CHL	C1B-CHB-C4A	-3.18	123.82	130.12
42	Y	619	NEX	C28-C29-C30	3.18	123.82	118.94
44	CC	522	DGD	O3G-C1D-C2D	3.18	113.27	108.30
40	44	612	LUT	C1-C6-C5	-3.18	118.14	122.61
32	B	606	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
32	Aa	407	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
39	3	601	CHL	C1B-CHB-C4A	-3.18	123.82	130.12
32	D	404	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
32	33	613	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
41	y	301	XAT	C19-C9-C8	3.17	123.08	118.08
32	r	601	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
41	NN	617	XAT	C20-C13-C12	3.17	123.08	118.08
32	Rr	609	CLA	CMB-C2B-C3B	3.17	130.61	124.68
32	1	610	CLA	CMB-C2B-C1B	-3.17	123.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	r	602	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
34	H	101	BCR	C29-C30-C25	3.17	115.36	110.48
40	YY	615	LUT	C18-C5-C4	3.17	120.23	114.36
32	Y	614	CLA	C4A-NA-C1A	3.17	108.13	106.71
32	b	609	CLA	CMB-C2B-C3B	3.17	130.61	124.68
32	3	610	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
34	BB	616	BCR	C38-C26-C27	3.17	119.70	113.62
32	B	622	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
32	a	406	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
32	y	316	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
41	Nn	308	XAT	C38-C25-C26	-3.17	116.96	122.26
32	B	610	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
36	SS	301	LHG	O7-C7-C8	3.16	119.62	110.80
39	r	607	CHL	C4A-NA-C1A	3.16	108.13	106.71
32	2	602	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
32	Gg	311	CLA	CMB-C2B-C3B	3.16	130.59	124.68
34	B	613	BCR	C36-C18-C17	-3.16	118.50	122.92
32	1	609	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
34	Cc	517	BCR	C33-C5-C4	3.16	119.69	113.62
32	g	612	CLA	CMB-C2B-C3B	3.16	130.59	124.68
34	c	515	BCR	C33-C5-C4	3.16	119.68	113.62
32	R	601	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
32	n	612	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
39	11	608	CHL	C1B-CHB-C4A	-3.16	123.87	130.12
32	1	603	CLA	C4A-NA-C1A	3.16	108.12	106.71
32	GG	603	CLA	C4A-NA-C1A	3.16	108.12	106.71
32	GG	603	CLA	C1B-CHB-C4A	-3.16	123.87	130.12
42	Y	617	NEX	C28-C29-C30	3.16	123.78	118.94
42	RR	317	NEX	C26-C27-C28	-3.15	119.33	125.99
39	Ss	606	CHL	C4A-NA-C1A	3.15	108.12	106.71
32	Nn	304	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
41	r	615	XAT	C39-C29-C28	3.15	123.04	118.08
34	TT	101	BCR	C38-C26-C25	-3.15	120.99	124.53
39	NN	605	CHL	O2D-CGD-O1D	-3.15	117.68	123.84
32	Dd	401	CLA	CMB-C2B-C3B	3.15	130.57	124.68
32	b	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
34	b	619	BCR	C37-C22-C23	3.15	123.04	118.08
32	s	611	CLA	CMB-C2B-C3B	3.15	130.56	124.68
39	G	607	CHL	CHB-C4A-NA	3.15	128.86	124.51
32	1	602	CLA	CMB-C2B-C3B	3.15	130.56	124.68
41	y	302	XAT	C25-C24-C23	3.14	118.97	112.75
41	44	613	XAT	C26-C27-C28	-3.14	119.34	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	11	604	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
34	Bb	619	BCR	C40-C30-C25	-3.14	105.20	110.30
32	B	604	CLA	CMB-C2B-C3B	3.14	130.56	124.68
39	44	605	CHL	CHB-C4A-NA	3.14	128.86	124.51
41	g	619	XAT	C38-C25-C26	-3.14	117.00	122.26
32	33	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
32	Yy	610	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
32	N	612	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
32	YY	610	CLA	C4A-NA-C1A	3.14	108.12	106.71
34	Dd	403	BCR	C28-C27-C26	-3.14	108.47	114.08
41	Gg	301	XAT	C38-C25-C26	-3.14	117.00	122.26
32	AA	406	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
32	YY	612	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
32	Gg	311	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
32	1	604	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
34	d	403	BCR	C28-C27-C26	-3.14	108.47	114.08
34	Bb	617	BCR	C37-C22-C23	3.14	123.02	118.08
32	GG	610	CLA	C4A-NA-C1A	3.14	108.12	106.71
39	Nn	311	CHL	CHB-C4A-NA	3.14	128.85	124.51
32	G	610	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
39	N	609	CHL	C1B-CHB-C4A	-3.13	123.91	130.12
36	A	414	LHG	O7-C7-C8	3.13	118.25	111.50
39	RR	306	CHL	C1B-CHB-C4A	-3.13	123.91	130.12
40	22	614	LUT	C38-C25-C24	-3.13	116.86	123.56
32	RR	311	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
32	BB	607	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
32	g	602	CLA	CHD-C1D-ND	-3.13	121.58	124.45
39	Nn	315	CHL	CHB-C4A-NA	3.13	128.84	124.51
32	4	310	CLA	C4A-NA-C1A	3.13	108.11	106.71
32	YY	612	CLA	C2A-C1A-CHA	3.13	129.33	123.86
32	CC	512	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
32	CC	502	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
41	Rr	615	XAT	C6-C7-C8	-3.13	119.38	125.99
39	y	307	CHL	CHB-C4A-NA	3.13	128.84	124.51
32	Bb	603	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
32	R	608	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
32	22	609	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
34	H	101	BCR	C2-C1-C6	3.12	115.29	110.48
34	CC	515	BCR	C27-C26-C25	-3.12	118.20	122.73
32	BB	604	CLA	C4A-NA-C1A	3.12	108.11	106.71
39	33	606	CHL	C4A-NA-C1A	3.12	108.11	106.71
32	s	602	CLA	C1B-CHB-C4A	-3.12	123.94	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	YY	614	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
32	1	612	CLA	CMB-C2B-C3B	3.12	130.51	124.68
39	11	607	CHL	CBD-CHA-C1A	3.12	132.17	128.50
39	R	605	CHL	C2A-C3A-C4A	-3.12	96.83	101.87
32	g	603	CLA	C4A-NA-C1A	3.12	108.11	106.71
42	Gg	318	NEX	C26-C27-C28	3.11	132.58	125.99
34	C	516	BCR	C38-C26-C25	-3.11	121.03	124.53
32	Bb	611	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
42	NN	618	NEX	C28-C29-C30	3.11	123.72	118.94
36	EE	101	LHG	O7-C7-C8	3.11	118.20	111.50
39	GG	606	CHL	C4A-NA-C1A	3.11	108.10	106.71
32	b	611	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
32	c	508	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
39	Gg	310	CHL	C1B-CHB-C4A	-3.11	123.96	130.12
32	B	606	CLA	CMB-C2B-C3B	3.11	130.49	124.68
39	Yy	605	CHL	CHB-C4A-NA	3.11	128.81	124.51
39	11	605	CHL	C1B-CHB-C4A	-3.11	123.96	130.12
32	NN	612	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
32	3	611	CLA	C4A-NA-C1A	3.11	108.10	106.71
37	A	412	SQD	O47-C7-C8	3.11	118.20	111.50
42	Rr	616	NEX	C26-C27-C28	-3.11	119.43	125.99
32	b	614	CLA	CMB-C2B-C3B	3.10	130.49	124.68
32	CC	509	CLA	CMB-C2B-C3B	3.10	130.49	124.68
34	Bb	617	BCR	C27-C26-C25	-3.10	118.22	122.73
32	g	614	CLA	C4A-NA-C1A	3.10	108.10	106.71
32	C	513	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
32	N	612	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
32	BB	605	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
32	d	401	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
32	BB	602	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
32	c	513	CLA	CMB-C2B-C3B	3.10	130.48	124.68
34	Bb	617	BCR	C33-C5-C4	3.10	119.57	113.62
32	22	602	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
32	G	603	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
39	Y	605	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
39	33	607	CHL	C4A-NA-C1A	3.10	108.10	106.71
32	S	608	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
32	CC	502	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
34	b	617	BCR	C15-C16-C17	-3.10	117.13	123.47
34	k	101	BCR	C30-C25-C26	-3.10	118.25	122.61
32	c	512	CLA	CMB-C2B-C3B	3.10	130.47	124.68
34	b	619	BCR	C1-C6-C5	-3.10	118.25	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	609	CLA	C1B-CHB-C4A	-3.10	123.99	130.12
32	B	620	CLA	CMB-C2B-C1B	-3.10	123.71	128.46
34	H	101	BCR	C32-C1-C6	-3.10	105.28	110.30
34	BB	618	BCR	C38-C26-C25	-3.10	121.05	124.53
32	4	303	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
34	h	101	BCR	C35-C13-C12	3.10	122.95	118.08
32	Aa	406	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
36	0	201	LHG	O7-C7-C8	3.09	118.17	111.50
32	33	602	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
40	Yy	615	LUT	C36-C21-C26	3.09	114.23	109.55
32	B	620	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
32	Bb	602	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
39	G	608	CHL	O2D-CGD-O1D	-3.09	117.79	123.84
40	NN	616	LUT	C22-C23-C24	-3.09	108.22	111.74
40	Ss	614	LUT	C1-C6-C7	3.09	124.53	115.78
42	g	617	NEX	C17-C1-C6	-3.09	107.70	110.47
42	R	617	NEX	C26-C27-C28	-3.09	119.46	125.99
39	Ss	606	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
34	B	616	BCR	C27-C26-C25	-3.09	118.25	122.73
32	C	507	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
34	Bb	619	BCR	C1-C6-C5	-3.09	118.27	122.61
32	Bb	610	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
32	4	310	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
39	r	605	CHL	CHB-C4A-NA	3.08	128.78	124.51
32	Dd	401	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
32	a	407	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
41	4	314	XAT	C26-C27-C28	-3.08	119.47	125.99
39	2	607	CHL	C4A-NA-C1A	3.08	108.09	106.71
32	Y	614	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
32	BB	604	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
44	c	517	DGD	O1G-C1A-C2A	3.08	121.58	111.91
32	BB	615	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
32	b	604	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
32	2	602	CLA	C4A-NA-C1A	3.08	108.09	106.71
39	YY	601	CHL	C4A-NA-C1A	3.08	108.09	106.71
40	Yy	615	LUT	C1-C6-C7	3.08	124.49	115.78
32	b	608	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
40	SS	315	LUT	C3-C4-C5	-3.08	105.72	111.85
34	Bb	617	BCR	C40-C30-C25	3.08	115.29	110.30
32	s	609	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
32	G	612	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
32	4	312	CLA	CMB-C2B-C1B	-3.08	123.74	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BB	602	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
40	Y	615	LUT	C18-C5-C4	3.07	120.05	114.36
34	B	614	BCR	C33-C5-C4	3.07	119.52	113.62
34	h	101	BCR	C38-C26-C25	-3.07	121.08	124.53
32	c	502	CLA	CMB-C2B-C3B	3.07	130.43	124.68
42	Y	619	NEX	C26-C27-C28	-3.07	119.50	125.99
32	Rr	613	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
32	22	613	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
32	c	502	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
32	Cc	504	CLA	CMB-C2B-C3B	3.07	130.42	124.68
44	Cc	519	DGD	O1G-C1A-C2A	3.07	121.54	111.91
32	11	610	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
41	Rr	615	XAT	C26-C27-C28	-3.07	119.51	125.99
32	d	401	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
32	BB	603	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
39	2	605	CHL	C4A-NA-C1A	3.06	108.08	106.71
32	Yy	603	CLA	CMB-C2B-C3B	3.06	130.41	124.68
32	Cc	514	CLA	CMB-C2B-C3B	3.06	130.41	124.68
32	b	608	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
41	Nn	308	XAT	C19-C9-C8	3.06	122.90	118.08
32	NN	614	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
36	22	615	LHG	O7-C7-C8	3.06	118.09	111.50
32	c	506	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
37	BB	621	SQD	O8-S-O7	3.06	118.75	111.27
32	B	624	CLA	CMB-C2B-C3B	3.06	130.40	124.68
32	2	609	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
32	s	609	CLA	CMB-C2B-C3B	3.06	130.40	124.68
32	YY	603	CLA	CMB-C2B-C3B	3.06	130.40	124.68
34	T	101	BCR	C37-C22-C23	3.06	122.89	118.08
32	CC	513	CLA	CMB-C2B-C3B	3.06	130.40	124.68
39	Ss	601	CHL	CHB-C4A-NA	3.06	128.74	124.51
41	g	619	XAT	C6-C7-C8	-3.05	119.53	125.99
44	D	411	DGD	O1G-C1A-C2A	3.05	121.49	111.91
32	RR	302	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
32	1	609	CLA	C4A-NA-C1A	3.05	108.08	106.71
32	DD	401	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
32	R	612	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
44	B	603	DGD	O1G-C1A-C2A	3.05	121.49	111.91
39	Rr	605	CHL	C4A-NA-C1A	3.05	108.08	106.71
32	11	602	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
32	g	611	CLA	CMB-C2B-C3B	3.05	130.39	124.68
42	RR	317	NEX	C28-C29-C30	3.05	123.62	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Ss	609	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
32	Cc	513	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
40	Yy	615	LUT	C17-C1-C6	-3.05	105.35	110.30
32	g	613	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
39	Rr	606	CHL	C4A-NA-C1A	3.05	108.08	106.71
32	Cc	510	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
32	c	505	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
32	Dd	401	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
39	Y	605	CHL	CHB-C4A-NA	3.05	128.73	124.51
32	Bb	615	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
42	Y	617	NEX	C26-C27-C28	-3.05	119.55	125.99
32	CC	503	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
32	11	609	CLA	CBD-CHA-C1A	3.04	132.09	128.50
35	D	407	PL9	C20-C19-C21	-3.04	110.15	115.27
32	N	614	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
39	NN	609	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
32	Ss	611	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
32	CC	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
32	b	603	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
32	Cc	508	CLA	CMB-C2B-C3B	3.04	130.37	124.68
32	3	609	CLA	C1D-ND-C4D	-3.04	104.17	106.33
32	Rr	609	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
32	r	613	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
32	YY	610	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
32	Cc	504	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
42	y	319	NEX	C28-C29-C30	3.04	123.60	118.94
40	Nn	307	LUT	C3-C4-C5	-3.04	105.80	111.85
34	CC	516	BCR	C38-C26-C27	3.04	119.45	113.62
32	R	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
32	b	608	CLA	CMB-C2B-C3B	3.04	130.36	124.68
32	s	609	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
32	RR	312	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
32	R	611	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
32	D	401	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
39	G	606	CHL	C4A-NA-C1A	3.03	108.07	106.71
32	44	611	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
32	R	602	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
41	44	613	XAT	O24-C25-C38	3.03	118.69	115.06
32	B	611	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
32	g	610	CLA	C4A-NA-C1A	3.03	108.07	106.71
34	A	409	BCR	C36-C18-C19	3.03	122.85	118.08
41	Gg	301	XAT	C6-C7-C8	-3.03	119.58	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	604	CLA	O2D-CGD-CBD	3.03	116.65	111.27
32	g	614	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
39	2	601	CHL	CBD-CHA-C1A	3.03	132.07	128.50
32	CC	509	CLA	O2D-CGD-CBD	3.03	116.65	111.27
32	CC	503	CLA	CBA-CAA-C2A	3.03	122.80	113.86
32	Rr	610	CLA	CMB-C2B-C3B	3.03	130.34	124.68
32	b	601	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
32	Rr	602	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
35	DD	406	PL9	C20-C19-C21	-3.03	110.18	115.27
42	N	618	NEX	C28-C29-C30	3.03	123.58	118.94
32	11	603	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
39	GG	609	CHL	O2D-CGD-O1D	-3.02	117.92	123.84
39	s	606	CHL	O2D-CGD-O1D	-3.02	117.92	123.84
32	C	510	CLA	O2D-CGD-CBD	3.02	116.64	111.27
34	C	517	BCR	C38-C26-C27	3.02	119.42	113.62
42	g	617	NEX	C28-C29-C30	3.02	123.58	118.94
32	Rr	604	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
34	D	406	BCR	C33-C5-C6	-3.02	121.13	124.53
41	g	619	XAT	C20-C13-C12	3.02	122.84	118.08
32	r	604	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
39	2	601	CHL	C4A-NA-C1A	3.02	108.06	106.71
32	SS	312	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
32	c	505	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
32	B	621	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
32	B	609	CLA	CMB-C2B-C3B	3.02	130.33	124.68
32	33	603	CLA	CMB-C2B-C3B	3.02	130.32	124.68
32	Bb	608	CLA	CMB-C2B-C3B	3.02	130.32	124.68
34	T	101	BCR	C38-C26-C25	-3.02	121.14	124.53
32	S	609	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
38	C	521	LMG	C8-O7-C10	-3.02	110.36	117.79
32	N	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
42	Y	619	NEX	C17-C1-C6	-3.02	107.77	110.47
32	Bb	612	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
32	Ss	603	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
39	NN	605	CHL	CHB-C4A-NA	3.01	128.68	124.51
32	Ss	609	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
36	Rr	617	LHG	O8-C23-C24	3.01	121.37	111.91
32	2	609	CLA	CMB-C2B-C3B	3.01	130.32	124.68
32	Gg	315	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
32	33	609	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
32	Gg	313	CLA	CHB-C4A-NA	3.01	128.68	124.51
37	B	617	SQD	O8-S-O7	3.01	118.63	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Gg	307	CHL	CHB-C4A-NA	3.01	128.68	124.51
34	DD	405	BCR	C33-C5-C6	-3.01	121.15	124.53
40	y	317	LUT	C36-C21-C26	3.01	114.11	109.55
32	C	507	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
32	Bb	608	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
34	D	406	BCR	C37-C22-C23	3.01	122.82	118.08
32	Ss	612	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
32	11	613	CLA	CBD-CHA-C1A	3.01	132.05	128.50
32	C	505	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
32	s	612	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
34	Bb	617	BCR	C15-C16-C17	-3.01	117.31	123.47
34	BB	620	BCR	C27-C26-C25	-3.01	118.36	122.73
32	C	505	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
40	Y	615	LUT	C2-C3-C4	-3.01	106.19	110.30
34	Kk	101	BCR	C33-C5-C4	3.01	119.39	113.62
32	44	609	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
34	B	616	BCR	C33-C5-C4	3.01	119.39	113.62
40	R	615	LUT	C17-C1-C6	-3.01	105.42	110.30
32	22	613	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
32	Cc	507	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
32	4	311	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
32	Rr	604	CLA	C4A-NA-C1A	3.01	108.06	106.71
39	NN	609	CHL	C4A-NA-C1A	3.01	108.06	106.71
32	c	501	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
32	B	624	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
32	Nn	312	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
32	S	603	CLA	CMB-C2B-C3B	3.00	130.30	124.68
32	3	611	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
32	Bb	615	CLA	CHB-C4A-NA	3.00	128.66	124.51
39	R	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
44	BB	625	DGD	O1G-C1A-C2A	3.00	121.33	111.91
32	r	611	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
32	NN	602	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
39	YY	605	CHL	C4A-NA-C1A	3.00	108.06	106.71
32	Aa	407	CLA	CMB-C2B-C3B	3.00	130.29	124.68
32	22	604	CLA	CBD-CHA-C1A	3.00	132.04	128.50
32	Y	614	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
32	CC	504	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
39	G	601	CHL	C4A-NA-C1A	3.00	108.05	106.71
32	B	604	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
32	22	602	CLA	CBD-CHA-C1A	3.00	132.03	128.50
39	22	601	CHL	CBD-CHA-C1A	3.00	132.03	128.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Rr	608	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
32	AA	406	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
32	B	607	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
32	Gg	311	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
34	K	102	BCR	C33-C5-C6	-2.99	121.17	124.53
36	AA	414	LHG	O7-C7-C8	2.99	117.95	111.50
32	11	604	CLA	O2D-CGD-CBD	2.99	116.59	111.27
32	33	613	CLA	CBD-CHA-C1A	2.99	132.03	128.50
39	g	601	CHL	CHB-C4A-NA	2.99	128.65	124.51
32	B	619	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
34	k	101	BCR	C36-C18-C19	2.99	122.79	118.08
34	BB	618	BCR	C33-C5-C4	2.99	119.36	113.62
39	1	606	CHL	O2D-CGD-O1D	-2.99	117.99	123.84
32	YY	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
32	A	406	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
32	Rr	602	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
41	Yy	619	XAT	C40-C33-C34	-2.99	118.73	122.92
39	NN	605	CHL	C1B-CHB-C4A	-2.99	124.20	130.12
36	CC	523	LHG	O8-C23-C24	2.99	121.29	111.91
39	Y	601	CHL	CHB-C4A-NA	2.99	128.65	124.51
32	r	609	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
39	1	607	CHL	CBD-CHA-C1A	2.99	132.02	128.50
34	AA	409	BCR	C36-C18-C19	2.99	122.78	118.08
42	Rr	616	NEX	C20-C13-C14	-2.99	118.74	122.92
32	s	611	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
32	r	604	CLA	C4A-NA-C1A	2.99	108.05	106.71
32	3	613	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
32	22	609	CLA	CBD-CHA-C1A	2.98	132.02	128.50
42	Y	619	NEX	C20-C13-C14	-2.98	118.74	122.92
42	Nn	309	NEX	C20-C13-C14	-2.98	118.74	122.92
39	y	308	CHL	CHB-C4A-NA	2.98	128.64	124.51
32	Nn	314	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
39	S	601	CHL	C4A-NA-C1A	2.98	108.05	106.71
39	GG	607	CHL	CHB-C4A-NA	2.98	128.64	124.51
33	A	407	PHO	O1D-CGD-CBD	2.98	129.71	124.74
39	SS	302	CHL	CHB-C4A-NA	2.98	128.63	124.51
32	BB	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
32	Y	612	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
40	2	614	LUT	C38-C25-C24	-2.98	117.18	123.56
39	s	607	CHL	C4A-NA-C1A	2.98	108.05	106.71
32	2	612	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
41	r	615	XAT	C19-C9-C8	2.98	122.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	608	CHL	CHB-C4A-NA	2.98	128.63	124.51
39	NN	608	CHL	CHB-C4A-NA	2.98	128.63	124.51
34	Cc	516	BCR	C1-C6-C5	-2.98	118.42	122.61
32	s	603	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
39	Y	608	CHL	CHB-C4A-NA	2.98	128.63	124.51
32	BB	611	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
41	GG	619	XAT	C38-C25-C26	-2.98	117.27	122.26
32	2	609	CLA	CBD-CHA-C1A	2.98	132.01	128.50
34	Kk	101	BCR	C36-C18-C19	2.98	122.77	118.08
39	Y	606	CHL	C4A-NA-C1A	2.98	108.04	106.71
42	Yy	617	NEX	C40-C33-C32	2.98	122.77	118.08
32	SS	309	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
41	r	615	XAT	C26-C27-C28	-2.97	119.70	125.99
42	Yy	617	NEX	C28-C29-C30	2.97	123.51	118.94
40	Yy	616	LUT	C3-C4-C5	-2.97	105.93	111.85
42	Gg	318	NEX	C39-C29-C28	2.97	122.76	118.08
32	c	513	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
39	GG	609	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
32	n	612	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
32	n	604	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
32	BB	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
41	GG	617	XAT	C6-C7-C8	-2.97	119.71	125.99
32	C	514	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
39	g	606	CHL	CHB-C4A-NA	2.97	128.62	124.51
32	G	613	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
32	RR	308	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
39	33	608	CHL	C1B-CHB-C4A	-2.97	124.24	130.12
32	s	610	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
32	b	601	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
32	c	501	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
33	AA	407	PHO	O1D-CGD-CBD	2.96	129.68	124.74
32	Nn	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
42	n	617	NEX	C15-C35-C34	-2.96	117.40	123.47
32	Yy	614	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
39	Nn	318	CHL	CHB-C4A-NA	2.96	128.61	124.51
32	C	515	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
39	4	308	CHL	C1B-CHB-C4A	-2.96	124.25	130.12
39	N	609	CHL	CMB-C2B-C3B	2.96	130.22	124.68
32	S	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
32	1	613	CLA	CBD-CHA-C1A	2.96	131.99	128.50
32	c	507	CLA	CMB-C2B-C3B	2.96	130.21	124.68
32	CC	511	CLA	O2D-CGD-O1D	-2.96	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Bb	601	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
40	Ss	615	LUT	C35-C15-C14	-2.96	117.42	123.47
39	g	609	CHL	C1B-CHB-C4A	-2.96	124.26	130.12
32	y	316	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
32	YY	614	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
32	b	615	CLA	CHB-C4A-NA	2.96	128.60	124.51
32	S	608	CLA	C4A-NA-C1A	2.96	108.03	106.71
32	S	602	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
41	GG	617	XAT	C40-C33-C32	2.96	122.73	118.08
32	33	604	CLA	CMB-C2B-C3B	2.96	130.21	124.68
36	AA	411	LHG	C5-O7-C7	-2.95	110.52	117.79
40	y	318	LUT	C36-C21-C26	2.95	114.02	109.55
44	B	601	DGD	C2G-O2G-C1B	-2.95	110.52	117.79
32	44	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
39	44	605	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
32	G	610	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
39	1	605	CHL	C1B-CHB-C4A	-2.95	124.27	130.12
32	2	610	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
32	Gg	315	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
32	G	603	CLA	C4A-NA-C1A	2.95	108.03	106.71
42	n	617	NEX	C28-C29-C30	2.95	123.47	118.94
32	G	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
32	Y	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
37	L	101	SQD	O48-C23-C24	2.95	121.17	111.91
39	y	311	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
32	44	610	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
32	Bb	614	CLA	CMB-C2B-C3B	2.95	130.20	124.68
32	Yy	611	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
32	11	609	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
32	1	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
32	BB	606	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
32	11	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
32	4	303	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
32	Ss	611	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
32	Yy	613	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
38	a	412	LMG	O8-C28-C29	2.95	121.16	111.91
32	C	504	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
41	y	301	XAT	C36-C21-C22	-2.95	103.86	108.98
32	Cc	509	CLA	CMB-C2B-C3B	2.95	130.19	124.68
32	Yy	604	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
32	b	610	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
39	RR	307	CHL	CHB-C4A-NA	2.95	128.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	604	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
32	2	602	CLA	CHD-C1D-ND	-2.95	121.75	124.45
32	b	602	CLA	C4A-NA-C1A	2.94	108.03	106.71
32	SS	310	CLA	C1B-CHB-C4A	-2.94	124.28	130.12
32	g	612	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
32	B	619	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
39	Yy	609	CHL	C1B-CHB-C4A	-2.94	124.29	130.12
41	N	617	XAT	O24-C25-C38	2.94	118.58	115.06
41	g	619	XAT	O4-C5-C18	2.94	118.58	115.06
32	Nn	302	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
39	YY	608	CHL	CHB-C4A-NA	2.94	128.58	124.51
44	c	517	DGD	C2G-O2G-C1B	-2.94	110.55	117.79
32	Yy	610	CLA	CMB-C2B-C3B	2.94	130.18	124.68
32	R	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
39	S	601	CHL	CHB-C4A-NA	2.94	128.58	124.51
36	A	413	LHG	O8-C23-C24	2.94	121.14	111.91
32	33	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
32	r	613	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
32	SS	304	CLA	CMB-C2B-C3B	2.94	130.18	124.68
32	Cc	514	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
32	Ss	610	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
32	33	604	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
39	44	607	CHL	O2D-CGD-O1D	-2.94	118.09	123.84
39	Yy	606	CHL	CHB-C4A-NA	2.94	128.58	124.51
42	g	617	NEX	C37-C21-C36	-2.94	103.03	107.37
32	Ss	602	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
32	Ss	604	CLA	CMB-C2B-C3B	2.94	130.18	124.68
32	CC	513	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
34	K	102	BCR	C16-C15-C14	-2.94	117.45	123.47
32	SS	305	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
34	C	516	BCR	C31-C1-C6	2.94	115.06	110.30
39	11	606	CHL	O2D-CGD-O1D	-2.94	118.09	123.84
32	11	609	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
39	R	605	CHL	CAA-C2A-C1A	-2.94	102.35	111.97
32	a	407	CLA	CMB-C2B-C3B	2.94	130.17	124.68
32	BB	614	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
41	G	619	XAT	C38-C25-C26	-2.93	117.34	122.26
32	S	611	CLA	CHB-C4A-NA	2.93	128.57	124.51
41	Gg	301	XAT	O4-C5-C18	2.93	118.57	115.06
32	33	602	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
32	C	515	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
32	A	406	CLA	C1B-CHB-C4A	-2.93	124.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	506	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
34	B	616	BCR	C3-C4-C5	-2.93	108.84	114.08
37	LL	102	SQD	O48-C23-C24	2.93	121.11	111.91
32	11	603	CLA	CMB-C2B-C3B	2.93	130.16	124.68
42	Nn	309	NEX	C28-C29-C30	2.93	123.44	118.94
32	C	503	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
39	Rr	606	CHL	C1B-CHB-C4A	-2.93	124.31	130.12
32	3	609	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
40	s	615	LUT	C35-C15-C14	-2.93	117.47	123.47
32	C	503	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
34	XX	202	BCR	C32-C1-C6	2.93	115.05	110.30
32	22	609	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
32	r	612	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
37	L	102	SQD	O9-S-C6	2.93	110.42	106.94
32	Rr	613	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
32	N	614	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
32	SS	305	CLA	CMB-C2B-C3B	2.93	130.16	124.68
32	c	507	CLA	CHB-C4A-NA	2.93	128.56	124.51
32	BB	615	CLA	CMB-C2B-C3B	2.93	130.15	124.68
32	22	613	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
32	BB	614	CLA	CHB-C4A-NA	2.93	128.56	124.51
39	YY	601	CHL	CHB-C4A-NA	2.93	128.56	124.51
32	c	507	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
32	R	613	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
42	Rr	616	NEX	C17-C1-C6	-2.93	107.85	110.47
32	n	611	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
44	BB	624	DGD	O1G-C1A-C2A	2.92	121.09	111.91
32	Cc	510	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
32	r	608	CLA	CMB-C2B-C3B	2.92	130.15	124.68
32	BB	614	CLA	CMB-C2B-C3B	2.92	130.15	124.68
39	Gg	302	CHL	CHB-C4A-NA	2.92	128.55	124.51
32	SS	314	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
32	4	304	CLA	CHB-C4A-NA	2.92	128.55	124.51
32	22	613	CLA	CBD-CHA-C1A	2.92	131.94	128.50
32	2	604	CLA	CBD-CHA-C1A	2.92	131.94	128.50
32	N	613	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
32	33	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
35	d	404	PL9	C7-C3-C4	2.92	119.25	116.88
35	Dd	404	PL9	C7-C3-C4	2.92	119.25	116.88
32	g	611	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
34	c	516	BCR	C37-C22-C23	2.92	122.68	118.08
32	1	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	SS	312	CLA	CHB-C4A-NA	2.92	128.55	124.51
32	S	604	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
39	S	606	CHL	CHB-C4A-NA	2.92	128.55	124.51
32	n	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
41	r	615	XAT	C18-C5-C6	-2.92	117.37	122.26
32	1	612	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
34	Kk	101	BCR	C34-C9-C10	-2.92	118.84	122.92
32	r	604	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	4	310	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	CC	504	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	Bb	606	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	N	602	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
32	b	606	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	11	610	CLA	CBD-CHA-C1A	2.92	131.94	128.50
32	NN	611	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
39	22	606	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
32	Bb	604	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
41	Gg	301	XAT	C20-C13-C12	2.92	122.67	118.08
32	C	507	CLA	CMB-C2B-C1B	-2.91	123.98	128.46
35	Dd	404	PL9	C20-C19-C21	-2.91	110.37	115.27
32	3	613	CLA	CBD-CHA-C1A	2.91	131.94	128.50
32	b	614	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
32	B	618	CLA	CMB-C2B-C1B	-2.91	123.98	128.46
40	n	615	LUT	C2-C3-C4	-2.91	106.31	110.30
39	N	609	CHL	C2A-C1A-CHA	2.91	128.95	123.86
35	D	407	PL9	C40-C39-C41	-2.91	110.37	115.27
42	n	617	NEX	C20-C13-C14	-2.91	118.84	122.92
39	n	606	CHL	CHB-C4A-NA	2.91	128.54	124.51
32	3	604	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
32	b	615	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
32	Bb	614	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
39	3	605	CHL	C4A-NA-C1A	2.91	108.02	106.71
32	22	611	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
32	Cc	503	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	c	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	y	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	RR	302	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
32	Nn	302	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	RR	303	CLA	CHB-C4A-NA	2.91	128.53	124.51
39	N	605	CHL	CHB-C4A-NA	2.91	128.53	124.51
39	Nn	316	CHL	CHB-C4A-NA	2.91	128.53	124.51
32	N	611	CLA	CMB-C2B-C1B	-2.91	124.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Nn	309	NEX	C15-C35-C34	-2.91	117.52	123.47
39	22	605	CHL	C4A-NA-C1A	2.91	108.01	106.71
40	n	615	LUT	C17-C1-C6	-2.91	105.58	110.30
32	BB	605	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
32	3	603	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
32	CC	508	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
32	2	602	CLA	CMB-C2B-C3B	2.91	130.12	124.68
32	Bb	603	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
32	B	609	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
32	B	622	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
32	SS	303	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
32	3	602	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
32	b	612	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
32	Cc	507	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
32	C	510	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
39	N	609	CHL	O2D-CGD-O1D	-2.90	118.16	123.84
39	33	601	CHL	C1B-CHB-C4A	-2.90	124.37	130.12
44	B	601	DGD	O1G-C1A-C2A	2.90	121.02	111.91
40	R	615	LUT	C19-C9-C8	2.90	122.65	118.08
32	CC	506	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
35	d	404	PL9	C20-C19-C21	-2.90	110.39	115.27
32	S	610	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
32	b	611	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	4	308	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
40	YY	615	LUT	C2-C3-C4	-2.90	106.33	110.30
39	3	607	CHL	C4A-NA-C1A	2.90	108.01	106.71
32	g	603	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
32	g	610	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
32	3	611	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
34	CC	515	BCR	C28-C27-C26	-2.90	108.90	114.08
32	44	604	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
32	Gg	312	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
39	S	607	CHL	CHB-C4A-NA	2.90	128.52	124.51
32	SS	314	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
32	R	613	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
32	Ss	612	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	33	605	CHL	C4A-NA-C1A	2.90	108.01	106.71
32	r	608	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
37	BB	621	SQD	C45-O47-C7	-2.90	110.66	117.79
39	RR	305	CHL	CAA-C2A-C1A	-2.89	102.49	111.97
40	Ss	615	LUT	C38-C25-C24	-2.89	117.36	123.56
32	44	602	CLA	CMB-C2B-C1B	-2.89	124.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	SS	315	LUT	C1-C6-C5	-2.89	118.54	122.61
39	Y	608	CHL	O2D-CGD-O1D	-2.89	118.18	123.84
32	n	602	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
32	33	612	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
41	Yy	619	XAT	C36-C21-C22	-2.89	103.96	108.98
32	DD	401	CLA	CMB-C2B-C3B	2.89	130.09	124.68
32	Rr	601	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
32	3	611	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	Gg	306	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
39	Gg	308	CHL	CHB-C4A-NA	2.89	128.51	124.51
32	D	401	CLA	CMB-C2B-C3B	2.89	130.09	124.68
32	Rr	609	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	33	603	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
32	1	610	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	RR	302	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	4	303	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
32	c	509	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	2	613	CLA	CBD-CHA-C1A	2.89	131.91	128.50
39	GG	605	CHL	CHB-C4A-NA	2.89	128.51	124.51
34	Hh	101	BCR	C38-C26-C25	-2.89	121.28	124.53
32	n	610	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	CC	514	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
39	Nn	315	CHL	O2D-CGD-CBD	2.89	116.40	111.27
32	Y	613	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
39	22	606	CHL	C4A-NA-C1A	2.89	108.00	106.71
32	s	611	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
39	Yy	608	CHL	CHB-C4A-NA	2.89	128.50	124.51
44	BB	623	DGD	O1G-C1A-C2A	2.89	120.97	111.91
32	c	508	CLA	CMB-C2B-C3B	2.89	130.08	124.68
44	CC	519	DGD	O1G-C1A-C2A	2.89	120.96	111.91
32	BB	601	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
39	22	608	CHL	CHB-C4A-NA	2.89	128.50	124.51
39	G	605	CHL	CHB-C4A-NA	2.89	128.50	124.51
32	R	601	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	G	606	CHL	CHB-C4A-NA	2.88	128.50	124.51
32	d	402	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
32	s	608	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
37	B	602	SQD	O48-C23-C24	2.88	120.96	111.91
32	b	604	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	Y	612	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
39	g	607	CHL	CHB-C4A-NA	2.88	128.50	124.51
32	Rr	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	GG	613	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	Nn	303	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	NN	614	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
39	22	607	CHL	C4A-NA-C1A	2.88	108.00	106.71
32	33	611	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
32	B	610	CLA	CHB-C4A-NA	2.88	128.50	124.51
32	r	609	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
32	s	602	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
32	RR	303	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
32	YY	602	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
32	GG	610	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	44	606	CHL	CHB-C4A-NA	2.88	128.50	124.51
39	N	606	CHL	CHB-C4A-NA	2.88	128.50	124.51
39	r	607	CHL	CHB-C4A-NA	2.88	128.50	124.51
39	y	310	CHL	CHB-C4A-NA	2.88	128.50	124.51
32	11	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	Cc	509	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
32	3	602	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
39	N	605	CHL	C1B-CHB-C4A	-2.88	124.41	130.12
35	A	410	PL9	C25-C24-C26	-2.88	110.42	115.27
32	3	603	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
32	c	508	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
39	g	605	CHL	C1B-CHB-C4A	-2.88	124.41	130.12
44	C	520	DGD	O1G-C1A-C2A	2.88	120.94	111.91
32	1	602	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
32	c	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
34	b	617	BCR	C27-C26-C25	-2.88	118.55	122.73
40	NN	616	LUT	C38-C25-C24	-2.88	117.40	123.56
32	Ss	602	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
34	B	612	BCR	C15-C16-C17	-2.88	117.58	123.47
32	44	610	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
32	Nn	303	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
39	Yy	609	CHL	O2D-CGD-O1D	-2.88	118.21	123.84
32	22	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
32	BB	611	CLA	CMB-C2B-C3B	2.88	130.06	124.68
32	S	613	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
40	Rr	614	LUT	C1-C6-C5	-2.88	118.56	122.61
39	RR	305	CHL	O2D-CGD-O1D	-2.88	118.22	123.84
39	Gg	302	CHL	O2D-CGD-O1D	-2.88	118.22	123.84
32	C	514	CLA	CHB-C4A-NA	2.88	128.49	124.51
32	Bb	606	CLA	C1B-CHB-C4A	-2.88	124.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	411	LHG	C5-O7-C7	-2.87	110.71	117.79
44	BB	624	DGD	C2G-O2G-C1B	-2.87	110.71	117.79
39	y	309	CHL	CHB-C4A-NA	2.87	128.49	124.51
42	g	617	NEX	C38-C25-C26	-2.87	117.44	122.26
32	Cc	503	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
32	Yy	613	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	Rr	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	R	602	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	B	607	CLA	CMB-C2B-C3B	2.87	130.06	124.68
39	NN	606	CHL	CHB-C4A-NA	2.87	128.49	124.51
38	Aa	412	LMG	O8-C28-C29	2.87	120.92	111.91
40	G	616	LUT	C19-C9-C8	2.87	122.60	118.08
32	R	602	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
32	C	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	Nn	313	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
39	YY	606	CHL	CHB-C4A-NA	2.87	128.48	124.51
32	Bb	605	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
32	44	603	CLA	CHB-C4A-NA	2.87	128.48	124.51
32	11	611	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
39	R	606	CHL	C1B-CHB-C4A	-2.87	124.43	130.12
39	N	608	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
32	3	610	CLA	CMB-C2B-C3B	2.87	130.05	124.68
32	Bb	616	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
34	B	613	BCR	C38-C26-C25	-2.87	121.31	124.53
41	4	314	XAT	O24-C25-C38	2.87	118.50	115.06
35	DD	406	PL9	C40-C39-C41	-2.87	110.44	115.27
32	2	613	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
34	b	617	BCR	C33-C5-C4	2.87	119.13	113.62
46	e	101	HEM	C1B-NB-C4B	2.87	108.04	105.07
32	1	603	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
32	Rr	603	CLA	CMB-C2B-C3B	2.87	130.04	124.68
33	D	402	PHO	O1D-CGD-CBD	2.87	129.52	124.74
32	Bb	603	CLA	CMB-C2B-C3B	2.87	130.04	124.68
32	Ss	604	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
32	b	605	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	g	614	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	4	307	CHL	CHB-C4A-NA	2.87	128.48	124.51
39	GG	606	CHL	CHB-C4A-NA	2.87	128.48	124.51
32	c	510	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	11	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	2	612	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
32	g	614	CLA	C1B-CHB-C4A	-2.87	124.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Yy	614	CLA	CMB-C2B-C3B	2.87	130.04	124.68
35	D	407	PL9	C35-C34-C36	-2.87	110.45	115.27
39	g	609	CHL	O2D-CGD-O1D	-2.87	118.24	123.84
39	G	608	CHL	CHB-C4A-NA	2.87	128.47	124.51
42	Gg	318	NEX	C36-C21-C26	2.86	117.78	110.05
36	DD	407	LHG	O8-C23-C24	2.86	120.90	111.91
34	BB	616	BCR	C28-C27-C26	-2.86	108.96	114.08
32	3	610	CLA	CHD-C1D-ND	-2.86	121.82	124.45
39	SS	307	CHL	CHB-C4A-NA	2.86	128.47	124.51
32	AA	406	CLA	CMB-C2B-C3B	2.86	130.03	124.68
34	BB	616	BCR	C15-C16-C17	-2.86	117.61	123.47
32	RR	313	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
32	G	602	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
32	Dd	402	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
34	C	516	BCR	C37-C22-C23	2.86	122.59	118.08
39	Yy	605	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
32	B	619	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
39	g	601	CHL	C4A-NA-C1A	2.86	107.99	106.71
39	N	608	CHL	CHB-C4A-NA	2.86	128.47	124.51
39	Y	607	CHL	CHB-C4A-NA	2.86	128.47	124.51
36	3	614	LHG	C5-O7-C7	-2.86	110.75	117.79
32	r	601	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	NN	601	CHL	O2D-CGD-O1D	-2.86	118.25	123.84
41	Nn	308	XAT	C6-C7-C8	-2.86	119.95	125.99
40	S	614	LUT	C1-C6-C5	-2.86	118.59	122.61
39	l	605	CHL	O2D-CGD-CBD	2.86	116.35	111.27
46	e	101	HEM	C3B-C2B-C1B	2.86	108.61	106.49
41	y	302	XAT	C6-C7-C8	-2.86	119.95	125.99
32	r	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
32	C	507	CLA	C4A-NA-C1A	2.86	107.99	106.71
32	NN	602	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
32	B	623	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
40	Nn	306	LUT	C17-C1-C6	-2.86	105.66	110.30
32	b	606	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
32	33	611	CLA	CMB-C2B-C3B	2.86	130.02	124.68
39	s	605	CHL	CHB-C4A-NA	2.86	128.46	124.51
40	Nn	306	LUT	C2-C3-C4	-2.86	106.39	110.30
32	r	601	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
32	N	604	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
32	2	612	CLA	CMB-C2B-C3B	2.85	130.02	124.68
32	3	604	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	SS	309	CLA	O2D-CGD-O1D	-2.85	118.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	613	CLA	C1B-CHB-C4A	-2.85	124.46	130.12
39	GG	608	CHL	O2D-CGD-O1D	-2.85	118.26	123.84
39	N	607	CHL	O2D-CGD-O1D	-2.85	118.26	123.84
34	CC	515	BCR	C37-C22-C23	2.85	122.57	118.08
42	N	618	NEX	C15-C35-C34	-2.85	117.63	123.47
37	B	617	SQD	C45-O47-C7	-2.85	110.77	117.79
39	g	608	CHL	CHB-C4A-NA	2.85	128.46	124.51
32	1	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	Rr	602	CLA	C4A-NA-C1A	2.85	107.99	106.71
39	Y	601	CHL	C4A-NA-C1A	2.85	107.99	106.71
32	Ss	608	CLA	CMB-C2B-C3B	2.85	130.01	124.68
36	d	405	LHG	O8-C23-C24	2.85	120.85	111.91
32	11	613	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
32	Gg	304	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
46	E	101	HEM	C4B-CHC-C1C	2.85	126.32	122.56
32	Cc	515	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
33	Aa	409	PHO	O1D-CGD-CBD	2.85	129.49	124.74
32	NN	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
32	Bb	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
42	Y	619	NEX	C15-C35-C34	-2.85	117.64	123.47
32	g	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
32	Cc	510	CLA	CMB-C2B-C3B	2.85	130.01	124.68
41	44	613	XAT	C35-C15-C14	-2.85	117.64	123.47
32	y	306	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	D	408	LHG	O8-C23-C24	2.85	120.85	111.91
32	B	618	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
32	S	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
32	DD	404	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	NN	608	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
34	CC	515	BCR	C31-C1-C6	2.85	114.92	110.30
32	Rr	601	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
32	SS	309	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
41	Rr	615	XAT	C18-C5-C6	-2.85	117.49	122.26
39	s	605	CHL	C1B-CHB-C4A	-2.85	124.48	130.12
32	b	615	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
32	Yy	612	CLA	CHB-C4A-NA	2.85	128.45	124.51
40	Y	616	LUT	C18-C5-C6	-2.85	121.33	124.53
32	GG	612	CLA	CHB-C4A-NA	2.85	128.45	124.51
32	r	604	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
32	r	611	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
32	22	610	CLA	CMB-C2B-C3B	2.84	130.00	124.68
42	y	319	NEX	C15-C35-C34	-2.84	117.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	606	CHL	O2D-CGD-O1D	-2.84	118.28	123.84
32	44	604	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	G	612	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	c	513	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
39	Ss	605	CHL	C1B-CHB-C4A	-2.84	124.49	130.12
32	22	610	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	Bb	602	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	44	609	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	S	609	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
32	Yy	612	CLA	CMB-C2B-C3B	2.84	130.00	124.68
32	11	611	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
32	R	609	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
39	NN	609	CHL	O2D-CGD-O1D	-2.84	118.28	123.84
39	Gg	310	CHL	O2D-CGD-O1D	-2.84	118.28	123.84
34	c	514	BCR	C1-C6-C5	-2.84	118.61	122.61
37	C	501	SQD	O48-C23-C24	2.84	120.82	111.91
39	NN	601	CHL	C1B-CHB-C4A	-2.84	124.49	130.12
32	22	612	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
32	Y	602	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
32	Cc	506	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
39	33	601	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
32	Aa	405	CLA	CHB-C4A-NA	2.84	128.44	124.51
32	g	602	CLA	C1D-ND-C4D	-2.84	104.32	106.33
41	G	619	XAT	C6-C7-C8	-2.84	119.99	125.99
39	22	605	CHL	CBD-CHA-C1A	2.84	131.84	128.50
32	CC	509	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
32	3	613	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
34	T	101	BCR	C15-C14-C13	-2.84	123.26	127.31
39	YY	605	CHL	CHB-C4A-NA	2.84	128.43	124.51
39	Y	609	CHL	CHB-C4A-NA	2.84	128.43	124.51
32	2	603	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
32	Y	610	CLA	CMB-C2B-C3B	2.83	129.98	124.68
39	n	609	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
35	Dd	404	PL9	C35-C34-C36	-2.83	110.50	115.27
34	c	516	BCR	C27-C26-C25	-2.83	118.62	122.73
32	y	315	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
32	3	602	CLA	CBD-CHA-C1A	2.83	131.84	128.50
32	G	612	CLA	CMB-C2B-C3B	2.83	129.98	124.68
39	Gg	306	CHL	C2A-C1A-CHA	2.83	128.81	123.86
32	Aa	406	CLA	C1D-ND-C4D	-2.83	104.32	106.33
32	11	610	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
32	C	509	CLA	CMB-C2B-C1B	-2.83	124.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	613	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
32	S	611	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
32	YY	603	CLA	CHB-C4A-NA	2.83	128.43	124.51
39	Rr	607	CHL	CHB-C4A-NA	2.83	128.43	124.51
34	DD	405	BCR	C37-C22-C23	2.83	122.54	118.08
40	GG	616	LUT	C19-C9-C8	2.83	122.54	118.08
32	B	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
34	h	101	BCR	C29-C30-C25	2.83	114.84	110.48
34	XX	202	BCR	C29-C30-C25	2.83	114.84	110.48
39	GG	601	CHL	CHB-C4A-NA	2.83	128.43	124.51
32	n	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
32	S	602	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
39	Y	606	CHL	CHB-C4A-NA	2.83	128.43	124.51
32	22	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
32	S	604	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
34	Hh	101	BCR	C36-C18-C17	-2.83	118.96	122.92
32	Rr	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
32	2	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
32	4	311	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
39	Ss	605	CHL	O2D-CGD-O1D	-2.83	118.31	123.84
44	Cc	519	DGD	C2G-O2G-C1B	-2.83	110.82	117.79
32	CC	510	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	22	603	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
32	Rr	603	CLA	CHB-C4A-NA	2.83	128.42	124.51
32	3	609	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
32	c	509	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
32	Rr	608	CLA	CMB-C2B-C3B	2.83	129.97	124.68
32	Ss	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	RR	304	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
42	Y	619	NEX	C5-C6-C1	2.83	122.50	119.70
39	g	605	CHL	C2A-C1A-CHA	2.83	128.80	123.86
32	RR	311	CLA	CMB-C2B-C3B	2.83	129.97	124.68
32	b	608	CLA	C4A-NA-C1A	2.83	107.98	106.71
39	Gg	308	CHL	C4A-NA-C1A	2.83	107.98	106.71
39	11	601	CHL	C1B-CHB-C4A	-2.83	124.52	130.12
32	R	604	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
32	N	612	CLA	CMB-C2B-C3B	2.83	129.97	124.68
46	Ee	101	HEM	C3B-C2B-C1B	2.83	108.58	106.49
34	C	517	BCR	C27-C26-C25	-2.83	118.63	122.73
36	r	616	LHG	O8-C23-C24	2.83	120.78	111.91
32	S	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	Nn	313	CLA	CMB-C2B-C3B	2.83	129.97	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	605	CHL	O2D-CGD-CBD	2.83	116.29	111.27
34	b	619	BCR	C30-C25-C26	-2.83	118.63	122.61
32	4	305	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	YY	613	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
32	Aa	405	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
34	b	619	BCR	C29-C30-C25	2.83	114.83	110.48
32	S	609	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
32	CC	511	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
39	Gg	309	CHL	CHB-C4A-NA	2.82	128.42	124.51
33	a	409	PHO	O1D-CGD-CBD	2.82	129.44	124.74
32	CC	506	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
32	Bb	602	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
32	Ss	602	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
32	BB	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	YY	605	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
32	YY	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
41	G	619	XAT	O4-C5-C18	2.82	118.44	115.06
32	y	314	CLA	CHB-C4A-NA	2.82	128.41	124.51
39	Rr	606	CHL	CHB-C4A-NA	2.82	128.41	124.51
32	a	407	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
32	1	613	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
32	B	610	CLA	CMB-C2B-C3B	2.82	129.96	124.68
39	Rr	605	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
39	s	605	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
34	XX	202	BCR	C37-C22-C23	2.82	122.52	118.08
32	11	604	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
32	b	602	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
39	n	605	CHL	C4A-NA-C1A	2.82	107.97	106.71
39	G	605	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
39	Ss	605	CHL	CHB-C4A-NA	2.82	128.41	124.51
32	b	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
32	s	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
32	Cc	510	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
32	33	602	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
32	2	611	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
39	Rr	605	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
39	2	606	CHL	C4A-NA-C1A	2.82	107.97	106.71
32	22	611	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
39	3	601	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
40	s	614	LUT	C38-C25-C24	-2.82	117.53	123.56
32	44	604	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
32	22	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Nn	319	CHL	C1B-CHB-C4A	-2.82	124.54	130.12
34	h	101	BCR	C16-C15-C14	-2.82	117.70	123.47
32	n	612	CLA	CMB-C2B-C3B	2.82	129.95	124.68
32	RR	313	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
32	D	405	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
34	T	101	BCR	C30-C25-C26	-2.82	118.65	122.61
32	Nn	305	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
41	Yy	619	XAT	C6-C7-C8	-2.82	120.04	125.99
40	r	614	LUT	C1-C6-C5	-2.82	118.65	122.61
32	g	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
39	3	605	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
32	Y	603	CLA	CMB-C2B-C3B	2.82	129.94	124.68
39	SS	308	CHL	C1B-CHB-C4A	-2.81	124.54	130.12
40	G	616	LUT	C36-C21-C26	2.81	113.81	109.55
41	y	301	XAT	C24-C23-C22	-2.81	105.34	110.77
34	Cc	518	BCR	C1-C6-C5	-2.81	118.65	122.61
32	y	315	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
39	3	607	CHL	CBD-CHA-C1A	2.81	131.82	128.50
32	c	511	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	Dd	405	LHG	O8-C23-C24	2.81	120.74	111.91
32	a	410	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
32	c	510	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
34	TT	101	BCR	C19-C18-C17	-2.81	114.62	118.94
32	y	305	CLA	CMB-C2B-C3B	2.81	129.94	124.68
32	Ss	612	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
42	Rr	616	NEX	C2-C1-C6	2.81	111.94	109.21
32	1	611	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
34	B	612	BCR	C37-C22-C23	2.81	122.51	118.08
39	33	601	CHL	C4A-NA-C1A	2.81	107.97	106.71
32	Bb	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
39	22	601	CHL	CHB-C4A-NA	2.81	128.40	124.51
32	b	602	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
32	SS	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	NN	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	s	612	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
32	Cc	507	CLA	CMB-C2B-C3B	2.81	129.94	124.68
41	Nn	308	XAT	C20-C13-C12	2.81	122.50	118.08
40	Gg	316	LUT	C1-C6-C5	-2.81	118.66	122.61
32	RR	309	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
32	SS	311	CLA	CMB-C2B-C3B	2.81	129.93	124.68
39	11	607	CHL	C4A-NA-C1A	2.81	107.97	106.71
32	N	602	CLA	CHB-C4A-NA	2.81	128.39	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	606	CHL	CHB-C4A-NA	2.81	128.39	124.51
33	D	402	PHO	O2D-CGD-O1D	-2.81	118.35	123.84
36	Nn	310	LHG	O8-C23-C24	2.81	120.71	111.91
32	C	512	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
32	BB	609	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
39	YY	607	CHL	CHB-C4A-NA	2.81	128.39	124.51
40	SS	315	LUT	C38-C25-C24	-2.81	117.56	123.56
37	Aa	413	SQD	O48-C23-C24	2.81	120.71	111.91
32	44	609	CLA	CMB-C2B-C3B	2.81	129.93	124.68
32	R	614	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
39	Yy	606	CHL	O2D-CGD-O1D	-2.80	118.35	123.84
32	S	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
32	11	613	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
32	NN	604	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
42	R	617	NEX	C15-C35-C34	-2.80	117.73	123.47
32	AA	408	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
32	3	603	CLA	CBD-CHA-C1A	2.80	131.80	128.50
39	GG	605	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
39	GG	606	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
32	GG	612	CLA	CMB-C2B-C3B	2.80	129.92	124.68
39	2	601	CHL	CHB-C4A-NA	2.80	128.39	124.51
39	3	606	CHL	CHB-C4A-NA	2.80	128.39	124.51
32	11	611	CLA	CBD-CHA-C1A	2.80	131.80	128.50
32	S	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
32	y	316	CLA	CMB-C2B-C3B	2.80	129.92	124.68
39	NN	607	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
39	2	607	CHL	CHB-C4A-NA	2.80	128.38	124.51
32	A	408	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
32	b	606	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
41	RR	316	XAT	C26-C27-C28	-2.80	120.07	125.99
32	N	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
32	Y	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	YY	608	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
39	Gg	309	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
32	Cc	512	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
39	Ss	607	CHL	CHB-C4A-NA	2.80	128.38	124.51
39	N	601	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
32	NN	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	s	604	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
34	B	614	BCR	C3-C4-C5	-2.80	109.08	114.08
32	Gg	312	CLA	CBA-CAA-C2A	2.80	122.12	113.86
39	n	605	CHL	CHB-C4A-NA	2.80	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	607	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
32	4	304	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
40	22	614	LUT	C15-C35-C34	2.80	129.21	123.47
32	SS	303	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
39	YY	601	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
32	BB	608	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
39	Rr	605	CHL	CHB-C4A-NA	2.80	128.38	124.51
34	h	101	BCR	C11-C10-C9	-2.80	123.32	127.31
39	s	601	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
32	r	603	CLA	CHB-C4A-NA	2.80	128.38	124.51
42	RR	317	NEX	C15-C35-C34	-2.80	117.75	123.47
32	CC	508	CLA	CHB-C4A-NA	2.80	128.38	124.51
32	Ss	608	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
39	YY	609	CHL	C1B-CHB-C4A	-2.80	124.58	130.12
32	Nn	301	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	c	501	CLA	C4-C3-C5	2.80	119.97	115.27
39	33	601	CHL	CHB-C4A-NA	2.79	128.38	124.51
32	A	406	CLA	CMB-C2B-C3B	2.79	129.91	124.68
32	NN	604	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
32	Gg	315	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
32	2	611	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
32	SS	312	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	CC	505	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
39	s	601	CHL	CHB-C4A-NA	2.79	128.37	124.51
39	SS	306	CHL	CHB-C4A-NA	2.79	128.37	124.51
34	c	515	BCR	C24-C23-C22	-2.79	122.02	126.23
35	AA	410	PL9	C25-C24-C26	-2.79	110.57	115.27
32	Gg	313	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
32	11	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	3	612	CLA	CBD-CHA-C1A	2.79	131.79	128.50
39	3	605	CHL	CHB-C4A-NA	2.79	128.37	124.51
34	CC	517	BCR	C29-C30-C25	2.79	114.78	110.48
32	BB	606	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
32	a	405	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
32	CC	513	CLA	CHB-C4A-NA	2.79	128.37	124.51
34	XX	202	BCR	C30-C25-C26	-2.79	118.69	122.61
39	11	607	CHL	C2A-C1A-CHA	2.79	127.03	122.71
32	N	604	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	22	607	CHL	CHB-C4A-NA	2.79	128.37	124.51
32	G	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
40	Yy	616	LUT	C7-C8-C9	-2.79	122.02	126.23
32	r	601	CLA	CMB-C2B-C3B	2.79	129.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	101	LHG	C5-O7-C7	-2.79	112.70	117.90
32	N	602	CLA	O2D-CGD-CBD	2.79	116.22	111.27
32	Aa	407	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
36	G	618	LHG	C5-O7-C7	-2.79	110.93	117.79
32	R	609	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
32	c	503	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
39	NN	601	CHL	CHB-C4A-NA	2.79	128.36	124.51
39	33	605	CHL	CBD-CHA-C1A	2.79	131.78	128.50
32	y	316	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
32	2	603	CLA	CMB-C2B-C3B	2.78	129.89	124.68
32	s	613	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
32	B	623	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
32	YY	610	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
39	g	608	CHL	O2D-CGD-O1D	-2.78	118.39	123.84
39	GG	601	CHL	O2D-CGD-O1D	-2.78	118.39	123.84
32	22	613	CLA	CMB-C2B-C3B	2.78	129.89	124.68
32	Yy	612	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
39	S	605	CHL	O2D-CGD-O1D	-2.78	118.39	123.84
37	L	102	SQD	O48-C23-C24	2.78	120.64	111.91
39	G	601	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
32	Rr	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
32	44	615	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
32	Gg	312	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
32	G	614	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
39	2	605	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
39	2	605	CHL	CBD-CHA-C1A	2.78	131.78	128.50
32	3	604	CLA	CMB-C2B-C3B	2.78	129.88	124.68
32	Gg	313	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
39	44	605	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
40	Ss	614	LUT	C38-C25-C24	-2.78	117.61	123.56
32	SS	304	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
39	SS	306	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
32	Aa	410	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
32	B	606	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
32	R	608	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
39	33	605	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
34	b	618	BCR	C29-C30-C25	2.78	114.76	110.48
32	11	603	CLA	C4A-NA-C1A	2.78	107.95	106.71
32	33	612	CLA	CBD-CHA-C1A	2.78	131.77	128.50
32	c	508	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
35	D	407	PL9	C25-C24-C26	-2.78	110.60	115.27
32	Gg	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	3	606	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
32	22	612	CLA	CBD-CHA-C1A	2.78	131.77	128.50
32	44	609	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
32	s	612	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
32	BB	601	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
33	DD	402	PHO	O1D-CGD-CBD	2.78	129.36	124.74
32	r	613	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
32	3	612	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
34	Bb	619	BCR	C29-C30-C25	2.77	114.75	110.48
32	Rr	611	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
39	44	606	CHL	O2D-CGD-O1D	-2.77	118.41	123.84
39	22	601	CHL	O2D-CGD-O1D	-2.77	118.41	123.84
32	y	314	CLA	CMB-C2B-C3B	2.77	129.87	124.68
32	BB	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
39	2	608	CHL	CHB-C4A-NA	2.77	128.35	124.51
32	NN	613	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
39	22	605	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
32	Rr	602	CLA	C1D-ND-C4D	-2.77	104.36	106.33
40	y	318	LUT	C38-C25-C24	-2.77	117.63	123.56
32	44	603	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
32	33	610	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
32	22	604	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
32	1	610	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
39	11	607	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
32	CC	502	CLA	CMB-C2B-C3B	2.77	129.87	124.68
32	Yy	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
41	y	302	XAT	C20-C13-C14	-2.77	119.04	122.92
32	2	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
32	b	603	CLA	CMB-C2B-C3B	2.77	129.86	124.68
32	33	609	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
41	R	616	XAT	C26-C27-C28	-2.77	120.13	125.99
32	GG	614	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
32	C	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
32	SS	310	CLA	CMB-C2B-C3B	2.77	129.86	124.68
32	Yy	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
34	T	101	BCR	C3-C4-C5	-2.77	109.13	114.08
32	GG	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
32	RR	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
39	G	609	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
32	Bb	606	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
32	33	613	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
32	N	613	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	KK	103	BCR	C40-C30-C25	2.77	114.79	110.30
39	Nn	317	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
39	S	607	CHL	O2D-CGD-O1D	-2.77	118.43	123.84
39	33	608	CHL	O2D-CGD-O1D	-2.77	118.43	123.84
32	Rr	611	CLA	CMB-C2B-C3B	2.77	129.86	124.68
39	33	605	CHL	CHB-C4A-NA	2.77	128.34	124.51
32	c	503	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
39	22	601	CHL	C4A-NA-C1A	2.77	107.95	106.71
40	22	614	LUT	C36-C21-C26	2.77	113.74	109.55
32	11	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
32	22	612	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
32	3	612	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
34	TT	101	BCR	C30-C25-C26	-2.77	118.72	122.61
39	GG	608	CHL	CHB-C4A-NA	2.77	128.34	124.51
40	s	614	LUT	C19-C9-C8	2.77	122.43	118.08
32	Nn	312	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
34	Hh	101	BCR	C36-C18-C19	2.76	122.43	118.08
39	S	601	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
32	1	604	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
32	44	611	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
39	G	608	CHL	C2A-C1A-CHA	2.76	128.68	123.85
39	S	605	CHL	CHB-C4A-NA	2.76	128.33	124.51
32	B	622	CLA	CMB-C2B-C3B	2.76	129.85	124.68
32	33	603	CLA	CBD-CHA-C1A	2.76	131.75	128.50
32	r	610	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
34	Cc	517	BCR	C24-C23-C22	-2.76	122.06	126.23
32	S	612	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
32	AA	405	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
32	C	505	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
32	b	603	CLA	C4A-NA-C1A	2.76	107.95	106.71
32	RR	309	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
32	Rr	604	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
32	Y	603	CLA	CHB-C4A-NA	2.76	128.33	124.51
40	2	614	LUT	C16-C1-C6	2.76	114.78	110.30
32	Rr	612	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
39	44	606	CHL	C1B-CHB-C4A	-2.76	124.65	130.12
34	TT	101	BCR	C15-C14-C13	-2.76	123.37	127.31
32	YY	604	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
37	LL	101	SQD	O48-C23-C24	2.76	120.56	111.91
32	b	616	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
39	Y	609	CHL	C1B-CHB-C4A	-2.76	124.65	130.12
32	B	624	CLA	O2A-CGA-O1A	-2.76	116.63	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	11	612	CLA	C4A-NA-C1A	2.76	107.95	106.71
39	RR	305	CHL	C4A-NA-C1A	2.76	107.95	106.71
32	n	612	CLA	CHB-C4A-NA	2.76	128.33	124.51
39	4	306	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
32	4	305	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
39	Nn	315	CHL	C1B-CHB-C4A	-2.76	124.66	130.12
40	s	615	LUT	C38-C25-C24	-2.76	117.66	123.56
32	GG	604	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
32	Cc	508	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
32	22	604	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
39	G	609	CHL	C1B-CHB-C4A	-2.76	124.66	130.12
32	Cc	513	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
39	33	607	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
39	4	302	CHL	C4A-NA-C1A	2.76	107.94	106.71
39	22	608	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
40	R	615	LUT	C16-C1-C6	2.76	114.77	110.30
32	c	504	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
32	Cc	512	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
42	Rr	616	NEX	C15-C35-C34	-2.75	117.83	123.47
32	Bb	602	CLA	C4A-NA-C1A	2.75	107.94	106.71
32	c	501	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
32	g	611	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
32	4	312	CLA	CMB-C2B-C3B	2.75	129.83	124.68
32	CC	511	CLA	CMB-C2B-C3B	2.75	129.83	124.68
32	A	405	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
39	4	307	CHL	C1B-CHB-C4A	-2.75	124.67	130.12
35	Dd	404	PL9	C30-C29-C31	-2.75	110.64	115.27
32	r	602	CLA	C4A-NA-C1A	2.75	107.94	106.71
39	Yy	601	CHL	C1B-CHB-C4A	-2.75	124.67	130.12
32	Rr	608	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	R	606	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
34	B	612	BCR	C27-C26-C25	-2.75	118.74	122.73
39	YY	609	CHL	CHB-C4A-NA	2.75	128.32	124.51
41	y	301	XAT	C6-C7-C8	-2.75	120.18	125.99
32	NN	613	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
32	44	610	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	Nn	319	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
34	h	101	BCR	C38-C26-C27	2.75	118.90	113.62
32	3	611	CLA	CBD-CHA-C1A	2.75	131.74	128.50
39	11	601	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
34	Cc	516	BCR	C36-C18-C17	-2.75	119.07	122.92
32	G	614	CLA	CMB-C2B-C1B	-2.75	124.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	511	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
32	G	614	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
41	r	615	XAT	C40-C33-C32	2.75	122.41	118.08
32	n	614	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
32	NN	612	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
34	BB	620	BCR	C16-C15-C14	-2.75	117.85	123.47
38	AA	415	LMG	O8-C28-C29	2.75	120.52	111.91
32	g	604	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
39	Gg	307	CHL	O2D-CGD-O1D	-2.75	118.47	123.84
32	n	603	CLA	CMB-C2B-C3B	2.75	129.81	124.68
39	g	607	CHL	C4A-NA-C1A	2.74	107.94	106.71
32	44	603	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
32	N	603	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
39	YY	609	CHL	O2D-CGD-O1D	-2.74	118.47	123.84
34	C	518	BCR	C29-C30-C25	2.74	114.70	110.48
39	GG	609	CHL	CHB-C4A-NA	2.74	128.31	124.51
38	b	620	LMG	O8-C28-C29	2.74	120.52	111.91
34	C	518	BCR	C30-C25-C26	-2.74	118.75	122.61
34	CC	516	BCR	C38-C26-C25	-2.74	121.45	124.53
32	GG	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
32	N	613	CLA	CMB-C2B-C3B	2.74	129.81	124.68
32	g	614	CLA	CMB-C2B-C3B	2.74	129.81	124.68
34	Hh	101	BCR	C29-C30-C25	2.74	114.70	110.48
32	r	609	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
33	a	408	PHO	O2D-CGD-O1D	-2.74	118.48	123.84
39	33	607	CHL	C1B-CHB-C4A	-2.74	124.69	130.12
39	1	601	CHL	C1B-CHB-C4A	-2.74	124.69	130.12
32	Ss	604	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
32	Bb	603	CLA	C4A-NA-C1A	2.74	107.94	106.71
32	44	611	CLA	CMB-C2B-C3B	2.74	129.81	124.68
32	D	404	CLA	CHB-C4A-NA	2.74	128.30	124.51
32	Bb	616	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	s	607	CHL	CHB-C4A-NA	2.74	128.30	124.51
32	y	305	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
42	NN	618	NEX	C15-C35-C34	-2.74	117.86	123.47
39	R	605	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
39	3	607	CHL	C1B-CHB-C4A	-2.74	124.69	130.12
39	1	607	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
39	g	605	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
32	n	613	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
32	C	509	CLA	CHB-C4A-NA	2.74	128.30	124.51
36	BB	622	LHG	O8-C23-C24	2.74	120.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	615	LUT	C16-C1-C6	2.74	114.74	110.30
32	Cc	513	CLA	CHD-C1D-ND	-2.74	121.94	124.45
34	B	614	BCR	C36-C18-C17	-2.74	119.09	122.92
32	G	604	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
32	Rr	601	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
32	BB	610	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
32	Bb	601	CLA	CMB-C2B-C3B	2.74	129.80	124.68
40	GG	616	LUT	C36-C21-C26	2.74	113.69	109.55
35	DD	406	PL9	C35-C34-C36	-2.74	110.67	115.27
39	44	608	CHL	C4A-NA-C1A	2.74	107.94	106.71
34	H	101	BCR	C37-C22-C23	-2.74	113.77	118.08
32	Y	602	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
39	33	606	CHL	O2D-CGD-O1D	-2.74	118.49	123.84
39	2	607	CHL	O2D-CGD-O1D	-2.74	118.49	123.84
39	n	601	CHL	O2D-CGD-O1D	-2.74	118.49	123.84
32	G	610	CLA	CHB-C4A-NA	2.73	128.29	124.51
39	n	609	CHL	CHB-C4A-NA	2.73	128.29	124.51
32	11	604	CLA	CMB-C2B-C3B	2.73	129.79	124.68
32	CC	504	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
39	r	605	CHL	CMB-C2B-C1B	-2.73	124.26	128.46
39	Yy	601	CHL	CHB-C4A-NA	2.73	128.29	124.51
34	c	515	BCR	C15-C16-C17	-2.73	117.88	123.47
32	4	310	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
34	c	516	BCR	C1-C6-C5	-2.73	118.76	122.61
40	Ss	614	LUT	C36-C21-C26	2.73	113.68	109.55
34	Cc	517	BCR	C15-C16-C17	-2.73	117.88	123.47
32	RR	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	11	607	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
40	Y	615	LUT	C38-C25-C24	-2.73	117.71	123.56
32	R	603	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
39	Gg	306	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
38	A	415	LMG	O8-C28-C29	2.73	120.48	111.91
34	BB	618	BCR	C3-C4-C5	-2.73	109.20	114.08
32	3	602	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
32	r	610	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
32	B	610	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
41	Gg	301	XAT	C39-C29-C28	2.73	122.38	118.08
39	22	605	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
39	Rr	607	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
32	r	608	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
32	33	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
32	SS	303	CLA	O2D-CGD-O1D	-2.73	118.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	607	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
32	Cc	509	CLA	CHB-C4A-NA	2.73	128.28	124.51
39	33	607	CHL	CHB-C4A-NA	2.73	128.28	124.51
33	Aa	409	PHO	O2D-CGD-O1D	-2.73	118.50	123.84
32	Cc	513	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
35	A	410	PL9	C35-C34-C36	-2.73	110.68	115.27
32	g	612	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
39	Nn	311	CHL	O2D-CGD-O1D	-2.73	118.51	123.84
39	4	302	CHL	CHB-C4A-NA	2.73	128.28	124.51
39	22	608	CHL	C4A-NA-C1A	2.73	107.93	106.71
38	Cc	501	LMG	C4-C3-C2	2.73	115.58	110.82
32	4	312	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
32	GG	611	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
32	44	603	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
32	G	612	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
32	Nn	302	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
39	GG	608	CHL	C1B-CHB-C4A	-2.73	124.72	130.12
32	s	603	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
32	Cc	511	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
32	Gg	305	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
32	GG	612	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
39	G	608	CHL	C1B-CHB-C4A	-2.72	124.72	130.12
32	Gg	312	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
33	Aa	408	PHO	O2D-CGD-O1D	-2.72	118.51	123.84
32	Yy	613	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
32	Nn	305	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
40	Gg	316	LUT	C17-C1-C6	-2.72	105.88	110.30
32	NN	610	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
32	Ss	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	4	304	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	Ss	603	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
42	Y	617	NEX	C40-C33-C32	2.72	122.37	118.08
32	SS	311	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	C	512	CLA	CMB-C2B-C3B	2.72	129.77	124.68
32	BB	608	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
32	2	604	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
32	Yy	611	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
32	Y	611	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	s	604	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	S	606	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
39	SS	302	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
32	BB	613	CLA	CMB-C2B-C3B	2.72	129.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	616	BCR	C37-C22-C23	2.72	122.36	118.08
32	c	506	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
32	33	609	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	r	603	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
32	RR	311	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
32	c	506	CLA	CMB-C2B-C3B	2.72	129.76	124.68
34	B	614	BCR	C38-C26-C25	-2.72	121.47	124.53
32	Bb	611	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
33	a	409	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
34	Bb	618	BCR	C29-C30-C25	2.72	114.66	110.48
46	EE	102	HEM	C4B-CHC-C1C	2.72	126.14	122.56
39	NN	609	CHL	C2A-C1A-CHA	2.72	128.61	123.86
32	Y	604	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
32	1	611	CLA	CBD-CHA-C1A	2.72	131.70	128.50
39	Y	609	CHL	O2D-CGD-O1D	-2.72	118.53	123.84
32	NN	614	CLA	CMB-C2B-C3B	2.72	129.76	124.68
32	CC	508	CLA	O2D-CGD-CBD	2.72	116.09	111.27
39	G	605	CHL	C1B-CHB-C4A	-2.72	124.74	130.12
32	Rr	603	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	R	611	CLA	CMB-C2B-C3B	2.72	129.76	124.68
32	Ss	613	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
39	g	607	CHL	O2D-CGD-O1D	-2.71	118.53	123.84
32	CC	511	CLA	CHB-C4A-NA	2.71	128.27	124.51
34	c	514	BCR	C2-C1-C6	2.71	114.66	110.48
39	n	601	CHL	C1B-CHB-C4A	-2.71	124.74	130.12
32	S	608	CLA	CMB-C2B-C3B	2.71	129.76	124.68
32	NN	612	CLA	CMB-C2B-C3B	2.71	129.75	124.68
34	XX	202	BCR	C36-C18-C17	-2.71	119.12	122.92
32	GG	614	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
39	NN	601	CHL	CMB-C2B-C3B	2.71	129.75	124.68
39	22	608	CHL	C1B-CHB-C4A	-2.71	124.74	130.12
32	22	603	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
32	R	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
46	Ee	101	HEM	C1B-NB-C4B	2.71	107.88	105.07
39	2	607	CHL	CBD-CHA-C1A	2.71	131.70	128.50
32	C	503	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
32	c	502	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
32	CC	502	CLA	CHB-C4A-NA	2.71	128.26	124.51
32	N	614	CLA	CMB-C2B-C3B	2.71	129.75	124.68
32	Rr	612	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
39	RR	306	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
32	1	603	CLA	CBD-CHA-C1A	2.71	131.69	128.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	CC	508	CLA	CMB-C2B-C3B	2.71	129.75	124.68
32	GG	614	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
39	22	607	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
39	n	607	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
42	R	617	NEX	C17-C1-C6	-2.71	108.05	110.47
39	g	601	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
32	B	605	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
34	BB	617	BCR	C15-C16-C17	-2.71	117.93	123.47
32	N	614	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	Cc	506	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	YY	614	CLA	CMB-C2B-C3B	2.71	129.75	124.68
32	22	604	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
32	Gg	315	CLA	CMB-C2B-C3B	2.71	129.74	124.68
39	22	606	CHL	O2D-CGD-O1D	-2.71	118.55	123.84
32	N	612	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
32	n	602	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
32	YY	602	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
32	SS	313	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
34	XX	202	BCR	C7-C8-C9	-2.71	122.15	126.23
32	Bb	613	CLA	CHB-C4A-NA	2.71	128.25	124.51
39	g	609	CHL	CHB-C4A-NA	2.71	128.25	124.51
32	s	610	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
40	RR	315	LUT	C3-C4-C5	-2.71	106.46	111.85
44	a	415	DGD	O5D-C1E-C2E	2.71	112.53	108.30
39	22	605	CHL	CHB-C4A-NA	2.71	128.25	124.51
32	Cc	505	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
36	n	618	LHG	O8-C23-C24	2.70	120.40	111.91
39	l	601	CHL	O2D-CGD-O1D	-2.70	118.55	123.84
39	Gg	308	CHL	O2D-CGD-O1D	-2.70	118.55	123.84
32	Gg	303	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
32	s	613	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
32	Y	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
32	Cc	508	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
32	BB	604	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
32	N	613	CLA	CHD-C1D-ND	-2.70	121.97	124.45
32	3	610	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
40	Nn	306	LUT	C36-C21-C26	2.70	113.64	109.55
32	D	405	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	b	611	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	c	504	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	Cc	504	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
36	SS	301	LHG	O8-C23-C24	2.70	120.39	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	GG	605	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
41	GG	619	XAT	C6-C7-C8	-2.70	120.28	125.99
39	SS	308	CHL	CHB-C4A-NA	2.70	128.25	124.51
40	S	614	LUT	C38-C25-C24	-2.70	117.78	123.56
32	B	620	CLA	CMB-C2B-C3B	2.70	129.73	124.68
32	4	304	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
39	2	601	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
32	B	620	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	11	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
32	33	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
42	Rr	616	NEX	C40-C33-C32	2.70	122.33	118.08
32	b	615	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	BB	605	CLA	CMB-C2B-C3B	2.70	129.73	124.68
32	b	601	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	Nn	304	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
32	Rr	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
32	2	604	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
32	N	611	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
39	n	609	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
32	S	603	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
32	Y	602	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
41	NN	617	XAT	C40-C33-C34	-2.70	119.14	122.92
39	RR	307	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
40	Yy	616	LUT	C19-C9-C8	2.70	122.33	118.08
32	N	611	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
32	y	313	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
32	n	612	CLA	C4A-NA-C1A	2.70	107.92	106.71
34	T	101	BCR	C29-C30-C25	2.70	114.63	110.48
32	r	611	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
34	Hh	101	BCR	C16-C15-C14	-2.70	117.95	123.47
32	a	405	CLA	CHB-C4A-NA	2.69	128.24	124.51
32	S	604	CLA	CMB-C2B-C3B	2.69	129.72	124.68
32	R	614	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
32	11	602	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
32	b	609	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
32	2	610	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
34	D	406	BCR	C36-C18-C19	2.69	122.32	118.08
32	r	602	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
32	Y	614	CLA	CMB-C2B-C3B	2.69	129.72	124.68
32	G	611	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
36	s	616	LHG	O8-C23-C24	2.69	120.36	111.91
35	Dd	404	PL9	C40-C39-C41	-2.69	110.74	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	506	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
37	CC	501	SQD	O48-C23-C24	2.69	120.36	111.91
32	Bb	611	CLA	CMB-C2B-C3B	2.69	129.71	124.68
32	Bb	612	CLA	CMB-C2B-C3B	2.69	129.71	124.68
39	1	601	CHL	CBD-CHA-C1A	2.69	131.67	128.50
39	3	608	CHL	O2D-CGD-O1D	-2.69	118.58	123.84
39	R	607	CHL	O2D-CGD-O1D	-2.69	118.58	123.84
32	Bb	604	CLA	CMB-C2B-C3B	2.69	129.71	124.68
32	c	511	CLA	CHD-C1D-ND	-2.69	121.98	124.45
39	1	607	CHL	CHB-C4A-NA	2.69	128.23	124.51
39	2	606	CHL	C1B-CHB-C4A	-2.69	124.79	130.12
32	33	602	CLA	CBD-CHA-C1A	2.69	131.67	128.50
32	G	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	R	611	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
32	Ss	609	CLA	CMB-C2B-C3B	2.69	129.71	124.68
34	Dd	403	BCR	C33-C5-C4	2.69	118.78	113.62
32	1	613	CLA	CHD-C1D-ND	-2.69	121.98	124.45
32	G	602	CLA	CHD-C1D-ND	-2.69	121.98	124.45
32	SS	312	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
41	G	617	XAT	C20-C13-C12	2.69	122.31	118.08
32	SS	312	CLA	CMB-C2B-C3B	2.69	129.71	124.68
32	Yy	603	CLA	CHB-C4A-NA	2.69	128.23	124.51
32	11	609	CLA	CMB-C2B-C3B	2.69	129.71	124.68
39	N	601	CHL	CHB-C4A-NA	2.69	128.23	124.51
32	Rr	603	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
32	Ss	610	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
44	h	102	DGD	O1G-C1A-C2A	2.69	120.34	111.91
39	YY	606	CHL	C4A-NA-C1A	2.69	107.91	106.71
32	Rr	611	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
32	2	603	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
39	Nn	318	CHL	O2D-CGD-O1D	-2.69	118.59	123.84
41	G	617	XAT	C39-C29-C28	-2.69	113.85	118.08
39	SS	308	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
32	C	504	CLA	CBA-CAA-C2A	2.68	121.79	113.86
39	3	605	CHL	CBD-CHA-C1A	2.68	131.66	128.50
39	4	307	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
32	Yy	602	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
39	G	608	CHL	C4A-NA-C1A	2.68	107.91	106.71
44	Aa	401	DGD	O5D-C1E-C2E	2.68	112.49	108.30
32	SS	304	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	y	314	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
32	B	608	CLA	O2D-CGD-O1D	-2.68	118.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	306	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	3	610	CLA	CBD-CHA-C1A	2.68	131.66	128.50
32	RR	314	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
32	RR	310	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	Bb	601	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	b	616	CLA	CHB-C4A-NA	2.68	128.22	124.51
32	s	608	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	3	608	CHL	CHB-C4A-NA	2.68	128.22	124.51
41	G	617	XAT	C6-C7-C8	-2.68	120.33	125.99
32	c	506	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	R	608	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	b	610	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
39	3	607	CHL	CHB-C4A-NA	2.68	128.22	124.51
34	CC	515	BCR	C38-C26-C25	-2.68	121.52	124.53
32	YY	611	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	33	610	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	NN	611	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	C	511	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
40	y	318	LUT	C7-C8-C9	-2.68	122.19	126.23
32	Gg	313	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	S	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
39	y	303	CHL	C1B-CHB-C4A	-2.68	124.81	130.12
32	4	312	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
36	Gg	319	LHG	O8-C23-C24	2.68	120.31	111.91
32	R	608	CLA	CMB-C2B-C3B	2.68	129.68	124.68
32	Rr	610	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
34	C	516	BCR	C27-C26-C25	-2.68	118.85	122.73
32	1	604	CLA	CMB-C2B-C3B	2.68	129.68	124.68
32	Yy	604	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
32	y	304	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
32	BB	603	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
32	CC	505	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
39	Rr	607	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
39	S	607	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
39	Y	605	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
32	RR	304	CLA	O2D-CGD-CBD	2.67	116.02	111.27
34	Cc	516	BCR	C2-C1-C6	2.67	114.60	110.48
34	CC	517	BCR	C30-C25-C26	-2.67	118.85	122.61
41	NN	617	XAT	O24-C25-C38	2.67	118.26	115.06
32	Y	610	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
39	y	308	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
42	NN	618	NEX	C11-C10-C9	-2.67	123.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Nn	307	LUT	C36-C21-C26	2.67	113.59	109.55
32	NN	612	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
32	YY	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
39	s	607	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
34	C	517	BCR	C15-C16-C17	-2.67	118.00	123.47
42	Gg	318	NEX	C28-C29-C30	2.67	123.04	118.94
40	2	614	LUT	C36-C21-C26	2.67	113.59	109.55
35	d	404	PL9	C40-C39-C41	-2.67	110.78	115.27
32	Y	604	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
34	b	617	BCR	C40-C30-C25	2.67	114.63	110.30
32	Ss	608	CLA	CHB-C4A-NA	2.67	128.21	124.51
32	b	605	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
32	Nn	314	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
40	N	615	LUT	C38-C25-C24	-2.67	117.85	123.56
39	n	606	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
32	Yy	602	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
39	2	606	CHL	CBD-CHA-C1A	2.67	131.65	128.50
32	NN	610	CLA	C4A-NA-C1A	2.67	107.91	106.71
39	G	609	CHL	CHB-C4A-NA	2.67	128.20	124.51
32	BB	613	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
39	3	608	CHL	C1B-CHB-C4A	-2.67	124.83	130.12
32	y	313	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
32	AA	405	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
32	r	602	CLA	C1D-ND-C4D	-2.67	104.44	106.33
34	C	516	BCR	C28-C27-C26	-2.67	109.31	114.08
32	Gg	314	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
39	R	606	CHL	CMB-C2B-C1B	-2.67	124.36	128.46
32	B	622	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
32	Cc	514	CLA	CHB-C4A-NA	2.67	128.20	124.51
32	NN	610	CLA	CMB-C2B-C3B	2.67	129.67	124.68
34	C	517	BCR	C28-C27-C26	-2.67	109.32	114.08
32	b	610	CLA	CMB-C2B-C3B	2.67	129.66	124.68
32	R	613	CLA	CMB-C2B-C3B	2.66	129.66	124.68
35	AA	410	PL9	C30-C29-C31	-2.66	110.79	115.27
32	SS	311	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
34	CC	516	BCR	C27-C26-C25	-2.66	118.86	122.73
32	N	604	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
32	GG	613	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
32	RR	310	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
34	Hh	101	BCR	C34-C9-C8	-2.66	113.88	118.08
32	GG	603	CLA	CMB-C2B-C3B	2.66	129.66	124.68
32	BB	612	CLA	CHB-C4A-NA	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	606	CHL	CHB-C4A-NA	2.66	128.19	124.51
32	RR	311	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
32	2	611	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
41	4	314	XAT	C40-C33-C34	-2.66	119.20	122.92
40	n	616	LUT	C36-C21-C26	2.66	113.58	109.55
40	Rr	614	LUT	C38-C25-C24	-2.66	117.87	123.56
32	Nn	312	CLA	O2D-CGD-CBD	2.66	116.00	111.27
42	NN	618	NEX	C40-C33-C34	-2.66	119.20	122.92
39	44	601	CHL	C1B-CHB-C4A	-2.66	124.85	130.12
32	NN	602	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	RR	311	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	Ss	610	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
34	H	101	BCR	C16-C15-C14	-2.66	118.03	123.47
34	Aa	411	BCR	C37-C22-C23	2.66	122.27	118.08
32	DD	401	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
39	44	601	CHL	CHB-C4A-NA	2.66	128.19	124.51
39	y	303	CHL	CHB-C4A-NA	2.66	128.19	124.51
39	2	606	CHL	O2D-CGD-O1D	-2.66	118.64	123.84
39	Gg	310	CHL	CHB-C4A-NA	2.66	128.19	124.51
35	AA	410	PL9	C35-C34-C36	-2.66	110.80	115.27
34	BB	618	BCR	C36-C18-C17	-2.66	119.20	122.92
39	33	608	CHL	CHB-C4A-NA	2.66	128.19	124.51
34	a	411	BCR	C37-C22-C23	2.66	122.26	118.08
38	Bb	620	LMG	O8-C28-C29	2.66	120.25	111.91
39	NN	606	CHL	O2D-CGD-O1D	-2.66	118.64	123.84
32	3	611	CLA	CMB-C2B-C3B	2.66	129.65	124.68
39	11	608	CHL	C4A-NA-C1A	2.66	107.90	106.71
40	Gg	317	LUT	C38-C25-C24	-2.66	117.88	123.56
35	AA	410	PL9	C53-C6-C1	2.66	120.42	114.99
34	B	613	BCR	C15-C16-C17	-2.66	118.03	123.47
32	NN	602	CLA	O2D-CGD-CBD	2.66	115.99	111.27
32	D	401	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
39	Y	601	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
32	r	612	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
39	3	606	CHL	C1B-CHB-C4A	-2.65	124.86	130.12
39	y	309	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
39	33	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
32	SS	310	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
39	2	608	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
36	4	315	LHG	C5-O7-C7	-2.65	112.95	117.90
35	A	410	PL9	C53-C6-C1	2.65	120.41	114.99
32	CC	514	CLA	O2D-CGD-O1D	-2.65	118.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	22	611	CLA	CBD-CHA-C1A	2.65	131.63	128.50
34	TT	101	BCR	C3-C4-C5	-2.65	109.34	114.08
34	DD	405	BCR	C33-C5-C4	2.65	118.71	113.62
32	YY	614	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
39	3	607	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
36	JJ	101	LHG	O8-C23-C24	2.65	120.23	111.91
39	n	608	CHL	O2D-CGD-O1D	-2.65	118.65	123.84
32	n	611	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
32	C	509	CLA	CMB-C2B-C3B	2.65	129.64	124.68
32	B	609	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
39	s	601	CHL	C1B-CHB-C4A	-2.65	124.87	130.12
34	d	403	BCR	C33-C5-C4	2.65	118.71	113.62
41	GG	619	XAT	O4-C5-C18	2.65	118.23	115.06
36	d	406	LHG	O8-C23-C24	2.65	120.22	111.91
32	Bb	616	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
32	s	610	CLA	CMB-C2B-C3B	2.65	129.64	124.68
32	3	610	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
39	YY	606	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
42	Y	617	NEX	C15-C35-C34	-2.65	118.05	123.47
39	1	607	CHL	C1B-CHB-C4A	-2.65	124.87	130.12
32	NN	602	CLA	CMB-C2B-C3B	2.65	129.63	124.68
39	4	309	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
32	R	603	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
39	SS	307	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
34	BB	620	BCR	C33-C5-C4	2.65	118.70	113.62
32	RR	308	CLA	CMB-C2B-C3B	2.65	129.63	124.68
32	Bb	610	CLA	CMB-C2B-C3B	2.65	129.63	124.68
36	g	618	LHG	O8-C23-C24	2.65	120.22	111.91
46	Ee	101	HEM	C4D-ND-C1D	2.65	107.81	105.07
32	b	611	CLA	CMB-C2B-C3B	2.65	129.63	124.68
32	b	613	CLA	CHB-C4A-NA	2.65	128.17	124.51
40	n	616	LUT	C38-C25-C24	-2.65	117.90	123.56
34	T	101	BCR	C19-C18-C17	-2.65	114.88	118.94
32	Nn	312	CLA	CHB-C4A-NA	2.65	128.17	124.51
34	c	516	BCR	C2-C1-C6	2.65	114.55	110.48
32	Bb	616	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
32	CC	503	CLA	CMB-C2B-C3B	2.65	129.63	124.68
40	Yy	616	LUT	C38-C25-C24	-2.65	117.90	123.56
34	AA	409	BCR	C2-C1-C6	2.65	114.55	110.48
34	KK	103	BCR	C16-C15-C14	-2.64	118.06	123.47
39	y	309	CHL	C1B-CHB-C4A	-2.64	124.88	130.12
32	BB	603	CLA	CMB-C2B-C3B	2.64	129.62	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	CC	507	CLA	CBA-CAA-C2A	2.64	121.67	113.86
32	4	311	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	BB	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
32	Bb	614	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
32	y	312	CLA	CHB-C4A-NA	2.64	128.17	124.51
39	Nn	319	CHL	CHB-C4A-NA	2.64	128.17	124.51
32	YY	613	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
44	Cc	519	DGD	O6D-C5D-C6D	2.64	112.00	106.67
35	DD	406	PL9	C53-C6-C1	2.64	120.39	114.99
32	33	610	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	Dd	402	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	Y	614	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
32	CC	512	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
40	Gg	317	LUT	C17-C1-C6	-2.64	106.02	110.30
32	c	505	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	GG	603	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
34	CC	516	BCR	C15-C16-C17	-2.64	118.07	123.47
40	Yy	616	LUT	C36-C21-C26	2.64	113.54	109.55
32	R	610	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
32	BB	602	CLA	CMB-C2B-C3B	2.64	129.62	124.68
32	Bb	609	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
40	s	614	LUT	C8-C9-C10	-2.64	114.89	118.94
32	d	402	CLA	CMB-C2B-C3B	2.64	129.61	124.68
32	44	615	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
39	GG	606	CHL	C1B-CHB-C4A	-2.64	124.89	130.12
32	a	410	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
39	2	605	CHL	CHB-C4A-NA	2.64	128.16	124.51
36	Dd	406	LHG	O8-C23-C24	2.64	120.18	111.91
32	Yy	611	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
32	DD	404	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
34	D	406	BCR	C33-C5-C4	2.64	118.68	113.62
40	Nn	306	LUT	C38-C25-C24	-2.64	117.92	123.56
32	g	610	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
32	BB	615	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
39	44	607	CHL	C1B-CHB-C4A	-2.64	124.90	130.12
35	d	404	PL9	C30-C29-C31	-2.64	110.84	115.27
32	b	614	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
32	Bb	610	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
39	2	608	CHL	C1B-CHB-C4A	-2.64	124.90	130.12
32	y	304	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
32	N	602	CLA	CMB-C2B-C3B	2.63	129.61	124.68
32	B	605	CLA	C1B-CHB-C4A	-2.63	124.90	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Bb	605	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
38	b	621	LMG	O8-C28-C29	2.63	120.17	111.91
32	Cc	505	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
39	Y	601	CHL	C1B-CHB-C4A	-2.63	124.90	130.12
39	YY	606	CHL	C1B-CHB-C4A	-2.63	124.90	130.12
32	R	611	CLA	CHB-C4A-NA	2.63	128.15	124.51
32	GG	604	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
32	NN	604	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
41	R	616	XAT	C35-C15-C14	-2.63	118.08	123.47
32	22	612	CLA	CMB-C2B-C3B	2.63	129.60	124.68
39	2	605	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
35	DD	406	PL9	C30-C29-C31	-2.63	110.85	115.27
32	YY	603	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
38	Bb	621	LMG	O8-C28-C29	2.63	120.16	111.91
44	Hh	102	DGD	O1G-C1A-C2A	2.63	120.16	111.91
40	G	615	LUT	C38-C25-C24	-2.63	117.93	123.56
32	11	612	CLA	CBC-CAC-C3C	2.63	119.68	112.43
32	BB	608	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
32	4	303	CLA	CMB-C2B-C3B	2.63	129.60	124.68
39	N	601	CHL	CMB-C2B-C1B	-2.63	124.42	128.46
32	RR	313	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
39	Ss	601	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
32	Yy	603	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
39	N	601	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
33	DD	402	PHO	O2D-CGD-O1D	-2.63	118.70	123.84
32	1	602	CLA	CBD-CHA-C1A	2.63	131.60	128.50
32	Y	612	CLA	CMB-C2B-C3B	2.63	129.59	124.68
36	AA	414	LHG	O8-C23-C24	2.63	120.15	111.91
32	Gg	303	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
32	33	612	CLA	CHD-C1D-ND	-2.63	122.04	124.45
39	1	608	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
40	y	317	LUT	C38-C25-C24	-2.63	117.94	123.56
32	B	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
32	33	611	CLA	CBD-CHA-C1A	2.63	131.59	128.50
32	YY	604	CLA	O2D-CGD-CBD	2.63	115.93	111.27
34	KK	103	BCR	C30-C25-C24	2.63	123.20	115.78
34	K	102	BCR	C40-C30-C25	2.63	114.56	110.30
39	y	311	CHL	C1B-CHB-C4A	-2.62	124.92	130.12
39	G	601	CHL	CHB-C4A-NA	2.62	128.14	124.51
32	b	615	CLA	CMB-C2B-C3B	2.62	129.59	124.68
41	4	314	XAT	O4-C5-C18	2.62	118.20	115.06
39	44	608	CHL	O2D-CGD-O1D	-2.62	118.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	610	CLA	CBD-CHA-C1A	2.62	131.59	128.50
34	B	616	BCR	C16-C15-C14	-2.62	118.10	123.47
32	44	611	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
32	G	603	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
32	b	607	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
39	Yy	605	CHL	C1B-CHB-C4A	-2.62	124.92	130.12
32	C	508	CLA	CBA-CAA-C2A	2.62	121.60	113.86
40	n	616	LUT	C7-C8-C9	-2.62	122.27	126.23
32	RR	303	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
32	Rr	601	CLA	CMB-C2B-C3B	2.62	129.58	124.68
32	G	603	CLA	CMB-C2B-C3B	2.62	129.58	124.68
32	Y	603	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
41	NN	617	XAT	C6-C7-C8	-2.62	120.45	125.99
32	r	611	CLA	CMB-C2B-C3B	2.62	129.58	124.68
33	Aa	408	PHO	O1D-CGD-CBD	2.62	129.10	124.74
32	c	507	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
32	1	610	CLA	CMB-C2B-C3B	2.62	129.58	124.68
40	g	616	LUT	C38-C25-C24	-2.62	117.96	123.56
34	Aa	411	BCR	C36-C18-C17	-2.62	119.25	122.92
32	Gg	314	CLA	CBD-CHA-C1A	2.62	131.59	128.50
34	Cc	518	BCR	C27-C26-C25	-2.62	118.93	122.73
32	YY	612	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
32	GG	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
34	H	101	BCR	C20-C21-C22	-2.62	123.58	127.31
32	RR	302	CLA	CMB-C2B-C3B	2.62	129.57	124.68
40	2	614	LUT	C2-C3-C4	-2.62	106.72	110.30
32	BB	602	CLA	CHB-C4A-NA	2.62	128.13	124.51
32	s	602	CLA	CMB-C2B-C3B	2.62	129.57	124.68
32	S	608	CLA	CHD-C1D-ND	-2.62	122.05	124.45
32	2	603	CLA	CBD-CHA-C1A	2.62	131.58	128.50
32	Gg	304	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
32	b	613	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
32	AA	406	CLA	CHD-C1D-ND	-2.61	122.05	124.45
34	TT	101	BCR	C24-C23-C22	-2.61	122.28	126.23
32	R	610	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
39	G	606	CHL	C1B-CHB-C4A	-2.61	124.94	130.12
32	44	611	CLA	CHB-C4A-NA	2.61	128.13	124.51
34	A	409	BCR	C2-C1-C6	2.61	114.50	110.48
34	CC	516	BCR	C28-C27-C26	-2.61	109.41	114.08
37	C	501	SQD	O7-S-C6	2.61	110.04	106.94
39	r	605	CHL	C1B-CHB-C4A	-2.61	124.94	130.12
36	J	101	LHG	O8-C23-C24	2.61	120.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	513	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
32	Gg	305	CLA	CHD-C1D-ND	-2.61	122.05	124.45
32	BB	609	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
40	Gg	317	LUT	C36-C21-C26	2.61	113.50	109.55
32	Cc	514	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
32	44	610	CLA	CMB-C2B-C3B	2.61	129.56	124.68
32	11	613	CLA	CMB-C2B-C3B	2.61	129.56	124.68
32	C	514	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
40	NN	615	LUT	C38-C25-C24	-2.61	117.98	123.56
40	Ss	615	LUT	C18-C5-C6	2.61	127.46	124.53
32	B	619	CLA	CHB-C4A-NA	2.61	128.12	124.51
32	GG	610	CLA	CHD-C1D-ND	-2.61	122.06	124.45
39	g	607	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
32	Y	613	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
32	Ss	603	CLA	CMB-C2B-C3B	2.61	129.56	124.68
40	r	614	LUT	C38-C25-C24	-2.61	117.98	123.56
32	Ss	610	CLA	CMB-C2B-C3B	2.61	129.55	124.68
32	BB	608	CLA	CAA-C2A-C1A	-2.61	103.44	111.97
32	22	611	CLA	CHD-C1D-ND	-2.61	122.06	124.45
32	11	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
37	CC	501	SQD	C45-O47-C7	-2.60	111.38	117.79
39	YY	605	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
39	YY	607	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
39	S	605	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
32	Aa	405	CLA	CAC-C3C-C4C	2.60	128.19	124.81
32	NN	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
32	Bb	607	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
39	Ss	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
32	C	513	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
32	c	512	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
39	y	310	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
32	Bb	615	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
41	r	615	XAT	C6-C7-C8	-2.60	120.49	125.99
32	b	604	CLA	CMB-C2B-C3B	2.60	129.54	124.68
32	BB	607	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
32	S	602	CLA	CMB-C2B-C3B	2.60	129.54	124.68
33	A	407	PHO	CMB-C2B-C3B	2.60	129.54	124.68
39	33	607	CHL	CBD-CHA-C1A	2.60	131.56	128.50
32	B	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	Gg	306	CHL	CHB-C4A-NA	2.60	128.11	124.51
34	K	102	BCR	C27-C26-C25	-2.60	118.96	122.73
39	y	307	CHL	C1B-CHB-C4A	-2.60	124.97	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	408	PHO	O1D-CGD-CBD	2.60	129.07	124.74
42	YY	617	NEX	C15-C35-C34	-2.60	118.15	123.47
32	33	610	CLA	CBD-CHA-C1A	2.60	131.56	128.50
32	s	603	CLA	CMB-C2B-C3B	2.60	129.54	124.68
32	s	610	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
32	NN	614	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
32	2	602	CLA	CBD-CHA-C1A	2.60	131.56	128.50
32	RR	303	CLA	CMB-C2B-C3B	2.60	129.54	124.68
32	Nn	312	CLA	CMB-C2B-C3B	2.60	129.54	124.68
41	Yy	619	XAT	C38-C25-C26	-2.60	117.91	122.26
46	e	101	HEM	C4D-ND-C1D	2.60	107.76	105.07
34	Hh	101	BCR	C11-C10-C9	-2.60	123.60	127.31
39	4	302	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
40	n	615	LUT	C38-C25-C24	-2.60	118.00	123.56
36	3	614	LHG	O8-C23-C24	2.60	120.06	111.91
32	c	512	CLA	CHB-C4A-NA	2.60	128.10	124.51
32	s	602	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
32	22	603	CLA	CBD-CHA-C1A	2.60	131.56	128.50
39	11	606	CHL	CBD-CHA-C1A	2.60	131.56	128.50
32	RR	309	CLA	CHB-C4A-NA	2.60	128.10	124.51
39	Y	607	CHL	C1B-CHB-C4A	-2.60	124.98	130.12
32	Y	611	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
32	CC	510	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
34	C	518	BCR	C37-C22-C23	2.59	122.17	118.08
46	Ee	101	HEM	C4B-CHC-C1C	2.59	125.98	122.56
32	CC	511	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
32	Dd	402	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
39	y	311	CHL	CHB-C4A-NA	2.59	128.10	124.51
32	c	503	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
32	1	604	CLA	CBD-CHA-C1A	2.59	131.56	128.50
40	S	614	LUT	C18-C5-C4	2.59	119.16	114.36
32	CC	503	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
39	44	607	CHL	CHB-C4A-NA	2.59	128.10	124.51
39	11	605	CHL	CHB-C4A-NA	2.59	128.10	124.51
32	b	616	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
32	2	609	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
32	Yy	610	CLA	CHB-C4A-NA	2.59	128.09	124.51
32	CC	503	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
35	A	410	PL9	C20-C19-C21	-2.59	110.92	115.27
40	Nn	307	LUT	C19-C9-C8	2.59	122.16	118.08
34	D	406	BCR	C3-C4-C5	-2.59	109.45	114.08
32	Nn	303	CLA	CMB-C2B-C3B	2.59	129.52	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Bb	613	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
39	Gg	302	CHL	C1B-CHB-C4A	-2.59	124.99	130.12
32	b	606	CLA	CMB-C2B-C3B	2.59	129.52	124.68
39	22	601	CHL	C1B-CHB-C4A	-2.59	124.99	130.12
39	Gg	308	CHL	C1B-CHB-C4A	-2.59	124.99	130.12
32	r	602	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
32	Y	612	CLA	CED-O2D-CGD	2.59	121.79	115.94
32	c	504	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	11	607	CHL	CHB-C4A-NA	2.59	128.09	124.51
32	s	612	CLA	CMB-C2B-C3B	2.59	129.52	124.68
32	y	313	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
32	d	402	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
40	G	615	LUT	C36-C21-C26	2.59	113.46	109.55
32	c	505	CLA	C4A-NA-C1A	2.58	107.87	106.71
32	r	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
32	4	312	CLA	CHB-C4A-NA	2.58	128.09	124.51
32	Cc	506	CLA	CHB-C4A-NA	2.58	128.09	124.51
32	n	614	CLA	CHD-C1D-ND	-2.58	122.08	124.45
32	22	611	CLA	CMB-C2B-C3B	2.58	129.51	124.68
35	D	407	PL9	C53-C6-C1	2.58	120.27	114.99
32	R	609	CLA	CHB-C4A-NA	2.58	128.09	124.51
32	BB	606	CLA	CMB-C2B-C1B	-2.58	124.49	128.46
32	RR	308	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
32	XX	201	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
32	C	503	CLA	CHD-C1D-ND	-2.58	122.08	124.45
32	CC	510	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
32	r	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
34	Bb	619	BCR	C27-C26-C25	-2.58	118.98	122.73
34	Aa	411	BCR	C2-C1-C6	2.58	114.46	110.48
32	r	609	CLA	CMB-C2B-C3B	2.58	129.51	124.68
32	33	604	CLA	CBD-CHA-C1A	2.58	131.54	128.50
32	g	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
32	3	603	CLA	CMB-C2B-C3B	2.58	129.51	124.68
32	b	604	CLA	C4-C3-C5	2.58	119.61	115.27
39	Ss	607	CHL	O2D-CGD-O1D	-2.58	118.79	123.84
32	n	612	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
32	y	304	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
40	2	614	LUT	C19-C9-C8	2.58	122.14	118.08
32	SS	309	CLA	CMB-C2B-C3B	2.58	129.50	124.68
32	C	504	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
39	2	601	CHL	C1B-CHB-C4A	-2.58	125.01	130.12
32	R	604	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	11	610	CLA	CMB-C2B-C3B	2.58	129.50	124.68
36	11	614	LHG	O8-C23-C24	2.58	120.00	111.91
32	2	611	CLA	CBD-CHA-C1A	2.58	131.54	128.50
32	b	601	CLA	CMB-C2B-C3B	2.58	129.50	124.68
40	y	318	LUT	C3-C4-C5	-2.58	106.72	111.85
32	RR	313	CLA	CMB-C2B-C3B	2.58	129.50	124.68
34	Bb	618	BCR	C15-C16-C17	-2.58	118.20	123.47
35	Dd	404	PL9	C53-C6-C1	2.58	120.26	114.99
34	TT	101	BCR	C29-C30-C25	2.58	114.45	110.48
32	CC	513	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
39	Nn	311	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
39	Nn	317	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
32	y	312	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
41	g	619	XAT	C39-C29-C28	2.57	122.13	118.08
32	YY	611	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
32	GG	610	CLA	CHB-C4A-NA	2.57	128.07	124.51
32	S	610	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
32	YY	602	CLA	CMB-C2B-C3B	2.57	129.49	124.68
34	Kk	101	BCR	C16-C15-C14	-2.57	118.21	123.47
39	g	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
32	S	611	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
32	R	612	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
32	1	613	CLA	CMB-C2B-C3B	2.57	129.49	124.68
32	r	613	CLA	CHD-C1D-ND	-2.57	122.09	124.45
39	22	606	CHL	CBD-CHA-C1A	2.57	131.53	128.50
32	C	509	CLA	O2D-CGD-CBD	2.57	115.83	111.27
32	Bb	604	CLA	C4-C3-C5	2.57	119.59	115.27
32	3	609	CLA	CMB-C2B-C3B	2.57	129.48	124.68
32	b	616	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
42	N	618	NEX	C40-C33-C34	-2.57	119.33	122.92
32	C	508	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
32	R	613	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
41	Yy	619	XAT	C24-C23-C22	-2.57	105.81	110.77
32	X	201	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
41	GG	617	XAT	C39-C29-C28	-2.57	114.03	118.08
32	Ss	602	CLA	CMB-C2B-C3B	2.57	129.48	124.68
32	Nn	305	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
32	Nn	305	CLA	CHD-C1D-ND	-2.57	122.09	124.45
36	Y	618	LHG	O8-C23-C24	2.57	119.96	111.91
34	a	411	BCR	C2-C1-C6	2.57	114.43	110.48
32	SS	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
32	c	501	CLA	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	102	BCR	C30-C25-C24	2.57	123.04	115.78
32	XX	201	CLA	CMA-C3A-C2A	-2.57	110.11	116.10
32	A	405	CLA	CHB-C4A-NA	2.57	128.06	124.51
35	d	404	PL9	C53-C6-C1	2.56	120.23	114.99
32	CC	505	CLA	CHD-C1D-ND	-2.56	122.10	124.45
32	CC	512	CLA	CMB-C2B-C1B	-2.56	124.52	128.46
32	YY	604	CLA	CMB-C2B-C1B	-2.56	124.52	128.46
42	N	618	NEX	C11-C10-C9	-2.56	123.65	127.31
32	R	604	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
32	SS	314	CLA	CMB-C2B-C3B	2.56	129.47	124.68
34	DD	405	BCR	C3-C4-C5	-2.56	109.50	114.08
39	R	605	CHL	C4A-NA-C1A	2.56	107.86	106.71
32	b	612	CLA	CMB-C2B-C3B	2.56	129.47	124.68
40	Gg	316	LUT	C36-C21-C26	2.56	113.43	109.55
32	c	513	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	Bb	606	CLA	CMB-C2B-C3B	2.56	129.47	124.68
32	3	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
41	y	302	XAT	C19-C9-C10	-2.56	119.34	122.92
32	C	508	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
32	YY	614	CLA	CHB-C4A-NA	2.56	128.05	124.51
34	CC	515	BCR	C34-C9-C8	-2.56	114.04	118.08
32	R	602	CLA	CMB-C2B-C3B	2.56	129.47	124.68
32	YY	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	CC	509	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	GG	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
40	YY	616	LUT	C38-C25-C24	-2.56	118.08	123.56
44	CC	518	DGD	O1G-C1A-C2A	2.56	119.94	111.91
32	DD	403	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	C	510	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	c	511	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
32	Cc	509	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
39	N	607	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
32	Ss	603	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
39	Nn	316	CHL	O2D-CGD-O1D	-2.56	118.84	123.84
32	CC	510	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	SS	304	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	Ss	613	CLA	CMB-C2B-C1B	-2.56	124.54	128.46
39	N	606	CHL	O2D-CGD-O1D	-2.56	118.84	123.84
41	Nn	308	XAT	C15-C35-C34	-2.56	118.24	123.47
32	n	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	R	609	CLA	CMB-C2B-C3B	2.55	129.46	124.68
32	CC	507	CLA	O2D-CGD-O1D	-2.55	118.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	613	CLA	CMB-C2B-C3B	2.55	129.46	124.68
39	RR	307	CHL	C1B-CHB-C4A	-2.55	125.06	130.12
32	c	509	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
42	Yy	617	NEX	C20-C13-C14	-2.55	119.35	122.92
44	Aa	401	DGD	O1G-C1A-C2A	2.55	119.92	111.91
32	Y	602	CLA	CMB-C2B-C3B	2.55	129.45	124.68
32	SS	303	CLA	CMB-C2B-C3B	2.55	129.45	124.68
39	3	601	CHL	CHB-C4A-NA	2.55	128.04	124.51
36	A	414	LHG	O8-C23-C24	2.55	119.91	111.91
44	a	415	DGD	O1G-C1A-C2A	2.55	119.91	111.91
32	Gg	312	CLA	CMB-C2B-C3B	2.55	129.45	124.68
32	Gg	313	CLA	CMB-C2B-C3B	2.55	129.45	124.68
32	Nn	303	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
32	2	612	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
40	RR	315	LUT	C19-C9-C8	2.55	122.09	118.08
32	44	602	CLA	CMB-C2B-C3B	2.55	129.45	124.68
32	CC	508	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
39	GG	608	CHL	C2A-C1A-CHA	2.55	128.30	123.85
32	BB	607	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	G	611	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
32	CC	507	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
34	B	614	BCR	C37-C22-C21	-2.55	119.36	122.92
40	Nn	307	LUT	C38-C25-C24	-2.55	118.11	123.56
35	d	404	PL9	C35-C34-C36	-2.55	110.99	115.27
32	11	603	CLA	CBD-CHA-C1A	2.55	131.50	128.50
41	N	617	XAT	C6-C7-C8	-2.55	120.61	125.99
44	CC	522	DGD	O1G-C1A-C2A	2.55	119.90	111.91
40	s	615	LUT	C17-C1-C6	-2.55	106.17	110.30
32	1	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
32	g	603	CLA	CMB-C2B-C3B	2.55	129.44	124.68
32	Nn	302	CLA	CMB-C2B-C3B	2.55	129.44	124.68
32	Gg	312	CLA	O2A-C1-C2	-2.55	101.95	108.64
32	g	610	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
32	N	610	CLA	C4A-NA-C1A	2.54	107.85	106.71
32	Cc	513	CLA	CMB-C2B-C3B	2.54	129.44	124.68
32	C	504	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	B	607	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	BB	609	CLA	C5-C3-C2	2.54	126.27	121.12
39	Yy	608	CHL	C1B-CHB-C4A	-2.54	125.08	130.12
32	XX	201	CLA	CHD-C1D-ND	-2.54	122.12	124.45
32	y	305	CLA	CHB-C4A-NA	2.54	128.03	124.51
40	4	313	LUT	C36-C21-C26	2.54	113.39	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	604	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
41	Rr	615	XAT	C16-C1-C2	-2.54	104.57	108.98
32	C	511	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
40	NN	615	LUT	C2-C3-C4	-2.54	106.83	110.30
32	AA	405	CLA	CHB-C4A-NA	2.54	128.02	124.51
32	1l	602	CLA	CHD-C1D-ND	-2.54	122.12	124.45
39	Ss	601	CHL	C1B-CHB-C4A	-2.54	125.09	130.12
39	SS	302	CHL	C1B-CHB-C4A	-2.54	125.09	130.12
32	Nn	301	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
34	c	516	BCR	C8-C7-C6	-2.54	120.07	127.20
39	Yy	608	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
41	G	619	XAT	C20-C13-C14	-2.54	119.37	122.92
32	NN	611	CLA	CMB-C2B-C3B	2.54	129.43	124.68
39	g	606	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
32	4	310	CLA	CMB-C2B-C3B	2.54	129.43	124.68
39	S	601	CHL	C1B-CHB-C4A	-2.54	125.09	130.12
32	B	608	CLA	CHB-C4A-NA	2.54	128.02	124.51
32	Cc	515	CLA	CHB-C4A-NA	2.54	128.02	124.51
40	N	615	LUT	C17-C1-C6	-2.54	106.19	110.30
40	GG	615	LUT	C36-C21-C26	2.54	113.39	109.55
42	Yy	617	NEX	C15-C35-C34	-2.54	118.28	123.47
32	B	618	CLA	CMB-C2B-C3B	2.54	129.42	124.68
32	C	504	CLA	CMB-C2B-C3B	2.53	129.42	124.68
32	Bb	604	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
32	n	613	CLA	CMB-C2B-C3B	2.53	129.42	124.68
32	C	509	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
32	44	604	CLA	CMB-C2B-C3B	2.53	129.42	124.68
32	N	611	CLA	CMB-C2B-C3B	2.53	129.42	124.68
32	n	602	CLA	O2D-CGD-CBD	2.53	115.77	111.27
39	YY	607	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
32	b	612	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	DD	401	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	GG	611	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
38	j	101	LMG	O8-C28-C29	2.53	119.85	111.91
43	C	502	LMU	C1B-O1B-C4'	-2.53	111.70	117.96
40	N	616	LUT	C19-C9-C8	2.53	122.06	118.08
32	c	509	CLA	CMB-C2B-C3B	2.53	129.41	124.68
32	R	613	CLA	CAC-C3C-C4C	2.53	128.09	124.81
32	s	608	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
32	CC	502	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
38	Cc	501	LMG	C1-C2-C3	2.53	115.26	110.00
34	K	102	BCR	C38-C26-C27	2.53	118.47	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	SS	311	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	Bb	602	CLA	CMB-C2B-C3B	2.53	129.41	124.68
32	Bb	607	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
34	C	516	BCR	C34-C9-C8	-2.53	114.10	118.08
39	NN	607	CHL	C1B-CHB-C4A	-2.53	125.11	130.12
40	N	616	LUT	C15-C35-C34	-2.53	118.30	123.47
32	s	603	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
32	n	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
32	Nn	304	CLA	CMB-C2B-C3B	2.52	129.40	124.68
39	R	607	CHL	C1B-CHB-C4A	-2.52	125.12	130.12
39	n	607	CHL	C1B-CHB-C4A	-2.52	125.12	130.12
32	44	603	CLA	CMB-C2B-C3B	2.52	129.40	124.68
32	C	507	CLA	CMB-C2B-C3B	2.52	129.40	124.68
32	b	606	CLA	CHB-C4A-NA	2.52	128.00	124.51
40	Y	616	LUT	C38-C25-C24	-2.52	118.16	123.56
34	Bb	619	BCR	C37-C22-C21	-2.52	119.39	122.92
38	Dd	408	LMG	O8-C28-C29	2.52	119.83	111.91
32	BB	612	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
32	b	607	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
35	D	407	PL9	C7-C3-C4	2.52	118.93	116.88
40	Y	616	LUT	C18-C5-C4	2.52	119.03	114.36
35	D	407	PL9	C30-C29-C31	-2.52	111.03	115.27
32	C	512	CLA	CHB-C4A-NA	2.52	128.00	124.51
32	S	603	CLA	CHB-C4A-NA	2.52	128.00	124.51
32	N	611	CLA	CHB-C4A-NA	2.52	128.00	124.51
34	DD	405	BCR	C36-C18-C19	2.52	122.05	118.08
32	Cc	503	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	NN	601	CHL	C3C-C4C-NC	-2.52	107.75	110.57
39	11	601	CHL	CHB-C4A-NA	2.52	128.00	124.51
32	BB	601	CLA	CMB-C2B-C3B	2.52	129.39	124.68
39	Gg	309	CHL	C1B-CHB-C4A	-2.52	125.13	130.12
41	RR	316	XAT	C35-C15-C14	-2.52	118.32	123.47
39	g	601	CHL	C1B-CHB-C4A	-2.52	125.13	130.12
34	BB	617	BCR	C38-C26-C25	-2.52	121.70	124.53
32	B	611	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
39	Gg	307	CHL	C1B-CHB-C4A	-2.52	125.14	130.12
32	C	511	CLA	CHB-C4A-NA	2.52	127.99	124.51
32	BB	615	CLA	CHB-C4A-NA	2.52	127.99	124.51
32	33	610	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
34	c	516	BCR	C33-C5-C4	2.51	118.45	113.62
32	GG	611	CLA	O2D-CGD-O1D	-2.51	118.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	22	608	CHL	CBD-CHA-C1A	2.51	131.46	128.50
35	DD	406	PL9	C25-C24-C26	-2.51	111.04	115.27
32	3	602	CLA	CMB-C2B-C3B	2.51	129.38	124.68
39	RR	305	CHL	CHD-C1D-ND	-2.51	122.14	124.45
35	A	410	PL9	C40-C39-C41	-2.51	111.04	115.27
32	Ss	612	CLA	CMB-C2B-C3B	2.51	129.38	124.68
36	CC	521	LHG	O8-C23-C24	2.51	119.79	111.91
32	Rr	609	CLA	CHB-C4A-NA	2.51	127.99	124.51
39	4	308	CHL	C2A-C1A-CHA	2.51	128.25	123.86
32	S	613	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
32	CC	503	CLA	CHD-C1D-ND	-2.51	122.14	124.45
32	Cc	508	CLA	C4-C3-C5	2.51	119.50	115.27
40	y	318	LUT	C19-C9-C8	2.51	122.03	118.08
39	Yy	601	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
32	c	506	CLA	C4-C3-C5	2.51	119.50	115.27
32	g	613	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
32	Nn	304	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
34	c	514	BCR	C34-C9-C8	-2.51	114.12	118.08
34	CC	517	BCR	C37-C22-C23	2.51	122.03	118.08
39	N	609	CHL	CHB-C4A-NA	2.51	127.98	124.51
34	b	618	BCR	C15-C16-C17	-2.51	118.33	123.47
32	S	610	CLA	CMB-C2B-C3B	2.51	129.37	124.68
33	A	407	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
39	33	606	CHL	CBD-CHA-C1A	2.51	131.46	128.50
36	II	101	LHG	O8-C23-C24	2.51	119.78	111.91
32	B	621	CLA	CHD-C1D-ND	-2.51	122.15	124.45
41	r	615	XAT	C16-C1-C2	-2.51	104.62	108.98
32	c	511	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
40	Y	616	LUT	C40-C33-C32	2.51	122.03	118.08
32	YY	611	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
34	Aa	411	BCR	C30-C25-C26	-2.51	119.08	122.61
32	GG	613	CLA	CAC-C3C-C4C	2.51	128.06	124.81
32	S	612	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
32	RR	304	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
32	s	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	c	516	BCR	C37-C22-C21	-2.51	119.41	122.92
37	A	412	SQD	O7-S-C6	2.51	109.92	106.94
32	R	614	CLA	CMB-C2B-C3B	2.51	129.37	124.68
39	Yy	609	CHL	CHB-C4A-NA	2.51	127.98	124.51
39	n	605	CHL	O2D-CGD-CBD	2.50	115.72	111.27
36	GG	618	LHG	C5-O7-C7	-2.50	111.63	117.79
32	X	201	CLA	CHD-C1D-ND	-2.50	122.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	602	CLA	CHD-C1D-ND	-2.50	122.15	124.45
32	Bb	602	CLA	CHD-C1D-ND	-2.50	122.15	124.45
39	3	605	CHL	C1B-CHB-C4A	-2.50	125.16	130.12
39	Y	606	CHL	O2D-CGD-O1D	-2.50	118.94	123.84
39	R	605	CHL	CHB-C4A-NA	2.50	127.97	124.51
32	B	605	CLA	C5-C3-C2	2.50	126.18	121.12
41	Rr	615	XAT	C39-C29-C28	2.50	122.02	118.08
39	22	607	CHL	C1B-CHB-C4A	-2.50	125.16	130.12
34	TT	101	BCR	C37-C22-C23	2.50	122.02	118.08
39	11	608	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
40	RR	315	LUT	C15-C35-C34	-2.50	118.35	123.47
33	D	402	PHO	CMB-C2B-C3B	2.50	129.36	124.68
32	y	305	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
32	C	512	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
32	Ss	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
32	r	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
39	Nn	318	CHL	C1B-CHB-C4A	-2.50	125.17	130.12
39	NN	601	CHL	CAC-C3C-C4C	2.50	128.05	124.81
40	RR	315	LUT	C38-C25-C24	-2.50	118.21	123.56
36	Ss	616	LHG	O8-C23-C24	2.50	119.75	111.91
34	a	411	BCR	C30-C25-C26	-2.50	119.10	122.61
39	33	605	CHL	C1B-CHB-C4A	-2.50	125.17	130.12
41	y	301	XAT	C39-C29-C30	-2.50	119.42	122.92
34	K	102	BCR	C36-C18-C19	2.50	122.01	118.08
32	a	407	CLA	CHD-C1D-ND	-2.50	122.16	124.45
32	n	604	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
32	BB	604	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
32	Yy	614	CLA	CHB-C4A-NA	2.50	127.96	124.51
32	33	603	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
39	2	607	CHL	C1B-CHB-C4A	-2.50	125.17	130.12
32	Cc	505	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
34	Bb	618	BCR	C36-C18-C17	-2.49	119.43	122.92
39	g	608	CHL	C1B-CHB-C4A	-2.49	125.18	130.12
39	11	608	CHL	CBD-CHA-C1A	2.49	131.44	128.50
41	4	314	XAT	C35-C15-C14	-2.49	118.37	123.47
32	y	312	CLA	C4A-NA-C1A	2.49	107.83	106.71
36	AA	411	LHG	O8-C23-C24	2.49	119.73	111.91
39	s	607	CHL	C1B-CHB-C4A	-2.49	125.18	130.12
32	11	612	CLA	C1D-ND-C4D	-2.49	104.56	106.33
40	Ss	615	LUT	C17-C1-C6	-2.49	106.26	110.30
32	Yy	603	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
39	Y	606	CHL	C1B-CHB-C4A	-2.49	125.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YY	618	LHG	O8-C23-C24	2.49	119.73	111.91
34	C	517	BCR	C38-C26-C25	-2.49	121.73	124.53
32	D	401	CLA	CHB-C4A-NA	2.49	127.96	124.51
32	s	613	CLA	CMB-C2B-C3B	2.49	129.34	124.68
32	RR	312	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
42	Rr	616	NEX	C5-C6-C1	2.49	122.17	119.70
40	R	615	LUT	C38-C25-C24	-2.49	118.23	123.56
39	4	308	CHL	CHB-C4A-NA	2.49	127.96	124.51
37	l	102	SQD	O48-C23-C24	2.49	119.72	111.91
32	SS	314	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
32	CC	506	CLA	CAC-C3C-C4C	2.49	128.04	124.81
32	C	506	CLA	CMB-C2B-C3B	2.49	129.34	124.68
32	Cc	508	CLA	CHB-C4A-NA	2.49	127.95	124.51
39	4	306	CHL	C1B-CHB-C4A	-2.49	125.19	130.12
32	YY	602	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
32	B	608	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
40	2	614	LUT	C17-C1-C6	-2.49	106.26	110.30
37	l	102	SQD	O7-S-C6	2.49	109.90	106.94
32	s	611	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
34	Bb	617	BCR	C24-C23-C22	-2.49	122.47	126.23
39	N	608	CHL	C1B-CHB-C4A	-2.49	125.19	130.12
39	n	608	CHL	C1B-CHB-C4A	-2.49	125.19	130.12
32	BB	607	CLA	CHD-C1D-ND	-2.49	122.17	124.45
32	S	609	CLA	CMB-C2B-C3B	2.49	129.33	124.68
32	YY	610	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
39	Ss	607	CHL	C1B-CHB-C4A	-2.49	125.19	130.12
32	n	602	CLA	CMB-C2B-C3B	2.49	129.33	124.68
32	CC	507	CLA	CHB-C4A-NA	2.49	127.95	124.51
32	GG	613	CLA	CBD-CHA-C1A	2.48	131.43	128.50
32	44	604	CLA	CHB-C4A-NA	2.48	127.95	124.51
32	G	602	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
32	DD	401	CLA	O2D-CGD-CBD	2.48	115.68	111.27
32	NN	612	CLA	CHB-C4A-NA	2.48	127.95	124.51
32	y	312	CLA	CMB-C2B-C3B	2.48	129.32	124.68
39	Y	607	CHL	O2D-CGD-O1D	-2.48	118.98	123.84
32	Bb	609	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
32	y	316	CLA	CHB-C4A-NA	2.48	127.94	124.51
37	B	617	SQD	O48-C23-C24	2.48	119.69	111.91
32	r	613	CLA	CMB-C2B-C3B	2.48	129.32	124.68
42	YY	617	NEX	C40-C33-C32	2.48	121.98	118.08
32	Bb	606	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
39	NN	608	CHL	C1B-CHB-C4A	-2.48	125.21	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	G	617	XAT	C40-C33-C32	2.48	121.98	118.08
32	Gg	311	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	B	613	BCR	C37-C22-C21	-2.48	119.45	122.92
32	Y	610	CLA	CAA-C2A-C1A	-2.48	103.86	111.97
32	33	613	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
40	s	615	LUT	C19-C9-C8	2.48	121.98	118.08
32	n	611	CLA	CMB-C2B-C3B	2.48	129.31	124.68
32	R	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
32	22	602	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
40	NN	616	LUT	C19-C9-C8	2.47	121.97	118.08
32	Rr	601	CLA	CHB-C4A-NA	2.47	127.93	124.51
32	C	503	CLA	CHB-C4A-NA	2.47	127.93	124.51
37	Ll	101	SQD	O7-S-C6	2.47	109.88	106.94
32	3	609	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
34	d	403	BCR	C4-C5-C6	-2.47	119.14	122.73
32	Yy	611	CLA	CMB-C2B-C3B	2.47	129.31	124.68
39	y	303	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
32	b	610	CLA	CHD-C1D-ND	-2.47	122.18	124.45
32	c	504	CLA	CHD-C1D-ND	-2.47	122.18	124.45
32	X	201	CLA	CMB-C2B-C3B	2.47	129.30	124.68
32	r	602	CLA	CMB-C2B-C3B	2.47	129.30	124.68
42	g	617	NEX	C36-C21-C26	2.47	116.72	110.05
35	Dd	404	PL9	C25-C24-C26	-2.47	111.11	115.27
32	RR	310	CLA	CHB-C4A-NA	2.47	127.93	124.51
37	BB	621	SQD	O48-C23-C24	2.47	119.66	111.91
32	2	611	CLA	CHD-C1D-ND	-2.47	122.18	124.45
32	Aa	407	CLA	CHD-C1D-ND	-2.47	122.18	124.45
32	c	506	CLA	CHB-C4A-NA	2.47	127.93	124.51
32	Gg	304	CLA	CMB-C2B-C3B	2.47	129.30	124.68
39	Y	608	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
39	1	601	CHL	CHB-C4A-NA	2.47	127.93	124.51
32	1	602	CLA	CHD-C1D-ND	-2.47	122.18	124.45
32	Ss	611	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
39	3	606	CHL	CBD-CHA-C1A	2.47	131.41	128.50
42	RR	317	NEX	C17-C1-C6	-2.47	108.26	110.47
34	C	516	BCR	C11-C10-C9	-2.47	123.79	127.31
36	G	618	LHG	O8-C23-C24	2.47	119.65	111.91
32	n	613	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
39	NN	605	CHL	O2D-CGD-CBD	2.47	115.65	111.27
32	BB	601	CLA	CHD-C1D-ND	-2.47	122.19	124.45
46	e	101	HEM	C4B-CHC-C1C	2.47	125.81	122.56
34	K	102	BCR	C7-C8-C9	-2.47	122.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	607	CHL	O2A-CGA-O1A	-2.46	117.37	123.59
32	y	306	CLA	CHB-C4A-NA	2.46	127.92	124.51
32	11	602	CLA	CBD-CHA-C1A	2.46	131.40	128.50
42	YY	617	NEX	C20-C13-C14	-2.46	119.47	122.92
32	11	613	CLA	CHD-C1D-ND	-2.46	122.19	124.45
33	AA	407	PHO	O2D-CGD-O1D	-2.46	119.02	123.84
35	AA	410	PL9	C7-C3-C2	-2.46	120.06	123.30
32	r	602	CLA	CHB-C4A-NA	2.46	127.92	124.51
32	y	315	CLA	CHB-C4A-NA	2.46	127.92	124.51
36	A	411	LHG	O8-C23-C24	2.46	119.63	111.91
32	B	621	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
41	4	314	XAT	C39-C29-C30	-2.46	119.48	122.92
32	4	311	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
32	Yy	604	CLA	CHD-C1D-ND	-2.46	122.19	124.45
32	S	611	CLA	CMB-C2B-C3B	2.46	129.28	124.68
32	Rr	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
39	11	608	CHL	CHB-C4A-NA	2.46	127.91	124.51
34	b	618	BCR	C36-C18-C17	-2.46	119.48	122.92
32	22	603	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
32	B	619	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
32	N	604	CLA	CMB-C2B-C3B	2.46	129.28	124.68
33	AA	407	PHO	C5-C3-C2	2.46	126.09	121.12
39	RR	306	CHL	C3C-C4C-NC	-2.46	107.81	110.57
32	3	602	CLA	CHD-C1D-ND	-2.46	122.19	124.45
35	AA	410	PL9	C20-C19-C21	-2.46	111.14	115.27
40	g	615	LUT	C36-C21-C26	2.46	113.27	109.55
39	N	606	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
32	Rr	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
32	Y	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
32	RR	304	CLA	CHB-C4A-NA	2.46	127.91	124.51
38	WW	201	LMG	O8-C28-C29	2.46	119.62	111.91
34	CC	516	BCR	C24-C23-C22	-2.46	122.52	126.23
32	CC	504	CLA	CMB-C2B-C3B	2.46	129.28	124.68
38	W	201	LMG	O8-C28-C29	2.46	119.62	111.91
40	G	616	LUT	C38-C25-C24	-2.46	118.30	123.56
32	c	501	CLA	C6-C5-C3	2.46	119.90	113.45
32	3	612	CLA	CHD-C1D-ND	-2.46	122.20	124.45
40	Yy	615	LUT	C38-C25-C24	-2.46	118.30	123.56
32	Bb	606	CLA	CHB-C4A-NA	2.46	127.91	124.51
40	N	616	LUT	C22-C23-C24	-2.46	108.95	111.74
42	Rr	616	NEX	C32-C33-C34	-2.46	115.17	118.94
32	c	503	CLA	CMB-C2B-C3B	2.46	129.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Nn	301	CLA	CHB-C4A-NA	2.46	127.91	124.51
32	c	503	CLA	CHD-C1D-ND	-2.45	122.20	124.45
32	RR	314	CLA	CAC-C3C-C4C	2.45	128.00	124.81
32	N	612	CLA	CHB-C4A-NA	2.45	127.91	124.51
42	Nn	309	NEX	C32-C33-C34	-2.45	115.17	118.94
39	G	607	CHL	C1B-CHB-C4A	-2.45	125.26	130.12
39	GG	608	CHL	C4A-NA-C1A	2.45	107.81	106.71
39	GG	607	CHL	C1B-CHB-C4A	-2.45	125.26	130.12
39	22	606	CHL	CHB-C4A-NA	2.45	127.90	124.51
32	Ss	604	CLA	CHD-C1D-ND	-2.45	122.20	124.45
32	Yy	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
32	3	604	CLA	CBD-CHA-C1A	2.45	131.39	128.50
40	n	615	LUT	C36-C21-C26	2.45	113.26	109.55
32	A	408	CLA	CHB-C4A-NA	2.45	127.90	124.51
32	BB	611	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
32	B	619	CLA	CMB-C2B-C3B	2.45	129.26	124.68
36	33	614	LHG	O8-C23-C24	2.45	119.60	111.91
32	R	614	CLA	CHD-C1D-ND	-2.45	122.20	124.45
32	G	604	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
32	BB	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
32	RR	309	CLA	CHD-C1D-ND	-2.45	122.20	124.45
34	Dd	403	BCR	C4-C5-C6	-2.45	119.17	122.73
37	Ll	101	SQD	O48-C23-C24	2.45	119.59	111.91
32	b	612	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
32	G	614	CLA	CMB-C2B-C3B	2.45	129.26	124.68
34	DD	405	BCR	C29-C30-C25	2.45	114.25	110.48
32	G	613	CLA	CBD-CHA-C1A	2.45	131.38	128.50
32	r	601	CLA	CHB-C4A-NA	2.45	127.90	124.51
39	4	302	CHL	CMB-C2B-C1B	-2.45	124.70	128.46
32	C	511	CLA	CMB-C2B-C3B	2.45	129.25	124.68
32	Cc	511	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
36	K	101	LHG	O8-C23-C24	2.45	119.58	111.91
32	11	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
32	Aa	410	CLA	CHB-C4A-NA	2.44	127.89	124.51
32	NN	602	CLA	CAC-C3C-C4C	2.44	127.98	124.81
32	Yy	610	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
32	n	614	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
36	KK	101	LHG	O8-C23-C24	2.44	119.58	111.91
32	r	609	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	d	404	PL9	C25-C24-C26	-2.44	111.16	115.27
32	C	506	CLA	CHD-C1D-ND	-2.44	122.21	124.45
34	Hh	101	BCR	C12-C13-C14	-2.44	115.19	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	11	611	CLA	CHD-C1D-ND	-2.44	122.21	124.45
41	44	613	XAT	C12-C13-C14	-2.44	115.19	118.94
44	C	519	DGD	O1G-C1A-C2A	2.44	119.57	111.91
32	44	602	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
34	BB	617	BCR	C37-C22-C21	-2.44	119.50	122.92
32	BB	605	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
32	Ss	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
39	44	608	CHL	CHB-C4A-NA	2.44	127.89	124.51
32	Aa	410	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
34	Cc	517	BCR	C3-C4-C5	-2.44	109.72	114.08
32	YY	613	CLA	CMB-C2B-C3B	2.44	129.24	124.68
40	N	616	LUT	C7-C8-C9	-2.44	122.55	126.23
32	y	314	CLA	C5-C3-C2	2.44	126.05	121.12
39	1	606	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
32	RR	314	CLA	CMB-C2B-C3B	2.44	129.24	124.68
32	NN	613	CLA	CHB-C4A-NA	2.44	127.88	124.51
40	Gg	316	LUT	C38-C25-C24	-2.44	118.34	123.56
32	a	405	CLA	CAC-C3C-C4C	2.44	127.97	124.81
32	C	508	CLA	CHB-C4A-NA	2.44	127.88	124.51
41	Rr	615	XAT	O4-C5-C6	-2.43	56.94	58.96
39	YY	608	CHL	C1B-CHB-C4A	-2.43	125.30	130.12
32	Rr	613	CLA	CHD-C1D-ND	-2.43	122.22	124.45
32	g	603	CLA	CMB-C2B-C1B	-2.43	124.72	128.46
46	E	101	HEM	CBA-CAA-C2A	-2.43	108.47	112.62
32	b	606	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
32	Bb	612	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
40	SS	315	LUT	C35-C15-C14	-2.43	118.49	123.47
40	YY	615	LUT	C35-C15-C14	-2.43	118.49	123.47
34	KK	103	BCR	C36-C18-C19	2.43	121.91	118.08
32	BB	608	CLA	CHB-C4A-NA	2.43	127.87	124.51
34	Cc	518	BCR	C37-C22-C21	-2.43	119.52	122.92
32	s	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
32	GG	614	CLA	CMB-C2B-C3B	2.43	129.22	124.68
40	g	616	LUT	C19-C9-C8	2.43	121.91	118.08
38	C	521	LMG	O8-C28-C29	2.43	119.53	111.91
32	Cc	511	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
32	CC	506	CLA	CMB-C2B-C3B	2.43	129.22	124.68
32	Ss	608	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
39	44	601	CHL	C4A-NA-C1A	2.43	107.80	106.71
32	22	604	CLA	CMB-C2B-C3B	2.43	129.22	124.68
33	DD	402	PHO	CMB-C2B-C3B	2.43	129.22	124.68
42	Gg	318	NEX	C12-C13-C14	-2.43	115.22	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	410	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
39	s	601	CHL	C1-C2-C3	-2.43	121.84	126.04
40	2	614	LUT	C15-C35-C34	2.43	128.45	123.47
32	a	410	CLA	CHB-C4A-NA	2.43	127.87	124.51
32	Bb	605	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
39	11	601	CHL	CBD-CHA-C1A	2.43	131.36	128.50
32	Y	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
32	CC	505	CLA	CMB-C2B-C3B	2.43	129.22	124.68
32	2	613	CLA	CHD-C1D-ND	-2.43	122.22	124.45
32	4	304	CLA	CMB-C2B-C3B	2.43	129.22	124.68
34	B	613	BCR	C33-C5-C6	-2.42	121.81	124.53
40	Ss	615	LUT	C12-C13-C14	-2.42	115.22	118.94
38	AA	415	LMG	C8-O7-C10	-2.42	111.82	117.79
40	Gg	317	LUT	C19-C9-C8	2.42	121.90	118.08
32	BB	614	CLA	C5-C3-C2	2.42	126.02	121.12
32	RR	314	CLA	O2D-CGD-CBD	2.42	115.58	111.27
34	CC	517	BCR	C36-C18-C17	-2.42	119.53	122.92
39	NN	609	CHL	CHB-C4A-NA	2.42	127.86	124.51
32	22	602	CLA	CMB-C2B-C3B	2.42	129.21	124.68
39	SS	307	CHL	C1B-CHB-C4A	-2.42	125.32	130.12
32	Nn	305	CLA	CMB-C2B-C3B	2.42	129.21	124.68
34	T	101	BCR	C38-C26-C27	2.42	118.27	113.62
36	C	522	LHG	O8-C23-C24	2.42	119.51	111.91
32	Cc	506	CLA	CHD-C1D-ND	-2.42	122.23	124.45
32	BB	601	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
39	3	608	CHL	CBD-CHA-C1A	2.42	131.35	128.50
32	X	201	CLA	CMA-C3A-C2A	-2.42	110.45	116.10
34	a	411	BCR	C36-C18-C17	-2.42	119.53	122.92
32	Ss	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	B	622	CLA	CHB-C4A-NA	2.42	127.86	124.51
35	DD	406	PL9	C7-C3-C4	2.42	118.84	116.88
40	Ss	614	LUT	C8-C9-C10	-2.42	115.23	118.94
32	Bb	615	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
36	Gg	319	LHG	C5-O7-C7	-2.42	111.83	117.79
40	N	615	LUT	C20-C13-C12	2.42	121.89	118.08
32	S	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
34	BB	620	BCR	C12-C13-C14	-2.42	115.23	118.94
32	Aa	410	CLA	CHD-C1D-ND	-2.42	122.23	124.45
38	CC	520	LMG	O8-C28-C29	2.42	119.50	111.91
32	Cc	511	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	2	611	CLA	CMB-C2B-C3B	2.42	129.21	124.68
32	g	613	CLA	CBD-CHA-C1A	2.42	131.35	128.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	GG	615	LUT	C38-C25-C24	-2.42	118.38	123.56
32	1	610	CLA	CHD-C1D-ND	-2.42	122.23	124.45
32	3	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
34	Cc	516	BCR	C11-C10-C9	-2.42	123.86	127.31
40	RR	315	LUT	C7-C8-C9	-2.42	122.58	126.23
32	Aa	406	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	Rr	613	CLA	CMB-C2B-C3B	2.42	129.20	124.68
32	33	609	CLA	CMB-C2B-C3B	2.42	129.20	124.68
32	RR	309	CLA	CMB-C2B-C3B	2.42	129.20	124.68
32	Bb	612	CLA	CHB-C4A-NA	2.42	127.85	124.51
37	Ll	101	SQD	O8-S-C6	2.42	109.59	105.74
40	22	614	LUT	C39-C29-C30	2.42	126.31	122.92
40	s	614	LUT	C12-C13-C14	-2.42	115.23	118.94
32	NN	604	CLA	CMB-C2B-C3B	2.42	129.20	124.68
32	B	605	CLA	CHB-C4A-NA	2.42	127.85	124.51
32	BB	615	CLA	CAA-C2A-C3A	-2.42	110.46	116.10
41	Nn	308	XAT	C25-C24-C23	2.42	117.53	112.75
32	CC	508	CLA	C5-C3-C2	2.42	126.00	121.12
39	33	606	CHL	C1B-CHB-C4A	-2.42	125.33	130.12
39	GG	601	CHL	C1B-CHB-C4A	-2.42	125.33	130.12
32	C	505	CLA	CMB-C2B-C3B	2.41	129.20	124.68
39	YY	601	CHL	C1B-CHB-C4A	-2.41	125.33	130.12
42	NN	618	NEX	C20-C13-C14	-2.41	119.54	122.92
39	44	601	CHL	CMB-C2B-C1B	-2.41	124.75	128.46
44	Cc	519	DGD	C6E-C5E-C4E	-2.41	107.35	113.00
39	GG	605	CHL	C4A-NA-C1A	2.41	107.79	106.71
34	CC	516	BCR	C37-C22-C23	2.41	121.88	118.08
42	Yy	617	NEX	C32-C33-C34	-2.41	115.24	118.94
37	LL	101	SQD	O8-S-C6	2.41	109.58	105.74
32	R	612	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
32	Y	604	CLA	CMB-C2B-C3B	2.41	129.19	124.68
40	44	612	LUT	C38-C25-C24	-2.41	118.40	123.56
36	y	320	LHG	O8-C23-C24	2.41	119.47	111.91
34	k	101	BCR	C16-C15-C14	-2.41	118.53	123.47
32	33	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
44	c	517	DGD	O6D-C5D-C6D	2.41	111.53	106.67
32	GG	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
40	Gg	317	LUT	C16-C1-C6	2.41	114.21	110.30
39	11	606	CHL	C1B-CHB-C4A	-2.41	125.34	130.12
34	Hh	101	BCR	C38-C26-C27	2.41	118.24	113.62
39	1	606	CHL	CBD-CHA-C1A	2.41	131.34	128.50
32	R	603	CLA	CMB-C2B-C3B	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
32	11	612	CLA	CMA-C3A-C2A	-2.41	107.46	114.44
32	AA	408	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	BB	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	r	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	BB	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	Bb	616	CLA	CMB-C2B-C3B	2.41	129.18	124.68
32	RR	304	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
32	Gg	304	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
34	DD	405	BCR	C38-C26-C27	2.41	118.24	113.62
42	RR	317	NEX	C11-C10-C9	-2.41	123.88	127.31
32	SS	313	CLA	CHB-C4A-NA	2.41	127.84	124.51
33	Aa	409	PHO	CMC-C2C-C3C	2.41	129.48	124.94
41	y	301	XAT	O24-C25-C26	-2.41	56.97	58.96
32	CC	510	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
32	NN	603	CLA	CAA-C2A-C3A	-2.41	108.25	114.26
40	GG	616	LUT	C38-C25-C24	-2.40	118.41	123.56
39	33	608	CHL	C4A-NA-C1A	2.40	107.79	106.71
32	Aa	406	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
39	g	606	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
36	1	614	LHG	O8-C23-C24	2.40	119.45	111.91
32	2	602	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	D	406	BCR	C38-C26-C27	2.40	118.23	113.62
41	R	616	XAT	C8-C9-C10	-2.40	115.25	118.94
39	NN	606	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
32	Y	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	b	602	CLA	CMB-C2B-C3B	2.40	129.17	124.68
36	N	619	LHG	O8-C23-C24	2.40	119.44	111.91
32	B	610	CLA	C5-C3-C2	2.40	125.98	121.12
32	BB	609	CLA	CMB-C2B-C3B	2.40	129.17	124.68
40	g	615	LUT	C38-C25-C24	-2.40	118.42	123.56
34	KK	103	BCR	C34-C9-C10	-2.40	119.56	122.92
32	RR	313	CLA	CAC-C3C-C4C	2.40	127.92	124.81
41	y	301	XAT	C38-C25-C24	-2.40	111.58	114.28
46	Ee	101	HEM	CMC-C2C-C3C	2.40	129.17	124.68
39	2	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
40	Y	615	LUT	C35-C15-C14	-2.40	118.56	123.47
32	BB	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
41	GG	617	XAT	C20-C13-C12	2.40	121.86	118.08
32	Y	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	Bb	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	S	606	CHL	C1B-CHB-C4A	-2.40	125.37	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	YY	610	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
32	Rr	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	22	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
32	c	508	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	22	612	CLA	CHD-C1D-ND	-2.40	122.25	124.45
34	D	406	BCR	C38-C26-C25	-2.39	121.84	124.53
32	BB	609	CLA	CHB-C4A-NA	2.39	127.82	124.51
41	y	302	XAT	C15-C35-C34	-2.39	118.57	123.47
32	Yy	602	CLA	CMB-C2B-C3B	2.39	129.16	124.68
32	BB	602	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
32	RR	303	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
32	B	608	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
32	Yy	613	CLA	CMB-C2B-C3B	2.39	129.15	124.68
32	S	609	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	Y	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	s	604	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	b	607	CLA	CHD-C1D-ND	-2.39	122.26	124.45
41	Yy	619	XAT	C38-C25-C24	-2.39	111.59	114.28
42	RR	317	NEX	C32-C33-C34	-2.39	115.27	118.94
32	Yy	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	n	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	a	410	CLA	CMB-C2B-C3B	2.39	129.15	124.68
32	B	607	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
39	RR	306	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
32	Gg	304	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
32	BB	615	CLA	O2D-CGD-CBD	2.39	115.51	111.27
32	B	605	CLA	O2D-CGD-CBD	2.39	115.51	111.27
32	S	612	CLA	CHB-C4A-NA	2.39	127.81	124.51
32	y	304	CLA	CHB-C4A-NA	2.39	127.81	124.51
34	AA	409	BCR	C36-C18-C17	-2.39	119.58	122.92
32	r	610	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
32	NN	610	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
33	a	409	PHO	CMB-C2B-C3B	2.39	129.14	124.68
32	G	613	CLA	CHD-C1D-ND	-2.39	122.26	124.45
32	C	511	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
32	g	604	CLA	CHD-C1D-ND	-2.39	122.26	124.45
34	C	517	BCR	C24-C23-C22	-2.39	122.63	126.23
39	R	606	CHL	CHB-C4A-NA	2.38	127.81	124.51
32	XX	201	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
32	G	604	CLA	CHD-C1D-ND	-2.38	122.26	124.45
34	H	101	BCR	C38-C26-C27	2.38	118.20	113.62
42	Gg	318	NEX	C38-C25-C26	-2.38	118.27	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	YY	610	CLA	CMB-C2B-C3B	2.38	129.14	124.68
32	y	316	CLA	CHD-C1D-ND	-2.38	122.26	124.45
41	Rr	615	XAT	C4-C3-C2	-2.38	106.17	110.77
39	22	607	CHL	CBD-CHA-C1A	2.38	131.31	128.50
34	B	612	BCR	C28-C27-C26	-2.38	109.82	114.08
32	B	620	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
32	D	405	CLA	CHB-C4A-NA	2.38	127.81	124.51
40	Ss	615	LUT	C20-C13-C12	2.38	121.83	118.08
32	Aa	407	CLA	CHB-C4A-NA	2.38	127.80	124.51
32	CC	510	CLA	CMB-C2B-C3B	2.38	129.13	124.68
40	2	614	LUT	C22-C23-C24	-2.38	109.03	111.74
32	B	611	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
39	4	302	CHL	O2D-CGD-O1D	-2.38	118.69	124.09
39	N	605	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
32	22	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
32	SS	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
32	Yy	614	CLA	CHD-C1D-ND	-2.38	122.27	124.45
32	r	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
32	2	612	CLA	CHD-C1D-ND	-2.38	122.27	124.45
32	AA	405	CLA	CAC-C3C-C4C	2.38	127.89	124.81
41	y	302	XAT	C26-C27-C28	-2.38	120.97	125.99
32	2	613	CLA	CHB-C4A-NA	2.37	127.80	124.51
39	Gg	310	CHL	CAC-C3C-C4C	2.37	127.89	124.81
32	3	613	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
32	Ss	613	CLA	CHD-C1D-ND	-2.37	122.27	124.45
32	C	509	CLA	C5-C3-C2	2.37	125.92	121.12
32	R	604	CLA	CMB-C2B-C3B	2.37	129.12	124.68
33	AA	407	PHO	CMB-C2B-C3B	2.37	129.12	124.68
39	11	606	CHL	CHB-C4A-NA	2.37	127.79	124.51
32	YY	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
34	c	515	BCR	C3-C4-C5	-2.37	109.84	114.08
32	22	613	CLA	CHD-C1D-ND	-2.37	122.28	124.45
32	C	504	CLA	CHD-C1D-ND	-2.37	122.28	124.45
32	NN	614	CLA	CHD-C1D-ND	-2.37	122.28	124.45
40	N	615	LUT	C12-C13-C14	-2.37	115.30	118.94
39	44	601	CHL	O2D-CGD-O1D	-2.37	118.71	124.09
39	RR	306	CHL	CHB-C4A-NA	2.37	127.79	124.51
39	G	607	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
40	s	615	LUT	C20-C13-C12	2.37	121.81	118.08
37	BB	621	SQD	O5-C5-C4	-2.37	105.39	109.69
39	1	608	CHL	CHB-C4A-NA	2.37	127.79	124.51
39	Ss	606	CHL	C2A-C1A-CHA	2.37	128.00	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	613	CLA	CHB-C4A-NA	2.37	127.79	124.51
46	EE	102	HEM	C4D-ND-C1D	2.37	107.52	105.07
32	D	404	CLA	O2D-CGD-CBD	2.37	115.47	111.27
32	CC	514	CLA	CHB-C4A-NA	2.37	127.78	124.51
39	Yy	607	CHL	C1B-CHB-C4A	-2.37	125.43	130.12
42	R	617	NEX	C11-C10-C9	-2.37	123.93	127.31
32	B	605	CLA	CMB-C2B-C3B	2.37	129.10	124.68
32	Gg	304	CLA	CHB-C4A-NA	2.37	127.78	124.51
32	B	623	CLA	CMB-C2B-C1B	-2.36	124.83	128.46
36	NN	619	LHG	O8-C23-C24	2.36	119.33	111.91
32	B	623	CLA	CHB-C4A-NA	2.36	127.78	124.51
34	C	517	BCR	C37-C22-C23	2.36	121.80	118.08
46	Ee	101	HEM	C4C-CHD-C1D	2.36	125.68	122.56
32	Gg	315	CLA	CHB-C4A-NA	2.36	127.78	124.51
32	Bb	604	CLA	CHD-C1D-ND	-2.36	122.28	124.45
40	Ss	615	LUT	C8-C9-C10	-2.36	115.32	118.94
42	Y	619	NEX	C32-C33-C34	-2.36	115.32	118.94
41	N	617	XAT	C36-C21-C22	-2.36	104.88	108.98
32	Nn	301	CLA	CMB-C2B-C3B	2.36	129.10	124.68
32	g	603	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
39	2	608	CHL	CBD-CHA-C1A	2.36	131.28	128.50
40	g	616	LUT	C36-C21-C26	2.36	113.12	109.55
39	RR	305	CHL	CAA-CBA-CGA	-2.36	106.36	113.25
32	YY	602	CLA	CHD-C1D-ND	-2.36	122.29	124.45
32	y	304	CLA	CMB-C2B-C3B	2.36	129.09	124.68
34	b	617	BCR	C3-C4-C5	-2.36	109.87	114.08
32	B	624	CLA	CHD-C1D-ND	-2.36	122.29	124.45
39	1	608	CHL	CAC-C3C-C4C	2.36	127.87	124.81
37	LL	101	SQD	O9-S-C6	2.36	109.74	106.94
32	BB	608	CLA	CMB-C2B-C3B	2.36	129.09	124.68
39	Nn	317	CHL	C5-C3-C2	2.36	125.89	121.12
32	N	614	CLA	CHD-C1D-ND	-2.36	122.29	124.45
32	B	618	CLA	CHD-C1D-ND	-2.36	122.29	124.45
32	B	621	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
32	Aa	405	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
35	A	410	PL9	C30-C29-C31	-2.36	111.31	115.27
39	g	609	CHL	CAC-C3C-C4C	2.36	127.87	124.81
32	Nn	304	CLA	CHB-C4A-NA	2.36	127.77	124.51
32	33	603	CLA	CHD-C1D-ND	-2.36	122.29	124.45
32	Gg	311	CLA	CHD-C1D-ND	-2.36	122.29	124.45
32	Aa	406	CLA	O2D-CGD-CBD	2.36	115.45	111.27
32	b	605	CLA	C5-C3-C2	2.36	125.88	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	415	LMG	C8-O7-C10	-2.36	111.99	117.79
34	Dd	403	BCR	C33-C5-C6	-2.36	121.88	124.53
32	B	606	CLA	CHB-C4A-NA	2.36	127.77	124.51
32	3	613	CLA	CHD-C1D-ND	-2.35	122.29	124.45
42	Y	617	NEX	C20-C13-C14	-2.35	119.62	122.92
39	33	608	CHL	CBD-CHA-C1A	2.35	131.27	128.50
32	BB	609	CLA	CAC-C3C-C4C	2.35	127.86	124.81
32	B	605	CLA	CAC-C3C-C4C	2.35	127.86	124.81
32	c	502	CLA	C5-C3-C2	2.35	125.88	121.12
32	Cc	515	CLA	CHD-C1D-ND	-2.35	122.29	124.45
34	H	101	BCR	C33-C5-C6	2.35	127.17	124.53
32	b	602	CLA	O1D-CGD-CBD	2.35	129.30	124.48
32	C	507	CLA	CAC-C3C-C4C	2.35	127.86	124.81
39	R	605	CHL	CAA-CBA-CGA	-2.35	106.38	113.25
41	G	617	XAT	C35-C15-C14	-2.35	118.66	123.47
46	e	101	HEM	CMC-C2C-C3C	2.35	129.08	124.68
36	EE	101	LHG	O8-C23-C24	2.35	119.29	111.91
34	BB	617	BCR	C33-C5-C6	-2.35	121.89	124.53
40	Gg	317	LUT	C2-C3-C4	-2.35	107.09	110.30
41	Gg	301	XAT	C31-C30-C29	-2.35	123.95	127.31
36	GG	618	LHG	O8-C23-C24	2.35	119.28	111.91
32	4	305	CLA	CHB-C4A-NA	2.35	127.76	124.51
40	R	615	LUT	C15-C35-C34	-2.35	118.66	123.47
32	a	406	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
32	Nn	301	CLA	CAC-C3C-C4C	2.35	127.86	124.81
34	TT	101	BCR	C38-C26-C27	2.35	118.13	113.62
32	B	611	CLA	CAA-C2A-C3A	-2.35	110.61	116.10
36	Yy	618	LHG	O8-C23-C24	2.35	119.28	111.91
32	33	602	CLA	CHD-C1D-ND	-2.35	122.30	124.45
32	B	618	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
32	RR	310	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
32	NN	603	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
32	a	406	CLA	O2D-CGD-CBD	2.35	115.44	111.27
32	Yy	612	CLA	C5-C3-C2	2.35	125.87	121.12
34	XX	202	BCR	C1-C6-C7	2.35	122.42	115.78
34	Bb	619	BCR	C33-C5-C6	-2.35	121.89	124.53
34	C	518	BCR	C36-C18-C17	-2.35	119.64	122.92
32	44	615	CLA	CHB-C4A-NA	2.35	127.76	124.51
34	KK	103	BCR	C33-C5-C6	-2.35	121.89	124.53
32	a	406	CLA	C1D-ND-C4D	-2.35	104.67	106.33
33	Aa	409	PHO	CMB-C2B-C3B	2.34	129.06	124.68
32	11	603	CLA	CHD-C1D-ND	-2.34	122.30	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	YY	615	LUT	C38-C25-C24	-2.34	118.54	123.56
34	CC	515	BCR	C11-C10-C9	-2.34	123.97	127.31
43	KK	102	LMU	C1'-O5'-C5'	2.34	118.29	113.69
39	r	607	CHL	O2A-CGA-O1A	-2.34	117.68	123.59
32	2	613	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
32	g	613	CLA	CHD-C1D-ND	-2.34	122.30	124.45
32	s	613	CLA	CHD-C1D-ND	-2.34	122.30	124.45
32	1	610	CLA	CBD-CHA-C1A	2.34	131.26	128.50
32	R	614	CLA	O2D-CGD-CBD	2.34	115.43	111.27
37	LL	102	SQD	O9-S-C6	2.34	109.72	106.94
32	b	614	CLA	CHD-C1D-ND	-2.34	122.30	124.45
41	GG	617	XAT	C35-C15-C14	-2.34	118.68	123.47
39	N	601	CHL	CAC-C3C-C4C	2.34	127.85	124.81
32	B	611	CLA	O2D-CGD-CBD	2.34	115.43	111.27
40	Ss	615	LUT	C3-C4-C5	-2.34	107.19	111.85
32	Gg	305	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
40	Ss	614	LUT	C12-C13-C14	-2.34	115.35	118.94
40	G	616	LUT	C20-C13-C12	2.34	121.76	118.08
32	B	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
43	R	618	LMU	C1-O1'-C1'	2.34	117.72	113.84
32	A	405	CLA	CAC-C3C-C4C	2.34	127.84	124.81
32	N	610	CLA	CHB-C4A-NA	2.34	127.75	124.51
39	r	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
32	r	602	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	b	605	CLA	CHD-C1D-ND	-2.34	122.31	124.45
32	CC	502	CLA	CBA-CAA-C2A	2.34	120.77	113.86
32	b	604	CLA	CHB-C4A-NA	2.34	127.75	124.51
32	BB	603	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
41	GG	619	XAT	C12-C13-C14	-2.34	115.36	118.94
32	n	602	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	RR	302	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	y	306	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
36	Dd	407	LHG	O8-C23-C24	2.33	119.23	111.91
34	Dd	403	BCR	C27-C26-C25	-2.33	119.34	122.73
34	A	409	BCR	C40-C30-C25	-2.33	106.51	110.30
32	Y	612	CLA	C5-C3-C2	2.33	125.84	121.12
32	s	609	CLA	CHB-C4A-NA	2.33	127.74	124.51
32	Bb	614	CLA	CHD-C1D-ND	-2.33	122.31	124.45
34	D	406	BCR	C29-C30-C25	2.33	114.07	110.48
32	CC	504	CLA	CHB-C4A-NA	2.33	127.74	124.51
34	BB	620	BCR	C24-C23-C22	-2.33	122.71	126.23
32	C	503	CLA	CMB-C2B-C3B	2.33	129.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	616	LUT	C38-C25-C24	-2.33	118.57	123.56
32	B	624	CLA	CHB-C4A-NA	2.33	127.74	124.51
32	Bb	609	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
32	Bb	604	CLA	CHB-C4A-NA	2.33	127.74	124.51
32	BB	609	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
34	c	515	BCR	C39-C30-C25	-2.33	106.52	110.30
34	c	515	BCR	C38-C26-C27	2.33	118.09	113.62
34	A	409	BCR	C36-C18-C17	-2.33	119.66	122.92
34	CC	515	BCR	C2-C3-C4	-2.33	106.17	111.38
32	s	602	CLA	CHB-C4A-NA	2.33	127.74	124.51
32	BB	606	CLA	CHB-C4A-NA	2.33	127.74	124.51
42	Y	617	NEX	C17-C1-C6	-2.33	108.39	110.47
32	3	604	CLA	CHD-C1D-ND	-2.33	122.31	124.45
32	SS	303	CLA	CHD-C1D-ND	-2.33	122.31	124.45
32	C	515	CLA	CHB-C4A-NA	2.33	127.73	124.51
37	A	412	SQD	O8-S-C6	2.33	109.45	105.74
32	g	602	CLA	CED-O2D-CGD	-2.33	110.67	115.94
40	n	615	LUT	C15-C35-C34	-2.33	118.70	123.47
32	CC	506	CLA	CHB-C4A-NA	2.33	127.73	124.51
40	y	318	LUT	C20-C13-C12	2.33	121.75	118.08
40	4	313	LUT	C38-C25-C24	-2.33	118.57	123.56
32	Aa	410	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
34	b	619	BCR	C2-C1-C6	2.33	114.07	110.48
32	Nn	313	CLA	CHB-C4A-NA	2.33	127.73	124.51
39	SS	306	CHL	C1B-CHB-C4A	-2.33	125.50	130.12
39	44	607	CHL	C2A-C1A-CHA	2.33	127.93	123.86
32	RR	314	CLA	CHB-C4A-NA	2.33	127.73	124.51
32	S	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
32	c	509	CLA	CHB-C4A-NA	2.33	127.73	124.51
32	R	610	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
32	CC	512	CLA	CMB-C2B-C3B	2.33	129.03	124.68
32	Yy	604	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
32	d	401	CLA	CHB-C4A-NA	2.33	127.73	124.51
34	B	613	BCR	C33-C5-C4	2.33	118.08	113.62
32	Rr	611	CLA	CHB-C4A-NA	2.32	127.73	124.51
32	b	607	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
40	R	615	LUT	C32-C33-C34	-2.32	115.37	118.94
32	r	612	CLA	CHD-C1D-ND	-2.32	122.32	124.45
32	b	609	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
32	s	602	CLA	CHD-C1D-ND	-2.32	122.32	124.45
40	YY	616	LUT	C19-C9-C8	2.32	121.74	118.08
32	Bb	605	CLA	C5-C3-C2	2.32	125.82	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Ss	602	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	NN	612	CLA	CAA-C2A-C3A	-2.32	108.46	114.26
36	JJ	101	LHG	C5-O7-C7	-2.32	112.08	117.79
32	Rr	602	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	n	610	CLA	CHB-C4A-NA	2.32	127.72	124.51
34	DD	405	BCR	C38-C26-C25	-2.32	121.92	124.53
32	33	609	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	b	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	YY	612	CLA	CHB-C4A-NA	2.32	127.72	124.51
34	Bb	619	BCR	C2-C1-C6	2.32	114.05	110.48
32	B	605	CLA	CHD-C1D-ND	-2.32	122.32	124.45
32	Cc	504	CLA	C5-C3-C2	2.32	125.81	121.12
41	g	619	XAT	C12-C13-C14	-2.32	115.38	118.94
32	Y	604	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	Cc	506	CLA	CAC-C3C-C4C	2.32	127.82	124.81
32	SS	314	CLA	CHD-C1D-ND	-2.32	122.32	124.45
35	A	410	PL9	C7-C3-C2	-2.32	120.25	123.30
32	g	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
33	a	408	PHO	CMB-C2B-C3B	2.32	129.01	124.68
32	B	605	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
32	Ss	613	CLA	CMB-C2B-C3B	2.32	129.01	124.68
40	Rr	614	LUT	C15-C35-C34	-2.32	118.73	123.47
39	4	309	CHL	C2A-C1A-CHA	2.32	127.91	123.86
39	N	609	CHL	C3C-C4C-NC	-2.32	107.97	110.57
42	N	618	NEX	C15-C14-C13	-2.32	124.00	127.31
40	S	614	LUT	C15-C35-C34	-2.32	118.73	123.47
32	Nn	304	CLA	CHD-C1D-ND	-2.32	122.33	124.45
32	Cc	508	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
32	S	602	CLA	CHB-C4A-NA	2.32	127.71	124.51
32	b	605	CLA	CHB-C4A-NA	2.32	127.71	124.51
40	G	616	LUT	C35-C15-C14	-2.32	118.73	123.47
32	C	513	CLA	CMB-C2B-C3B	2.32	129.01	124.68
40	22	614	LUT	C22-C23-C24	-2.32	109.11	111.74
34	Cc	517	BCR	C27-C26-C25	-2.31	119.37	122.73
34	Hh	101	BCR	C2-C3-C4	-2.31	106.20	111.38
34	c	516	BCR	C15-C16-C17	-2.31	118.73	123.47
32	S	602	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
36	l	101	LHG	O8-C23-C24	2.31	119.17	111.91
32	4	310	CLA	CHB-C4A-NA	2.31	127.71	124.51
32	N	603	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
32	YY	612	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
32	b	605	CLA	CMB-C2B-C1B	-2.31	124.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	304	CLA	CAC-C3C-C4C	2.31	127.81	124.81
32	B	609	CLA	C1-C2-C3	-2.31	122.04	126.04
40	r	614	LUT	C19-C9-C8	2.31	121.72	118.08
32	S	613	CLA	CHB-C4A-NA	2.31	127.71	124.51
32	Nn	314	CLA	CHD-C1D-ND	-2.31	122.33	124.45
32	g	603	CLA	CHB-C4A-NA	2.31	127.71	124.51
42	YY	617	NEX	C17-C1-C6	-2.31	108.40	110.47
32	RR	302	CLA	O2D-CGD-CBD	2.31	115.37	111.27
32	Dd	402	CLA	CHB-C4A-NA	2.31	127.71	124.51
32	Rr	602	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
40	Ss	615	LUT	C2-C3-C4	-2.31	107.14	110.30
44	CC	518	DGD	O6D-C5D-C6D	2.31	111.33	106.67
32	A	405	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
32	s	604	CLA	CHD-C1D-ND	-2.31	122.33	124.45
32	2	613	CLA	CMB-C2B-C3B	2.31	129.00	124.68
32	A	406	CLA	CHB-C4A-NA	2.31	127.70	124.51
32	R	612	CLA	CHD-C1D-ND	-2.31	122.33	124.45
32	GG	611	CLA	CMB-C2B-C3B	2.31	129.00	124.68
32	BB	609	CLA	O2D-CGD-CBD	2.31	115.37	111.27
45	D	403	BCT	O3-C-O1	-2.31	113.56	119.55
46	e	101	HEM	CHC-C4B-C3B	2.31	128.10	124.57
44	C	523	DGD	O1G-C1A-C2A	2.31	119.15	111.91
40	RR	315	LUT	C32-C33-C34	-2.31	115.40	118.94
32	CC	505	CLA	CHB-C4A-NA	2.31	127.70	124.51
34	Cc	518	BCR	C15-C16-C17	-2.31	118.75	123.47
37	AA	412	SQD	O7-S-C6	2.31	109.68	106.94
42	y	319	NEX	C32-C33-C34	-2.31	115.40	118.94
32	YY	610	CLA	CHB-C4A-NA	2.31	127.70	124.51
34	C	518	BCR	C24-C23-C22	-2.31	122.75	126.23
32	Gg	312	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
32	n	604	CLA	CHD-C1D-ND	-2.30	122.34	124.45
42	Y	617	NEX	C32-C33-C34	-2.30	115.41	118.94
39	Rr	607	CHL	O2A-CGA-O1A	-2.30	117.78	123.59
36	g	618	LHG	C5-O7-C7	-2.30	112.12	117.79
32	3	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
34	C	518	BCR	C27-C26-C25	-2.30	119.39	122.73
34	k	101	BCR	C8-C9-C10	2.30	122.47	118.94
34	d	403	BCR	C27-C26-C25	-2.30	119.39	122.73
32	y	306	CLA	CHD-C1D-ND	-2.30	122.34	124.45
37	L	101	SQD	O9-S-C6	2.30	109.67	106.94
32	g	604	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
32	AA	406	CLA	CHB-C4A-NA	2.30	127.69	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	102	BCR	C23-C22-C21	-2.30	115.41	118.94
42	N	618	NEX	C20-C13-C14	-2.30	119.70	122.92
32	C	507	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
32	GG	613	CLA	CHD-C1D-ND	-2.30	122.34	124.45
32	22	611	CLA	CHB-C4A-NA	2.30	127.69	124.51
32	Bb	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
39	YY	609	CHL	C4A-NA-C1A	2.30	107.74	106.71
32	44	602	CLA	CHB-C4A-NA	2.30	127.69	124.51
32	SS	303	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
32	C	513	CLA	CHB-C4A-NA	2.30	127.69	124.51
40	22	614	LUT	C19-C9-C8	2.30	121.70	118.08
32	b	616	CLA	CMB-C2B-C3B	2.30	128.98	124.68
32	S	613	CLA	CHD-C1D-ND	-2.30	122.34	124.45
39	NN	609	CHL	C3C-C4C-NC	-2.30	107.99	110.57
40	Gg	317	LUT	C15-C35-C34	-2.30	118.77	123.47
32	n	610	CLA	C4A-NA-C1A	2.30	107.74	106.71
32	R	609	CLA	CHD-C1D-ND	-2.30	122.34	124.45
41	N	617	XAT	C15-C35-C34	-2.30	118.77	123.47
38	a	412	LMG	C8-O7-C10	-2.30	112.14	117.79
34	b	619	BCR	C37-C22-C21	-2.30	119.71	122.92
41	Nn	308	XAT	C39-C29-C30	-2.30	119.71	122.92
40	GG	616	LUT	C35-C15-C14	-2.30	118.77	123.47
32	BB	606	CLA	CMB-C2B-C3B	2.30	128.97	124.68
32	RR	310	CLA	CMB-C2B-C3B	2.30	128.97	124.68
32	BB	609	CLA	CHD-C1D-ND	-2.29	122.34	124.45
39	Yy	606	CHL	C1B-CHB-C4A	-2.29	125.57	130.12
39	y	310	CHL	O2D-CGD-O1D	-2.29	119.35	123.84
32	g	611	CLA	CHB-C4A-NA	2.29	127.68	124.51
32	c	506	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
32	B	608	CLA	CMB-C2B-C3B	2.29	128.97	124.68
32	YY	604	CLA	CMB-C2B-C3B	2.29	128.97	124.68
32	SS	309	CLA	CHB-C4A-NA	2.29	127.68	124.51
32	b	604	CLA	CHD-C1D-ND	-2.29	122.35	124.45
32	s	608	CLA	CHD-C1D-ND	-2.29	122.35	124.45
34	T	101	BCR	C4-C5-C6	-2.29	119.40	122.73
40	Nn	307	LUT	C15-C35-C34	-2.29	118.78	123.47
40	NN	615	LUT	C20-C13-C12	2.29	121.69	118.08
32	Dd	401	CLA	CHB-C4A-NA	2.29	127.68	124.51
39	r	606	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
41	g	619	XAT	C31-C30-C29	-2.29	124.04	127.31
32	Y	610	CLA	CBA-CAA-C2A	2.29	120.62	113.86
46	EE	102	HEM	CBA-CAA-C2A	-2.29	108.72	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	609	CHL	CAC-C3C-C4C	2.29	127.78	124.81
37	B	602	SQD	O8-S-C6	2.29	109.38	105.74
40	Y	616	LUT	C15-C35-C34	-2.29	118.79	123.47
39	YY	607	CHL	OMC-CMC-C2C	-2.29	120.52	125.69
41	G	619	XAT	C39-C29-C28	2.29	121.68	118.08
32	Bb	607	CLA	CHD-C1D-ND	-2.29	122.35	124.45
32	BB	614	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
32	b	607	CLA	CHB-C4A-NA	2.28	127.67	124.51
34	K	102	BCR	C16-C17-C18	-2.28	124.05	127.31
42	n	617	NEX	C32-C33-C34	-2.28	115.44	118.94
40	Y	616	LUT	C36-C21-C26	2.28	113.00	109.55
39	Gg	306	CHL	OMC-CMC-C2C	-2.28	120.52	125.69
32	SS	305	CLA	CHB-C4A-NA	2.28	127.67	124.51
34	BB	618	BCR	C37-C22-C21	-2.28	119.72	122.92
34	b	617	BCR	C39-C30-C25	-2.28	106.59	110.30
32	b	609	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
32	YY	613	CLA	CHB-C4A-NA	2.28	127.67	124.51
32	33	613	CLA	CHD-C1D-ND	-2.28	122.36	124.45
32	BB	604	CLA	CHD-C1D-ND	-2.28	122.36	124.45
34	XX	202	BCR	C16-C15-C14	-2.28	118.80	123.47
39	GG	607	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
32	3	612	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
32	RR	304	CLA	CED-O2D-CGD	2.28	121.10	115.94
41	y	302	XAT	C39-C29-C30	-2.28	119.73	122.92
32	s	609	CLA	CHD-C1D-ND	-2.28	122.36	124.45
34	T	101	BCR	C23-C22-C21	-2.28	115.44	118.94
32	DD	401	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
36	22	615	LHG	O8-C23-C24	2.28	119.06	111.91
32	Cc	505	CLA	CHD-C1D-ND	-2.28	122.36	124.45
38	c	519	LMG	O8-C28-C29	2.28	119.06	111.91
32	B	618	CLA	O2D-CGD-CBD	2.28	115.32	111.27
32	RR	302	CLA	CHB-C4A-NA	2.28	127.66	124.51
32	NN	613	CLA	CHD-C1D-ND	-2.28	122.36	124.45
32	A	406	CLA	CHD-C1D-ND	-2.28	122.36	124.45
34	B	612	BCR	C2-C1-C6	2.28	113.99	110.48
34	AA	409	BCR	C37-C22-C23	-2.28	114.49	118.08
32	b	603	CLA	CHB-C4A-NA	2.28	127.66	124.51
39	33	606	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
32	Nn	305	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
32	Ss	610	CLA	CHB-C4A-NA	2.28	127.66	124.51
34	Cc	516	BCR	C34-C9-C8	-2.28	114.49	118.08
32	g	610	CLA	CMB-C2B-C3B	2.28	128.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	r	615	XAT	O4-C5-C6	-2.27	57.08	58.96
42	n	617	NEX	C15-C14-C13	-2.27	124.06	127.31
41	Yy	619	XAT	C39-C29-C30	-2.27	119.74	122.92
46	E	101	HEM	C4D-ND-C1D	2.27	107.42	105.07
32	N	610	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
39	Nn	317	CHL	O2A-CGA-O1A	-2.27	117.86	123.59
32	Yy	604	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	2	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	N	614	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	a	406	CLA	CHB-C4A-NA	2.27	127.65	124.51
39	RR	305	CHL	CHB-C4A-NA	2.27	127.65	124.51
34	b	617	BCR	C24-C23-C22	-2.27	122.80	126.23
32	Nn	313	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
39	2	608	CHL	C4A-NA-C1A	2.27	107.73	106.71
32	c	502	CLA	CHD-C1D-ND	-2.27	122.37	124.45
39	RR	306	CHL	C2A-C3A-C4A	-2.27	98.20	101.87
32	Bb	608	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	CC	502	CLA	CHD-C1D-ND	-2.27	122.37	124.45
32	SS	314	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	S	602	CLA	CHD-C1D-ND	-2.27	122.37	124.45
32	RR	312	CLA	CHD-C1D-ND	-2.27	122.37	124.45
39	33	605	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
40	n	616	LUT	C19-C9-C8	2.27	121.65	118.08
32	44	604	CLA	CHD-C1D-ND	-2.27	122.37	124.45
32	n	602	CLA	CHD-C1D-ND	-2.27	122.37	124.45
39	y	308	CHL	C1B-CHB-C4A	-2.27	125.63	130.12
34	Dd	403	BCR	C15-C16-C17	-2.27	118.83	123.47
32	SS	309	CLA	CHD-C1D-ND	-2.27	122.37	124.45
32	r	610	CLA	CMB-C2B-C3B	2.27	128.92	124.68
32	y	313	CLA	CMB-C2B-C3B	2.27	128.92	124.68
39	NN	609	CHL	CMB-C2B-C3B	2.27	128.92	124.68
34	A	409	BCR	C27-C26-C25	-2.27	119.44	122.73
39	Y	607	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
32	Aa	406	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
40	y	318	LUT	C40-C33-C32	2.27	121.65	118.08
33	Aa	408	PHO	CMB-C2B-C3B	2.27	128.92	124.68
32	g	602	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
39	YY	609	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
32	y	315	CLA	CHD-C1D-ND	-2.26	122.37	124.45
32	Cc	503	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
39	n	608	CHL	O2A-CGA-O1A	-2.26	117.88	123.59
32	BB	605	CLA	C1-C2-C3	-2.26	122.13	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Nn	314	CLA	CMB-C2B-C1B	-2.26	124.98	128.46
37	l	102	SQD	O8-S-C6	2.26	109.35	105.74
32	b	601	CLA	C1-C2-C3	-2.26	122.13	126.04
32	b	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
32	d	402	CLA	CHB-C4A-NA	2.26	127.64	124.51
34	BB	620	BCR	C20-C21-C22	-2.26	124.08	127.31
32	22	609	CLA	CHD-C1D-ND	-2.26	122.38	124.45
32	33	604	CLA	CHD-C1D-ND	-2.26	122.38	124.45
34	XX	202	BCR	C31-C1-C6	-2.26	106.63	110.30
40	Nn	307	LUT	C7-C8-C9	-2.26	122.82	126.23
39	n	607	CHL	C1-C2-C3	-2.26	122.13	126.04
34	AA	409	BCR	C20-C21-C22	-2.26	124.08	127.31
39	y	311	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
37	B	617	SQD	O5-C5-C4	-2.26	105.59	109.69
32	BB	613	CLA	CHD-C1D-ND	-2.26	122.38	124.45
32	n	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
32	33	613	CLA	CMB-C2B-C3B	2.26	128.91	124.68
34	BB	617	BCR	C33-C5-C4	2.26	117.96	113.62
34	Cc	516	BCR	C38-C26-C27	2.26	117.96	113.62
39	Yy	607	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
34	BB	620	BCR	C35-C13-C12	2.26	121.64	118.08
34	d	403	BCR	C33-C5-C6	-2.26	121.99	124.53
34	B	616	BCR	C12-C13-C14	-2.26	115.48	118.94
34	B	616	BCR	C16-C17-C18	-2.26	124.09	127.31
40	R	615	LUT	C36-C21-C26	2.26	112.96	109.55
39	n	606	CHL	C1B-CHB-C4A	-2.26	125.65	130.12
38	Cc	501	LMG	O8-C28-C29	2.26	118.99	111.91
38	a	412	LMG	O1-C1-C2	2.26	111.83	108.30
32	b	606	CLA	CHD-C1D-ND	-2.26	122.38	124.45
32	GG	612	CLA	CHD-C1D-ND	-2.26	122.38	124.45
32	G	613	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
32	Rr	608	CLA	CHB-C4A-NA	2.26	127.63	124.51
46	Ee	101	HEM	CHC-C4B-C3B	2.25	128.02	124.57
32	44	609	CLA	CHB-C4A-NA	2.25	127.63	124.51
32	Ss	602	CLA	CHD-C1D-ND	-2.25	122.38	124.45
32	a	407	CLA	CHB-C4A-NA	2.25	127.63	124.51
32	Nn	314	CLA	CHB-C4A-NA	2.25	127.63	124.51
40	Rr	614	LUT	C19-C9-C8	2.25	121.63	118.08
32	Dd	402	CLA	CHD-C1D-ND	-2.25	122.38	124.45
39	Gg	308	CHL	O2A-CGA-O1A	-2.25	117.91	123.59
40	S	614	LUT	C19-C9-C8	2.25	121.62	118.08
41	R	616	XAT	C24-C23-C22	-2.25	106.43	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	514	BCR	C11-C10-C9	-2.25	124.10	127.31
34	K	102	BCR	C12-C13-C14	-2.25	115.49	118.94
40	N	615	LUT	C18-C5-C6	-2.25	122.00	124.53
32	g	614	CLA	CHD-C1D-ND	-2.25	122.39	124.45
32	Bb	609	CLA	CHD-C1D-ND	-2.25	122.39	124.45
32	Nn	302	CLA	CHD-C1D-ND	-2.25	122.39	124.45
32	C	506	CLA	CHB-C4A-NA	2.25	127.62	124.51
32	s	602	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
36	0	201	LHG	O8-C23-C24	2.25	118.97	111.91
32	2	611	CLA	CHB-C4A-NA	2.25	127.62	124.51
32	B	610	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
32	Bb	610	CLA	CHD-C1D-ND	-2.25	122.39	124.45
39	Ss	601	CHL	O2A-CGA-O1A	-2.25	117.92	123.59
32	4	305	CLA	CHD-C1D-ND	-2.25	122.39	124.45
32	RR	313	CLA	CHD-C1D-ND	-2.25	122.39	124.45
32	R	602	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
32	b	610	CLA	CHB-C4A-NA	2.25	127.62	124.51
40	N	615	LUT	C15-C35-C34	-2.25	118.87	123.47
32	Bb	607	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
32	Bb	603	CLA	CHB-C4A-NA	2.25	127.62	124.51
32	Ss	609	CLA	CHD-C1D-ND	-2.24	122.39	124.45
36	D	410	LHG	O8-C23-C24	2.24	118.95	111.91
37	Aa	413	SQD	O8-S-C6	2.24	109.32	105.74
32	Bb	608	CLA	CHD-C1D-ND	-2.24	122.39	124.45
41	Gg	301	XAT	C12-C13-C14	-2.24	115.50	118.94
32	Cc	512	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	3	610	CLA	CAC-C3C-C4C	2.24	127.72	124.81
32	Y	602	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
45	a	413	BCT	O3-C-O1	-2.24	113.73	119.55
39	1	608	CHL	C1D-CHD-C4C	-2.24	121.22	126.06
34	CC	516	BCR	C40-C30-C25	2.24	113.94	110.30
41	y	301	XAT	C19-C9-C10	-2.24	119.78	122.92
32	R	603	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
32	Cc	510	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	Yy	611	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	n	611	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	Gg	305	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	DD	403	CLA	O2D-CGD-CBD	2.24	115.25	111.27
41	Yy	619	XAT	O24-C25-C26	-2.24	57.10	58.96
40	NN	615	LUT	C12-C13-C14	-2.24	115.50	118.94
32	Y	612	CLA	O2D-CGD-CBD	2.24	115.25	111.27
32	AA	408	CLA	C1-C2-C3	-2.24	122.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	n	610	CLA	C1D-ND-C4D	-2.24	104.74	106.33
39	G	601	CHL	C1B-CHB-C4A	-2.24	125.68	130.12
34	C	518	BCR	C37-C22-C21	-2.24	119.79	122.92
32	Cc	514	CLA	CHD-C1D-ND	-2.24	122.40	124.45
34	C	518	BCR	C20-C21-C22	-2.24	124.11	127.31
32	C	505	CLA	C6-C5-C3	2.24	119.33	113.45
33	Aa	408	PHO	C5-C3-C2	2.24	125.65	121.12
32	B	609	CLA	CHD-C1D-ND	-2.24	122.40	124.45
32	Bb	605	CLA	CHD-C1D-ND	-2.24	122.40	124.45
32	B	620	CLA	CHB-C4A-NA	2.24	127.61	124.51
40	Y	615	LUT	C21-C26-C27	-2.24	109.87	112.70
32	BB	613	CLA	C1-C2-C3	-2.24	122.17	126.04
32	Cc	511	CLA	CMB-C2B-C3B	2.24	128.86	124.68
32	Nn	301	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
34	Cc	517	BCR	C37-C22-C23	2.24	121.60	118.08
43	R	618	LMU	C1'-O5'-C5'	2.24	118.08	113.69
32	Gg	314	CLA	CHB-C4A-NA	2.24	127.60	124.51
32	BB	601	CLA	O2D-CGD-CBD	2.24	115.24	111.27
33	A	407	PHO	C5-C3-C2	2.24	125.64	121.12
32	22	603	CLA	CHD-C1D-ND	-2.24	122.40	124.45
46	E	101	HEM	C1B-NB-C4B	2.23	107.38	105.07
34	B	616	BCR	C29-C28-C27	-2.23	106.38	111.38
40	SS	315	LUT	C18-C5-C6	-2.23	122.02	124.53
40	N	616	LUT	C17-C1-C6	-2.23	106.67	110.30
40	g	615	LUT	C17-C1-C6	-2.23	106.67	110.30
38	b	621	LMG	C8-O7-C10	-2.23	112.29	117.79
32	Bb	613	CLA	CHD-C1D-ND	-2.23	122.40	124.45
32	G	612	CLA	CAC-C3C-C4C	2.23	127.71	124.81
41	G	619	XAT	C12-C13-C14	-2.23	115.52	118.94
32	R	614	CLA	CHB-C4A-NA	2.23	127.60	124.51
32	GG	613	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
41	Yy	619	XAT	C20-C13-C12	2.23	121.59	118.08
39	r	606	CHL	C2A-C1A-CHA	2.23	127.76	123.86
32	RR	304	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
40	y	317	LUT	C1-C2-C3	2.23	118.68	113.64
39	N	609	CHL	O2D-CGD-CBD	2.23	115.23	111.27
39	11	607	CHL	CAC-C3C-C4C	2.23	127.70	124.81
32	33	612	CLA	CMB-C2B-C3B	2.23	128.85	124.68
32	Rr	610	CLA	CHB-C4A-NA	2.23	127.60	124.51
32	11	610	CLA	CHB-C4A-NA	2.23	127.60	124.51
40	s	615	LUT	C12-C13-C14	-2.23	115.52	118.94
40	s	615	LUT	C36-C21-C26	2.23	112.92	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	44	608	CHL	OMC-CMC-C2C	-2.23	120.64	125.69
32	YY	614	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
32	N	612	CLA	CAA-C2A-C3A	-2.23	108.69	114.26
40	n	616	LUT	C12-C13-C14	-2.23	115.52	118.94
32	N	604	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	Bb	607	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	b	608	CLA	CHD-C1D-ND	-2.23	122.41	124.45
39	1	608	CHL	CBD-CHA-C1A	2.23	131.12	128.50
32	b	601	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	NN	604	CLA	CHB-C4A-NA	2.23	127.59	124.51
41	GG	619	XAT	C20-C13-C14	-2.23	119.80	122.92
37	C	501	SQD	O9-S-C6	2.23	109.59	106.94
41	N	617	XAT	C16-C1-C2	-2.23	105.11	108.98
32	CC	503	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	SS	310	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	YY	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
34	c	514	BCR	C15-C16-C17	-2.23	118.91	123.47
34	Bb	617	BCR	C39-C30-C25	-2.23	106.69	110.30
32	BB	610	CLA	C11-C10-C8	-2.23	108.72	115.92
32	C	508	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
39	Y	609	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
39	Nn	316	CHL	C1B-CHB-C4A	-2.22	125.71	130.12
32	Cc	507	CLA	CHD-C1D-ND	-2.22	122.41	124.45
32	33	611	CLA	CHD-C1D-ND	-2.22	122.41	124.45
32	c	509	CLA	CHD-C1D-ND	-2.22	122.41	124.45
32	c	502	CLA	CHB-C4A-NA	2.22	127.59	124.51
39	g	607	CHL	O2A-CGA-O1A	-2.22	117.98	123.59
39	Yy	609	CHL	CAC-C3C-C4C	2.22	127.69	124.81
32	YY	612	CLA	C5-C3-C2	2.22	125.61	121.12
40	44	612	LUT	C36-C21-C26	2.22	112.91	109.55
34	h	101	BCR	C27-C26-C25	-2.22	119.50	122.73
38	Bb	621	LMG	O1-C1-C2	2.22	111.77	108.30
34	A	409	BCR	C20-C21-C22	-2.22	124.14	127.31
32	B	611	CLA	CMB-C2B-C3B	2.22	128.83	124.68
32	Aa	410	CLA	CMB-C2B-C3B	2.22	128.83	124.68
32	r	611	CLA	CHB-C4A-NA	2.22	127.58	124.51
32	Y	604	CLA	CHD-C1D-ND	-2.22	122.42	124.45
32	GG	614	CLA	CHD-C1D-ND	-2.22	122.42	124.45
32	BB	603	CLA	CHB-C4A-NA	2.22	127.58	124.51
32	Nn	302	CLA	CHB-C4A-NA	2.22	127.58	124.51
32	s	609	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
32	Bb	605	CLA	CHB-C4A-NA	2.22	127.58	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	616	BCR	C2-C1-C6	2.22	113.89	110.48
37	LL	102	SQD	O8-S-C6	2.22	109.27	105.74
32	2	604	CLA	CHD-C1D-ND	-2.22	122.42	124.45
32	G	603	CLA	CHD-C1D-ND	-2.22	122.42	124.45
32	R	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
34	CC	515	BCR	C33-C5-C6	-2.22	122.04	124.53
32	BB	612	CLA	CMB-C2B-C3B	2.22	128.82	124.68
32	b	609	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	A	409	BCR	C37-C22-C23	-2.22	114.58	118.08
39	11	605	CHL	CBD-CHA-C1A	2.22	131.11	128.50
36	DD	408	LHG	O8-C23-C24	2.22	118.86	111.91
34	H	101	BCR	C24-C23-C22	-2.22	122.89	126.23
32	G	604	CLA	CHB-C4A-NA	2.22	127.58	124.51
39	g	605	CHL	OMC-CMC-C2C	-2.21	120.68	125.69
39	Y	609	CHL	O2A-CGA-O1A	-2.21	118.00	123.59
32	Gg	314	CLA	CHD-C1D-ND	-2.21	122.42	124.45
41	44	613	XAT	C8-C9-C10	-2.21	115.54	118.94
41	NN	617	XAT	C16-C1-C2	-2.21	105.14	108.98
32	Nn	312	CLA	CAC-C3C-C4C	2.21	127.68	124.81
39	GG	609	CHL	CAC-C3C-C4C	2.21	127.68	124.81
34	KK	103	BCR	C39-C30-C25	-2.21	106.71	110.30
32	N	602	CLA	CHD-C1D-ND	-2.21	122.42	124.45
32	Y	602	CLA	CHD-C1D-ND	-2.21	122.42	124.45
32	4	303	CLA	O2D-CGD-CBD	2.21	115.20	111.27
32	3	613	CLA	CMB-C2B-C3B	2.21	128.82	124.68
34	c	516	BCR	C29-C30-C25	2.21	113.89	110.48
41	R	616	XAT	C12-C13-C14	-2.21	115.55	118.94
32	R	610	CLA	CMB-C2B-C3B	2.21	128.82	124.68
32	YY	612	CLA	CMB-C2B-C3B	2.21	128.82	124.68
32	SS	305	CLA	CAC-C3C-C4C	2.21	127.68	124.81
34	BB	618	BCR	C32-C1-C6	-2.21	106.71	110.30
32	22	602	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
32	Gg	312	CLA	CHB-C4A-NA	2.21	127.57	124.51
34	d	403	BCR	C15-C16-C17	-2.21	118.94	123.47
38	b	621	LMG	O1-C1-C2	2.21	111.75	108.30
36	D	409	LHG	O8-C23-C24	2.21	118.84	111.91
32	Bb	615	CLA	CMB-C2B-C3B	2.21	128.81	124.68
39	NN	609	CHL	O2D-CGD-CBD	2.21	115.20	111.27
39	R	606	CHL	C3C-C4C-NC	-2.21	108.09	110.57
34	D	406	BCR	C16-C15-C14	-2.21	118.95	123.47
32	g	613	CLA	CAC-C3C-C4C	2.21	127.68	124.81
33	a	408	PHO	C5-C3-C2	2.21	125.59	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	605	CHL	CAA-C2A-C3A	2.21	118.83	112.78
34	c	516	BCR	C32-C1-C6	-2.21	106.71	110.30
32	DD	404	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
32	22	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
42	Y	619	NEX	C11-C10-C9	-2.21	124.16	127.31
41	y	301	XAT	C15-C35-C34	-2.21	118.95	123.47
32	YY	612	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
34	KK	103	BCR	C38-C26-C27	2.21	117.86	113.62
32	s	612	CLA	CHB-C4A-NA	2.21	127.57	124.51
32	4	311	CLA	CHB-C4A-NA	2.21	127.57	124.51
45	AA	413	BCT	O3-C-O1	-2.21	113.82	119.55
32	GG	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
39	YY	608	CHL	CMB-C2B-C1B	-2.21	125.07	128.46
32	y	306	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
32	CC	514	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
41	Nn	308	XAT	C19-C9-C10	-2.21	119.83	122.92
34	c	514	BCR	C2-C3-C4	-2.21	106.44	111.38
40	R	615	LUT	C20-C13-C12	2.21	121.56	118.08
39	Nn	319	CHL	CAC-C3C-C4C	2.21	127.67	124.81
40	44	612	LUT	C35-C15-C14	-2.21	118.95	123.47
41	R	616	XAT	C36-C21-C22	-2.21	105.15	108.98
34	h	101	BCR	C34-C9-C10	-2.21	119.83	122.92
32	g	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
36	Yy	618	LHG	C5-O7-C7	-2.21	112.36	117.79
40	N	616	LUT	C16-C1-C6	2.20	113.88	110.30
32	CC	504	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
32	AA	408	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
32	NN	610	CLA	CHB-C4A-NA	2.20	127.56	124.51
32	2	609	CLA	CHD-C1D-ND	-2.20	122.43	124.45
37	L	101	SQD	O8-S-C6	2.20	109.25	105.74
42	Gg	318	NEX	C20-C13-C14	-2.20	119.84	122.92
32	G	611	CLA	CHB-C4A-NA	2.20	127.56	124.51
34	KK	103	BCR	C12-C13-C14	-2.20	115.56	118.94
32	C	515	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
39	Yy	607	CHL	O1D-CGD-CBD	2.20	128.99	124.48
32	S	602	CLA	CBA-CAA-C2A	2.20	120.36	113.86
34	AA	409	BCR	C2-C3-C4	-2.20	106.46	111.38
40	4	313	LUT	C35-C15-C14	-2.20	118.96	123.47
33	A	407	PHO	C1B-NB-C4B	2.20	111.61	107.09
34	c	514	BCR	C38-C26-C27	2.20	117.84	113.62
32	Bb	608	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
42	Nn	309	NEX	C15-C14-C13	-2.20	124.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	R	617	NEX	C32-C33-C34	-2.20	115.56	118.94
32	Rr	612	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
32	Nn	312	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
32	BB	612	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
41	RR	316	XAT	C24-C23-C22	-2.20	106.52	110.77
39	3	606	CHL	CAC-C3C-C4C	2.20	127.66	124.81
34	Dd	403	BCR	C1-C6-C7	2.20	122.00	115.78
32	4	303	CLA	CHB-C4A-NA	2.20	127.55	124.51
32	n	603	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
40	RR	315	LUT	C36-C21-C26	2.20	112.87	109.55
39	R	606	CHL	C2A-C3A-C4A	-2.20	98.32	101.87
42	YY	617	NEX	C32-C33-C34	-2.20	115.57	118.94
32	Y	613	CLA	CHD-C1D-ND	-2.20	122.44	124.45
32	Bb	615	CLA	CHD-C1D-ND	-2.20	122.44	124.45
39	Nn	316	CHL	O2A-CGA-O1A	-2.20	118.05	123.59
40	NN	616	LUT	C17-C1-C6	-2.20	106.74	110.30
39	22	601	CHL	CMB-C2B-C1B	-2.20	125.09	128.46
32	r	608	CLA	CHB-C4A-NA	2.20	127.55	124.51
39	s	606	CHL	C2A-C1A-CHA	2.20	127.70	123.86
32	Yy	603	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
39	Rr	606	CHL	O2D-CGD-O1D	-2.20	119.55	123.84
32	RR	310	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
32	s	610	CLA	CHB-C4A-NA	2.20	127.55	124.51
39	N	606	CHL	CAC-C3C-C4C	2.20	127.66	124.81
42	g	617	NEX	C12-C13-C14	-2.19	115.57	118.94
34	B	612	BCR	C38-C26-C27	2.19	117.83	113.62
32	33	612	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
34	H	101	BCR	C36-C18-C17	-2.19	119.85	122.92
41	y	301	XAT	C40-C33-C34	-2.19	119.85	122.92
39	NN	601	CHL	C2C-C3C-C4C	2.19	108.05	106.49
32	Y	614	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
42	Yy	617	NEX	C15-C14-C13	-2.19	124.18	127.31
34	Cc	516	BCR	C15-C16-C17	-2.19	118.98	123.47
32	G	614	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	B	604	CLA	CHB-C4A-NA	2.19	127.55	124.51
32	a	405	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
33	Aa	409	PHO	O2A-CGA-O1A	-2.19	118.06	123.59
34	b	618	BCR	C37-C22-C21	-2.19	119.85	122.92
32	CC	502	CLA	O2D-CGD-CBD	2.19	115.16	111.27
38	m	101	LMG	O8-C28-C29	2.19	118.79	111.91
34	C	518	BCR	C7-C6-C5	-2.19	116.15	121.46
32	G	610	CLA	O2A-CGA-O1A	-2.19	118.06	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	NN	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	NN	614	CLA	CHB-C4A-NA	2.19	127.54	124.51
34	BB	620	BCR	C16-C17-C18	-2.19	124.18	127.31
34	T	101	BCR	C40-C30-C25	-2.19	106.74	110.30
32	Rr	601	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	GG	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
34	C	516	BCR	C2-C3-C4	-2.19	106.48	111.38
32	33	613	CLA	O2D-CGD-CBD	2.19	115.16	111.27
32	DD	404	CLA	CHB-C4A-NA	2.19	127.54	124.51
34	DD	405	BCR	C27-C26-C25	-2.19	119.55	122.73
44	B	601	DGD	O6D-C5D-C6D	2.19	111.09	106.67
32	Yy	613	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	b	609	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	Cc	512	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	b	608	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	c	502	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
32	CC	507	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
34	DD	405	BCR	C16-C15-C14	-2.19	118.99	123.47
36	a	414	LHG	O8-C23-C24	2.19	118.78	111.91
36	D	410	LHG	C5-O7-C7	-2.19	112.40	117.79
32	NN	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	Cc	504	CLA	CHD-C1D-ND	-2.19	122.44	124.45
39	4	309	CHL	CHB-C4A-NA	2.19	127.54	124.51
39	YY	609	CHL	O2A-CGA-O1A	-2.19	118.07	123.59
32	n	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	b	613	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	Ss	611	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	22	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
32	a	406	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
32	c	510	CLA	CHB-C4A-NA	2.19	127.53	124.51
41	Rr	615	XAT	C35-C15-C14	-2.19	119.00	123.47
32	G	602	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	R	610	CLA	CHB-C4A-NA	2.18	127.53	124.51
39	GG	605	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
33	A	407	PHO	CMC-C2C-C3C	2.18	129.06	124.94
32	C	507	CLA	CHB-C4A-NA	2.18	127.53	124.51
42	n	617	NEX	C40-C33-C34	-2.18	119.86	122.92
32	3	612	CLA	CMB-C2B-C3B	2.18	128.76	124.68
32	Y	612	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
32	Y	613	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
34	C	518	BCR	C4-C5-C6	-2.18	119.56	122.73
34	CC	517	BCR	C4-C5-C6	-2.18	119.56	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Yy	616	LUT	C20-C13-C12	2.18	121.52	118.08
32	Bb	606	CLA	CHD-C1D-ND	-2.18	122.45	124.45
32	C	505	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	Bb	601	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	Bb	603	CLA	CBA-CAA-C2A	2.18	120.30	113.86
32	Yy	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45
32	BB	608	CLA	CHD-C1D-ND	-2.18	122.45	124.45
42	Y	619	NEX	C15-C14-C13	-2.18	124.20	127.31
32	g	611	CLA	C4-C3-C5	2.18	118.94	115.27
37	AA	412	SQD	O9-S-C6	2.18	109.53	106.94
32	CC	512	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	c	512	CLA	CHD-C1D-ND	-2.18	122.45	124.45
34	c	514	BCR	C36-C18-C17	-2.18	119.87	122.92
34	Bb	618	BCR	C37-C22-C21	-2.18	119.87	122.92
32	N	603	CLA	CAA-C2A-C3A	-2.18	108.81	114.26
40	Y	616	LUT	C7-C8-C9	-2.18	122.94	126.23
34	h	101	BCR	C4-C5-C6	-2.18	119.57	122.73
39	Y	605	CHL	O1D-CGD-CBD	2.18	128.94	124.48
40	r	614	LUT	C36-C21-C26	2.18	112.85	109.55
32	b	602	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
32	G	614	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	N	602	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
34	CC	516	BCR	C2-C1-C6	2.18	113.83	110.48
32	g	611	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
32	D	401	CLA	O2D-CGD-CBD	2.18	115.14	111.27
32	Y	602	CLA	CAC-C3C-C4C	2.18	127.64	124.81
41	Rr	615	XAT	C24-C23-C22	-2.18	106.57	110.77
32	Bb	604	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
34	BB	618	BCR	C16-C15-C14	-2.18	119.01	123.47
32	BB	611	CLA	C2D-C1D-ND	-2.18	108.50	110.10
32	A	408	CLA	C1-C2-C3	-2.18	122.28	126.04
32	NN	610	CLA	CHD-C1D-ND	-2.18	122.45	124.45
37	C	501	SQD	O48-C23-O10	-2.18	118.10	123.59
34	K	102	BCR	C39-C30-C25	-2.18	106.77	110.30
32	3	610	CLA	CHB-C4A-NA	2.18	127.52	124.51
44	BB	625	DGD	C2G-O2G-C1B	-2.18	112.44	117.79
32	Cc	504	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
41	RR	316	XAT	C36-C21-C22	-2.17	105.21	108.98
32	YY	612	CLA	O2D-CGD-CBD	2.17	115.13	111.27
40	Ss	614	LUT	C19-C9-C8	2.17	121.50	118.08
32	n	614	CLA	CHB-C4A-NA	2.17	127.52	124.51
32	NN	603	CLA	CHD-C1D-ND	-2.17	122.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	309	CHL	CAC-C3C-C4C	2.17	127.63	124.81
32	b	603	CLA	CBA-CAA-C2A	2.17	120.28	113.86
32	N	603	CLA	CHB-C4A-NA	2.17	127.52	124.51
32	s	611	CLA	CHB-C4A-NA	2.17	127.52	124.51
39	Yy	601	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
32	n	602	CLA	CAC-C3C-C4C	2.17	127.63	124.81
34	Bb	618	BCR	C33-C5-C6	-2.17	122.09	124.53
40	r	614	LUT	C15-C35-C34	-2.17	119.03	123.47
32	11	611	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	RR	308	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	Cc	507	CLA	CHB-C4A-NA	2.17	127.51	124.51
42	Rr	616	NEX	C11-C10-C9	-2.17	124.21	127.31
37	B	602	SQD	O9-S-C6	2.17	109.52	106.94
32	CC	504	CLA	CHD-C1D-ND	-2.17	122.46	124.45
39	n	606	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
39	Nn	319	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
34	b	619	BCR	C15-C16-C17	-2.17	119.03	123.47
34	TT	101	BCR	C4-C5-C6	-2.17	119.58	122.73
32	RR	309	CLA	CBA-CAA-C2A	2.17	120.27	113.86
32	SS	312	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
32	AA	406	CLA	O2D-CGD-CBD	2.17	115.12	111.27
32	1	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	B	621	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	y	315	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
32	s	609	CLA	O2D-CGD-CBD	2.17	115.12	111.27
44	c	517	DGD	O1G-C1A-O1A	-2.17	118.13	123.59
34	Bb	617	BCR	C3-C4-C5	-2.17	110.21	114.08
32	GG	602	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
34	b	618	BCR	C29-C28-C27	-2.16	106.54	111.38
32	GG	610	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
32	R	608	CLA	CHD-C1D-ND	-2.16	122.47	124.45
44	BB	624	DGD	O6D-C5D-C6D	2.16	111.03	106.67
41	RR	316	XAT	C4-C3-C2	-2.16	106.60	110.77
32	N	610	CLA	CBA-CAA-C2A	2.16	120.25	113.86
37	CC	501	SQD	O7-S-C6	2.16	109.51	106.94
41	RR	316	XAT	C8-C9-C10	-2.16	115.62	118.94
32	RR	312	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	B	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
32	11	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	n	614	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
40	Yy	616	LUT	C40-C33-C32	2.16	121.48	118.08
41	4	314	XAT	C12-C13-C14	-2.16	115.62	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	YY	611	CLA	CMB-C2B-C3B	2.16	128.72	124.68
40	s	614	LUT	C36-C21-C26	2.16	112.82	109.55
32	n	611	CLA	CHD-C1D-ND	-2.16	122.47	124.45
39	R	605	CHL	CHD-C1D-ND	-2.16	122.47	124.45
32	b	608	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
32	l	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	G	613	CLA	CHB-C4A-NA	2.16	127.50	124.51
34	AA	409	BCR	C40-C30-C25	-2.16	106.80	110.30
33	AA	407	PHO	C1B-NB-C4B	2.16	111.52	107.09
36	Ll	102	LHG	O8-C23-C24	2.16	118.68	111.91
32	NN	602	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
37	L	101	SQD	O7-S-C6	2.16	109.50	106.94
33	D	402	PHO	C1B-NB-C4B	2.16	111.52	107.09
32	GG	604	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
32	BB	604	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	N	603	CLA	CHD-C1D-ND	-2.16	122.47	124.45
32	Y	604	CLA	O2D-CGD-CBD	2.16	115.10	111.27
32	DD	404	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	Aa	411	BCR	C38-C26-C25	-2.16	122.11	124.53
32	R	608	CLA	CHB-C4A-NA	2.16	127.49	124.51
39	33	608	CHL	CAC-C3C-C4C	2.16	127.61	124.81
40	R	615	LUT	C28-C29-C30	-2.16	115.63	118.94
32	Bb	602	CLA	CHB-C4A-NA	2.16	127.49	124.51
40	Ss	614	LUT	C16-C1-C6	2.15	113.79	110.30
32	44	610	CLA	CHD-C1D-ND	-2.15	122.47	124.45
32	Ss	612	CLA	CHB-C4A-NA	2.15	127.49	124.51
39	Y	609	CHL	C1-C2-C3	-2.15	122.32	126.04
32	NN	604	CLA	CHD-C1D-ND	-2.15	122.47	124.45
32	YY	604	CLA	CHD-C1D-ND	-2.15	122.47	124.45
32	C	505	CLA	CHD-C1D-ND	-2.15	122.48	124.45
32	R	613	CLA	CHD-C1D-ND	-2.15	122.48	124.45
42	RR	317	NEX	C40-C33-C32	2.15	121.47	118.08
32	Ss	608	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
40	GG	616	LUT	C20-C13-C12	2.15	121.47	118.08
40	YY	616	LUT	C36-C21-C26	2.15	112.80	109.55
32	N	604	CLA	CHD-C1D-ND	-2.15	122.48	124.45
34	A	409	BCR	C2-C3-C4	-2.15	106.57	111.38
32	a	410	CLA	CHD-C1D-ND	-2.15	122.48	124.45
41	R	616	XAT	C4-C3-C2	-2.15	106.62	110.77
32	n	610	CLA	CMC-C2C-C1C	2.15	128.31	125.04
34	b	619	BCR	C38-C26-C25	-2.15	122.11	124.53
33	a	409	PHO	O2A-CGA-O1A	-2.15	118.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	602	CLA	CHB-C4A-NA	2.15	127.48	124.51
41	GG	619	XAT	C26-C27-C28	-2.15	121.45	125.99
32	b	615	CLA	CHD-C1D-ND	-2.15	122.48	124.45
38	Aa	412	LMG	O1-C1-C2	2.15	111.66	108.30
32	Bb	609	CLA	CHB-C4A-NA	2.15	127.48	124.51
32	11	612	CLA	C2D-C1D-ND	-2.15	108.52	110.10
39	GG	606	CHL	CAC-C3C-C4C	2.15	127.60	124.81
32	g	613	CLA	CHB-C4A-NA	2.15	127.48	124.51
39	22	605	CHL	C2A-C1A-CHA	2.15	126.04	122.71
32	N	610	CLA	CMB-C2B-C3B	2.15	128.70	124.68
32	S	611	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
32	y	313	CLA	CHB-C4A-NA	2.15	127.48	124.51
32	GG	614	CLA	CHB-C4A-NA	2.15	127.48	124.51
39	SS	308	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
39	N	609	CHL	CAC-C3C-C4C	2.15	127.59	124.81
39	NN	609	CHL	CAC-C3C-C4C	2.15	127.59	124.81
32	Nn	305	CLA	CHB-C4A-NA	2.15	127.48	124.51
39	1	605	CHL	C1D-CHD-C4C	-2.15	121.43	126.06
32	b	604	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
32	g	610	CLA	CHB-C4A-NA	2.14	127.48	124.51
32	RR	313	CLA	CHB-C4A-NA	2.14	127.48	124.51
40	4	313	LUT	C19-C9-C8	2.14	121.46	118.08
32	Bb	602	CLA	O1D-CGD-CBD	2.14	128.87	124.48
32	GG	612	CLA	CAC-C3C-C4C	2.14	127.59	124.81
39	N	601	CHL	C4A-NA-C1A	2.14	107.67	106.71
32	BB	610	CLA	C4-C3-C5	2.14	118.87	115.27
39	11	607	CHL	C3C-C4C-NC	-2.14	108.17	110.57
34	c	514	BCR	C38-C26-C25	-2.14	122.12	124.53
41	G	617	XAT	C31-C30-C29	-2.14	124.25	127.31
39	y	311	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
32	d	402	CLA	CHD-C1D-ND	-2.14	122.49	124.45
32	CC	509	CLA	CHD-C1D-ND	-2.14	122.49	124.45
40	YY	616	LUT	C20-C13-C12	2.14	121.45	118.08
37	L	101	SQD	C45-O47-C7	-2.14	112.52	117.79
32	AA	408	CLA	CHD-C1D-ND	-2.14	122.49	124.45
32	Gg	312	CLA	CHD-C1D-ND	-2.14	122.49	124.45
32	D	401	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
32	R	609	CLA	CBA-CAA-C2A	2.14	120.18	113.86
32	B	606	CLA	C11-C10-C8	-2.14	109.00	115.92
38	Aa	412	LMG	C8-O7-C10	-2.14	112.53	117.79
39	g	601	CHL	CAC-C3C-C4C	2.14	127.58	124.81
32	Aa	407	CLA	O2D-CGD-CBD	2.14	115.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Bb	603	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
32	44	610	CLA	CHB-C4A-NA	2.14	127.47	124.51
32	22	604	CLA	CHB-C4A-NA	2.14	127.47	124.51
32	Cc	505	CLA	CHB-C4A-NA	2.14	127.47	124.51
32	Gg	303	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
39	22	607	CHL	CAC-C3C-C4C	2.14	127.58	124.81
32	C	503	CLA	CBA-CAA-C2A	2.14	120.17	113.86
34	Bb	619	BCR	C15-C16-C17	-2.14	119.10	123.47
39	4	309	CHL	CHD-C1D-ND	-2.14	122.49	124.45
32	Cc	505	CLA	CMB-C2B-C3B	2.14	128.67	124.68
32	Bb	613	CLA	O1D-CGD-CBD	2.14	128.85	124.48
40	G	616	LUT	C12-C13-C14	-2.14	115.66	118.94
32	n	610	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
32	Cc	506	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
32	Bb	605	CLA	CMB-C2B-C3B	2.14	128.67	124.68
42	Rr	616	NEX	C15-C14-C13	-2.13	124.26	127.31
40	YY	616	LUT	C15-C35-C34	-2.13	119.10	123.47
39	y	307	CHL	O1D-CGD-CBD	2.13	128.85	124.48
32	b	606	CLA	O1D-CGD-CBD	2.13	128.85	124.48
32	s	611	CLA	C2A-C1A-CHA	2.13	127.59	123.86
40	G	615	LUT	C35-C15-C14	-2.13	119.10	123.47
32	YY	603	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
34	Bb	618	BCR	C29-C28-C27	-2.13	106.61	111.38
32	1	611	CLA	CHD-C1D-ND	-2.13	122.49	124.45
32	Cc	503	CLA	CHD-C1D-ND	-2.13	122.49	124.45
32	GG	602	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
39	N	609	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
34	KK	103	BCR	C2-C1-C6	2.13	113.76	110.48
32	Ss	608	CLA	CHD-C1D-ND	-2.13	122.50	124.45
32	2	610	CLA	CHD-C1D-ND	-2.13	122.50	124.45
32	Gg	315	CLA	CHD-C1D-ND	-2.13	122.50	124.45
39	11	605	CHL	CHD-C1D-ND	-2.13	122.50	124.45
39	4	308	CHL	C3C-C4C-NC	-2.13	108.18	110.57
34	Hh	101	BCR	C4-C5-C6	-2.13	119.64	122.73
34	BB	620	BCR	C19-C18-C17	-2.13	115.67	118.94
32	Aa	410	CLA	CBA-CAA-C2A	2.13	120.15	113.86
32	Y	612	CLA	C4A-NA-C1A	2.13	107.66	106.71
34	BB	616	BCR	C34-C9-C8	2.13	121.43	118.08
32	Aa	406	CLA	CMB-C2B-C3B	2.13	128.66	124.68
44	Cc	519	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
32	BB	604	CLA	C6-C5-C3	2.13	119.04	113.45
40	Gg	317	LUT	C40-C33-C32	2.13	121.43	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	503	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
34	Cc	516	BCR	C38-C26-C25	-2.13	122.14	124.53
41	G	619	XAT	C26-C27-C28	-2.13	121.49	125.99
39	Yy	606	CHL	CAC-C3C-C4C	2.13	127.57	124.81
32	S	612	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
32	RR	314	CLA	CHD-C1D-ND	-2.13	122.50	124.45
34	D	406	BCR	C27-C26-C25	-2.13	119.64	122.73
42	g	617	NEX	C20-C13-C14	-2.13	119.94	122.92
32	Y	603	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	3	608	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
39	y	307	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
39	y	303	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
32	a	405	CLA	CHD-C1D-ND	-2.13	122.50	124.45
40	RR	315	LUT	C11-C10-C9	-2.13	124.28	127.31
41	GG	617	XAT	C31-C30-C29	-2.13	124.28	127.31
34	Hh	101	BCR	C37-C22-C23	2.12	121.42	118.08
33	AA	407	PHO	CMC-C2C-C3C	2.12	128.95	124.94
40	Nn	306	LUT	C15-C35-C34	-2.12	119.12	123.47
34	d	403	BCR	C12-C13-C14	-2.12	115.68	118.94
40	22	614	LUT	C31-C30-C29	-2.12	124.28	127.31
34	C	518	BCR	C34-C9-C8	2.12	121.42	118.08
32	C	510	CLA	CHD-C1D-ND	-2.12	122.50	124.45
37	LL	102	SQD	C45-O47-C7	-2.12	112.56	117.79
39	y	303	CHL	C3A-C2A-C1A	-2.12	98.16	101.34
40	Yy	615	LUT	C1-C2-C3	2.12	118.44	113.64
39	G	601	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
32	Cc	511	CLA	C4-C3-C5	2.12	118.84	115.27
32	a	407	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
32	g	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
41	G	619	XAT	C31-C30-C29	-2.12	124.28	127.31
32	r	612	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
34	B	613	BCR	C29-C28-C27	-2.12	106.64	111.38
32	n	603	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
40	Yy	616	LUT	C15-C35-C34	-2.12	119.13	123.47
34	C	517	BCR	C2-C1-C6	2.12	113.75	110.48
41	Rr	615	XAT	C12-C13-C14	-2.12	115.69	118.94
32	1	611	CLA	C2A-C1A-CHA	2.12	126.00	122.71
32	Yy	610	CLA	C4A-NA-C1A	2.12	107.66	106.71
32	1	609	CLA	O1D-CGD-CBD	2.12	128.82	124.48
32	BB	603	CLA	O2D-CGD-CBD	2.12	115.03	111.27
32	n	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
40	Y	615	LUT	C8-C9-C10	-2.12	115.69	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Cc	517	BCR	C39-C30-C25	-2.12	106.86	110.30
39	GG	601	CHL	O2A-CGA-O1A	-2.12	118.25	123.59
32	B	623	CLA	CMB-C2B-C3B	2.12	128.64	124.68
32	11	604	CLA	C2A-C1A-CHA	2.12	125.99	122.71
45	Aa	414	BCT	O3-C-O1	-2.12	114.06	119.55
34	CC	517	BCR	C7-C6-C5	-2.12	116.33	121.46
32	b	611	CLA	CHD-C1D-ND	-2.12	122.51	124.45
32	4	311	CLA	CHD-C1D-ND	-2.12	122.51	124.45
32	b	603	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
40	Yy	615	LUT	C35-C15-C14	-2.12	119.14	123.47
32	Aa	405	CLA	C5-C3-C2	2.12	125.40	121.12
38	Bb	621	LMG	C8-O7-C10	-2.12	112.58	117.79
32	2	604	CLA	CHB-C4A-NA	2.12	127.44	124.51
38	Mm	101	LMG	O8-C28-C29	2.12	118.55	111.91
32	Bb	609	CLA	C1-C2-C3	-2.12	122.39	126.04
39	N	607	CHL	C1-C2-C3	-2.12	122.39	126.04
39	YY	607	CHL	O2D-CGD-CBD	2.11	115.03	111.27
32	c	501	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
42	R	617	NEX	C20-C13-C14	-2.11	119.96	122.92
39	n	605	CHL	C1D-CHD-C4C	-2.11	121.50	126.06
32	R	610	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
32	Bb	606	CLA	O1D-CGD-CBD	2.11	128.81	124.48
32	D	405	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
32	SS	313	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
32	B	618	CLA	CHB-C4A-NA	2.11	127.44	124.51
32	Aa	405	CLA	C2A-C1A-CHA	2.11	127.56	123.86
32	Rr	609	CLA	C4-C3-C5	2.11	118.83	115.27
32	S	604	CLA	CHD-C1D-ND	-2.11	122.51	124.45
34	D	406	BCR	C7-C6-C5	-2.11	116.34	121.46
32	b	613	CLA	O1D-CGD-CBD	2.11	128.81	124.48
33	Aa	408	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
36	l	101	LHG	C5-O7-C7	-2.11	112.59	117.79
34	c	514	BCR	C29-C30-C25	2.11	113.73	110.48
32	Bb	611	CLA	CHB-C4A-NA	2.11	127.43	124.51
46	EE	102	HEM	C1B-NB-C4B	2.11	107.25	105.07
32	s	603	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
42	Gg	318	NEX	C37-C21-C36	-2.11	104.26	107.37
32	Nn	314	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
32	D	405	CLA	CHD-C1D-ND	-2.11	122.51	124.45
34	d	403	BCR	C40-C30-C25	2.11	113.72	110.30
32	2	612	CLA	CHB-C4A-NA	2.11	127.43	124.51
32	BB	601	CLA	CHB-C4A-NA	2.11	127.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	610	CLA	C4A-NA-C1A	2.11	107.66	106.71
32	SS	304	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
39	Rr	606	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
34	BB	616	BCR	C33-C5-C6	-2.11	122.16	124.53
44	B	603	DGD	C2G-O2G-C1B	-2.11	112.59	117.79
32	RR	302	CLA	C1-C2-C3	-2.11	122.39	126.04
32	Ss	603	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	R	602	CLA	CAA-C2A-C3A	2.11	118.56	112.78
46	e	101	HEM	C4C-CHD-C1D	2.11	125.34	122.56
32	g	614	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
39	Yy	605	CHL	O2A-CGA-O1A	-2.11	118.27	123.59
46	EE	102	HEM	C4C-CHD-C1D	2.11	125.34	122.56
37	Aa	413	SQD	O9-S-C6	2.11	109.45	106.94
32	Bb	611	CLA	CHD-C1D-ND	-2.11	122.52	124.45
32	33	610	CLA	CHB-C4A-NA	2.11	127.43	124.51
32	GG	604	CLA	CHB-C4A-NA	2.11	127.43	124.51
32	g	612	CLA	CAC-C3C-C4C	2.11	127.55	124.81
39	4	307	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
32	d	401	CLA	CAC-C3C-C4C	2.11	127.55	124.81
32	R	612	CLA	O2D-CGD-CBD	2.11	115.01	111.27
32	Rr	601	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
39	G	608	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
32	C	505	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
32	Aa	406	CLA	CMC-C2C-C1C	2.11	128.25	125.04
32	S	612	CLA	CHD-C1D-ND	-2.11	122.52	124.45
34	KK	103	BCR	C16-C17-C18	-2.11	124.31	127.31
32	R	612	CLA	CMB-C2B-C3B	2.11	128.62	124.68
32	c	506	CLA	CHD-C1D-ND	-2.10	122.52	124.45
32	A	408	CLA	O1D-CGD-CBD	2.10	128.79	124.48
36	11	614	LHG	C5-O7-C7	-2.10	112.61	117.79
32	22	610	CLA	CHB-C4A-NA	2.10	127.42	124.51
34	CC	517	BCR	C20-C21-C22	-2.10	124.31	127.31
40	G	615	LUT	C40-C33-C32	2.10	121.39	118.08
34	h	101	BCR	C12-C13-C14	-2.10	115.71	118.94
37	Aa	413	SQD	O7-S-C6	2.10	109.44	106.94
32	Cc	513	CLA	C1-C2-C3	-2.10	122.41	126.04
32	Rr	604	CLA	CHD-C1D-ND	-2.10	122.52	124.45
40	44	612	LUT	C19-C9-C8	2.10	121.39	118.08
32	Cc	506	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
34	BB	620	BCR	C8-C9-C10	-2.10	115.71	118.94
40	GG	616	LUT	C12-C13-C14	-2.10	115.71	118.94
32	Cc	514	CLA	O2A-CGA-O1A	-2.10	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	101	BCR	C37-C22-C23	2.10	121.39	118.08
32	Nn	313	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
39	NN	607	CHL	C1-C2-C3	-2.10	122.41	126.04
39	44	607	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
39	RR	305	CHL	CAA-C2A-C3A	2.10	118.53	112.78
41	NN	617	XAT	C36-C21-C22	-2.10	105.33	108.98
39	Y	605	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
36	Yy	618	LHG	O7-C7-O9	-2.10	118.62	123.70
36	Ll	102	LHG	C5-O7-C7	-2.10	112.62	117.79
39	n	605	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
40	RR	315	LUT	C20-C13-C12	2.10	121.39	118.08
32	11	609	CLA	CAC-C3C-C4C	2.10	127.53	124.81
32	44	602	CLA	CHD-C1D-ND	-2.10	122.52	124.45
40	NN	615	LUT	C1-C6-C5	-2.10	119.66	122.61
40	R	615	LUT	C12-C13-C14	-2.10	115.72	118.94
32	YY	614	CLA	CAA-C2A-C3A	2.10	118.53	112.78
33	DD	402	PHO	C1B-NB-C4B	2.10	111.40	107.09
32	22	603	CLA	CMB-C2B-C3B	2.10	128.61	124.68
37	LL	102	SQD	O7-S-C6	2.10	109.43	106.94
32	g	602	CLA	C2D-C1D-ND	2.10	111.65	110.10
32	Ss	613	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
32	Gg	304	CLA	CHD-C1D-ND	-2.10	122.53	124.45
44	CC	522	DGD	O2G-C1B-O1B	-2.10	118.63	123.70
40	SS	315	LUT	C7-C8-C9	-2.10	123.06	126.23
33	a	408	PHO	O2A-CGA-O1A	-2.10	118.30	123.59
32	D	404	CLA	CAC-C3C-C4C	2.10	127.53	124.81
32	NN	610	CLA	CBA-CAA-C2A	2.10	120.06	113.86
37	B	602	SQD	O7-S-C6	2.10	109.43	106.94
42	Y	617	NEX	C15-C14-C13	-2.10	124.32	127.31
32	2	610	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
39	Y	609	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
34	Aa	411	BCR	C37-C22-C21	-2.10	119.99	122.92
41	Rr	615	XAT	C19-C9-C10	-2.10	119.99	122.92
40	S	614	LUT	C7-C8-C9	-2.10	123.07	126.23
32	Ss	609	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
32	r	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
32	Rr	608	CLA	CBA-CAA-C2A	2.10	120.05	113.86
34	Cc	516	BCR	C27-C26-C25	-2.10	119.69	122.73
32	Nn	303	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
41	Yy	619	XAT	C16-C1-C2	-2.10	105.34	108.98
34	KK	103	BCR	C23-C22-C21	-2.10	115.73	118.94
39	Nn	318	CHL	CMB-C2B-C1B	-2.09	125.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	604	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	c	513	CLA	CHD-C1D-ND	-2.09	122.53	124.45
32	Nn	301	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	11	601	CHL	CHD-C1D-ND	-2.09	122.53	124.45
32	c	504	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	Ss	604	CLA	CHB-C4A-NA	2.09	127.41	124.51
39	GG	608	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
34	B	616	BCR	C20-C21-C22	-2.09	124.32	127.31
32	Rr	604	CLA	CAA-C2A-C1A	-2.09	105.11	111.97
32	A	406	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
39	G	605	CHL	C4A-NA-C1A	2.09	107.65	106.71
32	SS	305	CLA	CHD-C1D-ND	-2.09	122.53	124.45
32	CC	503	CLA	C4-C3-C5	2.09	118.79	115.27
39	y	307	CHL	O2A-CGA-O1A	-2.09	118.31	123.59
39	Y	608	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
32	Y	613	CLA	CMB-C2B-C3B	2.09	128.59	124.68
32	S	608	CLA	CHB-C4A-NA	2.09	127.40	124.51
37	L	102	SQD	O4-C4-C5	2.09	114.49	109.30
32	b	601	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	n	604	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
40	NN	616	LUT	C16-C1-C6	2.09	113.69	110.30
32	NN	604	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
32	c	512	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
38	j	101	LMG	O1-C1-C2	2.09	111.57	108.30
42	YY	617	NEX	C15-C14-C13	-2.09	124.33	127.31
34	B	612	BCR	C19-C18-C17	-2.09	115.73	118.94
40	s	615	LUT	C8-C9-C10	-2.09	115.73	118.94
32	Cc	508	CLA	CHD-C1D-ND	-2.09	122.53	124.45
32	Y	610	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
32	b	616	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
38	c	519	LMG	O8-C28-O10	-2.09	118.32	123.59
39	Yy	608	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
32	Bb	613	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
34	k	101	BCR	C28-C27-C26	-2.09	110.35	114.08
32	Bb	616	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
32	BB	602	CLA	CAA-C2A-C3A	2.09	118.49	112.78
32	Gg	311	CLA	CMC-C2C-C1C	2.09	128.22	125.04
32	11	612	CLA	CMC-C2C-C1C	-2.09	121.86	125.04
41	Rr	615	XAT	C16-C1-C6	2.09	115.68	110.05
39	GG	606	CHL	CMB-C2B-C1B	-2.09	125.26	128.46
32	33	611	CLA	CHB-C4A-NA	2.09	127.40	124.51
32	s	610	CLA	CHD-C1D-ND	-2.09	122.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	512	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
39	Yy	605	CHL	O1D-CGD-CBD	2.08	128.75	124.48
32	Ss	610	CLA	CHD-C1D-ND	-2.08	122.54	124.45
34	b	617	BCR	C29-C30-C25	2.08	113.69	110.48
32	CC	504	CLA	C6-C5-C3	2.08	118.92	113.45
32	Gg	315	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
39	RR	306	CHL	CHA-C1A-NA	-2.08	121.63	126.40
32	CC	510	CLA	CHD-C1D-ND	-2.08	122.54	124.45
32	CC	512	CLA	CHD-C1D-ND	-2.08	122.54	124.45
32	Bb	601	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	G	606	CHL	CAC-C3C-C4C	2.08	127.51	124.81
32	AA	406	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
32	B	622	CLA	C1-C2-C3	-2.08	122.44	126.04
34	XX	202	BCR	C38-C26-C25	-2.08	122.19	124.53
32	c	502	CLA	C4-C3-C2	-2.08	118.34	123.68
34	Dd	403	BCR	C19-C18-C17	-2.08	115.75	118.94
40	g	616	LUT	C28-C29-C30	-2.08	115.75	118.94
39	Yy	605	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
40	Gg	316	LUT	C35-C15-C14	-2.08	119.21	123.47
32	Ss	608	CLA	CAA-C2A-C3A	2.08	118.47	112.78
32	n	610	CLA	CAC-C3C-C4C	2.08	127.51	124.81
39	11	605	CHL	C3A-C4A-CHB	-2.08	118.53	124.01
32	r	612	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	y	311	CHL	O2D-CGD-CBD	2.08	114.97	111.27
32	N	604	CLA	CMA-C3A-C2A	-2.08	111.24	116.10
40	y	317	LUT	C16-C1-C6	2.08	113.67	110.30
40	GG	615	LUT	C15-C35-C34	-2.08	119.21	123.47
32	D	401	CLA	C4-C3-C5	2.08	118.77	115.27
40	r	614	LUT	C20-C13-C12	2.08	121.35	118.08
38	Dd	408	LMG	C8-O7-C10	-2.08	112.67	117.79
32	2	603	CLA	CHD-C1D-ND	-2.08	122.54	124.45
32	CC	514	CLA	CHD-C1D-ND	-2.08	122.54	124.45
32	BB	613	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	3	605	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
41	Yy	619	XAT	C15-C35-C34	-2.08	119.22	123.47
32	Cc	513	CLA	CHB-C4A-NA	2.08	127.39	124.51
39	s	607	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
34	DD	405	BCR	C7-C6-C5	-2.08	116.43	121.46
32	r	611	CLA	O1D-CGD-CBD	2.08	128.74	124.48
36	AA	411	LHG	O7-C7-O9	-2.08	118.68	123.70
39	R	605	CHL	C3C-C4C-NC	-2.08	108.24	110.57
34	B	616	BCR	C19-C18-C17	-2.08	115.75	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	622	CLA	CHD-C1D-ND	-2.08	122.55	124.45
32	A	405	CLA	O1D-CGD-CBD	2.08	128.73	124.48
32	S	603	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
34	Cc	517	BCR	C36-C18-C17	-2.08	120.01	122.92
32	Nn	312	CLA	CHD-C1D-ND	-2.08	122.55	124.45
32	CC	511	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
32	B	623	CLA	CHD-C1D-ND	-2.08	122.55	124.45
34	b	618	BCR	C33-C5-C6	-2.07	122.20	124.53
36	A	413	LHG	O8-C23-O10	-2.07	118.36	123.59
39	YY	606	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
34	TT	101	BCR	C29-C28-C27	-2.07	106.74	111.38
39	y	310	CHL	O2A-CGA-O1A	-2.07	118.36	123.59
34	k	101	BCR	C12-C13-C14	-2.07	115.76	118.94
41	y	301	XAT	C16-C1-C2	-2.07	105.38	108.98
39	Yy	601	CHL	C3A-C2A-C1A	-2.07	98.23	101.34
32	y	314	CLA	C4A-NA-C1A	2.07	107.64	106.71
32	l	603	CLA	CHD-C1D-ND	-2.07	122.55	124.45
39	Gg	306	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
40	NN	616	LUT	C15-C35-C34	-2.07	119.23	123.47
34	k	101	BCR	C7-C8-C9	-2.07	123.10	126.23
40	y	317	LUT	C35-C15-C14	-2.07	119.23	123.47
39	S	607	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
32	Cc	508	CLA	C1-C2-C3	-2.07	122.46	126.04
34	d	403	BCR	C1-C6-C7	2.07	121.64	115.78
32	s	612	CLA	CHD-C1D-ND	-2.07	122.55	124.45
32	BB	602	CLA	O1D-CGD-CBD	2.07	128.72	124.48
38	Cc	501	LMG	O8-C28-O10	-2.07	118.37	123.59
32	s	604	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
34	Dd	403	BCR	C30-C25-C24	2.07	121.63	115.78
32	n	612	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
40	YY	616	LUT	C7-C8-C9	-2.07	123.11	126.23
33	D	402	PHO	CMC-C2C-C3C	2.07	128.84	124.94
32	Y	614	CLA	CAA-C2A-C3A	2.07	118.44	112.78
32	DD	401	CLA	CHD-C1D-ND	-2.07	122.55	124.45
34	BB	616	BCR	C19-C18-C17	-2.07	115.77	118.94
39	N	601	CHL	C3C-C4C-NC	-2.07	108.25	110.57
32	Yy	612	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
34	B	616	BCR	C8-C9-C10	-2.07	115.77	118.94
37	L	102	SQD	O8-S-C6	2.07	109.03	105.74
40	Rr	614	LUT	C36-C21-C26	2.07	112.68	109.55
34	d	403	BCR	C30-C25-C24	2.07	121.62	115.78
39	YY	608	CHL	O2A-CGA-O1A	-2.07	118.38	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Ss	615	LUT	C28-C29-C30	-2.07	115.77	118.94
32	b	601	CLA	CAA-C2A-C3A	2.07	118.44	112.78
32	r	601	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
33	DD	402	PHO	O2A-CGA-O1A	-2.07	118.38	123.59
32	G	613	CLA	CMB-C2B-C3B	2.07	128.54	124.68
32	n	610	CLA	CMB-C2B-C3B	2.07	128.54	124.68
32	y	314	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
40	Y	616	LUT	C20-C13-C12	2.07	121.33	118.08
32	2	610	CLA	CMB-C2B-C3B	2.07	128.54	124.68
39	Yy	608	CHL	CMB-C2B-C1B	-2.07	125.29	128.46
41	Rr	615	XAT	C20-C13-C14	-2.07	120.03	122.92
32	b	611	CLA	CHB-C4A-NA	2.06	127.37	124.51
39	y	310	CHL	CMB-C2B-C1B	-2.06	125.29	128.46
34	H	101	BCR	C16-C17-C18	-2.06	124.36	127.31
32	SS	303	CLA	CBA-CAA-C2A	2.06	119.95	113.86
34	Bb	617	BCR	C38-C26-C27	2.06	117.58	113.62
32	Cc	510	CLA	CHD-C1D-ND	-2.06	122.56	124.45
34	Cc	518	BCR	C7-C8-C9	-2.06	123.12	126.23
32	SS	311	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
32	Ss	602	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
32	b	613	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
36	CC	523	LHG	O8-C23-O10	-2.06	118.39	123.59
34	XX	202	BCR	C35-C13-C12	2.06	121.33	118.08
40	g	616	LUT	C15-C35-C34	-2.06	119.25	123.47
38	BB	619	LMG	O8-C28-C29	2.06	118.38	111.91
32	4	304	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
34	a	411	BCR	C4-C5-C6	-2.06	119.74	122.73
32	n	602	CLA	CAA-C2A-C3A	2.06	118.42	112.78
39	G	607	CHL	CAC-C3C-C4C	2.06	127.48	124.81
40	y	318	LUT	C11-C10-C9	-2.06	124.37	127.31
32	YY	611	CLA	C2D-C1D-ND	-2.06	108.58	110.10
32	AA	405	CLA	O2A-C1-C2	-2.06	103.22	108.64
32	d	401	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	Cc	511	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	N	612	CLA	CAC-C3C-C4C	2.06	127.48	124.81
32	YY	612	CLA	C4-C3-C2	-2.06	118.39	123.68
39	YY	609	CHL	CMB-C2B-C1B	-2.06	125.30	128.46
40	Y	616	LUT	C19-C9-C8	2.06	121.32	118.08
44	D	411	DGD	O1G-C1A-O1A	-2.06	118.39	123.59
32	11	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	B	610	CLA	O2D-CGD-CBD	2.06	114.93	111.27
39	s	601	CHL	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
32	3	603	CLA	CHB-C4A-NA	2.06	127.36	124.51
32	N	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	Dd	401	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	NN	611	CLA	CBA-CAA-C2A	2.06	119.94	113.86
32	c	501	CLA	CMB-C2B-C3B	2.06	128.53	124.68
41	N	617	XAT	C39-C29-C28	2.06	121.32	118.08
41	R	616	XAT	C39-C29-C30	-2.06	120.04	122.92
32	A	408	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
32	a	406	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
32	B	621	CLA	C6-C5-C3	2.06	118.85	113.45
32	BB	614	CLA	O2D-CGD-CBD	2.06	114.92	111.27
32	B	609	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
34	Aa	411	BCR	C29-C28-C27	-2.06	106.78	111.38
32	b	601	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	RR	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
32	s	608	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
32	d	401	CLA	O2D-CGD-CBD	2.05	114.92	111.27
44	c	518	DGD	O1G-C1A-C2A	2.05	118.36	111.91
32	c	510	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
34	B	614	BCR	C16-C15-C14	-2.05	119.27	123.47
40	s	615	LUT	C28-C29-C30	-2.05	115.79	118.94
32	y	316	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
40	Rr	614	LUT	C28-C29-C30	-2.05	115.79	118.94
39	Ss	607	CHL	CMB-C2B-C1B	-2.05	125.31	128.46
39	N	608	CHL	CMB-C2B-C1B	-2.05	125.31	128.46
32	B	619	CLA	CAA-C2A-C3A	2.05	118.40	112.78
34	B	612	BCR	C34-C9-C8	2.05	121.31	118.08
32	N	610	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
32	g	610	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
34	a	411	BCR	C37-C22-C21	-2.05	120.05	122.92
32	GG	602	CLA	CHB-C4A-NA	2.05	127.35	124.51
32	YY	613	CLA	CHD-C1D-ND	-2.05	122.57	124.45
34	BB	617	BCR	C29-C28-C27	-2.05	106.79	111.38
42	N	618	NEX	C32-C33-C34	-2.05	115.79	118.94
40	y	318	LUT	C15-C35-C34	-2.05	119.27	123.47
39	3	605	CHL	CAC-C3C-C4C	2.05	127.47	124.81
39	44	606	CHL	CMB-C2B-C1B	-2.05	125.31	128.46
32	BB	604	CLA	CMB-C2B-C3B	2.05	128.52	124.68
32	BB	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
40	GG	615	LUT	C17-C1-C6	-2.05	106.97	110.30
32	CC	505	CLA	O2A-CGA-O1A	-2.05	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	NN	611	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
39	n	608	CHL	CMB-C2B-C1B	-2.05	125.31	128.46
32	g	612	CLA	C2A-C1A-CHA	2.05	127.44	123.86
41	4	314	XAT	C4-C3-C2	-2.05	106.81	110.77
44	CC	518	DGD	C6E-C5E-C4E	-2.05	108.20	113.00
34	CC	517	BCR	C24-C23-C22	-2.05	123.14	126.23
40	NN	616	LUT	C37-C21-C22	-2.05	105.55	109.44
32	44	602	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
39	Y	608	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
32	Ss	611	CLA	C2A-C1A-CHA	2.05	127.44	123.86
34	CC	517	BCR	C27-C26-C25	-2.05	119.76	122.73
33	AA	407	PHO	O2A-CGA-O1A	-2.05	118.42	123.59
33	A	407	PHO	O2A-CGA-O1A	-2.05	118.42	123.59
39	s	607	CHL	CMB-C2B-C1B	-2.05	125.32	128.46
32	2	603	CLA	CHB-C4A-NA	2.05	127.34	124.51
32	g	611	CLA	C2A-C1A-CHA	2.05	127.44	123.86
32	C	515	CLA	O2D-CGD-CBD	2.05	114.91	111.27
42	R	617	NEX	C2-C1-C6	2.05	111.20	109.21
34	k	101	BCR	C35-C13-C12	2.05	121.30	118.08
32	c	507	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	Cc	504	CLA	CHB-C4A-NA	2.05	127.34	124.51
32	N	611	CLA	CBA-CAA-C2A	2.05	119.91	113.86
32	b	607	CLA	CMB-C2B-C3B	2.05	128.51	124.68
40	g	616	LUT	C16-C1-C6	2.05	113.62	110.30
32	Rr	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
41	GG	619	XAT	C39-C29-C28	2.05	121.30	118.08
32	B	624	CLA	C1-O2A-CGA	2.05	121.81	116.44
32	c	505	CLA	CHB-C4A-NA	2.05	127.34	124.51
41	NN	617	XAT	C26-C27-C28	-2.05	121.67	125.99
34	CC	515	BCR	C15-C16-C17	-2.04	119.28	123.47
39	2	608	CHL	CMB-C2B-C1B	-2.04	125.32	128.46
32	3	609	CLA	CHB-C4A-NA	2.04	127.34	124.51
41	RR	316	XAT	C12-C13-C14	-2.04	115.80	118.94
40	RR	315	LUT	C28-C29-C30	-2.04	115.81	118.94
32	R	613	CLA	CHB-C4A-NA	2.04	127.34	124.51
36	N	619	LHG	O7-C7-O9	-2.04	118.76	123.70
39	3	606	CHL	CMB-C2B-C1B	-2.04	125.32	128.46
39	r	606	CHL	C3C-C4C-NC	-2.04	108.28	110.57
32	Bb	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
41	44	613	XAT	C28-C29-C30	-2.04	115.81	118.94
36	KK	101	LHG	C5-O7-C7	-2.04	112.76	117.79
44	Cc	519	DGD	O2G-C1B-O1B	-2.04	118.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	r	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
32	BB	604	CLA	C4-C3-C5	2.04	118.70	115.27
41	Nn	308	XAT	C16-C1-C2	-2.04	105.44	108.98
40	g	616	LUT	C35-C15-C14	-2.04	119.30	123.47
32	c	502	CLA	O2D-CGD-CBD	2.04	114.89	111.27
39	n	609	CHL	O2D-CGD-CBD	2.04	114.89	111.27
32	n	602	CLA	C1-C2-C3	-2.04	122.52	126.04
32	RR	304	CLA	CMB-C2B-C3B	2.04	128.49	124.68
32	SS	313	CLA	CHD-C1D-ND	-2.04	122.58	124.45
32	Nn	304	CLA	O1D-CGD-CBD	2.04	128.65	124.48
39	Y	606	CHL	CMB-C2B-C1B	-2.04	125.33	128.46
41	GG	617	XAT	O24-C25-C26	-2.04	57.27	58.96
42	NN	618	NEX	C32-C33-C34	-2.04	115.81	118.94
39	RR	305	CHL	CBA-CAA-C2A	2.04	119.88	113.86
32	N	611	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	Bb	610	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	CC	505	CLA	O2D-CGD-CBD	2.04	114.89	111.27
42	RR	317	NEX	C20-C13-C14	-2.04	120.07	122.92
32	d	402	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	C	514	CLA	C4-C3-C2	-2.04	118.46	123.68
39	n	609	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
44	C	519	DGD	O6D-C5D-C6D	2.04	110.77	106.67
32	Cc	509	CLA	C5-C3-C2	2.03	125.23	121.12
32	33	603	CLA	CHB-C4A-NA	2.03	127.33	124.51
34	TT	101	BCR	C40-C30-C25	-2.03	107.00	110.30
41	GG	617	XAT	C12-C13-C14	-2.03	115.82	118.94
32	b	612	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
32	GG	603	CLA	CHD-C1D-ND	-2.03	122.58	124.45
42	g	617	NEX	C10-C11-C12	-2.03	116.87	123.22
32	3	611	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	Ss	612	CLA	O2D-CGD-CBD	2.03	114.88	111.27
32	c	501	CLA	C11-C12-C13	-2.03	109.35	115.92
34	B	616	BCR	C24-C23-C22	-2.03	123.16	126.23
34	Hh	101	BCR	C7-C6-C5	-2.03	116.54	121.46
32	Yy	603	CLA	CHA-C1A-NA	-2.03	121.74	126.40
32	c	507	CLA	C5-C3-C2	2.03	125.23	121.12
34	d	403	BCR	C19-C18-C17	-2.03	115.82	118.94
39	22	608	CHL	CMB-C2B-C1B	-2.03	125.34	128.46
39	33	601	CHL	C3A-C4A-CHB	-2.03	118.66	124.01
32	YY	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
32	Nn	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
41	N	617	XAT	C26-C27-C28	-2.03	121.70	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	RR	306	CHL	CMB-C2B-C1B	-2.03	125.34	128.46
32	SS	314	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
32	CC	508	CLA	C2A-C1A-CHA	2.03	127.41	123.86
32	B	619	CLA	O1D-CGD-CBD	2.03	128.64	124.48
34	k	101	BCR	C31-C1-C6	-2.03	107.01	110.30
32	BB	614	CLA	C4-C3-C2	-2.03	118.47	123.68
39	GG	601	CHL	CAC-C3C-C4C	2.03	127.44	124.81
34	h	101	BCR	C34-C9-C8	-2.03	114.88	118.08
40	Y	616	LUT	C2-C3-C4	2.03	113.08	110.30
38	Bb	621	LMG	O7-C10-O9	-2.03	118.80	123.70
32	GG	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
32	44	602	CLA	CBA-CAA-C2A	2.03	119.85	113.86
32	A	408	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	BB	605	CLA	O1D-CGD-CBD	2.03	128.63	124.48
40	NN	615	LUT	C36-C21-C26	2.03	112.62	109.55
39	G	608	CHL	O1D-CGD-CBD	2.03	128.63	124.48
32	22	602	CLA	CHB-C4A-NA	2.03	127.32	124.51
34	H	101	BCR	C4-C5-C6	-2.03	119.79	122.73
32	BB	609	CLA	C4-C3-C2	-2.03	118.48	123.68
40	Yy	615	LUT	C12-C13-C14	-2.03	115.83	118.94
32	Gg	313	CLA	CHA-C1A-NA	-2.03	121.75	126.40
39	G	606	CHL	CMB-C2B-C1B	-2.03	125.35	128.46
34	a	411	BCR	C29-C28-C27	-2.03	106.85	111.38
38	Cc	501	LMG	O7-C10-O9	-2.03	118.80	123.70
42	Yy	617	NEX	C2-C1-C6	2.03	111.18	109.21
39	R	606	CHL	CHA-C1A-NA	-2.03	121.76	126.40
32	S	604	CLA	CAC-C3C-C4C	2.03	127.44	124.81
32	c	505	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	CC	506	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
40	y	317	LUT	C1-C6-C7	2.03	121.51	115.78
32	33	602	CLA	CHB-C4A-NA	2.03	127.31	124.51
38	c	519	LMG	C4-C3-C2	2.03	114.36	110.82
39	YY	605	CHL	CMB-C2B-C1B	-2.03	125.35	128.46
32	AA	408	CLA	O1D-CGD-CBD	2.03	128.63	124.48
41	Yy	619	XAT	C19-C9-C8	2.03	121.27	118.08
32	4	303	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
39	4	308	CHL	O2A-CGA-O1A	-2.02	118.25	123.30
32	B	620	CLA	O2D-CGD-CBD	2.02	114.87	111.27
39	N	607	CHL	CAC-C3C-C4C	2.02	127.44	124.81
32	Ss	604	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
32	33	604	CLA	CHB-C4A-NA	2.02	127.31	124.51
32	3	602	CLA	CHB-C4A-NA	2.02	127.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	GG	613	CLA	CMB-C2B-C3B	2.02	128.46	124.68
34	Bb	619	BCR	C39-C30-C25	2.02	113.58	110.30
39	2	607	CHL	CMB-C2B-C1B	-2.02	125.35	128.46
32	3	611	CLA	CHB-C4A-NA	2.02	127.31	124.51
32	B	605	CLA	C4-C3-C2	-2.02	118.49	123.68
32	Nn	303	CLA	CHA-C1A-NA	-2.02	121.77	126.40
33	D	402	PHO	O2A-CGA-O1A	-2.02	118.49	123.59
34	Cc	516	BCR	C24-C25-C26	-2.02	116.57	121.46
34	T	101	BCR	C29-C28-C27	-2.02	106.86	111.38
34	Dd	403	BCR	C12-C13-C14	-2.02	115.84	118.94
40	GG	615	LUT	C32-C33-C34	-2.02	115.84	118.94
39	3	608	CHL	CAC-C3C-C4C	2.02	127.43	124.81
39	g	601	CHL	C1-C2-C3	-2.02	122.55	126.04
32	YY	612	CLA	C2A-C3A-C4A	-2.02	98.61	101.87
34	B	616	BCR	C35-C13-C12	2.02	121.26	118.08
39	33	605	CHL	CMB-C2B-C1B	-2.02	125.36	128.46
39	RR	305	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
32	YY	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	g	605	CHL	CMB-C2B-C1B	-2.02	125.36	128.46
32	Nn	301	CLA	CBA-CAA-C2A	2.02	119.82	113.86
44	c	517	DGD	C6E-C5E-C4E	-2.02	108.27	113.00
34	T	101	BCR	C21-C20-C19	-2.02	116.92	123.22
39	Y	607	CHL	O2D-CGD-CBD	2.02	114.86	111.27
40	G	616	LUT	C32-C33-C34	-2.02	115.84	118.94
32	4	305	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
32	BB	615	CLA	CAC-C3C-C4C	2.02	127.43	124.81
32	11	602	CLA	CHB-C4A-NA	2.02	127.30	124.51
39	Y	601	CHL	C3C-C4C-NC	-2.02	108.31	110.57
40	Y	615	LUT	C32-C33-C34	-2.02	115.84	118.94
38	B	615	LMG	O8-C28-C29	2.02	118.24	111.91
40	Rr	614	LUT	C18-C5-C6	-2.02	122.26	124.53
32	BB	610	CLA	O1D-CGD-CBD	2.02	128.61	124.48
34	Cc	516	BCR	C29-C30-C25	2.02	113.59	110.48
32	s	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
32	Aa	407	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
32	CC	508	CLA	C4-C3-C2	-2.02	118.50	123.68
39	Gg	309	CHL	CMB-C2B-C1B	-2.02	125.36	128.46
33	A	407	PHO	C1-C2-C3	-2.02	122.56	126.04
40	n	616	LUT	C15-C35-C34	-2.02	119.34	123.47
32	Yy	614	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
34	B	612	BCR	C36-C18-C17	-2.02	120.10	122.92
40	Yy	616	LUT	C11-C10-C9	-2.02	124.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	622	CLA	O1D-CGD-CBD	2.02	128.61	124.48
40	SS	315	LUT	C11-C10-C9	-2.02	124.43	127.31
40	RR	315	LUT	C12-C13-C14	-2.01	115.85	118.94
39	NN	608	CHL	CMB-C2B-C1B	-2.01	125.37	128.46
32	c	510	CLA	CHD-C1D-ND	-2.01	122.60	124.45
35	AA	410	PL9	C40-C39-C41	-2.01	111.88	115.27
40	NN	615	LUT	C15-C35-C34	-2.01	119.35	123.47
34	c	515	BCR	C36-C18-C17	-2.01	120.10	122.92
32	NN	611	CLA	CHD-C1D-ND	-2.01	122.60	124.45
39	g	608	CHL	CMB-C2B-C1B	-2.01	125.37	128.46
34	B	614	BCR	C32-C1-C6	-2.01	107.03	110.30
39	RR	306	CHL	CAA-C2A-C3A	2.01	118.29	112.78
32	n	614	CLA	O2D-CGD-CBD	2.01	114.84	111.27
32	B	621	CLA	CAC-C3C-C4C	2.01	127.42	124.81
34	C	518	BCR	C33-C5-C4	2.01	117.48	113.62
37	LL	101	SQD	O7-S-C6	2.01	109.33	106.94
32	G	610	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
39	33	606	CHL	CAC-C3C-C4C	2.01	127.42	124.81
32	r	602	CLA	C1-C2-C3	-2.01	122.56	126.04
40	Ss	614	LUT	C1-C2-C3	2.01	118.19	113.64
39	S	601	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
32	B	621	CLA	CMB-C2B-C3B	2.01	128.44	124.68
34	Kk	101	BCR	C16-C17-C18	-2.01	124.44	127.31
32	G	612	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
32	Gg	313	CLA	CAC-C3C-C4C	2.01	127.42	124.81
32	B	606	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
41	Rr	615	XAT	C28-C29-C30	-2.01	115.86	118.94
39	R	606	CHL	CAA-C2A-C3A	2.01	118.28	112.78
39	y	308	CHL	CMB-C2B-C1B	-2.01	125.38	128.46
43	R	618	LMU	C3B-C4B-C5B	-2.01	106.65	110.24
34	AA	409	BCR	C27-C26-C25	-2.01	119.81	122.73
34	Dd	403	BCR	C23-C22-C21	-2.01	115.86	118.94
39	Yy	609	CHL	O2D-CGD-CBD	2.01	114.84	111.27
32	Ss	611	CLA	CHA-C1A-NA	-2.01	121.80	126.40
34	Kk	101	BCR	C7-C6-C5	2.01	126.33	121.46
32	Bb	610	CLA	O1D-CGD-CBD	2.01	128.59	124.48
39	YY	609	CHL	C1-C2-C3	-2.01	122.57	126.04
32	Bb	601	CLA	CBA-CAA-C2A	2.01	119.79	113.86
39	Gg	302	CHL	C4A-NA-C1A	2.01	107.61	106.71
32	G	613	CLA	CAC-C3C-C4C	2.01	127.42	124.81
32	NN	612	CLA	CAC-C3C-C4C	2.01	127.42	124.81
32	Cc	503	CLA	C6-C7-C8	2.01	122.41	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	605	CHL	CMB-C2B-C1B	-2.01	125.38	128.46
34	D	406	BCR	C12-C13-C14	-2.01	115.86	118.94
40	Yy	615	LUT	C16-C1-C6	2.01	113.56	110.30
32	b	611	CLA	O2D-CGD-CBD	2.01	114.83	111.27
32	G	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
32	Y	611	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
32	Nn	314	CLA	CMB-C2B-C3B	2.01	128.43	124.68
32	c	508	CLA	C1-C2-C3	-2.01	122.57	126.04
38	c	519	LMG	O7-C10-O9	-2.01	118.85	123.70
34	C	516	BCR	C36-C18-C17	-2.01	120.11	122.92
32	Rr	612	CLA	CHD-C1D-ND	-2.01	122.61	124.45
32	g	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
38	c	519	LMG	C8-O7-C10	-2.01	112.85	117.79
32	Cc	512	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
32	C	511	CLA	CHD-C1D-ND	-2.01	122.61	124.45
32	RR	302	CLA	CAA-C2A-C3A	2.01	118.27	112.78
34	c	514	BCR	C27-C26-C25	-2.00	119.82	122.73
39	Nn	315	CHL	O2A-CGA-O1A	-2.00	118.53	123.59
40	RR	315	LUT	C16-C1-C6	2.00	113.55	110.30
42	y	319	NEX	C24-C23-C22	-2.00	106.90	110.77
32	R	603	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
32	YY	613	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	Ss	601	CHL	CMB-C2B-C1B	-2.00	125.39	128.46
39	SS	302	CHL	O2A-CGA-O1A	-2.00	118.54	123.59
32	c	506	CLA	C1-C2-C3	-2.00	122.58	126.04
32	c	508	CLA	CHD-C1D-ND	-2.00	122.61	124.45
32	n	603	CLA	CHD-C1D-ND	-2.00	122.61	124.45
32	b	607	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	Ss	607	CHL	O2A-CGA-O1A	-2.00	118.54	123.59
44	CC	519	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
41	44	613	XAT	C32-C33-C34	-2.00	115.87	118.94
32	BB	607	CLA	C1-C2-C3	-2.00	122.58	126.04
32	y	316	CLA	CAA-C2A-C3A	2.00	118.25	112.78
32	SS	304	CLA	O1A-CGA-CBA	2.00	129.51	123.08
38	F	101	LMG	O8-C28-C29	2.00	118.19	111.91
32	AA	408	CLA	CMB-C2B-C3B	2.00	128.42	124.68

All (780) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	406	CLA	ND

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Mol	Chain	Res	Type	Atom
32	A	408	CLA	ND
32	Rr	601	CLA	ND
32	Rr	602	CLA	ND
32	Rr	603	CLA	ND
32	Rr	604	CLA	ND
32	Rr	608	CLA	ND
32	Rr	609	CLA	ND
32	Rr	610	CLA	ND
32	Rr	611	CLA	ND
32	Rr	612	CLA	ND
32	Rr	613	CLA	ND
32	Ss	602	CLA	ND
32	Ss	603	CLA	ND
32	Ss	604	CLA	ND
32	Ss	608	CLA	ND
32	Ss	609	CLA	ND
32	Ss	610	CLA	ND
32	Ss	611	CLA	ND
32	Ss	612	CLA	ND
32	Ss	613	CLA	ND
32	Yy	602	CLA	ND
32	Yy	603	CLA	ND
32	Yy	604	CLA	ND
32	Yy	610	CLA	ND
32	Yy	611	CLA	ND
32	Yy	612	CLA	ND
32	Yy	613	CLA	ND
32	Yy	614	CLA	ND
32	44	602	CLA	ND
32	44	603	CLA	ND
32	44	604	CLA	ND
32	44	609	CLA	ND
32	44	610	CLA	ND
32	44	611	CLA	ND
32	44	615	CLA	ND
32	11	602	CLA	ND
32	11	603	CLA	ND
32	11	604	CLA	ND
32	11	609	CLA	ND
32	11	610	CLA	ND
32	11	611	CLA	ND
32	11	612	CLA	ND

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Mol	Chain	Res	Type	Atom
32	11	613	CLA	ND
32	22	602	CLA	ND
32	22	603	CLA	ND
32	22	604	CLA	ND
32	22	609	CLA	ND
32	22	610	CLA	ND
32	22	611	CLA	ND
32	22	612	CLA	ND
32	22	613	CLA	ND
32	33	602	CLA	ND
32	33	603	CLA	ND
32	33	604	CLA	ND
32	33	609	CLA	ND
32	33	610	CLA	ND
32	33	611	CLA	ND
32	33	612	CLA	ND
32	33	613	CLA	ND
32	1	602	CLA	ND
32	1	603	CLA	ND
32	1	604	CLA	ND
32	1	609	CLA	ND
32	1	610	CLA	ND
32	1	611	CLA	ND
32	1	612	CLA	ND
32	1	613	CLA	ND
32	2	602	CLA	ND
32	2	603	CLA	ND
32	2	604	CLA	ND
32	2	609	CLA	ND
32	2	610	CLA	ND
32	2	611	CLA	ND
32	2	612	CLA	ND
32	2	613	CLA	ND
32	3	602	CLA	ND
32	3	603	CLA	ND
32	3	604	CLA	ND
32	3	609	CLA	ND
32	3	610	CLA	ND
32	3	611	CLA	ND
32	3	612	CLA	ND
32	3	613	CLA	ND
32	C	503	CLA	ND

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Mol	Chain	Res	Type	Atom
32	C	505	CLA	ND
32	C	506	CLA	ND
32	C	507	CLA	ND
32	C	508	CLA	ND
32	C	509	CLA	ND
32	C	510	CLA	ND
32	C	511	CLA	ND
32	C	512	CLA	ND
32	C	513	CLA	ND
32	C	514	CLA	ND
32	C	515	CLA	ND
32	D	401	CLA	ND
32	D	404	CLA	ND
32	D	405	CLA	ND
32	G	602	CLA	ND
32	G	603	CLA	ND
32	G	604	CLA	ND
32	G	610	CLA	ND
32	G	611	CLA	ND
32	G	612	CLA	ND
32	G	613	CLA	ND
32	G	614	CLA	ND
32	N	602	CLA	ND
32	N	603	CLA	ND
32	N	604	CLA	ND
32	N	610	CLA	ND
32	N	611	CLA	ND
32	N	612	CLA	ND
32	N	613	CLA	ND
32	N	614	CLA	ND
32	R	601	CLA	ND
32	R	602	CLA	ND
32	R	603	CLA	ND
32	R	604	CLA	ND
32	R	608	CLA	ND
32	R	609	CLA	ND
32	R	610	CLA	ND
32	R	611	CLA	ND
32	R	612	CLA	ND
32	R	613	CLA	ND
32	S	602	CLA	ND
32	S	603	CLA	ND

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Mol	Chain	Res	Type	Atom
32	S	604	CLA	ND
32	S	608	CLA	ND
32	S	609	CLA	ND
32	S	610	CLA	ND
32	S	611	CLA	ND
32	S	612	CLA	ND
32	S	613	CLA	ND
32	X	201	CLA	ND
32	Y	602	CLA	ND
32	Y	603	CLA	ND
32	Y	610	CLA	ND
32	Y	611	CLA	ND
32	Y	612	CLA	ND
32	Y	613	CLA	ND
32	Y	614	CLA	ND
32	a	405	CLA	ND
32	a	406	CLA	ND
32	a	407	CLA	ND
32	a	410	CLA	ND
32	b	601	CLA	ND
32	b	602	CLA	ND
32	b	603	CLA	ND
32	b	604	CLA	ND
32	b	605	CLA	ND
32	b	606	CLA	ND
32	b	607	CLA	ND
32	b	608	CLA	ND
32	b	609	CLA	ND
32	b	610	CLA	ND
32	b	611	CLA	ND
32	b	612	CLA	ND
32	b	613	CLA	ND
32	b	614	CLA	ND
32	b	615	CLA	ND
32	b	616	CLA	ND
32	c	501	CLA	ND
32	c	502	CLA	ND
32	c	503	CLA	ND
32	c	504	CLA	ND
32	c	505	CLA	ND
32	c	506	CLA	ND
32	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
32	c	508	CLA	ND
32	c	509	CLA	ND
32	c	510	CLA	ND
32	c	511	CLA	ND
32	c	512	CLA	ND
32	c	513	CLA	ND
32	d	402	CLA	ND
32	g	603	CLA	ND
32	g	604	CLA	ND
32	g	610	CLA	ND
32	g	611	CLA	ND
32	g	612	CLA	ND
32	g	613	CLA	ND
32	g	614	CLA	ND
32	n	602	CLA	ND
32	n	603	CLA	ND
32	n	604	CLA	ND
32	n	610	CLA	ND
32	n	611	CLA	ND
32	n	612	CLA	ND
32	n	613	CLA	ND
32	n	614	CLA	ND
32	r	601	CLA	ND
32	r	602	CLA	ND
32	r	603	CLA	ND
32	r	604	CLA	ND
32	r	608	CLA	ND
32	r	609	CLA	ND
32	r	610	CLA	ND
32	r	611	CLA	ND
32	r	612	CLA	ND
32	r	613	CLA	ND
32	s	602	CLA	ND
32	s	603	CLA	ND
32	s	604	CLA	ND
32	s	608	CLA	ND
32	s	609	CLA	ND
32	s	610	CLA	ND
32	s	611	CLA	ND
32	s	612	CLA	ND
32	s	613	CLA	ND
32	y	304	CLA	ND

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Mol	Chain	Res	Type	Atom
32	y	305	CLA	ND
32	y	306	CLA	ND
32	y	312	CLA	ND
32	y	313	CLA	ND
32	y	314	CLA	ND
32	y	315	CLA	ND
32	y	316	CLA	ND
32	4	303	CLA	ND
32	4	304	CLA	ND
32	4	305	CLA	ND
32	4	310	CLA	ND
32	4	311	CLA	ND
32	4	312	CLA	ND
32	AA	405	CLA	ND
32	AA	406	CLA	ND
32	AA	408	CLA	ND
32	BB	601	CLA	ND
32	BB	602	CLA	ND
32	BB	603	CLA	ND
32	BB	604	CLA	ND
32	BB	605	CLA	ND
32	BB	606	CLA	ND
32	BB	607	CLA	ND
32	BB	608	CLA	ND
32	BB	610	CLA	ND
32	BB	611	CLA	ND
32	BB	612	CLA	ND
32	BB	613	CLA	ND
32	BB	614	CLA	ND
32	BB	615	CLA	ND
32	CC	502	CLA	ND
32	CC	504	CLA	ND
32	CC	505	CLA	ND
32	CC	506	CLA	ND
32	CC	507	CLA	ND
32	CC	508	CLA	ND
32	CC	509	CLA	ND
32	CC	510	CLA	ND
32	CC	511	CLA	ND
32	CC	512	CLA	ND
32	CC	513	CLA	ND
32	CC	514	CLA	ND

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Mol	Chain	Res	Type	Atom
32	DD	401	CLA	ND
32	DD	403	CLA	ND
32	DD	404	CLA	ND
32	B	604	CLA	ND
32	B	606	CLA	ND
32	B	607	CLA	ND
32	B	608	CLA	ND
32	B	609	CLA	ND
32	B	610	CLA	ND
32	B	611	CLA	ND
32	B	618	CLA	ND
32	B	619	CLA	ND
32	B	620	CLA	ND
32	B	621	CLA	ND
32	B	622	CLA	ND
32	B	623	CLA	ND
32	B	624	CLA	ND
32	GG	602	CLA	ND
32	GG	603	CLA	ND
32	GG	604	CLA	ND
32	GG	610	CLA	ND
32	GG	611	CLA	ND
32	GG	612	CLA	ND
32	GG	613	CLA	ND
32	GG	614	CLA	ND
32	NN	602	CLA	ND
32	NN	603	CLA	ND
32	NN	604	CLA	ND
32	NN	610	CLA	ND
32	NN	611	CLA	ND
32	NN	612	CLA	ND
32	NN	613	CLA	ND
32	NN	614	CLA	ND
32	RR	302	CLA	ND
32	RR	303	CLA	ND
32	RR	304	CLA	ND
32	RR	308	CLA	ND
32	RR	309	CLA	ND
32	RR	310	CLA	ND
32	RR	311	CLA	ND
32	RR	312	CLA	ND
32	RR	313	CLA	ND

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Mol	Chain	Res	Type	Atom
32	SS	303	CLA	ND
32	SS	304	CLA	ND
32	SS	305	CLA	ND
32	SS	309	CLA	ND
32	SS	310	CLA	ND
32	SS	311	CLA	ND
32	SS	312	CLA	ND
32	SS	313	CLA	ND
32	SS	314	CLA	ND
32	XX	201	CLA	ND
32	YY	602	CLA	ND
32	YY	603	CLA	ND
32	YY	610	CLA	ND
32	YY	611	CLA	ND
32	YY	612	CLA	ND
32	YY	613	CLA	ND
32	YY	614	CLA	ND
32	Aa	405	CLA	ND
32	Aa	406	CLA	ND
32	Aa	407	CLA	ND
32	Aa	410	CLA	ND
32	Bb	601	CLA	ND
32	Bb	602	CLA	ND
32	Bb	603	CLA	ND
32	Bb	604	CLA	ND
32	Bb	605	CLA	ND
32	Bb	606	CLA	ND
32	Bb	607	CLA	ND
32	Bb	608	CLA	ND
32	Bb	609	CLA	ND
32	Bb	610	CLA	ND
32	Bb	611	CLA	ND
32	Bb	612	CLA	ND
32	Bb	613	CLA	ND
32	Bb	614	CLA	ND
32	Bb	615	CLA	ND
32	Bb	616	CLA	ND
32	Cc	503	CLA	ND
32	Cc	505	CLA	ND
32	Cc	506	CLA	ND
32	Cc	507	CLA	ND
32	Cc	508	CLA	ND

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Mol	Chain	Res	Type	Atom
32	Cc	509	CLA	ND
32	Cc	510	CLA	ND
32	Cc	511	CLA	ND
32	Cc	512	CLA	ND
32	Cc	513	CLA	ND
32	Cc	514	CLA	ND
32	Cc	515	CLA	ND
32	Dd	402	CLA	ND
32	Gg	304	CLA	ND
32	Gg	305	CLA	ND
32	Gg	311	CLA	ND
32	Gg	312	CLA	ND
32	Gg	313	CLA	ND
32	Gg	314	CLA	ND
32	Gg	315	CLA	ND
32	Nn	301	CLA	ND
32	Nn	302	CLA	ND
32	Nn	303	CLA	ND
32	Nn	304	CLA	ND
32	Nn	312	CLA	ND
32	Nn	313	CLA	ND
32	Nn	314	CLA	ND
39	Rr	605	CHL	ND
39	Rr	605	CHL	NA
39	Rr	605	CHL	NC
39	Rr	606	CHL	ND
39	Rr	606	CHL	NA
39	Rr	606	CHL	NC
39	Rr	607	CHL	ND
39	Rr	607	CHL	NA
39	Rr	607	CHL	NC
39	Ss	601	CHL	ND
39	Ss	601	CHL	NA
39	Ss	601	CHL	NC
39	Ss	605	CHL	ND
39	Ss	605	CHL	NA
39	Ss	605	CHL	NC
39	Ss	606	CHL	ND
39	Ss	606	CHL	NA
39	Ss	606	CHL	NC
39	Ss	607	CHL	ND
39	Ss	607	CHL	NA

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Mol	Chain	Res	Type	Atom
39	Ss	607	CHL	NC
39	Yy	601	CHL	ND
39	Yy	601	CHL	NA
39	Yy	601	CHL	NC
39	Yy	605	CHL	ND
39	Yy	605	CHL	NA
39	Yy	605	CHL	NC
39	Yy	606	CHL	ND
39	Yy	606	CHL	NA
39	Yy	606	CHL	NC
39	Yy	607	CHL	ND
39	Yy	607	CHL	NA
39	Yy	607	CHL	NC
39	Yy	608	CHL	ND
39	Yy	608	CHL	NA
39	Yy	608	CHL	NC
39	Yy	609	CHL	ND
39	Yy	609	CHL	NA
39	Yy	609	CHL	NC
39	44	601	CHL	ND
39	44	601	CHL	NA
39	44	601	CHL	NC
39	44	605	CHL	ND
39	44	605	CHL	NA
39	44	605	CHL	NC
39	44	606	CHL	ND
39	44	606	CHL	NA
39	44	606	CHL	NC
39	44	607	CHL	ND
39	44	607	CHL	NA
39	44	607	CHL	NC
39	44	608	CHL	ND
39	44	608	CHL	NA
39	44	608	CHL	NC
39	11	601	CHL	ND
39	11	601	CHL	NA
39	11	601	CHL	NC
39	11	605	CHL	ND
39	11	605	CHL	NA
39	11	605	CHL	NC
39	11	606	CHL	ND
39	11	606	CHL	NA

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Mol	Chain	Res	Type	Atom
39	11	606	CHL	NC
39	11	607	CHL	ND
39	11	607	CHL	NA
39	11	607	CHL	NC
39	11	608	CHL	ND
39	11	608	CHL	NA
39	11	608	CHL	NC
39	22	601	CHL	ND
39	22	601	CHL	NA
39	22	601	CHL	NC
39	22	605	CHL	ND
39	22	605	CHL	NA
39	22	605	CHL	NC
39	22	606	CHL	ND
39	22	606	CHL	NA
39	22	606	CHL	NC
39	22	607	CHL	ND
39	22	607	CHL	NA
39	22	607	CHL	NC
39	22	608	CHL	ND
39	22	608	CHL	NA
39	22	608	CHL	NC
39	33	601	CHL	ND
39	33	601	CHL	NA
39	33	601	CHL	NC
39	33	605	CHL	ND
39	33	605	CHL	NA
39	33	605	CHL	NC
39	33	606	CHL	ND
39	33	606	CHL	NA
39	33	606	CHL	NC
39	33	607	CHL	ND
39	33	607	CHL	NA
39	33	607	CHL	NC
39	33	608	CHL	ND
39	33	608	CHL	NA
39	33	608	CHL	NC
39	1	601	CHL	ND
39	1	601	CHL	NA
39	1	601	CHL	NC
39	1	605	CHL	ND
39	1	605	CHL	NA

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Mol	Chain	Res	Type	Atom
39	1	605	CHL	NC
39	1	606	CHL	ND
39	1	606	CHL	NA
39	1	606	CHL	NC
39	1	607	CHL	ND
39	1	607	CHL	NA
39	1	607	CHL	NC
39	1	608	CHL	ND
39	1	608	CHL	NA
39	1	608	CHL	NC
39	2	601	CHL	ND
39	2	601	CHL	NA
39	2	601	CHL	NC
39	2	605	CHL	ND
39	2	605	CHL	NA
39	2	605	CHL	NC
39	2	606	CHL	ND
39	2	606	CHL	NA
39	2	606	CHL	NC
39	2	607	CHL	ND
39	2	607	CHL	NA
39	2	607	CHL	NC
39	2	608	CHL	ND
39	2	608	CHL	NA
39	2	608	CHL	NC
39	3	601	CHL	ND
39	3	601	CHL	NA
39	3	601	CHL	NC
39	3	605	CHL	ND
39	3	605	CHL	NA
39	3	605	CHL	NC
39	3	606	CHL	ND
39	3	606	CHL	NA
39	3	606	CHL	NC
39	3	607	CHL	ND
39	3	607	CHL	NA
39	3	607	CHL	NC
39	3	608	CHL	ND
39	3	608	CHL	NA
39	3	608	CHL	NC
39	G	601	CHL	ND
39	G	601	CHL	NA

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

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

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

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Mol	Chain	Res	Type	Atom
39	s	606	CHL	NC
39	s	607	CHL	ND
39	s	607	CHL	NA
39	s	607	CHL	NC
39	y	303	CHL	ND
39	y	303	CHL	NA
39	y	303	CHL	NC
39	y	307	CHL	ND
39	y	307	CHL	NA
39	y	307	CHL	NC
39	y	308	CHL	ND
39	y	308	CHL	NA
39	y	308	CHL	NC
39	y	309	CHL	ND
39	y	309	CHL	NA
39	y	309	CHL	NC
39	y	310	CHL	ND
39	y	310	CHL	NA
39	y	310	CHL	NC
39	y	311	CHL	ND
39	y	311	CHL	NA
39	y	311	CHL	NC
39	4	302	CHL	ND
39	4	302	CHL	NA
39	4	302	CHL	NC
39	4	306	CHL	ND
39	4	306	CHL	NA
39	4	306	CHL	NC
39	4	307	CHL	ND
39	4	307	CHL	NA
39	4	307	CHL	NC
39	4	308	CHL	ND
39	4	308	CHL	NA
39	4	308	CHL	NC
39	4	309	CHL	ND
39	4	309	CHL	NA
39	4	309	CHL	NC
39	GG	601	CHL	ND
39	GG	601	CHL	NA
39	GG	601	CHL	NC
39	GG	605	CHL	ND
39	GG	605	CHL	NA

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Mol	Chain	Res	Type	Atom
39	GG	605	CHL	NC
39	GG	606	CHL	ND
39	GG	606	CHL	NA
39	GG	606	CHL	NC
39	GG	607	CHL	ND
39	GG	607	CHL	NA
39	GG	607	CHL	NC
39	GG	608	CHL	ND
39	GG	608	CHL	NA
39	GG	608	CHL	NC
39	GG	609	CHL	ND
39	GG	609	CHL	NA
39	GG	609	CHL	NC
39	NN	601	CHL	ND
39	NN	601	CHL	NA
39	NN	601	CHL	NC
39	NN	605	CHL	ND
39	NN	605	CHL	NA
39	NN	605	CHL	NC
39	NN	606	CHL	ND
39	NN	606	CHL	NA
39	NN	606	CHL	NC
39	NN	607	CHL	ND
39	NN	607	CHL	NA
39	NN	607	CHL	NC
39	NN	608	CHL	ND
39	NN	608	CHL	NA
39	NN	608	CHL	NC
39	NN	609	CHL	ND
39	NN	609	CHL	NA
39	NN	609	CHL	NC
39	RR	305	CHL	ND
39	RR	305	CHL	NA
39	RR	305	CHL	NC
39	RR	306	CHL	ND
39	RR	306	CHL	NA
39	RR	306	CHL	NC
39	RR	307	CHL	ND
39	RR	307	CHL	NA
39	RR	307	CHL	NC
39	SS	302	CHL	ND
39	SS	302	CHL	NA

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Mol	Chain	Res	Type	Atom
39	SS	302	CHL	NC
39	SS	306	CHL	ND
39	SS	306	CHL	NA
39	SS	306	CHL	NC
39	SS	307	CHL	ND
39	SS	307	CHL	NA
39	SS	307	CHL	NC
39	SS	308	CHL	ND
39	SS	308	CHL	NA
39	SS	308	CHL	NC
39	YY	601	CHL	ND
39	YY	601	CHL	NA
39	YY	601	CHL	NC
39	YY	605	CHL	ND
39	YY	605	CHL	NA
39	YY	605	CHL	NC
39	YY	606	CHL	ND
39	YY	606	CHL	NA
39	YY	606	CHL	NC
39	YY	607	CHL	ND
39	YY	607	CHL	NA
39	YY	607	CHL	NC
39	YY	608	CHL	ND
39	YY	608	CHL	NA
39	YY	608	CHL	NC
39	YY	609	CHL	ND
39	YY	609	CHL	NA
39	YY	609	CHL	NC
39	Gg	302	CHL	ND
39	Gg	302	CHL	NA
39	Gg	302	CHL	NC
39	Gg	306	CHL	ND
39	Gg	306	CHL	NA
39	Gg	306	CHL	NC
39	Gg	307	CHL	ND
39	Gg	307	CHL	NA
39	Gg	307	CHL	NC
39	Gg	308	CHL	ND
39	Gg	308	CHL	NA
39	Gg	308	CHL	NC
39	Gg	309	CHL	ND
39	Gg	309	CHL	NA

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Mol	Chain	Res	Type	Atom
39	Gg	309	CHL	NC
39	Gg	310	CHL	ND
39	Gg	310	CHL	NA
39	Gg	310	CHL	NC
39	Nn	311	CHL	ND
39	Nn	311	CHL	NA
39	Nn	311	CHL	NC
39	Nn	315	CHL	ND
39	Nn	315	CHL	NA
39	Nn	315	CHL	NC
39	Nn	316	CHL	ND
39	Nn	316	CHL	NA
39	Nn	316	CHL	NC
39	Nn	317	CHL	ND
39	Nn	317	CHL	NA
39	Nn	317	CHL	NC
39	Nn	318	CHL	ND
39	Nn	318	CHL	NA
39	Nn	318	CHL	NC
39	Nn	319	CHL	ND
39	Nn	319	CHL	NA
39	Nn	319	CHL	NC

