



Full wwPDB EM Validation Report ⓘ

Dec 22, 2022 – 06:33 pm GMT

PDB ID : 7PI0
EMDB ID : EMD-13429
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-19
Resolution : 2.43 Å(reported)
Based on initial model : 6KAC

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

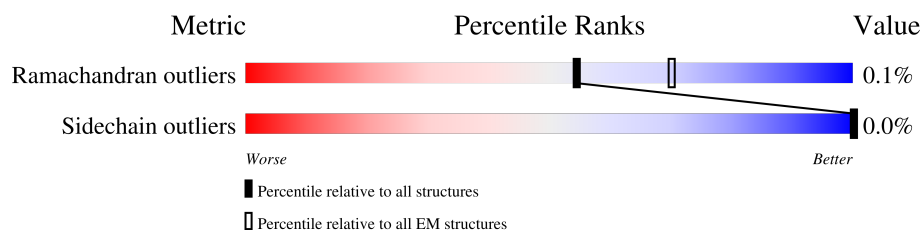
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.


















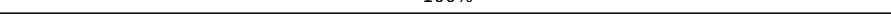
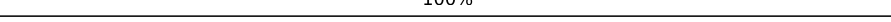
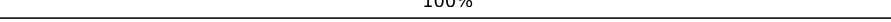

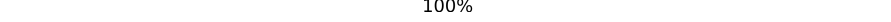
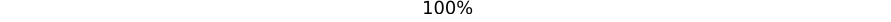
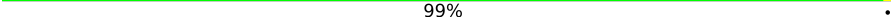
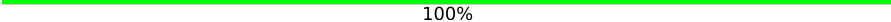


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	336	
1	a	336	
2	B	484	
2	b	484	
3	V	32	
3	v	32	
4	C	449	
4	c	449	
5	D	348	

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Mol	Chain	Length	Quality of chain
5	d	348	 100%
6	E	76	 100%
6	e	76	 100%
7	F	31	 100%
7	f	31	 100%
8	H	67	 100%
8	h	67	 100%
9	I	35	 100%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 100%
12	l	38	 100%
13	M	31	 100%
13	m	31	 100%
14	O	238	 100%
14	o	238	 100%
15	P	187	 100%
15	p	187	 99%
16	T	30	 100%
16	t	30	 100%
17	W	44	 100%
17	w	44	 100%

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Mol	Chain	Length	Quality of chain
18	X	30	 100%
18	x	30	 100%
19	Z	61	 100%
19	z	61	 100%
20	N	222	 100%
20	n	222	 100%
21	G	221	 100%
21	g	221	 100%
22	R	196	 99%
22	r	196	 99%
23	S	243	 100%
23	s	243	 100%
24	Y	222	 99%
24	y	222	 100%
25	U	27	 100%
25	u	27	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	S	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	c	512	X	-	-	-
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-
29	CLA	r	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
44	RRX	H	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	RRX	h	101	X	-	-	-
45	CHL	G	601	X	-	-	-
45	CHL	G	605	X	-	-	-
45	CHL	G	606	X	-	-	-
45	CHL	G	607	X	-	-	-
45	CHL	G	608	X	-	-	-
45	CHL	G	609	X	-	-	-
45	CHL	N	601	X	-	-	-
45	CHL	N	605	X	-	-	-
45	CHL	N	606	X	-	-	-
45	CHL	N	607	X	-	-	-
45	CHL	N	608	X	-	-	-
45	CHL	N	609	X	-	-	-
45	CHL	R	606	X	-	-	-
45	CHL	R	607	X	-	-	-
45	CHL	S	601	X	-	-	-
45	CHL	S	606	X	-	-	-
45	CHL	S	607	X	-	-	-
45	CHL	S	608	X	-	-	-
45	CHL	Y	601	X	-	-	-
45	CHL	Y	605	X	-	-	-
45	CHL	Y	606	X	-	-	-
45	CHL	Y	607	X	-	-	-
45	CHL	Y	609	X	-	-	-
45	CHL	g	601	X	-	-	-
45	CHL	g	605	X	-	-	-
45	CHL	g	606	X	-	-	-
45	CHL	g	607	X	-	-	-
45	CHL	g	608	X	-	-	-
45	CHL	g	609	X	-	-	-
45	CHL	n	601	X	-	-	-
45	CHL	n	605	X	-	-	-
45	CHL	n	606	X	-	-	-
45	CHL	n	607	X	-	-	-
45	CHL	n	608	X	-	-	-
45	CHL	n	609	X	-	-	-
45	CHL	r	606	X	-	-	-
45	CHL	r	607	X	-	-	-
45	CHL	s	601	X	-	-	-
45	CHL	s	606	X	-	-	-
45	CHL	s	607	X	-	-	-
45	CHL	s	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CHL	y	601	X	-	-	-
45	CHL	y	605	X	-	-	-
45	CHL	y	606	X	-	-	-
45	CHL	y	607	X	-	-	-
45	CHL	y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-
48	XAT	R	621	X	-	-	-
48	XAT	Y	622	X	-	-	-
48	XAT	g	622	X	-	-	-
48	XAT	n	622	X	-	-	-
48	XAT	r	621	X	-	-	-
48	XAT	y	622	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 77465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		
1	a	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

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

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

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

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

- Molecule 13 is a protein called PsbM.

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

- Molecule 14 is a protein called PsbO.

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

- Molecule 15 is a protein called PsbP.

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

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

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

- Molecule 17 is a protein called PsbW.

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

- Molecule 18 is a protein called PsbX.

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

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

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

- Molecule 20 is a protein called LHCII M3.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 22 is a protein called CP29.

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

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

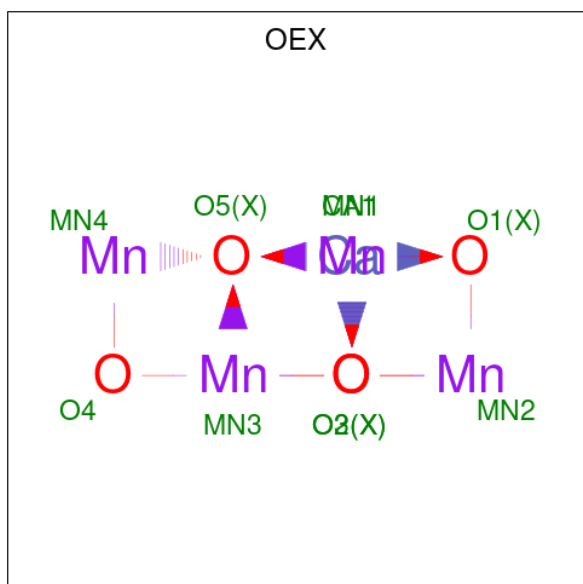
- Molecule 24 is a protein called LHCII M1.

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

- Molecule 25 is a protein called PsbU.

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

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

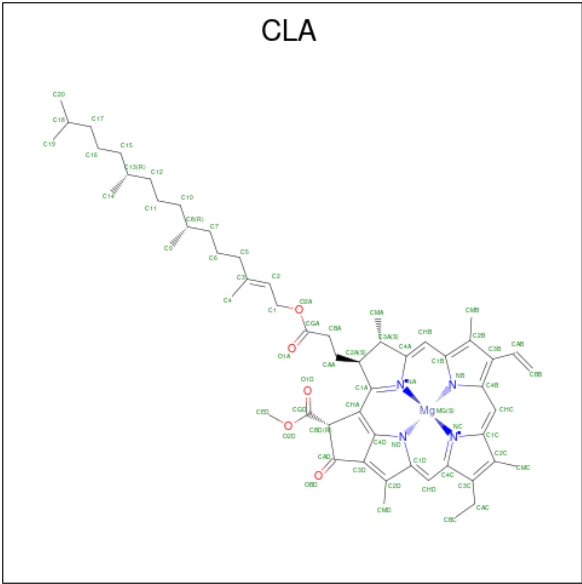
- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	D	1	Total	C	Mg	N	O	0
			125	105	2	8	10	
29	D	1	Total	C	Mg	N	O	0
			125	105	2	8	10	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	G	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	S	1	Total 620	C 510	Mg 11	N 44	O 55	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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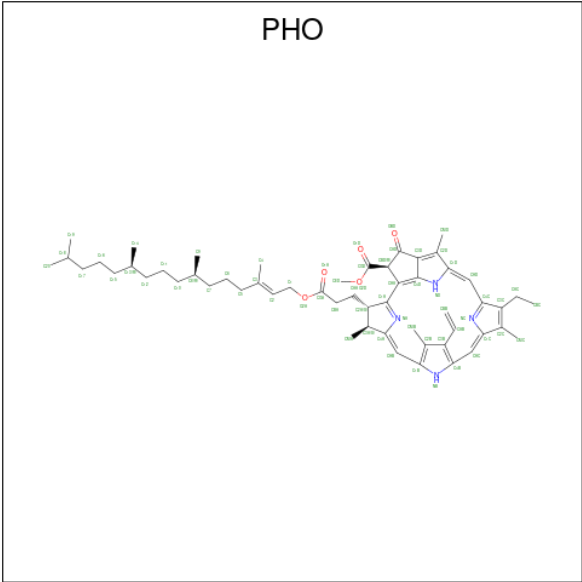
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0

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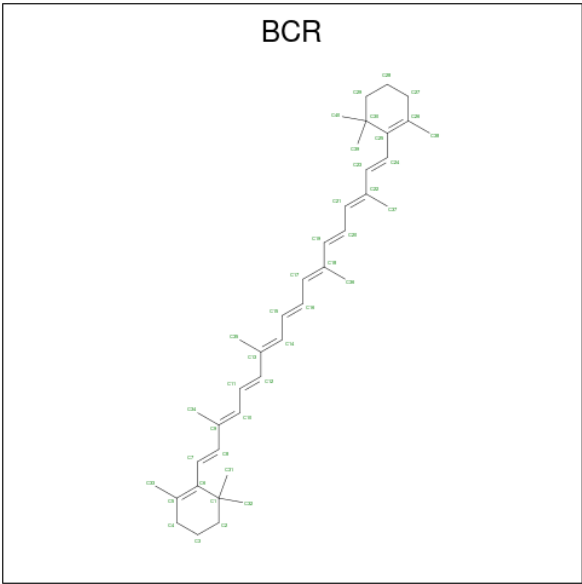
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C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

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).

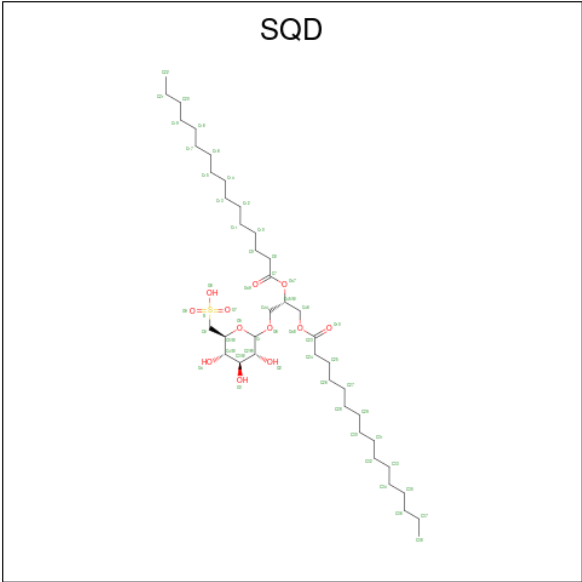


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 80 80	0
31	B	1	Total C 80 80	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 80 80	0
31	b	1	Total C 80 80	0
31	c	1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

- Molecule 32 is SODIUM ION (three-letter code: NA) (formula: Na).

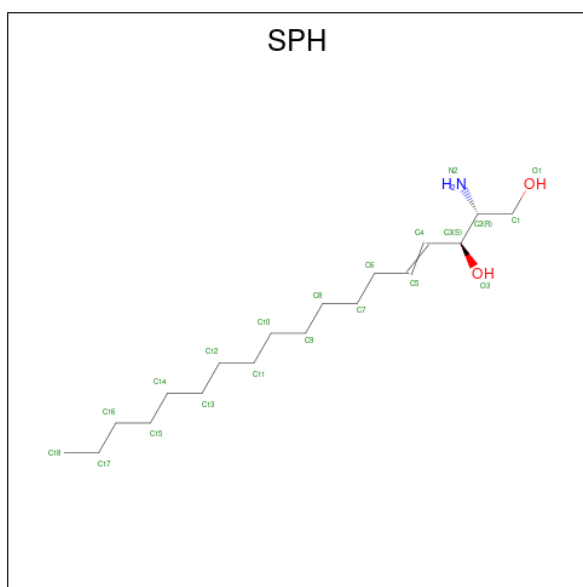
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Na 1 1	0
32	a	1	Total Na 1 1	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



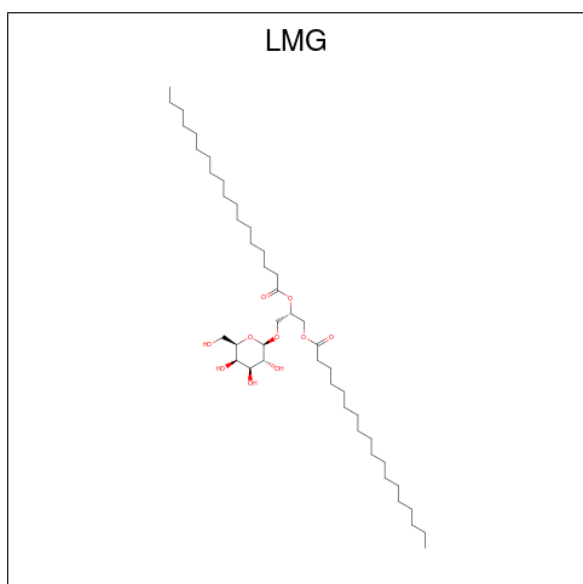
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			42	29	12	1	
33	B	1	Total	C	O	S	0
			96	70	24	2	
33	B	1	Total	C	O	S	0
			96	70	24	2	
33	C	1	Total	C	O	S	0
			36	23	12	1	
33	M	1	Total	C	O	S	0
			42	29	12	1	
33	a	1	Total	C	O	S	0
			51	38	12	1	
33	b	1	Total	C	O	S	0
			96	70	24	2	
33	b	1	Total	C	O	S	0
			96	70	24	2	
33	c	1	Total	C	O	S	0
			54	41	12	1	
33	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 34 is SPHINGOSINE (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



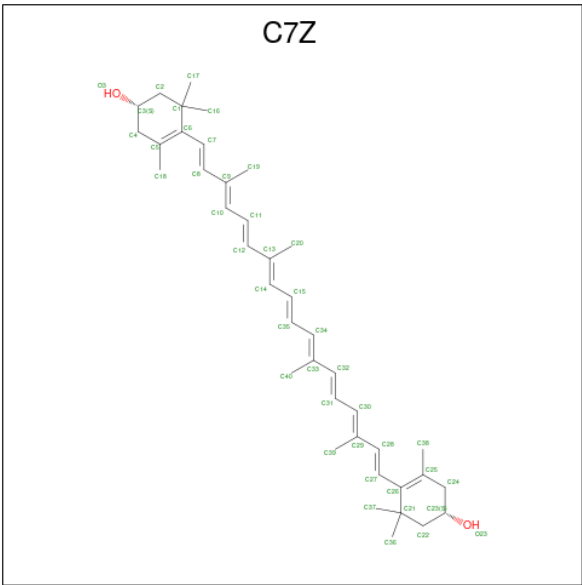
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			21	18	1	2	
34	Y	1	Total	C	N	O	0
			21	18	1	2	
34	a	1	Total	C	N	O	0
			21	18	1	2	
34	y	1	Total	C	N	O	0
			21	18	1	2	

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



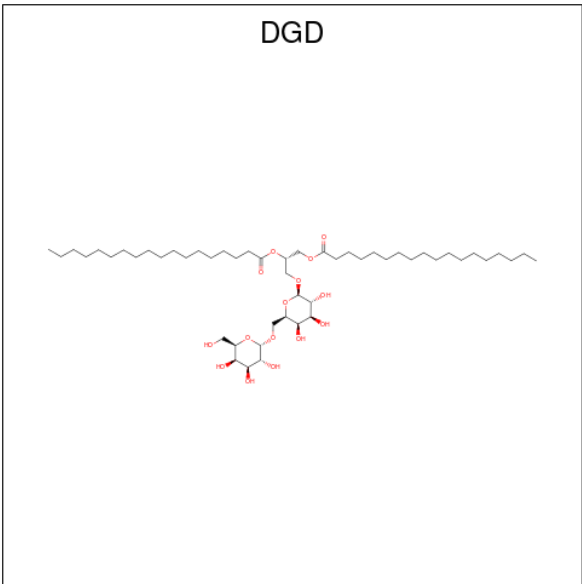
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			40	30	10	
35	B	1	Total	C	O	0
			44	34	10	
35	C	1	Total	C	O	0
			144	114	30	
35	C	1	Total	C	O	0
			144	114	30	
35	C	1	Total	C	O	0
			144	114	30	
35	D	1	Total	C	O	0
			42	32	10	
35	H	1	Total	C	O	0
			48	38	10	
35	W	1	Total	C	O	0
			39	29	10	
35	a	1	Total	C	O	0
			48	38	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			106	86	20	
35	c	1	Total	C	O	0
			106	86	20	
35	d	1	Total	C	O	0
			46	36	10	
35	h	1	Total	C	O	0
			48	38	10	
35	w	1	Total	C	O	0
			39	29	10	

- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



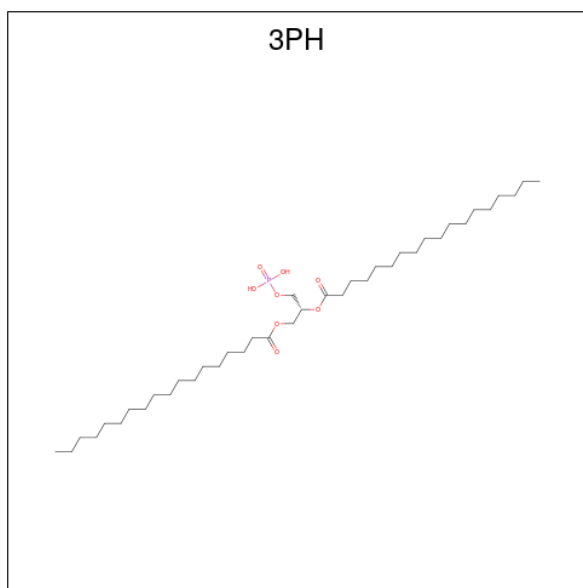
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			43	28	15	

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Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			157	112	45	
37	C	1	Total	C	O	0
			157	112	45	
37	C	1	Total	C	O	0
			157	112	45	
37	b	1	Total	C	O	0
			43	28	15	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



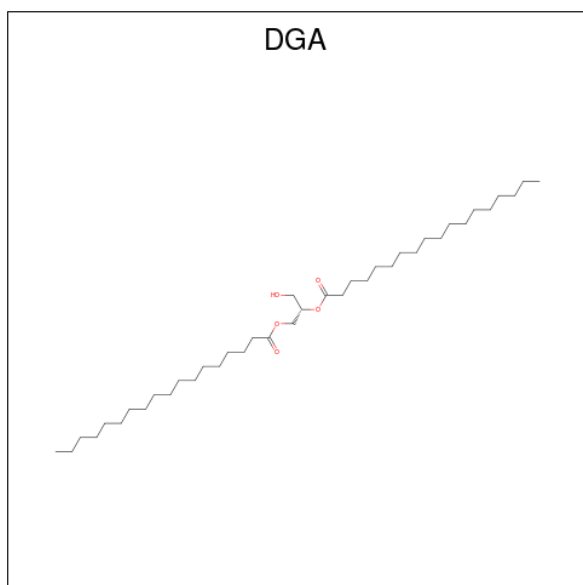
Mol	Chain	Residues	Atoms				AltConf
38	B	1	Total	C	O	P	0
			48	39	8	1	
38	T	1	Total	C	O	P	0
			48	39	8	1	
38	S	1	Total	C	O	P	0
			30	21	8	1	
38	b	1	Total	C	O	P	0
			39	30	8	1	

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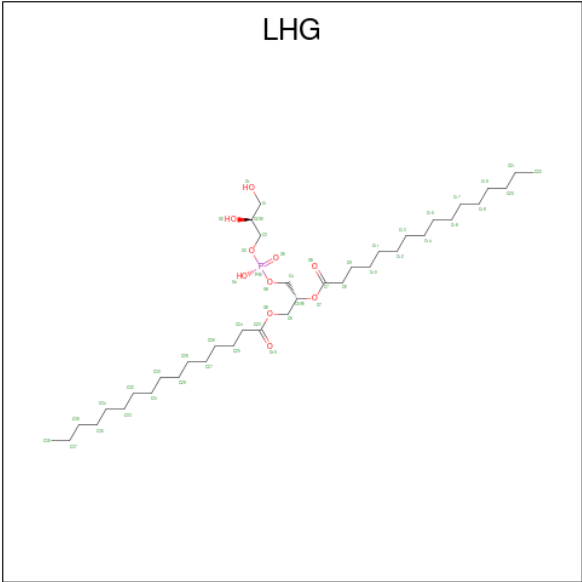
Mol	Chain	Residues	Atoms				AltConf
38	t	1	Total	C	O	P	0
			48	39	8	1	
38	s	1	Total	C	O	P	0
			48	39	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
39	B	1	Total	C	O		0
			37	32	5		
39	C	1	Total	C	O		0
			44	39	5		
39	J	1	Total	C	O		0
			29	24	5		
39	b	1	Total	C	O		0
			44	39	5		
39	c	1	Total	C	O		0
			44	39	5		
39	j	1	Total	C	O		0
			29	24	5		

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



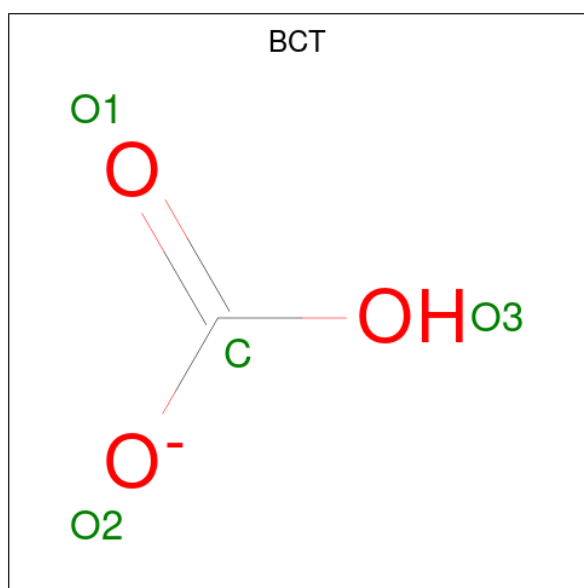
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	O	P	0
			35	24	10	1	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	L	1	Total	C	O	P	0
			49	38	10	1	
40	N	1	Total	C	O	P	0
			49	38	10	1	
40	G	1	Total	C	O	P	0
			49	38	10	1	
40	S	1	Total	C	O	P	0
			45	34	10	1	
40	Y	1	Total	C	O	P	0
			49	38	10	1	
40	c	1	Total	C	O	P	0
			85	63	20	2	
40	c	1	Total	C	O	P	0
			85	63	20	2	
40	d	1	Total	C	O	P	0
			132	99	30	3	
40	d	1	Total	C	O	P	0
			132	99	30	3	
40	d	1	Total	C	O	P	0
			132	99	30	3	

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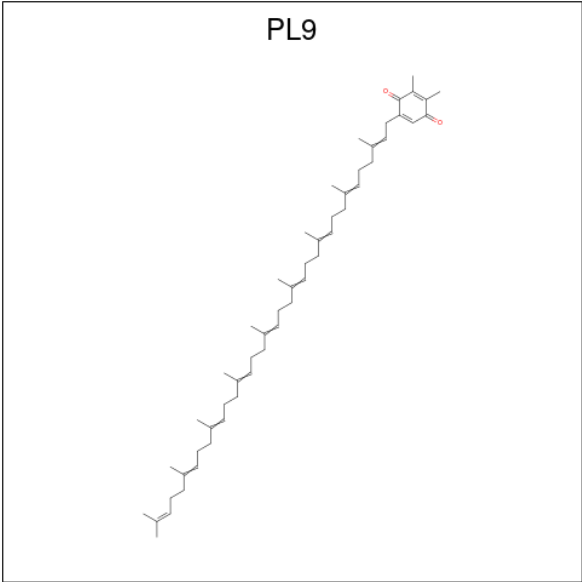
Mol	Chain	Residues	Atoms				AltConf
40	l	1	Total	C	O	P	0
			49	38	10	1	
40	n	1	Total	C	O	P	0
			42	31	10	1	
40	g	1	Total	C	O	P	0
			49	38	10	1	
40	s	1	Total	C	O	P	0
			45	34	10	1	
40	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



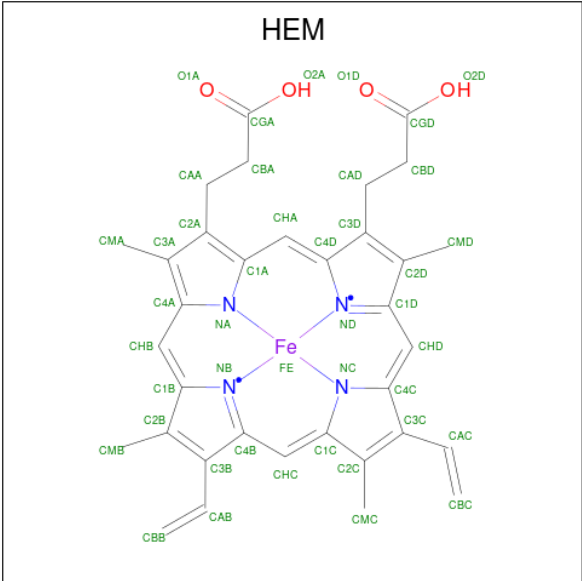
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			4	1	3	
41	d	1	Total	C	O	0
			4	1	3	

- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			55	53	2	
42	d	1	Total	C	O	0
			55	53	2	

- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



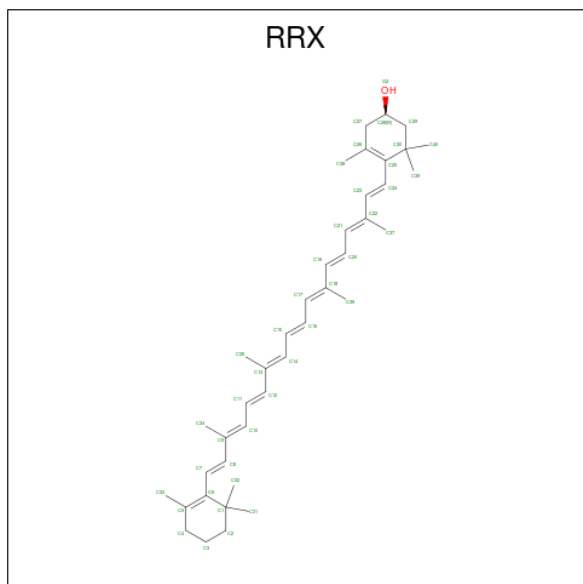
Mol	Chain	Residues	Atoms					AltConf
43	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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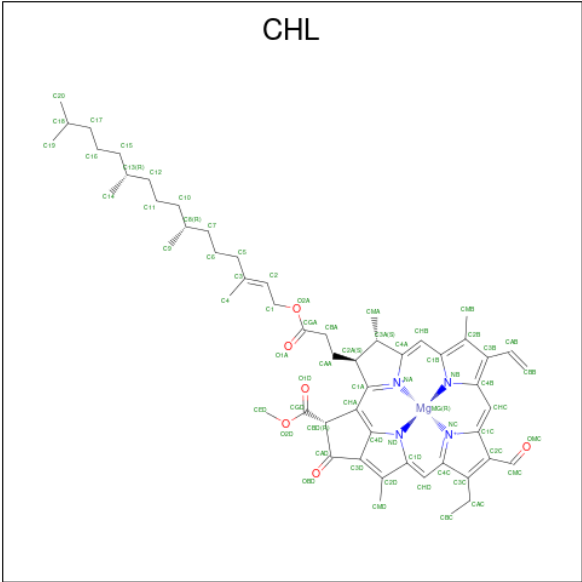
Mol	Chain	Residues	Atoms					AltConf
43	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
44	H	1	Total	C	O	0
			41	40	1	
44	h	1	Total	C	O	0
			41	40	1	

- Molecule 45 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	R	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	R	1	Total	C	Mg	N	O	0
			94	74	2	8	10	

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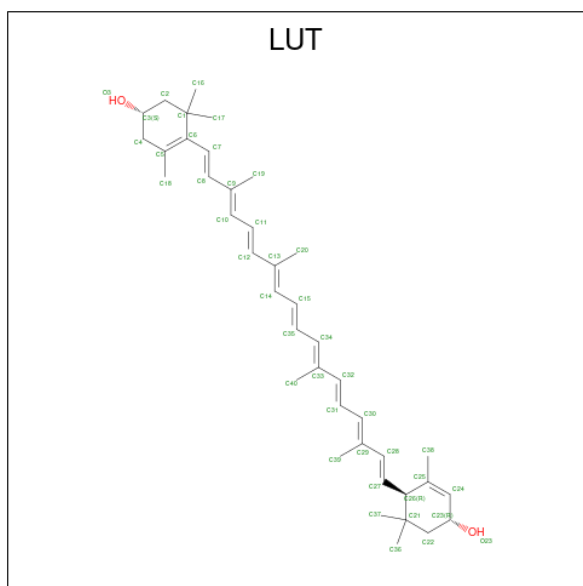
Mol	Chain	Residues	Atoms					AltConf
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	

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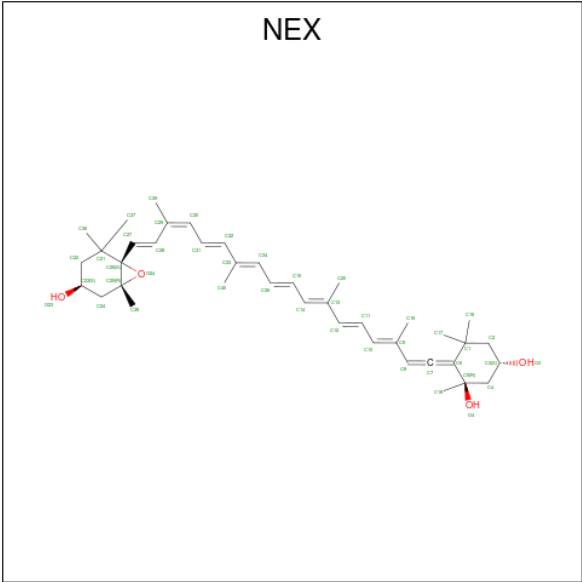
Mol	Chain	Residues	Atoms					AltConf
45	r	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	r	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	

- Molecule 46 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



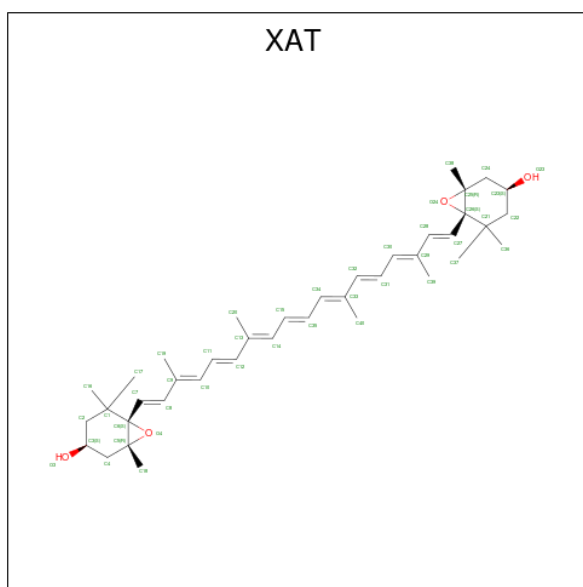
Mol	Chain	Residues	Atoms			AltConf
46	N	1	Total	C	O	0
			84	80	4	
46	N	1	Total	C	O	0
			84	80	4	
46	G	1	Total	C	O	0
			84	80	4	
46	G	1	Total	C	O	0
			84	80	4	
46	R	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			84	80	4	
46	S	1	Total	C	O	0
			84	80	4	
46	Y	1	Total	C	O	0
			84	80	4	
46	Y	1	Total	C	O	0
			84	80	4	
46	n	1	Total	C	O	0
			84	80	4	
46	n	1	Total	C	O	0
			84	80	4	
46	g	1	Total	C	O	0
			84	80	4	
46	g	1	Total	C	O	0
			84	80	4	
46	r	1	Total	C	O	0
			42	40	2	
46	s	1	Total	C	O	0
			84	80	4	
46	s	1	Total	C	O	0
			84	80	4	
46	y	1	Total	C	O	0
			84	80	4	
46	y	1	Total	C	O	0
			84	80	4	

- Molecule 47 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			44	40	4	
47	G	1	Total	C	O	0
			44	40	4	
47	R	1	Total	C	O	0
			27	25	2	
47	S	1	Total	C	O	0
			44	40	4	
47	Y	1	Total	C	O	0
			44	40	4	
47	n	1	Total	C	O	0
			44	40	4	
47	g	1	Total	C	O	0
			44	40	4	
47	r	1	Total	C	O	0
			27	25	2	
47	s	1	Total	C	O	0
			44	40	4	
47	y	1	Total	C	O	0
			44	40	4	

- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
49	R	1	Total 35	C 24	O 11	0
49	r	1	Total 35	C 24	O 11	0

- Molecule 50 is (2S)-3-[[(R)- (2-aminoethoxy) (hydroxy) phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



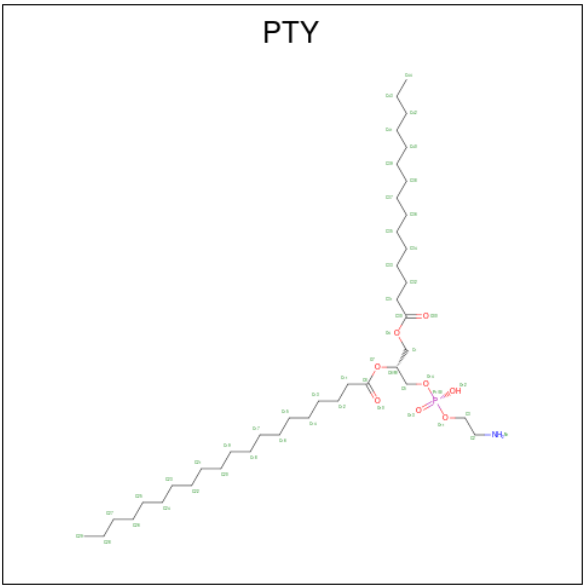
Mol	Chain	Residues	Atoms					AltConf
50	S	1	Total	C	N	O	P	0
			20	11	1	7	1	

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Mol	Chain	Residues	Atoms					AltConf
50	s	1	Total	C	N	O	P	0
			19	10	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	27	Total	O	0
			93	93	
52	A	7	Total	O	0
			93	93	
52	A	7	Total	O	0
			93	93	
52	A	22	Total	O	0
			93	93	

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Mol	Chain	Residues	Atoms		AltConf
52	A	10	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	2	Total 93	O 93	0
52	A	2	Total 93	O 93	0
52	A	4	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	B	6	Total 125	O 125	0
52	B	11	Total 125	O 125	0
52	B	12	Total 125	O 125	0
52	B	4	Total 125	O 125	0
52	B	1	Total 125	O 125	0

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Mol	Chain	Residues	Atoms		AltConf
52	B	40	Total 125	O 125	0
52	B	16	Total 125	O 125	0
52	B	2	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	9	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	4	Total 125	O 125	0
52	B	2	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	5	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	V	5	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
52	V	1	Total 6	O 6	0
52	C	3	Total 113	O 113	0
52	C	3	Total 113	O 113	0
52	C	15	Total 113	O 113	0
52	C	56	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	3	Total 113	O 113	0
52	C	2	Total 113	O 113	0
52	C	12	Total 113	O 113	0
52	C	3	Total 113	O 113	0
52	C	3	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0

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Mol	Chain	Residues	Atoms		AltConf
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	3	Total 77	O 77	0
52	D	6	Total 77	O 77	0
52	D	8	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	3	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	11	Total 77	O 77	0
52	D	12	Total 77	O 77	0
52	D	9	Total 77	O 77	0

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Mol	Chain	Residues	Atoms		AltConf
52	D	5	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	E	1	Total 18	O 18	0
52	E	1	Total 18	O 18	0
52	E	15	Total 18	O 18	0
52	E	1	Total 18	O 18	0
52	F	1	Total 1	O 1	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	13	Total 19	O 19	0
52	I	1	Total 6	O 6	0
52	I	2	Total 6	O 6	0
52	I	3	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
52	J	3	Total 4	O 4	0
52	J	1	Total 4	O 4	0
52	K	1	Total 10	O 10	0
52	K	9	Total 10	O 10	0
52	L	6	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	M	1	Total 8	O 8	0
52	M	1	Total 8	O 8	0
52	M	1	Total 8	O 8	0
52	M	3	Total 8	O 8	0
52	M	2	Total 8	O 8	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	2	Total 79	O 79	0
52	O	1	Total 79	O 79	0

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Mol	Chain	Residues	Atoms		AltConf
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	18	Total 79	O 79	0
52	O	5	Total 79	O 79	0
52	O	18	Total 79	O 79	0
52	O	10	Total 79	O 79	0
52	O	9	Total 79	O 79	0
52	O	6	Total 79	O 79	0
52	O	2	Total 79	O 79	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	13	Total 25	O 25	0
52	P	7	Total 25	O 25	0
52	T	1	Total 5	O 5	0
52	T	2	Total 5	O 5	0
52	T	2	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
52	W	1	Total 8	O 8	0
52	W	1	Total 8	O 8	0
52	W	2	Total 8	O 8	0
52	W	4	Total 8	O 8	0
52	X	3	Total 3	O 3	0
52	Z	1	Total 4	O 4	0
52	Z	3	Total 4	O 4	0
52	N	27	Total 61	O 61	0
52	N	11	Total 61	O 61	0
52	N	10	Total 61	O 61	0
52	N	6	Total 61	O 61	0
52	N	5	Total 61	O 61	0
52	N	1	Total 61	O 61	0
52	N	1	Total 61	O 61	0
52	G	1	Total 60	O 60	0
52	G	1	Total 60	O 60	0
52	G	7	Total 60	O 60	0
52	G	37	Total 60	O 60	0
52	G	14	Total 60	O 60	0
52	R	1	Total 35	O 35	0
52	R	29	Total 35	O 35	0

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Mol	Chain	Residues	Atoms		AltConf
52	R	4	Total 35	O 35	0
52	R	1	Total 35	O 35	0
52	S	1	Total 33	O 33	0
52	S	29	Total 33	O 33	0
52	S	3	Total 33	O 33	0
52	Y	1	Total 56	O 56	0
52	Y	1	Total 56	O 56	0
52	Y	1	Total 56	O 56	0
52	Y	21	Total 56	O 56	0
52	Y	21	Total 56	O 56	0
52	Y	11	Total 56	O 56	0
52	U	1	Total 8	O 8	0
52	U	7	Total 8	O 8	0
52	a	15	Total 91	O 91	0
52	a	5	Total 91	O 91	0
52	a	20	Total 91	O 91	0
52	a	9	Total 91	O 91	0
52	a	2	Total 91	O 91	0
52	a	6	Total 91	O 91	0
52	a	9	Total 91	O 91	0
52	a	4	Total 91	O 91	0

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Mol	Chain	Residues	Atoms		AltConf
52	a	5	Total 91	O 91	0
52	a	6	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	2	Total 91	O 91	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	48	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	21	Total 115	O 115	0
52	b	2	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	8	Total 115	O 115	0
52	b	2	Total 115	O 115	0
52	b	1	Total 115	O 115	0

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Mol	Chain	Residues	Atoms		AltConf
52	b	6	Total 115	O 115	0
52	b	7	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	11	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	v	1	Total 2	O 2	0
52	v	1	Total 2	O 2	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	16	Total 101	O 101	0
52	c	14	Total 101	O 101	0
52	c	20	Total 101	O 101	0
52	c	2	Total 101	O 101	0
52	c	21	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	2	Total 101	O 101	0

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Mol	Chain	Residues	Atoms		AltConf
52	c	16	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	3	Total 65	O 65	0
52	d	28	Total 65	O 65	0
52	d	11	Total 65	O 65	0
52	d	12	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	5	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	e	1	Total 20	O 20	0
52	e	6	Total 20	O 20	0
52	e	11	Total 20	O 20	0
52	e	2	Total 20	O 20	0

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Mol	Chain	Residues	Atoms		AltConf
52	f	3	Total 3	O 3	0
52	h	1	Total 20	O 20	0
52	h	2	Total 20	O 20	0
52	h	1	Total 20	O 20	0
52	h	1	Total 20	O 20	0
52	h	9	Total 20	O 20	0
52	h	4	Total 20	O 20	0
52	h	2	Total 20	O 20	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	9	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	j	3	Total 3	O 3	0
52	k	5	Total 8	O 8	0
52	k	3	Total 8	O 8	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0

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Mol	Chain	Residues	Atoms	AltConf
52	l	1	Total O 10 10	0
52	l	5	Total O 10 10	0
52	m	1	Total O 7 7	0
52	m	1	Total O 7 7	0
52	m	2	Total O 7 7	0
52	m	3	Total O 7 7	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	29	Total O 81 81	0
52	o	1	Total O 81 81	0
52	o	15	Total O 81 81	0
52	o	7	Total O 81 81	0
52	o	8	Total O 81 81	0
52	o	13	Total O 81 81	0
52	o	1	Total O 81 81	0
52	p	1	Total O 68 68	0

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Mol	Chain	Residues	Atoms		AltConf
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	13	Total 68	O 68	0
52	p	34	Total 68	O 68	0
52	p	13	Total 68	O 68	0
52	t	2	Total 2	O 2	0
52	w	1	Total 10	O 10	0
52	w	1	Total 10	O 10	0
52	w	4	Total 10	O 10	0
52	w	2	Total 10	O 10	0
52	w	2	Total 10	O 10	0
52	x	9	Total 9	O 9	0
52	z	1	Total 8	O 8	0
52	z	6	Total 8	O 8	0
52	z	1	Total 8	O 8	0
52	n	1	Total 36	O 36	0

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Mol	Chain	Residues	Atoms		AltConf
52	n	19	Total 36	O 36	0
52	n	7	Total 36	O 36	0
52	n	6	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	g	2	Total 31	O 31	0
52	g	24	Total 31	O 31	0
52	g	5	Total 31	O 31	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	11	Total 38	O 38	0
52	r	21	Total 38	O 38	0
52	s	1	Total 39	O 39	0
52	s	24	Total 39	O 39	0
52	s	10	Total 39	O 39	0
52	s	4	Total 39	O 39	0

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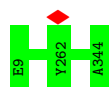
Mol	Chain	Residues	Atoms		AltConf
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	29	Total 63	O 63	0
52	y	26	Total 63	O 63	0
52	y	4	Total 63	O 63	0
52	u	1	Total 7	O 7	0
52	u	1	Total 7	O 7	0
52	u	5	Total 7	O 7	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0

3 Residue-property plots

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

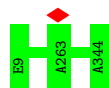
- Molecule 1: Photosystem II protein D1

Chain A:  100%



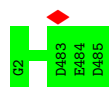
- Molecule 1: Photosystem II protein D1

Chain a:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  100%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%

There are no outlier residues recorded for this chain.

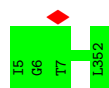
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Photosystem II D2 protein

Chain D:  100%



- Molecule 5: Photosystem II D2 protein

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

Chain I:  100%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain J:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: PsbM

Chain M:  100%

There are no outlier residues recorded for this chain.

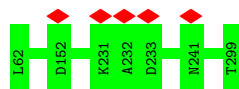
- Molecule 13: PsbM

Chain m:  100%

There are no outlier residues recorded for this chain.

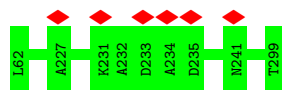
- Molecule 14: PsbO

Chain O:  100%



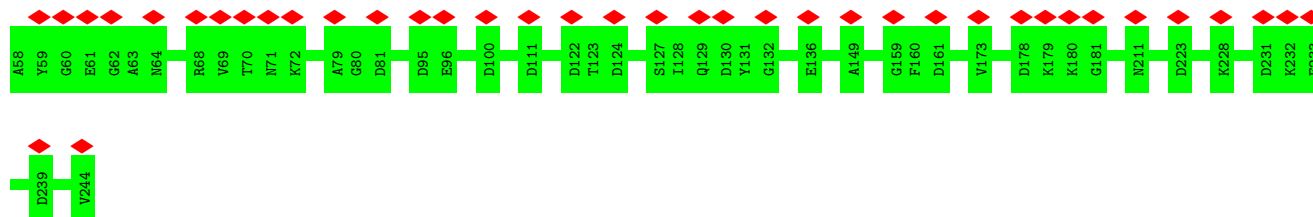
- Molecule 14: PsbO

Chain o:  100%



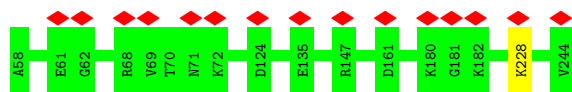
- Molecule 15: PsbP

Chain P:  21% 100%



- Molecule 15: PsbP

Chain p:  8% 99%



- Molecule 16: Photosystem II reaction center protein T

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: Photosystem II reaction center protein T

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: PsbW

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: PsbW

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: PsbX

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: PsbX

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: LHCII M3

Chain N:  100%



- Molecule 20: LHCII M3

Chain n: 100%



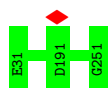
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G: 100%

There are no outlier residues recorded for this chain.

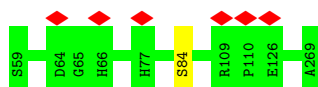
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain g: 100%



- Molecule 22: CP29

Chain R: 99%



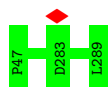
- Molecule 22: CP29

Chain r: 99%



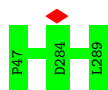
- Molecule 23: CP26

Chain S: 100%



- Molecule 23: CP26

Chain s: 100%



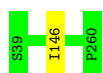
- Molecule 24: LHCII M1

Chain Y:  99%



- Molecule 24: LHCII M1

Chain y:  100%



- Molecule 25: PsbU

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: PsbU

Chain u:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-16.255	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.896, 0.896, 0.896	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/2717	0.50	0/3707
1	a	0.33	0/2717	0.50	0/3707
2	B	0.31	0/3906	0.50	0/5319
2	b	0.31	0/3906	0.50	0/5319
3	V	0.25	0/228	0.46	0/311
3	v	0.24	0/228	0.47	0/311
4	C	0.30	0/3602	0.49	0/4913
4	c	0.31	0/3602	0.49	0/4913
5	D	0.30	0/2860	0.49	0/3899
5	d	0.32	0/2860	0.49	0/3899
6	E	0.29	0/639	0.53	0/870
6	e	0.29	0/639	0.52	0/870
7	F	0.27	0/259	0.49	0/351
7	f	0.26	0/259	0.48	0/351
8	H	0.28	0/513	0.50	0/703
8	h	0.29	0/513	0.48	0/703
9	I	0.32	0/287	0.48	0/386
9	i	0.32	0/287	0.48	0/386
10	J	0.25	0/272	0.43	0/369
10	j	0.26	0/272	0.48	0/369
11	K	0.33	0/308	0.50	0/423
11	k	0.34	0/308	0.53	0/423
12	L	0.31	0/321	0.47	0/435
12	l	0.33	0/321	0.46	0/435
13	M	0.31	0/237	0.49	0/323
13	m	0.30	0/237	0.49	0/323
14	O	0.29	0/1855	0.54	0/2505
14	o	0.29	0/1855	0.55	0/2505
15	P	0.27	0/1473	0.53	0/1988
15	p	0.28	0/1473	0.52	0/1988
16	T	0.34	0/254	0.47	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.33	0/254	0.46	0/342
17	W	0.27	0/339	0.50	0/460
17	w	0.29	0/339	0.49	0/460
18	X	0.28	0/202	0.43	0/276
18	x	0.27	0/202	0.41	0/276
19	Z	0.26	0/469	0.40	0/641
19	z	0.26	0/469	0.42	0/641
20	N	0.29	0/1751	0.47	0/2386
20	n	0.29	0/1751	0.45	0/2386
21	G	0.27	0/1725	0.47	0/2348
21	g	0.28	0/1725	0.47	0/2348
22	R	0.27	0/1506	0.49	0/2035
22	r	0.27	0/1506	0.48	0/2035
23	S	0.28	0/1903	0.49	0/2590
23	s	0.29	0/1903	0.49	0/2590
24	Y	0.28	0/1715	0.48	1/2338 (0.0%)
24	y	0.29	0/1715	0.46	0/2338
25	U	0.27	0/224	0.58	0/298
25	u	0.35	0/224	0.75	0/298
All	All	0.30	0/59130	0.49	1/80432 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
24	Y	78	ALA	C-N-CA	-5.42	108.14	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
1	a	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	B	481/484 (99%)	470 (98%)	11 (2%)	0	100	100
2	b	481/484 (99%)	468 (97%)	13 (3%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
4	c	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
5	D	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	d	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
6	E	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h	65/67 (97%)	65 (100%)	0	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
14	o	236/238 (99%)	218 (92%)	18 (8%)	0	100	100
15	P	185/187 (99%)	175 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
16	t	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	34
20	n	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	34
21	G	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
21	g	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	R	191/196 (97%)	178 (93%)	13 (7%)	0	100	100
22	r	191/196 (97%)	174 (91%)	16 (8%)	1 (0%)	29	34
23	S	241/243 (99%)	228 (95%)	13 (5%)	0	100	100
23	s	241/243 (99%)	220 (91%)	21 (9%)	0	100	100
24	Y	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	29	34
24	y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	34
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	7334/7442 (98%)	7065 (96%)	264 (4%)	5 (0%)	54	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	r	176	LEU
24	y	146	ILE
24	Y	146	ILE
20	n	145	ILE
20	N	145	ILE

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	275/275 (100%)	275 (100%)	0	100	100
1	a	275/275 (100%)	275 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	150 (99%)	1 (1%)	84	90
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5934/5934 (100%)	5933 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
15	p	228	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
20	N	148	GLN
2	b	394	GLN
15	p	71	ASN
19	z	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	b	218	2	3,7,8	0.88	0	1,8,10	0.59	0
22	SEP	R	84	22	8,9,10	1.50	1 (12%)	8,12,14	1.64	2 (25%)
2	CSD	B	218	2	3,7,8	0.83	0	1,8,10	0.58	0
22	SEP	r	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.53	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	b	218	2	-	1/2/6/8	-
22	SEP	R	84	22	-	1/5/8/10	-
2	CSD	B	218	2	-	1/2/6/8	-
22	SEP	r	84	22	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.35	1.61	1.50
22	r	84	SEP	P-O1P	3.33	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	84	SEP	P-OG-CB	-3.02	109.98	118.30
22	r	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	R	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	r	84	SEP	P-OG-CB	-2.25	112.11	118.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	r	84	SEP	N-CA-CB-OG
22	r	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P
22	r	84	SEP	CB-OG-P-O3P
2	B	218	CSD	N-CA-CB-SG
2	b	218	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 8 are monoatomic - leaving 346 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
41	BCT	D	401	-	2,3,3	1.32	0	2,3,3	2.60	2 (100%)
46	LUT	n	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.89	12 (23%)
47	NEX	N	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.61	11 (22%)
38	3PH	T	101	-	47,47,47	0.84	3 (6%)	51,52,52	1.12	2 (3%)
45	CHL	n	606	-	66,74,74	0.95	3 (4%)	73,114,114	1.12	7 (9%)
29	CLA	r	608	-	60,68,73	1.06	4 (6%)	70,107,113	1.10	4 (5%)
29	CLA	s	610	23	65,73,73	1.01	4 (6%)	76,113,113	1.12	5 (6%)
29	CLA	S	610	23	65,73,73	1.02	3 (4%)	76,113,113	1.05	3 (3%)
29	CLA	S	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.02	3 (3%)
45	CHL	N	605	20	66,74,74	0.86	3 (4%)	73,114,114	1.21	7 (9%)
45	CHL	N	609	20	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	r	602	22	60,68,73	1.05	3 (5%)	70,107,113	1.11	4 (5%)
29	CLA	Y	608	52	50,58,73	1.15	3 (6%)	58,95,113	1.09	3 (5%)
33	SQD	B	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
29	CLA	B	606	-	65,73,73	1.00	3 (4%)	76,113,113	1.13	3 (3%)
46	LUT	s	621	-	42,43,43	2.29	1 (2%)	51,60,60	1.92	12 (23%)
34	SPH	A	414	-	19,20,20	0.64	0	18,21,21	1.07	1 (5%)
39	DGA	J	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.24	2 (6%)
29	CLA	n	613	20	65,73,73	1.01	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	a	405	-	65,73,73	1.03	3 (4%)	76,113,113	1.18	5 (6%)
45	CHL	S	601	23	46,54,74	1.06	4 (8%)	49,90,114	1.41	7 (14%)
31	BCR	a	411	-	41,41,41	1.83	5 (12%)	56,56,56	4.25	15 (26%)
29	CLA	B	614	-	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
40	LHG	l	101	-	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
31	BCR	c	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	20 (35%)
29	CLA	b	613	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	2 (2%)
35	LMG	C	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.04	2 (3%)
29	CLA	g	602	21	65,73,73	1.03	3 (4%)	76,113,113	0.99	3 (3%)
29	CLA	n	610	20	65,73,73	1.03	4 (6%)	76,113,113	1.16	6 (7%)
29	CLA	a	406	52	65,73,73	1.01	3 (4%)	76,113,113	1.08	6 (7%)
33	SQD	b	626	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
29	CLA	C	501	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
46	LUT	S	621	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
29	CLA	n	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.07	5 (6%)
46	LUT	R	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.01	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	c	503	-	65,73,73	1.03	3 (4%)	76,113,113	0.95	4 (5%)
29	CLA	N	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.89	3 (3%)
29	CLA	D	402	-	65,73,73	1.01	3 (4%)	76,113,113	1.02	2 (2%)
45	CHL	g	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.38	10 (19%)
29	CLA	b	610	-	65,73,73	1.02	3 (4%)	76,113,113	1.07	4 (5%)
29	CLA	s	612	23	45,53,73	1.23	3 (6%)	52,89,113	1.12	3 (5%)
46	LUT	G	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	13 (25%)
45	CHL	G	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.26	10 (13%)
45	CHL	n	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.25	9 (12%)
31	BCR	B	618	-	41,41,41	1.86	5 (12%)	56,56,56	4.22	19 (33%)
29	CLA	r	603	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	7 (10%)
29	CLA	c	501	-	65,73,73	1.02	3 (4%)	76,113,113	1.02	5 (6%)
29	CLA	R	602	22	60,68,73	1.06	3 (5%)	70,107,113	1.09	4 (5%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
29	CLA	b	609	-	65,73,73	0.99	3 (4%)	76,113,113	0.98	1 (1%)
45	CHL	y	601	24	66,74,74	0.89	3 (4%)	73,114,114	1.19	10 (13%)
45	CHL	y	607	-	66,74,74	0.79	2 (3%)	73,114,114	1.27	11 (15%)
45	CHL	y	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	8 (16%)
29	CLA	C	507	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	3 (3%)
29	CLA	s	617	23	50,58,73	1.16	3 (6%)	58,95,113	1.21	6 (10%)
38	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.10	2 (3%)
26	OEX	a	401	52,1,4	0,15,15	-	-	-	-	-
35	LMG	A	413	-	40,40,55	0.76	2 (5%)	48,48,63	1.15	4 (8%)
29	CLA	d	402	-	65,73,73	1.01	4 (6%)	76,113,113	1.03	2 (2%)
50	LPX	s	625	-	18,18,29	1.23	2 (11%)	20,22,33	1.03	1 (5%)
29	CLA	Y	614	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	3 (3%)
29	CLA	B	610	-	65,73,73	1.02	4 (6%)	76,113,113	1.05	3 (3%)
45	CHL	n	605	20	66,74,74	0.91	4 (6%)	73,114,114	1.25	12 (16%)
29	CLA	S	609	23	60,68,73	1.06	3 (5%)	70,107,113	1.08	3 (4%)
29	CLA	b	606	-	65,73,73	1.01	3 (4%)	76,113,113	1.14	4 (5%)
29	CLA	b	614	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	2 (2%)
35	LMG	c	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.11	3 (5%)
45	CHL	G	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.26	11 (15%)
51	PTY	y	627	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
33	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	Y	606	-	66,74,74	0.94	4 (6%)	73,114,114	1.15	9 (12%)
29	CLA	n	612	20	45,53,73	1.23	3 (6%)	52,89,113	1.10	4 (7%)
29	CLA	G	611	-	65,73,73	1.02	3 (4%)	76,113,113	1.06	3 (3%)
29	CLA	Y	602	24	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
47	NEX	n	623	-	38,46,46	3.36	9 (23%)	50,70,70	1.60	10 (20%)
48	XAT	G	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	B	602	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
43	HEM	f	101	7,6	41,50,50	1.44	4 (9%)	45,82,82	1.30	4 (8%)
29	CLA	R	608	-	60,68,73	1.06	4 (6%)	70,107,113	1.04	3 (4%)
45	CHL	y	606	52	51,59,74	0.97	3 (5%)	55,96,114	1.39	11 (20%)
29	CLA	y	611	40	65,73,73	1.02	3 (4%)	76,113,113	0.96	3 (3%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	13 (23%)
29	CLA	Y	612	24	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
46	LUT	r	620	-	42,43,43	2.42	2 (4%)	51,60,60	1.94	14 (27%)
34	SPH	a	414	-	19,20,20	0.65	0	18,21,21	1.08	1 (5%)
45	CHL	N	601	20	66,74,74	0.82	3 (4%)	73,114,114	1.23	10 (13%)
47	NEX	Y	623	-	38,46,46	3.31	9 (23%)	50,70,70	1.84	11 (22%)
45	CHL	r	606	-	44,52,74	1.07	3 (6%)	46,87,114	1.35	8 (17%)
29	CLA	A	410	-	60,68,73	1.04	3 (5%)	70,107,113	1.10	4 (5%)
48	XAT	R	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.87	13 (24%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.02	2 (4%)
30	PHO	a	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.25	5 (10%)
31	BCR	c	515	-	41,41,41	1.82	5 (12%)	56,56,56	4.17	19 (33%)
29	CLA	B	617	-	55,63,73	1.10	4 (7%)	64,101,113	1.08	3 (4%)
29	CLA	B	605	-	65,73,73	1.01	3 (4%)	76,113,113	1.21	6 (7%)
48	XAT	N	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.00	14 (25%)
36	C7Z	b	620	-	43,43,43	5.29	27 (62%)	58,60,60	2.41	24 (41%)
35	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.08	3 (5%)
29	CLA	R	612	-	50,58,73	1.17	3 (6%)	58,95,113	1.08	4 (6%)
29	CLA	y	602	24	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	s	609	-	60,68,73	1.05	3 (5%)	70,107,113	1.08	3 (4%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.04	2 (4%)
33	SQD	b	621	-	41,42,54	0.87	0	50,53,65	0.96	3 (6%)
29	CLA	N	604	-	65,73,73	1.01	3 (4%)	76,113,113	1.02	4 (5%)
29	CLA	S	604	-	55,63,73	1.11	3 (5%)	64,101,113	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	DGD	c	520	-	60,60,67	1.06	6 (10%)	74,74,81	0.95	2 (2%)
46	LUT	g	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.96	13 (25%)
33	SQD	m	101	-	41,42,54	0.88	0	50,53,65	0.96	3 (6%)
45	CHL	Y	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.22	10 (13%)
29	CLA	R	603	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	5 (7%)
37	DGD	c	519	-	63,63,67	1.11	7 (11%)	77,77,81	0.94	3 (3%)
29	CLA	Y	603	-	65,73,73	1.02	3 (4%)	76,113,113	0.93	2 (2%)
29	CLA	C	511	4	65,73,73	1.04	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	b	616	-	65,73,73	1.01	3 (4%)	76,113,113	0.91	2 (2%)
40	LHG	d	410	-	38,38,48	0.41	0	41,44,54	1.09	2 (4%)
35	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
46	LUT	N	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	12 (23%)
40	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.05	2 (4%)
45	CHL	N	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.14	9 (12%)
29	CLA	b	602	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	4 (5%)
45	CHL	g	605	21	48,56,74	1.00	3 (6%)	51,92,114	1.31	9 (17%)
29	CLA	B	607	-	65,73,73	1.02	3 (4%)	76,113,113	1.05	4 (5%)
45	CHL	s	608	-	61,69,74	0.88	3 (4%)	67,108,114	1.26	10 (14%)
49	LMT	R	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.18	5 (10%)
29	CLA	c	511	4	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
29	CLA	b	617	-	65,73,73	1.01	4 (6%)	76,113,113	0.98	3 (3%)
29	CLA	B	603	-	65,73,73	1.00	3 (4%)	76,113,113	1.06	2 (2%)
29	CLA	g	610	21	65,73,73	1.01	4 (6%)	76,113,113	1.25	5 (6%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.08	1 (5%)
29	CLA	C	510	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	3 (3%)
45	CHL	S	607	-	43,51,74	1.03	3 (6%)	45,86,114	1.47	9 (20%)
29	CLA	B	608	52	65,73,73	0.99	3 (4%)	76,113,113	1.01	3 (3%)
51	PTY	Y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.45	2 (9%)
45	CHL	Y	609	24	66,74,74	0.84	3 (4%)	73,114,114	1.27	11 (15%)
46	LUT	Y	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	15 (29%)
46	LUT	g	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	12 (23%)
31	BCR	A	411	-	41,41,41	1.84	5 (12%)	56,56,56	4.27	15 (26%)
29	CLA	C	509	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
33	SQD	C	526	-	35,36,54	0.94	0	44,47,65	1.04	2 (4%)
29	CLA	C	504	52	55,63,73	1.08	3 (5%)	64,101,113	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	S	602	23	60,68,73	1.06	3 (5%)	70,107,113	0.99	4 (5%)
29	CLA	r	612	-	51,59,73	1.17	3 (5%)	59,96,113	1.24	5 (8%)
35	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.07	3 (5%)
40	LHG	g	624	29	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
40	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
29	CLA	b	612	-	65,73,73	1.03	3 (4%)	76,113,113	1.08	4 (5%)
40	LHG	n	624	-	41,41,48	0.41	0	44,47,54	1.15	4 (9%)
40	LHG	c	497	-	37,37,48	0.44	0	40,43,54	1.16	3 (7%)
45	CHL	g	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.36	14 (19%)
47	NEX	S	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.80	13 (26%)
29	CLA	A	406	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	d	403	-	65,73,73	1.02	3 (4%)	76,113,113	1.09	5 (6%)
29	CLA	a	407	52	49,57,73	1.15	3 (6%)	55,93,113	1.18	4 (7%)
48	XAT	r	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.89	11 (20%)
29	CLA	g	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.00	2 (2%)
29	CLA	r	609	22	60,68,73	1.08	3 (5%)	70,107,113	1.04	4 (5%)
29	CLA	c	509	-	65,73,73	1.03	3 (4%)	76,113,113	1.06	4 (5%)
36	C7Z	B	620	-	43,43,43	5.30	27 (62%)	58,60,60	2.46	23 (39%)
29	CLA	c	510	-	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)
29	CLA	G	602	21	65,73,73	1.04	3 (4%)	76,113,113	0.96	3 (3%)
50	LPX	S	625	-	19,19,29	1.20	2 (10%)	21,23,33	1.04	1 (4%)
51	PTY	y	626	-	49,49,49	0.88	4 (8%)	52,54,54	1.05	2 (3%)
34	SPH	y	625	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
45	CHL	g	608	-	44,52,74	1.06	3 (6%)	46,87,114	1.46	10 (21%)
45	CHL	G	609	21	66,74,74	0.86	3 (4%)	73,114,114	1.24	12 (16%)
37	DGD	C	520	-	54,54,67	0.93	4 (7%)	68,68,81	0.90	2 (2%)
29	CLA	s	605	23	50,58,73	1.14	3 (6%)	58,95,113	1.24	6 (10%)
45	CHL	n	608	-	50,58,74	0.93	2 (4%)	52,94,114	1.44	11 (21%)
29	CLA	s	604	-	55,63,73	1.10	3 (5%)	64,101,113	1.20	3 (4%)
45	CHL	y	609	24	66,74,74	0.86	3 (4%)	73,114,114	1.35	12 (16%)
29	CLA	b	608	52	65,73,73	0.99	3 (4%)	76,113,113	1.09	2 (2%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	1.23	3 (5%)
29	CLA	C	502	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
29	CLA	s	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.06	4 (5%)
51	PTY	Y	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	h	102	-	48,48,55	0.99	4 (8%)	56,56,63	1.11	2 (3%)
44	RRX	h	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.50	23 (40%)
31	BCR	C	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
30	PHO	A	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.20	4 (8%)
31	BCR	D	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.13	14 (25%)
29	CLA	b	615	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
29	CLA	c	505	-	65,73,73	1.02	4 (6%)	76,113,113	1.08	3 (3%)
29	CLA	G	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.91	1 (1%)
46	LUT	S	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.85	10 (19%)
29	CLA	y	608	-	50,58,73	1.16	3 (6%)	58,95,113	1.08	3 (5%)
40	LHG	y	624	29	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
30	PHO	A	408	-	51,69,69	0.98	4 (7%)	47,99,99	1.20	5 (10%)
45	CHL	S	606	-	44,52,74	1.08	3 (6%)	46,87,114	1.34	7 (15%)
29	CLA	A	407	-	50,58,73	1.15	3 (6%)	58,95,113	1.09	4 (6%)
29	CLA	a	410	-	60,68,73	1.03	3 (5%)	70,107,113	1.11	5 (7%)
45	CHL	G	606	-	50,58,74	1.03	4 (8%)	52,94,114	1.41	9 (17%)
29	CLA	C	508	-	65,73,73	1.01	3 (4%)	76,113,113	1.08	5 (6%)
45	CHL	Y	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	9 (18%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
47	NEX	g	623	-	38,46,46	3.29	9 (23%)	50,70,70	1.87	13 (26%)
29	CLA	g	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.09	4 (7%)
35	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.16	3 (6%)
29	CLA	N	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.00	5 (6%)
47	NEX	y	623	-	38,46,46	3.31	11 (28%)	50,70,70	1.82	13 (26%)
29	CLA	B	613	-	65,73,73	1.00	3 (4%)	76,113,113	1.05	2 (2%)
29	CLA	y	614	-	65,73,73	1.03	3 (4%)	76,113,113	1.02	5 (6%)
29	CLA	g	603	-	65,73,73	1.01	3 (4%)	76,113,113	0.98	3 (3%)
44	RRX	H	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.58	22 (38%)
40	LHG	s	624	29	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
40	LHG	G	624	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
29	CLA	y	603	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	2 (2%)
33	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	c	504	-	65,73,73	0.98	3 (4%)	76,113,113	1.05	3 (3%)
35	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.12	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G	612	21	43,51,73	1.22	3 (6%)	49,86,113	1.06	3 (6%)
35	LMG	C	527	-	42,42,55	0.78	2 (4%)	50,50,63	1.17	4 (8%)
45	CHL	N	607	-	66,74,74	0.89	3 (4%)	73,114,114	1.25	12 (16%)
49	LMT	r	625	-	36,36,36	1.24	6 (16%)	47,47,47	1.16	4 (8%)
29	CLA	b	604	-	65,73,73	1.00	3 (4%)	76,113,113	1.12	3 (3%)
29	CLA	g	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
47	NEX	G	623	-	38,46,46	3.31	9 (23%)	50,70,70	1.83	15 (30%)
29	CLA	C	512	-	65,73,73	1.02	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	c	508	-	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
35	LMG	w	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
29	CLA	G	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.94	3 (3%)
37	DGD	b	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.19	5 (8%)
45	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.44	10 (19%)
45	CHL	s	607	-	43,51,74	1.09	3 (6%)	45,86,114	1.45	7 (15%)
46	LUT	y	620	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	13 (25%)
29	CLA	C	506	-	65,73,73	1.01	3 (4%)	76,113,113	0.94	3 (3%)
40	LHG	C	525	-	34,34,48	0.44	0	37,40,54	1.17	2 (5%)
29	CLA	N	612	20	45,53,73	1.22	3 (6%)	52,89,113	1.03	4 (7%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	18 (32%)
29	CLA	G	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.02	2 (3%)
29	CLA	N	613	20	65,73,73	1.03	3 (4%)	76,113,113	0.96	2 (2%)
47	NEX	R	622	-	24,28,46	3.24	6 (25%)	32,42,70	1.76	7 (21%)
45	CHL	s	601	23	46,54,74	1.05	4 (8%)	49,90,114	1.41	9 (18%)
29	CLA	B	609	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	2 (2%)
37	DGD	C	518	-	52,52,67	1.02	4 (7%)	66,66,81	0.93	2 (3%)
39	DGA	B	625	-	36,36,43	1.19	2 (5%)	38,38,45	1.30	3 (7%)
31	BCR	B	619	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
29	CLA	C	513	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	2 (2%)
29	CLA	C	503	-	65,73,73	1.03	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	g	604	-	49,57,73	1.16	3 (6%)	55,93,113	1.11	3 (5%)
29	CLA	D	403	-	60,68,73	1.07	3 (5%)	70,107,113	1.14	4 (5%)
31	BCR	C	514	-	41,41,41	1.82	4 (9%)	56,56,56	4.21	14 (25%)
29	CLA	N	611	40	49,57,73	1.17	3 (6%)	55,93,113	1.09	3 (5%)
29	CLA	y	613	24	65,73,73	1.00	3 (4%)	76,113,113	0.89	1 (1%)
29	CLA	s	602	23	60,68,73	1.05	3 (5%)	70,107,113	1.14	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	d	404	-	41,41,41	1.82	4 (9%)	56,56,56	4.27	17 (30%)
40	LHG	S	624	29	44,44,48	0.41	0	47,50,54	1.04	3 (6%)
45	CHL	n	609	20	66,74,74	0.82	2 (3%)	73,114,114	1.31	12 (16%)
29	CLA	N	614	-	49,57,73	1.16	3 (6%)	55,93,113	1.05	4 (7%)
29	CLA	c	507	52	65,73,73	1.03	4 (6%)	76,113,113	1.10	4 (5%)
45	CHL	S	608	-	61,69,74	0.90	3 (4%)	67,108,114	1.36	12 (17%)
45	CHL	n	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.26	12 (16%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.94	2 (2%)
39	DGA	c	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	A	405	-	65,73,73	1.01	3 (4%)	76,113,113	1.05	4 (5%)
48	XAT	n	622	-	39,47,47	0.73	1 (2%)	54,74,74	2.03	13 (24%)
29	CLA	B	615	-	65,73,73	1.04	3 (4%)	76,113,113	1.08	3 (3%)
41	BCT	d	401	27	2,3,3	1.15	0	2,3,3	4.30	2 (100%)
29	CLA	B	612	-	65,73,73	1.02	3 (4%)	76,113,113	1.11	5 (6%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.18	2 (3%)
29	CLA	b	607	-	57,65,73	1.07	3 (5%)	66,103,113	1.08	3 (4%)
29	CLA	S	612	23	45,53,73	1.23	3 (6%)	52,89,113	1.03	4 (7%)
45	CHL	Y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.23	10 (13%)
45	CHL	g	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
29	CLA	c	502	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	4 (5%)
29	CLA	n	604	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	3 (3%)
29	CLA	N	610	-	65,73,73	1.01	3 (4%)	76,113,113	1.11	3 (3%)
29	CLA	G	610	21	65,73,73	1.02	3 (4%)	76,113,113	1.21	5 (6%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
48	XAT	g	622	-	39,47,47	0.73	1 (2%)	54,74,74	1.99	13 (24%)
40	LHG	Y	624	29	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
29	CLA	n	611	-	49,57,73	1.16	3 (6%)	55,93,113	1.04	3 (5%)
38	3PH	S	626	-	29,29,47	1.09	4 (13%)	33,34,52	1.24	2 (6%)
29	CLA	y	610	24	65,73,73	1.00	4 (6%)	76,113,113	1.11	4 (5%)
47	NEX	s	623	-	38,46,46	3.36	9 (23%)	50,70,70	1.67	10 (20%)
29	CLA	s	614	-	55,63,73	1.10	3 (5%)	64,101,113	1.03	3 (4%)
33	SQD	M	101	-	41,42,54	0.89	0	50,53,65	0.96	3 (6%)
46	LUT	n	621	-	42,43,43	2.32	1 (2%)	51,60,60	1.81	12 (23%)
29	CLA	r	604	-	49,57,73	1.15	3 (6%)	55,93,113	1.03	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G	604	-	49,57,73	1.19	3 (6%)	55,93,113	1.07	4 (7%)
33	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.93	2 (3%)
29	CLA	s	603	-	65,73,73	1.02	4 (6%)	76,113,113	1.17	5 (6%)
29	CLA	c	513	-	65,73,73	1.01	3 (4%)	76,113,113	1.04	3 (3%)
30	PHO	a	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.22	5 (10%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	R	604	-	49,57,73	1.16	3 (6%)	55,93,113	1.03	1 (1%)
39	DGA	C	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.49	3 (6%)
35	LMG	H	102	-	48,48,55	0.99	4 (8%)	56,56,63	1.08	2 (3%)
31	BCR	b	619	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
29	CLA	S	605	23	50,58,73	1.15	3 (6%)	58,95,113	1.32	3 (5%)
45	CHL	R	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.39	9 (17%)
29	CLA	b	603	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	3 (3%)
29	CLA	y	612	24	65,73,73	1.01	3 (4%)	76,113,113	1.02	3 (3%)
46	LUT	N	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.88	13 (25%)
29	CLA	r	610	22	60,68,73	1.07	3 (5%)	70,107,113	1.17	5 (7%)
29	CLA	c	512	-	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
29	CLA	b	611	52	65,73,73	1.01	3 (4%)	76,113,113	0.92	1 (1%)
35	LMG	D	411	-	42,42,55	0.76	2 (4%)	50,50,63	0.97	2 (4%)
46	LUT	Y	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
29	CLA	Y	613	24	65,73,73	1.01	3 (4%)	76,113,113	0.88	1 (1%)
46	LUT	G	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.93	11 (21%)
48	XAT	Y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.75	20 (37%)
42	PL9	D	405	-	55,55,55	1.34	6 (10%)	68,69,69	1.47	11 (16%)
35	LMG	d	411	-	46,46,55	0.91	3 (6%)	54,54,63	1.05	2 (3%)
33	SQD	A	412	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
45	CHL	G	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.39	8 (15%)
29	CLA	S	603	-	65,73,73	1.03	4 (6%)	76,113,113	1.18	7 (9%)
45	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.40	8 (17%)
47	NEX	r	622	-	24,28,46	3.23	6 (25%)	32,42,70	1.83	7 (21%)
29	CLA	S	617	23	50,58,73	1.18	3 (6%)	58,95,113	1.27	6 (10%)
29	CLA	Y	604	52	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)
29	CLA	b	605	-	65,73,73	1.02	4 (6%)	76,113,113	1.22	5 (6%)
29	CLA	B	604	-	65,73,73	0.99	3 (4%)	76,113,113	1.12	5 (6%)
29	CLA	S	614	-	50,58,73	1.16	3 (6%)	58,95,113	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	s	613	23	55,63,73	1.11	3 (5%)	64,101,113	1.10	3 (4%)
29	CLA	S	613	23	55,63,73	1.12	3 (5%)	64,101,113	1.14	3 (4%)
29	CLA	Y	611	40	65,73,73	1.01	3 (4%)	76,113,113	1.01	6 (7%)
29	CLA	g	612	21	43,51,73	1.20	3 (6%)	49,86,113	1.11	2 (4%)
29	CLA	y	604	52	65,73,73	1.00	3 (4%)	76,113,113	1.11	5 (6%)
42	PL9	d	405	-	55,55,55	1.28	5 (9%)	68,69,69	1.51	11 (16%)
29	CLA	c	506	-	60,68,73	1.05	3 (5%)	70,107,113	1.10	5 (7%)
29	CLA	B	616	-	65,73,73	1.00	3 (4%)	76,113,113	0.89	2 (2%)
46	LUT	s	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.99	15 (29%)
29	CLA	R	609	22	46,54,73	1.19	3 (6%)	53,90,113	1.19	4 (7%)
29	CLA	B	611	52	65,73,73	1.01	3 (4%)	76,113,113	0.93	2 (2%)
37	DGD	C	519	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	3 (4%)
38	3PH	b	624	-	38,38,47	0.96	4 (10%)	42,43,52	1.17	2 (4%)
45	CHL	g	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
45	CHL	s	606	-	44,52,74	0.98	2 (4%)	46,87,114	1.45	8 (17%)
31	BCR	b	618	-	41,41,41	1.85	4 (9%)	56,56,56	4.22	15 (26%)
37	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
29	CLA	n	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.20	3 (5%)
43	HEM	F	101	7,6	41,50,50	1.45	3 (7%)	45,82,82	1.36	5 (11%)
46	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	13 (25%)
48	XAT	y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
26	OEX	A	401	52,1,4	0,15,15	-	-	-	-	-
29	CLA	Y	610	24	65,73,73	1.01	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	n	603	-	65,73,73	1.01	3 (4%)	76,113,113	1.00	4 (5%)
29	CLA	C	505	-	60,68,73	1.07	4 (6%)	70,107,113	1.04	2 (2%)
31	BCR	c	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	19 (33%)
40	LHG	N	624	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)
35	LMG	b	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.07	2 (3%)
29	CLA	R	610	22	60,68,73	1.06	3 (5%)	70,107,113	1.08	4 (5%)
45	CHL	r	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.44	8 (15%)
45	CHL	R	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	8 (17%)

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	LUT	n	620	-	-	4/29/67/67	0/2/2/2
47	NEX	N	623	-	-	2/27/83/83	1/3/3/3
38	3PH	T	101	-	-	27/49/49/49	-
45	CHL	n	606	-	4/4/20/26	9/39/137/137	-
29	CLA	r	608	-	1/1/14/20	13/31/109/115	-
29	CLA	s	610	23	1/1/15/20	11/37/115/115	-
29	CLA	S	610	23	1/1/15/20	10/37/115/115	-
29	CLA	S	611	40	1/1/15/20	17/37/115/115	-
45	CHL	N	605	20	4/4/20/26	15/39/137/137	-
45	CHL	N	609	20	4/4/20/26	6/39/137/137	-
29	CLA	r	602	22	1/1/14/20	7/31/109/115	-
29	CLA	Y	608	52	1/1/12/20	8/19/97/115	-
33	SQD	B	626	-	-	14/49/69/69	0/1/1/1
29	CLA	B	606	-	1/1/15/20	8/37/115/115	-
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
34	SPH	A	414	-	-	10/21/21/21	-
39	DGA	J	101	-	-	14/30/30/45	-
29	CLA	n	613	20	-	14/37/115/115	-
29	CLA	a	405	-	1/1/15/20	12/37/115/115	-
45	CHL	S	601	23	3/3/16/26	3/15/113/137	-
31	BCR	a	411	-	-	9/29/63/63	0/2/2/2
29	CLA	B	614	-	1/1/15/20	11/37/115/115	-
40	LHG	l	101	-	-	31/53/53/53	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	b	613	-	1/1/15/20	10/37/115/115	-
35	LMG	C	523	-	-	21/50/70/70	0/1/1/1
29	CLA	g	602	21	1/1/15/20	16/37/115/115	-
29	CLA	n	610	20	1/1/15/20	11/37/115/115	-
29	CLA	a	406	52	1/1/15/20	15/37/115/115	-
33	SQD	b	626	-	-	19/49/69/69	0/1/1/1
29	CLA	C	501	-	-	13/37/115/115	-
46	LUT	S	621	-	-	3/29/67/67	0/2/2/2
29	CLA	n	602	20	1/1/15/20	11/37/115/115	-
46	LUT	R	620	-	-	5/29/67/67	0/2/2/2
29	CLA	c	503	-	-	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	603	-	1/1/15/20	21/37/115/115	-
29	CLA	D	402	-	1/1/15/20	6/37/115/115	-
45	CHL	g	606	-	3/3/16/26	3/20/118/137	-
29	CLA	b	610	-	1/1/15/20	5/37/115/115	-
29	CLA	s	612	23	1/1/11/20	2/13/91/115	-
46	LUT	G	620	-	-	0/29/67/67	0/2/2/2
45	CHL	G	601	21	4/4/20/26	11/39/137/137	-
45	CHL	n	601	20	4/4/20/26	12/39/137/137	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
29	CLA	r	603	-	-	12/31/109/115	-
29	CLA	c	501	-	-	13/37/115/115	-
29	CLA	R	602	22	1/1/14/20	6/31/109/115	-
39	DGA	j	101	-	-	16/30/30/45	-
29	CLA	b	609	-	-	4/37/115/115	-
45	CHL	y	601	24	4/4/20/26	8/39/137/137	-
45	CHL	y	607	-	4/4/20/26	12/39/137/137	-
45	CHL	y	605	24	3/3/16/26	4/15/113/137	-
29	CLA	C	507	52	1/1/15/20	12/37/115/115	-
29	CLA	s	617	23	1/1/12/20	5/19/97/115	-
38	3PH	s	626	-	-	23/49/49/49	-
35	LMG	A	413	-	-	10/35/55/70	0/1/1/1
29	CLA	d	402	-	1/1/15/20	5/37/115/115	-
50	LPX	s	625	-	-	10/20/20/31	-
29	CLA	Y	614	-	1/1/15/20	13/37/115/115	-
29	CLA	B	610	-	1/1/15/20	12/37/115/115	-
45	CHL	n	605	20	4/4/20/26	11/39/137/137	-
29	CLA	S	609	23	1/1/14/20	9/31/109/115	-
29	CLA	b	606	-	1/1/15/20	9/37/115/115	-
29	CLA	b	614	-	1/1/15/20	11/37/115/115	-
45	CHL	G	607	-	4/4/20/26	13/39/137/137	-
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
51	PTY	y	627	-	-	14/20/20/53	-
33	SQD	B	621	-	-	14/37/57/69	0/1/1/1
45	CHL	Y	606	-	4/4/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	n	612	20	1/1/11/20	6/13/91/115	-
29	CLA	G	611	-	1/1/15/20	11/37/115/115	-
29	CLA	Y	602	24	1/1/15/20	12/37/115/115	-
48	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
47	NEX	n	623	-	-	2/27/83/83	1/3/3/3
29	CLA	B	602	-	1/1/15/20	18/37/115/115	-
43	HEM	f	101	7,6	-	1/12/54/54	-
29	CLA	R	608	-	1/1/14/20	11/31/109/115	-
45	CHL	y	606	52	3/3/17/26	2/21/119/137	-
29	CLA	y	611	40	1/1/15/20	6/37/115/115	-
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
29	CLA	Y	612	24	1/1/15/20	13/37/115/115	-
46	LUT	r	620	-	-	5/29/67/67	0/2/2/2
34	SPH	a	414	-	-	11/21/21/21	-
45	CHL	N	601	20	4/4/20/26	9/39/137/137	-
47	NEX	Y	623	-	-	8/27/83/83	0/3/3/3
45	CHL	r	606	-	3/3/15/26	4/13/111/137	-
48	XAT	R	621	-	2/2/12/26	0/31/93/93	0/4/4/4
29	CLA	A	410	-	-	8/31/109/115	-
40	LHG	D	408	-	-	16/48/48/53	-
30	PHO	a	409	-	-	6/37/103/103	0/5/6/6
31	BCR	c	515	-	-	13/29/63/63	0/2/2/2
29	CLA	B	617	-	1/1/13/20	11/25/103/115	-
29	CLA	B	605	-	1/1/15/20	16/37/115/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
36	C7Z	b	620	-	1/1/12/26	7/29/67/67	0/2/2/2
35	LMG	B	622	-	-	13/39/59/70	0/1/1/1
29	CLA	R	612	-	1/1/12/20	9/19/97/115	-
29	CLA	y	602	24	1/1/15/20	6/37/115/115	-
29	CLA	s	609	-	1/1/14/20	17/31/109/115	-
40	LHG	D	410	-	-	18/43/43/53	-
33	SQD	b	621	-	-	13/37/57/69	0/1/1/1
29	CLA	N	604	-	1/1/15/20	8/37/115/115	-
29	CLA	S	604	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	c	520	-	-	8/48/88/95	0/2/2/2
46	LUT	g	620	-	-	2/29/67/67	0/2/2/2
33	SQD	m	101	-	-	21/37/57/69	0/1/1/1
45	CHL	Y	601	24	4/4/20/26	5/39/137/137	-
29	CLA	R	603	-	-	11/31/109/115	-
37	DGD	c	519	-	-	17/51/91/95	0/2/2/2
29	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
29	CLA	C	511	4	1/1/15/20	5/37/115/115	-
29	CLA	b	616	-	1/1/15/20	12/37/115/115	-
40	LHG	d	410	-	-	21/43/43/53	-
35	LMG	c	523	-	-	13/50/70/70	0/1/1/1
46	LUT	N	621	-	-	3/29/67/67	0/2/2/2
40	LHG	d	408	-	-	22/48/48/53	-
45	CHL	N	606	-	4/4/20/26	9/39/137/137	-
29	CLA	b	602	-	1/1/15/20	22/37/115/115	-
45	CHL	g	605	21	3/3/16/26	4/18/116/137	-
29	CLA	B	607	-	1/1/15/20	14/37/115/115	-
45	CHL	s	608	-	4/4/19/26	5/33/131/137	-
49	LMT	R	625	-	-	2/21/61/61	0/2/2/2
29	CLA	c	511	4	-	12/37/115/115	-
29	CLA	b	617	-	1/1/15/20	15/37/115/115	-
29	CLA	B	603	-	1/1/15/20	4/37/115/115	-
29	CLA	g	610	21	1/1/15/20	5/37/115/115	-
34	SPH	Y	625	-	-	11/21/21/21	-
29	CLA	C	510	-	1/1/15/20	14/37/115/115	-
45	CHL	S	607	-	3/3/15/26	0/12/110/137	-
29	CLA	B	608	52	1/1/15/20	23/37/115/115	-
51	PTY	Y	627	-	-	12/20/20/53	-
45	CHL	Y	609	24	4/4/20/26	6/39/137/137	-
46	LUT	Y	620	-	-	2/29/67/67	0/2/2/2
46	LUT	g	621	-	-	1/29/67/67	0/2/2/2
31	BCR	A	411	-	-	9/29/63/63	0/2/2/2
29	CLA	C	509	-	1/1/15/20	16/37/115/115	-
33	SQD	C	526	-	-	12/31/51/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	504	52	1/1/13/20	8/25/103/115	-
29	CLA	S	602	23	1/1/14/20	10/31/109/115	-
29	CLA	r	612	-	1/1/12/20	9/21/99/115	-
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
40	LHG	g	624	29	-	30/53/53/53	-
40	LHG	d	409	-	-	22/53/53/53	-
29	CLA	b	612	-	-	12/37/115/115	-
40	LHG	n	624	-	-	30/46/46/53	-
40	LHG	c	497	-	-	19/42/42/53	-
45	CHL	g	607	-	4/4/20/26	10/39/137/137	-
47	NEX	S	623	-	-	2/27/83/83	0/3/3/3
29	CLA	A	406	52	1/1/15/20	16/37/115/115	-
29	CLA	d	403	-	1/1/15/20	10/37/115/115	-
48	XAT	r	621	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	a	407	52	-	5/18/96/115	-
29	CLA	g	611	40	1/1/15/20	8/37/115/115	-
29	CLA	r	609	22	1/1/14/20	13/31/109/115	-
29	CLA	c	509	-	1/1/15/20	14/37/115/115	-
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	c	510	-	1/1/15/20	9/37/115/115	-
29	CLA	G	602	21	1/1/15/20	14/37/115/115	-
50	LPX	S	625	-	-	7/21/21/31	-
51	PTY	y	626	-	-	28/53/53/53	-
34	SPH	y	625	-	-	3/21/21/21	-
45	CHL	g	608	-	3/3/15/26	0/13/111/137	-
45	CHL	G	609	21	4/4/20/26	11/39/137/137	-
37	DGD	C	520	-	-	5/42/82/95	0/2/2/2
29	CLA	s	605	23	-	6/19/97/115	-
45	CHL	n	608	-	3/3/16/26	3/20/118/137	-
29	CLA	s	604	-	1/1/13/20	11/25/103/115	-
45	CHL	y	609	24	4/4/20/26	6/39/137/137	-
29	CLA	b	608	52	1/1/15/20	7/37/115/115	-
40	LHG	L	101	-	-	33/53/53/53	-
29	CLA	C	502	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	611	40	1/1/15/20	14/37/115/115	-
51	PTY	Y	626	-	-	18/53/53/53	-
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
44	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
31	BCR	C	515	-	-	10/29/63/63	0/2/2/2
30	PHO	A	409	-	-	4/37/103/103	0/5/6/6
31	BCR	D	404	-	-	12/29/63/63	0/2/2/2
29	CLA	b	615	-	1/1/15/20	13/37/115/115	-
29	CLA	c	505	-	1/1/15/20	18/37/115/115	-
29	CLA	G	613	21	1/1/15/20	10/37/115/115	-
46	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	y	608	-	1/1/12/20	8/19/97/115	-
40	LHG	y	624	29	-	28/53/53/53	-
40	LHG	c	525	-	-	30/51/51/53	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
45	CHL	S	606	-	3/3/15/26	1/13/111/137	-
29	CLA	A	407	-	1/1/12/20	8/19/97/115	-
45	CHL	G	606	-	3/3/16/26	5/20/118/137	-
29	CLA	a	410	-	-	8/31/109/115	-
29	CLA	C	508	-	1/1/15/20	7/37/115/115	-
45	CHL	Y	605	24	3/3/16/26	5/15/113/137	-
38	3PH	B	624	-	-	20/49/49/49	-
47	NEX	g	623	-	-	5/27/83/83	0/3/3/3
29	CLA	g	614	-	1/1/11/20	9/18/96/115	-
35	LMG	W	201	-	-	16/34/54/70	0/1/1/1
29	CLA	N	602	20	1/1/15/20	14/37/115/115	-
47	NEX	y	623	-	-	8/27/83/83	0/3/3/3
29	CLA	B	613	-	1/1/15/20	9/37/115/115	-
29	CLA	y	614	-	1/1/15/20	14/37/115/115	-
29	CLA	g	603	-	1/1/15/20	20/37/115/115	-
44	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
40	LHG	s	624	29	-	22/49/49/53	-
40	LHG	G	624	-	-	29/53/53/53	-
29	CLA	y	603	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SQD	c	526	-	-	15/49/69/69	0/1/1/1
29	CLA	c	504	-	1/1/15/20	12/37/115/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
29	CLA	G	612	21	1/1/10/20	3/11/89/115	-
35	LMG	C	527	-	-	19/37/57/70	0/1/1/1
45	CHL	N	607	-	4/4/20/26	12/39/137/137	-
49	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	b	604	-	1/1/15/20	8/37/115/115	-
29	CLA	g	613	21	-	21/37/115/115	-
47	NEX	G	623	-	-	4/27/83/83	0/3/3/3
29	CLA	C	512	-	1/1/15/20	17/37/115/115	-
29	CLA	c	508	-	1/1/15/20	6/37/115/115	-
35	LMG	w	201	-	-	17/34/54/70	0/1/1/1
29	CLA	G	603	-	1/1/15/20	10/37/115/115	-
37	DGD	b	623	-	-	8/32/72/95	0/2/2/2
45	CHL	N	608	-	3/3/16/26	5/20/118/137	-
45	CHL	s	607	-	3/3/15/26	0/12/110/137	-
46	LUT	y	620	-	-	2/29/67/67	0/2/2/2
29	CLA	C	506	-	-	8/37/115/115	-
40	LHG	C	525	-	-	23/39/39/53	-
29	CLA	N	612	20	1/1/11/20	4/13/91/115	-
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2
29	CLA	G	614	-	1/1/11/20	7/18/96/115	-
29	CLA	N	613	20	1/1/15/20	13/37/115/115	-
47	NEX	R	622	-	-	9/19/50/83	0/2/2/3
45	CHL	s	601	23	3/3/16/26	4/15/113/137	-
29	CLA	B	609	-	1/1/15/20	7/37/115/115	-
37	DGD	C	518	-	-	8/40/80/95	0/2/2/2
39	DGA	B	625	-	-	19/38/38/45	-
31	BCR	B	619	-	-	13/29/63/63	0/2/2/2
29	CLA	g	604	-	1/1/11/20	8/18/96/115	-
29	CLA	C	503	-	-	11/37/115/115	-
29	CLA	C	513	-	-	13/37/115/115	-
29	CLA	D	403	-	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	514	-	-	13/29/63/63	0/2/2/2
29	CLA	N	611	40	1/1/11/20	4/18/96/115	-
29	CLA	y	613	24	-	8/37/115/115	-
29	CLA	s	602	23	1/1/14/20	6/31/109/115	-
31	BCR	d	404	-	-	11/29/63/63	0/2/2/2
40	LHG	S	624	29	-	15/49/49/53	-
45	CHL	n	609	20	4/4/20/26	7/39/137/137	-
29	CLA	N	614	-	1/1/11/20	8/18/96/115	-
29	CLA	c	507	52	1/1/15/20	13/37/115/115	-
45	CHL	S	608	-	4/4/19/26	7/33/131/137	-
45	CHL	n	607	-	4/4/20/26	11/39/137/137	-
40	LHG	D	409	-	-	18/53/53/53	-
37	DGD	c	518	-	-	10/44/84/95	0/2/2/2
39	DGA	c	524	-	-	27/45/45/45	-
29	CLA	A	405	-	1/1/15/20	12/37/115/115	-
48	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	B	615	-	1/1/15/20	11/37/115/115	-
29	CLA	B	612	-	-	11/37/115/115	-
38	3PH	t	101	-	-	25/49/49/49	-
29	CLA	b	607	-	1/1/13/20	11/28/106/115	-
29	CLA	S	612	23	1/1/11/20	3/13/91/115	-
45	CHL	Y	607	-	4/4/20/26	11/39/137/137	-
45	CHL	g	609	21	4/4/20/26	8/39/137/137	-
29	CLA	c	502	-	1/1/15/20	11/37/115/115	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
29	CLA	N	610	-	1/1/15/20	13/37/115/115	-
29	CLA	G	610	21	1/1/15/20	5/37/115/115	-
31	BCR	C	516	-	-	11/29/63/63	0/2/2/2
48	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
40	LHG	Y	624	29	-	28/53/53/53	-
29	CLA	n	611	-	1/1/11/20	5/18/96/115	-
38	3PH	S	626	-	-	7/31/31/49	-
29	CLA	y	610	24	1/1/15/20	6/37/115/115	-
47	NEX	s	623	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	614	-	1/1/13/20	6/25/103/115	-
33	SQD	M	101	-	-	20/37/57/69	0/1/1/1
46	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	r	604	-	1/1/11/20	9/18/96/115	-
29	CLA	G	604	-	1/1/11/20	9/18/96/115	-
33	SQD	a	412	-	-	17/46/66/69	0/1/1/1
29	CLA	s	603	-	-	14/37/115/115	-
29	CLA	c	513	-	-	12/37/115/115	-
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
39	DGA	b	625	-	-	19/45/45/45	-
29	CLA	R	604	-	1/1/11/20	6/18/96/115	-
39	DGA	C	524	-	-	23/45/45/45	-
35	LMG	H	102	-	-	17/43/63/70	0/1/1/1
31	BCR	b	619	-	-	12/29/63/63	0/2/2/2
29	CLA	S	605	23	1/1/12/20	7/19/97/115	-
45	CHL	R	607	-	3/3/16/26	6/20/118/137	-
29	CLA	b	603	-	1/1/15/20	8/37/115/115	-
29	CLA	y	612	24	1/1/15/20	12/37/115/115	-
46	LUT	N	620	-	-	3/29/67/67	0/2/2/2
29	CLA	r	610	22	1/1/14/20	7/31/109/115	-
29	CLA	c	512	-	1/1/15/20	15/37/115/115	-
29	CLA	b	611	52	1/1/15/20	6/37/115/115	-
35	LMG	D	411	-	-	3/37/57/70	0/1/1/1
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	Y	613	24	1/1/15/20	18/37/115/115	-
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
48	XAT	Y	622	-	1/1/12/26	0/31/93/93	0/4/4/4
42	PL9	D	405	-	-	10/53/73/73	0/1/1/1
35	LMG	d	411	-	-	7/41/61/70	0/1/1/1
33	SQD	A	412	-	-	9/37/57/69	0/1/1/1
45	CHL	G	605	21	3/3/16/26	6/18/116/137	-
29	CLA	S	603	-	1/1/15/20	17/37/115/115	-
45	CHL	G	608	-	3/3/15/26	1/13/111/137	-
47	NEX	r	622	-	-	5/19/50/83	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	617	23	1/1/12/20	6/19/97/115	-
29	CLA	Y	604	52	1/1/15/20	15/37/115/115	-
29	CLA	b	605	-	1/1/15/20	12/37/115/115	-
29	CLA	B	604	-	1/1/15/20	10/37/115/115	-
29	CLA	S	614	-	1/1/12/20	8/19/97/115	-
29	CLA	s	613	23	1/1/13/20	11/25/103/115	-
29	CLA	S	613	23	1/1/13/20	11/25/103/115	-
29	CLA	Y	611	40	1/1/15/20	9/37/115/115	-
29	CLA	g	612	21	-	2/11/89/115	-
29	CLA	y	604	52	1/1/15/20	15/37/115/115	-
42	PL9	d	405	-	-	11/53/73/73	0/1/1/1
29	CLA	c	506	-	-	9/31/109/115	-
29	CLA	B	616	-	1/1/15/20	9/37/115/115	-
46	LUT	s	620	-	-	4/29/67/67	0/2/2/2
29	CLA	R	609	22	1/1/11/20	8/15/93/115	-
29	CLA	B	611	52	1/1/15/20	7/37/115/115	-
37	DGD	C	519	-	-	11/42/82/95	0/2/2/2
45	CHL	g	601	21	4/4/20/26	10/39/137/137	-
38	3PH	b	624	-	-	28/40/40/49	-
45	CHL	s	606	-	3/3/15/26	1/13/111/137	-
31	BCR	b	618	-	-	11/29/63/63	0/2/2/2
37	DGD	B	623	-	-	13/32/72/95	0/2/2/2
29	CLA	n	614	-	1/1/11/20	3/18/96/115	-
43	HEM	F	101	7,6	-	1/12/54/54	-
46	LUT	y	621	-	-	1/29/67/67	0/2/2/2
48	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	Y	610	24	1/1/15/20	4/37/115/115	-
29	CLA	n	603	-	1/1/15/20	12/37/115/115	-
29	CLA	C	505	-	1/1/14/20	14/31/109/115	-
31	BCR	c	516	-	-	12/29/63/63	0/2/2/2
40	LHG	N	624	29	-	30/53/53/53	-
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1
29	CLA	R	610	22	1/1/14/20	11/31/109/115	-
45	CHL	r	607	-	3/3/16/26	5/20/118/137	-
45	CHL	R	606	-	3/3/15/26	4/13/111/137	-

All (1090) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	H	101	RRX	C26-C25	15.61	1.61	1.34
44	h	101	RRX	C26-C25	15.51	1.61	1.34
36	B	620	C7Z	C25-C26	15.39	1.61	1.34
36	b	620	C7Z	C25-C26	15.36	1.61	1.34
36	B	620	C7Z	C5-C6	14.83	1.60	1.34
36	b	620	C7Z	C5-C6	14.79	1.60	1.34
44	h	101	RRX	C5-C6	14.78	1.60	1.34
44	H	101	RRX	C5-C6	14.77	1.60	1.34
46	r	620	LUT	C24-C25	14.73	1.51	1.33
46	G	620	LUT	C24-C25	14.58	1.51	1.33
46	y	620	LUT	C24-C25	14.55	1.51	1.33
46	Y	620	LUT	C24-C25	14.55	1.51	1.33
46	N	620	LUT	C24-C25	14.52	1.51	1.33
46	g	621	LUT	C24-C25	14.51	1.51	1.33
46	Y	621	LUT	C24-C25	14.48	1.51	1.33
46	s	620	LUT	C24-C25	14.45	1.51	1.33
46	R	620	LUT	C24-C25	14.45	1.51	1.33
46	y	621	LUT	C24-C25	14.41	1.51	1.33
46	N	621	LUT	C24-C25	14.41	1.51	1.33
46	G	621	LUT	C24-C25	14.41	1.51	1.33
46	n	620	LUT	C24-C25	14.36	1.51	1.33
46	n	621	LUT	C24-C25	14.25	1.50	1.33
46	g	620	LUT	C24-C25	14.19	1.50	1.33
46	S	621	LUT	C24-C25	14.12	1.50	1.33
46	s	621	LUT	C24-C25	14.02	1.50	1.33
46	S	620	LUT	C24-C25	13.79	1.50	1.33
36	B	620	C7Z	C24-C23	11.53	1.72	1.52
36	b	620	C7Z	C24-C23	11.41	1.72	1.52
36	B	620	C7Z	C2-C3	-10.64	1.37	1.52
36	b	620	C7Z	C22-C23	-10.60	1.37	1.52
36	B	620	C7Z	C22-C23	-10.50	1.37	1.52
44	H	101	RRX	C29-C28	-10.47	1.37	1.52
44	h	101	RRX	C29-C28	-10.40	1.37	1.52
36	b	620	C7Z	C2-C3	-10.38	1.37	1.52
36	b	620	C7Z	C4-C3	8.32	1.66	1.52
36	B	620	C7Z	C4-C3	8.27	1.66	1.52
44	h	101	RRX	C27-C28	7.93	1.66	1.52
44	H	101	RRX	C27-C28	7.91	1.66	1.52
47	R	622	NEX	C30-C29	-7.63	1.25	1.35
47	g	623	NEX	C10-C9	-7.62	1.25	1.35
47	n	623	NEX	C34-C33	-7.58	1.25	1.35
47	n	623	NEX	C14-C13	-7.58	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	s	623	NEX	C14-C13	-7.56	1.25	1.35
47	n	623	NEX	C10-C9	-7.50	1.25	1.35
47	Y	623	NEX	C30-C29	-7.47	1.25	1.35
47	s	623	NEX	C34-C33	-7.47	1.25	1.35
47	N	623	NEX	C14-C13	-7.47	1.25	1.35
47	r	622	NEX	C34-C33	-7.47	1.25	1.35
47	r	622	NEX	C30-C29	-7.46	1.25	1.35
47	S	623	NEX	C14-C13	-7.46	1.25	1.35
47	N	623	NEX	C34-C33	-7.45	1.25	1.35
47	g	623	NEX	C14-C13	-7.44	1.25	1.35
47	n	623	NEX	C30-C29	-7.43	1.25	1.35
47	R	622	NEX	C34-C33	-7.42	1.25	1.35
47	N	623	NEX	C30-C29	-7.41	1.26	1.35
47	s	623	NEX	C30-C29	-7.40	1.26	1.35
47	s	623	NEX	C10-C9	-7.39	1.26	1.35
47	G	623	NEX	C34-C33	-7.38	1.26	1.35
47	Y	623	NEX	C34-C33	-7.37	1.26	1.35
47	S	623	NEX	C30-C29	-7.36	1.26	1.35
47	g	623	NEX	C30-C29	-7.36	1.26	1.35
47	G	623	NEX	C14-C13	-7.35	1.26	1.35
47	S	623	NEX	C34-C33	-7.35	1.26	1.35
47	Y	623	NEX	C14-C13	-7.34	1.26	1.35
47	G	623	NEX	C10-C9	-7.34	1.26	1.35
47	y	623	NEX	C14-C13	-7.32	1.26	1.35
47	y	623	NEX	C34-C33	-7.32	1.26	1.35
47	y	623	NEX	C30-C29	-7.32	1.26	1.35
47	S	623	NEX	C10-C9	-7.31	1.26	1.35
47	N	623	NEX	C10-C9	-7.31	1.26	1.35
47	G	623	NEX	C30-C29	-7.30	1.26	1.35
47	y	623	NEX	C10-C9	-7.28	1.26	1.35
47	Y	623	NEX	C10-C9	-7.22	1.26	1.35
47	g	623	NEX	C34-C33	-7.21	1.26	1.35
31	c	516	BCR	C10-C9	7.08	1.45	1.35
31	C	516	BCR	C10-C9	7.07	1.45	1.35
31	D	404	BCR	C10-C9	7.00	1.45	1.35
31	c	514	BCR	C10-C9	6.91	1.44	1.35
47	n	623	NEX	C35-C15	-6.85	1.18	1.36
31	d	404	BCR	C10-C9	6.83	1.44	1.35
47	s	623	NEX	C35-C15	-6.80	1.18	1.36
47	R	622	NEX	C35-C15	-6.79	1.18	1.36
47	N	623	NEX	C35-C15	-6.78	1.18	1.36
47	r	622	NEX	C35-C15	-6.76	1.18	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S	623	NEX	C35-C15	-6.75	1.18	1.36
47	g	623	NEX	C35-C15	-6.73	1.18	1.36
31	b	618	BCR	C10-C9	6.73	1.44	1.35
47	Y	623	NEX	C35-C15	-6.71	1.18	1.36
47	G	623	NEX	C35-C15	-6.71	1.18	1.36
47	y	623	NEX	C35-C15	-6.71	1.18	1.36
31	C	517	BCR	C10-C9	6.70	1.44	1.35
31	c	517	BCR	C10-C9	6.66	1.44	1.35
31	C	514	BCR	C10-C9	6.56	1.44	1.35
31	C	515	BCR	C10-C9	6.54	1.44	1.35
31	B	618	BCR	C10-C9	6.52	1.44	1.35
44	H	101	RRX	C2-C3	-6.50	1.36	1.52
44	h	101	RRX	C2-C3	-6.47	1.36	1.52
31	A	411	BCR	C10-C9	6.43	1.44	1.35
31	B	619	BCR	C10-C9	6.42	1.44	1.35
31	b	619	BCR	C10-C9	6.41	1.44	1.35
31	c	515	BCR	C10-C9	6.33	1.44	1.35
47	n	623	NEX	C11-C12	-6.32	1.18	1.34
47	s	623	NEX	C11-C12	-6.32	1.18	1.34
47	s	623	NEX	C31-C32	-6.31	1.18	1.34
47	n	623	NEX	C31-C32	-6.29	1.18	1.34
47	S	623	NEX	C31-C32	-6.29	1.18	1.34
47	R	622	NEX	C31-C32	-6.28	1.18	1.34
31	a	411	BCR	C10-C9	6.27	1.44	1.35
47	G	623	NEX	C11-C12	-6.24	1.18	1.34
47	Y	623	NEX	C31-C32	-6.23	1.18	1.34
47	y	623	NEX	C31-C32	-6.23	1.18	1.34
47	r	622	NEX	C31-C32	-6.22	1.18	1.34
47	y	623	NEX	C11-C12	-6.22	1.18	1.34
47	g	623	NEX	C31-C32	-6.21	1.18	1.34
47	g	623	NEX	C11-C12	-6.21	1.18	1.34
47	N	623	NEX	C11-C12	-6.21	1.18	1.34
47	N	623	NEX	C31-C32	-6.20	1.18	1.34
47	S	623	NEX	C11-C12	-6.19	1.18	1.34
47	Y	623	NEX	C11-C12	-6.19	1.18	1.34
47	G	623	NEX	C31-C32	-6.13	1.18	1.34
44	H	101	RRX	C1-C6	-5.95	1.45	1.53
44	h	101	RRX	C1-C6	-5.90	1.45	1.53
31	D	404	BCR	C24-C23	5.73	1.50	1.33
31	c	516	BCR	C24-C23	5.72	1.50	1.33
31	C	516	BCR	C24-C23	5.69	1.50	1.33
31	b	619	BCR	C24-C23	5.67	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	404	BCR	C24-C23	5.67	1.50	1.33
31	B	619	BCR	C24-C23	5.66	1.50	1.33
47	s	623	NEX	C7-C8	5.61	1.41	1.32
31	c	517	BCR	C24-C23	5.59	1.50	1.33
31	C	517	BCR	C24-C23	5.57	1.49	1.33
31	b	619	BCR	C11-C12	-5.56	1.20	1.34
31	B	619	BCR	C11-C12	-5.56	1.20	1.34
31	a	411	BCR	C11-C12	-5.54	1.20	1.34
31	C	514	BCR	C24-C23	5.54	1.49	1.33
31	c	514	BCR	C24-C23	5.53	1.49	1.33
36	b	620	C7Z	C12-C13	5.53	1.57	1.45
31	c	515	BCR	C11-C12	-5.51	1.20	1.34
31	A	411	BCR	C24-C23	5.50	1.49	1.33
31	a	411	BCR	C24-C23	5.48	1.49	1.33
31	C	515	BCR	C24-C23	5.47	1.49	1.33
31	A	411	BCR	C11-C12	-5.47	1.20	1.34
47	S	623	NEX	C7-C8	5.47	1.41	1.32
47	N	623	NEX	C7-C8	5.47	1.41	1.32
36	B	620	C7Z	C12-C13	5.46	1.57	1.45
31	B	618	BCR	C11-C12	-5.45	1.20	1.34
47	Y	623	NEX	C7-C8	5.45	1.41	1.32
47	y	623	NEX	C7-C8	5.44	1.41	1.32
31	c	517	BCR	C11-C12	-5.41	1.20	1.34
31	C	517	BCR	C11-C12	-5.41	1.20	1.34
44	H	101	RRX	C30-C25	-5.39	1.46	1.53
31	b	618	BCR	C11-C12	-5.38	1.20	1.34
31	C	514	BCR	C11-C12	-5.38	1.20	1.34
31	c	515	BCR	C24-C23	5.37	1.49	1.33
47	G	623	NEX	C7-C8	5.36	1.40	1.32
31	B	618	BCR	C24-C23	5.34	1.49	1.33
36	b	620	C7Z	C24-C25	-5.33	1.42	1.51
47	S	623	NEX	C28-C29	-5.33	1.34	1.45
44	h	101	RRX	C30-C25	-5.33	1.46	1.53
31	C	515	BCR	C11-C12	-5.30	1.20	1.34
47	n	623	NEX	C7-C8	5.29	1.40	1.32
31	c	514	BCR	C11-C12	-5.29	1.21	1.34
31	b	618	BCR	C24-C23	5.28	1.49	1.33
36	B	620	C7Z	C24-C25	-5.27	1.42	1.51
47	s	623	NEX	C28-C29	-5.27	1.34	1.45
47	r	622	NEX	C28-C29	-5.27	1.34	1.45
47	R	622	NEX	C28-C29	-5.26	1.34	1.45
36	b	620	C7Z	C1-C6	-5.26	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	404	BCR	C11-C12	-5.24	1.21	1.34
47	g	623	NEX	C28-C29	-5.23	1.34	1.45
47	Y	623	NEX	C28-C29	-5.23	1.34	1.45
31	D	404	BCR	C11-C12	-5.20	1.21	1.34
47	n	623	NEX	C28-C29	-5.18	1.34	1.45
31	C	516	BCR	C11-C12	-5.16	1.21	1.34
47	G	623	NEX	C28-C29	-5.16	1.34	1.45
44	h	101	RRX	C2-C1	5.15	1.66	1.54
47	y	623	NEX	C28-C29	-5.15	1.34	1.45
31	c	516	BCR	C11-C12	-5.14	1.21	1.34
47	N	623	NEX	C28-C29	-5.10	1.35	1.45
44	H	101	RRX	C2-C1	5.10	1.65	1.54
44	h	101	RRX	C19-C18	5.05	1.56	1.45
36	B	620	C7Z	C1-C6	-5.05	1.46	1.53
44	H	101	RRX	C19-C18	4.97	1.56	1.45
47	g	623	NEX	C7-C8	4.88	1.40	1.32
42	D	405	PL9	C7-C3	-4.73	1.46	1.51
44	h	101	RRX	C8-C9	4.72	1.56	1.45
36	b	620	C7Z	C28-C29	4.70	1.56	1.45
31	a	411	BCR	C16-C17	-4.65	1.29	1.43
36	B	620	C7Z	C28-C29	4.65	1.55	1.45
44	H	101	RRX	C8-C9	4.63	1.55	1.45
31	A	411	BCR	C16-C17	-4.63	1.29	1.43
31	c	515	BCR	C16-C17	-4.63	1.29	1.43
31	B	618	BCR	C16-C17	-4.57	1.29	1.43
31	B	619	BCR	C16-C17	-4.56	1.29	1.43
31	b	619	BCR	C16-C17	-4.54	1.29	1.43
31	C	517	BCR	C16-C17	-4.50	1.29	1.43
31	c	517	BCR	C16-C17	-4.50	1.29	1.43
31	C	515	BCR	C16-C17	-4.50	1.29	1.43
36	b	620	C7Z	C32-C33	4.50	1.55	1.45
31	b	618	BCR	C16-C17	-4.49	1.29	1.43
36	B	620	C7Z	C4-C5	-4.48	1.44	1.51
36	B	620	C7Z	C32-C33	4.47	1.55	1.45
36	b	620	C7Z	C4-C5	-4.45	1.44	1.51
44	h	101	RRX	C12-C13	4.44	1.55	1.45
31	C	514	BCR	C16-C17	-4.43	1.29	1.43
31	D	404	BCR	C16-C17	-4.41	1.29	1.43
31	c	514	BCR	C16-C17	-4.40	1.29	1.43
44	h	101	RRX	C27-C26	-4.36	1.44	1.51
31	c	516	BCR	C16-C17	-4.36	1.29	1.43
31	C	516	BCR	C16-C17	-4.30	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	H	101	RRX	C12-C13	4.30	1.55	1.45
44	H	101	RRX	C27-C26	-4.29	1.44	1.51
37	B	623	DGD	O1G-C1A	4.28	1.45	1.33
37	C	518	DGD	O1G-C1A	4.25	1.45	1.33
31	d	404	BCR	C16-C17	-4.25	1.30	1.43
37	c	518	DGD	O1G-C1A	4.24	1.45	1.33
37	b	623	DGD	O1G-C1A	4.24	1.45	1.33
44	H	101	RRX	C3-C4	4.23	1.65	1.52
44	h	101	RRX	C3-C4	4.22	1.65	1.52
37	C	520	DGD	O1G-C1A	4.19	1.45	1.33
36	b	620	C7Z	C31-C30	4.16	1.56	1.43
37	C	519	DGD	O1G-C1A	4.14	1.45	1.33
36	B	620	C7Z	C31-C30	4.10	1.56	1.43
37	c	520	DGD	O1G-C1A	4.10	1.45	1.33
36	b	620	C7Z	C11-C10	4.10	1.56	1.43
36	b	620	C7Z	C8-C9	4.07	1.54	1.45
37	c	519	DGD	O1G-C1A	4.06	1.45	1.33
36	B	620	C7Z	C11-C10	4.03	1.55	1.43
36	B	620	C7Z	C8-C9	4.03	1.54	1.45
44	h	101	RRX	C20-C21	4.01	1.55	1.43
43	F	101	HEM	C3C-CAC	4.00	1.56	1.47
42	d	405	PL9	C7-C3	-3.91	1.47	1.51
43	f	101	HEM	C3C-CAC	3.91	1.55	1.47
44	H	101	RRX	C20-C21	3.91	1.55	1.43
42	D	405	PL9	C3-C4	-3.88	1.43	1.49
36	b	620	C7Z	C22-C21	3.87	1.67	1.54
29	G	603	CLA	C1D-ND	3.87	1.42	1.37
29	N	614	CLA	C1D-ND	3.85	1.42	1.37
36	B	620	C7Z	C22-C21	3.84	1.66	1.54
29	N	603	CLA	C1D-ND	3.80	1.42	1.37
44	h	101	RRX	C15-C14	3.80	1.55	1.43
29	C	505	CLA	C4D-ND	-3.79	1.32	1.37
29	C	513	CLA	C1D-ND	3.77	1.42	1.37
29	d	402	CLA	C4D-ND	-3.76	1.32	1.37
47	r	622	NEX	C14-C13	-3.76	1.26	1.35
47	R	622	NEX	C14-C13	-3.75	1.26	1.35
29	N	611	CLA	C1D-ND	3.75	1.42	1.37
44	H	101	RRX	C15-C14	3.75	1.55	1.43
29	r	609	CLA	C4D-ND	-3.74	1.32	1.37
44	h	101	RRX	C23-C22	3.74	1.54	1.45
29	s	617	CLA	C1D-ND	3.74	1.42	1.37
29	S	617	CLA	C1D-ND	3.73	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	614	CLA	C4D-ND	-3.73	1.32	1.37
29	a	407	CLA	C4D-ND	-3.73	1.32	1.37
29	B	610	CLA	C4D-ND	-3.73	1.32	1.37
43	f	101	HEM	C3C-C2C	-3.72	1.35	1.40
29	G	604	CLA	C1D-ND	3.71	1.42	1.37
29	y	611	CLA	C1D-ND	3.70	1.42	1.37
29	a	405	CLA	C4D-ND	-3.70	1.32	1.37
29	g	614	CLA	C1D-ND	3.69	1.42	1.37
29	g	611	CLA	C1D-ND	3.69	1.42	1.37
29	B	614	CLA	C4D-ND	-3.69	1.32	1.37
29	S	613	CLA	C1D-ND	3.68	1.42	1.37
29	r	604	CLA	C1D-ND	3.68	1.42	1.37
29	G	612	CLA	C1D-ND	3.67	1.42	1.37
29	B	617	CLA	C4D-ND	-3.66	1.32	1.37
29	C	511	CLA	C1D-ND	3.66	1.42	1.37
29	R	608	CLA	C4D-ND	-3.66	1.32	1.37
29	b	617	CLA	C4D-ND	-3.66	1.32	1.37
29	C	501	CLA	C1D-ND	3.66	1.42	1.37
29	Y	608	CLA	C4D-ND	-3.65	1.32	1.37
29	G	611	CLA	C1D-ND	3.65	1.42	1.37
29	s	609	CLA	C1D-ND	3.65	1.42	1.37
29	r	612	CLA	C1D-ND	3.65	1.42	1.37
29	R	609	CLA	C4D-ND	-3.65	1.32	1.37
29	y	602	CLA	C1D-ND	3.65	1.42	1.37
29	b	614	CLA	C4D-ND	-3.65	1.32	1.37
29	c	503	CLA	C4D-ND	-3.64	1.32	1.37
29	B	615	CLA	C4D-ND	-3.64	1.32	1.37
44	H	101	RRX	C23-C22	3.64	1.53	1.45
29	Y	603	CLA	C1D-ND	3.64	1.42	1.37
29	s	611	CLA	C1D-ND	3.63	1.42	1.37
43	F	101	HEM	C3C-C2C	-3.63	1.35	1.40
29	y	614	CLA	C4D-ND	-3.62	1.32	1.37
29	n	603	CLA	C1D-ND	3.62	1.42	1.37
29	y	613	CLA	C1D-ND	3.62	1.42	1.37
29	S	611	CLA	C1D-ND	3.62	1.42	1.37
29	S	604	CLA	C1D-ND	3.62	1.42	1.37
29	a	406	CLA	C4D-ND	-3.61	1.32	1.37
29	n	614	CLA	C4D-ND	-3.61	1.32	1.37
29	s	613	CLA	C1D-ND	3.61	1.42	1.37
29	c	505	CLA	C4D-ND	-3.61	1.32	1.37
29	R	612	CLA	C1D-ND	3.60	1.42	1.37
29	b	615	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	615	CLA	C1D-ND	3.59	1.42	1.37
29	Y	611	CLA	C1D-ND	3.59	1.42	1.37
29	n	613	CLA	C1D-ND	3.59	1.42	1.37
29	B	609	CLA	C1D-ND	3.59	1.42	1.37
29	C	503	CLA	C1D-ND	3.59	1.42	1.37
29	Y	613	CLA	C1D-ND	3.59	1.42	1.37
39	B	625	DGA	OG2-CB1	3.59	1.44	1.34
29	y	608	CLA	C4D-ND	-3.58	1.32	1.37
29	c	513	CLA	C1D-ND	3.58	1.42	1.37
29	r	608	CLA	C4D-ND	-3.58	1.32	1.37
29	n	611	CLA	C1D-ND	3.58	1.42	1.37
29	b	615	CLA	C4D-ND	-3.58	1.32	1.37
29	c	502	CLA	C4D-ND	-3.57	1.32	1.37
29	b	606	CLA	C4D-ND	-3.57	1.32	1.37
29	N	613	CLA	C1D-ND	3.57	1.42	1.37
29	b	616	CLA	C1D-ND	3.57	1.42	1.37
29	C	508	CLA	C4D-ND	-3.57	1.32	1.37
29	D	402	CLA	C4D-ND	-3.57	1.32	1.37
29	g	613	CLA	C1D-ND	3.57	1.42	1.37
29	D	403	CLA	C1D-ND	3.57	1.42	1.37
29	b	603	CLA	C4D-ND	-3.57	1.32	1.37
29	c	511	CLA	C1D-ND	3.56	1.42	1.37
36	b	620	C7Z	C15-C14	3.56	1.54	1.43
29	c	507	CLA	C4D-ND	-3.56	1.32	1.37
39	b	625	DGA	OG2-CB1	3.56	1.44	1.34
29	Y	602	CLA	C1D-ND	3.56	1.42	1.37
29	n	602	CLA	C1D-ND	3.56	1.42	1.37
29	G	602	CLA	C1D-ND	3.55	1.42	1.37
29	N	602	CLA	C4D-ND	-3.55	1.32	1.37
29	G	602	CLA	C4D-ND	-3.55	1.32	1.37
29	b	610	CLA	C4D-ND	-3.55	1.32	1.37
29	C	504	CLA	C1D-ND	3.55	1.42	1.37
29	B	612	CLA	C4D-ND	-3.55	1.32	1.37
29	G	610	CLA	C1D-ND	3.55	1.42	1.37
29	B	607	CLA	C1D-ND	3.54	1.42	1.37
29	R	603	CLA	C1D-ND	3.54	1.42	1.37
42	d	405	PL9	C3-C4	-3.54	1.43	1.49
29	c	510	CLA	C4D-ND	-3.54	1.32	1.37
29	g	603	CLA	C1D-ND	3.54	1.42	1.37
29	S	605	CLA	C1D-ND	3.54	1.42	1.37
29	B	605	CLA	C1D-ND	3.54	1.42	1.37
29	d	403	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	616	CLA	C1D-ND	3.54	1.42	1.37
29	S	612	CLA	C1D-ND	3.53	1.42	1.37
29	r	603	CLA	C1D-ND	3.53	1.42	1.37
29	n	612	CLA	C1D-ND	3.53	1.42	1.37
29	A	406	CLA	C1D-ND	3.53	1.42	1.37
29	g	602	CLA	C1D-ND	3.53	1.42	1.37
29	y	603	CLA	C1D-ND	3.52	1.42	1.37
29	S	609	CLA	C1D-ND	3.52	1.42	1.37
36	B	620	C7Z	C7-C6	3.52	1.57	1.45
36	b	620	C7Z	C2-C1	3.51	1.65	1.54
29	R	602	CLA	C1D-ND	3.51	1.42	1.37
29	C	509	CLA	C1D-ND	3.51	1.42	1.37
29	b	612	CLA	C4D-ND	-3.51	1.32	1.37
29	s	605	CLA	C1D-ND	3.51	1.42	1.37
29	S	610	CLA	C1D-ND	3.51	1.42	1.37
29	B	608	CLA	C4D-ND	-3.50	1.32	1.37
29	g	612	CLA	C1D-ND	3.50	1.42	1.37
29	B	606	CLA	C4D-ND	-3.50	1.32	1.37
29	C	503	CLA	C4D-ND	-3.50	1.32	1.37
29	b	609	CLA	C1D-ND	3.50	1.42	1.37
29	S	602	CLA	C4D-ND	-3.50	1.32	1.37
29	c	506	CLA	C4D-ND	-3.50	1.32	1.37
29	G	614	CLA	C1D-ND	3.50	1.42	1.37
29	c	501	CLA	C1D-ND	3.50	1.42	1.37
29	b	608	CLA	C4D-ND	-3.50	1.32	1.37
29	B	613	CLA	C4D-ND	-3.50	1.32	1.37
29	r	609	CLA	C1D-ND	3.50	1.42	1.37
29	S	617	CLA	C4D-ND	-3.49	1.32	1.37
29	n	602	CLA	C4D-ND	-3.49	1.32	1.37
29	n	610	CLA	C4D-ND	-3.49	1.32	1.37
29	y	608	CLA	C1D-ND	3.49	1.42	1.37
39	J	101	DGA	OG2-CB1	3.49	1.44	1.34
29	c	504	CLA	C4D-ND	-3.49	1.32	1.37
29	c	508	CLA	C4D-ND	-3.49	1.32	1.37
29	N	612	CLA	C1D-ND	3.49	1.42	1.37
29	A	405	CLA	C4D-ND	-3.48	1.32	1.37
29	g	603	CLA	C4D-ND	-3.48	1.32	1.37
29	r	602	CLA	C4D-ND	-3.48	1.32	1.37
29	N	610	CLA	C1D-ND	3.48	1.42	1.37
29	b	611	CLA	C1D-ND	3.48	1.42	1.37
29	n	604	CLA	C1D-ND	3.48	1.42	1.37
29	a	410	CLA	C4D-ND	-3.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	509	CLA	C4D-ND	-3.47	1.32	1.37
29	B	602	CLA	C1D-ND	3.47	1.42	1.37
44	h	101	RRX	C11-C10	3.47	1.54	1.43
29	r	603	CLA	C4D-ND	-3.47	1.32	1.37
29	C	502	CLA	C1D-ND	3.47	1.42	1.37
29	C	507	CLA	C4D-ND	-3.47	1.32	1.37
36	B	620	C7Z	C15-C14	3.47	1.54	1.43
29	Y	614	CLA	C4D-ND	-3.47	1.32	1.37
29	c	509	CLA	C1D-ND	3.47	1.42	1.37
29	s	614	CLA	C1D-ND	3.47	1.42	1.37
29	n	603	CLA	C4D-ND	-3.47	1.32	1.37
29	D	403	CLA	C4D-ND	-3.47	1.32	1.37
36	B	620	C7Z	C2-C1	3.47	1.65	1.54
29	c	503	CLA	C1D-ND	3.46	1.42	1.37
29	s	612	CLA	C1D-ND	3.46	1.42	1.37
29	G	613	CLA	C1D-ND	3.46	1.42	1.37
29	s	610	CLA	C1D-ND	3.46	1.42	1.37
29	b	613	CLA	C4D-ND	-3.46	1.32	1.37
29	c	505	CLA	C1D-ND	3.46	1.42	1.37
29	B	603	CLA	C4D-ND	-3.45	1.32	1.37
29	r	610	CLA	C1D-ND	3.45	1.42	1.37
29	c	509	CLA	C4D-ND	-3.45	1.33	1.37
29	S	602	CLA	C1D-ND	3.45	1.42	1.37
36	b	620	C7Z	C7-C6	3.45	1.57	1.45
29	s	602	CLA	C1D-ND	3.44	1.42	1.37
29	A	410	CLA	C4D-ND	-3.44	1.33	1.37
29	B	611	CLA	C1D-ND	3.44	1.42	1.37
29	Y	604	CLA	C1D-ND	3.44	1.42	1.37
29	b	612	CLA	C1D-ND	3.44	1.42	1.37
29	A	407	CLA	C1D-ND	3.44	1.42	1.37
29	s	602	CLA	C4D-ND	-3.44	1.33	1.37
29	y	612	CLA	C4D-ND	-3.44	1.33	1.37
29	N	604	CLA	C1D-ND	3.43	1.42	1.37
29	R	612	CLA	C4D-ND	-3.43	1.33	1.37
29	s	614	CLA	C4D-ND	-3.43	1.33	1.37
29	G	604	CLA	C4D-ND	-3.43	1.33	1.37
29	Y	612	CLA	C1D-ND	3.43	1.42	1.37
29	b	604	CLA	C4D-ND	-3.43	1.33	1.37
29	b	607	CLA	C4D-ND	-3.43	1.33	1.37
29	Y	612	CLA	C4D-ND	-3.43	1.33	1.37
29	C	506	CLA	C1D-ND	3.43	1.42	1.37
29	r	602	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	602	CLA	C4D-ND	-3.43	1.33	1.37
29	C	502	CLA	C4D-ND	-3.43	1.33	1.37
44	H	101	RRX	C11-C10	3.43	1.54	1.43
29	c	508	CLA	C1D-ND	3.42	1.42	1.37
29	S	603	CLA	C4D-ND	-3.42	1.33	1.37
39	j	101	DGA	OG2-CB1	3.42	1.43	1.34
29	A	407	CLA	C4D-ND	-3.42	1.33	1.37
29	n	612	CLA	C4D-ND	-3.42	1.33	1.37
29	C	507	CLA	C1D-ND	3.42	1.42	1.37
29	d	403	CLA	C4D-ND	-3.41	1.33	1.37
29	b	602	CLA	C1D-ND	3.41	1.42	1.37
36	b	620	C7Z	C27-C26	3.41	1.57	1.45
29	G	614	CLA	C4D-ND	-3.41	1.33	1.37
29	s	610	CLA	C4D-ND	-3.41	1.33	1.37
29	S	613	CLA	C4D-ND	-3.40	1.33	1.37
29	C	512	CLA	C1D-ND	3.40	1.42	1.37
29	R	609	CLA	C1D-ND	3.40	1.42	1.37
29	Y	614	CLA	C1D-ND	3.40	1.42	1.37
29	c	506	CLA	C1D-ND	3.40	1.42	1.37
29	B	604	CLA	C4D-ND	-3.40	1.33	1.37
36	B	620	C7Z	C27-C26	3.40	1.57	1.45
29	c	512	CLA	C4D-ND	-3.40	1.33	1.37
29	y	604	CLA	C1D-ND	3.39	1.42	1.37
36	b	620	C7Z	C35-C34	3.39	1.54	1.43
29	N	604	CLA	C4D-ND	-3.39	1.33	1.37
29	R	608	CLA	C1D-ND	3.39	1.42	1.37
29	g	604	CLA	C4D-ND	-3.39	1.33	1.37
29	y	610	CLA	C4D-ND	-3.39	1.33	1.37
29	c	507	CLA	C1D-ND	3.39	1.42	1.37
29	R	604	CLA	C4D-ND	-3.39	1.33	1.37
29	R	610	CLA	C4D-ND	-3.39	1.33	1.37
29	r	610	CLA	C4D-ND	-3.39	1.33	1.37
29	y	614	CLA	C1D-ND	3.39	1.41	1.37
29	g	610	CLA	C4D-ND	-3.38	1.33	1.37
29	y	611	CLA	C4D-ND	-3.38	1.33	1.37
29	R	610	CLA	C1D-ND	3.38	1.41	1.37
39	C	524	DGA	OG2-CB1	3.38	1.43	1.34
29	r	612	CLA	C4D-ND	-3.38	1.33	1.37
39	c	524	DGA	OG2-CB1	3.38	1.43	1.34
29	r	608	CLA	C1D-ND	3.38	1.41	1.37
45	G	607	CHL	CBB-CAB	3.38	1.51	1.29
29	n	610	CLA	C1D-ND	3.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	612	CLA	C4D-ND	-3.38	1.33	1.37
29	C	512	CLA	C4D-ND	-3.38	1.33	1.37
29	n	614	CLA	C1D-ND	3.38	1.41	1.37
29	b	611	CLA	C4D-ND	-3.38	1.33	1.37
29	N	602	CLA	C1D-ND	3.38	1.41	1.37
29	A	410	CLA	C1D-ND	3.37	1.41	1.37
29	C	510	CLA	C1D-ND	3.37	1.41	1.37
29	s	603	CLA	C1D-ND	3.37	1.41	1.37
29	g	610	CLA	C1D-ND	3.37	1.41	1.37
29	y	603	CLA	C4D-ND	-3.37	1.33	1.37
29	g	604	CLA	C1D-ND	3.37	1.41	1.37
29	R	603	CLA	C4D-ND	-3.37	1.33	1.37
29	s	611	CLA	C4D-ND	-3.37	1.33	1.37
45	Y	601	CHL	CBB-CAB	3.36	1.51	1.29
29	g	611	CLA	C4D-ND	-3.36	1.33	1.37
45	G	605	CHL	CBB-CAB	3.36	1.51	1.29
45	n	609	CHL	CBB-CAB	3.36	1.51	1.29
29	s	604	CLA	C4D-ND	-3.36	1.33	1.37
29	C	508	CLA	C1D-ND	3.35	1.41	1.37
29	B	611	CLA	C4D-ND	-3.35	1.33	1.37
29	a	406	CLA	C1D-ND	3.35	1.41	1.37
45	g	605	CHL	CBB-CAB	3.35	1.51	1.29
29	c	501	CLA	C4D-ND	-3.35	1.33	1.37
29	s	604	CLA	C1D-ND	3.35	1.41	1.37
29	C	506	CLA	C4D-ND	-3.35	1.33	1.37
29	Y	610	CLA	C4D-ND	-3.35	1.33	1.37
35	b	622	LMG	C22-C21	-3.35	1.32	1.51
45	N	608	CHL	CBB-CAB	3.34	1.51	1.29
29	B	603	CLA	C1D-ND	3.34	1.41	1.37
29	Y	603	CLA	C4D-ND	-3.34	1.33	1.37
29	C	501	CLA	C4D-ND	-3.34	1.33	1.37
29	b	609	CLA	C4D-ND	-3.34	1.33	1.37
45	G	605	CHL	C4B-NB	3.34	1.38	1.35
45	g	607	CHL	CBB-CAB	3.34	1.51	1.29
29	Y	608	CLA	C1D-ND	3.34	1.41	1.37
39	c	524	DGA	OG1-CA1	3.34	1.43	1.33
29	A	406	CLA	C4D-ND	-3.34	1.33	1.37
29	N	613	CLA	C4D-ND	-3.33	1.33	1.37
29	C	504	CLA	C4D-ND	-3.33	1.33	1.37
29	S	611	CLA	C4D-ND	-3.33	1.33	1.37
45	g	608	CHL	CBB-CAB	3.33	1.51	1.29
29	a	410	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	620	C7Z	C35-C34	3.33	1.53	1.43
29	c	502	CLA	C1D-ND	3.33	1.41	1.37
29	S	610	CLA	C4D-ND	-3.33	1.33	1.37
29	c	512	CLA	C1D-ND	3.32	1.41	1.37
45	y	601	CHL	CBB-CAB	3.32	1.51	1.29
29	b	606	CLA	C1D-ND	3.32	1.41	1.37
45	Y	605	CHL	CBB-CAB	3.32	1.51	1.29
29	B	607	CLA	C4D-ND	-3.32	1.33	1.37
29	R	602	CLA	C4D-ND	-3.32	1.33	1.37
45	y	605	CHL	CBB-CAB	3.32	1.51	1.29
45	n	601	CHL	CBB-CAB	3.32	1.51	1.29
45	N	609	CHL	CBB-CAB	3.32	1.51	1.29
45	s	606	CHL	CBB-CAB	3.32	1.51	1.29
29	G	612	CLA	C4D-ND	-3.32	1.33	1.37
45	y	609	CHL	CBB-CAB	3.32	1.51	1.29
45	N	601	CHL	CBB-CAB	3.32	1.51	1.29
45	g	601	CHL	CBB-CAB	3.31	1.51	1.29
45	Y	609	CHL	CBB-CAB	3.31	1.51	1.29
45	n	608	CHL	CBB-CAB	3.31	1.51	1.29
29	Y	613	CLA	C4D-ND	-3.31	1.33	1.37
29	B	612	CLA	C1D-ND	3.31	1.41	1.37
45	G	601	CHL	CBB-CAB	3.31	1.51	1.29
29	Y	610	CLA	C1D-ND	3.31	1.41	1.37
29	S	605	CLA	C4D-ND	-3.31	1.33	1.37
45	G	609	CHL	CBB-CAB	3.30	1.51	1.29
29	B	617	CLA	C1D-ND	3.30	1.41	1.37
29	S	614	CLA	C1D-ND	3.30	1.41	1.37
29	g	612	CLA	C4D-ND	-3.30	1.33	1.37
45	g	609	CHL	CBB-CAB	3.30	1.51	1.29
45	S	607	CHL	CBB-CAB	3.30	1.51	1.29
37	c	520	DGD	CAB-C9B	-3.30	1.33	1.51
29	n	613	CLA	C4D-ND	-3.30	1.33	1.37
29	C	505	CLA	C1D-ND	3.30	1.41	1.37
29	y	610	CLA	C1D-ND	3.30	1.41	1.37
44	h	101	RRX	C16-C17	3.30	1.53	1.43
29	Y	611	CLA	C4D-ND	-3.30	1.33	1.37
29	B	609	CLA	C4D-ND	-3.29	1.33	1.37
29	S	604	CLA	C4D-ND	-3.29	1.33	1.37
45	N	605	CHL	CBB-CAB	3.29	1.51	1.29
29	Y	604	CLA	C4D-ND	-3.29	1.33	1.37
29	c	504	CLA	C1D-ND	3.29	1.41	1.37
39	J	101	DGA	OG1-CA1	3.29	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	609	CLA	C4D-ND	-3.29	1.33	1.37
35	B	622	LMG	C22-C21	-3.29	1.33	1.51
39	C	524	DGA	OG1-CA1	3.28	1.42	1.33
39	B	625	DGA	OG1-CA1	3.28	1.42	1.33
29	s	605	CLA	C4D-ND	-3.28	1.33	1.37
29	R	604	CLA	C1D-ND	3.28	1.41	1.37
29	r	610	CLA	CHC-C1C	3.28	1.43	1.35
29	B	610	CLA	C1D-ND	3.28	1.41	1.37
37	c	519	DGD	CAB-C9B	-3.28	1.33	1.51
39	j	101	DGA	OG1-CA1	3.27	1.42	1.33
35	c	523	LMG	C40-C39	-3.27	1.33	1.51
29	b	605	CLA	C1D-ND	3.27	1.41	1.37
29	y	612	CLA	C1D-ND	3.27	1.41	1.37
29	C	510	CLA	C4D-ND	-3.27	1.33	1.37
35	b	622	LMG	C19-C18	-3.27	1.33	1.51
45	n	605	CHL	CBB-CAB	3.27	1.50	1.29
29	b	610	CLA	C1D-ND	3.26	1.41	1.37
35	B	622	LMG	C19-C18	-3.26	1.33	1.51
35	c	521	LMG	C40-C39	-3.26	1.33	1.51
45	S	601	CHL	C4B-NB	3.26	1.38	1.35
35	C	521	LMG	C40-C39	-3.26	1.33	1.51
29	S	612	CLA	C4D-ND	-3.26	1.33	1.37
45	S	608	CHL	CBB-CAB	3.26	1.50	1.29
29	b	617	CLA	C1D-ND	3.26	1.41	1.37
45	Y	607	CHL	CBB-CAB	3.26	1.50	1.29
37	c	519	DGD	CDA-CCA	-3.26	1.33	1.51
29	a	407	CLA	C1D-ND	3.26	1.41	1.37
35	H	102	LMG	C19-C18	-3.26	1.33	1.51
29	b	603	CLA	C1D-ND	3.26	1.41	1.37
35	h	102	LMG	C19-C18	-3.25	1.33	1.51
29	g	610	CLA	CHC-C1C	3.25	1.43	1.35
29	R	610	CLA	CHC-C1C	3.25	1.43	1.35
29	Y	602	CLA	C4D-ND	-3.25	1.33	1.37
29	N	610	CLA	C4D-ND	-3.25	1.33	1.37
29	y	604	CLA	C4D-ND	-3.25	1.33	1.37
29	s	613	CLA	C4D-ND	-3.25	1.33	1.37
35	c	521	LMG	C22-C21	-3.24	1.33	1.51
35	C	521	LMG	C19-C18	-3.24	1.33	1.51
29	n	610	CLA	CHC-C1C	3.24	1.43	1.35
37	C	518	DGD	CDB-CCB	-3.24	1.33	1.51
29	s	610	CLA	CHC-C1C	3.24	1.43	1.35
45	s	608	CHL	CBB-CAB	3.24	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	610	CLA	CHC-C1C	3.24	1.43	1.35
35	c	521	LMG	C37-C36	-3.24	1.33	1.51
37	C	519	DGD	CAB-C9B	-3.24	1.33	1.51
29	G	611	CLA	C4D-ND	-3.23	1.33	1.37
35	c	523	LMG	C37-C36	-3.23	1.33	1.51
45	n	607	CHL	CBB-CAB	3.23	1.50	1.29
29	n	604	CLA	C4D-ND	-3.23	1.33	1.37
35	c	521	LMG	C19-C18	-3.23	1.33	1.51
35	D	411	LMG	C19-C18	-3.23	1.33	1.51
45	s	601	CHL	C4B-NB	3.23	1.38	1.35
39	b	625	DGA	OG1-CA1	3.23	1.42	1.33
29	d	402	CLA	CHC-C1C	3.23	1.43	1.35
35	C	521	LMG	C37-C36	-3.23	1.33	1.51
35	C	523	LMG	C25-C24	-3.23	1.33	1.51
37	C	520	DGD	CAA-C9A	-3.23	1.33	1.51
29	B	604	CLA	C1D-ND	3.23	1.41	1.37
29	B	608	CLA	C1D-ND	3.23	1.41	1.37
29	b	613	CLA	C1D-ND	3.23	1.41	1.37
37	c	518	DGD	CDB-CCB	-3.23	1.33	1.51
29	N	611	CLA	CHC-C1C	3.23	1.43	1.35
29	g	602	CLA	CHC-C1C	3.23	1.43	1.35
36	B	620	C7Z	C21-C26	-3.22	1.49	1.53
37	c	520	DGD	CAA-C9A	-3.22	1.33	1.51
35	C	523	LMG	C22-C21	-3.22	1.33	1.51
29	Y	602	CLA	CHC-C1C	3.22	1.43	1.35
29	c	510	CLA	C1D-ND	3.22	1.41	1.37
37	c	518	DGD	CAB-C9B	-3.22	1.33	1.51
37	c	519	DGD	CDB-CCB	-3.22	1.33	1.51
29	B	606	CLA	C1D-ND	3.22	1.41	1.37
29	N	611	CLA	C4D-ND	-3.22	1.33	1.37
29	G	610	CLA	C4D-ND	-3.22	1.33	1.37
45	R	606	CHL	CBB-CAB	3.22	1.50	1.29
35	C	527	LMG	C37-C36	-3.22	1.33	1.51
45	y	607	CHL	CBB-CAB	3.22	1.50	1.29
29	b	605	CLA	C4D-ND	-3.22	1.33	1.37
45	N	605	CHL	C4B-NB	3.22	1.38	1.35
44	H	101	RRX	C16-C17	3.21	1.53	1.43
45	G	601	CHL	C4B-NB	3.21	1.38	1.35
35	c	523	LMG	C43-C42	-3.21	1.33	1.51
45	S	606	CHL	C4B-NB	3.21	1.38	1.35
29	D	402	CLA	CHC-C1C	3.21	1.43	1.35
35	c	523	LMG	C19-C18	-3.21	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	413	LMG	C37-C36	-3.21	1.33	1.51
35	C	523	LMG	C40-C39	-3.21	1.33	1.51
35	C	523	LMG	C37-C36	-3.21	1.33	1.51
37	C	519	DGD	CDB-CCB	-3.21	1.33	1.51
35	c	523	LMG	C22-C21	-3.21	1.33	1.51
29	b	607	CLA	C1D-ND	3.21	1.41	1.37
29	G	602	CLA	CHC-C1C	3.21	1.43	1.35
29	G	611	CLA	CHC-C1C	3.21	1.43	1.35
35	d	411	LMG	C19-C18	-3.20	1.33	1.51
45	R	607	CHL	CBB-CAB	3.20	1.50	1.29
29	S	617	CLA	CHC-C1C	3.20	1.43	1.35
37	C	518	DGD	CAB-C9B	-3.20	1.33	1.51
45	S	606	CHL	CBB-CAB	3.20	1.50	1.29
29	b	604	CLA	C1D-ND	3.20	1.41	1.37
29	s	603	CLA	C4D-ND	-3.20	1.33	1.37
36	B	620	C7Z	C38-C25	3.20	1.56	1.50
35	c	523	LMG	C25-C24	-3.20	1.33	1.51
35	a	413	LMG	C40-C39	-3.20	1.33	1.51
37	c	519	DGD	CAA-C9A	-3.20	1.33	1.51
35	w	201	LMG	C37-C36	-3.20	1.33	1.51
35	W	201	LMG	C37-C36	-3.20	1.33	1.51
29	g	613	CLA	C4D-ND	-3.19	1.33	1.37
29	y	613	CLA	C4D-ND	-3.19	1.33	1.37
29	g	614	CLA	C4D-ND	-3.19	1.33	1.37
35	a	413	LMG	C19-C18	-3.19	1.33	1.51
45	r	606	CHL	CBB-CAB	3.19	1.50	1.29
29	N	610	CLA	CHC-C1C	3.19	1.43	1.35
35	C	523	LMG	C43-C42	-3.19	1.33	1.51
35	H	102	LMG	C40-C39	-3.18	1.33	1.51
29	s	617	CLA	C4D-ND	-3.18	1.33	1.37
45	G	608	CHL	CBB-CAB	3.18	1.50	1.29
45	R	607	CHL	C4B-NB	3.18	1.38	1.35
29	y	602	CLA	CHC-C1C	3.18	1.43	1.35
29	C	511	CLA	C4D-ND	-3.18	1.33	1.37
29	c	513	CLA	CHC-C1C	3.18	1.43	1.35
45	s	607	CHL	CBB-CAB	3.18	1.50	1.29
45	r	607	CHL	CBB-CAB	3.18	1.50	1.29
29	b	614	CLA	C1D-ND	3.18	1.41	1.37
35	H	102	LMG	C37-C36	-3.18	1.33	1.51
29	b	604	CLA	CHC-C1C	3.18	1.43	1.35
37	c	520	DGD	CDB-CCB	-3.18	1.33	1.51
29	N	612	CLA	C4D-ND	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	405	CLA	C1D-ND	3.18	1.41	1.37
29	B	604	CLA	CHC-C1C	3.18	1.43	1.35
29	G	604	CLA	CHC-C1C	3.18	1.43	1.35
29	B	602	CLA	C4D-ND	-3.18	1.33	1.37
29	b	608	CLA	C1D-ND	3.18	1.41	1.37
29	S	610	CLA	CHC-C1C	3.18	1.43	1.35
45	g	601	CHL	C4B-NB	3.17	1.38	1.35
29	G	613	CLA	C4D-ND	-3.17	1.33	1.37
29	S	611	CLA	CHC-C1C	3.17	1.43	1.35
35	h	102	LMG	C37-C36	-3.17	1.33	1.51
45	g	606	CHL	CBB-CAB	3.17	1.50	1.29
29	C	513	CLA	CHC-C1C	3.17	1.43	1.35
35	A	413	LMG	C19-C18	-3.17	1.33	1.51
45	G	608	CHL	C4B-NB	3.17	1.38	1.35
29	y	602	CLA	C4D-ND	-3.17	1.33	1.37
29	n	611	CLA	CHC-C1C	3.17	1.43	1.35
29	b	602	CLA	C4D-ND	-3.17	1.33	1.37
35	h	102	LMG	C40-C39	-3.16	1.33	1.51
29	g	611	CLA	CHC-C1C	3.16	1.43	1.35
29	N	612	CLA	CHC-C1C	3.16	1.43	1.35
29	N	602	CLA	CHC-C1C	3.16	1.43	1.35
29	r	604	CLA	C4D-ND	-3.16	1.33	1.37
44	h	101	RRX	C24-C25	3.16	1.56	1.45
29	s	611	CLA	CHC-C1C	3.16	1.43	1.35
29	n	611	CLA	C4D-ND	-3.15	1.33	1.37
35	d	411	LMG	C22-C21	-3.15	1.33	1.51
36	b	620	C7Z	C38-C25	3.15	1.56	1.50
44	H	101	RRX	C4-C5	-3.15	1.44	1.51
45	Y	605	CHL	C4B-NB	3.15	1.38	1.35
29	N	603	CLA	C4D-ND	-3.15	1.33	1.37
29	B	607	CLA	CHC-C1C	3.15	1.43	1.35
29	G	603	CLA	C4D-ND	-3.15	1.33	1.37
29	c	513	CLA	C4D-ND	-3.15	1.33	1.37
35	W	201	LMG	C40-C39	-3.14	1.33	1.51
29	B	613	CLA	C1D-ND	3.14	1.41	1.37
35	w	201	LMG	C40-C39	-3.14	1.33	1.51
29	s	609	CLA	C4D-ND	-3.14	1.33	1.37
29	b	613	CLA	CHC-C1C	3.14	1.43	1.35
35	C	523	LMG	C19-C18	-3.14	1.34	1.51
45	n	606	CHL	CBB-CAB	3.14	1.50	1.29
29	B	602	CLA	CHC-C1C	3.14	1.43	1.35
45	G	606	CHL	C4B-NB	3.14	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	616	CLA	CHC-C1C	3.14	1.43	1.35
29	s	617	CLA	CHC-C1C	3.13	1.43	1.35
45	N	607	CHL	CBB-CAB	3.13	1.50	1.29
29	B	614	CLA	C1D-ND	3.13	1.41	1.37
29	s	602	CLA	CHC-C1C	3.12	1.43	1.35
29	C	513	CLA	C4D-ND	-3.12	1.33	1.37
29	c	511	CLA	C4D-ND	-3.12	1.33	1.37
29	c	507	CLA	CHC-C1C	3.12	1.43	1.35
29	A	407	CLA	CHC-C1C	3.12	1.43	1.35
45	Y	606	CHL	C4B-NB	3.12	1.38	1.35
29	C	505	CLA	CHC-C1C	3.12	1.43	1.35
29	B	605	CLA	C4D-ND	-3.12	1.33	1.37
45	G	606	CHL	CBB-CAB	3.12	1.50	1.29
29	D	403	CLA	CHC-C1C	3.12	1.43	1.35
29	b	603	CLA	CHC-C1C	3.12	1.43	1.35
29	G	614	CLA	CHC-C1C	3.12	1.43	1.35
29	c	505	CLA	CHC-C1C	3.11	1.42	1.35
29	c	512	CLA	CHC-C1C	3.11	1.42	1.35
29	d	403	CLA	CHC-C1C	3.11	1.42	1.35
29	R	612	CLA	CHC-C1C	3.11	1.42	1.35
29	n	612	CLA	CHC-C1C	3.11	1.42	1.35
29	S	612	CLA	CHC-C1C	3.11	1.42	1.35
45	s	601	CHL	CBB-CAB	3.11	1.49	1.29
29	n	602	CLA	CHC-C1C	3.11	1.42	1.35
29	B	613	CLA	CHC-C1C	3.10	1.42	1.35
29	B	614	CLA	CHC-C1C	3.10	1.42	1.35
45	Y	606	CHL	CBB-CAB	3.10	1.49	1.29
29	S	609	CLA	CHC-C1C	3.10	1.42	1.35
29	R	602	CLA	CHC-C1C	3.10	1.42	1.35
29	c	509	CLA	CHC-C1C	3.10	1.42	1.35
29	b	602	CLA	CHC-C1C	3.10	1.42	1.35
29	C	512	CLA	CHC-C1C	3.10	1.42	1.35
45	N	606	CHL	C4B-NB	3.09	1.38	1.35
45	N	606	CHL	CBB-CAB	3.09	1.49	1.29
29	N	604	CLA	CHC-C1C	3.09	1.42	1.35
45	n	606	CHL	C3B-C2B	-3.09	1.36	1.40
45	S	607	CHL	C4B-NB	3.09	1.38	1.35
45	y	609	CHL	C4B-NB	3.09	1.38	1.35
29	n	614	CLA	CHC-C1C	3.09	1.42	1.35
29	S	605	CLA	CHC-C1C	3.09	1.42	1.35
29	C	504	CLA	CHC-C1C	3.09	1.42	1.35
29	y	610	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	612	CLA	CHC-C1C	3.09	1.42	1.35
45	y	605	CHL	C4B-NB	3.09	1.38	1.35
29	Y	613	CLA	CHC-C1C	3.09	1.42	1.35
29	b	616	CLA	C4D-ND	-3.09	1.33	1.37
29	s	614	CLA	CHC-C1C	3.09	1.42	1.35
44	H	101	RRX	C24-C25	3.09	1.56	1.45
44	h	101	RRX	C4-C5	-3.09	1.44	1.51
29	S	614	CLA	CHC-C1C	3.08	1.42	1.35
29	Y	610	CLA	CHC-C1C	3.08	1.42	1.35
29	a	405	CLA	C1D-ND	3.08	1.41	1.37
29	b	616	CLA	CHC-C1C	3.08	1.42	1.35
29	n	604	CLA	CHC-C1C	3.08	1.42	1.35
29	r	604	CLA	CHC-C1C	3.08	1.42	1.35
36	b	620	C7Z	C21-C26	-3.08	1.49	1.53
45	r	607	CHL	C4B-NB	3.08	1.38	1.35
29	b	609	CLA	CHC-C1C	3.08	1.42	1.35
29	B	603	CLA	CHC-C1C	3.08	1.42	1.35
29	C	501	CLA	CHC-C1C	3.07	1.42	1.35
29	g	614	CLA	CHC-C1C	3.07	1.42	1.35
29	B	609	CLA	CHC-C1C	3.07	1.42	1.35
29	A	410	CLA	CHC-C1C	3.07	1.42	1.35
29	C	502	CLA	CHC-C1C	3.07	1.42	1.35
29	b	615	CLA	CHC-C1C	3.07	1.42	1.35
45	S	601	CHL	CBB-CAB	3.07	1.49	1.29
29	b	607	CLA	CHC-C1C	3.07	1.42	1.35
45	s	607	CHL	C4B-NB	3.07	1.37	1.35
29	s	613	CLA	CHC-C1C	3.07	1.42	1.35
45	r	606	CHL	C4B-NB	3.06	1.37	1.35
29	y	613	CLA	CHC-C1C	3.06	1.42	1.35
29	g	603	CLA	CHC-C1C	3.06	1.42	1.35
29	y	614	CLA	CHC-C1C	3.06	1.42	1.35
29	C	503	CLA	CHC-C1C	3.06	1.42	1.35
29	b	610	CLA	CHC-C1C	3.06	1.42	1.35
29	Y	614	CLA	CHC-C1C	3.06	1.42	1.35
29	Y	604	CLA	CHC-C1C	3.06	1.42	1.35
29	C	507	CLA	CHC-C1C	3.06	1.42	1.35
29	a	407	CLA	CHC-C1C	3.06	1.42	1.35
29	g	604	CLA	CHC-C1C	3.06	1.42	1.35
29	c	501	CLA	CHC-C1C	3.06	1.42	1.35
29	S	602	CLA	CHC-C1C	3.06	1.42	1.35
43	F	101	HEM	CAB-C3B	3.06	1.55	1.47
29	S	603	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	611	CLA	CHC-C1C	3.05	1.42	1.35
29	C	509	CLA	CHC-C1C	3.05	1.42	1.35
44	h	101	RRX	C29-C30	3.05	1.64	1.54
29	y	611	CLA	CHC-C1C	3.05	1.42	1.35
29	B	616	CLA	C4D-ND	-3.05	1.33	1.37
43	f	101	HEM	CAB-C3B	3.05	1.55	1.47
29	B	615	CLA	CHC-C1C	3.04	1.42	1.35
29	C	511	CLA	CHC-C1C	3.04	1.42	1.35
29	a	410	CLA	CHC-C1C	3.04	1.42	1.35
29	G	603	CLA	CHC-C1C	3.04	1.42	1.35
29	S	613	CLA	CHC-C1C	3.04	1.42	1.35
29	N	613	CLA	CHC-C1C	3.04	1.42	1.35
29	R	608	CLA	CHC-C1C	3.04	1.42	1.35
29	c	511	CLA	CHC-C1C	3.04	1.42	1.35
29	b	614	CLA	CHC-C1C	3.04	1.42	1.35
29	R	609	CLA	CHC-C1C	3.04	1.42	1.35
45	y	601	CHL	C4B-NB	3.04	1.37	1.35
29	N	614	CLA	CHC-C1C	3.04	1.42	1.35
29	R	604	CLA	CHC-C1C	3.04	1.42	1.35
29	s	612	CLA	CHC-C1C	3.04	1.42	1.35
29	N	614	CLA	C4D-ND	-3.03	1.33	1.37
29	B	610	CLA	CHC-C1C	3.03	1.42	1.35
45	N	607	CHL	C3B-C2B	-3.03	1.36	1.40
45	G	609	CHL	C4B-NB	3.03	1.37	1.35
45	y	606	CHL	CBB-CAB	3.03	1.49	1.29
29	Y	603	CLA	CHC-C1C	3.03	1.42	1.35
45	Y	609	CHL	C4B-NB	3.03	1.37	1.35
29	s	605	CLA	CHC-C1C	3.03	1.42	1.35
45	g	609	CHL	C4B-NB	3.03	1.37	1.35
29	g	612	CLA	CHC-C1C	3.02	1.42	1.35
29	A	406	CLA	CHC-C1C	3.02	1.42	1.35
29	Y	608	CLA	CHC-C1C	3.02	1.42	1.35
29	r	602	CLA	CHC-C1C	3.02	1.42	1.35
45	N	601	CHL	C4B-NB	3.02	1.37	1.35
29	s	609	CLA	CHC-C1C	3.02	1.42	1.35
45	g	605	CHL	C4B-NB	3.01	1.37	1.35
45	Y	606	CHL	C3B-C2B	-3.01	1.36	1.40
45	n	601	CHL	C4B-NB	3.01	1.37	1.35
45	s	608	CHL	C4B-NB	3.01	1.37	1.35
29	r	612	CLA	CHC-C1C	3.00	1.42	1.35
29	N	603	CLA	CHC-C1C	3.00	1.42	1.35
29	r	608	CLA	CHC-C1C	3.00	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	g	606	CHL	C4B-NB	3.00	1.37	1.35
29	n	603	CLA	CHC-C1C	3.00	1.42	1.35
45	R	606	CHL	C4B-NB	3.00	1.37	1.35
45	S	608	CHL	C4B-NB	3.00	1.37	1.35
29	g	613	CLA	CHC-C1C	2.99	1.42	1.35
29	B	612	CLA	CHC-C1C	2.99	1.42	1.35
29	Y	612	CLA	CHC-C1C	2.99	1.42	1.35
29	C	510	CLA	CHC-C1C	2.99	1.42	1.35
29	y	604	CLA	CHC-C1C	2.99	1.42	1.35
29	s	603	CLA	CHC-C1C	2.99	1.42	1.35
29	y	603	CLA	CHC-C1C	2.98	1.42	1.35
29	A	405	CLA	CHC-C1C	2.98	1.42	1.35
45	g	608	CHL	C4B-NB	2.98	1.37	1.35
29	y	608	CLA	CHC-C1C	2.98	1.42	1.35
29	S	604	CLA	CHC-C1C	2.97	1.42	1.35
29	G	613	CLA	CHC-C1C	2.97	1.42	1.35
29	c	508	CLA	CHC-C1C	2.97	1.42	1.35
29	R	603	CLA	CHC-C1C	2.97	1.42	1.35
44	H	101	RRX	C29-C30	2.97	1.64	1.54
29	C	508	CLA	CHC-C1C	2.97	1.42	1.35
29	a	405	CLA	CHC-C1C	2.96	1.42	1.35
29	c	503	CLA	CHC-C1C	2.96	1.42	1.35
29	C	506	CLA	CHC-C1C	2.96	1.42	1.35
45	G	606	CHL	C3B-C2B	-2.96	1.36	1.40
44	h	101	RRX	C7-C6	2.96	1.55	1.45
29	a	406	CLA	CHC-C1C	2.96	1.42	1.35
29	c	504	CLA	CHC-C1C	2.96	1.42	1.35
45	r	606	CHL	C3B-C2B	-2.95	1.36	1.40
29	s	604	CLA	CHC-C1C	2.95	1.42	1.35
29	b	612	CLA	CHC-C1C	2.95	1.42	1.35
29	y	612	CLA	CHC-C1C	2.94	1.42	1.35
29	B	611	CLA	CHC-C1C	2.94	1.42	1.35
44	H	101	RRX	C7-C6	2.93	1.55	1.45
29	b	611	CLA	CHC-C1C	2.93	1.42	1.35
29	n	613	CLA	CHC-C1C	2.93	1.42	1.35
29	r	603	CLA	CHC-C1C	2.93	1.42	1.35
29	c	502	CLA	CHC-C1C	2.93	1.42	1.35
29	S	603	CLA	C1D-ND	2.92	1.41	1.37
42	d	405	PL9	C6-C1	-2.92	1.43	1.48
29	r	609	CLA	CHC-C1C	2.92	1.42	1.35
45	N	608	CHL	C4B-NB	2.90	1.37	1.35
29	b	617	CLA	CHC-C1C	2.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	608	CLA	CHC-C1C	2.90	1.42	1.35
45	n	606	CHL	C4B-NB	2.90	1.37	1.35
45	N	609	CHL	C4B-NB	2.89	1.37	1.35
45	n	605	CHL	C4B-NB	2.89	1.37	1.35
29	c	506	CLA	CHC-C1C	2.89	1.42	1.35
29	B	617	CLA	CHC-C1C	2.88	1.42	1.35
29	b	606	CLA	CHC-C1C	2.88	1.42	1.35
45	s	606	CHL	C4B-NB	2.87	1.37	1.35
29	B	606	CLA	CHC-C1C	2.87	1.42	1.35
42	D	405	PL9	C6-C1	-2.87	1.43	1.48
29	c	510	CLA	CHC-C1C	2.86	1.42	1.35
49	r	625	LMT	O3'-C3'	-2.86	1.36	1.43
29	D	402	CLA	C1D-ND	2.86	1.41	1.37
29	B	608	CLA	CHC-C1C	2.85	1.42	1.35
45	r	607	CHL	C3B-C2B	-2.83	1.36	1.40
45	N	607	CHL	C4B-NB	2.83	1.37	1.35
45	S	601	CHL	C3B-C2B	-2.83	1.36	1.40
50	s	625	LPX	P1-O1	2.82	1.70	1.59
45	G	607	CHL	C4B-NB	2.81	1.37	1.35
45	g	606	CHL	C3B-C2B	-2.81	1.36	1.40
45	R	607	CHL	C3B-C2B	-2.80	1.36	1.40
45	s	607	CHL	C3B-C2B	-2.79	1.36	1.40
45	Y	601	CHL	C4B-NB	2.79	1.37	1.35
49	R	625	LMT	O3'-C3'	-2.79	1.36	1.43
45	n	608	CHL	C4B-NB	2.79	1.37	1.35
45	g	607	CHL	C4B-NB	2.77	1.37	1.35
45	y	601	CHL	C3B-C2B	-2.77	1.36	1.40
29	B	605	CLA	CHC-C1C	2.77	1.42	1.35
45	N	606	CHL	C3B-C2B	-2.75	1.36	1.40
45	s	601	CHL	C3B-C2B	-2.74	1.36	1.40
45	R	606	CHL	C3B-C2B	-2.73	1.36	1.40
45	Y	607	CHL	C4B-NB	2.73	1.37	1.35
45	G	608	CHL	C3B-C2B	-2.73	1.36	1.40
29	b	605	CLA	CHC-C1C	2.73	1.42	1.35
45	S	606	CHL	C3B-C2B	-2.71	1.36	1.40
45	n	607	CHL	C4B-NB	2.71	1.37	1.35
44	H	101	RRX	C32-C1	2.70	1.59	1.53
50	S	625	LPX	P1-O1	2.68	1.70	1.59
44	h	101	RRX	C32-C1	2.67	1.59	1.53
45	y	606	CHL	C4B-NB	2.66	1.37	1.35
45	g	609	CHL	C3B-C2B	-2.65	1.36	1.40
45	n	609	CHL	C4B-NB	2.65	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	402	CLA	C1D-ND	2.64	1.41	1.37
30	a	408	PHO	CAC-C3C	-2.60	1.47	1.52
35	C	527	LMG	C40-C39	-2.59	1.33	1.51
30	A	409	PHO	CAC-C3C	-2.58	1.47	1.52
45	n	605	CHL	C3A-C2A	-2.58	1.47	1.54
45	n	605	CHL	C3B-C2B	-2.58	1.36	1.40
35	d	411	LMG	C37-C36	-2.57	1.33	1.51
30	a	409	PHO	CAC-C3C	-2.56	1.47	1.52
35	D	411	LMG	C37-C36	-2.55	1.33	1.51
49	r	625	LMT	O2'-C2'	-2.55	1.37	1.43
30	A	408	PHO	CAC-C3C	-2.55	1.47	1.52
49	R	625	LMT	O2'-C2'	-2.52	1.37	1.43
45	N	605	CHL	C3B-C2B	-2.52	1.36	1.40
38	B	624	3PH	O21-C2	-2.51	1.40	1.46
51	y	627	PTY	O7-C6	-2.50	1.40	1.46
51	y	626	PTY	O7-C6	-2.50	1.40	1.46
38	b	624	3PH	O21-C2	-2.49	1.40	1.46
42	D	405	PL9	C52-C5	-2.49	1.45	1.50
45	s	608	CHL	C3B-C2B	-2.49	1.36	1.40
38	b	624	3PH	O31-C31	2.47	1.40	1.33
45	y	607	CHL	C4B-NB	2.47	1.37	1.35
51	Y	627	PTY	O7-C6	-2.46	1.40	1.46
45	N	609	CHL	C3B-C2B	-2.46	1.37	1.40
45	G	609	CHL	C3B-C2B	-2.45	1.37	1.40
51	Y	626	PTY	O7-C6	-2.44	1.40	1.46
38	S	626	3PH	O21-C2	-2.43	1.40	1.46
38	B	624	3PH	O31-C31	2.43	1.40	1.33
44	H	101	RRX	C35-C13	2.42	1.55	1.50
49	r	625	LMT	O2B-C2B	-2.42	1.37	1.43
49	R	625	LMT	O2B-C2B	-2.42	1.37	1.43
36	B	620	C7Z	C20-C13	2.42	1.55	1.50
38	S	626	3PH	O31-C31	2.41	1.40	1.33
51	Y	626	PTY	O4-C30	2.41	1.40	1.33
44	h	101	RRX	C35-C13	2.41	1.55	1.50
38	s	626	3PH	O31-C31	2.40	1.40	1.33
51	y	626	PTY	O4-C30	2.40	1.40	1.33
36	b	620	C7Z	C20-C13	2.38	1.55	1.50
38	s	626	3PH	O21-C2	-2.38	1.40	1.46
36	B	620	C7Z	C10-C9	-2.38	1.32	1.35
29	S	603	CLA	MG-ND	-2.37	2.01	2.05
38	T	101	3PH	O31-C31	2.36	1.40	1.33
51	y	627	PTY	O7-C8	2.36	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S	608	CHL	C3B-C2B	-2.35	1.37	1.40
38	t	101	3PH	O31-C31	2.35	1.40	1.33
38	T	101	3PH	O21-C21	2.35	1.40	1.34
51	Y	627	PTY	O7-C8	2.33	1.40	1.35
48	g	622	XAT	O24-C25	-2.33	1.42	1.46
45	S	607	CHL	C3B-C2B	-2.32	1.37	1.40
45	Y	609	CHL	C3B-C2B	-2.32	1.37	1.40
45	g	601	CHL	C3B-C2B	-2.31	1.37	1.40
38	S	626	3PH	O21-C21	2.31	1.40	1.34
45	y	609	CHL	C3B-C2B	-2.31	1.37	1.40
45	g	605	CHL	C3B-C2B	-2.30	1.37	1.40
48	n	622	XAT	O24-C25	-2.30	1.42	1.46
38	s	626	3PH	O21-C21	2.29	1.40	1.34
45	Y	605	CHL	C3B-C2B	-2.28	1.37	1.40
38	t	101	3PH	O21-C2	-2.28	1.40	1.46
50	s	625	LPX	P1-O2	2.28	1.68	1.59
50	S	625	LPX	P1-O2	2.28	1.68	1.59
48	y	622	XAT	O24-C25	-2.28	1.43	1.46
38	t	101	3PH	O21-C21	2.27	1.40	1.34
49	r	625	LMT	O3B-C3B	-2.27	1.37	1.43
36	b	620	C7Z	C18-C5	2.27	1.54	1.50
48	G	622	XAT	O24-C25	-2.26	1.43	1.46
29	r	603	CLA	MG-ND	-2.26	2.01	2.05
45	y	605	CHL	C3B-C2B	-2.25	1.37	1.40
48	Y	622	XAT	O24-C25	-2.25	1.43	1.46
48	R	621	XAT	O24-C25	-2.25	1.43	1.46
30	a	408	PHO	CMC-C2C	-2.24	1.46	1.51
45	n	601	CHL	C3B-C2B	-2.24	1.37	1.40
48	N	622	XAT	O24-C25	-2.22	1.43	1.46
48	r	621	XAT	O24-C25	-2.21	1.43	1.46
45	N	601	CHL	C3B-C2B	-2.21	1.37	1.40
30	a	409	PHO	CMC-C2C	-2.21	1.46	1.51
36	B	620	C7Z	C18-C5	2.21	1.54	1.50
49	R	625	LMT	O3B-C3B	-2.21	1.37	1.43
45	G	605	CHL	C3B-C2B	-2.21	1.37	1.40
45	G	601	CHL	C3B-C2B	-2.20	1.37	1.40
36	b	620	C7Z	C10-C9	-2.20	1.32	1.35
39	c	524	DGA	OG2-CG2	-2.20	1.41	1.46
45	G	606	CHL	CHC-C1C	2.20	1.40	1.35
29	b	605	CLA	MG-ND	-2.20	2.01	2.05
49	R	625	LMT	O4'-C4B	-2.19	1.37	1.43
42	d	405	PL9	C52-C5	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	j	101	DGA	OG2-CG2	-2.18	1.41	1.46
45	S	601	CHL	CHC-C1C	2.18	1.40	1.35
51	Y	626	PTY	O7-C8	2.17	1.40	1.34
39	C	524	DGA	OG2-CG2	-2.17	1.41	1.46
38	S	626	3PH	O31-C3	-2.17	1.40	1.45
49	r	625	LMT	O4'-C4B	-2.16	1.37	1.43
45	g	608	CHL	C3B-C2B	-2.16	1.37	1.40
30	A	409	PHO	CMC-C2C	-2.16	1.46	1.51
38	B	624	3PH	O31-C3	-2.16	1.40	1.45
51	y	626	PTY	O7-C8	2.16	1.40	1.34
42	d	405	PL9	C53-C6	-2.15	1.46	1.50
51	y	626	PTY	O4-C1	-2.15	1.40	1.45
30	a	408	PHO	CMD-C2D	-2.14	1.46	1.51
31	B	619	BCR	C12-C13	-2.14	1.41	1.45
29	R	603	CLA	MG-ND	-2.14	2.01	2.05
45	N	606	CHL	CHC-C1C	2.13	1.40	1.35
38	b	624	3PH	O21-C21	2.13	1.40	1.34
30	A	408	PHO	CMC-C2C	-2.12	1.46	1.51
38	s	626	3PH	O31-C3	-2.12	1.40	1.45
29	s	603	CLA	MG-ND	-2.11	2.01	2.05
36	b	620	C7Z	C40-C33	2.11	1.55	1.50
31	c	515	BCR	C12-C13	-2.11	1.41	1.45
45	g	606	CHL	C3A-C2A	-2.11	1.48	1.54
46	r	620	LUT	C22-C21	-2.11	1.52	1.54
30	A	408	PHO	CMD-C2D	-2.10	1.46	1.51
38	T	101	3PH	O31-C3	-2.10	1.40	1.45
45	y	606	CHL	C3A-C2A	-2.10	1.48	1.54
31	b	619	BCR	C12-C13	-2.10	1.41	1.45
29	n	610	CLA	MG-ND	-2.10	2.01	2.05
42	D	405	PL9	C53-C6	-2.09	1.46	1.50
42	D	405	PL9	C7-C8	-2.09	1.47	1.50
38	B	624	3PH	O21-C21	2.09	1.40	1.34
38	b	624	3PH	O31-C3	-2.08	1.40	1.45
51	Y	627	PTY	O4-C1	-2.08	1.40	1.45
29	R	608	CLA	MG-ND	-2.08	2.01	2.05
45	s	601	CHL	CHC-C1C	2.08	1.40	1.35
36	B	620	C7Z	C40-C33	2.07	1.55	1.50
30	a	409	PHO	CMD-C2D	-2.07	1.46	1.51
38	t	101	3PH	O31-C3	-2.07	1.40	1.45
31	B	618	BCR	C12-C13	-2.06	1.41	1.45
30	A	409	PHO	CMD-C2D	-2.06	1.46	1.51
47	y	623	NEX	C1-C6	-2.06	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	610	CLA	MG-ND	-2.05	2.01	2.05
29	y	610	CLA	MG-ND	-2.05	2.01	2.05
49	r	625	LMT	O1'-C1'	-2.05	1.36	1.40
39	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
51	y	627	PTY	O4-C1	-2.05	1.40	1.45
29	C	505	CLA	MG-ND	-2.04	2.01	2.05
30	a	408	PHO	CMB-C2B	-2.04	1.46	1.51
29	g	610	CLA	MG-ND	-2.04	2.01	2.05
29	B	617	CLA	MG-ND	-2.04	2.01	2.05
35	H	102	LMG	C22-C21	-2.04	1.33	1.49
35	h	102	LMG	C22-C21	-2.03	1.33	1.49
31	a	411	BCR	C12-C13	-2.03	1.41	1.45
30	A	408	PHO	CMB-C2B	-2.03	1.46	1.51
29	s	610	CLA	MG-ND	-2.03	2.01	2.05
43	f	101	HEM	CMB-C2B	2.03	1.55	1.50
37	C	519	DGD	CGB-CFB	-2.03	1.33	1.49
37	c	518	DGD	CGB-CFB	-2.03	1.33	1.49
35	c	521	LMG	C43-C42	-2.03	1.33	1.49
45	Y	606	CHL	CHC-C1C	2.02	1.40	1.35
29	r	608	CLA	MG-ND	-2.02	2.01	2.05
37	c	520	DGD	CDA-CCA	-2.02	1.33	1.49
29	b	617	CLA	MG-ND	-2.02	2.01	2.05
37	C	520	DGD	CAB-C9B	-2.02	1.33	1.49
31	A	411	BCR	C12-C13	-2.02	1.41	1.45
29	d	402	CLA	MG-ND	-2.02	2.01	2.05
37	c	519	DGD	CGB-CFB	-2.02	1.33	1.49
35	c	521	LMG	C25-C24	-2.02	1.33	1.49
47	y	623	NEX	O24-C25	-2.01	1.43	1.46
37	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
35	C	521	LMG	C43-C42	-2.01	1.33	1.49
35	B	622	LMG	C25-C24	-2.01	1.33	1.49
37	c	520	DGD	CGB-CFB	-2.01	1.33	1.49
29	c	505	CLA	MG-ND	-2.01	2.01	2.05
29	c	507	CLA	MG-ND	-2.01	2.01	2.05
51	Y	626	PTY	O4-C1	-2.01	1.40	1.45
35	a	413	LMG	C22-C21	-2.01	1.33	1.49
37	C	520	DGD	CDA-CCA	-2.00	1.33	1.49
35	a	413	LMG	C43-C42	-2.00	1.33	1.49
35	A	413	LMG	C22-C21	-2.00	1.33	1.49
37	c	519	DGD	CGA-CFA	-2.00	1.33	1.49