All (5753) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	406	CLA	CHA-CBD-CGD-O1D
32	A	406	CLA	CHA-CBD-CGD-O2D
32	A	408	CLA	CHA-CBD-CGD-O1D
32	A	408	CLA	CHA-CBD-CGD-O2D
32	A	408	CLA	CAD-CBD-CGD-O1D
32	Rr	602	CLA	C1A-C2A-CAA-CBA
32	Rr	604	CLA	C1A-C2A-CAA-CBA
32	Rr	604	CLA	CHA-CBD-CGD-O1D
32	Rr	608	CLA	C1A-C2A-CAA-CBA
32	Rr	608	CLA	CBD-CGD-O2D-CED
32	Rr	609	CLA	C1A-C2A-CAA-CBA
32	Rr	609	CLA	C3A-C2A-CAA-CBA
32	Rr	609	CLA	CHA-CBD-CGD-O1D
32	Rr	609	CLA	CHA-CBD-CGD-O2D
32	Rr	610	CLA	C1A-C2A-CAA-CBA
32	Rr	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Rr	610	CLA	CHA-CBD-CGD-O1D
32	Rr	610	CLA	CHA-CBD-CGD-O2D
32	Rr	610	CLA	CAD-CBD-CGD-O1D
32	Rr	610	CLA	CAD-CBD-CGD-O2D
32	Rr	611	CLA	CBD-CGD-O2D-CED
32	Rr	612	CLA	C1A-C2A-CAA-CBA
32	Rr	613	CLA	CHA-CBD-CGD-O1D
32	Ss	604	CLA	CHA-CBD-CGD-O1D
32	Ss	604	CLA	CHA-CBD-CGD-O2D
32	Ss	604	CLA	CAD-CBD-CGD-O1D
32	Ss	608	CLA	C3A-C2A-CAA-CBA
32	Ss	609	CLA	C1A-C2A-CAA-CBA
32	Ss	609	CLA	C3A-C2A-CAA-CBA
32	Ss	611	CLA	CAD-CBD-CGD-O1D
32	Ss	611	CLA	CAD-CBD-CGD-O2D
32	Ss	612	CLA	CHA-CBD-CGD-O1D
32	Ss	612	CLA	CHA-CBD-CGD-O2D
32	Yy	602	CLA	C1A-C2A-CAA-CBA
32	Yy	602	CLA	C3A-C2A-CAA-CBA
32	Yy	604	CLA	C1A-C2A-CAA-CBA
32	Yy	604	CLA	C2A-CAA-CBA-CGA
32	Yy	610	CLA	C1A-C2A-CAA-CBA
32	Yy	610	CLA	C3A-C2A-CAA-CBA
32	Yy	611	CLA	C1A-C2A-CAA-CBA
32	Yy	612	CLA	CBD-CGD-O2D-CED
32	Yy	612	CLA	O1D-CGD-O2D-CED
32	Yy	613	CLA	CHA-CBD-CGD-O1D
32	Yy	613	CLA	CHA-CBD-CGD-O2D
32	Yy	614	CLA	C3A-C2A-CAA-CBA
32	44	603	CLA	C1A-C2A-CAA-CBA
32	44	603	CLA	CBD-CGD-O2D-CED
32	44	604	CLA	CBD-CGD-O2D-CED
32	44	609	CLA	C1A-C2A-CAA-CBA
32	44	609	CLA	C3A-C2A-CAA-CBA
32	44	609	CLA	CBD-CGD-O2D-CED
32	44	610	CLA	CBD-CGD-O2D-CED
32	44	615	CLA	CHA-CBD-CGD-O1D
32	11	603	CLA	CBD-CGD-O2D-CED
32	11	604	CLA	CBD-CGD-O2D-CED
32	11	604	CLA	O1D-CGD-O2D-CED
32	11	609	CLA	CBD-CGD-O2D-CED
32	11	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	11	613	CLA	CBD-CGD-O2D-CED
32	22	604	CLA	CBD-CGD-O2D-CED
32	22	610	CLA	C1A-C2A-CAA-CBA
32	22	610	CLA	CHA-CBD-CGD-O1D
32	22	610	CLA	CHA-CBD-CGD-O2D
32	22	610	CLA	CBD-CGD-O2D-CED
32	22	611	CLA	CBD-CGD-O2D-CED
32	22	613	CLA	CHA-CBD-CGD-O1D
32	22	613	CLA	CHA-CBD-CGD-O2D
32	33	610	CLA	CHA-CBD-CGD-O1D
32	33	610	CLA	CBD-CGD-O2D-CED
32	33	612	CLA	CBD-CGD-O2D-CED
32	33	613	CLA	CHA-CBD-CGD-O2D
32	1	603	CLA	CHA-CBD-CGD-O1D
32	1	603	CLA	CHA-CBD-CGD-O2D
32	1	603	CLA	CBD-CGD-O2D-CED
32	1	604	CLA	CBD-CGD-O2D-CED
32	1	609	CLA	CBD-CGD-O2D-CED
32	1	610	CLA	CHA-CBD-CGD-O1D
32	1	610	CLA	CHA-CBD-CGD-O2D
32	1	610	CLA	CAD-CBD-CGD-O1D
32	1	611	CLA	CBD-CGD-O2D-CED
32	2	603	CLA	CBD-CGD-O2D-CED
32	2	604	CLA	CBD-CGD-O2D-CED
32	2	610	CLA	CBD-CGD-O2D-CED
32	2	613	CLA	CBD-CGD-O2D-CED
32	3	610	CLA	CHA-CBD-CGD-O1D
32	3	610	CLA	CHA-CBD-CGD-O2D
32	3	610	CLA	CBD-CGD-O2D-CED
32	3	612	CLA	CHA-CBD-CGD-O1D
32	3	612	CLA	CHA-CBD-CGD-O2D
32	3	612	CLA	CBD-CGD-O2D-CED
32	C	503	CLA	C1A-C2A-CAA-CBA
32	C	503	CLA	C3A-C2A-CAA-CBA
32	C	504	CLA	C1A-C2A-CAA-CBA
32	C	507	CLA	CHA-CBD-CGD-O1D
32	C	507	CLA	CHA-CBD-CGD-O2D
32	C	507	CLA	CAD-CBD-CGD-O1D
32	C	508	CLA	C1A-C2A-CAA-CBA
32	C	508	CLA	C3A-C2A-CAA-CBA
32	C	508	CLA	CHA-CBD-CGD-O1D
32	C	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	C	508	CLA	CAD-CBD-CGD-O1D
32	C	508	CLA	CAD-CBD-CGD-O2D
32	C	508	CLA	CBD-CGD-O2D-CED
32	C	509	CLA	CHA-CBD-CGD-O1D
32	C	509	CLA	CHA-CBD-CGD-O2D
32	C	511	CLA	C1A-C2A-CAA-CBA
32	C	511	CLA	C3A-C2A-CAA-CBA
32	C	513	CLA	CHA-CBD-CGD-O1D
32	C	513	CLA	CHA-CBD-CGD-O2D
32	C	513	CLA	CAD-CBD-CGD-O1D
32	C	513	CLA	CAD-CBD-CGD-O2D
32	C	515	CLA	CHA-CBD-CGD-O1D
32	C	515	CLA	CHA-CBD-CGD-O2D
32	C	515	CLA	CBD-CGD-O2D-CED
32	G	602	CLA	CBD-CGD-O2D-CED
32	G	603	CLA	CBD-CGD-O2D-CED
32	G	611	CLA	CBD-CGD-O2D-CED
32	G	612	CLA	CBD-CGD-O2D-CED
32	G	613	CLA	CHA-CBD-CGD-O1D
32	G	613	CLA	CHA-CBD-CGD-O2D
32	G	613	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	C1A-C2A-CAA-CBA
32	N	602	CLA	C3A-C2A-CAA-CBA
32	N	603	CLA	CHA-CBD-CGD-O1D
32	N	603	CLA	CHA-CBD-CGD-O2D
32	N	603	CLA	CAD-CBD-CGD-O1D
32	N	603	CLA	CBD-CGD-O2D-CED
32	N	604	CLA	CHA-CBD-CGD-O1D
32	N	604	CLA	CBD-CGD-O2D-CED
32	N	610	CLA	C1A-C2A-CAA-CBA
32	N	611	CLA	C1A-C2A-CAA-CBA
32	N	611	CLA	C3A-C2A-CAA-CBA
32	N	612	CLA	CBD-CGD-O2D-CED
32	N	613	CLA	C1A-C2A-CAA-CBA
32	N	613	CLA	CBD-CGD-O2D-CED
32	N	614	CLA	CBD-CGD-O2D-CED
32	R	601	CLA	CHA-CBD-CGD-O1D
32	R	601	CLA	CHA-CBD-CGD-O2D
32	R	601	CLA	CAD-CBD-CGD-O1D
32	R	602	CLA	C3A-C2A-CAA-CBA
32	R	602	CLA	CHA-CBD-CGD-O1D
32	R	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	R	608	CLA	CBD-CGD-O2D-CED
32	R	609	CLA	C1A-C2A-CAA-CBA
32	R	609	CLA	C3A-C2A-CAA-CBA
32	R	609	CLA	CBD-CGD-O2D-CED
32	R	610	CLA	C1A-C2A-CAA-CBA
32	R	610	CLA	C3A-C2A-CAA-CBA
32	R	610	CLA	CHA-CBD-CGD-O1D
32	R	610	CLA	CHA-CBD-CGD-O2D
32	R	612	CLA	C1A-C2A-CAA-CBA
32	R	613	CLA	CHA-CBD-CGD-O1D
32	R	613	CLA	CHA-CBD-CGD-O2D
32	R	613	CLA	CBD-CGD-O2D-CED
32	R	614	CLA	CHA-CBD-CGD-O1D
32	R	614	CLA	CHA-CBD-CGD-O2D
32	S	602	CLA	C1A-C2A-CAA-CBA
32	S	604	CLA	C1A-C2A-CAA-CBA
32	S	608	CLA	CHA-CBD-CGD-O1D
32	S	608	CLA	CHA-CBD-CGD-O2D
32	S	608	CLA	CAD-CBD-CGD-O1D
32	S	609	CLA	CBD-CGD-O2D-CED
32	S	611	CLA	CBD-CGD-O2D-CED
32	S	612	CLA	CBD-CGD-O2D-CED
32	S	613	CLA	CHA-CBD-CGD-O1D
32	S	613	CLA	CHA-CBD-CGD-O2D
32	X	201	CLA	CBD-CGD-O2D-CED
32	Y	602	CLA	C1A-C2A-CAA-CBA
32	Y	602	CLA	C3A-C2A-CAA-CBA
32	Y	603	CLA	CBD-CGD-O2D-CED
32	Y	604	CLA	C2A-CAA-CBA-CGA
32	Y	610	CLA	C1A-C2A-CAA-CBA
32	Y	610	CLA	C3A-C2A-CAA-CBA
32	Y	610	CLA	CHA-CBD-CGD-O1D
32	Y	610	CLA	CHA-CBD-CGD-O2D
32	Y	612	CLA	CBD-CGD-O2D-CED
32	Y	613	CLA	CHA-CBD-CGD-O1D
32	Y	613	CLA	CHA-CBD-CGD-O2D
32	Y	614	CLA	C3A-C2A-CAA-CBA
32	a	406	CLA	CHA-CBD-CGD-O1D
32	a	406	CLA	CHA-CBD-CGD-O2D
32	a	407	CLA	CHA-CBD-CGD-O1D
32	a	407	CLA	CHA-CBD-CGD-O2D
32	a	410	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	a	410	CLA	CHA-CBD-CGD-O2D
32	a	410	CLA	CAD-CBD-CGD-O1D
32	b	601	CLA	C3A-C2A-CAA-CBA
32	b	601	CLA	CHA-CBD-CGD-O1D
32	b	601	CLA	CHA-CBD-CGD-O2D
32	b	601	CLA	CAD-CBD-CGD-O1D
32	b	601	CLA	CBD-CGD-O2D-CED
32	b	603	CLA	C1A-C2A-CAA-CBA
32	b	603	CLA	C3A-C2A-CAA-CBA
32	b	603	CLA	CHA-CBD-CGD-O1D
32	b	603	CLA	CHA-CBD-CGD-O2D
32	b	603	CLA	CBD-CGD-O2D-CED
32	b	608	CLA	CBD-CGD-O2D-CED
32	b	609	CLA	C1A-C2A-CAA-CBA
32	b	609	CLA	C3A-C2A-CAA-CBA
32	b	613	CLA	CBD-CGD-O2D-CED
32	b	614	CLA	CBD-CGD-O2D-CED
32	c	501	CLA	CHA-CBD-CGD-O1D
32	c	501	CLA	CHA-CBD-CGD-O2D
32	c	501	CLA	CAD-CBD-CGD-O1D
32	c	503	CLA	CBD-CGD-O2D-CED
32	c	504	CLA	CBD-CGD-O2D-CED
32	c	506	CLA	C1A-C2A-CAA-CBA
32	c	506	CLA	CHA-CBD-CGD-O1D
32	c	506	CLA	CHA-CBD-CGD-O2D
32	c	506	CLA	CAD-CBD-CGD-O1D
32	c	506	CLA	CBD-CGD-O2D-CED
32	c	507	CLA	CAD-CBD-CGD-O1D
32	c	507	CLA	CAD-CBD-CGD-O2D
32	c	511	CLA	CHA-CBD-CGD-O1D
32	c	511	CLA	CHA-CBD-CGD-O2D
32	c	511	CLA	CBD-CGD-O2D-CED
32	c	512	CLA	CBD-CGD-O2D-CED
32	c	513	CLA	C1A-C2A-CAA-CBA
32	c	513	CLA	CHA-CBD-CGD-O1D
32	c	513	CLA	CHA-CBD-CGD-O2D
32	c	513	CLA	CAD-CBD-CGD-O1D
32	d	402	CLA	CHA-CBD-CGD-O1D
32	d	402	CLA	CHA-CBD-CGD-O2D
32	g	603	CLA	CHA-CBD-CGD-O1D
32	g	603	CLA	CHA-CBD-CGD-O2D
32	g	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	g	604	CLA	C1A-C2A-CAA-CBA
32	g	604	CLA	CHA-CBD-CGD-O1D
32	g	604	CLA	CHA-CBD-CGD-O2D
32	g	604	CLA	CAD-CBD-CGD-O1D
32	g	604	CLA	CBD-CGD-O2D-CED
32	g	610	CLA	CHA-CBD-CGD-O1D
32	g	610	CLA	CHA-CBD-CGD-O2D
32	g	611	CLA	C1A-C2A-CAA-CBA
32	g	612	CLA	C1A-C2A-CAA-CBA
32	g	612	CLA	C3A-C2A-CAA-CBA
32	g	613	CLA	CBD-CGD-O2D-CED
32	g	614	CLA	CHA-CBD-CGD-O1D
32	n	602	CLA	C1A-C2A-CAA-CBA
32	n	602	CLA	C3A-C2A-CAA-CBA
32	n	602	CLA	CHA-CBD-CGD-O2D
32	n	603	CLA	CBD-CGD-O2D-CED
32	n	610	CLA	C1A-C2A-CAA-CBA
32	n	610	CLA	C3A-C2A-CAA-CBA
32	n	610	CLA	CBD-CGD-O2D-CED
32	n	612	CLA	CBD-CGD-O2D-CED
32	n	613	CLA	C1A-C2A-CAA-CBA
32	n	614	CLA	CBD-CGD-O2D-CED
32	r	602	CLA	C2A-CAA-CBA-CGA
32	r	604	CLA	C1A-C2A-CAA-CBA
32	r	604	CLA	CHA-CBD-CGD-O1D
32	r	604	CLA	CBD-CGD-O2D-CED
32	r	608	CLA	CBD-CGD-O2D-CED
32	r	609	CLA	C1A-C2A-CAA-CBA
32	r	609	CLA	C3A-C2A-CAA-CBA
32	r	609	CLA	CHA-CBD-CGD-O1D
32	r	609	CLA	CHA-CBD-CGD-O2D
32	r	610	CLA	C1A-C2A-CAA-CBA
32	r	611	CLA	CBD-CGD-O2D-CED
32	s	602	CLA	CHA-CBD-CGD-O1D
32	s	602	CLA	CHA-CBD-CGD-O2D
32	s	604	CLA	CHA-CBD-CGD-O1D
32	s	604	CLA	CHA-CBD-CGD-O2D
32	s	608	CLA	C1A-C2A-CAA-CBA
32	s	608	CLA	C3A-C2A-CAA-CBA
32	s	609	CLA	C1A-C2A-CAA-CBA
32	s	609	CLA	C3A-C2A-CAA-CBA
32	s	611	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	s	611	CLA	CAD-CBD-CGD-O2D
32	s	612	CLA	CHA-CBD-CGD-O1D
32	s	612	CLA	CHA-CBD-CGD-O2D
32	s	613	CLA	CBD-CGD-O2D-CED
32	y	304	CLA	C1A-C2A-CAA-CBA
32	y	304	CLA	C3A-C2A-CAA-CBA
32	y	312	CLA	C1A-C2A-CAA-CBA
32	y	312	CLA	C3A-C2A-CAA-CBA
32	y	313	CLA	C1A-C2A-CAA-CBA
32	y	314	CLA	CBD-CGD-O2D-CED
32	y	314	CLA	O1D-CGD-O2D-CED
32	y	315	CLA	CHA-CBD-CGD-O1D
32	y	315	CLA	CHA-CBD-CGD-O2D
32	y	316	CLA	C3A-C2A-CAA-CBA
32	4	303	CLA	C1A-C2A-CAA-CBA
32	4	304	CLA	C1A-C2A-CAA-CBA
32	4	304	CLA	C3A-C2A-CAA-CBA
32	4	304	CLA	CBD-CGD-O2D-CED
32	4	305	CLA	CBD-CGD-O2D-CED
32	4	310	CLA	C1A-C2A-CAA-CBA
32	4	310	CLA	C3A-C2A-CAA-CBA
32	4	310	CLA	CBD-CGD-O2D-CED
32	AA	405	CLA	CBD-CGD-O2D-CED
32	AA	408	CLA	CHA-CBD-CGD-O1D
32	AA	408	CLA	CHA-CBD-CGD-O2D
32	AA	408	CLA	CAD-CBD-CGD-O1D
32	BB	602	CLA	C3A-C2A-CAA-CBA
32	BB	602	CLA	CHA-CBD-CGD-O1D
32	BB	602	CLA	CHA-CBD-CGD-O2D
32	BB	602	CLA	CAD-CBD-CGD-O1D
32	BB	602	CLA	CAD-CBD-CGD-O2D
32	BB	605	CLA	CHA-CBD-CGD-O1D
32	BB	605	CLA	CHA-CBD-CGD-O2D
32	BB	605	CLA	CAD-CBD-CGD-O1D
32	BB	605	CLA	CAD-CBD-CGD-O2D
32	BB	606	CLA	CHA-CBD-CGD-O1D
32	BB	606	CLA	CHA-CBD-CGD-O2D
32	BB	608	CLA	CHA-CBD-CGD-O1D
32	BB	608	CLA	CHA-CBD-CGD-O2D
32	BB	608	CLA	CAD-CBD-CGD-O1D
32	BB	609	CLA	CHA-CBD-CGD-O1D
32	BB	609	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	BB	610	CLA	CHA-CBD-CGD-O1D
32	BB	610	CLA	CHA-CBD-CGD-O2D
32	BB	610	CLA	CAD-CBD-CGD-O1D
32	BB	610	CLA	CAD-CBD-CGD-O2D
32	BB	610	CLA	CBD-CGD-O2D-CED
32	BB	612	CLA	CBD-CGD-O2D-CED
32	BB	613	CLA	CHA-CBD-CGD-O1D
32	BB	613	CLA	CHA-CBD-CGD-O2D
32	BB	615	CLA	CHA-CBD-CGD-O2D
32	CC	502	CLA	C1A-C2A-CAA-CBA
32	CC	503	CLA	C1A-C2A-CAA-CBA
32	CC	506	CLA	CHA-CBD-CGD-O1D
32	CC	506	CLA	CHA-CBD-CGD-O2D
32	CC	506	CLA	CAD-CBD-CGD-O1D
32	CC	507	CLA	C1A-C2A-CAA-CBA
32	CC	507	CLA	C3A-C2A-CAA-CBA
32	CC	507	CLA	CHA-CBD-CGD-O1D
32	CC	507	CLA	CHA-CBD-CGD-O2D
32	CC	507	CLA	CAD-CBD-CGD-O1D
32	CC	507	CLA	CAD-CBD-CGD-O2D
32	CC	508	CLA	CHA-CBD-CGD-O1D
32	CC	508	CLA	CHA-CBD-CGD-O2D
32	CC	510	CLA	C1A-C2A-CAA-CBA
32	CC	510	CLA	C3A-C2A-CAA-CBA
32	CC	512	CLA	CHA-CBD-CGD-O1D
32	CC	512	CLA	CHA-CBD-CGD-O2D
32	CC	512	CLA	CAD-CBD-CGD-O1D
32	CC	512	CLA	CAD-CBD-CGD-O2D
32	CC	514	CLA	CHA-CBD-CGD-O1D
32	CC	514	CLA	CHA-CBD-CGD-O2D
32	CC	514	CLA	CBD-CGD-O2D-CED
32	B	604	CLA	C1A-C2A-CAA-CBA
32	B	604	CLA	CHA-CBD-CGD-O1D
32	B	604	CLA	CHA-CBD-CGD-O2D
32	B	605	CLA	CHA-CBD-CGD-O1D
32	B	605	CLA	CHA-CBD-CGD-O2D
32	B	606	CLA	CHA-CBD-CGD-O1D
32	B	606	CLA	CHA-CBD-CGD-O2D
32	B	606	CLA	CAD-CBD-CGD-O1D
32	B	606	CLA	CAD-CBD-CGD-O2D
32	B	606	CLA	CBD-CGD-O2D-CED
32	B	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	B	609	CLA	CHA-CBD-CGD-O1D
32	B	609	CLA	CHA-CBD-CGD-O2D
32	B	619	CLA	C3A-C2A-CAA-CBA
32	B	619	CLA	CHA-CBD-CGD-O1D
32	B	619	CLA	CHA-CBD-CGD-O2D
32	B	619	CLA	CAD-CBD-CGD-O1D
32	B	622	CLA	CHA-CBD-CGD-O1D
32	B	622	CLA	CHA-CBD-CGD-O2D
32	B	622	CLA	CAD-CBD-CGD-O1D
32	B	622	CLA	CAD-CBD-CGD-O2D
32	B	622	CLA	CBD-CGD-O2D-CED
32	B	623	CLA	CHA-CBD-CGD-O1D
32	B	623	CLA	CHA-CBD-CGD-O2D
32	GG	602	CLA	CBD-CGD-O2D-CED
32	GG	604	CLA	CBD-CGD-O2D-CED
32	GG	611	CLA	CBD-CGD-O2D-CED
32	GG	613	CLA	CBD-CGD-O2D-CED
32	NN	602	CLA	C1A-C2A-CAA-CBA
32	NN	602	CLA	C3A-C2A-CAA-CBA
32	NN	603	CLA	CHA-CBD-CGD-O1D
32	NN	603	CLA	CHA-CBD-CGD-O2D
32	NN	603	CLA	CAD-CBD-CGD-O1D
32	NN	603	CLA	CBD-CGD-O2D-CED
32	NN	604	CLA	CHA-CBD-CGD-O1D
32	NN	604	CLA	CHA-CBD-CGD-O2D
32	NN	610	CLA	C1A-C2A-CAA-CBA
32	NN	610	CLA	CBD-CGD-O2D-CED
32	NN	611	CLA	C1A-C2A-CAA-CBA
32	NN	611	CLA	C3A-C2A-CAA-CBA
32	NN	611	CLA	CHA-CBD-CGD-O1D
32	NN	611	CLA	CHA-CBD-CGD-O2D
32	NN	611	CLA	CAD-CBD-CGD-O1D
32	NN	611	CLA	CBD-CGD-O2D-CED
32	NN	613	CLA	C1A-C2A-CAA-CBA
32	NN	613	CLA	CBD-CGD-O2D-CED
32	NN	614	CLA	CBD-CGD-O2D-CED
32	RR	302	CLA	C1A-C2A-CAA-CBA
32	RR	302	CLA	C3A-C2A-CAA-CBA
32	RR	302	CLA	CHA-CBD-CGD-O1D
32	RR	302	CLA	CHA-CBD-CGD-O2D
32	RR	308	CLA	CBD-CGD-O2D-CED
32	RR	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	RR	309	CLA	C3A-C2A-CAA-CBA
32	RR	309	CLA	CBD-CGD-O2D-CED
32	RR	310	CLA	C1A-C2A-CAA-CBA
32	RR	310	CLA	C3A-C2A-CAA-CBA
32	RR	310	CLA	CHA-CBD-CGD-O1D
32	RR	310	CLA	CHA-CBD-CGD-O2D
32	RR	312	CLA	C1A-C2A-CAA-CBA
32	RR	313	CLA	CHA-CBD-CGD-O1D
32	RR	313	CLA	CHA-CBD-CGD-O2D
32	RR	313	CLA	CBD-CGD-O2D-CED
32	RR	314	CLA	CHA-CBD-CGD-O1D
32	SS	304	CLA	CBD-CGD-O2D-CED
32	SS	305	CLA	C1A-C2A-CAA-CBA
32	SS	310	CLA	CBD-CGD-O2D-CED
32	SS	312	CLA	CBD-CGD-O2D-CED
32	SS	313	CLA	CBD-CGD-O2D-CED
32	SS	314	CLA	CHA-CBD-CGD-O1D
32	SS	314	CLA	CHA-CBD-CGD-O2D
32	XX	201	CLA	CBD-CGD-O2D-CED
32	YY	602	CLA	C1A-C2A-CAA-CBA
32	YY	602	CLA	C3A-C2A-CAA-CBA
32	YY	603	CLA	CBD-CGD-O2D-CED
32	YY	610	CLA	C1A-C2A-CAA-CBA
32	YY	610	CLA	C3A-C2A-CAA-CBA
32	YY	610	CLA	CHA-CBD-CGD-O1D
32	YY	610	CLA	CHA-CBD-CGD-O2D
32	YY	610	CLA	CBD-CGD-O2D-CED
32	YY	611	CLA	CBD-CGD-O2D-CED
32	YY	612	CLA	CHA-CBD-CGD-O1D
32	YY	612	CLA	CHA-CBD-CGD-O2D
32	YY	612	CLA	CBD-CGD-O2D-CED
32	YY	613	CLA	CHA-CBD-CGD-O1D
32	YY	613	CLA	CHA-CBD-CGD-O2D
32	YY	614	CLA	C3A-C2A-CAA-CBA
32	Aa	405	CLA	C1A-C2A-CAA-CBA
32	Aa	405	CLA	CHA-CBD-CGD-O1D
32	Aa	405	CLA	CBD-CGD-O2D-CED
32	Aa	406	CLA	CHA-CBD-CGD-O1D
32	Aa	406	CLA	CHA-CBD-CGD-O2D
32	Aa	407	CLA	CHA-CBD-CGD-O1D
32	Aa	407	CLA	CHA-CBD-CGD-O2D
32	Aa	410	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	Aa	410	CLA	CHA-CBD-CGD-O2D
32	Aa	410	CLA	CAD-CBD-CGD-O1D
32	Bb	601	CLA	C3A-C2A-CAA-CBA
32	Bb	601	CLA	CHA-CBD-CGD-O1D
32	Bb	601	CLA	CHA-CBD-CGD-O2D
32	Bb	601	CLA	CBD-CGD-O2D-CED
32	Bb	603	CLA	C1A-C2A-CAA-CBA
32	Bb	603	CLA	C3A-C2A-CAA-CBA
32	Bb	603	CLA	CHA-CBD-CGD-O1D
32	Bb	603	CLA	CHA-CBD-CGD-O2D
32	Bb	603	CLA	CBD-CGD-O2D-CED
32	Bb	609	CLA	C1A-C2A-CAA-CBA
32	Bb	609	CLA	C3A-C2A-CAA-CBA
32	Bb	613	CLA	CBD-CGD-O2D-CED
32	Cc	503	CLA	C2A-CAA-CBA-CGA
32	Cc	503	CLA	CHA-CBD-CGD-O1D
32	Cc	503	CLA	CHA-CBD-CGD-O2D
32	Cc	504	CLA	CAD-CBD-CGD-O1D
32	Cc	504	CLA	CAD-CBD-CGD-O2D
32	Cc	506	CLA	CBD-CGD-O2D-CED
32	Cc	508	CLA	C1A-C2A-CAA-CBA
32	Cc	508	CLA	C3A-C2A-CAA-CBA
32	Cc	508	CLA	CHA-CBD-CGD-O1D
32	Cc	508	CLA	CHA-CBD-CGD-O2D
32	Cc	508	CLA	CAD-CBD-CGD-O1D
32	Cc	508	CLA	CAD-CBD-CGD-O2D
32	Cc	509	CLA	CAD-CBD-CGD-O1D
32	Cc	509	CLA	CAD-CBD-CGD-O2D
32	Cc	511	CLA	CHA-CBD-CGD-O1D
32	Cc	511	CLA	CAD-CBD-CGD-O1D
32	Cc	511	CLA	CAD-CBD-CGD-O2D
32	Cc	511	CLA	CBD-CGD-O2D-CED
32	Cc	513	CLA	CHA-CBD-CGD-O1D
32	Cc	513	CLA	CHA-CBD-CGD-O2D
32	Cc	513	CLA	CBD-CGD-O2D-CED
32	Cc	514	CLA	CBD-CGD-O2D-CED
32	Cc	515	CLA	C1A-C2A-CAA-CBA
32	Cc	515	CLA	CAD-CBD-CGD-O1D
32	Cc	515	CLA	CAD-CBD-CGD-O2D
32	Cc	515	CLA	CBD-CGD-O2D-CED
32	Dd	402	CLA	CHA-CBD-CGD-O1D
32	Dd	402	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	Gg	303	CLA	CHA-CBD-CGD-O1D
32	Gg	303	CLA	CHA-CBD-CGD-O2D
32	Gg	303	CLA	CAD-CBD-CGD-O1D
32	Gg	304	CLA	CHA-CBD-CGD-O1D
32	Gg	304	CLA	CHA-CBD-CGD-O2D
32	Gg	305	CLA	C1A-C2A-CAA-CBA
32	Gg	305	CLA	CHA-CBD-CGD-O1D
32	Gg	305	CLA	CHA-CBD-CGD-O2D
32	Gg	305	CLA	CBD-CGD-O2D-CED
32	Gg	311	CLA	CHA-CBD-CGD-O1D
32	Gg	311	CLA	CHA-CBD-CGD-O2D
32	Gg	311	CLA	CBD-CGD-O2D-CED
32	Gg	312	CLA	C1A-C2A-CAA-CBA
32	Gg	312	CLA	C2A-CAA-CBA-CGA
32	Gg	313	CLA	CBD-CGD-O2D-CED
32	Gg	314	CLA	CBD-CGD-O2D-CED
32	Gg	315	CLA	CHA-CBD-CGD-O1D
32	Nn	301	CLA	C1A-C2A-CAA-CBA
32	Nn	301	CLA	C3A-C2A-CAA-CBA
32	Nn	301	CLA	CBD-CGD-O2D-CED
32	Nn	303	CLA	CBD-CGD-O2D-CED
32	Nn	304	CLA	C1A-C2A-CAA-CBA
32	Nn	305	CLA	CBD-CGD-O2D-CED
32	Nn	312	CLA	C1A-C2A-CAA-CBA
32	Nn	312	CLA	C3A-C2A-CAA-CBA
32	Nn	312	CLA	CBD-CGD-O2D-CED
32	Nn	313	CLA	CBD-CGD-O2D-CED
33	a	409	PHO	C2A-CAA-CBA-CGA
33	Aa	409	PHO	C2A-CAA-CBA-CGA
34	C	516	BCR	C23-C24-C25-C26
34	C	517	BCR	C23-C24-C25-C26
34	K	102	BCR	C23-C24-C25-C26
34	K	102	BCR	C23-C24-C25-C30
34	T	101	BCR	C1-C6-C7-C8
34	T	101	BCR	C5-C6-C7-C8
34	a	411	BCR	C5-C6-C7-C8
34	b	617	BCR	C5-C6-C7-C8
34	b	617	BCR	C23-C24-C25-C26
34	b	617	BCR	C23-C24-C25-C30
34	c	515	BCR	C5-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C26
34	d	403	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	d	403	BCR	C23-C24-C25-C26
34	BB	616	BCR	C23-C24-C25-C26
34	BB	616	BCR	C23-C24-C25-C30
34	BB	620	BCR	C23-C24-C25-C26
34	CC	515	BCR	C23-C24-C25-C26
34	CC	516	BCR	C23-C24-C25-C26
34	B	612	BCR	C23-C24-C25-C26
34	B	612	BCR	C23-C24-C25-C30
34	B	616	BCR	C23-C24-C25-C26
34	B	616	BCR	C23-C24-C25-C30
34	KK	103	BCR	C23-C24-C25-C26
34	KK	103	BCR	C23-C24-C25-C30
34	TT	101	BCR	C1-C6-C7-C8
34	TT	101	BCR	C5-C6-C7-C8
34	XX	202	BCR	C1-C6-C7-C8
34	XX	202	BCR	C5-C6-C7-C8
34	Aa	411	BCR	C5-C6-C7-C8
34	Bb	617	BCR	C23-C24-C25-C26
34	Bb	617	BCR	C23-C24-C25-C30
34	Cc	517	BCR	C5-C6-C7-C8
34	Cc	517	BCR	C23-C24-C25-C26
34	Dd	403	BCR	C5-C6-C7-C8
34	Dd	403	BCR	C23-C24-C25-C26
34	Hh	101	BCR	C11-C12-C13-C14
34	Kk	101	BCR	C5-C6-C7-C8
34	Kk	101	BCR	C23-C24-C25-C26
34	Kk	101	BCR	C23-C24-C25-C30
35	A	410	PL9	C12-C11-C9-C8
35	A	410	PL9	C11-C12-C13-C14
35	A	410	PL9	C12-C13-C14-C15
35	A	410	PL9	C15-C14-C16-C17
35	A	410	PL9	C17-C18-C19-C21
35	A	410	PL9	C23-C24-C26-C27
35	A	410	PL9	C27-C28-C29-C31
35	A	410	PL9	C32-C33-C34-C35
35	A	410	PL9	C32-C33-C34-C36
35	A	410	PL9	C35-C34-C36-C37
35	A	410	PL9	C37-C38-C39-C40
35	A	410	PL9	C42-C43-C44-C45
35	A	410	PL9	C47-C48-C49-C50
35	A	410	PL9	C47-C48-C49-C51
35	D	407	PL9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
35	D	407	PL9	C17-C18-C19-C20
35	D	407	PL9	C17-C18-C19-C21
35	D	407	PL9	C20-C19-C21-C22
35	D	407	PL9	C25-C24-C26-C27
35	D	407	PL9	C27-C28-C29-C31
35	D	407	PL9	C32-C33-C34-C36
35	D	407	PL9	C40-C39-C41-C42
35	D	407	PL9	C42-C43-C44-C46
35	d	404	PL9	C7-C8-C9-C10
35	d	404	PL9	C12-C13-C14-C15
35	d	404	PL9	C18-C19-C21-C22
35	d	404	PL9	C22-C23-C24-C25
35	d	404	PL9	C22-C23-C24-C26
35	d	404	PL9	C27-C28-C29-C30
35	d	404	PL9	C27-C28-C29-C31
35	d	404	PL9	C37-C38-C39-C41
35	d	404	PL9	C38-C39-C41-C42
35	d	404	PL9	C42-C43-C44-C46
35	d	404	PL9	C45-C44-C46-C47
35	d	404	PL9	C47-C48-C49-C51
35	AA	410	PL9	C17-C18-C19-C20
35	AA	410	PL9	C20-C19-C21-C22
35	AA	410	PL9	C22-C23-C24-C25
35	AA	410	PL9	C22-C23-C24-C26
35	AA	410	PL9	C23-C24-C26-C27
35	AA	410	PL9	C27-C28-C29-C31
35	AA	410	PL9	C30-C29-C31-C32
35	AA	410	PL9	C37-C38-C39-C40
35	AA	410	PL9	C38-C39-C41-C42
35	AA	410	PL9	C47-C48-C49-C50
35	AA	410	PL9	C47-C48-C49-C51
35	DD	406	PL9	C7-C8-C9-C10
35	DD	406	PL9	C12-C11-C9-C10
35	DD	406	PL9	C17-C18-C19-C20
35	DD	406	PL9	C20-C19-C21-C22
35	DD	406	PL9	C22-C23-C24-C25
35	DD	406	PL9	C27-C28-C29-C31
35	DD	406	PL9	C32-C33-C34-C35
35	DD	406	PL9	C33-C34-C36-C37
35	DD	406	PL9	C37-C38-C39-C41
35	DD	406	PL9	C40-C39-C41-C42
35	DD	406	PL9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
35	Dd	404	PL9	C7-C8-C9-C11
35	Dd	404	PL9	C12-C13-C14-C16
35	Dd	404	PL9	C15-C14-C16-C17
35	Dd	404	PL9	C18-C19-C21-C22
35	Dd	404	PL9	C19-C21-C22-C23
35	Dd	404	PL9	C22-C23-C24-C25
35	Dd	404	PL9	C22-C23-C24-C26
35	Dd	404	PL9	C27-C28-C29-C30
35	Dd	404	PL9	C27-C28-C29-C31
35	Dd	404	PL9	C37-C38-C39-C41
35	Dd	404	PL9	C42-C43-C44-C46
35	Dd	404	PL9	C47-C48-C49-C51
36	A	411	LHG	C3-O3-P-O5
36	A	411	LHG	C4-O6-P-O3
36	A	413	LHG	C3-O3-P-O4
36	A	413	LHG	C4-O6-P-O3
36	A	413	LHG	C4-O6-P-O5
36	A	414	LHG	C3-O3-P-O6
36	Rr	617	LHG	C4-O6-P-O4
36	Ss	616	LHG	C4-O6-P-O3
36	Yy	618	LHG	O2-C2-C3-O3
36	Yy	618	LHG	C3-O3-P-O6
36	Yy	618	LHG	C4-O6-P-O3
36	44	614	LHG	C3-O3-P-O4
36	44	614	LHG	C3-O3-P-O5
36	44	614	LHG	C3-O3-P-O6
36	44	616	LHG	C3-O3-P-O6
36	44	616	LHG	C4-O6-P-O5
36	44	616	LHG	O9-C7-O7-C5
36	11	614	LHG	C3-O3-P-O4
36	11	614	LHG	C3-O3-P-O5
36	11	614	LHG	C4-O6-P-O4
36	22	615	LHG	C3-O3-P-O5
36	22	615	LHG	C4-O6-P-O3
36	22	615	LHG	C4-O6-P-O4
36	22	615	LHG	C4-O6-P-O5
36	33	614	LHG	C3-O3-P-O4
36	33	614	LHG	C3-O3-P-O5
36	33	614	LHG	C3-O3-P-O6
36	33	614	LHG	C4-O6-P-O4
36	1	614	LHG	C3-O3-P-O5
36	3	614	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	3	614	LHG	C3-O3-P-O5
36	3	614	LHG	C3-O3-P-O6
36	D	408	LHG	C3-O3-P-O5
36	D	408	LHG	C3-O3-P-O6
36	D	408	LHG	C4-O6-P-O3
36	D	408	LHG	C4-O6-P-O5
36	G	618	LHG	C8-C7-O7-C5
36	J	101	LHG	C3-O3-P-O4
36	J	101	LHG	C4-O6-P-O3
36	K	101	LHG	C4-O6-P-O4
36	N	619	LHG	C8-C7-O7-C5
36	Y	618	LHG	C3-O3-P-O6
36	Y	618	LHG	C4-O6-P-O3
36	d	405	LHG	C4-O6-P-O4
36	d	406	LHG	C3-O3-P-O4
36	d	406	LHG	C4-O6-P-O3
36	g	618	LHG	C1-C2-C3-O3
36	g	618	LHG	C3-O3-P-O5
36	l	101	LHG	C3-O3-P-O4
36	l	101	LHG	C3-O3-P-O5
36	l	101	LHG	C3-O3-P-O6
36	l	101	LHG	C4-O6-P-O5
36	n	618	LHG	C8-C7-O7-C5
36	r	616	LHG	C3-O3-P-O6
36	r	616	LHG	C4-O6-P-O4
36	s	616	LHG	C4-O6-P-O3
36	y	320	LHG	C3-O3-P-O4
36	y	320	LHG	C4-O6-P-O3
36	4	301	LHG	O1-C1-C2-C3
36	4	301	LHG	C4-O6-P-O5
36	4	301	LHG	O9-C7-O7-C5
36	4	315	LHG	C3-O3-P-O4
36	4	315	LHG	C3-O3-P-O5
36	4	315	LHG	C3-O3-P-O6
36	AA	411	LHG	C3-O3-P-O5
36	AA	411	LHG	C3-O3-P-O6
36	AA	411	LHG	C4-O6-P-O3
36	BB	622	LHG	C3-O3-P-O6
36	BB	622	LHG	C4-O6-P-O5
36	CC	521	LHG	C3-O3-P-O5
36	CC	521	LHG	C3-O3-P-O6
36	CC	523	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	CC	523	LHG	C4-O6-P-O3
36	CC	523	LHG	C4-O6-P-O5
36	DD	407	LHG	C3-O3-P-O6
36	DD	407	LHG	C4-O6-P-O3
36	DD	407	LHG	C4-O6-P-O5
36	GG	618	LHG	C8-C7-O7-C5
36	II	101	LHG	C4-O6-P-O3
36	II	101	LHG	C4-O6-P-O5
36	JJ	101	LHG	C3-O3-P-O4
36	NN	619	LHG	C3-O3-P-O6
36	NN	619	LHG	C8-C7-O7-C5
36	SS	301	LHG	C3-O3-P-O4
36	SS	301	LHG	C4-O6-P-O3
36	YY	618	LHG	C3-O3-P-O6
36	YY	618	LHG	C4-O6-P-O4
36	Dd	405	LHG	C4-O6-P-O4
36	Dd	406	LHG	C3-O3-P-O4
36	Dd	406	LHG	C4-O6-P-O3
36	Gg	319	LHG	C3-O3-P-O4
36	Ll	102	LHG	C3-O3-P-O4
36	Ll	102	LHG	C3-O3-P-O5
36	Ll	102	LHG	C3-O3-P-O6
36	Nn	310	LHG	C8-C7-O7-C5
37	A	412	SQD	O5-C5-C6-S
37	C	501	SQD	C2-C1-O6-C44
37	C	501	SQD	O5-C1-O6-C44
37	l	102	SQD	O5-C1-O6-C44
37	BB	621	SQD	C5-C6-S-O8
37	B	617	SQD	C5-C6-S-O8
37	Ll	101	SQD	O5-C1-O6-C44
38	b	621	LMG	O9-C10-O7-C8
38	Aa	412	LMG	O1-C7-C8-O7
38	Bb	621	LMG	O9-C10-O7-C8
38	Bb	621	LMG	C11-C10-O7-C8
39	Rr	605	CHL	C1A-C2A-CAA-CBA
39	Rr	605	CHL	CHA-CBD-CGD-O1D
39	Rr	605	CHL	CHA-CBD-CGD-O2D
39	Rr	606	CHL	CBD-CGD-O2D-CED
39	Rr	607	CHL	CHA-CBD-CGD-O1D
39	Ss	601	CHL	CBD-CGD-O2D-CED
39	Ss	605	CHL	C1A-C2A-CAA-CBA
39	Ss	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	Ss	606	CHL	CHA-CBD-CGD-O1D
39	Ss	606	CHL	CHA-CBD-CGD-O2D
39	Ss	606	CHL	CAD-CBD-CGD-O1D
39	Ss	606	CHL	CAD-CBD-CGD-O2D
39	Yy	601	CHL	CBD-CGD-O2D-CED
39	Yy	605	CHL	CHA-CBD-CGD-O1D
39	Yy	605	CHL	CHA-CBD-CGD-O2D
39	Yy	605	CHL	CAD-CBD-CGD-O1D
39	Yy	607	CHL	CBD-CGD-O2D-CED
39	Yy	608	CHL	CHA-CBD-CGD-O1D
39	Yy	608	CHL	CHA-CBD-CGD-O2D
39	44	605	CHL	CBD-CGD-O2D-CED
39	44	606	CHL	CBD-CGD-O2D-CED
39	44	607	CHL	CBD-CGD-O2D-CED
39	44	608	CHL	C1A-C2A-CAA-CBA
39	11	601	CHL	CBD-CGD-O2D-CED
39	11	606	CHL	CHA-CBD-CGD-O1D
39	11	606	CHL	CHA-CBD-CGD-O2D
39	11	607	CHL	CBD-CGD-O2D-CED
39	22	606	CHL	CBD-CGD-O2D-CED
39	22	608	CHL	CBD-CGD-O2D-CED
39	33	601	CHL	CHA-CBD-CGD-O1D
39	33	601	CHL	CBD-CGD-O2D-CED
39	33	605	CHL	CBD-CGD-O2D-CED
39	33	606	CHL	CHA-CBD-CGD-O1D
39	33	606	CHL	CBD-CGD-O2D-CED
39	33	607	CHL	CBD-CGD-O2D-CED
39	33	608	CHL	CBD-CGD-O2D-CED
39	1	601	CHL	CBD-CGD-O2D-CED
39	1	606	CHL	CHA-CBD-CGD-O1D
39	1	607	CHL	CBD-CGD-O2D-CED
39	2	608	CHL	CBD-CGD-O2D-CED
39	3	601	CHL	CBD-CGD-O2D-CED
39	3	605	CHL	CHA-CBD-CGD-O1D
39	3	606	CHL	CBD-CGD-O2D-CED
39	G	606	CHL	C1A-C2A-CAA-CBA
39	G	606	CHL	C3A-C2A-CAA-CBA
39	G	606	CHL	CBD-CGD-O2D-CED
39	G	607	CHL	CHA-CBD-CGD-O1D
39	G	607	CHL	CHA-CBD-CGD-O2D
39	G	607	CHL	CBD-CGD-O2D-CED
39	G	608	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	G	608	CHL	CAD-CBD-CGD-O2D
39	N	605	CHL	CHA-CBD-CGD-O1D
39	N	605	CHL	CHA-CBD-CGD-O2D
39	N	607	CHL	CHA-CBD-CGD-O1D
39	N	607	CHL	CHA-CBD-CGD-O2D
39	N	608	CHL	CBD-CGD-O2D-CED
39	N	609	CHL	CHA-CBD-CGD-O1D
39	N	609	CHL	CHA-CBD-CGD-O2D
39	R	605	CHL	C1A-C2A-CAA-CBA
39	R	605	CHL	C3A-C2A-CAA-CBA
39	R	606	CHL	C3A-C2A-CAA-CBA
39	R	606	CHL	CBD-CGD-O2D-CED
39	R	607	CHL	CHA-CBD-CGD-O1D
39	R	607	CHL	CHA-CBD-CGD-O2D
39	S	601	CHL	CBD-CGD-O2D-CED
39	S	605	CHL	CBD-CGD-O2D-CED
39	Y	601	CHL	CBD-CGD-O2D-CED
39	g	605	CHL	C1A-C2A-CAA-CBA
39	g	605	CHL	CBD-CGD-O2D-CED
39	g	606	CHL	C1A-C2A-CAA-CBA
39	g	606	CHL	C3A-C2A-CAA-CBA
39	g	606	CHL	CHA-CBD-CGD-O1D
39	g	606	CHL	CHA-CBD-CGD-O2D
39	g	606	CHL	CBD-CGD-O2D-CED
39	g	607	CHL	CBD-CGD-O2D-CED
39	g	609	CHL	C1A-C2A-CAA-CBA
39	g	609	CHL	CHA-CBD-CGD-O1D
39	g	609	CHL	CHA-CBD-CGD-O2D
39	n	601	CHL	CBD-CGD-O2D-CED
39	n	607	CHL	CHA-CBD-CGD-O1D
39	n	607	CHL	CHA-CBD-CGD-O2D
39	n	607	CHL	CBD-CGD-O2D-CED
39	n	608	CHL	CBD-CGD-O2D-CED
39	r	605	CHL	C1A-C2A-CAA-CBA
39	r	606	CHL	CBD-CGD-O2D-CED
39	r	607	CHL	CHA-CBD-CGD-O1D
39	r	607	CHL	CHA-CBD-CGD-O2D
39	s	601	CHL	CHA-CBD-CGD-O1D
39	s	601	CHL	CHA-CBD-CGD-O2D
39	s	601	CHL	CBD-CGD-O2D-CED
39	s	606	CHL	C1A-C2A-CAA-CBA
39	s	606	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	s	606	CHL	CHA-CBD-CGD-O2D
39	s	606	CHL	CAD-CBD-CGD-O1D
39	y	303	CHL	CBD-CGD-O2D-CED
39	y	307	CHL	CAD-CBD-CGD-O1D
39	y	307	CHL	CAD-CBD-CGD-O2D
39	y	309	CHL	CHA-CBD-CGD-O1D
39	y	309	CHL	CHA-CBD-CGD-O2D
39	y	310	CHL	CHA-CBD-CGD-O1D
39	y	310	CHL	CHA-CBD-CGD-O2D
39	4	306	CHL	CBD-CGD-O2D-CED
39	4	307	CHL	CBD-CGD-O2D-CED
39	4	308	CHL	CBD-CGD-O2D-CED
39	GG	606	CHL	C1A-C2A-CAA-CBA
39	GG	606	CHL	C3A-C2A-CAA-CBA
39	GG	606	CHL	CBD-CGD-O2D-CED
39	GG	607	CHL	CHA-CBD-CGD-O1D
39	GG	607	CHL	CHA-CBD-CGD-O2D
39	GG	607	CHL	CBD-CGD-O2D-CED
39	GG	608	CHL	CHA-CBD-CGD-O1D
39	GG	608	CHL	CHA-CBD-CGD-O2D
39	GG	608	CHL	CAD-CBD-CGD-O1D
39	GG	608	CHL	CBD-CGD-O2D-CED
39	GG	609	CHL	CBD-CGD-O2D-CED
39	NN	607	CHL	CHA-CBD-CGD-O1D
39	NN	607	CHL	CHA-CBD-CGD-O2D
39	NN	608	CHL	CBD-CGD-O2D-CED
39	NN	609	CHL	CHA-CBD-CGD-O1D
39	NN	609	CHL	CHA-CBD-CGD-O2D
39	RR	305	CHL	C3A-C2A-CAA-CBA
39	RR	306	CHL	C1A-C2A-CAA-CBA
39	RR	306	CHL	C3A-C2A-CAA-CBA
39	RR	306	CHL	CHA-CBD-CGD-O1D
39	RR	306	CHL	CHA-CBD-CGD-O2D
39	RR	306	CHL	CBD-CGD-O2D-CED
39	RR	307	CHL	CHA-CBD-CGD-O1D
39	RR	307	CHL	CHA-CBD-CGD-O2D
39	SS	302	CHL	CBD-CGD-O2D-CED
39	SS	308	CHL	CHA-CBD-CGD-O1D
39	SS	308	CHL	CBD-CGD-O2D-CED
39	YY	608	CHL	CBD-CGD-O2D-CED
39	Gg	302	CHL	CBD-CGD-O2D-CED
39	Gg	306	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	Gg	306	CHL	CBD-CGD-O2D-CED
39	Gg	307	CHL	C1A-C2A-CAA-CBA
39	Gg	307	CHL	C3A-C2A-CAA-CBA
39	Gg	307	CHL	CHA-CBD-CGD-O1D
39	Gg	307	CHL	CHA-CBD-CGD-O2D
39	Gg	308	CHL	CBD-CGD-O2D-CED
39	Gg	310	CHL	CHA-CBD-CGD-O1D
39	Gg	310	CHL	CHA-CBD-CGD-O2D
39	Gg	310	CHL	CBD-CGD-O2D-CED
39	Nn	311	CHL	CBD-CGD-O2D-CED
39	Nn	317	CHL	C1A-C2A-CAA-CBA
39	Nn	317	CHL	CHA-CBD-CGD-O1D
39	Nn	317	CHL	CHA-CBD-CGD-O2D
39	Nn	318	CHL	CBD-CGD-O2D-CED
40	Y	615	LUT	C21-C26-C27-C28
40	YY	615	LUT	C25-C26-C27-C28
41	Rr	615	XAT	C5-C6-C7-C8
41	Rr	615	XAT	O4-C6-C7-C8
41	Yy	619	XAT	C21-C26-C27-C28
41	Yy	619	XAT	C25-C26-C27-C28
41	Yy	619	XAT	O24-C26-C27-C28
41	G	617	XAT	C27-C28-C29-C30
41	G	617	XAT	C27-C28-C29-C39
41	G	619	XAT	O24-C26-C27-C28
41	g	619	XAT	O24-C26-C27-C28
41	r	615	XAT	O4-C6-C7-C8
41	y	301	XAT	C21-C26-C27-C28
41	y	301	XAT	C25-C26-C27-C28
41	y	301	XAT	O24-C26-C27-C28
41	y	302	XAT	O24-C26-C27-C28
41	GG	617	XAT	C27-C28-C29-C30
41	GG	617	XAT	C27-C28-C29-C39
41	GG	619	XAT	O24-C26-C27-C28
41	Gg	301	XAT	O24-C26-C27-C28
41	Nn	308	XAT	O24-C26-C27-C28
43	C	502	LMU	C2'-C1'-O1'-C1
43	C	502	LMU	O5'-C1'-O1'-C1
43	R	618	LMU	O5'-C1'-O1'-C1
44	a	415	DGD	O6D-C1D-O3G-C3G
44	CC	522	DGD	C2B-C1B-O2G-C2G
44	CC	522	DGD	O2G-C2G-C3G-O3G
44	CC	522	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
44	Aa	401	DGD	O6D-C1D-O3G-C3G
36	44	614	LHG	C8-C7-O7-C5
32	Rr	610	CLA	O1D-CGD-O2D-CED
32	Yy	603	CLA	O1D-CGD-O2D-CED
32	44	615	CLA	O1D-CGD-O2D-CED
32	11	611	CLA	O1D-CGD-O2D-CED
32	22	612	CLA	O1D-CGD-O2D-CED
32	1	609	CLA	O1D-CGD-O2D-CED
32	1	613	CLA	O1D-CGD-O2D-CED
32	2	612	CLA	O1D-CGD-O2D-CED
32	3	602	CLA	O1D-CGD-O2D-CED
32	C	508	CLA	O1D-CGD-O2D-CED
32	C	515	CLA	O1D-CGD-O2D-CED
32	G	604	CLA	O1D-CGD-O2D-CED
32	G	612	CLA	O1D-CGD-O2D-CED
32	N	610	CLA	O1D-CGD-O2D-CED
32	R	601	CLA	O1D-CGD-O2D-CED
32	R	610	CLA	O1D-CGD-O2D-CED
32	S	603	CLA	O1D-CGD-O2D-CED
32	X	201	CLA	O1D-CGD-O2D-CED
32	Y	603	CLA	O1D-CGD-O2D-CED
32	Y	612	CLA	O1D-CGD-O2D-CED
32	b	607	CLA	O1D-CGD-O2D-CED
32	c	506	CLA	O1D-CGD-O2D-CED
32	n	603	CLA	O1D-CGD-O2D-CED
32	s	604	CLA	O1D-CGD-O2D-CED
32	s	611	CLA	O1D-CGD-O2D-CED
32	CC	507	CLA	O1D-CGD-O2D-CED
32	GG	613	CLA	O1D-CGD-O2D-CED
32	RR	310	CLA	O1D-CGD-O2D-CED
32	SS	304	CLA	O1D-CGD-O2D-CED
32	YY	612	CLA	O1D-CGD-O2D-CED
32	Bb	609	CLA	O1D-CGD-O2D-CED
32	Bb	614	CLA	O1D-CGD-O2D-CED
32	Gg	303	CLA	O1D-CGD-O2D-CED
32	Gg	314	CLA	O1D-CGD-O2D-CED
32	Nn	301	CLA	O1D-CGD-O2D-CED
32	Nn	303	CLA	O1D-CGD-O2D-CED
32	Nn	313	CLA	O1D-CGD-O2D-CED
39	2	606	CHL	O1D-CGD-O2D-CED
39	G	605	CHL	O1D-CGD-O2D-CED
39	4	307	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	GG	605	CHL	O1D-CGD-O2D-CED
39	Nn	311	CHL	O1D-CGD-O2D-CED
39	Nn	317	CHL	O1D-CGD-O2D-CED
32	Rr	608	CLA	O1D-CGD-O2D-CED
32	Ss	604	CLA	O1D-CGD-O2D-CED
32	Ss	611	CLA	O1D-CGD-O2D-CED
32	44	603	CLA	O1D-CGD-O2D-CED
32	44	604	CLA	O1D-CGD-O2D-CED
32	44	609	CLA	O1D-CGD-O2D-CED
32	44	610	CLA	O1D-CGD-O2D-CED
32	11	609	CLA	O1D-CGD-O2D-CED
32	11	613	CLA	O1D-CGD-O2D-CED
32	22	611	CLA	O1D-CGD-O2D-CED
32	33	604	CLA	O1D-CGD-O2D-CED
32	33	610	CLA	O1D-CGD-O2D-CED
32	1	610	CLA	O1D-CGD-O2D-CED
32	1	611	CLA	O1D-CGD-O2D-CED
32	2	611	CLA	O1D-CGD-O2D-CED
32	3	610	CLA	O1D-CGD-O2D-CED
32	G	602	CLA	O1D-CGD-O2D-CED
32	G	611	CLA	O1D-CGD-O2D-CED
32	G	613	CLA	O1D-CGD-O2D-CED
32	R	608	CLA	O1D-CGD-O2D-CED
32	R	613	CLA	O1D-CGD-O2D-CED
32	S	609	CLA	O1D-CGD-O2D-CED
32	S	611	CLA	O1D-CGD-O2D-CED
32	b	614	CLA	O1D-CGD-O2D-CED
32	g	604	CLA	O1D-CGD-O2D-CED
32	g	611	CLA	O1D-CGD-O2D-CED
32	g	612	CLA	O1D-CGD-O2D-CED
32	g	613	CLA	O1D-CGD-O2D-CED
32	n	612	CLA	O1D-CGD-O2D-CED
32	n	614	CLA	O1D-CGD-O2D-CED
32	r	608	CLA	O1D-CGD-O2D-CED
32	s	610	CLA	O1D-CGD-O2D-CED
32	y	305	CLA	O1D-CGD-O2D-CED
32	4	304	CLA	O1D-CGD-O2D-CED
32	4	305	CLA	O1D-CGD-O2D-CED
32	4	310	CLA	O1D-CGD-O2D-CED
32	CC	514	CLA	O1D-CGD-O2D-CED
32	GG	602	CLA	O1D-CGD-O2D-CED
32	GG	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	GG	604	CLA	O1D-CGD-O2D-CED
32	GG	612	CLA	O1D-CGD-O2D-CED
32	RR	308	CLA	O1D-CGD-O2D-CED
32	RR	309	CLA	O1D-CGD-O2D-CED
32	RR	313	CLA	O1D-CGD-O2D-CED
32	SS	311	CLA	O1D-CGD-O2D-CED
32	SS	312	CLA	O1D-CGD-O2D-CED
32	XX	201	CLA	O1D-CGD-O2D-CED
32	YY	603	CLA	O1D-CGD-O2D-CED
32	Bb	607	CLA	O1D-CGD-O2D-CED
32	Cc	508	CLA	O1D-CGD-O2D-CED
32	Cc	514	CLA	O1D-CGD-O2D-CED
32	Gg	313	CLA	O1D-CGD-O2D-CED
39	Ss	601	CHL	O1D-CGD-O2D-CED
39	Yy	601	CHL	O1D-CGD-O2D-CED
39	44	605	CHL	O1D-CGD-O2D-CED
39	44	607	CHL	O1D-CGD-O2D-CED
39	11	607	CHL	O1D-CGD-O2D-CED
39	22	601	CHL	O1D-CGD-O2D-CED
39	22	605	CHL	O1D-CGD-O2D-CED
39	22	606	CHL	O1D-CGD-O2D-CED
39	33	601	CHL	O1D-CGD-O2D-CED
39	33	606	CHL	O1D-CGD-O2D-CED
39	1	607	CHL	O1D-CGD-O2D-CED
39	3	606	CHL	O1D-CGD-O2D-CED
39	G	606	CHL	O1D-CGD-O2D-CED
39	G	607	CHL	O1D-CGD-O2D-CED
39	G	609	CHL	O1D-CGD-O2D-CED
39	R	606	CHL	O1D-CGD-O2D-CED
39	g	601	CHL	O1D-CGD-O2D-CED
39	g	605	CHL	O1D-CGD-O2D-CED
39	n	601	CHL	O1D-CGD-O2D-CED
39	n	607	CHL	O1D-CGD-O2D-CED
39	y	303	CHL	O1D-CGD-O2D-CED
39	4	306	CHL	O1D-CGD-O2D-CED
39	4	308	CHL	O1D-CGD-O2D-CED
39	GG	606	CHL	O1D-CGD-O2D-CED
39	GG	607	CHL	O1D-CGD-O2D-CED
39	GG	609	CHL	O1D-CGD-O2D-CED
39	Gg	302	CHL	O1D-CGD-O2D-CED
39	Gg	306	CHL	O1D-CGD-O2D-CED
39	Gg	307	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	A	405	CLA	CBD-CGD-O2D-CED
32	Rr	604	CLA	CBD-CGD-O2D-CED
32	Rr	609	CLA	CBD-CGD-O2D-CED
32	Rr	610	CLA	CBD-CGD-O2D-CED
32	Ss	603	CLA	CBD-CGD-O2D-CED
32	Ss	604	CLA	CBD-CGD-O2D-CED
32	Ss	608	CLA	CBD-CGD-O2D-CED
32	Ss	609	CLA	CBD-CGD-O2D-CED
32	Ss	610	CLA	CBD-CGD-O2D-CED
32	Ss	611	CLA	CBD-CGD-O2D-CED
32	Ss	613	CLA	CBD-CGD-O2D-CED
32	Yy	603	CLA	CBD-CGD-O2D-CED
32	Yy	611	CLA	CBD-CGD-O2D-CED
32	Yy	614	CLA	CBD-CGD-O2D-CED
32	44	615	CLA	CBD-CGD-O2D-CED
32	11	602	CLA	CBD-CGD-O2D-CED
32	11	611	CLA	CBD-CGD-O2D-CED
32	22	603	CLA	CBD-CGD-O2D-CED
32	22	612	CLA	CBD-CGD-O2D-CED
32	33	602	CLA	CBD-CGD-O2D-CED
32	33	604	CLA	CBD-CGD-O2D-CED
32	33	613	CLA	CBD-CGD-O2D-CED
32	1	602	CLA	CBD-CGD-O2D-CED
32	1	610	CLA	CBD-CGD-O2D-CED
32	1	613	CLA	CBD-CGD-O2D-CED
32	2	611	CLA	CBD-CGD-O2D-CED
32	2	612	CLA	CBD-CGD-O2D-CED
32	3	602	CLA	CBD-CGD-O2D-CED
32	3	603	CLA	CBD-CGD-O2D-CED
32	3	604	CLA	CBD-CGD-O2D-CED
32	C	505	CLA	CBD-CGD-O2D-CED
32	C	513	CLA	CBD-CGD-O2D-CED
32	D	401	CLA	CBD-CGD-O2D-CED
32	G	604	CLA	CBD-CGD-O2D-CED
32	G	614	CLA	CBD-CGD-O2D-CED
32	N	610	CLA	CBD-CGD-O2D-CED
32	R	601	CLA	CBD-CGD-O2D-CED
32	R	610	CLA	CBD-CGD-O2D-CED
32	S	603	CLA	CBD-CGD-O2D-CED
32	S	608	CLA	CBD-CGD-O2D-CED
32	Y	610	CLA	CBD-CGD-O2D-CED
32	a	405	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	b	602	CLA	CBD-CGD-O2D-CED
32	b	605	CLA	CBD-CGD-O2D-CED
32	b	607	CLA	CBD-CGD-O2D-CED
32	b	609	CLA	CBD-CGD-O2D-CED
32	b	615	CLA	CBD-CGD-O2D-CED
32	c	509	CLA	CBD-CGD-O2D-CED
32	g	602	CLA	CBD-CGD-O2D-CED
32	g	611	CLA	CBD-CGD-O2D-CED
32	g	612	CLA	CBD-CGD-O2D-CED
32	g	614	CLA	CBD-CGD-O2D-CED
32	n	602	CLA	CBD-CGD-O2D-CED
32	n	611	CLA	CBD-CGD-O2D-CED
32	r	601	CLA	CBD-CGD-O2D-CED
32	r	609	CLA	CBD-CGD-O2D-CED
32	r	610	CLA	CBD-CGD-O2D-CED
32	r	612	CLA	CBD-CGD-O2D-CED
32	s	603	CLA	CBD-CGD-O2D-CED
32	s	604	CLA	CBD-CGD-O2D-CED
32	s	608	CLA	CBD-CGD-O2D-CED
32	s	610	CLA	CBD-CGD-O2D-CED
32	s	611	CLA	CBD-CGD-O2D-CED
32	y	305	CLA	CBD-CGD-O2D-CED
32	y	312	CLA	CBD-CGD-O2D-CED
32	y	313	CLA	CBD-CGD-O2D-CED
32	y	316	CLA	CBD-CGD-O2D-CED
32	BB	604	CLA	CBD-CGD-O2D-CED
32	BB	605	CLA	CBD-CGD-O2D-CED
32	BB	608	CLA	CBD-CGD-O2D-CED
32	BB	613	CLA	CBD-CGD-O2D-CED
32	CC	507	CLA	CBD-CGD-O2D-CED
32	CC	512	CLA	CBD-CGD-O2D-CED
32	B	604	CLA	CBD-CGD-O2D-CED
32	B	607	CLA	CBD-CGD-O2D-CED
32	B	621	CLA	CBD-CGD-O2D-CED
32	GG	603	CLA	CBD-CGD-O2D-CED
32	GG	610	CLA	CBD-CGD-O2D-CED
32	GG	612	CLA	CBD-CGD-O2D-CED
32	GG	614	CLA	CBD-CGD-O2D-CED
32	NN	604	CLA	CBD-CGD-O2D-CED
32	NN	612	CLA	CBD-CGD-O2D-CED
32	RR	310	CLA	CBD-CGD-O2D-CED
32	SS	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Bb	602	CLA	CBD-CGD-O2D-CED
32	Bb	605	CLA	CBD-CGD-O2D-CED
32	Bb	607	CLA	CBD-CGD-O2D-CED
32	Bb	609	CLA	CBD-CGD-O2D-CED
32	Bb	614	CLA	CBD-CGD-O2D-CED
32	Bb	615	CLA	CBD-CGD-O2D-CED
32	Cc	504	CLA	CBD-CGD-O2D-CED
32	Cc	508	CLA	CBD-CGD-O2D-CED
32	Cc	510	CLA	CBD-CGD-O2D-CED
32	Gg	303	CLA	CBD-CGD-O2D-CED
32	Gg	304	CLA	CBD-CGD-O2D-CED
32	Gg	312	CLA	CBD-CGD-O2D-CED
33	A	407	PHO	CBD-CGD-O2D-CED
39	Ss	605	CHL	CBD-CGD-O2D-CED
39	Ss	606	CHL	CBD-CGD-O2D-CED
39	Ss	607	CHL	CBD-CGD-O2D-CED
39	11	605	CHL	CBD-CGD-O2D-CED
39	11	608	CHL	CBD-CGD-O2D-CED
39	22	601	CHL	CBD-CGD-O2D-CED
39	22	605	CHL	CBD-CGD-O2D-CED
39	22	607	CHL	CBD-CGD-O2D-CED
39	2	601	CHL	CBD-CGD-O2D-CED
39	2	605	CHL	CBD-CGD-O2D-CED
39	2	606	CHL	CBD-CGD-O2D-CED
39	2	607	CHL	CBD-CGD-O2D-CED
39	3	608	CHL	CBD-CGD-O2D-CED
39	G	601	CHL	CBD-CGD-O2D-CED
39	G	605	CHL	CBD-CGD-O2D-CED
39	G	608	CHL	CBD-CGD-O2D-CED
39	G	609	CHL	CBD-CGD-O2D-CED
39	Y	607	CHL	CBD-CGD-O2D-CED
39	Y	608	CHL	CBD-CGD-O2D-CED
39	g	601	CHL	CBD-CGD-O2D-CED
39	g	608	CHL	CBD-CGD-O2D-CED
39	g	609	CHL	CBD-CGD-O2D-CED
39	s	606	CHL	CBD-CGD-O2D-CED
39	y	307	CHL	CBD-CGD-O2D-CED
39	GG	601	CHL	CBD-CGD-O2D-CED
39	GG	605	CHL	CBD-CGD-O2D-CED
39	SS	306	CHL	CBD-CGD-O2D-CED
39	YY	601	CHL	CBD-CGD-O2D-CED
39	YY	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	Gg	307	CHL	CBD-CGD-O2D-CED
39	Gg	309	CHL	CBD-CGD-O2D-CED
39	Nn	315	CHL	CBD-CGD-O2D-CED
39	Nn	317	CHL	CBD-CGD-O2D-CED
32	Ss	608	CLA	O1A-CGA-O2A-C1
32	C	512	CLA	O1A-CGA-O2A-C1
32	G	603	CLA	O1A-CGA-O2A-C1
32	N	610	CLA	O1A-CGA-O2A-C1
32	Y	602	CLA	O1A-CGA-O2A-C1
32	Y	610	CLA	O1A-CGA-O2A-C1
32	g	611	CLA	O1A-CGA-O2A-C1
32	n	610	CLA	O1A-CGA-O2A-C1
32	r	613	CLA	O1A-CGA-O2A-C1
32	CC	511	CLA	O1A-CGA-O2A-C1
32	B	624	CLA	O1A-CGA-O2A-C1
32	NN	610	CLA	O1A-CGA-O2A-C1
32	SS	312	CLA	O1A-CGA-O2A-C1
32	YY	602	CLA	O1A-CGA-O2A-C1
32	Gg	312	CLA	O1A-CGA-O2A-C1
32	Nn	301	CLA	O1A-CGA-O2A-C1
39	Y	605	CHL	O1A-CGA-O2A-C1
39	g	607	CHL	O1A-CGA-O2A-C1
39	Gg	308	CHL	O1A-CGA-O2A-C1
32	Rr	609	CLA	O1D-CGD-O2D-CED
32	22	610	CLA	O1D-CGD-O2D-CED
32	33	612	CLA	O1D-CGD-O2D-CED
32	3	612	CLA	O1D-CGD-O2D-CED
32	G	614	CLA	O1D-CGD-O2D-CED
32	N	612	CLA	O1D-CGD-O2D-CED
32	R	609	CLA	O1D-CGD-O2D-CED
32	a	405	CLA	O1D-CGD-O2D-CED
32	b	603	CLA	O1D-CGD-O2D-CED
32	b	609	CLA	O1D-CGD-O2D-CED
32	c	512	CLA	O1D-CGD-O2D-CED
32	g	614	CLA	O1D-CGD-O2D-CED
32	n	602	CLA	O1D-CGD-O2D-CED
32	n	610	CLA	O1D-CGD-O2D-CED
32	r	609	CLA	O1D-CGD-O2D-CED
32	GG	614	CLA	O1D-CGD-O2D-CED
32	NN	610	CLA	O1D-CGD-O2D-CED
32	YY	611	CLA	O1D-CGD-O2D-CED
32	Bb	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Cc	504	CLA	O1D-CGD-O2D-CED
32	Cc	511	CLA	O1D-CGD-O2D-CED
32	Cc	513	CLA	O1D-CGD-O2D-CED
32	Gg	305	CLA	O1D-CGD-O2D-CED
32	Gg	312	CLA	O1D-CGD-O2D-CED
32	Nn	305	CLA	O1D-CGD-O2D-CED
39	Rr	606	CHL	O1D-CGD-O2D-CED
39	Ss	606	CHL	O1D-CGD-O2D-CED
39	44	606	CHL	O1D-CGD-O2D-CED
39	2	601	CHL	O1D-CGD-O2D-CED
39	2	605	CHL	O1D-CGD-O2D-CED
39	2	607	CHL	O1D-CGD-O2D-CED
39	2	608	CHL	O1D-CGD-O2D-CED
39	3	601	CHL	O1D-CGD-O2D-CED
39	G	608	CHL	O1D-CGD-O2D-CED
39	S	605	CHL	O1D-CGD-O2D-CED
39	Y	607	CHL	O1D-CGD-O2D-CED
39	Y	608	CHL	O1D-CGD-O2D-CED
39	g	608	CHL	O1D-CGD-O2D-CED
39	g	609	CHL	O1D-CGD-O2D-CED
39	r	606	CHL	O1D-CGD-O2D-CED
39	s	601	CHL	O1D-CGD-O2D-CED
39	s	606	CHL	O1D-CGD-O2D-CED
39	GG	601	CHL	O1D-CGD-O2D-CED
39	RR	306	CHL	O1D-CGD-O2D-CED
39	SS	308	CHL	O1D-CGD-O2D-CED
39	YY	607	CHL	O1D-CGD-O2D-CED
32	Rr	611	CLA	O1D-CGD-O2D-CED
32	11	602	CLA	O1D-CGD-O2D-CED
32	11	603	CLA	O1D-CGD-O2D-CED
32	11	610	CLA	O1D-CGD-O2D-CED
32	22	603	CLA	O1D-CGD-O2D-CED
32	22	604	CLA	O1D-CGD-O2D-CED
32	2	603	CLA	O1D-CGD-O2D-CED
32	2	604	CLA	O1D-CGD-O2D-CED
32	2	610	CLA	O1D-CGD-O2D-CED
32	3	604	CLA	O1D-CGD-O2D-CED
32	G	603	CLA	O1D-CGD-O2D-CED
32	N	613	CLA	O1D-CGD-O2D-CED
32	b	601	CLA	O1D-CGD-O2D-CED
32	b	605	CLA	O1D-CGD-O2D-CED
32	b	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	b	613	CLA	O1D-CGD-O2D-CED
32	c	503	CLA	O1D-CGD-O2D-CED
32	c	511	CLA	O1D-CGD-O2D-CED
32	r	604	CLA	O1D-CGD-O2D-CED
32	r	610	CLA	O1D-CGD-O2D-CED
32	r	611	CLA	O1D-CGD-O2D-CED
32	s	613	CLA	O1D-CGD-O2D-CED
32	BB	610	CLA	O1D-CGD-O2D-CED
32	BB	612	CLA	O1D-CGD-O2D-CED
32	B	606	CLA	O1D-CGD-O2D-CED
32	B	608	CLA	O1D-CGD-O2D-CED
32	GG	611	CLA	O1D-CGD-O2D-CED
32	NN	612	CLA	O1D-CGD-O2D-CED
32	NN	613	CLA	O1D-CGD-O2D-CED
32	NN	614	CLA	O1D-CGD-O2D-CED
32	YY	610	CLA	O1D-CGD-O2D-CED
32	Bb	603	CLA	O1D-CGD-O2D-CED
32	Bb	605	CLA	O1D-CGD-O2D-CED
32	Bb	613	CLA	O1D-CGD-O2D-CED
32	Cc	506	CLA	O1D-CGD-O2D-CED
32	Gg	311	CLA	O1D-CGD-O2D-CED
39	33	605	CHL	O1D-CGD-O2D-CED
39	1	601	CHL	O1D-CGD-O2D-CED
39	Y	601	CHL	O1D-CGD-O2D-CED
39	g	607	CHL	O1D-CGD-O2D-CED
39	GG	608	CHL	O1D-CGD-O2D-CED
39	NN	608	CHL	O1D-CGD-O2D-CED
39	Gg	308	CHL	O1D-CGD-O2D-CED
39	Gg	309	CHL	O1D-CGD-O2D-CED
39	Gg	310	CHL	O1D-CGD-O2D-CED
32	S	611	CLA	CBA-CGA-O2A-C1
32	r	613	CLA	CBA-CGA-O2A-C1
32	Gg	312	CLA	CBA-CGA-O2A-C1
35	D	407	PL9	C47-C48-C49-C50
35	D	407	PL9	C47-C48-C49-C51
35	DD	406	PL9	C47-C48-C49-C50
35	DD	406	PL9	C47-C48-C49-C51
32	Rr	601	CLA	CBD-CGD-O2D-CED
32	22	613	CLA	CBD-CGD-O2D-CED
32	33	603	CLA	CBD-CGD-O2D-CED
32	33	611	CLA	CBD-CGD-O2D-CED
32	2	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	3	609	CLA	CBD-CGD-O2D-CED
32	3	611	CLA	CBD-CGD-O2D-CED
32	3	613	CLA	CBD-CGD-O2D-CED
32	C	506	CLA	CBD-CGD-O2D-CED
32	C	512	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	CBD-CGD-O2D-CED
32	S	602	CLA	CBD-CGD-O2D-CED
32	S	610	CLA	CBD-CGD-O2D-CED
32	Y	604	CLA	CBD-CGD-O2D-CED
32	Y	611	CLA	CBD-CGD-O2D-CED
32	b	612	CLA	CBD-CGD-O2D-CED
32	c	501	CLA	CBD-CGD-O2D-CED
32	c	508	CLA	CBD-CGD-O2D-CED
32	r	603	CLA	CBD-CGD-O2D-CED
32	s	602	CLA	CBD-CGD-O2D-CED
32	BB	602	CLA	CBD-CGD-O2D-CED
32	BB	603	CLA	CBD-CGD-O2D-CED
32	BB	614	CLA	CBD-CGD-O2D-CED
32	CC	504	CLA	CBD-CGD-O2D-CED
32	CC	511	CLA	CBD-CGD-O2D-CED
32	DD	401	CLA	CBD-CGD-O2D-CED
32	B	609	CLA	CBD-CGD-O2D-CED
32	B	610	CLA	CBD-CGD-O2D-CED
32	B	619	CLA	CBD-CGD-O2D-CED
32	B	620	CLA	CBD-CGD-O2D-CED
32	NN	602	CLA	CBD-CGD-O2D-CED
32	SS	309	CLA	CBD-CGD-O2D-CED
32	YY	602	CLA	CBD-CGD-O2D-CED
32	Cc	505	CLA	CBD-CGD-O2D-CED
32	Gg	315	CLA	CBD-CGD-O2D-CED
32	Nn	302	CLA	CBD-CGD-O2D-CED
33	AA	407	PHO	CBD-CGD-O2D-CED
39	Yy	605	CHL	CBD-CGD-O2D-CED
39	r	605	CHL	CBD-CGD-O2D-CED
39	s	605	CHL	CBD-CGD-O2D-CED
39	y	308	CHL	CBD-CGD-O2D-CED
39	NN	601	CHL	CBD-CGD-O2D-CED
39	NN	605	CHL	CBD-CGD-O2D-CED
39	YY	606	CHL	CBD-CGD-O2D-CED
32	Rr	608	CLA	O1A-CGA-O2A-C1
32	Rr	611	CLA	O1A-CGA-O2A-C1
32	Rr	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	Ss	602	CLA	O1A-CGA-O2A-C1
32	Ss	609	CLA	O1A-CGA-O2A-C1
32	Ss	611	CLA	O1A-CGA-O2A-C1
32	Ss	613	CLA	O1A-CGA-O2A-C1
32	Yy	610	CLA	O1A-CGA-O2A-C1
32	C	504	CLA	O1A-CGA-O2A-C1
32	C	511	CLA	O1A-CGA-O2A-C1
32	N	611	CLA	O1A-CGA-O2A-C1
32	S	611	CLA	O1A-CGA-O2A-C1
32	b	603	CLA	O1A-CGA-O2A-C1
32	b	612	CLA	O1A-CGA-O2A-C1
32	b	613	CLA	O1A-CGA-O2A-C1
32	c	503	CLA	O1A-CGA-O2A-C1
32	s	608	CLA	O1A-CGA-O2A-C1
32	s	611	CLA	O1A-CGA-O2A-C1
32	y	312	CLA	O1A-CGA-O2A-C1
32	BB	607	CLA	O1A-CGA-O2A-C1
32	CC	503	CLA	O1A-CGA-O2A-C1
32	CC	510	CLA	O1A-CGA-O2A-C1
32	GG	603	CLA	O1A-CGA-O2A-C1
32	NN	611	CLA	O1A-CGA-O2A-C1
32	YY	610	CLA	O1A-CGA-O2A-C1
32	Bb	603	CLA	O1A-CGA-O2A-C1
32	Bb	612	CLA	O1A-CGA-O2A-C1
32	Bb	613	CLA	O1A-CGA-O2A-C1
32	Cc	503	CLA	O1A-CGA-O2A-C1
39	Ss	601	CHL	O1A-CGA-O2A-C1
39	R	606	CHL	O1A-CGA-O2A-C1
39	n	601	CHL	O1A-CGA-O2A-C1
39	n	609	CHL	O1A-CGA-O2A-C1
39	YY	605	CHL	O1A-CGA-O2A-C1
39	Nn	311	CHL	O1A-CGA-O2A-C1
39	Nn	319	CHL	O1A-CGA-O2A-C1
32	1	603	CLA	O1D-CGD-O2D-CED
32	1	604	CLA	O1D-CGD-O2D-CED
32	N	614	CLA	O1D-CGD-O2D-CED
32	S	612	CLA	O1D-CGD-O2D-CED
32	AA	405	CLA	O1D-CGD-O2D-CED
32	SS	310	CLA	O1D-CGD-O2D-CED
32	SS	313	CLA	O1D-CGD-O2D-CED
32	Nn	312	CLA	O1D-CGD-O2D-CED
39	22	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	33	607	CHL	O1D-CGD-O2D-CED
39	N	608	CHL	O1D-CGD-O2D-CED
39	SS	302	CHL	O1D-CGD-O2D-CED
39	YY	608	CHL	O1D-CGD-O2D-CED
32	2	613	CLA	O1D-CGD-O2D-CED
32	N	603	CLA	O1D-CGD-O2D-CED
32	N	604	CLA	O1D-CGD-O2D-CED
32	c	504	CLA	O1D-CGD-O2D-CED
32	g	603	CLA	O1D-CGD-O2D-CED
32	B	622	CLA	O1D-CGD-O2D-CED
32	NN	603	CLA	O1D-CGD-O2D-CED
32	NN	611	CLA	O1D-CGD-O2D-CED
32	Aa	405	CLA	O1D-CGD-O2D-CED
32	Cc	515	CLA	O1D-CGD-O2D-CED
39	Yy	607	CHL	O1D-CGD-O2D-CED
39	11	601	CHL	O1D-CGD-O2D-CED
39	33	608	CHL	O1D-CGD-O2D-CED
39	S	601	CHL	O1D-CGD-O2D-CED
39	n	608	CHL	O1D-CGD-O2D-CED
39	Nn	318	CHL	O1D-CGD-O2D-CED
32	Ss	602	CLA	CBD-CGD-O2D-CED
32	11	612	CLA	CBD-CGD-O2D-CED
32	y	304	CLA	CBD-CGD-O2D-CED
32	Cc	503	CLA	CBD-CGD-O2D-CED
32	Nn	304	CLA	CBD-CGD-O2D-CED
39	N	609	CHL	CBD-CGD-O2D-CED
39	Y	605	CHL	CBD-CGD-O2D-CED
39	NN	609	CHL	CBD-CGD-O2D-CED
32	A	405	CLA	O1D-CGD-O2D-CED
39	g	606	CHL	O1D-CGD-O2D-CED
39	SS	306	CHL	O1D-CGD-O2D-CED
39	YY	601	CHL	O1D-CGD-O2D-CED
36	G	618	LHG	O9-C7-O7-C5
36	N	619	LHG	O9-C7-O7-C5
36	n	618	LHG	O9-C7-O7-C5
36	GG	618	LHG	O9-C7-O7-C5
36	NN	619	LHG	O9-C7-O7-C5
36	Nn	310	LHG	O9-C7-O7-C5
44	CC	522	DGD	O1B-C1B-O2G-C2G
32	A	405	CLA	O1A-CGA-O2A-C1
32	r	611	CLA	O1A-CGA-O2A-C1
32	AA	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	RR	306	CHL	O1A-CGA-O2A-C1
36	4	315	LHG	C8-C7-O7-C5
32	c	509	CLA	O1D-CGD-O2D-CED
32	C	508	CLA	C3-C5-C6-C7
32	C	514	CLA	C3-C5-C6-C7
32	R	609	CLA	C3-C5-C6-C7
32	Y	610	CLA	C3-C5-C6-C7
32	Y	613	CLA	C3-C5-C6-C7
32	b	604	CLA	C3-C5-C6-C7
32	b	605	CLA	C3-C5-C6-C7
32	b	614	CLA	C3-C5-C6-C7
32	b	615	CLA	C3-C5-C6-C7
32	d	401	CLA	C3-C5-C6-C7
32	r	602	CLA	C3-C5-C6-C7
32	y	314	CLA	C3-C5-C6-C7
32	BB	603	CLA	C3-C5-C6-C7
32	CC	507	CLA	C3-C5-C6-C7
32	CC	513	CLA	C3-C5-C6-C7
32	B	620	CLA	C3-C5-C6-C7
32	RR	309	CLA	C3-C5-C6-C7
32	YY	613	CLA	C3-C5-C6-C7
32	Bb	604	CLA	C3-C5-C6-C7
32	Bb	605	CLA	C3-C5-C6-C7
32	Bb	614	CLA	C3-C5-C6-C7
32	Nn	301	CLA	C3-C5-C6-C7
33	D	402	PHO	C3-C5-C6-C7
33	a	409	PHO	C3-C5-C6-C7
33	Aa	409	PHO	C3-C5-C6-C7
32	Ss	608	CLA	CBA-CGA-O2A-C1
32	Ss	609	CLA	CBA-CGA-O2A-C1
32	C	504	CLA	CBA-CGA-O2A-C1
32	C	511	CLA	CBA-CGA-O2A-C1
32	C	512	CLA	CBA-CGA-O2A-C1
32	G	603	CLA	CBA-CGA-O2A-C1
32	G	611	CLA	CBA-CGA-O2A-C1
32	N	610	CLA	CBA-CGA-O2A-C1
32	Y	602	CLA	CBA-CGA-O2A-C1
32	Y	610	CLA	CBA-CGA-O2A-C1
32	c	501	CLA	CBA-CGA-O2A-C1
32	c	503	CLA	CBA-CGA-O2A-C1
32	g	611	CLA	CBA-CGA-O2A-C1
32	n	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	n	610	CLA	CBA-CGA-O2A-C1
32	CC	503	CLA	CBA-CGA-O2A-C1
32	CC	504	CLA	CBA-CGA-O2A-C1
32	CC	510	CLA	CBA-CGA-O2A-C1
32	CC	511	CLA	CBA-CGA-O2A-C1
32	B	608	CLA	CBA-CGA-O2A-C1
32	B	624	CLA	CBA-CGA-O2A-C1
32	NN	610	CLA	CBA-CGA-O2A-C1
32	SS	312	CLA	CBA-CGA-O2A-C1
32	YY	602	CLA	CBA-CGA-O2A-C1
32	YY	610	CLA	CBA-CGA-O2A-C1
32	Nn	301	CLA	CBA-CGA-O2A-C1
37	L	101	SQD	C24-C23-O48-C46
37	LL	102	SQD	C24-C23-O48-C46
39	Y	605	CHL	CBA-CGA-O2A-C1
39	g	607	CHL	CBA-CGA-O2A-C1
39	n	601	CHL	CBA-CGA-O2A-C1
39	YY	605	CHL	CBA-CGA-O2A-C1
39	Gg	308	CHL	CBA-CGA-O2A-C1
39	Nn	311	CHL	CBA-CGA-O2A-C1
38	b	621	LMG	C11-C10-O7-C8
35	d	404	PL9	C47-C48-C49-C50
35	Dd	404	PL9	C47-C48-C49-C50
32	Ss	610	CLA	O1D-CGD-O2D-CED
32	C	505	CLA	O1D-CGD-O2D-CED
32	S	608	CLA	O1D-CGD-O2D-CED
32	r	601	CLA	O1D-CGD-O2D-CED
32	y	312	CLA	O1D-CGD-O2D-CED
32	y	316	CLA	O1D-CGD-O2D-CED
39	Nn	315	CHL	O1D-CGD-O2D-CED
32	r	613	CLA	CBD-CGD-O2D-CED
32	s	609	CLA	CBD-CGD-O2D-CED
32	B	624	CLA	CBD-CGD-O2D-CED
33	DD	402	PHO	CBD-CGD-O2D-CED
39	Yy	606	CHL	CBD-CGD-O2D-CED
39	R	607	CHL	CBD-CGD-O2D-CED
32	YY	612	CLA	O1A-CGA-O2A-C1
39	Ss	607	CHL	O1A-CGA-O2A-C1
38	Dd	408	LMG	O6-C5-C6-O5
32	Yy	614	CLA	O1D-CGD-O2D-CED
36	J	101	LHG	C8-C7-O7-C5
35	AA	410	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
35	DD	406	PL9	C25-C24-C26-C27
35	Dd	404	PL9	C45-C44-C46-C47
35	D	407	PL9	C13-C14-C16-C17
35	D	407	PL9	C38-C39-C41-C42
35	DD	406	PL9	C38-C39-C41-C42
35	Dd	404	PL9	C38-C39-C41-C42
32	Yy	613	CLA	CBD-CGD-O2D-CED
32	Y	614	CLA	CBD-CGD-O2D-CED
32	d	401	CLA	CBD-CGD-O2D-CED
32	4	311	CLA	CBD-CGD-O2D-CED
39	Rr	605	CHL	CBD-CGD-O2D-CED
39	N	601	CHL	CBD-CGD-O2D-CED
39	4	309	CHL	CBD-CGD-O2D-CED
39	YY	609	CHL	CBD-CGD-O2D-CED
32	Rr	601	CLA	C2A-CAA-CBA-CGA
32	Rr	608	CLA	C2A-CAA-CBA-CGA
32	Ss	610	CLA	C2A-CAA-CBA-CGA
32	44	611	CLA	C2A-CAA-CBA-CGA
32	D	404	CLA	C2A-CAA-CBA-CGA
32	R	604	CLA	C2A-CAA-CBA-CGA
32	b	606	CLA	C2A-CAA-CBA-CGA
32	b	616	CLA	C2A-CAA-CBA-CGA
32	r	601	CLA	C2A-CAA-CBA-CGA
32	s	602	CLA	C2A-CAA-CBA-CGA
32	s	610	CLA	C2A-CAA-CBA-CGA
32	4	312	CLA	C2A-CAA-CBA-CGA
32	BB	605	CLA	C2A-CAA-CBA-CGA
32	DD	403	CLA	C2A-CAA-CBA-CGA
32	B	605	CLA	C2A-CAA-CBA-CGA
32	RR	304	CLA	C2A-CAA-CBA-CGA
32	Bb	606	CLA	C2A-CAA-CBA-CGA
32	Bb	616	CLA	C2A-CAA-CBA-CGA
39	N	607	CHL	C2A-CAA-CBA-CGA
39	S	601	CHL	C2A-CAA-CBA-CGA
39	n	607	CHL	C2A-CAA-CBA-CGA
39	n	608	CHL	C2A-CAA-CBA-CGA
39	NN	607	CHL	C2A-CAA-CBA-CGA
39	SS	302	CHL	C2A-CAA-CBA-CGA
32	y	304	CLA	O1A-CGA-O2A-C1
37	L	101	SQD	O10-C23-O48-C46
32	Rr	604	CLA	O1D-CGD-O2D-CED
32	Ss	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	1	602	CLA	O1D-CGD-O2D-CED
32	y	313	CLA	O1D-CGD-O2D-CED
36	44	614	LHG	O9-C7-O7-C5
32	Rr	602	CLA	C3-C5-C6-C7
32	C	504	CLA	C3-C5-C6-C7
32	D	404	CLA	C3-C5-C6-C7
32	c	501	CLA	C3-C5-C6-C7
32	BB	604	CLA	C3-C5-C6-C7
32	CC	509	CLA	C3-C5-C6-C7
32	DD	403	CLA	C3-C5-C6-C7
32	B	621	CLA	C3-C5-C6-C7
32	Dd	401	CLA	C3-C5-C6-C7
39	Yy	609	CHL	C3-C5-C6-C7
39	N	607	CHL	C3-C5-C6-C7
32	A	405	CLA	CBA-CGA-O2A-C1
32	Rr	608	CLA	CBA-CGA-O2A-C1
32	Rr	611	CLA	CBA-CGA-O2A-C1
32	Rr	613	CLA	CBA-CGA-O2A-C1
32	Ss	602	CLA	CBA-CGA-O2A-C1
32	Ss	611	CLA	CBA-CGA-O2A-C1
32	Ss	613	CLA	CBA-CGA-O2A-C1
32	Yy	610	CLA	CBA-CGA-O2A-C1
32	N	611	CLA	CBA-CGA-O2A-C1
32	Y	603	CLA	CBA-CGA-O2A-C1
32	Y	612	CLA	CBA-CGA-O2A-C1
32	a	405	CLA	CBA-CGA-O2A-C1
32	b	603	CLA	CBA-CGA-O2A-C1
32	b	612	CLA	CBA-CGA-O2A-C1
32	b	613	CLA	CBA-CGA-O2A-C1
32	c	512	CLA	CBA-CGA-O2A-C1
32	r	611	CLA	CBA-CGA-O2A-C1
32	s	608	CLA	CBA-CGA-O2A-C1
32	s	611	CLA	CBA-CGA-O2A-C1
32	y	312	CLA	CBA-CGA-O2A-C1
32	AA	405	CLA	CBA-CGA-O2A-C1
32	AA	406	CLA	CBA-CGA-O2A-C1
32	BB	603	CLA	CBA-CGA-O2A-C1
32	BB	607	CLA	CBA-CGA-O2A-C1
32	BB	609	CLA	CBA-CGA-O2A-C1
32	BB	612	CLA	CBA-CGA-O2A-C1
32	B	605	CLA	CBA-CGA-O2A-C1
32	B	620	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	GG	603	CLA	CBA-CGA-O2A-C1
32	GG	611	CLA	CBA-CGA-O2A-C1
32	NN	611	CLA	CBA-CGA-O2A-C1
32	RR	310	CLA	CBA-CGA-O2A-C1
32	YY	603	CLA	CBA-CGA-O2A-C1
32	Bb	603	CLA	CBA-CGA-O2A-C1
32	Bb	609	CLA	CBA-CGA-O2A-C1
32	Bb	612	CLA	CBA-CGA-O2A-C1
32	Bb	613	CLA	CBA-CGA-O2A-C1
32	Cc	503	CLA	CBA-CGA-O2A-C1
32	Cc	514	CLA	CBA-CGA-O2A-C1
32	Gg	304	CLA	CBA-CGA-O2A-C1
32	Nn	305	CLA	CBA-CGA-O2A-C1
32	Nn	313	CLA	CBA-CGA-O2A-C1
33	A	407	PHO	CBA-CGA-O2A-C1
33	AA	407	PHO	CBA-CGA-O2A-C1
39	Ss	601	CHL	CBA-CGA-O2A-C1
39	R	606	CHL	CBA-CGA-O2A-C1
39	n	607	CHL	CBA-CGA-O2A-C1
39	n	609	CHL	CBA-CGA-O2A-C1
39	RR	306	CHL	CBA-CGA-O2A-C1
39	Nn	319	CHL	CBA-CGA-O2A-C1
44	CC	522	DGD	O6D-C5D-C6D-O5D
32	Ss	609	CLA	O1D-CGD-O2D-CED
32	BB	604	CLA	O1D-CGD-O2D-CED
32	BB	605	CLA	O1D-CGD-O2D-CED
39	G	601	CHL	O1D-CGD-O2D-CED
35	A	410	PL9	C7-C8-C9-C10
35	D	407	PL9	C7-C8-C9-C10
35	D	407	PL9	C22-C23-C24-C25
35	d	404	PL9	C32-C33-C34-C35
35	AA	410	PL9	C7-C8-C9-C10
35	AA	410	PL9	C12-C13-C14-C15
35	AA	410	PL9	C42-C43-C44-C45
35	DD	406	PL9	C12-C13-C14-C15
35	Dd	404	PL9	C32-C33-C34-C35
32	22	609	CLA	CBD-CGD-O2D-CED
32	Y	602	CLA	CBD-CGD-O2D-CED
32	n	604	CLA	CBD-CGD-O2D-CED
39	1	608	CHL	CBD-CGD-O2D-CED
32	Ss	613	CLA	O1D-CGD-O2D-CED
32	b	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	n	611	CLA	O1D-CGD-O2D-CED
32	s	603	CLA	O1D-CGD-O2D-CED
32	B	604	CLA	O1D-CGD-O2D-CED
32	GG	610	CLA	O1D-CGD-O2D-CED
32	NN	604	CLA	O1D-CGD-O2D-CED
33	A	407	PHO	O1D-CGD-O2D-CED
39	Ss	607	CHL	O1D-CGD-O2D-CED
39	3	608	CHL	O1D-CGD-O2D-CED
39	y	307	CHL	O1D-CGD-O2D-CED
35	A	410	PL9	C22-C23-C24-C26
35	A	410	PL9	C37-C38-C39-C41
35	D	407	PL9	C37-C38-C39-C41
35	d	404	PL9	C12-C13-C14-C16
35	d	404	PL9	C17-C18-C19-C21
35	AA	410	PL9	C17-C18-C19-C21
35	AA	410	PL9	C32-C33-C34-C36
35	AA	410	PL9	C37-C38-C39-C41
35	DD	406	PL9	C17-C18-C19-C21
35	Dd	404	PL9	C17-C18-C19-C21
44	C	523	DGD	C4E-C5E-C6E-O5E
32	A	406	CLA	O1A-CGA-O2A-C1
32	Ss	604	CLA	O1A-CGA-O2A-C1
32	G	610	CLA	O1A-CGA-O2A-C1
32	R	610	CLA	O1A-CGA-O2A-C1
32	Y	603	CLA	O1A-CGA-O2A-C1
32	a	410	CLA	O1A-CGA-O2A-C1
32	b	616	CLA	O1A-CGA-O2A-C1
32	n	603	CLA	O1A-CGA-O2A-C1
32	n	604	CLA	O1A-CGA-O2A-C1
32	r	608	CLA	O1A-CGA-O2A-C1
32	s	604	CLA	O1A-CGA-O2A-C1
32	s	609	CLA	O1A-CGA-O2A-C1
32	CC	504	CLA	O1A-CGA-O2A-C1
32	RR	310	CLA	O1A-CGA-O2A-C1
32	Aa	410	CLA	O1A-CGA-O2A-C1
32	Bb	608	CLA	O1A-CGA-O2A-C1
32	Bb	616	CLA	O1A-CGA-O2A-C1
32	Nn	305	CLA	O1A-CGA-O2A-C1
32	Nn	313	CLA	O1A-CGA-O2A-C1
32	Nn	314	CLA	O1A-CGA-O2A-C1
33	a	408	PHO	O1A-CGA-O2A-C1
33	Aa	408	PHO	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	LL	102	SQD	O10-C23-O48-C46
39	G	601	CHL	O1A-CGA-O2A-C1
39	n	608	CHL	O1A-CGA-O2A-C1
32	Gg	304	CLA	O1D-CGD-O2D-CED
43	RR	301	LMU	O5'-C5'-C6'-O6'
38	Dd	408	LMG	C4-C5-C6-O5
32	Rr	613	CLA	CBD-CGD-O2D-CED
32	2	609	CLA	CBD-CGD-O2D-CED
32	R	614	CLA	CBD-CGD-O2D-CED
32	c	507	CLA	CBD-CGD-O2D-CED
32	n	613	CLA	CBD-CGD-O2D-CED
32	BB	607	CLA	CBD-CGD-O2D-CED
32	CC	505	CLA	CBD-CGD-O2D-CED
32	B	623	CLA	CBD-CGD-O2D-CED
32	YY	604	CLA	CBD-CGD-O2D-CED
32	YY	614	CLA	CBD-CGD-O2D-CED
32	Bb	612	CLA	CBD-CGD-O2D-CED
32	Dd	402	CLA	CBD-CGD-O2D-CED
33	a	409	PHO	CBD-CGD-O2D-CED
33	Aa	409	PHO	CBD-CGD-O2D-CED
39	1	606	CHL	CBD-CGD-O2D-CED
39	N	605	CHL	CBD-CGD-O2D-CED
39	s	607	CHL	CBD-CGD-O2D-CED
39	y	309	CHL	CBD-CGD-O2D-CED
32	Y	610	CLA	O1D-CGD-O2D-CED
32	b	602	CLA	O1D-CGD-O2D-CED
32	BB	608	CLA	O1D-CGD-O2D-CED
39	11	608	CHL	O1D-CGD-O2D-CED
39	22	607	CHL	O1D-CGD-O2D-CED
36	K	101	LHG	O2-C2-C3-O3
36	g	618	LHG	O2-C2-C3-O3
36	y	320	LHG	O2-C2-C3-O3
36	KK	101	LHG	O2-C2-C3-O3
32	C	510	CLA	C3-C5-C6-C7
32	n	610	CLA	C3-C5-C6-C7
32	CC	503	CLA	C3-C5-C6-C7
32	Bb	603	CLA	C3-C5-C6-C7
33	DD	402	PHO	C3-C5-C6-C7
39	NN	607	CHL	C3-C5-C6-C7
32	A	406	CLA	CBA-CGA-O2A-C1
32	Ss	604	CLA	CBA-CGA-O2A-C1
32	Yy	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	C	508	CLA	CBA-CGA-O2A-C1
32	G	610	CLA	CBA-CGA-O2A-C1
32	R	608	CLA	CBA-CGA-O2A-C1
32	Y	614	CLA	CBA-CGA-O2A-C1
32	a	410	CLA	CBA-CGA-O2A-C1
32	b	608	CLA	CBA-CGA-O2A-C1
32	b	609	CLA	CBA-CGA-O2A-C1
32	b	616	CLA	CBA-CGA-O2A-C1
32	c	506	CLA	CBA-CGA-O2A-C1
32	c	510	CLA	CBA-CGA-O2A-C1
32	n	604	CLA	CBA-CGA-O2A-C1
32	n	612	CLA	CBA-CGA-O2A-C1
32	r	602	CLA	CBA-CGA-O2A-C1
32	s	602	CLA	CBA-CGA-O2A-C1
32	CC	506	CLA	CBA-CGA-O2A-C1
32	CC	507	CLA	CBA-CGA-O2A-C1
32	RR	308	CLA	CBA-CGA-O2A-C1
32	YY	612	CLA	CBA-CGA-O2A-C1
32	YY	614	CLA	CBA-CGA-O2A-C1
32	Aa	410	CLA	CBA-CGA-O2A-C1
32	Cc	508	CLA	CBA-CGA-O2A-C1
32	Nn	314	CLA	CBA-CGA-O2A-C1
39	Ss	607	CHL	CBA-CGA-O2A-C1
39	Yy	605	CHL	CBA-CGA-O2A-C1
39	G	601	CHL	CBA-CGA-O2A-C1
39	n	608	CHL	CBA-CGA-O2A-C1
39	s	607	CHL	CBA-CGA-O2A-C1
39	y	307	CHL	CBA-CGA-O2A-C1
39	GG	601	CHL	CBA-CGA-O2A-C1
32	Yy	602	CLA	O1A-CGA-O2A-C1
32	C	508	CLA	O1A-CGA-O2A-C1
32	G	611	CLA	O1A-CGA-O2A-C1
32	a	405	CLA	O1A-CGA-O2A-C1
32	b	608	CLA	O1A-CGA-O2A-C1
32	c	501	CLA	O1A-CGA-O2A-C1
32	c	512	CLA	O1A-CGA-O2A-C1
32	CC	507	CLA	O1A-CGA-O2A-C1
32	B	608	CLA	O1A-CGA-O2A-C1
33	A	407	PHO	O1A-CGA-O2A-C1
33	AA	407	PHO	O1A-CGA-O2A-C1
39	GG	601	CHL	O1A-CGA-O2A-C1
32	33	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	D	401	CLA	O1D-CGD-O2D-CED
32	r	612	CLA	O1D-CGD-O2D-CED
32	s	608	CLA	O1D-CGD-O2D-CED
32	CC	512	CLA	O1D-CGD-O2D-CED
32	B	621	CLA	O1D-CGD-O2D-CED
39	11	605	CHL	O1D-CGD-O2D-CED
36	g	618	LHG	C8-C7-O7-C5
36	KK	101	LHG	C8-C7-O7-C5
38	a	412	LMG	C11-C10-O7-C8
38	Aa	412	LMG	C11-C10-O7-C8
44	BB	624	DGD	C2B-C1B-O2G-C2G
32	b	604	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	CBD-CGD-O2D-CED
39	11	606	CHL	CBD-CGD-O2D-CED
39	1	605	CHL	CBD-CGD-O2D-CED
39	Y	609	CHL	CBD-CGD-O2D-CED
39	YY	605	CHL	CBD-CGD-O2D-CED
32	BB	609	CLA	O1A-CGA-O2A-C1
32	GG	611	CLA	O1A-CGA-O2A-C1
32	B	607	CLA	O1D-CGD-O2D-CED
39	NN	606	CHL	CBD-CGD-O2D-CED
32	Y	612	CLA	C3-C5-C6-C7
32	b	603	CLA	C3-C5-C6-C7
32	Bb	615	CLA	C3-C5-C6-C7
32	R	610	CLA	CBA-CGA-O2A-C1
32	c	509	CLA	CBA-CGA-O2A-C1
32	r	608	CLA	CBA-CGA-O2A-C1
32	s	604	CLA	CBA-CGA-O2A-C1
32	s	609	CLA	CBA-CGA-O2A-C1
32	y	304	CLA	CBA-CGA-O2A-C1
32	Bb	608	CLA	CBA-CGA-O2A-C1
32	Bb	616	CLA	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
33	Aa	408	PHO	CBA-CGA-O2A-C1
32	Yy	611	CLA	O1D-CGD-O2D-CED
32	C	513	CLA	O1D-CGD-O2D-CED
36	KK	101	LHG	O9-C7-O7-C5
43	RR	301	LMU	C4'-C5'-C6'-O6'
32	Y	612	CLA	O1A-CGA-O2A-C1
32	b	609	CLA	O1A-CGA-O2A-C1
32	c	506	CLA	O1A-CGA-O2A-C1
32	c	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	r	602	CLA	O1A-CGA-O2A-C1
32	AA	406	CLA	O1A-CGA-O2A-C1
32	BB	603	CLA	O1A-CGA-O2A-C1
32	BB	612	CLA	O1A-CGA-O2A-C1
32	B	605	CLA	O1A-CGA-O2A-C1
32	YY	603	CLA	O1A-CGA-O2A-C1
32	Cc	514	CLA	O1A-CGA-O2A-C1
39	s	607	CHL	O1A-CGA-O2A-C1
46	Ee	101	HEM	C3D-CAD-CBD-CGD
35	D	407	PL9	C12-C11-C9-C10
35	d	404	PL9	C12-C11-C9-C8
35	d	404	PL9	C13-C14-C16-C17
35	DD	406	PL9	C13-C14-C16-C17
32	BB	606	CLA	CBD-CGD-O2D-CED
32	RR	314	CLA	CBD-CGD-O2D-CED
32	Ss	602	CLA	C2A-CAA-CBA-CGA
32	BB	609	CLA	C2A-CAA-CBA-CGA
39	Ss	605	CHL	C2A-CAA-CBA-CGA
32	Ss	608	CLA	O1D-CGD-O2D-CED
32	33	613	CLA	O1D-CGD-O2D-CED
32	3	603	CLA	O1D-CGD-O2D-CED
39	Ss	605	CHL	O1D-CGD-O2D-CED
32	R	608	CLA	O1A-CGA-O2A-C1
32	Y	614	CLA	O1A-CGA-O2A-C1
32	c	509	CLA	O1A-CGA-O2A-C1
32	n	612	CLA	O1A-CGA-O2A-C1
32	CC	506	CLA	O1A-CGA-O2A-C1
32	B	620	CLA	O1A-CGA-O2A-C1
32	YY	614	CLA	O1A-CGA-O2A-C1
32	Bb	609	CLA	O1A-CGA-O2A-C1
32	Cc	508	CLA	O1A-CGA-O2A-C1
32	Gg	304	CLA	O1A-CGA-O2A-C1
39	n	607	CHL	O1A-CGA-O2A-C1
39	y	307	CHL	O1A-CGA-O2A-C1
37	L	102	SQD	O5-C1-O6-C44
37	LL	101	SQD	O5-C1-O6-C44
38	Aa	412	LMG	O6-C1-O1-C7
32	Bb	615	CLA	O1D-CGD-O2D-CED
35	A	410	PL9	C14-C16-C17-C18
35	A	410	PL9	C34-C36-C37-C38
35	A	410	PL9	C39-C41-C42-C43
35	D	407	PL9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	AA	410	PL9	C9-C11-C12-C13
35	DD	406	PL9	C14-C16-C17-C18
35	DD	406	PL9	C44-C46-C47-C48
32	C	503	CLA	CBA-CGA-O2A-C1
32	g	603	CLA	CBA-CGA-O2A-C1
32	g	614	CLA	CBA-CGA-O2A-C1
32	Cc	505	CLA	CBA-CGA-O2A-C1
32	Cc	511	CLA	CBA-CGA-O2A-C1
32	Gg	311	CLA	CBA-CGA-O2A-C1
32	Gg	315	CLA	CBA-CGA-O2A-C1
39	g	601	CHL	CBA-CGA-O2A-C1
32	Bb	608	CLA	CBD-CGD-O2D-CED
32	33	611	CLA	O1D-CGD-O2D-CED
32	BB	613	CLA	O1D-CGD-O2D-CED
32	CC	504	CLA	O1D-CGD-O2D-CED
32	DD	401	CLA	O1D-CGD-O2D-CED
32	B	609	CLA	O1D-CGD-O2D-CED
32	Bb	602	CLA	O1D-CGD-O2D-CED
32	Cc	510	CLA	O1D-CGD-O2D-CED
32	Nn	302	CLA	O1D-CGD-O2D-CED
39	Yy	605	CHL	O1D-CGD-O2D-CED
32	s	602	CLA	O1A-CGA-O2A-C1
32	RR	308	CLA	O1A-CGA-O2A-C1
39	Yy	605	CHL	O1A-CGA-O2A-C1
32	Rr	601	CLA	O1D-CGD-O2D-CED
32	2	602	CLA	O1D-CGD-O2D-CED
32	Y	611	CLA	O1D-CGD-O2D-CED
32	c	501	CLA	O1D-CGD-O2D-CED
32	BB	603	CLA	O1D-CGD-O2D-CED
32	SS	309	CLA	O1D-CGD-O2D-CED
39	r	605	CHL	O1D-CGD-O2D-CED
32	3	609	CLA	O1D-CGD-O2D-CED
32	S	602	CLA	O1D-CGD-O2D-CED
32	c	508	CLA	O1D-CGD-O2D-CED
39	YY	606	CHL	O1D-CGD-O2D-CED
36	K	101	LHG	C1-C2-C3-O3
36	KK	101	LHG	C1-C2-C3-O3
36	g	618	LHG	O9-C7-O7-C5
32	g	603	CLA	O1A-CGA-O2A-C1
32	g	614	CLA	O1A-CGA-O2A-C1
32	n	602	CLA	O1A-CGA-O2A-C1
32	Cc	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	Cc	511	CLA	O1A-CGA-O2A-C1
32	Gg	315	CLA	O1A-CGA-O2A-C1
39	g	601	CHL	O1A-CGA-O2A-C1
32	N	602	CLA	O1D-CGD-O2D-CED
32	S	610	CLA	O1D-CGD-O2D-CED
32	g	602	CLA	O1D-CGD-O2D-CED
32	B	619	CLA	O1D-CGD-O2D-CED
32	NN	602	CLA	O1D-CGD-O2D-CED
32	Rr	610	CLA	CBA-CGA-O2A-C1
32	Yy	603	CLA	CBA-CGA-O2A-C1
32	Yy	612	CLA	CBA-CGA-O2A-C1
32	Yy	614	CLA	CBA-CGA-O2A-C1
32	C	505	CLA	CBA-CGA-O2A-C1
32	C	506	CLA	CBA-CGA-O2A-C1
32	C	507	CLA	CBA-CGA-O2A-C1
32	D	405	CLA	CBA-CGA-O2A-C1
32	N	613	CLA	CBA-CGA-O2A-C1
32	R	602	CLA	CBA-CGA-O2A-C1
32	S	604	CLA	CBA-CGA-O2A-C1
32	S	610	CLA	CBA-CGA-O2A-C1
32	a	406	CLA	CBA-CGA-O2A-C1
32	b	610	CLA	CBA-CGA-O2A-C1
32	c	502	CLA	CBA-CGA-O2A-C1
32	c	505	CLA	CBA-CGA-O2A-C1
32	g	612	CLA	CBA-CGA-O2A-C1
32	n	602	CLA	CBA-CGA-O2A-C1
32	n	613	CLA	CBA-CGA-O2A-C1
32	r	610	CLA	CBA-CGA-O2A-C1
32	y	314	CLA	CBA-CGA-O2A-C1
32	y	316	CLA	CBA-CGA-O2A-C1
32	BB	602	CLA	CBA-CGA-O2A-C1
32	BB	605	CLA	CBA-CGA-O2A-C1
32	BB	614	CLA	CBA-CGA-O2A-C1
32	CC	502	CLA	CBA-CGA-O2A-C1
32	CC	505	CLA	CBA-CGA-O2A-C1
32	B	610	CLA	CBA-CGA-O2A-C1
32	B	619	CLA	CBA-CGA-O2A-C1
32	B	622	CLA	CBA-CGA-O2A-C1
32	GG	610	CLA	CBA-CGA-O2A-C1
32	NN	613	CLA	CBA-CGA-O2A-C1
32	RR	302	CLA	CBA-CGA-O2A-C1
32	SS	305	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	SS	311	CLA	CBA-CGA-O2A-C1
32	Aa	405	CLA	CBA-CGA-O2A-C1
32	Aa	406	CLA	CBA-CGA-O2A-C1
32	Bb	610	CLA	CBA-CGA-O2A-C1
32	Cc	507	CLA	CBA-CGA-O2A-C1
32	Cc	512	CLA	CBA-CGA-O2A-C1
32	Dd	402	CLA	CBA-CGA-O2A-C1
32	Nn	303	CLA	CBA-CGA-O2A-C1
32	Nn	304	CLA	CBA-CGA-O2A-C1
32	Nn	312	CLA	CBA-CGA-O2A-C1
39	Rr	606	CHL	CBA-CGA-O2A-C1
39	Rr	607	CHL	CBA-CGA-O2A-C1
39	Yy	609	CHL	CBA-CGA-O2A-C1
39	R	605	CHL	CBA-CGA-O2A-C1
39	S	601	CHL	CBA-CGA-O2A-C1
39	Y	608	CHL	CBA-CGA-O2A-C1
39	Y	609	CHL	CBA-CGA-O2A-C1
39	r	607	CHL	CBA-CGA-O2A-C1
39	s	601	CHL	CBA-CGA-O2A-C1
39	y	311	CHL	CBA-CGA-O2A-C1
39	RR	305	CHL	CBA-CGA-O2A-C1
39	YY	608	CHL	CBA-CGA-O2A-C1
39	YY	609	CHL	CBA-CGA-O2A-C1
39	Gg	302	CHL	CBA-CGA-O2A-C1
39	YY	601	CHL	C5-C6-C7-C8
32	44	602	CLA	CBD-CGD-O2D-CED
32	N	611	CLA	CBD-CGD-O2D-CED
32	Cc	509	CLA	CBD-CGD-O2D-CED
39	3	605	CHL	CBD-CGD-O2D-CED
32	S	604	CLA	O1A-CGA-O2A-C1
32	Y	602	CLA	C8-C10-C11-C12
32	b	612	CLA	C13-C15-C16-C17
32	g	603	CLA	C10-C11-C12-C13
32	r	609	CLA	C8-C10-C11-C12
32	BB	605	CLA	C5-C6-C7-C8
32	BB	614	CLA	C10-C11-C12-C13
32	B	610	CLA	C10-C11-C12-C13
32	NN	610	CLA	C5-C6-C7-C8
32	Gg	304	CLA	C10-C11-C12-C13
39	YY	601	CHL	C8-C10-C11-C12
36	BB	622	LHG	O2-C2-C3-O3
36	l	101	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
43	R	618	LMU	C2'-C1'-O1'-C1
32	Yy	603	CLA	O1A-CGA-O2A-C1
32	Yy	612	CLA	O1A-CGA-O2A-C1
32	B	619	CLA	O1A-CGA-O2A-C1
32	Aa	406	CLA	O1A-CGA-O2A-C1
32	Cc	507	CLA	O1A-CGA-O2A-C1
32	Nn	312	CLA	O1A-CGA-O2A-C1
44	C	523	DGD	O6E-C5E-C6E-O5E
35	D	407	PL9	C33-C34-C36-C37
35	Dd	404	PL9	C13-C14-C16-C17
32	C	511	CLA	C11-C12-C13-C14
32	Y	612	CLA	C6-C7-C8-C9
32	b	610	CLA	C6-C7-C8-C9
32	y	314	CLA	C11-C10-C8-C9
32	CC	510	CLA	C11-C12-C13-C14
32	Bb	610	CLA	C6-C7-C8-C9
32	Cc	503	CLA	C6-C7-C8-C9
32	s	602	CLA	O1D-CGD-O2D-CED
32	B	610	CLA	O1D-CGD-O2D-CED
32	B	620	CLA	O1D-CGD-O2D-CED
32	YY	602	CLA	O1D-CGD-O2D-CED
33	AA	407	PHO	O1D-CGD-O2D-CED
39	s	605	CHL	O1D-CGD-O2D-CED
39	y	308	CHL	O1D-CGD-O2D-CED
39	NN	605	CHL	O1D-CGD-O2D-CED
32	D	404	CLA	C4C-C3C-CAC-CBC
32	g	611	CLA	C2A-CAA-CBA-CGA
32	YY	604	CLA	C2A-CAA-CBA-CGA
34	C	516	BCR	C7-C8-C9-C34
34	c	514	BCR	C7-C8-C9-C34
34	h	101	BCR	C7-C8-C9-C34
34	CC	515	BCR	C7-C8-C9-C34
34	Cc	516	BCR	C7-C8-C9-C34
34	Hh	101	BCR	C7-C8-C9-C34
34	A	409	BCR	C21-C22-C23-C24
34	C	516	BCR	C7-C8-C9-C10
34	c	514	BCR	C7-C8-C9-C10
34	h	101	BCR	C7-C8-C9-C10
34	k	101	BCR	C7-C8-C9-C10
34	AA	409	BCR	C21-C22-C23-C24
34	CC	515	BCR	C7-C8-C9-C10
34	Cc	516	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	Hh	101	BCR	C7-C8-C9-C10
36	3	614	LHG	C8-C7-O7-C5
36	Gg	319	LHG	C8-C7-O7-C5
37	BB	621	SQD	C8-C7-O47-C45
44	B	601	DGD	C2B-C1B-O2G-C2G
44	D	411	DGD	C1A-C2A-C3A-C4A
44	BB	623	DGD	C1A-C2A-C3A-C4A
32	C	505	CLA	O1A-CGA-O2A-C1
32	C	507	CLA	O1A-CGA-O2A-C1
32	R	602	CLA	O1A-CGA-O2A-C1
32	c	505	CLA	O1A-CGA-O2A-C1
32	BB	602	CLA	O1A-CGA-O2A-C1
32	CC	505	CLA	O1A-CGA-O2A-C1
32	GG	610	CLA	O1A-CGA-O2A-C1
32	SS	305	CLA	O1A-CGA-O2A-C1
32	Cc	512	CLA	O1A-CGA-O2A-C1
39	Rr	606	CHL	O1A-CGA-O2A-C1
39	R	605	CHL	O1A-CGA-O2A-C1
39	Y	608	CHL	O1A-CGA-O2A-C1
39	r	607	CHL	O1A-CGA-O2A-C1
39	RR	305	CHL	O1A-CGA-O2A-C1
39	Gg	302	CHL	O1A-CGA-O2A-C1
32	BB	606	CLA	C5-C6-C7-C8
32	BB	610	CLA	C10-C11-C12-C13
32	CC	502	CLA	C5-C6-C7-C8
32	B	604	CLA	C5-C6-C7-C8
32	B	606	CLA	C10-C11-C12-C13
32	33	603	CLA	O1D-CGD-O2D-CED
32	3	611	CLA	O1D-CGD-O2D-CED
32	Y	604	CLA	O1D-CGD-O2D-CED
32	Gg	315	CLA	O1D-CGD-O2D-CED
32	Rr	612	CLA	CBA-CGA-O2A-C1
32	N	602	CLA	CBA-CGA-O2A-C1
32	NN	602	CLA	CBA-CGA-O2A-C1
36	N	619	LHG	C24-C23-O8-C6
32	Rr	609	CLA	C8-C10-C11-C12
32	N	610	CLA	C5-C6-C7-C8
32	b	615	CLA	C10-C11-C12-C13
32	c	503	CLA	C10-C11-C12-C13
32	y	312	CLA	C15-C16-C17-C18
32	y	315	CLA	C8-C10-C11-C12
32	YY	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	Bb	603	CLA	C5-C6-C7-C8
32	Bb	615	CLA	C10-C11-C12-C13
32	Cc	504	CLA	C15-C16-C17-C18
32	Cc	512	CLA	C5-C6-C7-C8
39	G	601	CHL	C5-C6-C7-C8
39	n	607	CHL	C15-C16-C17-C18
36	AA	414	LHG	C7-C8-C9-C10
36	II	101	LHG	C7-C8-C9-C10
36	Ll	102	LHG	C7-C8-C9-C10
32	CC	502	CLA	O1A-CGA-O2A-C1
32	DD	403	CLA	C4C-C3C-CAC-CBC
32	Yy	610	CLA	C15-C16-C17-C18
32	Y	612	CLA	C8-C10-C11-C12
32	BB	608	CLA	C5-C6-C7-C8
32	B	623	CLA	C5-C6-C7-C8
32	Bb	612	CLA	C13-C15-C16-C17
32	Cc	505	CLA	C10-C11-C12-C13
39	Yy	601	CHL	C13-C15-C16-C17
39	Yy	609	CHL	C5-C6-C7-C8
39	N	607	CHL	C10-C11-C12-C13
39	Y	601	CHL	C5-C6-C7-C8
39	Y	601	CHL	C8-C10-C11-C12
39	y	303	CHL	C13-C15-C16-C17
39	Nn	317	CHL	C15-C16-C17-C18
32	22	613	CLA	O1D-CGD-O2D-CED
32	3	613	CLA	O1D-CGD-O2D-CED
32	C	512	CLA	O1D-CGD-O2D-CED
32	N	613	CLA	O1A-CGA-O2A-C1
32	a	406	CLA	O1A-CGA-O2A-C1
32	BB	614	CLA	O1A-CGA-O2A-C1
32	Bb	610	CLA	O1A-CGA-O2A-C1
36	C	522	LHG	C7-C8-C9-C10
36	CC	521	LHG	C7-C8-C9-C10
38	b	621	LMG	C10-C11-C12-C13
38	Bb	621	LMG	C10-C11-C12-C13
44	C	523	DGD	C1A-C2A-C3A-C4A
38	c	519	LMG	C4-C5-C6-O5
32	y	315	CLA	CBD-CGD-O2D-CED
32	11	612	CLA	O1D-CGD-O2D-CED
32	C	506	CLA	O1D-CGD-O2D-CED
32	r	603	CLA	O1D-CGD-O2D-CED
32	Yy	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	b	611	CLA	C15-C16-C17-C18
32	Cc	503	CLA	C5-C6-C7-C8
39	y	303	CHL	C10-C11-C12-C13
36	NN	619	LHG	C24-C23-O8-C6
39	SS	302	CHL	CBA-CGA-O2A-C1
32	BB	614	CLA	O1D-CGD-O2D-CED
38	a	412	LMG	O9-C10-O7-C8
38	Aa	412	LMG	O9-C10-O7-C8
44	BB	624	DGD	O1B-C1B-O2G-C2G
32	Ss	611	CLA	C2-C1-O2A-CGA
32	s	611	CLA	C2-C1-O2A-CGA
32	Yy	610	CLA	C5-C6-C7-C8
32	BB	614	CLA	C5-C6-C7-C8
32	Aa	406	CLA	C13-C15-C16-C17
32	Bb	611	CLA	C15-C16-C17-C18
39	Y	601	CHL	C13-C15-C16-C17
39	n	607	CHL	C10-C11-C12-C13
44	Cc	520	DGD	C4D-C5D-C6D-O5D
32	Cc	505	CLA	O1D-CGD-O2D-CED
36	A	414	LHG	C7-C8-C9-C10
37	L	102	SQD	C7-C8-C9-C10
32	Aa	407	CLA	CBD-CGD-O2D-CED
32	Dd	401	CLA	CBD-CGD-O2D-CED
39	Y	606	CHL	CBD-CGD-O2D-CED
39	n	605	CHL	CBD-CGD-O2D-CED
32	Cc	515	CLA	C2A-CAA-CBA-CGA
37	B	617	SQD	C8-C7-O47-C45
38	C	521	LMG	C11-C10-O7-C8
32	b	603	CLA	C5-C6-C7-C8
32	B	610	CLA	C5-C6-C7-C8
32	b	612	CLA	O1D-CGD-O2D-CED
32	Nn	304	CLA	O1D-CGD-O2D-CED
39	N	609	CHL	O1D-CGD-O2D-CED
32	Y	610	CLA	C12-C13-C15-C16
32	b	609	CLA	C11-C12-C13-C15
32	AA	405	CLA	C11-C10-C8-C7
32	CC	510	CLA	C11-C12-C13-C15
32	B	623	CLA	C11-C10-C8-C7
32	Yy	614	CLA	O1A-CGA-O2A-C1
32	g	612	CLA	O1A-CGA-O2A-C1
32	r	610	CLA	O1A-CGA-O2A-C1
32	BB	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	B	622	CLA	O1A-CGA-O2A-C1
32	RR	302	CLA	O1A-CGA-O2A-C1
32	Aa	405	CLA	O1A-CGA-O2A-C1
32	Dd	402	CLA	O1A-CGA-O2A-C1
32	Gg	311	CLA	O1A-CGA-O2A-C1
39	S	601	CHL	O1A-CGA-O2A-C1
39	Y	609	CHL	O1A-CGA-O2A-C1
39	YY	608	CHL	O1A-CGA-O2A-C1
39	YY	609	CHL	O1A-CGA-O2A-C1
36	4	315	LHG	O9-C7-O7-C5
32	a	405	CLA	C2A-CAA-CBA-CGA
32	r	604	CLA	C2A-CAA-CBA-CGA
32	y	306	CLA	C2A-CAA-CBA-CGA
32	CC	511	CLA	C2A-CAA-CBA-CGA
32	B	622	CLA	C2A-CAA-CBA-CGA
39	s	605	CHL	C2A-CAA-CBA-CGA
32	y	304	CLA	O1D-CGD-O2D-CED
32	BB	602	CLA	O1D-CGD-O2D-CED
32	CC	511	CLA	O1D-CGD-O2D-CED
39	Y	605	CHL	O1D-CGD-O2D-CED
39	NN	601	CHL	O1D-CGD-O2D-CED
39	NN	609	CHL	O1D-CGD-O2D-CED
32	c	510	CLA	C5-C6-C7-C8
32	c	511	CLA	C10-C11-C12-C13
32	BB	608	CLA	C15-C16-C17-C18
39	Yy	601	CHL	C10-C11-C12-C13
39	GG	601	CHL	C5-C6-C7-C8
39	Nn	317	CHL	C10-C11-C12-C13
32	Rr	610	CLA	O1A-CGA-O2A-C1
32	D	405	CLA	O1A-CGA-O2A-C1
32	S	610	CLA	O1A-CGA-O2A-C1
32	c	502	CLA	O1A-CGA-O2A-C1
32	n	613	CLA	O1A-CGA-O2A-C1
32	y	314	CLA	O1A-CGA-O2A-C1
32	y	316	CLA	O1A-CGA-O2A-C1
32	B	610	CLA	O1A-CGA-O2A-C1
32	NN	613	CLA	O1A-CGA-O2A-C1
32	SS	311	CLA	O1A-CGA-O2A-C1
32	Nn	303	CLA	O1A-CGA-O2A-C1
39	Rr	607	CHL	O1A-CGA-O2A-C1
39	Yy	609	CHL	O1A-CGA-O2A-C1
39	s	601	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	y	311	CHL	O1A-CGA-O2A-C1
32	Bb	606	CLA	CBD-CGD-O2D-CED
43	KK	102	LMU	O5'-C1'-O1'-C1
32	C	503	CLA	C15-C16-C17-C18
32	C	512	CLA	C10-C11-C12-C13
32	Cc	509	CLA	C10-C11-C12-C13
32	Cc	503	CLA	O1D-CGD-O2D-CED
33	DD	402	PHO	O1D-CGD-O2D-CED
35	A	410	PL9	C29-C31-C32-C33
35	D	407	PL9	C29-C31-C32-C33
35	Dd	404	PL9	C44-C46-C47-C48
32	Ss	602	CLA	O1D-CGD-O2D-CED
32	B	624	CLA	O1D-CGD-O2D-CED
36	1	614	LHG	O2-C2-C3-O3
36	Gg	319	LHG	O9-C7-O7-C5
32	b	613	CLA	C3-C5-C6-C7
32	c	513	CLA	C2A-CAA-CBA-CGA
32	Yy	612	CLA	C10-C11-C12-C13
32	C	506	CLA	C15-C16-C17-C18
32	a	406	CLA	C13-C15-C16-C17
32	c	509	CLA	C10-C11-C12-C13
32	c	512	CLA	C15-C16-C17-C18
32	g	603	CLA	C13-C15-C16-C17
32	y	312	CLA	C5-C6-C7-C8
32	BB	607	CLA	C5-C6-C7-C8
32	CC	502	CLA	C15-C16-C17-C18
32	CC	505	CLA	C15-C16-C17-C18
32	CC	506	CLA	C5-C6-C7-C8
32	B	618	CLA	C10-C11-C12-C13
32	Bb	609	CLA	C5-C6-C7-C8
32	Gg	304	CLA	C13-C15-C16-C17
32	Bb	614	CLA	CBA-CGA-O2A-C1
39	r	606	CHL	CBA-CGA-O2A-C1
32	C	503	CLA	O1A-CGA-O2A-C1
32	C	506	CLA	O1A-CGA-O2A-C1
32	b	610	CLA	O1A-CGA-O2A-C1
32	Nn	304	CLA	O1A-CGA-O2A-C1
39	Yy	606	CHL	O1D-CGD-O2D-CED
32	C	513	CLA	C15-C16-C17-C18
32	b	615	CLA	C5-C6-C7-C8
32	c	507	CLA	C10-C11-C12-C13
32	y	314	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	B	624	CLA	C5-C6-C7-C8
32	Bb	615	CLA	C5-C6-C7-C8
32	Nn	312	CLA	C13-C15-C16-C17
33	a	409	PHO	C10-C11-C12-C13
33	Aa	409	PHO	C10-C11-C12-C13
39	G	601	CHL	C15-C16-C17-C18
39	y	311	CHL	C5-C6-C7-C8
32	d	401	CLA	O1D-CGD-O2D-CED
32	N	602	CLA	O1A-CGA-O2A-C1
32	NN	602	CLA	O1A-CGA-O2A-C1
36	l	101	LHG	C8-C7-O7-C5
44	c	518	DGD	C4D-C5D-C6D-O5D
32	C	507	CLA	C8-C10-C11-C12
32	R	602	CLA	C15-C16-C17-C18
32	b	609	CLA	C5-C6-C7-C8
32	c	502	CLA	C15-C16-C17-C18
32	c	505	CLA	C13-C15-C16-C17
32	B	605	CLA	C10-C11-C12-C13
32	RR	302	CLA	C15-C16-C17-C18
32	Cc	507	CLA	C13-C15-C16-C17
32	Cc	508	CLA	C10-C11-C12-C13
32	Cc	511	CLA	C8-C10-C11-C12
36	A	413	LHG	C3-O3-P-O6
36	Rr	617	LHG	C3-O3-P-O6
36	Rr	617	LHG	C4-O6-P-O3
36	11	614	LHG	C3-O3-P-O6
36	11	614	LHG	C4-O6-P-O3
36	C	522	LHG	C3-O3-P-O6
36	C	522	LHG	C4-O6-P-O3
36	D	410	LHG	C3-O3-P-O6
36	D	410	LHG	C4-O6-P-O3
36	J	101	LHG	C3-O3-P-O6
36	K	101	LHG	C3-O3-P-O6
36	K	101	LHG	C4-O6-P-O3
36	d	405	LHG	C4-O6-P-O3
36	d	406	LHG	C3-O3-P-O6
36	r	616	LHG	C4-O6-P-O3
36	y	320	LHG	C3-O3-P-O6
36	AA	414	LHG	C3-O3-P-O6
36	CC	521	LHG	C4-O6-P-O3
36	CC	523	LHG	C3-O3-P-O6
36	JJ	101	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	KK	101	LHG	C4-O6-P-O3
36	SS	301	LHG	C3-O3-P-O6
36	YY	618	LHG	C4-O6-P-O3
36	Dd	405	LHG	C4-O6-P-O3
36	Dd	406	LHG	C3-O3-P-O6
36	Gg	319	LHG	C3-O3-P-O6
38	m	101	LMG	C10-C11-C12-C13
44	C	519	DGD	C1B-C2B-C3B-C4B
39	y	311	CHL	C3-C5-C6-C7
36	J	101	LHG	O9-C7-O7-C5
32	S	612	CLA	CBA-CGA-O2A-C1
32	b	605	CLA	CBA-CGA-O2A-C1
32	b	614	CLA	CBA-CGA-O2A-C1
32	Bb	605	CLA	CBA-CGA-O2A-C1
39	Y	601	CHL	CBA-CGA-O2A-C1
32	Bb	605	CLA	C10-C11-C12-C13
32	Bb	613	CLA	C13-C15-C16-C17
32	Bb	615	CLA	C13-C15-C16-C17
39	YY	601	CHL	C13-C15-C16-C17
39	SS	302	CHL	O1A-CGA-O2A-C1
39	Ss	607	CHL	O2A-C1-C2-C3
39	s	607	CHL	O2A-C1-C2-C3
32	4	311	CLA	O1D-CGD-O2D-CED
36	Ll	102	LHG	C23-C24-C25-C26
44	Cc	519	DGD	C1B-C2B-C3B-C4B
32	r	613	CLA	O1D-CGD-O2D-CED
32	s	609	CLA	O1D-CGD-O2D-CED
39	Rr	605	CHL	O1D-CGD-O2D-CED
39	R	607	CHL	O1D-CGD-O2D-CED
36	Yy	618	LHG	C1-C2-C3-O3
36	1	614	LHG	C1-C2-C3-O3
36	y	320	LHG	C1-C2-C3-O3
36	3	614	LHG	O9-C7-O7-C5
36	l	101	LHG	O9-C7-O7-C5
37	BB	621	SQD	O49-C7-O47-C45
37	B	617	SQD	O49-C7-O47-C45
38	C	521	LMG	O9-C10-O7-C8
44	B	601	DGD	O1B-C1B-O2G-C2G
35	AA	410	PL9	C25-C24-C26-C27
32	AA	405	CLA	C5-C6-C7-C8
32	G	610	CLA	C2A-CAA-CBA-CGA
39	YY	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	CC	506	CLA	C3-C5-C6-C7
32	C	509	CLA	CBA-CGA-O2A-C1
32	C	514	CLA	CBA-CGA-O2A-C1
32	c	504	CLA	CBA-CGA-O2A-C1
32	g	610	CLA	CBA-CGA-O2A-C1
32	CC	508	CLA	CBA-CGA-O2A-C1
32	SS	303	CLA	CBA-CGA-O2A-C1
32	SS	313	CLA	CBA-CGA-O2A-C1
32	Cc	506	CLA	CBA-CGA-O2A-C1
32	Cc	510	CLA	CBA-CGA-O2A-C1
39	Ss	605	CHL	CBA-CGA-O2A-C1
39	n	605	CHL	CBA-CGA-O2A-C1
39	YY	601	CHL	CBA-CGA-O2A-C1
44	B	601	DGD	C2A-C1A-O1G-C1G
32	b	605	CLA	C10-C11-C12-C13
32	Cc	503	CLA	C13-C15-C16-C17
39	N	601	CHL	O1D-CGD-O2D-CED
36	d	406	LHG	C11-C10-C9-C8
32	Y	614	CLA	O1D-CGD-O2D-CED
32	CC	509	CLA	CBD-CGD-O2D-CED
36	AA	411	LHG	C8-C7-O7-C5
37	L	102	SQD	C8-C7-O47-C45
44	c	517	DGD	C2B-C1B-O2G-C2G
32	Bb	610	CLA	C13-C15-C16-C17
32	Cc	505	CLA	C3-C5-C6-C7
36	d	405	LHG	C28-C29-C30-C31
36	d	406	LHG	C31-C32-C33-C34
36	Dd	405	LHG	C28-C29-C30-C31
36	Dd	407	LHG	C25-C26-C27-C28
37	B	602	SQD	C25-C26-C27-C28
38	Mm	101	LMG	C39-C40-C41-C42
32	Yy	613	CLA	O1D-CGD-O2D-CED
39	4	309	CHL	O1D-CGD-O2D-CED
39	YY	609	CHL	O1D-CGD-O2D-CED
32	b	607	CLA	C16-C17-C18-C20
32	B	605	CLA	C16-C17-C18-C19
32	Bb	607	CLA	C16-C17-C18-C20
32	Gg	313	CLA	CBA-CGA-O2A-C1
44	BB	624	DGD	C2A-C1A-O1G-C1G
36	N	619	LHG	C10-C11-C12-C13
36	Y	618	LHG	C10-C11-C12-C13
36	a	414	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
36	NN	619	LHG	C10-C11-C12-C13
37	CC	501	SQD	C17-C18-C19-C20
44	BB	624	DGD	C7B-C8B-C9B-CAB
36	AA	411	LHG	O9-C7-O7-C5
37	L	102	SQD	O49-C7-O47-C45
32	b	601	CLA	C5-C6-C7-C8
32	Dd	402	CLA	C8-C10-C11-C12
39	GG	601	CHL	C15-C16-C17-C18
39	RR	307	CHL	CBD-CGD-O2D-CED
32	22	609	CLA	O1D-CGD-O2D-CED
32	n	604	CLA	O1D-CGD-O2D-CED
39	1	608	CHL	O1D-CGD-O2D-CED
32	Bb	605	CLA	O1A-CGA-O2A-C1
36	Dd	407	LHG	O6-C4-C5-O7
32	Y	602	CLA	O1D-CGD-O2D-CED
32	BB	607	CLA	O1D-CGD-O2D-CED
39	N	605	CHL	O1D-CGD-O2D-CED
39	s	607	CHL	O1D-CGD-O2D-CED
37	C	501	SQD	C18-C19-C20-C21
37	LL	101	SQD	C7-C8-C9-C10
33	Aa	409	PHO	O1D-CGD-O2D-CED
43	KK	102	LMU	C2'-C1'-O1'-C1
44	CC	522	DGD	C2D-C1D-O3G-C3G
38	Cc	501	LMG	C4-C5-C6-O5
36	Yy	618	LHG	C9-C10-C11-C12
36	Y	618	LHG	C25-C26-C27-C28
36	YY	618	LHG	C25-C26-C27-C28
44	B	601	DGD	C7B-C8B-C9B-CAB
32	b	615	CLA	C13-C15-C16-C17
32	SS	313	CLA	O1A-CGA-O2A-C1
36	N	619	LHG	O10-C23-O8-C6
32	g	611	CLA	C16-C17-C18-C20
32	BB	605	CLA	C16-C17-C18-C20
39	Nn	317	CHL	C16-C17-C18-C20
32	n	613	CLA	O1D-CGD-O2D-CED
32	Bb	612	CLA	O1D-CGD-O2D-CED
32	a	405	CLA	C4-C3-C5-C6
39	n	607	CHL	C4-C3-C5-C6
36	y	320	LHG	C9-C10-C11-C12
32	C	503	CLA	C11-C10-C8-C9
32	D	404	CLA	C14-C13-C15-C16
32	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	c	510	CLA	C11-C12-C13-C14
32	c	511	CLA	C6-C7-C8-C9
32	BB	603	CLA	C14-C13-C15-C16
32	B	620	CLA	C14-C13-C15-C16
32	B	622	CLA	C11-C10-C8-C9
32	Bb	602	CLA	C11-C10-C8-C9
33	a	409	PHO	O1D-CGD-O2D-CED
32	C	510	CLA	CBD-CGD-O2D-CED
44	c	518	DGD	O6D-C5D-C6D-O5D
44	Cc	520	DGD	O6D-C5D-C6D-O5D
38	Mm	101	LMG	C10-C11-C12-C13
36	Yy	618	LHG	C25-C26-C27-C28
37	B	602	SQD	C27-C28-C29-C30
38	m	101	LMG	C39-C40-C41-C42
44	h	102	DGD	C8B-C9B-CAB-CBB
39	NN	607	CHL	C10-C11-C12-C13
32	CC	503	CLA	C2A-CAA-CBA-CGA
39	Yy	601	CHL	C2A-CAA-CBA-CGA
39	Y	601	CHL	C2A-CAA-CBA-CGA
39	y	303	CHL	C2A-CAA-CBA-CGA
32	Rr	612	CLA	O1A-CGA-O2A-C1
36	NN	619	LHG	O10-C23-O8-C6
39	Ss	605	CHL	O1A-CGA-O2A-C1
39	r	606	CHL	O1A-CGA-O2A-C1
34	A	409	BCR	C37-C22-C23-C24
34	k	101	BCR	C7-C8-C9-C34
34	AA	409	BCR	C37-C22-C23-C24
32	RR	314	CLA	C4C-C3C-CAC-CBC
36	G	618	LHG	O1-C1-C2-C3
36	GG	618	LHG	O1-C1-C2-C3
34	H	101	BCR	C21-C22-C23-C24
32	C	511	CLA	C3-C5-C6-C7
32	CC	510	CLA	C3-C5-C6-C7
36	BB	622	LHG	O9-C7-O7-C5
36	CC	521	LHG	O9-C7-O7-C5
38	AA	415	LMG	O9-C10-O7-C8
38	CC	520	LMG	O9-C10-O7-C8
44	c	517	DGD	O1B-C1B-O2G-C2G
32	c	506	CLA	C10-C11-C12-C13
36	A	411	LHG	C8-C7-O7-C5
36	BB	622	LHG	C8-C7-O7-C5
36	CC	521	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
37	CC	501	SQD	C8-C7-O47-C45
37	LL	101	SQD	C8-C7-O47-C45
38	A	415	LMG	C11-C10-O7-C8
38	AA	415	LMG	C11-C10-O7-C8
38	CC	520	LMG	C11-C10-O7-C8
36	y	320	LHG	C25-C26-C27-C28
44	Aa	401	DGD	C2B-C3B-C4B-C5B
32	SS	303	CLA	CBD-CGD-O2D-CED
32	YY	614	CLA	O1D-CGD-O2D-CED
39	1	606	CHL	O1D-CGD-O2D-CED
36	Rr	617	LHG	C9-C10-C11-C12
38	b	620	LMG	C30-C31-C32-C33
44	a	415	DGD	C2B-C3B-C4B-C5B
32	b	607	CLA	C16-C17-C18-C19
32	B	622	CLA	C16-C17-C18-C20
32	Bb	607	CLA	C16-C17-C18-C19
32	YY	604	CLA	O1D-CGD-O2D-CED
35	d	404	PL9	C24-C26-C27-C28
35	DD	406	PL9	C39-C41-C42-C43
35	Dd	404	PL9	C24-C26-C27-C28
36	11	614	LHG	C26-C27-C28-C29
36	DD	408	LHG	C13-C14-C15-C16
36	YY	618	LHG	C13-C14-C15-C16
38	Bb	620	LMG	C30-C31-C32-C33
32	B	622	CLA	C5-C6-C7-C8
32	C	514	CLA	O1A-CGA-O2A-C1
32	b	605	CLA	O1A-CGA-O2A-C1
32	b	614	CLA	O1A-CGA-O2A-C1
32	Bb	614	CLA	O1A-CGA-O2A-C1
32	Cc	506	CLA	O1A-CGA-O2A-C1
39	n	605	CHL	O1A-CGA-O2A-C1
39	YY	601	CHL	O1A-CGA-O2A-C1
36	Ss	616	LHG	C15-C16-C17-C18
36	Yy	618	LHG	C24-C23-O8-C6
36	D	409	LHG	C13-C14-C15-C16
36	Dd	406	LHG	C9-C10-C11-C12
32	2	609	CLA	O1D-CGD-O2D-CED
32	c	507	CLA	O1D-CGD-O2D-CED
32	A	405	CLA	C3A-C2A-CAA-CBA
32	Rr	601	CLA	C3A-C2A-CAA-CBA
32	Rr	604	CLA	C3A-C2A-CAA-CBA
32	Rr	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Rr	612	CLA	C3A-C2A-CAA-CBA
32	Ss	603	CLA	C3A-C2A-CAA-CBA
32	44	603	CLA	C3A-C2A-CAA-CBA
32	44	611	CLA	C3A-C2A-CAA-CBA
32	C	504	CLA	C3A-C2A-CAA-CBA
32	C	505	CLA	C3A-C2A-CAA-CBA
32	G	602	CLA	C3A-C2A-CAA-CBA
32	R	604	CLA	C3A-C2A-CAA-CBA
32	R	611	CLA	C3A-C2A-CAA-CBA
32	a	405	CLA	C3A-C2A-CAA-CBA
32	b	616	CLA	C3A-C2A-CAA-CBA
32	c	510	CLA	C3A-C2A-CAA-CBA
32	d	401	CLA	C3A-C2A-CAA-CBA
32	n	603	CLA	C3A-C2A-CAA-CBA
32	n	613	CLA	C3A-C2A-CAA-CBA
32	r	601	CLA	C3A-C2A-CAA-CBA
32	r	610	CLA	C3A-C2A-CAA-CBA
32	r	611	CLA	C3A-C2A-CAA-CBA
32	s	603	CLA	C3A-C2A-CAA-CBA
32	4	312	CLA	C3A-C2A-CAA-CBA
32	AA	405	CLA	C3A-C2A-CAA-CBA
32	CC	503	CLA	C3A-C2A-CAA-CBA
32	CC	504	CLA	C3A-C2A-CAA-CBA
32	RR	304	CLA	C3A-C2A-CAA-CBA
32	RR	311	CLA	C3A-C2A-CAA-CBA
32	SS	305	CLA	C3A-C2A-CAA-CBA
32	Aa	405	CLA	C3A-C2A-CAA-CBA
32	Bb	616	CLA	C3A-C2A-CAA-CBA
32	Cc	512	CLA	C3A-C2A-CAA-CBA
32	Cc	515	CLA	C3A-C2A-CAA-CBA
32	Dd	401	CLA	C3A-C2A-CAA-CBA
32	Gg	312	CLA	C3A-C2A-CAA-CBA
32	Nn	304	CLA	C3A-C2A-CAA-CBA
32	Nn	313	CLA	C3A-C2A-CAA-CBA
39	Rr	605	CHL	C3A-C2A-CAA-CBA
39	Ss	605	CHL	C3A-C2A-CAA-CBA
39	Ss	606	CHL	C3A-C2A-CAA-CBA
39	44	607	CHL	C3A-C2A-CAA-CBA
39	44	608	CHL	C3A-C2A-CAA-CBA
39	Y	606	CHL	C3A-C2A-CAA-CBA
39	n	605	CHL	C3A-C2A-CAA-CBA
39	r	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	s	606	CHL	C3A-C2A-CAA-CBA
39	4	308	CHL	C3A-C2A-CAA-CBA
39	4	309	CHL	C3A-C2A-CAA-CBA
39	YY	606	CHL	C3A-C2A-CAA-CBA
39	Nn	315	CHL	C3A-C2A-CAA-CBA
39	Nn	317	CHL	C3A-C2A-CAA-CBA
37	Aa	413	SQD	C25-C26-C27-C28
32	Rr	613	CLA	O1D-CGD-O2D-CED
32	R	614	CLA	O1D-CGD-O2D-CED
32	S	612	CLA	O1A-CGA-O2A-C1
32	SS	303	CLA	O1A-CGA-O2A-C1
39	n	607	CHL	C16-C17-C18-C20
32	D	404	CLA	C2C-C3C-CAC-CBC
32	CC	505	CLA	O1D-CGD-O2D-CED
32	Dd	402	CLA	O1D-CGD-O2D-CED
38	A	415	LMG	O9-C10-O7-C8
37	l	102	SQD	C11-C10-C9-C8
37	Ll	101	SQD	C11-C10-C9-C8
32	c	501	CLA	O2A-C1-C2-C3
32	Bb	613	CLA	C3-C5-C6-C7
36	Nn	310	LHG	C23-C24-C25-C26
44	c	517	DGD	C1B-C2B-C3B-C4B
32	Nn	312	CLA	C8-C10-C11-C12
32	GG	611	CLA	C4-C3-C5-C6
32	a	407	CLA	CBA-CGA-O2A-C1
32	a	405	CLA	C2-C3-C5-C6
32	GG	611	CLA	C2-C3-C5-C6
39	n	607	CHL	C2-C3-C5-C6
36	11	614	LHG	C8-C7-O7-C5
36	D	410	LHG	C8-C7-O7-C5
37	L	101	SQD	C8-C7-O47-C45
37	AA	412	SQD	C8-C7-O47-C45
37	LL	102	SQD	C8-C7-O47-C45
38	c	519	LMG	C11-C10-O7-C8
38	Cc	501	LMG	C11-C10-O7-C8
38	Dd	408	LMG	C11-C10-O7-C8
44	Cc	519	DGD	C2B-C1B-O2G-C2G
32	b	606	CLA	O1D-CGD-O2D-CED
43	RR	301	LMU	O1'-C1-C2-C3
32	CC	511	CLA	C10-C11-C12-C13
32	c	504	CLA	O1A-CGA-O2A-C1
32	Gg	313	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	Y	601	CHL	O1A-CGA-O2A-C1
44	B	601	DGD	O1A-C1A-O1G-C1G
32	B	605	CLA	C16-C17-C18-C20
32	Cc	503	CLA	C16-C17-C18-C20
36	YY	618	LHG	C10-C11-C12-C13
32	c	511	CLA	C5-C6-C7-C8
32	BB	609	CLA	C10-C11-C12-C13
32	Bb	611	CLA	C10-C11-C12-C13
32	B	621	CLA	CBA-CGA-O2A-C1
37	Aa	413	SQD	C27-C28-C29-C30
32	C	509	CLA	O1A-CGA-O2A-C1
32	g	610	CLA	O1A-CGA-O2A-C1
32	CC	508	CLA	O1A-CGA-O2A-C1
32	Cc	510	CLA	O1A-CGA-O2A-C1
39	Yy	601	CHL	C8-C10-C11-C12
39	3	607	CHL	CBD-CGD-O2D-CED
38	c	519	LMG	O6-C5-C6-O5
38	Mm	101	LMG	C12-C13-C14-C15
36	A	411	LHG	O9-C7-O7-C5
36	11	614	LHG	O9-C7-O7-C5
36	D	410	LHG	O9-C7-O7-C5
36	JJ	101	LHG	O9-C7-O7-C5
37	CC	501	SQD	O49-C7-O47-C45
37	LL	101	SQD	O49-C7-O47-C45
37	LL	102	SQD	O49-C7-O47-C45
38	c	519	LMG	O9-C10-O7-C8
38	j	101	LMG	O9-C10-O7-C8
38	Cc	501	LMG	O9-C10-O7-C8
38	Dd	408	LMG	O9-C10-O7-C8
44	Cc	519	DGD	O1B-C1B-O2G-C2G
32	CC	510	CLA	C2-C1-O2A-CGA
32	Cc	514	CLA	C15-C16-C17-C18
44	BB	624	DGD	O1A-C1A-O1G-C1G
36	y	320	LHG	C7-C8-C9-C10
34	A	409	BCR	C1-C6-C7-C8
34	A	409	BCR	C5-C6-C7-C8
34	A	409	BCR	C23-C24-C25-C26
34	C	516	BCR	C5-C6-C7-C8
34	C	516	BCR	C23-C24-C25-C30
34	C	517	BCR	C1-C6-C7-C8
34	C	517	BCR	C5-C6-C7-C8
34	C	517	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
34	C	518	BCR	C23-C24-C25-C26
34	C	518	BCR	C23-C24-C25-C30
34	D	406	BCR	C23-C24-C25-C26
34	D	406	BCR	C23-C24-C25-C30
34	K	102	BCR	C5-C6-C7-C8
34	T	101	BCR	C23-C24-C25-C26
34	a	411	BCR	C1-C6-C7-C8
34	a	411	BCR	C23-C24-C25-C26
34	a	411	BCR	C23-C24-C25-C30
34	b	617	BCR	C1-C6-C7-C8
34	b	618	BCR	C1-C6-C7-C8
34	b	618	BCR	C5-C6-C7-C8
34	b	618	BCR	C23-C24-C25-C26
34	b	618	BCR	C23-C24-C25-C30
34	b	619	BCR	C1-C6-C7-C8
34	b	619	BCR	C5-C6-C7-C8
34	b	619	BCR	C23-C24-C25-C26
34	c	514	BCR	C5-C6-C7-C8
34	c	515	BCR	C1-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C30
34	c	516	BCR	C23-C24-C25-C26
34	d	403	BCR	C1-C6-C7-C8
34	d	403	BCR	C23-C24-C25-C30
34	h	101	BCR	C23-C24-C25-C26
34	h	101	BCR	C23-C24-C25-C30
34	k	101	BCR	C1-C6-C7-C8
34	k	101	BCR	C5-C6-C7-C8
34	k	101	BCR	C23-C24-C25-C26
34	k	101	BCR	C23-C24-C25-C30
34	AA	409	BCR	C1-C6-C7-C8
34	AA	409	BCR	C5-C6-C7-C8
34	BB	616	BCR	C1-C6-C7-C8
34	BB	616	BCR	C5-C6-C7-C8
34	BB	617	BCR	C1-C6-C7-C8
34	BB	617	BCR	C5-C6-C7-C8
34	BB	617	BCR	C23-C24-C25-C26
34	BB	617	BCR	C23-C24-C25-C30
34	BB	618	BCR	C1-C6-C7-C8
34	BB	618	BCR	C5-C6-C7-C8
34	BB	618	BCR	C23-C24-C25-C26
34	BB	620	BCR	C1-C6-C7-C8
34	BB	620	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	BB	620	BCR	C23-C24-C25-C30
34	CC	515	BCR	C5-C6-C7-C8
34	CC	515	BCR	C23-C24-C25-C30
34	CC	516	BCR	C1-C6-C7-C8
34	CC	516	BCR	C5-C6-C7-C8
34	CC	516	BCR	C23-C24-C25-C30
34	CC	517	BCR	C23-C24-C25-C26
34	CC	517	BCR	C23-C24-C25-C30
34	DD	405	BCR	C23-C24-C25-C26
34	DD	405	BCR	C23-C24-C25-C30
34	B	612	BCR	C1-C6-C7-C8
34	B	612	BCR	C5-C6-C7-C8
34	B	613	BCR	C1-C6-C7-C8
34	B	613	BCR	C5-C6-C7-C8
34	B	613	BCR	C23-C24-C25-C26
34	B	613	BCR	C23-C24-C25-C30
34	B	614	BCR	C1-C6-C7-C8
34	B	614	BCR	C5-C6-C7-C8
34	B	614	BCR	C23-C24-C25-C26
34	B	616	BCR	C1-C6-C7-C8
34	B	616	BCR	C5-C6-C7-C8
34	KK	103	BCR	C5-C6-C7-C8
34	TT	101	BCR	C23-C24-C25-C26
34	XX	202	BCR	C23-C24-C25-C26
34	XX	202	BCR	C23-C24-C25-C30
34	Aa	411	BCR	C1-C6-C7-C8
34	Aa	411	BCR	C23-C24-C25-C26
34	Aa	411	BCR	C23-C24-C25-C30
34	Bb	617	BCR	C1-C6-C7-C8
34	Bb	617	BCR	C5-C6-C7-C8
34	Bb	618	BCR	C1-C6-C7-C8
34	Bb	618	BCR	C5-C6-C7-C8
34	Bb	618	BCR	C23-C24-C25-C26
34	Bb	618	BCR	C23-C24-C25-C30
34	Bb	619	BCR	C5-C6-C7-C8
34	Cc	516	BCR	C5-C6-C7-C8
34	Cc	517	BCR	C1-C6-C7-C8
34	Cc	517	BCR	C23-C24-C25-C30
34	Cc	518	BCR	C23-C24-C25-C26
34	Dd	403	BCR	C1-C6-C7-C8
34	Dd	403	BCR	C23-C24-C25-C30
34	Hh	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
34	Hh	101	BCR	C23-C24-C25-C30
34	Kk	101	BCR	C1-C6-C7-C8
40	Rr	614	LUT	C5-C6-C7-C8
40	Ss	614	LUT	C5-C6-C7-C8
40	Yy	615	LUT	C5-C6-C7-C8
40	Yy	616	LUT	C5-C6-C7-C8
40	44	612	LUT	C5-C6-C7-C8
40	22	614	LUT	C5-C6-C7-C8
40	2	614	LUT	C5-C6-C7-C8
40	G	615	LUT	C5-C6-C7-C8
40	G	616	LUT	C1-C6-C7-C8
40	G	616	LUT	C5-C6-C7-C8
40	N	615	LUT	C5-C6-C7-C8
40	N	616	LUT	C5-C6-C7-C8
40	S	614	LUT	C5-C6-C7-C8
40	Y	615	LUT	C5-C6-C7-C8
40	Y	616	LUT	C1-C6-C7-C8
40	Y	616	LUT	C5-C6-C7-C8
40	g	615	LUT	C5-C6-C7-C8
40	g	616	LUT	C5-C6-C7-C8
40	n	616	LUT	C5-C6-C7-C8
40	r	614	LUT	C5-C6-C7-C8
40	s	614	LUT	C5-C6-C7-C8
40	s	615	LUT	C5-C6-C7-C8
40	y	317	LUT	C5-C6-C7-C8
40	y	318	LUT	C5-C6-C7-C8
40	4	313	LUT	C1-C6-C7-C8
40	4	313	LUT	C5-C6-C7-C8
40	GG	615	LUT	C5-C6-C7-C8
40	GG	616	LUT	C5-C6-C7-C8
40	NN	615	LUT	C5-C6-C7-C8
40	NN	616	LUT	C5-C6-C7-C8
40	RR	315	LUT	C5-C6-C7-C8
40	SS	315	LUT	C5-C6-C7-C8
40	YY	615	LUT	C5-C6-C7-C8
40	YY	616	LUT	C5-C6-C7-C8
40	Gg	316	LUT	C5-C6-C7-C8
40	Gg	317	LUT	C5-C6-C7-C8
40	Nn	307	LUT	C1-C6-C7-C8
40	Nn	307	LUT	C5-C6-C7-C8
32	Rr	602	CLA	CBA-CGA-O2A-C1
32	Ss	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	d	402	CLA	CBA-CGA-O2A-C1
32	s	603	CLA	CBA-CGA-O2A-C1
32	CC	513	CLA	CBA-CGA-O2A-C1
32	YY	613	CLA	CBA-CGA-O2A-C1
32	Aa	407	CLA	CBA-CGA-O2A-C1
39	Yy	601	CHL	CBA-CGA-O2A-C1
32	BB	611	CLA	C5-C6-C7-C8
32	B	623	CLA	C10-C11-C12-C13
32	YY	610	CLA	C5-C6-C7-C8
32	Cc	511	CLA	C10-C11-C12-C13
36	II	101	LHG	C8-C7-O7-C5
36	JJ	101	LHG	C8-C7-O7-C5
36	Dd	405	LHG	C8-C7-O7-C5
44	BB	625	DGD	C2B-C1B-O2G-C2G
44	B	603	DGD	C2B-C1B-O2G-C2G
39	y	309	CHL	O1D-CGD-O2D-CED
32	c	510	CLA	CBD-CGD-O2D-CED
43	C	502	LMU	O1'-C1-C2-C3
39	YY	605	CHL	O1D-CGD-O2D-CED
32	C	503	CLA	C11-C10-C8-C7
32	C	511	CLA	C11-C12-C13-C15
32	C	513	CLA	C6-C7-C8-C10
32	D	401	CLA	C11-C12-C13-C15
32	D	404	CLA	C6-C7-C8-C10
32	D	404	CLA	C12-C13-C15-C16
32	N	610	CLA	C11-C12-C13-C15
32	b	602	CLA	C11-C10-C8-C7
32	b	607	CLA	C11-C10-C8-C7
32	b	612	CLA	C6-C7-C8-C10
32	c	510	CLA	C11-C12-C13-C15
32	c	511	CLA	C6-C7-C8-C10
32	y	312	CLA	C11-C12-C13-C15
32	BB	606	CLA	C11-C10-C8-C7
32	DD	401	CLA	C11-C12-C13-C15
32	B	618	CLA	C6-C7-C8-C10
32	B	620	CLA	C12-C13-C15-C16
32	B	622	CLA	C11-C10-C8-C7
32	NN	610	CLA	C11-C12-C13-C15
32	Bb	602	CLA	C11-C10-C8-C7
32	Bb	607	CLA	C11-C10-C8-C7
32	Bb	608	CLA	C11-C12-C13-C15
32	Bb	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	Bb	612	CLA	C6-C7-C8-C10
39	n	607	CHL	C6-C7-C8-C10
32	a	407	CLA	O1A-CGA-O2A-C1
32	CC	512	CLA	C5-C6-C7-C8
32	Cc	509	CLA	C13-C15-C16-C17
32	B	623	CLA	O1D-CGD-O2D-CED
39	l	605	CHL	O1D-CGD-O2D-CED
39	Y	609	CHL	O1D-CGD-O2D-CED
36	Ll	102	LHG	O9-C7-O7-C5
37	L	101	SQD	O49-C7-O47-C45
38	B	615	LMG	O9-C10-O7-C8
32	C	510	CLA	CBA-CGA-O2A-C1
32	BB	604	CLA	CBA-CGA-O2A-C1
32	CC	509	CLA	CBA-CGA-O2A-C1
36	YY	618	LHG	C24-C23-O8-C6
39	Yy	608	CHL	CBA-CGA-O2A-C1
39	y	303	CHL	CBA-CGA-O2A-C1
39	y	310	CHL	CBA-CGA-O2A-C1
44	CC	522	DGD	C3B-C4B-C5B-C6B
32	Rr	602	CLA	C2A-CAA-CBA-CGA
32	c	501	CLA	C2A-CAA-CBA-CGA
32	c	505	CLA	C2A-CAA-CBA-CGA
32	c	510	CLA	C2A-CAA-CBA-CGA
32	r	610	CLA	C2A-CAA-CBA-CGA
32	4	305	CLA	C2A-CAA-CBA-CGA
32	CC	506	CLA	C2A-CAA-CBA-CGA
32	SS	313	CLA	C2A-CAA-CBA-CGA
32	YY	613	CLA	C2A-CAA-CBA-CGA
39	ll	606	CHL	O1D-CGD-O2D-CED
32	b	613	CLA	C13-C15-C16-C17
32	c	501	CLA	C13-C15-C16-C17
32	b	604	CLA	O1D-CGD-O2D-CED
44	D	411	DGD	C1B-C2B-C3B-C4B
32	44	602	CLA	O1D-CGD-O2D-CED
32	A	405	CLA	C5-C6-C7-C8
32	DD	403	CLA	C2C-C3C-CAC-CBC
32	RR	314	CLA	C2C-C3C-CAC-CBC
32	NN	602	CLA	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
39	NN	606	CHL	O1D-CGD-O2D-CED
36	Y	618	LHG	C13-C14-C15-C16
32	CC	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	Aa	407	CLA	O1A-CGA-O2A-C1
33	D	402	PHO	CBA-CGA-O2A-C1
32	Gg	312	CLA	C16-C17-C18-C20
37	CC	501	SQD	O5-C1-O6-C44
38	a	412	LMG	O6-C1-O1-C7
32	Rr	602	CLA	C15-C16-C17-C18
32	NN	602	CLA	C8-C10-C11-C12
39	y	303	CHL	C8-C10-C11-C12
32	Bb	608	CLA	O1D-CGD-O2D-CED
39	n	605	CHL	O1D-CGD-O2D-CED
35	D	407	PL9	C44-C46-C47-C48
35	d	404	PL9	C19-C21-C22-C23
36	33	614	LHG	C8-C7-O7-C5
36	K	101	LHG	C8-C7-O7-C5
36	d	405	LHG	C8-C7-O7-C5
36	Ll	102	LHG	C8-C7-O7-C5
37	A	412	SQD	C8-C7-O47-C45
38	j	101	LMG	C11-C10-O7-C8
38	BB	619	LMG	C11-C10-O7-C8
38	B	615	LMG	C11-C10-O7-C8
36	44	616	LHG	O6-C4-C5-O7
36	a	414	LHG	O6-C4-C5-O7
32	Rr	602	CLA	C8-C10-C11-C12
32	b	612	CLA	C8-C10-C11-C12
32	BB	606	CLA	C10-C11-C12-C13
32	Bb	612	CLA	C8-C10-C11-C12
38	C	521	LMG	C35-C36-C37-C38
36	d	405	LHG	O9-C7-O7-C5
37	AA	412	SQD	O49-C7-O47-C45
38	BB	619	LMG	O9-C10-O7-C8
37	CC	501	SQD	C2-C1-O6-C44
37	C	501	SQD	O47-C45-C46-O48
44	CC	519	DGD	O6E-C5E-C6E-O5E
32	c	513	CLA	CBD-CGD-O2D-CED
32	d	402	CLA	O1A-CGA-O2A-C1
32	YY	613	CLA	O1A-CGA-O2A-C1
43	KK	102	LMU	C3'-C4'-O1B-C1B
32	Yy	602	CLA	C10-C11-C12-C13
32	n	602	CLA	C8-C10-C11-C12
32	r	609	CLA	C15-C16-C17-C18
32	Bb	607	CLA	C5-C6-C7-C8
32	Cc	503	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	Bb	613	CLA	C4-C3-C5-C6
35	AA	410	PL9	C15-C14-C16-C17
37	B	602	SQD	C7-C8-C9-C10
32	B	622	CLA	C2-C3-C5-C6
32	Bb	613	CLA	C2-C3-C5-C6
35	D	407	PL9	C4-C3-C7-C8
35	DD	406	PL9	C4-C3-C7-C8
32	Rr	602	CLA	C6-C7-C8-C9
32	Yy	602	CLA	C11-C10-C8-C9
32	Yy	610	CLA	C11-C12-C13-C14
32	Yy	612	CLA	C11-C12-C13-C14
32	D	401	CLA	C11-C12-C13-C14
32	D	404	CLA	C6-C7-C8-C9
32	N	610	CLA	C11-C12-C13-C14
32	Y	610	CLA	C14-C13-C15-C16
32	b	607	CLA	C11-C10-C8-C9
32	b	609	CLA	C11-C12-C13-C14
32	b	613	CLA	C6-C7-C8-C9
32	c	503	CLA	C11-C10-C8-C9
32	d	401	CLA	C11-C12-C13-C14
32	AA	405	CLA	C11-C10-C8-C9
32	BB	605	CLA	C14-C13-C15-C16
32	BB	606	CLA	C11-C10-C8-C9
32	BB	611	CLA	C6-C7-C8-C9
32	DD	401	CLA	C11-C12-C13-C14
32	B	604	CLA	C11-C12-C13-C14
32	B	607	CLA	C6-C7-C8-C9
32	B	618	CLA	C6-C7-C8-C9
32	B	623	CLA	C11-C10-C8-C9
32	NN	610	CLA	C11-C12-C13-C14
32	Bb	607	CLA	C11-C10-C8-C9
32	Bb	610	CLA	C14-C13-C15-C16
32	Bb	613	CLA	C6-C7-C8-C9
32	Dd	401	CLA	C11-C12-C13-C14
39	n	607	CHL	C6-C7-C8-C9
39	y	303	CHL	C11-C12-C13-C14
39	Nn	317	CHL	C6-C7-C8-C9
32	RR	314	CLA	O1D-CGD-O2D-CED
32	Rr	602	CLA	O1A-CGA-O2A-C1
38	m	101	LMG	C12-C13-C14-C15
33	Aa	408	PHO	C3-C5-C6-C7
32	C	512	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	S	612	CLA	C2A-CAA-CBA-CGA
32	b	612	CLA	C2A-CAA-CBA-CGA
32	Cc	507	CLA	C2A-CAA-CBA-CGA
39	Nn	318	CHL	C2A-CAA-CBA-CGA
44	C	520	DGD	O6E-C5E-C6E-O5E
33	DD	402	PHO	CBA-CGA-O2A-C1
36	Dd	406	LHG	C24-C23-O8-C6
34	H	101	BCR	C37-C22-C23-C24
32	n	602	CLA	C13-C15-C16-C17
44	C	519	DGD	C5A-C6A-C7A-C8A
32	Ss	603	CLA	O1A-CGA-O2A-C1
32	s	603	CLA	O1A-CGA-O2A-C1
32	B	621	CLA	O1A-CGA-O2A-C1
36	Yy	618	LHG	O10-C23-O8-C6
39	Yy	601	CHL	O1A-CGA-O2A-C1
32	A	405	CLA	C1A-C2A-CAA-CBA
32	Rr	601	CLA	C1A-C2A-CAA-CBA
32	Rr	611	CLA	C1A-C2A-CAA-CBA
32	Rr	613	CLA	C1A-C2A-CAA-CBA
32	Ss	603	CLA	C1A-C2A-CAA-CBA
32	Ss	608	CLA	C1A-C2A-CAA-CBA
32	Yy	614	CLA	C1A-C2A-CAA-CBA
32	44	611	CLA	C1A-C2A-CAA-CBA
32	C	505	CLA	C1A-C2A-CAA-CBA
32	C	510	CLA	C1A-C2A-CAA-CBA
32	G	602	CLA	C1A-C2A-CAA-CBA
32	G	611	CLA	C1A-C2A-CAA-CBA
32	R	602	CLA	C1A-C2A-CAA-CBA
32	R	604	CLA	C1A-C2A-CAA-CBA
32	R	611	CLA	C1A-C2A-CAA-CBA
32	Y	604	CLA	C1A-C2A-CAA-CBA
32	Y	614	CLA	C1A-C2A-CAA-CBA
32	a	405	CLA	C1A-C2A-CAA-CBA
32	b	601	CLA	C1A-C2A-CAA-CBA
32	b	616	CLA	C1A-C2A-CAA-CBA
32	c	503	CLA	C1A-C2A-CAA-CBA
32	c	510	CLA	C1A-C2A-CAA-CBA
32	d	401	CLA	C1A-C2A-CAA-CBA
32	d	402	CLA	C1A-C2A-CAA-CBA
32	n	603	CLA	C1A-C2A-CAA-CBA
32	r	601	CLA	C1A-C2A-CAA-CBA
32	r	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	r	611	CLA	C1A-C2A-CAA-CBA
32	s	603	CLA	C1A-C2A-CAA-CBA
32	y	316	CLA	C1A-C2A-CAA-CBA
32	4	312	CLA	C1A-C2A-CAA-CBA
32	AA	405	CLA	C1A-C2A-CAA-CBA
32	BB	602	CLA	C1A-C2A-CAA-CBA
32	BB	604	CLA	C1A-C2A-CAA-CBA
32	BB	608	CLA	C1A-C2A-CAA-CBA
32	CC	504	CLA	C1A-C2A-CAA-CBA
32	CC	509	CLA	C1A-C2A-CAA-CBA
32	B	619	CLA	C1A-C2A-CAA-CBA
32	B	621	CLA	C1A-C2A-CAA-CBA
32	GG	611	CLA	C1A-C2A-CAA-CBA
32	RR	304	CLA	C1A-C2A-CAA-CBA
32	RR	311	CLA	C1A-C2A-CAA-CBA
32	SS	303	CLA	C1A-C2A-CAA-CBA
32	YY	614	CLA	C1A-C2A-CAA-CBA
32	Bb	601	CLA	C1A-C2A-CAA-CBA
32	Bb	616	CLA	C1A-C2A-CAA-CBA
32	Cc	504	CLA	C1A-C2A-CAA-CBA
32	Cc	512	CLA	C1A-C2A-CAA-CBA
32	Dd	401	CLA	C1A-C2A-CAA-CBA
32	Nn	313	CLA	C1A-C2A-CAA-CBA
38	F	101	LMG	O6-C5-C6-O5
38	DD	409	LMG	O6-C5-C6-O5
39	44	607	CHL	C1A-C2A-CAA-CBA
39	R	606	CHL	C1A-C2A-CAA-CBA
39	Y	606	CHL	C1A-C2A-CAA-CBA
39	n	605	CHL	C1A-C2A-CAA-CBA
39	4	308	CHL	C1A-C2A-CAA-CBA
39	4	309	CHL	C1A-C2A-CAA-CBA
39	RR	305	CHL	C1A-C2A-CAA-CBA
39	YY	606	CHL	C1A-C2A-CAA-CBA
39	Nn	315	CHL	C1A-C2A-CAA-CBA
32	Bb	601	CLA	C16-C17-C18-C20
32	Gg	312	CLA	C16-C17-C18-C19
36	33	614	LHG	O9-C7-O7-C5
36	K	101	LHG	O9-C7-O7-C5
36	II	101	LHG	O9-C7-O7-C5
36	Dd	405	LHG	O9-C7-O7-C5
36	Y	618	LHG	C11-C12-C13-C14
32	Yy	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	CC	505	CLA	C8-C10-C11-C12
32	B	622	CLA	C8-C10-C11-C12
32	YY	602	CLA	C5-C6-C7-C8
32	Bb	604	CLA	C10-C11-C12-C13
32	Bb	611	CLA	C5-C6-C7-C8
36	1	614	LHG	C3-O3-P-O6
36	1	614	LHG	C4-O6-P-O3
36	4	301	LHG	C3-O3-P-O6
36	BB	622	LHG	C4-O6-P-O3
36	Yy	618	LHG	C7-C8-C9-C10
37	Aa	413	SQD	C7-C8-C9-C10
32	N	611	CLA	O1D-CGD-O2D-CED
32	BB	606	CLA	O1D-CGD-O2D-CED
32	c	507	CLA	C13-C15-C16-C17
32	n	614	CLA	CBA-CGA-O2A-C1
36	Y	618	LHG	C24-C23-O8-C6
36	Yy	618	LHG	O6-C4-C5-C6
36	Y	618	LHG	O6-C4-C5-C6
36	a	414	LHG	O6-C4-C5-C6
36	y	320	LHG	O6-C4-C5-C6
36	YY	618	LHG	O6-C4-C5-C6
36	Dd	407	LHG	O6-C4-C5-C6
35	d	404	PL9	C42-C43-C44-C45
35	Dd	404	PL9	C12-C13-C14-C15
38	Cc	501	LMG	C28-C29-C30-C31
43	KK	102	LMU	C5'-C4'-O1B-C1B
32	b	611	CLA	C5-C6-C7-C8
32	g	611	CLA	C5-C6-C7-C8
32	g	611	CLA	C16-C17-C18-C19
32	BB	605	CLA	C16-C17-C18-C19
32	B	606	CLA	C16-C17-C18-C19
32	B	622	CLA	C16-C17-C18-C19
36	J	101	LHG	C24-C25-C26-C27
44	BB	623	DGD	C3B-C4B-C5B-C6B
32	Yy	610	CLA	C13-C15-C16-C17
32	B	608	CLA	C10-C11-C12-C13
39	N	601	CHL	C2A-CAA-CBA-CGA
32	b	607	CLA	CBA-CGA-O2A-C1
38	BB	619	LMG	O6-C5-C6-O5
38	B	615	LMG	O6-C5-C6-O5
44	h	102	DGD	O6E-C5E-C6E-O5E
44	BB	625	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
32	B	622	CLA	C4-C3-C5-C6
35	d	404	PL9	C30-C29-C31-C32
35	A	410	PL9	C38-C39-C41-C42
39	g	605	CHL	C3A-C2A-CAA-CBA
39	Gg	306	CHL	C3A-C2A-CAA-CBA
38	C	521	LMG	C32-C33-C34-C35
32	b	611	CLA	C10-C11-C12-C13
32	Cc	509	CLA	O1D-CGD-O2D-CED
44	BB	623	DGD	O6E-C5E-C6E-O5E
32	C	510	CLA	O1A-CGA-O2A-C1
33	D	402	PHO	O1A-CGA-O2A-C1
36	AA	411	LHG	C10-C11-C12-C13
44	Hh	102	DGD	C5A-C6A-C7A-C8A
32	44	604	CLA	C2A-CAA-CBA-CGA
32	Y	613	CLA	C2A-CAA-CBA-CGA
32	n	614	CLA	C2A-CAA-CBA-CGA
32	BB	610	CLA	C16-C17-C18-C19
32	Cc	503	CLA	C16-C17-C18-C19
39	3	605	CHL	O1D-CGD-O2D-CED
36	A	413	LHG	C4-C5-C6-O8
36	D	410	LHG	C4-C5-C6-O8
37	C	501	SQD	C44-C45-C46-O48
37	L	101	SQD	C44-C45-C46-O48
37	L	102	SQD	O6-C44-C45-C46
37	B	602	SQD	O6-C44-C45-C46
37	LL	102	SQD	C44-C45-C46-O48
38	C	521	LMG	O1-C7-C8-C9
38	BB	619	LMG	C7-C8-C9-O8
44	a	415	DGD	C1G-C2G-C3G-O3G
44	CC	522	DGD	C1G-C2G-C3G-O3G
44	D	411	DGD	O6E-C5E-C6E-O5E
32	CC	512	CLA	C15-C16-C17-C18
38	BB	619	LMG	C17-C18-C19-C20
44	Hh	102	DGD	C4B-C5B-C6B-C7B
32	CC	509	CLA	O1A-CGA-O2A-C1
32	y	304	CLA	C15-C16-C17-C18
32	CC	509	CLA	C10-C11-C12-C13
32	B	619	CLA	C10-C11-C12-C13
38	b	621	LMG	O6-C5-C6-O5
38	c	519	LMG	C28-C29-C30-C31
33	DD	402	PHO	O1A-CGA-O2A-C1
36	YY	618	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
39	Yy	608	CHL	O1A-CGA-O2A-C1
39	y	303	CHL	O1A-CGA-O2A-C1
39	y	310	CHL	O1A-CGA-O2A-C1
37	B	602	SQD	O5-C1-O6-C44
37	Aa	413	SQD	O5-C1-O6-C44
38	b	620	LMG	O6-C5-C6-O5
36	4	301	LHG	O1-C1-C2-O2
32	n	614	CLA	O1A-CGA-O2A-C1
38	Bb	621	LMG	O6-C5-C6-O5
36	Yy	618	LHG	C13-C14-C15-C16
37	C	501	SQD	C17-C18-C19-C20
32	C	513	CLA	C5-C6-C7-C8
32	Y	602	CLA	C5-C6-C7-C8
38	A	415	LMG	O6-C5-C6-O5
38	AA	415	LMG	O6-C5-C6-O5
38	Bb	620	LMG	O6-C5-C6-O5
32	g	611	CLA	C4-C3-C5-C6
32	CC	512	CLA	C4-C3-C5-C6
32	Bb	611	CLA	C4-C3-C5-C6
35	d	404	PL9	C25-C24-C26-C27
35	Dd	404	PL9	C30-C29-C31-C32
32	Dd	401	CLA	O1D-CGD-O2D-CED
36	K	101	LHG	C23-C24-C25-C26
32	B	606	CLA	C16-C17-C18-C20
32	Ss	612	CLA	CBA-CGA-O2A-C1
32	C	513	CLA	CBA-CGA-O2A-C1
32	G	602	CLA	CBA-CGA-O2A-C1
32	Y	613	CLA	CBA-CGA-O2A-C1
32	BB	613	CLA	CBA-CGA-O2A-C1
32	Dd	401	CLA	CBA-CGA-O2A-C1
33	a	409	PHO	CBA-CGA-O2A-C1
33	Aa	409	PHO	CBA-CGA-O2A-C1
36	22	615	LHG	C24-C23-O8-C6
36	n	618	LHG	C24-C23-O8-C6
38	C	521	LMG	O6-C5-C6-O5
43	R	618	LMU	O5'-C5'-C6'-O6'
36	r	616	LHG	C9-C10-C11-C12
44	Hh	102	DGD	O6E-C5E-C6E-O5E
32	Ss	612	CLA	C2A-CAA-CBA-CGA
32	SS	314	CLA	C2A-CAA-CBA-CGA
32	C	510	CLA	C10-C11-C12-C13
32	C	511	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
32	S	611	CLA	C2-C1-O2A-CGA
32	NN	610	CLA	C2-C1-O2A-CGA
39	Gg	308	CHL	C2-C1-O2A-CGA
32	y	315	CLA	O1D-CGD-O2D-CED
32	Bb	606	CLA	O1D-CGD-O2D-CED
32	Aa	407	CLA	O1D-CGD-O2D-CED
32	r	602	CLA	C15-C16-C17-C18
32	BB	612	CLA	C10-C11-C12-C13
32	n	611	CLA	CBA-CGA-O2A-C1
32	CC	512	CLA	CBA-CGA-O2A-C1
32	B	609	CLA	CBA-CGA-O2A-C1
32	Bb	607	CLA	CBA-CGA-O2A-C1
32	Bb	615	CLA	CBA-CGA-O2A-C1
32	Gg	303	CLA	CBA-CGA-O2A-C1
36	d	406	LHG	C24-C23-O8-C6
36	44	614	LHG	O6-C4-C5-O7
36	4	315	LHG	O6-C4-C5-O7
32	r	604	CLA	CAA-CBA-CGA-O2A
32	BB	610	CLA	C16-C17-C18-C20
38	m	101	LMG	C17-C18-C19-C20
32	C	503	CLA	C8-C10-C11-C12
32	BB	601	CLA	C13-C15-C16-C17
32	Bb	615	CLA	C15-C16-C17-C18
32	BB	604	CLA	O1A-CGA-O2A-C1
39	G	601	CHL	C3-C5-C6-C7
36	DD	408	LHG	C33-C34-C35-C36
36	D	410	LHG	O7-C5-C6-O8
36	y	320	LHG	O7-C5-C6-O8
38	C	521	LMG	O1-C7-C8-O7
38	a	412	LMG	O1-C7-C8-O7
44	a	415	DGD	O2G-C2G-C3G-O3G
44	Aa	401	DGD	O2G-C2G-C3G-O3G
44	CC	518	DGD	CCB-CDB-CEB-CFB
44	B	603	DGD	O1B-C1B-O2G-C2G
33	a	409	PHO	C15-C16-C17-C18
32	Y	613	CLA	O1A-CGA-O2A-C1
32	Bb	601	CLA	C16-C17-C18-C19
33	a	408	PHO	CHA-CBD-CGD-O1D
33	a	408	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O2D
37	L	101	SQD	C25-C26-C27-C28
38	m	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	C	513	CLA	C4-C3-C5-C6
32	b	611	CLA	C4-C3-C5-C6
32	Gg	312	CLA	C4-C3-C5-C6
35	Dd	404	PL9	C25-C24-C26-C27
32	Rr	602	CLA	C6-C7-C8-C10
32	Yy	602	CLA	C11-C10-C8-C7
32	Yy	610	CLA	C11-C12-C13-C15
32	Yy	612	CLA	C11-C12-C13-C15
32	C	505	CLA	C6-C7-C8-C10
32	R	609	CLA	C11-C12-C13-C15
32	Y	612	CLA	C6-C7-C8-C10
32	a	405	CLA	C12-C13-C15-C16
32	b	608	CLA	C11-C12-C13-C15
32	b	613	CLA	C6-C7-C8-C10
32	c	503	CLA	C11-C10-C8-C7
32	c	506	CLA	C11-C10-C8-C7
32	d	401	CLA	C11-C12-C13-C15
32	g	611	CLA	C2-C3-C5-C6
32	r	602	CLA	C6-C7-C8-C10
32	y	314	CLA	C11-C12-C13-C15
32	BB	605	CLA	C12-C13-C15-C16
32	BB	608	CLA	C11-C12-C13-C15
32	BB	609	CLA	C6-C7-C8-C10
32	BB	610	CLA	C6-C7-C8-C10
32	BB	611	CLA	C6-C7-C8-C10
32	BB	611	CLA	C12-C13-C15-C16
32	BB	612	CLA	C6-C7-C8-C10
32	CC	503	CLA	C6-C7-C8-C10
32	CC	508	CLA	C11-C10-C8-C7
32	DD	403	CLA	C6-C7-C8-C10
32	B	604	CLA	C11-C12-C13-C15
32	B	605	CLA	C6-C7-C8-C10
32	B	606	CLA	C6-C7-C8-C10
32	B	607	CLA	C6-C7-C8-C10
32	B	608	CLA	C6-C7-C8-C10
32	B	608	CLA	C12-C13-C15-C16
32	B	618	CLA	C12-C13-C15-C16
32	B	620	CLA	C11-C12-C13-C15
32	B	622	CLA	C12-C13-C15-C16
32	RR	302	CLA	C11-C12-C13-C15
32	RR	309	CLA	C11-C12-C13-C15
32	YY	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
32	YY	610	CLA	C6-C7-C8-C10
32	YY	610	CLA	C11-C12-C13-C15
32	YY	612	CLA	C11-C10-C8-C7
32	Aa	405	CLA	C12-C13-C15-C16
32	Bb	611	CLA	C2-C3-C5-C6
32	Bb	613	CLA	C6-C7-C8-C10
32	Cc	505	CLA	C11-C10-C8-C7
32	Cc	508	CLA	C11-C10-C8-C7
32	Cc	513	CLA	C11-C10-C8-C7
32	Dd	401	CLA	C11-C12-C13-C15
32	Gg	312	CLA	C2-C3-C5-C6
32	Gg	312	CLA	C11-C12-C13-C15
39	Yy	601	CHL	C11-C12-C13-C15
39	g	601	CHL	C6-C7-C8-C10
39	g	601	CHL	C11-C12-C13-C15
39	y	303	CHL	C11-C12-C13-C15
39	Nn	317	CHL	C6-C7-C8-C10
39	Nn	317	CHL	C12-C13-C15-C16
32	b	607	CLA	O1A-CGA-O2A-C1
44	CC	522	DGD	C7B-C8B-C9B-CAB
32	C	505	CLA	C6-C7-C8-C9
32	D	405	CLA	C14-C13-C15-C16
32	R	602	CLA	C11-C12-C13-C14
32	R	609	CLA	C11-C12-C13-C14
32	a	405	CLA	C14-C13-C15-C16
32	b	608	CLA	C11-C12-C13-C14
32	b	612	CLA	C11-C12-C13-C14
32	b	615	CLA	C11-C10-C8-C9
32	y	304	CLA	C11-C10-C8-C9
32	y	312	CLA	C11-C12-C13-C14
32	BB	608	CLA	C11-C12-C13-C14
32	BB	611	CLA	C14-C13-C15-C16
32	BB	612	CLA	C6-C7-C8-C9
32	BB	612	CLA	C14-C13-C15-C16
32	CC	502	CLA	C11-C10-C8-C9
32	B	606	CLA	C6-C7-C8-C9
32	B	607	CLA	C14-C13-C15-C16
32	B	608	CLA	C6-C7-C8-C9
32	B	618	CLA	C14-C13-C15-C16
32	B	622	CLA	C14-C13-C15-C16
32	RR	302	CLA	C11-C12-C13-C14
32	RR	309	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	YY	610	CLA	C11-C12-C13-C14
32	YY	612	CLA	C11-C10-C8-C9
32	Aa	405	CLA	C14-C13-C15-C16
32	Bb	608	CLA	C11-C12-C13-C14
32	Bb	612	CLA	C11-C12-C13-C14
32	Cc	505	CLA	C11-C10-C8-C9
32	Cc	511	CLA	C11-C10-C8-C9
33	D	402	PHO	C6-C7-C8-C9
33	a	409	PHO	C6-C7-C8-C9
33	DD	402	PHO	C6-C7-C8-C9
33	Aa	409	PHO	C6-C7-C8-C9
39	Yy	601	CHL	C11-C12-C13-C14
39	NN	607	CHL	C6-C7-C8-C9
39	N	607	CHL	CBD-CGD-O2D-CED
44	CC	522	DGD	C1B-C2B-C3B-C4B
36	d	406	LHG	C9-C10-C11-C12
32	CC	514	CLA	CBA-CGA-O2A-C1
39	Y	606	CHL	O1D-CGD-O2D-CED
32	C	515	CLA	C2A-CAA-CBA-CGA
32	BB	607	CLA	C2A-CAA-CBA-CGA
36	Dd	406	LHG	C11-C10-C9-C8
32	BB	613	CLA	O1A-CGA-O2A-C1
34	XX	202	BCR	C7-C8-C9-C34
36	y	320	LHG	C15-C16-C17-C18
34	TT	101	BCR	C21-C22-C23-C24
34	XX	202	BCR	C7-C8-C9-C10
32	Cc	513	CLA	C3-C5-C6-C7
32	CC	509	CLA	O1D-CGD-O2D-CED
32	BB	609	CLA	C8-C10-C11-C12
32	CC	506	CLA	C8-C10-C11-C12
32	Bb	610	CLA	C5-C6-C7-C8
32	Bb	616	CLA	C15-C16-C17-C18
44	CC	518	DGD	C2B-C1B-O2G-C2G
36	A	414	LHG	C11-C12-C13-C14
36	DD	407	LHG	C28-C29-C30-C31
32	R	609	CLA	CBA-CGA-O2A-C1
32	b	615	CLA	CBA-CGA-O2A-C1
32	RR	309	CLA	CBA-CGA-O2A-C1
32	RR	314	CLA	CBA-CGA-O2A-C1
36	0	201	LHG	C23-C24-C25-C26
32	b	610	CLA	C13-C15-C16-C17
44	CC	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
32	4	303	CLA	CBD-CGD-O2D-CED
32	CC	513	CLA	C8-C10-C11-C12
32	NN	602	CLA	C5-C6-C7-C8
36	44	614	LHG	O6-C4-C5-C6
36	D	408	LHG	O6-C4-C5-C6
36	DD	407	LHG	O6-C4-C5-C6
32	b	610	CLA	C3-C5-C6-C7
37	LL	102	SQD	C25-C26-C27-C28
44	Hh	102	DGD	C5B-C6B-C7B-C8B
44	CC	519	DGD	CAA-CBA-CCA-CDA
32	d	401	CLA	CBA-CGA-O2A-C1
32	DD	403	CLA	CBA-CGA-O2A-C1
32	Cc	504	CLA	CBA-CGA-O2A-C1
32	C	510	CLA	O1D-CGD-O2D-CED
36	n	618	LHG	C11-C10-C9-C8
44	D	411	DGD	CCB-CDB-CEB-CFB
32	b	604	CLA	C4-C3-C5-C6
32	C	513	CLA	C2-C3-C5-C6
32	b	611	CLA	C2-C3-C5-C6
32	CC	512	CLA	C2-C3-C5-C6
44	B	603	DGD	C1A-C2A-C3A-C4A
32	Cc	508	CLA	C15-C16-C17-C18
32	Dd	401	CLA	O1A-CGA-O2A-C1
36	Dd	406	LHG	O10-C23-O8-C6
44	D	411	DGD	C3B-C4B-C5B-C6B
36	Nn	310	LHG	C11-C10-C9-C8
32	SS	303	CLA	O1D-CGD-O2D-CED
32	D	404	CLA	CBA-CGA-O2A-C1
32	BB	606	CLA	CBA-CGA-O2A-C1
32	B	618	CLA	CBA-CGA-O2A-C1
36	r	616	LHG	C24-C23-O8-C6
37	Aa	413	SQD	C24-C23-O48-C46
39	s	605	CHL	CBA-CGA-O2A-C1
38	a	412	LMG	C10-C11-C12-C13
36	D	408	LHG	C28-C29-C30-C31
43	R	618	LMU	C5'-C4'-O1B-C1B
36	NN	619	LHG	C5-C4-O6-P
32	Rr	602	CLA	C3A-C2A-CAA-CBA
32	Rr	608	CLA	C3A-C2A-CAA-CBA
32	Yy	604	CLA	C3A-C2A-CAA-CBA
32	N	610	CLA	C3A-C2A-CAA-CBA
32	S	602	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	S	604	CLA	C3A-C2A-CAA-CBA
32	Y	604	CLA	C3A-C2A-CAA-CBA
32	c	506	CLA	C3A-C2A-CAA-CBA
32	c	513	CLA	C3A-C2A-CAA-CBA
32	y	305	CLA	C3A-C2A-CAA-CBA
32	4	303	CLA	C3A-C2A-CAA-CBA
32	AA	406	CLA	C3A-C2A-CAA-CBA
32	BB	608	CLA	C3A-C2A-CAA-CBA
32	CC	502	CLA	C3A-C2A-CAA-CBA
32	B	604	CLA	C3A-C2A-CAA-CBA
32	NN	610	CLA	C3A-C2A-CAA-CBA
32	NN	613	CLA	C3A-C2A-CAA-CBA
32	SS	303	CLA	C3A-C2A-CAA-CBA
43	KK	102	LMU	C2-C1-O1'-C1'
36	AA	414	LHG	C11-C12-C13-C14
37	Ll	101	SQD	C7-C8-C9-C10
32	D	405	CLA	C5-C6-C7-C8
32	c	508	CLA	C5-C6-C7-C8
32	B	605	CLA	C8-C10-C11-C12
32	c	501	CLA	C16-C17-C18-C20
32	r	609	CLA	CBA-CGA-O2A-C1
32	s	612	CLA	CBA-CGA-O2A-C1
36	A	414	LHG	C13-C14-C15-C16
38	Mm	101	LMG	C17-C18-C19-C20
38	Mm	101	LMG	C31-C32-C33-C34
32	b	603	CLA	C13-C15-C16-C17
32	Gg	312	CLA	C5-C6-C7-C8
36	CC	523	LHG	C4-C5-C6-O8
37	LL	101	SQD	O6-C44-C45-C46
37	Aa	413	SQD	O6-C44-C45-C46
38	a	412	LMG	O1-C7-C8-C9
38	Aa	412	LMG	O1-C7-C8-C9
44	Aa	401	DGD	C1G-C2G-C3G-O3G
37	A	412	SQD	O49-C7-O47-C45
36	Ll	102	LHG	C14-C15-C16-C17
32	Gg	303	CLA	O1A-CGA-O2A-C1
36	D	409	LHG	C10-C11-C12-C13
37	l	102	SQD	C30-C31-C32-C33
32	CC	513	CLA	O2A-C1-C2-C3
32	Bb	612	CLA	O2A-C1-C2-C3
36	YY	618	LHG	C11-C12-C13-C14
32	n	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	Bb	607	CLA	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
33	Aa	409	PHO	O1A-CGA-O2A-C1
36	Y	618	LHG	O10-C23-O8-C6
32	c	501	CLA	C4-C3-C5-C6
32	B	623	CLA	CBA-CGA-O2A-C1
32	c	506	CLA	C15-C16-C17-C18
32	BB	602	CLA	C10-C11-C12-C13
32	Bb	603	CLA	C13-C15-C16-C17
32	Gg	304	CLA	C8-C10-C11-C12
36	A	411	LHG	C3-O3-P-O6
36	4	301	LHG	C4-O6-P-O3
32	G	602	CLA	O1A-CGA-O2A-C1
32	B	609	CLA	O1A-CGA-O2A-C1
36	n	618	LHG	O10-C23-O8-C6
39	RR	307	CHL	O1D-CGD-O2D-CED
32	N	602	CLA	C3-C5-C6-C7
32	AA	408	CLA	C3-C5-C6-C7
32	Dd	402	CLA	C3-C5-C6-C7
36	G	618	LHG	O1-C1-C2-O2
36	11	614	LHG	O6-C4-C5-O7
36	3	614	LHG	O6-C4-C5-O7
36	4	301	LHG	O6-C4-C5-O7
36	CC	523	LHG	O6-C4-C5-O7
36	II	101	LHG	O6-C4-C5-O7
32	C	515	CLA	CBA-CGA-O2A-C1
32	Ss	612	CLA	O1A-CGA-O2A-C1
32	C	513	CLA	O1A-CGA-O2A-C1
32	CC	512	CLA	O1A-CGA-O2A-C1
32	D	404	CLA	C8-C10-C11-C12
32	b	615	CLA	C15-C16-C17-C18
37	A	412	SQD	O47-C7-C8-C9
36	J	101	LHG	O2-C2-C3-O3
36	AA	414	LHG	C13-C14-C15-C16
32	C	507	CLA	C5-C6-C7-C8
32	Bb	615	CLA	O1A-CGA-O2A-C1
43	R	618	LMU	C3'-C4'-O1B-C1B
37	L	101	SQD	O6-C44-C45-O47
37	L	101	SQD	O47-C45-C46-O48
37	LL	102	SQD	O6-C44-C45-O47
37	LL	102	SQD	O47-C45-C46-O48
32	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	D	409	LHG	C27-C28-C29-C30
32	c	501	CLA	C16-C17-C18-C19
35	d	404	PL9	C44-C46-C47-C48
32	C	510	CLA	C2-C1-O2A-CGA
32	r	613	CLA	C2-C1-O2A-CGA
32	GG	610	CLA	C2-C1-O2A-CGA
32	RR	302	CLA	C2-C1-O2A-CGA
32	SS	312	CLA	C2-C1-O2A-CGA
32	YY	612	CLA	C2-C1-O2A-CGA
38	c	519	LMG	C12-C13-C14-C15
32	b	616	CLA	C15-C16-C17-C18
32	BB	602	CLA	C15-C16-C17-C18
32	Bb	609	CLA	C10-C11-C12-C13
32	C	507	CLA	C14-C13-C15-C16
32	C	513	CLA	C6-C7-C8-C9
32	C	513	CLA	C11-C12-C13-C14
32	BB	610	CLA	C6-C7-C8-C9
32	CC	503	CLA	C11-C12-C13-C14
32	CC	504	CLA	C6-C7-C8-C9
32	CC	511	CLA	C6-C7-C8-C9
32	DD	403	CLA	C6-C7-C8-C9
32	DD	404	CLA	C14-C13-C15-C16
32	B	608	CLA	C14-C13-C15-C16
32	YY	610	CLA	C14-C13-C15-C16
32	Cc	512	CLA	C11-C12-C13-C14
32	Nn	301	CLA	C11-C12-C13-C14
33	Aa	409	PHO	C11-C12-C13-C14
39	G	601	CHL	C11-C12-C13-C14
39	Y	601	CHL	C11-C12-C13-C14
39	g	601	CHL	C6-C7-C8-C9
39	g	601	CHL	C11-C12-C13-C14
39	n	607	CHL	C14-C13-C15-C16
39	NN	607	CHL	C14-C13-C15-C16
39	YY	601	CHL	C11-C12-C13-C14
39	Gg	302	CHL	C11-C12-C13-C14
39	Nn	317	CHL	C14-C13-C15-C16
36	y	320	LHG	C13-C14-C15-C16
36	l	101	LHG	C14-C15-C16-C17
32	A	405	CLA	C8-C10-C11-C12
32	b	603	CLA	C8-C10-C11-C12
32	c	502	CLA	C13-C15-C16-C17
36	22	615	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
36	K	101	LHG	C5-C4-O6-P
36	N	619	LHG	C5-C4-O6-P
32	d	401	CLA	O1A-CGA-O2A-C1
36	22	615	LHG	O10-C23-O8-C6
36	d	406	LHG	O10-C23-O8-C6
32	Ss	613	CLA	C2A-CAA-CBA-CGA
32	CC	514	CLA	C2A-CAA-CBA-CGA
32	RR	302	CLA	C2A-CAA-CBA-CGA
32	b	601	CLA	C16-C17-C18-C20
32	Bb	606	CLA	C16-C17-C18-C20
39	n	607	CHL	C16-C17-C18-C19
32	Ss	603	CLA	O2A-C1-C2-C3
32	r	608	CLA	O2A-C1-C2-C3
32	r	610	CLA	O2A-C1-C2-C3
32	s	603	CLA	O2A-C1-C2-C3
32	s	613	CLA	O2A-C1-C2-C3
32	RR	310	CLA	O2A-C1-C2-C3
32	Nn	302	CLA	O2A-C1-C2-C3
32	Nn	314	CLA	O2A-C1-C2-C3
39	NN	609	CHL	O2A-C1-C2-C3
39	Nn	311	CHL	O2A-C1-C2-C3
34	H	101	BCR	C23-C24-C25-C26
34	b	619	BCR	C23-C24-C25-C30
34	AA	409	BCR	C23-C24-C25-C26
34	BB	618	BCR	C23-C24-C25-C30
34	B	614	BCR	C23-C24-C25-C30
34	KK	103	BCR	C1-C6-C7-C8
34	Bb	619	BCR	C1-C6-C7-C8
34	Cc	516	BCR	C1-C6-C7-C8
34	Cc	518	BCR	C23-C24-C25-C30
40	Rr	614	LUT	C1-C6-C7-C8
40	44	612	LUT	C1-C6-C7-C8
40	22	614	LUT	C1-C6-C7-C8
40	2	614	LUT	C1-C6-C7-C8
40	G	615	LUT	C1-C6-C7-C8
40	n	616	LUT	C1-C6-C7-C8
40	r	614	LUT	C1-C6-C7-C8
40	GG	616	LUT	C1-C6-C7-C8
40	SS	315	LUT	C1-C6-C7-C8
32	BB	609	CLA	C13-C15-C16-C17
34	Hh	101	BCR	C11-C12-C13-C35
40	y	317	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
32	CC	514	CLA	O1A-CGA-O2A-C1
39	3	607	CHL	O1D-CGD-O2D-CED
32	y	315	CLA	CBA-CGA-O2A-C1
32	N	612	CLA	C1A-C2A-CAA-CBA
32	NN	612	CLA	C1A-C2A-CAA-CBA
34	K	102	BCR	C7-C8-C9-C10
39	G	605	CHL	C1A-C2A-CAA-CBA
39	G	609	CHL	C1A-C2A-CAA-CBA
39	GG	605	CHL	C1A-C2A-CAA-CBA
39	GG	609	CHL	C1A-C2A-CAA-CBA
39	Gg	310	CHL	C1A-C2A-CAA-CBA
40	y	317	LUT	C7-C8-C9-C10
32	C	506	CLA	C8-C10-C11-C12
32	N	602	CLA	C8-C10-C11-C12
32	BB	603	CLA	C8-C10-C11-C12
32	Bb	602	CLA	C15-C16-C17-C18
38	BB	619	LMG	C33-C34-C35-C36
37	l	102	SQD	C7-C8-C9-C10
36	C	522	LHG	O9-C7-O7-C5
44	CC	518	DGD	O1B-C1B-O2G-C2G
36	C	522	LHG	C8-C7-O7-C5
39	SS	308	CHL	O2A-C1-C2-C3
32	A	405	CLA	C13-C15-C16-C17
38	DD	409	LMG	C31-C32-C33-C34
38	Cc	501	LMG	O6-C5-C6-O5
36	0	201	LHG	C14-C15-C16-C17
32	RR	309	CLA	O1A-CGA-O2A-C1
32	RR	314	CLA	O1A-CGA-O2A-C1
33	Aa	409	PHO	C15-C16-C17-C18
36	44	616	LHG	O6-C4-C5-C6
36	3	614	LHG	O6-C4-C5-C6
36	4	315	LHG	O6-C4-C5-C6
36	II	101	LHG	O6-C4-C5-C6
32	Rr	604	CLA	CAA-CBA-CGA-O2A
35	D	407	PL9	C30-C29-C31-C32
32	C	503	CLA	C6-C7-C8-C10
32	C	507	CLA	C12-C13-C15-C16
32	C	512	CLA	C6-C7-C8-C10
32	N	610	CLA	C12-C13-C15-C16
32	R	602	CLA	C11-C12-C13-C15
32	Y	602	CLA	C6-C7-C8-C10
32	b	602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	b	603	CLA	C11-C10-C8-C7
32	b	610	CLA	C6-C7-C8-C10
32	b	612	CLA	C11-C12-C13-C15
32	b	615	CLA	C11-C10-C8-C7
32	n	610	CLA	C11-C12-C13-C15
32	r	609	CLA	C11-C12-C13-C15
32	y	304	CLA	C11-C10-C8-C7
32	y	314	CLA	C11-C10-C8-C7
32	BB	603	CLA	C11-C12-C13-C15
32	BB	603	CLA	C12-C13-C15-C16
32	BB	605	CLA	C11-C10-C8-C7
32	BB	612	CLA	C12-C13-C15-C16
32	CC	502	CLA	C11-C10-C8-C7
32	CC	504	CLA	C6-C7-C8-C10
32	CC	506	CLA	C12-C13-C15-C16
32	CC	511	CLA	C6-C7-C8-C10
32	DD	404	CLA	C12-C13-C15-C16
32	B	607	CLA	C12-C13-C15-C16
32	YY	610	CLA	C12-C13-C15-C16
32	Bb	601	CLA	C11-C12-C13-C15
32	Bb	603	CLA	C11-C10-C8-C7
32	Bb	605	CLA	C12-C13-C15-C16
32	Bb	608	CLA	C11-C10-C8-C7
32	Bb	612	CLA	C11-C12-C13-C15
32	Cc	504	CLA	C11-C12-C13-C15
32	Cc	511	CLA	C11-C10-C8-C7
32	Nn	301	CLA	C11-C12-C13-C15
33	D	402	PHO	C6-C7-C8-C10
33	a	409	PHO	C6-C7-C8-C10
33	a	409	PHO	C11-C12-C13-C15
33	DD	402	PHO	C6-C7-C8-C10
33	Aa	409	PHO	C6-C7-C8-C10
39	Yy	609	CHL	C12-C13-C15-C16
39	G	601	CHL	C11-C12-C13-C15
39	Y	601	CHL	C11-C12-C13-C15
39	n	607	CHL	C12-C13-C15-C16
39	y	311	CHL	C12-C13-C15-C16
39	NN	607	CHL	C12-C13-C15-C16
39	YY	601	CHL	C11-C12-C13-C15
39	Gg	302	CHL	C11-C12-C13-C15
36	DD	408	LHG	C10-C11-C12-C13
32	Bb	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
39	Nn	317	CHL	C16-C17-C18-C19
36	A	411	LHG	C10-C11-C12-C13
32	b	607	CLA	C5-C6-C7-C8
32	DD	404	CLA	C5-C6-C7-C8
32	Aa	406	CLA	C8-C10-C11-C12
39	s	606	CHL	C2A-CAA-CBA-CGA
32	b	609	CLA	C13-C15-C16-C17
32	B	604	CLA	C15-C16-C17-C18
44	CC	522	DGD	C1A-C2A-C3A-C4A
38	B	615	LMG	C17-C18-C19-C20
32	r	609	CLA	O1A-CGA-O2A-C1
32	b	602	CLA	C16-C17-C18-C19
39	y	303	CHL	C16-C17-C18-C20
32	Bb	601	CLA	C5-C6-C7-C8
32	S	602	CLA	CBA-CGA-O2A-C1
32	g	602	CLA	CBA-CGA-O2A-C1
36	Nn	310	LHG	C24-C23-O8-C6
39	Nn	315	CHL	CBA-CGA-O2A-C1
36	Yy	618	LHG	C15-C16-C17-C18
36	s	616	LHG	C17-C18-C19-C20
38	F	101	LMG	C31-C32-C33-C34
36	Rr	617	LHG	C25-C26-C27-C28
32	g	603	CLA	C8-C10-C11-C12
32	Bb	607	CLA	C10-C11-C12-C13
44	BB	623	DGD	CDB-CEB-CFB-CGB
32	A	405	CLA	CAD-CBD-CGD-O2D
32	A	408	CLA	CAD-CBD-CGD-O2D
32	Rr	611	CLA	CAD-CBD-CGD-O2D
32	Ss	608	CLA	CAD-CBD-CGD-O2D
32	Ss	613	CLA	CAD-CBD-CGD-O2D
32	44	604	CLA	CAD-CBD-CGD-O2D
32	33	609	CLA	CAD-CBD-CGD-O2D
32	1	604	CLA	CAD-CBD-CGD-O2D
32	2	611	CLA	CAD-CBD-CGD-O2D
32	3	609	CLA	CAD-CBD-CGD-O2D
32	N	603	CLA	CAD-CBD-CGD-O2D
32	S	610	CLA	CAD-CBD-CGD-O2D
32	a	410	CLA	CAD-CBD-CGD-O2D
32	b	604	CLA	CAD-CBD-CGD-O2D
32	b	609	CLA	CAD-CBD-CGD-O2D
32	b	610	CLA	CAD-CBD-CGD-O2D
32	c	506	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	r	603	CLA	CAD-CBD-CGD-O2D
32	r	610	CLA	CAD-CBD-CGD-O2D
32	r	611	CLA	CAD-CBD-CGD-O2D
32	y	312	CLA	CAD-CBD-CGD-O2D
32	4	305	CLA	CAD-CBD-CGD-O2D
32	4	311	CLA	CAD-CBD-CGD-O2D
32	AA	408	CLA	CAD-CBD-CGD-O2D
32	B	619	CLA	CAD-CBD-CGD-O2D
32	GG	610	CLA	CAD-CBD-CGD-O2D
32	NN	611	CLA	CAD-CBD-CGD-O2D
32	NN	612	CLA	CAD-CBD-CGD-O2D
32	NN	614	CLA	CAD-CBD-CGD-O2D
32	RR	309	CLA	CAD-CBD-CGD-O2D
32	SS	310	CLA	CAD-CBD-CGD-O2D
32	Aa	410	CLA	CAD-CBD-CGD-O2D
32	Bb	604	CLA	CAD-CBD-CGD-O2D
32	Bb	610	CLA	CAD-CBD-CGD-O2D
32	Bb	616	CLA	CAD-CBD-CGD-O2D
32	Cc	506	CLA	CAD-CBD-CGD-O2D
32	Nn	301	CLA	CAD-CBD-CGD-O2D
39	Rr	606	CHL	CAD-CBD-CGD-O2D
39	Yy	601	CHL	CAD-CBD-CGD-O2D
39	Yy	605	CHL	CAD-CBD-CGD-O2D
39	Yy	606	CHL	CAD-CBD-CGD-O2D
39	11	601	CHL	CAD-CBD-CGD-O2D
39	33	607	CHL	CAD-CBD-CGD-O2D
39	33	608	CHL	CAD-CBD-CGD-O2D
39	G	601	CHL	CAD-CBD-CGD-O2D
39	N	608	CHL	CAD-CBD-CGD-O2D
39	S	605	CHL	CAD-CBD-CGD-O2D
39	S	606	CHL	CAD-CBD-CGD-O2D
39	S	607	CHL	CAD-CBD-CGD-O2D
39	Y	601	CHL	CAD-CBD-CGD-O2D
39	n	601	CHL	CAD-CBD-CGD-O2D
39	s	606	CHL	CAD-CBD-CGD-O2D
39	y	303	CHL	CAD-CBD-CGD-O2D
39	4	309	CHL	CAD-CBD-CGD-O2D
39	NN	608	CHL	CAD-CBD-CGD-O2D
39	SS	307	CHL	CAD-CBD-CGD-O2D
39	YY	601	CHL	CAD-CBD-CGD-O2D
32	CC	510	CLA	C10-C11-C12-C13
32	Bb	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
44	Aa	401	DGD	C2A-C1A-O1G-C1G
32	c	510	CLA	C4-C3-C5-C6
35	d	404	PL9	C35-C34-C36-C37
38	A	415	LMG	O6-C1-O1-C7
32	b	610	CLA	C5-C6-C7-C8
35	D	407	PL9	C39-C41-C42-C43
36	r	616	LHG	C4-C5-C6-O8
38	b	621	LMG	O1-C7-C8-C9
38	Bb	621	LMG	O1-C7-C8-C9
32	R	609	CLA	O1A-CGA-O2A-C1
44	C	523	DGD	C2B-C1B-O2G-C2G
36	A	413	LHG	O6-C4-C5-O7
36	33	614	LHG	O6-C4-C5-O7
36	D	408	LHG	O6-C4-C5-O7
36	AA	411	LHG	O6-C4-C5-O7
36	DD	407	LHG	O6-C4-C5-O7
32	c	510	CLA	C15-C16-C17-C18
32	Rr	601	CLA	O2A-C1-C2-C3
32	Ss	604	CLA	O2A-C1-C2-C3
32	R	601	CLA	O2A-C1-C2-C3
32	R	610	CLA	O2A-C1-C2-C3
32	R	611	CLA	O2A-C1-C2-C3
32	S	602	CLA	O2A-C1-C2-C3
32	Y	603	CLA	O2A-C1-C2-C3
32	r	601	CLA	O2A-C1-C2-C3
32	r	612	CLA	O2A-C1-C2-C3
32	s	604	CLA	O2A-C1-C2-C3
32	RR	311	CLA	O2A-C1-C2-C3
32	Gg	311	CLA	O2A-C1-C2-C3
39	N	609	CHL	O2A-C1-C2-C3
46	e	101	HEM	C4B-C3B-CAB-CBB
46	Ee	101	HEM	C4B-C3B-CAB-CBB
32	C	507	CLA	C2A-CAA-CBA-CGA
32	Bb	612	CLA	C2A-CAA-CBA-CGA
32	Nn	312	CLA	C2A-CAA-CBA-CGA
36	r	616	LHG	C25-C26-C27-C28
44	Aa	401	DGD	C5B-C6B-C7B-C8B
39	y	311	CHL	CBD-CGD-O2D-CED
32	b	601	CLA	C16-C17-C18-C19
32	b	602	CLA	C16-C17-C18-C20
32	CC	504	CLA	C16-C17-C18-C19
32	Bb	606	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	YY	601	CHL	C16-C17-C18-C20
36	CC	523	LHG	C24-C25-C26-C27
32	c	513	CLA	O1D-CGD-O2D-CED
38	Mm	101	LMG	O9-C10-O7-C8
32	Rr	604	CLA	CHA-CBD-CGD-O2D
32	Rr	613	CLA	CHA-CBD-CGD-O2D
32	Ss	602	CLA	CHA-CBD-CGD-O1D
32	Ss	602	CLA	CHA-CBD-CGD-O2D
32	Ss	610	CLA	CHA-CBD-CGD-O1D
32	Ss	610	CLA	CHA-CBD-CGD-O2D
32	Yy	604	CLA	CHA-CBD-CGD-O1D
32	Yy	604	CLA	CHA-CBD-CGD-O2D
32	44	602	CLA	CHA-CBD-CGD-O1D
32	44	615	CLA	CHA-CBD-CGD-O2D
32	11	603	CLA	CHA-CBD-CGD-O1D
32	11	603	CLA	CHA-CBD-CGD-O2D
32	22	602	CLA	CHA-CBD-CGD-O1D
32	22	602	CLA	CHA-CBD-CGD-O2D
32	22	609	CLA	CHA-CBD-CGD-O1D
32	22	609	CLA	CHA-CBD-CGD-O2D
32	33	610	CLA	CHA-CBD-CGD-O2D
32	33	611	CLA	CHA-CBD-CGD-O1D
32	33	611	CLA	CHA-CBD-CGD-O2D
32	33	613	CLA	CHA-CBD-CGD-O1D
32	3	611	CLA	CHA-CBD-CGD-O1D
32	3	611	CLA	CHA-CBD-CGD-O2D
32	3	613	CLA	CHA-CBD-CGD-O1D
32	3	613	CLA	CHA-CBD-CGD-O2D
32	C	505	CLA	CHA-CBD-CGD-O1D
32	C	505	CLA	CHA-CBD-CGD-O2D
32	C	514	CLA	CHA-CBD-CGD-O1D
32	C	514	CLA	CHA-CBD-CGD-O2D
32	D	401	CLA	CHA-CBD-CGD-O1D
32	G	604	CLA	CHA-CBD-CGD-O1D
32	G	604	CLA	CHA-CBD-CGD-O2D
32	N	602	CLA	CHA-CBD-CGD-O1D
32	N	602	CLA	CHA-CBD-CGD-O2D
32	N	604	CLA	CHA-CBD-CGD-O2D
32	R	611	CLA	CHA-CBD-CGD-O1D
32	R	611	CLA	CHA-CBD-CGD-O2D
32	Y	604	CLA	CHA-CBD-CGD-O1D
32	Y	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	Y	614	CLA	CHA-CBD-CGD-O1D
32	Y	614	CLA	CHA-CBD-CGD-O2D
32	b	602	CLA	CHA-CBD-CGD-O1D
32	b	602	CLA	CHA-CBD-CGD-O2D
32	b	615	CLA	CHA-CBD-CGD-O1D
32	c	502	CLA	CHA-CBD-CGD-O1D
32	c	502	CLA	CHA-CBD-CGD-O2D
32	c	505	CLA	CHA-CBD-CGD-O1D
32	c	505	CLA	CHA-CBD-CGD-O2D
32	c	509	CLA	CHA-CBD-CGD-O1D
32	c	509	CLA	CHA-CBD-CGD-O2D
32	g	612	CLA	CHA-CBD-CGD-O1D
32	g	612	CLA	CHA-CBD-CGD-O2D
32	g	614	CLA	CHA-CBD-CGD-O2D
32	n	602	CLA	CHA-CBD-CGD-O1D
32	r	604	CLA	CHA-CBD-CGD-O2D
32	s	610	CLA	CHA-CBD-CGD-O1D
32	s	610	CLA	CHA-CBD-CGD-O2D
32	y	306	CLA	CHA-CBD-CGD-O1D
32	y	306	CLA	CHA-CBD-CGD-O2D
32	4	303	CLA	CHA-CBD-CGD-O1D
32	4	303	CLA	CHA-CBD-CGD-O2D
32	4	311	CLA	CHA-CBD-CGD-O1D
32	BB	604	CLA	CHA-CBD-CGD-O1D
32	BB	604	CLA	CHA-CBD-CGD-O2D
32	BB	615	CLA	CHA-CBD-CGD-O1D
32	CC	504	CLA	CHA-CBD-CGD-O1D
32	CC	504	CLA	CHA-CBD-CGD-O2D
32	CC	513	CLA	CHA-CBD-CGD-O1D
32	CC	513	CLA	CHA-CBD-CGD-O2D
32	B	611	CLA	CHA-CBD-CGD-O1D
32	B	611	CLA	CHA-CBD-CGD-O2D
32	B	621	CLA	CHA-CBD-CGD-O1D
32	GG	604	CLA	CHA-CBD-CGD-O1D
32	GG	604	CLA	CHA-CBD-CGD-O2D
32	NN	602	CLA	CHA-CBD-CGD-O1D
32	NN	602	CLA	CHA-CBD-CGD-O2D
32	RR	311	CLA	CHA-CBD-CGD-O1D
32	RR	311	CLA	CHA-CBD-CGD-O2D
32	RR	314	CLA	CHA-CBD-CGD-O2D
32	SS	309	CLA	CHA-CBD-CGD-O1D
32	SS	309	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	YY	604	CLA	CHA-CBD-CGD-O1D
32	YY	614	CLA	CHA-CBD-CGD-O1D
32	YY	614	CLA	CHA-CBD-CGD-O2D
32	Aa	405	CLA	CHA-CBD-CGD-O2D
32	Bb	602	CLA	CHA-CBD-CGD-O1D
32	Bb	615	CLA	CHA-CBD-CGD-O1D
32	Cc	507	CLA	CHA-CBD-CGD-O1D
32	Cc	507	CLA	CHA-CBD-CGD-O2D
32	Cc	511	CLA	CHA-CBD-CGD-O2D
32	Gg	315	CLA	CHA-CBD-CGD-O2D
32	Nn	312	CLA	CHA-CBD-CGD-O1D
32	Nn	312	CLA	CHA-CBD-CGD-O2D
39	Rr	607	CHL	CHA-CBD-CGD-O2D
39	11	605	CHL	CHA-CBD-CGD-O1D
39	11	605	CHL	CHA-CBD-CGD-O2D
39	33	601	CHL	CHA-CBD-CGD-O2D
39	33	606	CHL	CHA-CBD-CGD-O2D
39	1	606	CHL	CHA-CBD-CGD-O2D
39	3	601	CHL	CHA-CBD-CGD-O1D
39	3	601	CHL	CHA-CBD-CGD-O2D
39	3	605	CHL	CHA-CBD-CGD-O2D
39	R	605	CHL	CHA-CBD-CGD-O1D
39	R	605	CHL	CHA-CBD-CGD-O2D
39	S	601	CHL	CHA-CBD-CGD-O1D
39	S	601	CHL	CHA-CBD-CGD-O2D
39	n	605	CHL	CHA-CBD-CGD-O1D
39	n	605	CHL	CHA-CBD-CGD-O2D
39	r	605	CHL	CHA-CBD-CGD-O1D
39	r	605	CHL	CHA-CBD-CGD-O2D
39	y	307	CHL	CHA-CBD-CGD-O1D
39	NN	605	CHL	CHA-CBD-CGD-O1D
39	NN	605	CHL	CHA-CBD-CGD-O2D
39	RR	305	CHL	CHA-CBD-CGD-O1D
39	RR	305	CHL	CHA-CBD-CGD-O2D
39	SS	302	CHL	CHA-CBD-CGD-O1D
39	SS	302	CHL	CHA-CBD-CGD-O2D
39	SS	308	CHL	CHA-CBD-CGD-O2D
39	Nn	318	CHL	CHA-CBD-CGD-O1D
32	Cc	512	CLA	C15-C16-C17-C18
32	D	404	CLA	O1A-CGA-O2A-C1
32	b	615	CLA	O1A-CGA-O2A-C1
32	s	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	BB	606	CLA	O1A-CGA-O2A-C1
32	DD	403	CLA	O1A-CGA-O2A-C1
32	Cc	504	CLA	O1A-CGA-O2A-C1
36	r	616	LHG	O10-C23-O8-C6
39	s	605	CHL	O1A-CGA-O2A-C1
37	L	101	SQD	C28-C29-C30-C31
37	LL	102	SQD	C12-C13-C14-C15
38	j	101	LMG	C29-C30-C31-C32
37	LL	102	SQD	C28-C29-C30-C31
36	YY	618	LHG	O7-C5-C6-O8
37	L	102	SQD	O6-C44-C45-O47
37	B	602	SQD	O6-C44-C45-O47
37	Aa	413	SQD	O6-C44-C45-O47
38	b	621	LMG	O7-C8-C9-O8
38	Bb	621	LMG	O7-C8-C9-O8
38	Mm	101	LMG	O1-C7-C8-O7
44	C	523	DGD	O2G-C2G-C3G-O3G
38	B	615	LMG	C30-C31-C32-C33
32	AA	405	CLA	C13-C15-C16-C17
32	g	602	CLA	O1A-CGA-O2A-C1
32	y	315	CLA	O1A-CGA-O2A-C1
32	B	618	CLA	O1A-CGA-O2A-C1
32	B	623	CLA	O1A-CGA-O2A-C1
37	Aa	413	SQD	O10-C23-O48-C46
44	C	520	DGD	C2A-C3A-C4A-C5A
39	N	607	CHL	O1D-CGD-O2D-CED
32	Bb	610	CLA	C3-C5-C6-C7
32	Bb	610	CLA	C15-C16-C17-C18
32	D	401	CLA	C4-C3-C5-C6
32	G	611	CLA	C4-C3-C5-C6
32	DD	401	CLA	C4-C3-C5-C6
35	D	407	PL9	C43-C44-C46-C47
35	d	404	PL9	C28-C29-C31-C32
32	4	303	CLA	O1D-CGD-O2D-CED
32	BB	601	CLA	CBA-CGA-O2A-C1
37	CC	501	SQD	C11-C10-C9-C8
38	b	620	LMG	O9-C10-O7-C8
38	m	101	LMG	O9-C10-O7-C8
32	C	504	CLA	C11-C12-C13-C14
32	C	512	CLA	C6-C7-C8-C9
32	b	601	CLA	C11-C12-C13-C14
32	n	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	BB	601	CLA	C6-C7-C8-C9
32	BB	601	CLA	C14-C13-C15-C16
32	CC	506	CLA	C14-C13-C15-C16
32	Bb	609	CLA	C11-C12-C13-C14
32	Bb	615	CLA	C11-C10-C8-C9
33	a	409	PHO	C11-C12-C13-C14
39	Yy	609	CHL	C14-C13-C15-C16
39	N	607	CHL	C14-C13-C15-C16
39	y	311	CHL	C14-C13-C15-C16
39	Gg	302	CHL	C6-C7-C8-C9
36	BB	622	LHG	C11-C10-C9-C8
37	L	101	SQD	C12-C13-C14-C15
32	DD	404	CLA	CBD-CGD-O2D-CED
32	C	515	CLA	O1A-CGA-O2A-C1
39	Nn	315	CHL	O1A-CGA-O2A-C1
44	Aa	401	DGD	O1A-C1A-O1G-C1G
36	g	618	LHG	C7-C8-C9-C10
38	a	412	LMG	C13-C14-C15-C16
44	h	102	DGD	C5A-C6A-C7A-C8A
44	CC	518	DGD	C2B-C3B-C4B-C5B
39	Yy	601	CHL	C16-C17-C18-C20
32	b	609	CLA	C2A-CAA-CBA-CGA
32	n	602	CLA	C2A-CAA-CBA-CGA
32	Cc	512	CLA	C2A-CAA-CBA-CGA
34	TT	101	BCR	C37-C22-C23-C24
44	BB	623	DGD	C1B-C2B-C3B-C4B
34	CC	516	BCR	C21-C22-C23-C24
40	Yy	616	LUT	C7-C8-C9-C10
36	r	616	LHG	C10-C11-C12-C13
32	44	602	CLA	C1A-C2A-CAA-CBA
32	BB	603	CLA	C1A-C2A-CAA-CBA
32	GG	602	CLA	C1A-C2A-CAA-CBA
32	Cc	505	CLA	C1A-C2A-CAA-CBA
32	Dd	402	CLA	C1A-C2A-CAA-CBA
39	YY	605	CHL	C1A-C2A-CAA-CBA
36	A	411	LHG	C23-C24-C25-C26
32	C	509	CLA	C13-C15-C16-C17
32	B	605	CLA	C13-C15-C16-C17
32	R	608	CLA	C2-C1-O2A-CGA
32	B	624	CLA	C2-C1-O2A-CGA
32	RR	308	CLA	C2-C1-O2A-CGA
39	s	605	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
32	c	508	CLA	CBA-CGA-O2A-C1
44	a	415	DGD	C2A-C1A-O1G-C1G
36	Ss	616	LHG	C3-O3-P-O6
36	D	409	LHG	C4-O6-P-O3
36	G	618	LHG	C4-O6-P-O3
36	N	619	LHG	C3-O3-P-O6
36	g	618	LHG	C3-O3-P-O6
36	GG	618	LHG	C4-O6-P-O3
36	JJ	101	LHG	C4-O6-P-O3
36	AA	411	LHG	C11-C10-C9-C8
32	CC	506	CLA	C4-C3-C5-C6
32	d	402	CLA	C3-C5-C6-C7
36	n	618	LHG	C5-C4-O6-P
36	Nn	310	LHG	C5-C4-O6-P
32	G	611	CLA	C2-C3-C5-C6
36	A	413	LHG	C24-C25-C26-C27
44	a	415	DGD	O1A-C1A-O1G-C1G
36	A	411	LHG	C4-O6-P-O4
36	A	414	LHG	C3-O3-P-O5
36	Rr	617	LHG	C3-O3-P-O4
36	Ss	616	LHG	C4-O6-P-O4
36	Yy	618	LHG	C3-O3-P-O4
36	Yy	618	LHG	C4-O6-P-O4
36	44	616	LHG	C3-O3-P-O4
36	1	614	LHG	C4-O6-P-O4
36	3	614	LHG	C4-O6-P-O4
36	C	522	LHG	C3-O3-P-O5
36	C	522	LHG	C4-O6-P-O5
36	D	410	LHG	C3-O3-P-O5
36	D	410	LHG	C4-O6-P-O5
36	J	101	LHG	C4-O6-P-O4
36	K	101	LHG	C3-O3-P-O4
36	K	101	LHG	C4-O6-P-O5
36	Y	618	LHG	C3-O3-P-O4
36	Y	618	LHG	C4-O6-P-O4
36	d	406	LHG	C4-O6-P-O4
36	r	616	LHG	C3-O3-P-O4
36	s	616	LHG	C4-O6-P-O4
36	y	320	LHG	C4-O6-P-O4
36	AA	411	LHG	C4-O6-P-O4
36	AA	414	LHG	C3-O3-P-O5
36	BB	622	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
36	CC	521	LHG	C4-O6-P-O5
36	DD	407	LHG	C3-O3-P-O5
36	KK	101	LHG	C4-O6-P-O5
36	NN	619	LHG	C3-O3-P-O4
36	SS	301	LHG	C4-O6-P-O4
36	YY	618	LHG	C3-O3-P-O4
36	Dd	406	LHG	C4-O6-P-O4
32	Y	602	CLA	C16-C17-C18-C20
32	c	505	CLA	C16-C17-C18-C20
32	CC	503	CLA	C16-C17-C18-C20
32	RR	302	CLA	C16-C17-C18-C20
32	YY	602	CLA	C16-C17-C18-C20
32	Cc	507	CLA	C16-C17-C18-C20
39	Y	609	CHL	C16-C17-C18-C20
39	YY	601	CHL	C16-C17-C18-C19
32	Ss	608	CLA	O2A-C1-C2-C3
32	G	610	CLA	O2A-C1-C2-C3
32	g	614	CLA	O2A-C1-C2-C3
32	r	611	CLA	O2A-C1-C2-C3
32	s	608	CLA	O2A-C1-C2-C3
32	Gg	315	CLA	O2A-C1-C2-C3
39	RR	306	CHL	O2A-C1-C2-C3
38	AA	415	LMG	O6-C1-O1-C7
36	11	614	LHG	O6-C4-C5-C6
36	AA	411	LHG	O6-C4-C5-C6
32	Bb	602	CLA	C5-C6-C7-C8
32	s	612	CLA	C2A-CAA-CBA-CGA
32	A	408	CLA	C3-C5-C6-C7
37	Ll	101	SQD	C30-C31-C32-C33
38	DD	409	LMG	C32-C33-C34-C35
44	a	415	DGD	C5B-C6B-C7B-C8B
37	Aa	413	SQD	C24-C25-C26-C27
38	WW	201	LMG	C38-C39-C40-C41
44	D	411	DGD	C7A-C8A-C9A-CAA
32	c	508	CLA	O1A-CGA-O2A-C1
38	b	620	LMG	C11-C10-O7-C8
32	b	606	CLA	C16-C17-C18-C20
39	YY	609	CHL	C16-C17-C18-C20
32	Rr	604	CLA	CAD-CBD-CGD-O1D
32	Ss	603	CLA	CAD-CBD-CGD-O1D
32	Ss	610	CLA	CAD-CBD-CGD-O1D
32	44	615	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	11	603	CLA	CAD-CBD-CGD-O1D
32	22	609	CLA	CAD-CBD-CGD-O1D
32	22	610	CLA	CAD-CBD-CGD-O1D
32	33	610	CLA	CAD-CBD-CGD-O1D
32	1	603	CLA	CAD-CBD-CGD-O1D
32	3	610	CLA	CAD-CBD-CGD-O1D
32	C	505	CLA	CAD-CBD-CGD-O1D
32	C	506	CLA	CAD-CBD-CGD-O1D
32	G	604	CLA	CAD-CBD-CGD-O1D
32	G	611	CLA	CAD-CBD-CGD-O1D
32	N	604	CLA	CAD-CBD-CGD-O1D
32	R	610	CLA	CAD-CBD-CGD-O1D
32	Y	614	CLA	CAD-CBD-CGD-O1D
32	b	602	CLA	CAD-CBD-CGD-O1D
32	b	603	CLA	CAD-CBD-CGD-O1D
32	b	613	CLA	CAD-CBD-CGD-O1D
32	c	502	CLA	CAD-CBD-CGD-O1D
32	c	505	CLA	CAD-CBD-CGD-O1D
32	c	509	CLA	CAD-CBD-CGD-O1D
32	g	614	CLA	CAD-CBD-CGD-O1D
32	n	612	CLA	CAD-CBD-CGD-O1D
32	r	604	CLA	CAD-CBD-CGD-O1D
32	s	602	CLA	CAD-CBD-CGD-O1D
32	s	603	CLA	CAD-CBD-CGD-O1D
32	s	604	CLA	CAD-CBD-CGD-O1D
32	s	610	CLA	CAD-CBD-CGD-O1D
32	BB	604	CLA	CAD-CBD-CGD-O1D
32	BB	606	CLA	CAD-CBD-CGD-O1D
32	CC	504	CLA	CAD-CBD-CGD-O1D
32	CC	505	CLA	CAD-CBD-CGD-O1D
32	B	604	CLA	CAD-CBD-CGD-O1D
32	B	621	CLA	CAD-CBD-CGD-O1D
32	B	623	CLA	CAD-CBD-CGD-O1D
32	GG	604	CLA	CAD-CBD-CGD-O1D
32	NN	604	CLA	CAD-CBD-CGD-O1D
32	RR	310	CLA	CAD-CBD-CGD-O1D
32	SS	309	CLA	CAD-CBD-CGD-O1D
32	YY	614	CLA	CAD-CBD-CGD-O1D
32	Bb	601	CLA	CAD-CBD-CGD-O1D
32	Bb	602	CLA	CAD-CBD-CGD-O1D
32	Bb	603	CLA	CAD-CBD-CGD-O1D
32	Bb	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	Cc	503	CLA	CAD-CBD-CGD-O1D
32	Cc	507	CLA	CAD-CBD-CGD-O1D
32	Gg	305	CLA	CAD-CBD-CGD-O1D
32	Gg	315	CLA	CAD-CBD-CGD-O1D
37	AA	412	SQD	O5-C5-C6-S
37	AA	412	SQD	C5-C6-S-O7
39	Rr	607	CHL	CAD-CBD-CGD-O1D
39	Yy	607	CHL	CAD-CBD-CGD-O1D
39	33	601	CHL	CAD-CBD-CGD-O1D
39	3	601	CHL	CAD-CBD-CGD-O1D
39	3	605	CHL	CAD-CBD-CGD-O1D
39	S	601	CHL	CAD-CBD-CGD-O1D
39	g	609	CHL	CAD-CBD-CGD-O1D
39	r	607	CHL	CAD-CBD-CGD-O1D
39	SS	302	CHL	CAD-CBD-CGD-O1D
39	Gg	310	CHL	CAD-CBD-CGD-O1D
39	Nn	318	CHL	CAD-CBD-CGD-O1D
36	D	410	LHG	C23-C24-C25-C26
32	GG	603	CLA	C5-C6-C7-C8
44	C	519	DGD	C2B-C3B-C4B-C5B
36	Dd	405	LHG	C25-C26-C27-C28
36	AA	411	LHG	C23-C24-C25-C26
32	R	602	CLA	C16-C17-C18-C20
32	c	506	CLA	C16-C17-C18-C20
32	b	613	CLA	C4-C3-C5-C6
35	DD	406	PL9	C35-C34-C36-C37
32	A	406	CLA	C3A-C2A-CAA-CBA
32	Rr	609	CLA	C11-C12-C13-C15
32	C	509	CLA	C11-C10-C8-C7
32	D	405	CLA	C12-C13-C15-C16
32	R	602	CLA	C12-C13-C15-C16
32	Y	610	CLA	C6-C7-C8-C10
32	b	601	CLA	C11-C12-C13-C15
32	b	604	CLA	C2-C3-C5-C6
32	b	608	CLA	C11-C10-C8-C7
32	b	609	CLA	C11-C10-C8-C7
32	c	502	CLA	C6-C7-C8-C10
32	g	611	CLA	C11-C12-C13-C15
32	n	610	CLA	C6-C7-C8-C10
32	BB	601	CLA	C12-C13-C15-C16
32	BB	602	CLA	C6-C7-C8-C10
32	BB	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
32	BB	610	CLA	C11-C10-C8-C7
32	CC	502	CLA	C6-C7-C8-C10
32	DD	401	CLA	C2-C3-C5-C6
32	B	606	CLA	C11-C10-C8-C7
32	B	619	CLA	C6-C7-C8-C10
32	B	624	CLA	C11-C10-C8-C7
32	NN	610	CLA	C12-C13-C15-C16
32	RR	302	CLA	C12-C13-C15-C16
32	Bb	615	CLA	C11-C10-C8-C7
32	Cc	503	CLA	C6-C7-C8-C10
32	Cc	505	CLA	C12-C13-C15-C16
33	Aa	409	PHO	C11-C12-C13-C15
36	A	411	LHG	O6-C4-C5-O7
36	Y	618	LHG	O6-C4-C5-O7
39	N	607	CHL	C11-C10-C8-C7
39	N	607	CHL	C12-C13-C15-C16
39	Y	609	CHL	C12-C13-C15-C16
39	GG	601	CHL	C11-C12-C13-C15
40	Y	615	LUT	C25-C26-C27-C28
36	EE	101	LHG	C15-C16-C17-C18
32	y	315	CLA	C3-C5-C6-C7
32	S	602	CLA	O1A-CGA-O2A-C1
35	D	407	PL9	C2-C3-C7-C8
35	DD	406	PL9	C2-C3-C7-C8
38	F	101	LMG	C32-C33-C34-C35
44	CC	518	DGD	C1B-C2B-C3B-C4B
37	C	501	SQD	C8-C7-O47-C45
36	d	405	LHG	C25-C26-C27-C28
32	Y	613	CLA	CBD-CGD-O2D-CED
32	R	611	CLA	C2A-CAA-CBA-CGA
32	y	315	CLA	C2A-CAA-CBA-CGA
39	Gg	302	CHL	C2A-CAA-CBA-CGA
32	G	603	CLA	C16-C17-C18-C20
32	GG	603	CLA	C16-C17-C18-C20
32	Dd	402	CLA	C16-C17-C18-C19
32	CC	508	CLA	C13-C15-C16-C17
38	m	101	LMG	O1-C7-C8-C9
38	Mm	101	LMG	O1-C7-C8-C9
36	A	413	LHG	O7-C5-C6-O8
37	LL	101	SQD	O6-C44-C45-O47
38	m	101	LMG	O1-C7-C8-O7
32	B	619	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	Aa	412	LMG	C13-C14-C15-C16
38	Mm	101	LMG	C33-C34-C35-C36
44	BB	623	DGD	C7A-C8A-C9A-CAA
32	C	514	CLA	O2A-C1-C2-C3
36	Nn	310	LHG	O10-C23-O8-C6
38	W	201	LMG	C29-C30-C31-C32
32	G	603	CLA	C5-C6-C7-C8
39	Yy	609	CHL	C8-C10-C11-C12
32	Gg	304	CLA	C3-C5-C6-C7
32	G	613	CLA	C4C-C3C-CAC-CBC
39	y	311	CHL	O1D-CGD-O2D-CED
32	CC	503	CLA	C4-C3-C5-C6
36	Yy	618	LHG	C31-C32-C33-C34
38	Dd	408	LMG	C29-C30-C31-C32
38	Mm	101	LMG	C11-C10-O7-C8
32	A	405	CLA	C11-C10-C8-C9
32	C	503	CLA	C11-C12-C13-C14
32	Y	602	CLA	C6-C7-C8-C9
32	b	603	CLA	C11-C10-C8-C9
32	b	616	CLA	C14-C13-C15-C16
32	c	506	CLA	C11-C10-C8-C9
32	r	602	CLA	C6-C7-C8-C9
32	r	609	CLA	C11-C12-C13-C14
32	y	314	CLA	C11-C12-C13-C14
32	BB	603	CLA	C11-C12-C13-C14
32	BB	605	CLA	C11-C10-C8-C9
32	CC	508	CLA	C11-C10-C8-C9
32	Bb	603	CLA	C11-C10-C8-C9
32	Bb	608	CLA	C11-C10-C8-C9
32	Cc	504	CLA	C11-C12-C13-C14
39	GG	601	CHL	C11-C12-C13-C14
44	C	523	DGD	O1B-C1B-O2G-C2G
35	d	404	PL9	C34-C36-C37-C38
32	Y	613	CLA	C11-C12-C13-C14
32	Gg	304	CLA	CAA-CBA-CGA-O2A
36	s	616	LHG	C11-C10-C9-C8
32	RR	302	CLA	C13-C15-C16-C17
32	Bb	602	CLA	C13-C15-C16-C17
32	BB	601	CLA	O1A-CGA-O2A-C1
32	Aa	406	CLA	C2C-C3C-CAC-CBC
32	A	405	CLA	C16-C17-C18-C20
32	C	505	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	y	303	CHL	C16-C17-C18-C19
36	A	414	LHG	C16-C17-C18-C19
34	c	515	BCR	C21-C22-C23-C24
34	c	516	BCR	C7-C8-C9-C10
32	G	603	CLA	C13-C15-C16-C17
36	AA	414	LHG	C16-C17-C18-C19
36	D	410	LHG	O2-C2-C3-O3
44	Hh	102	DGD	CDB-CEB-CFB-CGB
32	GG	603	CLA	C13-C15-C16-C17
36	11	614	LHG	C24-C25-C26-C27
36	l	101	LHG	C24-C25-C26-C27
38	C	521	LMG	C12-C13-C14-C15
32	C	503	CLA	C5-C6-C7-C8
32	b	601	CLA	C15-C16-C17-C18
32	AA	405	CLA	C8-C10-C11-C12
32	AA	408	CLA	C11-C12-C13-C15
44	CC	519	DGD	CBA-CCA-CDA-CEA
44	Cc	520	DGD	C9B-CAB-CBB-CCB
32	Dd	402	CLA	C5-C6-C7-C8
32	A	406	CLA	C1-C2-C3-C4
32	Rr	601	CLA	C1-C2-C3-C4
32	Rr	603	CLA	C1-C2-C3-C4
32	Rr	604	CLA	C1-C2-C3-C4
32	Rr	608	CLA	C1-C2-C3-C4
32	Rr	610	CLA	C1-C2-C3-C4
32	Rr	611	CLA	C1-C2-C3-C4
32	Rr	612	CLA	C1-C2-C3-C4
32	Rr	613	CLA	C1-C2-C3-C4
32	Ss	602	CLA	C1-C2-C3-C4
32	Ss	603	CLA	C1-C2-C3-C4
32	Ss	604	CLA	C1-C2-C3-C4
32	Ss	608	CLA	C1-C2-C3-C4
32	Ss	609	CLA	C1-C2-C3-C4
32	Ss	610	CLA	C1-C2-C3-C4
32	Ss	611	CLA	C1-C2-C3-C4
32	Ss	612	CLA	C1-C2-C3-C4
32	Ss	613	CLA	C1-C2-C3-C4
32	Yy	603	CLA	C1-C2-C3-C4
32	Yy	604	CLA	C1-C2-C3-C4
32	Yy	614	CLA	C1-C2-C3-C4
32	44	615	CLA	C1-C2-C3-C4
32	G	610	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	G	612	CLA	C1-C2-C3-C4
32	N	611	CLA	C1-C2-C3-C4
32	N	613	CLA	C1-C2-C3-C4
32	R	601	CLA	C1-C2-C3-C4
32	R	603	CLA	C1-C2-C3-C4
32	R	604	CLA	C1-C2-C3-C4
32	R	608	CLA	C1-C2-C3-C4
32	R	610	CLA	C1-C2-C3-C4
32	R	614	CLA	C1-C2-C3-C4
32	S	602	CLA	C1-C2-C3-C4
32	S	604	CLA	C1-C2-C3-C4
32	S	610	CLA	C1-C2-C3-C4
32	S	611	CLA	C1-C2-C3-C4
32	Y	603	CLA	C1-C2-C3-C4
32	Y	604	CLA	C1-C2-C3-C4
32	Y	614	CLA	C1-C2-C3-C4
32	a	407	CLA	C1-C2-C3-C4
32	g	610	CLA	C1-C2-C3-C4
32	g	612	CLA	C1-C2-C3-C4
32	g	614	CLA	C1-C2-C3-C4
32	n	603	CLA	C1-C2-C3-C4
32	n	604	CLA	C1-C2-C3-C4
32	n	612	CLA	C1-C2-C3-C4
32	n	613	CLA	C1-C2-C3-C4
32	n	614	CLA	C1-C2-C3-C4
32	r	601	CLA	C1-C2-C3-C4
32	r	603	CLA	C1-C2-C3-C4
32	r	604	CLA	C1-C2-C3-C4
32	r	608	CLA	C1-C2-C3-C4
32	r	610	CLA	C1-C2-C3-C4
32	r	611	CLA	C1-C2-C3-C4
32	r	612	CLA	C1-C2-C3-C4
32	r	613	CLA	C1-C2-C3-C4
32	s	602	CLA	C1-C2-C3-C4
32	s	603	CLA	C1-C2-C3-C4
32	s	604	CLA	C1-C2-C3-C4
32	s	608	CLA	C1-C2-C3-C4
32	s	609	CLA	C1-C2-C3-C4
32	s	610	CLA	C1-C2-C3-C4
32	s	611	CLA	C1-C2-C3-C4
32	s	612	CLA	C1-C2-C3-C4
32	s	613	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	y	305	CLA	C1-C2-C3-C4
32	y	306	CLA	C1-C2-C3-C4
32	y	316	CLA	C1-C2-C3-C4
32	AA	406	CLA	C1-C2-C3-C4
32	GG	610	CLA	C1-C2-C3-C4
32	GG	612	CLA	C1-C2-C3-C4
32	NN	611	CLA	C1-C2-C3-C4
32	NN	613	CLA	C1-C2-C3-C4
32	RR	303	CLA	C1-C2-C3-C4
32	RR	304	CLA	C1-C2-C3-C4
32	RR	308	CLA	C1-C2-C3-C4
32	RR	310	CLA	C1-C2-C3-C4
32	RR	314	CLA	C1-C2-C3-C4
32	SS	303	CLA	C1-C2-C3-C4
32	SS	305	CLA	C1-C2-C3-C4
32	SS	311	CLA	C1-C2-C3-C4
32	SS	312	CLA	C1-C2-C3-C4
32	SS	314	CLA	C1-C2-C3-C4
32	YY	603	CLA	C1-C2-C3-C4
32	YY	604	CLA	C1-C2-C3-C4
32	YY	614	CLA	C1-C2-C3-C4
32	Aa	407	CLA	C1-C2-C3-C4
32	Gg	311	CLA	C1-C2-C3-C4
32	Gg	313	CLA	C1-C2-C3-C4
32	Gg	315	CLA	C1-C2-C3-C4
32	Nn	303	CLA	C1-C2-C3-C4
32	Nn	304	CLA	C1-C2-C3-C4
32	Nn	305	CLA	C1-C2-C3-C4
32	Nn	313	CLA	C1-C2-C3-C4
32	Nn	314	CLA	C1-C2-C3-C4
39	Rr	607	CHL	C1-C2-C3-C4
39	Ss	605	CHL	C1-C2-C3-C4
39	Ss	606	CHL	C1-C2-C3-C4
39	Yy	608	CHL	C1-C2-C3-C4
39	R	606	CHL	C1-C2-C3-C4
39	R	607	CHL	C1-C2-C3-C4
39	Y	608	CHL	C1-C2-C3-C4
39	n	608	CHL	C1-C2-C3-C4
39	n	609	CHL	C1-C2-C3-C4
39	r	607	CHL	C1-C2-C3-C4
39	s	605	CHL	C1-C2-C3-C4
39	s	606	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
39	y	310	CHL	C1-C2-C3-C4
39	RR	306	CHL	C1-C2-C3-C4
39	RR	307	CHL	C1-C2-C3-C4
39	YY	608	CHL	C1-C2-C3-C4
39	Nn	318	CHL	C1-C2-C3-C4
39	Nn	319	CHL	C1-C2-C3-C4
32	R	614	CLA	O1A-CGA-O2A-C1
32	a	406	CLA	C2C-C3C-CAC-CBC
38	c	519	LMG	O7-C10-C11-C12
38	m	101	LMG	C33-C34-C35-C36
32	b	616	CLA	C8-C10-C11-C12
36	A	411	LHG	O6-C4-C5-C6
32	44	603	CLA	C2A-CAA-CBA-CGA
32	RR	311	CLA	C2A-CAA-CBA-CGA
32	Aa	405	CLA	C2A-CAA-CBA-CGA
32	Bb	609	CLA	C2A-CAA-CBA-CGA
36	Rr	617	LHG	O9-C7-O7-C5
37	C	501	SQD	O49-C7-O47-C45
38	Bb	620	LMG	O9-C10-O7-C8
32	Yy	602	CLA	C2-C1-O2A-CGA
32	N	610	CLA	C2-C1-O2A-CGA
32	Y	602	CLA	C2-C1-O2A-CGA
32	Y	610	CLA	C2-C1-O2A-CGA
32	y	304	CLA	C2-C1-O2A-CGA
32	CC	509	CLA	C2-C1-O2A-CGA
32	B	619	CLA	C2-C1-O2A-CGA
32	Cc	507	CLA	C2-C1-O2A-CGA
44	BB	623	DGD	C5B-C6B-C7B-C8B
44	Hh	102	DGD	C4A-C5A-C6A-C7A
39	Yy	601	CHL	C16-C17-C18-C19
37	AA	412	SQD	O47-C7-C8-C9
32	c	511	CLA	O1A-CGA-O2A-C1
37	L	102	SQD	C9-C10-C11-C12
38	WW	201	LMG	C12-C13-C14-C15
32	Cc	506	CLA	C5-C6-C7-C8
32	R	614	CLA	CBA-CGA-O2A-C1
32	DD	404	CLA	O1A-CGA-O2A-C1
36	Yy	618	LHG	O6-C4-C5-O7
36	y	320	LHG	O6-C4-C5-O7
36	YY	618	LHG	O6-C4-C5-O7
36	Nn	310	LHG	O6-C4-C5-O7
32	C	509	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	b	606	CLA	C16-C17-C18-C19
32	CC	504	CLA	C16-C17-C18-C20
32	NN	602	CLA	C13-C15-C16-C17
32	G	602	CLA	O2A-C1-C2-C3
32	n	604	CLA	O2A-C1-C2-C3
39	n	601	CHL	O2A-C1-C2-C3
32	Rr	609	CLA	C4-C3-C5-C6
32	Bb	604	CLA	C4-C3-C5-C6
36	Ll	102	LHG	C35-C36-C37-C38
34	c	516	BCR	C23-C24-C25-C30
40	YY	616	LUT	C1-C6-C7-C8
32	c	510	CLA	C2-C3-C5-C6
36	11	614	LHG	O10-C23-O8-C6
32	R	602	CLA	C13-C15-C16-C17
38	W	201	LMG	C12-C13-C14-C15
44	c	518	DGD	C9B-CAB-CBB-CCB
36	Nn	310	LHG	C11-C12-C13-C14
32	A	408	CLA	C11-C12-C13-C15
32	d	402	CLA	C16-C17-C18-C19
32	RR	302	CLA	C16-C17-C18-C19
32	Cc	508	CLA	C16-C17-C18-C20
44	BB	624	DGD	C2D-C1D-O3G-C3G
36	CC	523	LHG	O7-C5-C6-O8
38	BB	619	LMG	O7-C8-C9-O8
38	Bb	621	LMG	O1-C7-C8-O7
36	0	201	LHG	C32-C33-C34-C35
37	C	501	SQD	C11-C10-C9-C8
36	A	414	LHG	C4-O6-P-O3
36	44	616	LHG	C4-O6-P-O3
36	22	615	LHG	C3-O3-P-O6
36	0	201	LHG	C3-O3-P-O6
36	0	201	LHG	C4-O6-P-O3
36	D	409	LHG	C3-O3-P-O6
36	N	619	LHG	C4-O6-P-O3
36	a	414	LHG	C3-O3-P-O6
36	a	414	LHG	C4-O6-P-O3
36	d	405	LHG	C3-O3-P-O6
36	g	618	LHG	C4-O6-P-O3
36	l	101	LHG	C4-O6-P-O3
36	n	618	LHG	C3-O3-P-O6
36	n	618	LHG	C4-O6-P-O3
36	s	616	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	AA	414	LHG	C4-O6-P-O3
36	DD	408	LHG	C3-O3-P-O6
36	DD	408	LHG	C4-O6-P-O3
36	EE	101	LHG	C3-O3-P-O6
36	EE	101	LHG	C4-O6-P-O3
36	II	101	LHG	C3-O3-P-O6
36	KK	101	LHG	C3-O3-P-O6
36	NN	619	LHG	C4-O6-P-O3
36	Dd	405	LHG	C3-O3-P-O6
36	Dd	407	LHG	C3-O3-P-O6
36	Dd	407	LHG	C4-O6-P-O3
36	Gg	319	LHG	C4-O6-P-O3
36	Ll	102	LHG	C4-O6-P-O3
36	Nn	310	LHG	C3-O3-P-O6
36	Nn	310	LHG	C4-O6-P-O3
36	0	201	LHG	C15-C16-C17-C18
38	a	412	LMG	C11-C12-C13-C14
38	WW	201	LMG	C29-C30-C31-C32
32	CC	508	CLA	C16-C17-C18-C19
33	D	402	PHO	CHA-CBD-CGD-O1D
33	D	402	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O1D
33	DD	402	PHO	CHA-CBD-CGD-O1D
33	DD	402	PHO	CHA-CBD-CGD-O2D
33	Aa	408	PHO	CHA-CBD-CGD-O2D
33	Aa	409	PHO	CHA-CBD-CGD-O1D
33	Aa	409	PHO	CHA-CBD-CGD-O2D
36	A	411	LHG	C9-C10-C11-C12
44	Cc	520	DGD	C3B-C4B-C5B-C6B
32	B	605	CLA	C5-C6-C7-C8
36	y	320	LHG	C4-C5-C6-O8
37	LL	102	SQD	O6-C44-C45-C46
38	B	615	LMG	C7-C8-C9-O8
32	BB	610	CLA	C4-C3-C5-C6
32	Bb	601	CLA	C15-C16-C17-C18
32	C	508	CLA	C6-C7-C8-C10
32	C	513	CLA	C11-C12-C13-C15
32	D	401	CLA	C2-C3-C5-C6
32	c	501	CLA	C11-C12-C13-C15
32	BB	601	CLA	C6-C7-C8-C10
32	CC	503	CLA	C11-C12-C13-C15
32	CC	507	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
32	CC	512	CLA	C6-C7-C8-C10
32	Bb	609	CLA	C11-C12-C13-C15
32	Cc	512	CLA	C11-C12-C13-C15
32	Dd	401	CLA	C11-C10-C8-C7
32	Nn	301	CLA	C6-C7-C8-C10
35	Dd	404	PL9	C28-C29-C31-C32
39	NN	607	CHL	C6-C7-C8-C10
44	c	517	DGD	C2B-C3B-C4B-C5B
36	DD	408	LHG	C27-C28-C29-C30
32	C	503	CLA	C6-C7-C8-C9
32	C	509	CLA	C11-C10-C8-C9
32	Y	610	CLA	C6-C7-C8-C9
32	b	608	CLA	C11-C10-C8-C9
32	b	609	CLA	C11-C10-C8-C9
32	b	612	CLA	C6-C7-C8-C9
32	n	610	CLA	C6-C7-C8-C9
32	BB	602	CLA	C6-C7-C8-C9
32	BB	609	CLA	C6-C7-C8-C9
32	CC	502	CLA	C6-C7-C8-C9
32	B	605	CLA	C6-C7-C8-C9
32	B	619	CLA	C6-C7-C8-C9
32	B	620	CLA	C11-C12-C13-C14
32	YY	602	CLA	C6-C7-C8-C9
32	YY	610	CLA	C6-C7-C8-C9
32	Bb	601	CLA	C11-C12-C13-C14
32	Bb	612	CLA	C6-C7-C8-C9
32	Cc	505	CLA	C14-C13-C15-C16
32	Cc	508	CLA	C11-C10-C8-C9
32	Cc	513	CLA	C11-C10-C8-C9
44	C	519	DGD	C2B-C1B-O2G-C2G
32	Y	602	CLA	C16-C17-C18-C19
36	11	614	LHG	C24-C23-O8-C6
32	b	604	CLA	C10-C11-C12-C13
32	Bb	616	CLA	C8-C10-C11-C12
32	Cc	510	CLA	C5-C6-C7-C8
32	R	602	CLA	C16-C17-C18-C19
32	c	505	CLA	C16-C17-C18-C19
32	CC	503	CLA	C16-C17-C18-C19
32	YY	602	CLA	C16-C17-C18-C19
32	Dd	402	CLA	C16-C17-C18-C20
39	YY	609	CHL	C16-C17-C18-C19
36	l	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	Cc	506	CLA	C2C-C3C-CAC-CBC
36	0	201	LHG	C29-C30-C31-C32
36	Y	618	LHG	C7-C8-C9-C10
32	b	609	CLA	C10-C11-C12-C13
36	YY	618	LHG	C9-C10-C11-C12
32	Yy	603	CLA	O2A-C1-C2-C3
32	r	604	CLA	O2A-C1-C2-C3
32	s	609	CLA	O2A-C1-C2-C3
32	NN	611	CLA	O2A-C1-C2-C3
32	SS	303	CLA	O2A-C1-C2-C3
32	YY	603	CLA	O2A-C1-C2-C3
39	Rr	605	CHL	O2A-C1-C2-C3
39	R	606	CHL	O2A-C1-C2-C3
43	C	502	LMU	O5B-C5B-C6B-O6B
36	Ss	616	LHG	O9-C7-O7-C5
37	Ll	101	SQD	C10-C11-C12-C13
38	C	521	LMG	C33-C34-C35-C36
35	AA	410	PL9	C40-C39-C41-C42
32	Rr	609	CLA	O1A-CGA-O2A-C1
44	Hh	102	DGD	O2G-C1B-C2B-C3B
32	b	613	CLA	C2-C3-C5-C6
32	c	501	CLA	C2-C3-C5-C6
32	c	506	CLA	C16-C17-C18-C19
32	Cc	507	CLA	C16-C17-C18-C19
39	Y	609	CHL	C16-C17-C18-C19
32	Rr	609	CLA	CBA-CGA-O2A-C1
32	c	511	CLA	CBA-CGA-O2A-C1
36	Rr	617	LHG	C24-C23-O8-C6
44	Cc	520	DGD	C1A-C2A-C3A-C4A
32	R	613	CLA	C2C-C3C-CAC-CBC
32	Y	613	CLA	O1D-CGD-O2D-CED
36	NN	619	LHG	C13-C14-C15-C16
36	Ll	102	LHG	C24-C25-C26-C27
36	Dd	406	LHG	O7-C7-C8-C9
32	YY	602	CLA	C15-C16-C17-C18
32	DD	404	CLA	CBA-CGA-O2A-C1
37	B	602	SQD	C24-C23-O48-C46
32	G	603	CLA	C16-C17-C18-C19
32	GG	603	CLA	C16-C17-C18-C19
44	BB	624	DGD	O6D-C1D-O3G-C3G
32	g	613	CLA	C4C-C3C-CAC-CBC
44	C	519	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
39	NN	607	CHL	O1D-CGD-O2D-CED
35	D	407	PL9	C9-C11-C12-C13
39	NN	607	CHL	CBD-CGD-O2D-CED
32	C	511	CLA	C10-C11-C12-C13
32	C	514	CLA	C13-C15-C16-C17
37	Ll	101	SQD	C11-C12-C13-C14
36	n	618	LHG	O6-C4-C5-O7
36	KK	101	LHG	O6-C4-C5-O7
38	W	201	LMG	C38-C39-C40-C41
38	Cc	501	LMG	C12-C13-C14-C15
44	Hh	102	DGD	C9B-CAB-CBB-CCB
39	Yy	609	CHL	C16-C17-C18-C20
32	Bb	601	CLA	CAA-CBA-CGA-O2A
36	l	614	LHG	C25-C26-C27-C28
36	Y	618	LHG	C18-C19-C20-C21
37	l	102	SQD	C10-C11-C12-C13
32	C	505	CLA	C4-C3-C5-C6
32	c	503	CLA	C13-C15-C16-C17
32	BB	609	CLA	C5-C6-C7-C8
36	y	320	LHG	C10-C11-C12-C13
36	Dd	406	LHG	C24-C25-C26-C27
32	b	601	CLA	O1A-CGA-O2A-C1
37	B	602	SQD	O10-C23-O48-C46
36	DD	408	LHG	C17-C18-C19-C20
32	44	611	CLA	CAA-CBA-CGA-O1A
32	D	405	CLA	C2-C1-O2A-CGA
32	n	603	CLA	C2-C1-O2A-CGA
32	n	614	CLA	C2-C1-O2A-CGA
32	r	602	CLA	C2-C1-O2A-CGA
32	s	602	CLA	C2-C1-O2A-CGA
32	RR	314	CLA	C2-C1-O2A-CGA
32	YY	602	CLA	C2-C1-O2A-CGA
32	Nn	313	CLA	C2-C1-O2A-CGA
39	Y	609	CHL	C2-C1-O2A-CGA
39	YY	609	CHL	C2-C1-O2A-CGA
36	DD	408	LHG	C19-C20-C21-C22
37	Aa	413	SQD	C32-C33-C34-C35
36	Ss	616	LHG	C11-C10-C9-C8
37	LL	101	SQD	C9-C10-C11-C12
32	b	607	CLA	C10-C11-C12-C13
32	Yy	613	CLA	C2A-CAA-CBA-CGA
39	Y	609	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	Ll	102	LHG	C31-C32-C33-C34
37	C	501	SQD	C15-C16-C17-C18
32	44	602	CLA	C3A-C2A-CAA-CBA
32	N	613	CLA	C3A-C2A-CAA-CBA
32	g	611	CLA	C3A-C2A-CAA-CBA
32	r	604	CLA	C3A-C2A-CAA-CBA
32	r	608	CLA	C3A-C2A-CAA-CBA
32	Ss	609	CLA	O2A-C1-C2-C3
32	n	611	CLA	O2A-C1-C2-C3
32	n	614	CLA	O2A-C1-C2-C3
32	Nn	305	CLA	O2A-C1-C2-C3
39	Y	608	CHL	O2A-C1-C2-C3
39	n	606	CHL	O2A-C1-C2-C3
39	r	605	CHL	O2A-C1-C2-C3
38	Cc	501	LMG	O7-C10-C11-C12
32	r	604	CLA	CAA-CBA-CGA-O1A
32	CC	506	CLA	C2-C3-C5-C6
35	A	410	PL9	C4-C3-C7-C8
32	C	508	CLA	C6-C7-C8-C9
32	CC	507	CLA	C6-C7-C8-C9
32	CC	512	CLA	C6-C7-C8-C9
32	Bb	616	CLA	C14-C13-C15-C16
33	A	407	PHO	C14-C13-C15-C16
33	AA	407	PHO	C14-C13-C15-C16
32	d	402	CLA	C16-C17-C18-C20
32	Cc	508	CLA	C16-C17-C18-C19
38	B	615	LMG	C16-C17-C18-C19
32	44	611	CLA	CAA-CBA-CGA-O2A
36	Dd	405	LHG	C33-C34-C35-C36
36	AA	411	LHG	C9-C10-C11-C12
38	a	412	LMG	C31-C32-C33-C34
38	b	621	LMG	C7-C8-C9-O8
38	Bb	621	LMG	C7-C8-C9-O8
40	22	614	LUT	C20-C13-C14-C15
40	2	614	LUT	C20-C13-C14-C15
40	YY	615	LUT	C21-C26-C27-C28
42	Rr	616	NEX	C39-C29-C30-C31
42	Yy	617	NEX	C39-C29-C30-C31
42	N	618	NEX	C39-C29-C30-C31
42	R	617	NEX	C39-C29-C30-C31
42	Y	617	NEX	C39-C29-C30-C31
42	Y	619	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
42	g	617	NEX	C39-C29-C30-C31
42	n	617	NEX	C39-C29-C30-C31
42	y	319	NEX	C39-C29-C30-C31
42	NN	618	NEX	C39-C29-C30-C31
42	RR	317	NEX	C39-C29-C30-C31
42	YY	617	NEX	C39-C29-C30-C31
42	Gg	318	NEX	C39-C29-C30-C31
42	Nn	309	NEX	C39-C29-C30-C31
32	CC	502	CLA	C3-C5-C6-C7
39	Ss	606	CHL	C2A-CAA-CBA-CGA
36	A	411	LHG	C11-C10-C9-C8
32	c	509	CLA	C16-C17-C18-C19
32	AA	408	CLA	C11-C12-C13-C14
32	b	612	CLA	O2A-C1-C2-C3
32	Aa	405	CLA	O2A-C1-C2-C3
32	Cc	503	CLA	O2A-C1-C2-C3
38	WW	201	LMG	O6-C1-O1-C7
44	Cc	519	DGD	O6D-C1D-O3G-C3G
36	s	616	LHG	C9-C10-C11-C12
32	44	610	CLA	CAA-CBA-CGA-O2A
32	4	303	CLA	CAA-CBA-CGA-O1A
36	D	408	LHG	C27-C28-C29-C30
36	CC	523	LHG	C30-C31-C32-C33
37	C	501	SQD	C16-C17-C18-C19
32	Y	602	CLA	C15-C16-C17-C18
33	a	409	PHO	C8-C10-C11-C12
34	Cc	517	BCR	C21-C22-C23-C24
36	d	405	LHG	C33-C34-C35-C36
44	CC	518	DGD	CAB-CBB-CCB-CDB
32	B	606	CLA	C5-C6-C7-C8
32	BB	604	CLA	C4-C3-C5-C6
32	Cc	512	CLA	C4-C3-C5-C6
32	A	406	CLA	C1A-C2A-CAA-CBA
32	y	305	CLA	C1A-C2A-CAA-CBA
32	AA	406	CLA	C1A-C2A-CAA-CBA
32	DD	404	CLA	C1A-C2A-CAA-CBA
32	YY	604	CLA	C1A-C2A-CAA-CBA
32	Gg	313	CLA	C1A-C2A-CAA-CBA
39	Y	605	CHL	C1A-C2A-CAA-CBA
39	s	601	CHL	C1A-C2A-CAA-CBA
36	Y	618	LHG	C31-C32-C33-C34
37	B	602	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
32	A	405	CLA	C11-C10-C8-C7
32	A	405	CLA	C12-C13-C15-C16
32	C	504	CLA	C6-C7-C8-C10
32	C	504	CLA	C11-C12-C13-C15
32	b	604	CLA	C12-C13-C15-C16
32	b	605	CLA	C12-C13-C15-C16
32	b	606	CLA	C11-C10-C8-C7
32	c	510	CLA	C12-C13-C15-C16
32	c	512	CLA	C11-C10-C8-C7
32	r	602	CLA	C11-C10-C8-C7
32	AA	405	CLA	C12-C13-C15-C16
32	BB	602	CLA	C12-C13-C15-C16
32	BB	604	CLA	C11-C10-C8-C7
32	B	619	CLA	C12-C13-C15-C16
32	Bb	604	CLA	C12-C13-C15-C16
32	Bb	609	CLA	C11-C10-C8-C7
32	Cc	514	CLA	C11-C10-C8-C7
32	Dd	402	CLA	C12-C13-C15-C16
33	A	407	PHO	C6-C7-C8-C10
39	YY	609	CHL	C12-C13-C15-C16
32	C	511	CLA	C8-C10-C11-C12
32	4	312	CLA	CAA-CBA-CGA-O1A
39	44	608	CHL	CAA-CBA-CGA-O1A
44	c	518	DGD	C3B-C4B-C5B-C6B
36	r	616	LHG	C31-C32-C33-C34
36	A	413	LHG	C30-C31-C32-C33
36	n	618	LHG	C11-C12-C13-C14
32	4	303	CLA	CAA-CBA-CGA-O2A
32	CC	512	CLA	C8-C10-C11-C12
32	C	504	CLA	C16-C17-C18-C20
32	a	405	CLA	C16-C17-C18-C20
32	AA	405	CLA	C16-C17-C18-C20
32	Aa	410	CLA	C11-C12-C13-C15
39	Y	601	CHL	C16-C17-C18-C20
36	d	406	LHG	C24-C25-C26-C27
36	Ll	102	LHG	C9-C10-C11-C12
32	g	603	CLA	C3-C5-C6-C7
32	b	614	CLA	C2A-CAA-CBA-CGA
32	YY	612	CLA	C2A-CAA-CBA-CGA
32	Aa	406	CLA	C2A-CAA-CBA-CGA
32	Bb	614	CLA	C2A-CAA-CBA-CGA
44	BB	625	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
32	CC	508	CLA	C10-C11-C12-C13
32	Bb	605	CLA	C15-C16-C17-C18
39	Rr	607	CHL	CAA-CBA-CGA-O2A
39	44	608	CHL	CAA-CBA-CGA-O2A
36	Yy	618	LHG	C10-C11-C12-C13
36	0	201	LHG	C28-C29-C30-C31
36	DD	407	LHG	C27-C28-C29-C30
38	C	521	LMG	C18-C19-C20-C21
32	Rr	604	CLA	O2A-C1-C2-C3
32	Rr	611	CLA	O2A-C1-C2-C3
32	Ss	612	CLA	O2A-C1-C2-C3
32	s	612	CLA	O2A-C1-C2-C3
39	R	607	CHL	O2A-C1-C2-C3
39	g	607	CHL	O2A-C1-C2-C3
39	RR	307	CHL	O2A-C1-C2-C3
39	Gg	308	CHL	O2A-C1-C2-C3
32	CC	510	CLA	C8-C10-C11-C12
32	CC	513	CLA	C13-C15-C16-C17
33	Aa	409	PHO	C8-C10-C11-C12
32	b	601	CLA	CBA-CGA-O2A-C1
36	33	614	LHG	O6-C4-C5-C6
36	Nn	310	LHG	O6-C4-C5-C6
35	D	407	PL9	C32-C33-C34-C35
38	m	101	LMG	C11-C10-O7-C8
37	L	101	SQD	C45-C46-O48-C23
39	y	311	CHL	C16-C17-C18-C20
32	A	408	CLA	C8-C10-C11-C12
32	G	603	CLA	C10-C11-C12-C13
46	Ee	101	HEM	CAA-CBA-CGA-O2A
36	Y	618	LHG	C16-C17-C18-C19
32	C	504	CLA	C4-C3-C5-C6
33	A	407	PHO	C2-C3-C5-C6
35	AA	410	PL9	C12-C11-C9-C8
36	YY	618	LHG	C31-C32-C33-C34
32	N	602	CLA	C5-C6-C7-C8
32	b	606	CLA	C5-C6-C7-C8
36	AA	414	LHG	C23-C24-C25-C26
36	Yy	618	LHG	O9-C7-O7-C5
36	II	101	LHG	C24-C25-C26-C27
38	W	201	LMG	C33-C34-C35-C36
40	22	614	LUT	C12-C13-C14-C15
40	2	614	LUT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
42	Rr	616	NEX	C28-C29-C30-C31
42	Yy	617	NEX	C28-C29-C30-C31
42	N	618	NEX	C28-C29-C30-C31
42	R	617	NEX	C28-C29-C30-C31
42	Y	617	NEX	C28-C29-C30-C31
42	Y	619	NEX	C28-C29-C30-C31
42	g	617	NEX	C28-C29-C30-C31
42	n	617	NEX	C28-C29-C30-C31
42	y	319	NEX	C28-C29-C30-C31
42	NN	618	NEX	C28-C29-C30-C31
42	RR	317	NEX	C28-C29-C30-C31
42	YY	617	NEX	C28-C29-C30-C31
42	Gg	318	NEX	C28-C29-C30-C31
42	Nn	309	NEX	C28-C29-C30-C31
32	C	512	CLA	C13-C15-C16-C17
36	0	201	LHG	C27-C28-C29-C30
36	A	414	LHG	O7-C5-C6-O8
36	l	101	LHG	O7-C5-C6-O8
36	EE	101	LHG	O7-C5-C6-O8
36	Ll	102	LHG	O7-C5-C6-O8
38	CC	520	LMG	O1-C7-C8-O7
44	B	603	DGD	CCA-CDA-CEA-CFA
39	NN	601	CHL	C2A-CAA-CBA-CGA
38	Aa	412	LMG	C29-C30-C31-C32
44	C	519	DGD	CAB-CBB-CCB-CDB
44	CC	518	DGD	C7B-C8B-C9B-CAB
32	C	514	CLA	C8-C10-C11-C12
38	BB	619	LMG	C12-C13-C14-C15
32	Cc	509	CLA	O1A-CGA-O2A-C1
35	AA	410	PL9	C14-C16-C17-C18
36	N	619	LHG	C1-C2-C3-O3
39	44	605	CHL	CAA-CBA-CGA-O2A
32	C	507	CLA	C4-C3-C5-C6
35	Dd	404	PL9	C12-C11-C9-C10
36	YY	618	LHG	C16-C17-C18-C19
32	c	505	CLA	C2-C1-O2A-CGA
32	BB	602	CLA	C2-C1-O2A-CGA
32	Rr	609	CLA	C2-C3-C5-C6
32	BB	610	CLA	C2-C3-C5-C6
36	Rr	617	LHG	O10-C23-O8-C6
32	C	513	CLA	C8-C10-C11-C12
33	DD	402	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
39	44	605	CHL	CAA-CBA-CGA-O1A
36	1	614	LHG	O8-C23-C24-C25
32	CC	502	CLA	C11-C12-C13-C14
32	CC	509	CLA	C14-C13-C15-C16
32	DD	403	CLA	C14-C13-C15-C16
33	Aa	408	PHO	C11-C10-C8-C9
38	a	412	LMG	C29-C30-C31-C32
36	y	320	LHG	C5-C4-O6-P
36	11	614	LHG	O7-C7-C8-C9
36	AA	414	LHG	C15-C16-C17-C18
32	Dd	401	CLA	C5-C6-C7-C8
33	a	408	PHO	O1D-CGD-O2D-CED
32	A	408	CLA	C11-C12-C13-C14
32	C	509	CLA	C16-C17-C18-C20
32	4	312	CLA	CAA-CBA-CGA-O2A
32	N	611	CLA	O2A-C1-C2-C3
32	Gg	303	CLA	O2A-C1-C2-C3
44	Cc	519	DGD	C2B-C3B-C4B-C5B
34	K	102	BCR	C1-C6-C7-C8
34	c	514	BCR	C1-C6-C7-C8
40	Ss	614	LUT	C1-C6-C7-C8
40	Yy	616	LUT	C1-C6-C7-C8
40	N	616	LUT	C1-C6-C7-C8
40	g	616	LUT	C1-C6-C7-C8
40	n	615	LUT	C5-C6-C7-C8
40	s	615	LUT	C1-C6-C7-C8
40	GG	615	LUT	C1-C6-C7-C8
40	NN	616	LUT	C1-C6-C7-C8
40	Nn	306	LUT	C5-C6-C7-C8
32	B	618	CLA	C13-C15-C16-C17
34	c	516	BCR	C7-C8-C9-C34
32	44	610	CLA	CAA-CBA-CGA-O1A
32	S	603	CLA	CAA-CBA-CGA-O2A
46	Ee	101	HEM	CAA-CBA-CGA-O1A
46	Ee	101	HEM	CAD-CBD-CGD-O2D
32	GG	603	CLA	C10-C11-C12-C13
32	Y	613	CLA	C4-C3-C5-C6
32	Cc	511	CLA	C4-C3-C5-C6
32	G	604	CLA	C1A-C2A-CAA-CBA
32	Y	611	CLA	C1A-C2A-CAA-CBA
39	S	607	CHL	C1A-C2A-CAA-CBA
39	Y	601	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	N	610	CLA	C15-C16-C17-C18
32	g	603	CLA	C5-C6-C7-C8
44	h	102	DGD	C4A-C5A-C6A-C7A
32	CC	503	CLA	C2-C3-C5-C6
32	Aa	405	CLA	C2-C3-C5-C6
32	g	603	CLA	CAA-CBA-CGA-O2A
39	44	607	CHL	CAA-CBA-CGA-O2A
39	4	302	CHL	CAA-CBA-CGA-O2A
32	n	602	CLA	C5-C6-C7-C8
37	C	501	SQD	C45-C44-O6-C1
38	Bb	620	LMG	C11-C10-O7-C8
32	DD	404	CLA	O1D-CGD-O2D-CED
39	4	308	CHL	CAA-CBA-CGA-O2A
32	Yy	613	CLA	O1A-CGA-O2A-C1
36	EE	101	LHG	C16-C17-C18-C19
44	B	603	DGD	O6D-C5D-C6D-O5D
32	Bb	607	CLA	C15-C16-C17-C18
33	a	408	PHO	CBD-CGD-O2D-CED
32	Cc	509	CLA	CBA-CGA-O2A-C1
32	GG	613	CLA	C4C-C3C-CAC-CBC
36	N	619	LHG	C13-C14-C15-C16
32	44	603	CLA	CAA-CBA-CGA-O2A
39	44	607	CHL	CAA-CBA-CGA-O1A
39	4	308	CHL	CAA-CBA-CGA-O1A
32	C	510	CLA	C13-C15-C16-C17
44	BB	623	DGD	C9B-CAB-CBB-CCB
36	4	301	LHG	O6-C4-C5-C6
32	B	621	CLA	C4-C3-C5-C6
35	AA	410	PL9	C35-C34-C36-C37
32	C	503	CLA	C11-C12-C13-C15
32	C	505	CLA	C2-C3-C5-C6
32	DD	403	CLA	C12-C13-C15-C16
32	Bb	604	CLA	C2-C3-C5-C6
32	Cc	511	CLA	C2-C3-C5-C6
32	r	604	CLA	O1A-CGA-O2A-C1
36	y	320	LHG	C31-C32-C33-C34
32	d	402	CLA	C5-C6-C7-C8
39	r	607	CHL	CAA-CBA-CGA-O2A
44	Cc	519	DGD	C2D-C1D-O3G-C3G
32	Yy	602	CLA	C16-C17-C18-C20
32	c	509	CLA	C16-C17-C18-C20
32	CC	508	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
37	Ll	101	SQD	C18-C19-C20-C21
36	BB	622	LHG	C1-C2-C3-O3
35	Dd	404	PL9	C42-C43-C44-C45
38	b	621	LMG	O1-C7-C8-O7
32	y	315	CLA	C11-C12-C13-C14
33	D	402	PHO	C8-C10-C11-C12
32	Rr	603	CLA	O2A-C1-C2-C3
32	Ss	611	CLA	O2A-C1-C2-C3
32	44	615	CLA	O2A-C1-C2-C3
32	R	603	CLA	O2A-C1-C2-C3
32	R	608	CLA	O2A-C1-C2-C3
32	S	611	CLA	O2A-C1-C2-C3
32	g	602	CLA	O2A-C1-C2-C3
32	r	603	CLA	O2A-C1-C2-C3
32	r	613	CLA	O2A-C1-C2-C3
32	GG	602	CLA	O2A-C1-C2-C3
32	SS	305	CLA	O2A-C1-C2-C3
32	SS	312	CLA	O2A-C1-C2-C3
32	Gg	313	CLA	O2A-C1-C2-C3
39	Rr	607	CHL	O2A-C1-C2-C3
39	Yy	608	CHL	O2A-C1-C2-C3
32	44	615	CLA	CAA-CBA-CGA-O2A
32	a	410	CLA	CAA-CBA-CGA-O2A
37	L	102	SQD	O47-C7-C8-C9
37	LL	101	SQD	O47-C7-C8-C9
44	h	102	DGD	C5B-C6B-C7B-C8B
39	g	601	CHL	C2A-CAA-CBA-CGA
32	C	509	CLA	C10-C11-C12-C13
32	BB	601	CLA	C10-C11-C12-C13
32	C	505	CLA	C16-C17-C18-C20
35	A	410	PL9	C36-C37-C38-C39
32	Yy	613	CLA	CBA-CGA-O2A-C1
32	r	604	CLA	CBA-CGA-O2A-C1
37	l	102	SQD	C18-C19-C20-C21
36	Gg	319	LHG	C7-C8-C9-C10
36	Nn	310	LHG	O8-C23-C24-C25
37	L	101	SQD	O47-C7-C8-C9
37	BB	621	SQD	O47-C7-C8-C9
37	B	617	SQD	O47-C7-C8-C9
44	C	520	DGD	O6D-C5D-C6D-O5D
32	c	509	CLA	C4-C3-C5-C6
32	YY	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
35	Dd	404	PL9	C35-C34-C36-C37
36	JJ	101	LHG	C11-C10-C9-C8
37	l	102	SQD	C11-C12-C13-C14
39	4	307	CHL	CAA-CBA-CGA-O2A
32	Y	613	CLA	C2-C3-C5-C6
32	g	603	CLA	C16-C17-C18-C20
32	b	607	CLA	C15-C16-C17-C18
32	Ss	602	CLA	CAA-CBA-CGA-O2A
32	DD	403	CLA	CAA-CBA-CGA-O2A
32	Gg	313	CLA	CAA-CBA-CGA-O2A
36	GG	618	LHG	O7-C7-C8-C9
37	LL	102	SQD	O47-C7-C8-C9
32	A	405	CLA	C14-C13-C15-C16
32	R	602	CLA	C14-C13-C15-C16
32	b	602	CLA	C14-C13-C15-C16
32	c	502	CLA	C6-C7-C8-C9
32	c	508	CLA	C6-C7-C8-C9
32	g	611	CLA	C11-C12-C13-C14
32	g	611	CLA	C14-C13-C15-C16
32	r	602	CLA	C11-C10-C8-C9
32	BB	607	CLA	C6-C7-C8-C9
32	BB	607	CLA	C11-C10-C8-C9
32	BB	610	CLA	C11-C10-C8-C9
32	B	606	CLA	C11-C10-C8-C9
32	NN	610	CLA	C14-C13-C15-C16
32	Bb	611	CLA	C6-C7-C8-C9
32	Gg	312	CLA	C11-C12-C13-C14
32	Gg	312	CLA	C14-C13-C15-C16
39	G	601	CHL	C11-C10-C8-C9
39	N	607	CHL	C11-C10-C8-C9
39	Y	609	CHL	C14-C13-C15-C16
32	44	603	CLA	CAA-CBA-CGA-O1A
32	y	306	CLA	C3A-C2A-CAA-CBA
32	YY	604	CLA	C3A-C2A-CAA-CBA
39	s	601	CHL	C3A-C2A-CAA-CBA
36	DD	407	LHG	C31-C32-C33-C34
36	C	522	LHG	O2-C2-C3-O3
32	Y	603	CLA	CAA-CBA-CGA-O2A
32	BB	607	CLA	CAA-CBA-CGA-O2A
32	Aa	410	CLA	CAA-CBA-CGA-O2A
32	Bb	609	CLA	CAA-CBA-CGA-O2A
37	CC	501	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	LL	102	SQD	O48-C23-C24-C25
39	Yy	609	CHL	CAA-CBA-CGA-O2A
36	Rr	617	LHG	C31-C32-C33-C34
36	EE	101	LHG	C14-C15-C16-C17
38	m	101	LMG	C32-C33-C34-C35
32	Rr	608	CLA	CAD-CBD-CGD-O2D
32	Rr	612	CLA	CAD-CBD-CGD-O2D
32	Ss	604	CLA	CAD-CBD-CGD-O2D
32	11	604	CLA	CAD-CBD-CGD-O2D
32	11	610	CLA	CAD-CBD-CGD-O2D
32	22	612	CLA	CAD-CBD-CGD-O2D
32	33	604	CLA	CAD-CBD-CGD-O2D
32	1	602	CLA	CAD-CBD-CGD-O2D
32	1	610	CLA	CAD-CBD-CGD-O2D
32	1	612	CLA	CAD-CBD-CGD-O2D
32	2	603	CLA	CAD-CBD-CGD-O2D
32	2	604	CLA	CAD-CBD-CGD-O2D
32	2	610	CLA	CAD-CBD-CGD-O2D
32	3	604	CLA	CAD-CBD-CGD-O2D
32	C	507	CLA	CAD-CBD-CGD-O2D
32	C	510	CLA	CAD-CBD-CGD-O2D
32	D	401	CLA	CAD-CBD-CGD-O2D
32	D	404	CLA	CAD-CBD-CGD-O2D
32	N	611	CLA	CAD-CBD-CGD-O2D
32	N	613	CLA	CAD-CBD-CGD-O2D
32	N	614	CLA	CAD-CBD-CGD-O2D
32	R	601	CLA	CAD-CBD-CGD-O2D
32	R	603	CLA	CAD-CBD-CGD-O2D
32	R	609	CLA	CAD-CBD-CGD-O2D
32	S	608	CLA	CAD-CBD-CGD-O2D
32	b	601	CLA	CAD-CBD-CGD-O2D
32	b	614	CLA	CAD-CBD-CGD-O2D
32	c	508	CLA	CAD-CBD-CGD-O2D
32	c	512	CLA	CAD-CBD-CGD-O2D
32	c	513	CLA	CAD-CBD-CGD-O2D
32	d	401	CLA	CAD-CBD-CGD-O2D
32	n	610	CLA	CAD-CBD-CGD-O2D
32	r	608	CLA	CAD-CBD-CGD-O2D
32	s	608	CLA	CAD-CBD-CGD-O2D
32	BB	601	CLA	CAD-CBD-CGD-O2D
32	BB	607	CLA	CAD-CBD-CGD-O2D
32	BB	608	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	CC	506	CLA	CAD-CBD-CGD-O2D
32	CC	509	CLA	CAD-CBD-CGD-O2D
32	DD	403	CLA	CAD-CBD-CGD-O2D
32	B	618	CLA	CAD-CBD-CGD-O2D
32	GG	614	CLA	CAD-CBD-CGD-O2D
32	NN	603	CLA	CAD-CBD-CGD-O2D
32	NN	613	CLA	CAD-CBD-CGD-O2D
32	RR	303	CLA	CAD-CBD-CGD-O2D
32	YY	604	CLA	CAD-CBD-CGD-O2D
32	Bb	609	CLA	CAD-CBD-CGD-O2D
32	Bb	614	CLA	CAD-CBD-CGD-O2D
32	Cc	514	CLA	CAD-CBD-CGD-O2D
32	Gg	312	CLA	CAD-CBD-CGD-O2D
33	A	407	PHO	CAD-CBD-CGD-O2D
39	44	605	CHL	CAD-CBD-CGD-O2D
39	22	601	CHL	CAD-CBD-CGD-O2D
39	22	607	CHL	CAD-CBD-CGD-O2D
39	33	605	CHL	CAD-CBD-CGD-O2D
39	2	608	CHL	CAD-CBD-CGD-O2D
39	3	608	CHL	CAD-CBD-CGD-O2D
39	G	606	CHL	CAD-CBD-CGD-O2D
39	N	606	CHL	CAD-CBD-CGD-O2D
39	Y	605	CHL	CAD-CBD-CGD-O2D
39	g	601	CHL	CAD-CBD-CGD-O2D
39	GG	601	CHL	CAD-CBD-CGD-O2D
39	GG	606	CHL	CAD-CBD-CGD-O2D
39	GG	608	CHL	CAD-CBD-CGD-O2D
39	GG	609	CHL	CAD-CBD-CGD-O2D
39	NN	606	CHL	CAD-CBD-CGD-O2D
39	SS	306	CHL	CAD-CBD-CGD-O2D
39	YY	605	CHL	CAD-CBD-CGD-O2D
39	YY	606	CHL	CAD-CBD-CGD-O2D
39	Gg	309	CHL	CAD-CBD-CGD-O2D
39	Nn	311	CHL	CAD-CBD-CGD-O2D
36	Rr	617	LHG	C8-C7-O7-C5
32	C	504	CLA	C16-C17-C18-C19
32	a	405	CLA	C16-C17-C18-C19
32	S	613	CLA	CAA-CBA-CGA-O2A
39	44	606	CHL	CAA-CBA-CGA-O2A
39	GG	607	CHL	CAA-CBA-CGA-O2A
44	h	102	DGD	C1B-C2B-C3B-C4B
32	Rr	601	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	n	618	LHG	O8-C23-C24-C25
37	L	101	SQD	O48-C23-C24-C25
32	BB	609	CLA	C4C-C3C-CAC-CBC
37	B	602	SQD	C32-C33-C34-C35
32	AA	408	CLA	C8-C10-C11-C12
32	Gg	304	CLA	C5-C6-C7-C8
32	B	606	CLA	C4-C3-C5-C6
32	Cc	511	CLA	C16-C17-C18-C19
32	S	603	CLA	CAA-CBA-CGA-O1A
39	44	601	CHL	CAA-CBA-CGA-O2A
39	4	302	CHL	CAA-CBA-CGA-O1A
39	4	306	CHL	CAA-CBA-CGA-O2A
39	4	309	CHL	CAA-CBA-CGA-O2A
32	C	504	CLA	C2-C3-C5-C6
32	Cc	512	CLA	C2-C3-C5-C6
35	DD	406	PL9	C28-C29-C31-C32
32	R	602	CLA	CAA-CBA-CGA-O2A
32	GG	602	CLA	CAA-CBA-CGA-O2A
36	G	618	LHG	O7-C7-C8-C9
36	II	101	LHG	O7-C7-C8-C9
36	JJ	101	LHG	O7-C7-C8-C9
37	l	102	SQD	O47-C7-C8-C9
37	Ll	101	SQD	O47-C7-C8-C9
44	a	415	DGD	O2G-C1B-C2B-C3B
44	Cc	519	DGD	C3A-C4A-C5A-C6A
44	Hh	102	DGD	C2A-C3A-C4A-C5A
34	C	517	BCR	C21-C22-C23-C24
34	h	101	BCR	C11-C12-C13-C14
34	BB	620	BCR	C21-C22-C23-C24
34	Bb	617	BCR	C21-C22-C23-C24
34	Cc	518	BCR	C7-C8-C9-C10
40	Yy	615	LUT	C7-C8-C9-C10
40	N	616	LUT	C7-C8-C9-C10
40	n	616	LUT	C7-C8-C9-C10
40	y	318	LUT	C7-C8-C9-C10
40	RR	315	LUT	C7-C8-C9-C10
35	d	404	PL9	C9-C11-C12-C13
32	B	607	CLA	C5-C6-C7-C8
44	c	518	DGD	C1A-C2A-C3A-C4A
42	Rr	616	NEX	O24-C26-C27-C28
42	Yy	617	NEX	O24-C26-C27-C28
42	Y	619	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
42	n	617	NEX	O24-C26-C27-C28
42	y	319	NEX	O24-C26-C27-C28
42	RR	317	NEX	O24-C26-C27-C28
32	4	305	CLA	CAA-CBA-CGA-O1A
32	4	305	CLA	CAA-CBA-CGA-O2A
46	Ee	101	HEM	CAD-CBD-CGD-O1D
44	Cc	520	DGD	C2A-C3A-C4A-C5A
36	Nn	310	LHG	C18-C19-C20-C21
36	N	619	LHG	O6-C4-C5-O7
32	G	610	CLA	CAA-CBA-CGA-O2A
32	b	613	CLA	CAA-CBA-CGA-O2A
32	g	612	CLA	CAA-CBA-CGA-O2A
32	r	601	CLA	CAA-CBA-CGA-O2A
32	BB	601	CLA	CAA-CBA-CGA-O2A
32	Bb	613	CLA	CAA-CBA-CGA-O2A
39	GG	601	CHL	CAA-CBA-CGA-O2A
44	Aa	401	DGD	O2G-C1B-C2B-C3B
32	a	410	CLA	C11-C12-C13-C15
32	Bb	610	CLA	C16-C17-C18-C20
32	Ss	602	CLA	O2A-C1-C2-C3
32	G	612	CLA	O2A-C1-C2-C3
32	Y	614	CLA	O2A-C1-C2-C3
32	s	602	CLA	O2A-C1-C2-C3
32	s	611	CLA	O2A-C1-C2-C3
32	y	316	CLA	O2A-C1-C2-C3
32	RR	308	CLA	O2A-C1-C2-C3
32	RR	314	CLA	O2A-C1-C2-C3
32	Aa	407	CLA	O2A-C1-C2-C3
39	R	605	CHL	O2A-C1-C2-C3
39	n	608	CHL	O2A-C1-C2-C3
39	r	607	CHL	O2A-C1-C2-C3
39	s	605	CHL	O2A-C1-C2-C3
39	y	310	CHL	O2A-C1-C2-C3
39	YY	608	CHL	O2A-C1-C2-C3
39	Nn	316	CHL	O2A-C1-C2-C3
32	44	602	CLA	CAA-CBA-CGA-O2A
32	44	604	CLA	CAA-CBA-CGA-O1A
32	44	604	CLA	CAA-CBA-CGA-O2A
32	CC	502	CLA	C8-C10-C11-C12
32	C	507	CLA	O2A-C1-C2-C3
32	C	511	CLA	O2A-C1-C2-C3
32	a	405	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	b	602	CLA	O2A-C1-C2-C3
32	b	603	CLA	O2A-C1-C2-C3
32	b	613	CLA	O2A-C1-C2-C3
32	BB	612	CLA	O2A-C1-C2-C3
32	BB	614	CLA	O2A-C1-C2-C3
32	CC	510	CLA	O2A-C1-C2-C3
32	B	608	CLA	O2A-C1-C2-C3
32	B	610	CLA	O2A-C1-C2-C3
32	Bb	602	CLA	O2A-C1-C2-C3
32	Bb	603	CLA	O2A-C1-C2-C3
32	Bb	613	CLA	O2A-C1-C2-C3
33	D	402	PHO	O2A-C1-C2-C3
33	a	409	PHO	O2A-C1-C2-C3
33	DD	402	PHO	O2A-C1-C2-C3
33	Aa	409	PHO	O2A-C1-C2-C3
39	Yy	601	CHL	O2A-C1-C2-C3
39	Y	601	CHL	O2A-C1-C2-C3
39	y	303	CHL	O2A-C1-C2-C3
39	YY	601	CHL	O2A-C1-C2-C3
32	BB	613	CLA	C2A-CAA-CBA-CGA
32	B	624	CLA	C2A-CAA-CBA-CGA
32	CC	509	CLA	C5-C6-C7-C8
44	C	519	DGD	C7B-C8B-C9B-CAB
32	Ss	612	CLA	CAA-CBA-CGA-O2A
32	r	608	CLA	CAA-CBA-CGA-O2A
32	r	611	CLA	CAA-CBA-CGA-O2A
32	GG	612	CLA	CAA-CBA-CGA-O2A
39	RR	307	CHL	CAA-CBA-CGA-O2A
32	S	613	CLA	CAA-CBA-CGA-O1A
39	G	607	CHL	CAA-CBA-CGA-O2A
46	e	101	HEM	CAA-CBA-CGA-O2A
36	D	409	LHG	C19-C20-C21-C22
44	D	411	DGD	C9B-CAB-CBB-CCB
32	c	510	CLA	C16-C17-C18-C19
32	Bb	610	CLA	C16-C17-C18-C19
39	Yy	609	CHL	C16-C17-C18-C19
36	y	320	LHG	O9-C7-O7-C5
44	c	518	DGD	C5B-C6B-C7B-C8B
32	Yy	604	CLA	O1D-CGD-O2D-CED
32	Rr	601	CLA	CHA-CBD-CGD-O1D
32	Rr	601	CLA	CHA-CBD-CGD-O2D
32	Rr	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	Rr	602	CLA	CHA-CBD-CGD-O2D
32	Rr	603	CLA	CHA-CBD-CGD-O1D
32	Rr	603	CLA	CHA-CBD-CGD-O2D
32	Ss	611	CLA	CHA-CBD-CGD-O2D
32	Yy	602	CLA	CHA-CBD-CGD-O2D
32	44	602	CLA	CHA-CBD-CGD-O2D
32	44	603	CLA	CHA-CBD-CGD-O2D
32	44	609	CLA	CHA-CBD-CGD-O2D
32	44	610	CLA	CHA-CBD-CGD-O1D
32	44	610	CLA	CHA-CBD-CGD-O2D
32	11	604	CLA	CHA-CBD-CGD-O1D
32	11	612	CLA	CHA-CBD-CGD-O1D
32	33	603	CLA	CHA-CBD-CGD-O1D
32	33	603	CLA	CHA-CBD-CGD-O2D
32	33	612	CLA	CHA-CBD-CGD-O1D
32	33	612	CLA	CHA-CBD-CGD-O2D
32	2	602	CLA	CHA-CBD-CGD-O1D
32	2	602	CLA	CHA-CBD-CGD-O2D
32	3	603	CLA	CHA-CBD-CGD-O2D
32	C	504	CLA	CHA-CBD-CGD-O1D
32	C	510	CLA	CHA-CBD-CGD-O1D
32	C	511	CLA	CHA-CBD-CGD-O2D
32	G	612	CLA	CHA-CBD-CGD-O1D
32	G	612	CLA	CHA-CBD-CGD-O2D
32	R	604	CLA	CHA-CBD-CGD-O1D
32	R	608	CLA	CHA-CBD-CGD-O1D
32	R	608	CLA	CHA-CBD-CGD-O2D
32	S	602	CLA	CHA-CBD-CGD-O1D
32	S	604	CLA	CHA-CBD-CGD-O2D
32	S	611	CLA	CHA-CBD-CGD-O1D
32	S	611	CLA	CHA-CBD-CGD-O2D
32	X	201	CLA	CHA-CBD-CGD-O1D
32	Y	602	CLA	CHA-CBD-CGD-O1D
32	b	605	CLA	CHA-CBD-CGD-O1D
32	b	612	CLA	CHA-CBD-CGD-O2D
32	b	615	CLA	CHA-CBD-CGD-O2D
32	c	507	CLA	CHA-CBD-CGD-O1D
32	c	507	CLA	CHA-CBD-CGD-O2D
32	g	602	CLA	CHA-CBD-CGD-O1D
32	g	602	CLA	CHA-CBD-CGD-O2D
32	g	613	CLA	CHA-CBD-CGD-O1D
32	g	613	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	n	613	CLA	CHA-CBD-CGD-O1D
32	n	613	CLA	CHA-CBD-CGD-O2D
32	r	601	CLA	CHA-CBD-CGD-O2D
32	r	602	CLA	CHA-CBD-CGD-O1D
32	r	602	CLA	CHA-CBD-CGD-O2D
32	r	613	CLA	CHA-CBD-CGD-O1D
32	r	613	CLA	CHA-CBD-CGD-O2D
32	4	304	CLA	CHA-CBD-CGD-O1D
32	4	310	CLA	CHA-CBD-CGD-O1D
32	4	310	CLA	CHA-CBD-CGD-O2D
32	4	312	CLA	CHA-CBD-CGD-O1D
32	4	312	CLA	CHA-CBD-CGD-O2D
32	BB	603	CLA	CHA-CBD-CGD-O1D
32	BB	612	CLA	CHA-CBD-CGD-O1D
32	BB	612	CLA	CHA-CBD-CGD-O2D
32	CC	503	CLA	CHA-CBD-CGD-O1D
32	CC	509	CLA	CHA-CBD-CGD-O1D
32	CC	509	CLA	CHA-CBD-CGD-O2D
32	CC	510	CLA	CHA-CBD-CGD-O1D
32	B	608	CLA	CHA-CBD-CGD-O1D
32	B	608	CLA	CHA-CBD-CGD-O2D
32	B	621	CLA	CHA-CBD-CGD-O2D
32	GG	602	CLA	CHA-CBD-CGD-O1D
32	GG	612	CLA	CHA-CBD-CGD-O1D
32	GG	612	CLA	CHA-CBD-CGD-O2D
32	RR	304	CLA	CHA-CBD-CGD-O2D
32	RR	308	CLA	CHA-CBD-CGD-O2D
32	SS	304	CLA	CHA-CBD-CGD-O1D
32	SS	305	CLA	CHA-CBD-CGD-O1D
32	SS	305	CLA	CHA-CBD-CGD-O2D
32	SS	312	CLA	CHA-CBD-CGD-O2D
32	SS	313	CLA	CHA-CBD-CGD-O1D
32	SS	313	CLA	CHA-CBD-CGD-O2D
32	YY	604	CLA	CHA-CBD-CGD-O2D
32	Bb	602	CLA	CHA-CBD-CGD-O2D
32	Bb	605	CLA	CHA-CBD-CGD-O1D
32	Bb	605	CLA	CHA-CBD-CGD-O2D
32	Bb	612	CLA	CHA-CBD-CGD-O1D
32	Bb	612	CLA	CHA-CBD-CGD-O2D
32	Bb	615	CLA	CHA-CBD-CGD-O2D
32	Cc	504	CLA	CHA-CBD-CGD-O1D
32	Cc	504	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	Cc	505	CLA	CHA-CBD-CGD-O1D
32	Cc	509	CLA	CHA-CBD-CGD-O1D
32	Cc	509	CLA	CHA-CBD-CGD-O2D
32	Cc	515	CLA	CHA-CBD-CGD-O1D
32	Cc	515	CLA	CHA-CBD-CGD-O2D
32	Gg	313	CLA	CHA-CBD-CGD-O1D
32	Gg	313	CLA	CHA-CBD-CGD-O2D
32	Nn	304	CLA	CHA-CBD-CGD-O1D
32	Nn	304	CLA	CHA-CBD-CGD-O2D
39	Ss	601	CHL	CHA-CBD-CGD-O1D
39	Ss	601	CHL	CHA-CBD-CGD-O2D
39	Ss	605	CHL	CHA-CBD-CGD-O1D
39	Ss	607	CHL	CHA-CBD-CGD-O1D
39	1	601	CHL	CHA-CBD-CGD-O1D
39	1	605	CHL	CHA-CBD-CGD-O1D
39	1	605	CHL	CHA-CBD-CGD-O2D
39	1	608	CHL	CHA-CBD-CGD-O2D
39	2	607	CHL	CHA-CBD-CGD-O1D
39	3	606	CHL	CHA-CBD-CGD-O1D
39	3	606	CHL	CHA-CBD-CGD-O2D
39	G	605	CHL	CHA-CBD-CGD-O1D
39	G	608	CHL	CHA-CBD-CGD-O1D
39	G	608	CHL	CHA-CBD-CGD-O2D
39	g	605	CHL	CHA-CBD-CGD-O1D
39	g	605	CHL	CHA-CBD-CGD-O2D
39	n	608	CHL	CHA-CBD-CGD-O1D
39	n	609	CHL	CHA-CBD-CGD-O1D
39	n	609	CHL	CHA-CBD-CGD-O2D
39	s	605	CHL	CHA-CBD-CGD-O2D
39	s	607	CHL	CHA-CBD-CGD-O1D
39	s	607	CHL	CHA-CBD-CGD-O2D
39	y	307	CHL	CHA-CBD-CGD-O2D
39	Gg	306	CHL	CHA-CBD-CGD-O1D
39	Gg	306	CHL	CHA-CBD-CGD-O2D
39	Nn	318	CHL	CHA-CBD-CGD-O2D
39	Nn	319	CHL	CHA-CBD-CGD-O1D
39	Nn	319	CHL	CHA-CBD-CGD-O2D
32	44	602	CLA	CAA-CBA-CGA-O1A
39	4	306	CHL	CAA-CBA-CGA-O1A
39	4	309	CHL	CAA-CBA-CGA-O1A
32	r	609	CLA	C4-C3-C5-C6
32	y	315	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	A	407	PHO	C4-C3-C5-C6
32	Y	610	CLA	CAA-CBA-CGA-O2A
32	b	616	CLA	CAA-CBA-CGA-O2A
32	SS	314	CLA	CAA-CBA-CGA-O2A
39	y	311	CHL	CAA-CBA-CGA-O2A
32	YY	613	CLA	C2-C3-C5-C6
35	DD	406	PL9	C43-C44-C46-C47
36	D	408	LHG	C29-C30-C31-C32
36	CC	523	LHG	O6-C4-C5-C6
36	DD	408	LHG	O6-C4-C5-C6
39	44	606	CHL	CAA-CBA-CGA-O1A
39	G	607	CHL	CAA-CBA-CGA-O1A
37	LL	102	SQD	C45-C46-O48-C23
32	A	406	CLA	CAA-CBA-CGA-O2A
32	Ss	609	CLA	CAA-CBA-CGA-O2A
32	c	508	CLA	CAA-CBA-CGA-O2A
32	B	618	CLA	CAA-CBA-CGA-O2A
32	B	624	CLA	CAA-CBA-CGA-O2A
32	Bb	616	CLA	CAA-CBA-CGA-O2A
32	Cc	509	CLA	CAA-CBA-CGA-O2A
36	3	614	LHG	O7-C7-C8-C9
39	R	607	CHL	CAA-CBA-CGA-O2A
39	Gg	302	CHL	CAA-CBA-CGA-O2A
36	s	616	LHG	C13-C14-C15-C16
36	44	616	LHG	O7-C5-C6-O8
36	0	201	LHG	O7-C5-C6-O8
36	Y	618	LHG	O7-C5-C6-O8
36	AA	414	LHG	O7-C5-C6-O8
37	A	412	SQD	O47-C45-C46-O48
44	Hh	102	DGD	C1B-C2B-C3B-C4B
44	B	601	DGD	CCB-CDB-CEB-CFB
44	B	603	DGD	C2A-C3A-C4A-C5A
39	4	307	CHL	CAA-CBA-CGA-O1A
36	J	101	LHG	C26-C27-C28-C29
44	Hh	102	DGD	C7B-C8B-C9B-CAB
32	Rr	608	CLA	CAA-CBA-CGA-O2A
32	Yy	604	CLA	CAA-CBA-CGA-O2A
32	G	612	CLA	CAA-CBA-CGA-O2A
32	b	605	CLA	CAA-CBA-CGA-O2A
32	BB	612	CLA	CAA-CBA-CGA-O2A
32	YY	604	CLA	CAA-CBA-CGA-O2A
36	JJ	101	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
39	Ss	605	CHL	CAA-CBA-CGA-O2A
39	G	601	CHL	CAA-CBA-CGA-O2A
39	g	601	CHL	CAA-CBA-CGA-O2A
39	s	601	CHL	CAA-CBA-CGA-O2A
44	CC	518	DGD	O2G-C1B-C2B-C3B
38	BB	619	LMG	C16-C17-C18-C19
39	YY	609	CHL	C2A-CAA-CBA-CGA
39	GG	607	CHL	CAA-CBA-CGA-O1A
33	Aa	408	PHO	CHA-CBD-CGD-O1D
32	Y	612	CLA	C15-C16-C17-C18
38	WW	201	LMG	C29-C28-O8-C9
44	C	520	DGD	CDA-CEA-CFA-CGA
44	c	517	DGD	C3A-C4A-C5A-C6A
36	Ss	616	LHG	C8-C7-O7-C5
32	r	603	CLA	CAA-CBA-CGA-O2A
32	s	612	CLA	CAA-CBA-CGA-O2A
32	B	608	CLA	CAA-CBA-CGA-O2A
36	s	616	LHG	O8-C23-C24-C25
44	Cc	520	DGD	C5B-C6B-C7B-C8B
32	D	404	CLA	C11-C12-C13-C15
32	R	602	CLA	C6-C7-C8-C10
32	c	509	CLA	C2-C3-C5-C6
32	d	401	CLA	C11-C10-C8-C7
32	BB	604	CLA	C2-C3-C5-C6
32	CC	509	CLA	C12-C13-C15-C16
32	B	606	CLA	C2-C3-C5-C6
32	B	621	CLA	C11-C10-C8-C7
32	Bb	603	CLA	C12-C13-C15-C16
32	Cc	504	CLA	C6-C7-C8-C10
32	Cc	512	CLA	C12-C13-C15-C16
33	AA	407	PHO	C6-C7-C8-C10
32	y	304	CLA	C16-C17-C18-C20
32	Cc	512	CLA	C16-C17-C18-C19
32	Gg	304	CLA	C16-C17-C18-C20
35	AA	410	PL9	C4-C3-C7-C8
35	Dd	404	PL9	C4-C3-C7-C8
38	B	615	LMG	C12-C13-C14-C15
38	Dd	408	LMG	O6-C1-O1-C7
32	b	609	CLA	CAA-CBA-CGA-O2A
32	c	507	CLA	CAA-CBA-CGA-O2A
44	C	523	DGD	C6B-C7B-C8B-C9B
32	Rr	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	D	404	CLA	C11-C12-C13-C14
32	N	610	CLA	C14-C13-C15-C16
32	R	602	CLA	C6-C7-C8-C9
32	a	405	CLA	C11-C10-C8-C9
32	b	604	CLA	C14-C13-C15-C16
32	b	606	CLA	C11-C10-C8-C9
32	b	611	CLA	C6-C7-C8-C9
32	AA	405	CLA	C14-C13-C15-C16
32	BB	602	CLA	C11-C10-C8-C9
32	BB	604	CLA	C11-C10-C8-C9
32	B	610	CLA	C11-C12-C13-C14
32	B	619	CLA	C11-C10-C8-C9
32	B	619	CLA	C14-C13-C15-C16
32	B	624	CLA	C11-C10-C8-C9
32	RR	302	CLA	C14-C13-C15-C16
32	Bb	604	CLA	C14-C13-C15-C16
32	Bb	605	CLA	C14-C13-C15-C16
32	Bb	609	CLA	C11-C10-C8-C9
32	Cc	504	CLA	C6-C7-C8-C9
32	Cc	510	CLA	C6-C7-C8-C9
32	Cc	514	CLA	C11-C10-C8-C9
32	Dd	401	CLA	C11-C10-C8-C9
32	Nn	301	CLA	C6-C7-C8-C9
33	A	407	PHO	C6-C7-C8-C9
32	Gg	313	CLA	CAA-CBA-CGA-O1A
37	BB	621	SQD	O49-C7-C8-C9
32	YY	612	CLA	C8-C10-C11-C12
32	Rr	612	CLA	O2A-C1-C2-C3
32	Yy	614	CLA	O2A-C1-C2-C3
32	S	604	CLA	O2A-C1-C2-C3
32	S	610	CLA	O2A-C1-C2-C3
32	a	407	CLA	O2A-C1-C2-C3
32	g	610	CLA	O2A-C1-C2-C3
32	n	612	CLA	O2A-C1-C2-C3
32	GG	612	CLA	O2A-C1-C2-C3
32	RR	303	CLA	O2A-C1-C2-C3
32	SS	311	CLA	O2A-C1-C2-C3
32	YY	614	CLA	O2A-C1-C2-C3
39	Rr	606	CHL	O2A-C1-C2-C3
39	Ss	605	CHL	O2A-C1-C2-C3
39	Ss	606	CHL	O2A-C1-C2-C3
39	n	609	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
36	D	409	LHG	C17-C18-C19-C20
36	DD	407	LHG	C29-C30-C31-C32
38	W	201	LMG	C29-C28-O8-C9
32	GG	603	CLA	CAA-CBA-CGA-O2A
36	D	408	LHG	O8-C23-C24-C25
37	C	501	SQD	C4-C5-C6-S
37	AA	412	SQD	C5-C6-S-O8
37	CC	501	SQD	C4-C5-C6-S
32	c	510	CLA	C16-C17-C18-C20
32	Aa	410	CLA	C11-C12-C13-C14
32	Cc	511	CLA	C16-C17-C18-C20
36	A	414	LHG	C15-C16-C17-C18
36	l	101	LHG	C31-C32-C33-C34
36	Yy	618	LHG	C8-C7-O7-C5
32	a	406	CLA	C2A-CAA-CBA-CGA
32	g	603	CLA	C2A-CAA-CBA-CGA
32	B	607	CLA	C2A-CAA-CBA-CGA
32	B	609	CLA	C2A-CAA-CBA-CGA
36	DD	408	LHG	C7-C8-C9-C10
36	n	618	LHG	O10-C23-C24-C25
37	LL	102	SQD	O10-C23-C24-C25
44	a	415	DGD	O1B-C1B-C2B-C3B
32	D	404	CLA	CAA-CBA-CGA-O2A
36	Ss	616	LHG	O8-C23-C24-C25
36	r	616	LHG	O8-C23-C24-C25
36	DD	407	LHG	O8-C23-C24-C25
37	C	501	SQD	O47-C7-C8-C9
32	CC	506	CLA	C4C-C3C-CAC-CBC
37	L	102	SQD	C13-C14-C15-C16
36	EE	101	LHG	C9-C10-C11-C12
39	44	601	CHL	CAA-CBA-CGA-O1A
37	B	617	SQD	O49-C7-C8-C9
39	NN	607	CHL	C13-C15-C16-C17
32	Yy	602	CLA	C16-C17-C18-C19
32	Cc	512	CLA	C16-C17-C18-C20
39	y	311	CHL	C16-C17-C18-C19
36	22	615	LHG	C24-C25-C26-C27
32	Aa	405	CLA	C4-C3-C5-C6
32	a	406	CLA	CAA-CBA-CGA-O2A
32	SS	303	CLA	CAA-CBA-CGA-O2A
32	Cc	508	CLA	C8-C10-C11-C12
38	m	101	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	Ss	602	CLA	CAA-CBA-CGA-O1A
32	D	404	CLA	CAA-CBA-CGA-O1A
32	BB	607	CLA	CAA-CBA-CGA-O1A
37	A	412	SQD	O49-C7-C8-C9
37	L	101	SQD	O10-C23-C24-C25
37	l	102	SQD	O49-C7-C8-C9
40	n	615	LUT	C11-C12-C13-C14
36	11	614	LHG	C25-C26-C27-C28
32	C	515	CLA	C1A-C2A-CAA-CBA
32	G	603	CLA	C1A-C2A-CAA-CBA
32	a	406	CLA	C1A-C2A-CAA-CBA
32	y	306	CLA	C1A-C2A-CAA-CBA
32	CC	514	CLA	C1A-C2A-CAA-CBA
32	B	620	CLA	C1A-C2A-CAA-CBA
32	YY	612	CLA	C1A-C2A-CAA-CBA
32	Aa	406	CLA	C1A-C2A-CAA-CBA
32	Gg	303	CLA	C1A-C2A-CAA-CBA
39	Yy	605	CHL	C1A-C2A-CAA-CBA
32	G	610	CLA	CAA-CBA-CGA-O1A
37	L	101	SQD	O49-C7-C8-C9
37	LL	102	SQD	O49-C7-C8-C9
37	Ll	101	SQD	O49-C7-C8-C9
32	c	506	CLA	C8-C10-C11-C12
32	BB	606	CLA	C2-C1-O2A-CGA
38	BB	619	LMG	C30-C31-C32-C33
36	y	320	LHG	C24-C23-O8-C6
32	Y	603	CLA	CAA-CBA-CGA-O1A
32	Bb	609	CLA	CAA-CBA-CGA-O1A
36	II	101	LHG	O9-C7-C8-C9
36	JJ	101	LHG	O9-C7-C8-C9
37	LL	101	SQD	O49-C7-C8-C9
32	4	311	CLA	CAA-CBA-CGA-O1A
36	YY	618	LHG	C4-C5-C6-O8
37	L	101	SQD	O6-C44-C45-C46
44	C	523	DGD	C1G-C2G-C3G-O3G
44	Cc	519	DGD	C1G-C2G-C3G-O3G
32	Bb	605	CLA	CAA-CBA-CGA-O2A
32	A	405	CLA	C2A-CAA-CBA-CGA
32	Bb	608	CLA	C2A-CAA-CBA-CGA
36	33	614	LHG	C4-O6-P-O3
32	Rr	601	CLA	CAA-CBA-CGA-O1A
32	Rr	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	44	615	CLA	CAA-CBA-CGA-O1A
32	a	410	CLA	CAA-CBA-CGA-O1A
32	DD	403	CLA	CAA-CBA-CGA-O1A
36	3	614	LHG	O9-C7-C8-C9
36	GG	618	LHG	O9-C7-C8-C9
37	L	102	SQD	O49-C7-C8-C9
39	R	607	CHL	CAA-CBA-CGA-O1A
39	y	311	CHL	CAA-CBA-CGA-O1A
36	A	413	LHG	C27-C28-C29-C30
32	Rr	603	CLA	CAA-CBA-CGA-O2A
32	g	611	CLA	CAA-CBA-CGA-O2A
32	y	306	CLA	CAA-CBA-CGA-O2A
32	AA	406	CLA	CAA-CBA-CGA-O2A
32	a	406	CLA	C8-C10-C11-C12
36	AA	411	LHG	C5-C4-O6-P
44	h	102	DGD	C2A-C3A-C4A-C5A
32	Yy	604	CLA	CAA-CBA-CGA-O1A
32	s	612	CLA	CAA-CBA-CGA-O1A
36	Nn	310	LHG	O10-C23-C24-C25
38	WW	201	LMG	C2-C1-O1-C7
32	Bb	606	CLA	C5-C6-C7-C8
36	33	614	LHG	C4-O6-P-O5
36	3	614	LHG	C4-O6-P-O5
36	0	201	LHG	C3-O3-P-O5
36	d	405	LHG	C3-O3-P-O5
36	g	618	LHG	C4-O6-P-O5
36	4	301	LHG	C3-O3-P-O4
36	4	315	LHG	C4-O6-P-O5
36	EE	101	LHG	C3-O3-P-O5
36	EE	101	LHG	C4-O6-P-O5
36	Dd	405	LHG	C3-O3-P-O5
36	Gg	319	LHG	C4-O6-P-O5
36	Ll	102	LHG	C4-O6-P-O5
32	g	603	CLA	C16-C17-C18-C19
32	B	605	CLA	C4C-C3C-CAC-CBC
32	A	406	CLA	CAA-CBA-CGA-O1A
32	Ss	612	CLA	CAA-CBA-CGA-O1A
32	Y	610	CLA	CAA-CBA-CGA-O1A
32	c	507	CLA	CAA-CBA-CGA-O1A
32	g	612	CLA	CAA-CBA-CGA-O1A
32	r	611	CLA	CAA-CBA-CGA-O1A
32	B	624	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	GG	612	CLA	CAA-CBA-CGA-O1A
32	YY	604	CLA	CAA-CBA-CGA-O1A
32	Bb	616	CLA	CAA-CBA-CGA-O1A
32	Cc	509	CLA	CAA-CBA-CGA-O1A
36	G	618	LHG	O9-C7-C8-C9
37	CC	501	SQD	O49-C7-C8-C9
39	GG	601	CHL	CAA-CBA-CGA-O1A
32	Ss	610	CLA	O2A-C1-C2-C3
32	Yy	604	CLA	O2A-C1-C2-C3
32	R	614	CLA	O2A-C1-C2-C3
32	S	612	CLA	O2A-C1-C2-C3
32	n	603	CLA	O2A-C1-C2-C3
32	s	610	CLA	O2A-C1-C2-C3
32	NN	613	CLA	O2A-C1-C2-C3
32	SS	313	CLA	O2A-C1-C2-C3
39	s	606	CHL	O2A-C1-C2-C3
39	RR	305	CHL	O2A-C1-C2-C3
39	Nn	319	CHL	O2A-C1-C2-C3
36	A	413	LHG	O6-C4-C5-C6
36	DD	407	LHG	C24-C25-C26-C27
44	CC	519	DGD	O6D-C5D-C6D-O5D
46	e	101	HEM	CAA-CBA-CGA-O1A
34	C	516	BCR	C1-C6-C7-C8
34	h	101	BCR	C1-C6-C7-C8
34	h	101	BCR	C5-C6-C7-C8
34	CC	515	BCR	C1-C6-C7-C8
34	Hh	101	BCR	C1-C6-C7-C8
34	Hh	101	BCR	C5-C6-C7-C8
40	Yy	615	LUT	C1-C6-C7-C8
40	S	614	LUT	C1-C6-C7-C8
40	Y	615	LUT	C1-C6-C7-C8
40	s	614	LUT	C1-C6-C7-C8
40	NN	615	LUT	C1-C6-C7-C8
40	YY	615	LUT	C1-C6-C7-C8
40	Gg	316	LUT	C1-C6-C7-C8
36	Nn	310	LHG	C19-C20-C21-C22
44	BB	624	DGD	CCB-CDB-CEB-CFB
32	d	402	CLA	C13-C15-C16-C17
36	D	408	LHG	C23-C24-C25-C26
42	g	617	NEX	C26-C27-C28-C29
42	Gg	318	NEX	C26-C27-C28-C29
32	R	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	b	609	CLA	CAA-CBA-CGA-O1A
32	b	616	CLA	CAA-CBA-CGA-O1A
32	r	608	CLA	CAA-CBA-CGA-O1A
32	B	608	CLA	CAA-CBA-CGA-O1A
32	Aa	410	CLA	CAA-CBA-CGA-O1A
37	C	501	SQD	O49-C7-C8-C9
39	Yy	609	CHL	CAA-CBA-CGA-O1A
39	G	601	CHL	CAA-CBA-CGA-O1A
39	RR	307	CHL	CAA-CBA-CGA-O1A
32	R	613	CLA	C4C-C3C-CAC-CBC
36	C	522	LHG	O7-C7-C8-C9
36	YY	618	LHG	O7-C7-C8-C9
39	r	605	CHL	CAA-CBA-CGA-O2A
32	Ss	609	CLA	CAA-CBA-CGA-O1A
32	r	601	CLA	CAA-CBA-CGA-O1A
32	SS	314	CLA	CAA-CBA-CGA-O1A
32	Bb	613	CLA	CAA-CBA-CGA-O1A
39	g	601	CHL	CAA-CBA-CGA-O1A
39	s	601	CHL	CAA-CBA-CGA-O1A
37	l	102	SQD	O10-C23-O48-C46
35	DD	406	PL9	C32-C33-C34-C36
36	YY	618	LHG	C11-C10-C9-C8
37	CC	501	SQD	C19-C20-C21-C22
32	NN	602	CLA	CAA-CBA-CGA-O2A
32	Aa	406	CLA	CAA-CBA-CGA-O2A
32	Gg	312	CLA	CAA-CBA-CGA-O2A
36	A	414	LHG	O8-C23-C24-C25
36	Y	618	LHG	O7-C7-C8-C9
39	RR	306	CHL	CAA-CBA-CGA-O2A
33	Aa	408	PHO	O1D-CGD-O2D-CED
32	b	613	CLA	CAA-CBA-CGA-O1A
32	GG	602	CLA	CAA-CBA-CGA-O1A
44	Aa	401	DGD	O1B-C1B-C2B-C3B
32	Yy	613	CLA	C4-C3-C5-C6
39	N	607	CHL	C13-C15-C16-C17
32	C	512	CLA	C16-C17-C18-C20
36	D	408	LHG	C25-C26-C27-C28
36	DD	407	LHG	C25-C26-C27-C28
44	C	519	DGD	C6B-C7B-C8B-C9B
32	33	612	CLA	CAD-CBD-CGD-O1D
32	C	504	CLA	CAD-CBD-CGD-O1D
32	Y	602	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	b	615	CLA	CAD-CBD-CGD-O1D
32	c	508	CLA	CAD-CBD-CGD-O1D
32	g	613	CLA	CAD-CBD-CGD-O1D
32	n	603	CLA	CAD-CBD-CGD-O1D
32	n	613	CLA	CAD-CBD-CGD-O1D
32	r	602	CLA	CAD-CBD-CGD-O1D
32	BB	603	CLA	CAD-CBD-CGD-O1D
32	BB	615	CLA	CAD-CBD-CGD-O1D
32	CC	503	CLA	CAD-CBD-CGD-O1D
32	B	611	CLA	CAD-CBD-CGD-O1D
32	GG	611	CLA	CAD-CBD-CGD-O1D
32	GG	613	CLA	CAD-CBD-CGD-O1D
32	RR	312	CLA	CAD-CBD-CGD-O1D
32	Bb	615	CLA	CAD-CBD-CGD-O1D
32	Cc	505	CLA	CAD-CBD-CGD-O1D
32	Nn	303	CLA	CAD-CBD-CGD-O1D
32	Nn	312	CLA	CAD-CBD-CGD-O1D
32	Nn	313	CLA	CAD-CBD-CGD-O1D
37	C	501	SQD	O5-C5-C6-S
37	CC	501	SQD	O5-C5-C6-S
39	Ss	601	CHL	CAD-CBD-CGD-O1D
39	44	607	CHL	CAD-CBD-CGD-O1D
39	1	601	CHL	CAD-CBD-CGD-O1D
39	2	607	CHL	CAD-CBD-CGD-O1D
39	n	608	CHL	CAD-CBD-CGD-O1D
39	4	306	CHL	CAD-CBD-CGD-O1D
39	NN	605	CHL	CAD-CBD-CGD-O1D
39	RR	305	CHL	CAD-CBD-CGD-O1D
39	Nn	319	CHL	CAD-CBD-CGD-O1D
32	Rr	608	CLA	CAA-CBA-CGA-O1A
32	c	508	CLA	CAA-CBA-CGA-O1A
32	r	603	CLA	CAA-CBA-CGA-O1A
32	SS	303	CLA	CAA-CBA-CGA-O1A
36	r	616	LHG	O10-C23-C24-C25
39	Gg	302	CHL	CAA-CBA-CGA-O1A
44	C	519	DGD	CDB-CEB-CFB-CGB
32	N	602	CLA	CAA-CBA-CGA-O2A
32	Y	604	CLA	CAA-CBA-CGA-O2A
32	YY	603	CLA	CAA-CBA-CGA-O2A
38	W	201	LMG	O7-C10-C11-C12
38	WW	201	LMG	O7-C10-C11-C12
32	BB	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	Bb	609	CLA	C15-C16-C17-C18
32	C	510	CLA	C14-C13-C15-C16
32	b	602	CLA	C6-C7-C8-C9
32	b	604	CLA	C6-C7-C8-C9
32	b	605	CLA	C14-C13-C15-C16
32	b	610	CLA	C14-C13-C15-C16
32	b	616	CLA	C11-C12-C13-C14
32	c	501	CLA	C11-C12-C13-C14
32	c	510	CLA	C14-C13-C15-C16
32	c	512	CLA	C11-C10-C8-C9
32	g	603	CLA	C11-C12-C13-C14
32	BB	602	CLA	C14-C13-C15-C16
32	BB	614	CLA	C11-C12-C13-C14
32	Bb	604	CLA	C6-C7-C8-C9
32	Cc	512	CLA	C14-C13-C15-C16
32	Cc	513	CLA	C14-C13-C15-C16
32	Dd	402	CLA	C14-C13-C15-C16
33	a	408	PHO	C11-C10-C8-C9
39	G	601	CHL	C6-C7-C8-C9
39	YY	609	CHL	C14-C13-C15-C16
36	GG	618	LHG	O1-C1-C2-O2
32	G	612	CLA	CAA-CBA-CGA-O1A
39	Ss	605	CHL	CAA-CBA-CGA-O1A
44	CC	518	DGD	O1B-C1B-C2B-C3B
32	CC	509	CLA	C16-C17-C18-C20
32	Bb	612	CLA	C16-C17-C18-C20
32	Rr	611	CLA	CAA-CBA-CGA-O2A
32	y	304	CLA	CAA-CBA-CGA-O2A
32	CC	506	CLA	CAA-CBA-CGA-O2A
32	B	619	CLA	CAA-CBA-CGA-O2A
32	Cc	507	CLA	CAA-CBA-CGA-O2A
38	b	621	LMG	C11-C12-C13-C14
36	33	614	LHG	C24-C25-C26-C27
36	y	320	LHG	O10-C23-O8-C6
32	y	306	CLA	CAA-CBA-CGA-O1A
32	BB	611	CLA	C2A-CAA-CBA-CGA
32	Yy	602	CLA	CAA-CBA-CGA-O2A
32	Y	602	CLA	CAA-CBA-CGA-O2A
32	r	602	CLA	CAA-CBA-CGA-O2A
32	BB	602	CLA	CAA-CBA-CGA-O2A
32	Nn	305	CLA	CAA-CBA-CGA-O2A
33	AA	407	PHO	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	N	602	CLA	C13-C15-C16-C17
39	Gg	302	CHL	C10-C11-C12-C13
32	Y	604	CLA	CAA-CBA-CGA-O1A
32	3	610	CLA	C2C-C3C-CAC-CBC
32	BB	608	CLA	C4-C3-C5-C6
38	DD	409	LMG	C11-C12-C13-C14
44	CC	519	DGD	C2A-C3A-C4A-C5A
32	Yy	602	CLA	C12-C13-C15-C16
32	Yy	610	CLA	C6-C7-C8-C10
32	C	510	CLA	C11-C12-C13-C15
32	C	513	CLA	C11-C10-C8-C7
32	Y	610	CLA	C11-C12-C13-C15
32	Y	613	CLA	C6-C7-C8-C10
32	b	602	CLA	C6-C7-C8-C10
32	b	604	CLA	C6-C7-C8-C10
32	b	611	CLA	C6-C7-C8-C10
32	b	616	CLA	C11-C12-C13-C15
32	c	501	CLA	C11-C10-C8-C7
32	c	506	CLA	C12-C13-C15-C16
32	c	508	CLA	C6-C7-C8-C10
32	y	312	CLA	C6-C7-C8-C10
32	BB	602	CLA	C11-C10-C8-C7
32	CC	502	CLA	C11-C12-C13-C15
32	CC	512	CLA	C11-C10-C8-C7
32	B	605	CLA	C12-C13-C15-C16
32	B	610	CLA	C11-C12-C13-C15
32	B	619	CLA	C11-C10-C8-C7
32	B	621	CLA	C2-C3-C5-C6
32	RR	302	CLA	C6-C7-C8-C10
32	Bb	604	CLA	C6-C7-C8-C10
32	Bb	606	CLA	C11-C10-C8-C7
32	Bb	610	CLA	C6-C7-C8-C10
32	Bb	611	CLA	C6-C7-C8-C10
32	Bb	616	CLA	C11-C12-C13-C15
32	Cc	508	CLA	C12-C13-C15-C16
32	Cc	510	CLA	C6-C7-C8-C10
32	Cc	513	CLA	C12-C13-C15-C16
32	Gg	303	CLA	C3A-C2A-CAA-CBA
32	Gg	313	CLA	C3A-C2A-CAA-CBA
35	AA	410	PL9	C18-C19-C21-C22
39	N	609	CHL	C3A-C2A-CAA-CBA
39	NN	609	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	Gg	302	CHL	C6-C7-C8-C10
32	b	605	CLA	CAA-CBA-CGA-O1A
32	AA	406	CLA	CAA-CBA-CGA-O1A
32	c	505	CLA	CAA-CBA-CGA-O2A
32	y	314	CLA	CAA-CBA-CGA-O2A
32	CC	502	CLA	CAA-CBA-CGA-O2A
32	Cc	510	CLA	CAA-CBA-CGA-O2A
36	y	320	LHG	O8-C23-C24-C25
39	Rr	605	CHL	CAA-CBA-CGA-O2A
44	h	102	DGD	O2G-C1B-C2B-C3B
36	J	101	LHG	C25-C26-C27-C28
44	Hh	102	DGD	C3B-C4B-C5B-C6B
32	Rr	608	CLA	O2A-C1-C2-C3
32	Y	604	CLA	O2A-C1-C2-C3
32	g	612	CLA	O2A-C1-C2-C3
32	SS	314	CLA	O2A-C1-C2-C3
32	Nn	313	CLA	O2A-C1-C2-C3
37	AA	412	SQD	O48-C23-C24-C25
40	SS	315	LUT	C11-C12-C13-C14
32	Rr	603	CLA	CAA-CBA-CGA-O1A
32	Rr	611	CLA	CAA-CBA-CGA-O1A
32	Y	602	CLA	CAA-CBA-CGA-O1A
32	a	406	CLA	CAA-CBA-CGA-O1A
32	c	505	CLA	CAA-CBA-CGA-O1A
36	DD	407	LHG	O10-C23-C24-C25
44	C	523	DGD	CAB-CBB-CCB-CDB
44	CC	518	DGD	CDB-CEB-CFB-CGB
32	y	304	CLA	C16-C17-C18-C19
32	G	602	CLA	CAA-CBA-CGA-O2A
32	Y	612	CLA	CAA-CBA-CGA-O2A
33	A	407	PHO	CAA-CBA-CGA-O2A
36	11	614	LHG	O8-C23-C24-C25
32	CC	504	CLA	C8-C10-C11-C12
32	Bb	614	CLA	C15-C16-C17-C18
32	B	619	CLA	CAA-CBA-CGA-O1A
32	NN	602	CLA	CAA-CBA-CGA-O1A
32	Aa	406	CLA	CAA-CBA-CGA-O1A
32	Cc	507	CLA	CAA-CBA-CGA-O1A
36	D	408	LHG	O10-C23-C24-C25
36	y	320	LHG	C8-C7-O7-C5
32	C	505	CLA	C8-C10-C11-C12
32	YY	613	CLA	C8-C10-C11-C12

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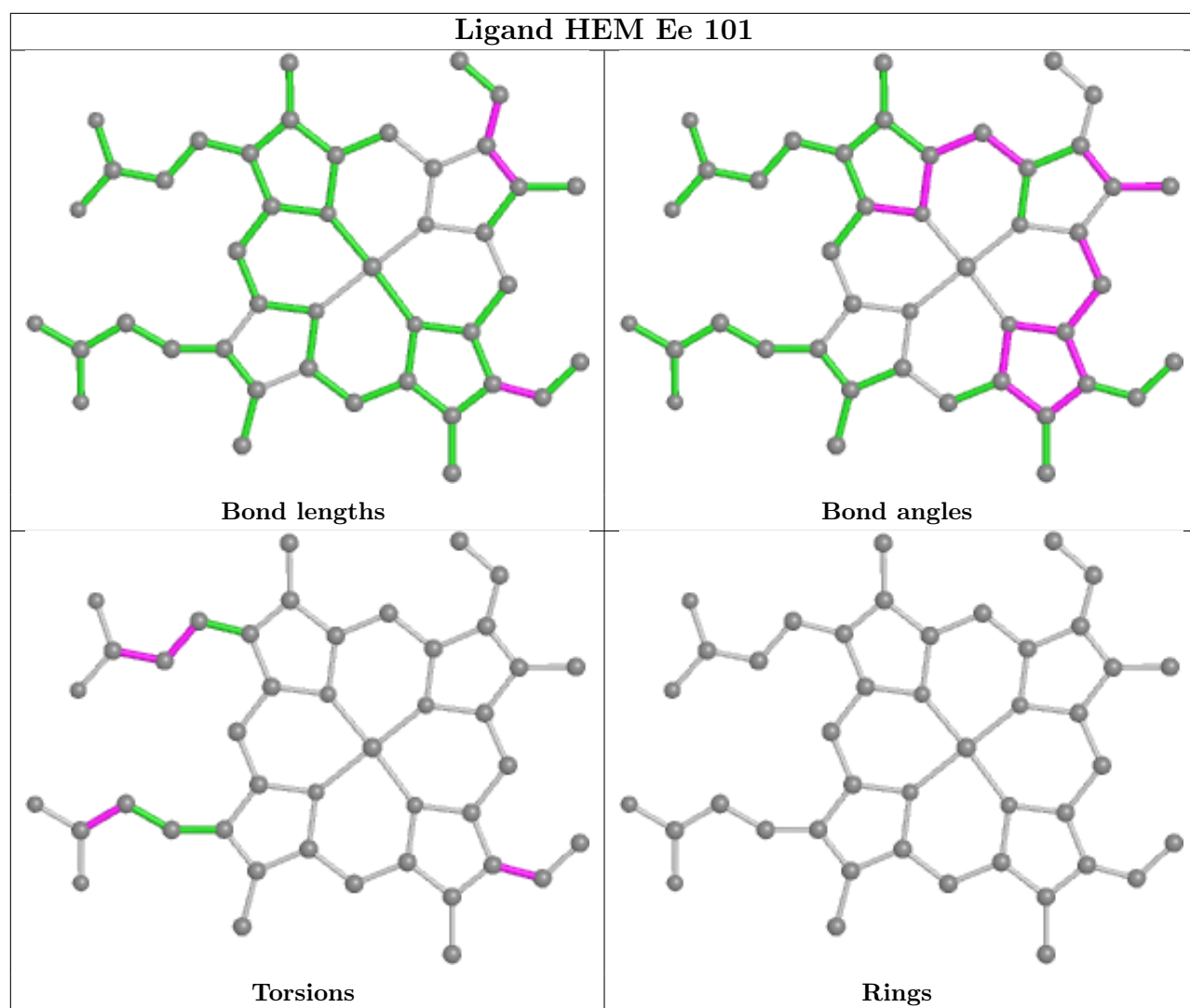
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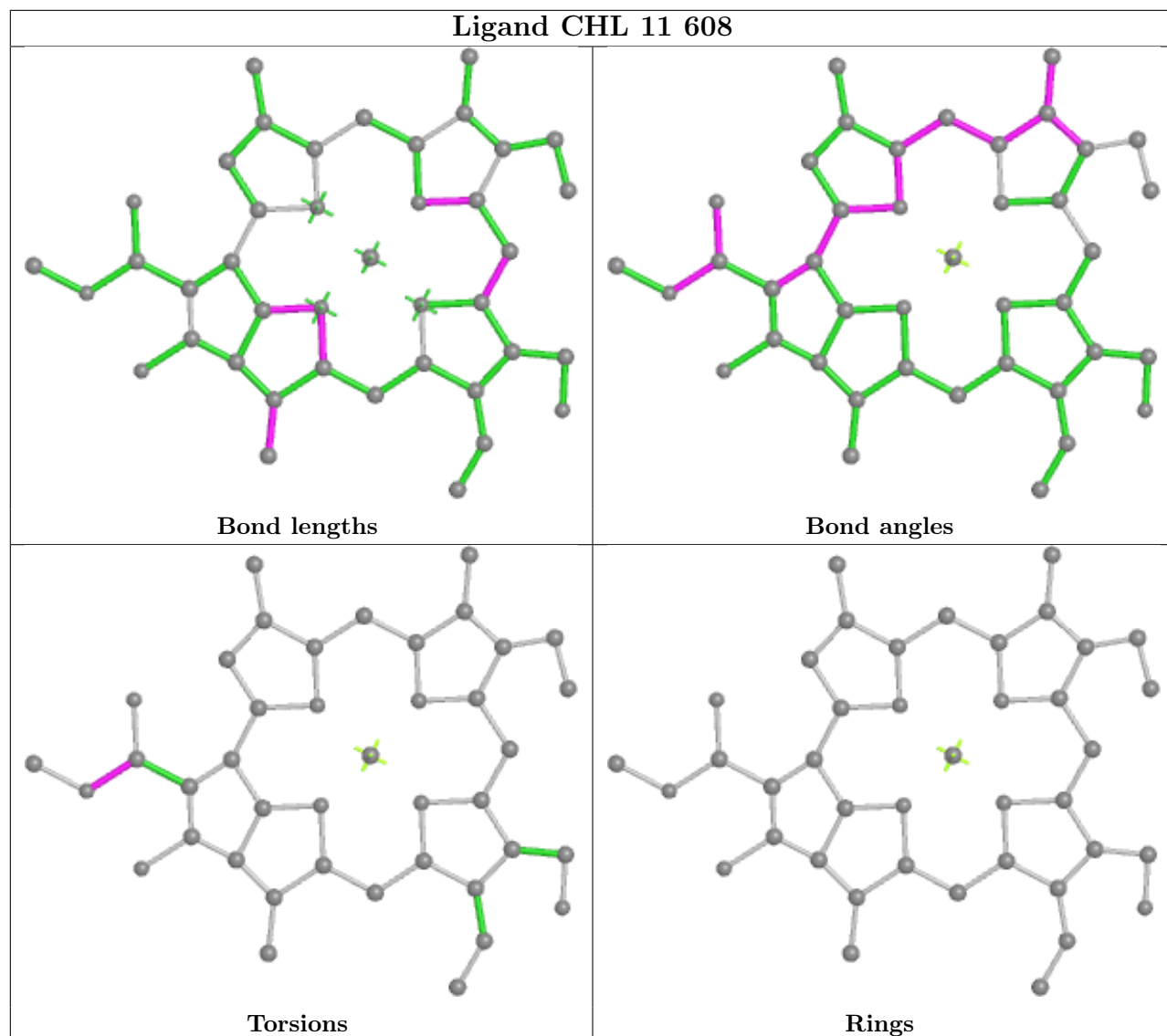
Mol	Chain	Res	Type	Atoms
32	Yy	612	CLA	CAA-CBA-CGA-O2A
32	YY	602	CLA	CAA-CBA-CGA-O2A
32	Gg	311	CLA	CAA-CBA-CGA-O2A
38	m	101	LMG	O8-C28-C29-C30
32	CC	509	CLA	C13-C15-C16-C17
32	Yy	602	CLA	CAA-CBA-CGA-O1A
32	N	602	CLA	CAA-CBA-CGA-O1A
32	g	611	CLA	CAA-CBA-CGA-O1A
32	BB	612	CLA	CAA-CBA-CGA-O1A
36	Ss	616	LHG	O10-C23-C24-C25
36	s	616	LHG	O10-C23-C24-C25
32	CC	510	CLA	C2A-CAA-CBA-CGA
44	BB	624	DGD	C2B-C3B-C4B-C5B
38	WW	201	LMG	O10-C28-O8-C9
32	Y	613	CLA	C8-C10-C11-C12
32	BB	602	CLA	C5-C6-C7-C8
32	BB	609	CLA	C15-C16-C17-C18
32	Y	612	CLA	CAA-CBA-CGA-O1A
32	CC	506	CLA	CAA-CBA-CGA-O1A
32	Bb	605	CLA	CAA-CBA-CGA-O1A
32	G	603	CLA	CAA-CBA-CGA-O2A
32	n	602	CLA	CAA-CBA-CGA-O2A
32	s	611	CLA	CAA-CBA-CGA-O2A
32	Nn	312	CLA	CAA-CBA-CGA-O2A
32	4	311	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

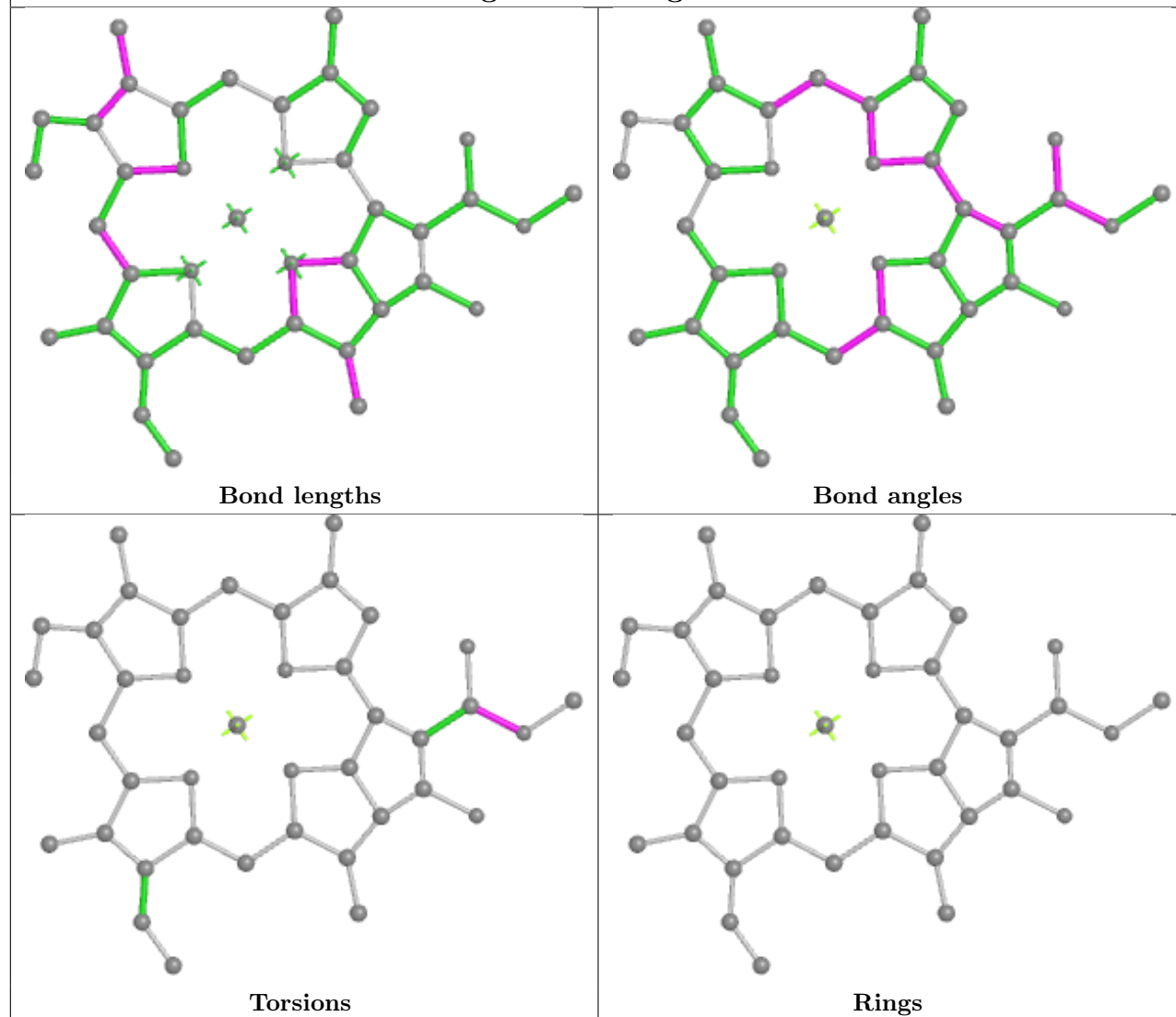
No monomer is involved in short contacts.

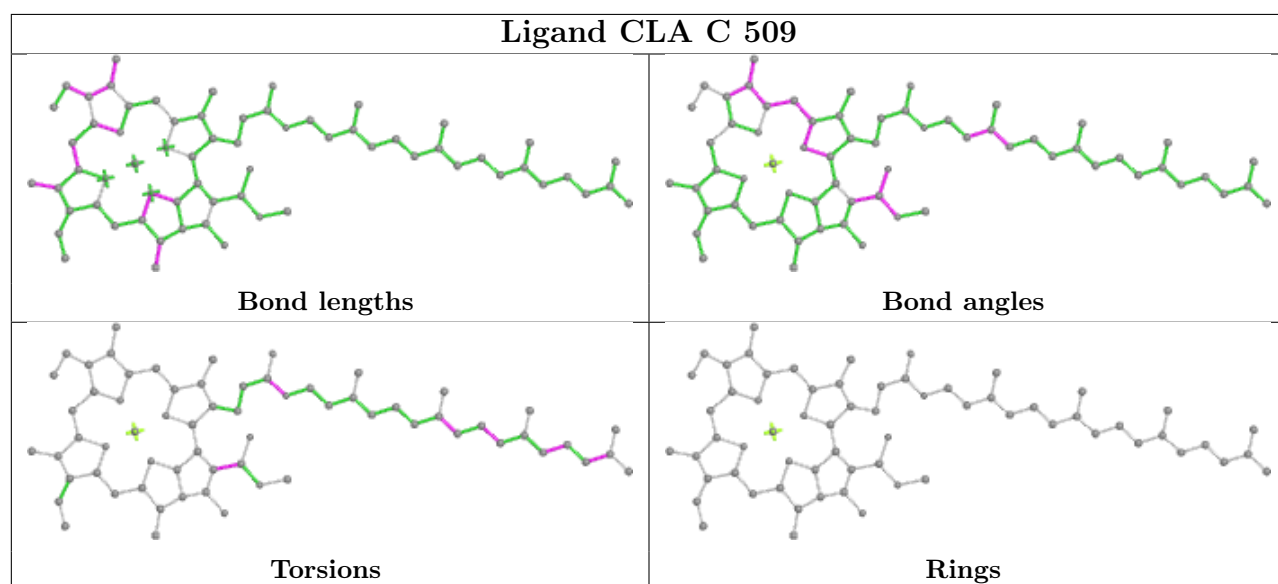
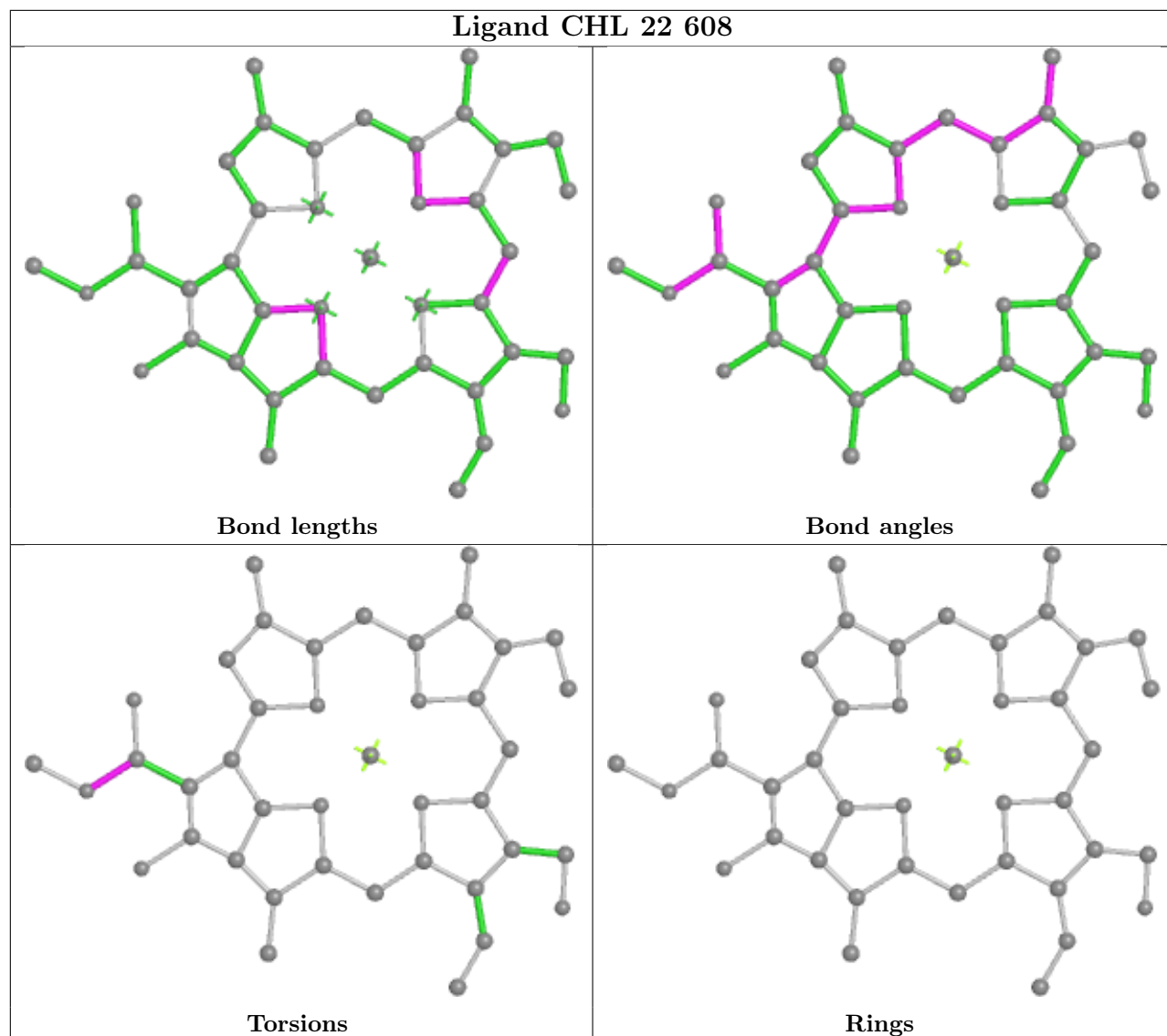
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



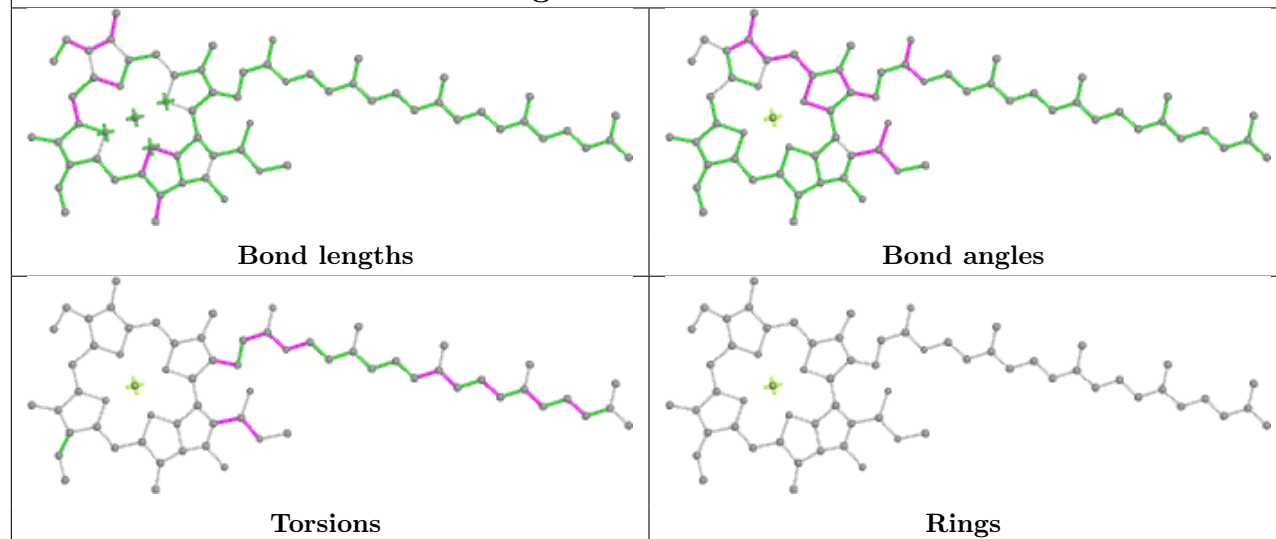


## Ligand CLA Gg 314

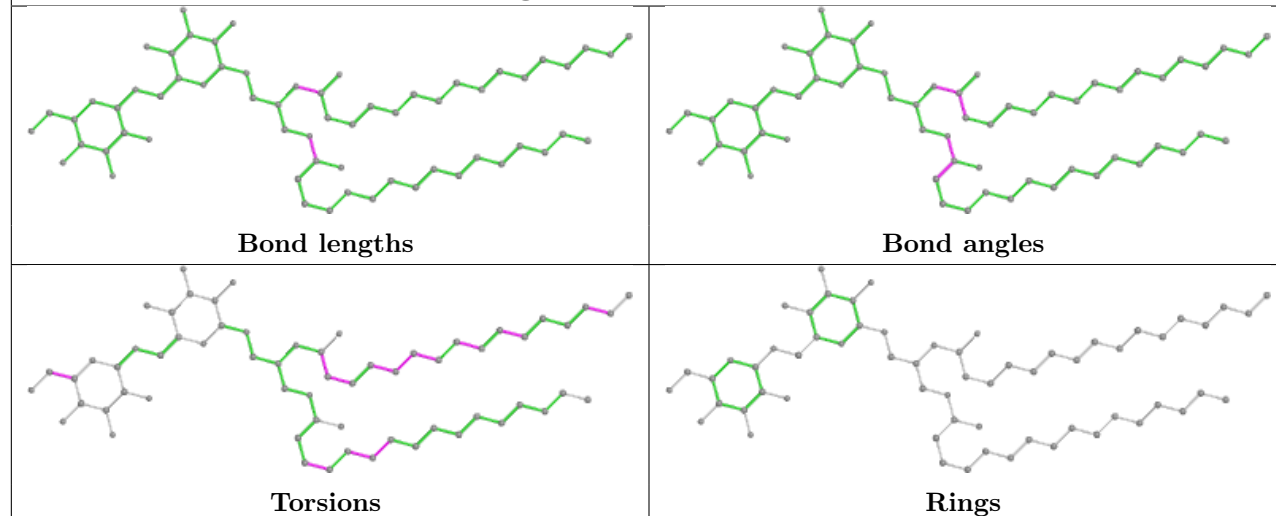




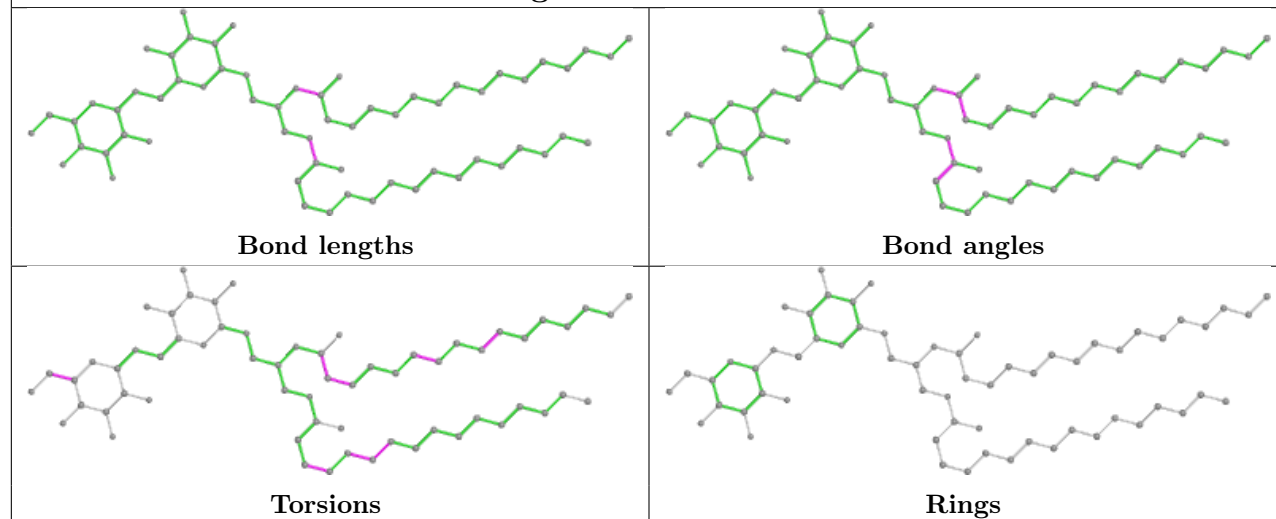
## Ligand CLA B 619



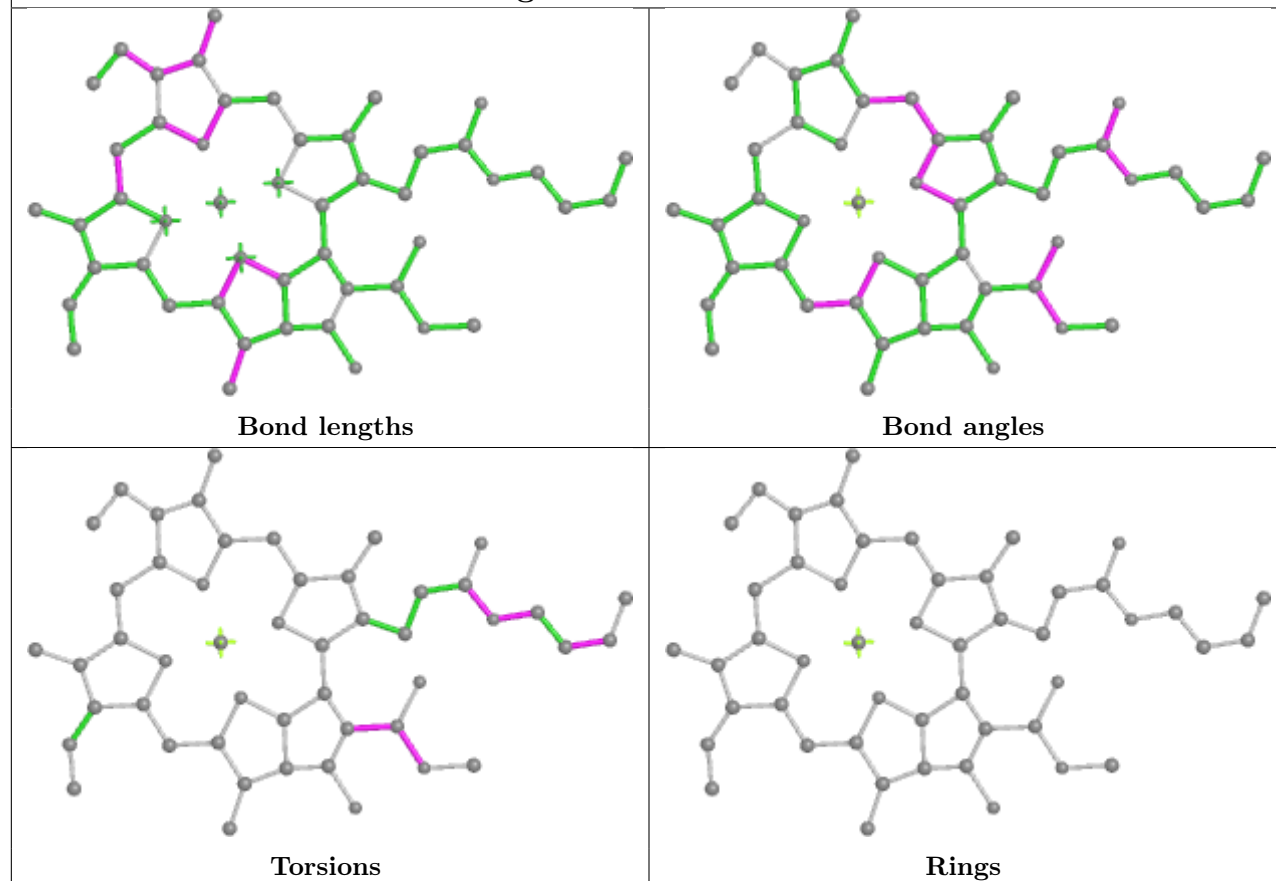
## Ligand DGD Hh 102



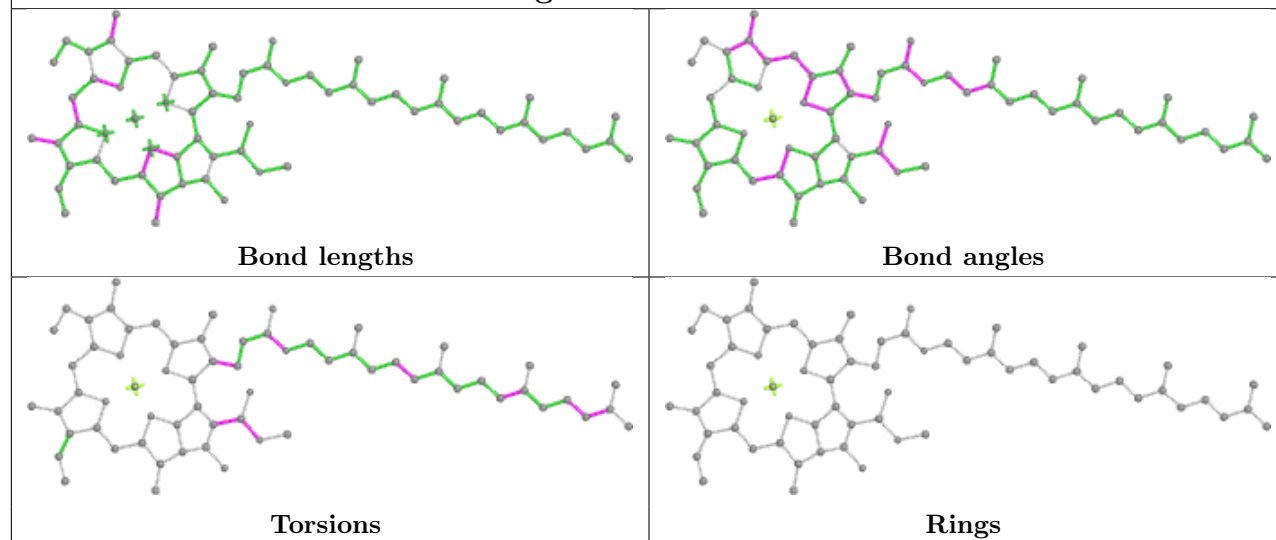
## Ligand DGD h 102

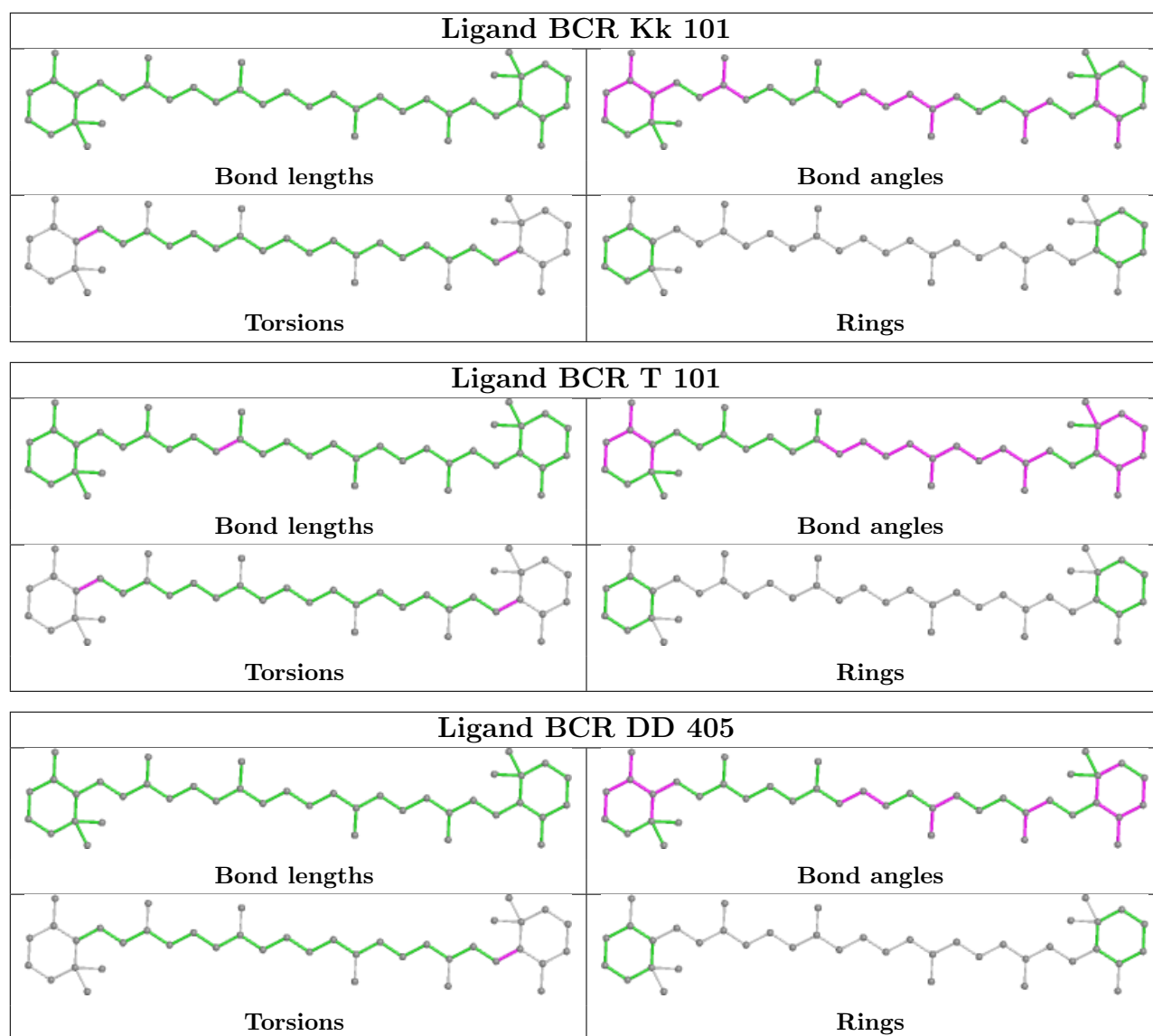


## Ligand CLA GG 610



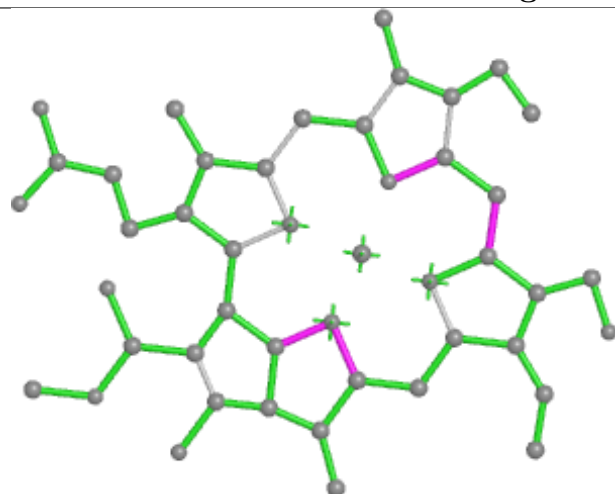
## Ligand CLA b 601



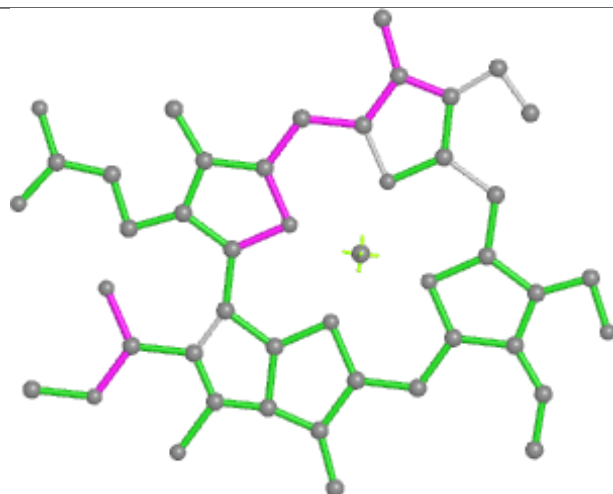




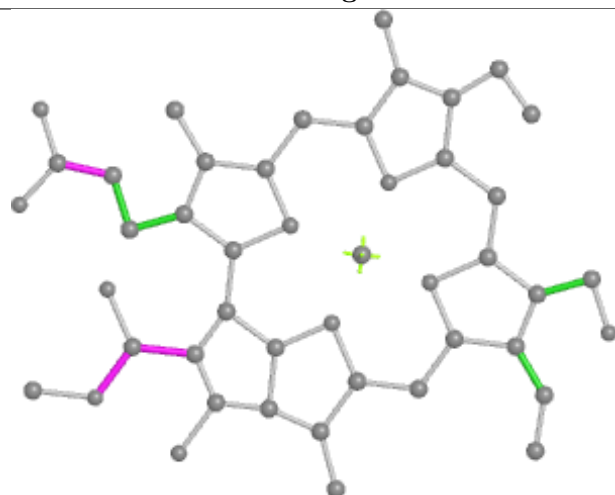
## Ligand CHL 4 306



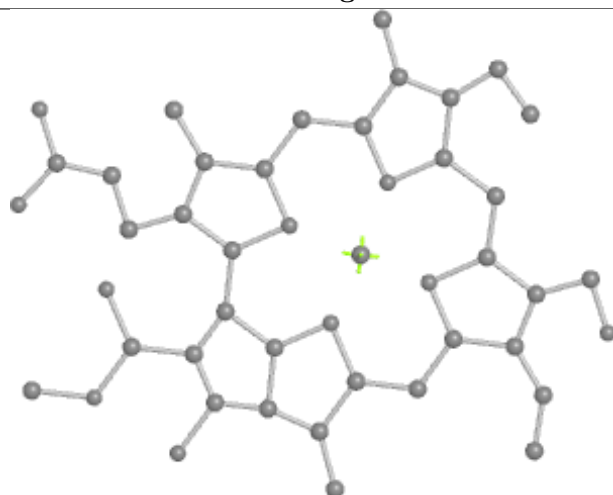
Bond lengths



Bond angles

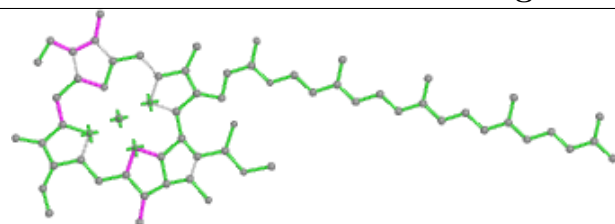


Torsions

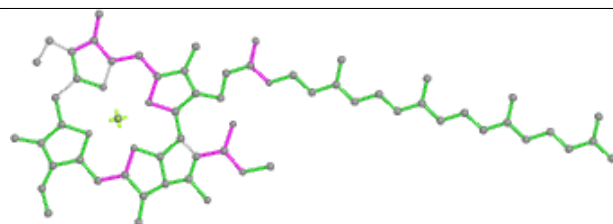


Rings

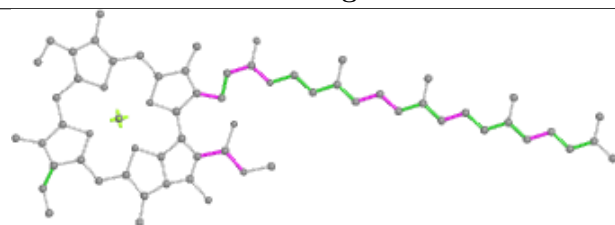
## Ligand CLA N 602



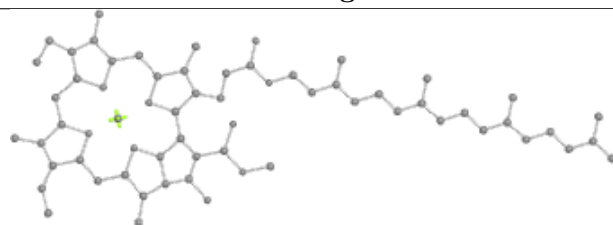
Bond lengths



Bond angles

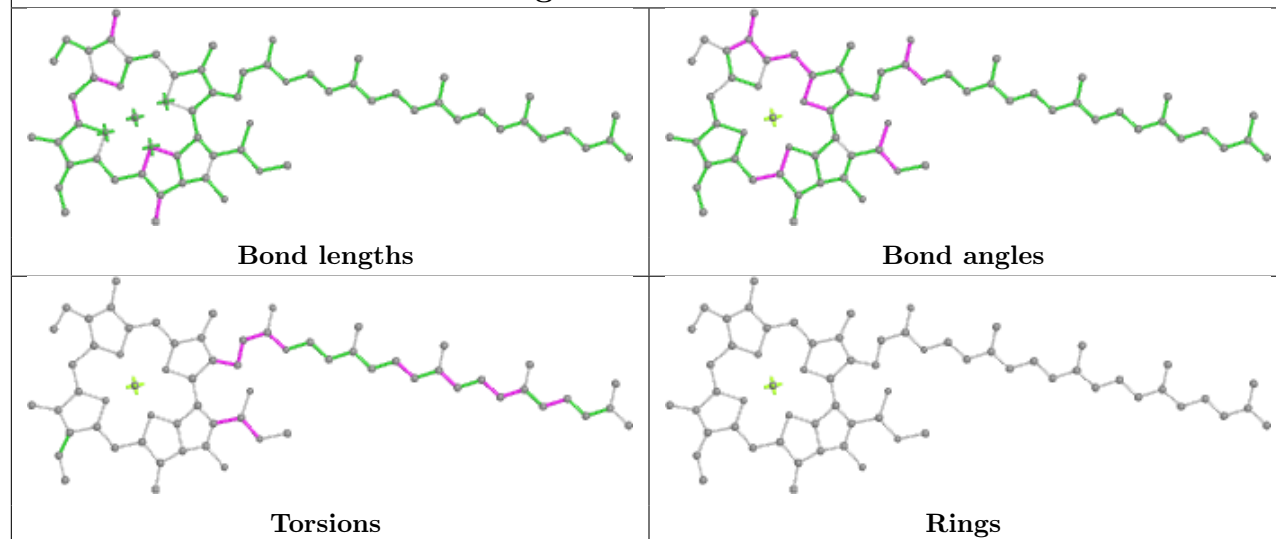


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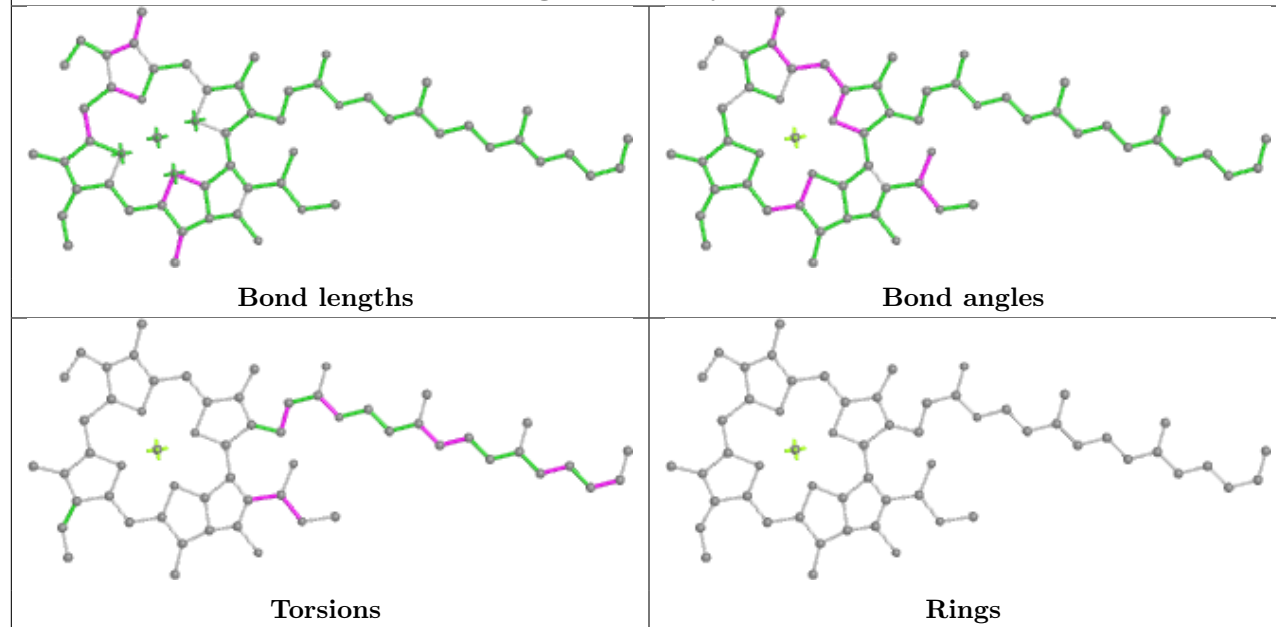


Rings

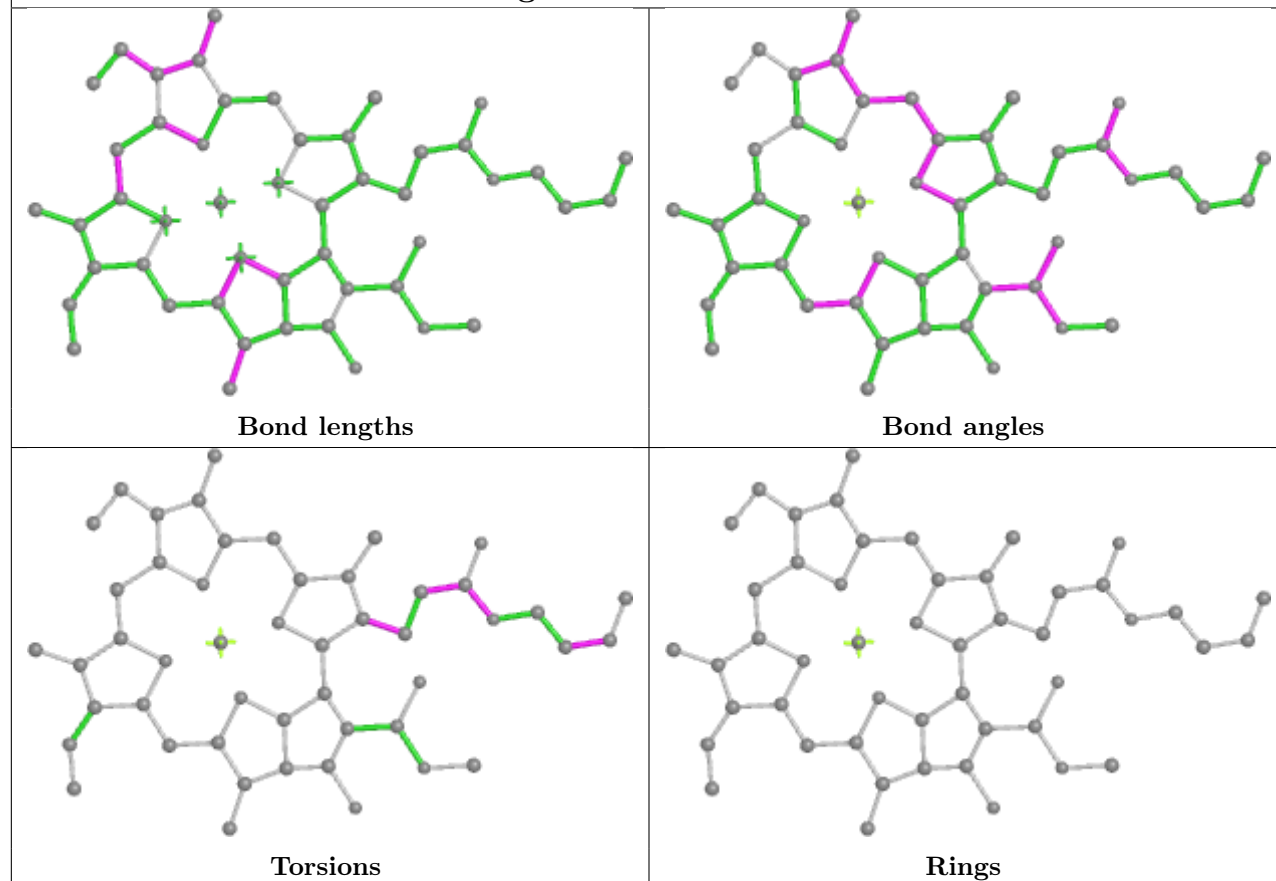
## Ligand CLA b 609



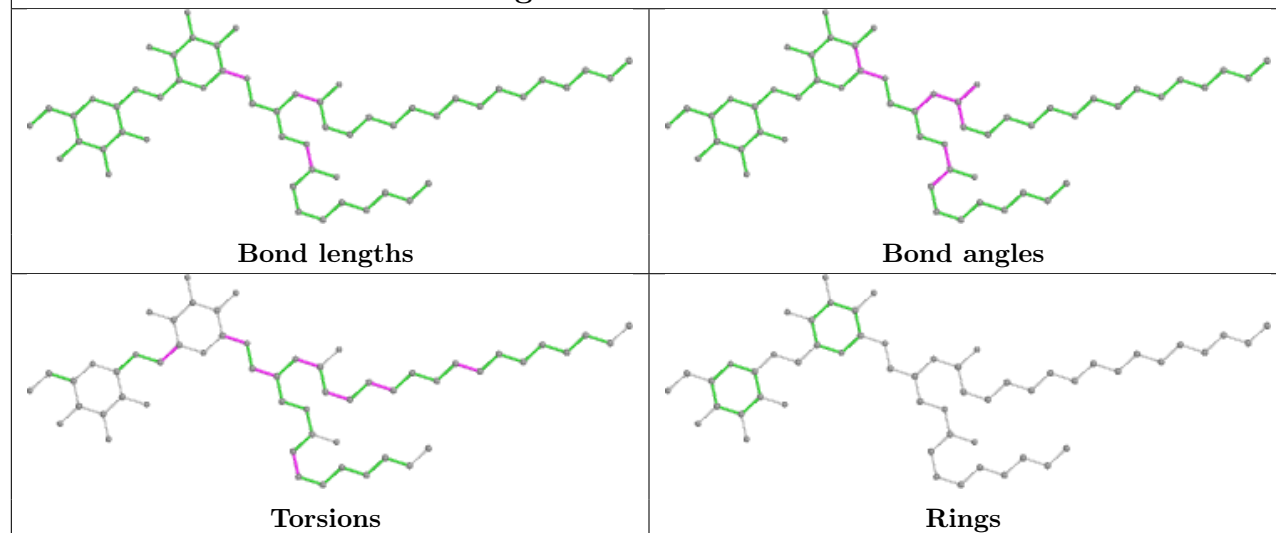
## Ligand CLA y 315

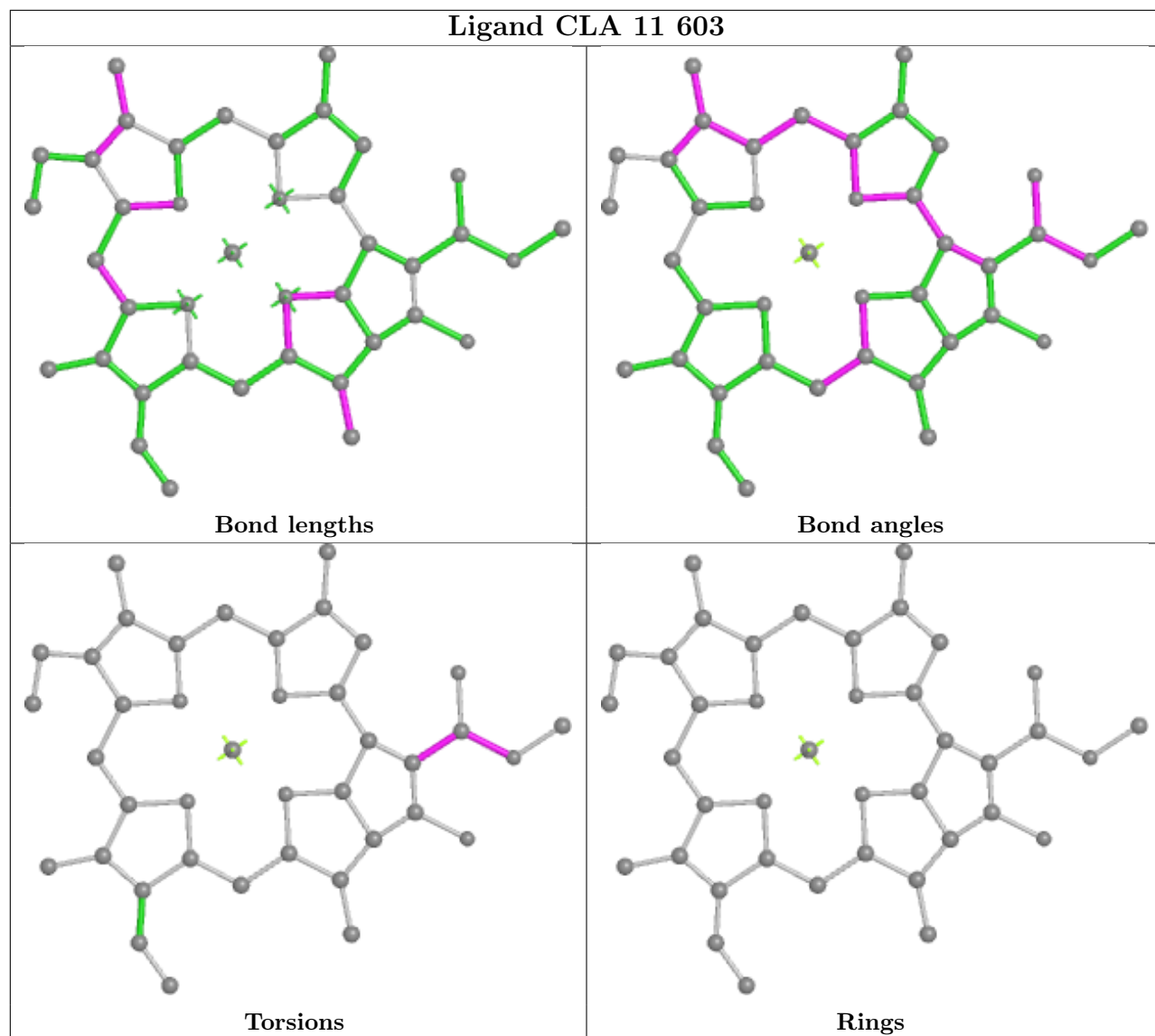


## Ligand CLA AA 406

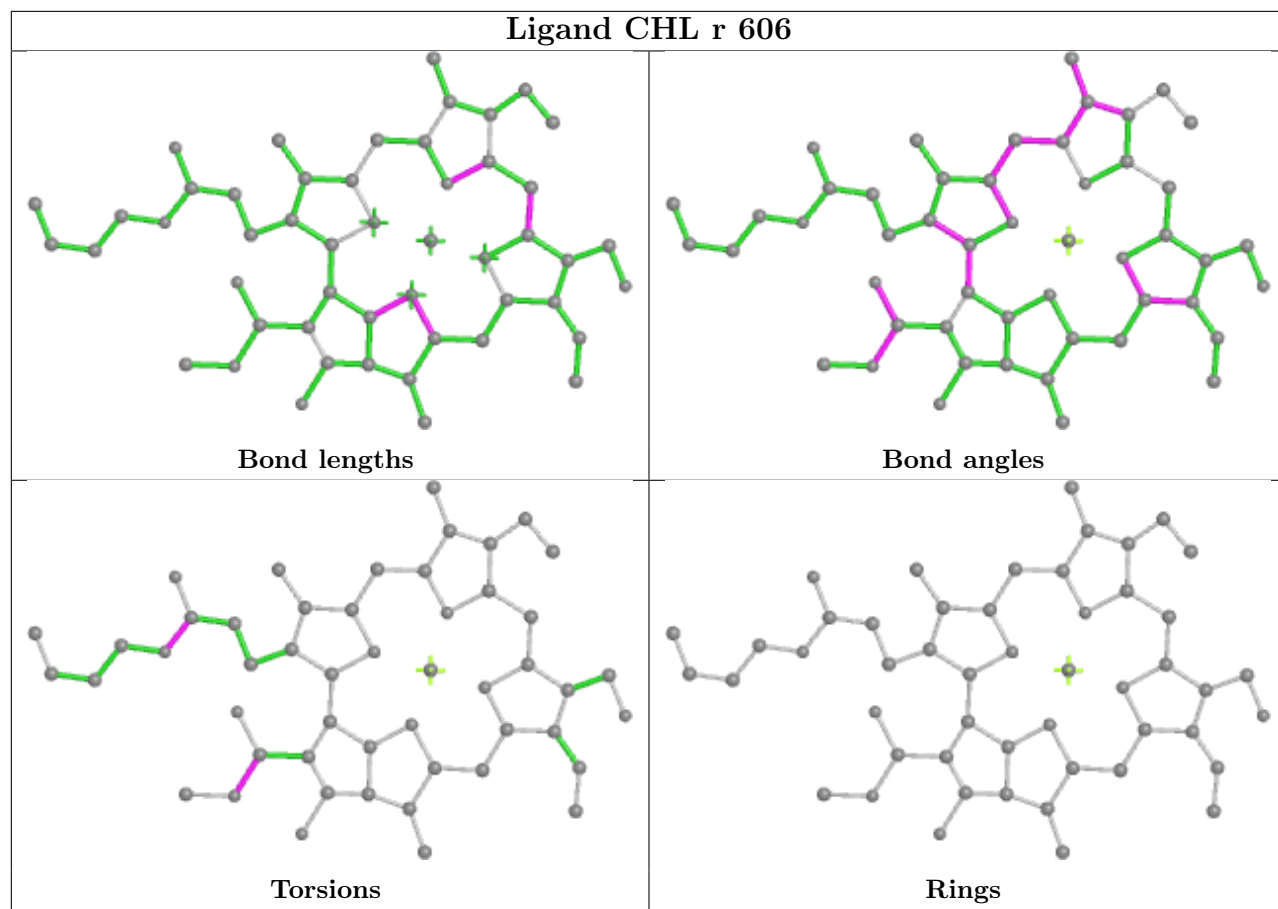


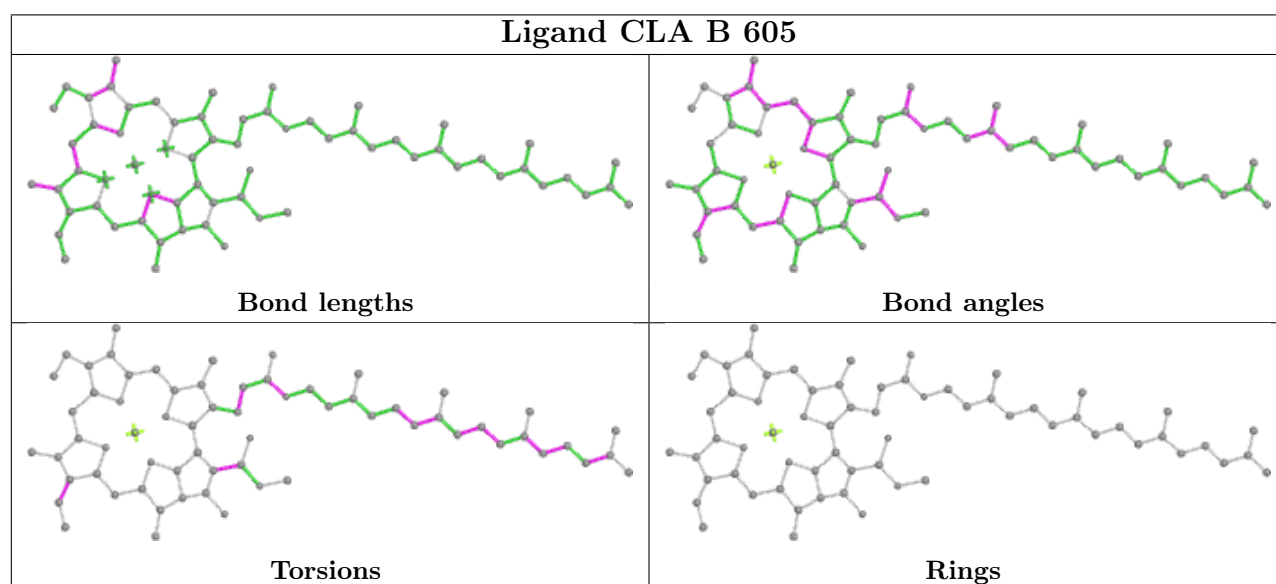
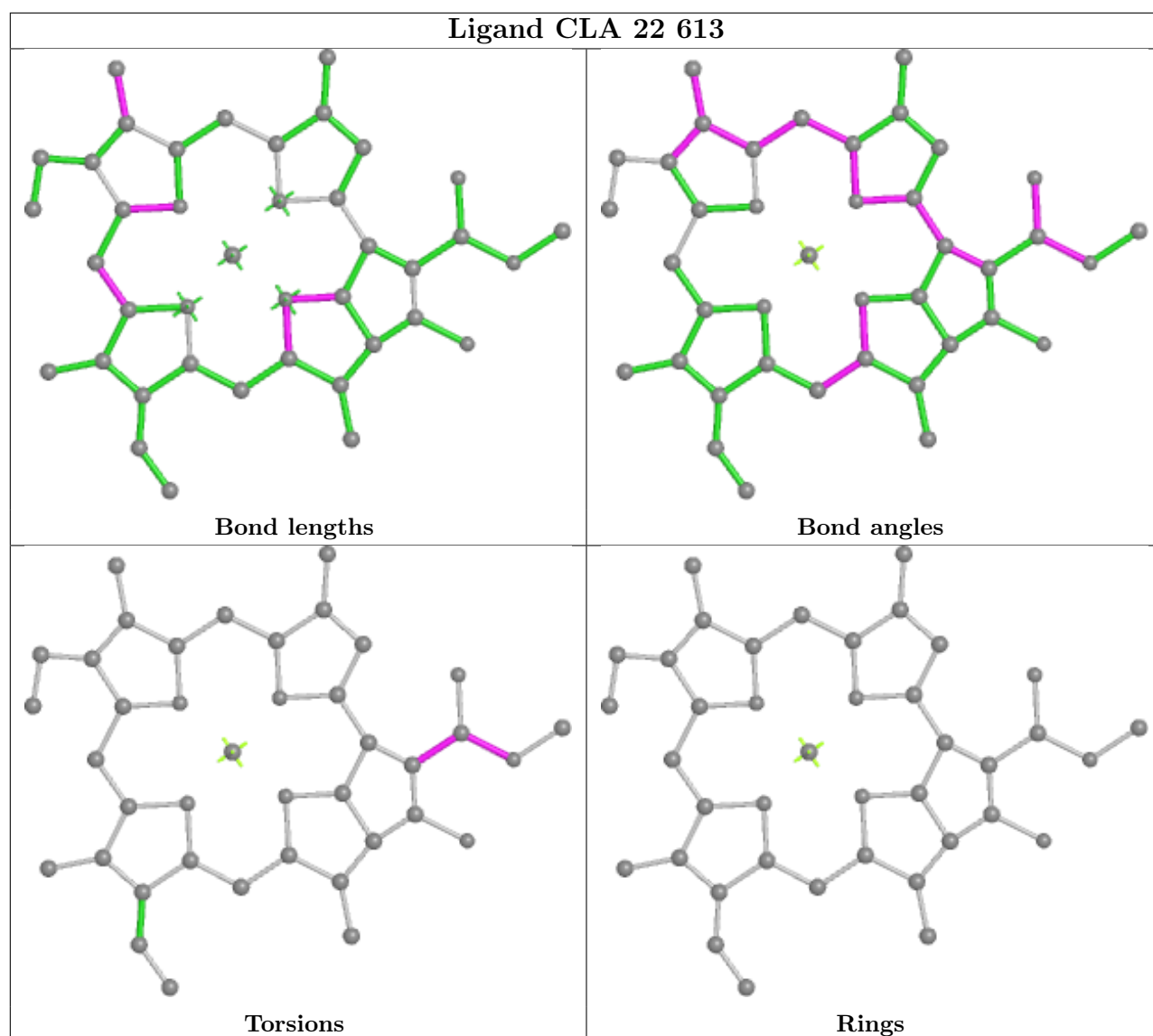
## Ligand DGD CC 522

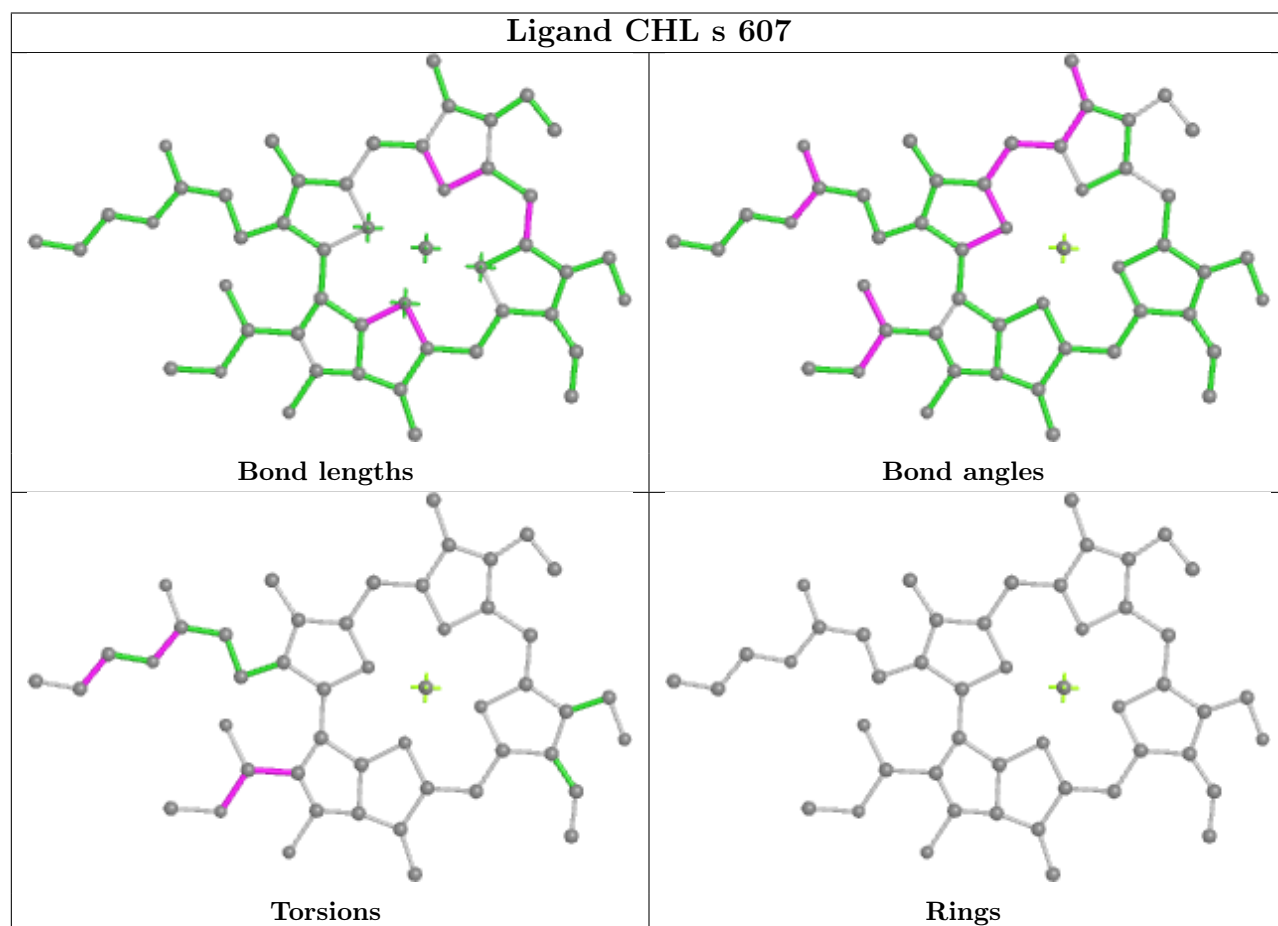
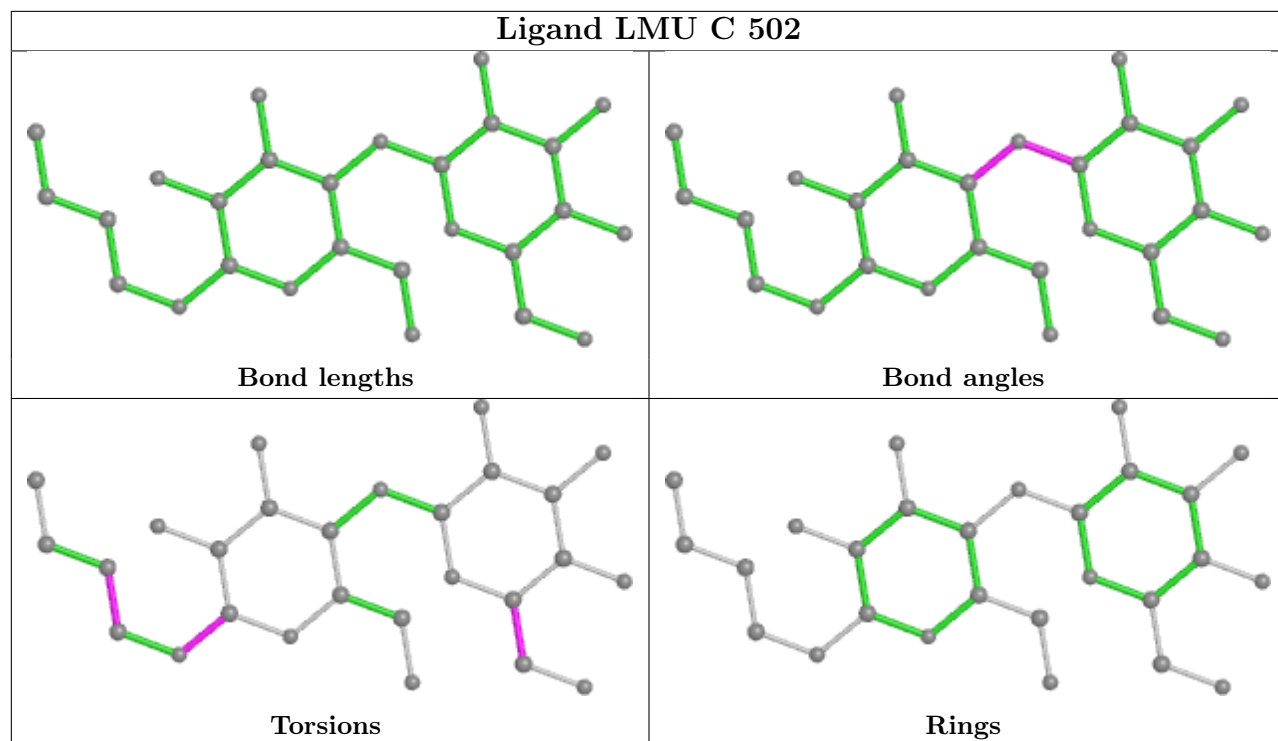


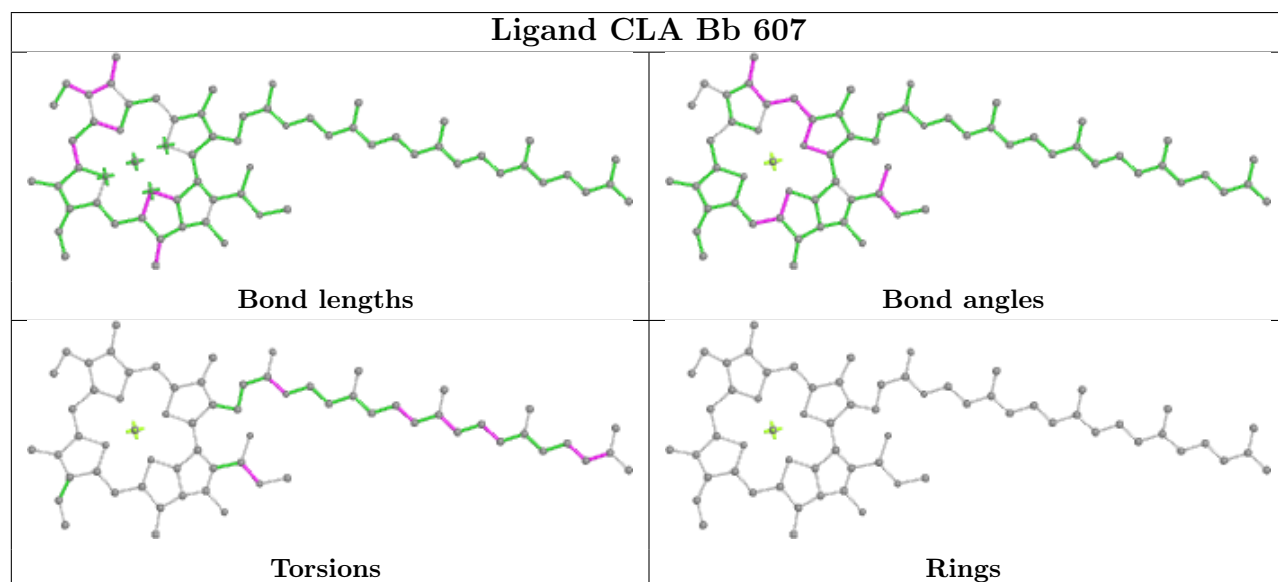
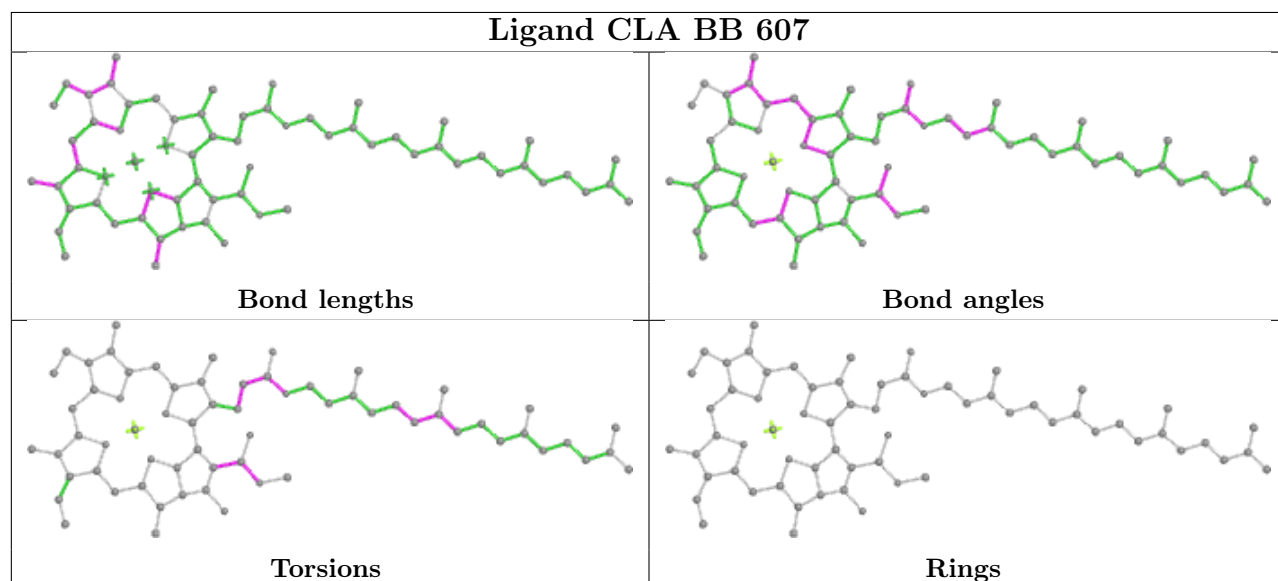
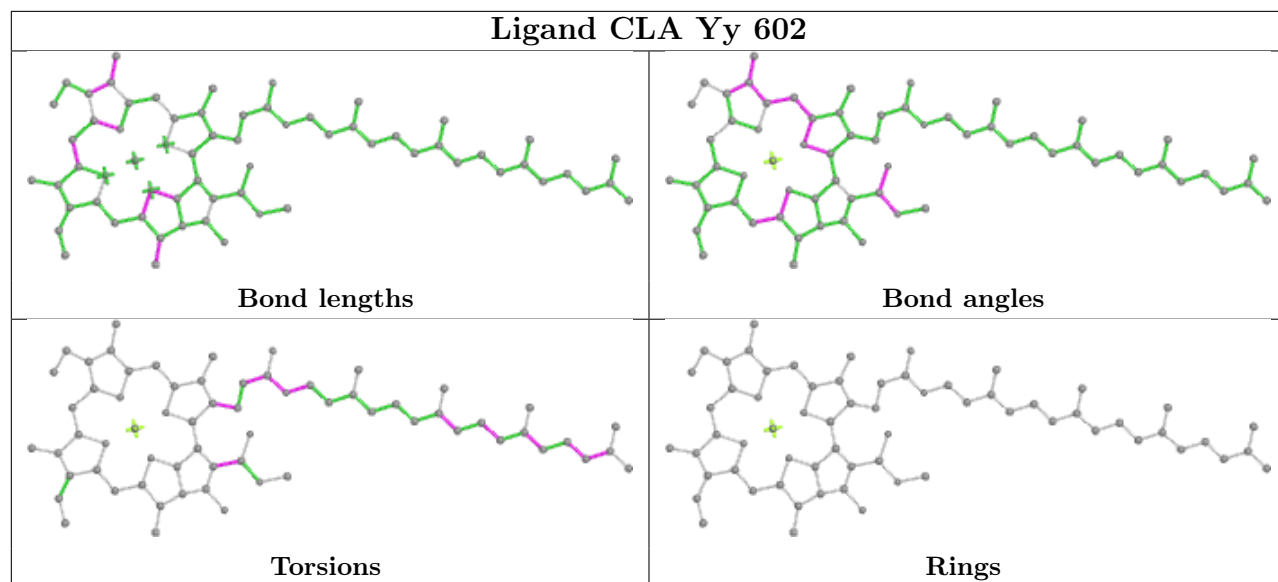


## Ligand CHL r 606

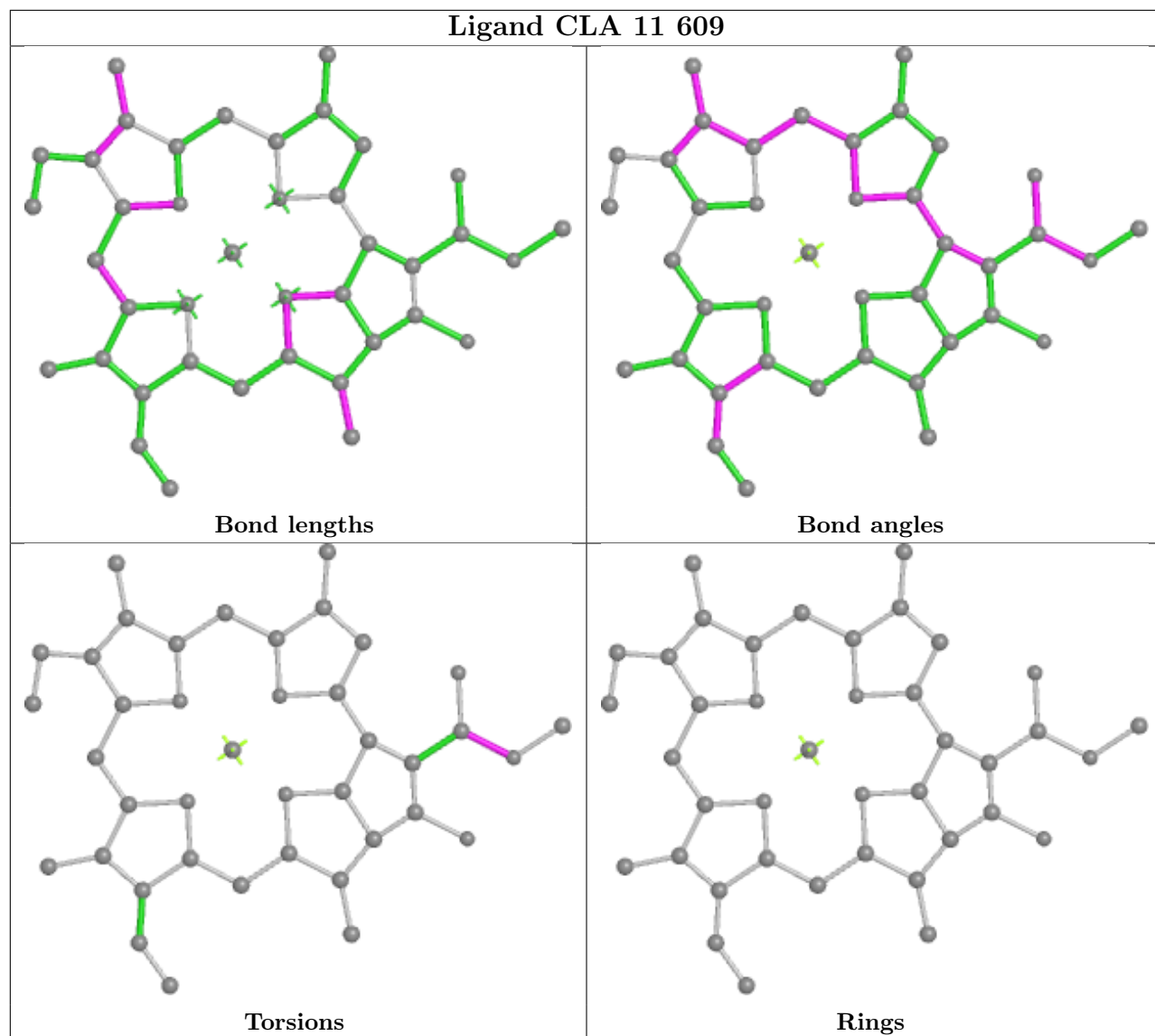


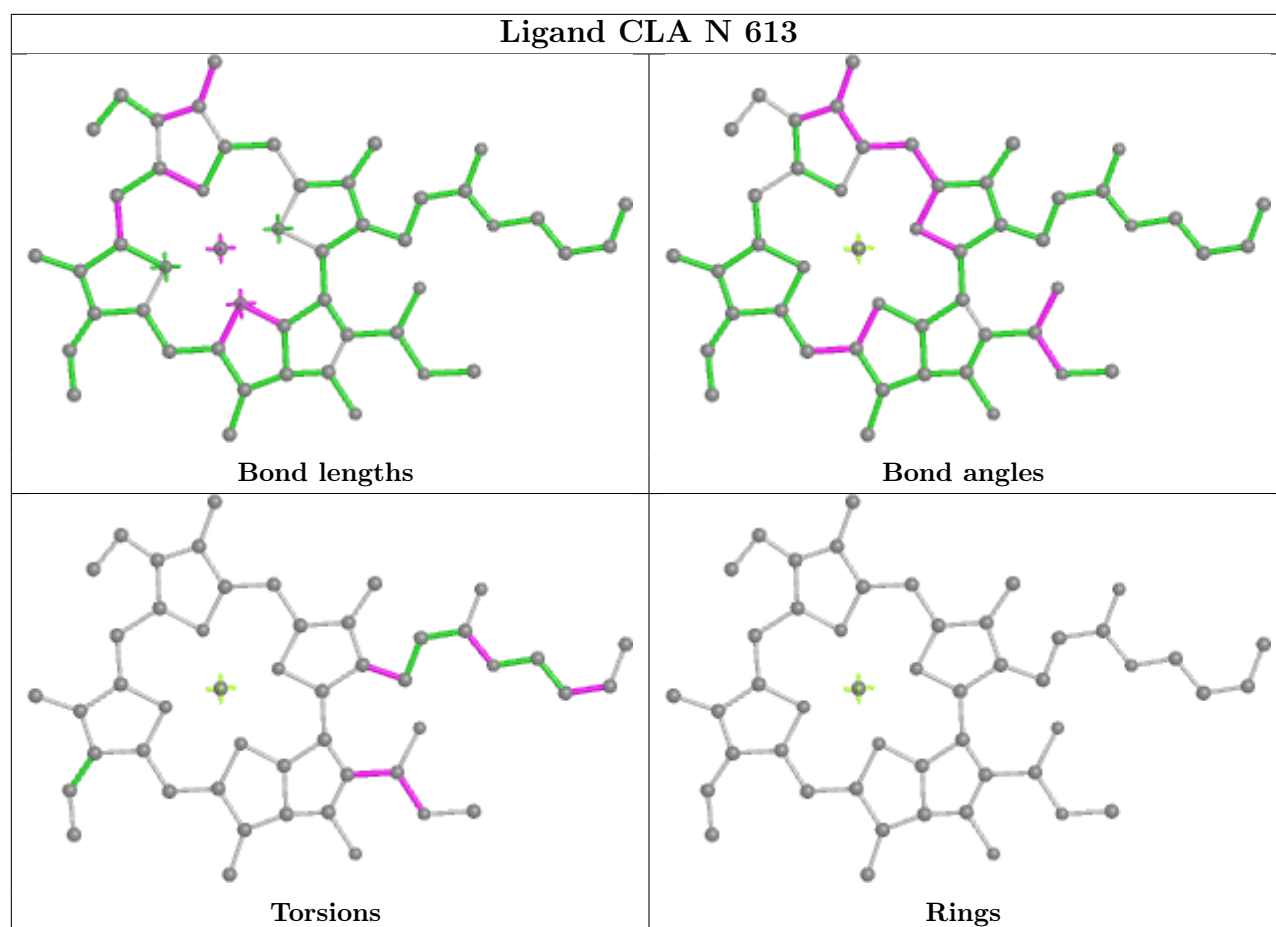


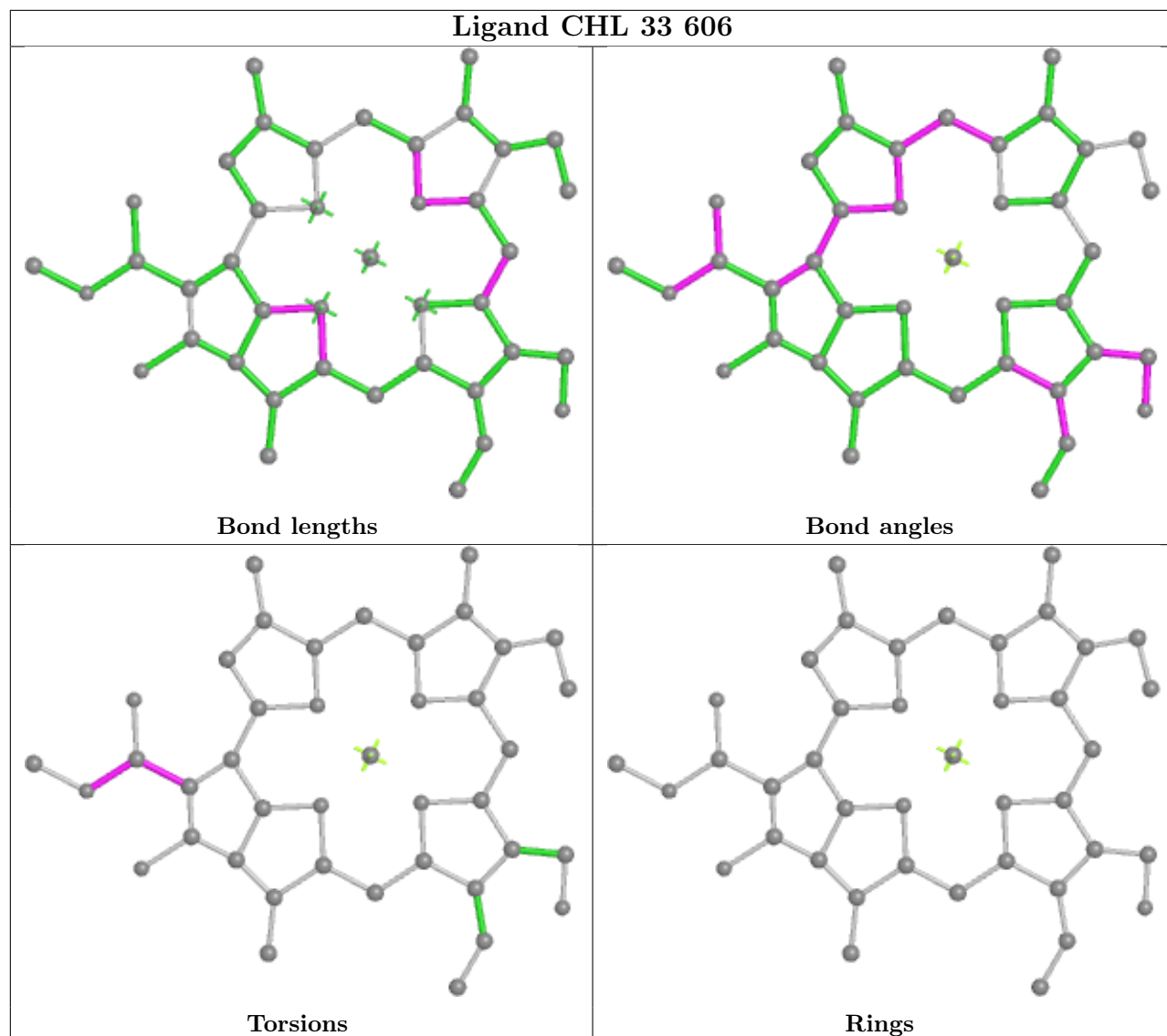


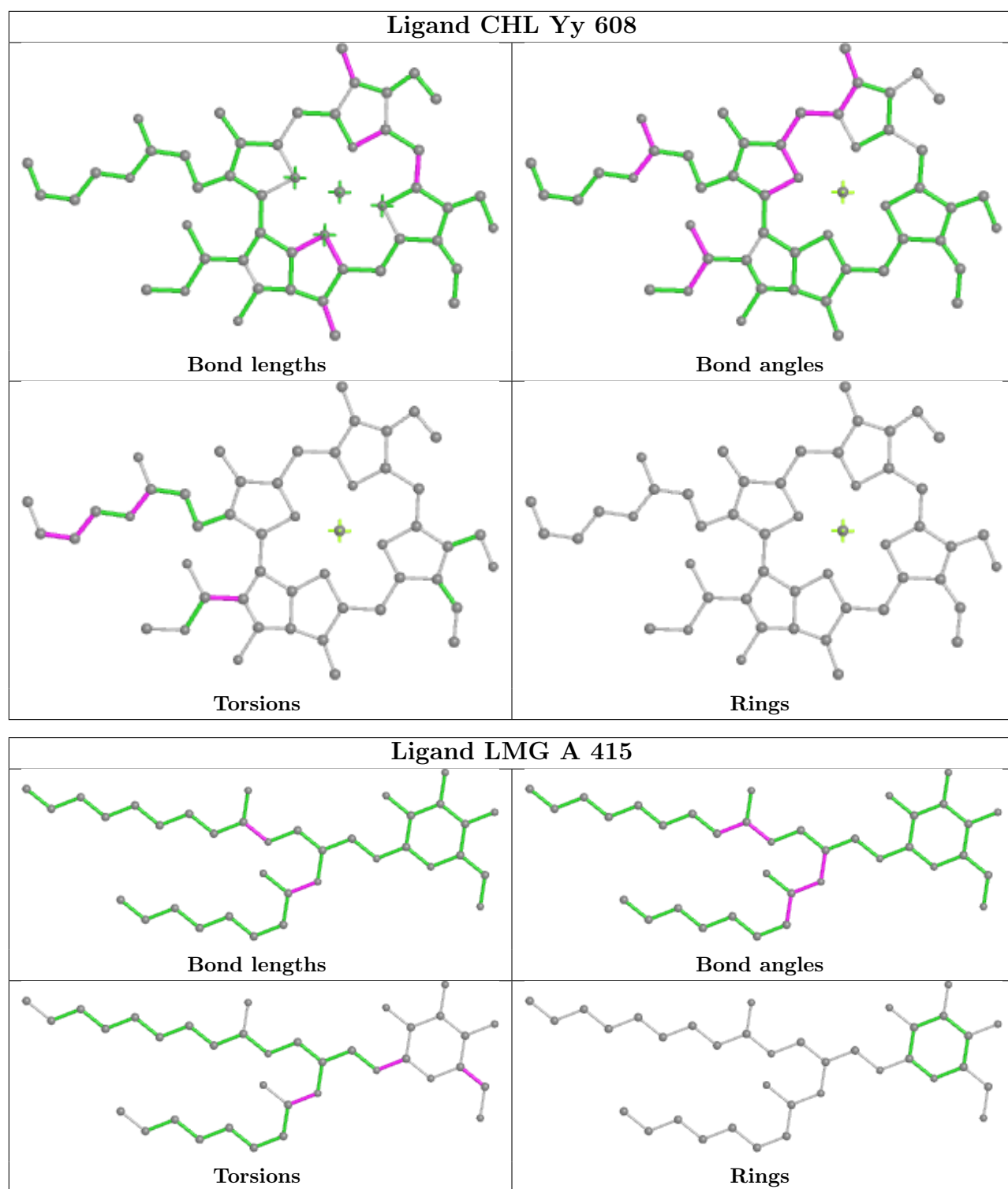


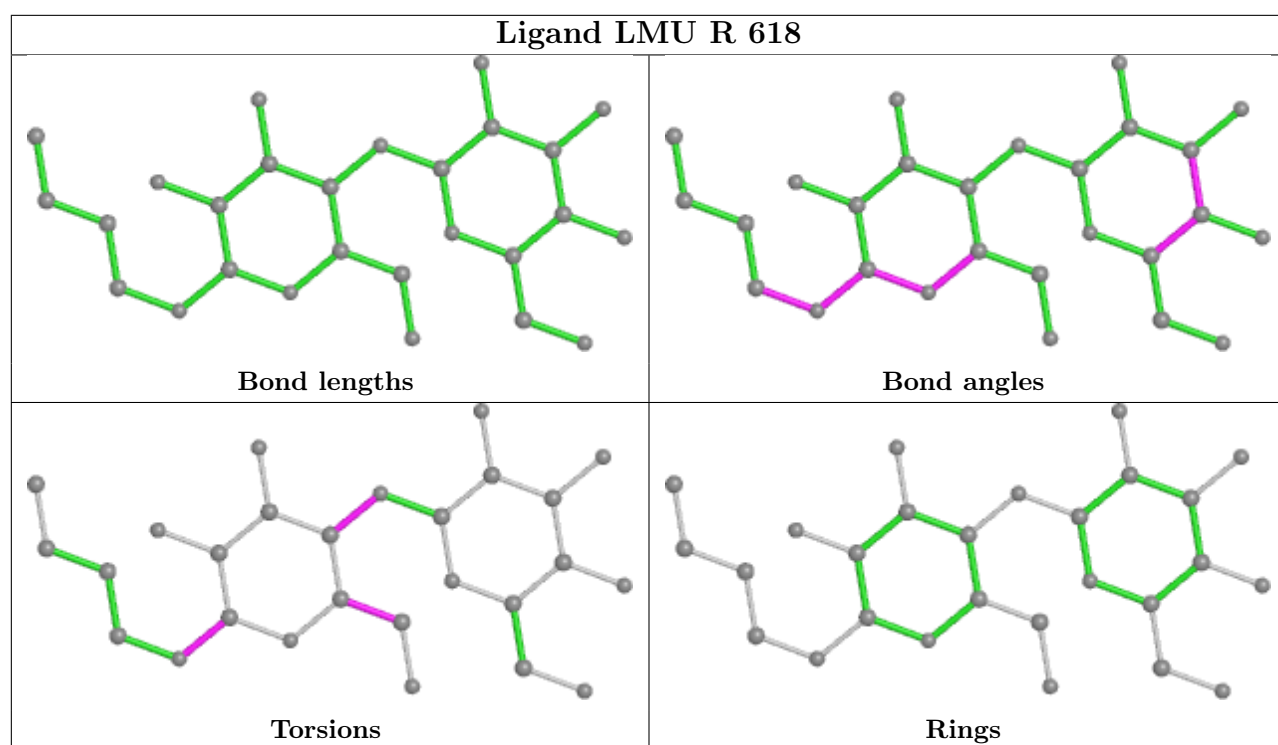
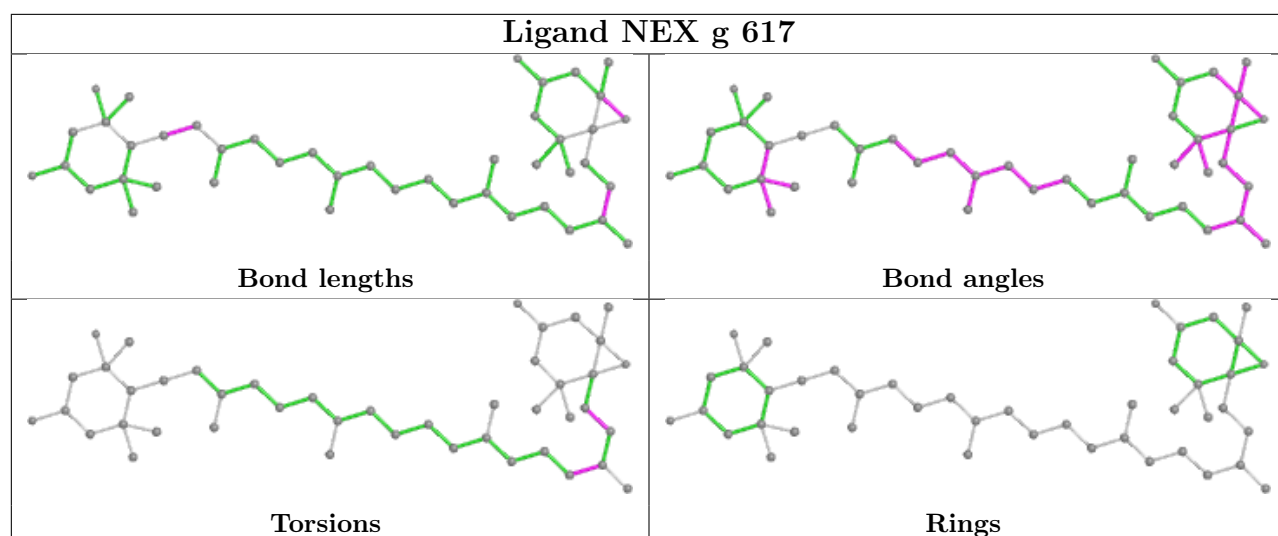




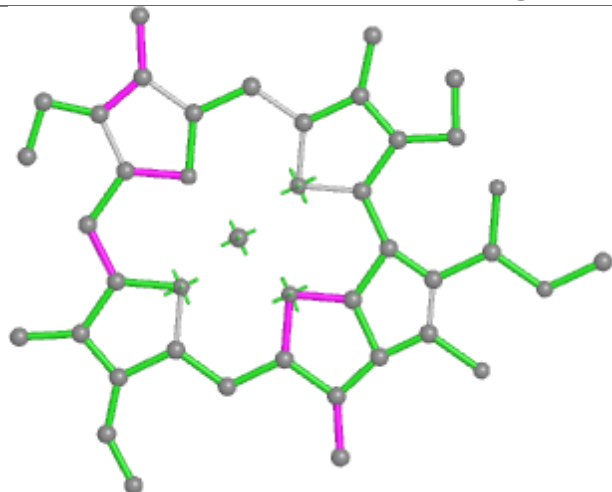




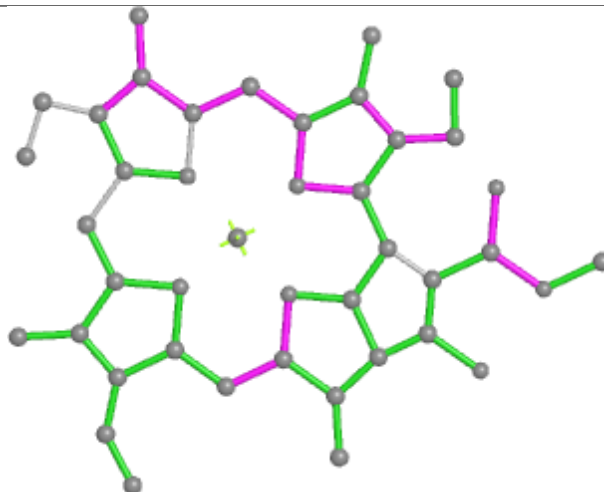




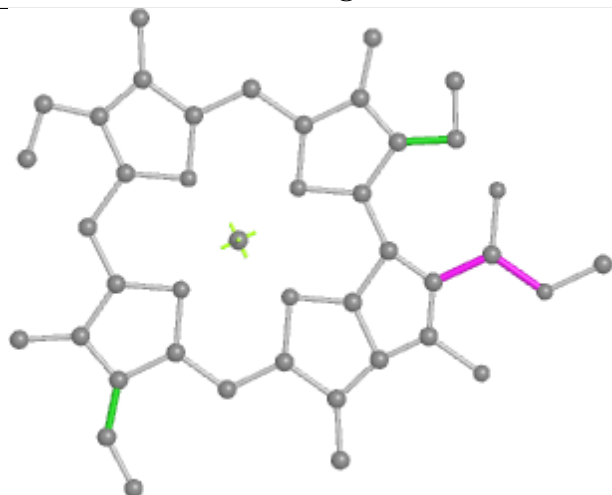
## Ligand CLA N 603



Bond lengths



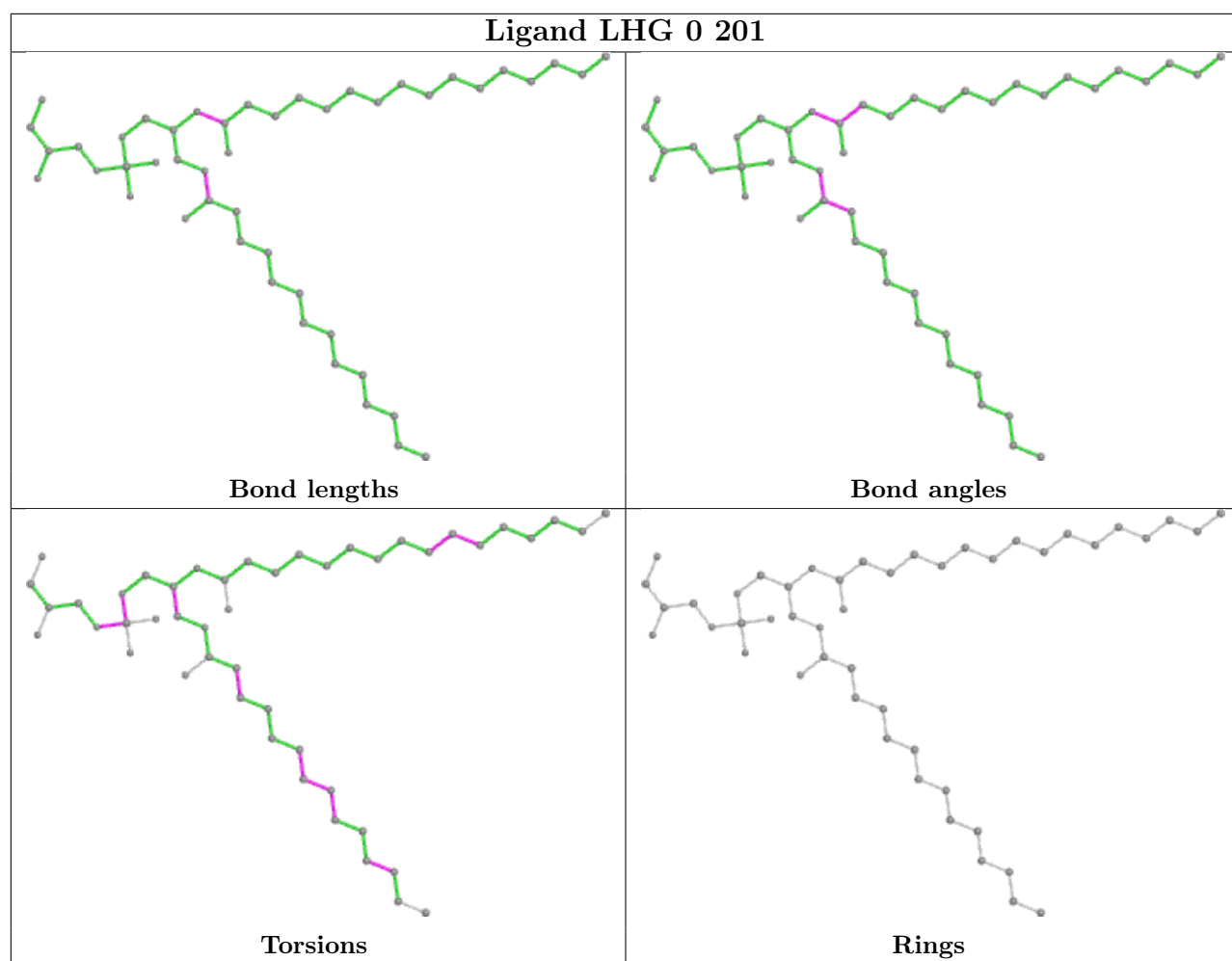
Bond angles

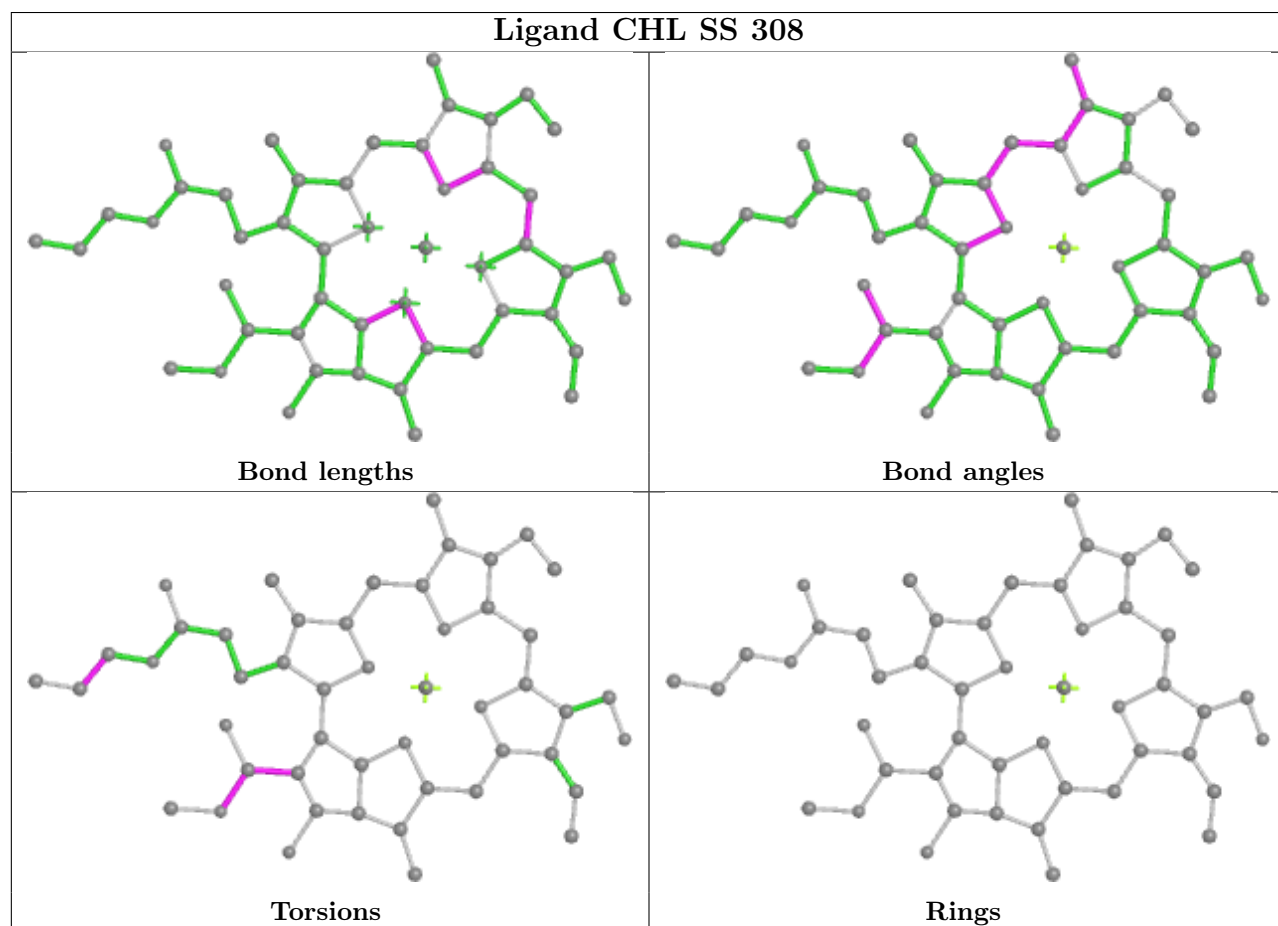
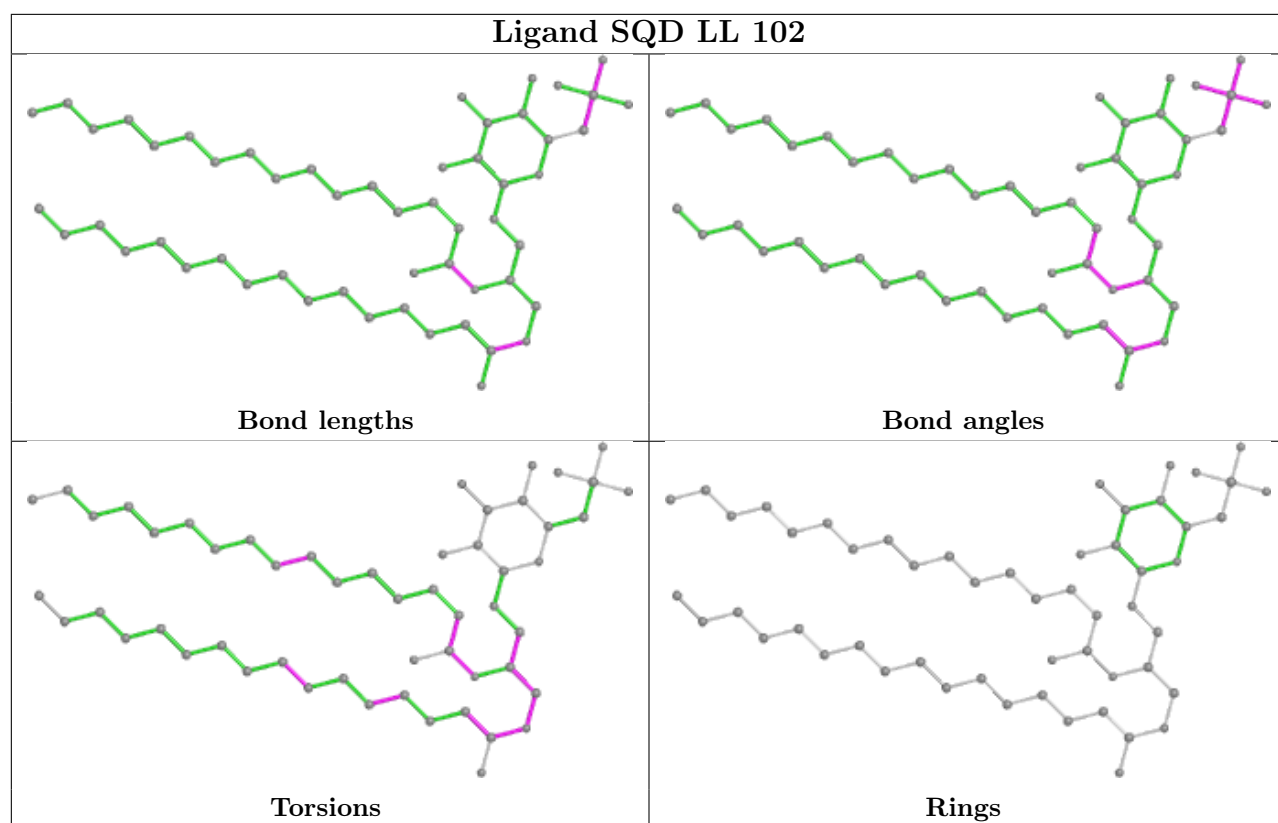


Torsions

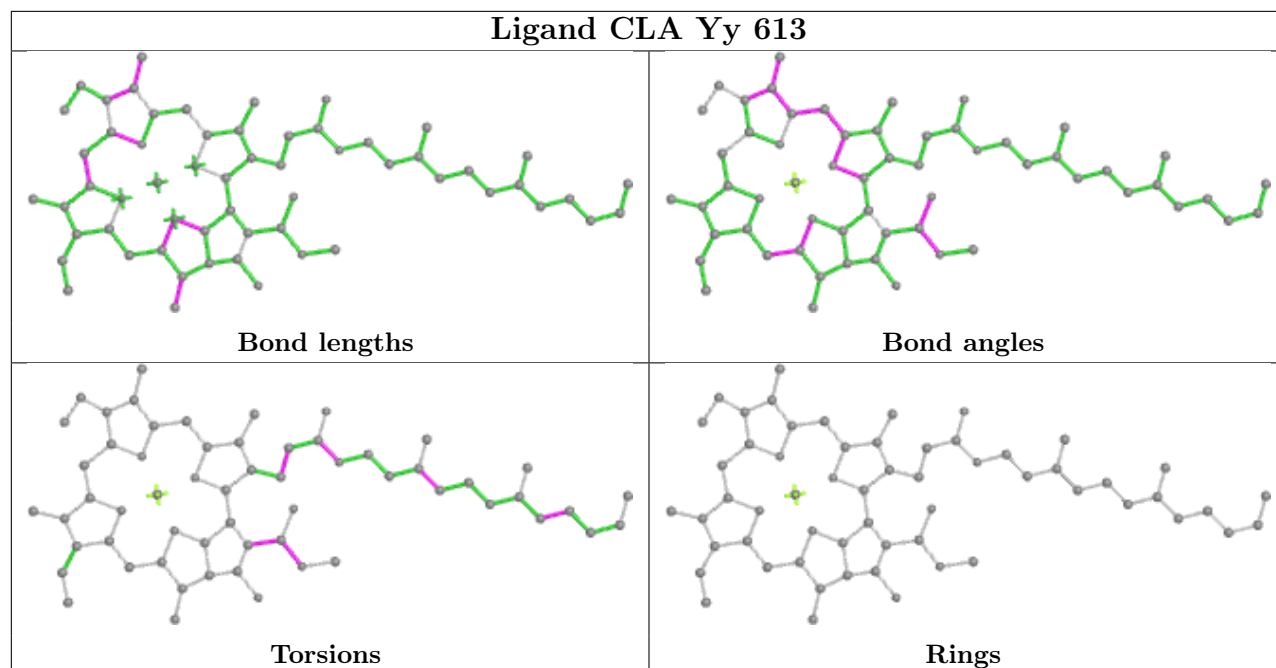
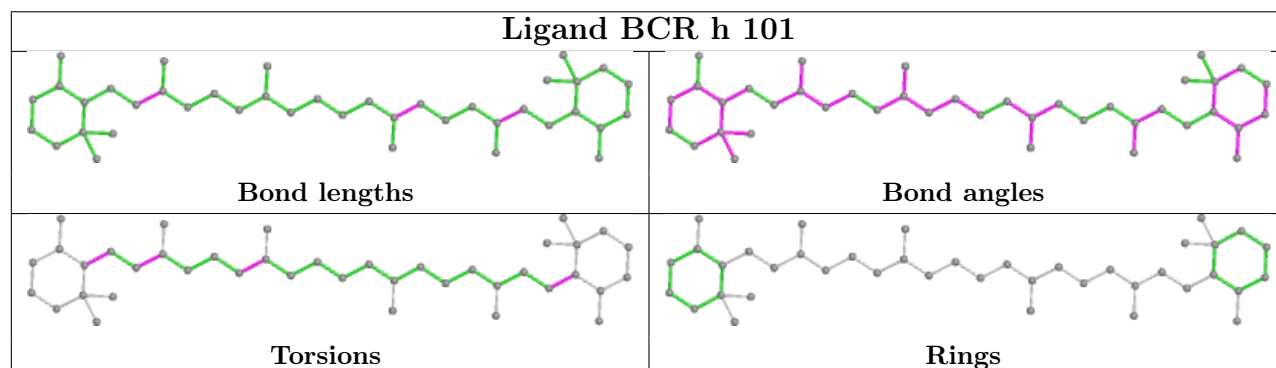
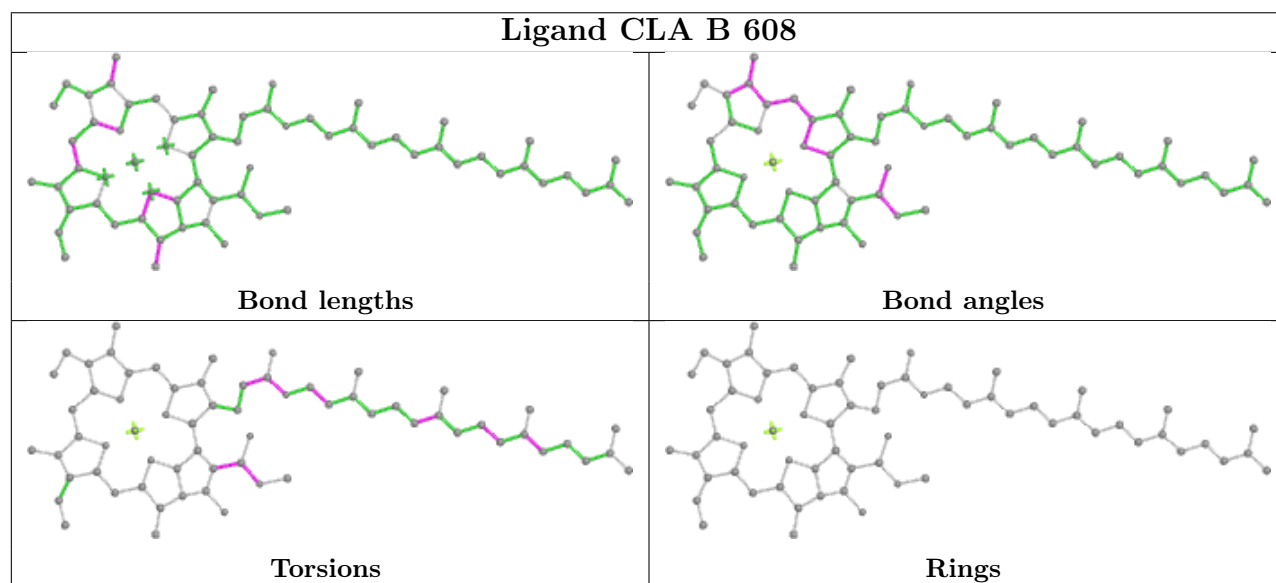


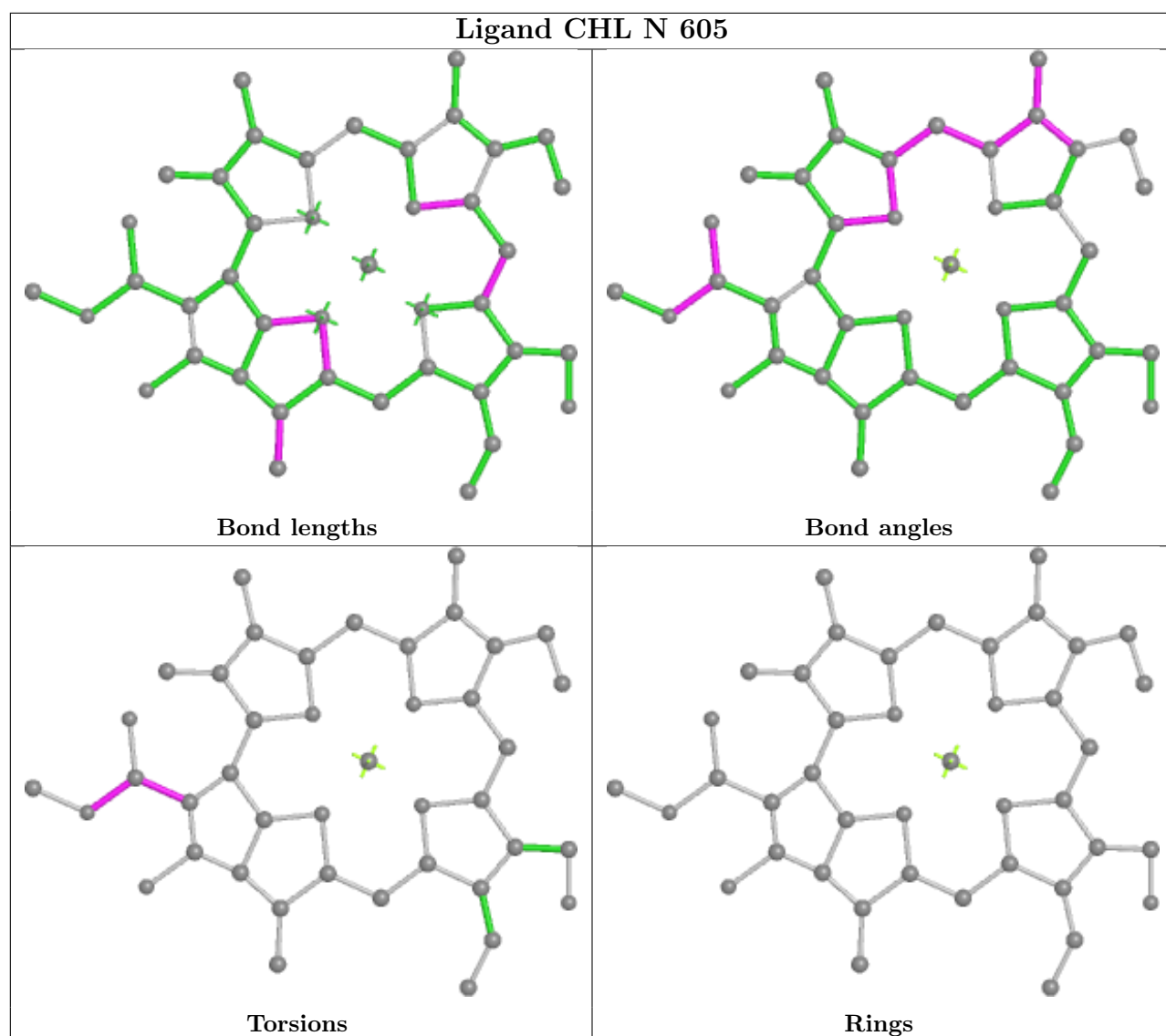
Rings



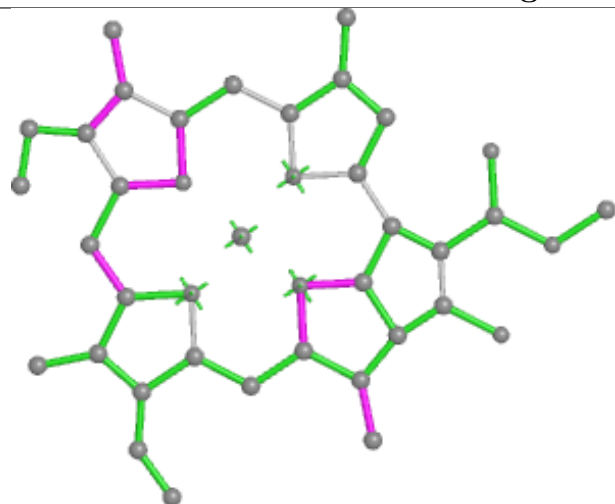




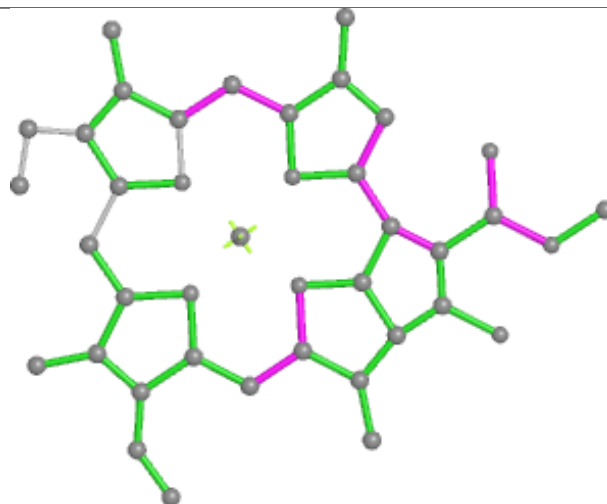
**Ligand CLA Yy 613****Ligand BCR h 101****Ligand CLA B 608**



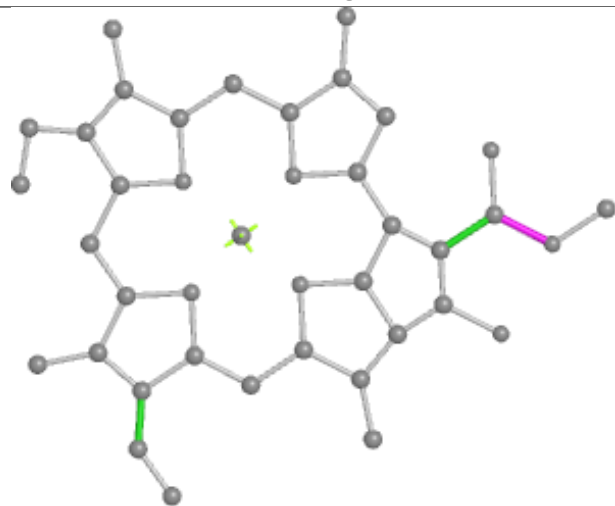
## Ligand CLA 1 611



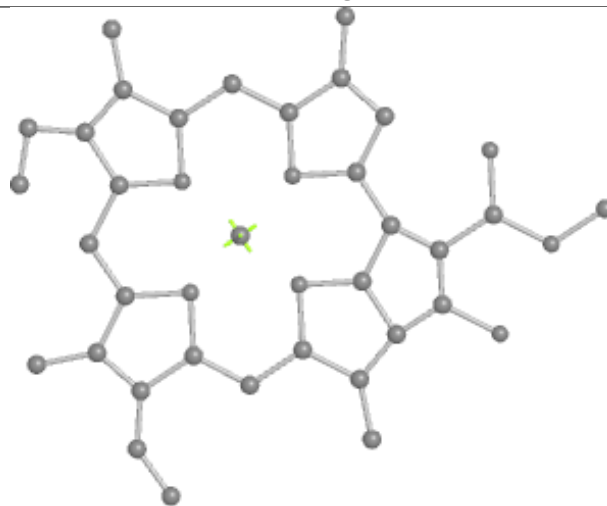
Bond lengths



Bond angles

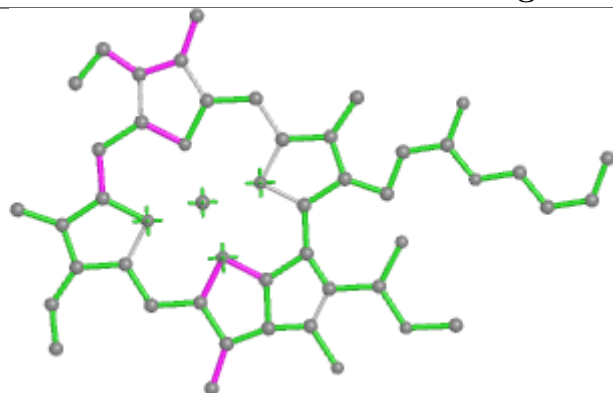


Torsions

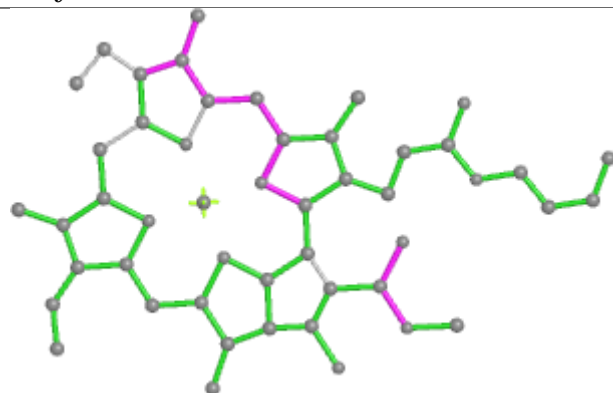


Rings

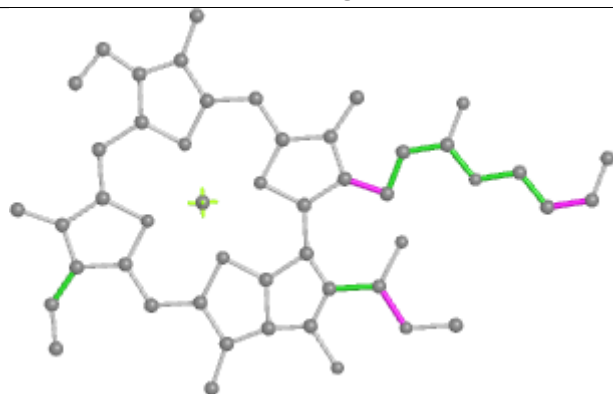
## Ligand CLA y 305



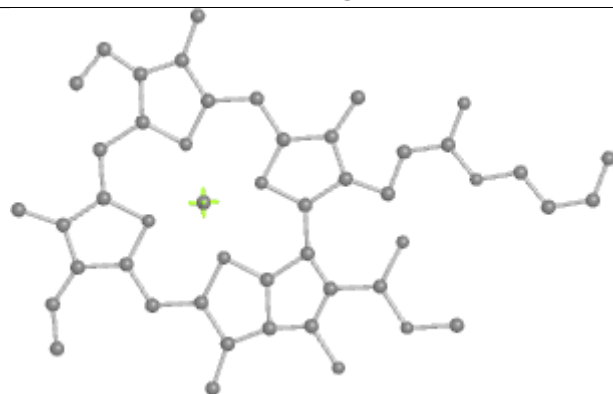
Bond lengths



Bond angles

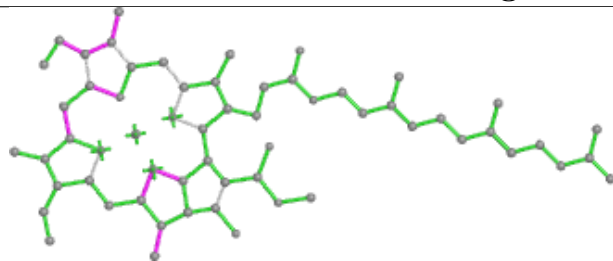


Torsions

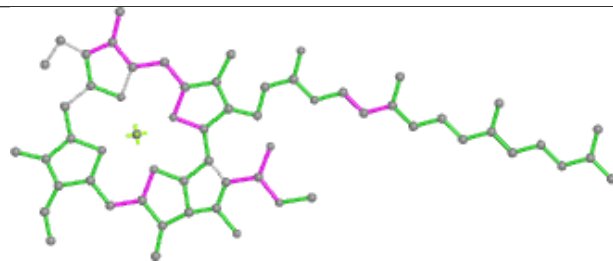


Rings

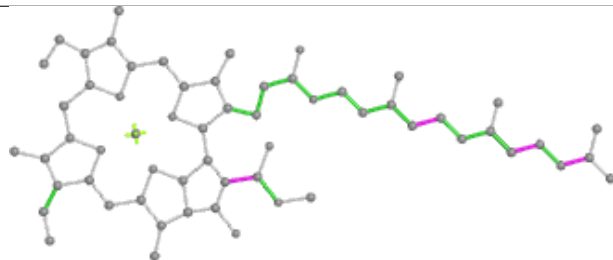
## Ligand CLA AA 408



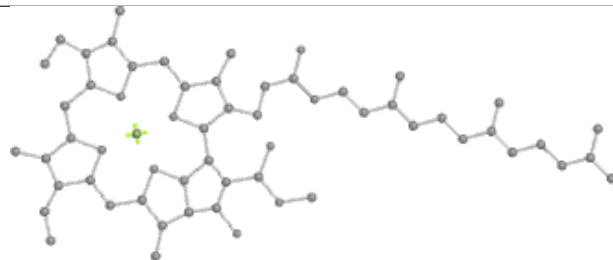
Bond lengths



Bond angles

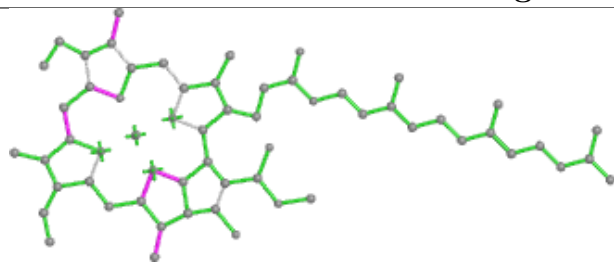


Torsions

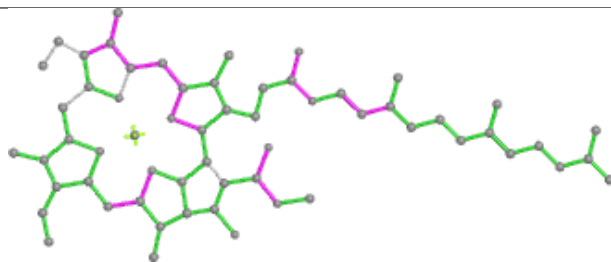


Rings

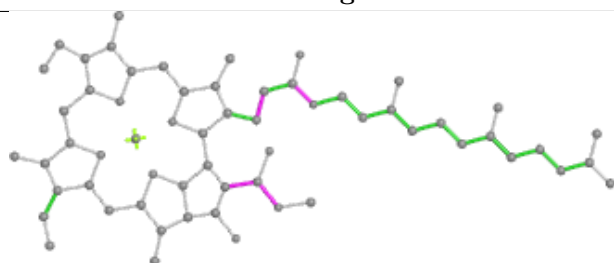
## Ligand CLA B 609



Bond lengths



Bond angles

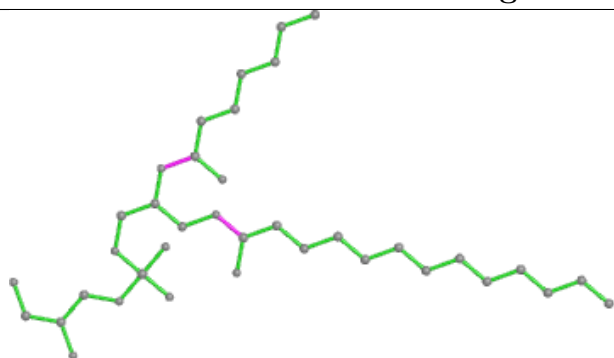


Torsions

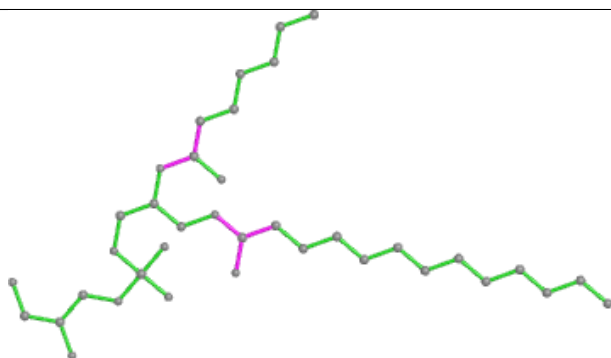


Rings

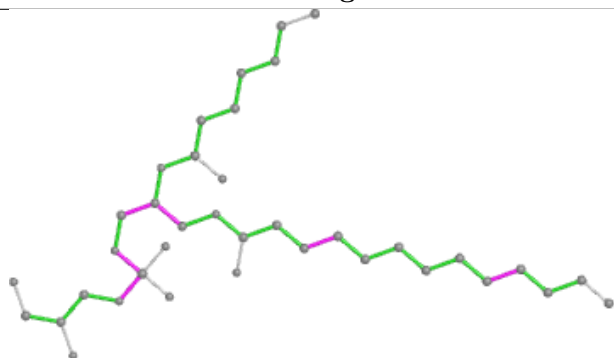
## Ligand LHG CC 523



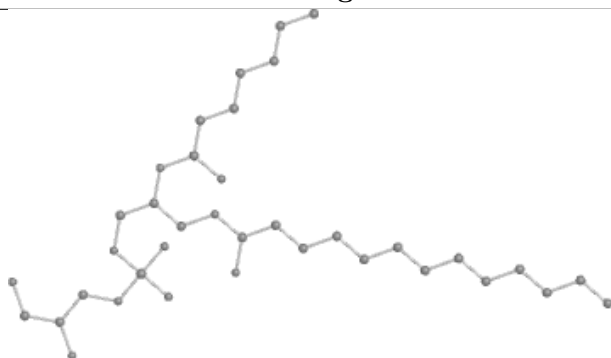
Bond lengths



Bond angles

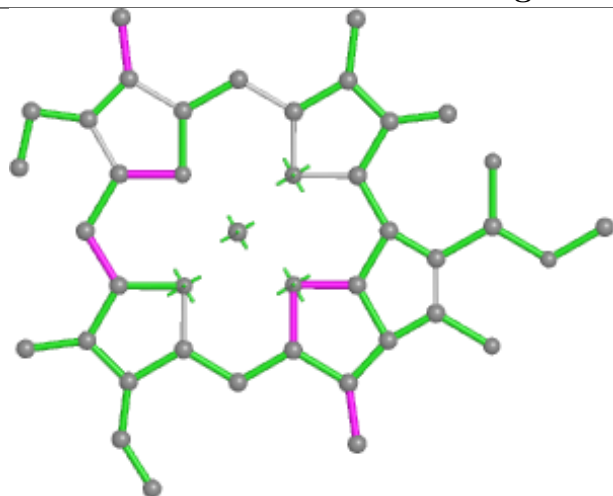


Torsions

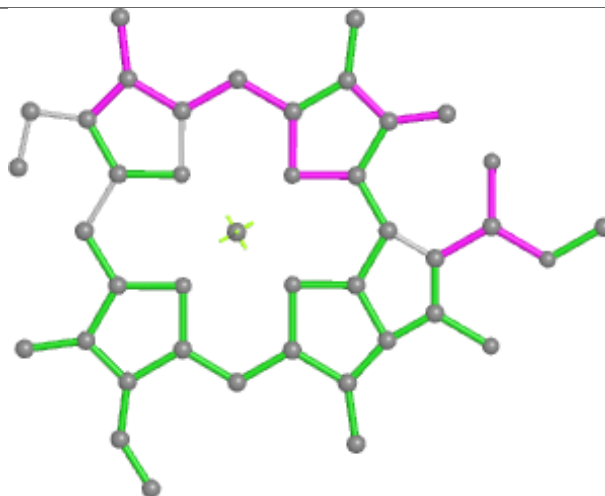


Rings

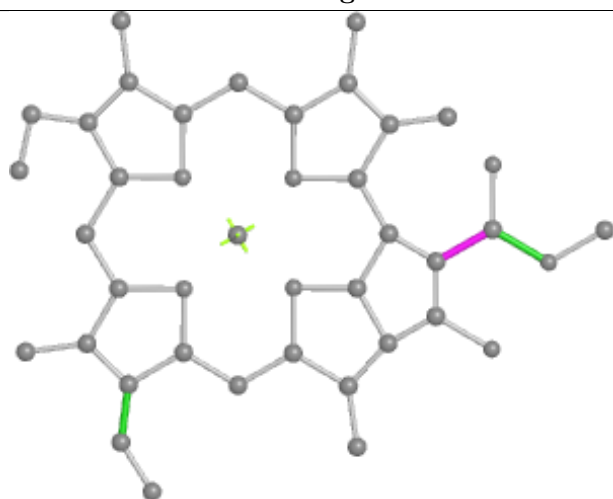
## Ligand CLA B 611



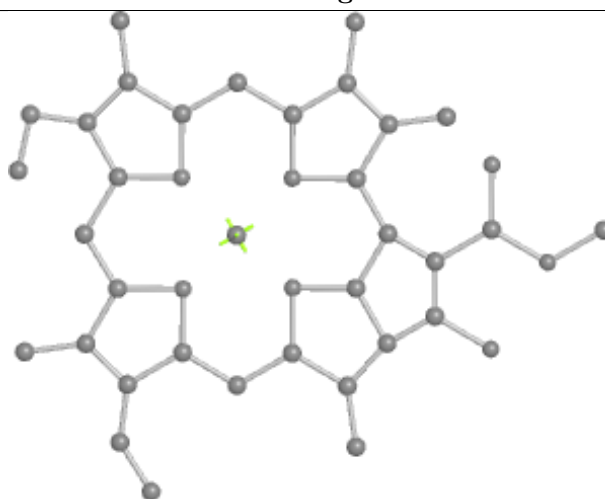
Bond lengths



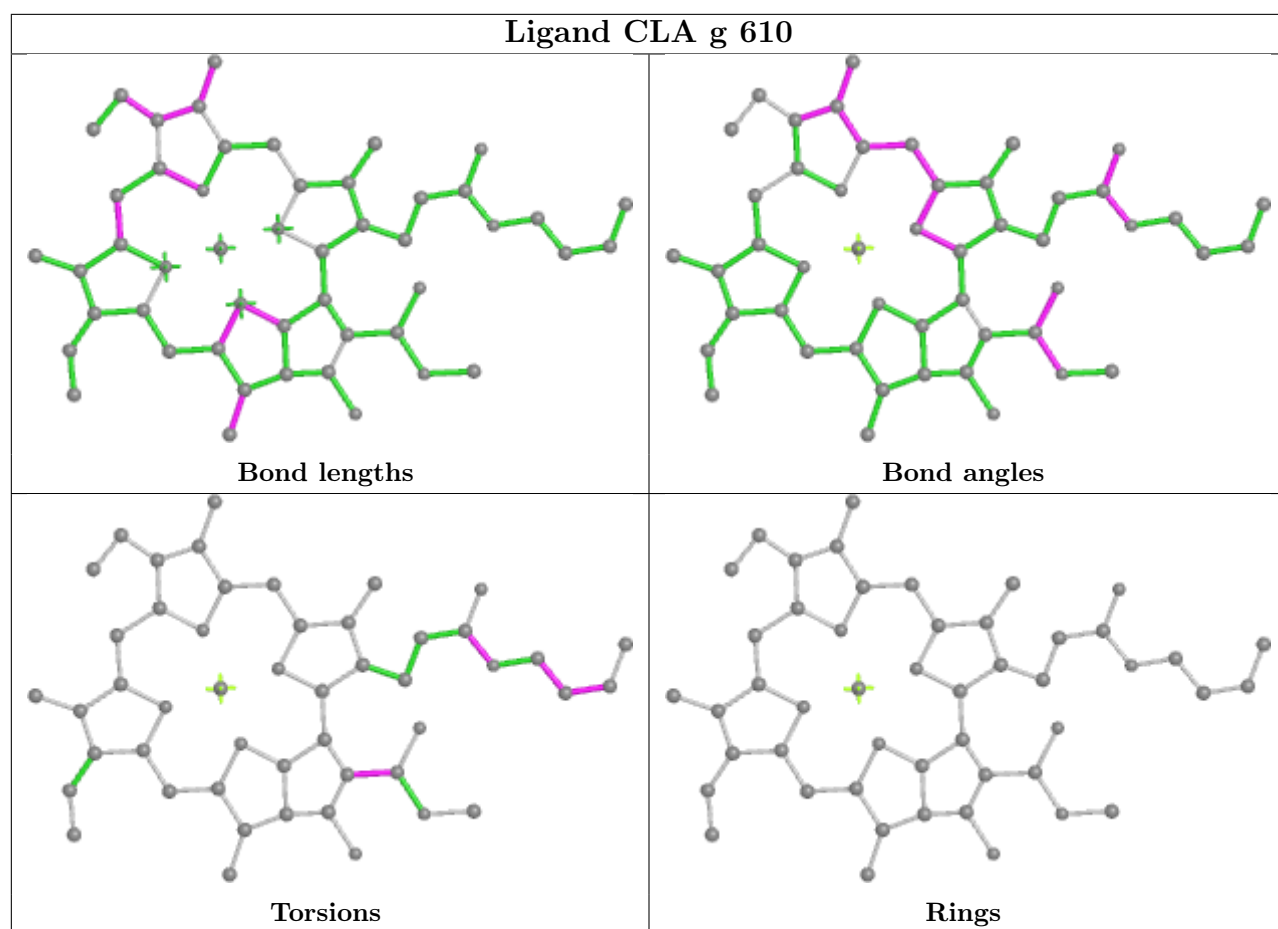
Bond angles



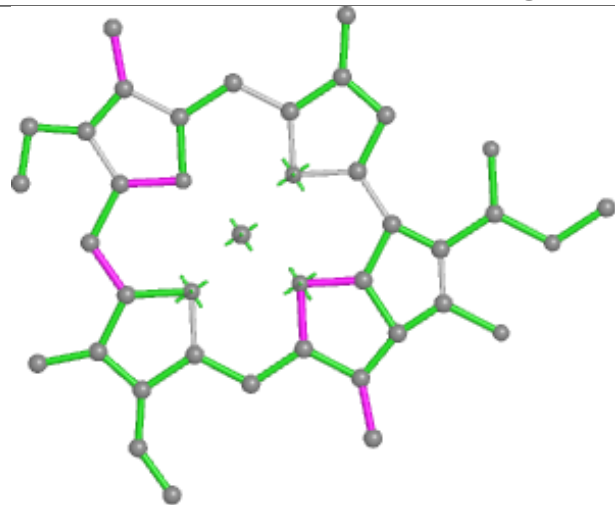
Torsions



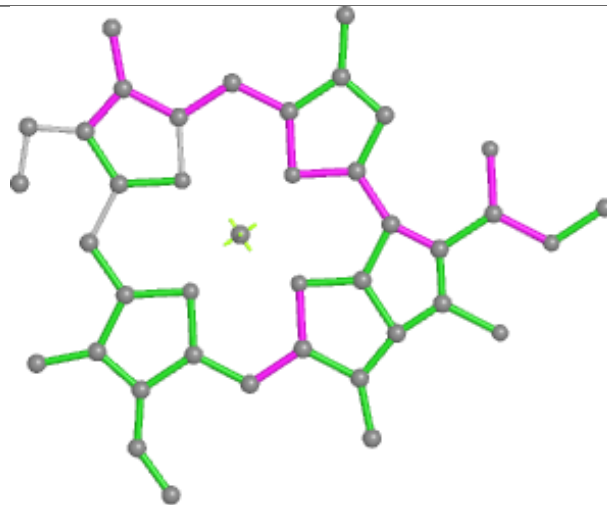
Rings



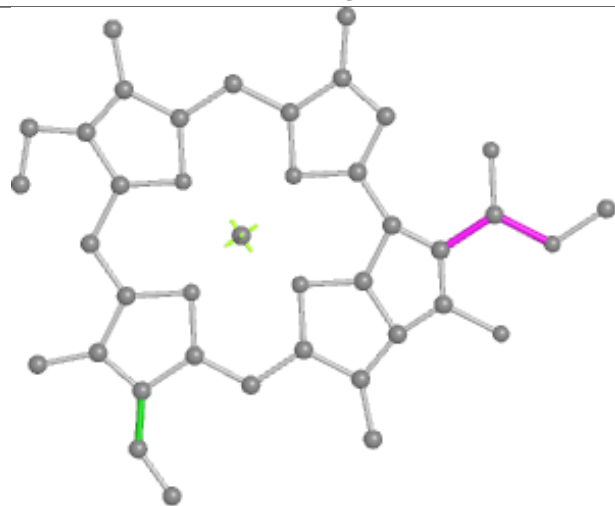
## Ligand CLA 3 611



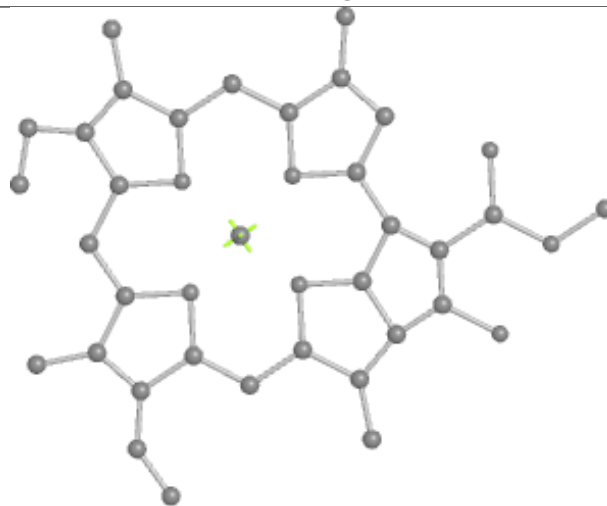
Bond lengths



Bond angles

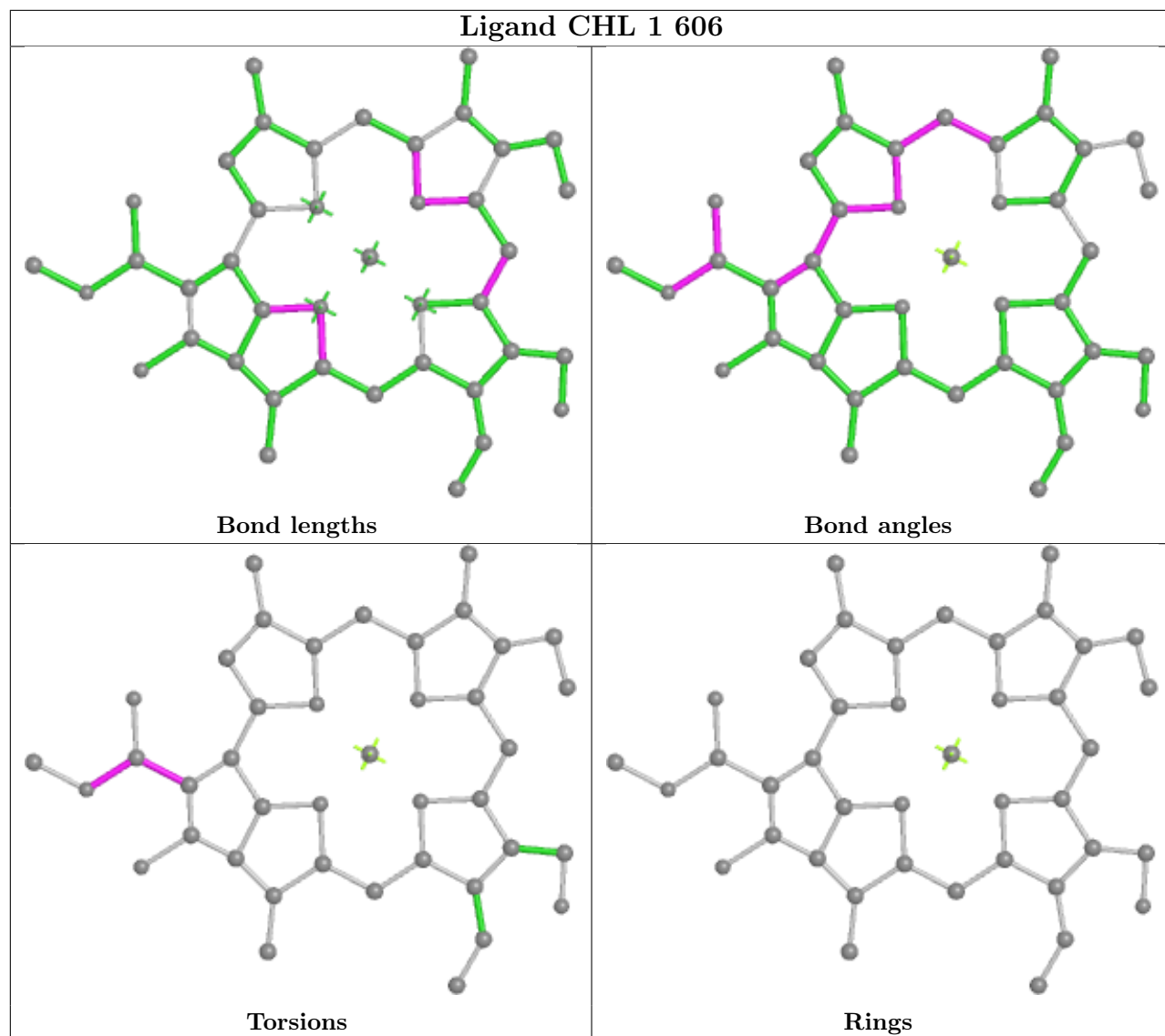


Torsions

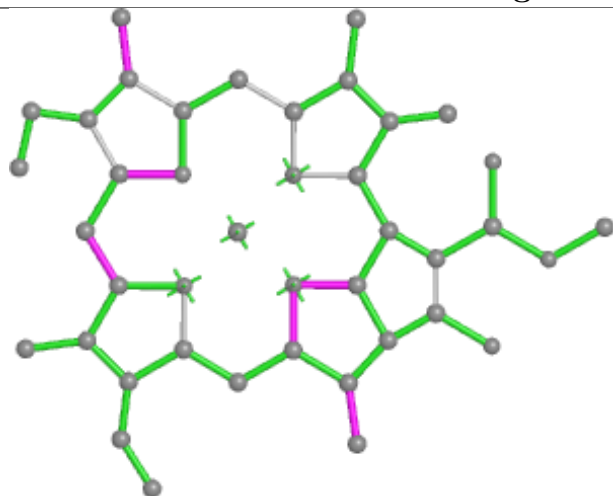


Rings

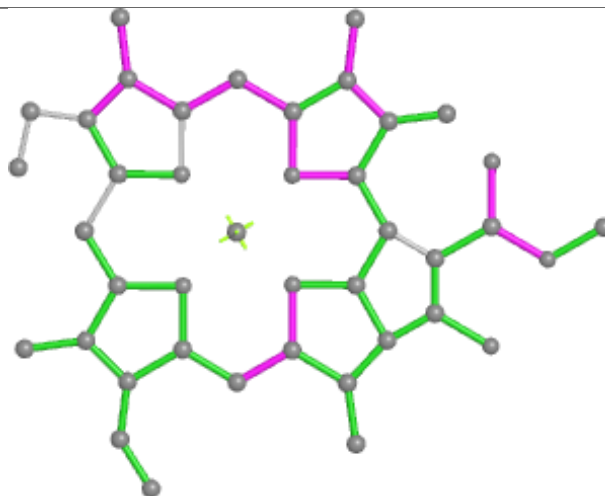




## Ligand CLA N 604



Bond lengths



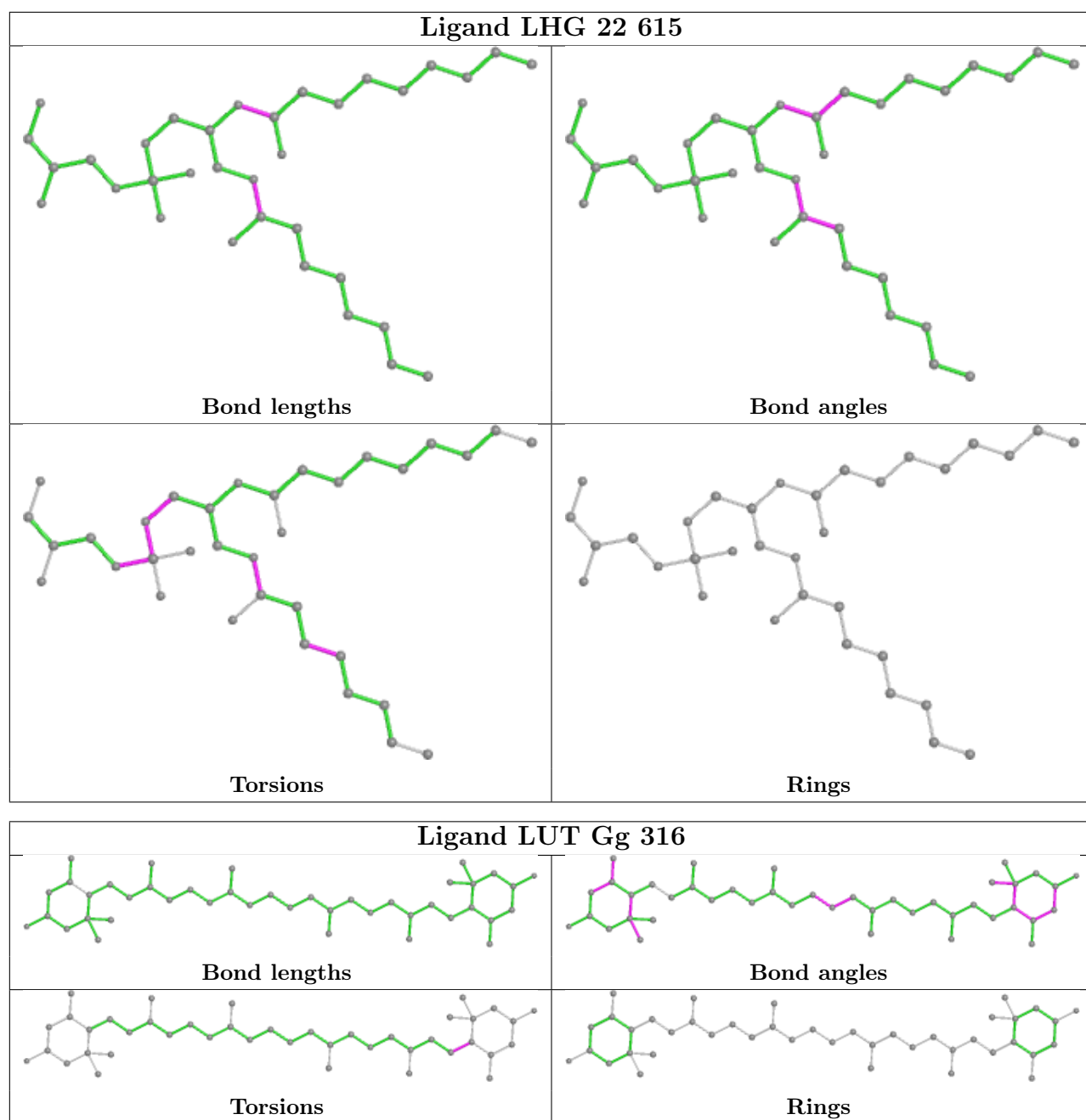
Bond angles



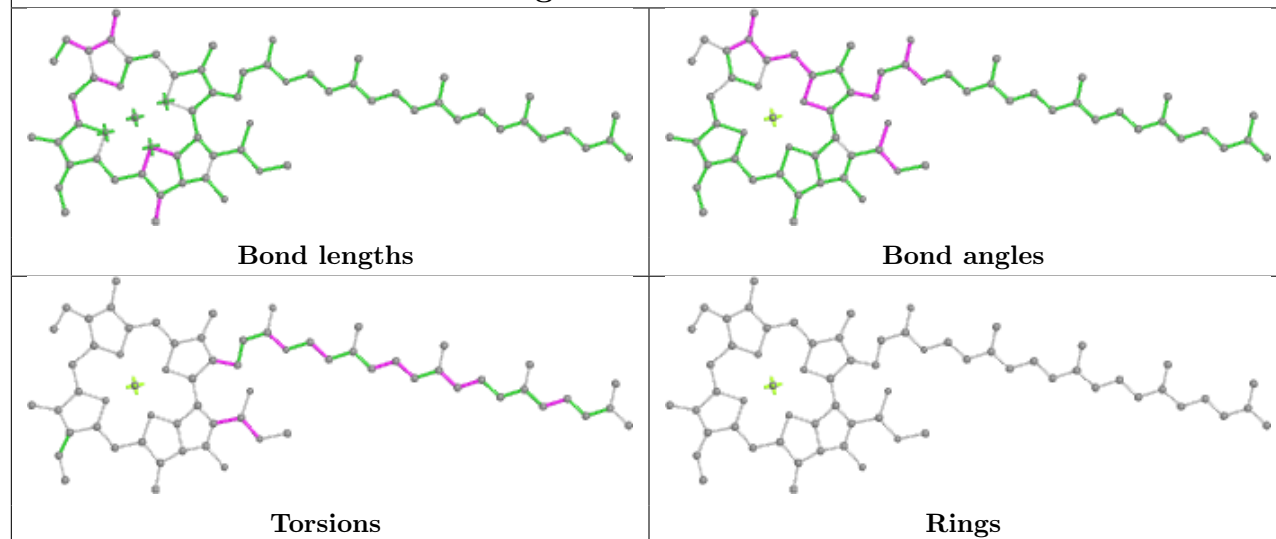
Torsions



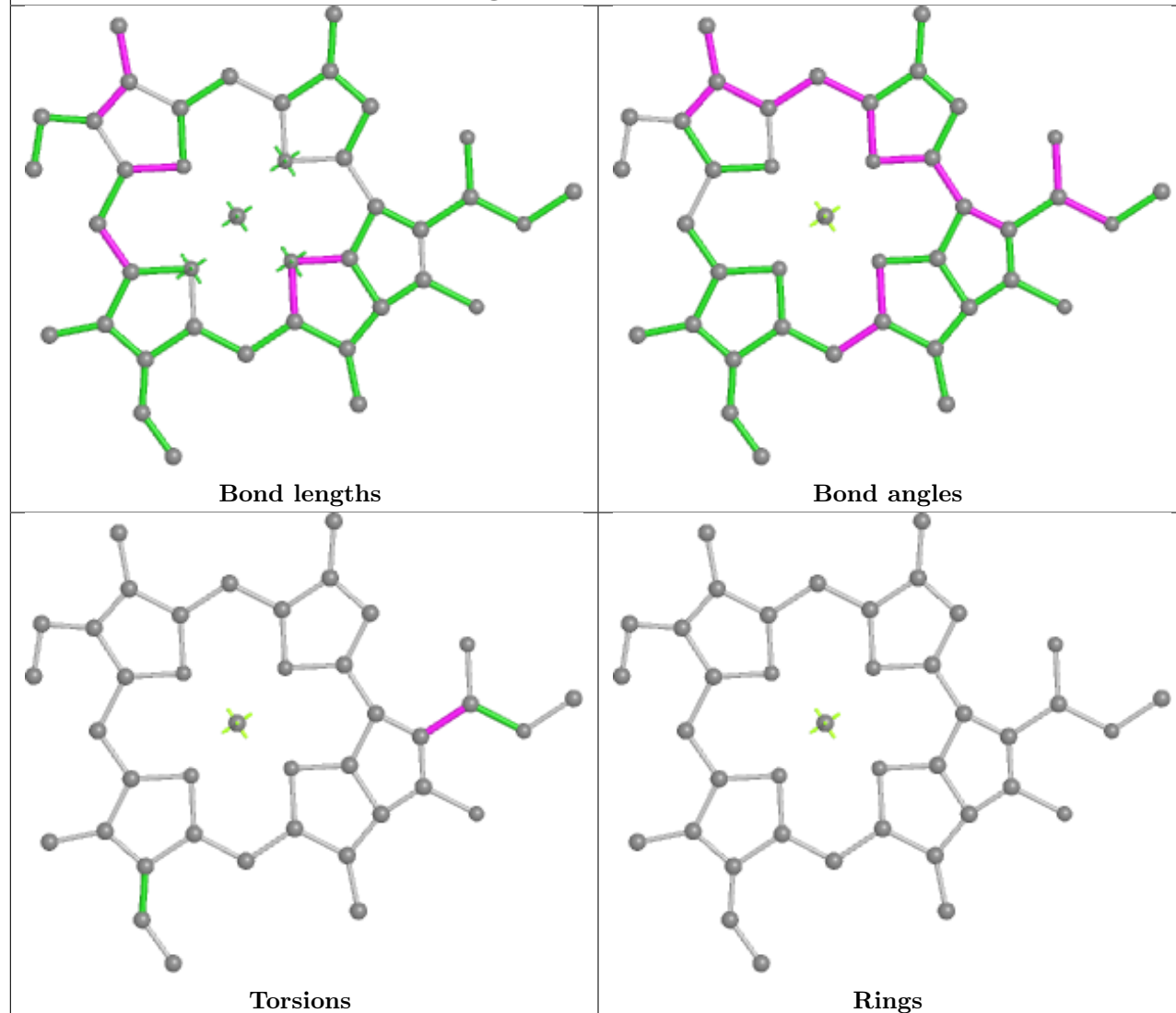
Rings



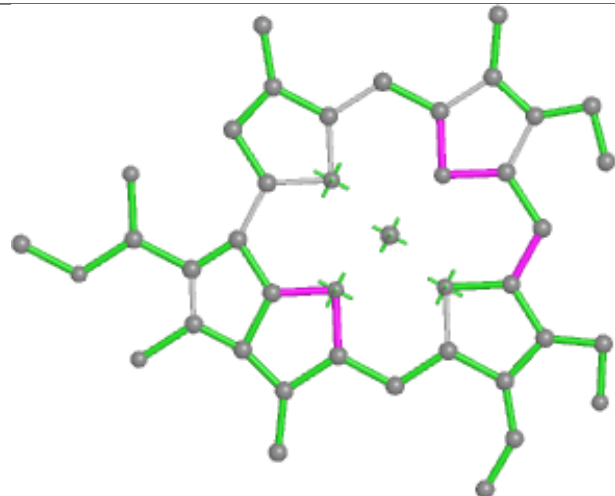
## Ligand CLA b 603



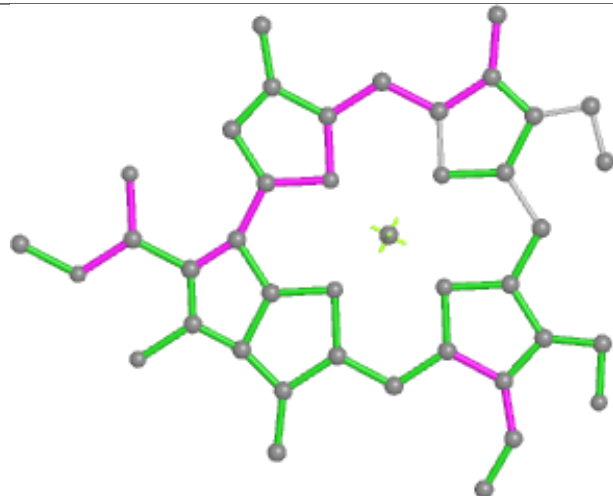
## Ligand CLA 22 602



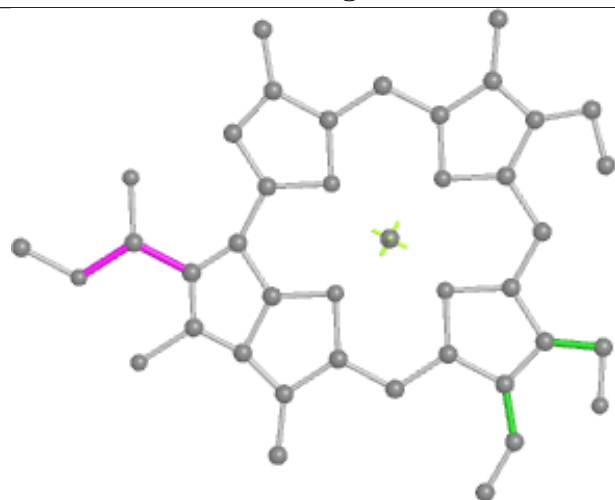
## Ligand CHL 3 606



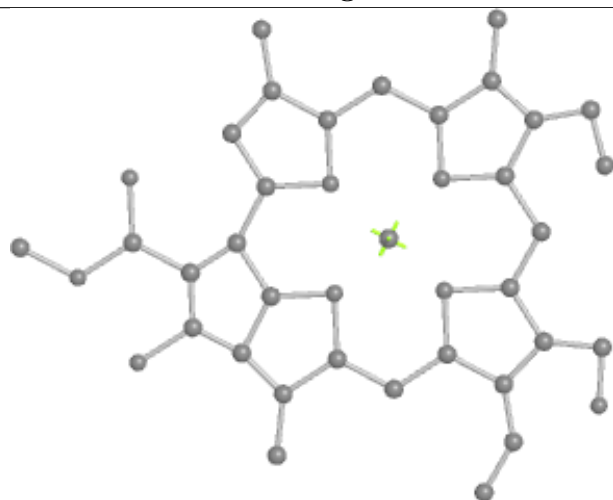
Bond lengths



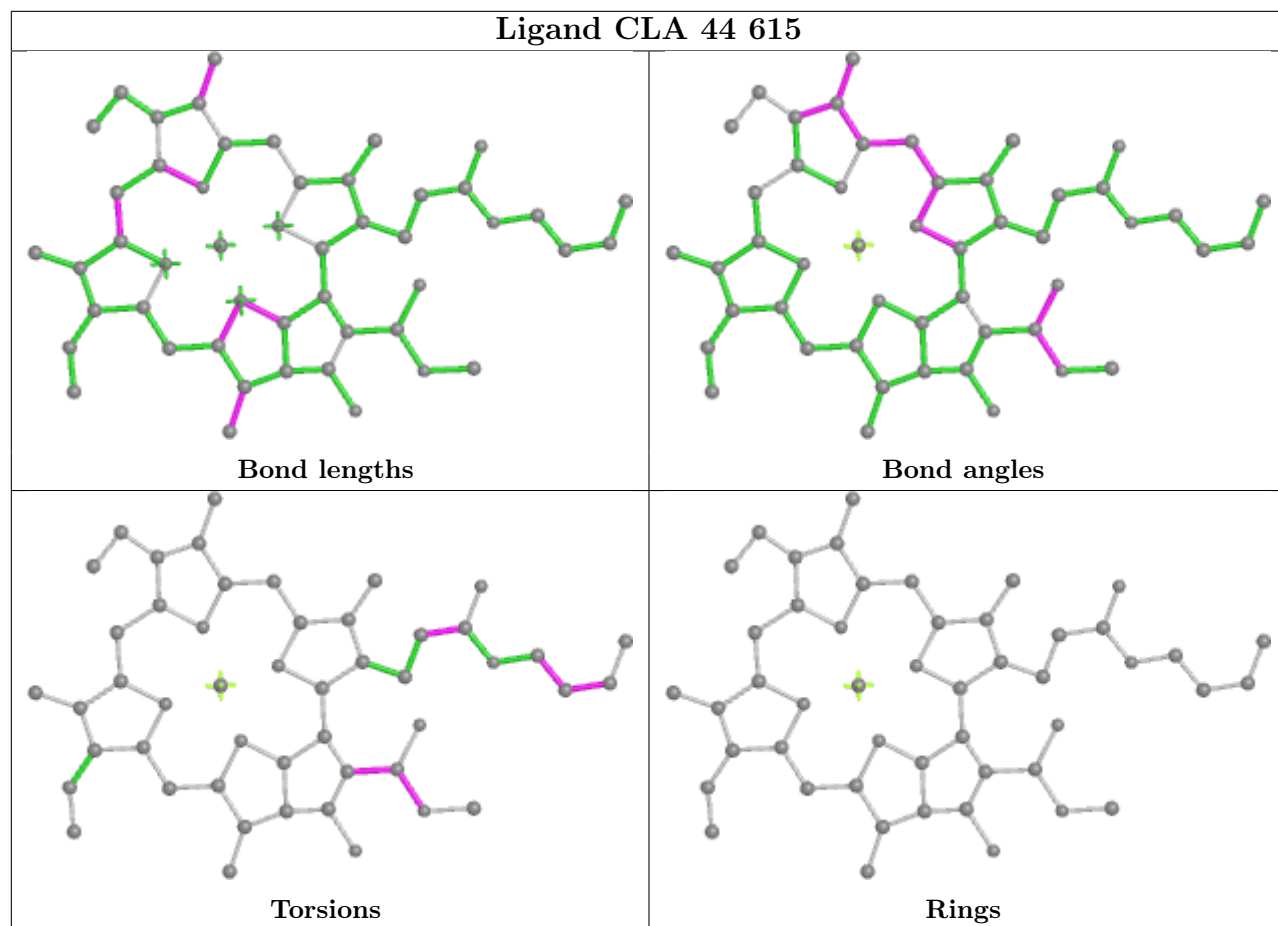
Bond angles



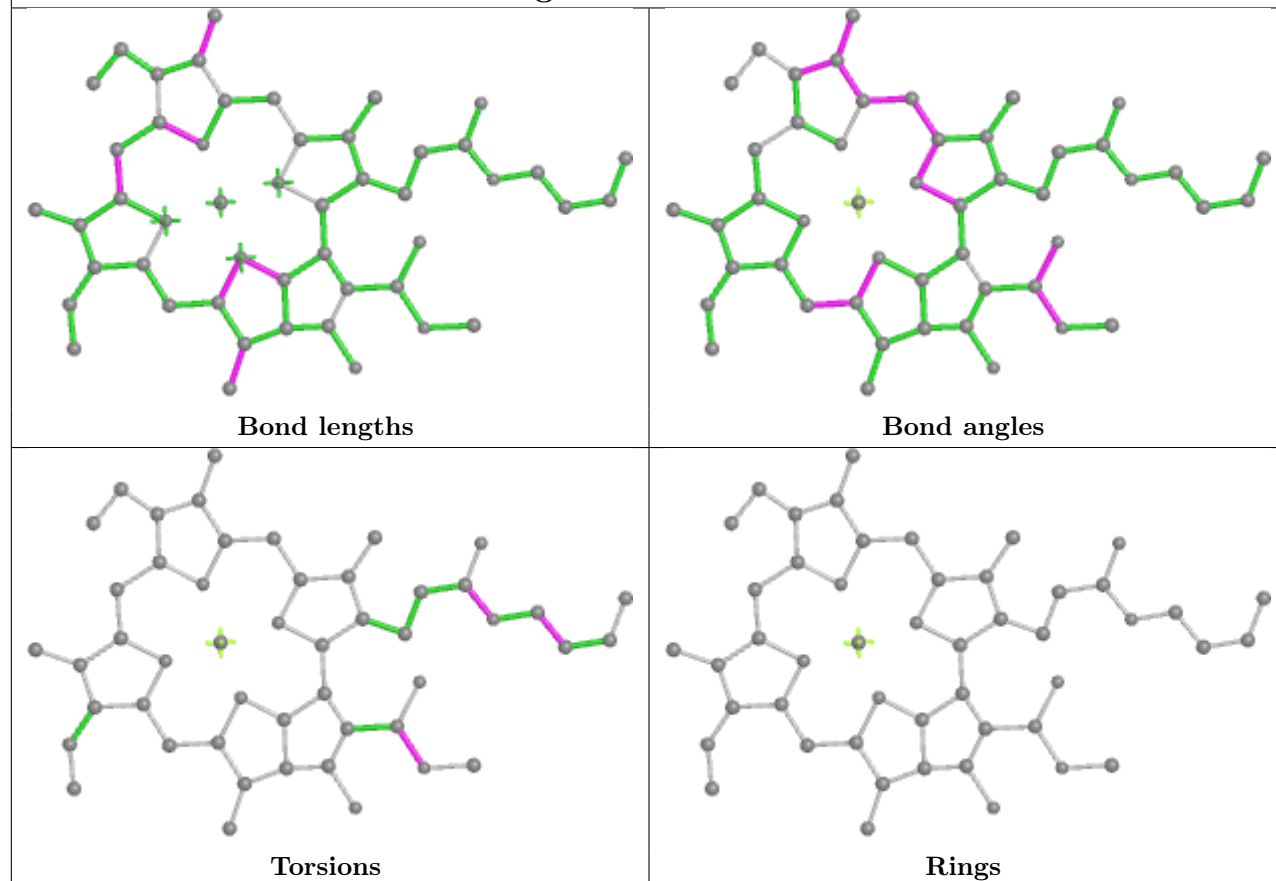
Torsions



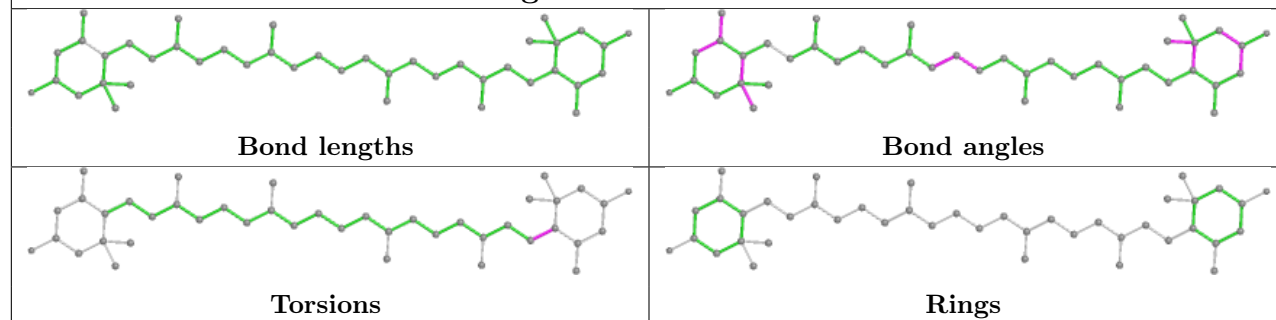
Rings



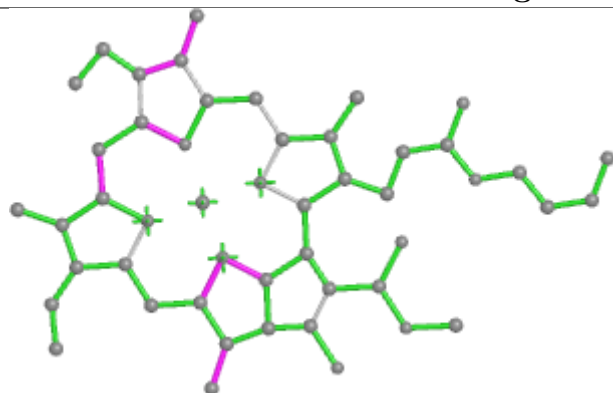
## Ligand CLA n 611



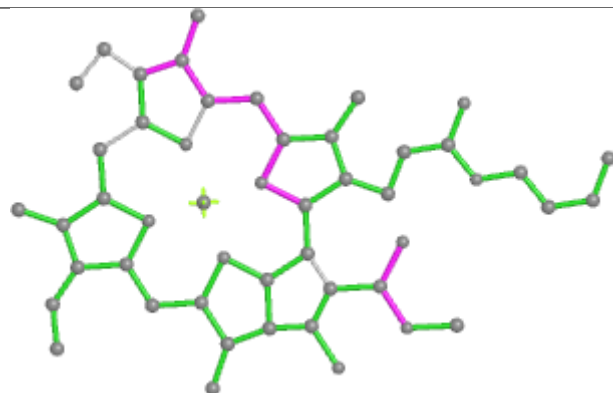
## Ligand LUT Nn 306



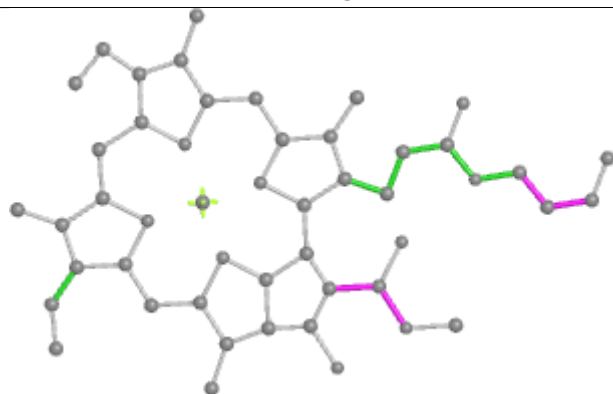
## Ligand CLA R 601



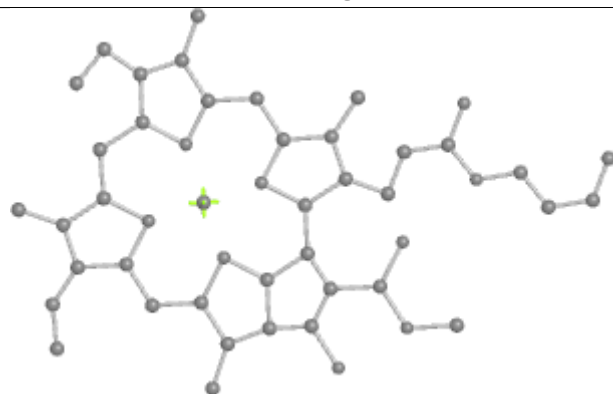
Bond lengths



Bond angles

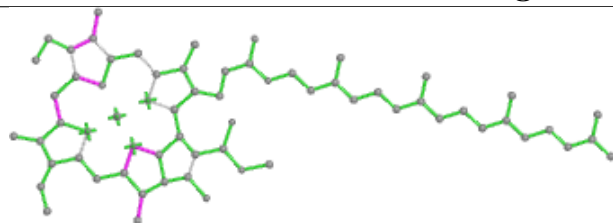


Torsions

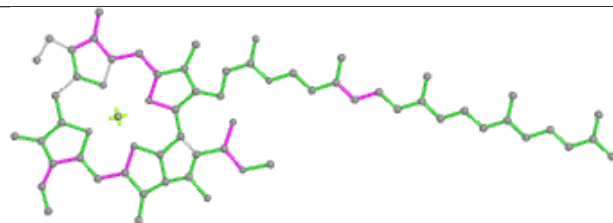


Rings

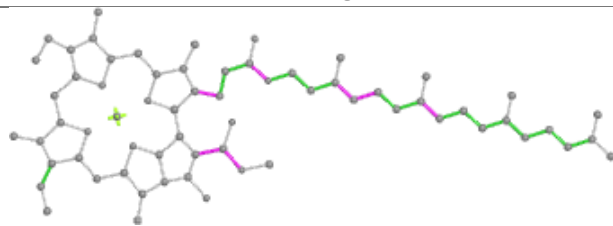
## Ligand CLA B 621



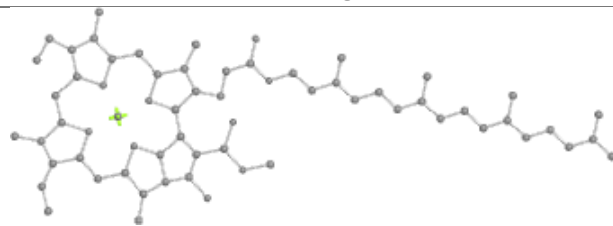
Bond lengths



Bond angles

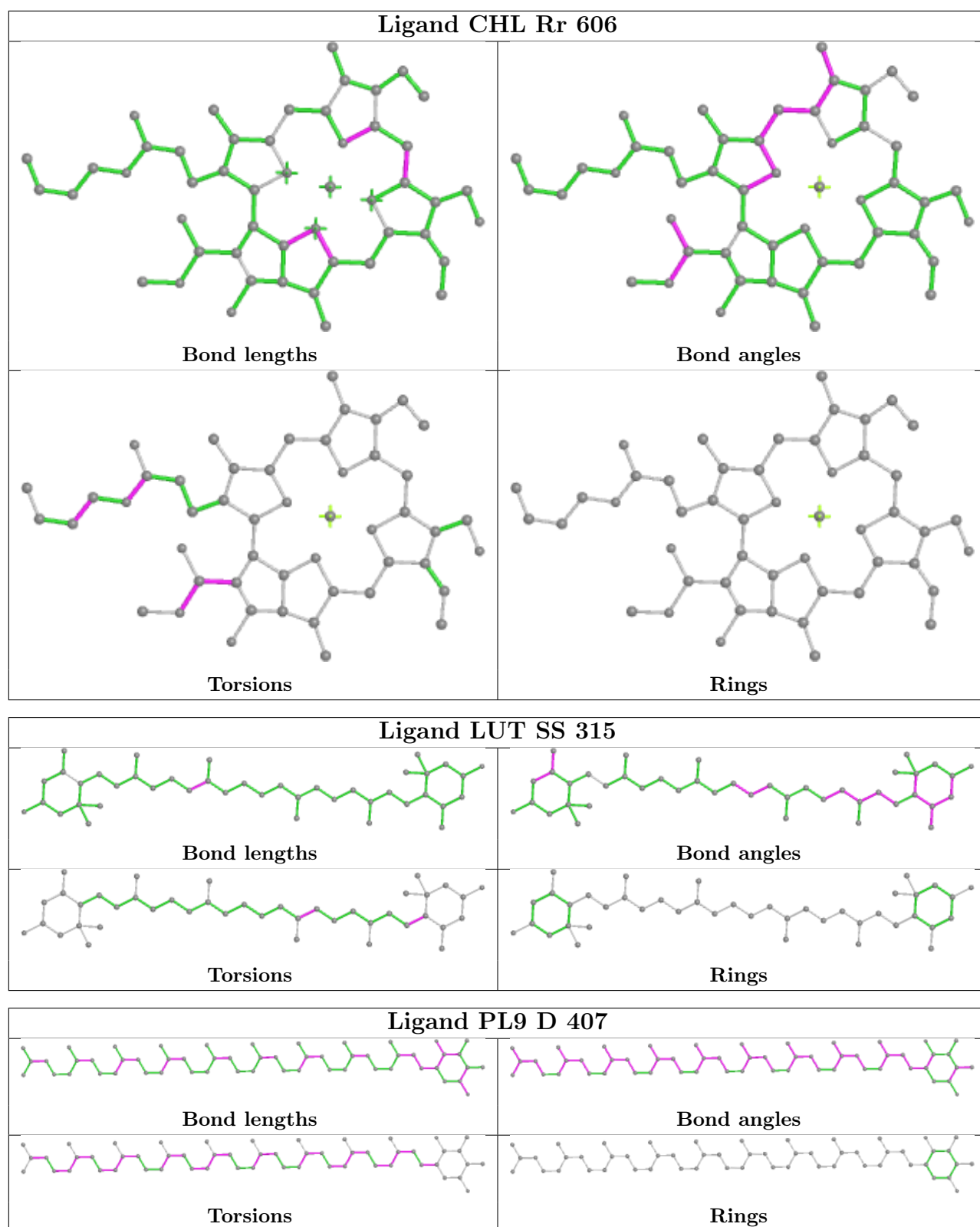


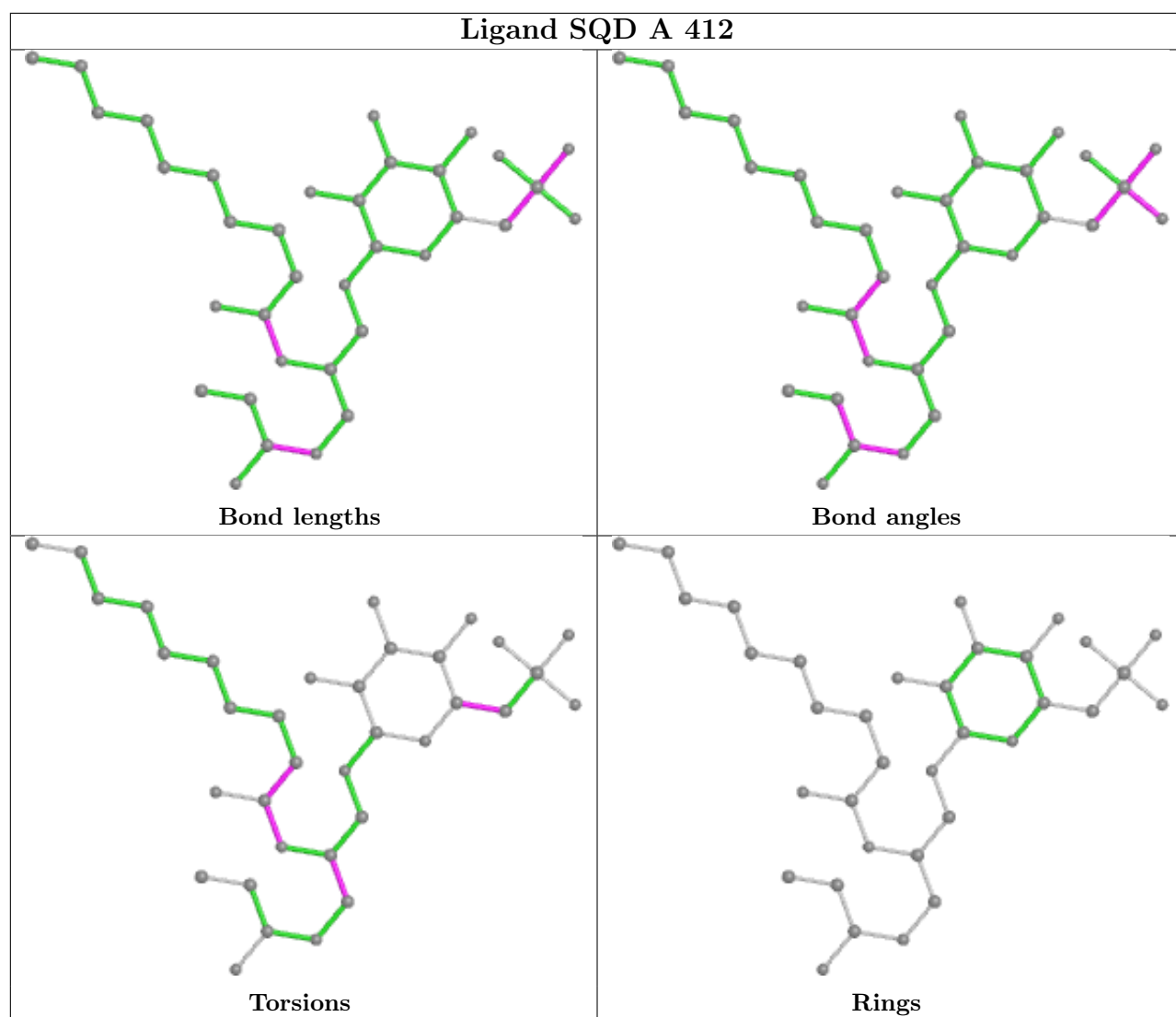
Torsions



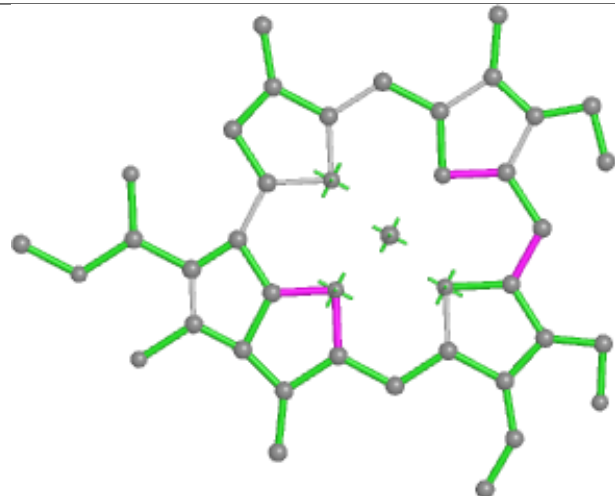
Rings



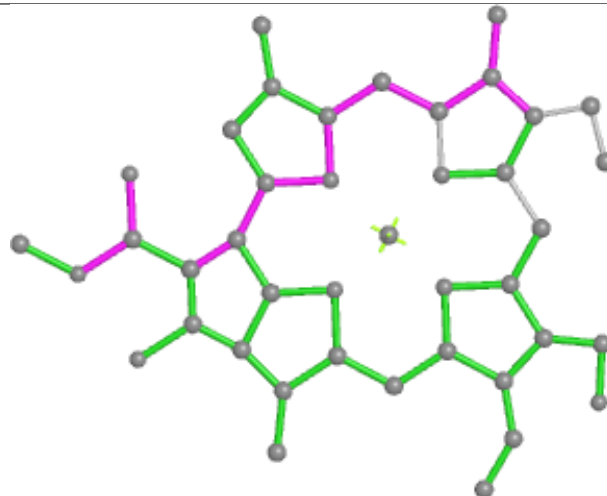




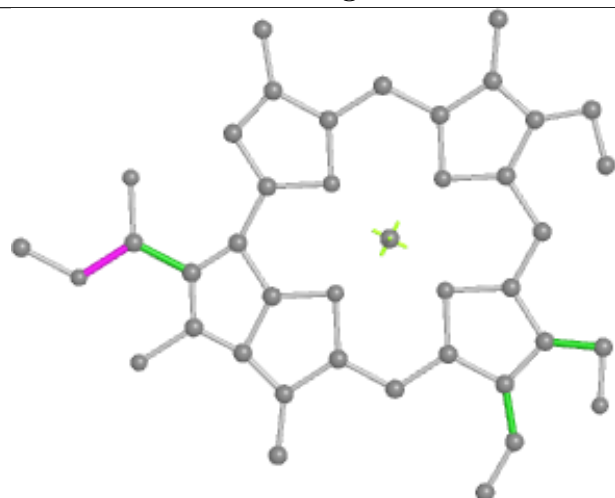
## Ligand CHL 1 607



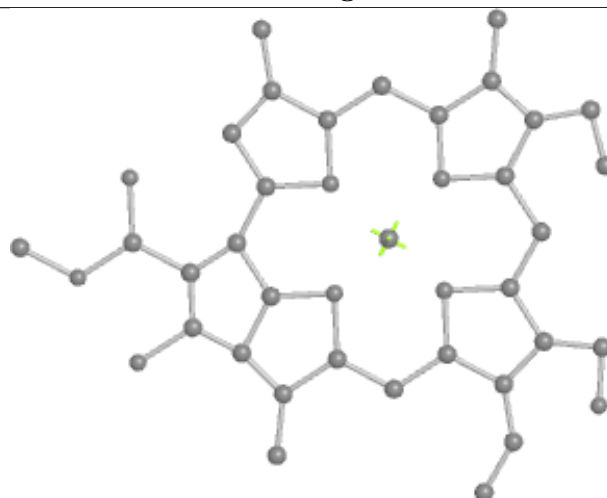
Bond lengths



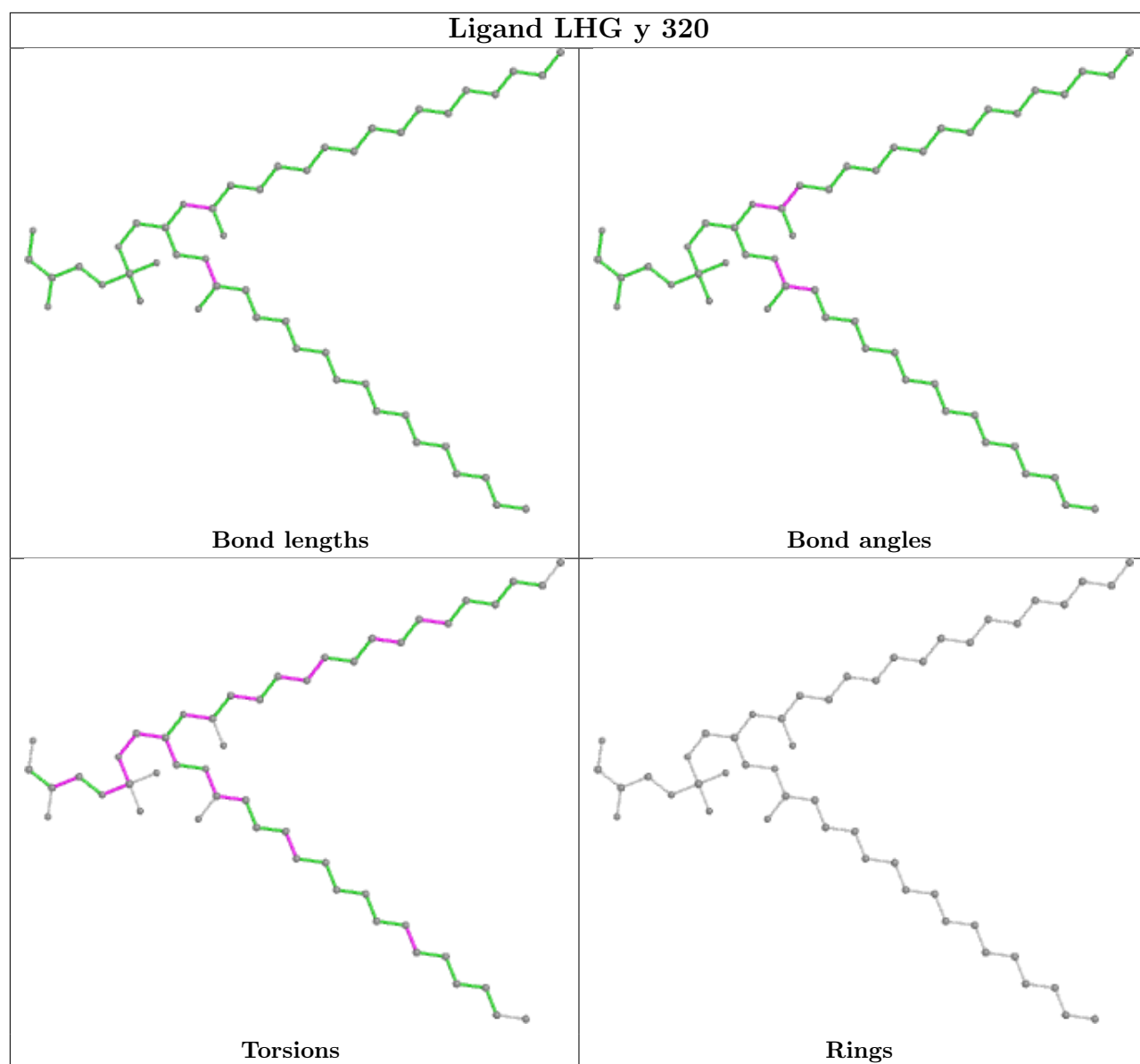
Bond angles

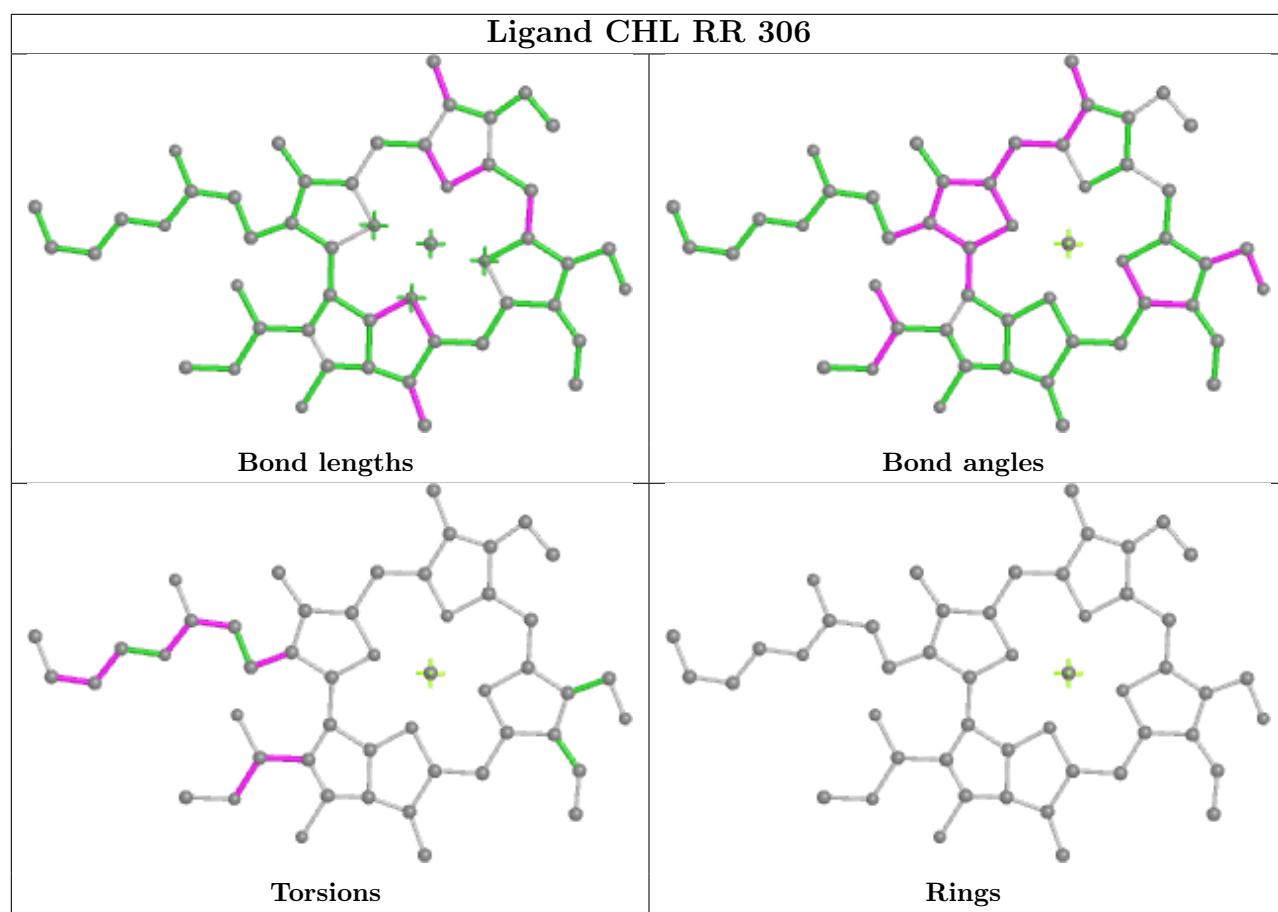


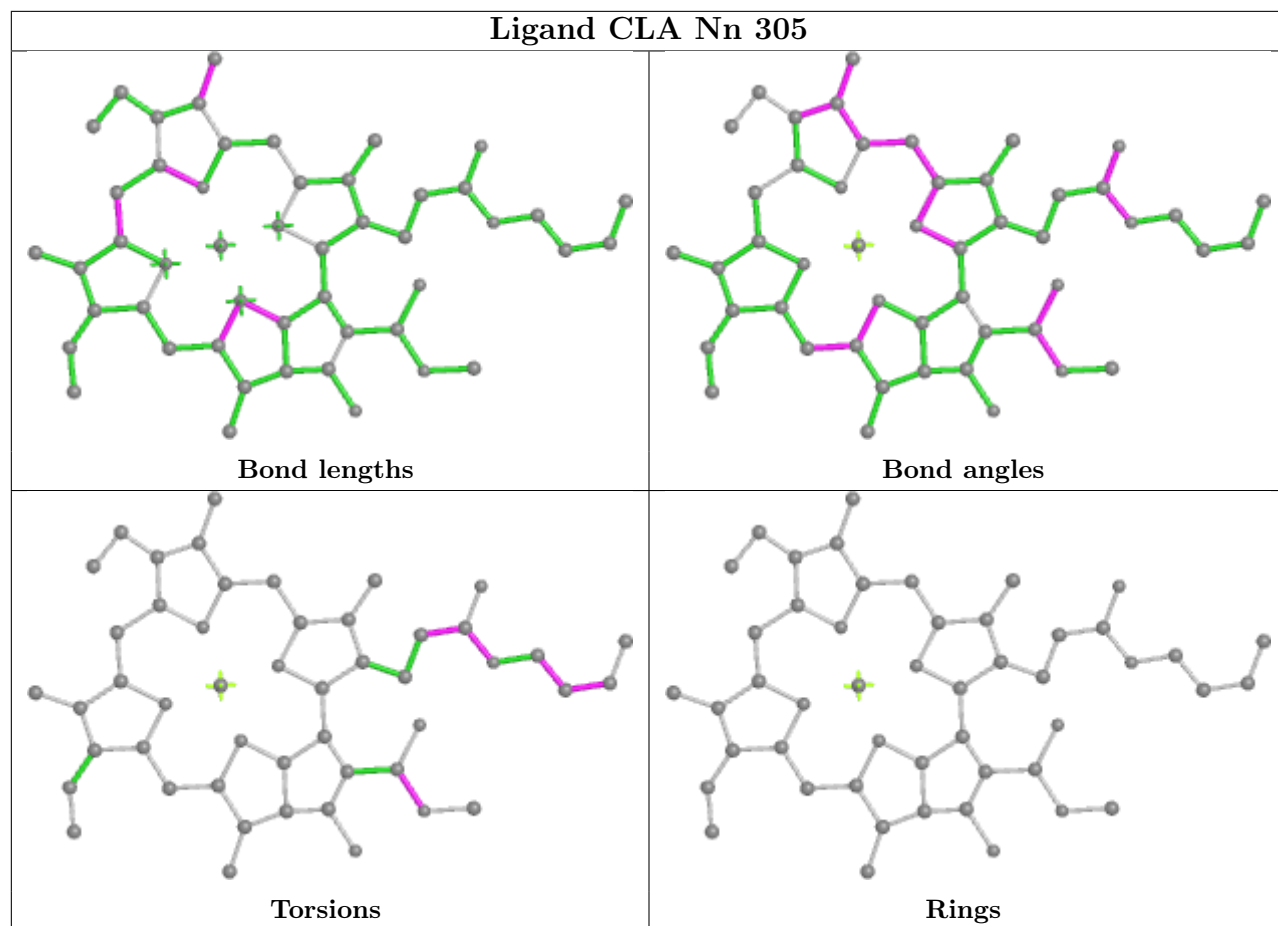
Torsions



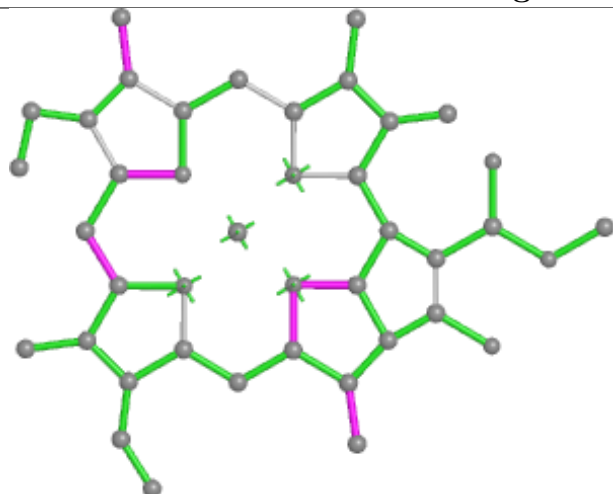
Rings



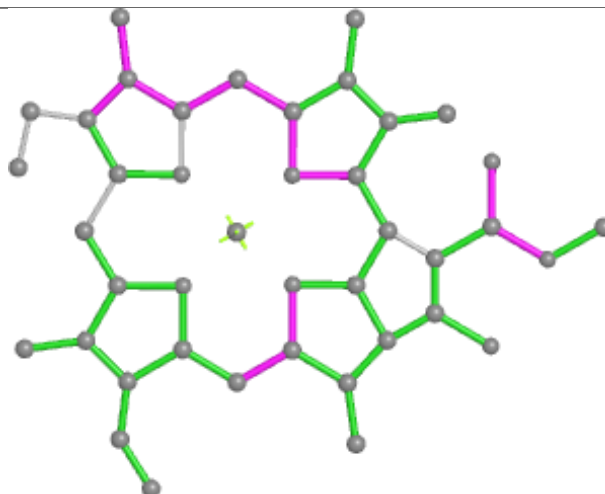




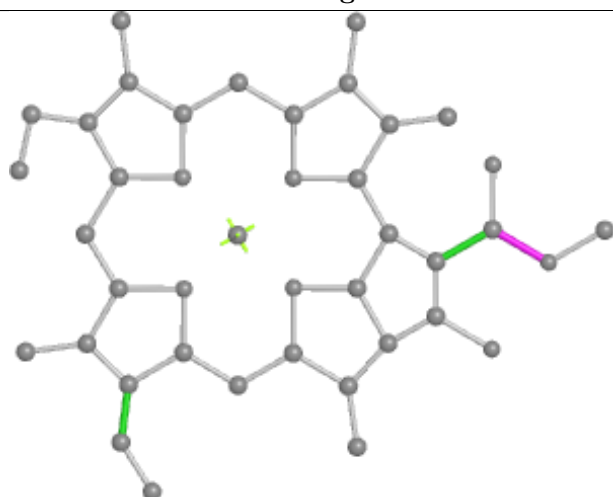
## Ligand CLA G 614



Bond lengths



Bond angles

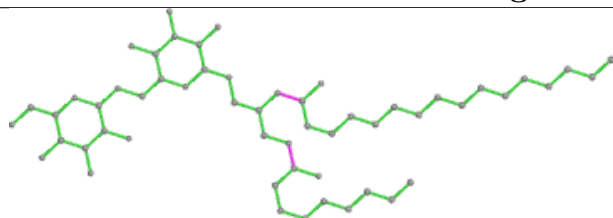


Torsions

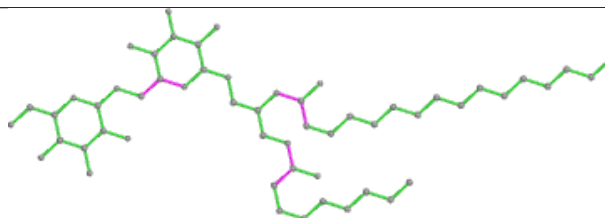


Rings

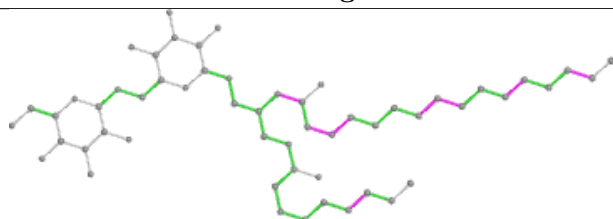
## Ligand DGD C 519



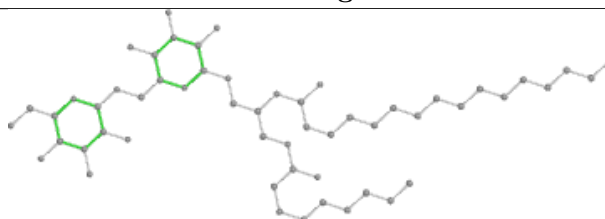
Bond lengths



Bond angles

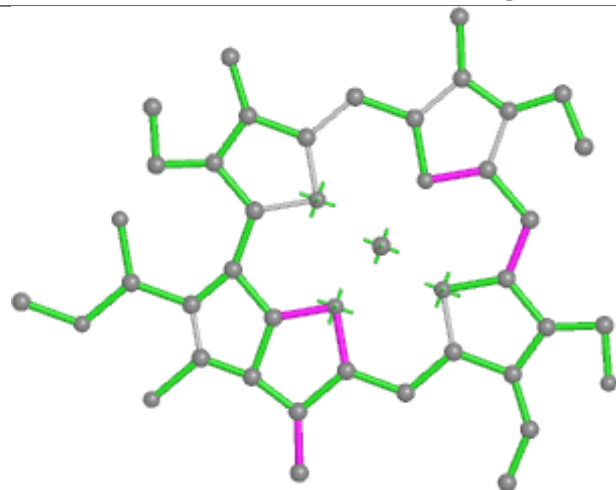


Torsions

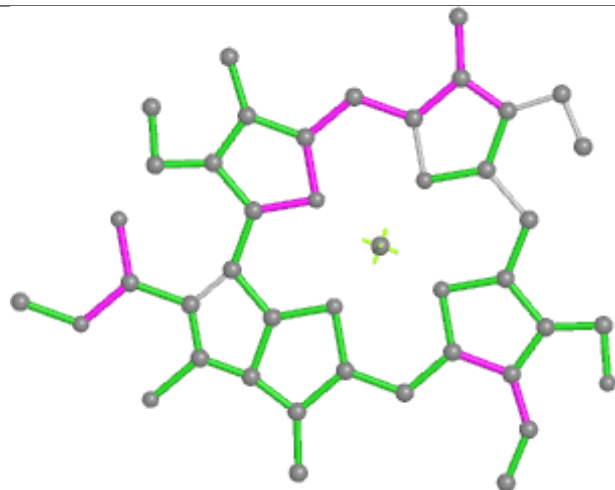


Rings

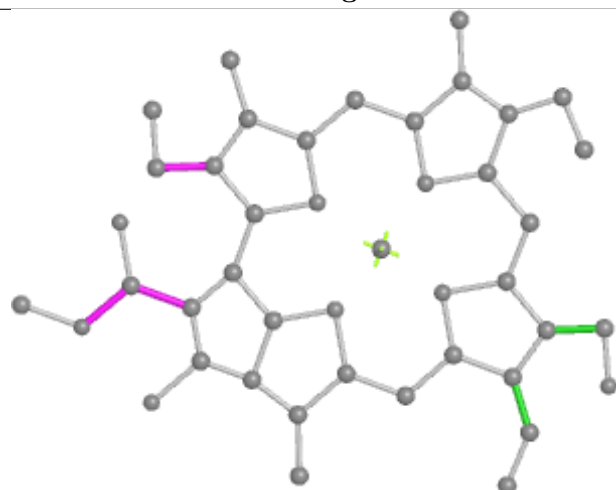
## Ligand CHL GG 609



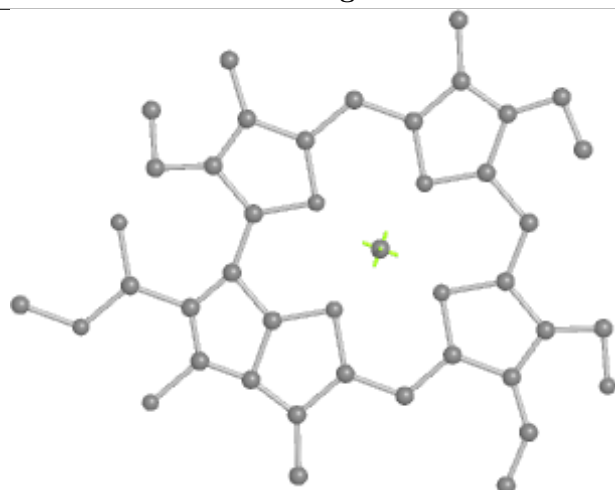
Bond lengths



Bond angles



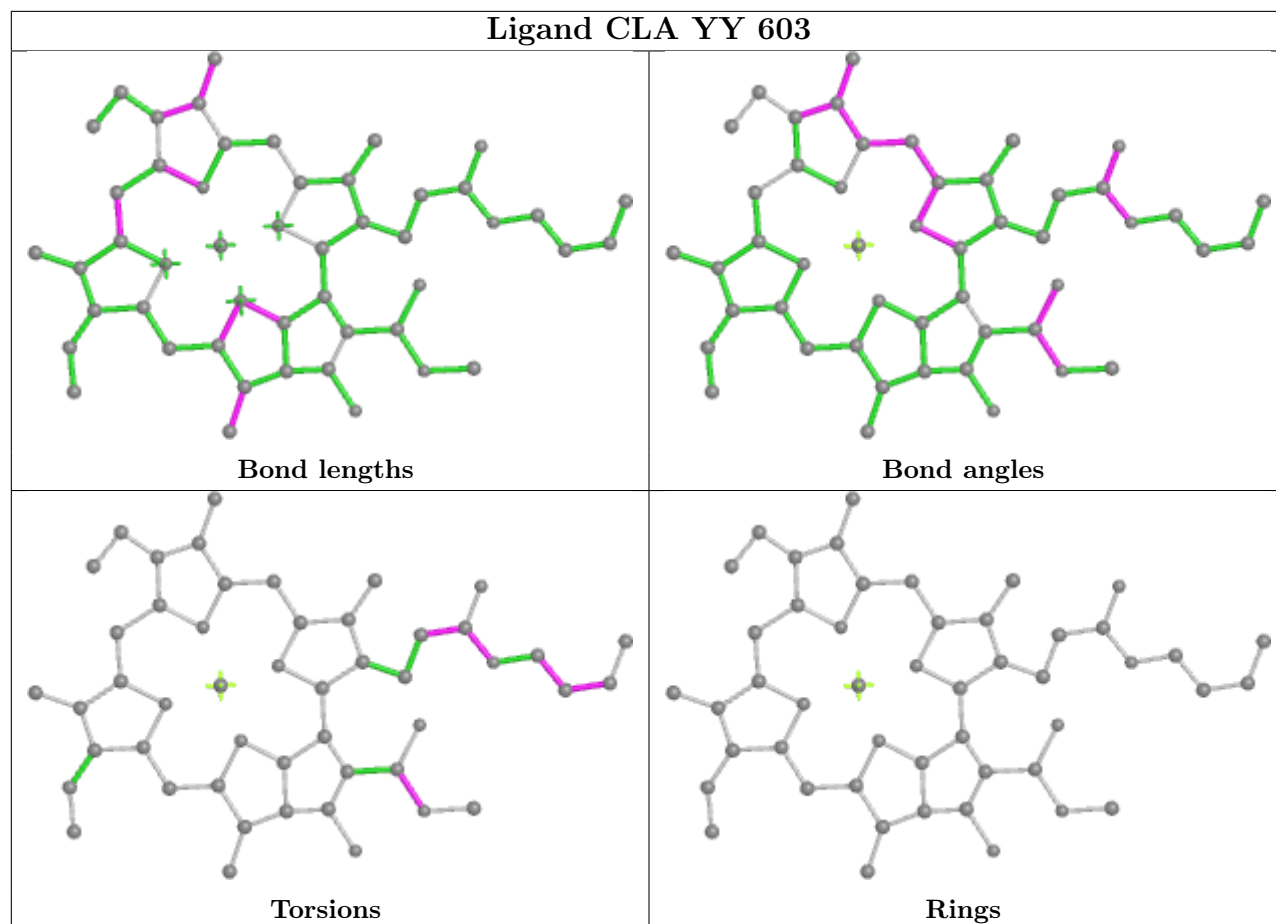
Torsions

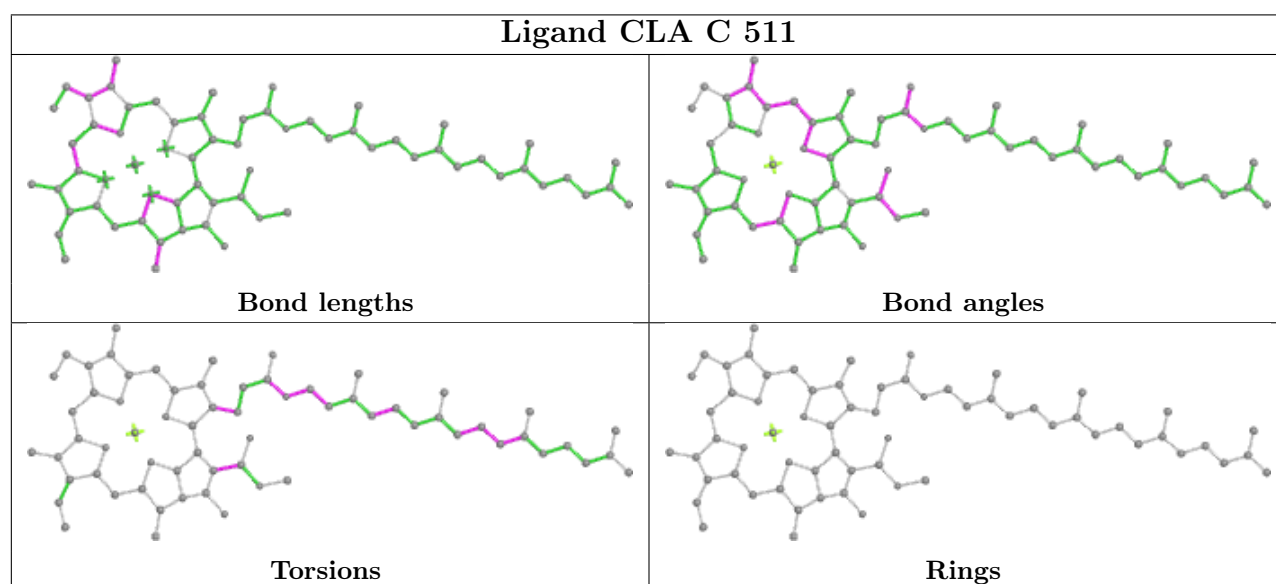
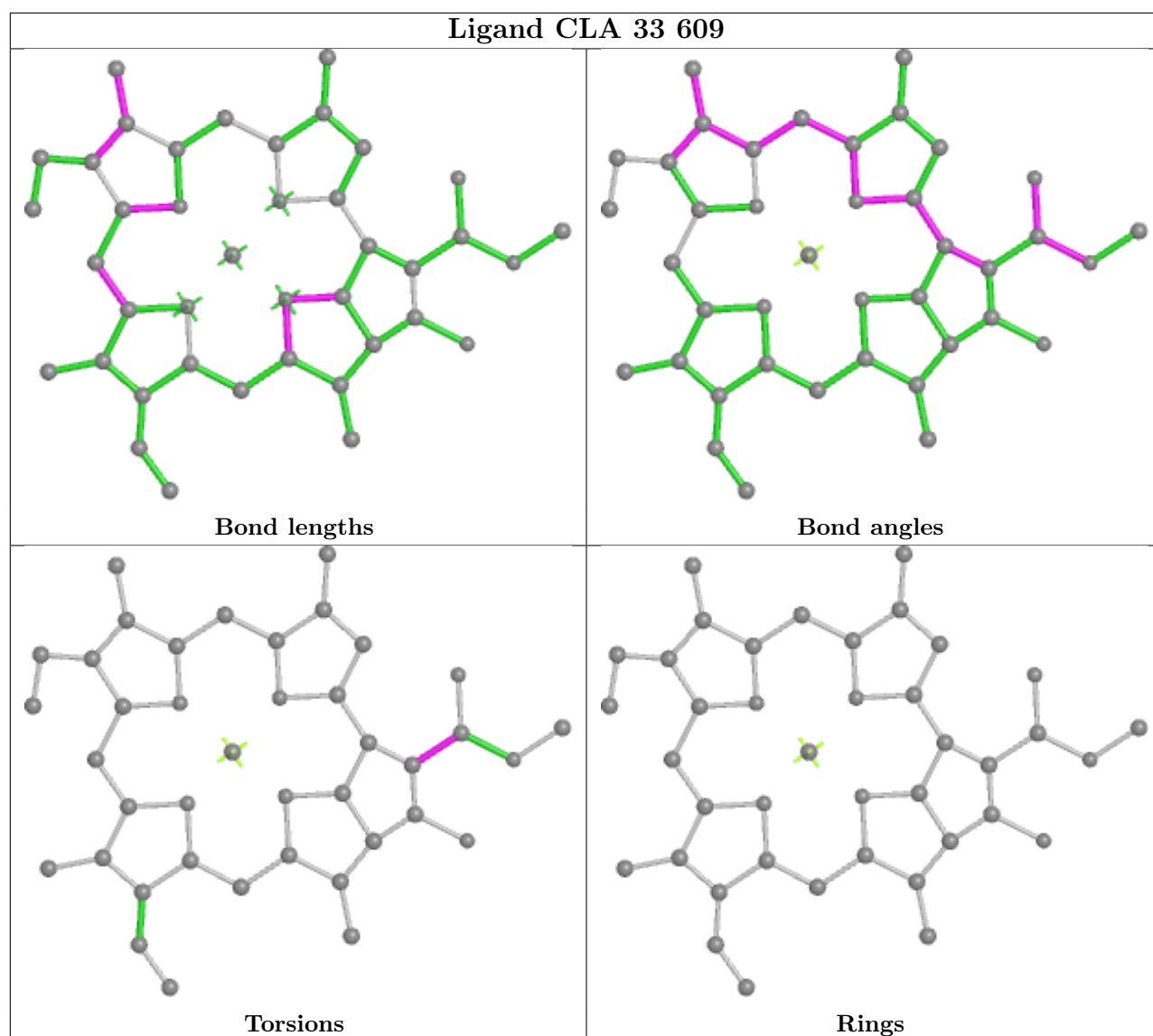


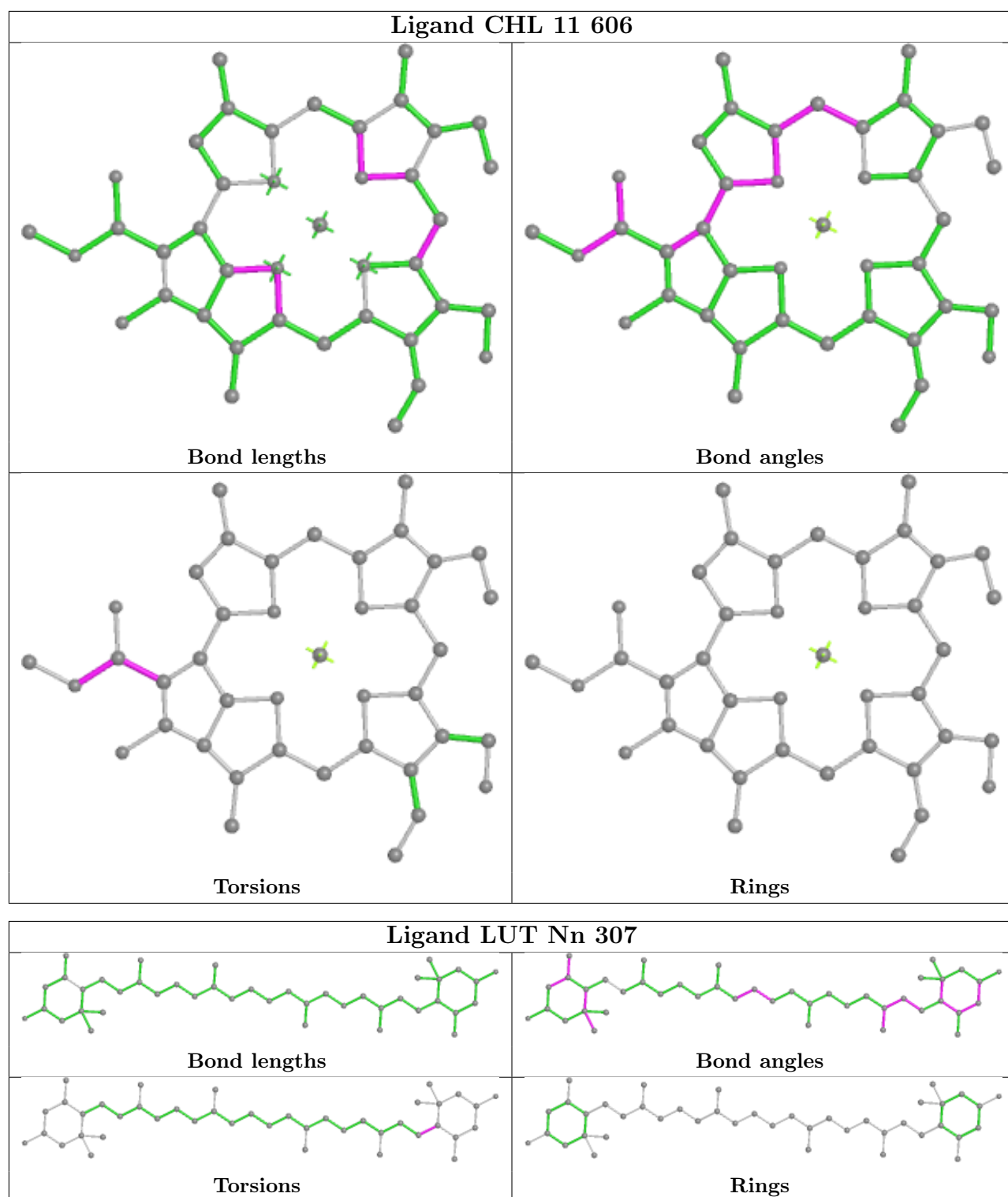
Rings

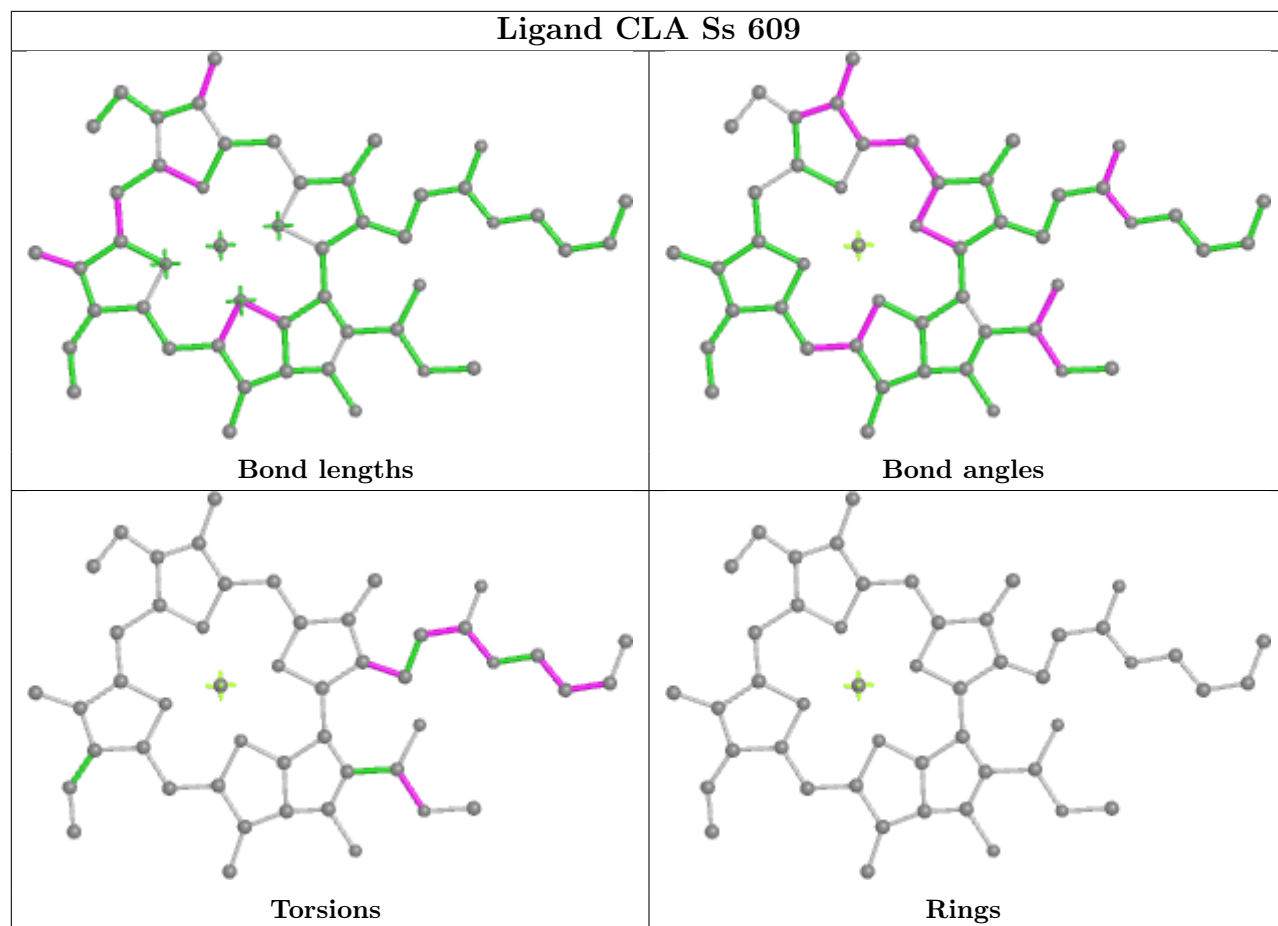


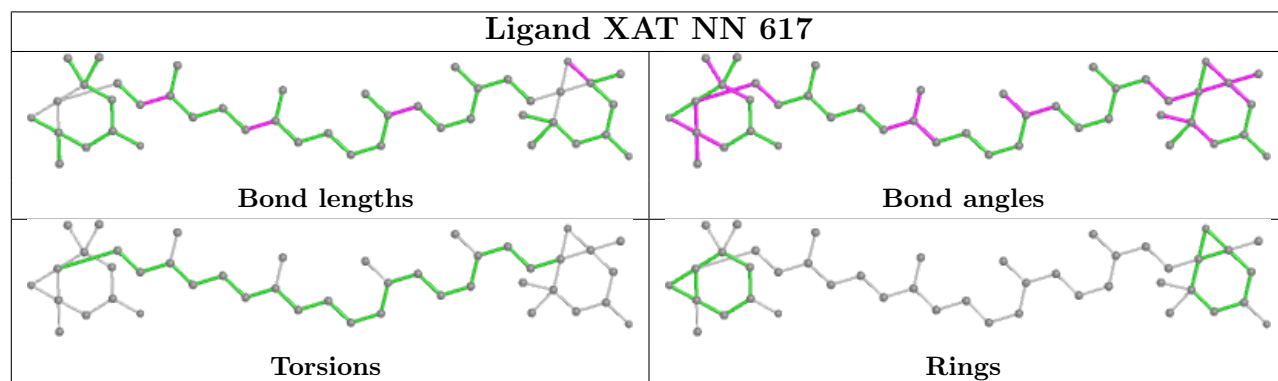
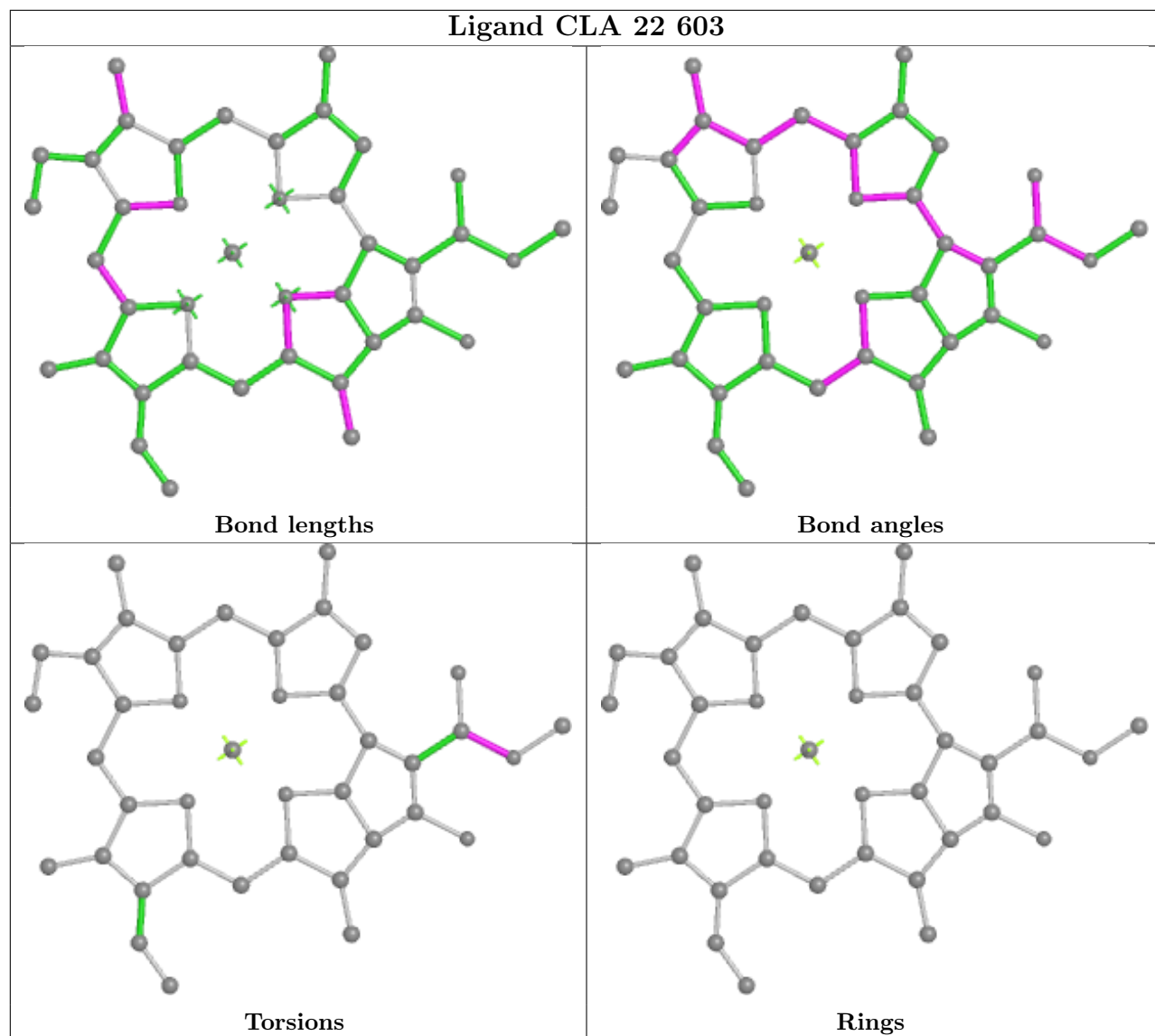
## Ligand CLA YY 603

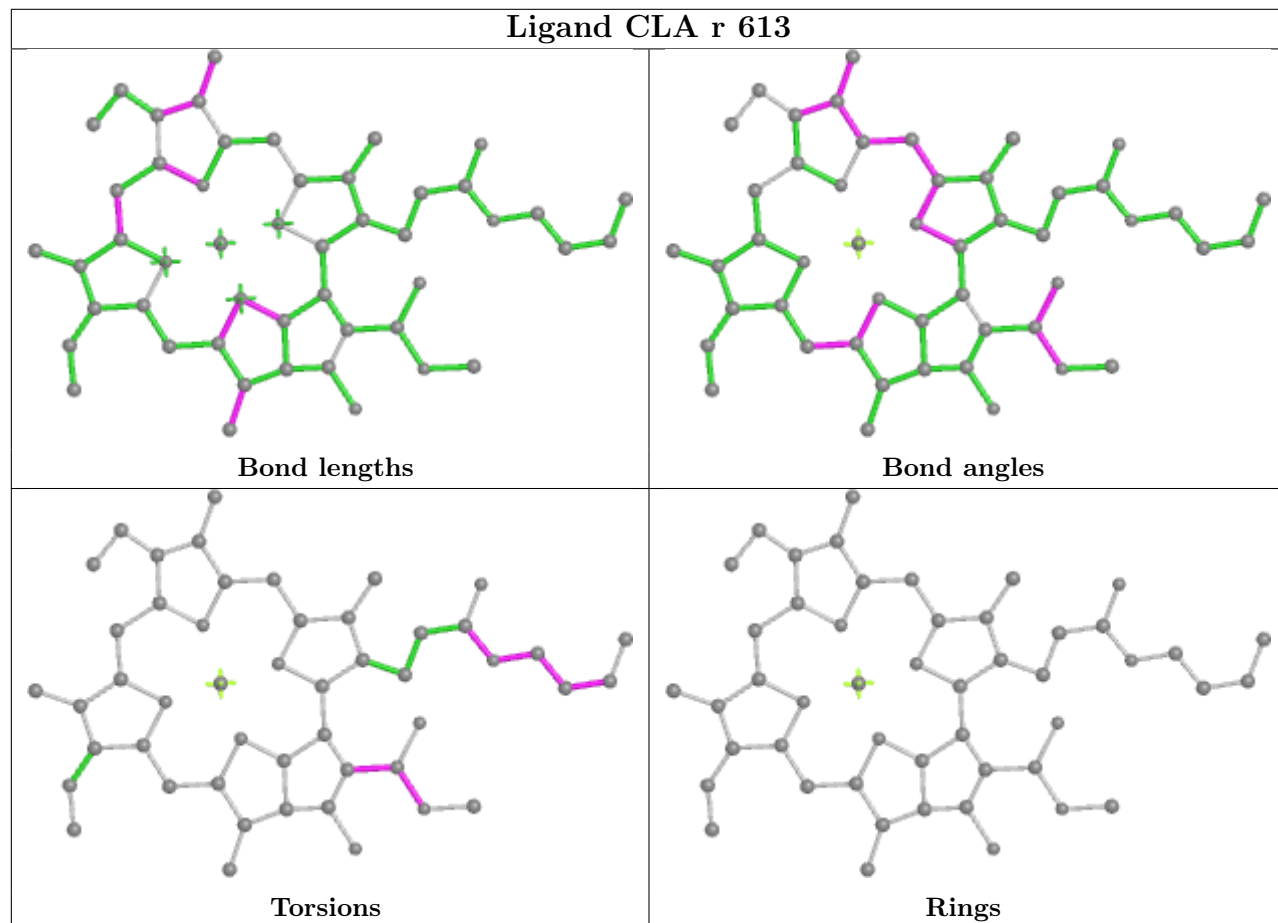
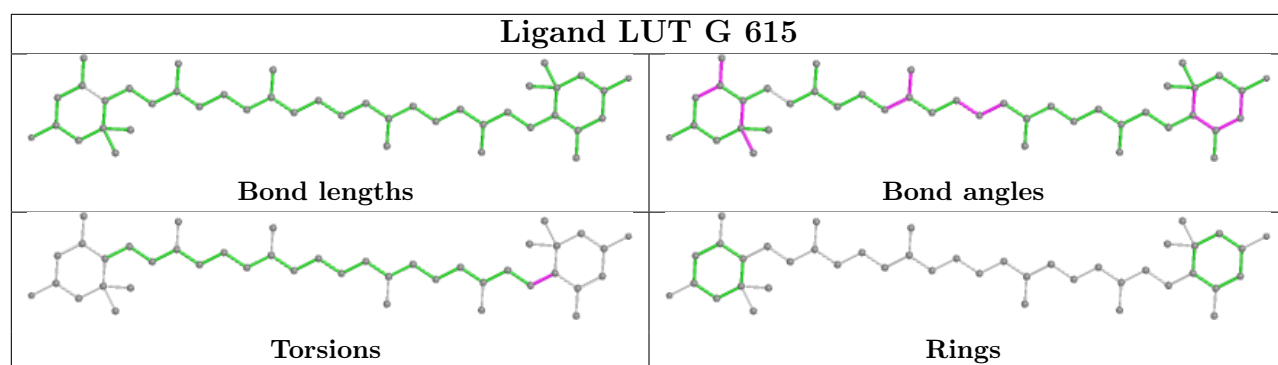


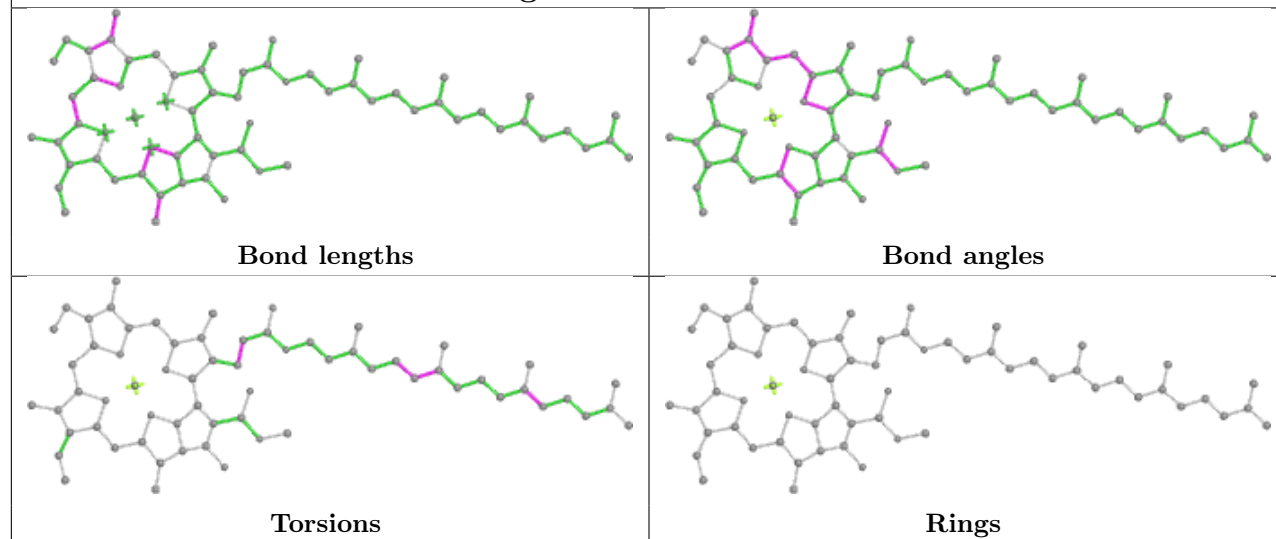
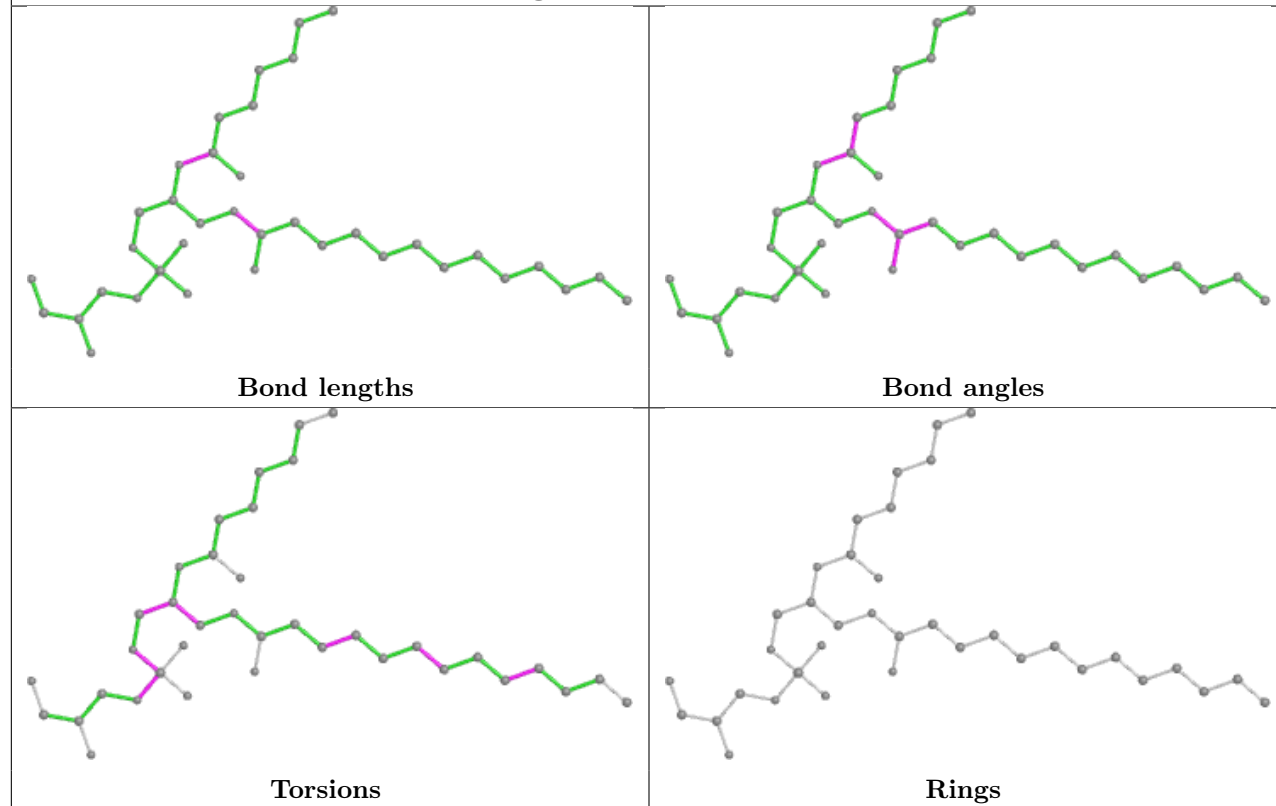


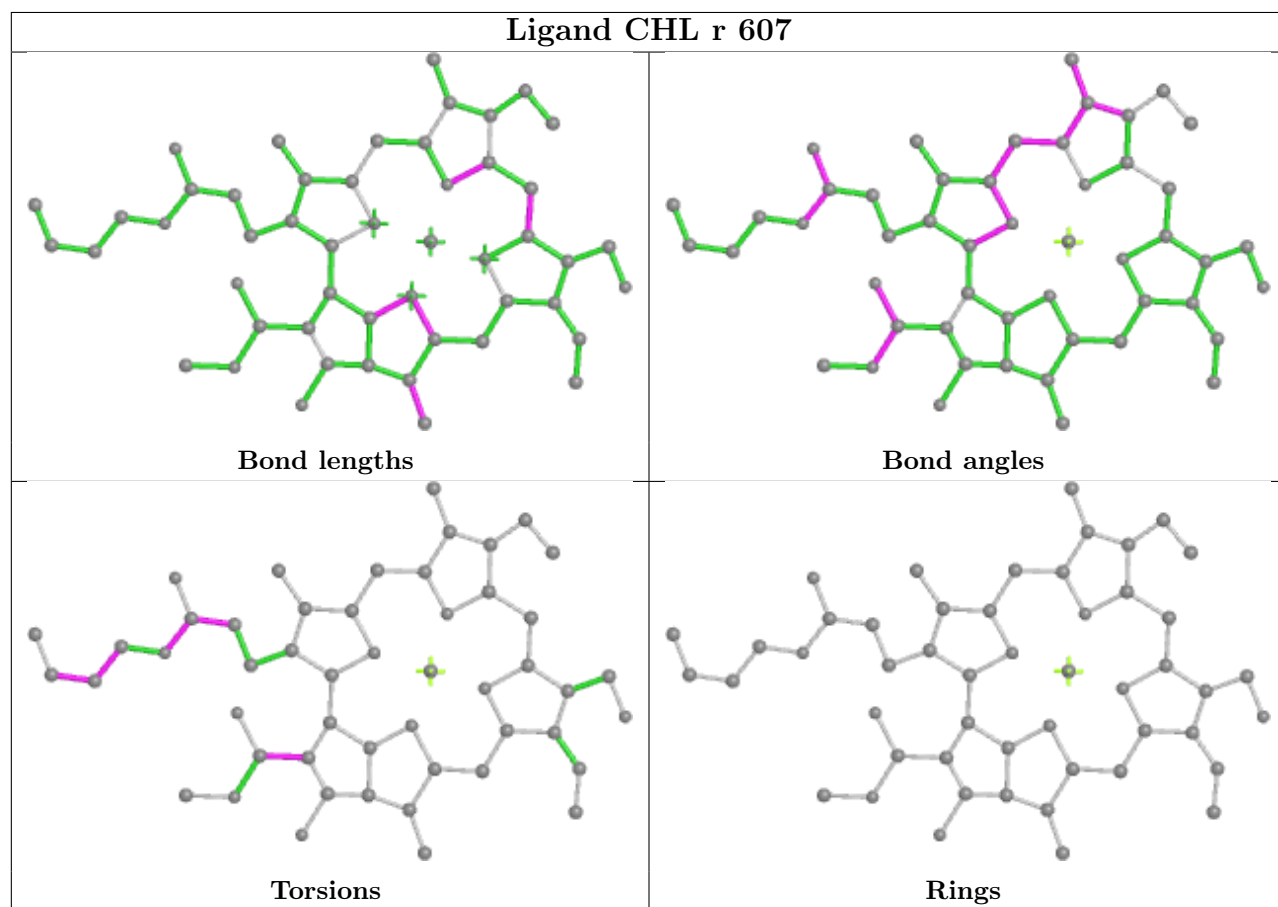
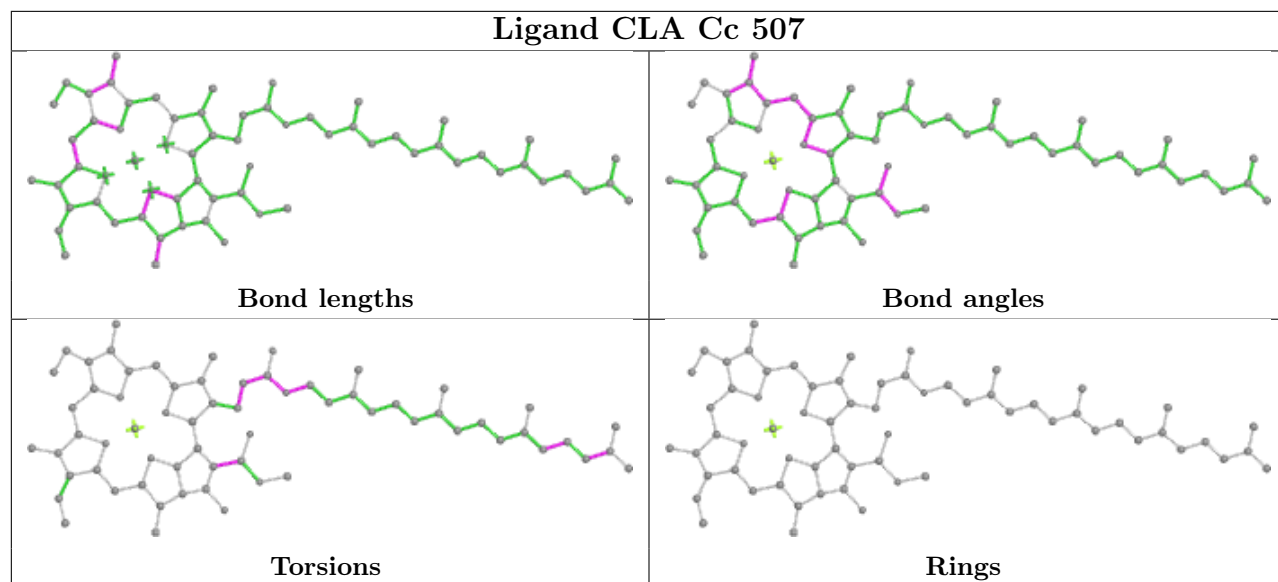






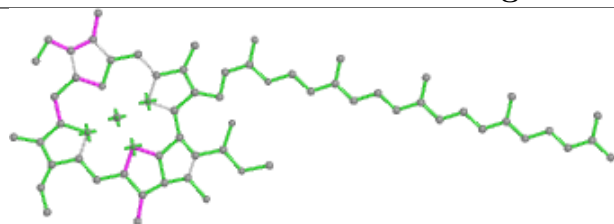


**Ligand CLA BB 611****Ligand LHG A 413**

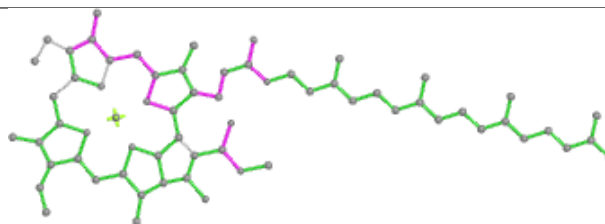




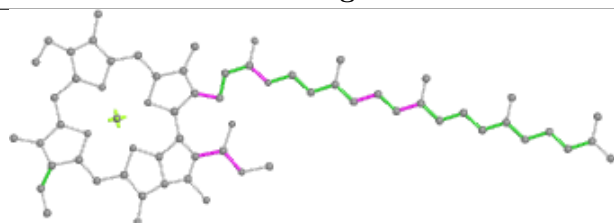
## Ligand CLA CC 507



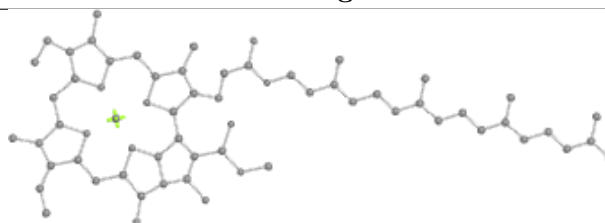
Bond lengths



Bond angles

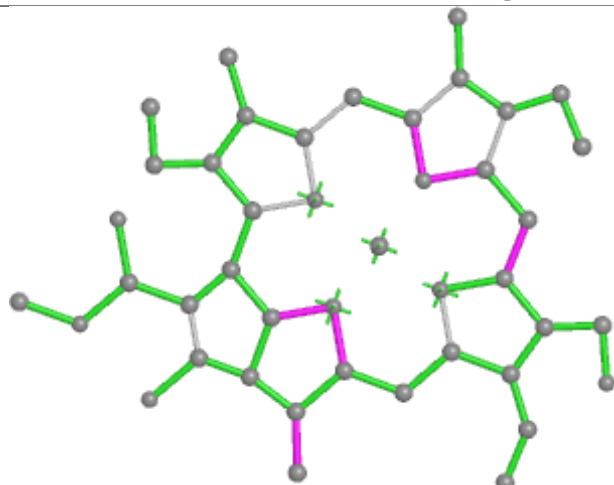


Torsions

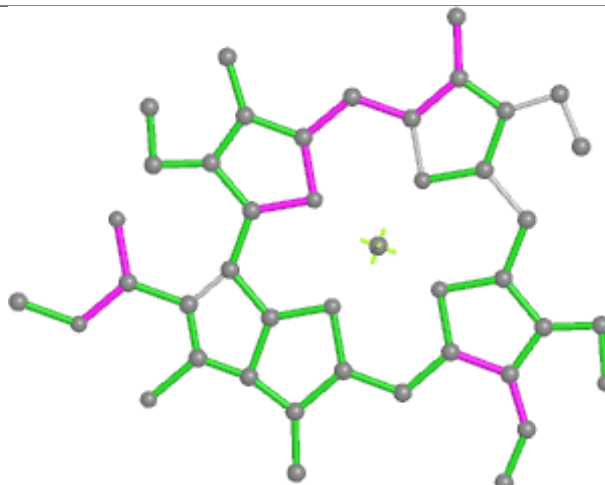


Rings

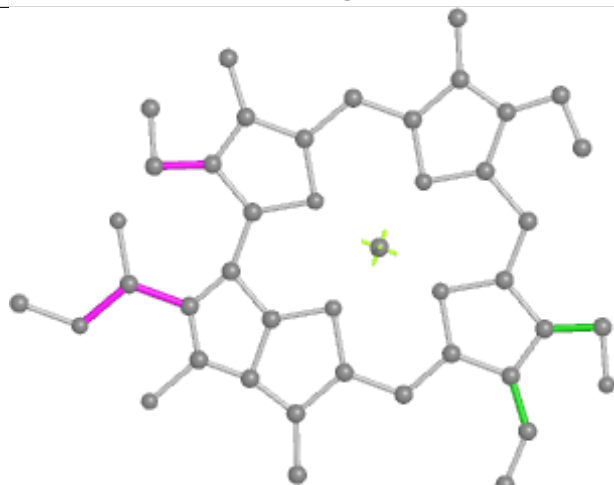
## Ligand CHL GG 606



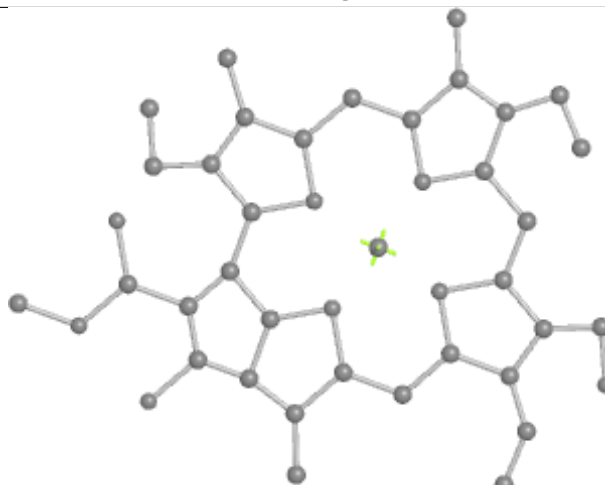
Bond lengths



Bond angles

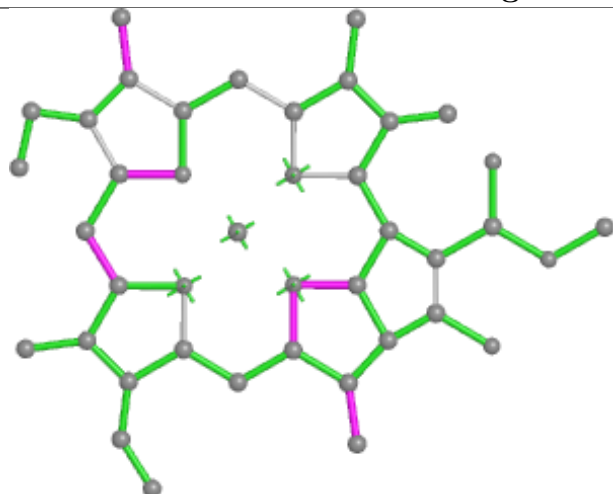


Torsions

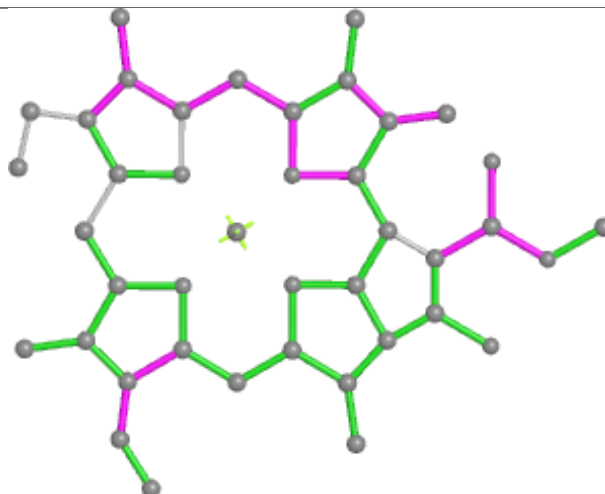


Rings

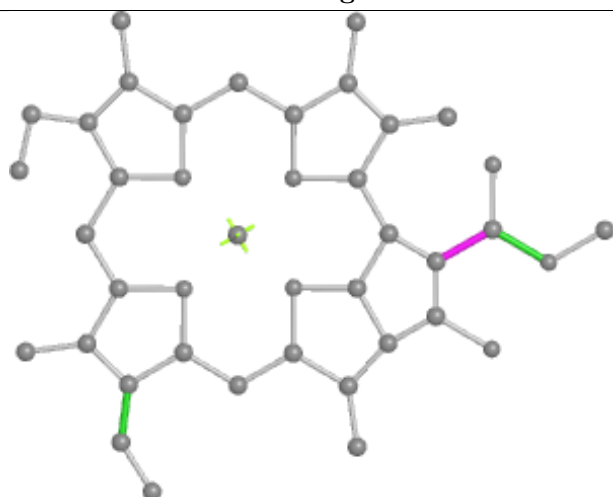
## Ligand CLA BB 615



Bond lengths



Bond angles

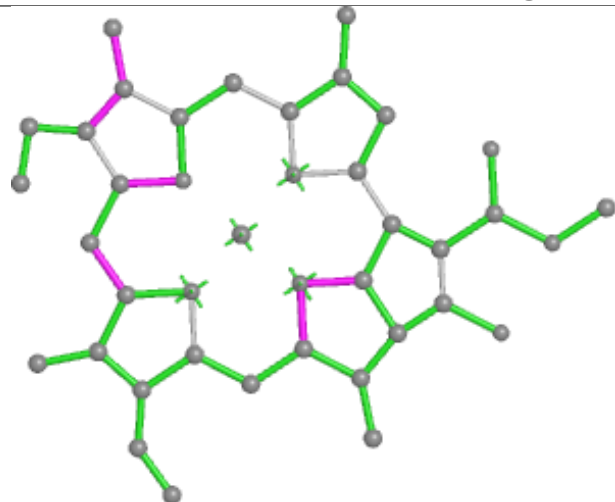


Torsions

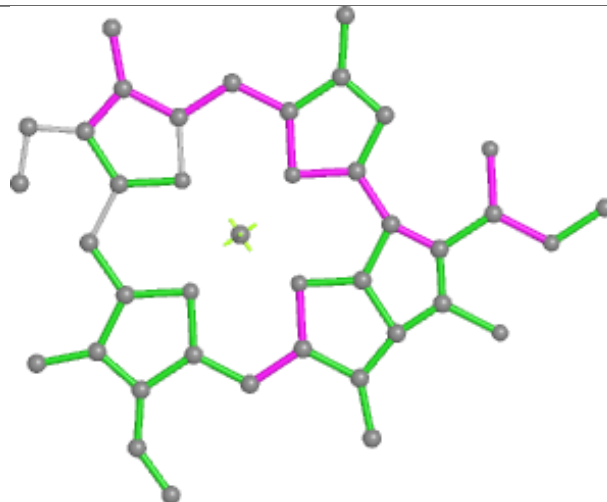


Rings

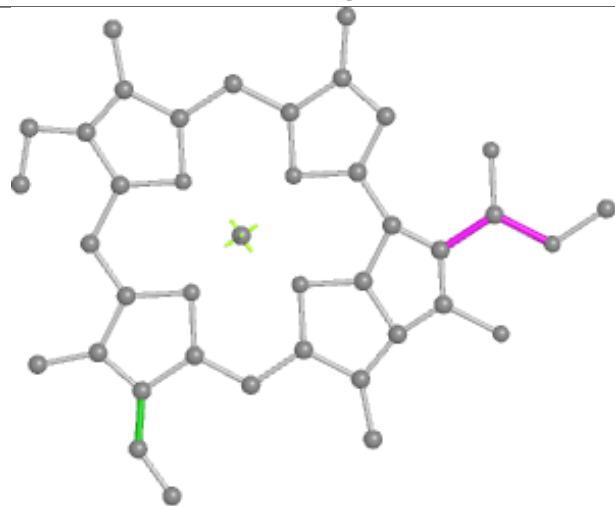
## Ligand CLA 2 602



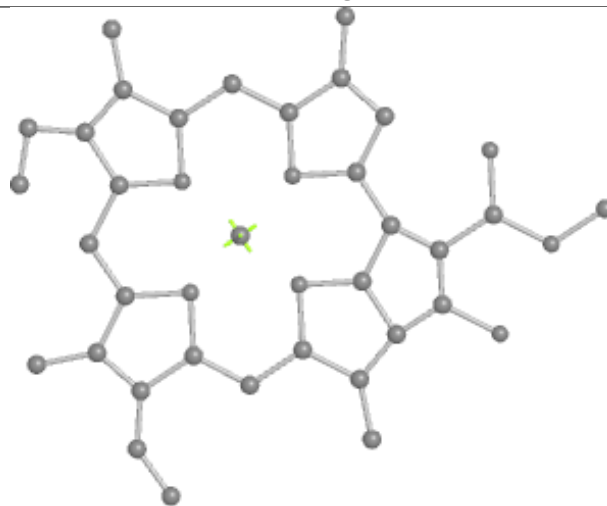
Bond lengths



Bond angles

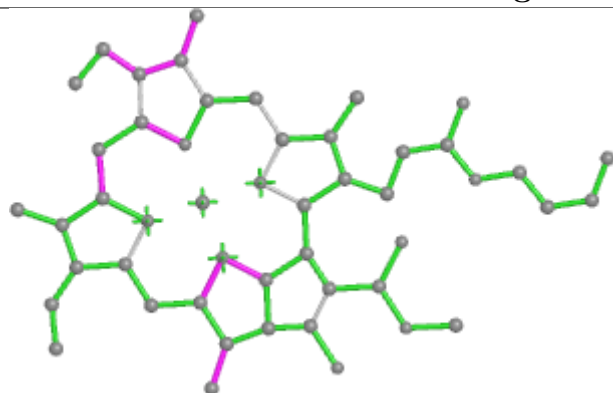


Torsions

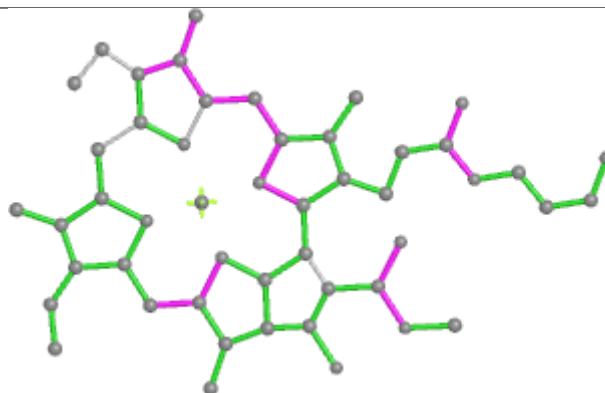


Rings

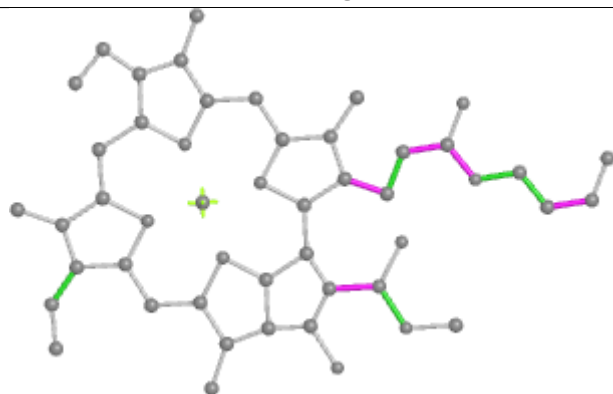
## Ligand CLA A 406



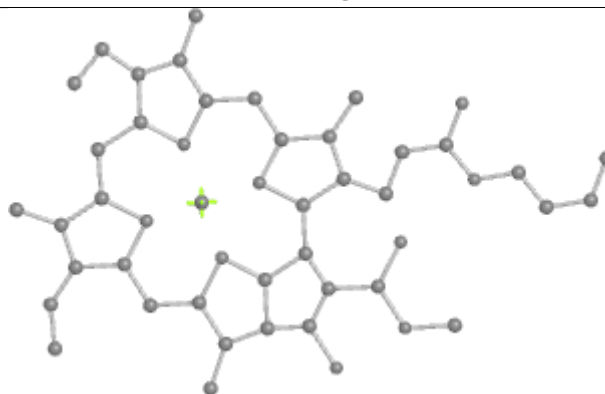
Bond lengths



Bond angles

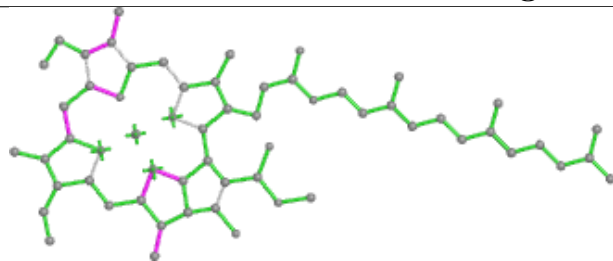


Torsions

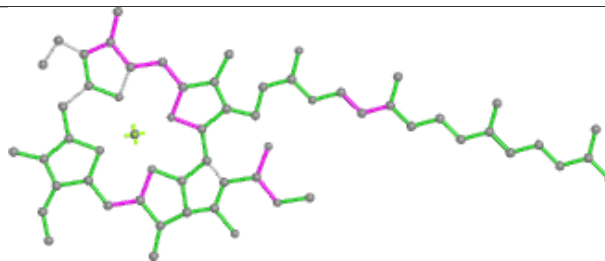


Rings

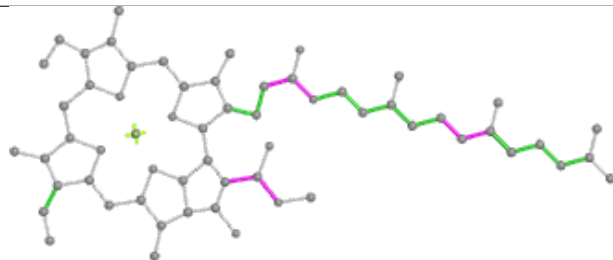
## Ligand CLA c 508



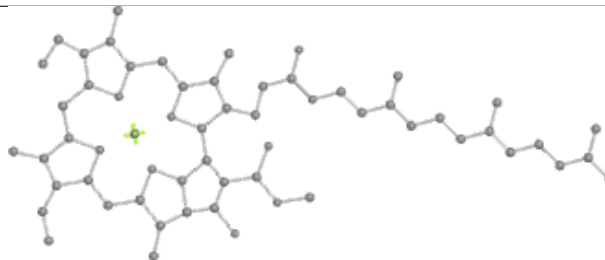
Bond lengths



Bond angles

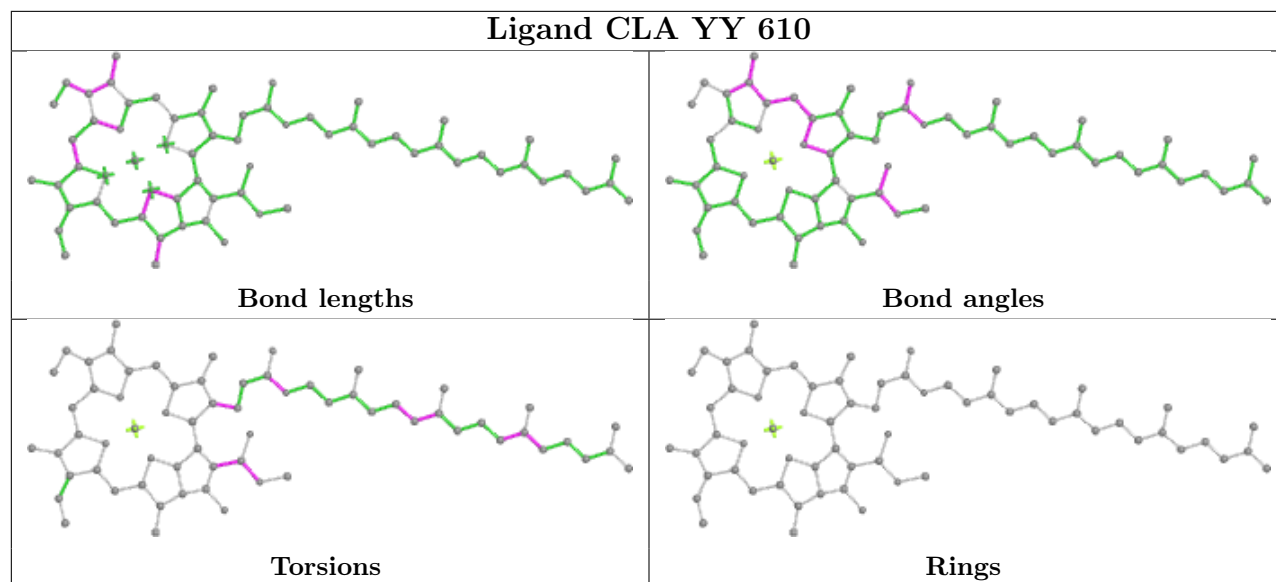


Torsions

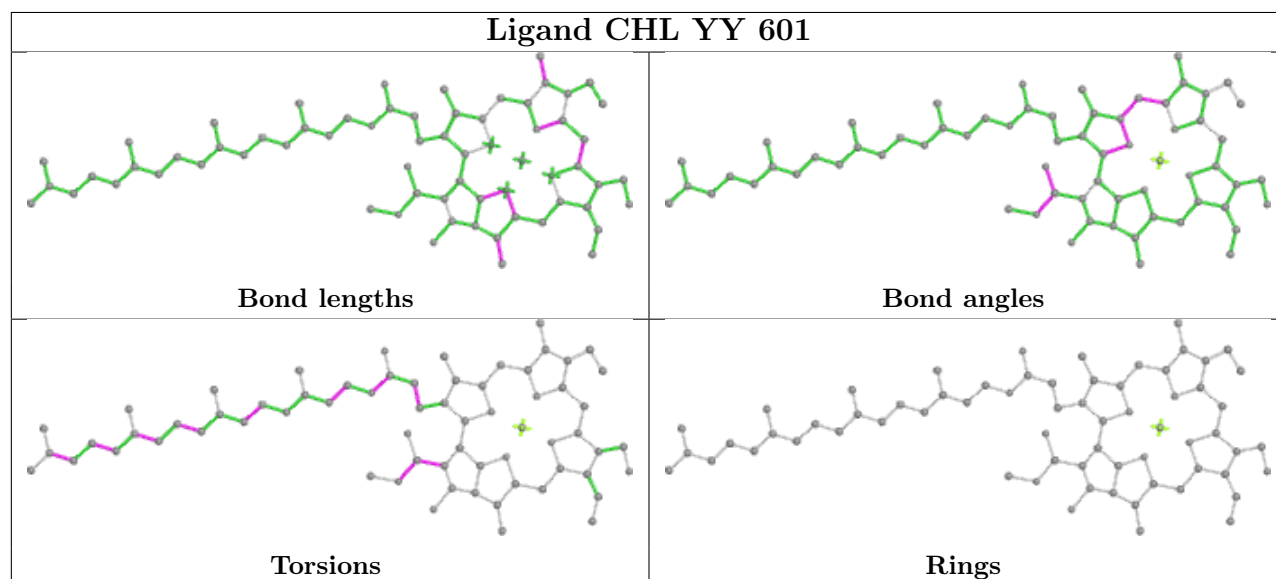


Rings

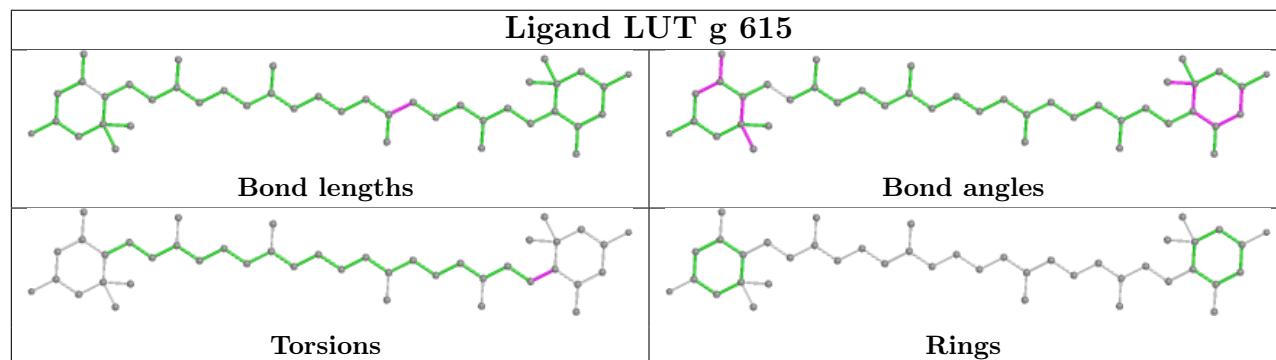
## Ligand CLA YY 610

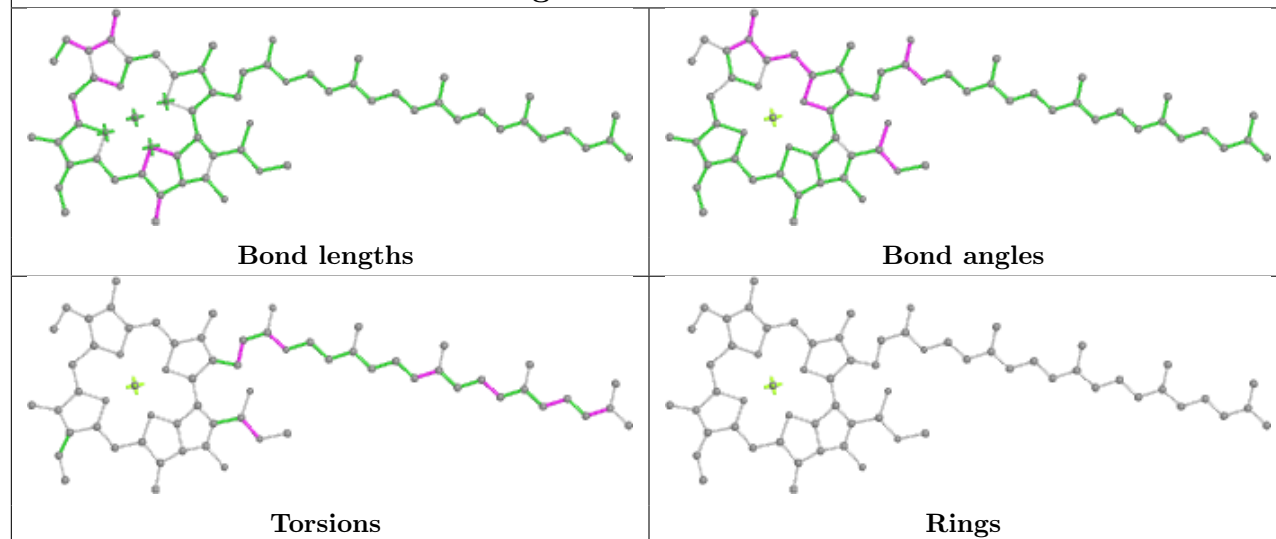
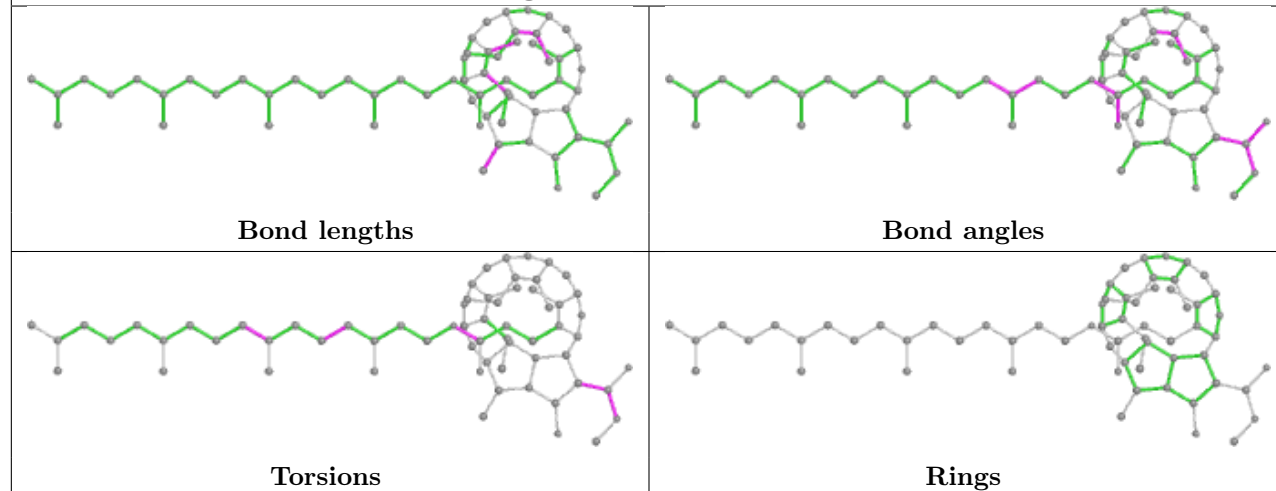


## Ligand CHL YY 601

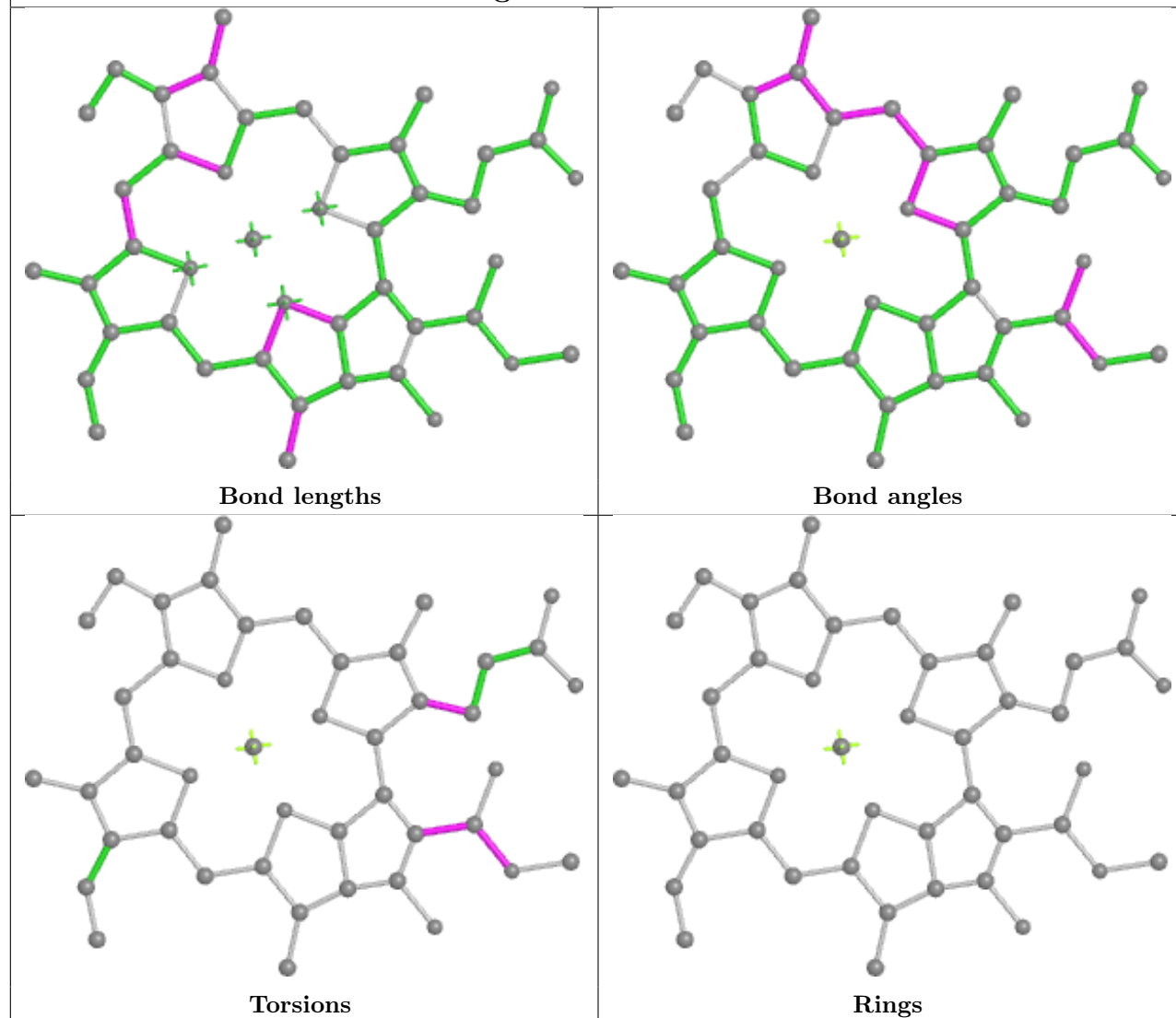


## Ligand LUT g 615

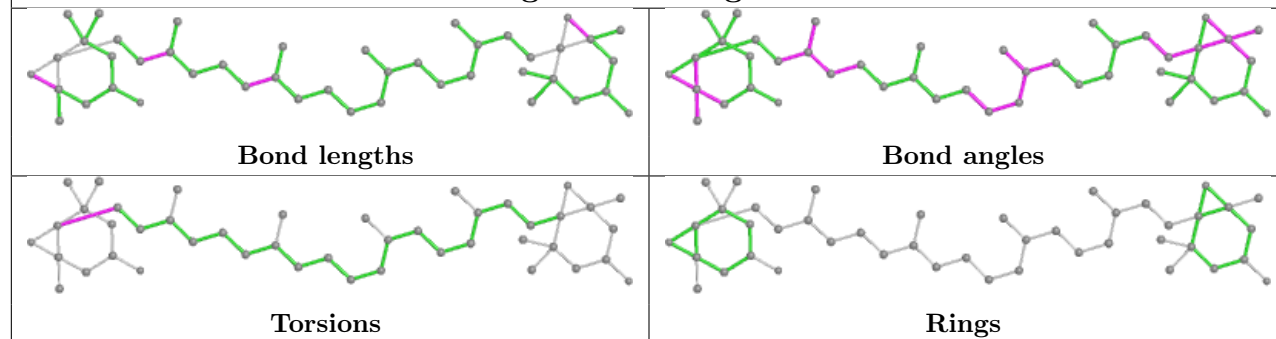


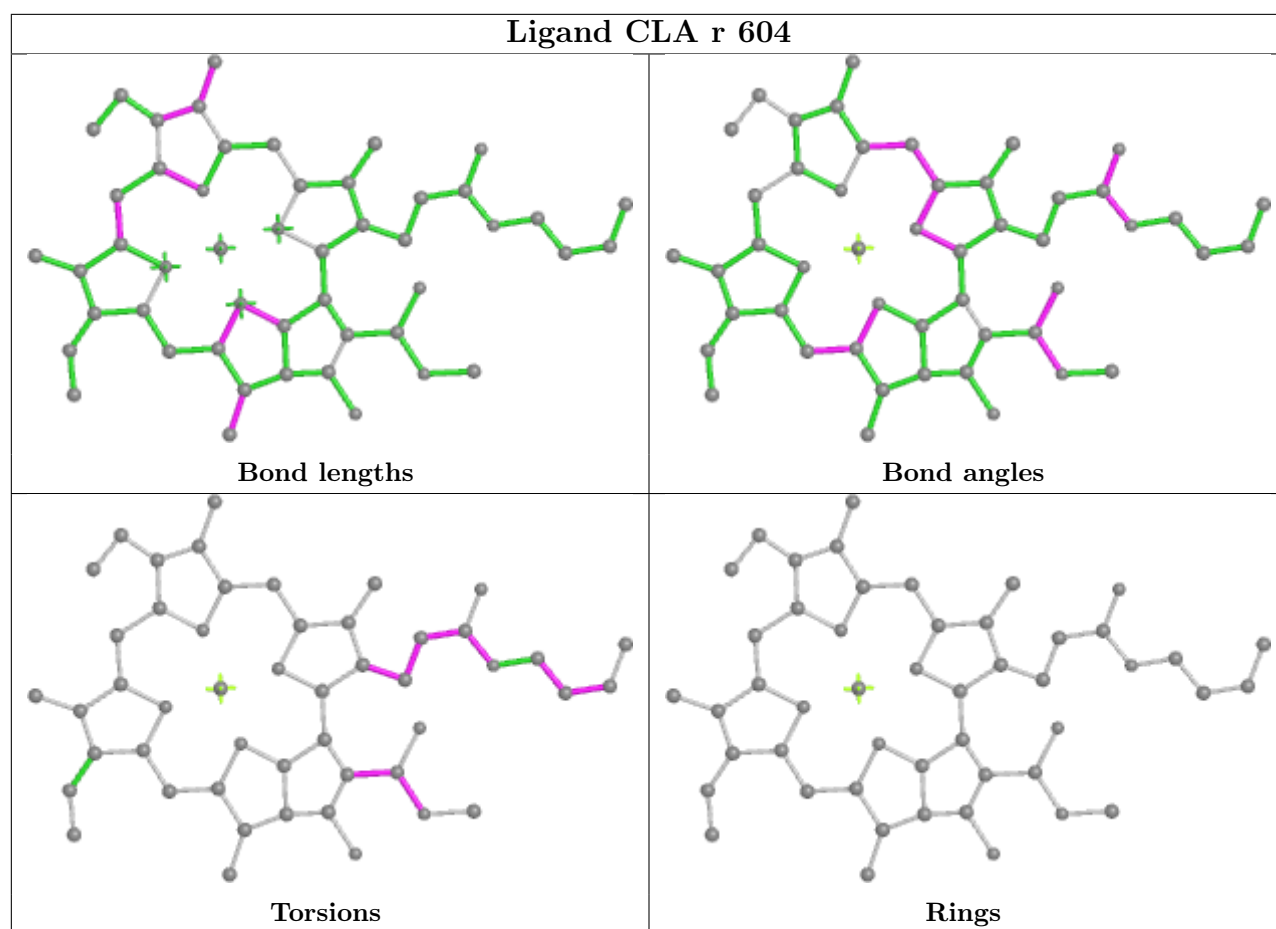
**Ligand CLA C 512****Ligand PHO Aa 408**

## Ligand CLA 4 310



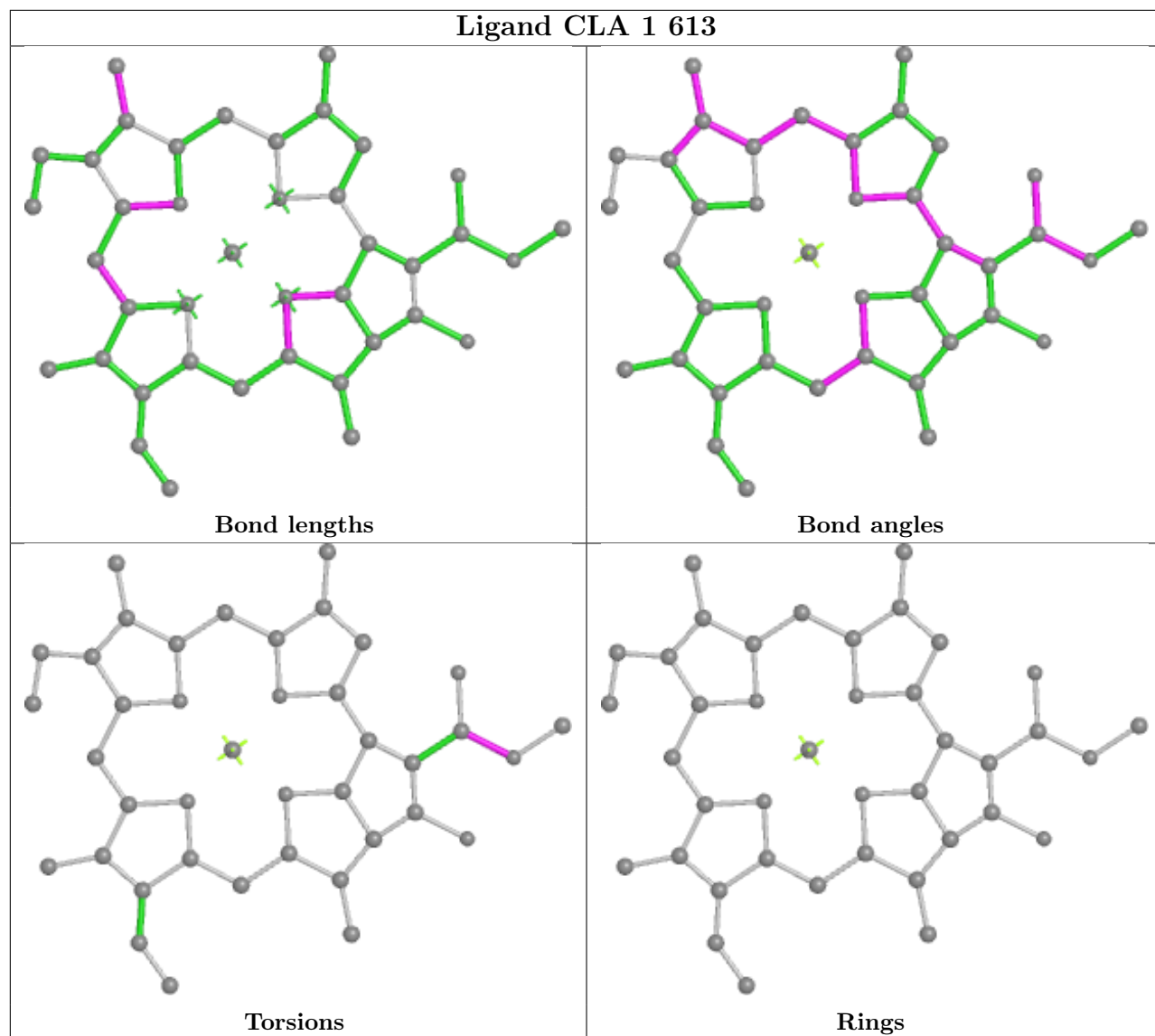
## Ligand XAT Gg 301



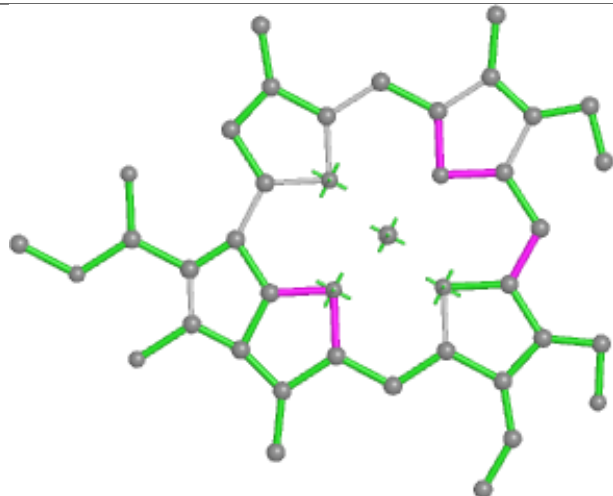




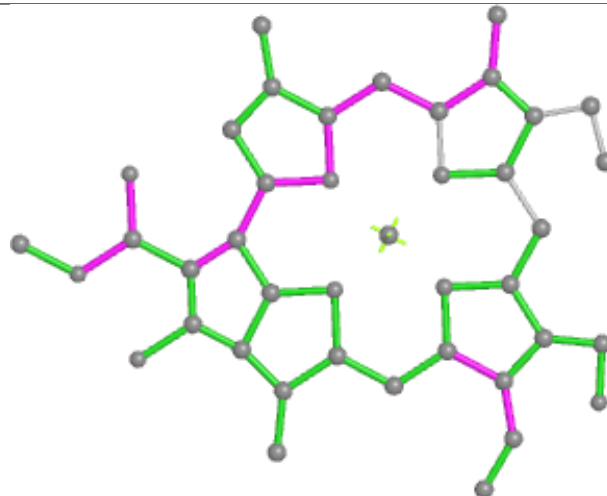
## Ligand CLA 1 613



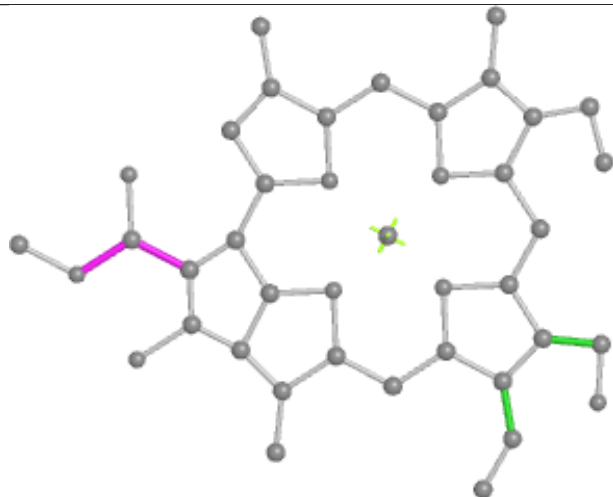
## Ligand CHL 3 605



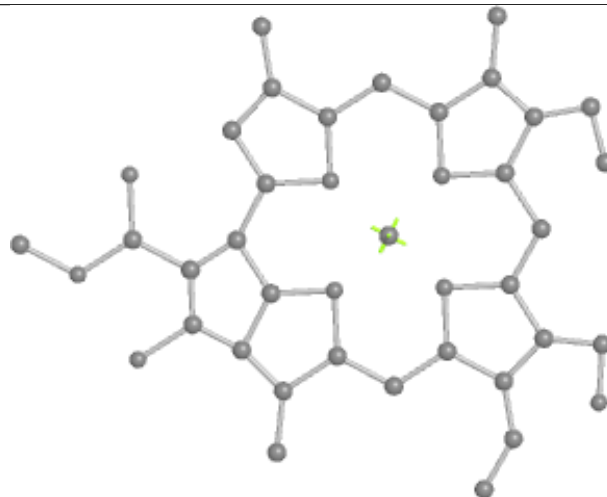
Bond lengths



Bond angles

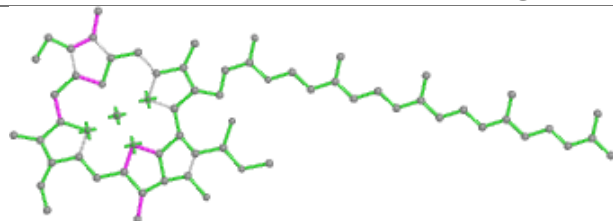


Torsions

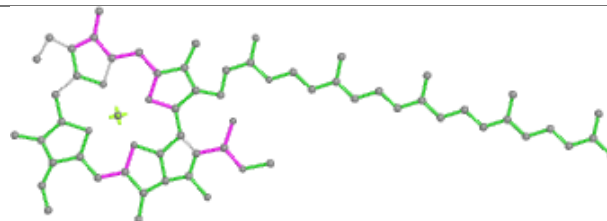


Rings

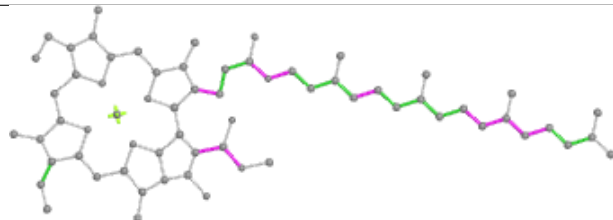
## Ligand CLA C 510



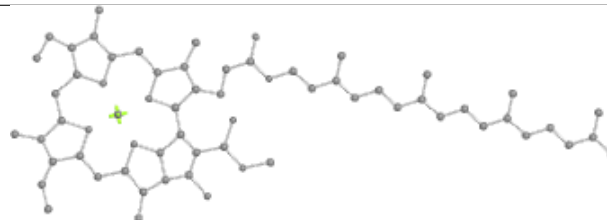
Bond lengths



Bond angles

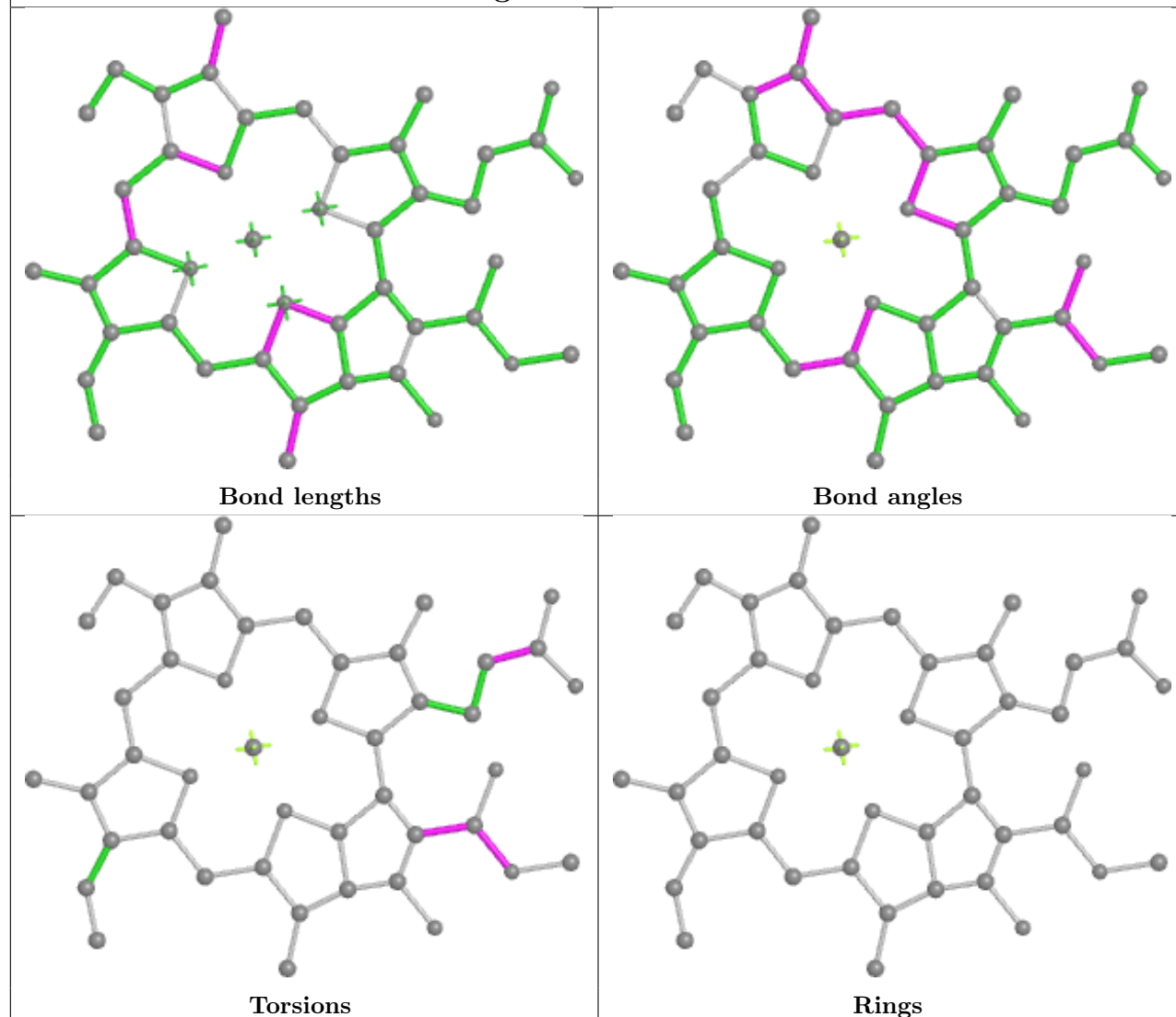


Torsions

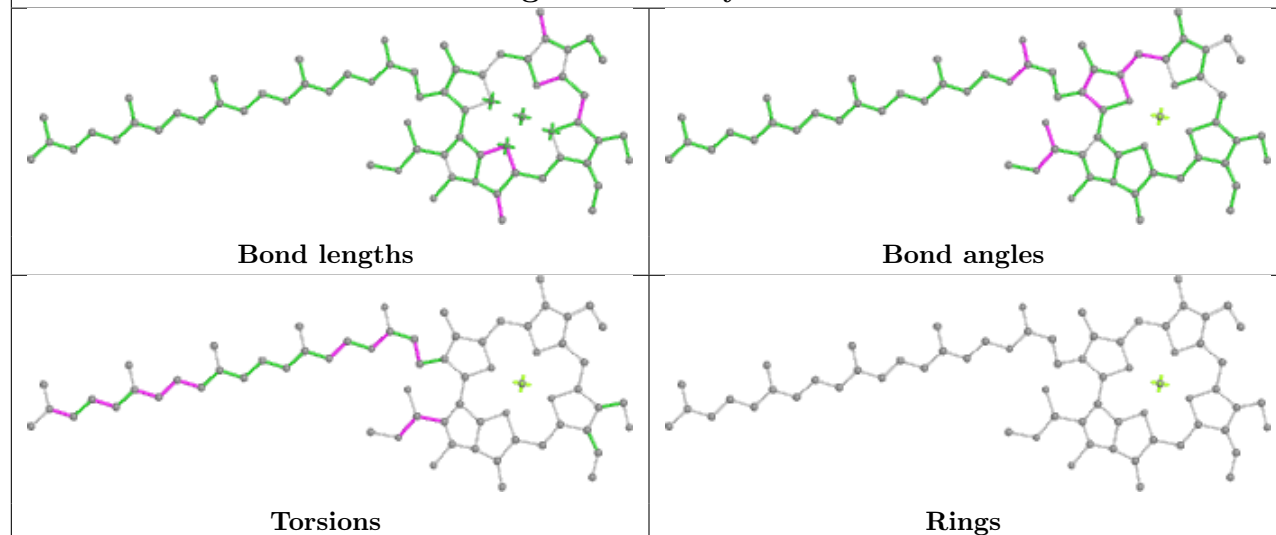


Rings

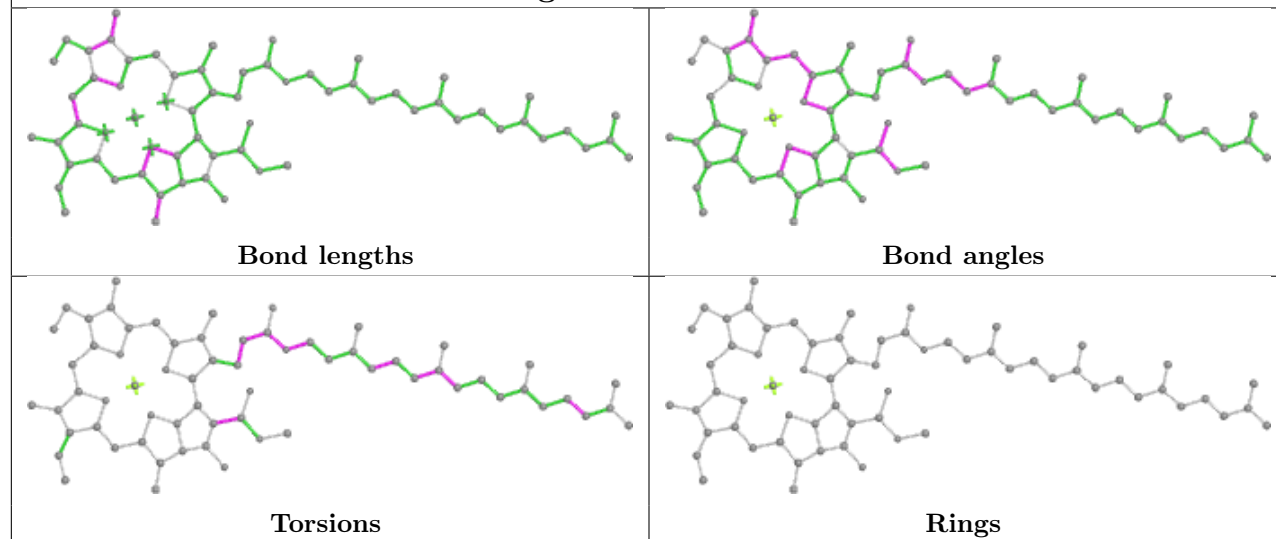
## Ligand CLA 4 311



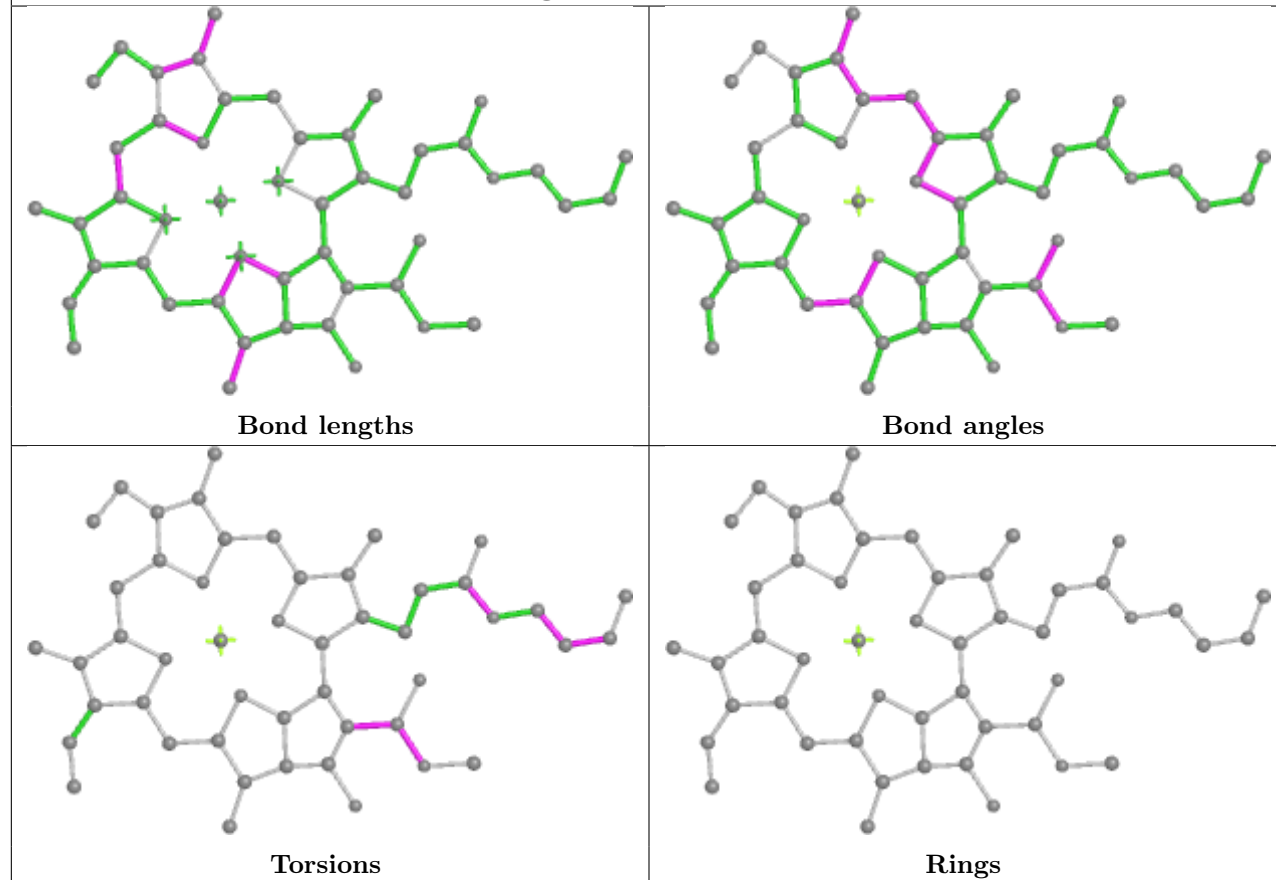
## Ligand CHL Yy 601

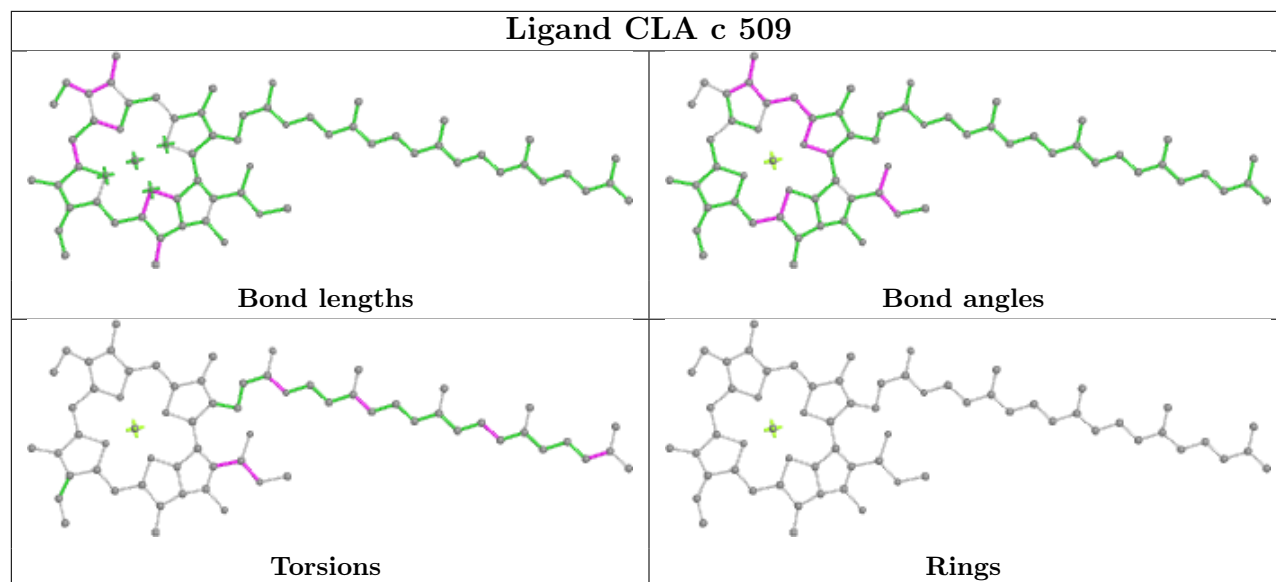
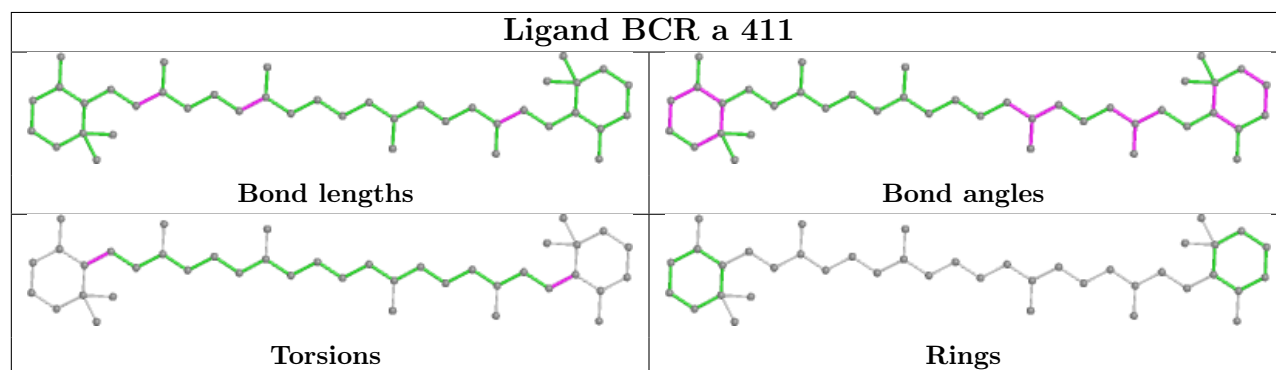


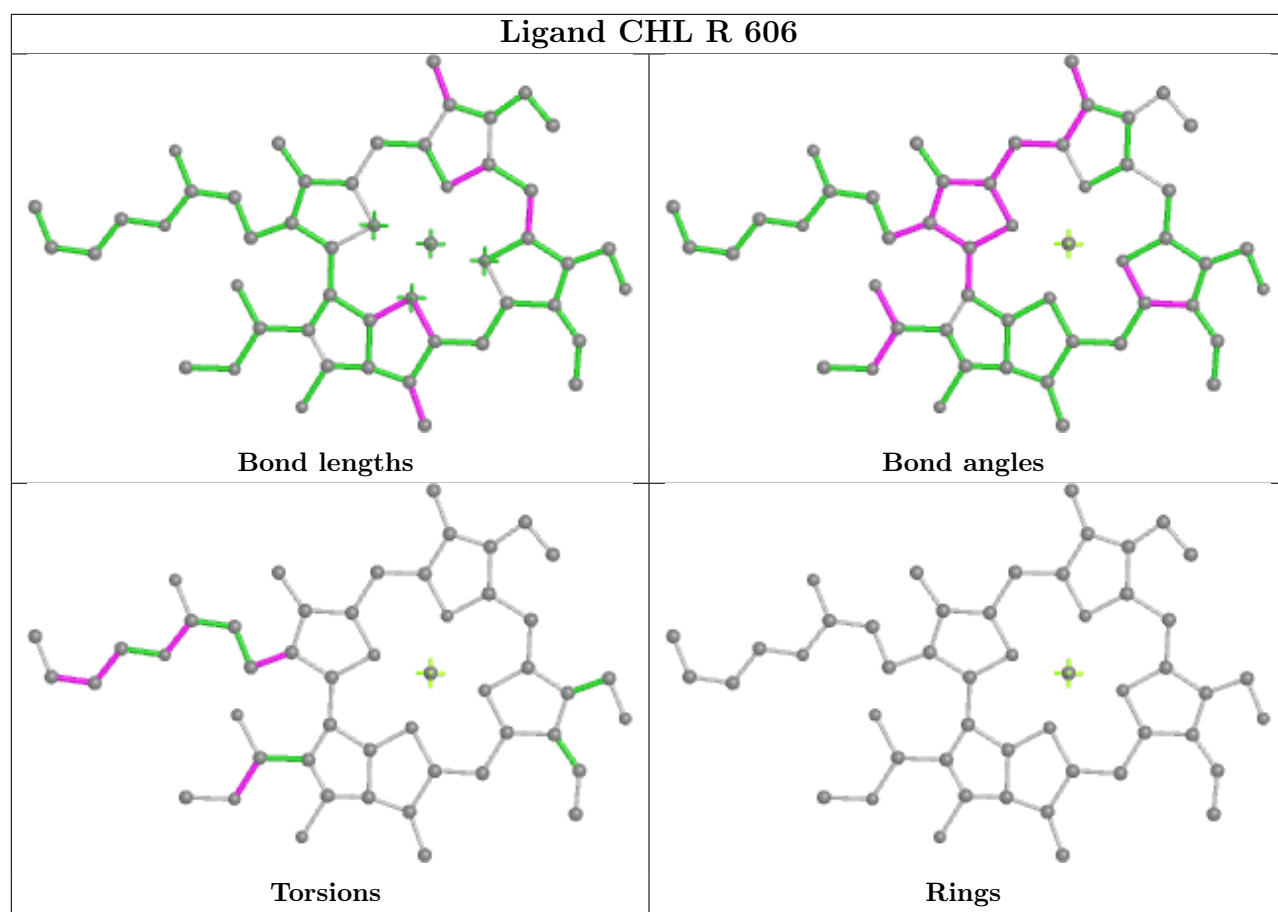
## Ligand CLA r 602

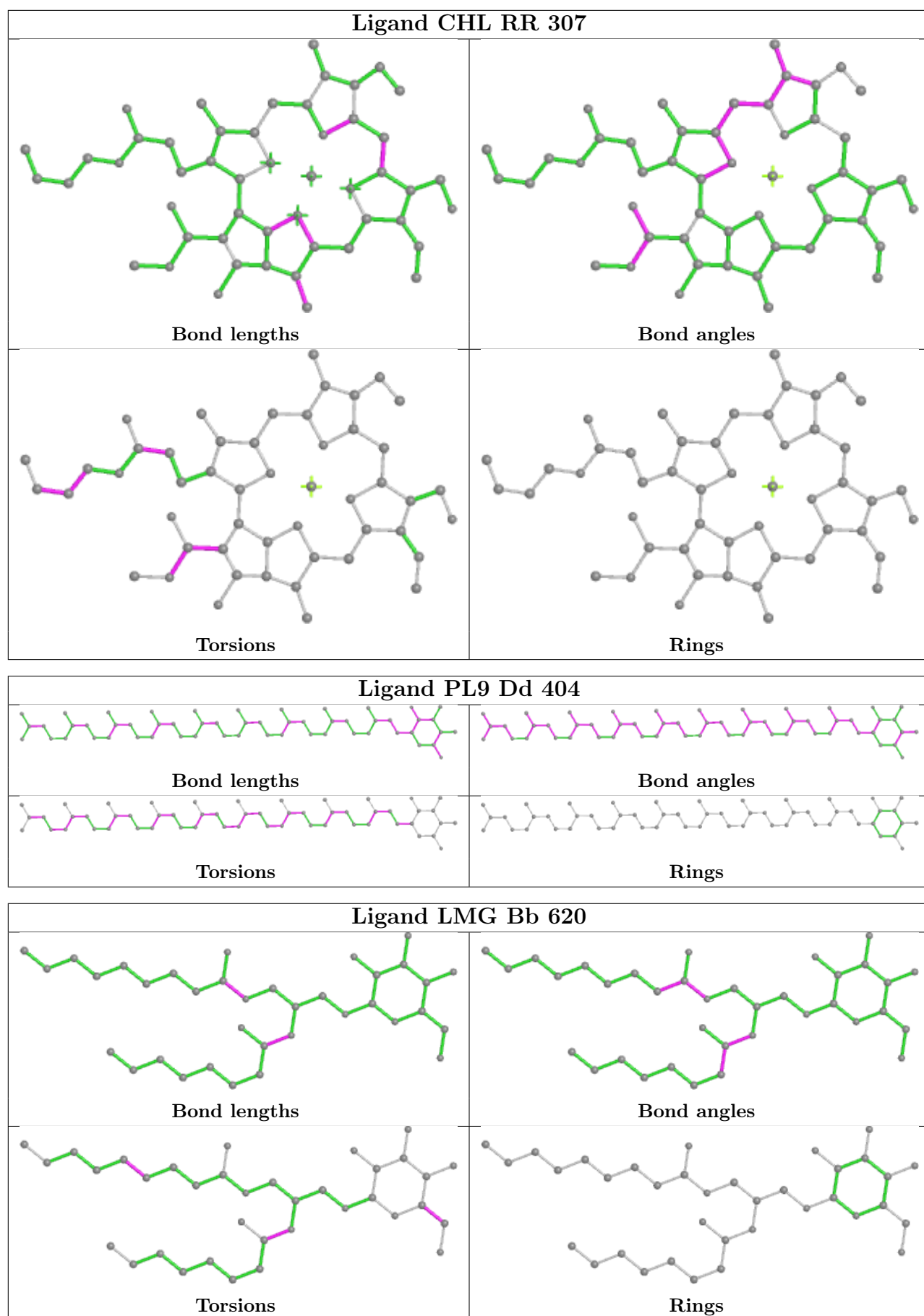


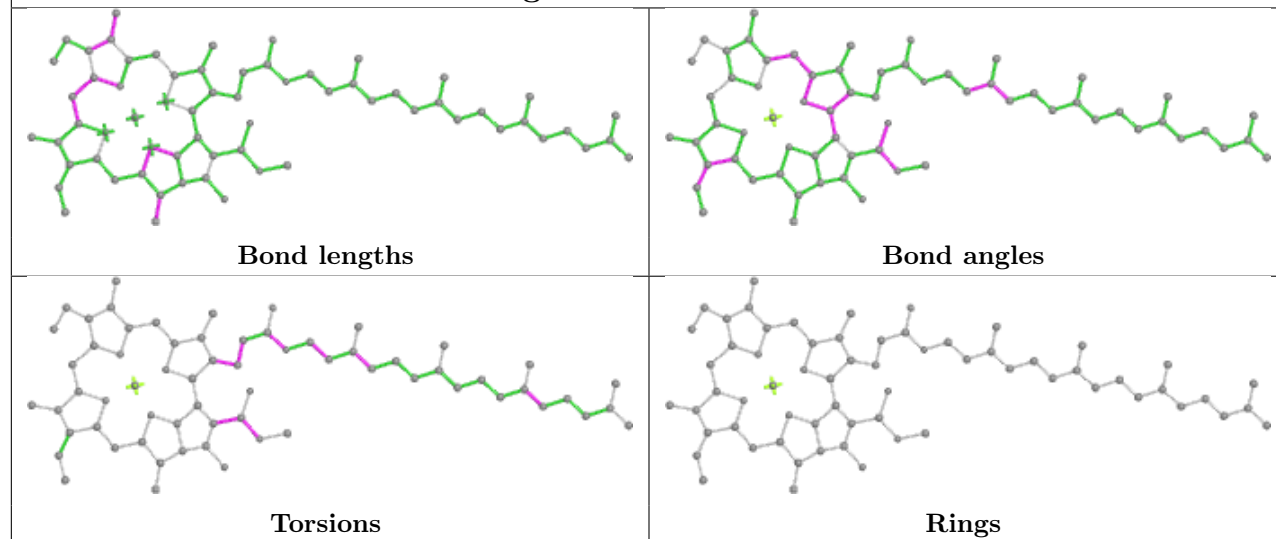
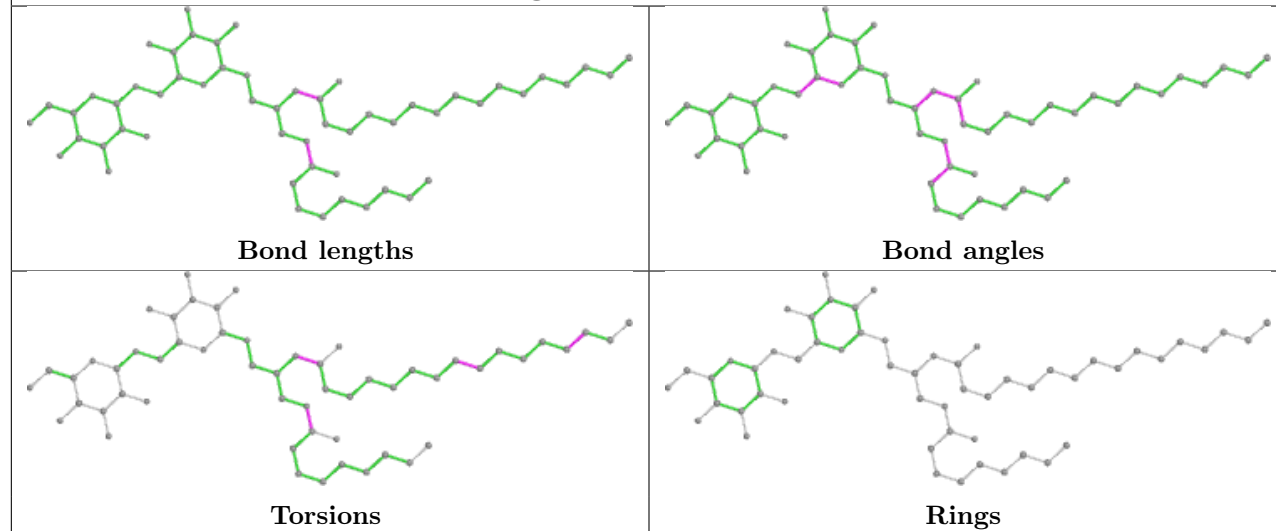
## Ligand CLA s 604



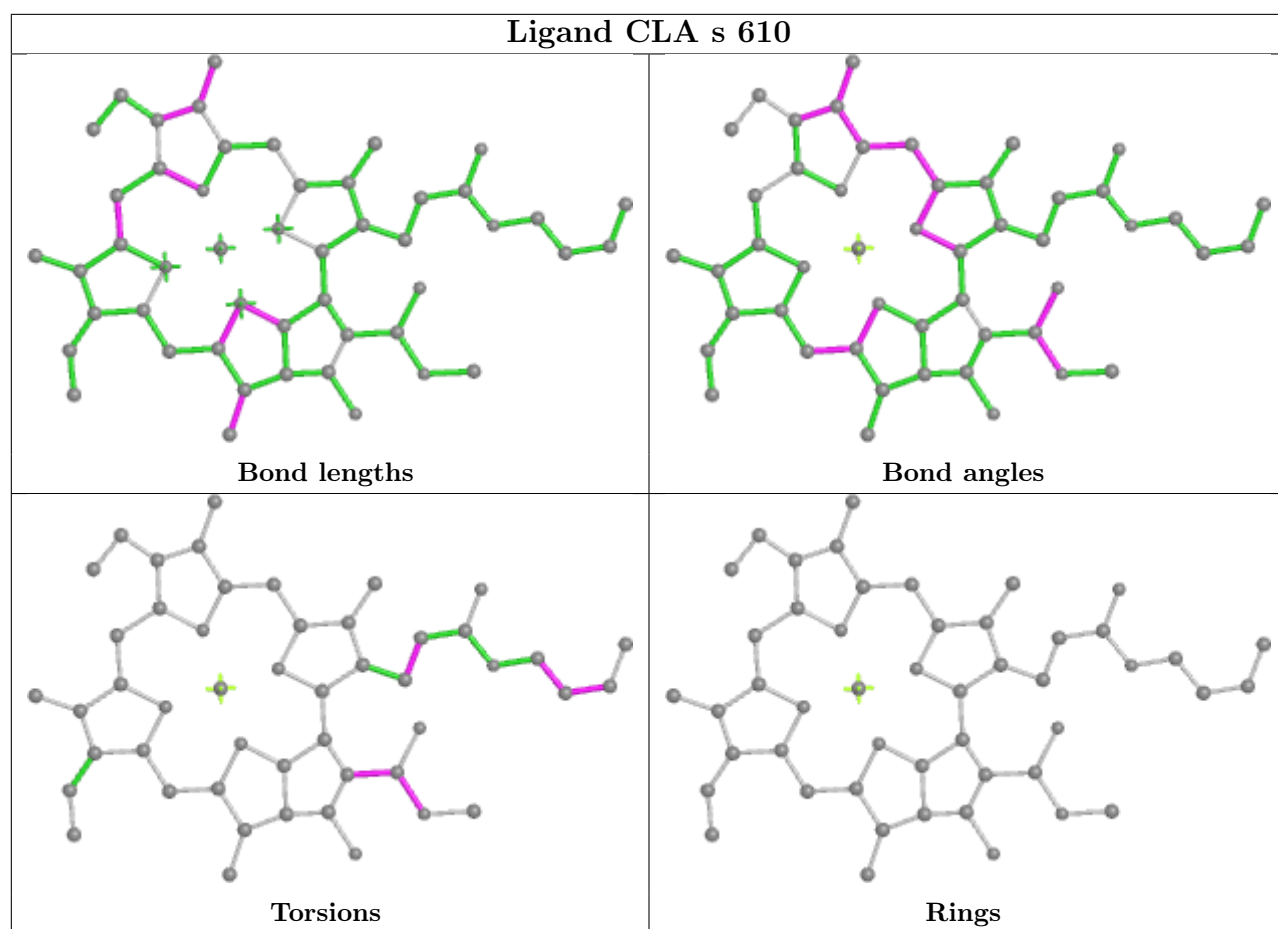
**Ligand CLA c 509****Ligand BCR a 411**



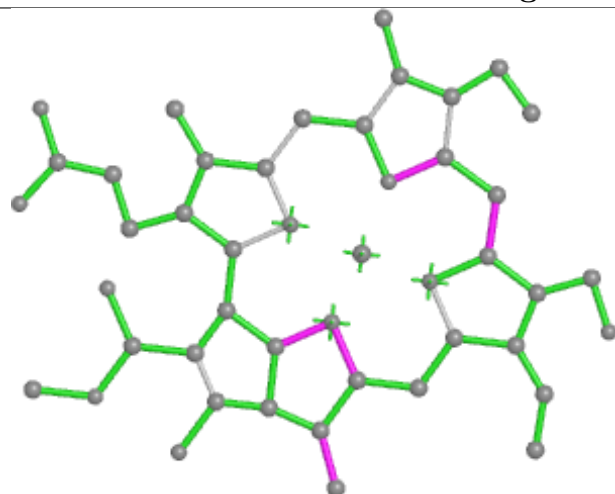


**Ligand CLA Aa 405****Ligand DGD B 601**

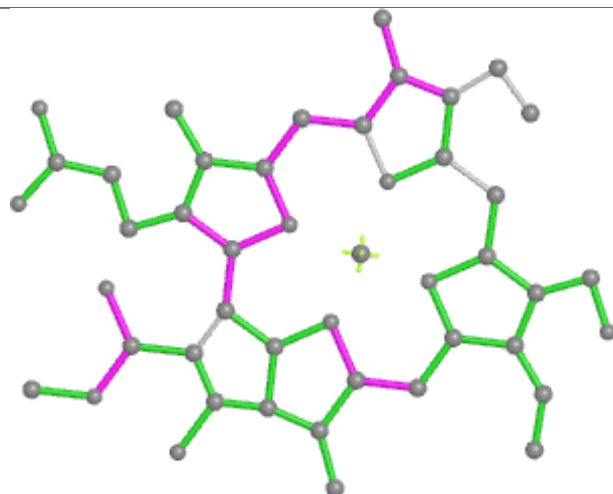




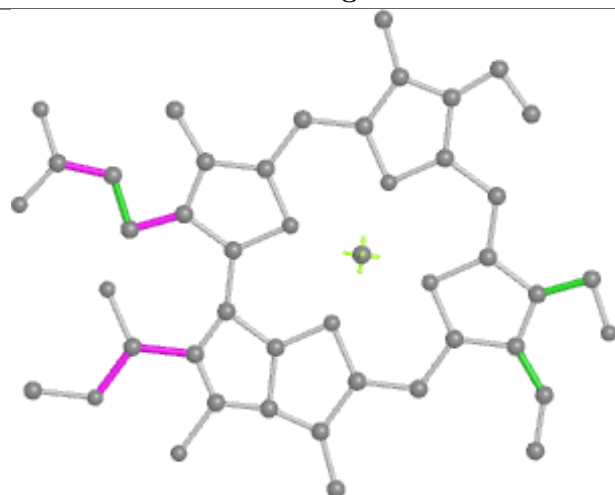
## Ligand CHL 4 309



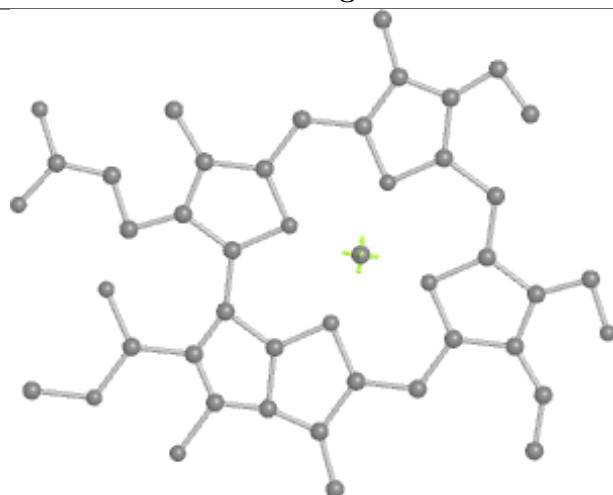
Bond lengths



Bond angles

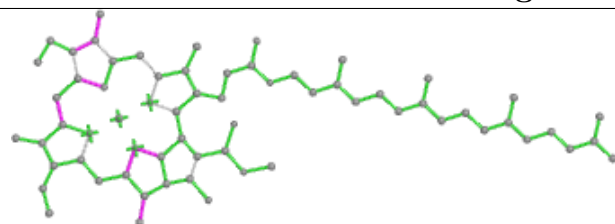


Torsions

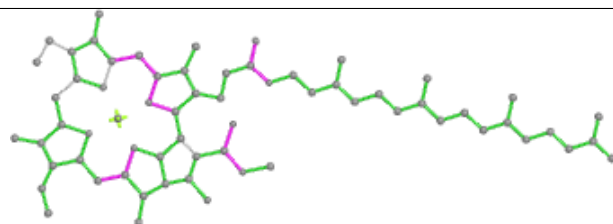


Rings

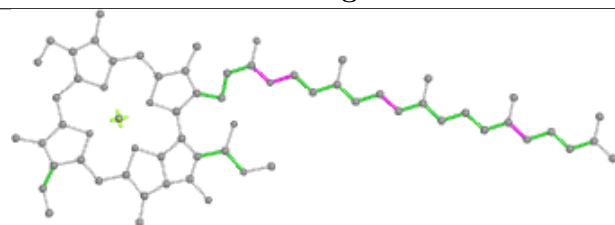
## Ligand CLA D 405



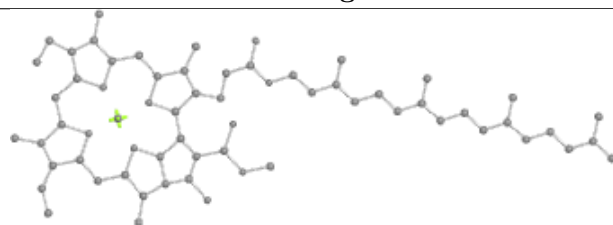
Bond lengths



Bond angles

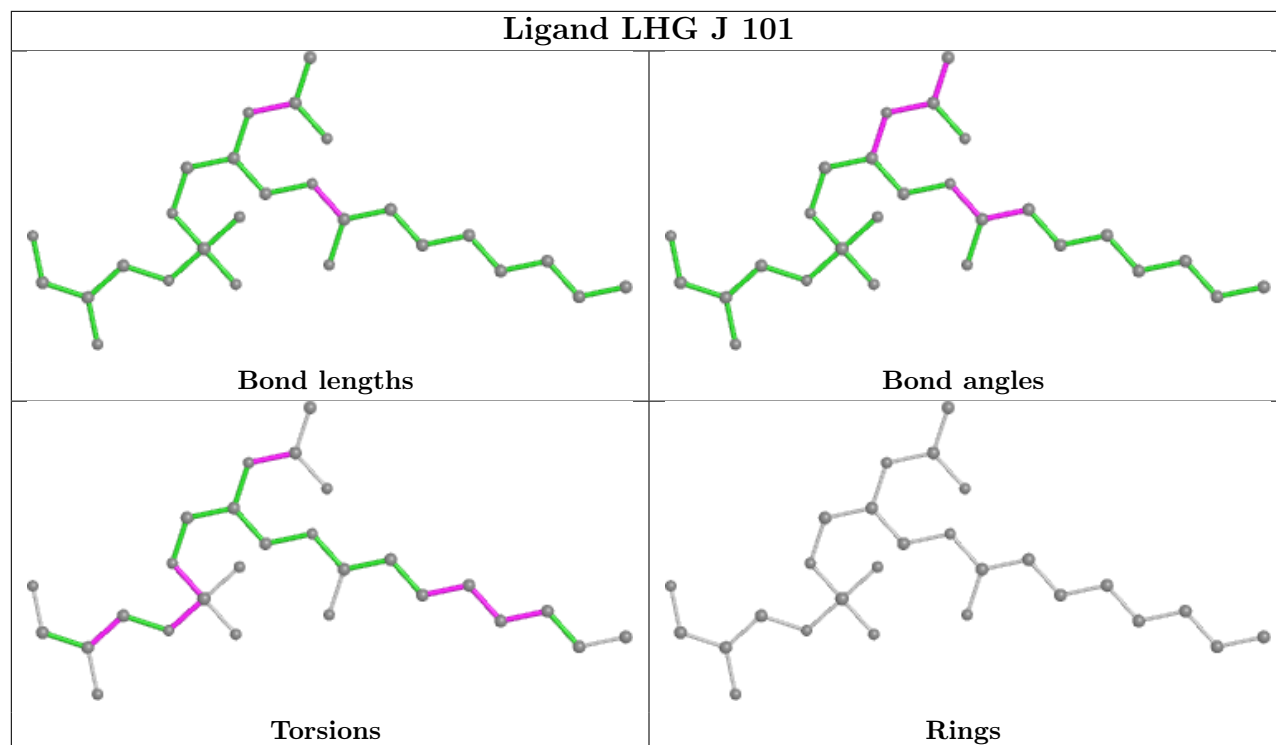


Torsions

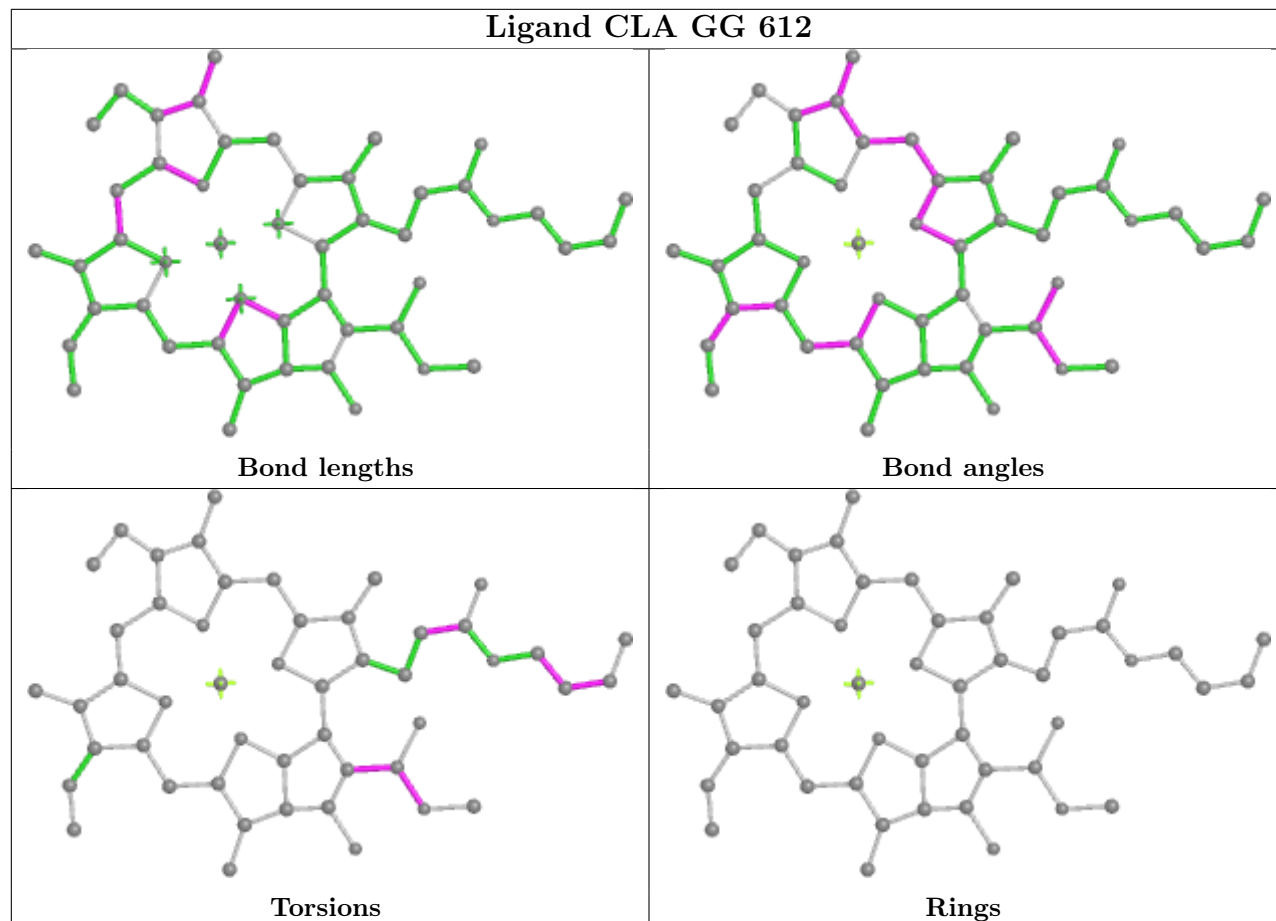


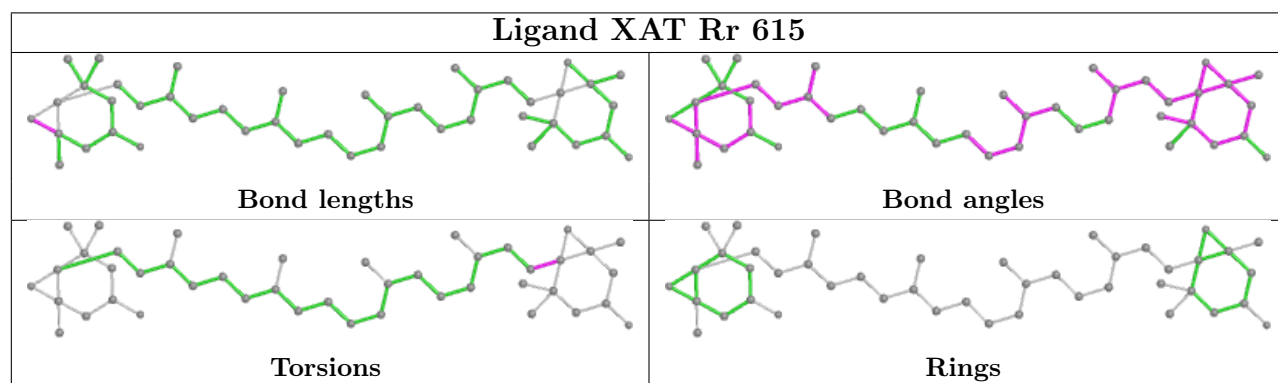
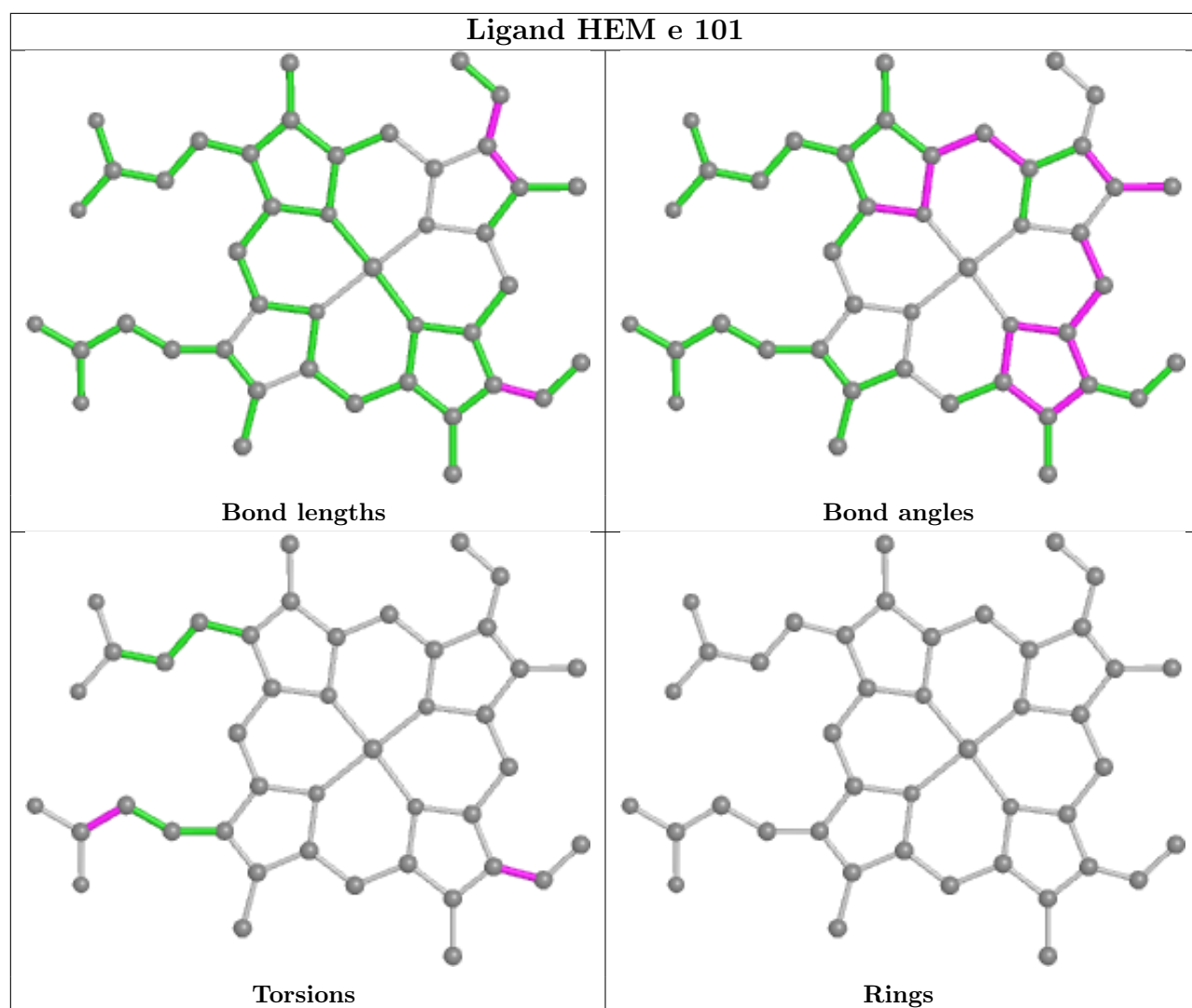
Rings

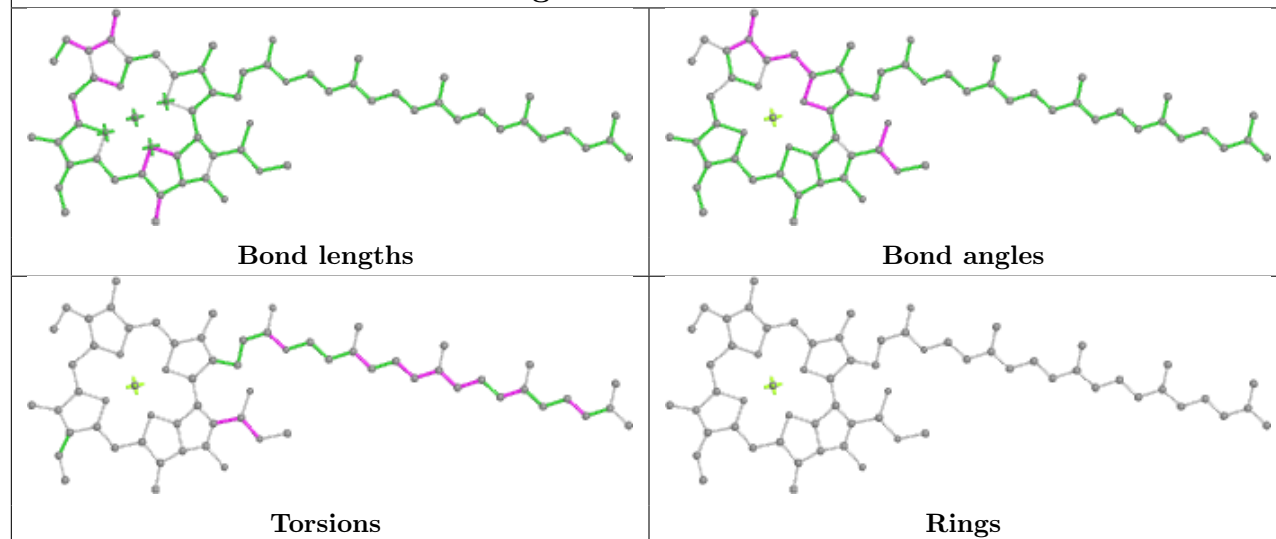
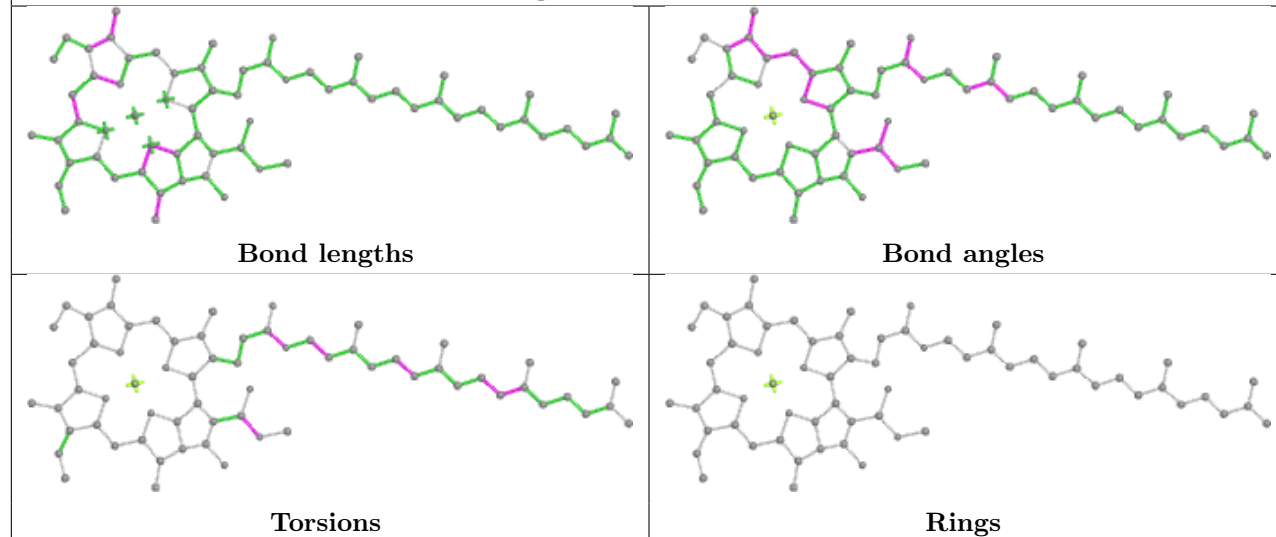
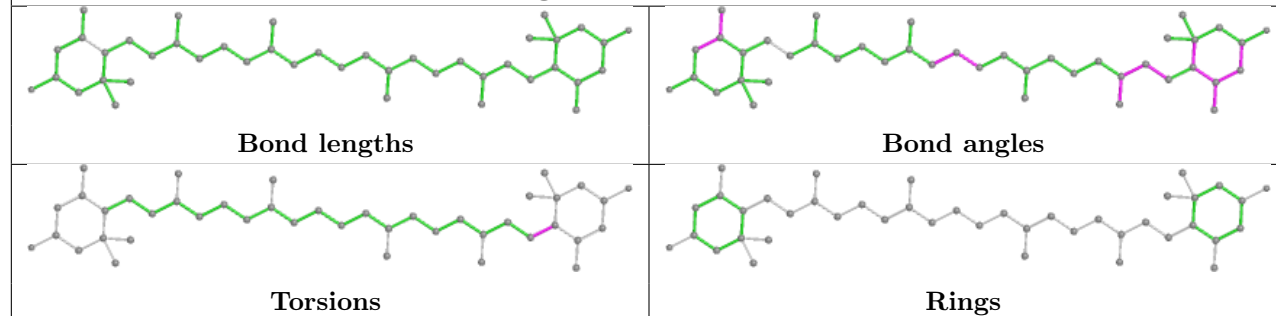
## Ligand LHG J 101

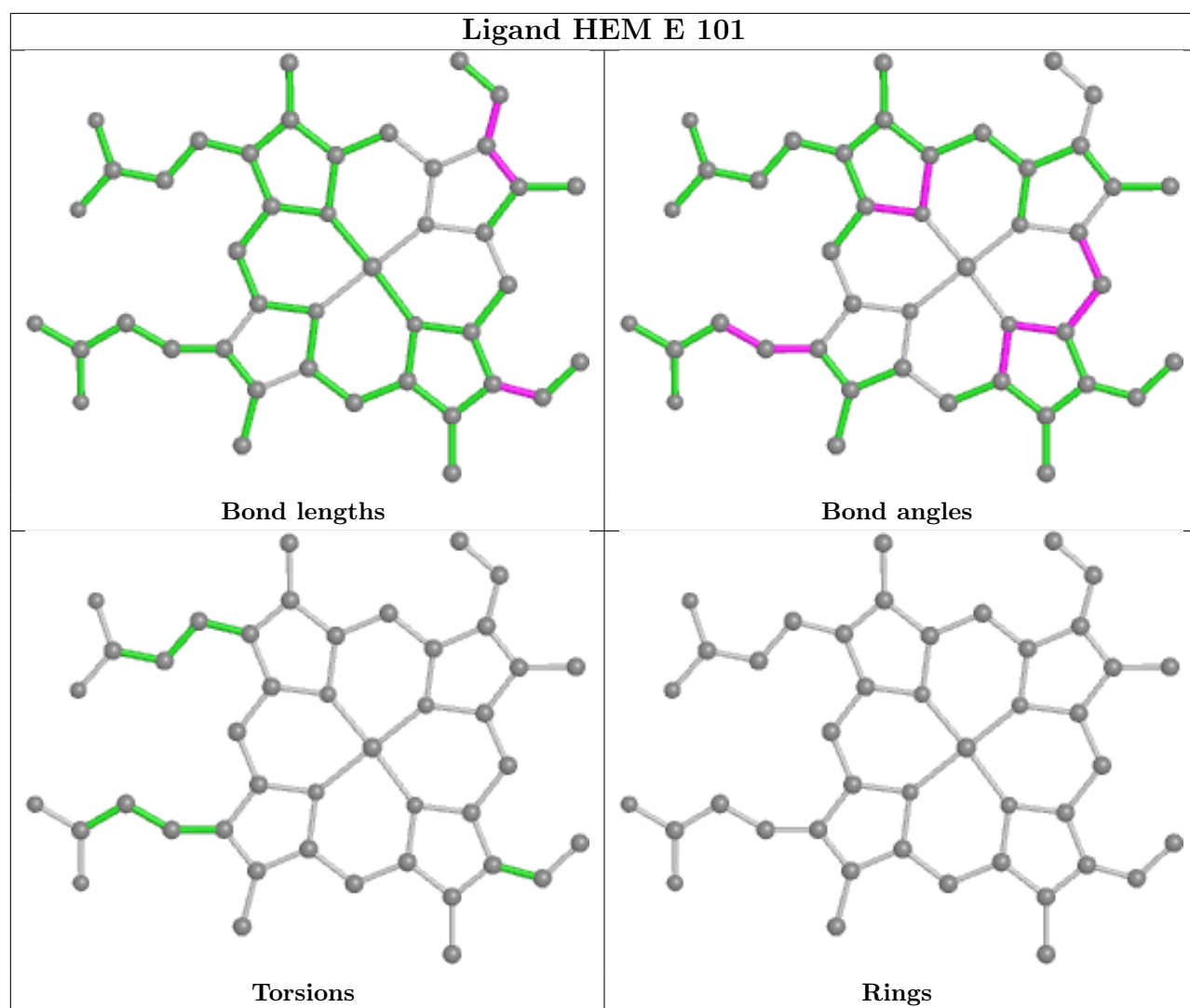


## Ligand CLA GG 612

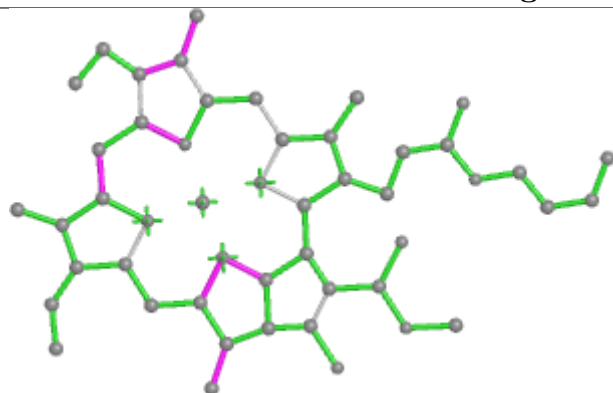




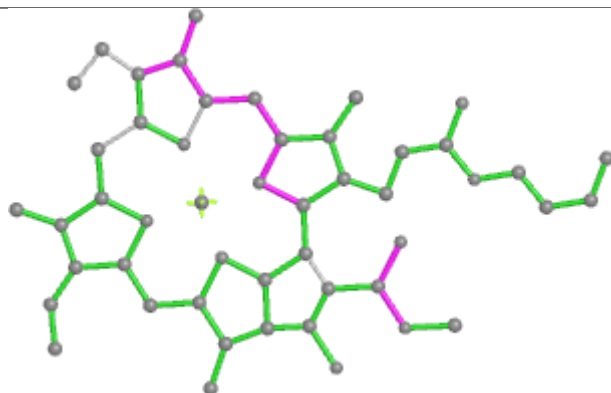
**Ligand CLA C 513****Ligand CLA B 610****Ligand LUT S 614**



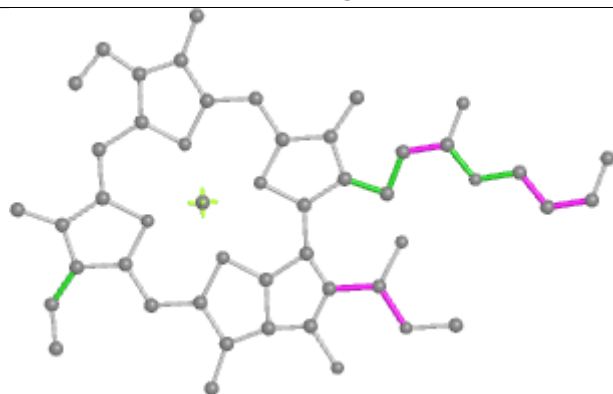
## Ligand CLA r 603



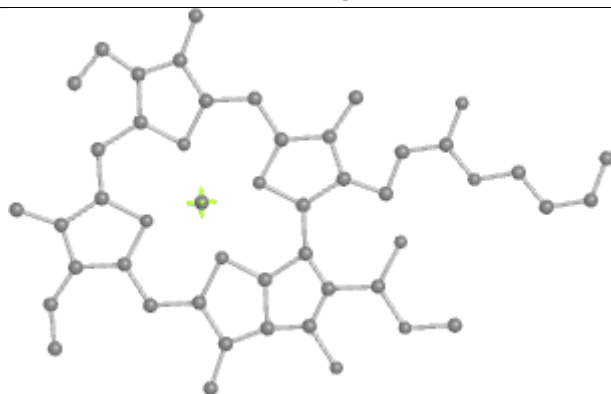
Bond lengths



Bond angles

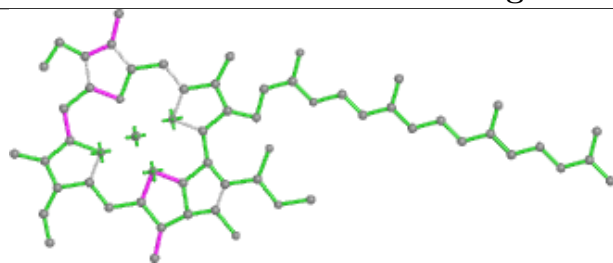


Torsions

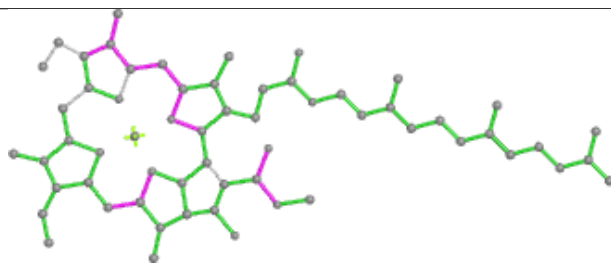


Rings

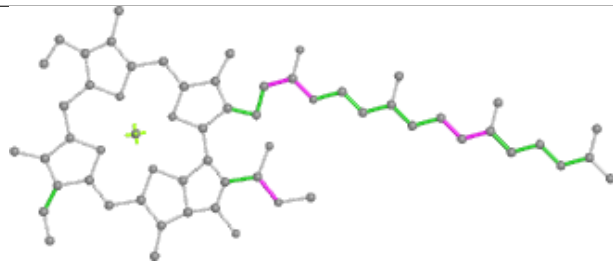
## Ligand CLA Cc 510



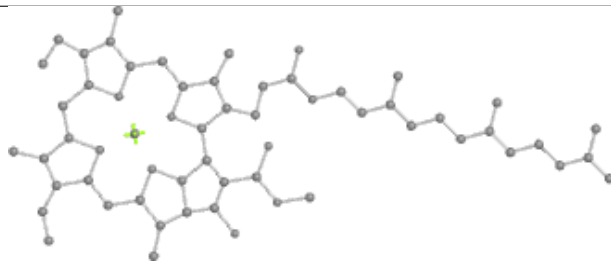
Bond lengths



Bond angles

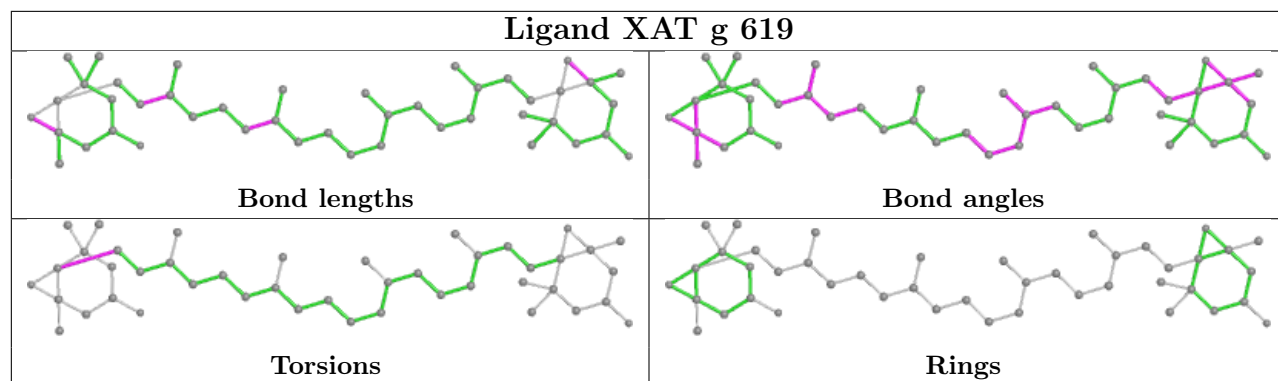


Torsions

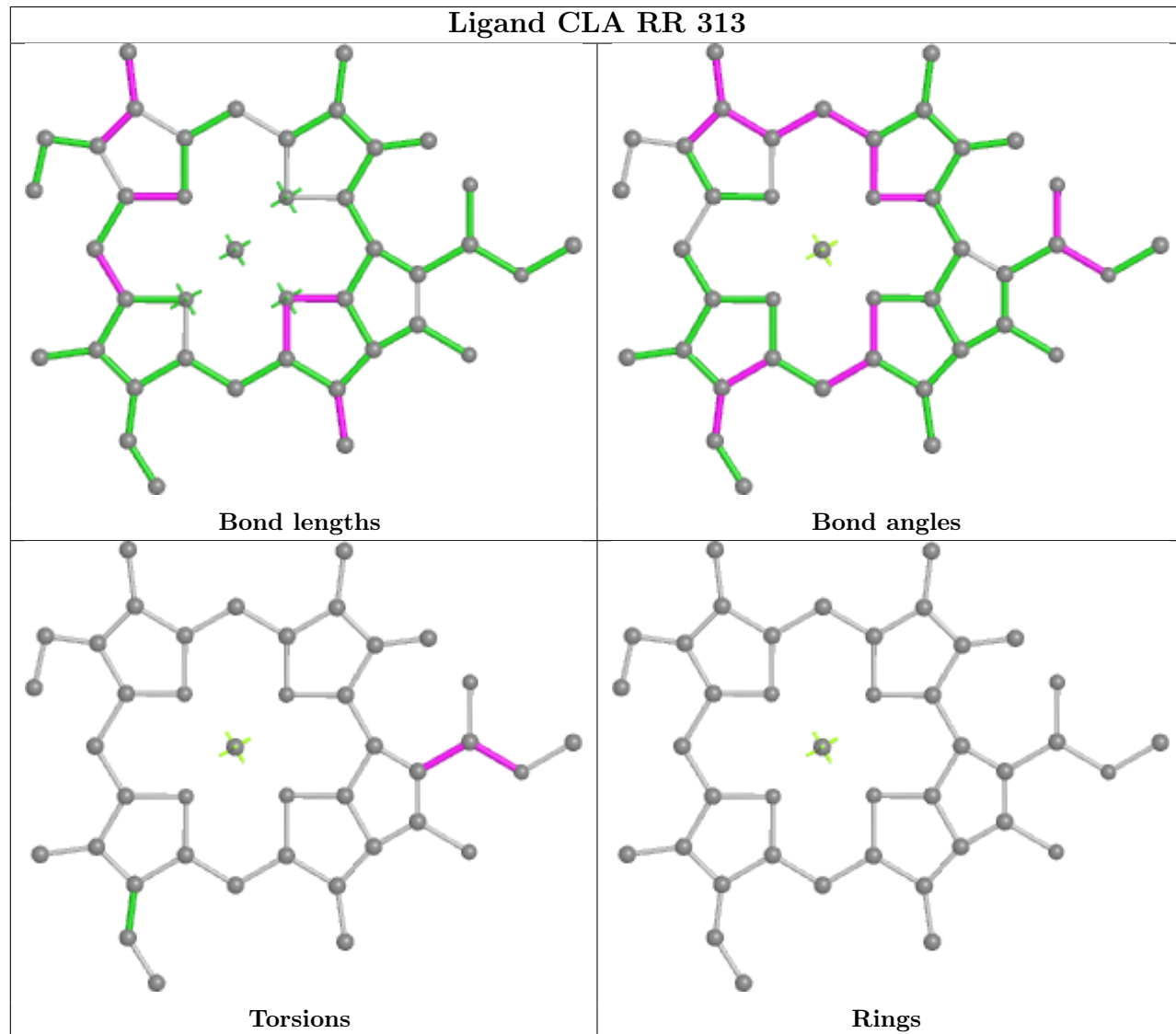


Rings

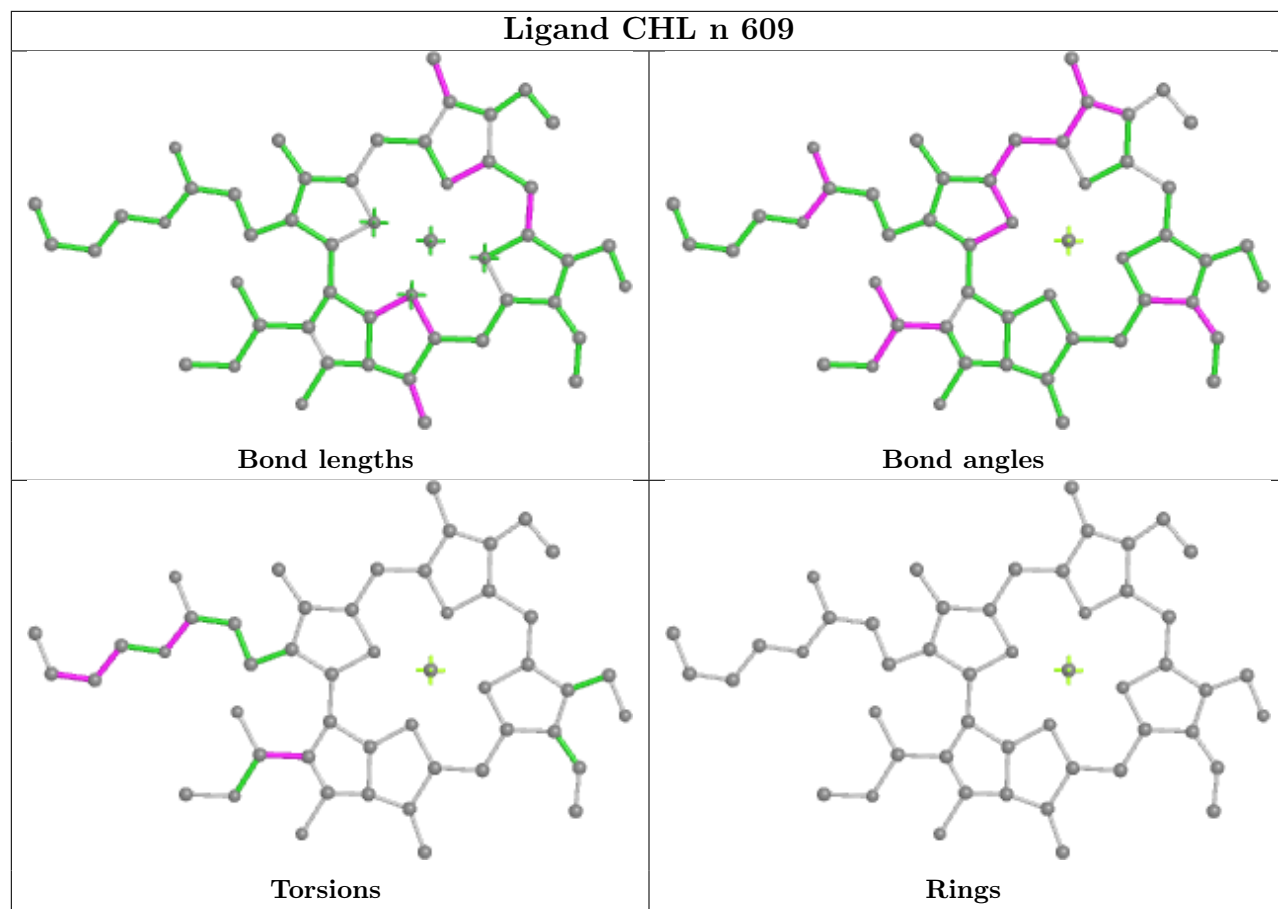
## Ligand XAT g 619

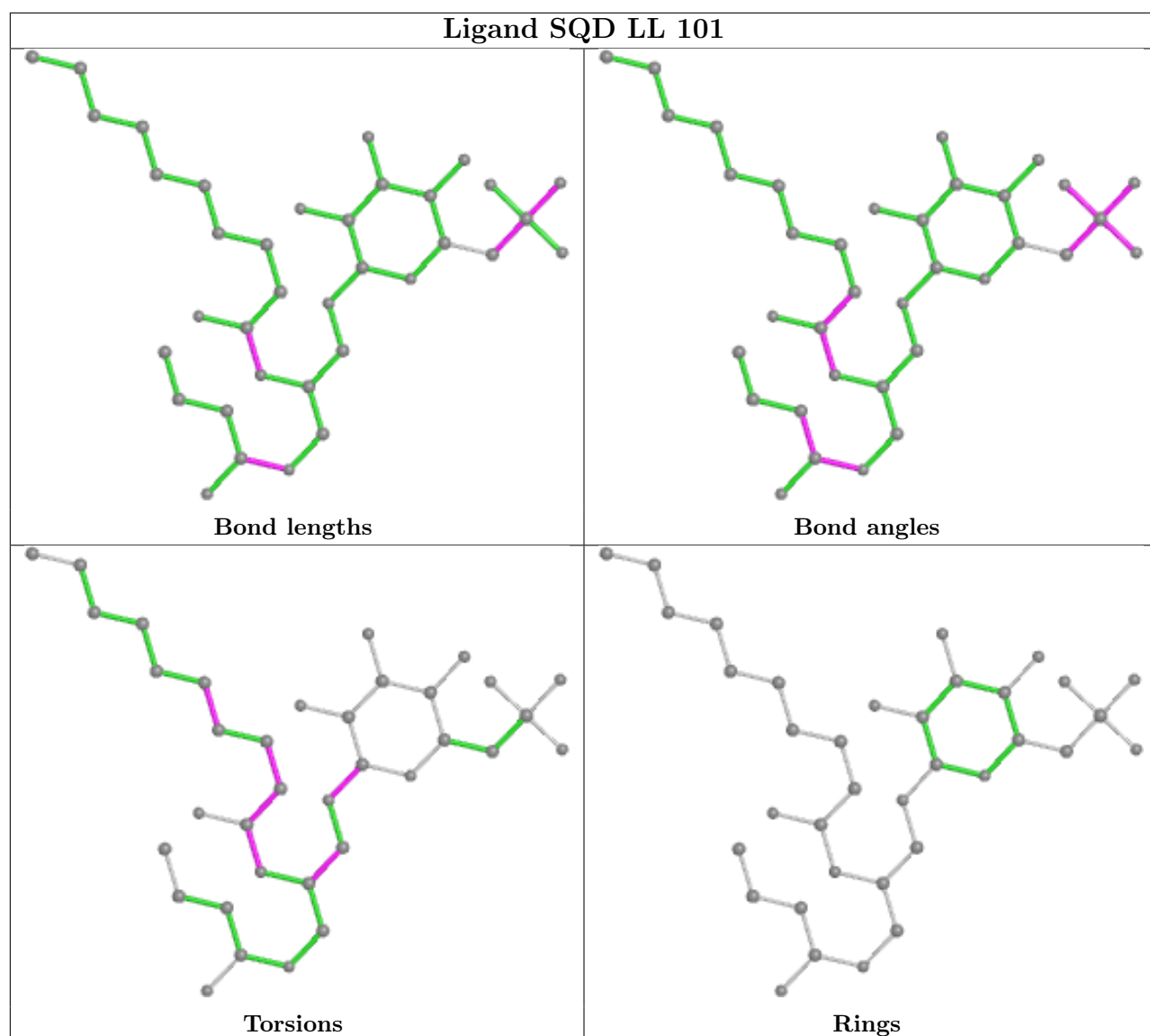


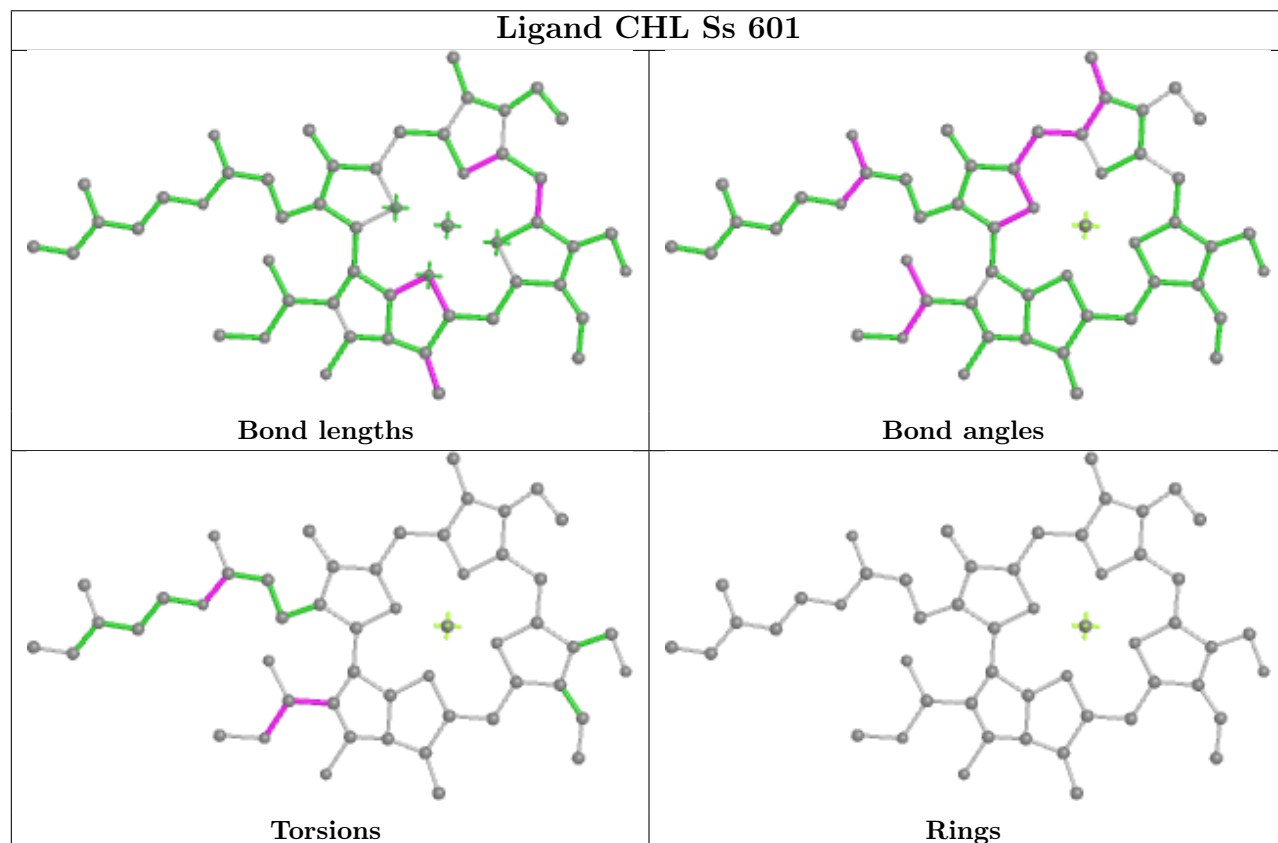
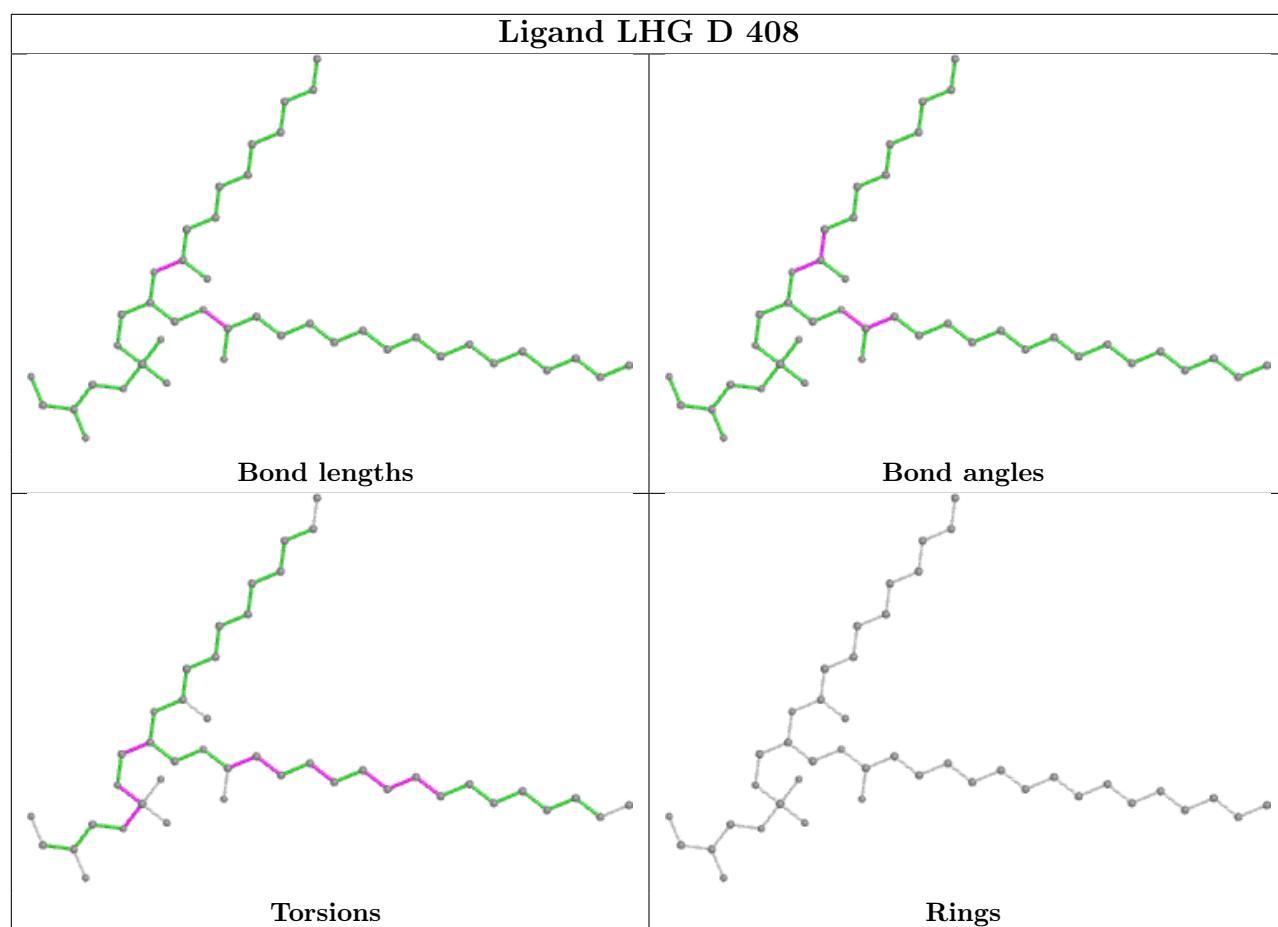
## Ligand CLA RR 313



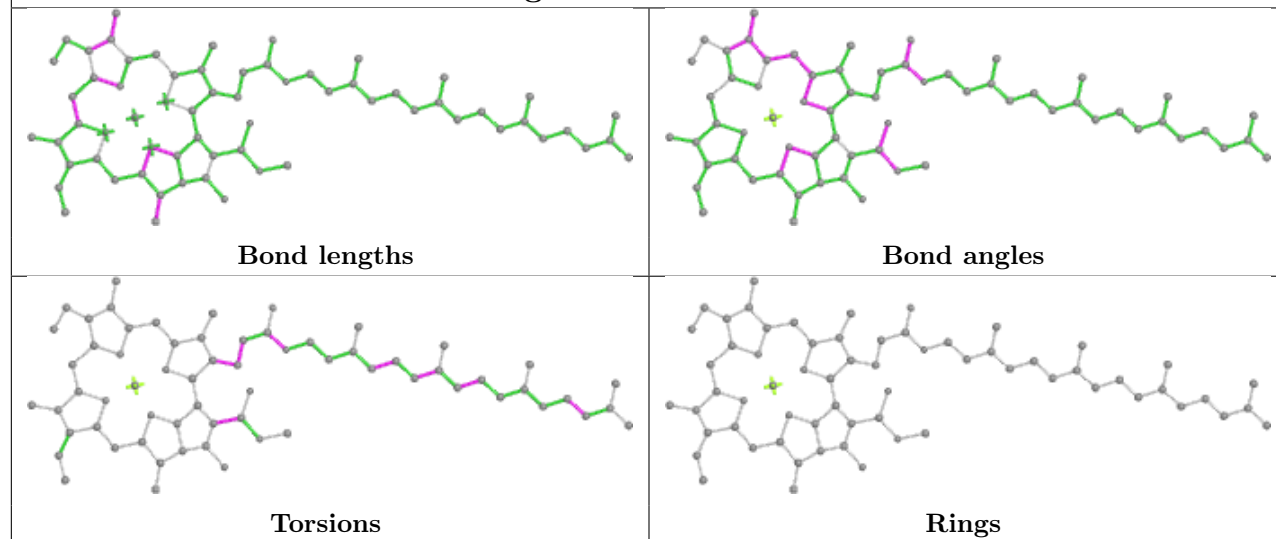




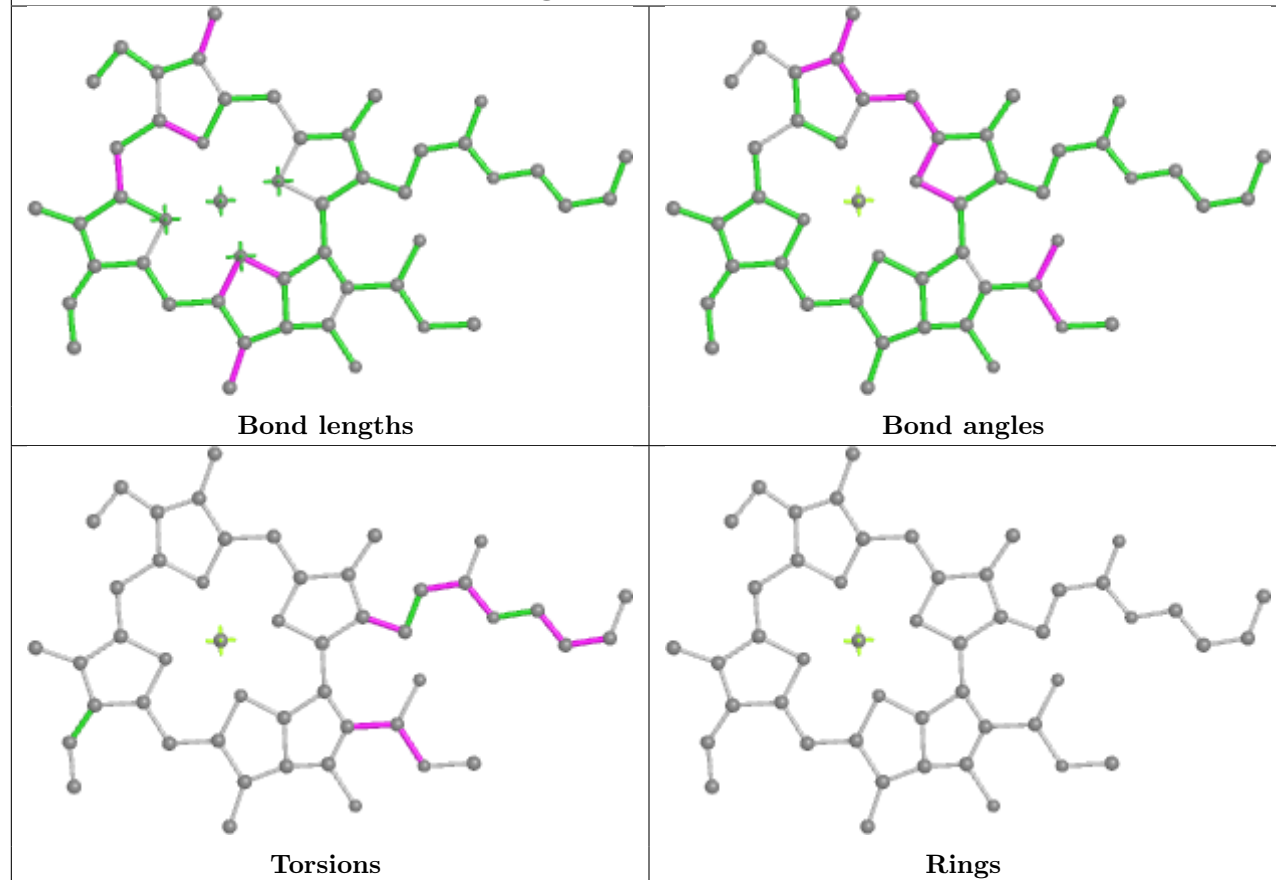


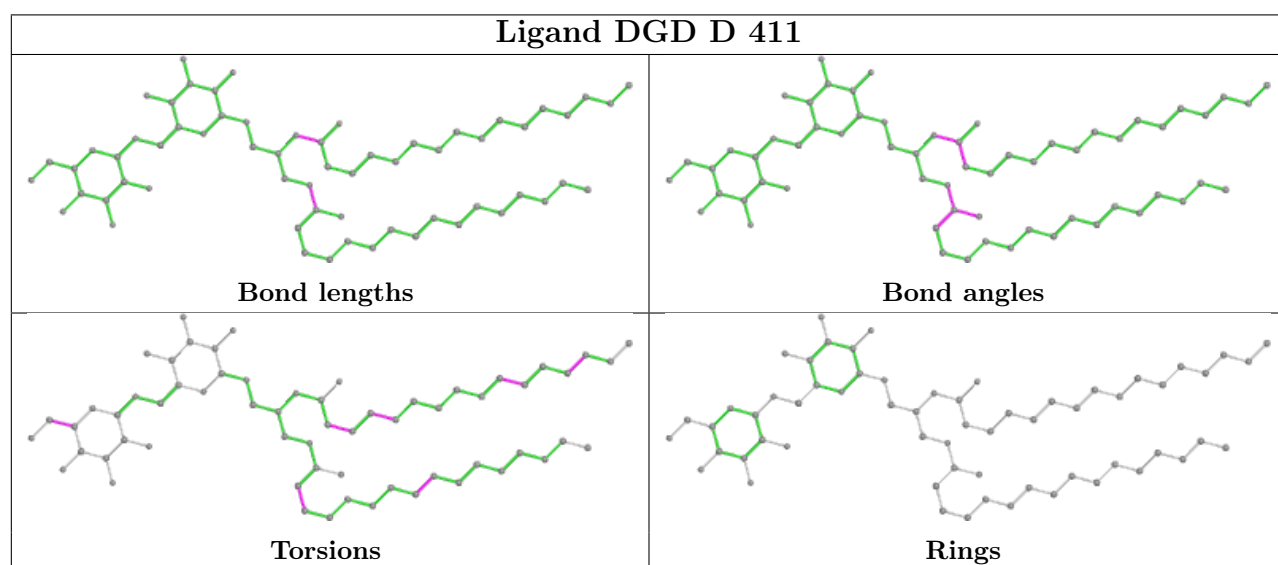
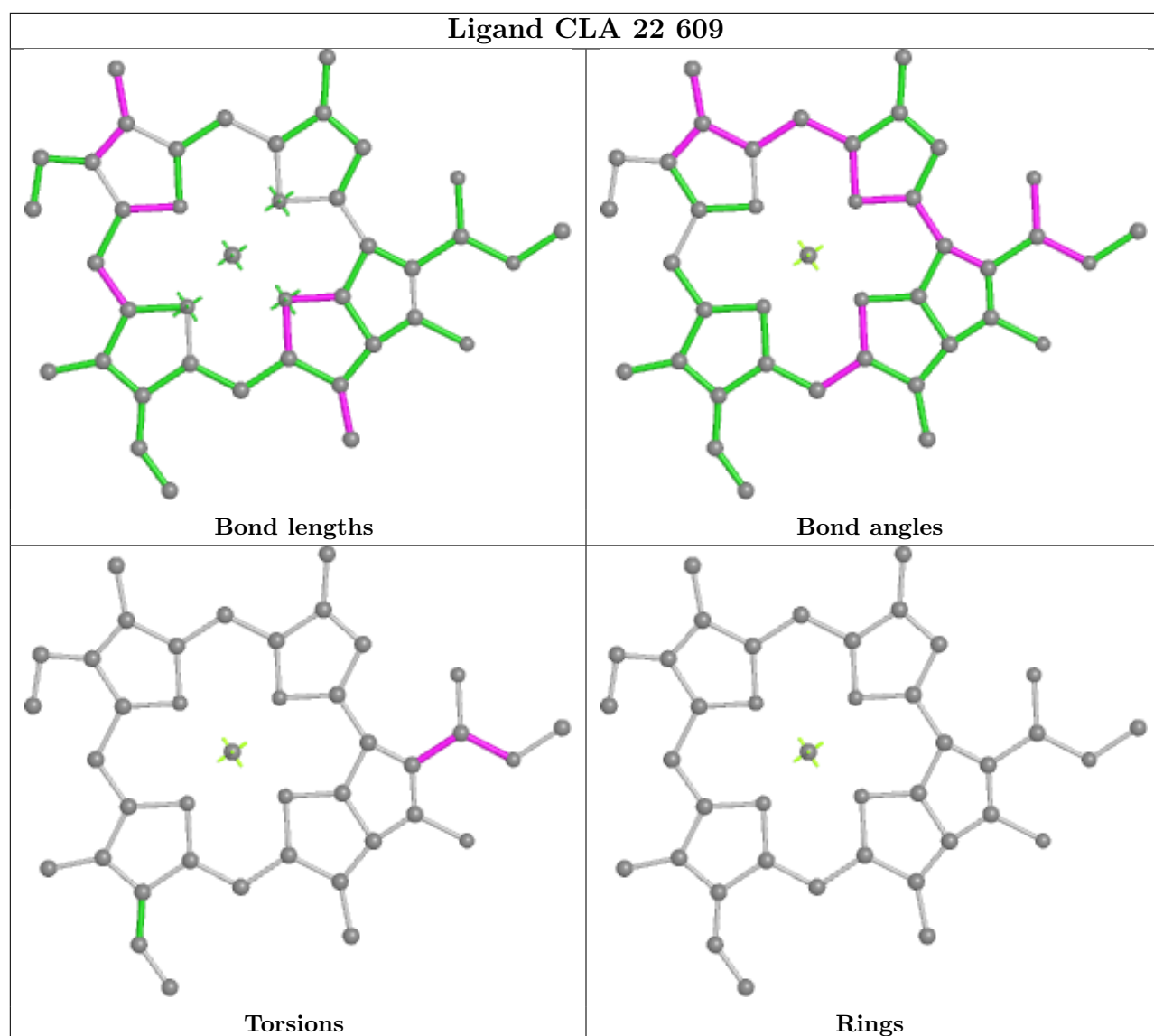


## Ligand CLA Rr 602

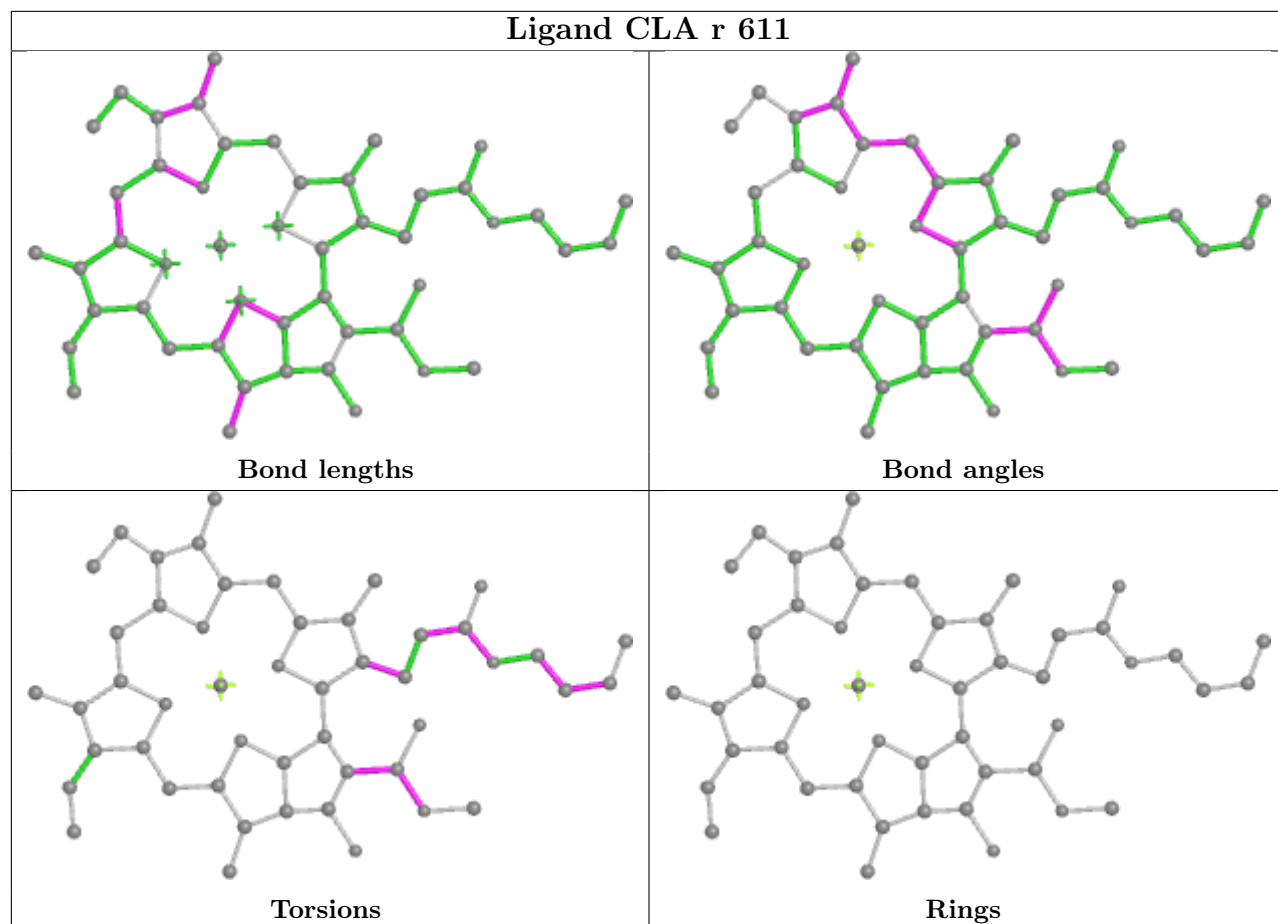


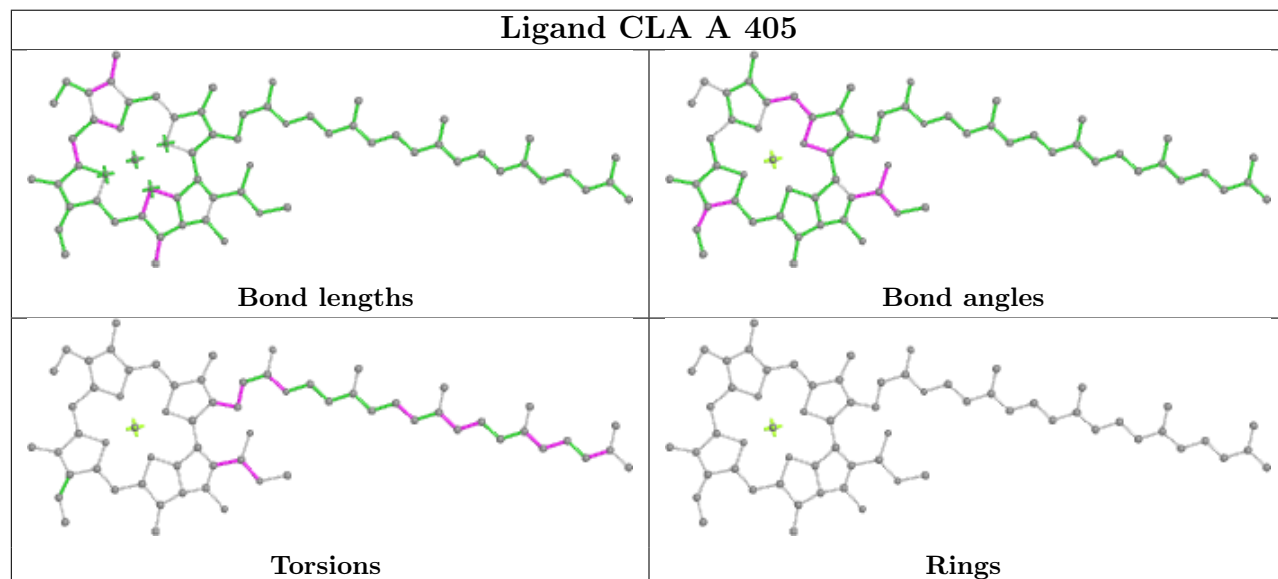
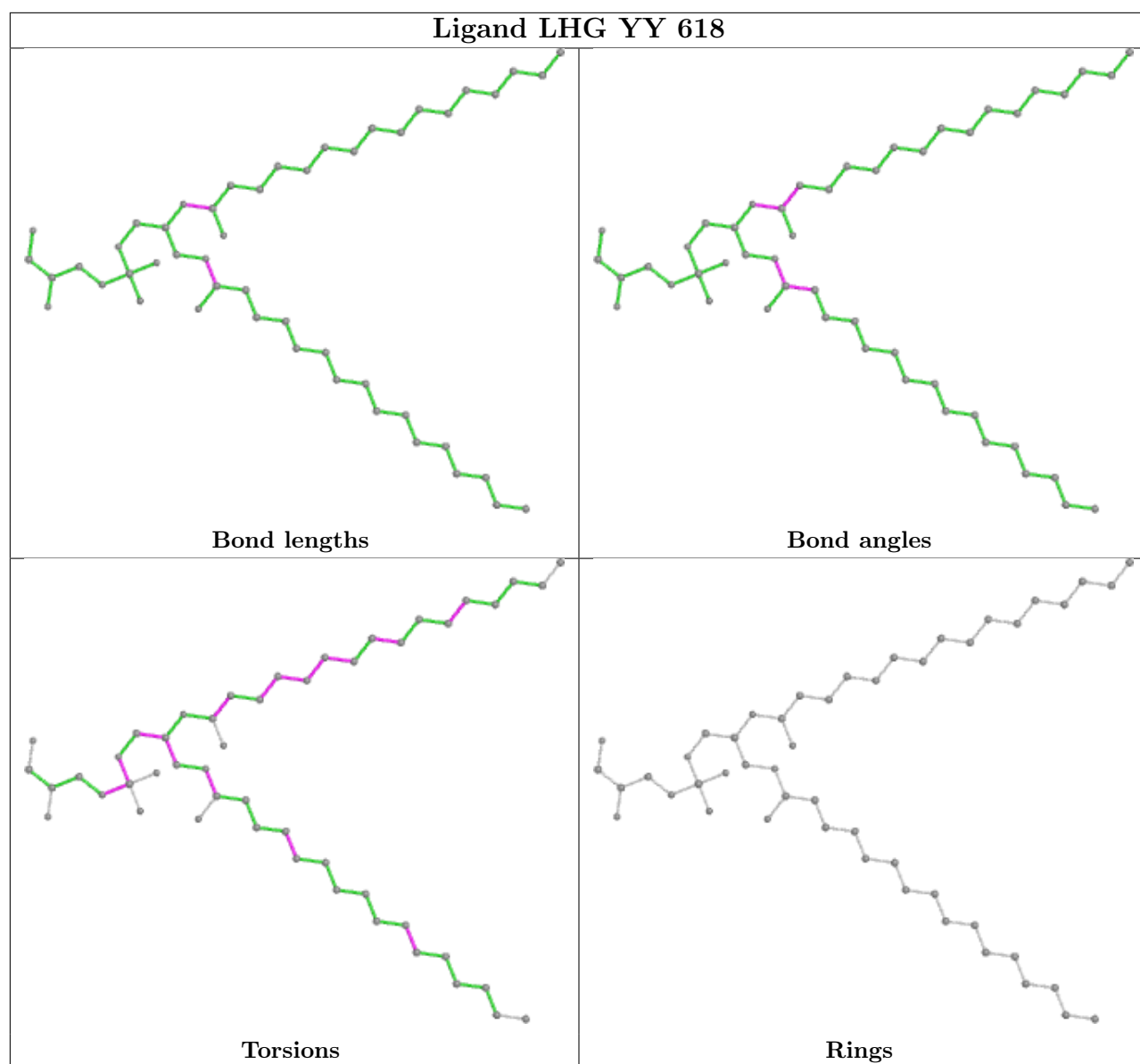
## Ligand CLA r 608

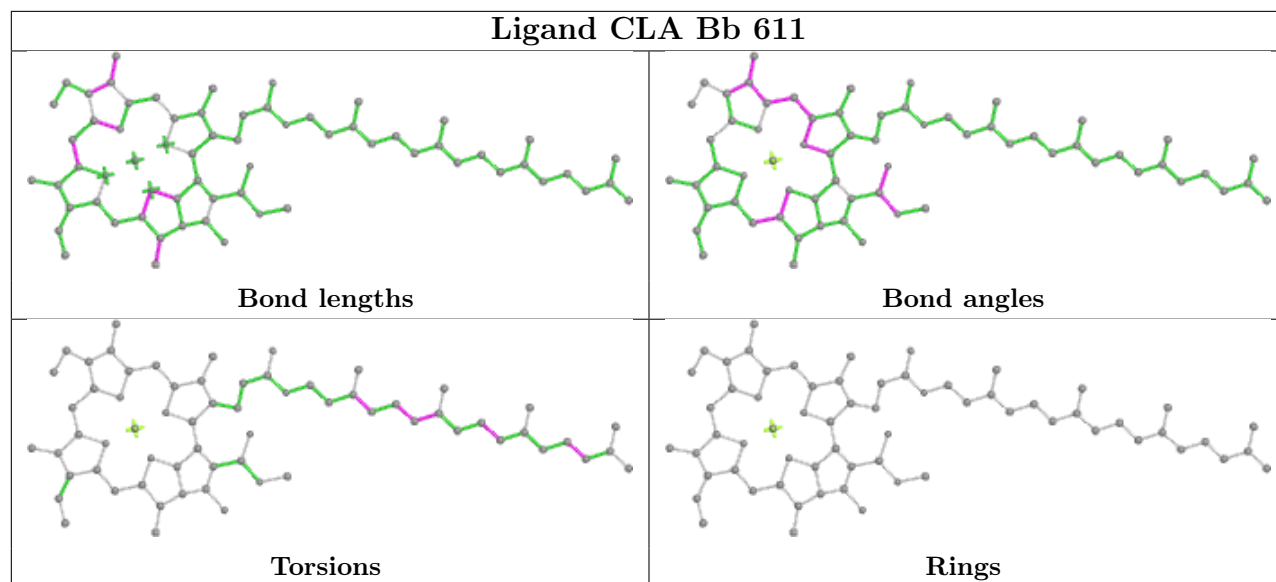
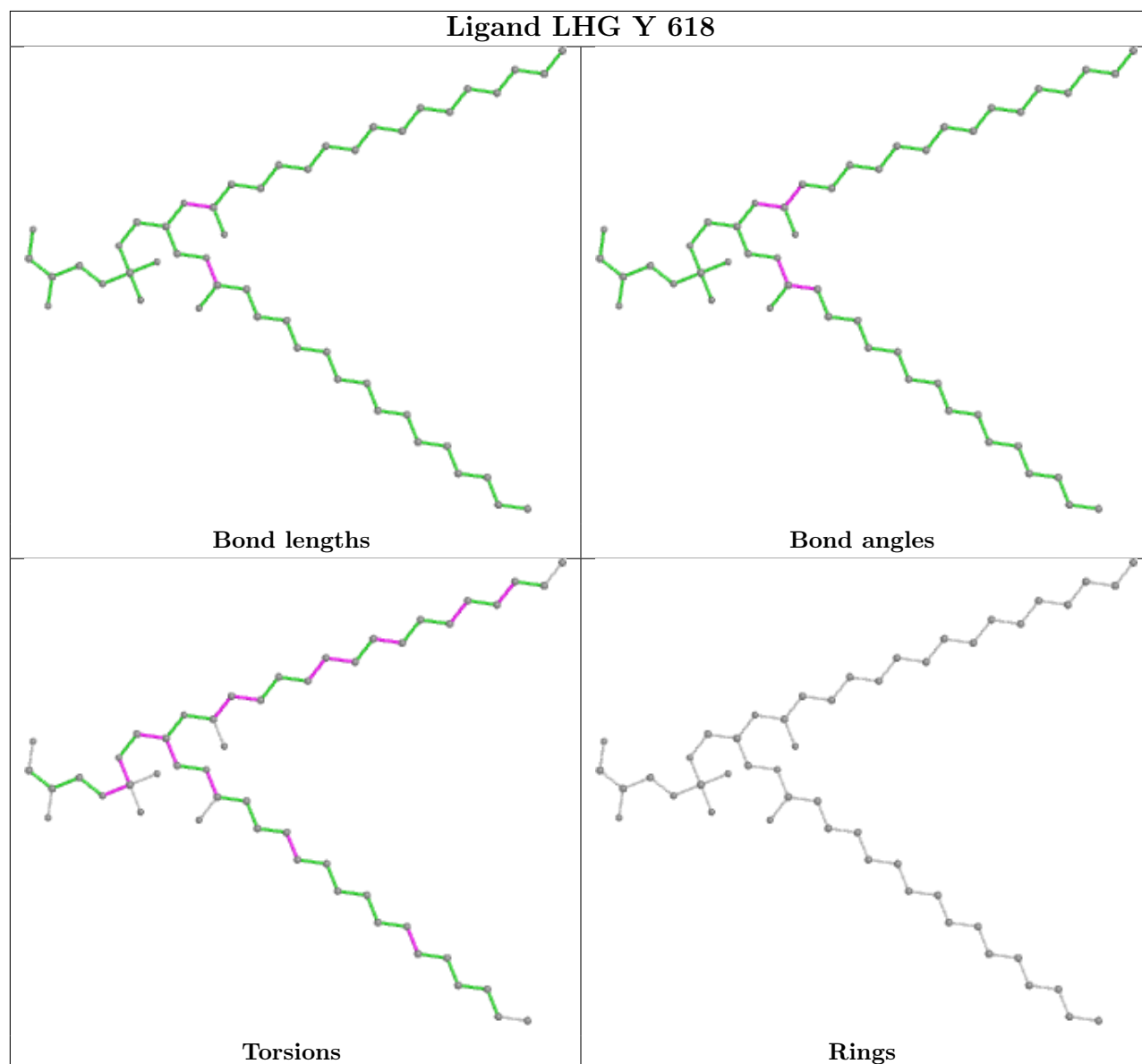