All (2038) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	404	BCR	C10-C11-C12	17.66	178.32	123.22
31	C	517	BCR	C10-C11-C12	17.51	177.86	123.22
31	c	517	BCR	C10-C11-C12	17.44	177.64	123.22
31	b	618	BCR	C10-C11-C12	17.38	177.47	123.22
31	b	619	BCR	C10-C11-C12	17.35	177.38	123.22
31	B	619	BCR	C10-C11-C12	17.21	176.91	123.22
31	D	404	BCR	C10-C11-C12	17.20	176.89	123.22
31	c	516	BCR	C10-C11-C12	17.11	176.63	123.22
31	C	516	BCR	C10-C11-C12	16.95	176.10	123.22
31	C	514	BCR	C10-C11-C12	16.93	176.05	123.22
31	c	515	BCR	C10-C11-C12	16.90	175.95	123.22
31	c	514	BCR	C10-C11-C12	16.90	175.95	123.22
48	Y	622	XAT	C37-C21-C36	-16.82	82.56	107.37
31	C	515	BCR	C10-C11-C12	16.71	175.35	123.22
48	y	622	XAT	C37-C21-C36	-16.67	82.78	107.37
31	B	618	BCR	C10-C11-C12	16.64	175.15	123.22
31	a	411	BCR	C10-C11-C12	16.54	174.83	123.22
31	A	411	BCR	C10-C11-C12	16.48	174.65	123.22
31	c	514	BCR	C11-C10-C9	14.43	147.90	127.31
31	c	516	BCR	C11-C10-C9	13.59	146.70	127.31
31	C	516	BCR	C11-C10-C9	13.59	146.70	127.31
31	a	411	BCR	C11-C10-C9	13.23	146.19	127.31
31	A	411	BCR	C11-C10-C9	13.22	146.17	127.31
31	C	514	BCR	C11-C10-C9	13.16	146.09	127.31
31	d	404	BCR	C21-C20-C19	13.14	164.21	123.22
31	b	618	BCR	C11-C10-C9	13.04	145.91	127.31
31	B	618	BCR	C11-C10-C9	12.51	145.17	127.31
48	y	622	XAT	C37-C21-C22	-12.49	87.28	108.98
31	A	411	BCR	C11-C12-C13	12.28	160.91	126.42
48	Y	622	XAT	C37-C21-C22	-12.26	87.67	108.98
31	a	411	BCR	C11-C12-C13	12.24	160.81	126.42
31	A	411	BCR	C21-C20-C19	12.15	161.13	123.22
31	C	515	BCR	C11-C10-C9	12.15	144.65	127.31
31	B	618	BCR	C11-C12-C13	12.14	160.51	126.42
31	c	517	BCR	C11-C10-C9	12.12	144.61	127.31
31	C	515	BCR	C11-C12-C13	12.11	160.44	126.42
31	C	514	BCR	C16-C15-C14	12.06	148.18	123.47
31	a	411	BCR	C21-C20-C19	12.05	160.82	123.22
31	c	517	BCR	C21-C20-C19	12.04	160.78	123.22
31	C	517	BCR	C21-C20-C19	12.03	160.75	123.22
31	C	517	BCR	C11-C10-C9	11.92	144.33	127.31
31	c	514	BCR	C16-C15-C14	11.78	147.60	123.47
31	c	515	BCR	C11-C10-C9	11.71	144.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	619	BCR	C11-C10-C9	11.69	143.99	127.31
31	C	515	BCR	C16-C15-C14	11.69	147.41	123.47
31	d	404	BCR	C16-C15-C14	11.67	147.38	123.47
31	D	404	BCR	C11-C12-C13	11.63	159.08	126.42
31	b	619	BCR	C11-C10-C9	11.43	143.62	127.31
31	C	516	BCR	C11-C12-C13	11.43	158.51	126.42
31	D	404	BCR	C11-C10-C9	11.41	143.60	127.31
31	c	516	BCR	C21-C20-C19	11.35	158.65	123.22
31	c	517	BCR	C16-C15-C14	11.34	146.71	123.47
31	c	515	BCR	C16-C15-C14	11.24	146.51	123.47
31	d	404	BCR	C11-C10-C9	11.22	143.32	127.31
31	c	516	BCR	C11-C12-C13	11.20	157.87	126.42
31	c	514	BCR	C21-C20-C19	11.18	158.10	123.22
31	b	618	BCR	C16-C15-C14	11.17	146.36	123.47
31	b	619	BCR	C21-C20-C19	11.17	158.08	123.22
31	C	517	BCR	C16-C15-C14	11.15	146.31	123.47
31	b	619	BCR	C16-C15-C14	11.11	146.22	123.47
31	D	404	BCR	C21-C20-C19	11.10	157.85	123.22
31	C	516	BCR	C21-C20-C19	11.05	157.72	123.22
31	c	514	BCR	C11-C12-C13	10.97	157.24	126.42
31	C	514	BCR	C21-C20-C19	10.92	157.28	123.22
31	b	619	BCR	C11-C12-C13	10.86	156.93	126.42
31	B	619	BCR	C11-C12-C13	10.83	156.84	126.42
31	B	619	BCR	C21-C20-C19	10.79	156.89	123.22
31	c	517	BCR	C11-C12-C13	10.78	156.69	126.42
31	B	619	BCR	C16-C15-C14	10.77	145.53	123.47
31	b	618	BCR	C21-C20-C19	10.76	156.80	123.22
31	C	517	BCR	C11-C12-C13	10.75	156.61	126.42
31	d	404	BCR	C11-C12-C13	10.69	156.44	126.42
31	c	515	BCR	C11-C12-C13	10.66	156.35	126.42
31	A	411	BCR	C16-C15-C14	10.55	145.09	123.47
31	B	618	BCR	C21-C20-C19	10.52	156.05	123.22
31	C	516	BCR	C16-C15-C14	10.47	144.91	123.47
31	c	516	BCR	C16-C15-C14	10.46	144.90	123.47
31	b	618	BCR	C11-C12-C13	10.39	155.60	126.42
31	a	411	BCR	C16-C15-C14	10.34	144.66	123.47
31	D	404	BCR	C16-C15-C14	10.31	144.60	123.47
31	C	515	BCR	C21-C20-C19	10.28	155.30	123.22
31	C	514	BCR	C11-C12-C13	10.01	154.54	126.42
31	c	515	BCR	C21-C20-C19	10.00	154.42	123.22
31	B	618	BCR	C16-C15-C14	9.66	143.25	123.47
31	c	515	BCR	C20-C19-C18	9.57	153.29	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	515	BCR	C20-C19-C18	9.24	152.37	126.42
31	B	618	BCR	C20-C19-C18	8.58	150.52	126.42
31	C	514	BCR	C20-C19-C18	8.49	150.28	126.42
31	b	618	BCR	C20-C19-C18	8.37	149.93	126.42
31	B	619	BCR	C20-C19-C18	8.30	149.74	126.42
31	c	514	BCR	C20-C19-C18	8.20	149.45	126.42
31	c	516	BCR	C20-C19-C18	8.11	149.20	126.42
31	C	516	BCR	C20-C19-C18	8.09	149.15	126.42
31	D	404	BCR	C20-C19-C18	8.05	149.04	126.42
31	b	619	BCR	C20-C19-C18	8.00	148.88	126.42
44	H	101	RRX	C20-C21-C22	-7.63	116.41	127.31
31	c	517	BCR	C20-C19-C18	7.62	147.84	126.42
31	C	517	BCR	C20-C19-C18	7.59	147.74	126.42
48	Y	622	XAT	C36-C21-C22	7.46	121.94	108.98
31	A	411	BCR	C20-C19-C18	7.41	147.24	126.42
31	a	411	BCR	C20-C19-C18	7.40	147.19	126.42
48	Y	622	XAT	C37-C21-C26	-7.26	90.45	110.05
48	y	622	XAT	C37-C21-C26	-7.25	90.48	110.05
48	y	622	XAT	C36-C21-C22	7.20	121.50	108.98
44	h	101	RRX	C11-C10-C9	-7.02	117.30	127.31
44	h	101	RRX	C20-C21-C22	-6.92	117.44	127.31
44	H	101	RRX	C11-C10-C9	-6.85	117.53	127.31
39	b	625	DGA	CDB-CCB-CBB	-6.82	79.81	114.42
36	B	620	C7Z	C11-C10-C9	-6.77	117.64	127.31
29	g	610	CLA	C4A-NA-C1A	6.68	109.71	106.71
39	C	524	DGA	CDB-CCB-CBB	-6.62	80.82	114.42
39	c	524	DGA	CDB-CCB-CBB	-6.62	80.83	114.42
44	H	101	RRX	C15-C14-C13	-6.59	117.91	127.31
48	N	622	XAT	C31-C30-C29	-6.47	118.08	127.31
44	h	101	RRX	C16-C17-C18	-6.32	118.30	127.31
31	d	404	BCR	C20-C19-C18	6.31	144.14	126.42
36	b	620	C7Z	C11-C10-C9	-6.23	118.41	127.31
29	G	610	CLA	C4A-NA-C1A	6.17	109.48	106.71
48	y	622	XAT	C31-C30-C29	-6.10	118.60	127.31
48	g	622	XAT	C15-C14-C13	-6.07	118.65	127.31
48	G	622	XAT	C31-C30-C29	-6.04	118.69	127.31
29	b	605	CLA	C4A-NA-C1A	6.04	109.42	106.71
44	h	101	RRX	C15-C14-C13	-6.03	118.70	127.31
46	g	620	LUT	C21-C26-C25	6.01	122.19	111.42
48	Y	622	XAT	C31-C30-C29	-6.00	118.75	127.31
44	H	101	RRX	C24-C23-C22	-5.98	117.20	126.23
29	S	605	CLA	C4A-NA-C1A	5.85	109.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	620	LUT	C21-C26-C25	5.83	121.86	111.42
48	g	622	XAT	C31-C30-C29	-5.83	118.99	127.31
46	g	621	LUT	C21-C26-C25	5.81	121.82	111.42
46	s	620	LUT	C21-C26-C25	5.78	121.78	111.42
46	G	621	LUT	C21-C26-C25	5.78	121.77	111.42
46	G	620	LUT	C21-C26-C25	5.72	121.67	111.42
29	s	603	CLA	C4A-NA-C1A	5.71	109.27	106.71
46	N	620	LUT	C21-C26-C25	5.70	121.63	111.42
46	N	621	LUT	C21-C26-C25	5.68	121.59	111.42
48	n	622	XAT	C31-C30-C29	-5.63	119.27	127.31
46	y	620	LUT	C21-C26-C25	5.62	121.49	111.42
40	L	101	LHG	O7-C7-C8	5.58	123.53	111.50
36	B	620	C7Z	C18-C5-C6	-5.58	118.26	124.53
29	C	507	CLA	C4A-NA-C1A	5.54	109.20	106.71
36	b	620	C7Z	C18-C5-C6	-5.51	118.34	124.53
29	N	610	CLA	C4A-NA-C1A	5.51	109.19	106.71
46	Y	621	LUT	C21-C26-C25	5.49	121.26	111.42
29	b	608	CLA	C4A-NA-C1A	5.45	109.16	106.71
36	B	620	C7Z	C35-C34-C33	-5.45	119.54	127.31
48	G	622	XAT	C15-C14-C13	-5.41	119.58	127.31
44	H	101	RRX	C16-C17-C18	-5.39	119.62	127.31
46	n	621	LUT	C21-C26-C25	5.38	121.05	111.42
46	S	621	LUT	C21-C26-C25	5.35	121.00	111.42
46	y	621	LUT	C21-C26-C25	5.33	120.97	111.42
48	Y	622	XAT	C15-C14-C13	-5.32	119.72	127.31
46	s	621	LUT	C21-C26-C25	5.29	120.89	111.42
48	n	622	XAT	C15-C14-C13	-5.24	119.83	127.31
48	r	621	XAT	C31-C30-C29	-5.22	119.86	127.31
46	n	620	LUT	C21-C26-C25	5.19	120.72	111.42
29	y	610	CLA	C4A-NA-C1A	5.18	109.04	106.71
48	N	622	XAT	C15-C14-C13	-5.15	119.96	127.31
36	b	620	C7Z	C35-C34-C33	-5.11	120.02	127.31
41	d	401	BCT	O2-C-O1	5.11	132.80	119.55
29	s	604	CLA	C4A-NA-C1A	5.11	109.00	106.71
29	B	605	CLA	C4A-NA-C1A	5.09	109.00	106.71
48	y	622	XAT	C15-C14-C13	-5.07	120.07	127.31
47	S	623	NEX	C2-C1-C6	5.06	114.13	109.21
48	R	621	XAT	C31-C30-C29	-5.03	120.13	127.31
46	S	620	LUT	C21-C26-C25	5.02	120.42	111.42
46	S	620	LUT	C21-C26-C27	5.00	119.02	112.70
29	r	602	CLA	C4A-NA-C1A	5.00	108.95	106.71
29	B	606	CLA	C4A-NA-C1A	4.98	108.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	507	CLA	C4A-NA-C1A	4.98	108.94	106.71
29	b	606	CLA	C4A-NA-C1A	4.98	108.94	106.71
42	d	405	PL9	C7-C3-C4	4.97	120.92	116.88
51	Y	627	PTY	O7-C8-C11	4.97	120.23	111.09
51	y	627	PTY	O7-C8-C11	4.96	120.22	111.09
29	R	602	CLA	C4A-NA-C1A	4.93	108.92	106.71
29	r	608	CLA	C4A-NA-C1A	4.91	108.91	106.71
46	r	620	LUT	C21-C26-C25	4.90	120.20	111.42
47	Y	623	NEX	C2-C1-C6	4.88	113.96	109.21
29	c	502	CLA	C4A-NA-C1A	4.87	108.89	106.71
29	Y	610	CLA	C4A-NA-C1A	4.83	108.88	106.71
36	B	620	C7Z	C38-C25-C26	-4.83	119.11	124.53
46	R	620	LUT	C21-C26-C25	4.82	120.05	111.42
29	d	403	CLA	C4A-NA-C1A	4.82	108.87	106.71
36	b	620	C7Z	C1-C6-C5	-4.81	115.84	122.61
29	B	608	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	b	604	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	B	604	CLA	C4A-NA-C1A	4.80	108.86	106.71
29	c	511	CLA	C4A-NA-C1A	4.79	108.86	106.71
37	b	623	DGD	O2G-C1B-C2B	4.77	121.79	111.50
29	G	611	CLA	C4A-NA-C1A	4.76	108.85	106.71
29	C	502	CLA	C4A-NA-C1A	4.76	108.84	106.71
29	D	403	CLA	C4A-NA-C1A	4.73	108.83	106.71
47	r	622	NEX	C38-C25-C24	4.72	119.59	114.28
48	n	622	XAT	C38-C25-C24	4.71	119.58	114.28
42	D	405	PL9	C7-C3-C4	4.69	120.69	116.88
36	b	620	C7Z	C38-C25-C26	-4.69	119.26	124.53
46	y	621	LUT	C22-C23-C24	-4.68	106.41	111.74
29	s	617	CLA	C4A-NA-C1A	4.68	108.81	106.71
48	n	622	XAT	C18-C5-C4	4.68	119.54	114.28
47	S	623	NEX	C38-C25-C24	4.67	119.53	114.28
46	n	621	LUT	C21-C26-C27	4.65	118.58	112.70
29	n	610	CLA	C4A-NA-C1A	4.65	108.80	106.71
29	s	602	CLA	C4A-NA-C1A	4.64	108.79	106.71
46	n	620	LUT	C21-C26-C27	4.64	118.57	112.70
48	Y	622	XAT	C18-C5-C4	4.64	119.50	114.28
29	c	505	CLA	C4A-NA-C1A	4.63	108.79	106.71
47	Y	623	NEX	C38-C25-C24	4.63	119.49	114.28
47	y	623	NEX	C38-C25-C24	4.62	119.48	114.28
35	A	413	LMG	O7-C10-C11	4.62	121.46	111.50
46	r	620	LUT	C21-C26-C27	4.62	118.54	112.70
29	S	613	CLA	C4A-NA-C1A	4.62	108.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	610	CLA	C4A-NA-C1A	4.61	108.78	106.71
29	y	602	CLA	C4A-NA-C1A	4.60	108.78	106.71
46	y	621	LUT	C21-C26-C27	4.60	118.52	112.70
47	s	623	NEX	C38-C25-C24	4.60	119.45	114.28
29	g	612	CLA	C4A-NA-C1A	4.59	108.77	106.71
47	R	622	NEX	C38-C25-C24	4.59	119.44	114.28
35	W	201	LMG	O7-C10-C11	4.58	121.38	111.50
46	N	621	LUT	C21-C26-C27	4.58	118.48	112.70
47	g	623	NEX	C27-C28-C29	-4.57	118.44	125.53
48	Y	622	XAT	C38-C25-C24	4.55	119.40	114.28
47	n	623	NEX	C27-C28-C29	-4.55	118.47	125.53
47	G	623	NEX	C38-C25-C24	4.54	119.39	114.28
29	s	605	CLA	C4A-NA-C1A	4.54	108.75	106.71
29	y	604	CLA	C4A-NA-C1A	4.54	108.75	106.71
38	t	101	3PH	O21-C21-C22	4.53	121.26	111.50
47	G	623	NEX	C27-C28-C29	-4.53	118.50	125.53
29	s	609	CLA	C4A-NA-C1A	4.52	108.74	106.71
48	N	622	XAT	C18-C5-C4	4.52	119.36	114.28
48	N	622	XAT	C38-C25-C24	4.52	119.36	114.28
29	B	607	CLA	C4A-NA-C1A	4.52	108.74	106.71
36	B	620	C7Z	C7-C8-C9	-4.50	119.44	126.23
29	B	617	CLA	C4A-NA-C1A	4.49	108.72	106.71
36	B	620	C7Z	C1-C6-C5	-4.48	116.31	122.61
48	G	622	XAT	C18-C5-C4	4.46	119.30	114.28
46	g	621	LUT	C21-C26-C27	4.46	118.33	112.70
47	r	622	NEX	C27-C28-C29	-4.45	118.62	125.53
29	S	610	CLA	C4A-NA-C1A	4.44	108.70	106.71
38	S	626	3PH	O21-C21-C22	4.44	121.06	111.50
36	b	620	C7Z	C15-C14-C13	-4.43	120.99	127.31
31	C	516	BCR	C33-C5-C6	-4.43	119.55	124.53
46	R	620	LUT	C21-C26-C27	4.41	118.28	112.70
47	N	623	NEX	C38-C25-C24	4.41	119.25	114.28
29	a	405	CLA	C4A-NA-C1A	4.41	108.69	106.71
29	b	610	CLA	C4A-NA-C1A	4.41	108.69	106.71
48	g	622	XAT	C7-C8-C9	-4.41	118.69	125.53
29	Y	614	CLA	C4A-NA-C1A	4.40	108.68	106.71
29	d	402	CLA	CHD-C1D-ND	-4.39	120.42	124.45
48	G	622	XAT	C7-C8-C9	-4.38	118.73	125.53
37	B	623	DGD	O2G-C1B-C2B	4.38	120.95	111.50
29	S	617	CLA	C4A-NA-C1A	4.38	108.68	106.71
48	g	622	XAT	C18-C5-C4	4.37	119.20	114.28
47	g	623	NEX	C38-C25-C24	4.37	119.19	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	n	623	NEX	C38-C25-C24	4.36	119.18	114.28
48	R	621	XAT	C38-C25-C24	4.35	119.18	114.28
29	r	610	CLA	C4A-NA-C1A	4.34	108.66	106.71
29	b	607	CLA	C4A-NA-C1A	4.34	108.66	106.71
48	y	622	XAT	C18-C5-C4	4.33	119.15	114.28
45	y	609	CHL	C2C-C3C-C4C	4.33	109.58	106.49
35	C	527	LMG	O7-C10-C11	4.32	120.82	111.50
46	s	620	LUT	C21-C26-C27	4.32	118.16	112.70
36	B	620	C7Z	C15-C14-C13	-4.31	121.16	127.31
29	n	614	CLA	C4A-NA-C1A	4.30	108.64	106.71
29	c	504	CLA	C4A-NA-C1A	4.30	108.64	106.71
47	y	623	NEX	C27-C28-C29	-4.30	118.86	125.53
40	N	624	LHG	O7-C7-C8	4.29	120.74	111.50
48	y	622	XAT	C7-C8-C9	-4.27	118.90	125.53
38	b	624	3PH	O21-C21-C22	4.27	120.71	111.50
46	S	621	LUT	C35-C34-C33	-4.27	121.21	127.31
47	Y	623	NEX	C27-C28-C29	-4.27	118.90	125.53
48	r	621	XAT	C18-C5-C4	4.27	119.08	114.28
29	g	611	CLA	C4A-NA-C1A	4.26	108.62	106.71
40	n	624	LHG	O7-C7-C8	4.26	120.69	111.50
40	C	525	LHG	O7-C7-C8	4.26	120.68	111.50
29	s	613	CLA	C4A-NA-C1A	4.26	108.62	106.71
29	g	614	CLA	C4A-NA-C1A	4.24	108.61	106.71
47	N	623	NEX	C27-C28-C29	-4.23	118.96	125.53
46	Y	621	LUT	C22-C23-C24	-4.23	106.93	111.74
47	R	622	NEX	C27-C28-C29	-4.23	118.97	125.53
48	y	622	XAT	C38-C25-C24	4.22	119.03	114.28
36	b	620	C7Z	C7-C8-C9	-4.21	119.88	126.23
29	R	604	CLA	CHD-C1D-ND	-4.21	120.59	124.45
46	Y	621	LUT	C21-C26-C27	4.19	117.99	112.70
29	n	614	CLA	CHD-C1D-ND	-4.19	120.61	124.45
44	h	101	RRX	C24-C23-C22	-4.18	119.91	126.23
29	S	611	CLA	C4A-NA-C1A	4.17	108.58	106.71
45	S	608	CHL	CHD-C1D-ND	-4.17	120.62	124.45
35	C	521	LMG	O7-C10-C11	4.16	120.46	111.50
46	g	621	LUT	C15-C14-C13	-4.15	121.38	127.31
29	S	603	CLA	C4A-NA-C1A	4.15	108.57	106.71
29	S	603	CLA	CHD-C1D-ND	-4.14	120.65	124.45
45	g	601	CHL	CHD-C1D-ND	-4.14	120.65	124.45
46	g	621	LUT	C35-C34-C33	-4.14	121.41	127.31
46	N	620	LUT	C21-C26-C27	4.13	117.93	112.70
46	g	620	LUT	C35-C34-C33	-4.13	121.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	620	LUT	C15-C14-C13	-4.12	121.43	127.31
45	n	609	CHL	CHD-C1D-ND	-4.12	120.67	124.45
48	r	621	XAT	C38-C25-C24	4.11	118.90	114.28
47	g	623	NEX	C17-C1-C6	-4.11	106.80	110.47
40	c	497	LHG	O7-C7-C8	4.10	120.34	111.50
29	B	610	CLA	C4A-NA-C1A	4.10	108.55	106.71
40	c	525	LHG	O7-C7-C8	4.09	120.33	111.50
40	S	624	LHG	O7-C7-C8	4.09	120.32	111.50
40	y	624	LHG	O7-C7-C8	4.09	120.32	111.50
45	y	609	CHL	CHD-C1D-ND	-4.09	120.70	124.45
45	Y	609	CHL	CHD-C1D-ND	-4.08	120.70	124.45
36	b	620	C7Z	C27-C28-C29	-4.08	120.07	126.23
38	s	626	3PH	O21-C21-C22	4.07	120.28	111.50
35	a	413	LMG	O7-C10-C11	4.07	120.27	111.50
46	r	620	LUT	C1-C6-C5	-4.07	116.89	122.61
48	y	622	XAT	C36-C21-C26	4.06	121.00	110.05
40	G	624	LHG	O7-C7-C8	4.05	120.24	111.50
46	R	620	LUT	C15-C14-C13	-4.04	121.54	127.31
29	B	603	CLA	C4A-NA-C1A	4.04	108.52	106.71
29	R	608	CLA	C4A-NA-C1A	4.04	108.52	106.71
46	s	621	LUT	C35-C34-C33	-4.04	121.55	127.31
29	S	617	CLA	CHD-C1D-ND	-4.03	120.75	124.45
29	S	609	CLA	C4A-NA-C1A	4.03	108.52	106.71
29	B	613	CLA	C4A-NA-C1A	4.02	108.51	106.71
29	A	406	CLA	C4A-NA-C1A	4.01	108.51	106.71
46	R	620	LUT	C18-C5-C6	-4.01	120.03	124.53
46	G	621	LUT	C15-C14-C13	-4.01	121.59	127.31
46	G	620	LUT	C22-C23-C24	-4.00	107.19	111.74
45	G	601	CHL	CHD-C1D-ND	-4.00	120.78	124.45
46	R	620	LUT	C11-C10-C9	-4.00	121.60	127.31
29	n	602	CLA	C4A-NA-C1A	3.99	108.50	106.71
45	n	605	CHL	CHD-C1D-ND	-3.99	120.79	124.45
38	B	624	3PH	O21-C21-C22	3.98	120.07	111.50
38	T	101	3PH	O21-C21-C22	3.98	120.07	111.50
35	h	102	LMG	O7-C10-C11	3.97	120.06	111.50
40	g	624	LHG	O7-C7-C8	3.97	120.06	111.50
29	c	513	CLA	C4A-NA-C1A	3.97	108.49	106.71
40	d	410	LHG	O7-C7-C8	3.97	120.05	111.50
47	S	623	NEX	C17-C1-C6	-3.96	106.93	110.47
40	s	624	LHG	O7-C7-C8	3.96	120.03	111.50
48	Y	622	XAT	C36-C21-C26	3.96	120.73	110.05
46	N	621	LUT	C22-C23-C24	-3.95	107.24	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	407	CLA	CHD-C1D-ND	-3.95	120.82	124.45
45	N	605	CHL	CHD-C1D-ND	-3.95	120.82	124.45
46	G	620	LUT	C21-C26-C27	3.95	117.70	112.70
48	r	621	XAT	C15-C14-C13	-3.95	121.68	127.31
45	y	609	CHL	C3C-C4C-NC	-3.95	106.14	110.57
29	C	508	CLA	CHD-C1D-ND	-3.94	120.83	124.45
47	S	623	NEX	C27-C28-C29	-3.94	119.42	125.53
46	g	621	LUT	C22-C23-C24	-3.93	107.26	111.74
39	J	101	DGA	OG2-CB1-CB2	3.93	119.97	111.50
29	N	614	CLA	C4A-NA-C1A	3.92	108.47	106.71
48	R	621	XAT	C18-C5-C4	3.92	118.69	114.28
46	Y	621	LUT	C15-C14-C13	-3.92	121.72	127.31
29	D	402	CLA	CHD-C1D-ND	-3.91	120.86	124.45
46	s	621	LUT	C21-C26-C27	3.91	117.64	112.70
36	b	620	C7Z	C31-C30-C29	-3.90	121.74	127.31
45	Y	606	CHL	CHD-C1D-ND	-3.90	120.87	124.45
36	B	620	C7Z	C27-C28-C29	-3.90	120.34	126.23
39	c	524	DGA	OG2-CB1-CB2	3.90	119.91	111.50
36	B	620	C7Z	C31-C30-C29	-3.90	121.75	127.31
29	C	504	CLA	C4A-NA-C1A	3.90	108.46	106.71
44	h	101	RRX	C38-C26-C25	-3.90	120.15	124.53
35	C	523	LMG	O7-C10-C11	3.89	119.89	111.50
40	D	410	LHG	O7-C7-C8	3.89	119.89	111.50
29	g	602	CLA	C4A-NA-C1A	3.88	108.45	106.71
47	s	623	NEX	C27-C28-C29	-3.87	119.52	125.53
45	G	609	CHL	CHD-C1D-ND	-3.87	120.89	124.45
39	B	625	DGA	OG2-CB1-CB2	3.87	119.85	111.50
39	b	625	DGA	OG2-CB1-CB2	3.87	119.84	111.50
47	G	623	NEX	C31-C30-C29	3.87	132.83	127.31
35	b	622	LMG	O7-C10-C11	3.86	119.83	111.50
45	Y	605	CHL	CHD-C1D-ND	-3.86	120.90	124.45
46	Y	621	LUT	C7-C8-C9	-3.86	120.40	126.23
29	G	612	CLA	C4A-NA-C1A	3.86	108.44	106.71
29	r	612	CLA	CHD-C1D-ND	-3.86	120.91	124.45
51	y	626	PTY	O7-C8-C11	3.86	119.81	111.50
48	r	621	XAT	O4-C5-C4	-3.86	110.49	113.38
51	Y	626	PTY	O7-C8-C11	3.85	119.81	111.50
48	R	621	XAT	C15-C14-C13	-3.85	121.81	127.31
46	y	621	LUT	C15-C14-C13	-3.85	121.82	127.31
46	S	621	LUT	C21-C26-C27	3.85	117.56	112.70
29	R	609	CLA	CHD-C1D-ND	-3.84	120.92	124.45
29	D	402	CLA	C4A-NA-C1A	3.84	108.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	521	LMG	O7-C10-C11	3.84	119.78	111.50
46	y	621	LUT	C35-C34-C33	-3.84	121.83	127.31
46	Y	621	LUT	C35-C34-C33	-3.84	121.83	127.31
39	C	524	DGA	OG2-CB1-CB2	3.83	119.77	111.50
39	j	101	DGA	OG2-CB1-CB2	3.83	119.76	111.50
29	S	613	CLA	CHD-C1D-ND	-3.83	120.94	124.45
46	G	621	LUT	C21-C26-C27	3.83	117.54	112.70
29	b	615	CLA	C4A-NA-C1A	3.81	108.42	106.71
46	g	621	LUT	C7-C8-C9	-3.81	120.48	126.23
45	g	609	CHL	CHD-C1D-ND	-3.80	120.96	124.45
29	B	615	CLA	C4A-NA-C1A	3.80	108.41	106.71
29	y	612	CLA	C4A-NA-C1A	3.80	108.41	106.71
37	c	518	DGD	O2G-C1B-C2B	3.80	119.69	111.50
29	S	602	CLA	CHD-C1D-ND	-3.80	120.96	124.45
46	G	621	LUT	C35-C34-C33	-3.79	121.89	127.31
37	C	520	DGD	O2G-C1B-C2B	3.79	119.67	111.50
46	n	621	LUT	C35-C34-C33	-3.79	121.90	127.31
35	H	102	LMG	O7-C10-C11	3.79	119.66	111.50
48	Y	622	XAT	C7-C8-C9	-3.79	119.66	125.53
29	S	614	CLA	CHD-C1D-ND	-3.78	120.98	124.45
29	B	615	CLA	CHD-C1D-ND	-3.78	120.98	124.45
29	C	509	CLA	CHD-C1D-ND	-3.78	120.98	124.45
46	s	620	LUT	C35-C34-C33	-3.78	121.91	127.31
40	d	408	LHG	O7-C7-C8	3.78	119.65	111.50
29	S	604	CLA	C4A-NA-C1A	3.78	108.41	106.71
29	R	610	CLA	C4A-NA-C1A	3.77	108.40	106.71
46	y	620	LUT	C15-C14-C13	-3.77	121.94	127.31
45	y	605	CHL	CHD-C1D-ND	-3.77	120.99	124.45
29	s	602	CLA	CHD-C1D-ND	-3.76	121.00	124.45
40	Y	624	LHG	O7-C7-C8	3.76	119.61	111.50
45	s	608	CHL	CHD-C1D-ND	-3.76	121.00	124.45
48	g	622	XAT	C38-C25-C24	3.76	118.51	114.28
39	B	625	DGA	CDB-CCB-CBB	-3.76	80.40	115.30
31	B	618	BCR	C33-C5-C4	3.76	120.84	113.62
37	c	520	DGD	O2G-C1B-C2B	3.76	119.60	111.50
31	A	411	BCR	C12-C13-C14	-3.76	113.18	118.94
29	a	406	CLA	CHD-C1D-ND	-3.76	121.00	124.45
46	N	621	LUT	C35-C34-C33	-3.75	121.95	127.31
29	s	611	CLA	C4A-NA-C1A	3.75	108.39	106.71
45	s	601	CHL	CHD-C1D-ND	-3.74	121.01	124.45
29	A	407	CLA	CHD-C1D-ND	-3.74	121.01	124.45
45	r	607	CHL	CHD-C1D-ND	-3.74	121.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	603	CLA	CHD-C1D-ND	-3.74	121.02	124.45
40	D	408	LHG	O7-C7-C8	3.74	119.56	111.50
45	g	606	CHL	CHD-C1D-ND	-3.73	121.02	124.45
29	C	510	CLA	CHD-C1D-ND	-3.73	121.03	124.45
29	Y	611	CLA	CHD-C1D-ND	-3.73	121.03	124.45
48	r	621	XAT	C6-C7-C8	-3.73	118.11	125.99
46	R	620	LUT	C35-C34-C33	-3.73	121.99	127.31
29	s	611	CLA	CHD-C1D-ND	-3.72	121.03	124.45
29	B	613	CLA	CHD-C1D-ND	-3.72	121.04	124.45
48	G	622	XAT	C38-C25-C24	3.72	118.46	114.28
29	R	609	CLA	C4A-NA-C1A	3.71	108.37	106.71
29	b	615	CLA	CHD-C1D-ND	-3.71	121.05	124.45
46	S	620	LUT	C15-C14-C13	-3.71	122.02	127.31
46	g	620	LUT	C15-C14-C13	-3.71	122.02	127.31
45	r	607	CHL	C3C-C4C-NC	-3.70	106.42	110.57
35	B	622	LMG	O7-C10-C11	3.70	119.48	111.50
45	N	608	CHL	CHD-C1D-ND	-3.70	121.05	124.45
45	S	607	CHL	CHD-C1D-ND	-3.70	121.06	124.45
29	Y	602	CLA	C4A-NA-C1A	3.69	108.37	106.71
44	h	101	RRX	C33-C5-C6	-3.69	120.38	124.53
33	a	412	SQD	O7-S-C6	-3.69	102.55	106.94
31	a	411	BCR	C12-C13-C14	-3.69	113.28	118.94
31	B	618	BCR	C33-C5-C6	-3.69	120.38	124.53
45	R	607	CHL	CHD-C1D-ND	-3.69	121.07	124.45
45	S	601	CHL	CHD-C1D-ND	-3.68	121.08	124.45
46	Y	620	LUT	C21-C26-C27	3.68	117.35	112.70
45	S	606	CHL	CHD-C1D-ND	-3.67	121.08	124.45
29	c	509	CLA	CHD-C1D-ND	-3.67	121.08	124.45
29	b	614	CLA	C4A-NA-C1A	3.67	108.36	106.71
45	N	607	CHL	CHD-C1D-ND	-3.67	121.08	124.45
29	G	602	CLA	CHD-C1D-ND	-3.67	121.08	124.45
29	d	402	CLA	C4A-NA-C1A	3.66	108.35	106.71
33	B	626	SQD	O7-S-C6	-3.66	102.59	106.94
35	d	411	LMG	O7-C10-C11	3.66	119.39	111.50
45	s	606	CHL	CHD-C1D-ND	-3.66	121.09	124.45
30	a	409	PHO	CMB-C2B-C3B	3.65	131.52	124.68
47	g	623	NEX	C31-C30-C29	3.65	132.53	127.31
33	A	412	SQD	O7-S-C6	-3.65	102.60	106.94
29	s	612	CLA	C4A-NA-C1A	3.65	108.35	106.71
45	n	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45
31	b	618	BCR	C23-C24-C25	-3.65	116.95	127.20
45	y	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	623	NEX	C2-C1-C6	3.65	112.76	109.21
29	s	610	CLA	CHD-C1D-ND	-3.65	121.10	124.45
31	C	516	BCR	C36-C18-C17	-3.65	117.81	122.92
48	R	621	XAT	O4-C5-C4	-3.65	110.64	113.38
29	c	508	CLA	CHD-C1D-ND	-3.65	121.10	124.45
45	G	601	CHL	C3C-C4C-NC	-3.64	106.48	110.57
29	R	608	CLA	CHD-C1D-ND	-3.64	121.11	124.45
45	G	605	CHL	C2C-C3C-C4C	3.64	109.08	106.49
29	c	509	CLA	C4A-NA-C1A	3.63	108.34	106.71
30	A	409	PHO	CMB-C2B-C3B	3.63	131.47	124.68
29	s	613	CLA	CHD-C1D-ND	-3.63	121.12	124.45
45	n	608	CHL	CHD-C1D-ND	-3.63	121.12	124.45
35	c	523	LMG	O7-C10-C11	3.62	119.30	111.50
46	y	621	LUT	C7-C8-C9	-3.62	120.77	126.23
46	r	620	LUT	C11-C10-C9	-3.61	122.16	127.31
47	s	623	NEX	C5-C4-C3	3.61	116.02	111.75
45	s	607	CHL	CHD-C1D-ND	-3.61	121.14	124.45
33	c	526	SQD	O7-S-C6	-3.61	102.65	106.94
31	A	411	BCR	C33-C5-C6	-3.60	120.48	124.53
29	y	611	CLA	CHD-C1D-ND	-3.60	121.14	124.45
47	g	623	NEX	C5-C6-C1	3.60	123.27	119.70
47	G	623	NEX	C2-C1-C6	3.60	112.71	109.21
29	n	612	CLA	CHD-C1D-ND	-3.60	121.15	124.45
46	N	620	LUT	C22-C23-C24	-3.60	107.65	111.74
29	B	610	CLA	CHD-C1D-ND	-3.60	121.15	124.45
44	H	101	RRX	C33-C5-C6	-3.60	120.49	124.53
29	N	611	CLA	CHD-C1D-ND	-3.59	121.15	124.45
46	s	621	LUT	C15-C14-C13	-3.59	122.18	127.31
36	B	620	C7Z	C1-C6-C7	3.59	125.93	115.78
40	d	409	LHG	O7-C7-C8	3.59	119.24	111.50
46	R	620	LUT	C7-C8-C9	-3.59	120.81	126.23
48	n	622	XAT	C6-C7-C8	-3.59	118.41	125.99
45	n	607	CHL	CHD-C1D-ND	-3.59	121.16	124.45
48	n	622	XAT	O4-C5-C4	-3.58	110.69	113.38
46	G	620	LUT	C35-C34-C33	-3.58	122.19	127.31
45	n	609	CHL	C3C-C4C-NC	-3.58	106.55	110.57
48	n	622	XAT	C7-C8-C9	-3.58	119.97	125.53
33	m	101	SQD	O7-S-C6	-3.58	102.68	106.94
46	g	621	LUT	C11-C10-C9	-3.58	122.20	127.31
45	g	607	CHL	C1-O2A-CGA	3.58	125.84	116.44
29	s	614	CLA	CHD-C1D-ND	-3.58	121.17	124.45
31	C	517	BCR	C28-C27-C26	-3.58	107.69	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	608	CLA	C4A-NA-C1A	3.58	108.31	106.71
29	S	605	CLA	CHD-C1D-ND	-3.58	121.17	124.45
46	N	620	LUT	C35-C34-C33	-3.57	122.21	127.31
29	C	509	CLA	C4A-NA-C1A	3.57	108.31	106.71
45	n	601	CHL	C3C-C4C-NC	-3.57	106.57	110.57
29	Y	608	CLA	CHD-C1D-ND	-3.57	121.17	124.45
29	Y	604	CLA	C4A-NA-C1A	3.57	108.31	106.71
48	N	622	XAT	C6-C7-C8	-3.57	118.45	125.99
31	B	618	BCR	C12-C13-C14	-3.56	113.47	118.94
29	B	614	CLA	C4A-NA-C1A	3.56	108.31	106.71
46	y	620	LUT	C21-C26-C27	3.56	117.20	112.70
45	n	605	CHL	C3C-C4C-NC	-3.56	106.58	110.57
29	b	609	CLA	CHD-C1D-ND	-3.56	121.18	124.45
29	s	612	CLA	CHD-C1D-ND	-3.56	121.19	124.45
46	S	621	LUT	C18-C5-C6	-3.56	120.53	124.53
47	G	623	NEX	C39-C29-C30	-3.56	117.94	122.92
45	G	608	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	y	614	CLA	CHD-C1D-ND	-3.55	121.19	124.45
29	n	613	CLA	C4A-NA-C1A	3.55	108.30	106.71
33	M	101	SQD	O7-S-C6	-3.55	102.72	106.94
29	B	612	CLA	C4A-NA-C1A	3.55	108.30	106.71
35	w	201	LMG	O7-C10-C11	3.55	119.14	111.50
47	Y	623	NEX	C17-C1-C6	-3.55	107.30	110.47
31	C	515	BCR	C23-C24-C25	-3.54	117.25	127.20
29	g	604	CLA	CHD-C1D-ND	-3.54	121.20	124.45
29	r	609	CLA	C4A-NA-C1A	3.53	108.30	106.71
29	S	609	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	Y	602	CLA	CHD-C1D-ND	-3.53	121.21	124.45
45	g	608	CHL	CHD-C1D-ND	-3.52	121.22	124.45
46	G	620	LUT	C15-C14-C13	-3.52	122.28	127.31
47	y	623	NEX	C39-C29-C30	-3.52	117.99	122.92
29	c	507	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	b	603	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	n	602	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	a	411	BCR	C33-C5-C6	-3.52	120.58	124.53
29	B	606	CLA	CHD-C1D-ND	-3.51	121.22	124.45
47	g	623	NEX	C39-C29-C30	-3.51	118.00	122.92
33	b	626	SQD	O7-S-C6	-3.51	102.77	106.94
29	c	501	CLA	C4A-NA-C1A	3.51	108.28	106.71
31	c	516	BCR	C36-C18-C17	-3.50	118.02	122.92
30	A	408	PHO	CMB-C2B-C3B	3.50	131.23	124.68
31	c	515	BCR	C23-C24-C25	-3.50	117.38	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	410	CLA	C4A-NA-C1A	3.50	108.28	106.71
29	r	609	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	s	617	CLA	CHD-C1D-ND	-3.49	121.24	124.45
45	G	601	CHL	C2C-C3C-C4C	3.49	108.98	106.49
45	g	607	CHL	CHD-C1D-ND	-3.49	121.24	124.45
47	r	622	NEX	C31-C30-C29	3.49	132.29	127.31
29	C	505	CLA	CHD-C1D-ND	-3.49	121.25	124.45
45	S	601	CHL	C3C-C4C-NC	-3.49	106.66	110.57
45	g	607	CHL	C1-C2-C3	-3.49	120.01	126.04
31	a	411	BCR	C23-C24-C25	-3.49	117.41	127.20
45	Y	601	CHL	CHD-C1D-ND	-3.48	121.25	124.45
45	g	601	CHL	C3C-C4C-NC	-3.48	106.66	110.57
46	s	621	LUT	C7-C8-C9	-3.48	120.97	126.23
29	y	610	CLA	CHD-C1D-ND	-3.48	121.26	124.45
37	C	519	DGD	O2G-C1B-C2B	3.48	119.00	111.50
33	C	526	SQD	O7-S-C6	-3.48	102.80	106.94
31	d	404	BCR	C19-C18-C17	3.48	124.28	118.94
37	C	518	DGD	O2G-C1B-C2B	3.48	118.99	111.50
29	y	608	CLA	CHD-C1D-ND	-3.47	121.26	124.45
29	C	505	CLA	C4A-NA-C1A	3.47	108.27	106.71
29	y	608	CLA	C4A-NA-C1A	3.47	108.27	106.71
45	G	606	CHL	C2C-C3C-C4C	3.47	108.97	106.49
31	c	516	BCR	C33-C5-C6	-3.47	120.63	124.53
46	g	620	LUT	C22-C23-C24	-3.47	107.80	111.74
45	y	607	CHL	C4A-NA-C1A	3.46	108.26	106.71
46	s	620	LUT	C7-C8-C9	-3.46	121.00	126.23
29	n	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
46	g	620	LUT	C7-C8-C9	-3.46	121.01	126.23
45	G	606	CHL	CHD-C1D-ND	-3.46	121.28	124.45
29	s	604	CLA	CHD-C1D-ND	-3.45	121.28	124.45
35	D	411	LMG	O7-C10-C11	3.45	118.94	111.50
48	n	622	XAT	O24-C25-C24	3.45	115.97	113.38
46	g	620	LUT	C21-C26-C27	3.45	117.06	112.70
45	N	609	CHL	C3C-C4C-NC	-3.45	106.70	110.57
29	B	604	CLA	CHD-C1D-ND	-3.44	121.29	124.45
29	B	603	CLA	CHD-C1D-ND	-3.44	121.29	124.45
46	n	620	LUT	C15-C14-C13	-3.44	122.40	127.31
46	s	620	LUT	C22-C23-C24	-3.44	107.82	111.74
33	B	621	SQD	O7-S-C6	-3.44	102.85	106.94
29	r	610	CLA	CHD-C1D-ND	-3.44	121.29	124.45
47	y	623	NEX	C31-C30-C29	3.44	132.22	127.31
30	a	408	PHO	CMB-C2B-C3B	3.44	131.11	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	603	CLA	CHD-C1D-ND	-3.43	121.30	124.45
29	C	513	CLA	C4A-NA-C1A	3.43	108.25	106.71
29	b	613	CLA	CHD-C1D-ND	-3.43	121.30	124.45
45	N	601	CHL	CHD-C1D-ND	-3.43	121.30	124.45
48	R	621	XAT	C6-C7-C8	-3.43	118.74	125.99
45	G	605	CHL	C3C-C4C-NC	-3.43	106.73	110.57
29	b	606	CLA	CHD-C1D-ND	-3.43	121.31	124.45
29	b	604	CLA	CHD-C1D-ND	-3.42	121.31	124.45
45	r	606	CHL	CHD-C1D-ND	-3.42	121.31	124.45
46	G	621	LUT	C7-C8-C9	-3.42	121.06	126.23
29	b	612	CLA	C4A-NA-C1A	3.42	108.25	106.71
46	S	620	LUT	C35-C34-C33	-3.42	122.42	127.31
29	g	611	CLA	CHD-C1D-ND	-3.42	121.31	124.45
45	y	606	CHL	CHD-C1D-ND	-3.41	121.32	124.45
33	b	621	SQD	O7-S-C6	-3.41	102.88	106.94
29	b	602	CLA	C4A-NA-C1A	3.41	108.24	106.71
47	R	622	NEX	C39-C29-C30	-3.40	118.16	122.92
29	G	604	CLA	CHD-C1D-ND	-3.40	121.33	124.45
45	R	606	CHL	CHD-C1D-ND	-3.40	121.33	124.45
47	N	623	NEX	C39-C29-C30	-3.39	118.17	122.92
48	G	622	XAT	C38-C25-C26	-3.39	116.58	122.26
31	A	411	BCR	C23-C24-C25	-3.39	117.67	127.20
36	B	620	C7Z	C28-C27-C26	-3.39	117.68	127.20
48	N	622	XAT	O4-C5-C4	-3.39	110.83	113.38
46	S	621	LUT	C15-C14-C13	-3.39	122.47	127.31
46	S	621	LUT	C22-C23-C24	-3.39	107.88	111.74
46	N	621	LUT	C7-C8-C9	-3.39	121.11	126.23
46	n	621	LUT	C7-C8-C9	-3.39	121.12	126.23
47	G	623	NEX	C17-C1-C6	-3.38	107.44	110.47
46	n	621	LUT	C15-C14-C13	-3.38	122.48	127.31
45	N	609	CHL	CHD-C1D-ND	-3.38	121.35	124.45
48	g	622	XAT	C38-C25-C26	-3.38	116.59	122.26
29	d	403	CLA	CHD-C1D-ND	-3.38	121.35	124.45
47	r	622	NEX	C39-C29-C30	-3.38	118.19	122.92
29	A	410	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	D	403	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	c	502	CLA	CHD-C1D-ND	-3.38	121.35	124.45
40	l	101	LHG	O7-C7-C8	3.37	118.77	111.50
31	B	618	BCR	C23-C24-C25	-3.37	117.72	127.20
29	b	614	CLA	CHD-C1D-ND	-3.37	121.35	124.45
45	N	605	CHL	C3C-C4C-NC	-3.37	106.79	110.57
29	r	608	CLA	CHD-C1D-ND	-3.37	121.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	527	LMG	O8-C28-C29	3.37	122.49	111.91
45	R	607	CHL	C3C-C4C-NC	-3.37	106.79	110.57
29	y	614	CLA	C4A-NA-C1A	3.37	108.22	106.71
44	H	101	RRX	C38-C26-C25	-3.37	120.75	124.53
46	N	620	LUT	C15-C14-C13	-3.36	122.52	127.31
29	A	406	CLA	CHD-C1D-ND	-3.36	121.37	124.45
45	n	607	CHL	C3C-C4C-NC	-3.36	106.81	110.57
29	Y	610	CLA	CHD-C1D-ND	-3.36	121.37	124.45
29	b	611	CLA	CHD-C1D-ND	-3.35	121.37	124.45
46	n	620	LUT	C35-C34-C33	-3.35	122.53	127.31
45	N	605	CHL	C2C-C3C-C4C	3.35	108.88	106.49
45	G	605	CHL	CHD-C1D-ND	-3.35	121.38	124.45
45	s	601	CHL	C3C-C4C-NC	-3.35	106.82	110.57
46	y	620	LUT	C35-C34-C33	-3.35	122.53	127.31
29	S	617	CLA	C2D-C1D-ND	-3.35	107.64	110.10
45	n	601	CHL	C2C-C3C-C4C	3.34	108.87	106.49
45	Y	609	CHL	C3C-C4C-NC	-3.34	106.82	110.57
29	G	610	CLA	CHD-C1D-ND	-3.34	121.38	124.45
29	N	604	CLA	C4A-NA-C1A	3.34	108.21	106.71
46	s	620	LUT	C15-C14-C13	-3.34	122.55	127.31
31	c	515	BCR	C12-C13-C14	-3.34	113.82	118.94
37	c	519	DGD	O2G-C1B-C2B	3.33	118.69	111.50
29	G	614	CLA	CHD-C1D-ND	-3.33	121.39	124.45
47	n	623	NEX	C39-C29-C30	-3.33	118.26	122.92
29	N	611	CLA	C4A-NA-C1A	3.33	108.20	106.71
29	g	613	CLA	CHD-C1D-ND	-3.33	121.40	124.45
29	B	611	CLA	CHD-C1D-ND	-3.33	121.40	124.45
45	S	608	CHL	C2C-C3C-C4C	3.32	108.86	106.49
46	G	621	LUT	C31-C30-C29	-3.32	122.57	127.31
47	Y	623	NEX	C39-C29-C30	-3.32	118.27	122.92
29	c	504	CLA	CHD-C1D-ND	-3.32	121.40	124.45
46	s	620	LUT	C35-C15-C14	-3.32	116.68	123.47
29	g	612	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	Y	612	CLA	C4A-NA-C1A	3.31	108.19	106.71
46	r	620	LUT	C15-C14-C13	-3.31	122.59	127.31
48	N	622	XAT	C7-C8-C9	-3.31	120.40	125.53
45	s	607	CHL	C2C-C3C-C4C	3.31	108.84	106.49
31	d	404	BCR	C36-C18-C17	-3.30	118.30	122.92
45	S	608	CHL	C3C-C4C-NC	-3.30	106.87	110.57
46	Y	620	LUT	C35-C34-C33	-3.30	122.60	127.31
31	c	515	BCR	C2-C1-C6	3.30	115.56	110.48
29	Y	612	CLA	CHD-C1D-ND	-3.30	121.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	621	LUT	C18-C5-C6	-3.30	120.83	124.53
45	S	607	CHL	C3C-C4C-NC	-3.30	106.88	110.57
45	N	601	CHL	C3C-C4C-NC	-3.29	106.88	110.57
29	c	510	CLA	CHD-C1D-ND	-3.29	121.43	124.45
41	d	401	BCT	O3-C-O1	-3.29	111.01	119.55
29	C	508	CLA	C4A-NA-C1A	3.29	108.19	106.71
29	N	613	CLA	C4A-NA-C1A	3.29	108.19	106.71
29	a	410	CLA	CHD-C1D-ND	-3.29	121.43	124.45
47	y	623	NEX	C5-C4-C3	3.28	115.63	111.75
31	a	411	BCR	C35-C13-C12	3.28	123.25	118.08
31	A	411	BCR	C35-C13-C12	3.28	123.25	118.08
45	s	607	CHL	C3C-C4C-NC	-3.28	106.89	110.57
29	g	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	S	610	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	n	611	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	D	404	BCR	C33-C5-C6	-3.28	120.84	124.53
31	C	515	BCR	C33-C5-C6	-3.28	120.84	124.53
29	g	602	CLA	CHD-C1D-ND	-3.28	121.44	124.45
45	S	601	CHL	C2C-C3C-C4C	3.28	108.83	106.49
29	r	602	CLA	CHD-C1D-ND	-3.28	121.44	124.45
47	s	623	NEX	C19-C9-C10	-3.28	118.33	122.92
29	s	609	CLA	CHD-C1D-ND	-3.27	121.45	124.45
47	N	623	NEX	C31-C30-C29	3.27	131.98	127.31
31	C	516	BCR	C19-C18-C17	3.26	123.94	118.94
31	B	618	BCR	C35-C13-C12	3.26	123.21	118.08
45	y	605	CHL	C3C-C4C-NC	-3.26	106.92	110.57
29	G	611	CLA	CHD-C1D-ND	-3.25	121.46	124.45
29	A	410	CLA	C4A-NA-C1A	3.25	108.17	106.71
36	b	620	C7Z	C28-C27-C26	-3.25	118.07	127.20
29	B	607	CLA	CHD-C1D-ND	-3.25	121.47	124.45
29	C	504	CLA	CHD-C1D-ND	-3.25	121.47	124.45
45	g	607	CHL	C3C-C4C-NC	-3.25	106.93	110.57
29	B	602	CLA	CHD-C1D-ND	-3.24	121.47	124.45
29	R	612	CLA	CHD-C1D-ND	-3.24	121.48	124.45
29	c	505	CLA	CHD-C1D-ND	-3.24	121.48	124.45
29	r	604	CLA	CHD-C1D-ND	-3.24	121.48	124.45
29	S	612	CLA	C4A-NA-C1A	3.24	108.16	106.71
29	b	613	CLA	C4A-NA-C1A	3.24	108.16	106.71
31	b	619	BCR	C33-C5-C6	-3.24	120.89	124.53
46	s	620	LUT	C18-C5-C6	-3.23	120.90	124.53
45	y	606	CHL	C1B-CHB-C4A	-3.23	123.72	130.12
45	r	607	CHL	C2C-C3C-C4C	3.23	108.79	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	g	601	CHL	C2C-C3C-C4C	3.23	108.79	106.49
29	B	609	CLA	CHD-C1D-ND	-3.23	121.49	124.45
46	n	620	LUT	C22-C23-C24	-3.23	108.07	111.74
29	C	513	CLA	CHD-C1D-ND	-3.22	121.49	124.45
42	d	405	PL9	C7-C3-C2	-3.22	119.07	123.30
42	D	405	PL9	C7-C3-C2	-3.22	119.07	123.30
29	r	612	CLA	C4A-NA-C1A	3.21	108.15	106.71
29	b	610	CLA	CHD-C1D-ND	-3.21	121.50	124.45
29	N	614	CLA	CHD-C1D-ND	-3.21	121.50	124.45
40	D	409	LHG	O7-C7-C8	3.21	118.42	111.50
29	S	604	CLA	CHD-C1D-ND	-3.21	121.50	124.45
46	G	621	LUT	C11-C10-C9	-3.21	122.73	127.31
29	C	507	CLA	CHD-C1D-ND	-3.21	121.51	124.45
45	G	607	CHL	CHD-C1D-ND	-3.21	121.51	124.45
31	d	404	BCR	C34-C9-C10	-3.20	118.44	122.92
45	S	607	CHL	C2C-C3C-C4C	3.20	108.77	106.49
45	G	608	CHL	C3C-C4C-NC	-3.20	106.98	110.57
47	y	623	NEX	C17-C1-C6	-3.20	107.61	110.47
29	B	616	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	C	511	CLA	CHD-C1D-ND	-3.19	121.52	124.45
45	G	606	CHL	C3C-C4C-NC	-3.19	107.00	110.57
31	b	618	BCR	C33-C5-C4	3.18	119.73	113.62
44	h	101	RRX	C4-C5-C6	-3.18	118.11	122.73
45	Y	601	CHL	C4A-NA-C1A	3.18	108.14	106.71
29	N	604	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	R	610	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	b	602	CLA	CHD-C1D-ND	-3.18	121.53	124.45
44	H	101	RRX	C4-C5-C6	-3.18	118.11	122.73
46	G	621	LUT	C22-C23-C24	-3.18	108.12	111.74
45	g	605	CHL	CHD-C1D-ND	-3.18	121.53	124.45
46	S	621	LUT	C7-C8-C9	-3.18	121.43	126.23
45	G	608	CHL	C2C-C3C-C4C	3.18	108.76	106.49
46	S	620	LUT	C7-C8-C9	-3.17	121.44	126.23
29	B	602	CLA	C4A-NA-C1A	3.17	108.13	106.71
29	N	602	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	C	514	BCR	C23-C24-C25	-3.16	118.32	127.20
46	g	621	LUT	C31-C30-C29	-3.16	122.80	127.31
45	n	606	CHL	CHD-C1D-ND	-3.16	121.55	124.45
46	r	620	LUT	C22-C23-C24	-3.16	108.15	111.74
45	y	607	CHL	C3C-C4C-NC	-3.16	107.03	110.57
36	b	620	C7Z	C1-C6-C7	3.15	124.70	115.78
29	B	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	y	606	CHL	CMA-C3A-C4A	3.15	120.25	111.77
29	Y	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45
31	B	619	BCR	C12-C13-C14	-3.15	114.11	118.94
45	y	606	CHL	C4D-CHA-C1A	3.15	125.08	121.25
48	n	622	XAT	C38-C25-C26	-3.15	116.98	122.26
46	Y	620	LUT	C22-C23-C24	-3.15	108.16	111.74
45	N	607	CHL	CHB-C4A-NA	3.15	128.87	124.51
29	S	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	y	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
48	N	622	XAT	C38-C25-C26	-3.15	116.99	122.26
29	y	602	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	S	611	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	N	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
44	h	101	RRX	C1-C6-C5	-3.14	118.20	122.61
45	Y	605	CHL	C3C-C4C-NC	-3.13	107.06	110.57
45	N	601	CHL	C2C-C3C-C4C	3.13	108.72	106.49
45	Y	607	CHL	CHD-C1D-ND	-3.13	121.58	124.45
29	c	513	CLA	CHD-C1D-ND	-3.13	121.58	124.45
31	c	517	BCR	C28-C27-C26	-3.13	108.49	114.08
29	g	610	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	c	506	CLA	CHD-C1D-ND	-3.12	121.59	124.45
45	S	608	CHL	C1-O2A-CGA	3.12	124.63	116.44
45	Y	606	CHL	CMA-C3A-C4A	3.12	120.16	111.77
31	B	619	BCR	C23-C24-C25	-3.12	118.44	127.20
31	D	404	BCR	C34-C9-C10	-3.12	118.55	122.92
46	N	621	LUT	C15-C14-C13	-3.12	122.86	127.31
29	b	616	CLA	CHD-C1D-ND	-3.12	121.59	124.45
29	y	604	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	B	619	BCR	C33-C5-C6	-3.12	121.03	124.53
45	N	609	CHL	CMA-C3A-C4A	3.11	120.14	111.77
45	S	606	CHL	CMA-C3A-C4A	3.11	120.14	111.77
29	G	612	CLA	CHD-C1D-ND	-3.11	121.59	124.45
45	y	607	CHL	CHB-C4A-NA	3.11	128.81	124.51
29	C	502	CLA	CHD-C1D-ND	-3.11	121.60	124.45
44	H	101	RRX	C1-C6-C5	-3.11	118.24	122.61
43	F	101	HEM	CMC-C2C-C3C	3.11	130.49	124.68
31	B	619	BCR	C23-C22-C21	-3.11	114.17	118.94
45	s	601	CHL	C2C-C3C-C4C	3.10	108.70	106.49
31	C	515	BCR	C12-C13-C14	-3.10	114.18	118.94
29	n	604	CLA	CHD-C1D-ND	-3.10	121.60	124.45
44	H	101	RRX	C33-C5-C4	3.09	119.56	113.62
46	r	620	LUT	C35-C34-C33	-3.09	122.90	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	621	LUT	C11-C10-C9	-3.09	122.90	127.31
47	y	623	NEX	C2-C1-C6	3.09	112.21	109.21
29	N	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
48	R	621	XAT	C38-C25-C26	-3.09	117.08	122.26
46	G	620	LUT	C7-C8-C9	-3.08	121.57	126.23
29	n	610	CLA	CHA-C1A-NA	-3.08	119.34	126.40
45	G	607	CHL	C4A-NA-C1A	3.08	108.09	106.71
31	c	516	BCR	C19-C18-C17	3.08	123.67	118.94
41	D	401	BCT	O2-C-O1	-3.08	111.56	119.55
46	S	620	LUT	C35-C15-C14	-3.08	117.17	123.47
45	N	608	CHL	C3C-C4C-NC	-3.08	107.12	110.57
45	n	607	CHL	C2C-C3C-C4C	3.08	108.68	106.49
45	Y	601	CHL	CHB-C4A-NA	3.07	128.76	124.51
46	y	620	LUT	C22-C23-C24	-3.07	108.24	111.74
29	s	605	CLA	CHD-C1D-ND	-3.07	121.63	124.45
46	n	620	LUT	C10-C11-C12	-3.07	113.63	123.22
45	n	605	CHL	C2C-C3C-C4C	3.07	108.68	106.49
49	r	625	LMT	O5B-C1B-C2B	3.07	116.85	110.35
29	n	603	CLA	CHD-C1D-ND	-3.07	121.64	124.45
45	s	606	CHL	C3C-C4C-NC	-3.07	107.13	110.57
49	R	625	LMT	O5B-C1B-C2B	3.07	116.84	110.35
45	n	608	CHL	C3C-C4C-NC	-3.07	107.13	110.57
29	B	612	CLA	CHD-C1D-ND	-3.07	121.64	124.45
45	R	607	CHL	CMA-C3A-C4A	3.06	120.01	111.77
45	y	601	CHL	CHB-C4A-NA	3.06	128.75	124.51
29	n	612	CLA	C4A-NA-C1A	3.06	108.08	106.71
48	R	621	XAT	C26-C27-C28	-3.06	119.53	125.99
45	Y	609	CHL	C2C-C3C-C4C	3.05	108.67	106.49
45	G	605	CHL	CMA-C3A-C4A	3.05	119.97	111.77
46	R	620	LUT	C18-C5-C4	3.05	120.00	114.36
31	B	619	BCR	C37-C22-C23	3.04	122.87	118.08
47	N	623	NEX	C5-C4-C3	3.04	115.35	111.75
45	Y	607	CHL	C3C-C4C-NC	-3.04	107.16	110.57
45	N	606	CHL	CHD-C1D-ND	-3.04	121.66	124.45
29	B	605	CLA	C1-C2-C3	-3.04	120.79	126.04
47	g	623	NEX	C5-C4-C3	-3.03	108.15	111.75
45	N	606	CHL	CMA-C3A-C4A	3.03	119.92	111.77
45	G	609	CHL	CMA-C3A-C4A	3.03	119.92	111.77
45	N	608	CHL	C2C-C3C-C4C	3.03	108.65	106.49
48	Y	622	XAT	O4-C5-C4	-3.03	111.11	113.38
31	C	514	BCR	C33-C5-C6	-3.03	121.13	124.53
45	N	609	CHL	C2C-C3C-C4C	3.02	108.64	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	r	607	CHL	CHD-C4C-C3C	3.02	129.28	124.84
47	s	623	NEX	C39-C29-C30	-3.02	118.69	122.92
45	N	608	CHL	CMA-C3A-C4A	3.02	119.89	111.77
44	h	101	RRX	C23-C24-C25	-3.02	118.72	127.20
29	Y	613	CLA	CHD-C1D-ND	-3.01	121.68	124.45
29	r	610	CLA	C1-C2-C3	-3.01	120.84	126.04
31	b	619	BCR	C23-C24-C25	-3.01	118.75	127.20
45	G	607	CHL	C3C-C4C-NC	-3.01	107.20	110.57
29	g	603	CLA	CHD-C1D-ND	-3.01	121.69	124.45
45	Y	601	CHL	C3C-C4C-NC	-3.00	107.20	110.57
47	s	623	NEX	C17-C1-C6	-3.00	107.78	110.47
44	H	101	RRX	C20-C19-C18	-3.00	117.98	126.42
45	S	607	CHL	CMA-C3A-C4A	3.00	119.84	111.77
46	s	621	LUT	C18-C5-C6	-3.00	121.16	124.53
29	C	501	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	C	515	BCR	C35-C13-C12	3.00	122.80	118.08
45	s	608	CHL	C3C-C4C-NC	-2.99	107.22	110.57
29	A	406	CLA	C1-C2-C3	-2.99	120.88	126.04
45	g	608	CHL	C3C-C4C-NC	-2.98	107.22	110.57
42	d	405	PL9	C7-C8-C9	-2.98	121.83	126.79
29	G	614	CLA	C4A-NA-C1A	2.98	108.05	106.71
45	g	608	CHL	CMA-C3A-C4A	2.98	119.78	111.77
45	n	609	CHL	CMA-C3A-C4A	2.98	119.78	111.77
45	g	606	CHL	CMA-C3A-C4A	2.98	119.78	111.77
48	r	621	XAT	C26-C27-C28	-2.98	119.70	125.99
45	Y	609	CHL	CMA-C3A-C4A	2.98	119.77	111.77
29	c	506	CLA	C1D-ND-C4D	-2.97	104.22	106.33
45	g	607	CHL	CMA-C3A-C4A	2.97	119.77	111.77
45	Y	601	CHL	CMA-C3A-C4A	2.97	119.76	111.77
45	R	606	CHL	CMA-C3A-C4A	2.97	119.75	111.77
29	b	607	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	c	501	CLA	CHD-C1D-ND	-2.97	121.73	124.45
30	a	409	PHO	O2D-CGD-O1D	-2.97	118.04	123.84
46	r	620	LUT	C18-C5-C4	2.96	119.85	114.36
45	n	608	CHL	CMA-C3A-C4A	2.96	119.74	111.77
45	g	601	CHL	CMA-C3A-C4A	2.96	119.74	111.77
44	h	101	RRX	C33-C5-C4	2.96	119.31	113.62
45	s	606	CHL	CMA-C3A-C4A	2.96	119.73	111.77
46	G	621	LUT	C18-C5-C6	-2.96	121.20	124.53
45	n	608	CHL	C2C-C3C-C4C	2.96	108.60	106.49
29	S	602	CLA	C4A-NA-C1A	2.96	108.04	106.71
44	h	101	RRX	C8-C7-C6	-2.96	118.90	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S	608	CHL	C1-C2-C3	-2.96	120.93	126.04
29	c	508	CLA	C4A-NA-C1A	2.96	108.03	106.71
29	r	604	CLA	C4A-NA-C1A	2.96	108.03	106.71
29	R	610	CLA	C1-C2-C3	-2.96	120.93	126.04
31	c	514	BCR	C36-C18-C17	-2.95	118.79	122.92
45	s	606	CHL	C2C-C3C-C4C	2.95	108.59	106.49
40	D	408	LHG	O8-C23-C24	2.95	121.16	111.91
29	S	603	CLA	C2D-C1D-ND	-2.95	107.93	110.10
46	Y	621	LUT	C11-C10-C9	-2.95	123.10	127.31
31	A	411	BCR	C38-C26-C25	-2.94	121.22	124.53
45	g	606	CHL	C1-O2A-CGA	2.94	124.17	116.44
46	y	621	LUT	C38-C25-C24	-2.94	117.26	123.56
45	n	607	CHL	CHB-C4A-NA	2.94	128.58	124.51
45	g	609	CHL	C1-O2A-CGA	2.94	124.15	116.44
45	g	605	CHL	CHB-C4A-NA	2.94	128.57	124.51
29	c	506	CLA	C4A-NA-C1A	2.94	108.03	106.71
44	H	101	RRX	C8-C7-C6	-2.93	118.96	127.20
29	n	603	CLA	C4A-NA-C1A	-2.93	105.39	106.71
47	n	623	NEX	C5-C4-C3	2.93	115.22	111.75
46	S	621	LUT	C35-C15-C14	-2.93	117.47	123.47
31	B	618	BCR	C8-C7-C6	-2.93	118.97	127.20
45	G	607	CHL	CMA-C3A-C4A	2.93	119.64	111.77
48	g	622	XAT	C26-C27-C28	-2.93	119.81	125.99
29	B	617	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	A	411	BCR	C37-C22-C23	2.92	122.68	118.08
45	r	606	CHL	CMA-C3A-C4A	2.92	119.62	111.77
36	b	620	C7Z	C11-C12-C13	-2.92	118.21	126.42
31	c	515	BCR	C35-C13-C12	2.92	122.68	118.08
45	N	607	CHL	C3C-C4C-NC	-2.92	107.30	110.57
45	R	607	CHL	C2C-C3C-C4C	2.92	108.57	106.49
47	R	622	NEX	C31-C30-C29	2.92	131.47	127.31
46	s	621	LUT	C22-C23-C24	-2.91	108.42	111.74
29	R	602	CLA	CHD-C1D-ND	-2.91	121.78	124.45
47	Y	623	NEX	C31-C30-C29	2.91	131.47	127.31
44	H	101	RRX	C7-C8-C9	-2.91	121.84	126.23
29	G	603	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	a	411	BCR	C37-C22-C23	2.91	122.66	118.08
45	G	606	CHL	CMA-C3A-C4A	2.90	119.58	111.77
48	y	622	XAT	C6-C7-C8	-2.90	119.85	125.99
45	y	606	CHL	C1-C2-C3	-2.90	122.06	126.75
45	N	606	CHL	C3C-C4C-NC	-2.90	107.32	110.57
35	C	521	LMG	O8-C28-C29	2.90	121.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N	620	LUT	C38-C25-C24	-2.90	117.36	123.56
46	n	620	LUT	C18-C5-C6	-2.90	121.27	124.53
42	D	405	PL9	C7-C8-C9	-2.90	121.97	126.79
44	h	101	RRX	C38-C26-C27	2.90	119.72	114.36
46	n	620	LUT	C7-C8-C9	-2.90	121.86	126.23
30	a	408	PHO	O2D-CGD-O1D	-2.90	118.18	123.84
29	b	605	CLA	CHA-C1A-NA	-2.89	119.77	126.40
35	C	523	LMG	O8-C28-C29	2.89	120.98	111.91
31	C	514	BCR	C36-C18-C17	-2.89	118.87	122.92
45	G	608	CHL	CMA-C3A-C4A	2.89	119.54	111.77
46	n	620	LUT	C31-C30-C29	-2.89	123.19	127.31
45	N	607	CHL	CHC-C1C-NC	2.89	128.58	124.20
45	n	605	CHL	C1-O2A-CGA	2.89	124.02	116.44
45	g	605	CHL	C3C-C4C-NC	-2.88	107.34	110.57
45	y	609	CHL	C4A-NA-C1A	2.88	108.00	106.71
46	s	621	LUT	C35-C15-C14	-2.88	117.57	123.47
48	r	621	XAT	O24-C25-C24	2.88	115.54	113.38
45	n	606	CHL	C1-C2-C3	-2.88	121.07	126.04
45	S	608	CHL	CMA-C3A-C4A	2.88	119.50	111.77
45	Y	607	CHL	CMA-C3A-C4A	2.88	119.50	111.77
47	n	623	NEX	C31-C30-C29	2.87	131.41	127.31
40	d	408	LHG	O8-C23-C24	2.87	120.93	111.91
45	s	608	CHL	C1B-CHB-C4A	-2.87	124.43	130.12
45	y	609	CHL	CMA-C3A-C4A	2.87	119.49	111.77
29	B	612	CLA	C1-C2-C3	-2.87	121.08	126.04
45	s	601	CHL	CMA-C3A-C4A	2.87	119.48	111.77
31	D	404	BCR	C35-C13-C12	2.87	122.59	118.08
45	s	608	CHL	CMA-C3A-C4A	2.87	119.47	111.77
45	N	601	CHL	C1-C2-C3	-2.86	121.09	126.04
45	n	609	CHL	C2C-C3C-C4C	2.86	108.53	106.49
46	N	621	LUT	C11-C10-C9	-2.86	123.23	127.31
45	N	601	CHL	CMA-C3A-C4A	2.86	119.46	111.77
45	n	601	CHL	C1-C2-C3	-2.86	121.10	126.04
48	Y	622	XAT	C6-C7-C8	-2.86	119.96	125.99
30	A	409	PHO	O1D-CGD-CBD	2.85	129.49	124.74
31	C	516	BCR	C35-C13-C12	2.85	122.57	118.08
31	C	515	BCR	C33-C5-C4	2.85	119.10	113.62
29	b	617	CLA	CHD-C1D-ND	-2.85	121.83	124.45
46	Y	621	LUT	C38-C25-C24	-2.85	117.46	123.56
45	y	601	CHL	C3C-C4C-NC	-2.85	107.37	110.57
31	c	514	BCR	C33-C5-C6	-2.85	121.33	124.53
45	N	609	CHL	CHB-C4A-NA	2.85	128.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G	622	XAT	C19-C9-C10	-2.85	118.93	122.92
29	a	407	CLA	C4A-NA-C1A	2.85	107.99	106.71
29	r	603	CLA	C4A-NA-C1A	2.85	107.99	106.71
48	y	622	XAT	C38-C25-C26	-2.85	117.49	122.26
48	N	622	XAT	O24-C25-C24	2.85	115.52	113.38
29	Y	604	CLA	CHD-C1D-ND	-2.84	121.84	124.45
46	y	621	LUT	C10-C11-C12	-2.84	114.35	123.22
45	Y	606	CHL	C1-O2A-CGA	2.84	123.90	116.44
45	y	601	CHL	CMA-C3A-C4A	2.84	119.40	111.77
46	g	620	LUT	C11-C10-C9	-2.84	123.26	127.31
47	S	623	NEX	C39-C29-C30	-2.84	118.95	122.92
45	g	605	CHL	CMA-C3A-C4A	2.84	119.40	111.77
36	B	620	C7Z	C11-C12-C13	-2.84	118.45	126.42
46	y	620	LUT	C10-C11-C12	-2.84	114.37	123.22
46	N	620	LUT	C10-C11-C12	-2.83	114.38	123.22
45	r	607	CHL	CMA-C3A-C4A	2.83	119.39	111.77
29	A	410	CLA	C1-C2-C3	-2.83	121.15	126.04
45	Y	607	CHL	C2C-C3C-C4C	2.83	108.51	106.49
29	g	604	CLA	C4A-NA-C1A	2.83	107.98	106.71
48	Y	622	XAT	C38-C25-C26	-2.83	117.52	122.26
45	s	607	CHL	CMA-C3A-C4A	2.83	119.38	111.77
46	S	620	LUT	C10-C11-C12	-2.83	114.39	123.22
29	c	506	CLA	C2D-C1D-ND	-2.83	108.02	110.10
45	n	601	CHL	CMA-C3A-C4A	2.83	119.37	111.77
45	g	609	CHL	CMA-C3A-C4A	2.83	119.37	111.77
45	s	608	CHL	C4D-CHA-C1A	2.82	124.68	121.25
36	b	620	C7Z	C24-C25-C26	-2.82	114.56	120.85
45	y	609	CHL	C1-O2A-CGA	2.82	123.84	116.44
29	G	613	CLA	CHD-C1D-ND	-2.82	121.86	124.45
46	y	621	LUT	C11-C10-C9	-2.82	123.29	127.31
43	F	101	HEM	C4D-ND-C1D	2.82	107.98	105.07
45	G	609	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
30	A	408	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
45	g	609	CHL	C3C-C4C-NC	-2.82	107.41	110.57
45	Y	605	CHL	CMA-C3A-C4A	2.82	119.35	111.77
46	g	620	LUT	C18-C5-C6	-2.81	121.37	124.53
29	b	612	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	c	512	CLA	CHD-C1D-ND	-2.81	121.87	124.45
47	s	623	NEX	C38-C25-C26	-2.81	117.55	122.26
29	y	613	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	A	405	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	Y	602	CLA	C1-C2-C3	-2.81	121.19	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R	609	CLA	C2D-C1D-ND	-2.81	108.03	110.10
29	c	510	CLA	C2D-C1D-ND	-2.81	108.03	110.10
46	N	621	LUT	C38-C25-C24	-2.81	117.55	123.56
46	Y	620	LUT	C10-C11-C12	-2.81	114.46	123.22
46	y	620	LUT	C18-C5-C6	-2.81	121.38	124.53
39	j	101	DGA	OG1-CA1-CA2	2.81	120.71	111.91
45	Y	609	CHL	C1-O2A-CGA	2.80	123.79	116.44
30	A	409	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
45	n	609	CHL	CHB-C4A-NA	2.80	128.38	124.51
50	s	625	LPX	O3-P1-O4	2.80	126.08	112.24
45	r	607	CHL	CHB-C4A-NA	2.80	128.38	124.51
46	s	621	LUT	C11-C10-C9	-2.80	123.32	127.31
45	g	608	CHL	C4D-CHA-C1A	2.80	124.65	121.25
46	y	620	LUT	C38-C25-C24	-2.80	117.58	123.56
29	N	613	CLA	CHD-C1D-ND	-2.79	121.89	124.45
45	Y	607	CHL	C4A-NA-C1A	2.79	107.96	106.71
45	G	607	CHL	CHB-C4A-NA	2.79	128.37	124.51
31	C	517	BCR	C27-C26-C25	-2.79	118.68	122.73
40	C	525	LHG	O8-C23-C24	2.79	120.67	111.91
45	s	606	CHL	C4D-CHA-C1A	2.79	124.65	121.25
35	h	102	LMG	O8-C28-C29	2.79	120.65	111.91
29	a	405	CLA	CHD-C1D-ND	-2.79	121.89	124.45
46	s	620	LUT	C39-C29-C28	2.78	122.47	118.08
46	S	621	LUT	C38-C25-C24	-2.78	117.60	123.56
40	L	101	LHG	O8-C23-C24	2.78	120.64	111.91
40	l	101	LHG	O8-C23-C24	2.78	120.64	111.91
43	f	101	HEM	CMC-C2C-C3C	2.78	129.88	124.68
46	S	620	LUT	C18-C5-C6	-2.78	121.41	124.53
29	R	603	CLA	CHD-C1D-ND	-2.78	121.90	124.45
44	H	101	RRX	C38-C26-C27	2.77	119.50	114.36
29	a	406	CLA	C1-C2-C3	-2.77	121.24	126.04
45	G	609	CHL	C3C-C4C-NC	-2.77	107.46	110.57
36	B	620	C7Z	C24-C25-C26	-2.77	114.67	120.85
45	G	601	CHL	CHB-C4A-NA	2.77	128.34	124.51
31	b	618	BCR	C33-C5-C6	-2.77	121.42	124.53
45	g	607	CHL	CHB-C4A-NA	2.77	128.34	124.51
45	G	601	CHL	CMA-C3A-C4A	2.76	119.20	111.77
45	g	609	CHL	C1B-CHB-C4A	-2.76	124.64	130.12
29	y	602	CLA	C1-C2-C3	-2.76	121.26	126.04
35	W	201	LMG	O8-C28-C29	2.76	120.58	111.91
46	Y	621	LUT	C31-C30-C29	-2.76	123.37	127.31
31	c	517	BCR	C36-C18-C17	-2.76	119.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	620	LUT	C10-C11-C12	-2.76	114.60	123.22
45	n	608	CHL	C1-O2A-CGA	2.76	123.68	116.44
30	a	409	PHO	O1D-CGD-CBD	2.75	129.33	124.74
45	n	601	CHL	CHB-C4A-NA	2.75	128.32	124.51
45	y	605	CHL	CMA-C3A-C4A	2.75	119.17	111.77
48	g	622	XAT	C19-C9-C10	-2.75	119.07	122.92
50	S	625	LPX	O3-P1-O4	2.75	125.83	112.24
45	N	608	CHL	C1-O2A-CGA	2.75	123.66	116.44
45	n	606	CHL	CMA-C3A-C4A	2.75	119.16	111.77
37	c	519	DGD	O1G-C1A-C2A	2.75	120.53	111.91
46	G	620	LUT	C11-C10-C9	-2.75	123.39	127.31
37	C	519	DGD	O1G-C1A-C2A	2.74	120.52	111.91
40	c	497	LHG	O8-C23-C24	2.74	120.52	111.91
45	N	606	CHL	C2C-C3C-C4C	2.74	108.44	106.49
29	b	612	CLA	C3C-C4C-NC	-2.74	107.49	110.57
45	Y	609	CHL	C4D-CHA-C1A	2.74	124.59	121.25
45	y	601	CHL	C1-C2-C3	-2.74	121.31	126.04
31	D	404	BCR	C12-C13-C14	-2.74	114.74	118.94
45	G	609	CHL	C1-O2A-CGA	2.74	123.62	116.44
49	R	625	LMT	C1B-C2B-C3B	2.74	115.69	110.00
45	N	608	CHL	C4D-CHA-C1A	2.74	124.58	121.25
45	y	607	CHL	C2C-C3C-C4C	2.73	108.44	106.49
37	C	518	DGD	O1G-C1A-C2A	2.73	120.48	111.91
45	G	607	CHL	C1-C2-C3	-2.73	121.32	126.04
45	y	607	CHL	CHD-C1D-ND	-2.73	121.95	124.45
47	S	623	NEX	C38-C25-C26	-2.73	117.69	122.26
38	b	624	3PH	O31-C31-C32	2.73	120.46	111.91
46	R	620	LUT	C8-C7-C6	-2.72	119.55	127.20
47	S	623	NEX	C20-C13-C14	-2.72	119.11	122.92
31	B	618	BCR	C4-C5-C6	-2.72	118.78	122.73
35	B	622	LMG	O8-C28-C29	2.72	120.45	111.91
48	r	621	XAT	C38-C25-C26	-2.72	117.70	122.26
31	c	514	BCR	C23-C24-C25	-2.72	119.57	127.20
46	y	620	LUT	C7-C8-C9	-2.72	122.13	126.23
45	G	605	CHL	CHB-C4A-NA	2.72	128.27	124.51
51	Y	626	PTY	O4-C30-C31	2.72	120.44	111.91
36	b	620	C7Z	C18-C5-C4	2.72	119.39	114.36
29	a	405	CLA	C1-C2-C3	2.72	130.74	126.04
31	c	516	BCR	C34-C9-C10	-2.72	119.12	122.92
45	G	601	CHL	C1-C2-C3	-2.72	121.35	126.04
45	G	606	CHL	C1-O2A-CGA	2.71	123.57	116.44
47	n	623	NEX	C40-C33-C34	-2.71	119.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	618	BCR	C1-C6-C5	-2.71	118.79	122.61
31	C	516	BCR	C34-C9-C10	-2.71	119.12	122.92
45	y	605	CHL	C2C-C3C-C4C	2.71	108.42	106.49
46	n	621	LUT	C18-C5-C6	-2.71	121.48	124.53
45	N	609	CHL	C1-O2A-CGA	2.71	123.56	116.44
29	g	610	CLA	C1-C2-C3	-2.71	121.36	126.04
46	r	620	LUT	C7-C8-C9	-2.71	122.14	126.23
45	N	601	CHL	CHB-C4A-NA	2.71	128.26	124.51
45	G	607	CHL	C1-O2A-CGA	2.71	123.55	116.44
31	b	619	BCR	C12-C13-C14	-2.71	114.79	118.94
31	D	404	BCR	C23-C24-C25	-2.71	119.60	127.20
48	y	622	XAT	C19-C9-C10	-2.71	119.13	122.92
29	c	508	CLA	C3C-C4C-NC	-2.71	107.54	110.57
46	Y	620	LUT	C38-C25-C24	-2.71	117.77	123.56
37	b	623	DGD	O6E-C5E-C4E	2.70	114.60	109.69
45	R	607	CHL	CHD-C4C-C3C	2.70	128.81	124.84
45	R	606	CHL	C4A-NA-C1A	2.70	107.92	106.71
45	n	609	CHL	C1-O2A-CGA	2.70	123.53	116.44
29	s	605	CLA	C3C-C4C-NC	-2.70	107.54	110.57
29	c	512	CLA	C4A-NA-C1A	2.70	107.92	106.71
35	c	521	LMG	O8-C28-C29	2.69	120.36	111.91
46	Y	620	LUT	C18-C5-C6	-2.69	121.50	124.53
45	S	601	CHL	CMA-C3A-C4A	2.69	119.00	111.77
38	S	626	3PH	O31-C31-C32	2.69	120.34	111.91
46	N	621	LUT	C18-C5-C6	-2.68	121.51	124.53
31	D	404	BCR	C36-C18-C17	-2.68	119.16	122.92
29	s	614	CLA	C4A-NA-C1A	2.68	107.91	106.71
31	a	411	BCR	C38-C26-C25	-2.68	121.51	124.53
31	b	619	BCR	C37-C22-C23	2.68	122.31	118.08
45	y	601	CHL	C1-O2A-CGA	2.68	123.48	116.44
29	A	405	CLA	C4A-NA-C1A	2.68	107.91	106.71
29	R	603	CLA	C4A-NA-C1A	2.68	107.91	106.71
31	B	619	BCR	C35-C13-C12	2.68	122.30	118.08
40	c	525	LHG	O8-C23-C24	2.68	120.31	111.91
29	C	501	CLA	C4A-NA-C1A	2.68	107.91	106.71
46	G	620	LUT	C38-C25-C24	-2.68	117.83	123.56
45	n	607	CHL	CMA-C3A-C4A	2.68	118.97	111.77
30	A	408	PHO	O1D-CGD-CBD	2.68	129.20	124.74
31	b	618	BCR	C4-C5-C6	-2.68	118.84	122.73
38	B	624	3PH	O31-C31-C32	2.68	120.31	111.91
48	G	622	XAT	C26-C27-C28	-2.68	120.33	125.99
46	G	620	LUT	C18-C5-C6	-2.68	121.52	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S	601	CHL	CHB-C4A-NA	2.67	128.21	124.51
46	Y	621	LUT	C10-C11-C12	-2.67	114.87	123.22
29	s	604	CLA	C1-C2-C3	-2.67	121.42	126.04
49	R	625	LMT	C3B-C4B-C5B	-2.67	105.47	110.24
46	N	620	LUT	C18-C5-C6	-2.67	121.53	124.53
45	n	608	CHL	C4D-CHA-C1A	2.67	124.50	121.25
29	a	410	CLA	C1-C2-C3	-2.67	121.43	126.04
44	h	101	RRX	C35-C13-C14	-2.67	119.19	122.92
45	g	607	CHL	C4A-NA-C1A	2.66	107.90	106.71
29	a	407	CLA	CHA-C1A-NA	-2.66	120.30	126.40
35	b	622	LMG	O8-C28-C29	2.66	120.27	111.91
37	c	520	DGD	O1G-C1A-C2A	2.66	120.26	111.91
40	d	409	LHG	O8-C23-C24	2.66	120.26	111.91
29	s	617	CLA	CHA-C1A-NA	-2.66	120.30	126.40
40	g	624	LHG	O8-C23-C24	2.66	120.25	111.91
44	H	101	RRX	C11-C12-C13	-2.66	118.95	126.42
29	N	603	CLA	CHD-C1D-ND	-2.66	122.01	124.45
36	B	620	C7Z	C35-C15-C14	-2.66	118.03	123.47
31	c	515	BCR	C3-C4-C5	-2.66	109.34	114.08
51	y	626	PTY	O4-C30-C31	2.66	120.24	111.91
45	n	605	CHL	CMA-C3A-C4A	2.65	118.91	111.77
29	r	610	CLA	C3C-C4C-NC	-2.65	107.60	110.57
29	b	612	CLA	C1-C2-C3	-2.65	121.46	126.04
29	Y	604	CLA	C1-C2-C3	-2.65	121.46	126.04
46	Y	621	LUT	C18-C5-C6	-2.65	121.55	124.53
29	r	612	CLA	CHA-C1A-NA	-2.65	120.33	126.40
31	c	516	BCR	C35-C13-C12	2.65	122.25	118.08
45	N	605	CHL	CHB-C4A-NA	2.65	128.18	124.51
29	S	614	CLA	C4A-NA-C1A	2.65	107.90	106.71
45	r	606	CHL	C4A-NA-C1A	2.64	107.89	106.71
29	G	610	CLA	CHA-C1A-NA	-2.64	120.35	126.40
38	t	101	3PH	O31-C31-C32	2.64	120.20	111.91
45	g	608	CHL	C2C-C3C-C4C	2.64	108.37	106.49
29	c	503	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	c	515	BCR	C33-C5-C4	2.64	118.68	113.62
45	s	607	CHL	CHB-C4A-NA	2.64	128.16	124.51
49	r	625	LMT	C1B-C2B-C3B	2.63	115.48	110.00
31	d	404	BCR	C33-C5-C4	2.63	118.67	113.62
35	A	413	LMG	C8-O7-C10	-2.63	111.31	117.79
40	G	624	LHG	O8-C23-C24	2.63	120.17	111.91
45	Y	609	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
45	S	606	CHL	C4D-CHA-C1A	2.63	124.45	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	c	524	DGA	OG1-CA1-CA2	2.63	120.15	111.91
45	n	606	CHL	CHB-C4A-NA	2.63	128.14	124.51
45	g	607	CHL	C1B-CHB-C4A	-2.63	124.92	130.12
37	C	520	DGD	O1G-C1A-C2A	2.62	120.14	111.91
31	C	517	BCR	C23-C24-C25	-2.62	119.83	127.20
47	S	623	NEX	C19-C9-C10	-2.62	119.25	122.92
46	n	620	LUT	C38-C25-C24	-2.62	117.95	123.56
46	G	620	LUT	C10-C11-C12	-2.62	115.04	123.22
45	Y	607	CHL	CHB-C4A-NA	2.62	128.13	124.51
45	y	607	CHL	C1-C2-C3	-2.62	121.51	126.04
46	s	620	LUT	C38-C25-C24	-2.62	117.96	123.56
46	y	621	LUT	C18-C5-C6	-2.62	121.59	124.53
29	C	503	CLA	CHD-C1D-ND	-2.62	122.05	124.45
30	a	408	PHO	O1D-CGD-CBD	2.62	129.09	124.74
29	R	603	CLA	CHA-C1A-NA	-2.61	120.41	126.40
45	N	607	CHL	C4A-NA-C1A	2.61	107.88	106.71
35	a	413	LMG	O8-C28-C29	2.61	120.10	111.91
45	G	607	CHL	C2C-C3C-C4C	2.61	108.35	106.49
46	R	620	LUT	C22-C23-C24	-2.61	108.77	111.74
45	s	608	CHL	C2C-C3C-C4C	2.61	108.35	106.49
29	r	603	CLA	CHA-C1A-NA	-2.61	120.43	126.40
45	n	608	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
45	Y	601	CHL	C1-O2A-CGA	2.60	123.28	116.44
46	s	620	LUT	C30-C31-C32	-2.60	115.09	123.22
45	Y	605	CHL	C2C-C3C-C4C	2.60	108.34	106.49
45	g	601	CHL	CHB-C4A-NA	2.60	128.11	124.51
48	G	622	XAT	C18-C5-C6	-2.60	117.91	122.26
45	r	606	CHL	CHB-C4A-NA	2.60	128.10	124.51
46	s	620	LUT	C10-C11-C12	-2.60	115.11	123.22
29	R	603	CLA	C2A-C1A-CHA	2.60	128.40	123.86
44	H	101	RRX	C35-C13-C14	-2.59	119.29	122.92
29	b	608	CLA	CHD-C1D-ND	-2.59	122.07	124.45
47	n	623	NEX	C19-C9-C10	-2.59	119.29	122.92
35	c	523	LMG	O8-C28-C29	2.59	120.04	111.91
45	Y	607	CHL	C1-C2-C3	-2.59	121.57	126.04
31	c	517	BCR	C31-C1-C6	-2.59	106.10	110.30
31	c	517	BCR	C23-C24-C25	-2.59	119.94	127.20
46	R	620	LUT	C1-C6-C5	-2.59	118.97	122.61
36	b	620	C7Z	C38-C25-C24	2.58	119.14	114.36
31	C	517	BCR	C2-C1-C6	2.58	114.46	110.48
29	Y	611	CLA	C4A-NA-C1A	2.58	107.87	106.71
29	C	508	CLA	C3C-C4C-NC	-2.58	107.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	N	605	CHL	C1-C2-C3	-2.58	121.58	126.04
31	C	514	BCR	C35-C13-C12	2.58	122.14	118.08
38	T	101	3PH	O31-C31-C32	2.58	120.00	111.91
40	D	409	LHG	C5-O7-C7	-2.58	111.45	117.79
45	G	609	CHL	C4D-CHA-C1A	2.58	124.38	121.25
45	r	607	CHL	C1-O2A-CGA	2.57	123.20	116.44
37	B	623	DGD	C1E-O6E-C5E	2.57	118.74	113.69
29	G	604	CLA	C4A-NA-C1A	2.57	107.86	106.71
29	s	603	CLA	CHD-C1D-ND	-2.57	122.09	124.45
45	N	606	CHL	C1-C2-C3	-2.57	121.60	126.04
45	R	606	CHL	CHB-C4A-NA	2.57	128.06	124.51
45	y	607	CHL	CMA-C3A-C4A	2.57	118.68	111.77
29	b	605	CLA	CAA-C2A-C1A	2.57	120.39	111.97
31	C	514	BCR	C12-C13-C14	-2.57	115.00	118.94
29	c	511	CLA	CHD-C1D-ND	-2.56	122.10	124.45
45	N	609	CHL	C4A-NA-C1A	2.56	107.86	106.71
29	C	512	CLA	CHD-C1D-ND	-2.56	122.10	124.45
45	G	609	CHL	CHC-C1C-NC	2.56	128.09	124.20
48	g	622	XAT	C6-C7-C8	-2.56	120.58	125.99
35	A	413	LMG	O8-C28-C29	2.56	119.95	111.91
45	G	606	CHL	CHB-C4A-NA	2.56	128.05	124.51
47	Y	623	NEX	C1-C2-C3	2.55	119.41	113.64
29	c	501	CLA	C1-C2-C3	-2.55	121.63	126.04
46	s	620	LUT	C11-C10-C9	-2.55	123.67	127.31
45	N	608	CHL	C1B-CHB-C4A	-2.55	125.07	130.12
47	s	623	NEX	C20-C13-C14	-2.55	119.35	122.92
39	J	101	DGA	OG1-CA1-CA2	2.55	119.90	111.91
29	B	608	CLA	CHD-C1D-ND	-2.55	122.11	124.45
45	n	607	CHL	C4A-NA-C1A	2.54	107.85	106.71
38	s	626	3PH	O31-C31-C32	2.54	119.89	111.91
45	g	601	CHL	C1-C2-C3	-2.54	121.64	126.04
31	C	517	BCR	C36-C18-C17	-2.54	119.37	122.92
40	L	101	LHG	O7-C7-O9	-2.54	117.57	123.70
36	B	620	C7Z	C38-C25-C24	2.54	119.06	114.36
47	Y	623	NEX	C20-C13-C14	-2.54	119.37	122.92
47	G	623	NEX	C16-C1-C6	-2.54	108.20	110.47
29	c	509	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
29	g	604	CLA	CHA-C1A-NA	-2.53	120.59	126.40
35	w	201	LMG	O8-C28-C29	2.53	119.86	111.91
45	n	605	CHL	C1B-CHB-C4A	-2.53	125.10	130.12
46	Y	620	LUT	C7-C8-C9	-2.53	122.41	126.23
46	g	620	LUT	C38-C25-C24	-2.53	118.14	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d	410	LHG	O8-C23-C24	2.53	119.86	111.91
45	g	607	CHL	C2C-C3C-C4C	2.53	108.29	106.49
29	b	605	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
47	N	623	NEX	C19-C9-C10	-2.53	119.38	122.92
48	n	622	XAT	C26-C27-C28	-2.53	120.64	125.99
47	g	623	NEX	C20-C13-C14	-2.53	119.38	122.92
45	R	607	CHL	C1-O2A-CGA	2.53	123.08	116.44
49	r	625	LMT	C3B-C4B-C5B	-2.53	105.73	110.24
40	s	624	LHG	O8-C23-C24	2.53	119.84	111.91
29	C	509	CLA	CHA-C1A-NA	-2.53	120.61	126.40
45	g	608	CHL	C1B-CHB-C4A	-2.53	125.11	130.12
40	N	624	LHG	O8-C23-C24	2.53	119.83	111.91
31	c	516	BCR	C2-C1-C6	2.52	114.37	110.48
35	C	521	LMG	C8-O7-C10	-2.52	111.58	117.79
46	s	621	LUT	C38-C25-C24	-2.52	118.16	123.56
29	C	501	CLA	C1-C2-C3	-2.52	121.68	126.04
45	y	609	CHL	C4D-CHA-C1A	2.52	124.32	121.25
45	N	607	CHL	CMA-C3A-C4A	2.52	118.55	111.77
44	h	101	RRX	C34-C9-C10	-2.52	119.39	122.92
45	N	605	CHL	CMA-C3A-C4A	2.52	118.54	111.77
29	y	604	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
29	n	603	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	b	619	BCR	C33-C5-C4	2.51	118.45	113.62
29	R	612	CLA	C1D-ND-C4D	-2.51	104.55	106.33
45	R	607	CHL	CHB-C4A-NA	2.51	127.98	124.51
45	Y	606	CHL	C1B-CHB-C4A	-2.51	125.14	130.12
43	f	101	HEM	C1B-NB-C4B	2.51	107.67	105.07
46	Y	620	LUT	C31-C30-C29	-2.51	123.73	127.31
47	S	623	NEX	C31-C30-C29	2.51	130.89	127.31
45	g	608	CHL	C4A-NA-C1A	2.51	107.83	106.71
46	y	621	LUT	C35-C15-C14	-2.51	118.34	123.47
31	c	517	BCR	C33-C5-C6	-2.51	121.71	124.53
29	C	506	CLA	CHD-C1D-ND	-2.51	122.15	124.45
47	N	623	NEX	C40-C33-C34	-2.50	119.41	122.92
39	C	524	DGA	OG1-CA1-CA2	2.50	119.76	111.91
40	c	497	LHG	C5-O7-C7	-2.50	111.63	117.79
29	s	603	CLA	CHA-C1A-NA	-2.50	120.67	126.40
29	c	509	CLA	CHA-C1A-NA	-2.50	120.67	126.40
31	c	516	BCR	C33-C5-C4	2.50	118.42	113.62
35	D	411	LMG	O8-C28-C29	2.50	119.75	111.91
29	R	603	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
40	n	624	LHG	C5-O7-C7	-2.49	111.65	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	610	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
31	c	517	BCR	C35-C13-C12	2.49	122.00	118.08
31	c	516	BCR	C3-C4-C5	-2.49	109.63	114.08
40	S	624	LHG	O8-C23-C24	2.49	119.72	111.91
31	c	517	BCR	C34-C9-C10	-2.49	119.44	122.92
42	d	405	PL9	C22-C23-C24	-2.49	121.67	127.66
45	g	609	CHL	C4D-CHA-C1A	2.49	124.28	121.25
31	c	516	BCR	C31-C1-C6	-2.48	106.27	110.30
29	n	604	CLA	C4A-NA-C1A	2.48	107.82	106.71
45	Y	607	CHL	C1-O2A-CGA	2.48	122.96	116.44
39	B	625	DGA	OG1-CA1-CA2	2.48	119.69	111.91
45	g	609	CHL	CHC-C1C-NC	2.48	127.97	124.20
29	y	604	CLA	C1-C2-C3	-2.48	121.76	126.04
47	y	623	NEX	C20-C13-C14	-2.48	119.45	122.92
46	r	620	LUT	C38-C25-C24	-2.48	118.26	123.56
40	n	624	LHG	O8-C23-C24	2.48	119.67	111.91
45	G	605	CHL	C4A-NA-C1A	2.47	107.82	106.71
45	y	609	CHL	CHB-C4A-NA	2.47	127.93	124.51
46	g	621	LUT	C38-C25-C24	-2.47	118.27	123.56
40	y	624	LHG	O8-C23-C24	2.47	119.66	111.91
45	N	607	CHL	C4D-CHA-C1A	2.47	124.25	121.25
44	H	101	RRX	C23-C22-C21	2.47	122.73	118.94
47	G	623	NEX	C40-C33-C34	-2.47	119.47	122.92
48	R	621	XAT	C7-C8-C9	-2.47	121.70	125.53
31	C	515	BCR	C34-C9-C10	-2.47	119.47	122.92
45	S	606	CHL	C1B-CHB-C4A	-2.46	125.23	130.12
45	S	607	CHL	CHB-C4A-NA	2.46	127.92	124.51
45	n	605	CHL	CHB-C4A-NA	2.46	127.92	124.51
31	b	619	BCR	C35-C13-C12	2.46	121.96	118.08
37	B	623	DGD	O1G-C1A-C2A	2.46	119.64	111.91
49	r	625	LMT	C3'-C4'-C5'	-2.46	105.28	110.93
29	r	603	CLA	C2A-C1A-CHA	2.46	128.16	123.86
46	Y	621	LUT	C36-C21-C26	-2.46	105.82	109.55
40	Y	624	LHG	O8-C23-C24	2.46	119.63	111.91
37	b	623	DGD	O1G-C1A-C2A	2.46	119.63	111.91
45	g	606	CHL	C4D-CHA-C1A	2.46	124.24	121.25
29	s	605	CLA	C2A-C1A-CHA	2.46	128.16	123.86
29	b	617	CLA	C4A-NA-C1A	2.46	107.81	106.71
45	S	608	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
29	C	509	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
47	g	623	NEX	C38-C25-C26	-2.45	118.15	122.26
45	s	601	CHL	CHB-C4A-NA	2.45	127.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	518	DGD	O1G-C1A-C2A	2.45	119.59	111.91
45	N	607	CHL	CHD-C4C-C3C	2.45	128.44	124.84
29	r	612	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
47	G	623	NEX	O24-C25-C38	-2.45	112.12	115.06
48	n	622	XAT	C19-C9-C10	-2.45	119.50	122.92
36	b	620	C7Z	C35-C15-C14	-2.45	118.46	123.47
45	N	601	CHL	C1-O2A-CGA	2.45	122.86	116.44
29	N	612	CLA	C4A-NA-C1A	2.44	107.80	106.71
47	n	623	NEX	C20-C13-C14	-2.44	119.50	122.92
45	Y	601	CHL	C1-C2-C3	-2.44	121.83	126.04
45	g	607	CHL	C4D-CHA-C1A	2.44	124.22	121.25
45	g	609	CHL	CHB-C4A-NA	2.44	127.88	124.51
40	y	624	LHG	C5-O7-C7	-2.44	111.79	117.79
31	c	516	BCR	C37-C22-C23	2.44	121.92	118.08
47	N	623	NEX	C38-C25-C26	-2.43	118.18	122.26
29	Y	610	CLA	CHA-C1A-NA	-2.43	120.83	126.40
47	n	623	NEX	C38-C25-C26	-2.43	118.19	122.26
49	R	625	LMT	C3'-C4'-C5'	-2.43	105.36	110.93
29	C	511	CLA	C4A-NA-C1A	2.43	107.80	106.71
48	N	622	XAT	C18-C5-C6	-2.43	118.19	122.26
31	c	515	BCR	C34-C9-C10	-2.43	119.52	122.92
29	G	604	CLA	CHA-C1A-NA	-2.43	120.84	126.40
44	H	101	RRX	C30-C29-C28	-2.43	108.16	113.64
29	N	603	CLA	CHA-C1A-NA	-2.43	120.84	126.40
45	G	608	CHL	CHB-C4A-NA	2.42	127.86	124.51
36	B	620	C7Z	C18-C5-C4	2.42	118.84	114.36
45	Y	605	CHL	C1B-CHB-C4A	-2.42	125.32	130.12
29	A	407	CLA	C4A-NA-C1A	2.42	107.80	106.71
45	N	601	CHL	C4A-NA-C1A	2.42	107.80	106.71
31	d	404	BCR	C37-C22-C21	-2.42	119.53	122.92
31	C	517	BCR	C33-C5-C6	-2.42	121.81	124.53
45	g	606	CHL	C3C-C4C-NC	-2.42	107.86	110.57
44	H	101	RRX	C23-C24-C25	-2.42	120.41	127.20
48	G	622	XAT	C6-C7-C8	-2.42	120.88	125.99
48	G	622	XAT	C39-C29-C30	-2.42	119.54	122.92
29	c	510	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	R	612	CLA	C1-C2-C3	-2.42	122.84	126.75
31	C	515	BCR	C38-C26-C25	-2.42	121.82	124.53
45	S	608	CHL	CHB-C4A-NA	2.41	127.85	124.51
47	g	623	NEX	C19-C9-C10	-2.41	119.54	122.92
45	y	601	CHL	C4A-NA-C1A	2.41	107.79	106.71
29	A	406	CLA	O2A-CGA-O1A	-2.41	117.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	610	CLA	CHA-C1A-NA	-2.41	120.88	126.40
45	g	606	CHL	C1B-CHB-C4A	-2.41	125.34	130.12
31	B	618	BCR	C36-C18-C17	-2.41	119.55	122.92
29	B	612	CLA	C3C-C4C-NC	-2.41	107.87	110.57
45	n	601	CHL	C1-O2A-CGA	2.41	122.77	116.44
34	A	414	SPH	C3-C4-C5	-2.41	119.42	124.79
31	d	404	BCR	C33-C5-C6	-2.41	121.82	124.53
47	S	623	NEX	C1-C2-C3	2.41	119.08	113.64
31	B	618	BCR	C37-C22-C23	2.41	121.87	118.08
47	G	623	NEX	C20-C13-C14	-2.41	119.55	122.92
42	D	405	PL9	C27-C28-C29	-2.40	121.87	127.66
34	y	625	SPH	C3-C4-C5	-2.40	119.43	124.79
47	G	623	NEX	C38-C25-C26	-2.40	118.23	122.26
35	d	411	LMG	O8-C28-C29	2.40	119.45	111.91
43	f	101	HEM	C4B-CHC-C1C	2.40	125.73	122.56
29	n	613	CLA	CHD-C1D-ND	-2.40	122.25	124.45
35	H	102	LMG	O8-C28-C29	2.40	119.44	111.91
29	g	610	CLA	CHA-C1A-NA	-2.40	120.91	126.40
46	y	621	LUT	C31-C30-C29	-2.40	123.89	127.31
37	b	623	DGD	C1E-O6E-C5E	2.40	118.39	113.69
42	d	405	PL9	C40-C39-C41	2.40	119.30	115.27
35	C	527	LMG	O8-C28-O10	-2.39	117.55	123.59
29	G	602	CLA	C1-C2-C3	-2.39	121.90	126.04
29	C	512	CLA	C4A-NA-C1A	2.39	107.78	106.71
29	B	607	CLA	C2D-C1D-ND	-2.39	108.34	110.10
29	A	405	CLA	C1-C2-C3	2.39	130.18	126.04
45	y	606	CHL	C3C-C4C-NC	-2.39	107.89	110.57
47	y	623	NEX	C38-C25-C26	-2.39	118.26	122.26
31	b	619	BCR	C23-C22-C21	-2.39	115.28	118.94
46	N	621	LUT	C10-C11-C12	-2.39	115.77	123.22
39	b	625	DGA	OG1-CA1-CA2	2.39	119.39	111.91
33	B	621	SQD	O3-C3-C2	-2.39	104.83	110.35
43	F	101	HEM	C4B-CHC-C1C	2.38	125.70	122.56
29	Y	604	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
45	y	607	CHL	C1-O2A-CGA	2.38	122.69	116.44
34	a	414	SPH	C3-C4-C5	-2.38	119.48	124.79
31	d	404	BCR	C28-C27-C26	-2.38	109.83	114.08
47	R	622	NEX	C20-C13-C12	2.38	119.86	114.60
45	n	606	CHL	C3C-C4C-NC	-2.38	107.90	110.57
29	G	603	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
29	c	503	CLA	C2D-C1D-ND	-2.38	108.35	110.10
30	a	408	PHO	CMC-C2C-C3C	2.37	129.42	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	511	CLA	CHA-C1A-NA	-2.37	120.96	126.40
46	n	621	LUT	C10-C11-C12	-2.37	115.81	123.22
35	a	413	LMG	C8-O7-C10	-2.37	111.95	117.79
40	y	624	LHG	C6-C5-C4	-2.37	106.18	111.79
29	b	603	CLA	C4A-NA-C1A	2.37	107.77	106.71
29	g	610	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
46	N	620	LUT	C7-C8-C9	-2.37	122.65	126.23
45	y	605	CHL	CHB-C4A-NA	2.37	127.79	124.51
46	y	620	LUT	C31-C30-C29	-2.37	123.93	127.31
45	g	606	CHL	CHB-C4A-NA	2.37	127.78	124.51
46	g	621	LUT	C10-C11-C12	-2.37	115.83	123.22
45	g	607	CHL	C3A-C2A-C1A	2.37	104.88	101.34
48	N	622	XAT	C39-C29-C30	-2.37	119.61	122.92
45	n	608	CHL	CHB-C4A-NA	2.37	127.78	124.51
31	c	515	BCR	C33-C5-C6	-2.37	121.87	124.53
29	N	602	CLA	C4A-NA-C1A	2.36	107.77	106.71
29	G	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
31	c	517	BCR	C2-C1-C6	2.36	114.12	110.48
29	n	614	CLA	CHA-C1A-NA	-2.36	120.99	126.40
31	A	411	BCR	C23-C22-C21	-2.36	115.32	118.94
47	G	623	NEX	C19-C9-C10	-2.36	119.62	122.92
42	d	405	PL9	C27-C28-C29	-2.36	121.98	127.66
43	F	101	HEM	C4C-CHD-C1D	2.36	125.67	122.56
45	n	609	CHL	C4A-NA-C1A	2.36	107.77	106.71
31	b	619	BCR	C36-C18-C17	-2.36	119.62	122.92
42	D	405	PL9	C22-C23-C24	-2.36	121.99	127.66
31	C	517	BCR	C33-C5-C4	2.35	118.14	113.62
45	y	606	CHL	C1-O2A-CGA	2.35	122.62	116.44
29	y	610	CLA	CHA-C1A-NA	-2.35	121.01	126.40
31	C	517	BCR	C34-C9-C10	-2.35	119.63	122.92
47	Y	623	NEX	C16-C1-C6	-2.35	108.37	110.47
44	H	101	RRX	C2-C1-C6	2.35	114.10	110.48
45	g	605	CHL	C4A-NA-C1A	2.35	107.76	106.71
45	y	605	CHL	C1B-CHB-C4A	-2.35	125.47	130.12
48	r	621	XAT	C7-C8-C9	-2.35	121.89	125.53
34	Y	625	SPH	C3-C4-C5	-2.35	119.55	124.79
46	S	620	LUT	C30-C31-C32	-2.35	115.89	123.22
29	a	405	CLA	C3C-C4C-NC	-2.35	107.94	110.57
45	Y	606	CHL	C3C-C4C-NC	-2.35	107.94	110.57
31	c	517	BCR	C3-C4-C5	-2.35	109.89	114.08
47	N	623	NEX	C17-C1-C6	-2.35	108.37	110.47
29	B	604	CLA	C2D-C1D-ND	-2.35	108.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	602	CLA	C1-C2-C3	-2.35	121.99	126.04
46	n	621	LUT	C22-C23-C24	-2.34	109.07	111.74
29	r	612	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
45	n	608	CHL	C4A-NA-C1A	2.34	107.76	106.71
29	g	602	CLA	C1-C2-C3	-2.34	121.99	126.04
45	N	607	CHL	C1B-CHB-C4A	-2.34	125.48	130.12
46	G	621	LUT	C10-C11-C12	-2.34	115.91	123.22
31	C	517	BCR	C3-C4-C5	-2.34	109.89	114.08
31	a	411	BCR	C23-C22-C21	-2.34	115.35	118.94
30	a	409	PHO	C1-C2-C3	-2.34	122.00	126.04
31	c	515	BCR	C38-C26-C25	-2.34	121.90	124.53
48	G	622	XAT	C40-C33-C34	-2.34	119.65	122.92
30	A	408	PHO	CMC-C2C-C3C	2.34	129.35	124.94
29	R	610	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
46	r	620	LUT	C37-C21-C26	2.34	113.08	109.55
31	C	517	BCR	C31-C1-C6	-2.34	106.51	110.30
45	n	609	CHL	CMB-C2B-C1B	-2.33	124.88	128.46
45	Y	606	CHL	C4D-CHA-C1A	2.33	124.09	121.25
45	N	608	CHL	C4A-NA-C1A	2.33	107.75	106.71
29	n	604	CLA	CHA-C1A-NA	-2.33	121.06	126.40
31	C	517	BCR	C35-C13-C12	2.33	121.75	118.08
45	Y	609	CHL	C1-C2-C3	-2.33	122.01	126.04
31	C	514	BCR	C38-C26-C25	-2.33	121.91	124.53
45	G	609	CHL	CHB-C4A-NA	2.33	127.73	124.51
47	Y	623	NEX	C38-C25-C26	-2.33	118.36	122.26
33	C	526	SQD	O3-C3-C2	-2.33	104.97	110.35
29	c	505	CLA	C1-C2-C3	-2.32	122.02	126.04
45	g	608	CHL	CHB-C4A-NA	2.32	127.72	124.51
45	N	607	CHL	C1-O2A-CGA	2.32	122.54	116.44
40	d	409	LHG	C5-O7-C7	-2.32	112.07	117.79
33	b	626	SQD	O3-C3-C2	-2.32	104.98	110.35
29	C	510	CLA	C2D-C1D-ND	-2.32	108.39	110.10
46	N	621	LUT	C35-C15-C14	-2.32	118.72	123.47
45	g	601	CHL	C1B-CHB-C4A	-2.32	125.53	130.12
48	Y	622	XAT	C19-C9-C10	-2.32	119.68	122.92
48	n	622	XAT	C18-C5-C6	-2.32	118.38	122.26
45	s	606	CHL	CMB-C2B-C1B	-2.31	124.91	128.46
47	r	622	NEX	C20-C13-C12	2.31	119.71	114.60
29	N	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	s	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	G	603	CLA	CHA-C1A-NA	-2.31	121.11	126.40
44	H	101	RRX	C34-C9-C10	-2.31	119.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	620	LUT	C11-C10-C9	-2.31	124.02	127.31
29	Y	602	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
31	b	618	BCR	C1-C6-C5	-2.31	119.36	122.61
45	n	607	CHL	CMB-C2B-C1B	-2.31	124.92	128.46
29	S	605	CLA	CHA-C1A-NA	-2.30	121.12	126.40
45	n	609	CHL	C1B-CHB-C4A	-2.30	125.55	130.12
45	s	606	CHL	CHB-C4A-NA	2.30	127.70	124.51
36	b	620	C7Z	C7-C6-C5	-2.30	115.89	121.46
45	n	609	CHL	C1-C2-C3	-2.30	122.06	126.04
29	Y	610	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
46	r	620	LUT	C37-C21-C22	-2.30	105.08	109.44
45	n	609	CHL	C4D-CHA-C1A	2.30	124.05	121.25
45	n	607	CHL	C1-O2A-CGA	2.30	122.48	116.44
47	y	623	NEX	C4-C3-C2	2.30	115.21	110.77
45	s	601	CHL	C1B-CHB-C4A	-2.30	125.56	130.12
31	C	517	BCR	C29-C30-C25	2.30	114.02	110.48
33	b	621	SQD	O3-C3-C2	-2.30	105.04	110.35
31	c	517	BCR	C27-C26-C25	-2.30	119.39	122.73
45	S	607	CHL	C4A-NA-C1A	2.30	107.74	106.71
29	S	602	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
29	y	608	CLA	CHA-C1A-NA	-2.30	121.14	126.40
45	s	601	CHL	C4D-CHA-C1A	2.30	124.04	121.25
29	C	502	CLA	C1-C2-C3	-2.29	122.08	126.04
31	d	404	BCR	C23-C24-C25	-2.29	120.76	127.20
47	g	623	NEX	O24-C25-C38	-2.29	112.31	115.06
45	Y	605	CHL	CHB-C4A-NA	2.29	127.68	124.51
29	B	602	CLA	CHA-C1A-NA	-2.29	121.15	126.40
48	R	621	XAT	O24-C25-C24	2.29	115.10	113.38
45	s	606	CHL	C1B-CHB-C4A	-2.29	125.58	130.12
29	B	612	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
44	H	101	RRX	C15-C16-C17	-2.29	118.79	123.47
29	n	603	CLA	CHA-C1A-NA	-2.29	121.16	126.40
45	Y	605	CHL	C4D-CHA-C1A	2.29	124.03	121.25
42	d	405	PL9	O1-C4-C3	-2.29	118.20	120.72
36	B	620	C7Z	C7-C6-C5	-2.29	115.92	121.46
45	S	608	CHL	CHD-C4C-C3C	2.29	128.20	124.84
48	R	621	XAT	C40-C33-C34	-2.29	119.72	122.92
48	g	622	XAT	C40-C33-C34	-2.29	119.72	122.92
47	s	623	NEX	C31-C30-C29	2.29	130.57	127.31
29	Y	604	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	C	516	BCR	C12-C13-C14	-2.28	115.44	118.94
29	y	604	CLA	CHA-C1A-NA	-2.28	121.17	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	G	609	CHL	CHD-C4C-C3C	2.28	128.20	124.84
47	r	622	NEX	C38-C25-C26	-2.28	118.43	122.26
31	c	517	BCR	C39-C30-C25	-2.28	106.60	110.30
45	N	608	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
40	N	624	LHG	C5-O7-C7	-2.28	112.18	117.79
31	c	516	BCR	C29-C28-C27	2.28	116.47	111.38
31	c	515	BCR	C4-C5-C6	-2.28	119.42	122.73
31	c	514	BCR	C19-C18-C17	2.28	122.44	118.94
47	G	623	NEX	C4-C3-C2	2.28	115.17	110.77
31	D	404	BCR	C37-C22-C23	2.28	121.67	118.08
45	y	607	CHL	CMB-C2B-C1B	-2.28	124.97	128.46
31	b	618	BCR	C35-C13-C12	2.28	121.66	118.08
44	h	101	RRX	C36-C18-C17	-2.28	119.74	122.92
40	D	410	LHG	O8-C23-C24	2.28	119.05	111.91
31	c	515	BCR	C31-C1-C6	-2.27	106.61	110.30
29	S	603	CLA	CHA-C1A-NA	-2.27	121.19	126.40
48	g	622	XAT	O24-C25-C24	2.27	115.09	113.38
29	G	610	CLA	C1-C2-C3	-2.27	122.11	126.04
31	B	619	BCR	C36-C18-C17	-2.27	119.74	122.92
29	c	507	CLA	CHA-C1A-NA	-2.27	121.20	126.40
44	h	101	RRX	C2-C1-C6	2.27	113.98	110.48
29	B	608	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	s	613	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
45	Y	609	CHL	CHD-C4C-C3C	2.27	128.18	124.84
45	g	607	CHL	CMB-C2B-C1B	-2.27	124.98	128.46
45	G	609	CHL	C1-C2-C3	-2.27	122.12	126.04
45	y	609	CHL	C1B-CHB-C4A	-2.27	125.63	130.12
29	r	609	CLA	CHA-C1A-NA	-2.27	121.21	126.40
45	g	606	CHL	CAA-C2A-C3A	-2.27	106.57	112.78
45	r	606	CHL	C1B-CHB-C4A	-2.26	125.63	130.12
45	R	606	CHL	C3C-C4C-NC	-2.26	108.03	110.57
51	Y	627	PTY	C6-O7-C8	-2.26	113.68	117.90
29	g	603	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
45	r	606	CHL	C3C-C4C-NC	-2.26	108.03	110.57
33	c	526	SQD	O3-C3-C2	-2.26	105.12	110.35
45	Y	607	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
45	n	608	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
46	G	621	LUT	C38-C25-C24	-2.26	118.73	123.56
46	Y	620	LUT	C15-C35-C34	-2.26	118.85	123.47
45	S	607	CHL	C4D-CHA-C1A	2.26	124.00	121.25
45	n	609	CHL	CHD-C4C-C3C	2.26	128.16	124.84
47	N	623	NEX	C20-C13-C14	-2.26	119.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	404	BCR	C38-C26-C27	2.26	117.95	113.62
45	G	607	CHL	CMB-C2B-C1B	-2.26	125.00	128.46
30	A	409	PHO	C1-C2-C3	-2.26	122.14	126.04
33	B	626	SQD	O3-C3-C2	-2.25	105.14	110.35
29	s	617	CLA	C2A-C1A-CHA	2.25	127.80	123.86
46	r	620	LUT	C18-C5-C6	-2.25	122.00	124.53
46	s	621	LUT	C10-C11-C12	-2.25	116.19	123.22
29	Y	608	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	s	610	CLA	C1-C2-C3	-2.25	122.15	126.04
37	c	519	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
48	N	622	XAT	C19-C9-C10	-2.25	119.77	122.92
31	c	517	BCR	C33-C5-C4	2.25	117.93	113.62
45	Y	609	CHL	CHB-C4A-NA	2.25	127.62	124.51
33	m	101	SQD	O3-C3-C2	-2.25	105.16	110.35
45	y	606	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
40	s	624	LHG	C5-O7-C7	-2.25	112.26	117.79
42	d	405	PL9	C20-C19-C21	2.25	119.05	115.27
48	r	621	XAT	C40-C33-C34	-2.24	119.78	122.92
29	c	507	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
29	B	610	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
45	r	606	CHL	C4D-CHA-C1A	2.24	123.98	121.25
33	a	412	SQD	O3-C3-C2	-2.24	105.17	110.35
29	B	602	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
29	r	608	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
47	S	623	NEX	C16-C1-C6	-2.24	108.47	110.47
46	n	620	LUT	C19-C9-C8	2.24	121.60	118.08
43	f	101	HEM	C4D-ND-C1D	2.24	107.38	105.07
48	y	622	XAT	C18-C5-C6	-2.23	118.52	122.26
45	S	606	CHL	C3C-C4C-NC	-2.23	108.07	110.57
31	d	404	BCR	C38-C26-C25	-2.23	122.02	124.53
47	G	623	NEX	C5-C4-C3	2.23	114.39	111.75
45	s	608	CHL	CHB-C4A-NA	2.23	127.60	124.51
31	C	516	BCR	C37-C22-C23	2.23	121.59	118.08
45	Y	601	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
46	Y	621	LUT	C35-C15-C14	-2.23	118.91	123.47
46	S	621	LUT	C10-C11-C12	-2.23	116.26	123.22
46	y	620	LUT	C39-C29-C28	2.23	121.59	118.08
29	a	406	CLA	C4A-NA-C1A	2.23	107.71	106.71
31	c	515	BCR	C34-C9-C8	2.23	121.59	118.08
45	G	605	CHL	C1-O2A-CGA	2.23	123.20	116.73
29	a	406	CLA	C1-O2A-CGA	2.23	122.29	116.44
33	A	412	SQD	O3-C3-C2	-2.23	105.20	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	605	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
42	D	405	PL9	O1-C4-C3	-2.23	118.27	120.72
31	B	618	BCR	C23-C22-C21	-2.22	115.53	118.94
29	s	617	CLA	C1-C2-C3	-2.22	123.15	126.75
46	R	620	LUT	C38-C25-C24	-2.22	118.80	123.56
31	d	404	BCR	C4-C5-C6	-2.22	119.50	122.73
46	n	621	LUT	C31-C30-C29	-2.22	124.14	127.31
31	c	514	BCR	C35-C13-C12	2.22	121.58	118.08
43	F	101	HEM	C1B-NB-C4B	2.22	107.37	105.07
29	N	614	CLA	CHA-C1A-NA	-2.22	121.31	126.40
29	y	610	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
44	h	101	RRX	C11-C12-C13	-2.22	120.19	126.42
29	b	610	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
45	G	606	CHL	C4D-CHA-C1A	2.22	123.95	121.25
47	r	622	NEX	C40-C33-C34	-2.21	119.82	122.92
29	B	604	CLA	C1-C2-C3	-2.21	122.22	126.04
31	B	619	BCR	C33-C5-C4	2.21	117.86	113.62
29	B	604	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
45	g	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
46	N	620	LUT	C19-C9-C8	2.21	121.55	118.08
29	R	602	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
44	h	101	RRX	C23-C22-C21	2.21	122.33	118.94
46	y	620	LUT	C11-C10-C9	-2.21	124.16	127.31
29	n	611	CLA	CHA-C1A-NA	-2.20	121.35	126.40
45	S	606	CHL	CHB-C4A-NA	2.20	127.56	124.51
33	M	101	SQD	O3-C3-C2	-2.20	105.25	110.35
29	S	613	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
29	a	406	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
45	G	608	CHL	C1B-CHB-C4A	-2.20	125.76	130.12
31	b	618	BCR	C34-C9-C10	-2.20	119.84	122.92
31	B	618	BCR	C1-C6-C7	2.20	122.00	115.78
29	Y	611	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
29	r	602	CLA	CHA-C1A-NA	-2.20	121.36	126.40
30	A	408	PHO	C1-C2-C3	-2.20	122.24	126.04
35	c	521	LMG	C8-O7-C10	-2.20	112.38	117.79
31	c	517	BCR	C29-C30-C25	2.20	113.86	110.48
46	g	621	LUT	C35-C15-C14	-2.20	118.97	123.47
29	r	603	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
48	Y	622	XAT	C39-C29-C30	-2.20	119.85	122.92
29	b	607	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
29	D	403	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
29	c	501	CLA	C3C-C4C-NC	-2.19	108.11	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	602	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
29	Y	611	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	S	603	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
45	G	607	CHL	C4D-CHA-C1A	2.19	123.91	121.25
31	C	514	BCR	C33-C5-C4	2.19	117.82	113.62
45	N	608	CHL	CHB-C4A-NA	2.19	127.53	124.51
44	h	101	RRX	C7-C8-C9	-2.19	122.93	126.23
48	Y	622	XAT	C20-C13-C14	-2.19	119.86	122.92
48	Y	622	XAT	C26-C27-C28	-2.19	121.37	125.99
45	R	606	CHL	C4D-CHA-C1A	2.18	123.91	121.25
29	b	615	CLA	C1-C2-C3	-2.18	122.27	126.04
42	D	405	PL9	C40-C39-C41	2.18	118.94	115.27
46	n	621	LUT	C35-C15-C14	-2.18	119.01	123.47
46	g	620	LUT	C39-C29-C28	2.18	121.51	118.08
33	m	101	SQD	O8-S-C6	-2.18	102.27	105.74
36	b	620	C7Z	C2-C3-C4	2.18	113.28	110.30
29	n	602	CLA	CHA-C1A-NA	-2.18	121.41	126.40
48	N	622	XAT	C26-C27-C28	-2.18	121.39	125.99
29	B	605	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	b	602	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	s	611	CLA	CHA-C1A-NA	-2.17	121.42	126.40
40	n	624	LHG	C6-C5-C4	-2.17	106.65	111.79
45	G	606	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
44	h	101	RRX	C30-C29-C28	-2.17	108.74	113.64
29	A	405	CLA	C3C-C4C-NC	-2.17	108.14	110.57
29	s	614	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
48	g	622	XAT	C39-C29-C30	-2.17	119.89	122.92
45	G	601	CHL	C1B-CHB-C4A	-2.17	125.82	130.12
45	N	609	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
45	g	609	CHL	C1-C2-C3	-2.17	122.29	126.04
48	y	622	XAT	C26-C27-C28	-2.17	121.41	125.99
36	B	620	C7Z	C30-C31-C32	-2.17	116.45	123.22
29	B	605	CLA	C4-C3-C5	2.17	118.92	115.27
31	b	618	BCR	C36-C18-C17	-2.17	119.89	122.92
29	s	610	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
29	a	410	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	s	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
35	C	527	LMG	O1-C1-C2	2.16	111.68	108.30
29	s	611	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
47	s	623	NEX	C40-C33-C34	-2.16	119.89	122.92
45	N	606	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
45	g	607	CHL	CHD-C4C-C3C	2.16	128.02	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	610	CLA	C1-C2-C3	-2.16	122.31	126.04
44	h	101	RRX	C15-C16-C17	-2.16	119.05	123.47
45	Y	609	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
29	a	406	CLA	CHA-C1A-NA	-2.16	121.45	126.40
40	N	624	LHG	C6-C5-C4	-2.16	106.68	111.79
45	N	609	CHL	C1-C2-C3	-2.16	122.31	126.04
29	r	608	CLA	CHA-C1A-NA	-2.16	121.45	126.40
45	G	608	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
29	y	614	CLA	C1-C2-C3	-2.16	122.31	126.04
29	b	606	CLA	C2D-C1D-ND	-2.16	108.51	110.10
47	y	623	NEX	O24-C25-C38	-2.16	112.47	115.06
29	g	614	CLA	CHA-C1A-NA	-2.15	121.46	126.40
45	n	606	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
31	A	411	BCR	C33-C5-C4	2.15	117.75	113.62
29	G	602	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
47	n	623	NEX	O24-C25-C38	-2.15	112.48	115.06
48	Y	622	XAT	C18-C5-C6	-2.15	118.66	122.26
29	B	607	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
42	d	405	PL9	C37-C38-C39	-2.15	122.49	127.66
29	Y	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
46	n	621	LUT	C38-C25-C24	-2.15	118.96	123.56
46	N	620	LUT	C30-C31-C32	-2.15	116.52	123.22
29	N	604	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
45	y	607	CHL	C4D-CHA-C1A	2.15	123.86	121.25
29	a	405	CLA	C2D-C1D-ND	-2.15	108.52	110.10
31	b	618	BCR	C37-C22-C23	2.15	121.46	118.08
29	y	611	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
45	Y	601	CHL	CHD-C4C-C3C	2.14	127.99	124.84
47	S	623	NEX	C26-C27-C28	-2.14	121.46	125.99
45	G	605	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
45	n	601	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
45	n	607	CHL	C4D-CHA-C1A	2.14	123.86	121.25
31	C	516	BCR	C29-C28-C27	2.14	116.16	111.38
45	N	606	CHL	CHB-C4A-NA	2.14	127.47	124.51
40	S	624	LHG	C5-O7-C7	-2.14	112.52	117.79
29	N	604	CLA	CHA-C1A-NA	-2.14	121.50	126.40
45	n	605	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
48	R	621	XAT	C27-C28-C29	2.14	128.85	125.53
45	y	606	CHL	C3A-C2A-C1A	2.14	104.54	101.34
48	g	622	XAT	C18-C5-C6	-2.14	118.68	122.26
29	c	512	CLA	C1-C2-C3	-2.14	122.35	126.04
40	G	624	LHG	C5-O7-C7	-2.13	112.53	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Y	606	CHL	CMB-C2B-C1B	-2.13	125.18	128.46
46	g	620	LUT	C15-C35-C34	-2.13	119.10	123.47
45	N	605	CHL	CMB-C2B-C1B	-2.13	125.18	128.46
29	n	602	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
45	g	606	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
46	y	620	LUT	C15-C35-C34	-2.13	119.11	123.47
29	b	605	CLA	CBA-CAA-C2A	2.13	120.16	113.86
29	r	609	CLA	C2D-C1D-ND	-2.13	108.53	110.10
29	G	612	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	n	612	CLA	CHA-C1A-NA	-2.13	121.52	126.40
45	y	609	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
29	b	604	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
45	n	605	CHL	C4D-CHA-C1A	2.13	123.84	121.25
29	S	612	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
48	Y	622	XAT	O24-C25-C38	-2.13	112.51	115.06
29	n	610	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
36	B	620	C7Z	C19-C9-C10	-2.13	119.95	122.92
46	G	620	LUT	C2-C3-C4	-2.12	107.40	110.30
45	s	601	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
45	S	608	CHL	CHD-C1D-C2D	2.12	129.94	125.48
45	G	601	CHL	CHD-C4C-C3C	2.12	127.96	124.84
45	r	607	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
45	s	607	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
45	n	607	CHL	C1B-CHB-C4A	-2.12	125.91	130.12
47	Y	623	NEX	O24-C25-C38	-2.12	112.51	115.06
45	S	608	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
29	R	602	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	C	507	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	B	606	CLA	C1-C2-C3	-2.12	122.38	126.04
40	D	409	LHG	O8-C23-C24	2.12	118.56	111.91
29	S	611	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	R	609	CLA	CHD-C1D-C2D	2.12	129.92	125.48
31	a	411	BCR	C33-C5-C4	2.12	117.69	113.62
35	A	413	LMG	O7-C10-O9	-2.12	118.58	123.70
46	R	620	LUT	C30-C31-C32	-2.12	116.61	123.22
45	y	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	Y	622	XAT	C40-C33-C34	-2.12	119.96	122.92
45	n	605	CHL	CHD-C4C-C3C	2.12	127.95	124.84
47	S	623	NEX	C4-C3-C2	2.12	114.86	110.77
31	C	515	BCR	C37-C22-C23	2.11	121.41	118.08
29	s	610	CLA	CHA-C1A-NA	-2.11	121.56	126.40
45	g	608	CHL	CMB-C2B-C1B	-2.11	125.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N	623	NEX	O24-C25-C38	-2.11	112.53	115.06
46	Y	620	LUT	C19-C9-C8	2.11	121.41	118.08
45	N	601	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
45	S	601	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
45	S	607	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
36	B	620	C7Z	C2-C3-C4	2.11	113.19	110.30
31	B	618	BCR	C34-C9-C8	2.11	121.40	118.08
45	G	609	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
29	r	603	CLA	CHD-C1D-ND	-2.11	122.52	124.45
46	S	621	LUT	C39-C29-C28	2.11	121.40	118.08
45	R	607	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
45	N	606	CHL	C4D-CHA-C1A	2.11	123.82	121.25
45	g	601	CHL	C4D-CHA-C1A	2.11	123.82	121.25
29	S	614	CLA	C1-C2-C3	-2.11	123.34	126.75
45	s	608	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
29	B	615	CLA	C1-C2-C3	-2.11	122.40	126.04
45	g	609	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
45	r	606	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
45	n	601	CHL	CHD-C4C-C3C	2.11	127.94	124.84
29	b	616	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
29	G	611	CLA	CHA-C1A-NA	-2.11	121.58	126.40
45	G	607	CHL	C1B-CHB-C4A	-2.10	125.95	130.12
33	B	621	SQD	O6-C1-C2	-2.10	105.02	108.30
47	R	622	NEX	C40-C33-C34	-2.10	119.98	122.92
46	G	620	LUT	C31-C30-C29	-2.10	124.31	127.31
45	y	605	CHL	C4D-CHA-C1A	2.10	123.81	121.25
45	R	607	CHL	C1B-CHB-C4A	-2.10	125.95	130.12
29	b	610	CLA	C1-C2-C3	-2.10	122.41	126.04
29	s	603	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
45	s	607	CHL	C4D-CHA-C1A	2.10	123.81	121.25
45	s	608	CHL	C4A-NA-C1A	2.10	107.65	106.71
42	D	405	PL9	C37-C38-C39	-2.10	122.61	127.66
29	d	403	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
45	Y	607	CHL	C4D-CHA-C1A	2.10	123.80	121.25
46	S	620	LUT	C40-C33-C32	2.10	121.38	118.08
45	G	601	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
45	s	608	CHL	CHD-C4C-C3C	2.10	127.92	124.84
29	c	508	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	S	603	CLA	C1-C2-C3	-2.09	122.42	126.04
47	G	623	NEX	C28-C29-C30	2.09	122.16	118.94
45	g	601	CHL	CHD-C4C-C3C	2.09	127.92	124.84
45	g	607	CHL	CHC-C1C-NC	2.09	127.38	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	s	620	LUT	C28-C29-C30	-2.09	115.73	118.94
48	n	622	XAT	C39-C29-C30	-2.09	119.99	122.92
29	d	403	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
45	g	608	CHL	CHC-C1C-NC	2.09	127.38	124.20
29	r	603	CLA	C2D-C1D-ND	-2.09	108.56	110.10
30	a	408	PHO	C1-C2-C3	-2.09	122.43	126.04
45	S	607	CHL	C1B-CHB-C4A	-2.09	125.97	130.12
45	N	607	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
45	Y	605	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	C	516	BCR	C33-C5-C4	2.09	117.63	113.62
45	Y	606	CHL	CHB-C4A-NA	2.09	127.40	124.51
45	g	601	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
46	S	621	LUT	C16-C1-C6	-2.09	106.91	110.30
29	d	403	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	g	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	N	611	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	g	614	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
45	g	605	CHL	CMB-C2B-C1B	-2.09	125.26	128.46
29	b	617	CLA	CHA-C1A-NA	-2.09	121.62	126.40
46	y	621	LUT	C36-C21-C26	-2.09	106.39	109.55
45	S	606	CHL	CMB-C2B-C1B	-2.09	125.26	128.46
44	h	101	RRX	C8-C9-C10	2.08	122.14	118.94
45	R	606	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
29	s	612	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
45	y	601	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
45	n	605	CHL	C1-C2-C3	-2.08	122.44	126.04
29	n	610	CLA	C2A-C1A-CHA	2.08	127.50	123.86
45	n	606	CHL	C3A-C2A-C1A	2.08	104.46	101.34
45	y	609	CHL	C1-C2-C3	-2.08	122.44	126.04
29	r	602	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
36	B	620	C7Z	C15-C35-C34	-2.08	119.22	123.47
45	y	606	CHL	CHC-C1C-NC	2.08	127.36	124.20
47	y	623	NEX	C40-C33-C34	-2.08	120.01	122.92
29	A	407	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	c	506	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
51	y	627	PTY	C6-O7-C8	-2.08	114.02	117.90
29	y	611	CLA	CHA-C1A-NA	-2.08	121.64	126.40
45	S	608	CHL	CHA-C4D-ND	2.08	136.84	132.50
45	Y	601	CHL	CHC-C1C-NC	2.08	127.35	124.20
31	C	514	BCR	C38-C26-C27	2.08	117.60	113.62
45	N	609	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
45	g	605	CHL	CHD-C4C-C3C	2.08	127.89	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	G	609	CHL	C4A-NA-C1A	2.08	107.64	106.71
29	a	407	CLA	C3C-C4C-NC	-2.07	108.24	110.57
46	G	620	LUT	C39-C29-C28	2.07	121.34	118.08
45	g	605	CHL	C1-O2A-CGA	2.07	122.75	116.73
29	S	617	CLA	C3C-C4C-NC	-2.07	108.25	110.57
46	r	620	LUT	C3-C4-C5	-2.07	107.72	111.85
29	N	602	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
37	b	623	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
45	R	606	CHL	C1B-CHB-C4A	-2.07	126.01	130.12
29	N	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
37	B	623	DGD	O6E-C5E-C4E	2.07	113.45	109.69
36	B	620	C7Z	C36-C21-C26	-2.07	106.94	110.30
29	S	617	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	c	501	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	Y	614	CLA	C1-C2-C3	-2.07	122.47	126.04
29	B	616	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	N	614	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
30	a	409	PHO	O2A-CGA-O1A	-2.07	118.38	123.59
45	y	601	CHL	CHC-C1C-NC	2.07	127.34	124.20
31	c	517	BCR	C12-C13-C14	-2.06	115.77	118.94
29	Y	611	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
37	C	519	DGD	O1G-C1A-O1A	-2.06	118.38	123.59
29	b	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
33	b	621	SQD	O8-S-C6	-2.06	102.45	105.74
29	C	512	CLA	C1-C2-C3	-2.06	122.48	126.04
29	A	407	CLA	CHA-C1A-NA	-2.06	121.68	126.40
45	n	607	CHL	CHD-C4C-C3C	2.06	127.87	124.84
29	c	503	CLA	C3C-C4C-NC	-2.06	108.26	110.57
29	r	603	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	c	516	BCR	C12-C13-C14	-2.06	115.78	118.94
35	W	201	LMG	O7-C10-O9	-2.06	118.73	123.70
46	Y	620	LUT	C39-C29-C28	2.06	121.32	118.08
42	D	405	PL9	O2-C1-C2	-2.06	117.07	121.78
31	c	516	BCR	C38-C26-C25	-2.06	122.22	124.53
42	D	405	PL9	O2-C1-C6	2.06	124.15	120.59
31	a	411	BCR	C36-C18-C17	-2.06	120.04	122.92
46	Y	620	LUT	C20-C13-C12	2.06	121.32	118.08
49	R	625	LMT	C1'-O5'-C5'	-2.06	109.65	113.69
29	C	503	CLA	C3C-C4C-NC	-2.06	108.27	110.57
29	y	603	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
36	b	620	C7Z	C36-C21-C26	-2.05	106.97	110.30
47	R	622	NEX	C38-C25-C26	-2.05	118.82	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	622	LMG	O7-C8-C9	2.05	115.84	108.40
45	s	601	CHL	CHC-C1C-NC	2.05	127.32	124.20
45	y	606	CHL	CHD-C4C-C3C	2.05	127.86	124.84
29	c	510	CLA	CHA-C1A-NA	-2.05	121.70	126.40
37	B	623	DGD	O2G-C1B-O1B	-2.05	118.74	123.70
29	y	614	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
48	y	622	XAT	C39-C29-C30	-2.05	120.05	122.92
40	g	624	LHG	C6-C5-C4	-2.05	106.94	111.79
36	B	620	C7Z	C21-C26-C25	-2.05	119.73	122.61
45	g	606	CHL	CHA-C1A-NA	-2.05	121.70	126.40
29	Y	603	CLA	C1-C2-C3	-2.05	122.50	126.04
29	a	410	CLA	C3C-C4C-NC	-2.05	108.27	110.57
29	C	506	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
46	s	620	LUT	C40-C33-C32	2.05	121.30	118.08
29	C	501	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	c	510	CLA	C1-C2-C3	-2.05	122.50	126.04
31	b	619	BCR	C34-C9-C10	-2.05	120.06	122.92
47	g	623	NEX	C28-C29-C30	2.05	122.08	118.94
48	y	622	XAT	C40-C33-C34	-2.04	120.06	122.92
47	y	623	NEX	C28-C29-C30	2.04	122.08	118.94
29	S	602	CLA	C1-C2-C3	-2.04	122.51	126.04
45	N	609	CHL	CHD-C4C-C3C	2.04	127.84	124.84
45	N	607	CHL	CMA-C3A-C2A	2.04	122.07	113.83
42	D	405	PL9	C20-C19-C21	2.04	118.71	115.27
29	N	602	CLA	C1-C2-C3	-2.04	122.51	126.04
45	S	601	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
36	b	620	C7Z	C30-C31-C32	-2.04	116.85	123.22
36	b	620	C7Z	C19-C9-C10	-2.04	120.07	122.92
42	d	405	PL9	O2-C1-C2	-2.04	117.11	121.78
29	B	605	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
29	C	508	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	b	606	CLA	C1-C2-C3	-2.04	122.52	126.04
29	A	410	CLA	C3C-C4C-NC	-2.04	108.29	110.57
29	C	510	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	C	506	CLA	C1D-ND-C4D	-2.04	104.89	106.33
29	S	603	CLA	CMD-C2D-C1D	-2.03	121.13	124.71
29	R	612	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	c	503	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
46	s	621	LUT	C39-C29-C28	2.03	121.28	118.08
29	c	513	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	n	611	CLA	C4A-NA-C1A	2.03	107.62	106.71
36	b	620	C7Z	C21-C26-C25	-2.03	119.75	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	514	BCR	C33-C5-C4	2.03	117.52	113.62
29	s	603	CLA	C2D-C1D-ND	-2.03	108.61	110.10
29	c	502	CLA	C1-C2-C3	-2.03	122.53	126.04
48	R	621	XAT	C24-C23-C22	-2.03	106.85	110.77
46	N	621	LUT	C31-C30-C29	-2.03	124.41	127.31
29	N	603	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
33	M	101	SQD	O8-S-C6	-2.03	102.51	105.74
31	c	514	BCR	C34-C9-C10	-2.03	120.08	122.92
45	g	601	CHL	C1-O2A-CGA	2.03	121.76	116.44
46	R	620	LUT	C1-C6-C7	2.03	121.51	115.78
45	n	605	CHL	C3A-C2A-C1A	2.03	104.37	101.34
29	S	609	CLA	CHA-C1A-NA	-2.03	121.76	126.40
29	S	612	CLA	CHA-C1A-NA	-2.03	121.76	126.40
29	n	612	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
45	G	606	CHL	CHA-C1A-NA	-2.02	121.76	126.40
29	g	613	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
48	N	622	XAT	C40-C33-C34	-2.02	120.09	122.92
42	d	405	PL9	C31-C32-C33	-2.02	105.23	111.88
46	g	620	LUT	C35-C15-C14	-2.02	119.33	123.47
45	N	606	CHL	C1-O2A-CGA	2.02	121.75	116.44
29	R	608	CLA	C2D-C1D-ND	-2.02	108.62	110.10
46	N	620	LUT	C39-C29-C28	2.02	121.26	118.08
45	y	601	CHL	CHD-C4C-C3C	2.02	127.81	124.84
29	c	502	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	G	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
36	b	620	C7Z	C31-C32-C33	-2.02	120.75	126.42
45	n	607	CHL	C3A-C2A-C1A	2.02	104.36	101.34
29	s	605	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
29	B	609	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	S	617	CLA	C1-C2-C3	-2.01	123.49	126.75
29	C	508	CLA	CHA-C1A-NA	-2.01	121.78	126.40
36	b	620	C7Z	C15-C35-C34	-2.01	119.35	123.47
45	g	605	CHL	C2C-C3C-C4C	2.01	107.92	106.49
29	C	503	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	y	612	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
45	G	608	CHL	C4D-CHA-C1A	2.01	123.70	121.25
46	N	620	LUT	C20-C13-C12	2.01	121.25	118.08
41	D	401	BCT	O3-C-O1	-2.01	114.32	119.55
29	b	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
46	n	620	LUT	C15-C35-C34	-2.01	119.35	123.47
45	n	608	CHL	CHD-C4C-C3C	2.01	127.80	124.84
35	C	521	LMG	O7-C10-O9	-2.01	118.84	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	612	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
29	B	617	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
45	y	607	CHL	CHD-C4C-C3C	2.01	127.80	124.84
45	Y	606	CHL	C3A-C2A-C1A	2.01	104.35	101.34
29	D	403	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	b	615	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	y	614	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	D	404	BCR	C19-C18-C17	2.01	122.02	118.94
45	Y	605	CHL	CHD-C4C-C3C	2.01	127.79	124.84
31	c	515	BCR	C37-C22-C23	2.01	121.24	118.08
29	c	504	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	s	605	CLA	CHA-C1A-NA	-2.01	121.81	126.40
29	B	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	A	411	BCR	C31-C1-C6	-2.00	107.05	110.30
45	y	609	CHL	CHD-C4C-C3C	2.00	127.79	124.84
29	s	617	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	Y	611	CLA	C3C-C4C-NC	-2.00	108.32	110.57
45	G	601	CHL	CHC-C1C-NC	2.00	127.24	124.20
29	n	610	CLA	C3C-C4C-NC	-2.00	108.33	110.57
31	B	619	BCR	C34-C9-C10	-2.00	120.12	122.92
45	N	601	CHL	CHD-C4C-C3C	2.00	127.78	124.84

All (311) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	B	602	CLA	ND
29	B	603	CLA	ND
29	B	604	CLA	ND
29	B	605	CLA	ND
29	B	606	CLA	ND
29	B	607	CLA	ND
29	B	608	CLA	ND
29	B	609	CLA	ND
29	B	610	CLA	ND
29	B	611	CLA	ND
29	B	613	CLA	ND
29	B	614	CLA	ND
29	B	615	CLA	ND
29	B	616	CLA	ND

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Mol	Chain	Res	Type	Atom
29	B	617	CLA	ND
29	C	502	CLA	ND
29	C	504	CLA	ND
29	C	505	CLA	ND
29	C	507	CLA	ND
29	C	508	CLA	ND
29	C	509	CLA	ND
29	C	510	CLA	ND
29	C	511	CLA	ND
29	C	512	CLA	ND
29	D	402	CLA	ND
29	D	403	CLA	ND
29	N	602	CLA	ND
29	N	603	CLA	ND
29	N	604	CLA	ND
29	N	610	CLA	ND
29	N	611	CLA	ND
29	N	612	CLA	ND
29	N	613	CLA	ND
29	N	614	CLA	ND
29	G	602	CLA	ND
29	G	603	CLA	ND
29	G	604	CLA	ND
29	G	610	CLA	ND
29	G	611	CLA	ND
29	G	612	CLA	ND
29	G	613	CLA	ND
29	G	614	CLA	ND
29	R	602	CLA	ND
29	R	604	CLA	ND
29	R	608	CLA	ND
29	R	609	CLA	ND
29	R	610	CLA	ND
29	R	612	CLA	ND
29	S	602	CLA	ND
29	S	603	CLA	ND
29	S	604	CLA	ND
29	S	605	CLA	ND
29	S	609	CLA	ND
29	S	610	CLA	ND
29	S	611	CLA	ND
29	S	612	CLA	ND

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Mol	Chain	Res	Type	Atom
29	S	613	CLA	ND
29	S	614	CLA	ND
29	S	617	CLA	ND
29	Y	602	CLA	ND
29	Y	603	CLA	ND
29	Y	604	CLA	ND
29	Y	608	CLA	ND
29	Y	610	CLA	ND
29	Y	611	CLA	ND
29	Y	612	CLA	ND
29	Y	613	CLA	ND
29	Y	614	CLA	ND
29	a	405	CLA	ND
29	a	406	CLA	ND
29	b	602	CLA	ND
29	b	603	CLA	ND
29	b	604	CLA	ND
29	b	605	CLA	ND
29	b	606	CLA	ND
29	b	607	CLA	ND
29	b	608	CLA	ND
29	b	610	CLA	ND
29	b	611	CLA	ND
29	b	613	CLA	ND
29	b	614	CLA	ND
29	b	615	CLA	ND
29	b	616	CLA	ND
29	b	617	CLA	ND
29	c	502	CLA	ND
29	c	504	CLA	ND
29	c	505	CLA	ND
29	c	507	CLA	ND
29	c	508	CLA	ND
29	c	509	CLA	ND
29	c	510	CLA	ND
29	c	512	CLA	ND
29	d	402	CLA	ND
29	d	403	CLA	ND
29	n	602	CLA	ND
29	n	603	CLA	ND
29	n	604	CLA	ND
29	n	610	CLA	ND