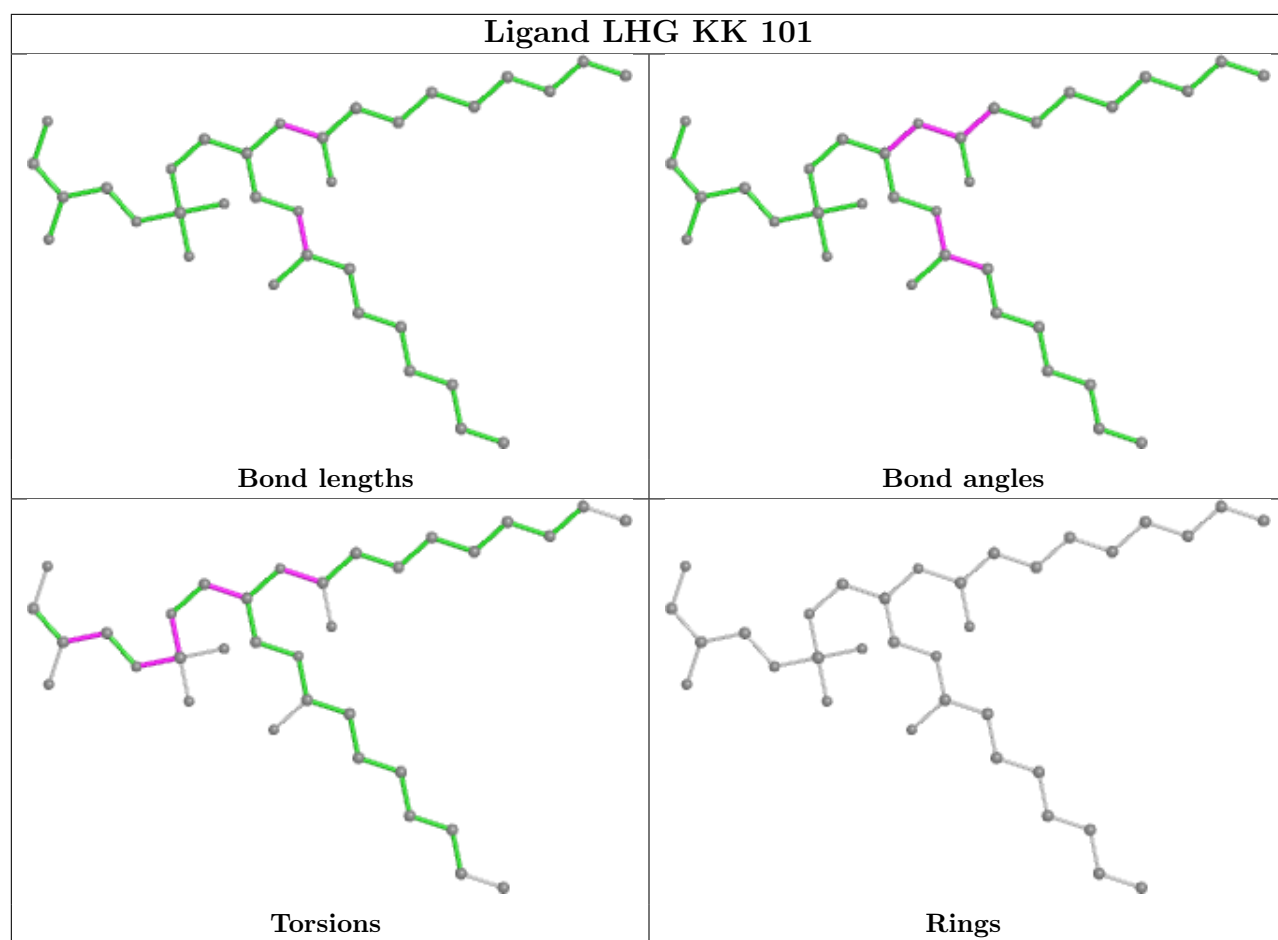
## Ligand CLA r 611



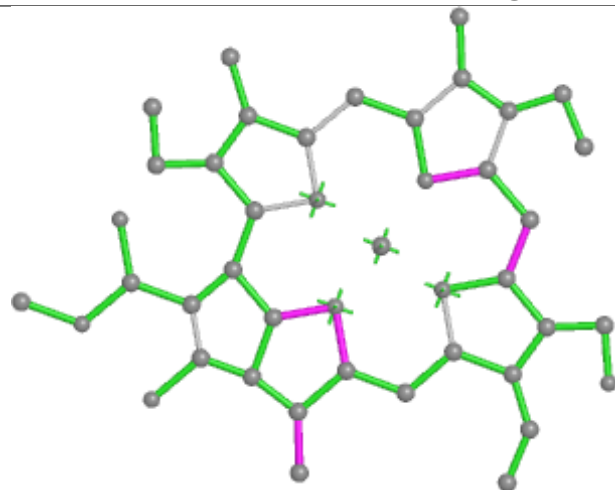


**Ligand CLA Bb 611****Ligand LHG Y 618**

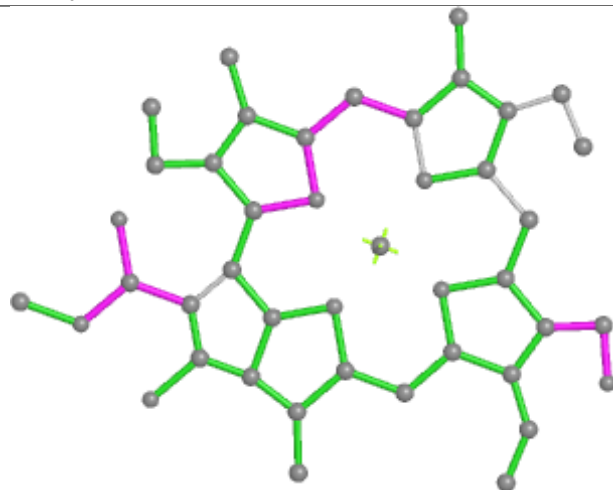




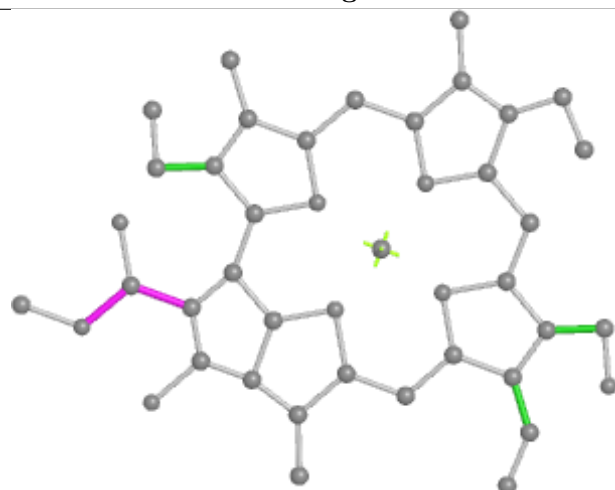
## Ligand CHL Yy 607



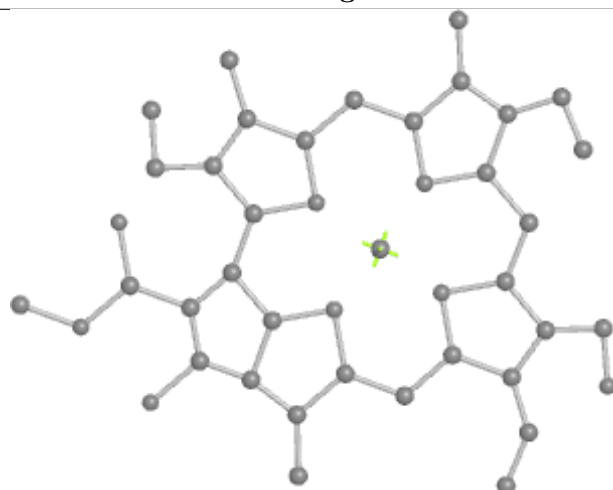
Bond lengths



Bond angles

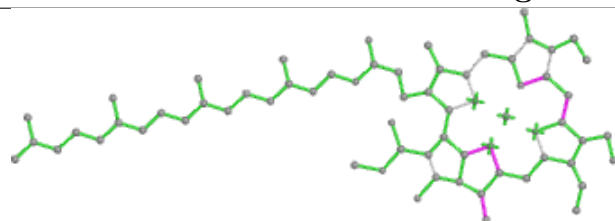


Torsions

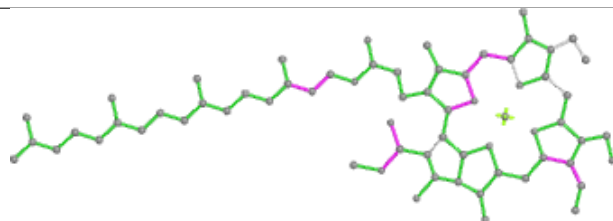


Rings

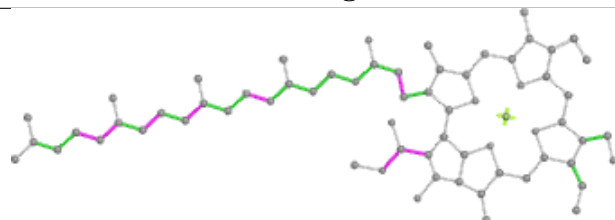
## Ligand CHL N 607



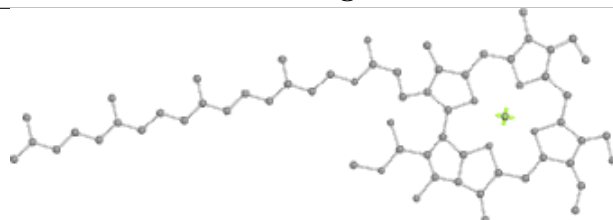
Bond lengths



Bond angles

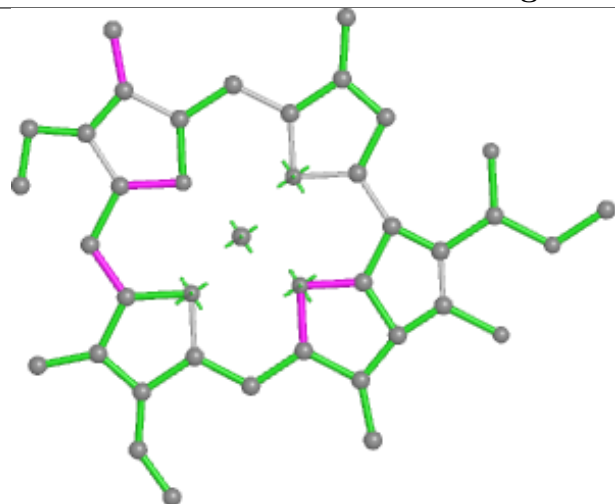


Torsions

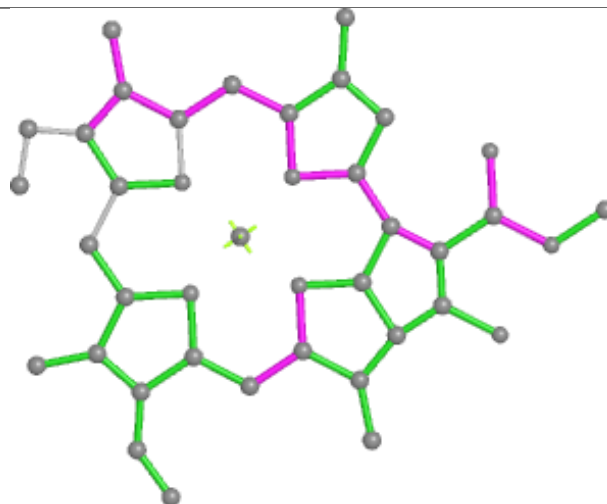


Rings

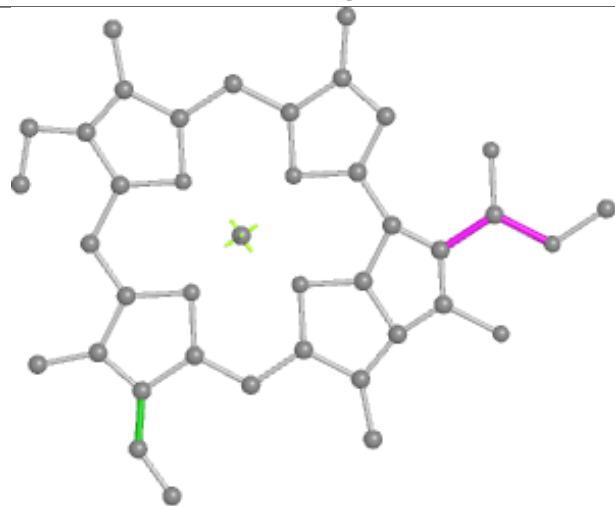
## Ligand CLA 1 610



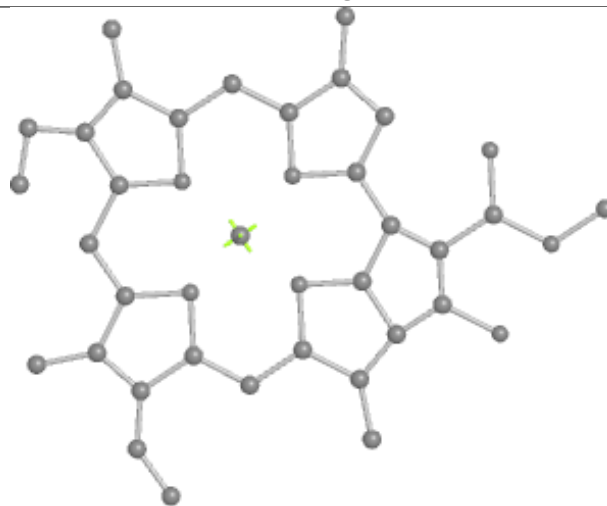
Bond lengths



Bond angles

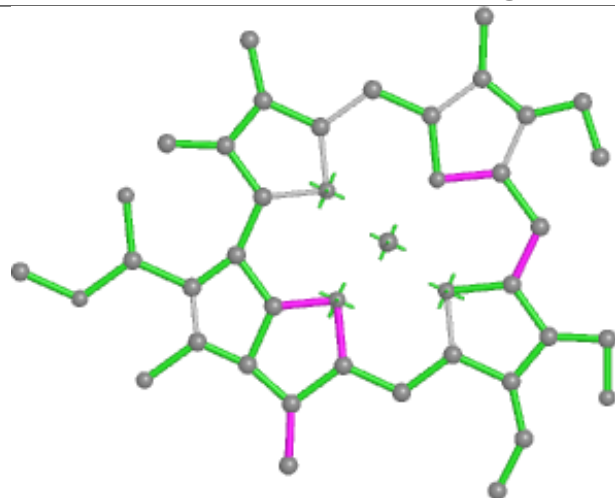


Torsions

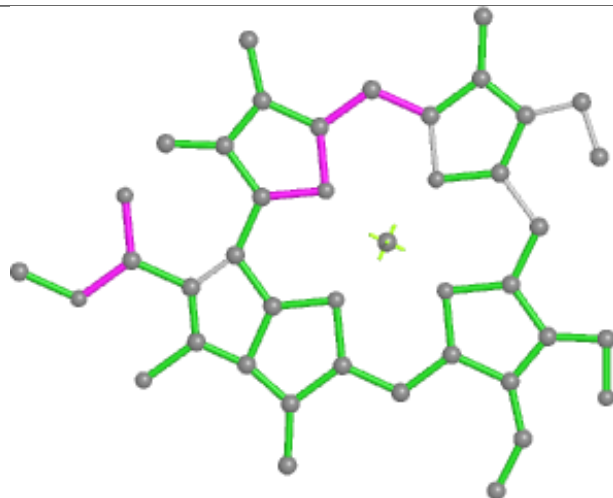


Rings

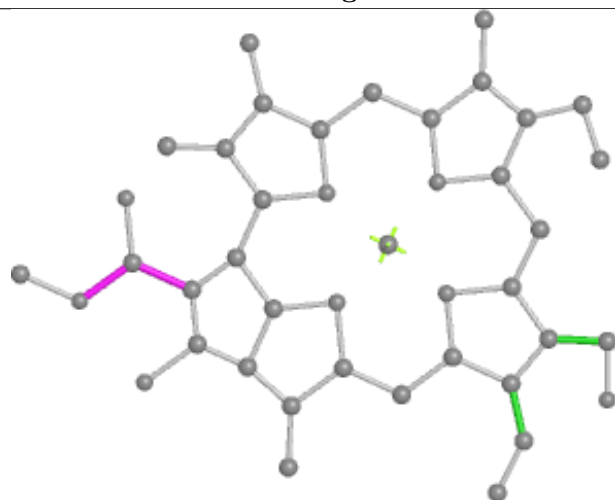
## Ligand CHL NN 606



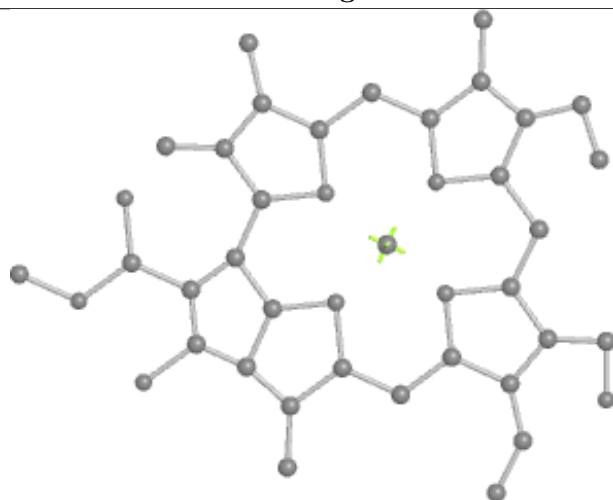
Bond lengths



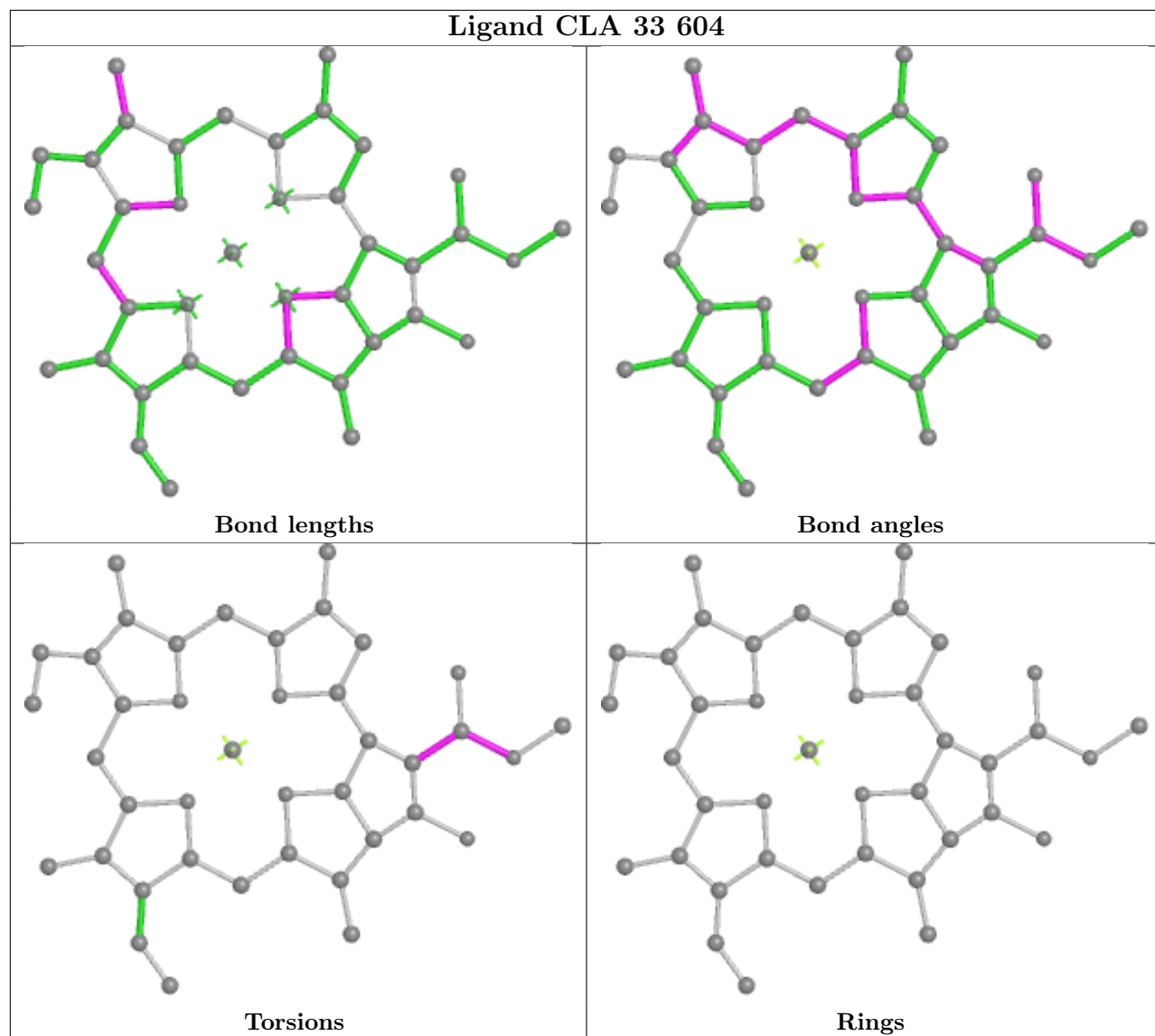
Bond angles



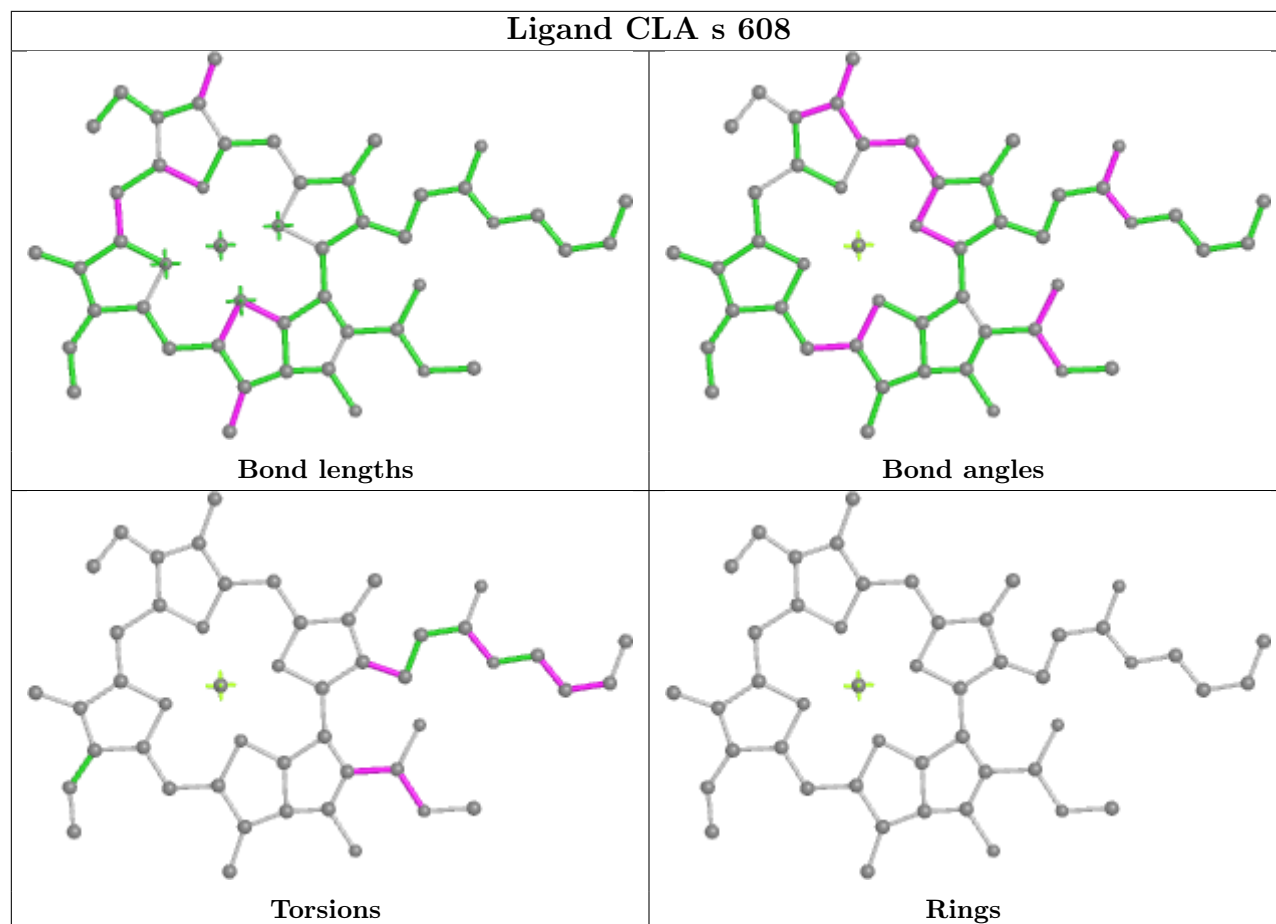
Torsions



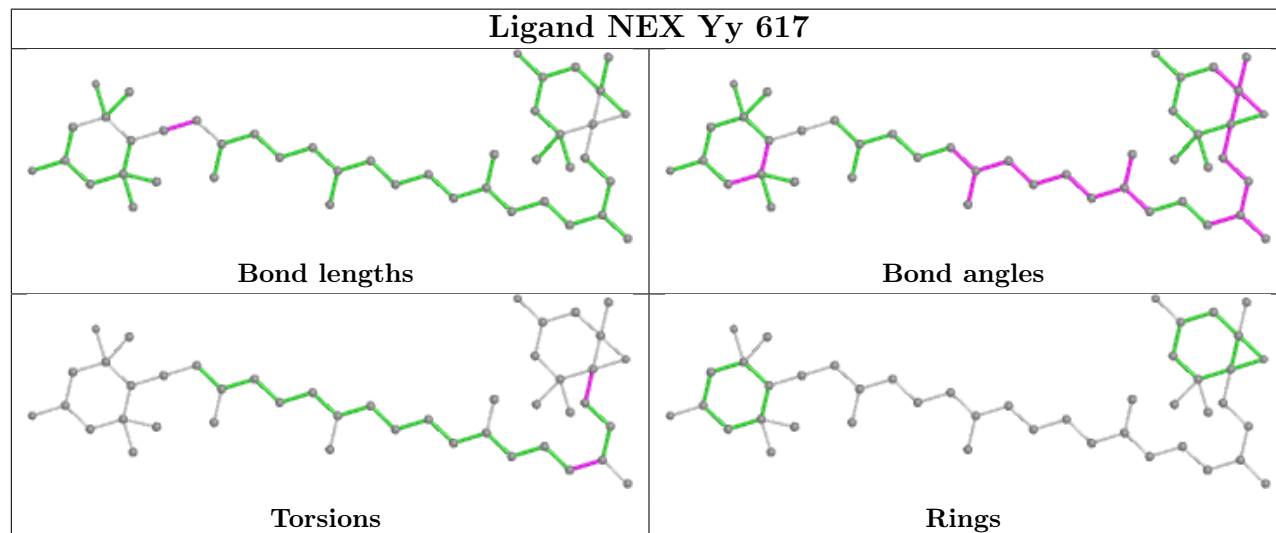
Rings

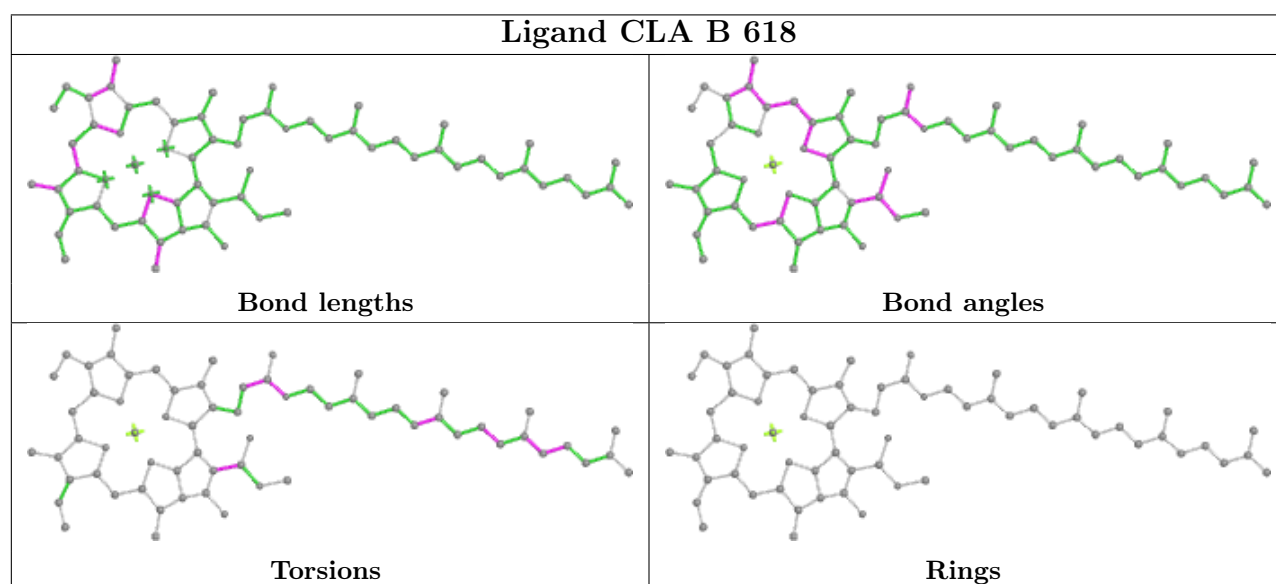
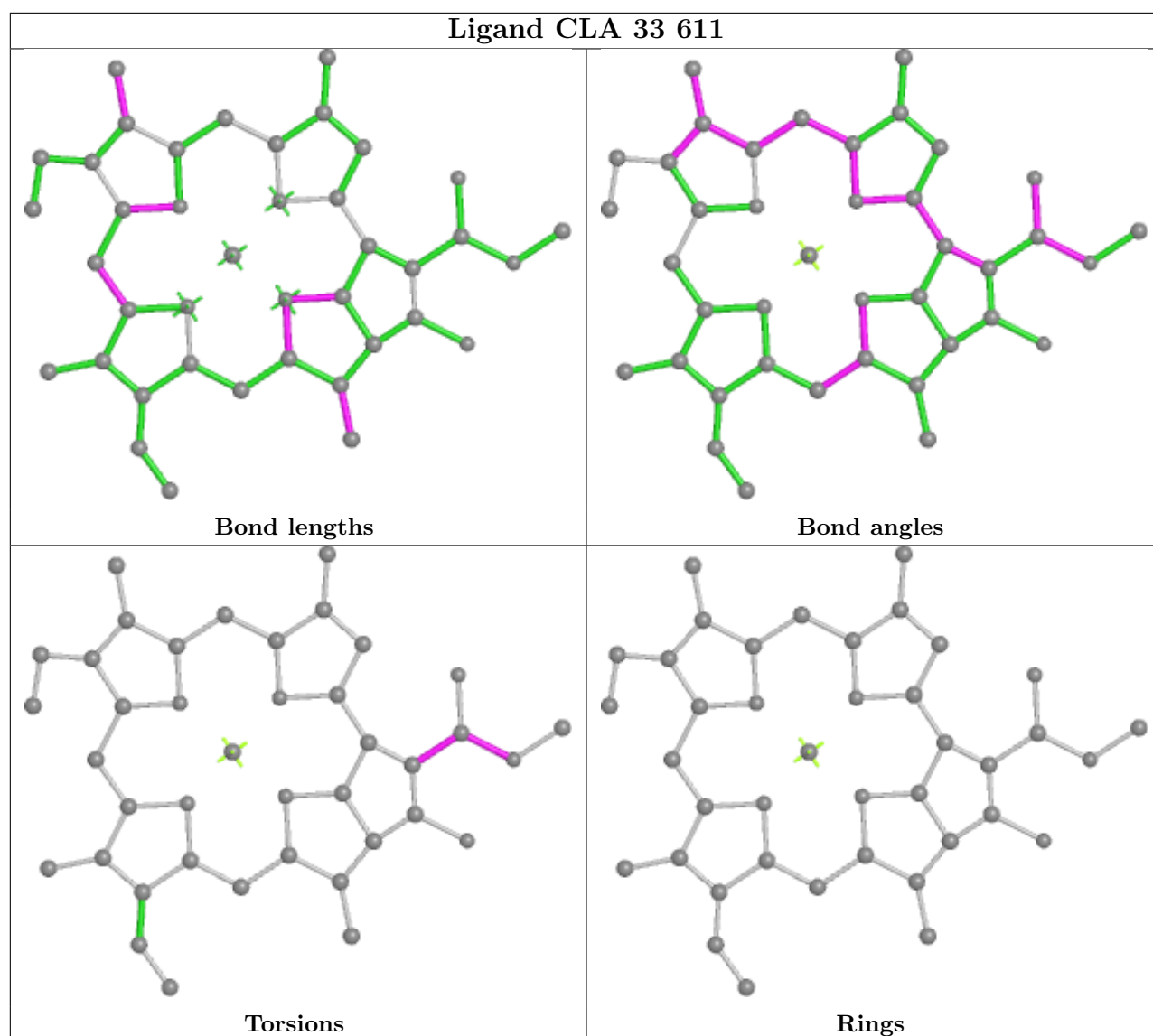


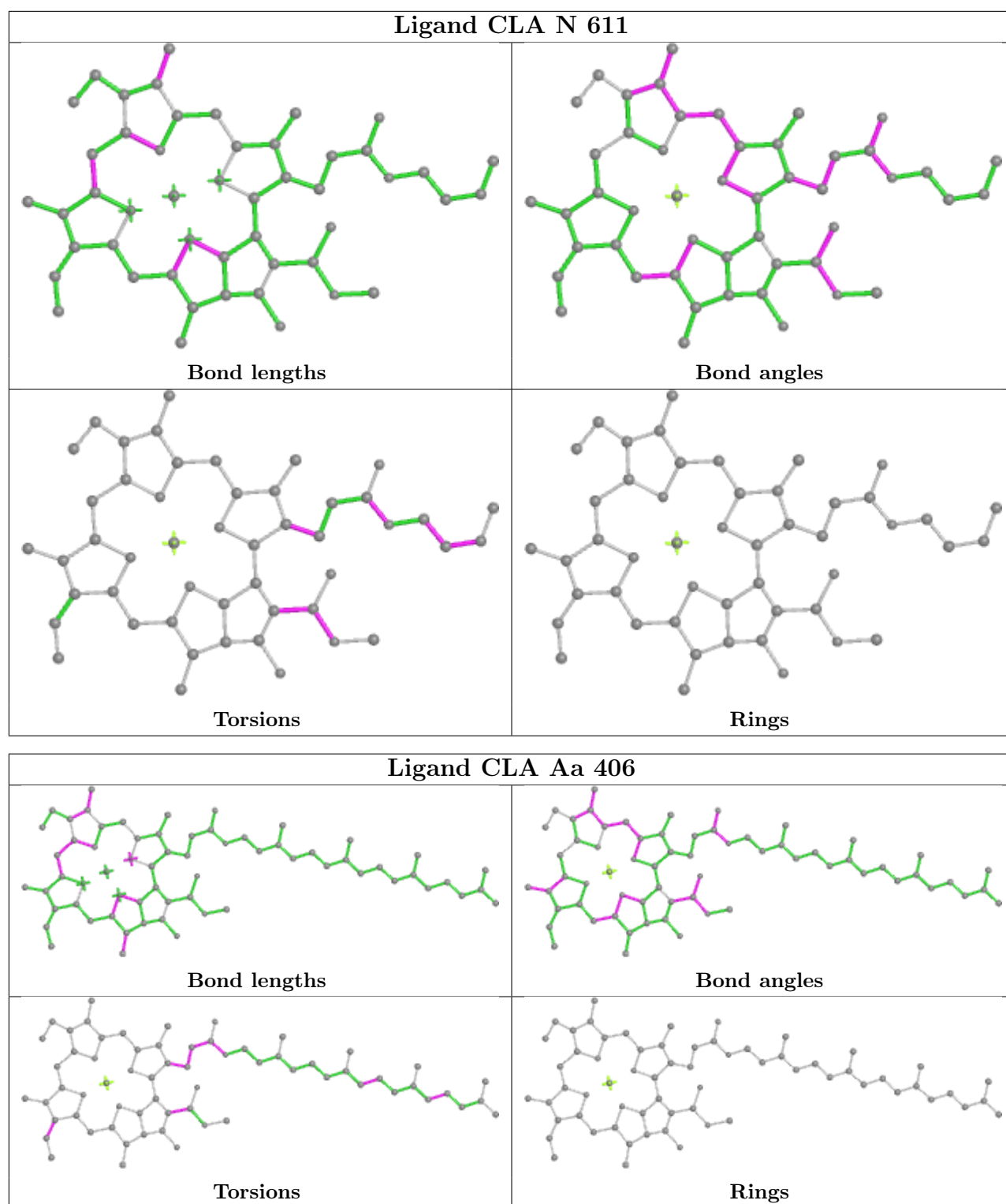
## Ligand CLA s 608



## Ligand NEX Yy 617

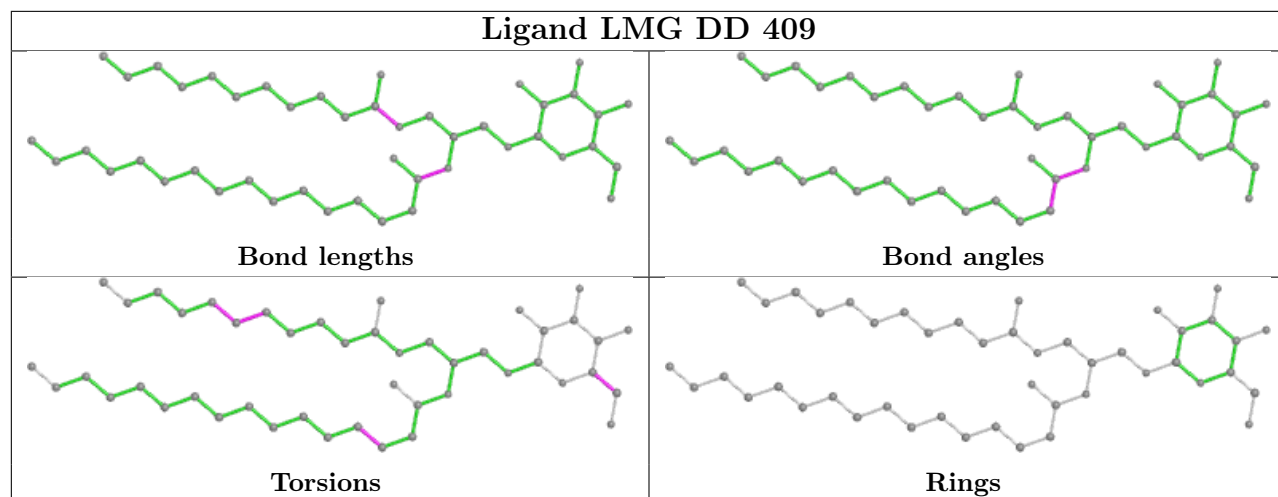




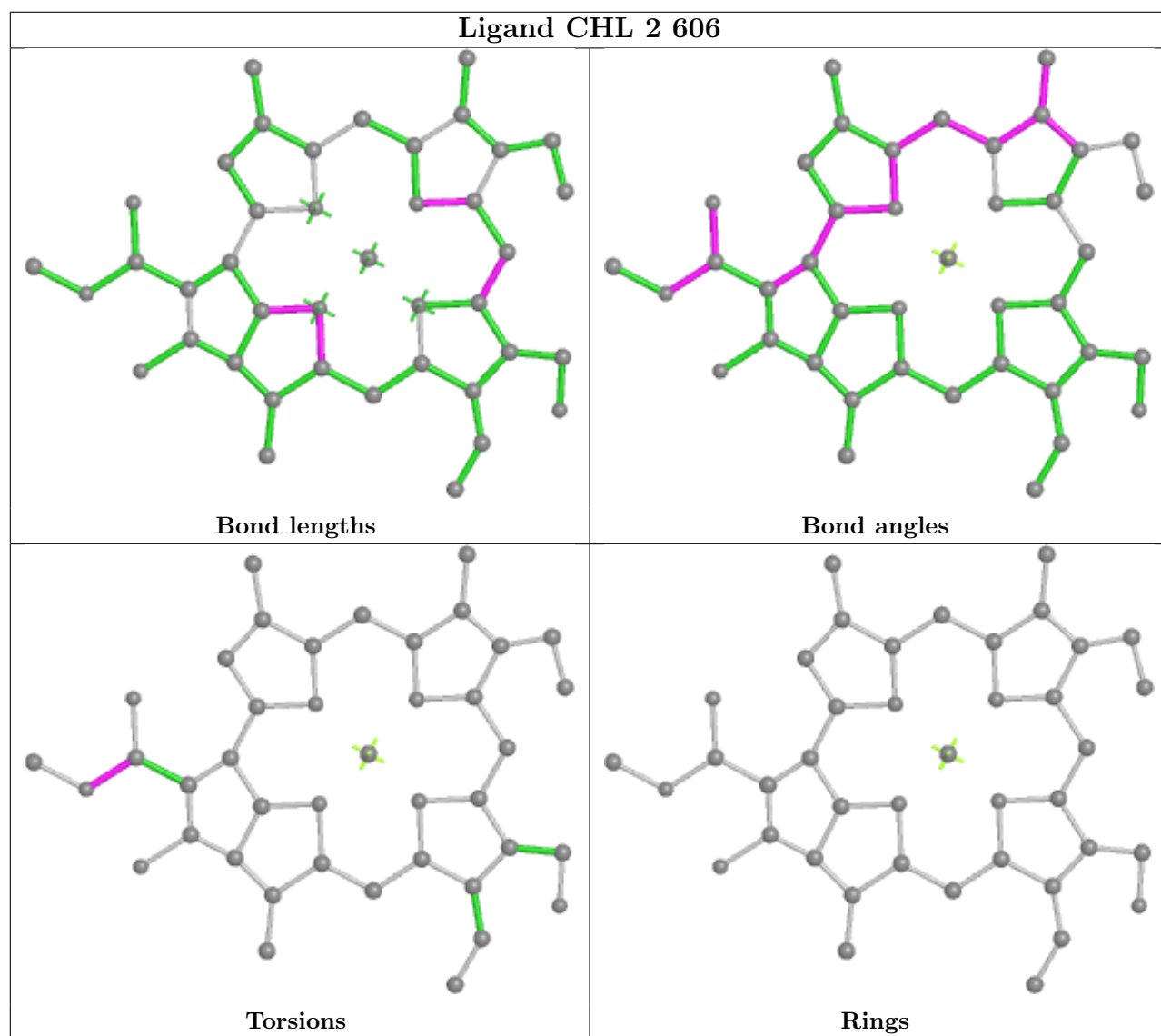




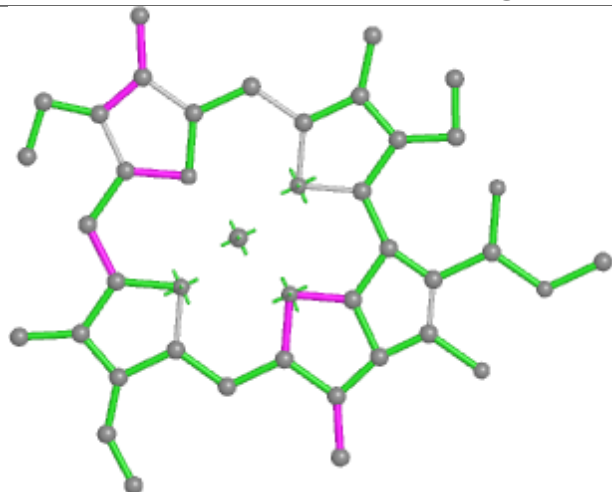
## Ligand LMG DD 409



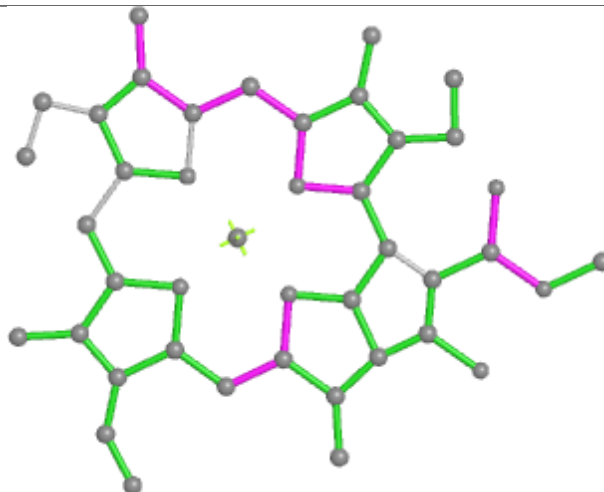
## Ligand CHL 2 606



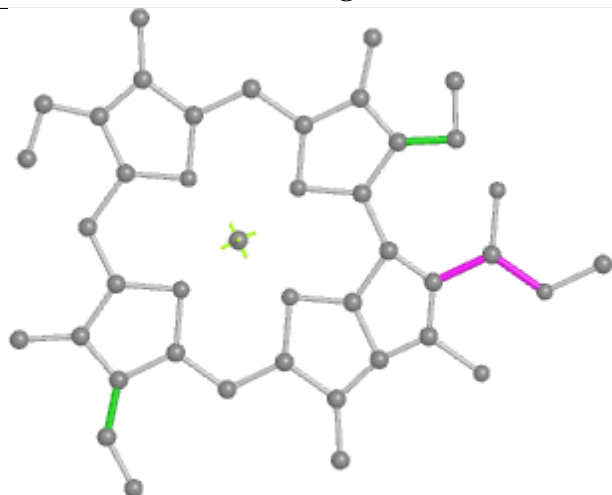
## Ligand CLA GG 604



Bond lengths



Bond angles

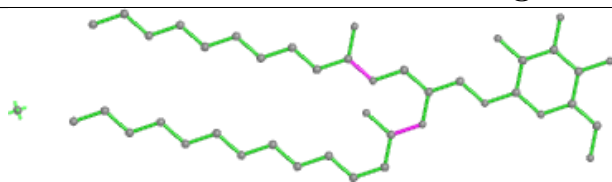


Torsions

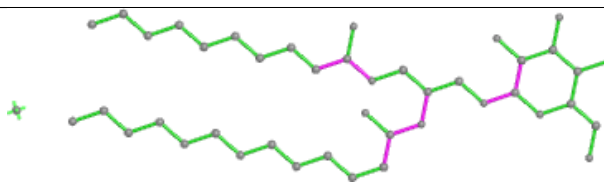


Rings

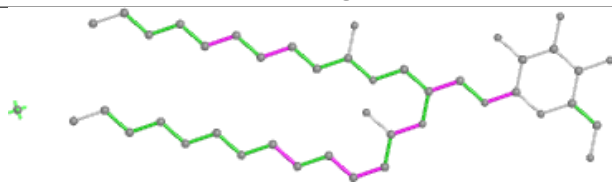
## Ligand LMG a 412



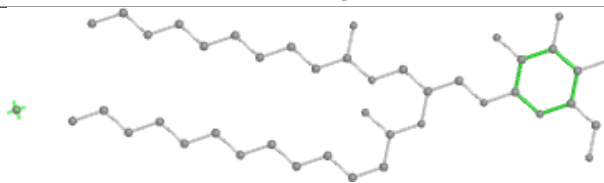
Bond lengths



Bond angles

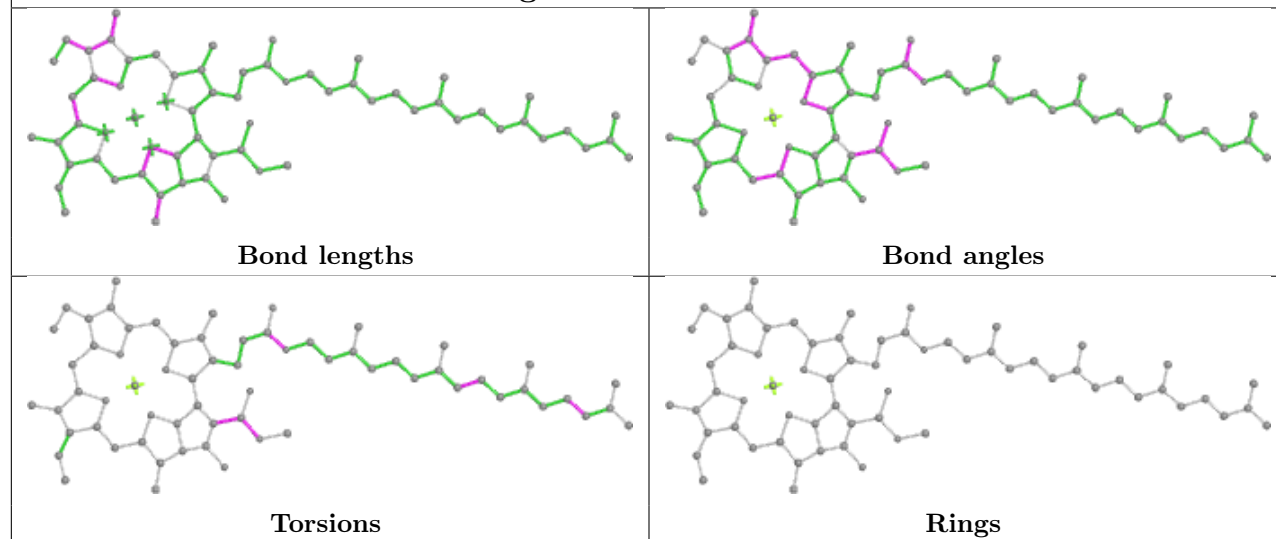


Torsions

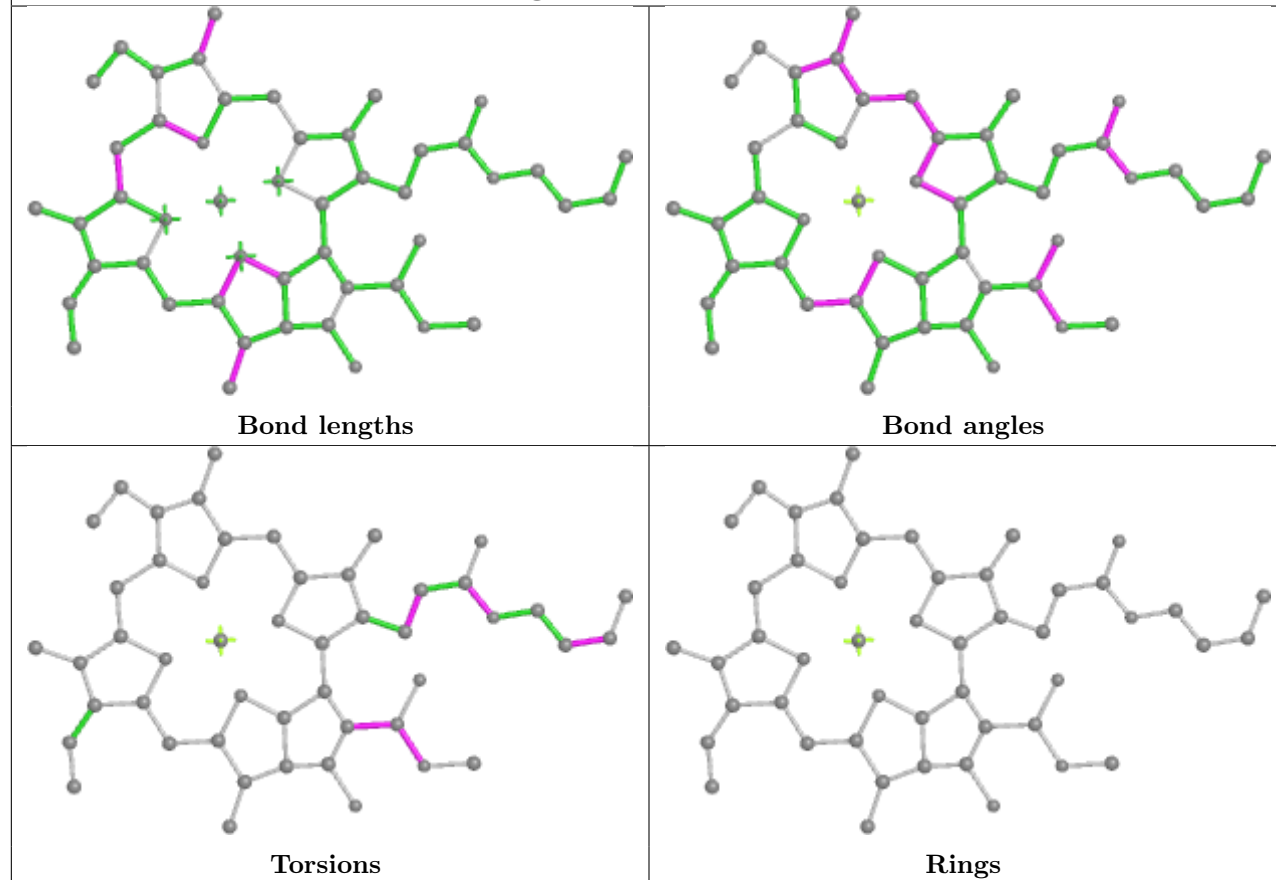


Rings

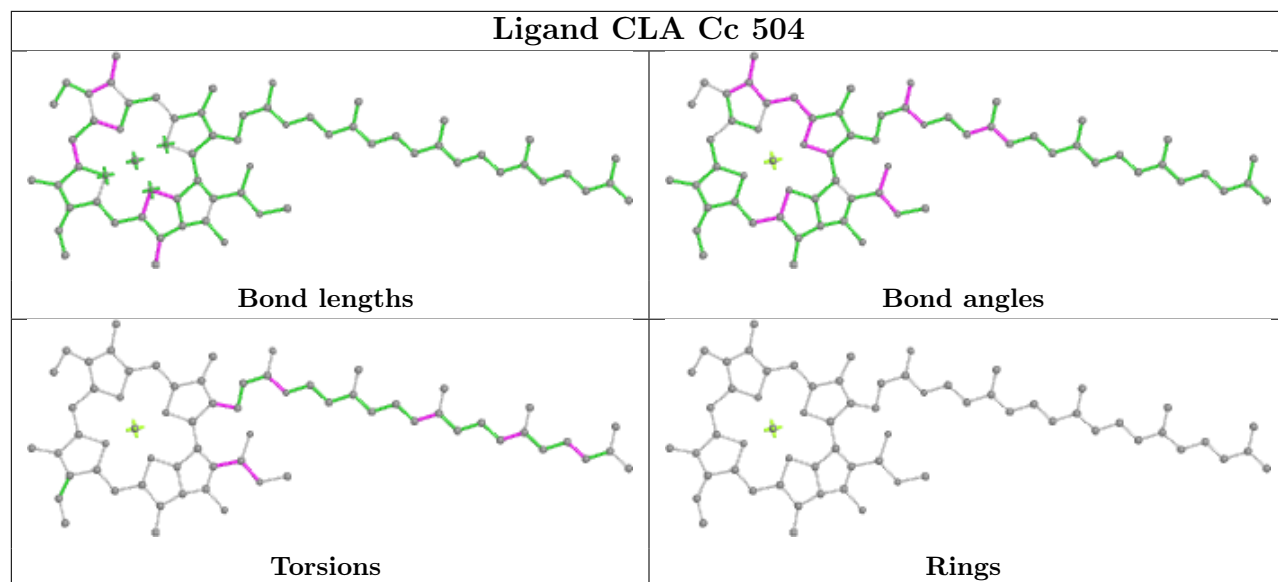
## Ligand CLA CC 505



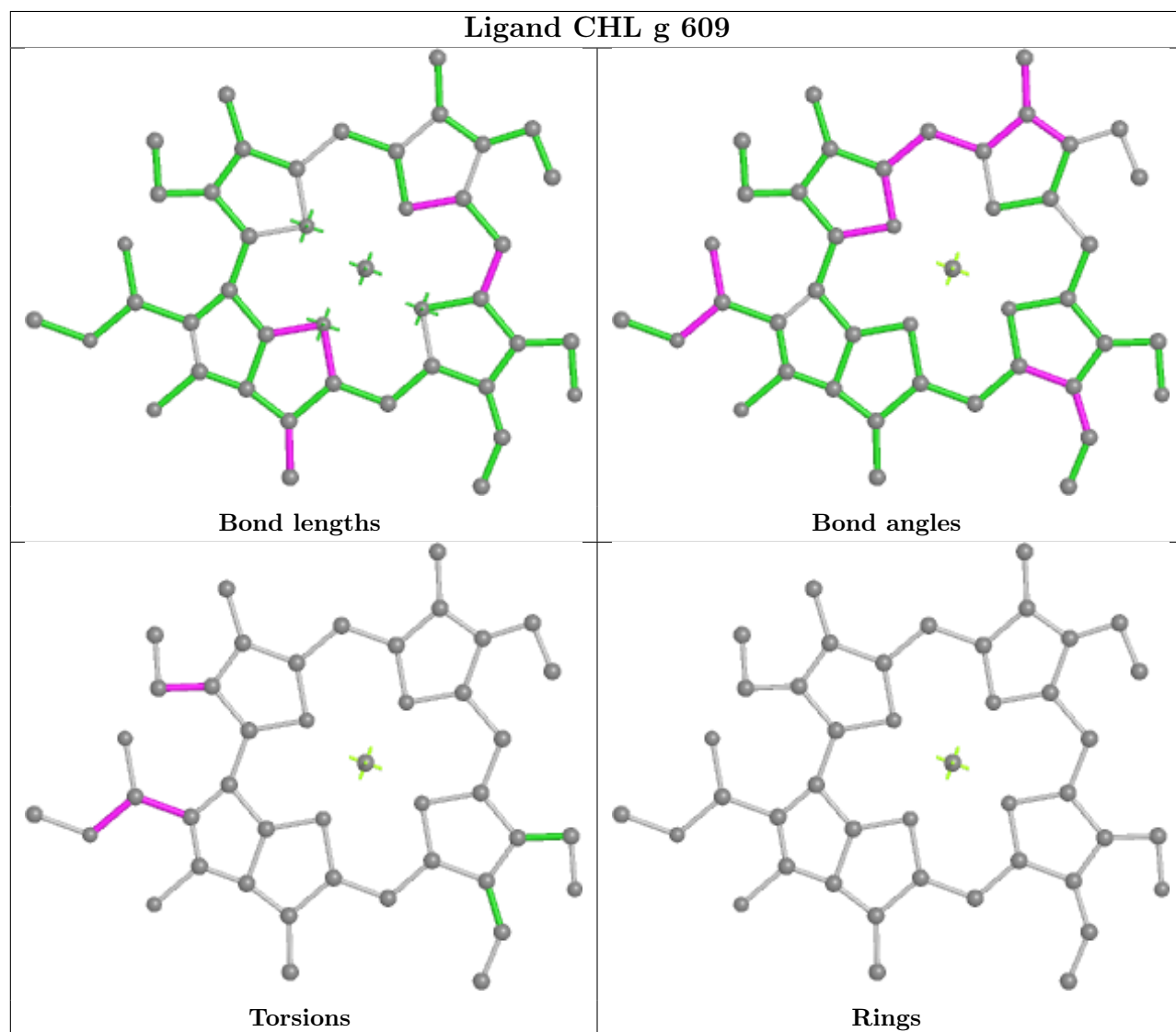
## Ligand CLA Ss 613



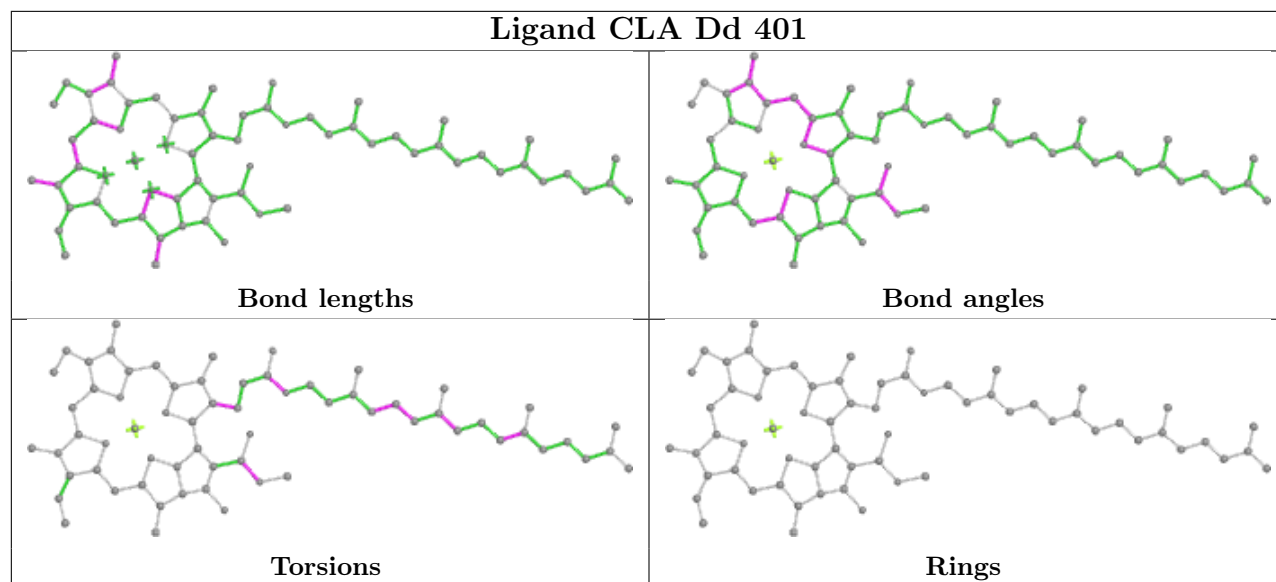
## Ligand CLA Cc 504



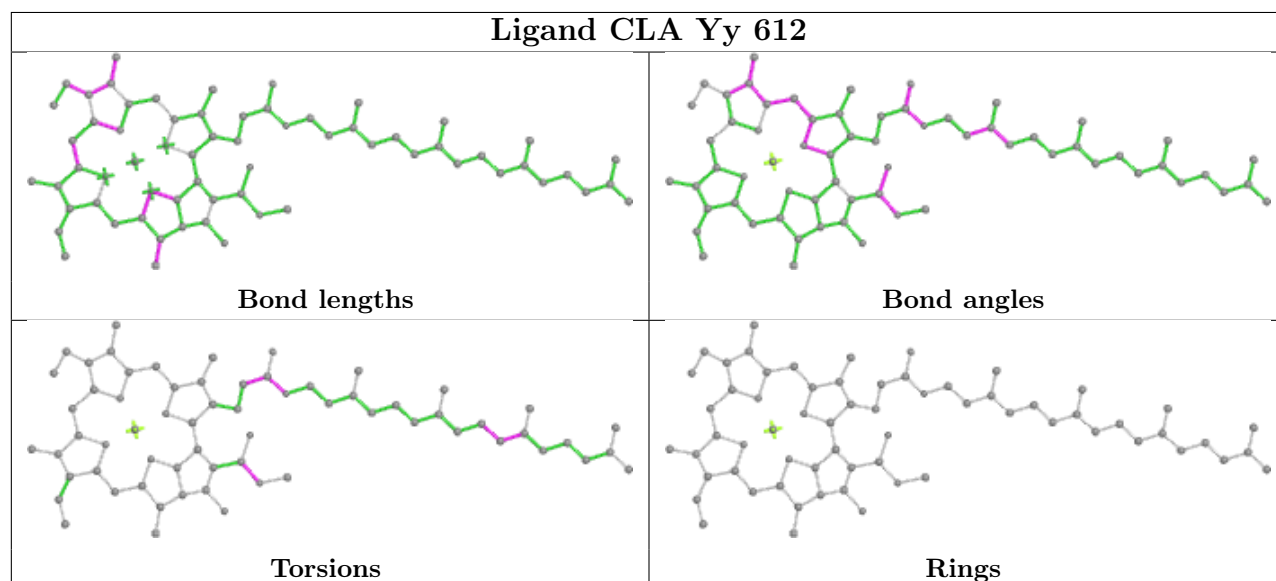
## Ligand CHL g 609



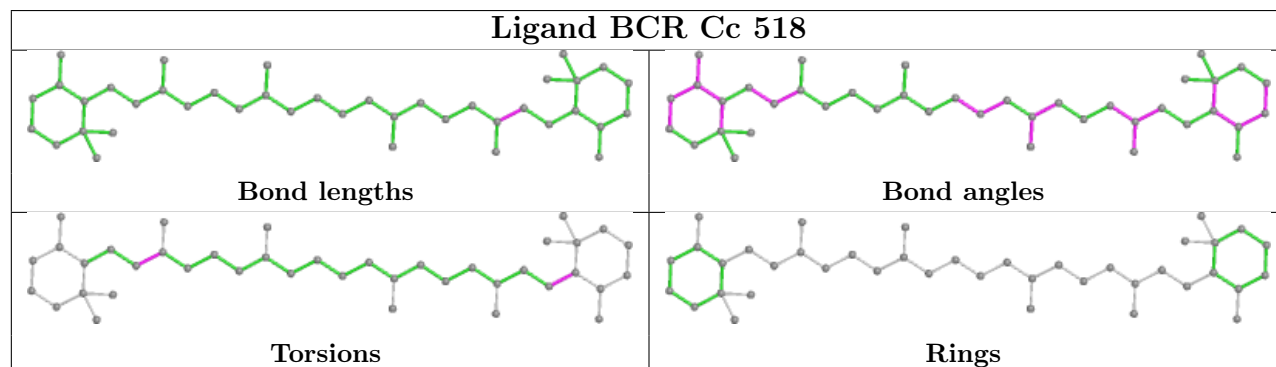
## Ligand CLA Dd 401



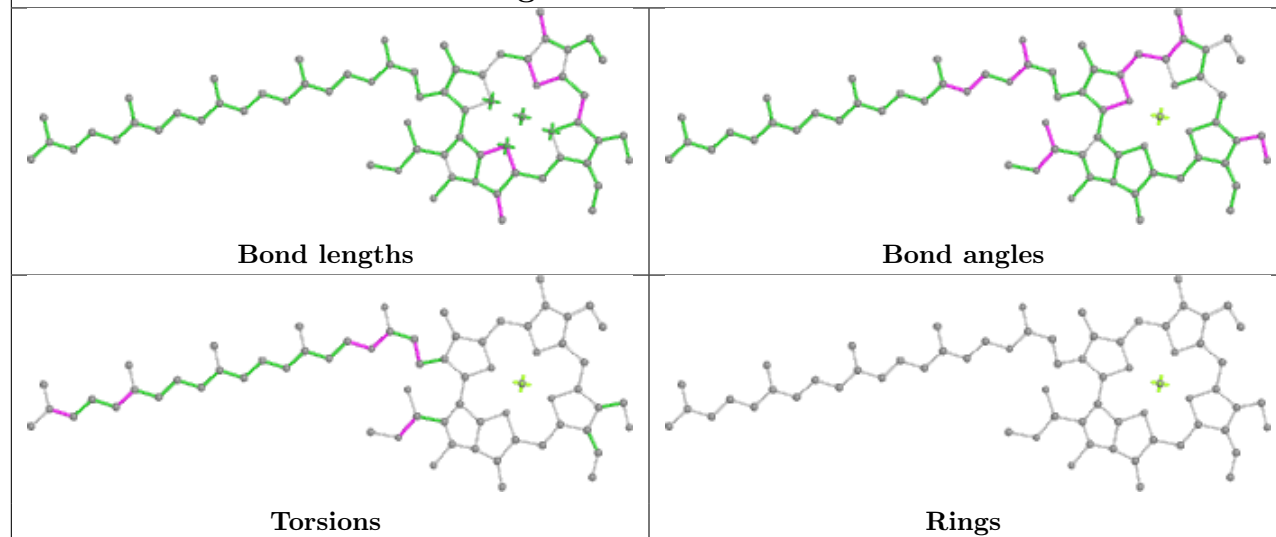
## Ligand CLA Yy 612



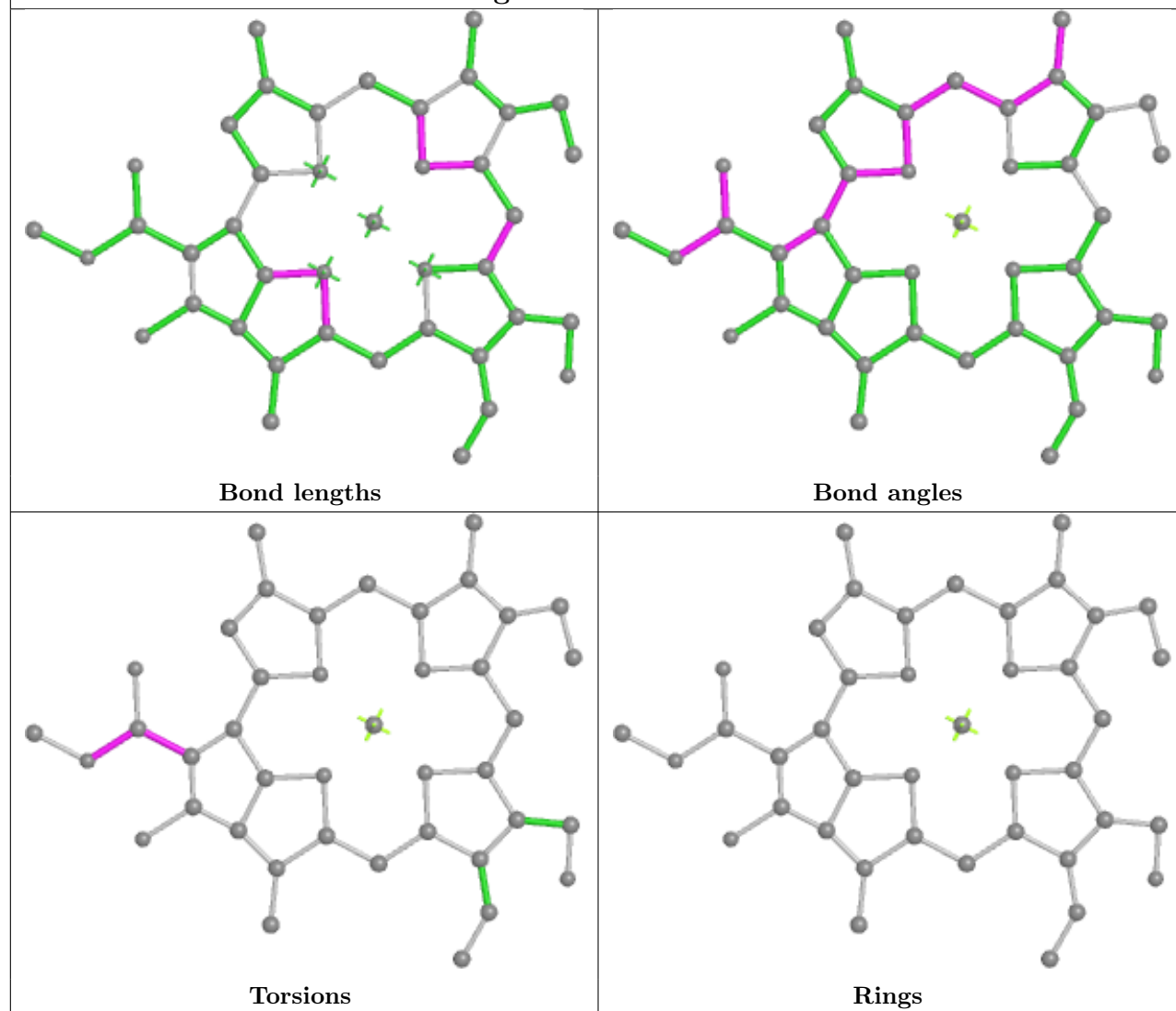
## Ligand BCR Cc 518

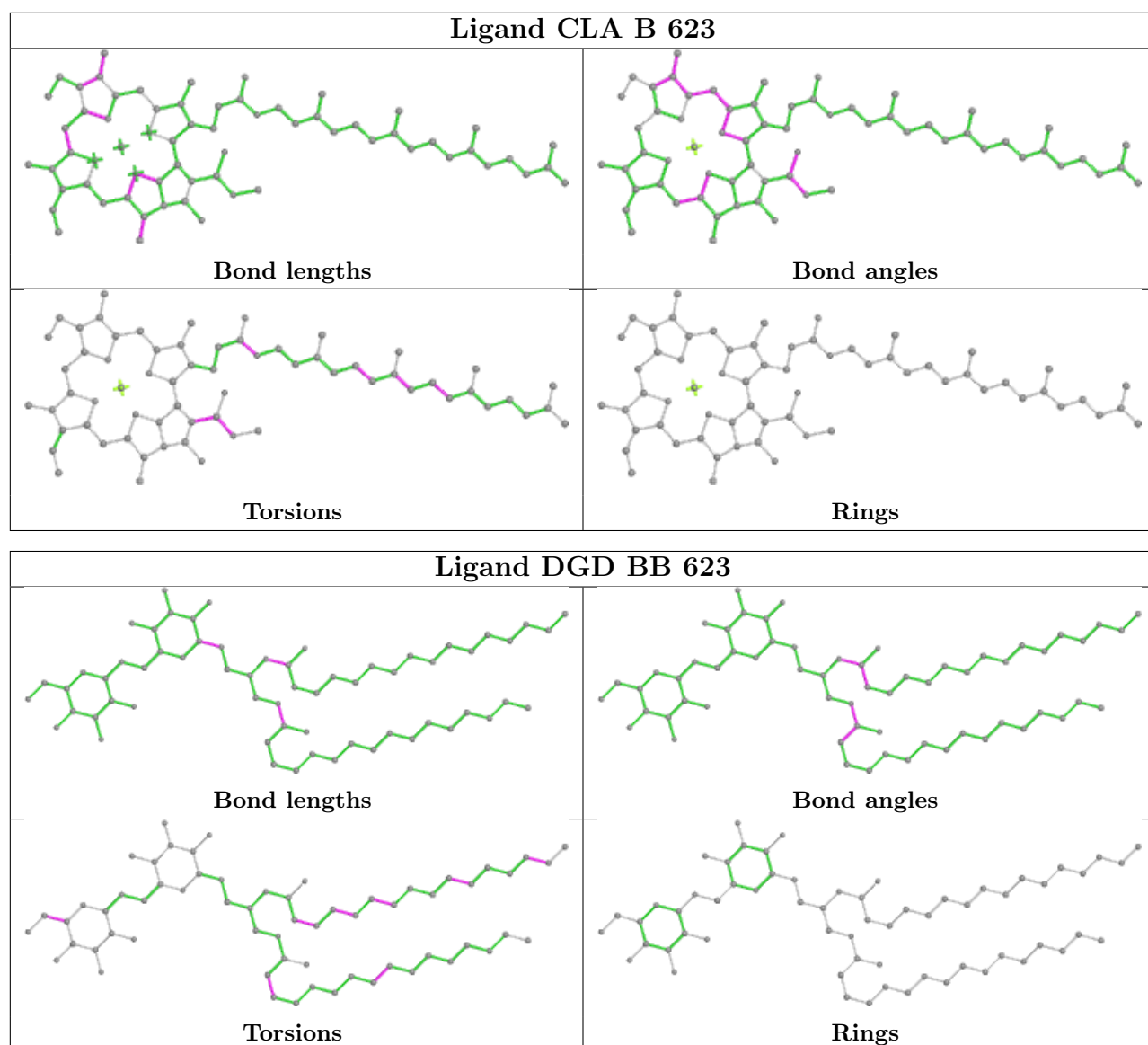


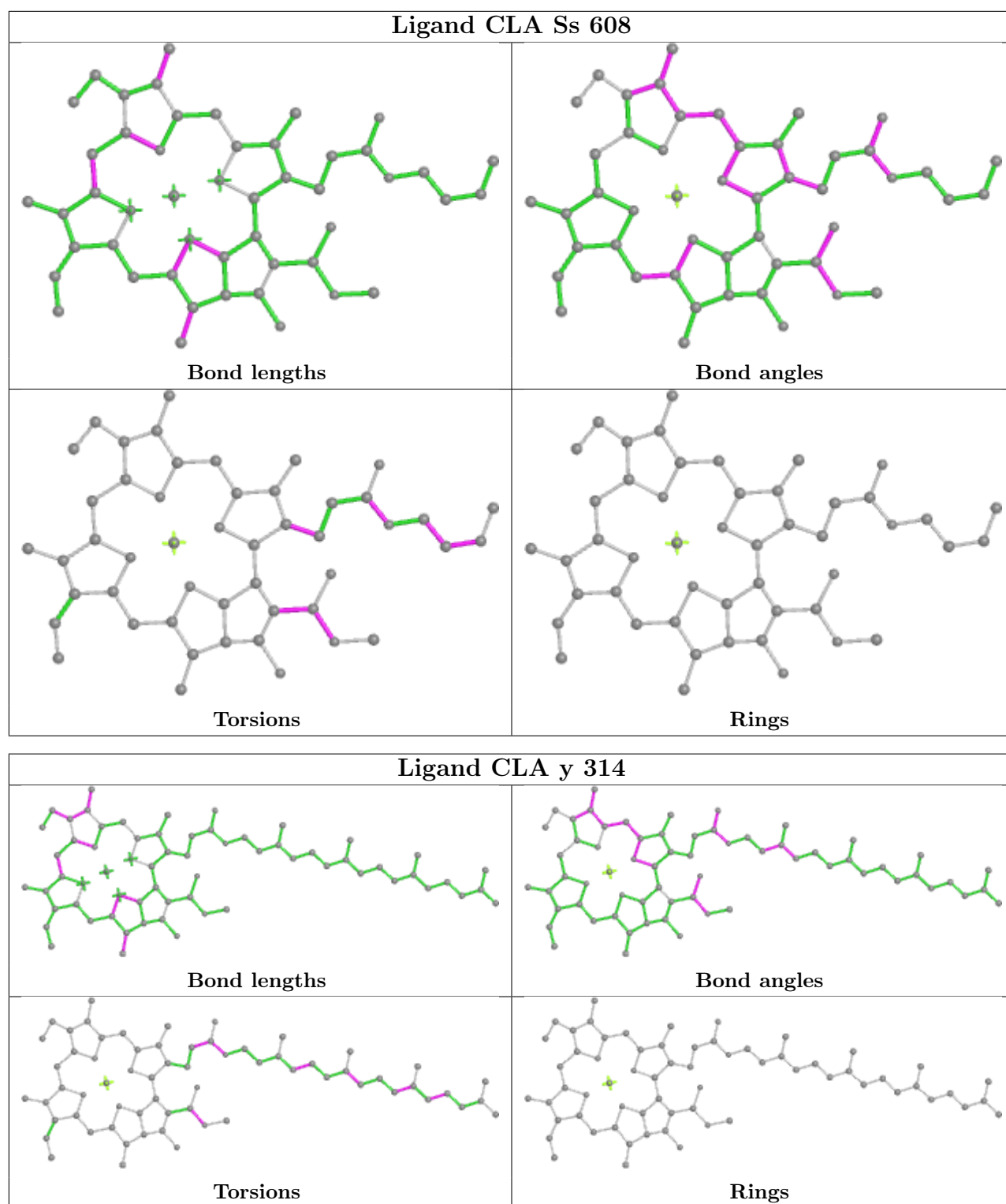
## Ligand CHL YY 609



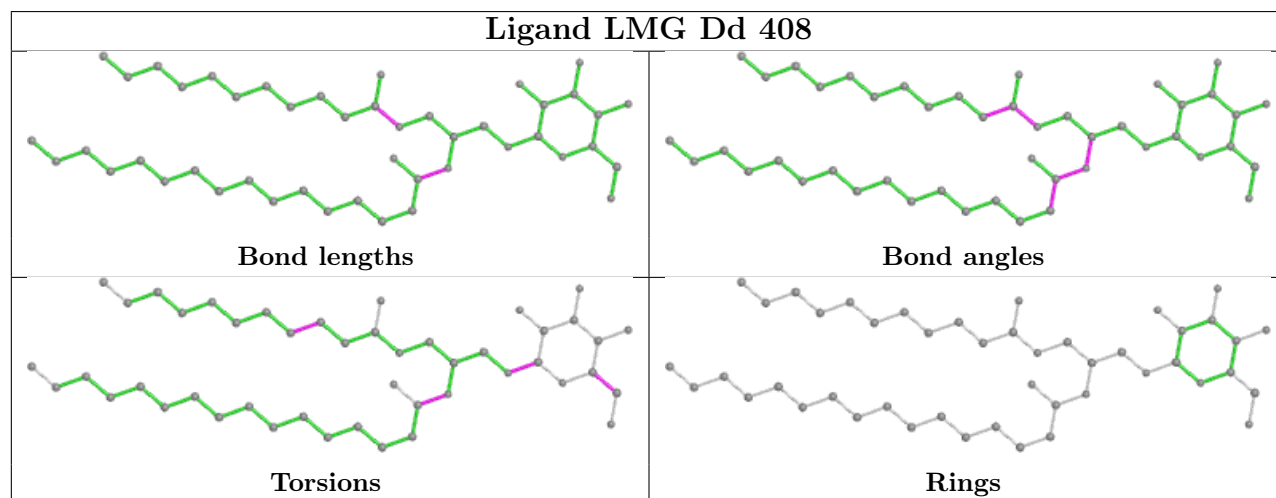
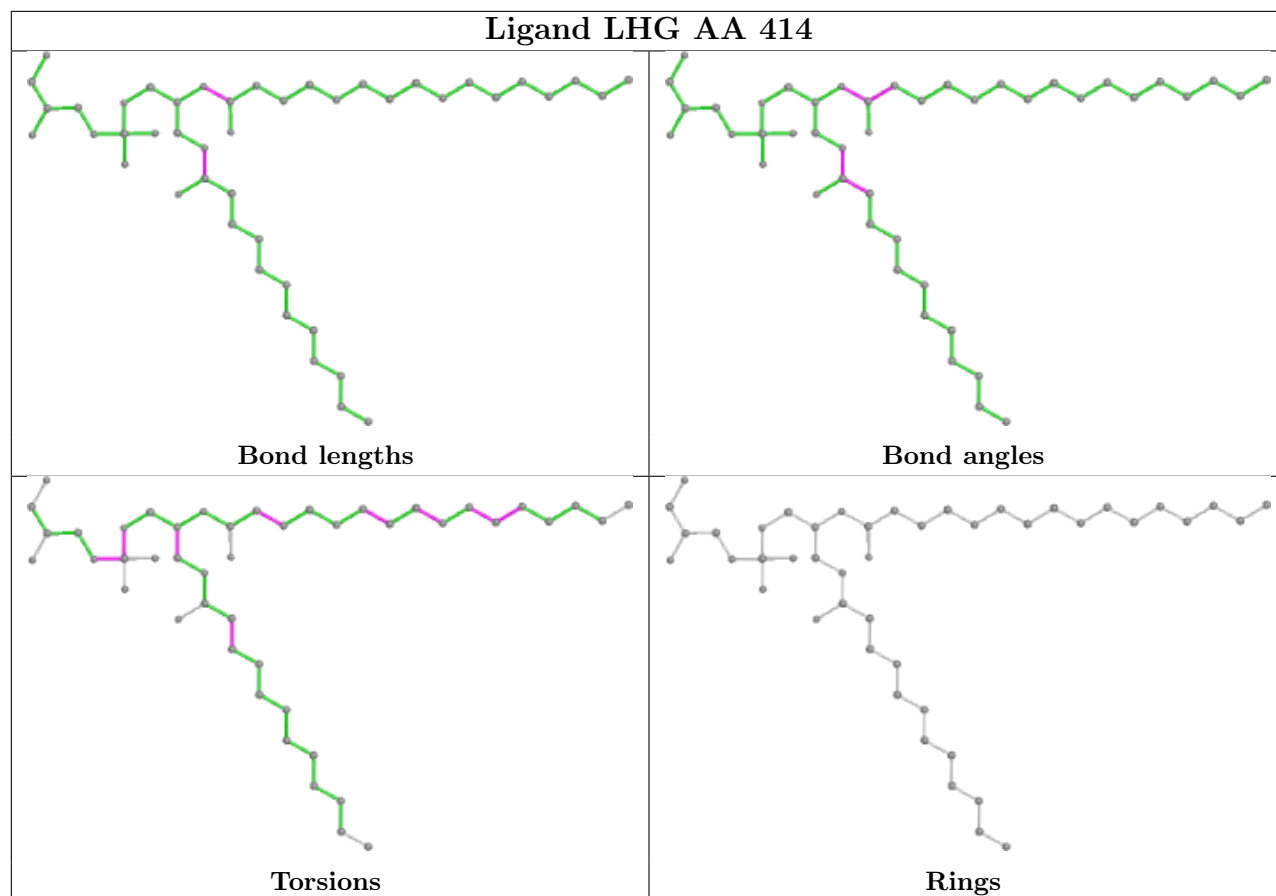
## Ligand CHL 2 607

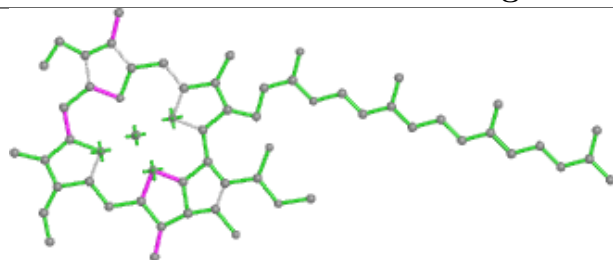




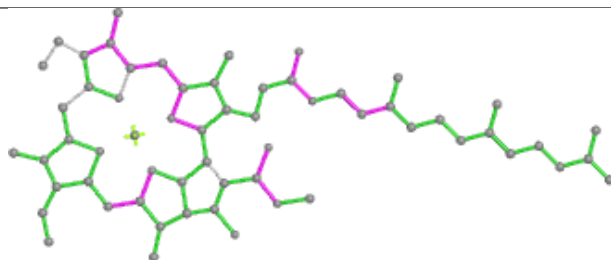




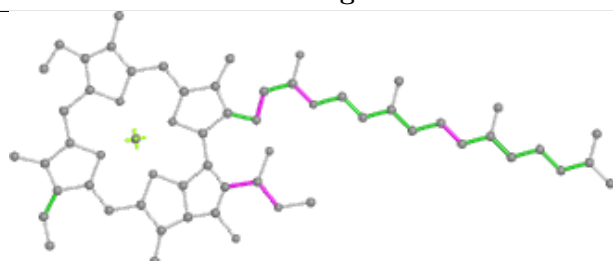


**Ligand CLA BB 613**

Bond lengths



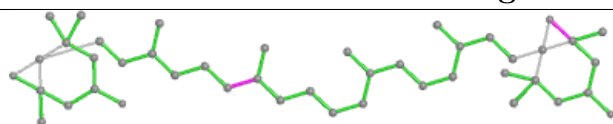
Bond angles



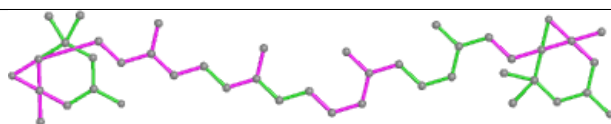
Torsions



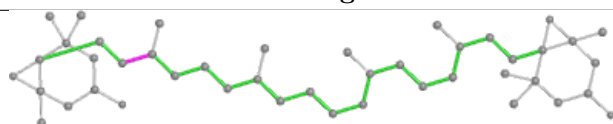
Rings

**Ligand XAT GG 617**

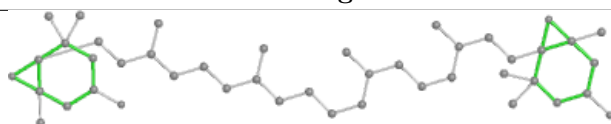
Bond lengths



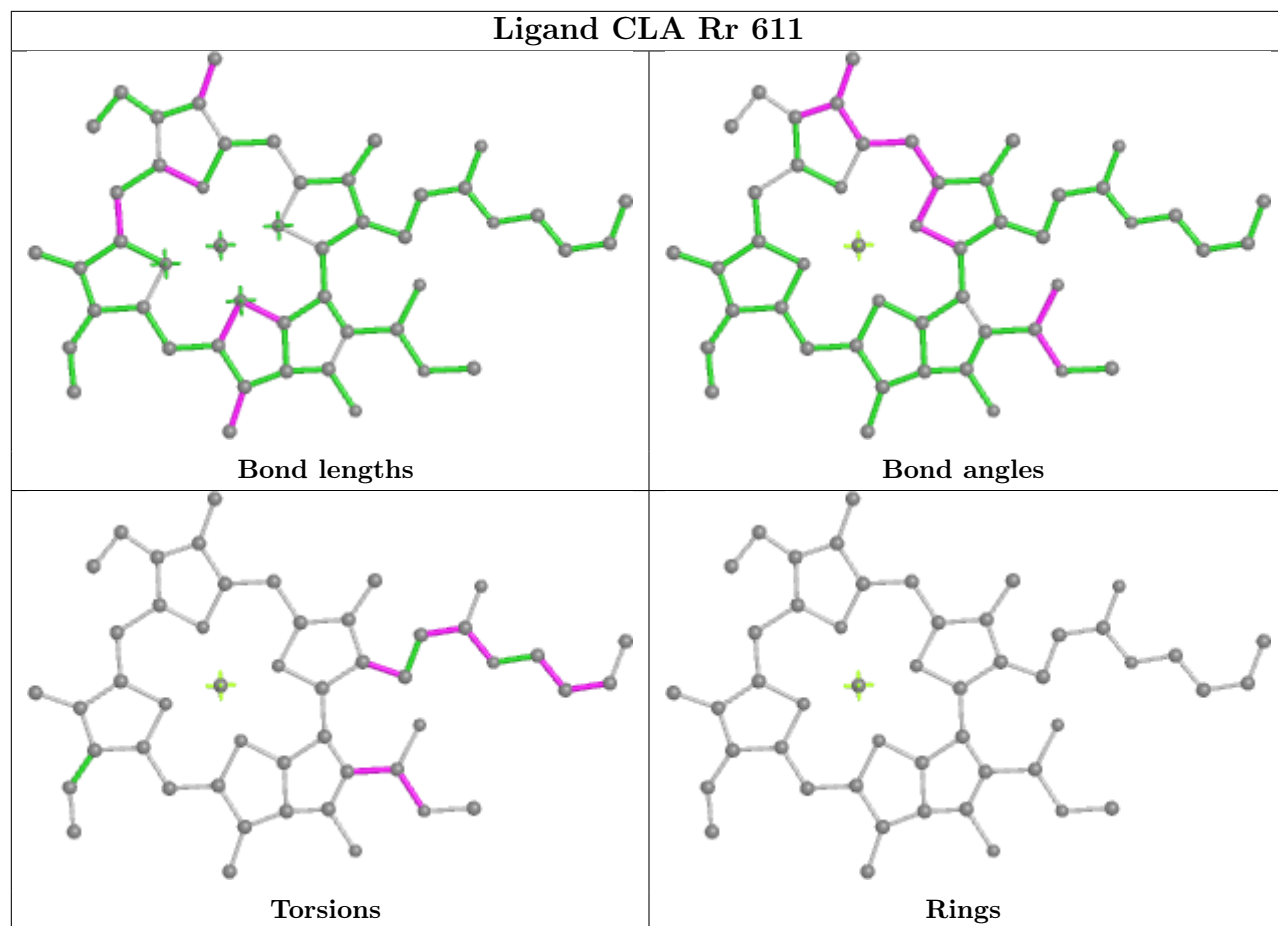
Bond angles



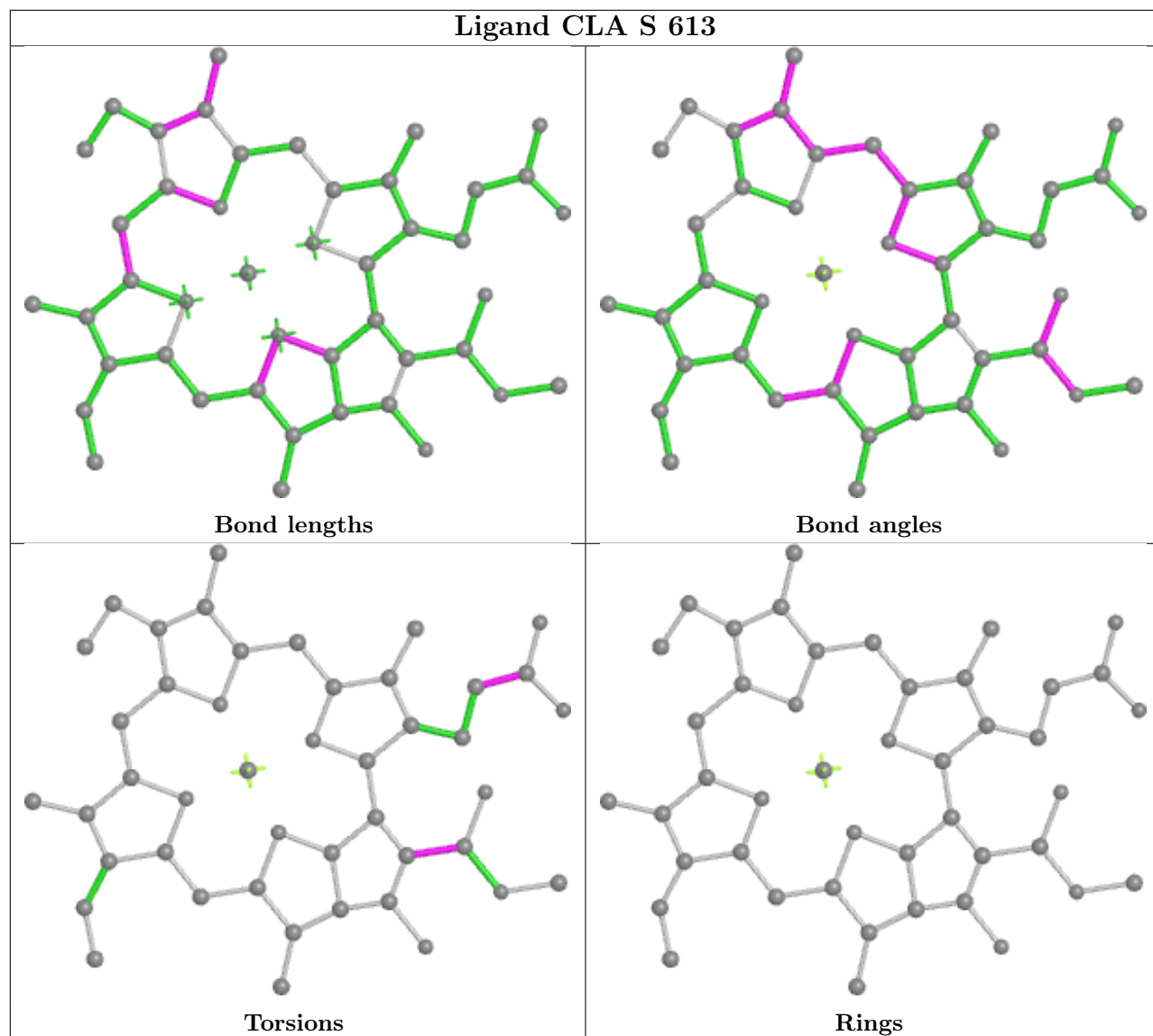
Torsions



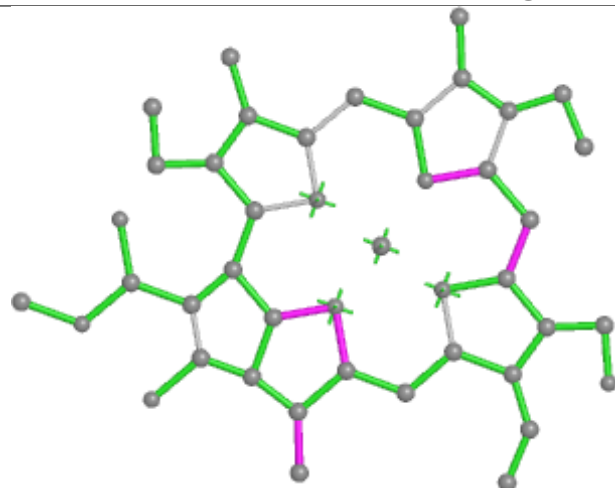
Rings



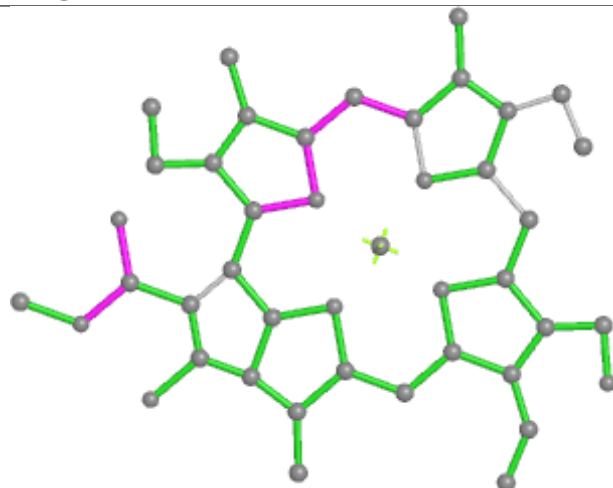
## Ligand CLA S 613



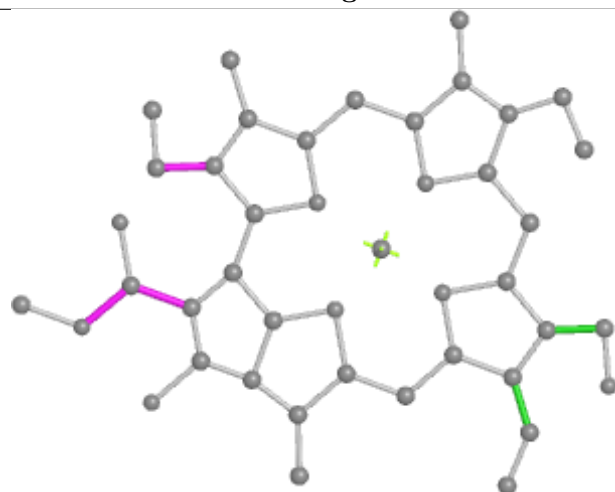
## Ligand CHL g 606



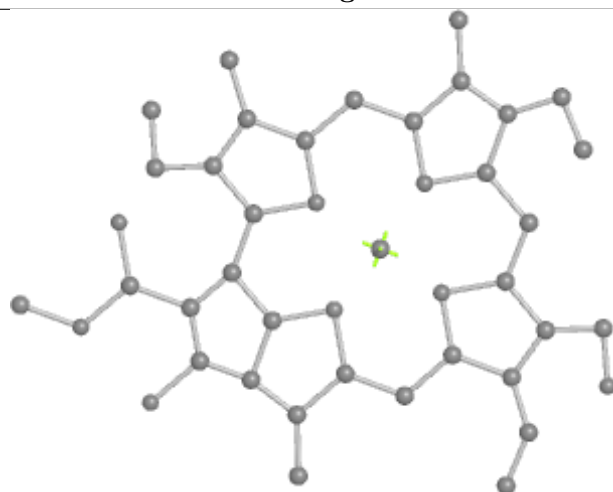
Bond lengths



Bond angles

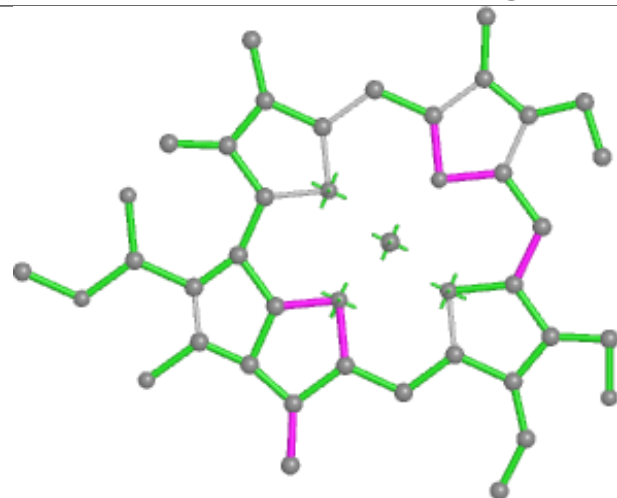


Torsions

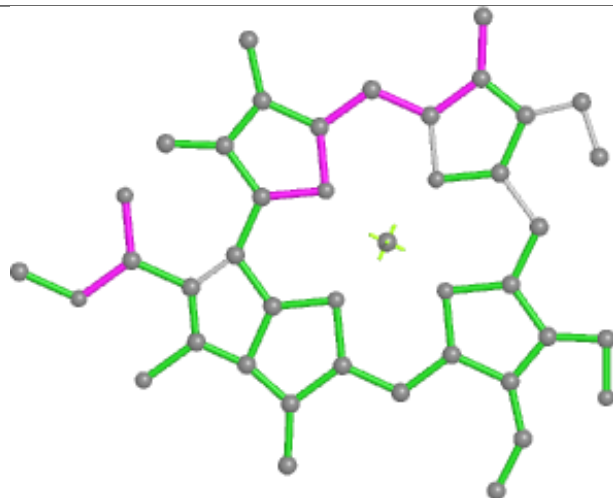


Rings

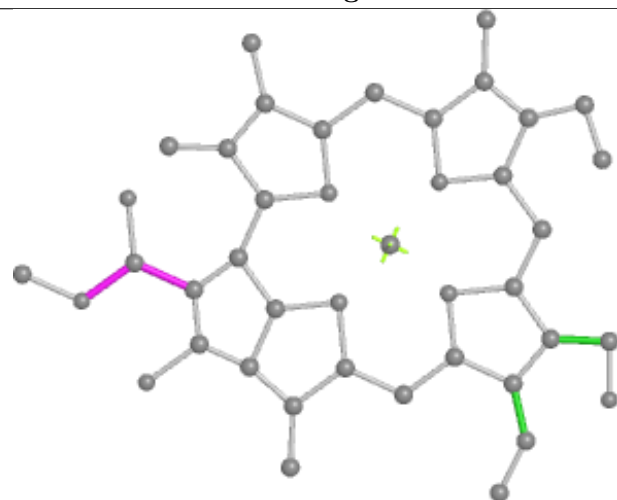
## Ligand CHL NN 608



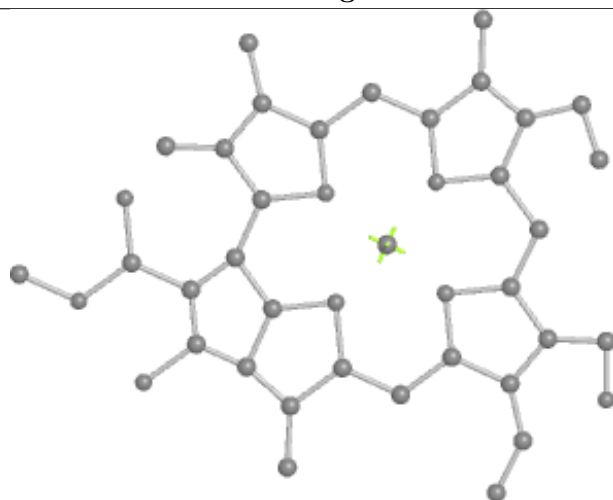
Bond lengths



Bond angles

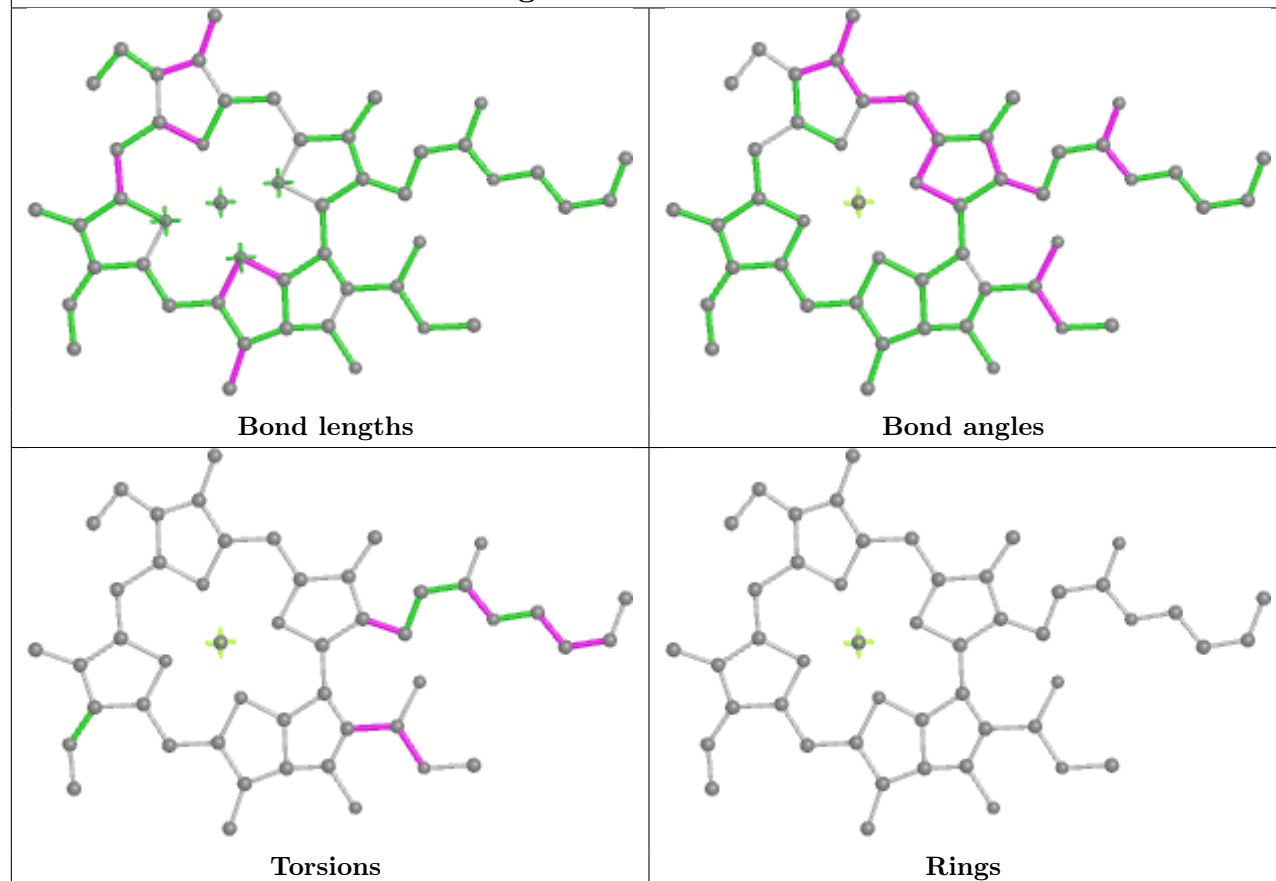


Torsions

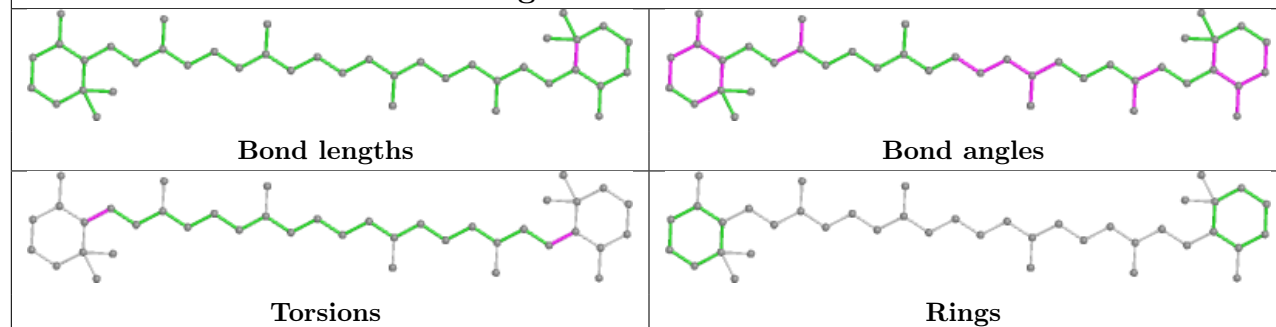


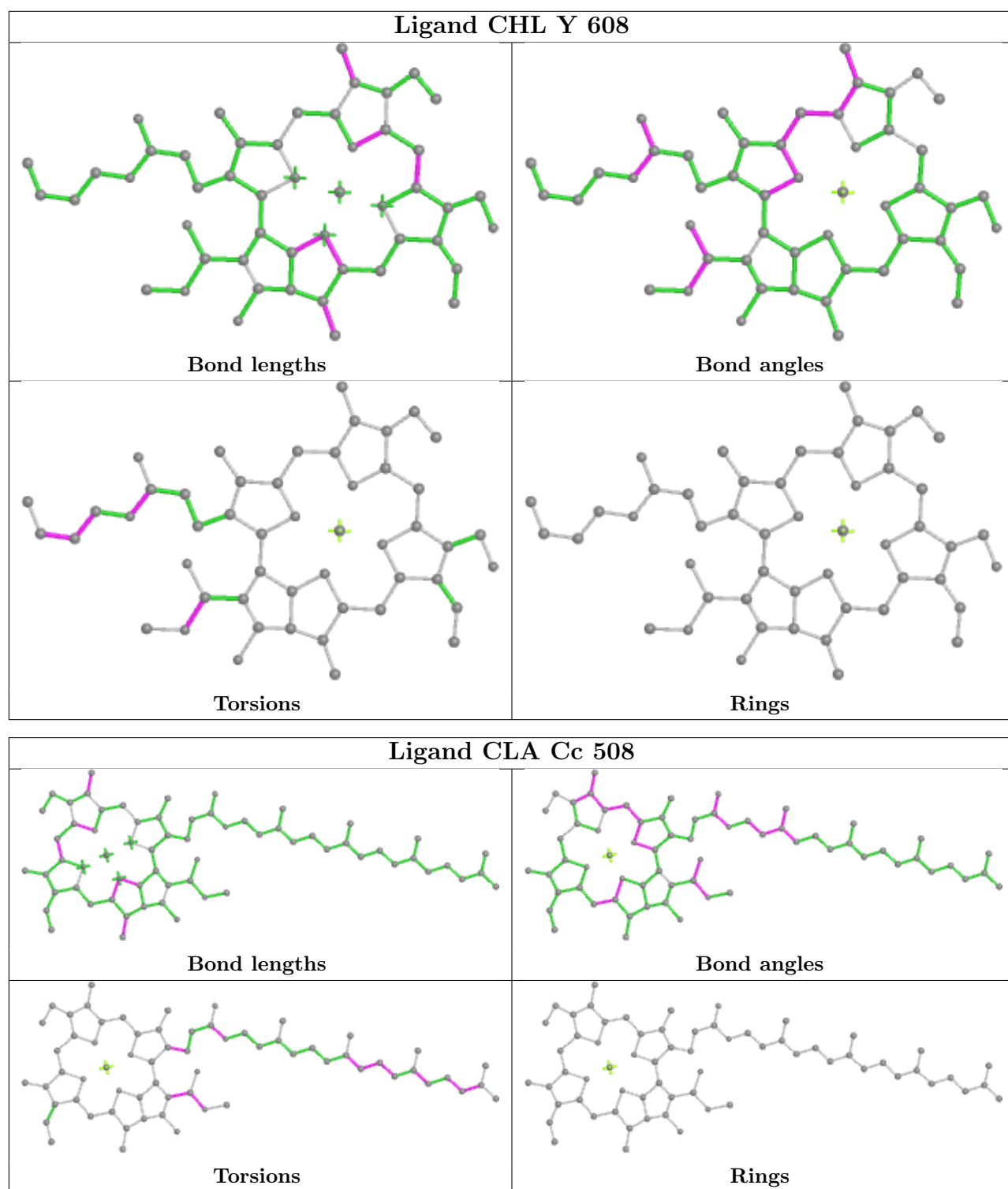
Rings

## Ligand CLA YY 614



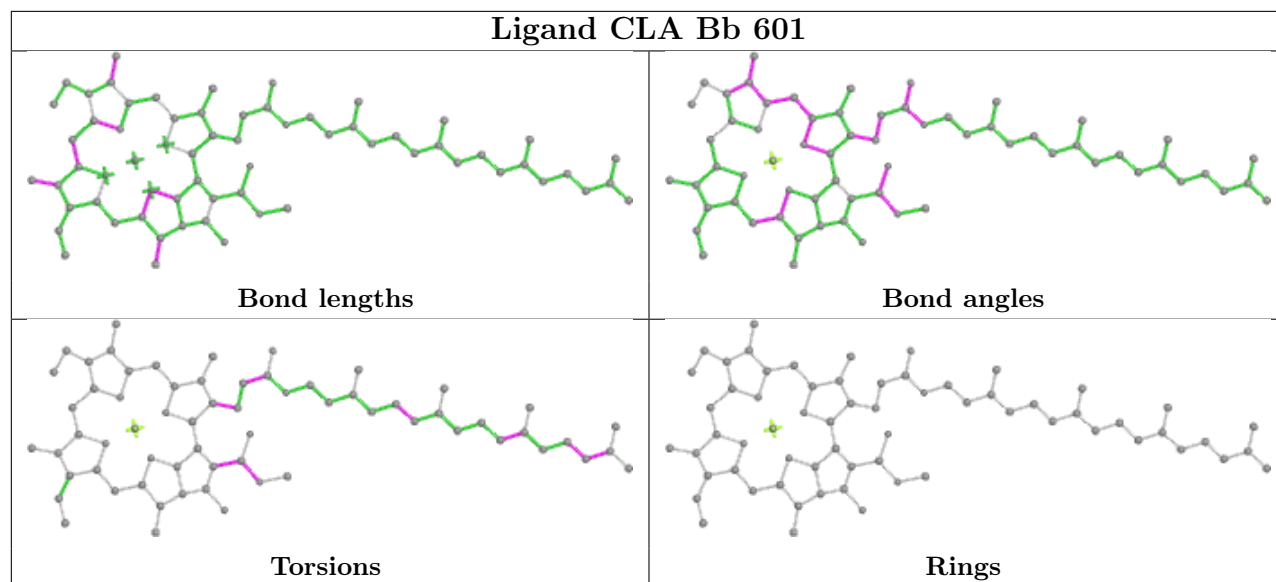
## Ligand BCR BB 616



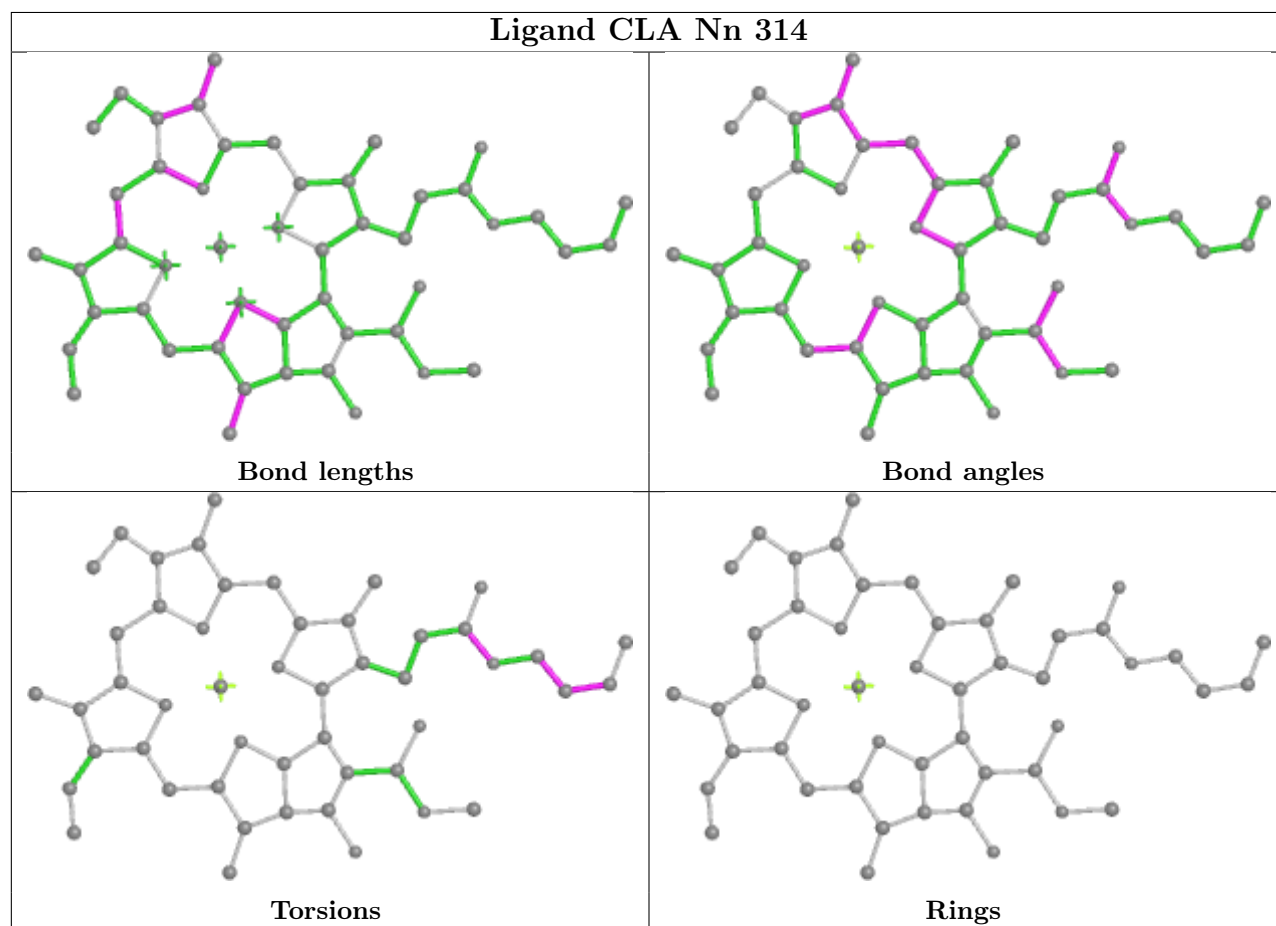




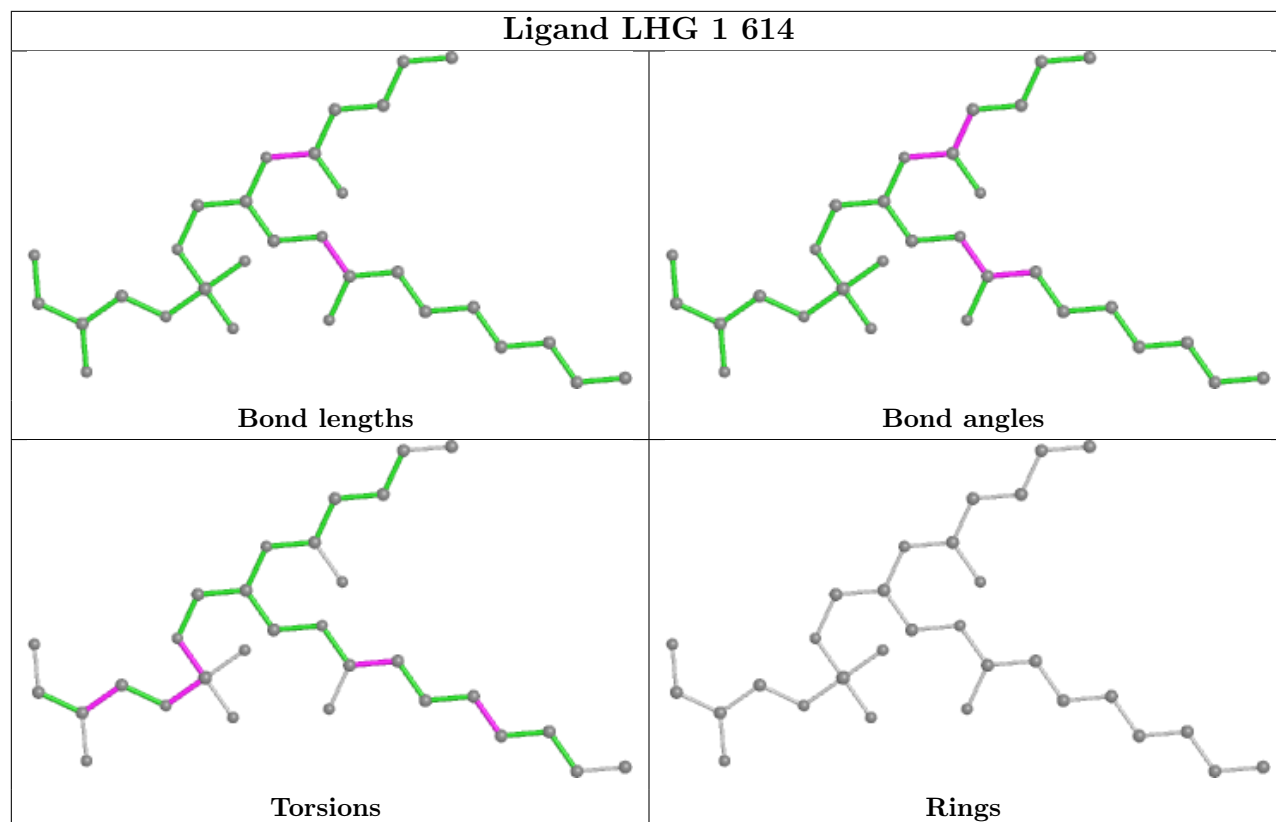
## Ligand CLA Bb 601



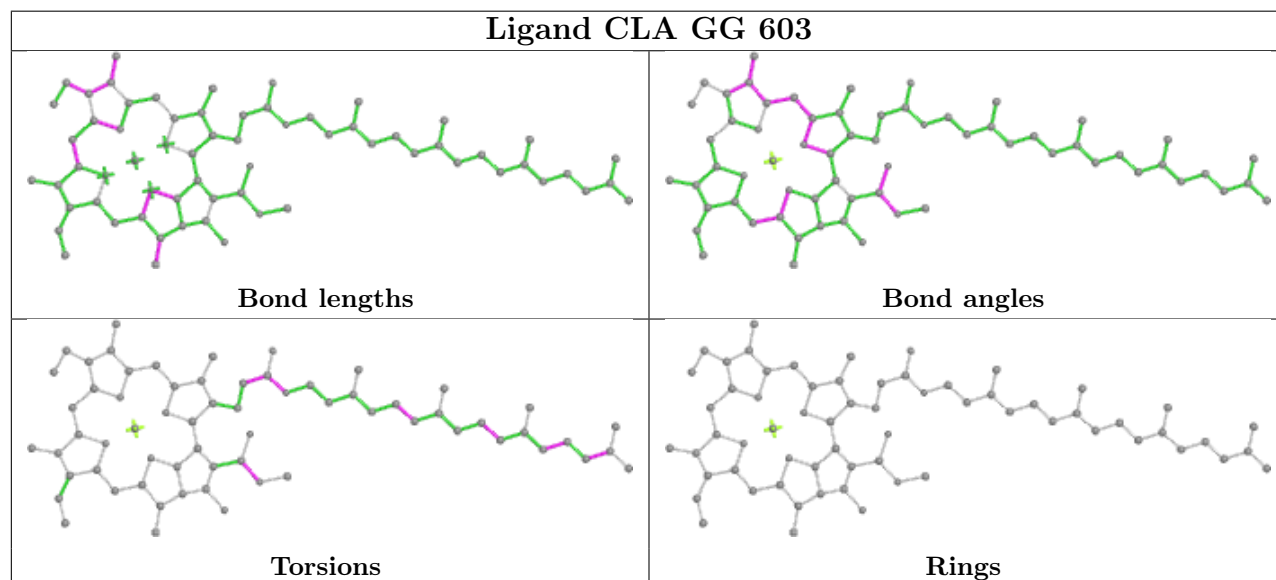
## Ligand CLA Nn 314



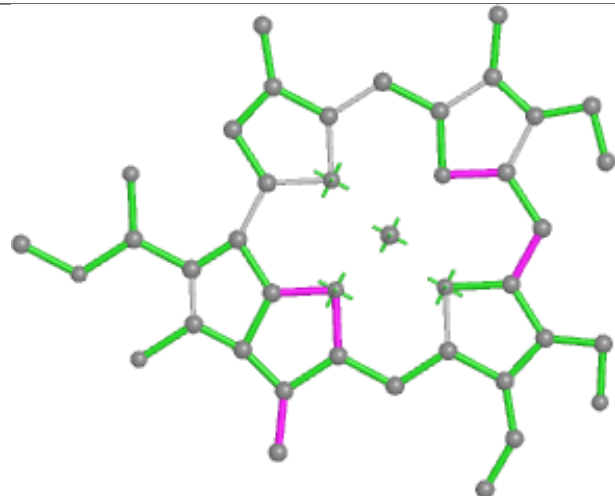
## Ligand LHG 1 614



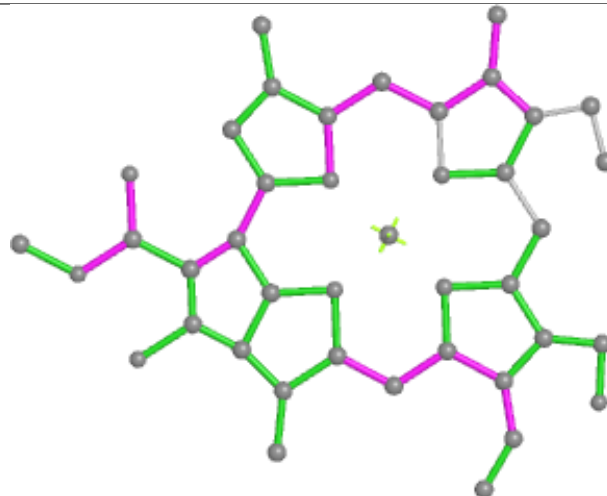
## Ligand CLA GG 603



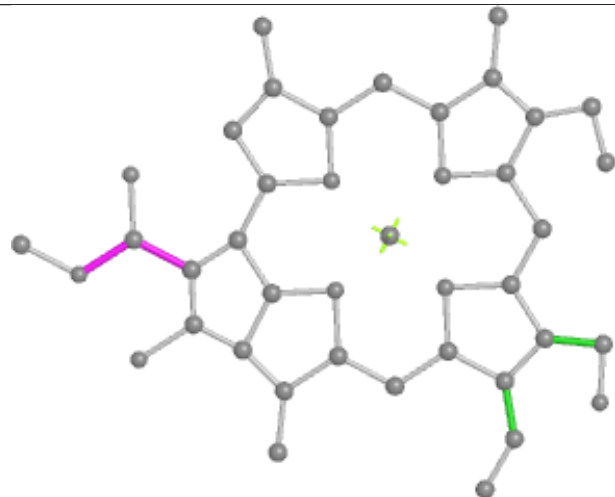
## Ligand CHL 1 608



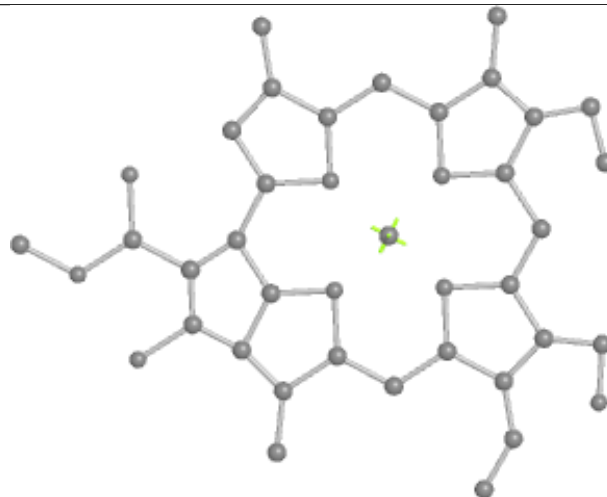
Bond lengths



Bond angles

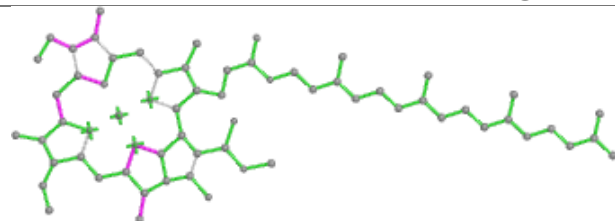


Torsions

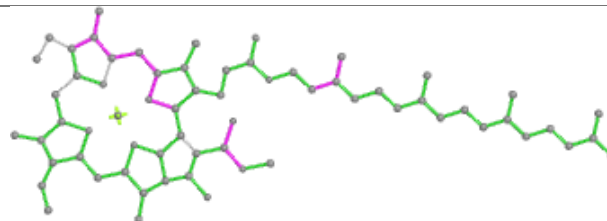


Rings

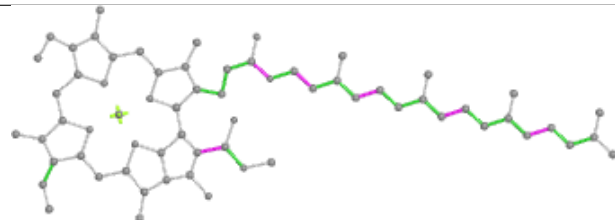
## Ligand CLA C 514



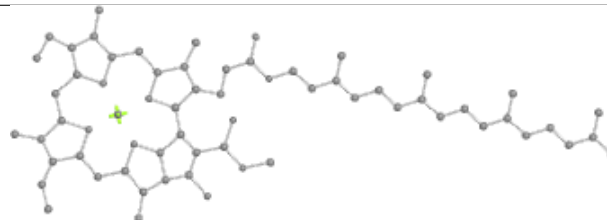
Bond lengths



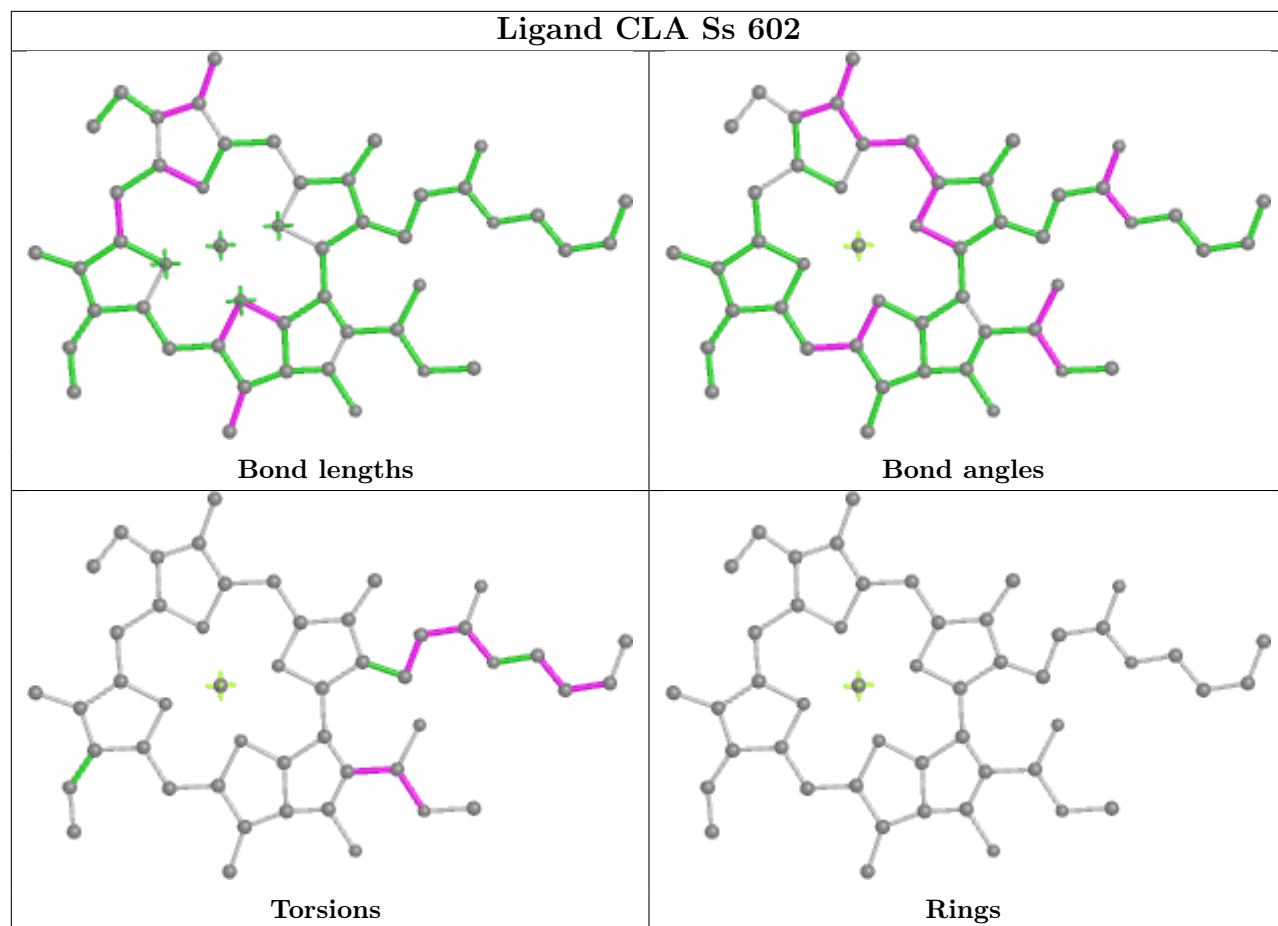
Bond angles

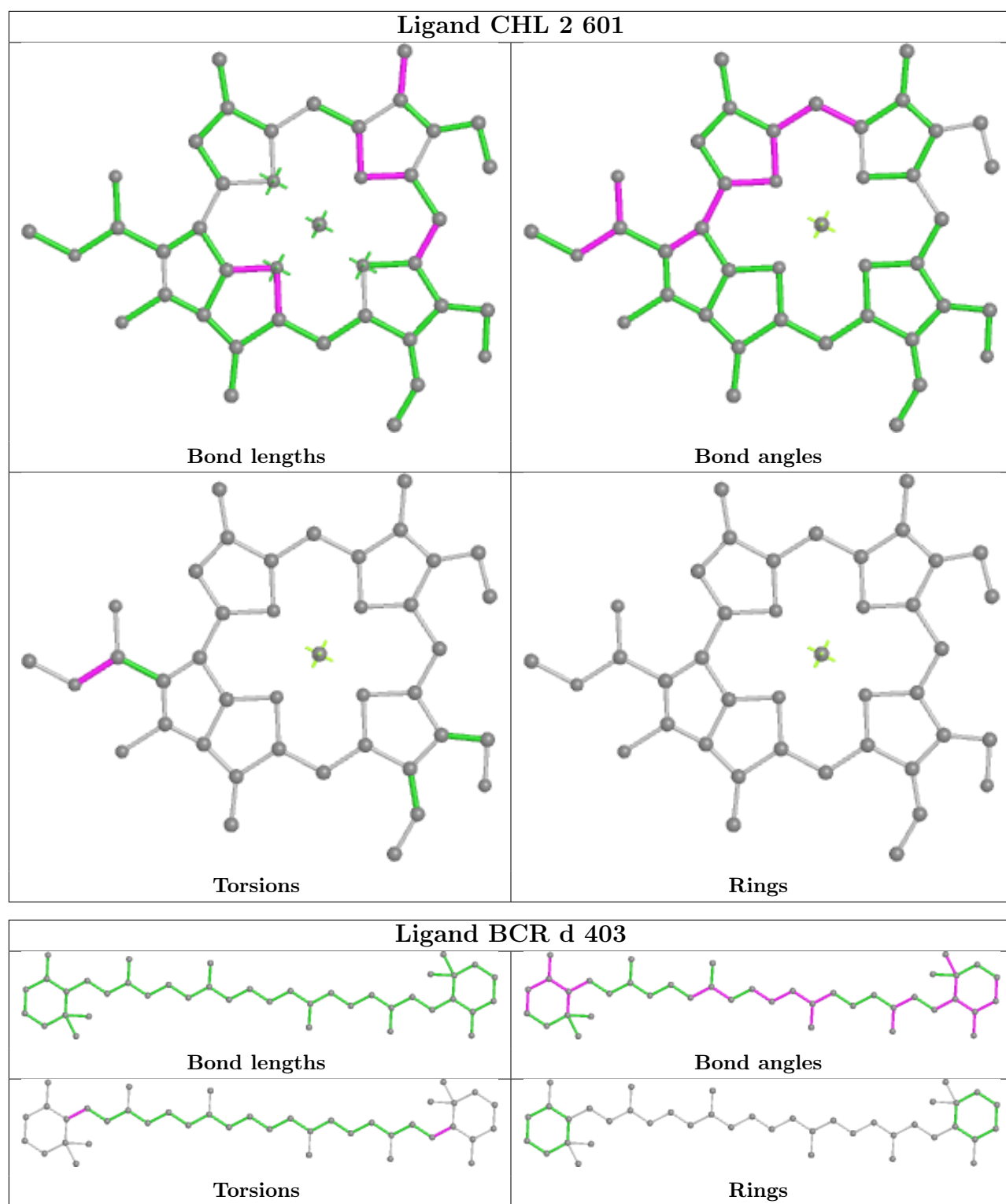


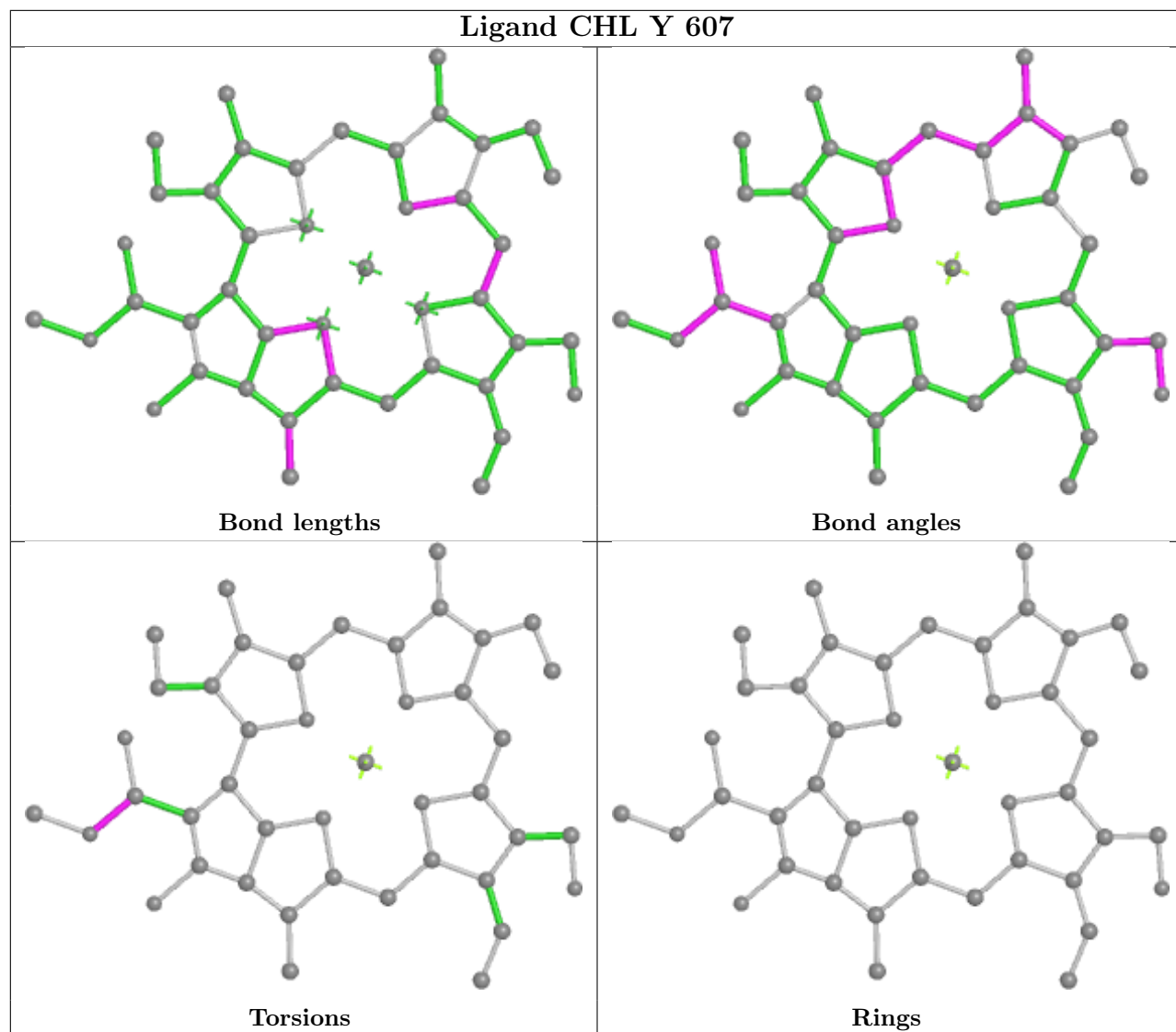
Torsions



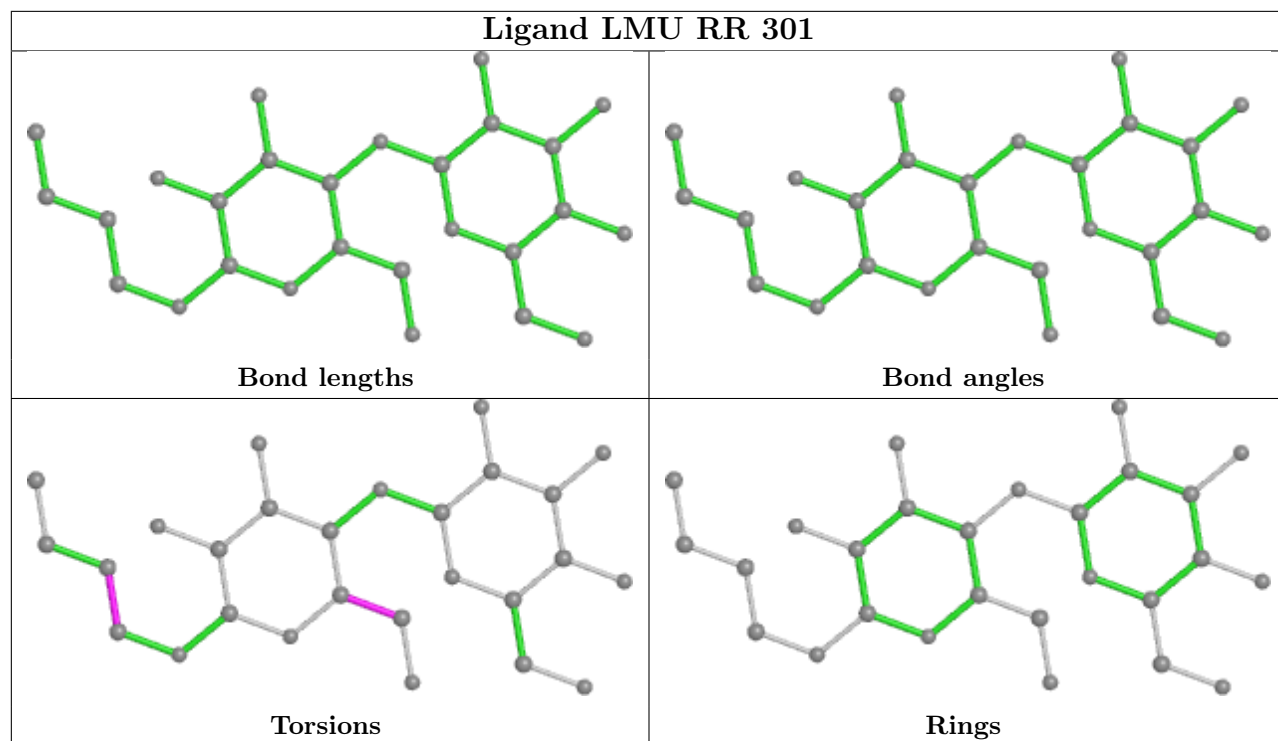
Rings



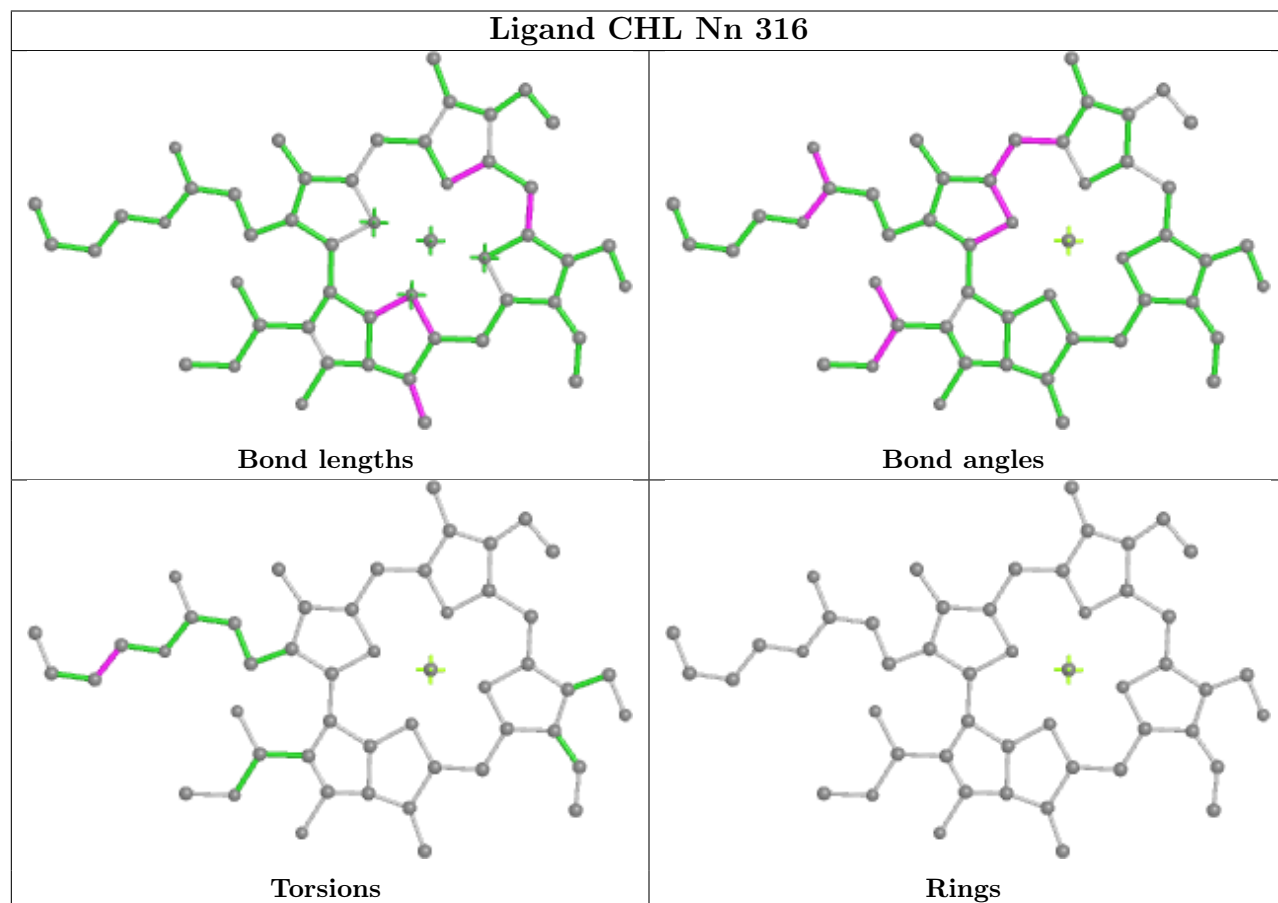


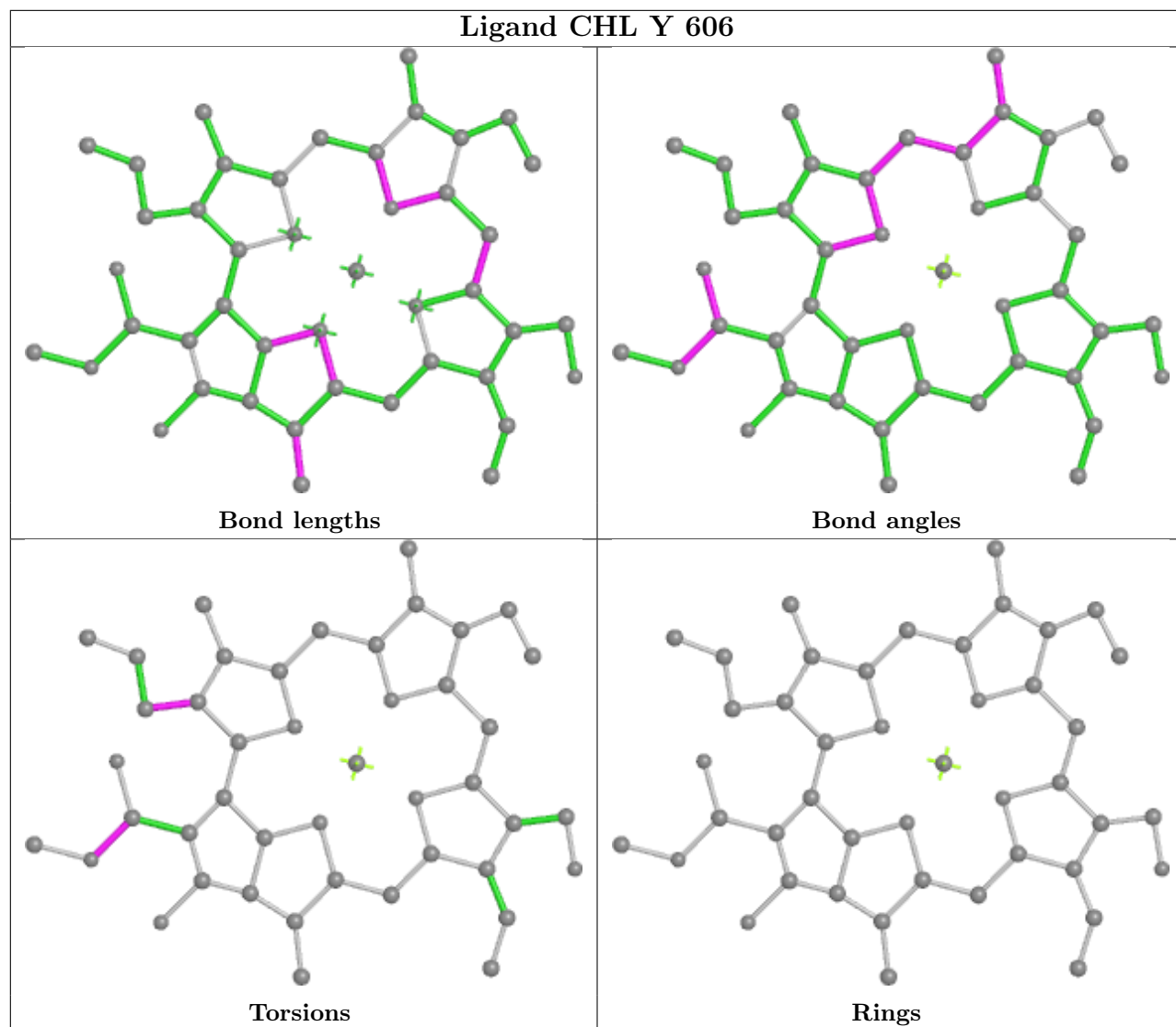


## Ligand LMU RR 301

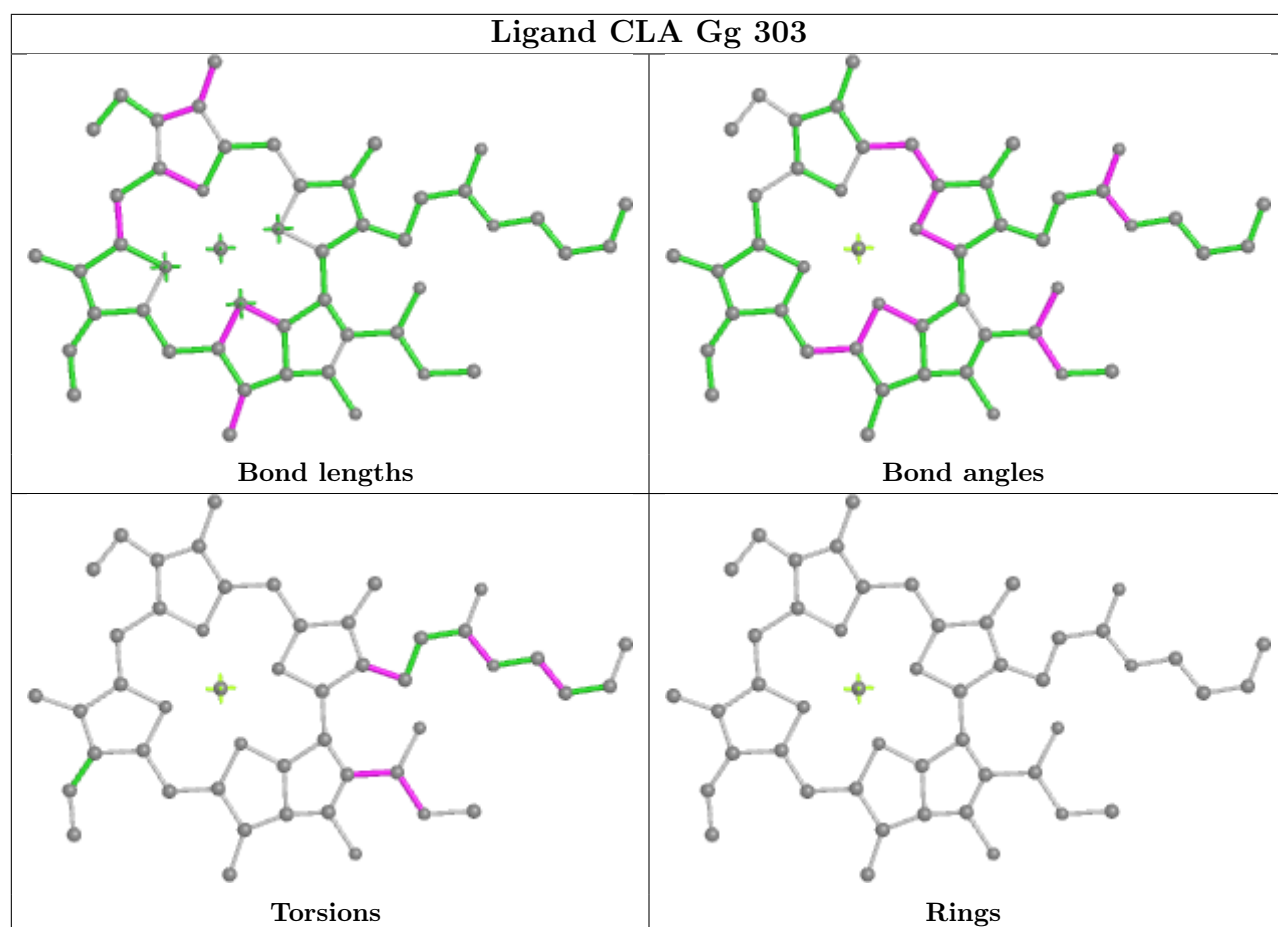


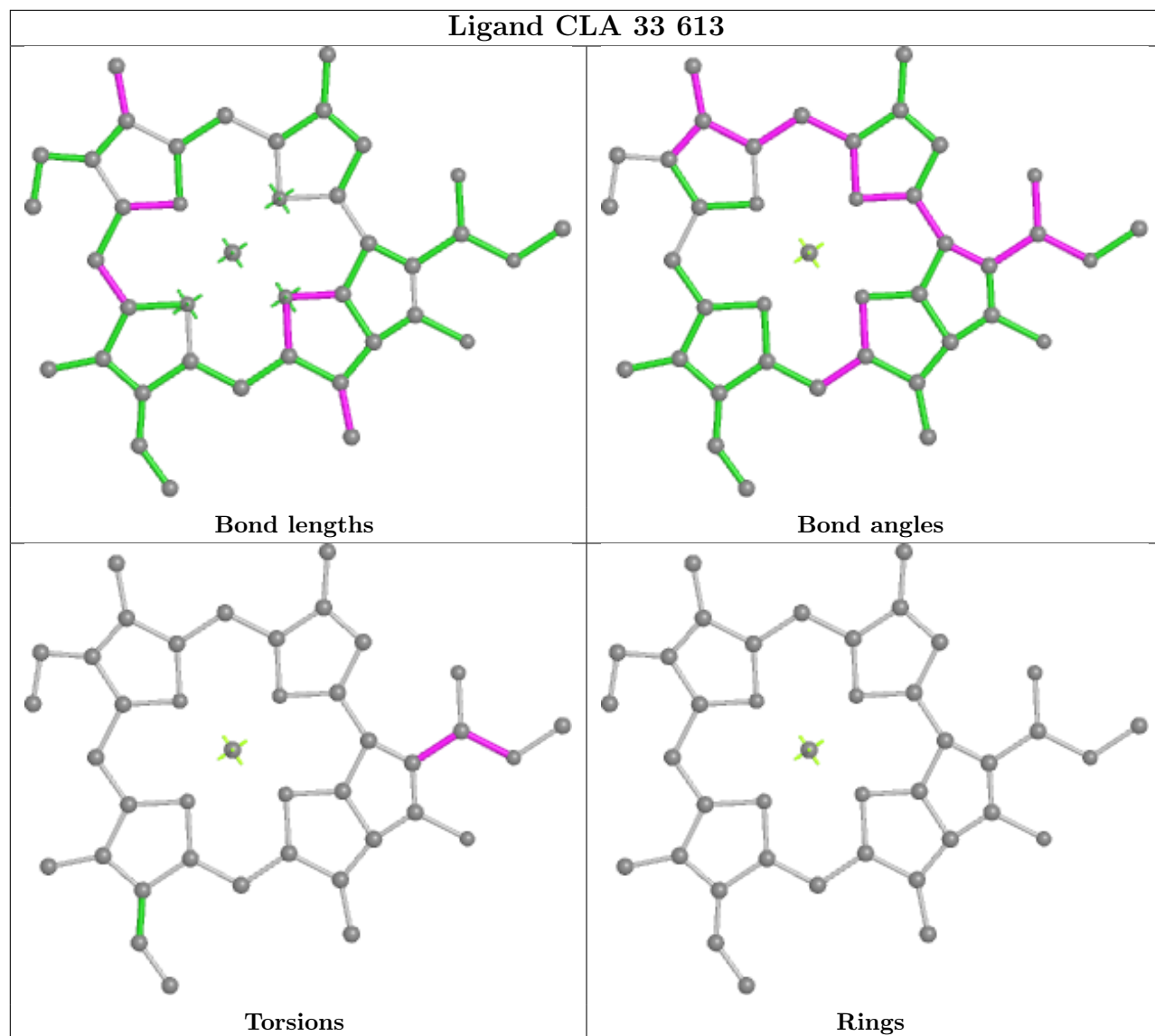
## Ligand CHL Nn 316

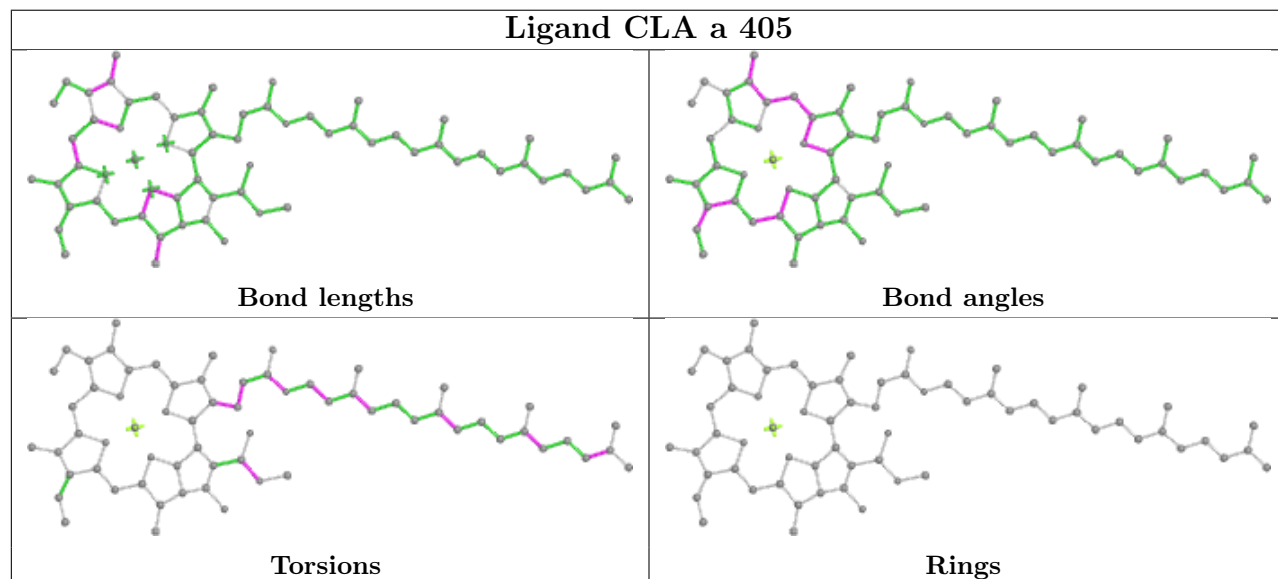
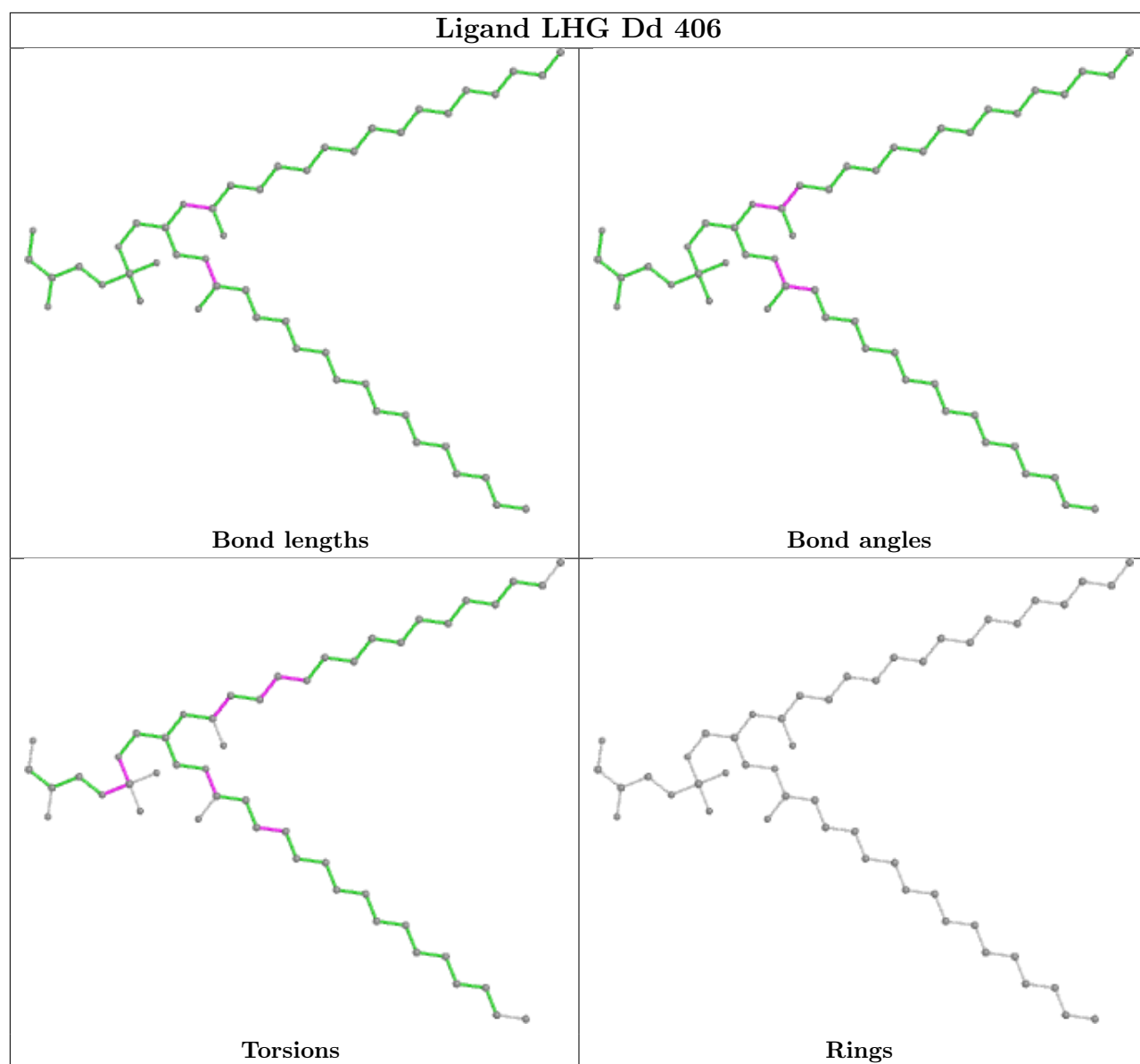


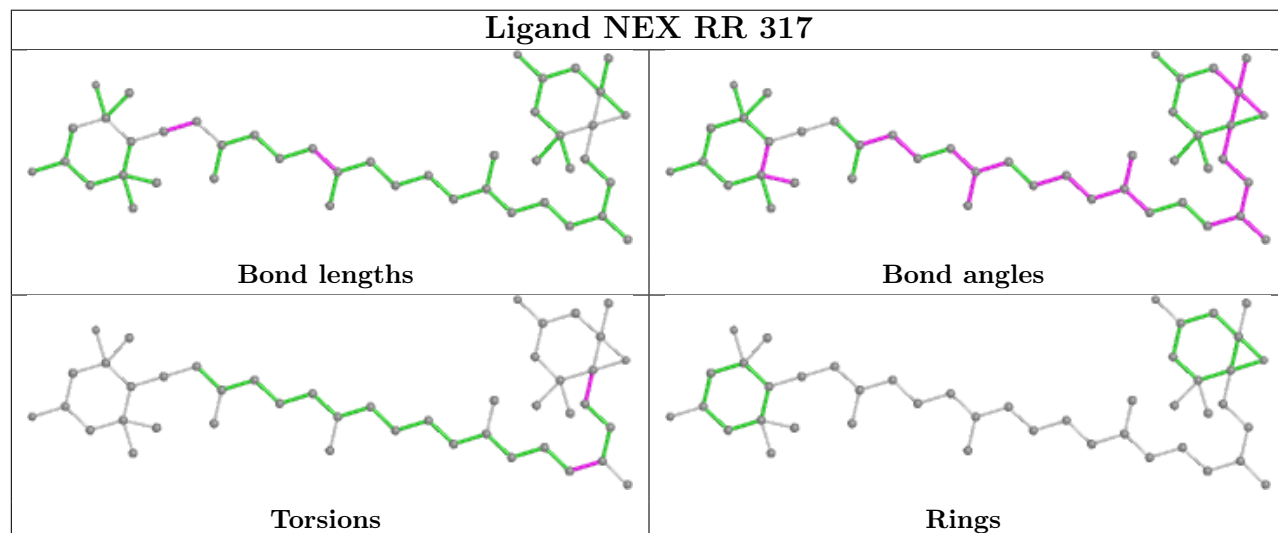
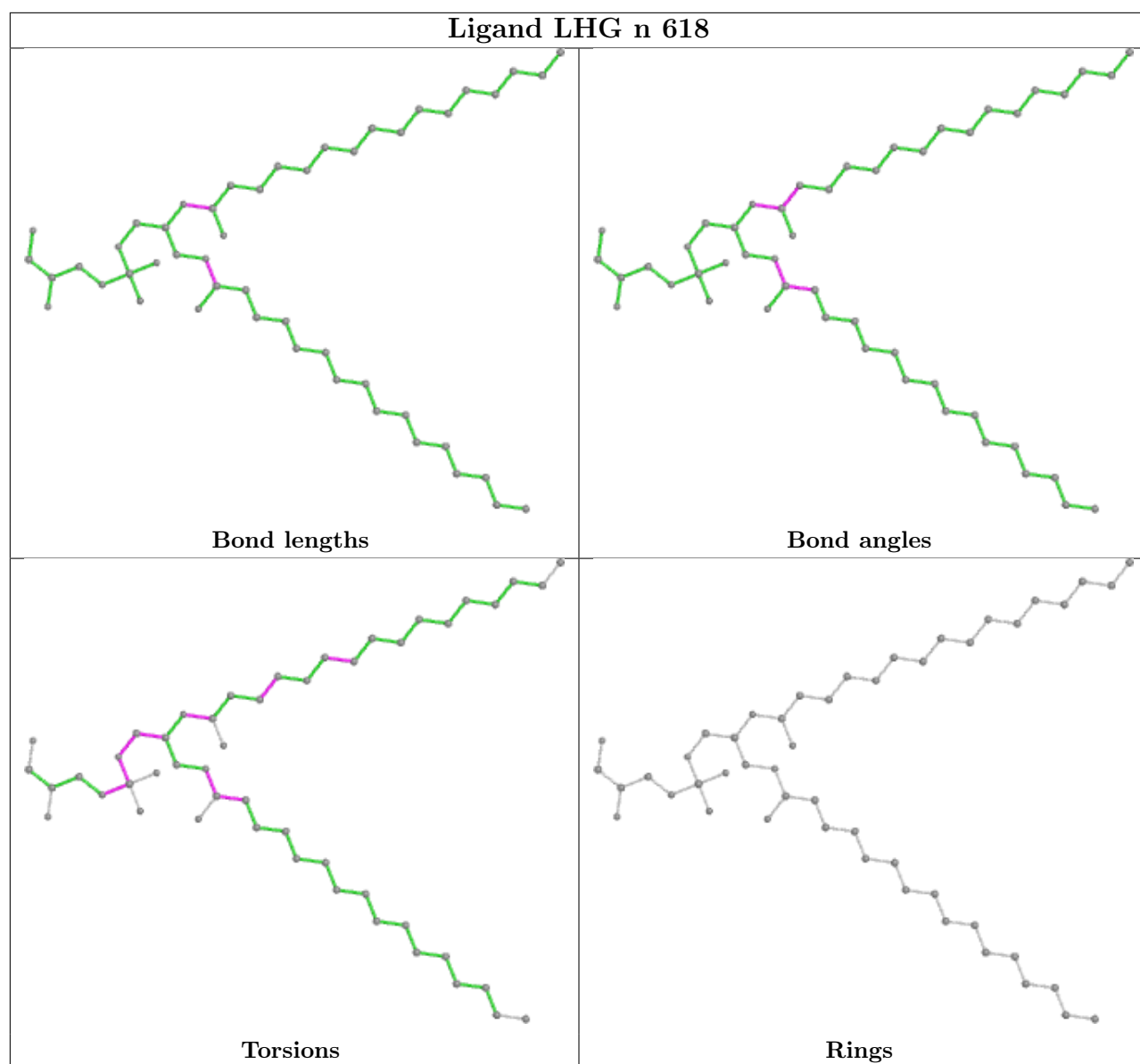


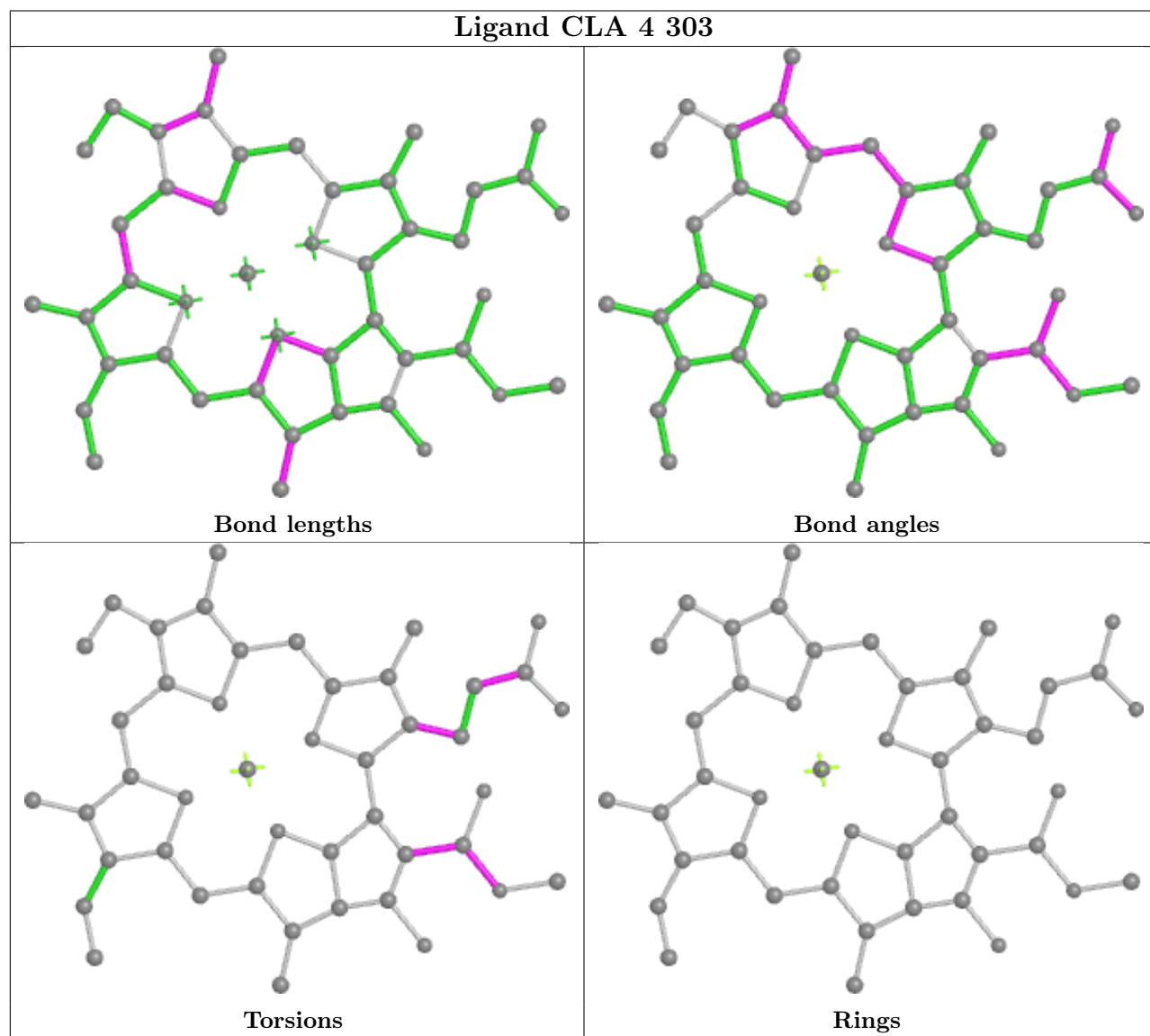
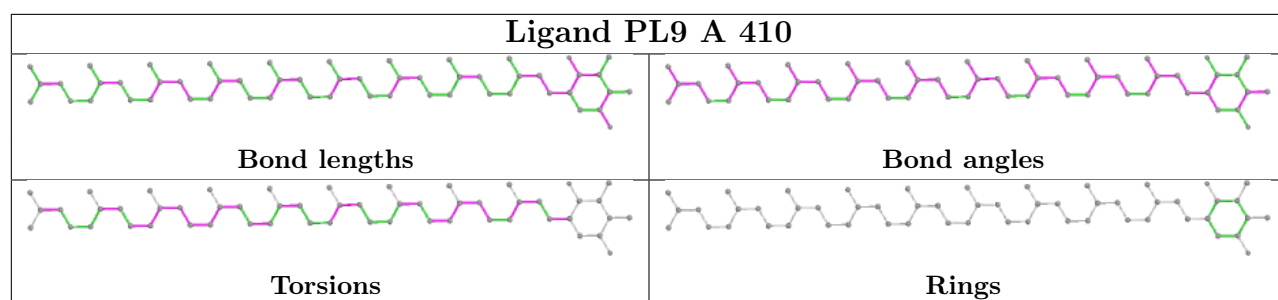




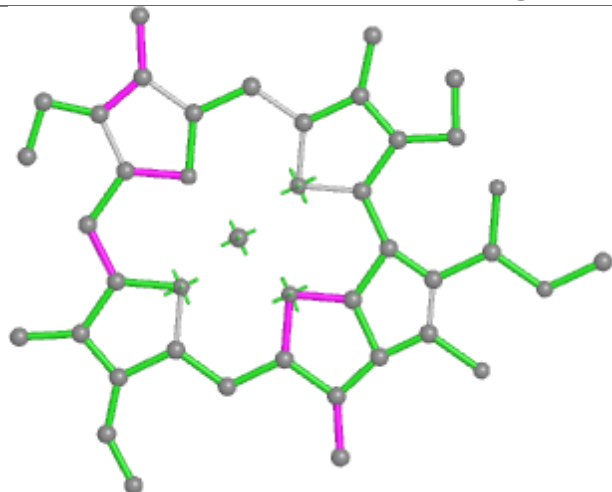




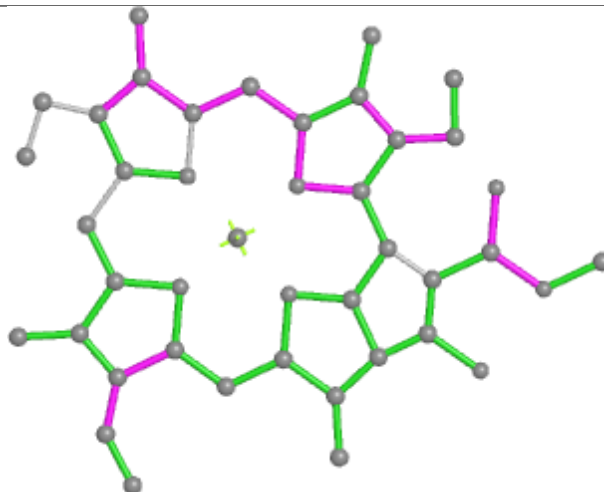




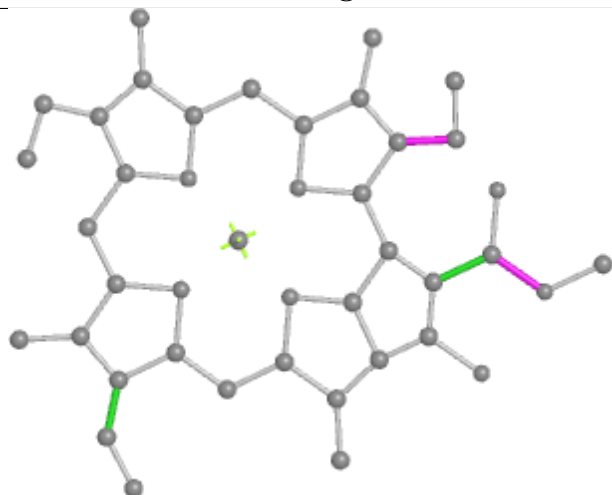
## Ligand CLA N 612



Bond lengths



Bond angles

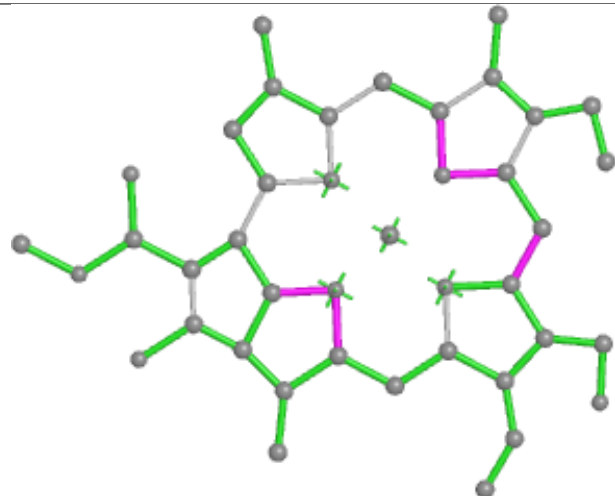


Torsions

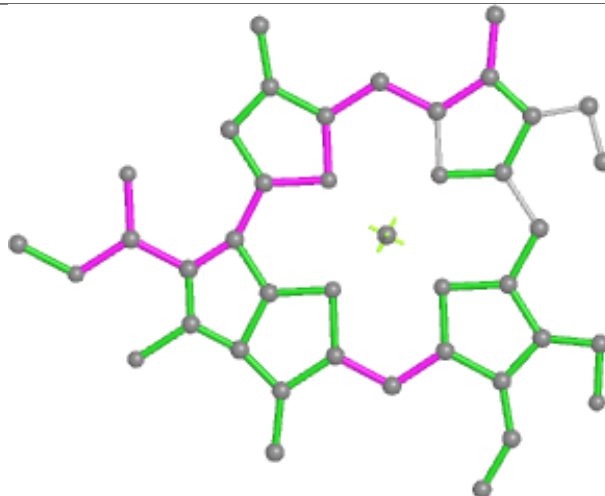


Rings

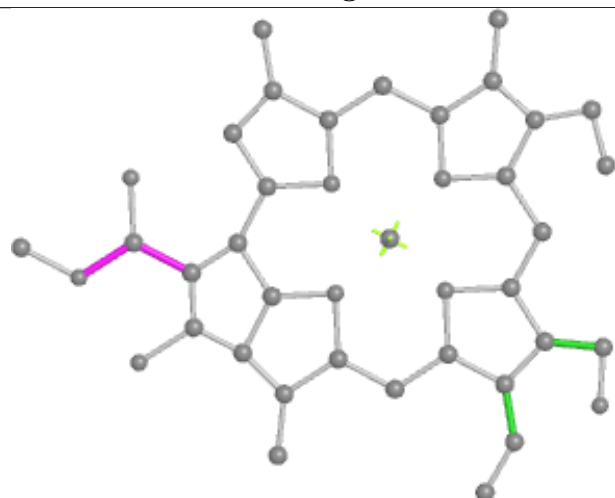
## Ligand CHL 1 605



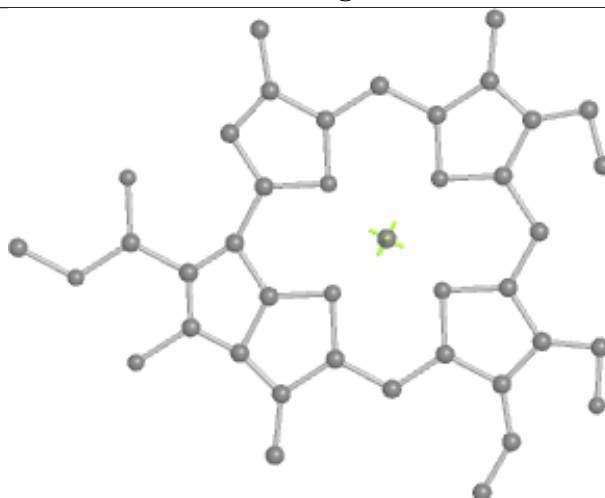
Bond lengths



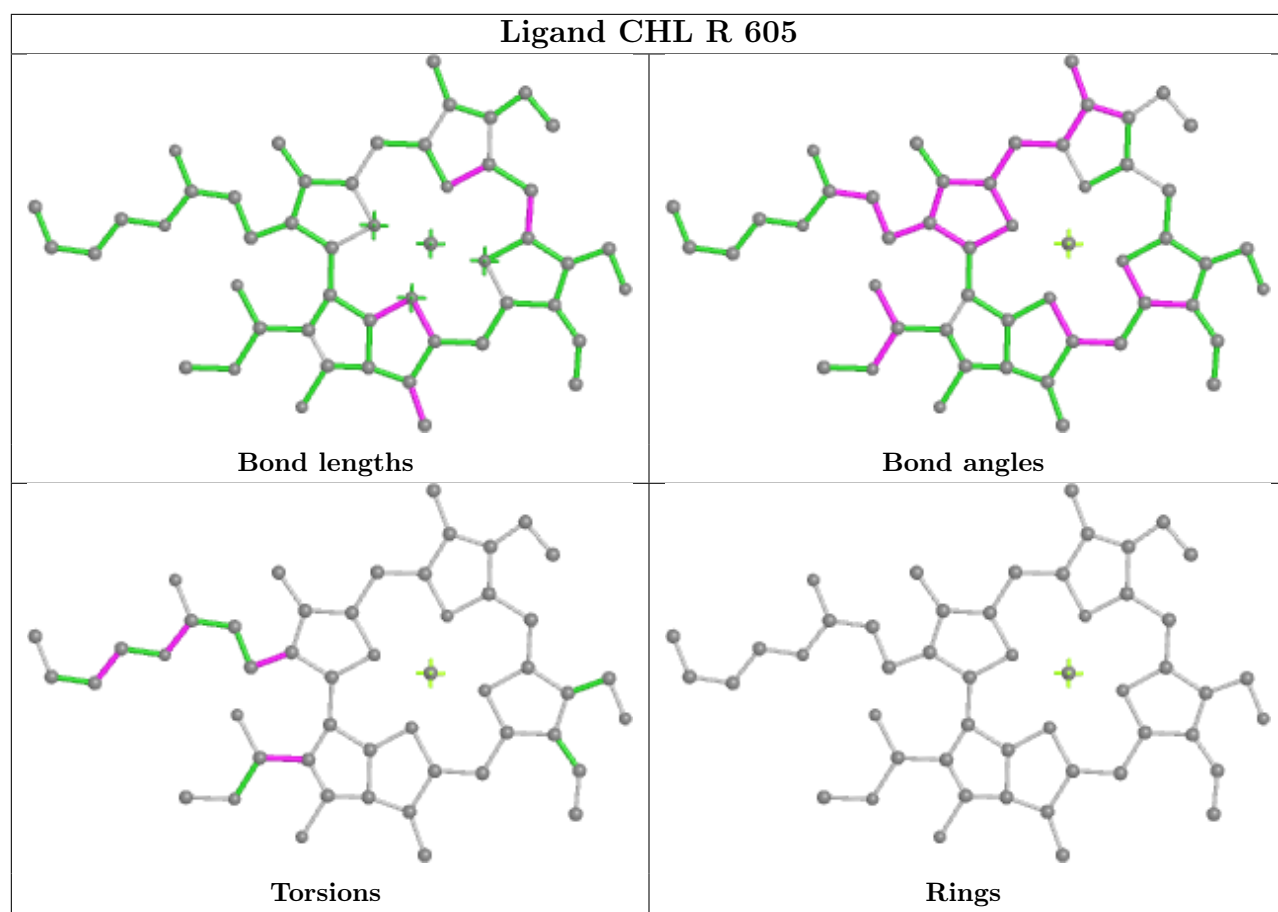
Bond angles



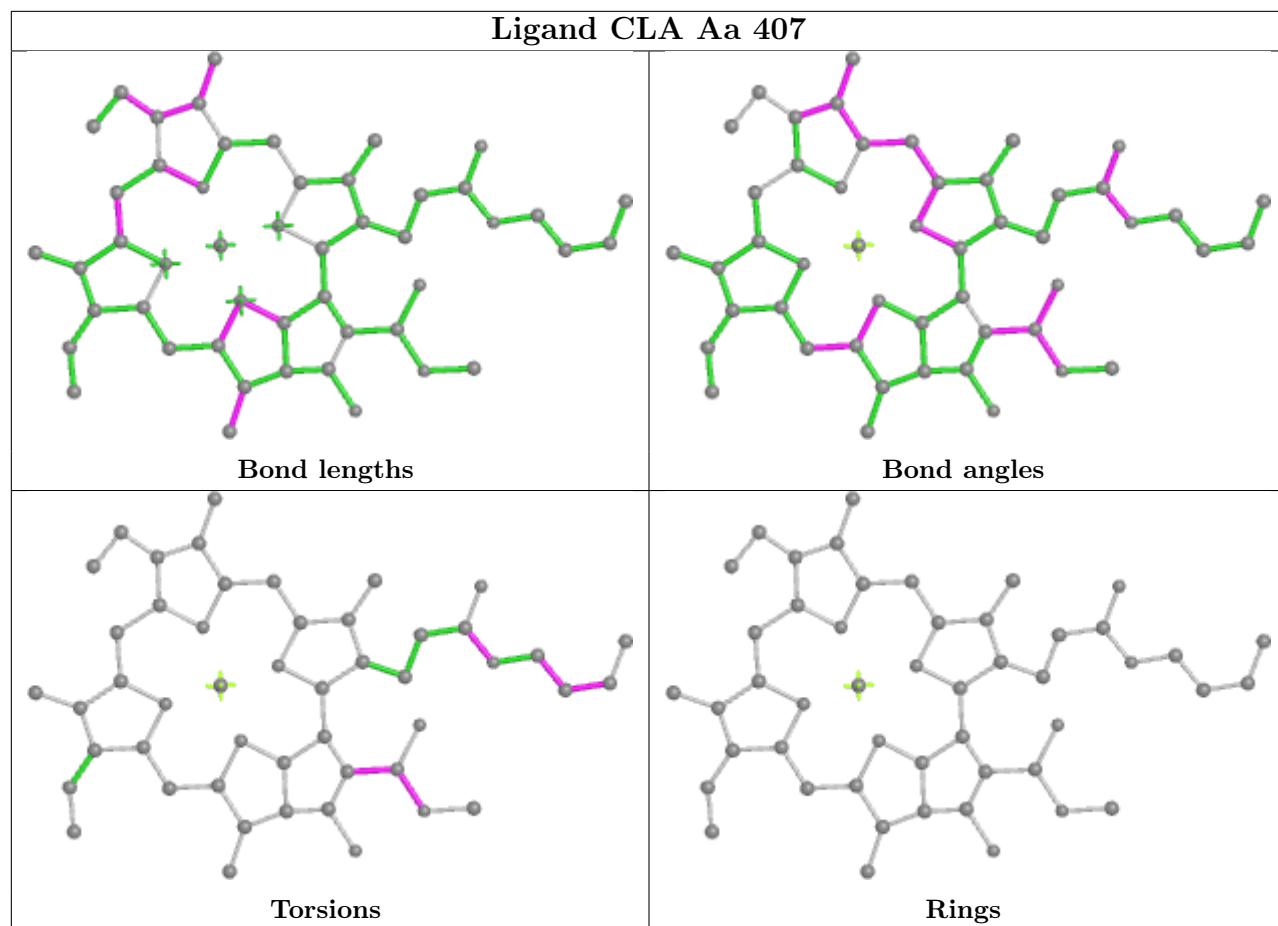
Torsions

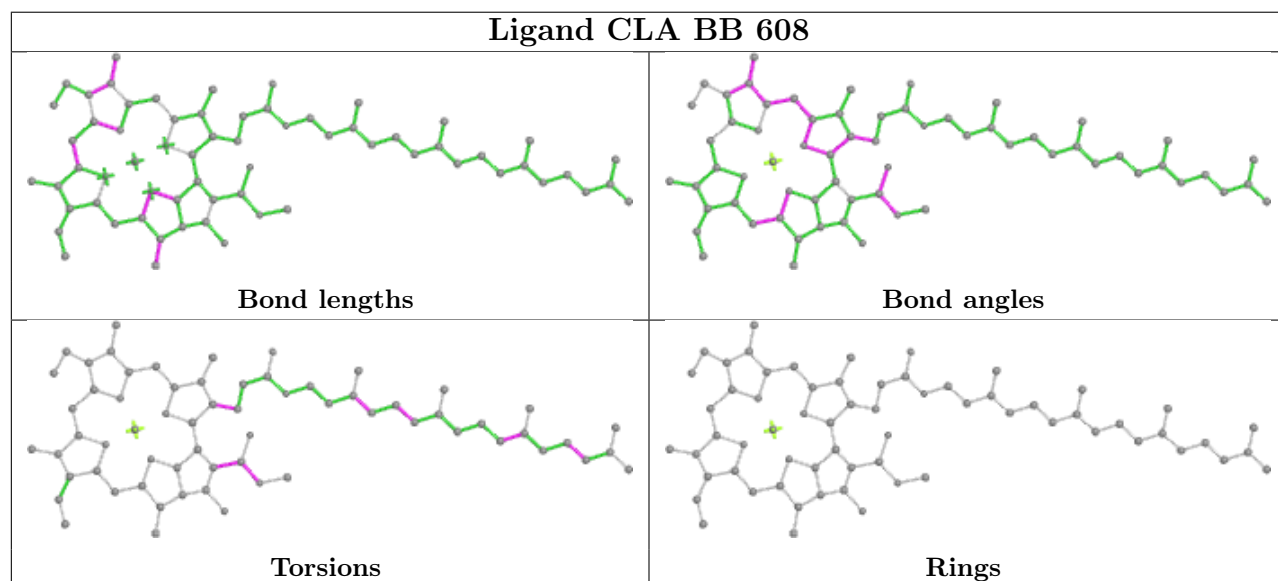
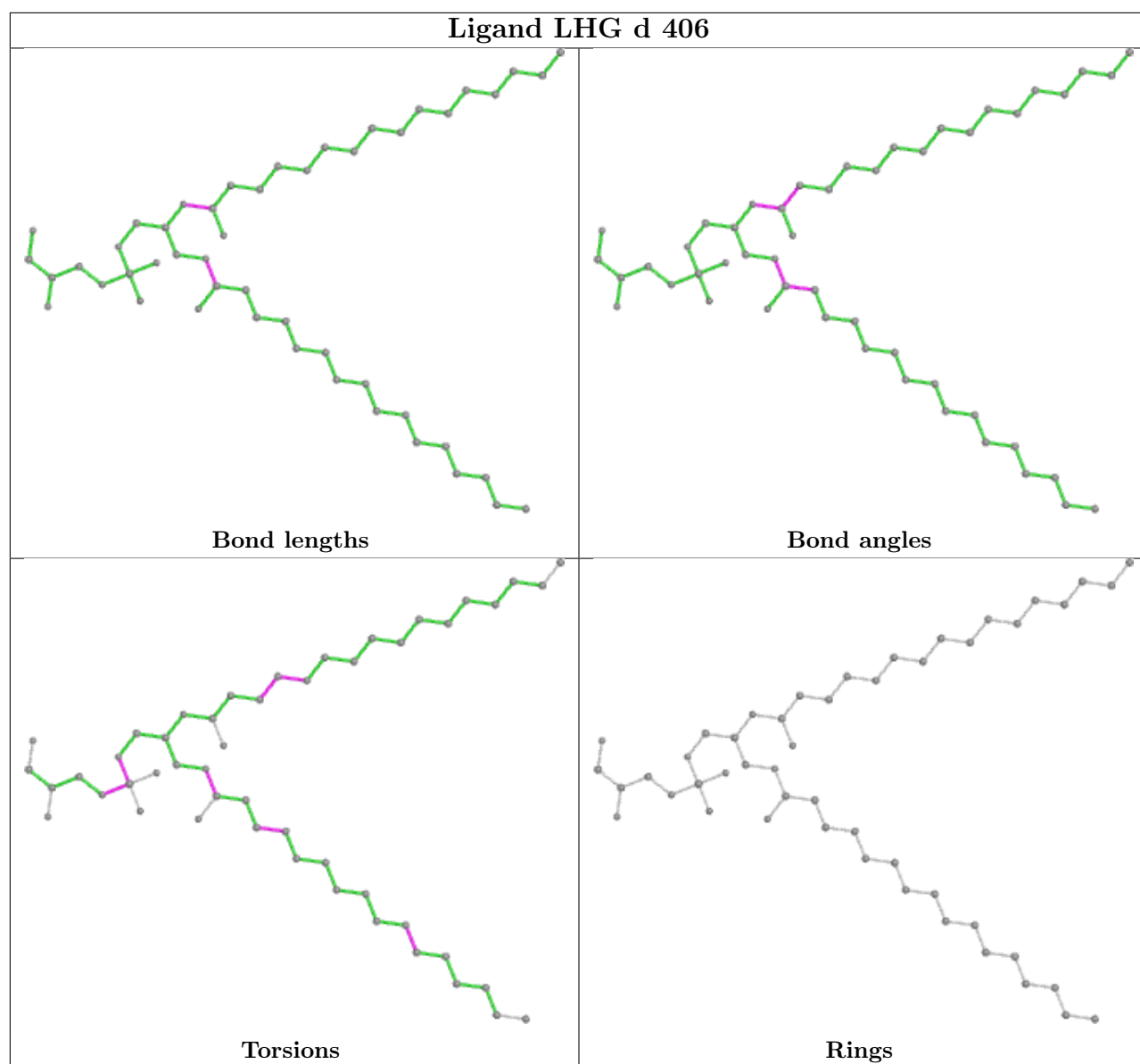


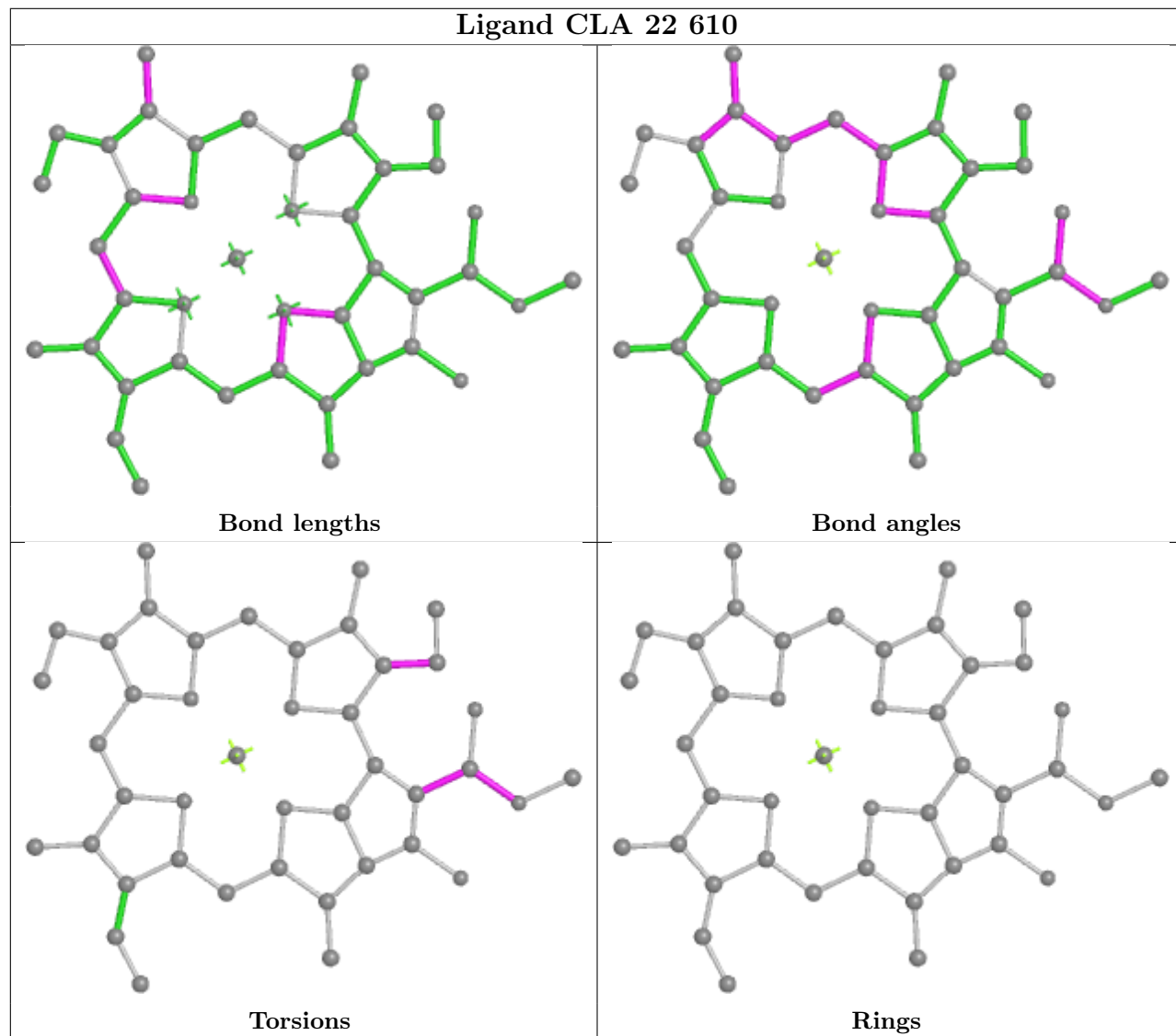
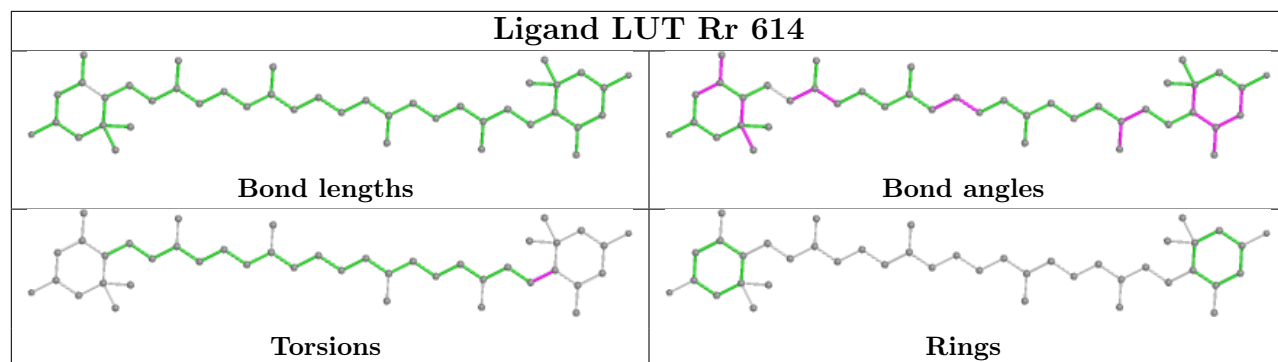
Rings

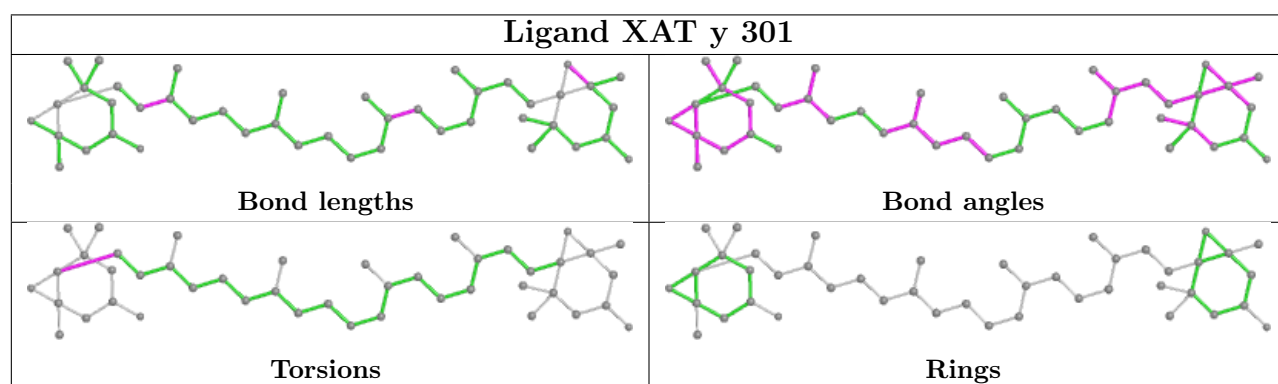
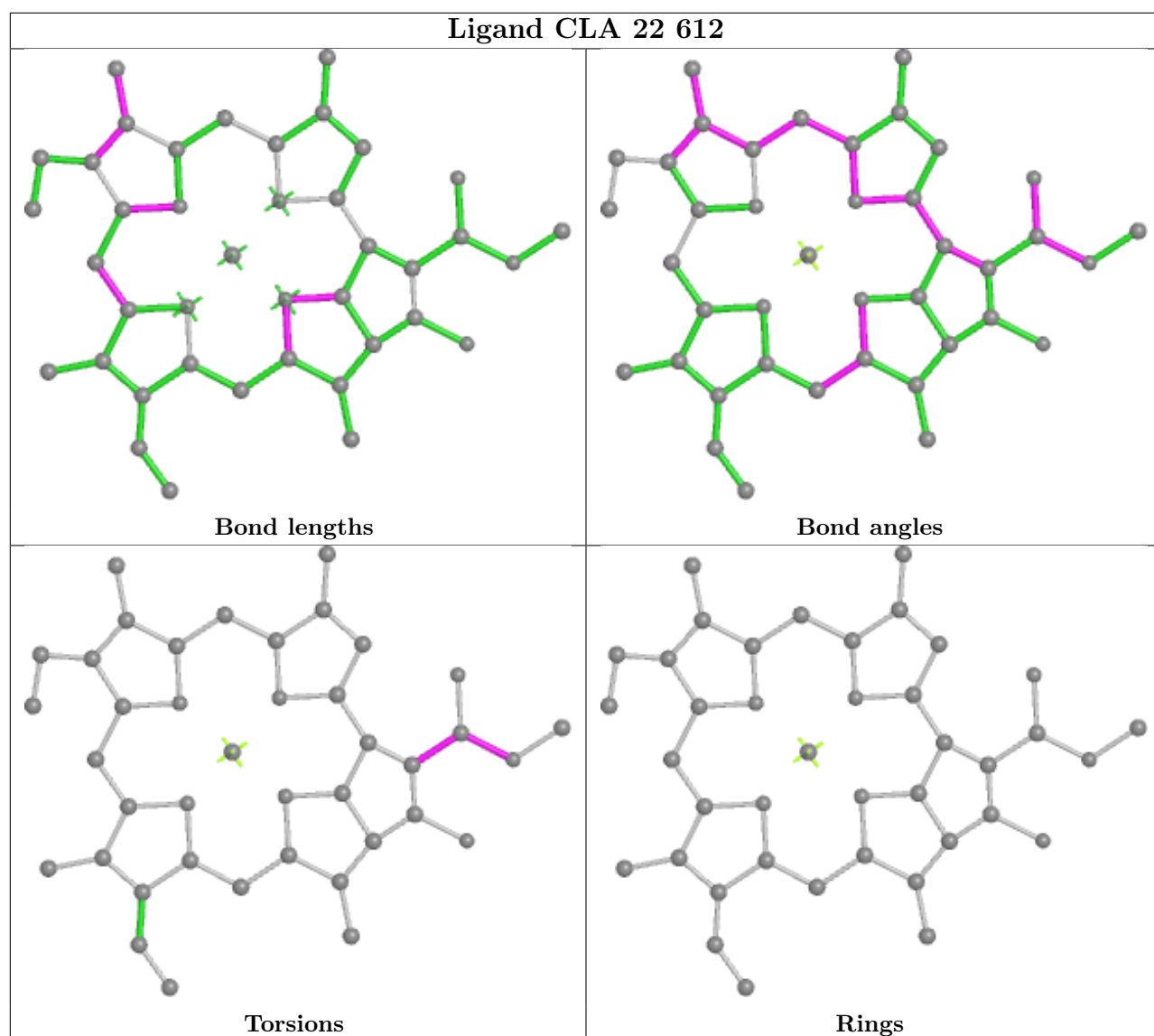


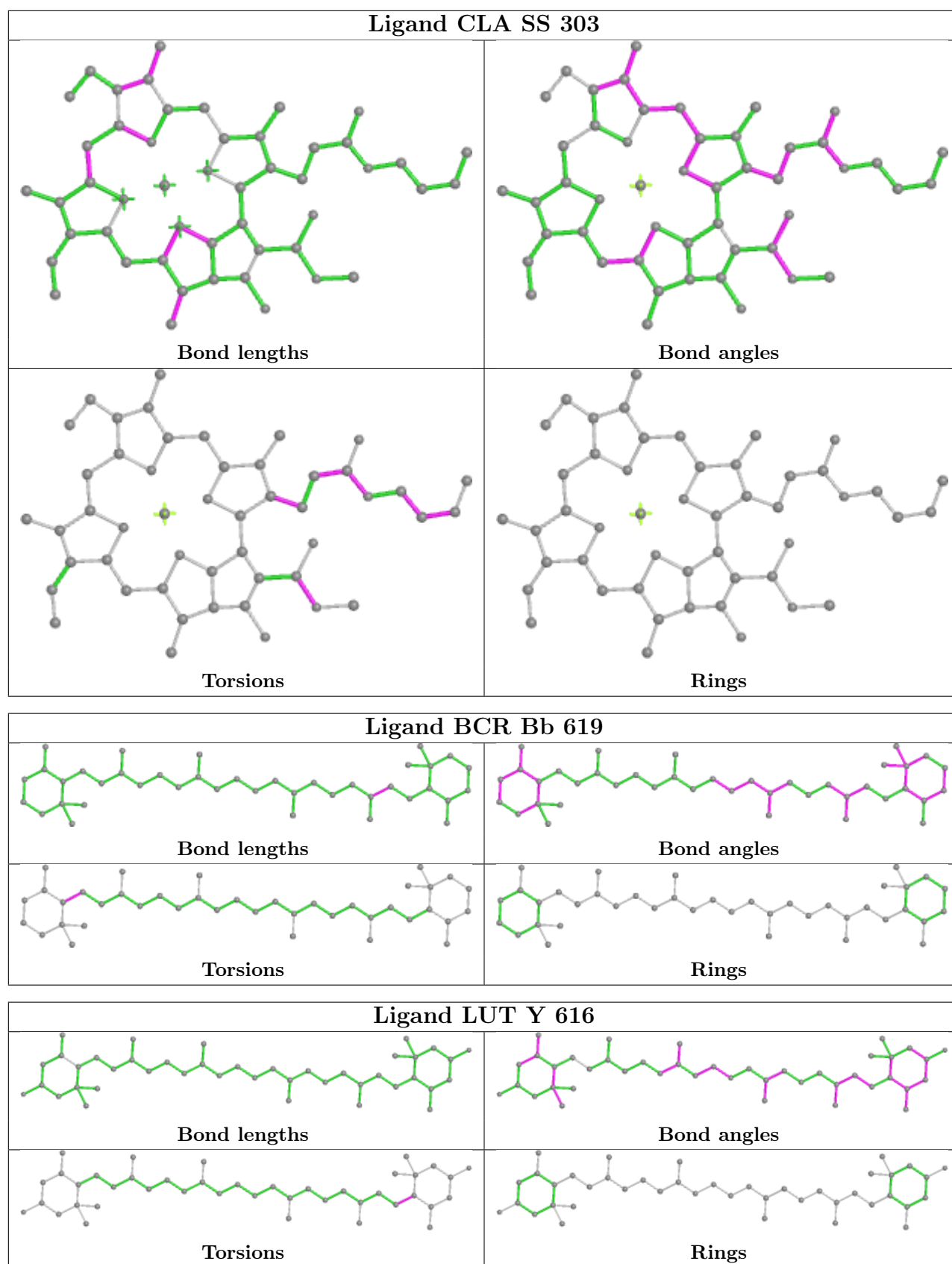




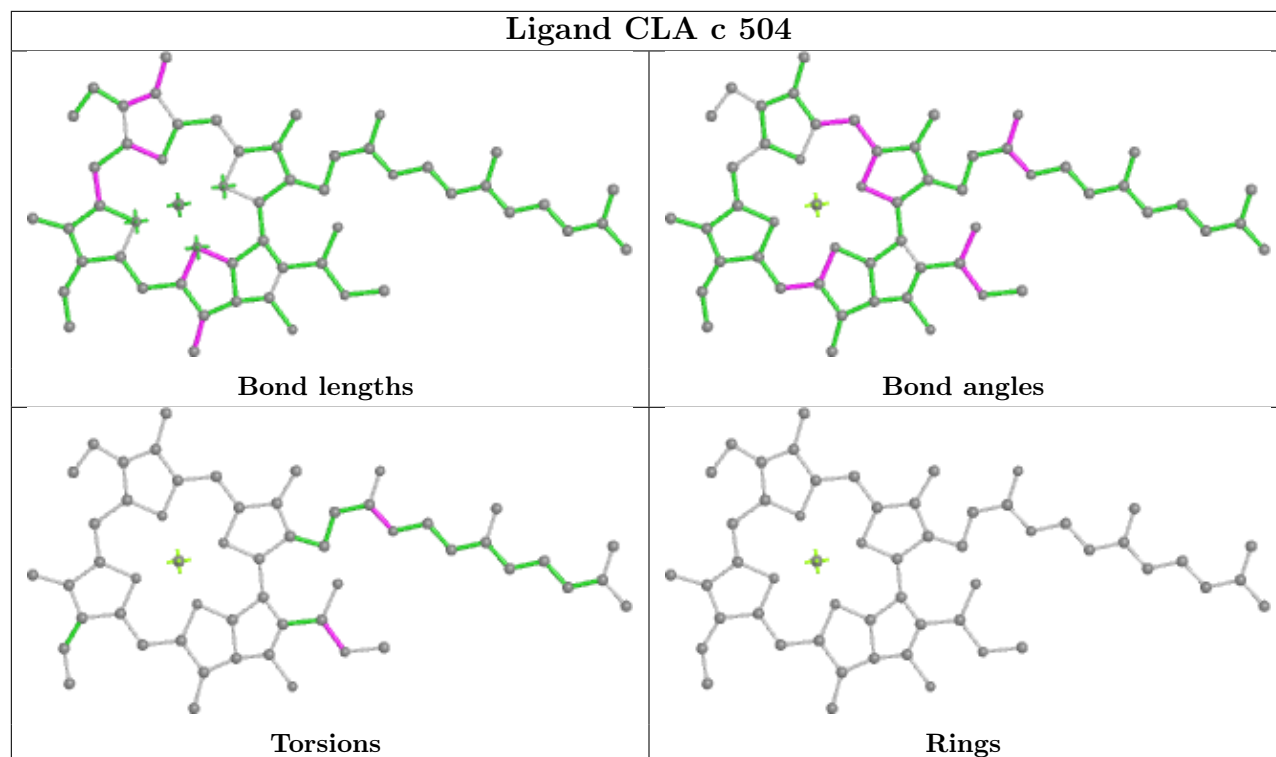




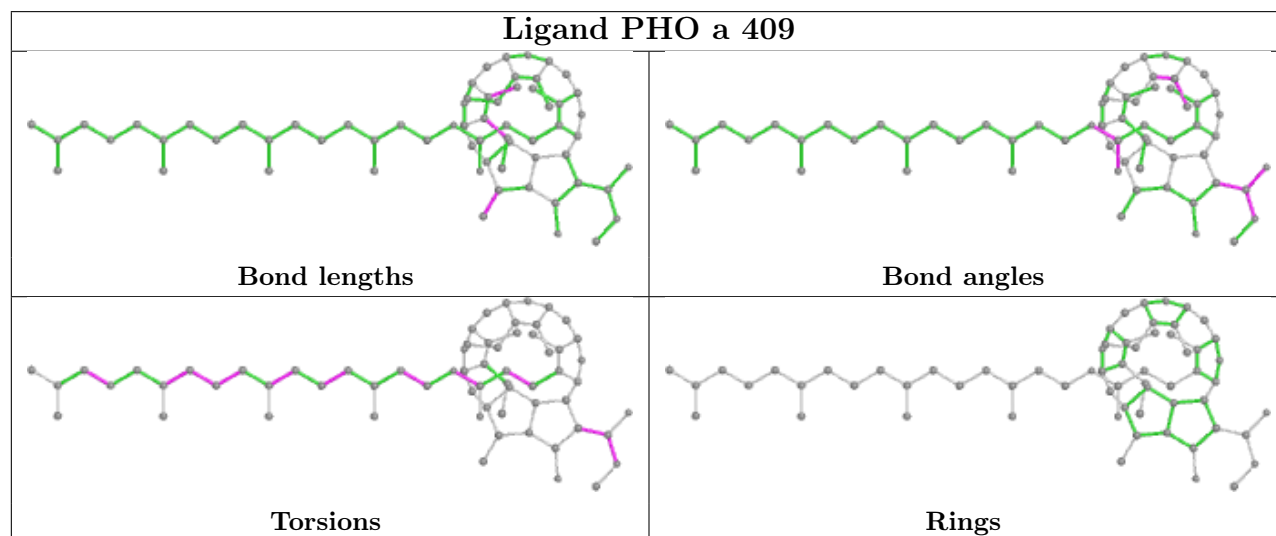




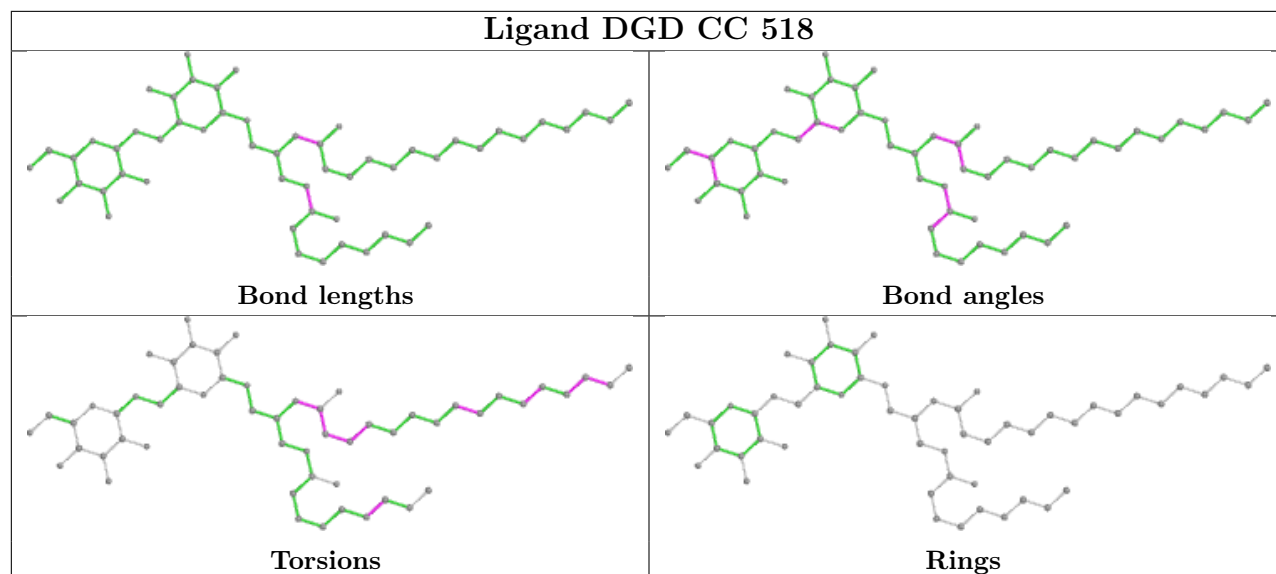
## Ligand CLA c 504



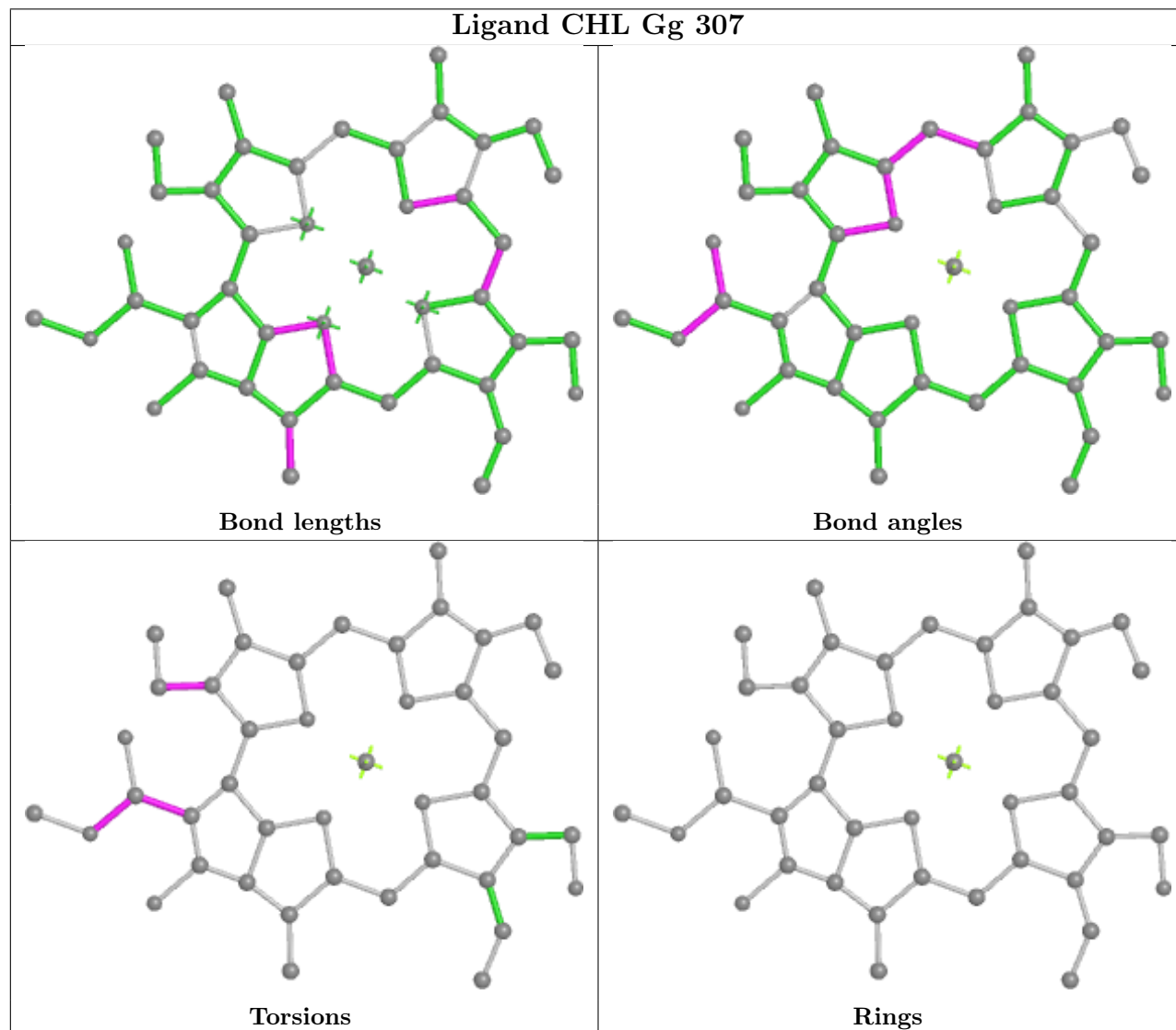
## Ligand PHO a 409



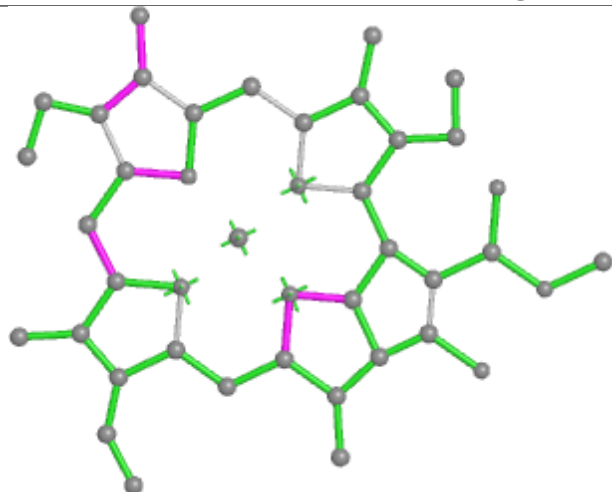
## Ligand DGD CC 518



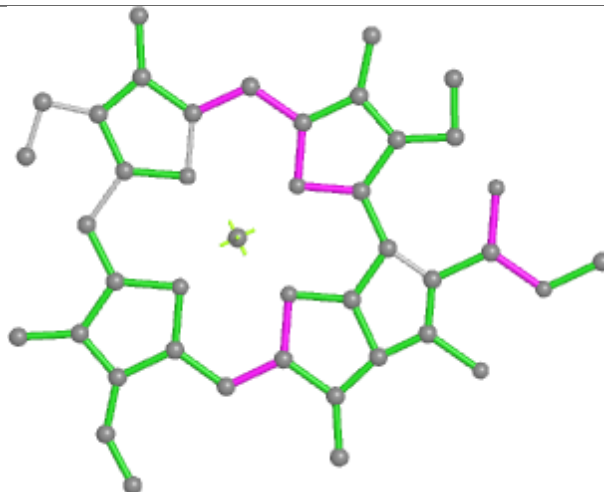
## Ligand CHL Gg 307



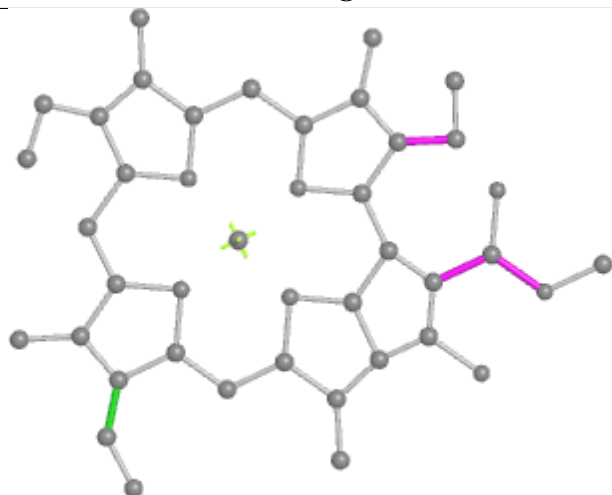
## Ligand CLA G 604



Bond lengths



Bond angles

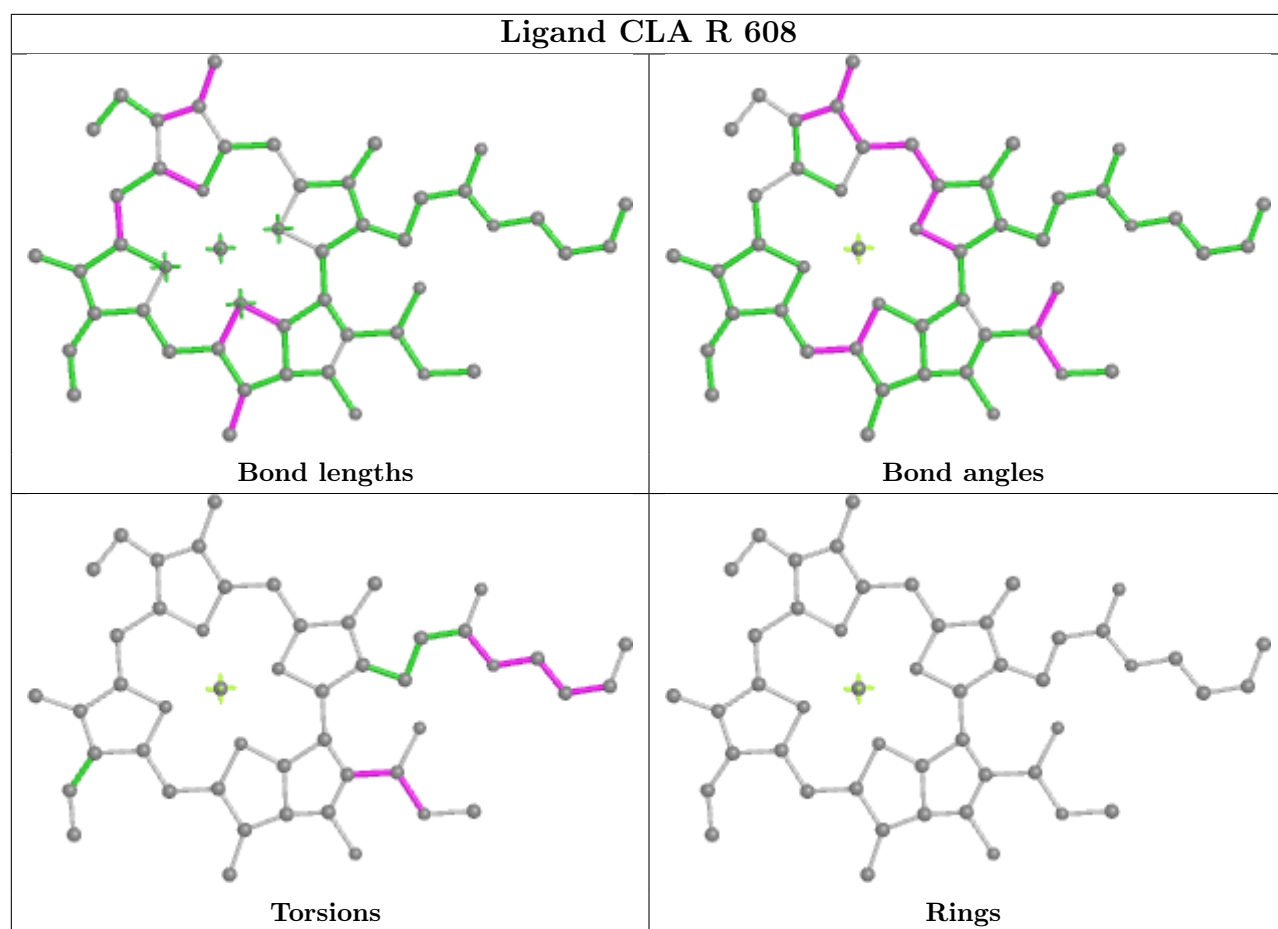


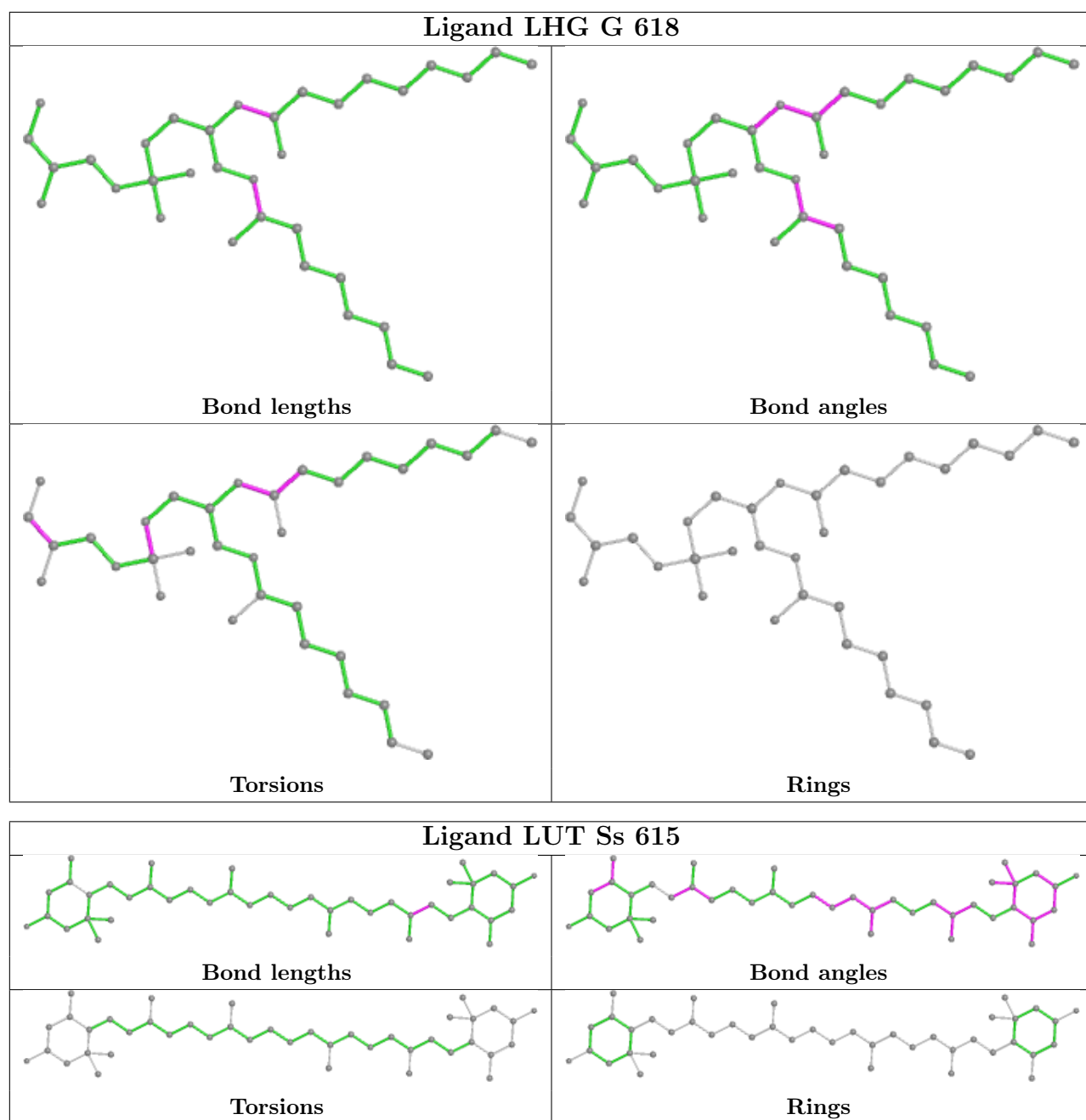
Torsions



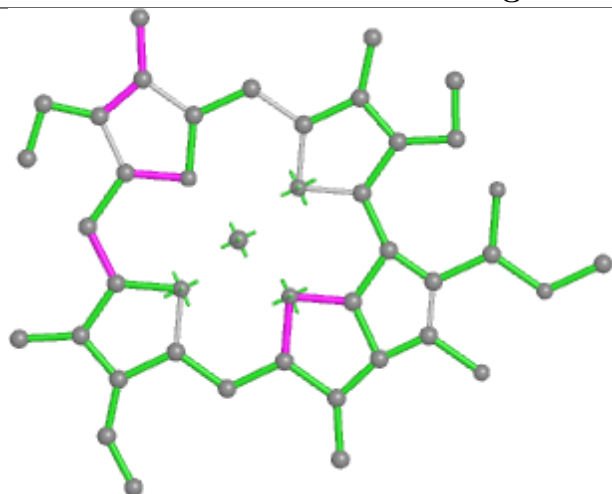
Rings



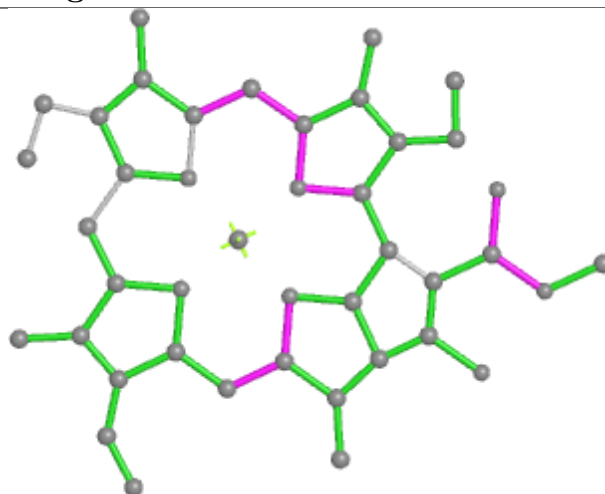




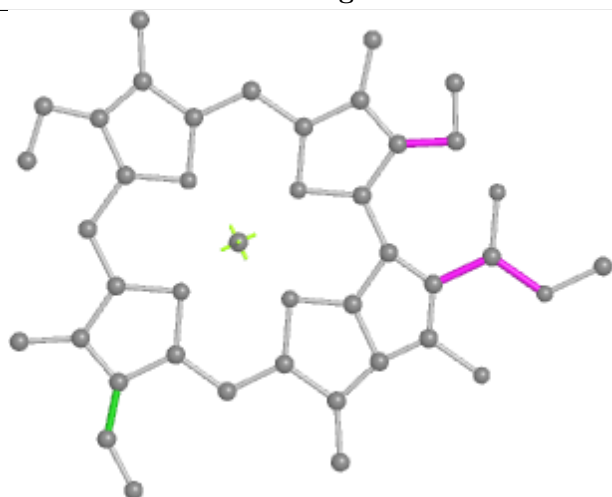
## Ligand CLA Gg 305



Bond lengths



Bond angles

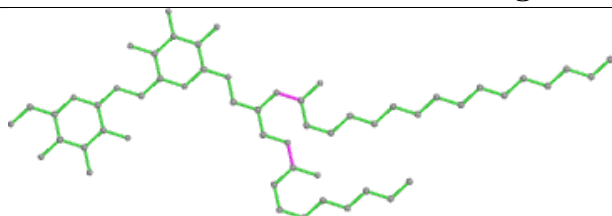


Torsions

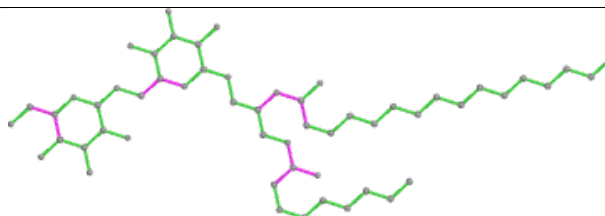


Rings

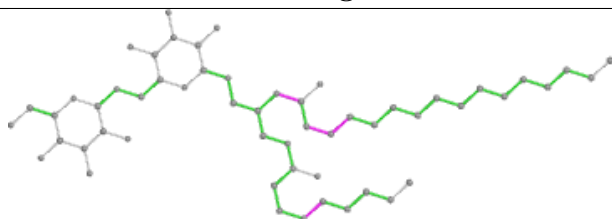
## Ligand DGD c 517



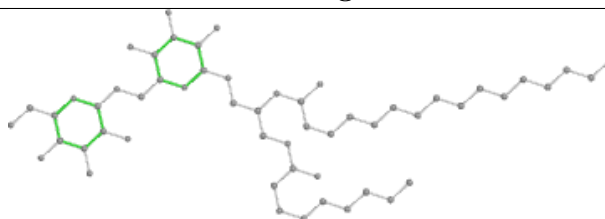
Bond lengths



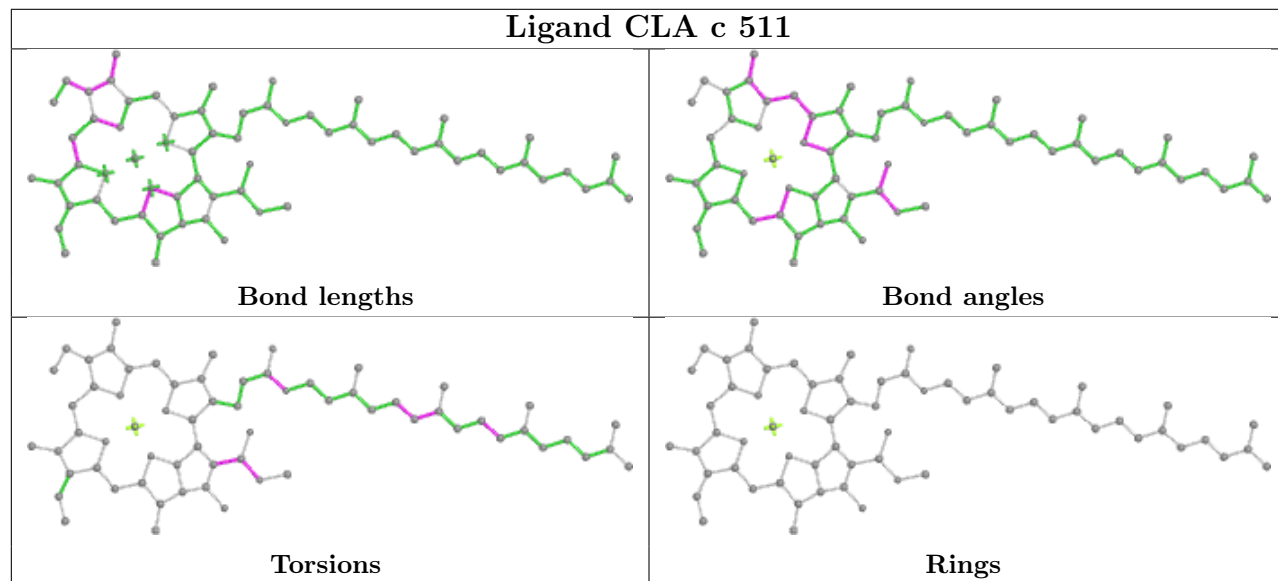
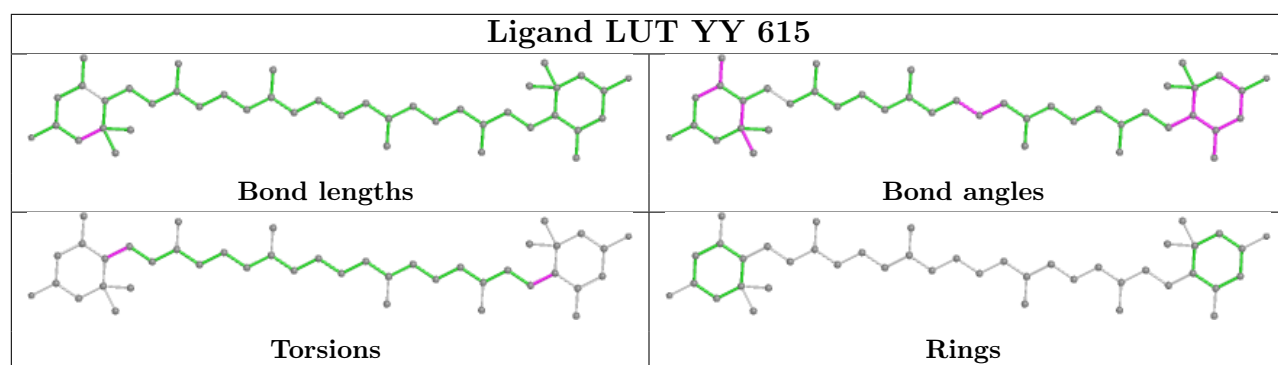
Bond angles



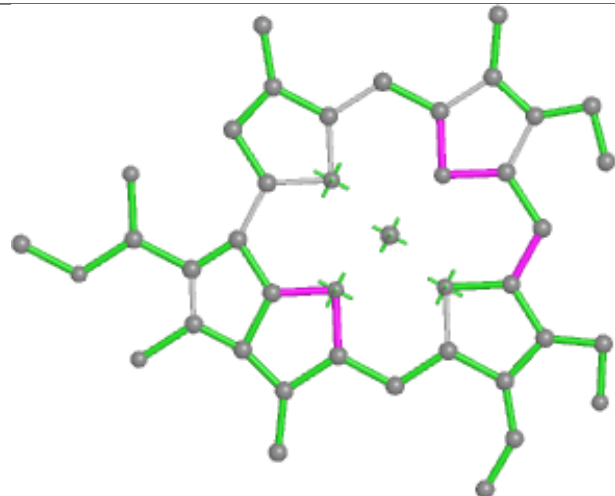
Torsions



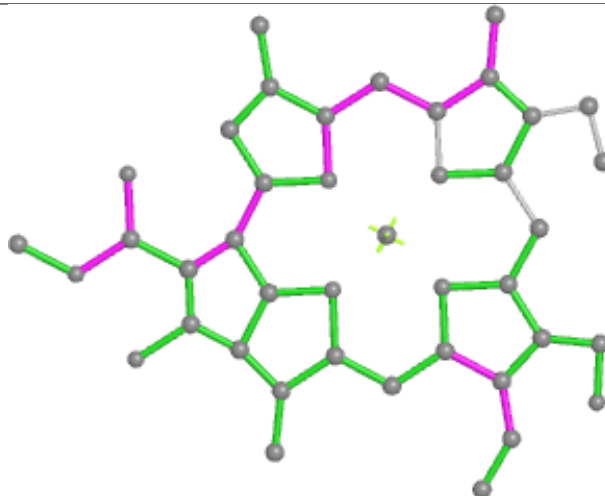
Rings



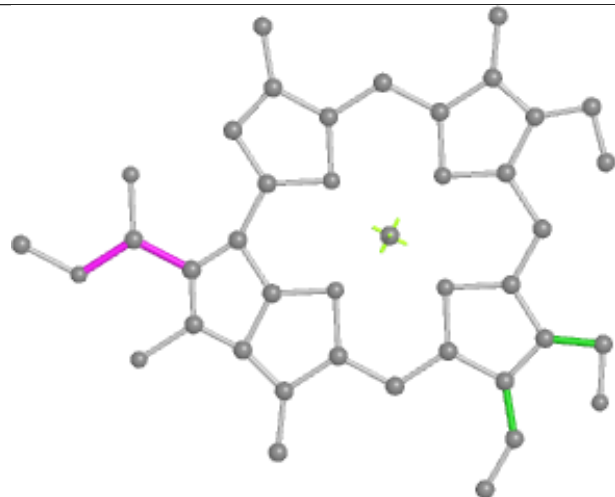
## Ligand CHL 3 608



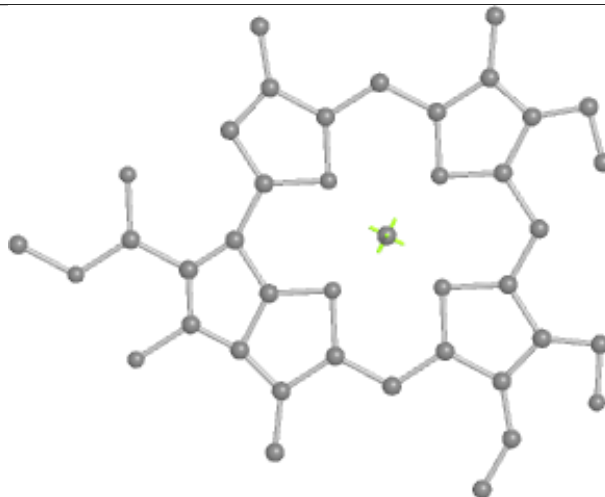
Bond lengths



Bond angles

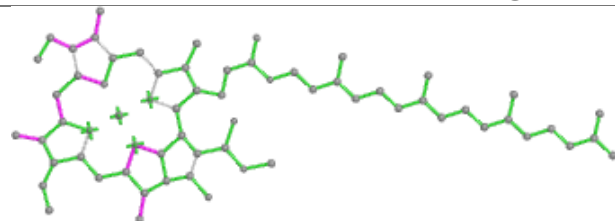


Torsions

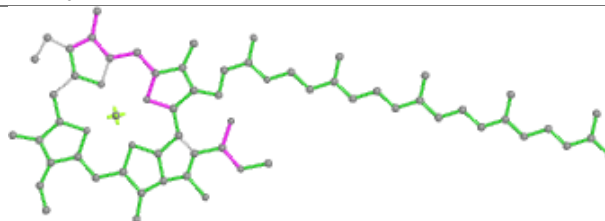


Rings

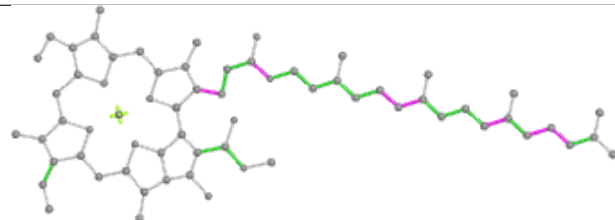
## Ligand CLA Yy 610



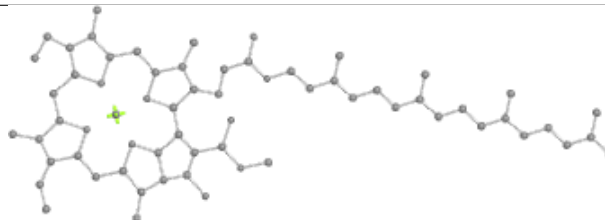
Bond lengths



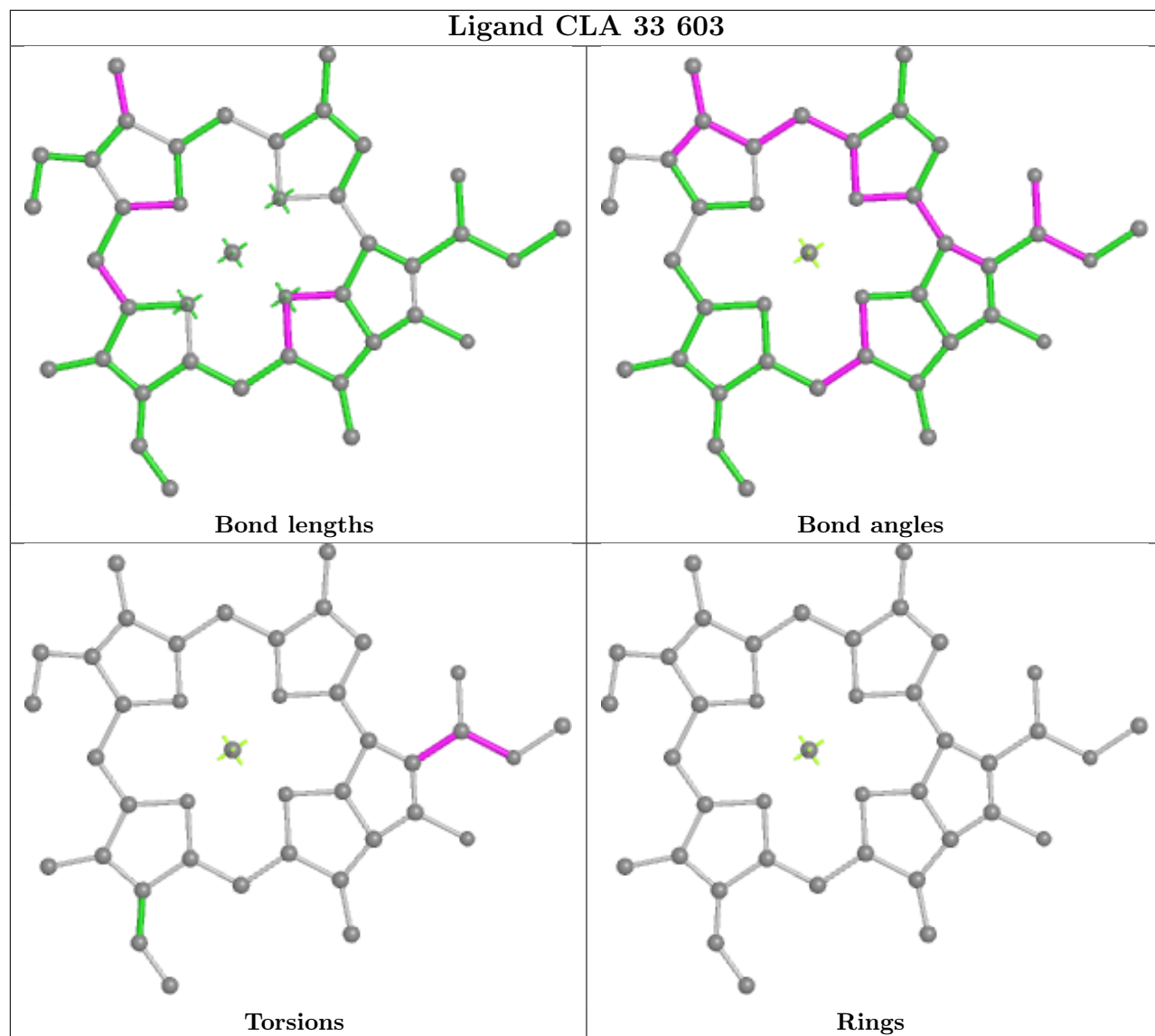
Bond angles



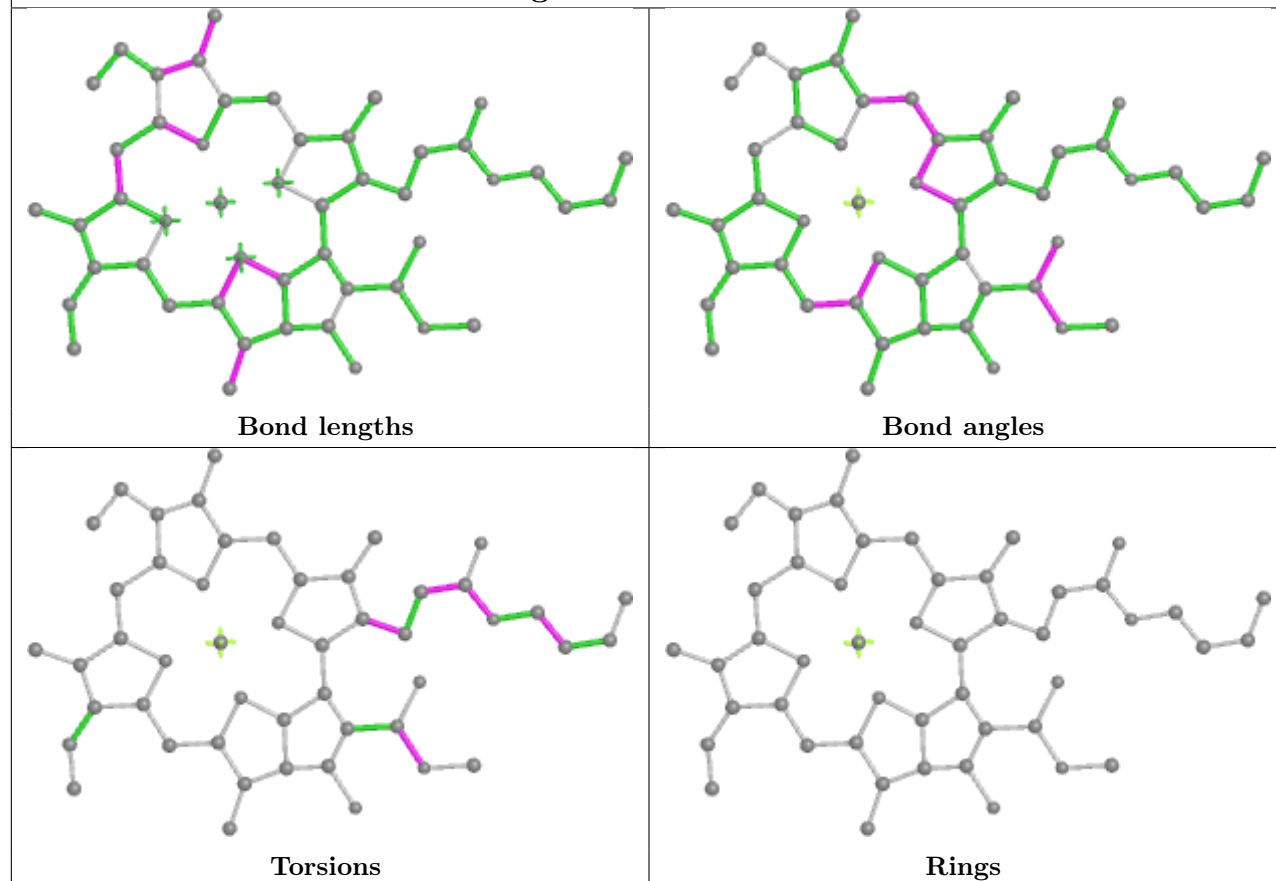
Torsions



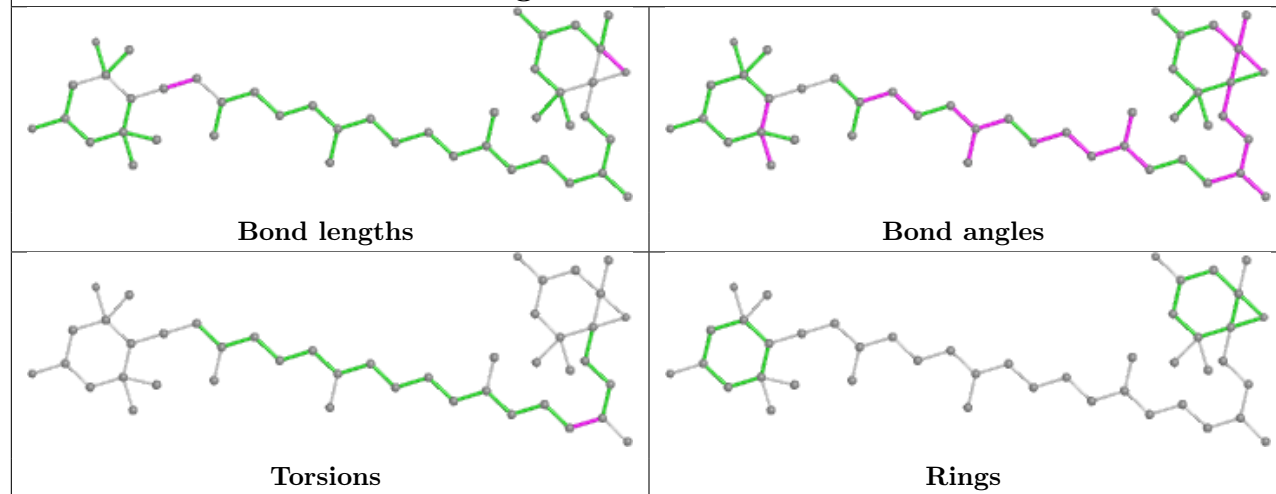
Rings



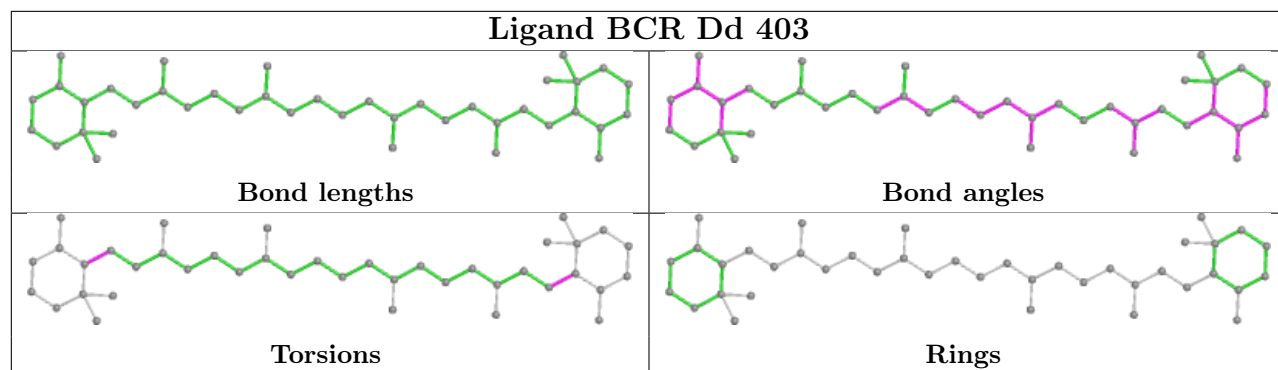
## Ligand CLA G 602



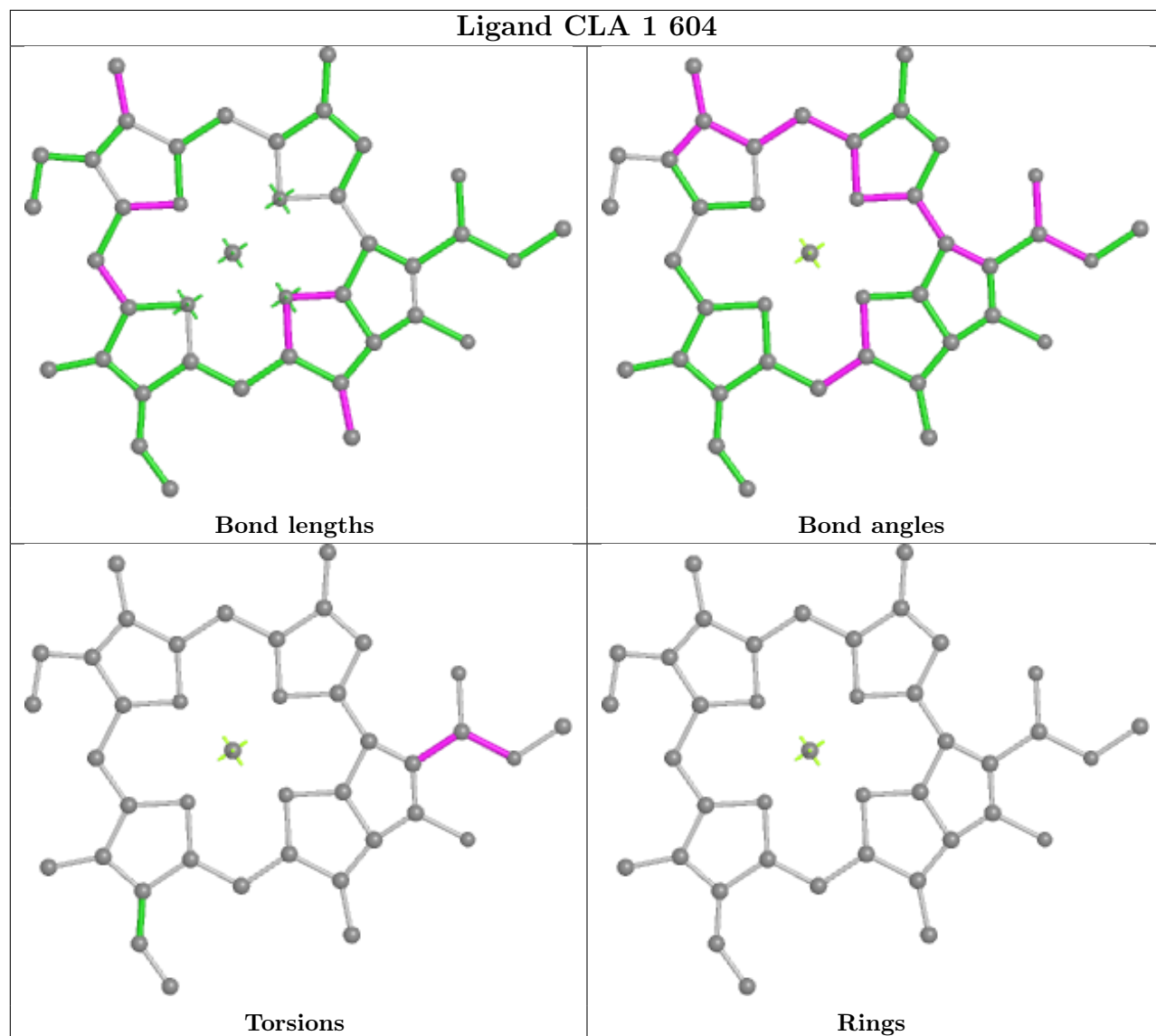
## Ligand NEX NN 618



## Ligand BCR Dd 403

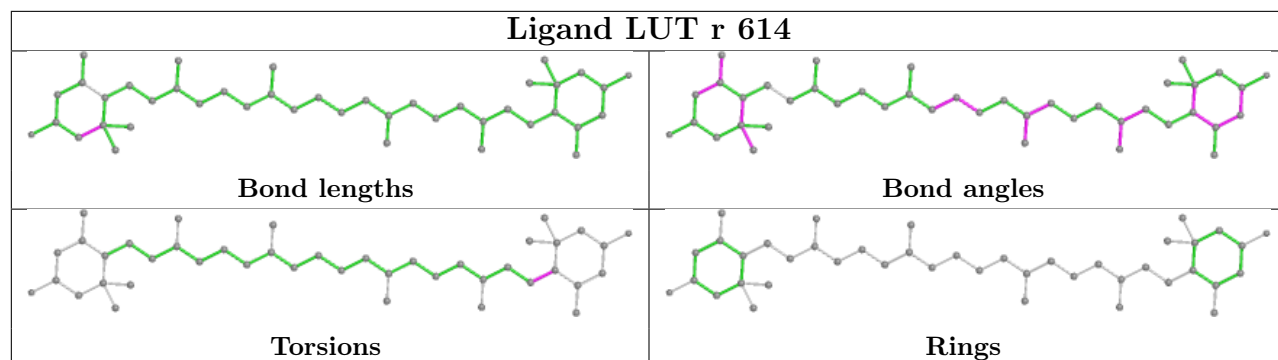


## Ligand CLA 1 604

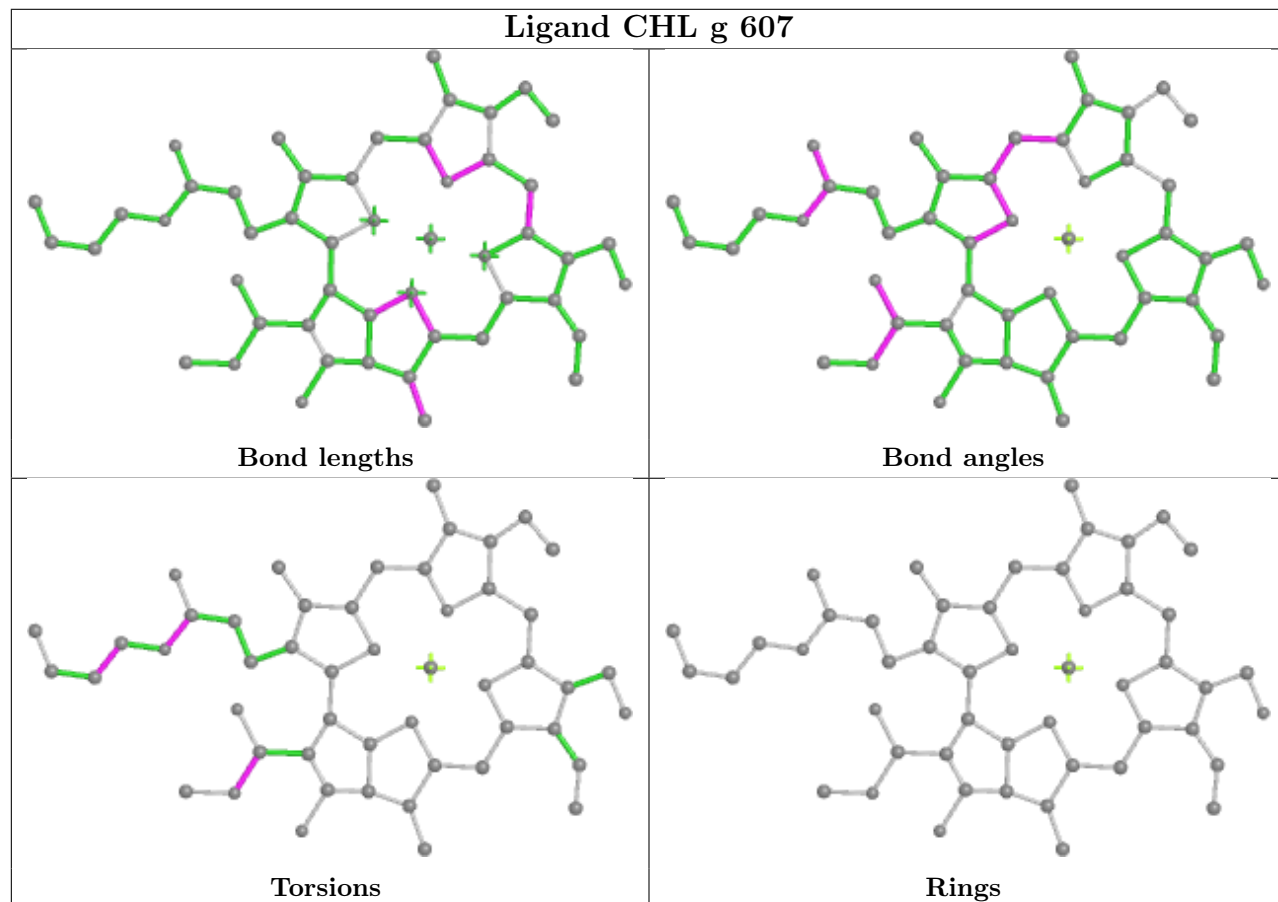




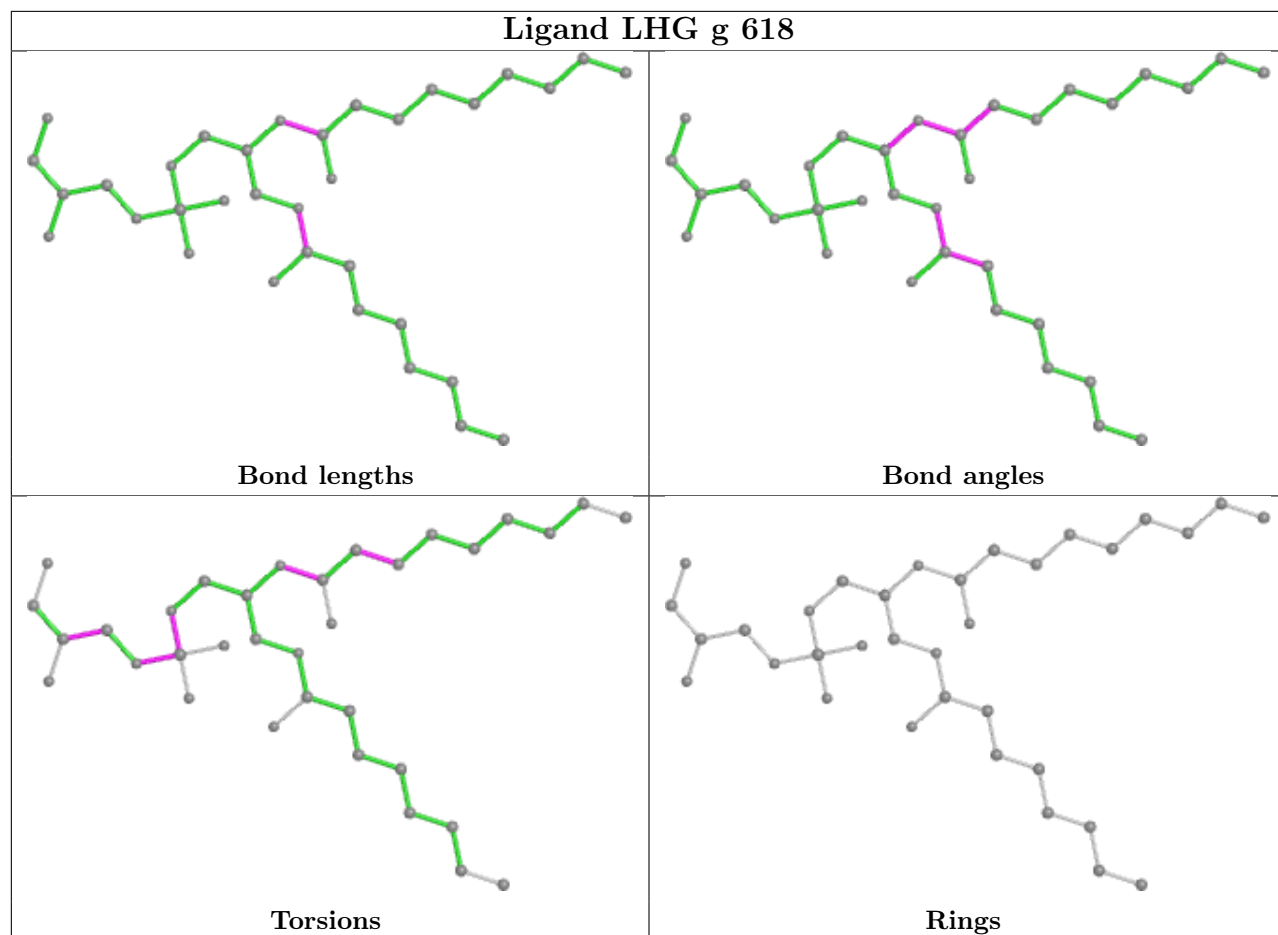
## Ligand LUT r 614



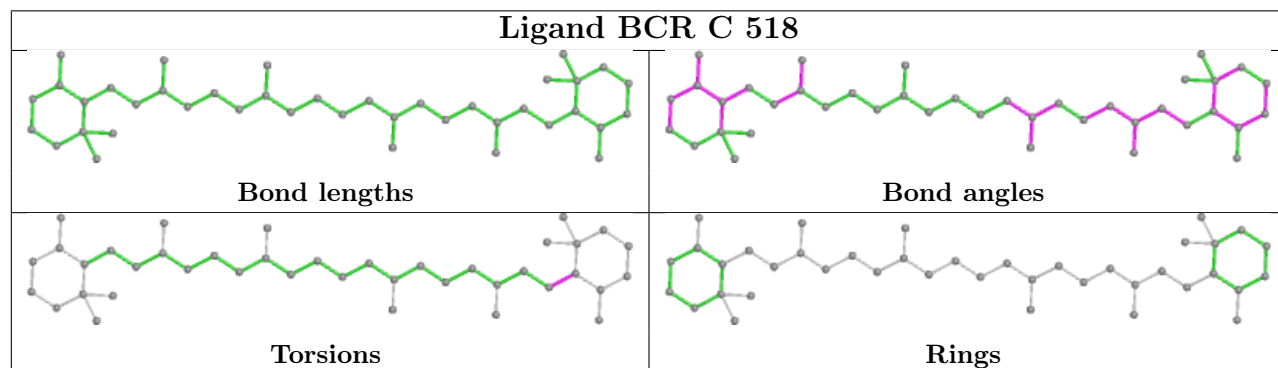
## Ligand CHL g 607



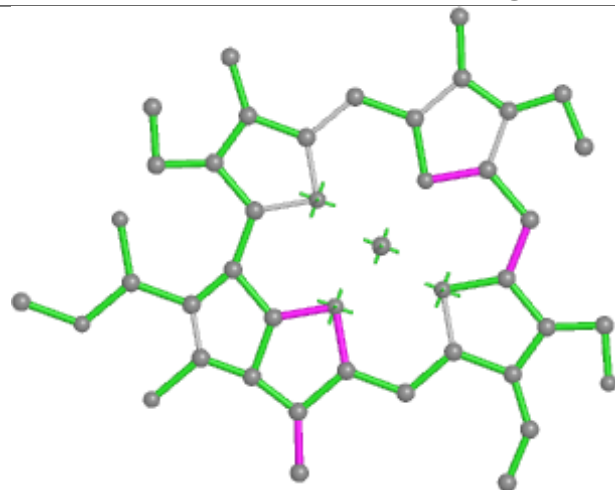
## Ligand LHG g 618



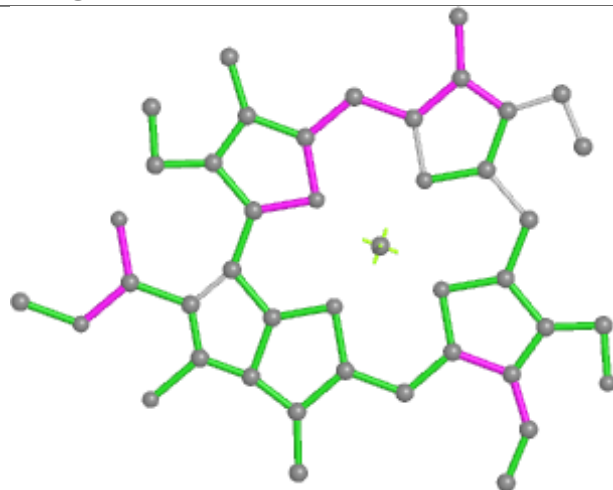
## Ligand BCR C 518



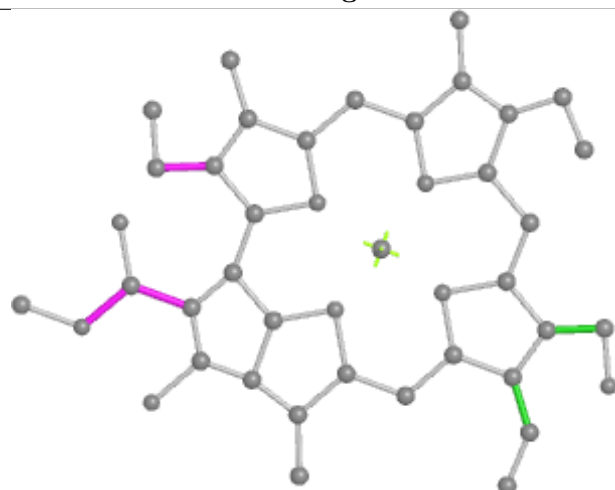
## Ligand CHL Gg 310



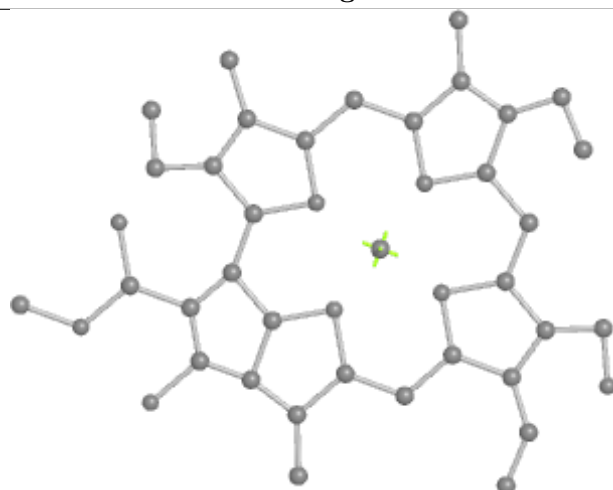
Bond lengths



Bond angles

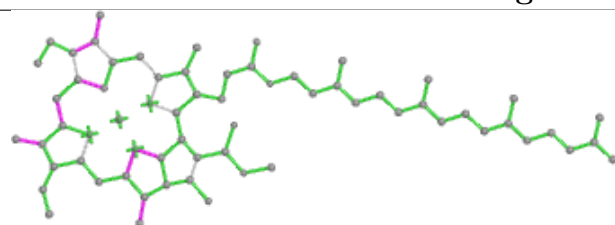


Torsions

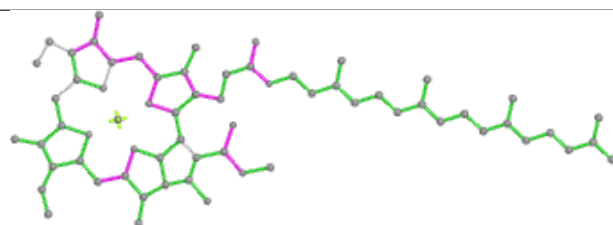


Rings

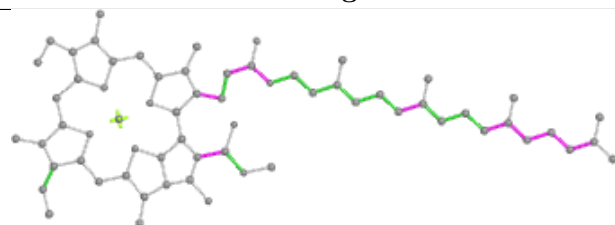
## Ligand CLA R 602



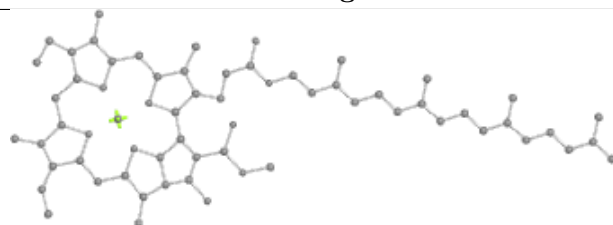
Bond lengths



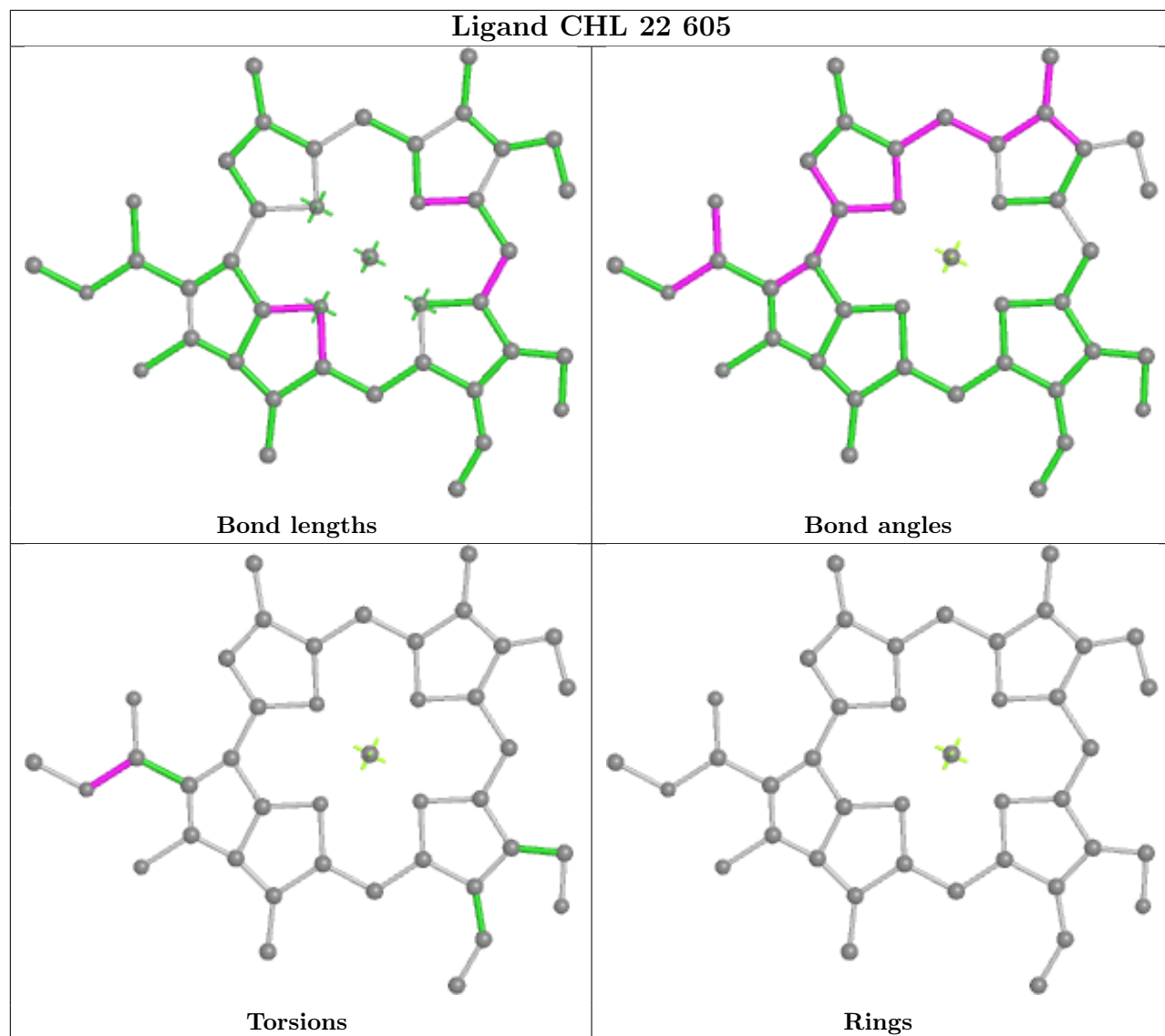
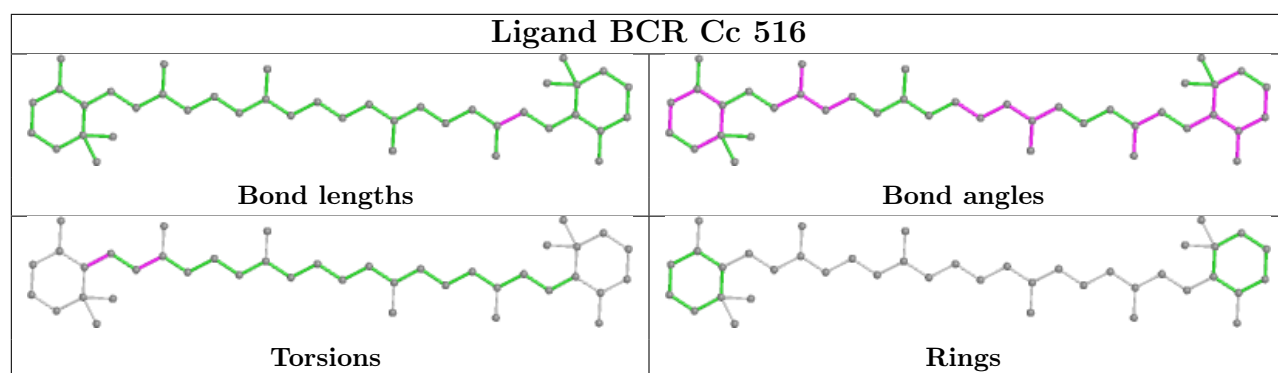
Bond angles

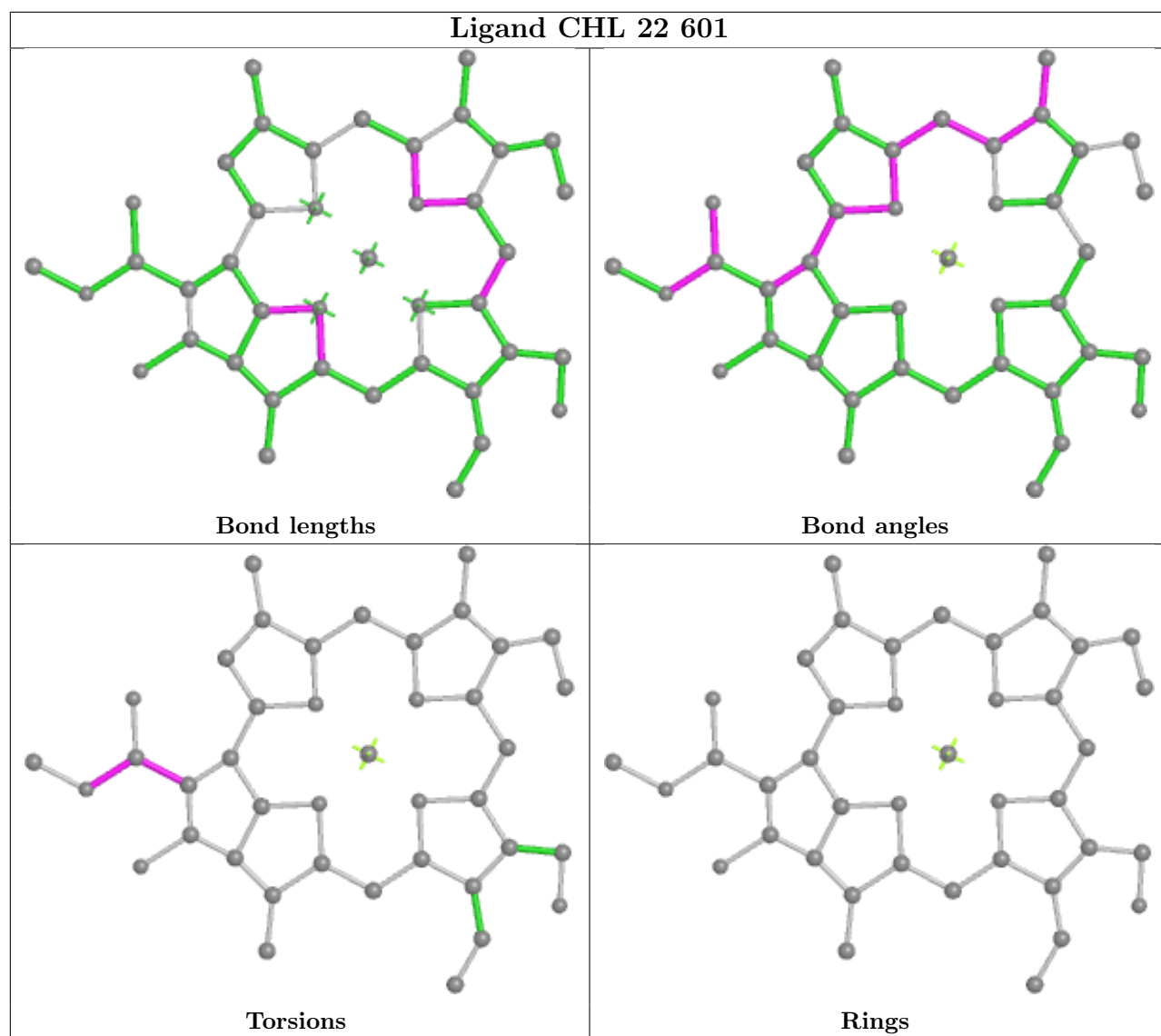
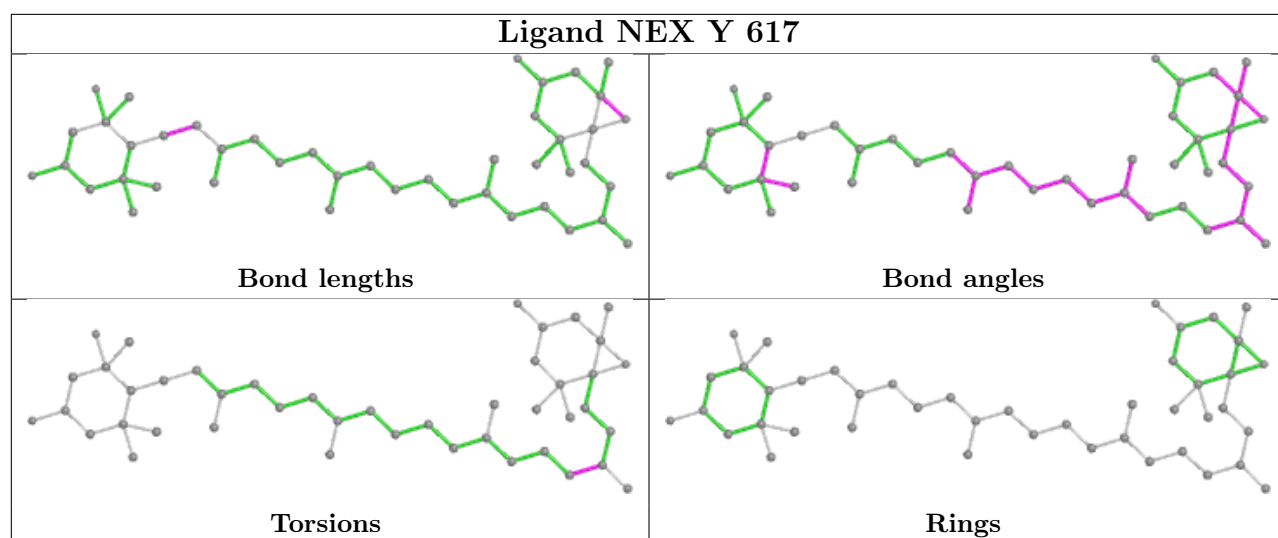


Torsions

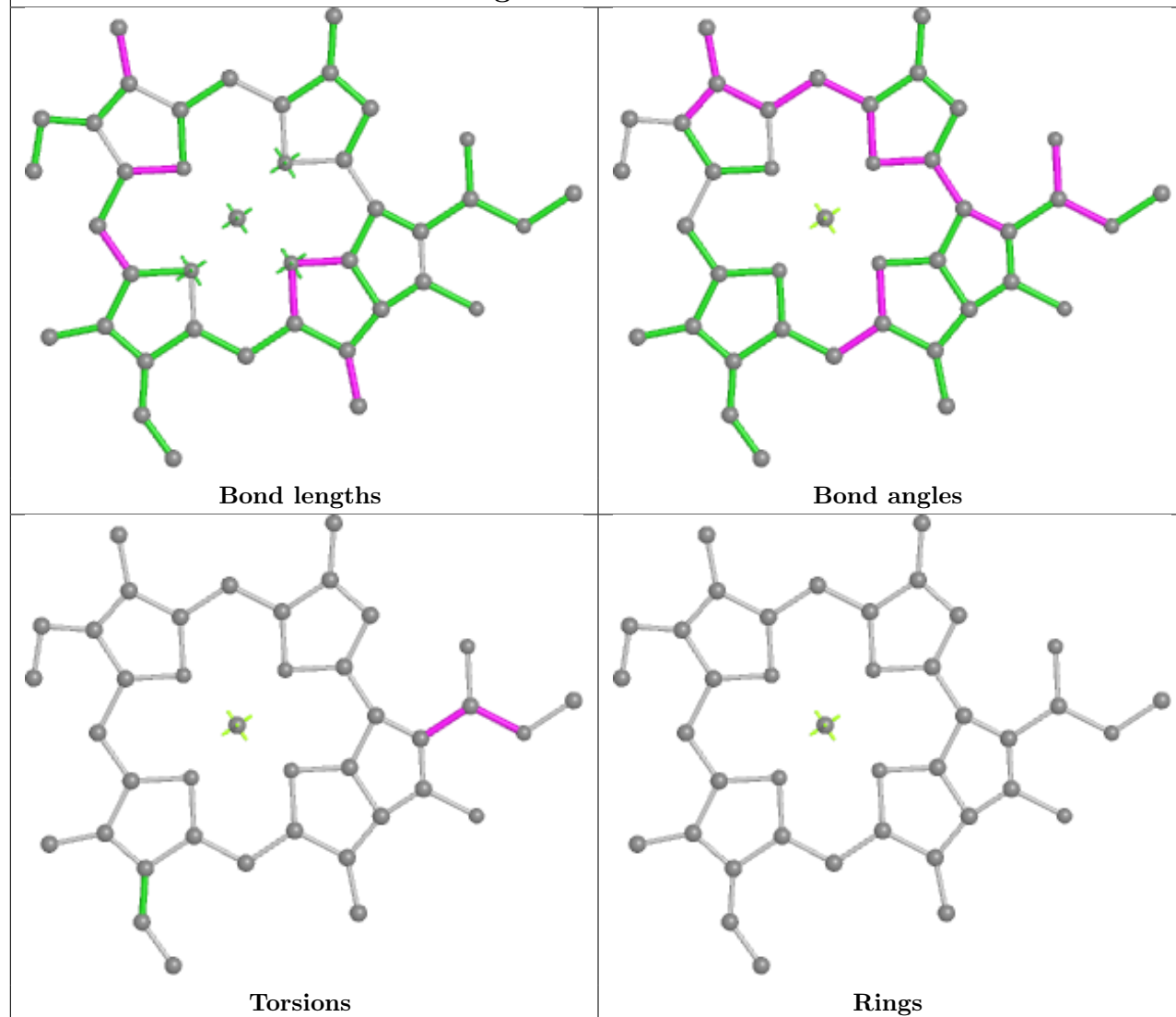


Rings

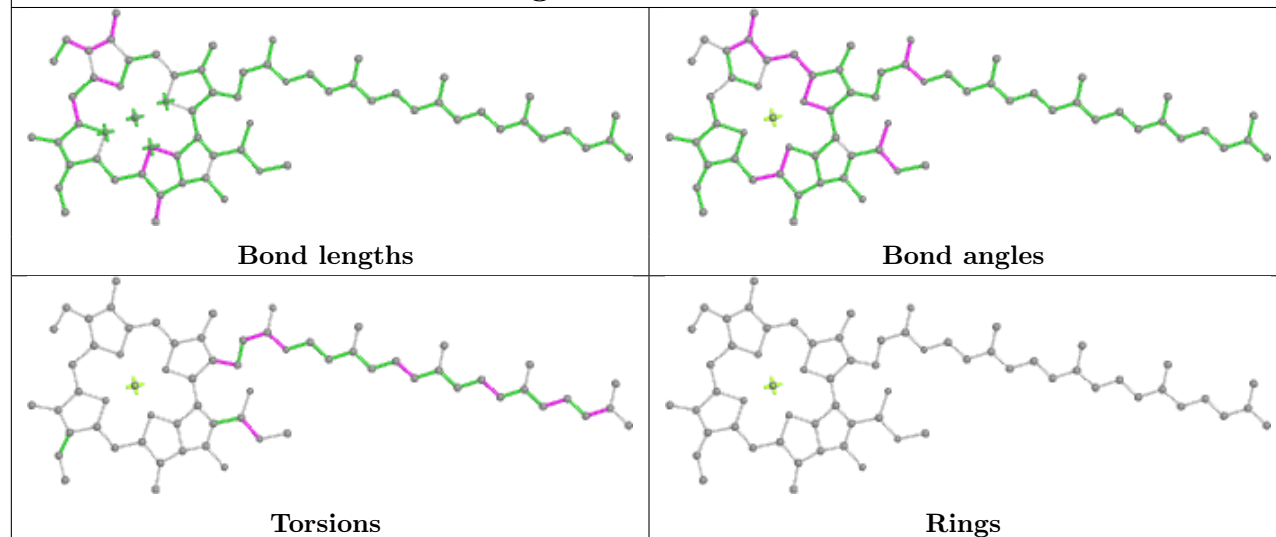




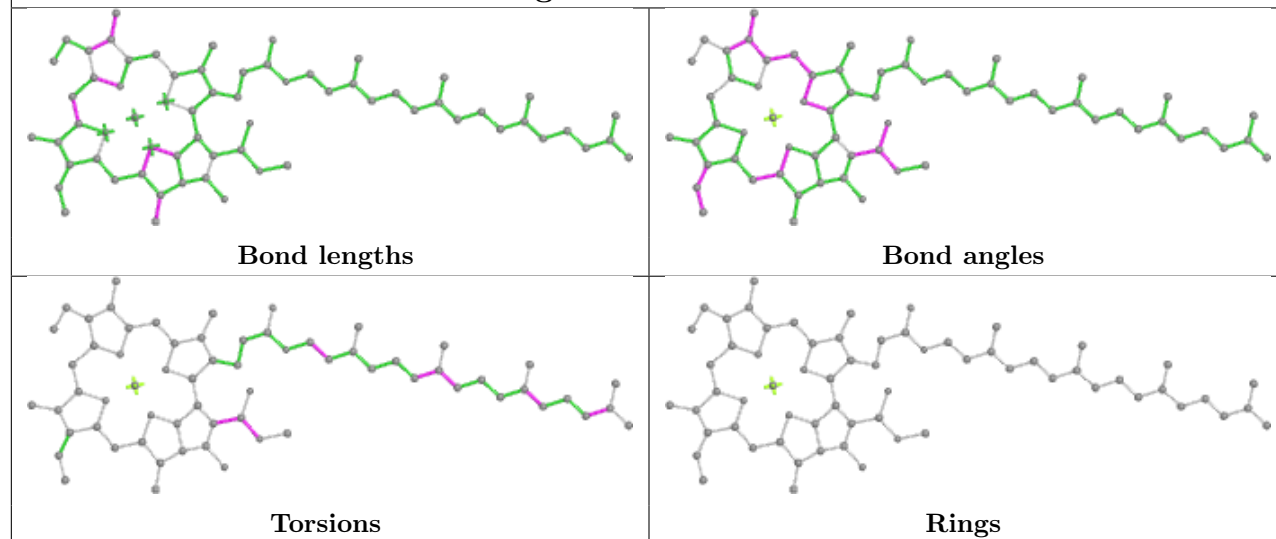
## Ligand CLA 2 610



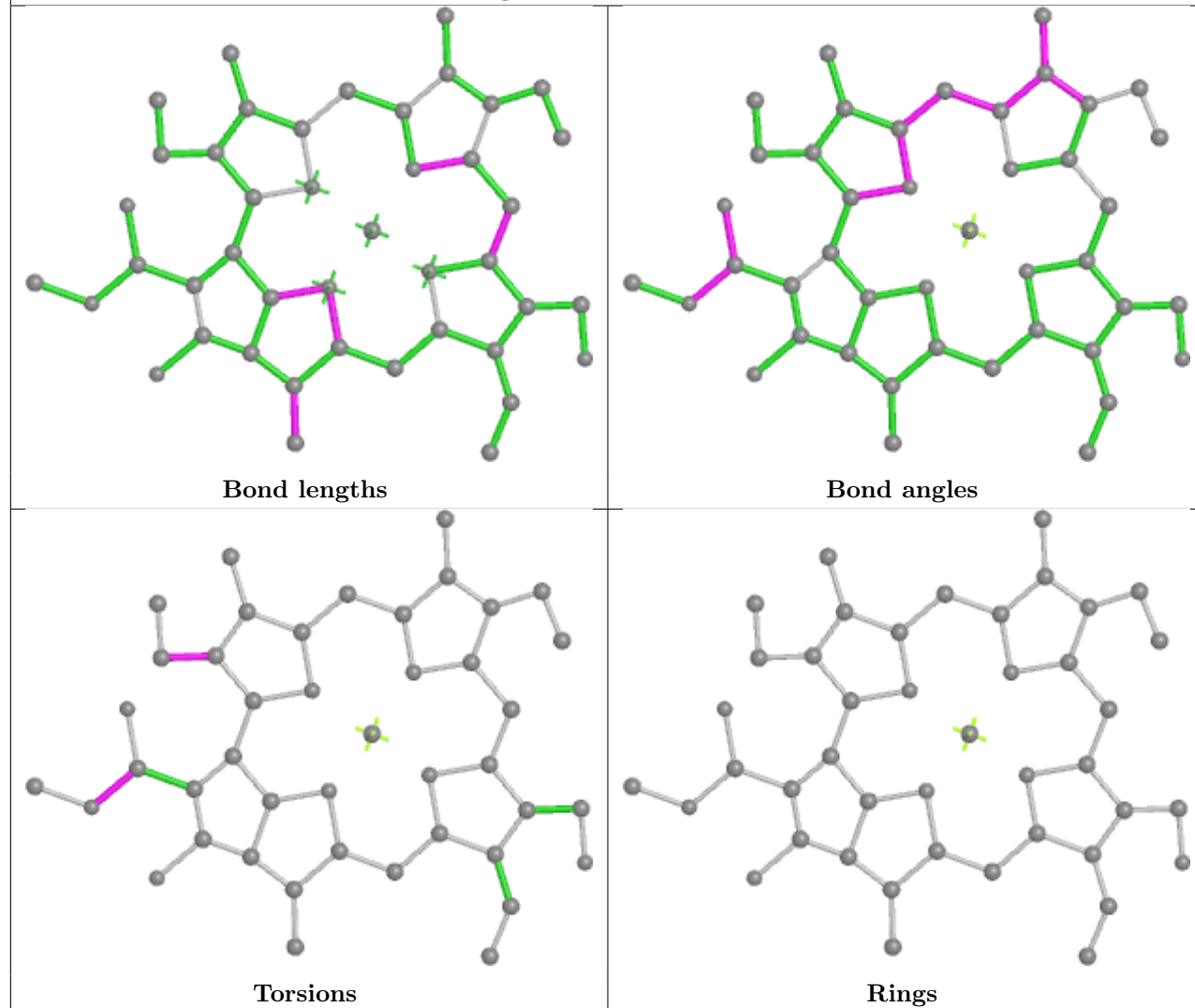
## Ligand CLA G 603



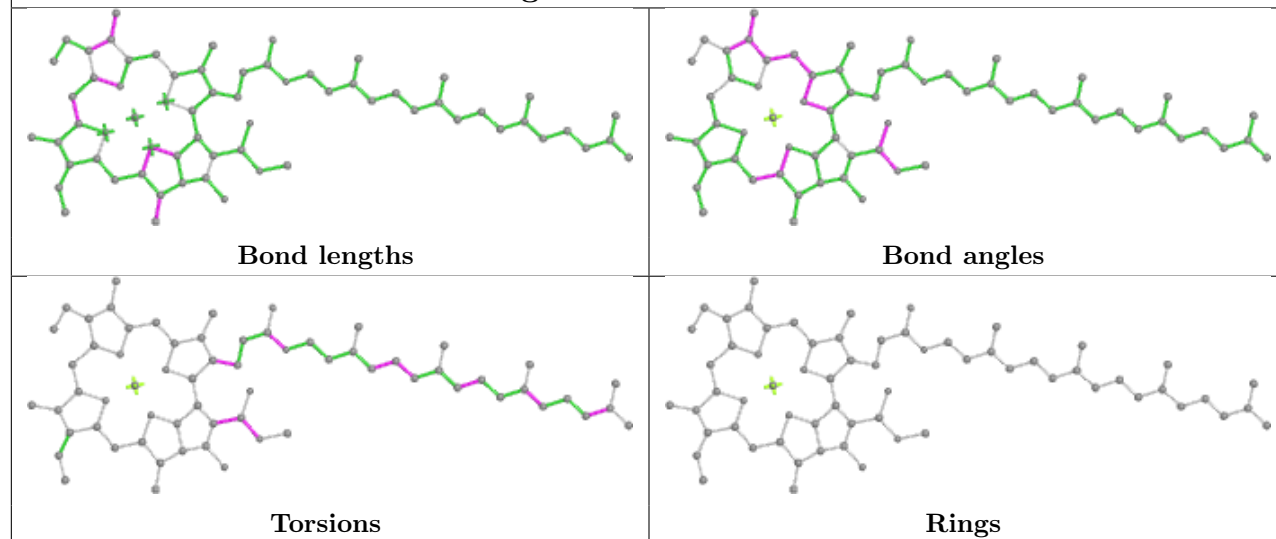
## Ligand CLA b 602



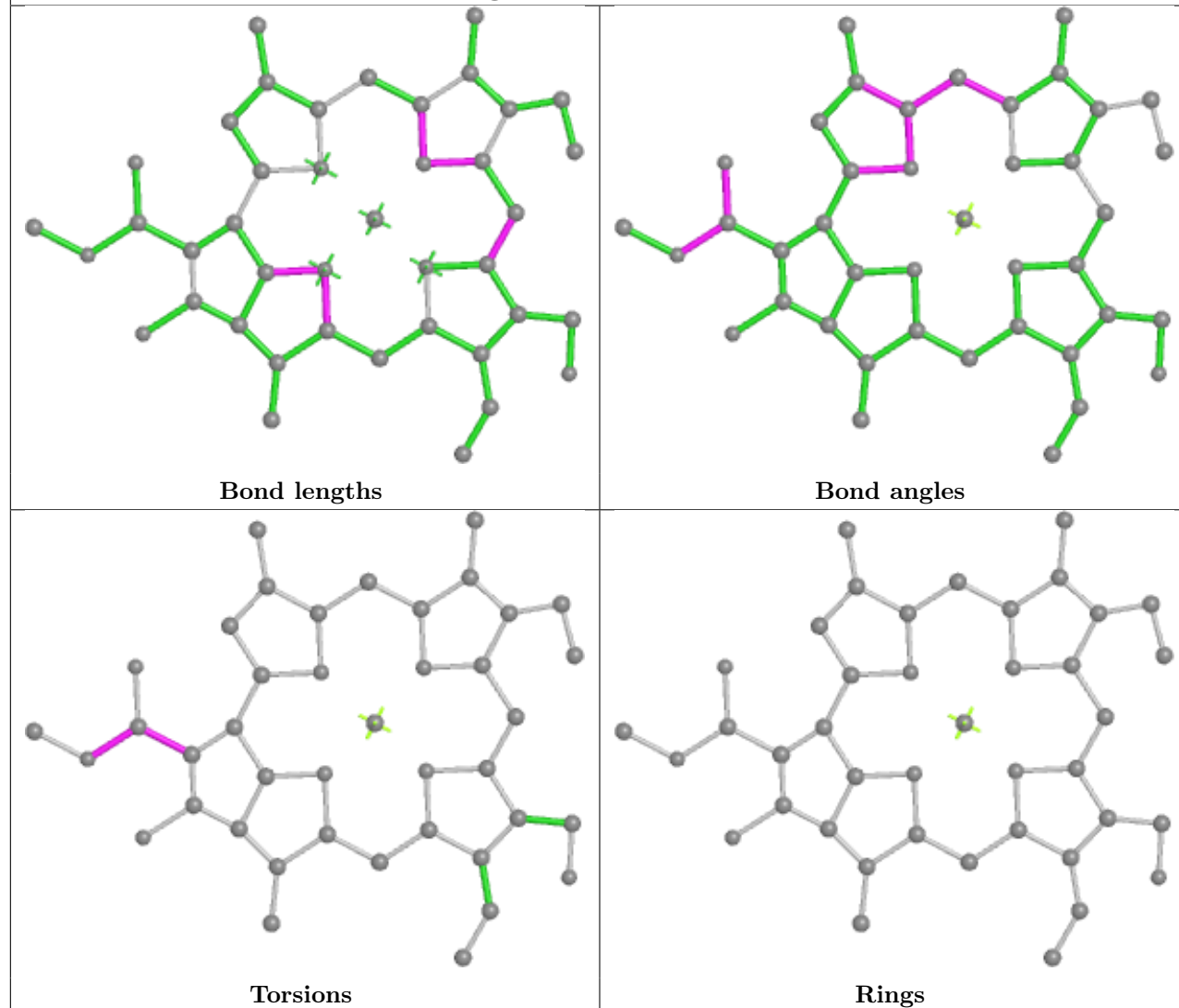
## Ligand CHL G 609



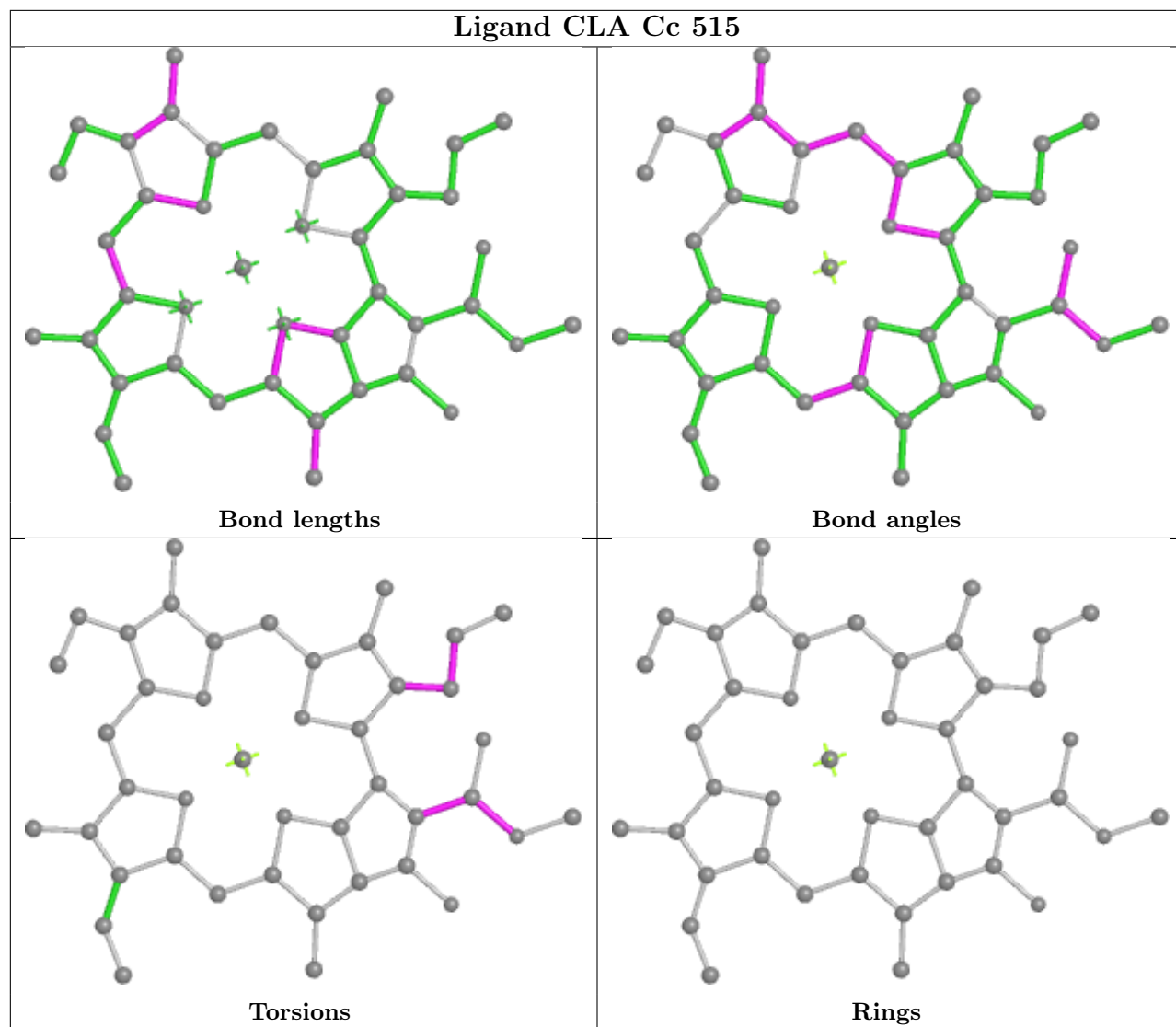
## Ligand CLA Dd 402



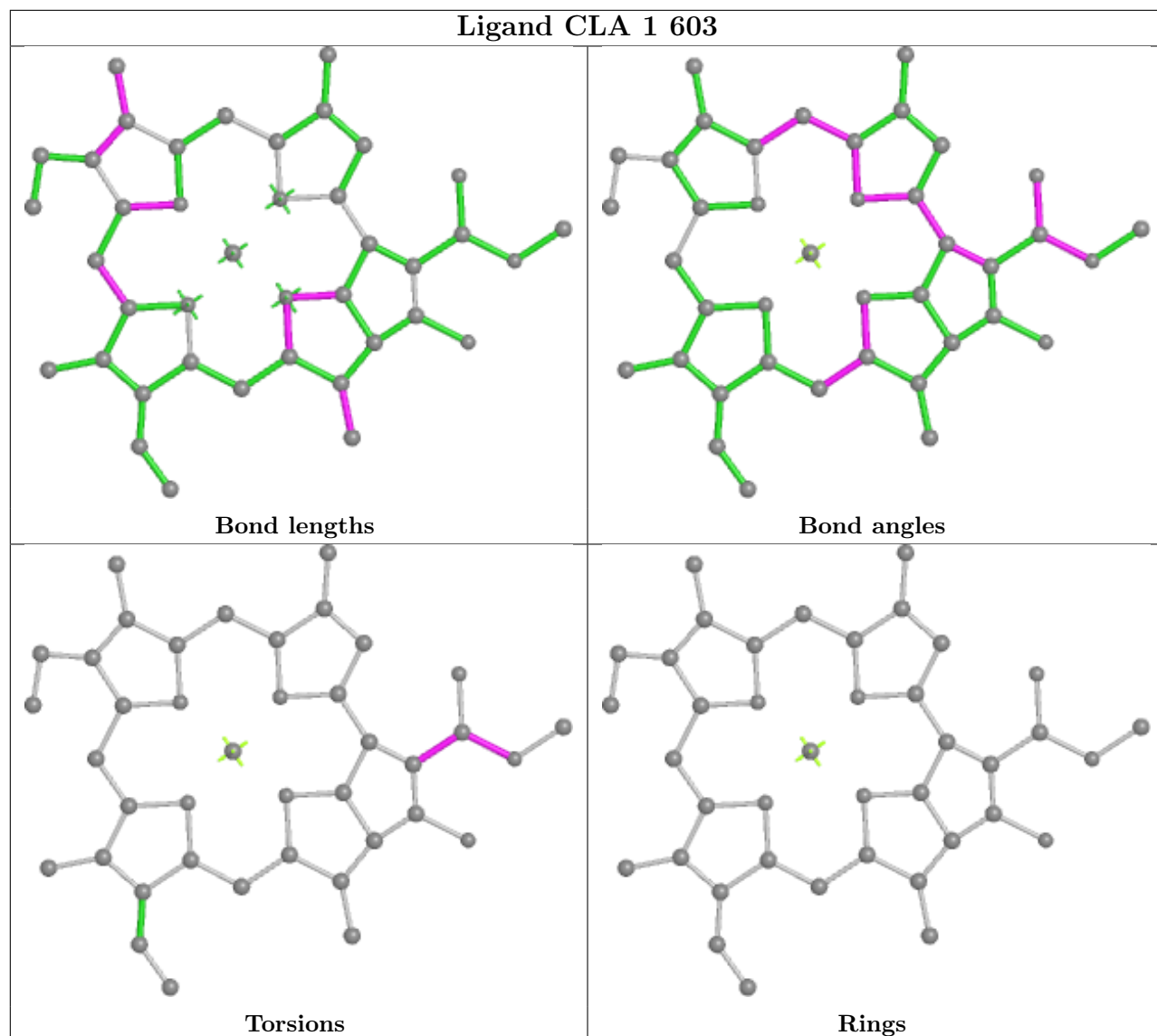
## Ligand CHL 33 601



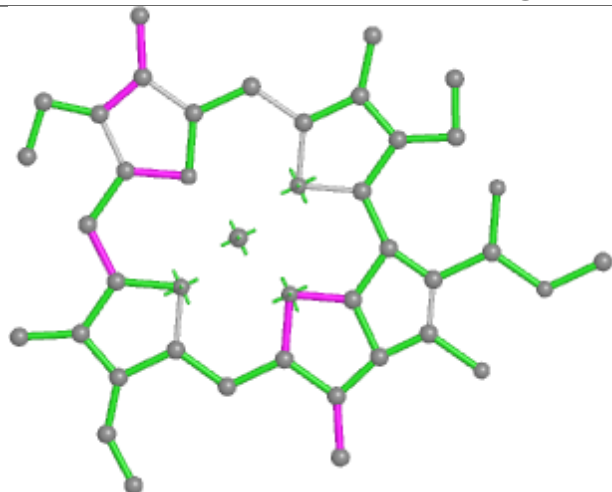




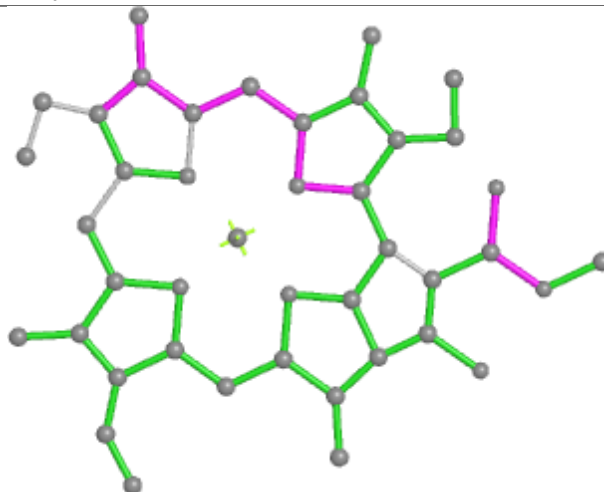
## Ligand CLA 1 603



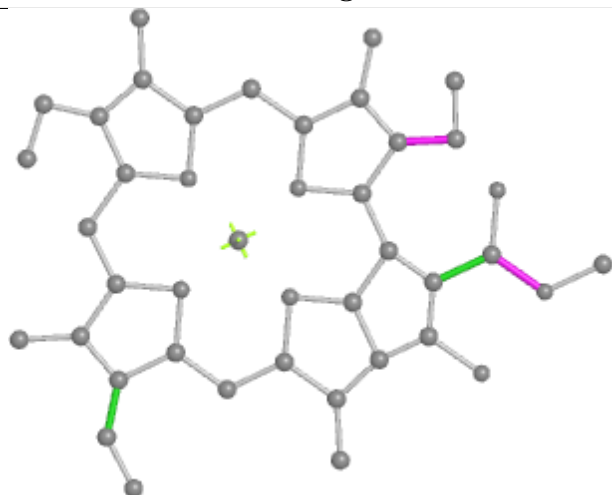
## Ligand CLA y 313



Bond lengths



Bond angles

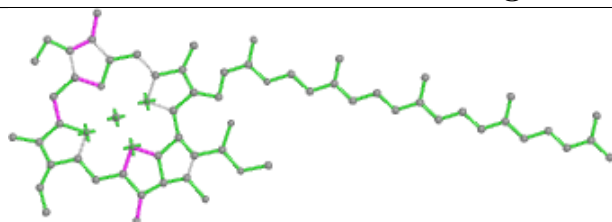


Torsions

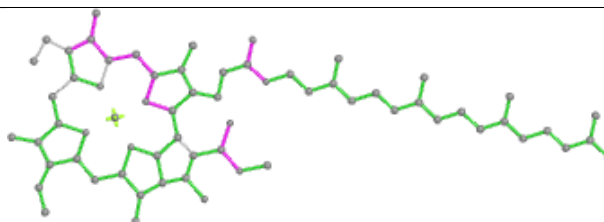


Rings

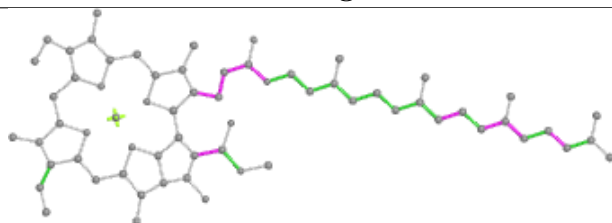
## Ligand CLA Bb 616



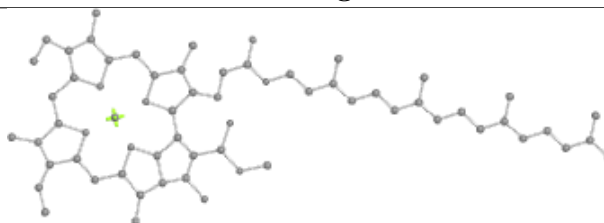
Bond lengths



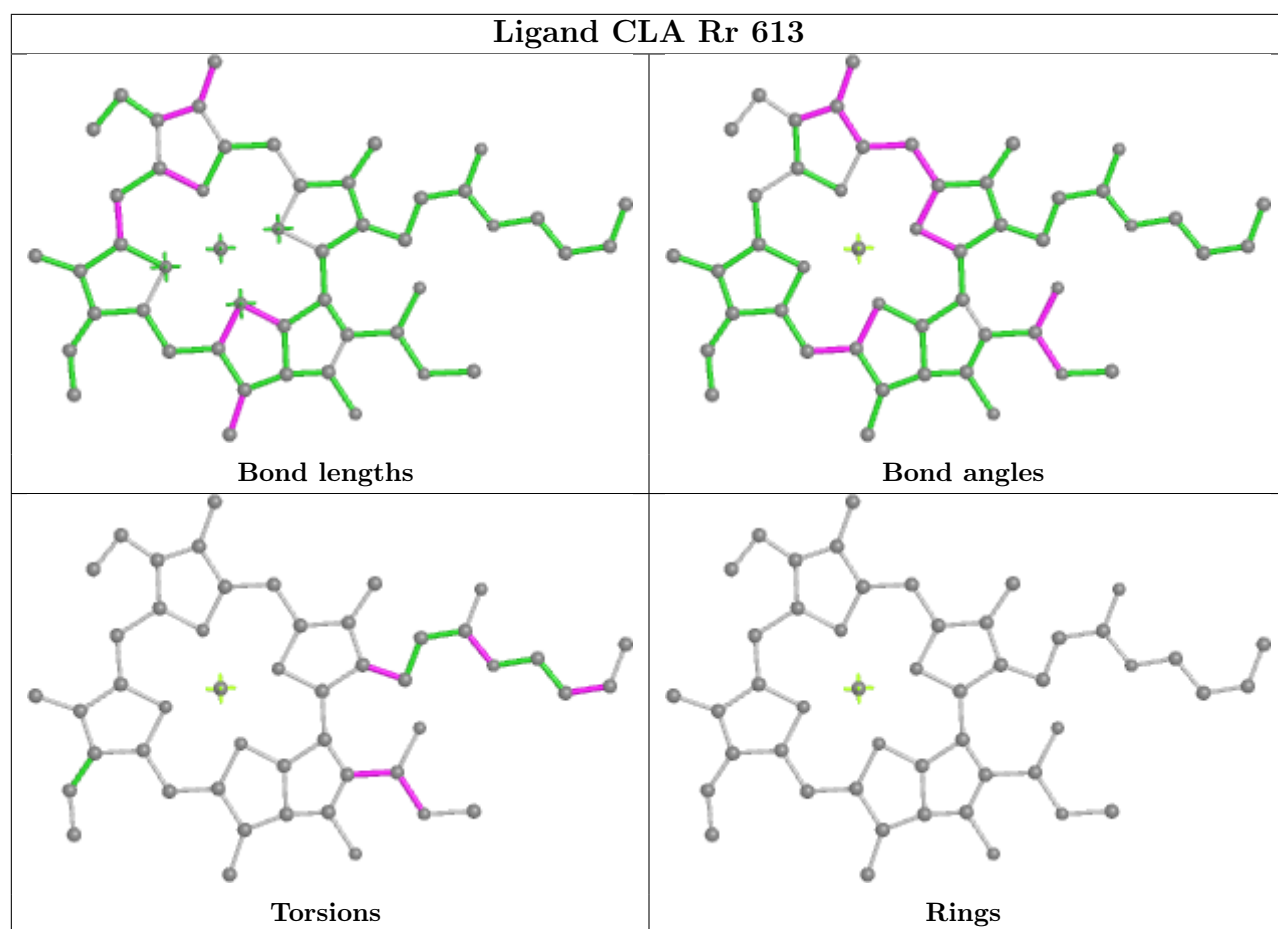
Bond angles

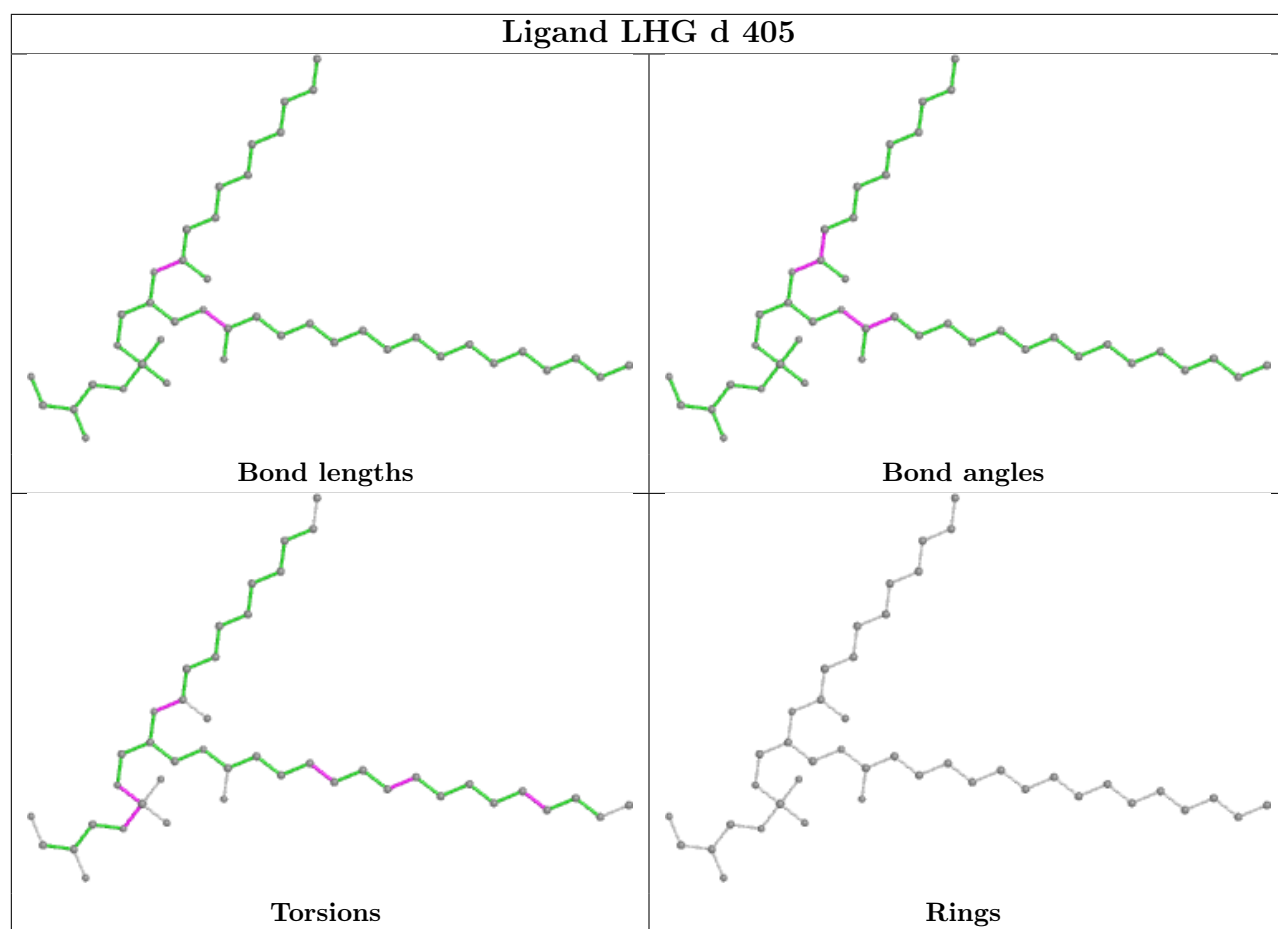


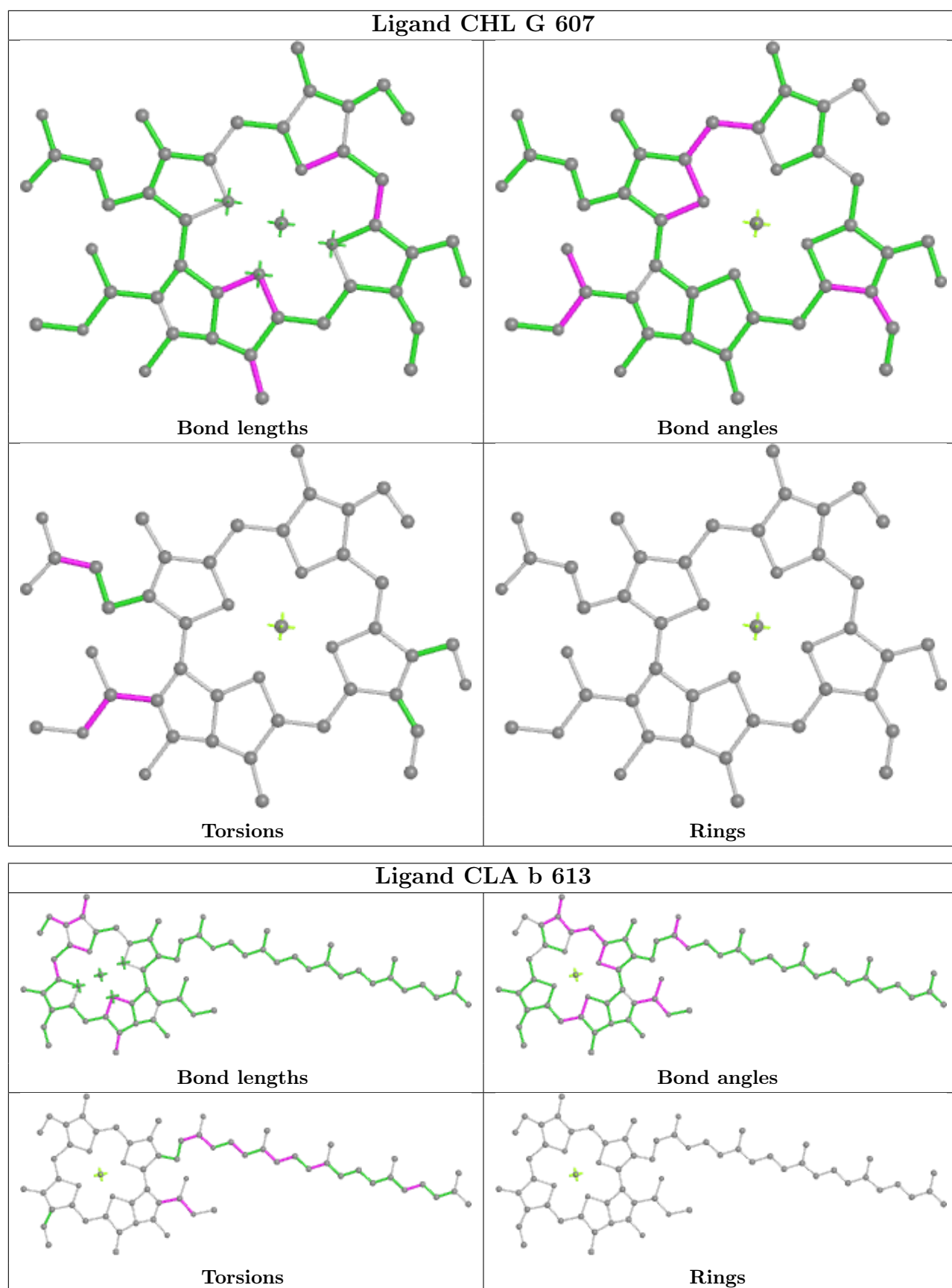
Torsions



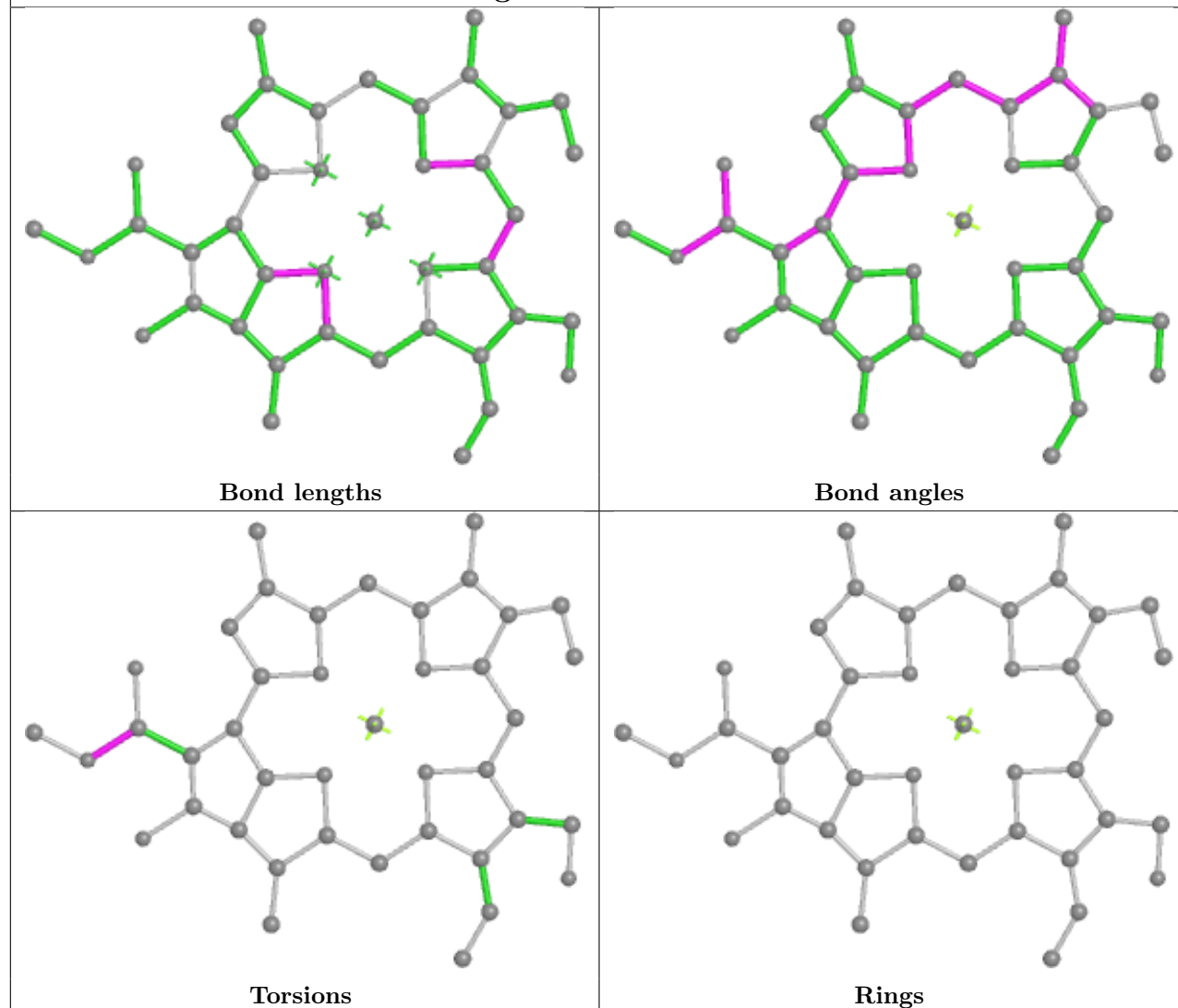
Rings



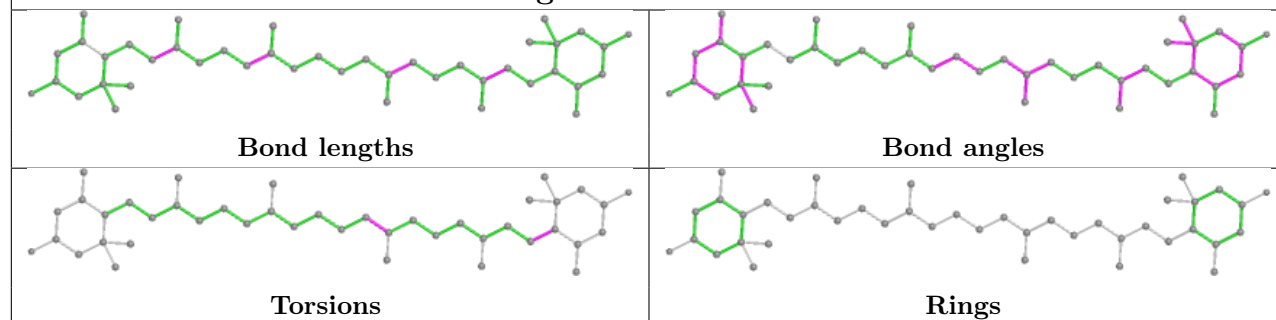




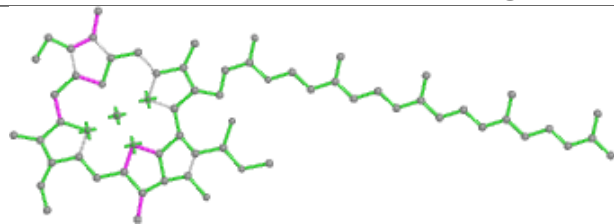
## Ligand CHL 2 605



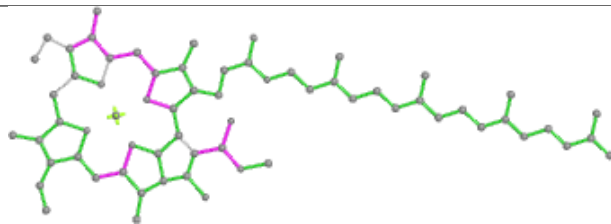
## Ligand LUT 2 614



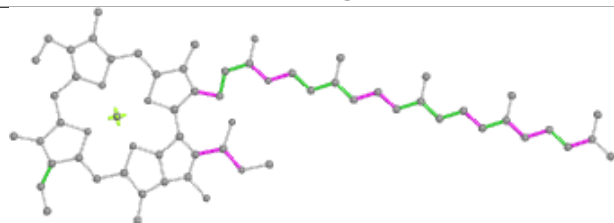
## Ligand CLA CC 509



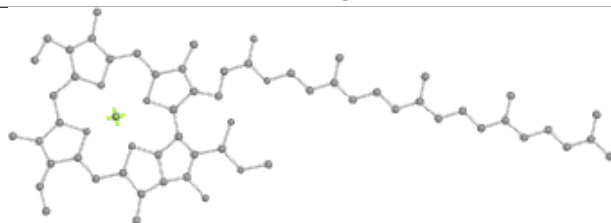
Bond lengths



Bond angles

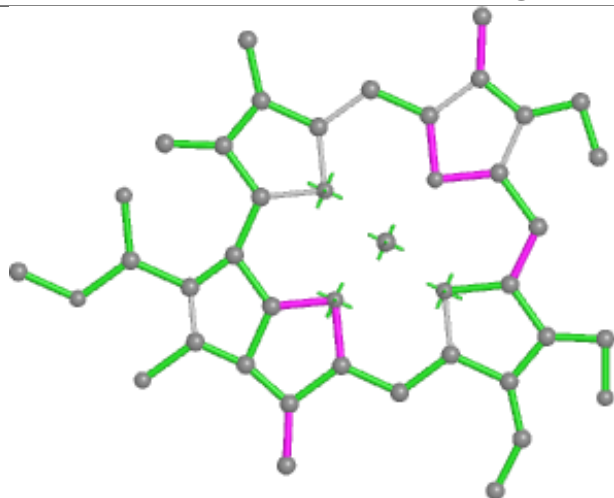


Torsions

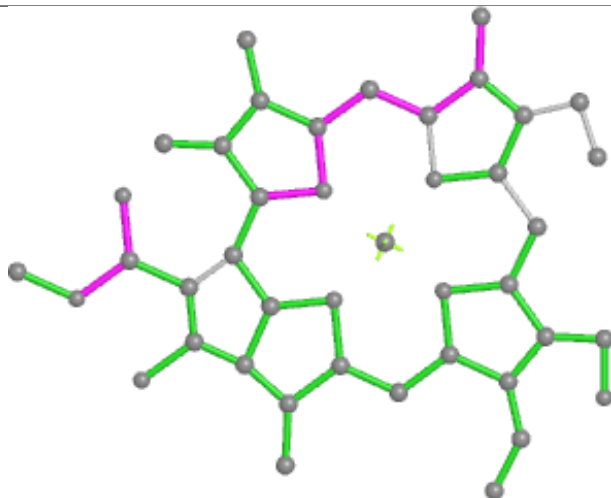


Rings

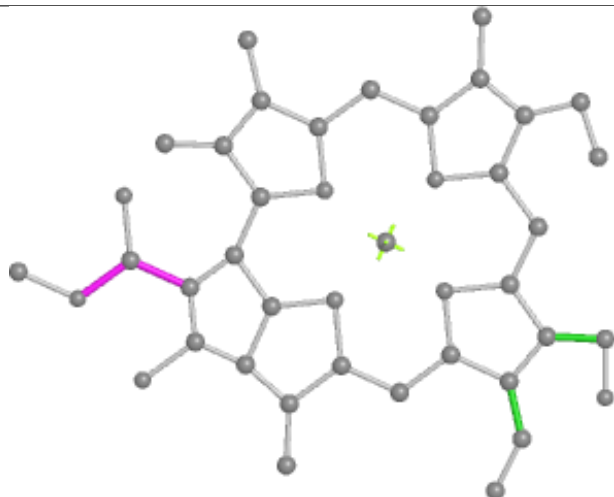
## Ligand CHL N 608



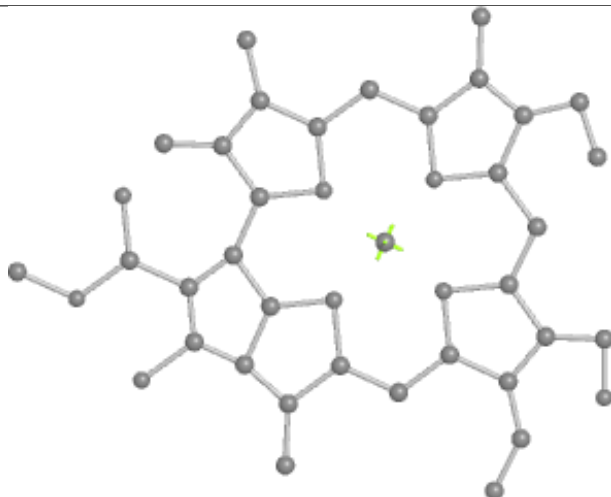
Bond lengths



Bond angles

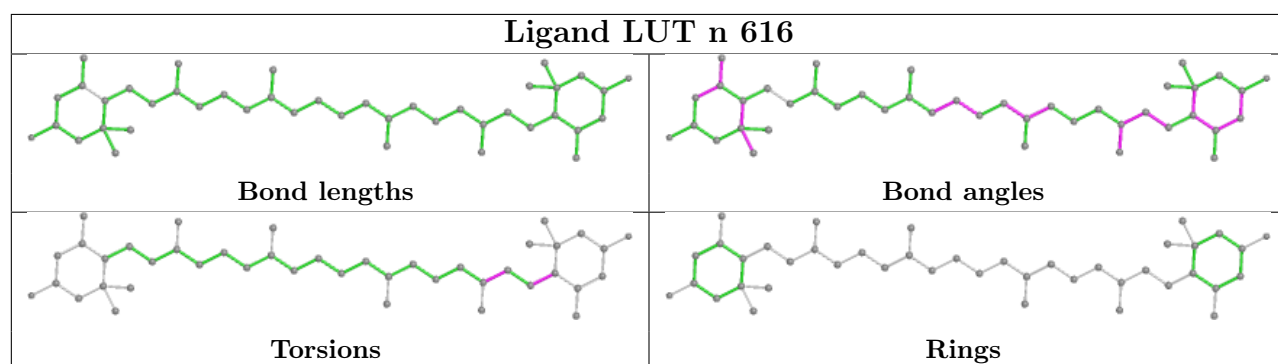
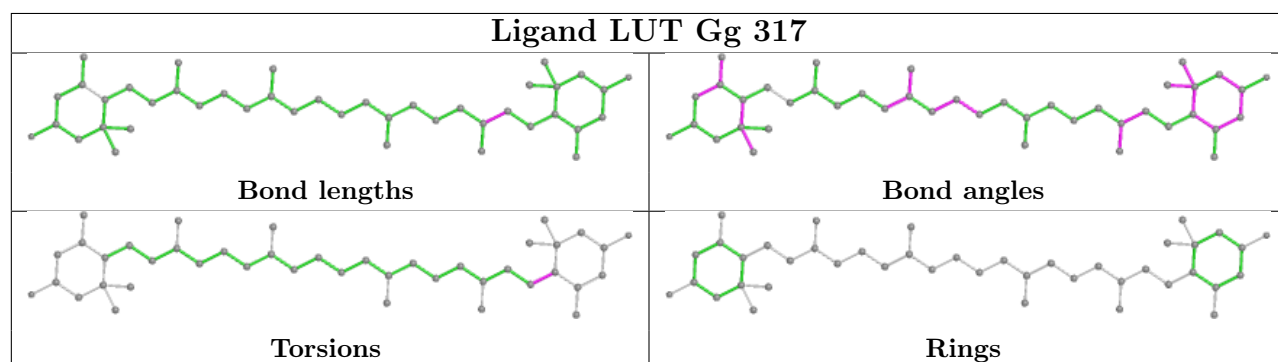
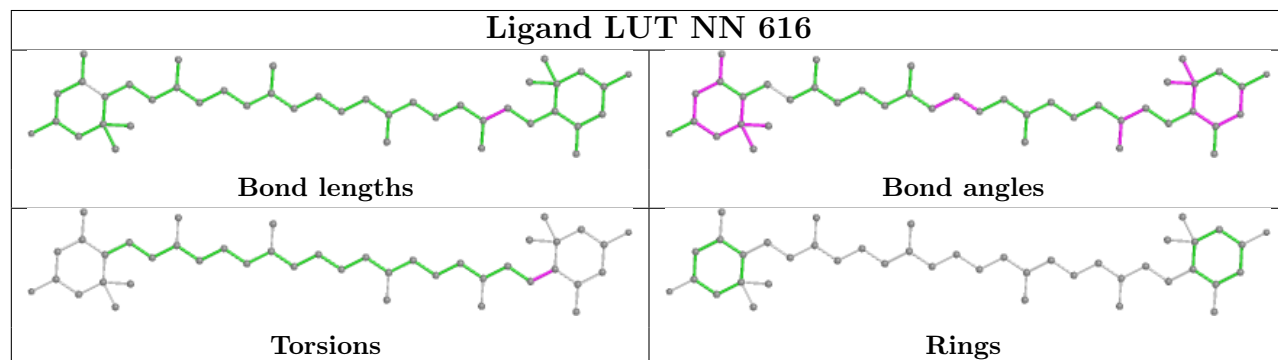
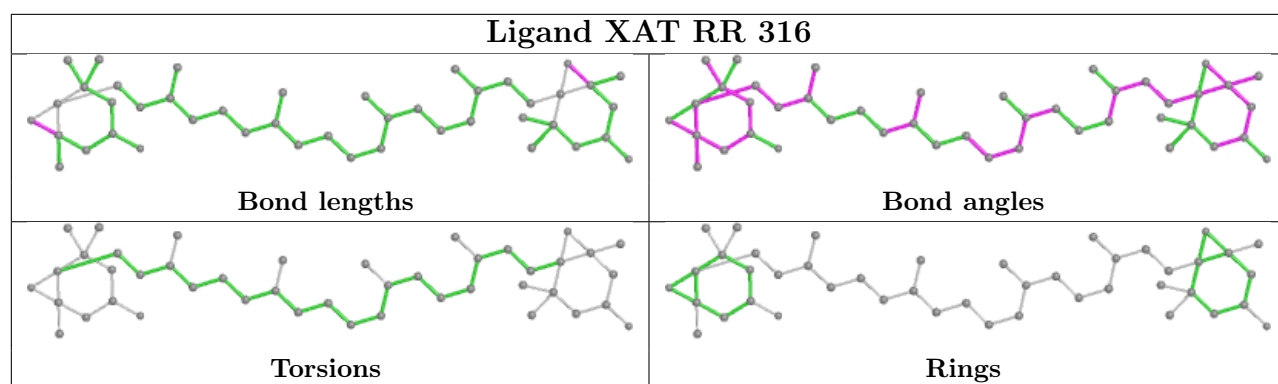