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Mol	Chain	Res	Type	Atom
29	n	611	CLA	ND
29	n	612	CLA	ND
29	n	614	CLA	ND
29	g	602	CLA	ND
29	g	603	CLA	ND
29	g	604	CLA	ND
29	g	610	CLA	ND
29	g	611	CLA	ND
29	g	614	CLA	ND
29	r	602	CLA	ND
29	r	604	CLA	ND
29	r	608	CLA	ND
29	r	609	CLA	ND
29	r	610	CLA	ND
29	r	612	CLA	ND
29	s	602	CLA	ND
29	s	604	CLA	ND
29	s	609	CLA	ND
29	s	610	CLA	ND
29	s	611	CLA	ND
29	s	612	CLA	ND
29	s	613	CLA	ND
29	s	614	CLA	ND
29	s	617	CLA	ND
29	y	602	CLA	ND
29	y	603	CLA	ND
29	y	604	CLA	ND
29	y	608	CLA	ND
29	y	610	CLA	ND
29	y	611	CLA	ND
29	y	612	CLA	ND
29	y	614	CLA	ND
36	B	620	C7Z	C3
36	b	620	C7Z	C3
44	H	101	RRX	C28
44	h	101	RRX	C28
45	N	601	CHL	NA
45	N	601	CHL	ND
45	N	601	CHL	C8
45	N	601	CHL	NC
45	N	605	CHL	NA
45	N	605	CHL	ND

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

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

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

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Mol	Chain	Res	Type	Atom
45	s	601	CHL	NA
45	s	601	CHL	ND
45	s	601	CHL	NC
45	s	606	CHL	NA
45	s	606	CHL	ND
45	s	606	CHL	NC
45	s	607	CHL	NA
45	s	607	CHL	ND
45	s	607	CHL	NC
45	s	608	CHL	NA
45	s	608	CHL	ND
45	s	608	CHL	C8
45	s	608	CHL	NC
45	y	601	CHL	NA
45	y	601	CHL	ND
45	y	601	CHL	C8
45	y	601	CHL	NC
45	y	605	CHL	NA
45	y	605	CHL	ND
45	y	605	CHL	NC
45	y	606	CHL	NA
45	y	606	CHL	ND
45	y	606	CHL	NC
45	y	607	CHL	NA
45	y	607	CHL	ND
45	y	607	CHL	C8
45	y	607	CHL	NC
45	y	609	CHL	NA
45	y	609	CHL	ND
45	y	609	CHL	C8
45	y	609	CHL	NC
48	N	622	XAT	C6
48	G	622	XAT	C6
48	G	622	XAT	C26
48	R	621	XAT	C6
48	R	621	XAT	C26
48	Y	622	XAT	C6
48	n	622	XAT	C6
48	g	622	XAT	C6
48	g	622	XAT	C26
48	r	621	XAT	C6
48	y	622	XAT	C6

All (3579) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D
29	A	407	CLA	C1A-C2A-CAA-CBA
29	A	407	CLA	C3A-C2A-CAA-CBA
29	A	407	CLA	CHA-CBD-CGD-O1D
29	A	407	CLA	CHA-CBD-CGD-O2D
29	B	602	CLA	C1A-C2A-CAA-CBA
29	B	602	CLA	CAD-CBD-CGD-O1D
29	B	602	CLA	CAD-CBD-CGD-O2D
29	B	605	CLA	C4-C3-C5-C6
29	B	607	CLA	CHA-CBD-CGD-O1D
29	B	608	CLA	C1A-C2A-CAA-CBA
29	B	608	CLA	C3A-C2A-CAA-CBA
29	B	608	CLA	C2-C3-C5-C6
29	B	608	CLA	C4-C3-C5-C6
29	C	501	CLA	CBD-CGD-O2D-CED
29	C	502	CLA	CHA-CBD-CGD-O1D
29	C	502	CLA	CHA-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O1D
29	C	504	CLA	C2-C3-C5-C6
29	C	504	CLA	C4-C3-C5-C6
29	C	508	CLA	CHA-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O2D
29	C	510	CLA	CBD-CGD-O2D-CED
29	C	513	CLA	C1A-C2A-CAA-CBA
29	C	513	CLA	C3A-C2A-CAA-CBA
29	N	610	CLA	C1A-C2A-CAA-CBA
29	N	610	CLA	C3A-C2A-CAA-CBA
29	N	613	CLA	CHA-CBD-CGD-O1D
29	N	613	CLA	CHA-CBD-CGD-O2D
29	N	613	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C1A-C2A-CAA-CBA
29	G	603	CLA	C3A-C2A-CAA-CBA
29	G	612	CLA	CBD-CGD-O2D-CED
29	G	613	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	G	613	CLA	CHA-CBD-CGD-O2D
29	G	614	CLA	C1A-C2A-CAA-CBA
29	R	603	CLA	C1A-C2A-CAA-CBA
29	R	603	CLA	C3A-C2A-CAA-CBA
29	R	603	CLA	CBA-CGA-O2A-C1
29	R	603	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O2D
29	R	603	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	O1D-CGD-O2D-CED
29	R	608	CLA	C1A-C2A-CAA-CBA
29	R	608	CLA	C3A-C2A-CAA-CBA
29	R	612	CLA	CBD-CGD-O2D-CED
29	S	602	CLA	C1A-C2A-CAA-CBA
29	S	602	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	C1A-C2A-CAA-CBA
29	S	603	CLA	C3A-C2A-CAA-CBA
29	S	603	CLA	C11-C12-C13-C14
29	S	605	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	C11-C10-C8-C9
29	S	610	CLA	C1A-C2A-CAA-CBA
29	S	610	CLA	C3A-C2A-CAA-CBA
29	S	610	CLA	C6-C7-C8-C10
29	S	611	CLA	C1A-C2A-CAA-CBA
29	S	611	CLA	C3A-C2A-CAA-CBA
29	S	613	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	C1A-C2A-CAA-CBA
29	Y	603	CLA	C3A-C2A-CAA-CBA
29	Y	608	CLA	C1A-C2A-CAA-CBA
29	Y	608	CLA	C2A-CAA-CBA-CGA
29	Y	611	CLA	O1A-CGA-O2A-C1
29	a	405	CLA	C2A-CAA-CBA-CGA
29	a	405	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	O2A-C1-C2-C3
29	a	406	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C3A-C2A-CAA-CBA
29	a	406	CLA	C2-C1-O2A-CGA
29	a	406	CLA	CHA-CBD-CGD-O1D
29	a	406	CLA	CHA-CBD-CGD-O2D
29	b	602	CLA	C11-C12-C13-C14
29	b	603	CLA	C2-C3-C5-C6
29	b	603	CLA	C4-C3-C5-C6
29	b	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	c	502	CLA	CHA-CBD-CGD-O1D
29	c	502	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	C6-C7-C8-C9
29	c	505	CLA	C11-C10-C8-C9
29	c	508	CLA	CHA-CBD-CGD-O1D
29	c	508	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	509	CLA	C6-C7-C8-C9
29	c	513	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	610	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C1A-C2A-CAA-CBA
29	g	613	CLA	CHA-CBD-CGD-O1D
29	g	613	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	C1A-C2A-CAA-CBA
29	r	603	CLA	C3A-C2A-CAA-CBA
29	r	603	CLA	CHA-CBD-CGD-O1D
29	r	603	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	C2-C3-C5-C6
29	r	608	CLA	C4-C3-C5-C6
29	r	609	CLA	C1A-C2A-CAA-CBA
29	r	609	CLA	CBD-CGD-O2D-CED
29	r	612	CLA	CBA-CGA-O2A-C1
29	r	612	CLA	O1A-CGA-O2A-C1
29	s	603	CLA	C1A-C2A-CAA-CBA
29	s	603	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C1A-C2A-CAA-CBA
29	s	609	CLA	C1A-C2A-CAA-CBA
29	s	609	CLA	C3A-C2A-CAA-CBA
29	s	610	CLA	C3A-C2A-CAA-CBA
29	y	604	CLA	CBD-CGD-O2D-CED
29	y	604	CLA	C6-C7-C8-C9
29	y	608	CLA	C1A-C2A-CAA-CBA
29	y	608	CLA	CBD-CGD-O2D-CED
30	A	409	PHO	C3A-C2A-CAA-CBA

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

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Mol	Chain	Res	Type	Atoms
31	b	618	BCR	C10-C11-C12-C13
31	b	618	BCR	C17-C18-C19-C20
31	b	618	BCR	C36-C18-C19-C20
31	b	618	BCR	C37-C22-C23-C24
31	b	619	BCR	C7-C8-C9-C10
31	b	619	BCR	C7-C8-C9-C34
31	b	619	BCR	C11-C10-C9-C8
31	b	619	BCR	C11-C10-C9-C34
31	b	619	BCR	C10-C11-C12-C13
31	c	516	BCR	C5-C6-C7-C8
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C11-C10-C9-C8
31	c	516	BCR	C11-C10-C9-C34
31	c	515	BCR	C1-C6-C7-C8
31	c	515	BCR	C11-C10-C9-C8
31	c	515	BCR	C11-C10-C9-C34
31	c	515	BCR	C10-C11-C12-C13
31	c	515	BCR	C11-C12-C13-C14
31	c	515	BCR	C11-C12-C13-C35
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	c	515	BCR	C23-C24-C25-C30
31	c	517	BCR	C11-C10-C9-C8
31	c	517	BCR	C11-C10-C9-C34
31	c	517	BCR	C10-C11-C12-C13
31	c	517	BCR	C17-C18-C19-C20
31	c	517	BCR	C36-C18-C19-C20
31	c	514	BCR	C7-C8-C9-C10
31	c	514	BCR	C7-C8-C9-C34
31	c	514	BCR	C11-C10-C9-C8
31	c	514	BCR	C11-C10-C9-C34
31	c	514	BCR	C10-C11-C12-C13
31	c	514	BCR	C36-C18-C19-C20
31	d	404	BCR	C11-C10-C9-C8
31	d	404	BCR	C11-C10-C9-C34
31	d	404	BCR	C10-C11-C12-C13
31	d	404	BCR	C21-C22-C23-C24
31	d	404	BCR	C37-C22-C23-C24
31	d	404	BCR	C23-C24-C25-C26
31	d	404	BCR	C23-C24-C25-C30
33	B	621	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
33	B	621	SQD	O5-C1-O6-C44
33	B	621	SQD	O5-C5-C6-S
33	B	626	SQD	C2-C1-O6-C44
33	B	626	SQD	O5-C1-O6-C44
33	B	626	SQD	C8-C7-O47-C45
33	B	626	SQD	C5-C6-S-O7
33	B	626	SQD	C5-C6-S-O8
33	B	626	SQD	C5-C6-S-O9
33	C	526	SQD	C5-C6-S-O9
33	M	101	SQD	C5-C6-S-O7
33	M	101	SQD	C5-C6-S-O8
33	M	101	SQD	C5-C6-S-O9
33	a	412	SQD	O5-C5-C6-S
33	b	621	SQD	C2-C1-O6-C44
33	b	621	SQD	O5-C1-O6-C44
33	b	626	SQD	C2-C1-O6-C44
33	b	626	SQD	O5-C1-O6-C44
33	c	526	SQD	O10-C23-O48-C46
33	c	526	SQD	O5-C5-C6-S
33	m	101	SQD	C2-C1-O6-C44
33	m	101	SQD	O5-C1-O6-C44
33	m	101	SQD	O5-C5-C6-S
33	m	101	SQD	C5-C6-S-O7
33	m	101	SQD	C5-C6-S-O8
33	m	101	SQD	C5-C6-S-O9
34	A	414	SPH	O1-C1-C2-C3
34	A	414	SPH	C1-C2-C3-O3
34	A	414	SPH	C1-C2-C3-C4
34	A	414	SPH	N2-C2-C3-C4
34	Y	625	SPH	O1-C1-C2-C3
34	Y	625	SPH	C2-C3-C4-C5
34	Y	625	SPH	O3-C3-C4-C5
34	a	414	SPH	C1-C2-C3-O3
34	a	414	SPH	C1-C2-C3-C4
34	a	414	SPH	N2-C2-C3-O3
34	a	414	SPH	N2-C2-C3-C4
35	A	413	LMG	O6-C1-O1-C7
35	B	622	LMG	O6-C1-O1-C7
35	C	527	LMG	C2-C1-O1-C7
35	C	527	LMG	O6-C1-O1-C7
35	C	527	LMG	O9-C10-O7-C8
35	C	527	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	W	201	LMG	O6-C1-O1-C7
35	W	201	LMG	C7-C8-O7-C10
35	W	201	LMG	C11-C10-O7-C8
35	a	413	LMG	O1-C7-C8-O7
35	b	622	LMG	O6-C1-O1-C7
35	w	201	LMG	O6-C1-O1-C7
36	B	620	C7Z	C5-C6-C7-C8
36	B	620	C7Z	C21-C26-C27-C28
36	b	620	C7Z	C1-C6-C7-C8
37	B	623	DGD	C2B-C1B-O2G-C2G
37	b	623	DGD	C2A-C1A-O1G-C1G
37	b	623	DGD	O1A-C1A-O1G-C1G
37	b	623	DGD	O1B-C1B-O2G-C2G
38	T	101	3PH	C1-O11-P-O13
38	T	101	3PH	C1-O11-P-O14
38	S	626	3PH	O22-C21-O21-C2
38	b	624	3PH	C1-O11-P-O13
38	b	624	3PH	C1-O11-P-O14
38	b	624	3PH	O11-C1-C2-O21
38	b	624	3PH	O22-C21-O21-C2
38	t	101	3PH	C1-O11-P-O13
38	t	101	3PH	C1-O11-P-O14
38	t	101	3PH	O22-C21-O21-C2
38	s	626	3PH	C22-C21-O21-C2
39	B	625	DGA	OB1-CB1-OG2-CG2
39	C	524	DGA	OG2-CG2-CG3-OXT
39	b	625	DGA	CG1-CG2-CG3-OXT
39	b	625	DGA	OG2-CG2-CG3-OXT
39	c	524	DGA	OG2-CG2-CG3-OXT
39	j	101	DGA	OG2-CG2-CG3-OXT
40	C	525	LHG	O1-C1-C2-C3
40	C	525	LHG	C1-C2-C3-O3
40	C	525	LHG	C3-O3-P-O4
40	C	525	LHG	C4-O6-P-O5
40	D	408	LHG	C4-O6-P-O5
40	D	409	LHG	C4-O6-P-O4
40	D	409	LHG	C4-O6-P-O5
40	D	410	LHG	C3-O3-P-O5
40	D	410	LHG	O7-C5-C6-O8
40	L	101	LHG	O1-C1-C2-C3
40	L	101	LHG	C1-C2-C3-O3
40	L	101	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
40	L	101	LHG	C8-C7-O7-C5
40	N	624	LHG	C3-O3-P-O5
40	N	624	LHG	C4-O6-P-O3
40	N	624	LHG	C4-O6-P-O4
40	N	624	LHG	C4-O6-P-O5
40	N	624	LHG	O7-C5-C6-O8
40	G	624	LHG	O1-C1-C2-O2
40	G	624	LHG	C4-O6-P-O4
40	G	624	LHG	O7-C5-C6-O8
40	Y	624	LHG	C1-C2-C3-O3
40	Y	624	LHG	C3-O3-P-O5
40	Y	624	LHG	C4-O6-P-O3
40	Y	624	LHG	C4-O6-P-O4
40	Y	624	LHG	C4-O6-P-O5
40	c	525	LHG	C1-C2-C3-O3
40	c	525	LHG	C4-O6-P-O4
40	c	497	LHG	C3-O3-P-O4
40	c	497	LHG	C3-O3-P-O5
40	c	497	LHG	C3-O3-P-O6
40	c	497	LHG	O9-C7-O7-C5
40	c	497	LHG	C8-C7-O7-C5
40	d	408	LHG	O1-C1-C2-C3
40	d	408	LHG	C1-C2-C3-O3
40	d	408	LHG	C3-O3-P-O5
40	d	408	LHG	C3-O3-P-O6
40	d	408	LHG	C4-O6-P-O5
40	d	410	LHG	C3-O3-P-O5
40	d	410	LHG	C4-O6-P-O5
40	d	410	LHG	O7-C5-C6-O8
40	d	409	LHG	C1-C2-C3-O3
40	d	409	LHG	C4-O6-P-O5
40	l	101	LHG	O1-C1-C2-C3
40	l	101	LHG	C3-O3-P-O4
40	l	101	LHG	C3-O3-P-O5
40	l	101	LHG	C4-O6-P-O3
40	l	101	LHG	C4-O6-P-O5
40	n	624	LHG	C3-O3-P-O5
40	n	624	LHG	C4-O6-P-O3
40	n	624	LHG	C4-O6-P-O4
40	n	624	LHG	C4-O6-P-O5
40	n	624	LHG	O7-C5-C6-O8
40	g	624	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
40	g	624	LHG	O7-C5-C6-O8
40	s	624	LHG	O1-C1-C2-C3
40	s	624	LHG	C4-O6-P-O4
40	y	624	LHG	O2-C2-C3-O3
40	y	624	LHG	C3-O3-P-O4
40	y	624	LHG	C3-O3-P-O5
40	y	624	LHG	C3-O3-P-O6
40	y	624	LHG	C4-O6-P-O5
42	D	405	PL9	C37-C38-C39-C40
42	D	405	PL9	C37-C38-C39-C41
42	d	405	PL9	C37-C38-C39-C40
42	d	405	PL9	C37-C38-C39-C41
44	H	101	RRX	C37-C22-C23-C24
44	H	101	RRX	C21-C22-C23-C24
44	h	101	RRX	C37-C22-C23-C24
44	h	101	RRX	C21-C22-C23-C24
44	h	101	RRX	C36-C18-C19-C20
44	h	101	RRX	C17-C18-C19-C20
44	h	101	RRX	C11-C12-C13-C35
45	N	609	CHL	CHA-CBD-CGD-O1D
45	N	609	CHL	CHA-CBD-CGD-O2D
45	G	601	CHL	CHA-CBD-CGD-O1D
45	G	601	CHL	CHA-CBD-CGD-O2D
45	G	605	CHL	CHA-CBD-CGD-O1D
45	G	605	CHL	CHA-CBD-CGD-O2D
45	G	609	CHL	CHA-CBD-CGD-O1D
45	G	609	CHL	CHA-CBD-CGD-O2D
45	Y	601	CHL	CHA-CBD-CGD-O1D
45	Y	601	CHL	CHA-CBD-CGD-O2D
45	n	601	CHL	C2-C3-C5-C6
45	n	601	CHL	C4-C3-C5-C6
45	n	605	CHL	C14-C13-C15-C16
45	n	606	CHL	C14-C13-C15-C16
45	g	601	CHL	C1A-C2A-CAA-CBA
45	g	601	CHL	C3A-C2A-CAA-CBA
45	g	601	CHL	CHA-CBD-CGD-O1D
45	g	601	CHL	CHA-CBD-CGD-O2D
45	g	607	CHL	C1A-C2A-CAA-CBA
45	g	607	CHL	C3A-C2A-CAA-CBA
45	g	609	CHL	C2-C3-C5-C6
45	g	609	CHL	C4-C3-C5-C6
45	y	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	y	601	CHL	CHA-CBD-CGD-O2D
45	y	609	CHL	C11-C12-C13-C14
46	N	621	LUT	C21-C26-C27-C28
46	R	620	LUT	C25-C26-C27-C28
46	S	620	LUT	C21-C26-C27-C28
46	Y	621	LUT	C21-C26-C27-C28
46	n	621	LUT	C21-C26-C27-C28
46	s	620	LUT	C21-C26-C27-C28
47	R	622	NEX	C12-C13-C14-C15
47	R	622	NEX	C32-C33-C34-C35
47	R	622	NEX	C40-C33-C34-C35
47	Y	623	NEX	C7-C8-C9-C10
47	Y	623	NEX	C10-C11-C12-C13
47	r	622	NEX	C12-C13-C14-C15
47	y	623	NEX	C7-C8-C9-C10
49	r	625	LMT	O5'-C1'-O1'-C1
49	r	625	LMT	C2-C1-O1'-C1'
50	S	625	LPX	C3-C4-C5-O6
50	S	625	LPX	C1-O2-P1-O3
50	s	625	LPX	C3-C4-C5-O6
50	s	625	LPX	C3-O1-P1-O3
50	s	625	LPX	C1-O2-P1-O4
51	Y	626	PTY	O4-C1-C6-O7
51	Y	626	PTY	N1-C2-C3-O11
51	Y	626	PTY	C3-O11-P1-O13
51	Y	626	PTY	C3-O11-P1-O14
51	Y	627	PTY	C3-O11-P1-O12
51	Y	627	PTY	C3-O11-P1-O13
51	y	626	PTY	N1-C2-C3-O11
51	y	627	PTY	N1-C2-C3-O11
51	y	627	PTY	C3-O11-P1-O12
51	Y	627	PTY	C11-C8-O7-C6
51	y	627	PTY	C11-C8-O7-C6
29	r	609	CLA	O1D-CGD-O2D-CED
29	s	613	CLA	O1D-CGD-O2D-CED
29	a	405	CLA	O1D-CGD-O2D-CED
29	r	603	CLA	O1D-CGD-O2D-CED
29	C	503	CLA	CBD-CGD-O2D-CED
29	R	609	CLA	CBD-CGD-O2D-CED
29	S	603	CLA	CBD-CGD-O2D-CED
29	S	617	CLA	CBD-CGD-O2D-CED
29	Y	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	b	606	CLA	CBD-CGD-O2D-CED
29	b	615	CLA	CBD-CGD-O2D-CED
29	c	502	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED
29	s	613	CLA	CBD-CGD-O2D-CED
29	B	602	CLA	O1A-CGA-O2A-C1
29	C	509	CLA	O1A-CGA-O2A-C1
29	R	603	CLA	O1A-CGA-O2A-C1
29	S	614	CLA	O1A-CGA-O2A-C1
29	n	611	CLA	O1A-CGA-O2A-C1
29	g	614	CLA	O1A-CGA-O2A-C1
29	r	608	CLA	O1A-CGA-O2A-C1
35	C	521	LMG	O10-C28-O8-C9
29	A	405	CLA	O1D-CGD-O2D-CED
29	C	503	CLA	O1D-CGD-O2D-CED
29	S	603	CLA	O1D-CGD-O2D-CED
29	S	613	CLA	O1D-CGD-O2D-CED
29	Y	608	CLA	O1D-CGD-O2D-CED
29	b	606	CLA	O1D-CGD-O2D-CED
40	L	101	LHG	C5-C6-O8-C23
29	C	501	CLA	O1D-CGD-O2D-CED
29	C	510	CLA	O1D-CGD-O2D-CED
29	N	613	CLA	O1D-CGD-O2D-CED
29	R	612	CLA	O1D-CGD-O2D-CED
29	S	614	CLA	CBA-CGA-O2A-C1
29	Y	604	CLA	CBA-CGA-O2A-C1
29	n	611	CLA	CBA-CGA-O2A-C1
29	g	614	CLA	CBA-CGA-O2A-C1
29	r	608	CLA	CBA-CGA-O2A-C1
29	s	611	CLA	CBA-CGA-O2A-C1
29	B	610	CLA	CBD-CGD-O2D-CED
29	B	615	CLA	CBD-CGD-O2D-CED
29	C	502	CLA	CBD-CGD-O2D-CED
29	D	403	CLA	CBD-CGD-O2D-CED
29	N	604	CLA	CBD-CGD-O2D-CED
29	G	610	CLA	CBD-CGD-O2D-CED
29	G	613	CLA	CBD-CGD-O2D-CED
29	Y	604	CLA	CBD-CGD-O2D-CED
29	c	510	CLA	CBD-CGD-O2D-CED
29	c	511	CLA	CBD-CGD-O2D-CED
29	y	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
51	Y	627	PTY	O10-C8-O7-C6
29	A	406	CLA	O1A-CGA-O2A-C1
29	C	513	CLA	O1A-CGA-O2A-C1
29	N	603	CLA	O1A-CGA-O2A-C1
29	N	611	CLA	O1A-CGA-O2A-C1
29	G	604	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1A-CGA-O2A-C1
29	S	605	CLA	O1A-CGA-O2A-C1
29	S	613	CLA	O1A-CGA-O2A-C1
29	Y	604	CLA	O1A-CGA-O2A-C1
29	Y	608	CLA	O1A-CGA-O2A-C1
29	c	509	CLA	O1A-CGA-O2A-C1
29	g	604	CLA	O1A-CGA-O2A-C1
29	g	611	CLA	O1A-CGA-O2A-C1
29	r	603	CLA	O1A-CGA-O2A-C1
29	s	611	CLA	O1A-CGA-O2A-C1
29	s	613	CLA	O1A-CGA-O2A-C1
29	s	614	CLA	O1A-CGA-O2A-C1
29	y	604	CLA	O1A-CGA-O2A-C1
29	y	611	CLA	O1A-CGA-O2A-C1
35	C	523	LMG	O10-C28-O8-C9
35	C	527	LMG	O10-C28-O8-C9
35	W	201	LMG	O10-C28-O8-C9
35	c	523	LMG	O10-C28-O8-C9
38	T	101	3PH	O32-C31-O31-C3
51	y	626	PTY	O30-C30-O4-C1
29	y	604	CLA	O1D-CGD-O2D-CED
51	y	627	PTY	O10-C8-O7-C6
29	G	612	CLA	O1D-CGD-O2D-CED
29	y	608	CLA	O1D-CGD-O2D-CED
51	Y	627	PTY	O30-C30-O4-C1
29	N	614	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	s	617	CLA	CBD-CGD-O2D-CED
33	B	626	SQD	O49-C7-O47-C45
35	B	622	LMG	O9-C10-O7-C8
35	W	201	LMG	O9-C10-O7-C8
35	b	622	LMG	O9-C10-O7-C8
37	B	623	DGD	O1B-C1B-O2G-C2G
38	T	101	3PH	O22-C21-O21-C2
38	s	626	3PH	O22-C21-O21-C2
39	b	625	DGA	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
29	y	603	CLA	O1A-CGA-O2A-C1
29	A	410	CLA	C3-C5-C6-C7
29	B	608	CLA	C3-C5-C6-C7
29	B	617	CLA	C3-C5-C6-C7
29	N	610	CLA	C3-C5-C6-C7
29	G	613	CLA	C3-C5-C6-C7
29	R	602	CLA	C3-C5-C6-C7
29	S	613	CLA	C3-C5-C6-C7
29	a	410	CLA	C3-C5-C6-C7
29	y	613	CLA	C3-C5-C6-C7
30	A	409	PHO	C3-C5-C6-C7
29	A	406	CLA	CBA-CGA-O2A-C1
29	B	602	CLA	CBA-CGA-O2A-C1
29	C	509	CLA	CBA-CGA-O2A-C1
29	C	512	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	CBA-CGA-O2A-C1
29	N	611	CLA	CBA-CGA-O2A-C1
29	N	614	CLA	CBA-CGA-O2A-C1
29	G	611	CLA	CBA-CGA-O2A-C1
29	S	605	CLA	CBA-CGA-O2A-C1
29	Y	611	CLA	CBA-CGA-O2A-C1
29	a	405	CLA	CBA-CGA-O2A-C1
29	d	403	CLA	CBA-CGA-O2A-C1
29	g	602	CLA	CBA-CGA-O2A-C1
29	g	611	CLA	CBA-CGA-O2A-C1
29	g	613	CLA	CBA-CGA-O2A-C1
29	r	603	CLA	CBA-CGA-O2A-C1
29	s	613	CLA	CBA-CGA-O2A-C1
29	y	604	CLA	CBA-CGA-O2A-C1
29	y	608	CLA	CBA-CGA-O2A-C1
33	c	526	SQD	C24-C23-O48-C46
35	C	521	LMG	C29-C28-O8-C9
35	C	523	LMG	C29-C28-O8-C9
35	W	201	LMG	C29-C28-O8-C9
35	c	523	LMG	C29-C28-O8-C9
35	B	622	LMG	C11-C10-O7-C8
35	b	622	LMG	C11-C10-O7-C8
37	b	623	DGD	C2B-C1B-O2G-C2G
38	T	101	3PH	C22-C21-O21-C2
38	S	626	3PH	C22-C21-O21-C2
38	b	624	3PH	C22-C21-O21-C2
38	t	101	3PH	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
39	B	625	DGA	CB2-CB1-OG2-CG2
29	S	617	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	CBD-CGD-O2D-CED
29	b	602	CLA	CBD-CGD-O2D-CED
29	A	407	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
51	y	627	PTY	C31-C30-O4-C1
29	R	609	CLA	CBA-CGA-O2A-C1
29	C	507	CLA	C4-C3-C5-C6
29	R	610	CLA	C4-C3-C5-C6
29	a	410	CLA	C4-C3-C5-C6
45	N	606	CHL	C4-C3-C5-C6
29	N	603	CLA	CBD-CGD-O2D-CED
29	d	403	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	C2A-CAA-CBA-CGA
29	R	612	CLA	C2A-CAA-CBA-CGA
29	s	617	CLA	C2A-CAA-CBA-CGA
45	N	606	CHL	C2A-CAA-CBA-CGA
45	N	608	CHL	C2A-CAA-CBA-CGA
45	Y	605	CHL	C2A-CAA-CBA-CGA
45	Y	607	CHL	C2A-CAA-CBA-CGA
45	s	601	CHL	C2A-CAA-CBA-CGA
29	D	403	CLA	O1A-CGA-O2A-C1
35	A	413	LMG	C17-C18-C19-C20
35	B	622	LMG	C17-C18-C19-C20
35	C	521	LMG	C35-C36-C37-C38
35	C	523	LMG	C17-C18-C19-C20
35	C	523	LMG	C41-C42-C43-C44
35	D	411	LMG	C17-C18-C19-C20
35	H	102	LMG	C35-C36-C37-C38
35	H	102	LMG	C38-C39-C40-C41
35	W	201	LMG	C35-C36-C37-C38
35	W	201	LMG	C38-C39-C40-C41
35	a	413	LMG	C17-C18-C19-C20
35	a	413	LMG	C35-C36-C37-C38
35	a	413	LMG	C38-C39-C40-C41
35	b	622	LMG	C17-C18-C19-C20
35	c	521	LMG	C17-C18-C19-C20
35	c	521	LMG	C20-C21-C22-C23
35	c	521	LMG	C35-C36-C37-C38
35	c	523	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	c	523	LMG	C20-C21-C22-C23
35	c	523	LMG	C23-C24-C25-C26
35	c	523	LMG	C41-C42-C43-C44
35	d	411	LMG	C17-C18-C19-C20
35	d	411	LMG	C20-C21-C22-C23
35	h	102	LMG	C35-C36-C37-C38
35	h	102	LMG	C38-C39-C40-C41
35	w	201	LMG	C35-C36-C37-C38
35	w	201	LMG	C38-C39-C40-C41
37	C	518	DGD	C8B-C9B-CAB-CBB
37	C	519	DGD	CBB-CCB-CDB-CEB
37	c	518	DGD	C8B-C9B-CAB-CBB
37	c	519	DGD	C8A-C9A-CAA-CBA
37	c	519	DGD	CBB-CCB-CDB-CEB
37	c	520	DGD	CBB-CCB-CDB-CEB
29	b	605	CLA	C3-C5-C6-C7
29	b	610	CLA	C3-C5-C6-C7
29	g	613	CLA	C3-C5-C6-C7
29	s	609	CLA	C3-C5-C6-C7
29	A	405	CLA	CBA-CGA-O2A-C1
29	C	513	CLA	CBA-CGA-O2A-C1
29	D	403	CLA	CBA-CGA-O2A-C1
29	G	604	CLA	CBA-CGA-O2A-C1
29	R	604	CLA	CBA-CGA-O2A-C1
29	R	608	CLA	CBA-CGA-O2A-C1
29	S	609	CLA	CBA-CGA-O2A-C1
29	S	613	CLA	CBA-CGA-O2A-C1
29	S	617	CLA	CBA-CGA-O2A-C1
29	Y	608	CLA	CBA-CGA-O2A-C1
29	c	509	CLA	CBA-CGA-O2A-C1
29	g	604	CLA	CBA-CGA-O2A-C1
29	s	614	CLA	CBA-CGA-O2A-C1
29	y	603	CLA	CBA-CGA-O2A-C1
29	y	611	CLA	CBA-CGA-O2A-C1
35	C	527	LMG	C29-C28-O8-C9
35	c	521	LMG	C29-C28-O8-C9
38	T	101	3PH	C32-C31-O31-C3
51	y	626	PTY	C31-C30-O4-C1
51	Y	627	PTY	C31-C30-O4-C1
29	c	502	CLA	O1D-CGD-O2D-CED
29	R	609	CLA	O1D-CGD-O2D-CED
29	A	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	608	CLA	O1A-CGA-O2A-C1
29	R	604	CLA	O1A-CGA-O2A-C1
29	R	608	CLA	O1A-CGA-O2A-C1
29	S	603	CLA	O1A-CGA-O2A-C1
29	Y	603	CLA	O1A-CGA-O2A-C1
29	a	405	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	O1A-CGA-O2A-C1
29	c	513	CLA	O1A-CGA-O2A-C1
29	d	403	CLA	O1A-CGA-O2A-C1
29	y	608	CLA	O1A-CGA-O2A-C1
35	c	521	LMG	O10-C28-O8-C9
40	L	101	LHG	O10-C23-O8-C6
40	l	101	LHG	O10-C23-O8-C6
29	R	609	CLA	O1A-CGA-O2A-C1
29	C	511	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	CBD-CGD-O2D-CED
29	S	611	CLA	CBD-CGD-O2D-CED
29	b	616	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CBD-CGD-O2D-CED
29	r	604	CLA	CBD-CGD-O2D-CED
29	s	603	CLA	CBD-CGD-O2D-CED
29	s	604	CLA	CBD-CGD-O2D-CED
40	C	525	LHG	O2-C2-C3-O3
40	D	408	LHG	O2-C2-C3-O3
40	L	101	LHG	O2-C2-C3-O3
40	N	624	LHG	O2-C2-C3-O3
40	Y	624	LHG	O2-C2-C3-O3
40	d	409	LHG	O2-C2-C3-O3
40	l	101	LHG	O2-C2-C3-O3
29	C	506	CLA	C3-C5-C6-C7
45	N	606	CHL	C3-C5-C6-C7
29	A	407	CLA	CBA-CGA-O2A-C1
29	B	608	CLA	CBA-CGA-O2A-C1
29	N	610	CLA	CBA-CGA-O2A-C1
29	G	602	CLA	CBA-CGA-O2A-C1
29	c	507	CLA	CBA-CGA-O2A-C1
29	n	613	CLA	CBA-CGA-O2A-C1
29	s	617	CLA	CBA-CGA-O2A-C1
38	t	101	3PH	C32-C31-O31-C3
40	l	101	LHG	C24-C23-O8-C6
29	C	512	CLA	O1A-CGA-O2A-C1
29	N	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	g	602	CLA	O1A-CGA-O2A-C1
29	g	613	CLA	O1A-CGA-O2A-C1
29	s	617	CLA	O1A-CGA-O2A-C1
29	b	615	CLA	O1D-CGD-O2D-CED
50	s	625	LPX	O5-C4-C5-O6
39	b	625	DGA	CB2-CB1-OG2-CG2
40	n	624	LHG	C8-C7-O7-C5
29	B	614	CLA	CBD-CGD-O2D-CED
29	B	617	CLA	CBD-CGD-O2D-CED
37	c	518	DGD	O6E-C5E-C6E-O5E
38	t	101	3PH	O32-C31-O31-C3
40	N	624	LHG	C11-C12-C13-C14
29	g	602	CLA	CBD-CGD-O2D-CED
29	B	605	CLA	C3-C5-C6-C7
29	S	610	CLA	C3-C5-C6-C7
29	n	613	CLA	C3-C5-C6-C7
45	g	601	CHL	C3-C5-C6-C7
29	B	617	CLA	CBA-CGA-O2A-C1
29	S	603	CLA	CBA-CGA-O2A-C1
29	Y	603	CLA	CBA-CGA-O2A-C1
29	a	406	CLA	CBA-CGA-O2A-C1
29	c	513	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	CBA-CGA-O2A-C1
40	L	101	LHG	C24-C23-O8-C6
29	n	604	CLA	O1D-CGD-O2D-CED
40	N	624	LHG	C13-C14-C15-C16
29	G	602	CLA	O1A-CGA-O2A-C1
29	n	613	CLA	O1A-CGA-O2A-C1
42	d	405	PL9	C47-C48-C49-C51
29	B	610	CLA	C4-C3-C5-C6
29	B	605	CLA	C2-C3-C5-C6
29	B	610	CLA	C2-C3-C5-C6
45	N	606	CHL	C2-C3-C5-C6
29	b	617	CLA	CBD-CGD-O2D-CED
40	L	101	LHG	C7-C8-C9-C10
29	r	609	CLA	C2A-CAA-CBA-CGA
45	n	608	CHL	C2A-CAA-CBA-CGA
45	y	605	CHL	C2A-CAA-CBA-CGA
29	B	617	CLA	O1A-CGA-O2A-C1
29	N	610	CLA	O1A-CGA-O2A-C1
29	S	609	CLA	O1A-CGA-O2A-C1
29	S	617	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	c	507	CLA	O1A-CGA-O2A-C1
35	a	413	LMG	O6-C1-O1-C7
42	D	405	PL9	C39-C41-C42-C43
42	d	405	PL9	C39-C41-C42-C43
49	r	625	LMT	O5B-C5B-C6B-O6B
29	B	610	CLA	O1D-CGD-O2D-CED
29	B	615	CLA	O1D-CGD-O2D-CED
29	N	604	CLA	O1D-CGD-O2D-CED
29	G	610	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
30	A	408	PHO	CBD-CGD-O2D-CED
29	C	502	CLA	O1D-CGD-O2D-CED
40	l	101	LHG	C1-C2-C3-O3
40	g	624	LHG	C1-C2-C3-O3
40	y	624	LHG	C1-C2-C3-O3
38	b	624	3PH	O32-C31-O31-C3
29	Y	604	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	CBA-CGA-O2A-C1
29	R	612	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	CBA-CGA-O2A-C1
29	g	603	CLA	CBA-CGA-O2A-C1
29	r	604	CLA	CBA-CGA-O2A-C1
29	s	605	CLA	CBA-CGA-O2A-C1
29	y	614	CLA	CBA-CGA-O2A-C1
33	M	101	SQD	C24-C23-O48-C46
33	m	101	SQD	C24-C23-O48-C46
37	C	520	DGD	C2A-C1A-O1G-C1G
38	b	624	3PH	C32-C31-O31-C3
40	D	410	LHG	C24-C23-O8-C6
50	S	625	LPX	C7-C6-O6-C5
29	G	614	CLA	CBD-CGD-O2D-CED
29	b	607	CLA	CBD-CGD-O2D-CED
29	y	614	CLA	CBD-CGD-O2D-CED
31	C	514	BCR	C9-C10-C11-C12
38	s	626	3PH	C31-C32-C33-C34
45	G	607	CHL	C10-C11-C12-C13
38	s	626	3PH	C34-C35-C36-C37
29	B	610	CLA	C5-C6-C7-C8
29	B	616	CLA	C13-C15-C16-C17
29	c	504	CLA	C13-C15-C16-C17
29	c	510	CLA	C8-C10-C11-C12
29	y	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
45	G	609	CHL	C8-C10-C11-C12
39	j	101	DGA	CB1-CB2-CB3-CB4
33	a	412	SQD	C2-C1-O6-C44
38	s	626	3PH	C32-C33-C34-C35
51	y	627	PTY	O30-C30-O4-C1
29	g	603	CLA	O1A-CGA-O2A-C1
29	s	605	CLA	O1A-CGA-O2A-C1
29	n	610	CLA	C4-C3-C5-C6
29	R	610	CLA	C2-C3-C5-C6
29	A	410	CLA	C6-C7-C8-C9
29	B	603	CLA	C14-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C9
29	B	610	CLA	C6-C7-C8-C9
29	B	614	CLA	C11-C12-C13-C14
29	B	616	CLA	C11-C10-C8-C9
29	C	501	CLA	C11-C12-C13-C14
29	C	506	CLA	C6-C7-C8-C9
29	C	509	CLA	C6-C7-C8-C9
29	C	513	CLA	C11-C10-C8-C9
29	N	604	CLA	C11-C12-C13-C14
29	G	611	CLA	C14-C13-C15-C16
29	R	602	CLA	C6-C7-C8-C9
29	R	610	CLA	C6-C7-C8-C9
29	S	602	CLA	C11-C10-C8-C9
29	S	611	CLA	C6-C7-C8-C9
29	Y	603	CLA	C6-C7-C8-C9
29	Y	604	CLA	C11-C10-C8-C9
29	Y	613	CLA	C6-C7-C8-C9
29	b	604	CLA	C11-C10-C8-C9
29	b	615	CLA	C11-C12-C13-C14
29	b	616	CLA	C11-C10-C8-C9
29	b	617	CLA	C14-C13-C15-C16
29	c	501	CLA	C11-C12-C13-C14
29	c	504	CLA	C11-C12-C13-C14
29	c	506	CLA	C6-C7-C8-C9
29	c	513	CLA	C11-C10-C8-C9
29	n	604	CLA	C14-C13-C15-C16
29	r	602	CLA	C6-C7-C8-C9
29	s	610	CLA	C6-C7-C8-C9
29	y	603	CLA	C6-C7-C8-C9
45	N	605	CHL	C14-C13-C15-C16
45	N	607	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
45	G	609	CHL	C14-C13-C15-C16
45	Y	607	CHL	C6-C7-C8-C9
45	Y	607	CHL	C14-C13-C15-C16
45	Y	609	CHL	C11-C12-C13-C14
45	n	601	CHL	C11-C10-C8-C9
45	n	609	CHL	C14-C13-C15-C16
45	g	601	CHL	C14-C13-C15-C16
45	g	609	CHL	C14-C13-C15-C16
45	y	607	CHL	C6-C7-C8-C9
45	y	607	CHL	C14-C13-C15-C16
29	D	403	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
29	A	405	CLA	C4C-C3C-CAC-CBC
29	B	614	CLA	C10-C11-C12-C13
29	C	509	CLA	C15-C16-C17-C18
29	N	613	CLA	C5-C6-C7-C8
45	S	608	CHL	C2A-CAA-CBA-CGA
31	A	411	BCR	C37-C22-C23-C24
31	D	404	BCR	C36-C18-C19-C20
31	b	619	BCR	C36-C18-C19-C20
44	H	101	RRX	C11-C12-C13-C35
44	h	101	RRX	C7-C8-C9-C34
46	R	620	LUT	C7-C8-C9-C19
31	c	516	BCR	C21-C22-C23-C24
44	h	101	RRX	C7-C8-C9-C10
29	c	510	CLA	O1D-CGD-O2D-CED
40	n	624	LHG	O9-C7-O7-C5
39	C	524	DGA	CB2-CB1-OG2-CG2
40	N	624	LHG	C8-C7-O7-C5
40	D	408	LHG	C31-C32-C33-C34
49	r	625	LMT	C4B-C5B-C6B-O6B
39	C	524	DGA	CA1-CA2-CA3-CA4
40	C	525	LHG	C23-C24-C25-C26
40	n	624	LHG	C23-C24-C25-C26
29	G	603	CLA	O1A-CGA-O2A-C1
29	R	612	CLA	O1A-CGA-O2A-C1
29	y	614	CLA	O1A-CGA-O2A-C1
40	D	410	LHG	O10-C23-O8-C6
50	S	625	LPX	O7-C6-O6-C5
29	C	504	CLA	C5-C6-C7-C8
29	C	513	CLA	C8-C10-C11-C12
29	G	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	Y	602	CLA	C13-C15-C16-C17
29	Y	613	CLA	C15-C16-C17-C18
29	b	604	CLA	C8-C10-C11-C12
29	y	604	CLA	C13-C15-C16-C17
45	G	607	CHL	C13-C15-C16-C17
45	Y	606	CHL	C5-C6-C7-C8
45	G	608	CHL	C2A-CAA-CBA-CGA
29	Y	612	CLA	CBA-CGA-O2A-C1
29	B	608	CLA	C8-C10-C11-C12
29	C	506	CLA	C5-C6-C7-C8
29	S	611	CLA	C15-C16-C17-C18
29	b	602	CLA	C10-C11-C12-C13
29	c	503	CLA	C15-C16-C17-C18
29	c	508	CLA	C5-C6-C7-C8
29	d	403	CLA	C8-C10-C11-C12
29	n	604	CLA	C8-C10-C11-C12
29	y	613	CLA	C15-C16-C17-C18
29	y	614	CLA	C8-C10-C11-C12
45	N	607	CHL	C8-C10-C11-C12
35	b	622	LMG	C28-C29-C30-C31
39	C	524	DGA	CB1-CB2-CB3-CB4
39	J	101	DGA	CB1-CB2-CB3-CB4
40	D	409	LHG	C23-C24-C25-C26
40	l	101	LHG	C23-C24-C25-C26
38	S	626	3PH	C32-C33-C34-C35
29	C	503	CLA	C15-C16-C17-C18
29	C	507	CLA	C15-C16-C17-C18
29	G	611	CLA	C10-C11-C12-C13
29	R	610	CLA	C5-C6-C7-C8
29	S	613	CLA	C5-C6-C7-C8
29	b	608	CLA	C10-C11-C12-C13
29	b	608	CLA	C13-C15-C16-C17
29	g	611	CLA	C10-C11-C12-C13
29	s	609	CLA	C10-C11-C12-C13
45	G	607	CHL	C15-C16-C17-C18
40	L	101	LHG	O1-C1-C2-O2
40	g	624	LHG	O1-C1-C2-O2
33	M	101	SQD	C7-C8-C9-C10
33	m	101	SQD	C7-C8-C9-C10
35	H	102	LMG	C28-C29-C30-C31
35	c	521	LMG	C28-C29-C30-C31
37	C	518	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
40	D	409	LHG	C7-C8-C9-C10
40	D	410	LHG	C23-C24-C25-C26
40	N	624	LHG	C7-C8-C9-C10
40	d	408	LHG	C7-C8-C9-C10
40	d	410	LHG	C23-C24-C25-C26
40	d	409	LHG	C7-C8-C9-C10
51	y	626	PTY	C8-C11-C12-C13
29	C	508	CLA	C5-C6-C7-C8
29	G	603	CLA	C5-C6-C7-C8
29	Y	611	CLA	C5-C6-C7-C8
29	Y	614	CLA	C8-C10-C11-C12
29	s	611	CLA	C15-C16-C17-C18
45	S	608	CHL	C5-C6-C7-C8
29	s	609	CLA	CBA-CGA-O2A-C1
29	C	509	CLA	C2-C1-O2A-CGA
29	B	608	CLA	C5-C6-C7-C8
29	C	503	CLA	C5-C6-C7-C8
29	Y	602	CLA	C15-C16-C17-C18
29	d	403	CLA	C10-C11-C12-C13
40	N	624	LHG	C23-C24-C25-C26
40	S	624	LHG	C23-C24-C25-C26
40	d	410	LHG	C7-C8-C9-C10
40	n	624	LHG	C7-C8-C9-C10
29	r	608	CLA	CBD-CGD-O2D-CED
45	S	606	CHL	C2A-CAA-CBA-CGA
40	S	624	LHG	C30-C31-C32-C33
43	F	101	HEM	C3D-CAD-CBD-CGD
29	B	604	CLA	C15-C16-C17-C18
29	B	606	CLA	C5-C6-C7-C8
29	N	613	CLA	C8-C10-C11-C12
29	Y	614	CLA	C5-C6-C7-C8
29	g	602	CLA	C13-C15-C16-C17
29	S	603	CLA	C11-C12-C13-C15
29	Y	603	CLA	C6-C7-C8-C10
29	b	614	CLA	C11-C10-C8-C7
29	n	602	CLA	C12-C13-C15-C16
29	n	610	CLA	C6-C7-C8-C10
29	n	610	CLA	C11-C12-C13-C15
29	r	609	CLA	C6-C7-C8-C10
29	y	614	CLA	C6-C7-C8-C10
45	Y	606	CHL	C12-C13-C15-C16
45	n	605	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
45	g	609	CHL	C12-C13-C15-C16
45	y	601	CHL	C12-C13-C15-C16
29	S	610	CLA	O1A-CGA-O2A-C1
29	r	604	CLA	O1A-CGA-O2A-C1
33	m	101	SQD	O10-C23-O48-C46
37	C	520	DGD	O1A-C1A-O1G-C1G
31	c	515	BCR	C19-C20-C21-C22
44	h	101	RRX	C19-C20-C21-C22
46	N	621	LUT	C29-C30-C31-C32
46	n	621	LUT	C29-C30-C31-C32
29	n	612	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	C2A-CAA-CBA-CGA
29	s	603	CLA	C2A-CAA-CBA-CGA
45	N	605	CHL	C2A-CAA-CBA-CGA
29	N	614	CLA	O1D-CGD-O2D-CED
29	y	603	CLA	O1D-CGD-O2D-CED
29	C	508	CLA	C15-C16-C17-C18
29	G	602	CLA	C8-C10-C11-C12
29	G	611	CLA	C13-C15-C16-C17
29	Y	610	CLA	C5-C6-C7-C8
29	b	610	CLA	C13-C15-C16-C17
29	b	610	CLA	C15-C16-C17-C18
29	b	617	CLA	C13-C15-C16-C17
29	c	503	CLA	C5-C6-C7-C8
29	g	602	CLA	C8-C10-C11-C12
29	r	608	CLA	C10-C11-C12-C13
33	M	101	SQD	O10-C23-O48-C46
29	G	611	CLA	CBD-CGD-O2D-CED
29	c	507	CLA	CBD-CGD-O2D-CED
33	M	101	SQD	O5-C1-O6-C44
37	B	623	DGD	O6D-C1D-O3G-C3G
29	B	608	CLA	C13-C15-C16-C17
29	y	612	CLA	C13-C15-C16-C17
45	Y	606	CHL	C15-C16-C17-C18
29	c	501	CLA	O1D-CGD-O2D-CED
29	s	617	CLA	O1D-CGD-O2D-CED
35	B	622	LMG	C28-C29-C30-C31
31	C	516	BCR	C10-C11-C12-C13
31	c	516	BCR	C10-C11-C12-C13
47	y	623	NEX	C10-C11-C12-C13
40	c	525	LHG	O2-C2-C3-O3
40	d	408	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
40	g	624	LHG	O2-C2-C3-O3
40	l	101	LHG	C5-C6-O8-C23
29	s	611	CLA	C10-C11-C12-C13
45	N	601	CHL	C13-C15-C16-C17
45	Y	607	CHL	C5-C6-C7-C8
29	b	617	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C2A-C1A-O1G-C1G
29	Y	612	CLA	O1A-CGA-O2A-C1
37	c	518	DGD	C1B-C2B-C3B-C4B
38	s	626	3PH	C21-C22-C23-C24
29	B	612	CLA	C13-C15-C16-C17
29	C	510	CLA	C15-C16-C17-C18
29	S	611	CLA	C5-C6-C7-C8
29	S	611	CLA	C8-C10-C11-C12
29	Y	612	CLA	C15-C16-C17-C18
29	Y	613	CLA	C5-C6-C7-C8
29	b	602	CLA	C13-C15-C16-C17
29	b	612	CLA	C13-C15-C16-C17
29	c	510	CLA	C15-C16-C17-C18
29	c	512	CLA	C5-C6-C7-C8
29	g	613	CLA	C13-C15-C16-C17
29	s	611	CLA	C8-C10-C11-C12
45	G	607	CHL	C5-C6-C7-C8
45	n	607	CHL	C15-C16-C17-C18
29	Y	614	CLA	O1D-CGD-O2D-CED
29	b	602	CLA	O1D-CGD-O2D-CED
33	b	621	SQD	C8-C7-O47-C45
33	m	101	SQD	C8-C7-O47-C45
29	B	602	CLA	C13-C15-C16-C17
29	Y	612	CLA	C13-C15-C16-C17
29	Y	613	CLA	C8-C10-C11-C12
29	b	606	CLA	C5-C6-C7-C8
29	b	616	CLA	C13-C15-C16-C17
29	b	617	CLA	C5-C6-C7-C8
29	c	504	CLA	C10-C11-C12-C13
29	c	509	CLA	C15-C16-C17-C18
29	g	603	CLA	C5-C6-C7-C8
29	y	612	CLA	C8-C10-C11-C12
45	s	608	CHL	C8-C10-C11-C12
45	y	607	CHL	C5-C6-C7-C8
40	C	525	LHG	C4-O6-P-O3
40	D	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
40	L	101	LHG	C4-O6-P-O3
40	G	624	LHG	C4-O6-P-O3
40	c	525	LHG	C4-O6-P-O3
40	d	409	LHG	C4-O6-P-O3
40	l	101	LHG	C3-O3-P-O6
40	g	624	LHG	C4-O6-P-O3
40	s	624	LHG	C4-O6-P-O3
40	y	624	LHG	C4-O6-P-O3
51	Y	626	PTY	C5-O14-P1-O11
51	Y	627	PTY	C3-O11-P1-O14
51	y	626	PTY	C3-O11-P1-O14
40	d	408	LHG	C23-C24-C25-C26
29	r	602	CLA	C3-C5-C6-C7
33	B	621	SQD	C24-C23-O48-C46
40	d	410	LHG	C24-C23-O8-C6
29	C	507	CLA	CBD-CGD-O2D-CED
29	C	507	CLA	C13-C15-C16-C17
29	N	603	CLA	C8-C10-C11-C12
29	b	603	CLA	C13-C15-C16-C17
45	N	605	CHL	C13-C15-C16-C17
45	g	607	CHL	C5-C6-C7-C8
37	c	520	DGD	C1A-C2A-C3A-C4A
37	C	518	DGD	O6E-C5E-C6E-O5E
33	b	621	SQD	O49-C7-O47-C45
33	m	101	SQD	O49-C7-O47-C45
39	C	524	DGA	OB1-CB1-OG2-CG2
40	N	624	LHG	O9-C7-O7-C5
29	B	617	CLA	C4-C3-C5-C6
29	b	604	CLA	C4-C3-C5-C6
29	s	610	CLA	C4-C3-C5-C6
45	G	609	CHL	C4-C3-C5-C6
29	a	410	CLA	C2-C3-C5-C6
29	Y	612	CLA	C8-C10-C11-C12
29	c	511	CLA	C8-C10-C11-C12
29	n	604	CLA	C13-C15-C16-C17
29	N	603	CLA	O1D-CGD-O2D-CED
29	C	507	CLA	C2A-CAA-CBA-CGA
29	R	608	CLA	C2A-CAA-CBA-CGA
29	S	602	CLA	C2A-CAA-CBA-CGA
29	S	614	CLA	C2A-CAA-CBA-CGA
29	r	604	CLA	C2A-CAA-CBA-CGA
29	s	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
45	Y	606	CHL	C2A-CAA-CBA-CGA
45	y	606	CHL	C2A-CAA-CBA-CGA
29	C	501	CLA	C16-C17-C18-C19
29	Y	613	CLA	C16-C17-C18-C20
37	c	518	DGD	C4E-C5E-C6E-O5E
29	b	602	CLA	CBA-CGA-O2A-C1
29	s	603	CLA	CBA-CGA-O2A-C1
29	s	610	CLA	CBA-CGA-O2A-C1
37	B	623	DGD	C2A-C1A-O1G-C1G
38	S	626	3PH	C32-C31-O31-C3
31	b	618	BCR	C9-C10-C11-C12
46	Y	621	LUT	C29-C30-C31-C32
46	y	621	LUT	C29-C30-C31-C32
38	t	101	3PH	C39-C3A-C3B-C3C
40	L	101	LHG	C9-C10-C11-C12
40	L	101	LHG	C33-C34-C35-C36
33	b	626	SQD	C8-C7-O47-C45
51	y	626	PTY	C11-C8-O7-C6
31	C	515	BCR	C11-C10-C9-C34
47	N	623	NEX	C39-C29-C30-C31
47	R	622	NEX	C39-C29-C30-C31
47	Y	623	NEX	C11-C10-C9-C19
47	Y	623	NEX	C39-C29-C30-C31
47	n	623	NEX	C39-C29-C30-C31
47	g	623	NEX	C11-C10-C9-C19
47	y	623	NEX	C11-C10-C9-C19
33	B	626	SQD	C12-C13-C14-C15
35	c	523	LMG	C29-C30-C31-C32
38	s	626	3PH	C24-C25-C26-C27
39	C	524	DGA	CCA-CDA-CEA-CFA
40	d	408	LHG	C25-C26-C27-C28
40	y	624	LHG	C28-C29-C30-C31
29	d	403	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C19
29	d	402	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C20
29	r	610	CLA	C11-C12-C13-C15
29	B	613	CLA	CBA-CGA-O2A-C1
33	c	526	SQD	C17-C18-C19-C20
34	Y	625	SPH	C14-C15-C16-C17
38	b	624	3PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
38	t	101	3PH	C32-C33-C34-C35
40	L	101	LHG	C11-C12-C13-C14
40	Y	624	LHG	C26-C27-C28-C29
40	c	525	LHG	C13-C14-C15-C16
40	l	101	LHG	C28-C29-C30-C31
40	n	624	LHG	C24-C25-C26-C27
40	s	624	LHG	C12-C13-C14-C15
35	B	622	LMG	C9-C8-O7-C10
33	M	101	SQD	O49-C7-O47-C45
33	b	626	SQD	O49-C7-O47-C45
51	y	626	PTY	O10-C8-O7-C6
29	a	406	CLA	C2C-C3C-CAC-CBC
37	C	519	DGD	C4B-C5B-C6B-C7B
38	s	626	3PH	C2A-C2B-C2C-C2D
39	j	101	DGA	CB6-CB7-CB8-CB9
40	y	624	LHG	C13-C14-C15-C16
37	c	519	DGD	C5A-C6A-C7A-C8A
38	B	624	3PH	C24-C25-C26-C27
38	B	624	3PH	C26-C27-C28-C29
38	T	101	3PH	C38-C39-C3A-C3B
38	b	624	3PH	C24-C25-C26-C27
40	C	525	LHG	C25-C26-C27-C28
40	c	525	LHG	C11-C12-C13-C14
40	n	624	LHG	C11-C12-C13-C14
40	g	624	LHG	C11-C12-C13-C14
29	b	609	CLA	C13-C15-C16-C17
29	c	505	CLA	C13-C15-C16-C17
29	s	603	CLA	C15-C16-C17-C18
43	f	101	HEM	C3D-CAD-CBD-CGD
39	B	625	DGA	CB5-CB6-CB7-CB8
40	D	409	LHG	C13-C14-C15-C16
40	N	624	LHG	C33-C34-C35-C36
40	s	624	LHG	C13-C14-C15-C16
45	S	608	CHL	C3-C5-C6-C7
40	L	101	LHG	C23-C24-C25-C26
29	r	604	CLA	O1D-CGD-O2D-CED
31	C	515	BCR	C11-C10-C9-C8
33	M	101	SQD	C2-C1-O6-C44
37	B	623	DGD	C2D-C1D-O3G-C3G
37	b	623	DGD	C2D-C1D-O3G-C3G
47	N	623	NEX	C28-C29-C30-C31
47	R	622	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
47	Y	623	NEX	C11-C10-C9-C8
47	Y	623	NEX	C28-C29-C30-C31
47	n	623	NEX	C28-C29-C30-C31
47	g	623	NEX	C11-C10-C9-C8
47	r	622	NEX	C28-C29-C30-C31
47	y	623	NEX	C11-C10-C9-C8
33	a	412	SQD	O47-C45-C46-O48
29	b	615	CLA	CBA-CGA-O2A-C1
38	s	626	3PH	C22-C23-C24-C25
39	c	524	DGA	CB4-CB5-CB6-CB7
40	D	410	LHG	C9-C10-C11-C12
40	Y	624	LHG	C33-C34-C35-C36
40	g	624	LHG	C9-C10-C11-C12
40	g	624	LHG	C13-C14-C15-C16
29	b	602	CLA	O1A-CGA-O2A-C1
29	s	609	CLA	O1A-CGA-O2A-C1
37	B	623	DGD	O1A-C1A-O1G-C1G
29	B	613	CLA	C16-C17-C18-C20
29	D	402	CLA	C16-C17-C18-C20
29	R	608	CLA	C11-C12-C13-C15
29	c	501	CLA	C16-C17-C18-C20
29	s	604	CLA	C6-C7-C8-C9
29	y	614	CLA	C16-C17-C18-C19
29	N	612	CLA	O1D-CGD-O2D-CED
29	N	603	CLA	C4-C3-C5-C6
29	G	613	CLA	C4-C3-C5-C6
34	Y	625	SPH	C11-C10-C9-C8
35	h	102	LMG	C12-C13-C14-C15
37	c	519	DGD	C4B-C5B-C6B-C7B
38	B	624	3PH	C29-C2A-C2B-C2C
38	B	624	3PH	C3C-C3D-C3E-C3F
40	Y	624	LHG	C11-C10-C9-C8
40	d	408	LHG	C11-C12-C13-C14
40	n	624	LHG	C14-C15-C16-C17
40	y	624	LHG	C11-C12-C13-C14
29	C	507	CLA	C2-C3-C5-C6
29	B	605	CLA	C11-C10-C8-C9
29	B	605	CLA	C11-C12-C13-C14
29	N	610	CLA	C6-C7-C8-C9
29	c	507	CLA	C6-C7-C8-C9
29	n	613	CLA	C14-C13-C15-C16
29	r	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
45	s	606	CHL	C2A-CAA-CBA-CGA
33	b	621	SQD	C25-C26-C27-C28
35	B	622	LMG	C15-C16-C17-C18
35	a	413	LMG	C39-C40-C41-C42
39	C	524	DGA	CA5-CA6-CA7-CA8
39	C	524	DGA	CA8-CA9-CAA-CBA
40	l	101	LHG	C26-C27-C28-C29
51	Y	626	PTY	C39-C40-C41-C42
29	R	608	CLA	C5-C6-C7-C8
29	g	613	CLA	C2A-CAA-CBA-CGA
29	s	604	CLA	C2A-CAA-CBA-CGA
45	n	605	CHL	C2A-CAA-CBA-CGA
31	B	619	BCR	C36-C18-C19-C20
31	C	516	BCR	C37-C22-C23-C24
31	c	516	BCR	C37-C22-C23-C24
36	b	620	C7Z	C7-C8-C9-C19
44	H	101	RRX	C7-C8-C9-C34
46	r	620	LUT	C7-C8-C9-C19
29	S	613	CLA	C4C-C3C-CAC-CBC
38	t	101	3PH	C2A-C2B-C2C-C2D
51	Y	626	PTY	C40-C41-C42-C43
40	D	408	LHG	O1-C1-C2-C3
40	D	409	LHG	O1-C1-C2-C3
40	G	624	LHG	O1-C1-C2-C3
40	S	624	LHG	O1-C1-C2-C3
40	Y	624	LHG	O1-C1-C2-C3
40	c	525	LHG	O1-C1-C2-C3
40	d	410	LHG	O1-C1-C2-C3
40	d	409	LHG	O1-C1-C2-C3
40	g	624	LHG	O1-C1-C2-C3
40	y	624	LHG	O1-C1-C2-C3
31	A	411	BCR	C17-C18-C19-C20
31	B	619	BCR	C11-C12-C13-C14
31	C	516	BCR	C21-C22-C23-C24
31	D	404	BCR	C11-C12-C13-C14
36	b	620	C7Z	C7-C8-C9-C10
44	H	101	RRX	C7-C8-C9-C10
44	h	101	RRX	C11-C12-C13-C14
46	r	620	LUT	C7-C8-C9-C10
29	C	512	CLA	C3-C5-C6-C7
29	s	604	CLA	O1D-CGD-O2D-CED
35	A	413	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	M	101	SQD	C8-C7-O47-C45
35	A	413	LMG	C11-C10-O7-C8
35	c	521	LMG	C11-C10-O7-C8
35	B	622	LMG	C11-C12-C13-C14
35	C	523	LMG	C18-C19-C20-C21
37	c	519	DGD	C7A-C8A-C9A-CAA
39	J	101	DGA	CB3-CB4-CB5-CB6
40	y	624	LHG	C29-C30-C31-C32
49	r	625	LMT	C11-C10-C9-C8
51	y	626	PTY	C31-C32-C33-C34
29	s	609	CLA	CBD-CGD-O2D-CED
35	h	102	LMG	C28-C29-C30-C31
39	B	625	DGA	CB1-CB2-CB3-CB4
29	g	613	CLA	O1D-CGD-O2D-CED
38	T	101	3PH	C22-C23-C24-C25
39	J	101	DGA	CA6-CA7-CA8-CA9
40	G	624	LHG	C24-C25-C26-C27
40	Y	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C16-C17-C18-C19
40	y	624	LHG	C31-C32-C33-C34
29	C	509	CLA	C16-C17-C18-C19
29	C	509	CLA	C16-C17-C18-C20
29	R	608	CLA	C11-C12-C13-C14
29	Y	614	CLA	C16-C17-C18-C20
29	a	410	CLA	C11-C12-C13-C14
29	a	410	CLA	C11-C12-C13-C15
29	b	602	CLA	C16-C17-C18-C20
29	c	509	CLA	C16-C17-C18-C19
29	c	509	CLA	C16-C17-C18-C20
29	c	512	CLA	C16-C17-C18-C20
29	d	402	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C20
29	s	604	CLA	C6-C7-C8-C10
30	a	408	PHO	C16-C17-C18-C20
33	a	412	SQD	O5-C1-O6-C44
37	b	623	DGD	O6D-C1D-O3G-C3G
29	B	612	CLA	C15-C16-C17-C18
29	C	512	CLA	C5-C6-C7-C8
29	a	405	CLA	C4C-C3C-CAC-CBC
33	B	621	SQD	C24-C25-C26-C27
33	B	626	SQD	C30-C31-C32-C33
38	B	624	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
38	t	101	3PH	C22-C23-C24-C25
38	t	101	3PH	C38-C39-C3A-C3B
40	D	408	LHG	C28-C29-C30-C31
40	N	624	LHG	C25-C26-C27-C28
40	G	624	LHG	C13-C14-C15-C16
40	c	525	LHG	C33-C34-C35-C36
40	d	409	LHG	C13-C14-C15-C16
40	l	101	LHG	C34-C35-C36-C37
40	g	624	LHG	C11-C10-C9-C8
51	Y	626	PTY	C36-C37-C38-C39
29	S	611	CLA	O1D-CGD-O2D-CED
35	b	622	LMG	C11-C12-C13-C14
38	t	101	3PH	C36-C37-C38-C39
39	B	625	DGA	CA4-CA5-CA6-CA7
39	C	524	DGA	CA6-CA7-CA8-CA9
39	J	101	DGA	CB5-CB6-CB7-CB8
40	s	624	LHG	C31-C32-C33-C34
35	C	523	LMG	C10-C11-C12-C13
29	Y	613	CLA	C10-C11-C12-C13
38	S	626	3PH	O32-C31-O31-C3
33	a	412	SQD	C10-C11-C12-C13
39	B	625	DGA	CB9-CAB-CBB-CCB
40	D	408	LHG	C24-C25-C26-C27
29	C	511	CLA	O1D-CGD-O2D-CED
29	d	403	CLA	C3-C5-C6-C7
29	r	603	CLA	C3-C5-C6-C7
33	b	621	SQD	C24-C23-O48-C46
40	d	409	LHG	C34-C35-C36-C37
29	N	603	CLA	C3A-C2A-CAA-CBA
29	G	614	CLA	C3A-C2A-CAA-CBA
29	R	612	CLA	C3A-C2A-CAA-CBA
29	S	605	CLA	C3A-C2A-CAA-CBA
29	S	614	CLA	C3A-C2A-CAA-CBA
29	Y	608	CLA	C3A-C2A-CAA-CBA
29	b	605	CLA	C3A-C2A-CAA-CBA
29	c	513	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C3A-C2A-CAA-CBA
29	g	603	CLA	C3A-C2A-CAA-CBA
29	r	609	CLA	C3A-C2A-CAA-CBA
29	r	612	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C3A-C2A-CAA-CBA
29	y	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	a	408	PHO	C3A-C2A-CAA-CBA
45	G	606	CHL	C3A-C2A-CAA-CBA
45	g	605	CHL	C3A-C2A-CAA-CBA
45	y	601	CHL	C3A-C2A-CAA-CBA
29	B	604	CLA	C10-C11-C12-C13
29	b	604	CLA	C15-C16-C17-C18
35	C	527	LMG	C14-C15-C16-C17
35	H	102	LMG	C13-C14-C15-C16
37	b	623	DGD	C3A-C4A-C5A-C6A
38	s	626	3PH	C2D-C2E-C2F-C2G
39	c	524	DGA	CB2-CB3-CB4-CB5
40	D	409	LHG	C10-C11-C12-C13
40	c	525	LHG	C27-C28-C29-C30
40	l	101	LHG	C14-C15-C16-C17
40	n	624	LHG	C13-C14-C15-C16
40	s	624	LHG	C30-C31-C32-C33
29	b	617	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	O1A-C1A-O1G-C1G
29	C	501	CLA	C16-C17-C18-C20
29	D	403	CLA	C11-C12-C13-C15
29	c	512	CLA	C16-C17-C18-C19
29	g	613	CLA	C16-C17-C18-C19
33	m	101	SQD	C11-C10-C9-C8
38	T	101	3PH	C28-C29-C2A-C2B
39	B	625	DGA	CB3-CB4-CB5-CB6
29	s	603	CLA	O1D-CGD-O2D-CED
35	c	523	LMG	O1-C7-C8-C9
35	d	411	LMG	C30-C31-C32-C33
39	j	101	DGA	CA4-CA5-CA6-CA7
40	d	409	LHG	C11-C12-C13-C14
51	Y	626	PTY	C15-C16-C17-C18
29	r	612	CLA	O2A-C1-C2-C3
47	R	622	NEX	C14-C15-C35-C34
29	A	406	CLA	C3-C5-C6-C7
45	G	601	CHL	C3-C5-C6-C7
49	r	625	LMT	C1-C2-C3-C4
45	r	607	CHL	C2C-C3C-CAC-CBC
33	B	621	SQD	O10-C23-O48-C46
29	c	510	CLA	C13-C15-C16-C17
29	y	603	CLA	C15-C16-C17-C18
29	c	504	CLA	C4-C3-C5-C6
29	B	615	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	N	603	CLA	C2-C3-C5-C6
29	G	613	CLA	C2-C3-C5-C6
29	Y	604	CLA	C2-C3-C5-C6
42	d	405	PL9	C13-C14-C16-C17
45	y	607	CHL	C2-C3-C5-C6
40	S	624	LHG	C8-C7-O7-C5
40	Y	624	LHG	C8-C7-O7-C5
40	y	624	LHG	C8-C7-O7-C5
35	C	527	LMG	C8-C9-O8-C28
40	C	525	LHG	O1-C1-C2-O2
40	D	409	LHG	O1-C1-C2-O2
40	d	408	LHG	O1-C1-C2-O2
40	d	410	LHG	O1-C1-C2-O2
40	l	101	LHG	O1-C1-C2-O2
40	y	624	LHG	O1-C1-C2-O2
35	c	521	LMG	C29-C30-C31-C32
38	s	626	3PH	C25-C26-C27-C28
40	d	408	LHG	C13-C14-C15-C16
49	r	625	LMT	C3-C4-C5-C6
29	s	610	CLA	O1A-CGA-O2A-C1
33	A	412	SQD	C7-C8-C9-C10
33	c	526	SQD	C23-C24-C25-C26
40	D	410	LHG	C7-C8-C9-C10
29	b	612	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C19
29	y	614	CLA	C16-C17-C18-C20
45	Y	606	CHL	C16-C17-C18-C19
34	a	414	SPH	C6-C7-C8-C9
40	n	624	LHG	O2-C2-C3-O3
45	n	601	CHL	C15-C16-C17-C18
38	B	624	3PH	C25-C26-C27-C28
38	t	101	3PH	C23-C24-C25-C26
39	c	524	DGA	CCB-CDB-CEB-CFB
40	d	409	LHG	C25-C26-C27-C28
40	g	624	LHG	C24-C25-C26-C27
40	y	624	LHG	C11-C10-C9-C8
51	y	626	PTY	C24-C25-C26-C27
29	s	603	CLA	O1A-CGA-O2A-C1
40	G	624	LHG	C23-C24-C25-C26
40	g	624	LHG	C23-C24-C25-C26
29	B	611	CLA	CBD-CGD-O2D-CED
35	c	521	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
40	Y	624	LHG	O9-C7-O7-C5
40	y	624	LHG	O9-C7-O7-C5
29	N	603	CLA	C2-C1-O2A-CGA
29	Y	608	CLA	C2-C1-O2A-CGA
29	b	602	CLA	C2-C1-O2A-CGA
29	s	611	CLA	C2-C1-O2A-CGA
37	c	518	DGD	C2B-C3B-C4B-C5B
38	T	101	3PH	C2D-C2E-C2F-C2G
40	G	624	LHG	C31-C32-C33-C34
40	y	624	LHG	C9-C10-C11-C12
29	C	512	CLA	C13-C15-C16-C17
29	g	603	CLA	C15-C16-C17-C18
29	B	613	CLA	O1A-CGA-O2A-C1
29	b	615	CLA	O1A-CGA-O2A-C1
40	d	410	LHG	O10-C23-O8-C6
29	B	602	CLA	C16-C17-C18-C20
29	r	610	CLA	C11-C12-C13-C14
31	A	411	BCR	C23-C24-C25-C26
31	A	411	BCR	C23-C24-C25-C30
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	C	515	BCR	C23-C24-C25-C26
31	C	516	BCR	C1-C6-C7-C8
31	D	404	BCR	C5-C6-C7-C8
31	D	404	BCR	C23-C24-C25-C26
31	D	404	BCR	C23-C24-C25-C30
31	a	411	BCR	C23-C24-C25-C26
31	a	411	BCR	C23-C24-C25-C30
31	b	618	BCR	C1-C6-C7-C8
31	b	618	BCR	C5-C6-C7-C8
31	c	516	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	d	404	BCR	C1-C6-C7-C8
31	d	404	BCR	C5-C6-C7-C8
36	B	620	C7Z	C1-C6-C7-C8
36	B	620	C7Z	C25-C26-C27-C28
36	b	620	C7Z	C5-C6-C7-C8
36	b	620	C7Z	C25-C26-C27-C28
44	H	101	RRX	C5-C6-C7-C8
40	D	409	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
51	y	626	PTY	C19-C20-C21-C22
29	b	616	CLA	O1D-CGD-O2D-CED
29	B	616	CLA	C8-C10-C11-C12
38	t	101	3PH	C2E-C2F-C2G-C2H
40	d	409	LHG	C23-C24-C25-C26
40	g	624	LHG	C7-C8-C9-C10
40	S	624	LHG	C26-C27-C28-C29
29	C	510	CLA	C13-C15-C16-C17
29	C	513	CLA	C15-C16-C17-C18
49	r	625	LMT	C5-C6-C7-C8
29	A	410	CLA	C4-C3-C5-C6
29	y	604	CLA	C4-C3-C5-C6
42	D	405	PL9	C15-C14-C16-C17
45	y	607	CHL	C4-C3-C5-C6
29	B	614	CLA	O1D-CGD-O2D-CED
29	B	602	CLA	C11-C10-C8-C7
29	B	603	CLA	C12-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C10
29	B	605	CLA	C11-C12-C13-C15
29	B	609	CLA	C11-C12-C13-C15
29	B	610	CLA	C11-C12-C13-C15
29	B	614	CLA	C11-C12-C13-C15
29	C	511	CLA	C6-C7-C8-C10
29	N	610	CLA	C6-C7-C8-C10
29	N	613	CLA	C11-C12-C13-C15
29	Y	604	CLA	C11-C10-C8-C7
29	Y	613	CLA	C6-C7-C8-C10
29	c	505	CLA	C2-C3-C5-C6
29	c	507	CLA	C6-C7-C8-C10
29	c	510	CLA	C12-C13-C15-C16
29	d	403	CLA	C11-C12-C13-C15
29	n	604	CLA	C12-C13-C15-C16
29	n	610	CLA	C12-C13-C15-C16
29	n	613	CLA	C12-C13-C15-C16
29	g	603	CLA	C6-C7-C8-C10
29	s	603	CLA	C11-C10-C8-C7
29	y	604	CLA	C2-C3-C5-C6
29	y	611	CLA	C12-C13-C15-C16
45	Y	607	CHL	C6-C7-C8-C10
45	n	609	CHL	C12-C13-C15-C16
45	g	607	CHL	C12-C13-C15-C16
45	y	609	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	B	615	CLA	O1A-CGA-O2A-C1
33	b	621	SQD	O10-C23-O48-C46
29	s	603	CLA	C2C-C3C-CAC-CBC
38	T	101	3PH	C2E-C2F-C2G-C2H
38	b	624	3PH	C28-C29-C2A-C2B
29	S	611	CLA	C10-C11-C12-C13
45	n	607	CHL	C8-C10-C11-C12
31	C	517	BCR	C9-C10-C11-C12
31	c	515	BCR	C9-C10-C11-C12
46	g	621	LUT	C29-C30-C31-C32
29	G	602	CLA	C16-C17-C18-C20
33	B	621	SQD	O49-C7-O47-C45
38	B	624	3PH	O22-C21-O21-C2
40	g	624	LHG	O9-C7-O7-C5
29	c	506	CLA	CBA-CGA-O2A-C1
38	B	624	3PH	C32-C31-O31-C3
39	J	101	DGA	CA2-CA1-OG1-CG1
34	A	414	SPH	C6-C7-C8-C9
29	N	613	CLA	C2A-CAA-CBA-CGA
29	S	613	CLA	C2A-CAA-CBA-CGA
45	R	607	CHL	C2A-CAA-CBA-CGA
45	r	607	CHL	C2A-CAA-CBA-CGA
45	y	607	CHL	C2A-CAA-CBA-CGA
29	b	612	CLA	C10-C11-C12-C13
29	c	505	CLA	C10-C11-C12-C13
29	s	609	CLA	C8-C10-C11-C12
34	Y	625	SPH	C6-C7-C8-C9
40	L	101	LHG	C17-C18-C19-C20
40	d	408	LHG	C28-C29-C30-C31
40	c	497	LHG	C7-C8-C9-C10
29	B	617	CLA	O1D-CGD-O2D-CED
33	M	101	SQD	C10-C11-C12-C13
33	M	101	SQD	C27-C28-C29-C30
34	a	414	SPH	C12-C13-C14-C15
38	t	101	3PH	C2D-C2E-C2F-C2G
39	b	625	DGA	CBB-CCB-CDB-CEB
40	n	624	LHG	C25-C26-C27-C28
38	T	101	3PH	C37-C38-C39-C3A
40	l	101	LHG	C13-C14-C15-C16
40	g	624	LHG	C31-C32-C33-C34
37	c	519	DGD	O6E-C5E-C6E-O5E
29	S	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	C	503	CLA	C16-C17-C18-C20
29	b	611	CLA	C16-C17-C18-C20
29	s	602	CLA	C11-C12-C13-C14
29	g	603	CLA	C13-C15-C16-C17
33	a	412	SQD	C11-C12-C13-C14
38	t	101	3PH	C37-C38-C39-C3A
39	b	625	DGA	CBB-CAB-CB9-CB8
40	c	525	LHG	C34-C35-C36-C37
40	d	408	LHG	C24-C25-C26-C27
35	c	523	LMG	C10-C11-C12-C13
33	A	412	SQD	C8-C7-O47-C45
33	B	621	SQD	C8-C7-O47-C45
33	c	526	SQD	C8-C7-O47-C45
35	C	521	LMG	C11-C10-O7-C8
35	C	523	LMG	C11-C10-O7-C8
35	a	413	LMG	C11-C10-O7-C8
38	B	624	3PH	C22-C21-O21-C2
40	C	525	LHG	C8-C7-O7-C5
40	G	624	LHG	C8-C7-O7-C5
40	g	624	LHG	C8-C7-O7-C5
40	s	624	LHG	C8-C7-O7-C5
35	A	413	LMG	C16-C17-C18-C19
29	b	612	CLA	C15-C16-C17-C18
29	c	512	CLA	C13-C15-C16-C17
29	R	610	CLA	CBD-CGD-O2D-CED
35	w	201	LMG	C36-C37-C38-C39
38	t	101	3PH	C27-C28-C29-C2A
40	d	410	LHG	C33-C34-C35-C36
50	s	625	LPX	O1-C3-C4-O5
35	C	521	LMG	O9-C10-O7-C8
35	C	523	LMG	O9-C10-O7-C8
35	a	413	LMG	O9-C10-O7-C8
40	C	525	LHG	O9-C7-O7-C5
40	G	624	LHG	O9-C7-O7-C5
40	G	624	LHG	C7-C8-C9-C10
40	Y	624	LHG	C7-C8-C9-C10
39	B	625	DGA	CA3-CA4-CA5-CA6
40	l	101	LHG	C33-C34-C35-C36
49	r	625	LMT	C4-C5-C6-C7
33	c	526	SQD	C2-C1-O6-C44
35	B	622	LMG	C2-C1-O1-C7
40	c	497	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
40	s	624	LHG	C28-C29-C30-C31
29	B	613	CLA	C16-C17-C18-C19
29	Y	613	CLA	C16-C17-C18-C19
33	M	101	SQD	C12-C13-C14-C15
33	b	626	SQD	C10-C11-C12-C13
35	D	411	LMG	O6-C5-C6-O5
49	R	625	LMT	O5'-C5'-C6'-O6'
49	r	625	LMT	O5'-C5'-C6'-O6'
45	Y	606	CHL	C10-C11-C12-C13
29	C	512	CLA	C4-C3-C5-C6
29	Y	604	CLA	C4-C3-C5-C6
42	d	405	PL9	C15-C14-C16-C17
45	N	601	CHL	C4-C3-C5-C6
37	c	519	DGD	C1B-C2B-C3B-C4B
51	y	626	PTY	C30-C31-C32-C33
29	B	617	CLA	C2-C3-C5-C6
29	b	604	CLA	C2-C3-C5-C6
29	c	504	CLA	C2-C3-C5-C6
29	n	610	CLA	C2-C3-C5-C6
29	s	610	CLA	C2-C3-C5-C6
45	G	609	CHL	C2-C3-C5-C6
29	B	609	CLA	C11-C12-C13-C14
29	B	610	CLA	C11-C12-C13-C14
29	C	510	CLA	C14-C13-C15-C16
29	C	511	CLA	C6-C7-C8-C9
29	C	513	CLA	C11-C12-C13-C14
29	N	604	CLA	C6-C7-C8-C9
29	G	602	CLA	C6-C7-C8-C9
29	Y	613	CLA	C14-C13-C15-C16
29	c	509	CLA	C14-C13-C15-C16
29	c	510	CLA	C14-C13-C15-C16
29	d	403	CLA	C11-C12-C13-C14
29	n	602	CLA	C14-C13-C15-C16
29	n	610	CLA	C6-C7-C8-C9
29	n	610	CLA	C11-C12-C13-C14
29	g	603	CLA	C6-C7-C8-C9
29	s	603	CLA	C11-C10-C8-C9
29	y	611	CLA	C14-C13-C15-C16
29	y	613	CLA	C11-C10-C8-C9
45	n	607	CHL	C11-C10-C8-C9
45	g	607	CHL	C14-C13-C15-C16
37	b	623	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
39	c	524	DGA	CAB-CBB-CCB-CDB
29	A	407	CLA	C2A-CAA-CBA-CGA
29	B	615	CLA	C2A-CAA-CBA-CGA
29	s	609	CLA	C2A-CAA-CBA-CGA
45	N	607	CHL	C2A-CAA-CBA-CGA
45	n	607	CHL	C2A-CAA-CBA-CGA
35	C	527	LMG	O6-C5-C6-O5
35	H	102	LMG	O6-C5-C6-O5
29	C	502	CLA	CBA-CGA-O2A-C1
37	C	519	DGD	C1B-C2B-C3B-C4B
29	g	602	CLA	O1D-CGD-O2D-CED
37	c	519	DGD	C9A-CAA-CBA-CCA
38	T	101	3PH	C3A-C3B-C3C-C3D
40	c	497	LHG	C28-C29-C30-C31
40	g	624	LHG	C28-C29-C30-C31
31	c	514	BCR	C17-C18-C19-C20
29	A	410	CLA	C1A-C2A-CAA-CBA
29	B	607	CLA	C1A-C2A-CAA-CBA
29	C	506	CLA	C1A-C2A-CAA-CBA
29	N	603	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C1A-C2A-CAA-CBA
29	G	604	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	C1A-C2A-CAA-CBA
29	G	611	CLA	C1A-C2A-CAA-CBA
29	R	609	CLA	C1A-C2A-CAA-CBA
29	R	610	CLA	C1A-C2A-CAA-CBA
29	R	612	CLA	C1A-C2A-CAA-CBA
29	Y	602	CLA	C1A-C2A-CAA-CBA
29	Y	604	CLA	C1A-C2A-CAA-CBA
29	a	410	CLA	C1A-C2A-CAA-CBA
29	b	602	CLA	C1A-C2A-CAA-CBA
29	b	607	CLA	C1A-C2A-CAA-CBA
29	b	612	CLA	C1A-C2A-CAA-CBA
29	c	501	CLA	C1A-C2A-CAA-CBA
29	c	506	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C1A-C2A-CAA-CBA
29	n	614	CLA	C1A-C2A-CAA-CBA
29	g	603	CLA	C1A-C2A-CAA-CBA
29	g	610	CLA	C1A-C2A-CAA-CBA
29	g	611	CLA	C1A-C2A-CAA-CBA
29	g	614	CLA	C1A-C2A-CAA-CBA
29	r	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	C1A-C2A-CAA-CBA
29	s	610	CLA	C1A-C2A-CAA-CBA
29	s	614	CLA	C1A-C2A-CAA-CBA
29	y	602	CLA	C1A-C2A-CAA-CBA
29	y	603	CLA	C1A-C2A-CAA-CBA
29	y	604	CLA	C1A-C2A-CAA-CBA
35	c	521	LMG	O6-C5-C6-O5
45	G	606	CHL	C1A-C2A-CAA-CBA
45	Y	605	CHL	C1A-C2A-CAA-CBA
45	g	605	CHL	C1A-C2A-CAA-CBA
45	y	601	CHL	C1A-C2A-CAA-CBA
29	B	611	CLA	C16-C17-C18-C20
29	D	402	CLA	C16-C17-C18-C19
29	D	403	CLA	C11-C12-C13-C14
29	S	609	CLA	C11-C12-C13-C15
29	b	611	CLA	C16-C17-C18-C19
29	b	612	CLA	C16-C17-C18-C19
29	s	602	CLA	C11-C12-C13-C15
29	s	613	CLA	C6-C7-C8-C9
30	A	408	PHO	C16-C17-C18-C20
33	c	526	SQD	O49-C7-O47-C45
40	S	624	LHG	O9-C7-O7-C5
35	c	523	LMG	C21-C22-C23-C24
38	t	101	3PH	C29-C2A-C2B-C2C
44	h	101	RRX	C15-C16-C17-C18
46	G	621	LUT	C29-C30-C31-C32
29	b	608	CLA	C15-C16-C17-C18
29	b	611	CLA	C15-C16-C17-C18
29	y	614	CLA	C13-C15-C16-C17
40	d	410	LHG	C3-O3-P-O6
40	n	624	LHG	C3-O3-P-O6
50	S	625	LPX	C1-O2-P1-O1
38	T	101	3PH	C31-C32-C33-C34
35	C	521	LMG	O6-C5-C6-O5
40	g	624	LHG	C26-C27-C28-C29
39	J	101	DGA	OA1-CA1-OG1-CG1
45	G	601	CHL	C15-C16-C17-C18
38	b	624	3PH	O11-C1-C2-C3
40	G	624	LHG	O6-C4-C5-C6
37	c	519	DGD	CCB-CDB-CEB-CFB
40	c	525	LHG	C15-C16-C17-C18
29	b	617	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	B	621	SQD	C26-C27-C28-C29
34	a	414	SPH	C7-C8-C9-C10
29	B	611	CLA	C15-C16-C17-C18
29	b	602	CLA	C16-C17-C18-C19
39	B	625	DGA	CA6-CA7-CA8-CA9
29	G	614	CLA	O1D-CGD-O2D-CED
33	m	101	SQD	C26-C27-C28-C29
38	s	626	3PH	C29-C2A-C2B-C2C
35	H	102	LMG	C10-C11-C12-C13
38	B	624	3PH	C21-C22-C23-C24
33	m	101	SQD	C27-C28-C29-C30
35	c	523	LMG	C18-C19-C20-C21
38	B	624	3PH	C2A-C2B-C2C-C2D
29	c	502	CLA	CBA-CGA-O2A-C1
37	C	518	DGD	C2A-C1A-O1G-C1G
29	c	505	CLA	C4-C3-C5-C6
29	C	509	CLA	C10-C11-C12-C13
29	b	616	CLA	C8-C10-C11-C12
29	G	604	CLA	CBD-CGD-O2D-CED
35	h	102	LMG	C36-C37-C38-C39
40	s	624	LHG	C34-C35-C36-C37
38	S	626	3PH	C21-C22-C23-C24
29	n	602	CLA	C2A-CAA-CBA-CGA
30	A	409	PHO	C2A-CAA-CBA-CGA
29	B	602	CLA	C16-C17-C18-C19
29	y	614	CLA	O1D-CGD-O2D-CED
33	M	101	SQD	C44-C45-C46-O48
35	A	413	LMG	O1-C7-C8-C9
35	C	521	LMG	C29-C30-C31-C32
35	C	523	LMG	C7-C8-C9-O8
35	H	102	LMG	C7-C8-C9-O8
38	B	624	3PH	C1-C2-C3-O31
38	T	101	3PH	C1-C2-C3-O31
38	s	626	3PH	C1-C2-C3-O31
39	C	524	DGA	OG1-CG1-CG2-CG3
40	C	525	LHG	C4-C5-C6-O8
40	D	410	LHG	C4-C5-C6-O8
40	G	624	LHG	C4-C5-C6-O8
40	Y	624	LHG	C29-C30-C31-C32
40	c	525	LHG	C4-C5-C6-O8
40	l	101	LHG	C4-C5-C6-O8
51	Y	627	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
29	b	606	CLA	C15-C16-C17-C18
38	B	624	3PH	C2C-C2D-C2E-C2F
40	C	525	LHG	C26-C27-C28-C29
40	l	101	LHG	C31-C32-C33-C34
40	g	624	LHG	C16-C17-C18-C19
35	W	201	LMG	C8-C7-O1-C1
35	w	201	LMG	C8-C7-O1-C1
37	C	519	DGD	C2G-C3G-O3G-C1D
37	C	519	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
30	A	408	PHO	O1D-CGD-O2D-CED
40	G	624	LHG	C9-C10-C11-C12
40	G	624	LHG	C11-C12-C13-C14
29	C	501	CLA	C10-C11-C12-C13
29	c	505	CLA	C5-C6-C7-C8
29	n	603	CLA	C5-C6-C7-C8
29	s	611	CLA	C5-C6-C7-C8
29	b	602	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	O1D-CGD-O2D-CED
37	B	623	DGD	O6E-C5E-C6E-O5E
29	c	506	CLA	O1A-CGA-O2A-C1
39	b	625	DGA	CB3-CB4-CB5-CB6
40	S	624	LHG	C9-C10-C11-C12
29	G	602	CLA	C16-C17-C18-C19
35	C	523	LMG	C16-C17-C18-C19
29	g	603	CLA	CBD-CGD-O2D-CED
35	h	102	LMG	O6-C5-C6-O5
37	C	519	DGD	O6E-C5E-C6E-O5E
40	s	624	LHG	O1-C1-C2-O2
37	C	519	DGD	CCB-CDB-CEB-CFB
51	y	626	PTY	C41-C42-C43-C44
29	N	603	CLA	C13-C15-C16-C17
38	B	624	3PH	O32-C31-O31-C3
35	a	413	LMG	C30-C31-C32-C33
50	S	625	LPX	O5-C4-C5-O6
35	h	102	LMG	C11-C10-O7-C8
40	L	101	LHG	C13-C14-C15-C16
29	y	602	CLA	C8-C10-C11-C12
35	d	411	LMG	O6-C5-C6-O5
47	r	622	NEX	C39-C29-C30-C31
29	s	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	y	614	CLA	C4-C3-C5-C6
45	G	607	CHL	C4-C3-C5-C6
30	a	408	PHO	C16-C17-C18-C19
45	N	605	CHL	C16-C17-C18-C19
29	b	613	CLA	CBA-CGA-O2A-C1
35	w	201	LMG	C29-C28-O8-C9
33	B	621	SQD	C25-C26-C27-C28
29	s	610	CLA	C8-C10-C11-C12
35	a	413	LMG	C15-C16-C17-C18
40	l	101	LHG	C35-C36-C37-C38
35	b	622	LMG	C9-C8-O7-C10
39	B	625	DGA	CG1-CG2-OG2-CB1
39	b	625	DGA	CG1-CG2-OG2-CB1
29	B	614	CLA	C2-C1-O2A-CGA
29	N	611	CLA	C2-C1-O2A-CGA
29	Y	604	CLA	C2-C1-O2A-CGA
29	n	603	CLA	C2-C1-O2A-CGA
45	g	607	CHL	C2-C1-O2A-CGA
40	N	624	LHG	C9-C10-C11-C12
30	a	409	PHO	C3-C5-C6-C7
34	Y	625	SPH	C11-C12-C13-C14
40	G	624	LHG	C35-C36-C37-C38
29	r	608	CLA	O1D-CGD-O2D-CED
45	N	605	CHL	C8-C10-C11-C12
38	T	101	3PH	C1-O11-P-O12
38	b	624	3PH	C1-O11-P-O12
38	t	101	3PH	C1-O11-P-O12
35	H	102	LMG	C36-C37-C38-C39
40	G	624	LHG	C16-C17-C18-C19
29	S	604	CLA	CBA-CGA-O2A-C1
38	s	626	3PH	C32-C31-O31-C3
29	C	502	CLA	O1A-CGA-O2A-C1
40	L	101	LHG	O6-C4-C5-O7
40	d	410	LHG	O6-C4-C5-O7
35	w	201	LMG	O7-C10-C11-C12
29	B	611	CLA	C16-C17-C18-C19
29	C	504	CLA	C6-C7-C8-C10
39	J	101	DGA	CB6-CB7-CB8-CB9
40	g	624	LHG	C35-C36-C37-C38
29	Y	612	CLA	C10-C11-C12-C13
29	b	615	CLA	C10-C11-C12-C13
29	g	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	C	523	LMG	C42-C43-C44-C45
40	Y	624	LHG	C16-C17-C18-C19
29	c	502	CLA	O1A-CGA-O2A-C1
37	C	518	DGD	O1A-C1A-O1G-C1G
37	B	623	DGD	C1A-C2A-C3A-C4A
29	B	608	CLA	C15-C16-C17-C18
29	B	614	CLA	C5-C6-C7-C8
29	c	509	CLA	C10-C11-C12-C13
29	s	611	CLA	C13-C15-C16-C17
37	c	519	DGD	C2E-C1E-O5D-C6D
39	j	101	DGA	CBB-CAB-CB9-CB8
40	Y	624	LHG	C34-C35-C36-C37
40	s	624	LHG	C33-C34-C35-C36
35	H	102	LMG	O7-C10-C11-C12
33	m	101	SQD	O47-C45-C46-O48
35	A	413	LMG	O1-C7-C8-O7
40	y	624	LHG	O7-C5-C6-O8
37	c	520	DGD	CCB-CDB-CEB-CFB
33	A	412	SQD	O49-C7-O47-C45
40	s	624	LHG	O9-C7-O7-C5
29	N	602	CLA	C10-C11-C12-C13
29	n	612	CLA	O1D-CGD-O2D-CED
37	c	518	DGD	C5B-C6B-C7B-C8B
38	b	624	3PH	C22-C23-C24-C25
29	A	410	CLA	C6-C7-C8-C10
29	A	410	CLA	C11-C10-C8-C7
29	B	604	CLA	C11-C12-C13-C15
29	B	610	CLA	C6-C7-C8-C10
29	B	616	CLA	C11-C12-C13-C15
29	C	501	CLA	C12-C13-C15-C16
29	C	509	CLA	C6-C7-C8-C10
29	C	509	CLA	C12-C13-C15-C16
29	C	510	CLA	C6-C7-C8-C10
29	C	510	CLA	C12-C13-C15-C16
29	C	513	CLA	C11-C12-C13-C15
29	D	402	CLA	C11-C12-C13-C15
29	D	403	CLA	C11-C10-C8-C7
29	N	604	CLA	C6-C7-C8-C10
29	N	604	CLA	C11-C12-C13-C15
29	N	610	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	G	602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	G	613	CLA	C12-C13-C15-C16
29	R	610	CLA	C6-C7-C8-C10
29	R	610	CLA	C11-C10-C8-C7
29	S	609	CLA	C11-C10-C8-C7
29	Y	602	CLA	C6-C7-C8-C10
29	Y	613	CLA	C11-C12-C13-C15
29	Y	613	CLA	C12-C13-C15-C16
29	b	607	CLA	C11-C10-C8-C7
29	b	617	CLA	C12-C13-C15-C16
29	c	501	CLA	C12-C13-C15-C16
29	c	503	CLA	C12-C13-C15-C16
29	c	504	CLA	C11-C10-C8-C7
29	c	506	CLA	C6-C7-C8-C10
29	c	507	CLA	C12-C13-C15-C16
29	c	509	CLA	C12-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C10-C8-C7
29	d	402	CLA	C11-C12-C13-C15
29	s	604	CLA	C2-C3-C5-C6
29	y	603	CLA	C6-C7-C8-C10
29	y	603	CLA	C12-C13-C15-C16
29	y	613	CLA	C11-C10-C8-C7
45	N	605	CHL	C11-C12-C13-C15
45	N	607	CHL	C11-C12-C13-C15
45	G	601	CHL	C11-C12-C13-C15
45	G	607	CHL	C2-C3-C5-C6
45	G	609	CHL	C12-C13-C15-C16
45	Y	606	CHL	C6-C7-C8-C10
45	Y	607	CHL	C12-C13-C15-C16
45	Y	609	CHL	C11-C12-C13-C15
45	Y	609	CHL	C12-C13-C15-C16
45	n	601	CHL	C11-C10-C8-C7
45	n	601	CHL	C11-C12-C13-C15
45	n	605	CHL	C11-C10-C8-C7
45	n	607	CHL	C11-C10-C8-C7
45	y	607	CHL	C6-C7-C8-C10
45	y	607	CHL	C12-C13-C15-C16
45	y	609	CHL	C12-C13-C15-C16
29	r	608	CLA	C3-C5-C6-C7
29	A	405	CLA	C14-C13-C15-C16
29	B	602	CLA	C6-C7-C8-C9
29	B	608	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	B	612	CLA	C14-C13-C15-C16
29	B	615	CLA	C6-C7-C8-C9
29	B	616	CLA	C11-C12-C13-C14
29	C	501	CLA	C14-C13-C15-C16
29	C	509	CLA	C14-C13-C15-C16
29	C	510	CLA	C6-C7-C8-C9
29	D	403	CLA	C11-C10-C8-C9
29	N	603	CLA	C6-C7-C8-C9
29	N	610	CLA	C11-C12-C13-C14
29	N	613	CLA	C11-C12-C13-C14
29	G	610	CLA	C11-C10-C8-C9
29	S	603	CLA	C11-C10-C8-C9
29	a	405	CLA	C14-C13-C15-C16
29	a	410	CLA	C11-C10-C8-C9
29	b	602	CLA	C11-C10-C8-C9
29	b	607	CLA	C11-C10-C8-C9
29	b	615	CLA	C6-C7-C8-C9
29	b	616	CLA	C11-C12-C13-C14
29	c	501	CLA	C14-C13-C15-C16
29	c	503	CLA	C11-C12-C13-C14
29	c	503	CLA	C14-C13-C15-C16
29	c	504	CLA	C11-C10-C8-C9
29	c	505	CLA	C14-C13-C15-C16
29	c	507	CLA	C14-C13-C15-C16
29	c	511	CLA	C11-C12-C13-C14
29	c	513	CLA	C6-C7-C8-C9
29	d	402	CLA	C11-C12-C13-C14
29	n	603	CLA	C11-C10-C8-C9
29	n	604	CLA	C6-C7-C8-C9
29	n	610	CLA	C14-C13-C15-C16
29	g	602	CLA	C6-C7-C8-C9
29	g	610	CLA	C11-C10-C8-C9
29	r	603	CLA	C11-C10-C8-C9
29	r	610	CLA	C11-C10-C8-C9
45	N	601	CHL	C11-C10-C8-C9
45	N	607	CHL	C11-C12-C13-C14
45	G	601	CHL	C11-C12-C13-C14
45	Y	606	CHL	C14-C13-C15-C16
45	n	605	CHL	C11-C10-C8-C9
45	n	605	CHL	C11-C12-C13-C14
45	y	609	CHL	C14-C13-C15-C16
31	B	619	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
31	b	619	BCR	C19-C20-C21-C22
29	R	608	CLA	CBD-CGD-O2D-CED
39	c	524	DGA	CDA-CEA-CFA-CGA
29	c	511	CLA	CBA-CGA-O2A-C1
42	d	405	PL9	C47-C48-C49-C50
36	B	620	C7Z	C7-C8-C9-C19
29	S	604	CLA	C6-C7-C8-C9
29	b	613	CLA	C16-C17-C18-C20
29	a	407	CLA	C2C-C3C-CAC-CBC
45	R	607	CHL	C2C-C3C-CAC-CBC
51	Y	626	PTY	C19-C20-C21-C22
31	b	618	BCR	C21-C22-C23-C24
31	b	619	BCR	C17-C18-C19-C20
36	B	620	C7Z	C7-C8-C9-C10
38	s	626	3PH	C35-C36-C37-C38
40	Y	624	LHG	C35-C36-C37-C38
40	d	409	LHG	C26-C27-C28-C29
40	D	408	LHG	C1-C2-C3-O3
29	B	606	CLA	C15-C16-C17-C18
40	c	525	LHG	C8-C7-O7-C5
39	B	625	DGA	CB4-CB5-CB6-CB7
40	N	624	LHG	C30-C31-C32-C33
29	B	606	CLA	CBA-CGA-O2A-C1
40	C	525	LHG	C24-C23-O8-C6
39	C	524	DGA	CB6-CB7-CB8-CB9
40	c	525	LHG	C30-C31-C32-C33
29	C	505	CLA	C5-C6-C7-C8
29	C	508	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
29	n	613	CLA	C13-C15-C16-C17
29	b	605	CLA	C4C-C3C-CAC-CBC
35	c	523	LMG	C13-C14-C15-C16
35	d	411	LMG	C18-C19-C20-C21
38	s	626	3PH	C3B-C3C-C3D-C3E
29	B	607	CLA	CBD-CGD-O2D-CED
37	c	519	DGD	O6E-C1E-O5D-C6D
29	y	612	CLA	C10-C11-C12-C13
38	B	624	3PH	O11-C1-C2-C3
40	D	409	LHG	O6-C4-C5-C6
40	D	410	LHG	O6-C4-C5-C6
40	L	101	LHG	O6-C4-C5-C6
40	c	525	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
40	d	410	LHG	O6-C4-C5-C6
40	l	101	LHG	O6-C4-C5-C6
40	g	624	LHG	O6-C4-C5-C6
51	Y	627	PTY	O14-C5-C6-C1
51	y	627	PTY	O14-C5-C6-C1
33	a	412	SQD	C28-C29-C30-C31
40	D	408	LHG	C7-C8-C9-C10
29	Y	604	CLA	C8-C10-C11-C12
45	N	606	CHL	C8-C10-C11-C12
45	Y	606	CHL	C13-C15-C16-C17
29	C	507	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
29	s	609	CLA	C4-C3-C5-C6
29	s	611	CLA	C4-C3-C5-C6
29	y	613	CLA	C4-C3-C5-C6
42	d	405	PL9	C40-C39-C41-C42
29	y	614	CLA	C2-C3-C5-C6
40	c	525	LHG	O9-C7-O7-C5
29	b	613	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1D-CGD-O2D-CED
45	s	608	CHL	C11-C12-C13-C15
38	S	626	3PH	C24-C25-C26-C27
39	J	101	DGA	CA4-CA5-CA6-CA7
40	L	101	LHG	C34-C35-C36-C37
40	Y	624	LHG	C11-C12-C13-C14
29	c	505	CLA	CBA-CGA-O2A-C1
38	b	624	3PH	C36-C37-C38-C39
39	c	524	DGA	CB7-CB8-CB9-CAB
40	y	624	LHG	C30-C31-C32-C33
30	a	409	PHO	C3A-C2A-CAA-CBA
45	N	601	CHL	C3A-C2A-CAA-CBA
45	G	601	CHL	C3A-C2A-CAA-CBA
45	Y	601	CHL	C3A-C2A-CAA-CBA
45	n	601	CHL	C3A-C2A-CAA-CBA
33	b	626	SQD	C27-C28-C29-C30
31	A	411	BCR	C19-C20-C21-C22
31	a	411	BCR	C19-C20-C21-C22
31	c	517	BCR	C9-C10-C11-C12
44	h	101	RRX	C9-C10-C11-C12
29	c	505	CLA	C8-C10-C11-C12
29	Y	614	CLA	CBA-CGA-O2A-C1
45	n	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	a	412	SQD	C44-C45-C46-O48
33	m	101	SQD	C44-C45-C46-O48
35	w	201	LMG	O1-C7-C8-C9
40	N	624	LHG	C4-C5-C6-O8
40	Y	624	LHG	C4-C5-C6-O8
40	c	497	LHG	C4-C5-C6-O8
40	n	624	LHG	C4-C5-C6-O8
40	g	624	LHG	C4-C5-C6-O8
40	y	624	LHG	C4-C5-C6-O8
51	Y	626	PTY	O4-C1-C6-C5
51	y	626	PTY	O4-C1-C6-C5
51	y	627	PTY	O4-C1-C6-C5
40	S	624	LHG	C31-C32-C33-C34
42	D	405	PL9	C47-C48-C49-C51
29	s	609	CLA	O1D-CGD-O2D-CED
39	c	524	DGA	CA5-CA6-CA7-CA8
29	c	512	CLA	C4-C3-C5-C6
29	Y	603	CLA	C16-C17-C18-C20
40	n	624	LHG	C9-C10-C11-C12
40	n	624	LHG	C28-C29-C30-C31
40	D	408	LHG	C4-O6-P-O3
51	y	627	PTY	C3-O11-P1-O14
35	w	201	LMG	O10-C28-O8-C9
38	s	626	3PH	O32-C31-O31-C3
29	g	603	CLA	C3-C5-C6-C7
29	s	604	CLA	C3-C5-C6-C7
45	S	601	CHL	C2A-CAA-CBA-CGA
40	D	408	LHG	O1-C1-C2-O2
40	Y	624	LHG	O1-C1-C2-O2
29	A	406	CLA	C5-C6-C7-C8
29	G	602	CLA	C15-C16-C17-C18
29	c	503	CLA	C13-C15-C16-C17
40	N	624	LHG	C28-C29-C30-C31
40	Y	624	LHG	C9-C10-C11-C12
40	c	525	LHG	C11-C10-C9-C8
40	c	497	LHG	C25-C26-C27-C28
40	c	525	LHG	O6-C4-C5-O7
40	c	497	LHG	O6-C4-C5-O7
51	Y	627	PTY	O14-C5-C6-O7
29	s	604	CLA	CBA-CGA-O2A-C1
40	N	624	LHG	C16-C17-C18-C19
29	S	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	b	613	CLA	C16-C17-C18-C19
45	N	605	CHL	C16-C17-C18-C20
45	N	607	CHL	C16-C17-C18-C20
45	Y	606	CHL	C16-C17-C18-C20
29	b	602	CLA	C15-C16-C17-C18
35	c	521	LMG	O7-C10-C11-C12
38	t	101	3PH	C25-C26-C27-C28
40	l	101	LHG	C29-C30-C31-C32
29	S	603	CLA	C2C-C3C-CAC-CBC
40	L	101	LHG	C28-C29-C30-C31
38	T	101	3PH	C24-C25-C26-C27
33	C	526	SQD	O6-C44-C45-O47
35	C	527	LMG	O1-C7-C8-O7
35	H	102	LMG	O7-C8-C9-O8
35	c	523	LMG	O1-C7-C8-O7
35	w	201	LMG	O7-C8-C9-O8
39	C	524	DGA	OG1-CG1-CG2-OG2
40	C	525	LHG	O7-C5-C6-O8
40	Y	624	LHG	O7-C5-C6-O8
35	H	102	LMG	C11-C10-O7-C8
29	C	504	CLA	C6-C7-C8-C9
29	S	604	CLA	C6-C7-C8-C10
34	y	625	SPH	C11-C12-C13-C14
37	C	519	DGD	O6E-C1E-O5D-C6D
29	B	602	CLA	C15-C16-C17-C18
29	S	610	CLA	C13-C15-C16-C17
39	c	524	DGA	CG1-CG2-CG3-OXT
39	j	101	DGA	CG1-CG2-CG3-OXT
40	N	624	LHG	C1-C2-C3-O3
40	d	408	LHG	C26-C27-C28-C29
35	h	102	LMG	O9-C10-O7-C8
29	D	402	CLA	C2-C1-O2A-CGA
29	b	605	CLA	C2-C1-O2A-CGA
29	B	611	CLA	O1D-CGD-O2D-CED
40	D	408	LHG	C25-C26-C27-C28
29	c	511	CLA	O1A-CGA-O2A-C1
29	B	604	CLA	C11-C12-C13-C14
29	C	512	CLA	C14-C13-C15-C16
29	D	402	CLA	C11-C12-C13-C14
29	N	604	CLA	C14-C13-C15-C16
29	R	610	CLA	C11-C10-C8-C9
29	S	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	Y	612	CLA	C11-C10-C8-C9
29	Y	613	CLA	C11-C12-C13-C14
29	b	603	CLA	C14-C13-C15-C16
29	b	611	CLA	C11-C12-C13-C14
29	c	507	CLA	C11-C10-C8-C9
29	r	608	CLA	C11-C10-C8-C9
45	G	609	CHL	C11-C10-C8-C9
35	W	201	LMG	C29-C30-C31-C32
38	T	101	3PH	C26-C27-C28-C29
40	s	624	LHG	C11-C12-C13-C14
29	Y	614	CLA	C13-C15-C16-C17
29	b	614	CLA	C5-C6-C7-C8
30	a	408	PHO	C1A-C2A-CAA-CBA
38	T	101	3PH	C2-C1-O11-P
38	b	624	3PH	C2-C1-O11-P
40	D	410	LHG	C2-C3-O3-P
40	l	101	LHG	C2-C3-O3-P
33	b	621	SQD	C11-C10-C9-C8
35	d	411	LMG	C19-C20-C21-C22
38	T	101	3PH	C36-C37-C38-C39
39	j	101	DGA	CB5-CB6-CB7-CB8
29	R	604	CLA	C2A-CAA-CBA-CGA
29	b	615	CLA	C2A-CAA-CBA-CGA
29	r	608	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C16-C17-C18-C20
29	g	611	CLA	C16-C17-C18-C20
29	s	613	CLA	C6-C7-C8-C10
30	A	408	PHO	C16-C17-C18-C19
31	B	619	BCR	C23-C24-C25-C26
31	B	619	BCR	C23-C24-C25-C30
31	C	517	BCR	C1-C6-C7-C8
31	C	517	BCR	C5-C6-C7-C8
31	c	515	BCR	C5-C6-C7-C8
31	c	517	BCR	C5-C6-C7-C8
36	b	620	C7Z	C21-C26-C27-C28
44	h	101	RRX	C23-C24-C25-C26
44	h	101	RRX	C5-C6-C7-C8
46	N	620	LUT	C1-C6-C7-C8
46	N	620	LUT	C5-C6-C7-C8
46	S	620	LUT	C5-C6-C7-C8
46	Y	620	LUT	C5-C6-C7-C8
38	T	101	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
38	s	626	3PH	C37-C38-C39-C3A
40	L	101	LHG	C30-C31-C32-C33
31	B	618	BCR	C17-C18-C19-C20
31	B	619	BCR	C17-C18-C19-C20
31	D	404	BCR	C17-C18-C19-C20
46	R	620	LUT	C7-C8-C9-C10
47	R	622	NEX	C20-C13-C14-C15
47	r	622	NEX	C20-C13-C14-C15
29	Y	603	CLA	C13-C15-C16-C17
35	H	102	LMG	O9-C10-O7-C8
39	C	524	DGA	CB9-CAB-CBB-CCB
29	S	609	CLA	C11-C12-C13-C14
40	N	624	LHG	C31-C32-C33-C34
29	A	407	CLA	C2C-C3C-CAC-CBC
35	b	622	LMG	C12-C13-C14-C15
42	D	405	PL9	C40-C39-C41-C42
35	C	523	LMG	C12-C13-C14-C15
49	r	625	LMT	C9-C10-C11-C12
29	A	405	CLA	C12-C13-C15-C16
29	A	410	CLA	C2-C3-C5-C6
29	B	602	CLA	C12-C13-C15-C16
29	B	605	CLA	C12-C13-C15-C16
29	B	607	CLA	C11-C10-C8-C7
29	B	608	CLA	C11-C12-C13-C15
29	B	612	CLA	C12-C13-C15-C16
29	B	615	CLA	C6-C7-C8-C10
29	B	616	CLA	C11-C10-C8-C7
29	C	505	CLA	C11-C10-C8-C7
29	C	506	CLA	C6-C7-C8-C10
29	C	512	CLA	C12-C13-C15-C16
29	N	602	CLA	C6-C7-C8-C10
29	N	602	CLA	C11-C12-C13-C15
29	N	603	CLA	C6-C7-C8-C10
29	N	603	CLA	C12-C13-C15-C16
29	N	613	CLA	C12-C13-C15-C16
29	G	610	CLA	C11-C10-C8-C7
29	R	602	CLA	C6-C7-C8-C10
29	S	602	CLA	C11-C10-C8-C7
29	S	603	CLA	C11-C10-C8-C7
29	S	603	CLA	C12-C13-C15-C16
29	Y	612	CLA	C11-C10-C8-C7
29	a	405	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	406	CLA	C6-C7-C8-C10
29	b	602	CLA	C11-C10-C8-C7
29	b	602	CLA	C11-C12-C13-C15
29	b	605	CLA	C11-C12-C13-C15
29	b	615	CLA	C6-C7-C8-C10
29	b	616	CLA	C11-C12-C13-C15
29	c	502	CLA	C11-C12-C13-C15
29	c	503	CLA	C11-C12-C13-C15
29	c	504	CLA	C6-C7-C8-C10
29	c	504	CLA	C11-C12-C13-C15
29	c	505	CLA	C12-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C12-C13-C15
29	n	603	CLA	C11-C10-C8-C7
29	n	603	CLA	C12-C13-C15-C16
29	n	604	CLA	C6-C7-C8-C10
29	g	602	CLA	C6-C7-C8-C10
29	g	602	CLA	C12-C13-C15-C16
29	g	603	CLA	C12-C13-C15-C16
29	g	610	CLA	C11-C10-C8-C7
29	r	603	CLA	C11-C10-C8-C7
29	r	610	CLA	C11-C10-C8-C7
29	y	602	CLA	C6-C7-C8-C10
29	y	604	CLA	C11-C10-C8-C7
29	y	612	CLA	C11-C10-C8-C7
45	N	605	CHL	C11-C10-C8-C7
45	N	607	CHL	C12-C13-C15-C16
45	G	607	CHL	C11-C12-C13-C15
45	G	609	CHL	C11-C12-C13-C15
45	n	605	CHL	C12-C13-C15-C16
45	n	606	CHL	C11-C12-C13-C15
45	n	606	CHL	C12-C13-C15-C16
45	g	601	CHL	C6-C7-C8-C10
45	g	601	CHL	C12-C13-C15-C16
45	g	609	CHL	C11-C12-C13-C15
29	N	610	CLA	C13-C15-C16-C17
31	C	515	BCR	C19-C20-C21-C22
31	c	514	BCR	C9-C10-C11-C12
31	d	404	BCR	C19-C20-C21-C22
46	S	621	LUT	C29-C30-C31-C32
46	r	620	LUT	C9-C10-C11-C12
46	s	621	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
47	R	622	NEX	C33-C34-C35-C15
29	C	503	CLA	C16-C17-C18-C19
39	B	625	DGA	CA1-CA2-CA3-CA4
39	C	524	DGA	CA4-CA5-CA6-CA7
29	G	603	CLA	C10-C11-C12-C13
30	A	408	PHO	C15-C16-C17-C18
29	S	604	CLA	C2A-CAA-CBA-CGA
29	S	609	CLA	C10-C11-C12-C13
39	j	101	DGA	CA1-CA2-CA3-CA4
29	b	617	CLA	C8-C10-C11-C12
29	c	503	CLA	C10-C11-C12-C13
45	n	606	CHL	C13-C15-C16-C17
45	n	607	CHL	C10-C11-C12-C13
29	Y	613	CLA	CBA-CGA-O2A-C1
39	C	524	DGA	CA3-CA4-CA5-CA6
40	d	409	LHG	C10-C11-C12-C13
40	s	624	LHG	C24-C25-C26-C27
40	D	408	LHG	C23-C24-C25-C26
33	B	621	SQD	C11-C10-C9-C8
34	a	414	SPH	C13-C14-C15-C16
38	t	101	3PH	C24-C25-C26-C27
40	s	624	LHG	C14-C15-C16-C17
29	B	605	CLA	C13-C15-C16-C17
29	B	606	CLA	CAD-CBD-CGD-O2D
29	B	609	CLA	CAD-CBD-CGD-O2D
29	B	611	CLA	CAD-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O2D
29	C	505	CLA	CAD-CBD-CGD-O2D
29	C	513	CLA	CAD-CBD-CGD-O2D
29	N	614	CLA	CAD-CBD-CGD-O2D
29	G	611	CLA	CAD-CBD-CGD-O2D
29	S	614	CLA	CAD-CBD-CGD-O2D
29	b	611	CLA	CAD-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O2D
29	c	513	CLA	CAD-CBD-CGD-O2D
29	g	602	CLA	CAD-CBD-CGD-O2D
29	r	602	CLA	CAD-CBD-CGD-O2D
29	r	609	CLA	CAD-CBD-CGD-O2D
29	s	609	CLA	CAD-CBD-CGD-O2D
29	y	603	CLA	CAD-CBD-CGD-O2D
29	y	614	CLA	CAD-CBD-CGD-O2D
30	a	408	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	M	101	SQD	C46-C45-O47-C7
33	b	621	SQD	C46-C45-O47-C7
45	n	605	CHL	CAD-CBD-CGD-O2D
47	Y	623	NEX	C7-C8-C9-C19
47	y	623	NEX	C7-C8-C9-C19
45	y	601	CHL	C3-C5-C6-C7
33	b	626	SQD	C30-C31-C32-C33
35	H	102	LMG	C12-C13-C14-C15
45	g	609	CHL	C13-C15-C16-C17
40	d	410	LHG	C25-C26-C27-C28
40	s	624	LHG	C29-C30-C31-C32
33	A	412	SQD	C24-C23-O48-C46
29	Y	603	CLA	C16-C17-C18-C19
37	C	520	DGD	C3A-C4A-C5A-C6A
29	D	403	CLA	C8-C10-C11-C12
29	Y	602	CLA	C8-C10-C11-C12
29	s	609	CLA	C5-C6-C7-C8
45	n	609	CHL	C8-C10-C11-C12
29	S	609	CLA	O1D-CGD-O2D-CED
33	A	412	SQD	O6-C44-C45-C46
33	a	412	SQD	O6-C44-C45-C46
35	a	413	LMG	O1-C7-C8-C9
35	a	413	LMG	C7-C8-C9-O8
39	J	101	DGA	OG1-CG1-CG2-CG3
39	c	524	DGA	OG1-CG1-CG2-CG3
40	d	410	LHG	C4-C5-C6-O8
29	B	605	CLA	CBD-CGD-O2D-CED
38	B	624	3PH	O11-C1-C2-O21
40	D	409	LHG	O6-C4-C5-O7
40	n	624	LHG	O6-C4-C5-O7
40	g	624	LHG	O6-C4-C5-O7
51	y	627	PTY	O14-C5-C6-O7
35	h	102	LMG	O7-C10-C11-C12
40	N	624	LHG	O8-C23-C24-C25
29	G	604	CLA	O2A-C1-C2-C3
29	n	614	CLA	O2A-C1-C2-C3
29	g	604	CLA	O2A-C1-C2-C3
29	c	501	CLA	C2A-CAA-CBA-CGA
29	B	605	CLA	C15-C16-C17-C18
29	g	610	CLA	C15-C16-C17-C18
29	C	505	CLA	CBD-CGD-O2D-CED
39	c	524	DGA	CEA-CFA-CGA-CHA