Torsions

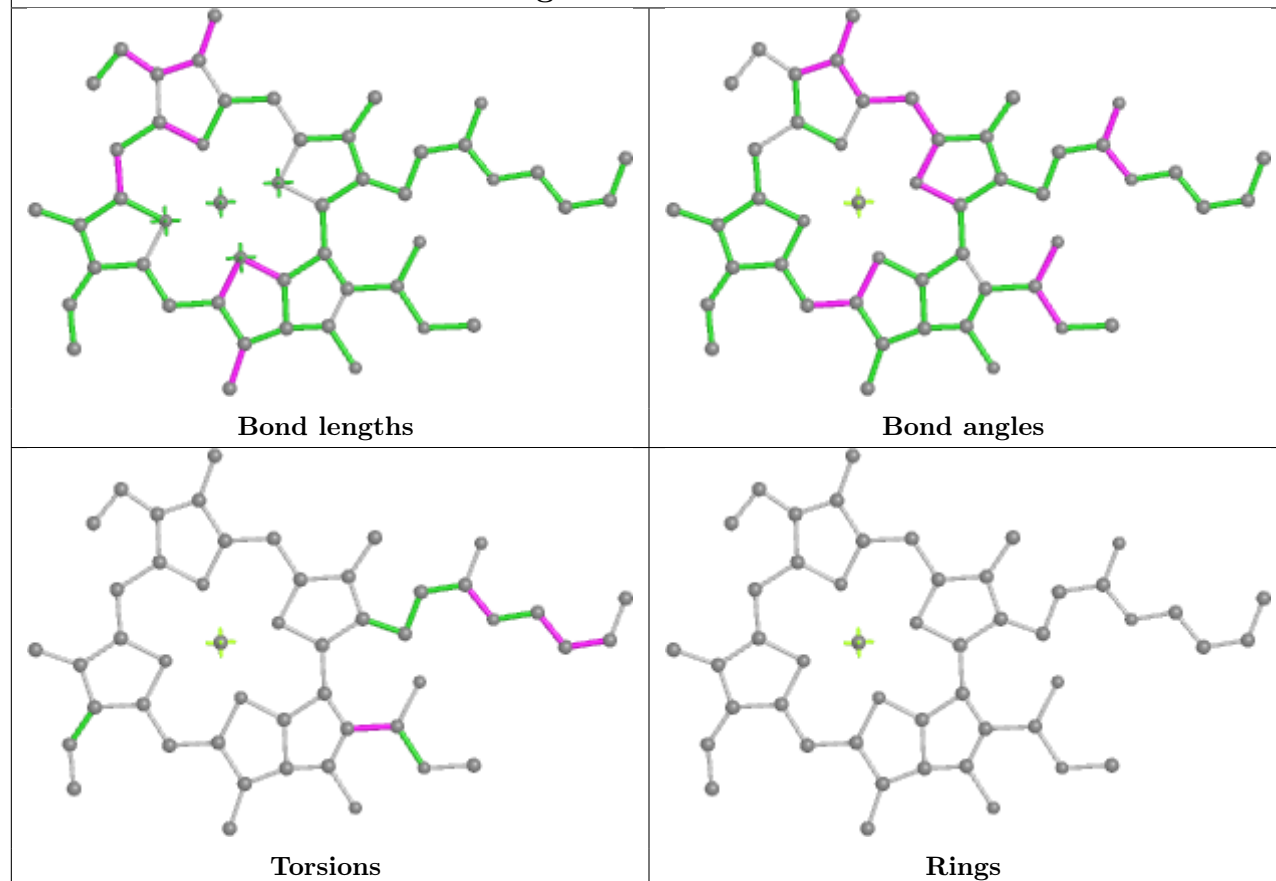


Rings

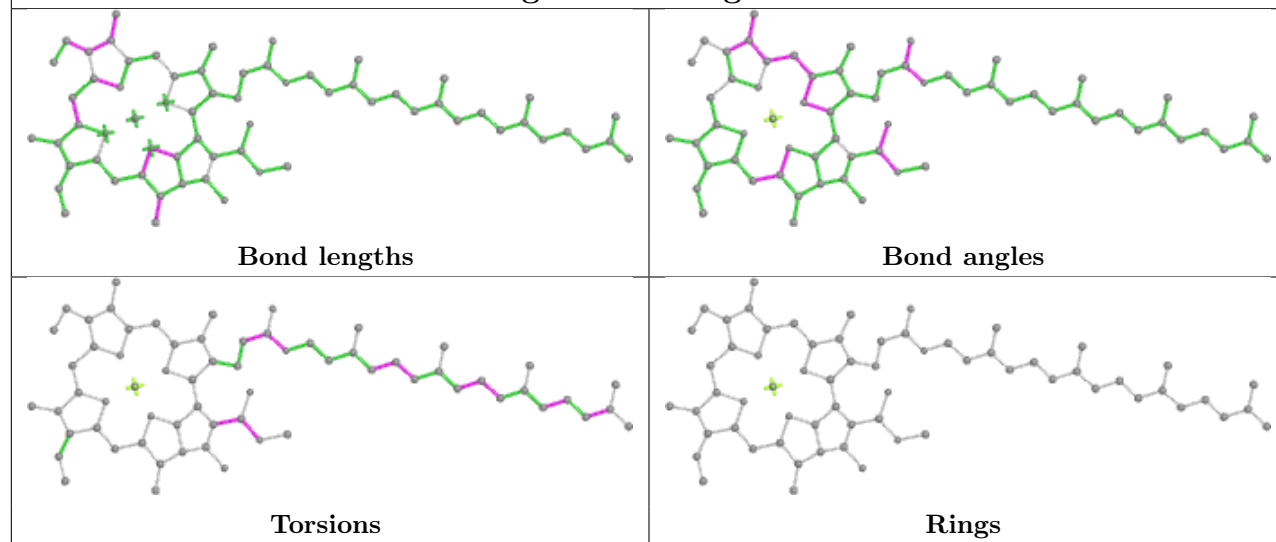


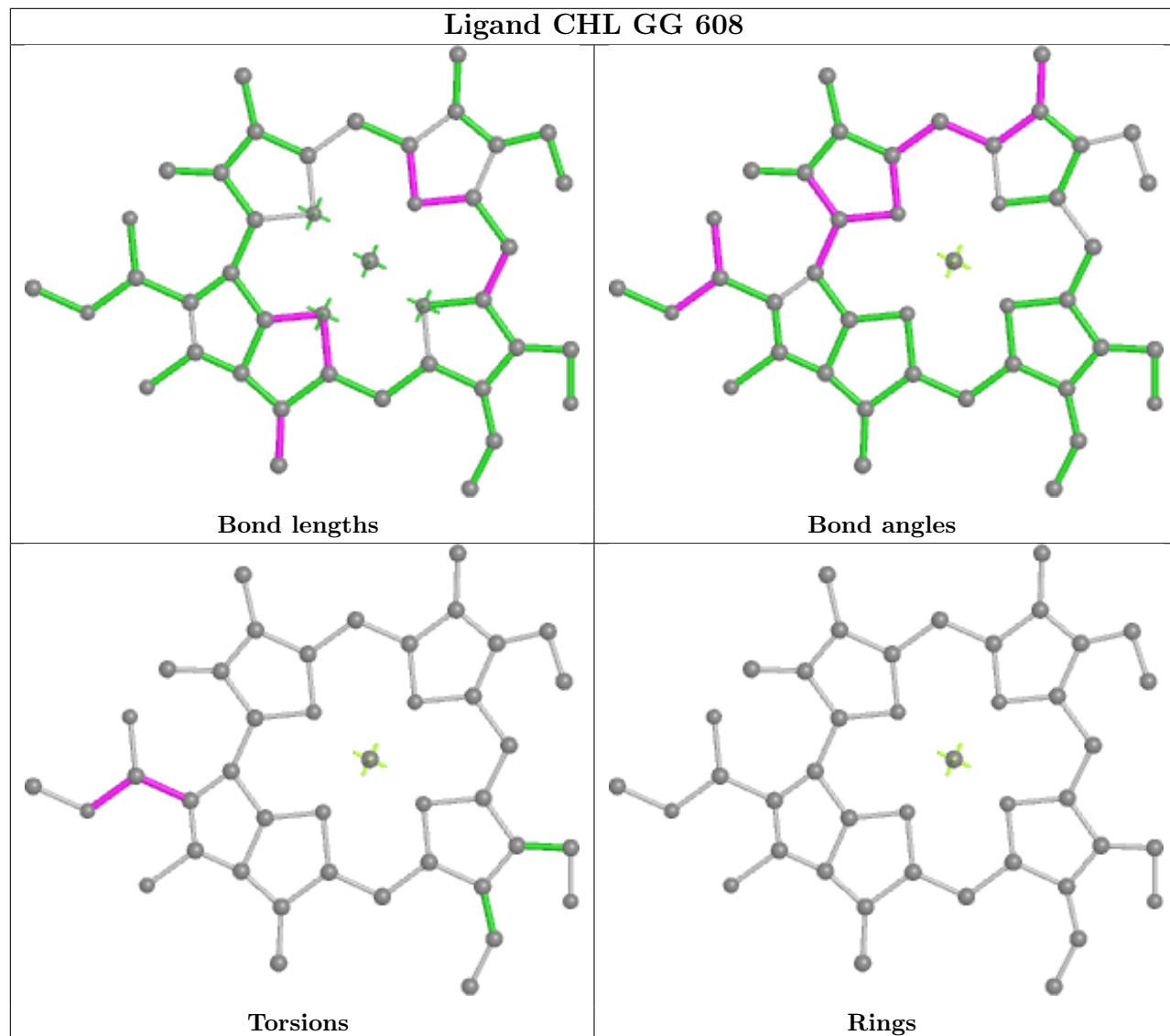
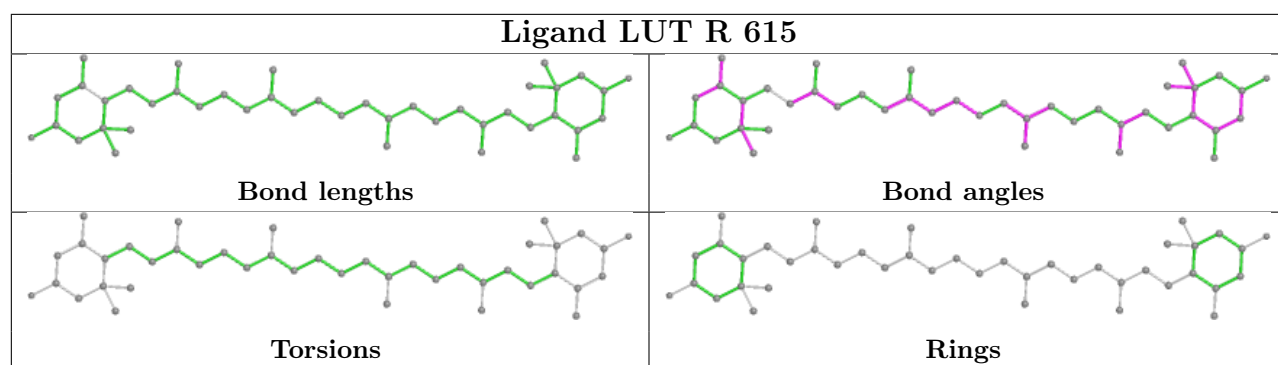


## Ligand CLA a 407

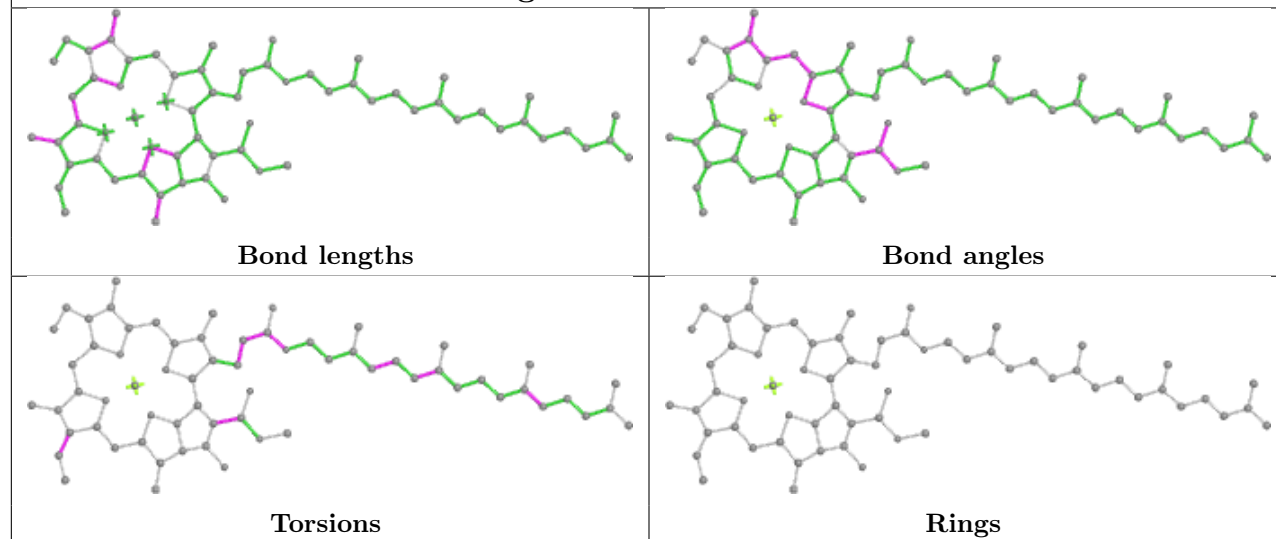


## Ligand CLA Gg 304

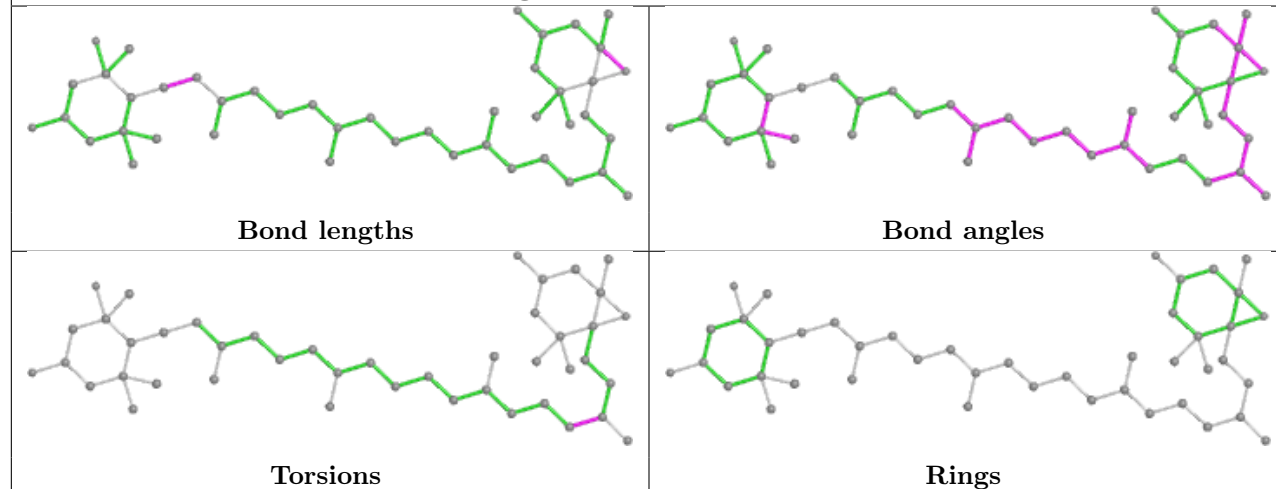




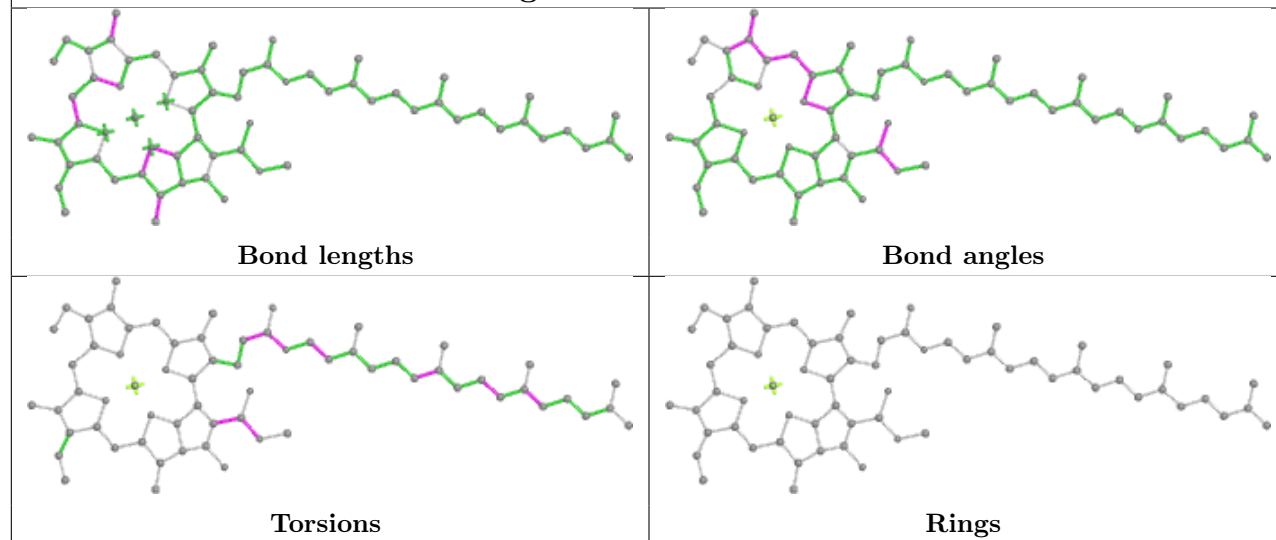
## Ligand CLA DD 403

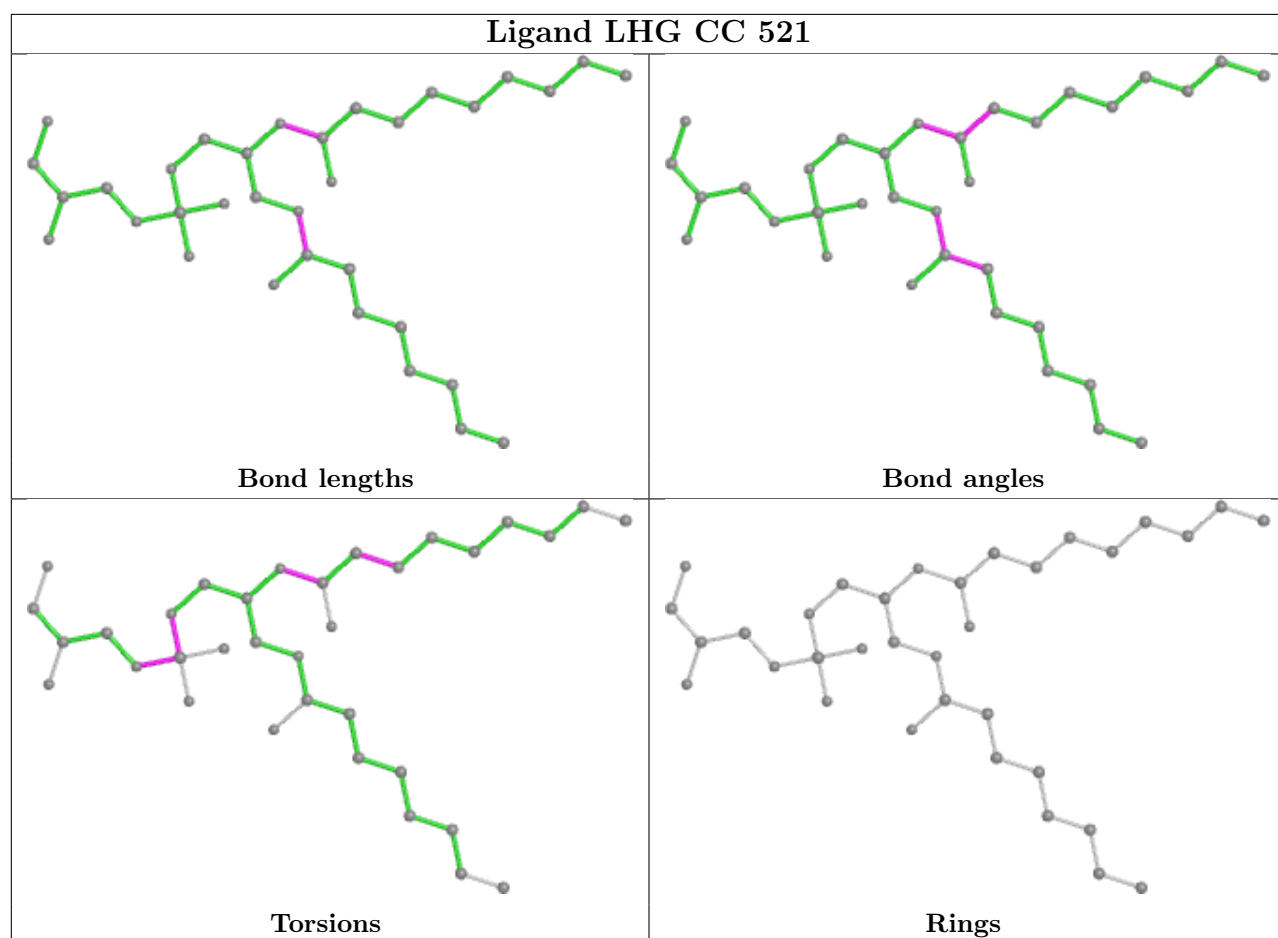


## Ligand NEX YY 617

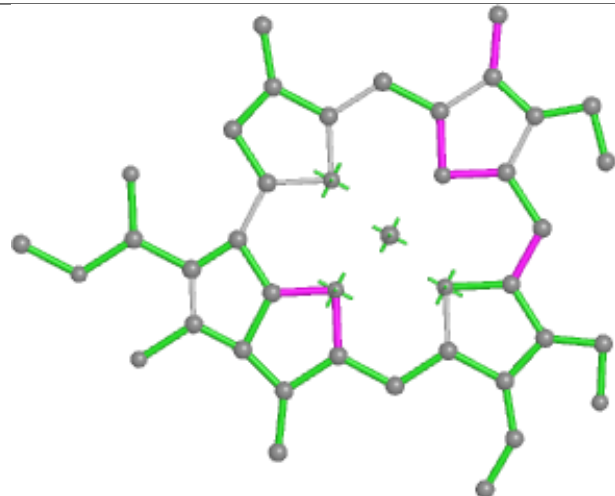


## Ligand CLA BB 612

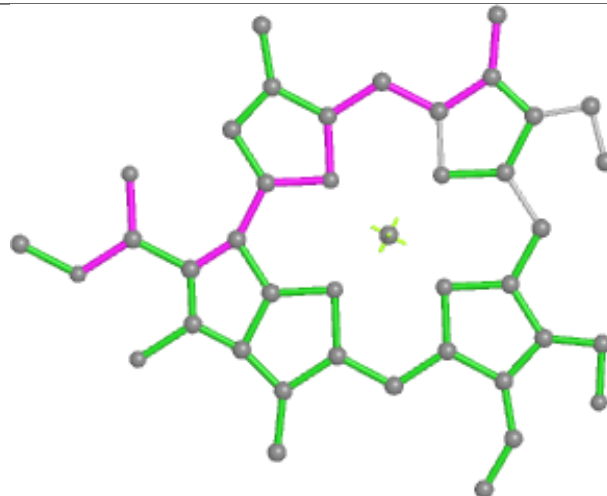




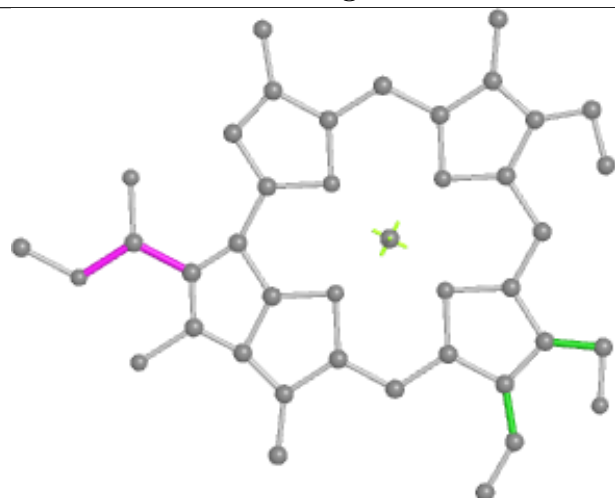
## Ligand CHL 2 608



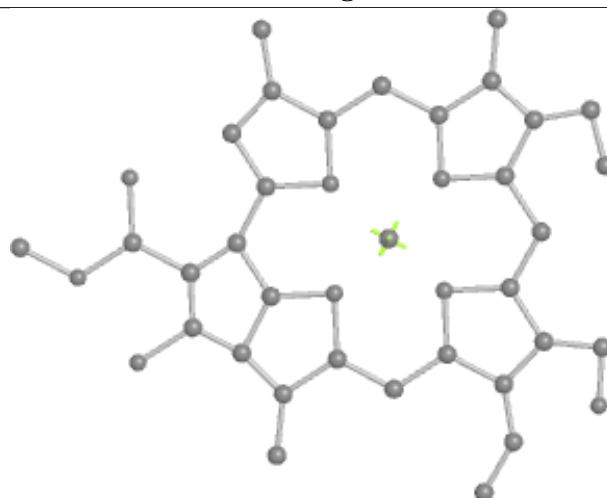
Bond lengths



Bond angles

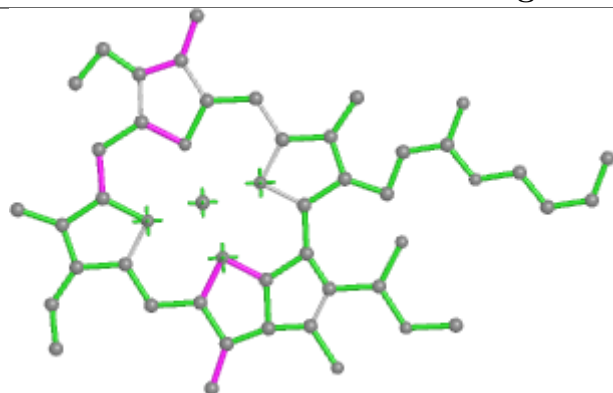


Torsions

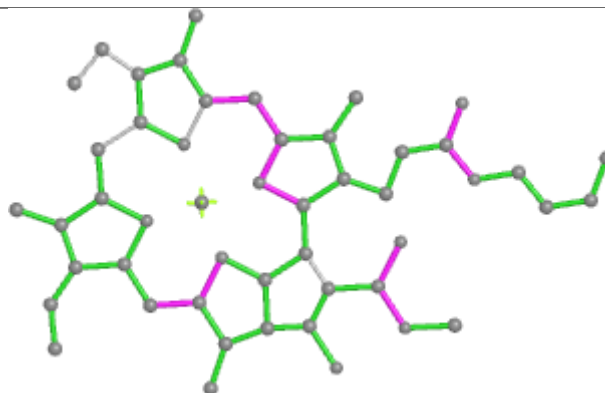


Rings

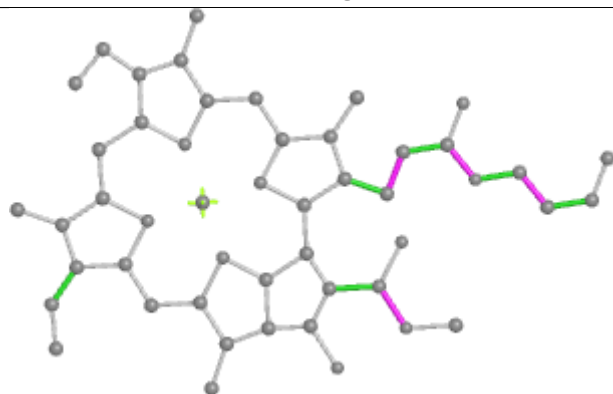
## Ligand CLA S 612



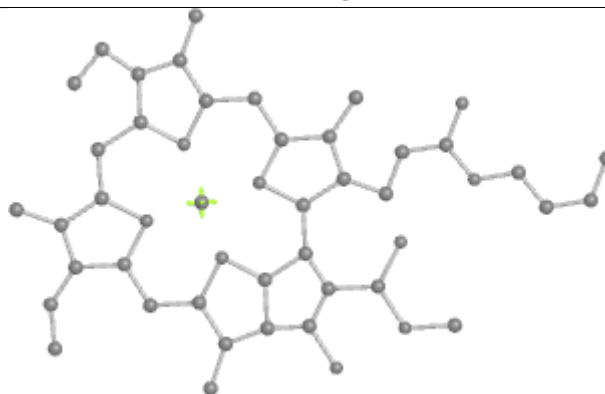
Bond lengths



Bond angles

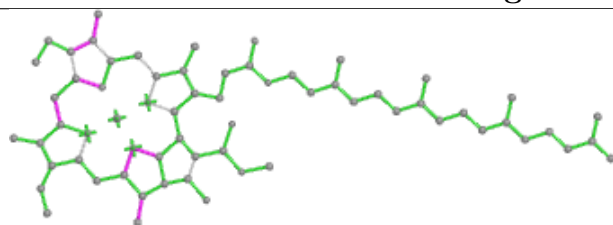


Torsions

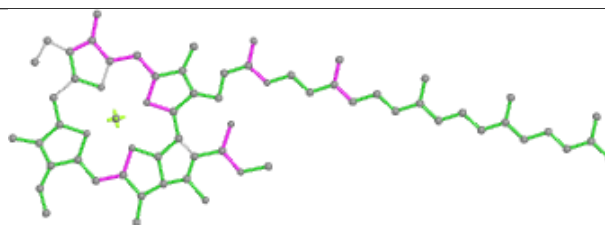


Rings

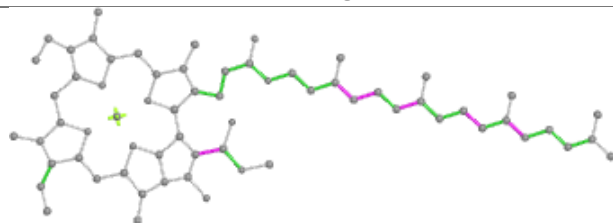
## Ligand CLA Bb 604



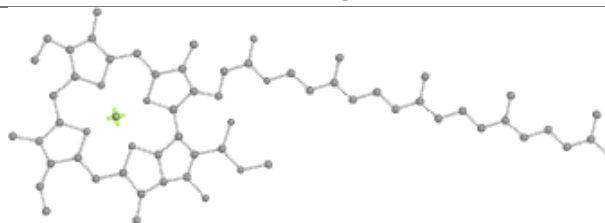
Bond lengths



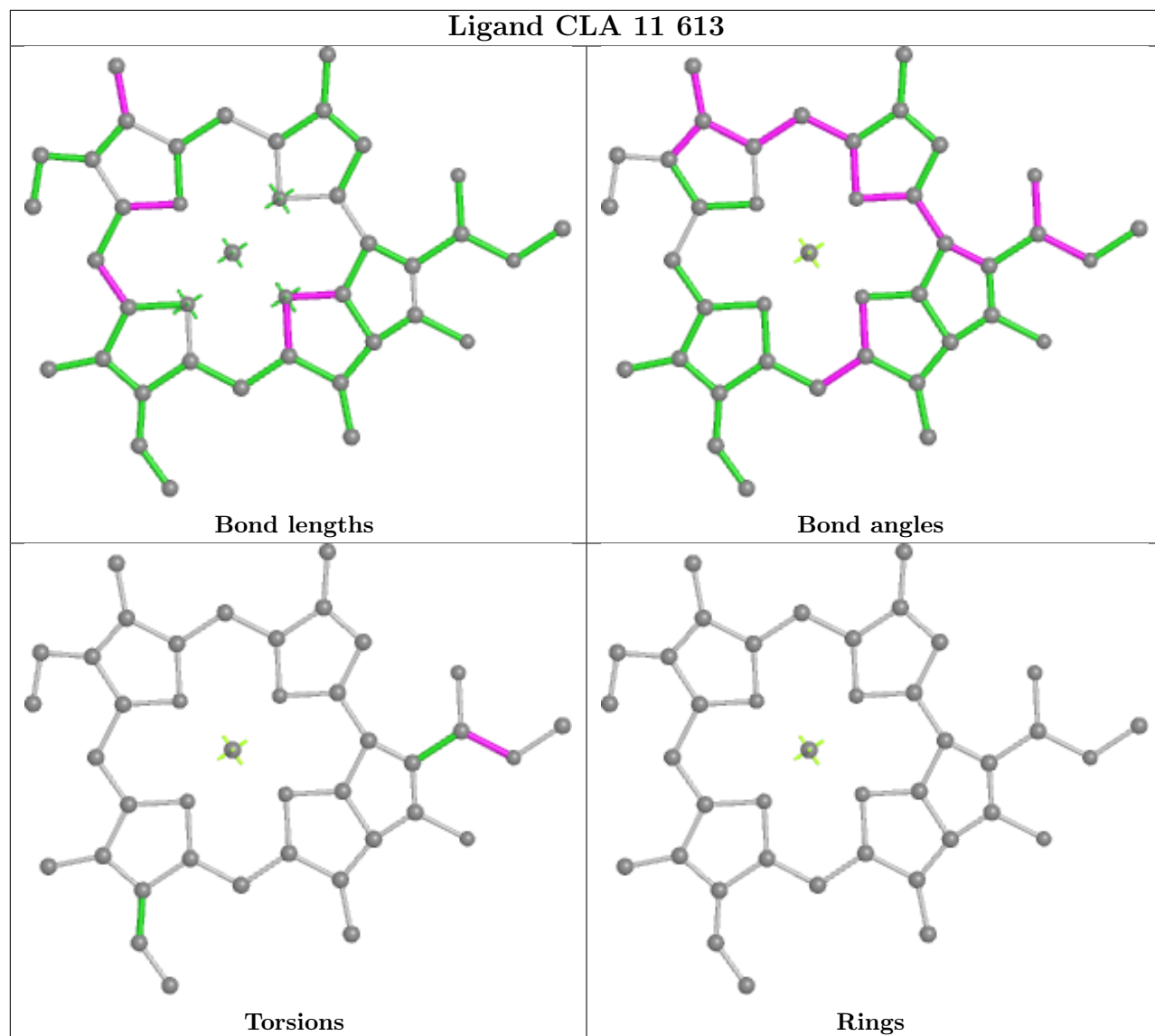
Bond angles



Torsions

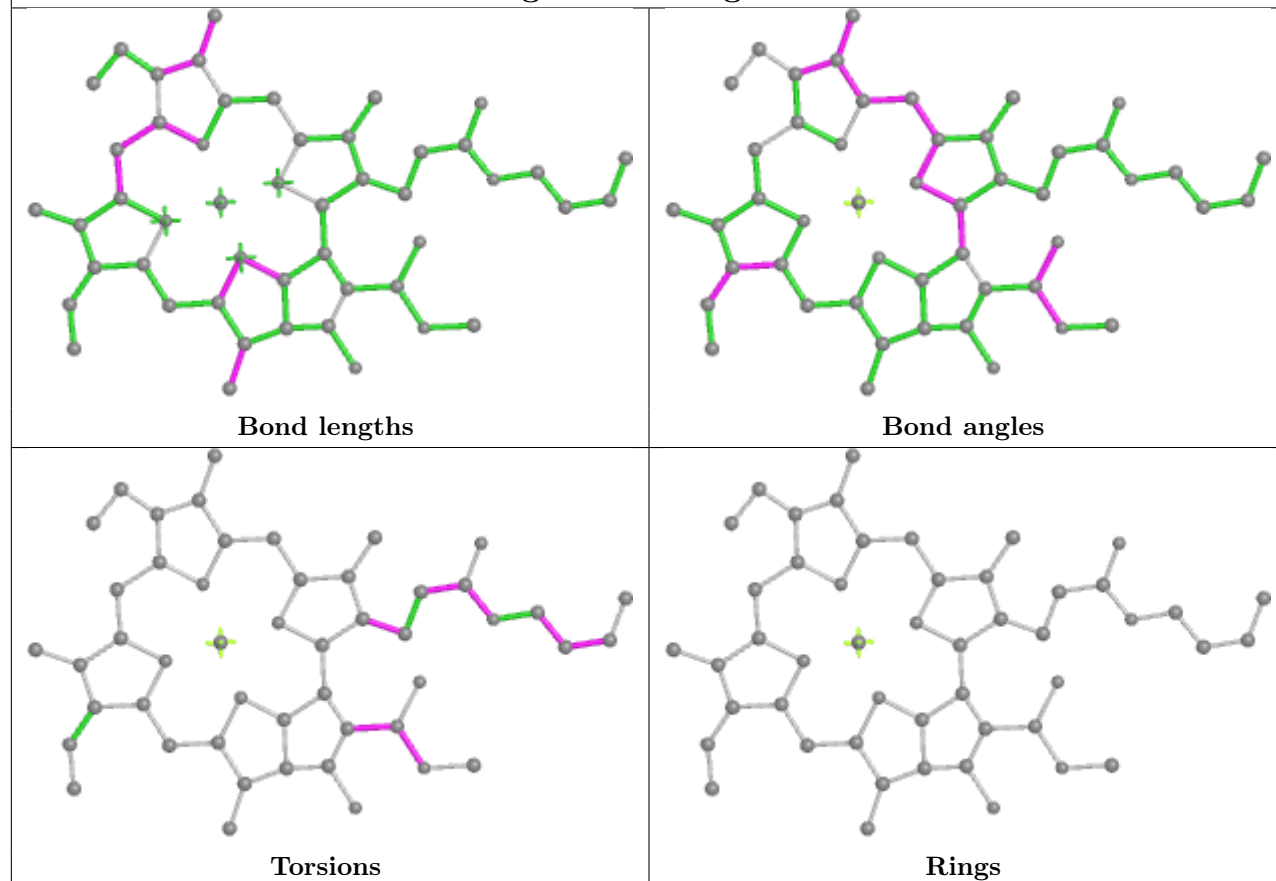


Rings

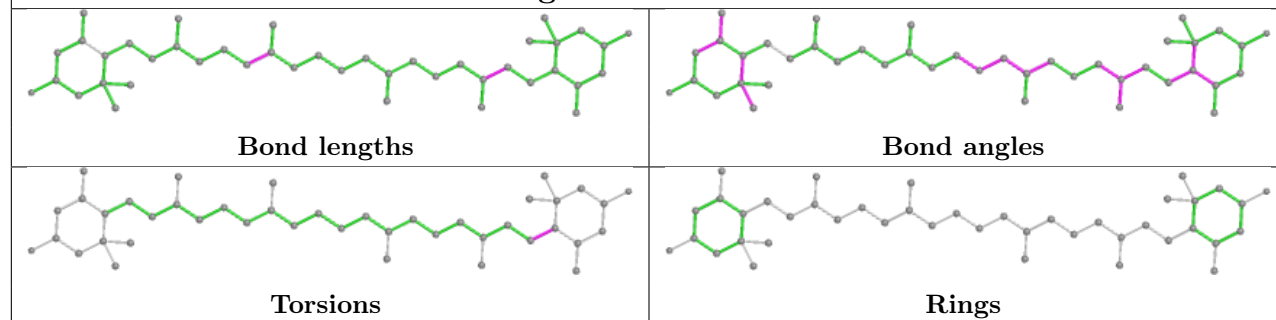


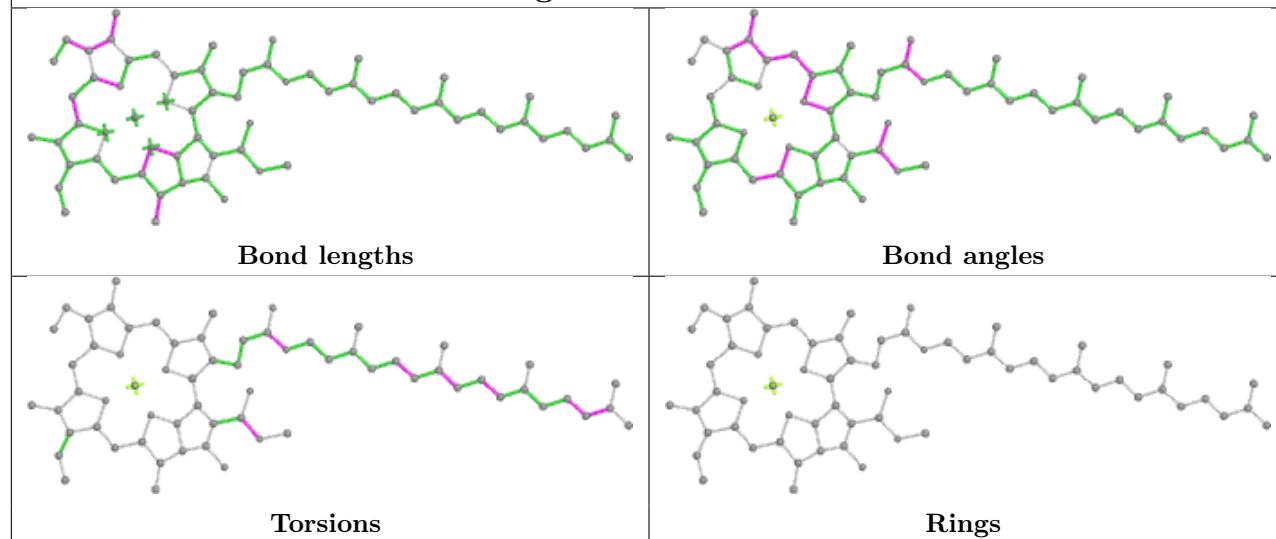
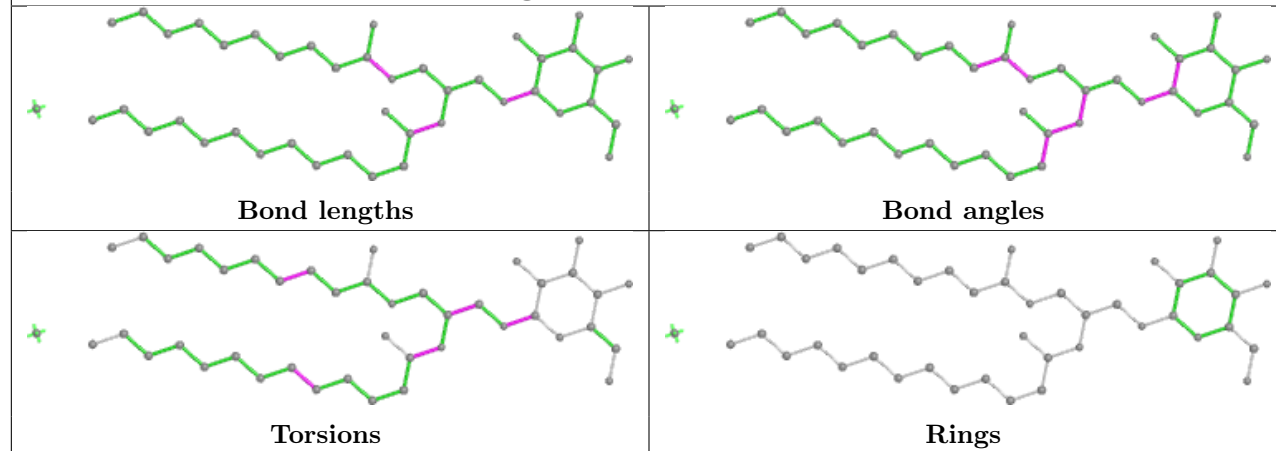


## Ligand CLA Gg 313

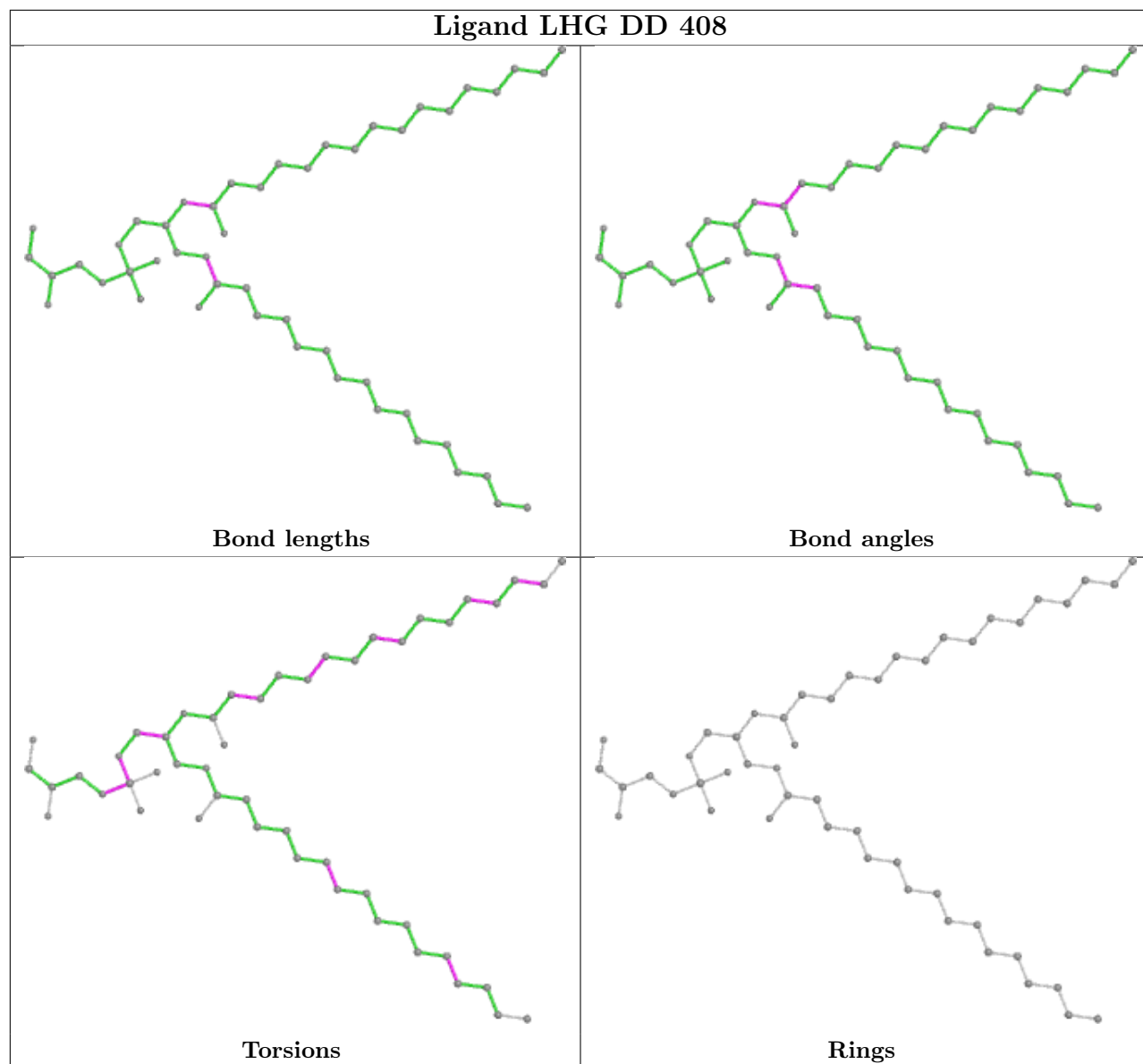


## Ligand LUT s 614

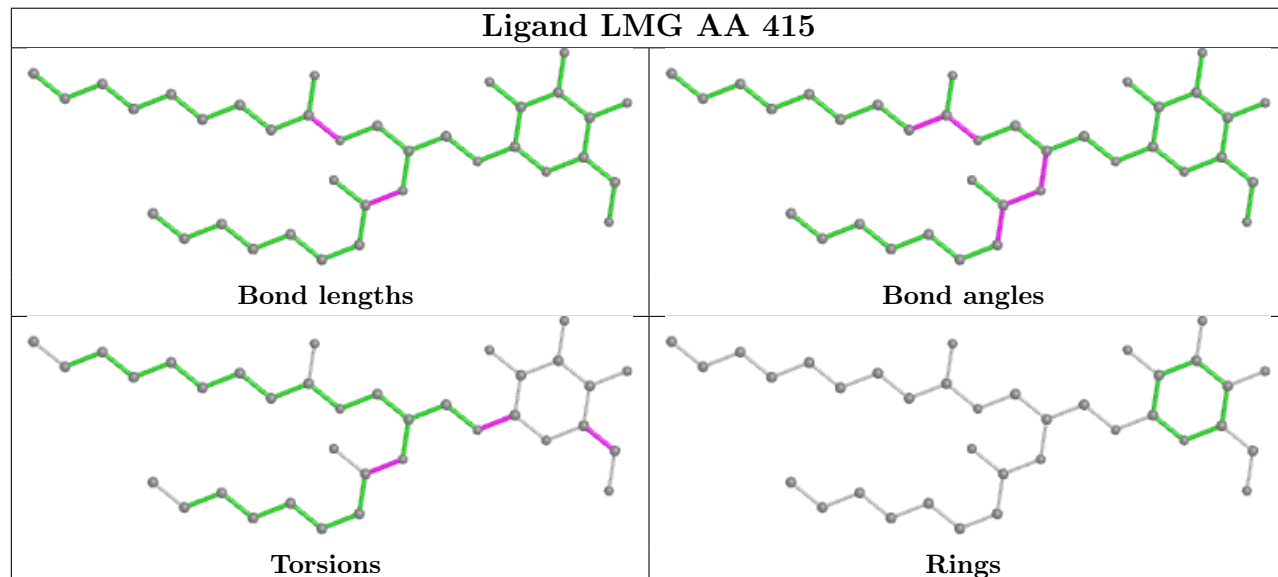


**Ligand CLA b 607****Ligand LMG Aa 412**

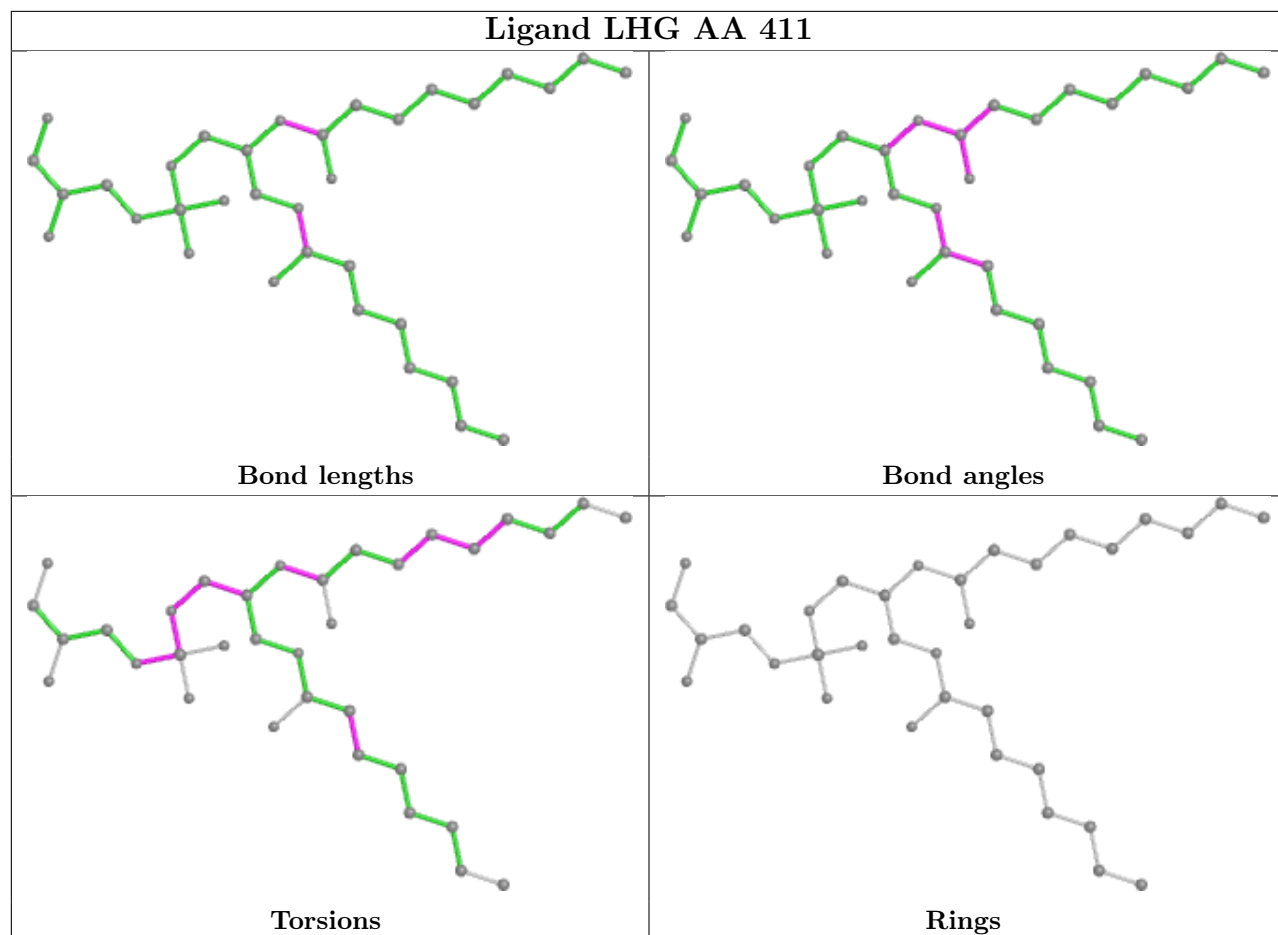
## Ligand LHG DD 408



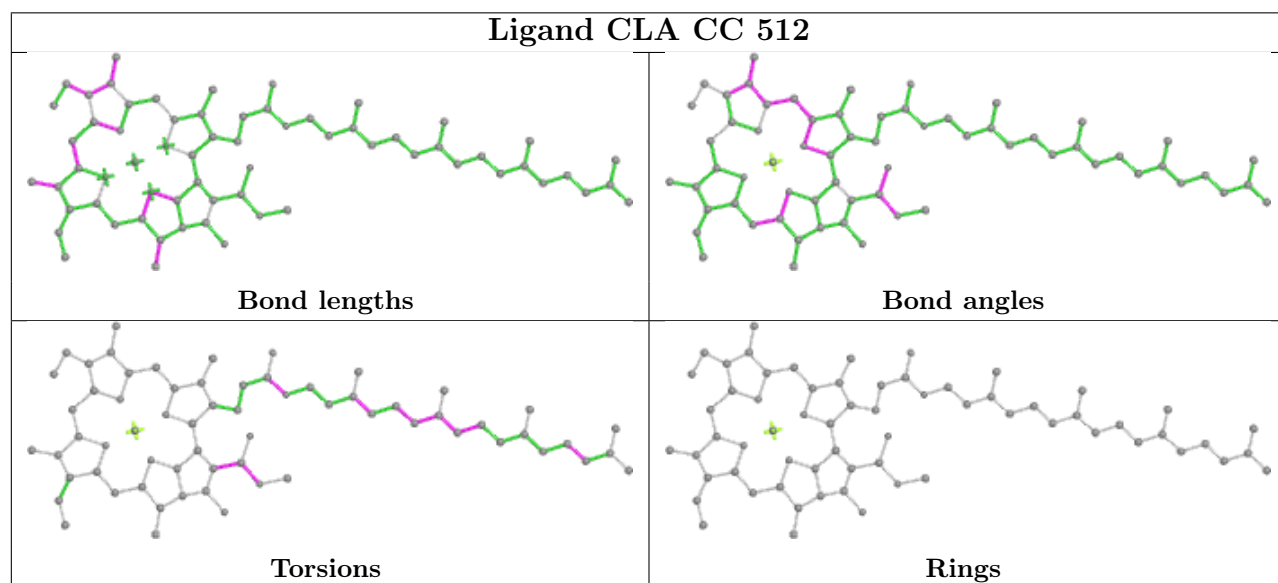
## Ligand LMG AA 415

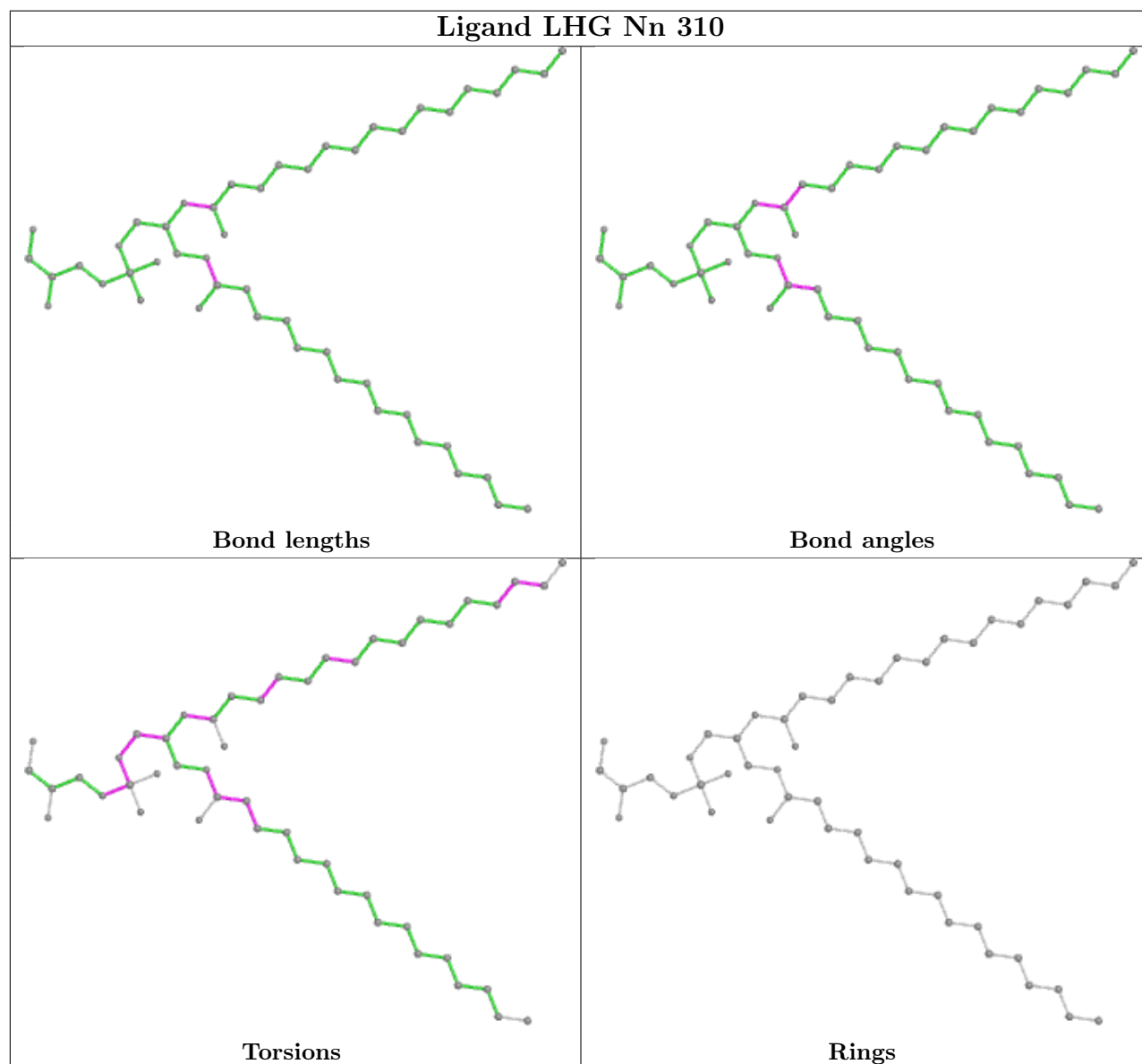
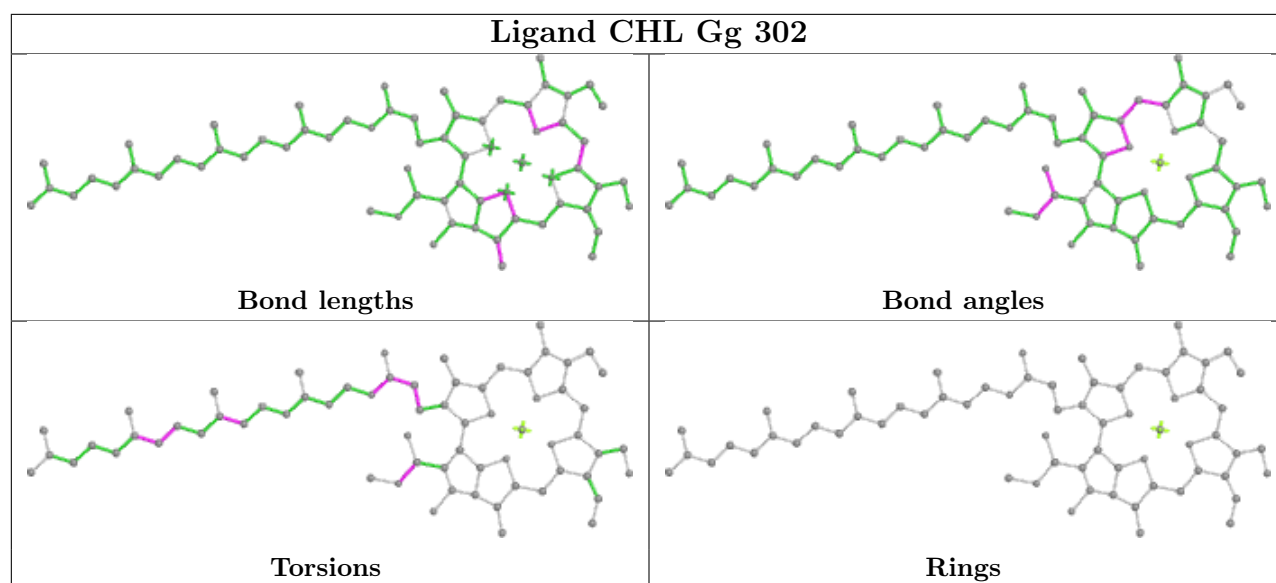


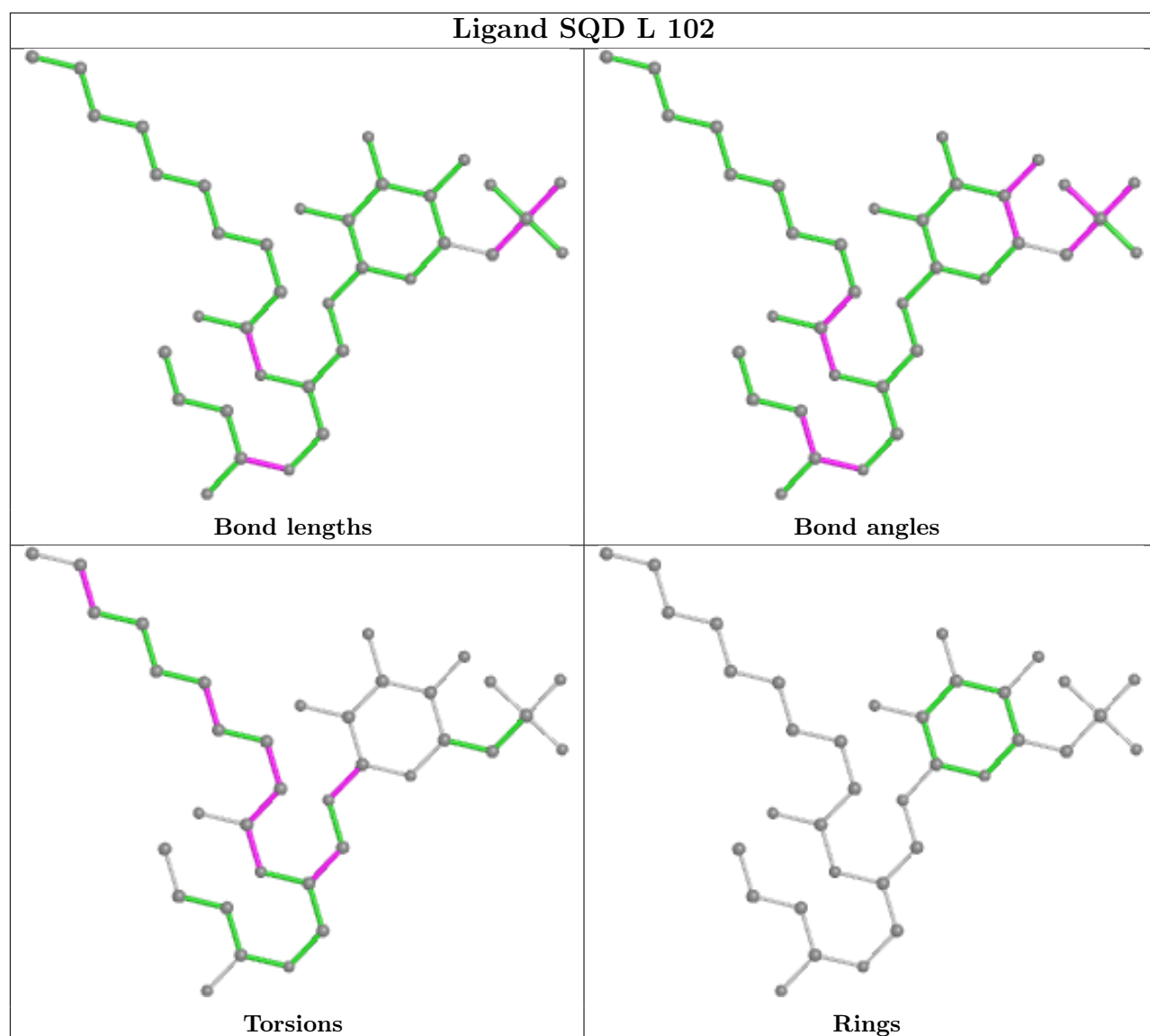
## Ligand LHG AA 411

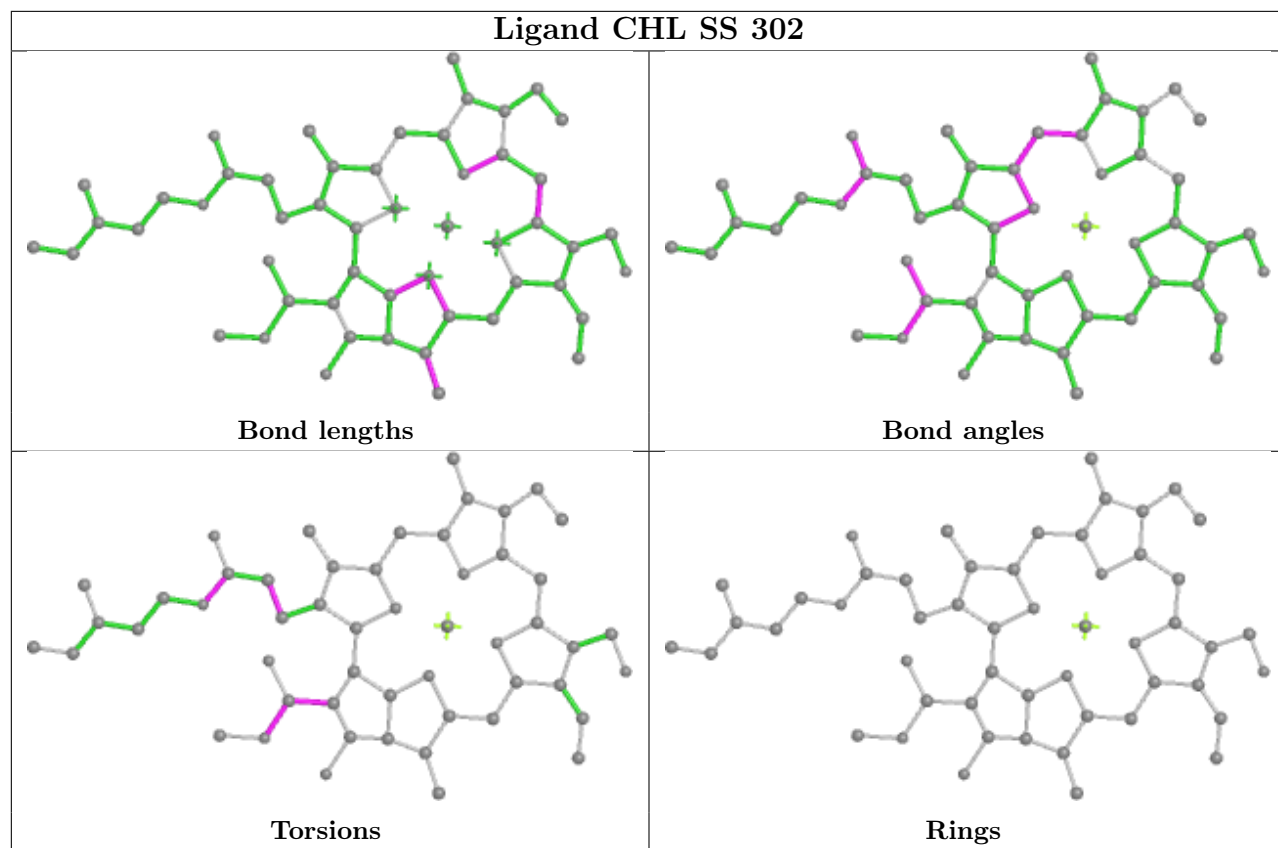


## Ligand CLA CC 512

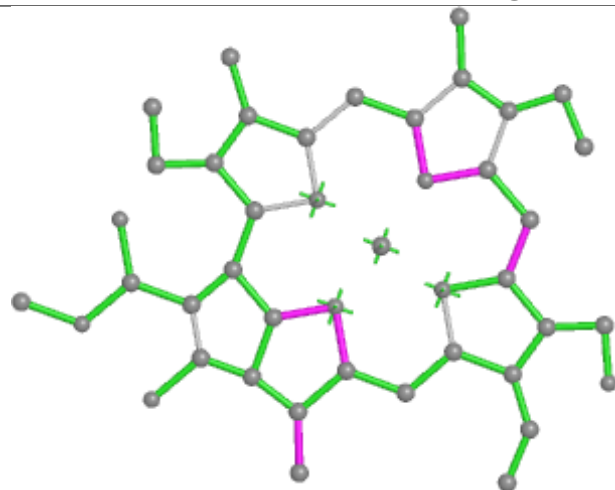




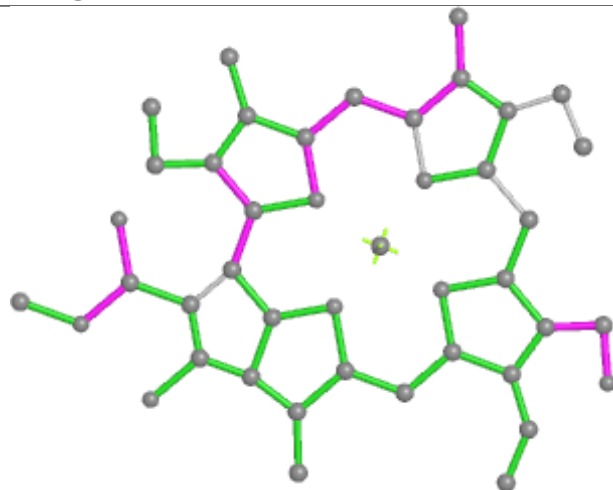




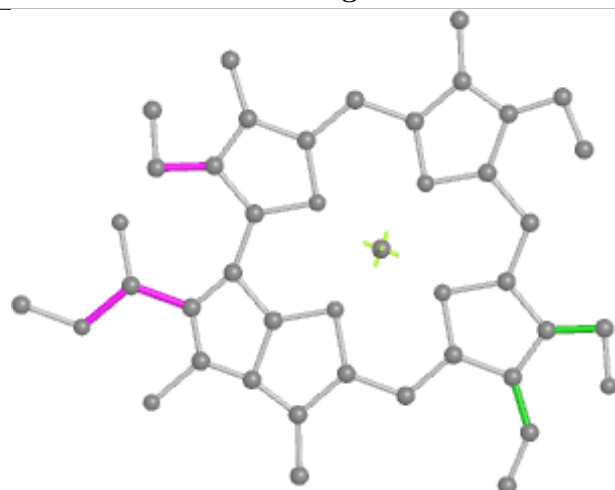
## Ligand CHL Gg 306



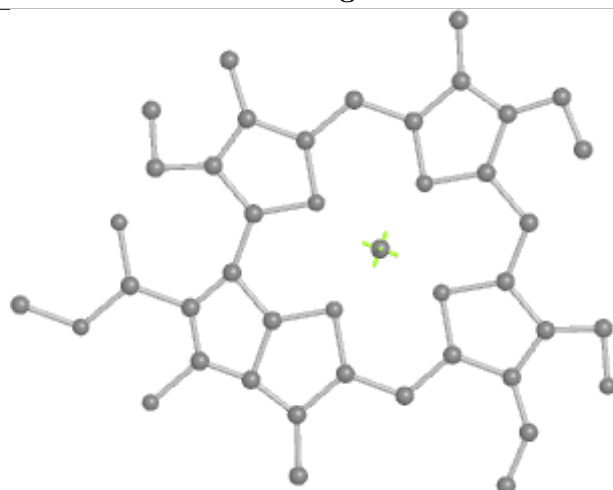
Bond lengths



Bond angles

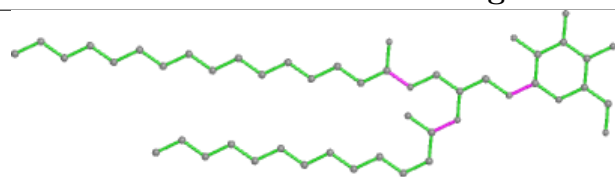


Torsions

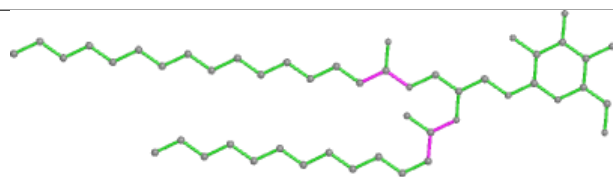


Rings

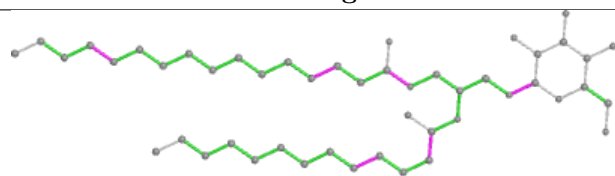
## Ligand LMG WW 201



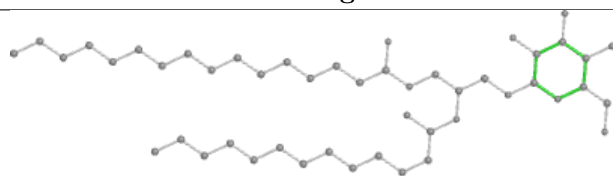
Bond lengths



Bond angles

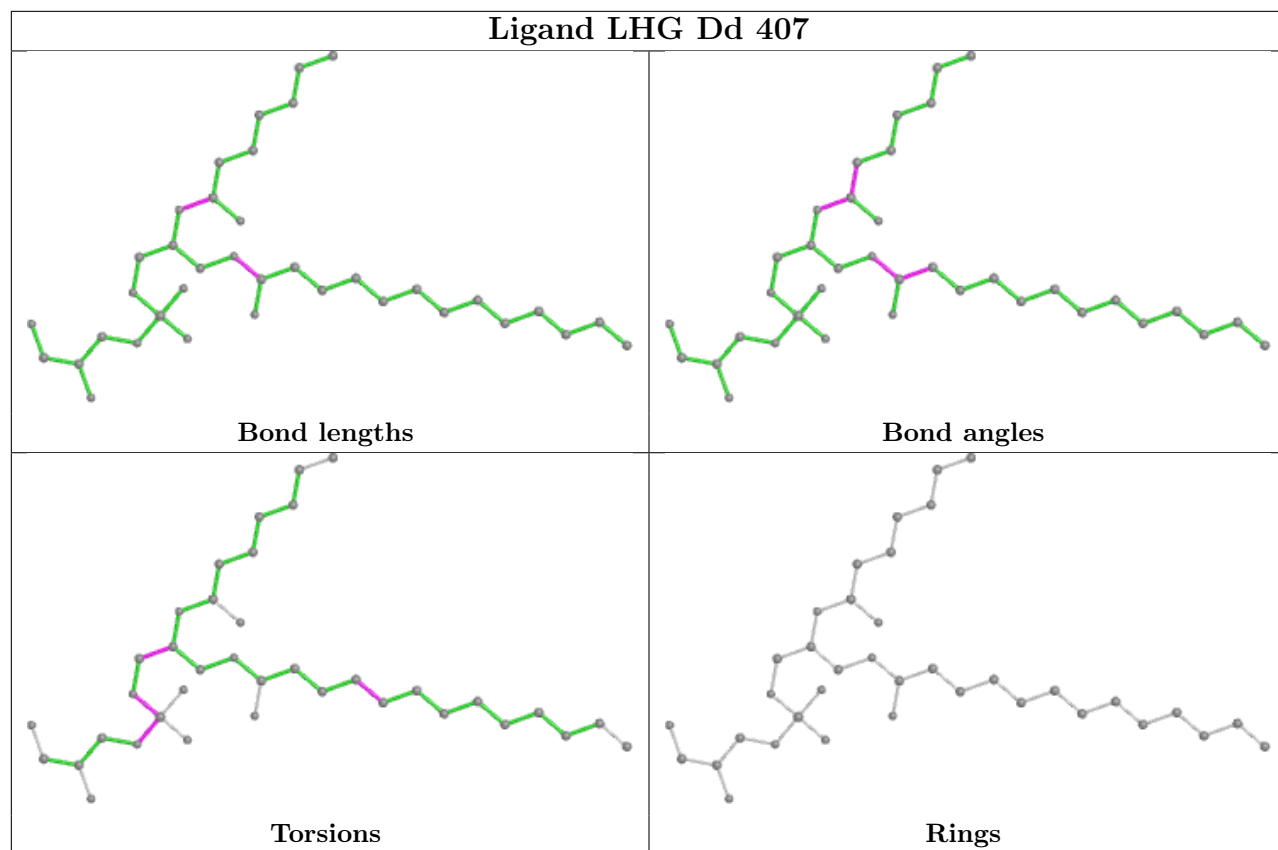


Torsions

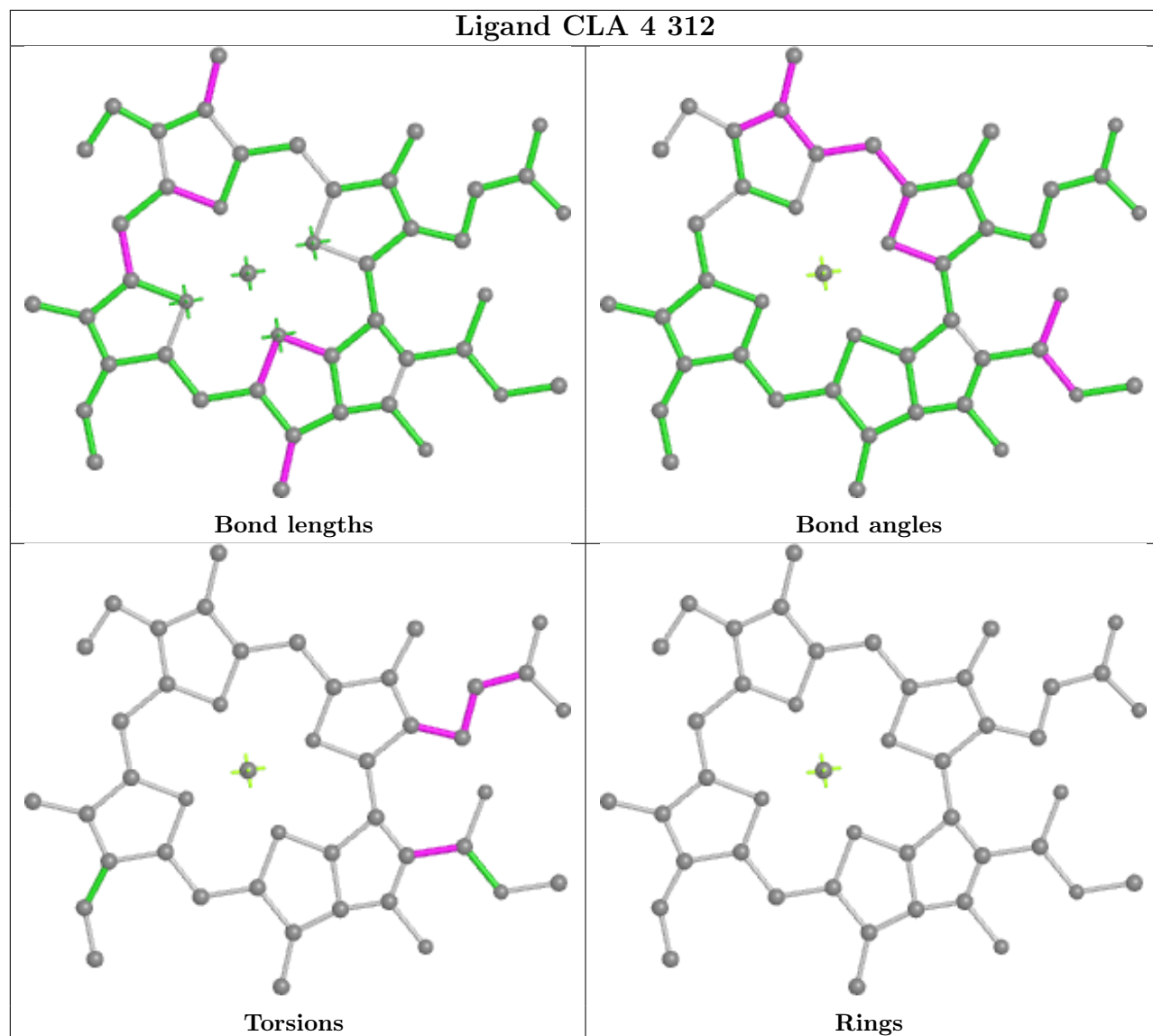


Rings

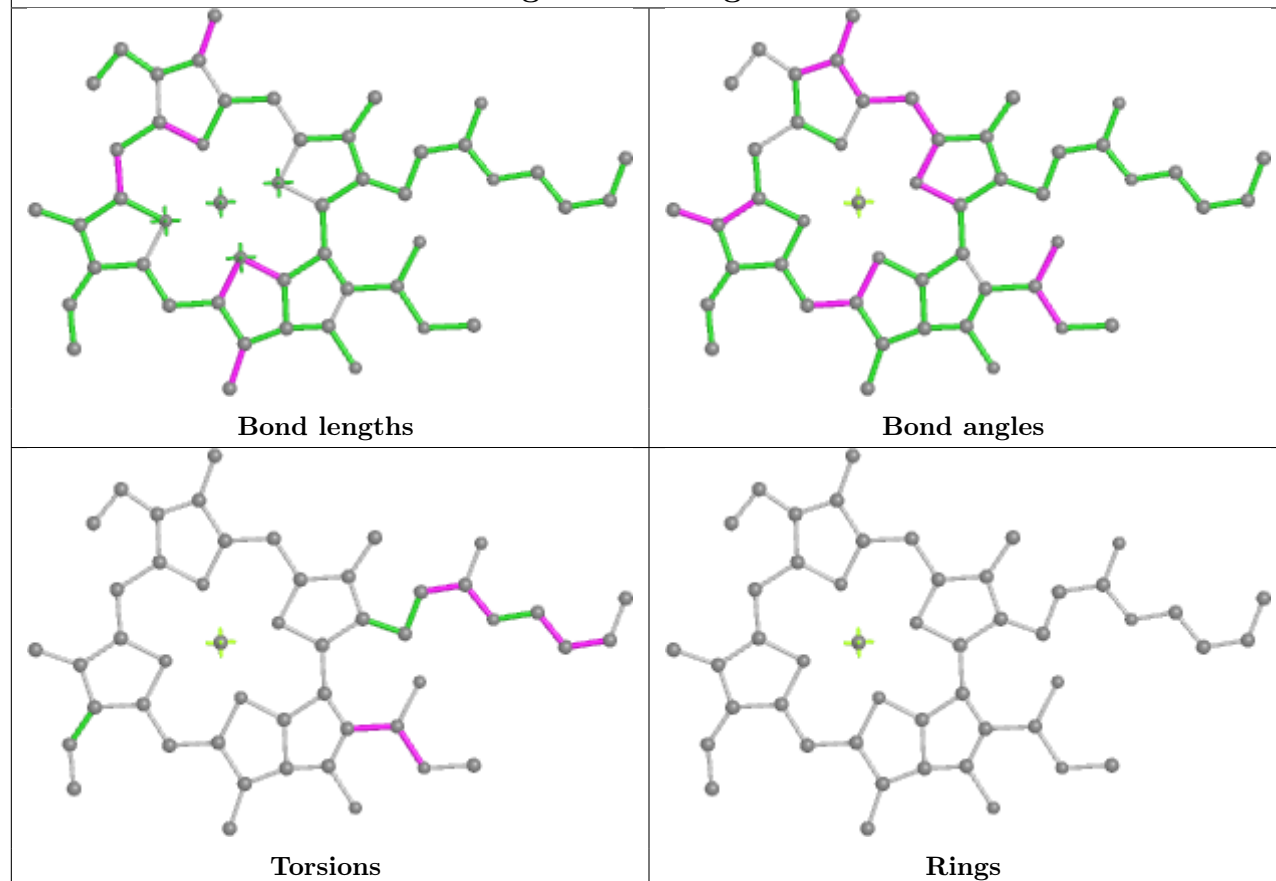




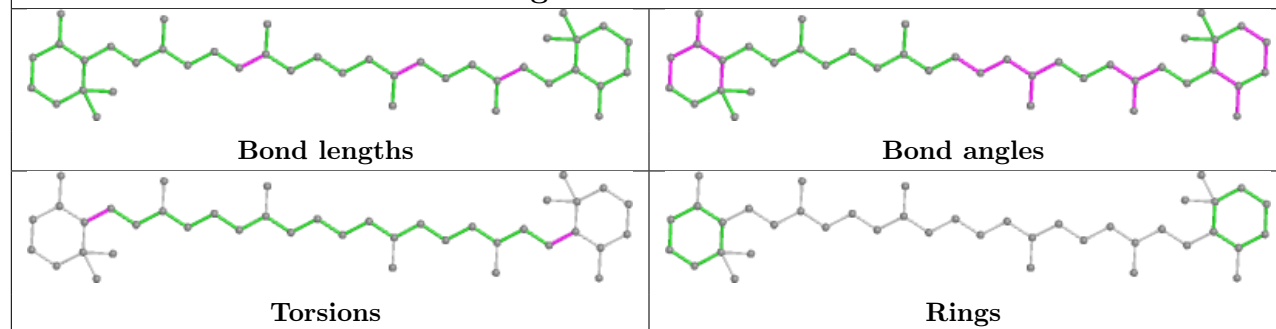
## Ligand CLA 4 312

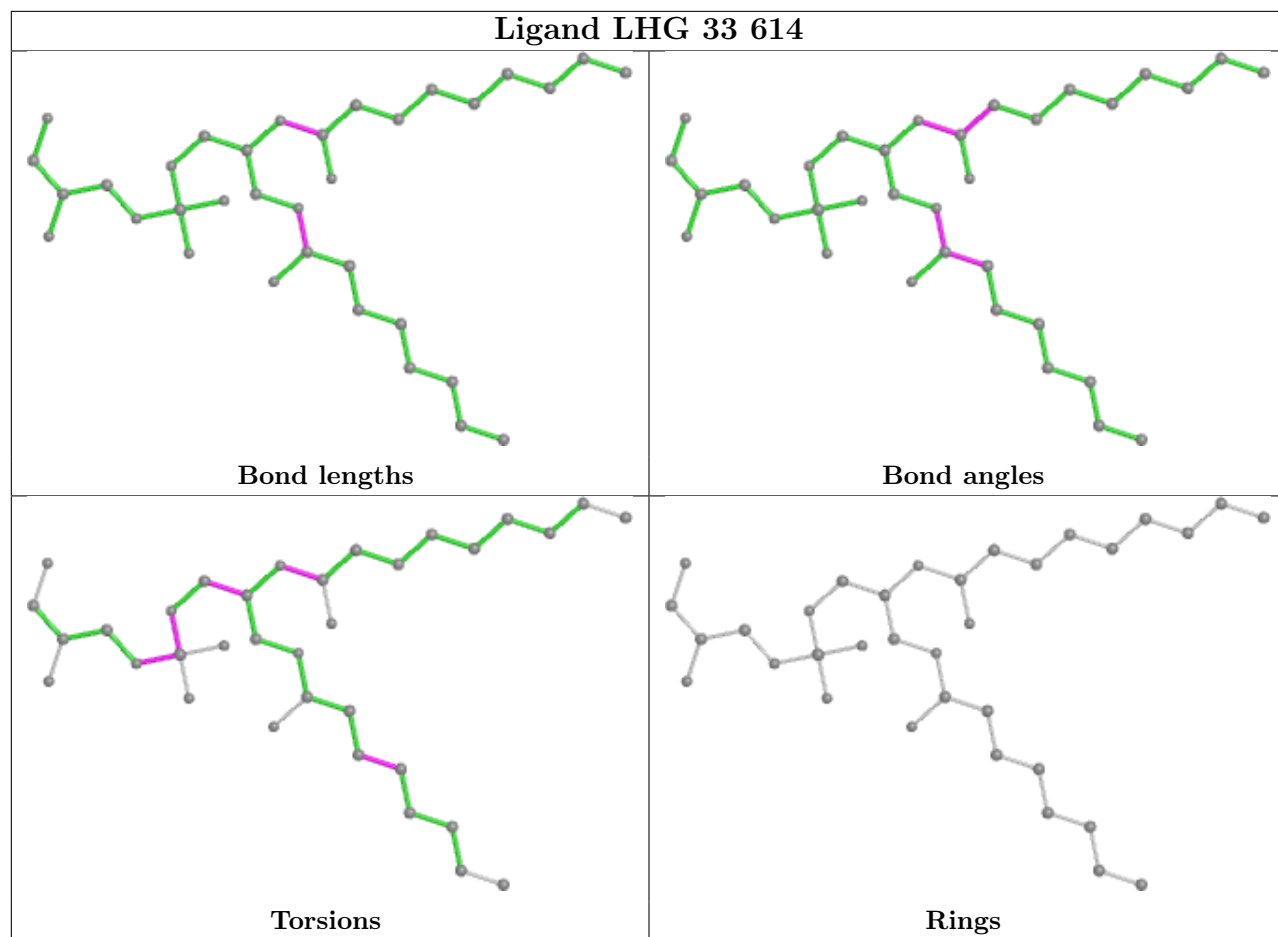


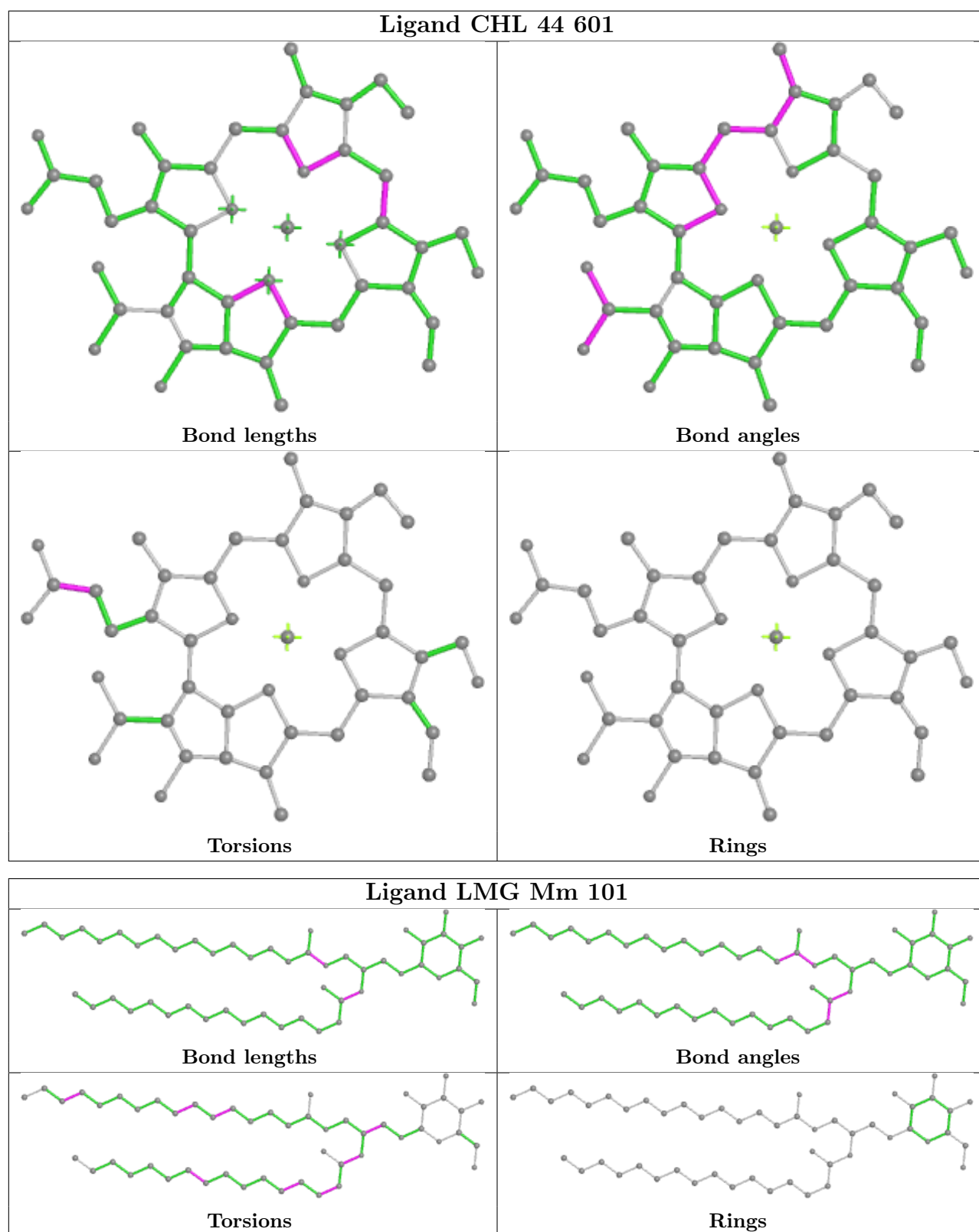
## Ligand CLA Gg 311

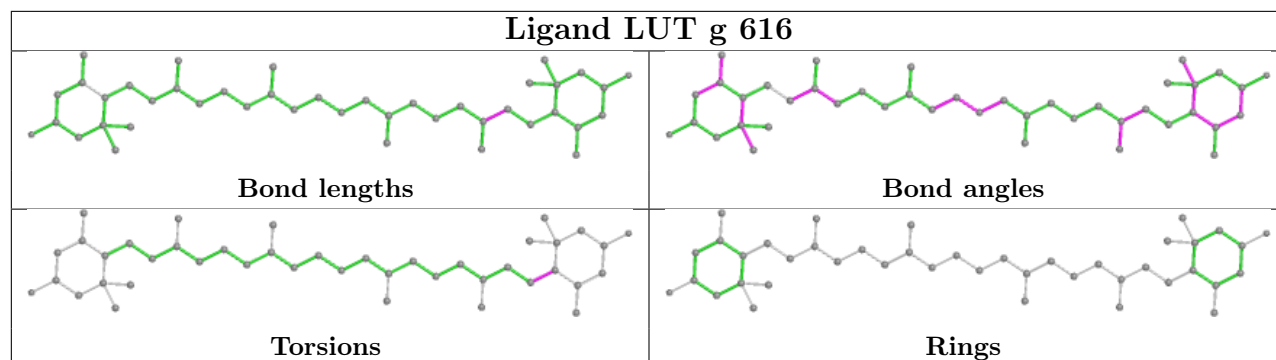
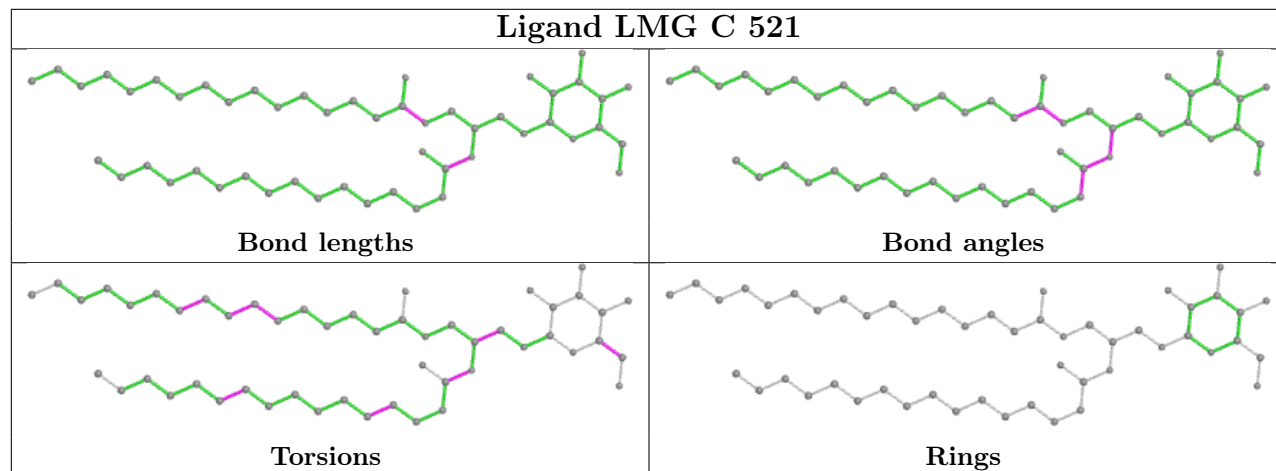
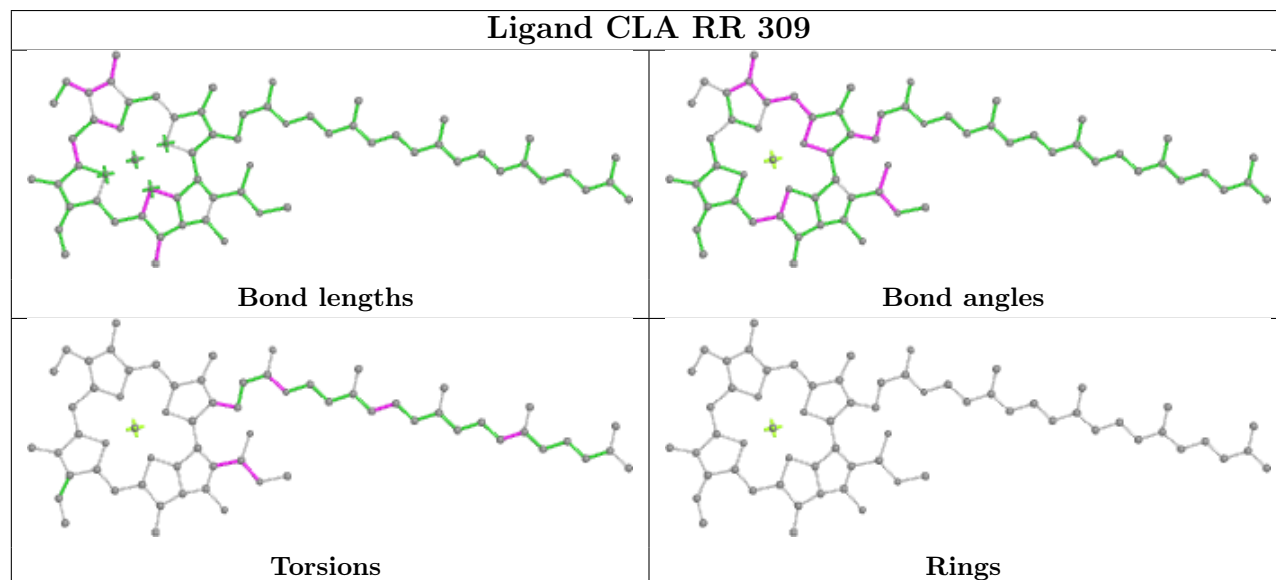


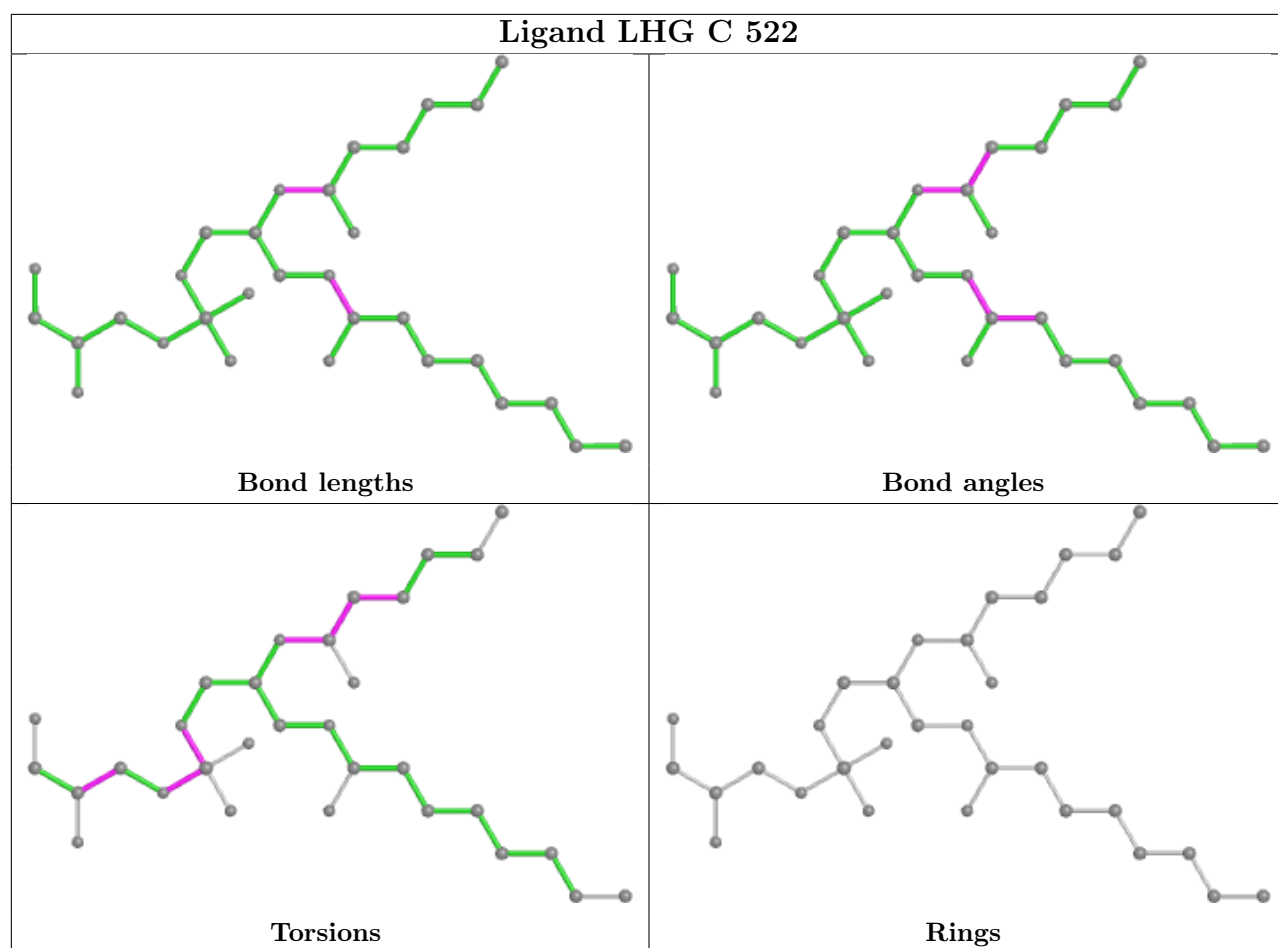
## Ligand BCR B 613



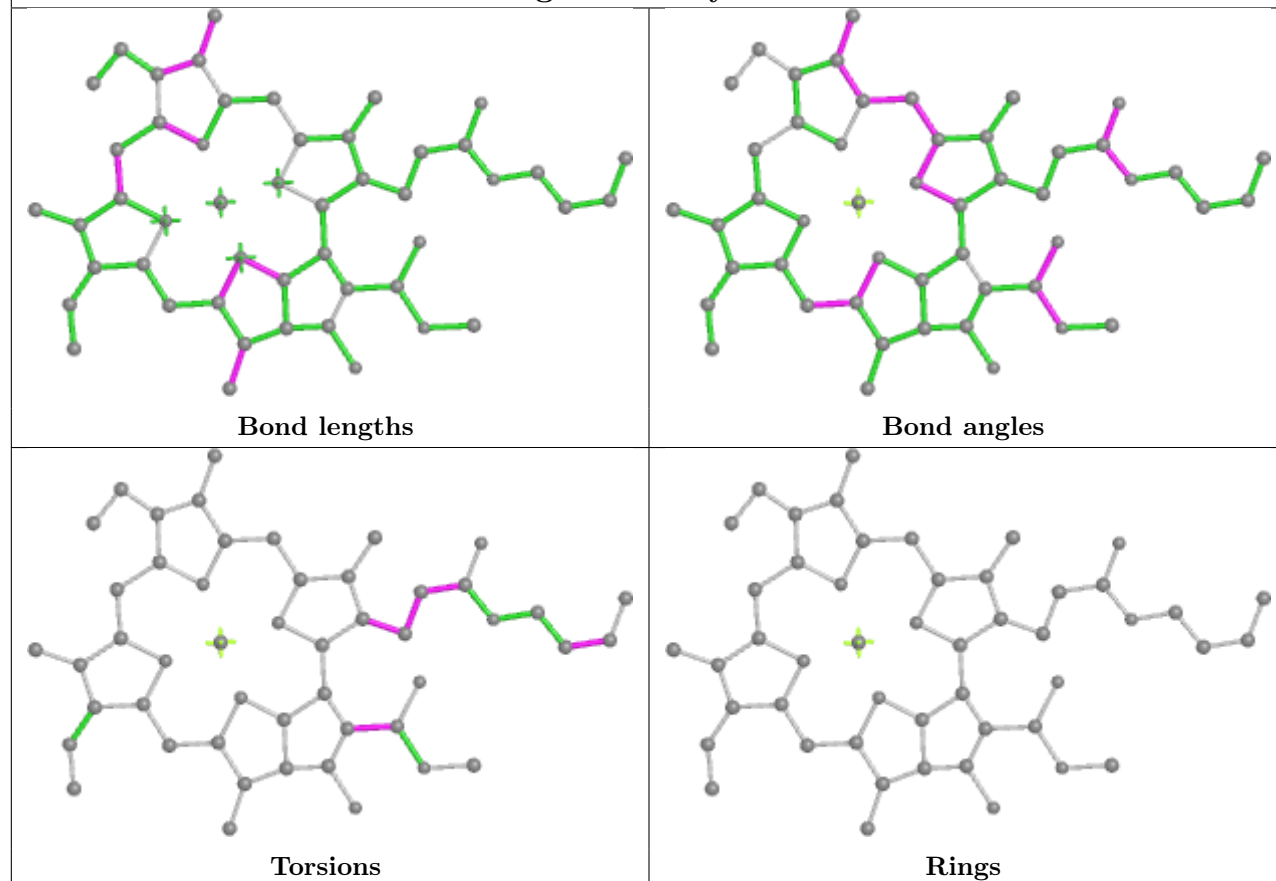




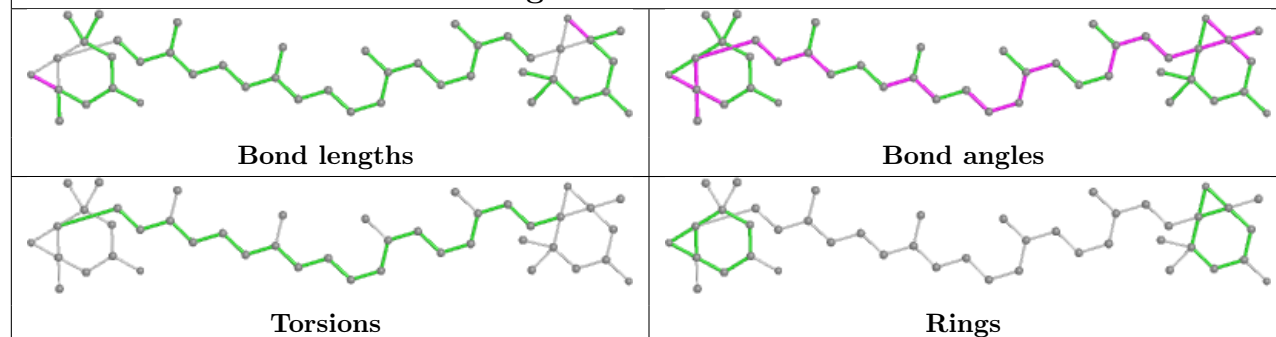
**Ligand LUT g 616****Ligand LMG C 521****Ligand CLA RR 309**



## Ligand CLA y 306

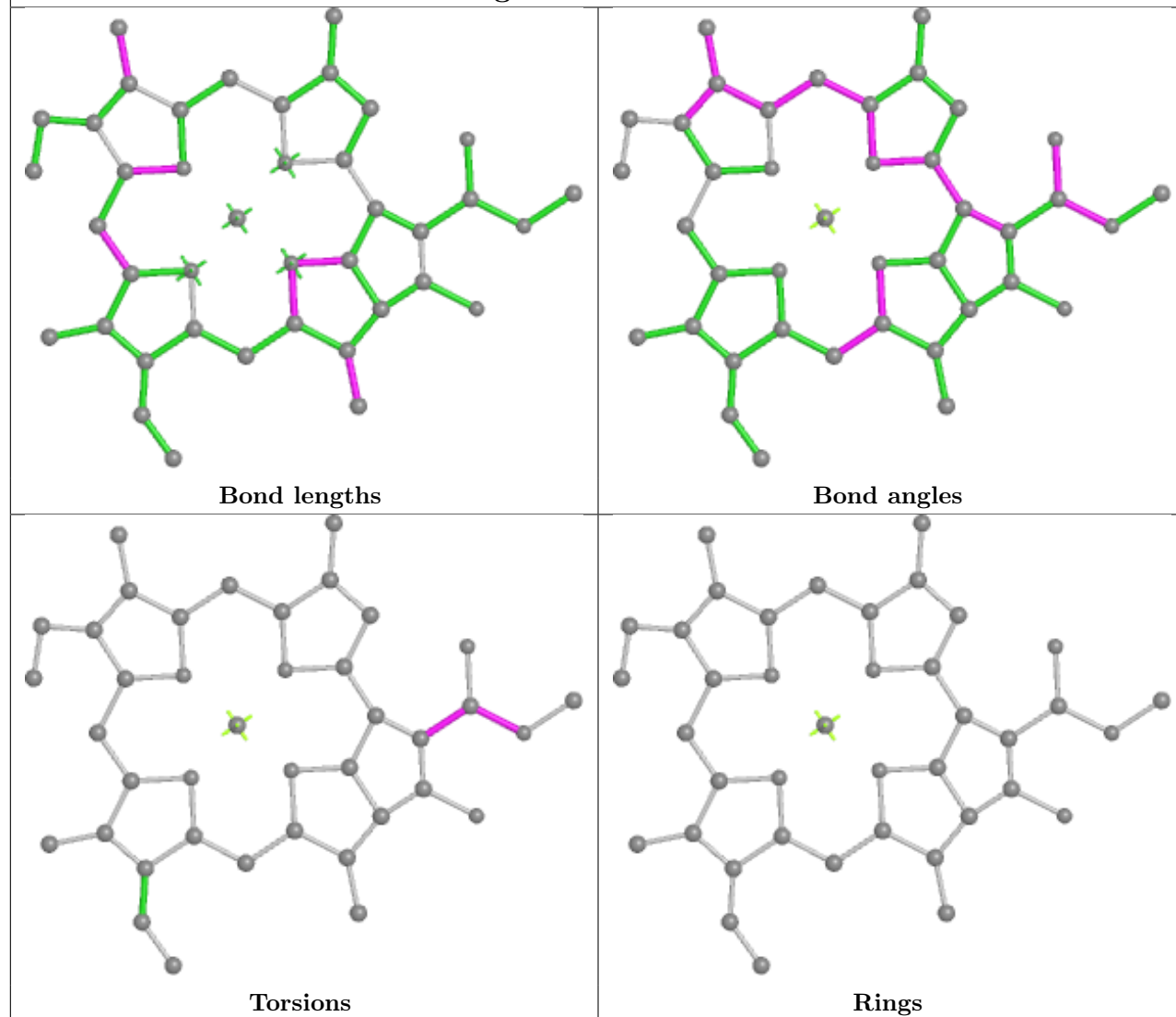


## Ligand XAT 44 613

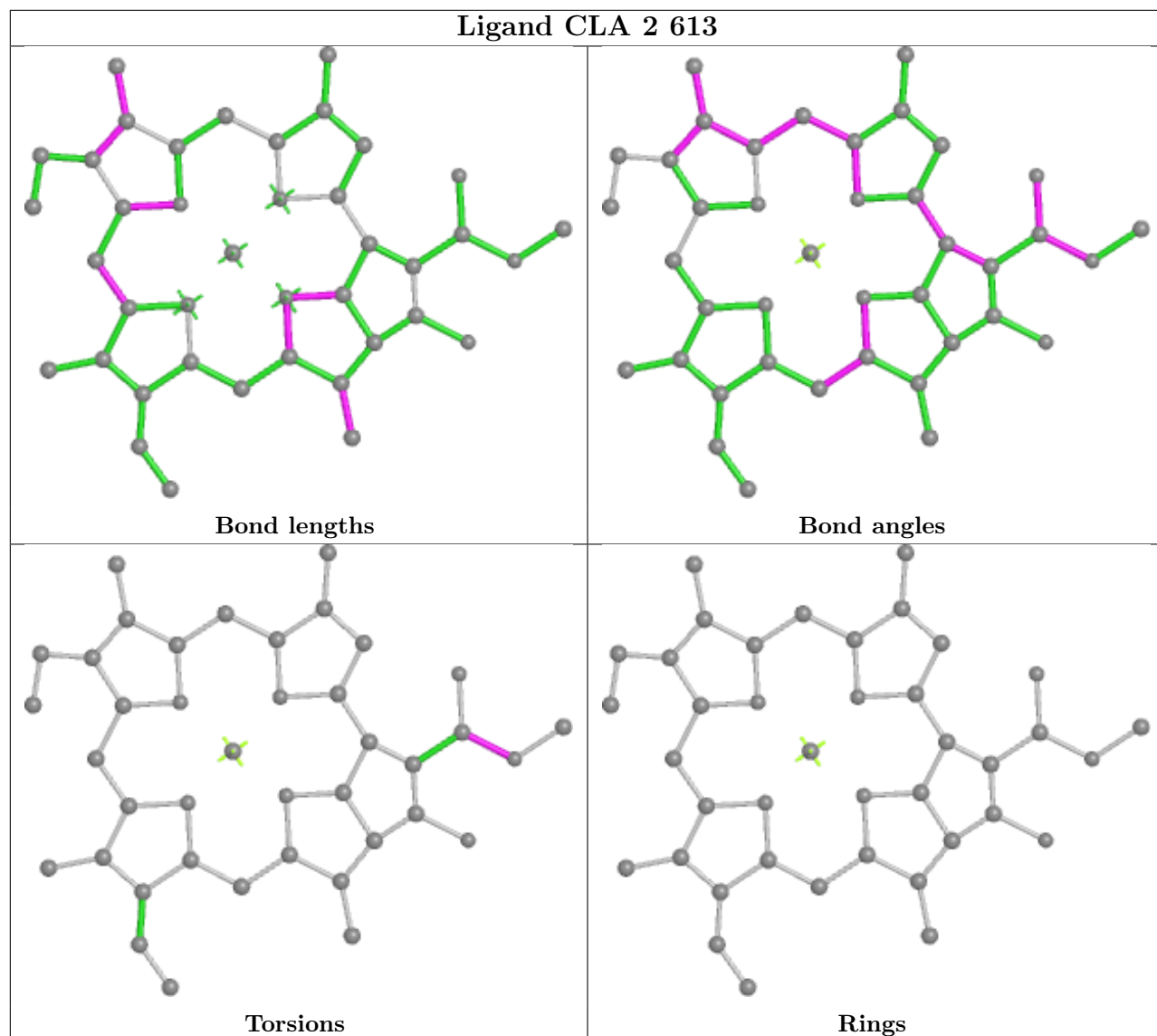




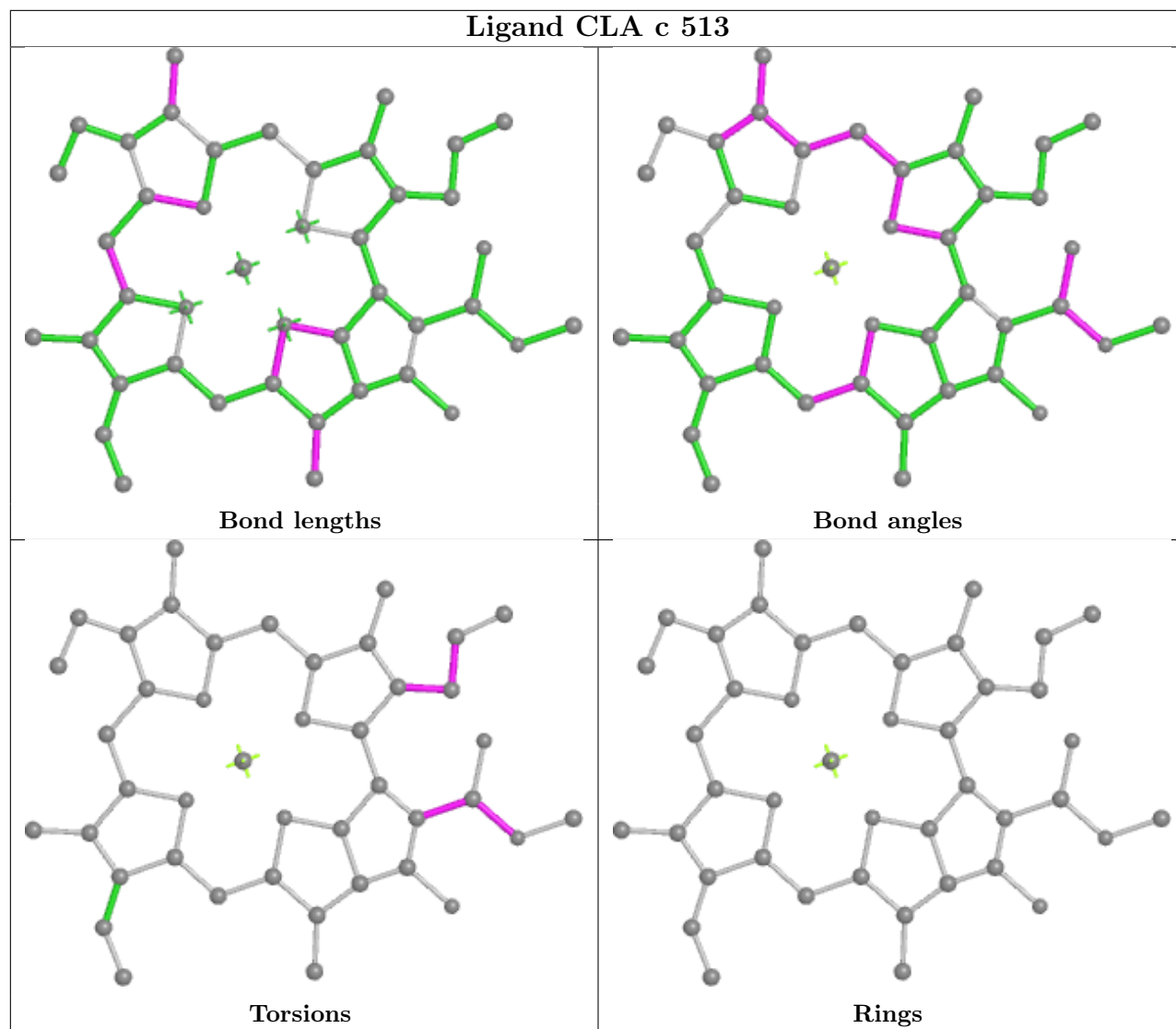
## Ligand CLA 3 613

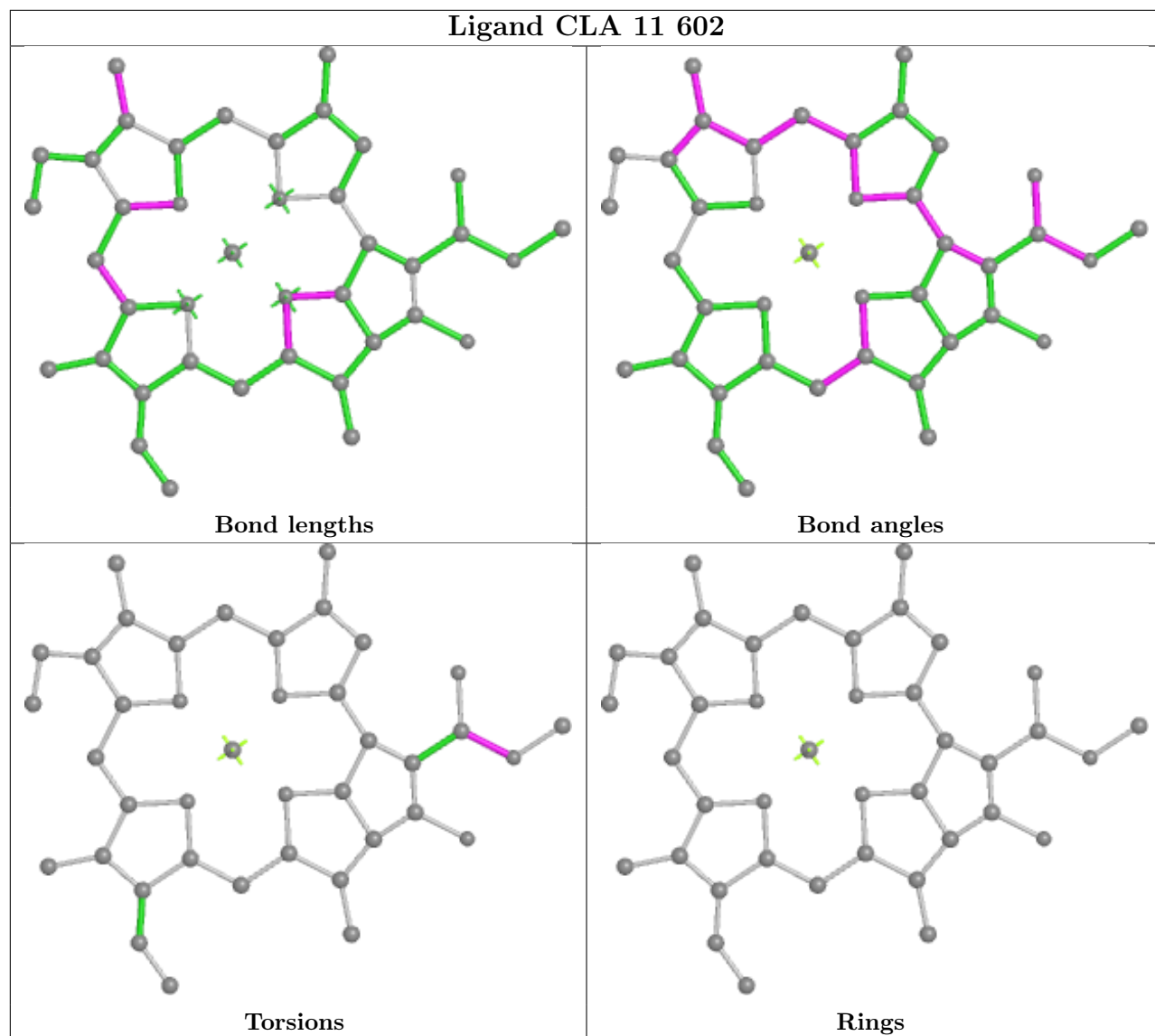


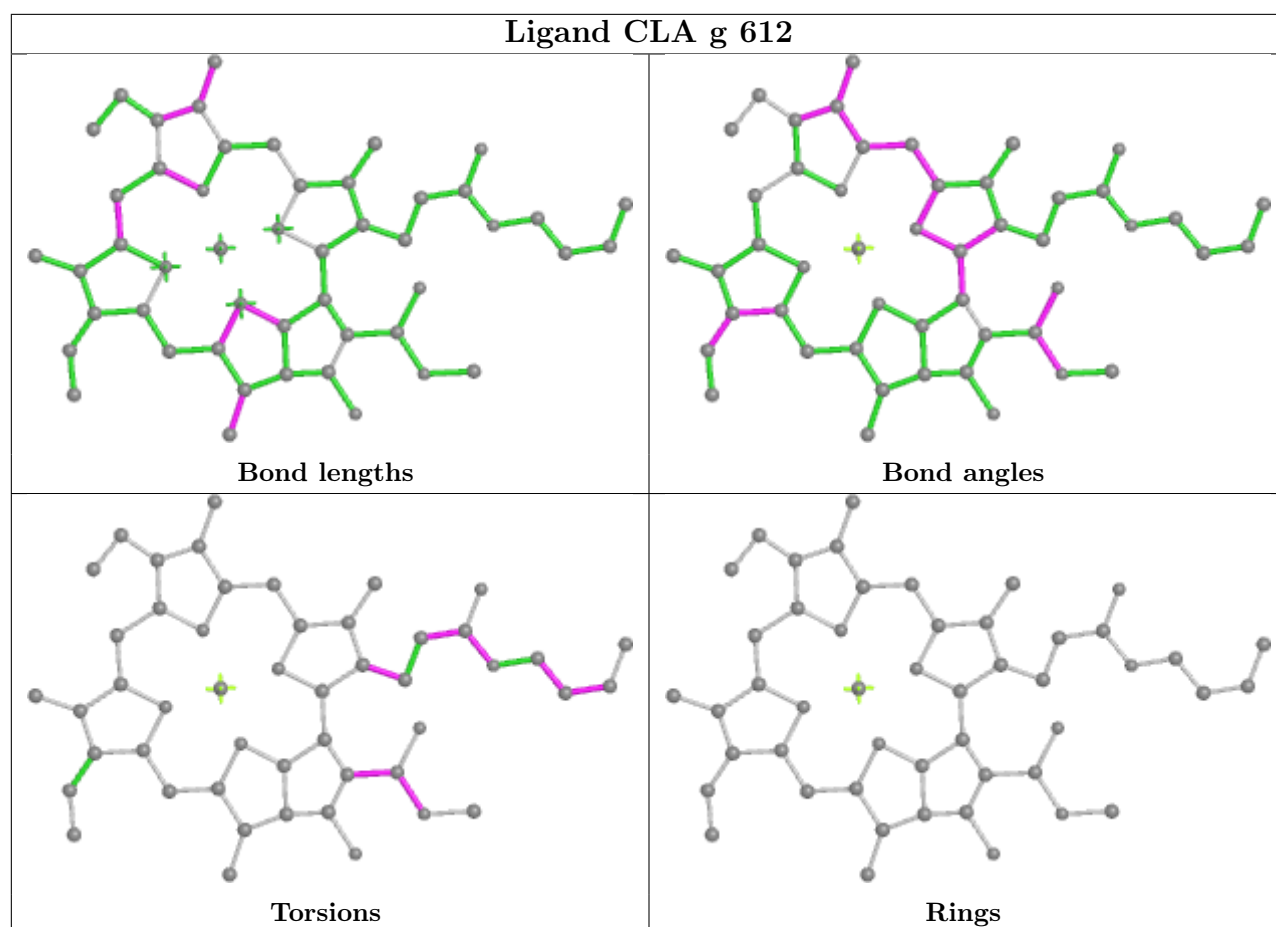
## Ligand CLA 2 613



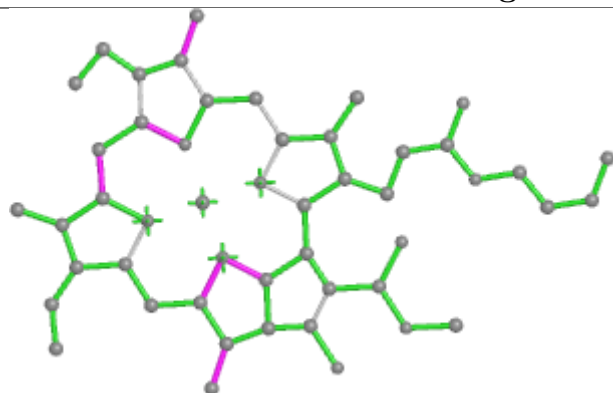
## Ligand CLA c 513



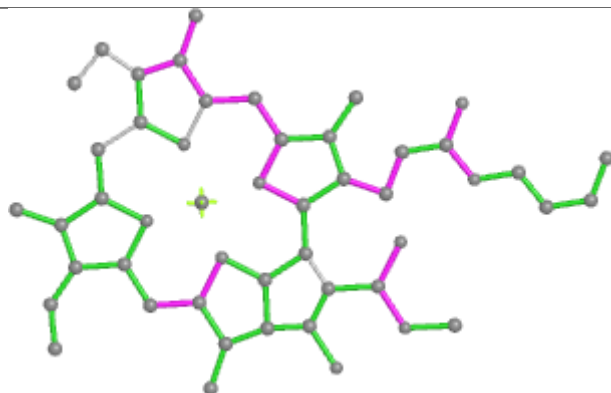




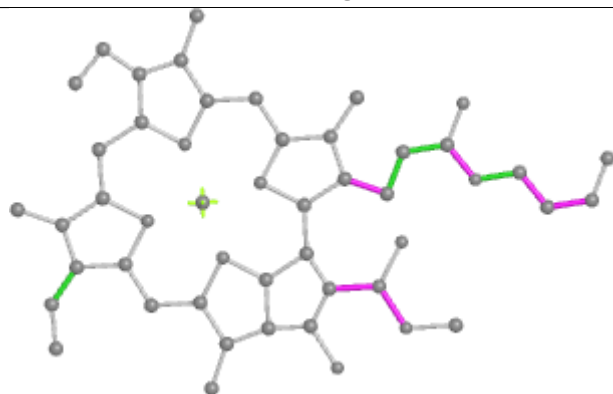
## Ligand CLA NN 611



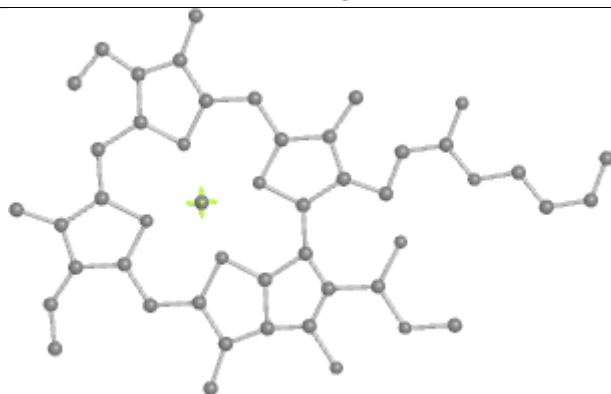
Bond lengths



Bond angles

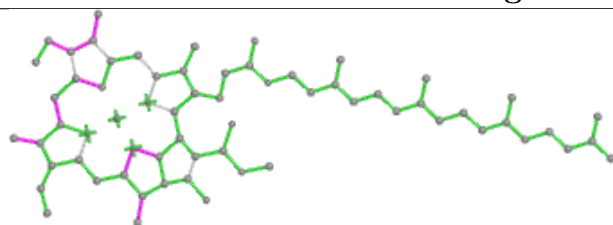


Torsions

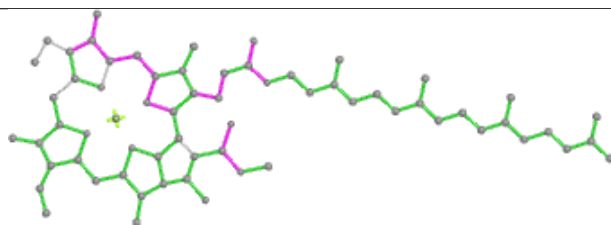


Rings

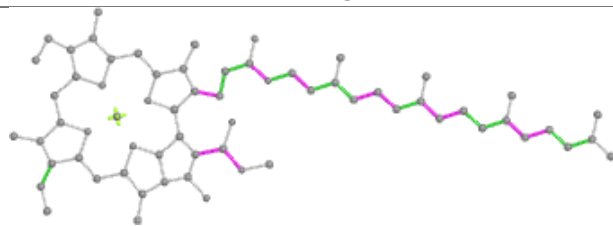
## Ligand CLA Bb 603



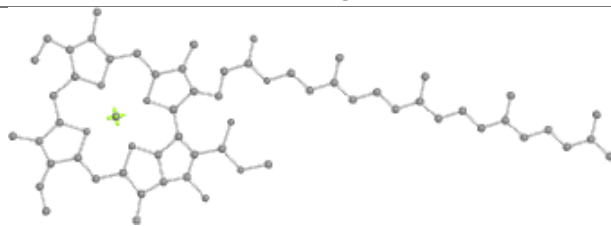
Bond lengths



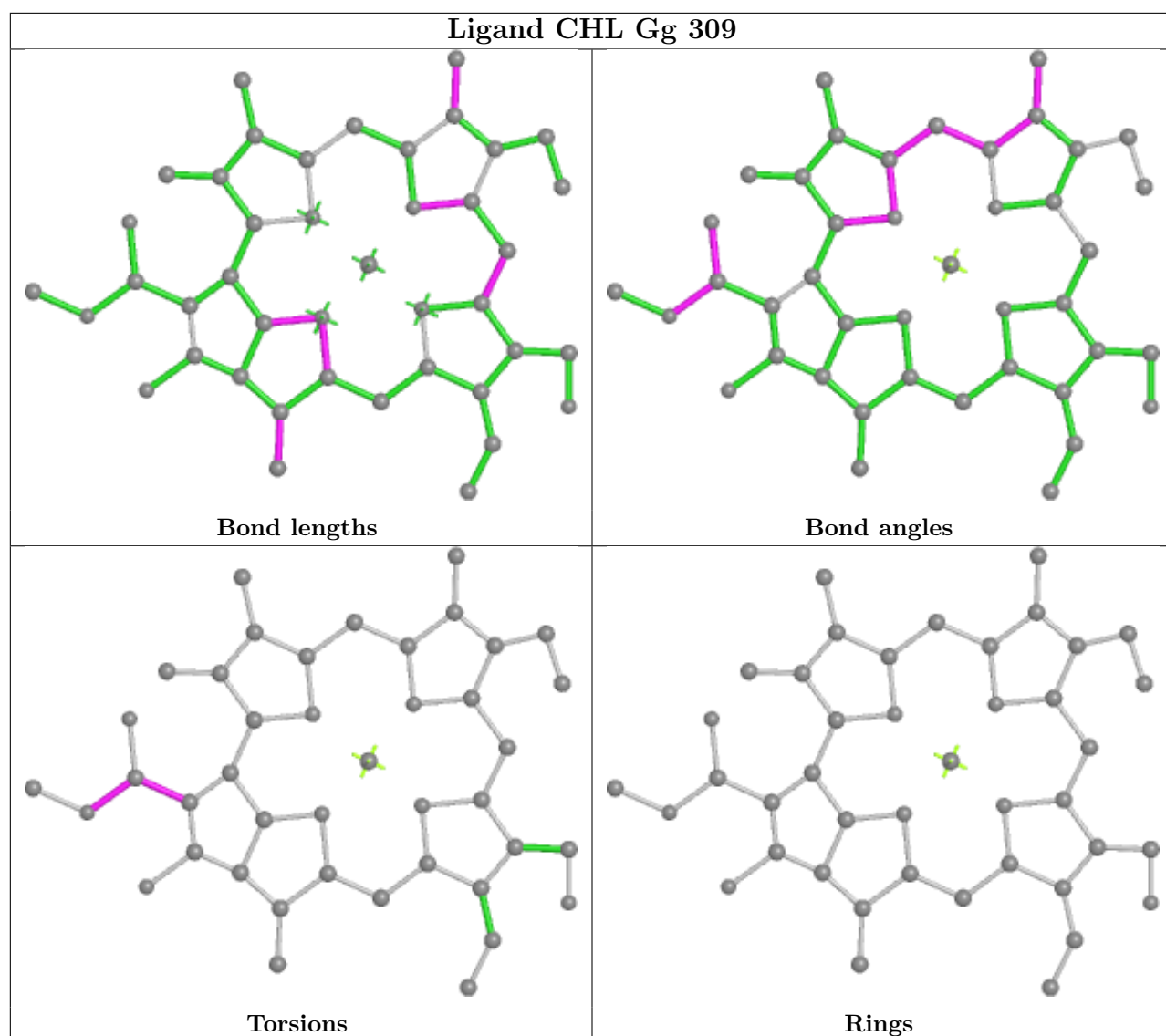
Bond angles

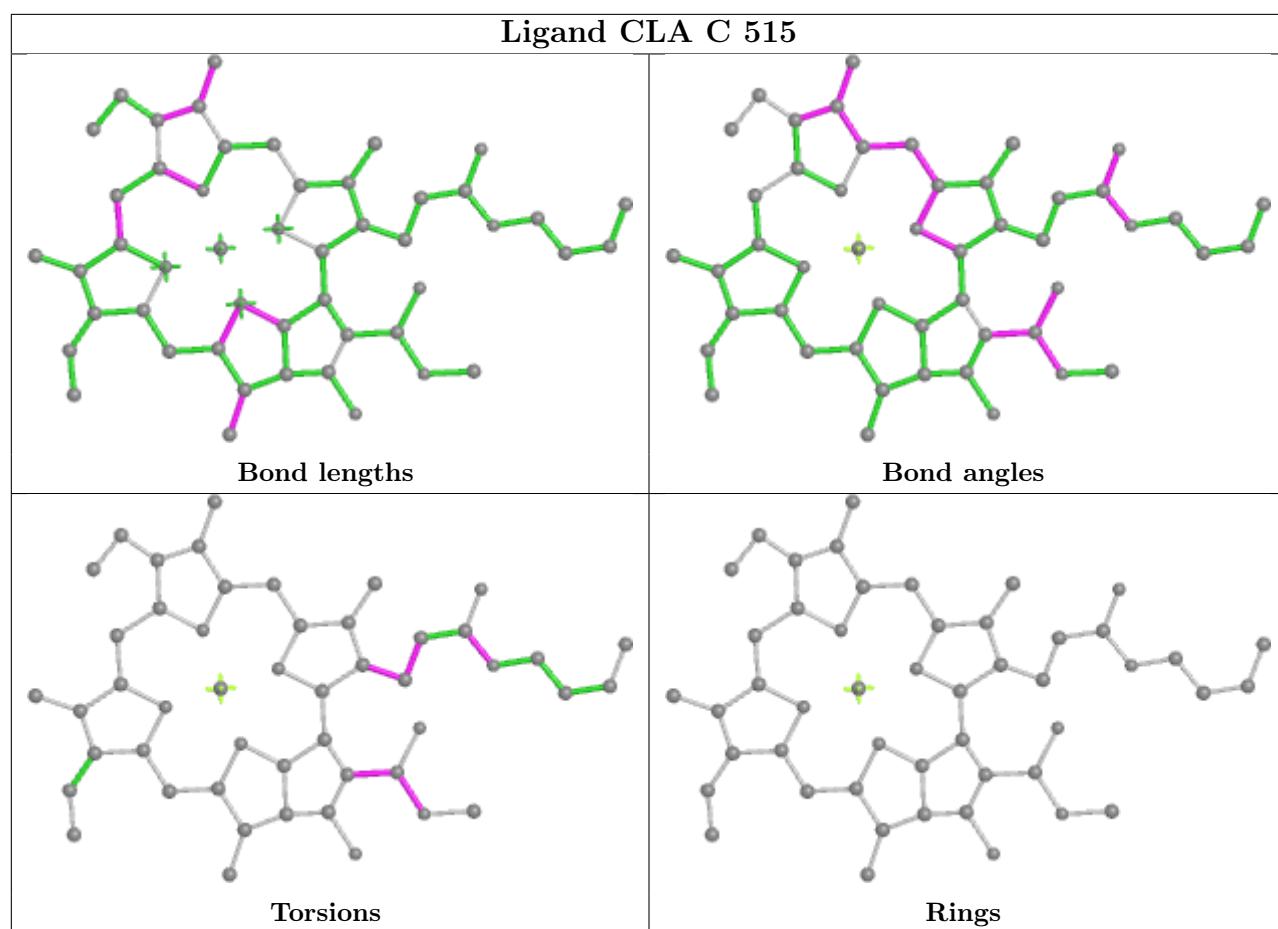


Torsions



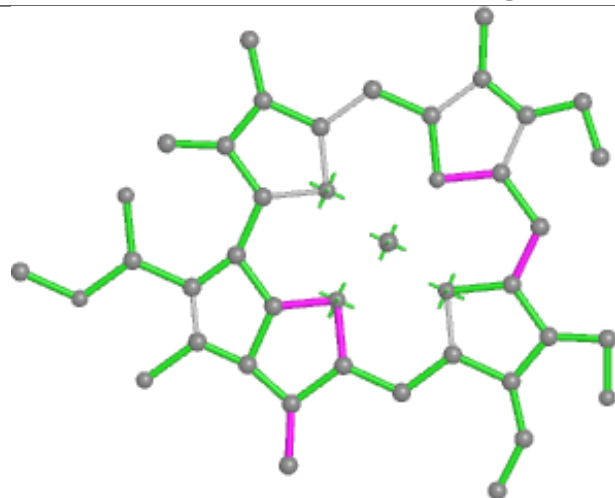
Rings



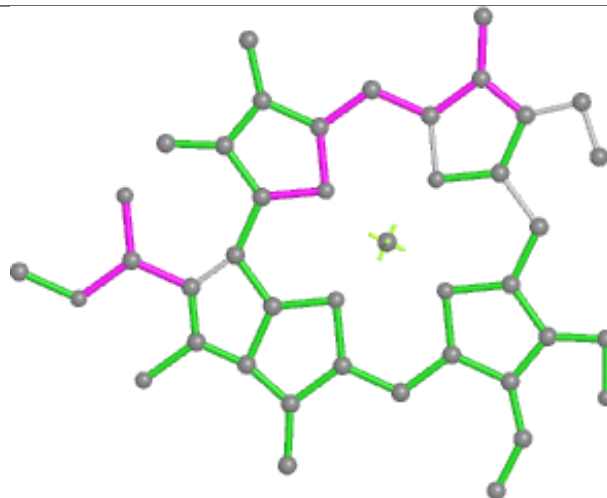




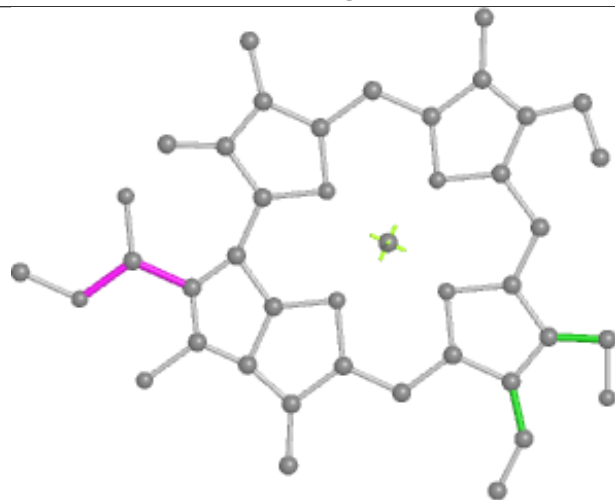
## Ligand CHL NN 605



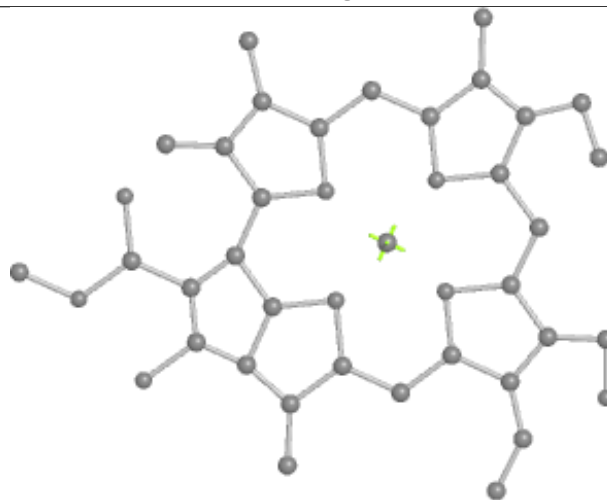
Bond lengths



Bond angles

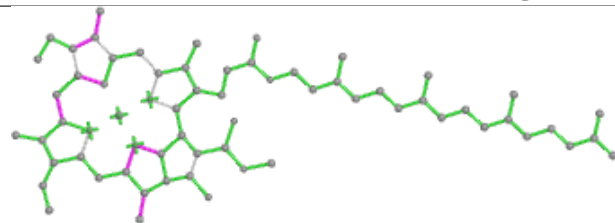


Torsions

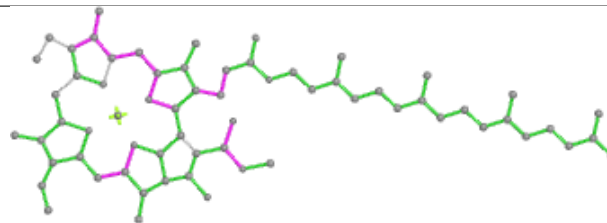


Rings

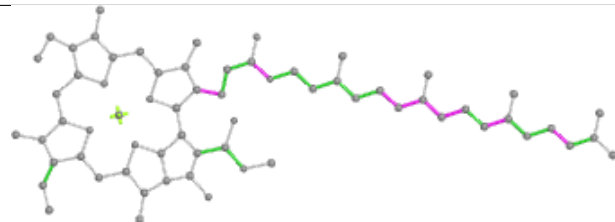
## Ligand CLA C 503



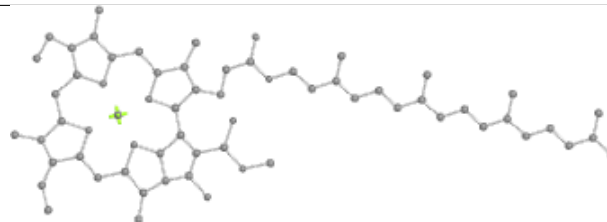
Bond lengths



Bond angles

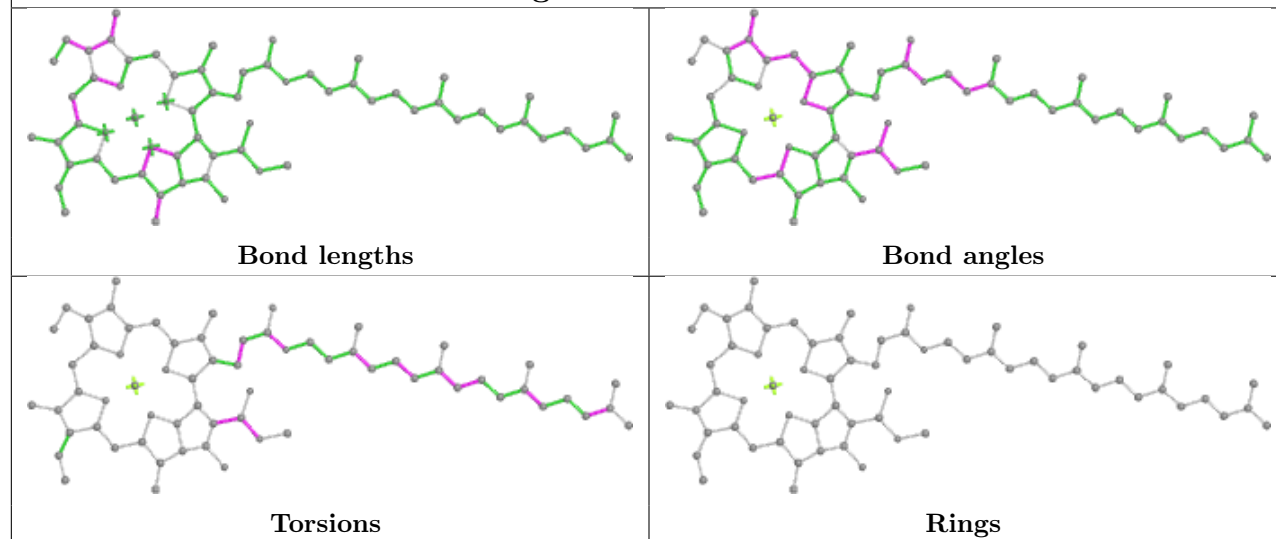


Torsions

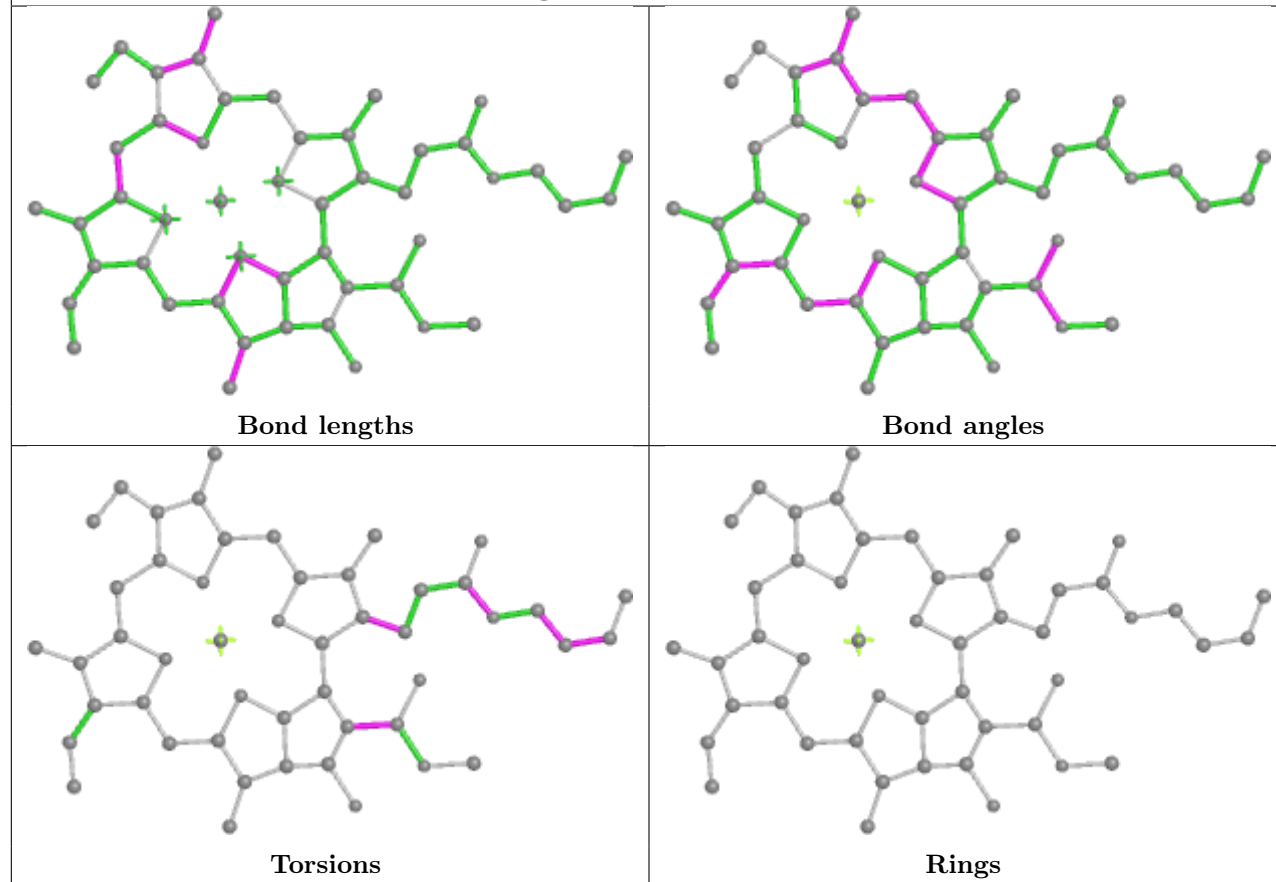


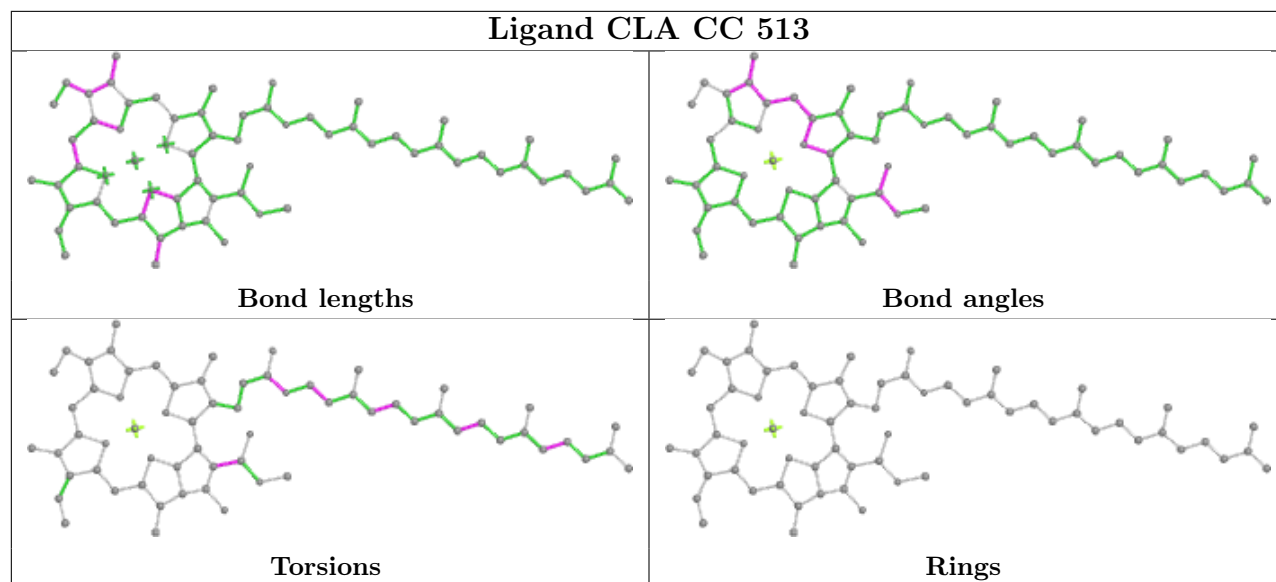
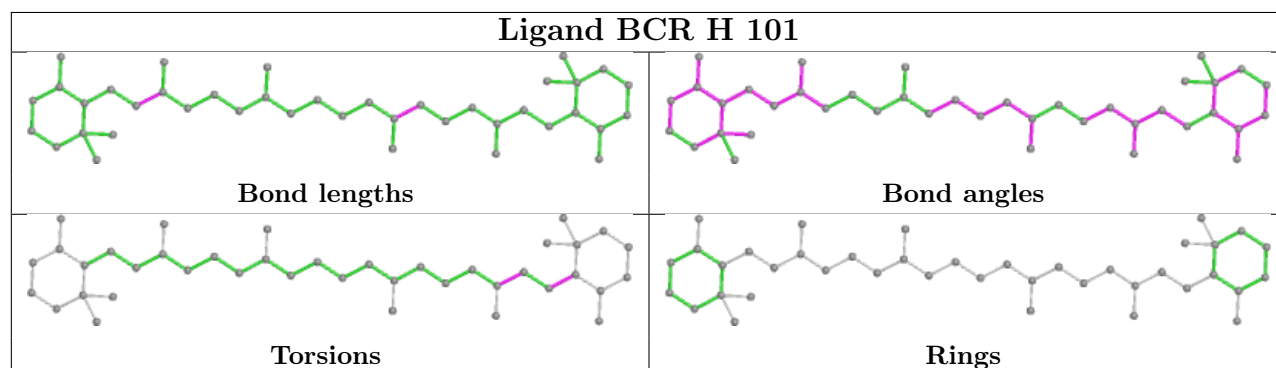
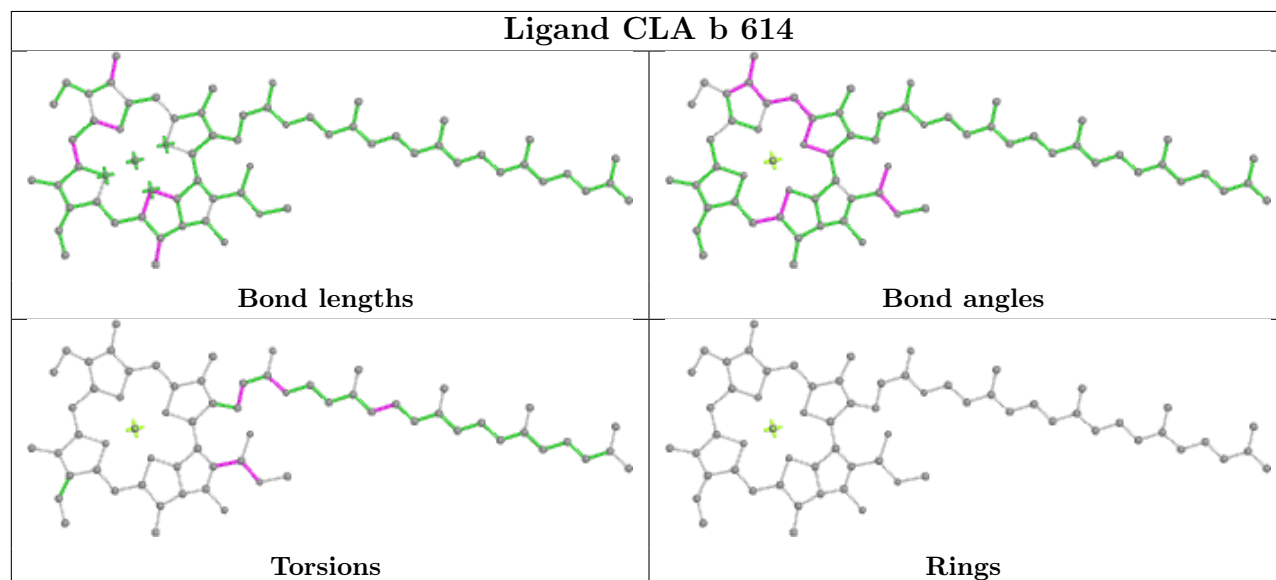
Rings

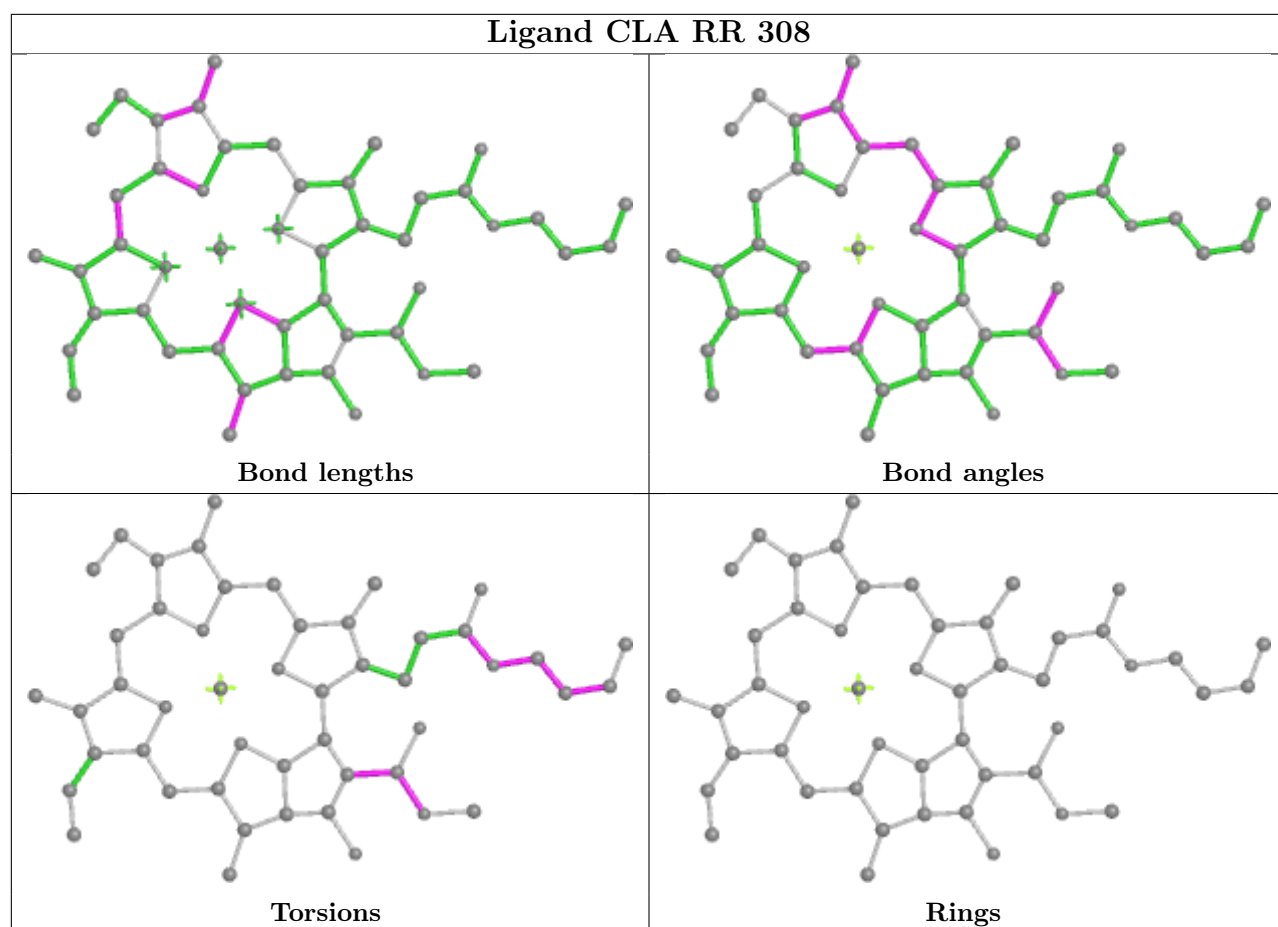
## Ligand CLA B 622

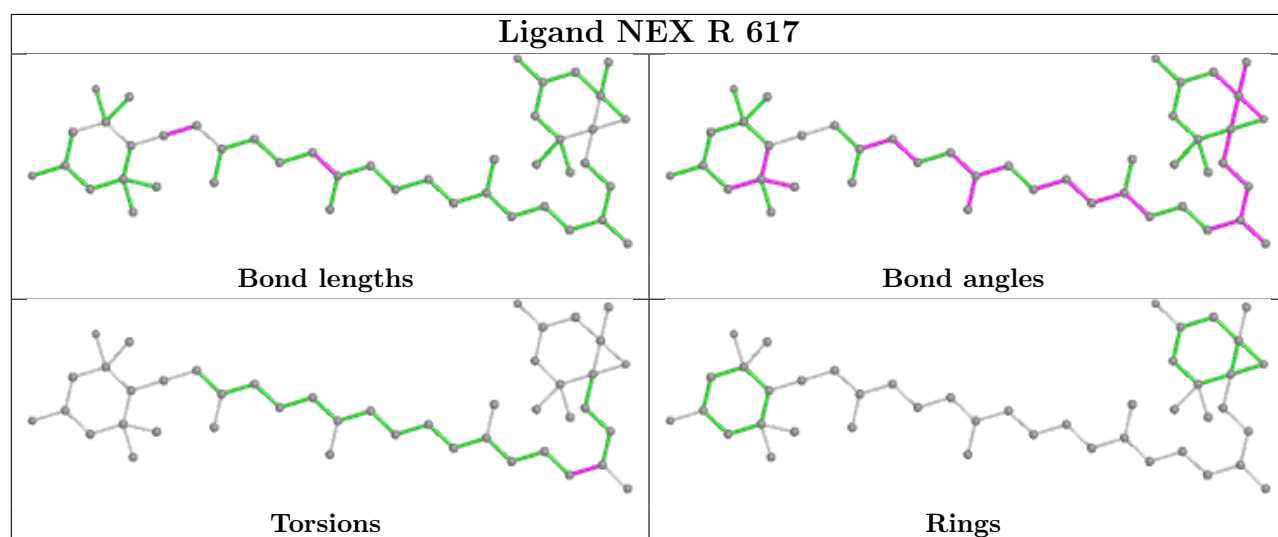
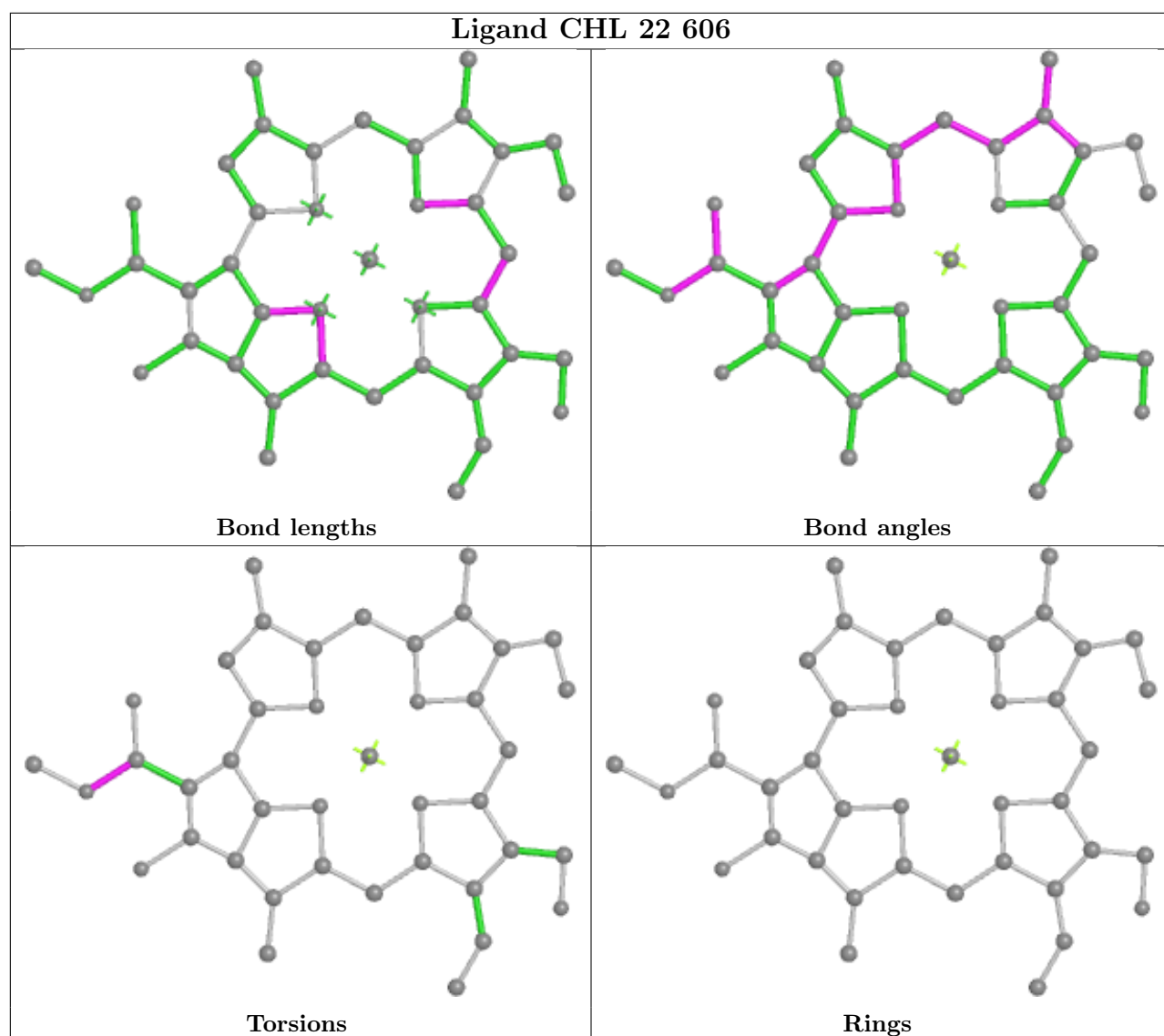


## Ligand CLA S 604

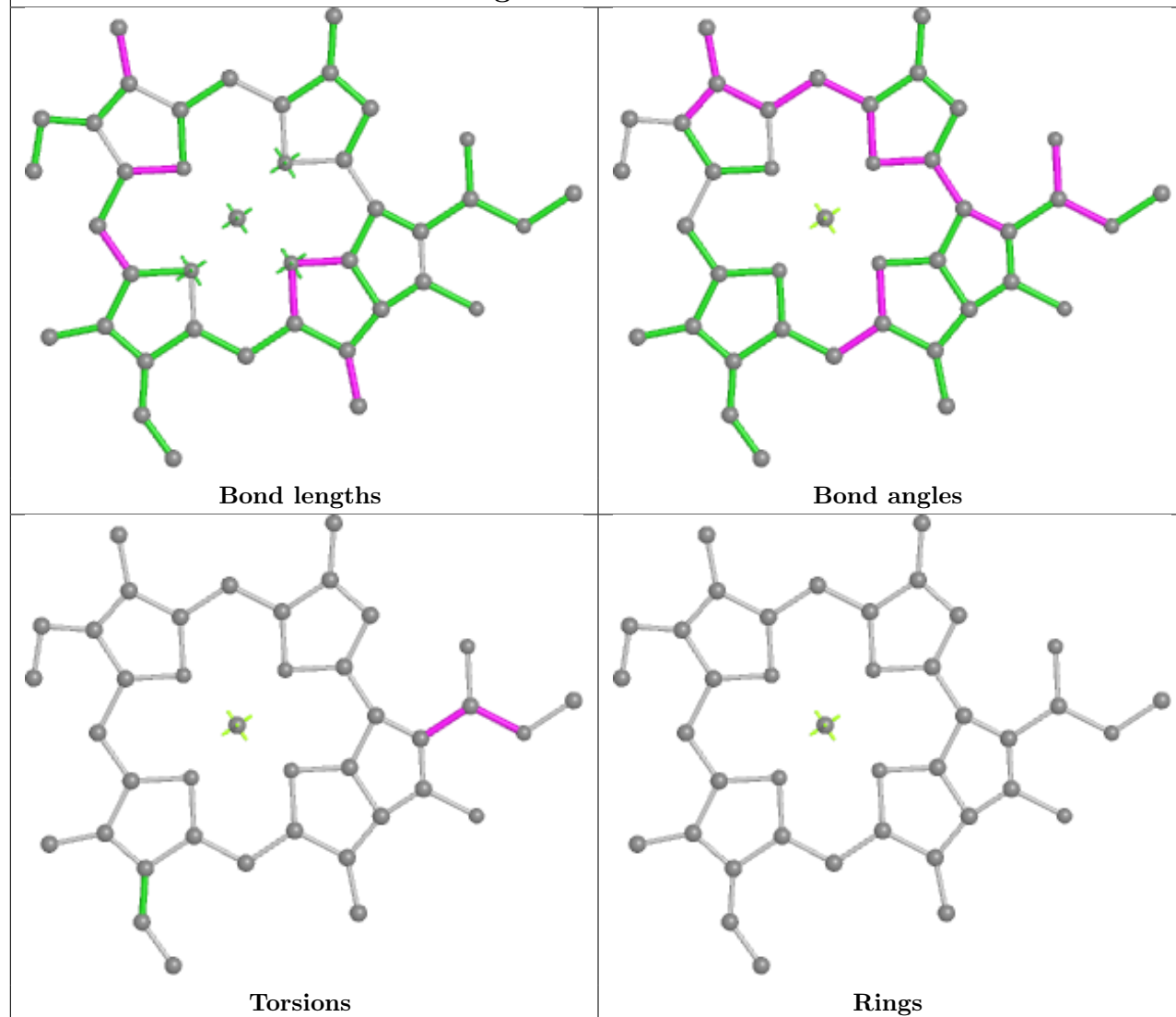


**Ligand CLA CC 513****Ligand BCR H 101****Ligand CLA b 614**

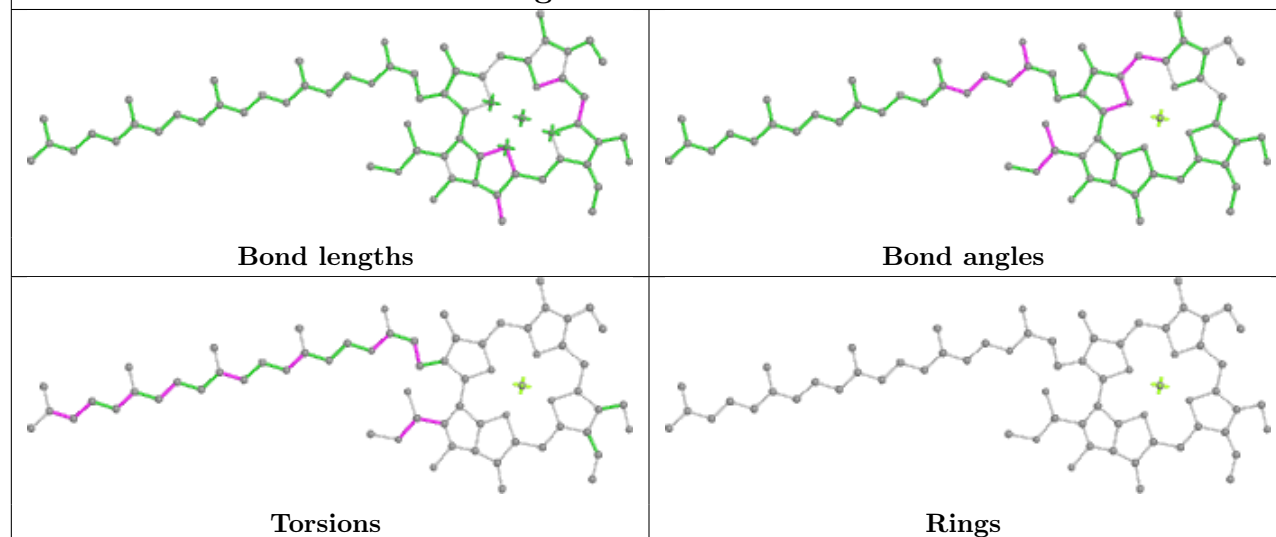




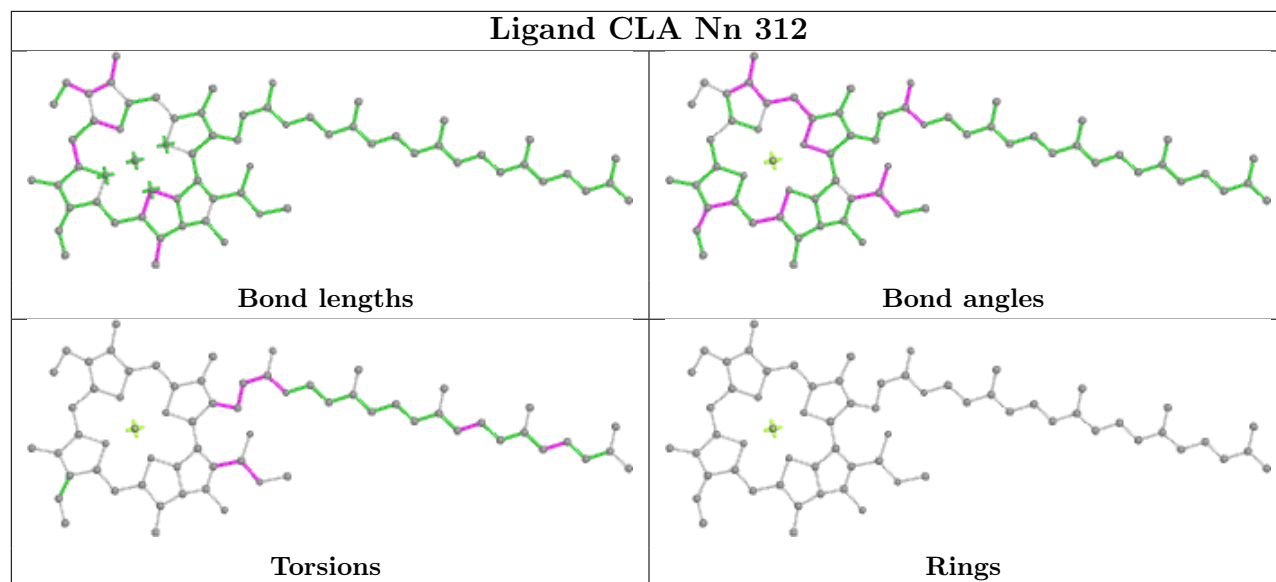
## Ligand CLA 2 604



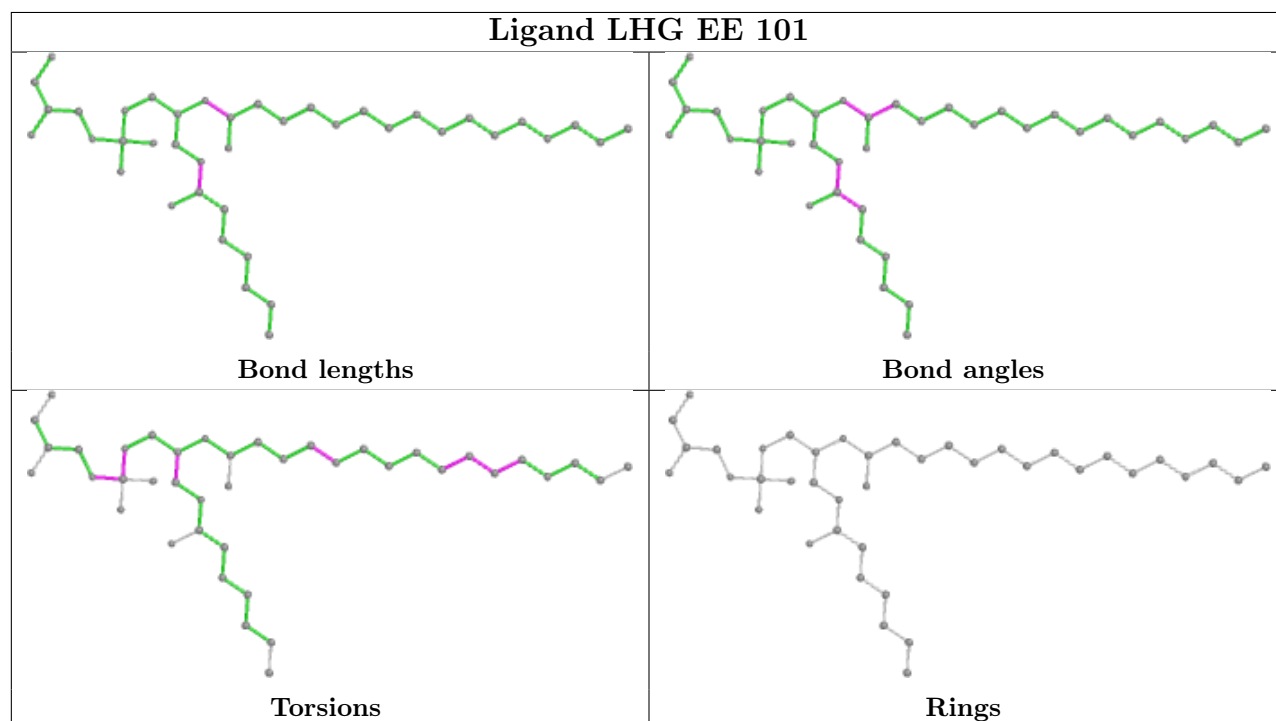
## Ligand CHL n 607



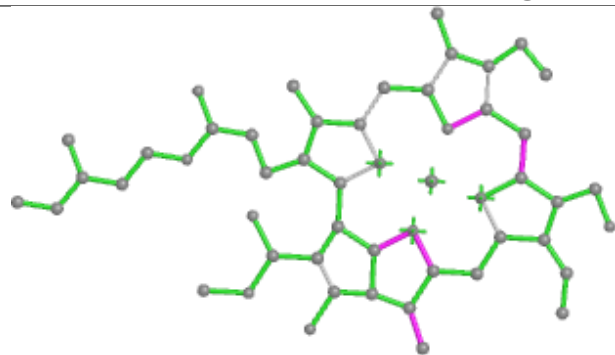
## Ligand CLA Nn 312



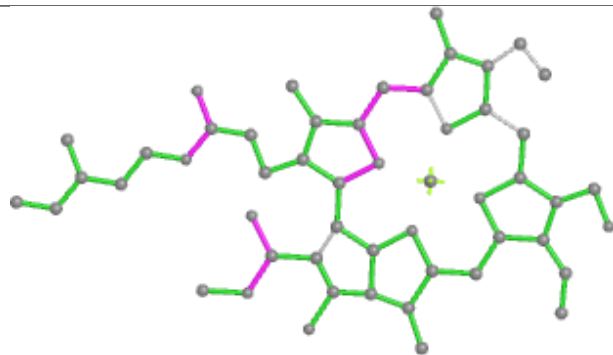
## Ligand LHG EE 101



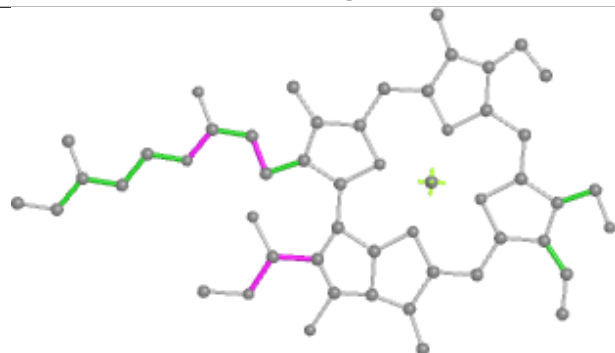
## Ligand CHL S 601



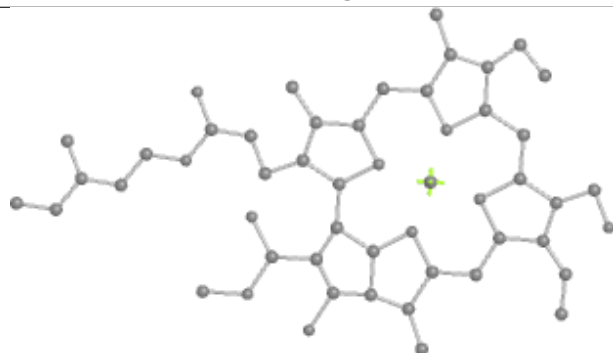
Bond lengths



Bond angles

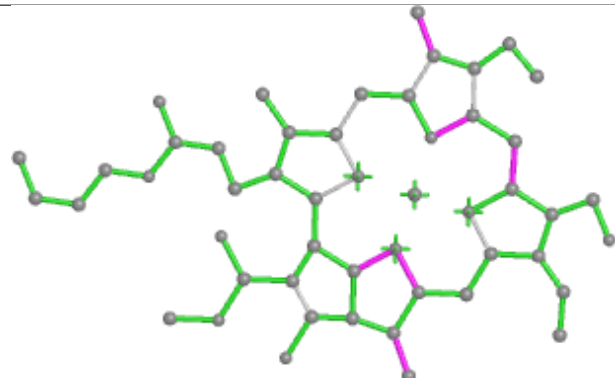


Torsions

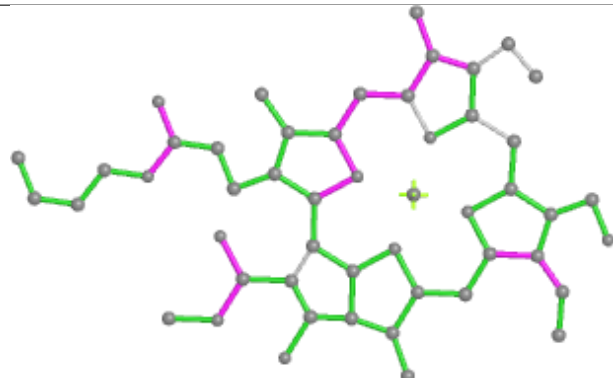


Rings

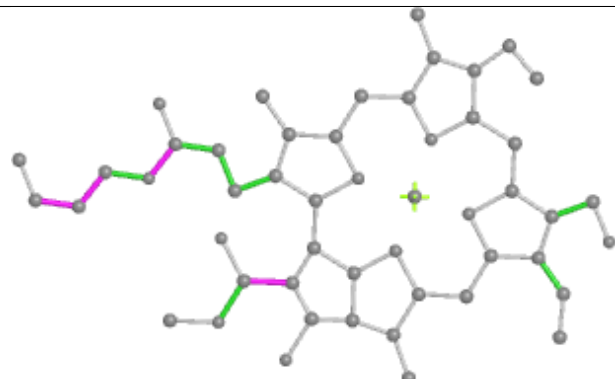
## Ligand CHL Nn 319



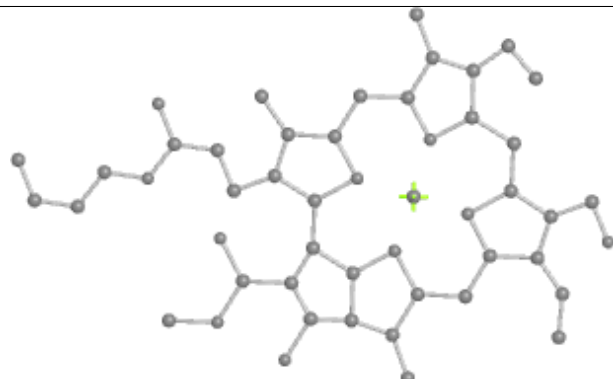
Bond lengths



Bond angles

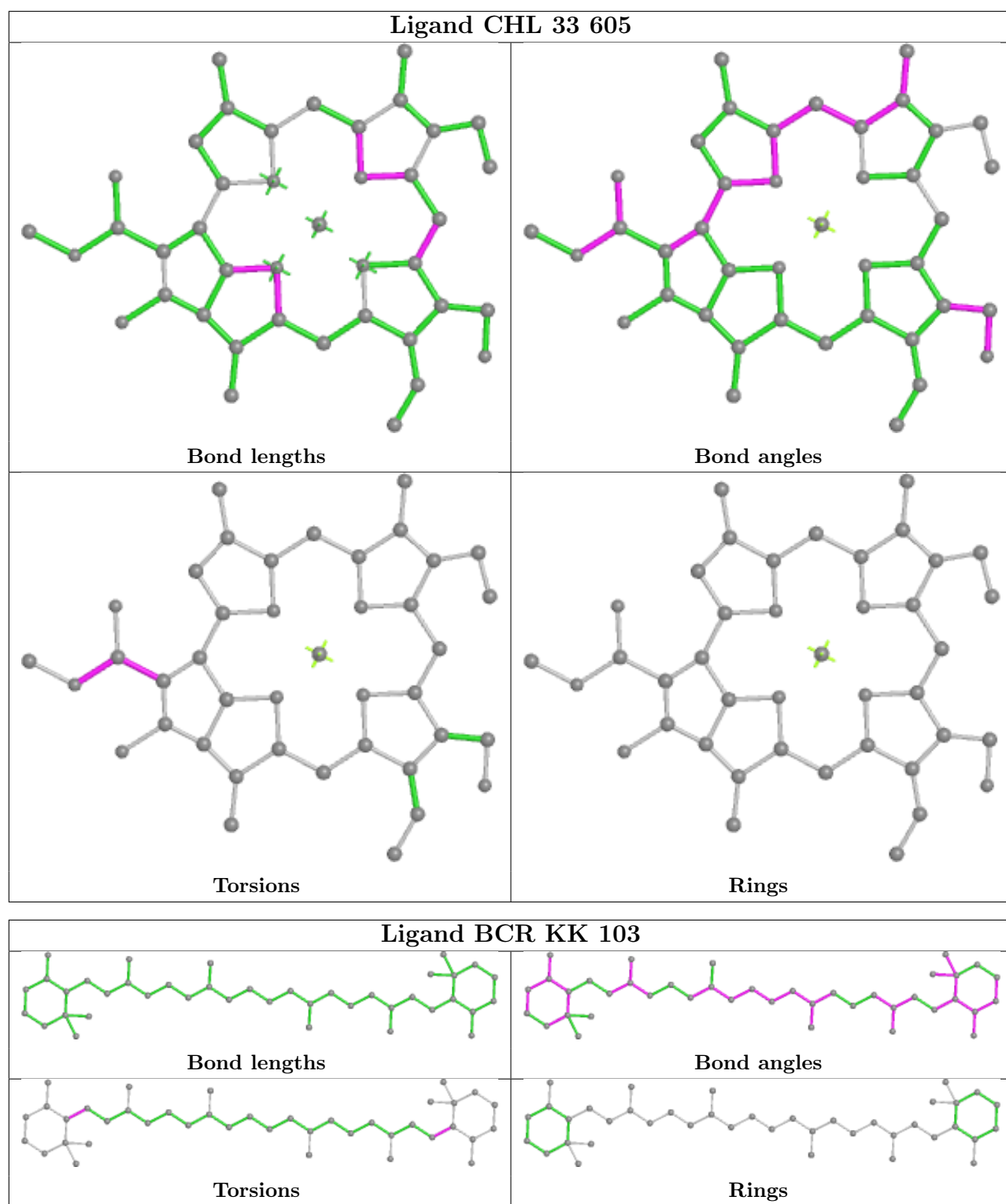


Torsions

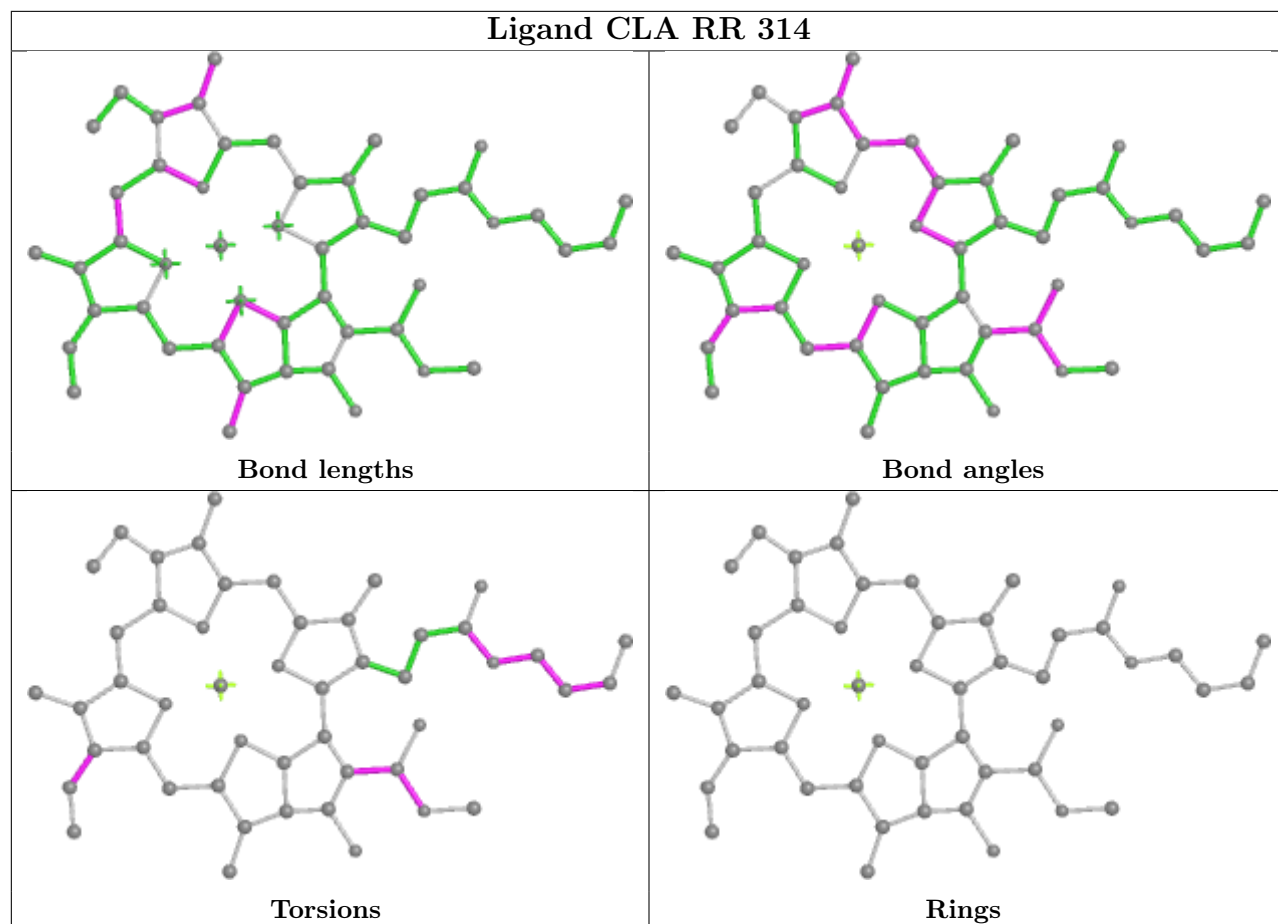


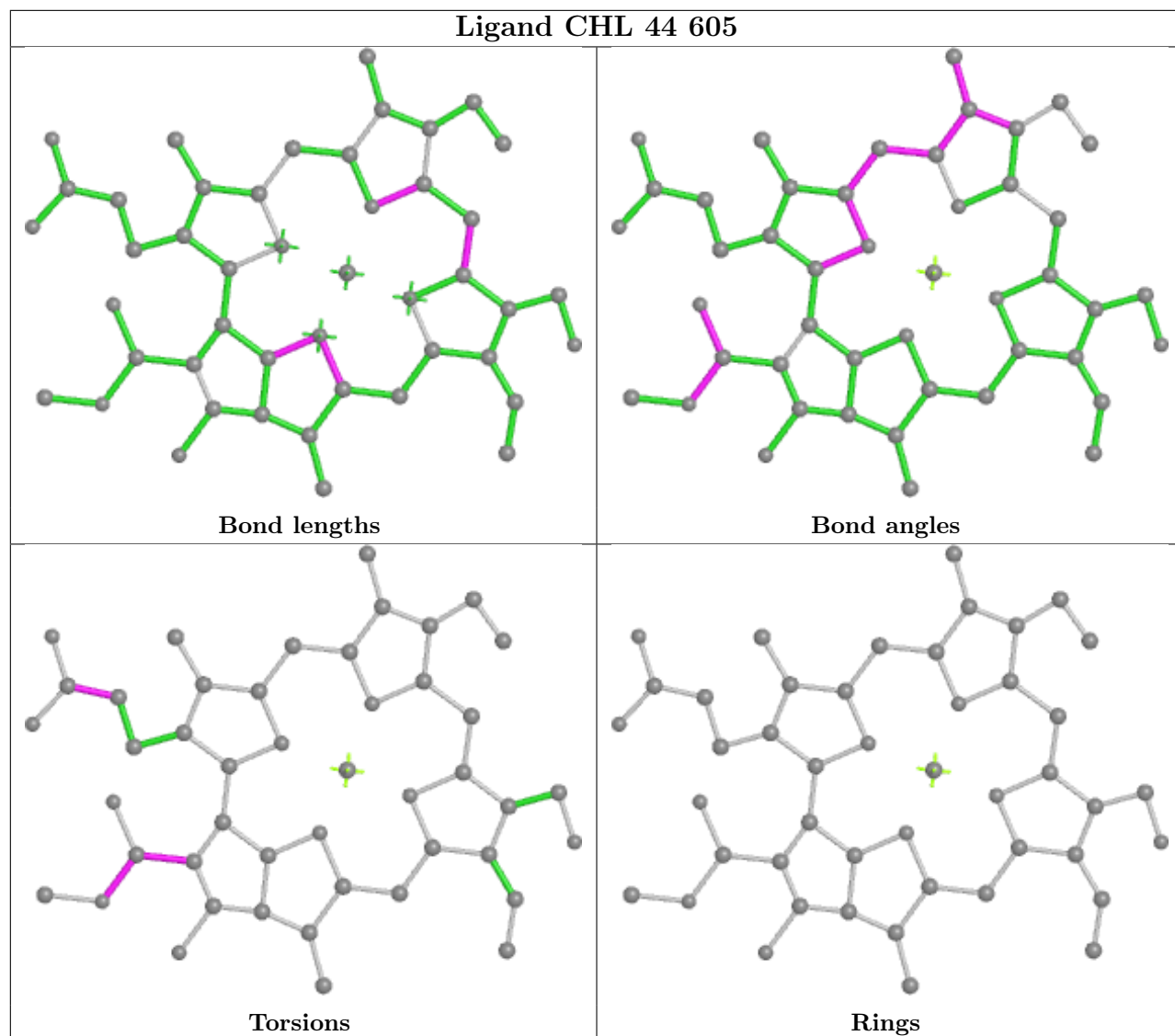
Rings

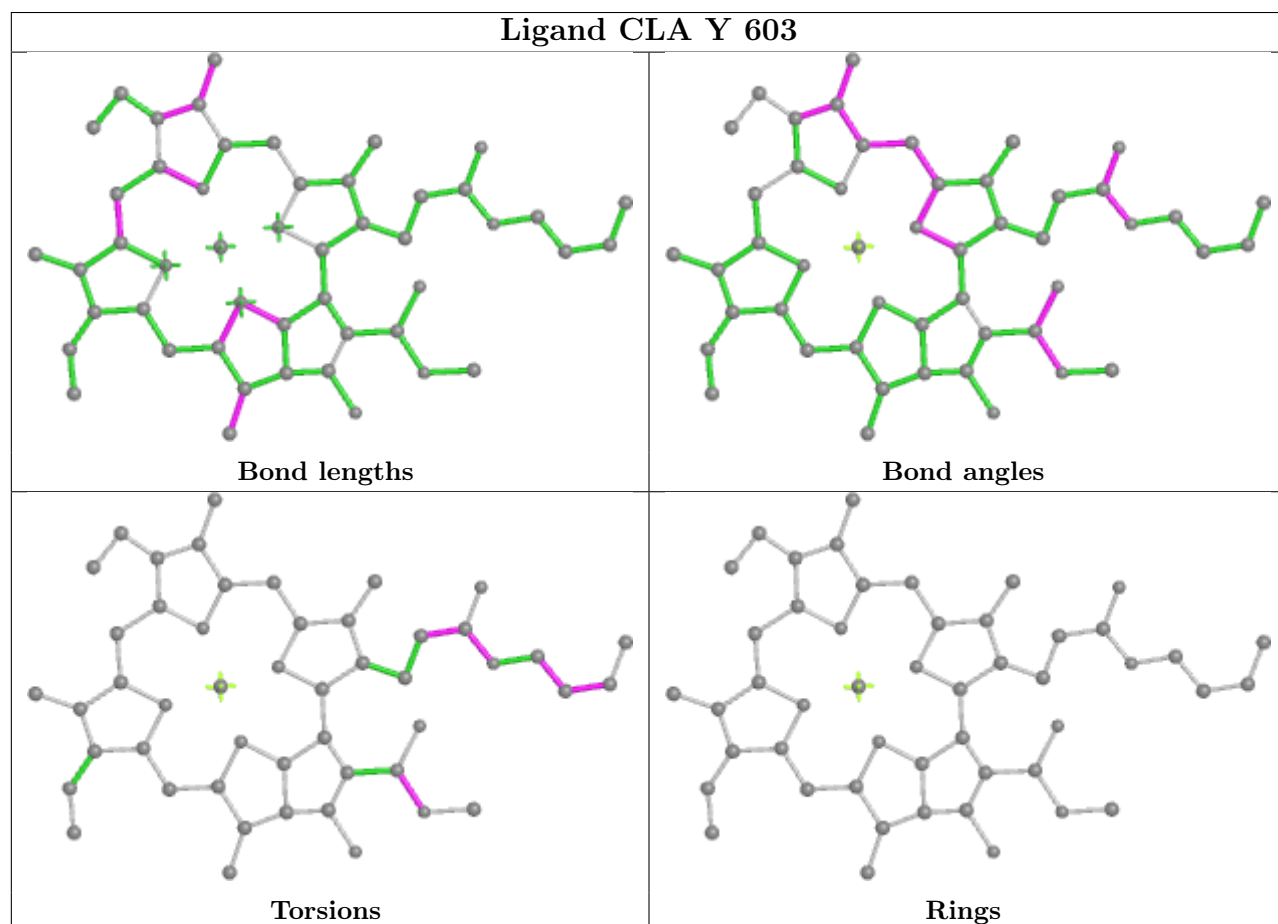
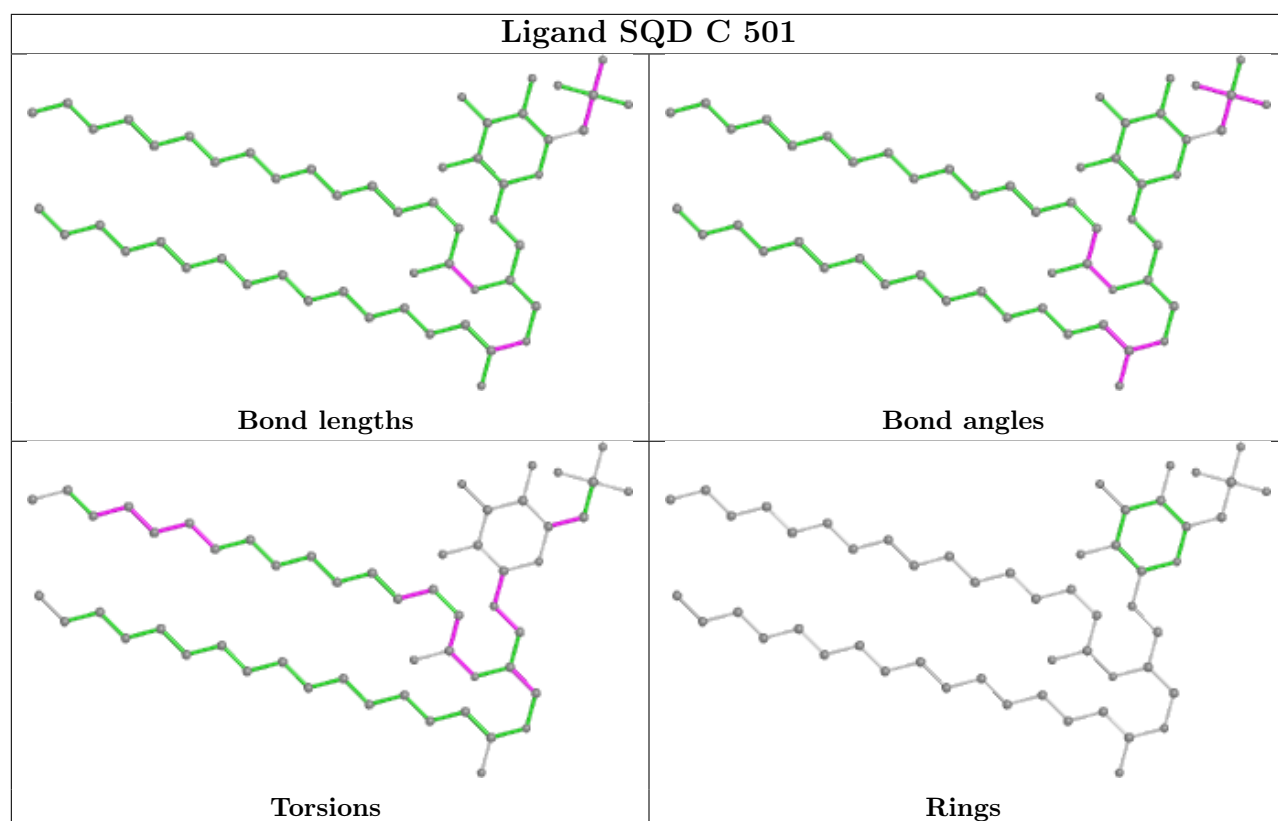




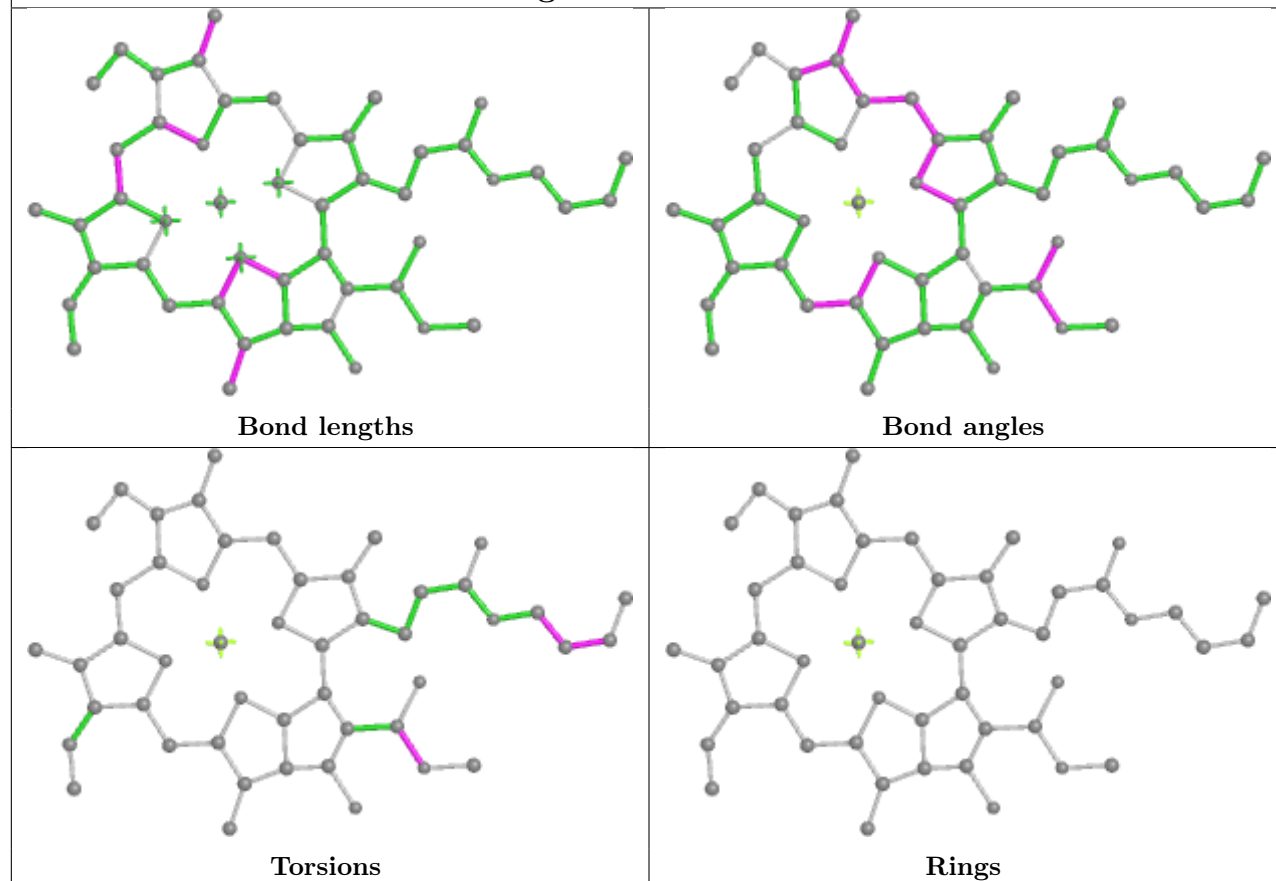
## Ligand CLA RR 314



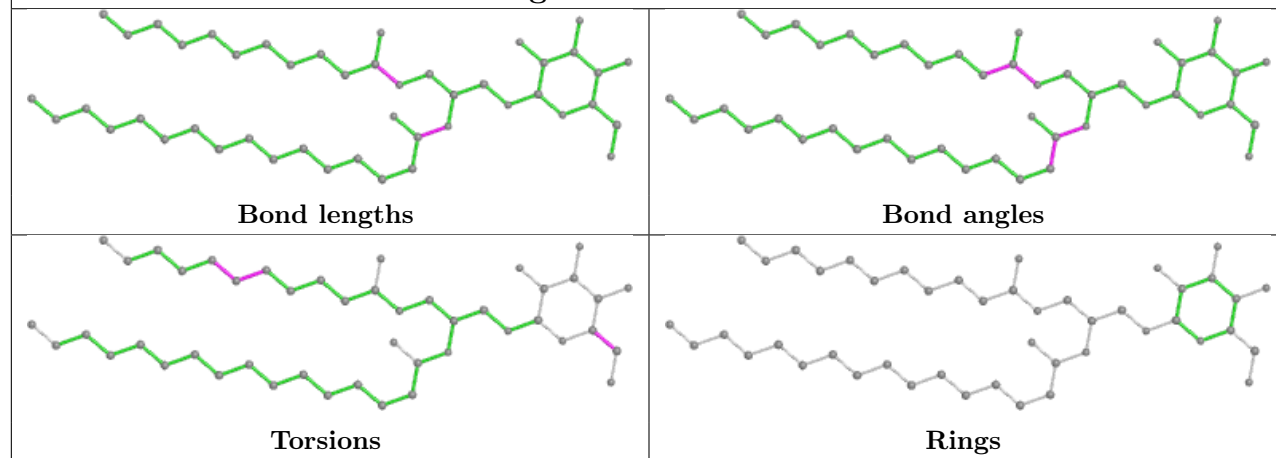


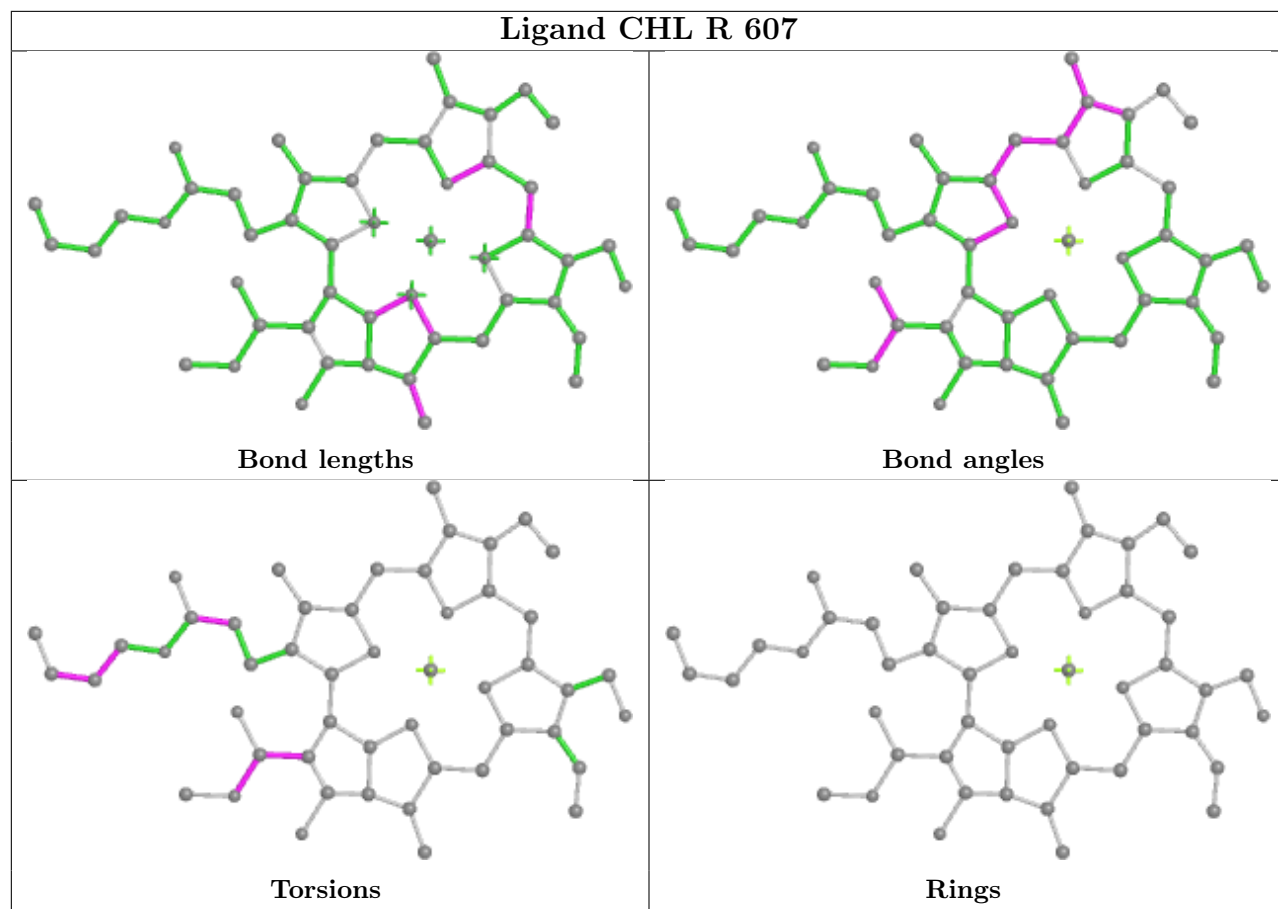


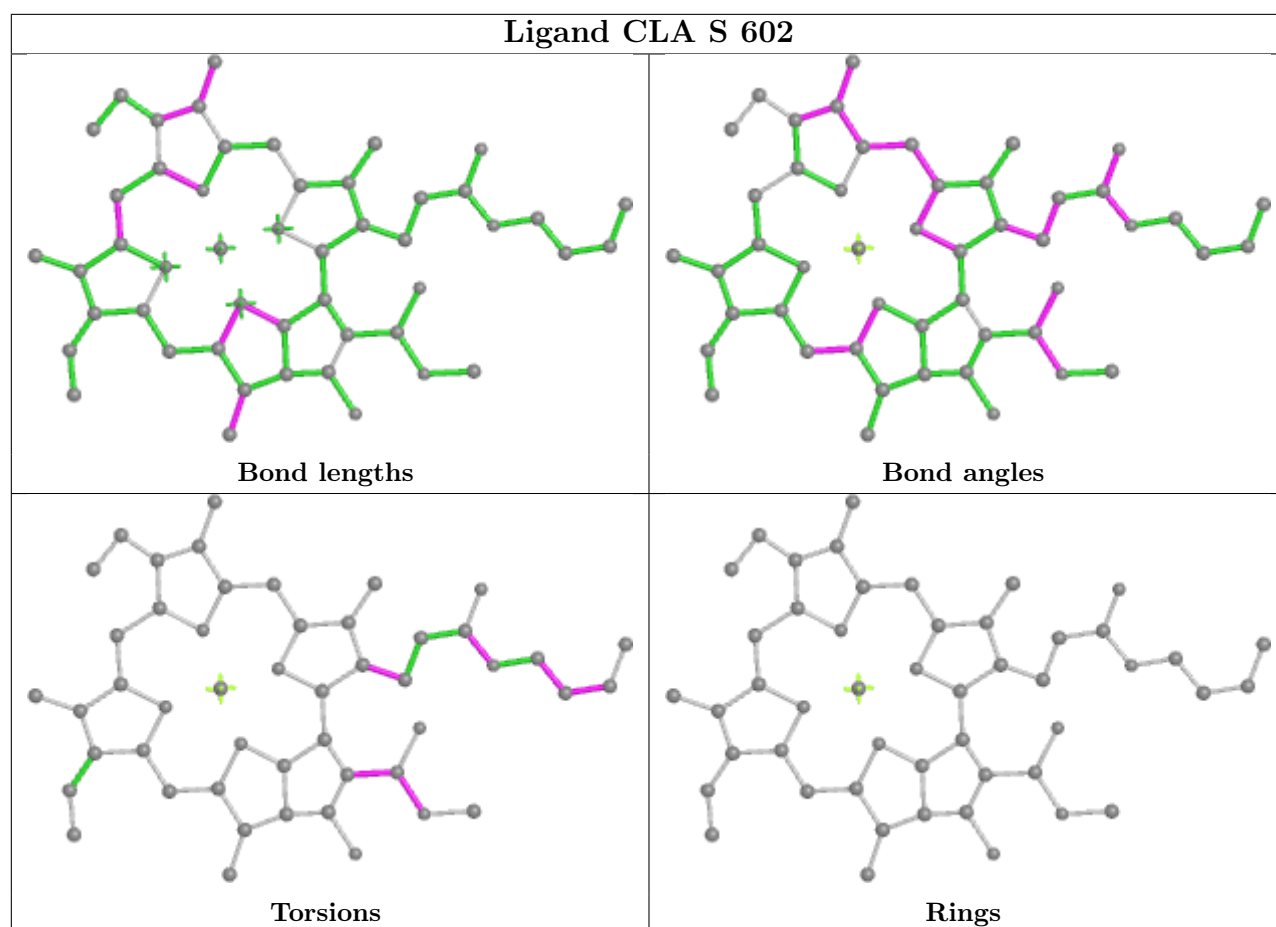
## Ligand CLA s 613

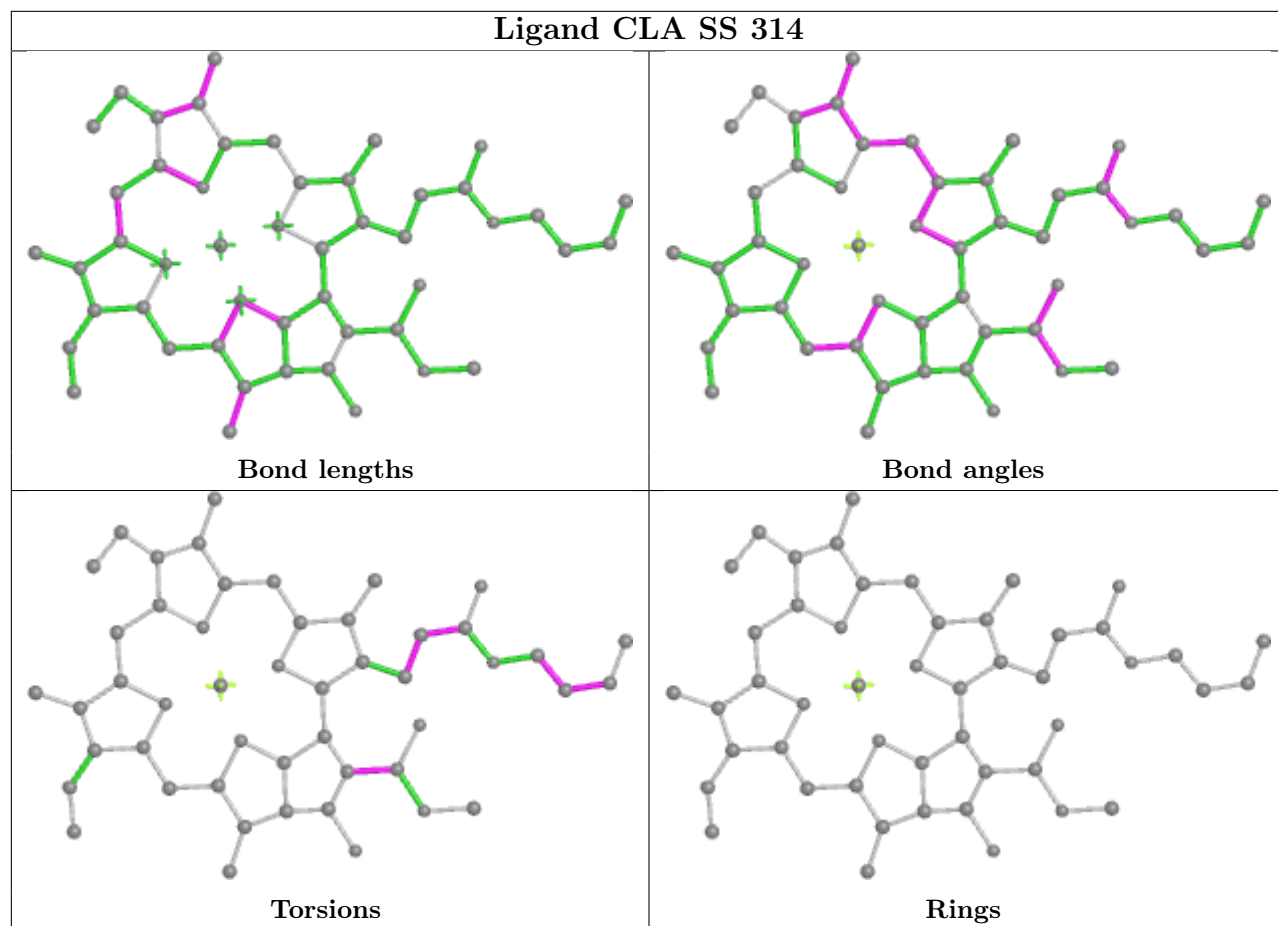


## Ligand LMG F 101



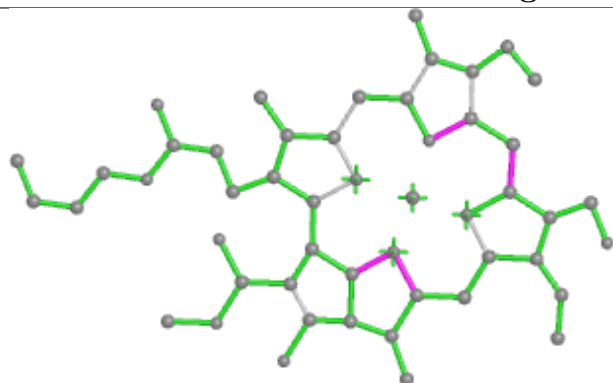




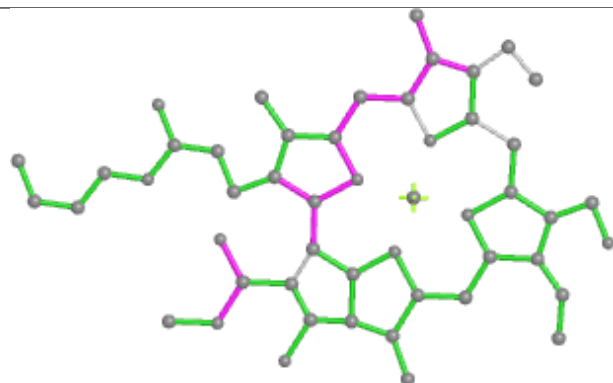




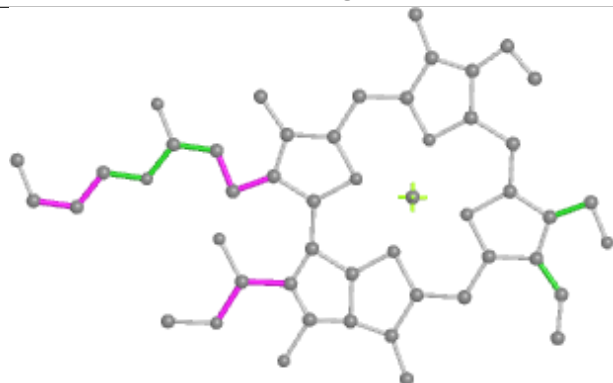
## Ligand CHL s 606



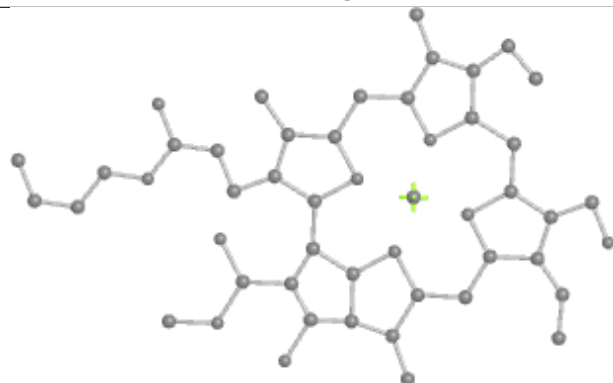
Bond lengths



Bond angles

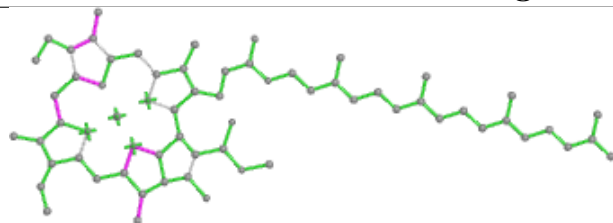


Torsions

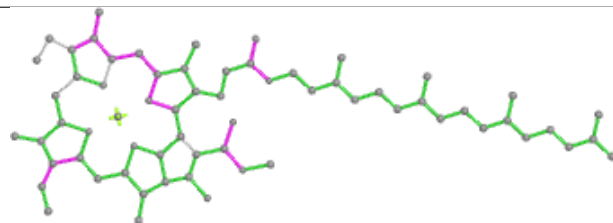


Rings

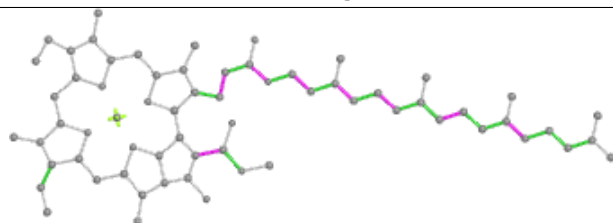
## Ligand CLA C 507



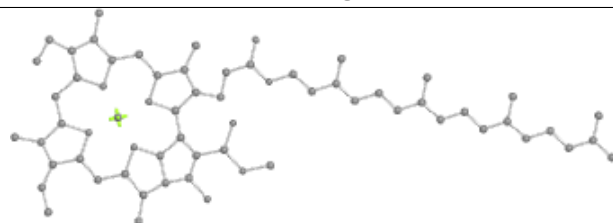
Bond lengths



Bond angles

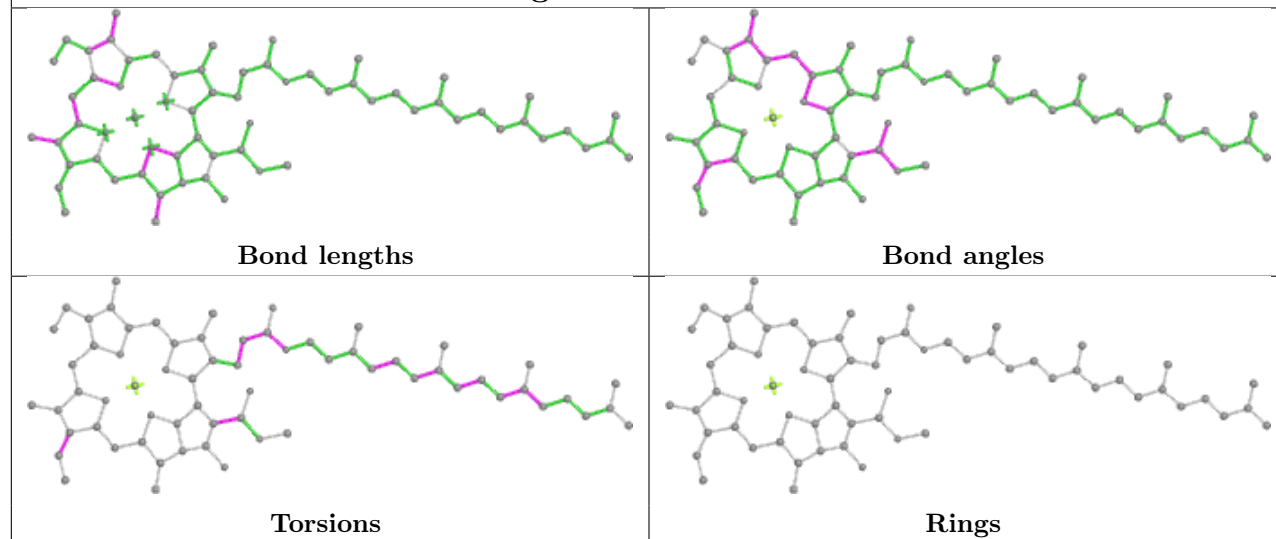


Torsions

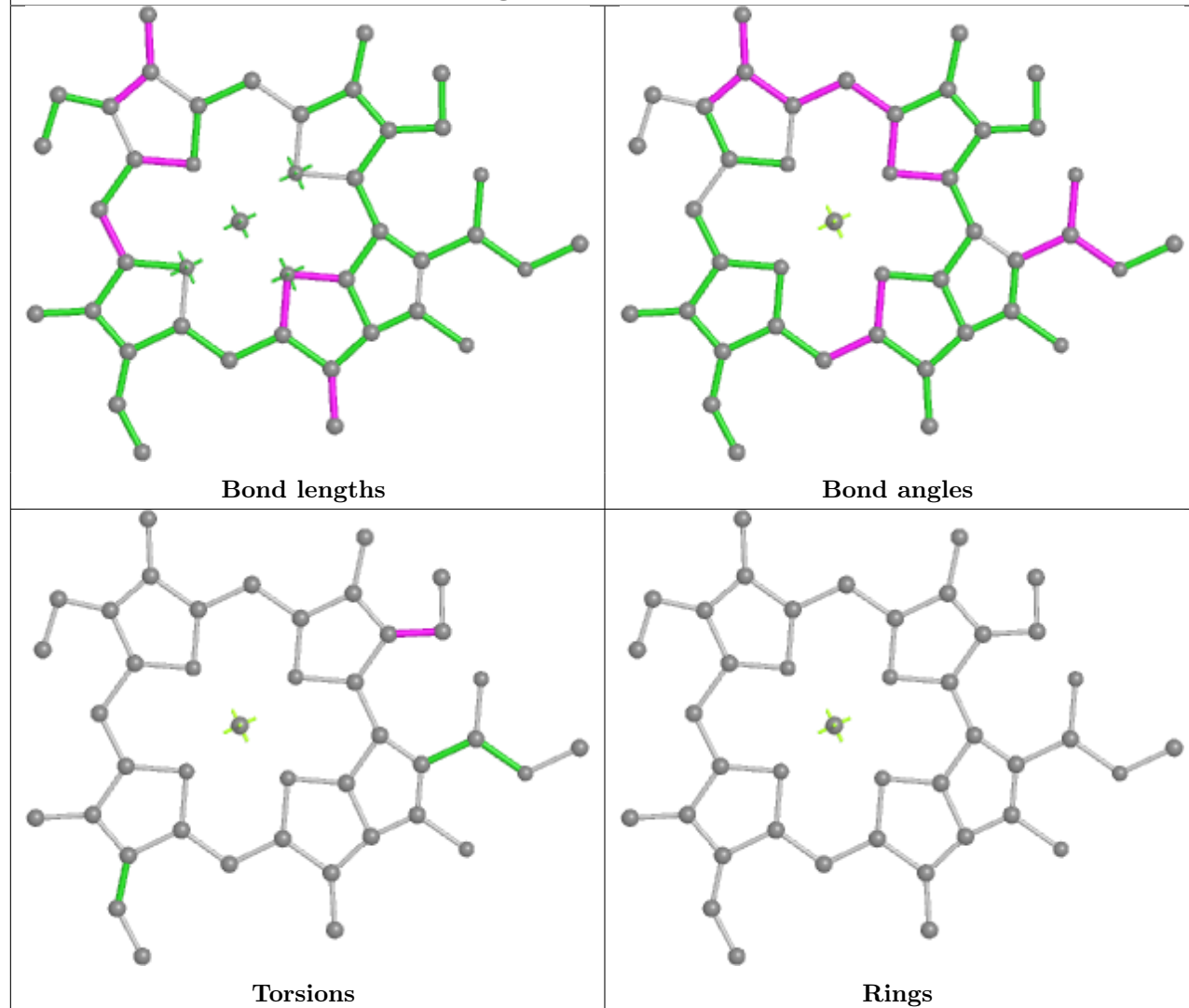


Rings

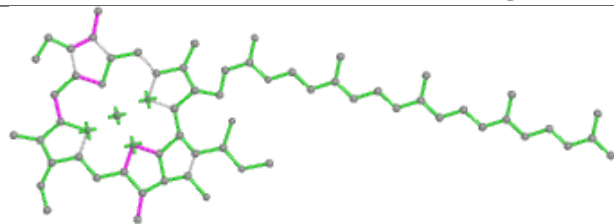
## Ligand CLA D 404



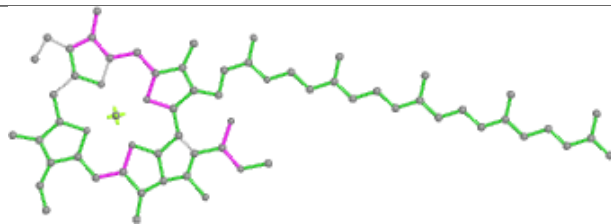
## Ligand CLA R 612



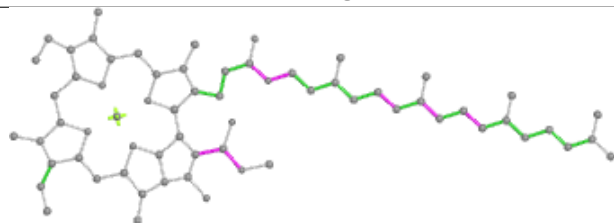
## Ligand CLA BB 606



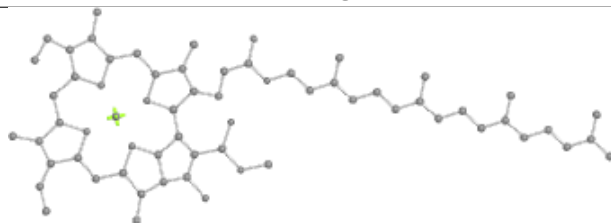
Bond lengths



Bond angles

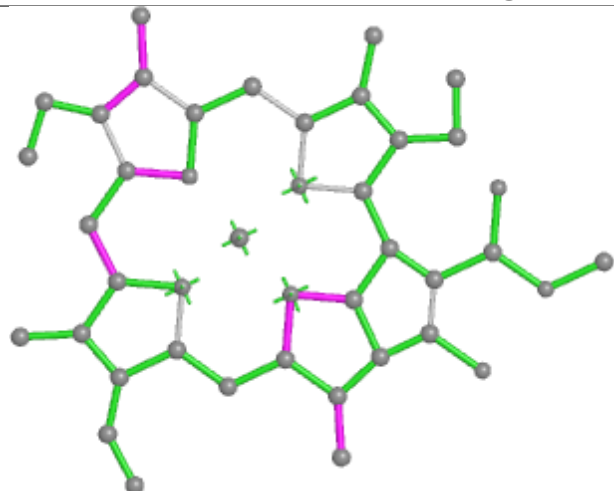


Torsions

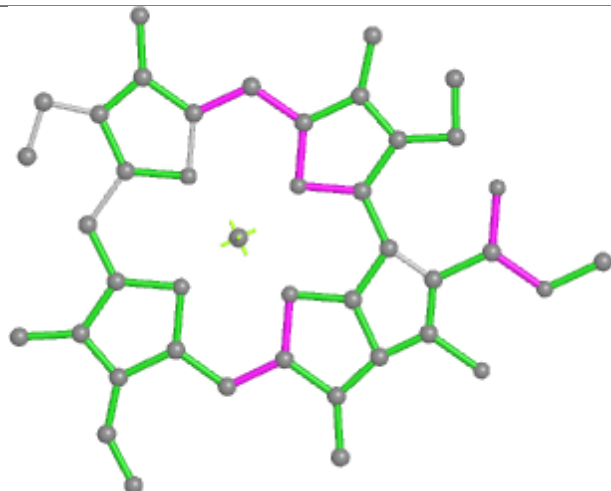


Rings

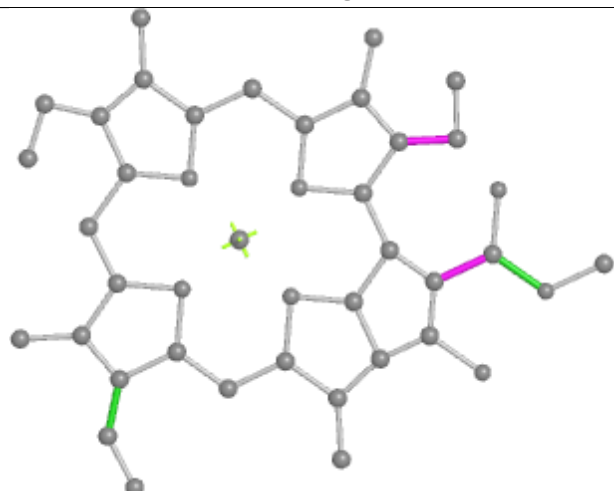
## Ligand CLA RR 312



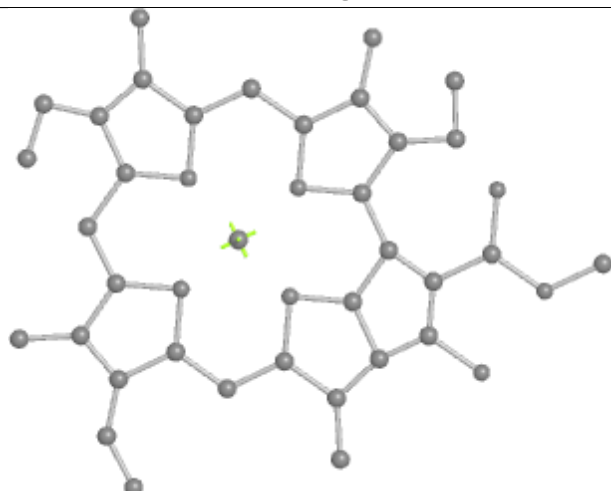
Bond lengths



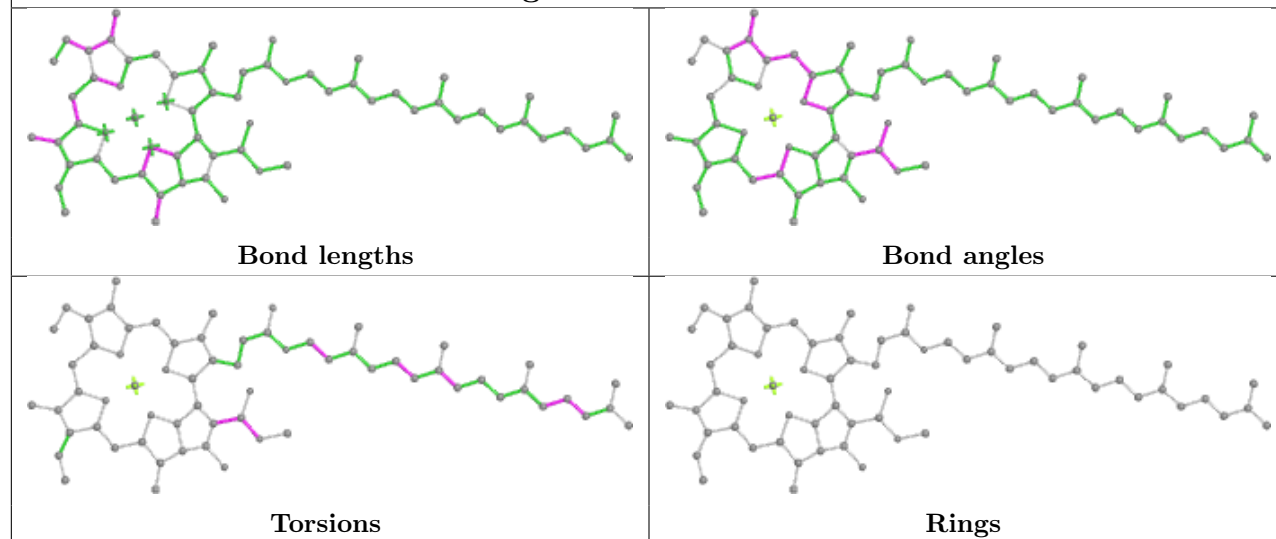
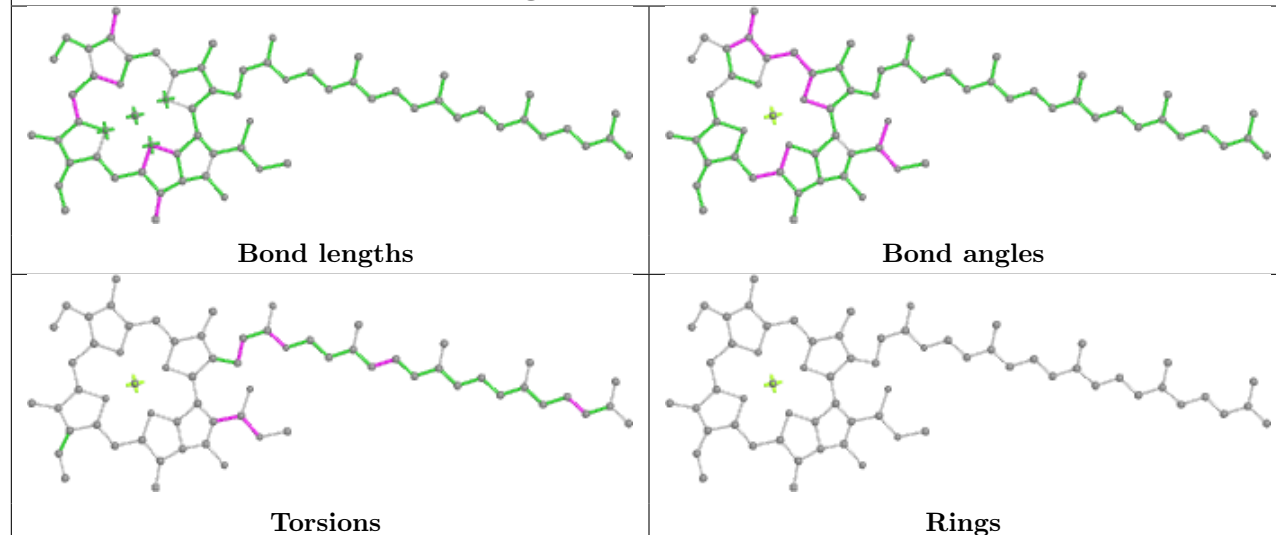
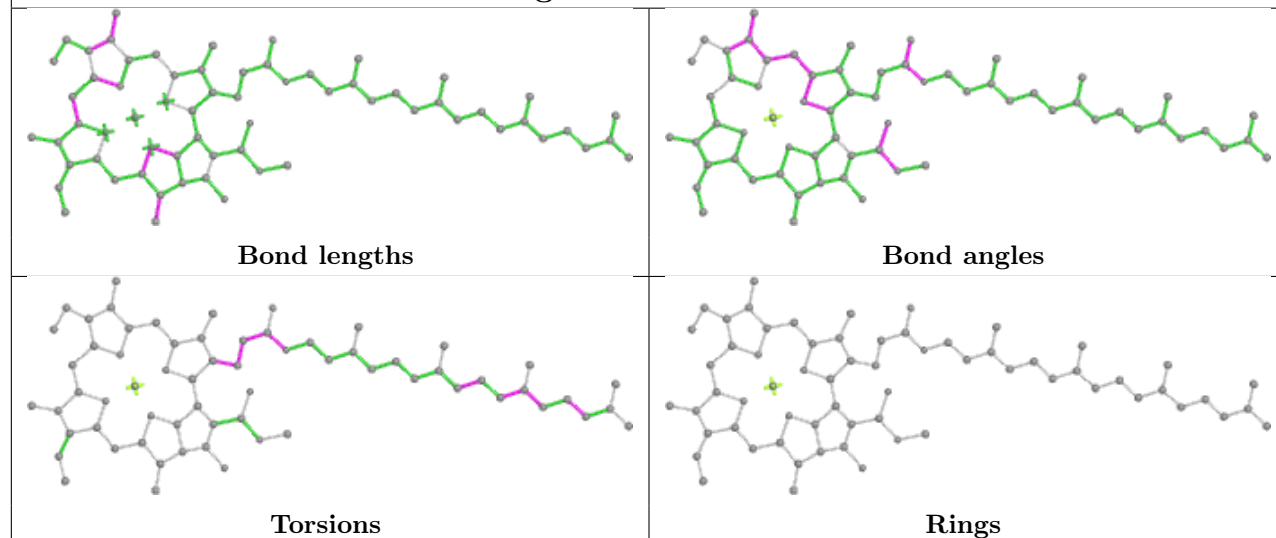
Bond angles



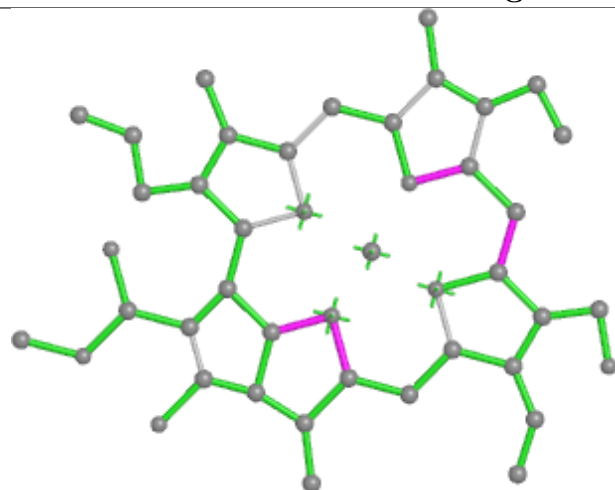
Torsions



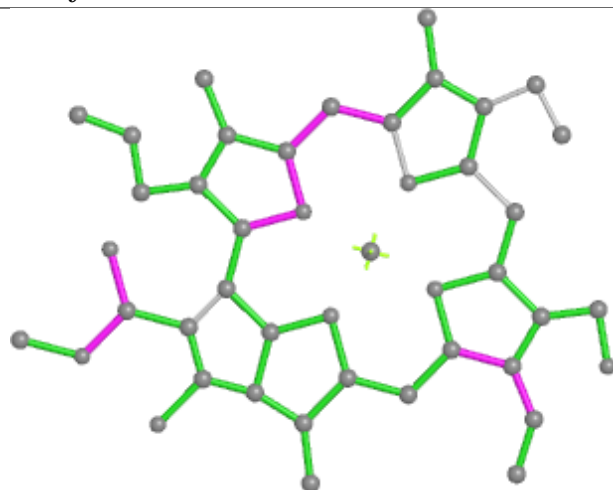
Rings

**Ligand CLA Bb 602****Ligand CLA Bb 614****Ligand CLA b 616**

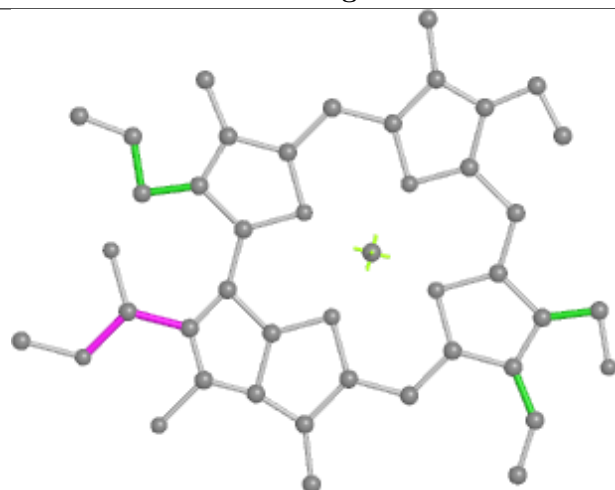
## Ligand CHL Yy 606



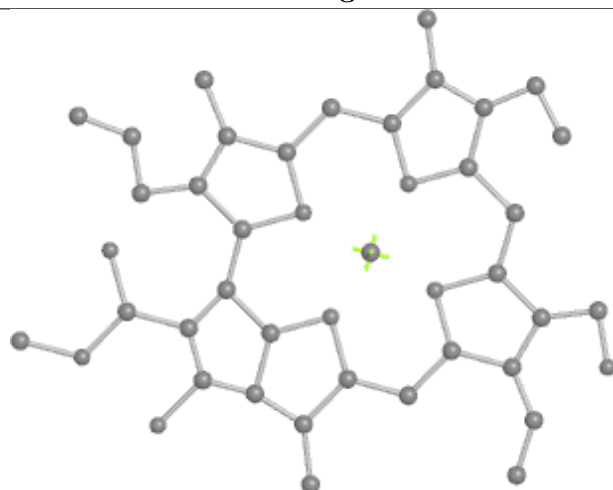
Bond lengths



Bond angles

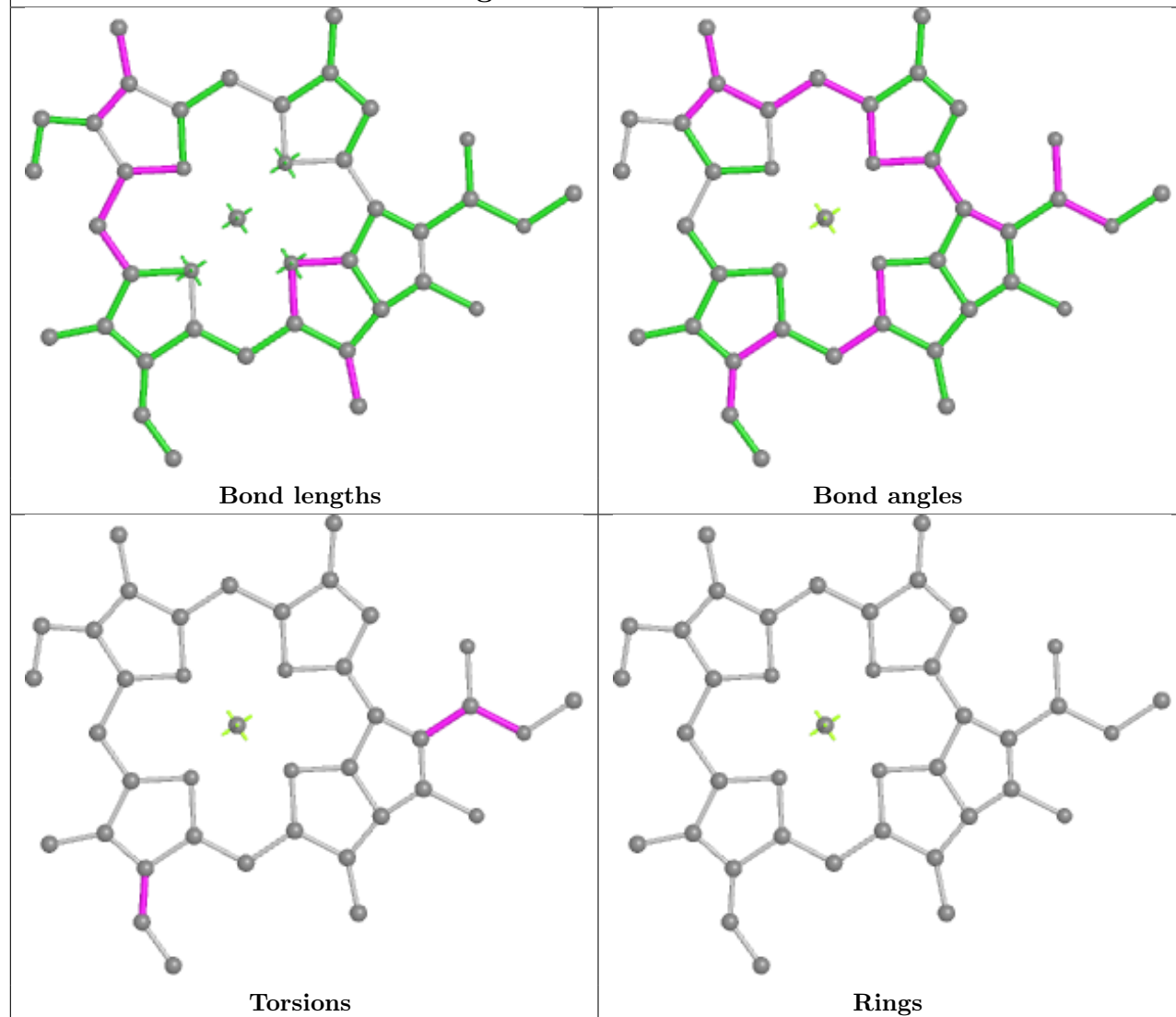


Torsions

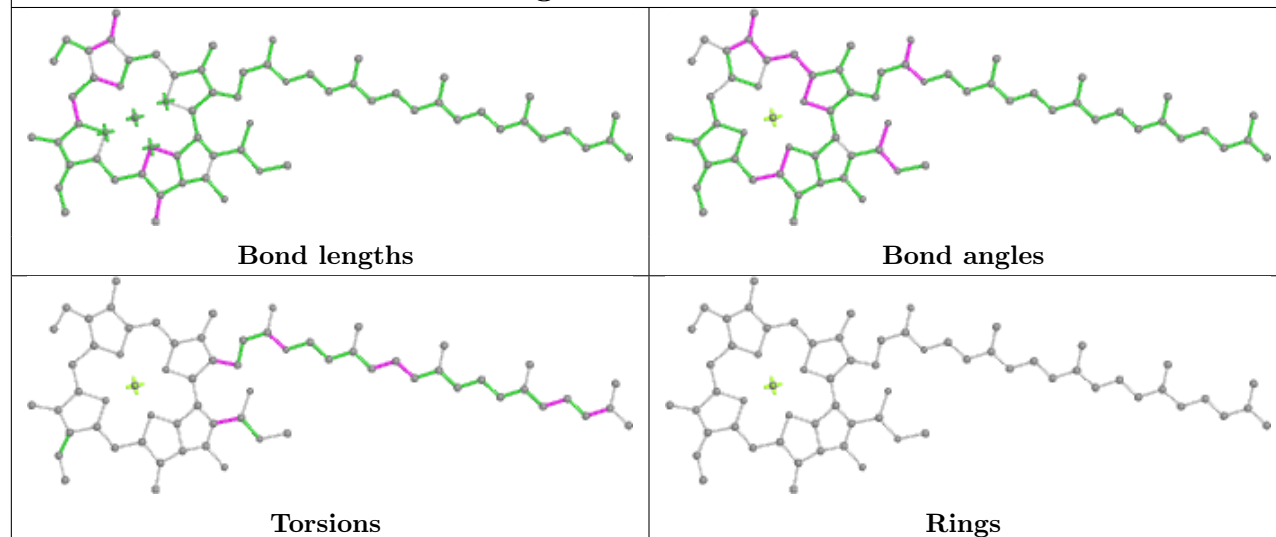


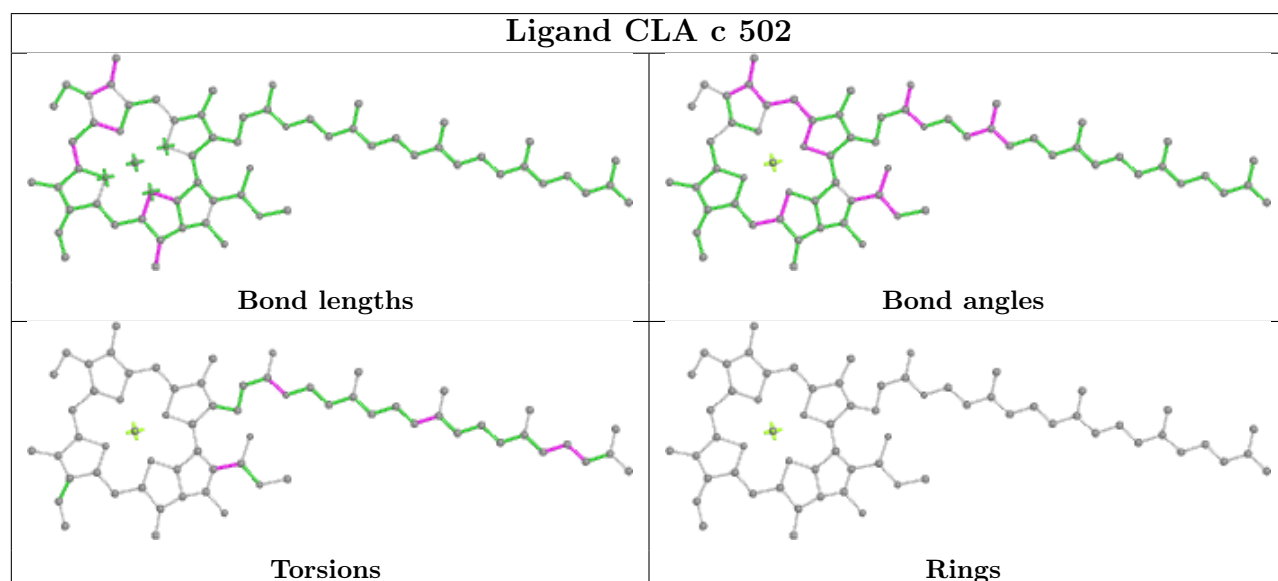
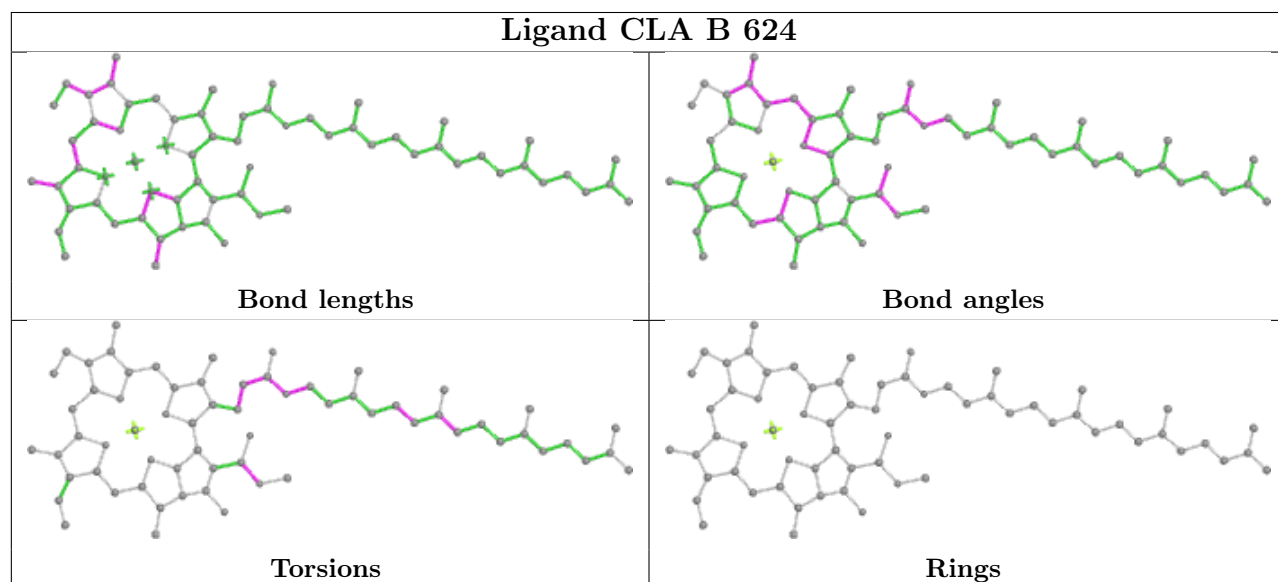
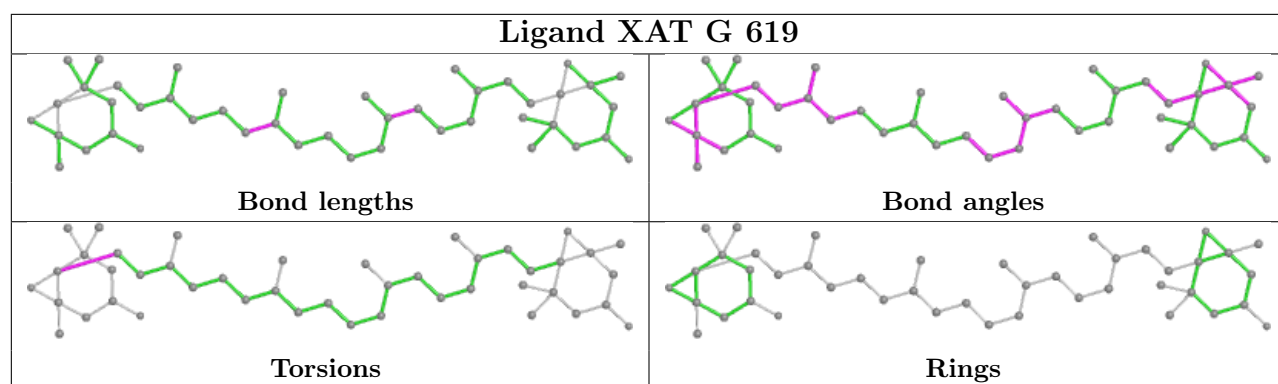
Rings

## Ligand CLA GG 613

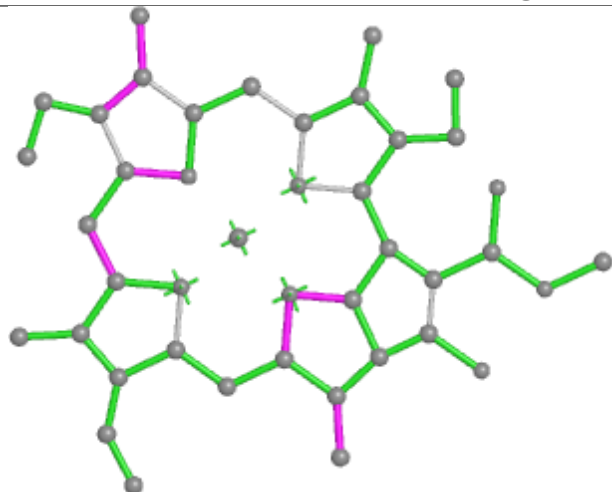


## Ligand CLA d 402

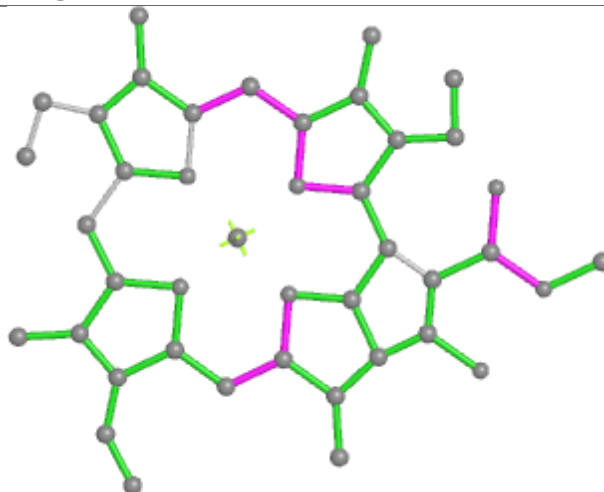




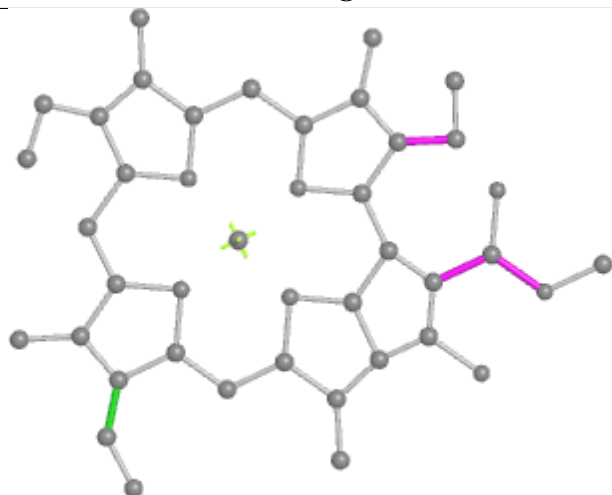
## Ligand CLA g 604



Bond lengths



Bond angles

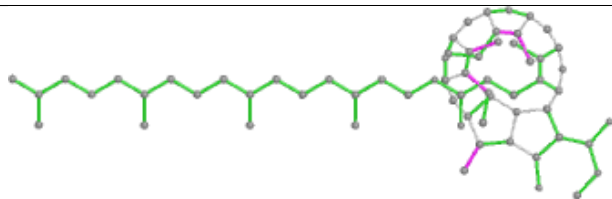


Torsions

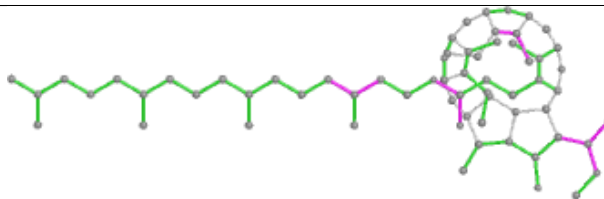


Rings

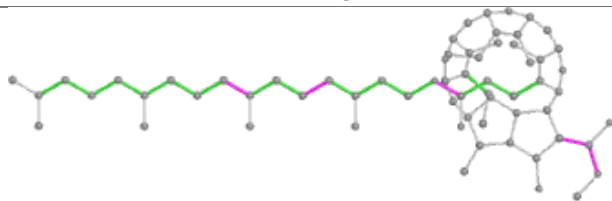
## Ligand PHO a 408



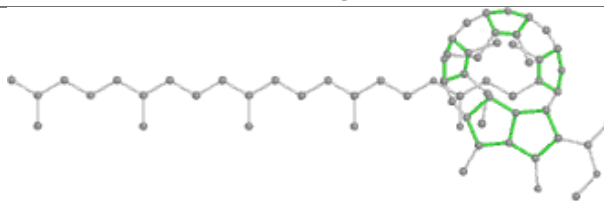
Bond lengths



Bond angles



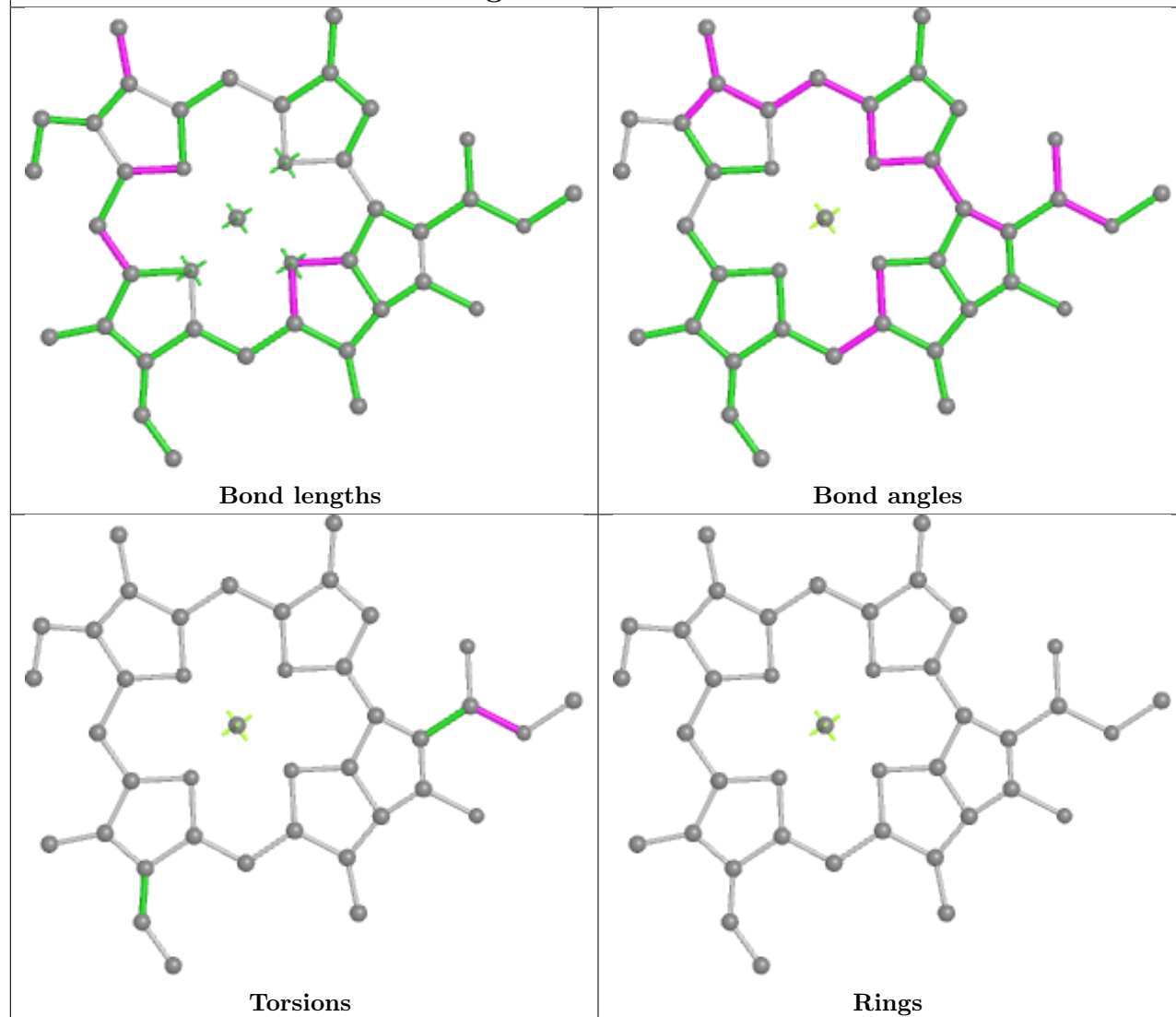
Torsions



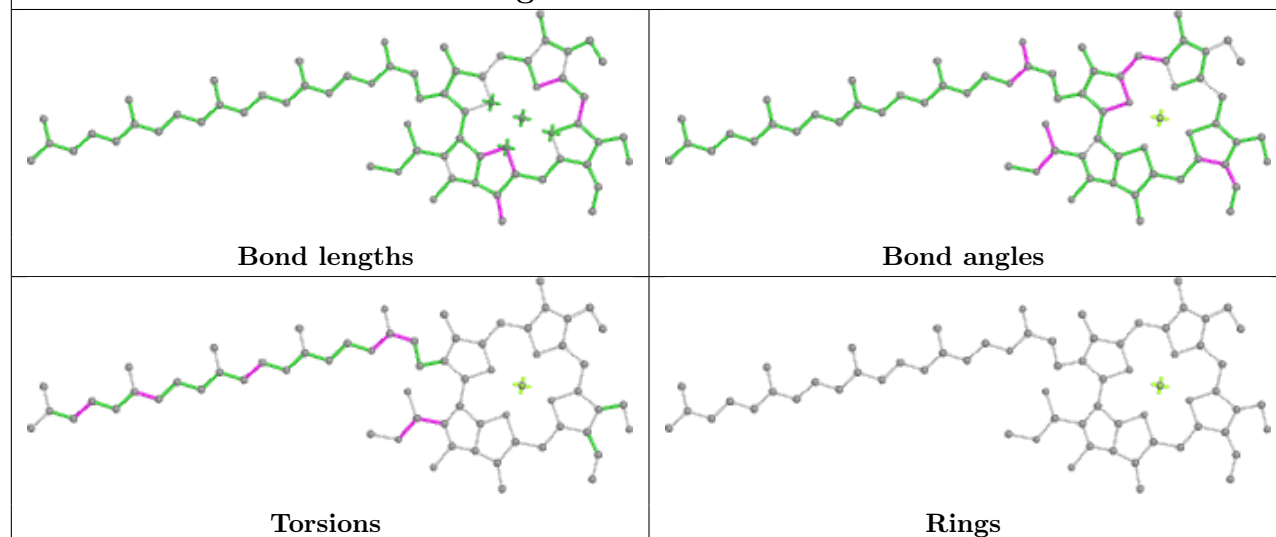
Rings



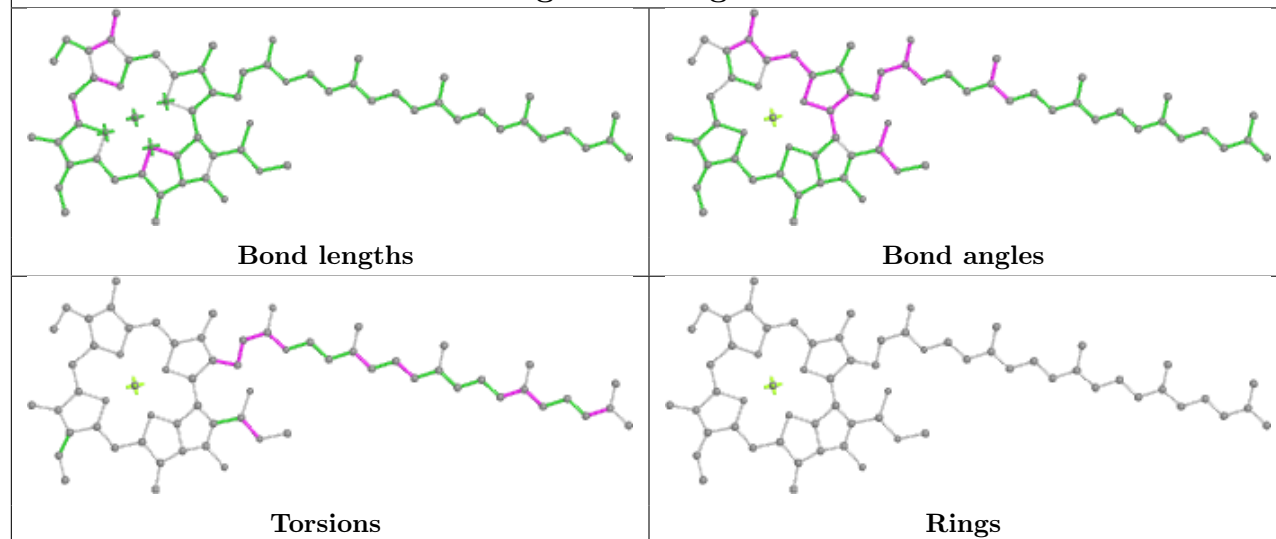
## Ligand CLA 33 602



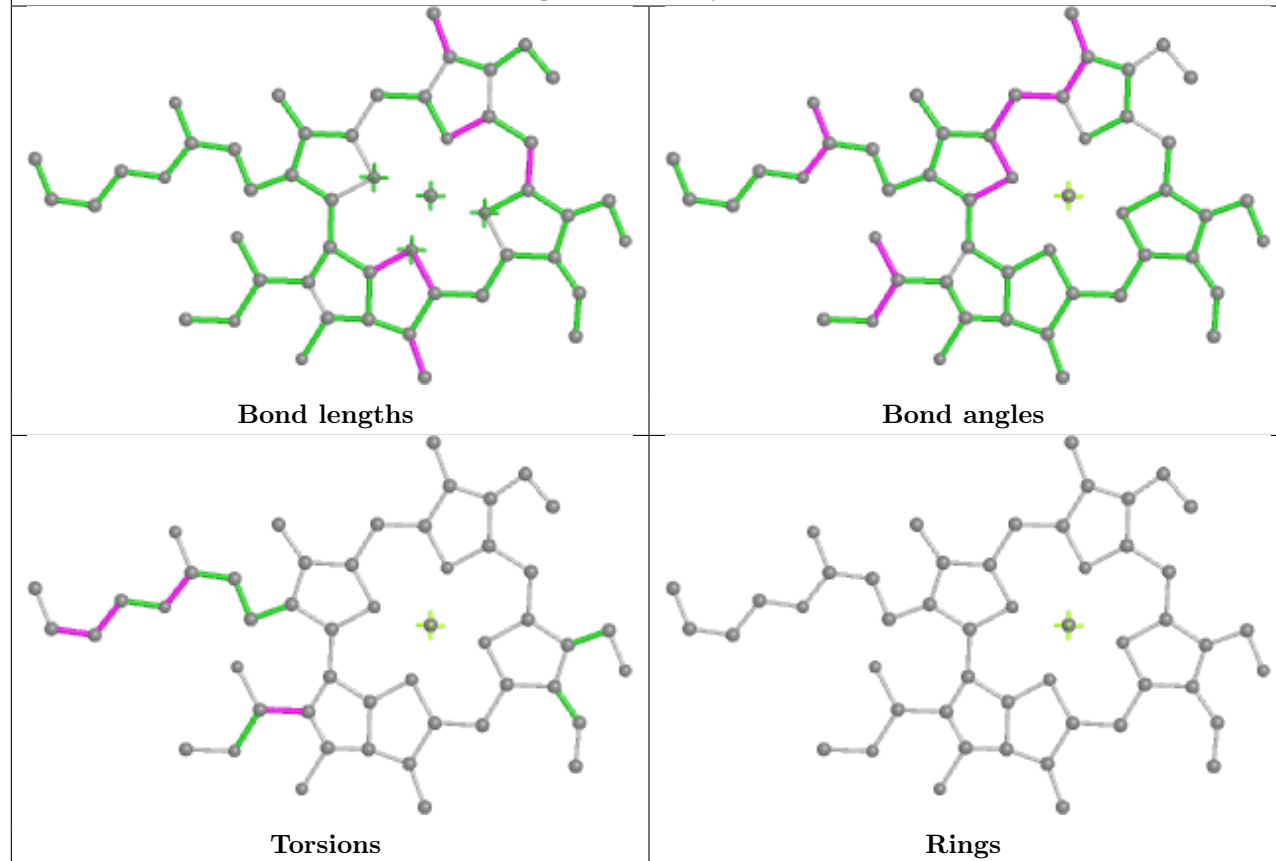
## Ligand CHL GG 601

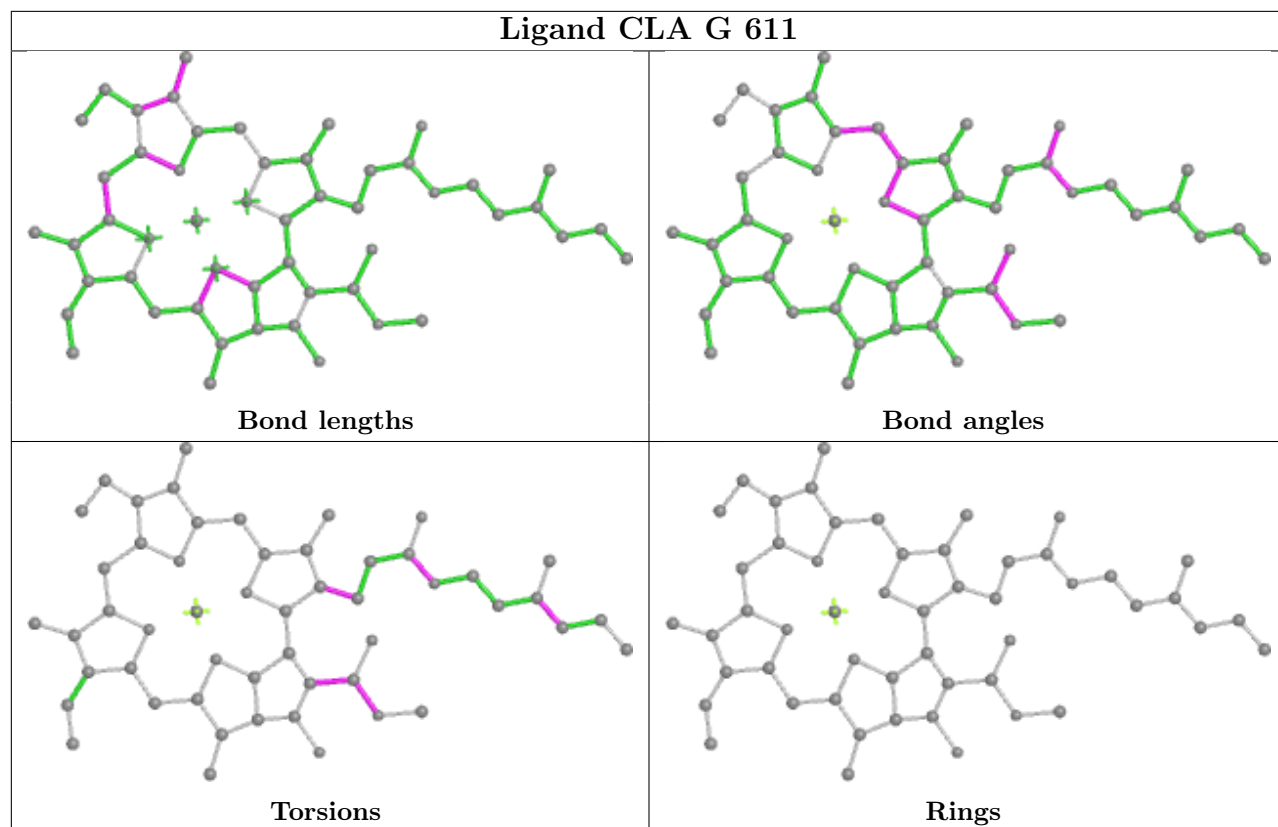


## Ligand CLA g 611

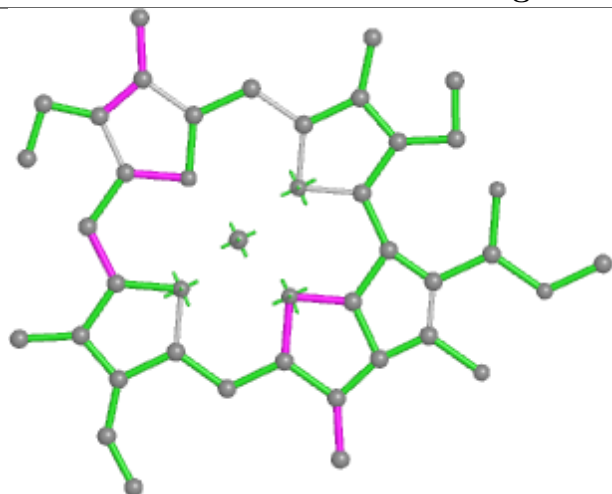


## Ligand CHL y 310

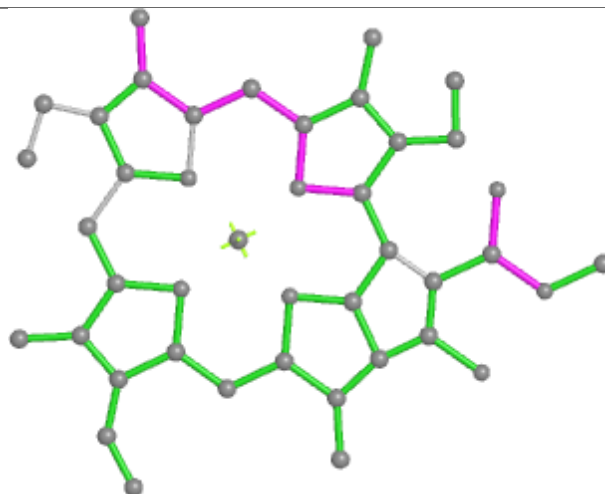




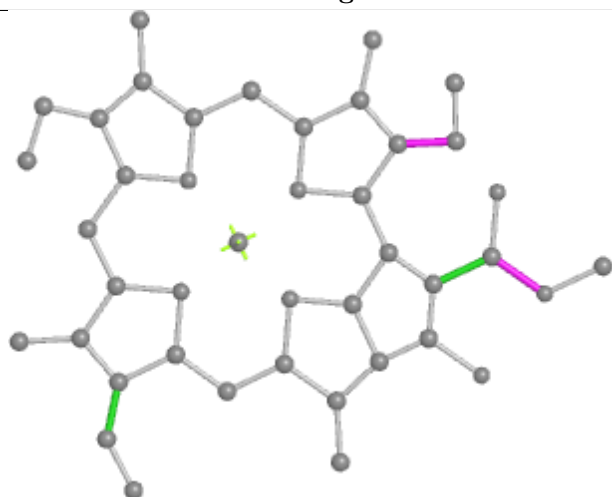
## Ligand CLA Y 611



Bond lengths



Bond angles

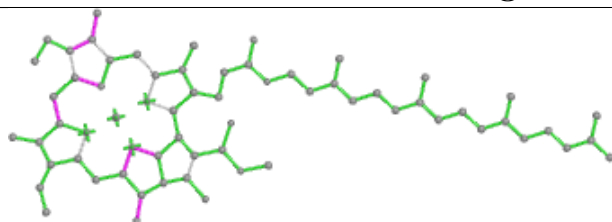


Torsions

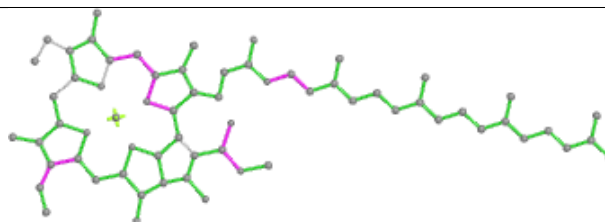


Rings

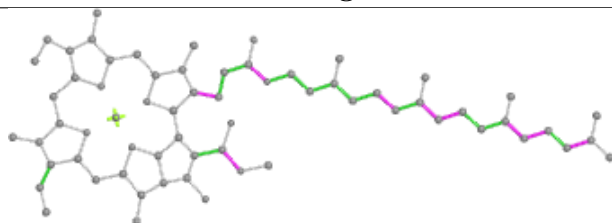
## Ligand CLA AA 405



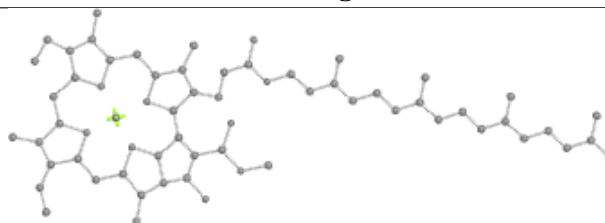
Bond lengths



Bond angles

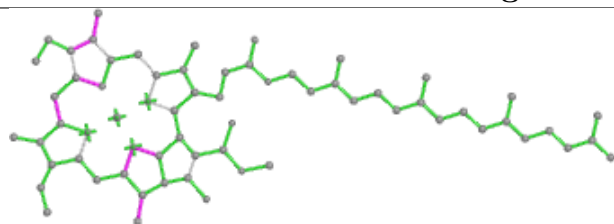


Torsions

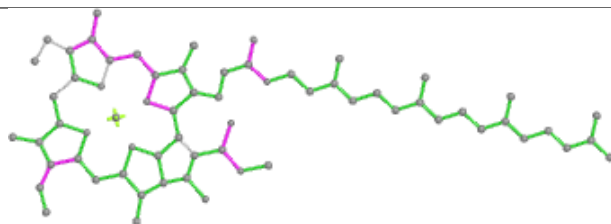


Rings

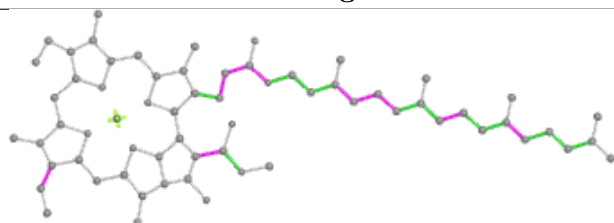
## Ligand CLA CC 506



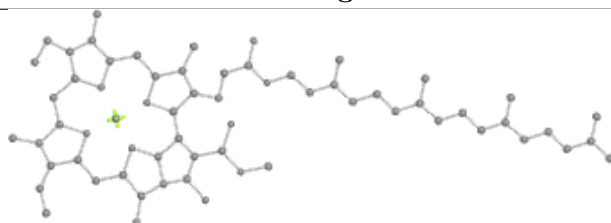
Bond lengths



Bond angles

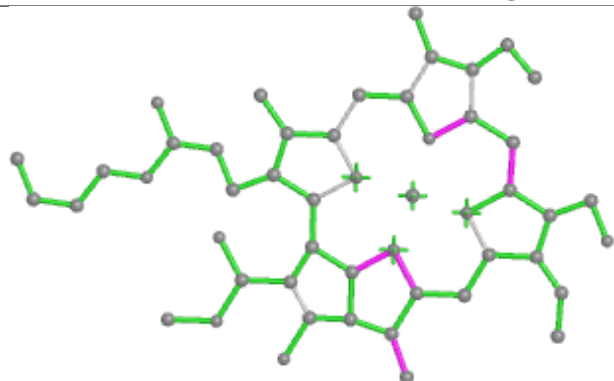


Torsions

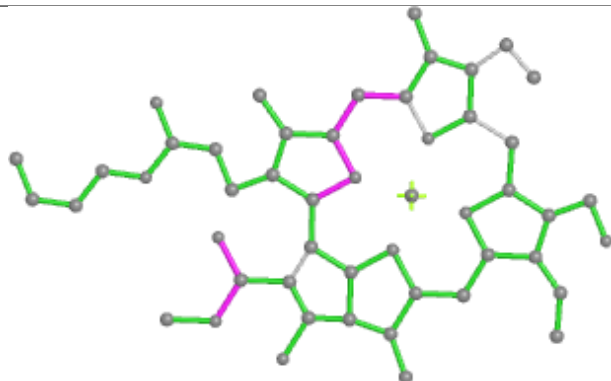


Rings

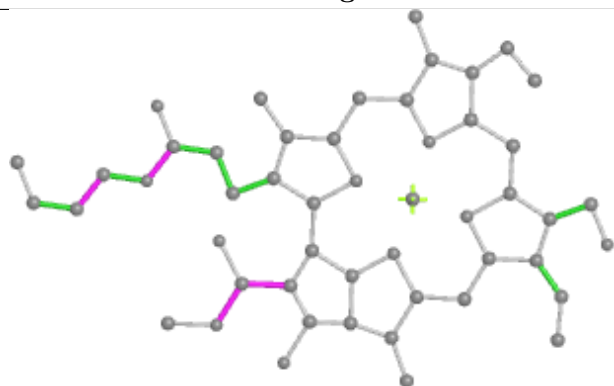
## Ligand CHL Nn 311



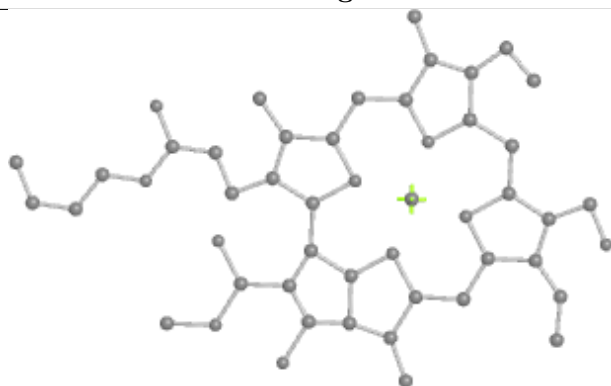
Bond lengths



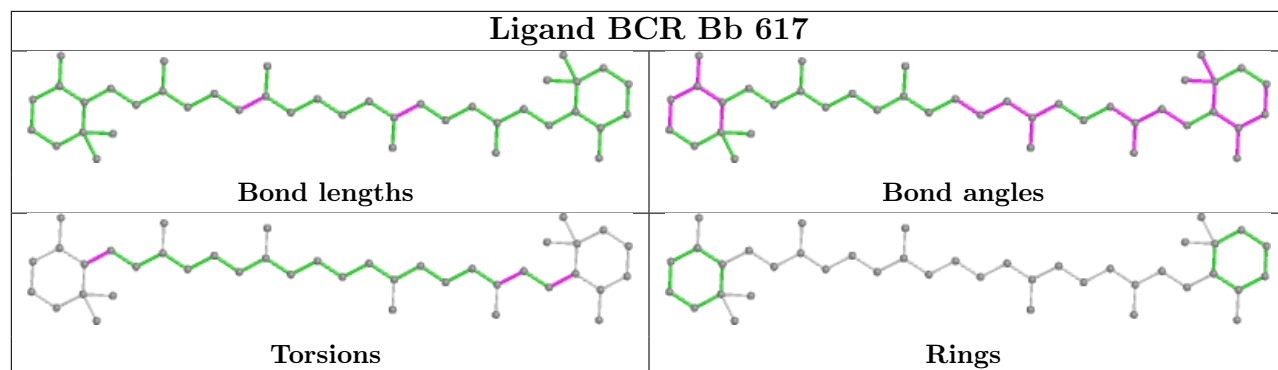
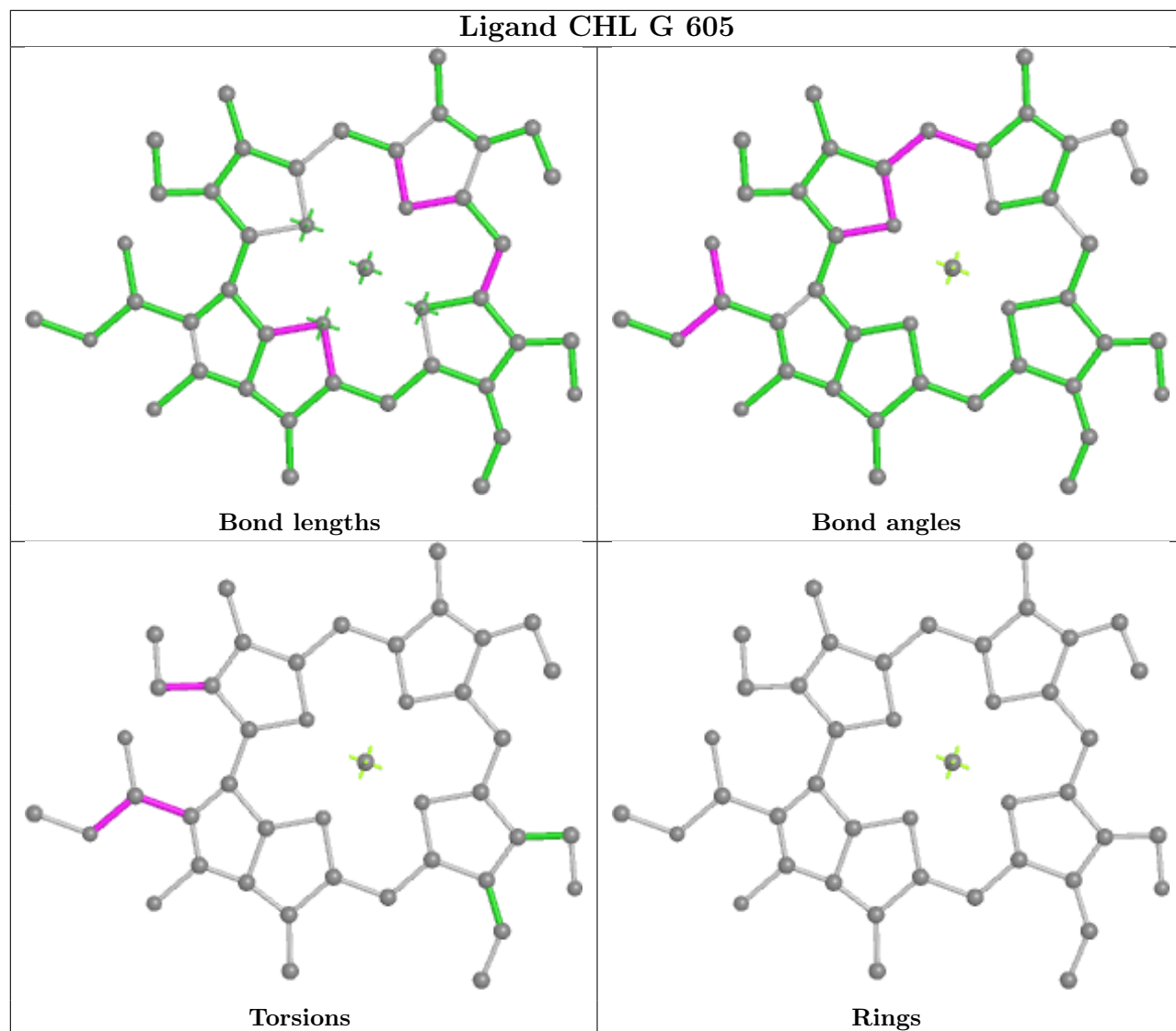
Bond angles

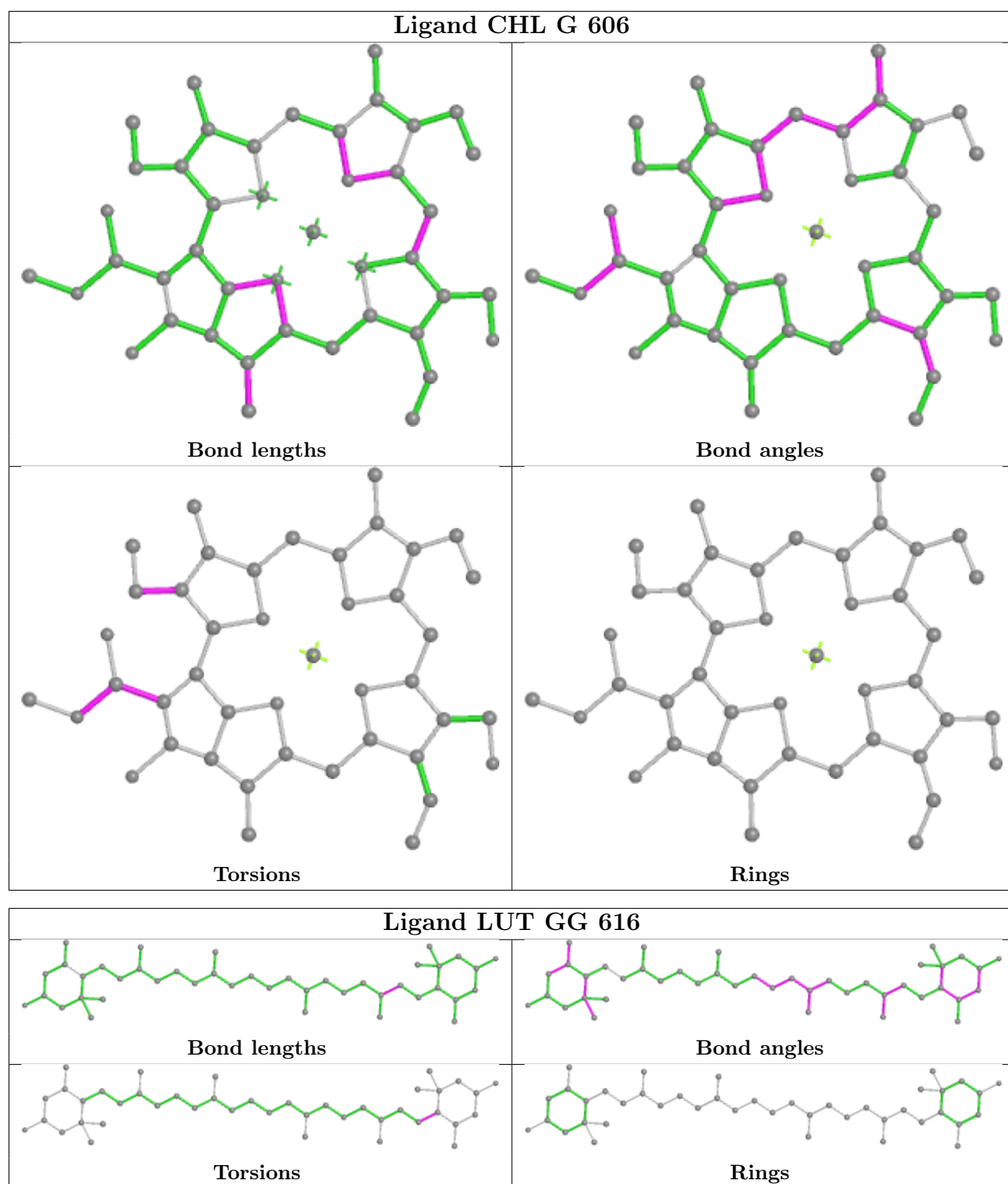


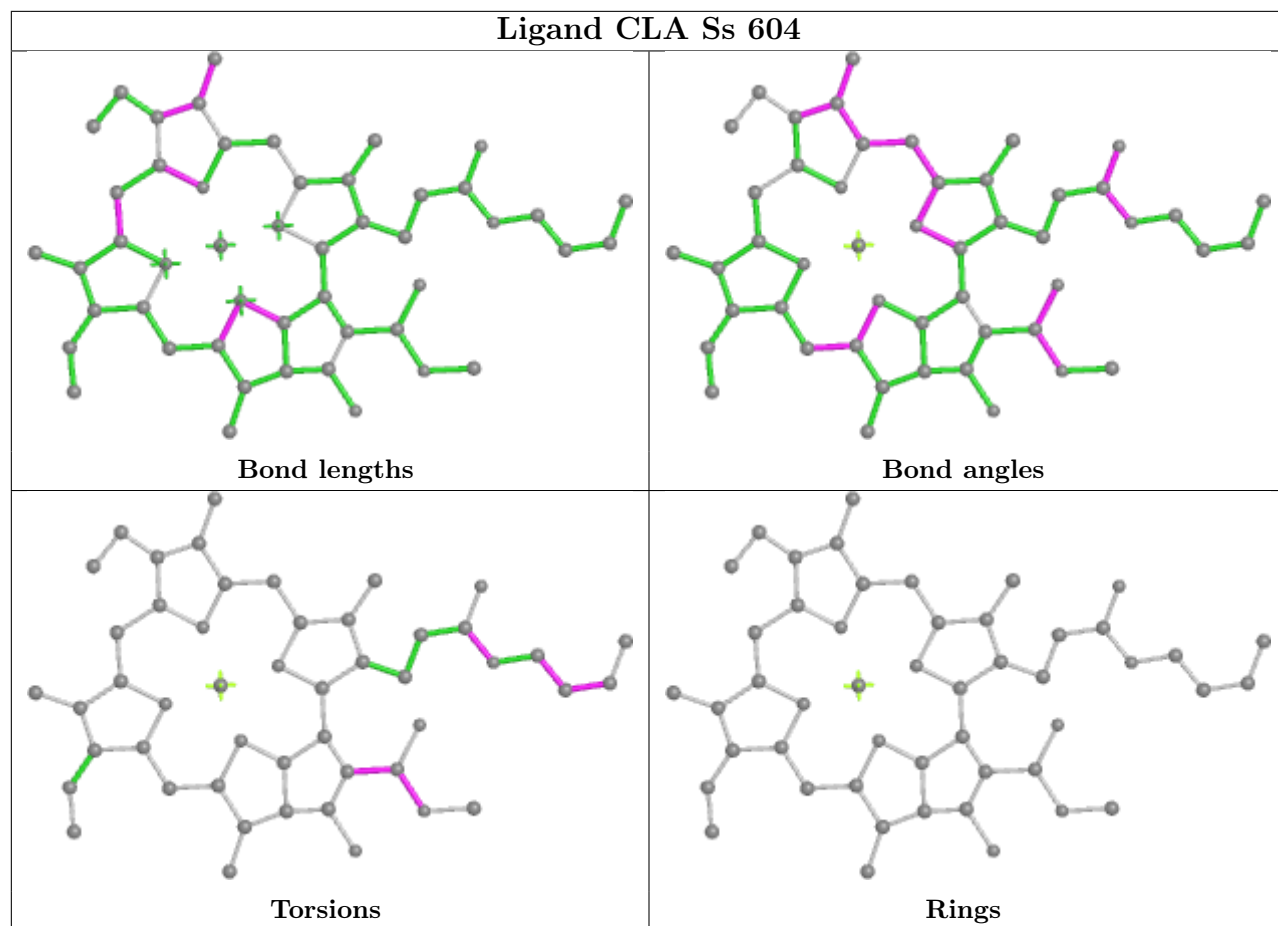
Torsions



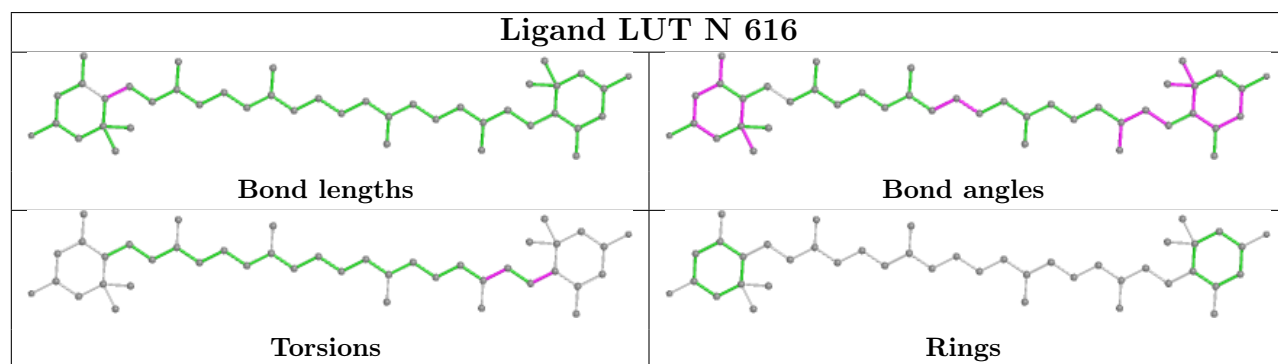
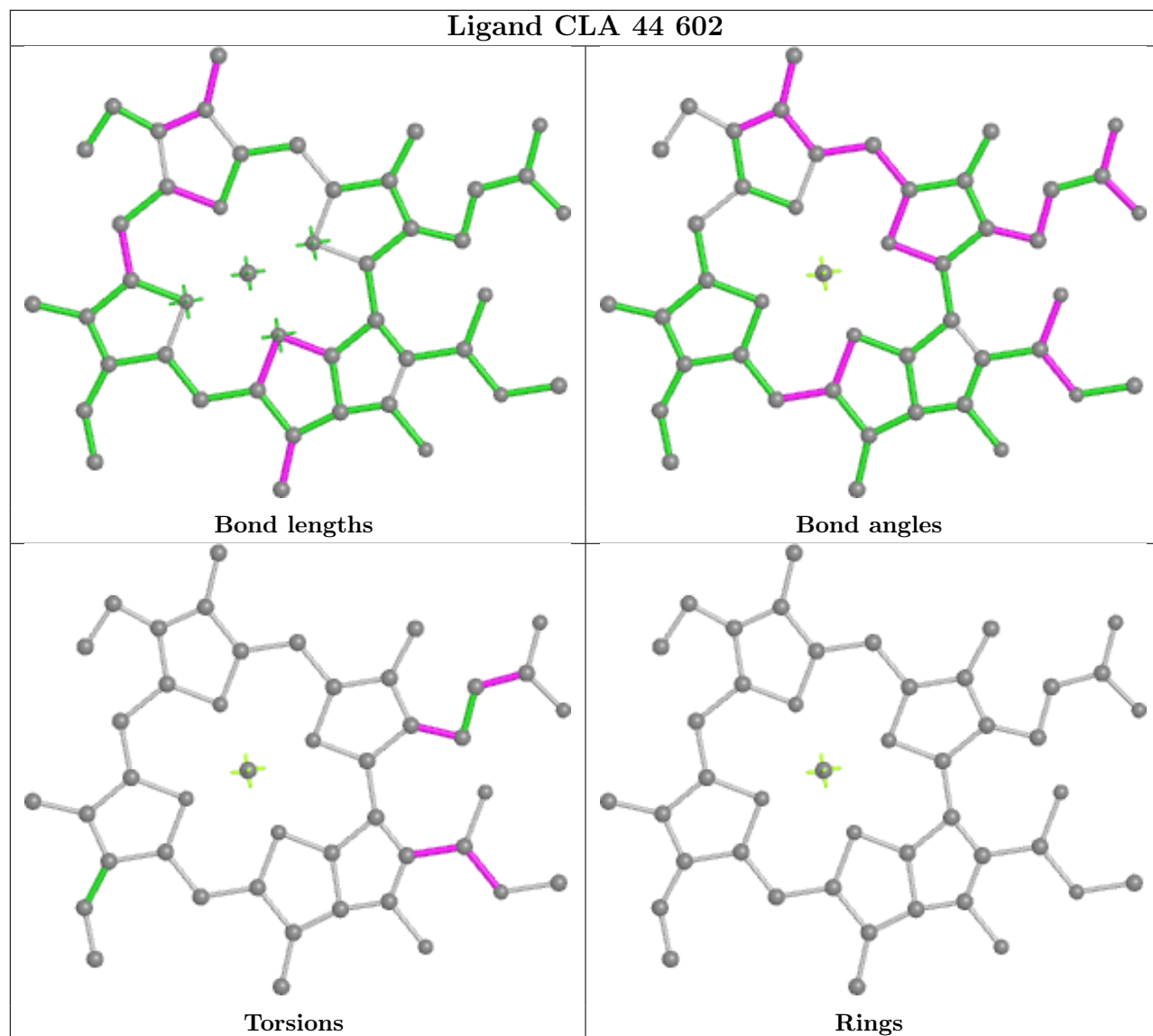
Rings

**Ligand BCR Bb 617****Ligand CHL G 605**

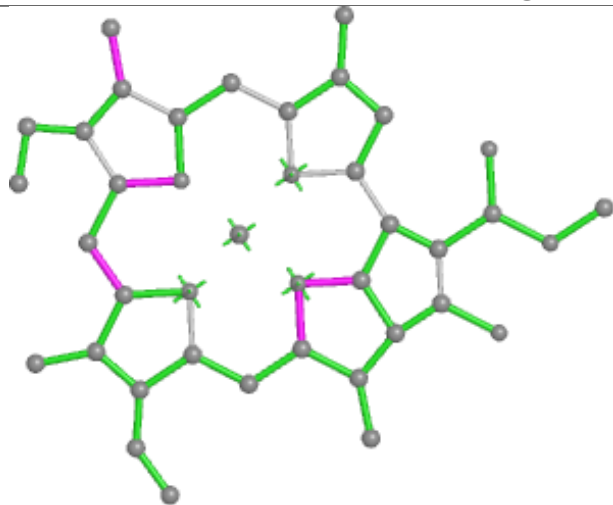




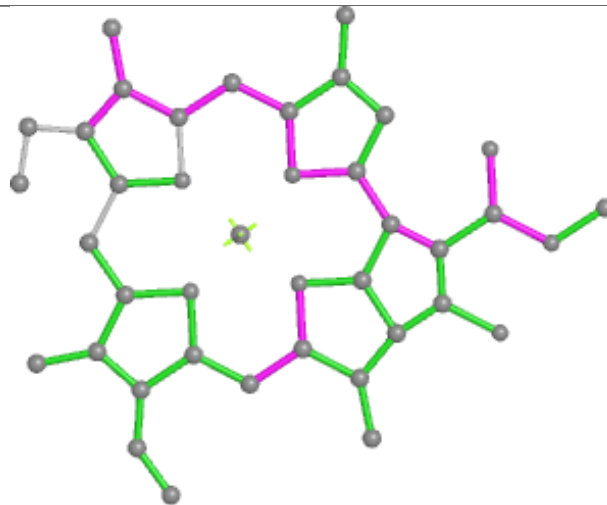




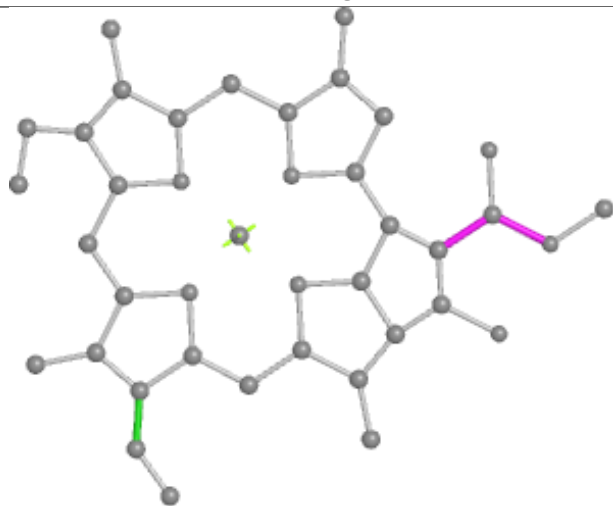
## Ligand CLA 3 604



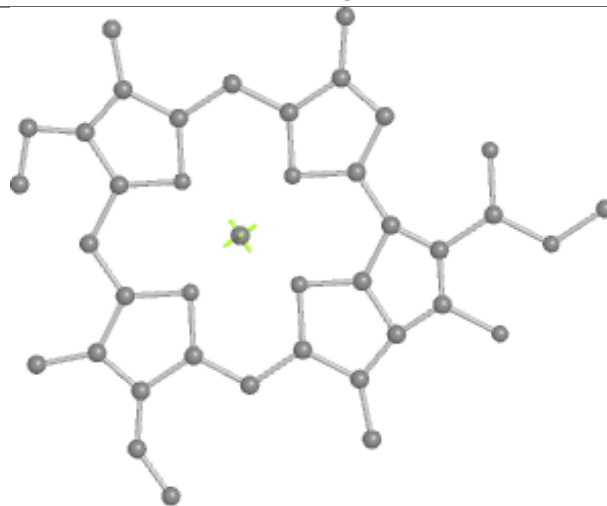
Bond lengths



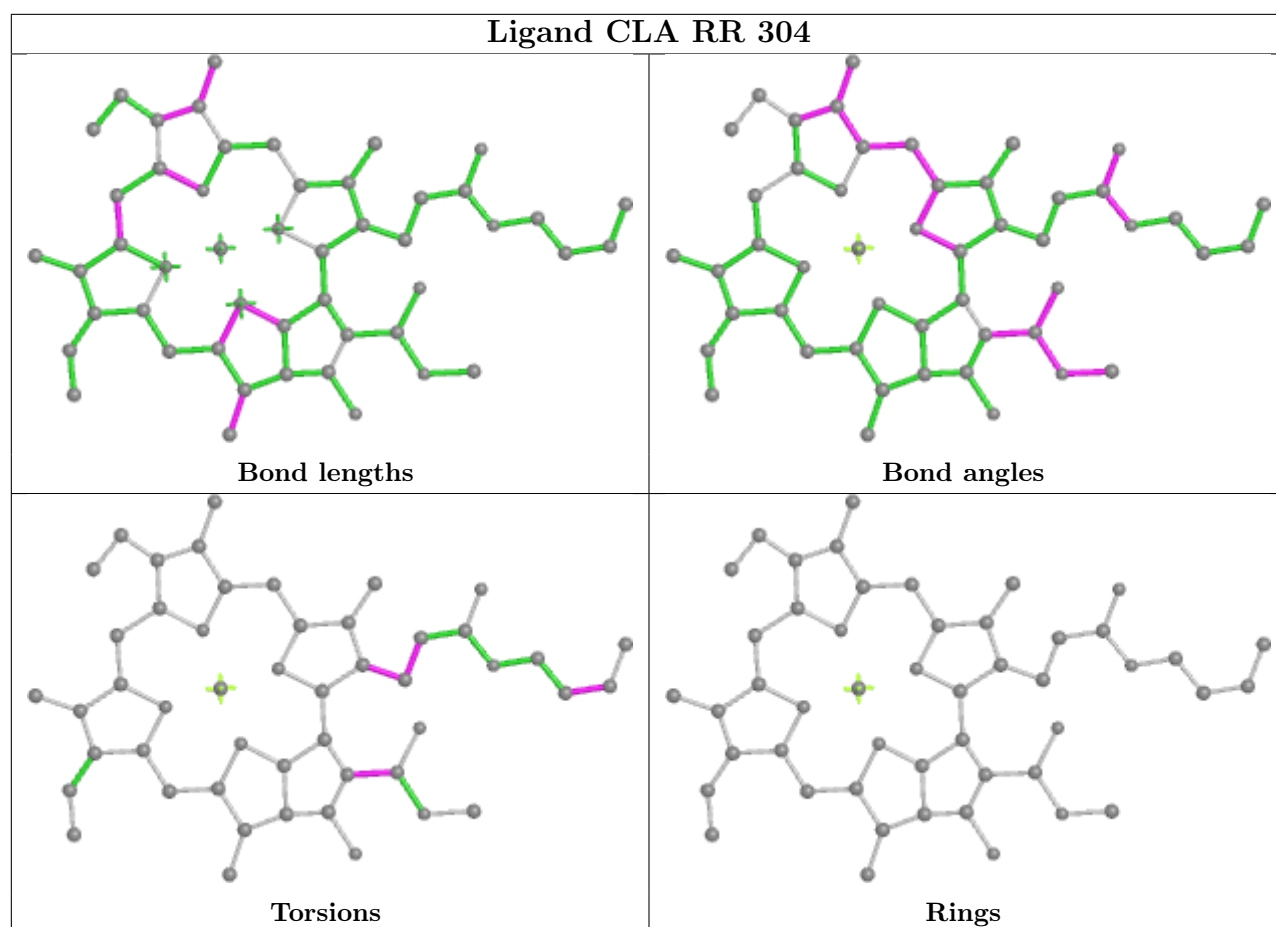
Bond angles

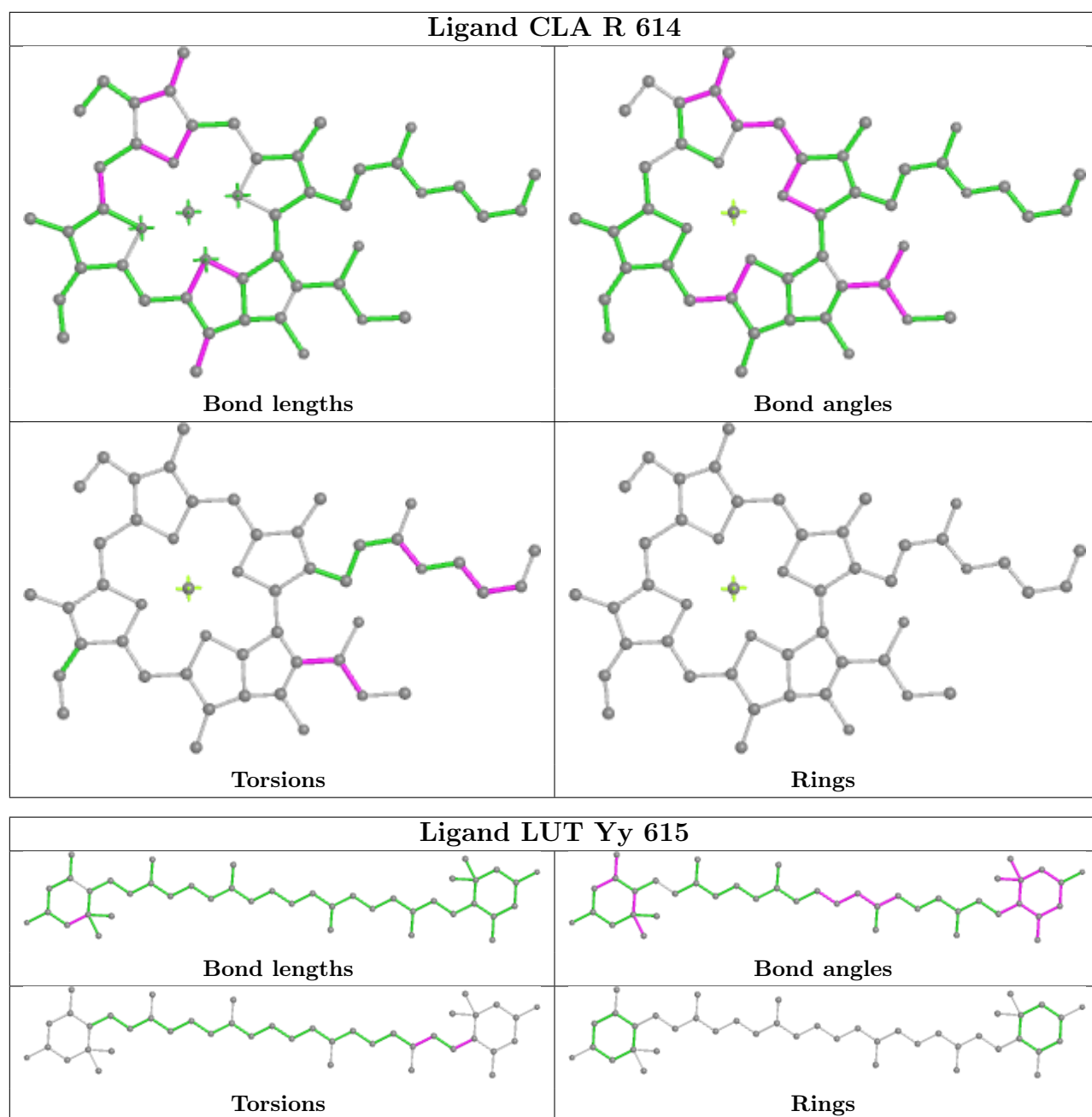


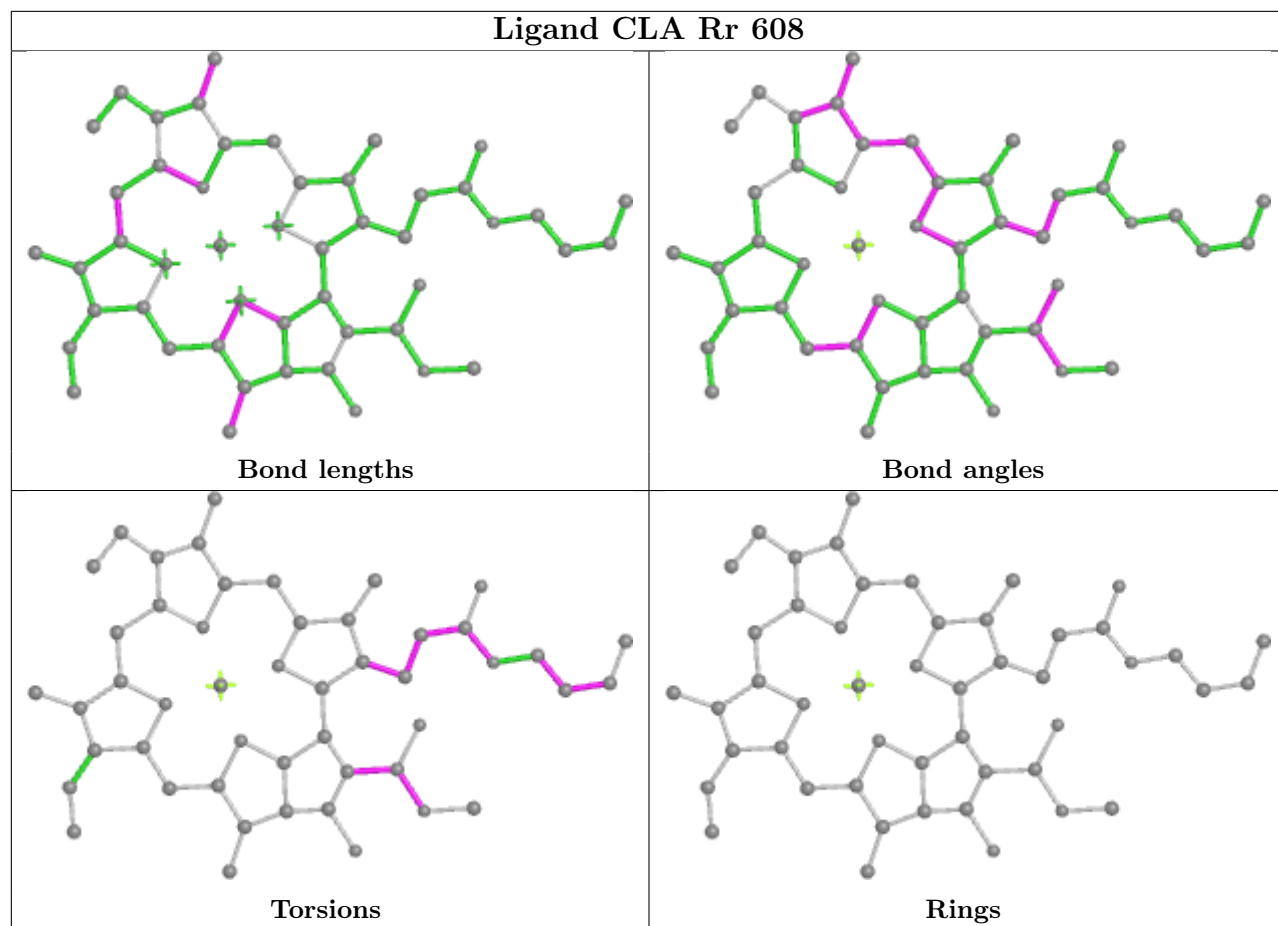
Torsions

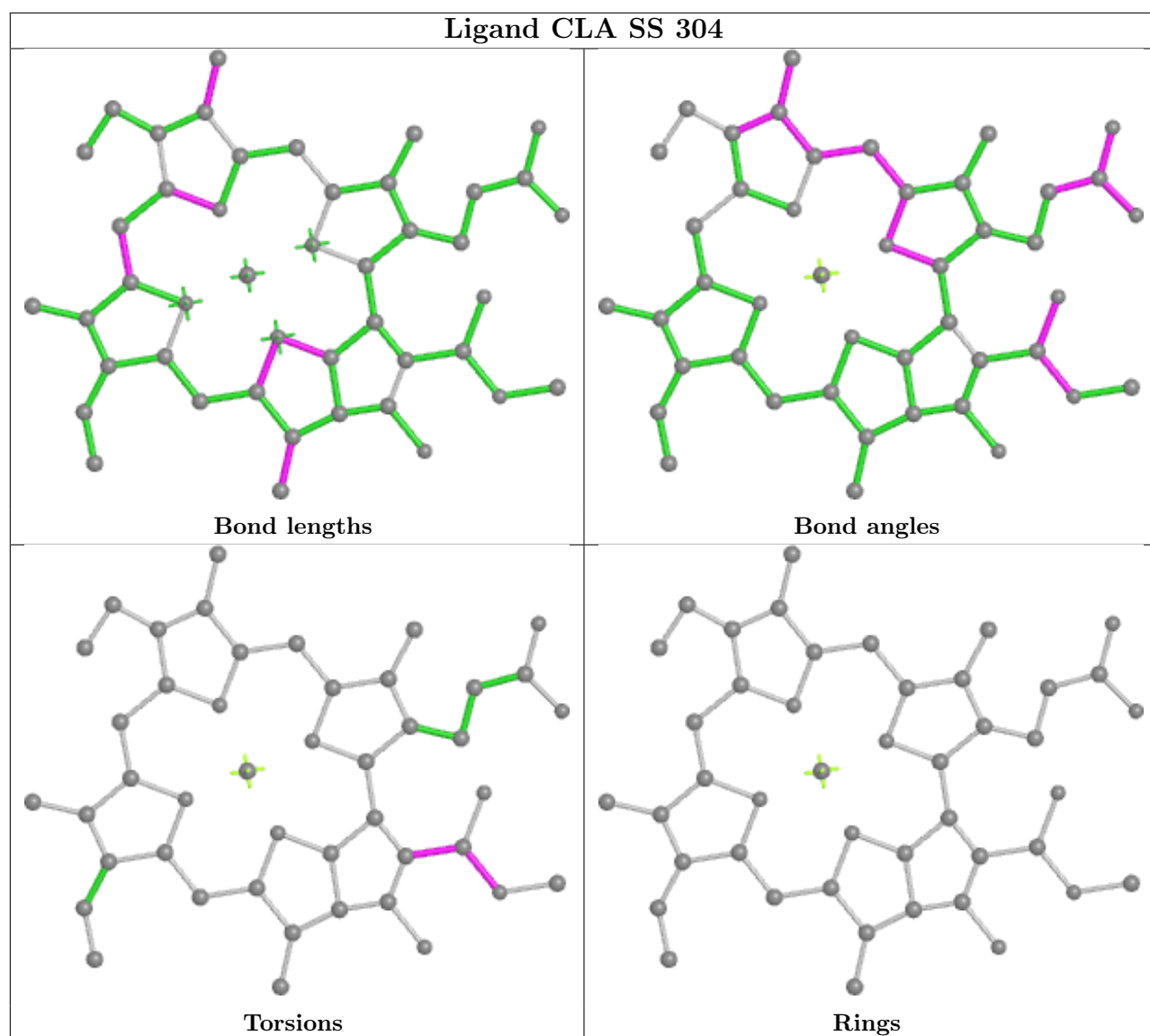


Rings

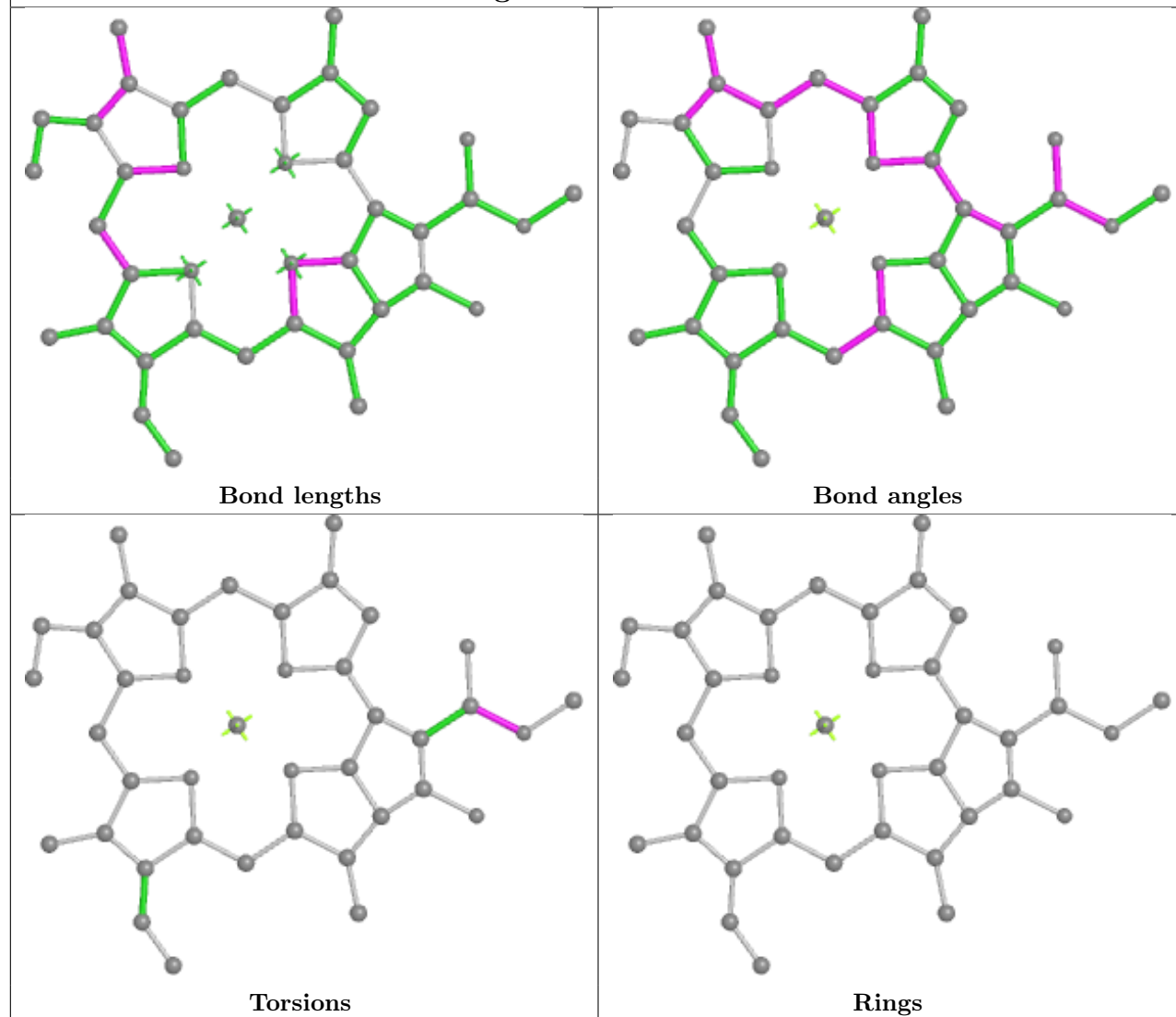




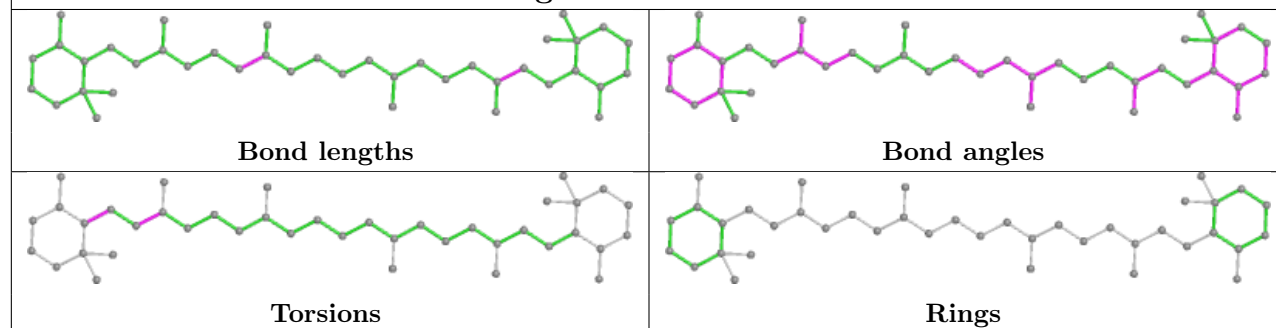


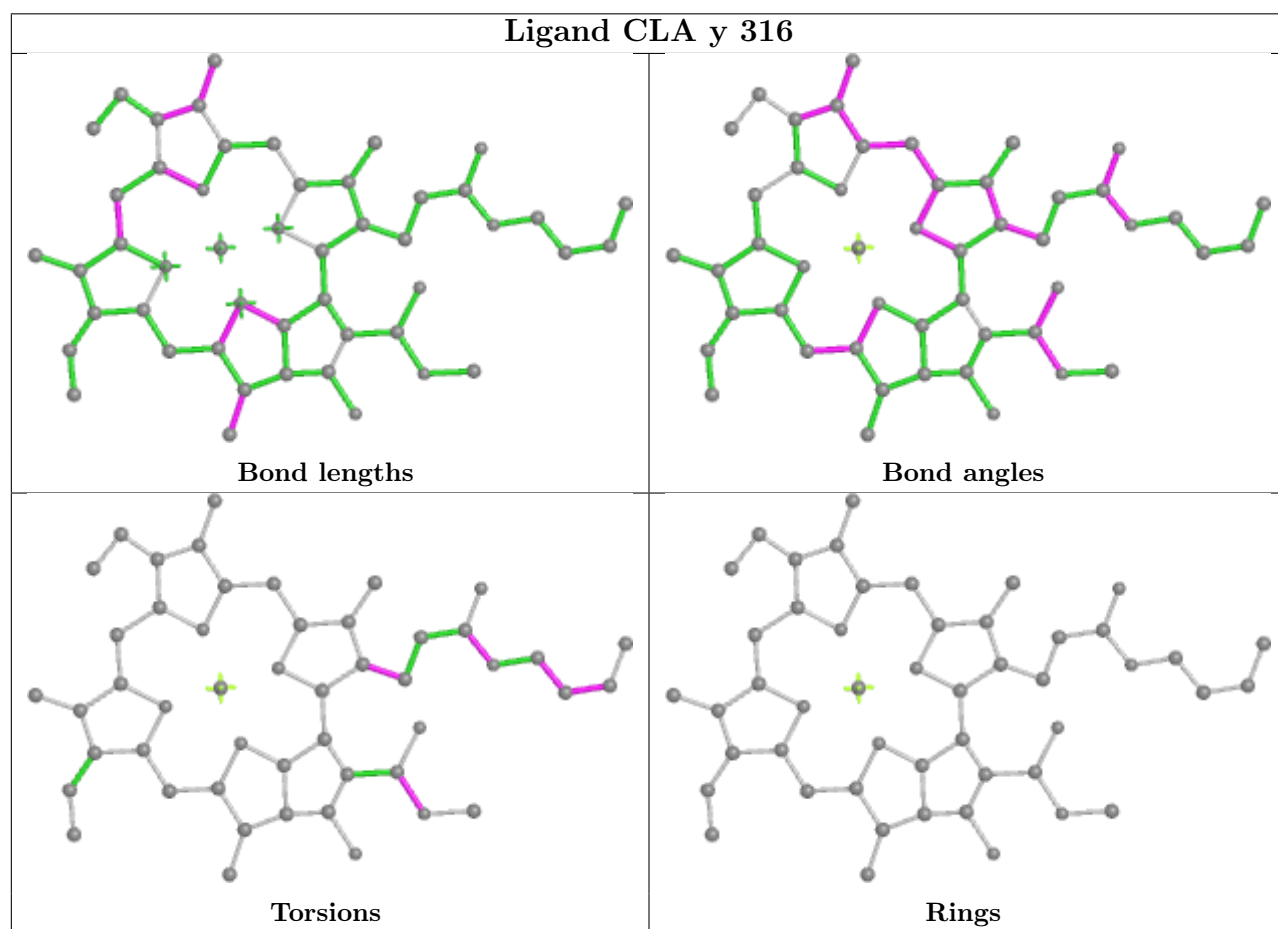
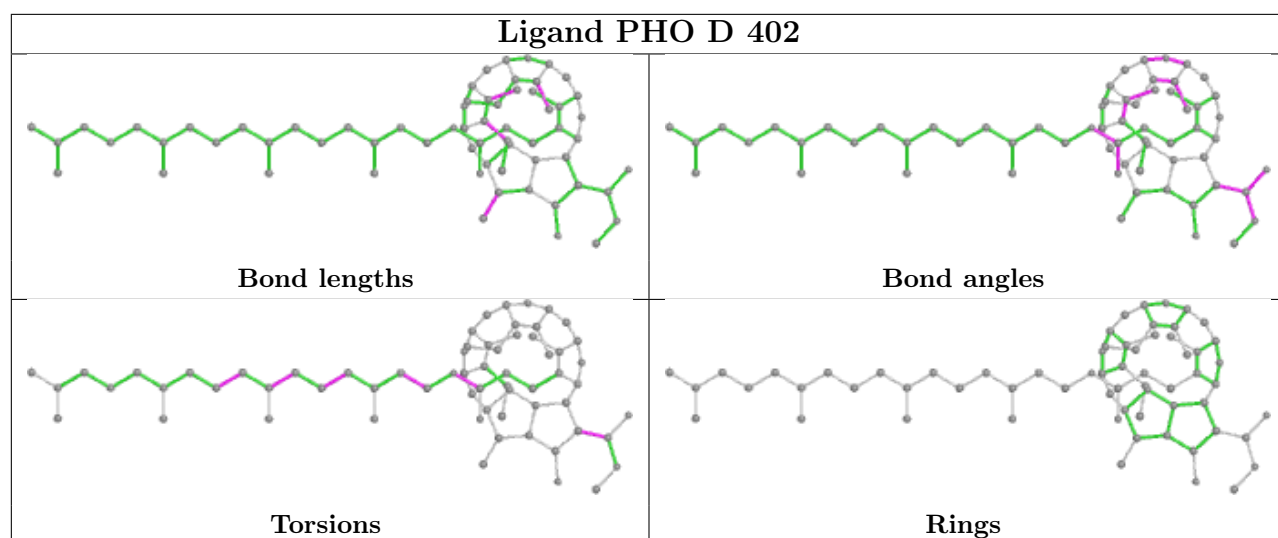


## Ligand CLA 3 602

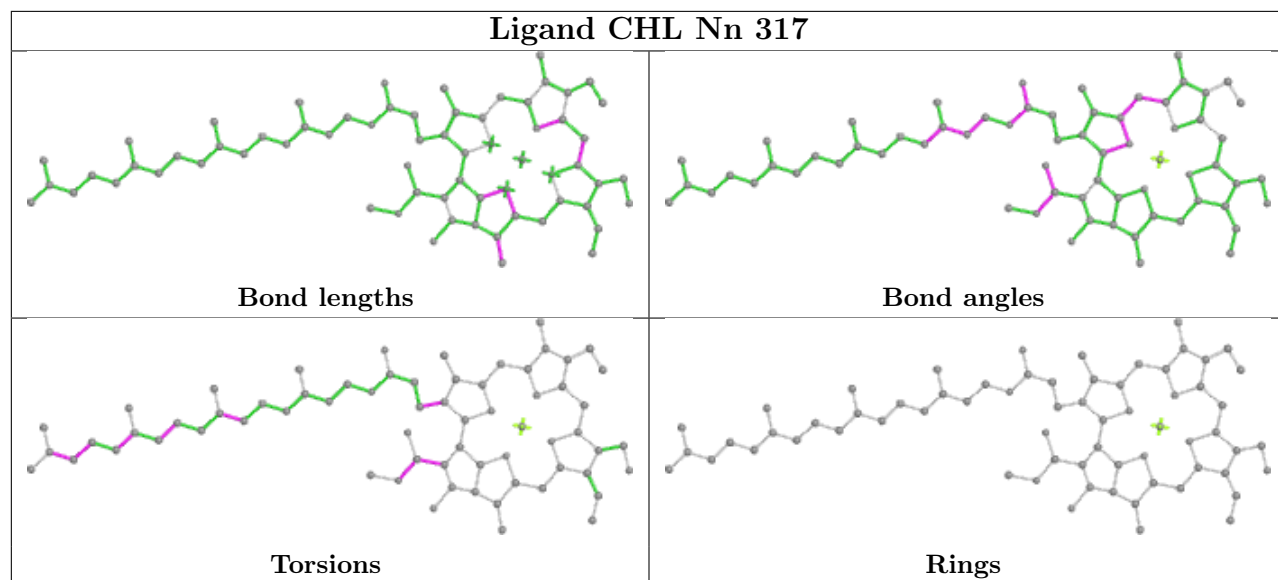
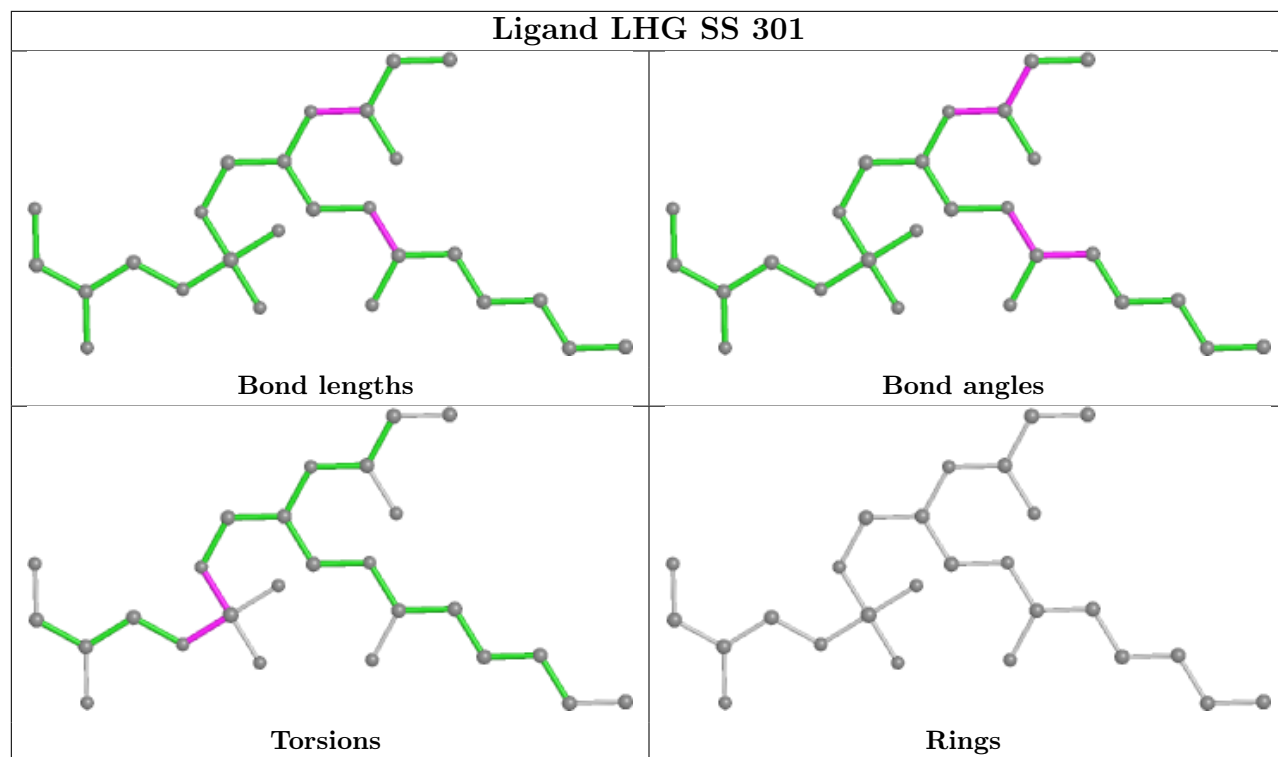


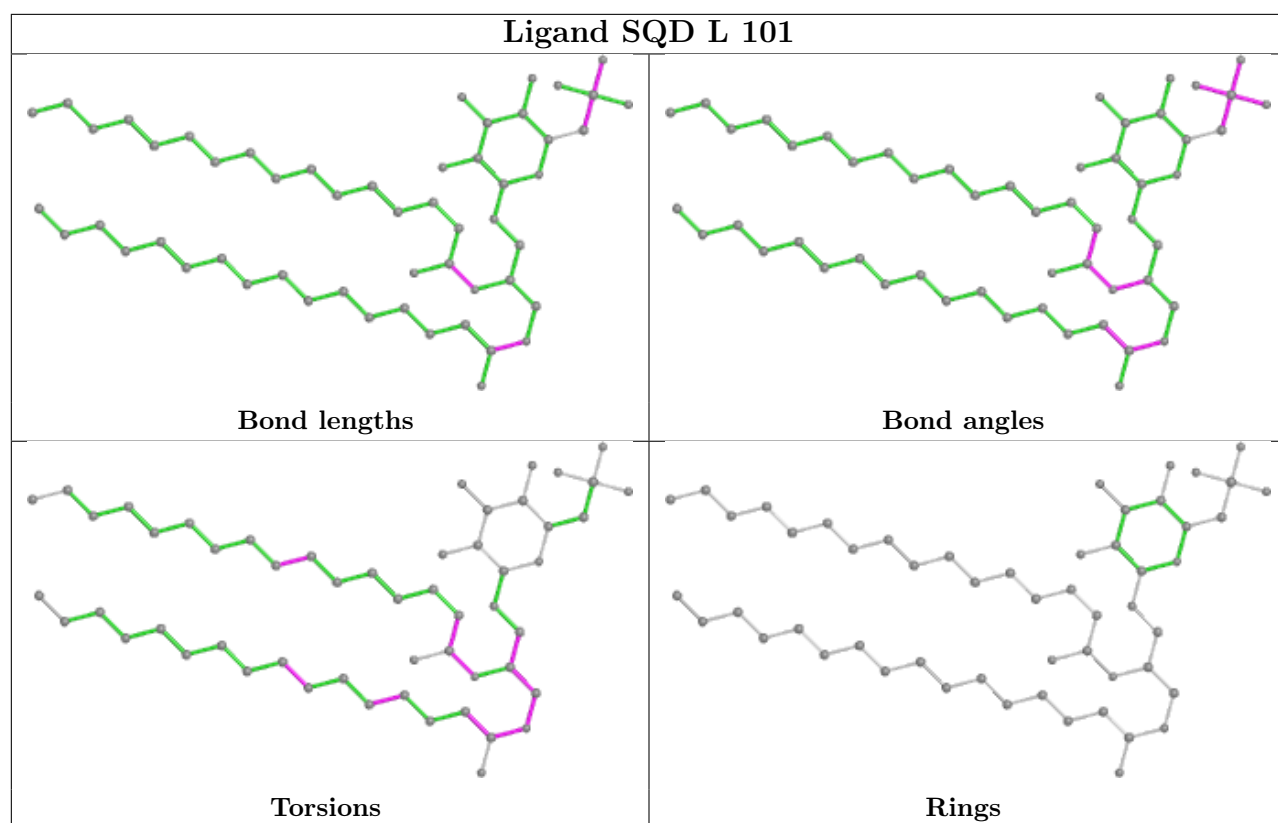
## Ligand BCR c 514



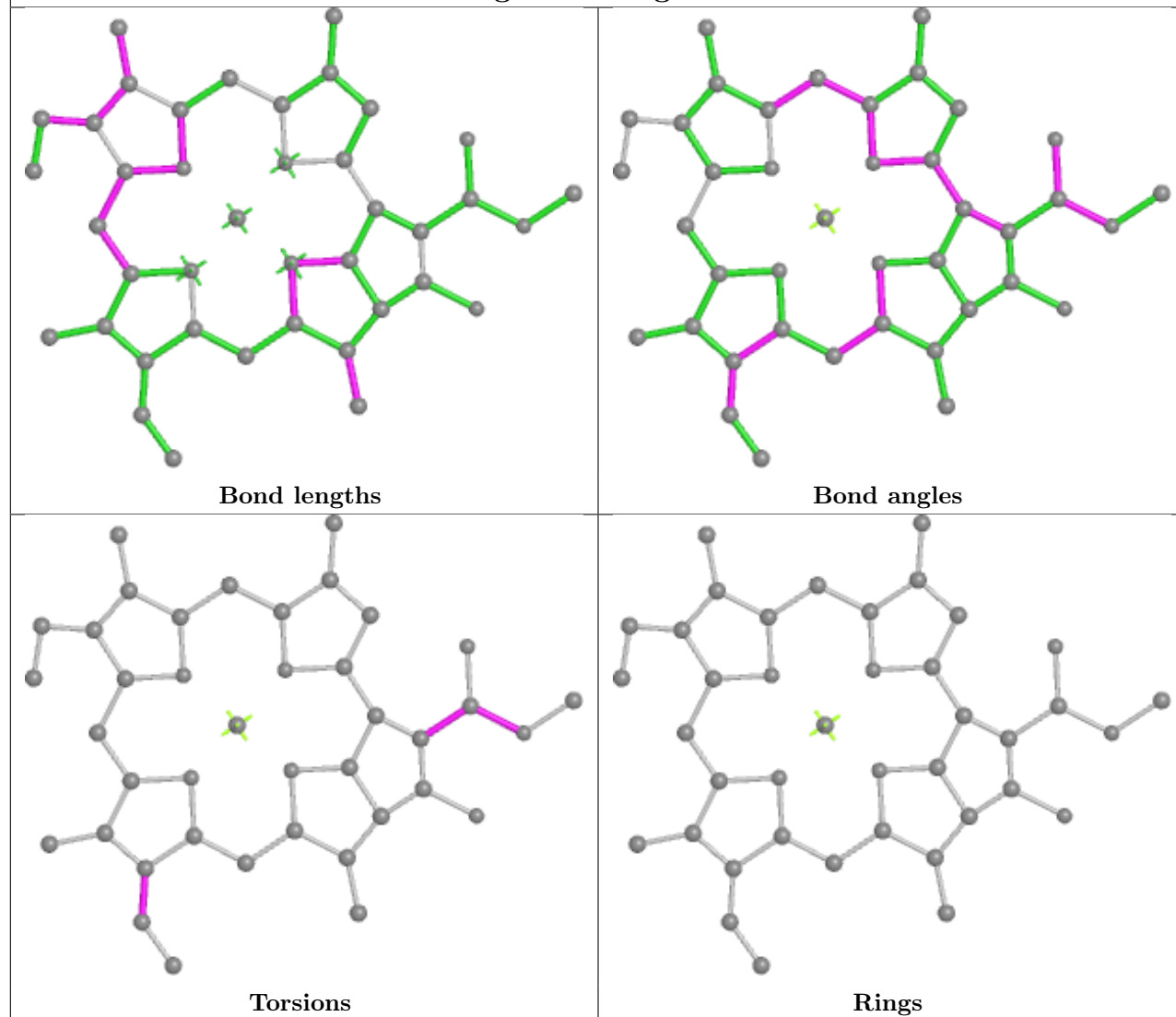




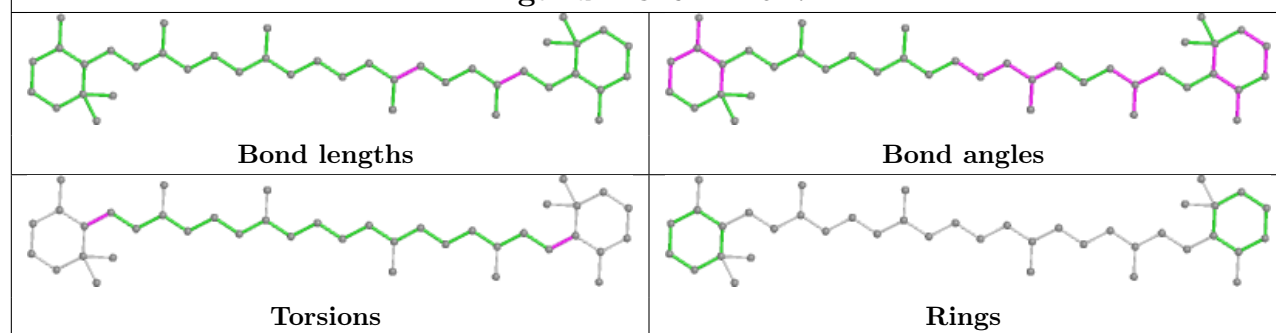




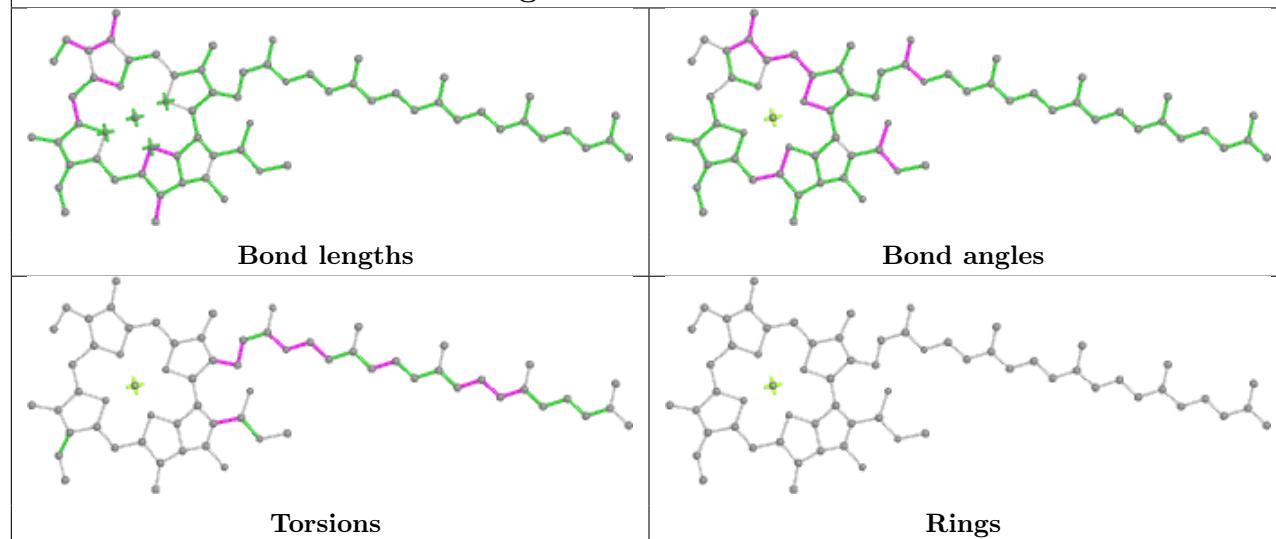
## Ligand CLA g 613



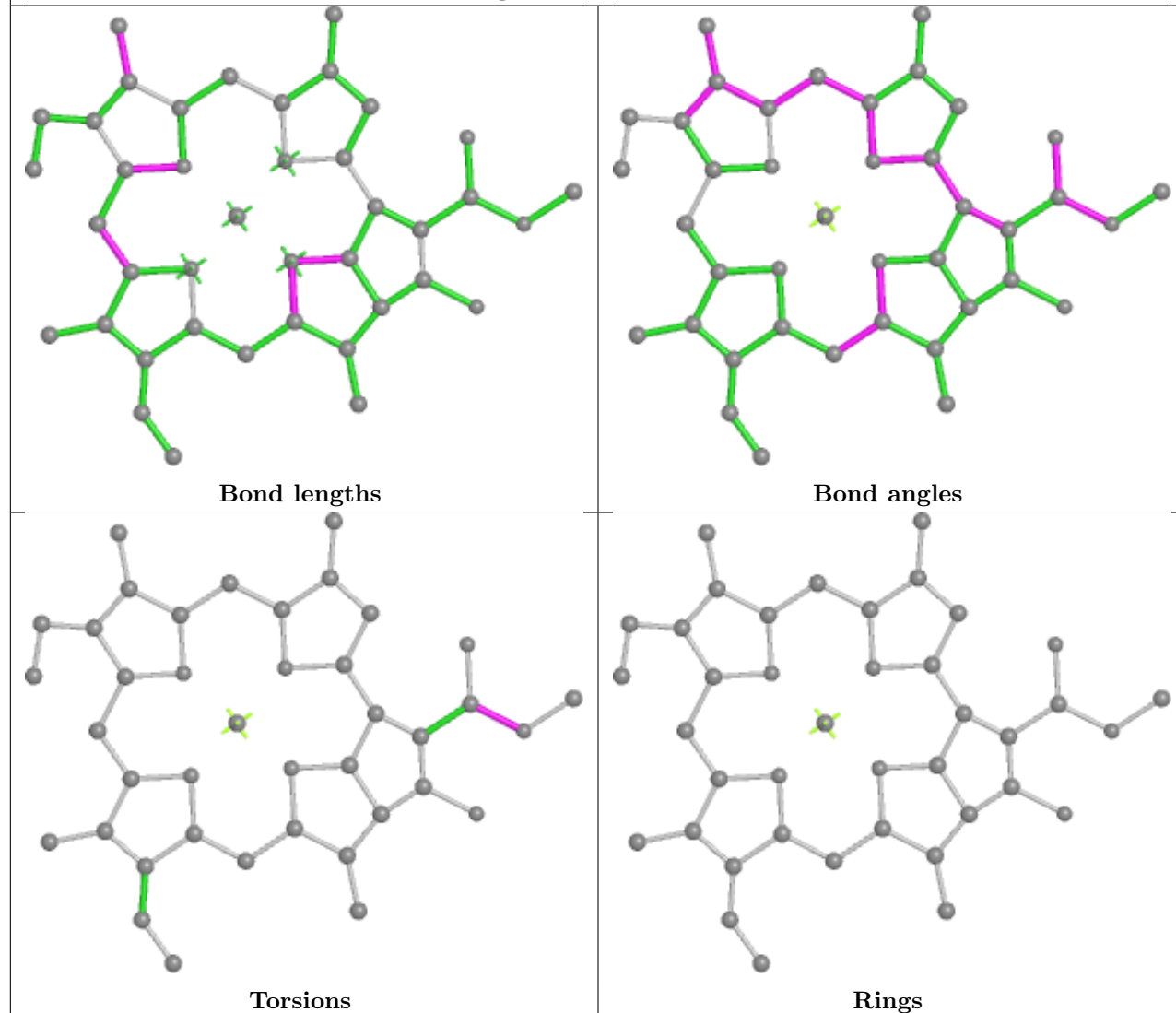
## Ligand BCR BB 617



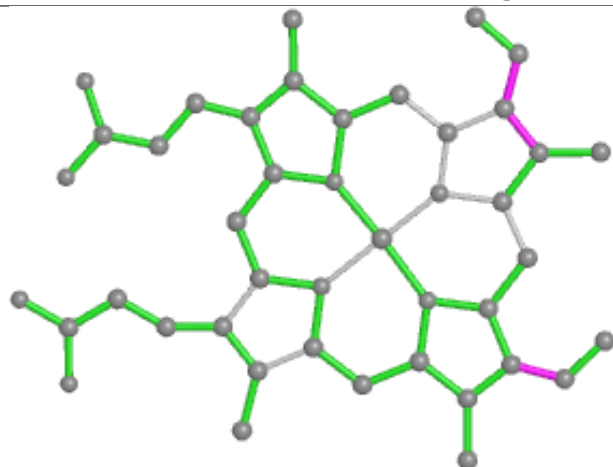
## Ligand CLA CC 510



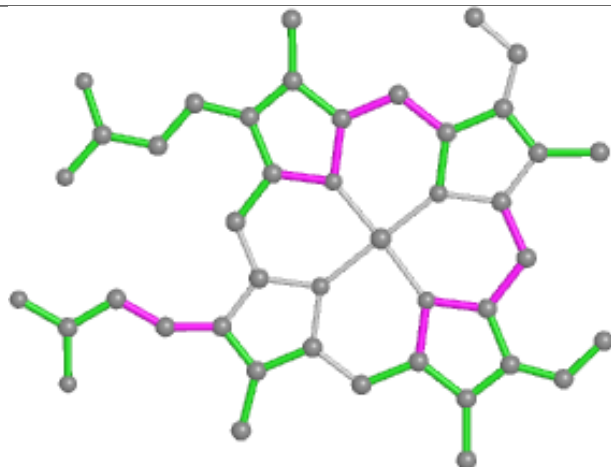
## Ligand CLA 2 612



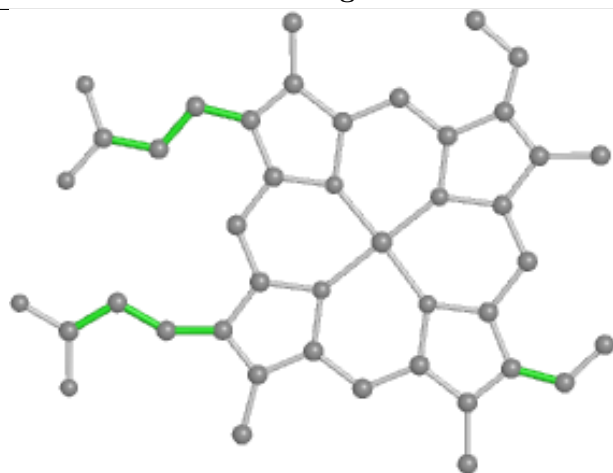
## Ligand HEM EE 102



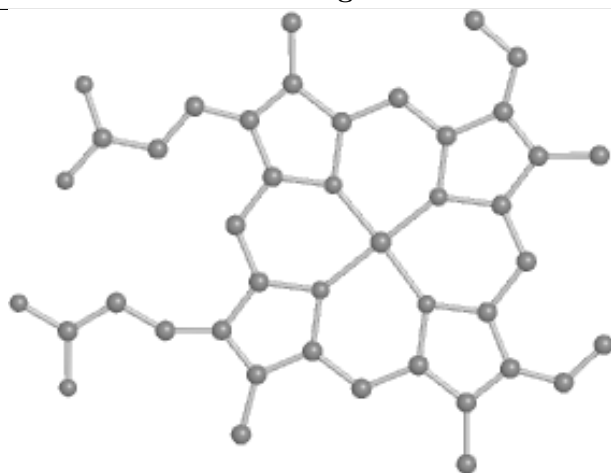
Bond lengths



Bond angles

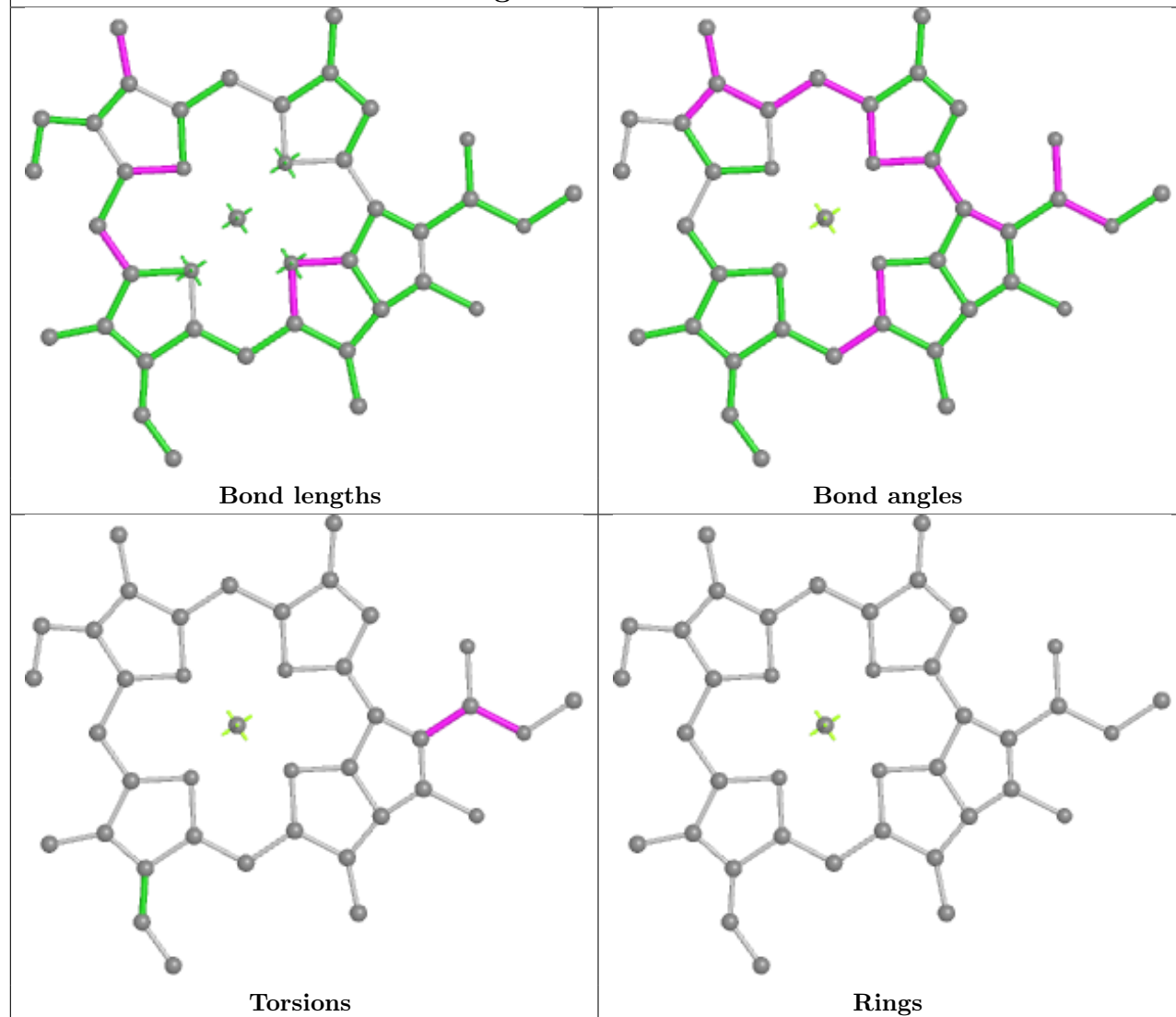


Torsions

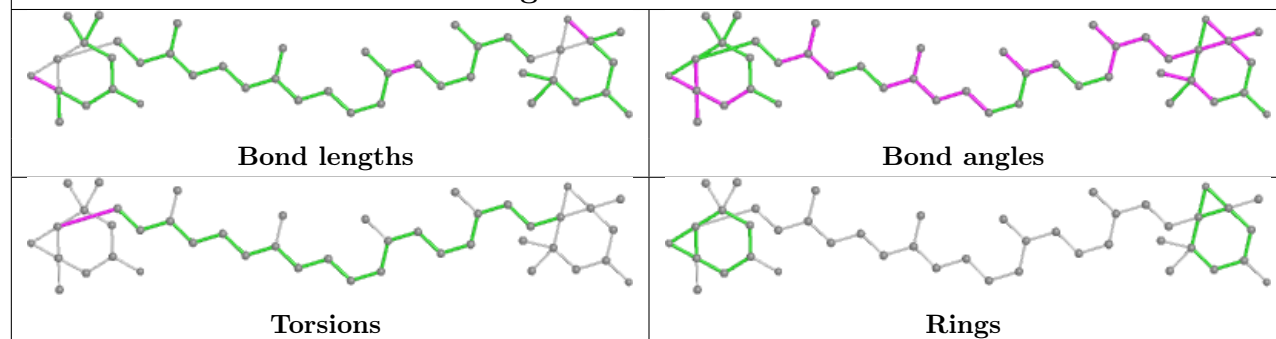


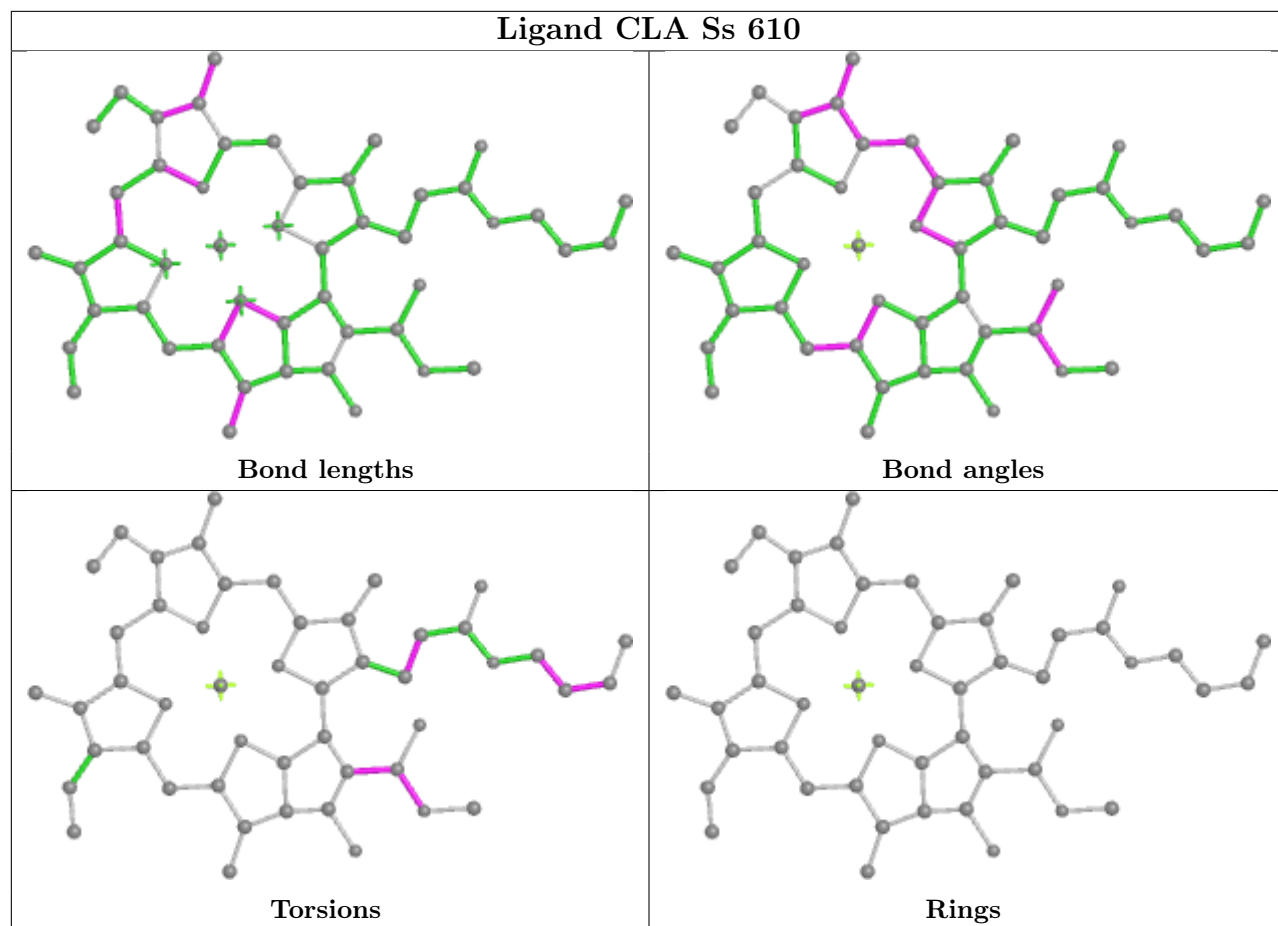
Rings

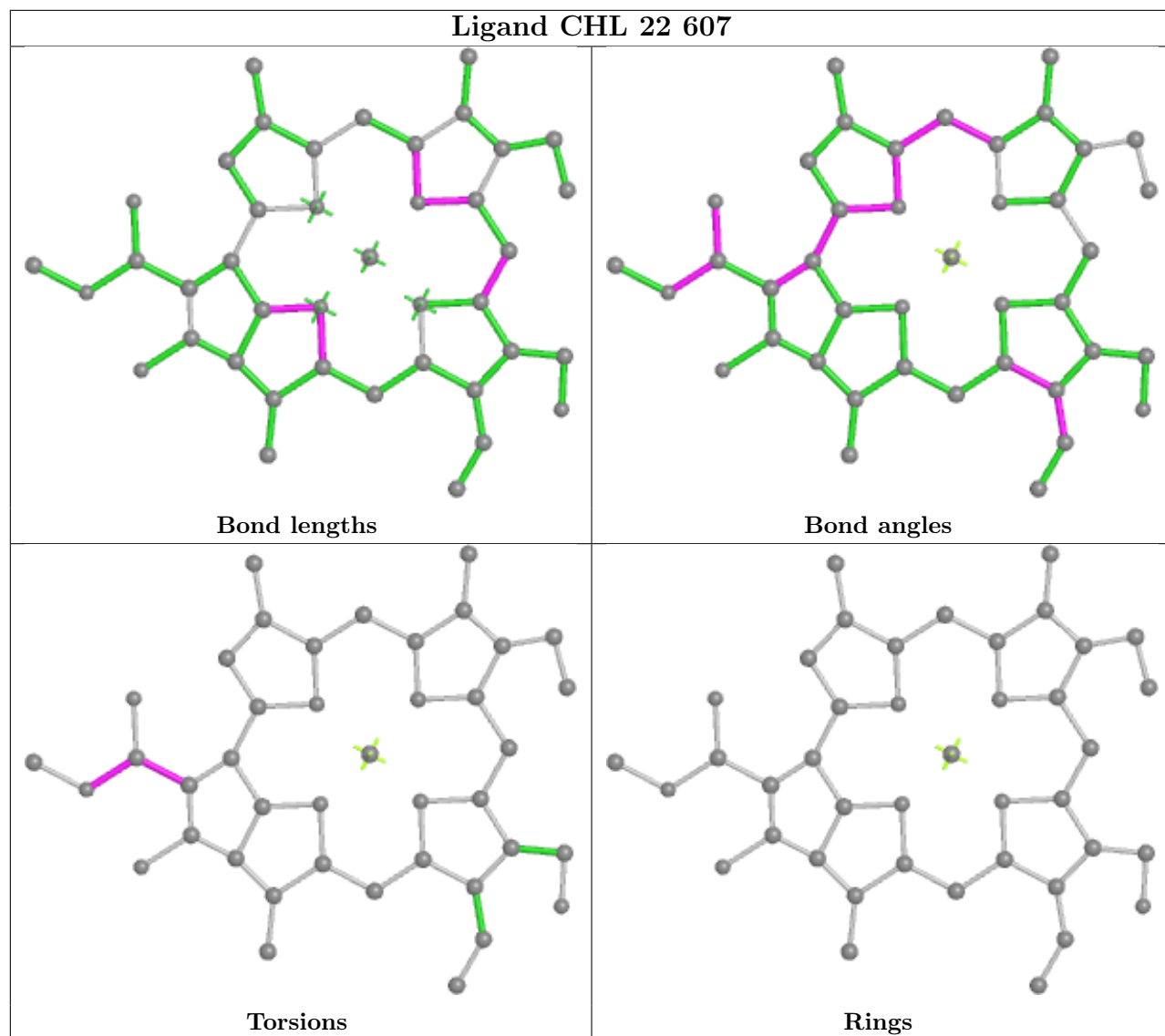
## Ligand CLA 3 603



## Ligand XAT Nn 308

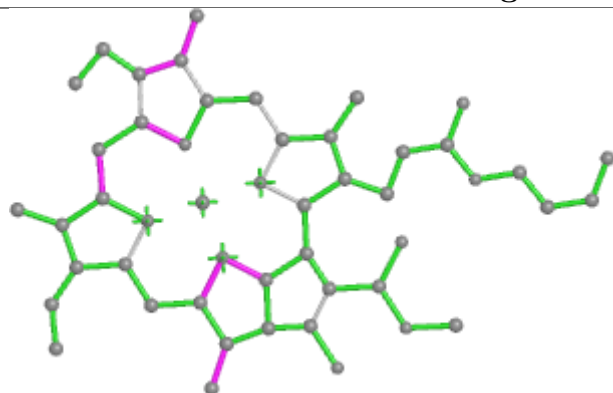




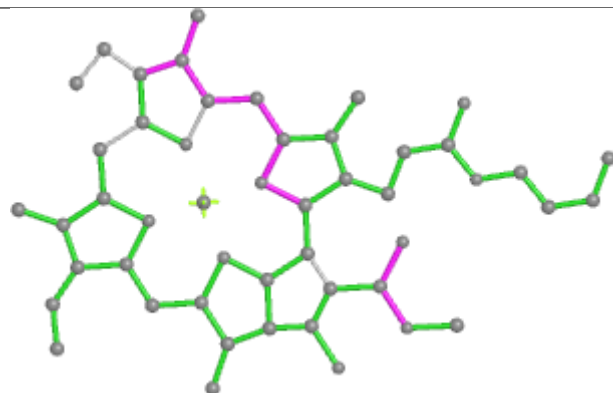




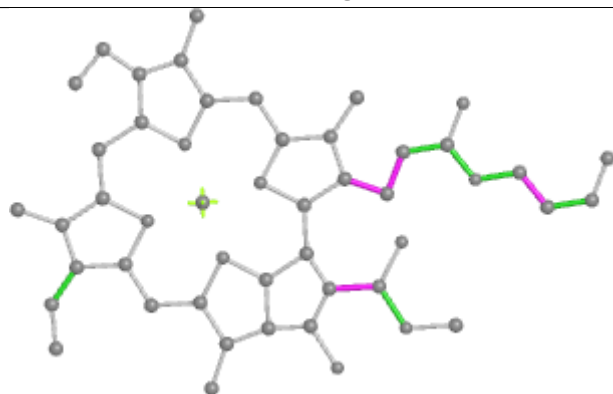
## Ligand CLA RR 311



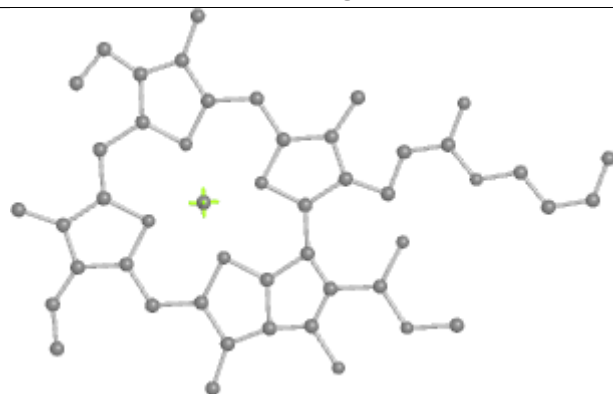
Bond lengths



Bond angles

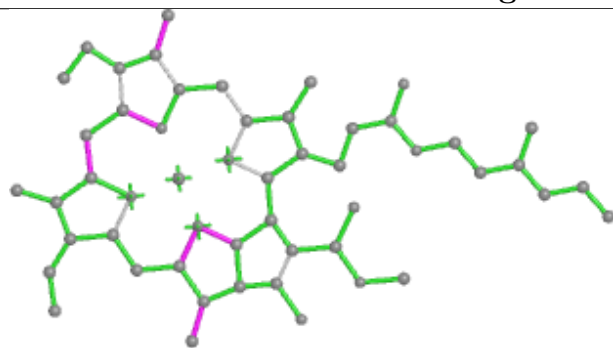


Torsions

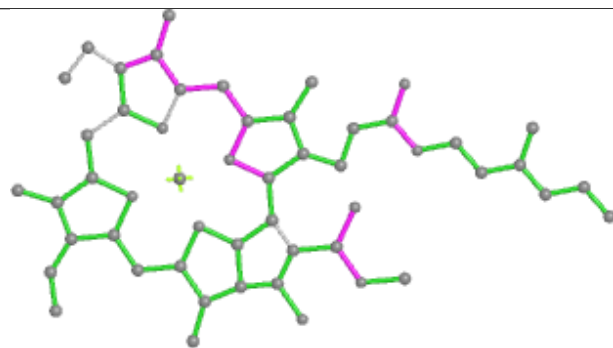


Rings

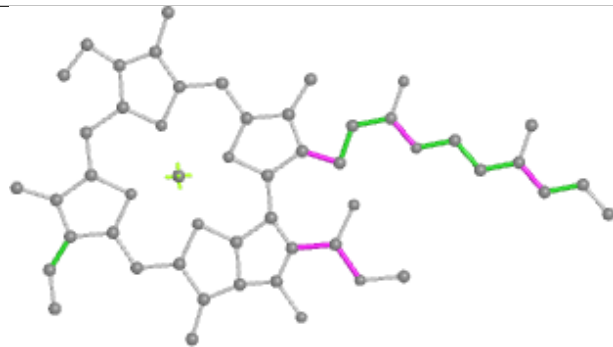
## Ligand CLA GG 611



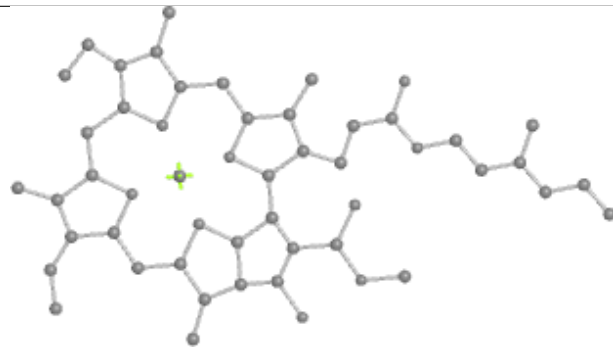
Bond lengths



Bond angles

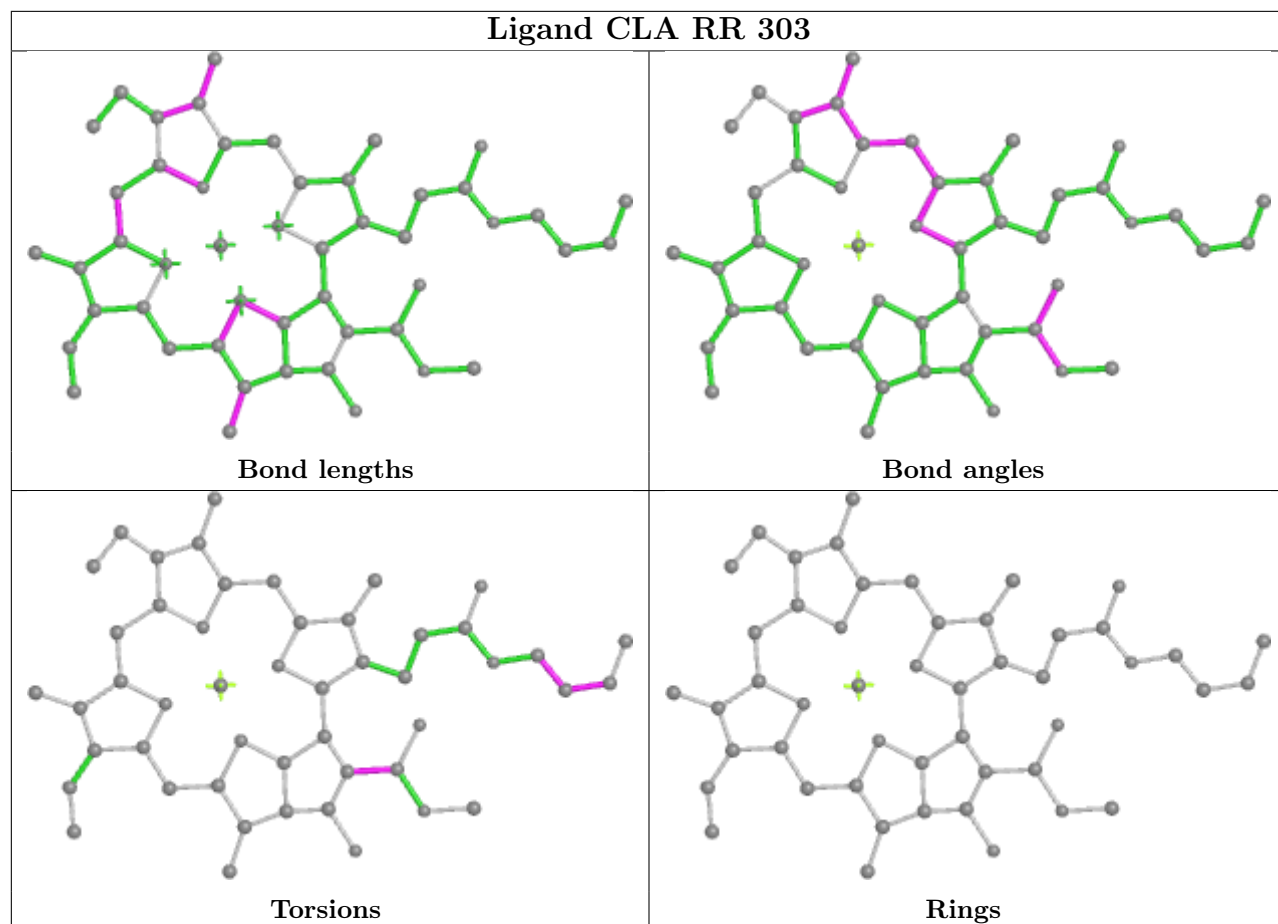


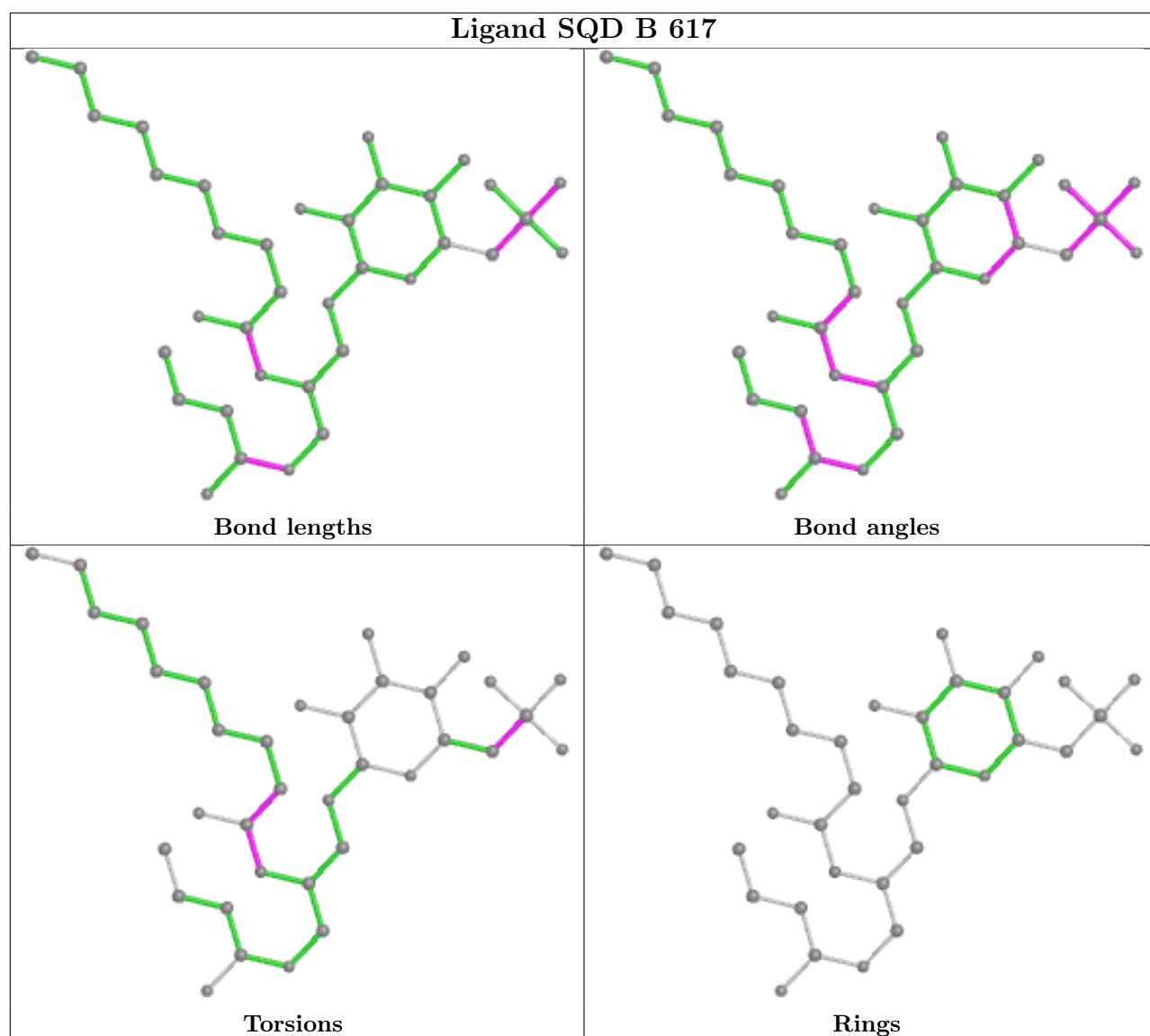
Torsions



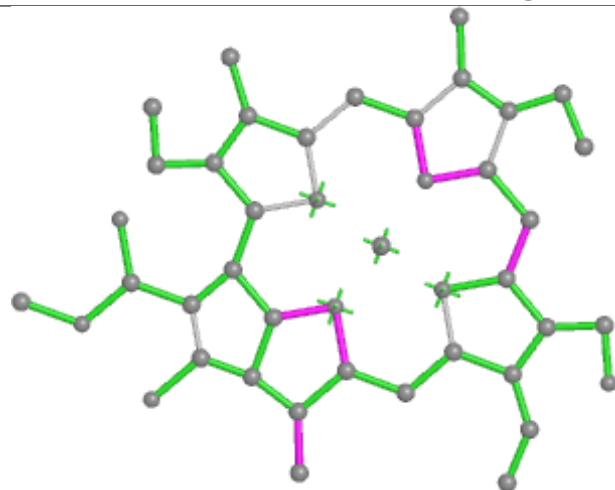
Rings

## Ligand CLA RR 303

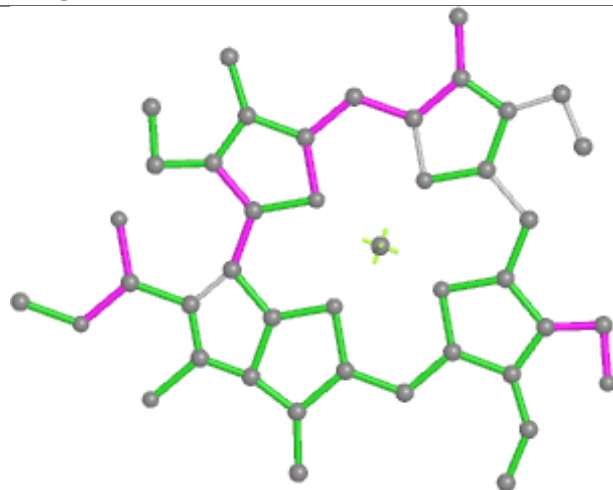




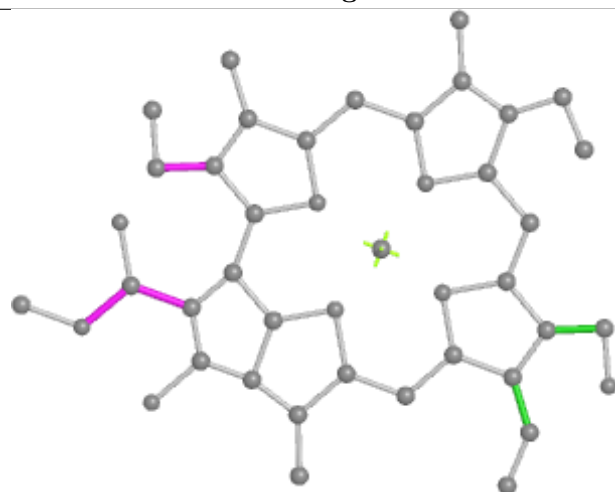
## Ligand CHL g 605



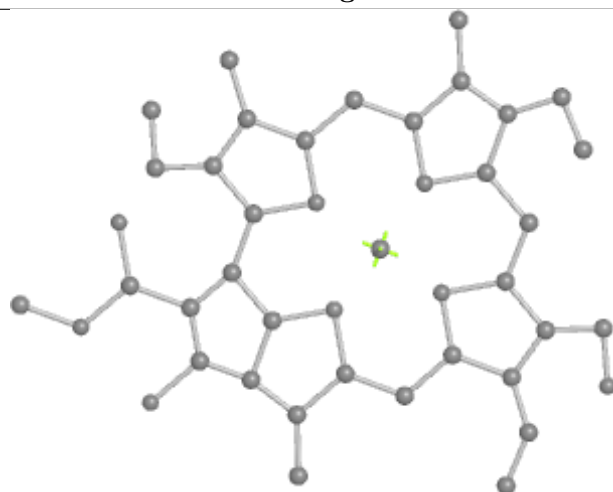
Bond lengths



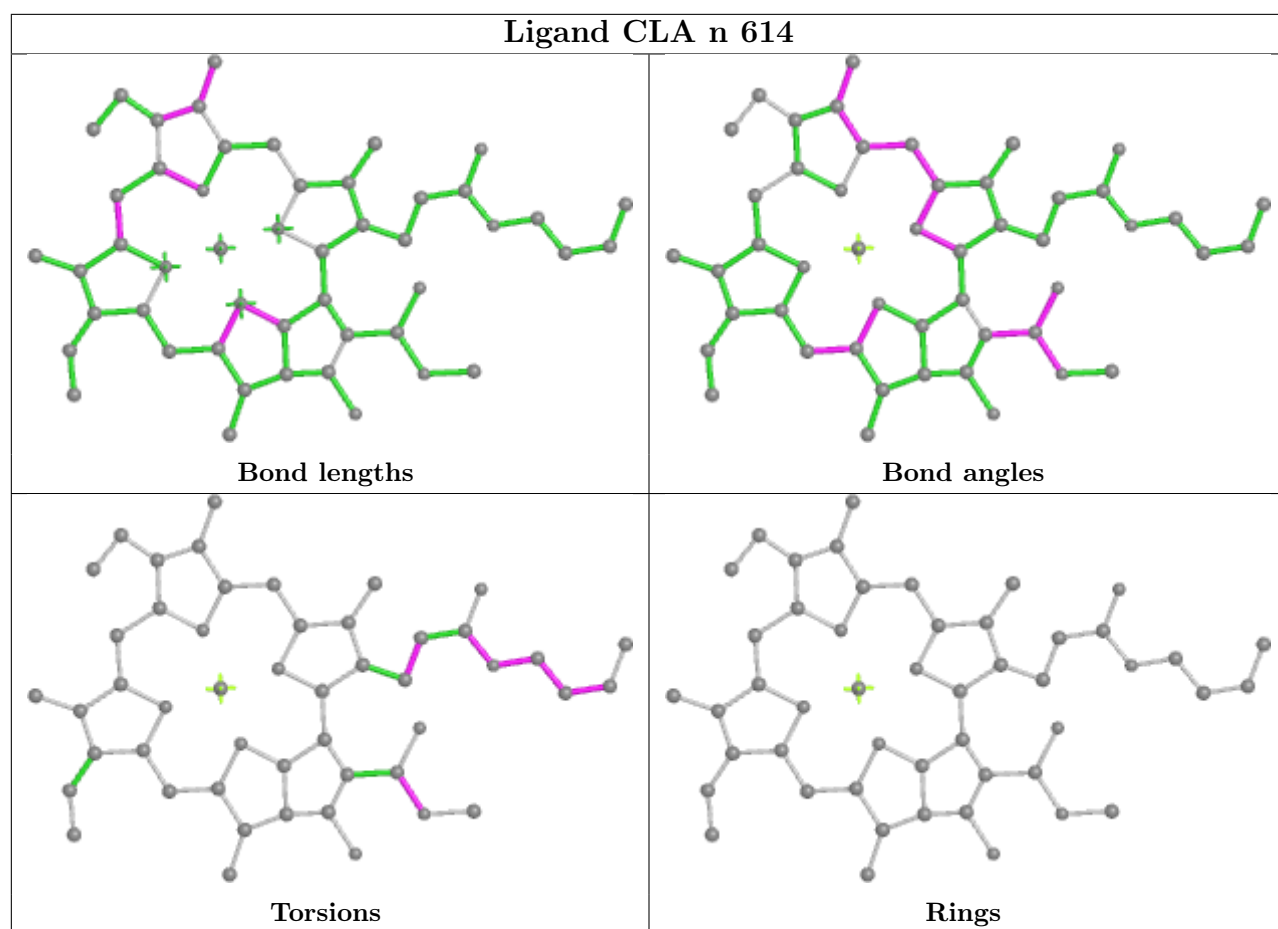
Bond angles

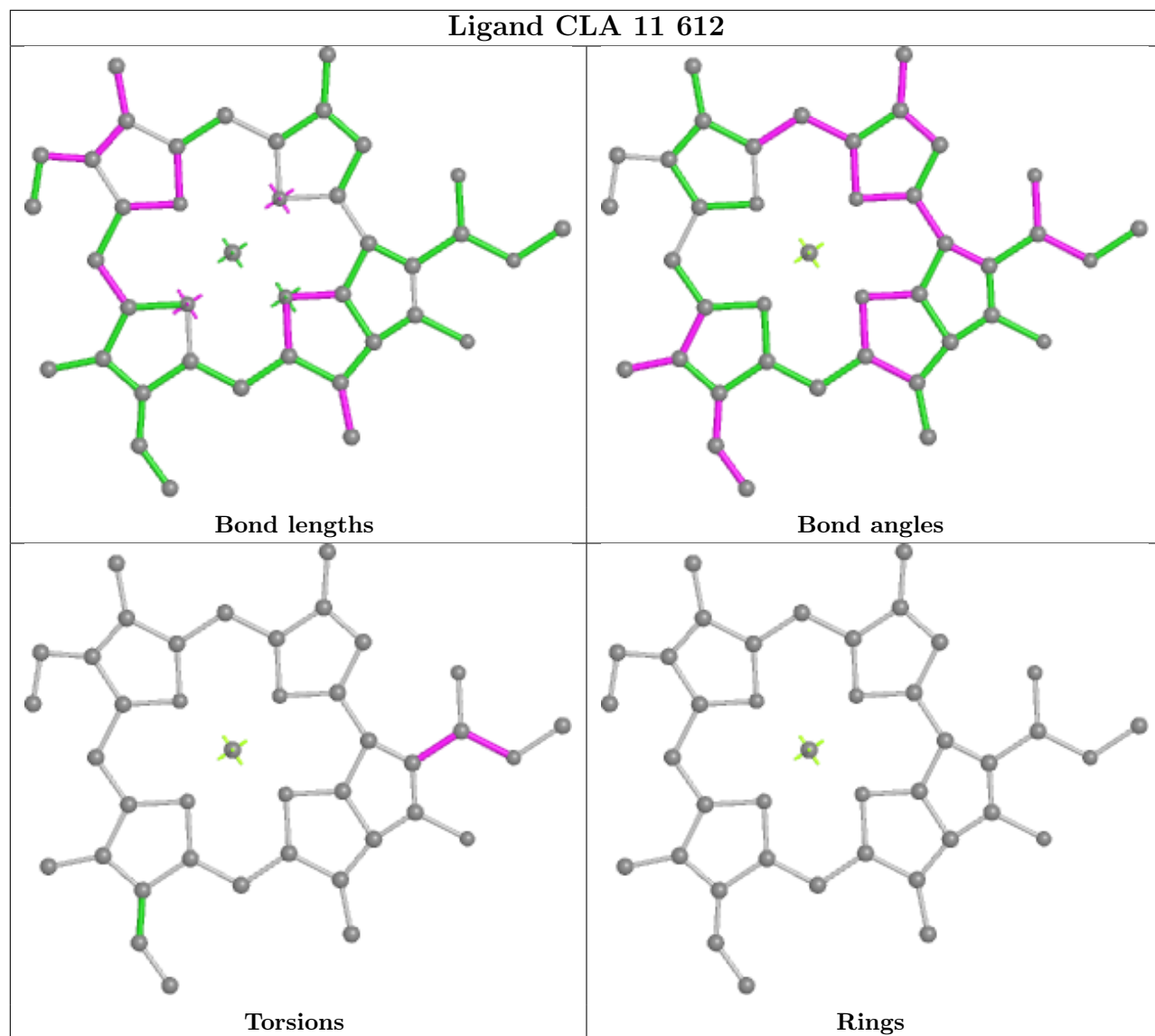


Torsions

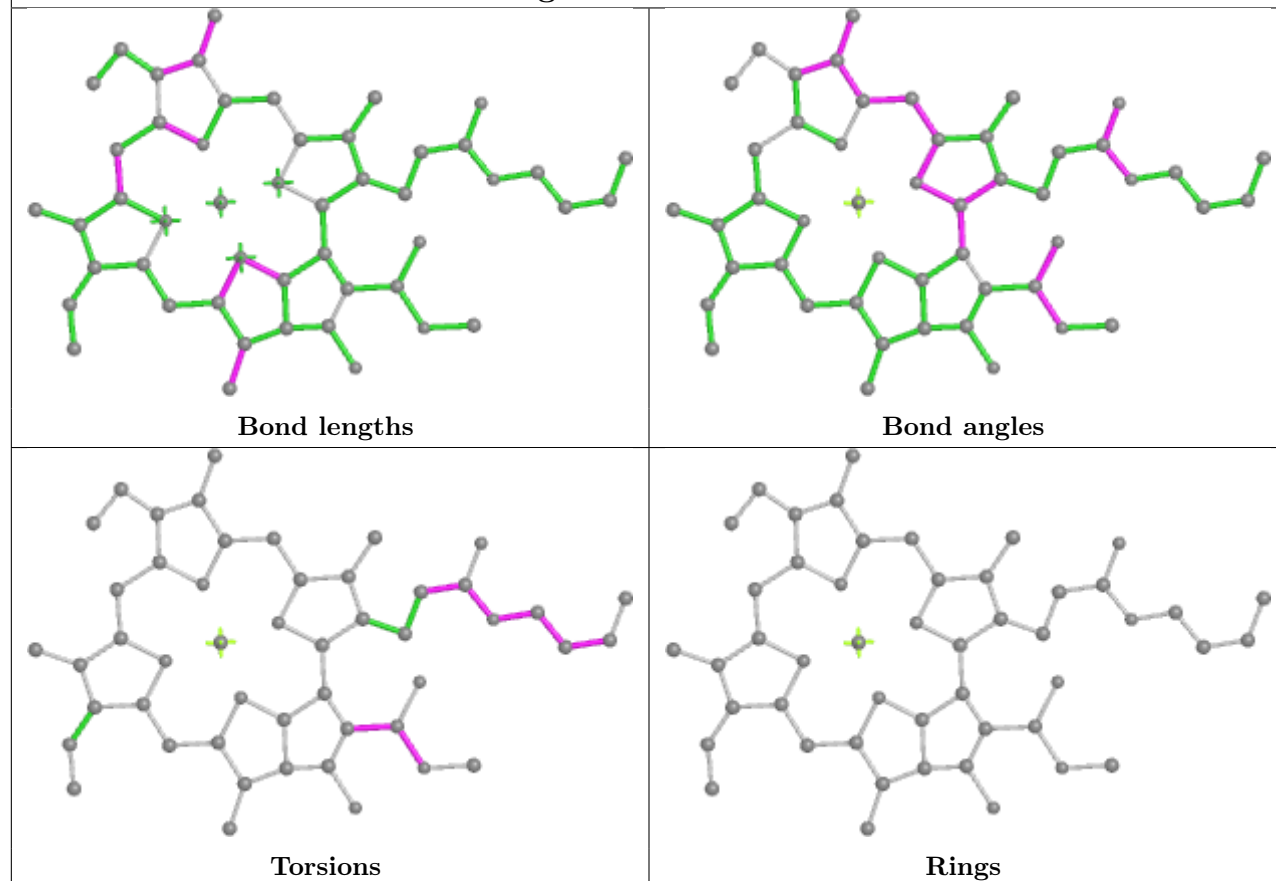


Rings

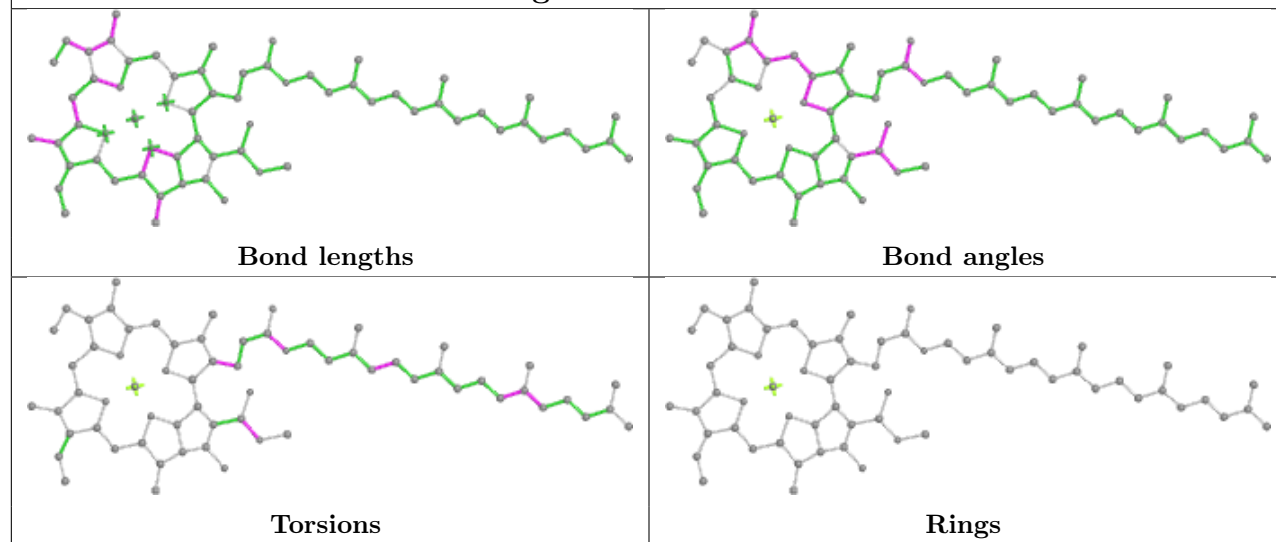


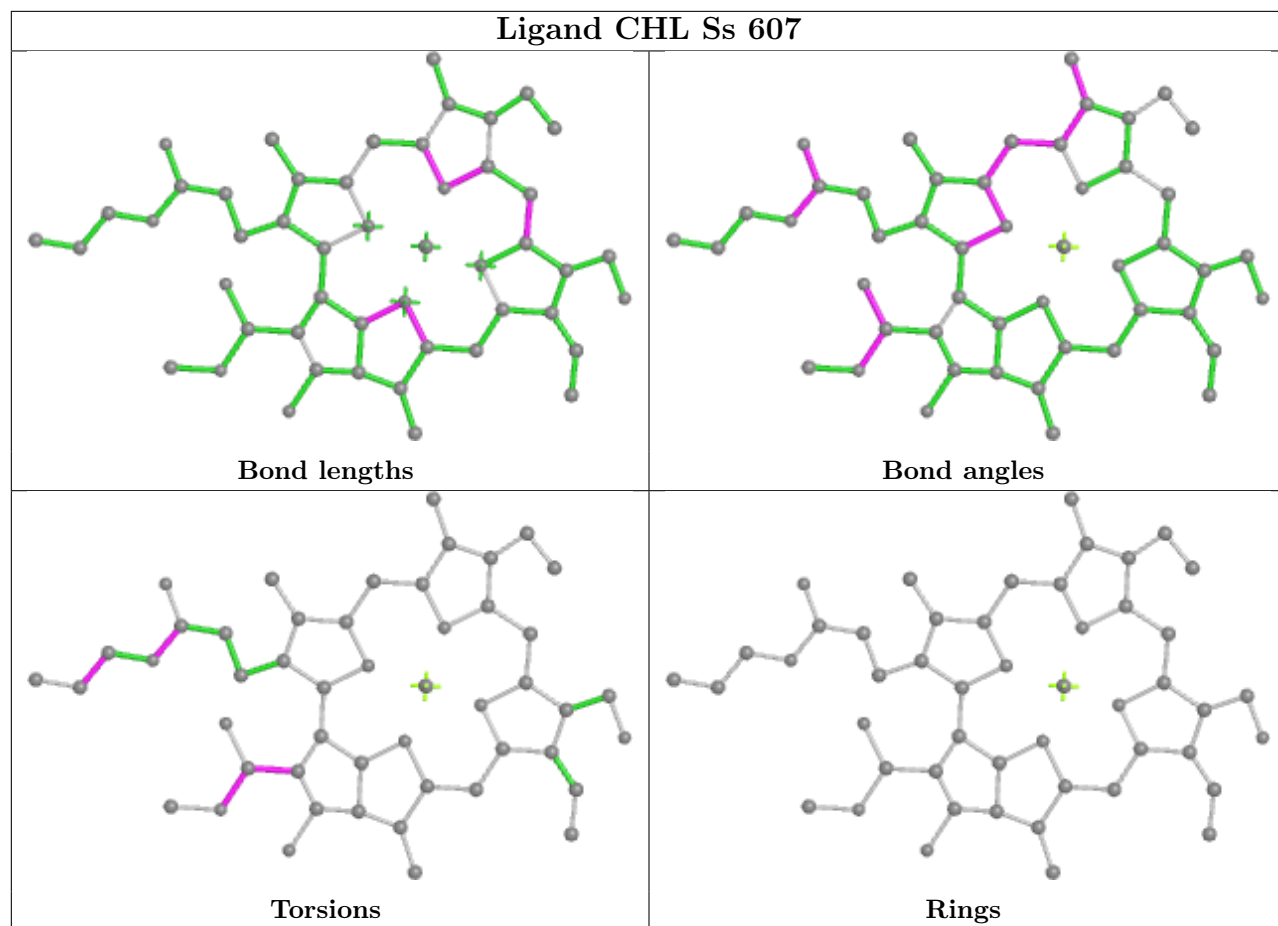


## Ligand CLA s 611



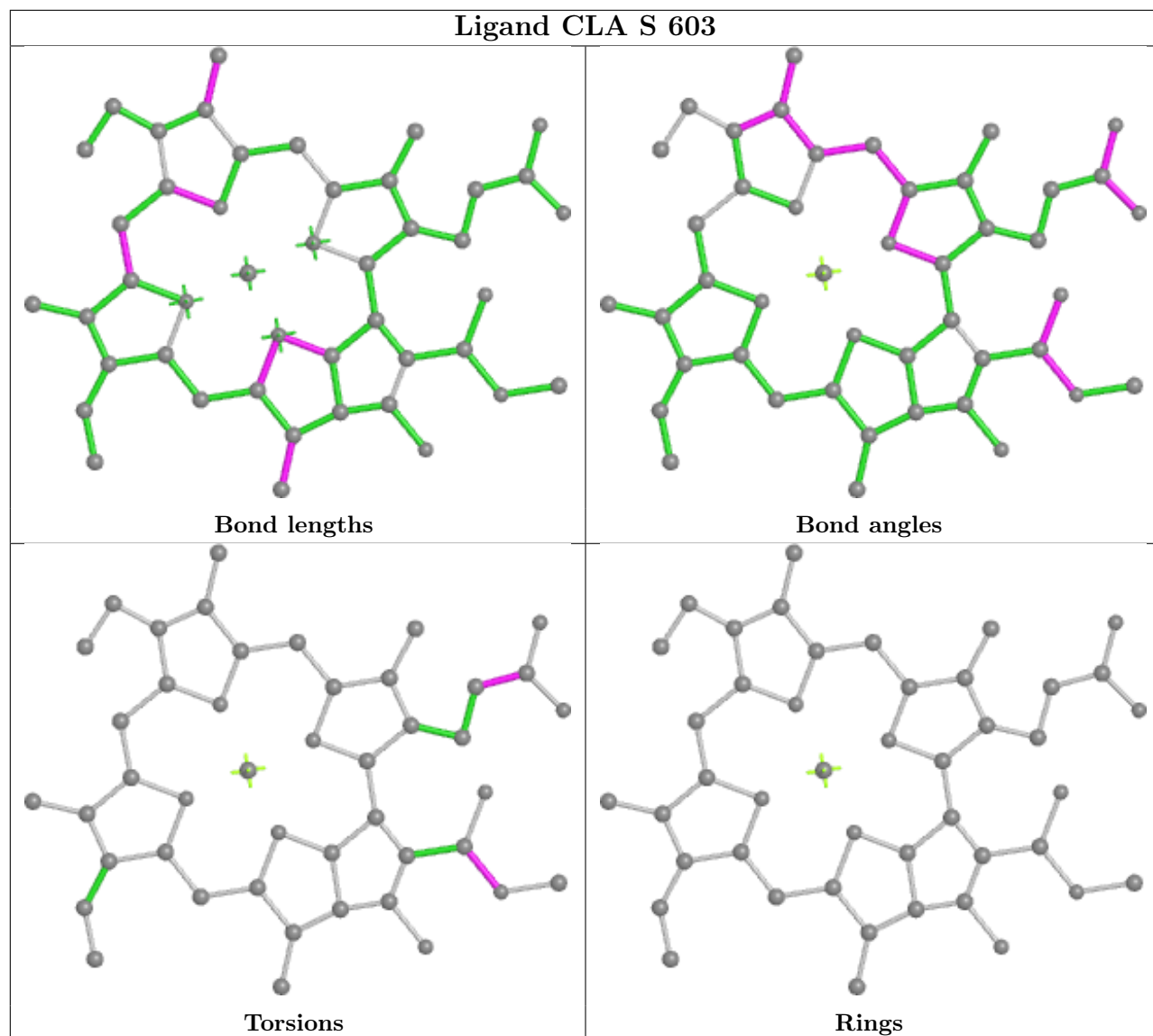
## Ligand CLA B 620



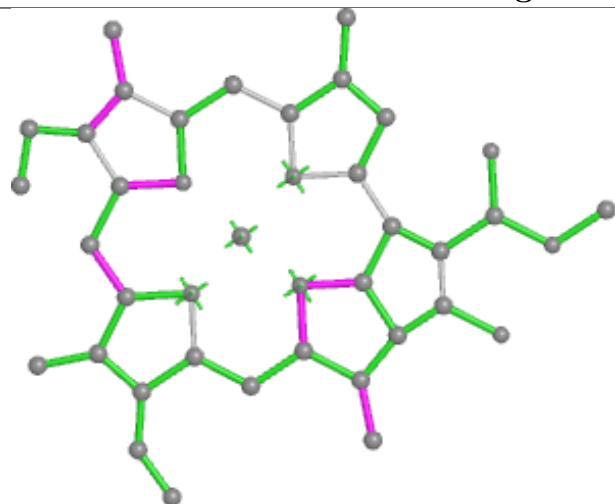




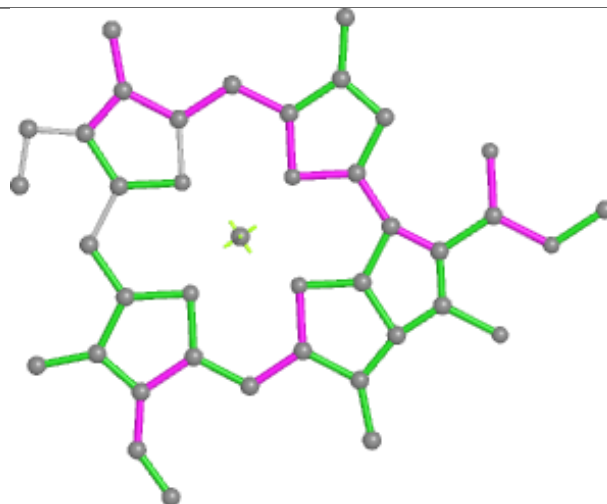
## Ligand CLA S 603



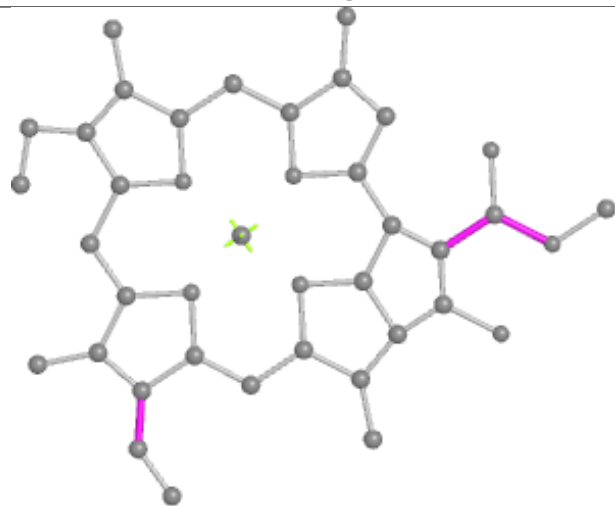
## Ligand CLA G 613



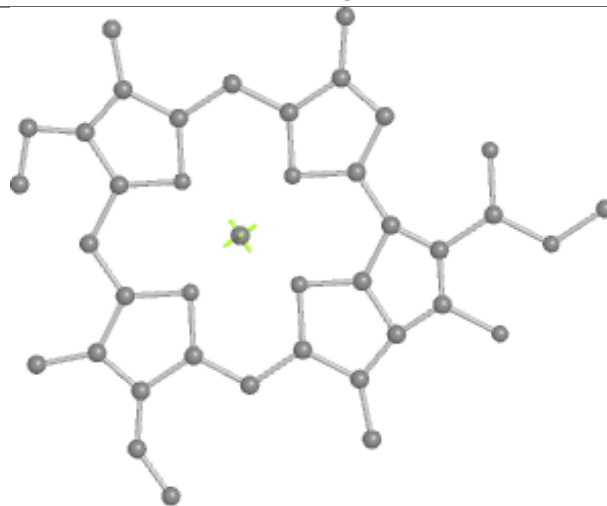
Bond lengths



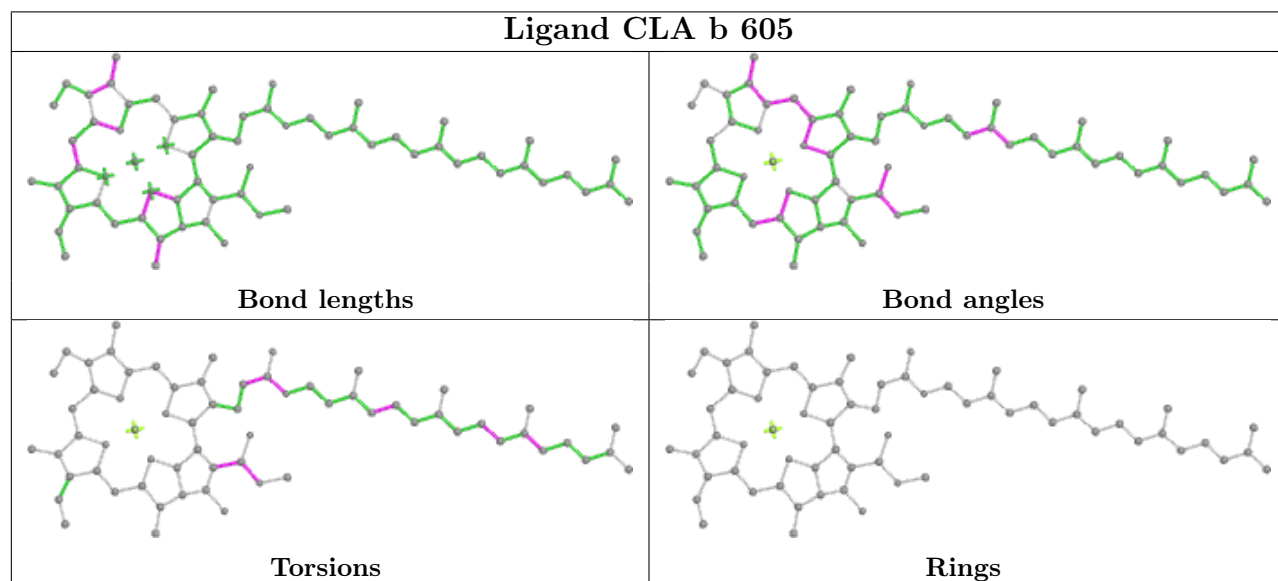
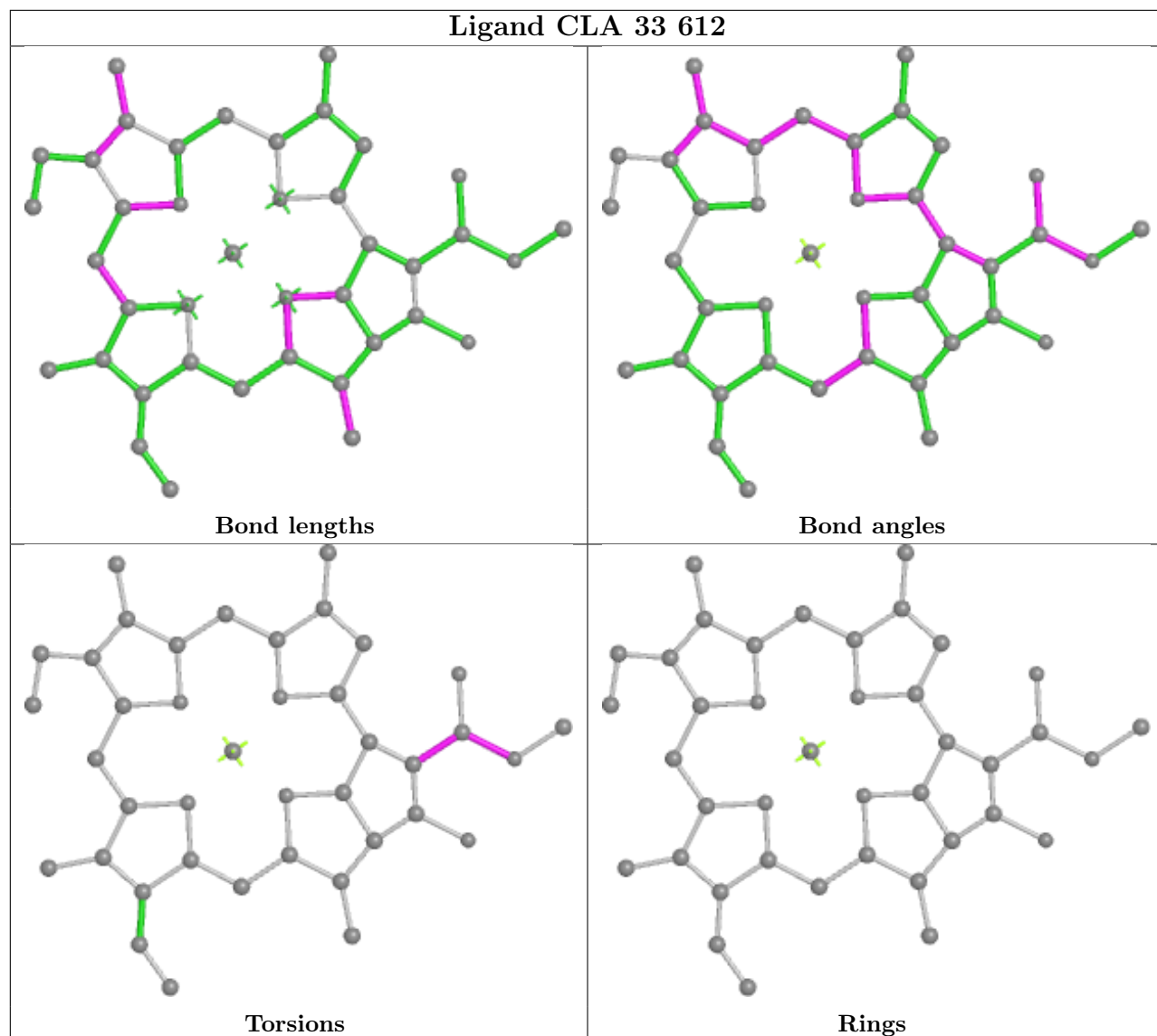
Bond angles

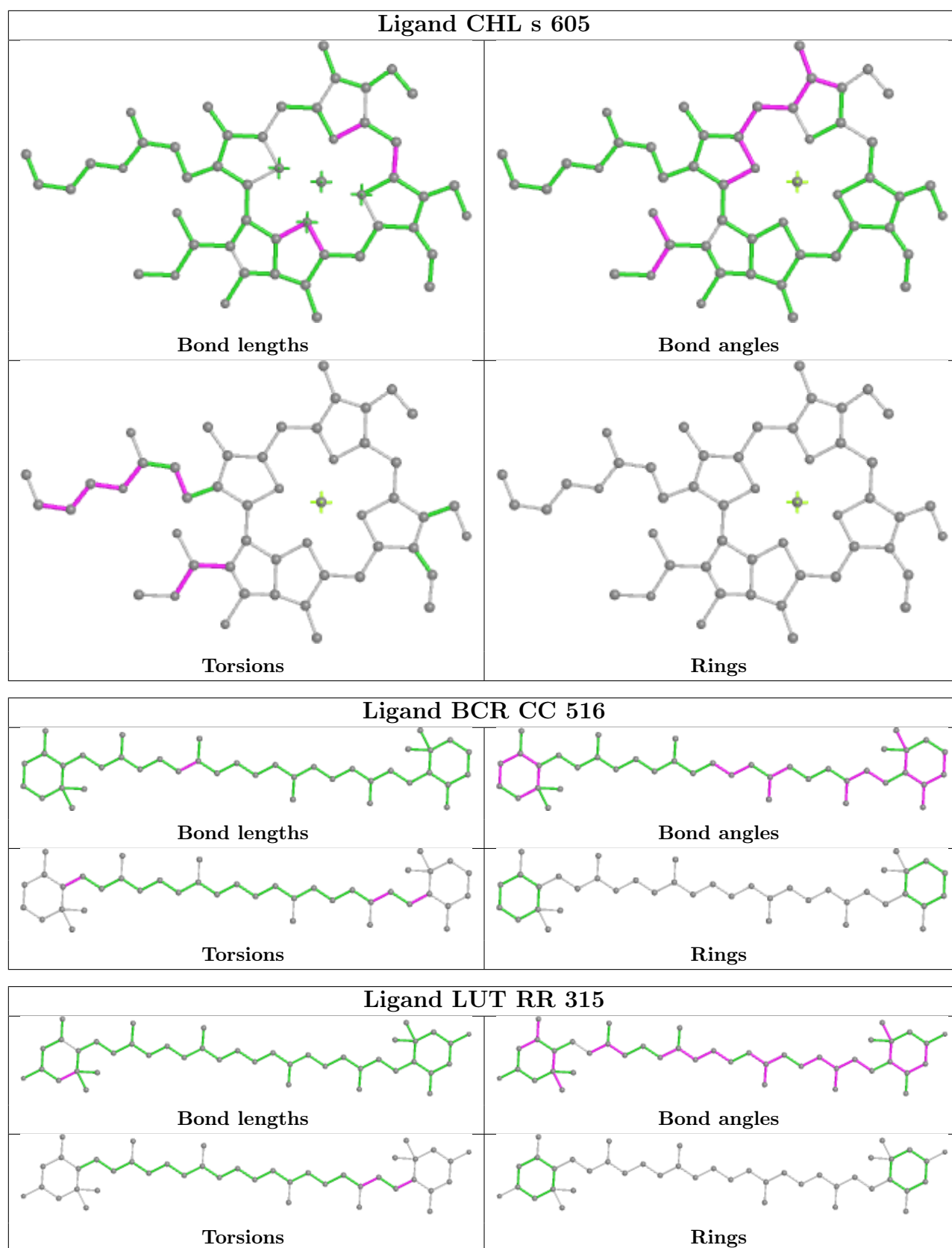


Torsions

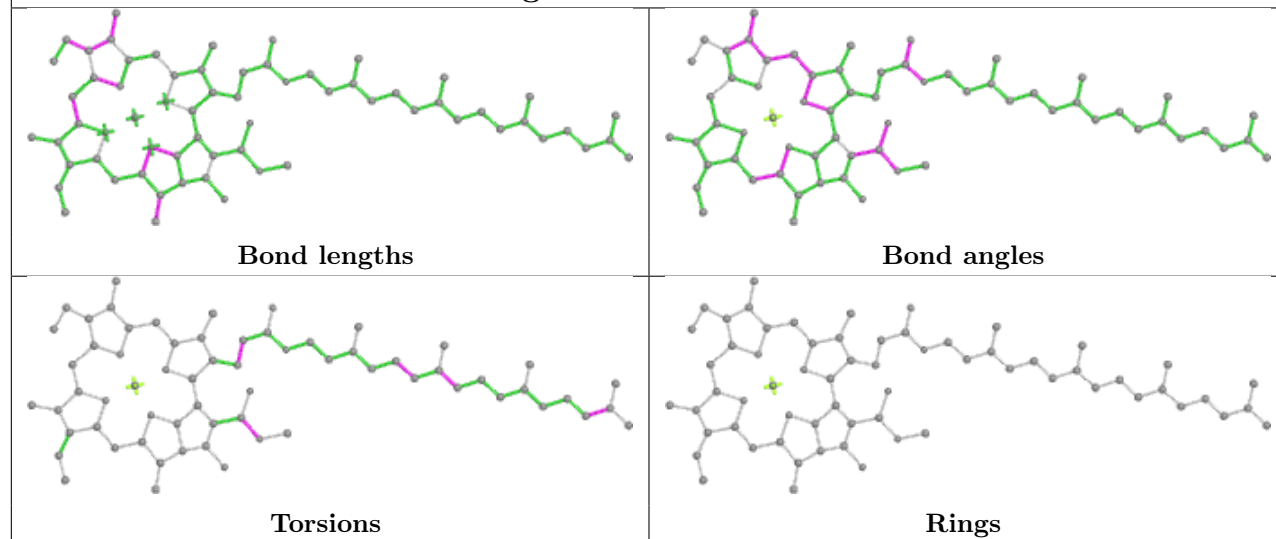


Rings

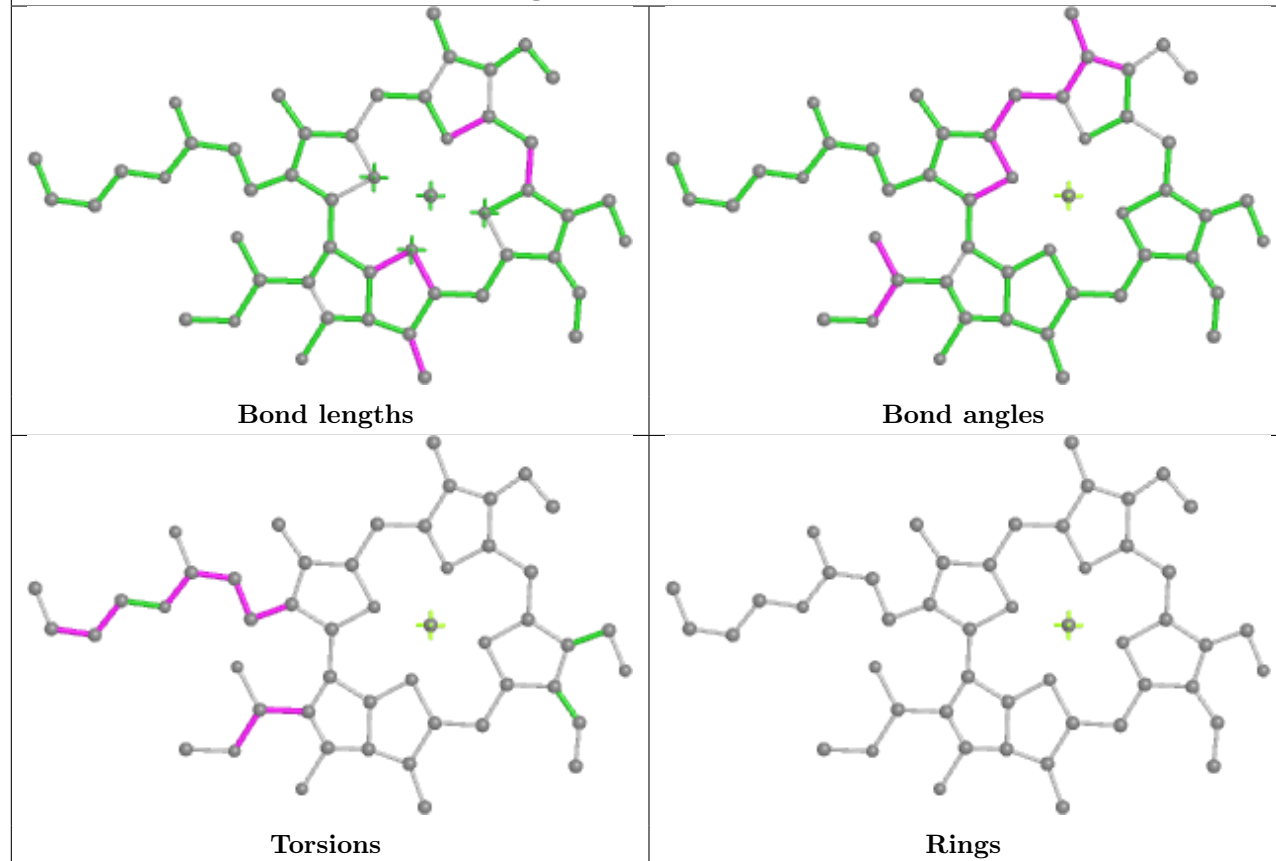




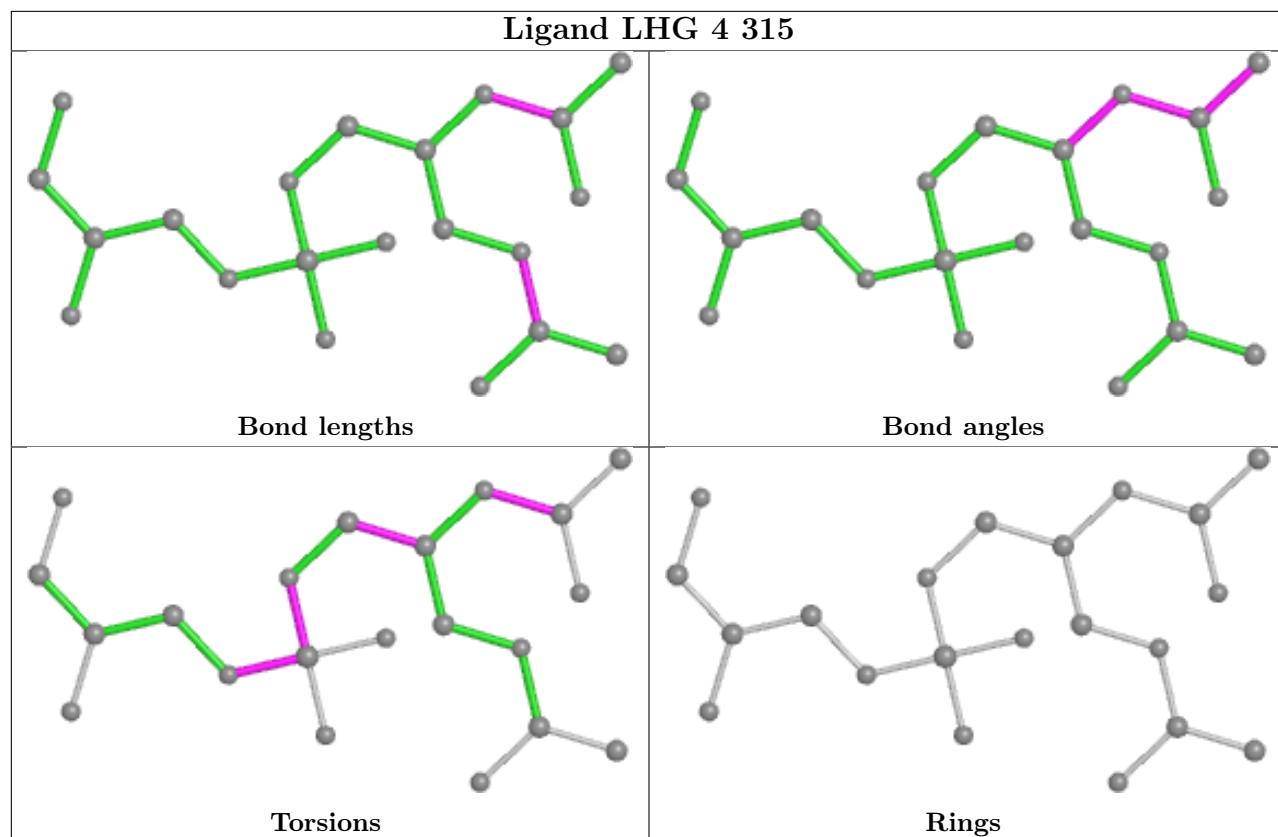
## Ligand CLA Bb 606



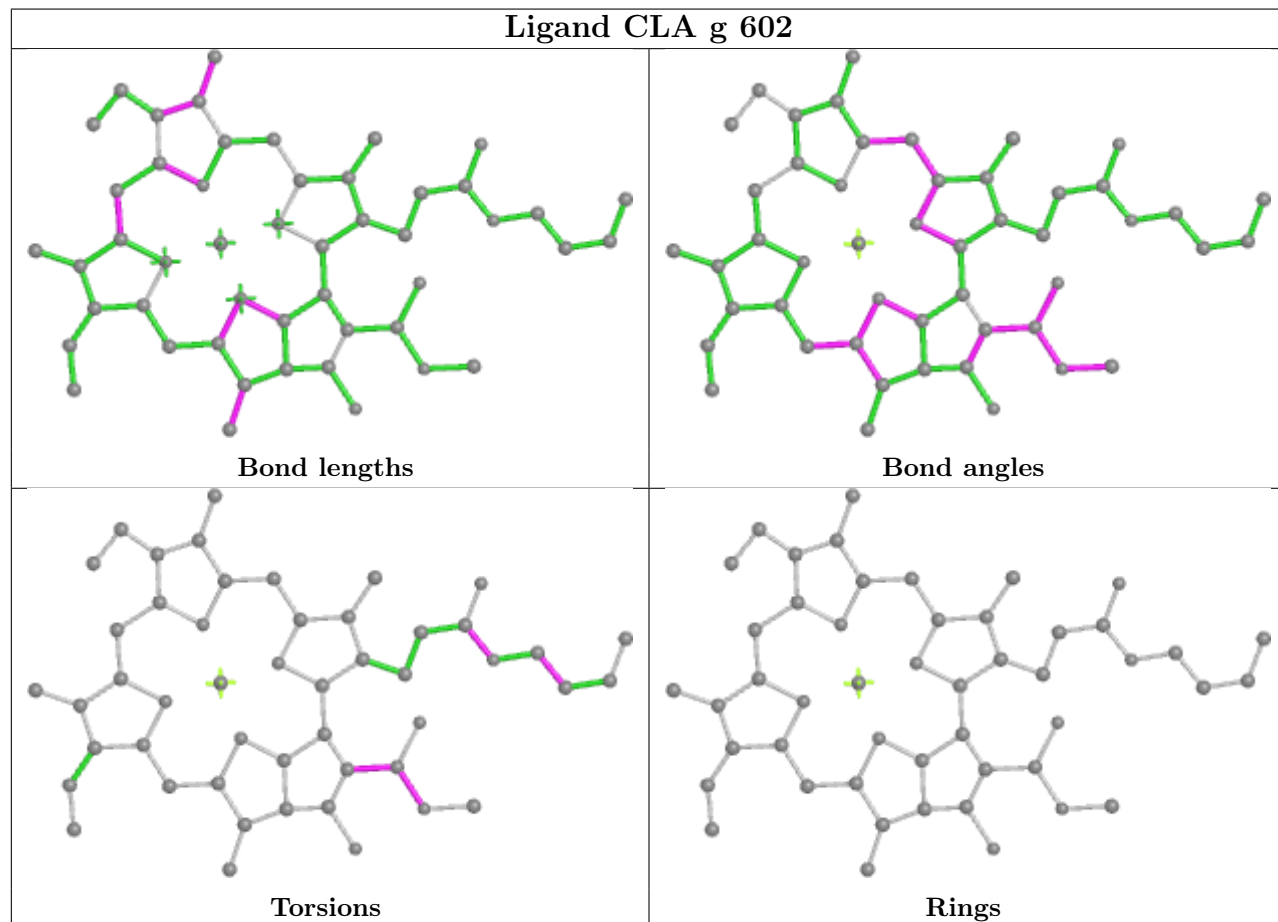
## Ligand CHL Ss 605



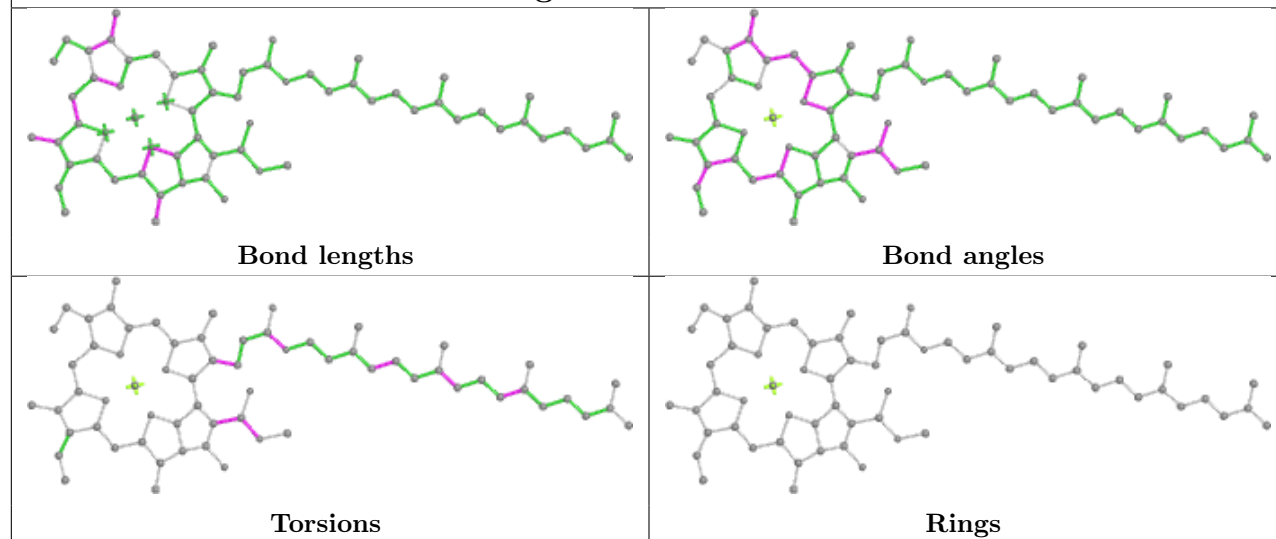
## Ligand LHG 4 315



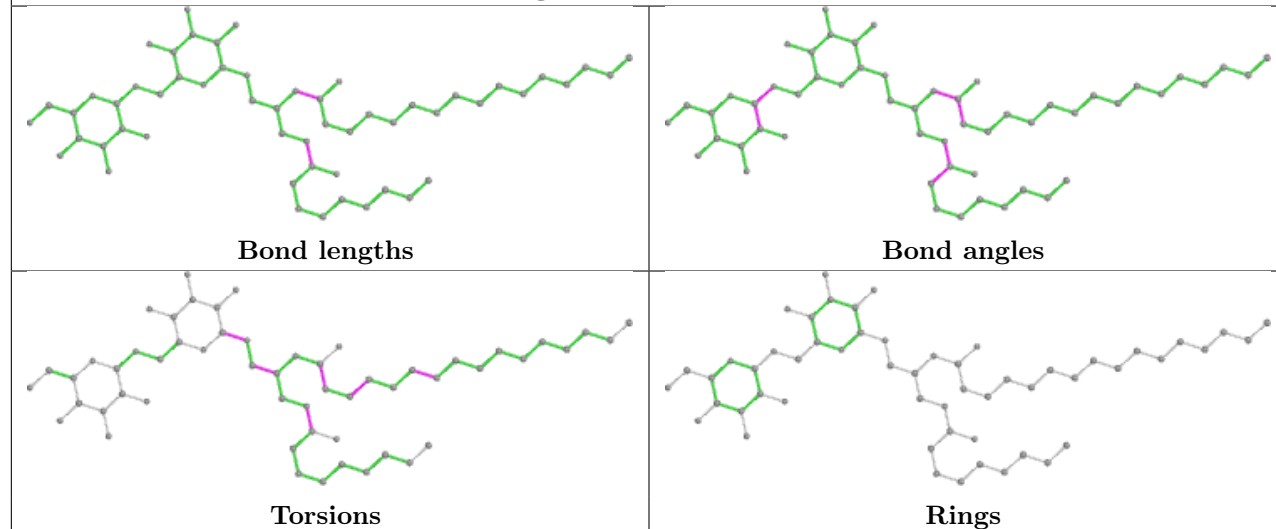
## Ligand CLA g 602



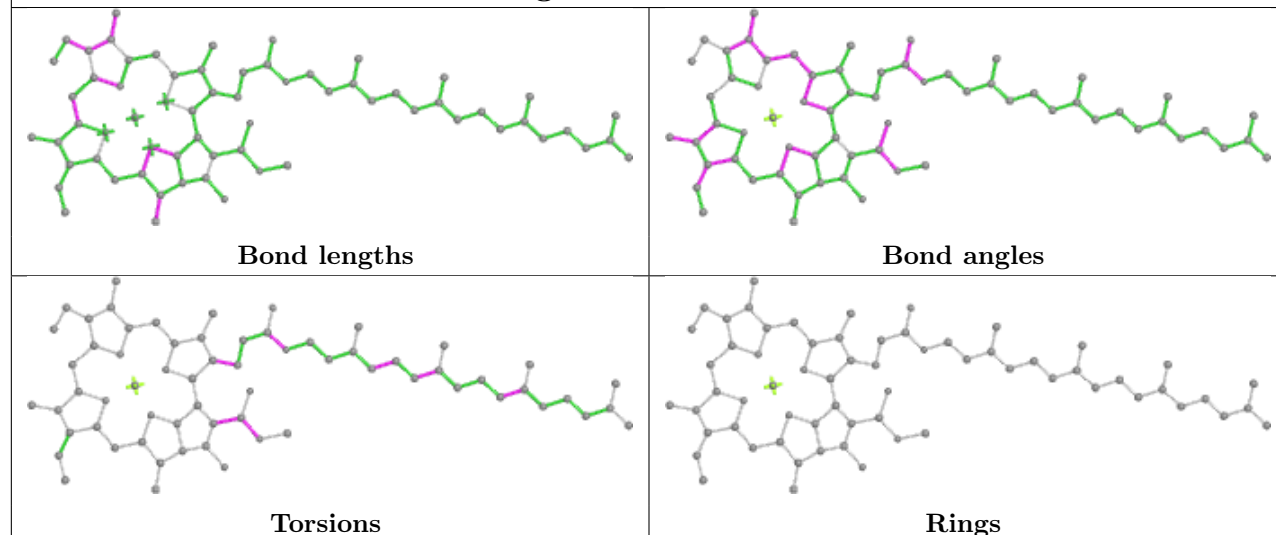
## Ligand CLA d 401

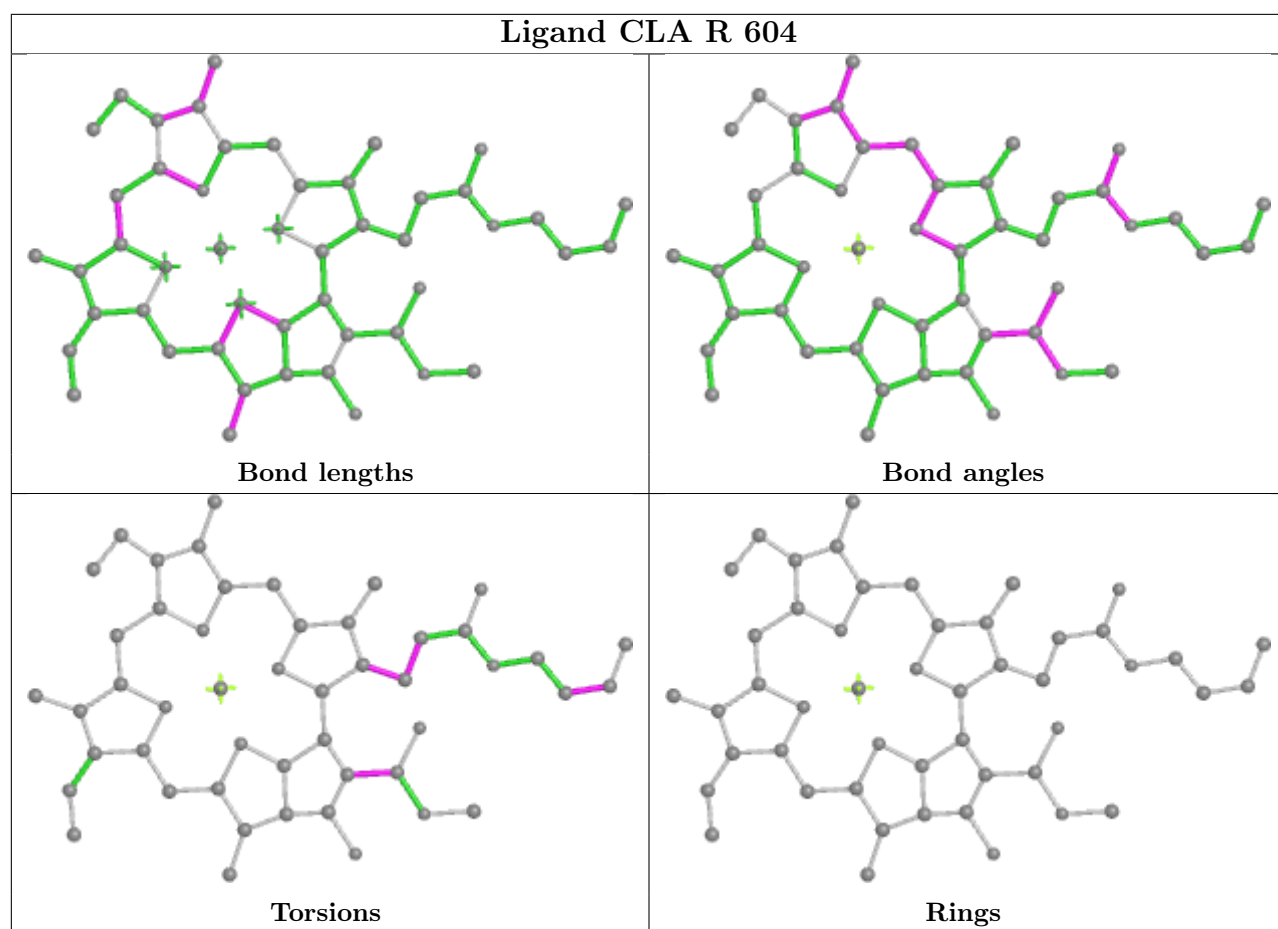


## Ligand DGD a 415



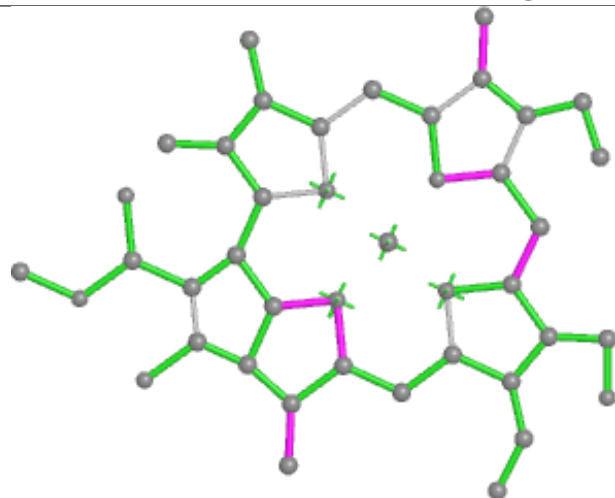
## Ligand CLA n 610



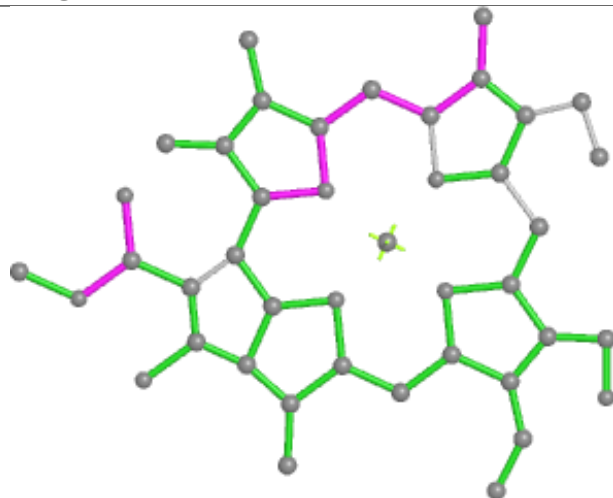




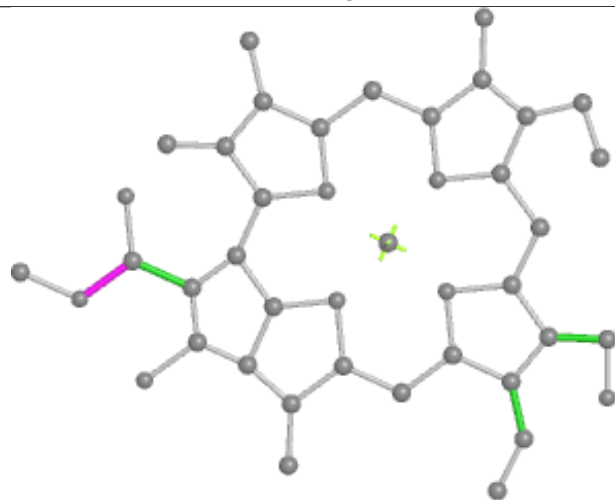
## Ligand CHL g 608



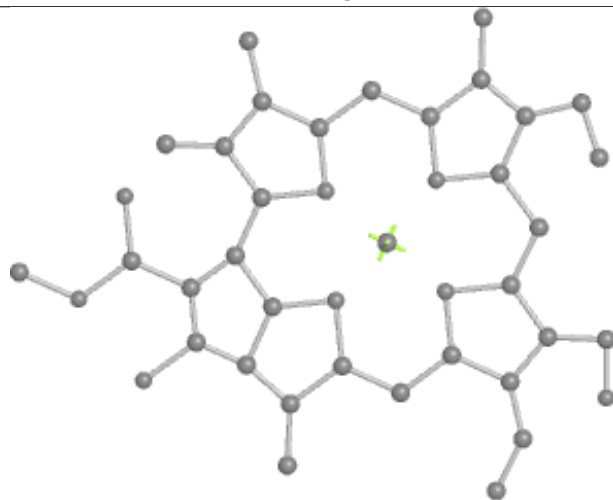
Bond lengths



Bond angles

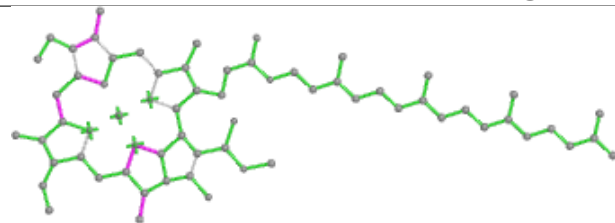


Torsions

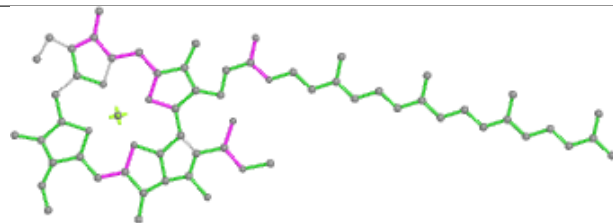


Rings

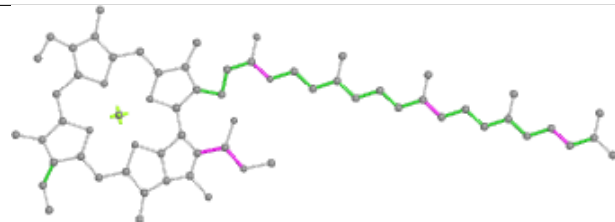
## Ligand CLA c 512



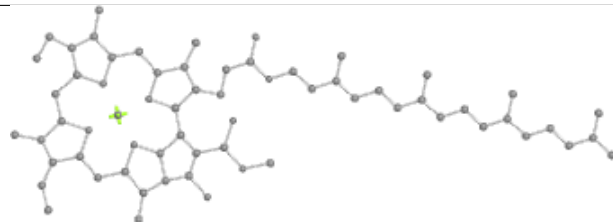
Bond lengths



Bond angles

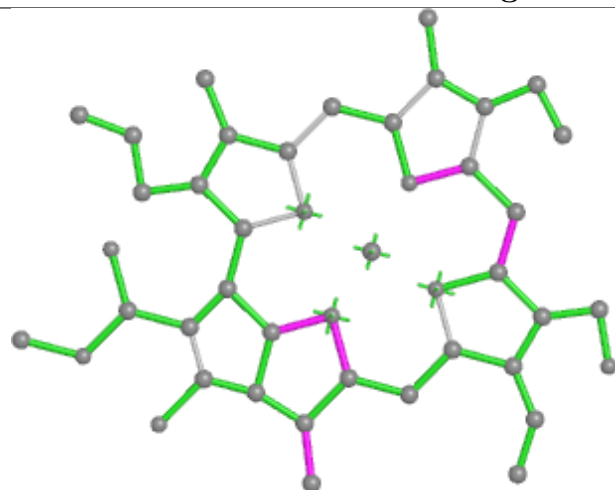


Torsions

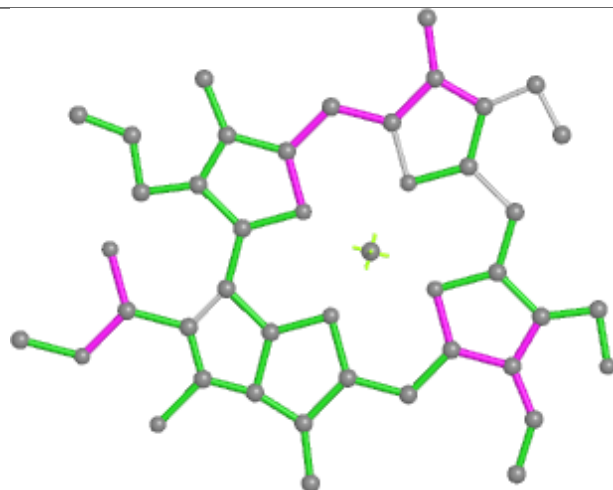


Rings

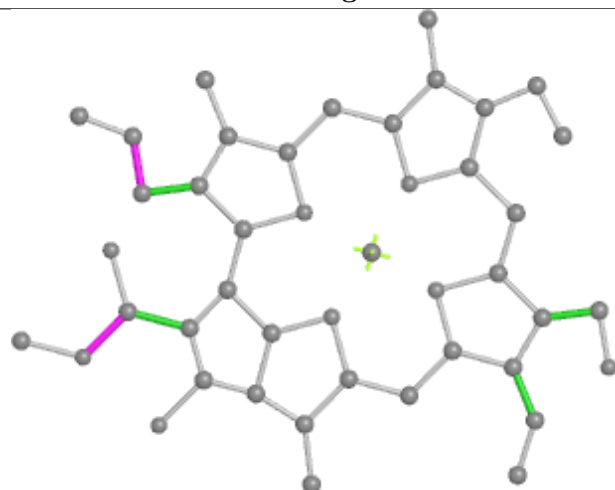
## Ligand CHL NN 601



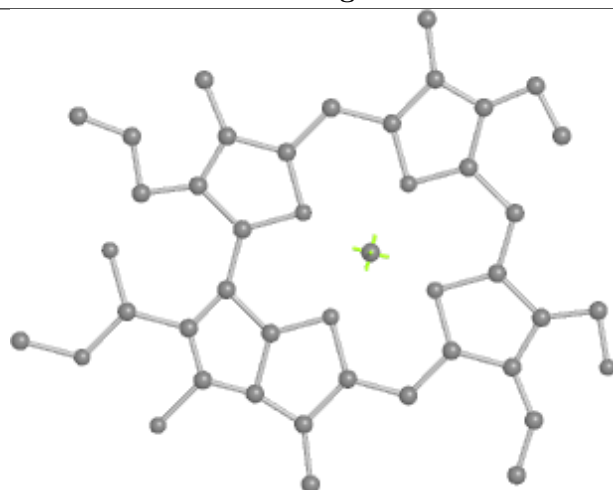
Bond lengths



Bond angles

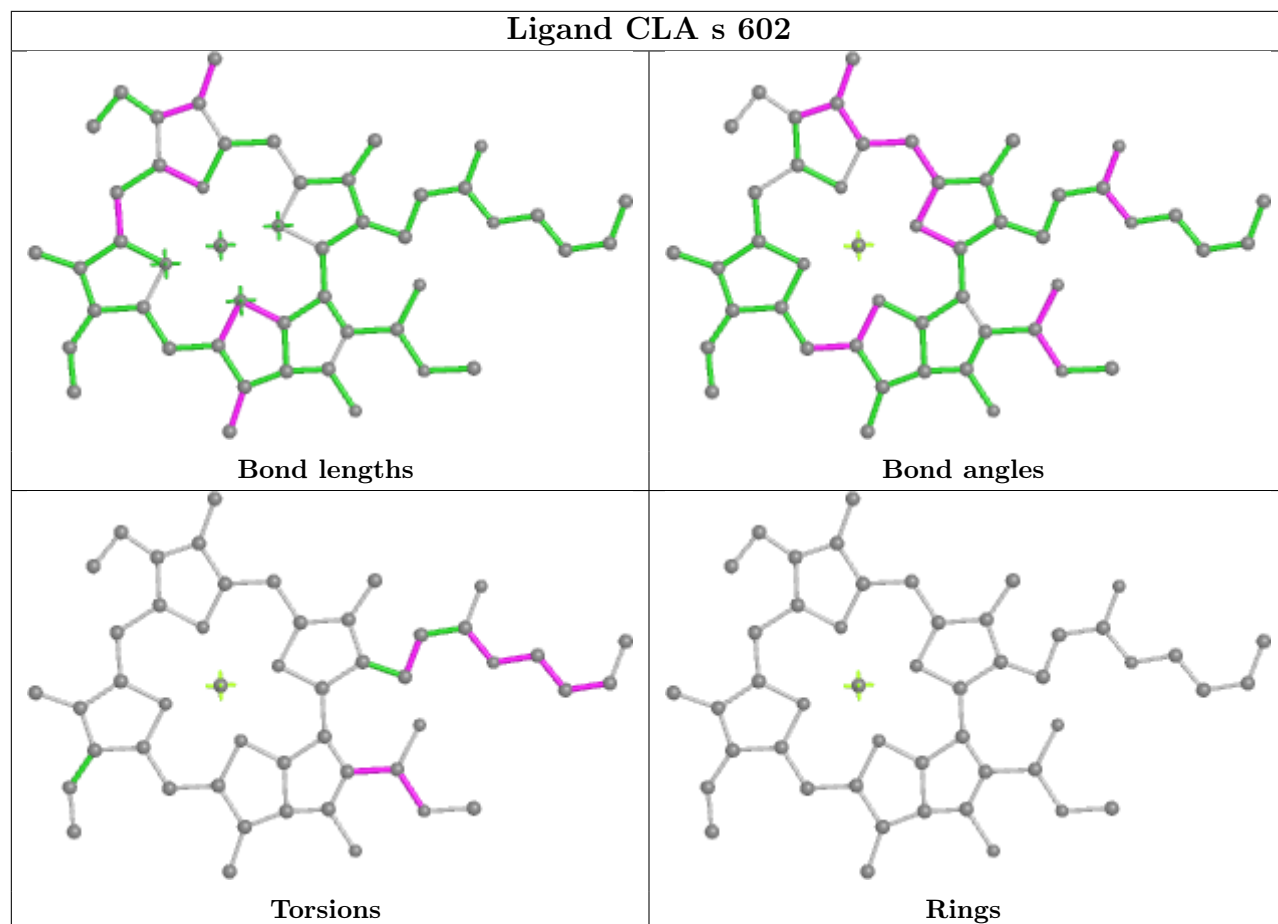


Torsions

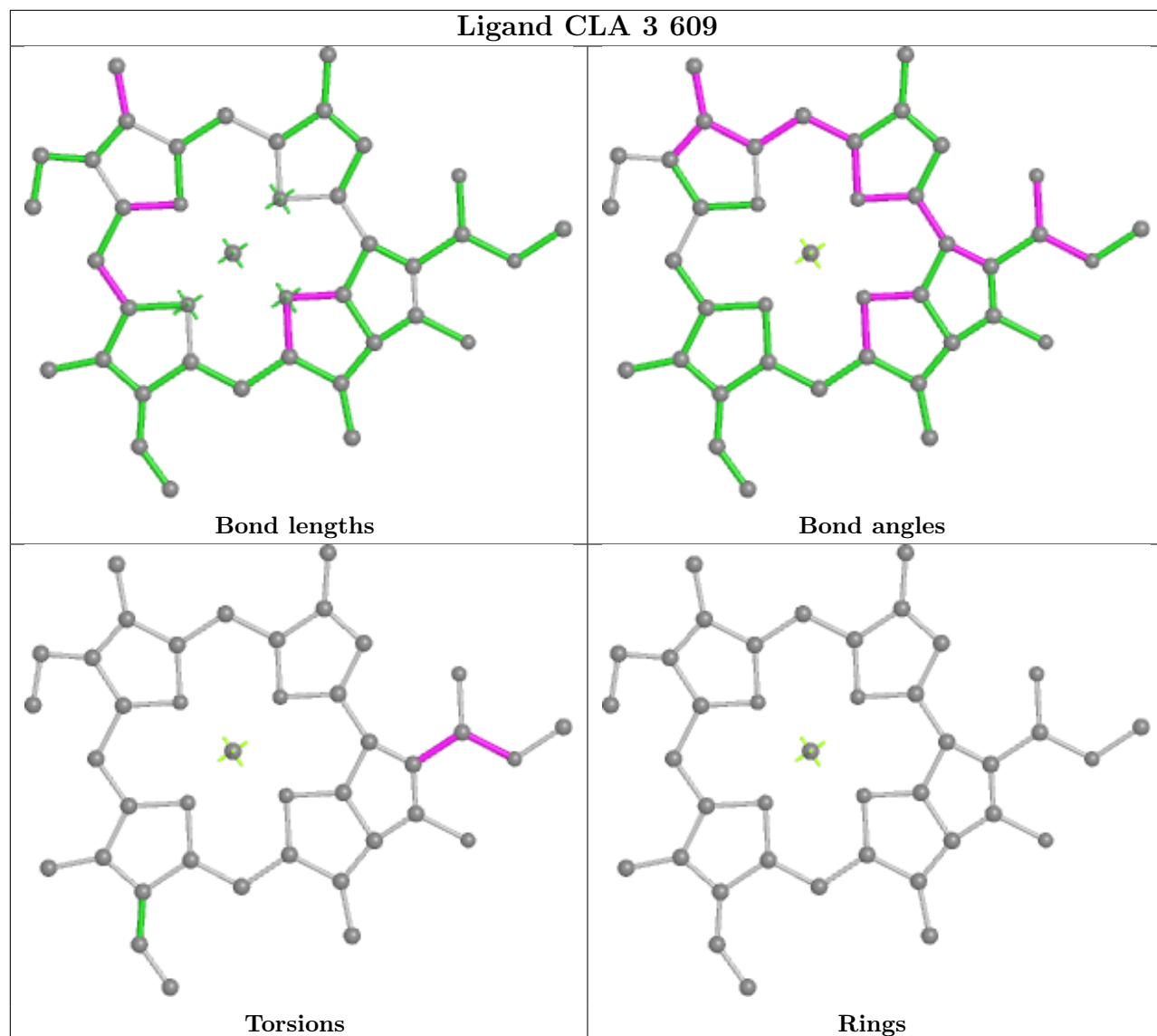


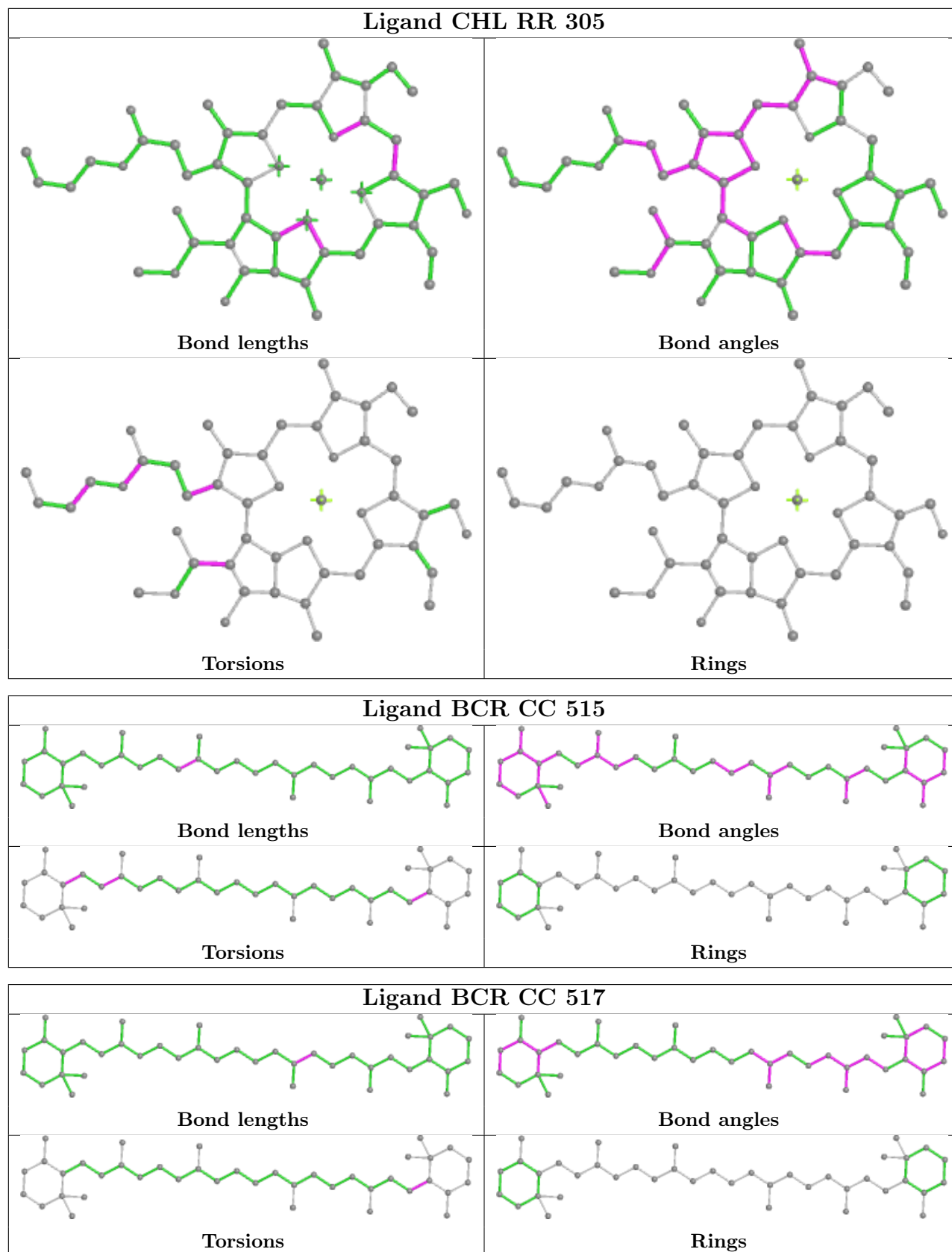
Rings

## Ligand CLA s 602

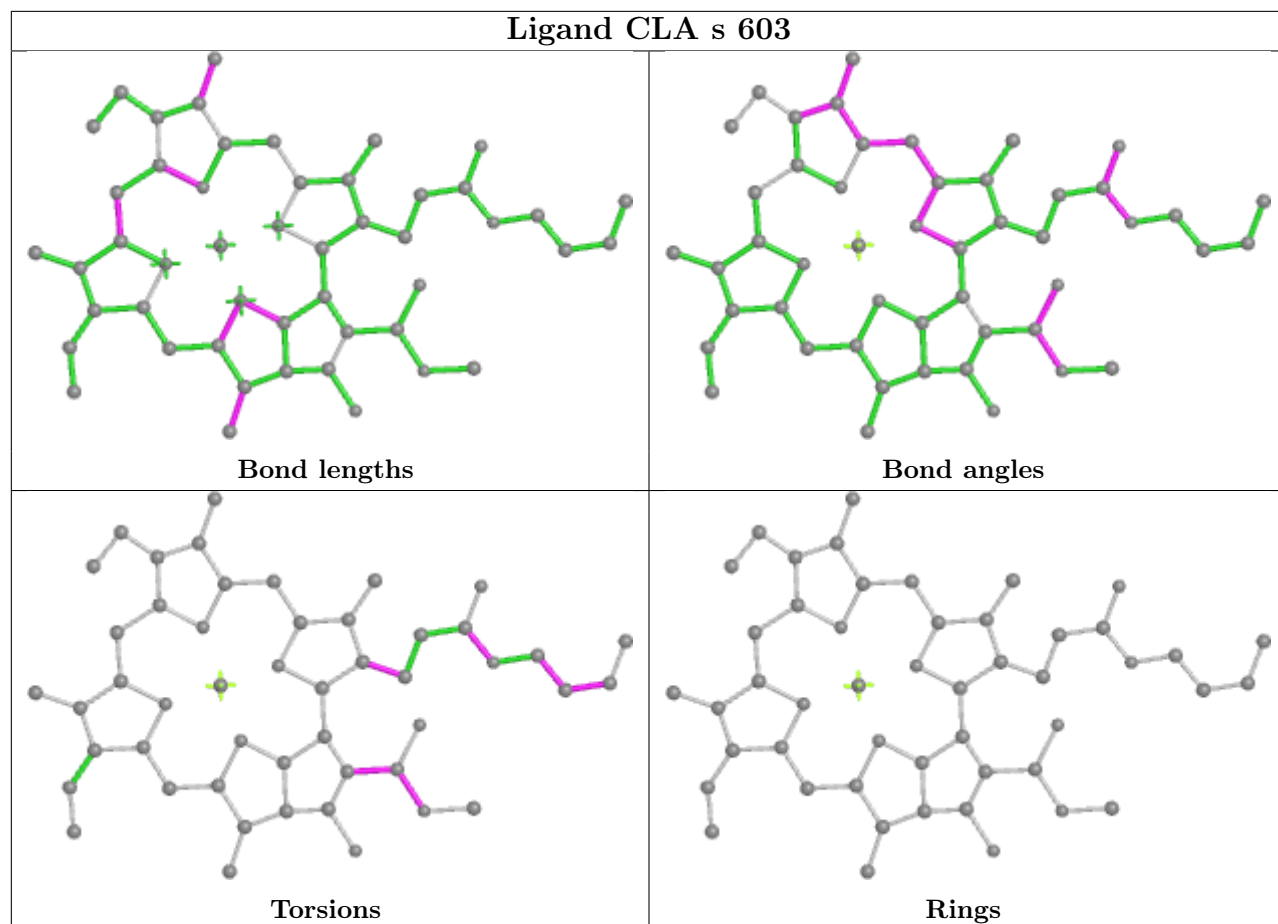


## Ligand CLA 3 609

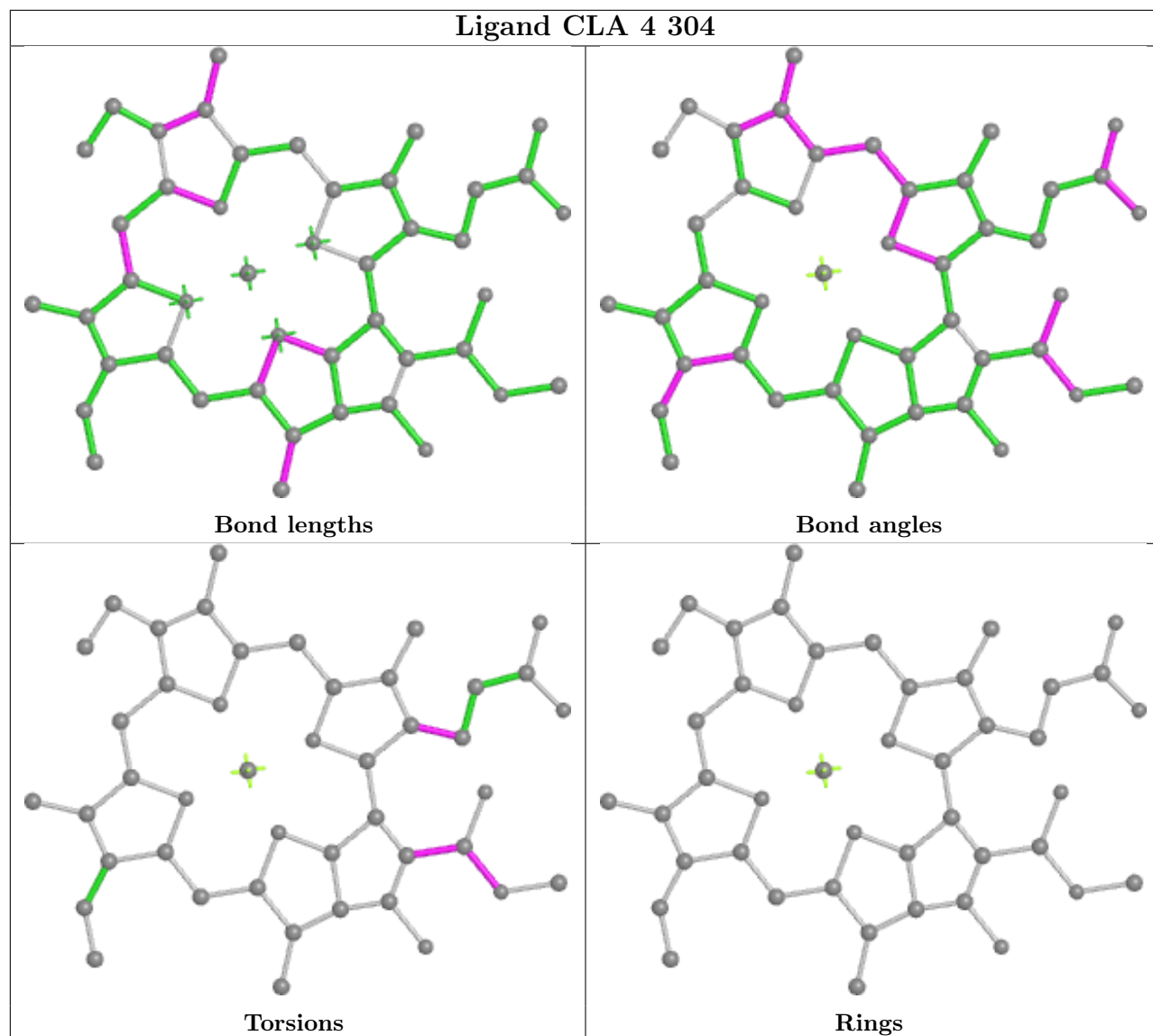


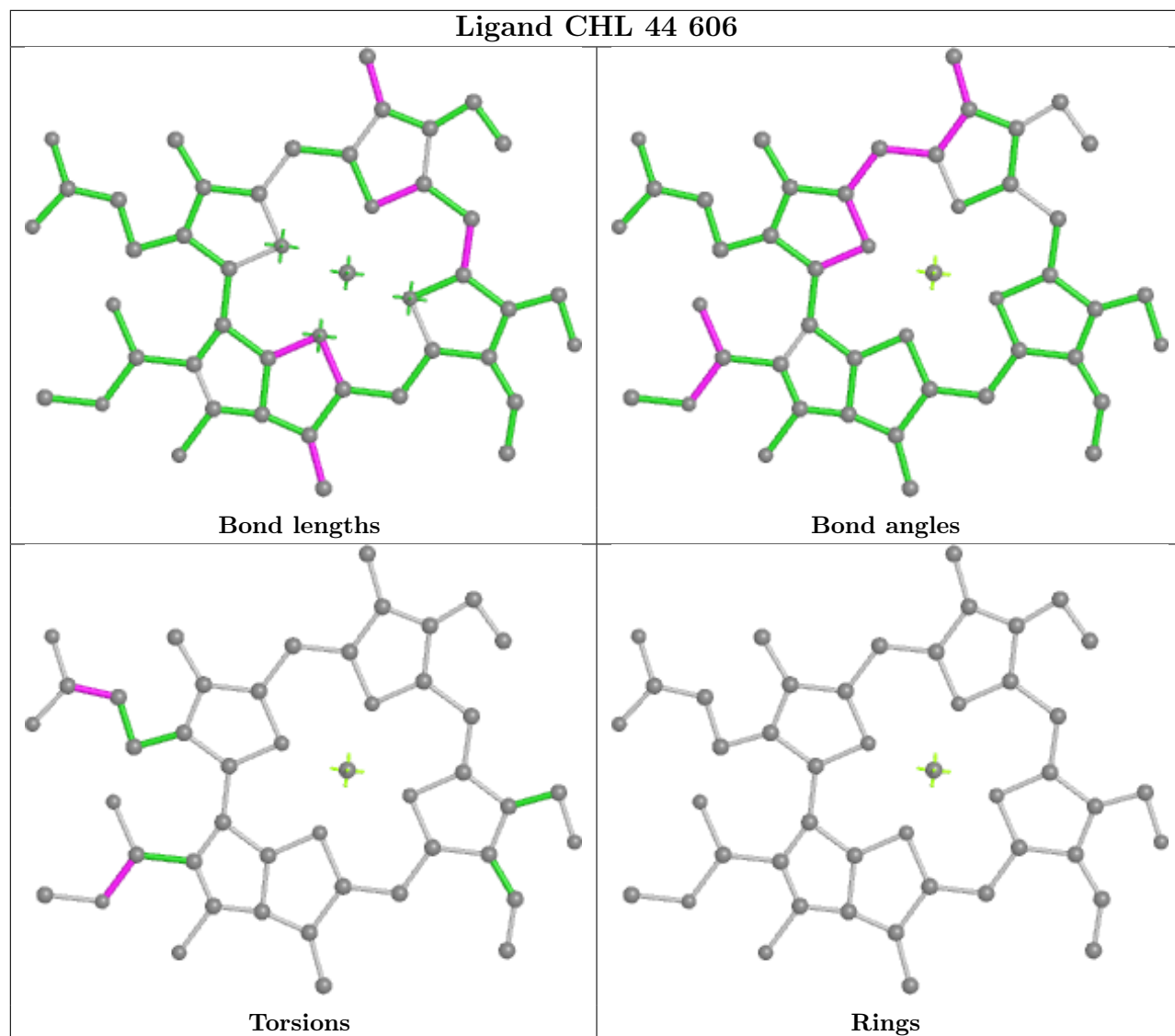


## Ligand CLA s 603



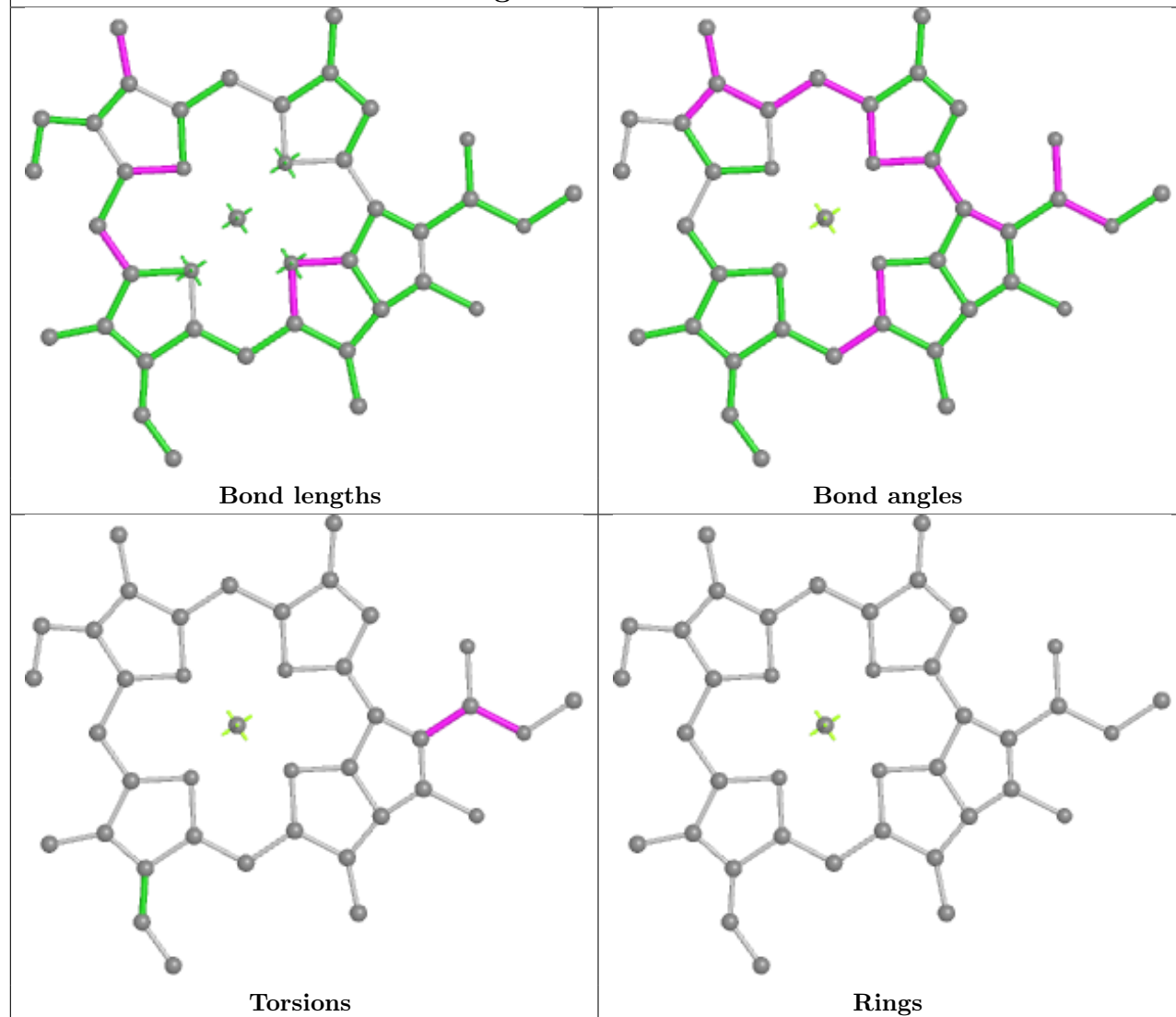
## Ligand CLA 4 304



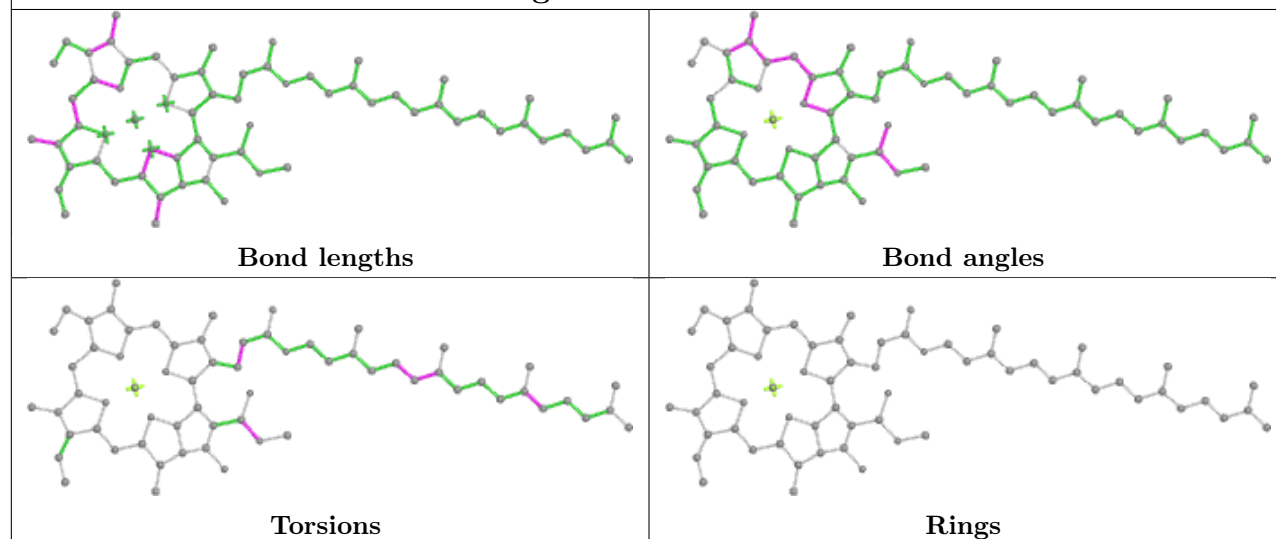


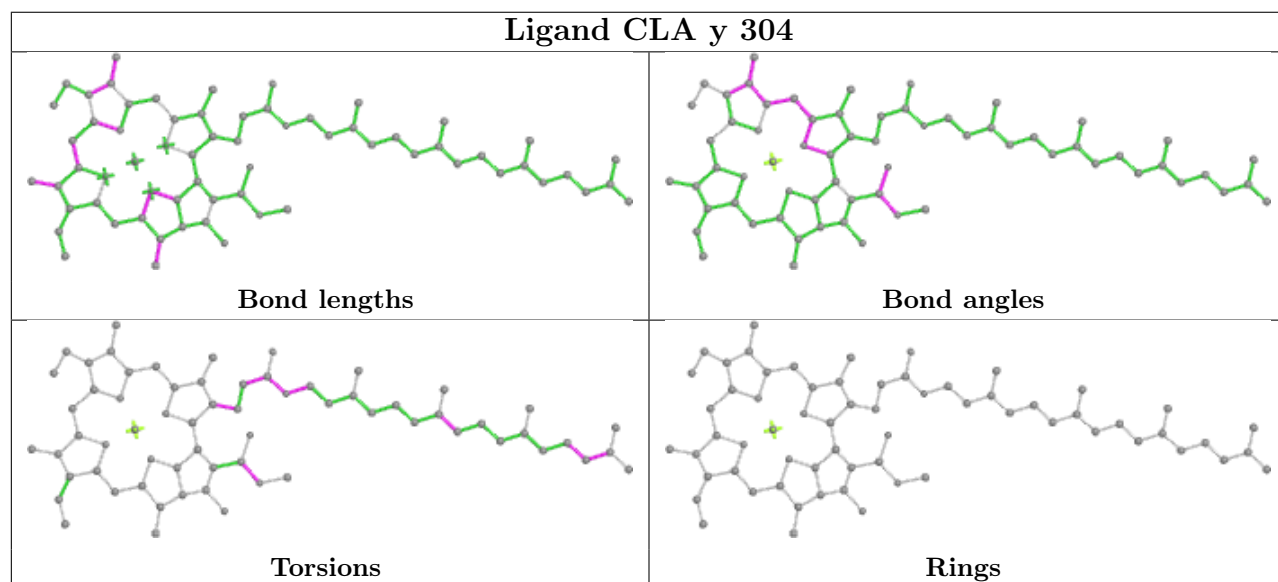
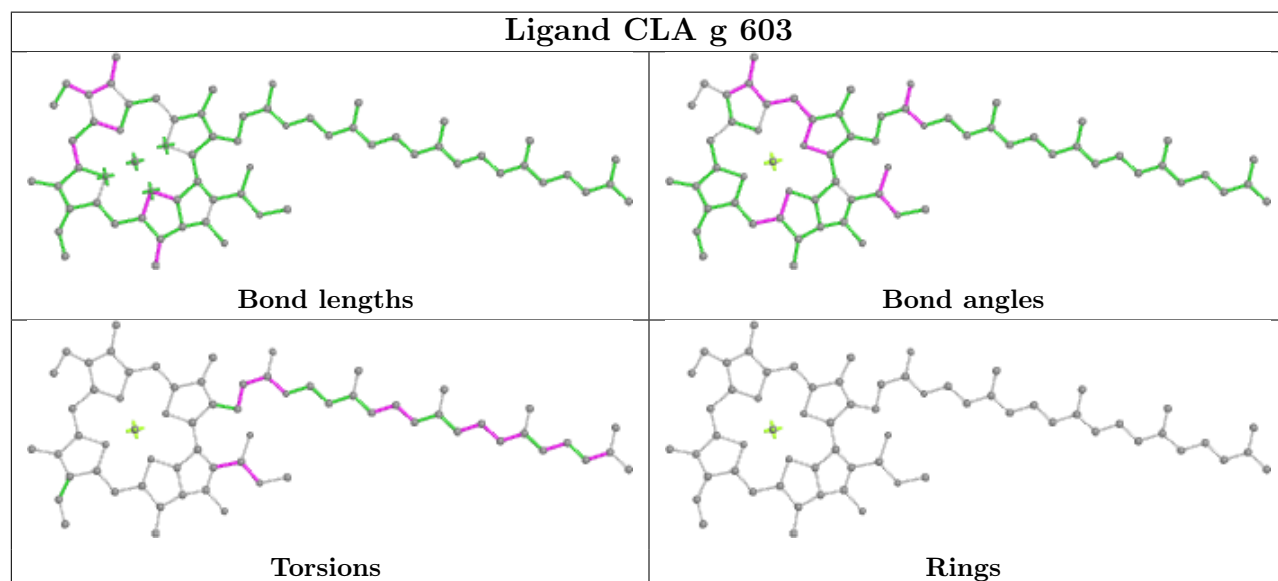
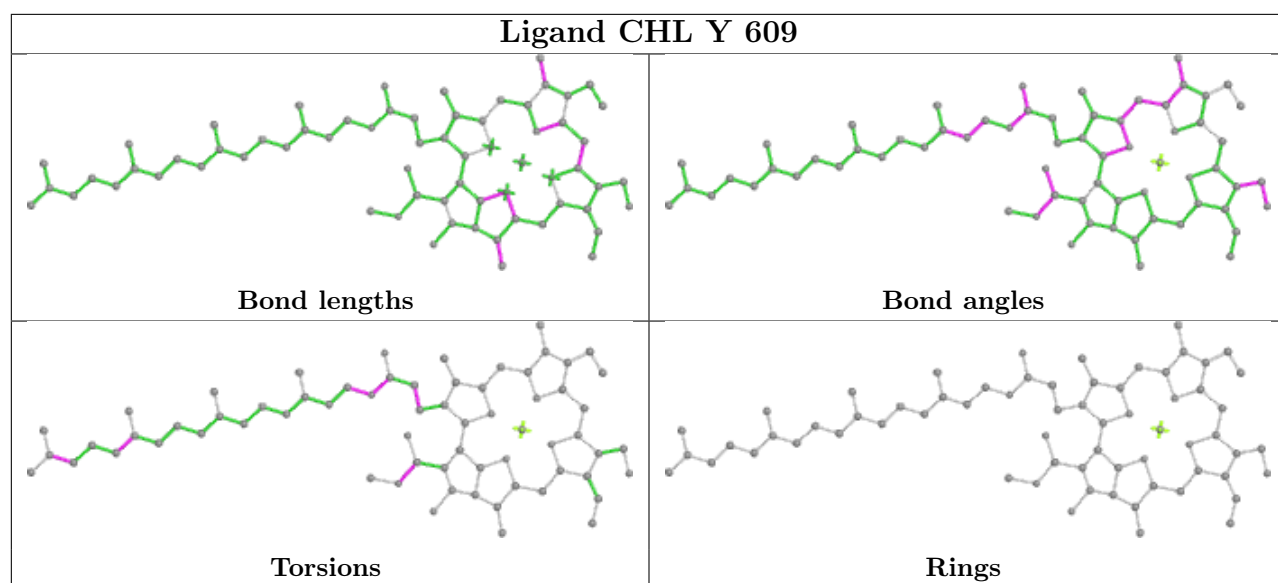


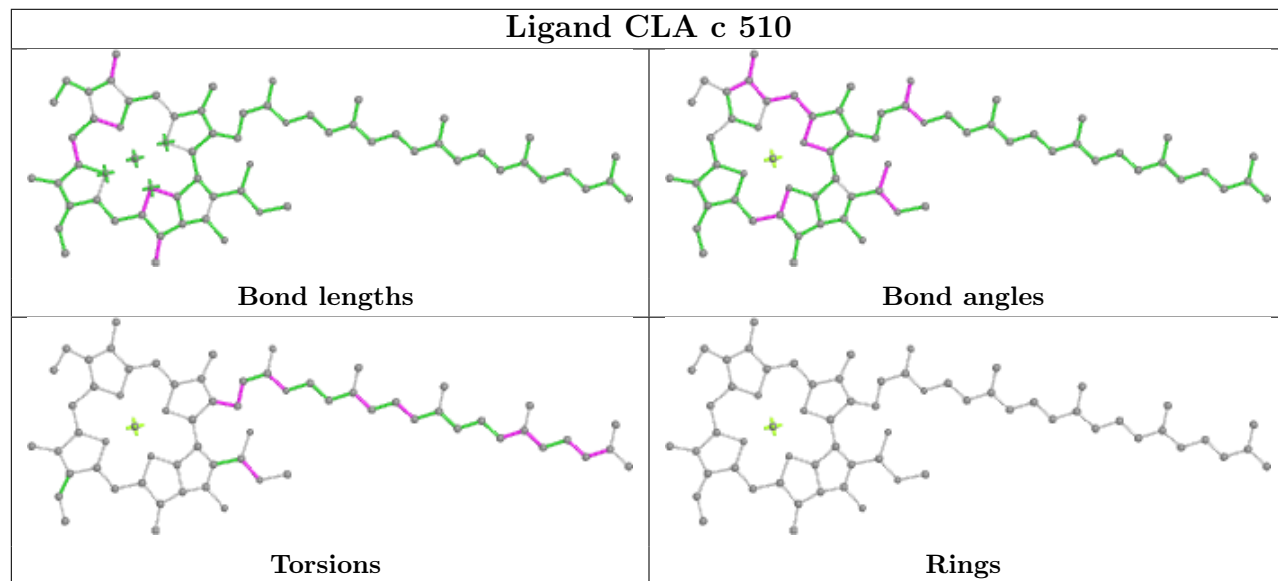
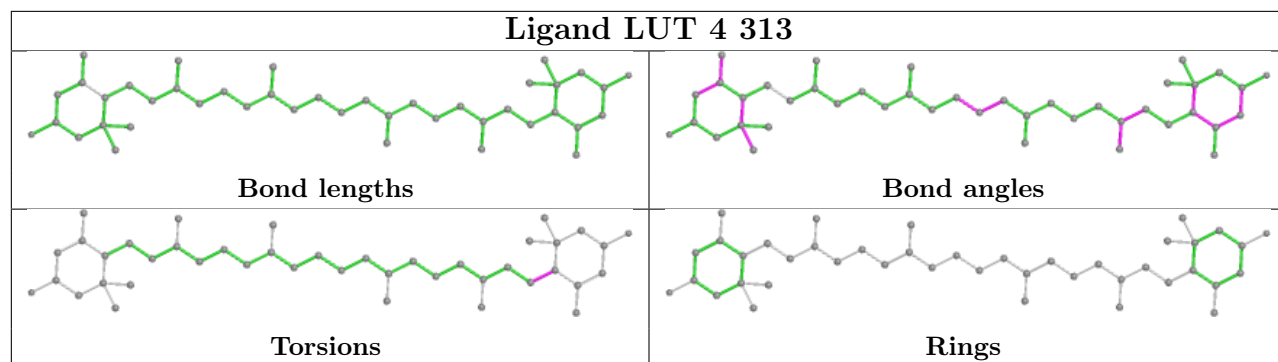
## Ligand CLA 2 611

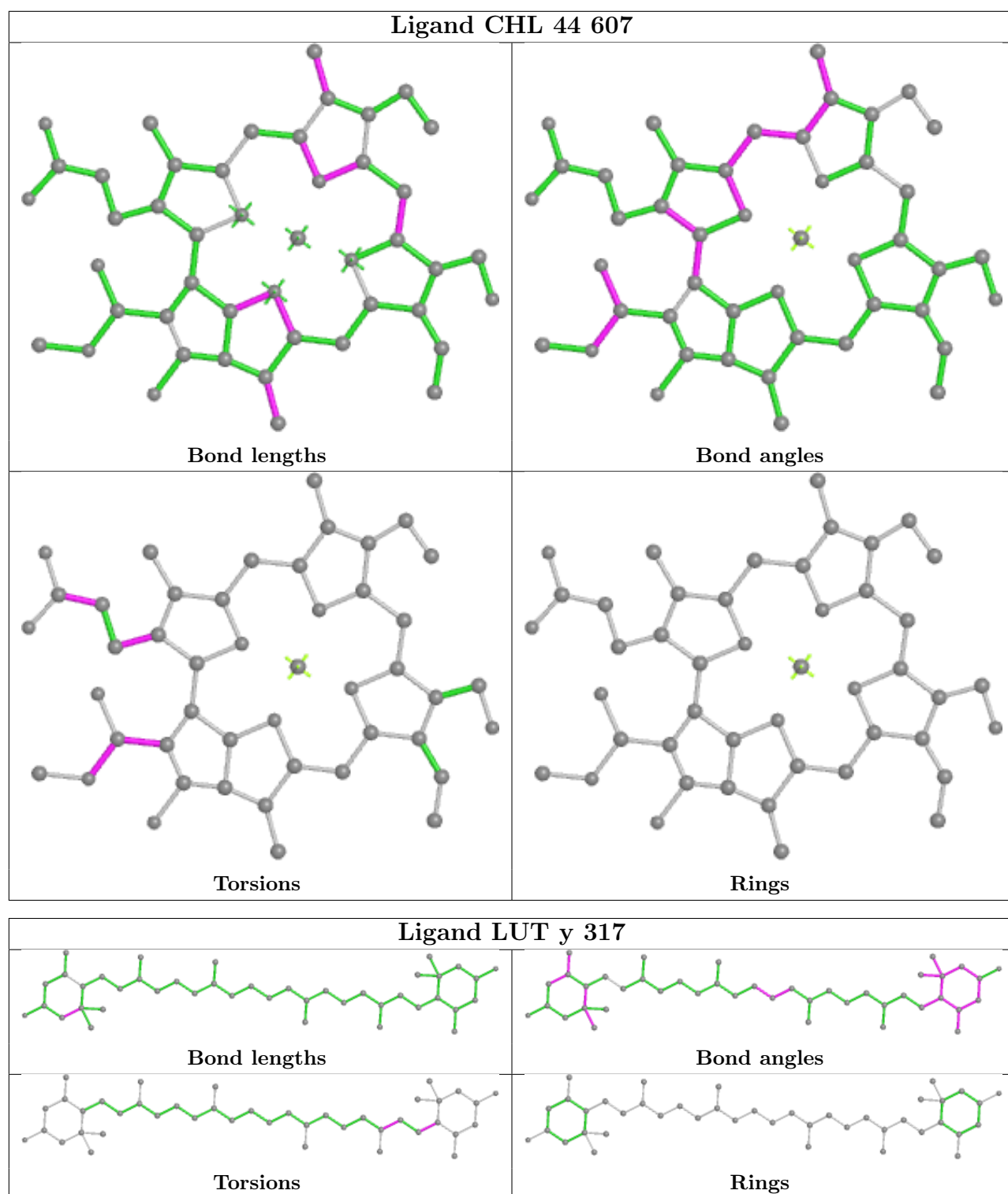


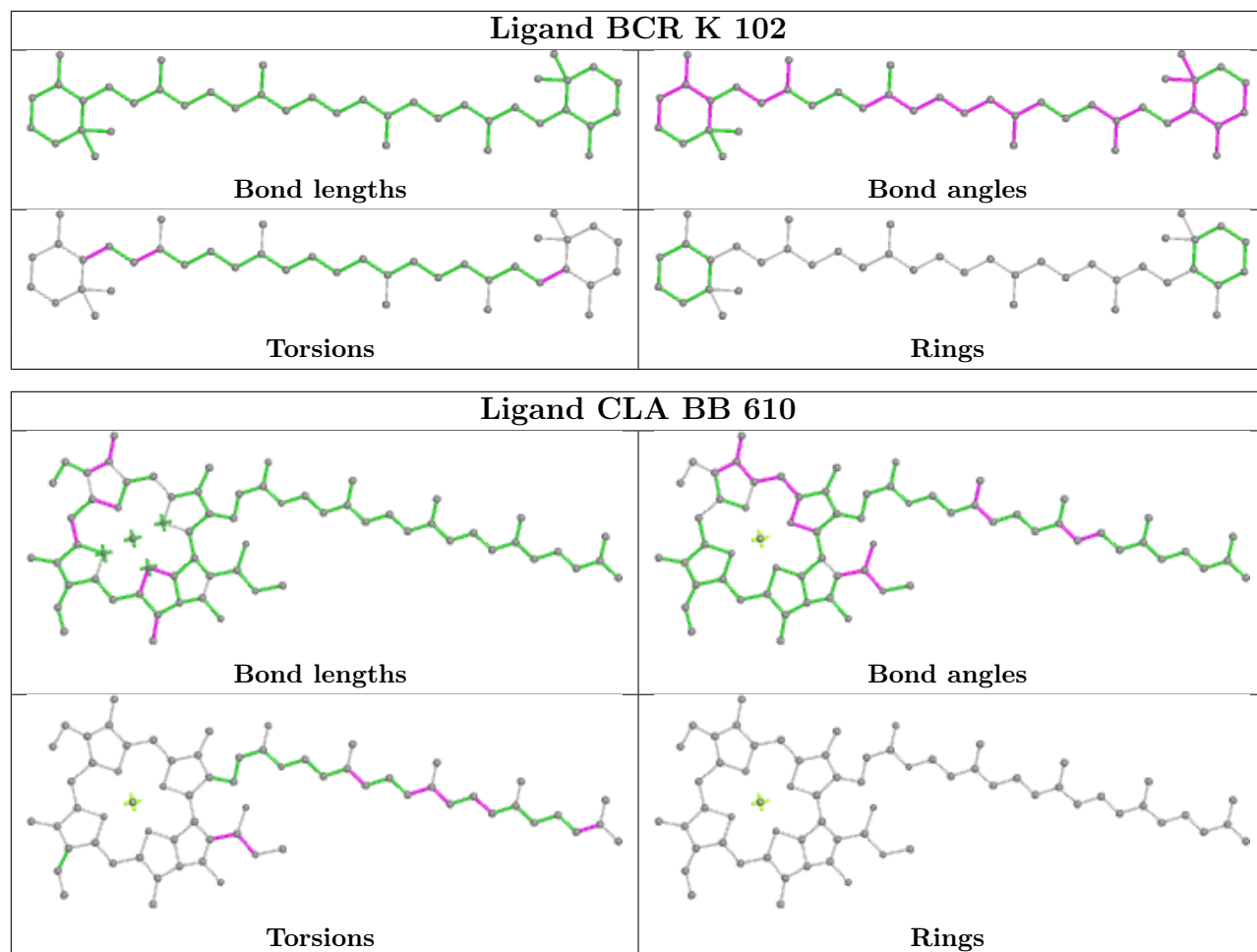
## Ligand CLA B 607

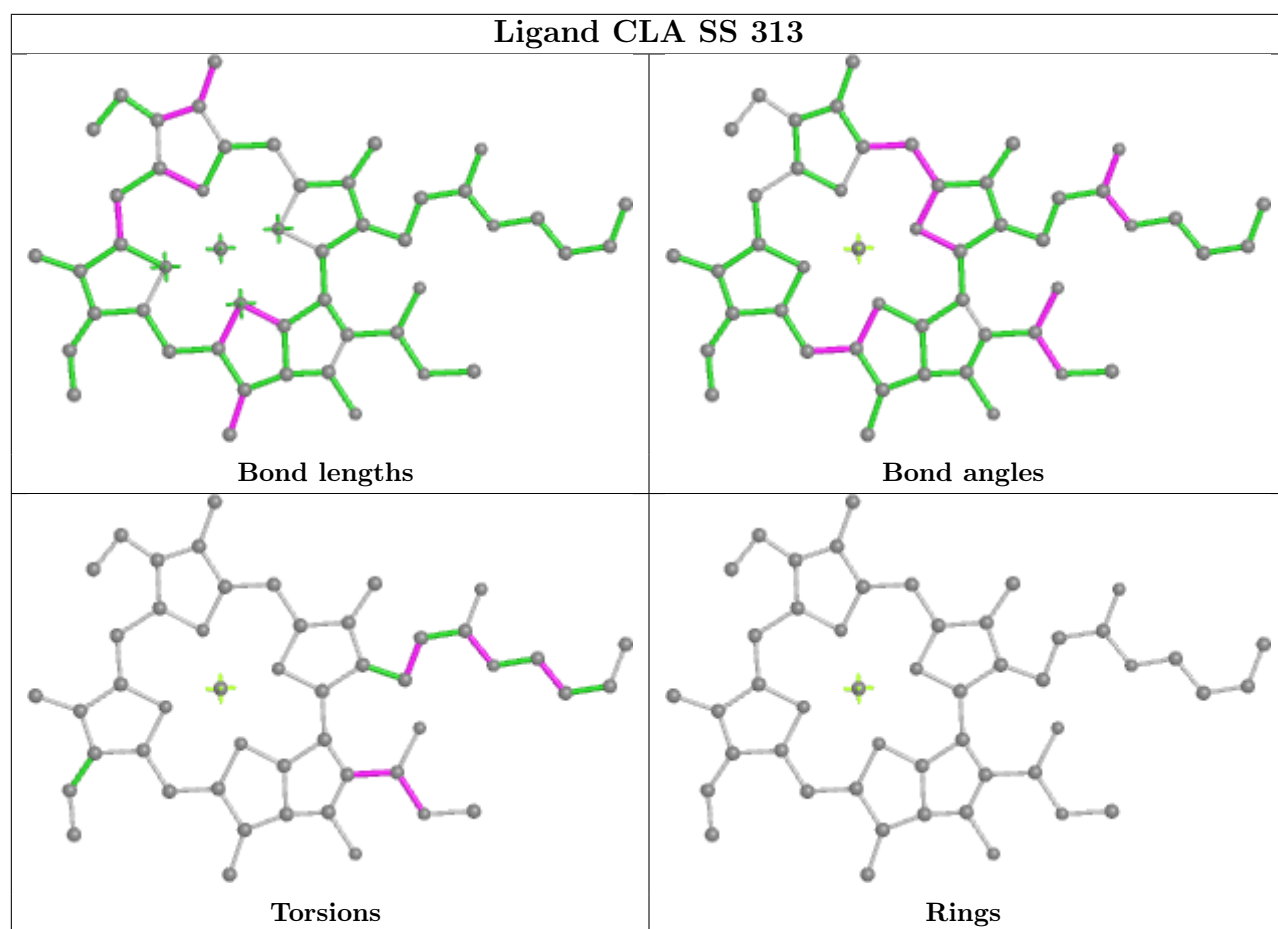




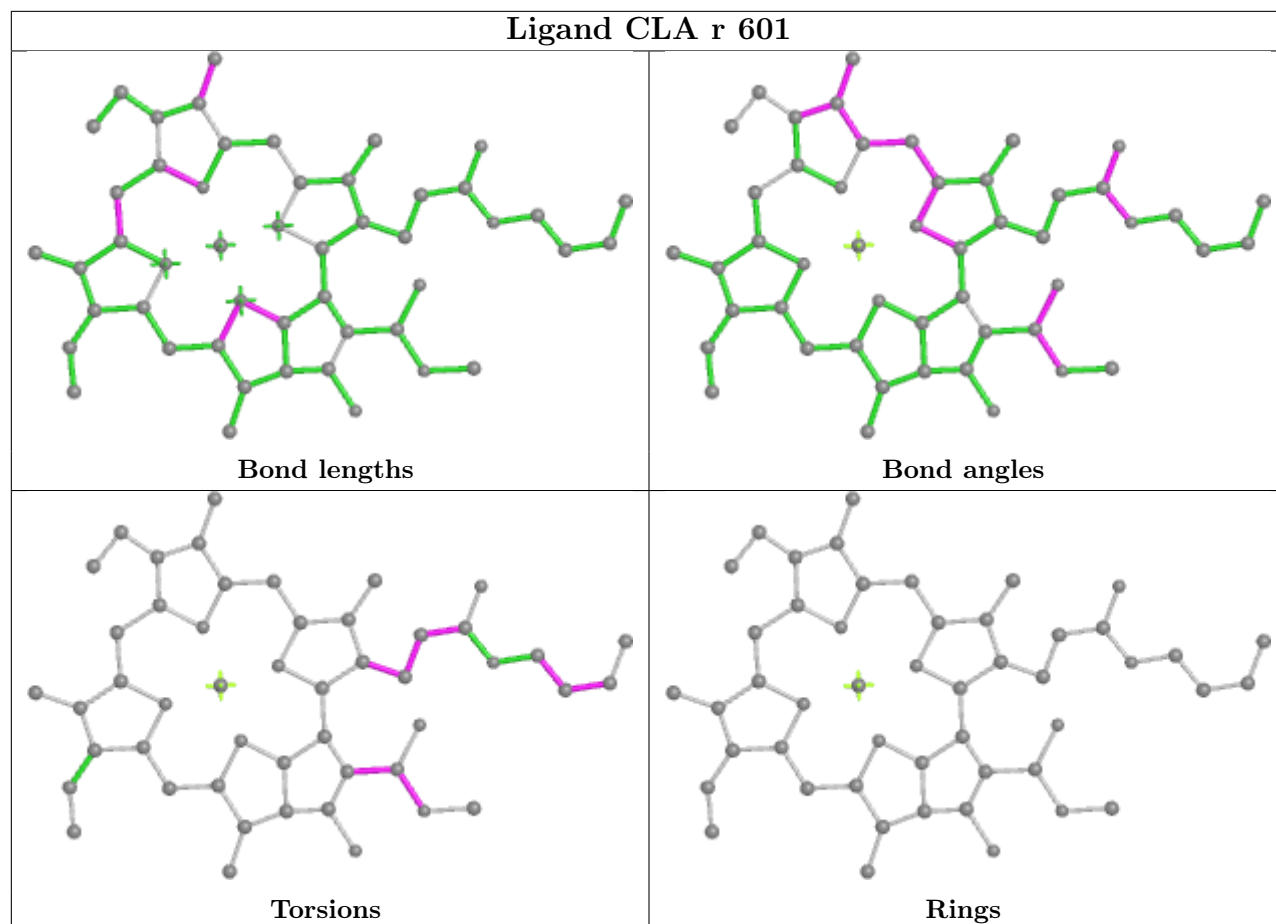


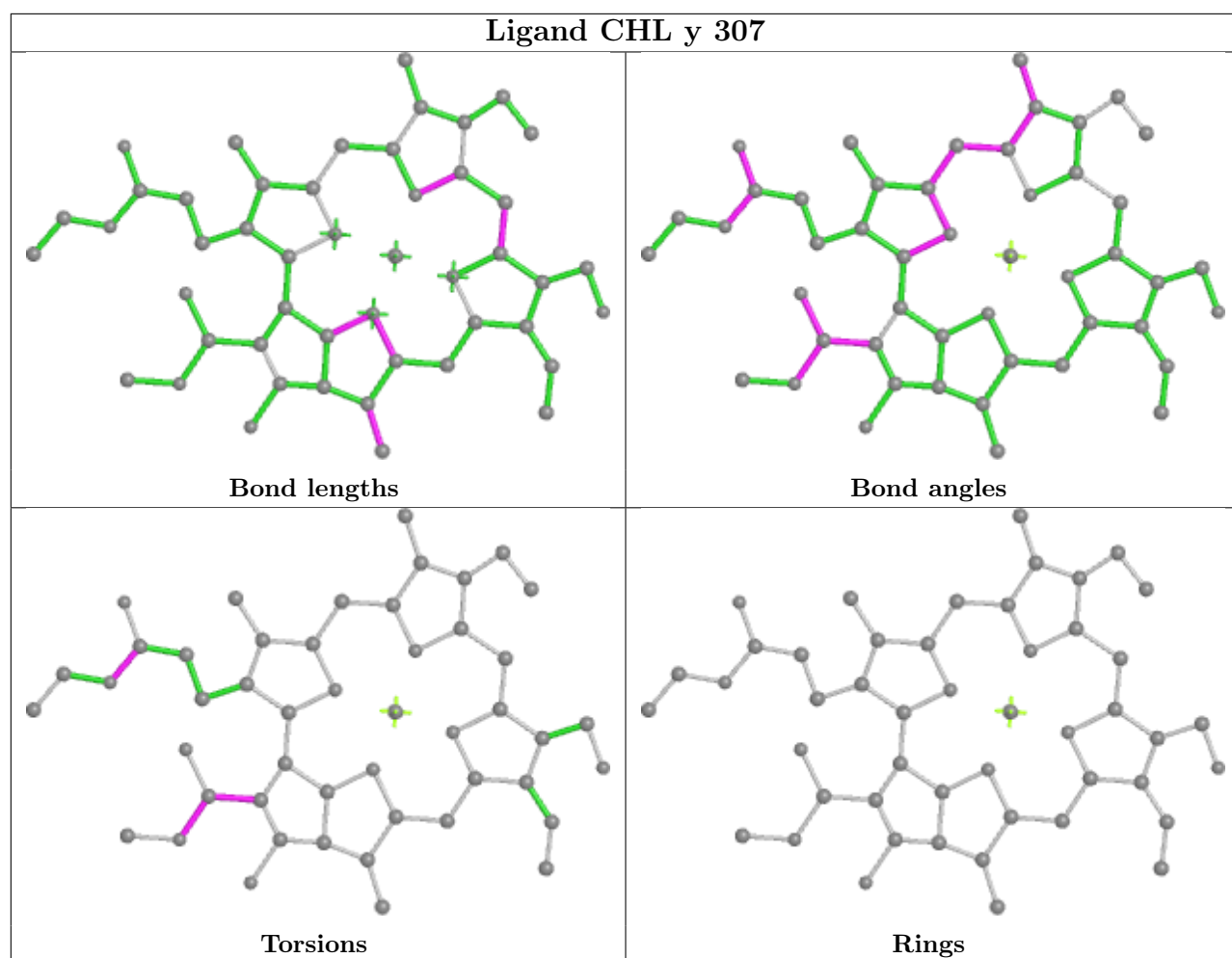




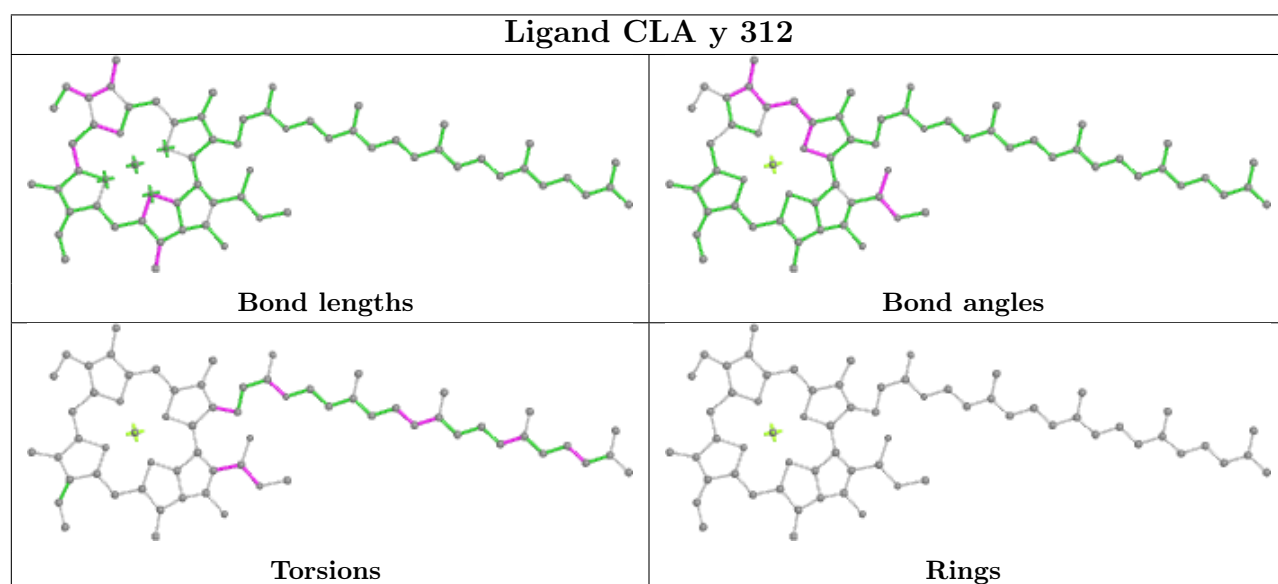
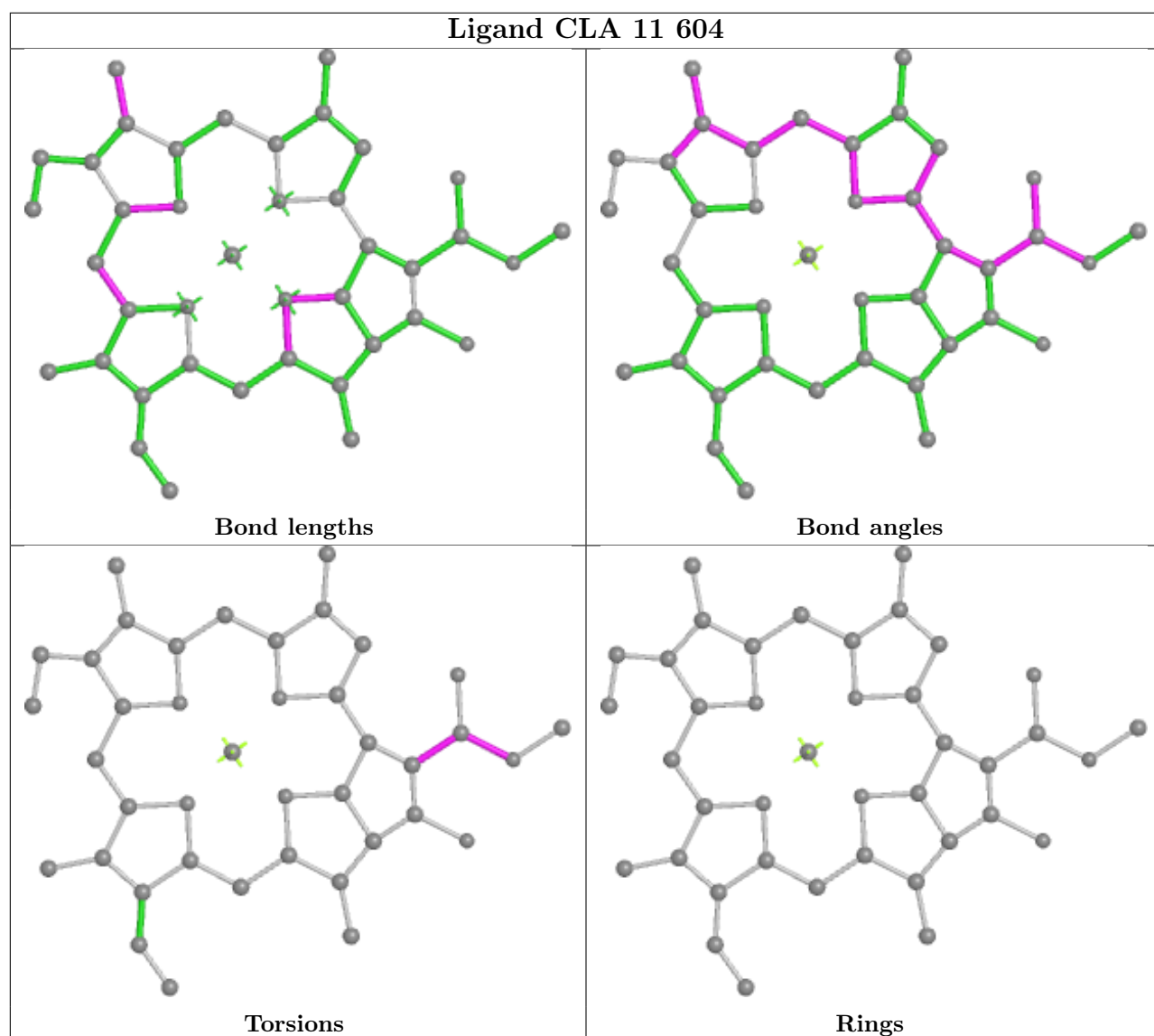


## Ligand CLA r 601

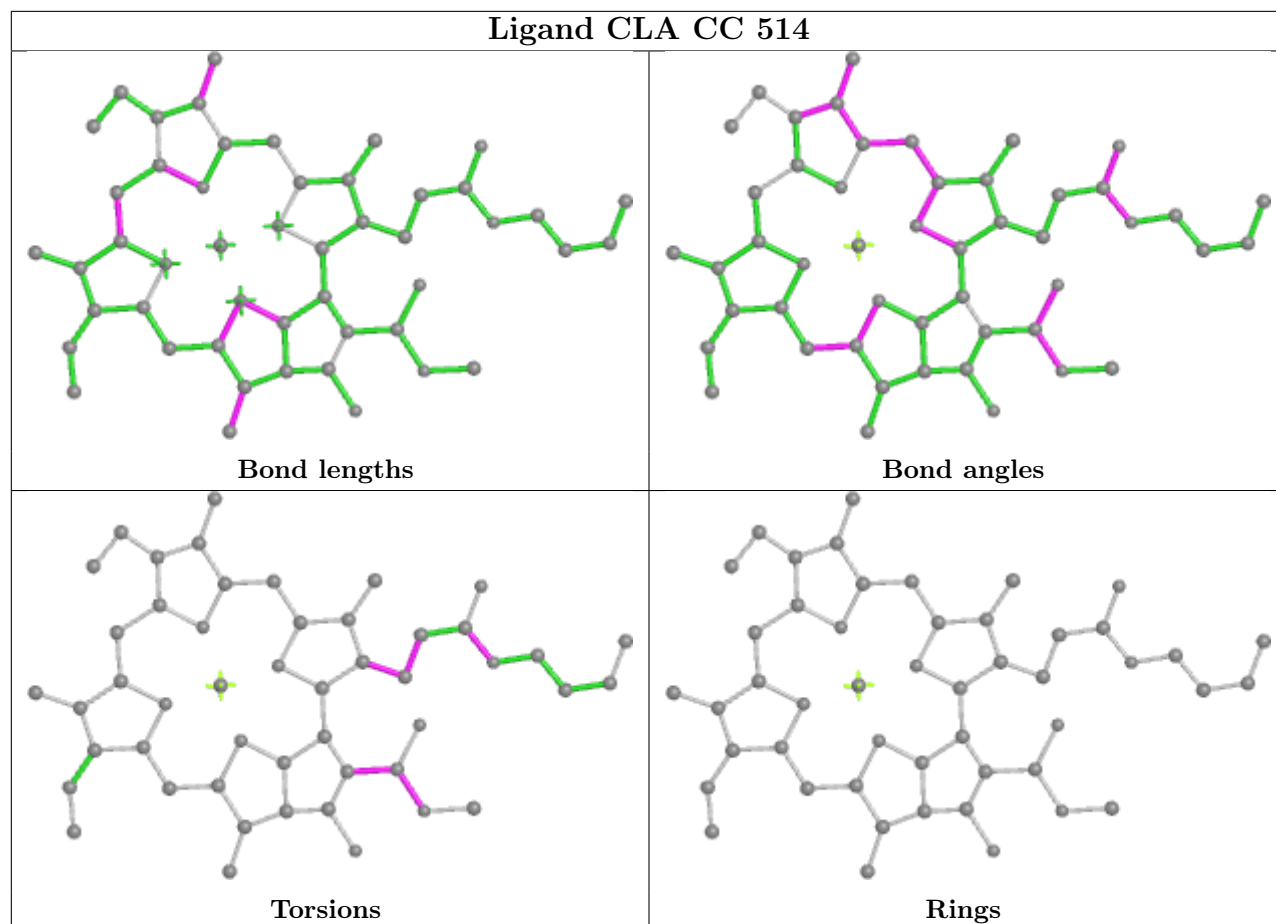




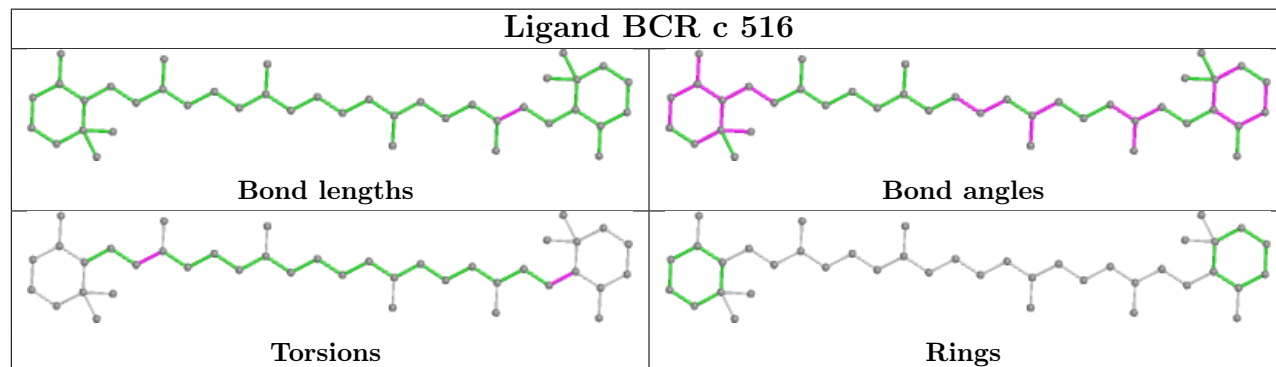




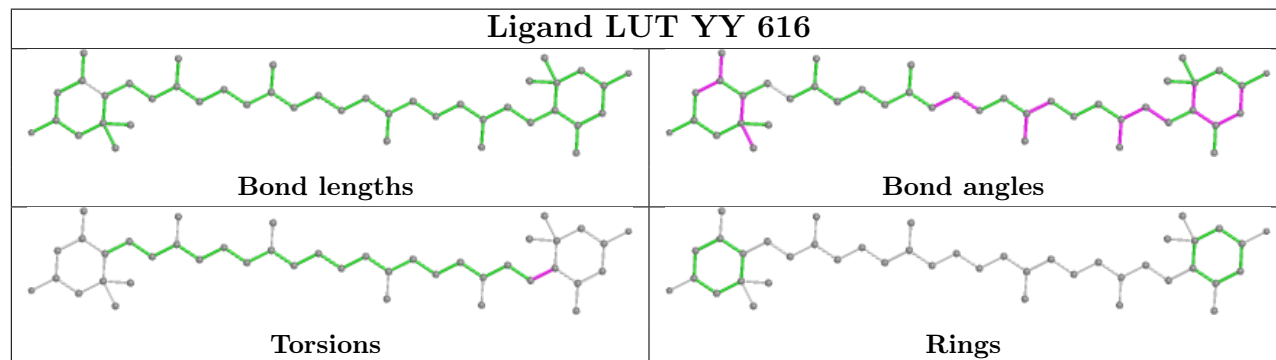
## Ligand CLA CC 514

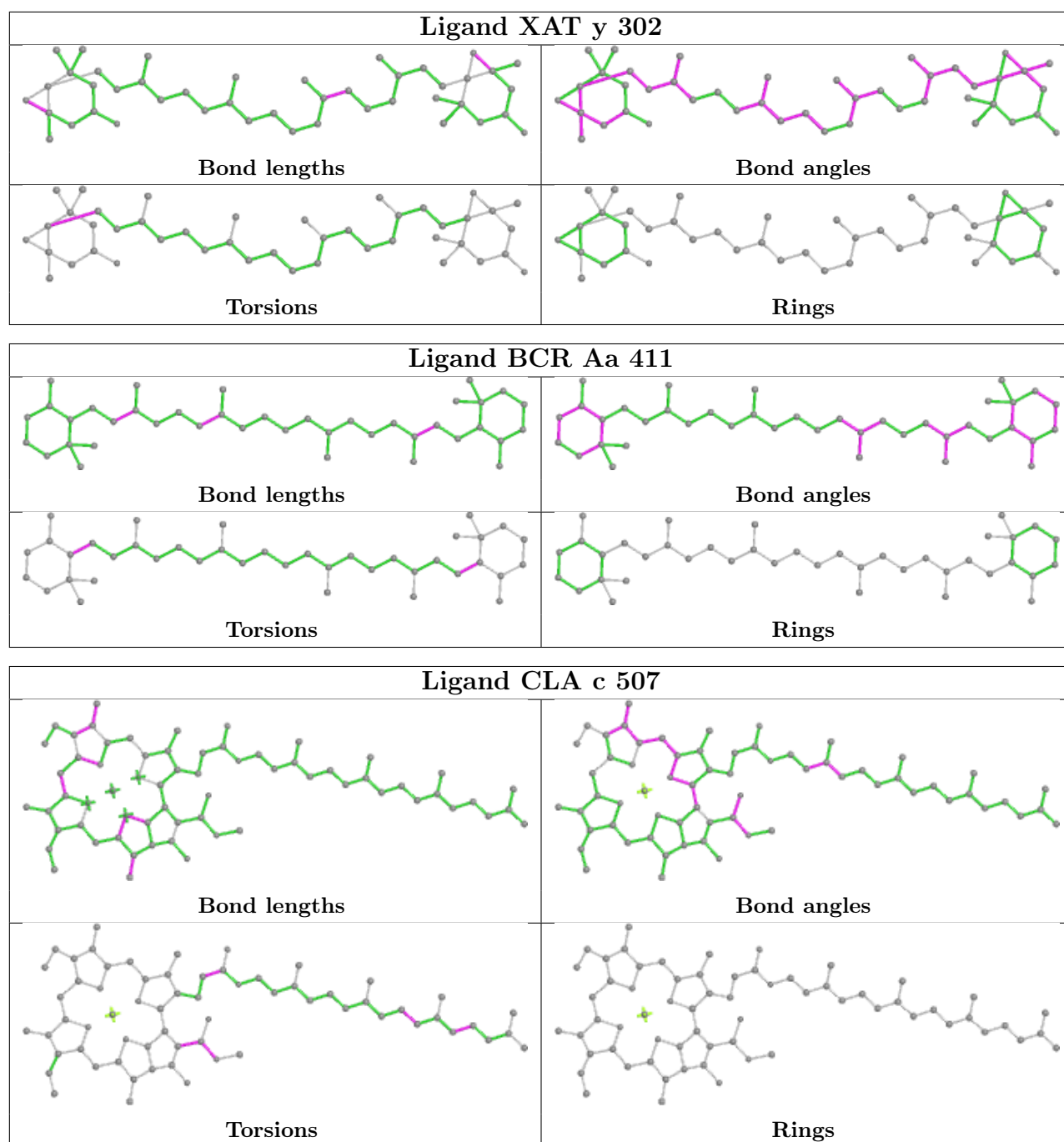


## Ligand BCR c 516

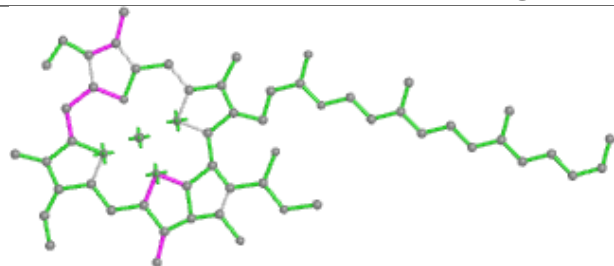


## Ligand LUT YY 616

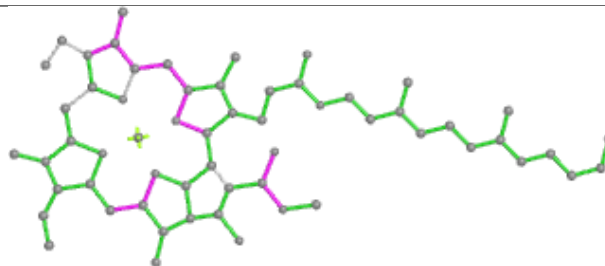




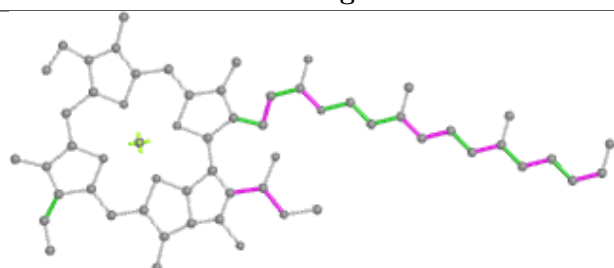
## Ligand CLA Y 613



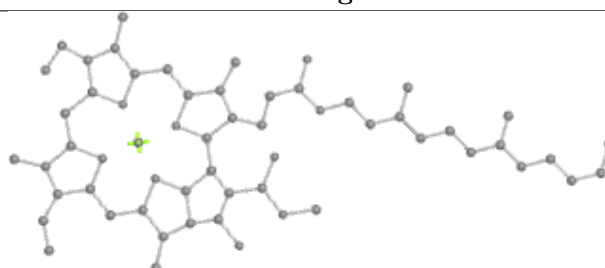
Bond lengths



Bond angles

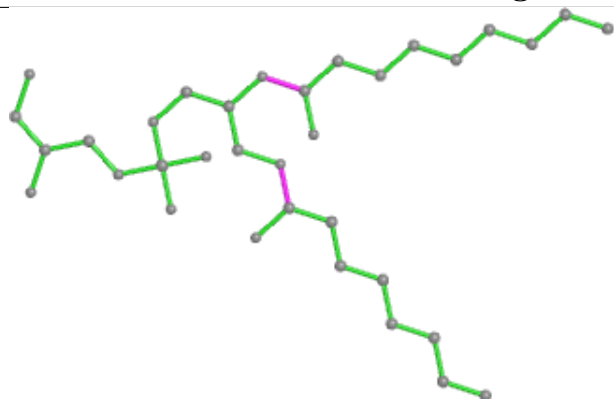


Torsions

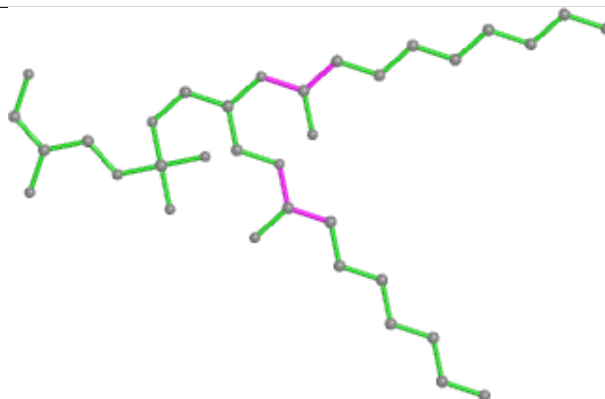


Rings

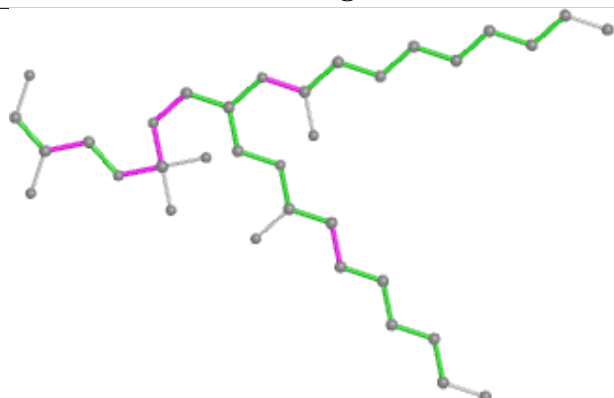
## Ligand LHG K 101



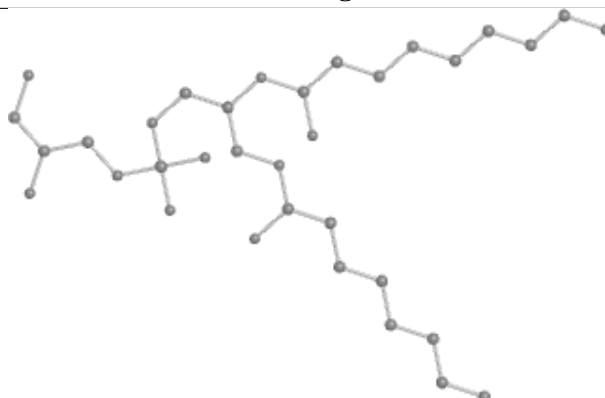
Bond lengths



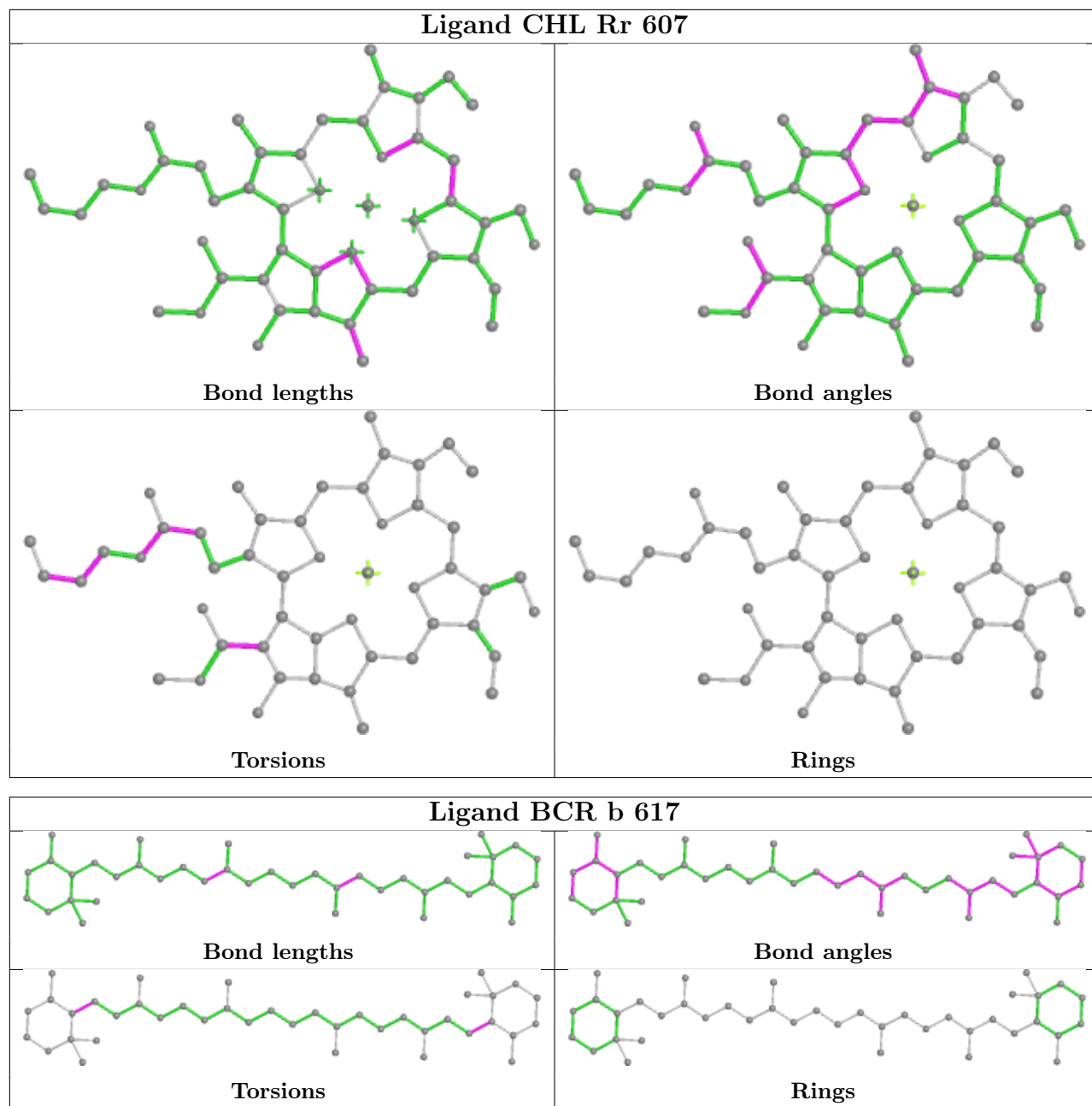
Bond angles



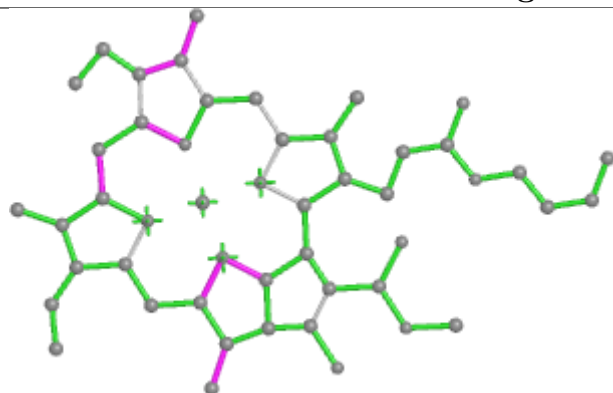
Torsions



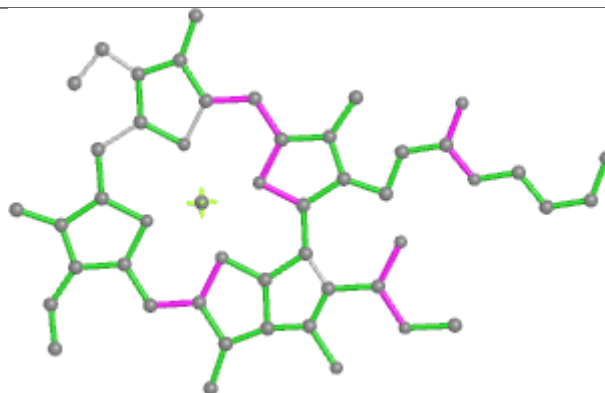
Rings



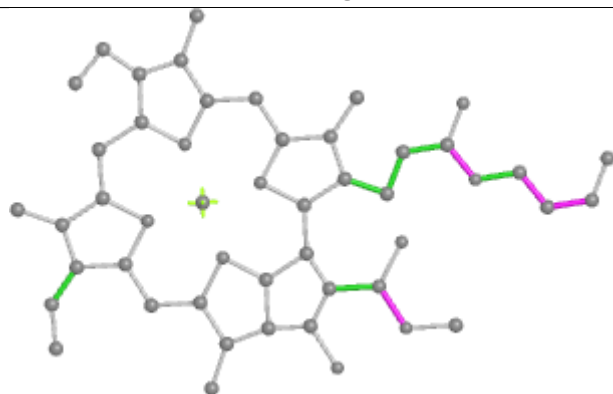
## Ligand CLA n 604



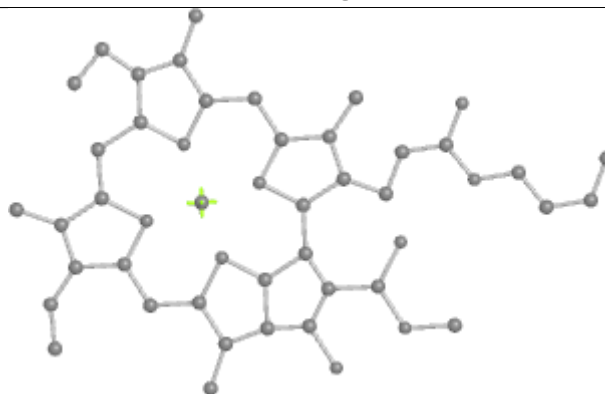
Bond lengths



Bond angles

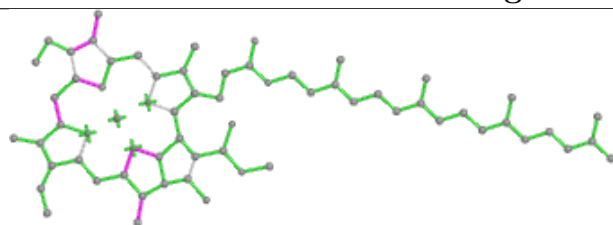


Torsions

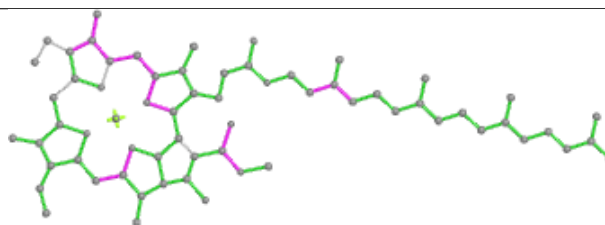


Rings

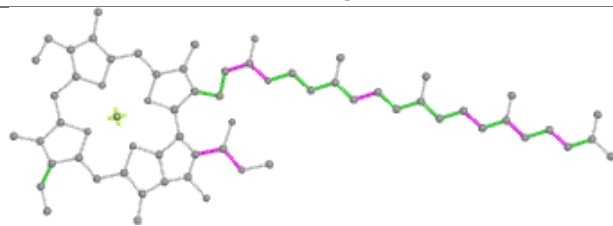
## Ligand CLA Bb 605



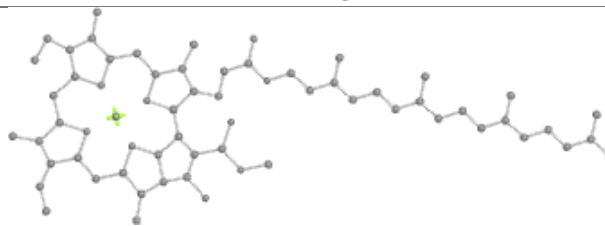
Bond lengths



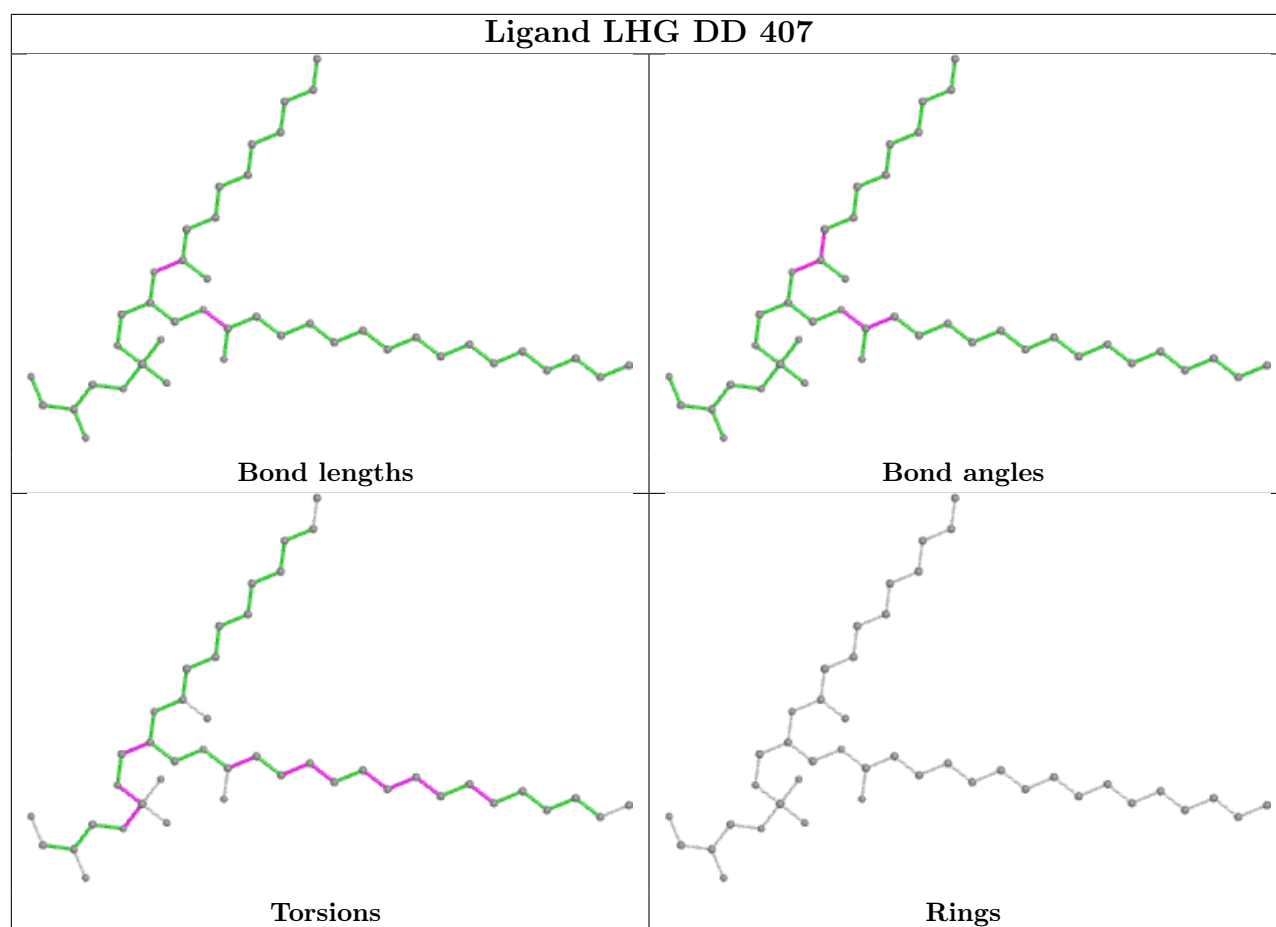
Bond angles

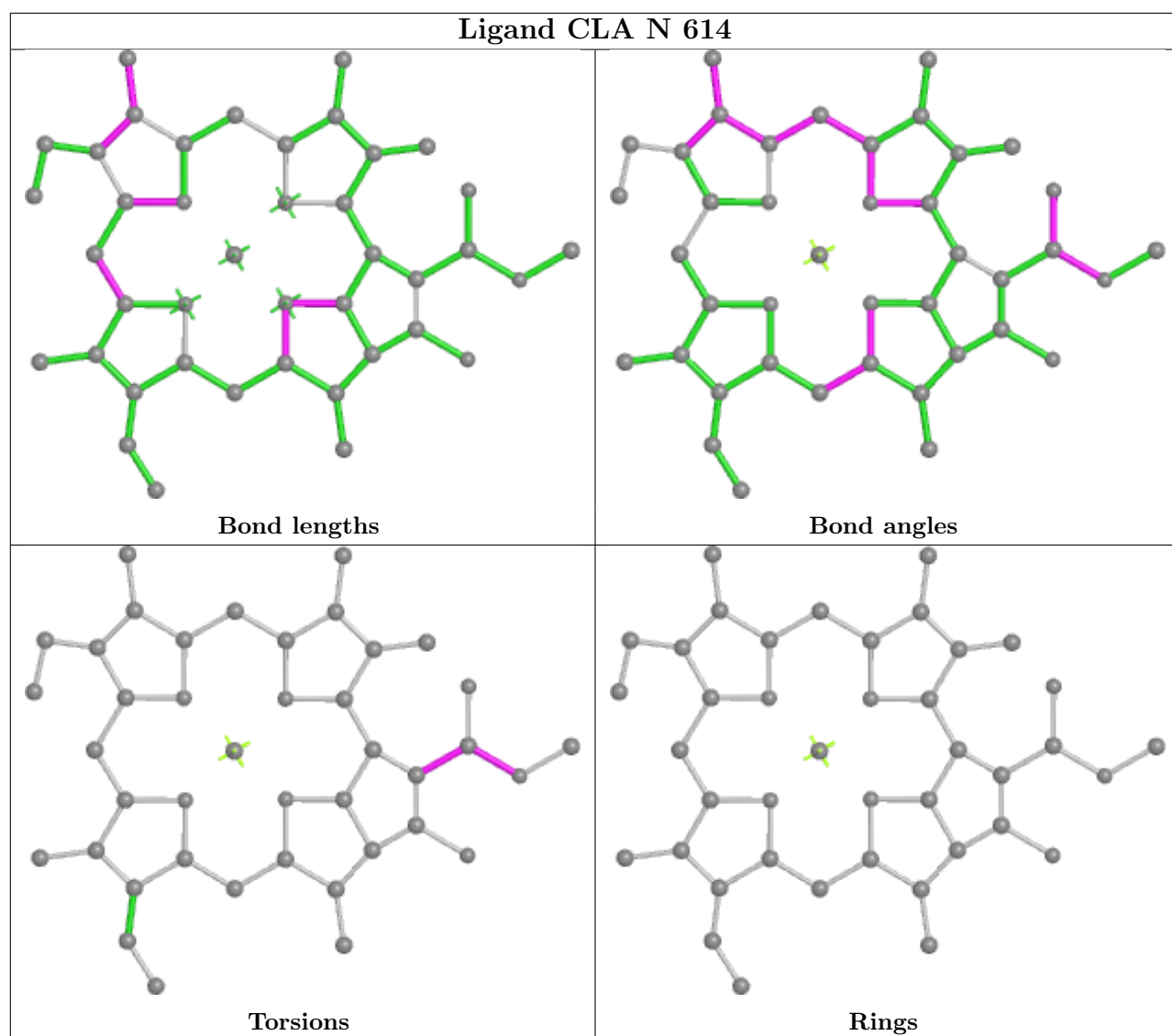


Torsions

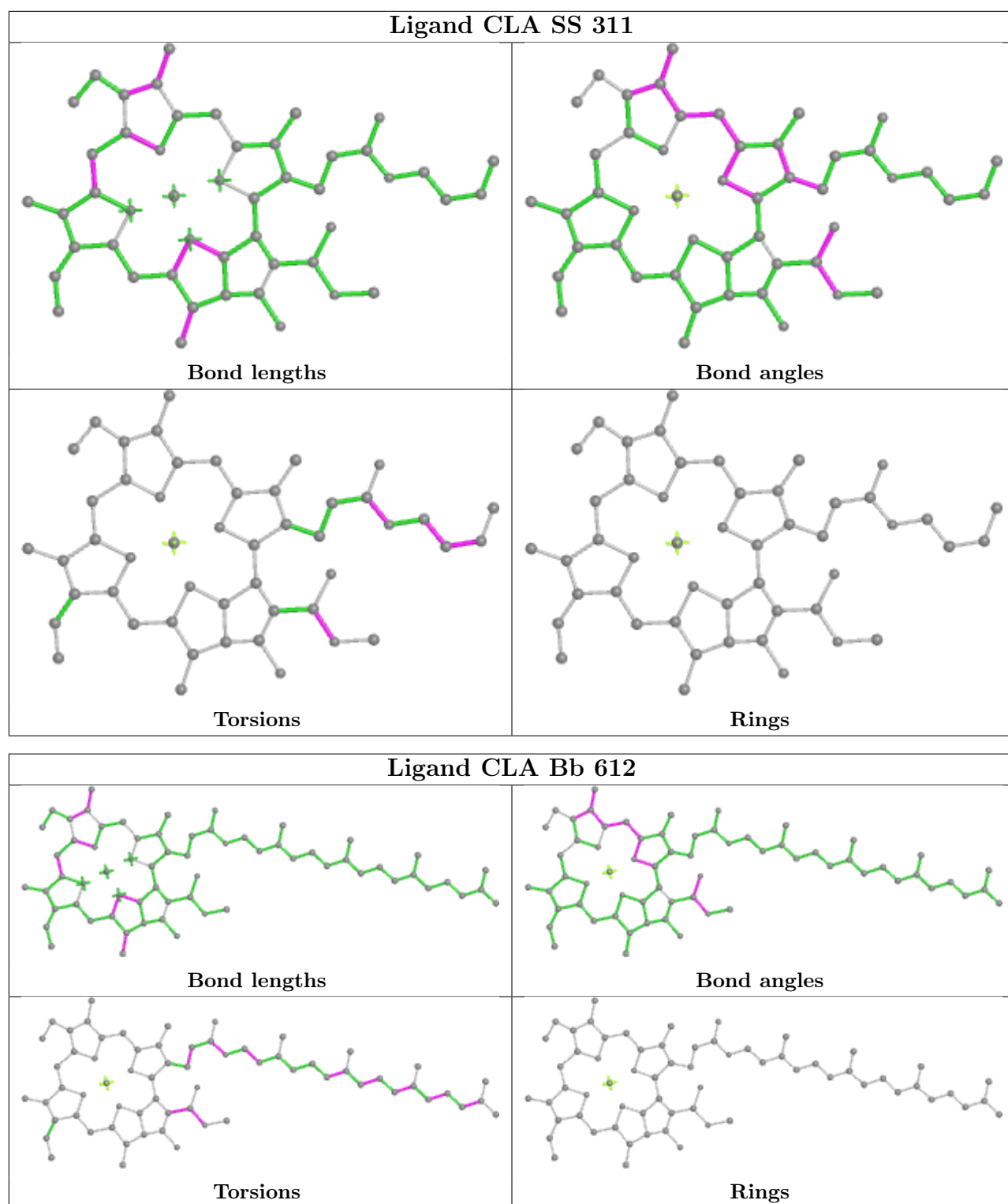


Rings

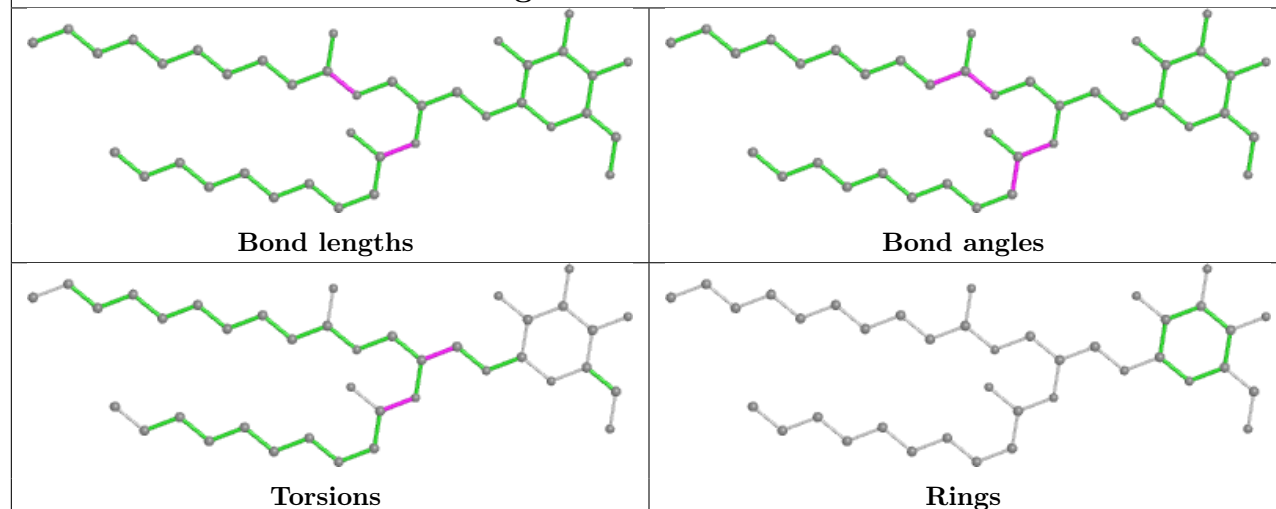








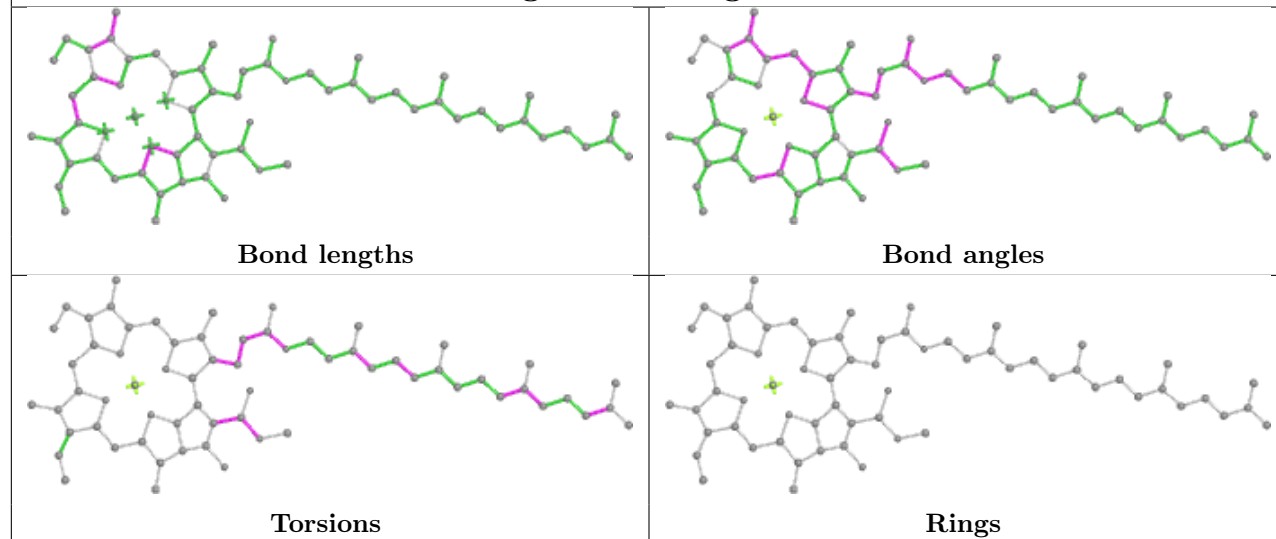
## Ligand LMG CC 520

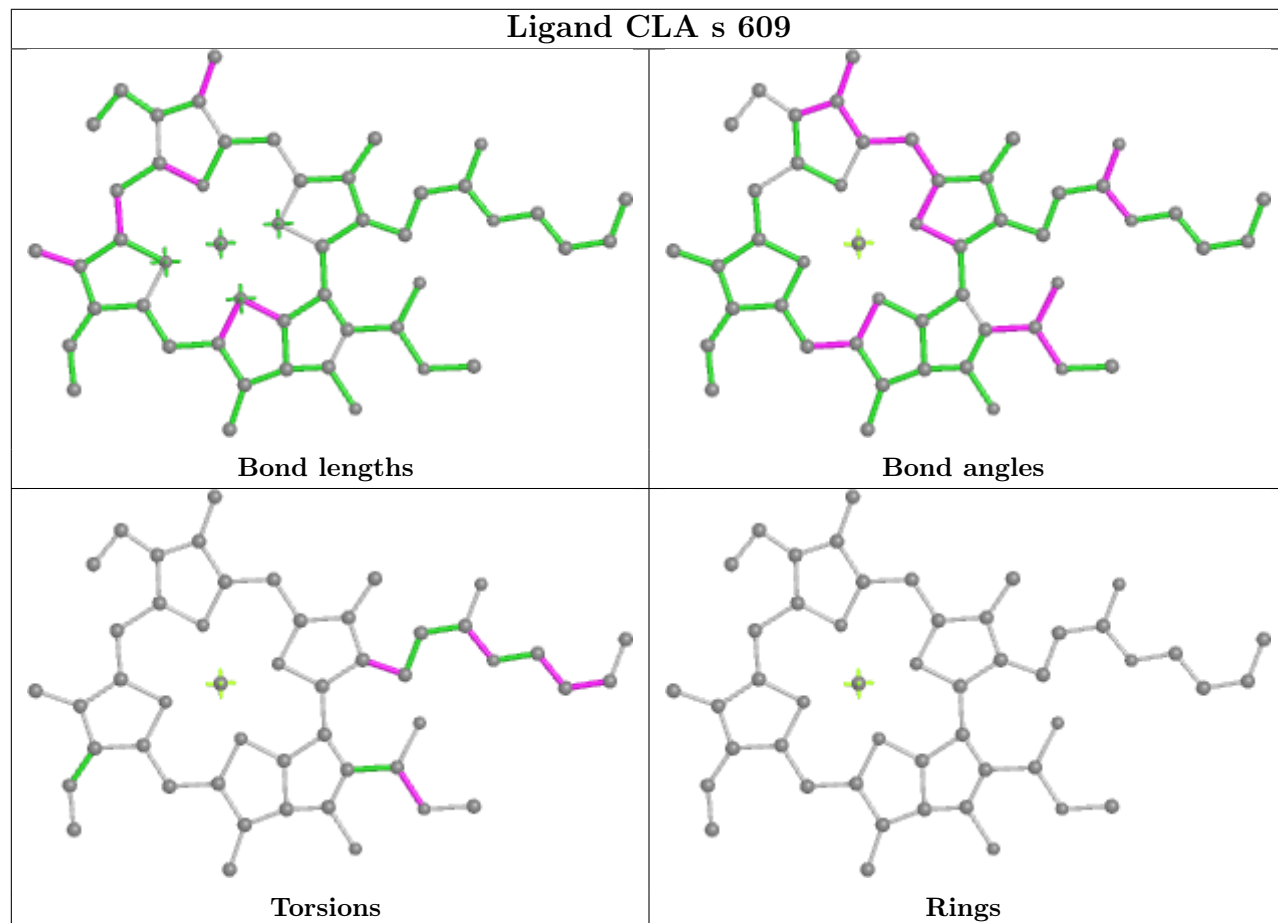
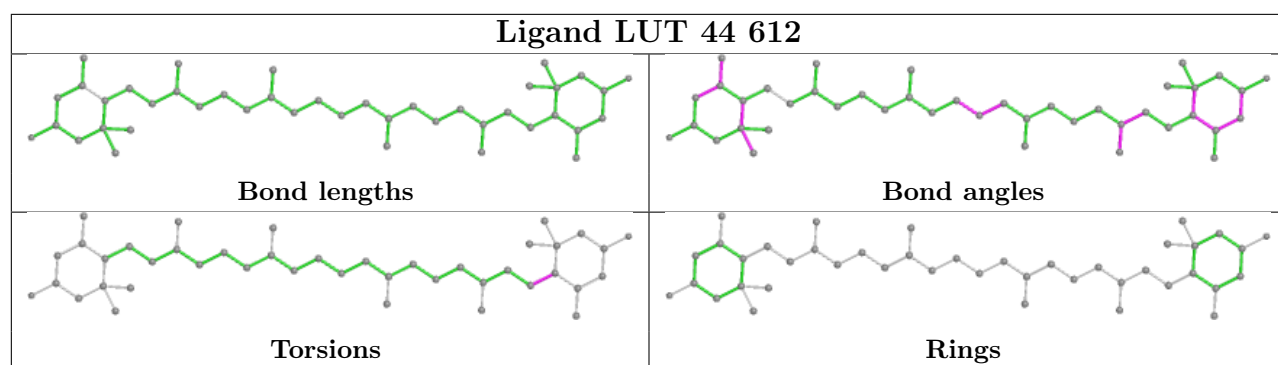


## Ligand LUT y 318

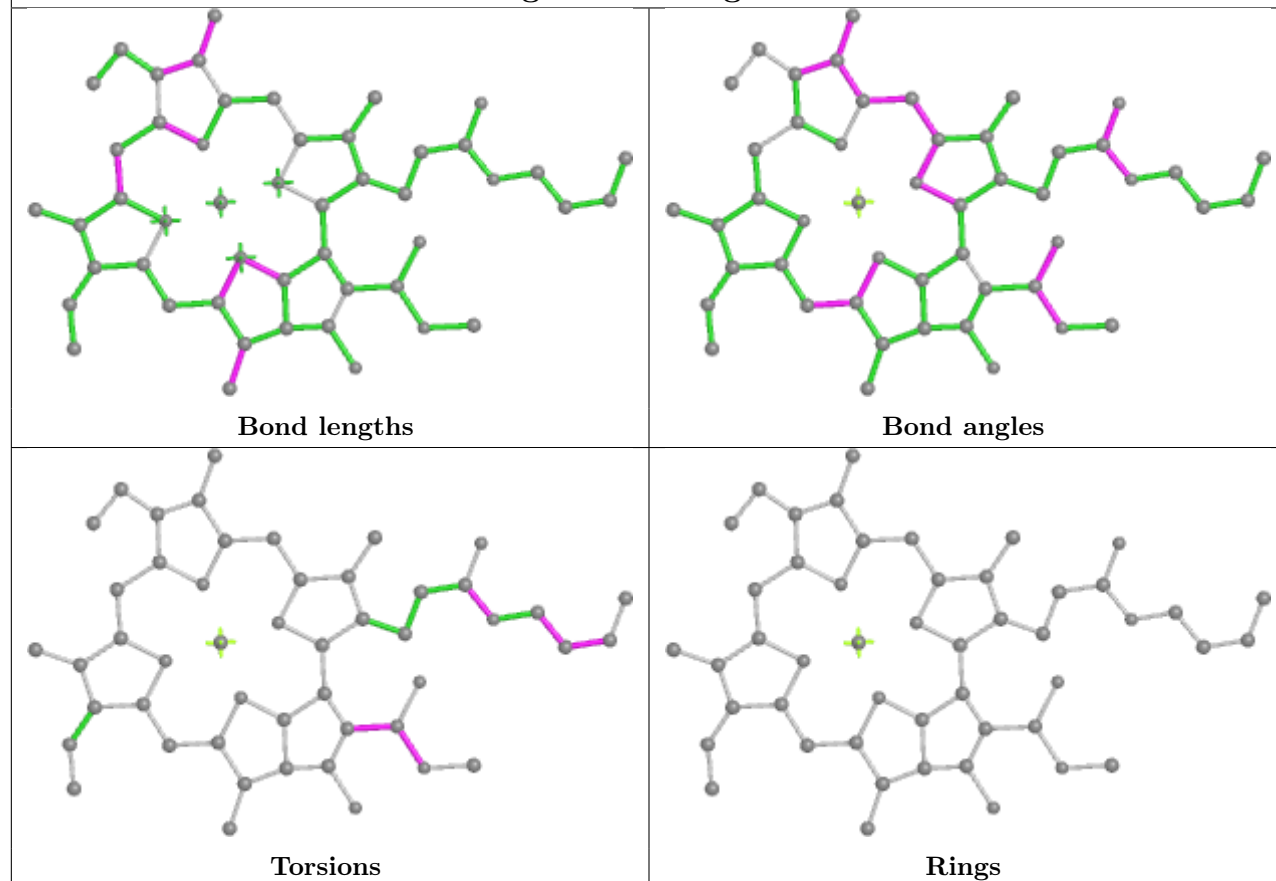


## Ligand CLA Gg 312

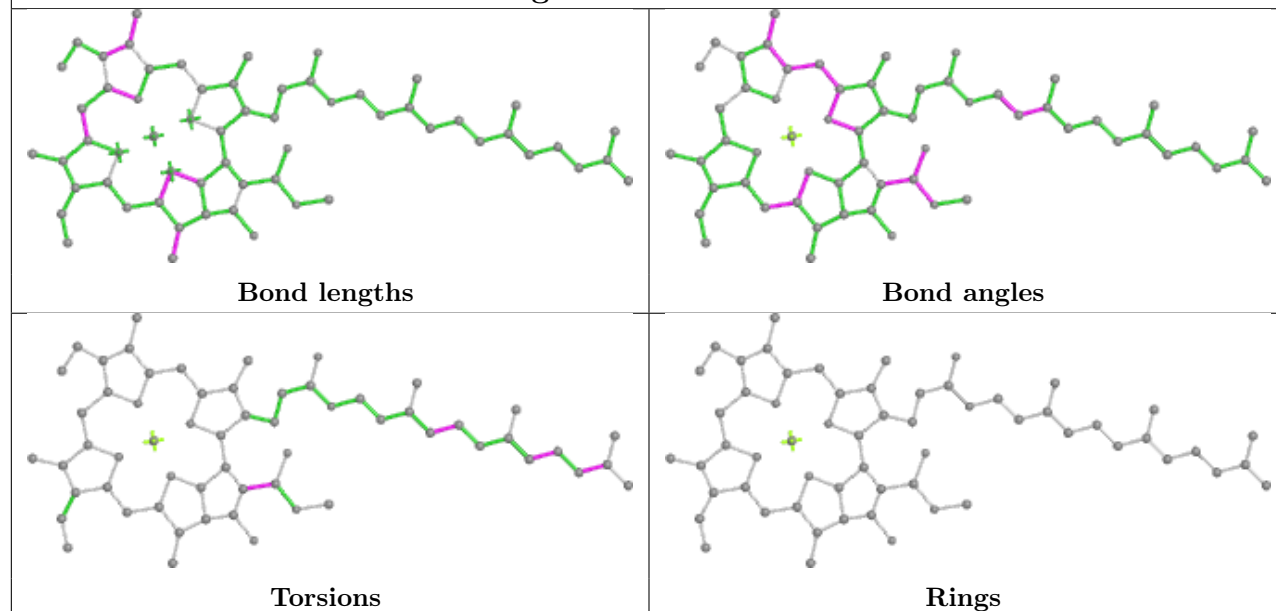




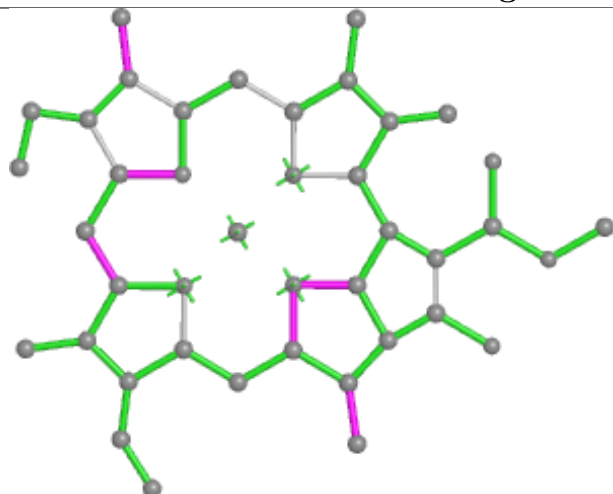
## Ligand CLA Gg 315



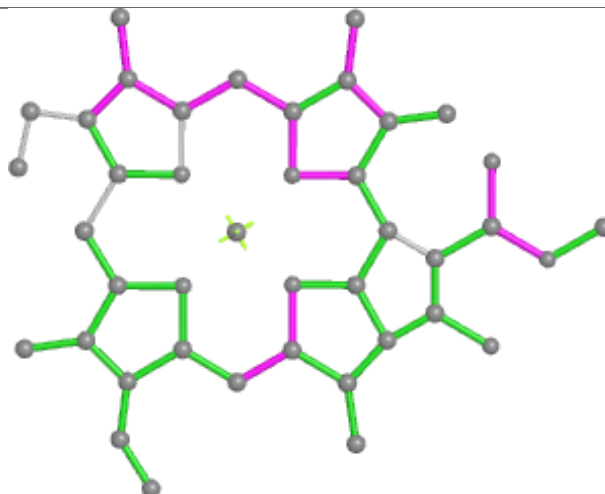
## Ligand CLA A 408



## Ligand CLA NN 604



Bond lengths



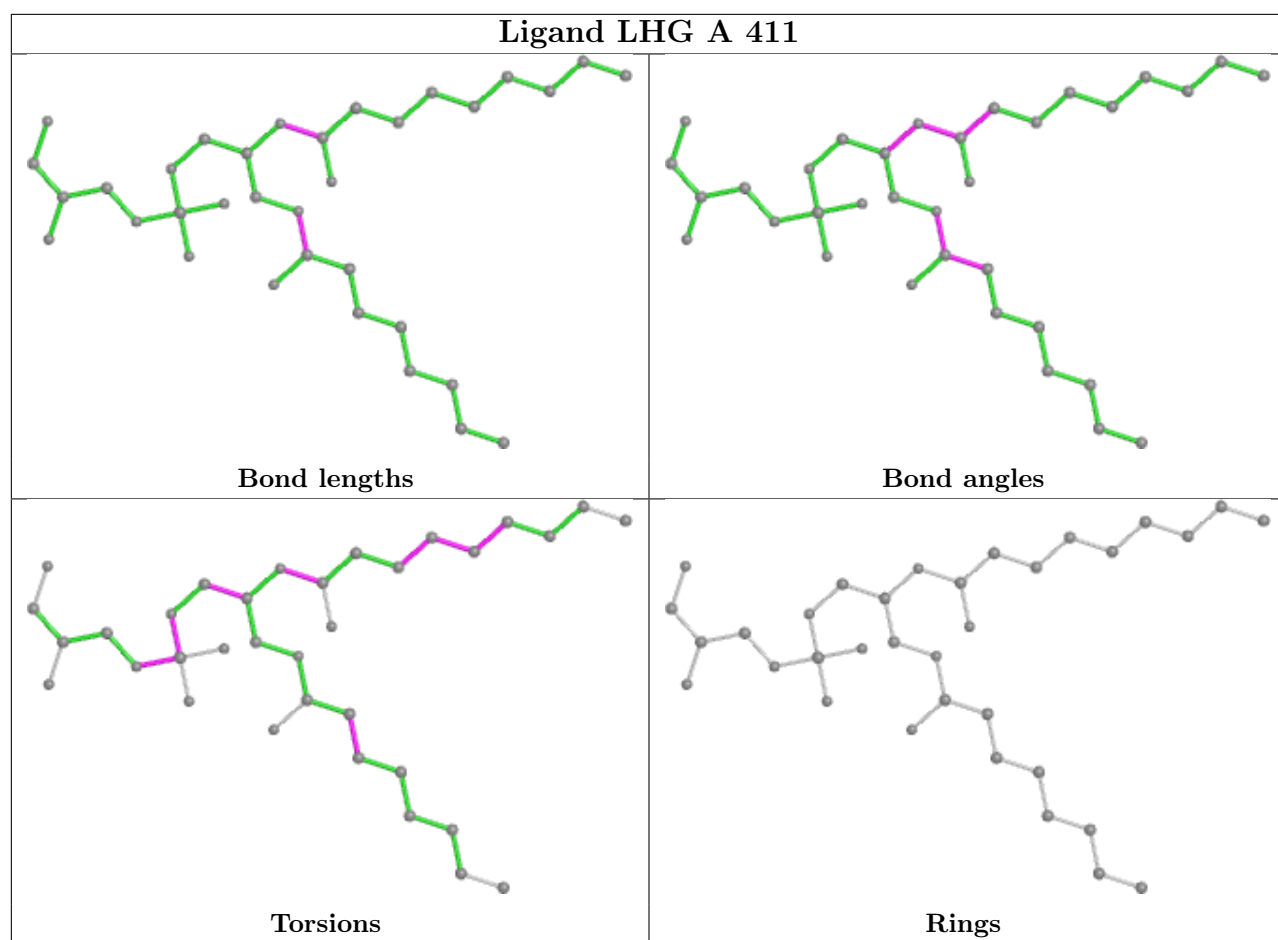
Bond angles

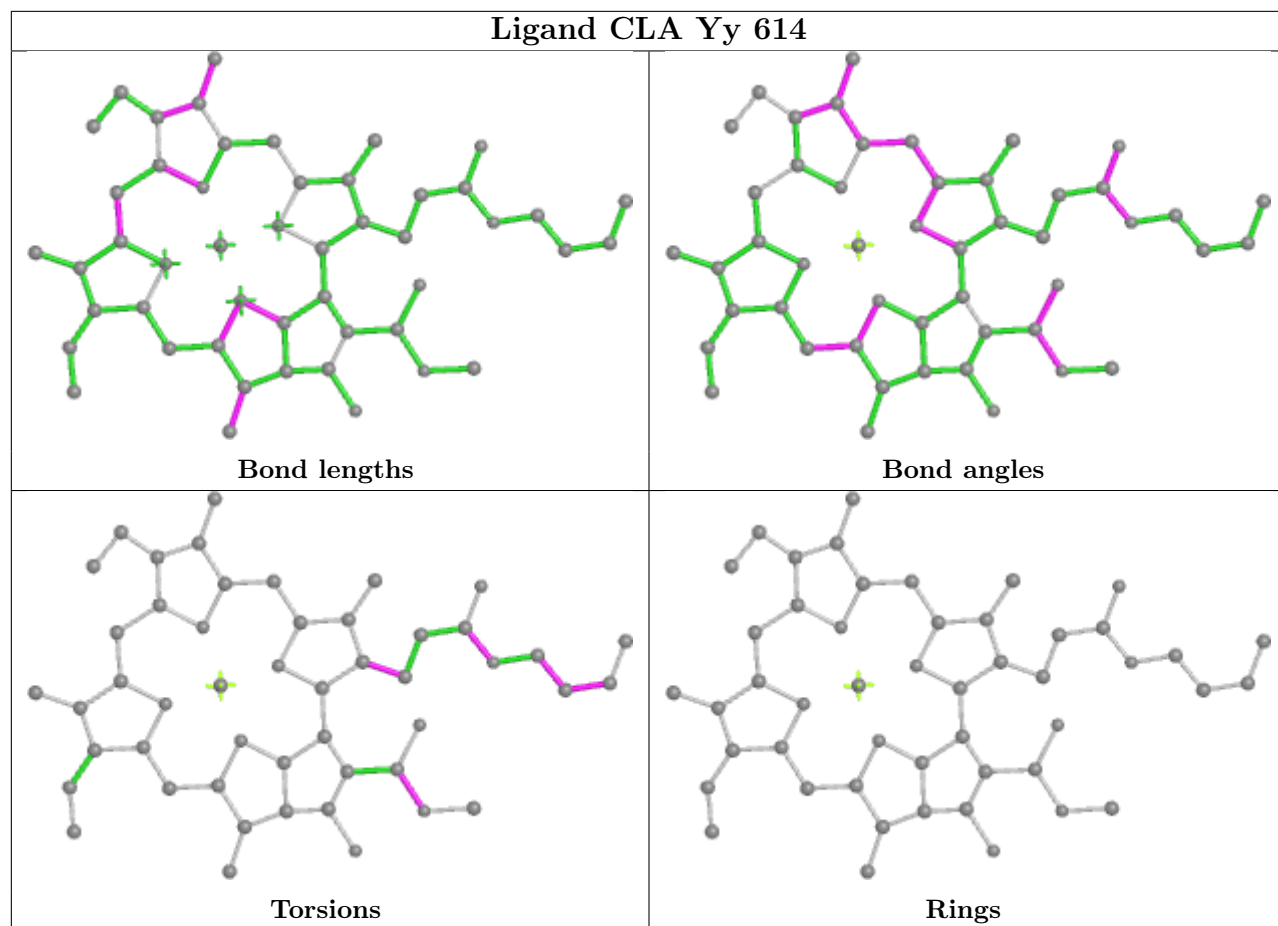


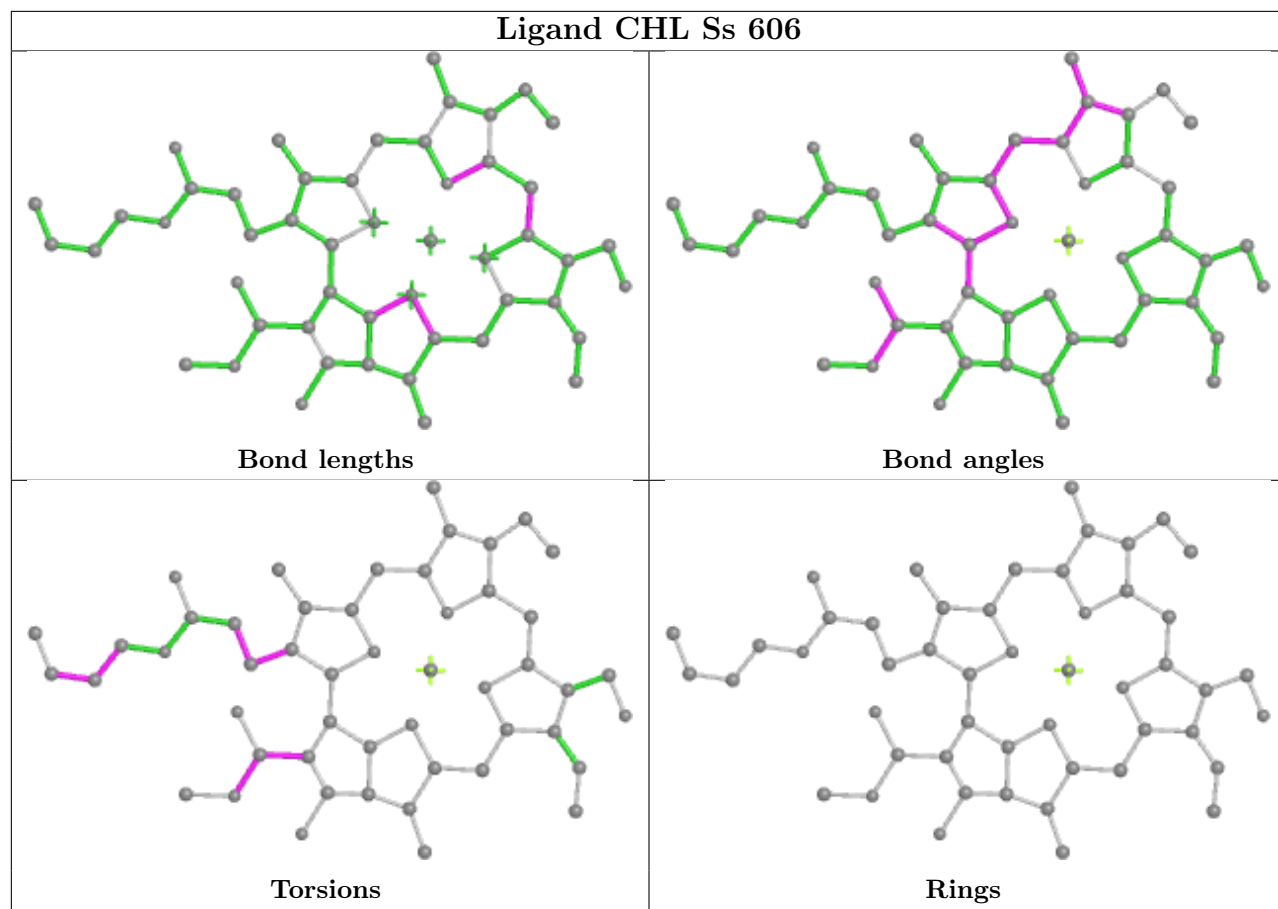
Torsions



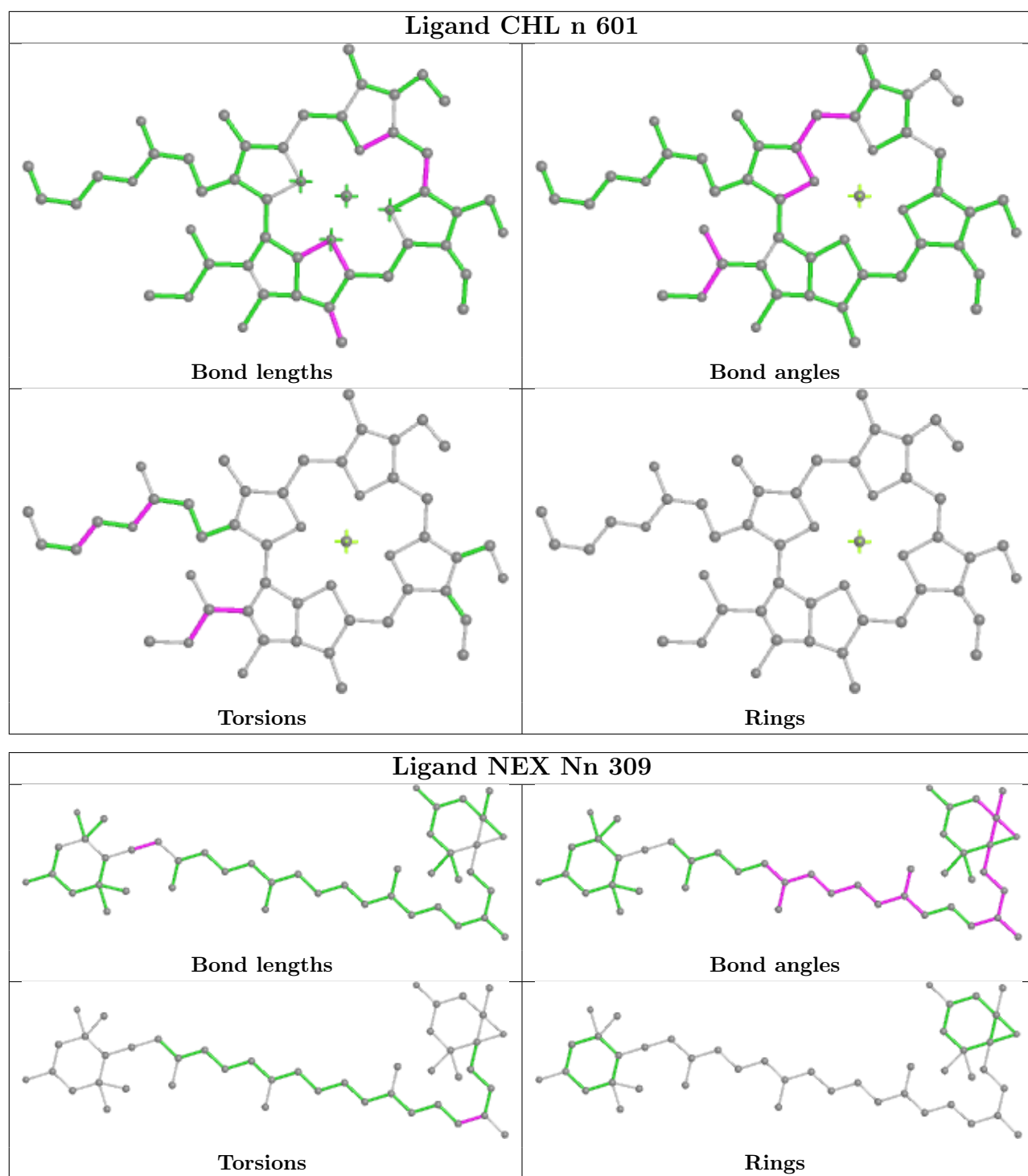
Rings



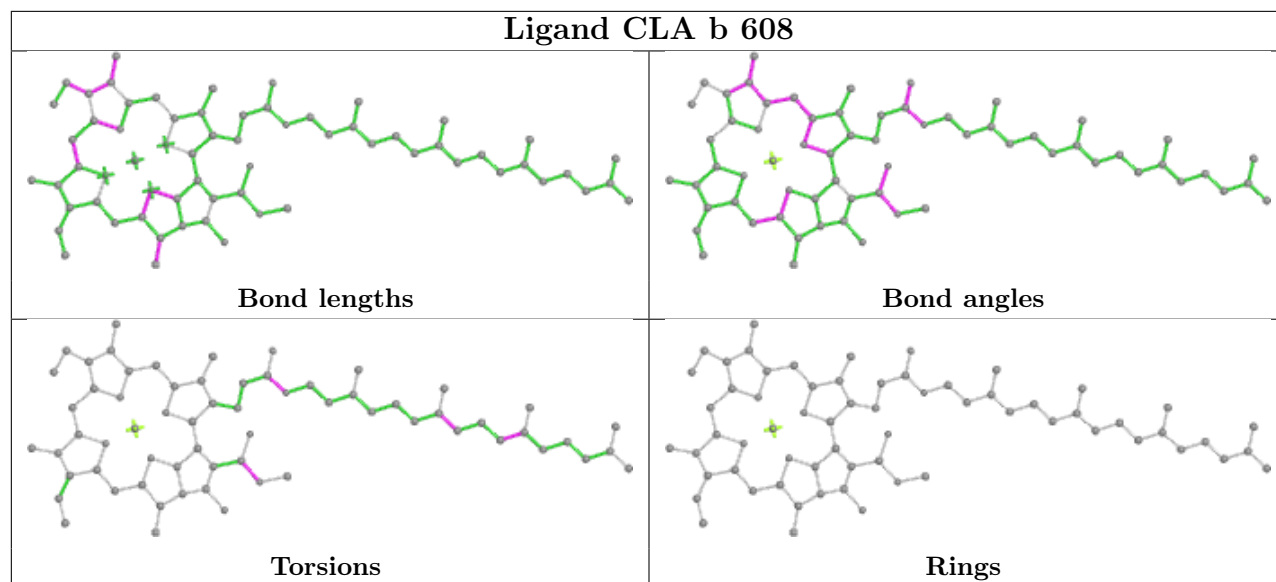




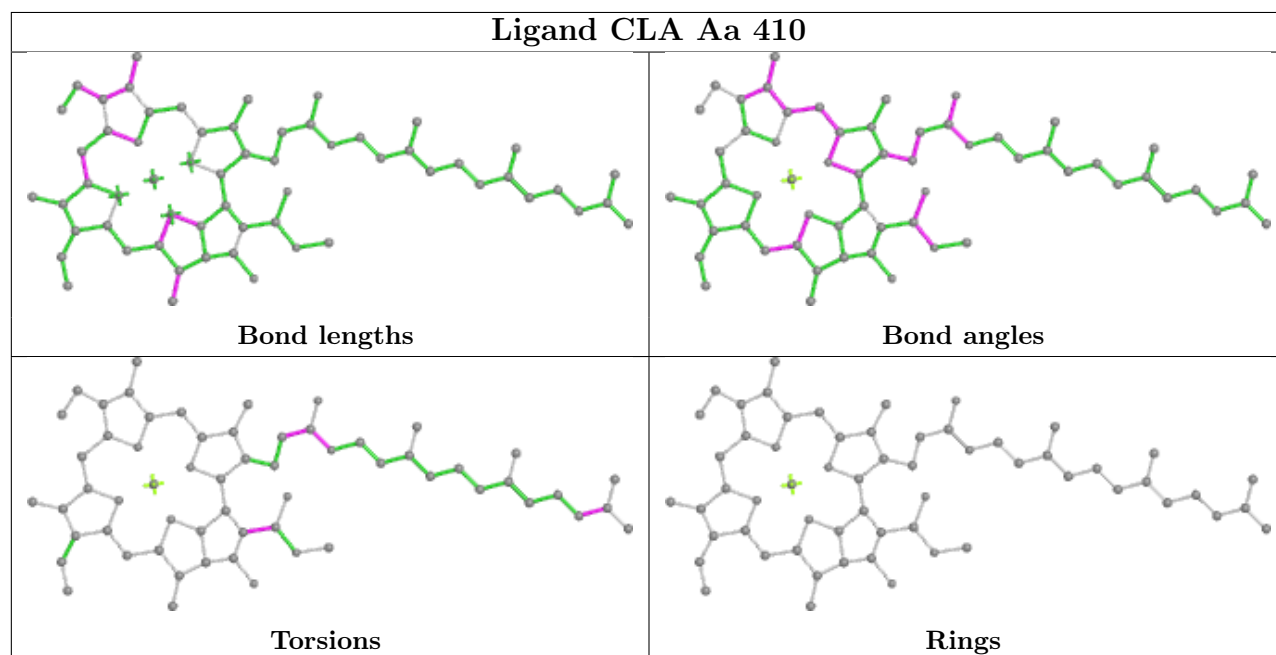


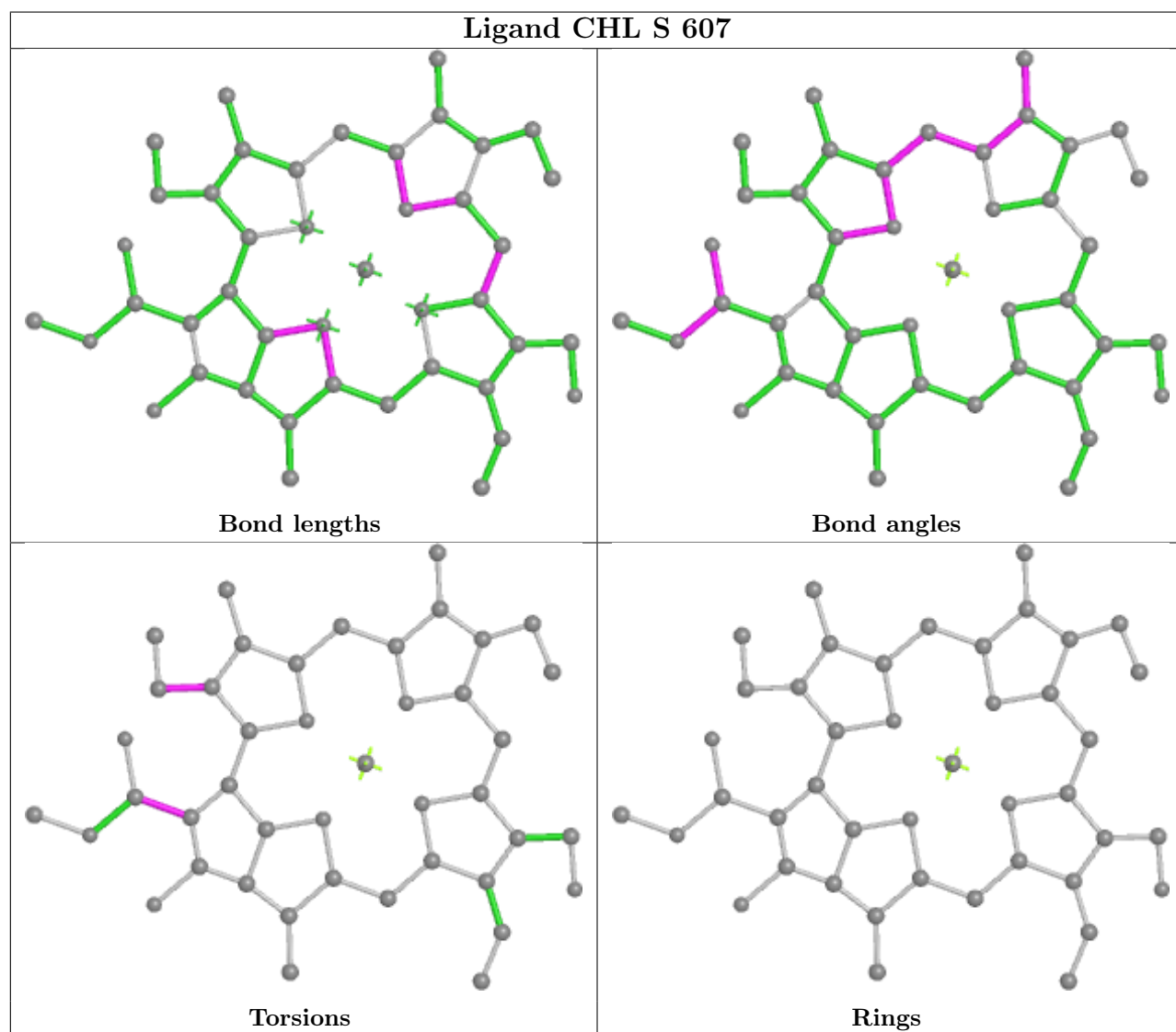
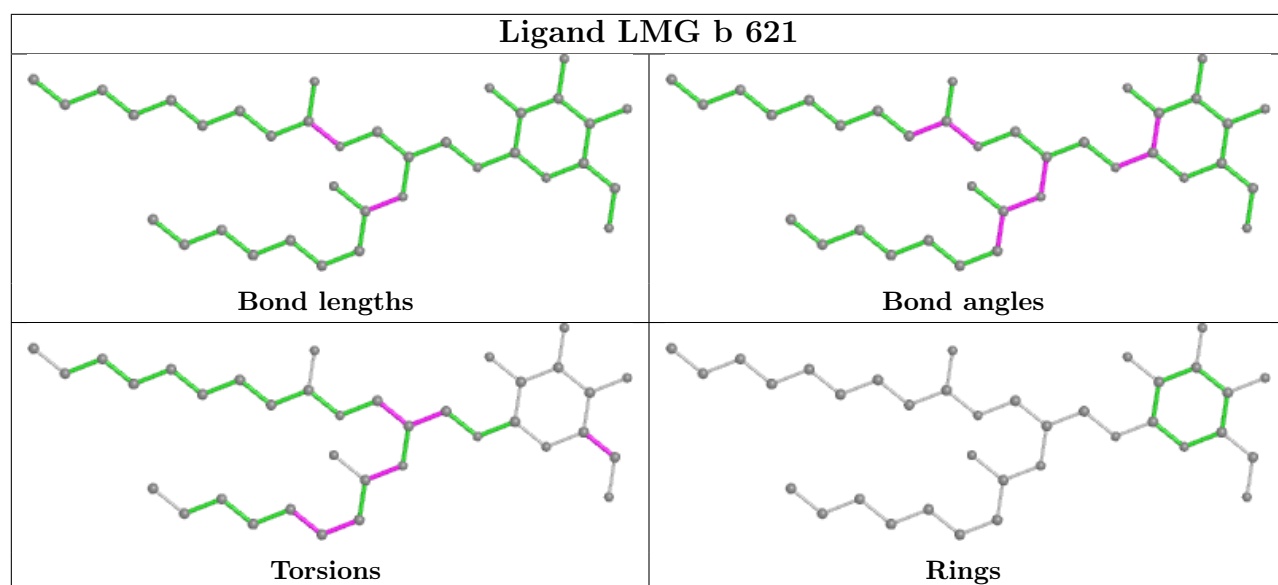


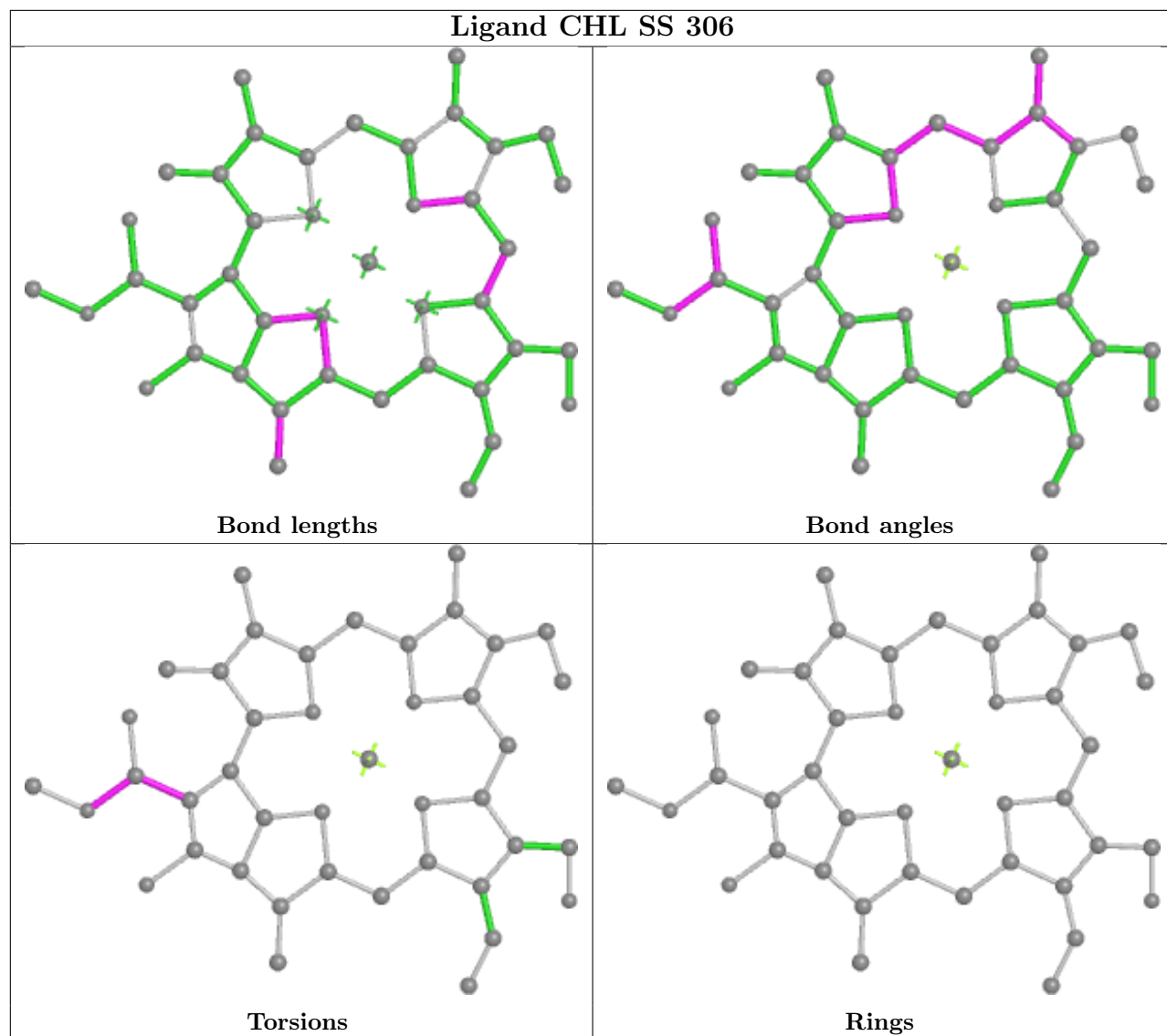
## Ligand CLA b 608



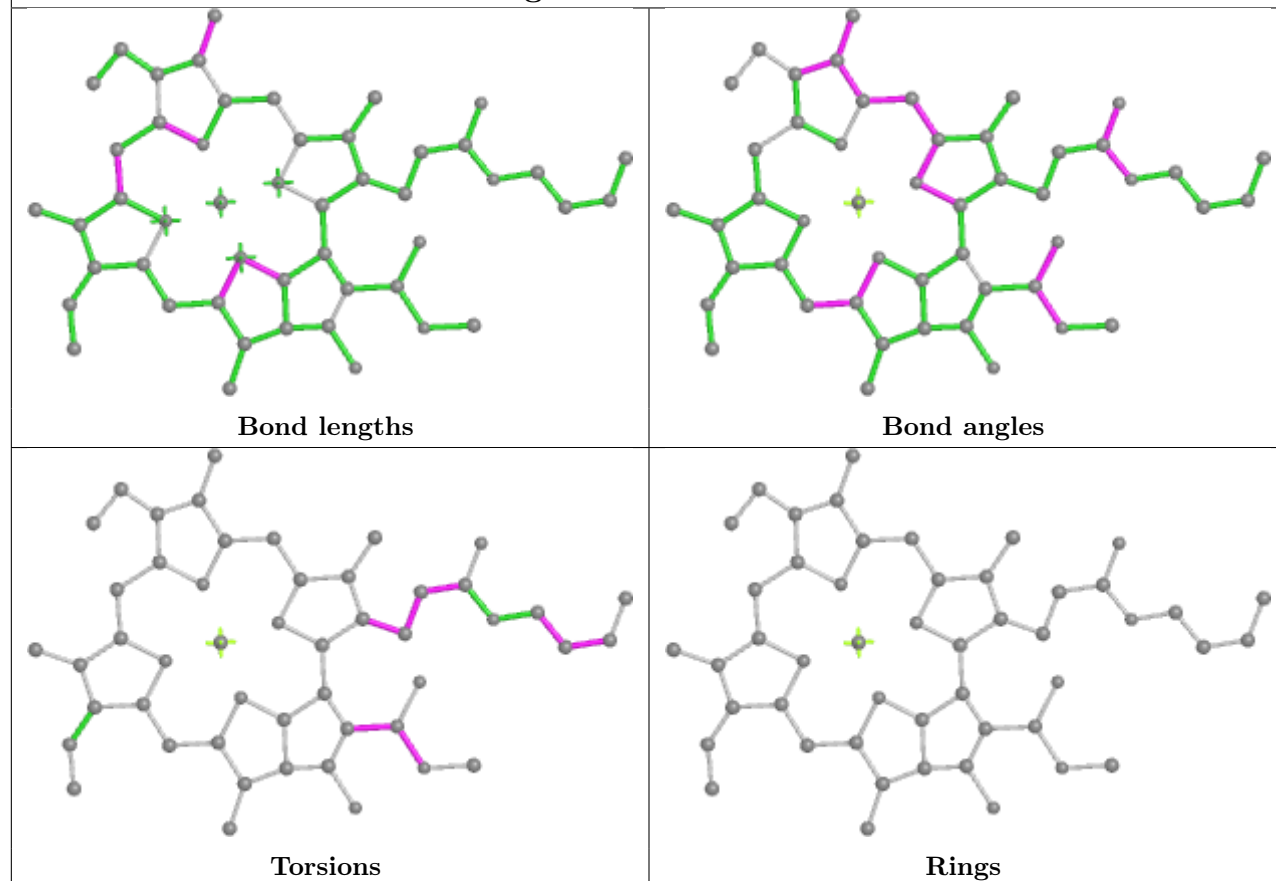
## Ligand CLA Aa 410



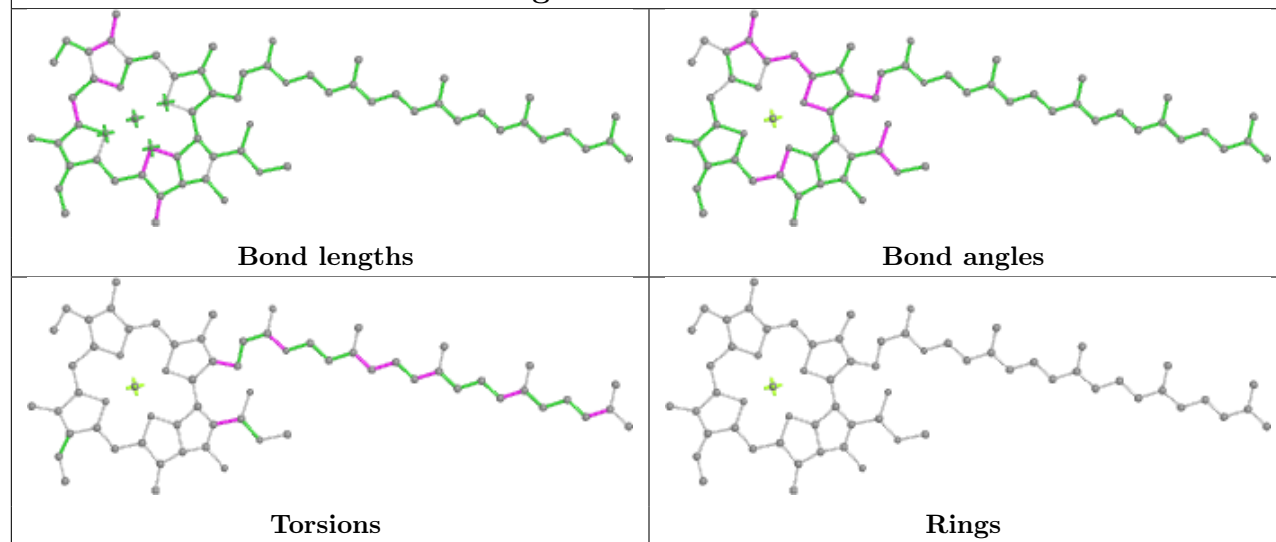




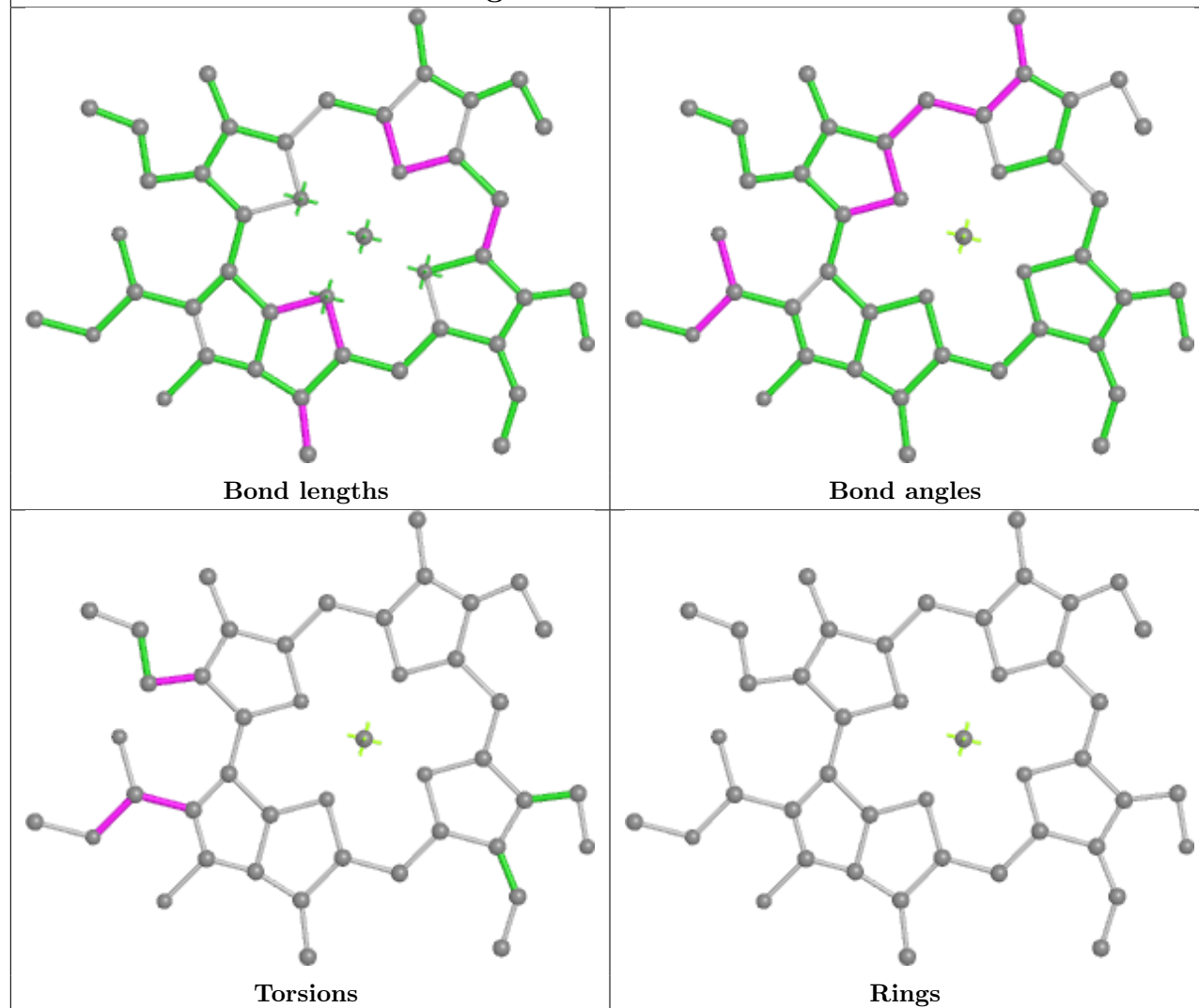
## Ligand CLA Rr 601



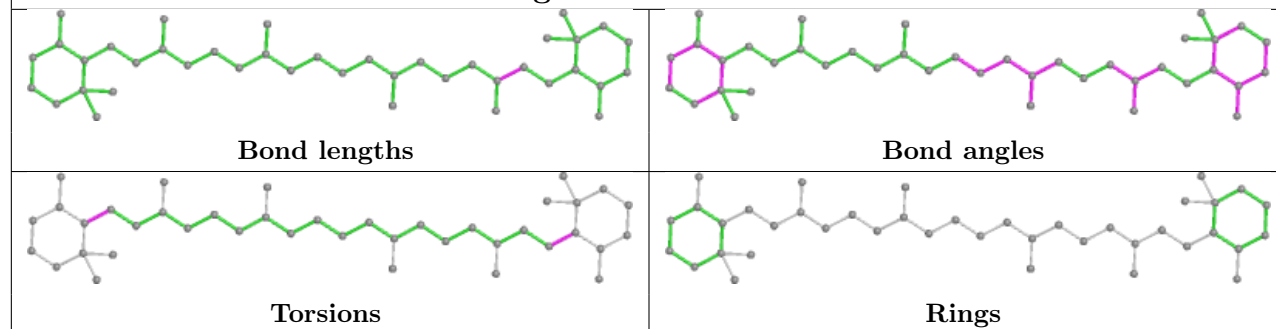
## Ligand CLA C 504

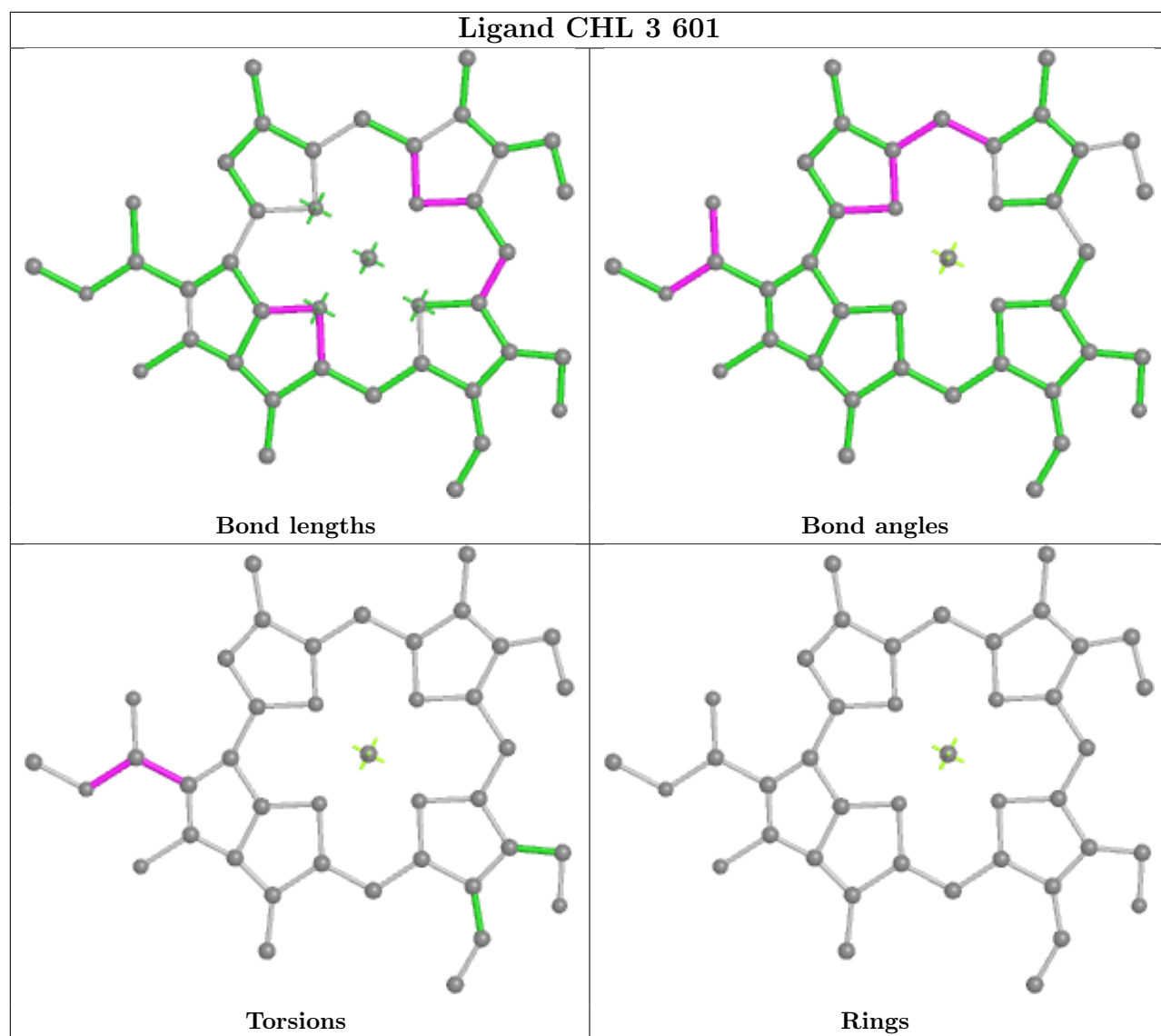
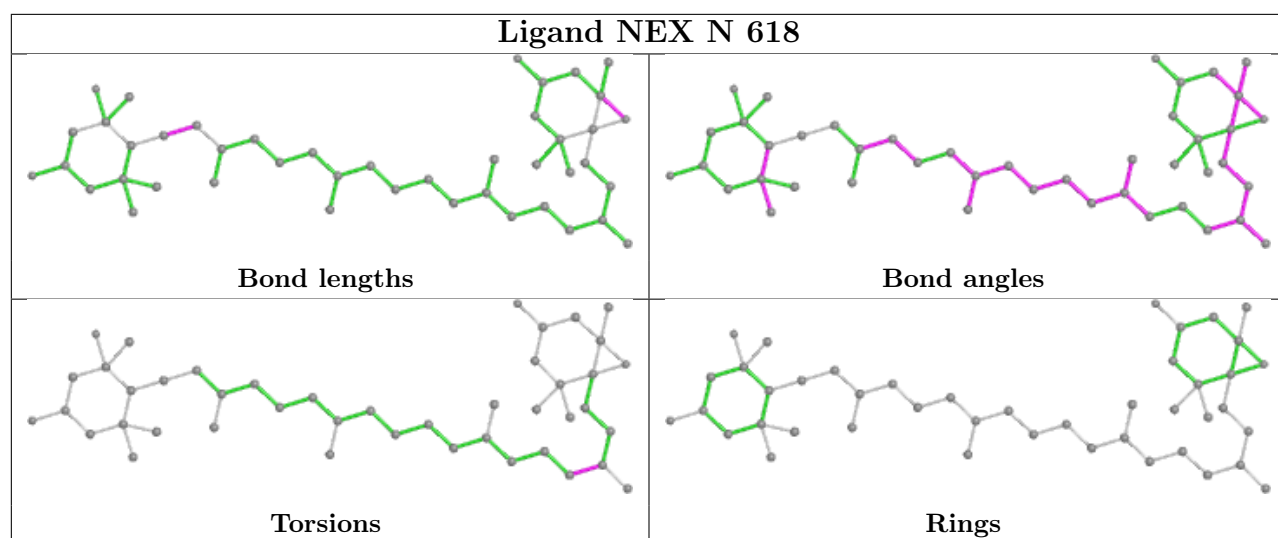


## Ligand CHL YY 606

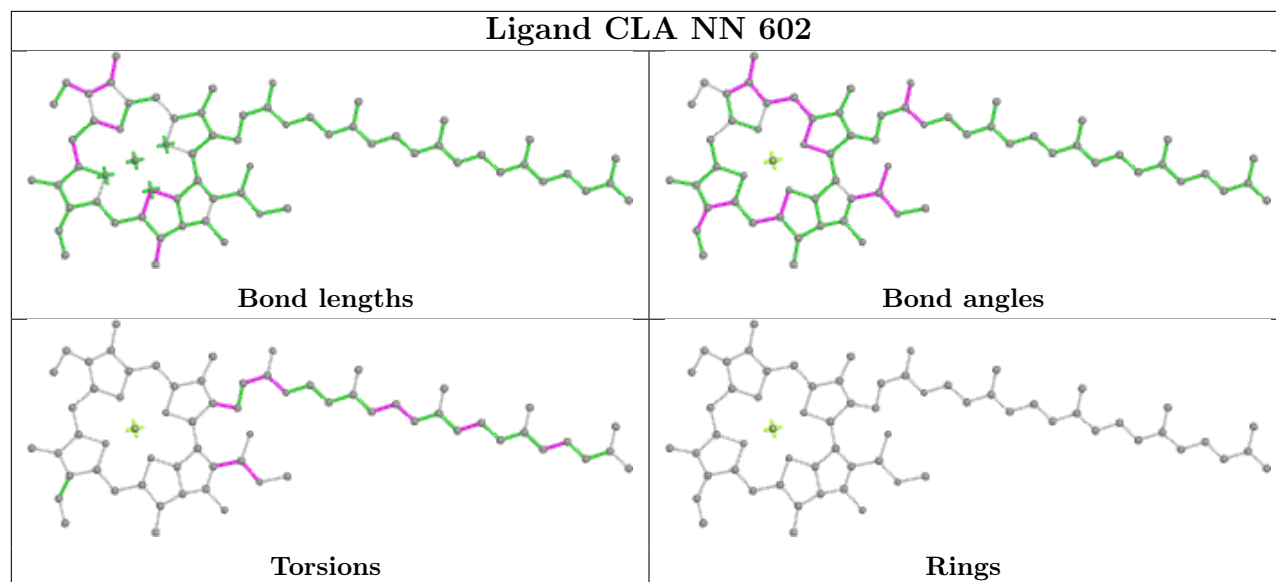


## Ligand BCR b 619

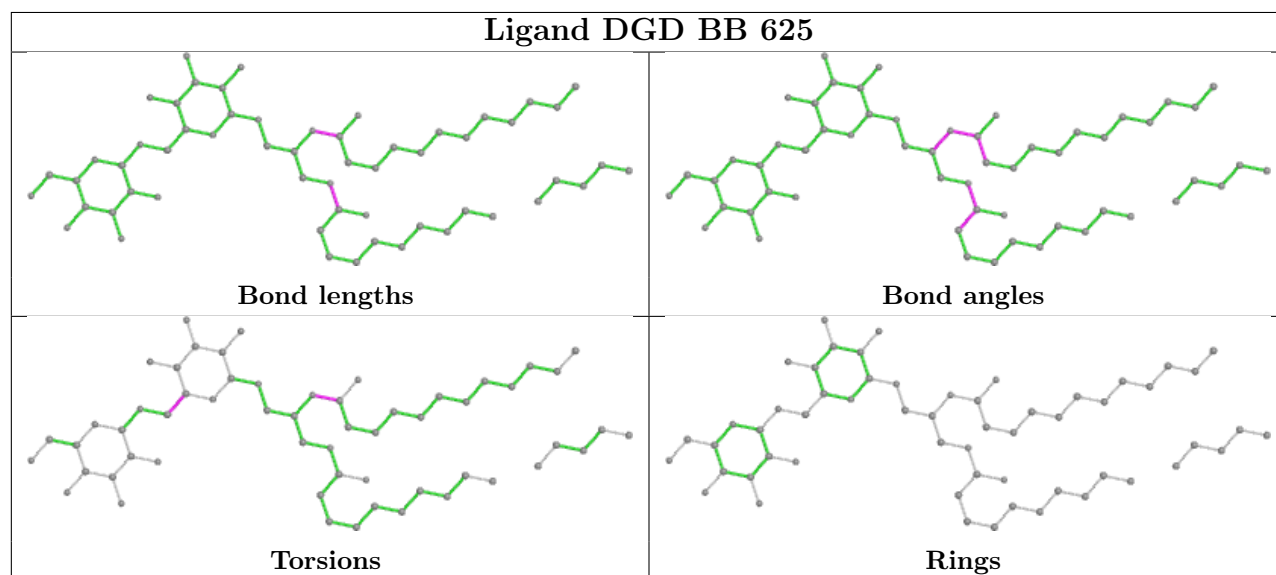




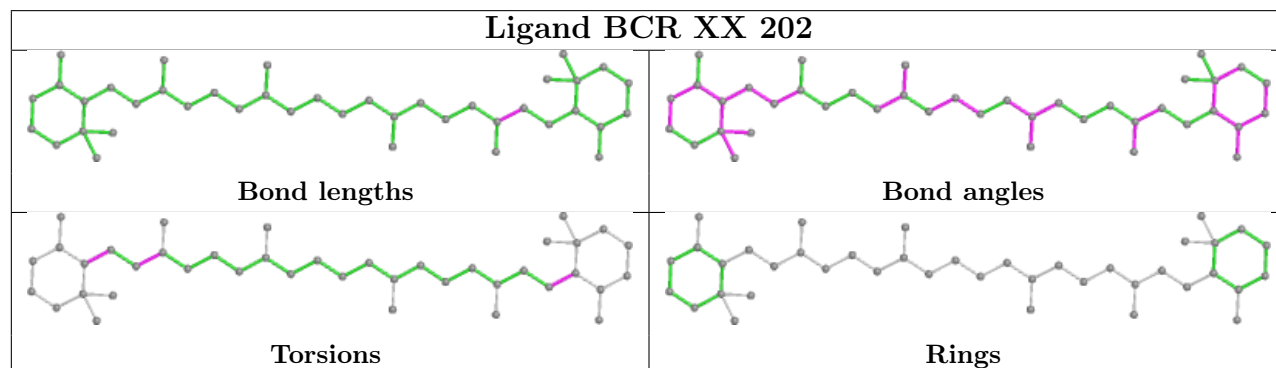
## Ligand CLA NN 602



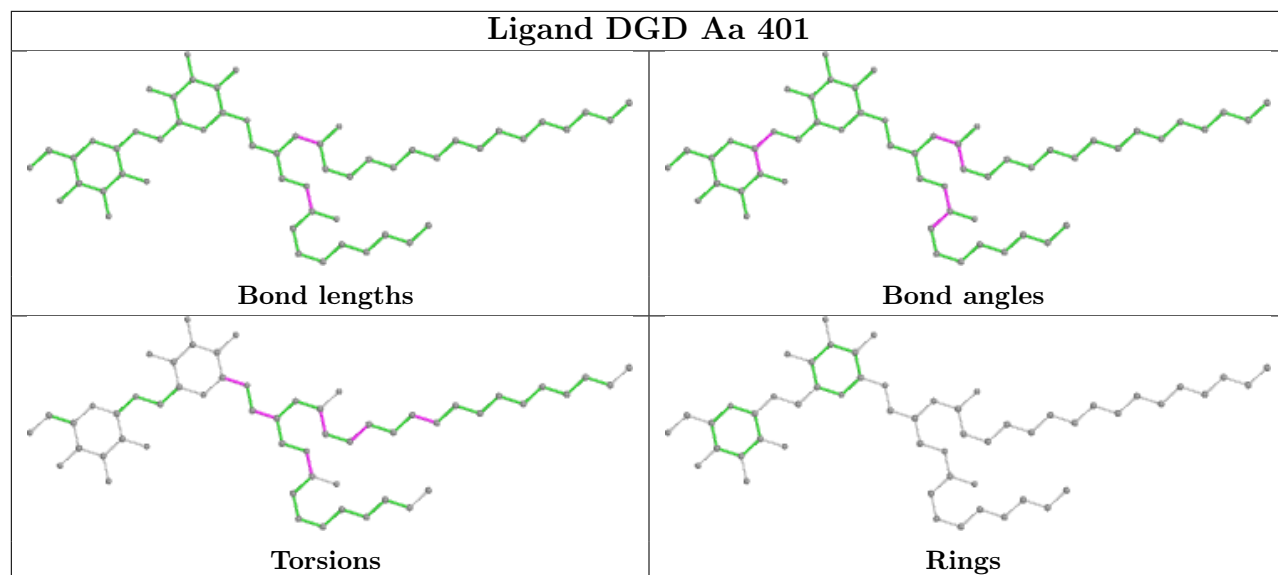
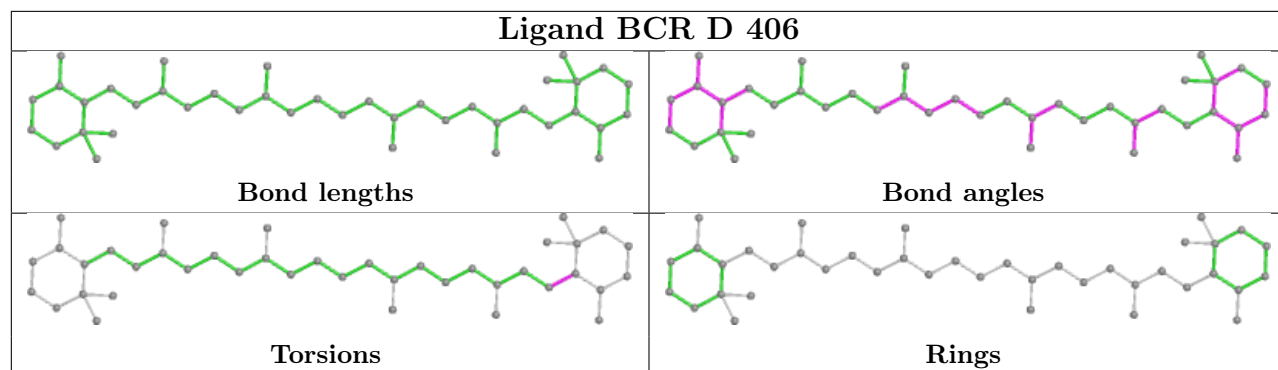
## Ligand DGD BB 625



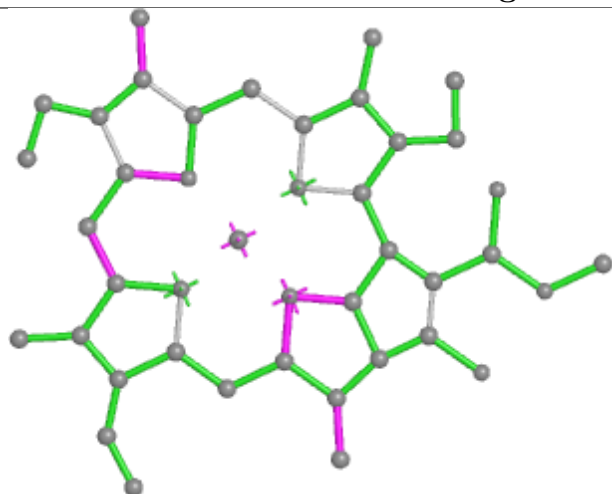
## Ligand BCR XX 202



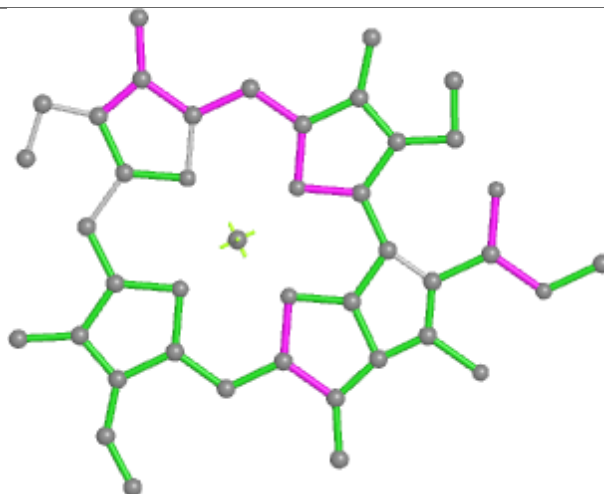




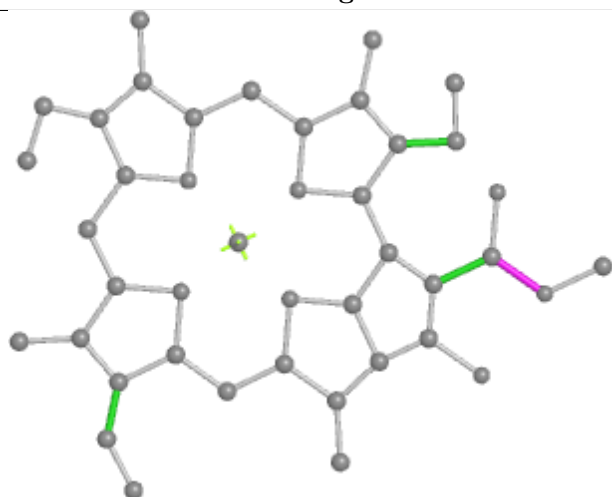
## Ligand CLA YY 611



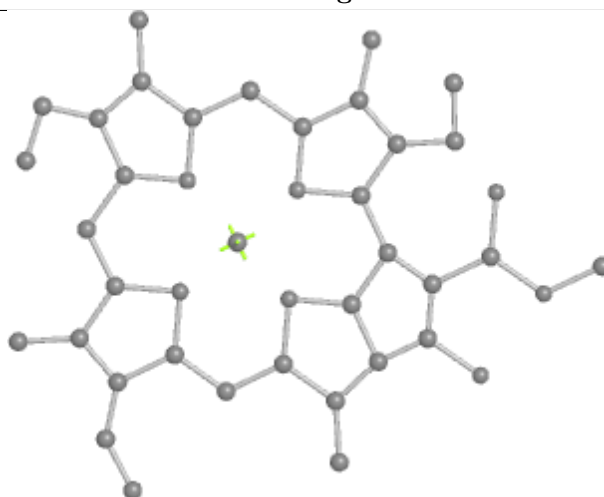
Bond lengths



Bond angles

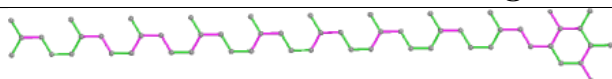


Torsions

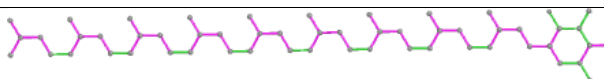


Rings

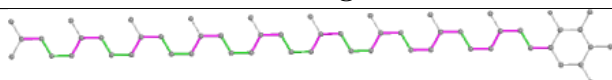
## Ligand PL9 AA 410



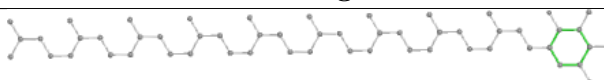
Bond lengths



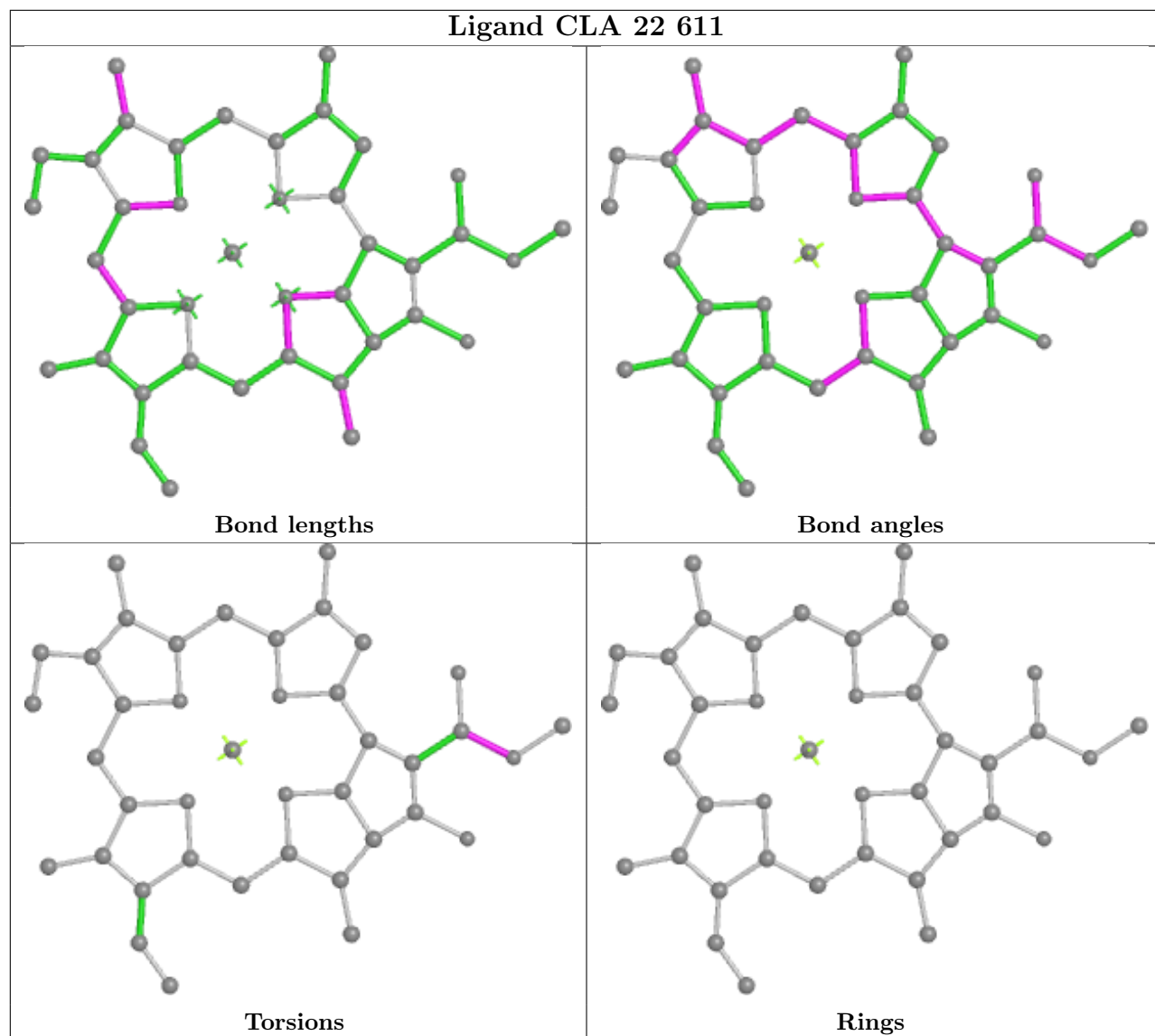
Bond angles

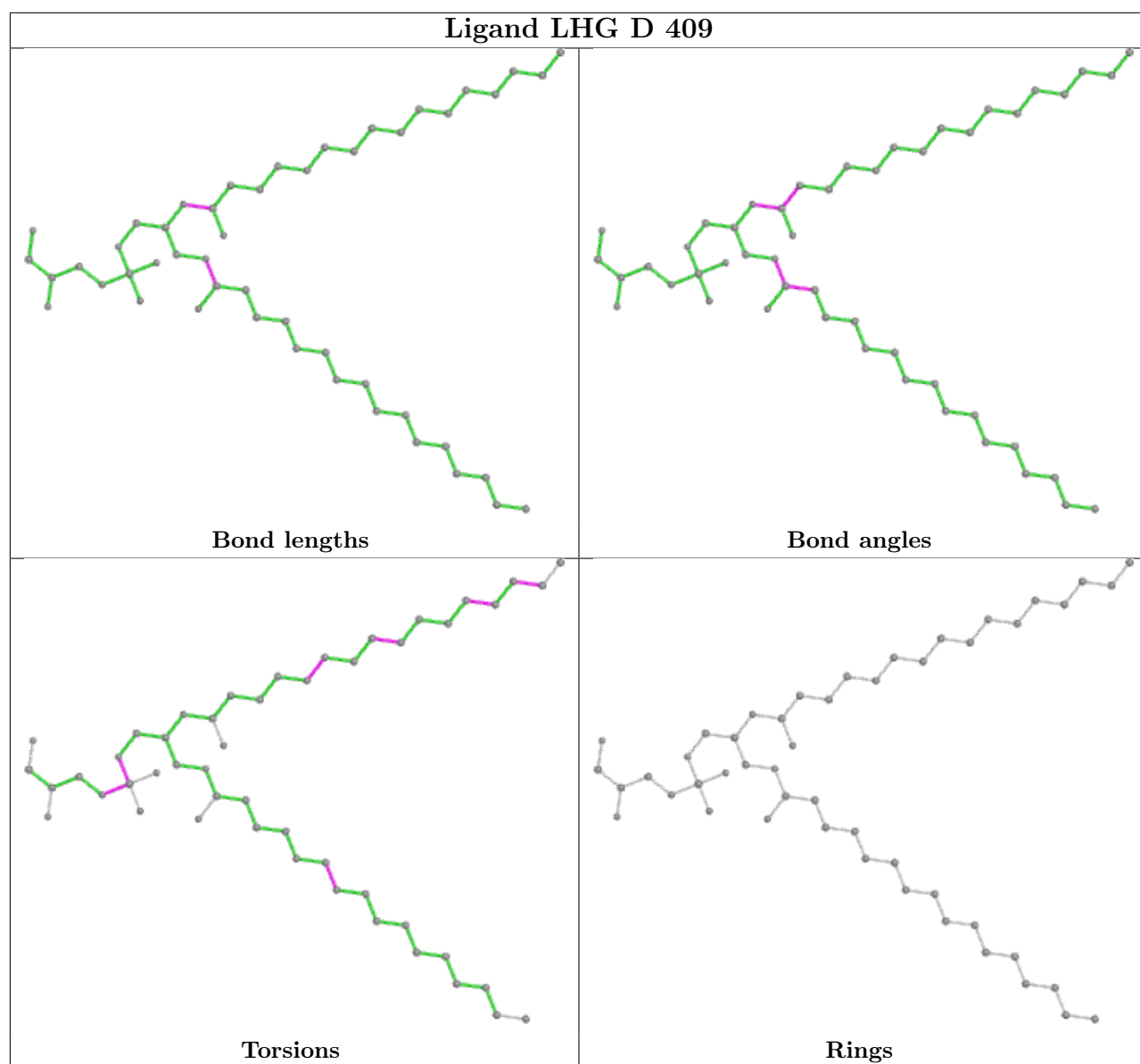


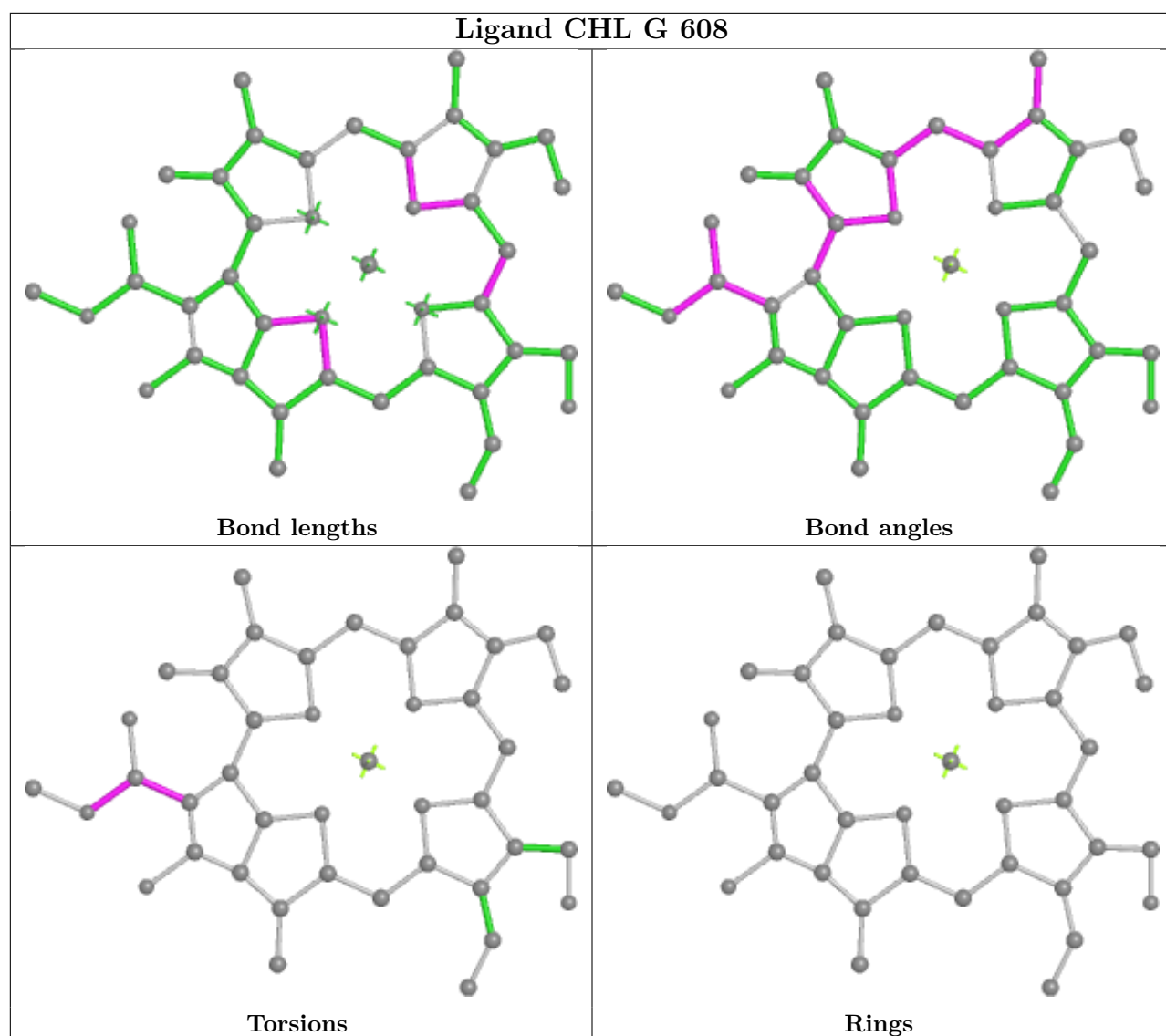
Torsions



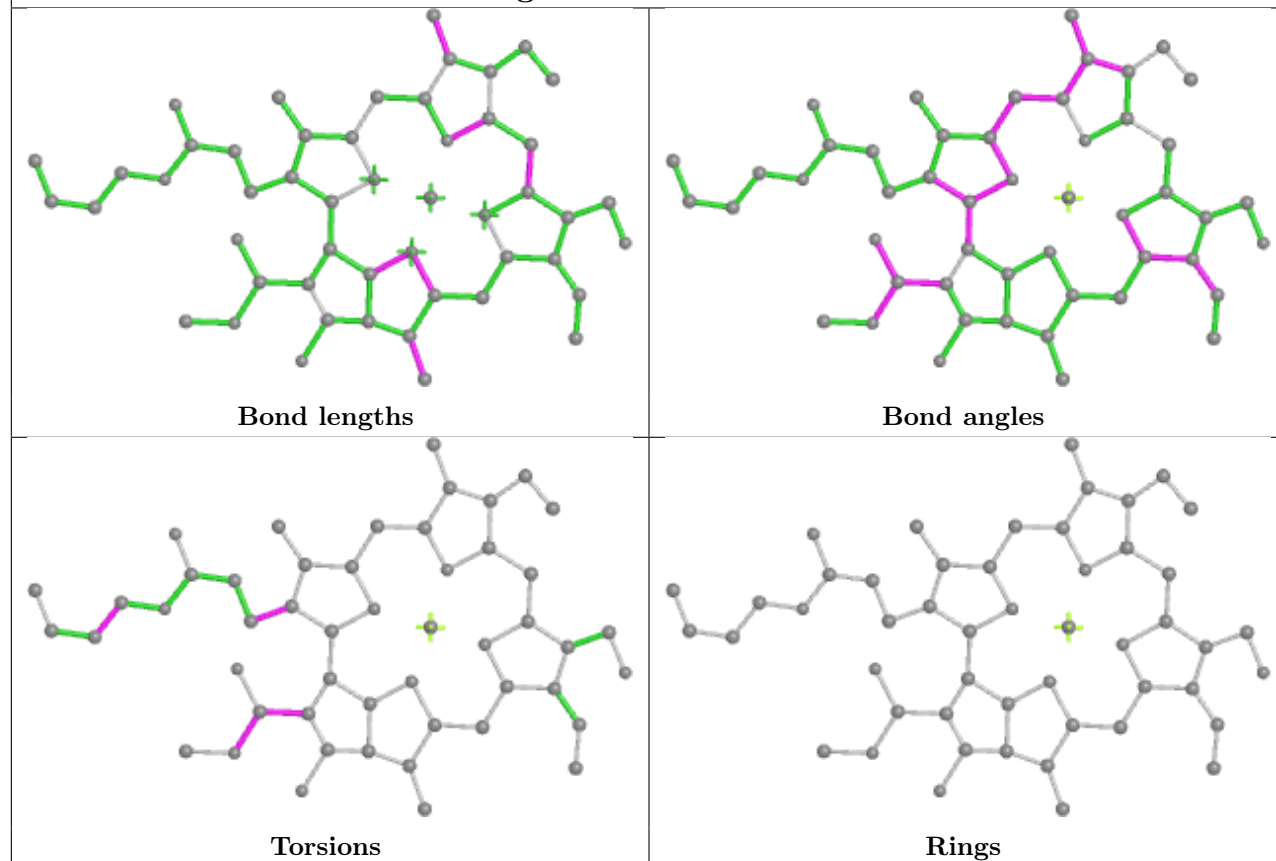
Rings



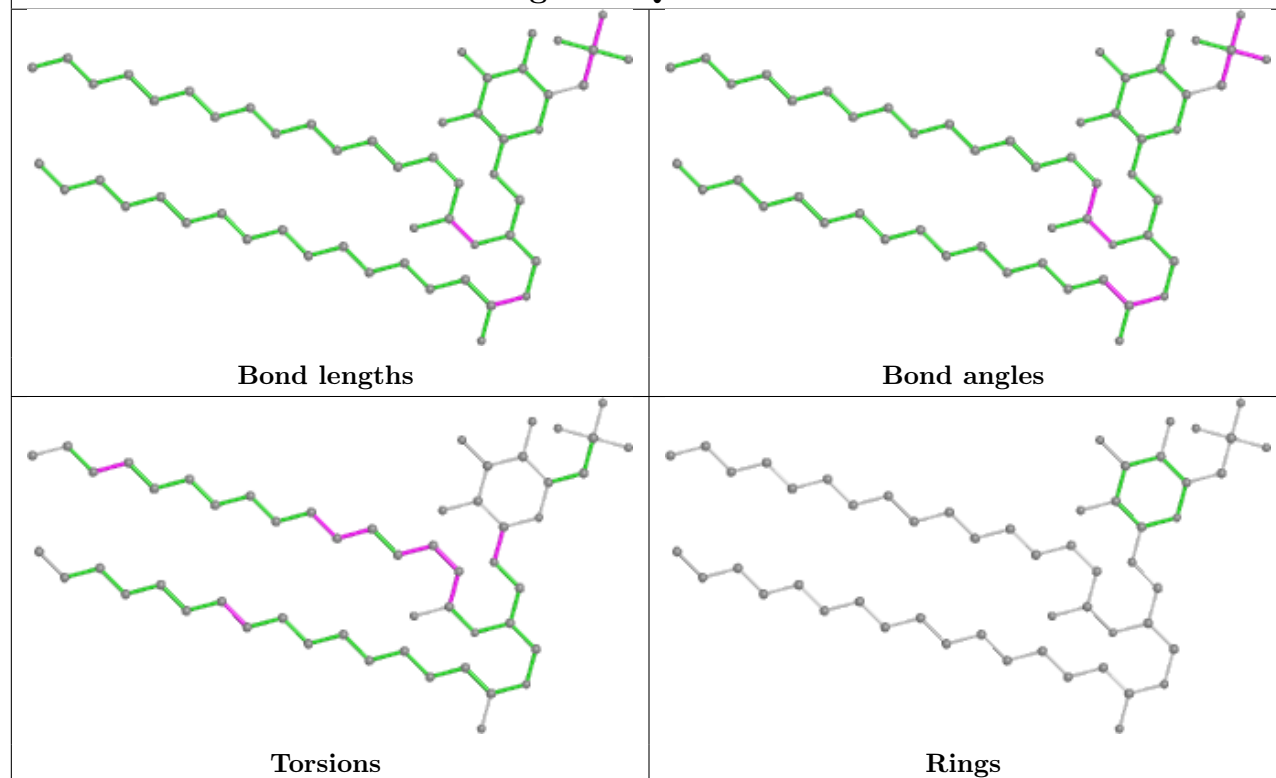




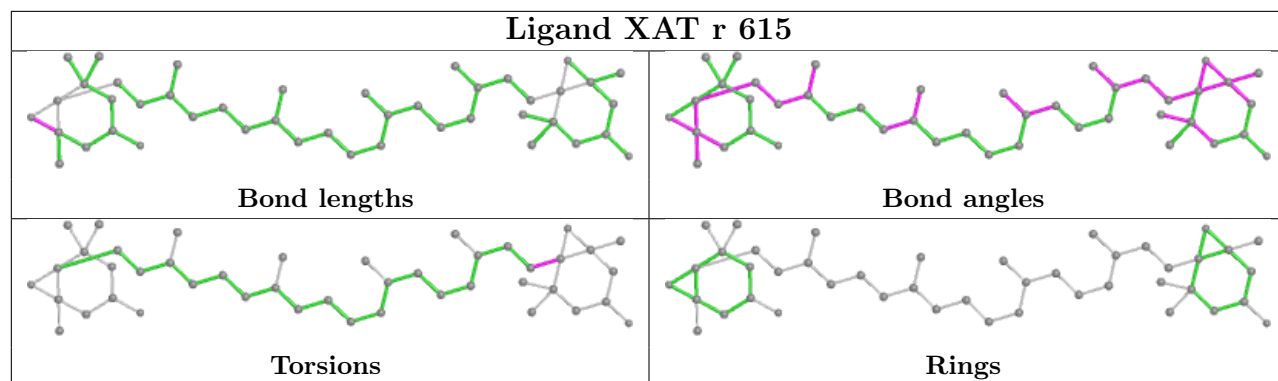
## Ligand CHL NN 609



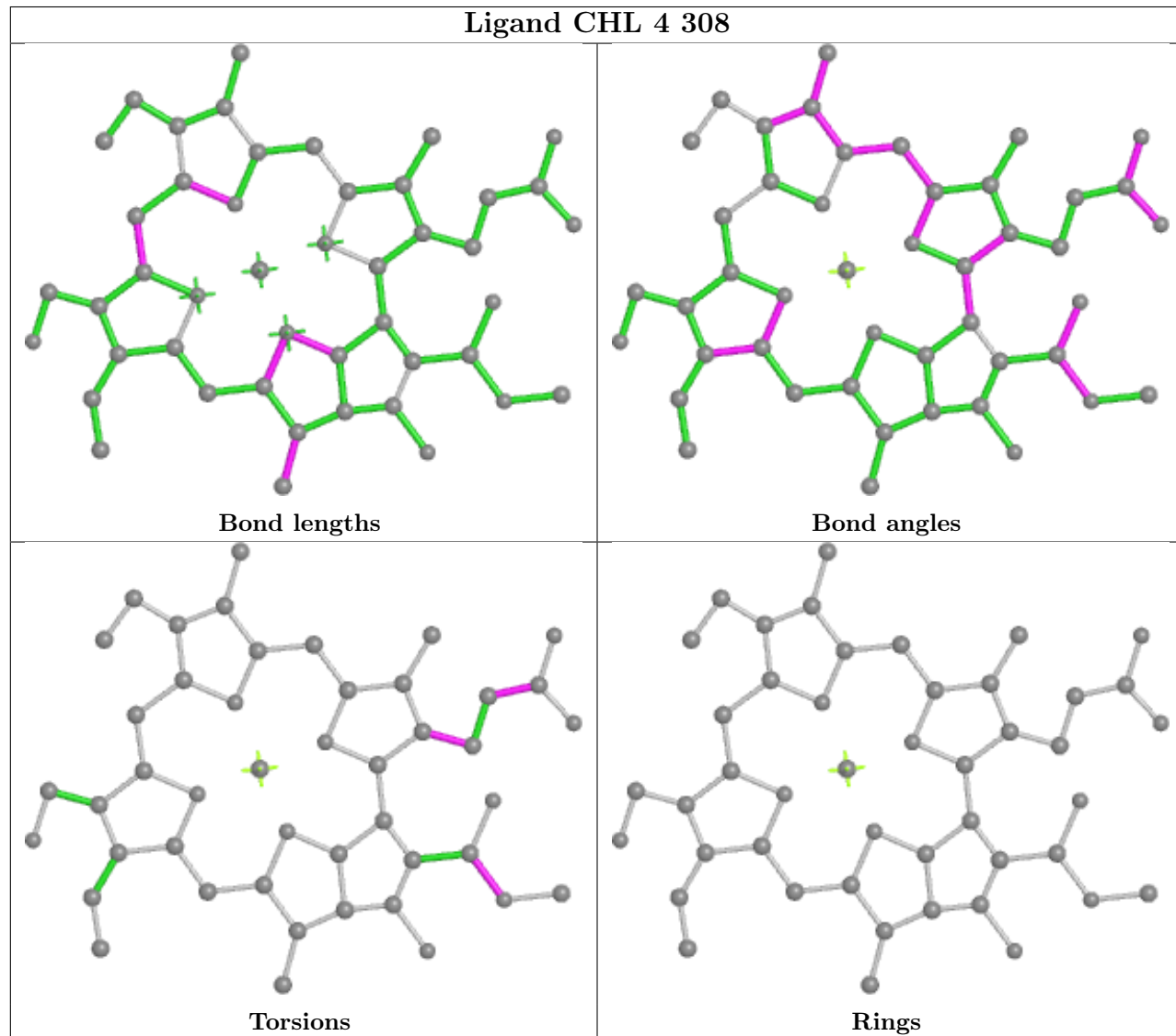
## Ligand SQD Ll 101

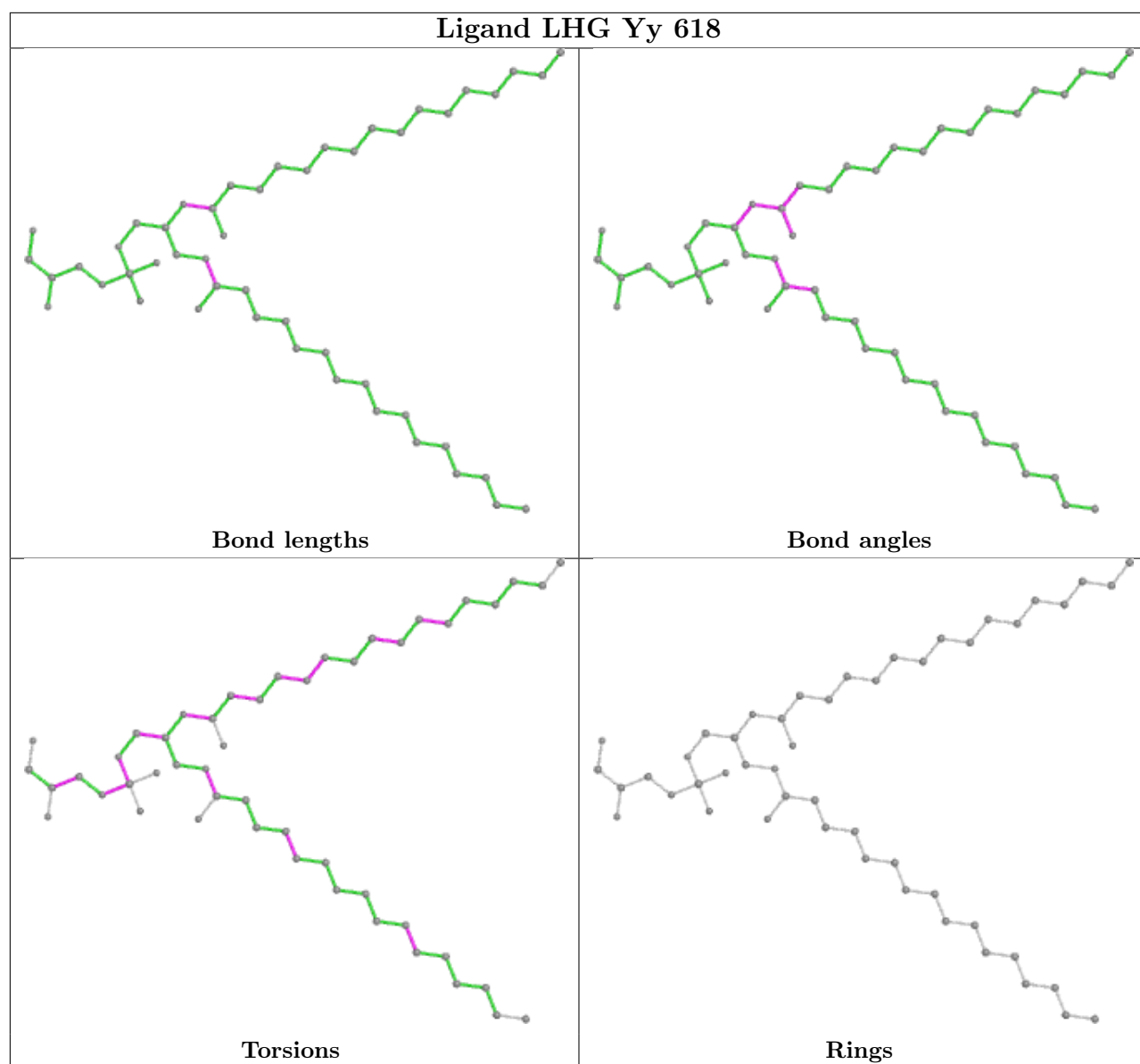


## Ligand XAT r 615

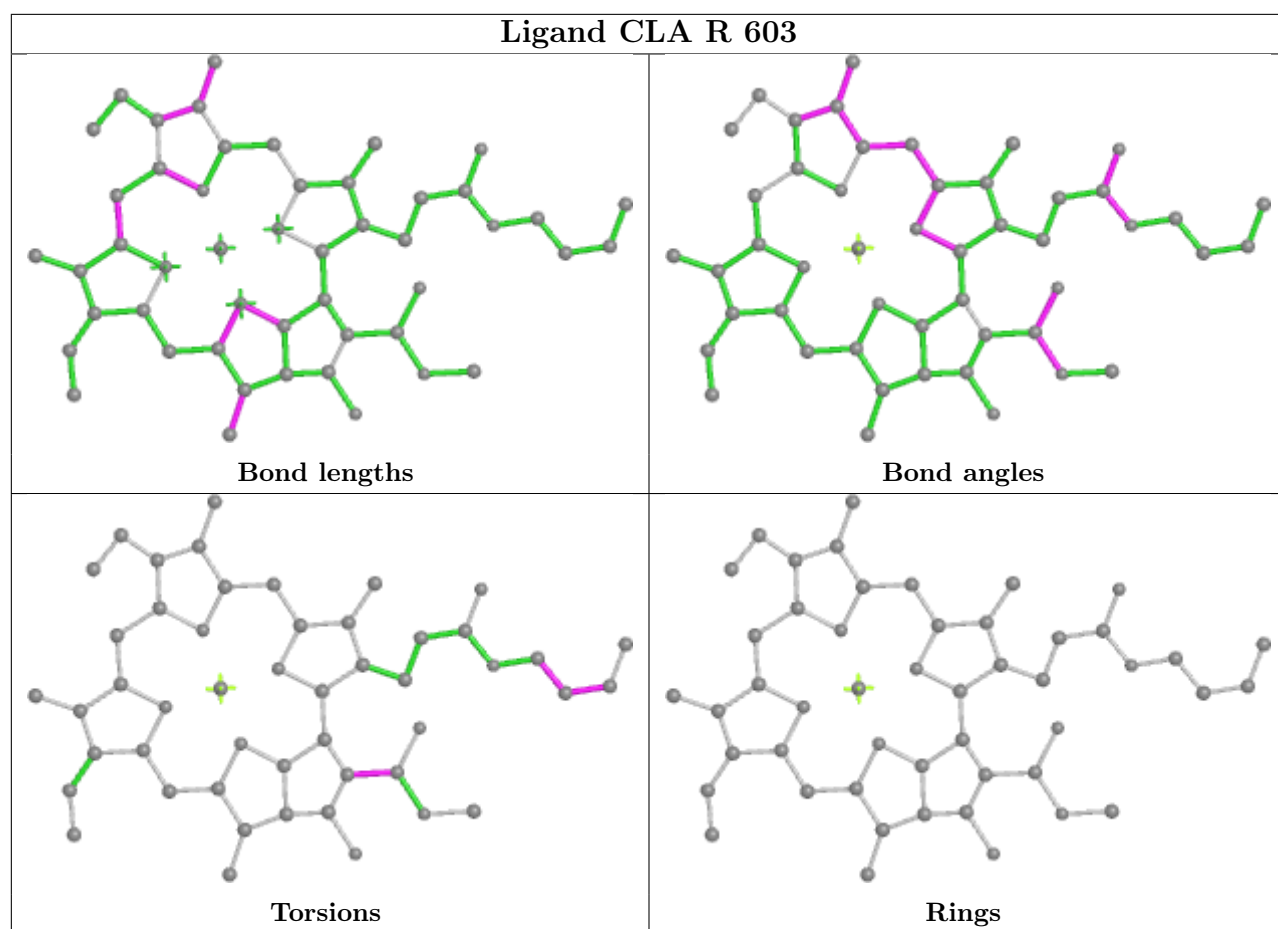


## Ligand CHL 4 308

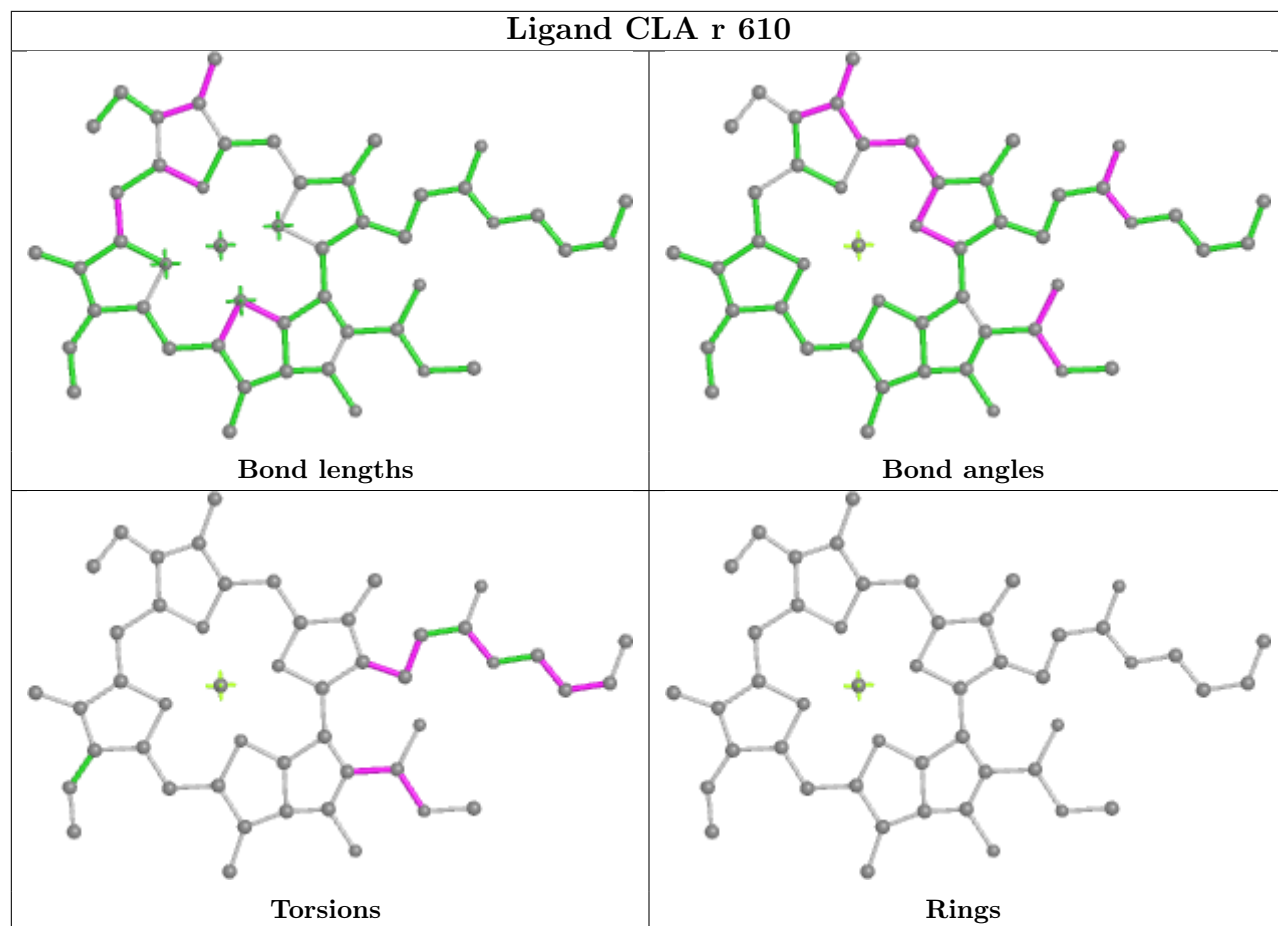




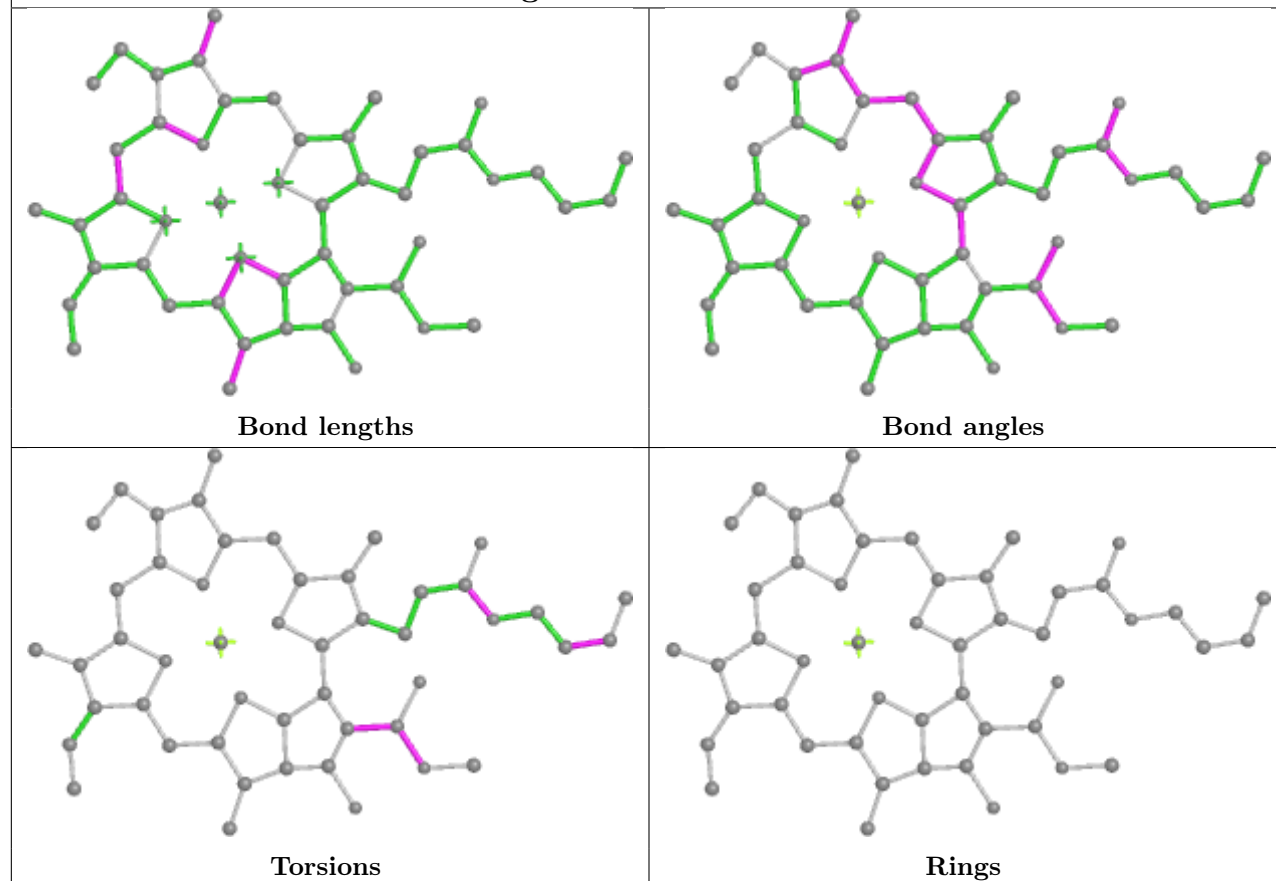




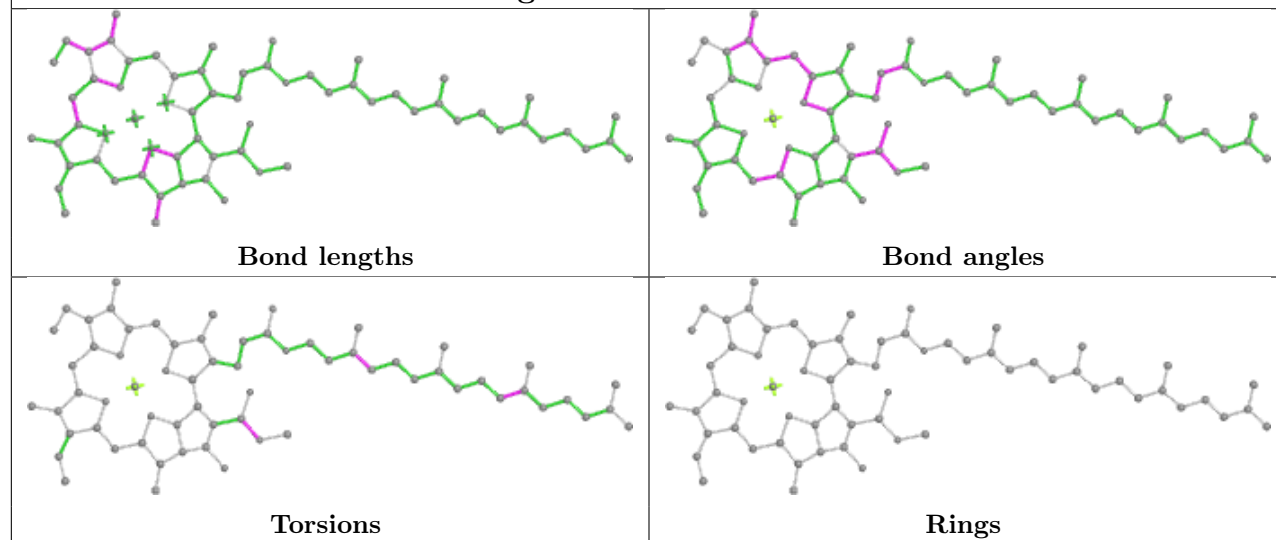
## Ligand CLA r 610

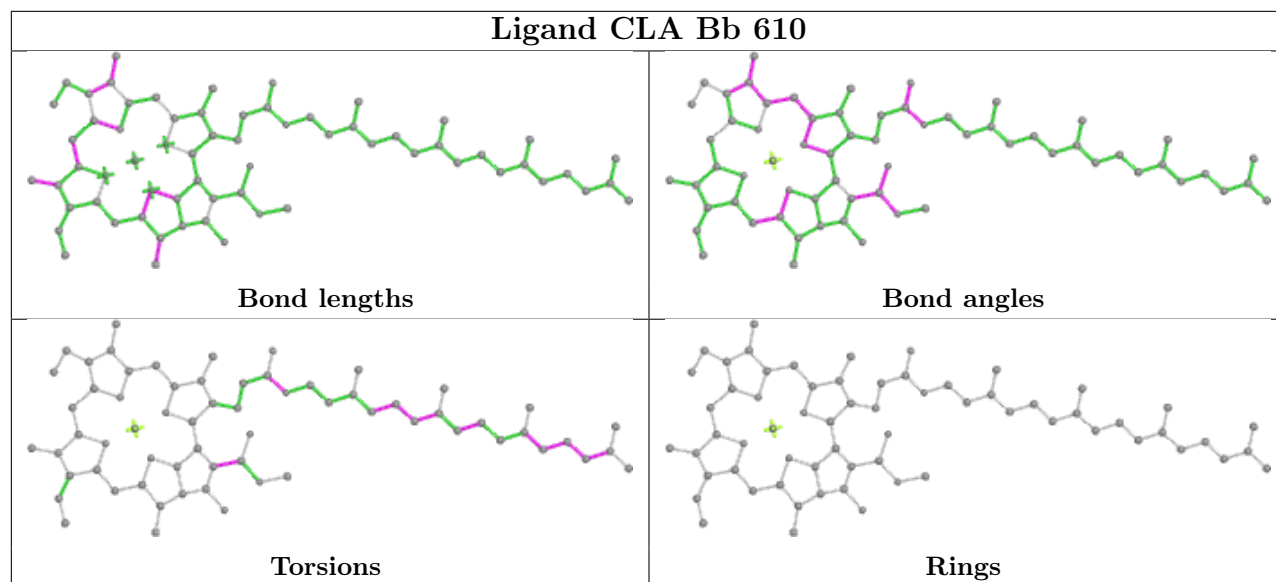
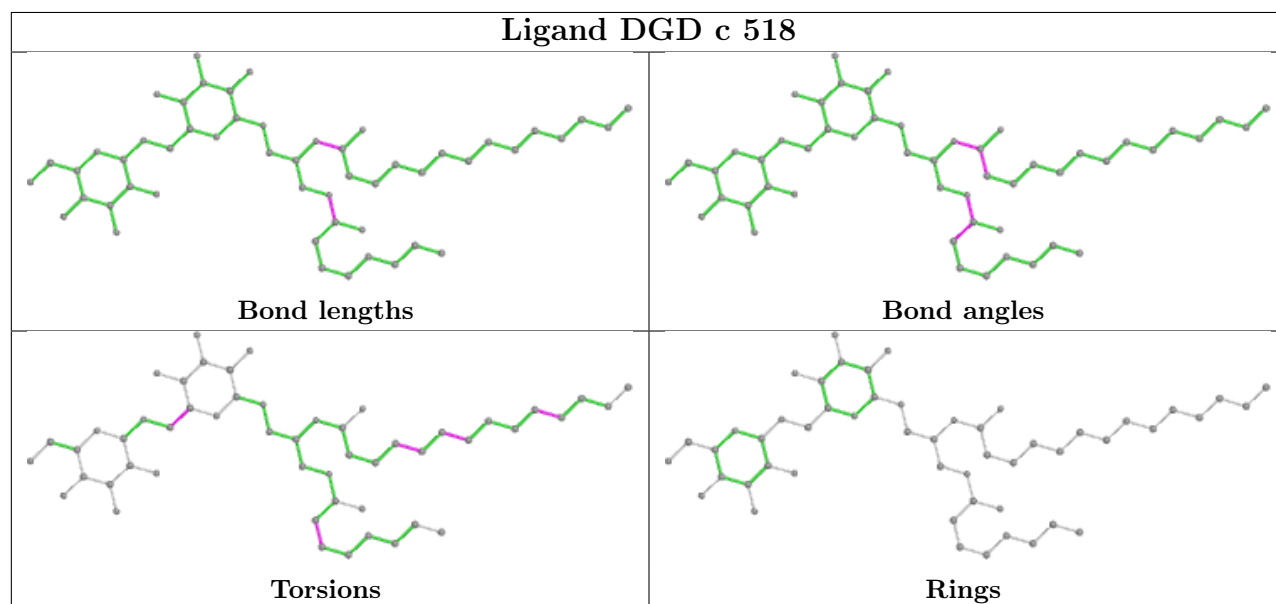