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Mol	Chain	Res	Type	Atoms
49	r	625	LMT	O1'-C1-C2-C3
29	B	607	CLA	CHA-CBD-CGD-O2D
29	B	608	CLA	CHA-CBD-CGD-O1D
29	B	608	CLA	CHA-CBD-CGD-O2D
29	C	504	CLA	CHA-CBD-CGD-O1D
29	S	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O2D
29	b	607	CLA	CHA-CBD-CGD-O1D
29	b	607	CLA	CHA-CBD-CGD-O2D
29	n	604	CLA	CHA-CBD-CGD-O1D
29	n	604	CLA	CHA-CBD-CGD-O2D
29	s	602	CLA	CHA-CBD-CGD-O1D
29	s	602	CLA	CHA-CBD-CGD-O2D
45	R	606	CHL	CHA-CBD-CGD-O1D
45	R	606	CHL	CHA-CBD-CGD-O2D
45	g	605	CHL	CHA-CBD-CGD-O1D
45	g	605	CHL	CHA-CBD-CGD-O2D
45	r	606	CHL	CHA-CBD-CGD-O1D
45	r	606	CHL	CHA-CBD-CGD-O2D
33	B	626	SQD	C24-C25-C26-C27
29	y	612	CLA	C3-C5-C6-C7
29	B	606	CLA	O1A-CGA-O2A-C1
29	Y	613	CLA	O1A-CGA-O2A-C1
29	Y	614	CLA	O1A-CGA-O2A-C1
29	c	505	CLA	O1A-CGA-O2A-C1
40	C	525	LHG	O10-C23-O8-C6
37	C	519	DGD	C2E-C1E-O5D-C6D
45	r	606	CHL	C2A-CAA-CBA-CGA
35	B	622	LMG	C31-C32-C33-C34
40	N	624	LHG	C35-C36-C37-C38
40	S	624	LHG	C24-C25-C26-C27
51	y	626	PTY	C37-C38-C39-C40
33	A	412	SQD	O6-C44-C45-O47
33	C	526	SQD	O47-C45-C46-O48
33	M	101	SQD	O47-C45-C46-O48
33	a	412	SQD	O6-C44-C45-O47
35	C	523	LMG	O1-C7-C8-O7
35	w	201	LMG	O1-C7-C8-O7
38	B	624	3PH	O21-C2-C3-O31
39	c	524	DGA	OG1-CG1-CG2-OG2
40	l	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
51	y	626	PTY	O4-C1-C6-O7
51	y	627	PTY	O4-C1-C6-O7
40	y	624	LHG	C26-C27-C28-C29
29	s	604	CLA	O1A-CGA-O2A-C1
38	b	624	3PH	C32-C33-C34-C35
35	c	521	LMG	C33-C34-C35-C36
38	b	624	3PH	C26-C27-C28-C29
40	l	101	LHG	C15-C16-C17-C18
29	g	613	CLA	C5-C6-C7-C8
40	D	410	LHG	C8-C7-O7-C5
45	Y	607	CHL	C4-C3-C5-C6
40	L	101	LHG	C10-C11-C12-C13
40	c	525	LHG	C7-C8-C9-C10
38	T	101	3PH	C3B-C3C-C3D-C3E
29	N	603	CLA	C15-C16-C17-C18
29	B	604	CLA	C6-C7-C8-C9
29	B	607	CLA	C11-C10-C8-C9
29	N	602	CLA	C11-C12-C13-C14
29	Y	612	CLA	C14-C13-C15-C16
29	b	612	CLA	C14-C13-C15-C16
29	b	614	CLA	C11-C10-C8-C9
29	c	513	CLA	C11-C12-C13-C14
29	g	602	CLA	C14-C13-C15-C16
29	y	604	CLA	C14-C13-C15-C16
29	y	612	CLA	C11-C10-C8-C9
45	N	605	CHL	C11-C12-C13-C14
45	G	601	CHL	C6-C7-C8-C9
45	Y	609	CHL	C14-C13-C15-C16
29	G	604	CLA	O1D-CGD-O2D-CED
33	c	526	SQD	C32-C33-C34-C35
29	g	603	CLA	O1D-CGD-O2D-CED
39	b	625	DGA	CB1-CB2-CB3-CB4
34	y	625	SPH	C11-C10-C9-C8
39	c	524	DGA	CDB-CEB-CFB-CGB
29	n	610	CLA	C5-C6-C7-C8
33	C	526	SQD	C5-C6-S-O8
33	a	412	SQD	C4-C5-C6-S
33	m	101	SQD	C4-C5-C6-S
38	B	624	3PH	C3B-C3C-C3D-C3E
31	a	411	BCR	C37-C22-C23-C24
29	c	507	CLA	C13-C15-C16-C17
29	r	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
40	d	408	LHG	C11-C10-C9-C8
40	y	624	LHG	C35-C36-C37-C38
31	A	411	BCR	C21-C22-C23-C24
44	H	101	RRX	C11-C12-C13-C14
35	C	527	LMG	C15-C16-C17-C18
29	R	610	CLA	O1D-CGD-O2D-CED
29	B	606	CLA	C1A-C2A-CAA-CBA
29	N	602	CLA	C1A-C2A-CAA-CBA
29	N	604	CLA	C1A-C2A-CAA-CBA
29	S	614	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	C1A-C2A-CAA-CBA
29	a	407	CLA	C1A-C2A-CAA-CBA
29	c	512	CLA	C1A-C2A-CAA-CBA
45	N	601	CHL	C1A-C2A-CAA-CBA
45	G	607	CHL	C1A-C2A-CAA-CBA
45	Y	601	CHL	C1A-C2A-CAA-CBA
45	n	601	CHL	C1A-C2A-CAA-CBA
45	g	609	CHL	C1A-C2A-CAA-CBA
45	Y	606	CHL	C8-C10-C11-C12
29	A	405	CLA	C2-C1-O2A-CGA
29	G	604	CLA	C2-C1-O2A-CGA
45	Y	606	CHL	C2-C1-O2A-CGA
29	C	505	CLA	CBA-CGA-O2A-C1
38	b	624	3PH	C27-C28-C29-C2A
39	C	524	DGA	CB7-CB8-CB9-CAB
40	G	624	LHG	C30-C31-C32-C33
47	r	622	NEX	C13-C14-C15-C35
40	C	525	LHG	C3-O3-P-O6
40	D	408	LHG	C3-O3-P-O6
40	L	101	LHG	C3-O3-P-O6
40	Y	624	LHG	C3-O3-P-O6
40	g	624	LHG	C3-O3-P-O6
50	s	625	LPX	C3-O1-P1-O2
40	c	497	LHG	C11-C12-C13-C14
35	C	527	LMG	C32-C33-C34-C35
39	c	524	DGA	CA8-CA9-CAA-CBA
45	Y	601	CHL	C3-C5-C6-C7
40	c	525	LHG	C2-C3-O3-P
40	c	497	LHG	C2-C3-O3-P
29	C	512	CLA	C2-C3-C5-C6
29	y	613	CLA	C2-C3-C5-C6
45	N	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	612	CLA	C4C-C3C-CAC-CBC
40	C	525	LHG	C3-O3-P-O5
40	C	525	LHG	C4-O6-P-O4
40	D	408	LHG	C4-O6-P-O4
40	D	410	LHG	C4-O6-P-O5
40	L	101	LHG	C4-O6-P-O4
40	L	101	LHG	C4-O6-P-O5
40	d	410	LHG	C3-O3-P-O4
40	d	409	LHG	C4-O6-P-O4
40	s	624	LHG	C4-O6-P-O5
40	y	624	LHG	C4-O6-P-O4
50	s	625	LPX	C3-O1-P1-O4
51	Y	626	PTY	C5-O14-P1-O12
51	y	626	PTY	C3-O11-P1-O12
51	y	627	PTY	C3-O11-P1-O13
29	C	505	CLA	C11-C12-C13-C14
29	g	611	CLA	C16-C17-C18-C19
34	Y	625	SPH	C10-C11-C12-C13
40	L	101	LHG	C11-C10-C9-C8
40	d	410	LHG	C34-C35-C36-C37
29	D	403	CLA	C10-C11-C12-C13
29	n	602	CLA	CBA-CGA-O2A-C1
40	N	624	LHG	O6-C4-C5-C6
40	c	497	LHG	O6-C4-C5-C6
51	y	626	PTY	O14-C5-C6-C1
29	R	608	CLA	O1D-CGD-O2D-CED
40	d	410	LHG	C11-C10-C9-C8
39	c	524	DGA	CA6-CA7-CA8-CA9
40	S	624	LHG	C29-C30-C31-C32
40	n	624	LHG	C26-C27-C28-C29
29	n	602	CLA	C15-C16-C17-C18
29	G	613	CLA	C2A-CAA-CBA-CGA
29	Y	613	CLA	C2A-CAA-CBA-CGA
29	R	608	CLA	C3-C5-C6-C7
35	C	527	LMG	C30-C31-C32-C33
35	W	201	LMG	C36-C37-C38-C39
45	N	607	CHL	C16-C17-C18-C19
35	c	521	LMG	C18-C19-C20-C21
29	B	608	CLA	CAD-CBD-CGD-O1D
29	C	504	CLA	CAD-CBD-CGD-O1D
29	n	604	CLA	CAD-CBD-CGD-O1D
29	r	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	C2-C3-C5-C6
29	s	602	CLA	CAD-CBD-CGD-O1D
33	C	526	SQD	C5-C6-S-O7
33	b	621	SQD	O5-C5-C6-S
45	N	609	CHL	CAD-CBD-CGD-O1D
45	R	606	CHL	CAD-CBD-CGD-O1D
45	r	606	CHL	CAD-CBD-CGD-O1D
51	y	626	PTY	C2-C3-O11-P1
51	y	627	PTY	C2-C3-O11-P1
39	b	625	DGA	CDB-CEB-CFB-CGB
39	c	524	DGA	CEB-CFB-CGB-CHB
38	b	624	3PH	C2B-C2C-C2D-C2E
30	a	408	PHO	C15-C16-C17-C18
40	D	409	LHG	C24-C23-O8-C6
33	A	412	SQD	O10-C23-O48-C46
45	N	605	CHL	C4-C3-C5-C6
29	B	613	CLA	C3A-C2A-CAA-CBA
29	C	501	CLA	C11-C12-C13-C15
29	C	502	CLA	C11-C12-C13-C15
29	C	505	CLA	C6-C7-C8-C10
29	C	509	CLA	C11-C10-C8-C7
29	C	512	CLA	C11-C10-C8-C7
29	N	602	CLA	C12-C13-C15-C16
29	N	603	CLA	C11-C10-C8-C7
29	N	614	CLA	C3A-C2A-CAA-CBA
29	Y	603	CLA	C11-C10-C8-C7
29	Y	611	CLA	C6-C7-C8-C10
29	b	602	CLA	C12-C13-C15-C16
29	b	608	CLA	C12-C13-C15-C16
29	b	612	CLA	C12-C13-C15-C16
29	b	616	CLA	C11-C10-C8-C7
29	c	501	CLA	C11-C12-C13-C15
29	c	505	CLA	C6-C7-C8-C10
29	c	511	CLA	C11-C12-C13-C15
29	g	603	CLA	C11-C10-C8-C7
29	g	613	CLA	C11-C12-C13-C15
29	r	602	CLA	C6-C7-C8-C10
29	s	611	CLA	C11-C10-C8-C7
29	y	604	CLA	C6-C7-C8-C10
40	D	410	LHG	O6-C4-C5-O7
40	N	624	LHG	O6-C4-C5-O7
40	l	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
45	N	605	CHL	C12-C13-C15-C16
45	N	606	CHL	C12-C13-C15-C16
45	G	601	CHL	C6-C7-C8-C10
45	Y	607	CHL	C11-C12-C13-C15
45	n	606	CHL	C11-C10-C8-C7
45	y	607	CHL	C11-C12-C13-C15
46	S	621	LUT	C25-C26-C27-C28
51	y	626	PTY	O14-C5-C6-O7
40	S	624	LHG	C15-C16-C17-C18
29	g	613	CLA	C15-C16-C17-C18
35	B	622	LMG	C18-C19-C20-C21
37	c	520	DGD	O6D-C5D-C6D-O5D
40	G	624	LHG	O8-C23-C24-C25
40	y	624	LHG	C23-C24-C25-C26
39	c	524	DGA	CB2-CB1-OG2-CG2
29	R	603	CLA	C2C-C3C-CAC-CBC
38	b	624	3PH	C35-C36-C37-C38
35	c	521	LMG	C32-C33-C34-C35
38	s	626	3PH	C3E-C3F-C3G-C3H
29	Y	602	CLA	C2A-CAA-CBA-CGA
29	B	616	CLA	C16-C17-C18-C20
40	s	624	LHG	C23-C24-C25-C26
37	C	520	DGD	O6D-C5D-C6D-O5D
34	A	414	SPH	O1-C1-C2-N2
34	Y	625	SPH	O1-C1-C2-N2
34	y	625	SPH	C1-C2-C3-O3
35	C	523	LMG	O1-C7-C8-C9
35	C	527	LMG	O1-C7-C8-C9
39	c	524	DGA	OB1-CB1-OG2-CG2
33	b	626	SQD	O6-C44-C45-O47
35	C	523	LMG	O7-C8-C9-O8
38	s	626	3PH	O21-C2-C3-O31
40	L	101	LHG	O7-C5-C6-O8
40	c	525	LHG	O7-C5-C6-O8
29	g	602	CLA	C15-C16-C17-C18
33	B	626	SQD	C25-C26-C27-C28
33	c	526	SQD	C28-C29-C30-C31
33	A	412	SQD	C45-C44-O6-C1
33	b	626	SQD	C45-C44-O6-C1
29	N	602	CLA	C16-C17-C18-C19
35	c	521	LMG	C15-C16-C17-C18
40	d	410	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
40	d	410	LHG	C24-C25-C26-C27
49	R	625	LMT	C6-C7-C8-C9
29	C	505	CLA	O1A-CGA-O2A-C1
29	Y	611	CLA	C13-C15-C16-C17
29	c	503	CLA	C8-C10-C11-C12
42	d	405	PL9	C45-C44-C46-C47
45	Y	606	CHL	C4-C3-C5-C6
35	h	102	LMG	C13-C14-C15-C16
29	B	602	CLA	C14-C13-C15-C16
29	B	605	CLA	C14-C13-C15-C16
29	B	608	CLA	C6-C7-C8-C9
29	B	611	CLA	C11-C12-C13-C14
29	B	615	CLA	C11-C10-C8-C9
29	C	508	CLA	C11-C12-C13-C14
29	N	603	CLA	C14-C13-C15-C16
29	N	613	CLA	C14-C13-C15-C16
29	G	603	CLA	C6-C7-C8-C9
29	G	613	CLA	C14-C13-C15-C16
29	S	610	CLA	C6-C7-C8-C9
29	Y	604	CLA	C14-C13-C15-C16
29	a	406	CLA	C6-C7-C8-C9
29	a	406	CLA	C11-C12-C13-C14
29	b	605	CLA	C11-C12-C13-C14
29	c	502	CLA	C11-C12-C13-C14
29	c	508	CLA	C11-C12-C13-C14
29	n	603	CLA	C14-C13-C15-C16
29	g	603	CLA	C14-C13-C15-C16
29	y	602	CLA	C6-C7-C8-C9
29	y	604	CLA	C11-C10-C8-C9
45	N	601	CHL	C14-C13-C15-C16
45	Y	606	CHL	C6-C7-C8-C9
45	n	609	CHL	C11-C12-C13-C14
45	g	601	CHL	C6-C7-C8-C9
29	B	607	CLA	O1D-CGD-O2D-CED
35	a	413	LMG	C11-C12-C13-C14
40	G	624	LHG	C28-C29-C30-C31
40	d	409	LHG	C11-C10-C9-C8
29	Y	611	CLA	C3-C5-C6-C7
35	C	523	LMG	C36-C37-C38-C39
40	G	624	LHG	C33-C34-C35-C36
40	d	408	LHG	C35-C36-C37-C38
40	s	624	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	n	602	CLA	O1A-CGA-O2A-C1
39	c	524	DGA	CB3-CB4-CB5-CB6
29	N	603	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C20
34	a	414	SPH	C9-C10-C11-C12
40	D	410	LHG	O9-C7-O7-C5
34	A	414	SPH	C10-C11-C12-C13
40	l	101	LHG	C30-C31-C32-C33
39	C	524	DGA	CBB-CAB-CB9-CB8
29	C	513	CLA	C16-C17-C18-C20
35	c	521	LMG	C19-C20-C21-C22
29	c	501	CLA	C10-C11-C12-C13
29	r	609	CLA	C8-C10-C11-C12
29	N	611	CLA	C1-C2-C3-C4
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4
29	n	611	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4
45	N	608	CHL	C1-C2-C3-C4
45	G	606	CHL	C1-C2-C3-C4
45	R	607	CHL	C1-C2-C3-C4
45	n	608	CHL	C1-C2-C3-C4
45	g	606	CHL	C1-C2-C3-C4
45	r	607	CHL	C1-C2-C3-C4
40	D	409	LHG	C31-C32-C33-C34
33	B	621	SQD	O47-C7-C8-C9
34	Y	625	SPH	C15-C16-C17-C18
33	B	621	SQD	C46-C45-O47-C7
33	m	101	SQD	C46-C45-O47-C7
35	C	527	LMG	C7-C8-O7-C10
38	T	101	3PH	C3-C2-O21-C21
38	t	101	3PH	C3-C2-O21-C21
29	R	609	CLA	C2A-CAA-CBA-CGA
29	S	605	CLA	C2A-CAA-CBA-CGA
29	S	617	CLA	C2A-CAA-CBA-CGA
45	G	607	CHL	C2A-CAA-CBA-CGA
39	c	524	DGA	CB9-CAB-CBB-CCB
29	S	610	CLA	C2-C1-O2A-CGA
29	b	609	CLA	C2-C1-O2A-CGA
29	b	614	CLA	C2-C1-O2A-CGA
29	d	402	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	n	611	CLA	C2-C1-O2A-CGA
45	N	607	CHL	C2-C1-O2A-CGA
45	G	607	CHL	C2-C1-O2A-CGA
45	n	607	CHL	C2-C1-O2A-CGA
45	y	606	CHL	C2-C1-O2A-CGA
39	c	524	DGA	CAA-CBA-CCA-CDA
35	w	201	LMG	C28-C29-C30-C31
39	c	524	DGA	CA3-CA4-CA5-CA6
40	c	525	LHG	C26-C27-C28-C29
33	m	101	SQD	O47-C7-C8-C9
45	S	608	CHL	CAA-CBA-CGA-O2A
29	N	602	CLA	C3-C5-C6-C7
29	Y	612	CLA	C3-C5-C6-C7
37	c	519	DGD	C6B-C7B-C8B-C9B
35	H	102	LMG	C29-C30-C31-C32
40	g	624	LHG	C29-C30-C31-C32
40	G	624	LHG	O6-C4-C5-O7
40	C	525	LHG	C29-C30-C31-C32
45	N	607	CHL	CAA-CBA-CGA-O2A
29	B	604	CLA	C4-C3-C5-C6
45	N	609	CHL	C4-C3-C5-C6
45	S	608	CHL	C4-C3-C5-C6
31	A	411	BCR	C5-C6-C7-C8
31	a	411	BCR	C5-C6-C7-C8
31	c	516	BCR	C23-C24-C25-C26
46	S	620	LUT	C1-C6-C7-C8
46	Y	620	LUT	C1-C6-C7-C8
46	n	620	LUT	C5-C6-C7-C8
45	y	607	CHL	C10-C11-C12-C13
29	B	605	CLA	C4C-C3C-CAC-CBC
40	S	624	LHG	C35-C36-C37-C38
33	a	412	SQD	C11-C10-C9-C8
35	w	201	LMG	C29-C30-C31-C32
38	T	101	3PH	C3F-C3G-C3H-C3I
39	b	625	DGA	CAB-CBB-CCB-CDB
29	B	612	CLA	C16-C17-C18-C20
29	S	613	CLA	C6-C7-C8-C9
51	Y	626	PTY	C35-C36-C37-C38
29	c	511	CLA	C2A-CAA-CBA-CGA
45	G	605	CHL	C2A-CAA-CBA-CGA
35	W	201	LMG	C2-C1-O1-C7
47	S	623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
51	Y	627	PTY	O4-C1-C6-O7
40	N	624	LHG	C3-O3-P-O6
40	G	624	LHG	C3-O3-P-O6
40	S	624	LHG	C3-O3-P-O6
40	c	525	LHG	C3-O3-P-O6
40	c	497	LHG	C4-O6-P-O3
40	d	408	LHG	C4-O6-P-O3
40	d	409	LHG	C3-O3-P-O6
40	s	624	LHG	C3-O3-P-O6
50	s	625	LPX	C1-O2-P1-O1
51	Y	627	PTY	C5-O14-P1-O11
51	y	626	PTY	C5-O14-P1-O11
51	y	627	PTY	C5-O14-P1-O11
35	b	622	LMG	C19-C20-C21-C22
29	s	609	CLA	C11-C12-C13-C14
30	a	409	PHO	CHA-CBD-CGD-O2D
40	n	624	LHG	C16-C17-C18-C19
33	C	526	SQD	O6-C44-C45-C46
33	C	526	SQD	C44-C45-C46-O48
38	b	624	3PH	C23-C24-C25-C26
39	c	524	DGA	CBB-CCB-CDB-CEB
29	B	608	CLA	C10-C11-C12-C13
29	B	604	CLA	C6-C7-C8-C10
29	C	508	CLA	C11-C12-C13-C15
29	G	603	CLA	C6-C7-C8-C10
29	Y	612	CLA	C12-C13-C15-C16
29	a	406	CLA	C11-C12-C13-C15
29	a	410	CLA	C11-C10-C8-C7
29	b	617	CLA	C6-C7-C8-C10
29	c	508	CLA	C11-C12-C13-C15
29	s	611	CLA	C2-C3-C5-C6
42	D	405	PL9	C13-C14-C16-C17
45	N	605	CHL	C2-C3-C5-C6
45	N	606	CHL	C11-C12-C13-C15
45	Y	606	CHL	C2-C3-C5-C6
35	C	527	LMG	C13-C14-C15-C16
40	d	408	LHG	C33-C34-C35-C36
29	C	502	CLA	C11-C12-C13-C14
29	C	505	CLA	C6-C7-C8-C9
29	C	512	CLA	C6-C7-C8-C9
29	C	512	CLA	C11-C10-C8-C9
29	N	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	G	602	CLA	C14-C13-C15-C16
29	Y	602	CLA	C6-C7-C8-C9
29	b	608	CLA	C14-C13-C15-C16
29	g	613	CLA	C11-C12-C13-C14
29	s	611	CLA	C11-C10-C8-C9
29	y	603	CLA	C14-C13-C15-C16
29	y	614	CLA	C6-C7-C8-C9
45	N	606	CHL	C14-C13-C15-C16
45	G	609	CHL	C11-C12-C13-C14
45	n	606	CHL	C11-C12-C13-C14
45	g	609	CHL	C11-C12-C13-C14
44	H	101	RRX	C9-C10-C11-C12
46	n	620	LUT	C29-C30-C31-C32
46	s	620	LUT	C29-C30-C31-C32
47	g	623	NEX	C9-C10-C11-C12
40	d	408	LHG	C29-C30-C31-C32
29	c	512	CLA	C10-C11-C12-C13
51	Y	626	PTY	C37-C38-C39-C40
29	b	613	CLA	C2A-CAA-CBA-CGA
40	Y	624	LHG	C17-C18-C19-C20
37	B	623	DGD	C1B-C2B-C3B-C4B
35	W	201	LMG	C37-C38-C39-C40
39	C	524	DGA	CA9-CAA-CBA-CCA
29	S	610	CLA	C8-C10-C11-C12
29	C	505	CLA	C11-C12-C13-C15
29	N	603	CLA	C16-C17-C18-C20
33	C	526	SQD	C24-C23-O48-C46
45	s	608	CHL	CAA-CBA-CGA-O2A
29	c	506	CLA	C5-C6-C7-C8
29	b	612	CLA	CBD-CGD-O2D-CED
40	c	525	LHG	C9-C10-C11-C12
29	N	614	CLA	O2A-C1-C2-C3
29	b	610	CLA	C4-C3-C5-C6
40	d	409	LHG	O1-C1-C2-O2
40	n	624	LHG	O8-C23-C24-C25
29	s	609	CLA	C2-C3-C5-C6
45	Y	607	CHL	C2-C3-C5-C6
29	R	610	CLA	C11-C12-C13-C14
29	C	507	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	CBA-CGA-O2A-C1
29	r	602	CLA	CBA-CGA-O2A-C1
37	c	519	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
40	C	525	LHG	C28-C29-C30-C31
45	s	601	CHL	CAA-CBA-CGA-O1A
40	g	624	LHG	C15-C16-C17-C18
38	T	101	3PH	C3D-C3E-C3F-C3G
39	C	524	DGA	CCB-CDB-CEB-CFB
40	D	408	LHG	C30-C31-C32-C33
40	y	624	LHG	C34-C35-C36-C37
33	C	526	SQD	O10-C23-O48-C46
29	a	407	CLA	CBA-CGA-O2A-C1
29	C	501	CLA	C2A-CAA-CBA-CGA
29	y	602	CLA	C2A-CAA-CBA-CGA
29	y	613	CLA	C2A-CAA-CBA-CGA
29	S	613	CLA	C6-C7-C8-C10
29	N	610	CLA	C5-C6-C7-C8
31	B	619	BCR	C9-C10-C11-C12
31	D	404	BCR	C13-C14-C15-C16
31	D	404	BCR	C19-C20-C21-C22
31	c	514	BCR	C13-C14-C15-C16
31	c	514	BCR	C19-C20-C21-C22
31	d	404	BCR	C9-C10-C11-C12
47	R	622	NEX	C13-C14-C15-C35
39	j	101	DGA	CB3-CB4-CB5-CB6
40	n	624	LHG	O6-C4-C5-C6
29	C	507	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	Y	612	CLA	C5-C6-C7-C8
29	R	609	CLA	C4C-C3C-CAC-CBC
33	b	626	SQD	C28-C29-C30-C31
29	N	602	CLA	C15-C16-C17-C18
40	c	497	LHG	C24-C25-C26-C27
29	N	610	CLA	C16-C17-C18-C20
29	b	602	CLA	CAA-CBA-CGA-O1A
29	B	606	CLA	C4-C3-C5-C6
29	Y	614	CLA	C4-C3-C5-C6
42	D	405	PL9	C45-C44-C46-C47
35	C	523	LMG	C34-C35-C36-C37
29	b	610	CLA	C2-C3-C5-C6
29	c	512	CLA	C2-C3-C5-C6
29	r	602	CLA	O1A-CGA-O2A-C1
29	a	405	CLA	C2-C1-O2A-CGA
29	n	613	CLA	C2-C1-O2A-CGA
29	r	604	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
34	A	414	SPH	C11-C10-C9-C8
37	c	518	DGD	C2A-C3A-C4A-C5A
29	B	617	CLA	C5-C6-C7-C8
29	C	501	CLA	C15-C16-C17-C18
29	C	512	CLA	C15-C16-C17-C18
29	C	510	CLA	C16-C17-C18-C20
29	n	602	CLA	C16-C17-C18-C20
29	y	610	CLA	C16-C17-C18-C20
29	B	607	CLA	C2A-CAA-CBA-CGA
29	b	606	CLA	C2A-CAA-CBA-CGA
29	y	610	CLA	C2A-CAA-CBA-CGA
35	h	102	LMG	O7-C8-C9-O8
38	T	101	3PH	O21-C2-C3-O31
35	w	201	LMG	C37-C38-C39-C40
45	n	607	CHL	CAA-CBA-CGA-O2A
35	a	413	LMG	C31-C32-C33-C34
40	D	409	LHG	C2-C3-O3-P
29	r	610	CLA	CBD-CGD-O2D-CED
51	y	626	PTY	C23-C24-C25-C26
29	S	602	CLA	C3A-C2A-CAA-CBA
29	c	512	CLA	C3A-C2A-CAA-CBA
45	Y	605	CHL	C3A-C2A-CAA-CBA
29	b	614	CLA	CBD-CGD-O2D-CED
29	y	612	CLA	CBA-CGA-O2A-C1
29	b	614	CLA	O1D-CGD-O2D-CED
33	a	412	SQD	C29-C30-C31-C32
37	c	520	DGD	C4A-C5A-C6A-C7A
40	l	101	LHG	C11-C10-C9-C8
45	R	606	CHL	C2A-CAA-CBA-CGA
45	n	609	CHL	C4-C3-C5-C6
29	n	603	CLA	C8-C10-C11-C12
39	c	524	DGA	CCA-CDA-CEA-CFA
40	D	409	LHG	C29-C30-C31-C32
40	G	624	LHG	C26-C27-C28-C29
40	c	525	LHG	C25-C26-C27-C28
29	B	604	CLA	C14-C13-C15-C16
29	C	503	CLA	C11-C10-C8-C9
29	a	405	CLA	C11-C12-C13-C14
29	b	605	CLA	C6-C7-C8-C9
29	g	613	CLA	C14-C13-C15-C16
29	r	608	CLA	C6-C7-C8-C9
29	s	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	y	612	CLA	C11-C12-C13-C14
30	a	409	PHO	C6-C7-C8-C9
45	N	606	CHL	C11-C12-C13-C14
45	N	609	CHL	C11-C12-C13-C14
45	n	609	CHL	C11-C10-C8-C9
29	n	604	CLA	C15-C16-C17-C18
29	g	612	CLA	C4C-C3C-CAC-CBC
40	D	410	LHG	C30-C31-C32-C33
40	c	525	LHG	C31-C32-C33-C34
33	b	626	SQD	O6-C44-C45-C46
35	A	413	LMG	C7-C8-C9-O8
35	h	102	LMG	C7-C8-C9-O8
40	L	101	LHG	C4-C5-C6-O8
46	G	621	LUT	C21-C26-C27-C28
47	G	623	NEX	C39-C29-C30-C31
47	S	623	NEX	C39-C29-C30-C31
47	g	623	NEX	C39-C29-C30-C31
47	s	623	NEX	C39-C29-C30-C31
47	y	623	NEX	C39-C29-C30-C31
35	C	523	LMG	C15-C16-C17-C18
29	B	605	CLA	O1D-CGD-O2D-CED
29	b	607	CLA	C2A-CAA-CBA-CGA
29	y	608	CLA	C2A-CAA-CBA-CGA
33	a	412	SQD	C15-C16-C17-C18
35	w	201	LMG	O9-C10-C11-C12
29	C	513	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C19
45	s	608	CHL	C11-C12-C13-C14
29	b	606	CLA	CBA-CGA-O2A-C1
29	C	505	CLA	O1D-CGD-O2D-CED
33	b	626	SQD	C12-C13-C14-C15
39	c	524	DGA	CFA-CGA-CHA-CIA
31	C	517	BCR	C7-C8-C9-C34
36	B	620	C7Z	C27-C28-C29-C39
46	r	620	LUT	C11-C12-C13-C20
29	b	603	CLA	C5-C6-C7-C8
29	C	509	CLA	CBD-CGD-O2D-CED
51	y	626	PTY	C17-C18-C19-C20
33	C	526	SQD	C7-C8-C9-C10
34	A	414	SPH	O3-C3-C4-C5
29	B	612	CLA	C1A-C2A-CAA-CBA
29	B	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	C	501	CLA	C1A-C2A-CAA-CBA
29	b	617	CLA	C1A-C2A-CAA-CBA
29	d	403	CLA	C1A-C2A-CAA-CBA
29	s	613	CLA	C1A-C2A-CAA-CBA
45	N	608	CHL	C1A-C2A-CAA-CBA
45	G	601	CHL	C1A-C2A-CAA-CBA
45	G	605	CHL	C1A-C2A-CAA-CBA
45	g	606	CHL	C1A-C2A-CAA-CBA
29	A	406	CLA	C11-C10-C8-C7
29	B	605	CLA	C11-C10-C8-C7
29	B	609	CLA	C6-C7-C8-C10
29	C	503	CLA	C12-C13-C15-C16
29	C	506	CLA	C11-C10-C8-C7
29	S	611	CLA	C6-C7-C8-C10
29	Y	604	CLA	C11-C12-C13-C15
29	Y	612	CLA	C6-C7-C8-C10
29	b	603	CLA	C11-C10-C8-C7
29	b	603	CLA	C12-C13-C15-C16
29	b	608	CLA	C11-C12-C13-C15
29	c	509	CLA	C11-C10-C8-C7
29	n	613	CLA	C11-C10-C8-C7
29	s	611	CLA	C11-C12-C13-C15
29	y	604	CLA	C12-C13-C15-C16
29	y	610	CLA	C12-C13-C15-C16
42	d	405	PL9	C43-C44-C46-C47
45	Y	606	CHL	C11-C12-C13-C15
45	g	607	CHL	C11-C10-C8-C7
29	a	407	CLA	O1A-CGA-O2A-C1
29	C	505	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C2A-CAA-CBA-CGA
37	C	518	DGD	O6D-C5D-C6D-O5D
29	b	602	CLA	C8-C10-C11-C12
40	D	410	LHG	C32-C33-C34-C35
45	N	608	CHL	O2A-C1-C2-C3
29	B	610	CLA	C15-C16-C17-C18
29	r	608	CLA	C5-C6-C7-C8
29	y	611	CLA	C13-C15-C16-C17
29	b	612	CLA	O1D-CGD-O2D-CED
29	b	605	CLA	C16-C17-C18-C20
29	s	610	CLA	C10-C11-C12-C13
29	n	612	CLA	CAA-CBA-CGA-O2A
29	Y	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	b	614	CLA	C4-C3-C5-C6
29	y	603	CLA	C4-C3-C5-C6
45	Y	609	CHL	C4-C3-C5-C6
45	g	607	CHL	C4-C3-C5-C6
45	y	609	CHL	C4-C3-C5-C6
29	C	509	CLA	C13-C15-C16-C17
29	b	612	CLA	C4C-C3C-CAC-CBC
45	y	605	CHL	CAA-CBA-CGA-O2A
29	y	612	CLA	O1A-CGA-O2A-C1
40	D	409	LHG	O10-C23-O8-C6
29	A	406	CLA	C4C-C3C-CAC-CBC
47	G	623	NEX	C28-C29-C30-C31
47	g	623	NEX	C28-C29-C30-C31
47	s	623	NEX	C28-C29-C30-C31
47	y	623	NEX	C28-C29-C30-C31
45	S	601	CHL	CAA-CBA-CGA-O1A
45	S	601	CHL	CAA-CBA-CGA-O2A
45	s	601	CHL	CAA-CBA-CGA-O2A
39	J	101	DGA	OG1-CG1-CG2-OG2
40	c	497	LHG	C26-C27-C28-C29
35	A	413	LMG	C11-C12-C13-C14
31	C	514	BCR	C15-C16-C17-C18
31	C	514	BCR	C19-C20-C21-C22
31	C	516	BCR	C9-C10-C11-C12
31	c	516	BCR	C9-C10-C11-C12
37	c	519	DGD	C3A-C4A-C5A-C6A
38	b	624	3PH	C21-C22-C23-C24
33	b	626	SQD	C11-C10-C9-C8
40	C	525	LHG	C24-C25-C26-C27
40	c	497	LHG	C30-C31-C32-C33
40	n	624	LHG	C18-C19-C20-C21
33	c	526	SQD	O5-C1-O6-C44
29	c	512	CLA	C15-C16-C17-C18
29	b	606	CLA	O1A-CGA-O2A-C1
39	B	625	DGA	CG1-CG2-CG3-OXT
39	C	524	DGA	CG1-CG2-CG3-OXT
29	C	509	CLA	O1D-CGD-O2D-CED
29	S	602	CLA	C4-C3-C5-C6
39	b	625	DGA	CBA-CCA-CDA-CEA
29	B	609	CLA	C2-C1-O2A-CGA
29	C	512	CLA	C2-C1-O2A-CGA
29	r	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	s	614	CLA	C2-C1-O2A-CGA
45	N	609	CHL	C2-C3-C5-C6
29	B	612	CLA	CBD-CGD-O2D-CED
33	b	626	SQD	C11-C12-C13-C14
39	b	625	DGA	CB7-CB8-CB9-CAB
29	S	611	CLA	C16-C17-C18-C19
29	s	609	CLA	C11-C12-C13-C15
29	A	406	CLA	C6-C7-C8-C9
29	B	602	CLA	C11-C12-C13-C14
29	C	507	CLA	C6-C7-C8-C9
29	n	612	CLA	CAA-CBA-CGA-O1A
45	N	607	CHL	C13-C15-C16-C17
29	r	612	CLA	C4-C3-C5-C6
35	H	102	LMG	C34-C35-C36-C37
40	d	409	LHG	C31-C32-C33-C34
29	B	604	CLA	C13-C15-C16-C17
29	b	605	CLA	C13-C15-C16-C17
29	y	613	CLA	C5-C6-C7-C8
29	a	407	CLA	C2A-CAA-CBA-CGA
29	c	503	CLA	C2A-CAA-CBA-CGA
29	s	605	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	O2A-C1-C2-C3
29	s	613	CLA	C4C-C3C-CAC-CBC
37	C	520	DGD	C9A-CAA-CBA-CCA
38	t	101	3PH	C2B-C2C-C2D-C2E
39	j	101	DGA	OA1-CA1-OG1-CG1
31	A	411	BCR	C1-C6-C7-C8
31	B	618	BCR	C23-C24-C25-C30
31	a	411	BCR	C1-C6-C7-C8
31	b	618	BCR	C23-C24-C25-C30
31	b	619	BCR	C23-C24-C25-C30
31	c	516	BCR	C23-C24-C25-C30
31	c	517	BCR	C1-C6-C7-C8
31	c	517	BCR	C23-C24-C25-C26
31	c	517	BCR	C23-C24-C25-C30
46	N	621	LUT	C1-C6-C7-C8
46	R	620	LUT	C1-C6-C7-C8
46	S	621	LUT	C1-C6-C7-C8
46	n	620	LUT	C1-C6-C7-C8
46	g	620	LUT	C1-C6-C7-C8
46	s	620	LUT	C1-C6-C7-C8
46	y	620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
46	y	620	LUT	C5-C6-C7-C8
38	s	626	3PH	C33-C34-C35-C36
35	A	413	LMG	O7-C10-C11-C12
40	g	624	LHG	O8-C23-C24-C25
33	b	621	SQD	O6-C44-C45-C46
45	y	605	CHL	CAA-CBA-CGA-O1A
29	Y	613	CLA	C13-C15-C16-C17
29	b	604	CLA	C13-C15-C16-C17
40	d	409	LHG	C12-C13-C14-C15
40	g	624	LHG	C30-C31-C32-C33
31	C	515	BCR	C13-C14-C15-C16
46	g	620	LUT	C29-C30-C31-C32
29	b	615	CLA	C4-C3-C5-C6
29	c	511	CLA	C4-C3-C5-C6
31	a	411	BCR	C21-C22-C23-C24
35	C	523	LMG	C11-C12-C13-C14
29	C	510	CLA	C2-C3-C5-C6
30	A	408	PHO	C2-C3-C5-C6
45	S	608	CHL	C2-C3-C5-C6
29	r	609	CLA	C4C-C3C-CAC-CBC
33	b	626	SQD	C9-C10-C11-C12
39	B	625	DGA	CA9-CAA-CBA-CCA
37	B	623	DGD	C2G-C3G-O3G-C1D
29	Y	603	CLA	C2C-C3C-CAC-CBC
33	B	626	SQD	C10-C11-C12-C13
51	y	626	PTY	C11-C12-C13-C14
45	S	608	CHL	C11-C12-C13-C15
29	R	602	CLA	C10-C11-C12-C13
29	n	602	CLA	C13-C15-C16-C17
29	B	612	CLA	O1D-CGD-O2D-CED
35	H	102	LMG	O9-C10-C11-C12
29	n	604	CLA	C2A-CAA-CBA-CGA
29	n	611	CLA	C2A-CAA-CBA-CGA
29	c	502	CLA	C13-C15-C16-C17
37	C	519	DGD	C3B-C4B-C5B-C6B
33	b	621	SQD	O47-C7-C8-C9
39	j	101	DGA	CA2-CA1-OG1-CG1
39	C	524	DGA	CAA-CBA-CCA-CDA
51	Y	626	PTY	C22-C23-C24-C25
45	G	609	CHL	C3-C5-C6-C7
29	R	603	CLA	C11-C12-C13-C15
29	B	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	b	621	SQD	C24-C25-C26-C27
35	c	521	LMG	C21-C22-C23-C24
29	B	614	CLA	C11-C10-C8-C7
29	C	505	CLA	C2-C3-C5-C6
29	C	507	CLA	C6-C7-C8-C10
29	Y	603	CLA	C2-C3-C5-C6
29	Y	604	CLA	C12-C13-C15-C16
29	c	511	CLA	C2-C3-C5-C6
29	g	613	CLA	C12-C13-C15-C16
45	n	609	CHL	C2-C3-C5-C6
29	c	501	CLA	C15-C16-C17-C18
39	j	101	DGA	CA7-CA8-CA9-CAA
40	G	624	LHG	C34-C35-C36-C37
40	c	525	LHG	O1-C1-C2-O2
38	T	101	3PH	C33-C34-C35-C36
40	l	101	LHG	C11-C12-C13-C14
46	N	620	LUT	C29-C30-C31-C32
29	S	605	CLA	CBD-CGD-O2D-CED
29	C	512	CLA	C16-C17-C18-C20
40	s	624	LHG	C2-C3-O3-P
37	B	623	DGD	O2G-C2G-C3G-O3G
29	S	603	CLA	C13-C15-C16-C17
45	N	607	CHL	C15-C16-C17-C18
29	S	612	CLA	CAA-CBA-CGA-O2A
45	G	606	CHL	O2A-C1-C2-C3
45	n	608	CHL	O2A-C1-C2-C3
29	a	406	CLA	CAA-CBA-CGA-O2A
29	b	614	CLA	CAA-CBA-CGA-O2A
29	g	614	CLA	CAA-CBA-CGA-O2A
35	C	523	LMG	O7-C10-C11-C12
50	s	625	LPX	O6-C6-C7-C8
51	Y	626	PTY	O4-C30-C31-C32
39	b	625	DGA	CA2-CA3-CA4-CA5
45	G	606	CHL	C2A-CAA-CBA-CGA
29	S	602	CLA	C11-C12-C13-C14
39	j	101	DGA	OG1-CA1-CA2-CA3
45	n	605	CHL	CAA-CBA-CGA-O2A
37	C	519	DGD	C2B-C3B-C4B-C5B
29	B	614	CLA	C4-C3-C5-C6
45	G	601	CHL	C4-C3-C5-C6
29	r	609	CLA	C5-C6-C7-C8
42	D	405	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
42	d	405	PL9	C38-C39-C41-C42
45	y	609	CHL	C2-C3-C5-C6
29	N	610	CLA	C16-C17-C18-C19
29	B	608	CLA	CAA-CBA-CGA-O2A
35	c	521	LMG	C14-C15-C16-C17
39	c	524	DGA	CFB-CGB-CHB-CIB
29	B	607	CLA	C14-C13-C15-C16
29	B	609	CLA	C6-C7-C8-C9
29	N	602	CLA	C6-C7-C8-C9
29	N	602	CLA	C14-C13-C15-C16
29	R	603	CLA	C6-C7-C8-C9
29	Y	611	CLA	C6-C7-C8-C9
29	b	602	CLA	C14-C13-C15-C16
29	b	604	CLA	C14-C13-C15-C16
29	b	614	CLA	C14-C13-C15-C16
29	b	617	CLA	C11-C10-C8-C9
29	g	603	CLA	C11-C10-C8-C9
29	g	611	CLA	C11-C12-C13-C14
29	g	611	CLA	C14-C13-C15-C16
29	y	610	CLA	C14-C13-C15-C16
45	N	605	CHL	C11-C10-C8-C9
45	n	601	CHL	C11-C12-C13-C14
45	n	606	CHL	C11-C10-C8-C9
45	g	607	CHL	C11-C10-C8-C9
45	y	601	CHL	C11-C10-C8-C9
45	y	607	CHL	C11-C12-C13-C14
40	c	525	LHG	C16-C17-C18-C19
40	D	409	LHG	C28-C29-C30-C31
40	G	624	LHG	C11-C10-C9-C8
29	b	617	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C3A-C2A-CAA-CBA
45	N	608	CHL	C3A-C2A-CAA-CBA
29	B	614	CLA	CAA-CBA-CGA-O2A
40	G	624	LHG	O7-C7-C8-C9
40	n	624	LHG	O7-C7-C8-C9
29	B	610	CLA	CAD-CBD-CGD-O2D
29	B	613	CLA	CAD-CBD-CGD-O2D
29	B	617	CLA	CAD-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O2D
29	G	612	CLA	CAD-CBD-CGD-O2D
29	G	614	CLA	CAD-CBD-CGD-O2D
29	R	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	S	611	CLA	CAD-CBD-CGD-O2D
29	S	612	CLA	CAD-CBD-CGD-O2D
29	S	617	CLA	CAD-CBD-CGD-O2D
29	Y	604	CLA	CAD-CBD-CGD-O2D
29	b	606	CLA	CAD-CBD-CGD-O2D
29	b	609	CLA	CAD-CBD-CGD-O2D
29	b	613	CLA	CAD-CBD-CGD-O2D
29	b	617	CLA	CAD-CBD-CGD-O2D
29	c	505	CLA	CAD-CBD-CGD-O2D
29	c	512	CLA	CAD-CBD-CGD-O2D
29	n	603	CLA	CAD-CBD-CGD-O2D
29	g	603	CLA	CAD-CBD-CGD-O2D
29	s	605	CLA	CAD-CBD-CGD-O2D
29	s	613	CLA	CAD-CBD-CGD-O2D
29	y	604	CLA	CAD-CBD-CGD-O2D
30	A	408	PHO	CAD-CBD-CGD-O2D
29	B	612	CLA	C16-C17-C18-C19
29	S	611	CLA	C16-C17-C18-C20
29	y	610	CLA	C16-C17-C18-C19
34	Y	625	SPH	C12-C13-C14-C15
40	L	101	LHG	C29-C30-C31-C32
40	d	409	LHG	C35-C36-C37-C38
40	D	410	LHG	C25-C26-C27-C28
40	d	409	LHG	C30-C31-C32-C33
30	a	409	PHO	C2-C1-O2A-CGA
35	D	411	LMG	C10-C11-C12-C13
29	R	609	CLA	CAA-CBA-CGA-O2A
29	R	612	CLA	CAA-CBA-CGA-O2A
29	S	611	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	CAA-CBA-CGA-O2A
29	s	603	CLA	CAA-CBA-CGA-O2A
33	c	526	SQD	O47-C7-C8-C9
45	N	605	CHL	CAA-CBA-CGA-O2A
35	h	102	LMG	C31-C32-C33-C34
29	C	510	CLA	C4-C3-C5-C6
29	y	603	CLA	C2-C3-C5-C6
45	Y	609	CHL	C2-C3-C5-C6
45	g	607	CHL	C2-C3-C5-C6
29	S	603	CLA	CAA-CBA-CGA-O2A
29	y	612	CLA	CAA-CBA-CGA-O2A
33	a	412	SQD	O48-C23-C24-C25
35	C	521	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	t	101	3PH	O31-C31-C32-C33
39	B	625	DGA	OG2-CB1-CB2-CB3
35	a	413	LMG	C18-C19-C20-C21
39	c	524	DGA	CB5-CB6-CB7-CB8
36	B	620	C7Z	C27-C28-C29-C30
46	R	620	LUT	C27-C28-C29-C30
35	b	622	LMG	C22-C23-C24-C25
35	w	201	LMG	C7-C8-C9-O8
48	y	622	XAT	O24-C26-C27-C28
29	B	612	CLA	C10-C11-C12-C13
29	N	613	CLA	CAA-CBA-CGA-O2A
29	R	604	CLA	CAA-CBA-CGA-O2A
29	c	507	CLA	CAA-CBA-CGA-O2A
37	c	518	DGD	O2G-C1B-C2B-C3B
29	B	608	CLA	C16-C17-C18-C20
40	S	624	LHG	C12-C13-C14-C15
33	B	621	SQD	C23-C24-C25-C26
40	N	624	LHG	C19-C20-C21-C22
29	N	603	CLA	O2A-C1-C2-C3
29	r	609	CLA	O2A-C1-C2-C3
29	s	614	CLA	O2A-C1-C2-C3
29	y	608	CLA	O2A-C1-C2-C3
45	n	605	CHL	O2A-C1-C2-C3
45	y	607	CHL	O2A-C1-C2-C3
51	y	626	PTY	C38-C39-C40-C41
29	B	616	CLA	CBA-CGA-O2A-C1
29	S	611	CLA	C2A-CAA-CBA-CGA
29	Y	610	CLA	C2A-CAA-CBA-CGA
29	c	505	CLA	C2A-CAA-CBA-CGA
29	s	610	CLA	C2A-CAA-CBA-CGA
29	B	607	CLA	C13-C15-C16-C17
29	B	615	CLA	CAA-CBA-CGA-O2A
39	b	625	DGA	OG2-CB1-CB2-CB3
40	N	624	LHG	O7-C7-C8-C9
40	D	410	LHG	C24-C25-C26-C27
34	a	414	SPH	C4-C5-C6-C7
29	B	608	CLA	C16-C17-C18-C19
29	b	605	CLA	C16-C17-C18-C19
29	n	602	CLA	C16-C17-C18-C19
29	S	605	CLA	O1D-CGD-O2D-CED
37	c	520	DGD	C2A-C3A-C4A-C5A
29	B	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	B	602	CLA	CHA-CBD-CGD-O2D
29	C	504	CLA	CHA-CBD-CGD-O2D
29	C	507	CLA	CHA-CBD-CGD-O2D
29	N	612	CLA	CHA-CBD-CGD-O1D
29	N	612	CLA	CHA-CBD-CGD-O2D
29	Y	602	CLA	CHA-CBD-CGD-O1D
29	Y	613	CLA	CHA-CBD-CGD-O1D
29	Y	613	CLA	CHA-CBD-CGD-O2D
29	b	611	CLA	CHA-CBD-CGD-O2D
29	b	616	CLA	CHA-CBD-CGD-O1D
29	b	616	CLA	CHA-CBD-CGD-O2D
29	c	504	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O1D
29	c	507	CLA	CHA-CBD-CGD-O2D
29	c	511	CLA	CHA-CBD-CGD-O1D
29	c	511	CLA	CHA-CBD-CGD-O2D
29	n	602	CLA	CHA-CBD-CGD-O1D
29	n	612	CLA	CHA-CBD-CGD-O1D
29	n	612	CLA	CHA-CBD-CGD-O2D
29	n	613	CLA	CHA-CBD-CGD-O1D
29	n	613	CLA	CHA-CBD-CGD-O2D
29	g	604	CLA	CHA-CBD-CGD-O1D
29	r	608	CLA	CHA-CBD-CGD-O2D
29	s	604	CLA	CHA-CBD-CGD-O1D
29	s	612	CLA	CHA-CBD-CGD-O1D
29	s	612	CLA	CHA-CBD-CGD-O2D
29	y	602	CLA	CHA-CBD-CGD-O2D
31	C	514	BCR	C13-C14-C15-C16
31	b	619	BCR	C9-C10-C11-C12
45	R	607	CHL	CHA-CBD-CGD-O1D
45	R	607	CHL	CHA-CBD-CGD-O2D
45	n	601	CHL	CHA-CBD-CGD-O1D
45	r	607	CHL	CHA-CBD-CGD-O1D
45	r	607	CHL	CHA-CBD-CGD-O2D
45	s	601	CHL	CHA-CBD-CGD-O2D
48	g	622	XAT	C29-C30-C31-C32
45	Y	607	CHL	C10-C11-C12-C13
30	A	408	PHO	C4-C3-C5-C6
40	d	409	LHG	C33-C34-C35-C36
42	D	405	PL9	C38-C39-C41-C42
33	m	101	SQD	C11-C12-C13-C14
29	A	405	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	B	617	CLA	CAA-CBA-CGA-O2A
29	G	603	CLA	CAA-CBA-CGA-O2A
29	S	614	CLA	CAA-CBA-CGA-O2A
29	b	613	CLA	CAA-CBA-CGA-O2A
29	r	604	CLA	CAA-CBA-CGA-O2A
39	B	625	DGA	OG1-CA1-CA2-CA3
45	G	605	CHL	CAA-CBA-CGA-O2A
35	d	411	LMG	C15-C16-C17-C18
29	c	512	CLA	CAA-CBA-CGA-O2A
35	c	521	LMG	O8-C28-C29-C30
37	B	623	DGD	O1G-C1A-C2A-C3A
40	Y	624	LHG	O8-C23-C24-C25
45	n	606	CHL	CAA-CBA-CGA-O2A
29	r	610	CLA	O1D-CGD-O2D-CED
29	C	510	CLA	C16-C17-C18-C19
30	A	409	PHO	CHA-CBD-CGD-O2D
30	a	408	PHO	CHA-CBD-CGD-O2D
30	a	409	PHO	CHA-CBD-CGD-O1D
34	A	414	SPH	N2-C2-C3-O3
35	c	521	LMG	O9-C10-C11-C12
35	C	527	LMG	O8-C28-C29-C30
35	a	413	LMG	O7-C10-C11-C12
40	L	101	LHG	C31-C32-C33-C34
37	c	519	DGD	C1A-C2A-C3A-C4A
40	n	624	LHG	C19-C20-C21-C22
29	B	604	CLA	C2-C3-C5-C6
29	S	611	CLA	C11-C10-C8-C7
29	Y	610	CLA	C12-C13-C15-C16
29	b	615	CLA	C11-C12-C13-C15
29	c	505	CLA	C11-C10-C8-C7
29	g	613	CLA	C6-C7-C8-C10
29	C	503	CLA	C10-C11-C12-C13
29	C	510	CLA	CAA-CBA-CGA-O2A
40	c	525	LHG	O7-C7-C8-C9
51	y	626	PTY	O4-C30-C31-C32
29	S	612	CLA	CAA-CBA-CGA-O1A
29	A	406	CLA	C11-C10-C8-C9
29	A	410	CLA	C11-C10-C8-C9
29	C	502	CLA	C6-C7-C8-C9
29	C	506	CLA	C11-C10-C8-C9
29	C	509	CLA	C11-C10-C8-C9
29	Y	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	603	CLA	C11-C10-C8-C9
29	b	617	CLA	C6-C7-C8-C9
29	c	505	CLA	C6-C7-C8-C9
29	n	613	CLA	C11-C10-C8-C9
29	g	613	CLA	C6-C7-C8-C9
29	s	611	CLA	C11-C12-C13-C14
45	G	607	CHL	C11-C12-C13-C14
45	n	607	CHL	C11-C12-C13-C14
31	c	514	BCR	C15-C16-C17-C18
40	N	624	LHG	C18-C19-C20-C21
48	G	622	XAT	C14-C15-C35-C34
45	Y	605	CHL	CAA-CBA-CGA-O2A
51	y	626	PTY	C13-C14-C15-C16
29	Y	602	CLA	CBA-CGA-O2A-C1
29	A	406	CLA	CAA-CBA-CGA-O2A
33	M	101	SQD	O47-C7-C8-C9
35	b	622	LMG	O7-C10-C11-C12
40	L	101	LHG	O7-C7-C8-C9
33	C	526	SQD	C4-C5-C6-S
33	b	626	SQD	C4-C5-C6-S
33	c	526	SQD	C4-C5-C6-S
29	B	616	CLA	O1A-CGA-O2A-C1
29	c	506	CLA	C10-C11-C12-C13
33	a	412	SQD	O10-C23-C24-C25
35	C	523	LMG	O9-C10-C11-C12
35	C	527	LMG	C11-C12-C13-C14
29	c	510	CLA	CAA-CBA-CGA-O2A
35	W	201	LMG	O8-C28-C29-C30
38	s	626	3PH	O21-C21-C22-C23
33	B	626	SQD	C19-C20-C21-C22
39	B	625	DGA	CA2-CA3-CA4-CA5
50	s	625	LPX	O7-C6-C7-C8
51	Y	626	PTY	O30-C30-C31-C32
29	R	604	CLA	CAA-CBA-CGA-O1A
29	R	612	CLA	CAA-CBA-CGA-O1A
29	c	510	CLA	CAA-CBA-CGA-O1A
29	y	612	CLA	CAA-CBA-CGA-O1A
38	s	626	3PH	O22-C21-C22-C23
40	n	624	LHG	O9-C7-C8-C9
45	n	605	CHL	CAA-CBA-CGA-O1A
31	C	517	BCR	C7-C8-C9-C10
31	C	516	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
36	b	620	C7Z	C27-C28-C29-C30
40	g	624	LHG	C33-C34-C35-C36
29	s	603	CLA	C8-C10-C11-C12
29	A	406	CLA	C2C-C3C-CAC-CBC
29	D	402	CLA	C1A-C2A-CAA-CBA
29	g	612	CLA	C1A-C2A-CAA-CBA
29	y	611	CLA	C1A-C2A-CAA-CBA
45	n	607	CHL	C1A-C2A-CAA-CBA
45	y	605	CHL	C1A-C2A-CAA-CBA
29	B	608	CLA	CAA-CBA-CGA-O1A
29	a	406	CLA	CAA-CBA-CGA-O1A
29	g	614	CLA	CAA-CBA-CGA-O1A
29	r	603	CLA	C2-C1-O2A-CGA
35	W	201	LMG	C32-C33-C34-C35
33	b	626	SQD	C24-C23-O48-C46
29	b	607	CLA	CAA-CBA-CGA-O1A
37	c	518	DGD	O1B-C1B-C2B-C3B
38	t	101	3PH	O32-C31-C32-C33
40	N	624	LHG	O9-C7-C8-C9
40	G	624	LHG	O9-C7-C8-C9
39	j	101	DGA	CB7-CB8-CB9-CAB
40	d	408	LHG	C30-C31-C32-C33
29	C	512	CLA	CAA-CBA-CGA-O2A
39	b	625	DGA	OG1-CA1-CA2-CA3
29	B	609	CLA	C2A-CAA-CBA-CGA
29	b	604	CLA	C2A-CAA-CBA-CGA
29	r	602	CLA	C2A-CAA-CBA-CGA
29	s	602	CLA	C2A-CAA-CBA-CGA
29	S	603	CLA	C16-C17-C18-C19
29	b	616	CLA	C16-C17-C18-C20
29	A	406	CLA	CAA-CBA-CGA-O1A
37	C	518	DGD	CCB-CDB-CEB-CFB
33	b	626	SQD	O10-C23-O48-C46
33	M	101	SQD	C11-C10-C9-C8
29	C	505	CLA	C4-C3-C5-C6
39	J	101	DGA	OG1-CA1-CA2-CA3
29	b	612	CLA	C8-C10-C11-C12
29	g	610	CLA	C8-C10-C11-C12
45	N	601	CHL	C8-C10-C11-C12
40	C	525	LHG	C2-C3-O3-P
40	Y	624	LHG	C32-C33-C34-C35
29	B	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
39	B	625	DGA	OA1-CA1-CA2-CA3
45	G	605	CHL	CAA-CBA-CGA-O1A
29	B	607	CLA	C8-C10-C11-C12
39	j	101	DGA	CB4-CB5-CB6-CB7
40	S	624	LHG	C3-O3-P-O5
40	d	408	LHG	C4-O6-P-O4
50	S	625	LPX	C1-O2-P1-O4
51	y	626	PTY	C5-O14-P1-O13
29	Y	611	CLA	C16-C17-C18-C19
40	d	410	LHG	C29-C30-C31-C32
29	B	615	CLA	CAA-CBA-CGA-O1A
29	S	603	CLA	CAA-CBA-CGA-O1A
29	b	613	CLA	CAA-CBA-CGA-O1A
29	b	614	CLA	CAA-CBA-CGA-O1A
39	j	101	DGA	OA1-CA1-CA2-CA3
51	y	626	PTY	O30-C30-C31-C32
29	R	604	CLA	O2A-C1-C2-C3
29	r	604	CLA	O2A-C1-C2-C3
29	n	613	CLA	CAA-CBA-CGA-O2A
35	a	413	LMG	C13-C14-C15-C16
35	w	201	LMG	C30-C31-C32-C33
31	B	618	BCR	C23-C24-C25-C26
31	b	619	BCR	C23-C24-C25-C26
46	s	620	LUT	C5-C6-C7-C8
29	N	613	CLA	CAA-CBA-CGA-O1A
29	s	603	CLA	CAA-CBA-CGA-O1A
33	c	526	SQD	O49-C7-C8-C9
35	W	201	LMG	O10-C28-C29-C30
39	b	625	DGA	OB1-CB1-CB2-CB3
35	H	102	LMG	C37-C38-C39-C40
29	C	501	CLA	CAA-CBA-CGA-O2A
33	B	626	SQD	C11-C12-C13-C14
29	G	602	CLA	C2A-CAA-CBA-CGA
29	R	602	CLA	C2A-CAA-CBA-CGA
29	S	611	CLA	CAA-CBA-CGA-O1A
29	Y	602	CLA	O1A-CGA-O2A-C1
38	B	624	3PH	C2E-C2F-C2G-C2H
29	B	607	CLA	CAA-CBA-CGA-O2A
45	y	601	CHL	C13-C15-C16-C17
34	a	414	SPH	C15-C16-C17-C18
38	b	624	3PH	C2C-C2D-C2E-C2F
29	r	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
39	B	625	DGA	OB1-CB1-CB2-CB3
29	S	604	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	C2-C3-C5-C6
29	B	602	CLA	C5-C6-C7-C8
29	C	506	CLA	CAD-CBD-CGD-O1D
29	C	511	CLA	CAD-CBD-CGD-O1D
29	G	604	CLA	CAD-CBD-CGD-O1D
29	S	604	CLA	CAD-CBD-CGD-O1D
29	b	607	CLA	C3-C5-C6-C7
29	b	608	CLA	CAD-CBD-CGD-O1D
29	b	616	CLA	CAD-CBD-CGD-O1D
29	c	503	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CAD-CBD-CGD-O1D
29	c	506	CLA	CAD-CBD-CGD-O1D
29	g	604	CLA	CAD-CBD-CGD-O1D
29	g	614	CLA	CAD-CBD-CGD-O1D
33	C	526	SQD	O5-C5-C6-S
33	M	101	SQD	O5-C5-C6-S
33	b	626	SQD	O5-C5-C6-S
38	b	624	3PH	C3-C2-O21-C21
45	N	601	CHL	CAD-CBD-CGD-O1D
45	R	607	CHL	CAD-CBD-CGD-O1D
45	n	601	CHL	CAD-CBD-CGD-O1D
51	Y	626	PTY	C2-C3-O11-P1
29	B	617	CLA	CAA-CBA-CGA-O1A
29	C	510	CLA	CAA-CBA-CGA-O1A
29	c	507	CLA	CAA-CBA-CGA-O1A
37	B	623	DGD	O1A-C1A-C2A-C3A
33	c	526	SQD	C27-C28-C29-C30
37	c	518	DGD	C4A-C5A-C6A-C7A
29	a	406	CLA	C15-C16-C17-C18
29	B	603	CLA	C11-C12-C13-C14
29	C	513	CLA	C6-C7-C8-C9
29	Y	614	CLA	C11-C10-C8-C9
29	b	606	CLA	C11-C12-C13-C14
29	b	609	CLA	C11-C12-C13-C14
29	b	613	CLA	C11-C10-C8-C9
29	c	505	CLA	C11-C12-C13-C14
29	c	509	CLA	C11-C10-C8-C9
45	Y	607	CHL	C11-C12-C13-C14
45	s	608	CHL	C6-C7-C8-C9
40	c	497	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
40	n	624	LHG	O1-C1-C2-O2
29	c	512	CLA	CAA-CBA-CGA-O1A
45	n	606	CHL	CAA-CBA-CGA-O1A
29	a	405	CLA	CAA-CBA-CGA-O2A
35	B	622	LMG	O7-C10-C11-C12
39	C	524	DGA	OG1-CA1-CA2-CA3
29	B	607	CLA	C10-C11-C12-C13
45	Y	605	CHL	CAA-CBA-CGA-O1A
49	r	625	LMT	C2-C3-C4-C5
29	G	603	CLA	CAA-CBA-CGA-O1A
29	S	614	CLA	CAA-CBA-CGA-O1A
29	B	615	CLA	C5-C6-C7-C8
40	D	408	LHG	C27-C28-C29-C30
29	B	613	CLA	CAA-CBA-CGA-O2A
29	G	614	CLA	CAA-CBA-CGA-O2A
29	c	501	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	O2G-C1B-C2B-C3B
38	b	624	3PH	O21-C21-C22-C23
39	J	101	DGA	OG2-CB1-CB2-CB3
40	y	624	LHG	O8-C23-C24-C25
39	b	625	DGA	OA1-CA1-OG1-CG1
29	c	509	CLA	C13-C15-C16-C17
35	c	521	LMG	O10-C28-C29-C30
40	L	101	LHG	O9-C7-C8-C9
40	Y	624	LHG	O10-C23-C24-C25
38	B	624	3PH	C2-C1-O11-P
29	g	613	CLA	C4-C3-C5-C6
45	g	601	CHL	C4-C3-C5-C6
29	B	610	CLA	C8-C10-C11-C12
29	B	602	CLA	C3A-C2A-CAA-CBA
29	B	606	CLA	C2-C3-C5-C6
29	B	607	CLA	C11-C12-C13-C15
29	B	608	CLA	C6-C7-C8-C10
29	Y	611	CLA	C11-C10-C8-C7
29	Y	614	CLA	C11-C10-C8-C7
29	b	605	CLA	C12-C13-C15-C16
29	b	613	CLA	C11-C10-C8-C7
29	b	614	CLA	C2-C3-C5-C6
29	c	505	CLA	C11-C12-C13-C15
29	c	508	CLA	C6-C7-C8-C10
29	s	610	CLA	C11-C10-C8-C7
29	y	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	y	612	CLA	C6-C7-C8-C10
45	G	607	CHL	C3A-C2A-CAA-CBA
29	A	405	CLA	CAA-CBA-CGA-O1A
35	a	413	LMG	O9-C10-C11-C12
38	b	624	3PH	O22-C21-C22-C23
39	J	101	DGA	OA1-CA1-CA2-CA3
39	b	625	DGA	OA1-CA1-CA2-CA3
29	b	615	CLA	CAA-CBA-CGA-O2A
29	g	603	CLA	CAA-CBA-CGA-O2A
33	a	412	SQD	O47-C7-C8-C9
31	b	619	BCR	C11-C12-C13-C14
36	B	620	C7Z	C11-C12-C13-C14
46	n	620	LUT	C27-C28-C29-C30
46	r	620	LUT	C11-C12-C13-C14
47	Y	623	NEX	C11-C12-C13-C14
47	y	623	NEX	C11-C12-C13-C14
29	g	603	CLA	CAA-CBA-CGA-O1A
47	G	623	NEX	C9-C10-C11-C12
47	G	623	NEX	C13-C14-C15-C35
29	S	613	CLA	C2C-C3C-CAC-CBC
35	C	521	LMG	C12-C13-C14-C15
40	n	624	LHG	C27-C28-C29-C30
29	n	614	CLA	CAA-CBA-CGA-O2A
33	A	412	SQD	O47-C7-C8-C9
45	G	607	CHL	CAA-CBA-CGA-O2A
29	y	603	CLA	C5-C6-C7-C8
29	y	614	CLA	C5-C6-C7-C8
45	n	607	CHL	C5-C6-C7-C8
35	B	622	LMG	O9-C10-C11-C12
35	b	622	LMG	O9-C10-C11-C12
39	C	524	DGA	OA1-CA1-CA2-CA3
40	c	525	LHG	O9-C7-C8-C9
29	Y	602	CLA	C10-C11-C12-C13
39	J	101	DGA	CA5-CA6-CA7-CA8
29	g	613	CLA	CAA-CBA-CGA-O2A
29	s	614	CLA	CAA-CBA-CGA-O2A
45	g	606	CHL	CAA-CBA-CGA-O2A
29	Y	602	CLA	C5-C6-C7-C8
29	C	512	CLA	CAA-CBA-CGA-O1A
29	b	615	CLA	CAA-CBA-CGA-O1A
29	C	503	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	C2A-CAA-CBA-CGA

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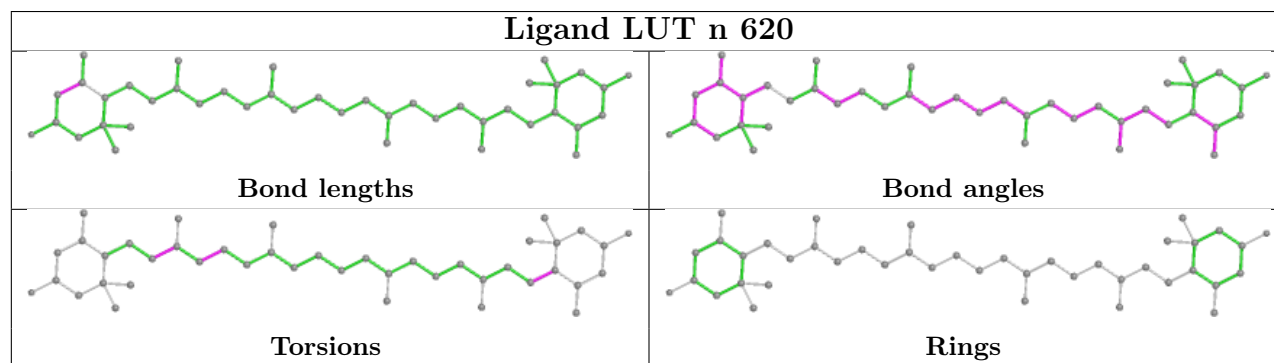
Mol	Chain	Res	Type	Atoms
29	S	602	CLA	C11-C12-C13-C15
29	N	602	CLA	C13-C15-C16-C17
45	N	605	CHL	C15-C16-C17-C18
33	M	101	SQD	C26-C27-C28-C29
33	m	101	SQD	C12-C13-C14-C15
38	b	624	3PH	C31-C32-C33-C34
35	C	527	LMG	O10-C28-C29-C30
38	b	624	3PH	C29-C2A-C2B-C2C
29	s	613	CLA	CAA-CBA-CGA-O2A

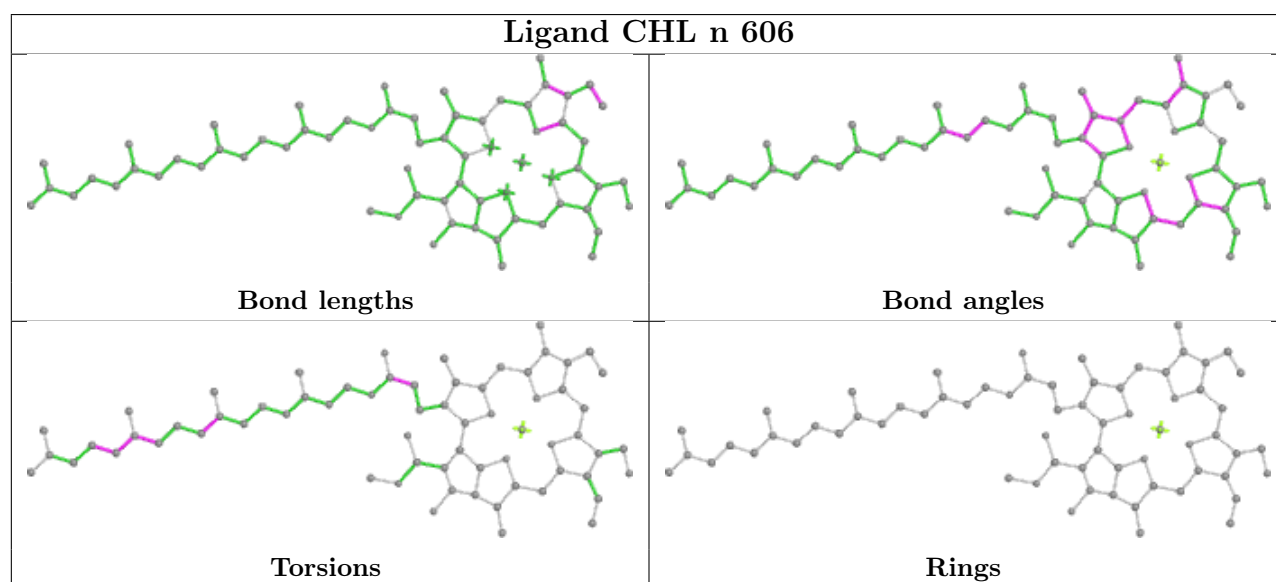
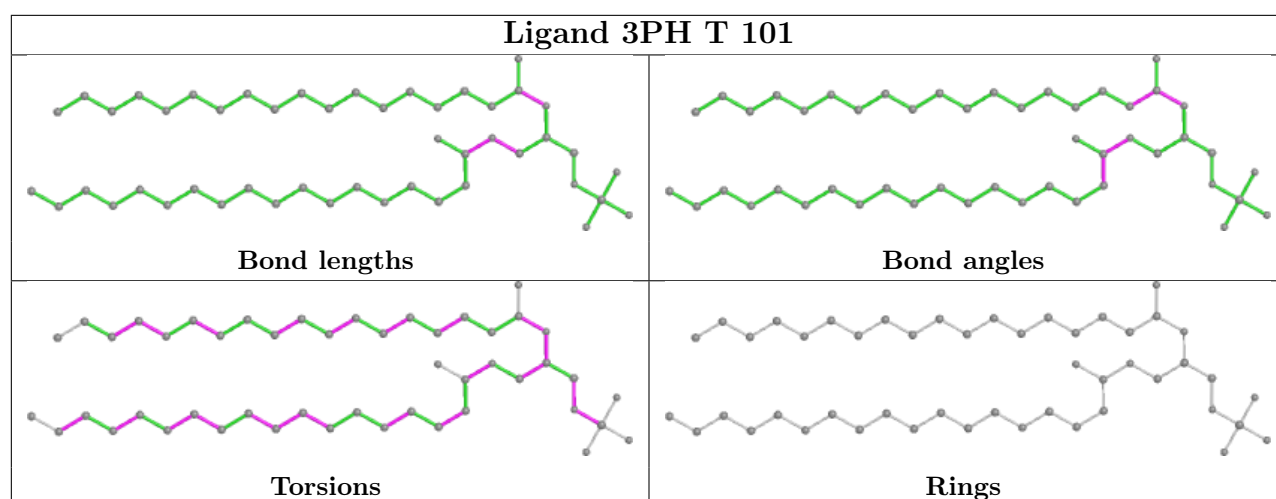
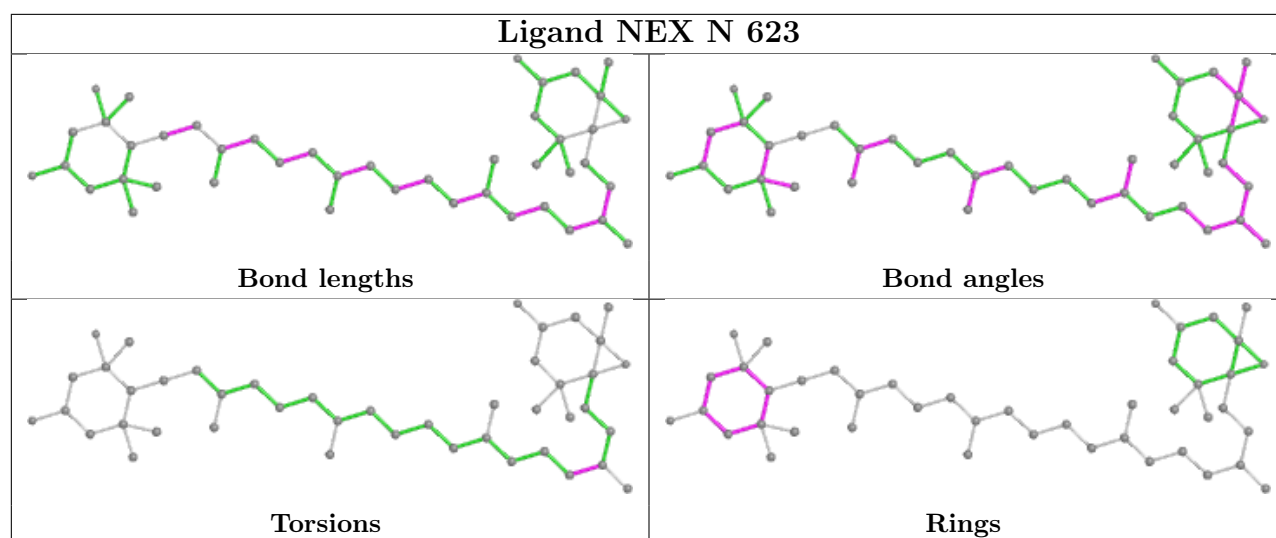
All (2) ring outliers are listed below:

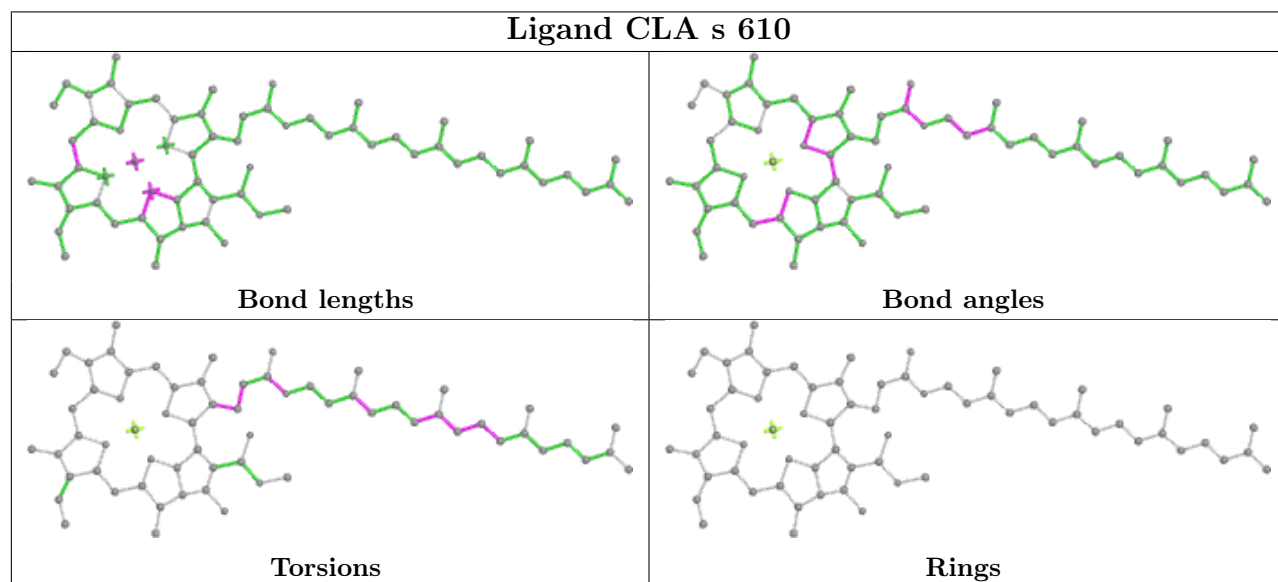
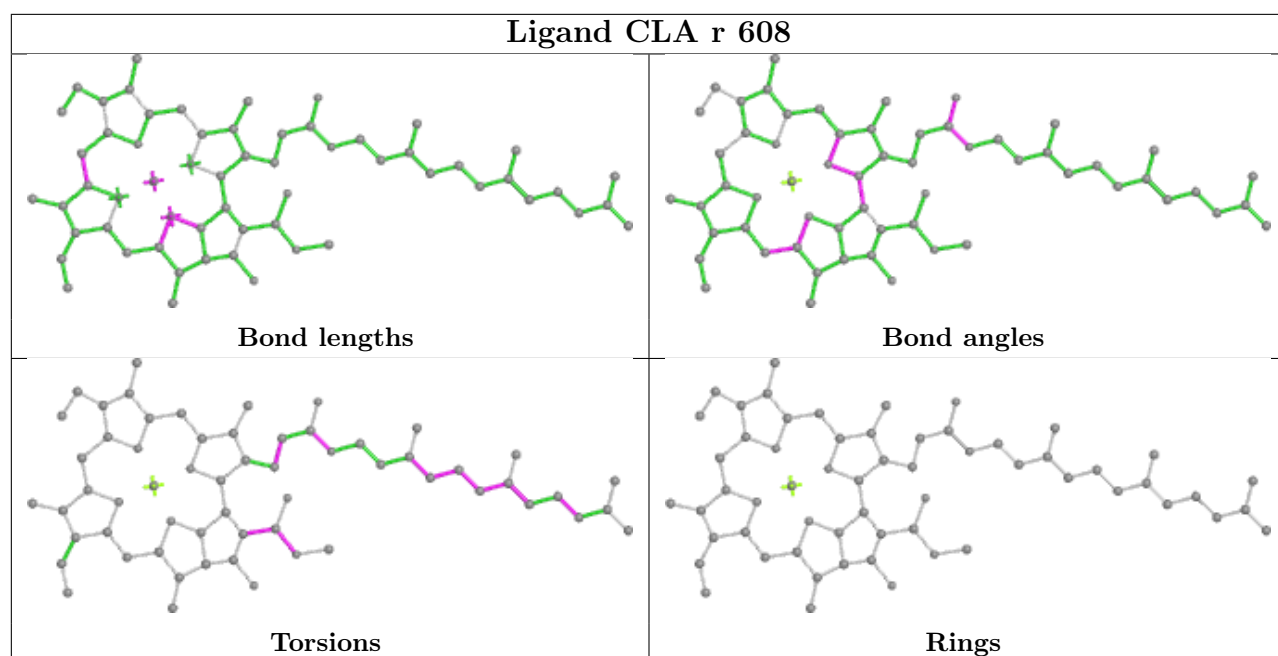
Mol	Chain	Res	Type	Atoms
47	n	623	NEX	C1-C2-C3-C4-C5-C6
47	N	623	NEX	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

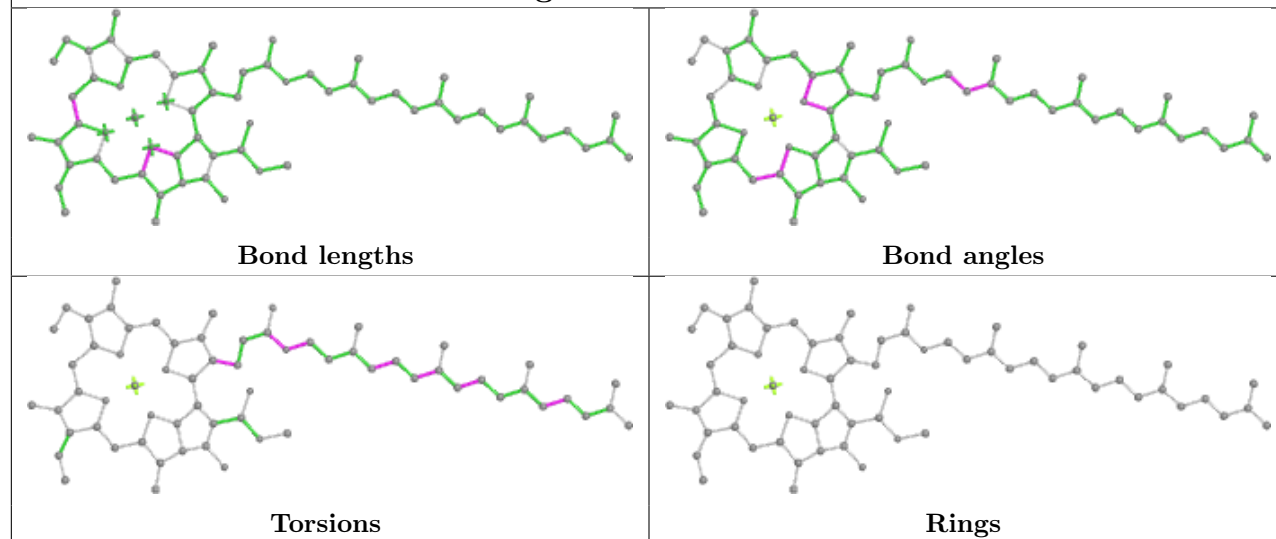
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



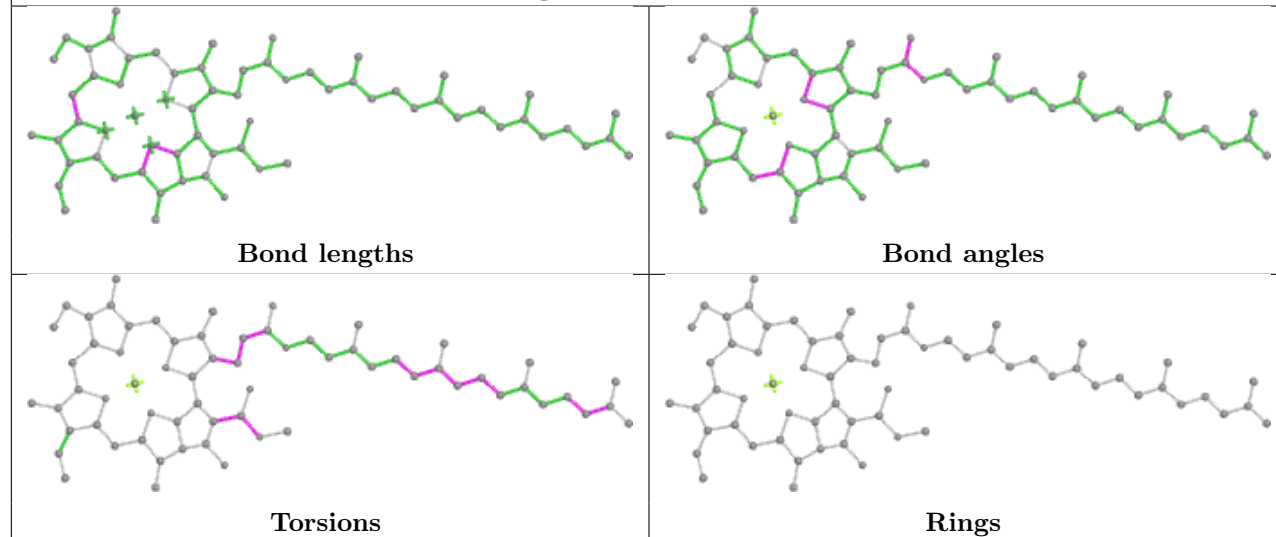




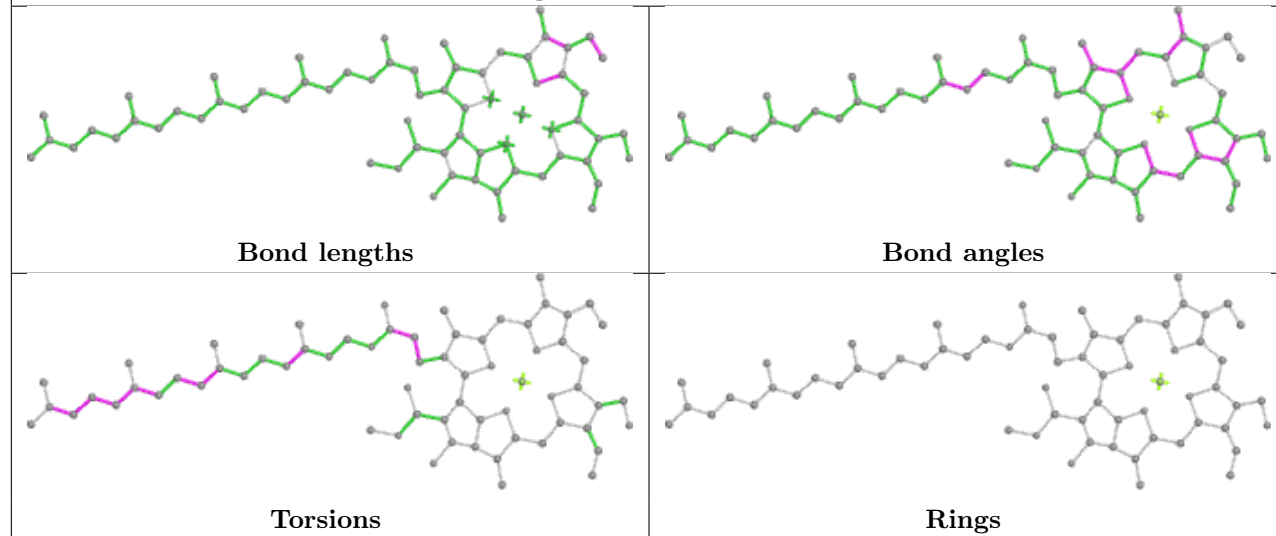
Ligand CLA S 610

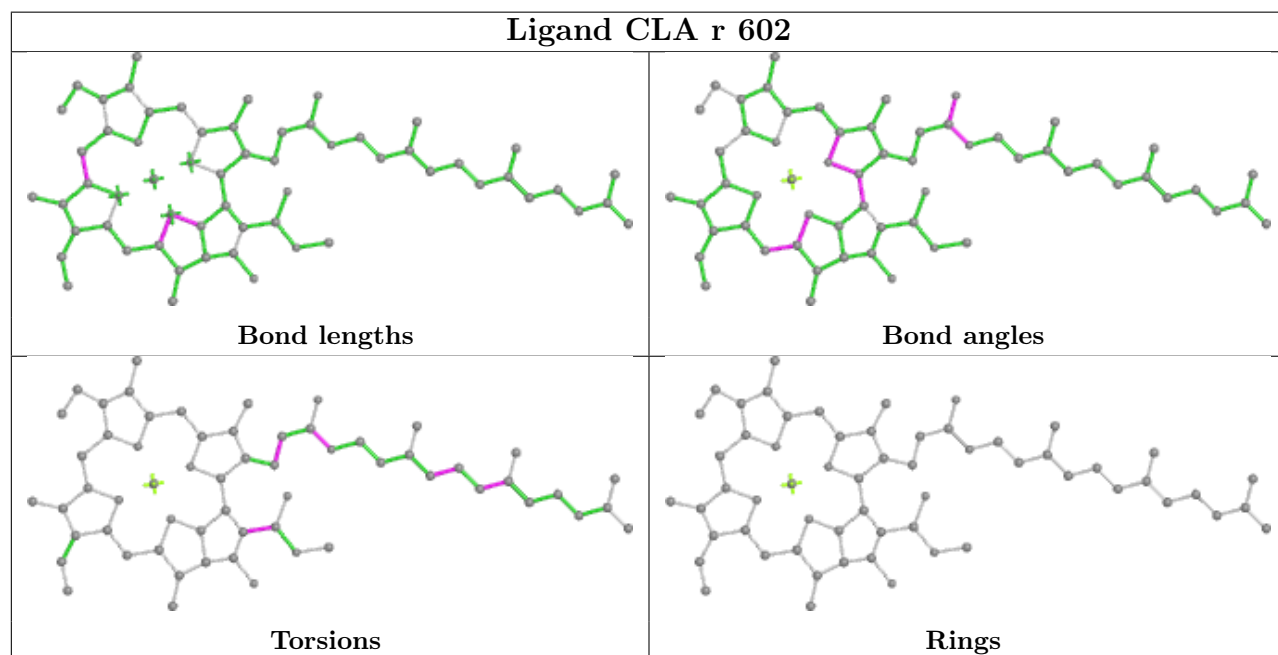
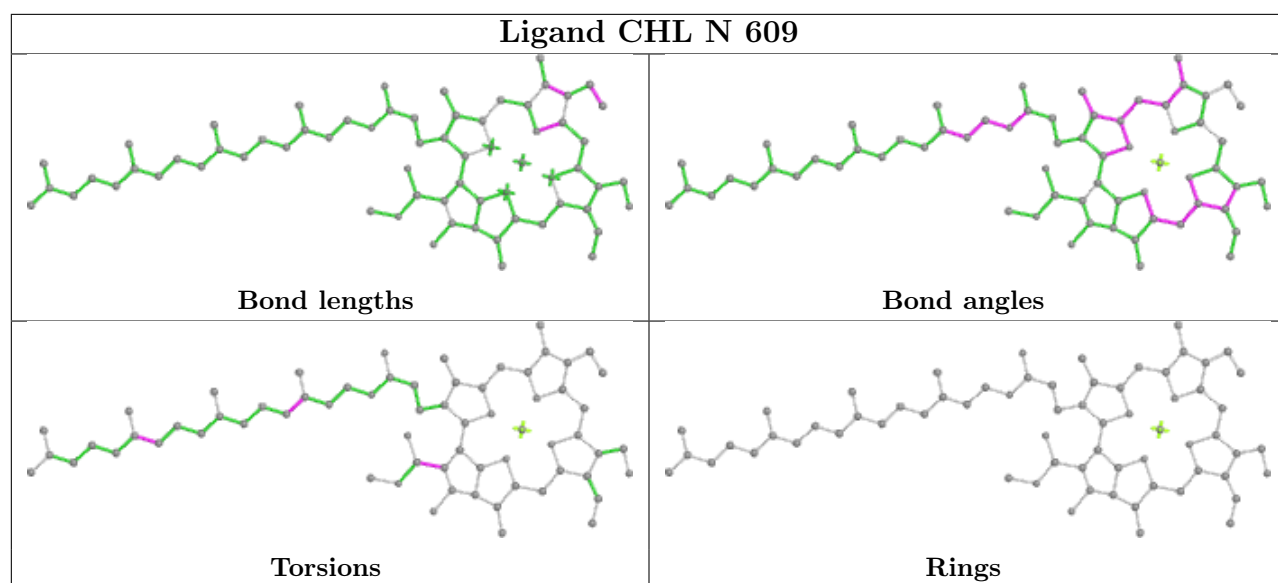


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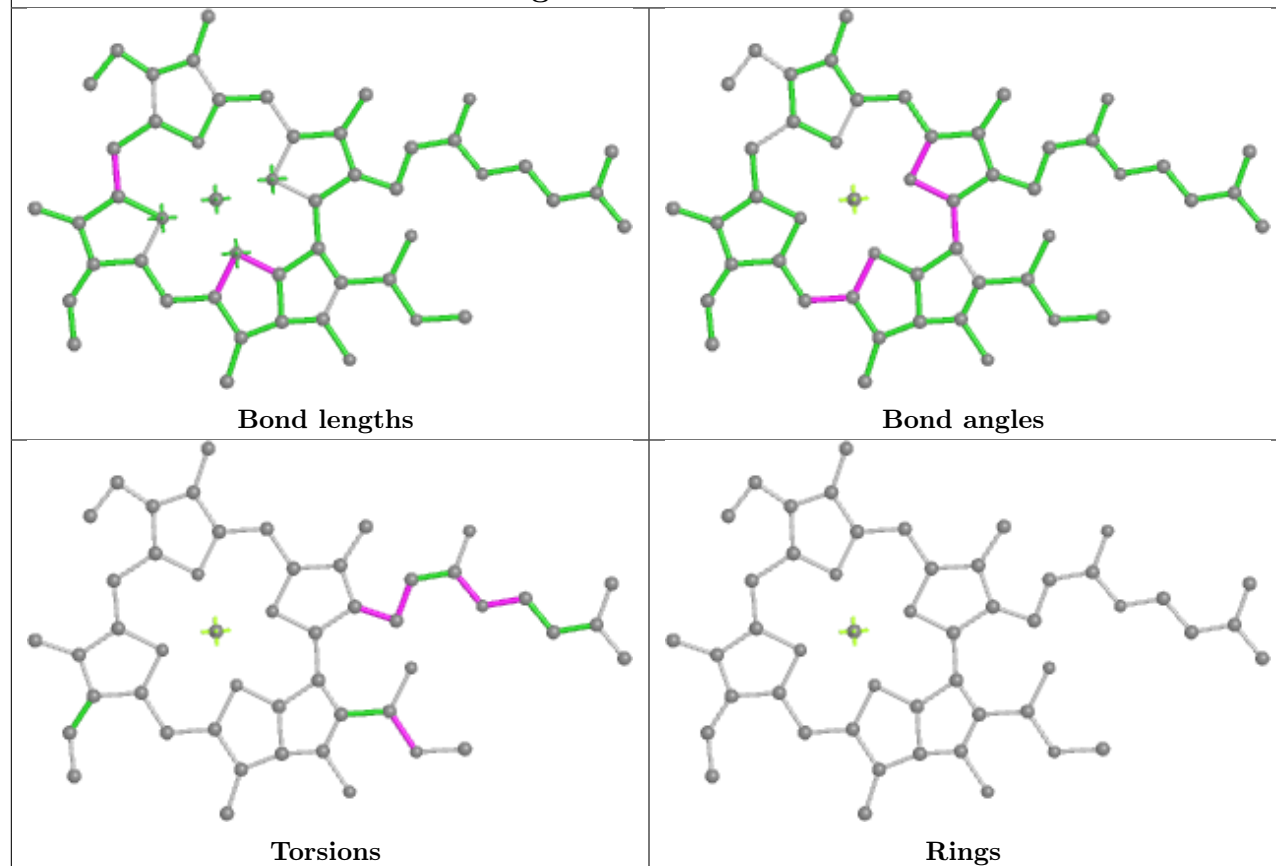


Ligand CHL N 605

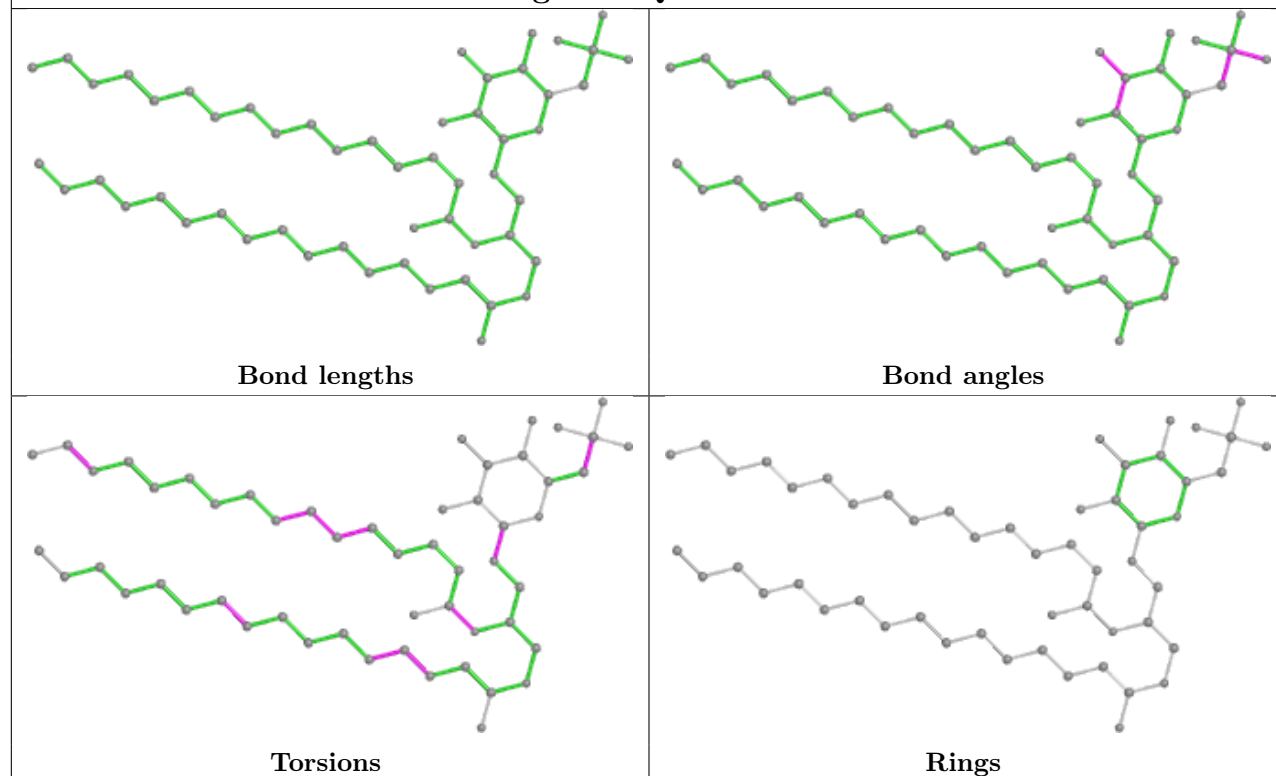


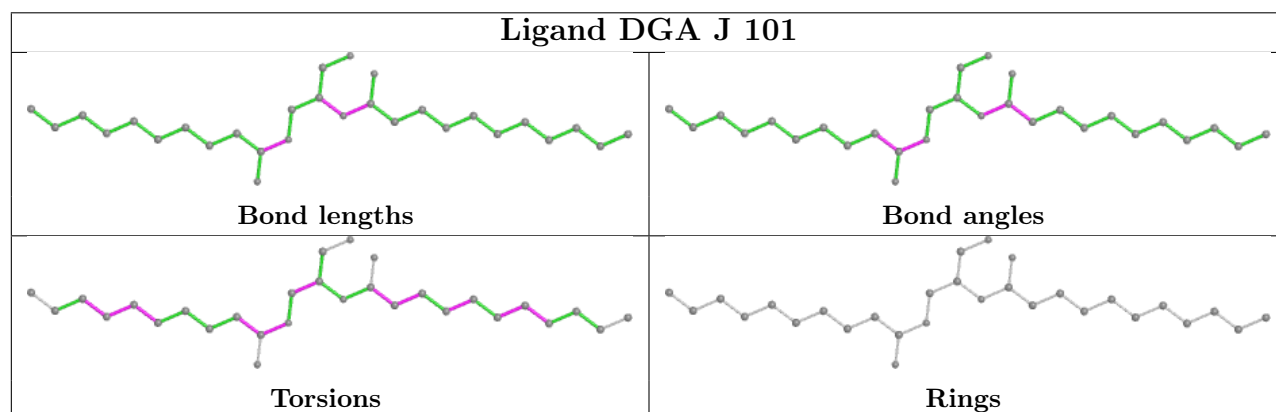
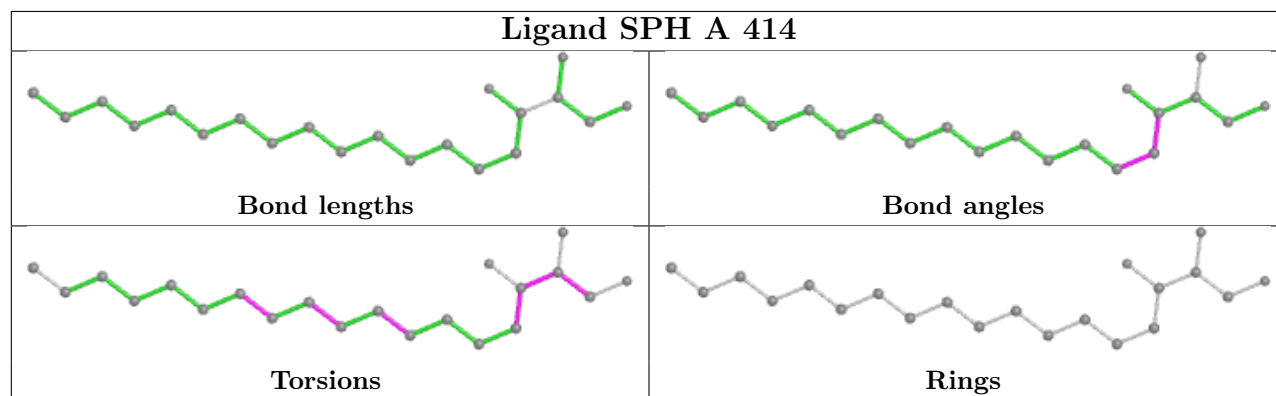
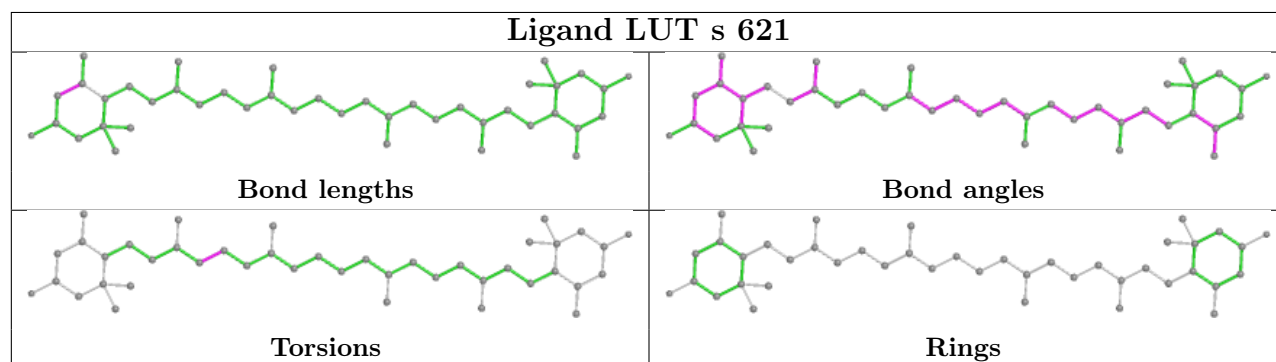
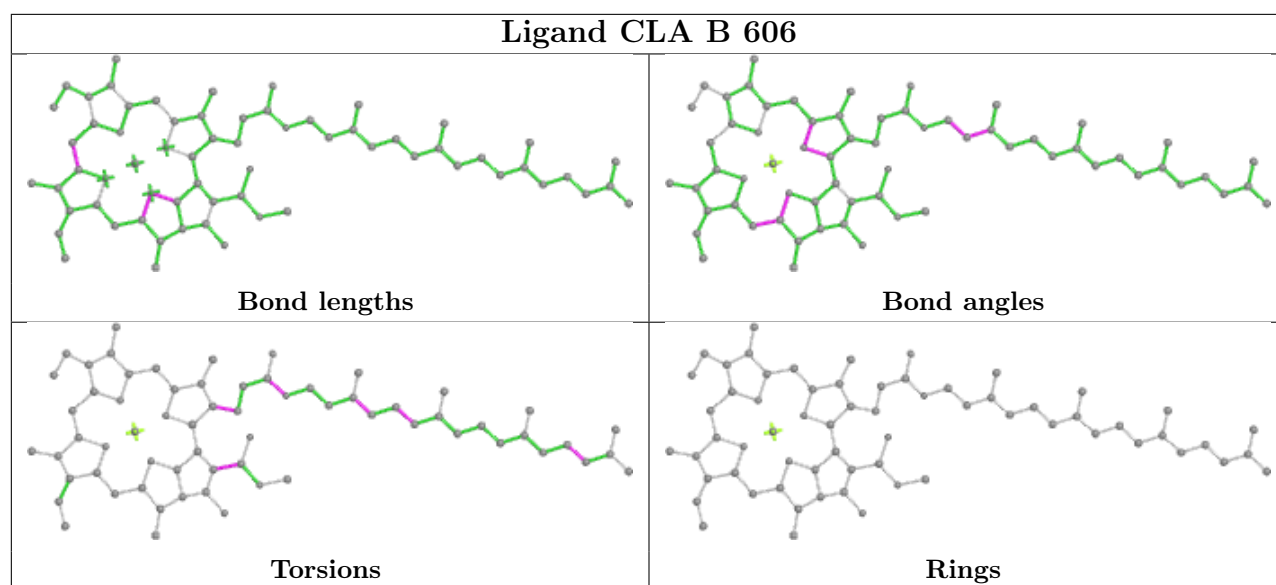


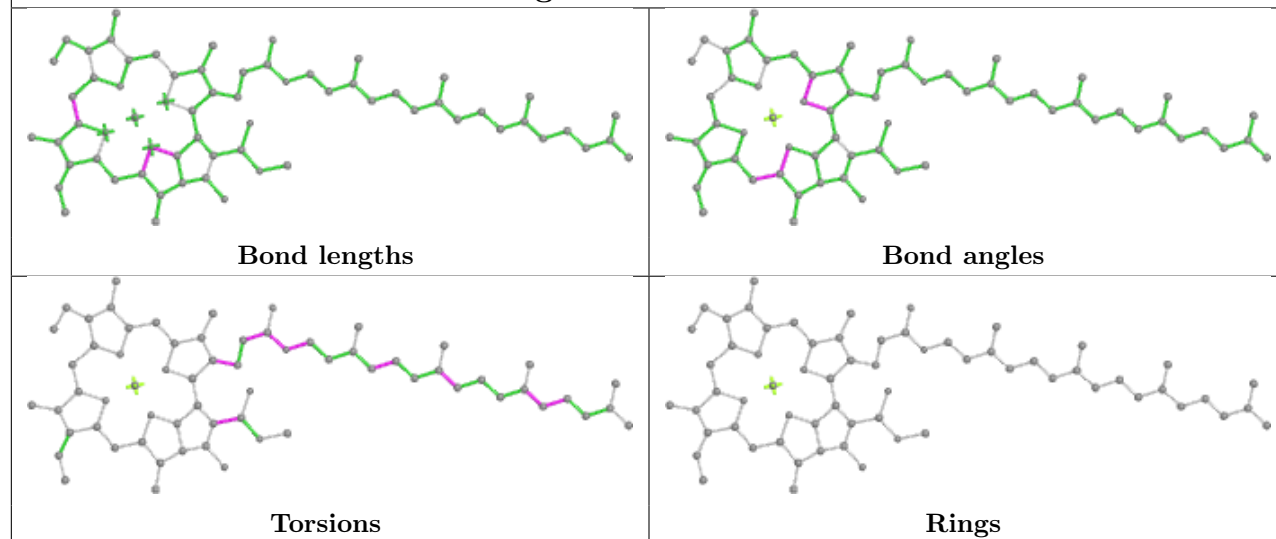
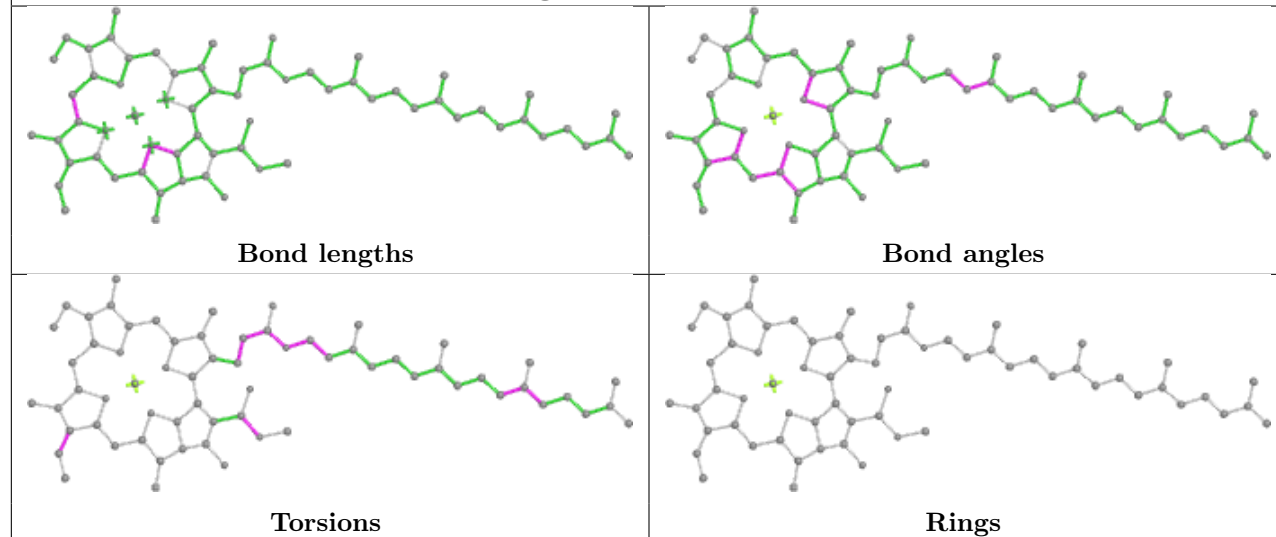
Ligand CLA Y 608



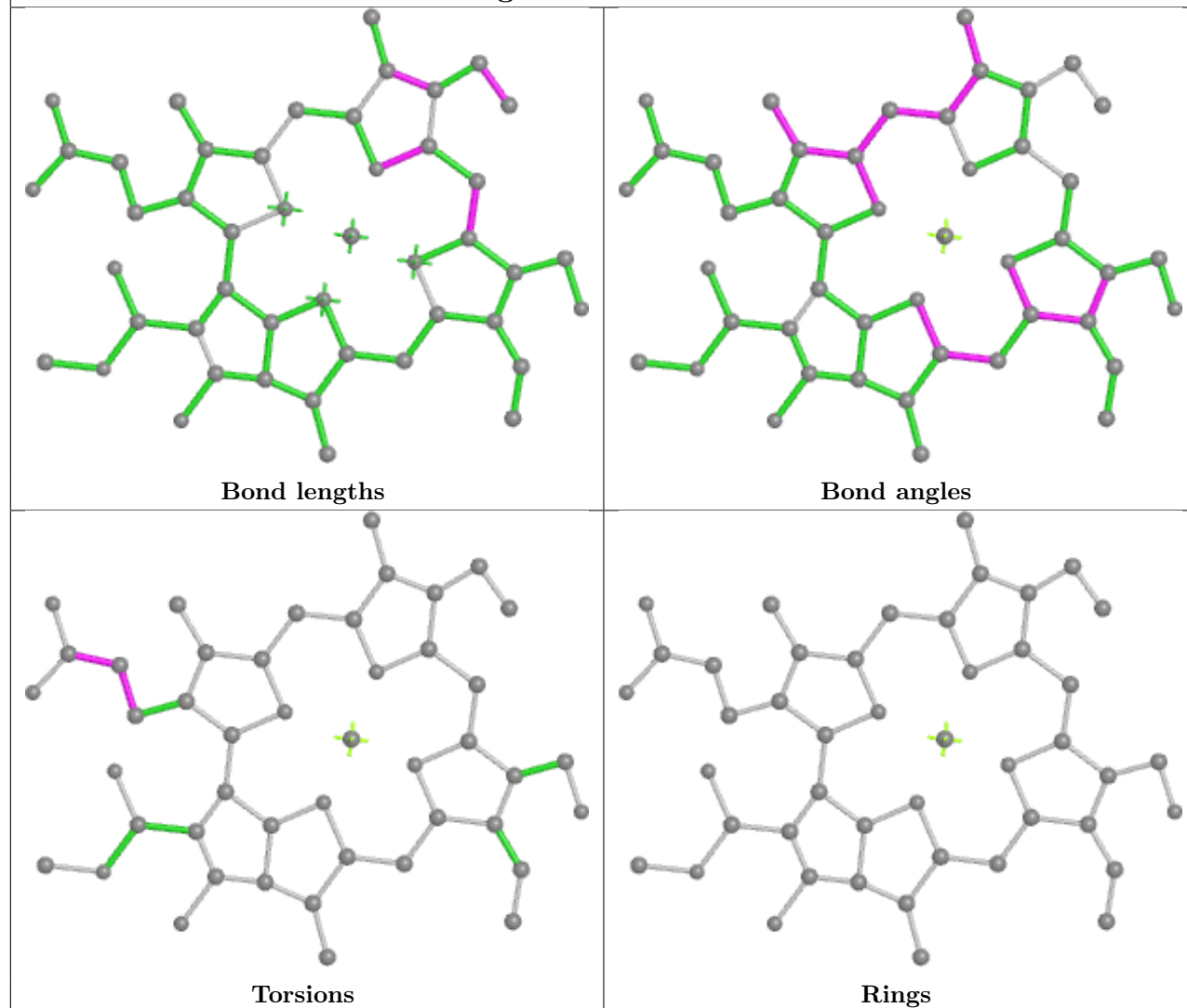
Ligand SQD B 626



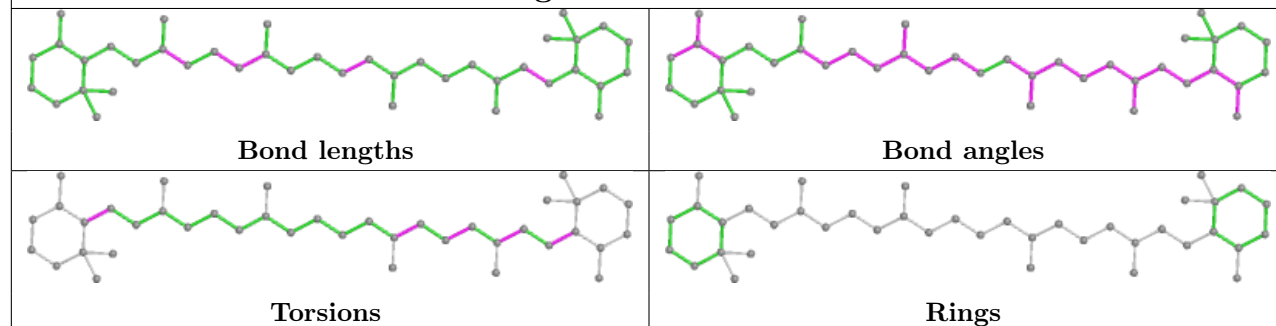


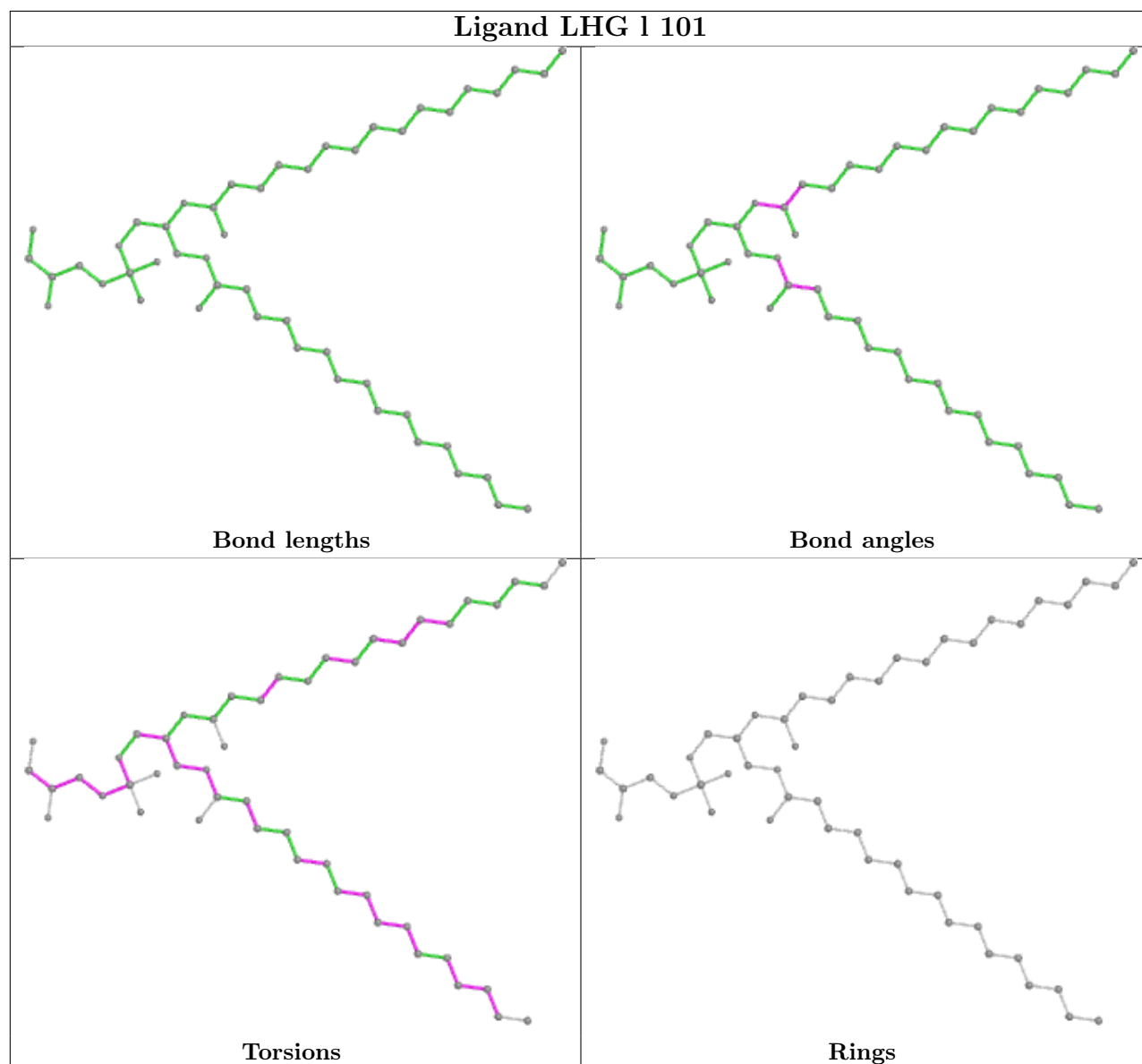
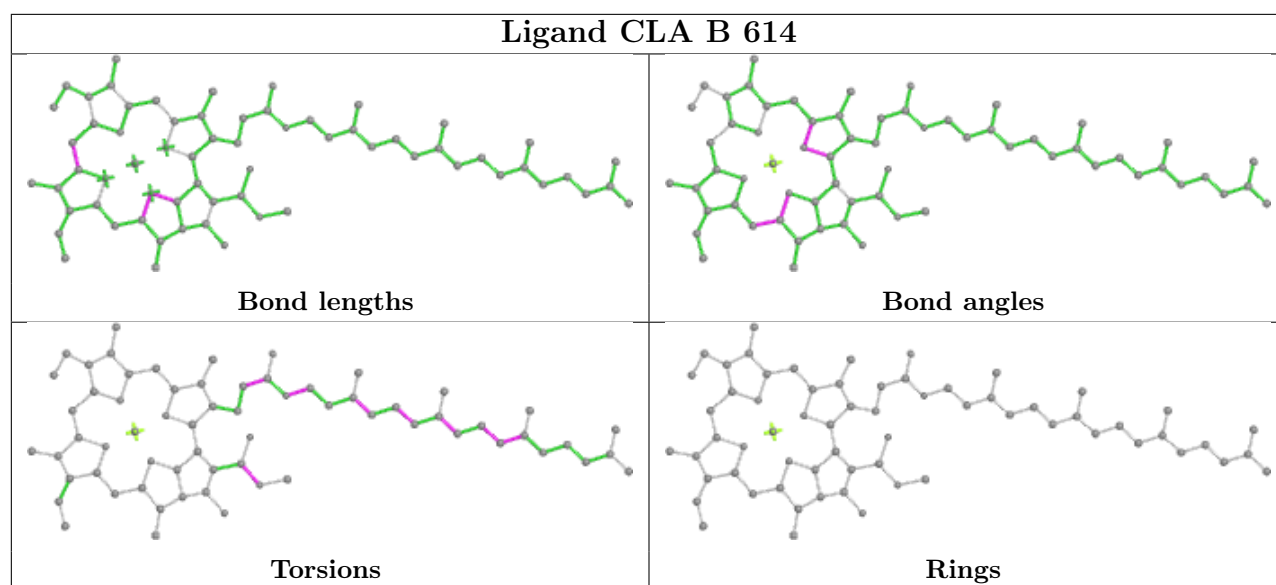
Ligand CLA n 613**Ligand CLA a 405**

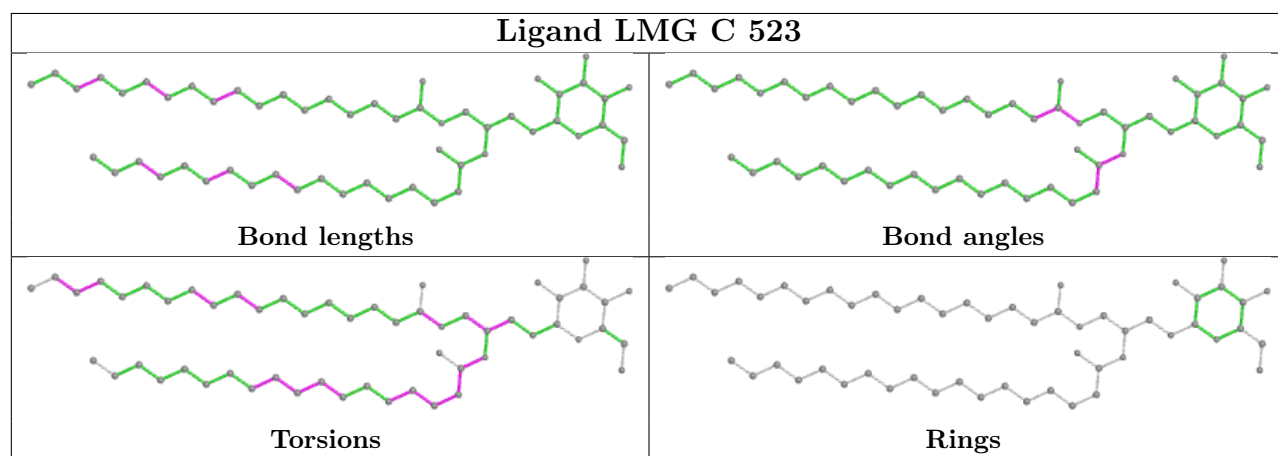
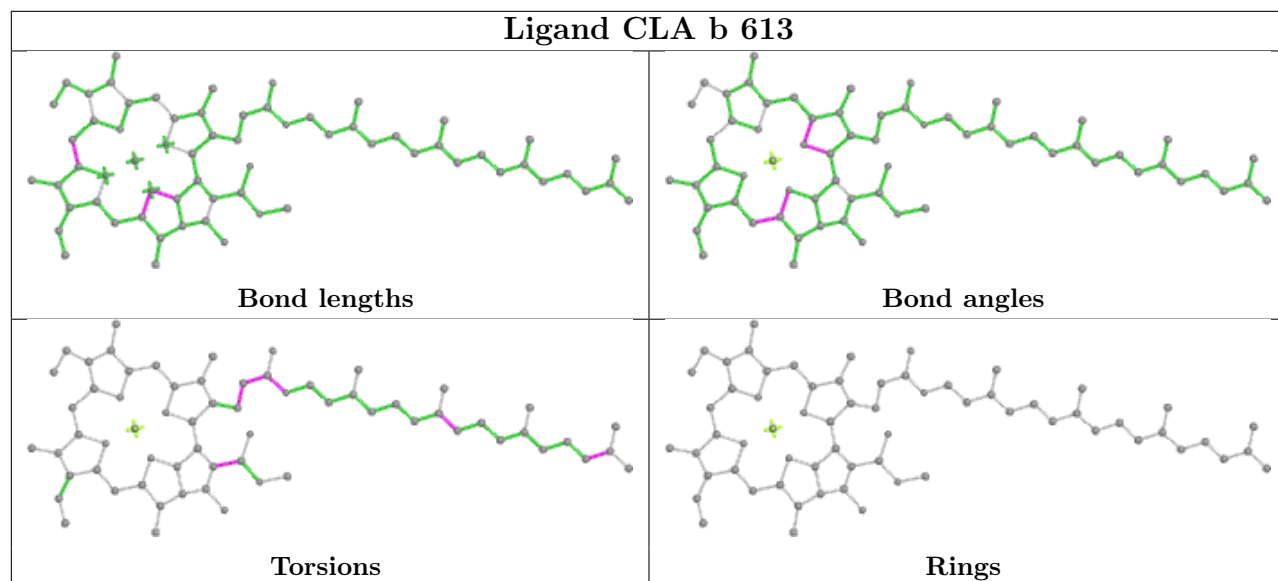
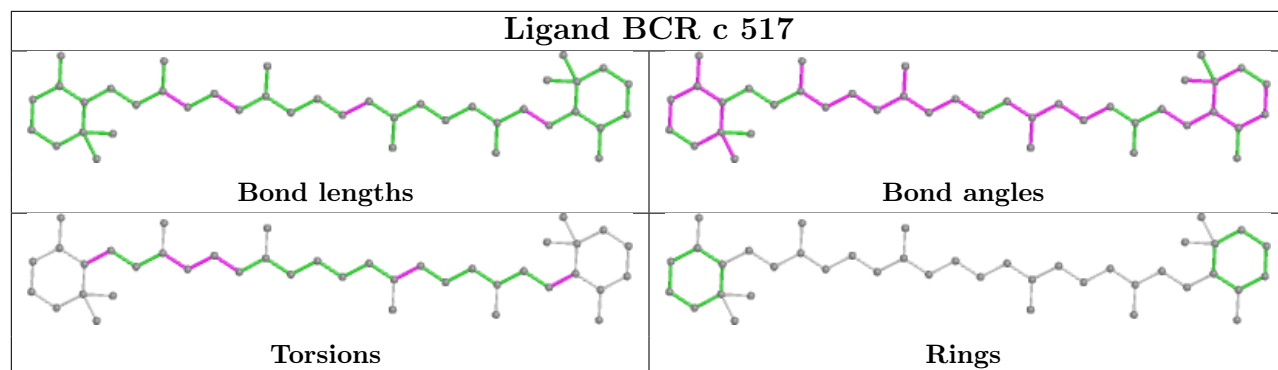
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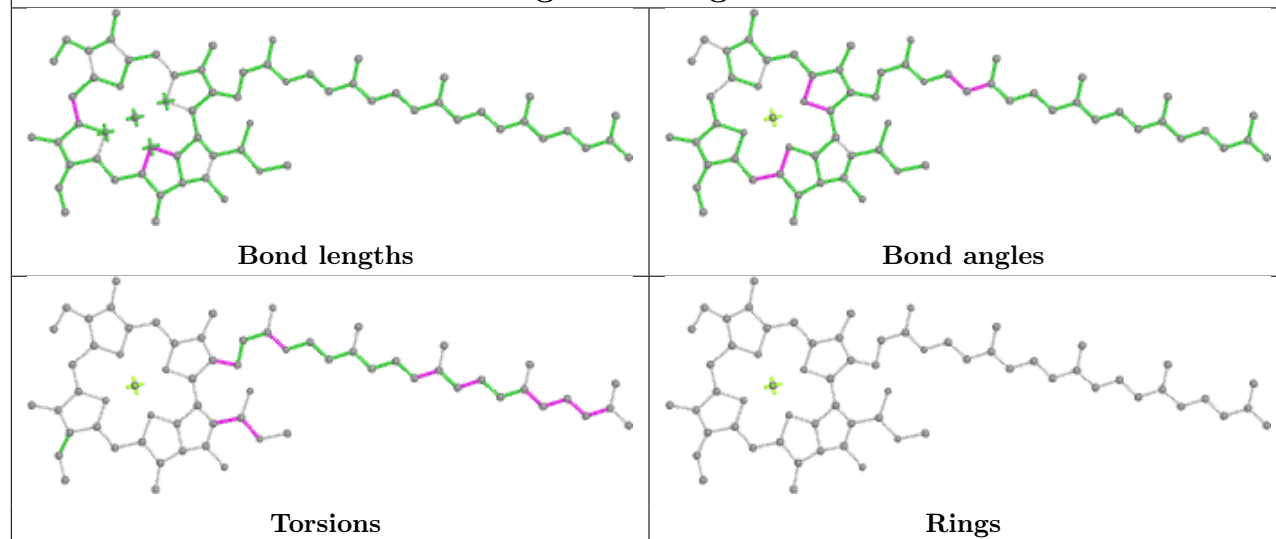
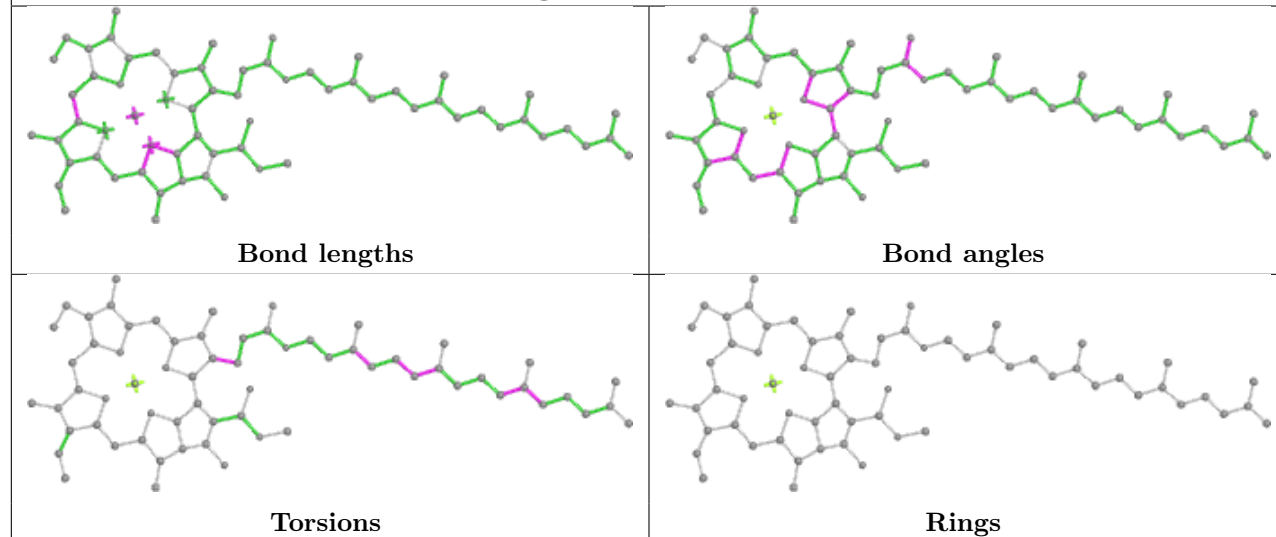
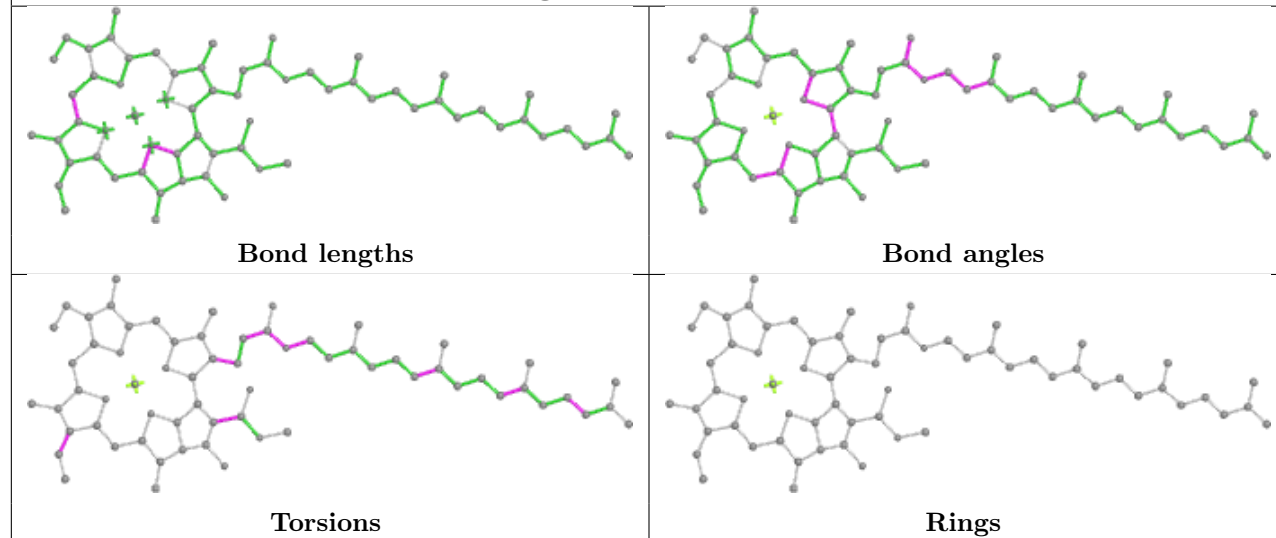


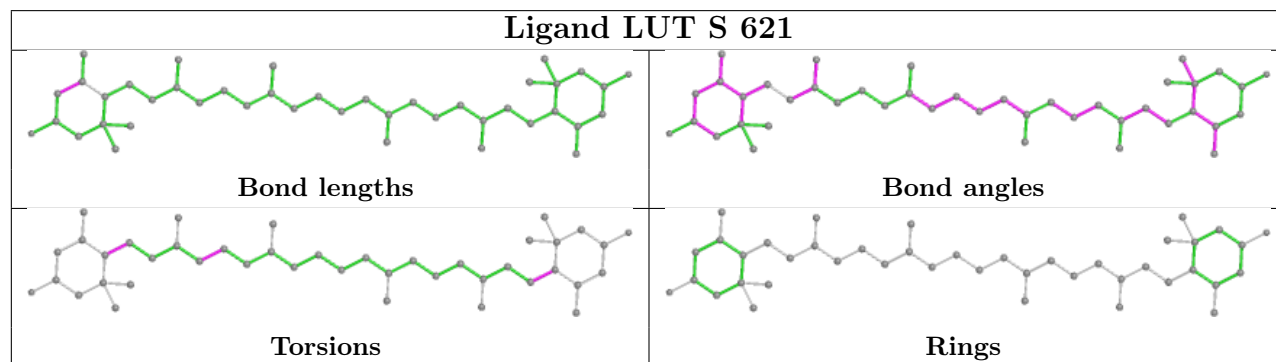
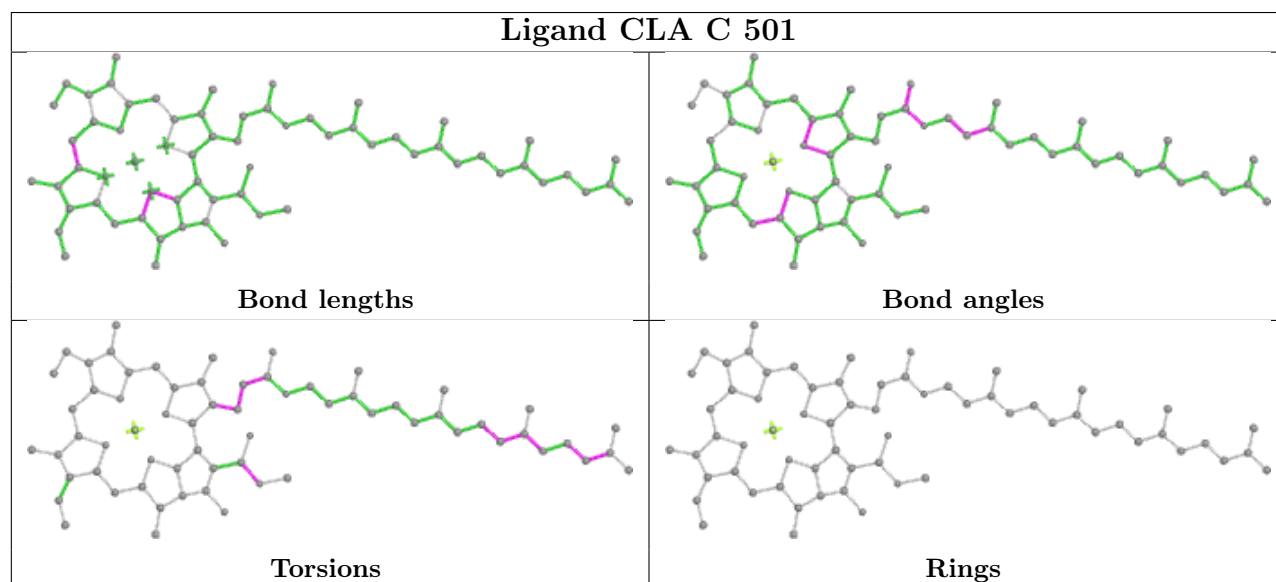
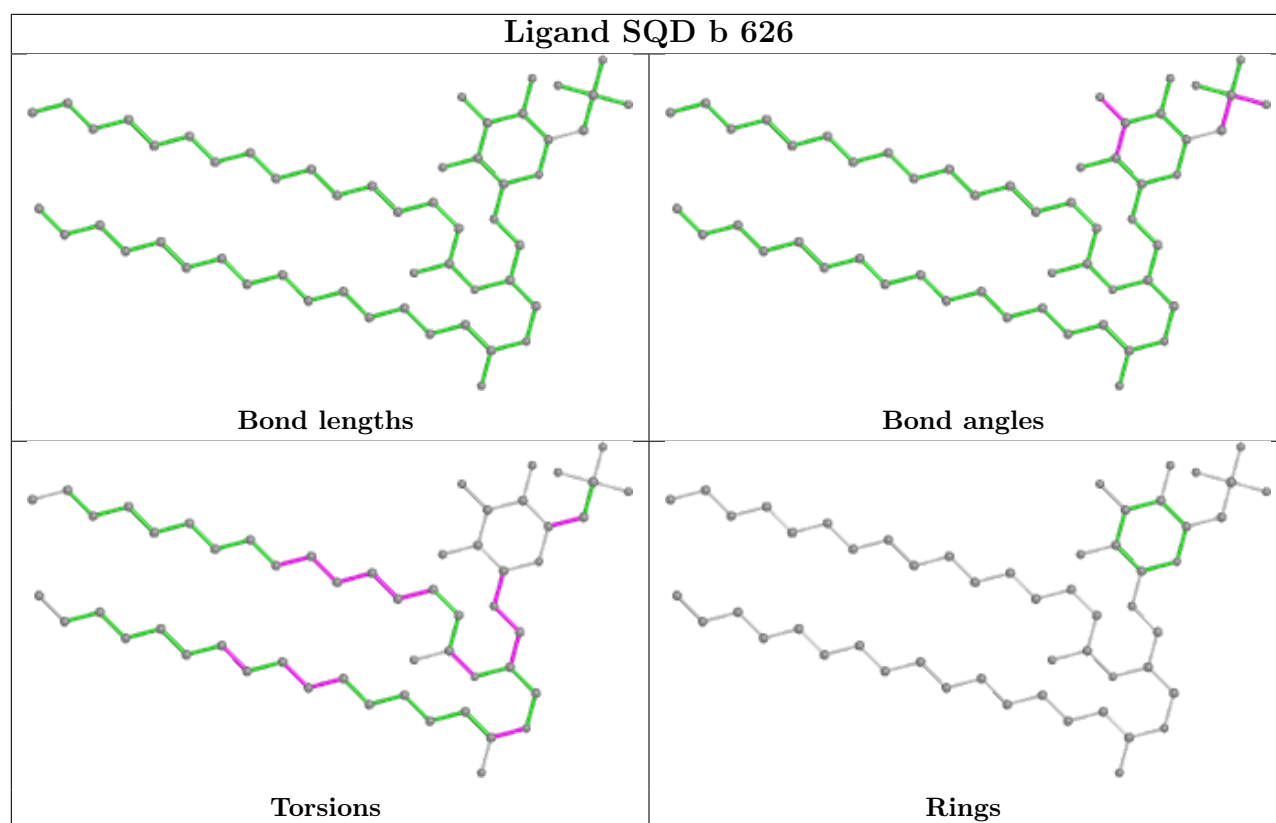
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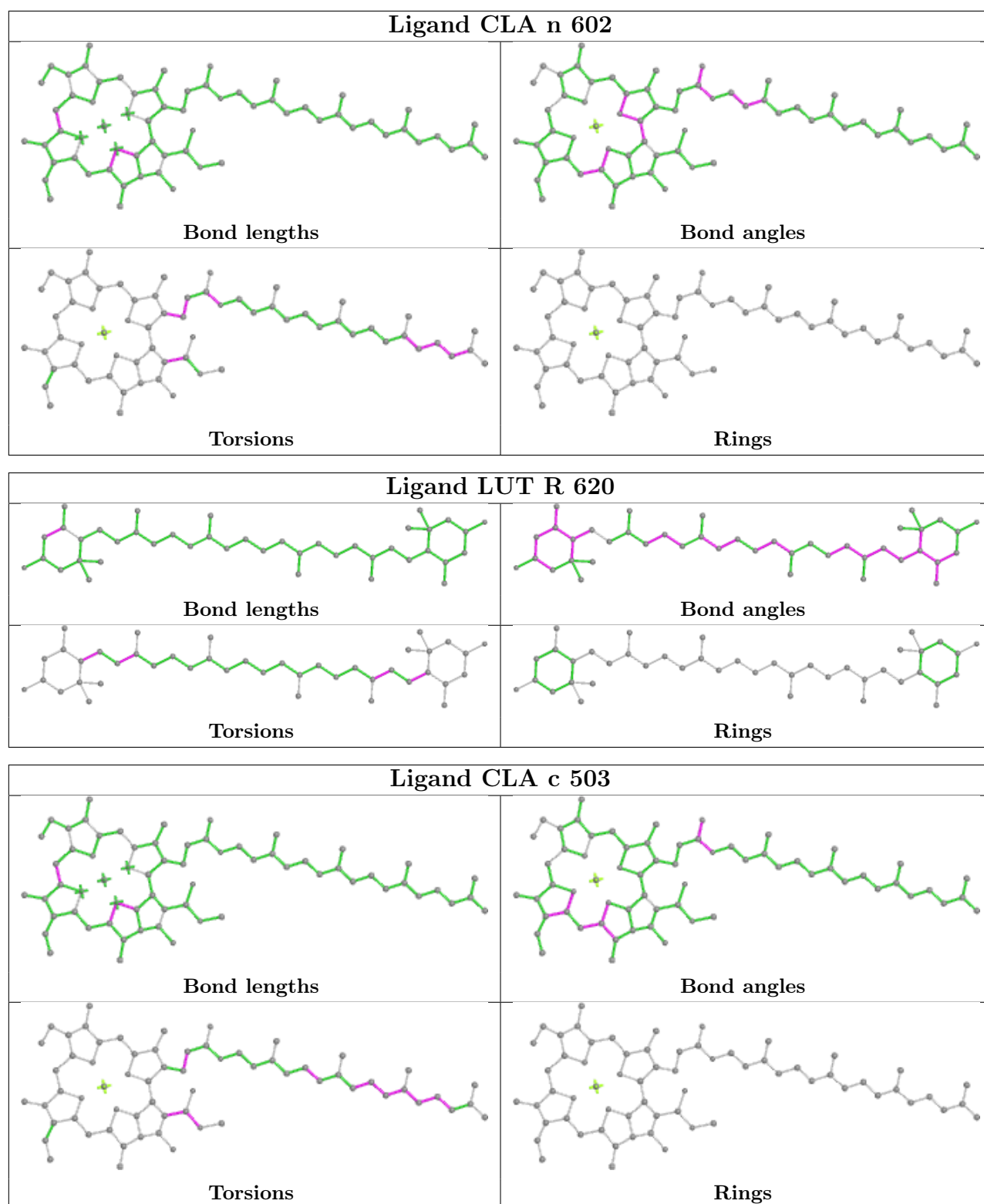


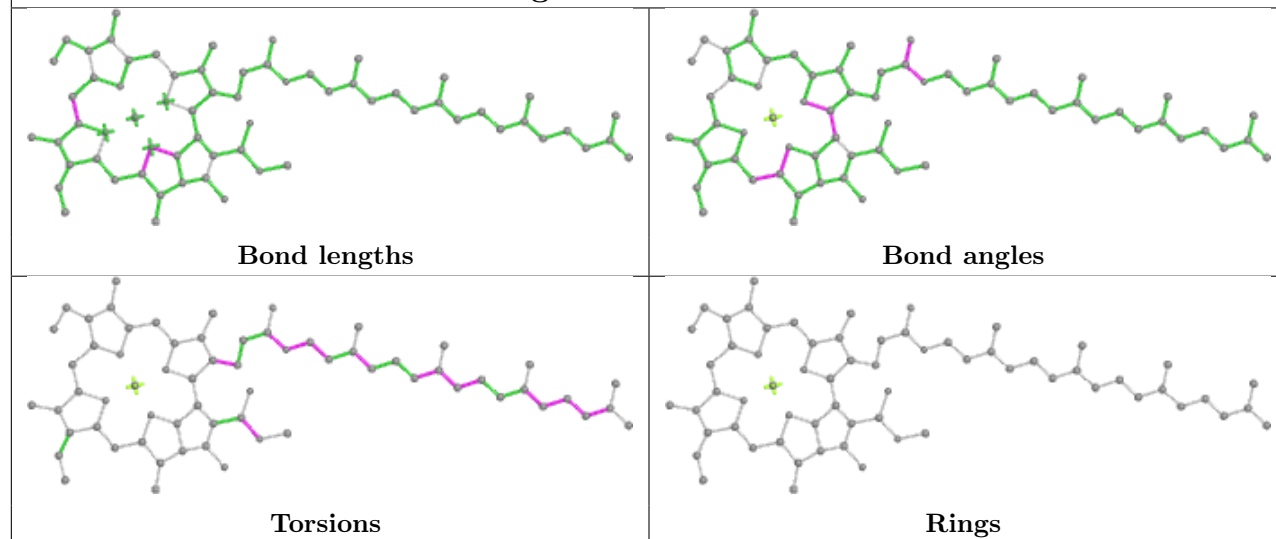
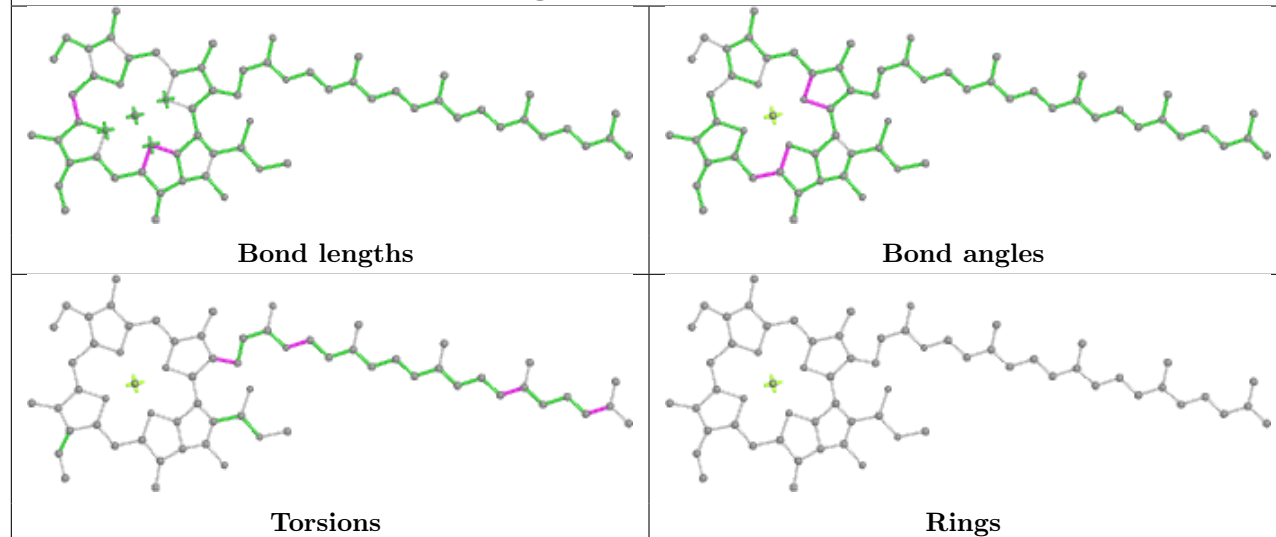


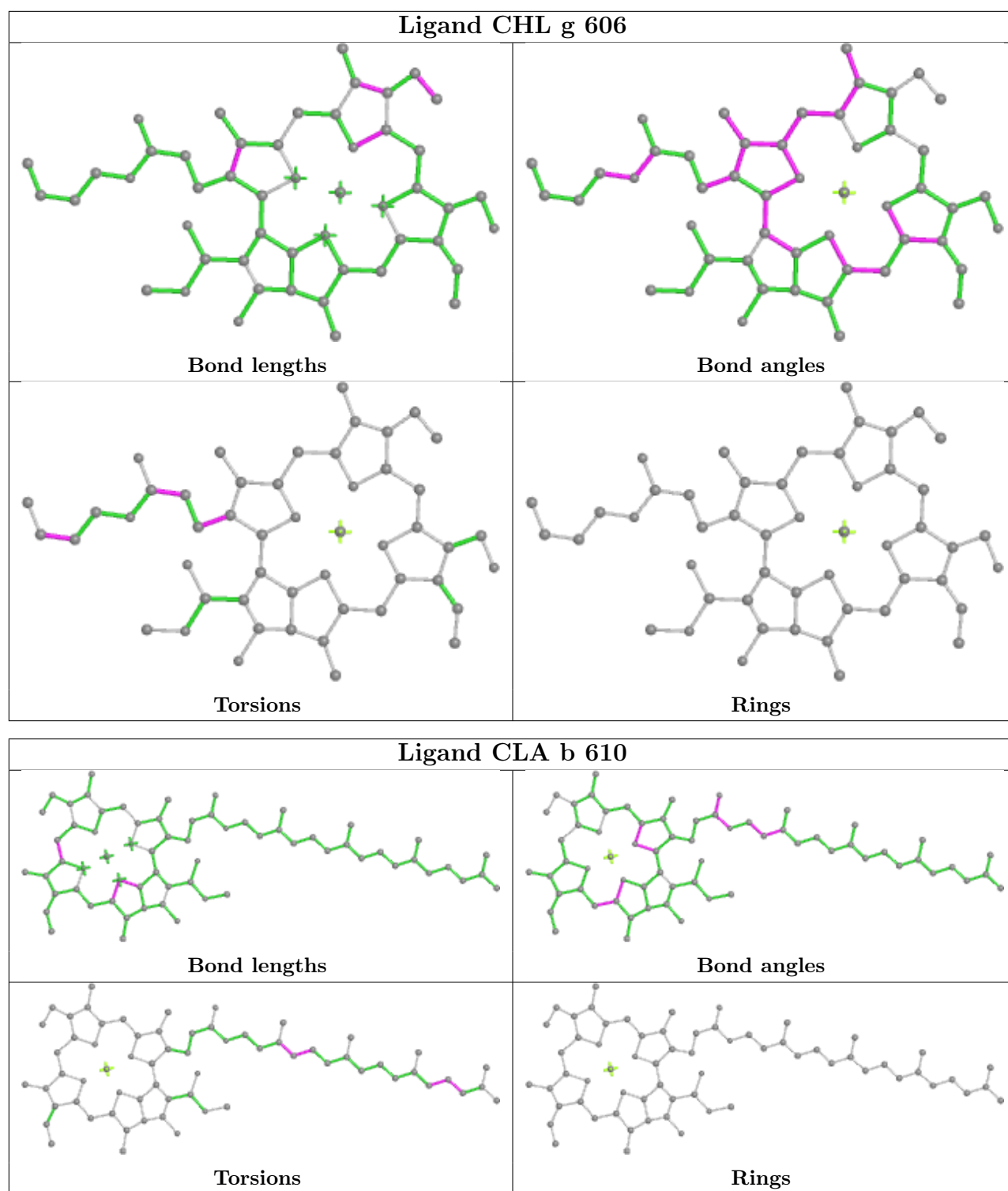


Ligand CLA g 602**Ligand CLA n 610****Ligand CLA a 406**

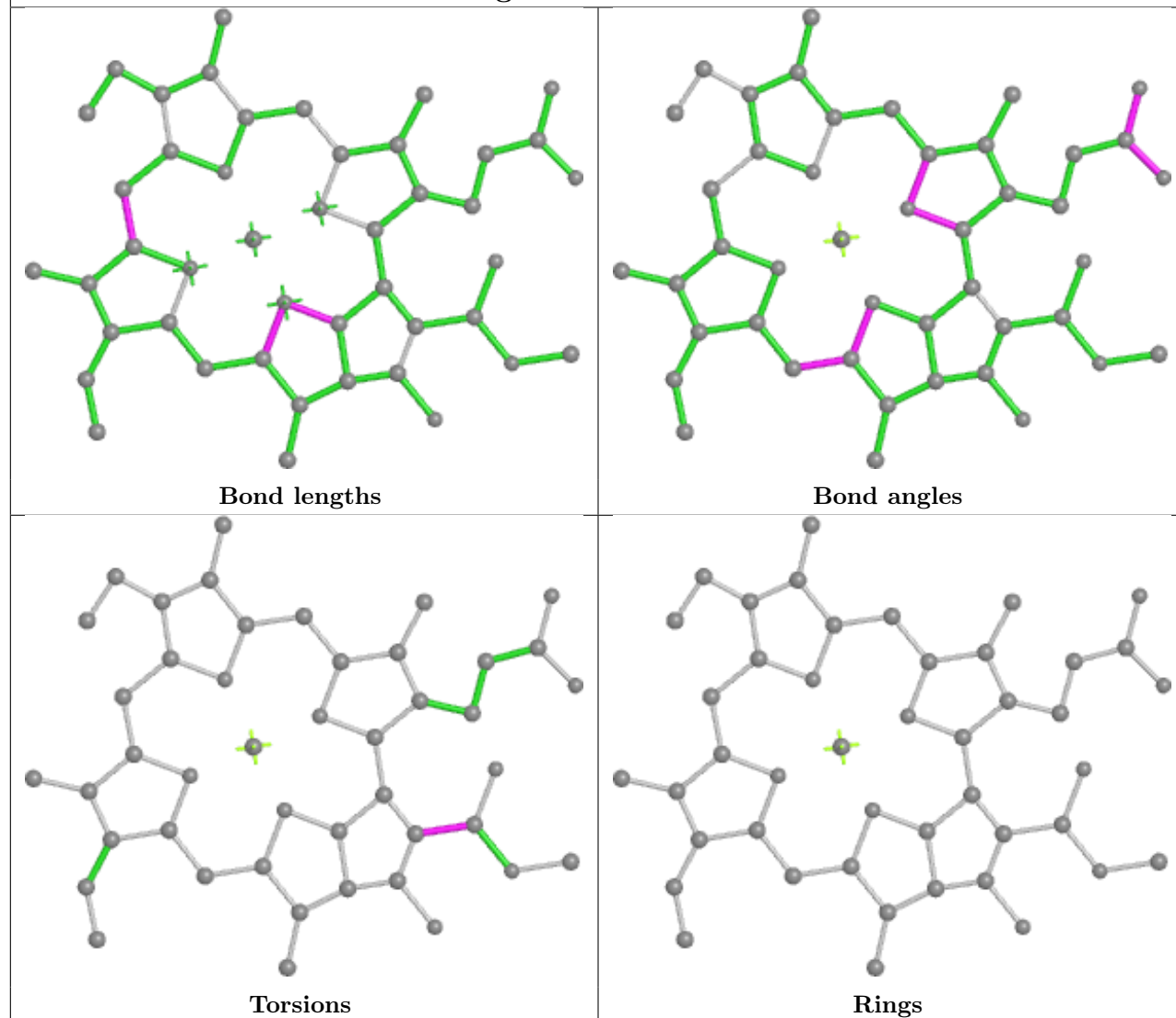




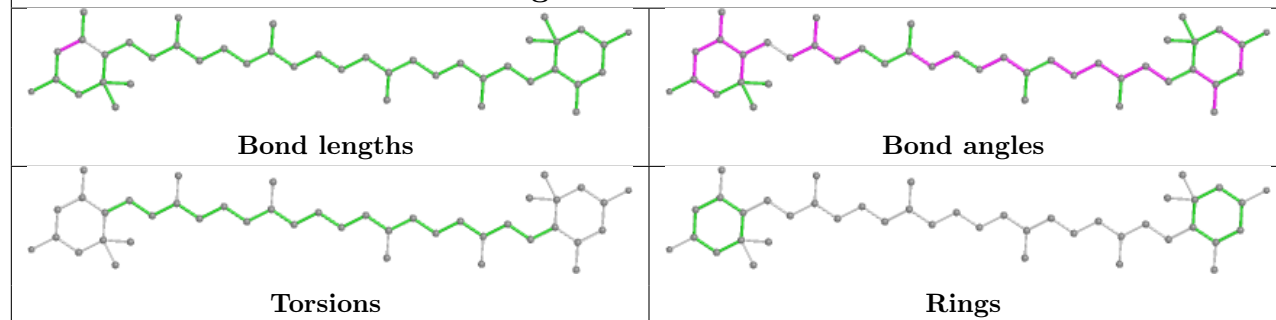
Ligand CLA N 603**Ligand CLA D 402**

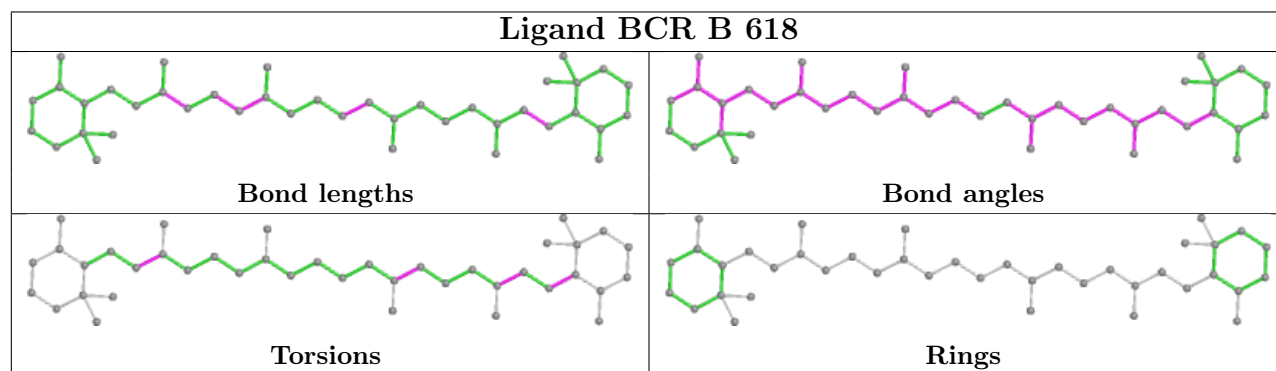
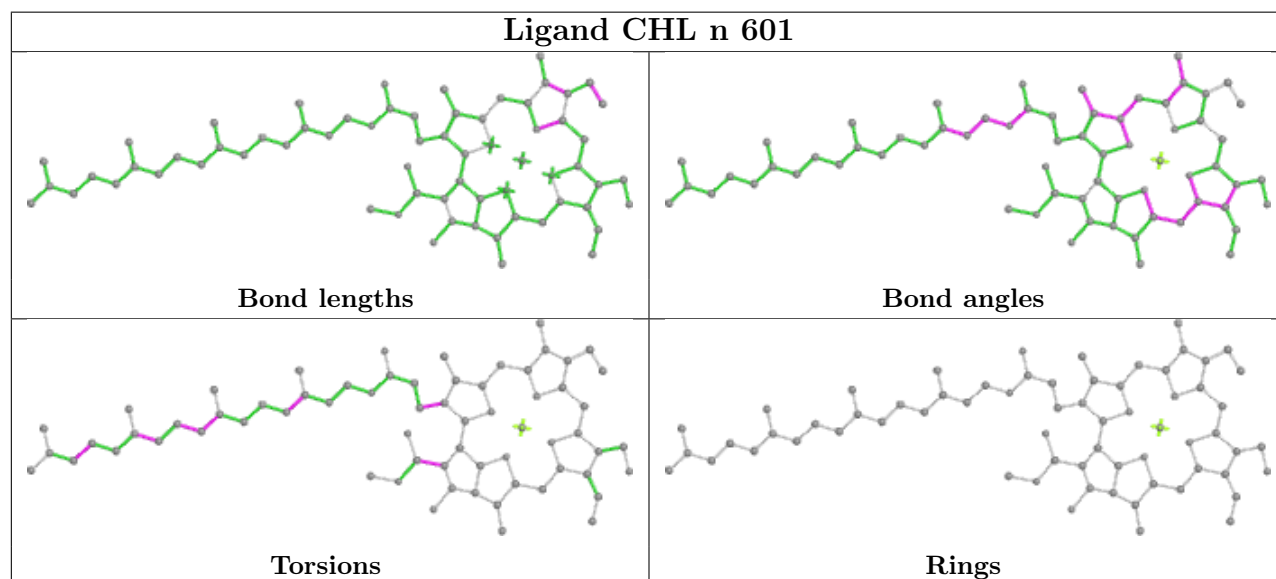
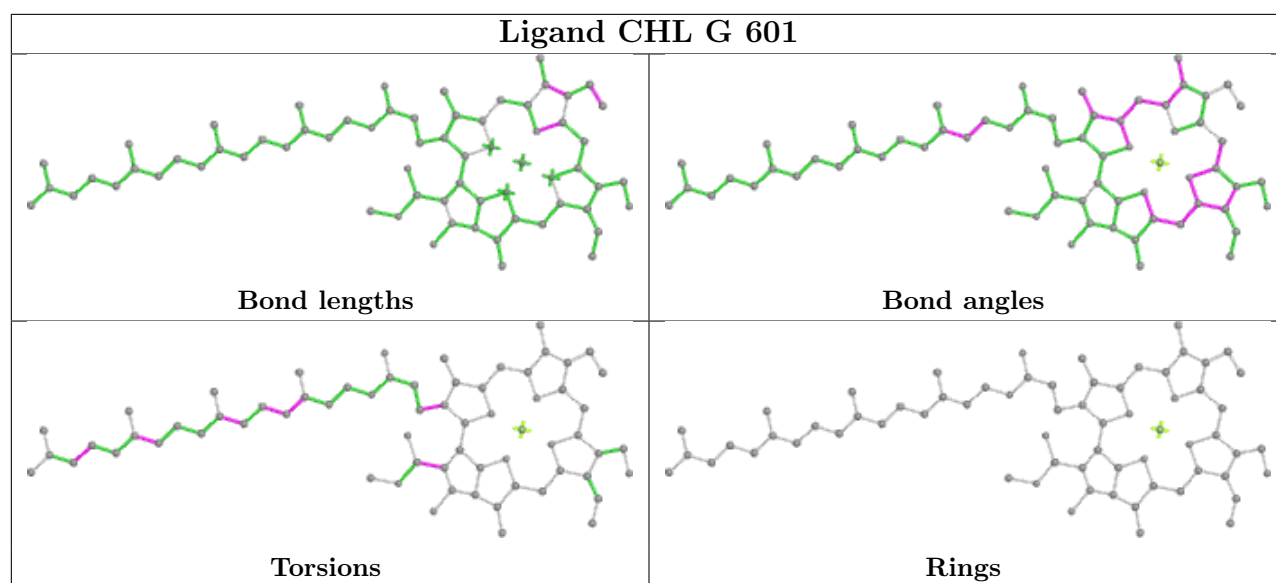


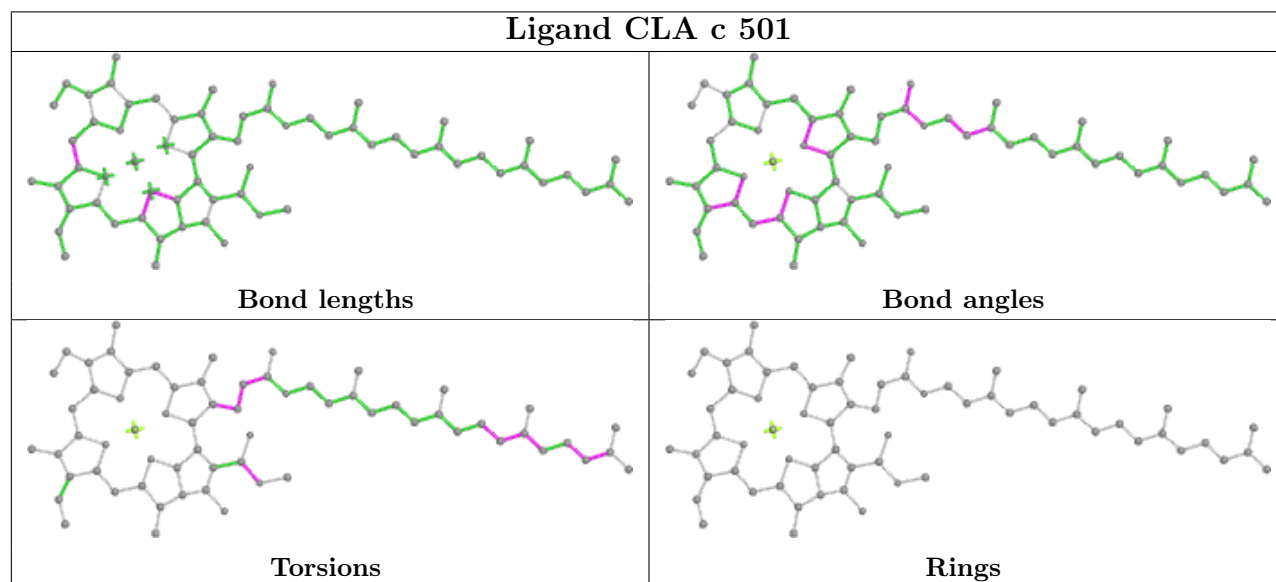
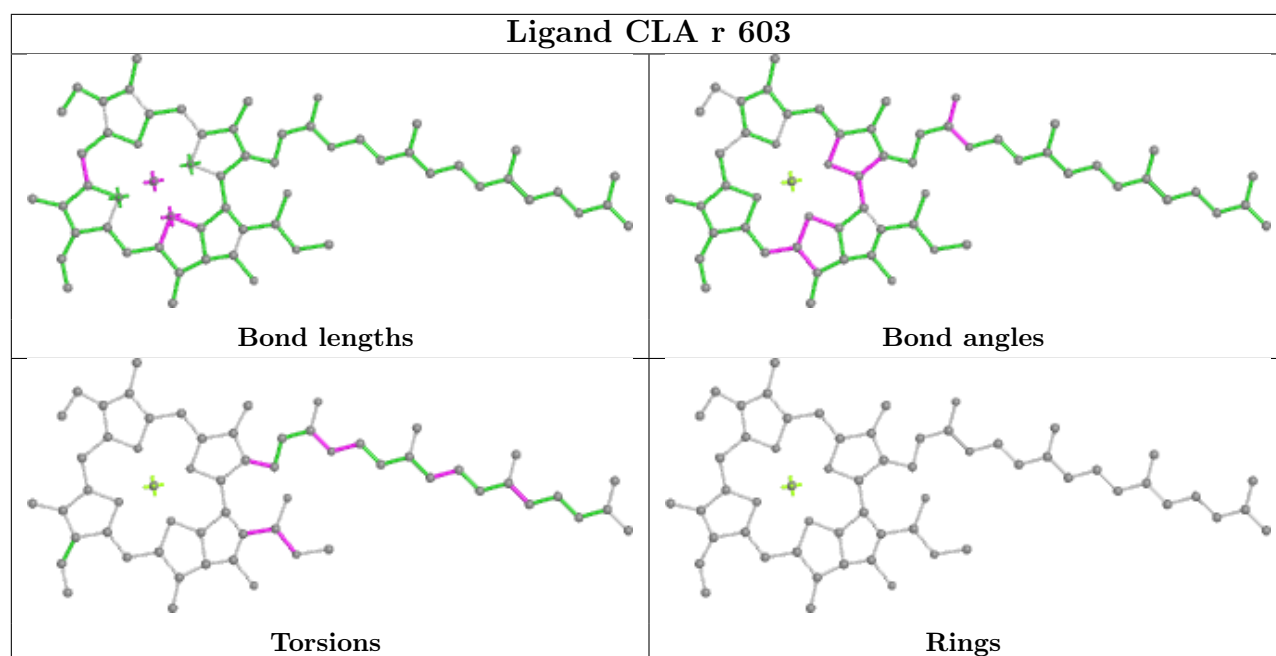
Ligand CLA s 612



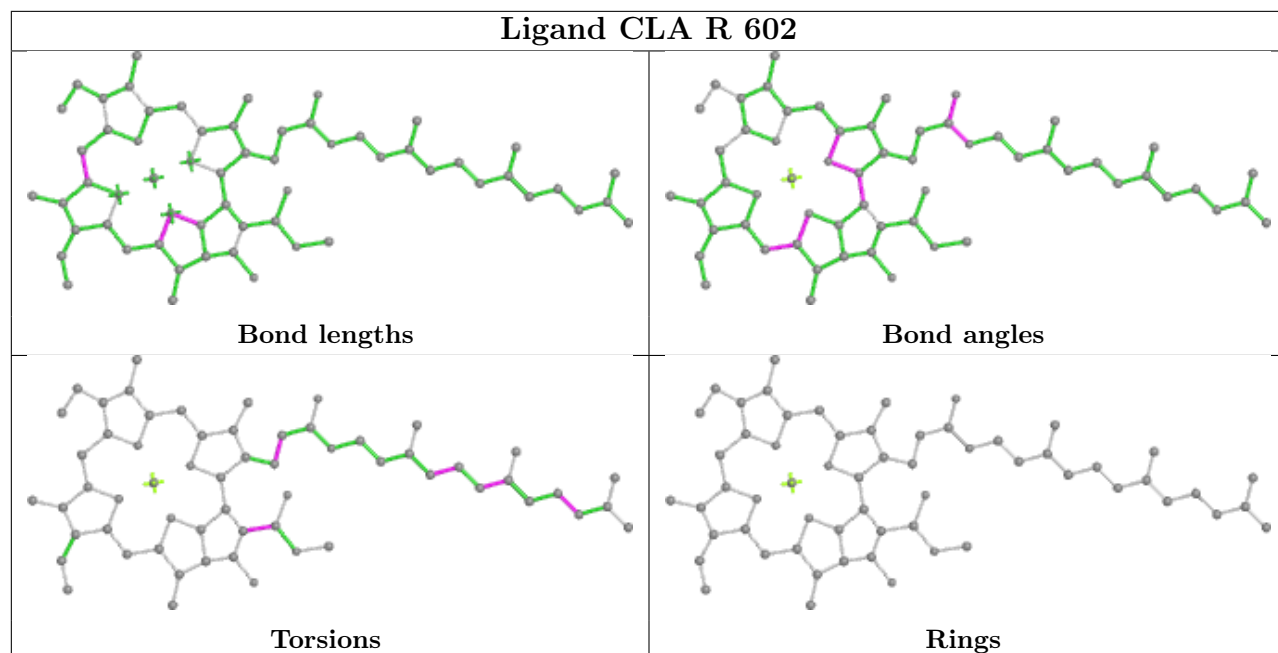
Ligand LUT G 620



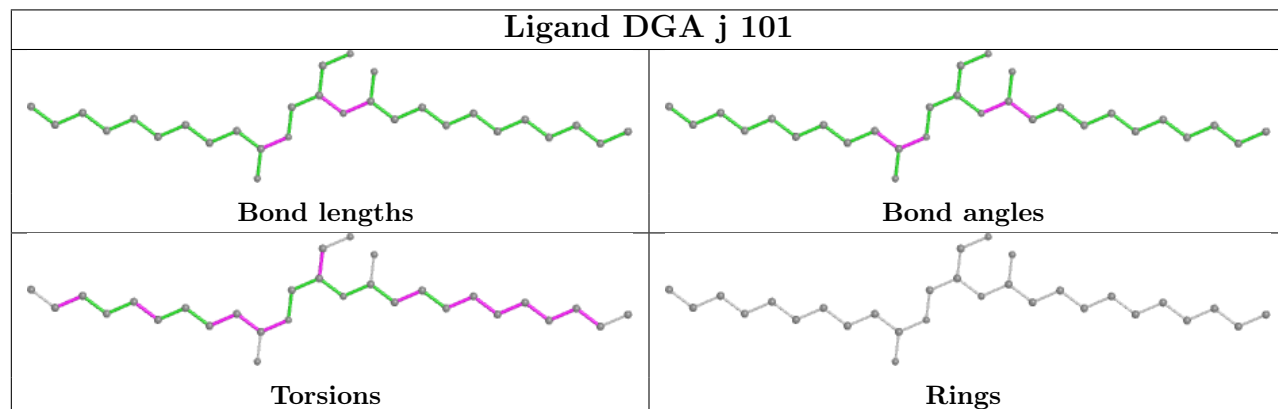




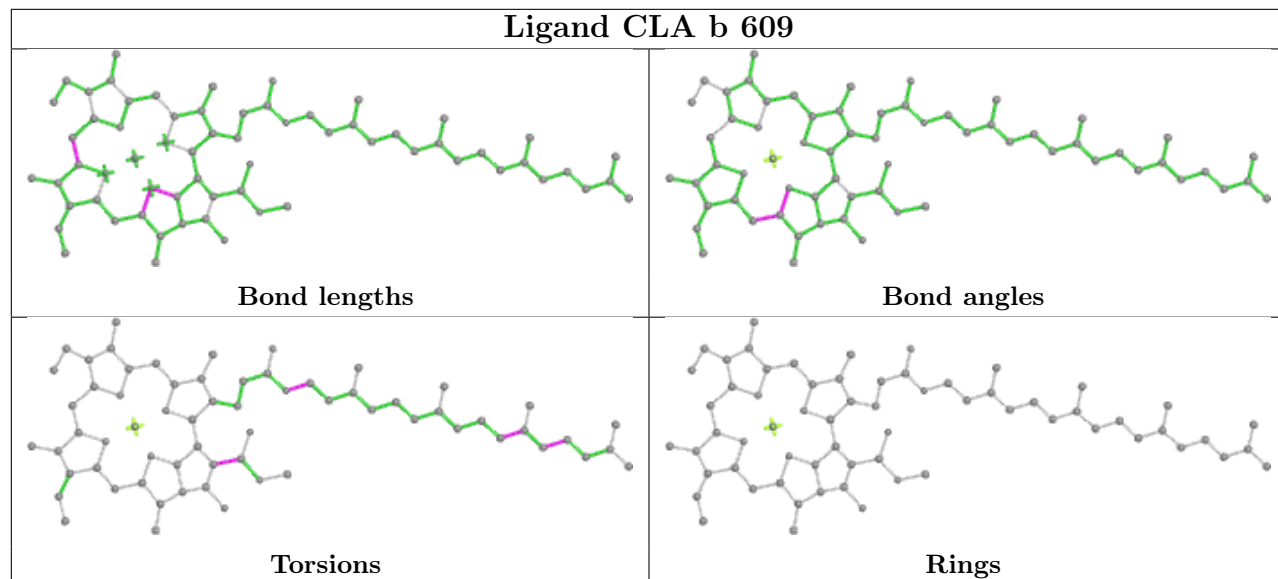
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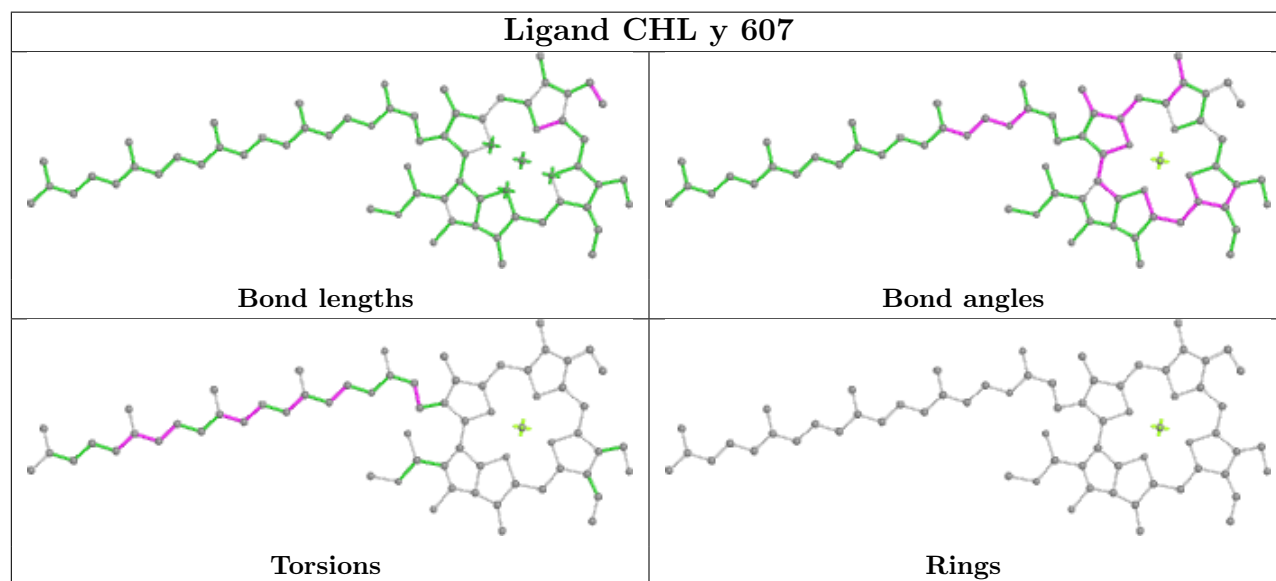
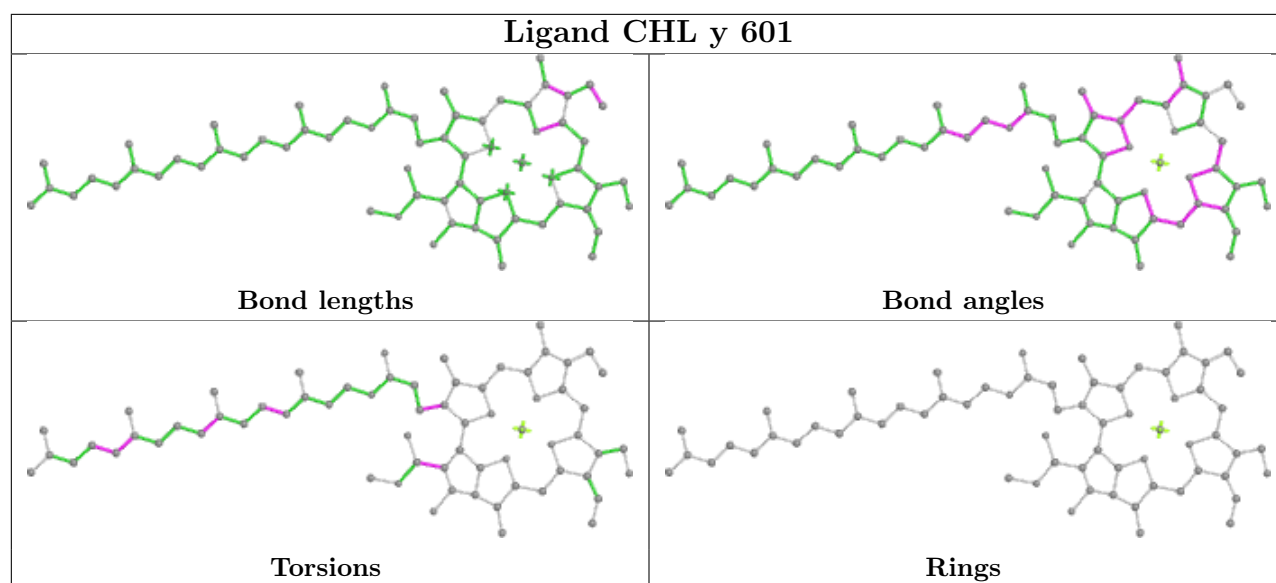


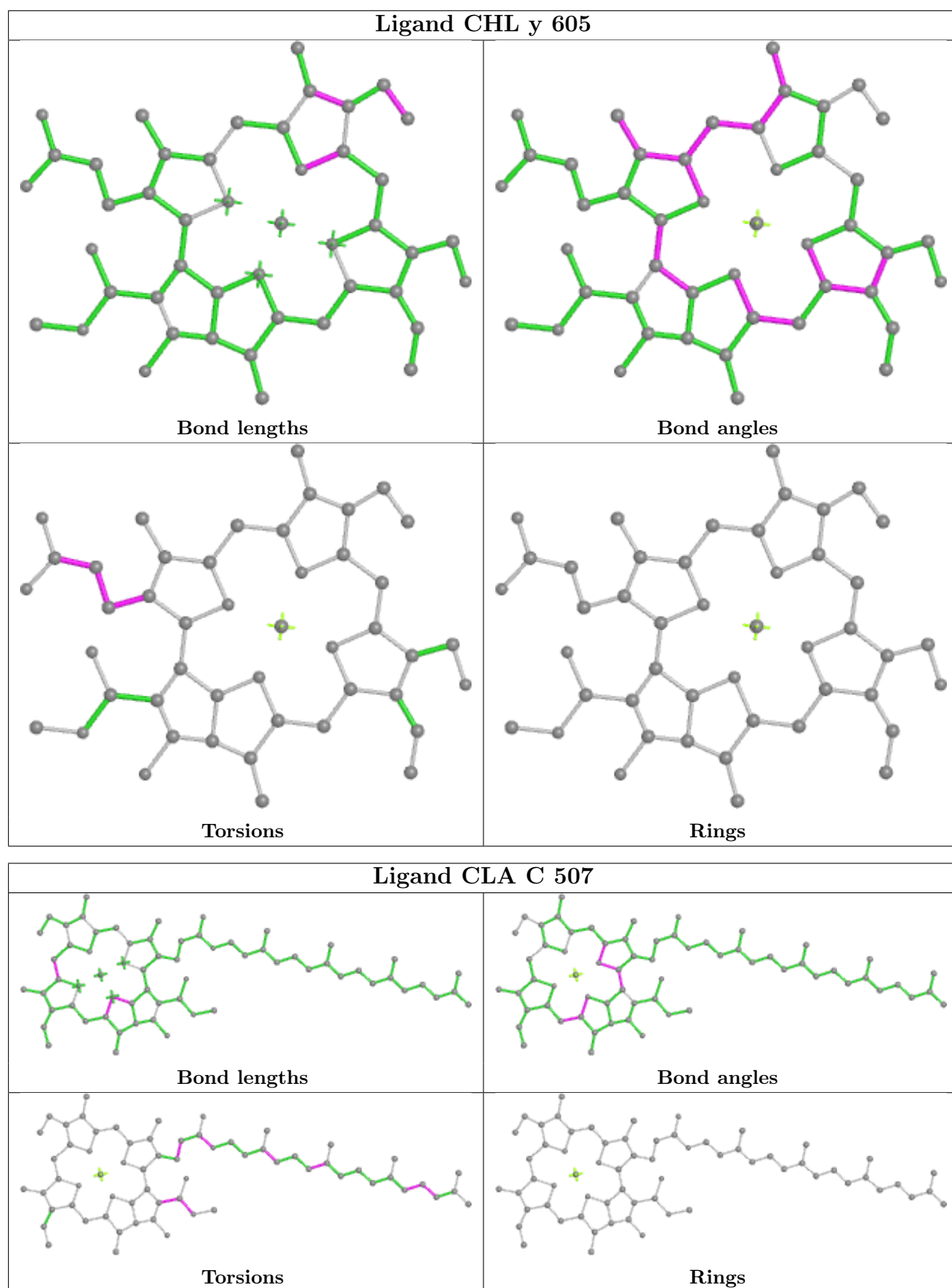
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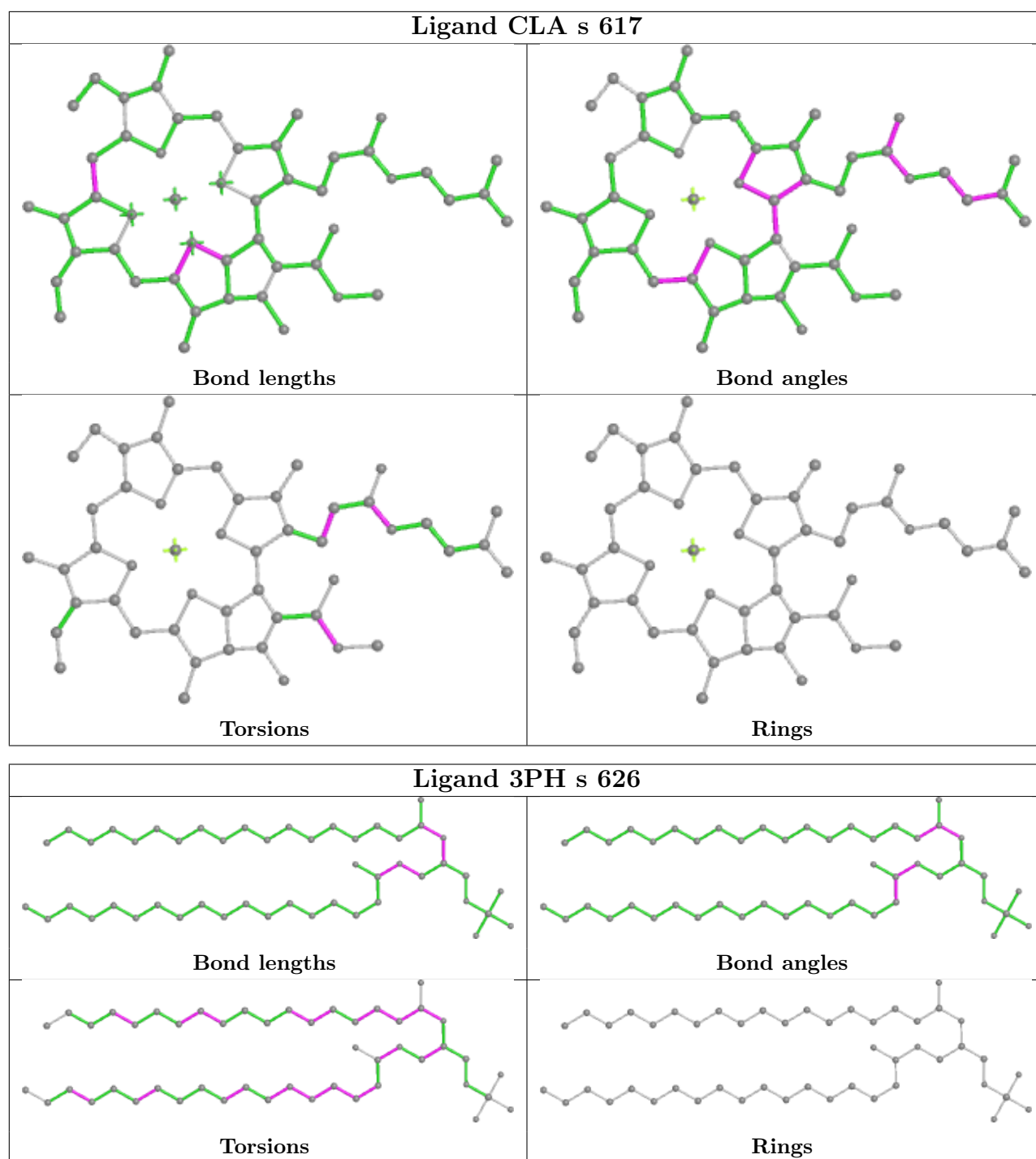


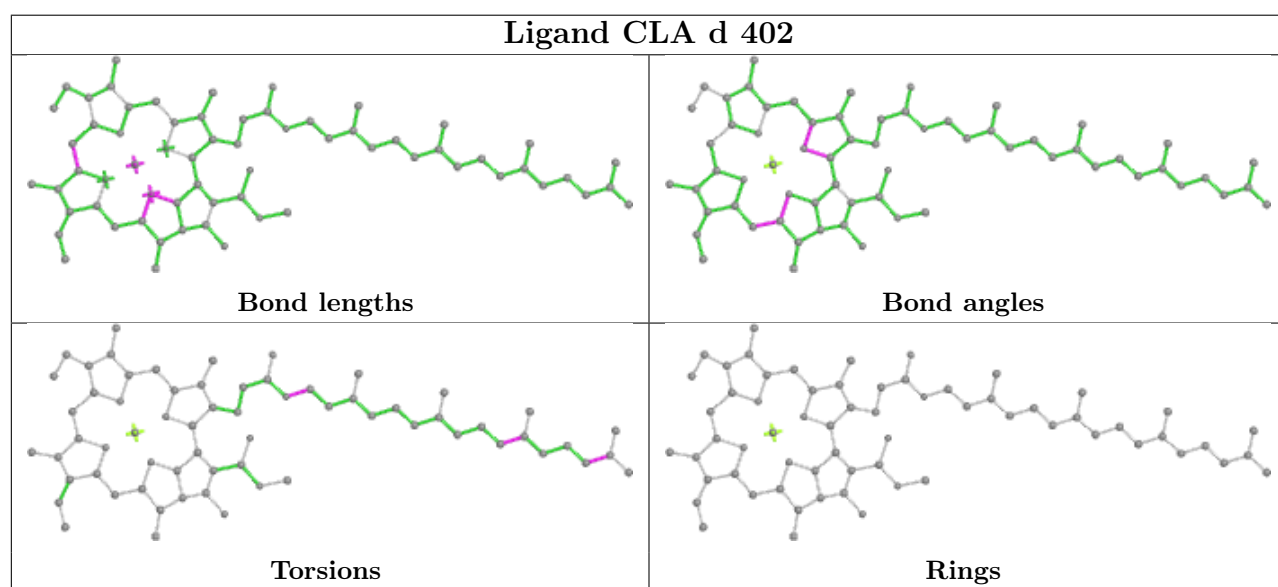
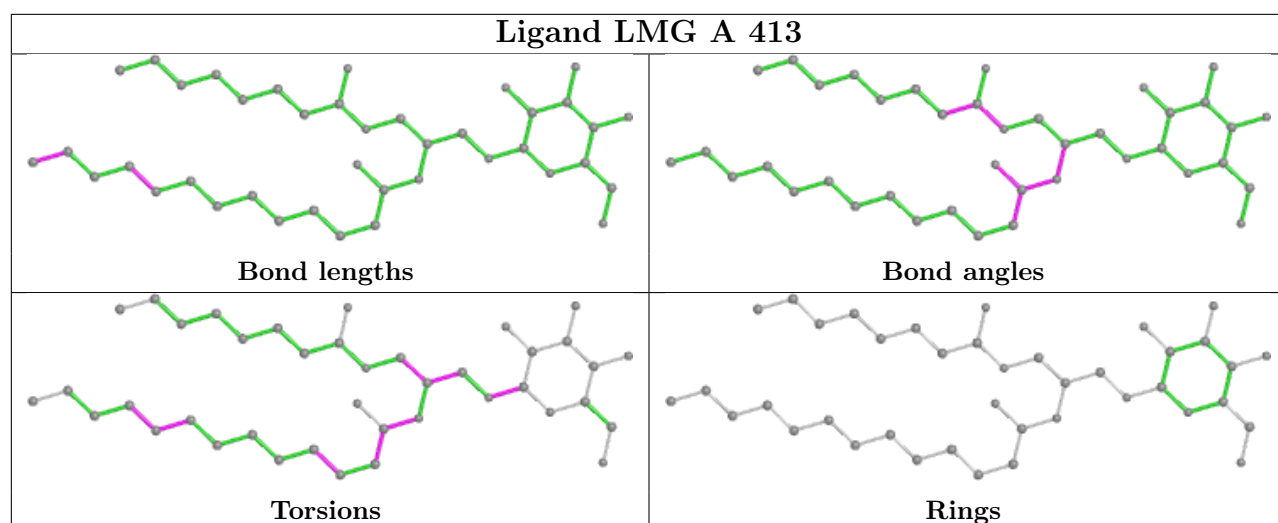
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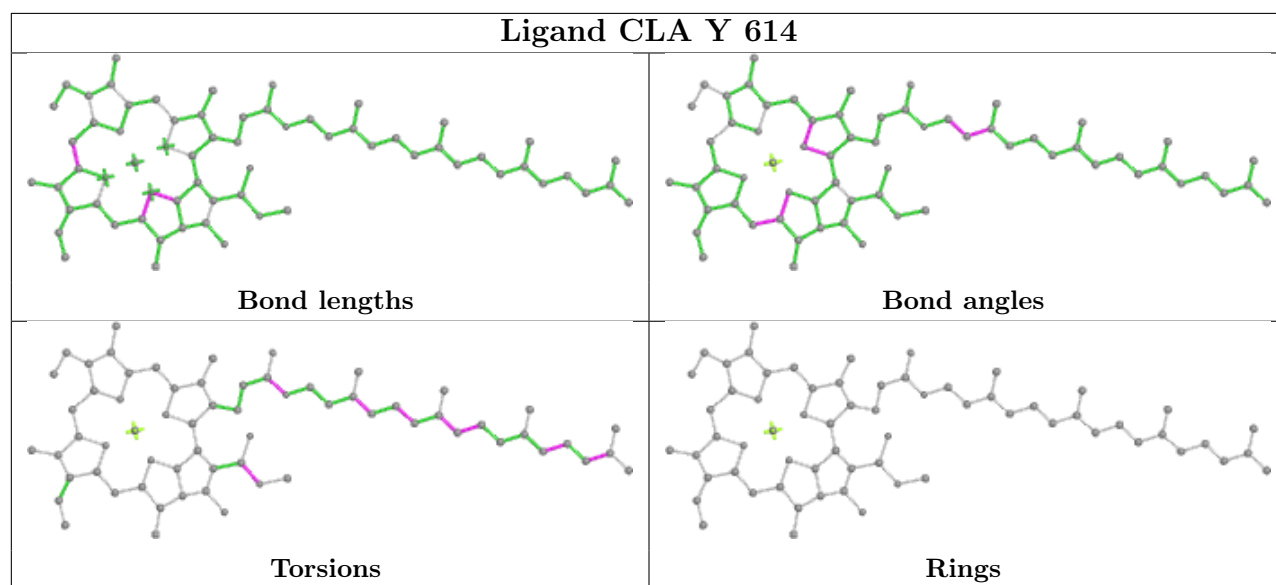
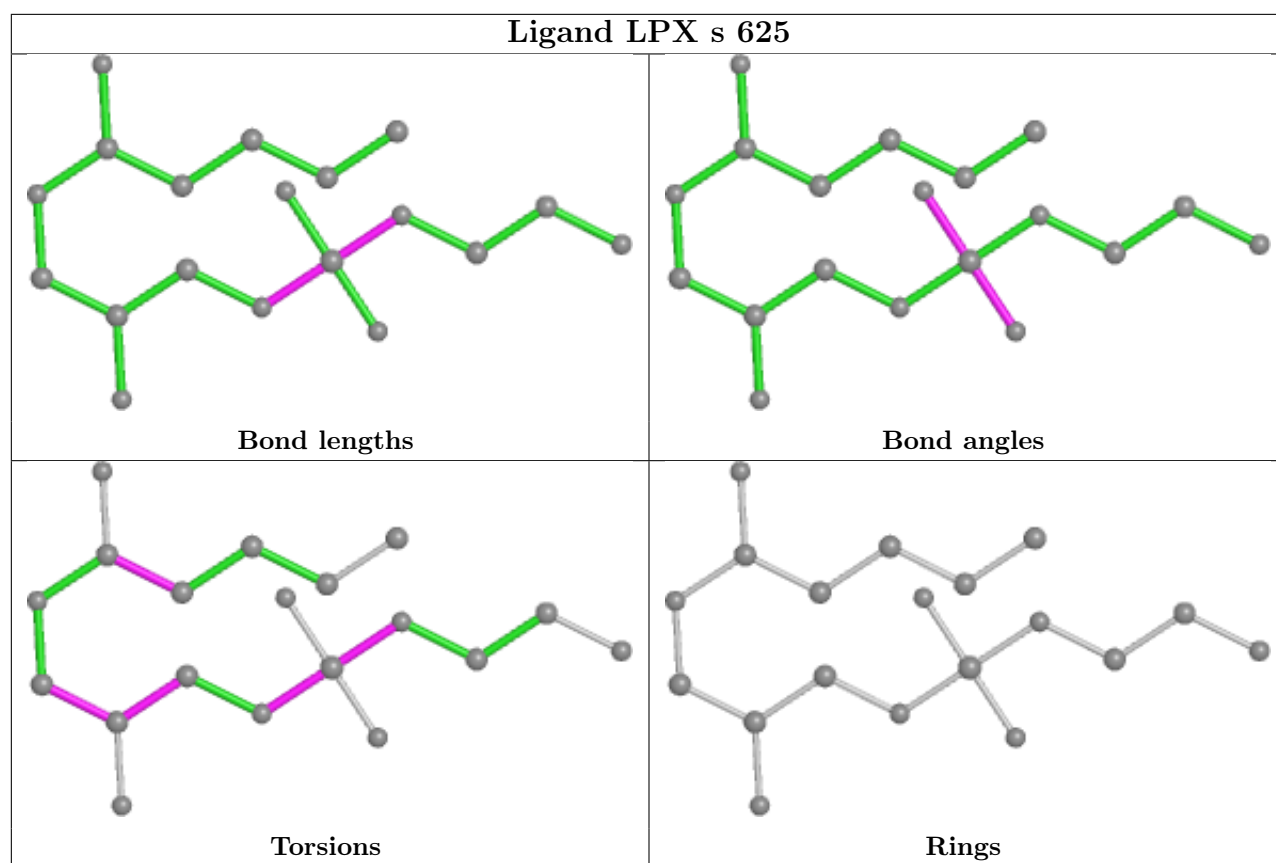