## Ligand CLA Nn 303

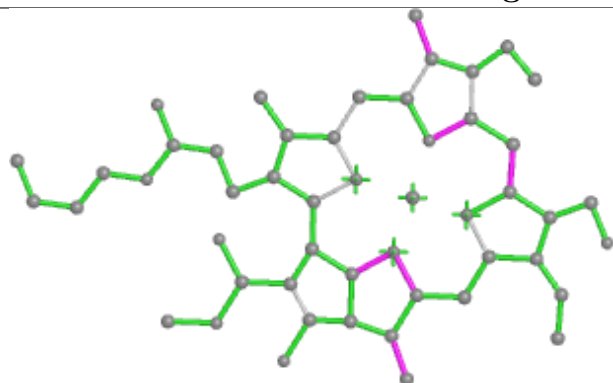


## Ligand CLA DD 401

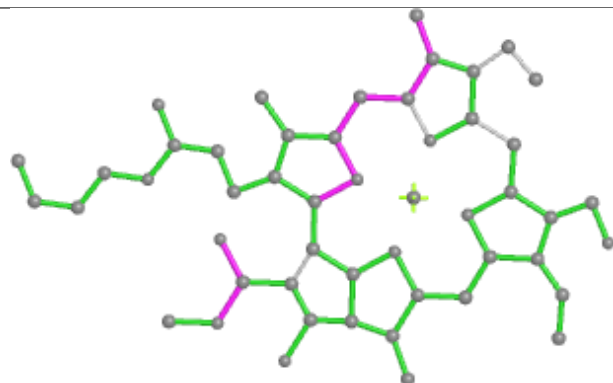


**Ligand CLA Bb 610****Ligand DGD c 518**

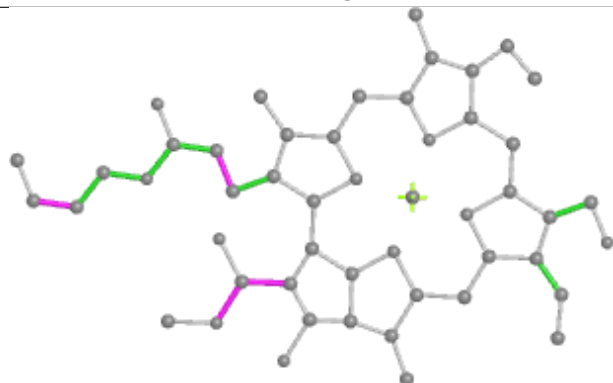
## Ligand CHL Nn 318



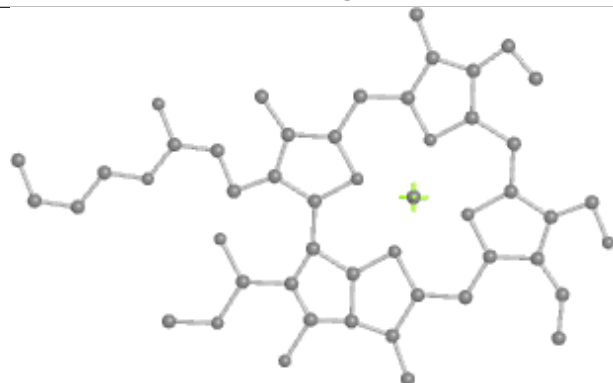
Bond lengths



Bond angles

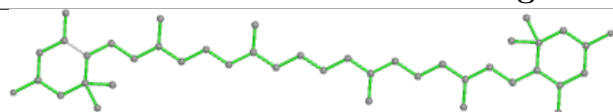


Torsions

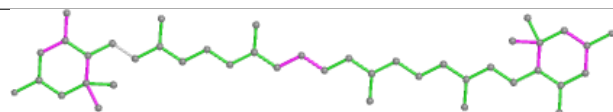


Rings

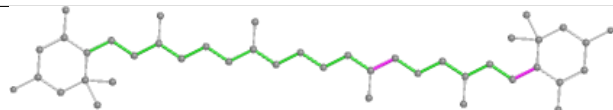
## Ligand LUT n 615



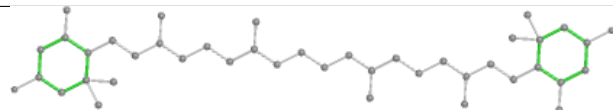
Bond lengths



Bond angles

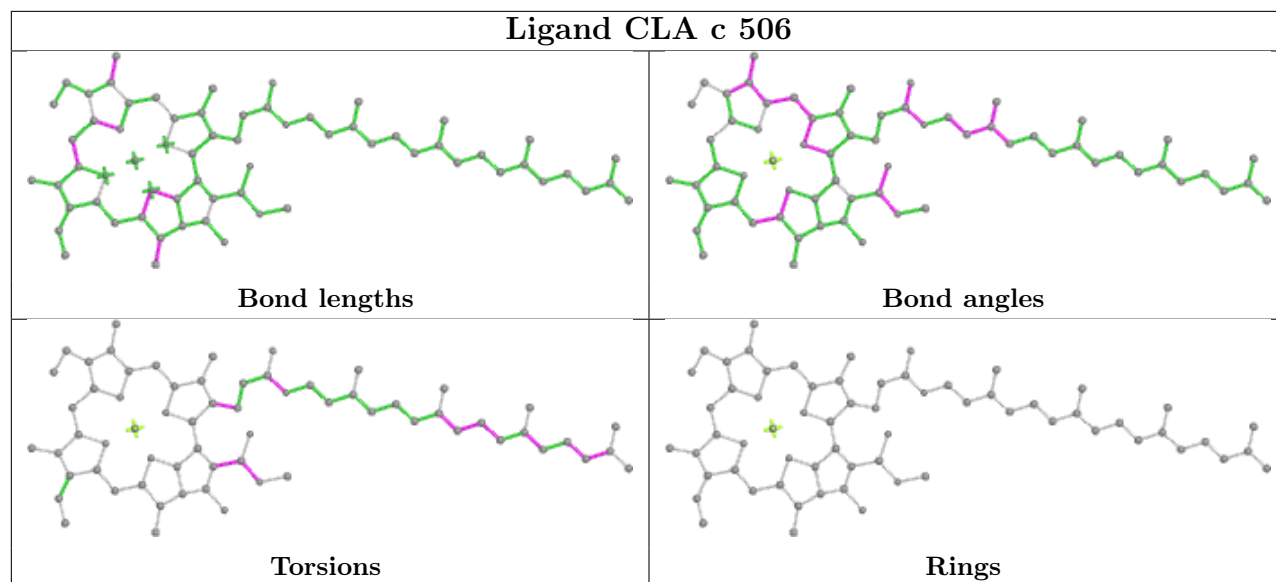


Torsions

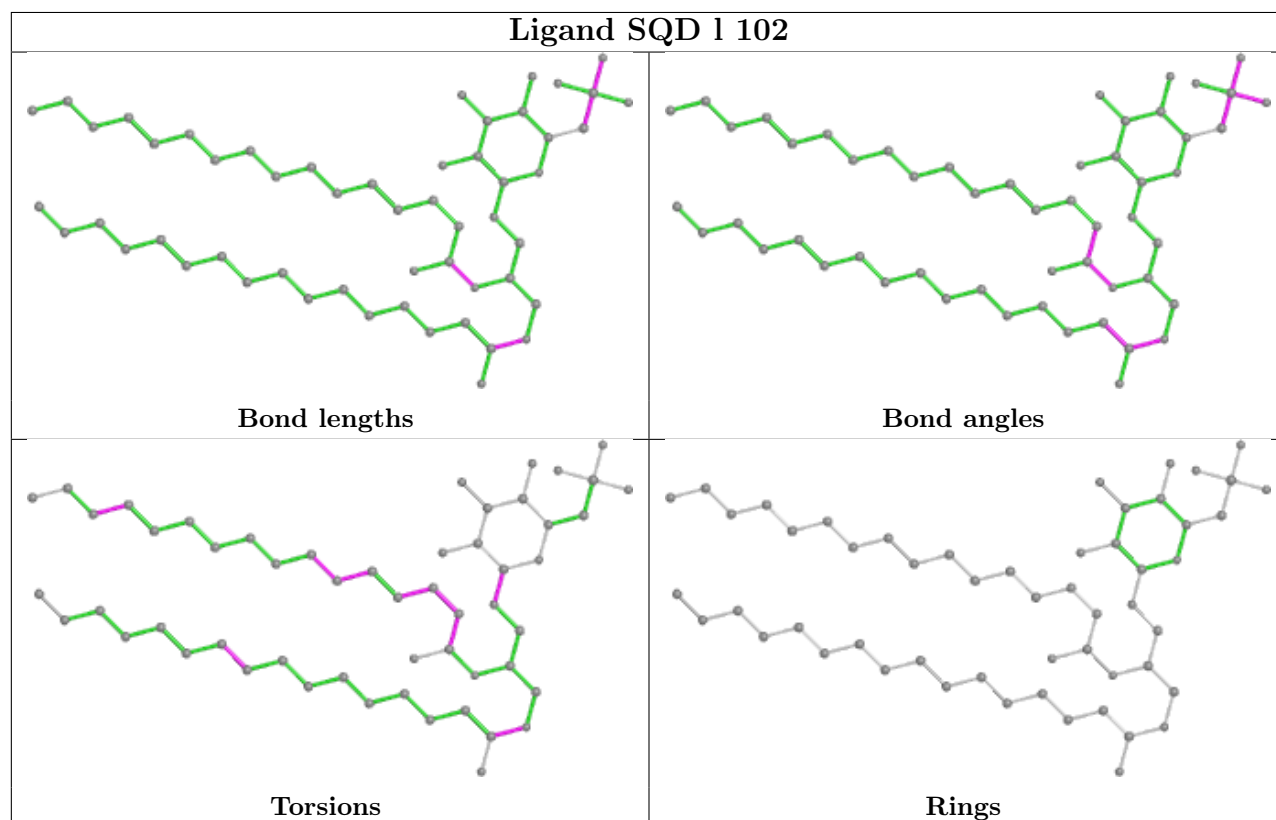


Rings

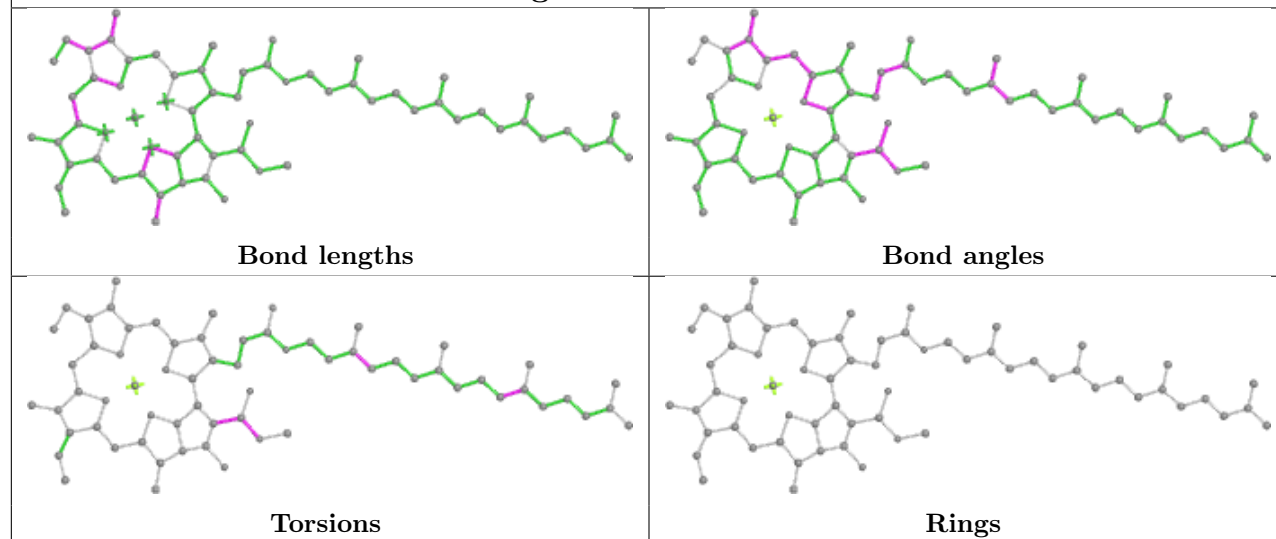
## Ligand CLA c 506



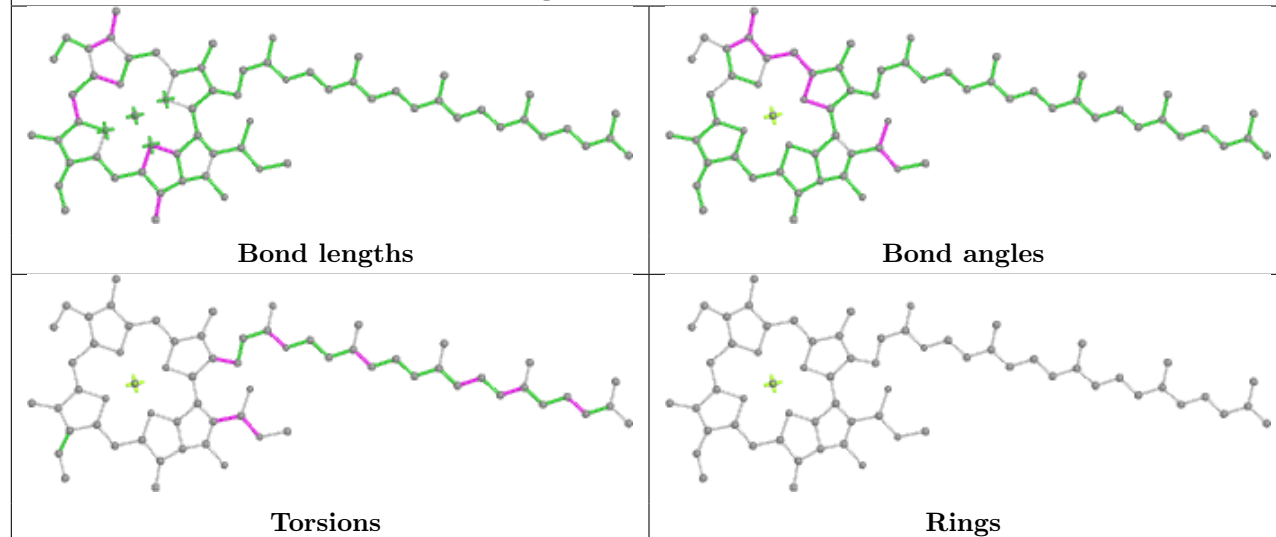
## Ligand SQD 1 102

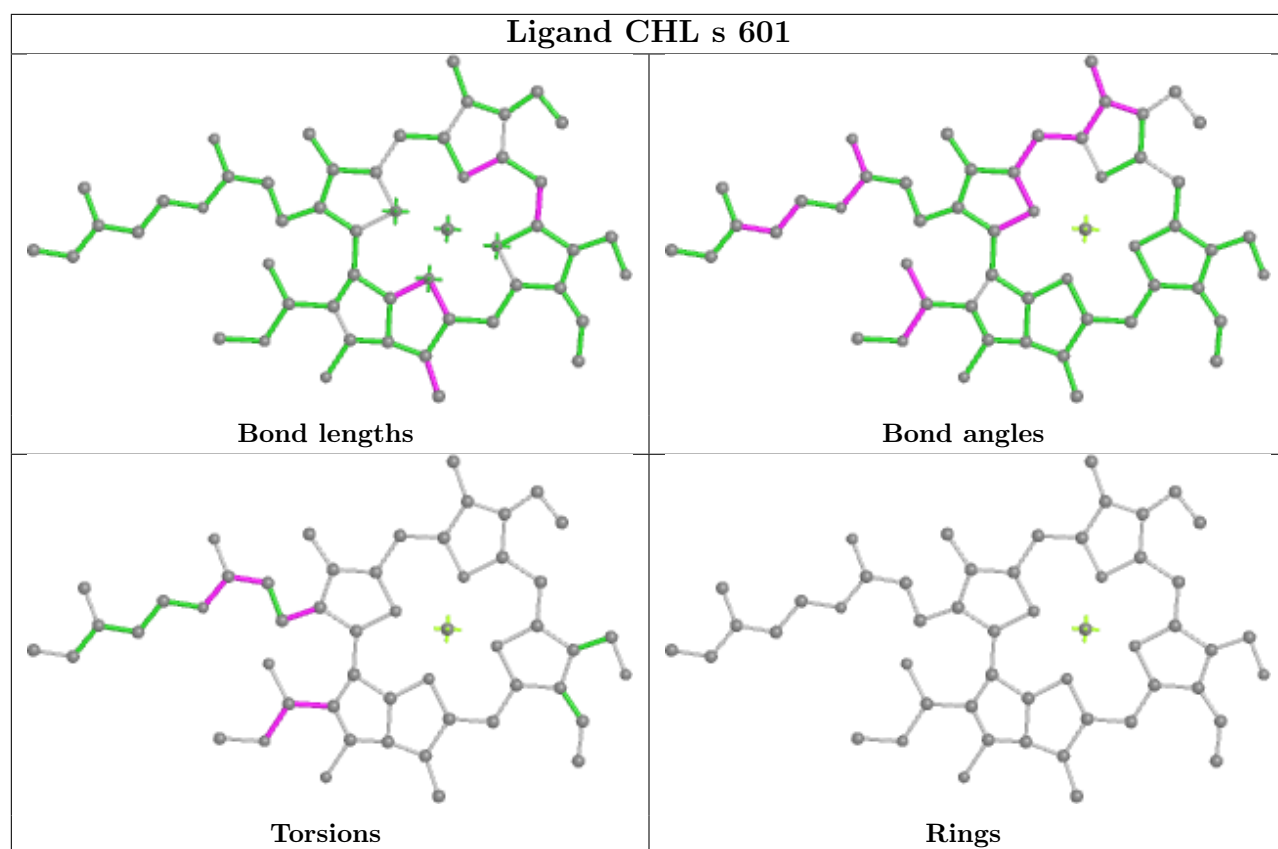


## Ligand CLA D 401

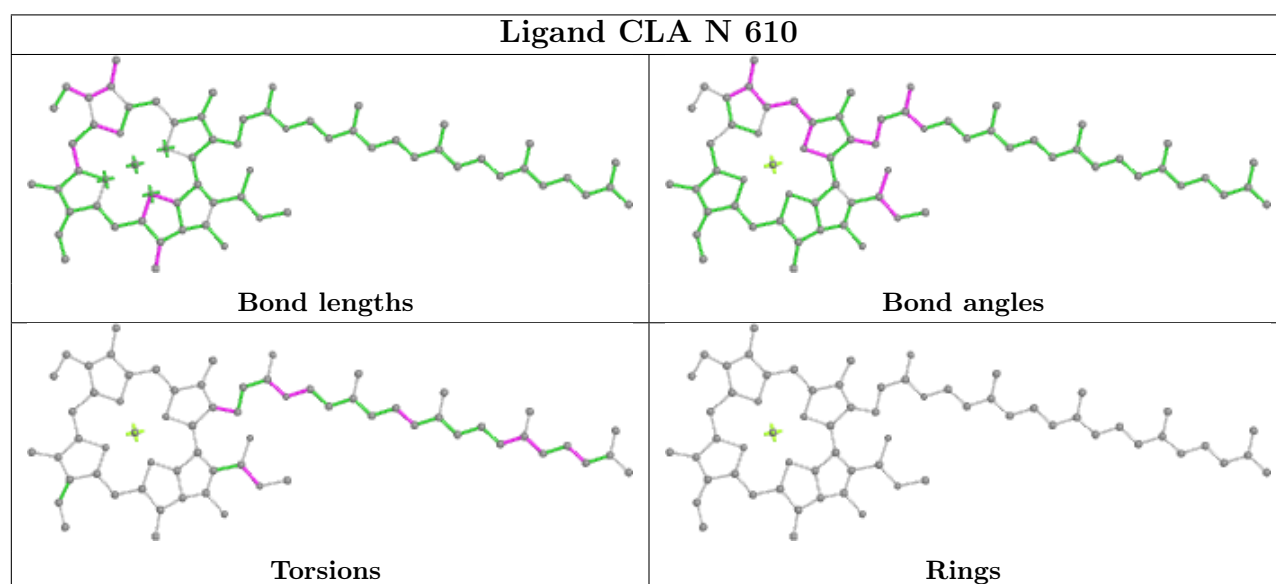
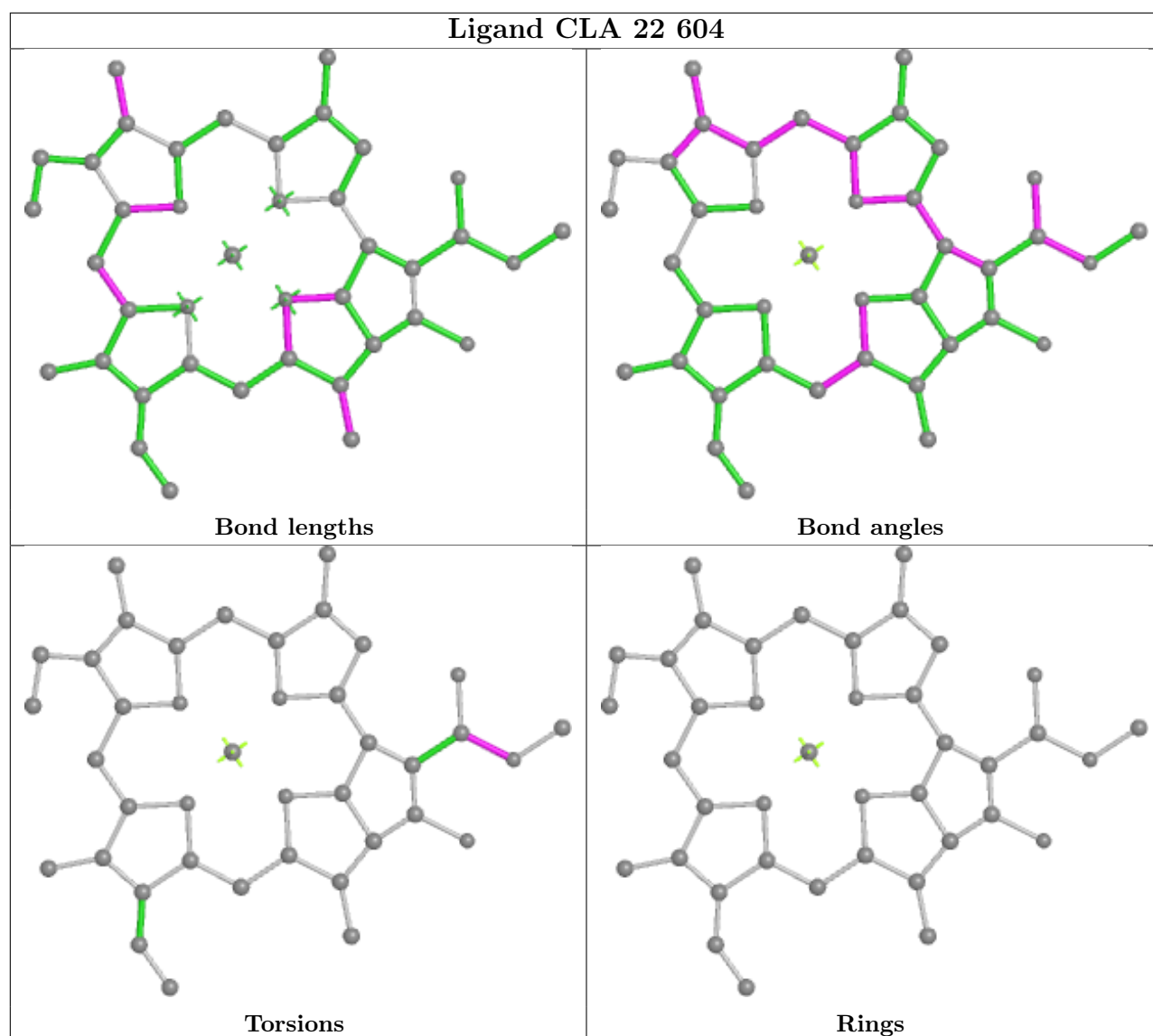


## Ligand CLA r 609

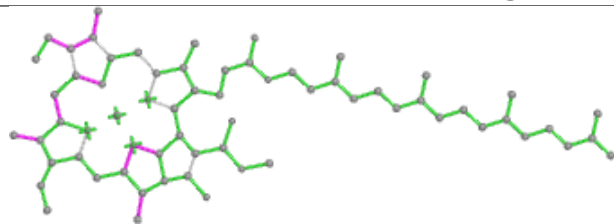




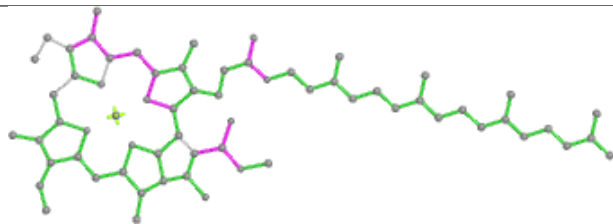




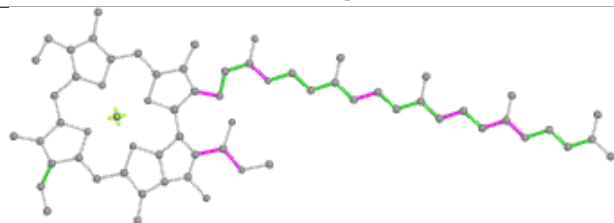
## Ligand CLA BB 603



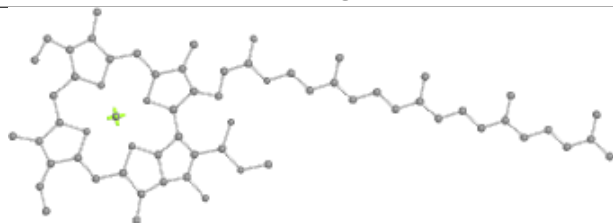
Bond lengths



Bond angles

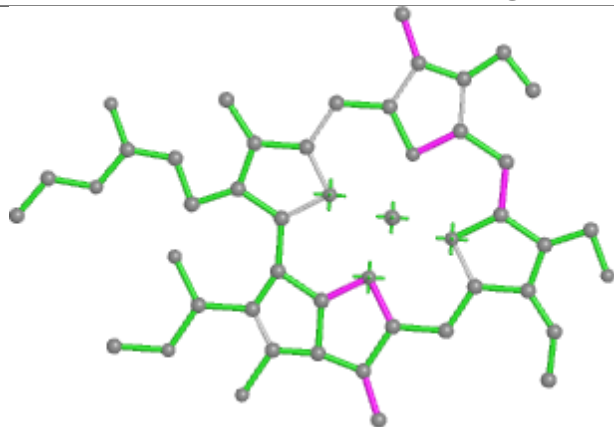


Torsions

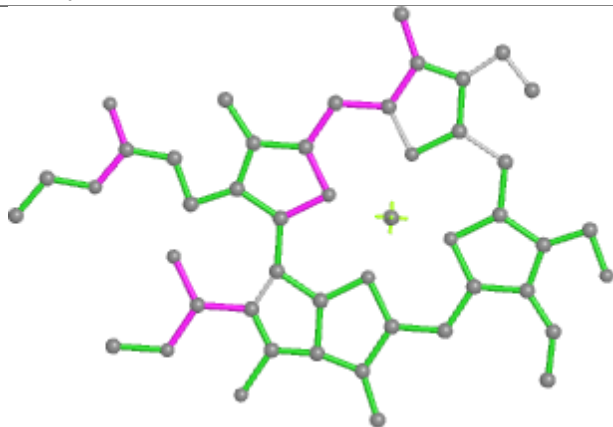


Rings

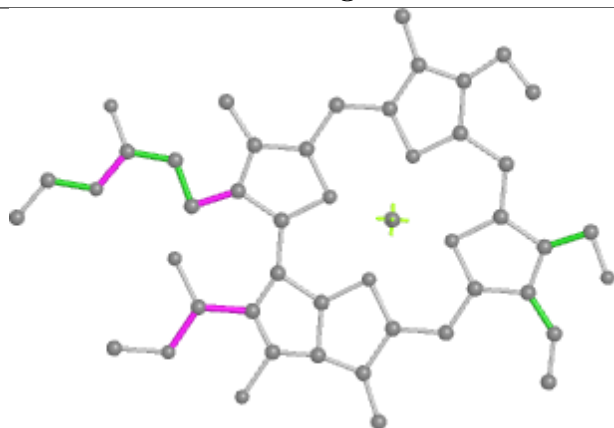
## Ligand CHL Yy 605



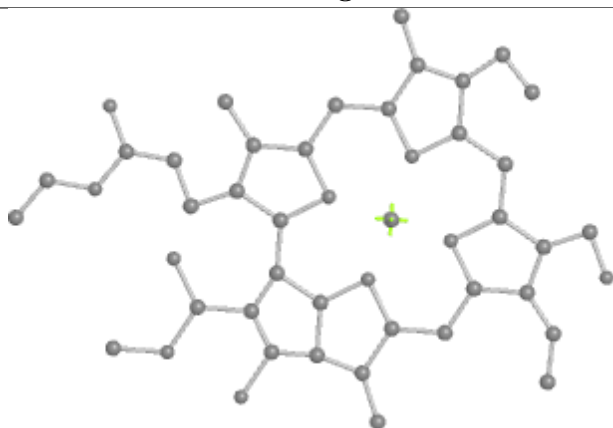
Bond lengths



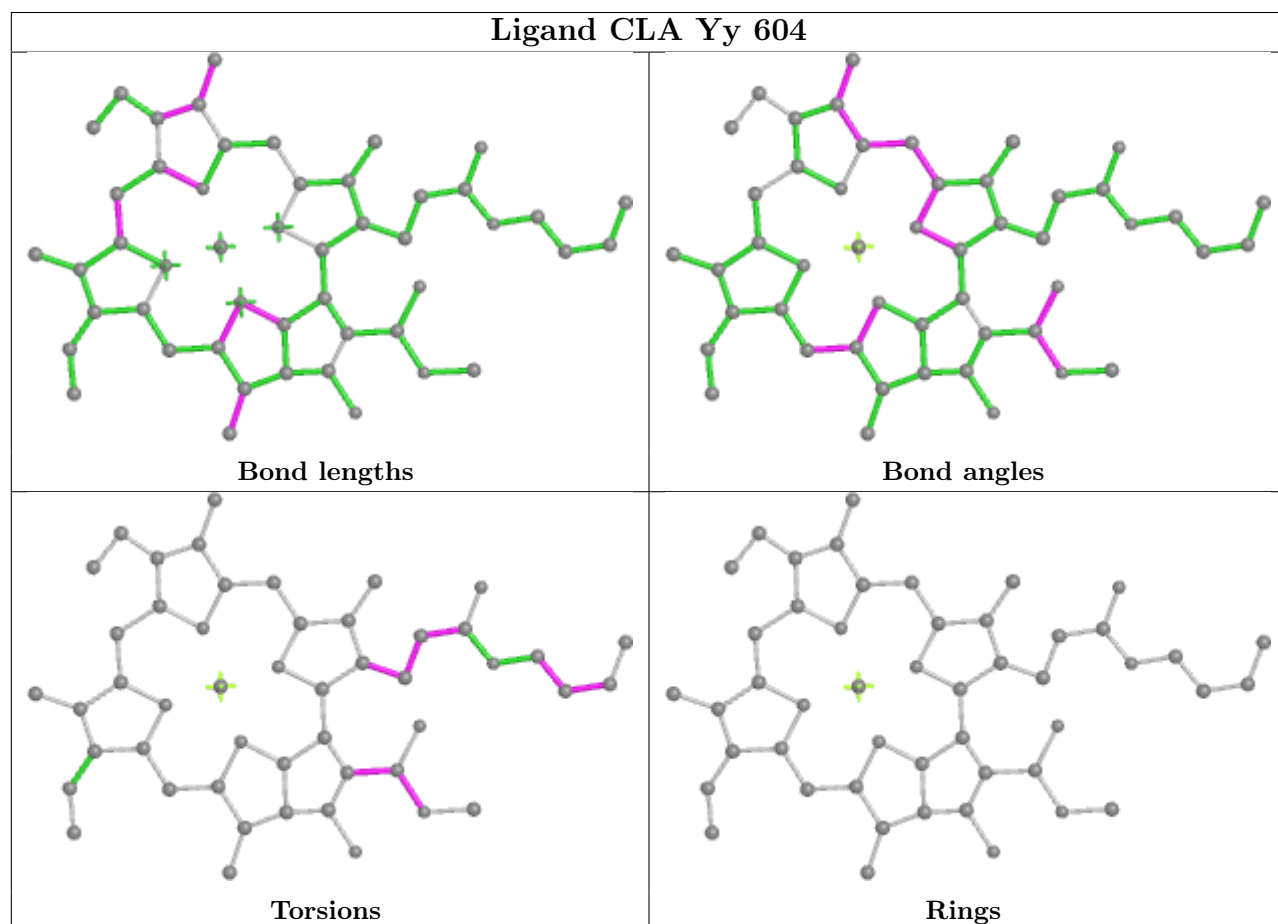
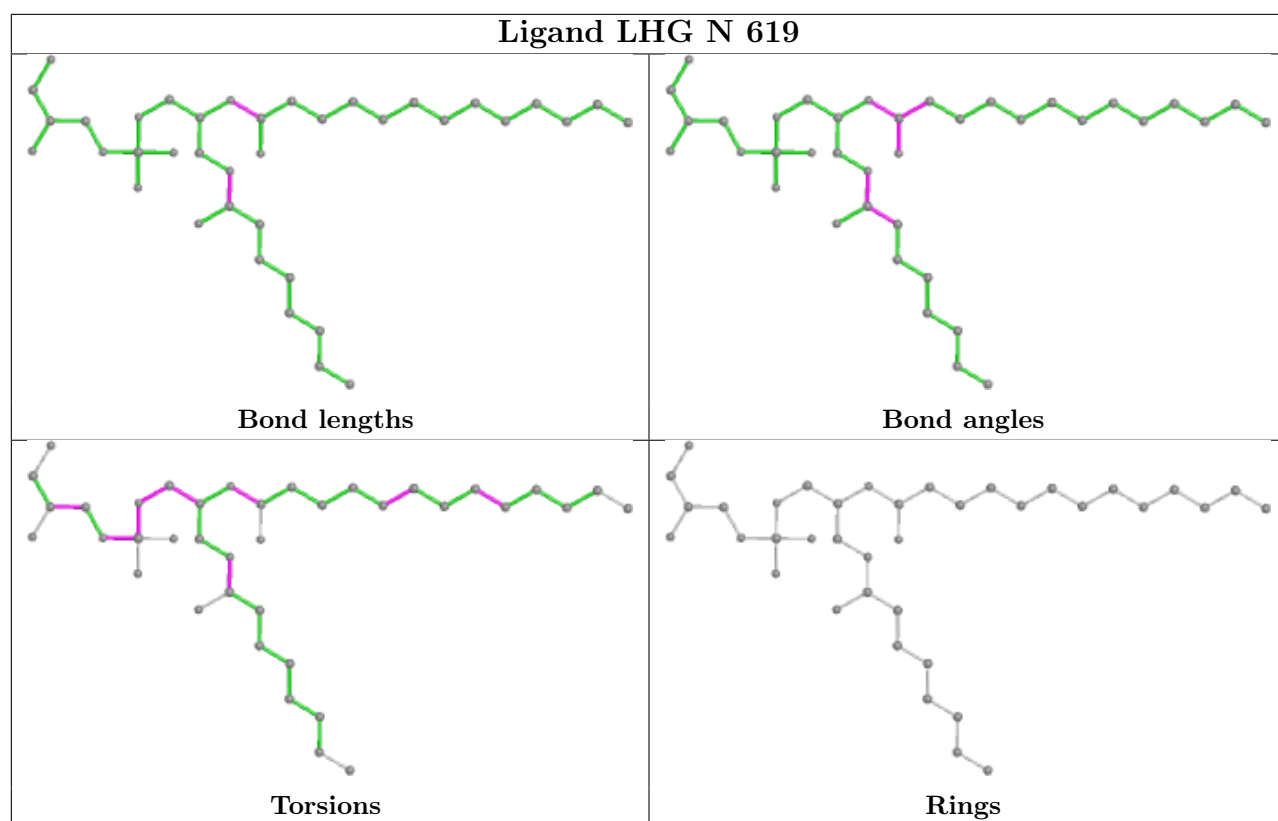
Bond angles

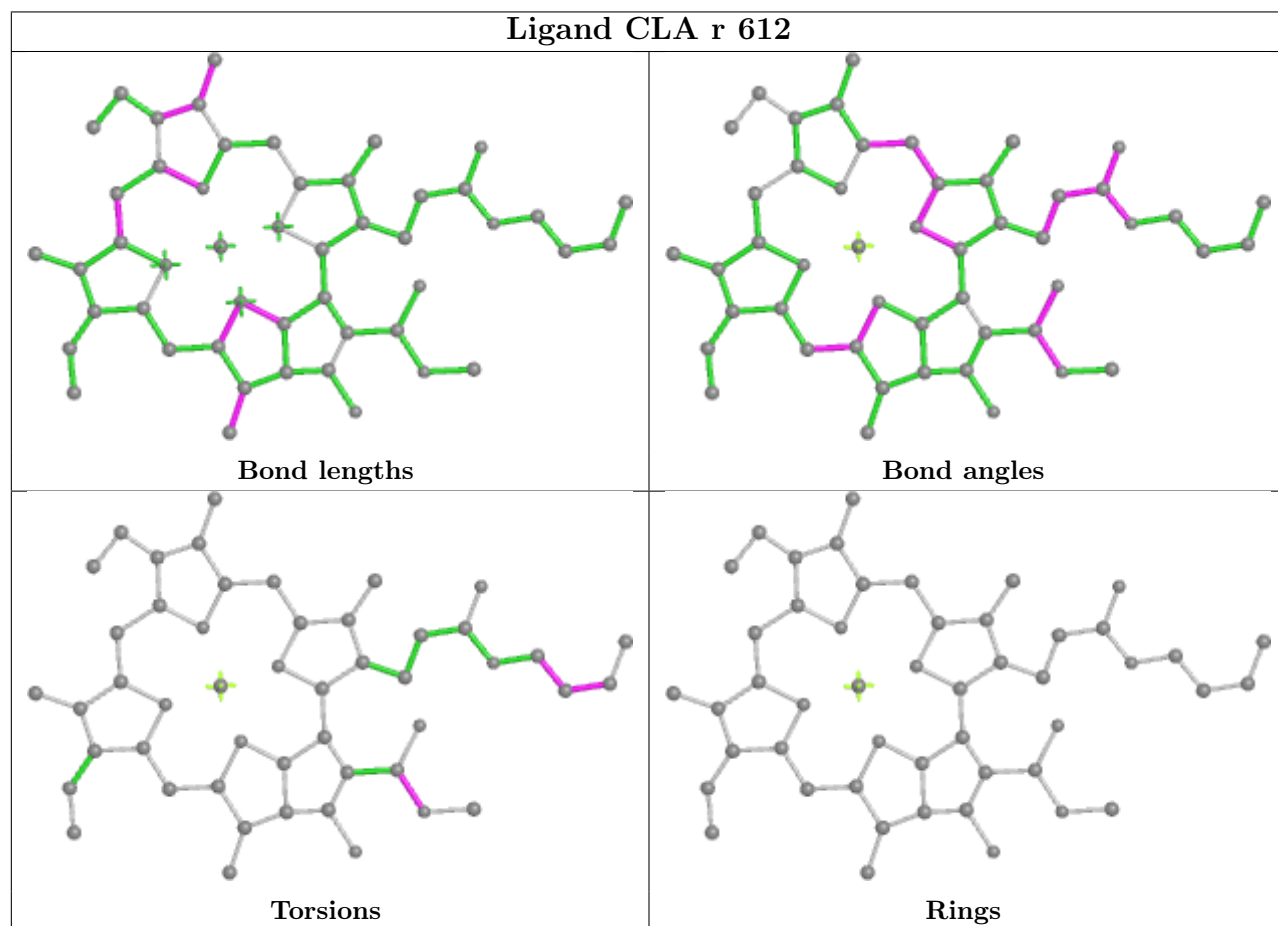
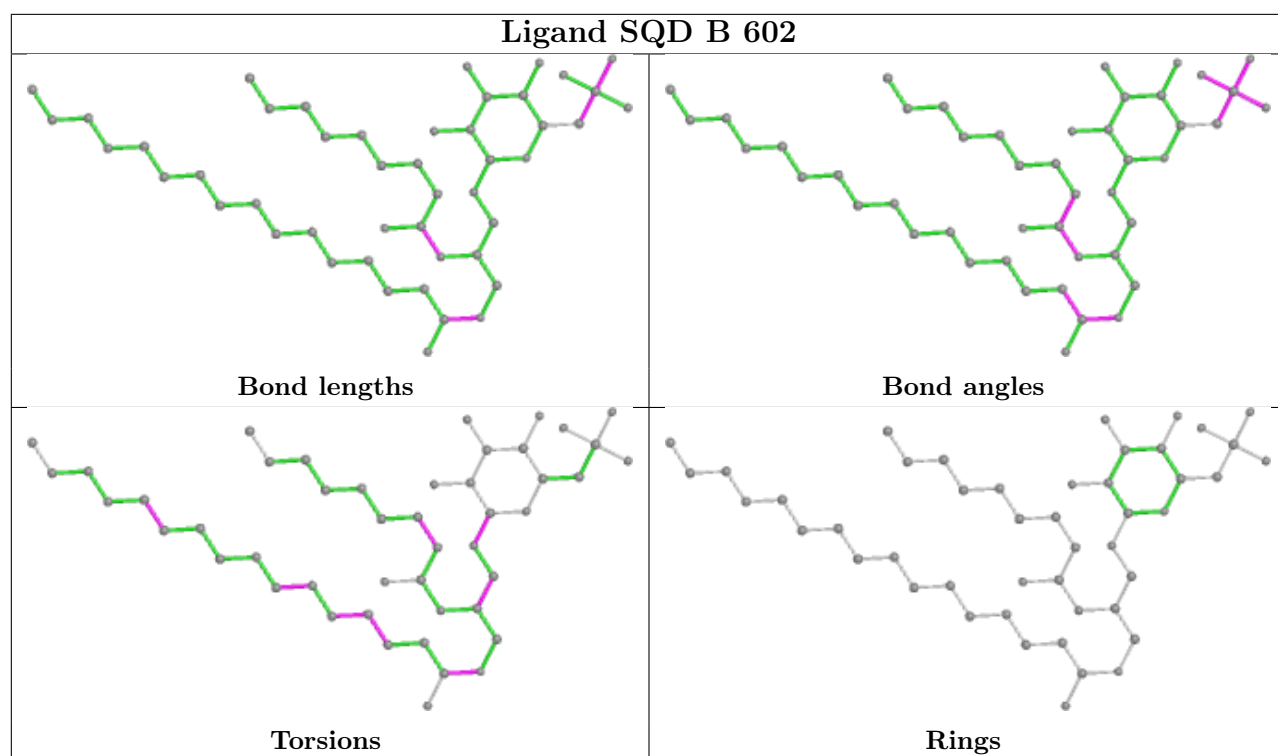


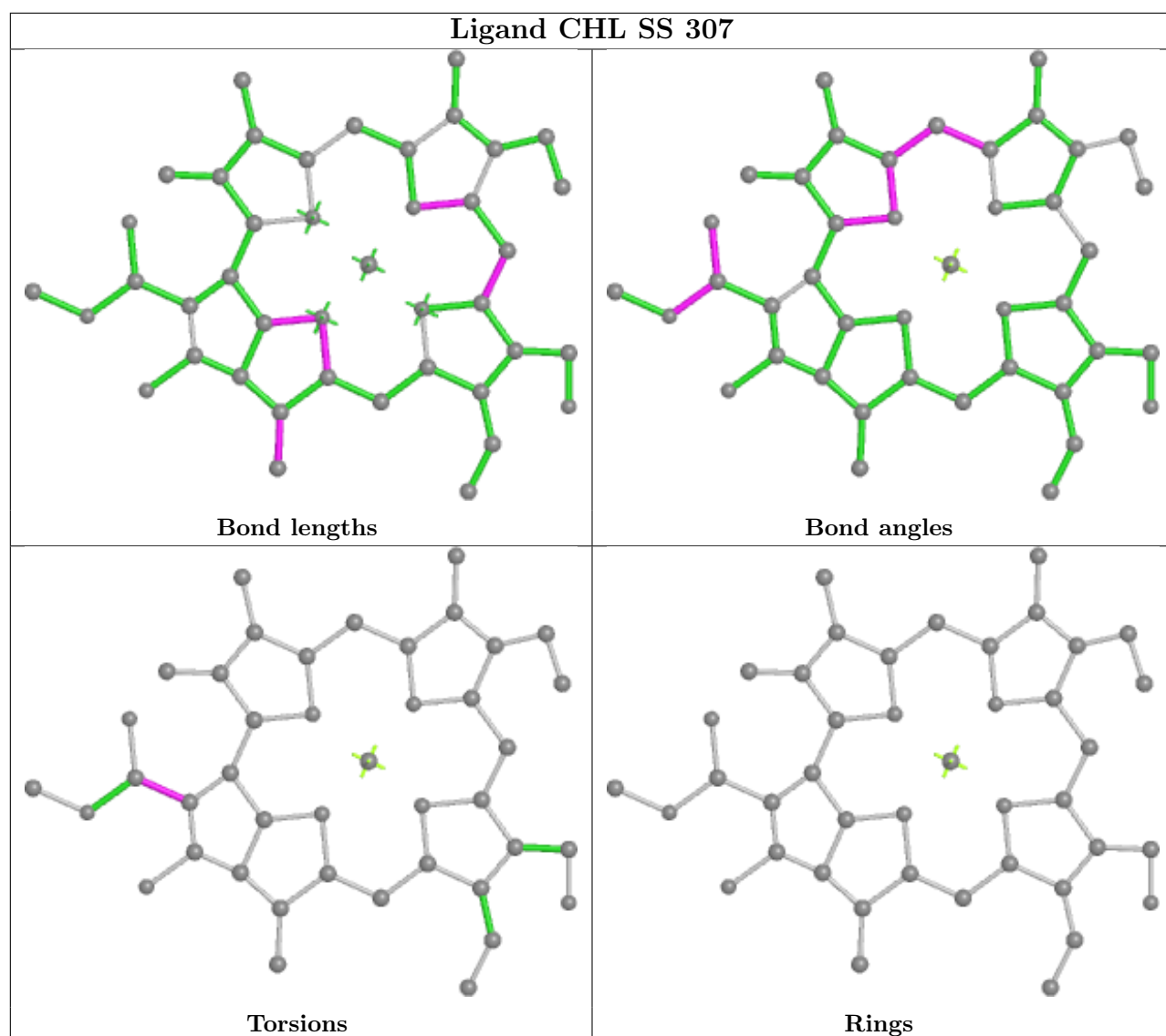
Torsions

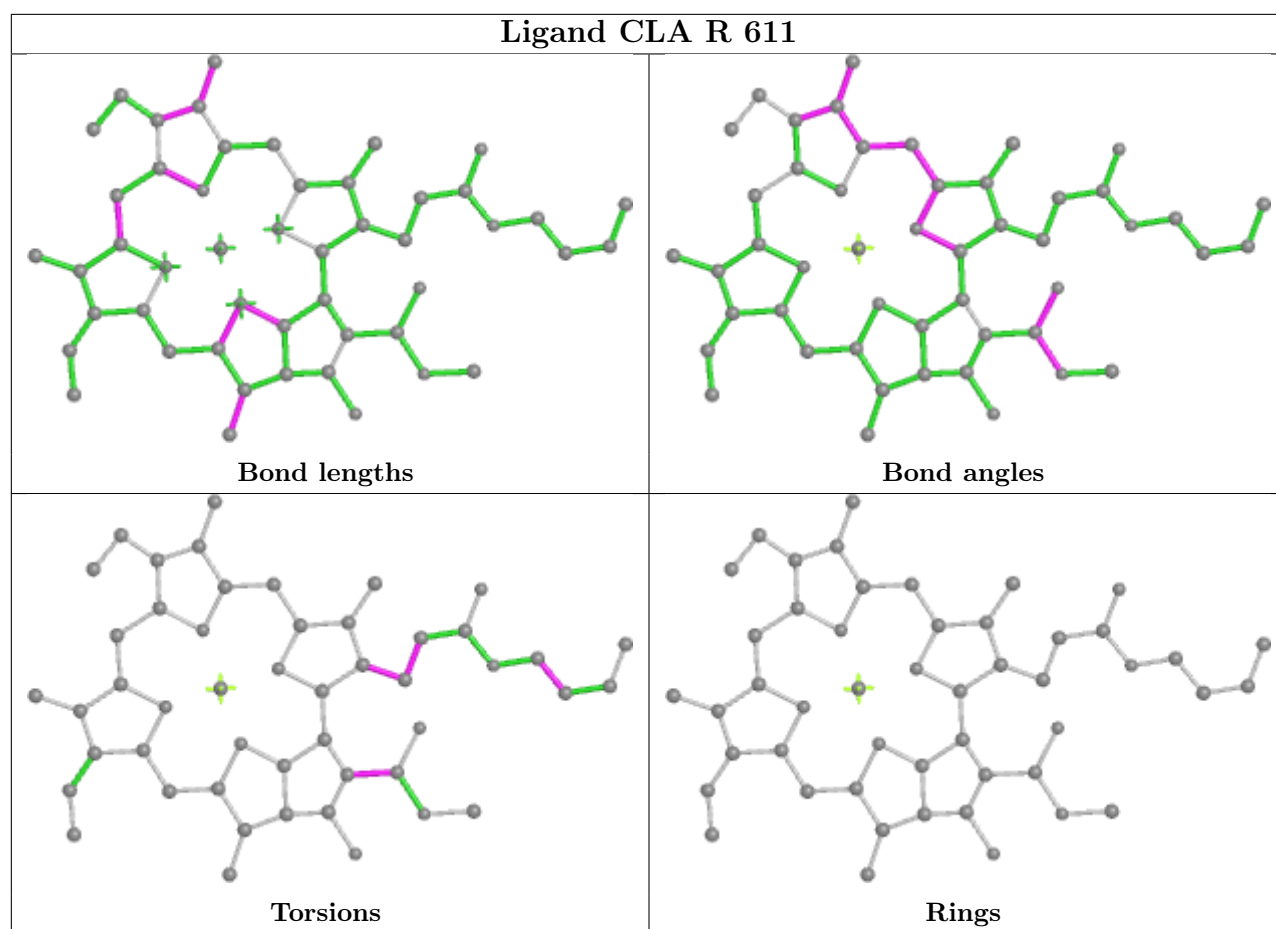


Rings

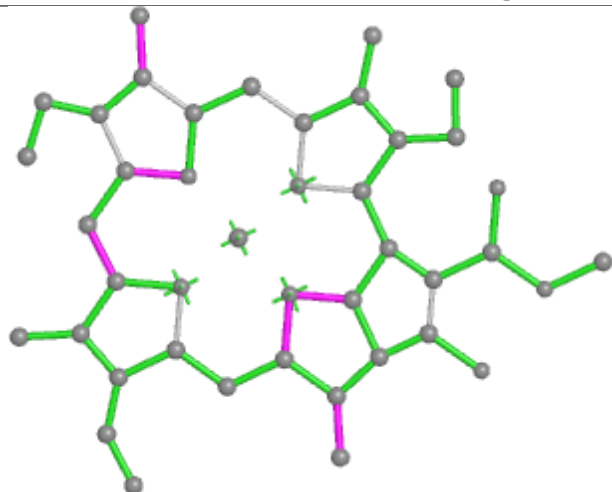




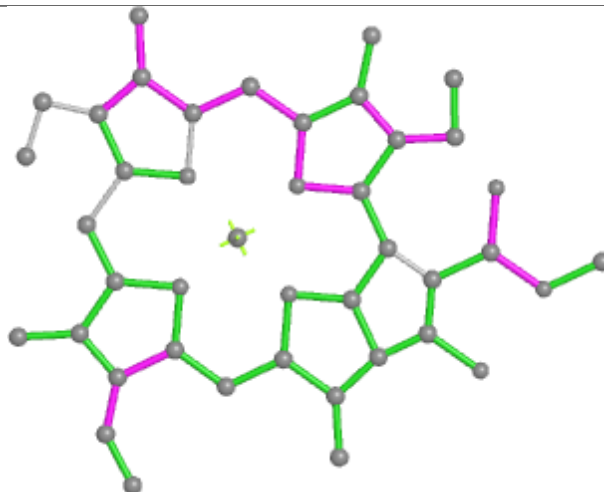




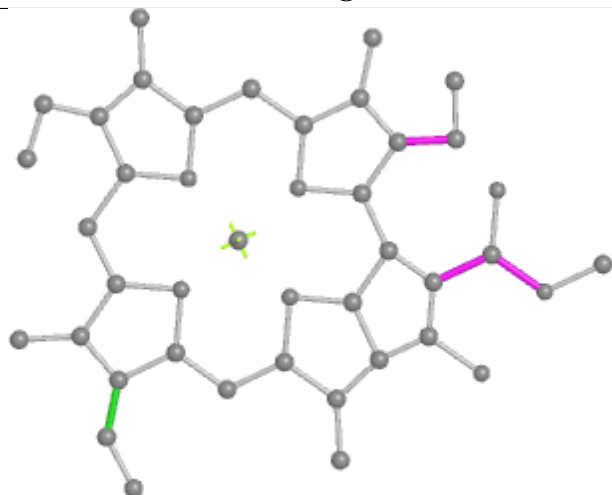
## Ligand CLA NN 612



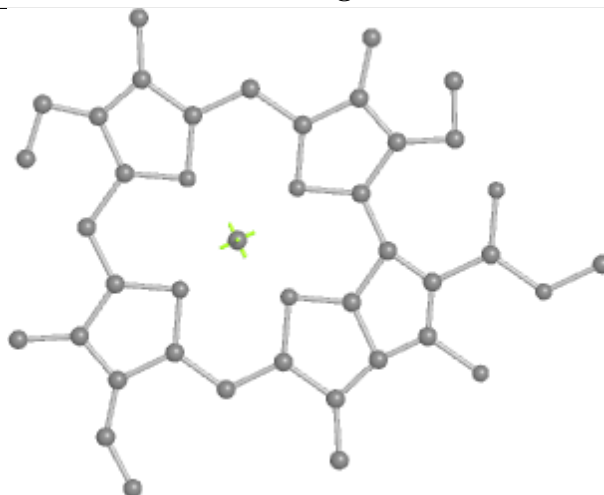
Bond lengths



Bond angles

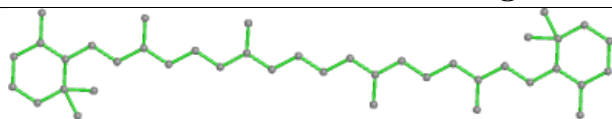


Torsions

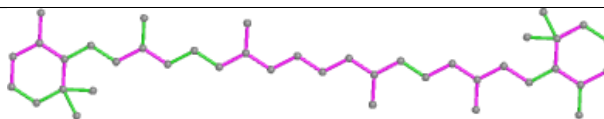


Rings

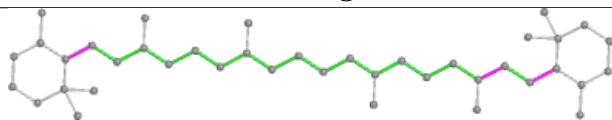
## Ligand BCR BB 620



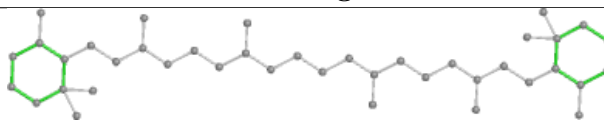
Bond lengths



Bond angles

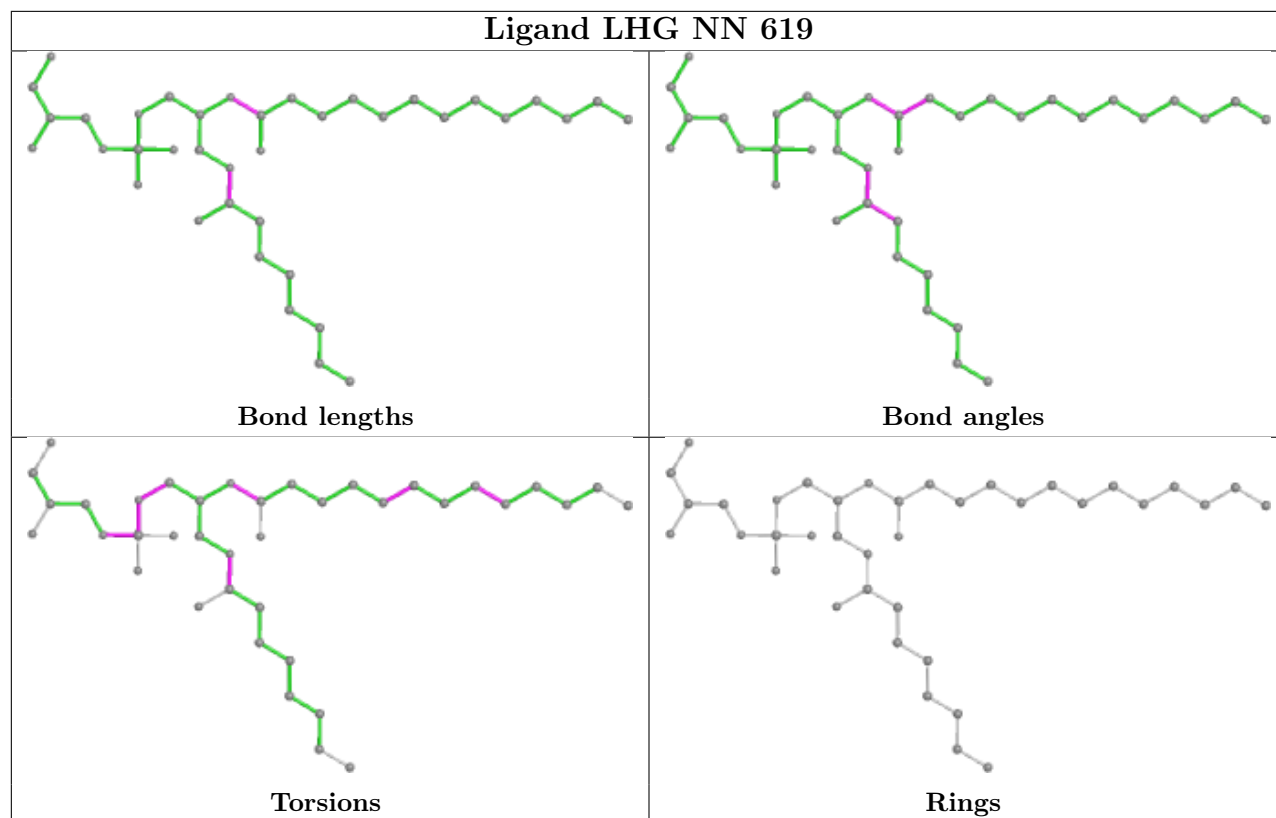


Torsions

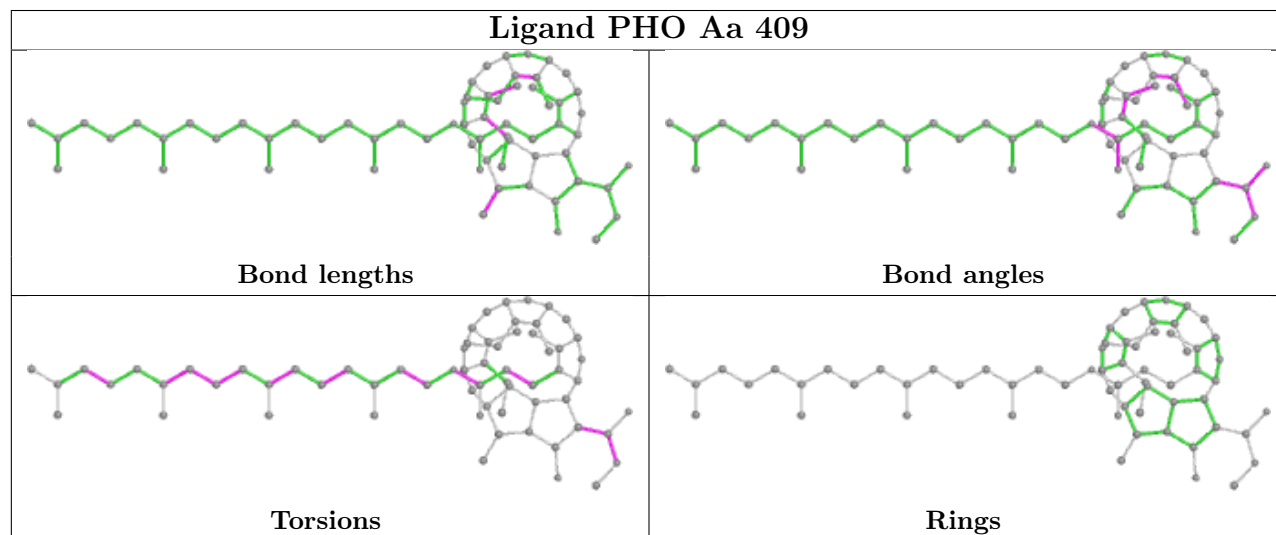


Rings

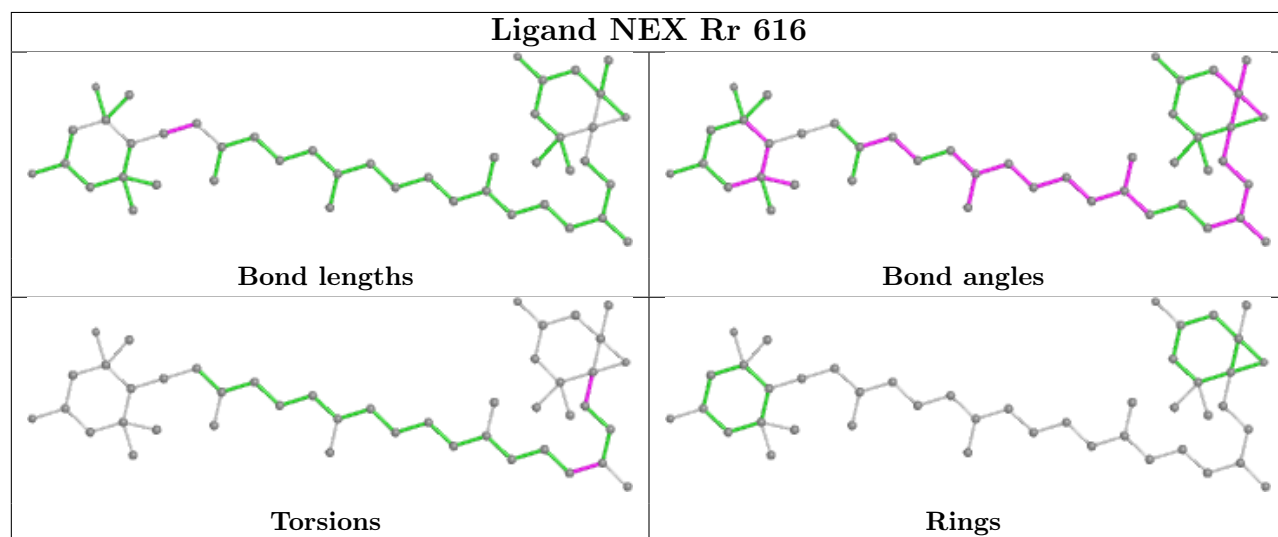
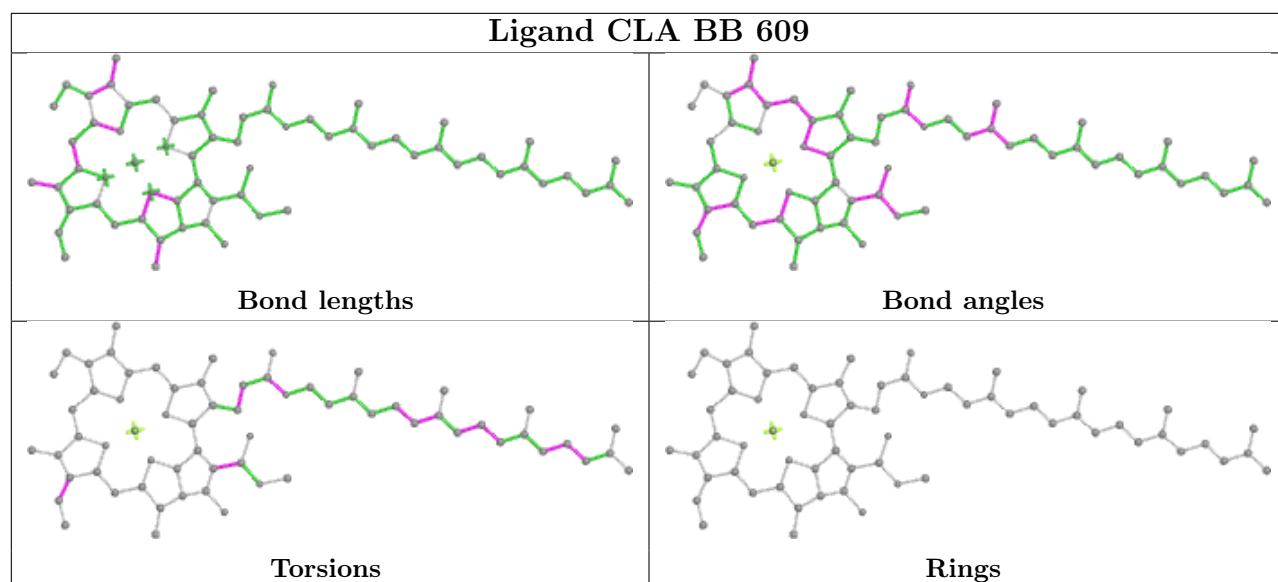
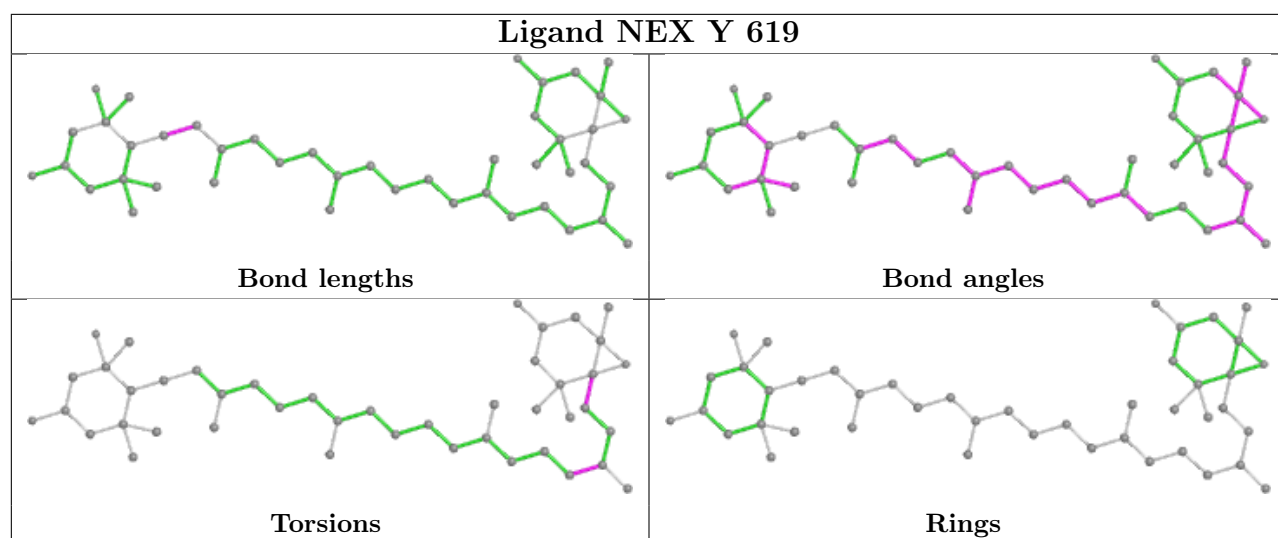
## Ligand LHG NN 619



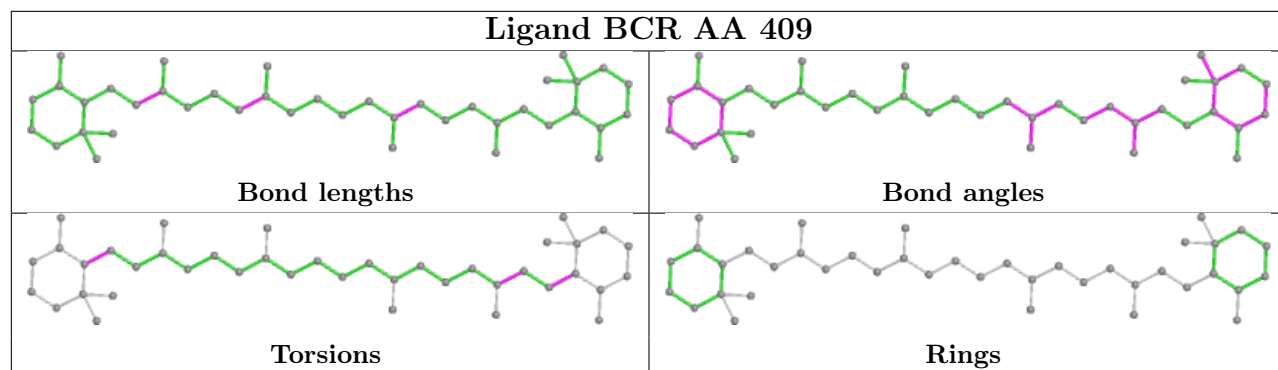
## Ligand PHO Aa 409



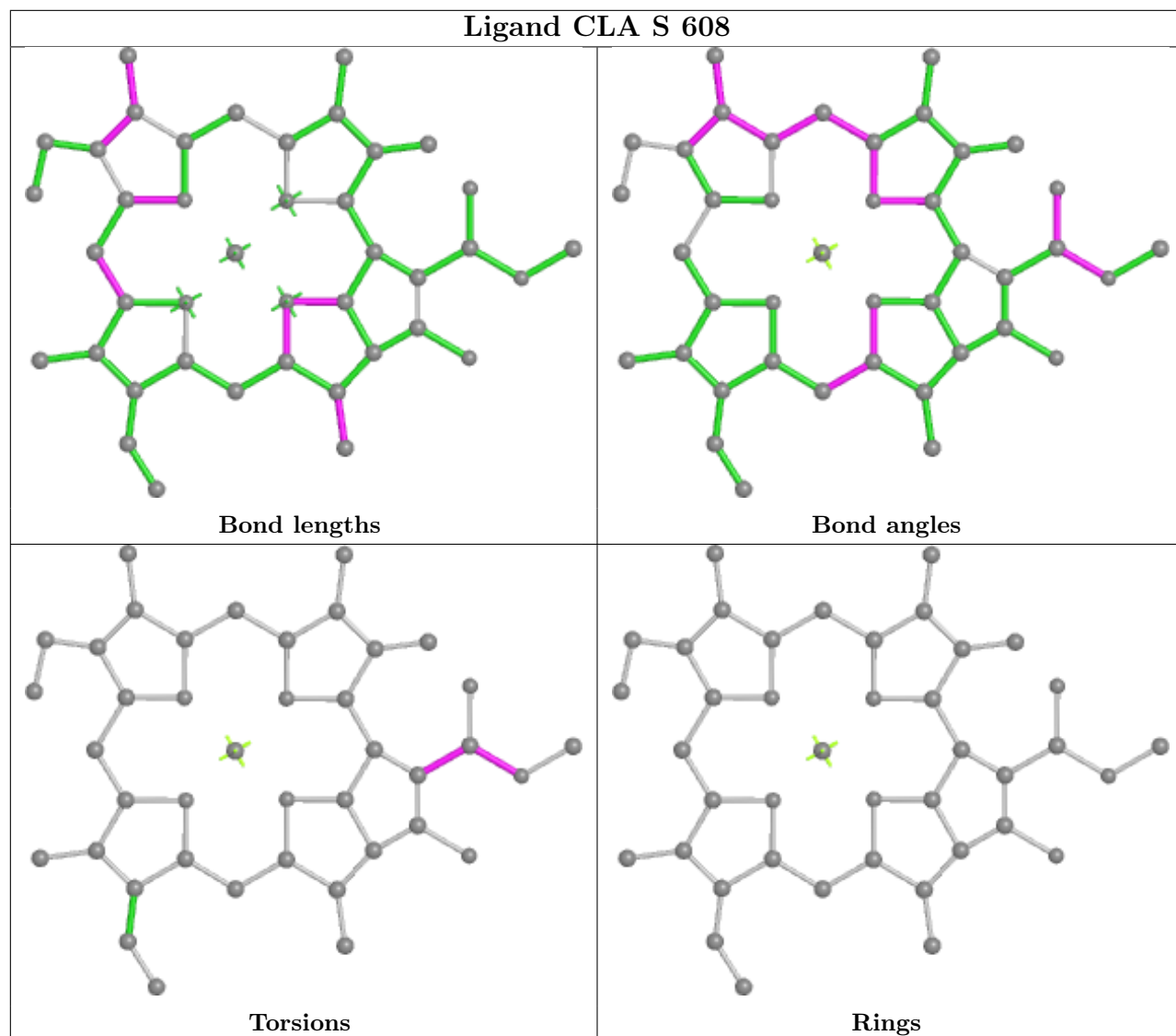




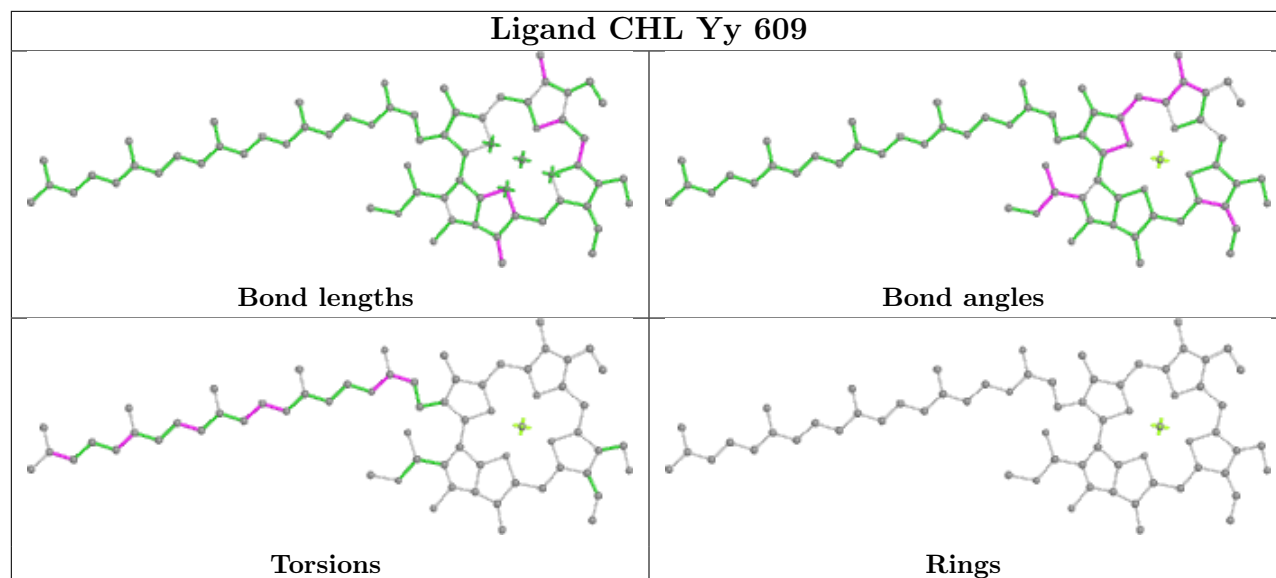
## Ligand BCR AA 409



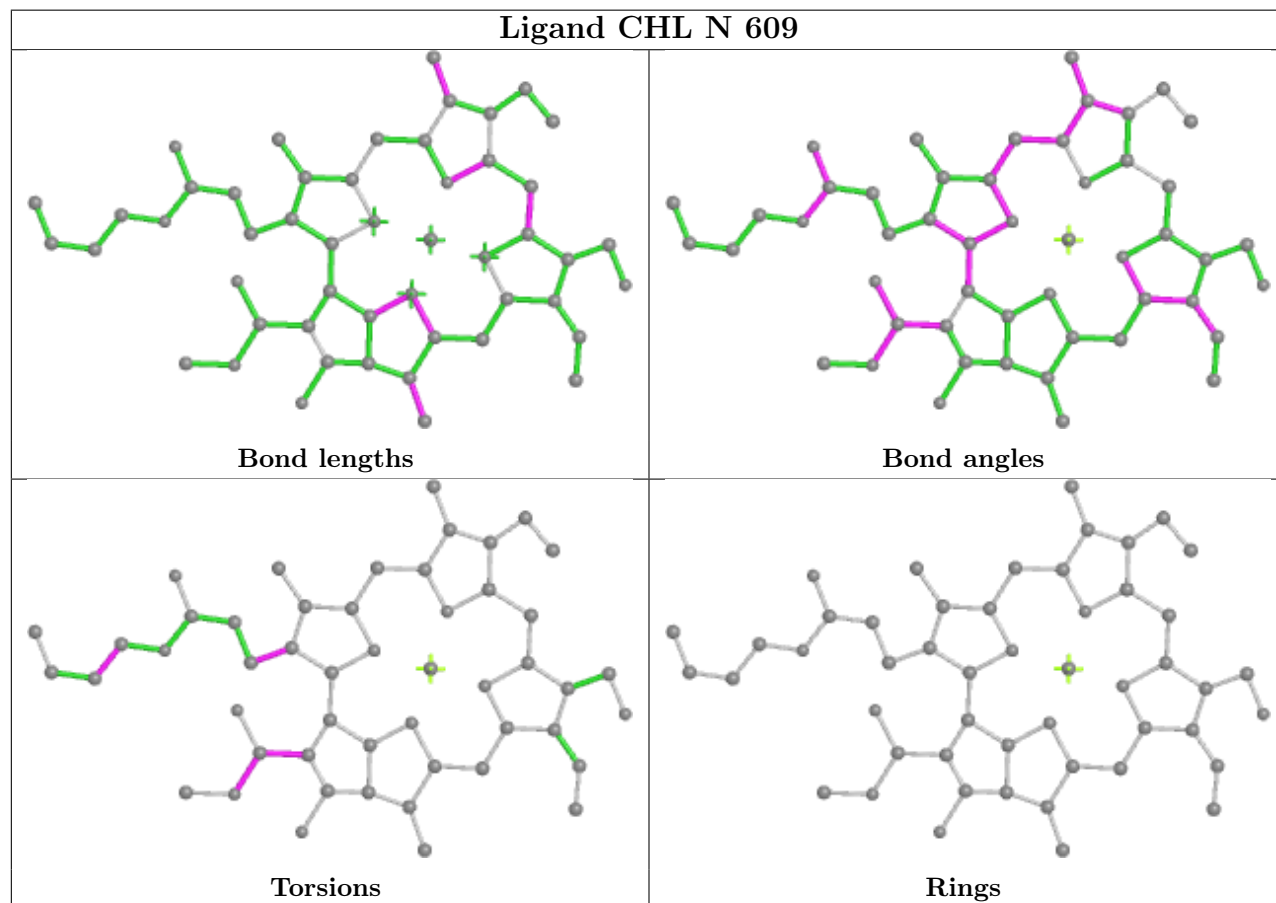
## Ligand CLA S 608

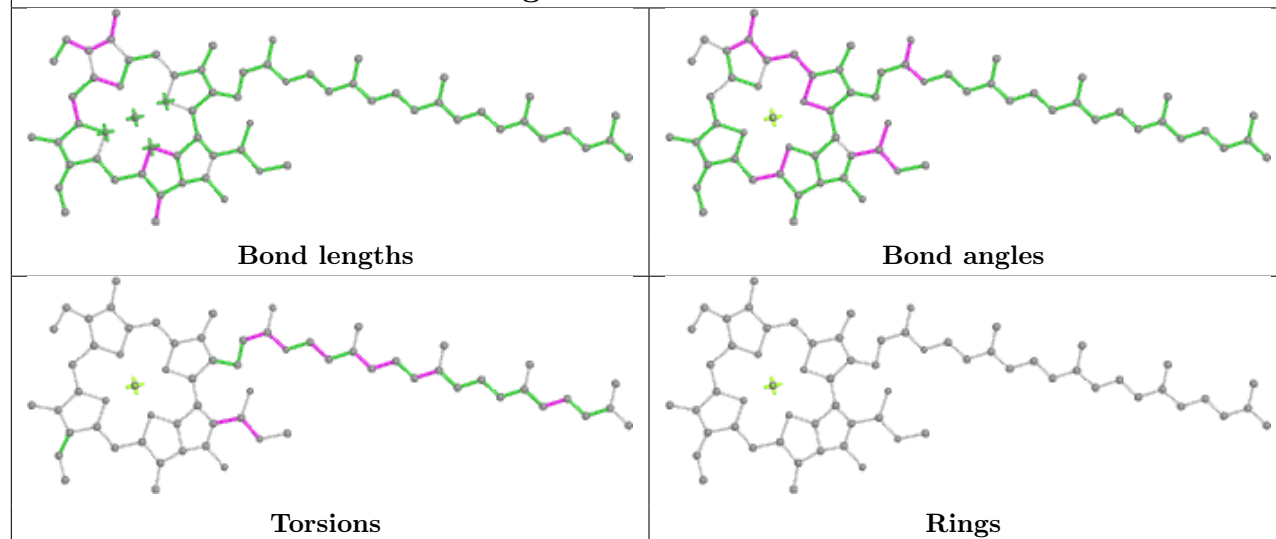
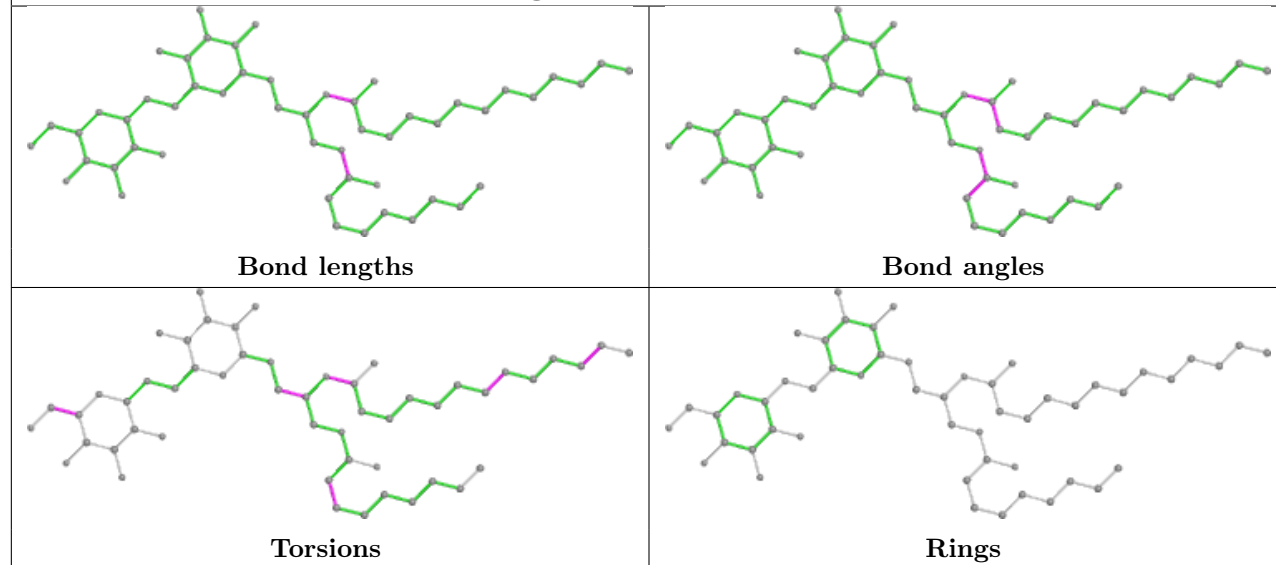


## Ligand CHL Yy 609

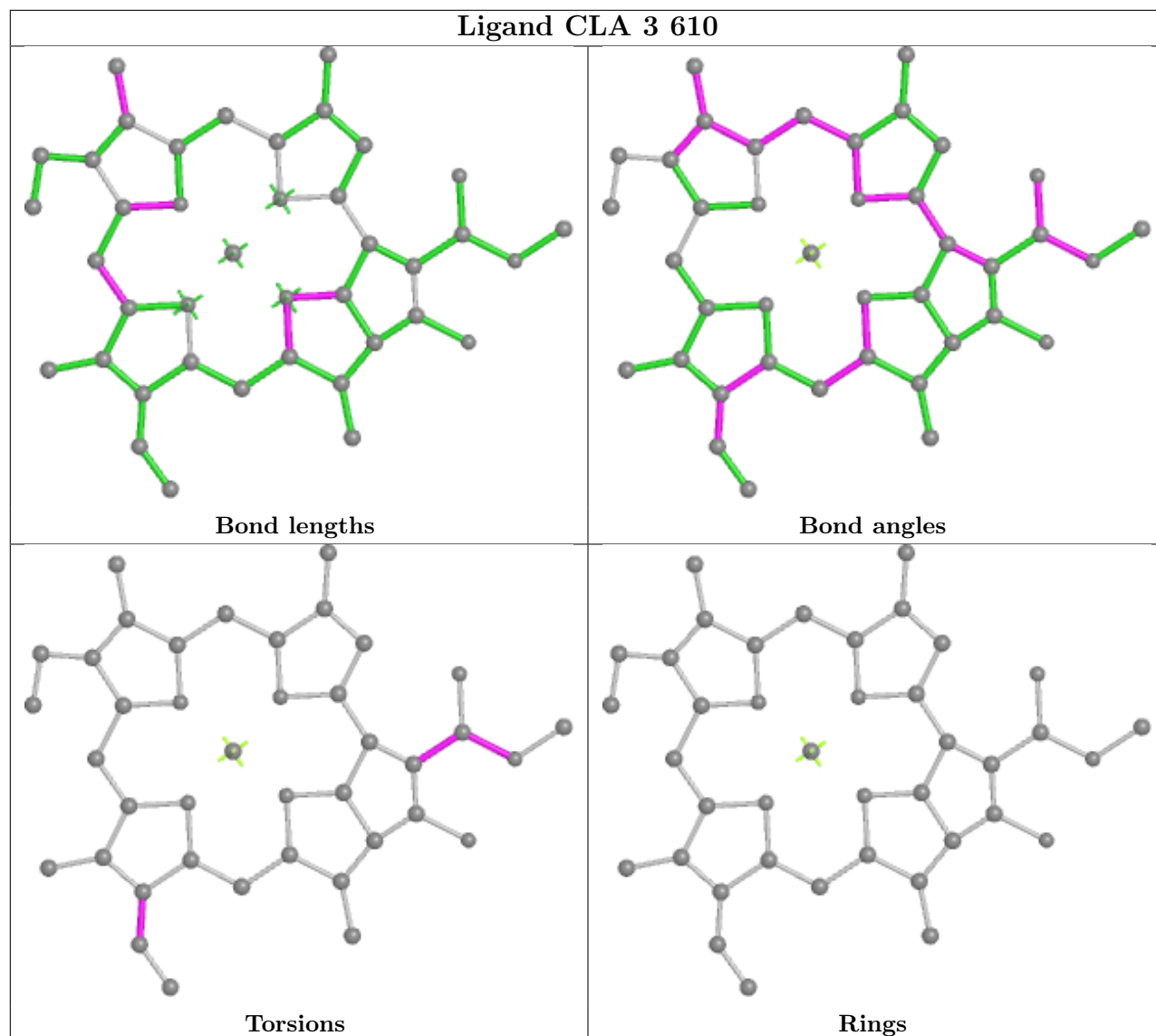


## Ligand CHL N 609

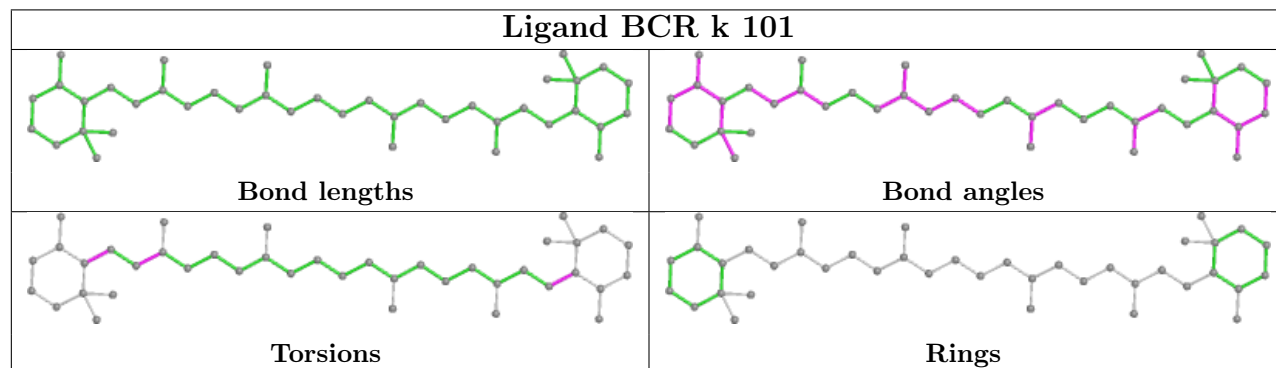


**Ligand CLA Bb 613****Ligand DGD C 523**

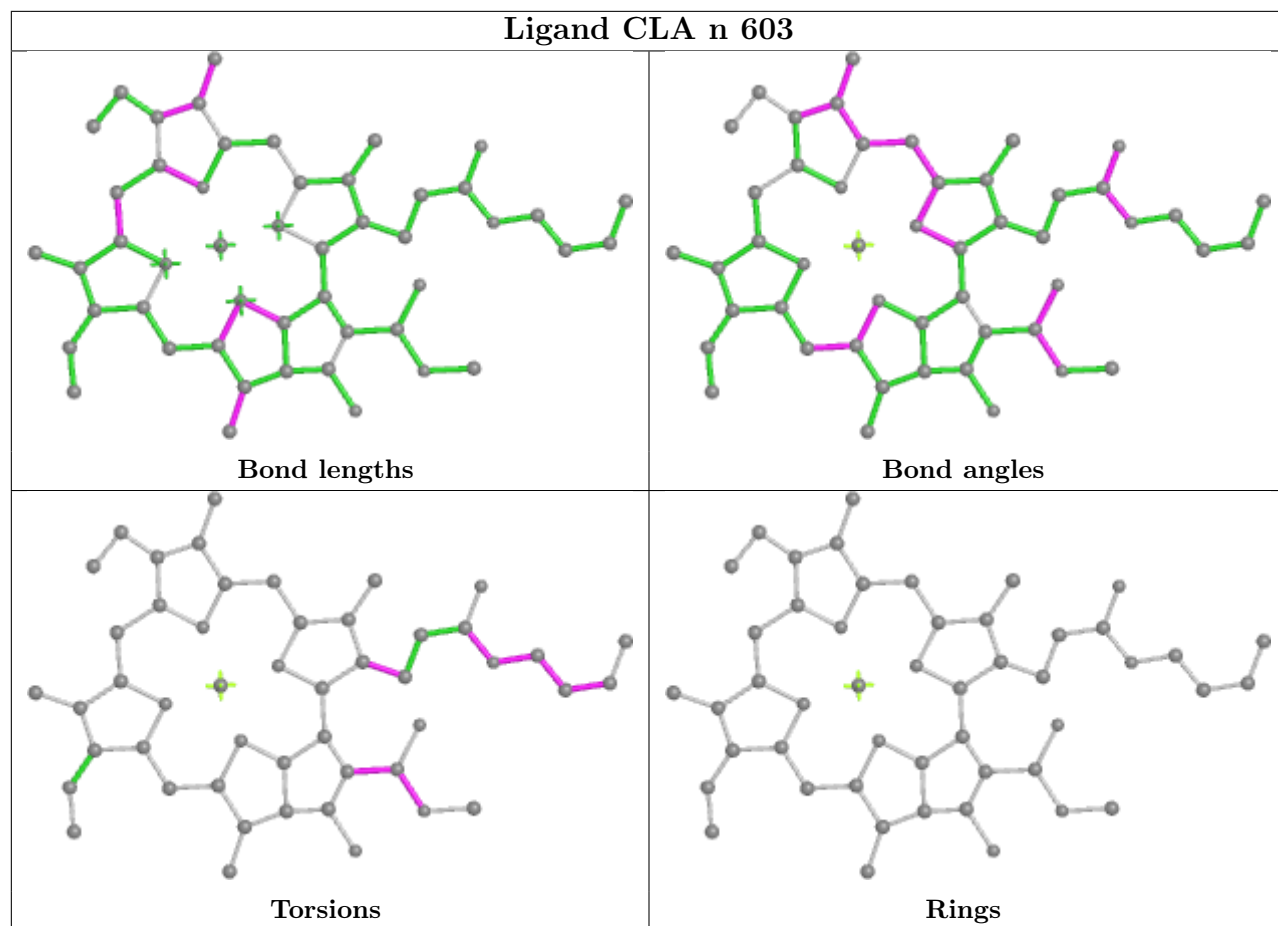
## Ligand CLA 3 610

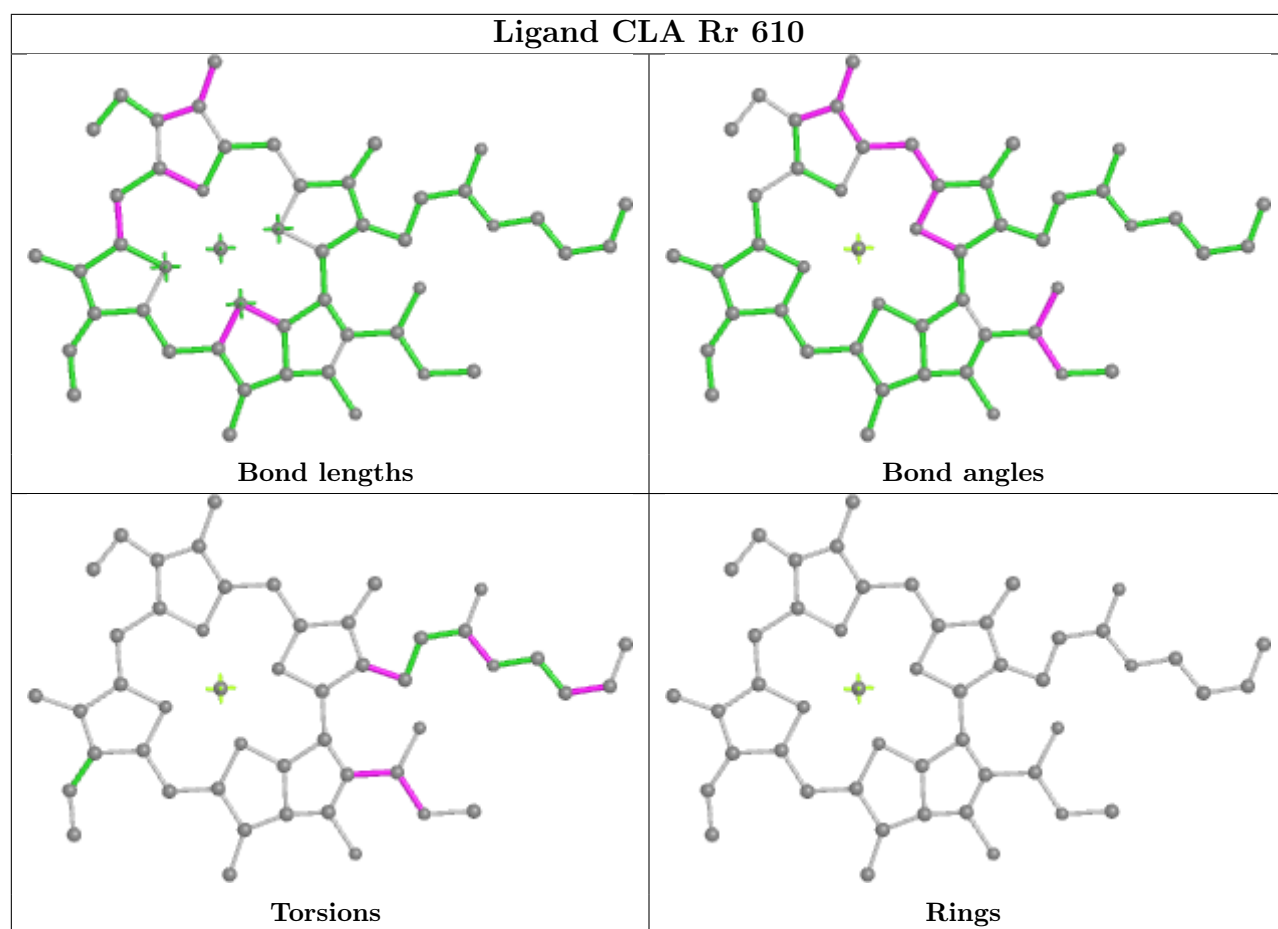


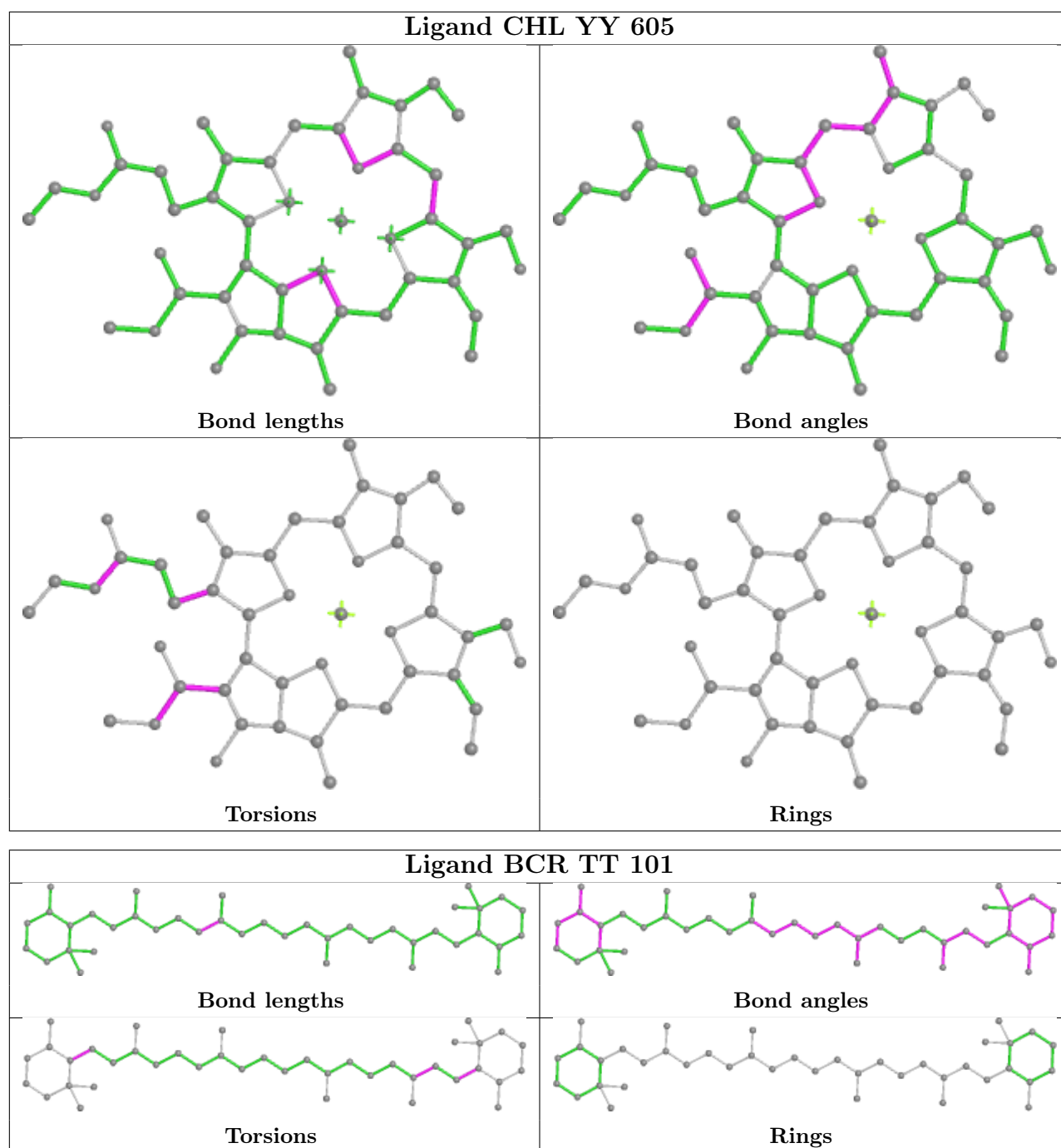
## Ligand BCR k 101



## Ligand CLA n 603

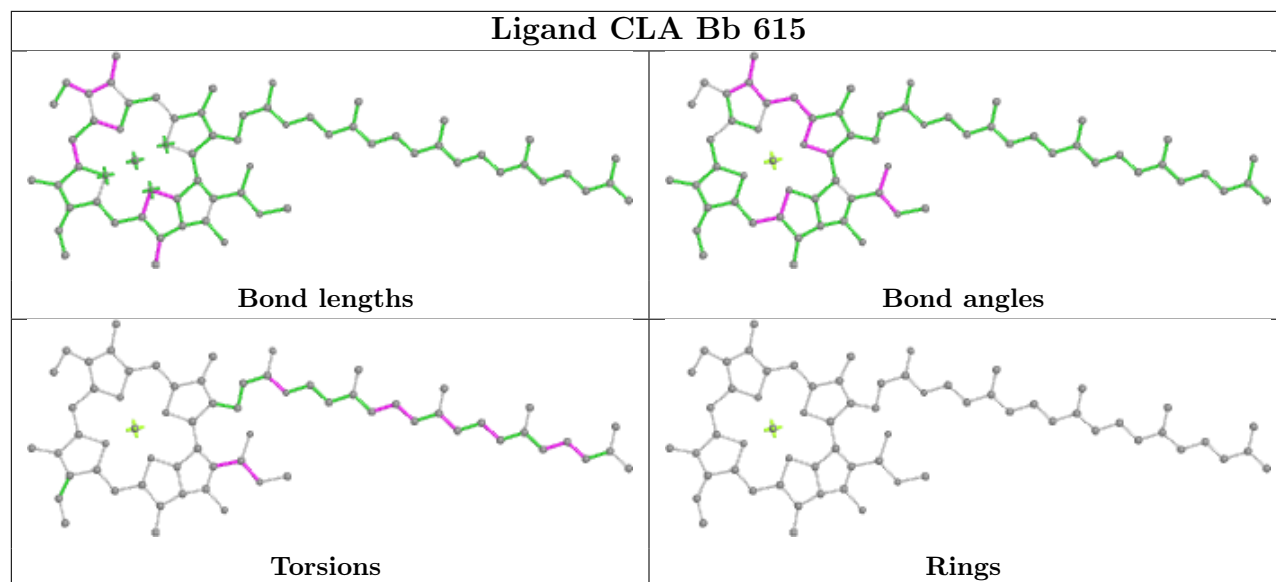




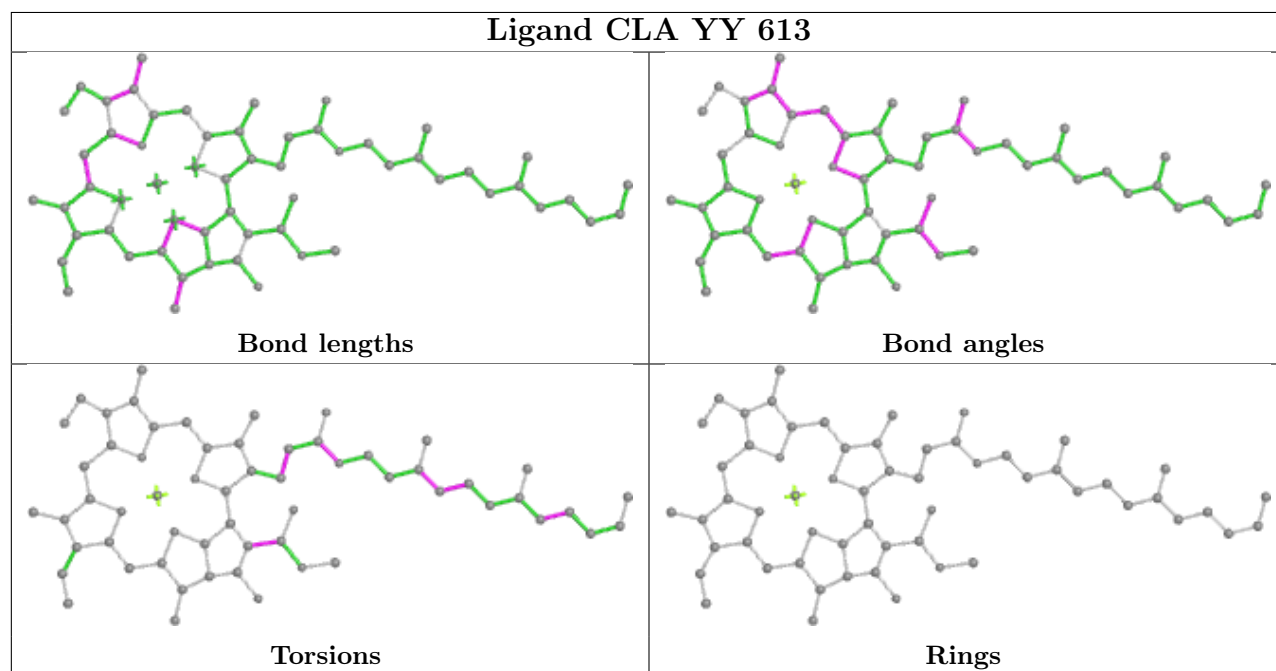




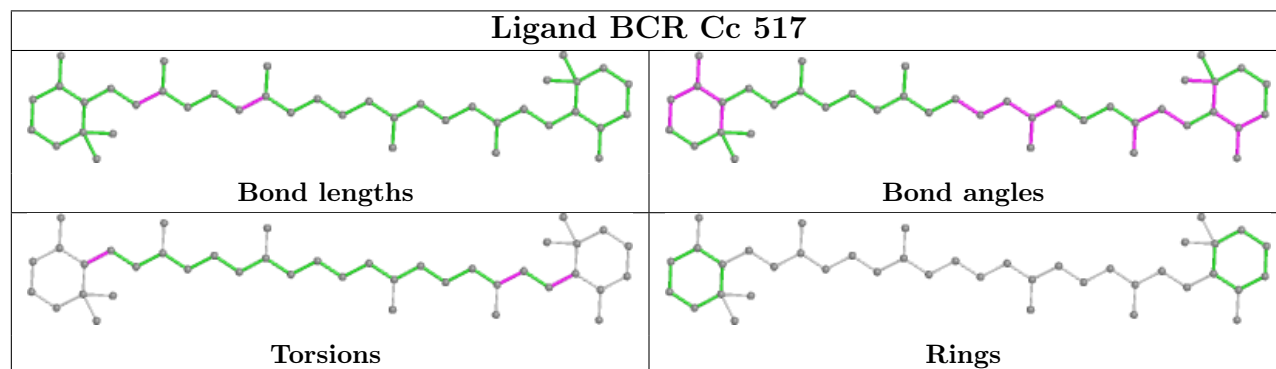
## Ligand CLA Bb 615

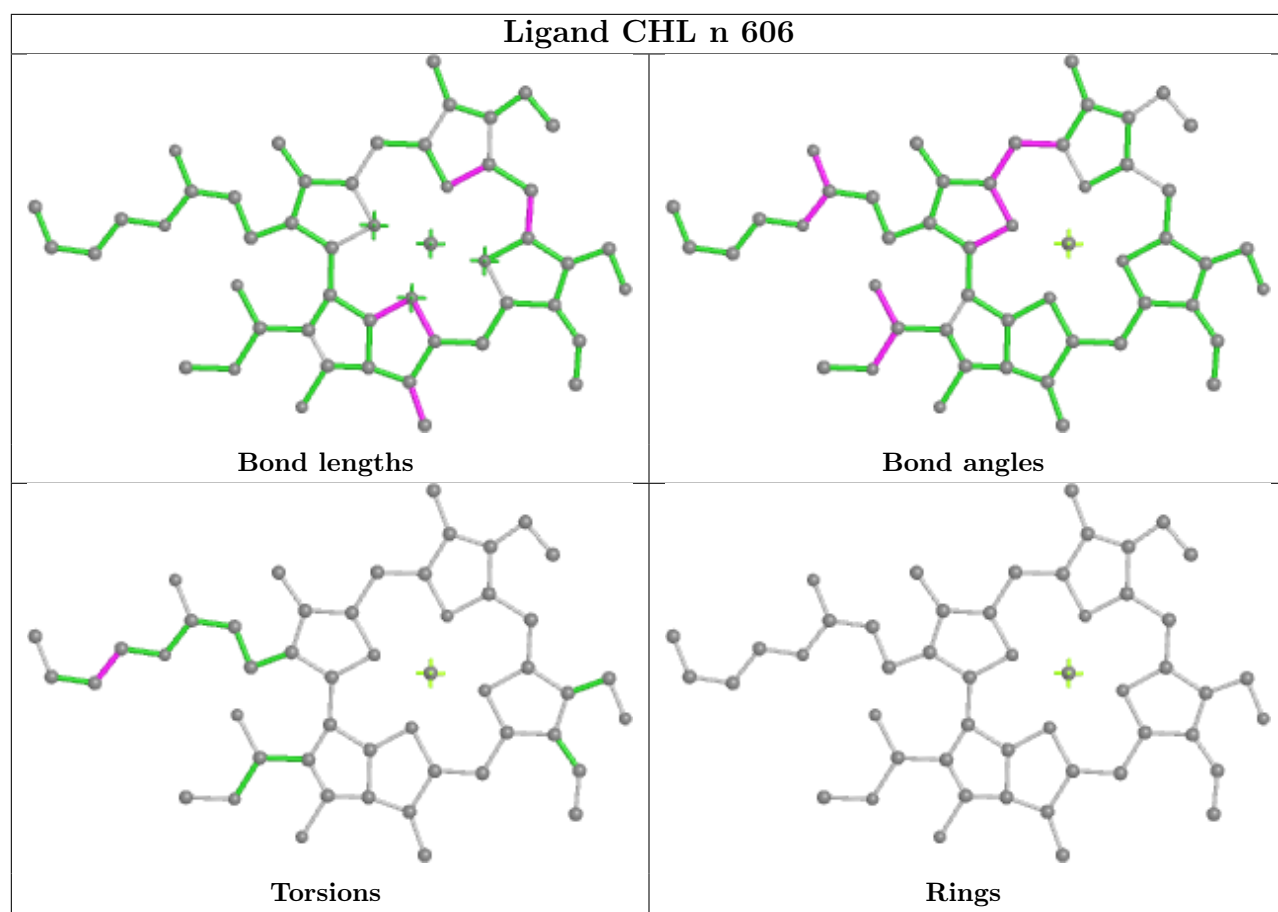


## Ligand CLA YY 613

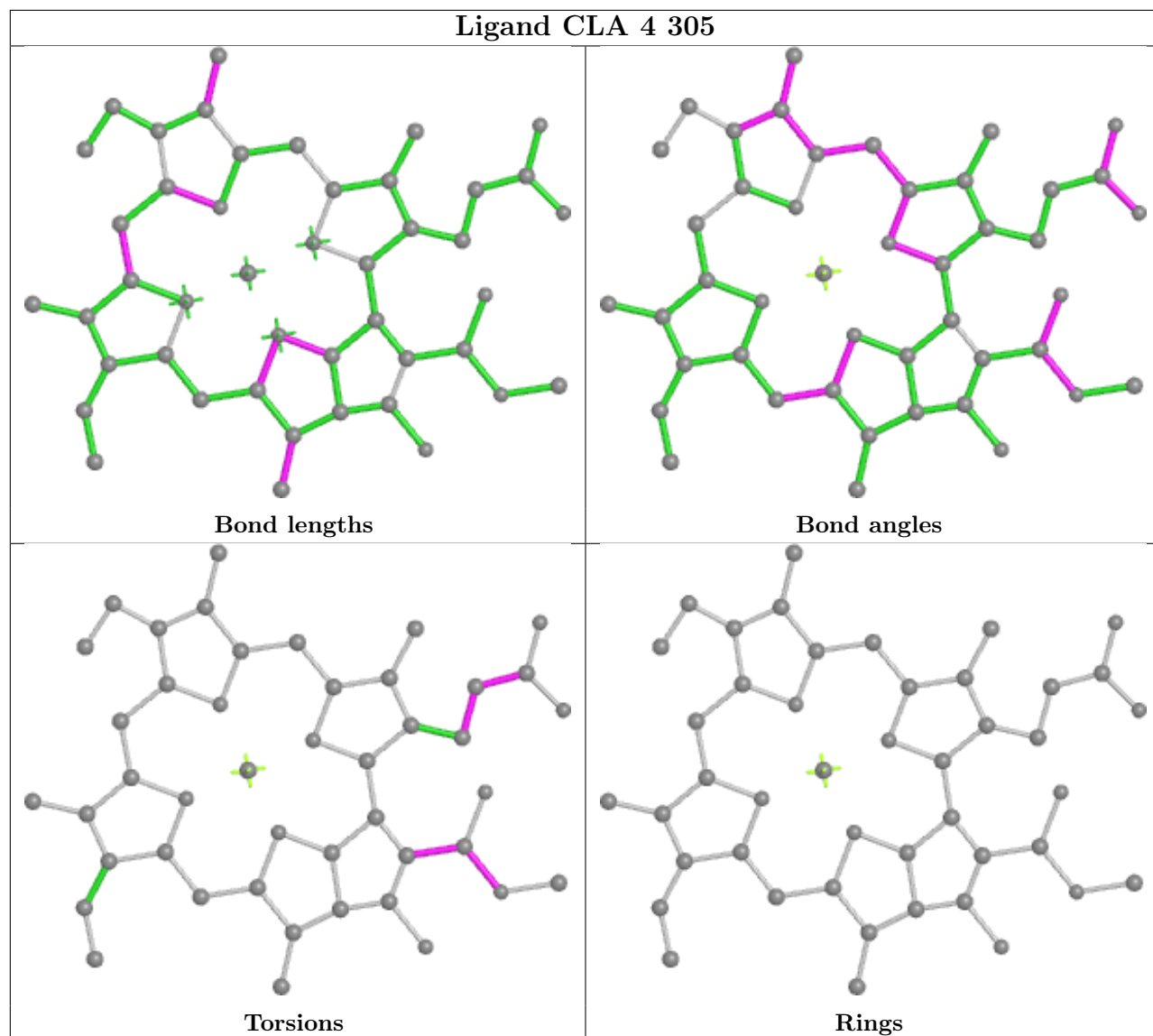


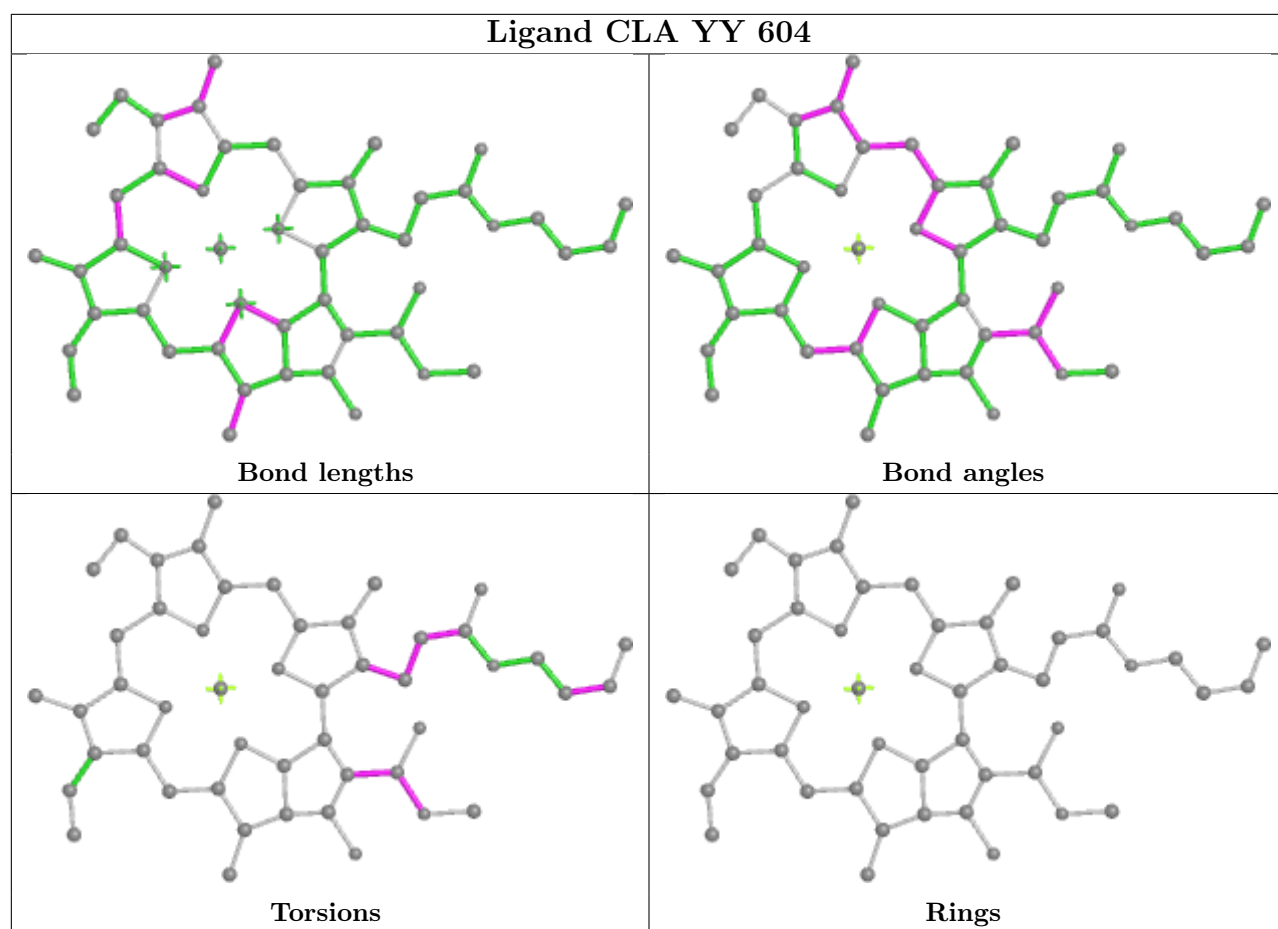
## Ligand BCR Cc 517

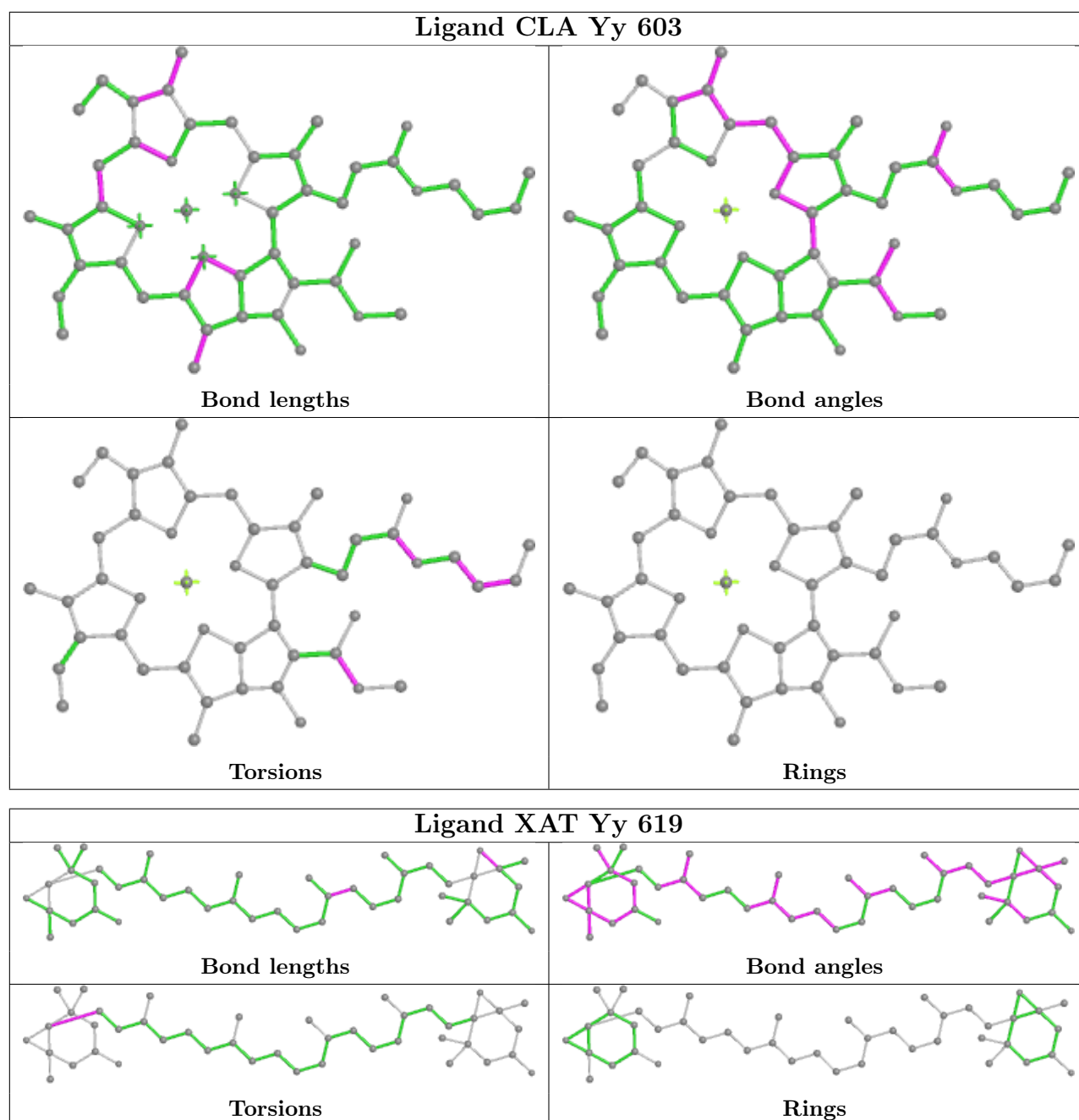




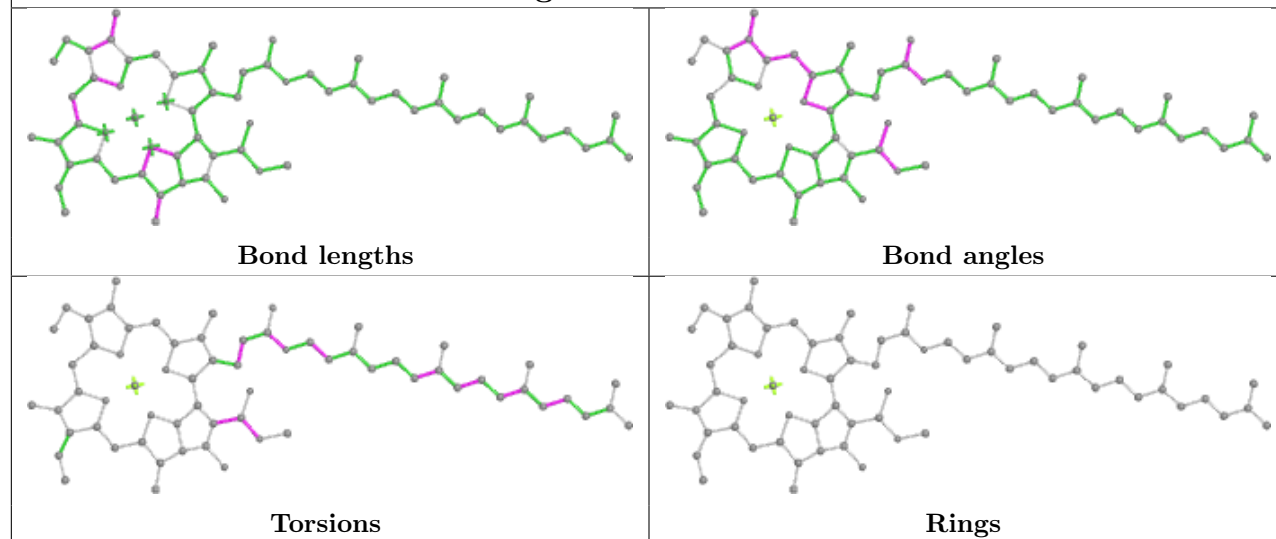
## Ligand CLA 4 305



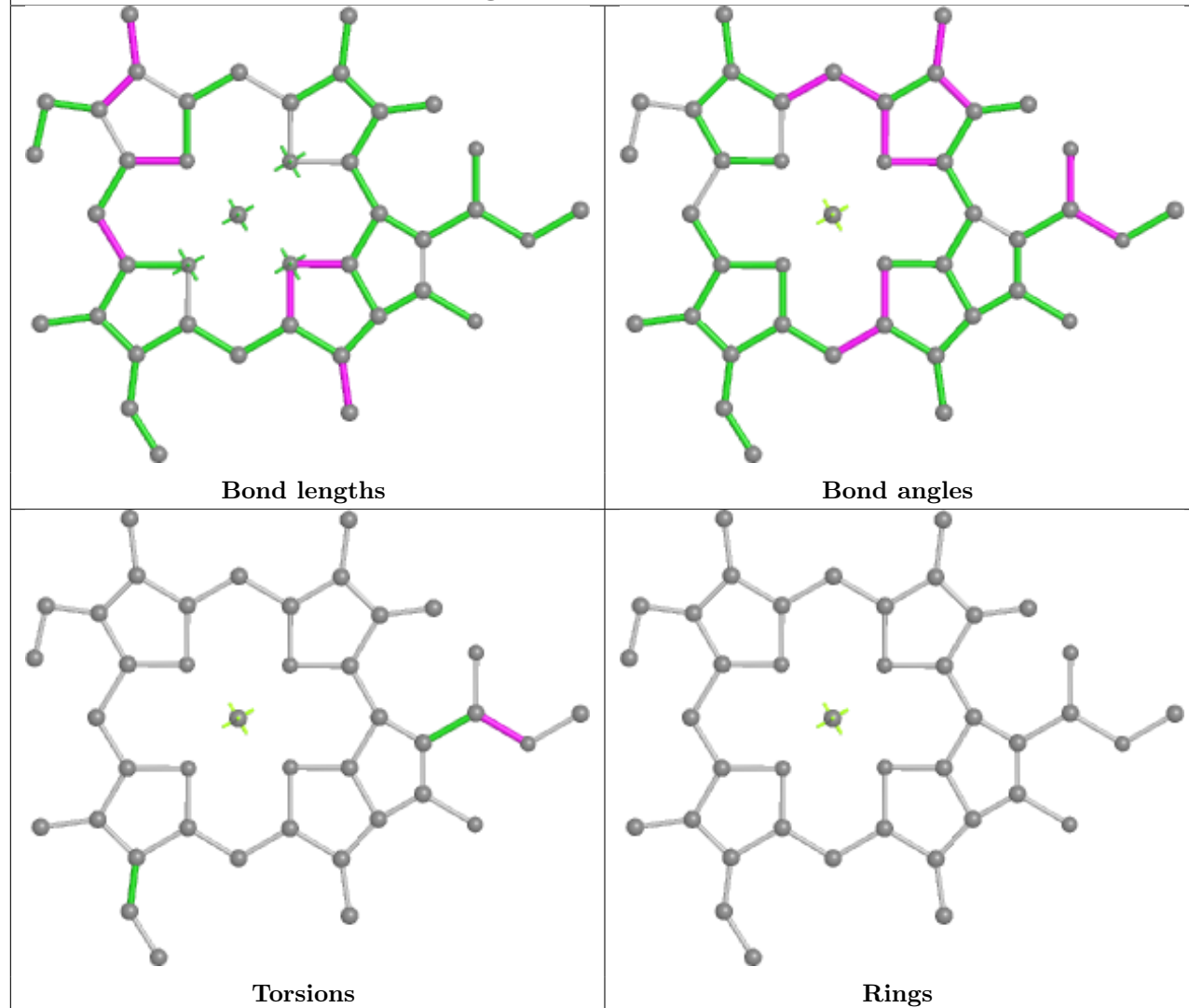




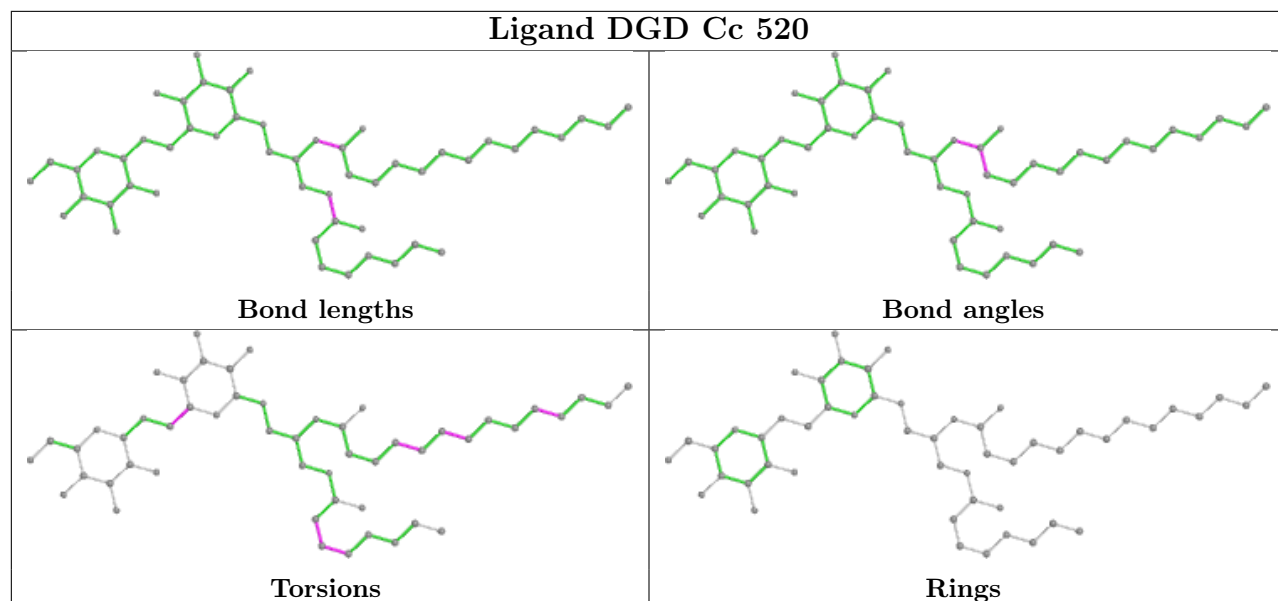
## Ligand CLA b 612



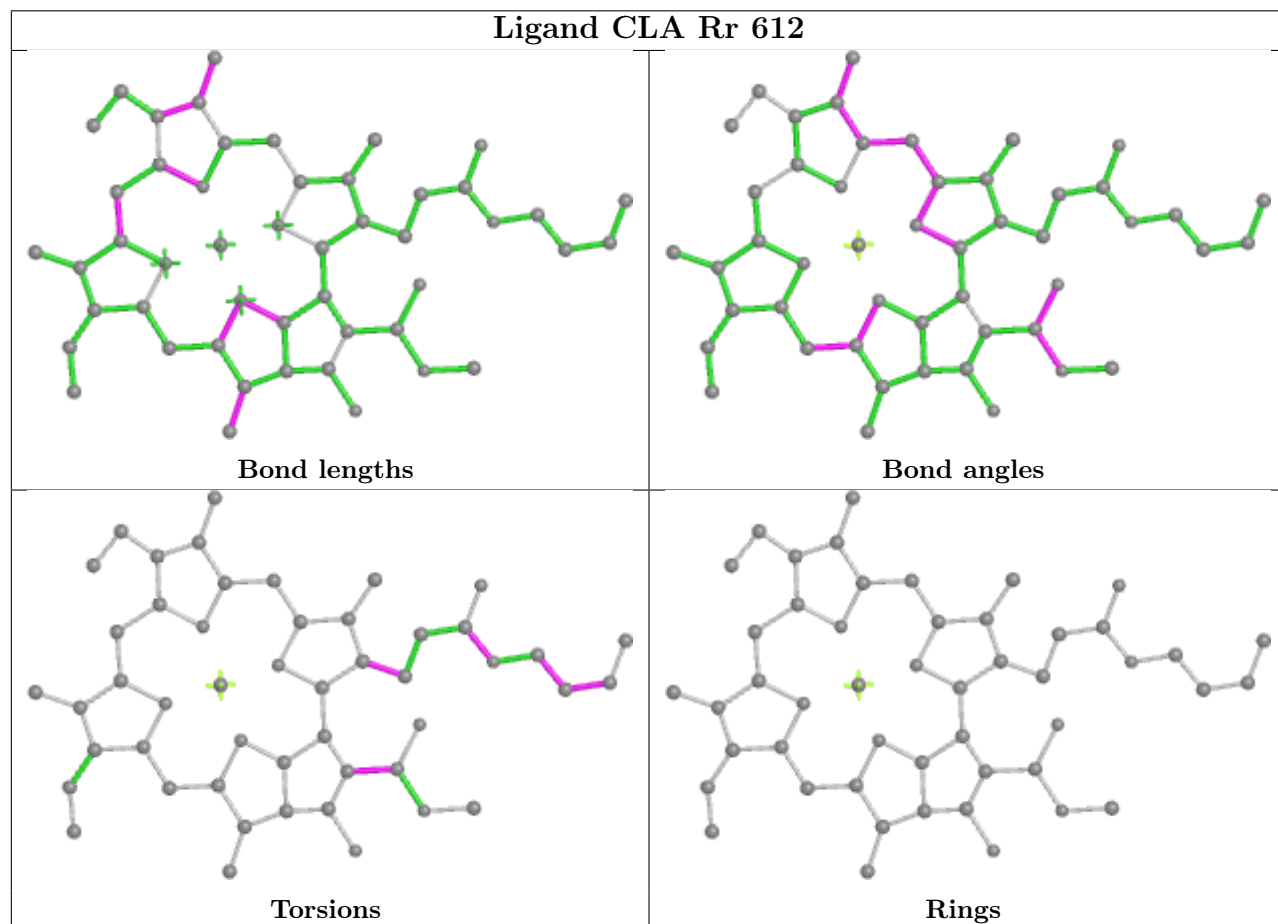
## Ligand CLA XX 201

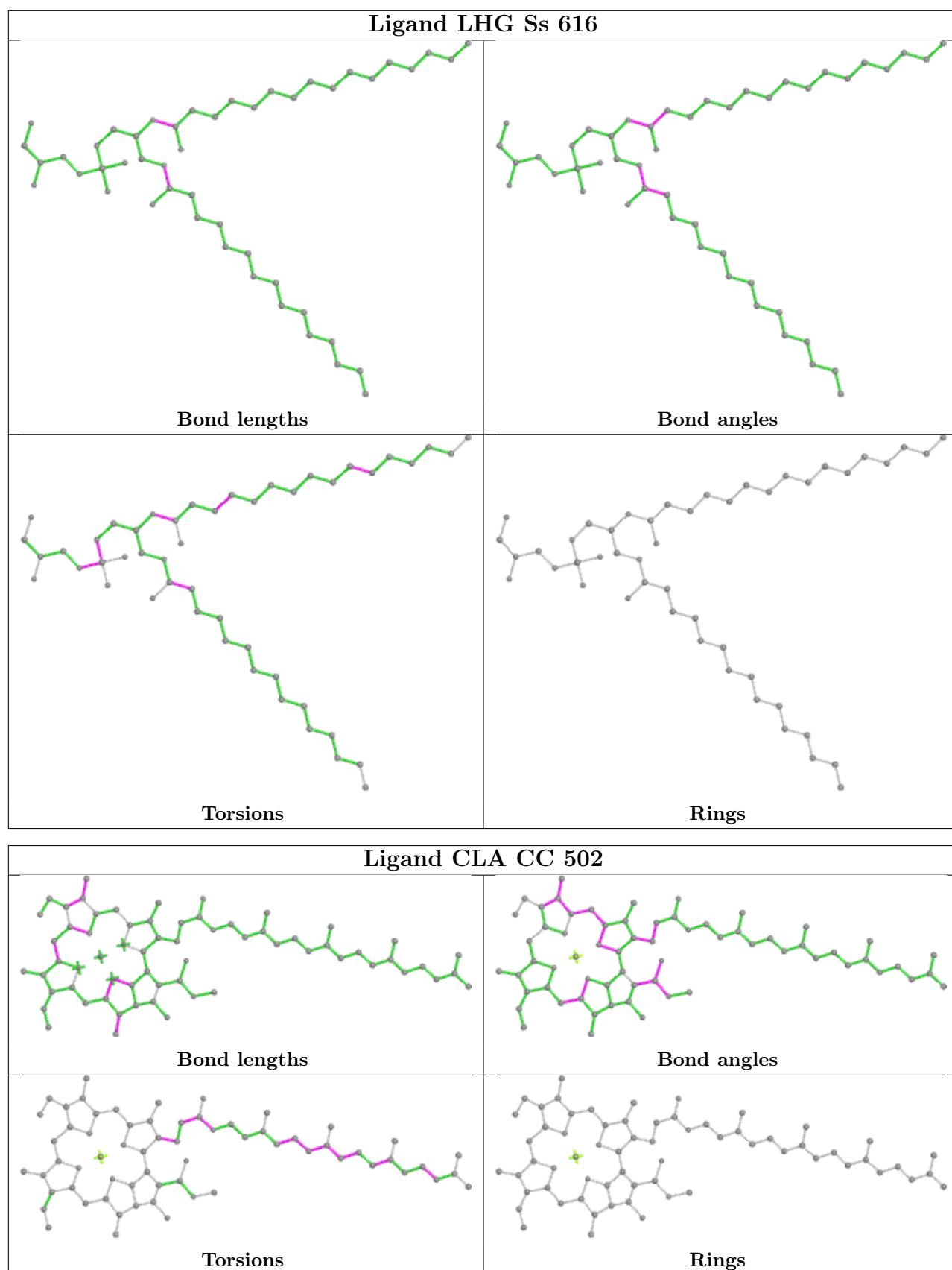


## Ligand DGD Cc 520

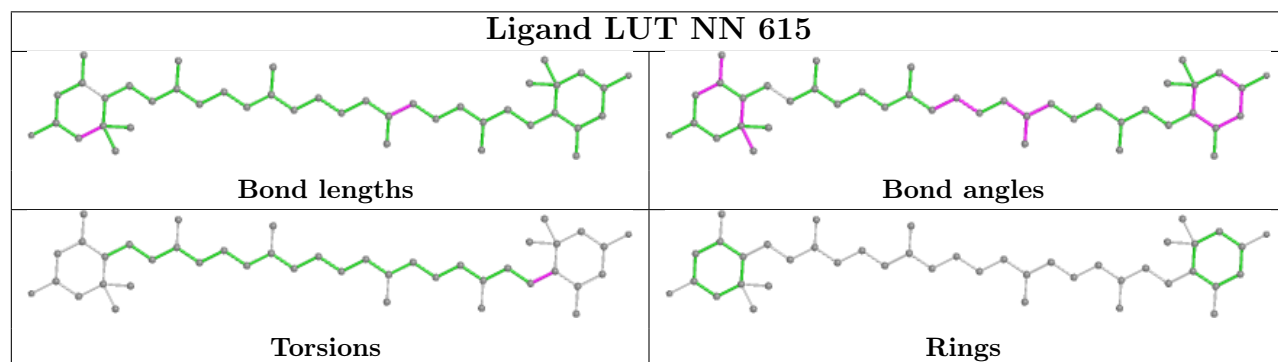
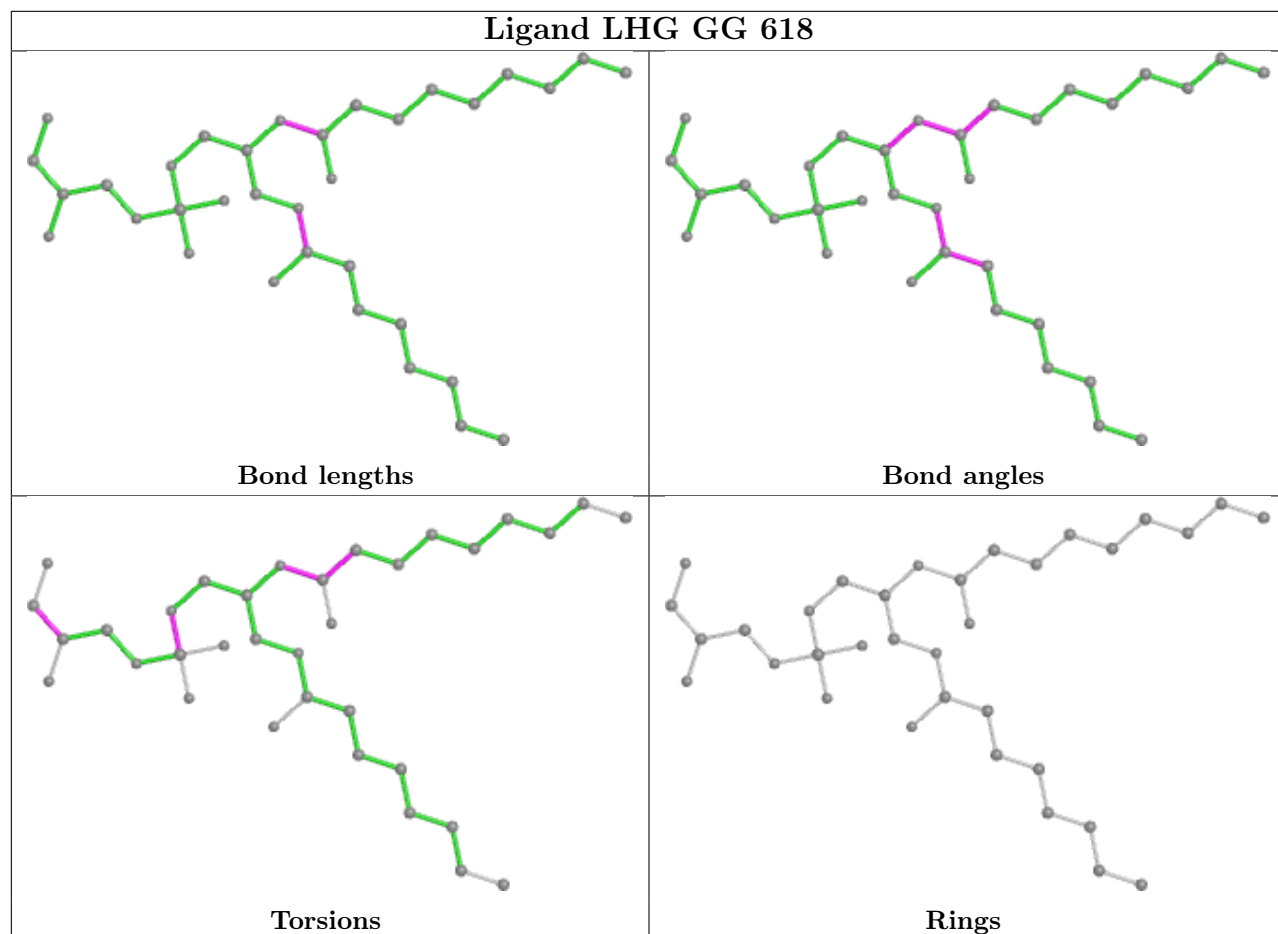
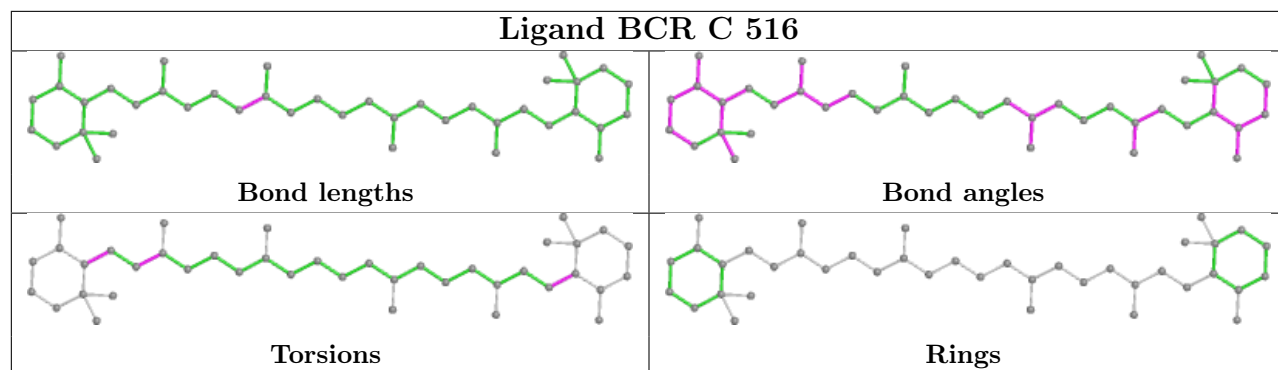


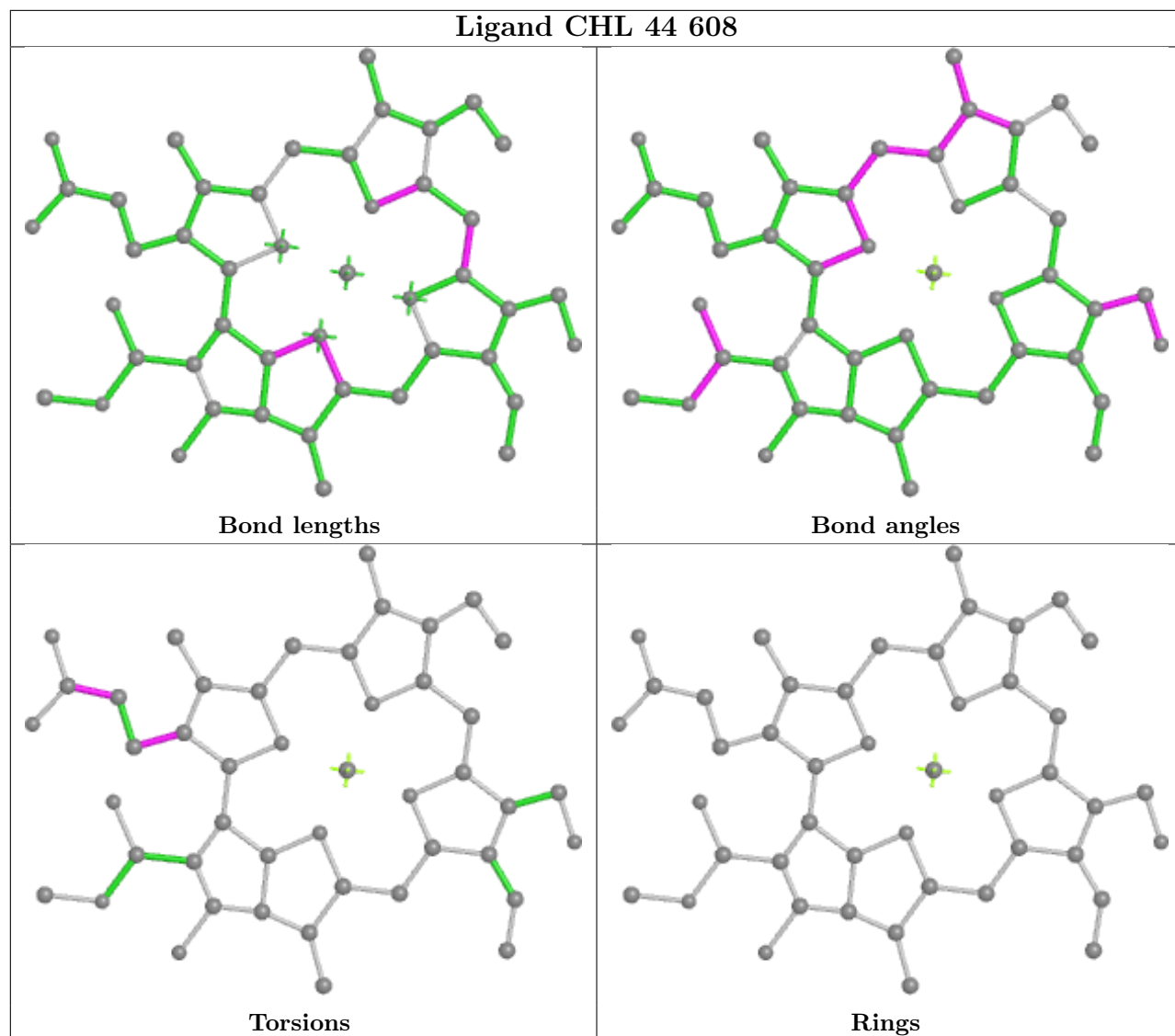
## Ligand CLA Rr 612



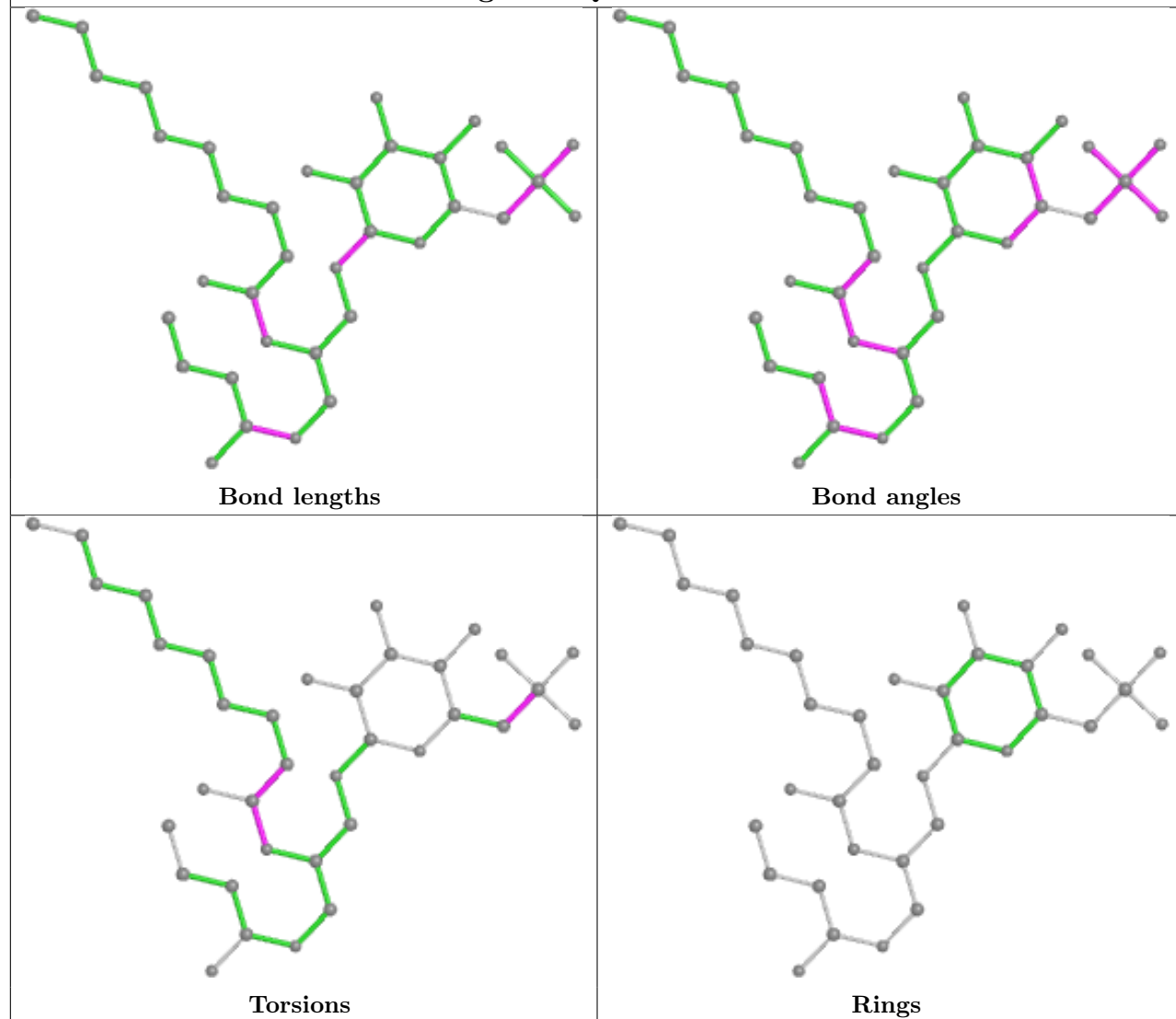




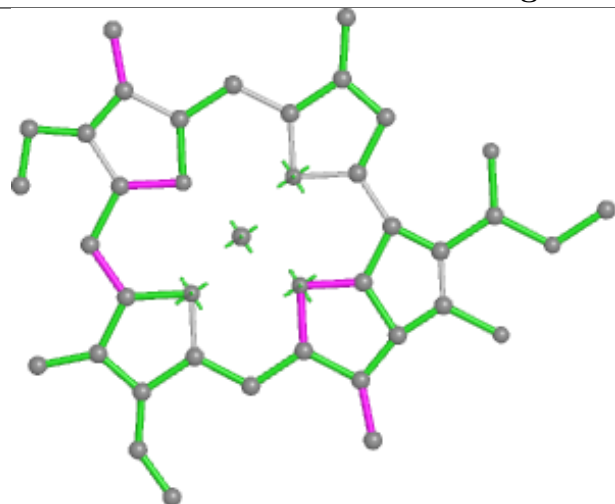




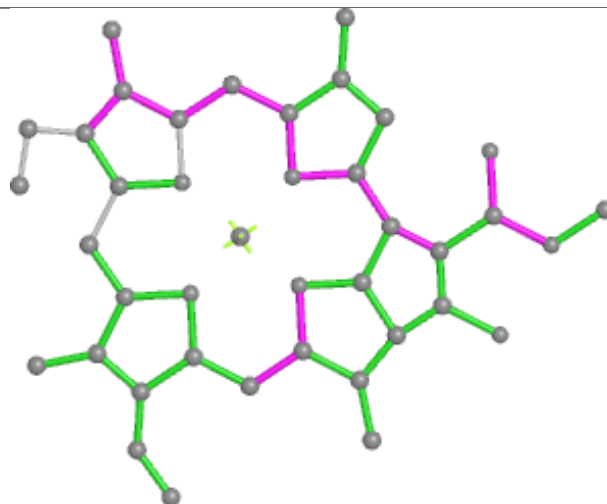
## Ligand SQD BB 621



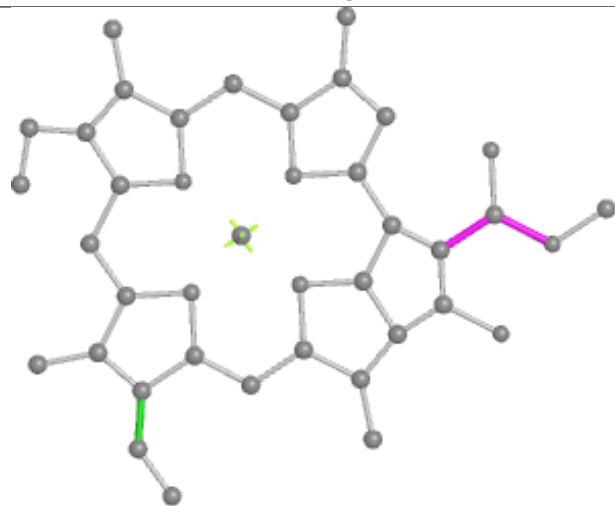
## Ligand CLA 2 603



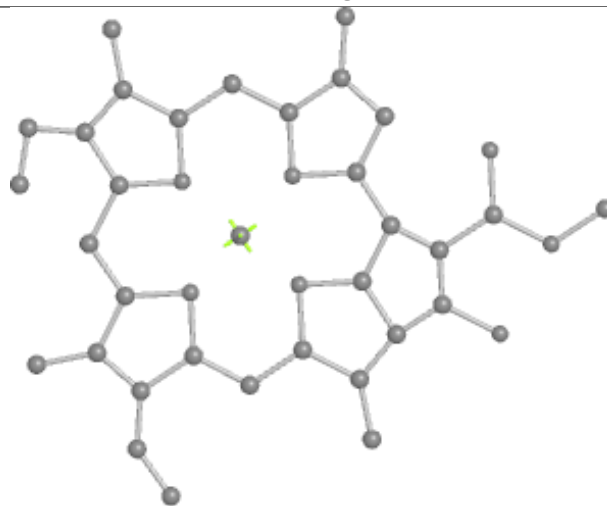
Bond lengths



Bond angles

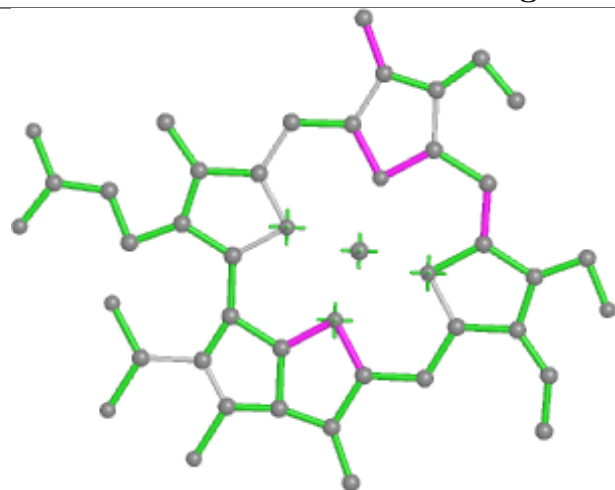


Torsions

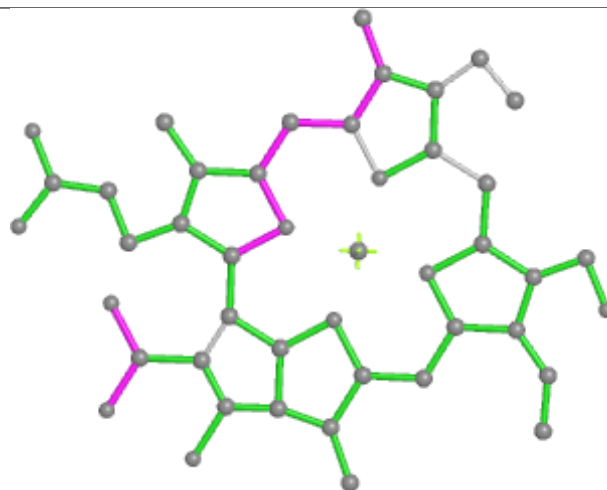


Rings

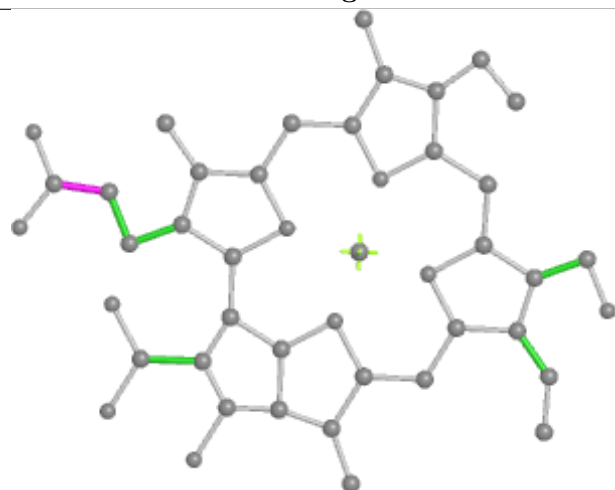
## Ligand CHL 4 302



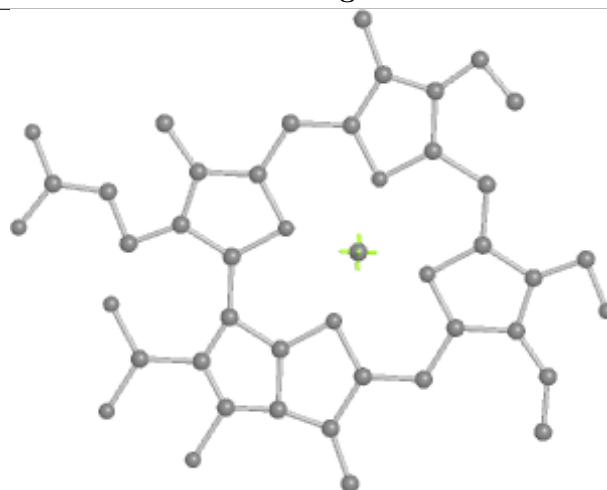
Bond lengths



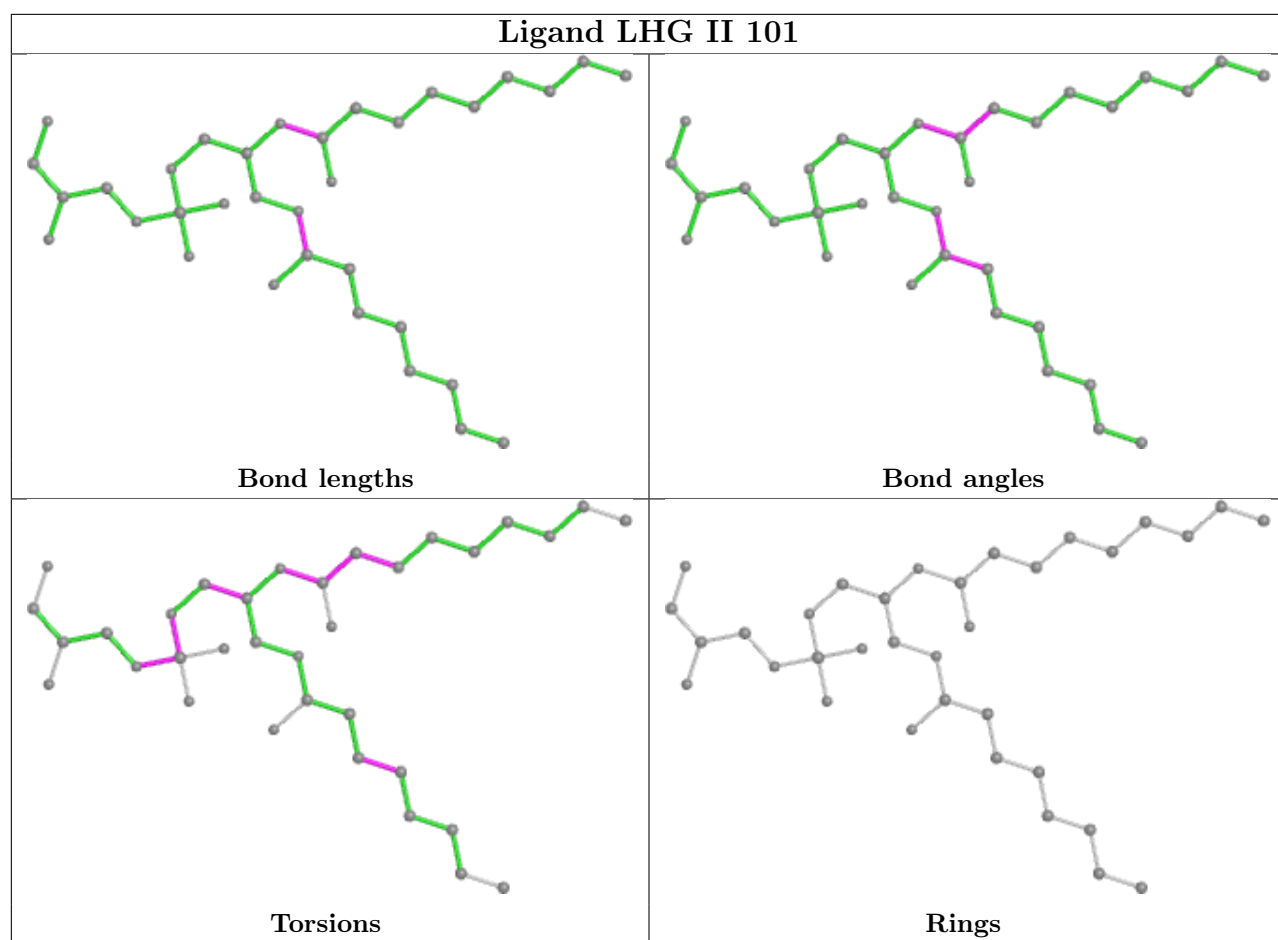
Bond angles

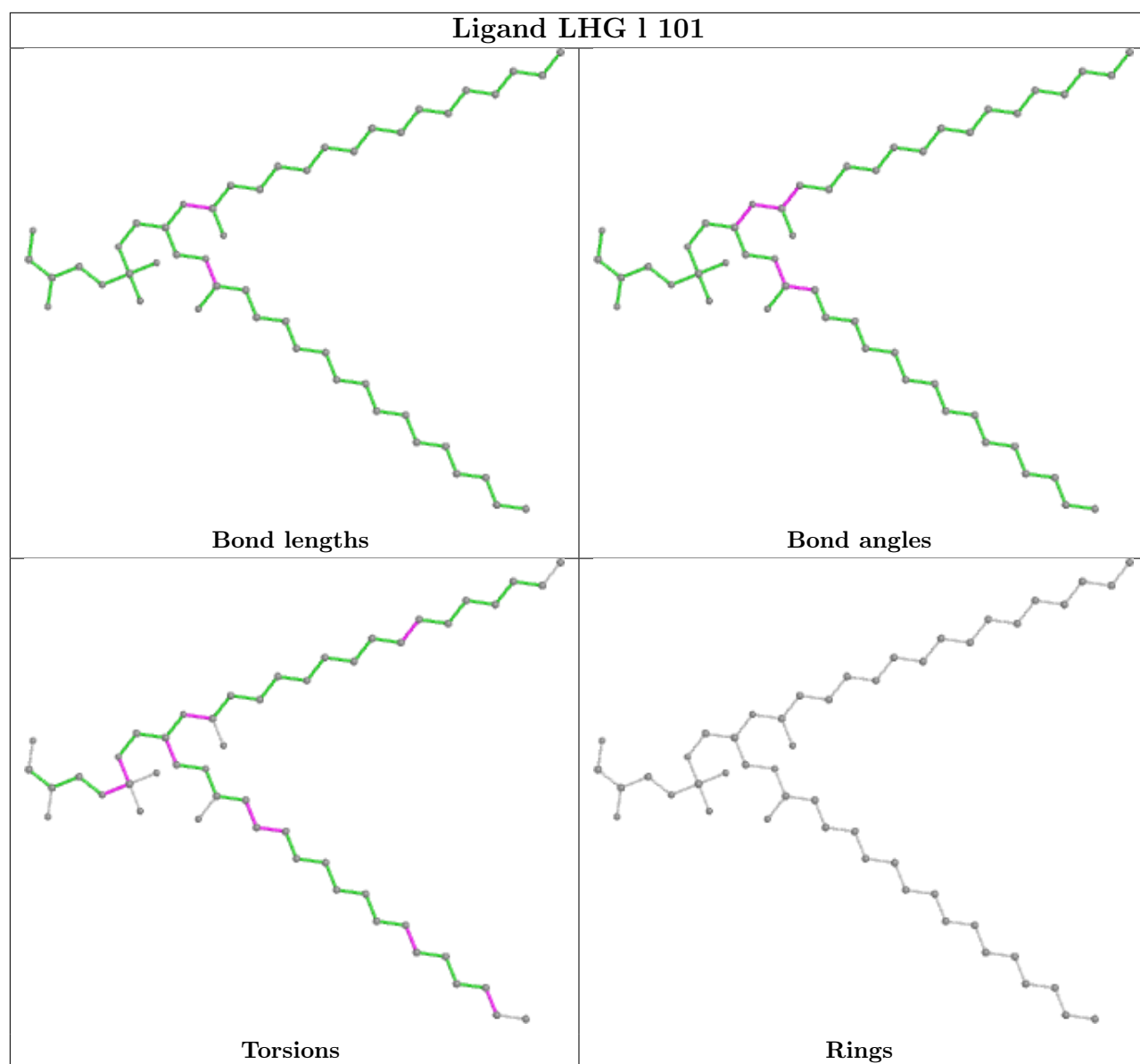


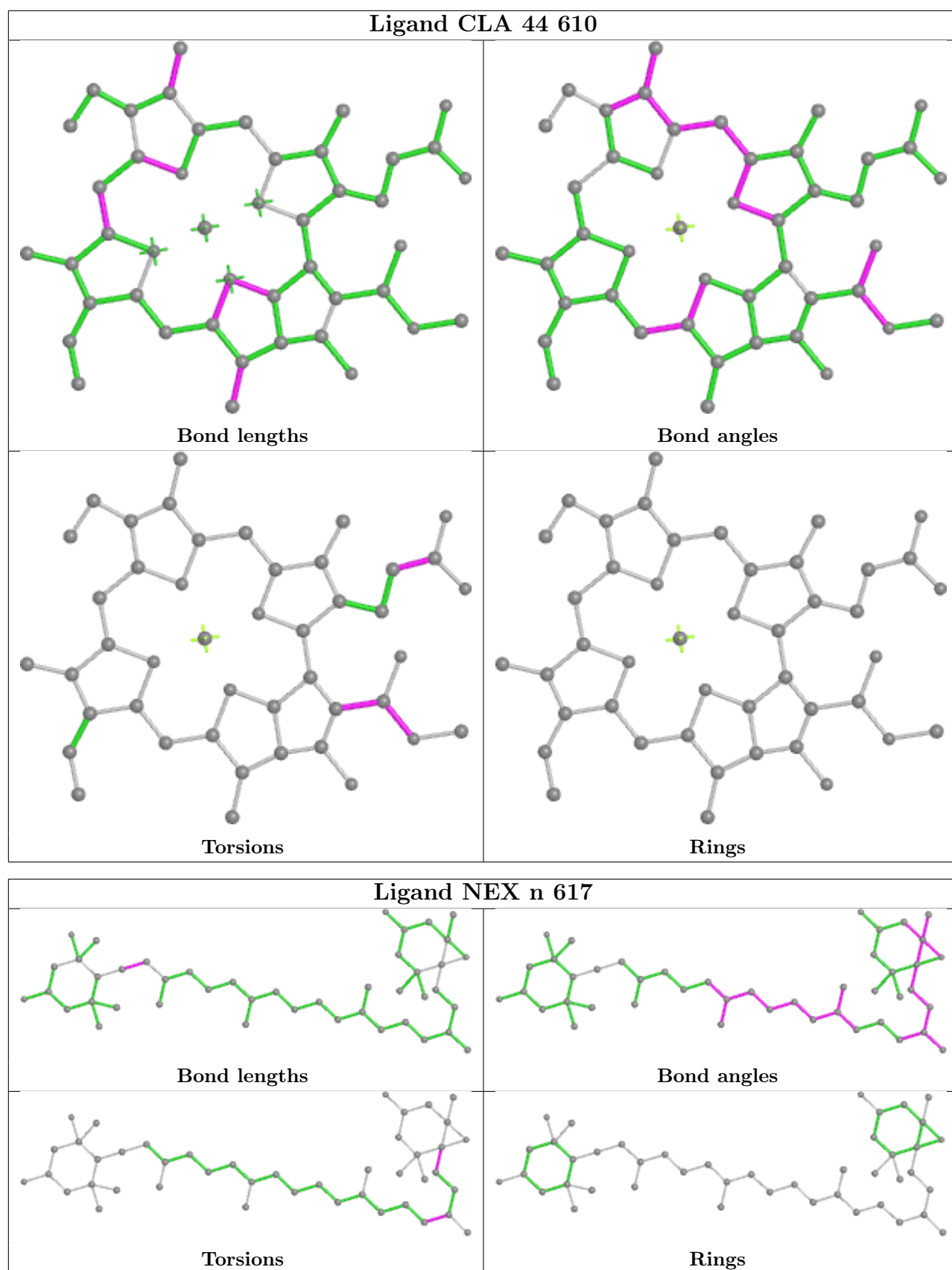
Torsions



Rings

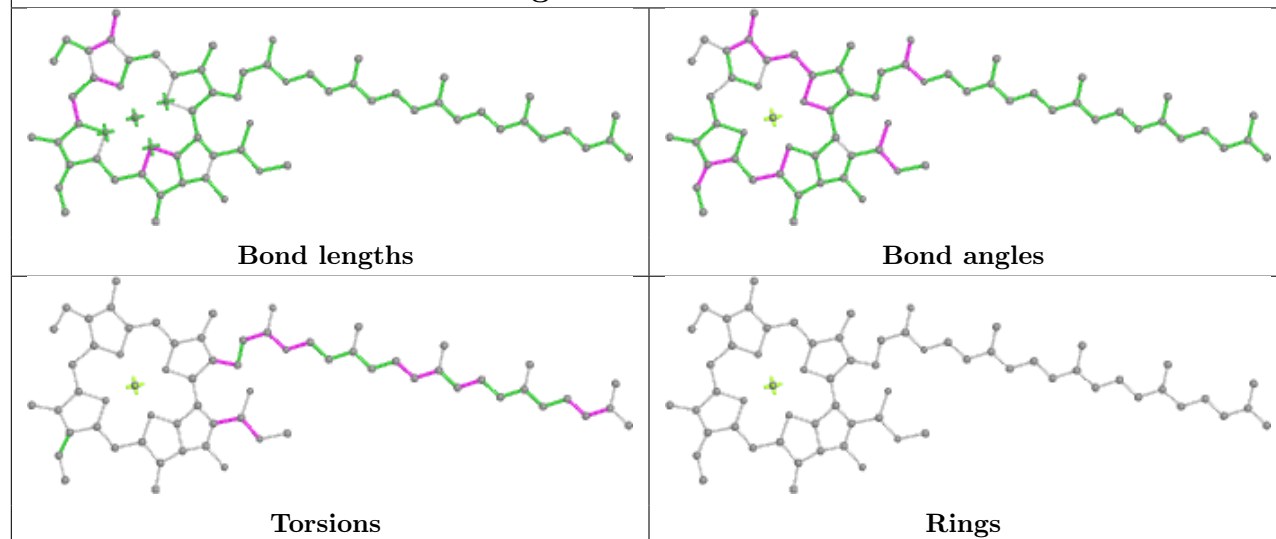




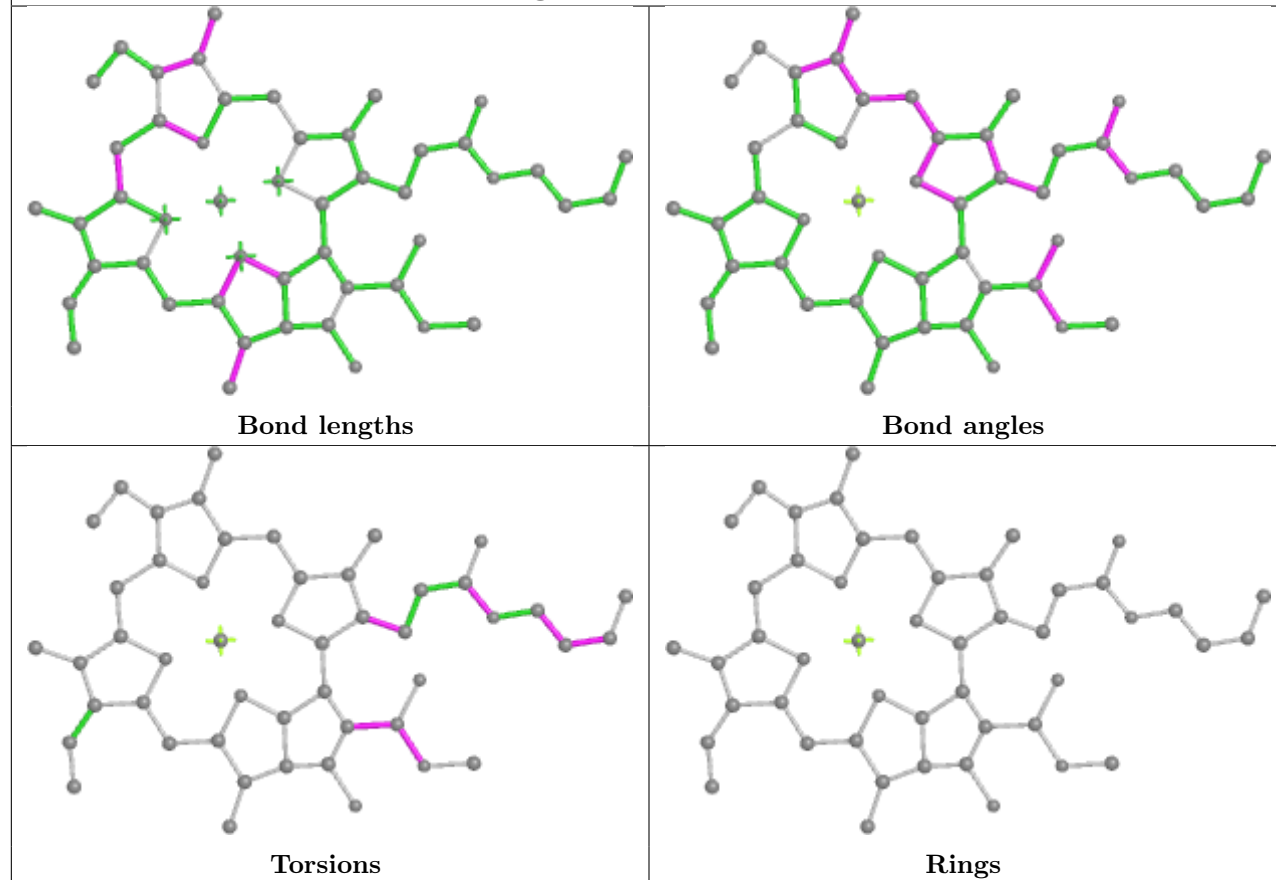


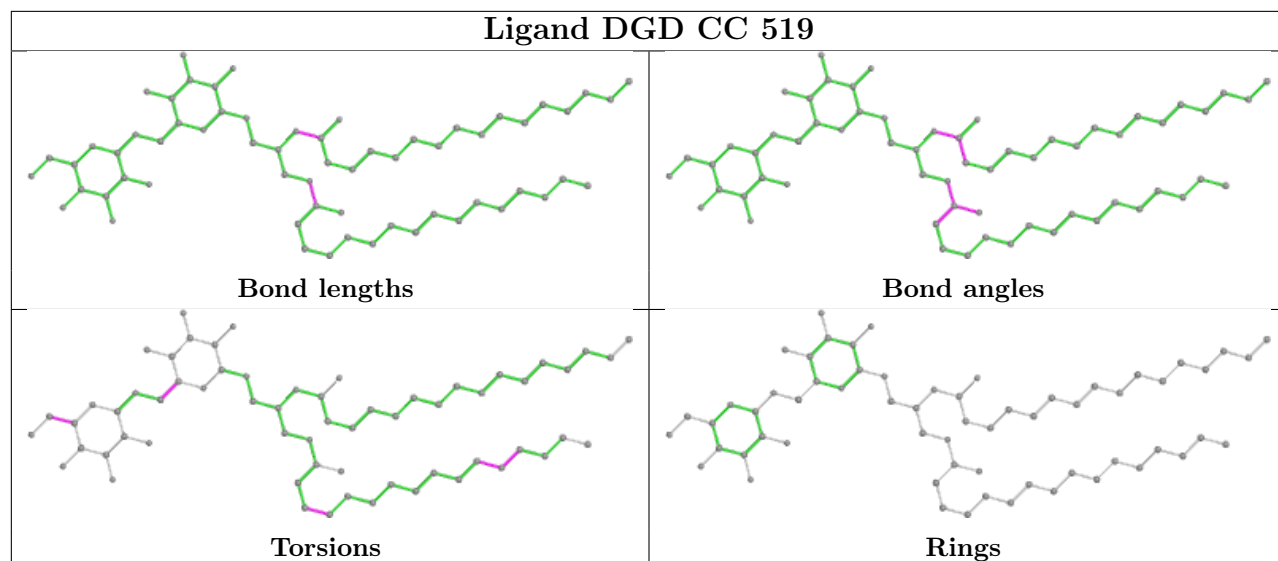
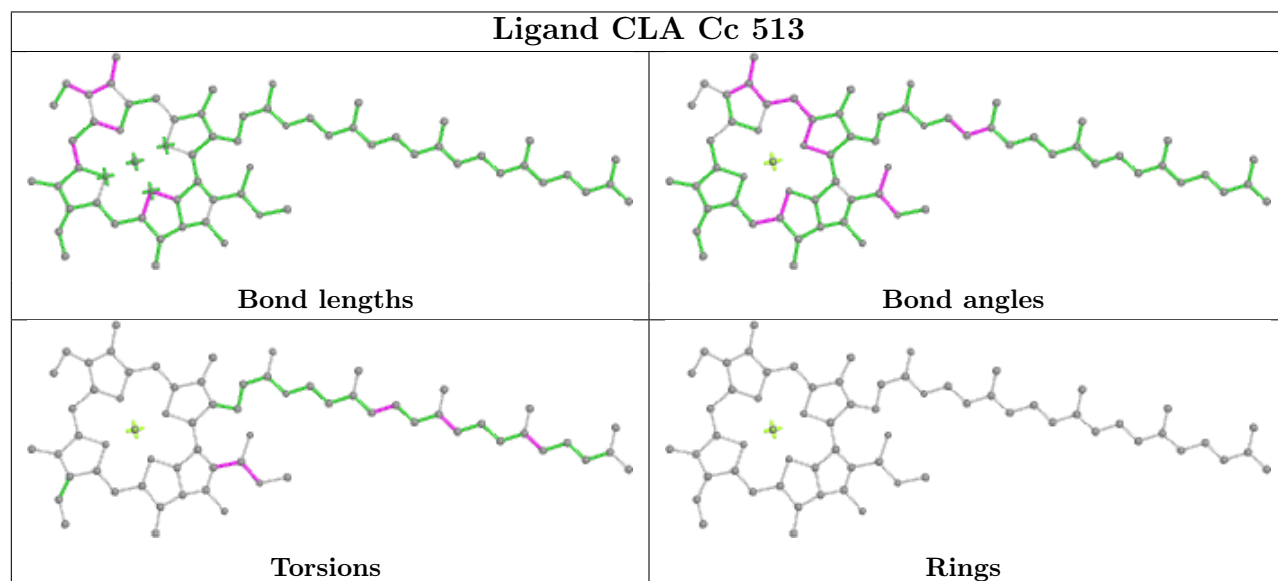


## Ligand CLA Y 602

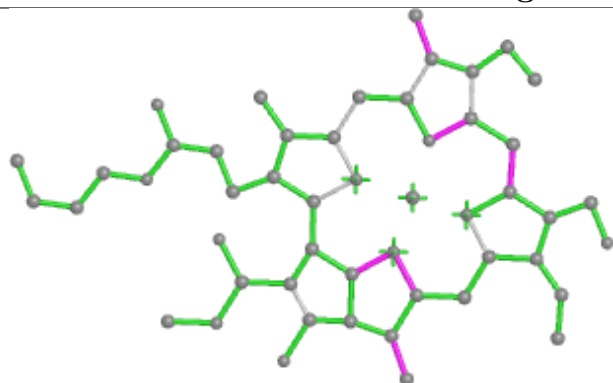


## Ligand CLA Y 614

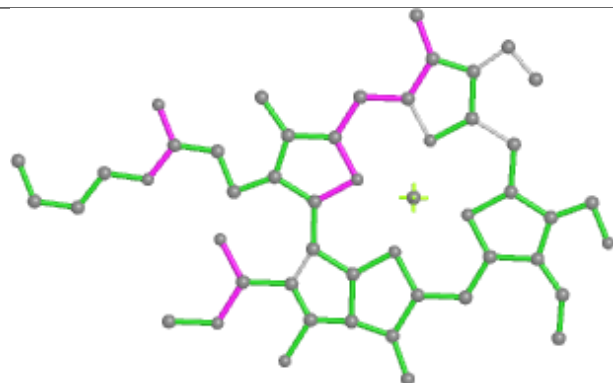


**Ligand DGD CC 519****Ligand CLA Cc 513**

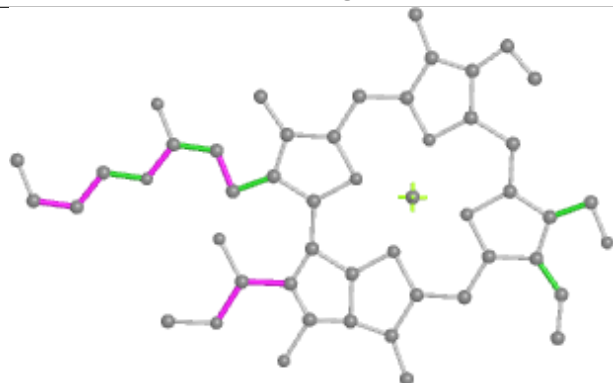
## Ligand CHL n 608



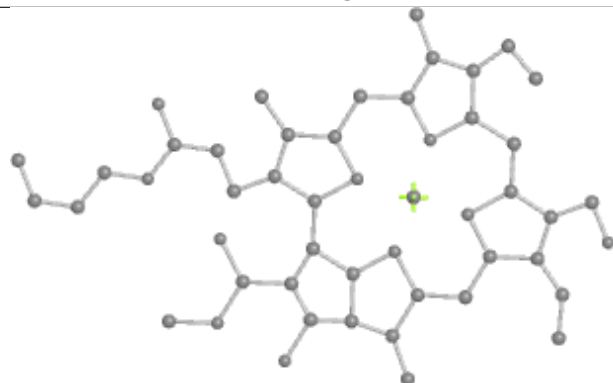
Bond lengths



Bond angles

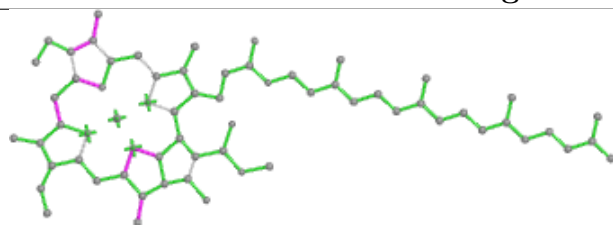


Torsions

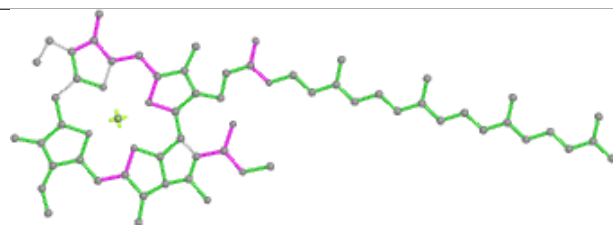


Rings

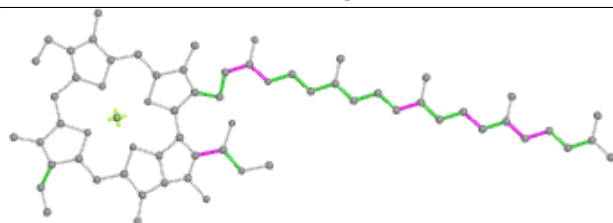
## Ligand CLA BB 601



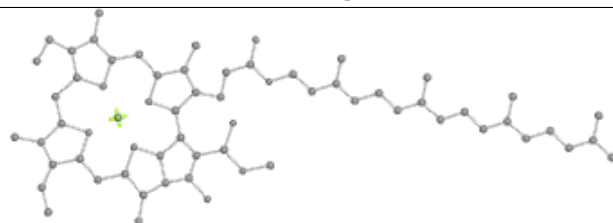
Bond lengths



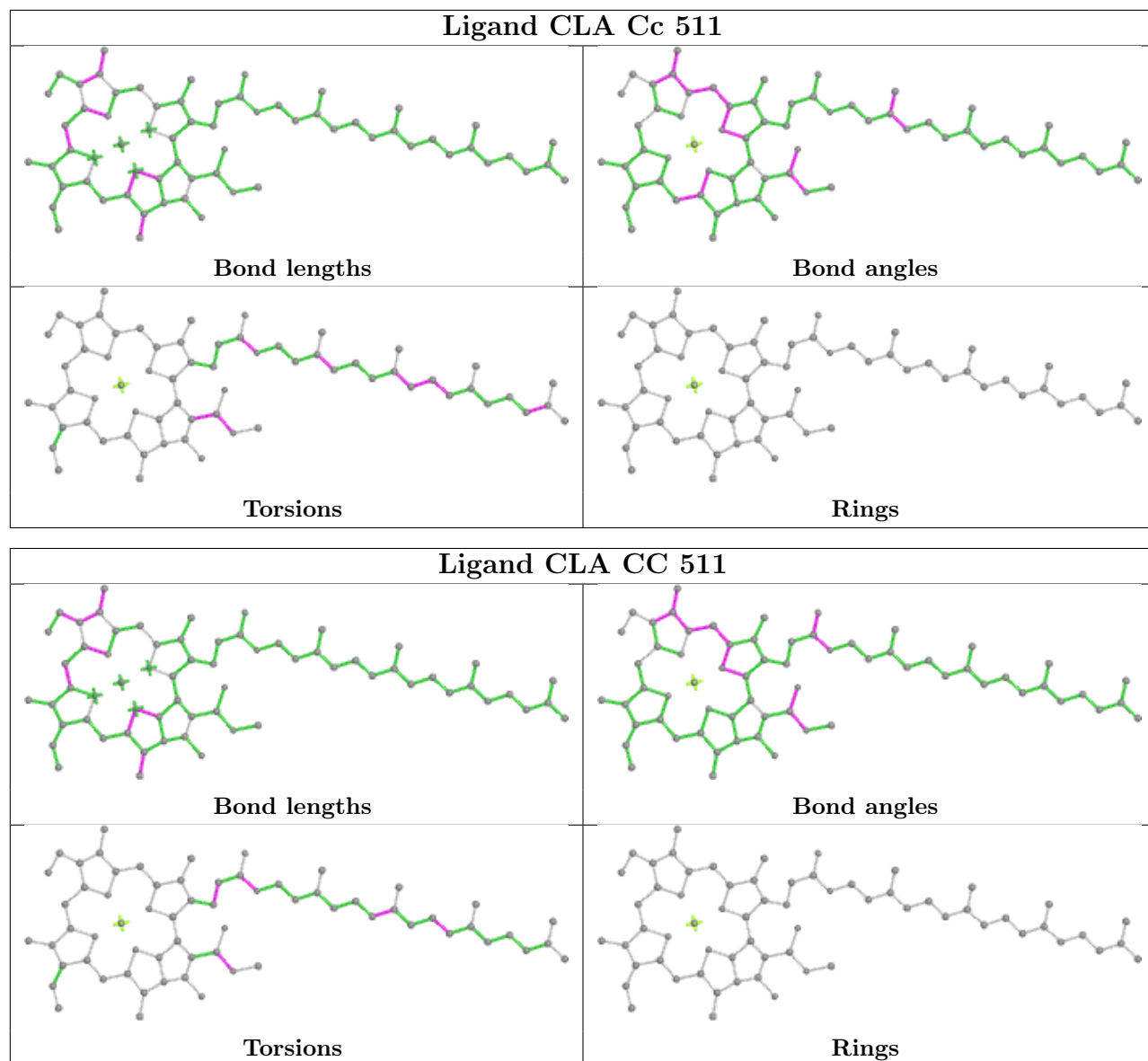
Bond angles

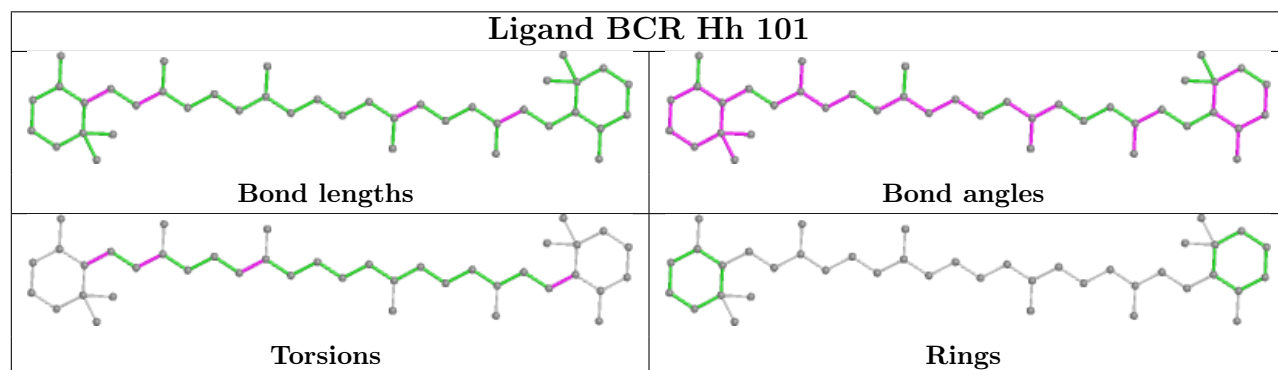
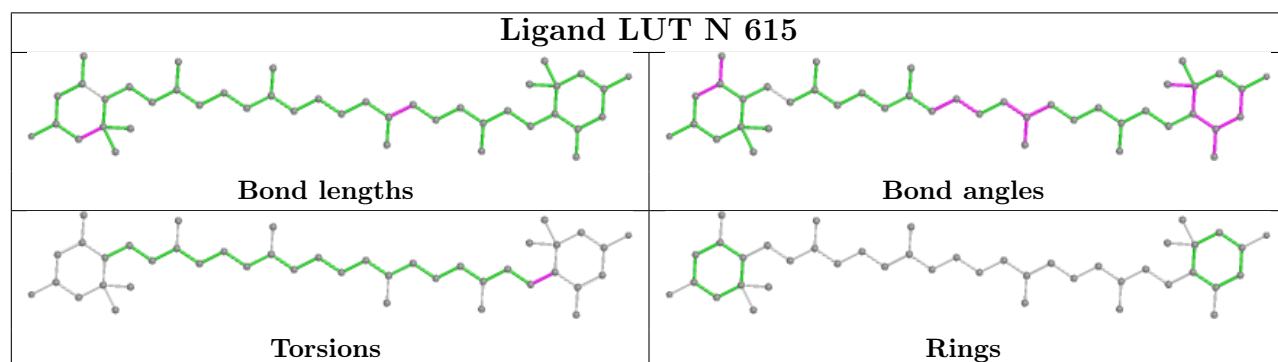
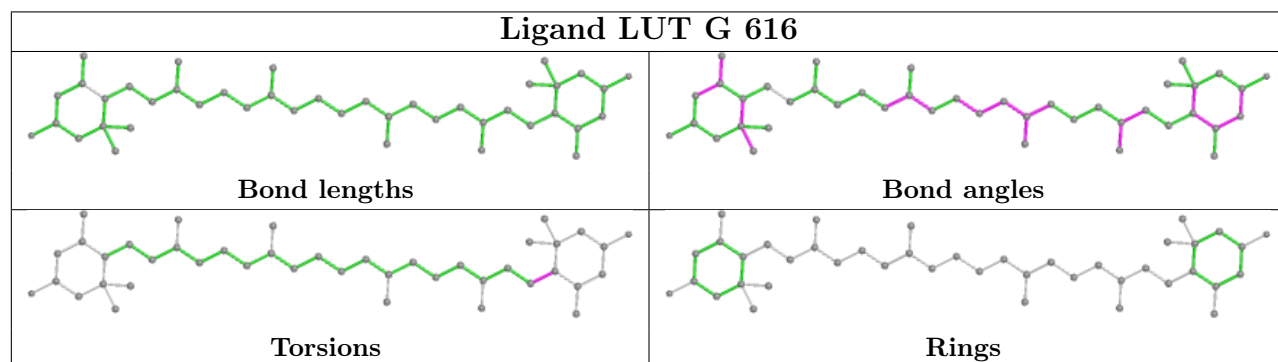
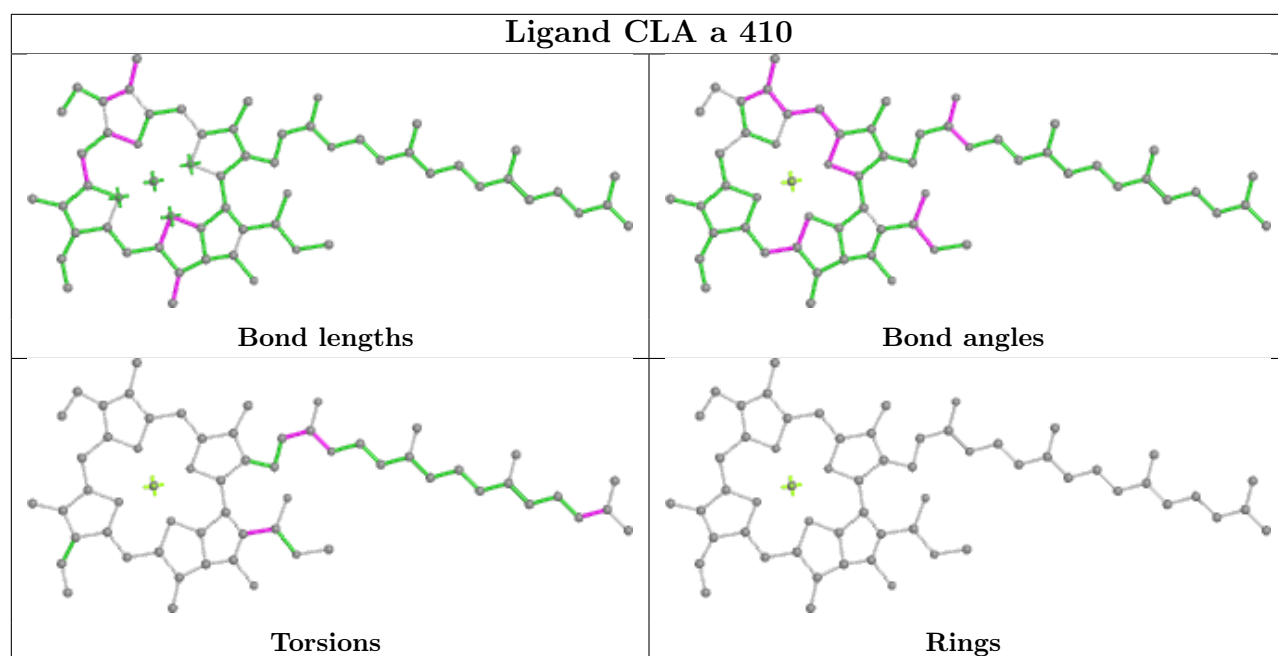


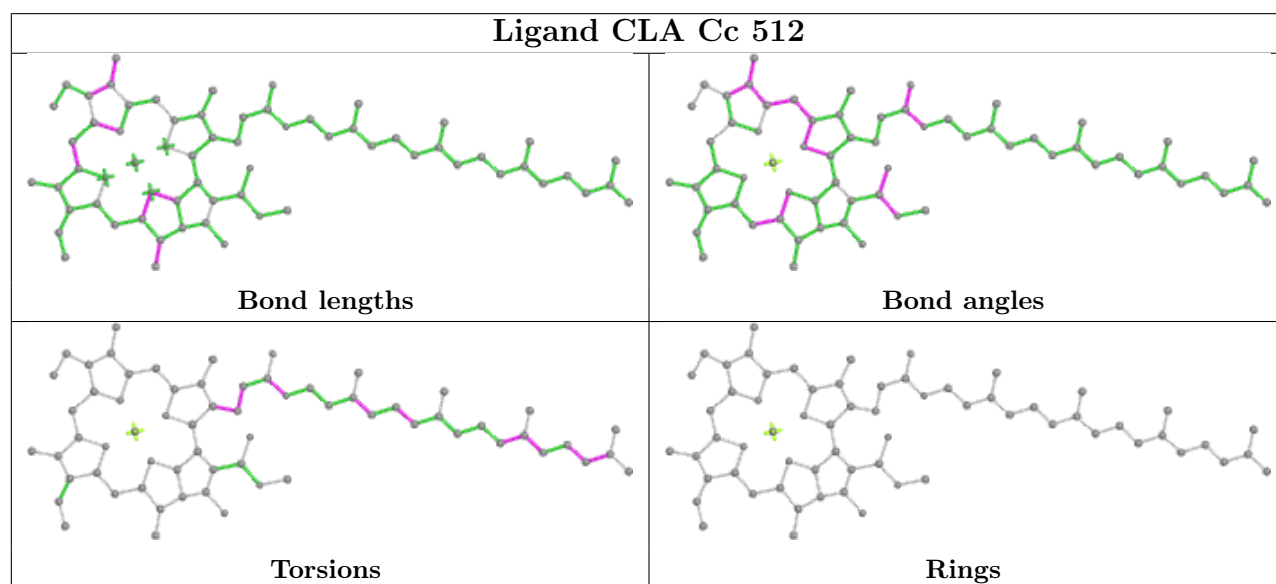
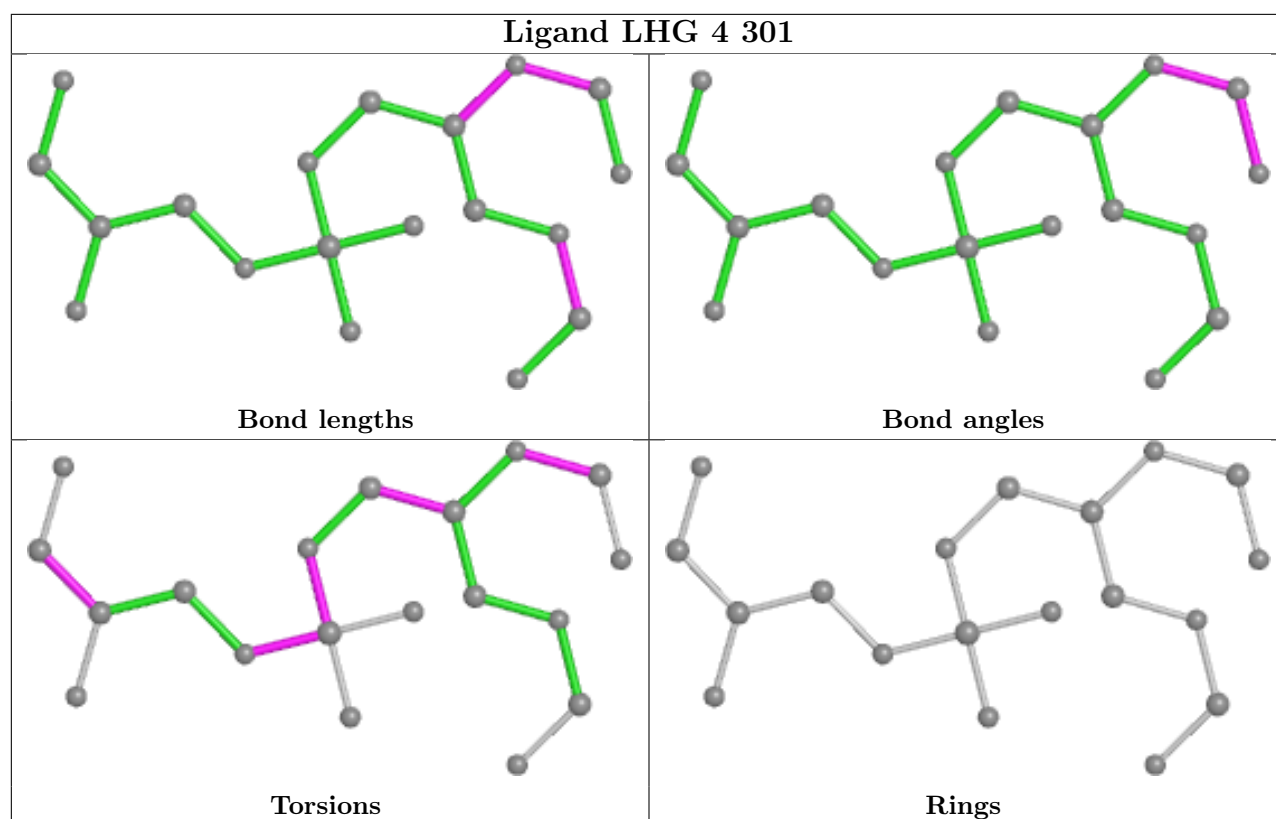
Torsions



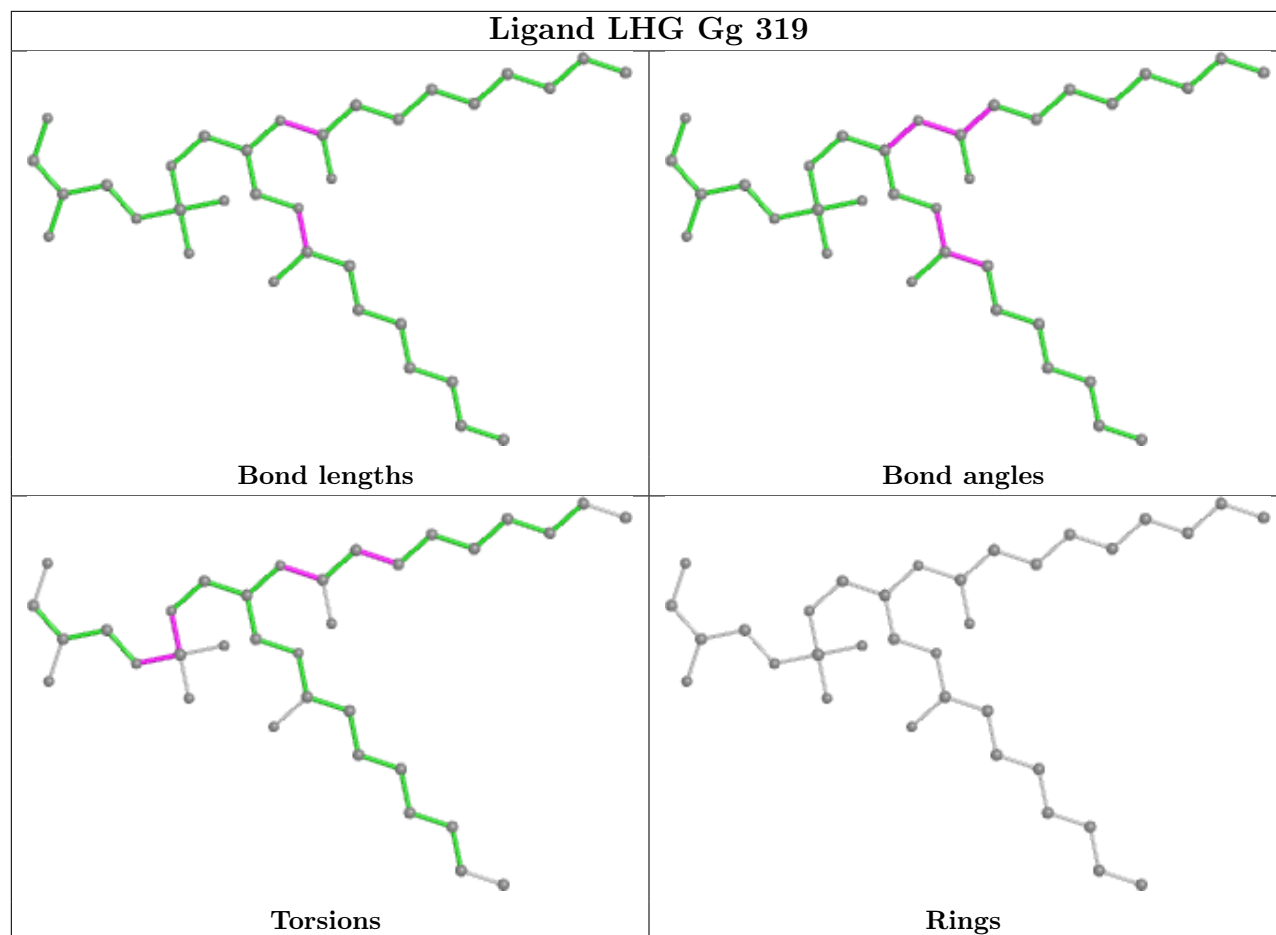
Rings



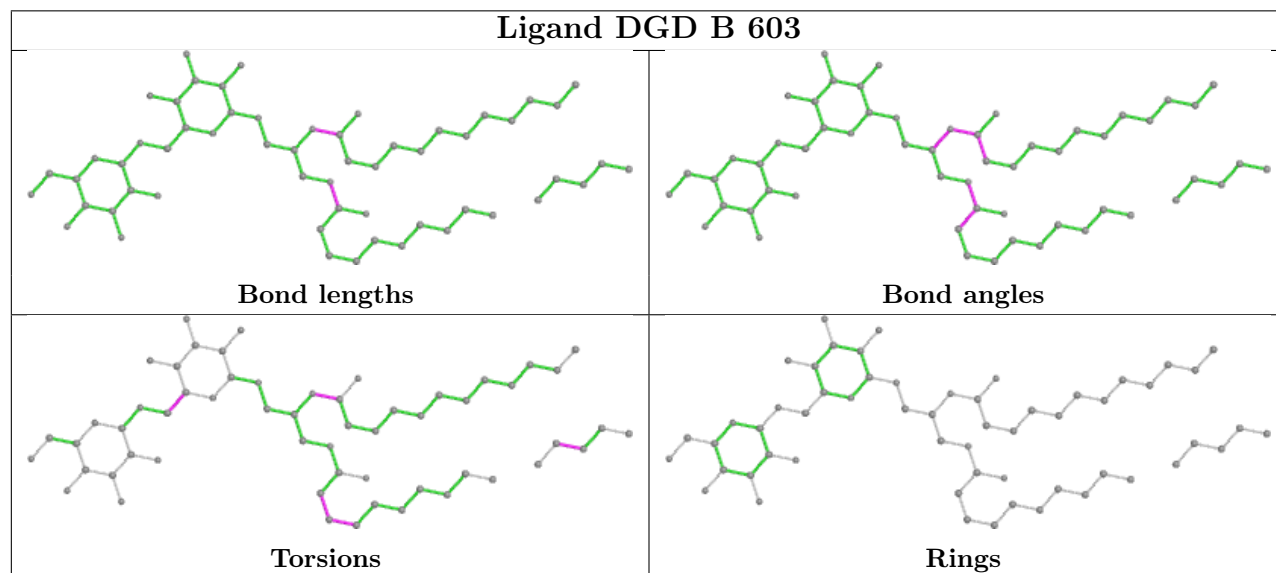




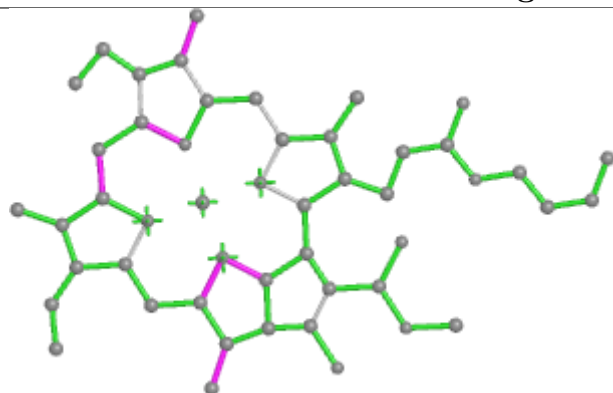
## Ligand LHG Gg 319



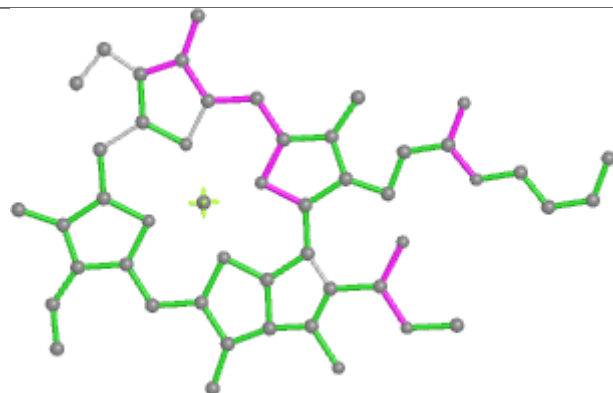
## Ligand DGD B 603



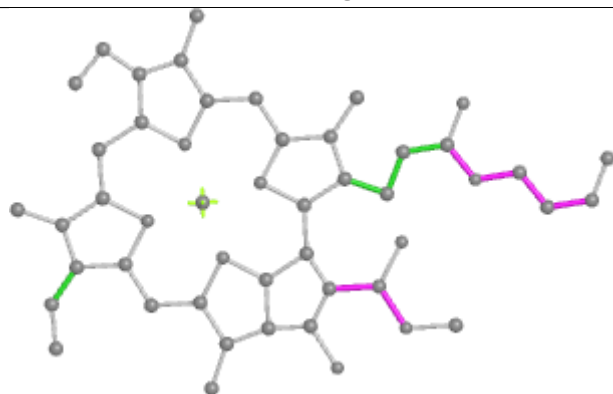
## Ligand CLA S 611



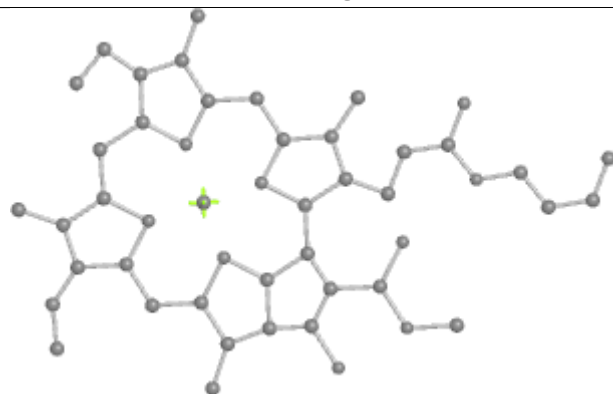
Bond lengths



Bond angles

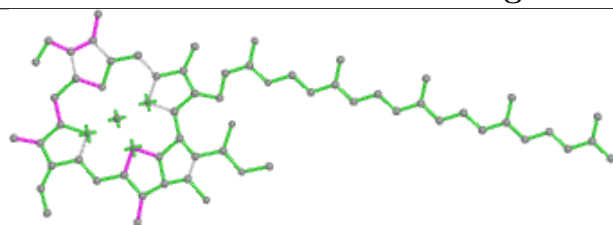


Torsions

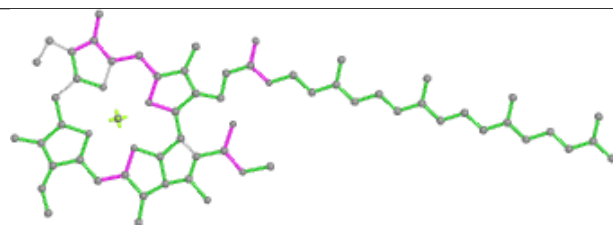


Rings

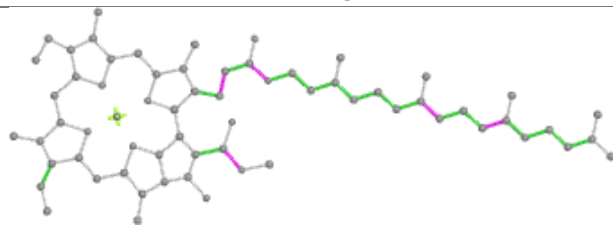
## Ligand CLA Bb 608



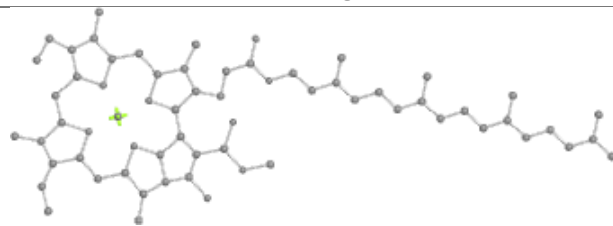
Bond lengths



Bond angles



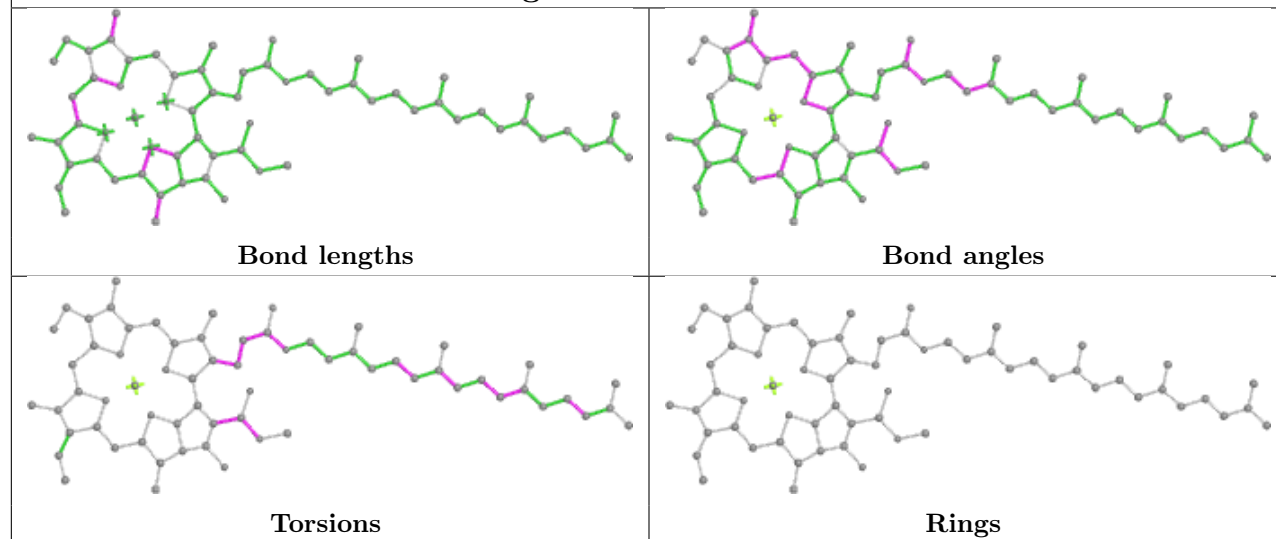
Torsions



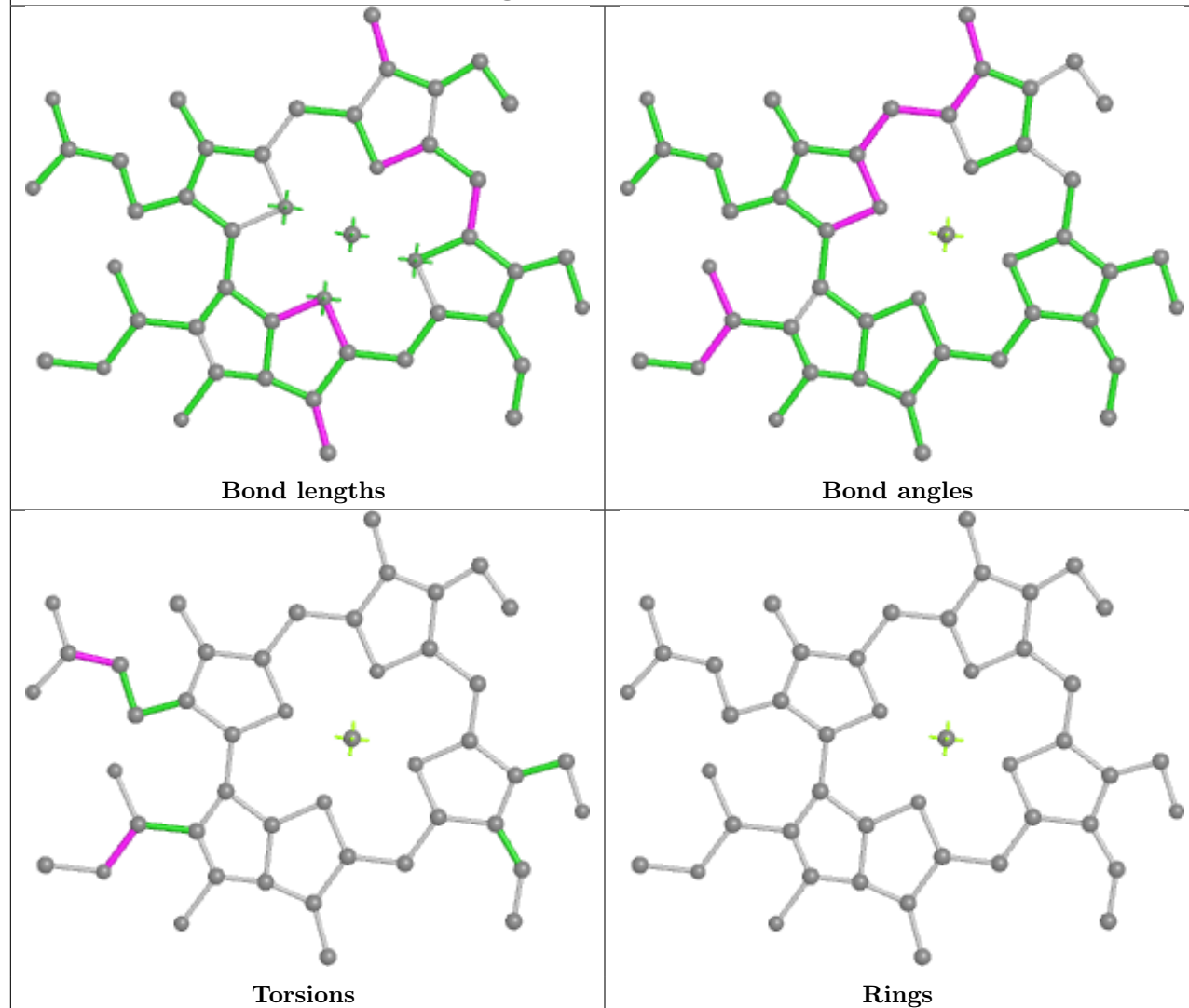
Rings



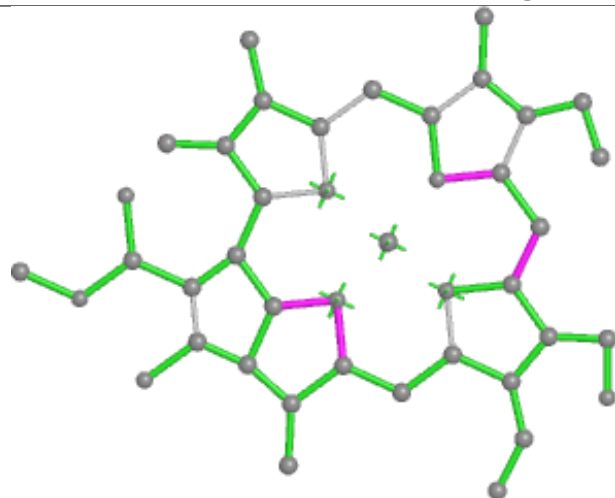
## Ligand CLA Bb 609



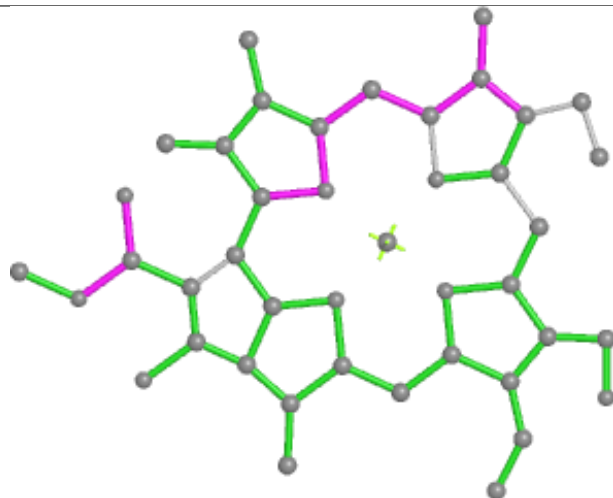
## Ligand CHL 4 307



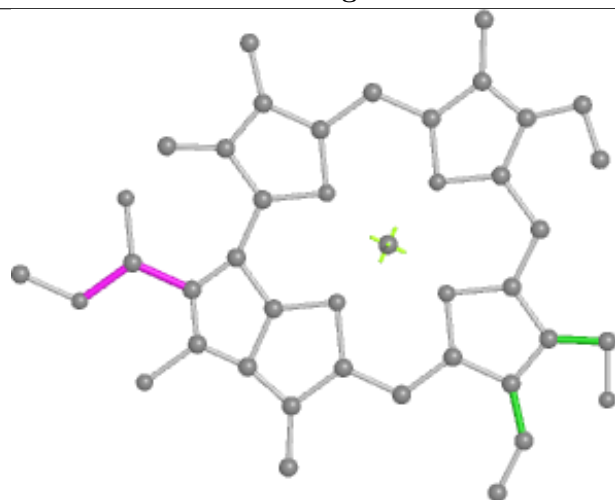
## Ligand CHL S 605



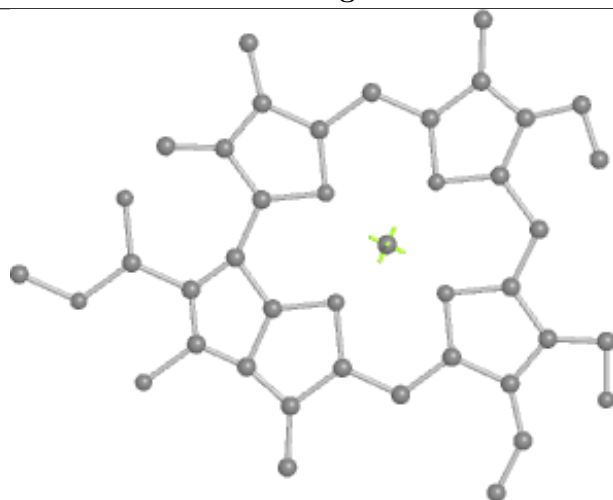
Bond lengths



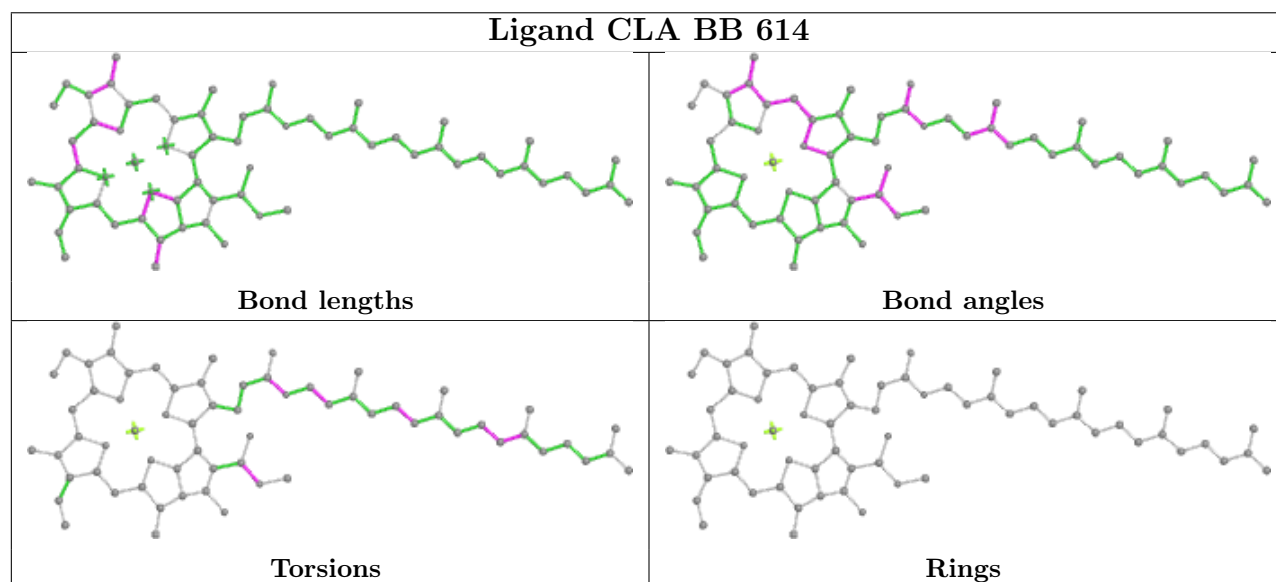
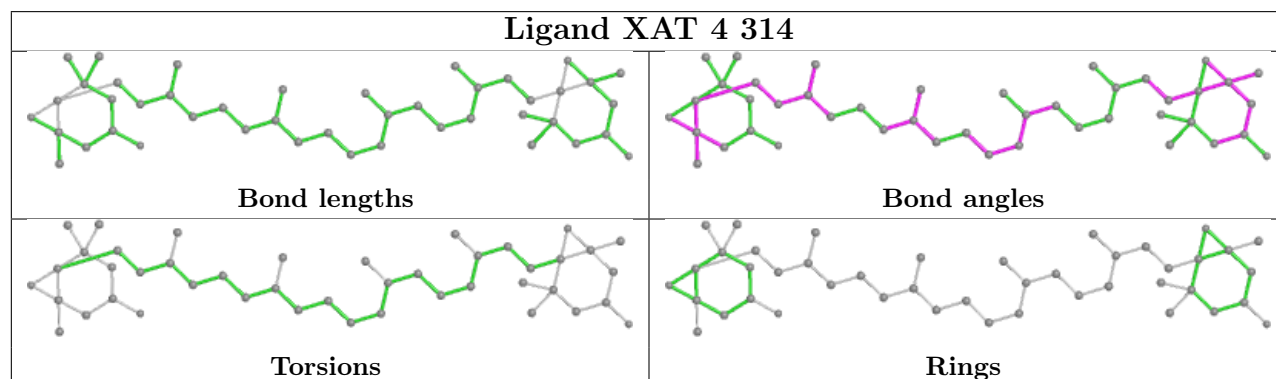
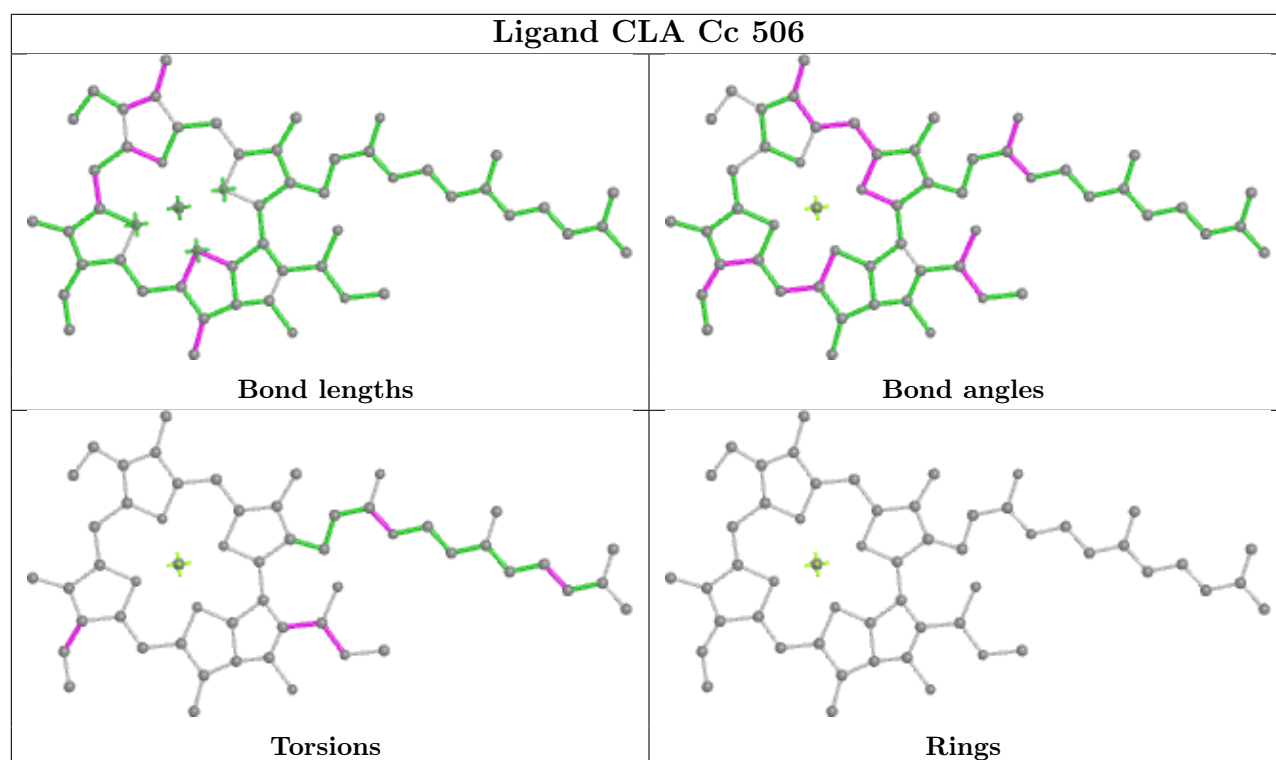
Bond angles

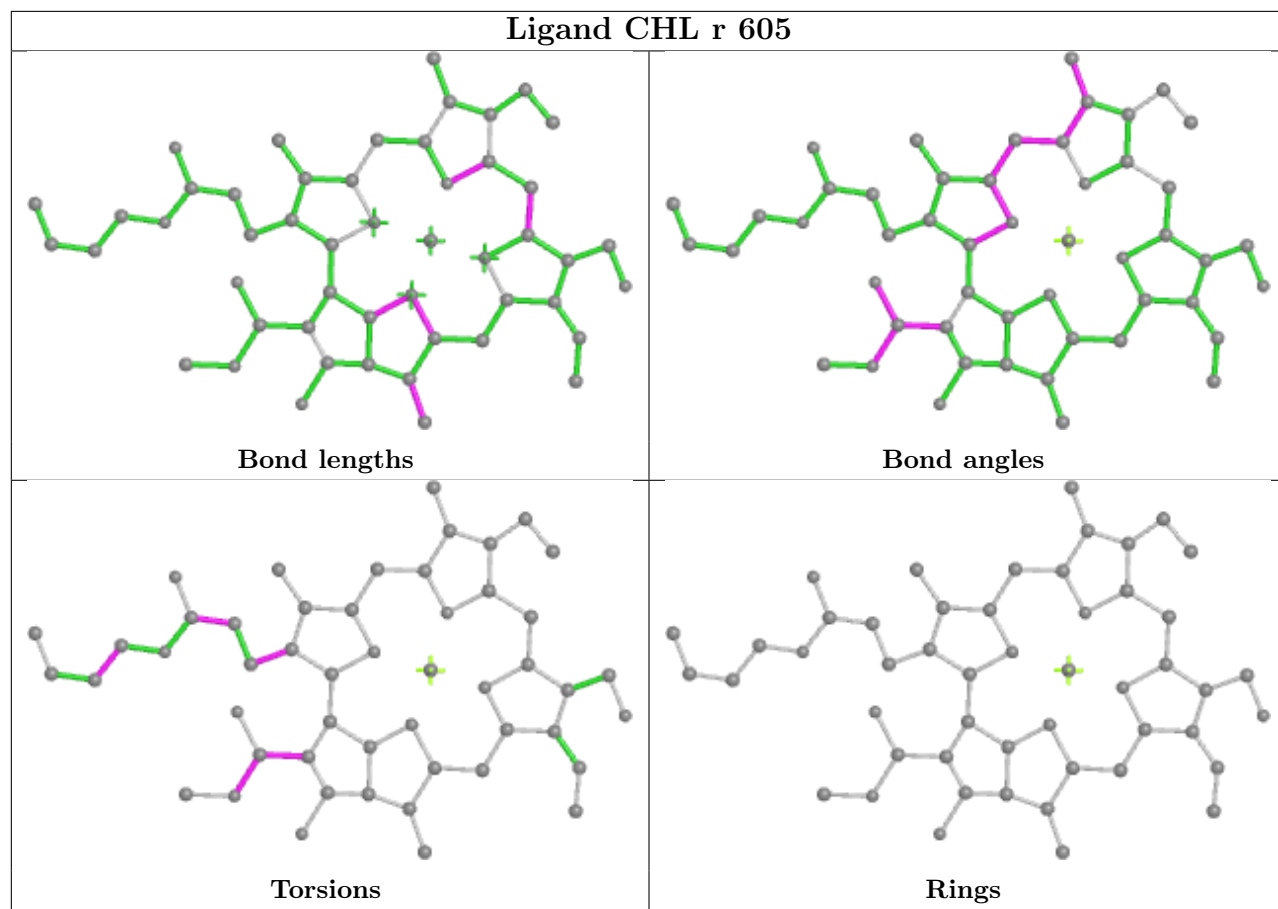


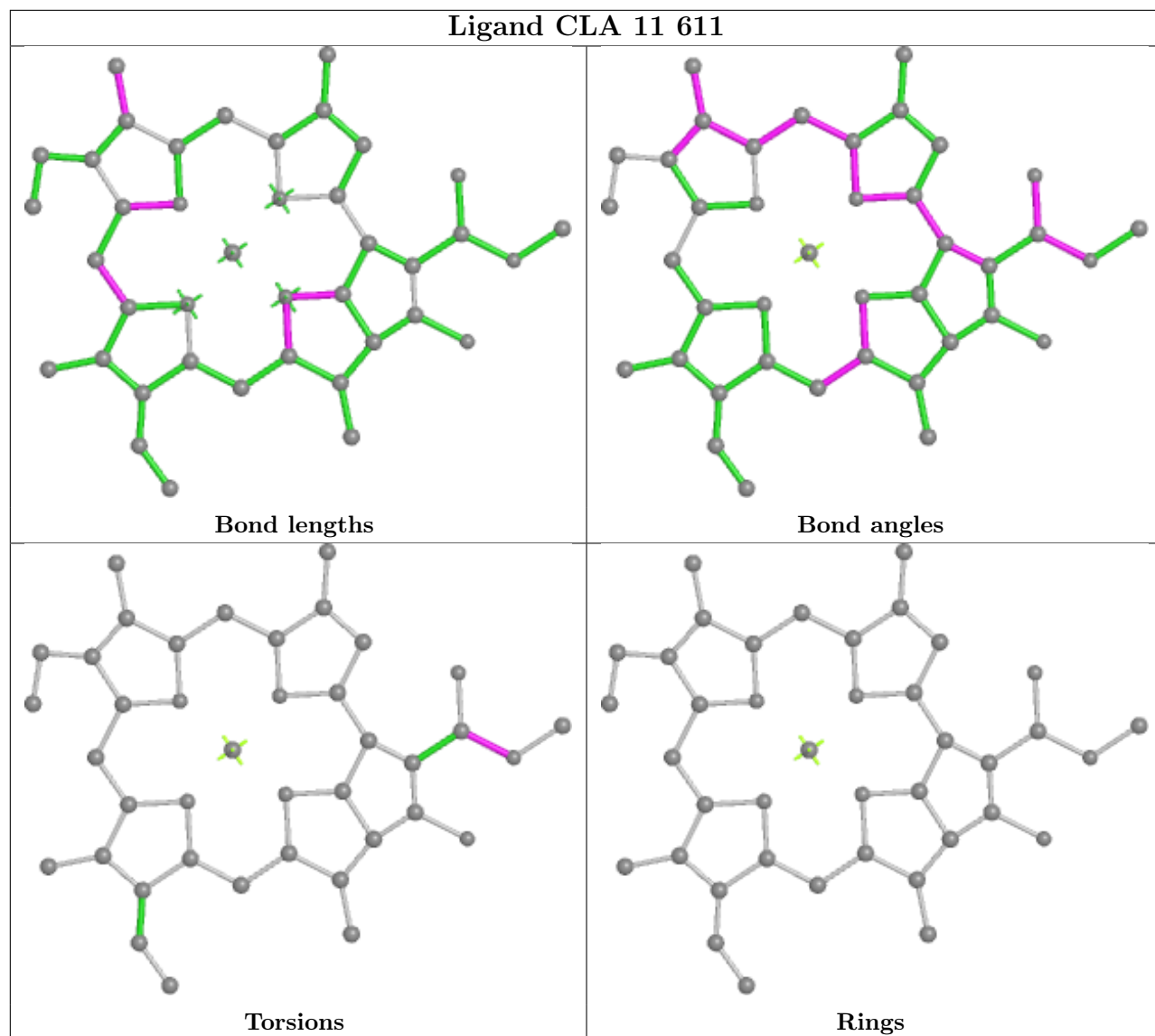
Torsions

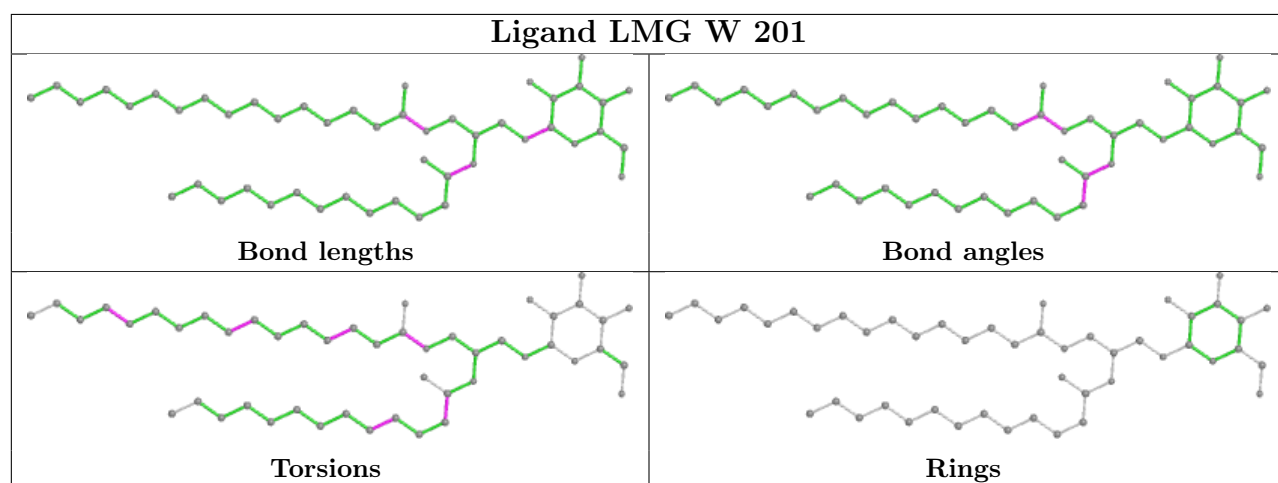
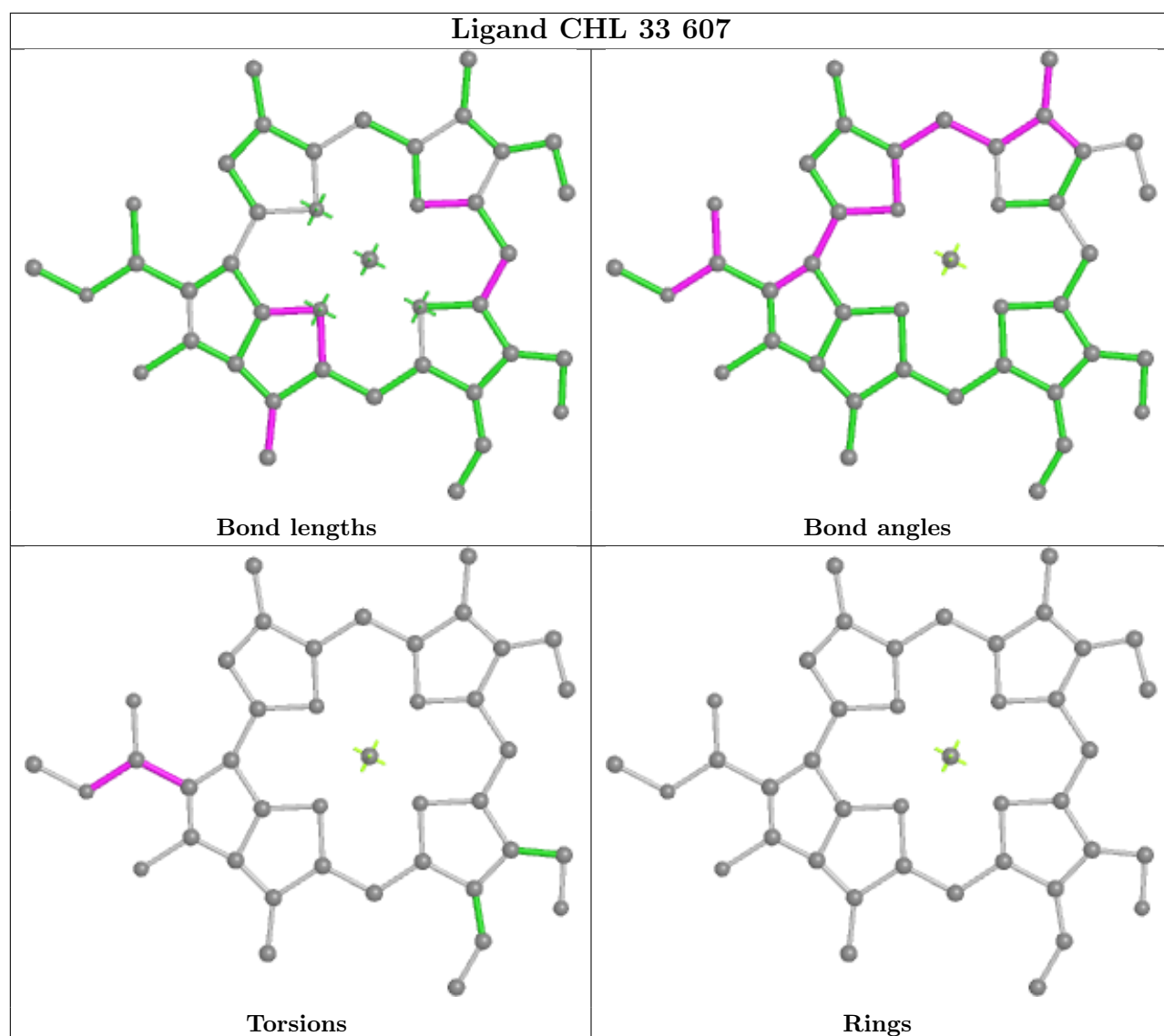


Rings

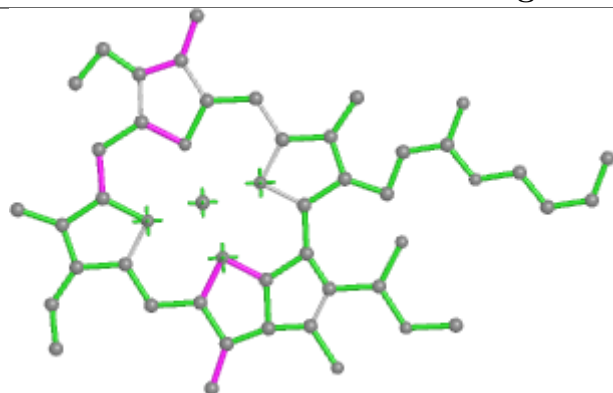




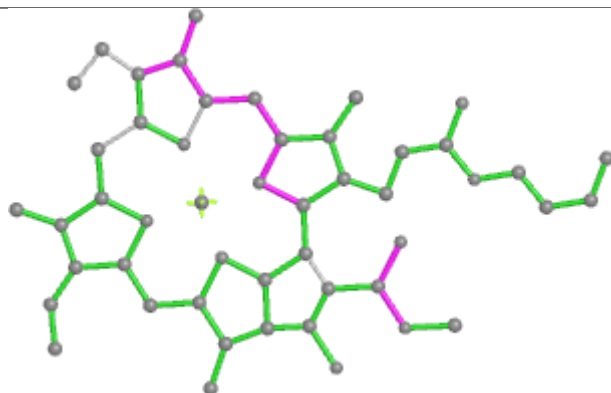




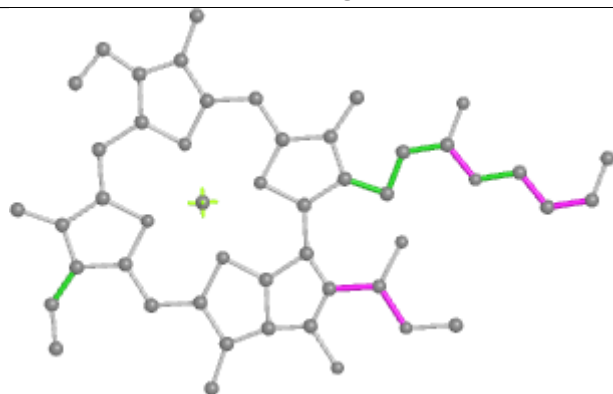
## Ligand CLA S 610



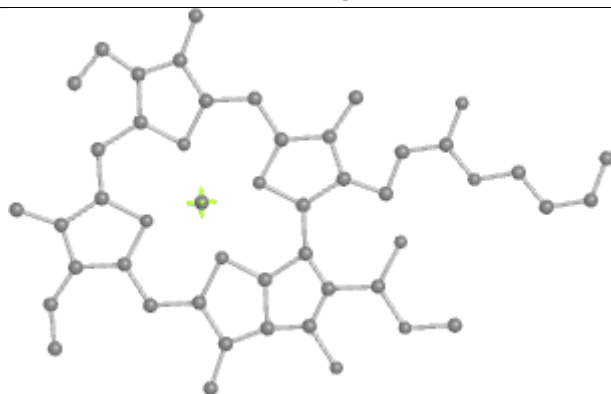
Bond lengths



Bond angles

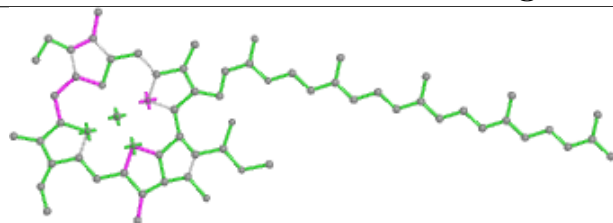


Torsions

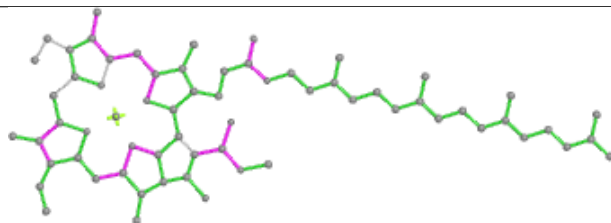


Rings

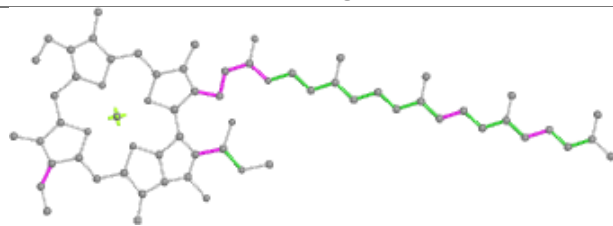
## Ligand CLA a 406



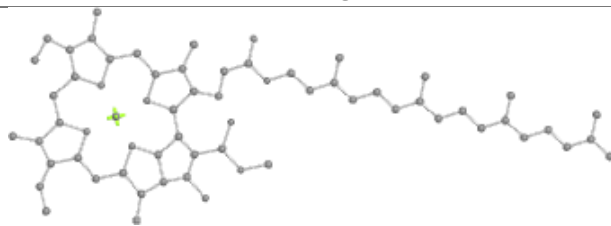
Bond lengths



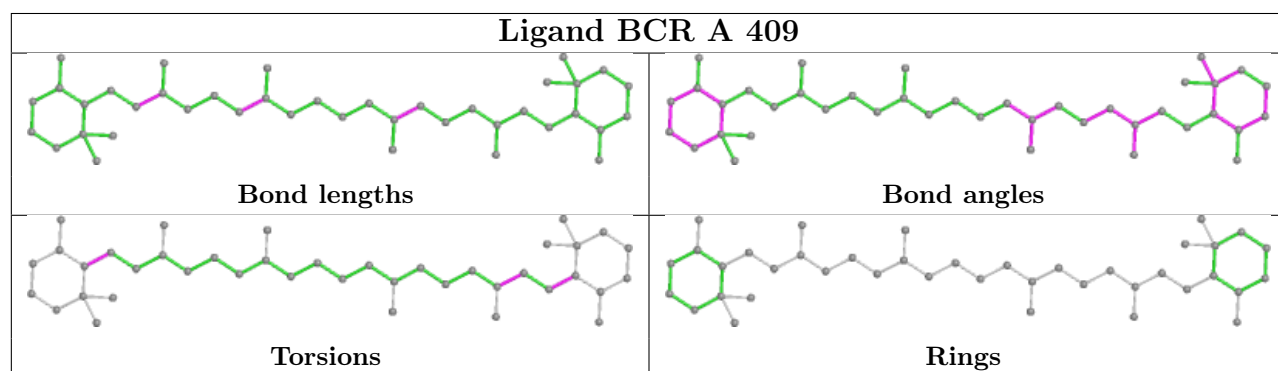
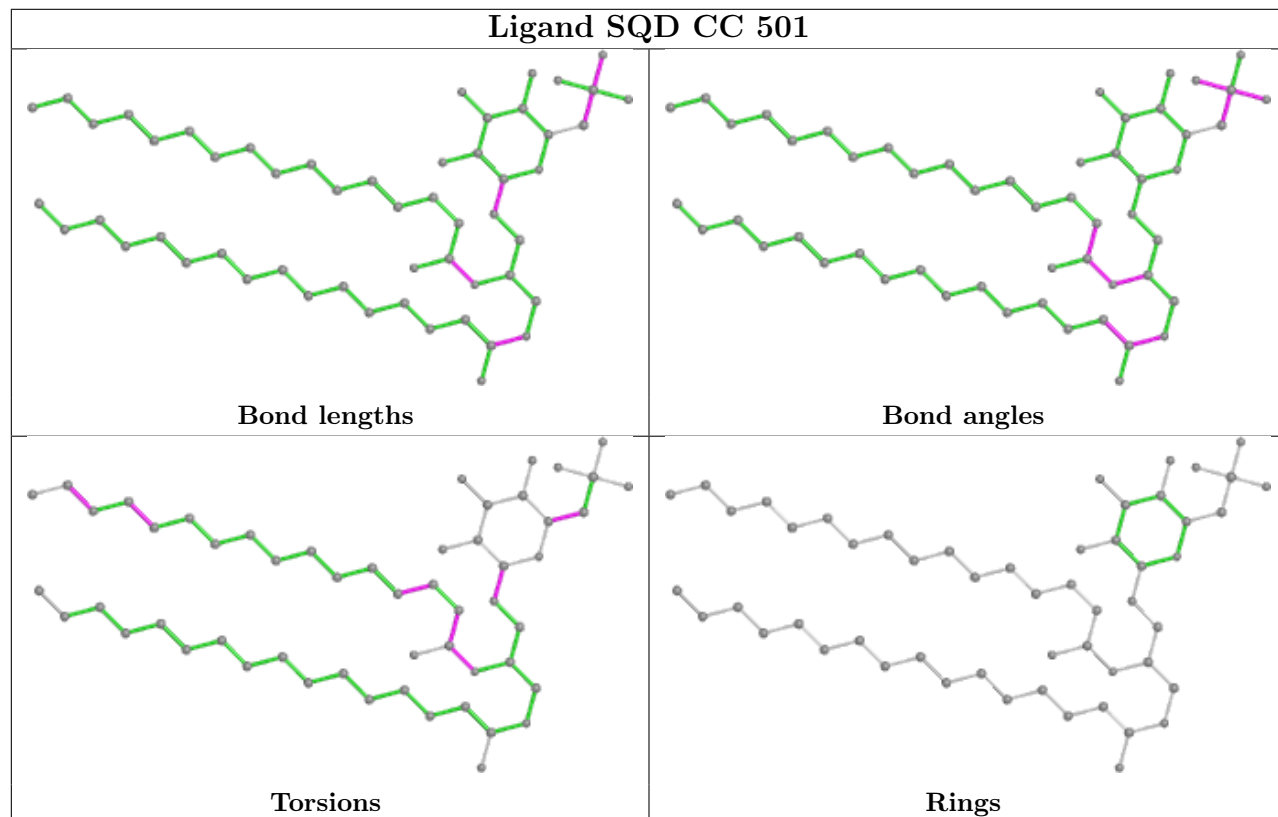
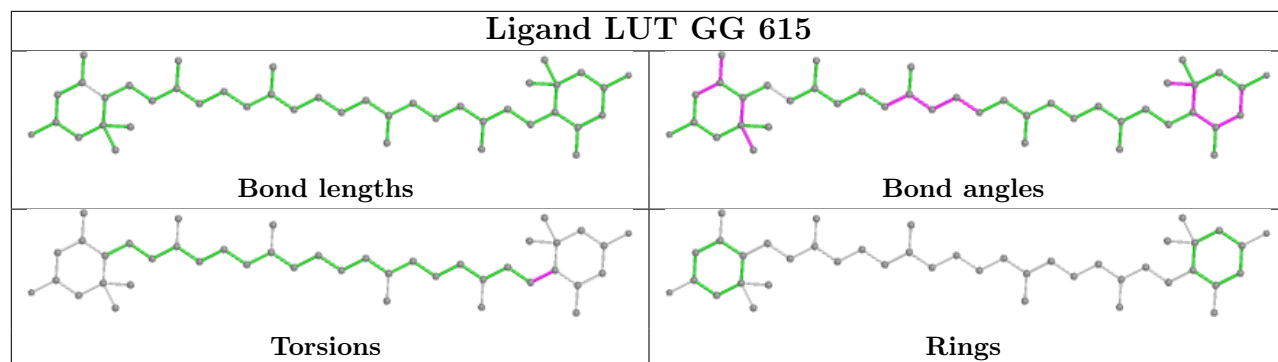
Bond angles



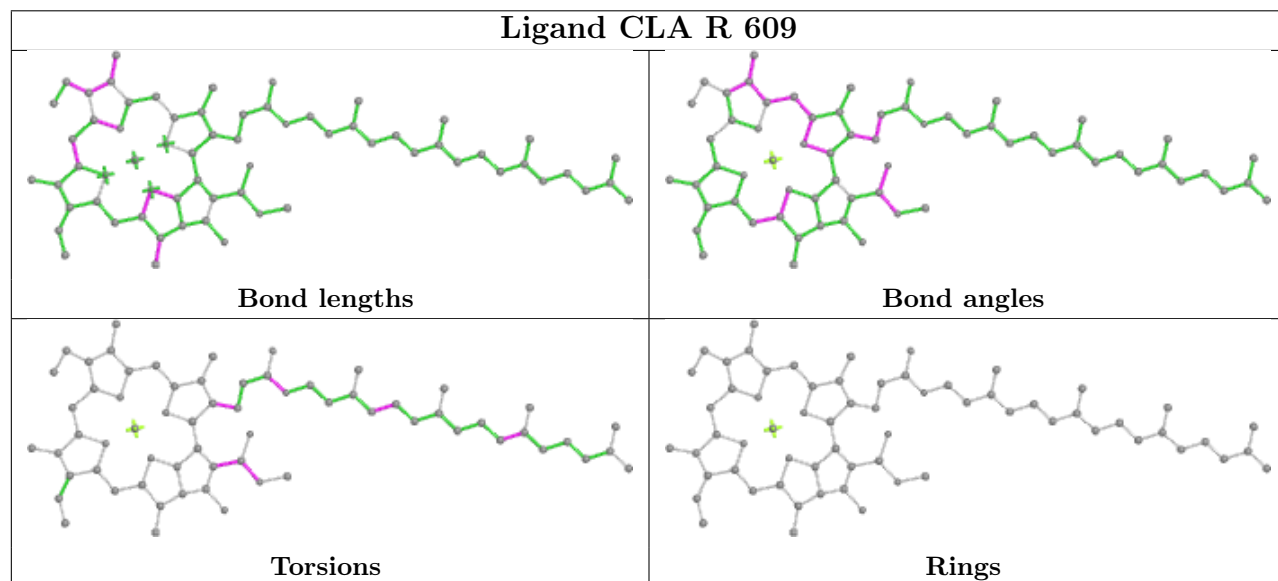
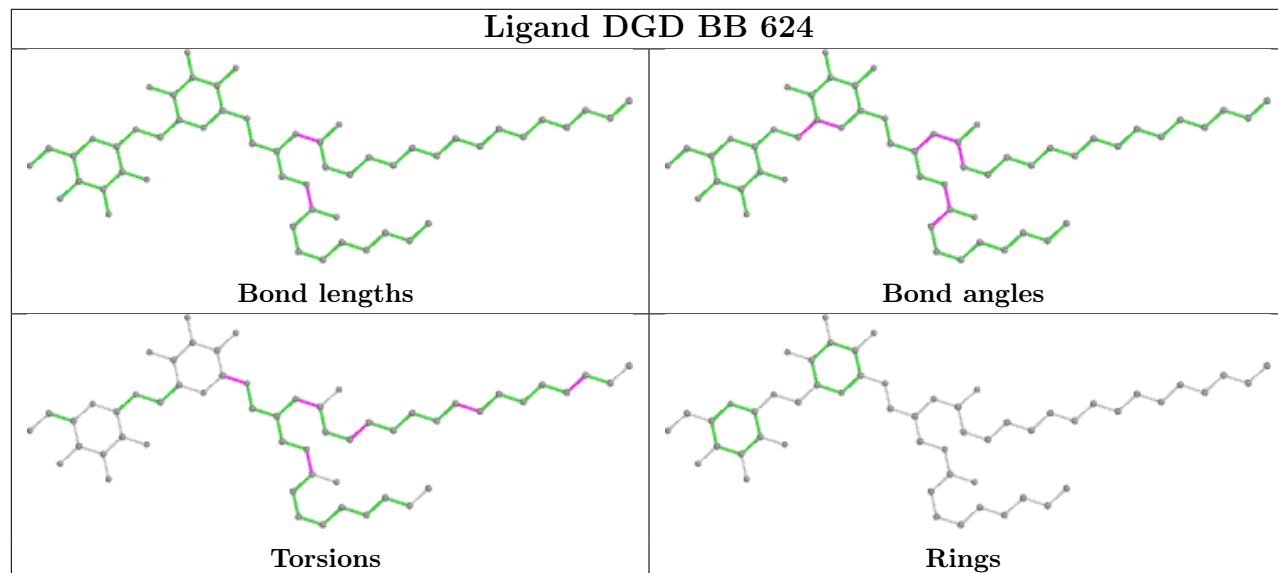
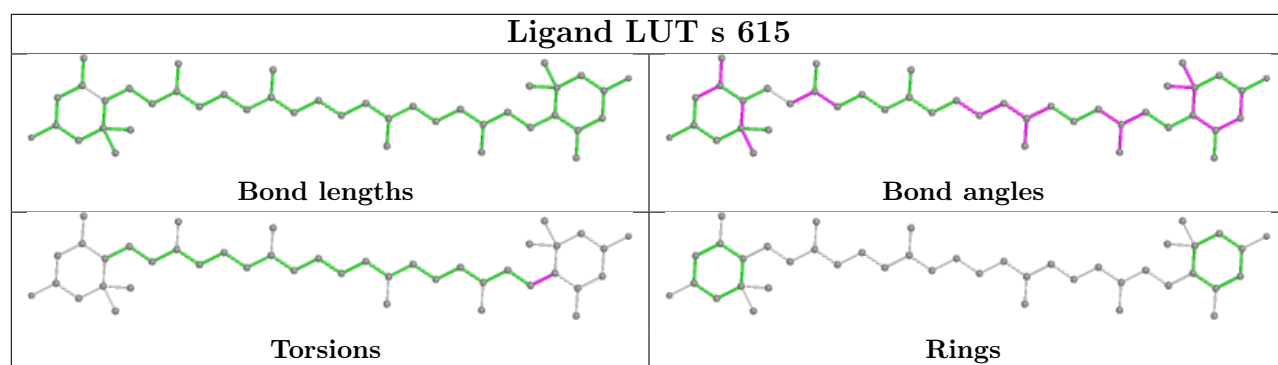
Torsions



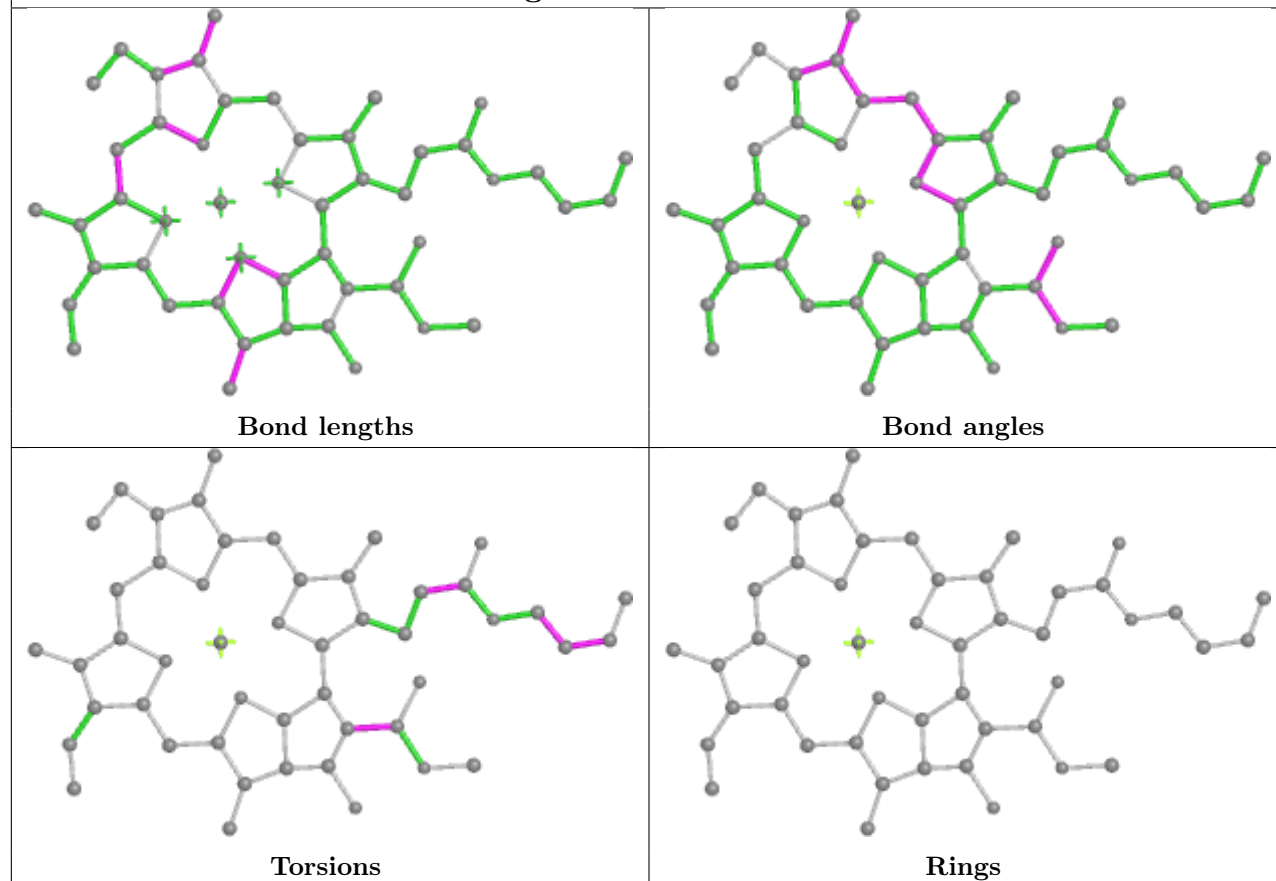
Rings



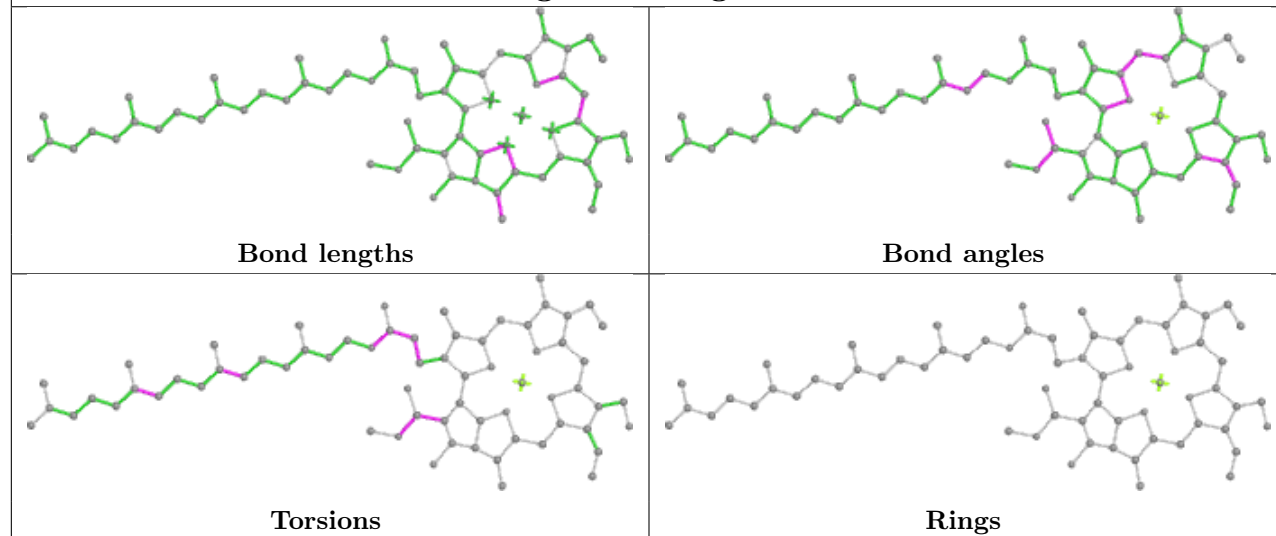


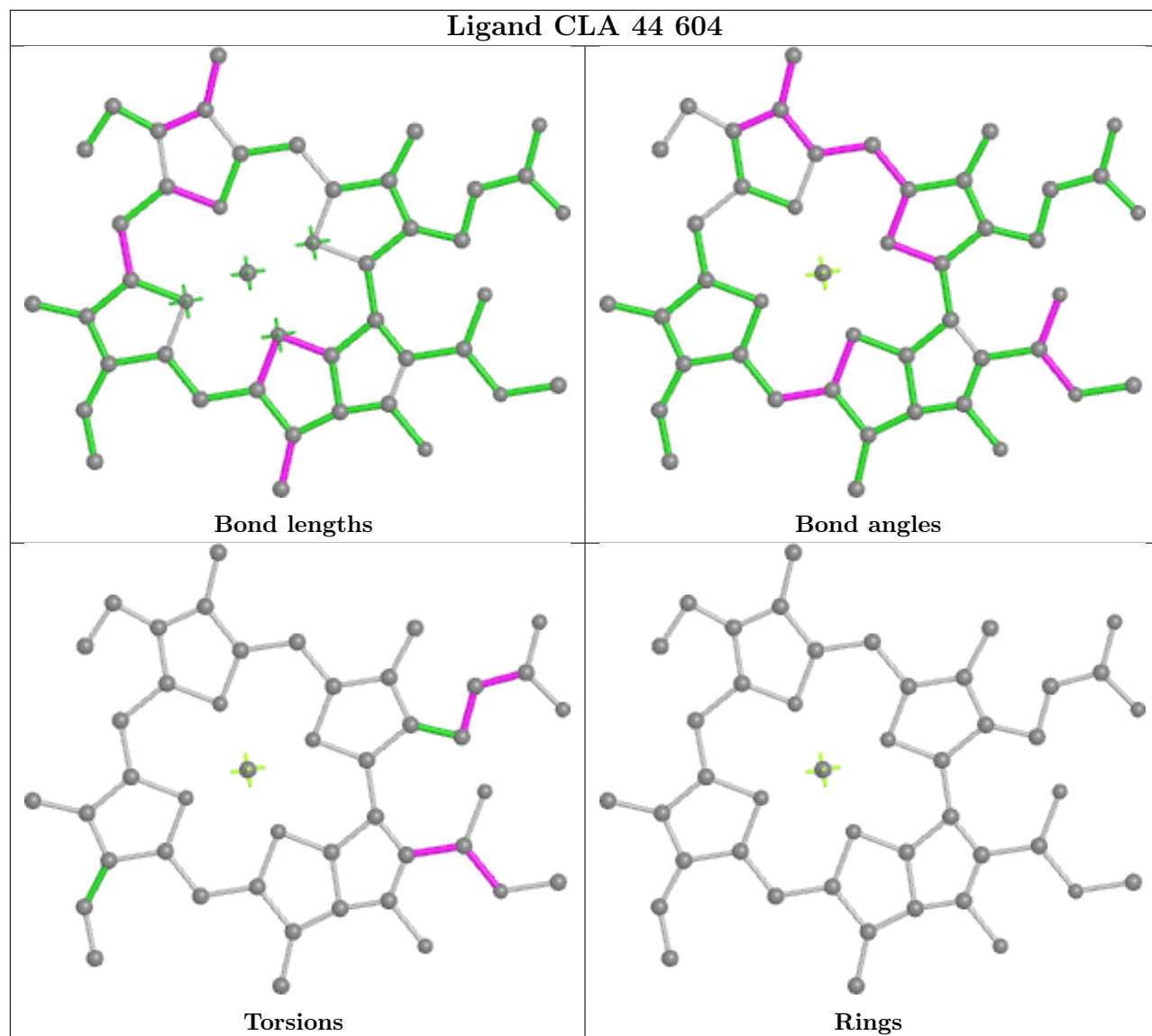
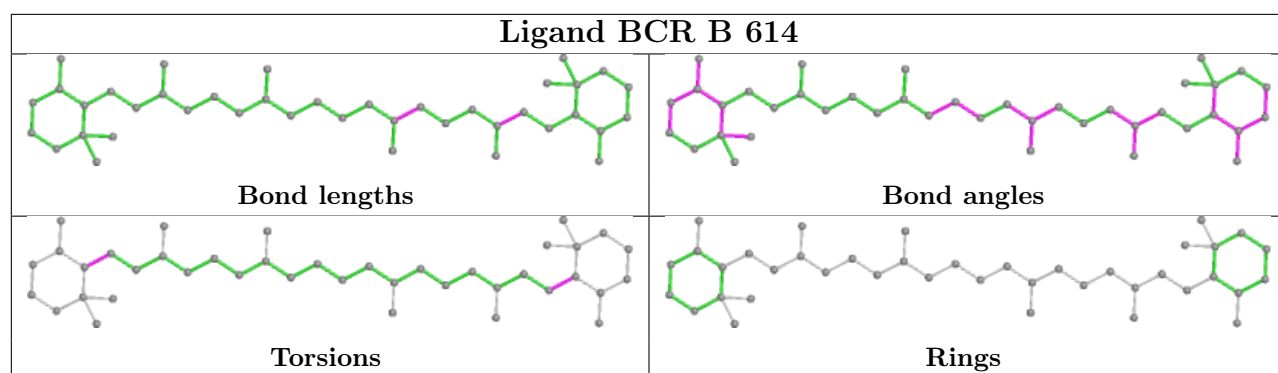


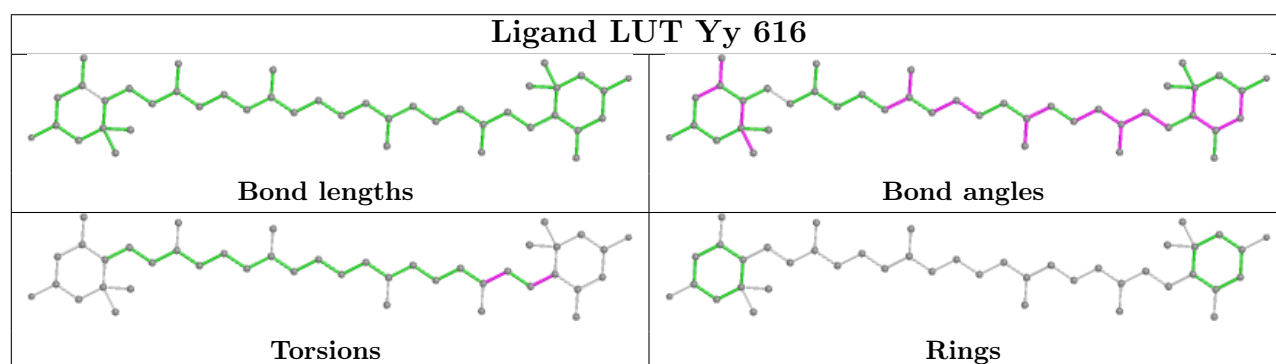
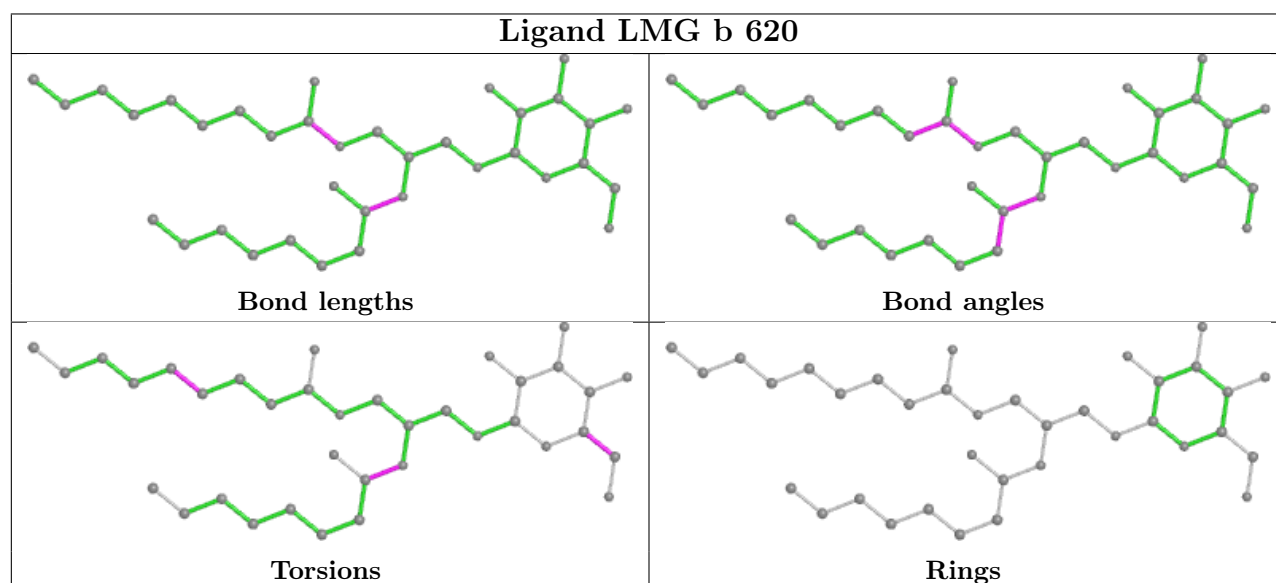
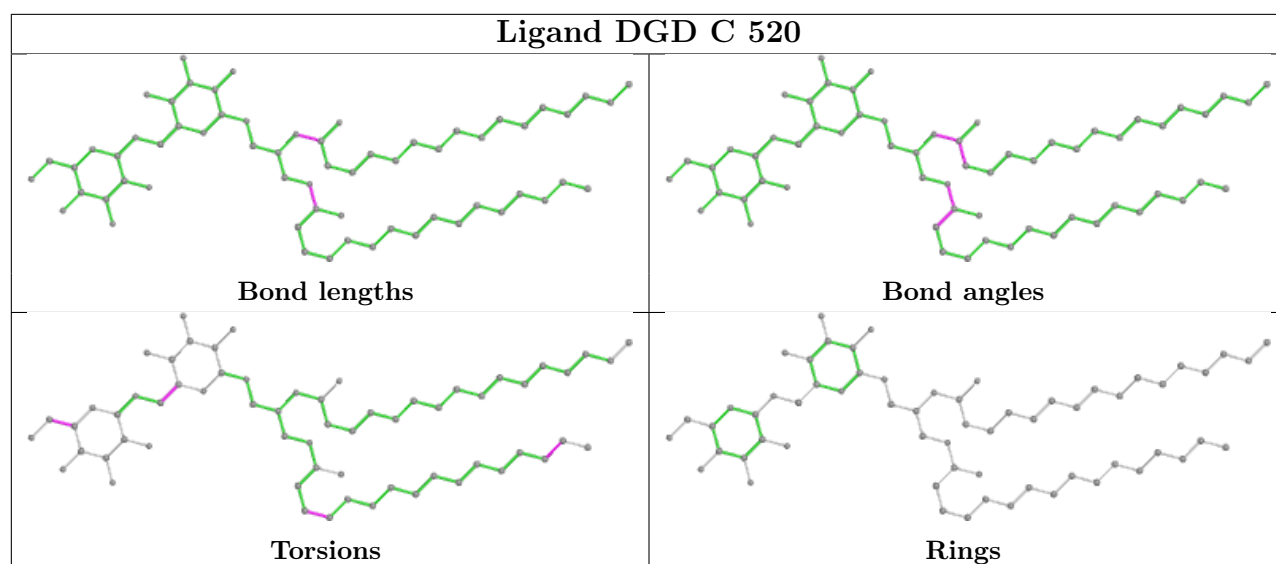
## Ligand CLA Rr 603

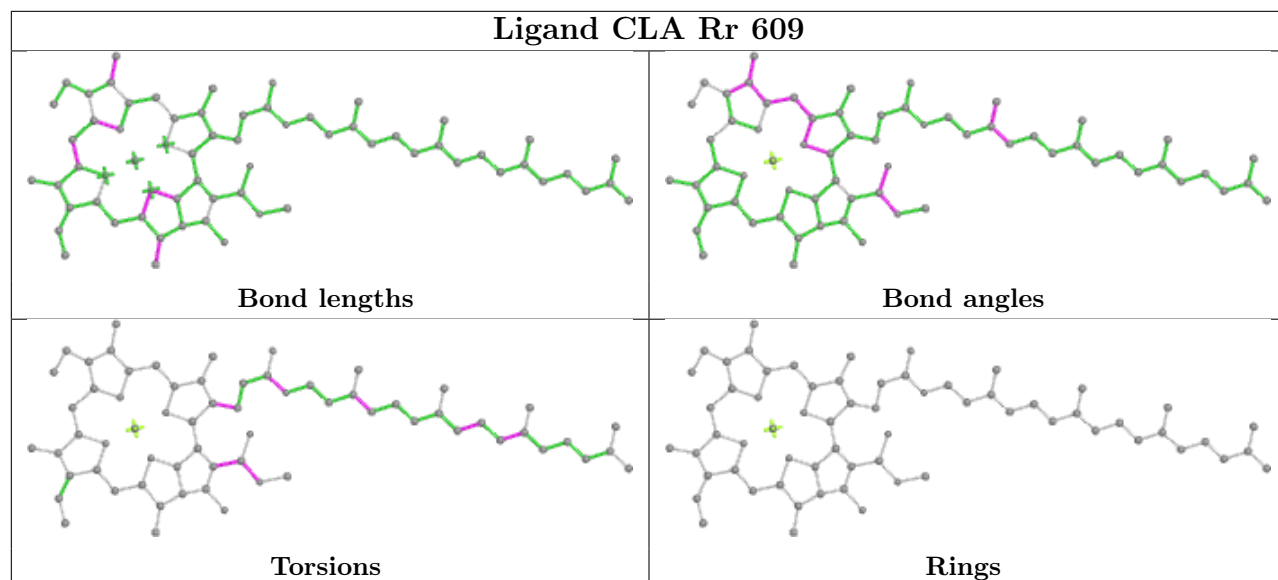
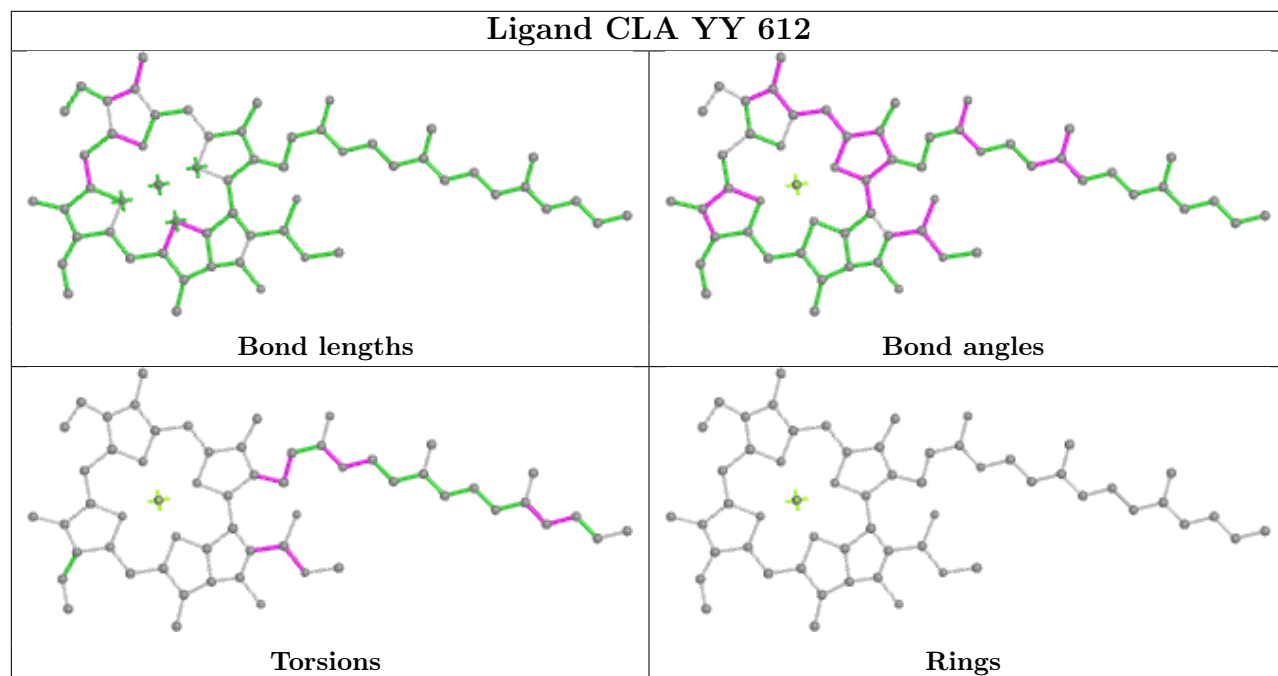
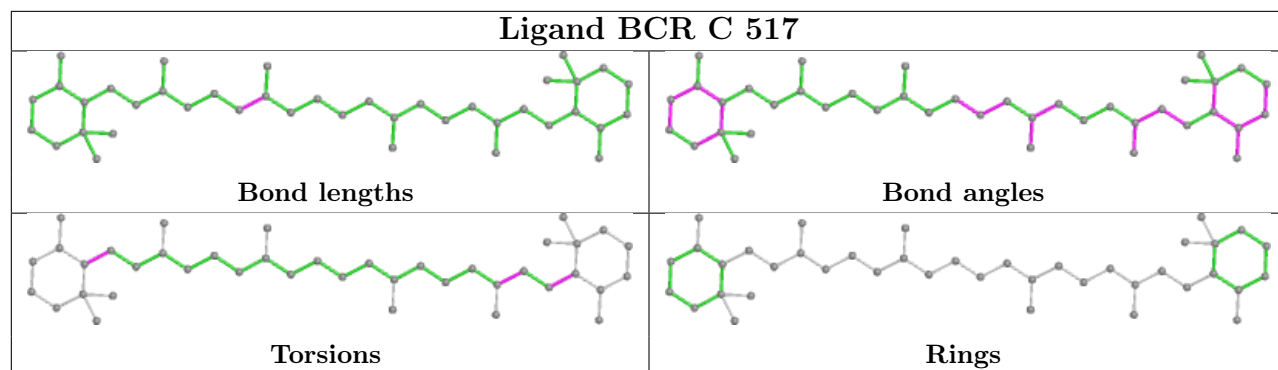


## Ligand CHL g 601

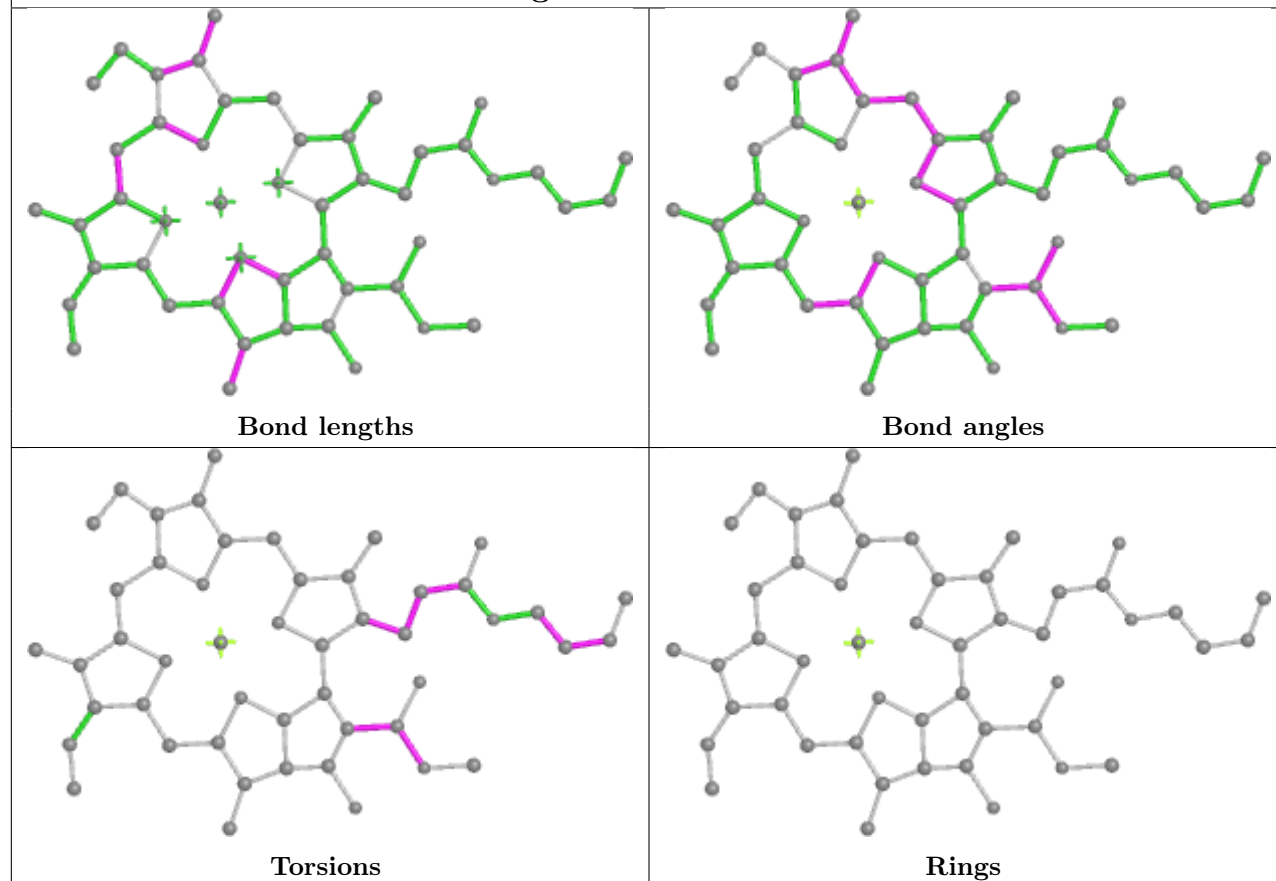




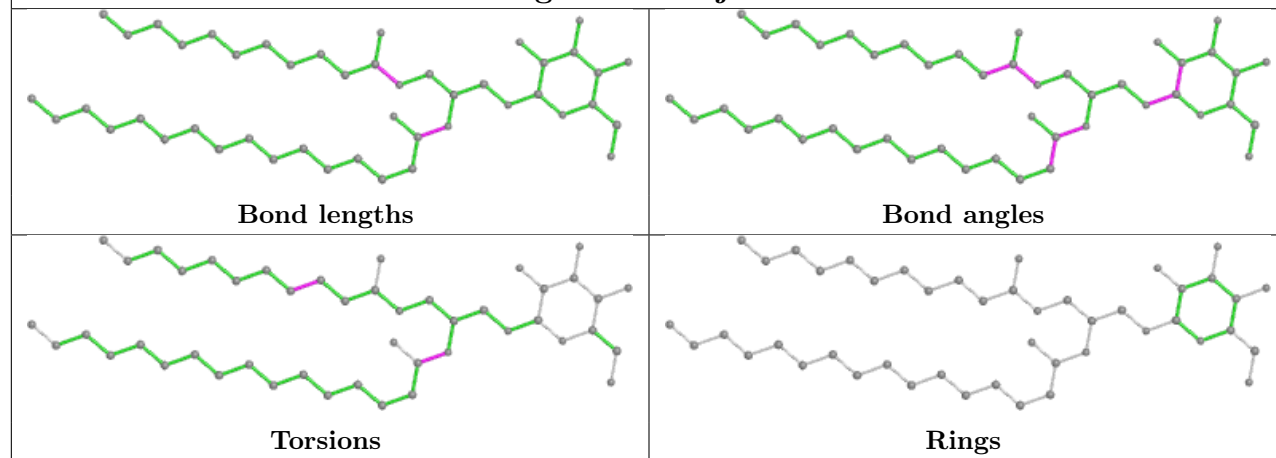




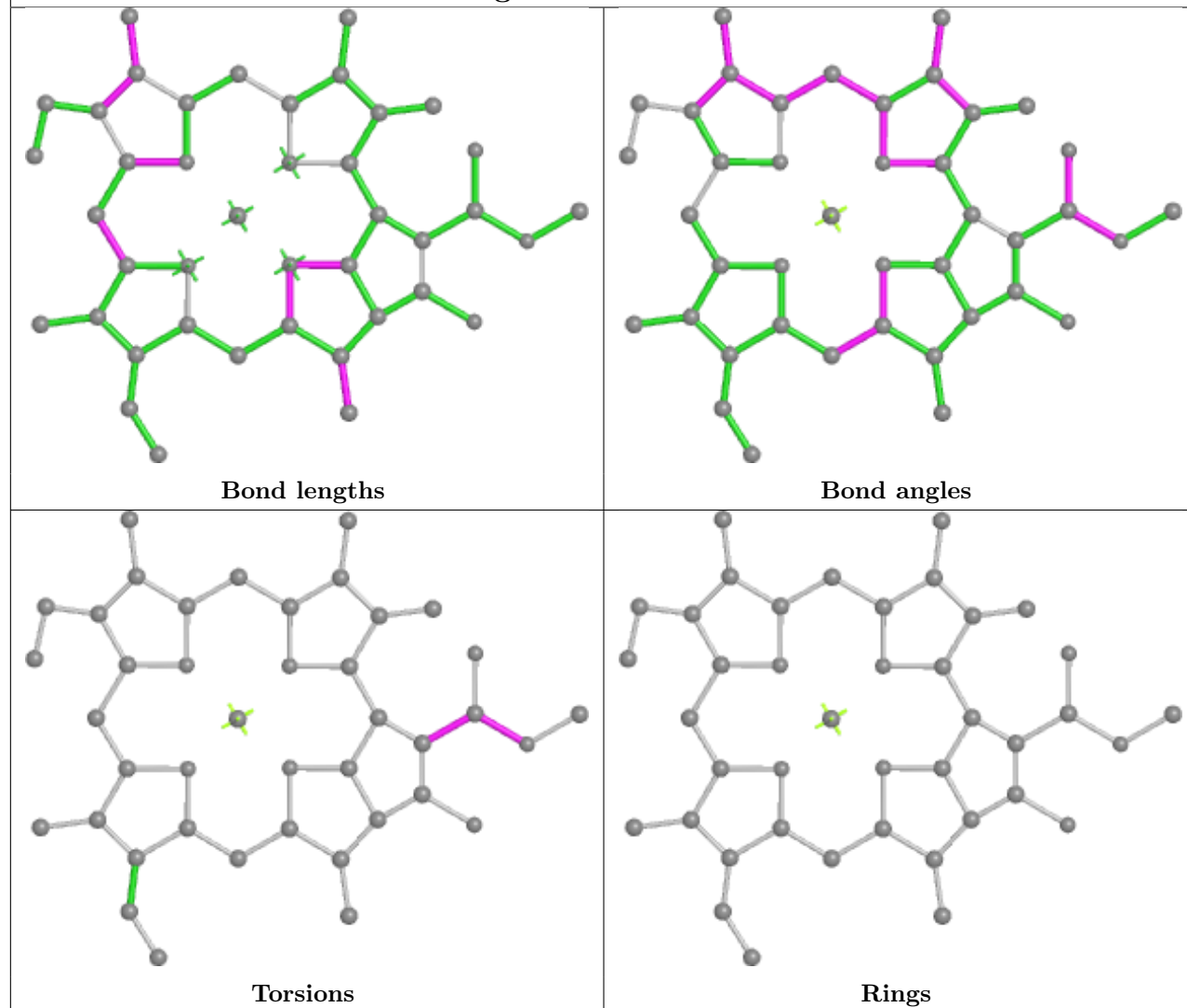
## Ligand CLA Y 604



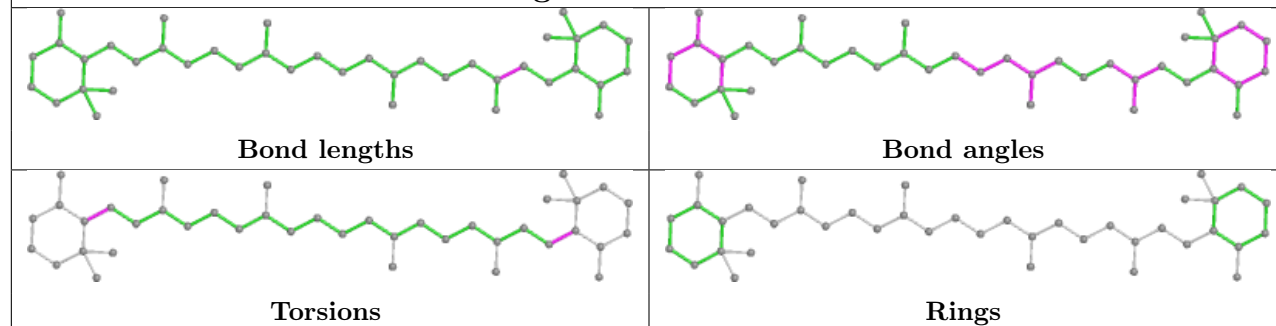
## Ligand LMG j 101



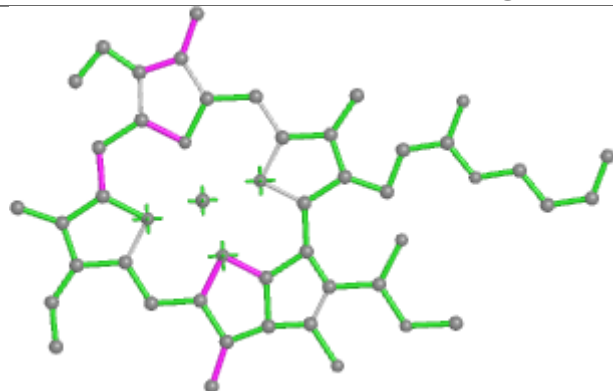
## Ligand CLA X 201



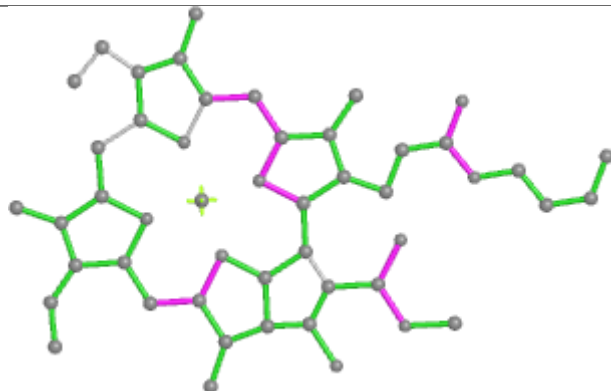
## Ligand BCR b 618



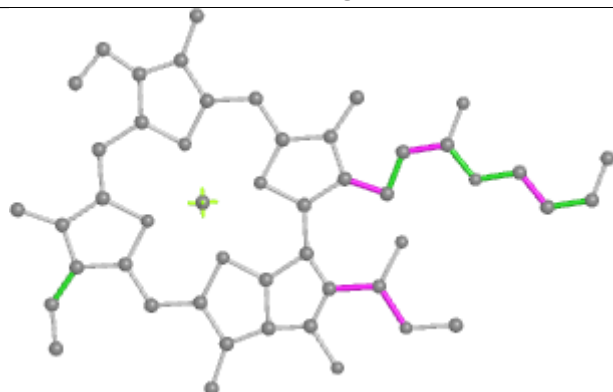
## Ligand CLA GG 602



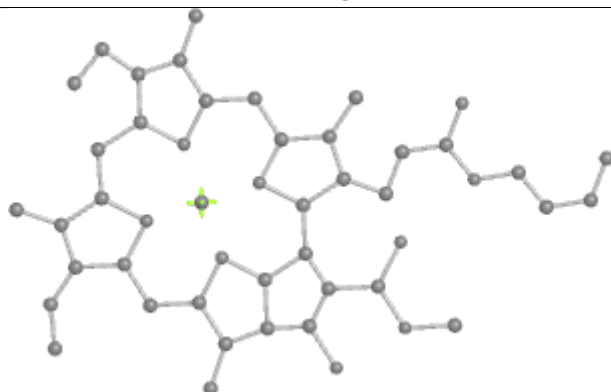
Bond lengths



Bond angles

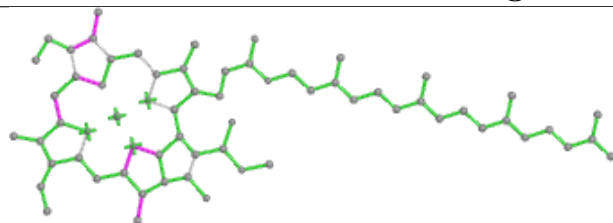


Torsions

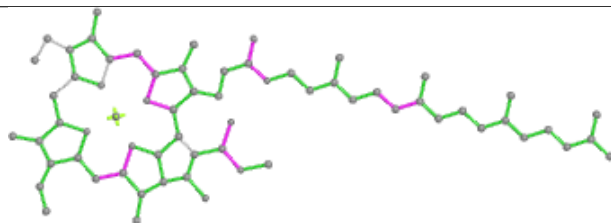


Rings

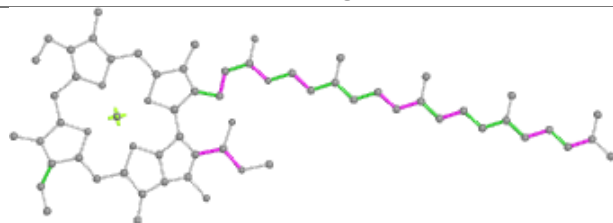
## Ligand CLA Cc 503



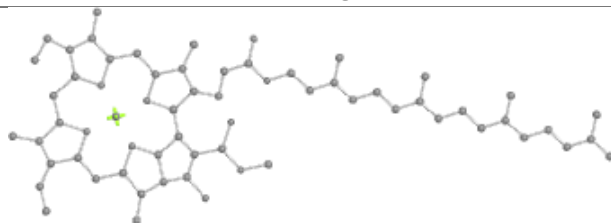
Bond lengths



Bond angles

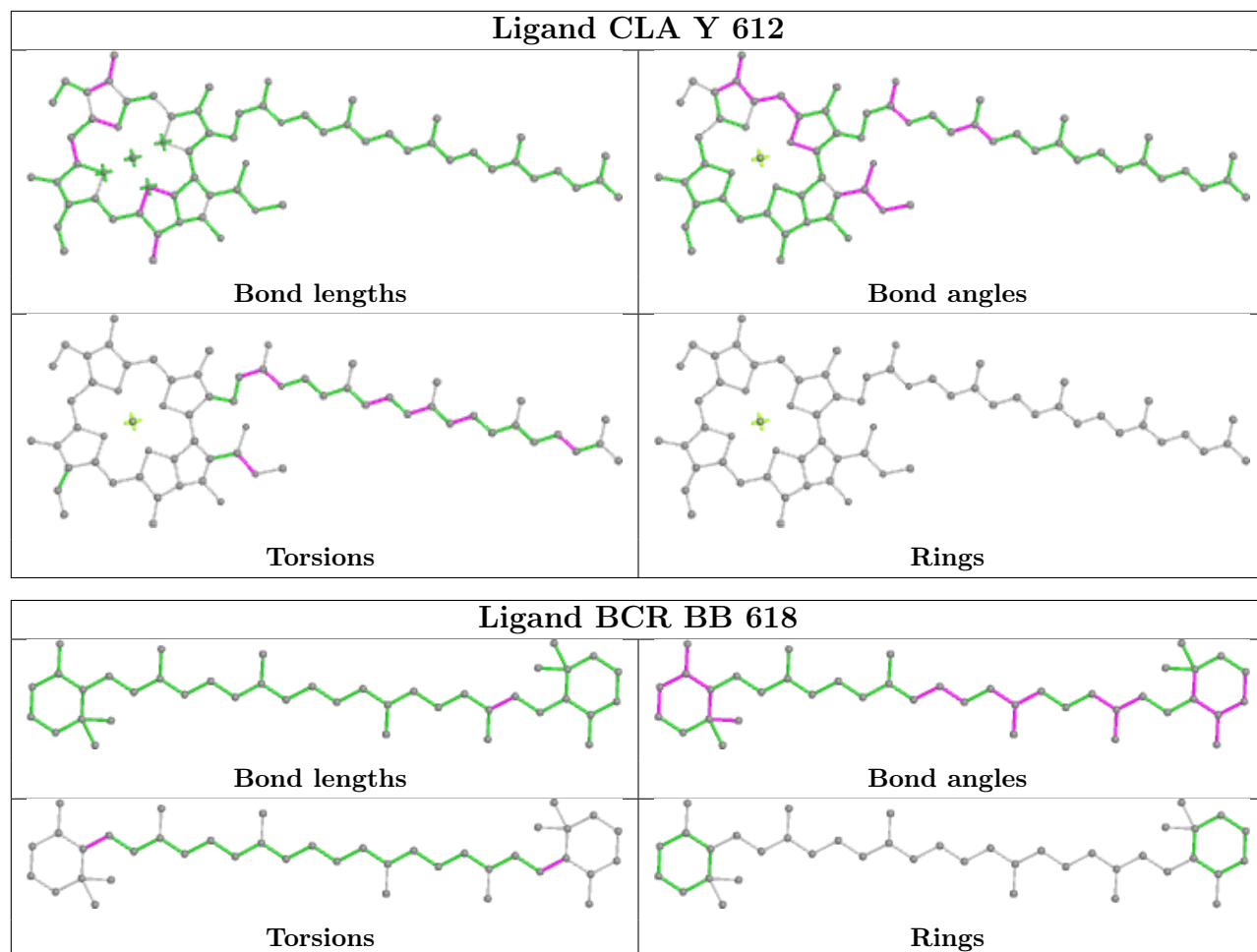


Torsions

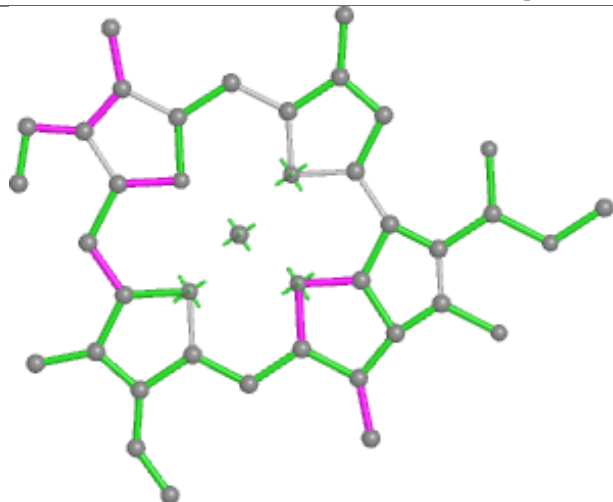


Rings

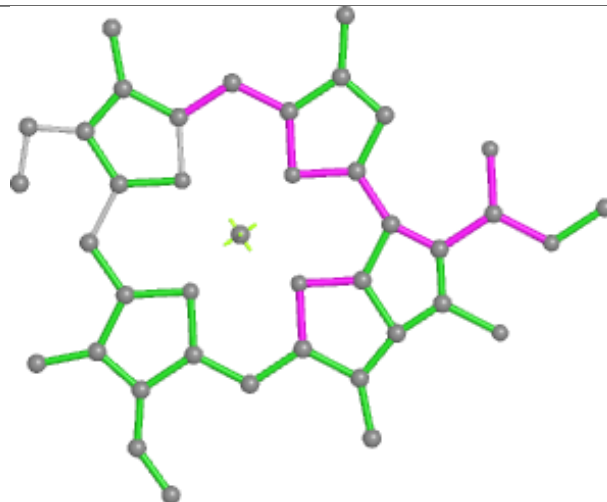




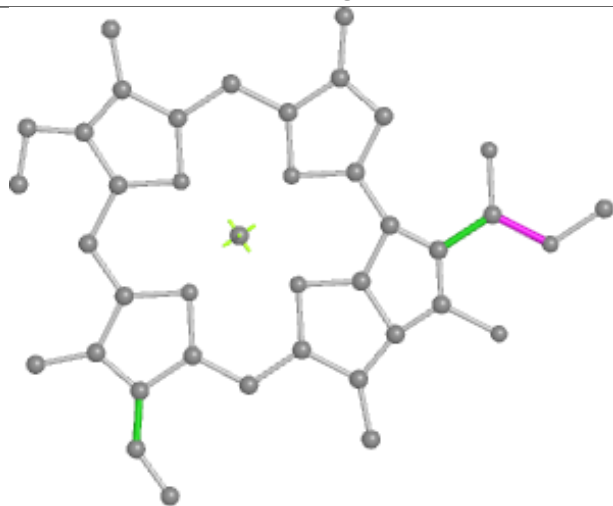
## Ligand CLA 1 609



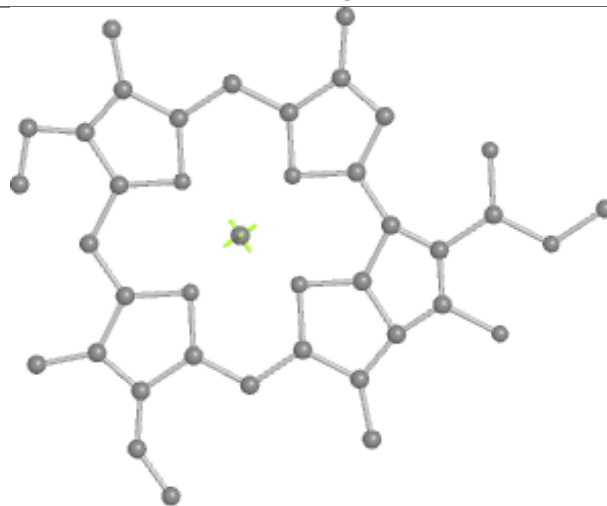
Bond lengths



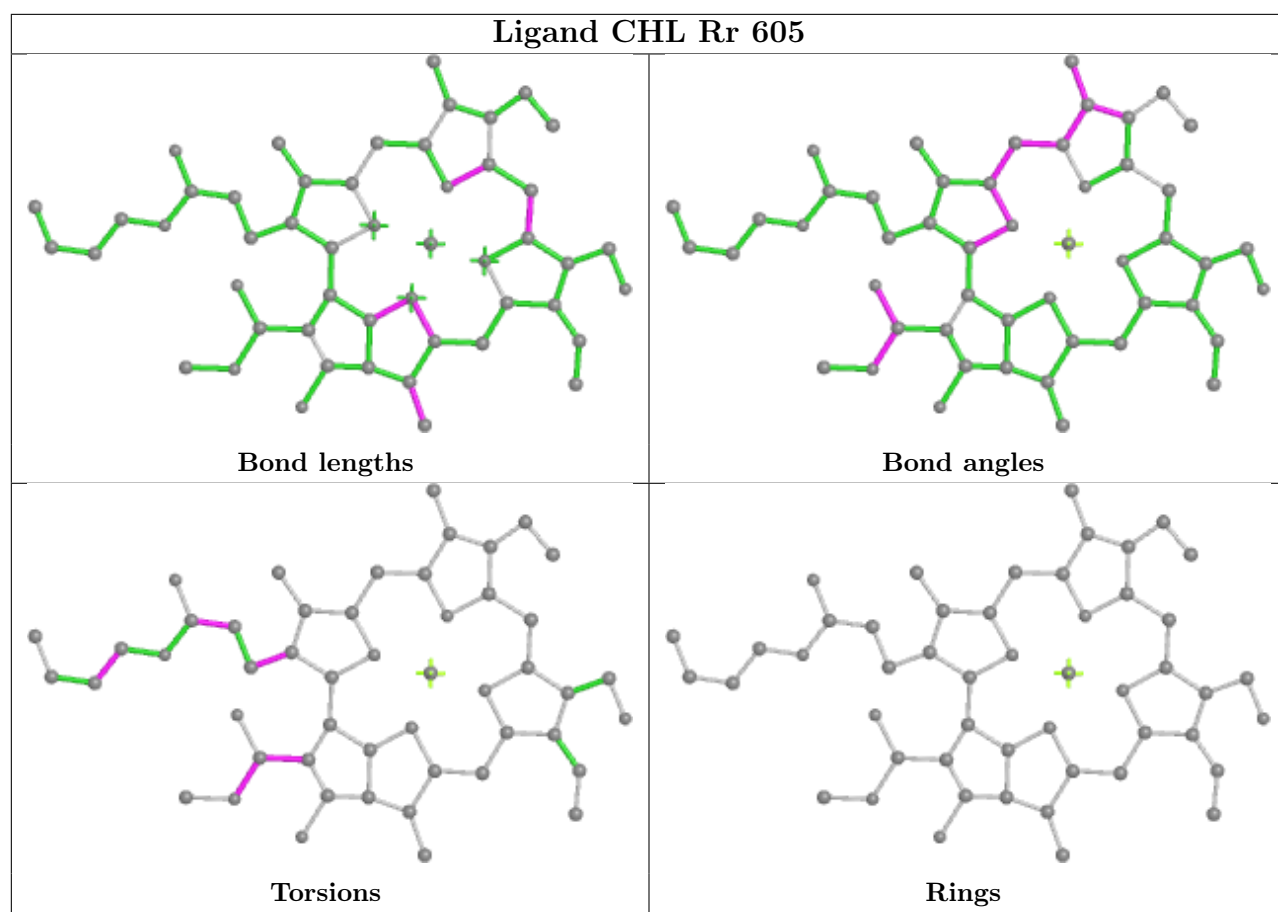
Bond angles

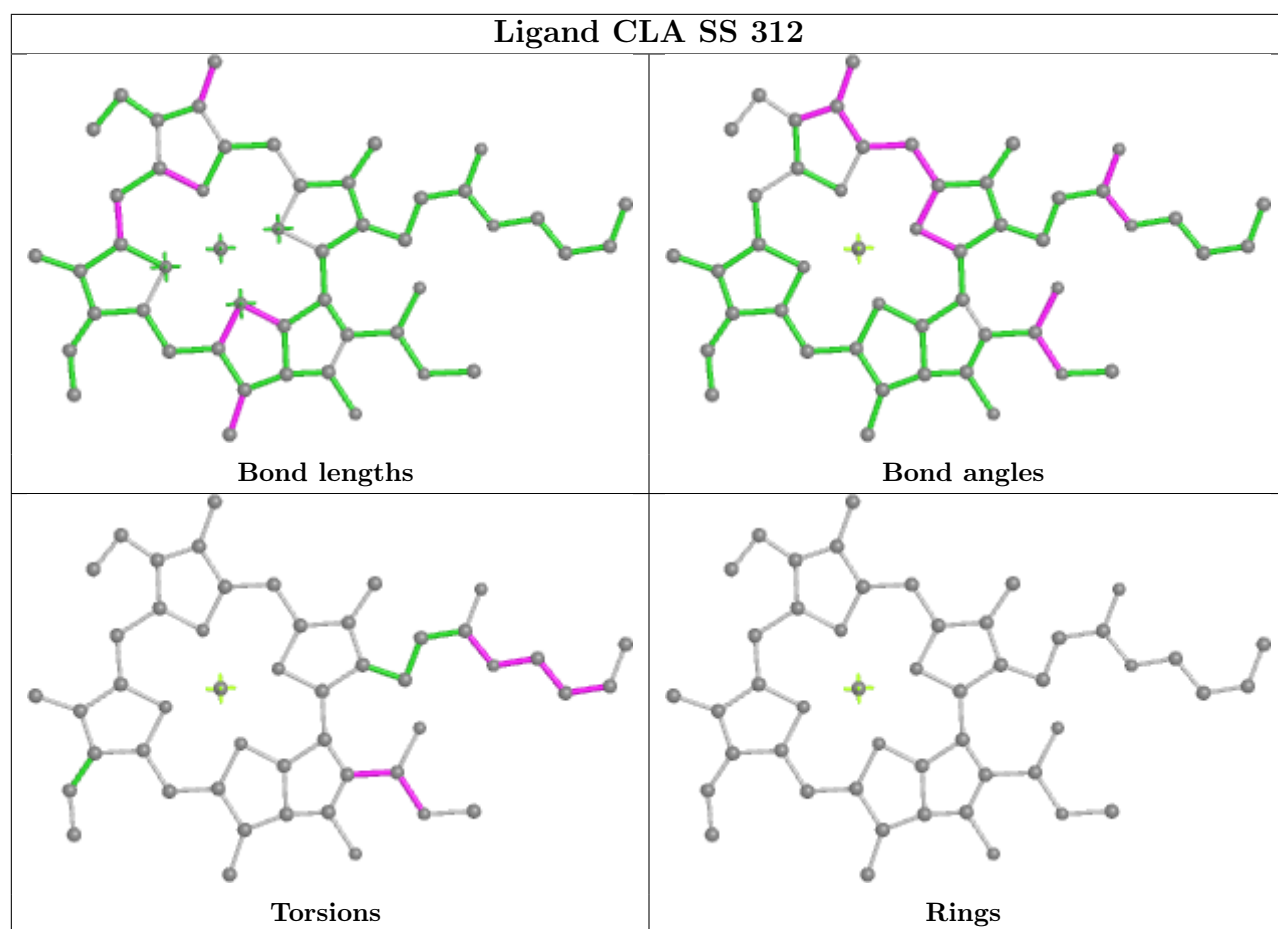


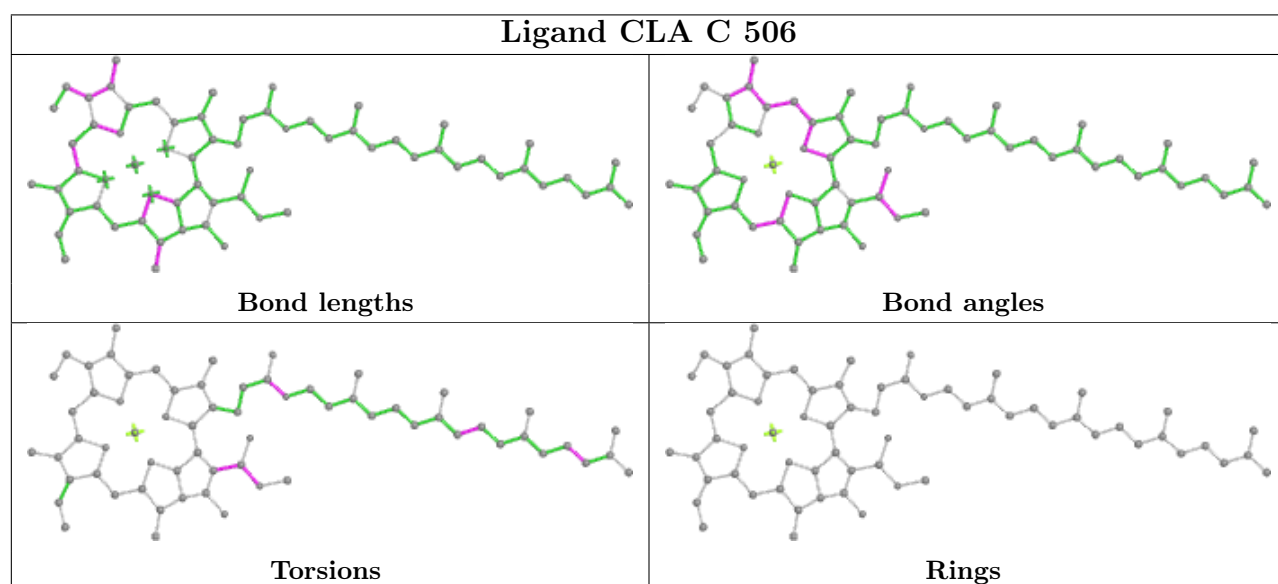
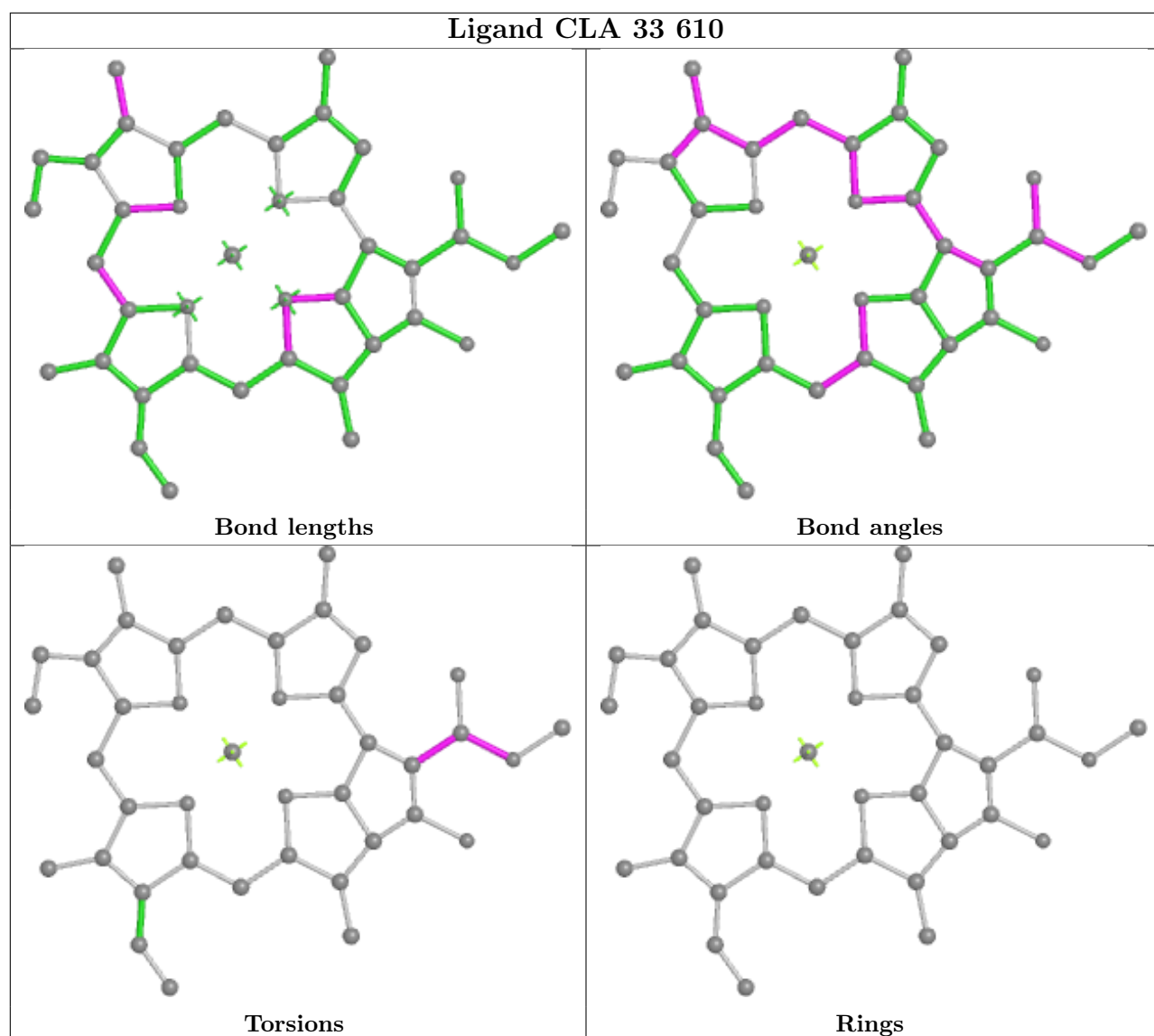
Torsions

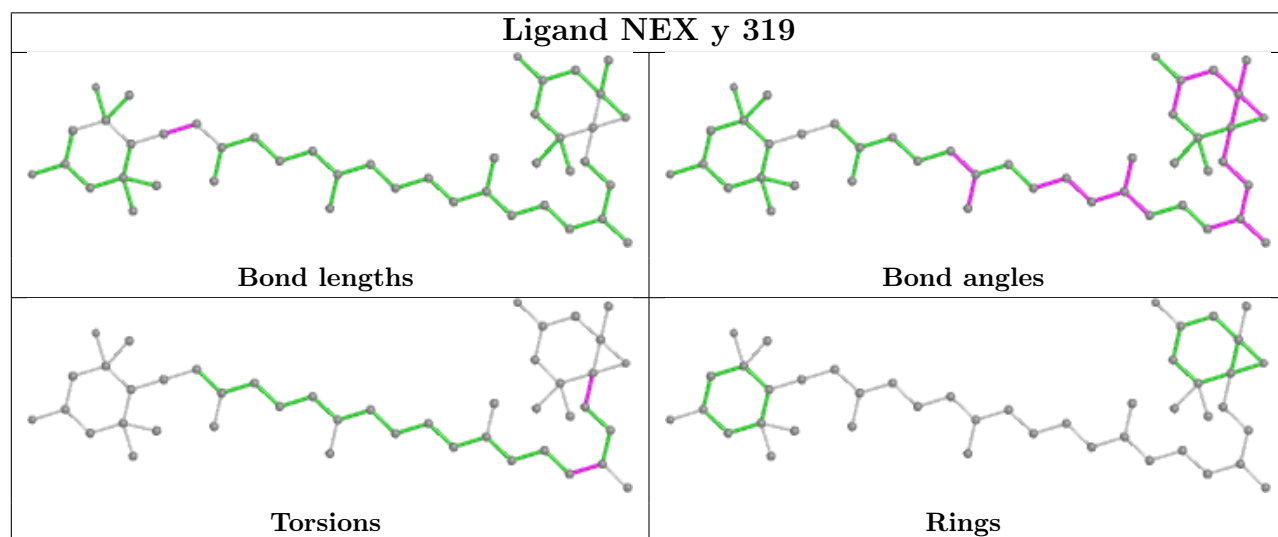
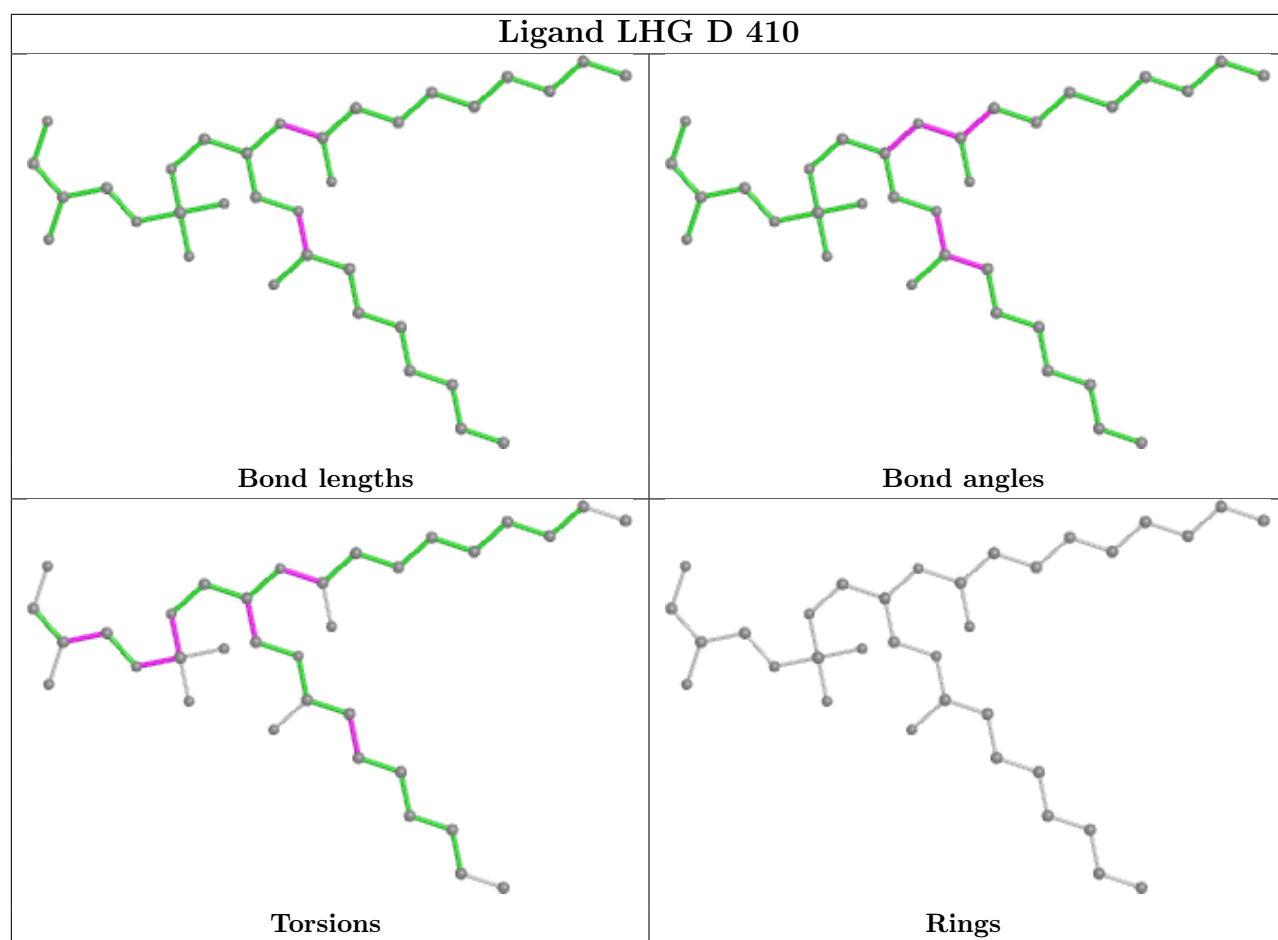