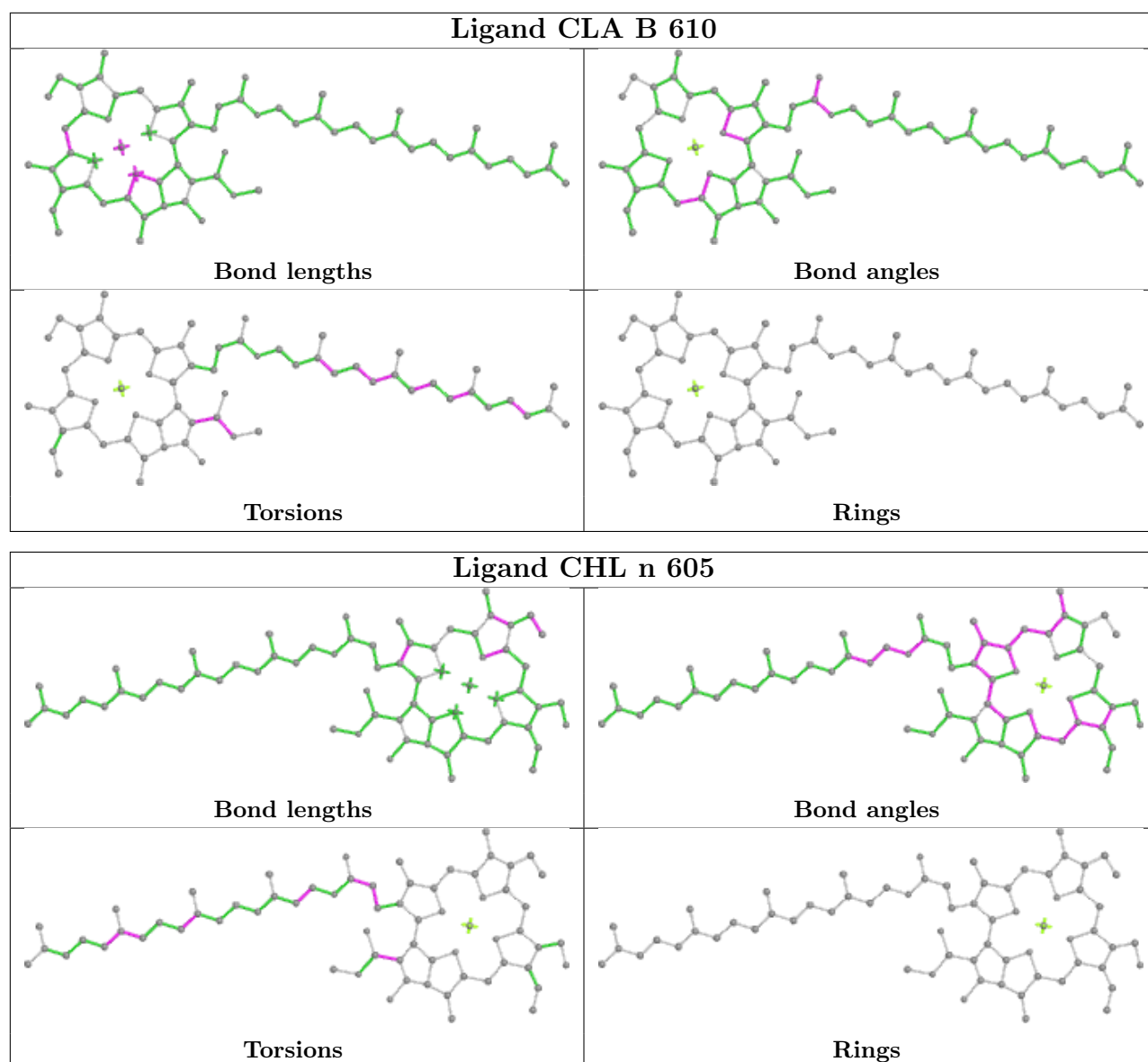


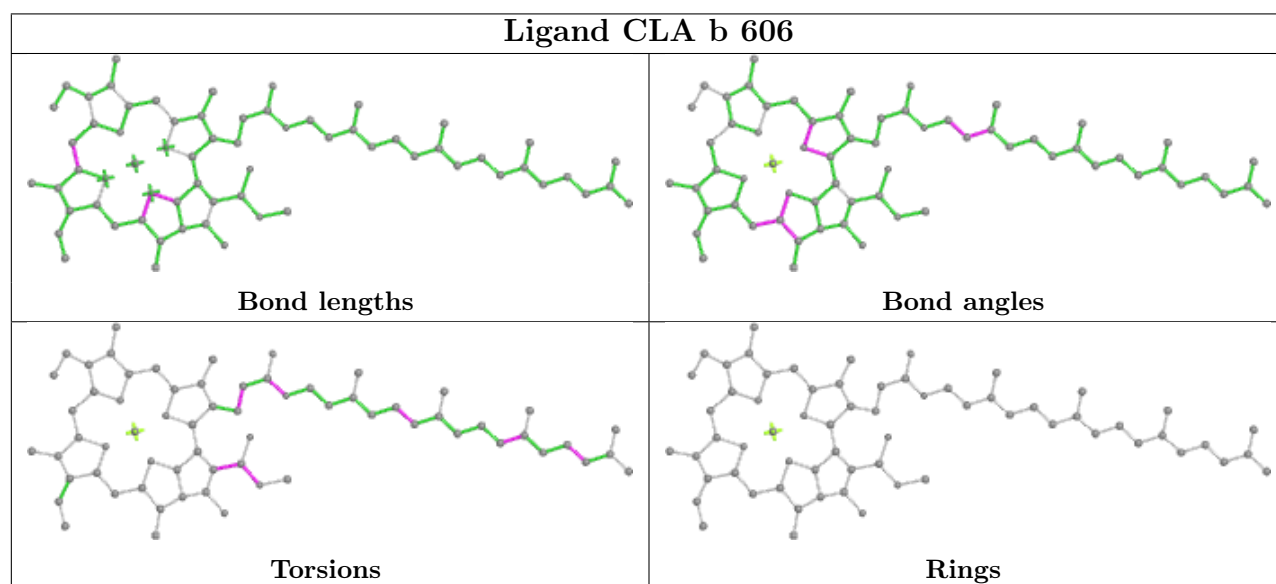
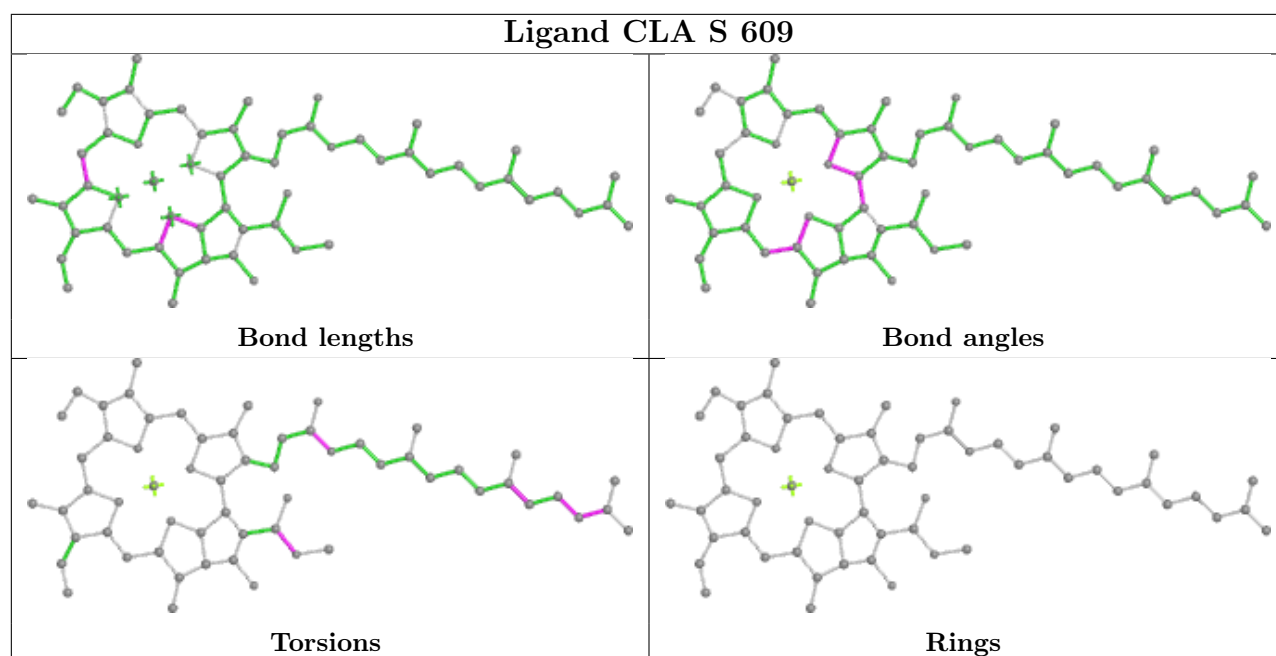


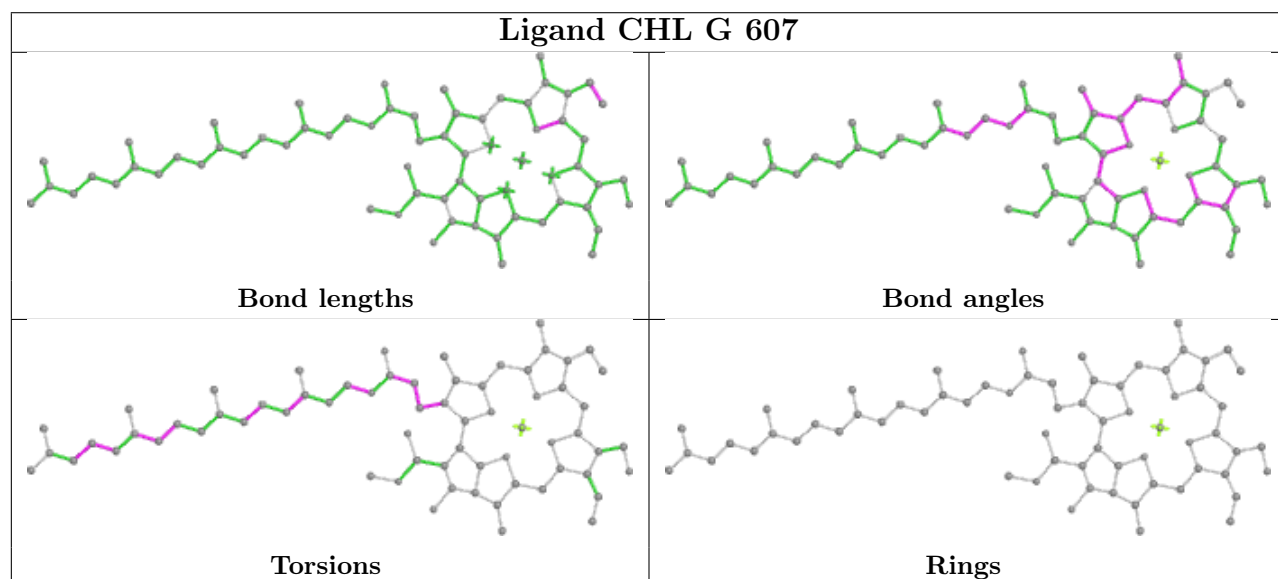
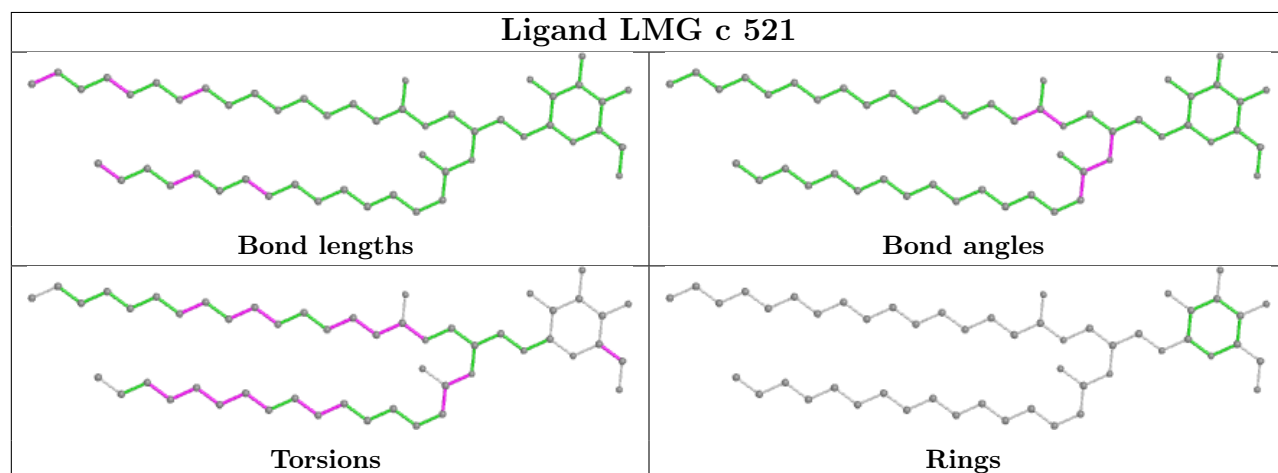
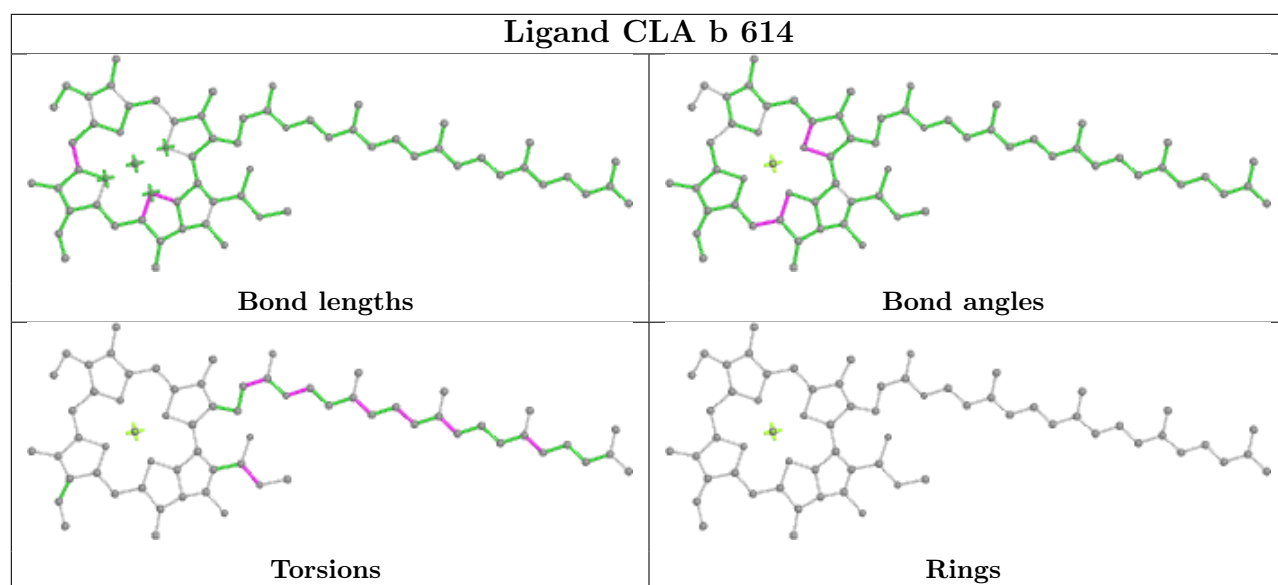


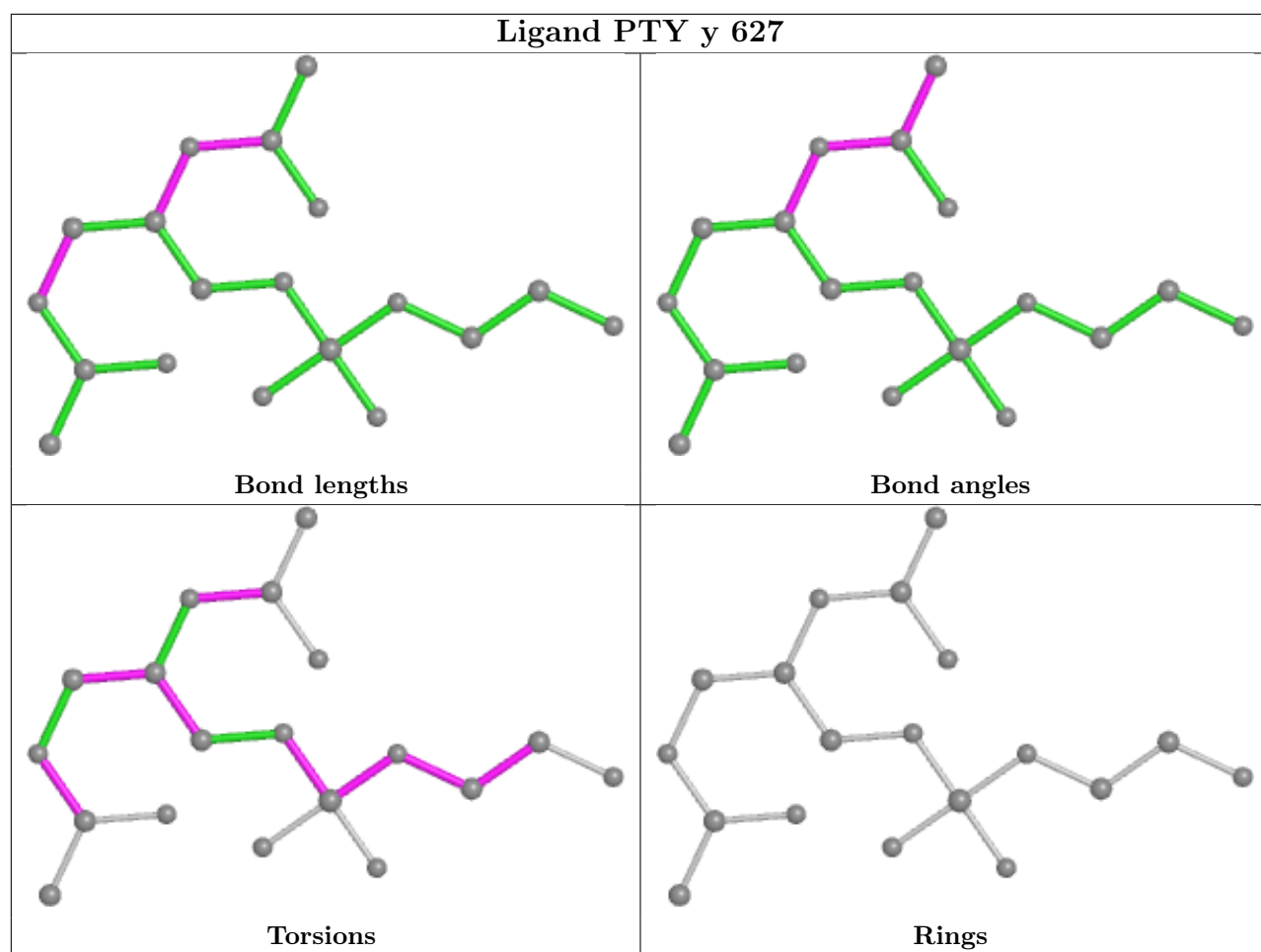


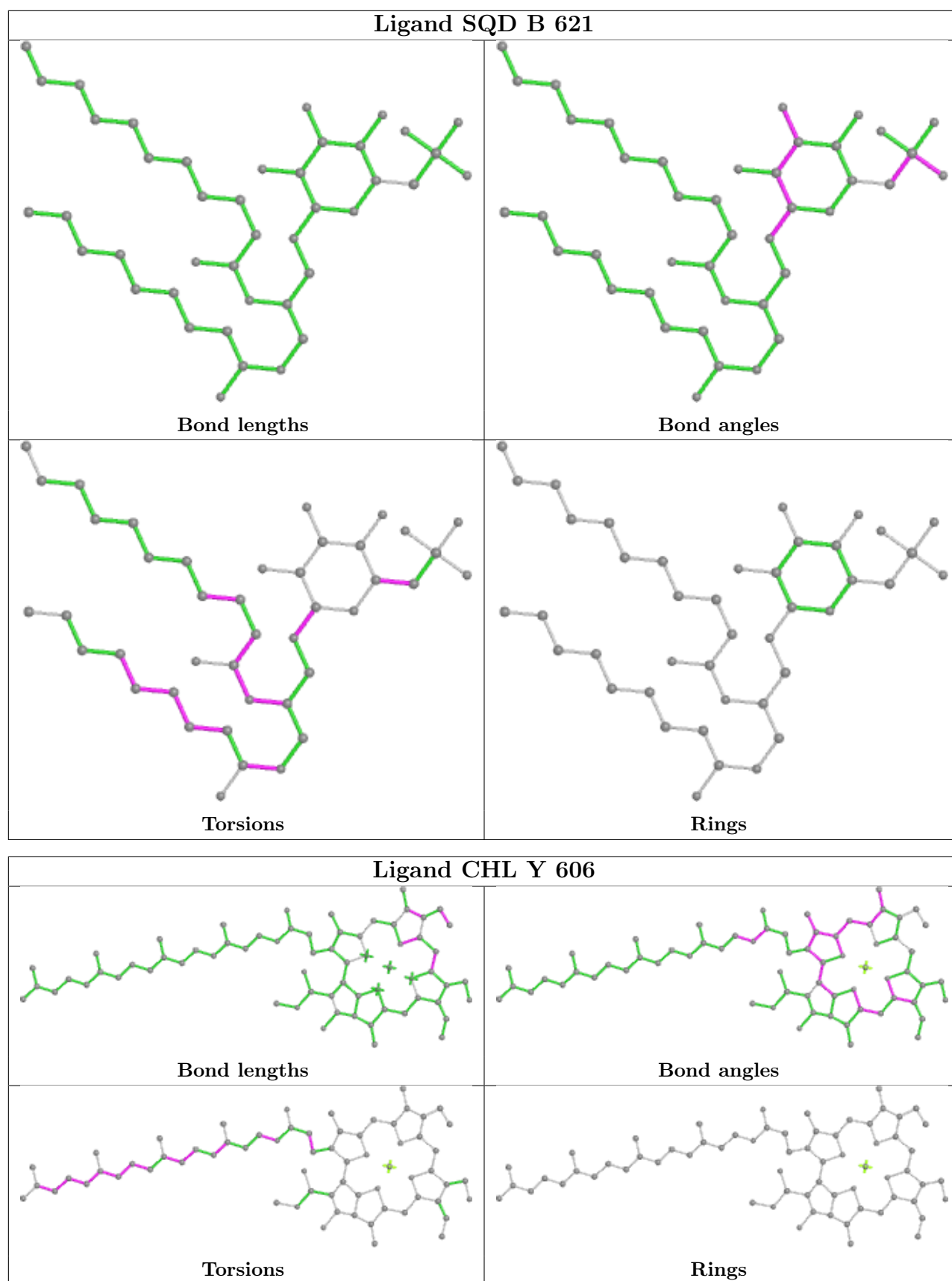




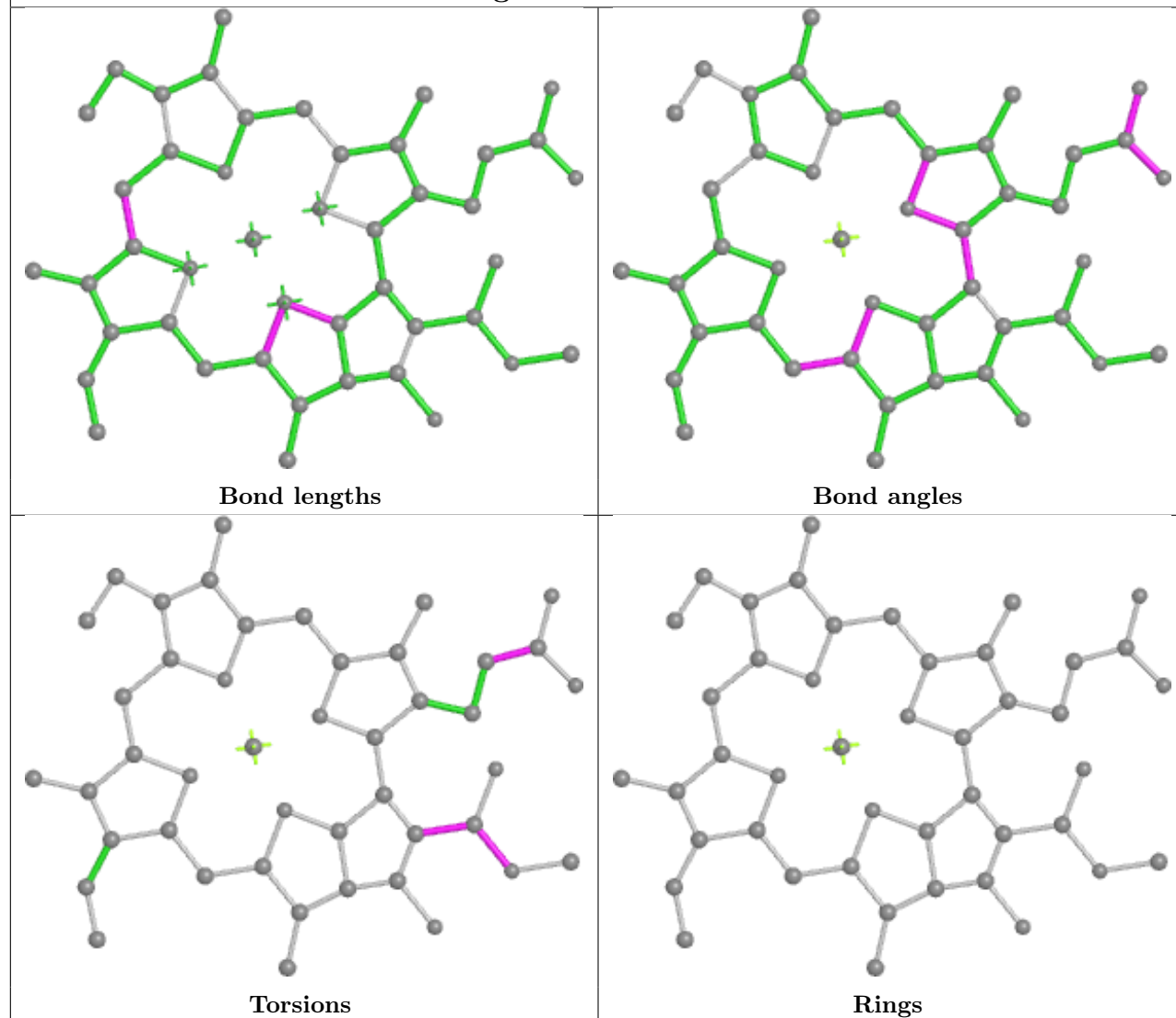




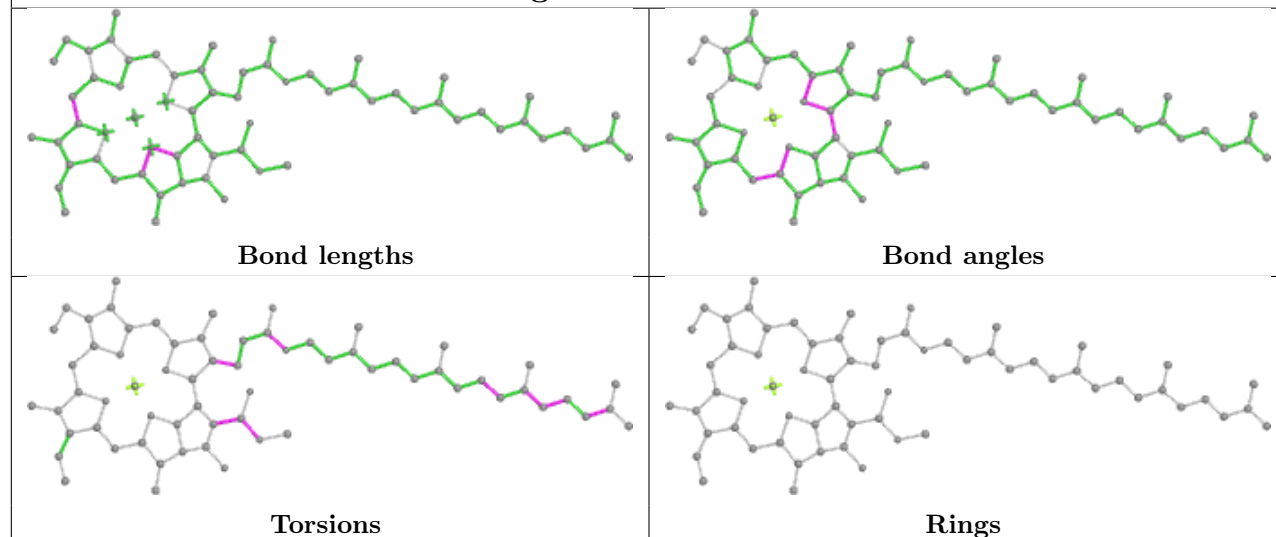




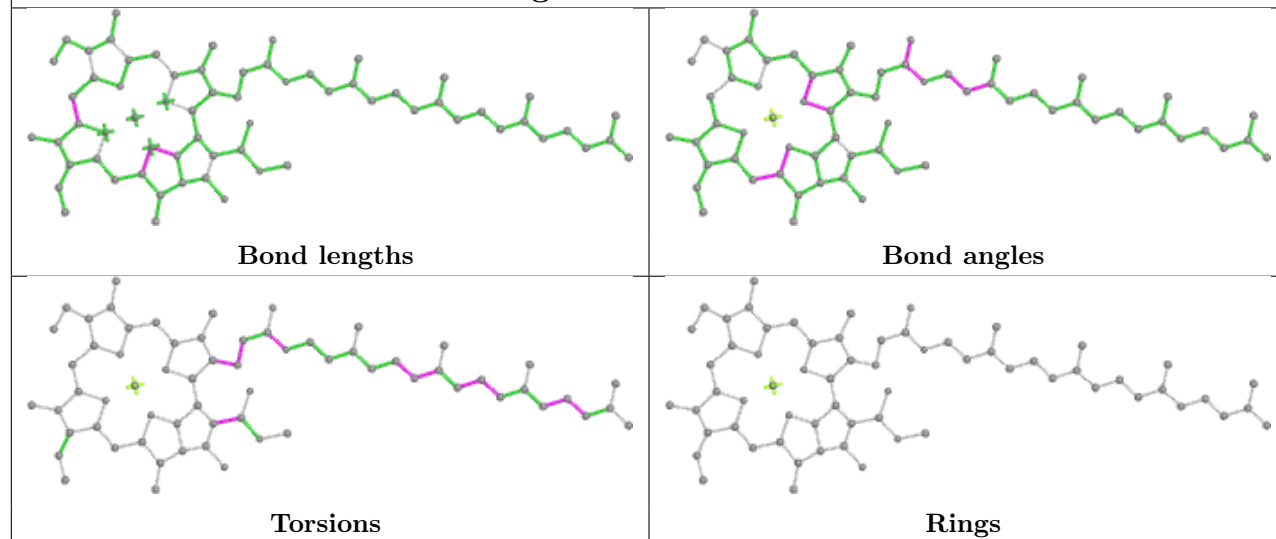
Ligand CLA n 612



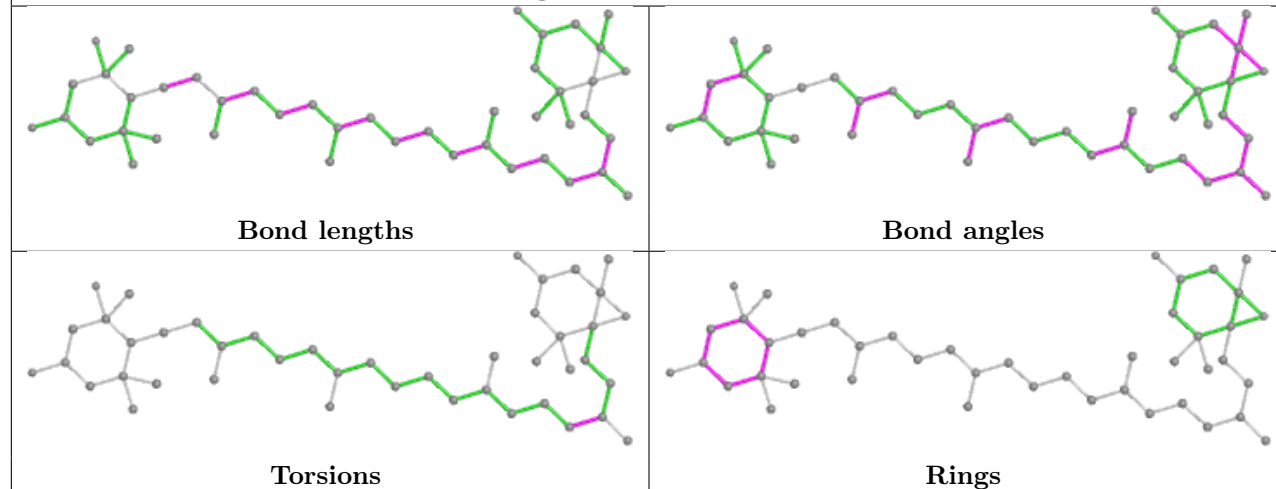
Ligand CLA G 611



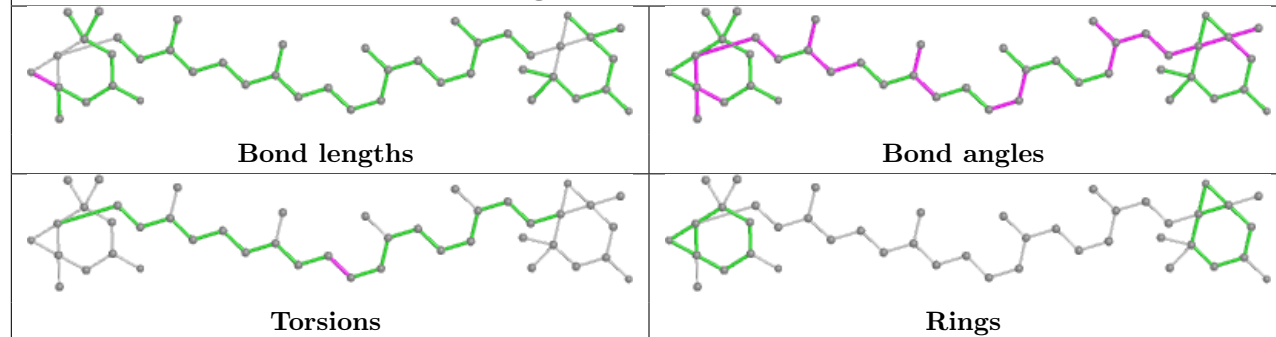
Ligand CLA Y 602

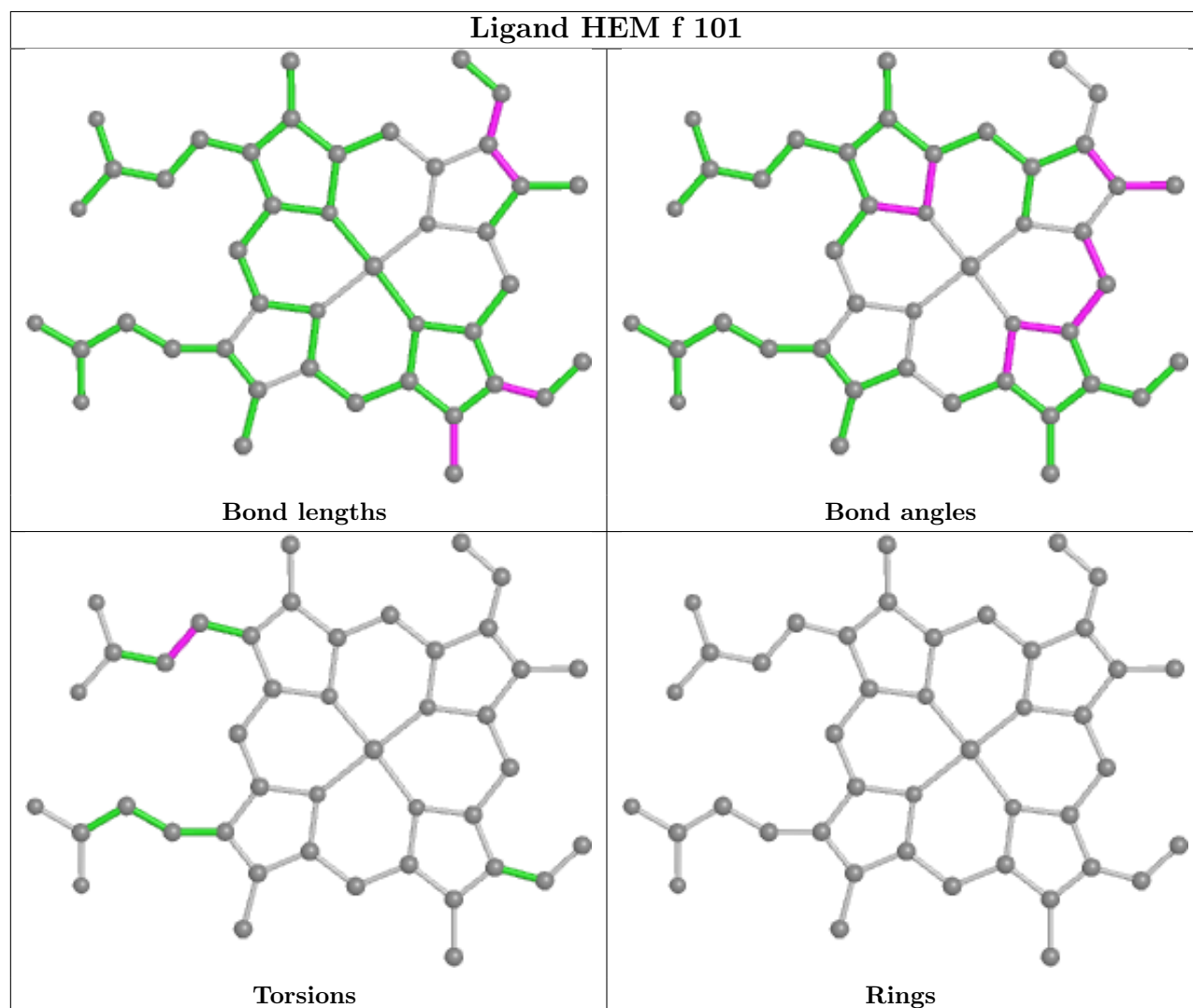
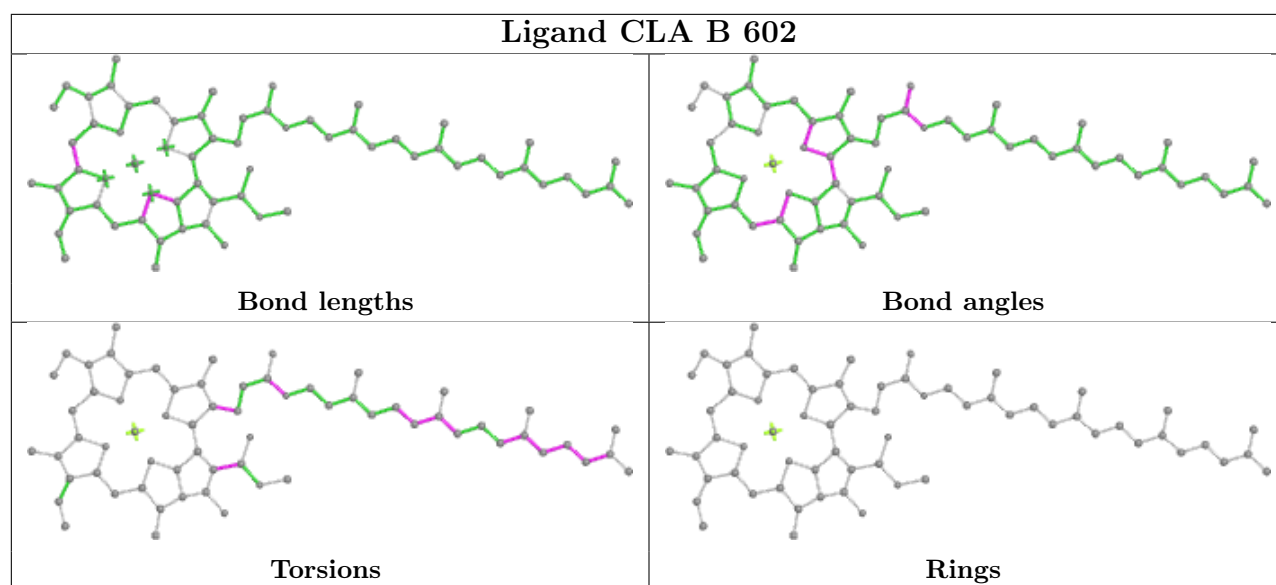


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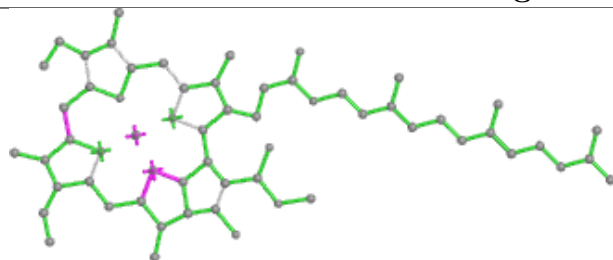


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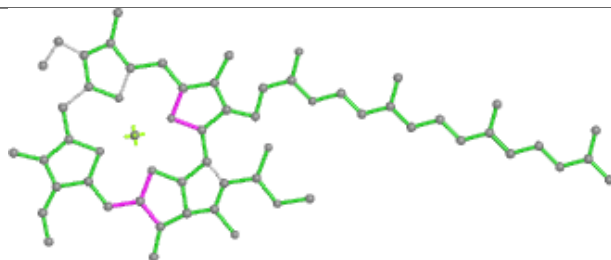




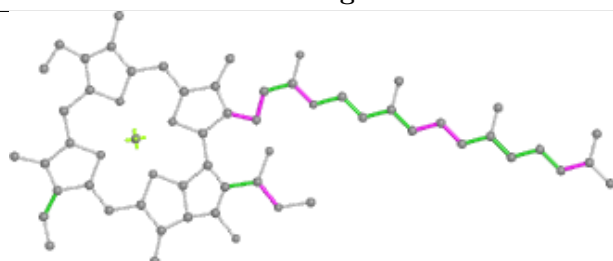
Ligand CLA R 608



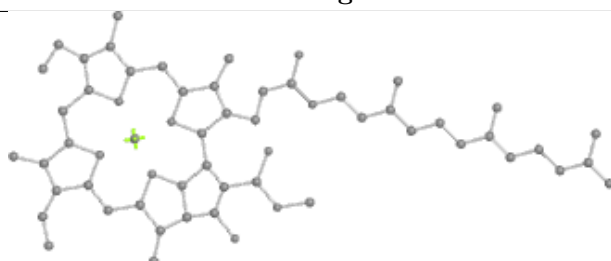
Bond lengths



Bond angles

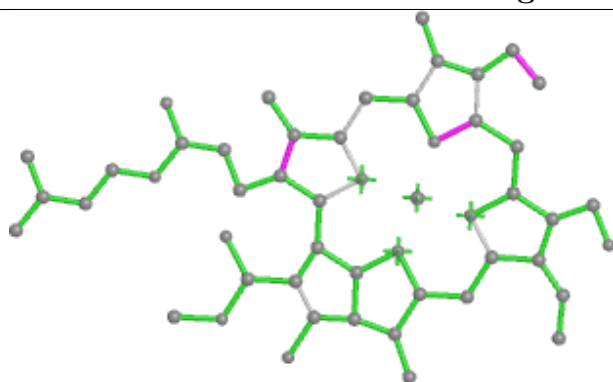


Torsions

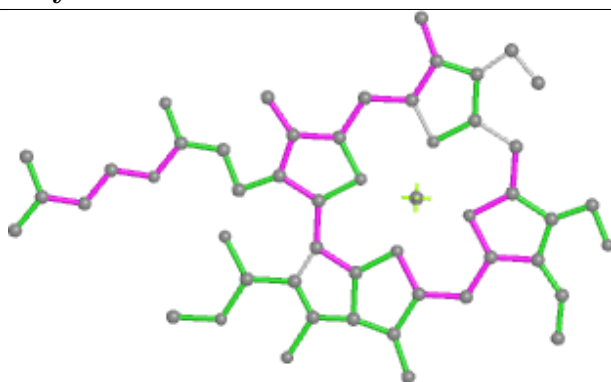


Rings

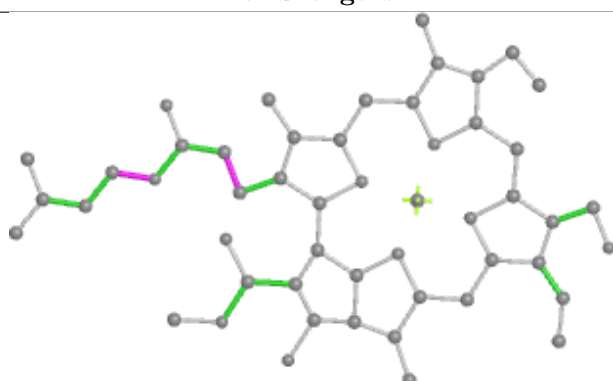
Ligand CHL y 606



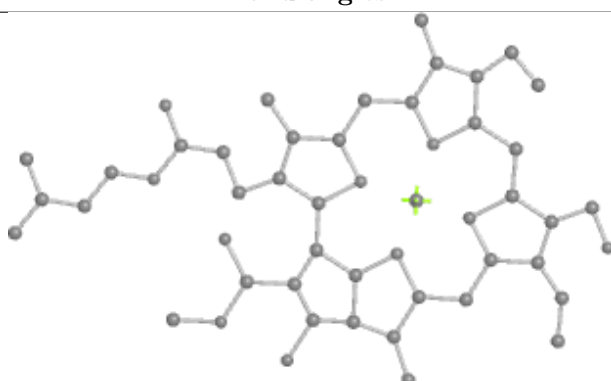
Bond lengths



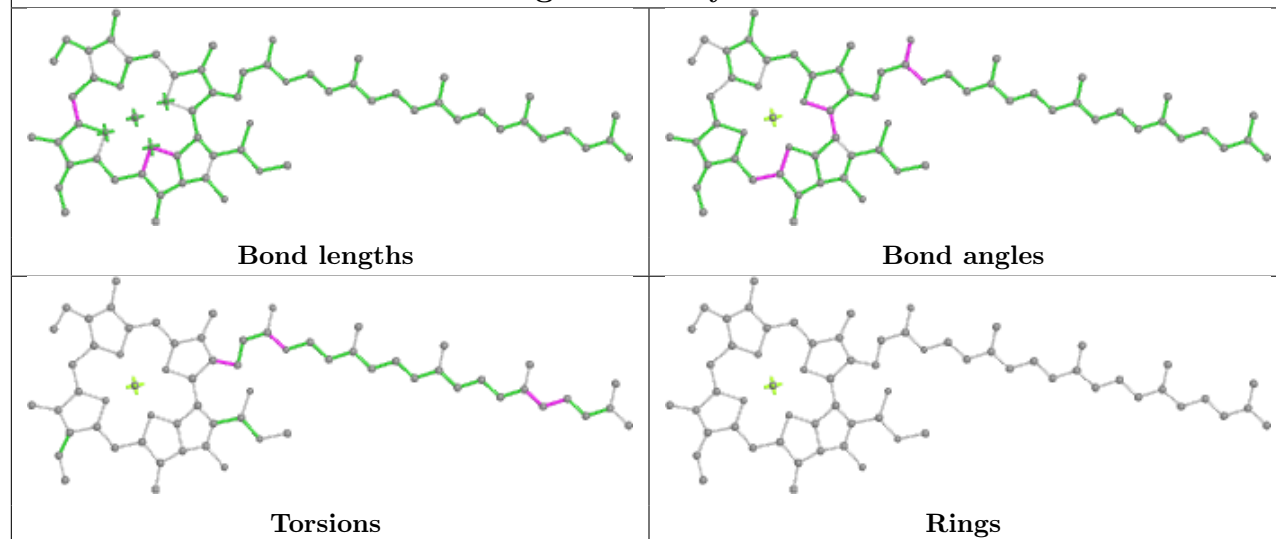
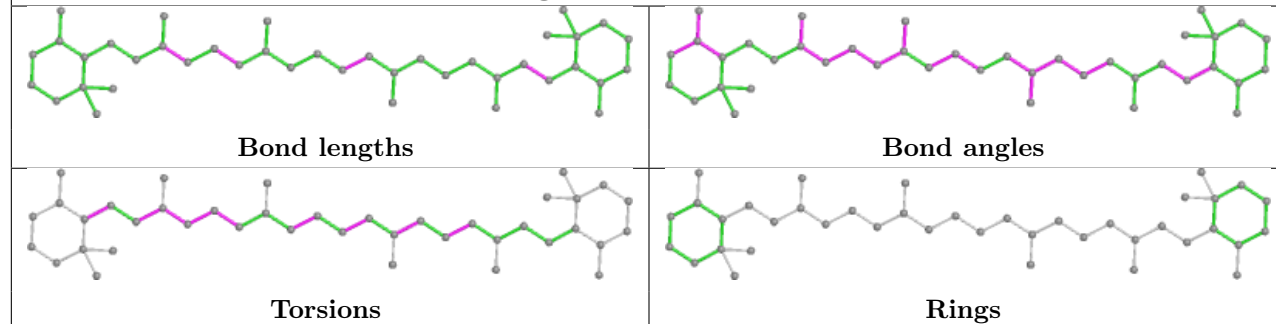
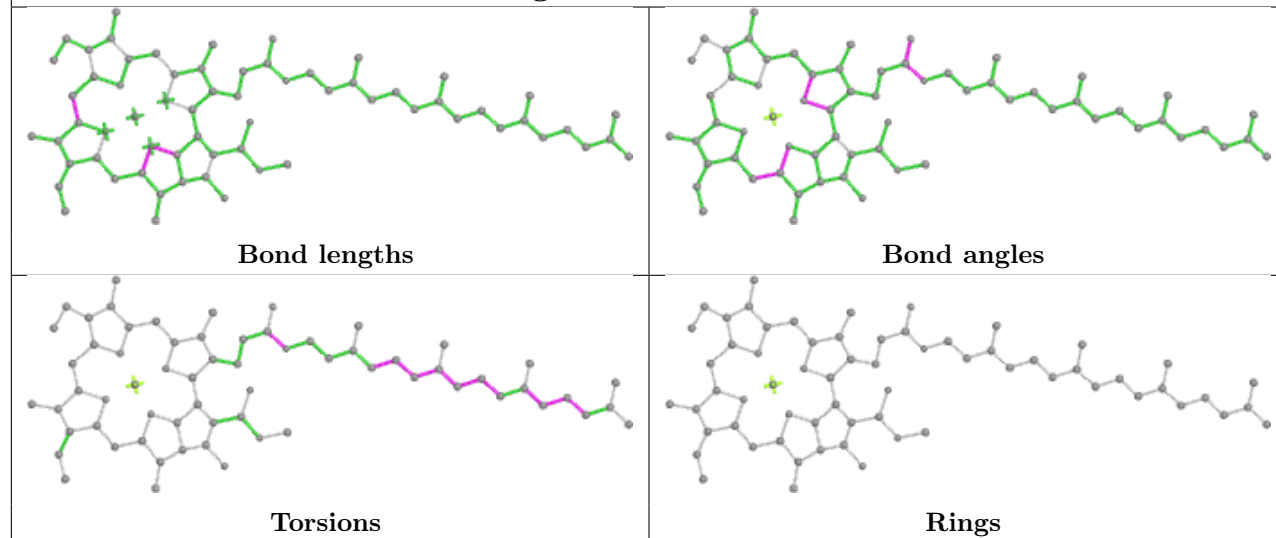
Bond angles

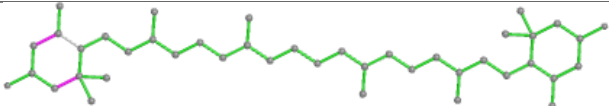
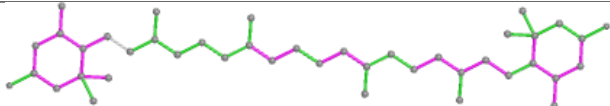
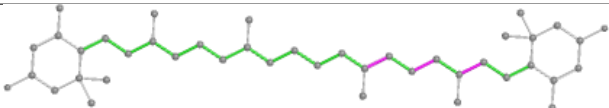
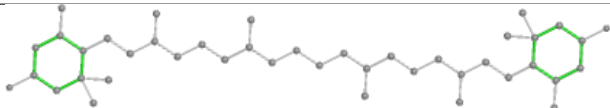


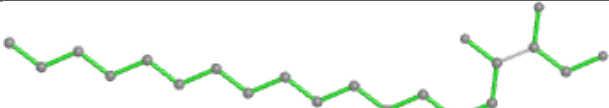
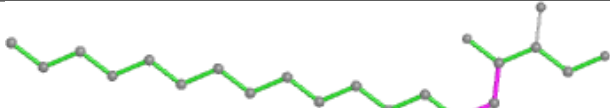
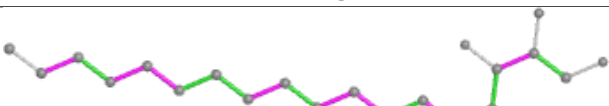
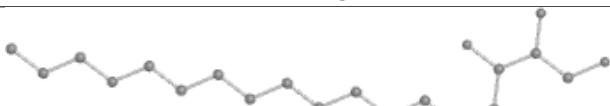
Torsions

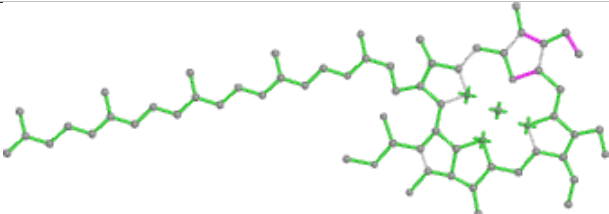
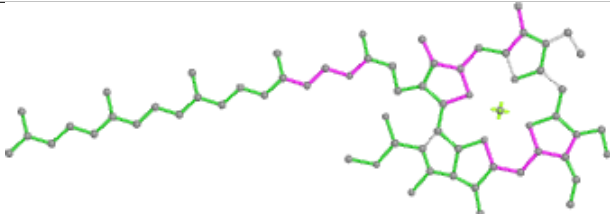
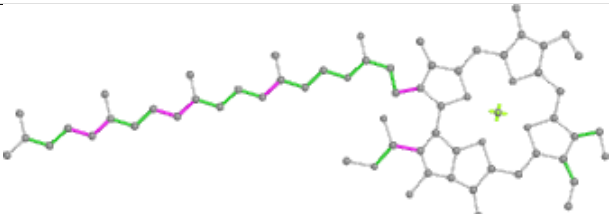
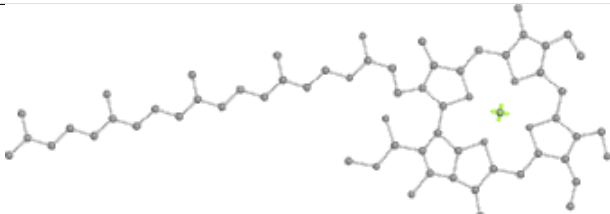


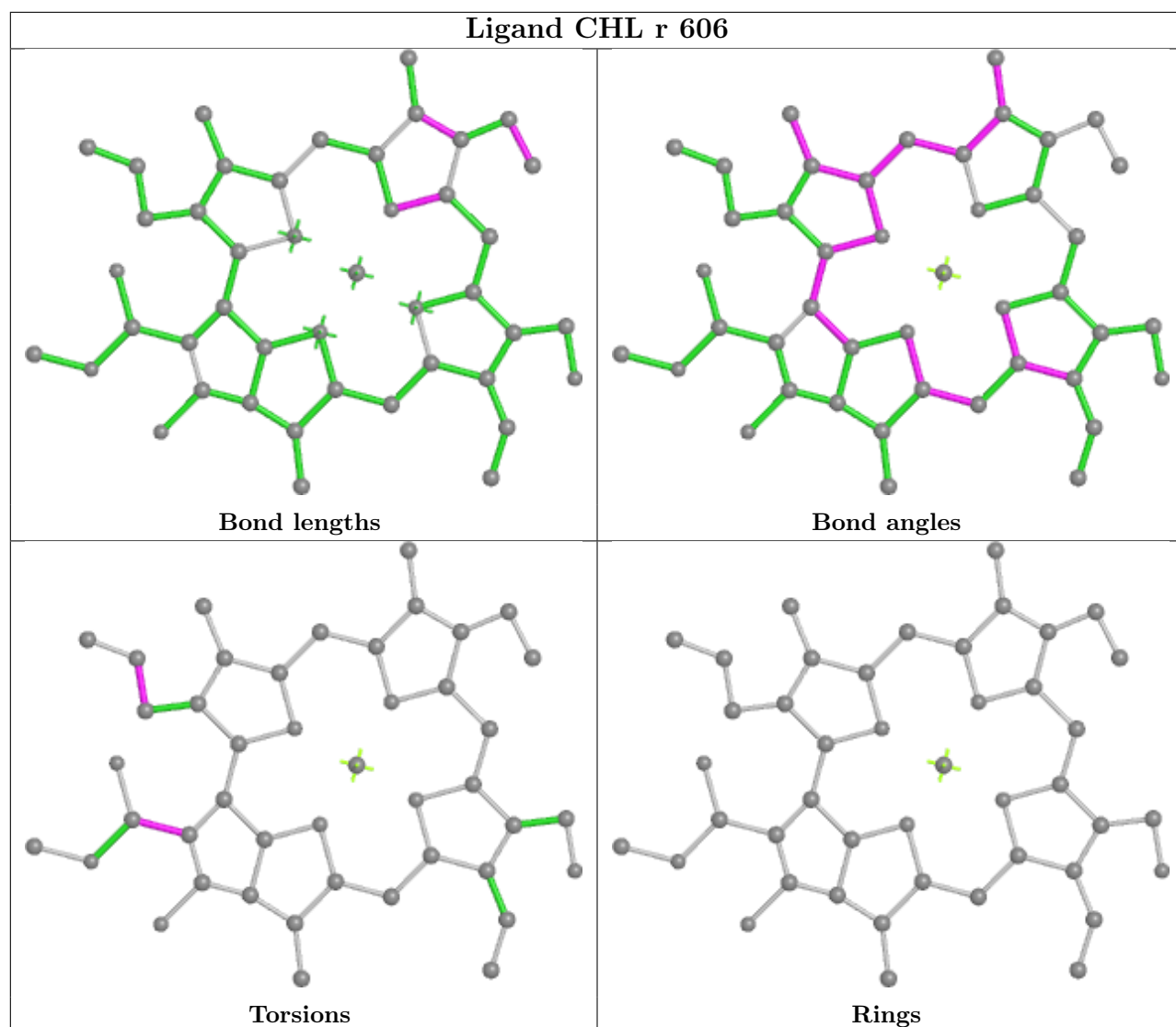
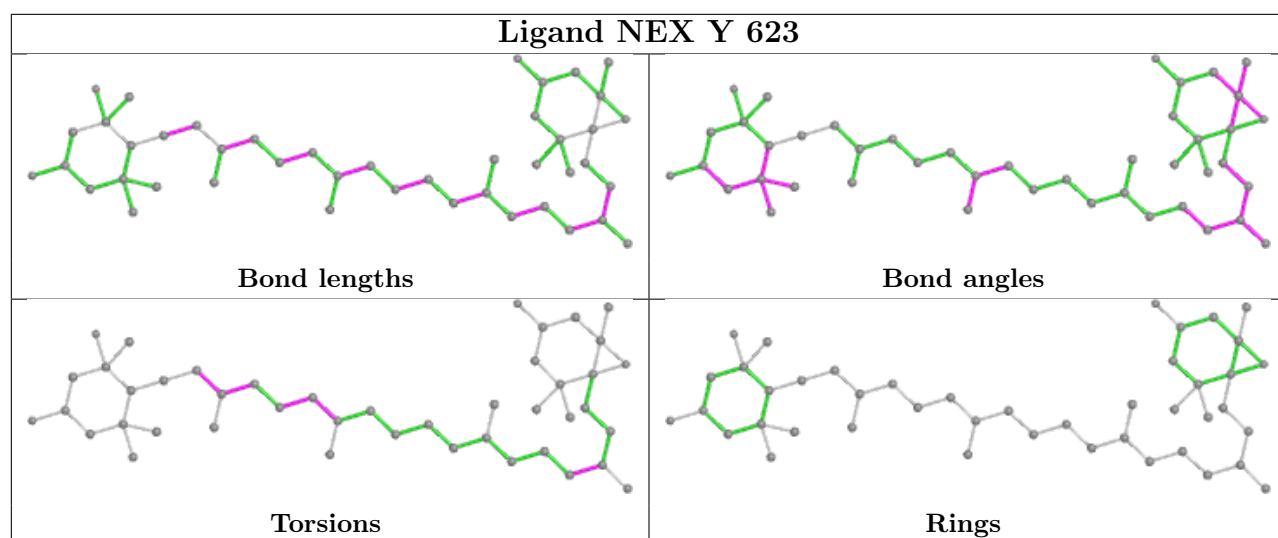
Rings

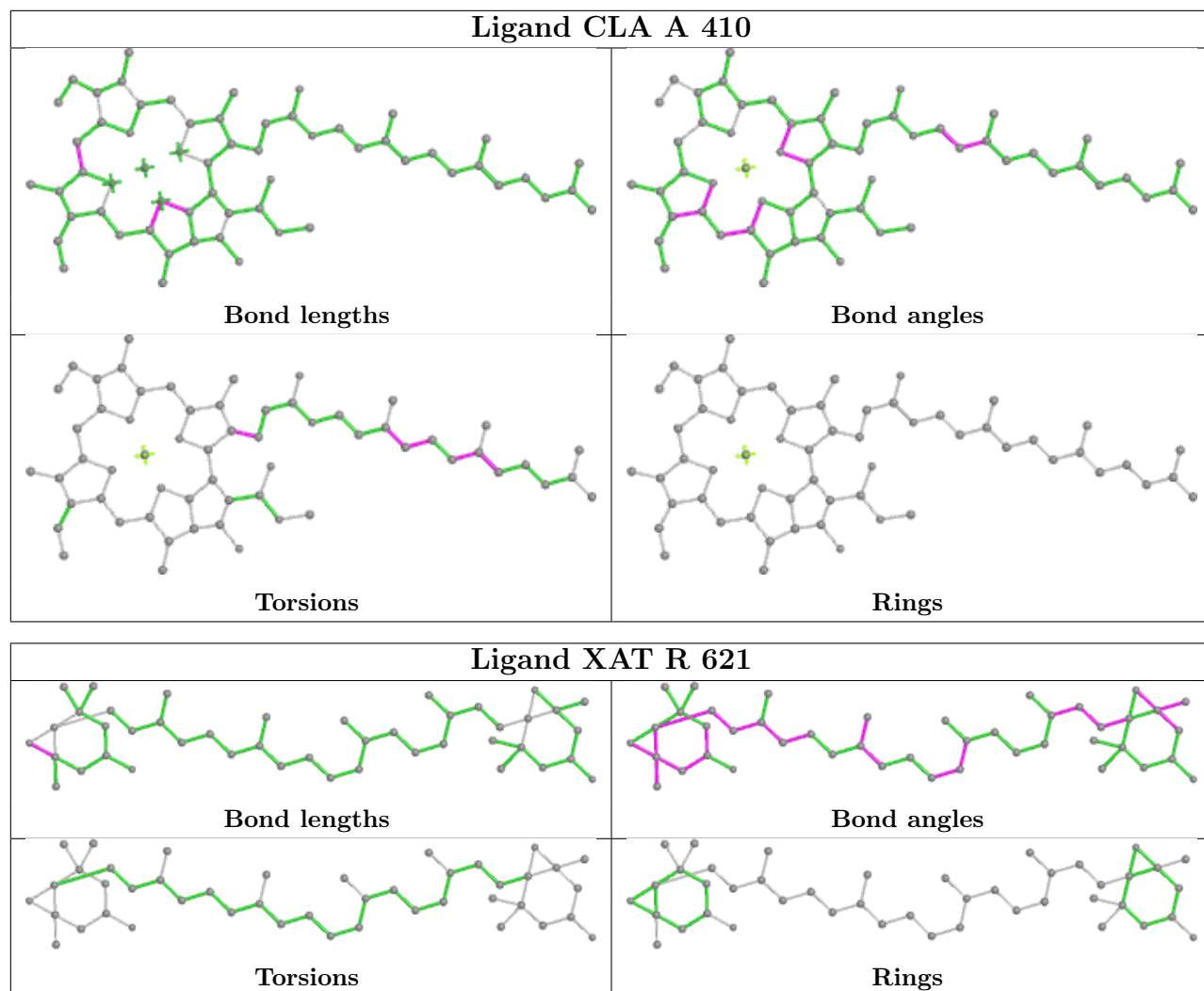
Ligand CLA y 611**Ligand BCR c 514****Ligand CLA Y 612**

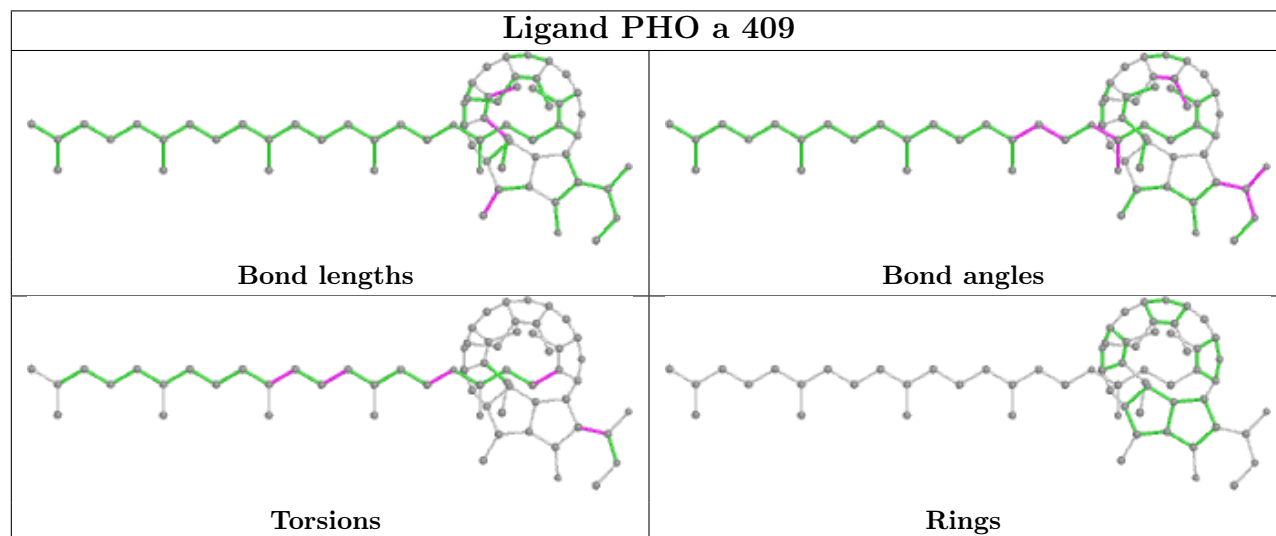
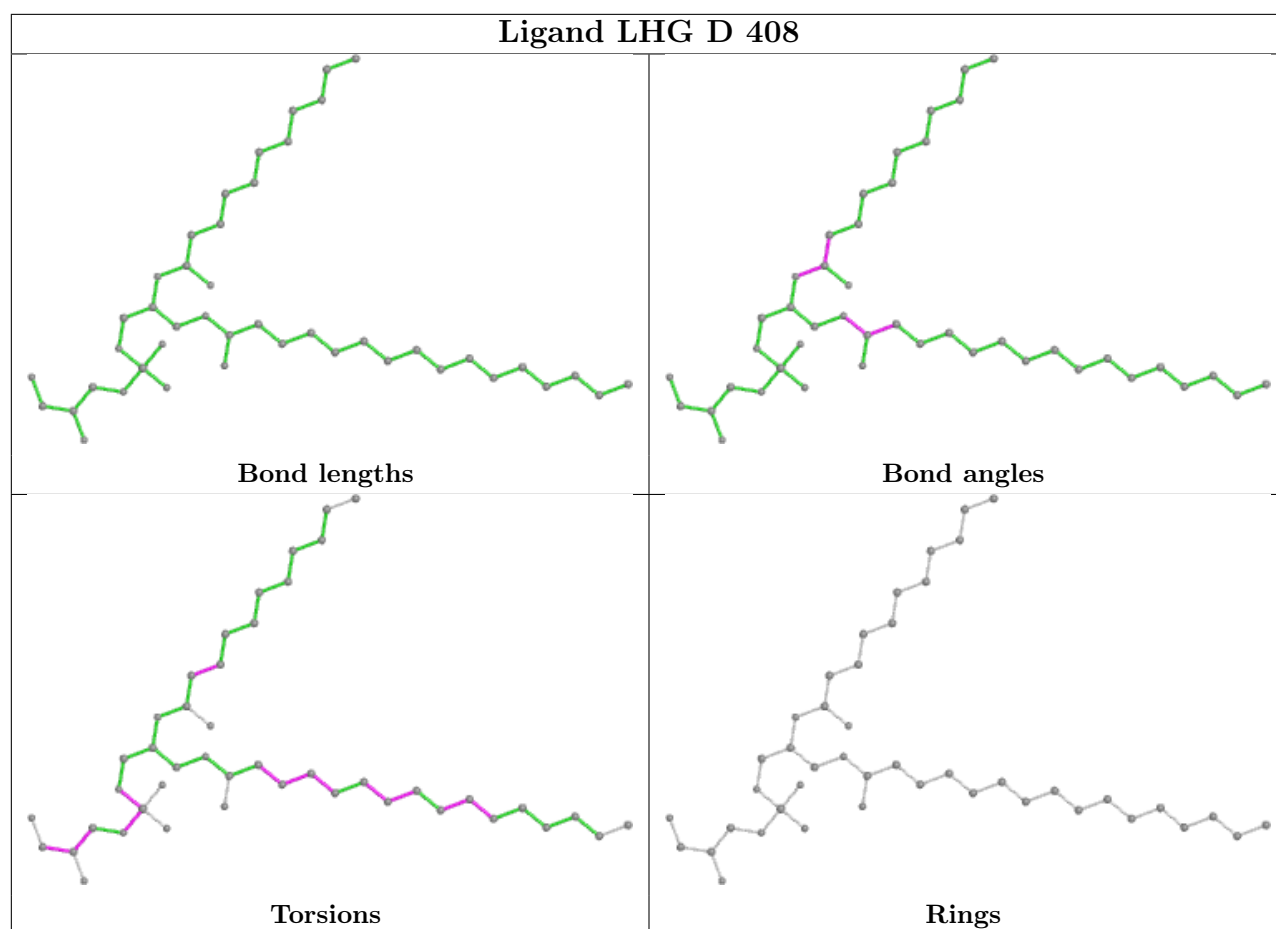
Ligand LUT r 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

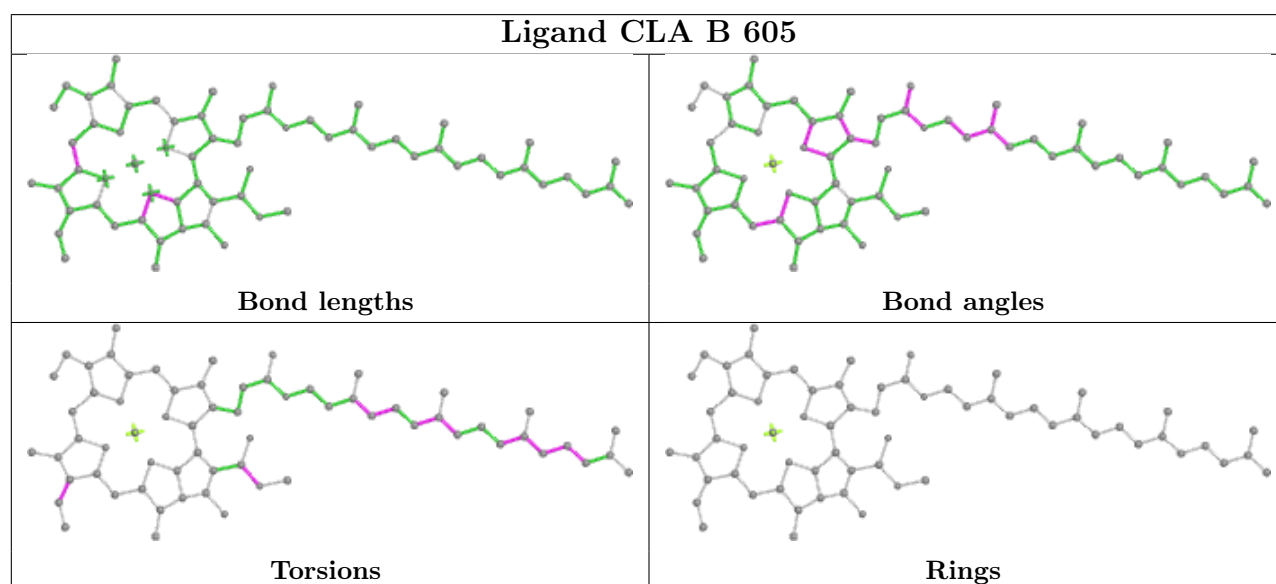
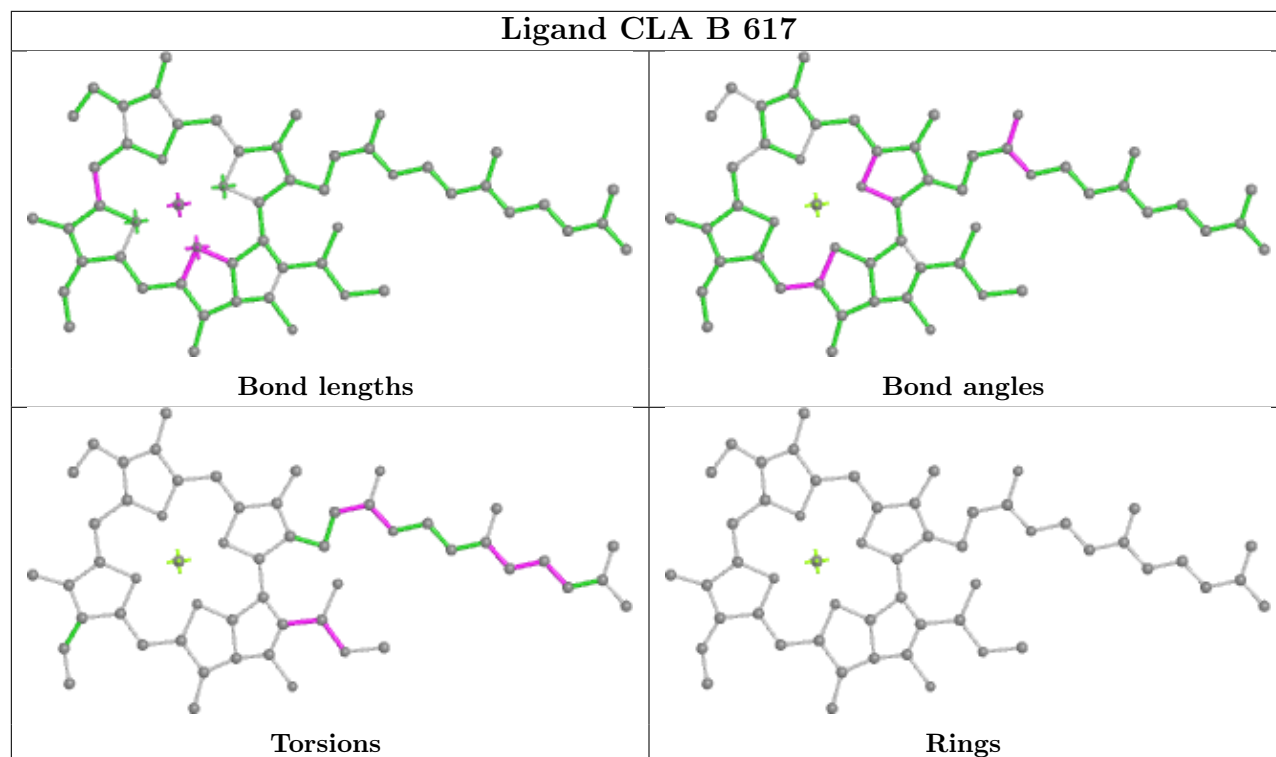
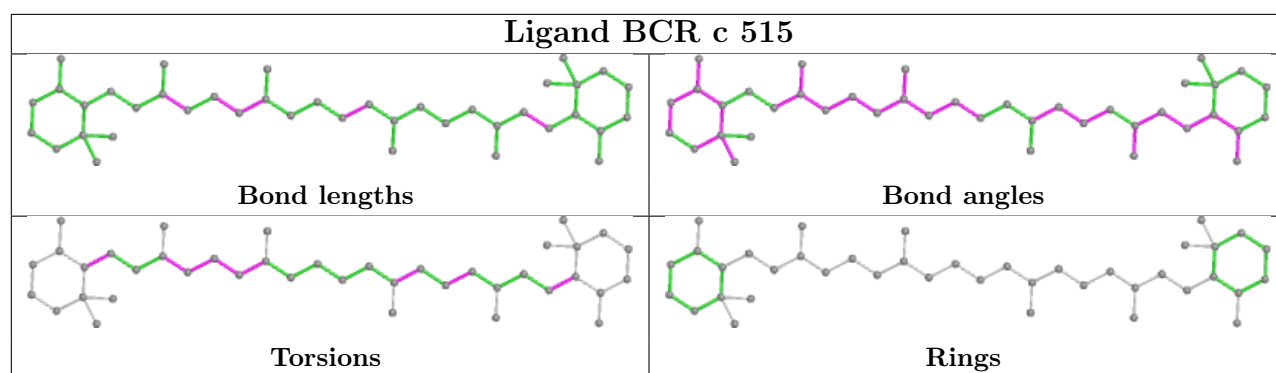
Ligand SPH a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

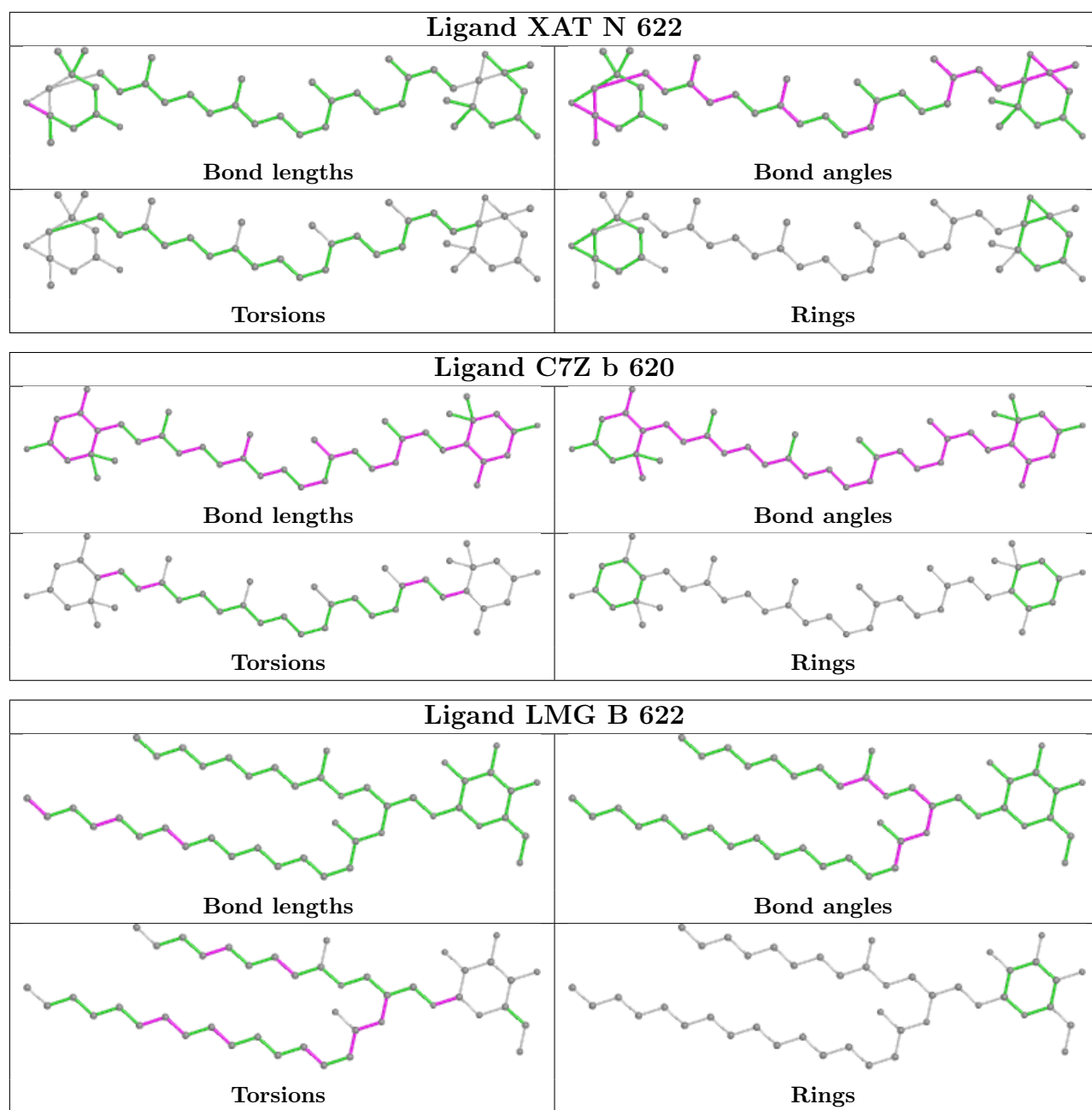
Ligand CHL N 601	
	
Bond lengths	Bond angles
	
Torsions	Rings



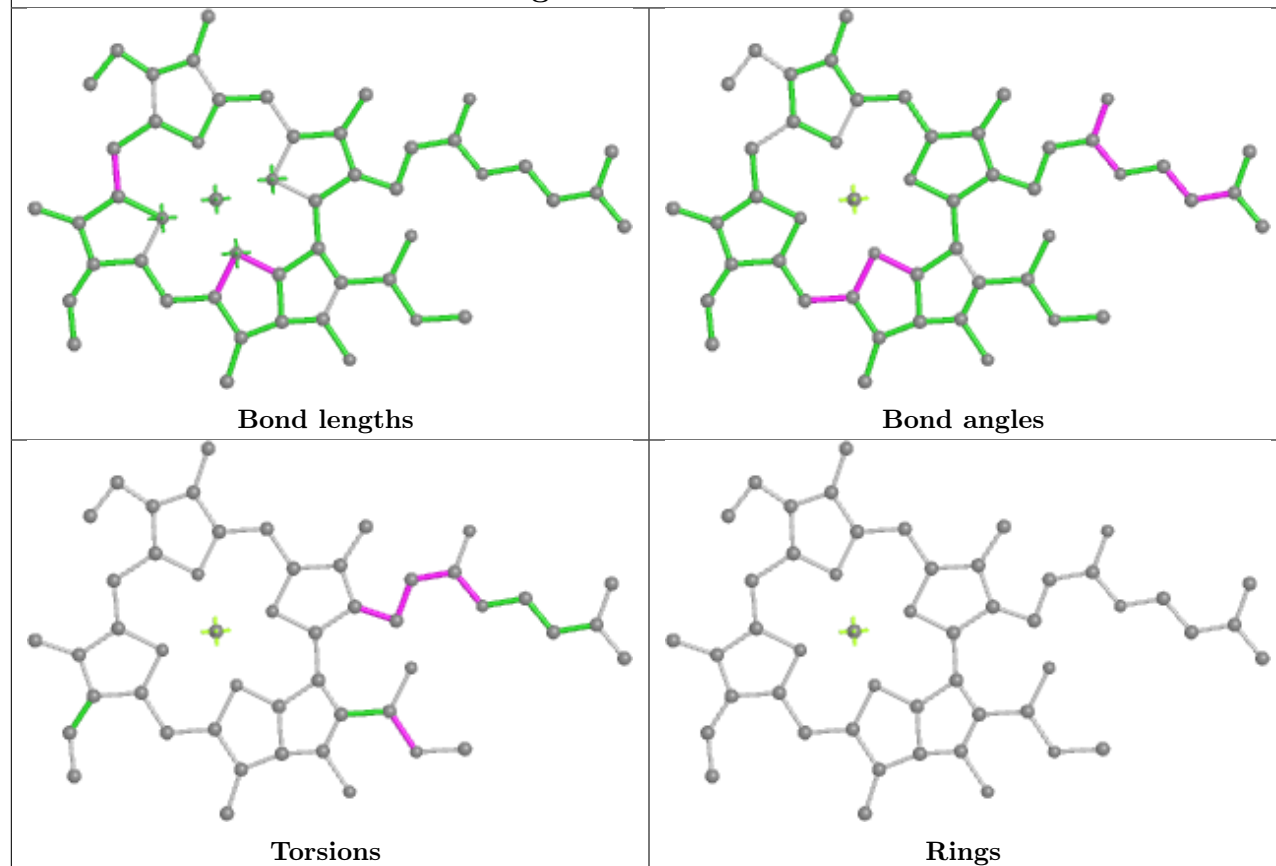




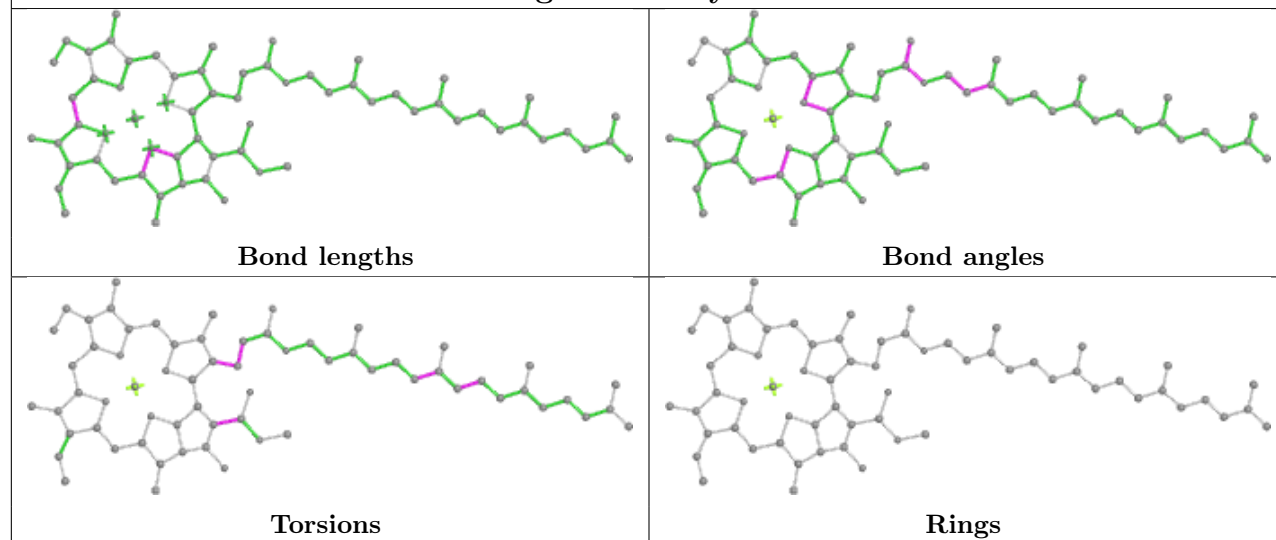




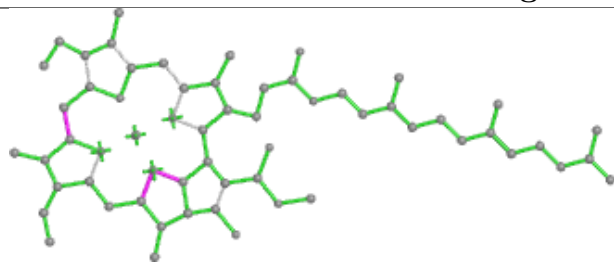
Ligand CLA R 612



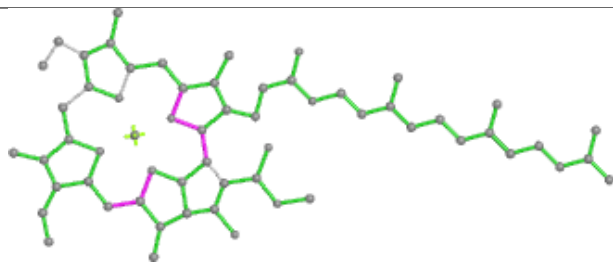
Ligand CLA y 602



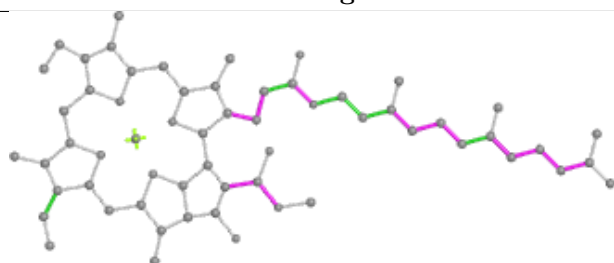
Ligand CLA s 609



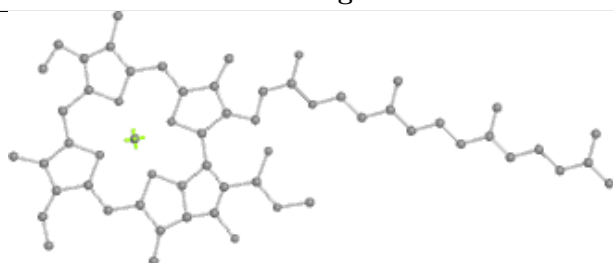
Bond lengths



Bond angles

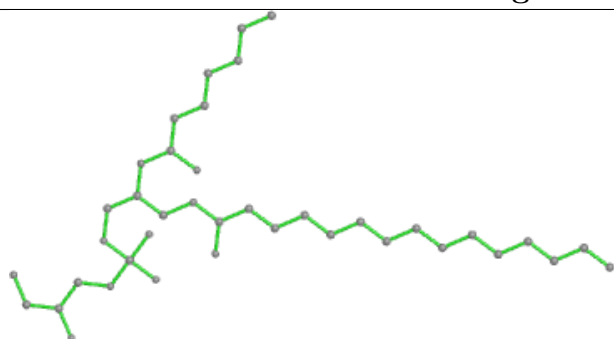


Torsions

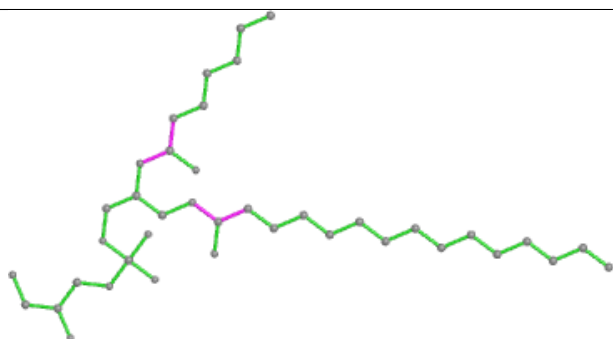


Rings

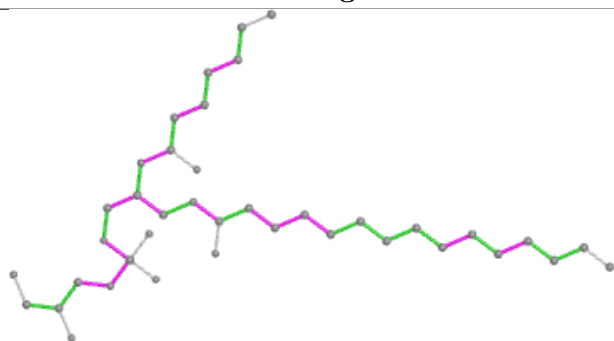
Ligand LHG D 410



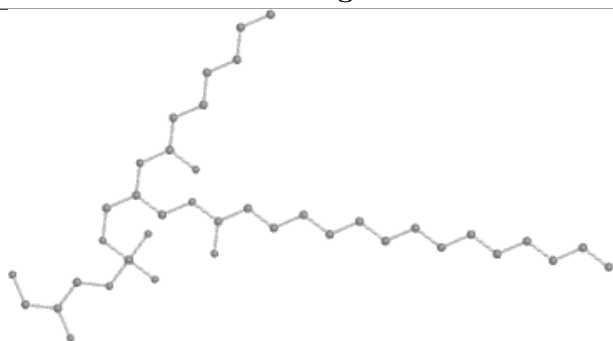
Bond lengths



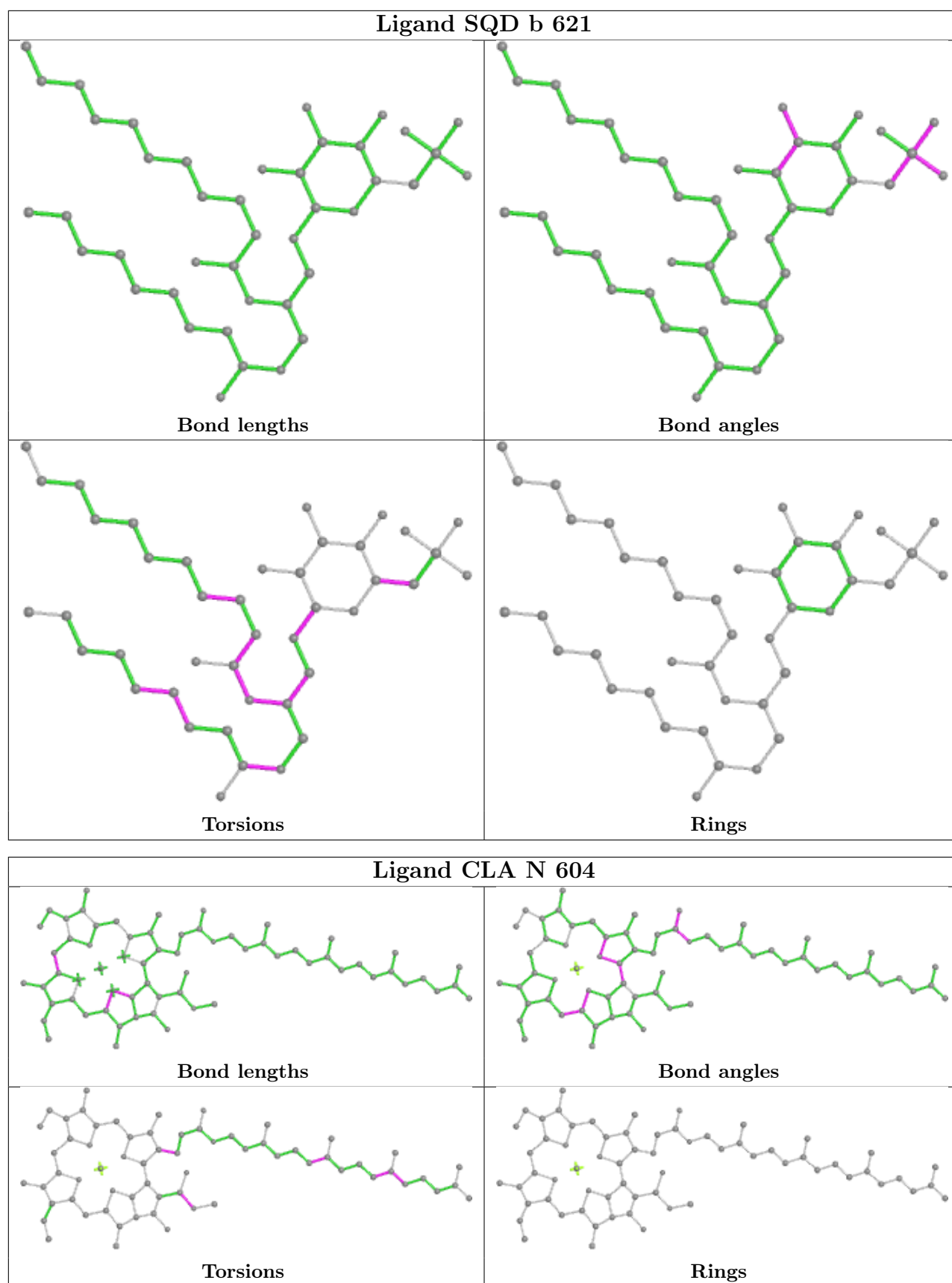
Bond angles

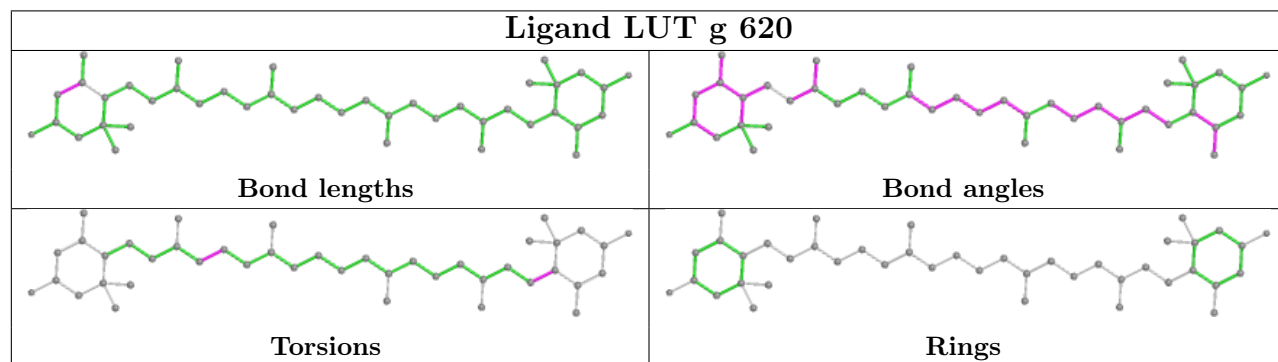
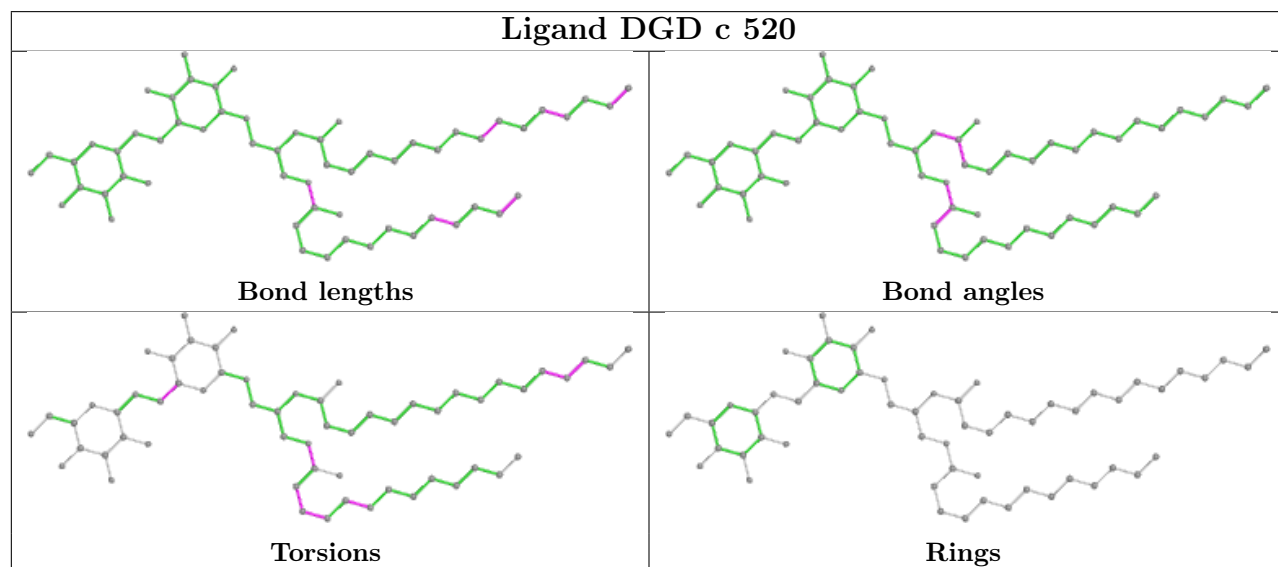
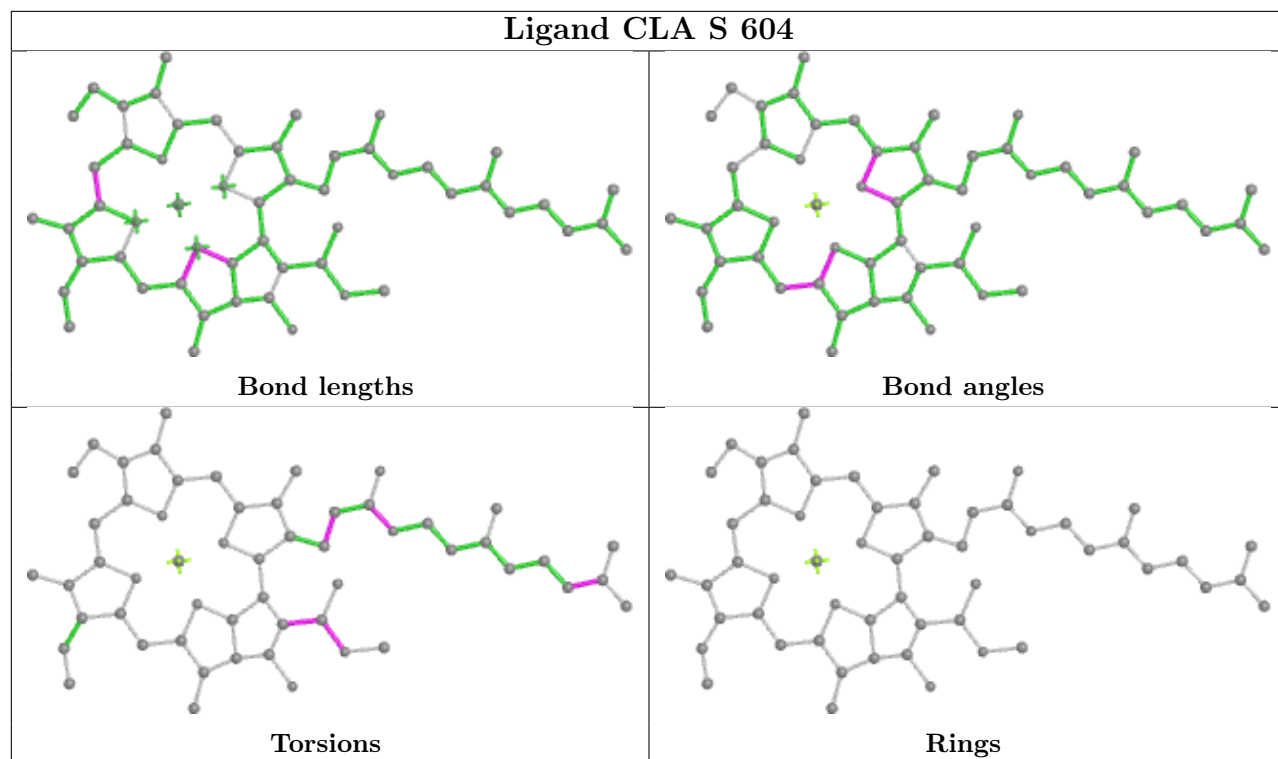


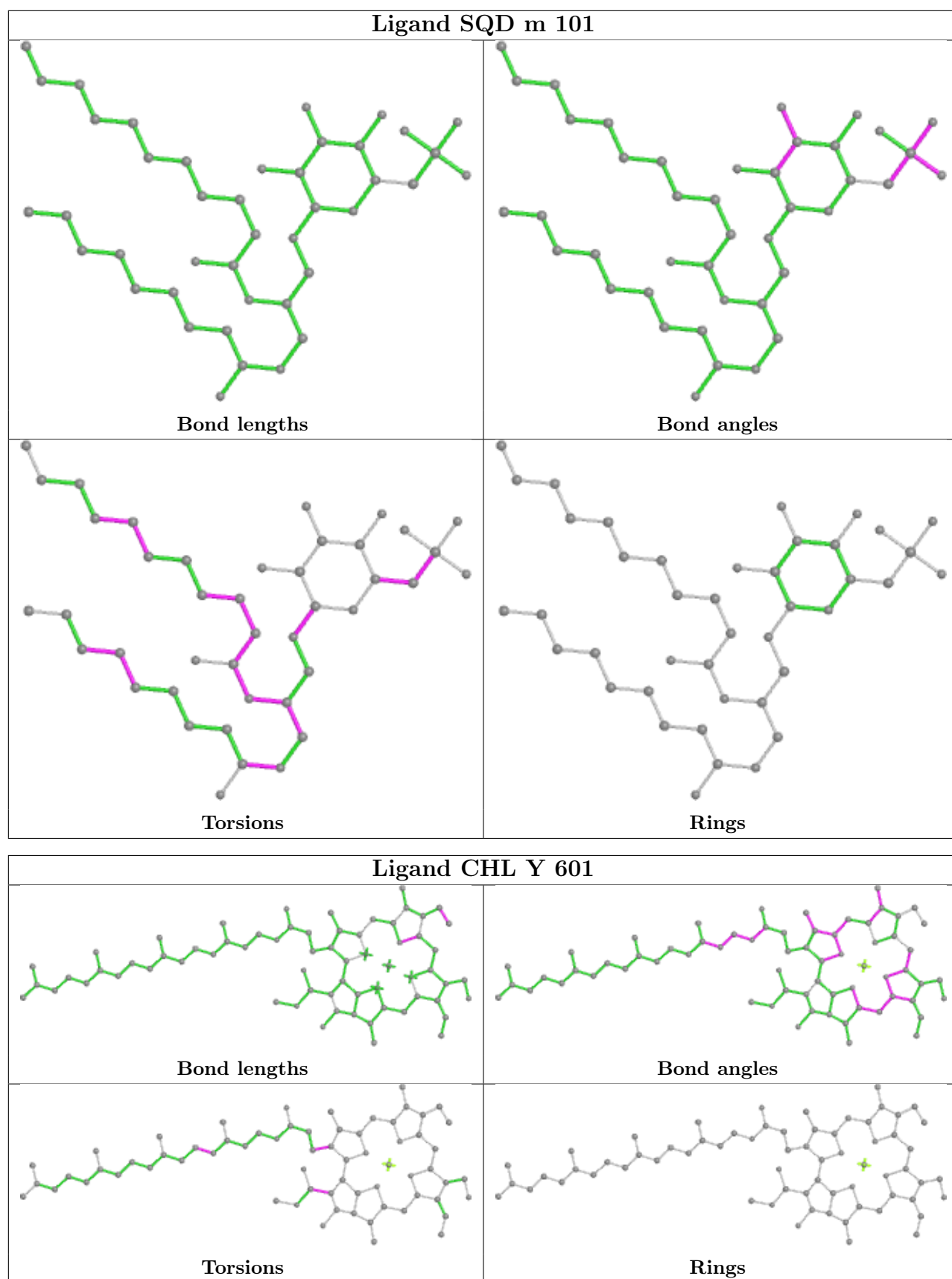
Torsions

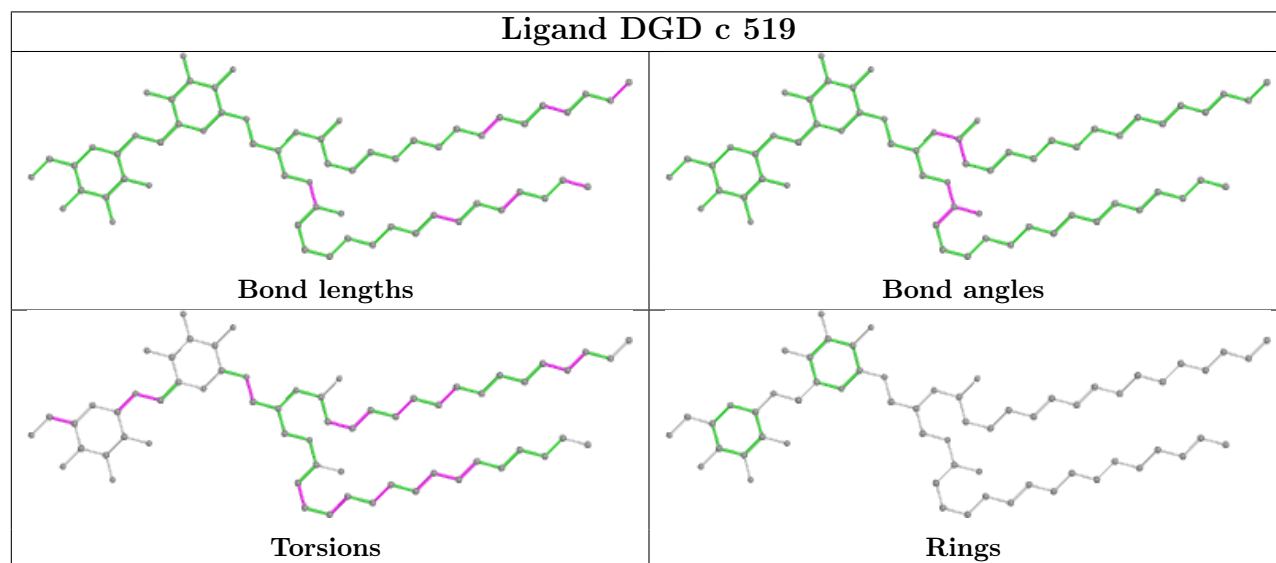
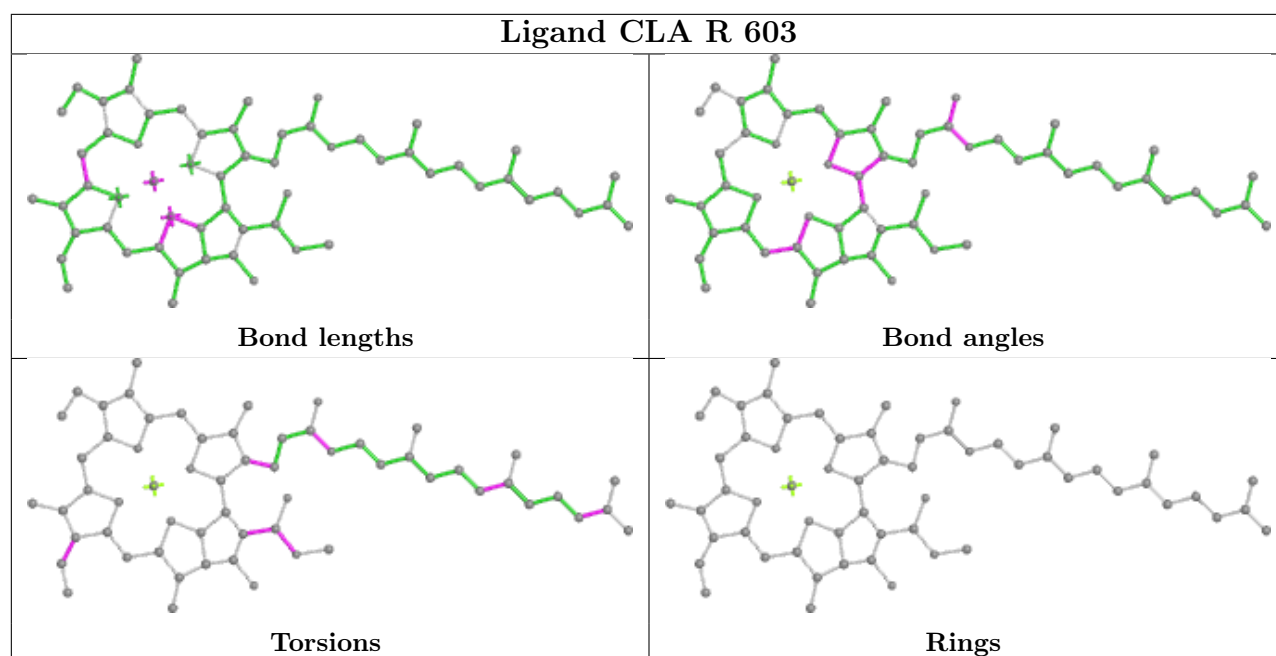