Rings

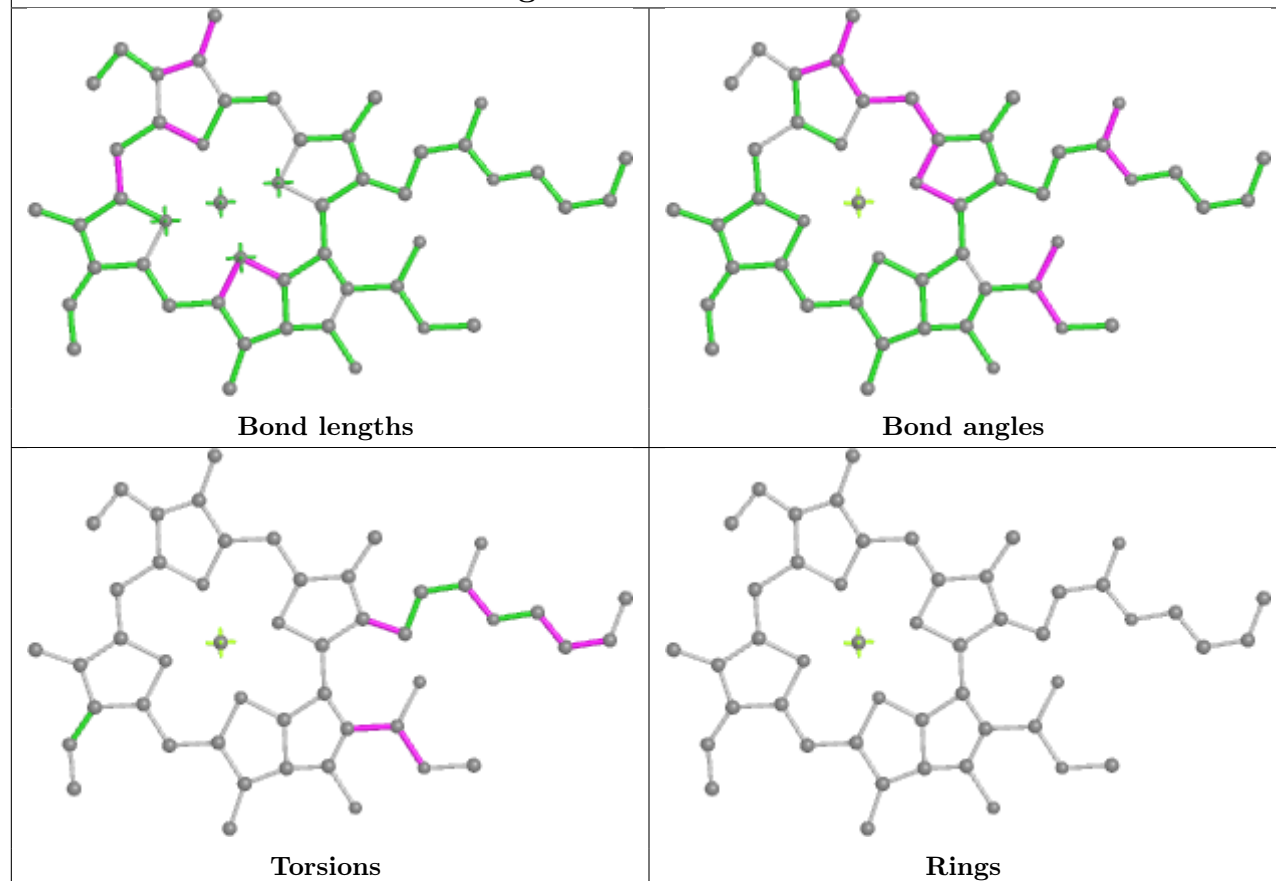




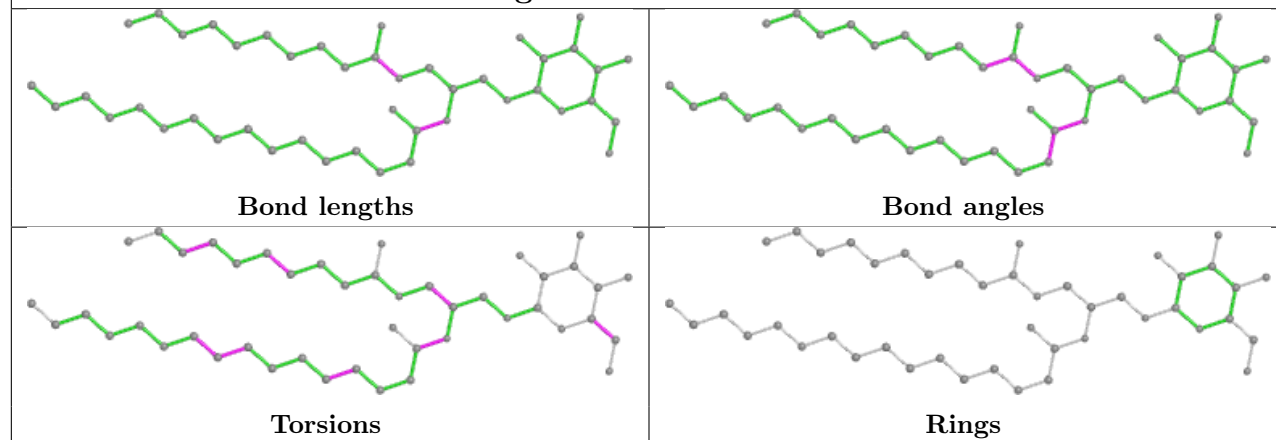


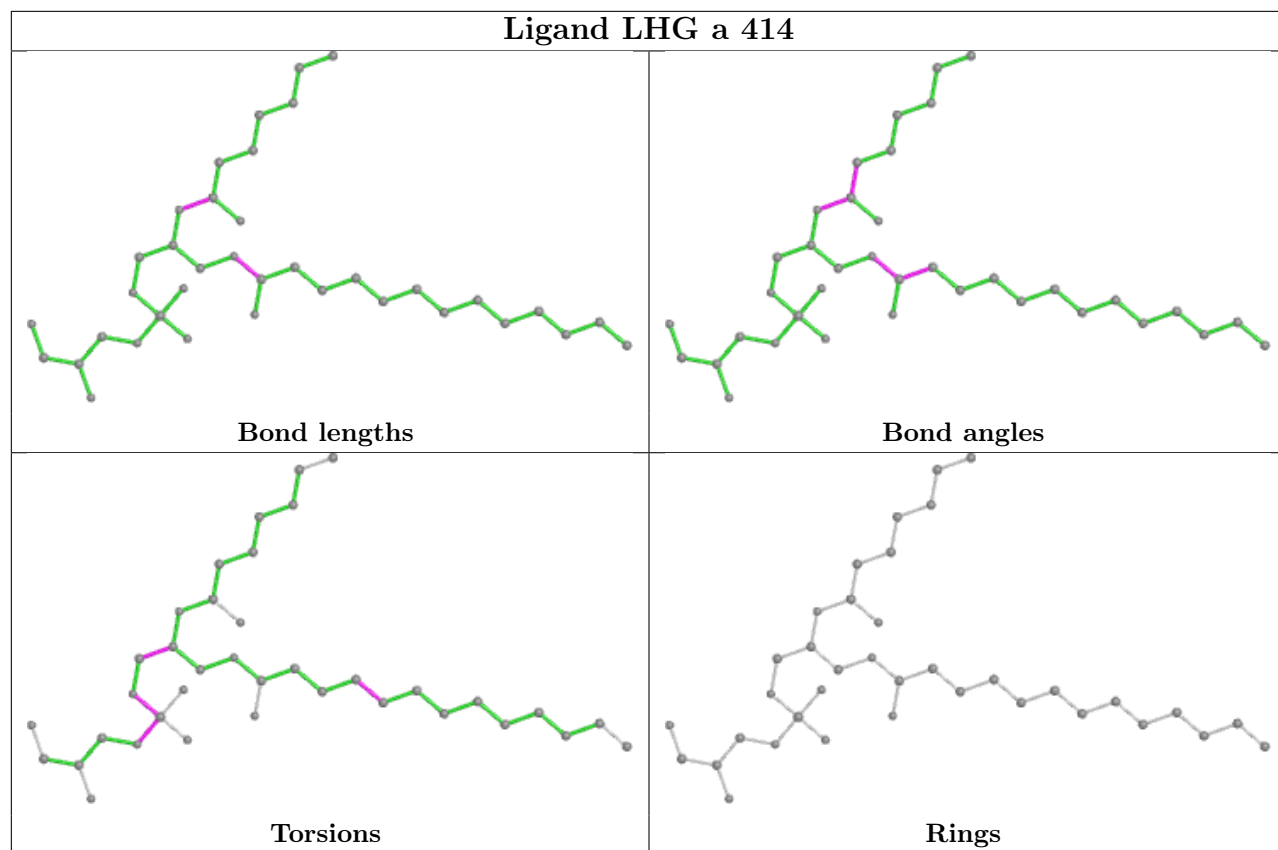


## Ligand CLA RR 310



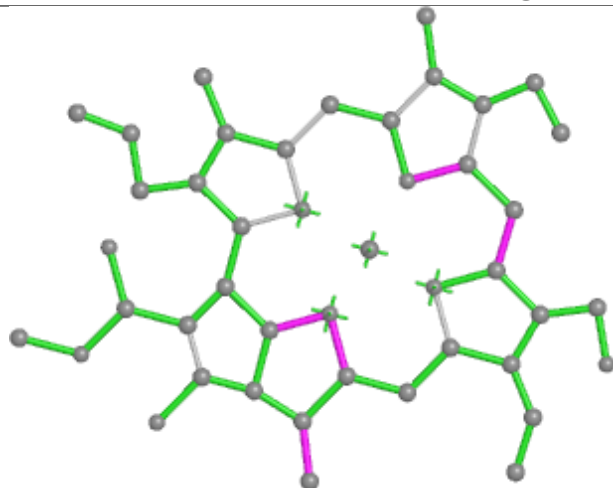
## Ligand LMG BB 619



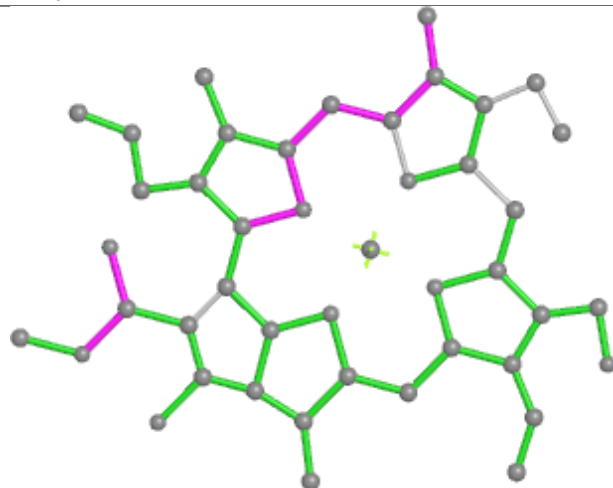




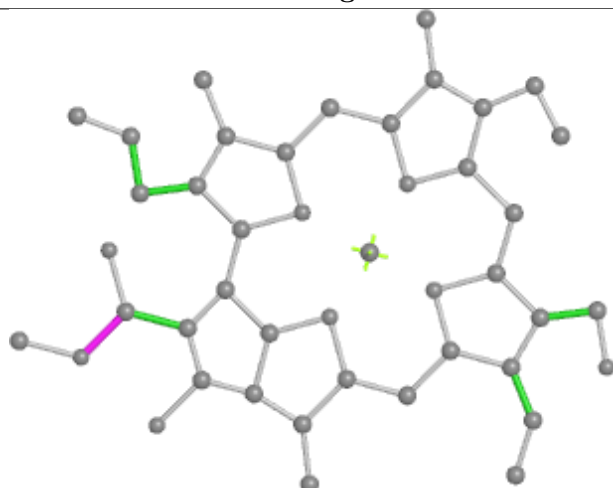
## Ligand CHL y 308



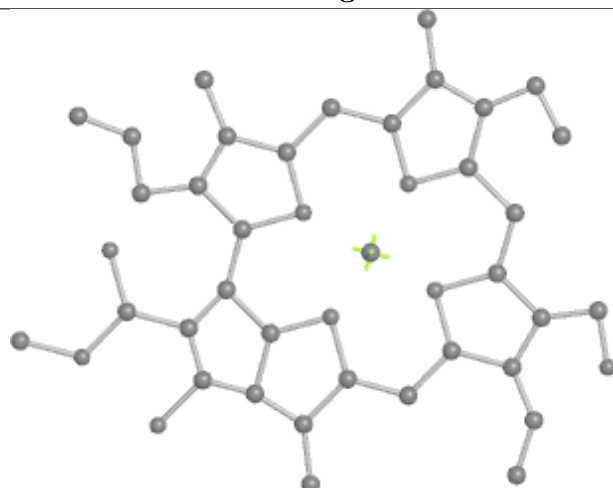
Bond lengths



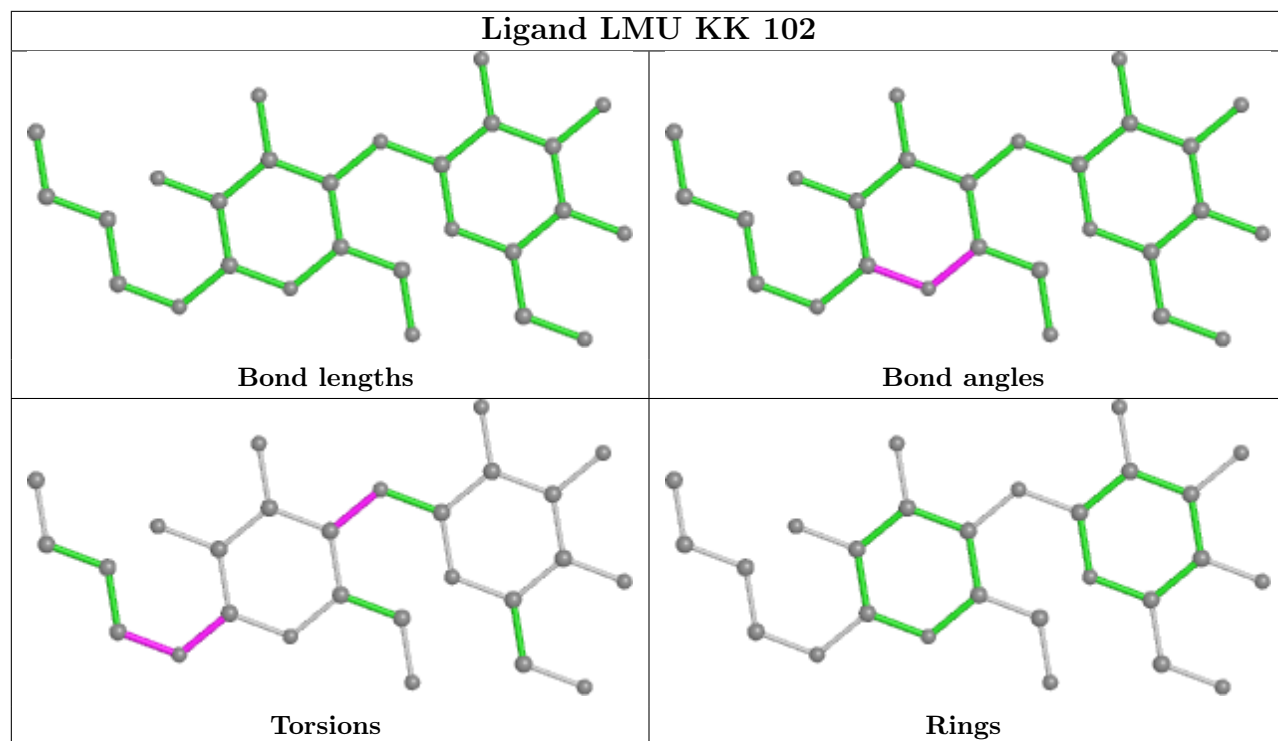
Bond angles

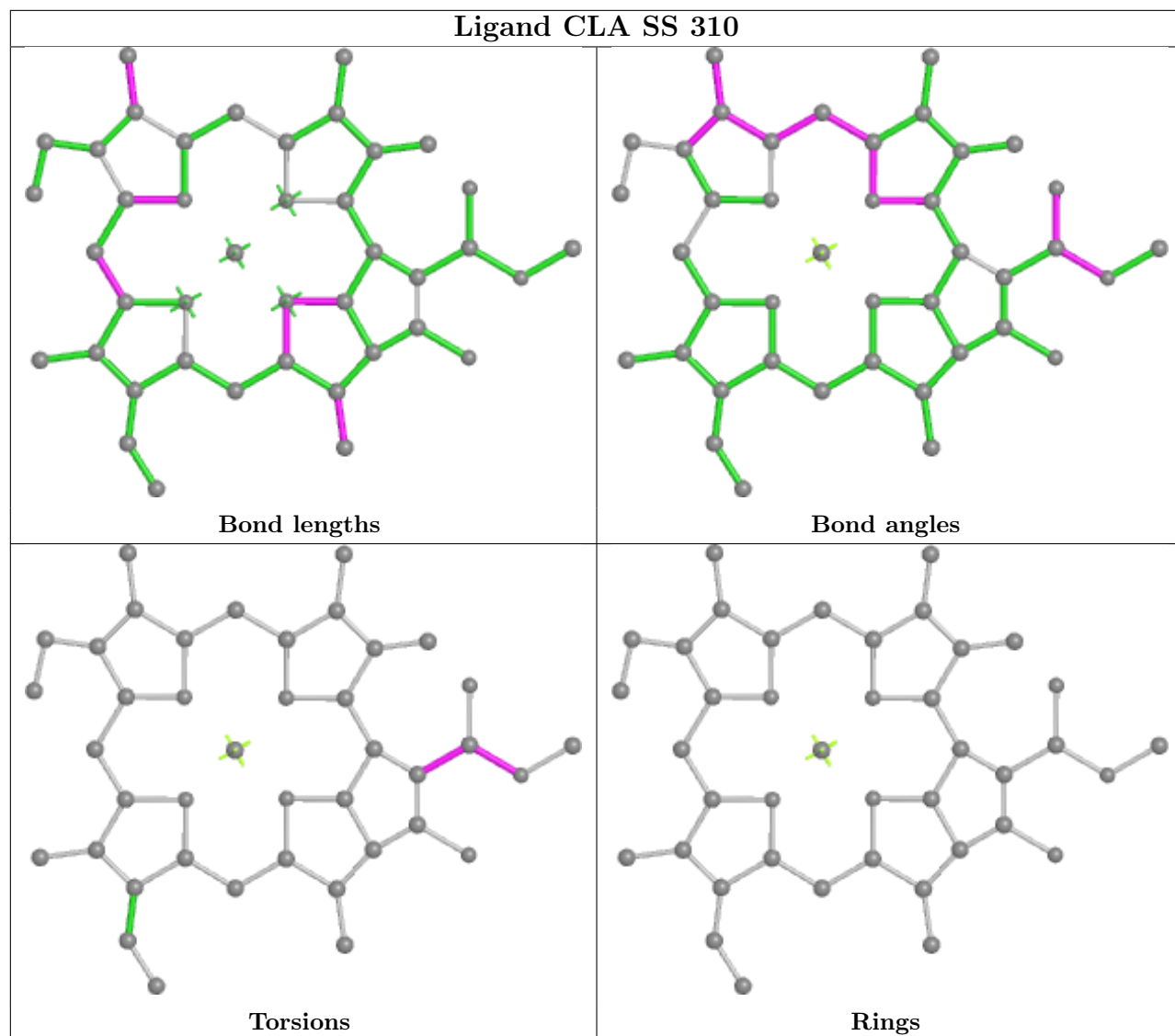


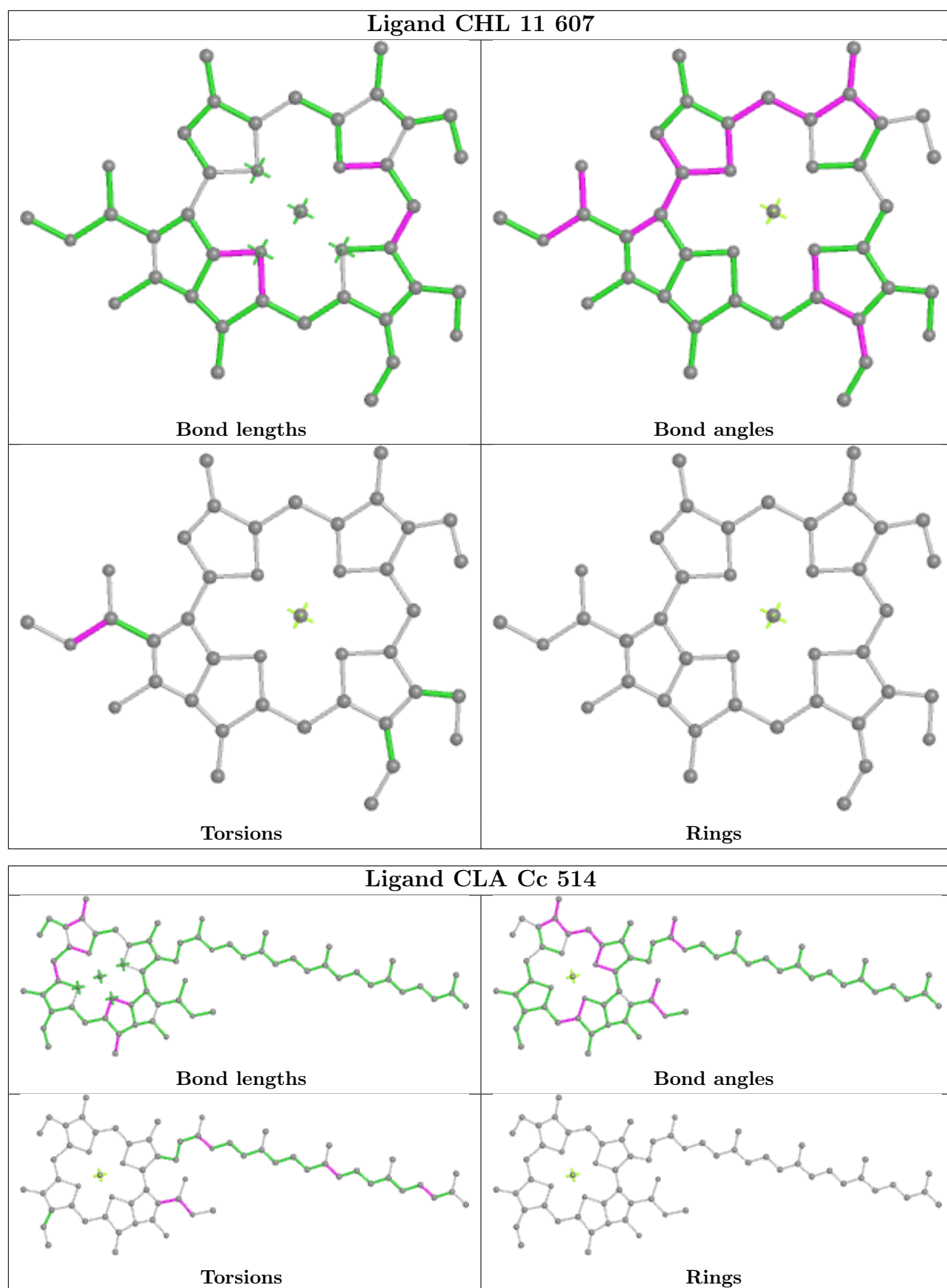
Torsions

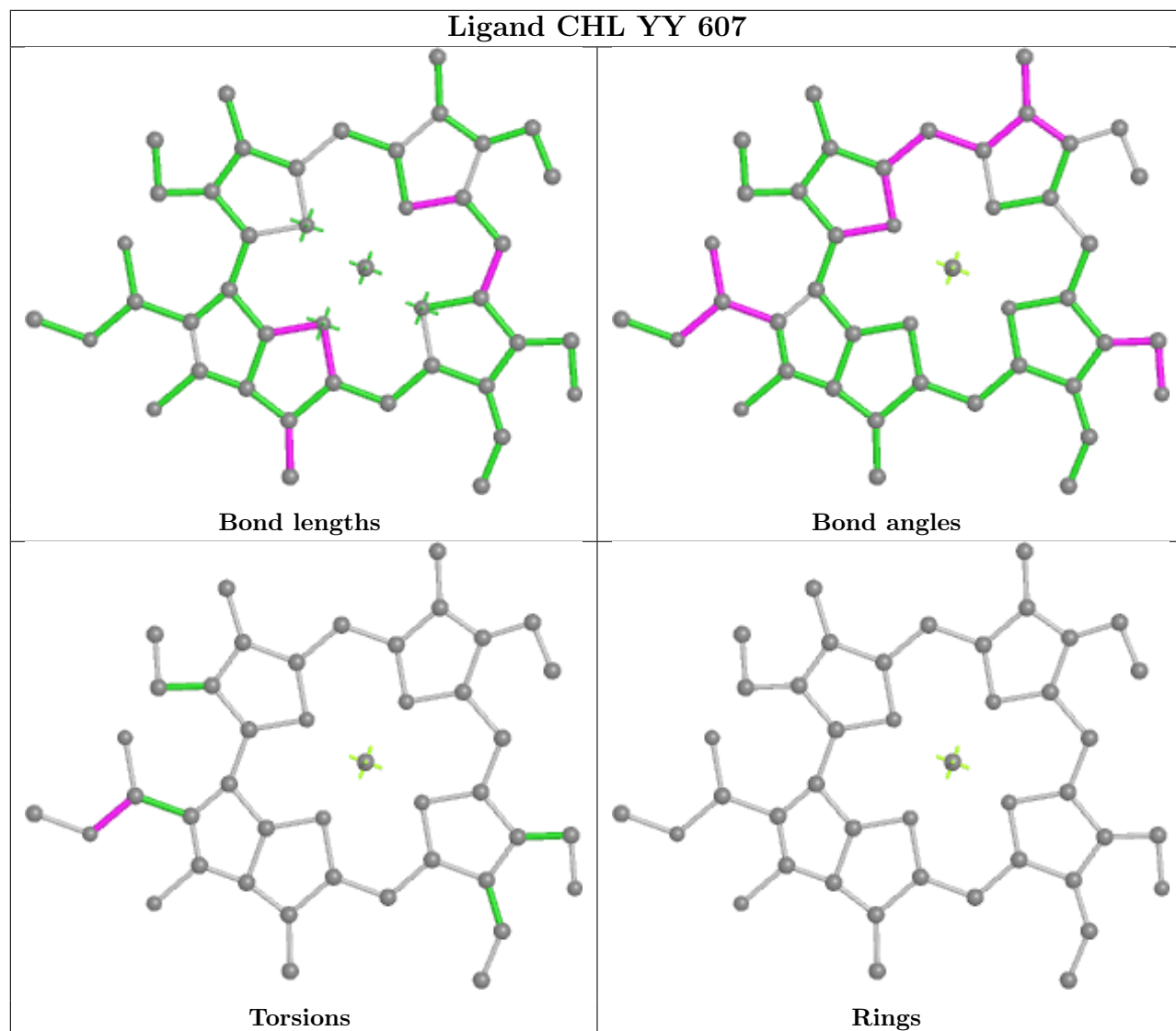
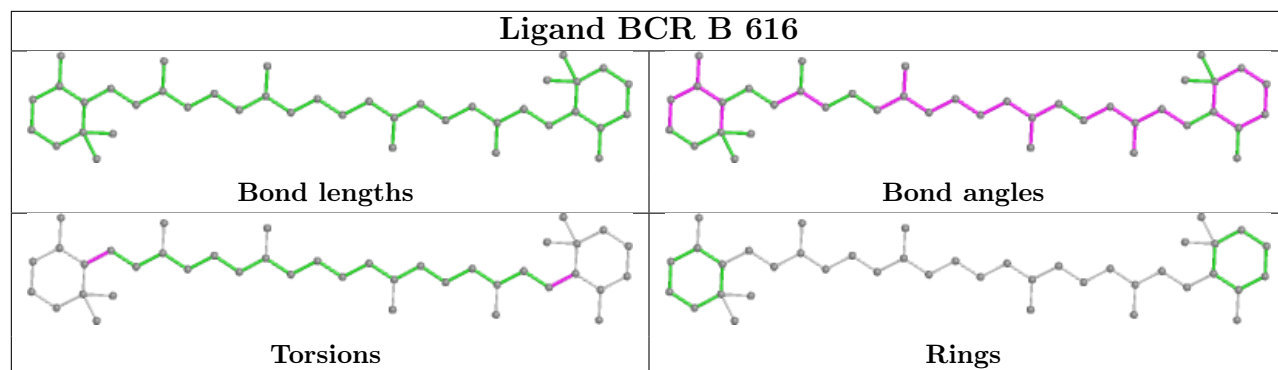


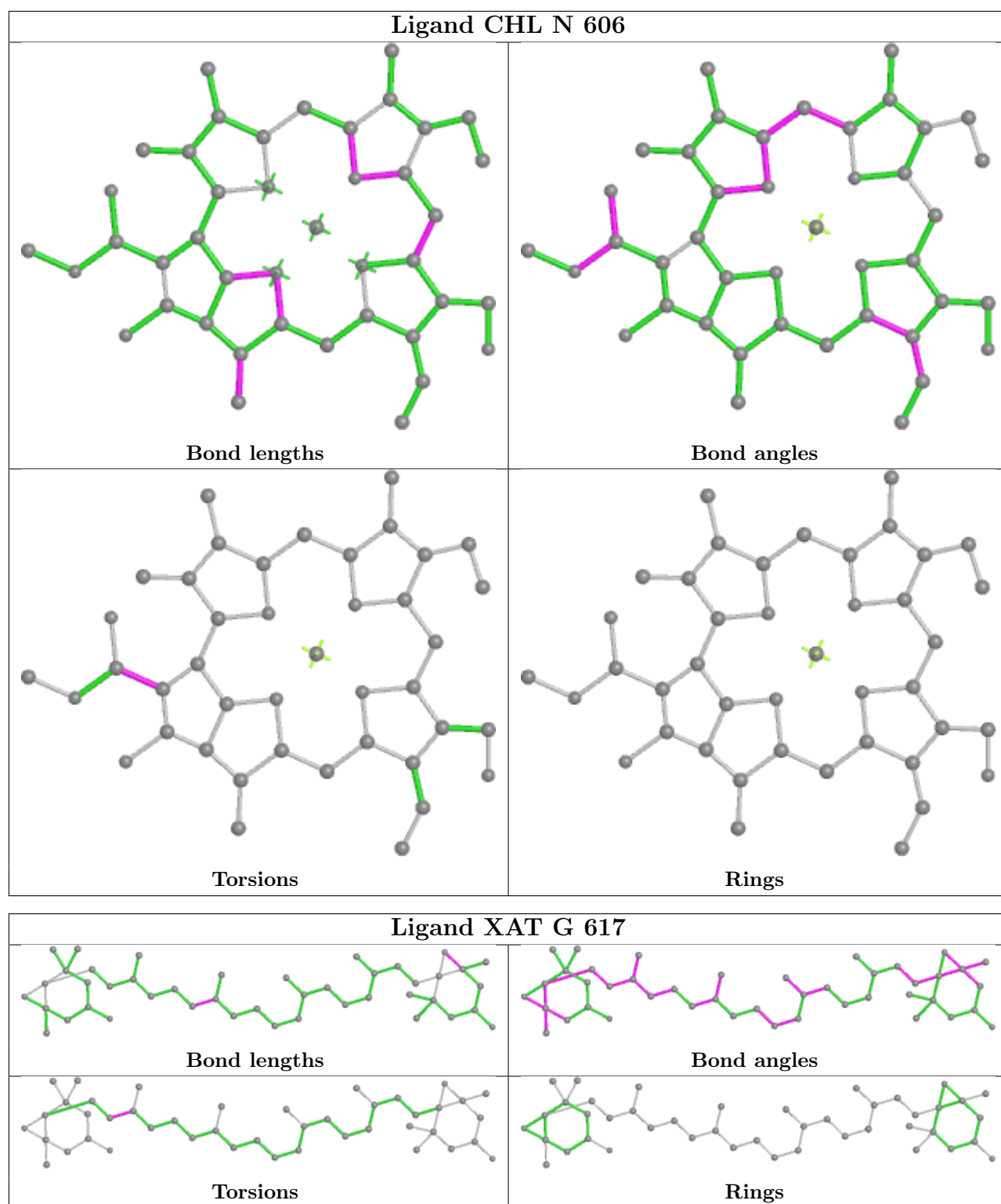
Rings

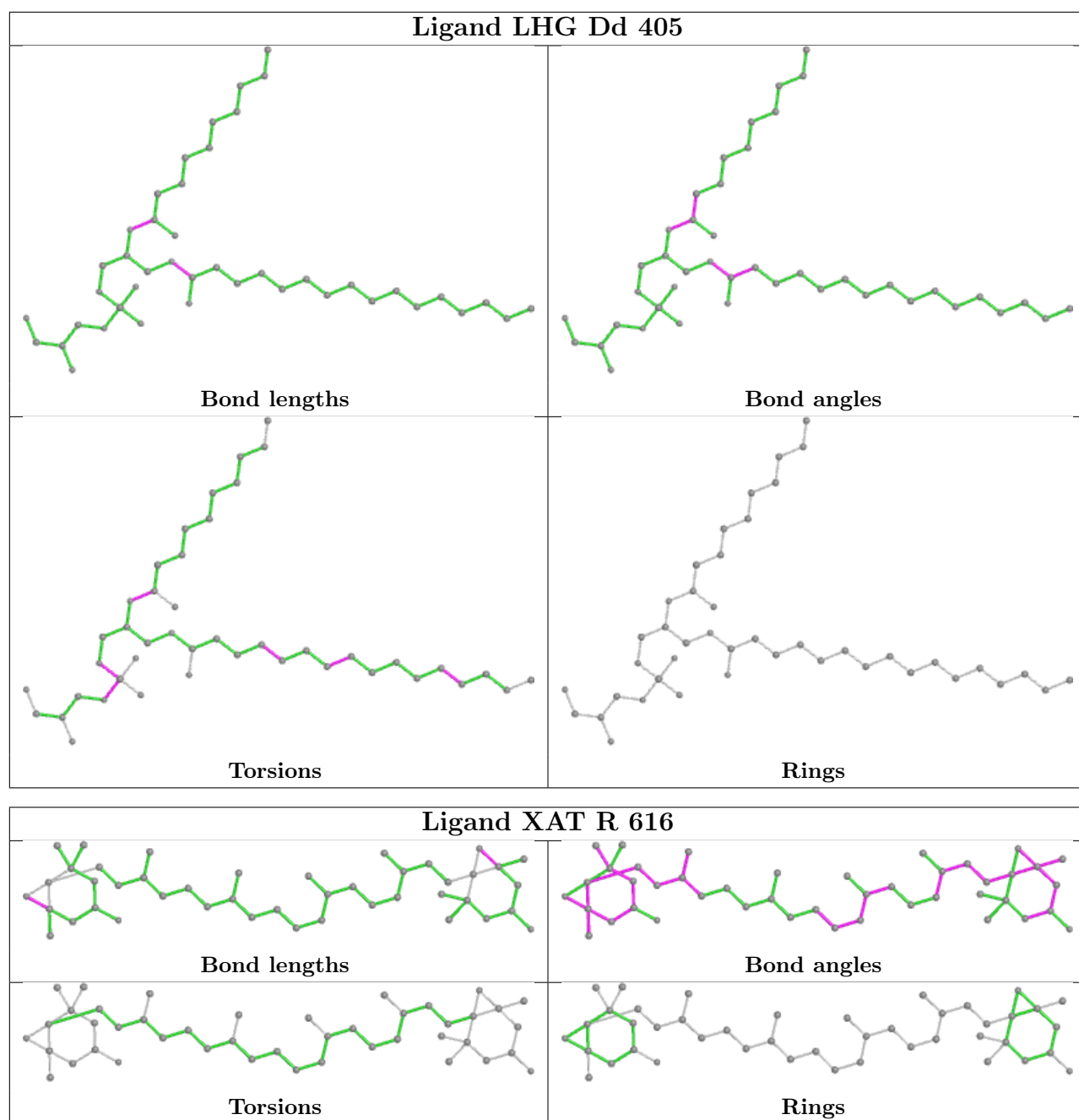


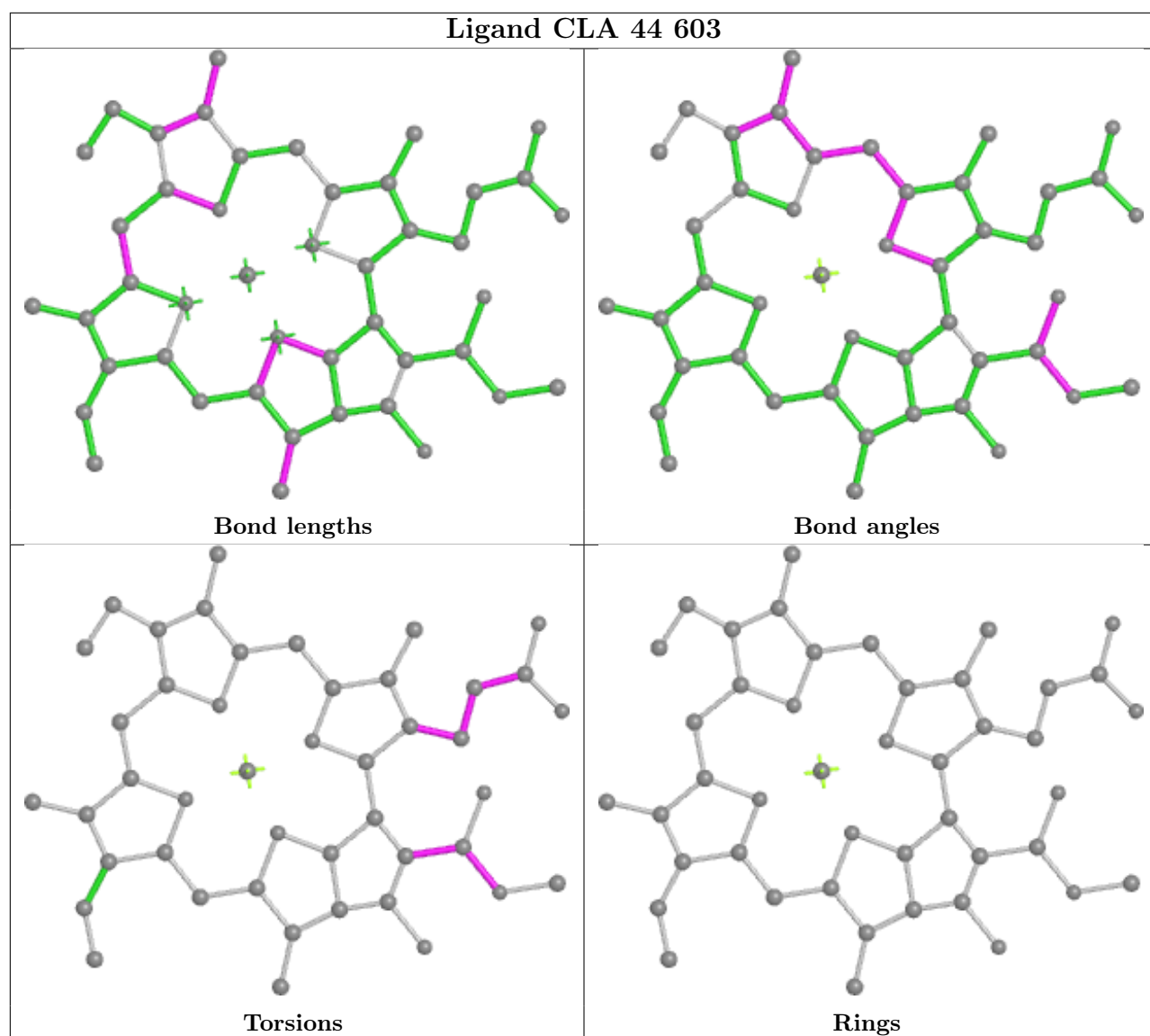






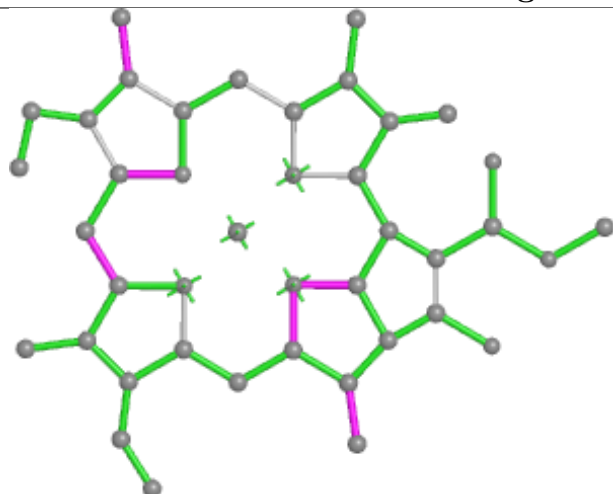




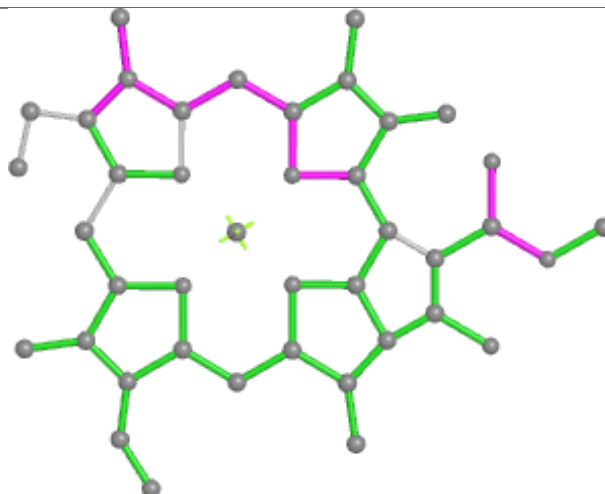




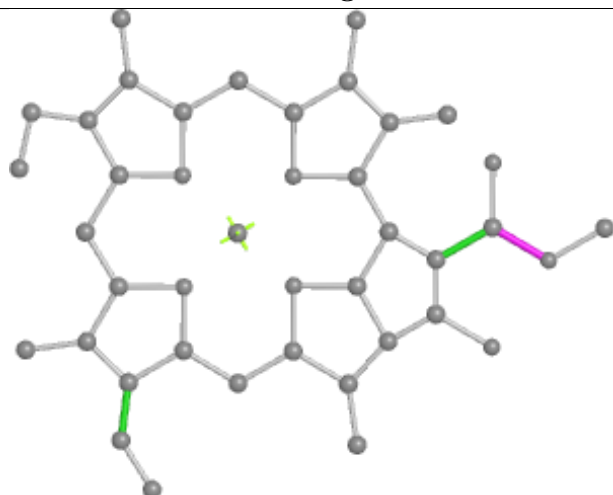
## Ligand CLA S 609



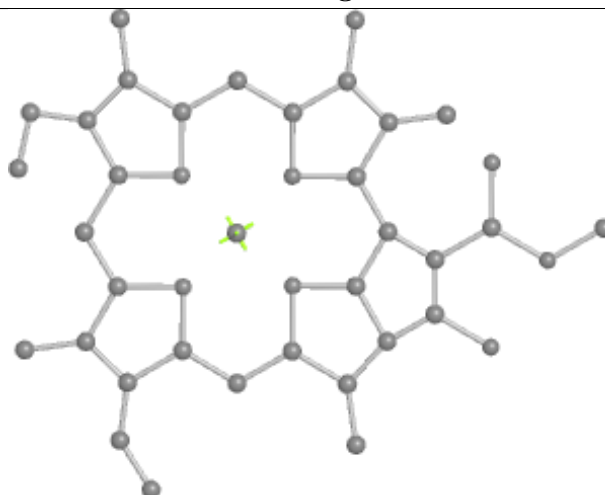
Bond lengths



Bond angles

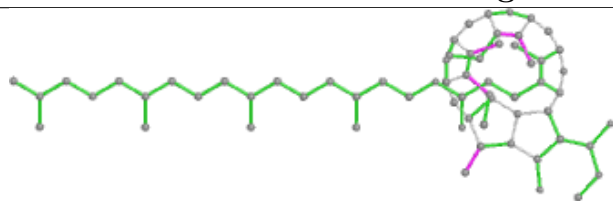


Torsions

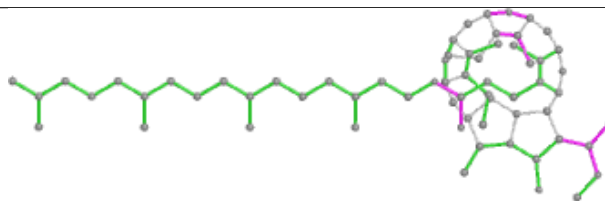


Rings

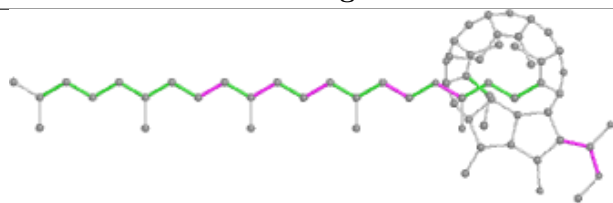
## Ligand PHO DD 402



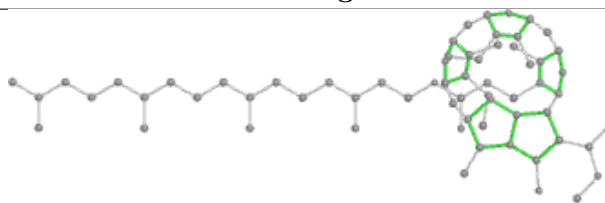
Bond lengths



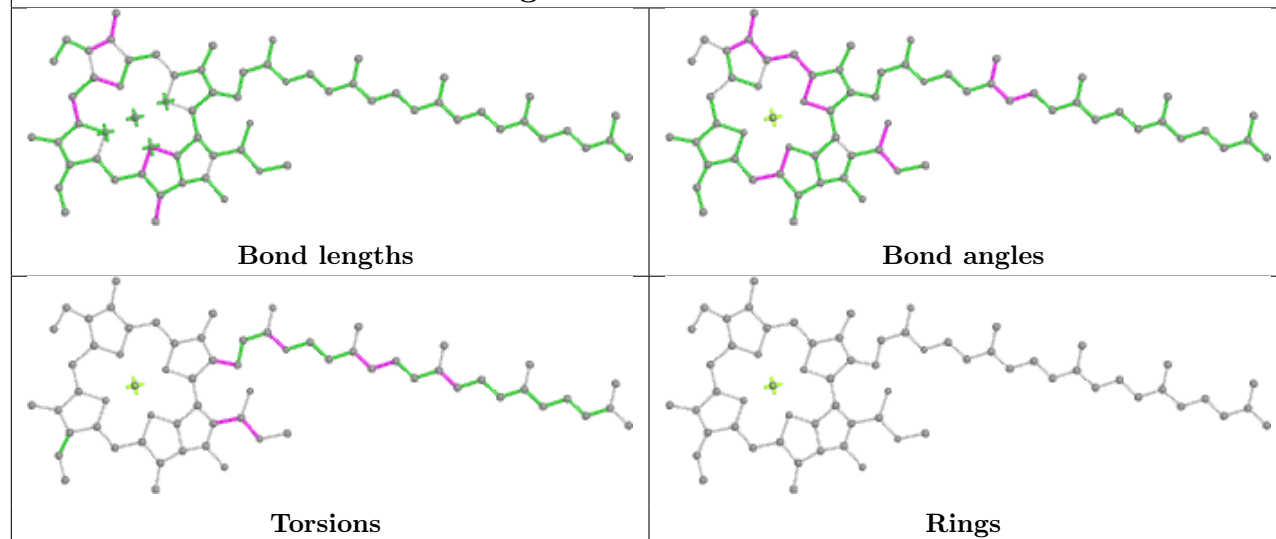
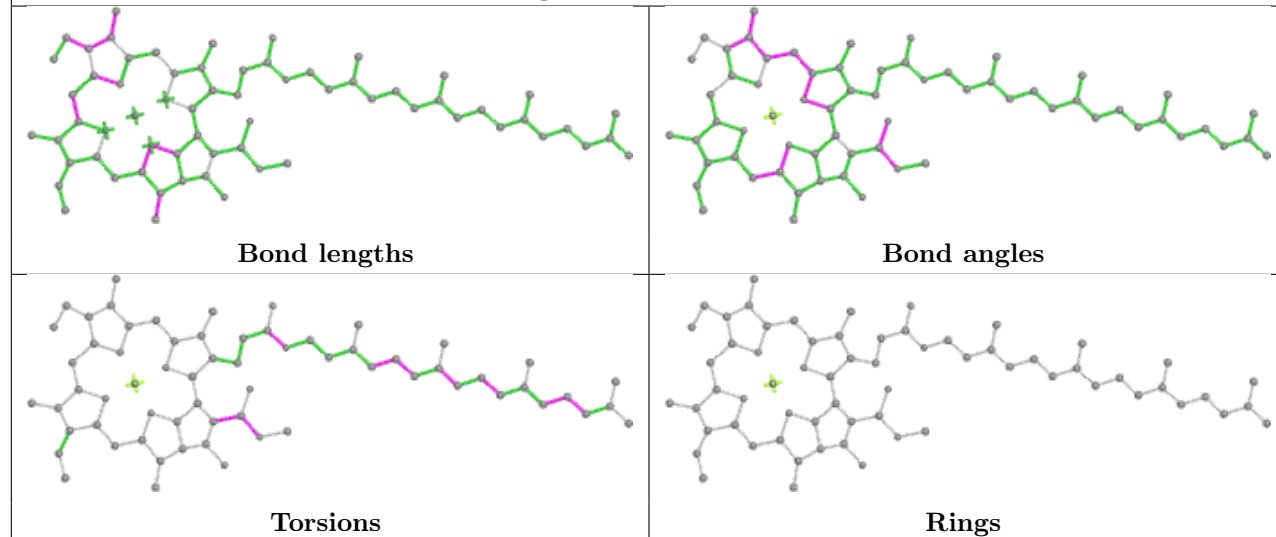
Bond angles



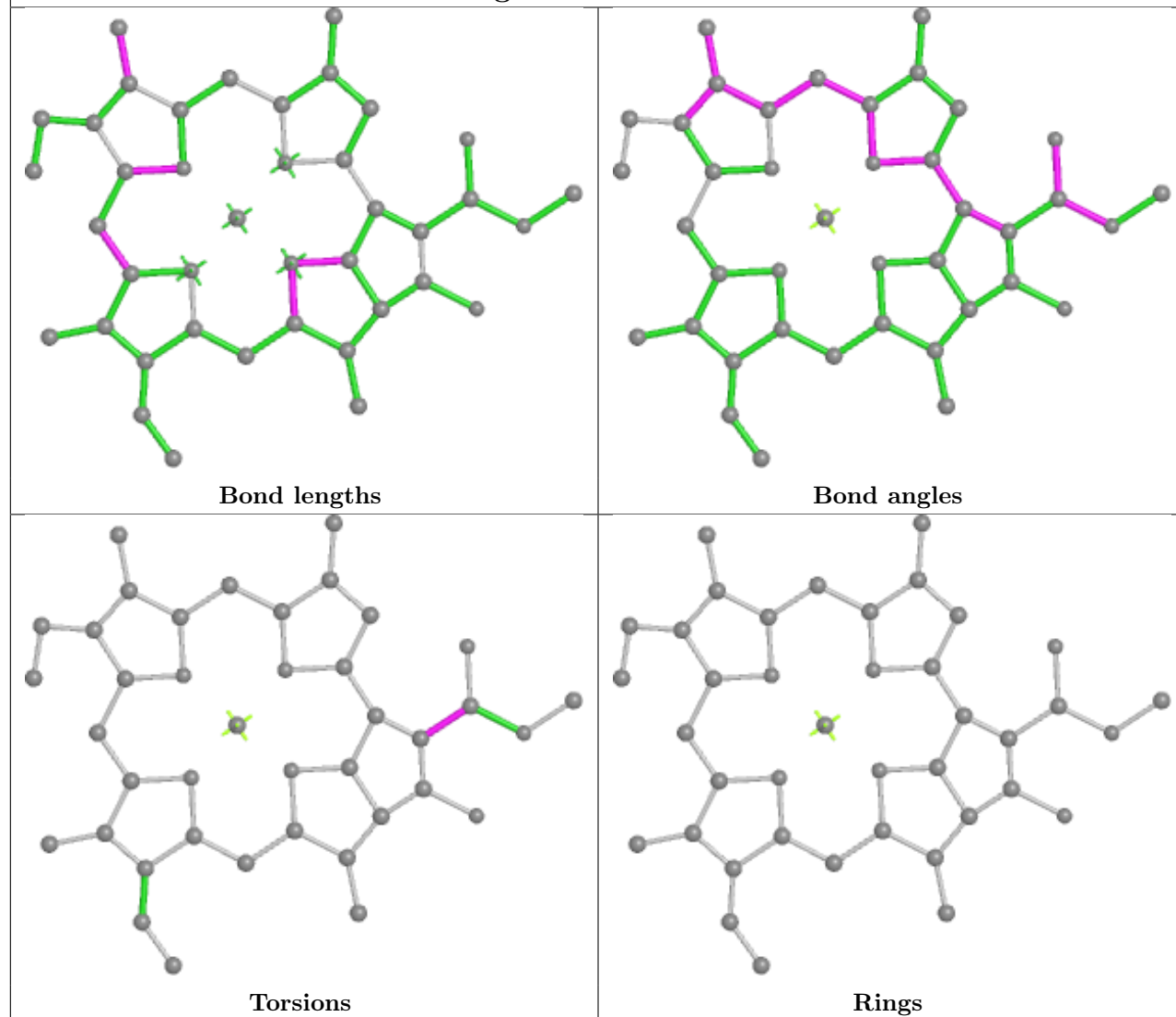
Torsions



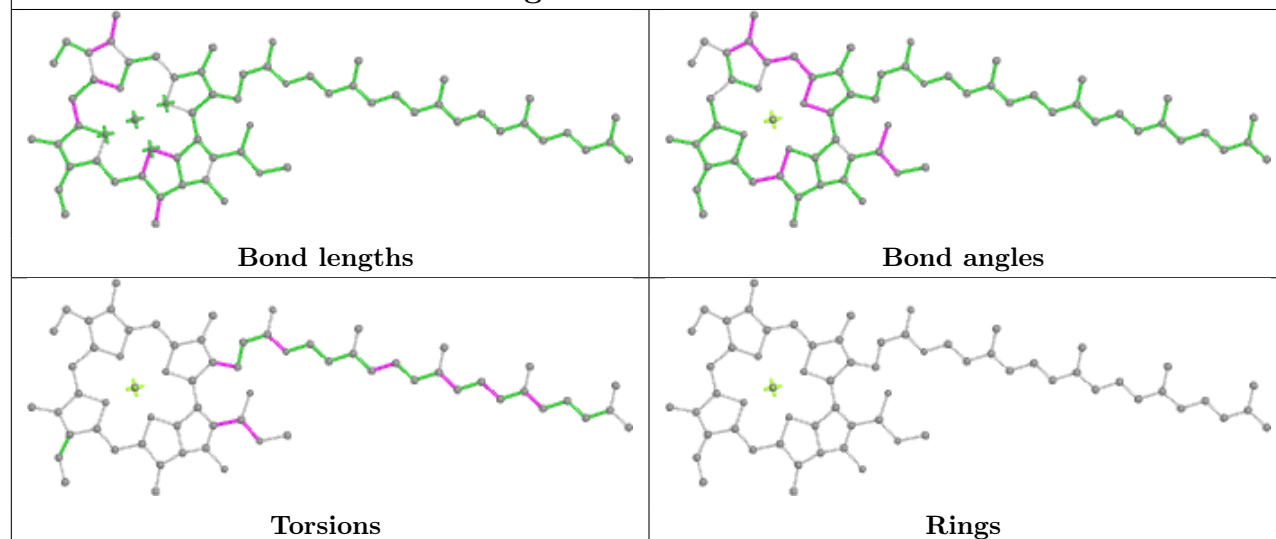
Rings

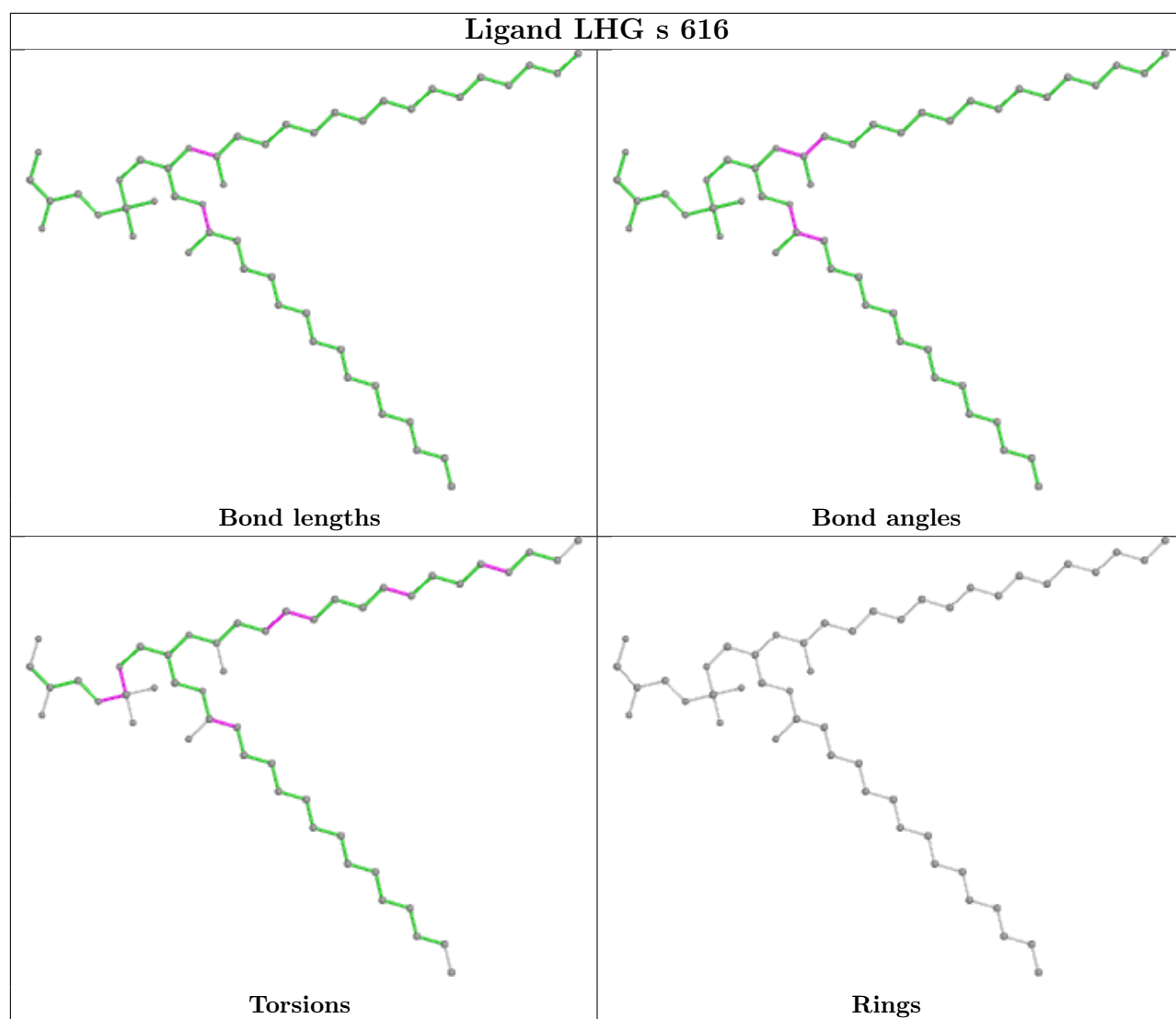
**Ligand CLA BB 604****Ligand CLA b 615**

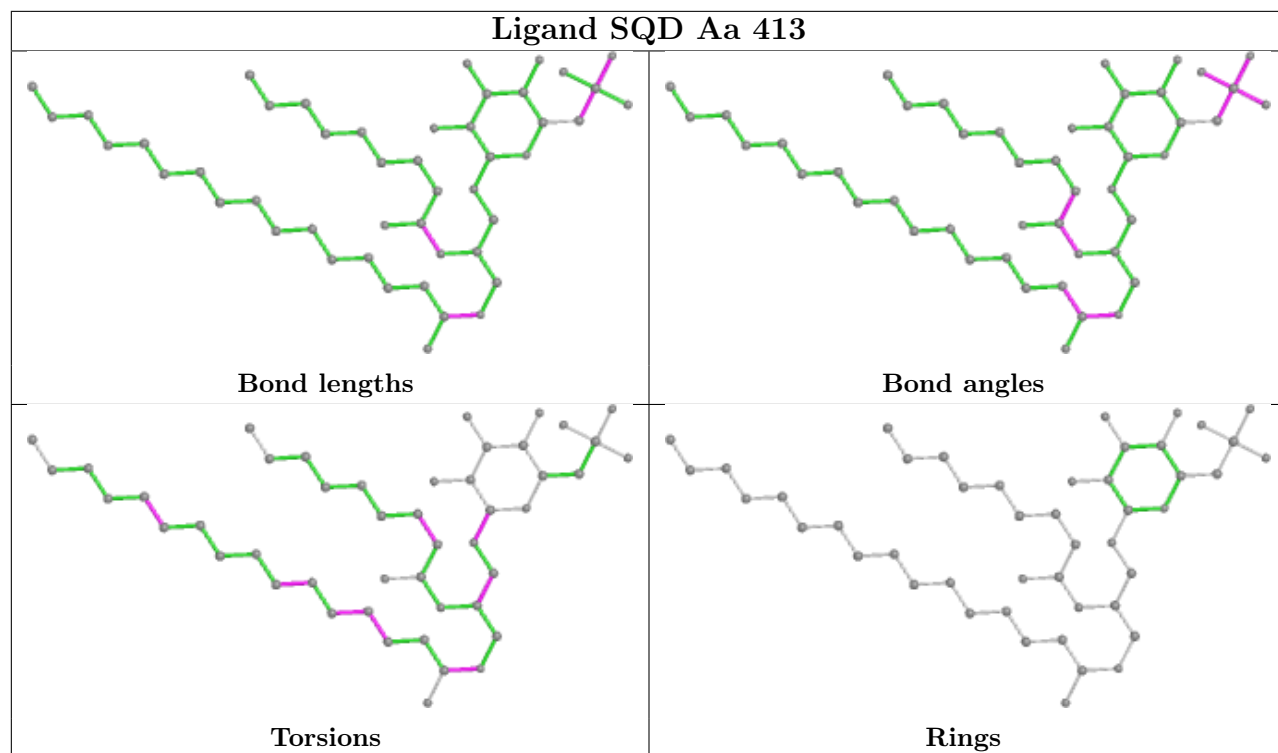
## Ligand CLA 1 612



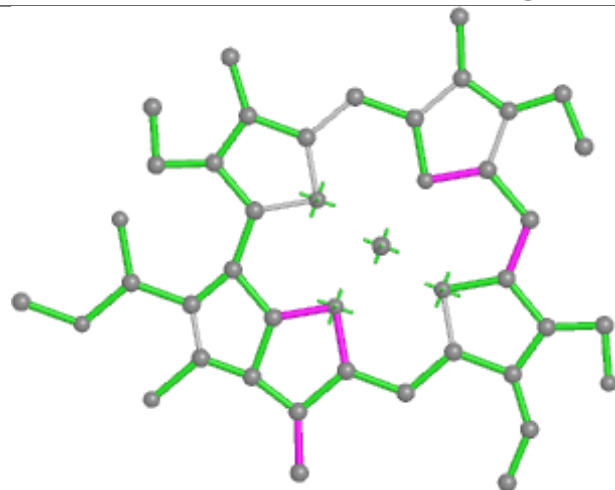
## Ligand CLA Cc 505



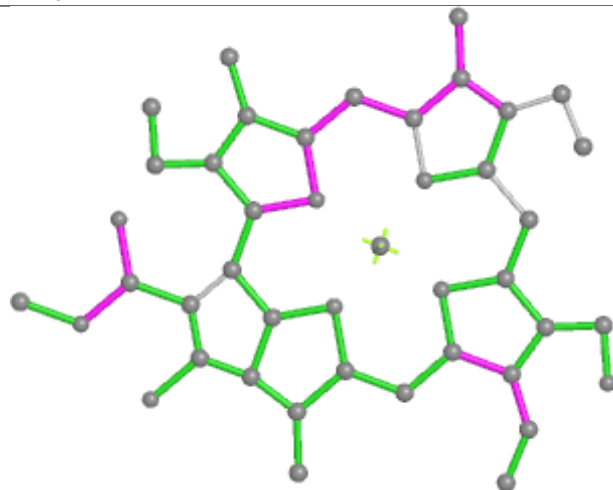




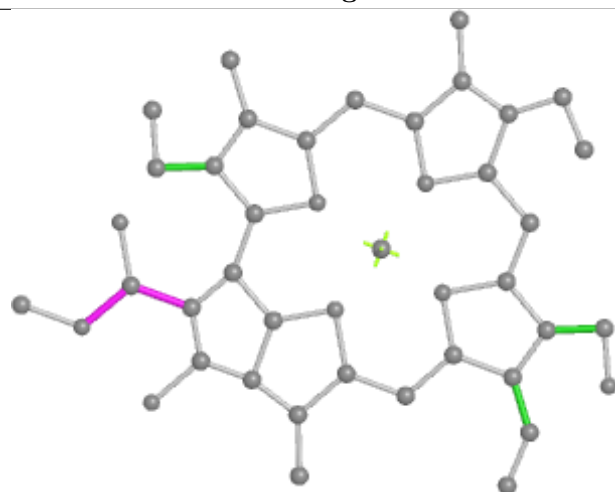
## Ligand CHL y 309



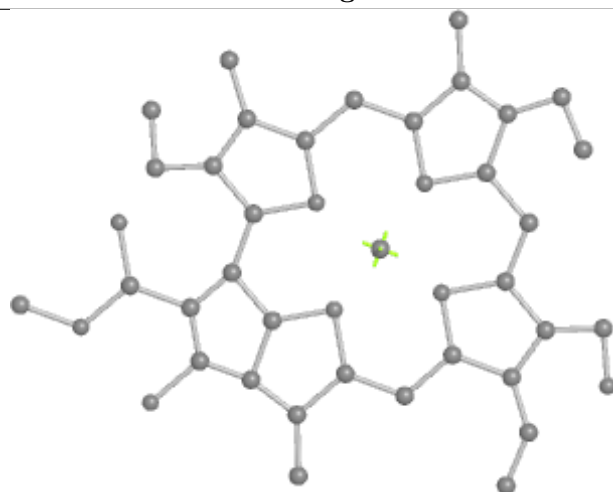
Bond lengths



Bond angles

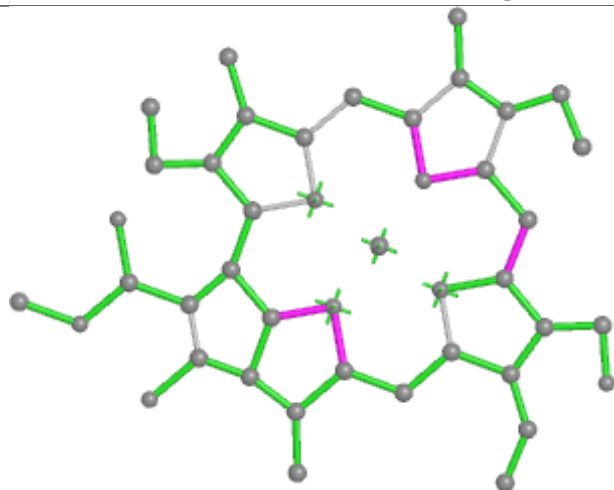


Torsions

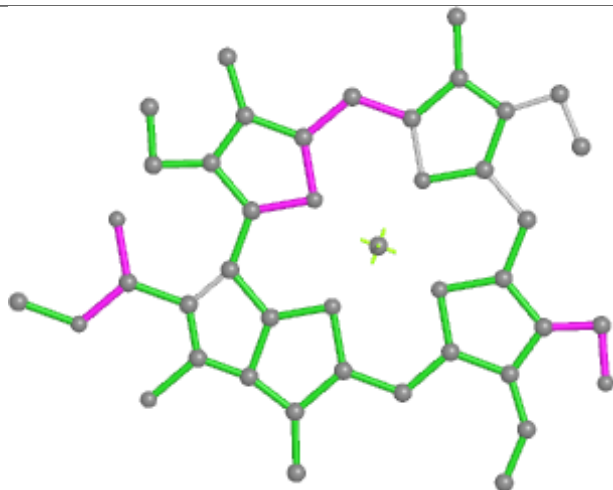


Rings

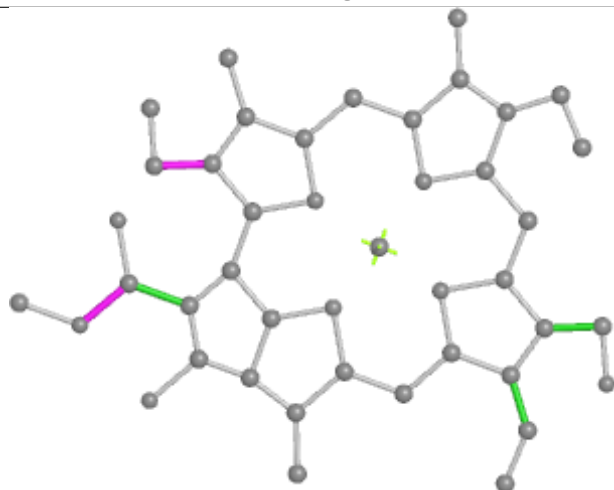
## Ligand CHL GG 605



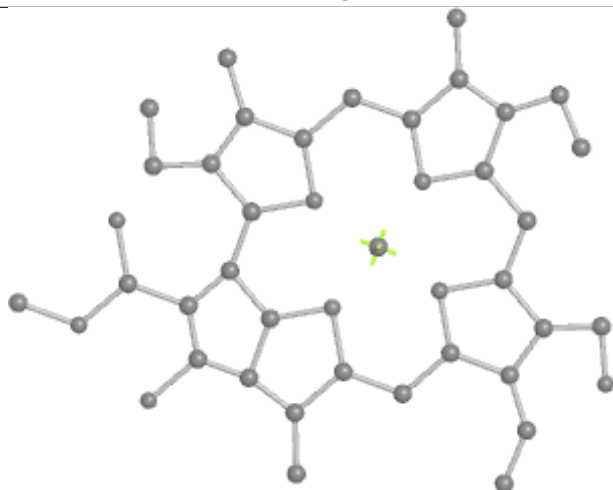
Bond lengths



Bond angles

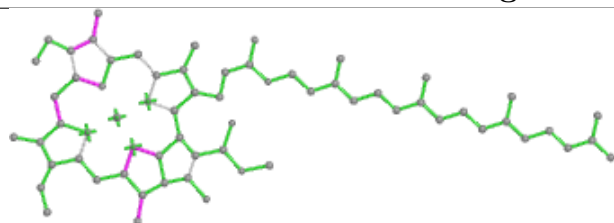


Torsions

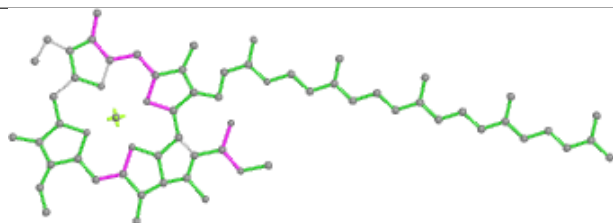


Rings

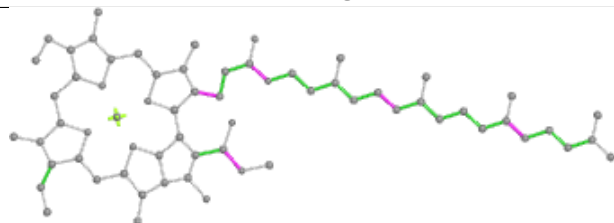
## Ligand CLA DD 404



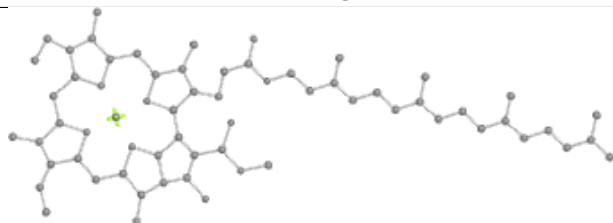
Bond lengths



Bond angles

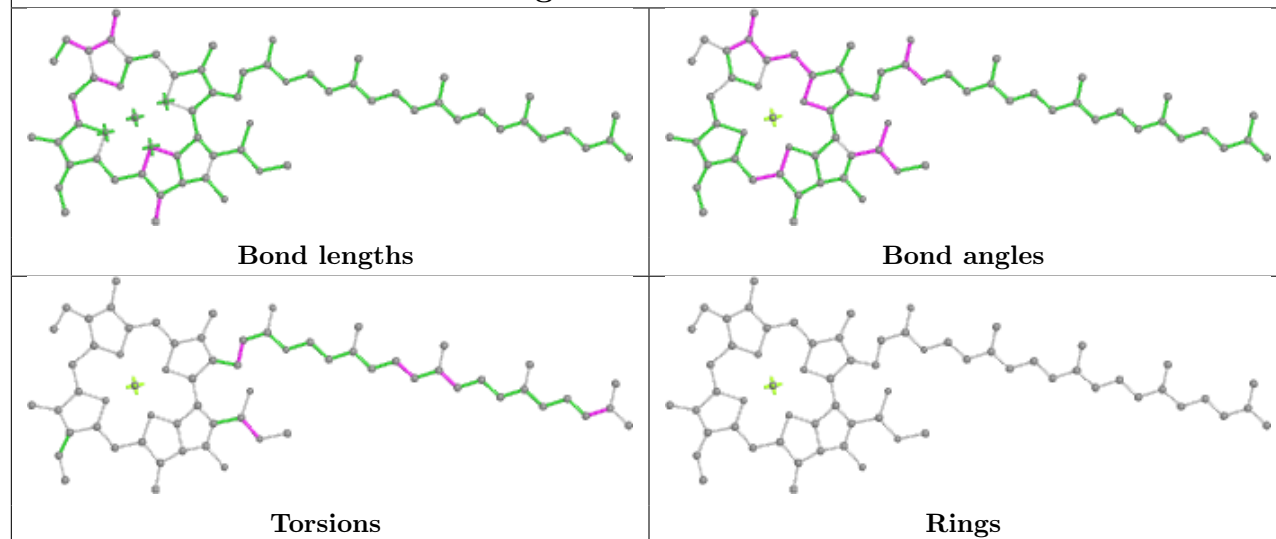


Torsions

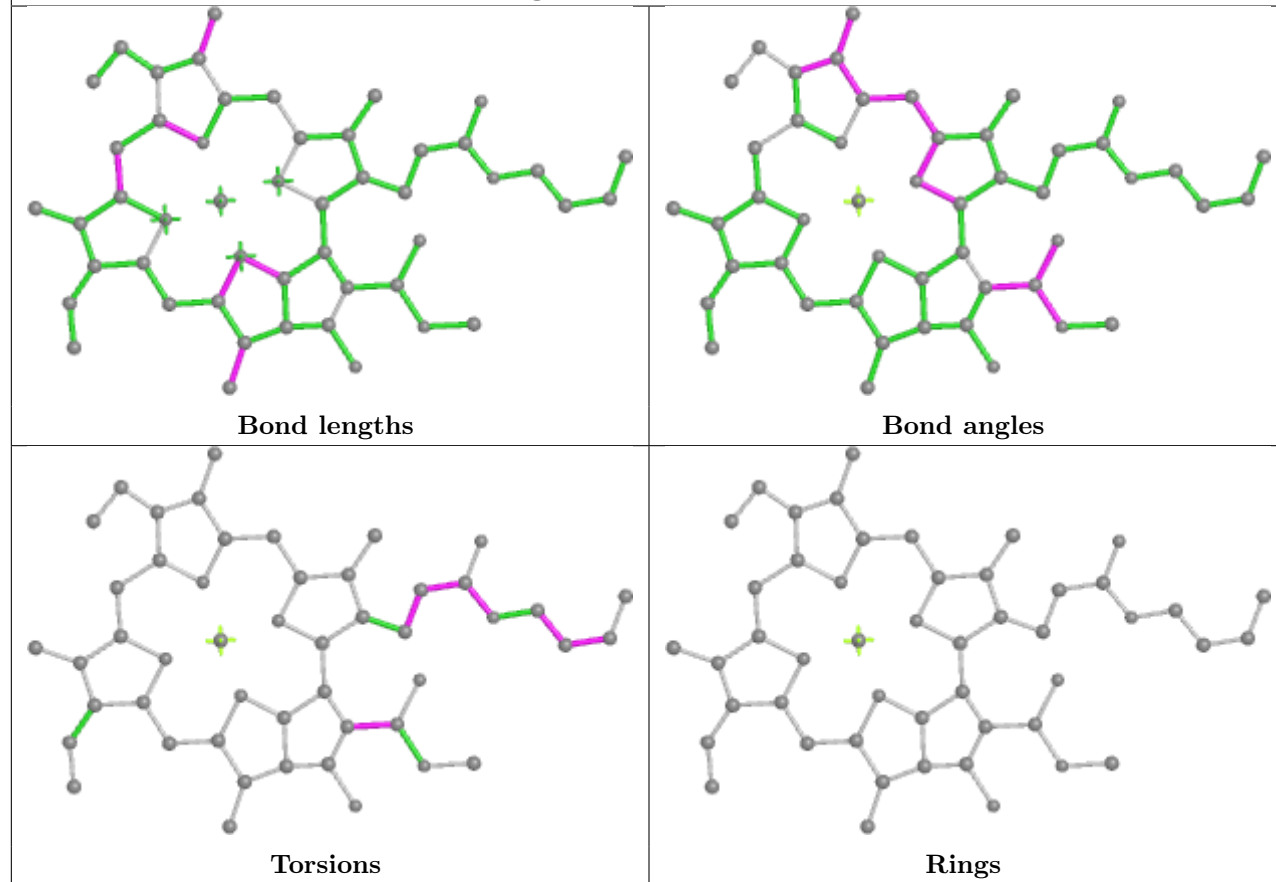


Rings

## Ligand CLA b 606

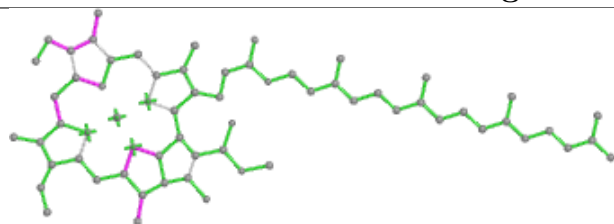


## Ligand CLA Ss 612

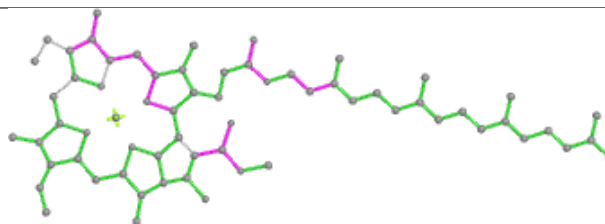




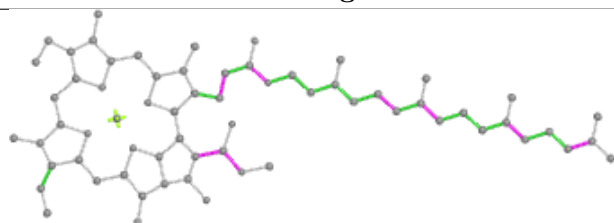
## Ligand CLA BB 605



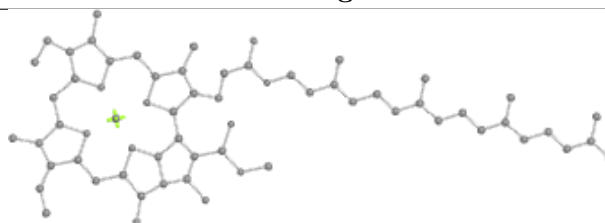
Bond lengths



Bond angles

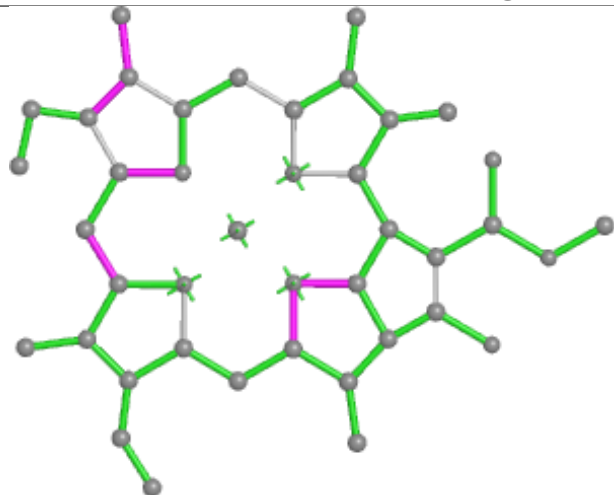


Torsions

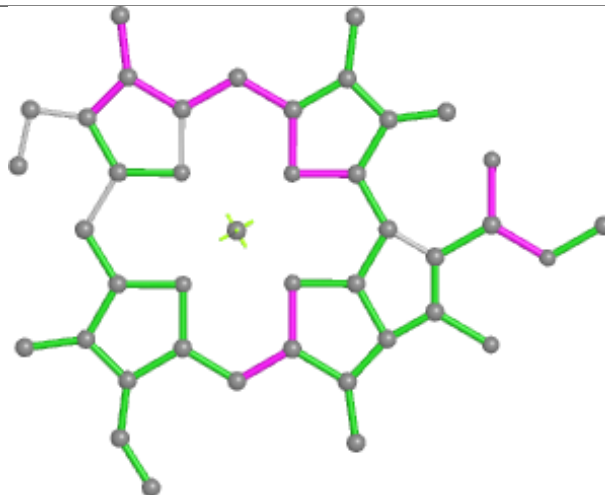


Rings

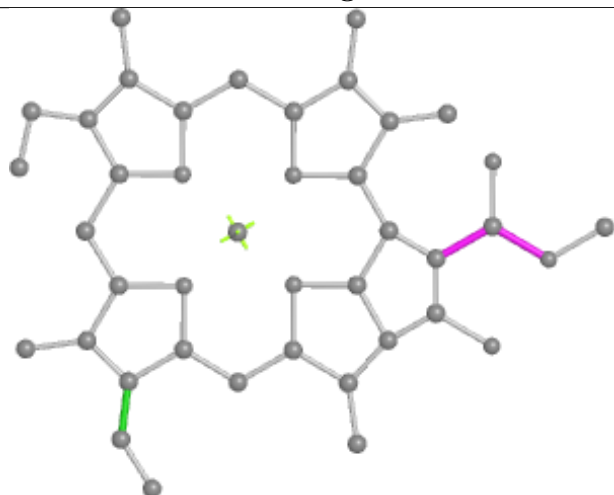
## Ligand CLA NN 614



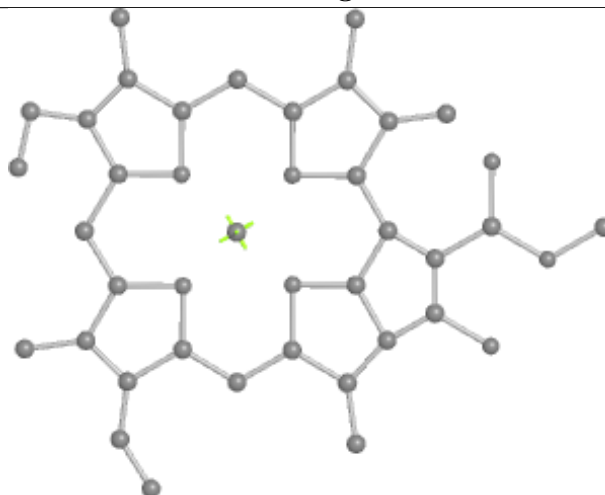
Bond lengths



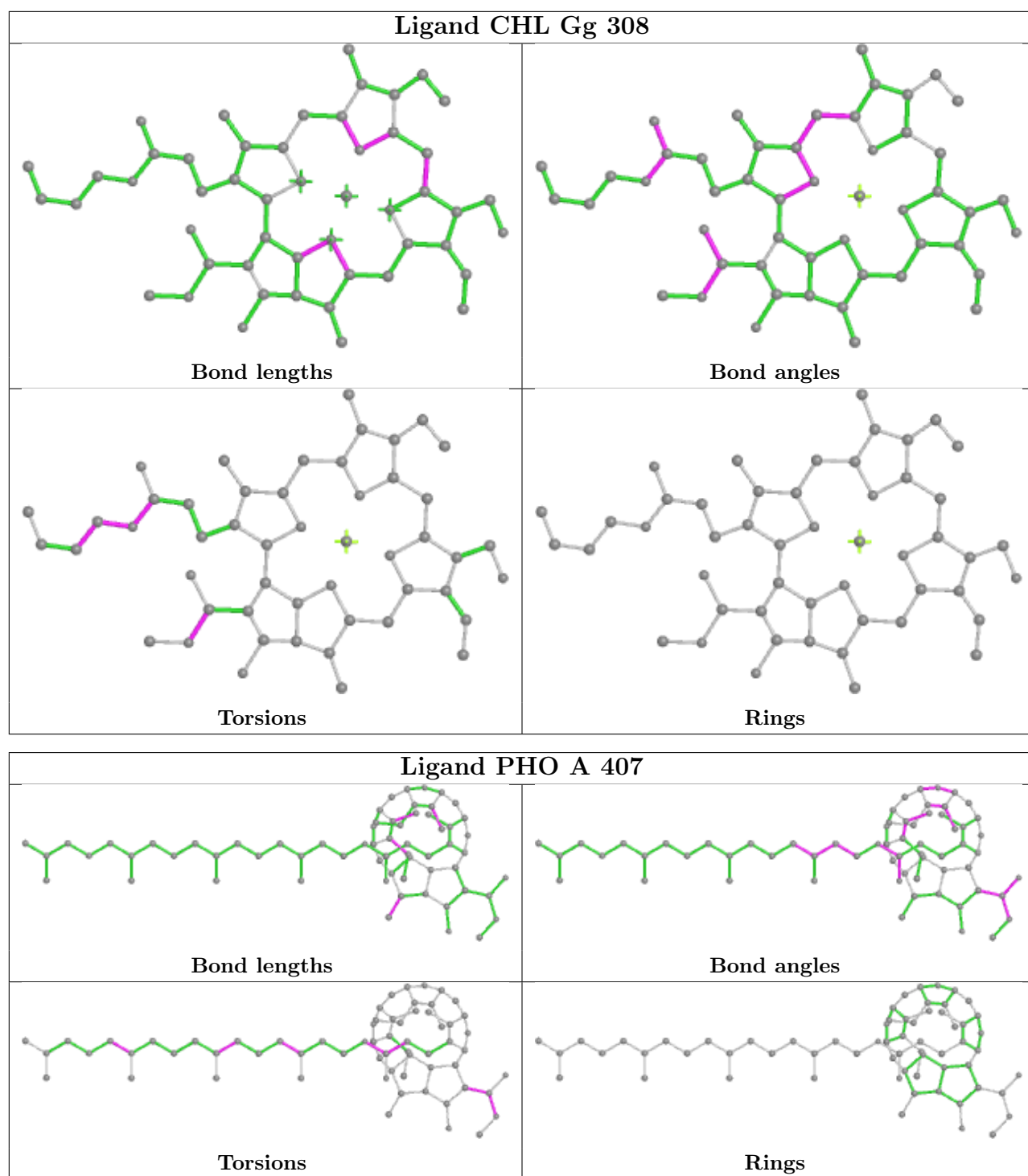
Bond angles



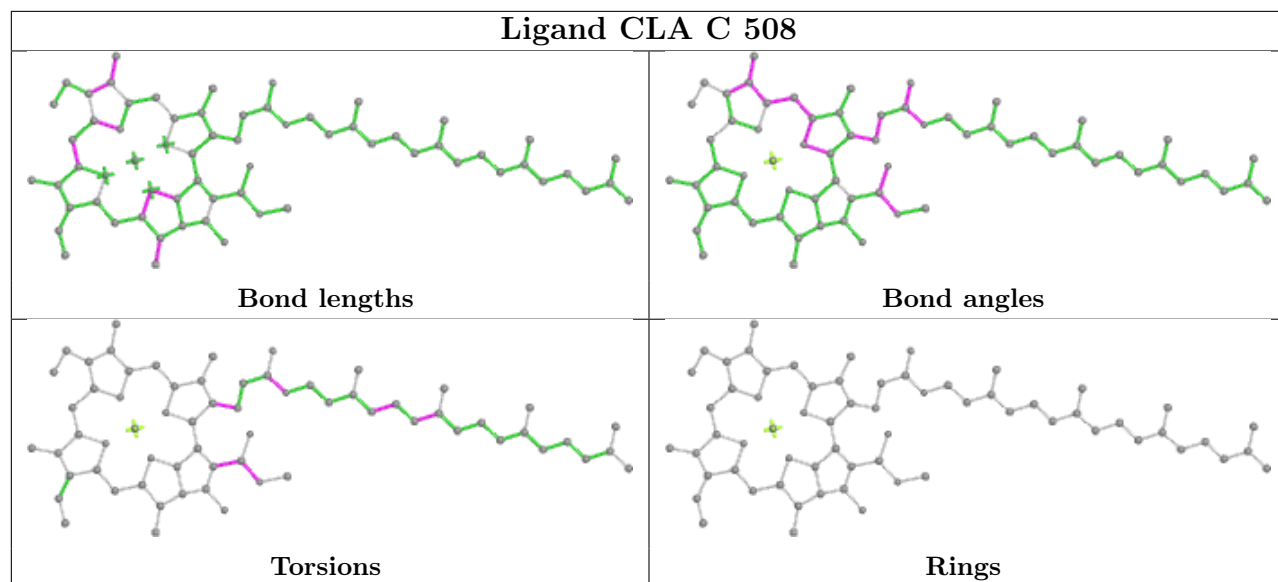
Torsions



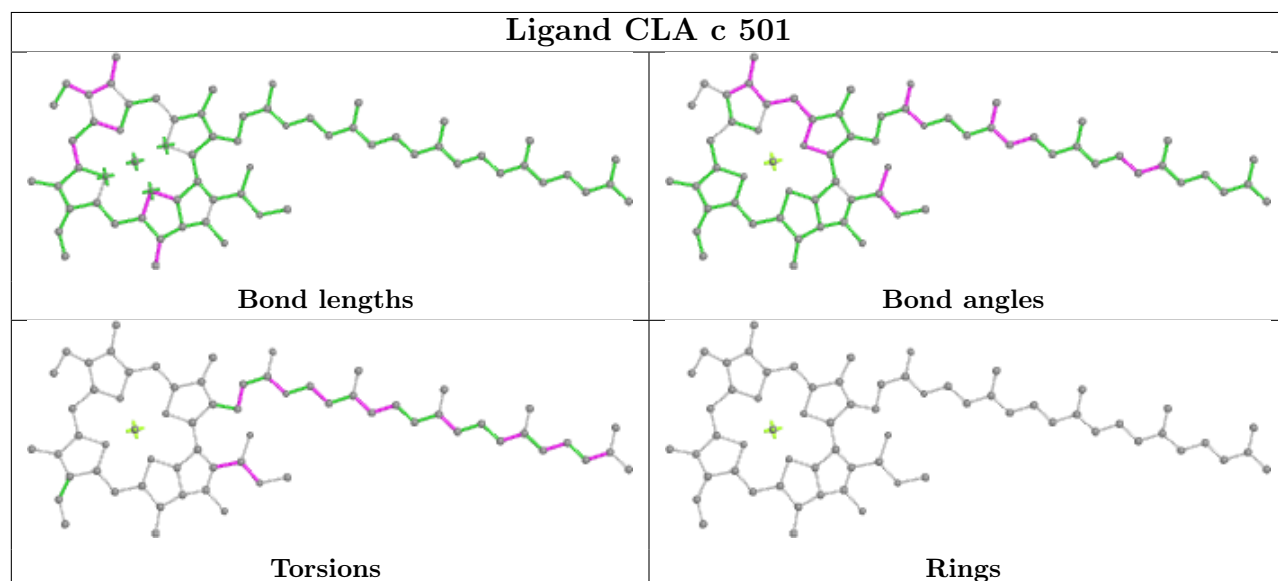
Rings



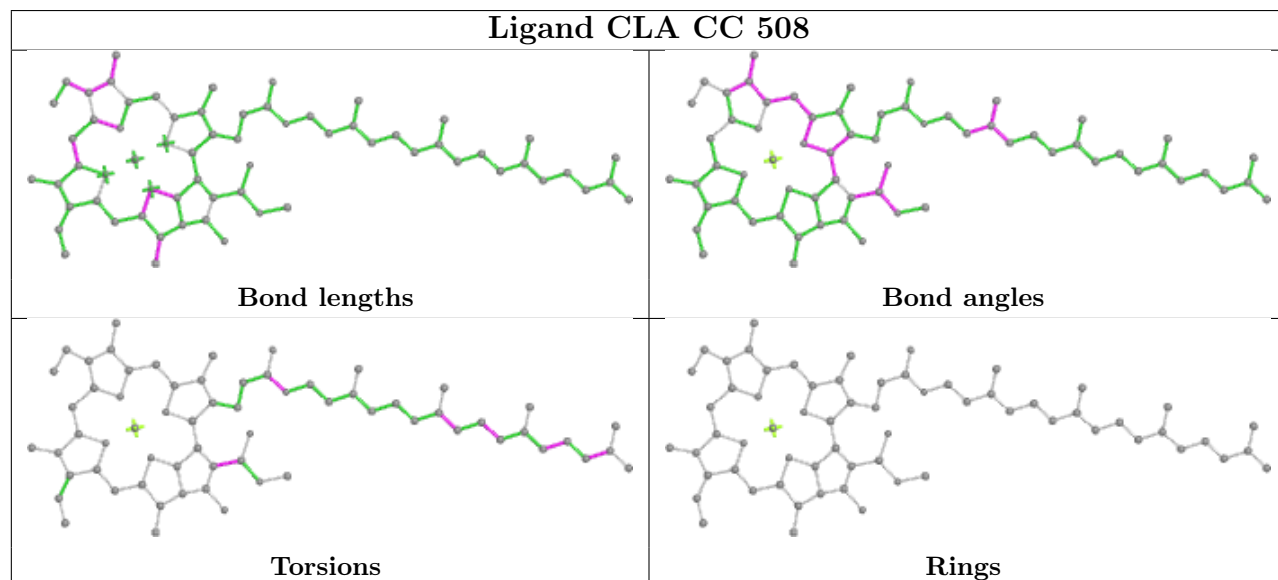
## Ligand CLA C 508



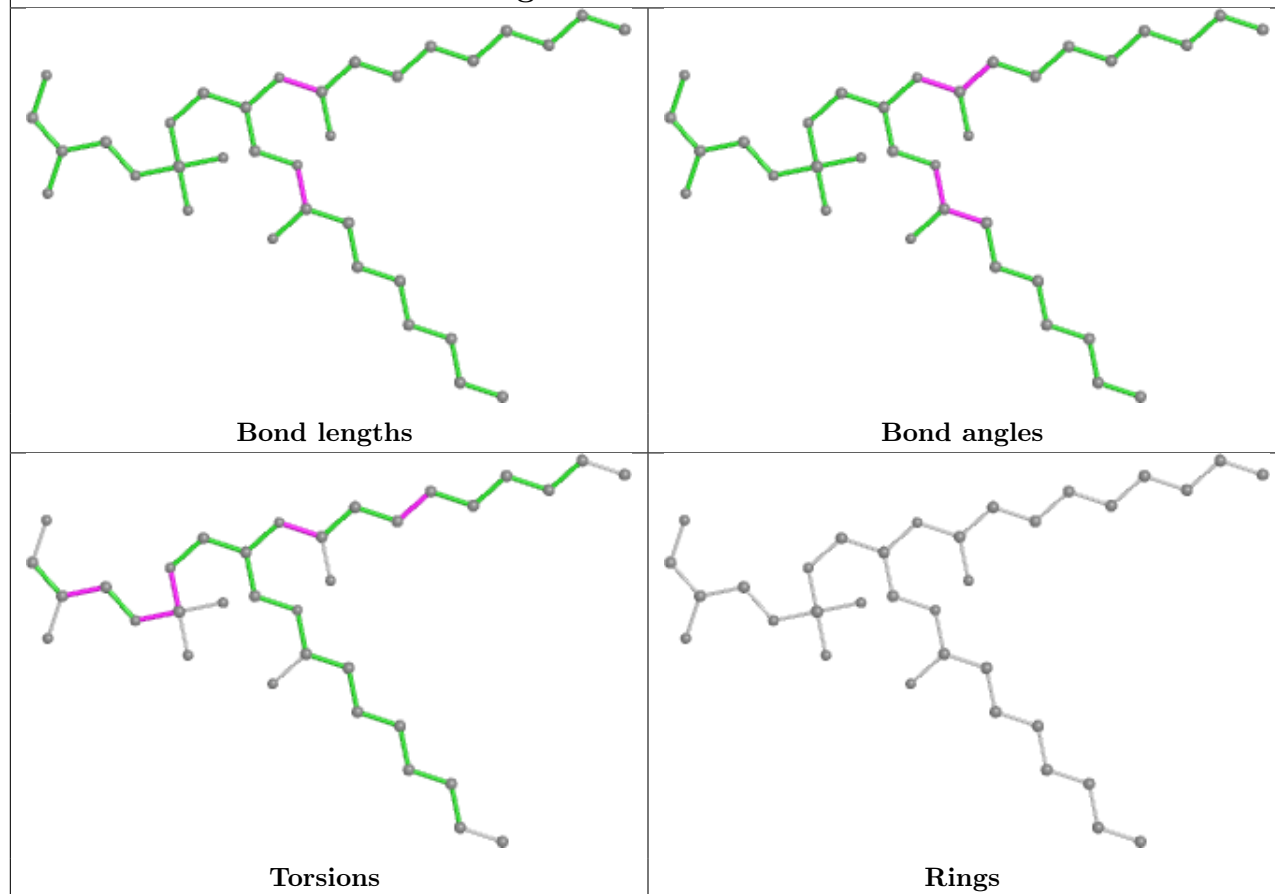
## Ligand CLA c 501



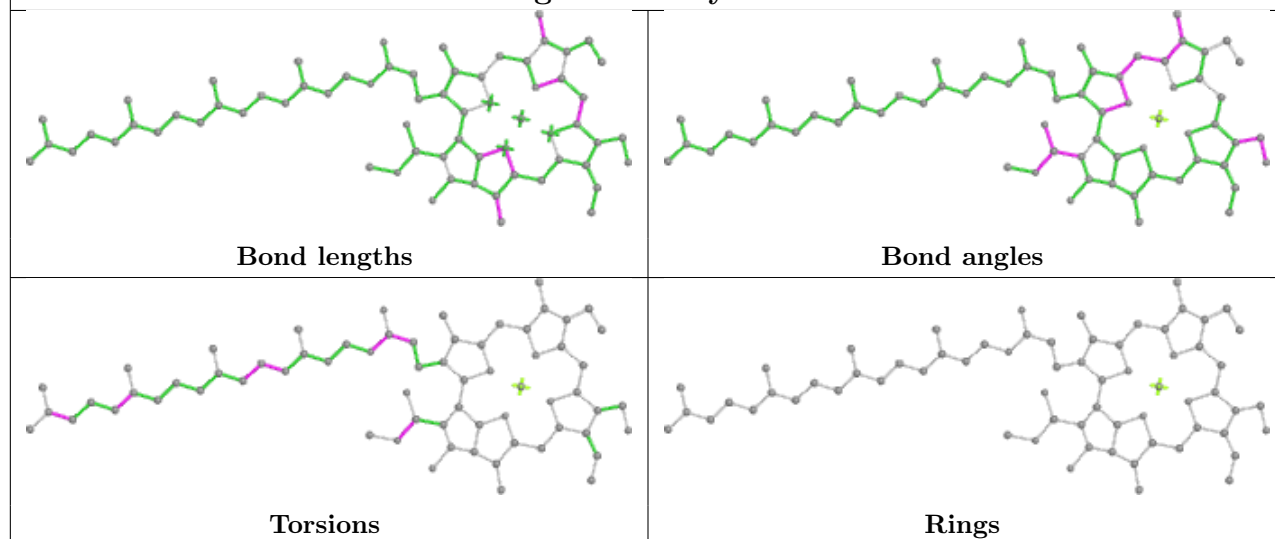
## Ligand CLA CC 508

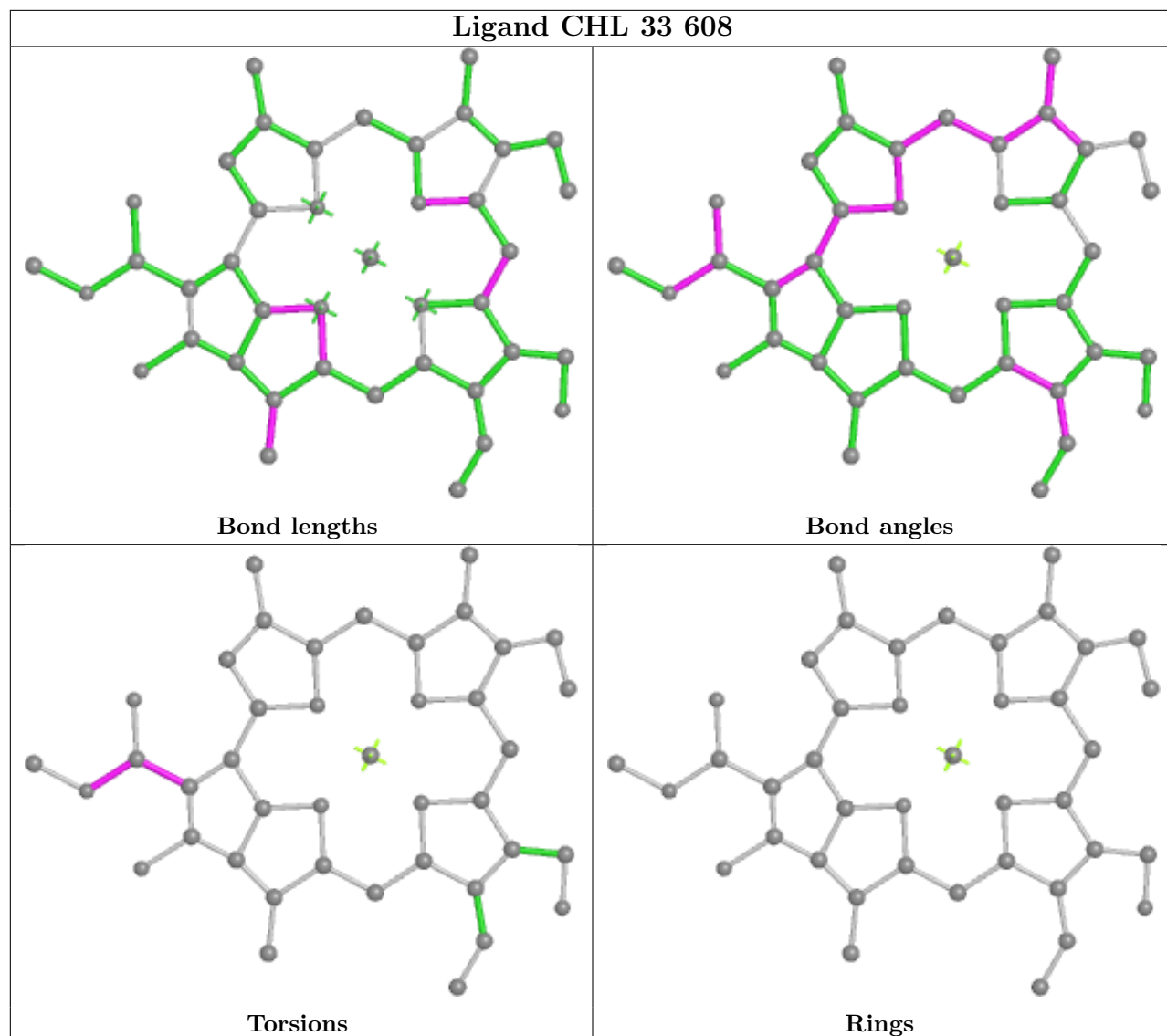


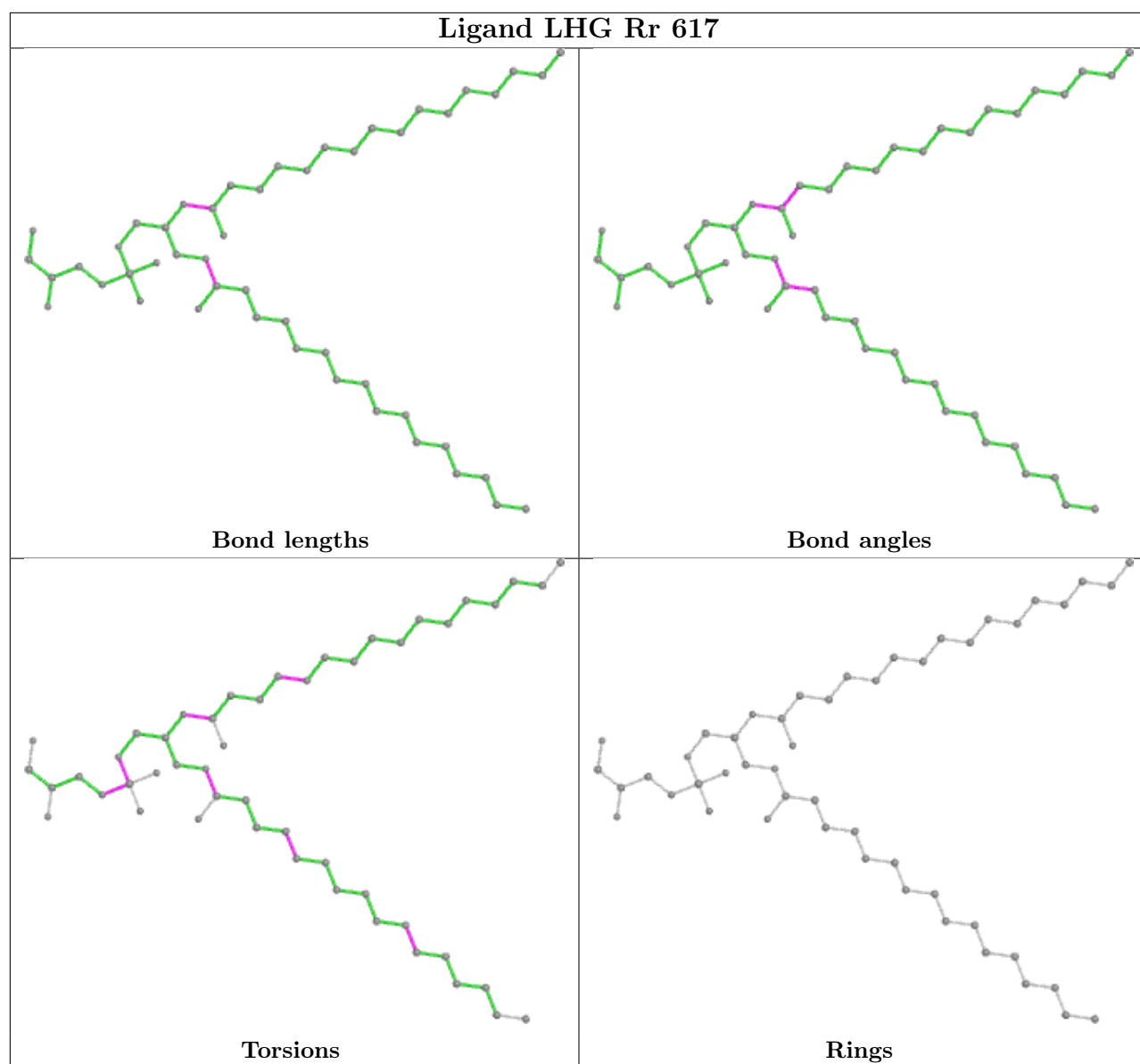
## Ligand LHG BB 622

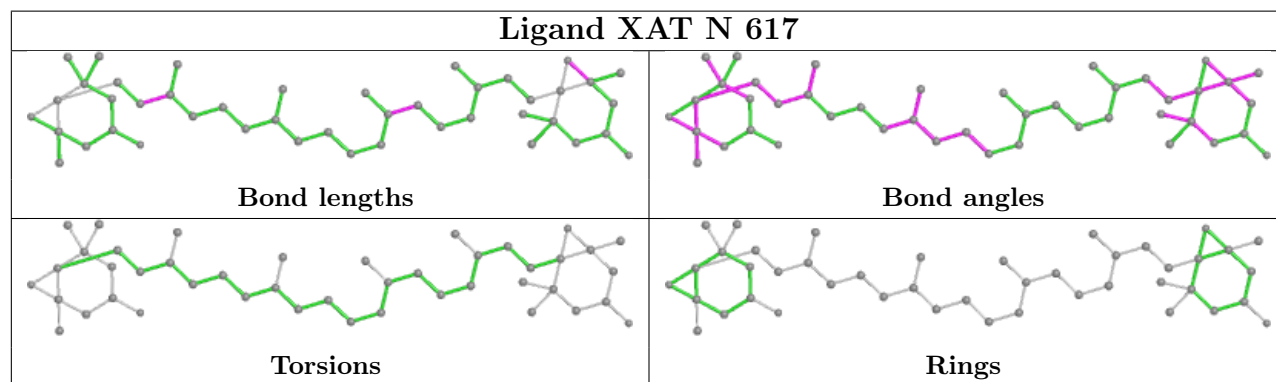
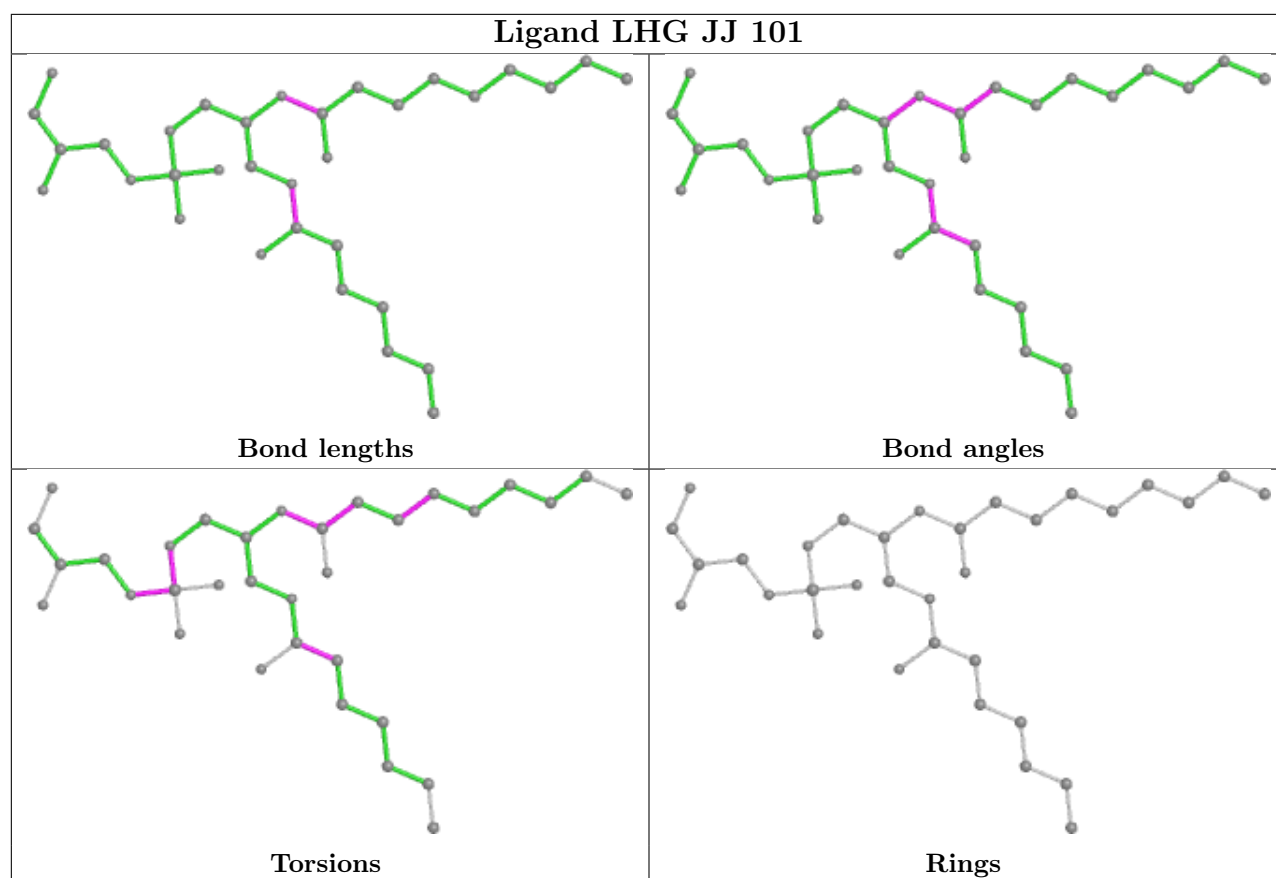


## Ligand CHL y 311

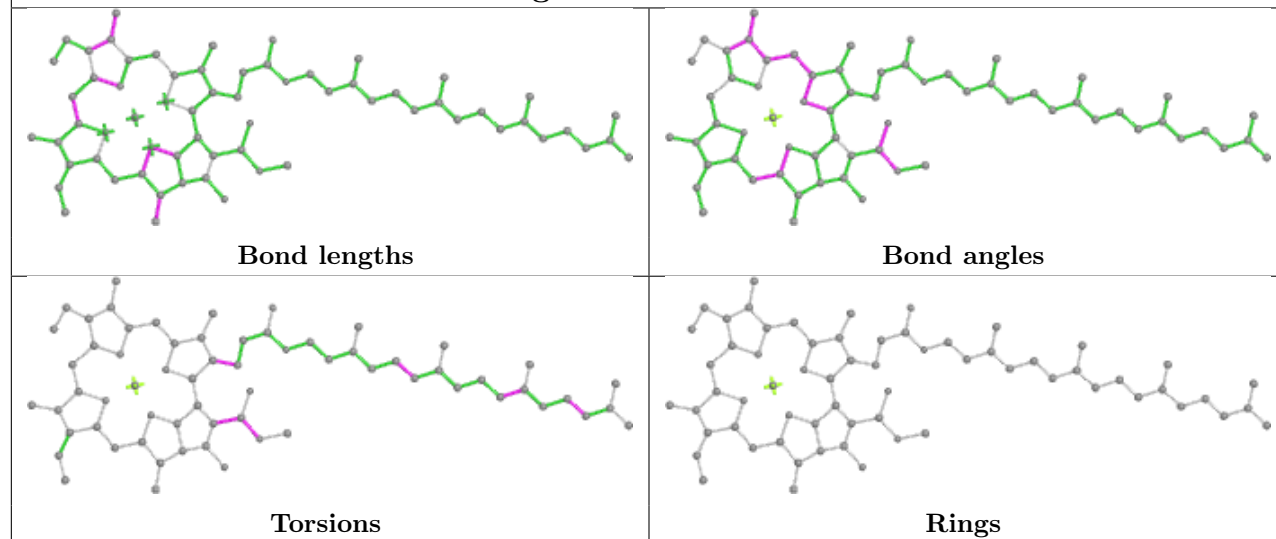




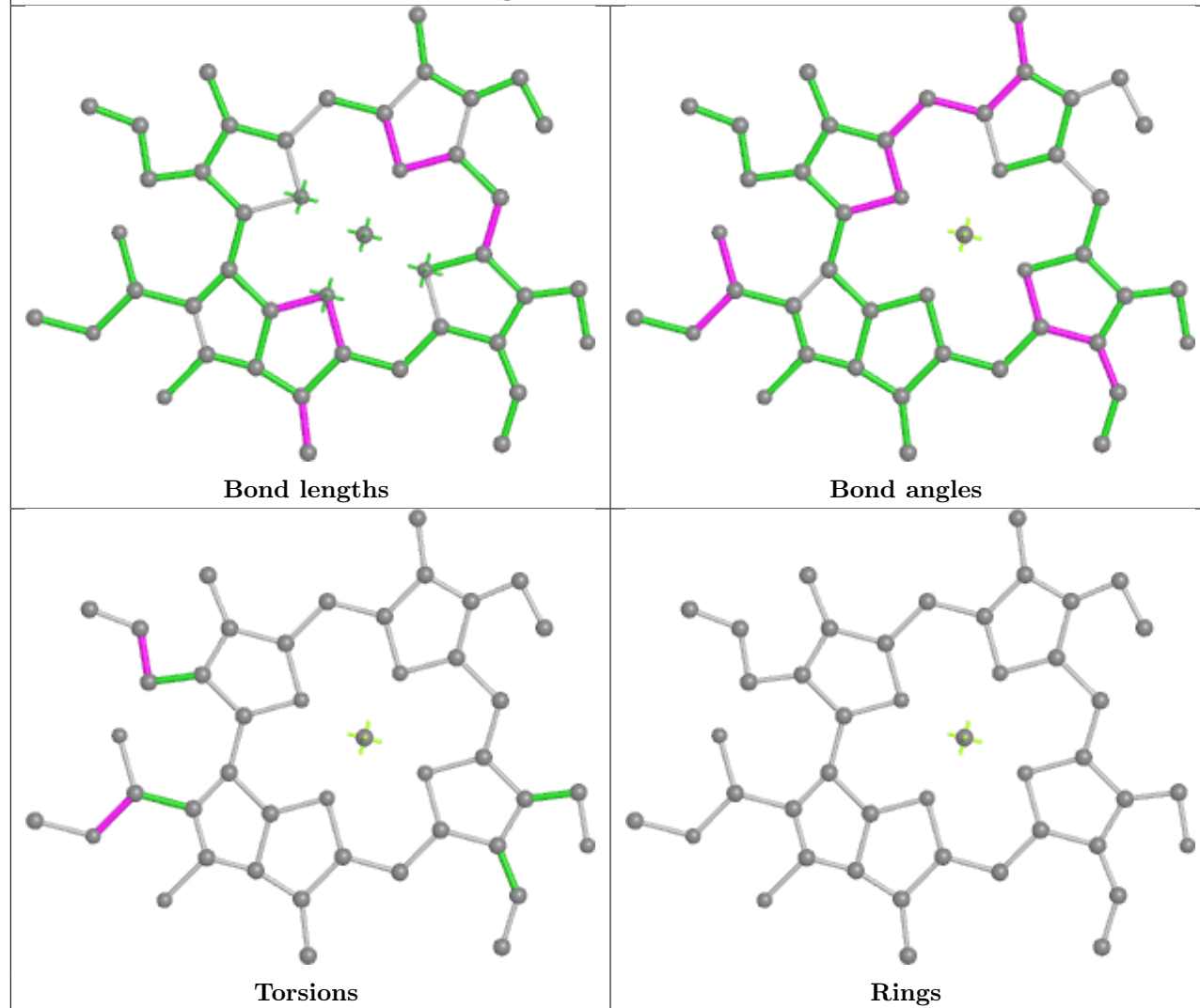




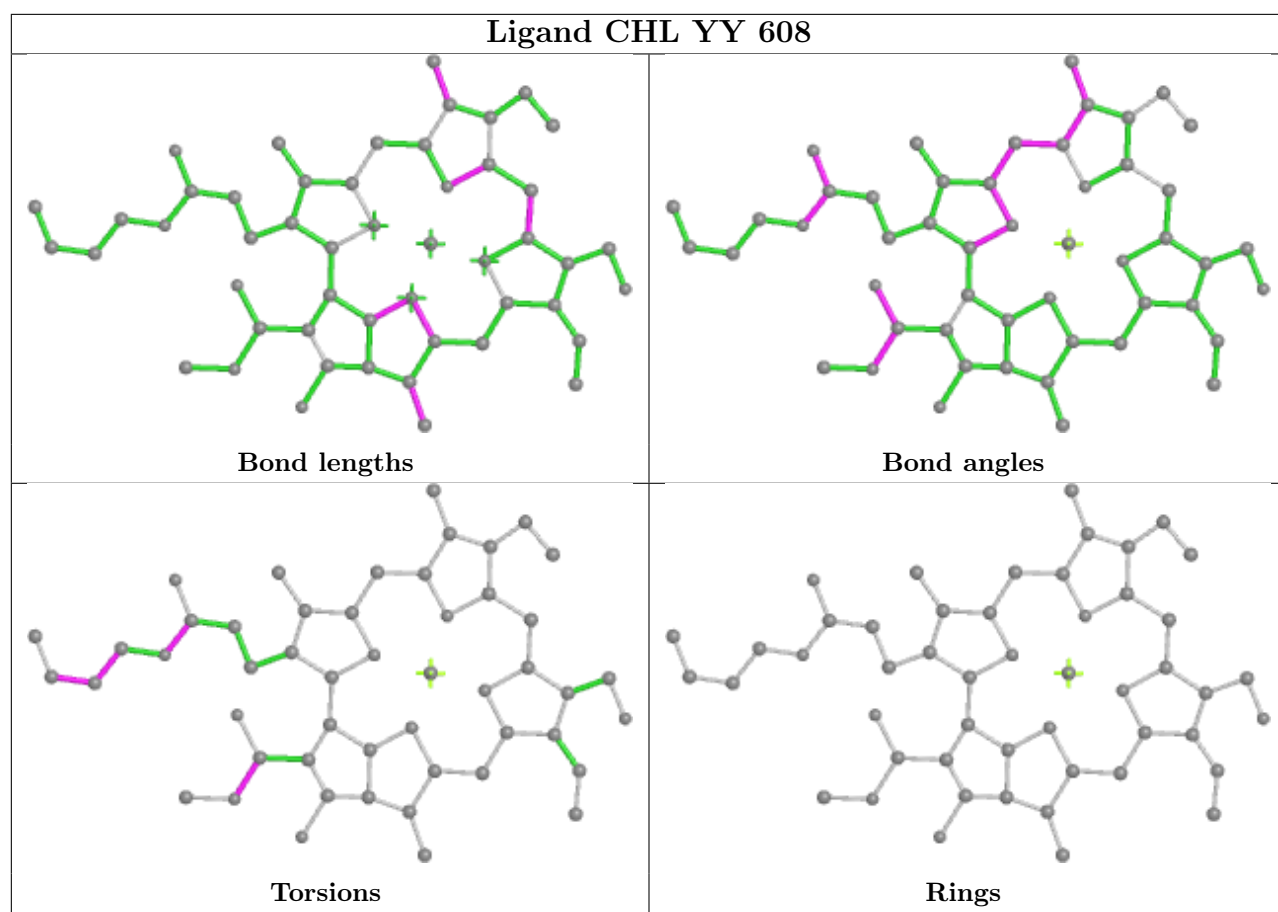
## Ligand CLA B 604

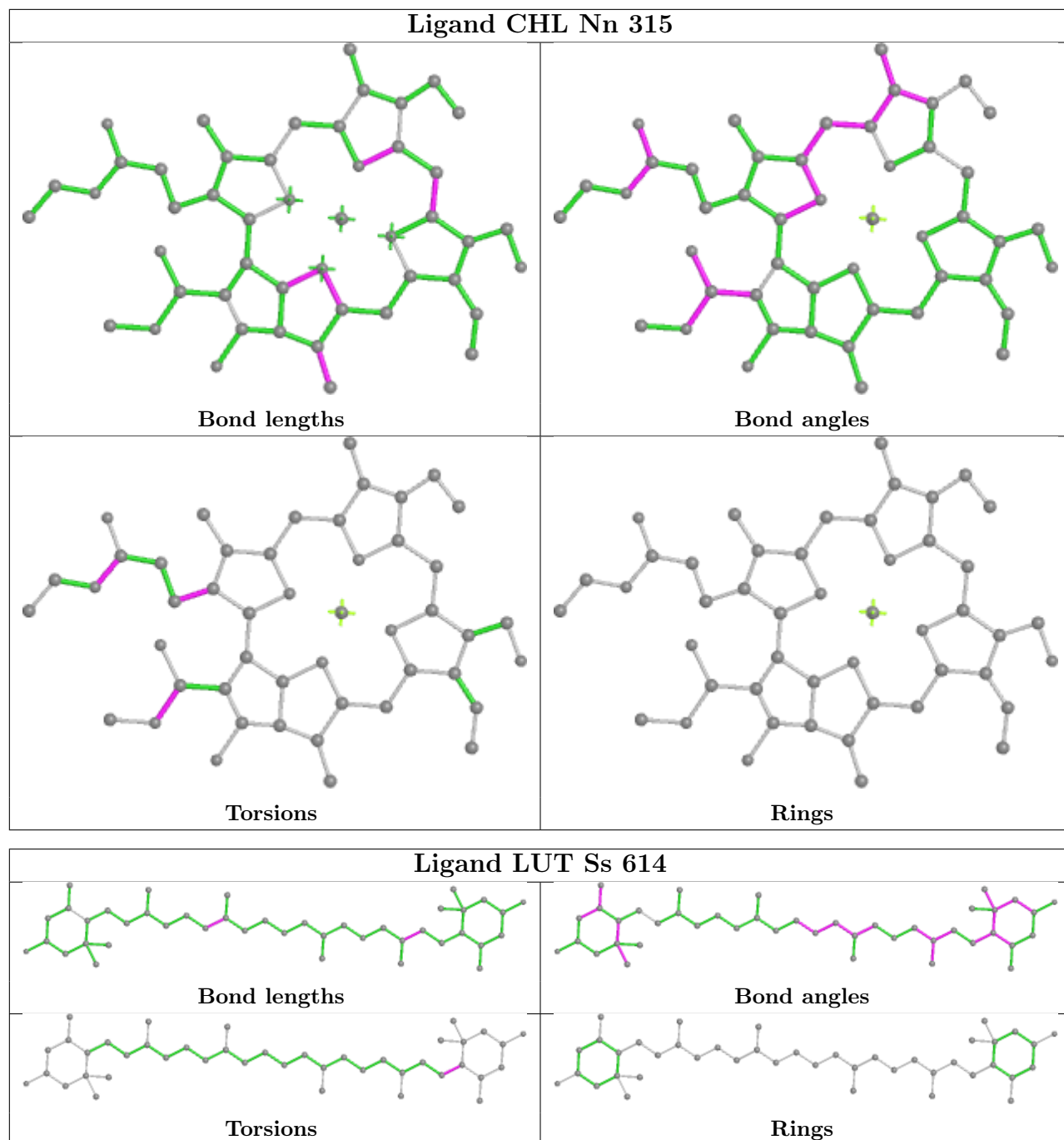


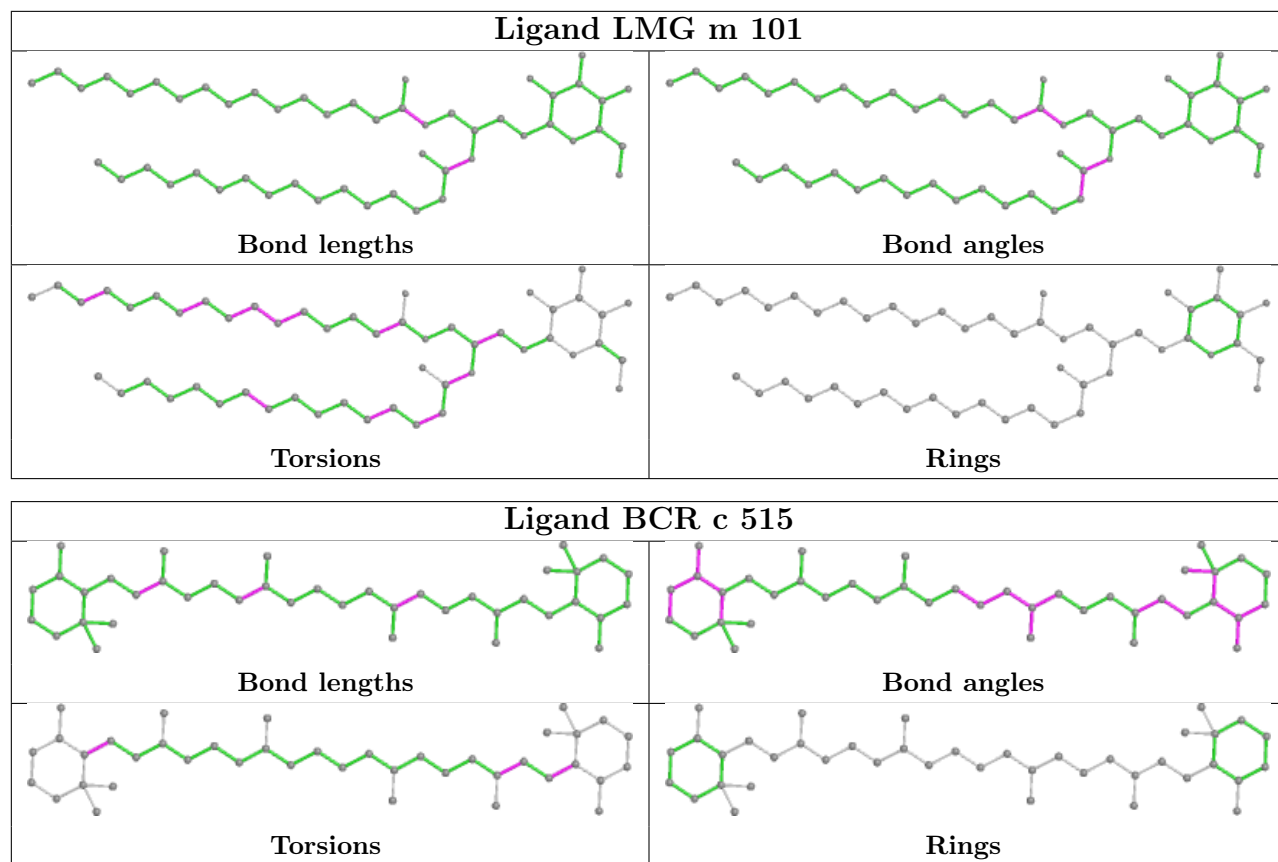
## Ligand CHL N 601

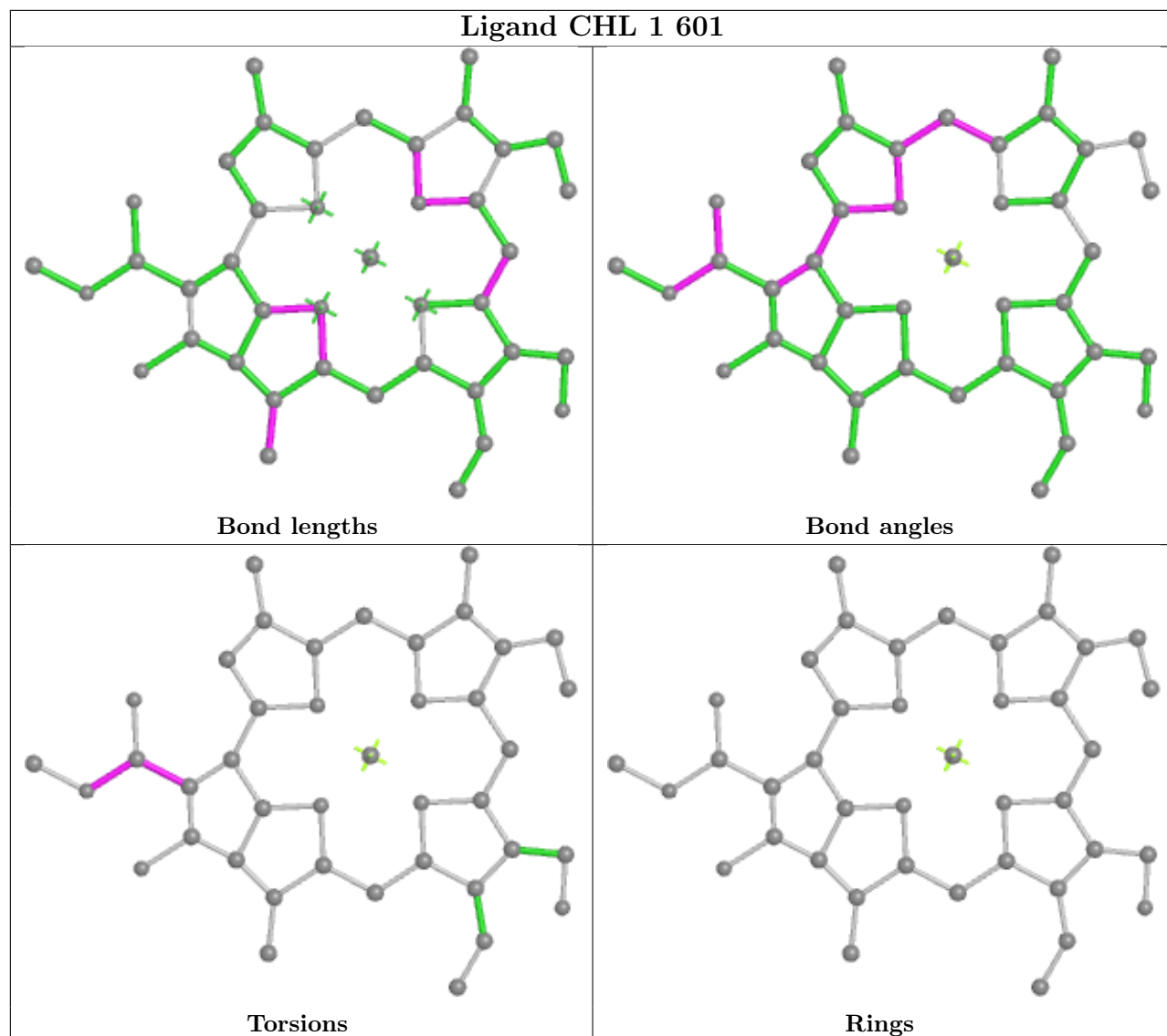


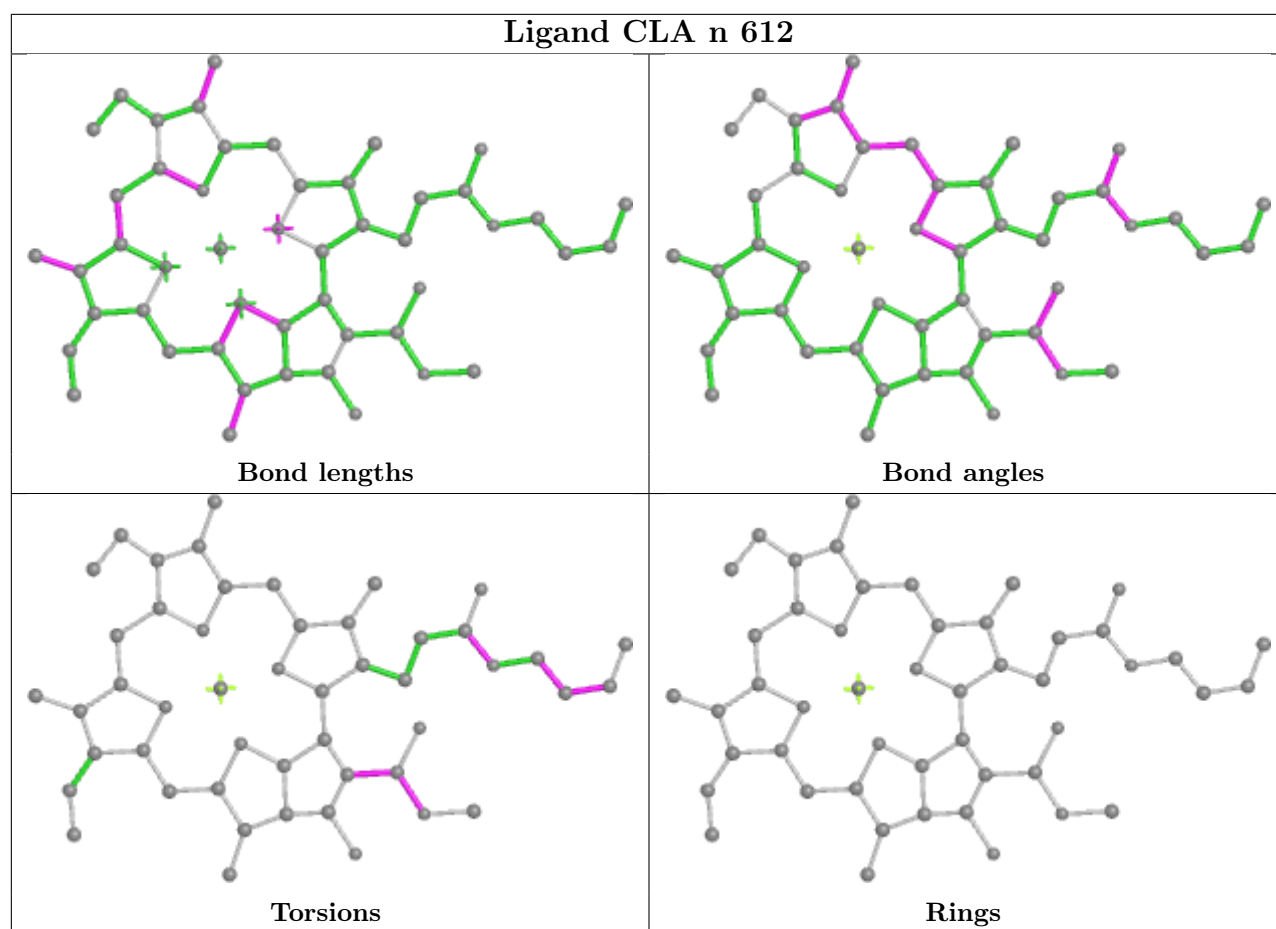




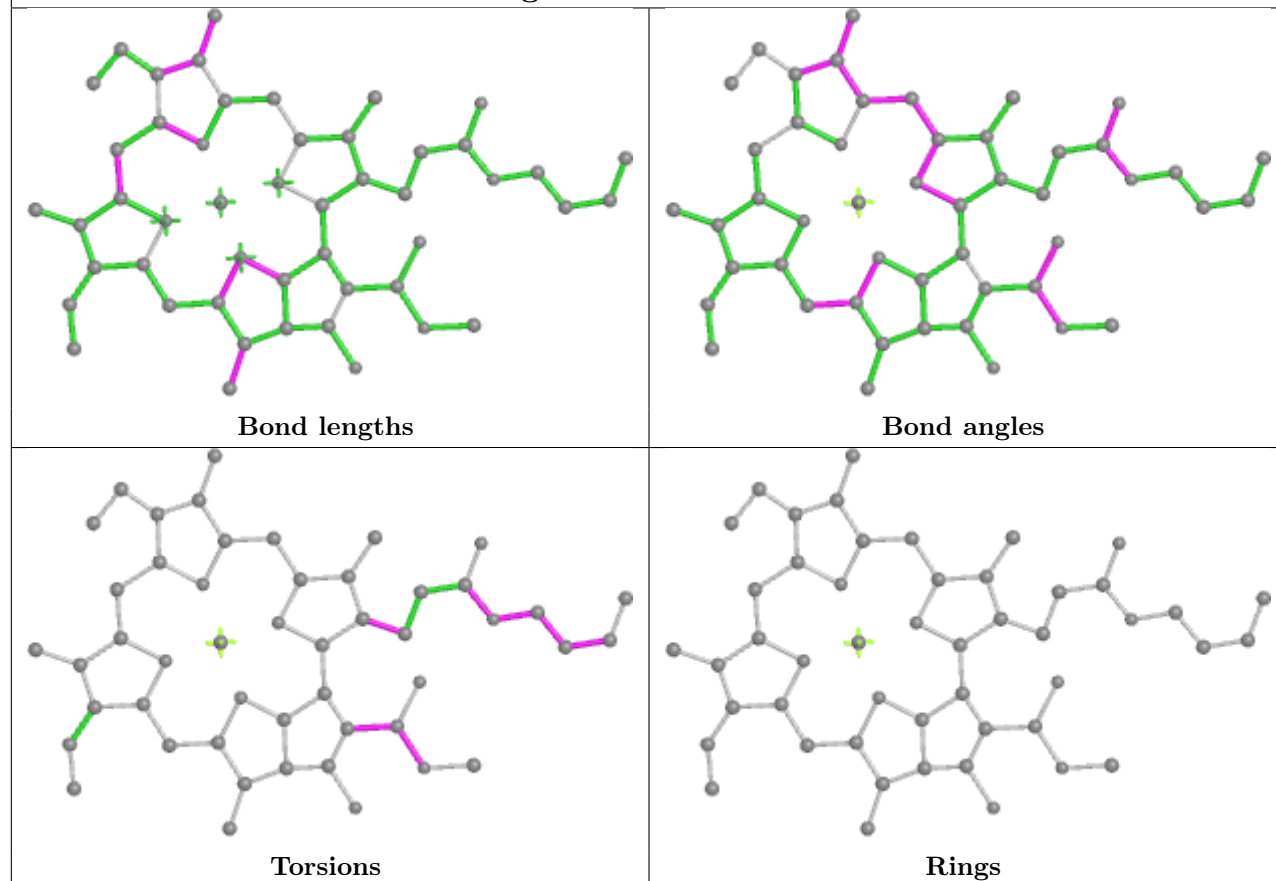




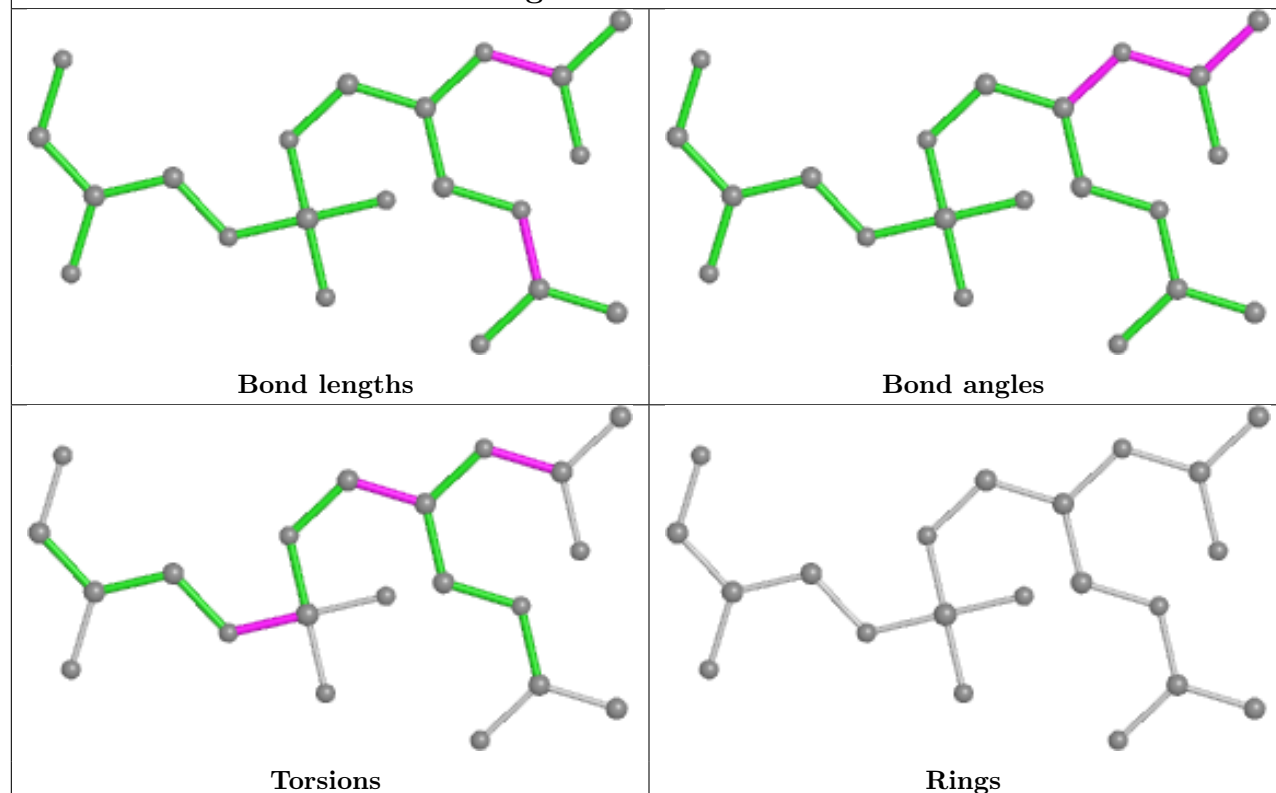


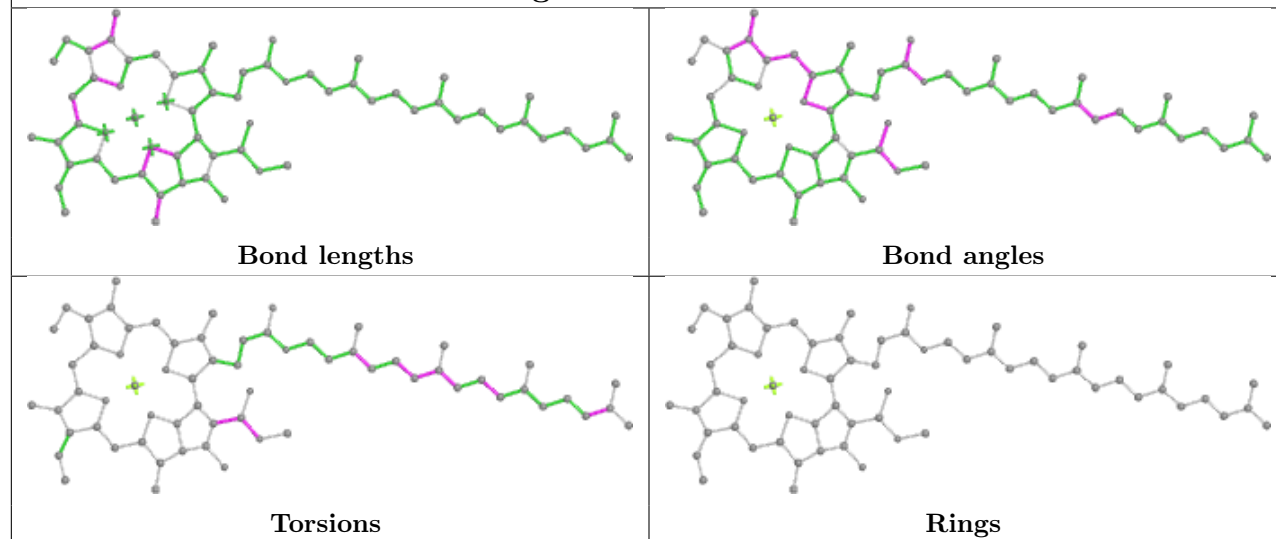
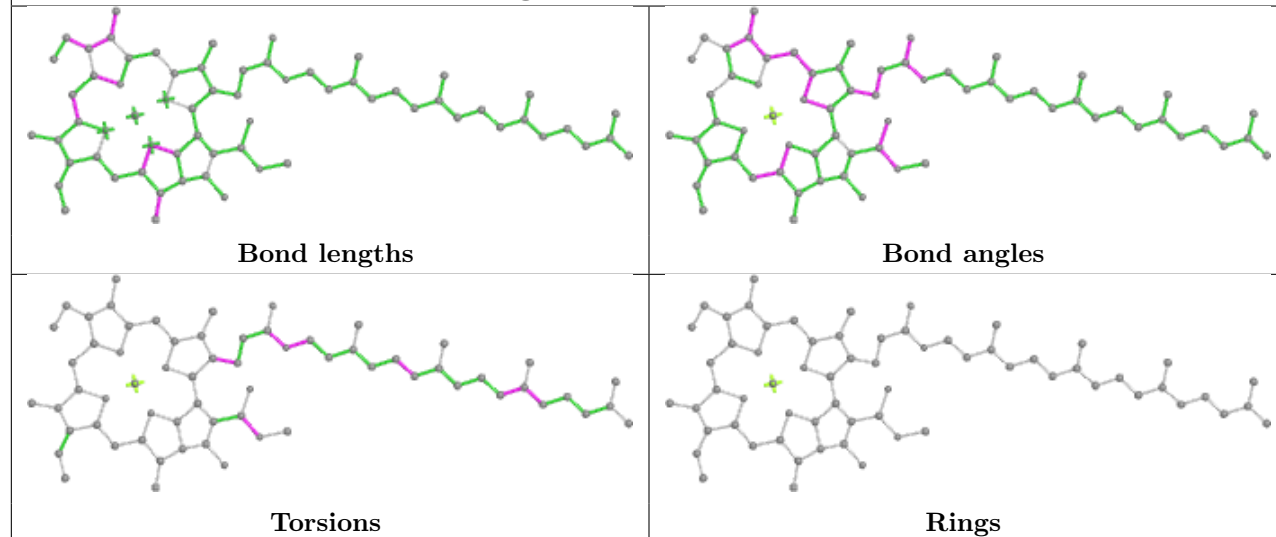
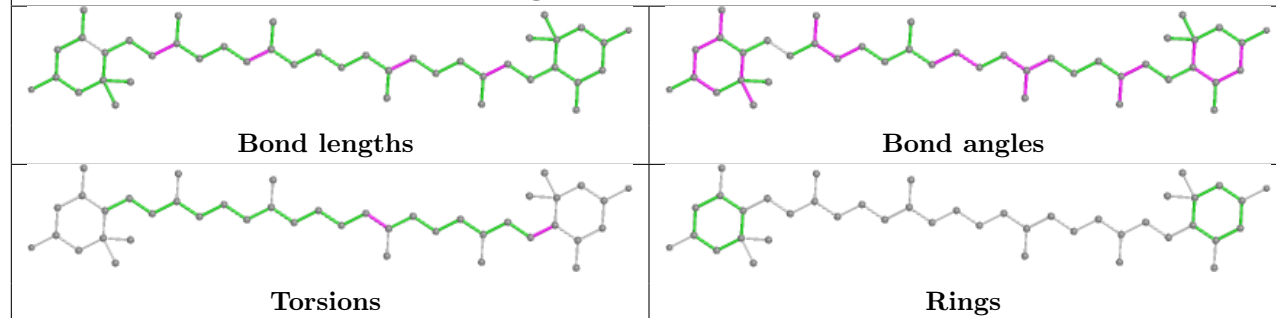


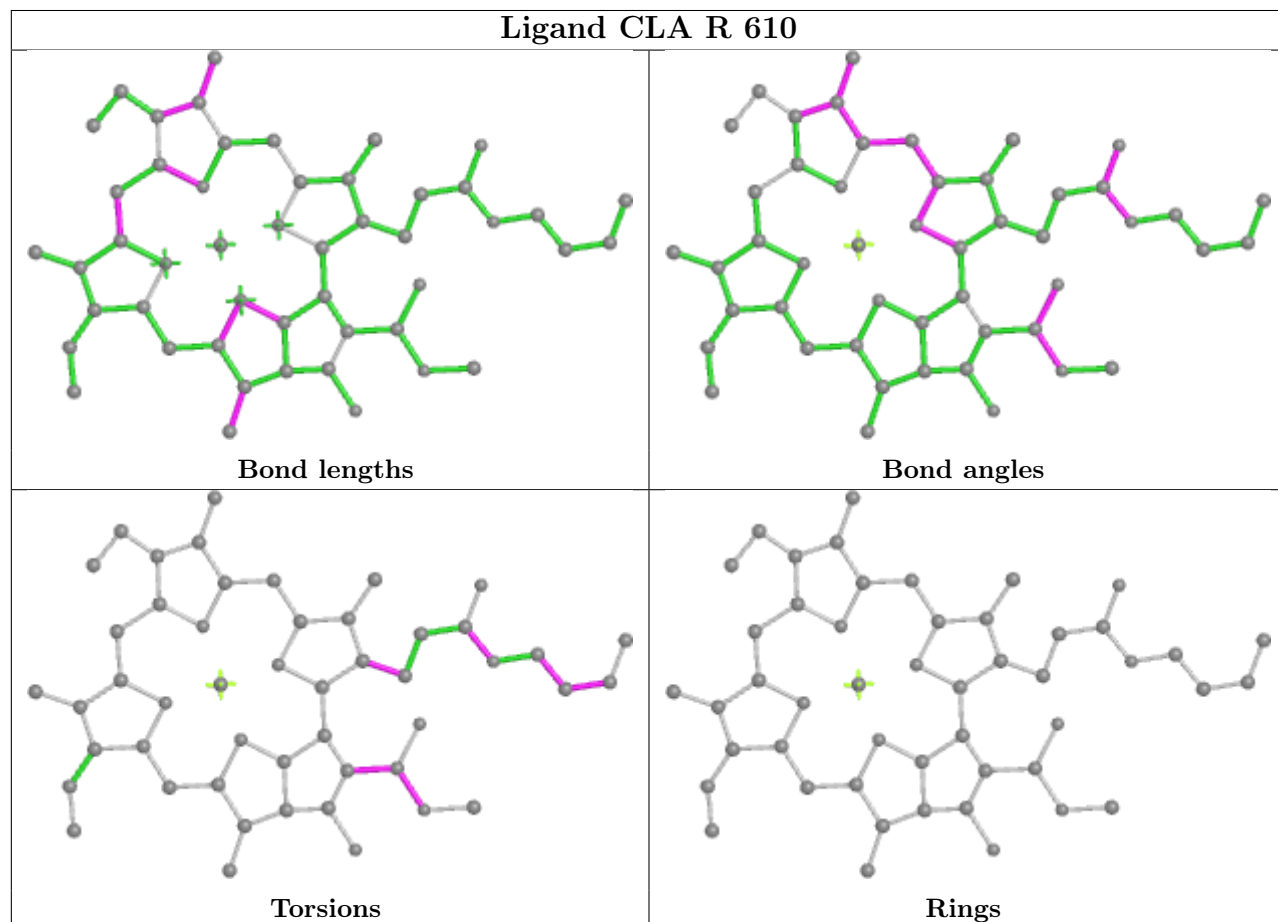
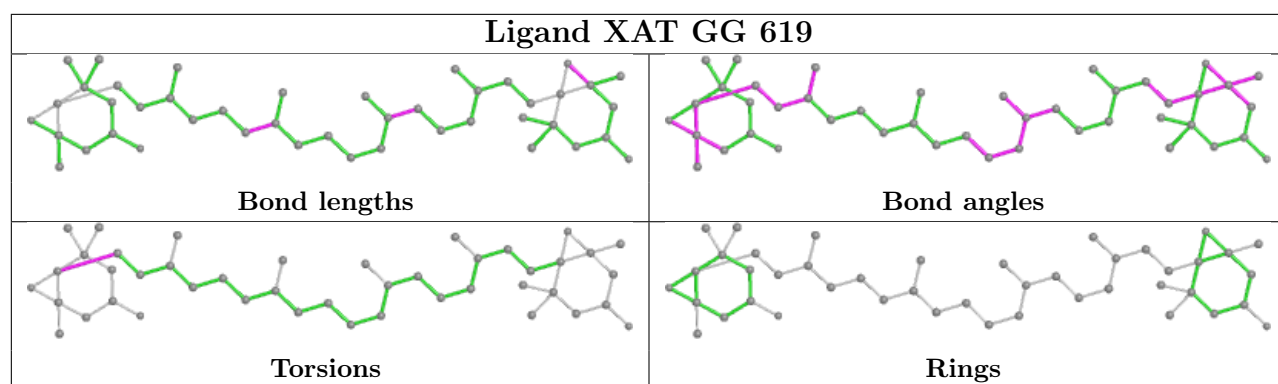
## Ligand CLA Nn 313



## Ligand LHG 44 614

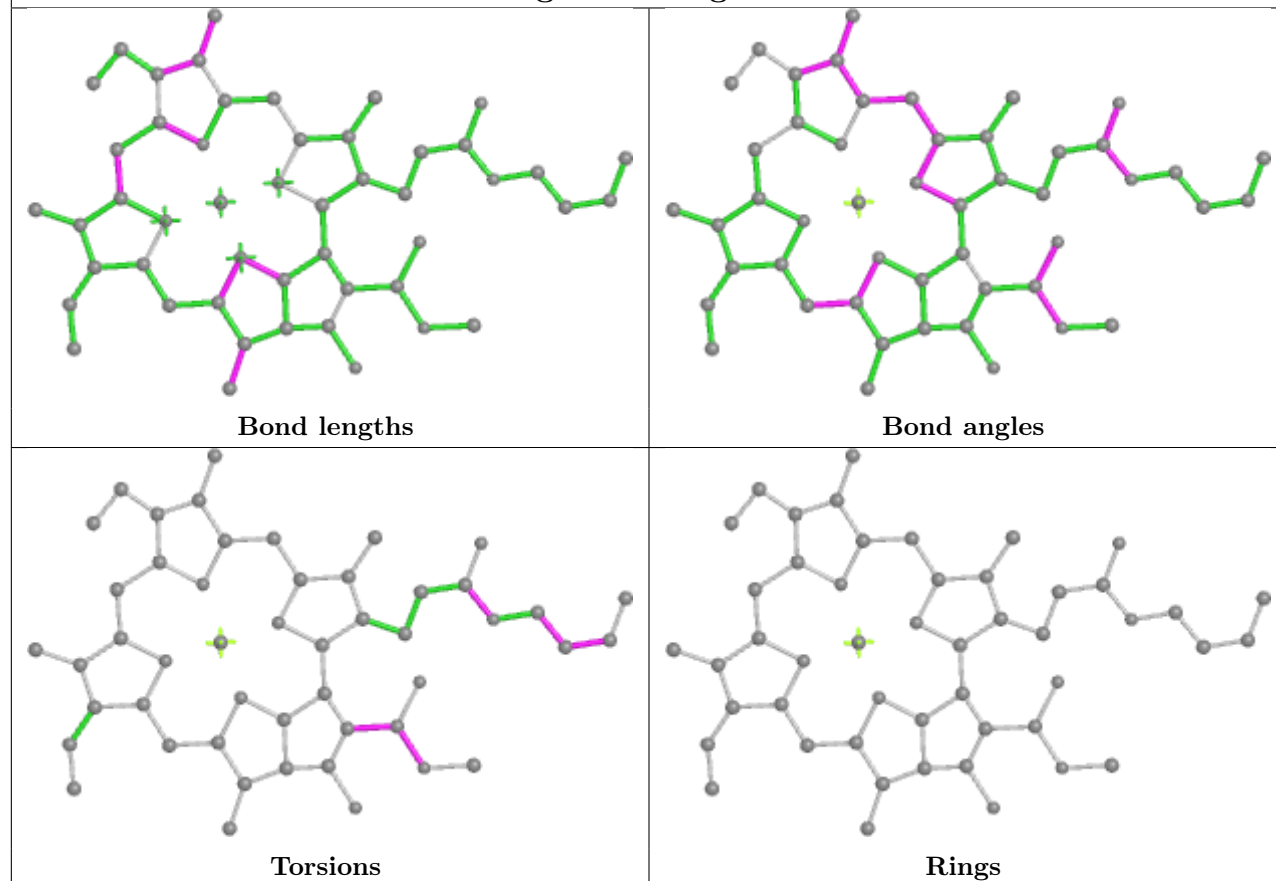


**Ligand CLA B 606****Ligand CLA NN 610****Ligand LUT 22 614**

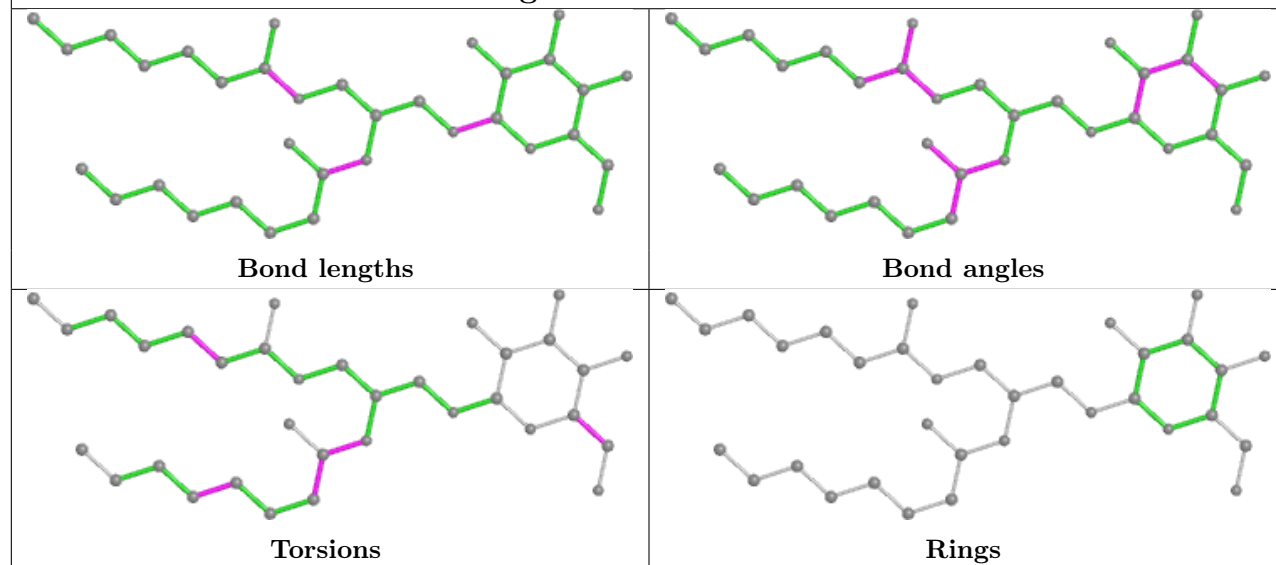




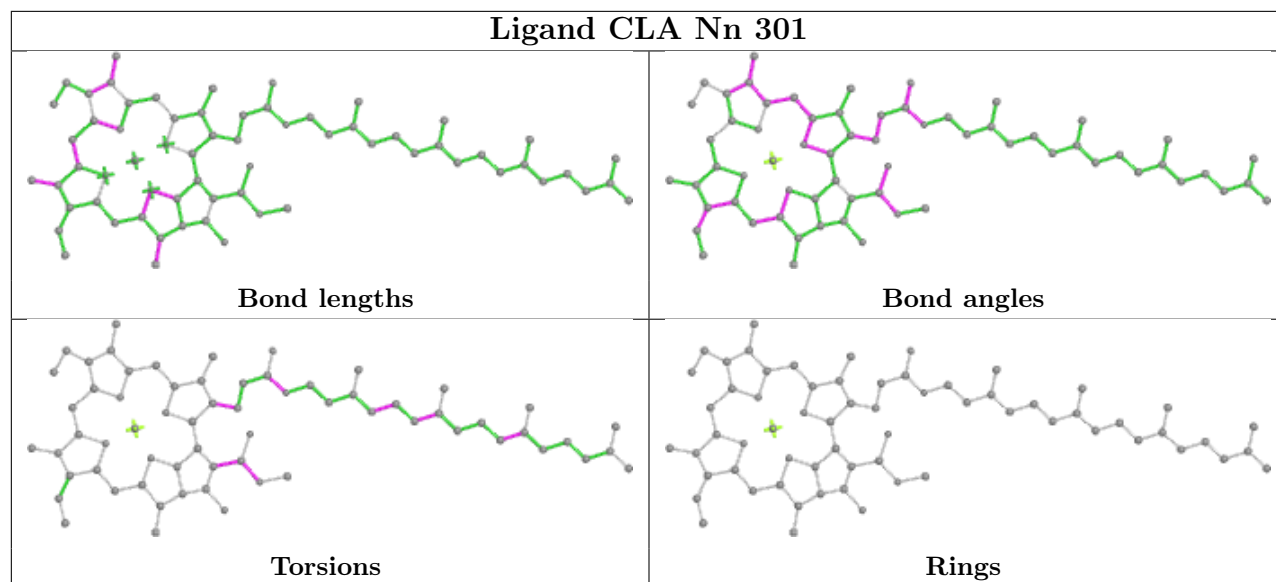
## Ligand CLA g 614



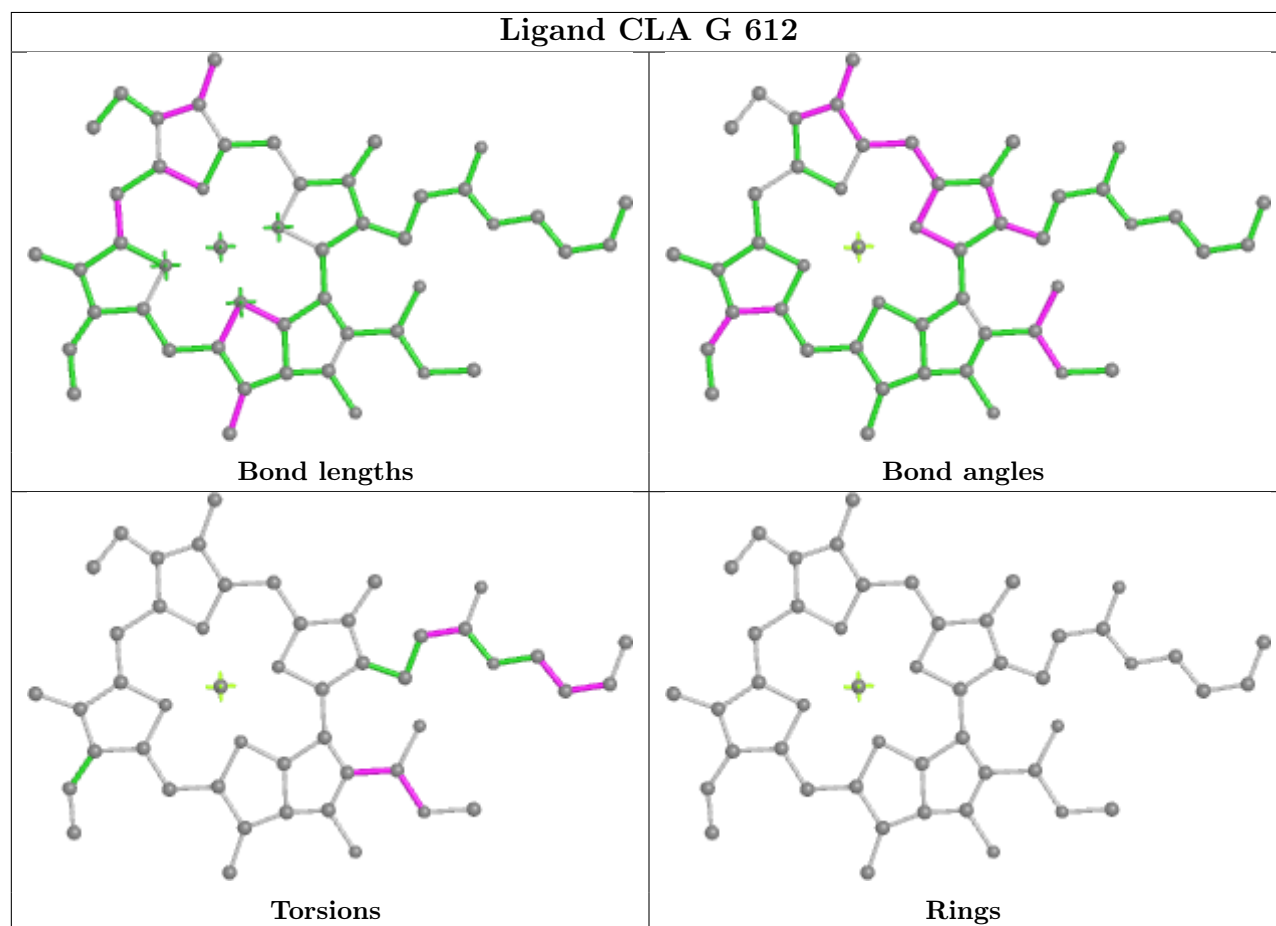
## Ligand LMG Cc 501



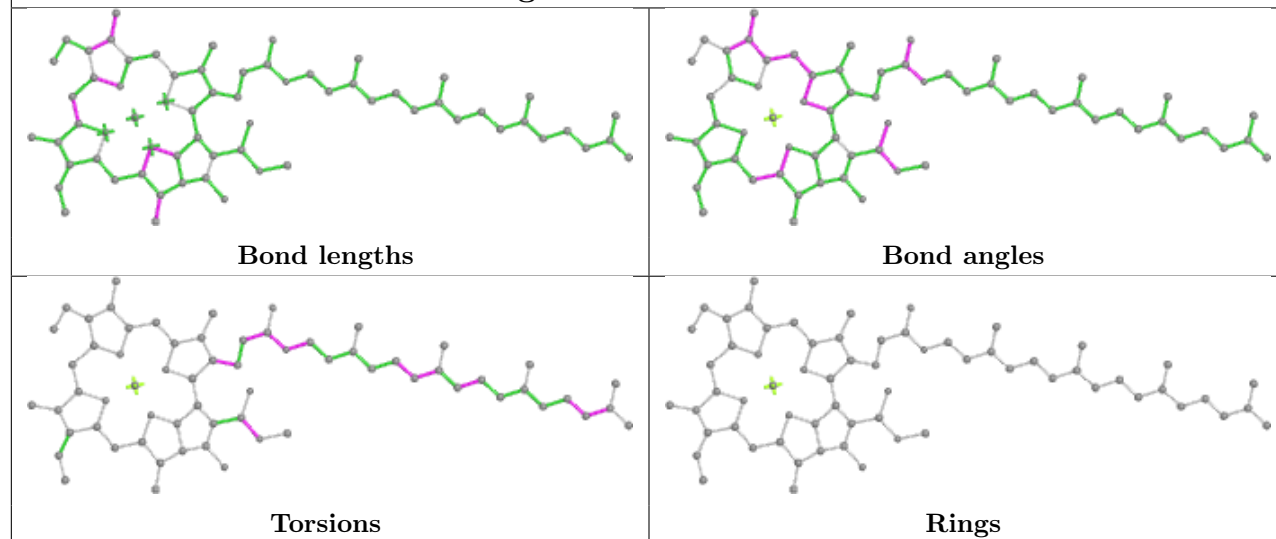
## Ligand CLA Nn 301



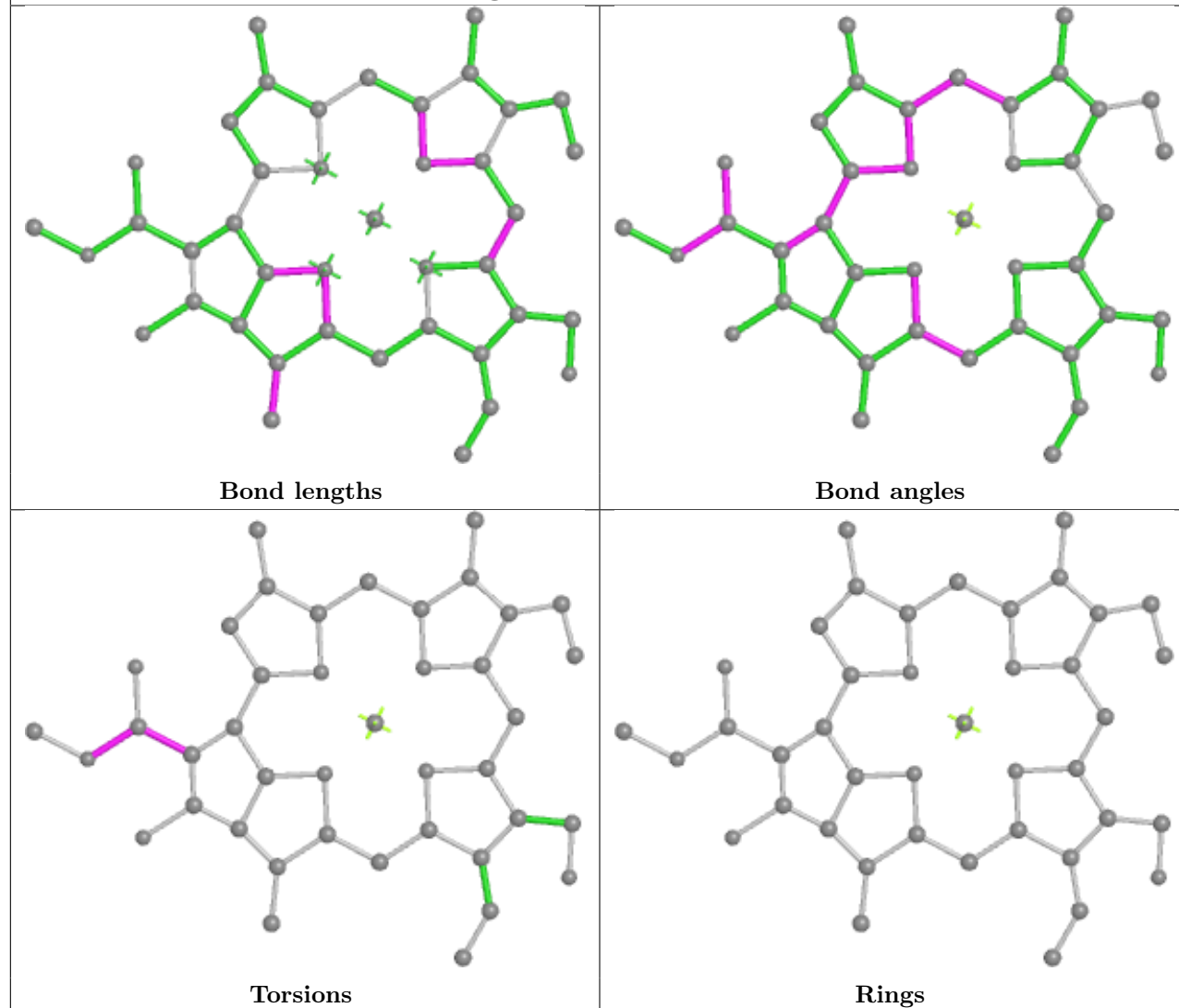
## Ligand CLA G 612



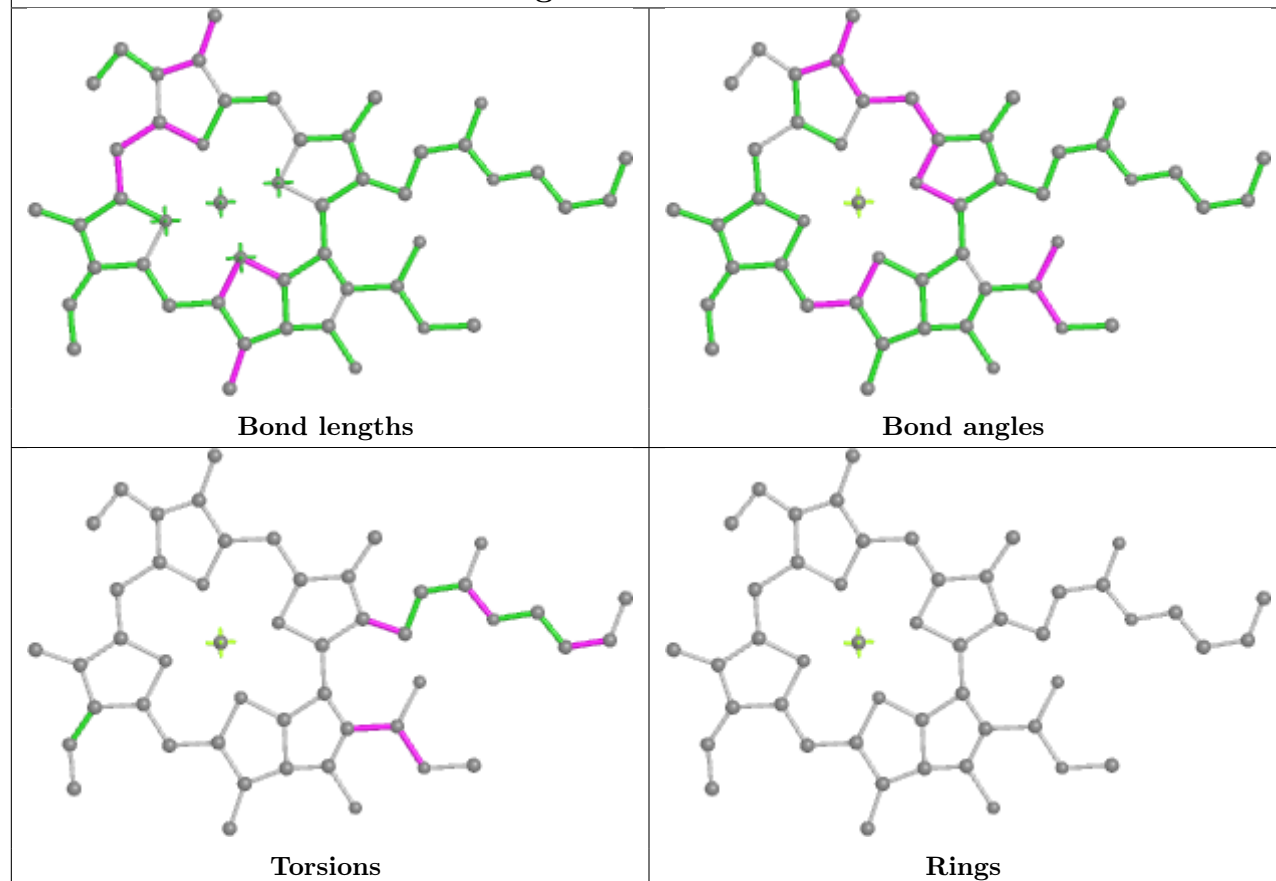
## Ligand CLA YY 602



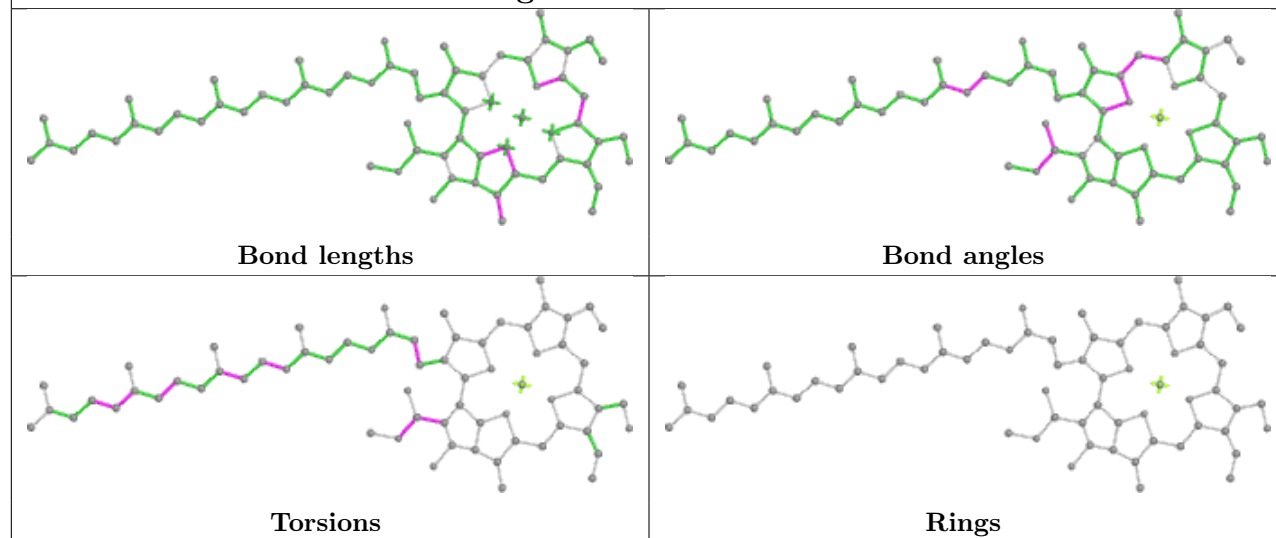
## Ligand CHL 11 601



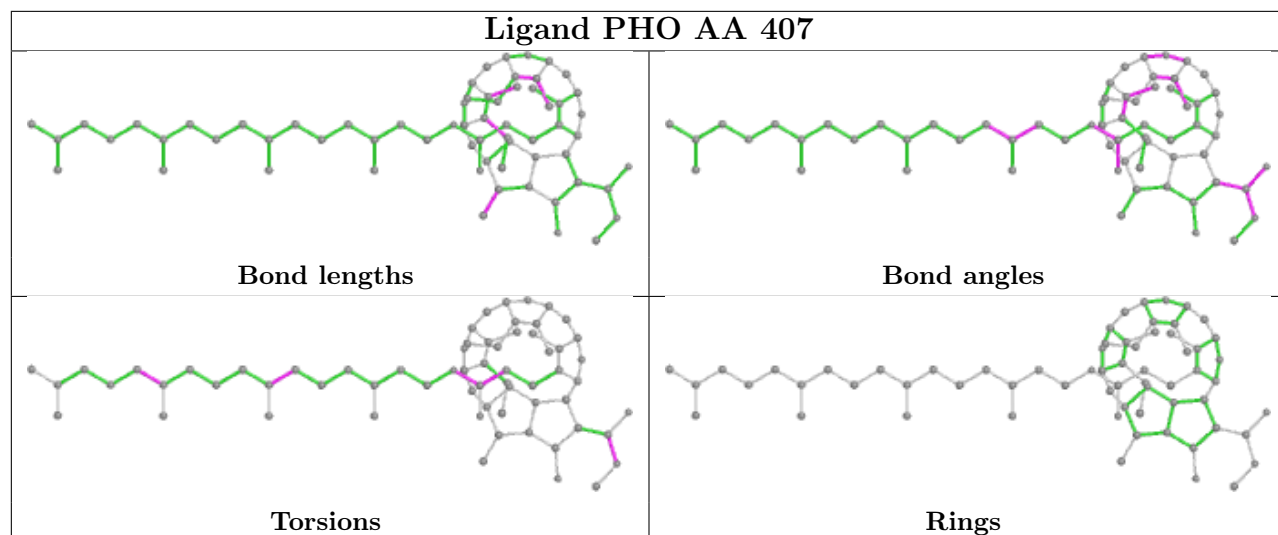
## Ligand CLA n 613



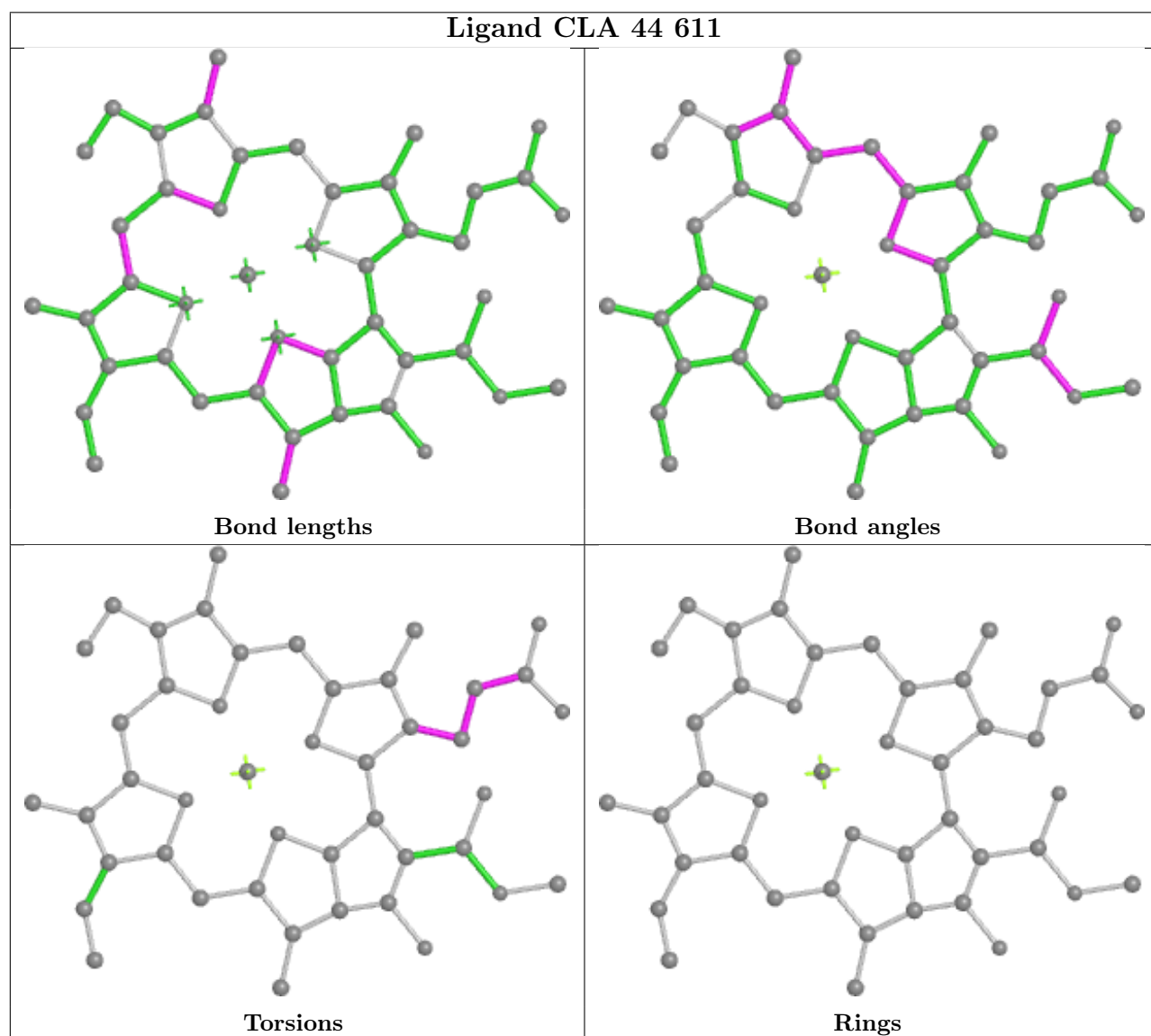
## Ligand CHL NN 607

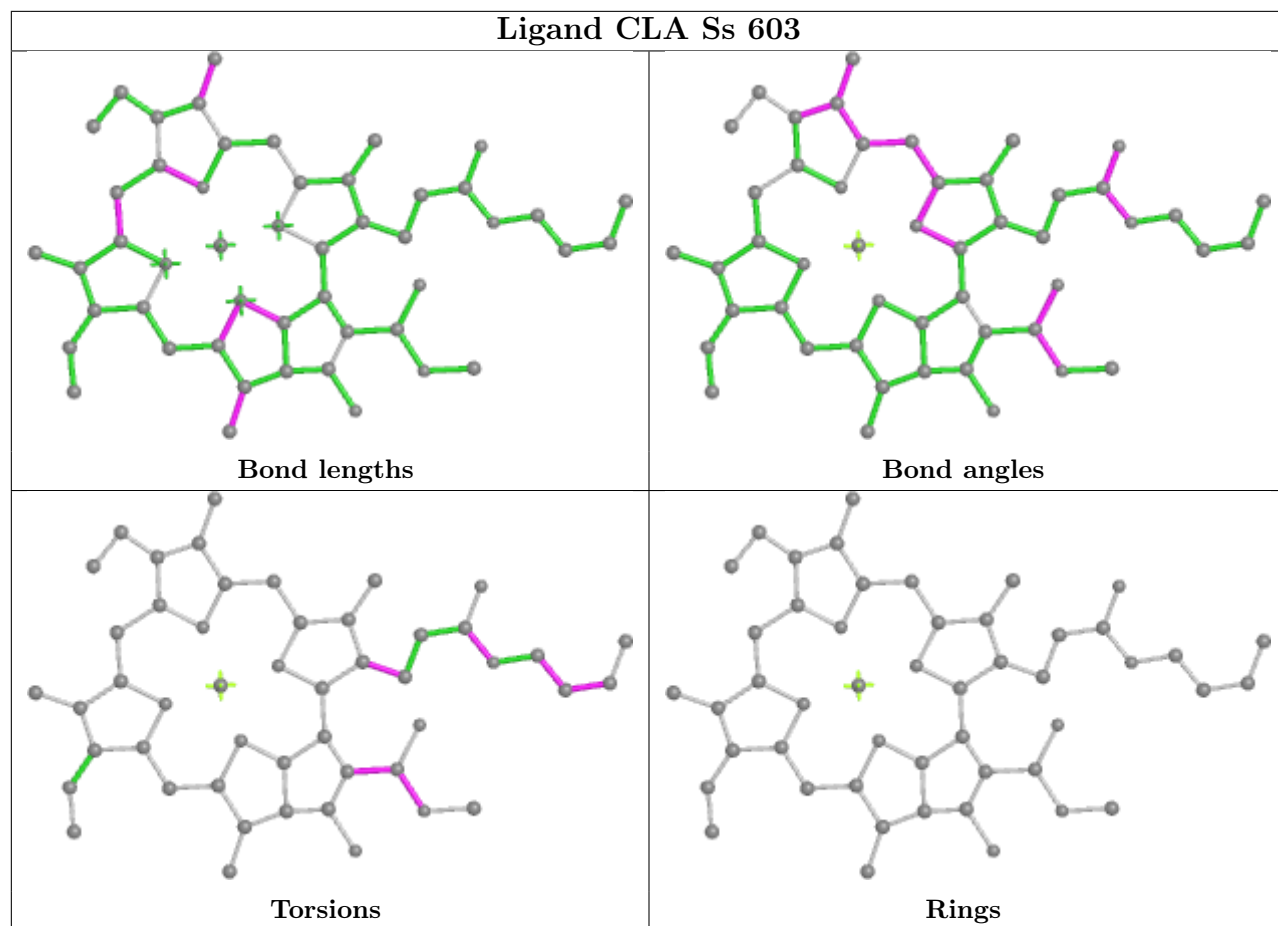


## Ligand PHO AA 407

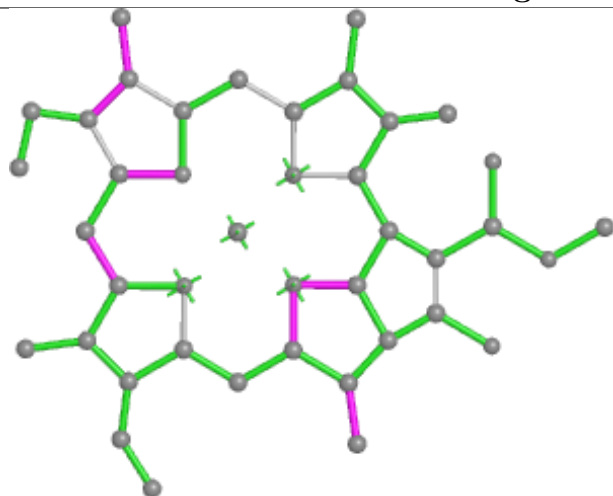


## Ligand CLA 44 611

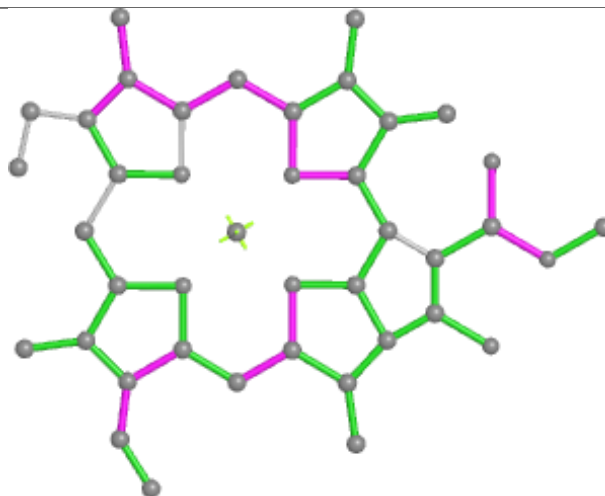




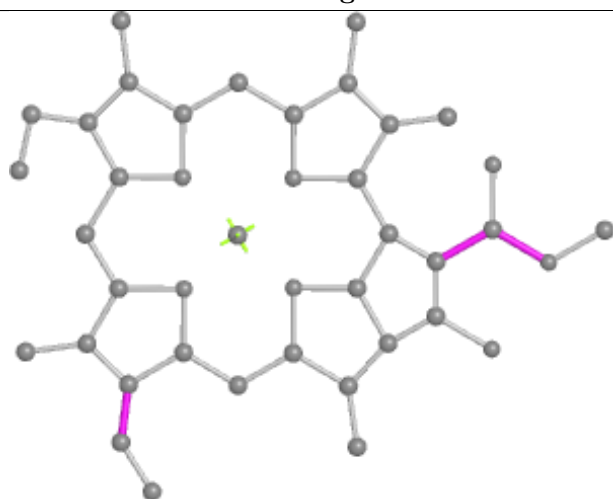
## Ligand CLA R 613



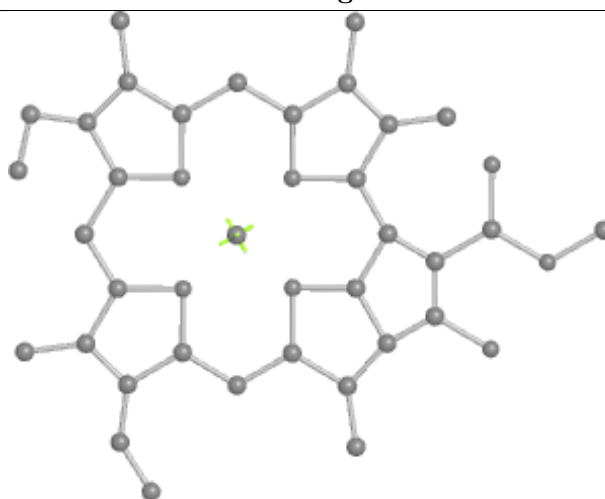
Bond lengths



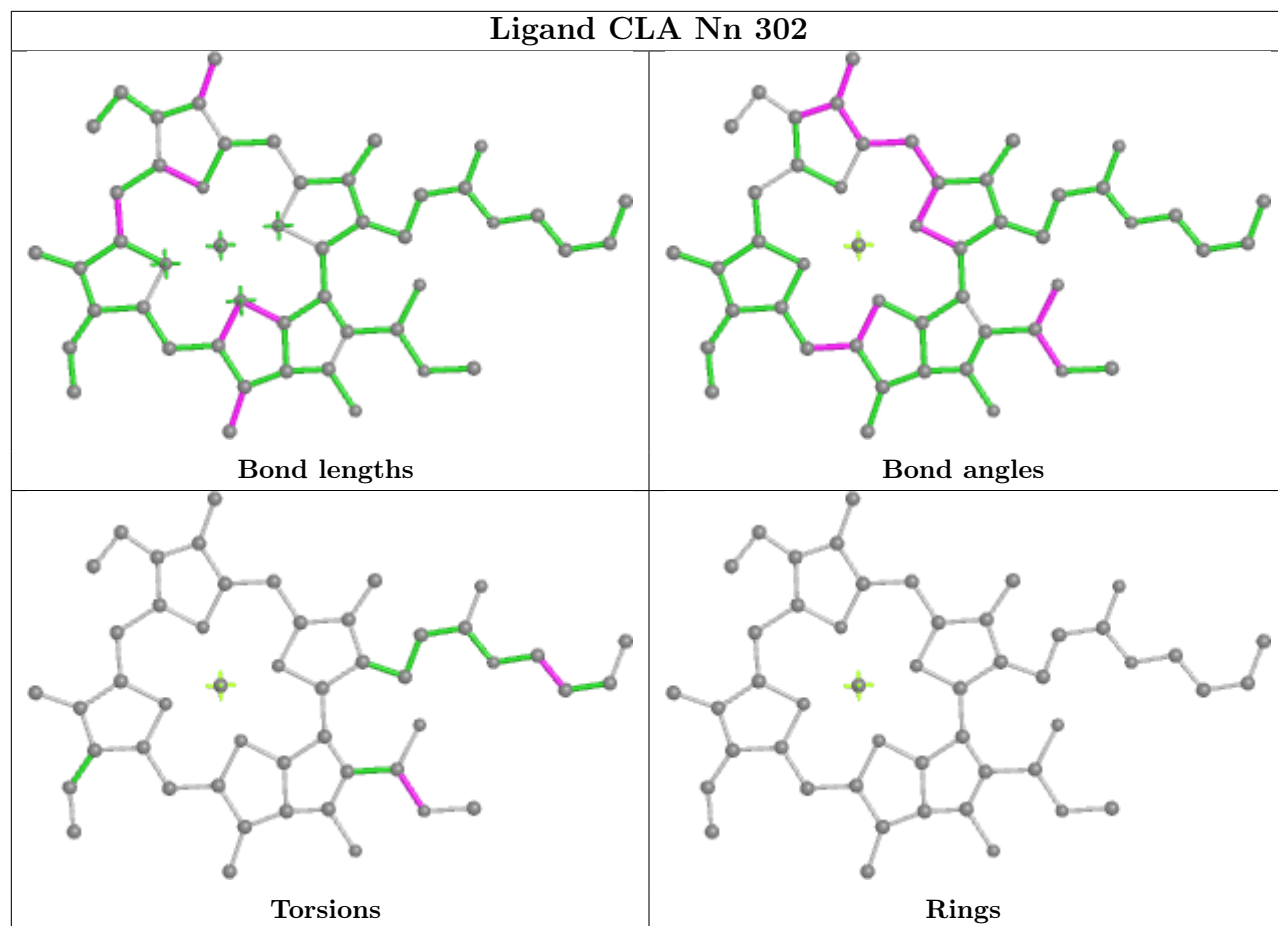
Bond angles



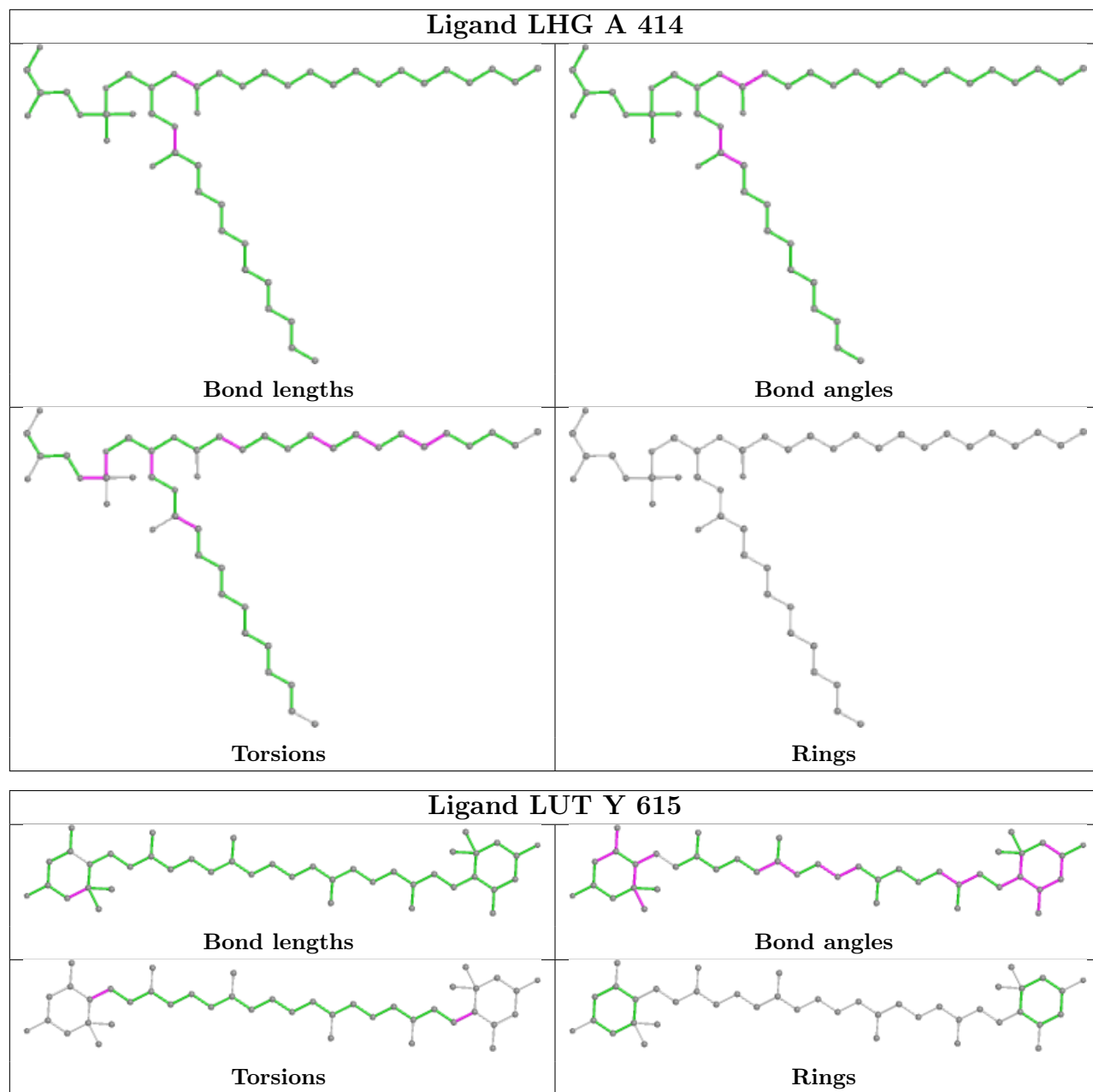
Torsions

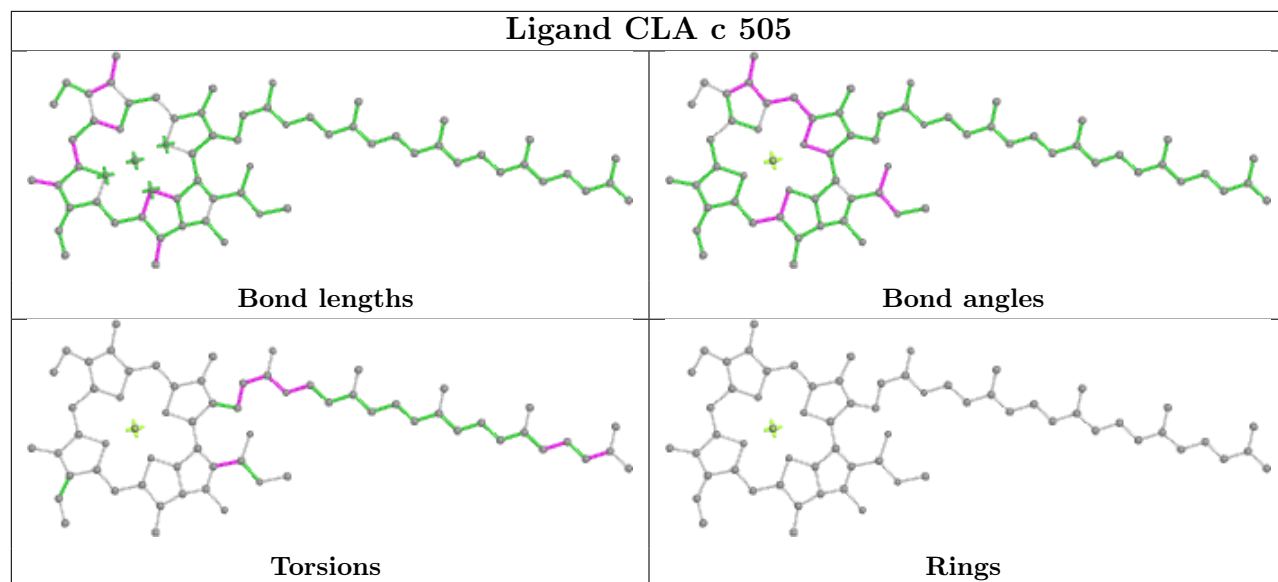
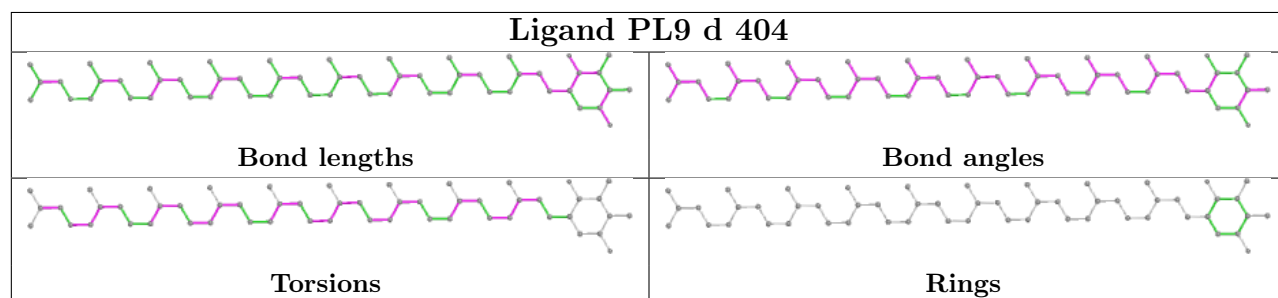


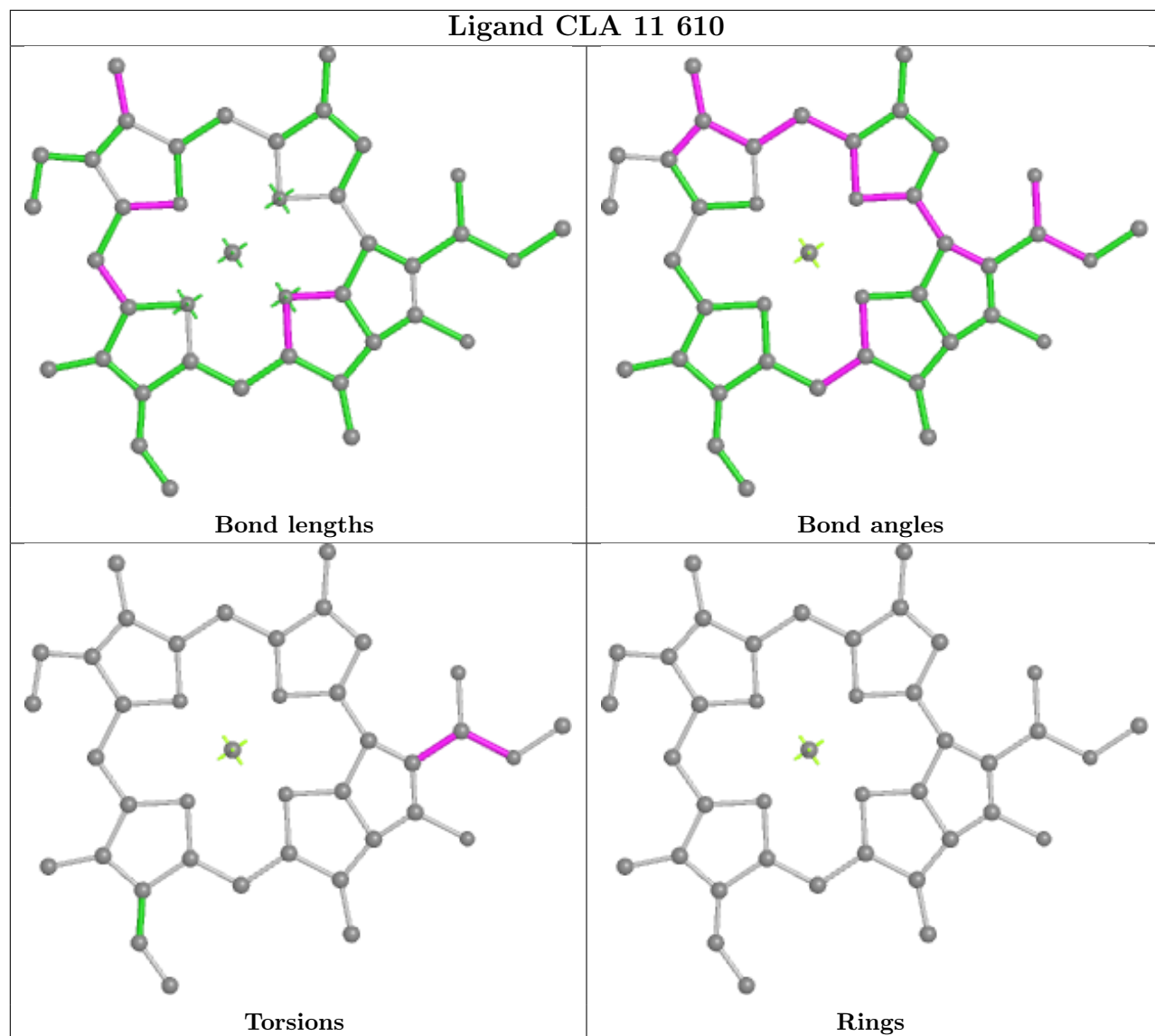
Rings

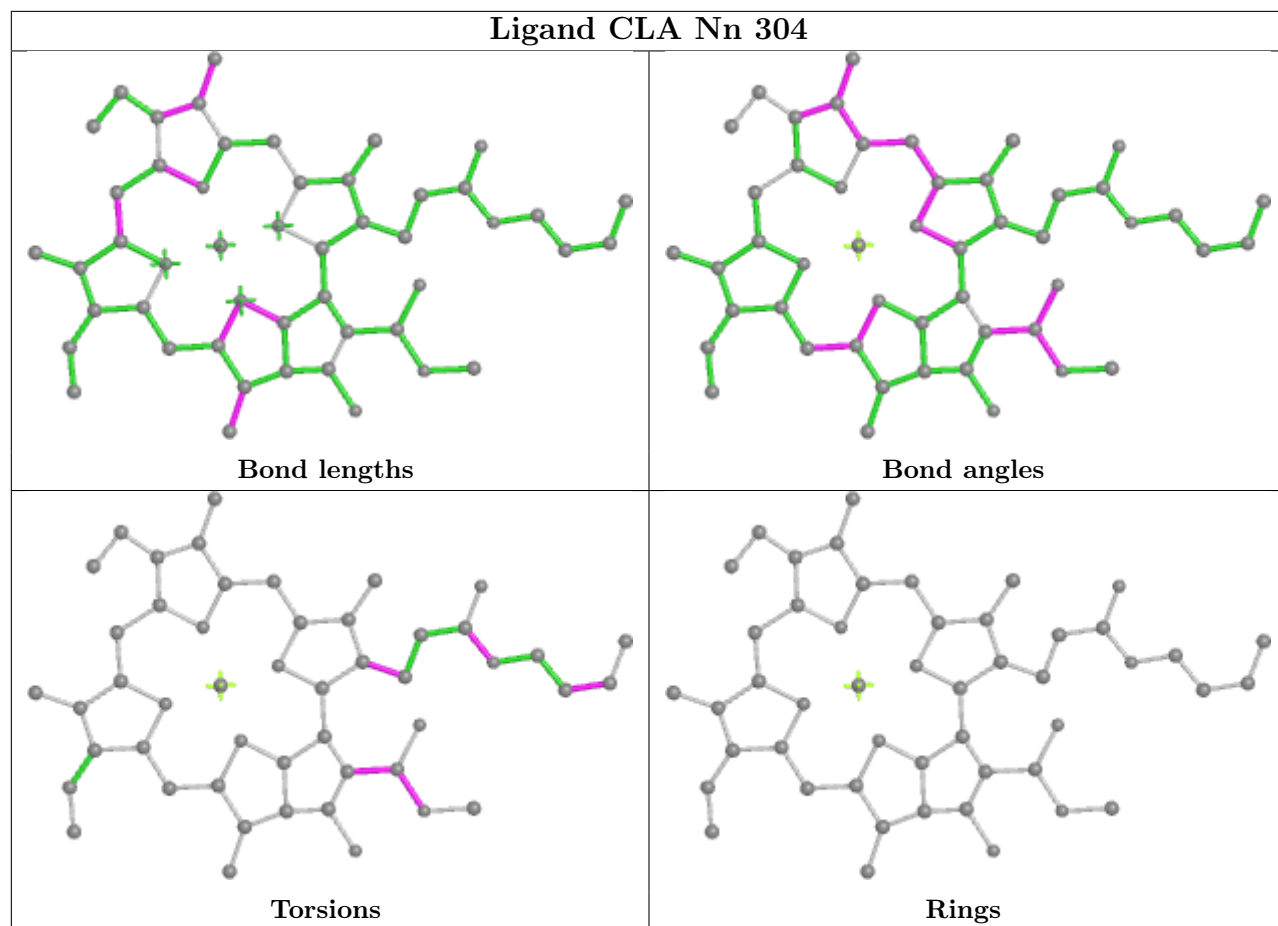




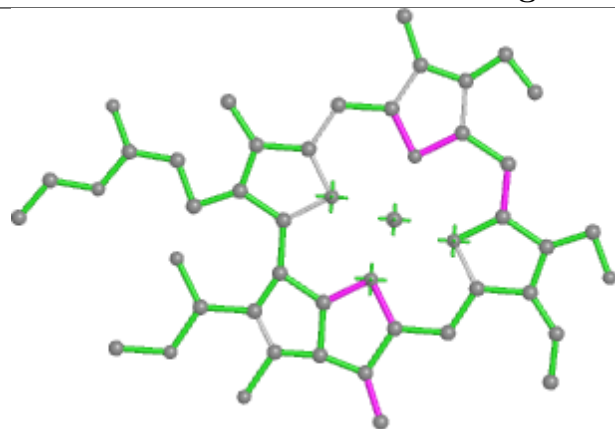


**Ligand CLA c 505****Ligand PL9 d 404**

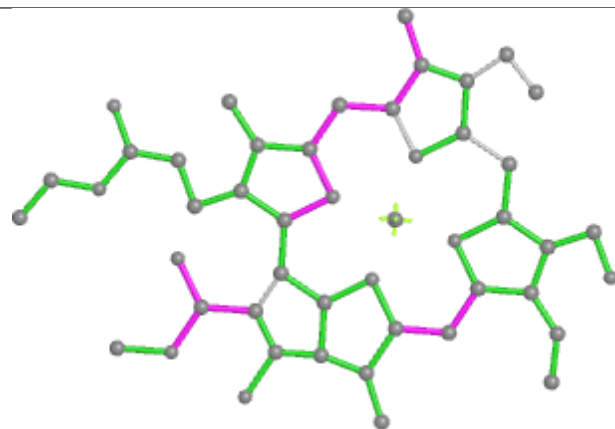




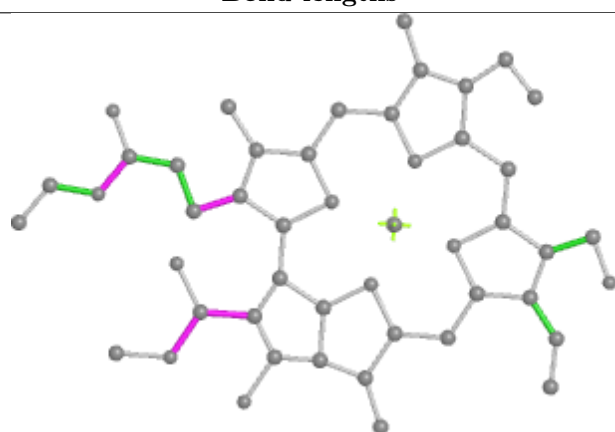
## Ligand CHL n 605



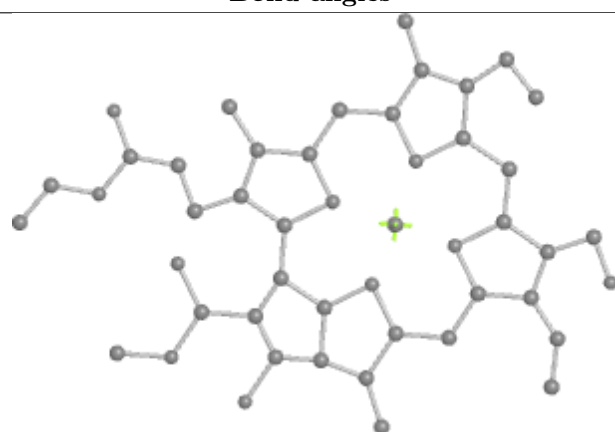
Bond lengths



Bond angles

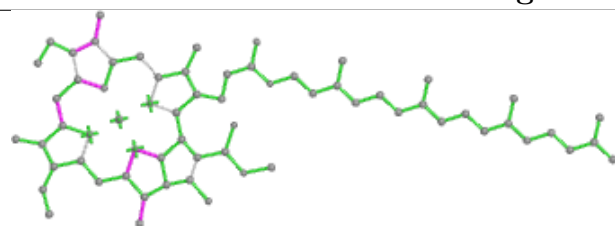


Torsions

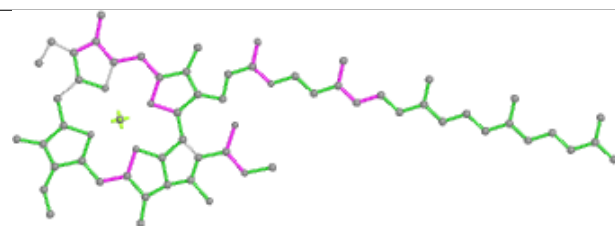


Rings

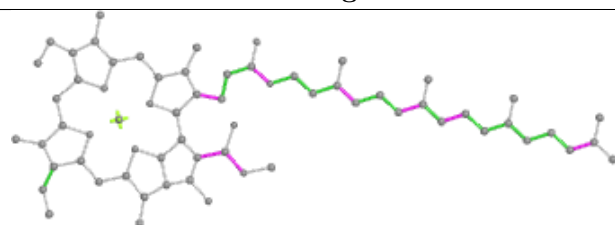
## Ligand CLA C 505



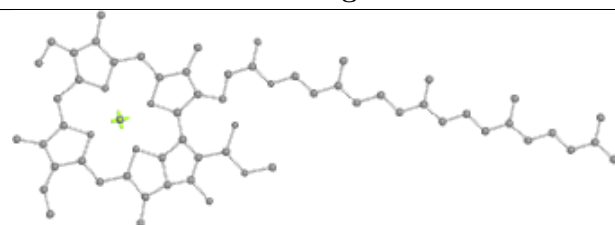
Bond lengths



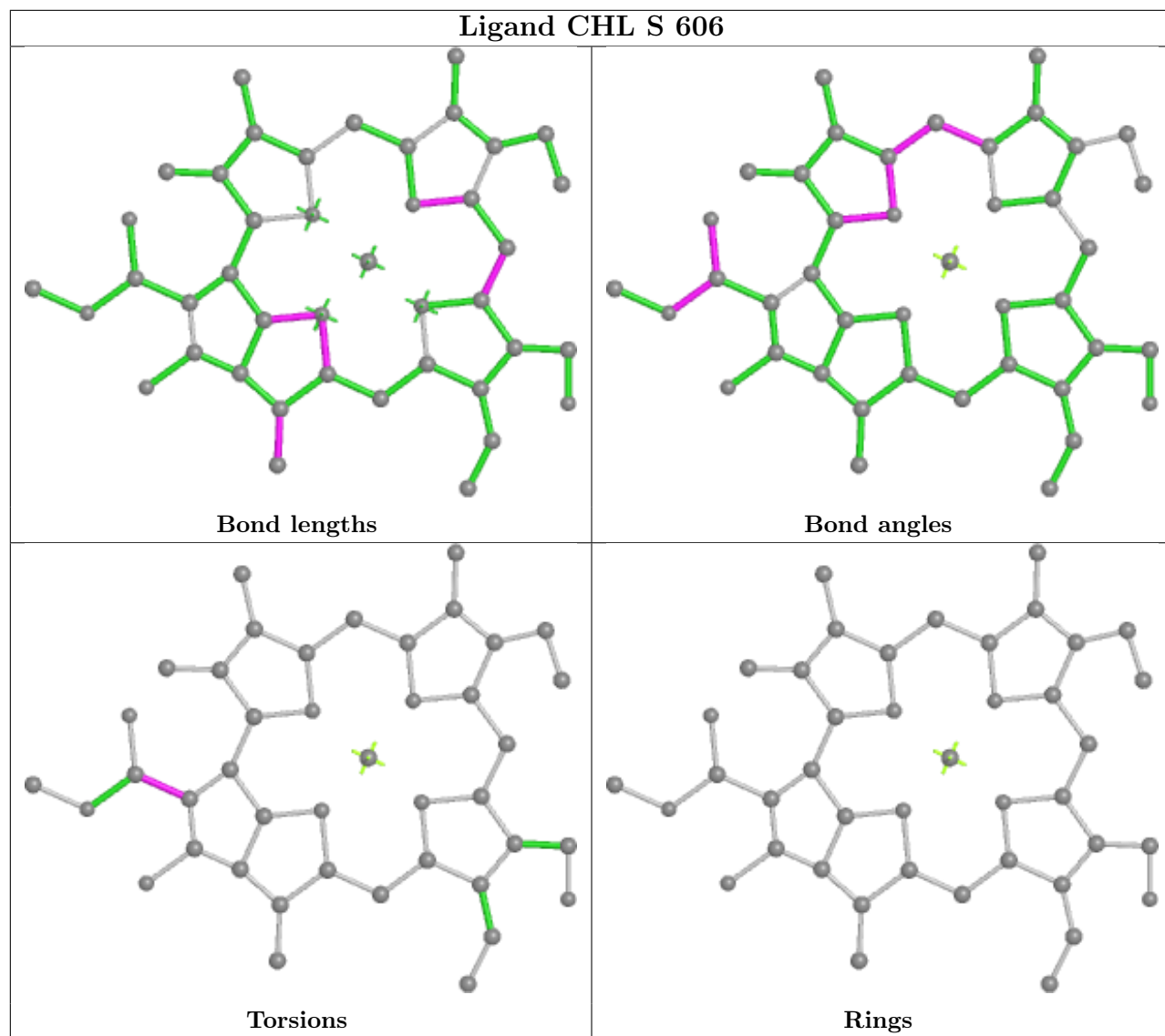
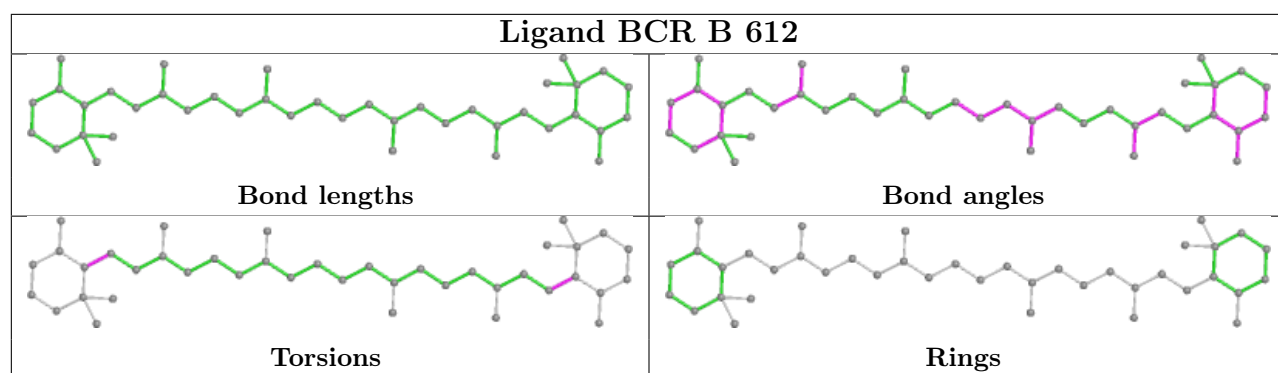
Bond angles



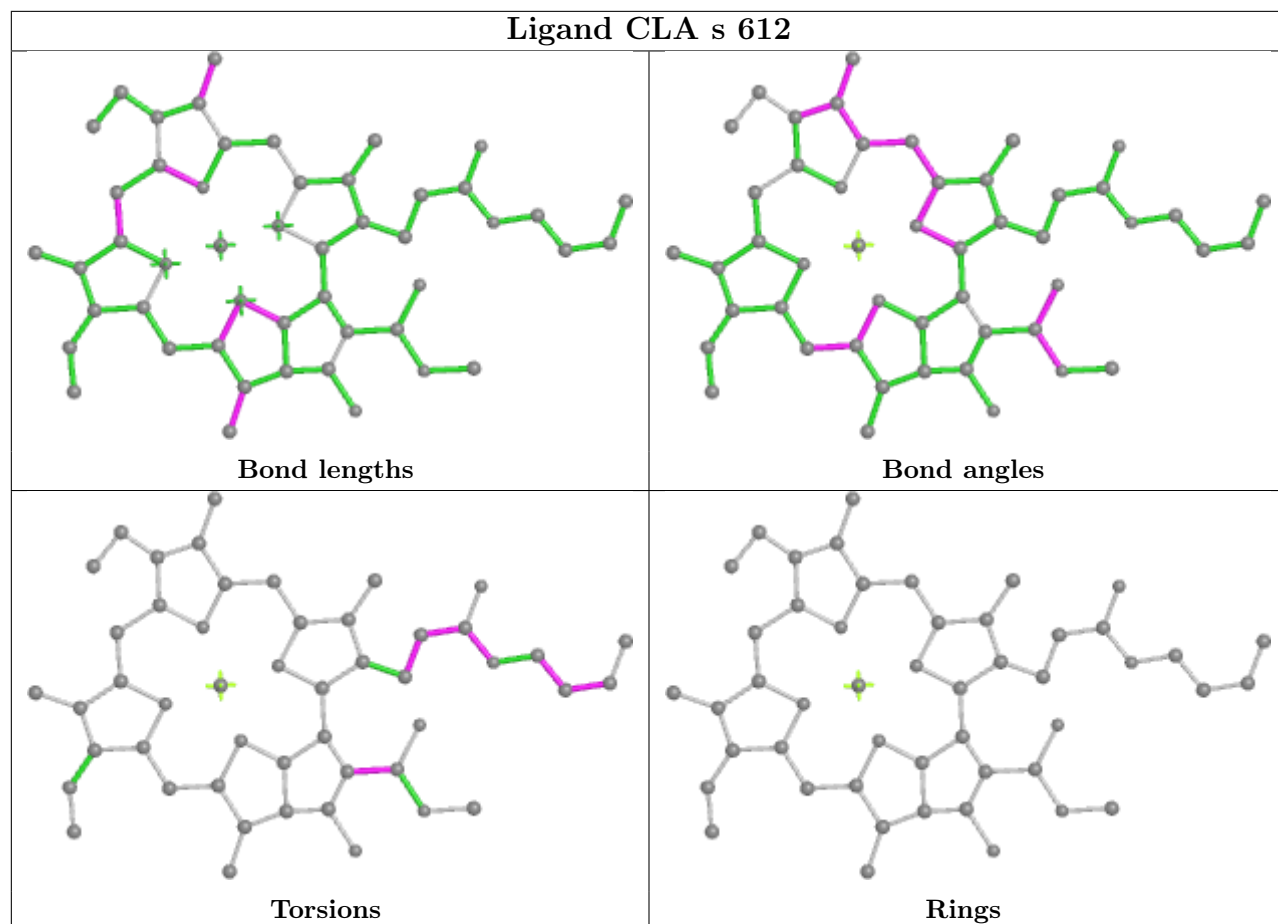
Torsions



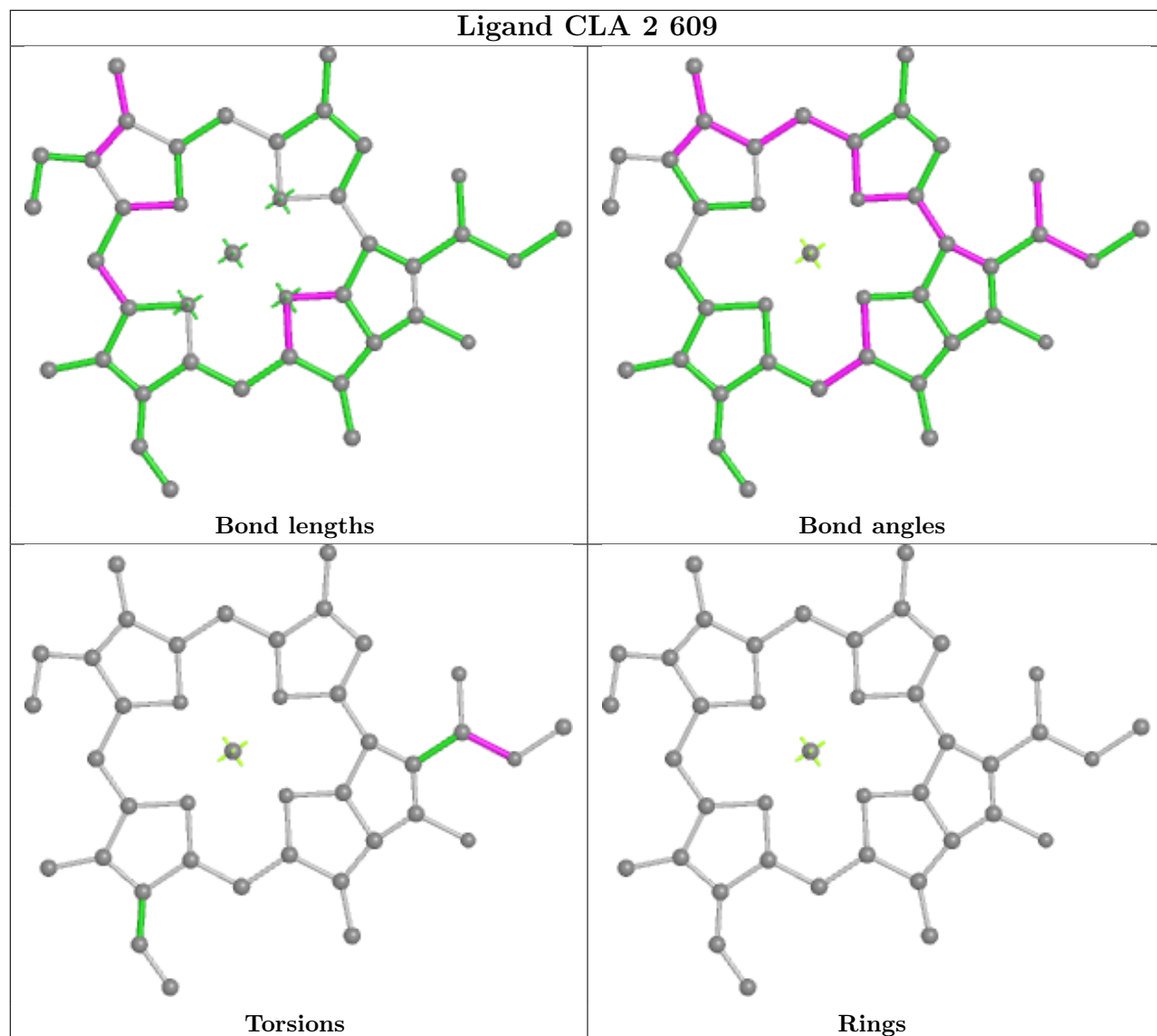
Rings



## Ligand CLA s 612

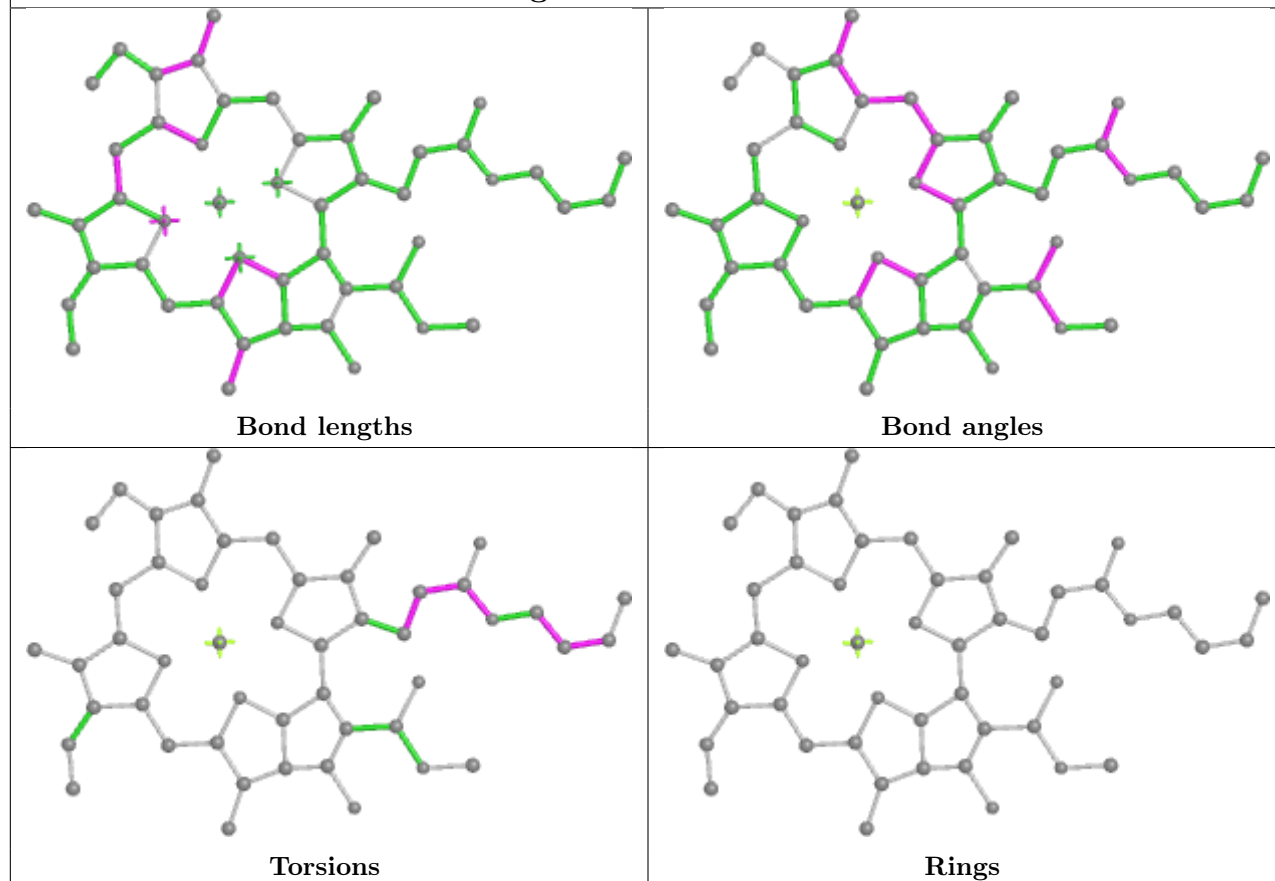


## Ligand CLA 2 609

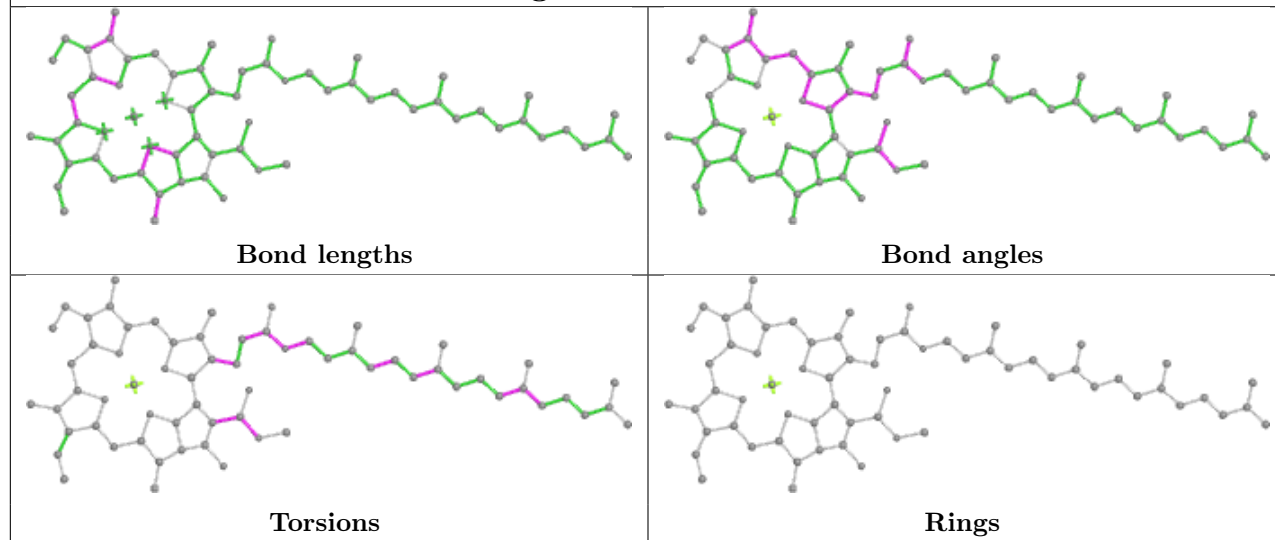


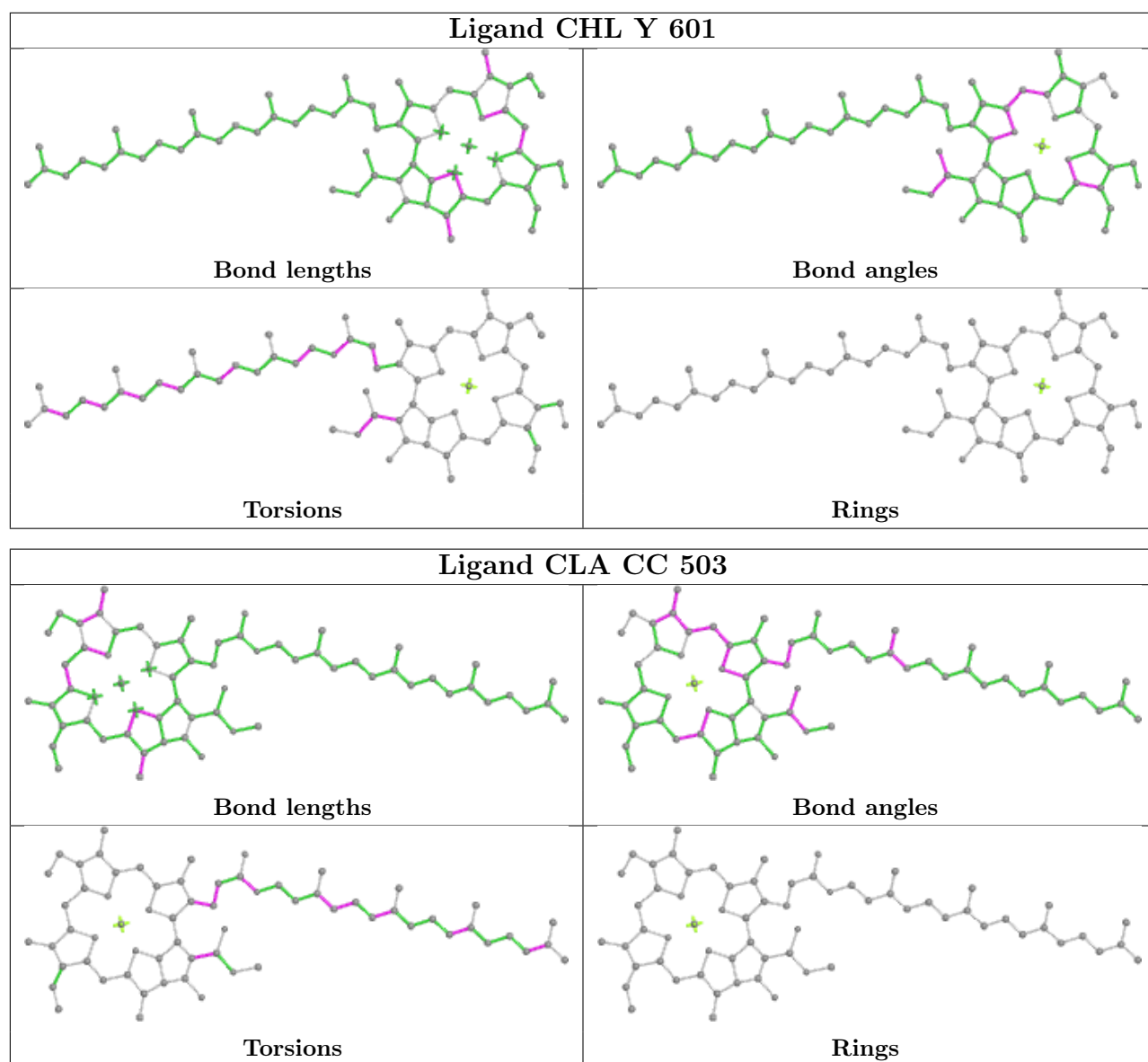


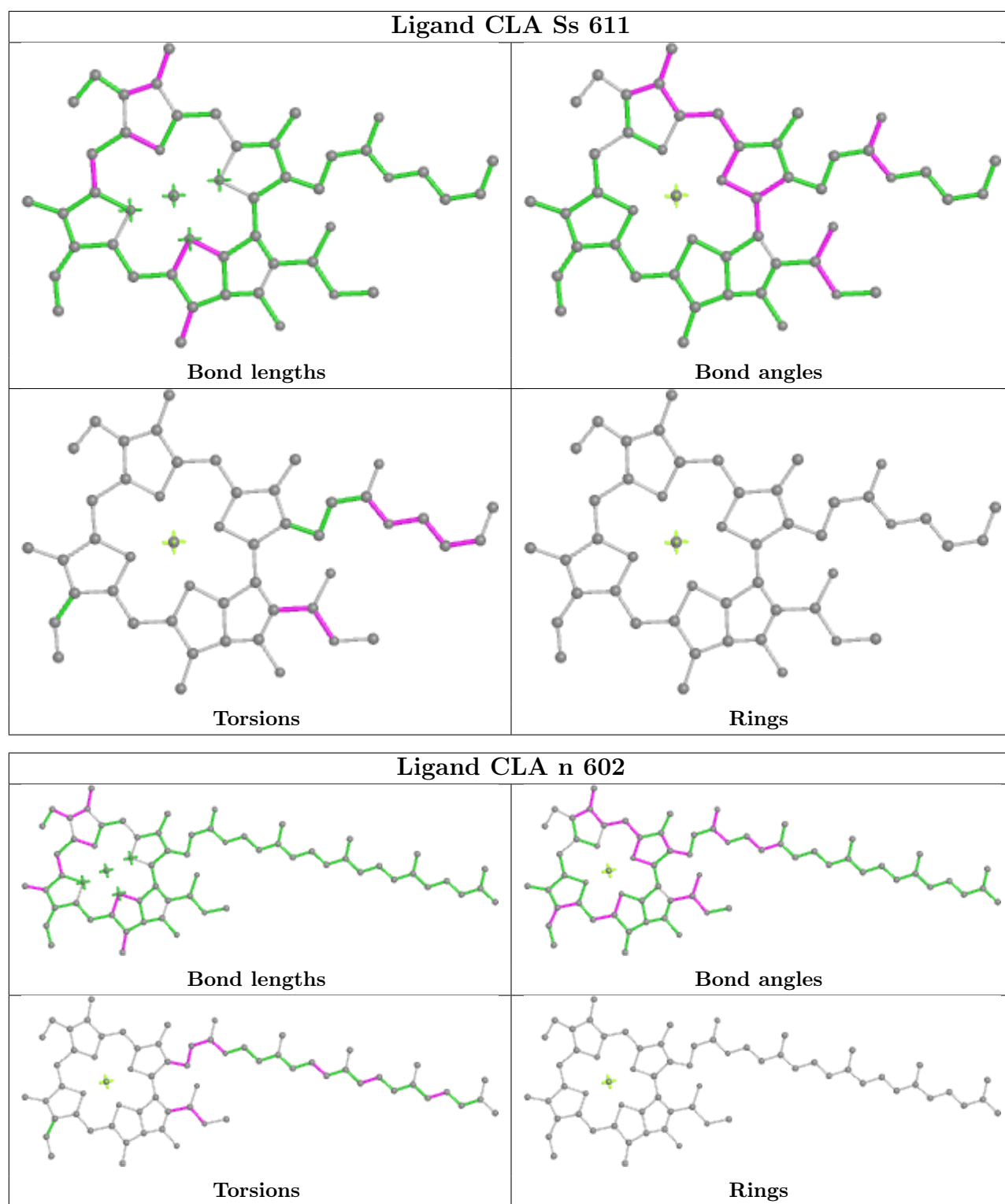
## Ligand CLA G 610



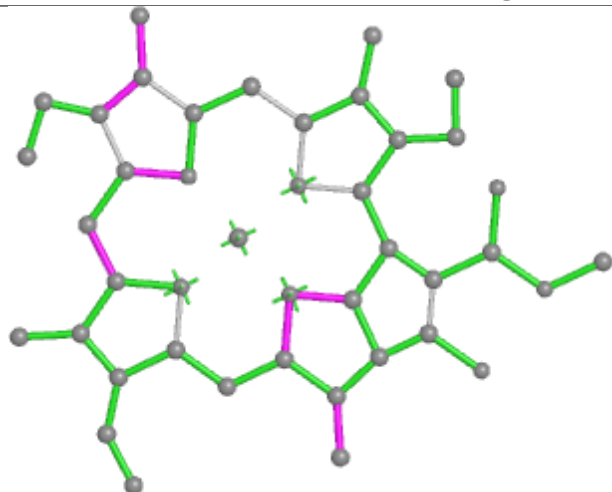
## Ligand CLA Y 610



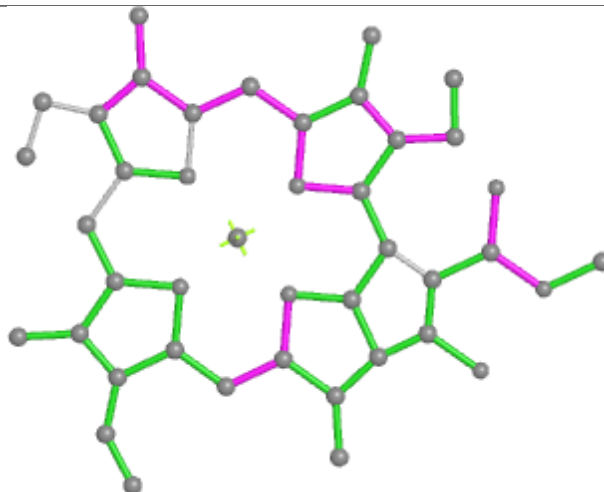




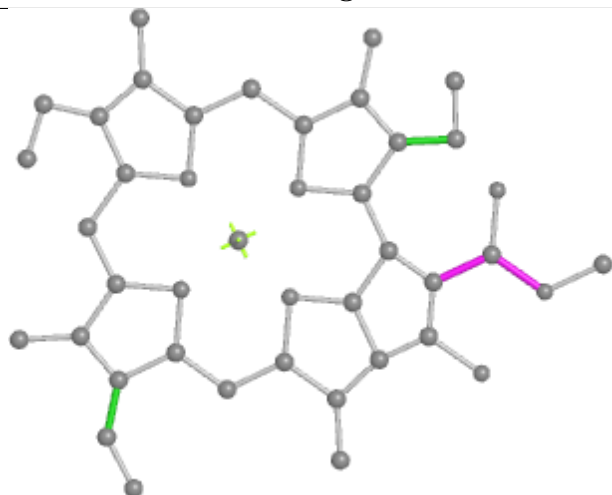
## Ligand CLA NN 603



Bond lengths



Bond angles

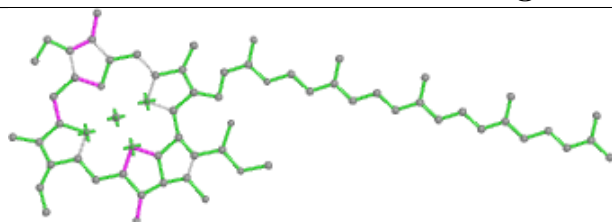


Torsions

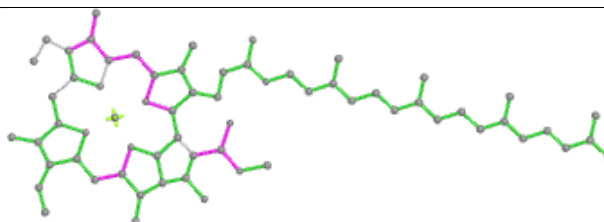


Rings

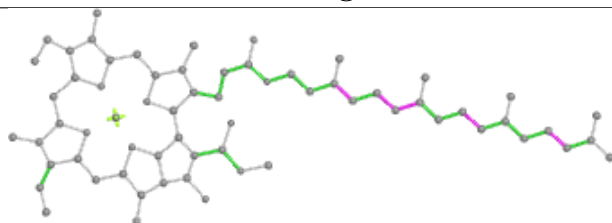
## Ligand CLA b 611



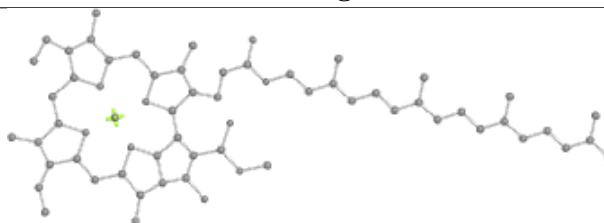
Bond lengths



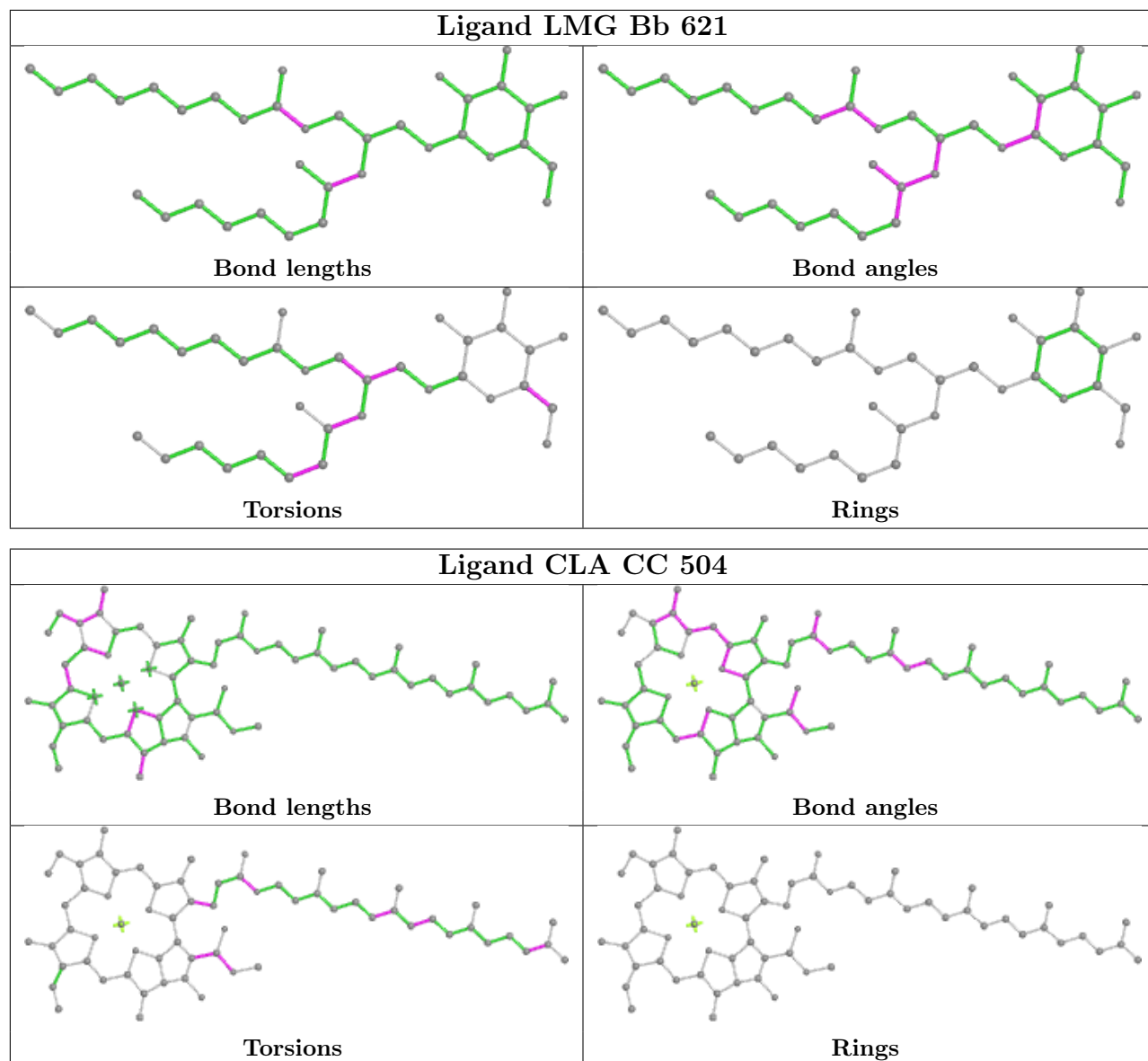
Bond angles

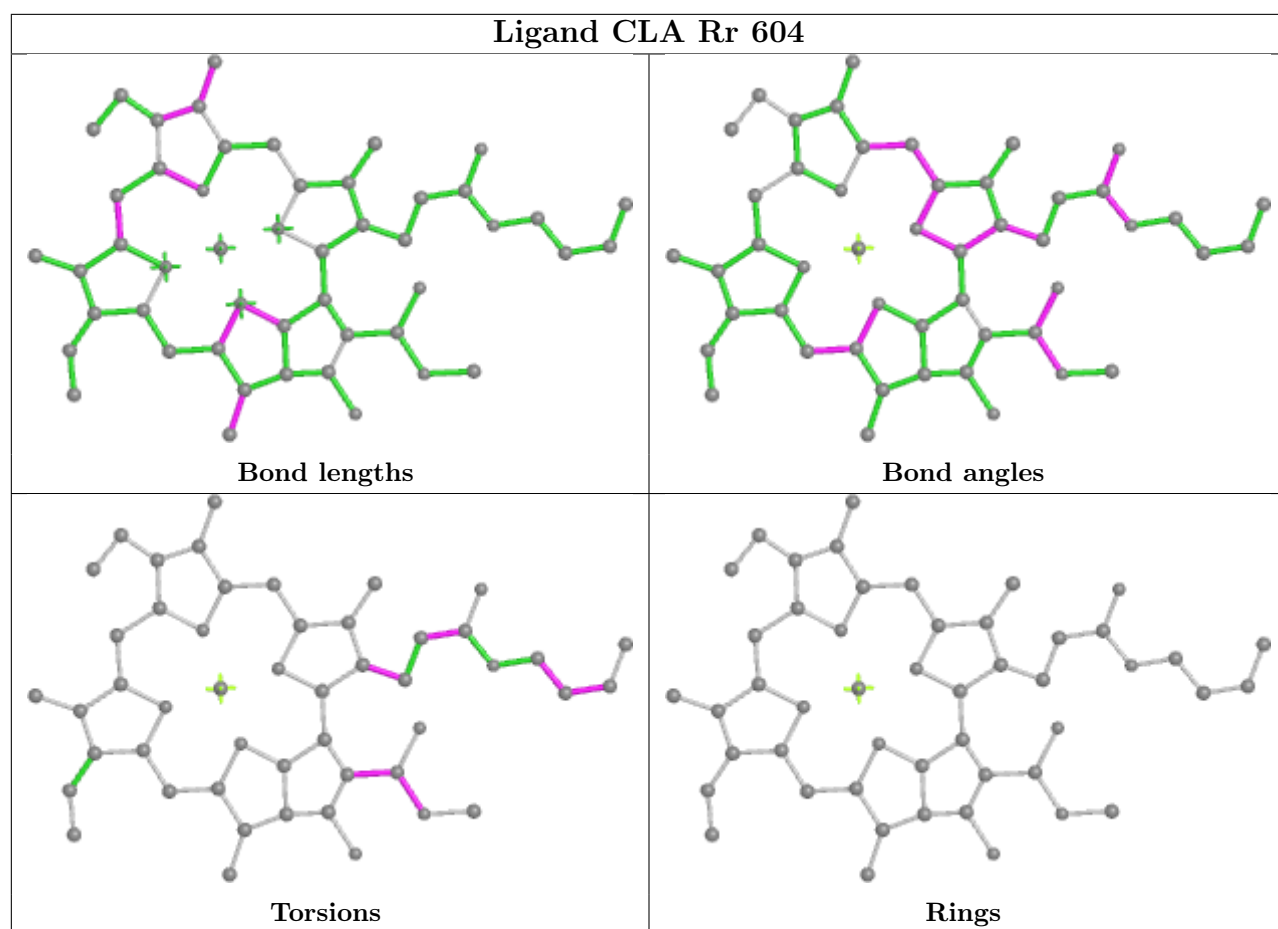


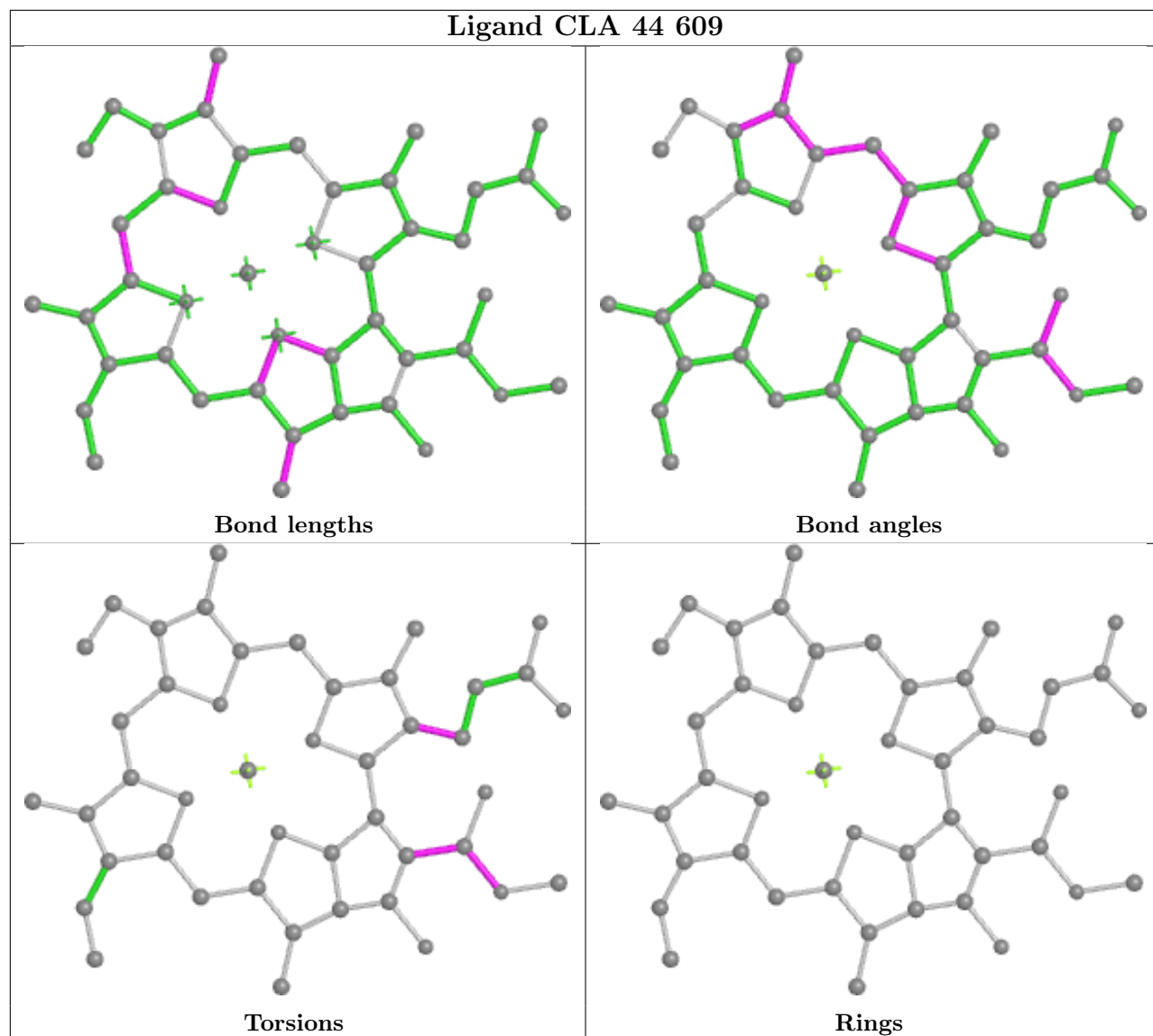
Torsions

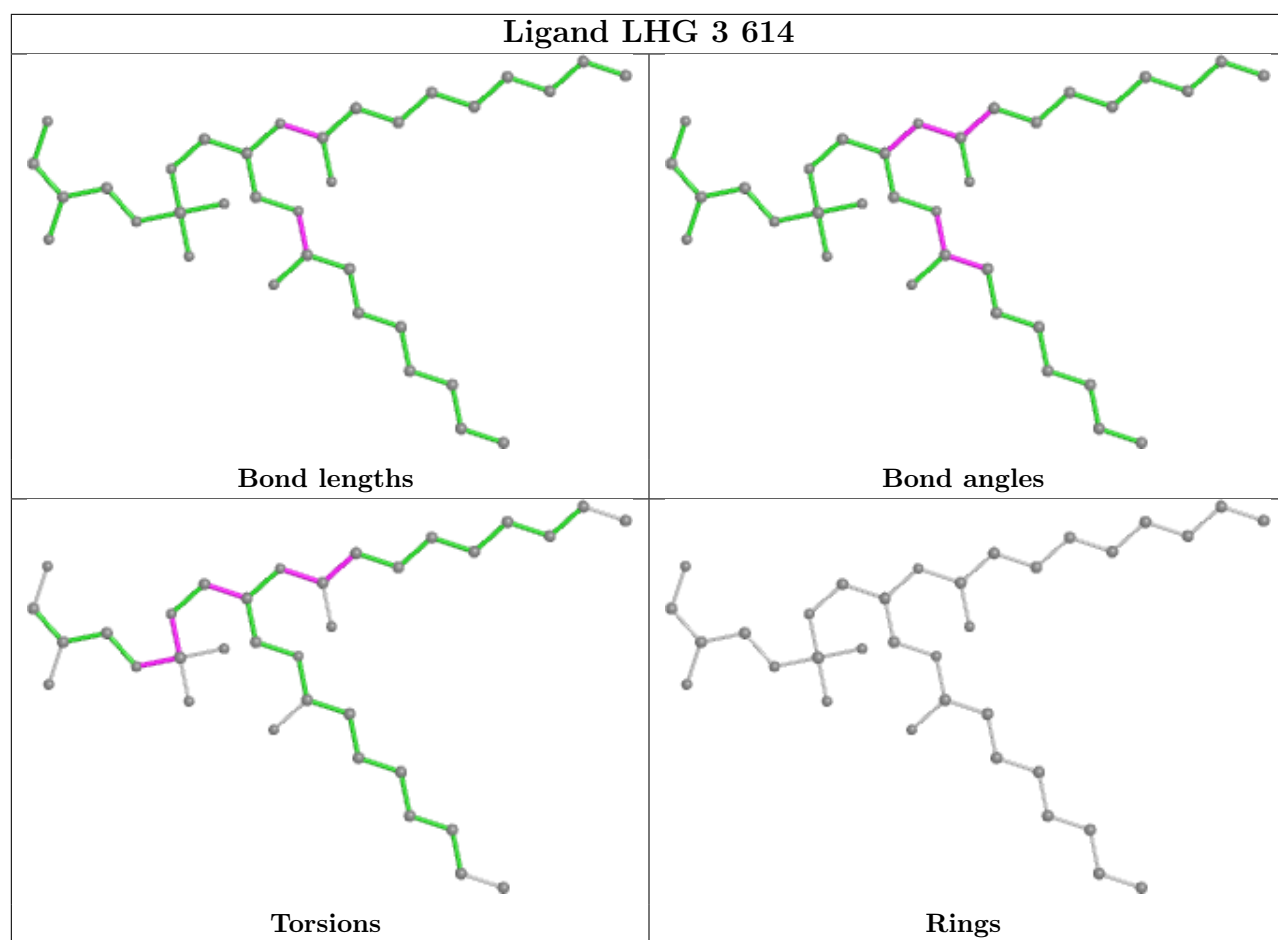


Rings

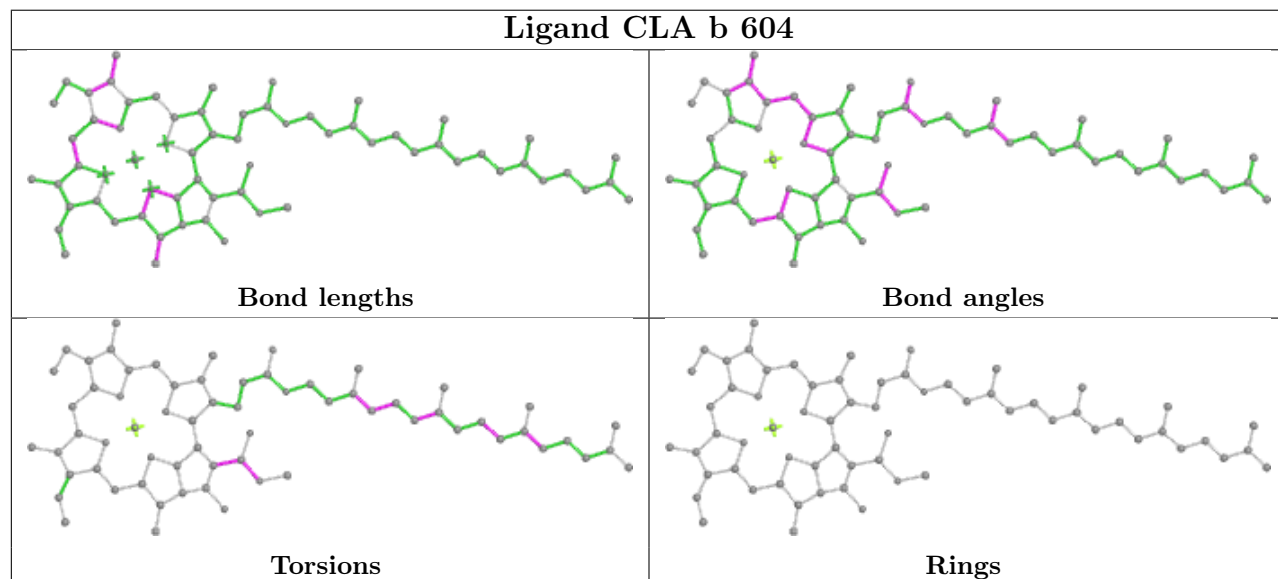
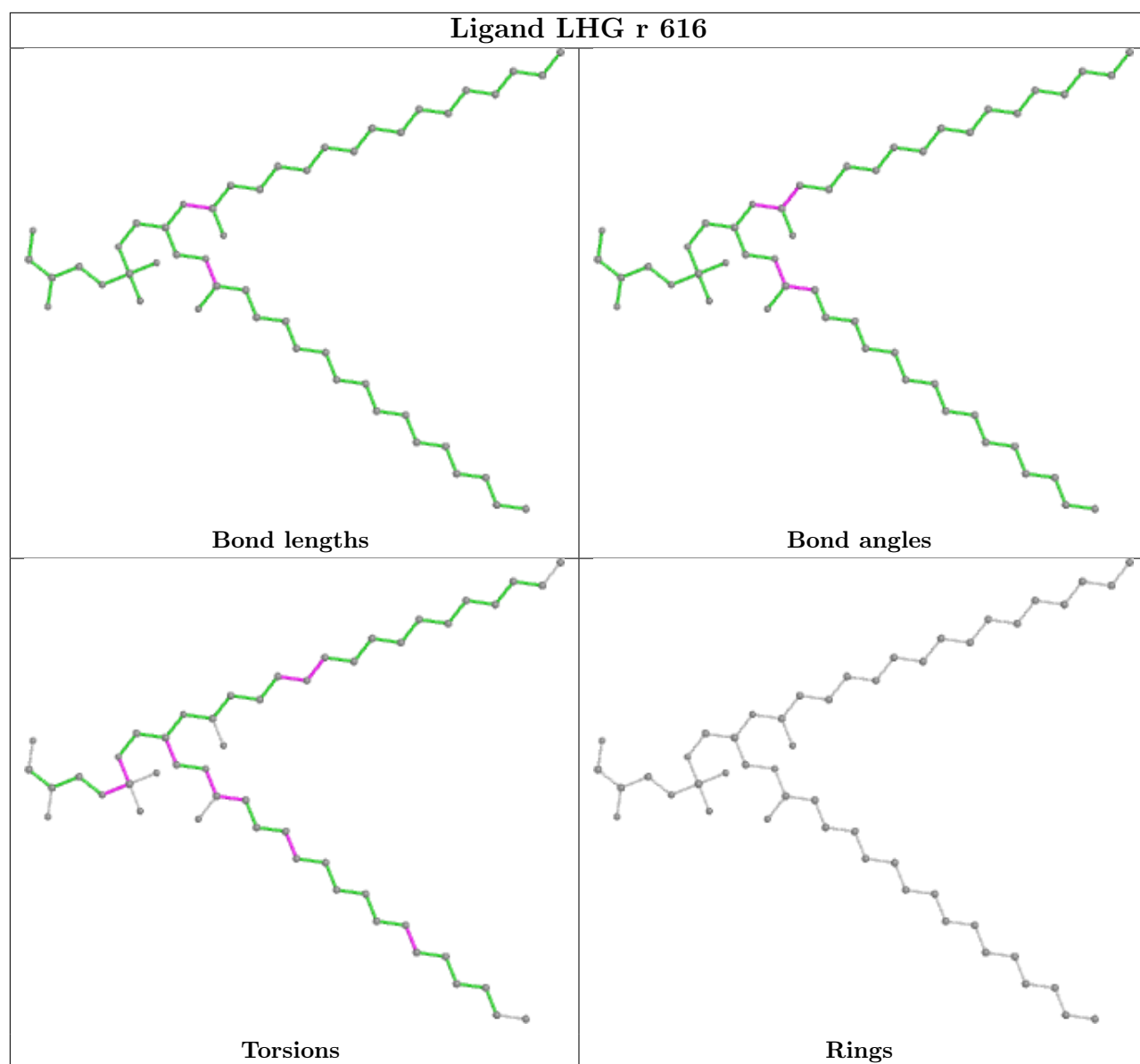




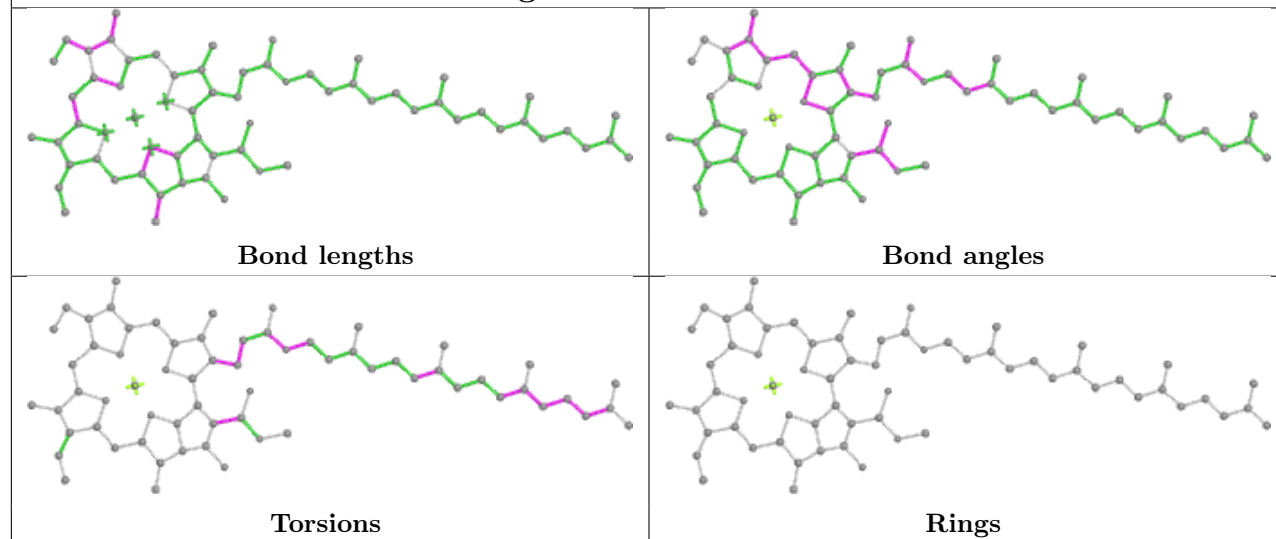




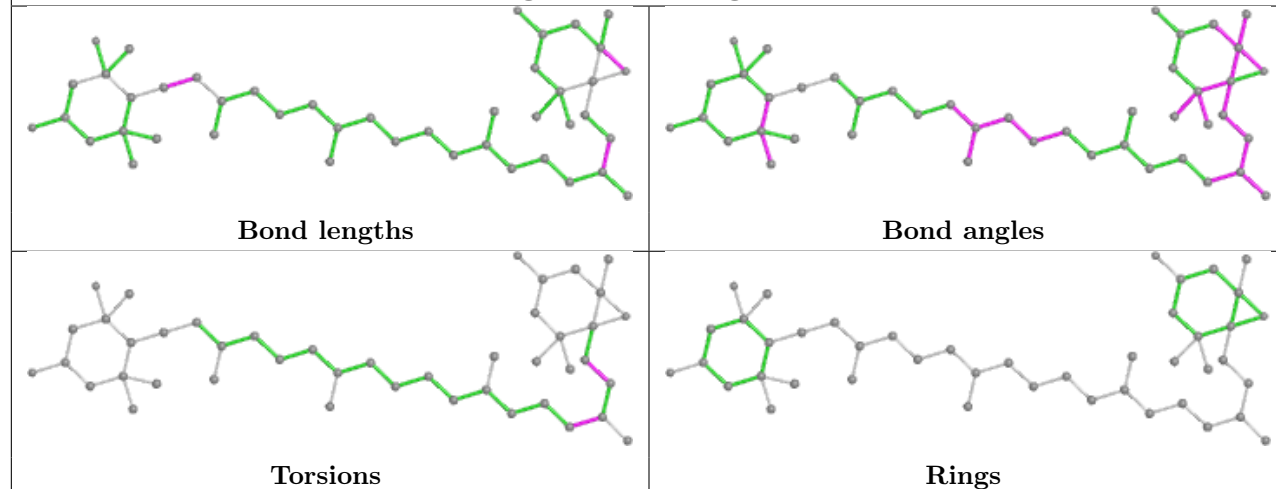




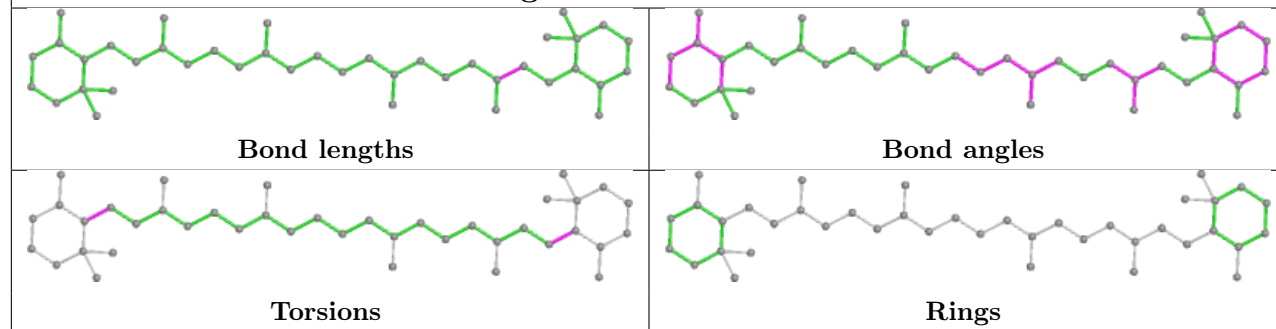
## Ligand CLA RR 302



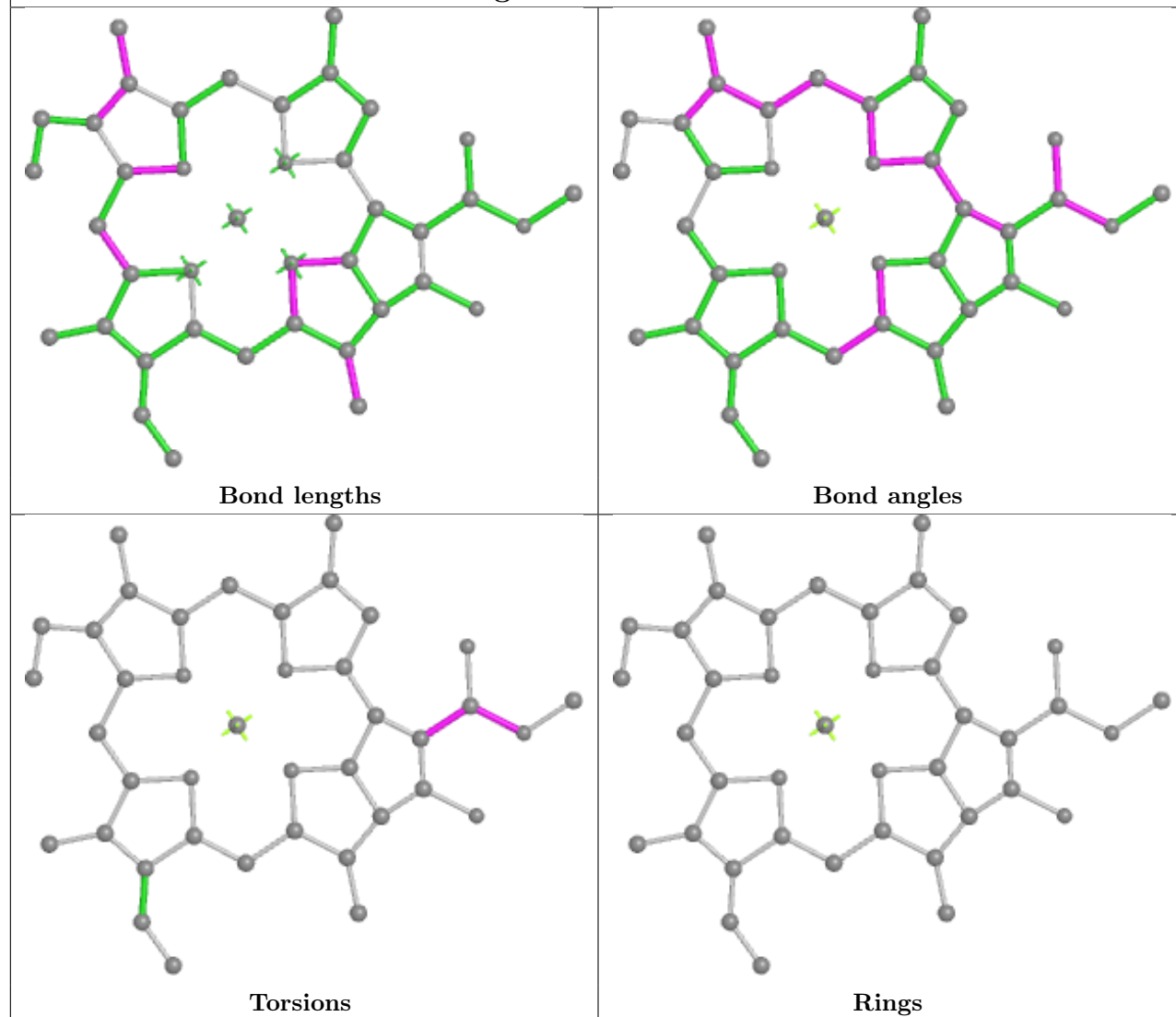
## Ligand NEX Gg 318

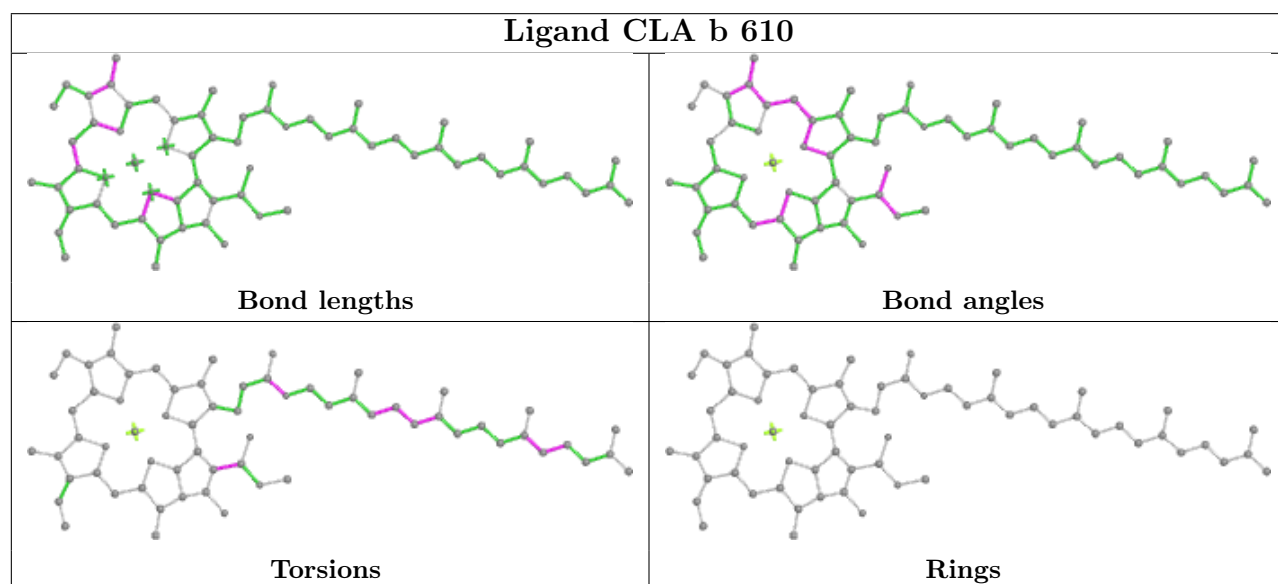
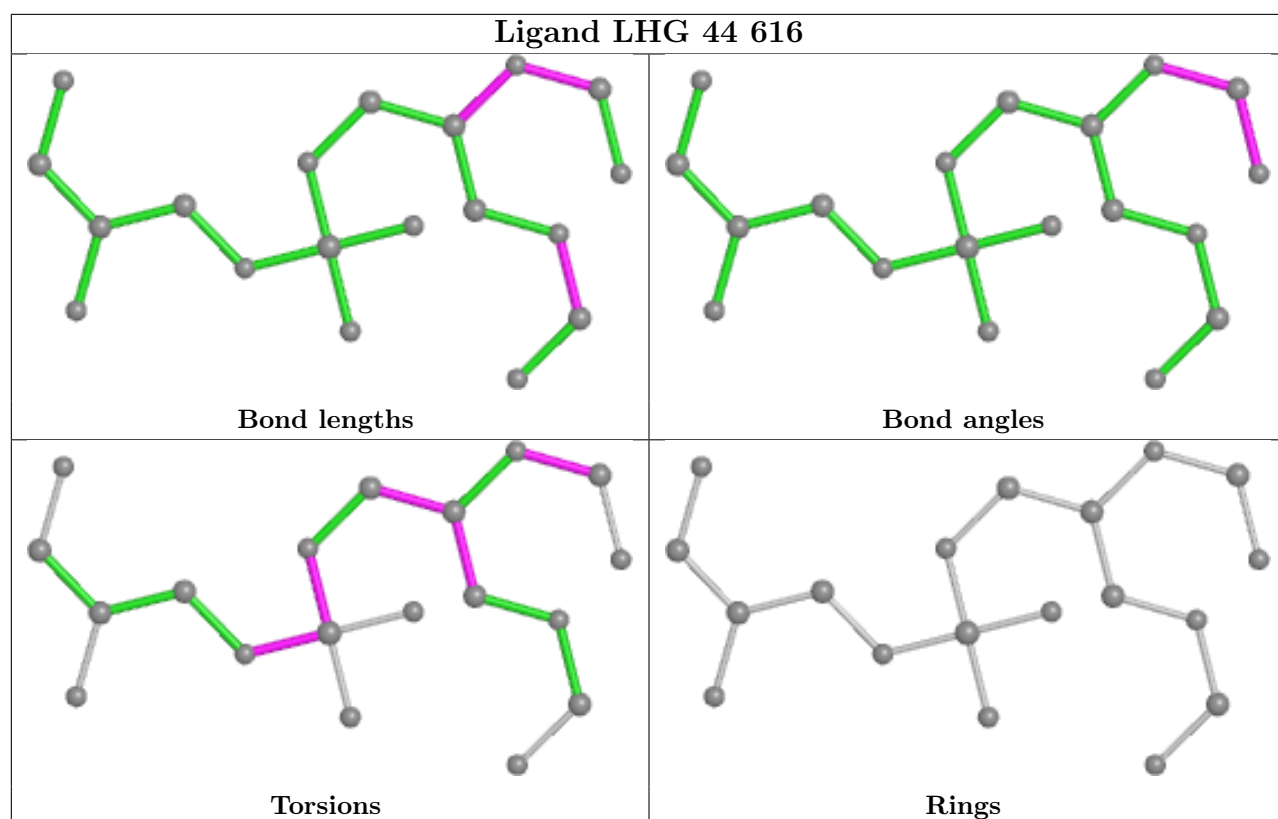


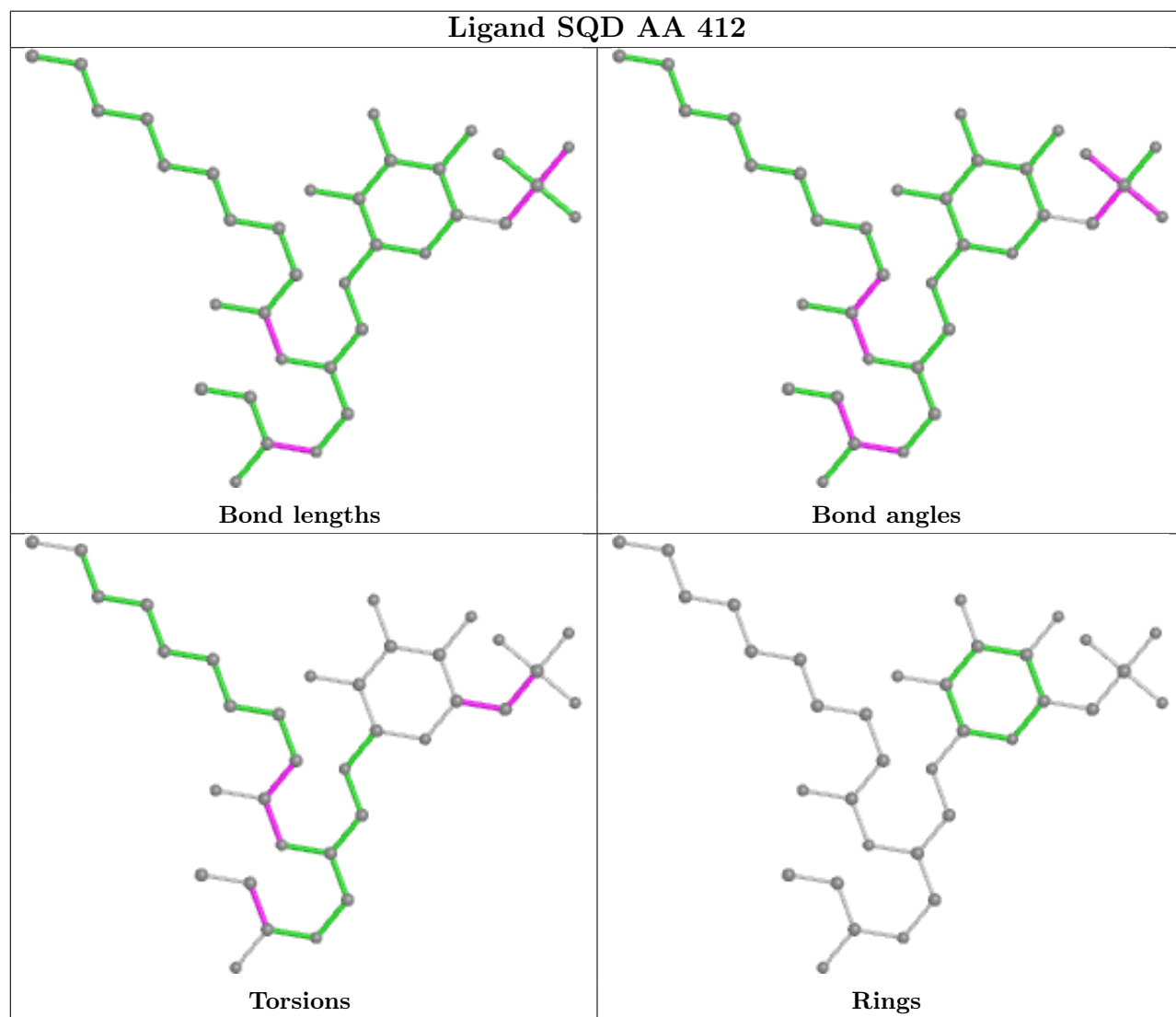
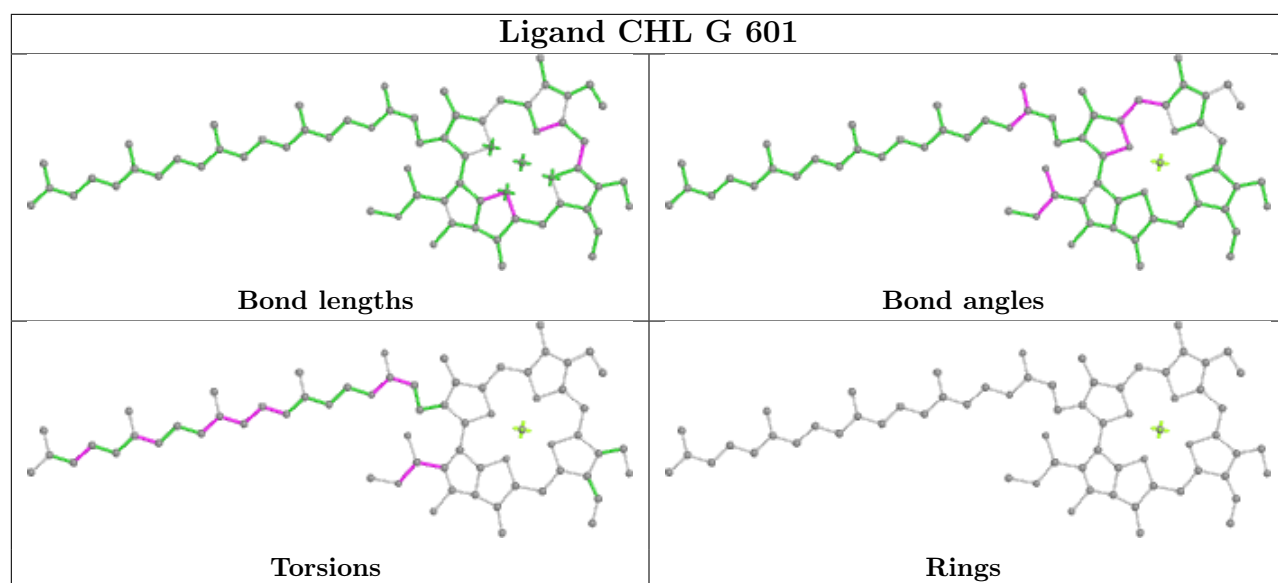
## Ligand BCR Bb 618



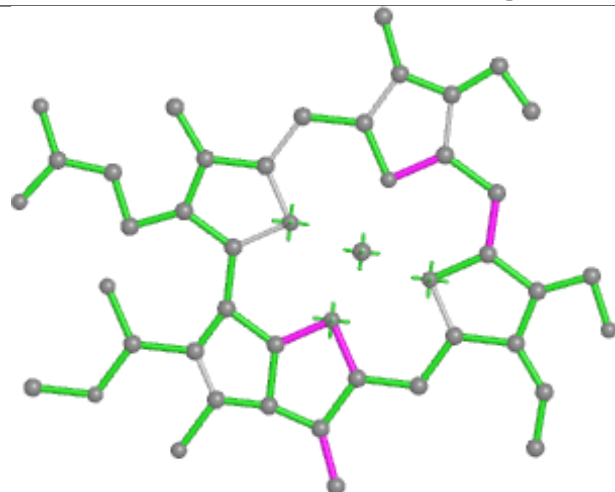
## Ligand CLA 3 612



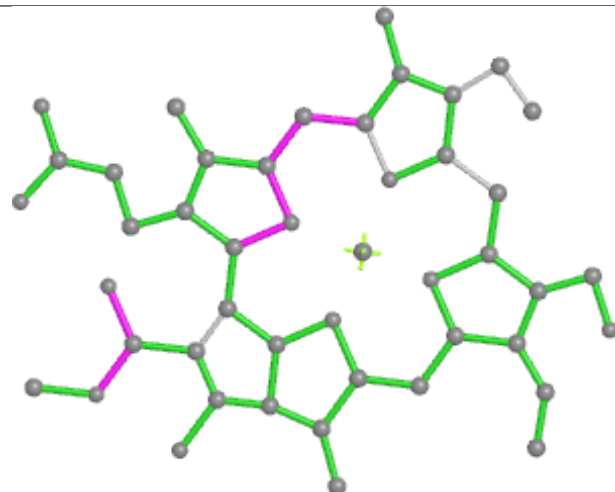




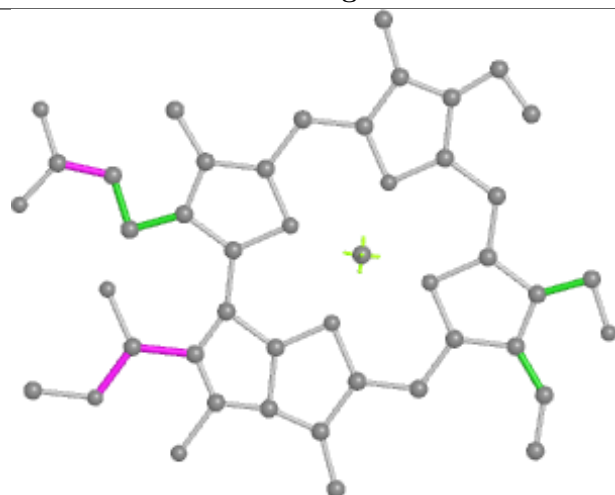
## Ligand CHL GG 607



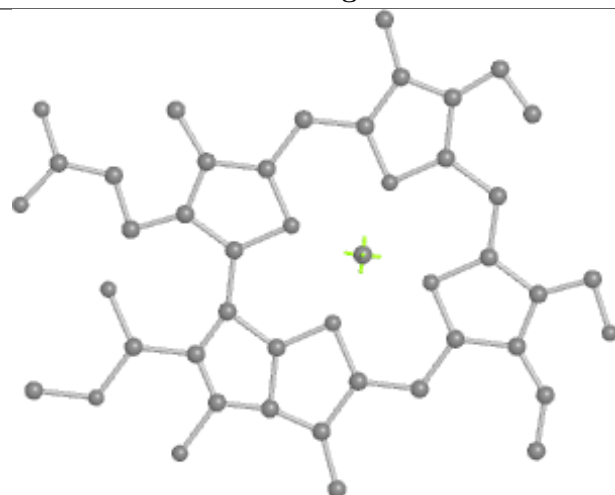
Bond lengths



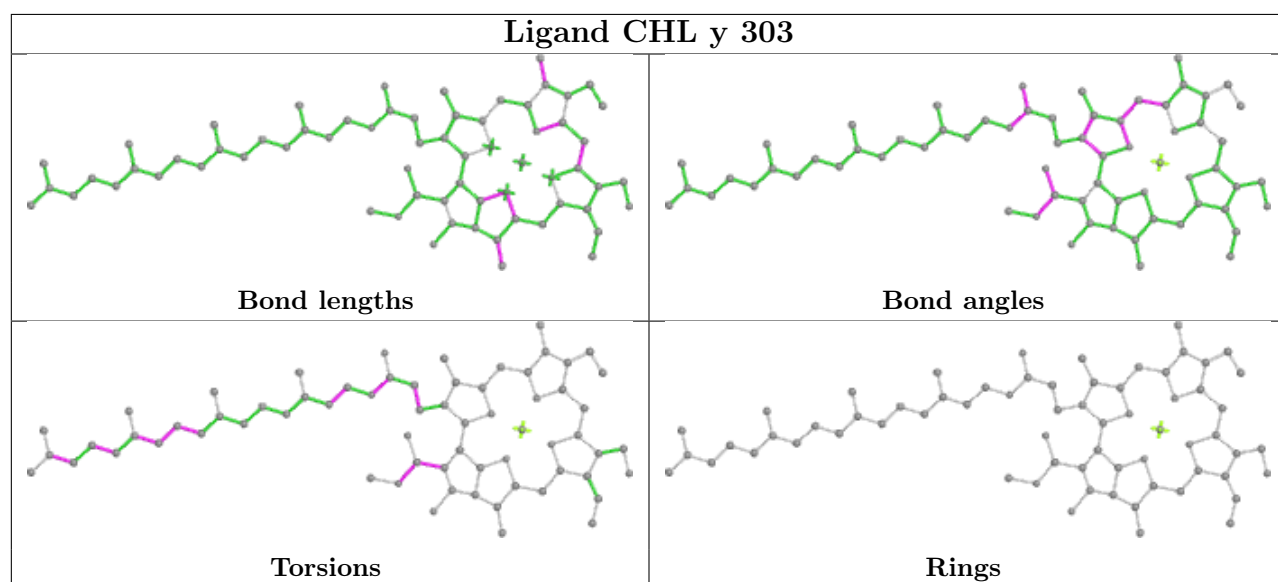
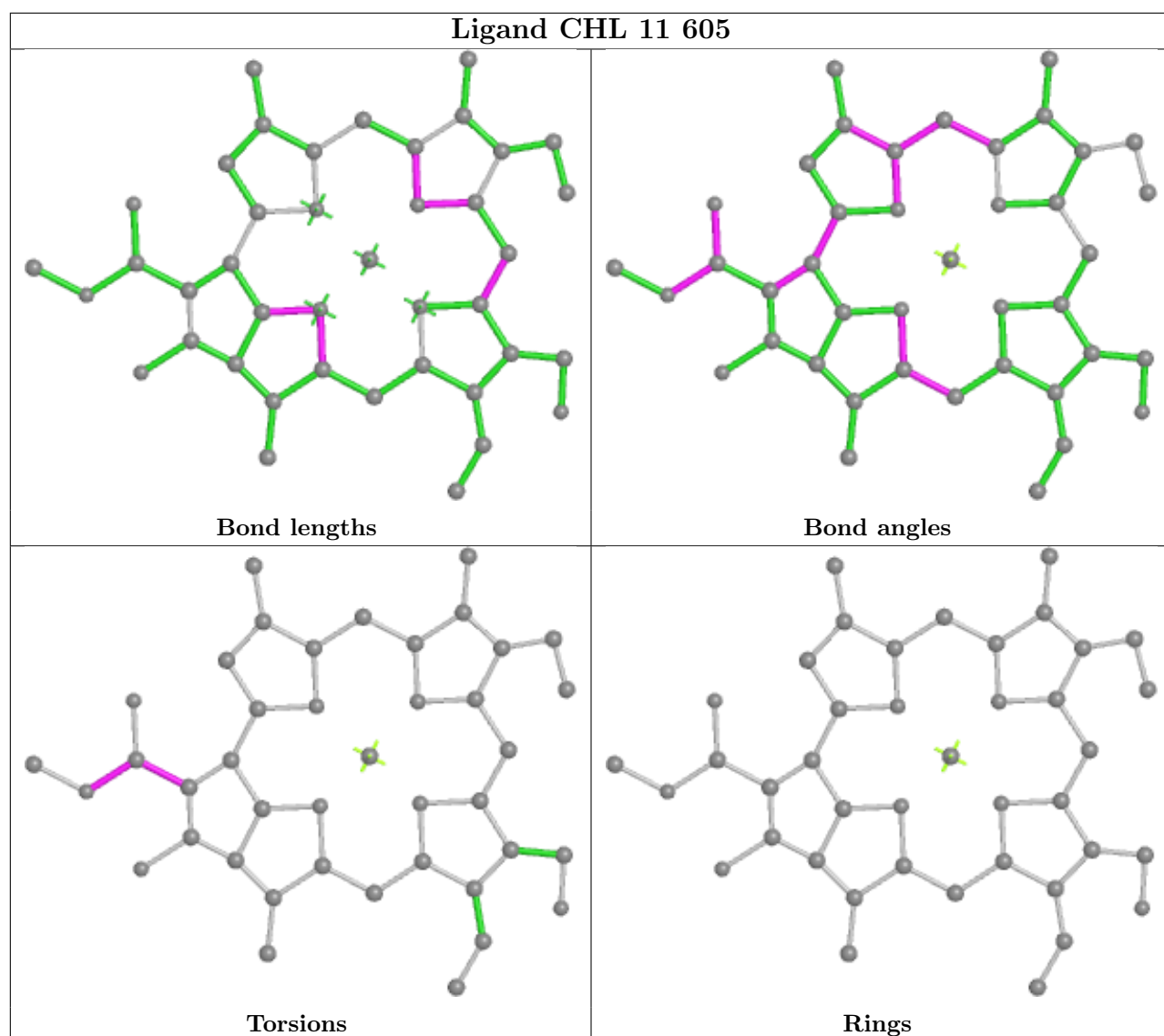
Bond angles



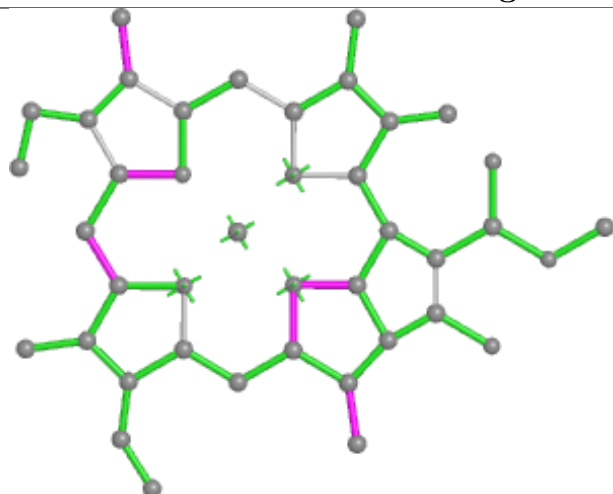
Torsions



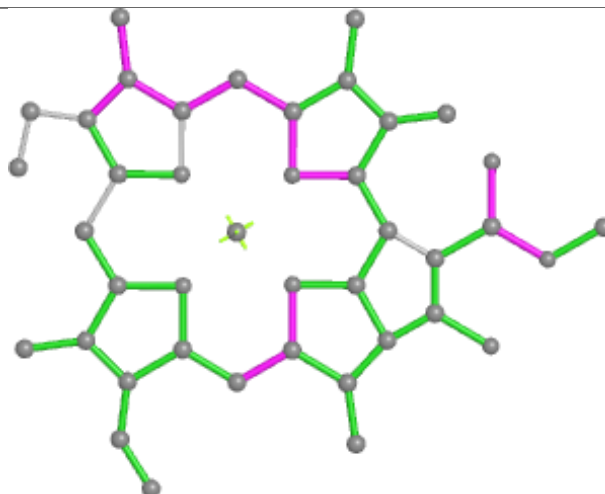
Rings



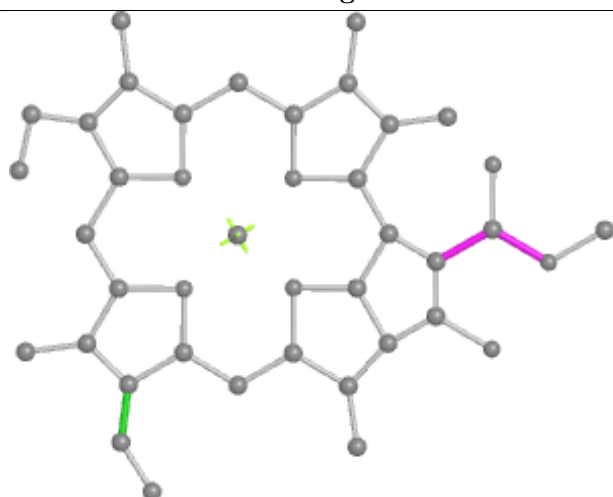
## Ligand CLA GG 614



Bond lengths



Bond angles

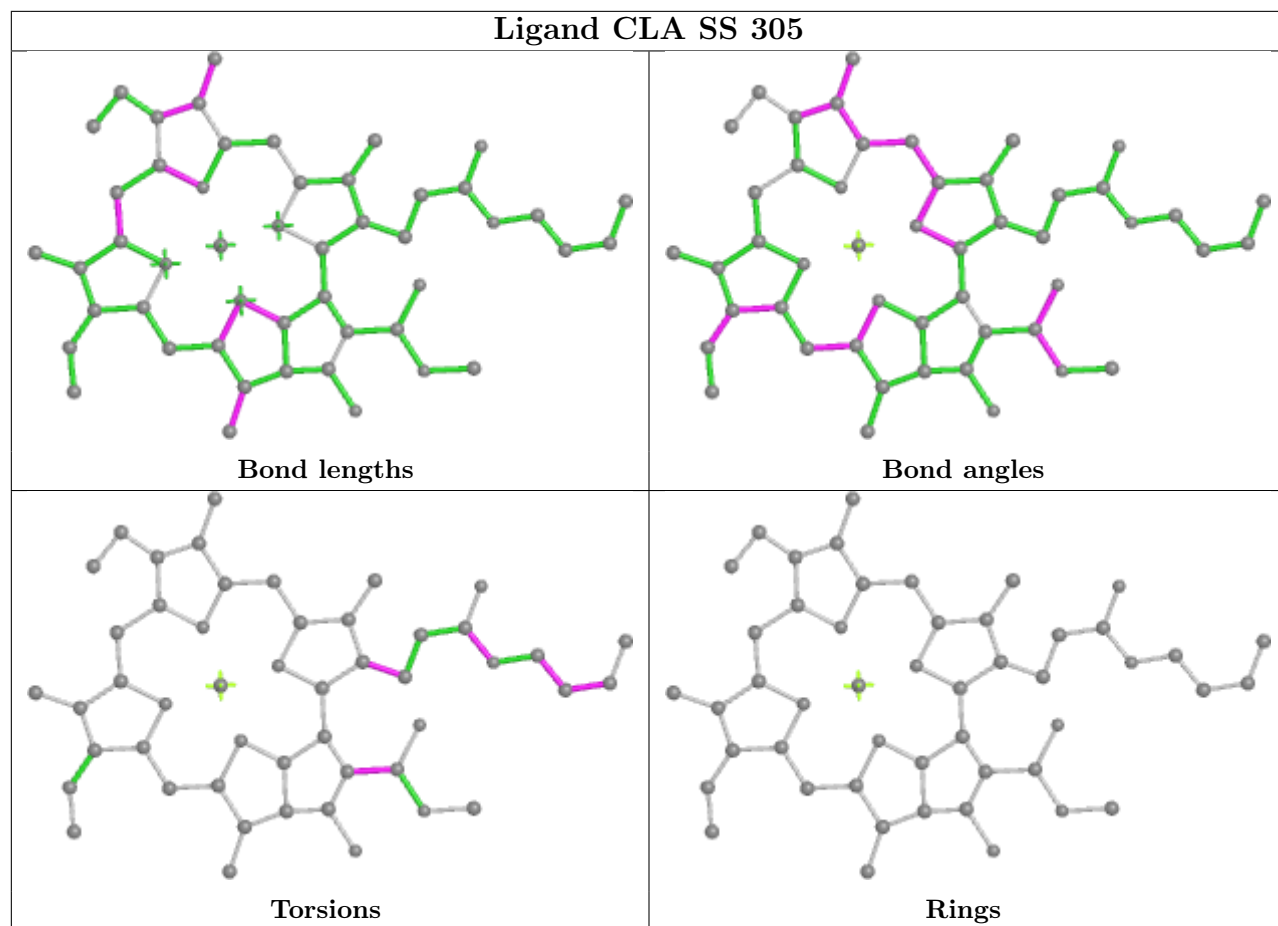


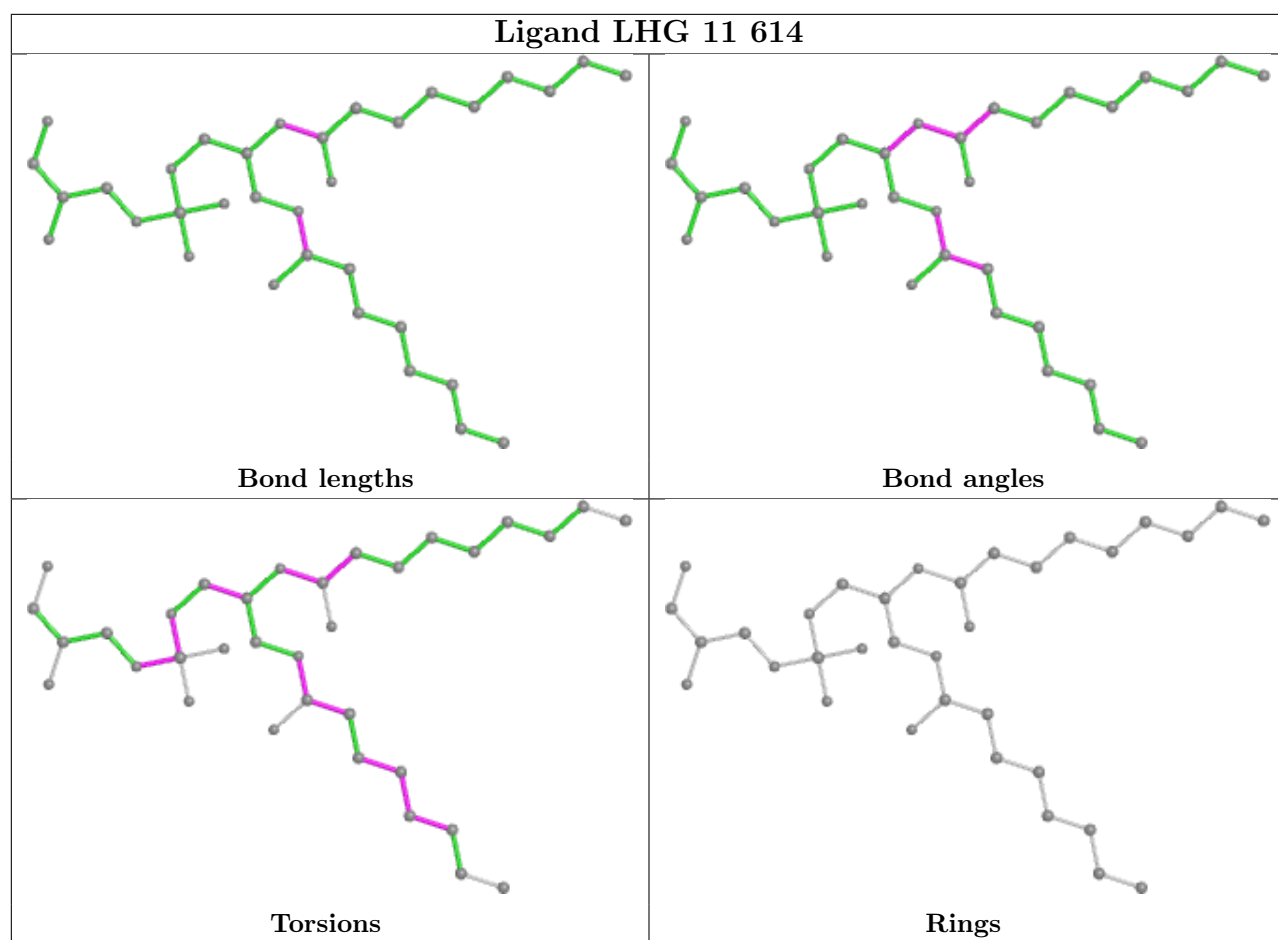
Torsions

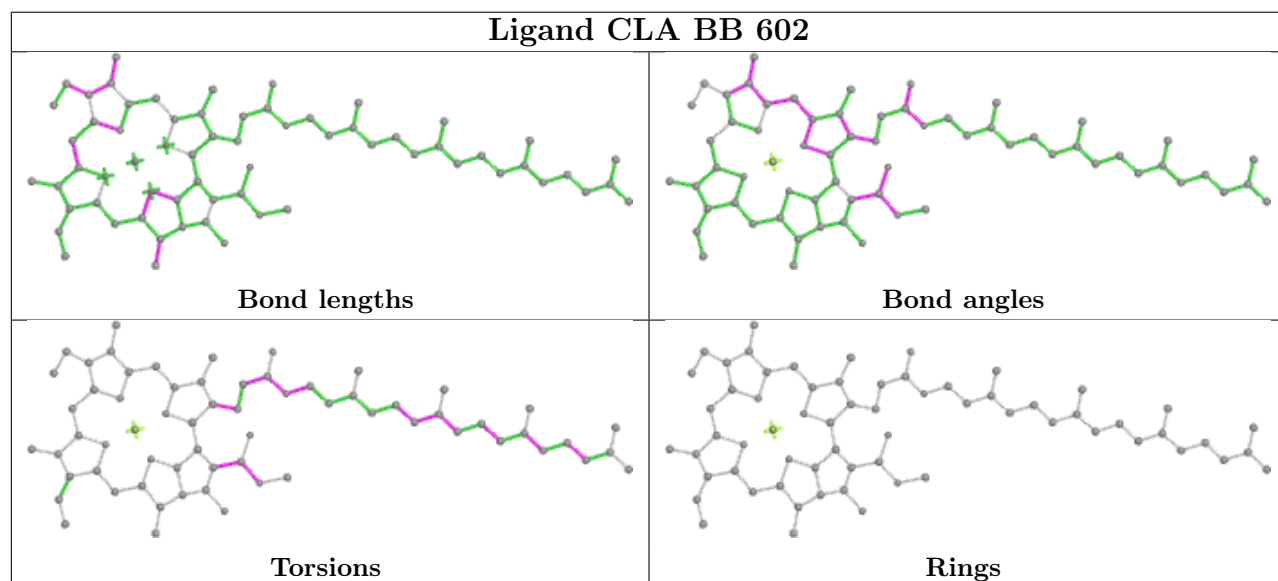
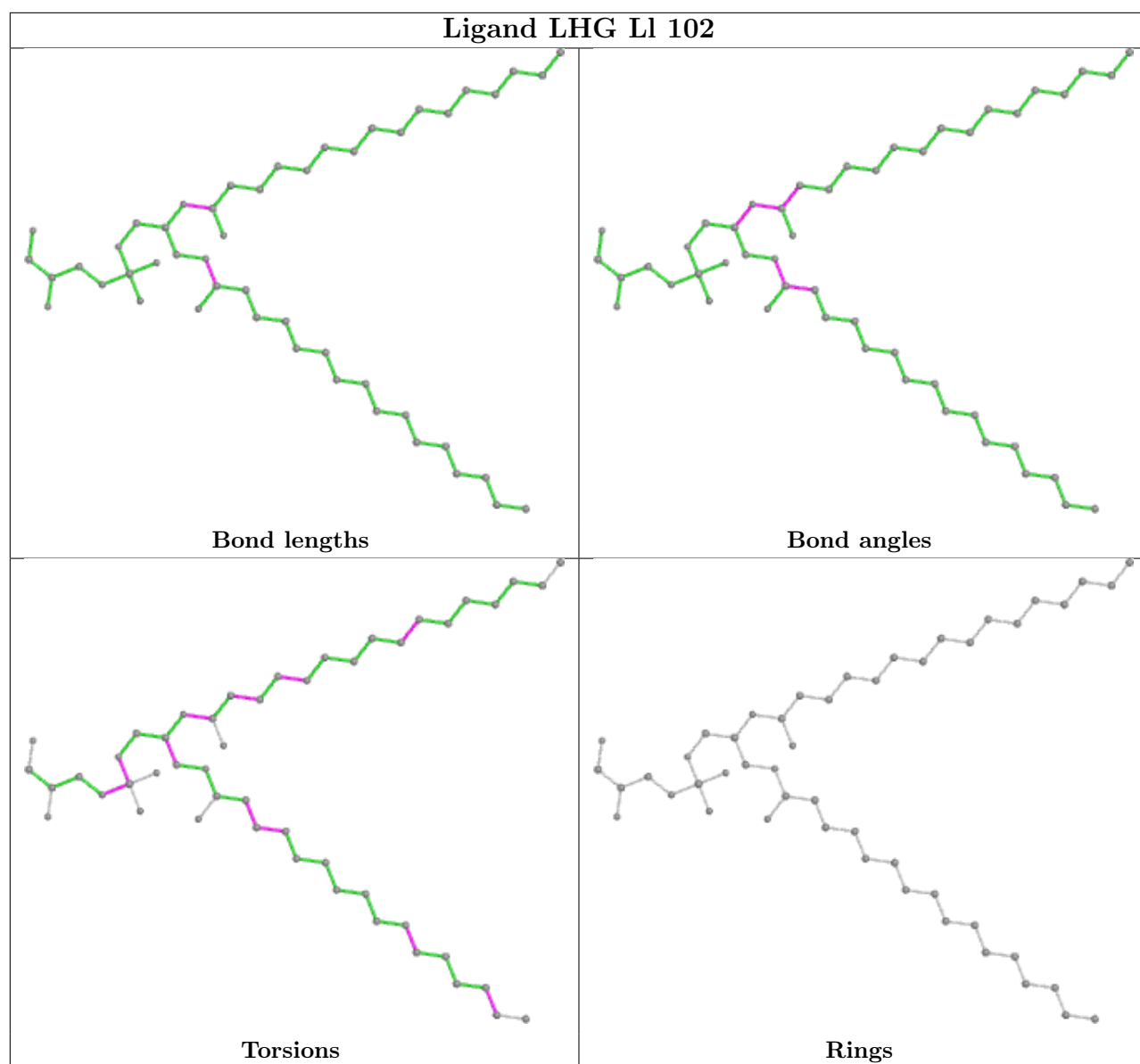


Rings

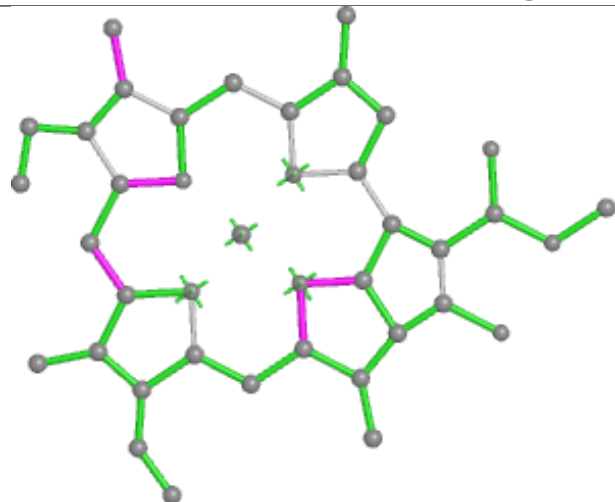




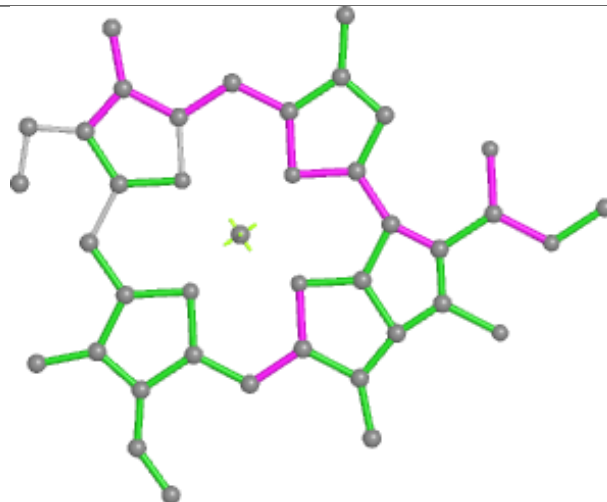




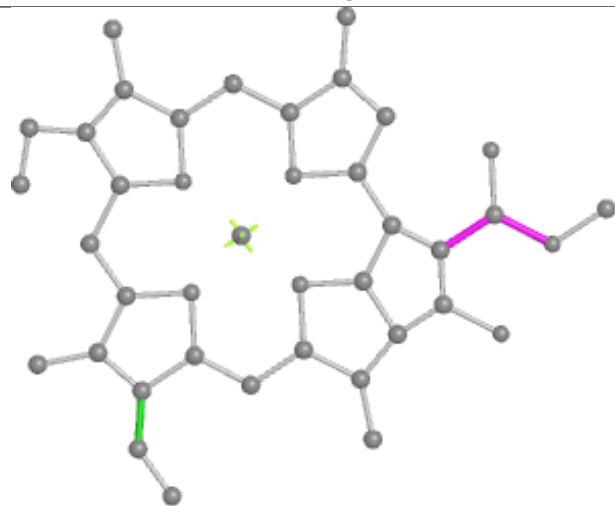
## Ligand CLA 1 602



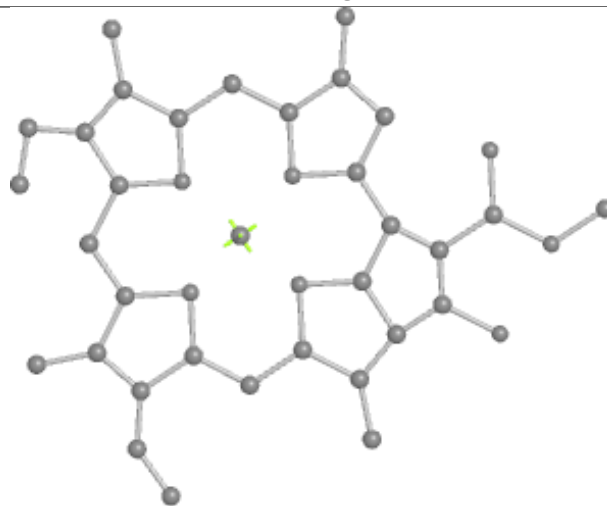
Bond lengths



Bond angles

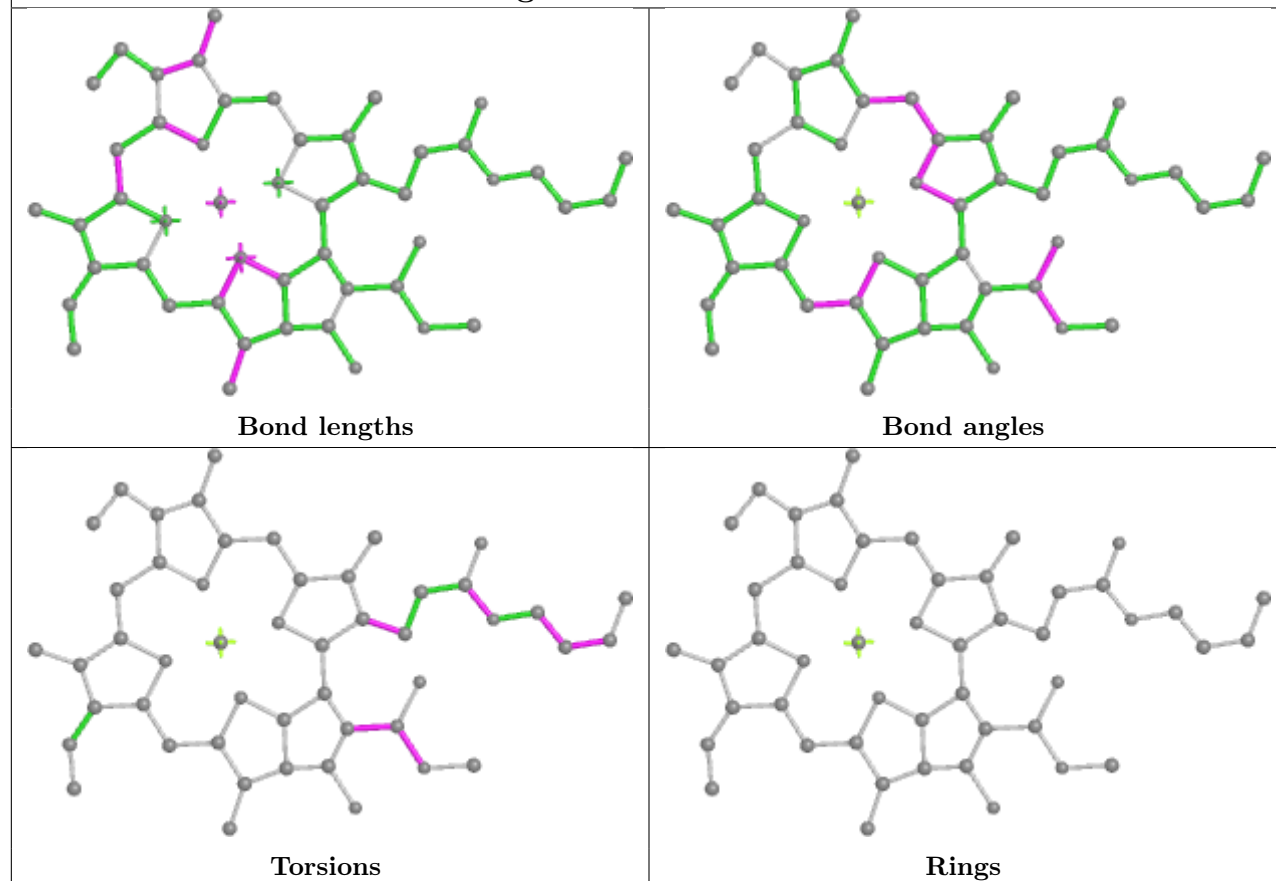


Torsions

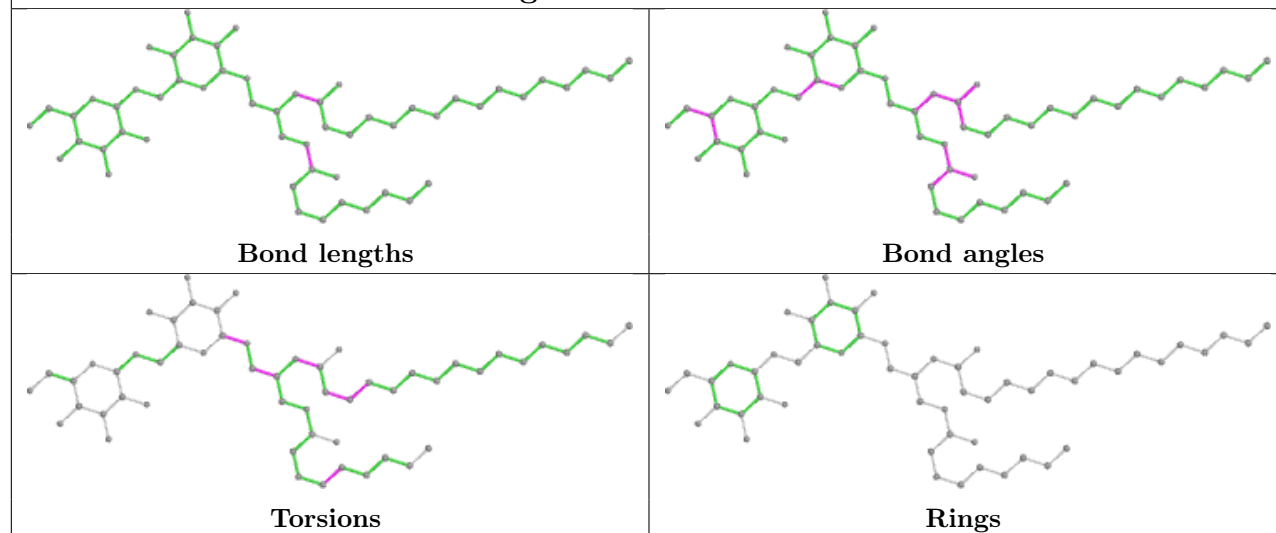


Rings

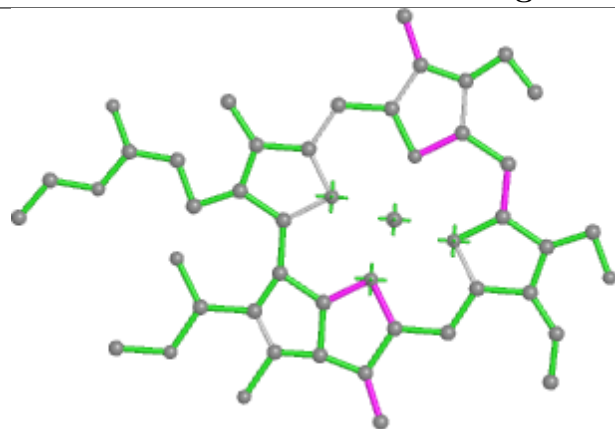
## Ligand CLA NN 613



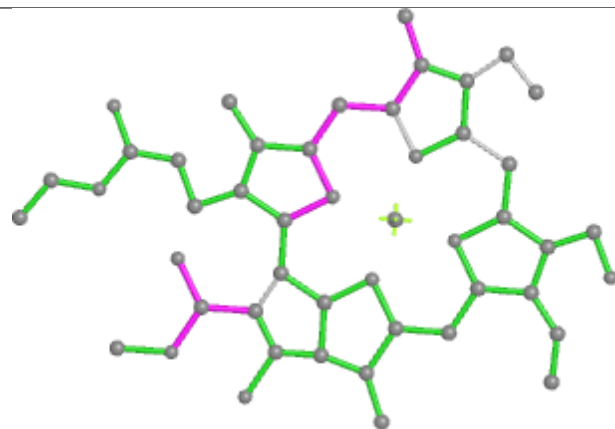
## Ligand DGD Cc 519



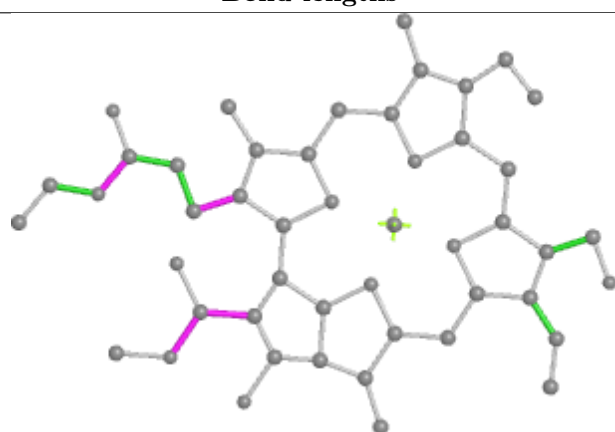
## Ligand CHL Y 605



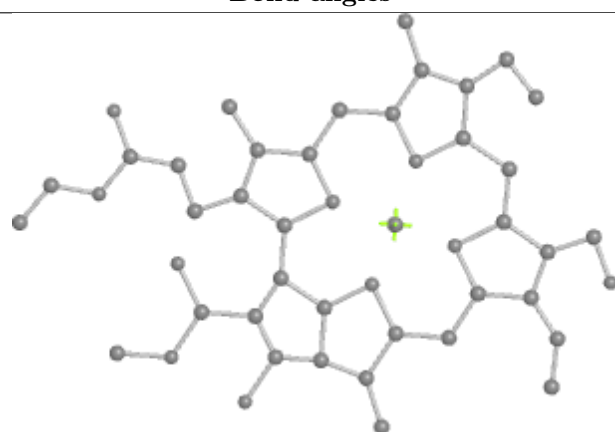
Bond lengths



Bond angles

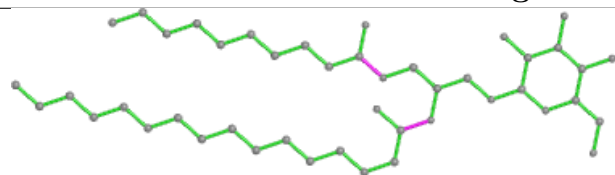


Torsions

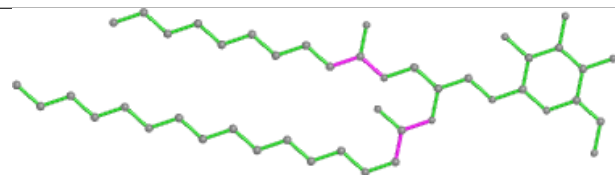


Rings

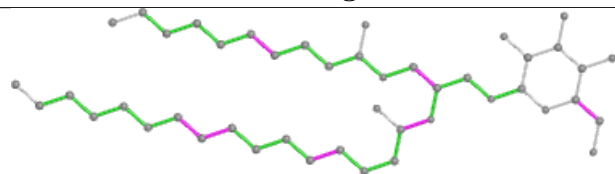
## Ligand LMG B 615



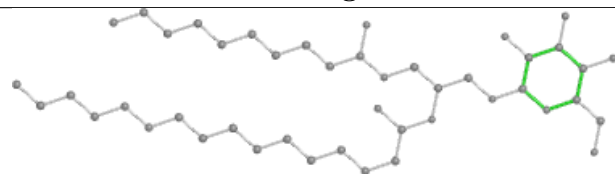
Bond lengths



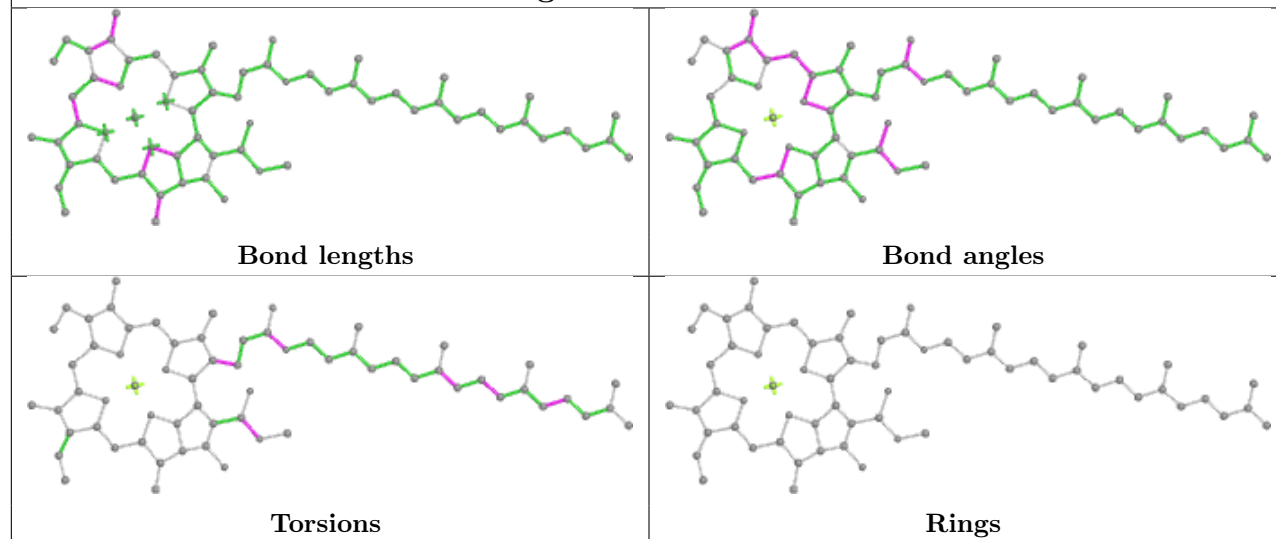
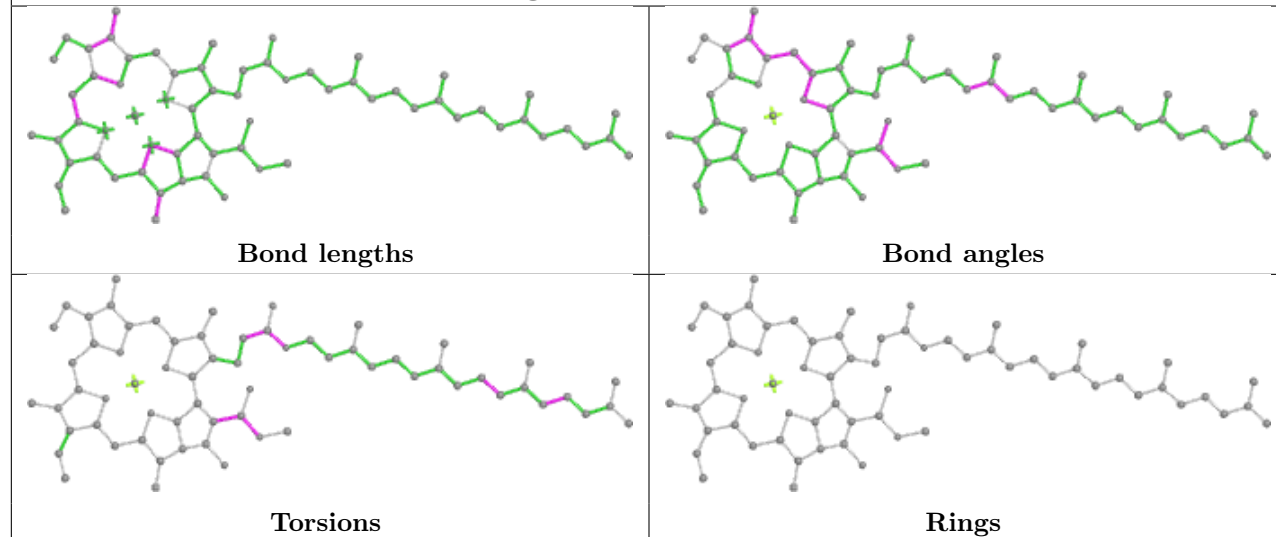
Bond angles



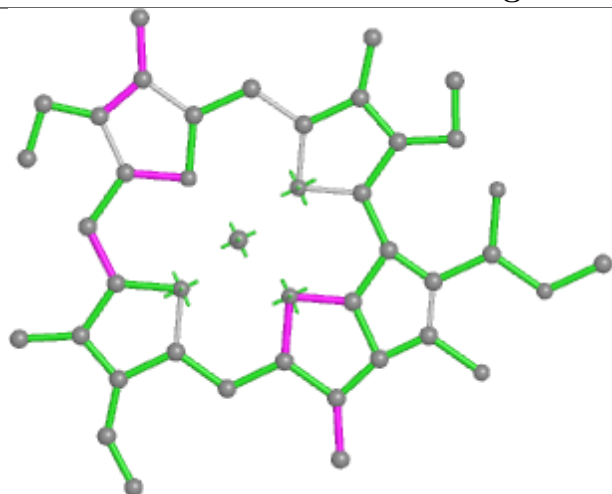
Torsions



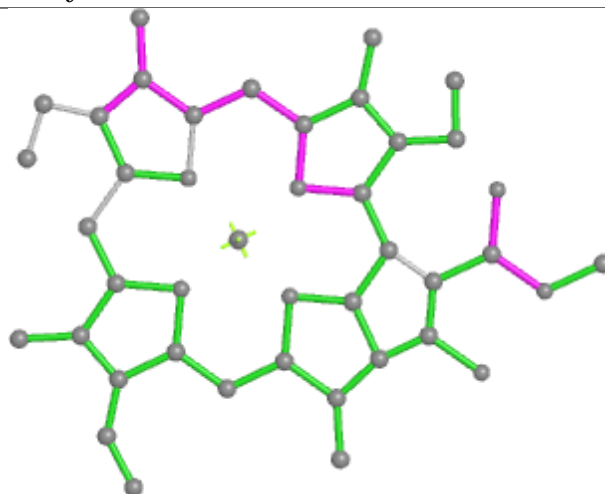
Rings

**Ligand CLA c 503****Ligand CLA Cc 509**

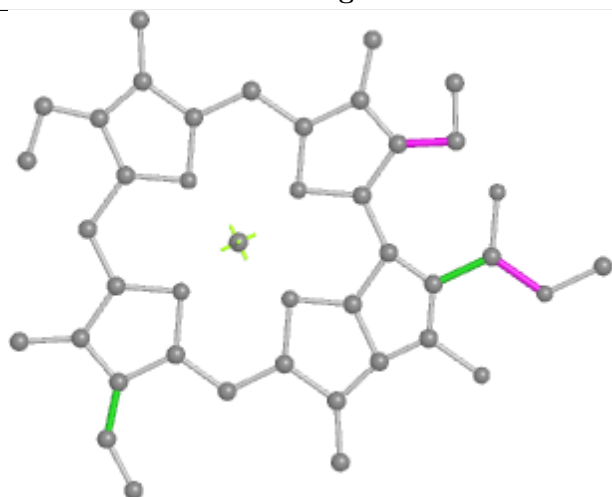
## Ligand CLA Yy 611



Bond lengths



Bond angles



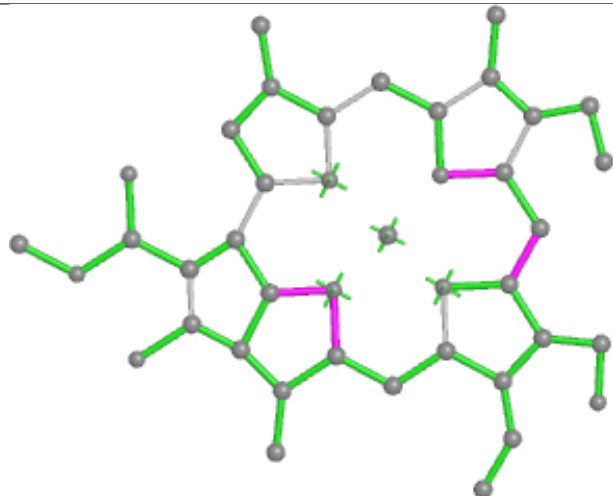
Torsions



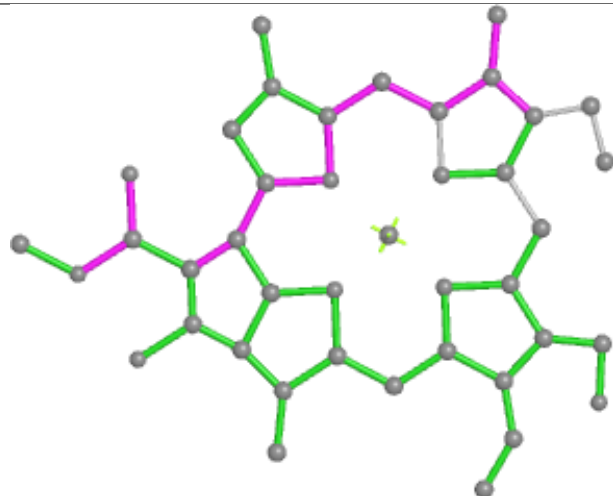
Rings



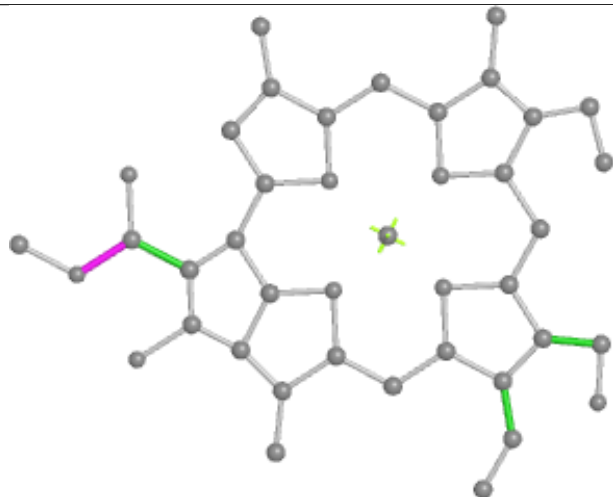
## Ligand CHL 3 607



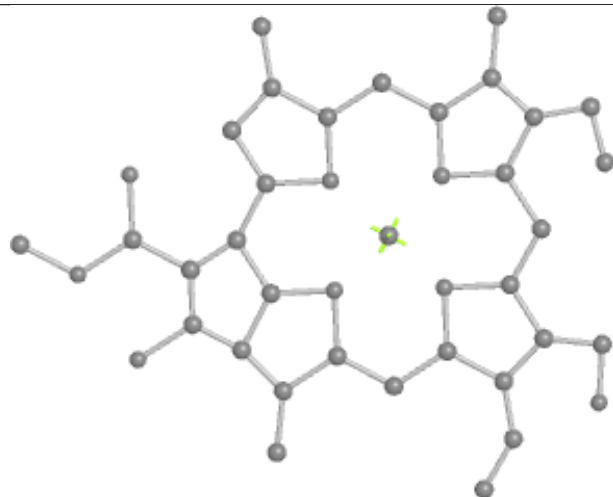
Bond lengths



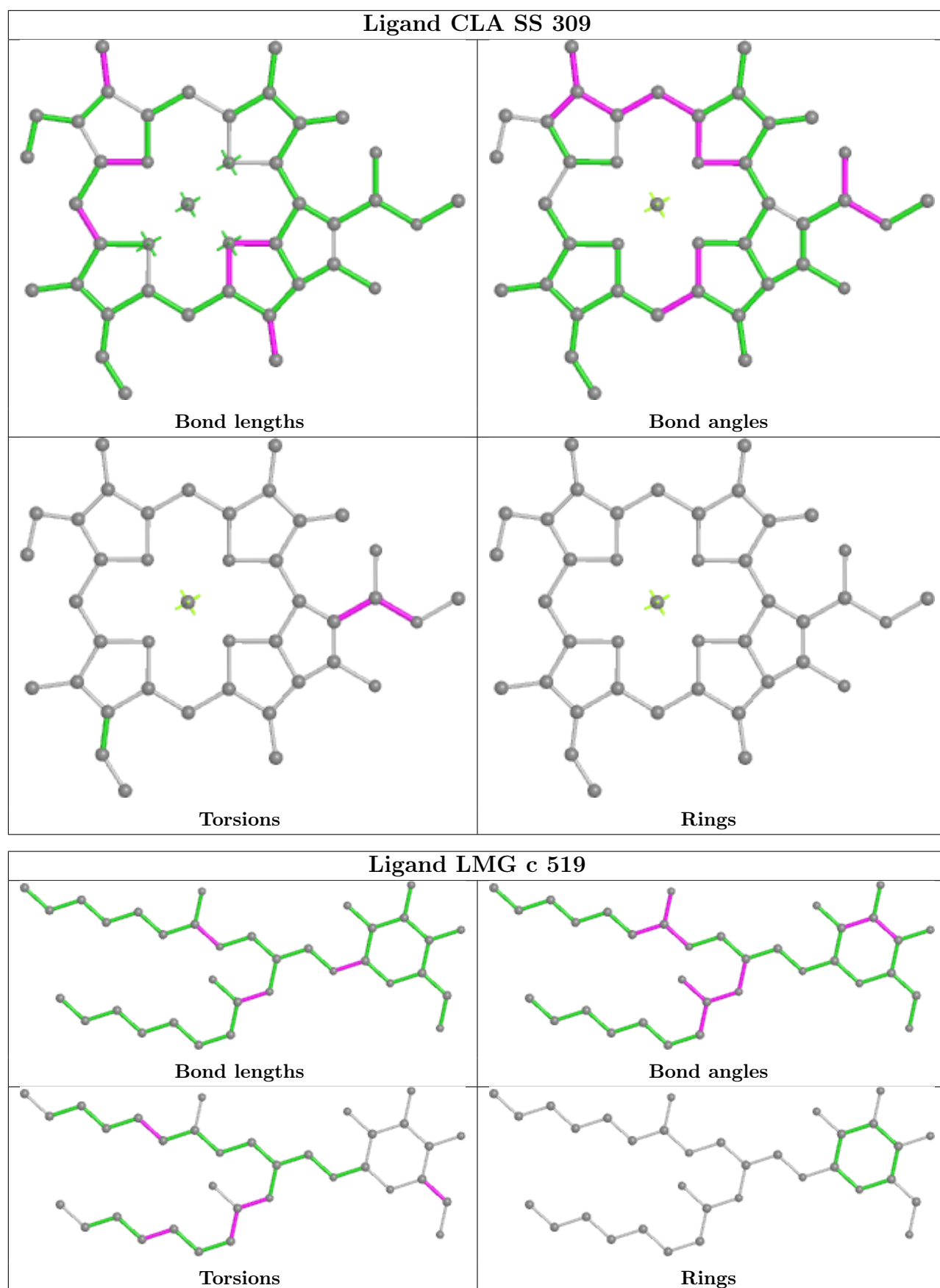
Bond angles

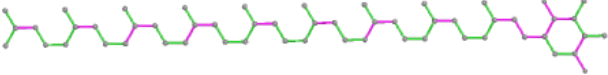
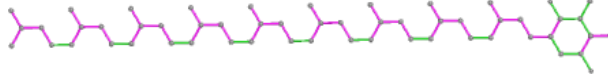
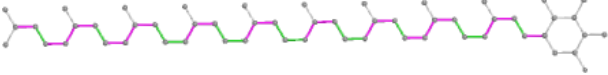
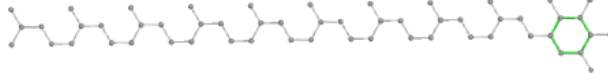


Torsions



Rings



Ligand PL9 DD 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39860. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit ⓘ

This section was not generated.