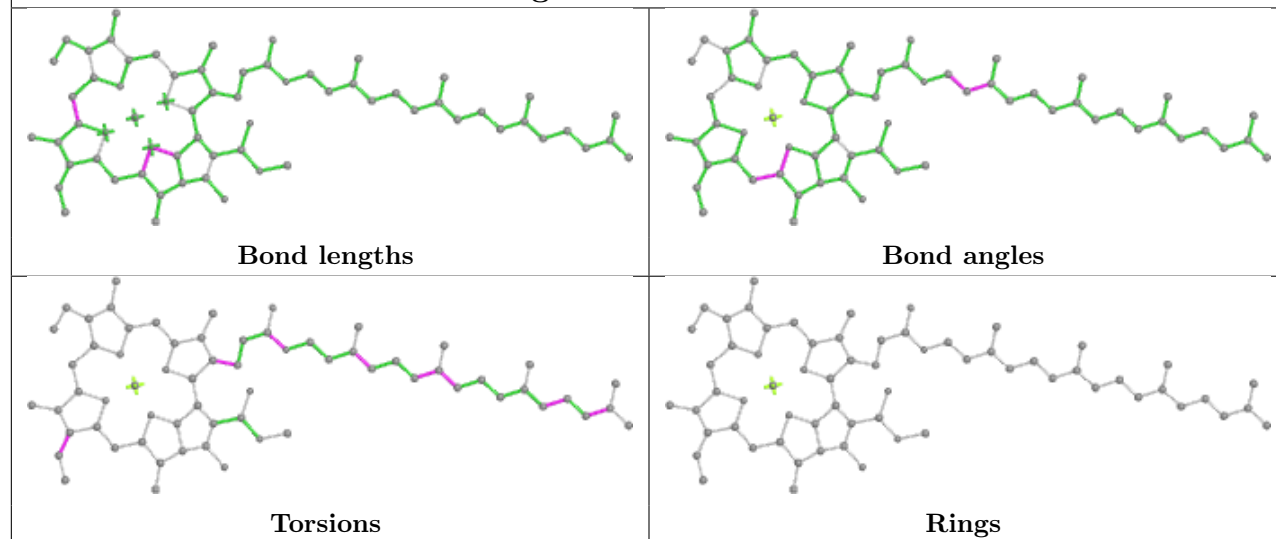
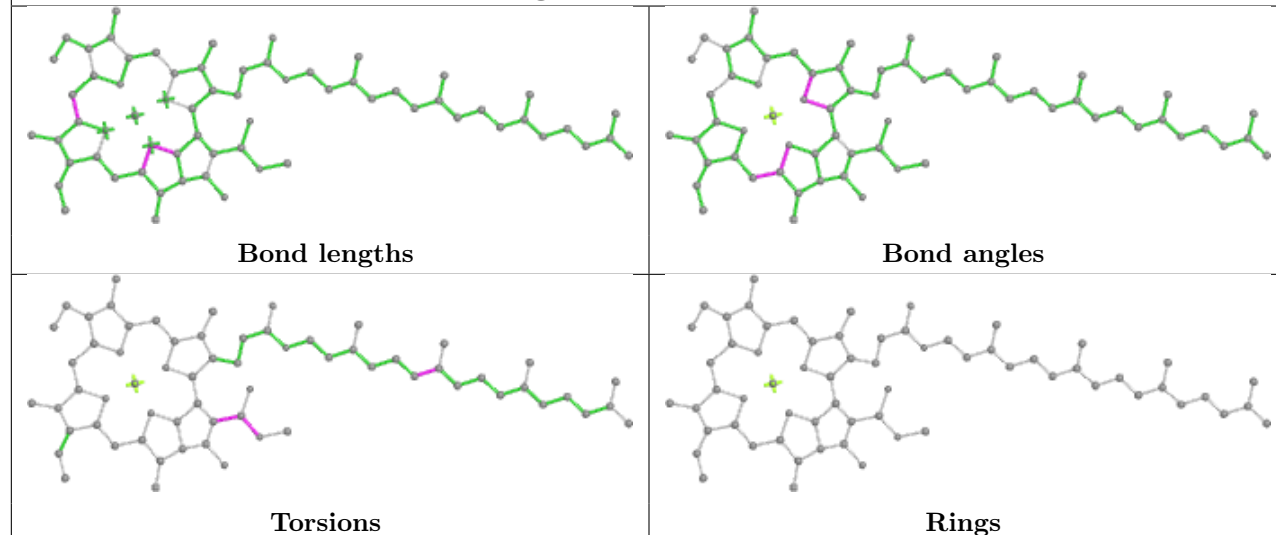
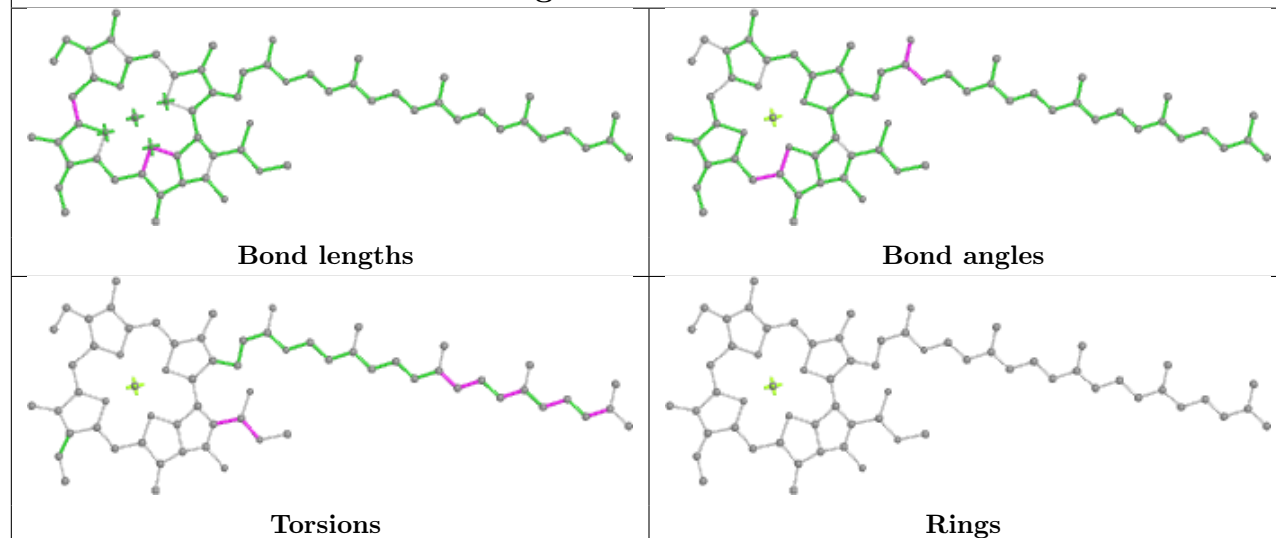
Rings

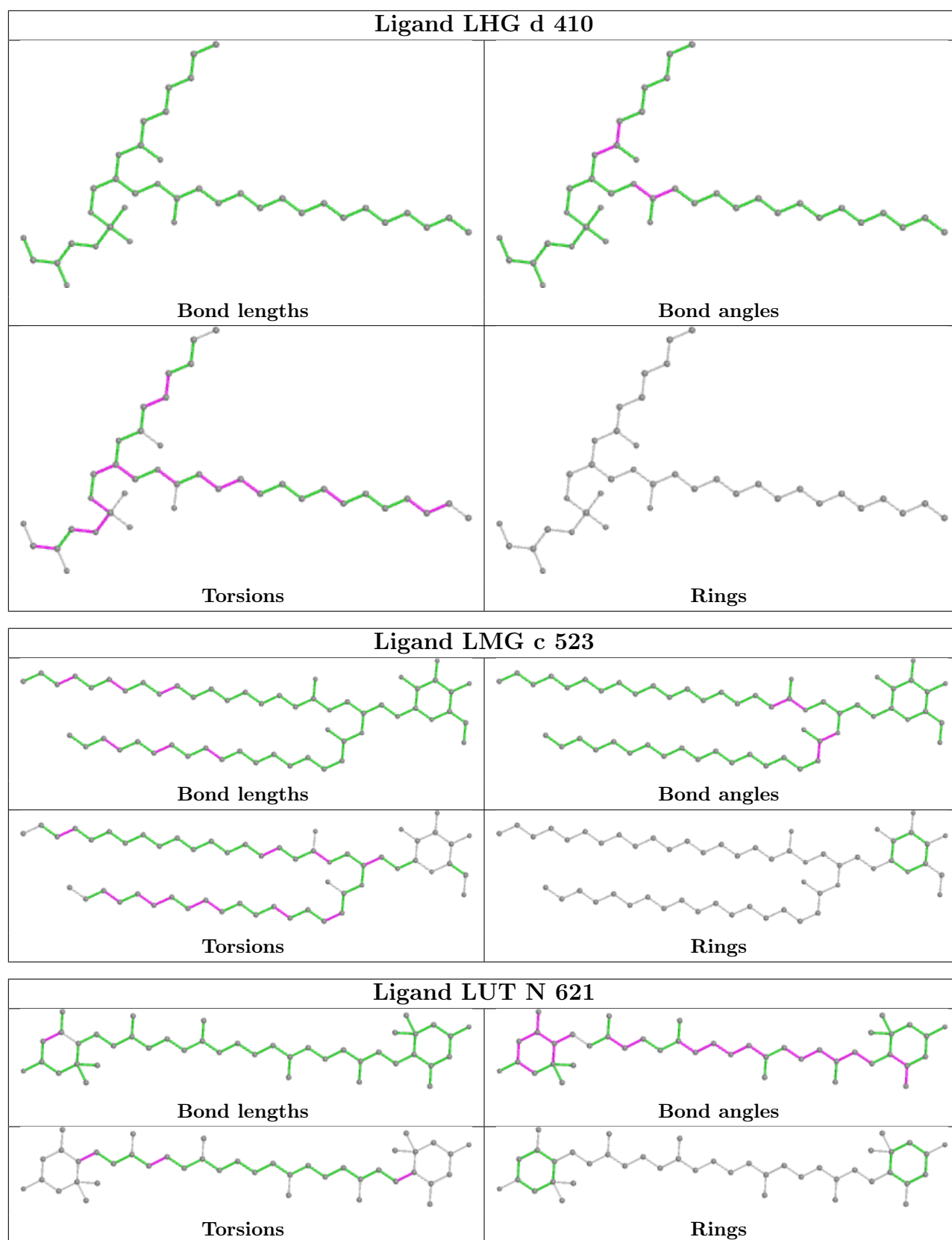




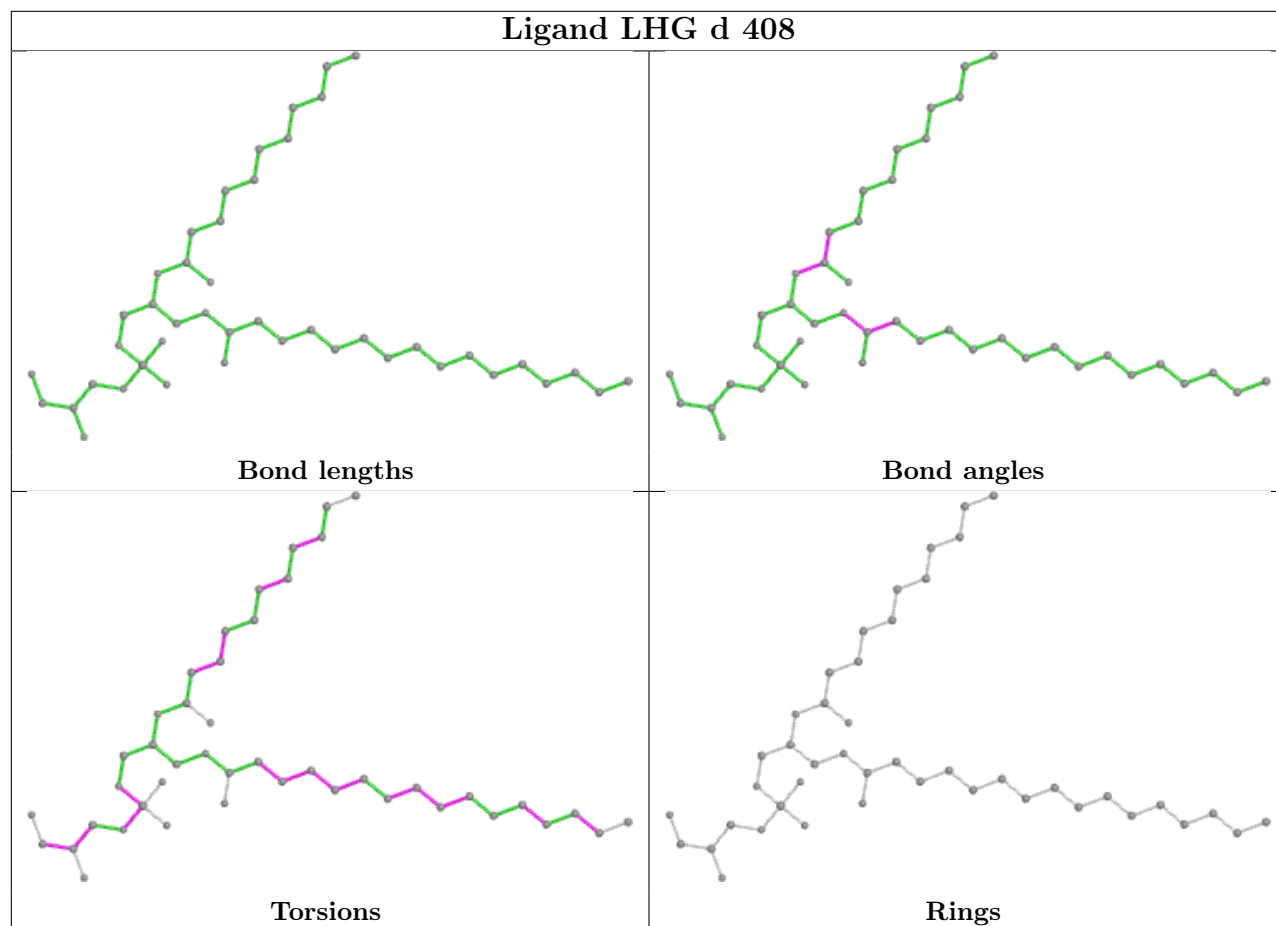




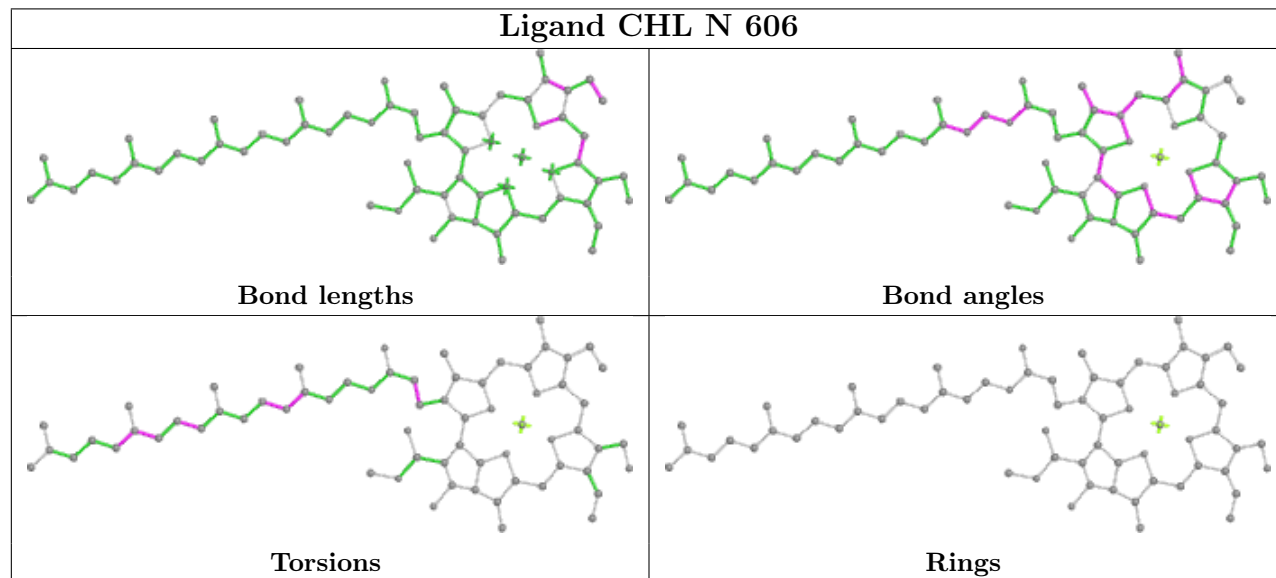
Ligand CLA Y 603**Ligand CLA C 511****Ligand CLA b 616**



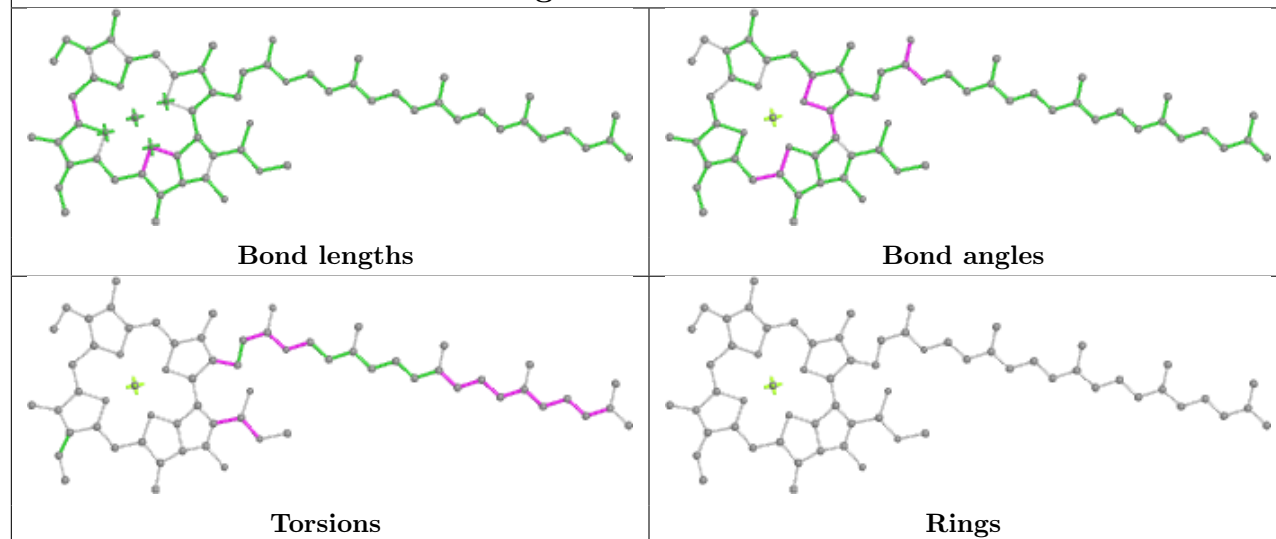
Ligand LHG d 408



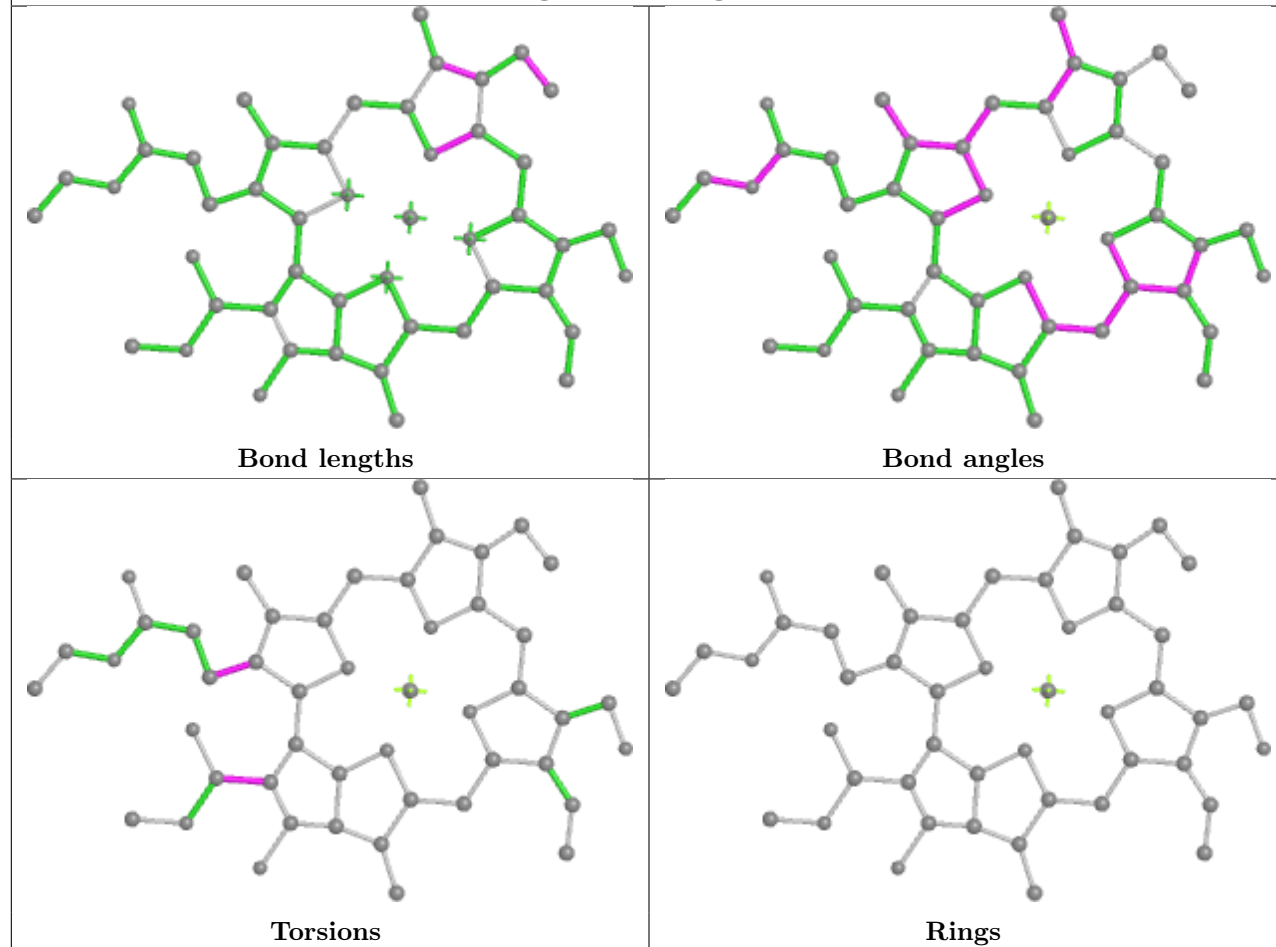
Ligand CHL N 606

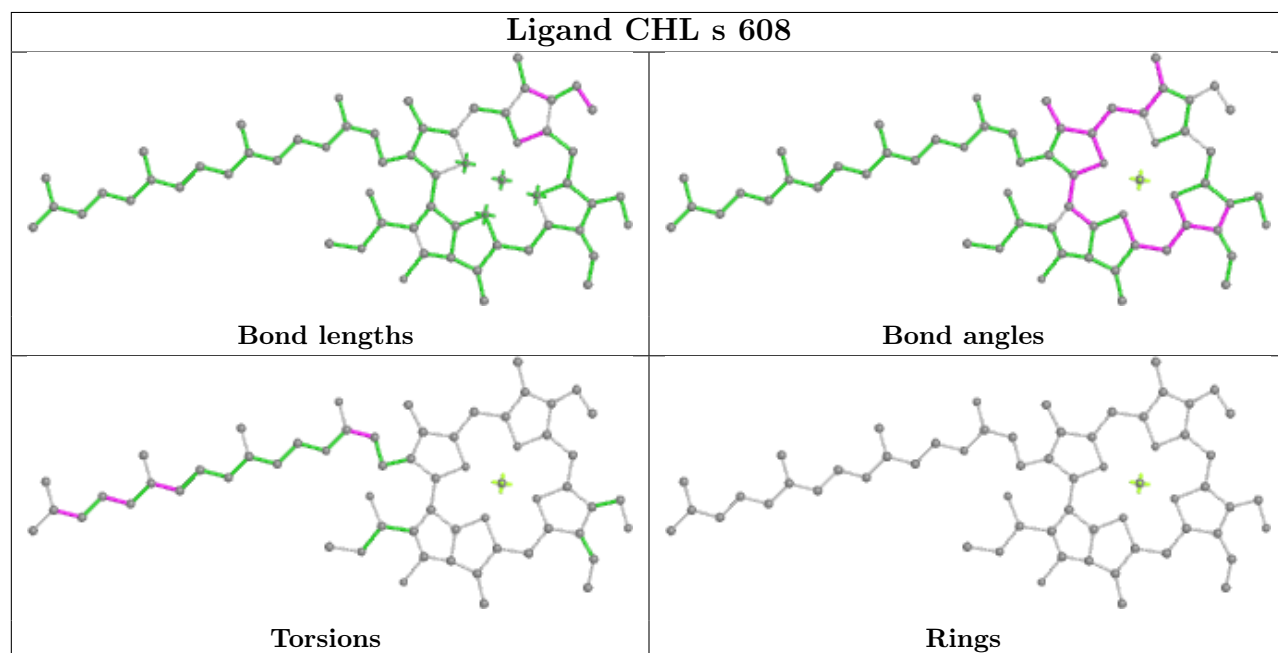
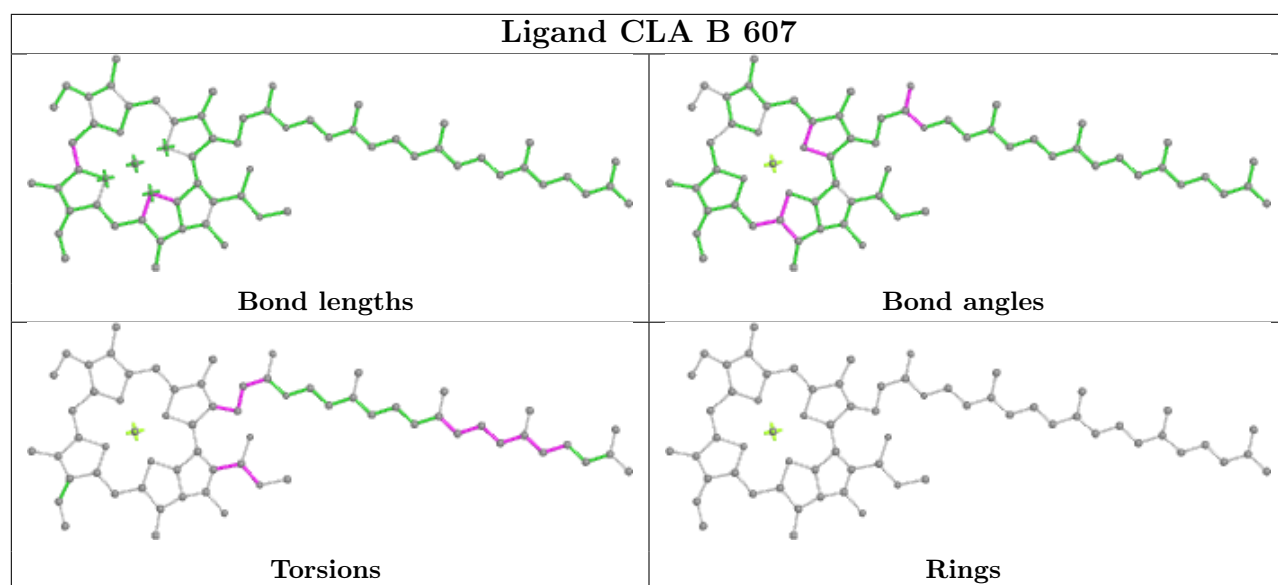


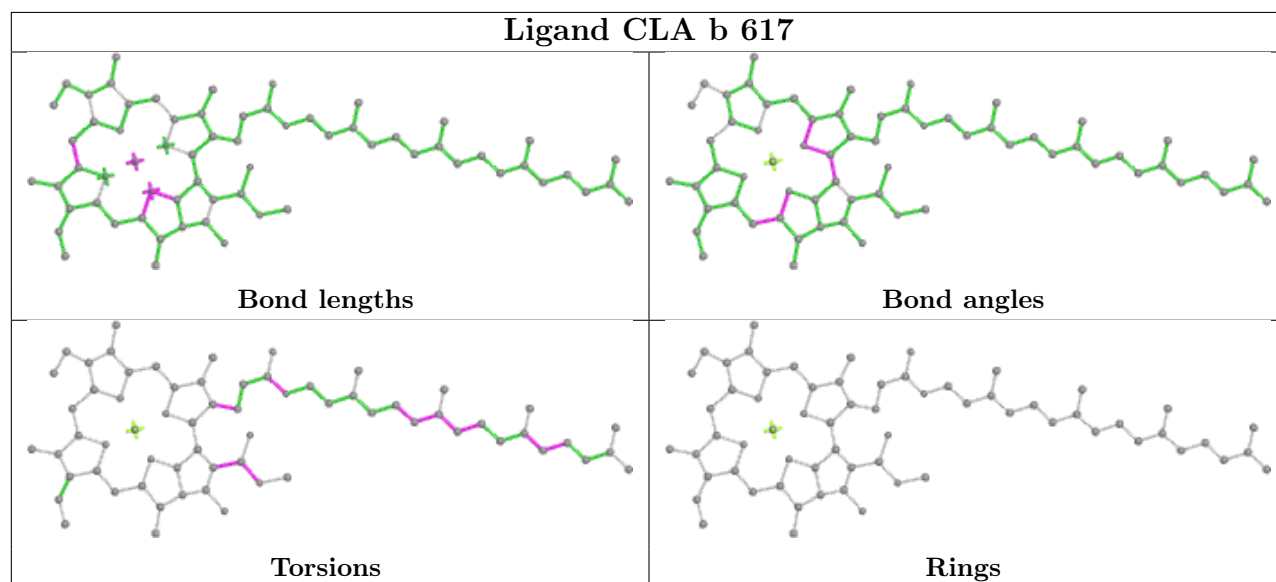
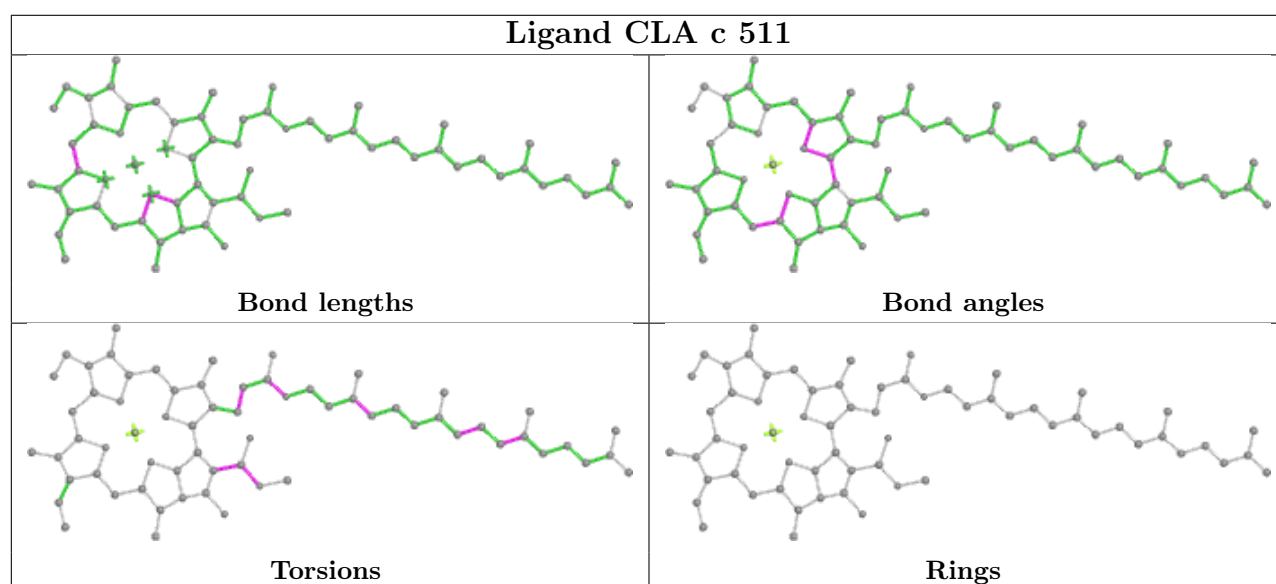
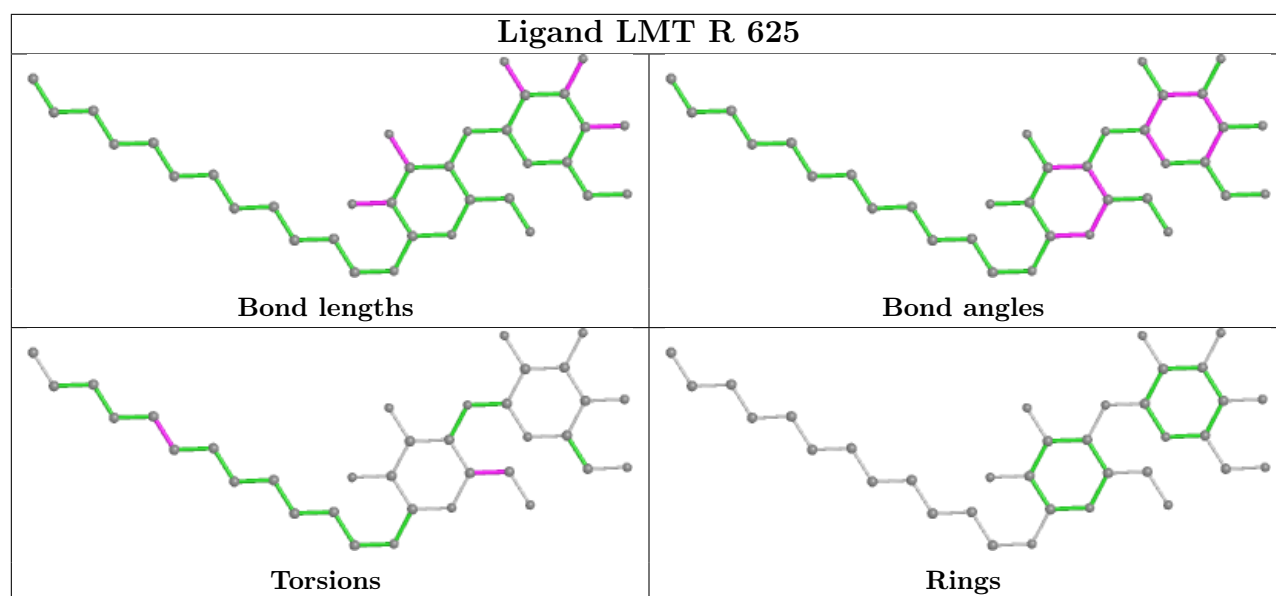
Ligand CLA b 602

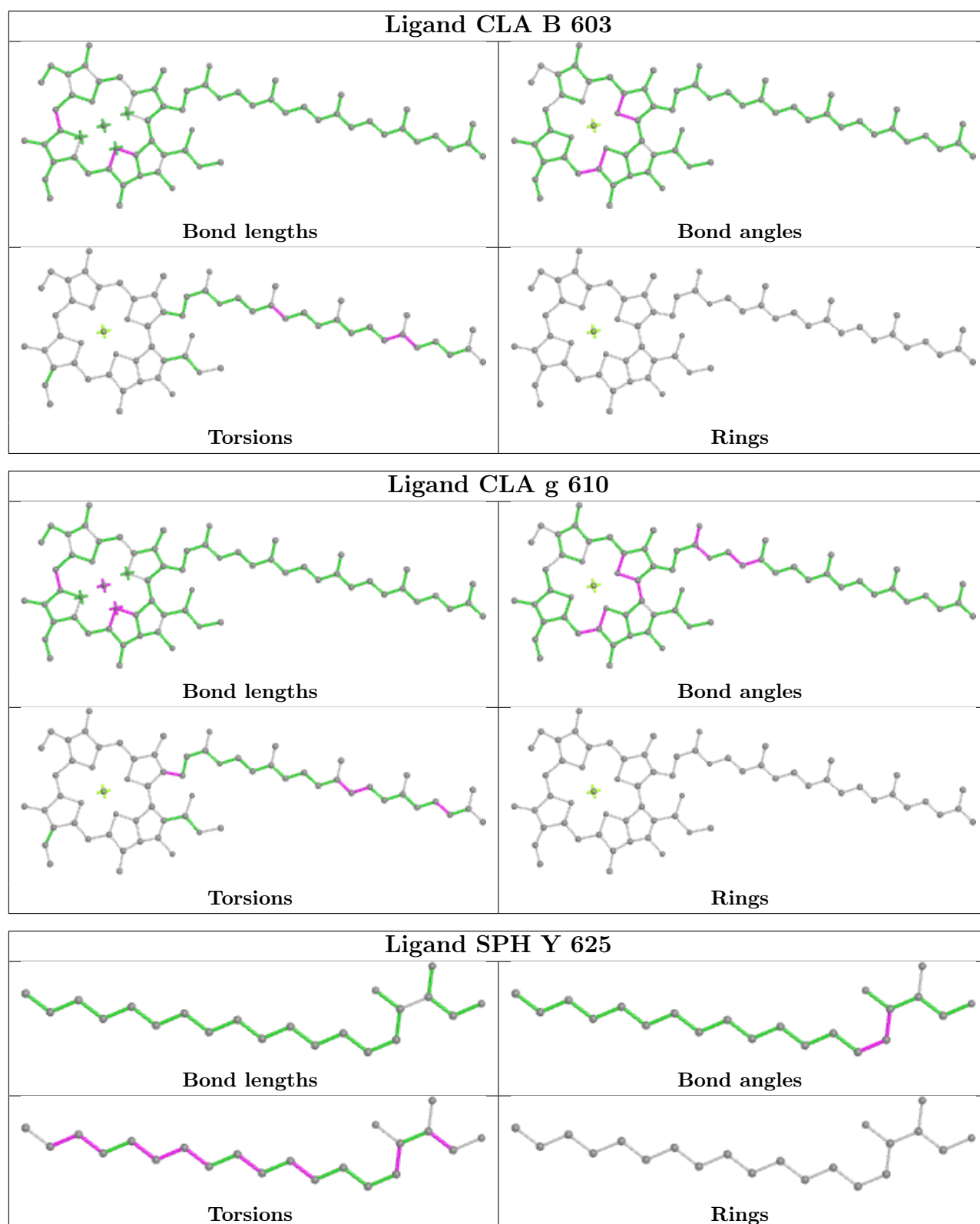


Ligand CHL g 605

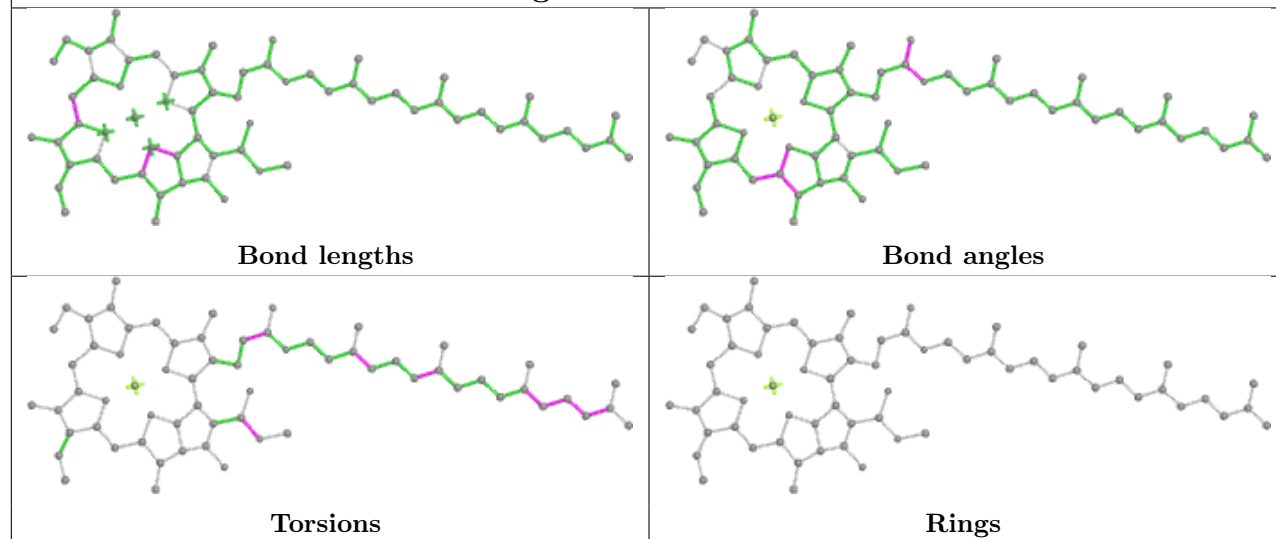




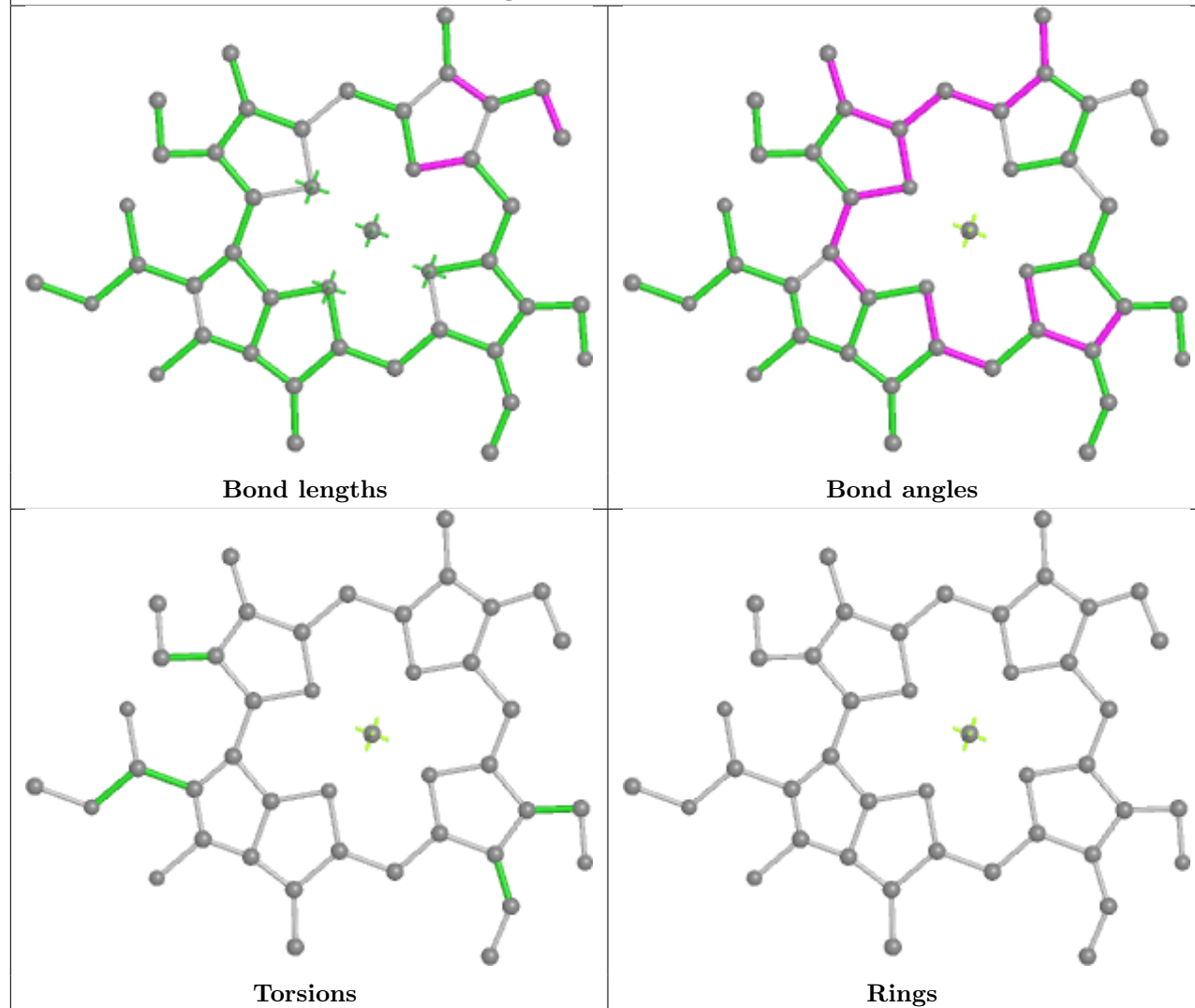




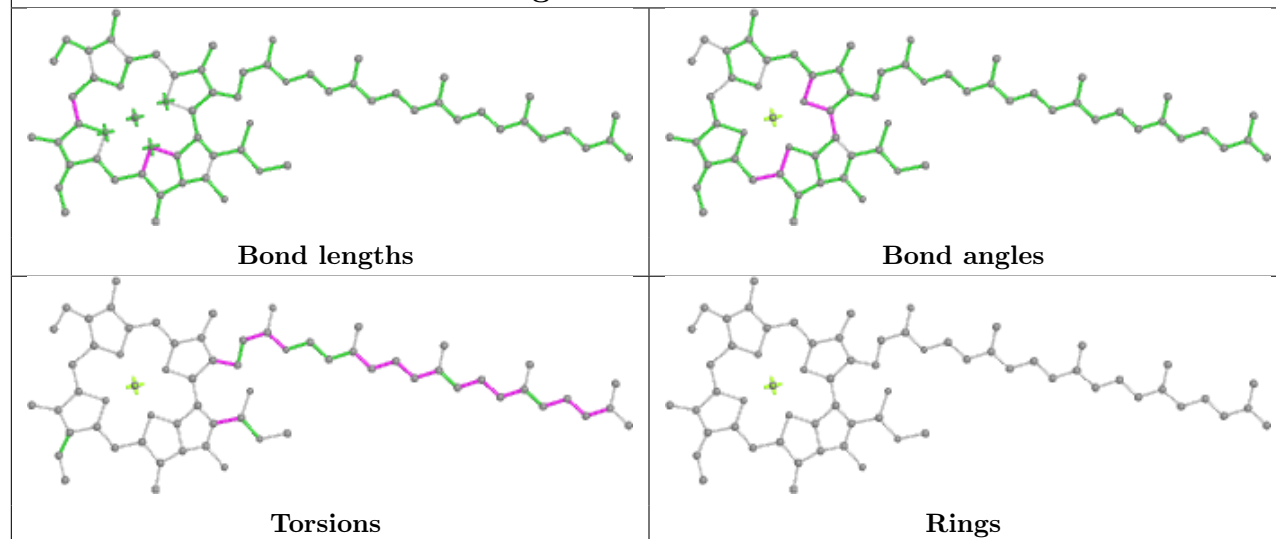
Ligand CLA C 510



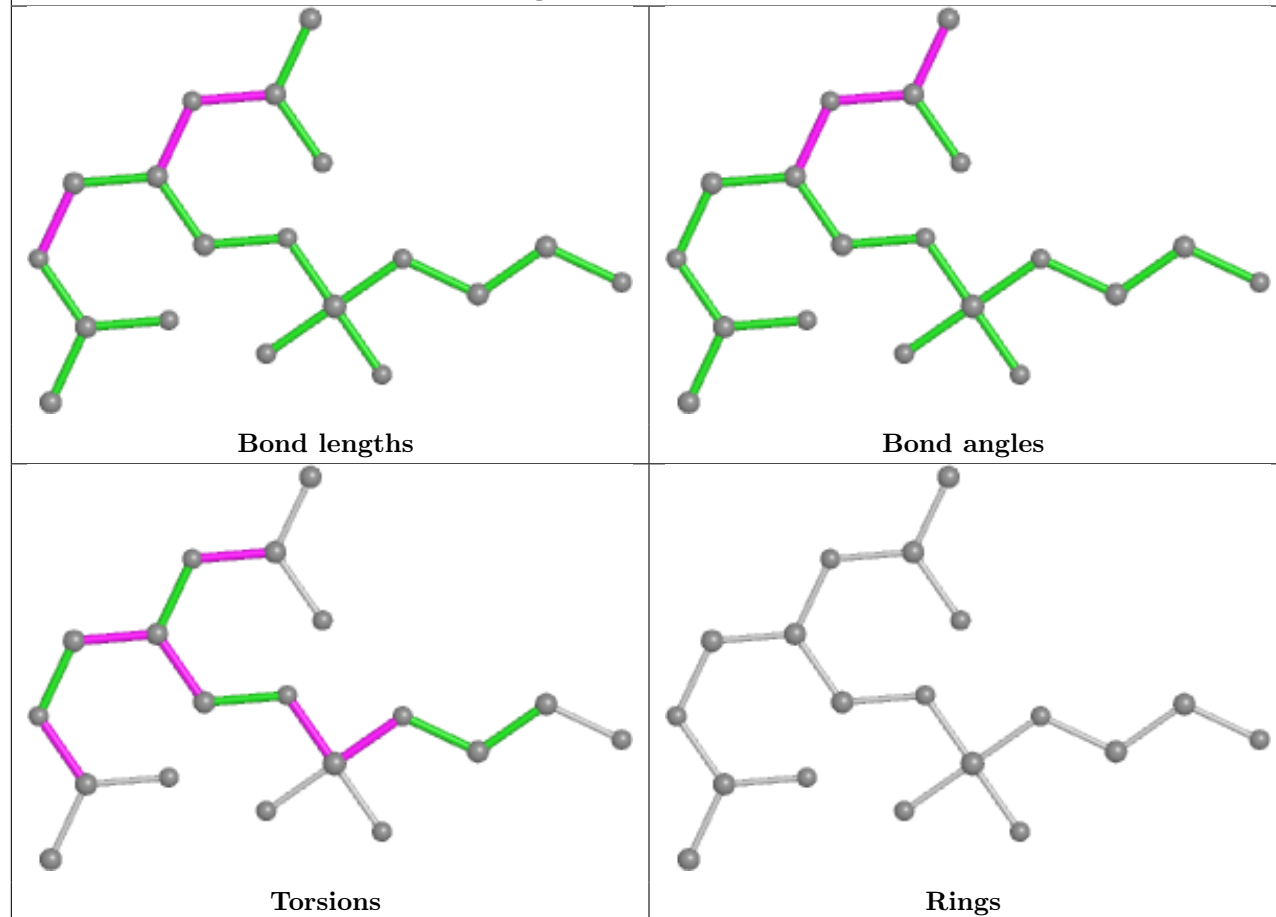
Ligand CHL S 607

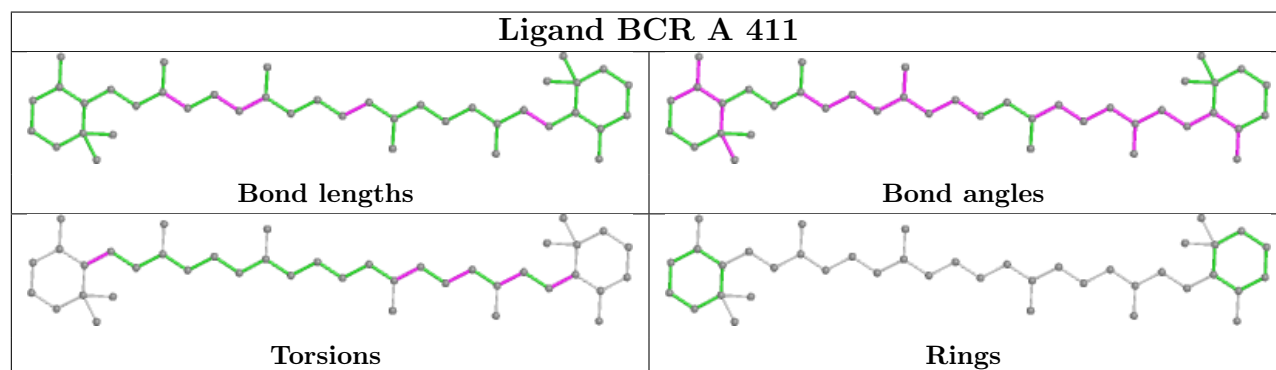
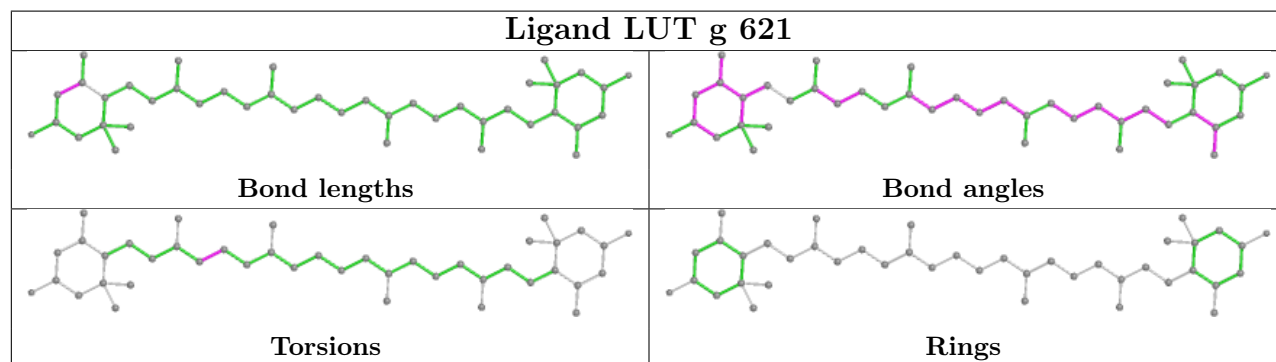
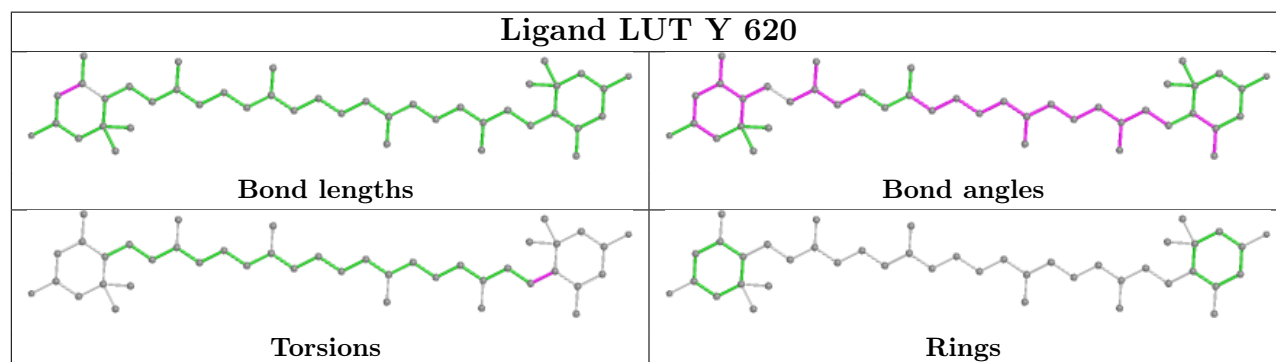
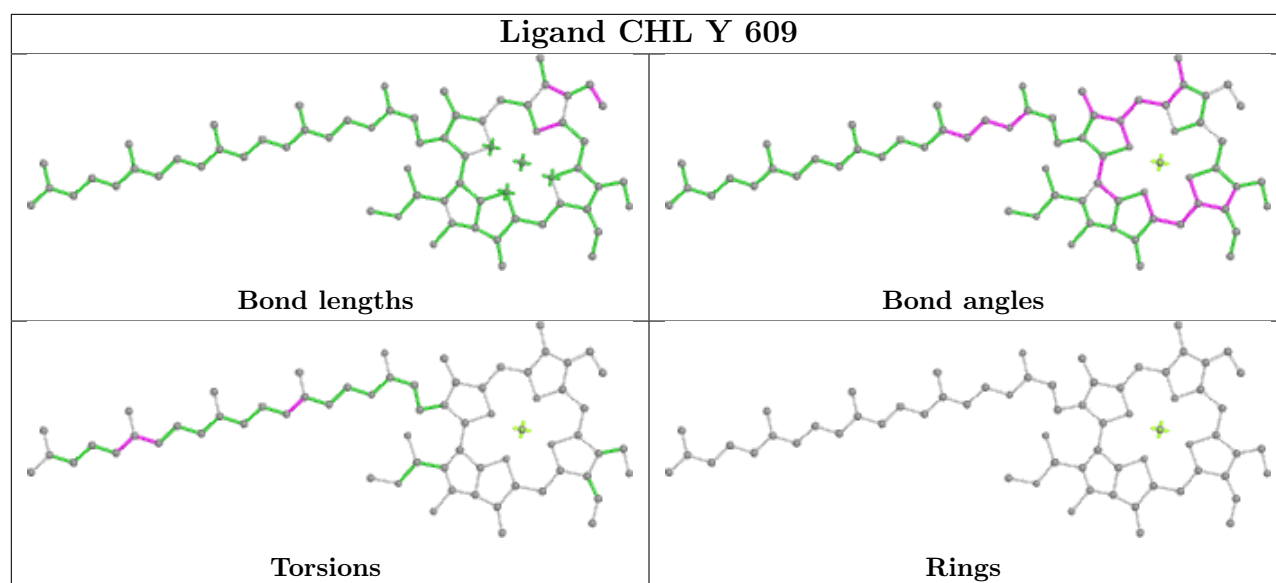


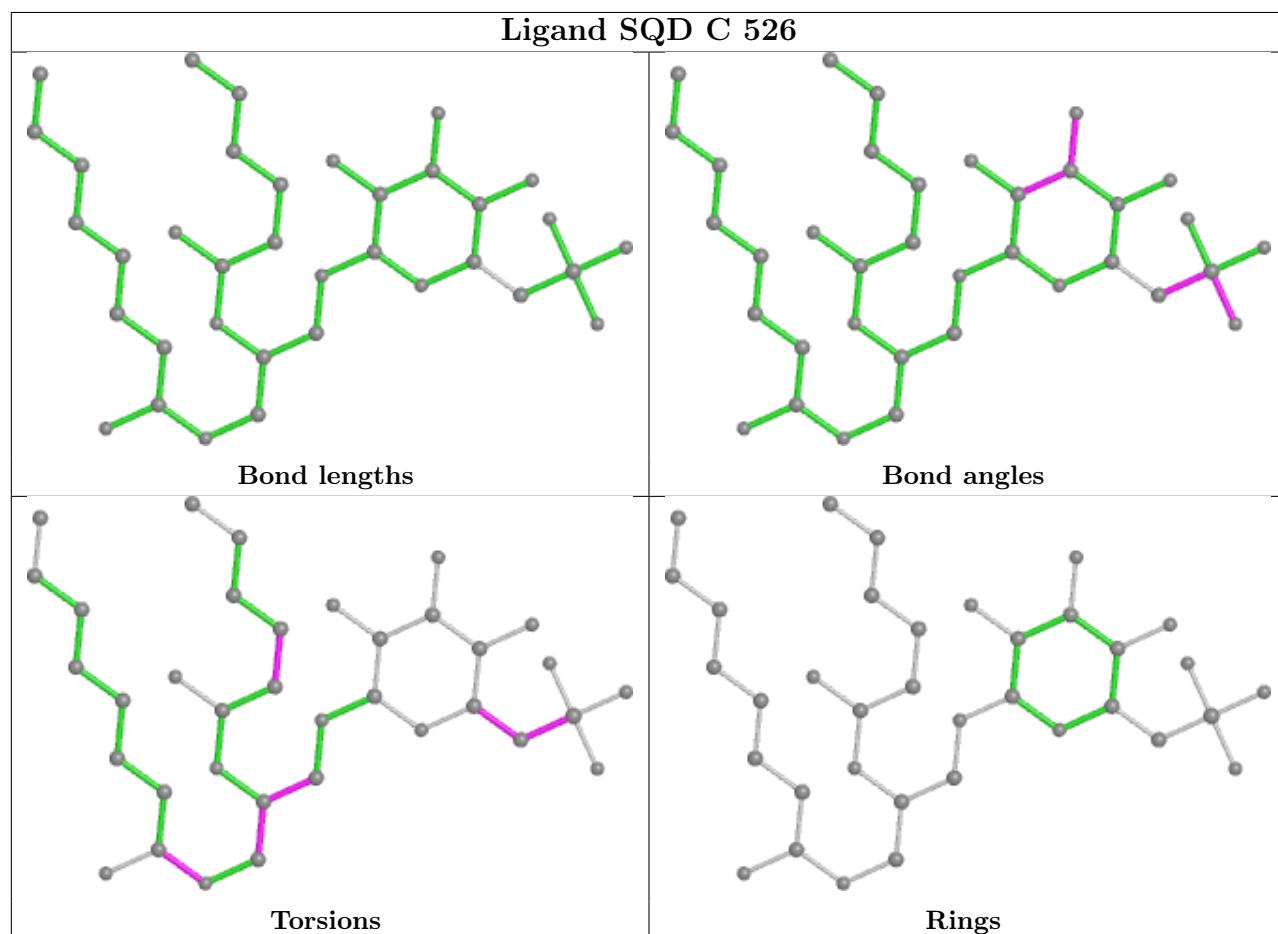
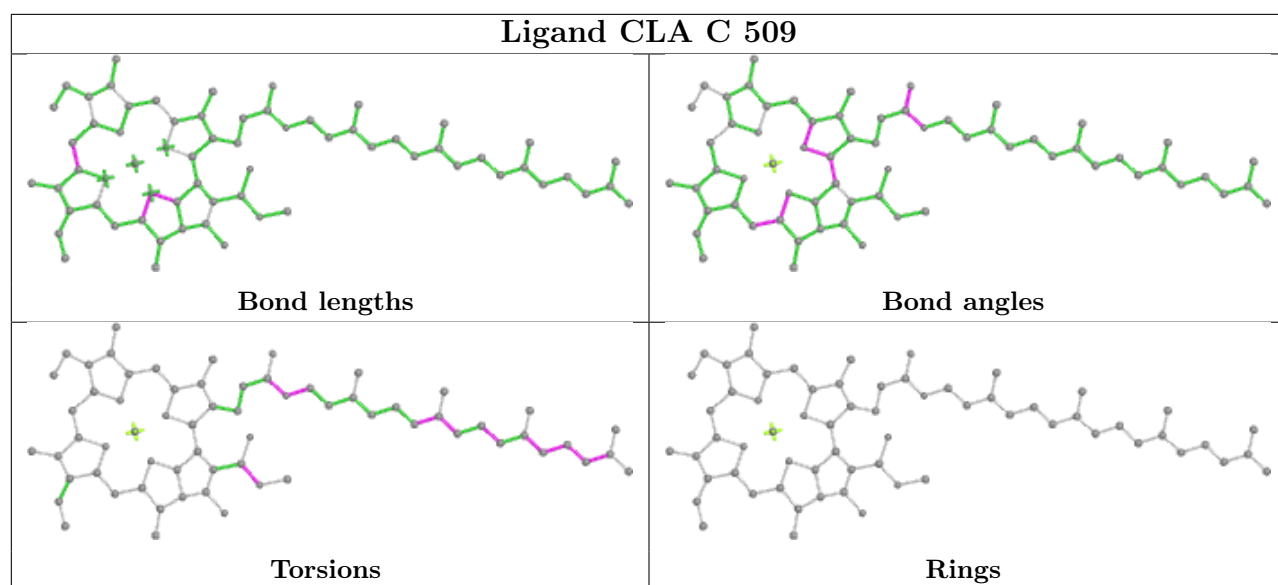
Ligand CLA B 608



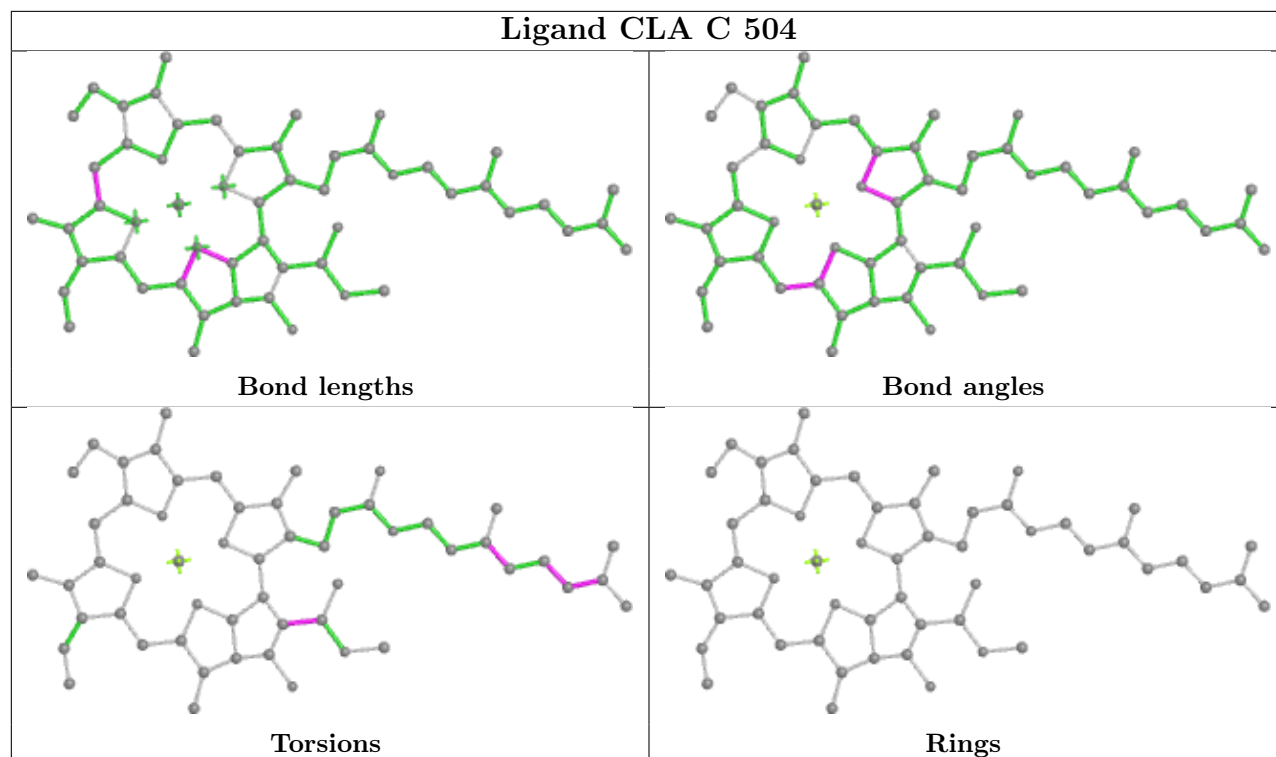
Ligand PTY Y 627



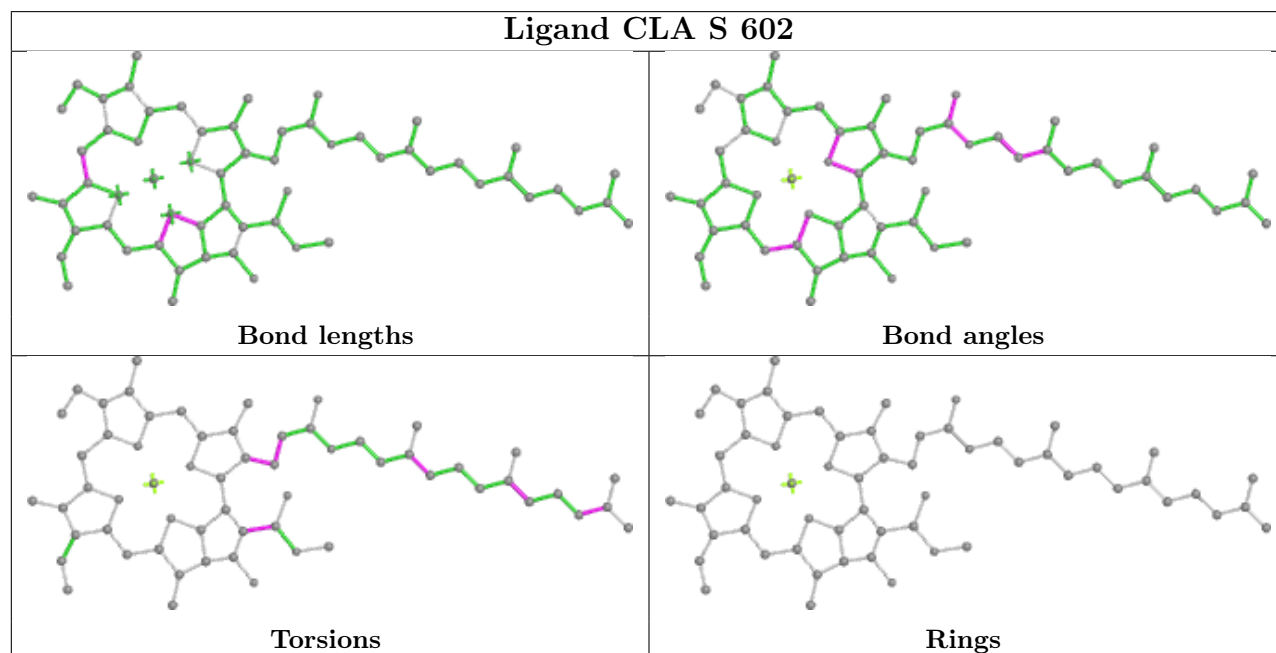


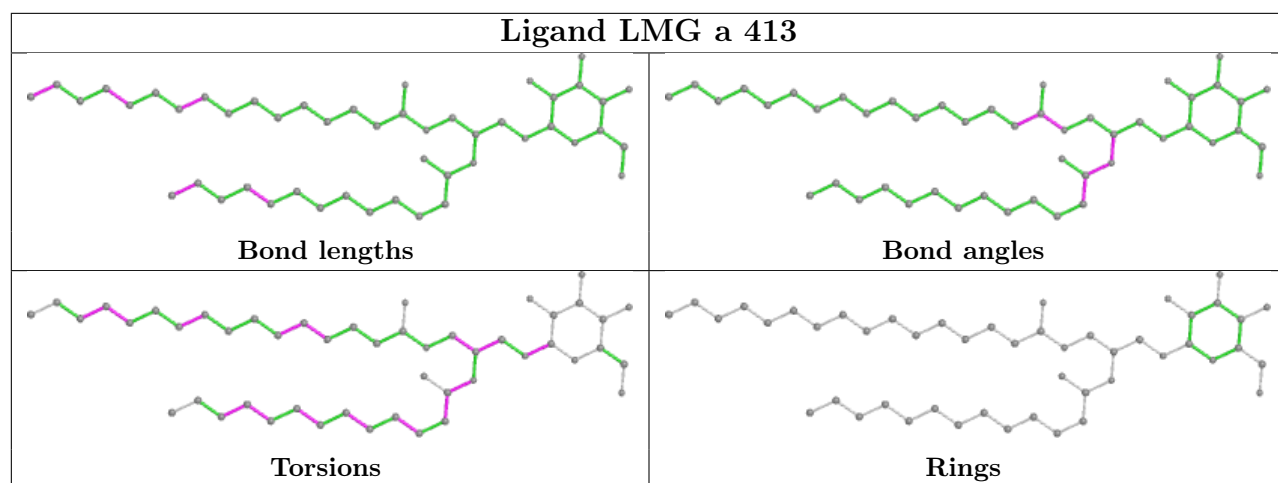
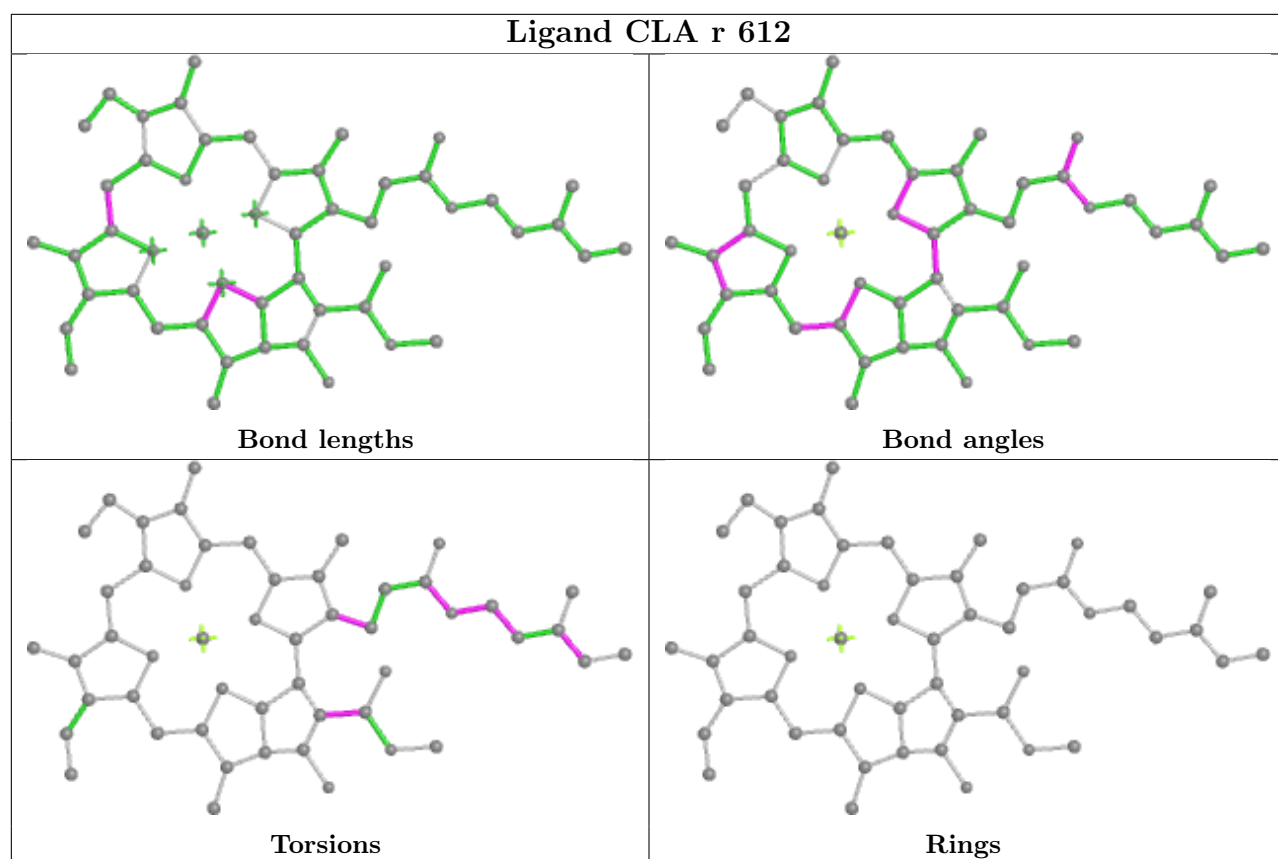


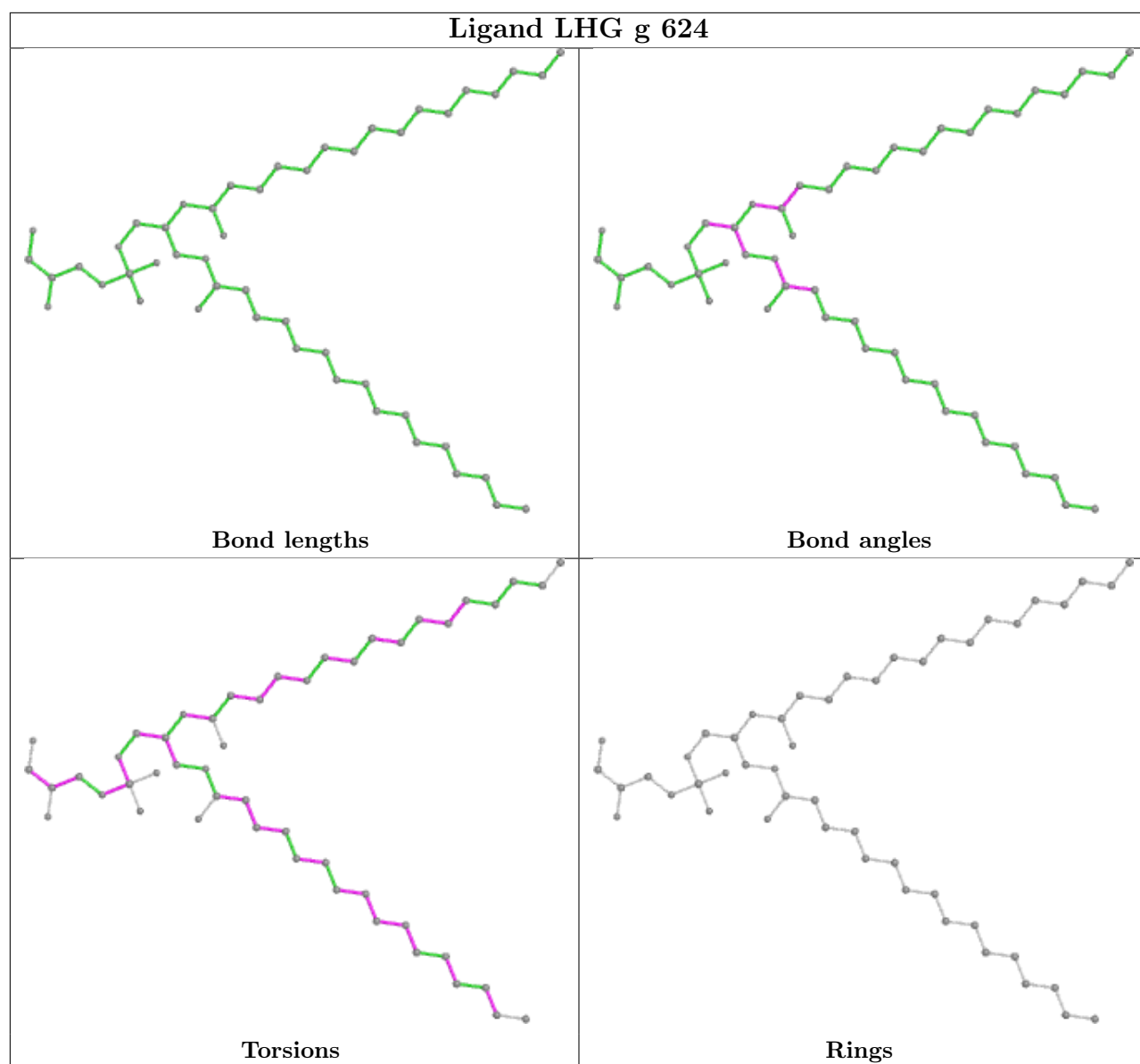
Ligand CLA C 504

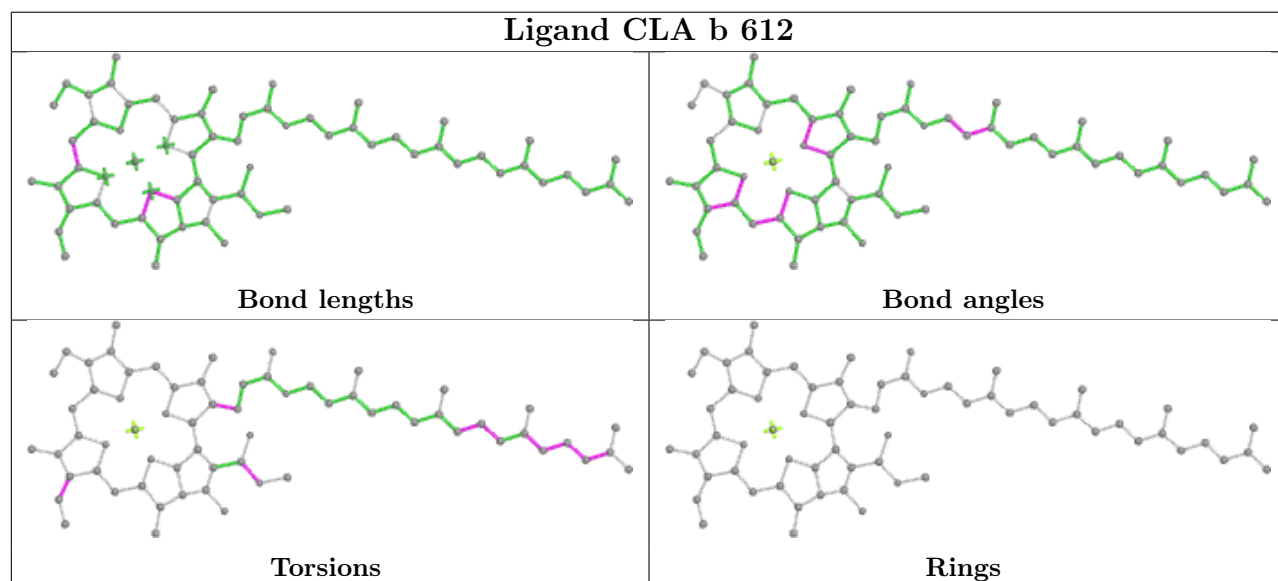
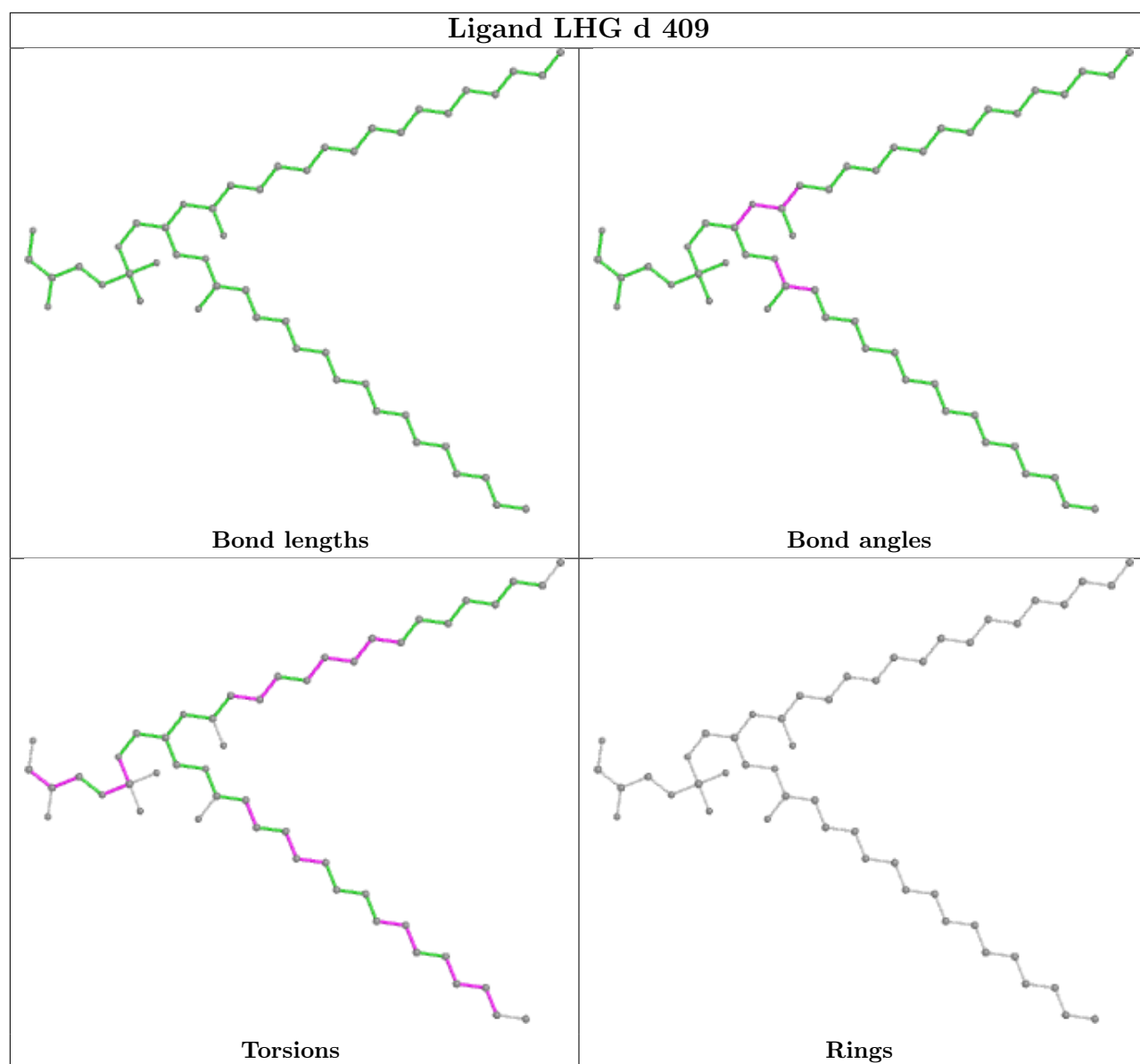


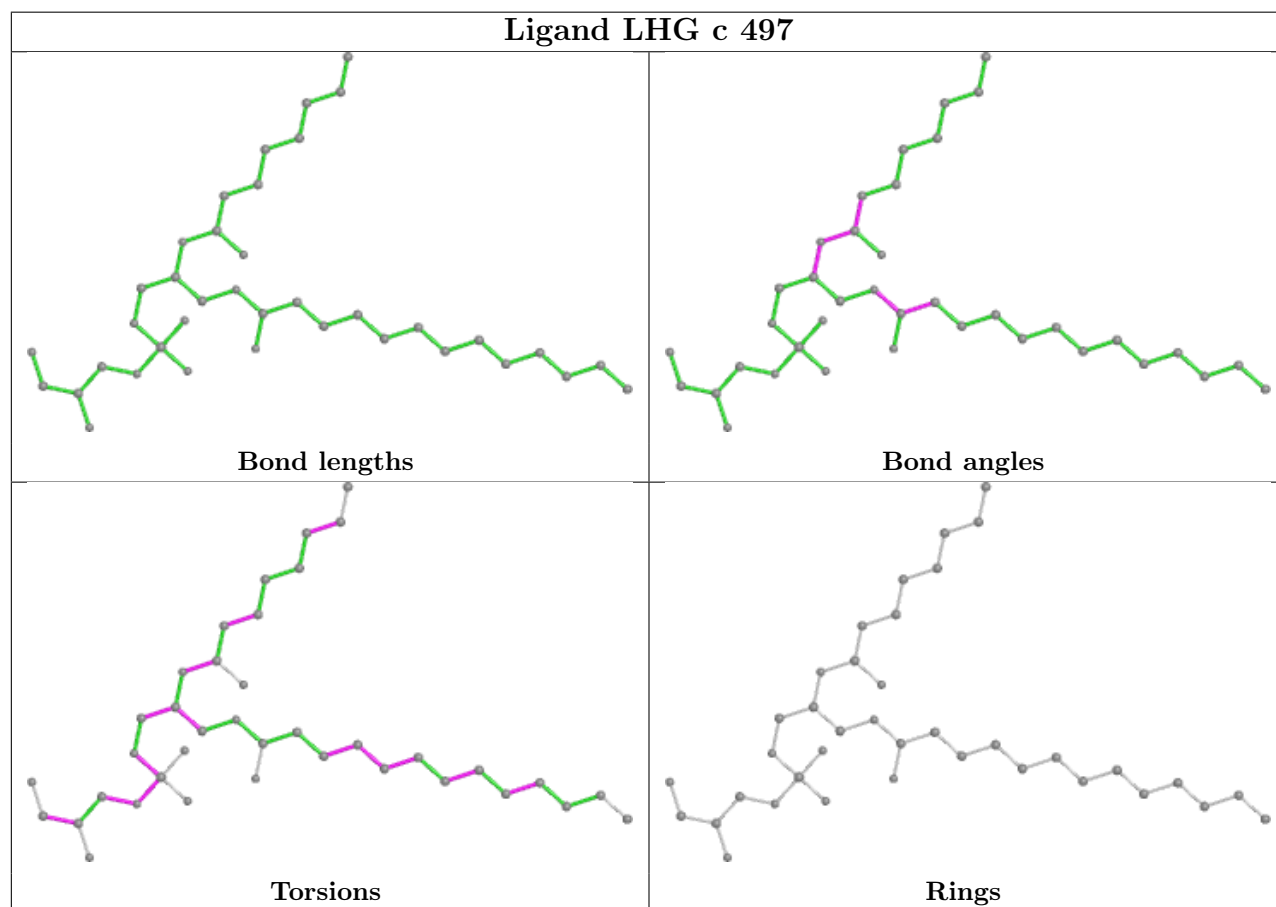
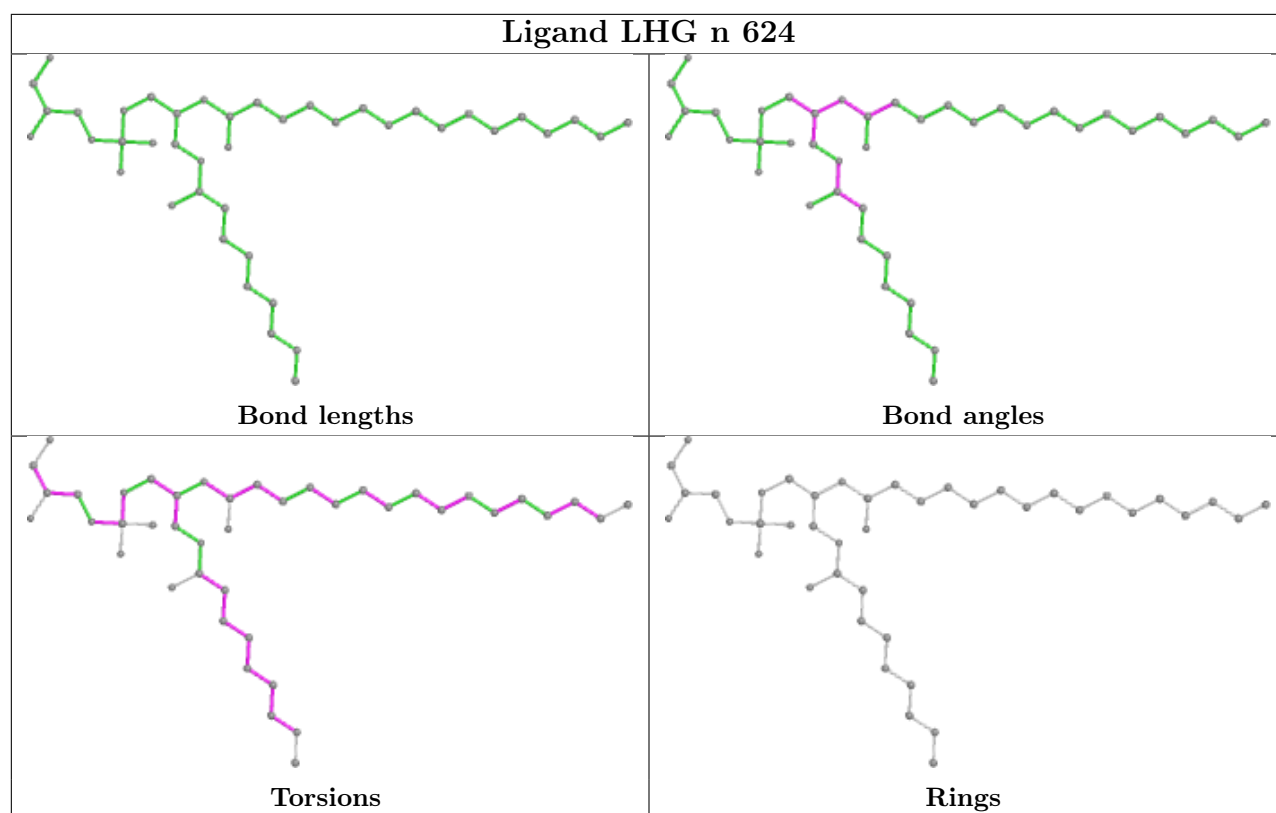
Ligand CLA S 602

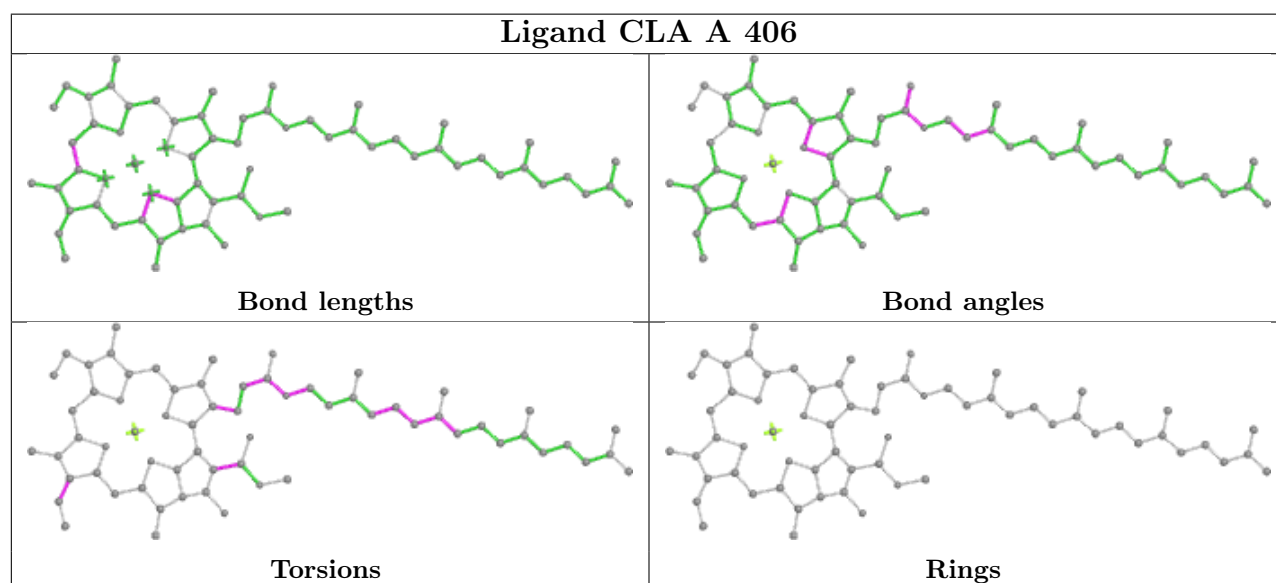
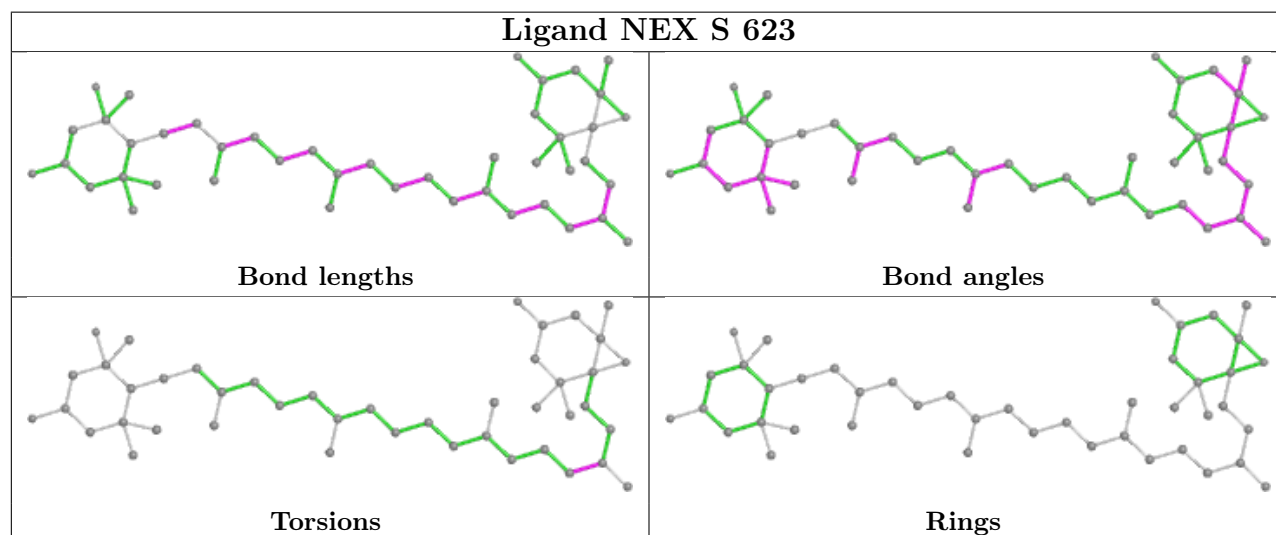
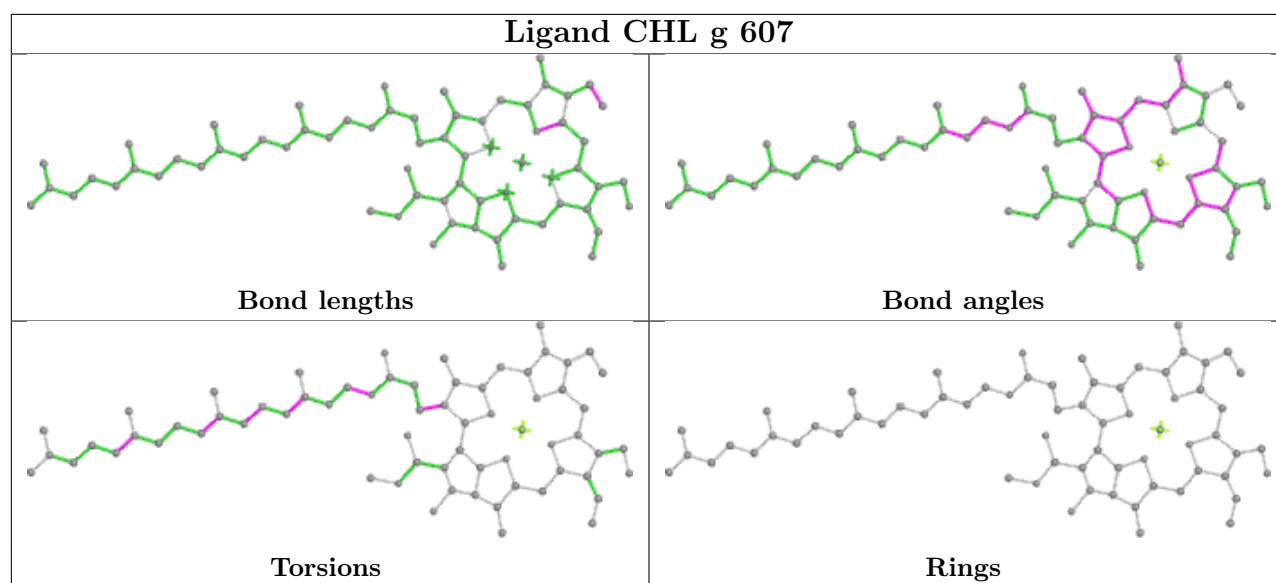




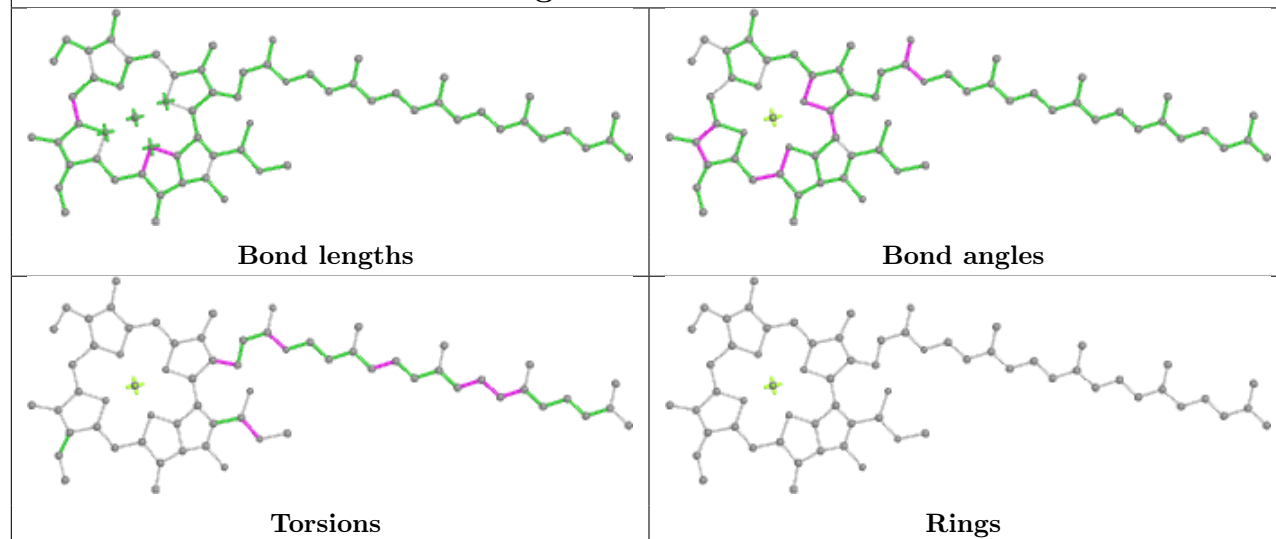




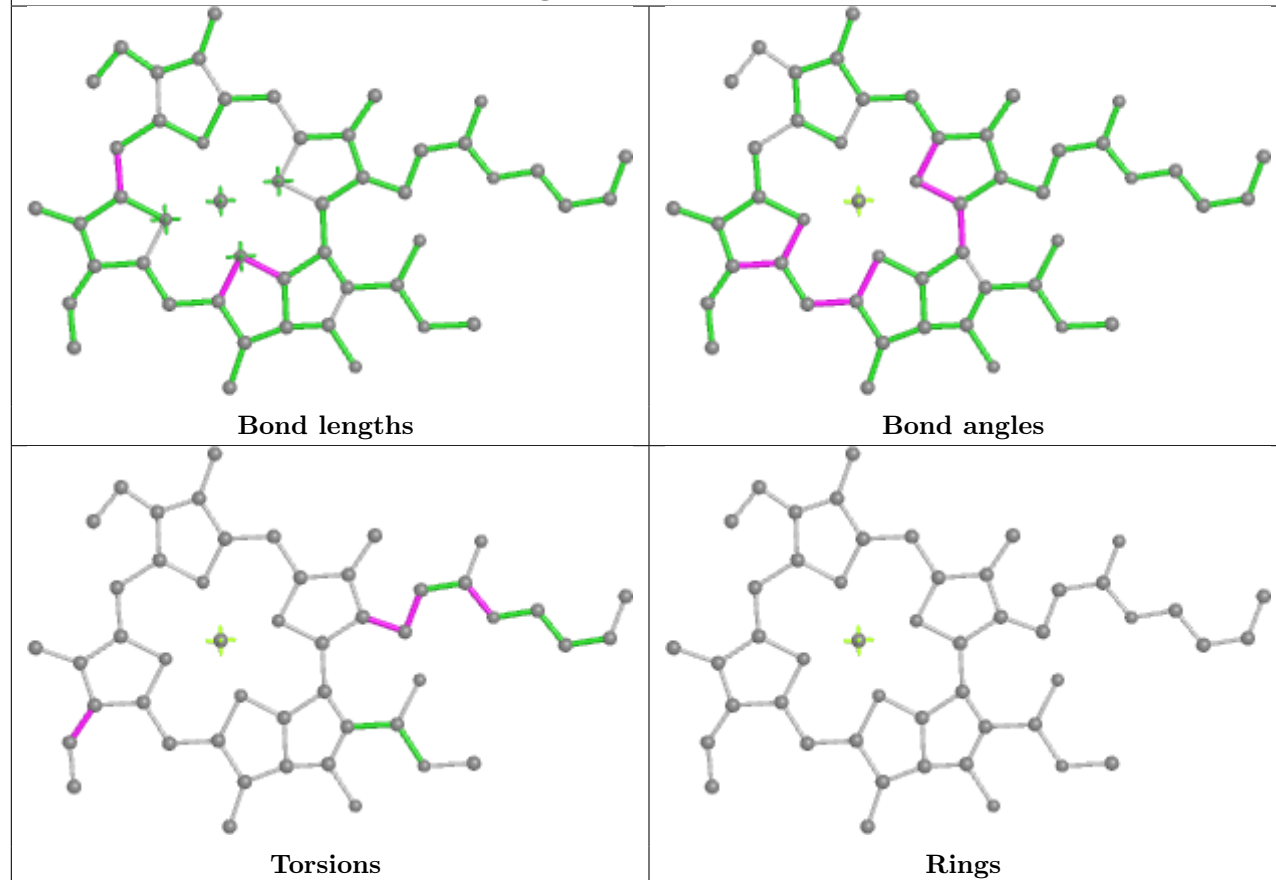


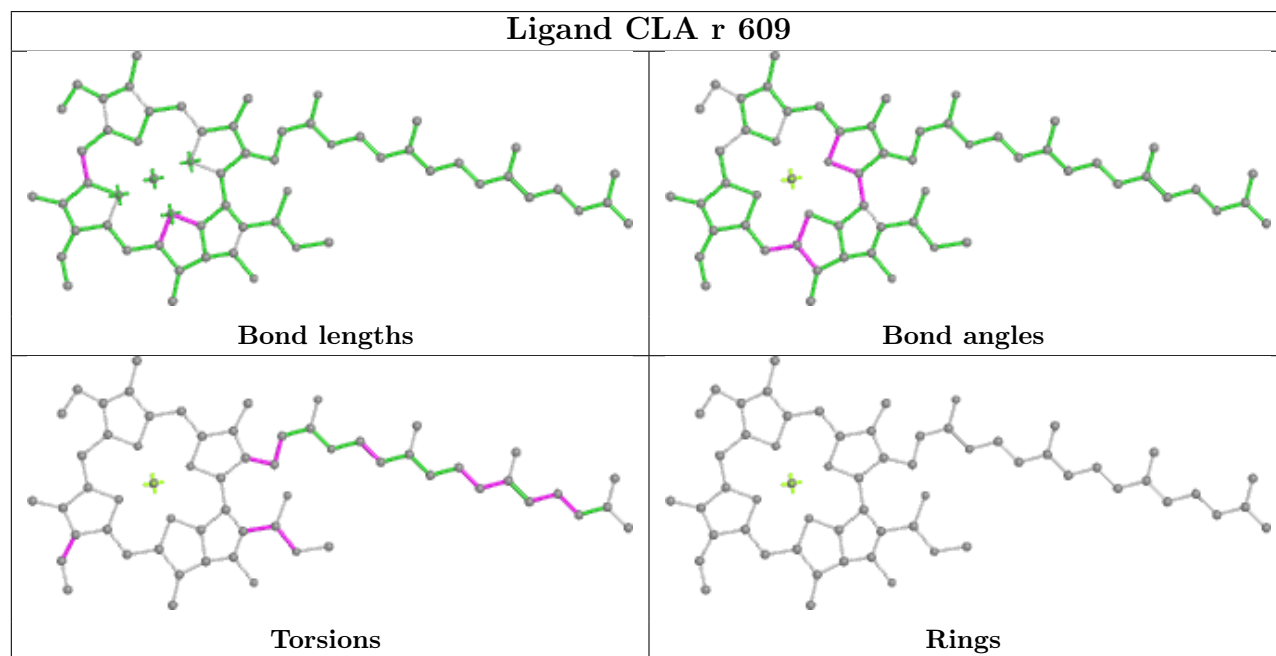
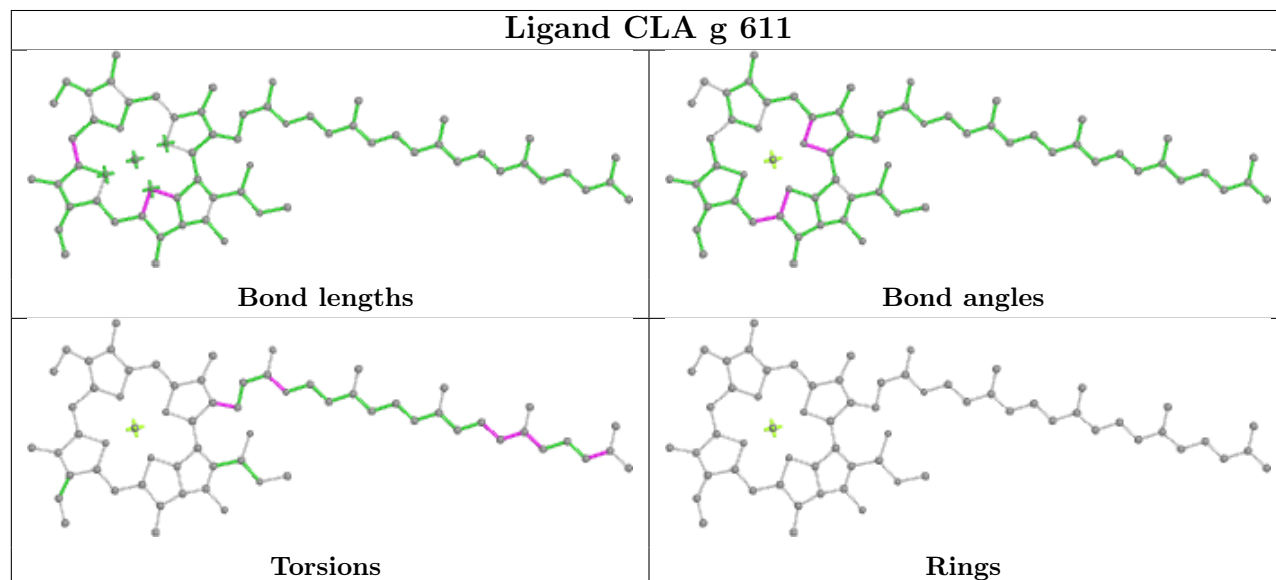
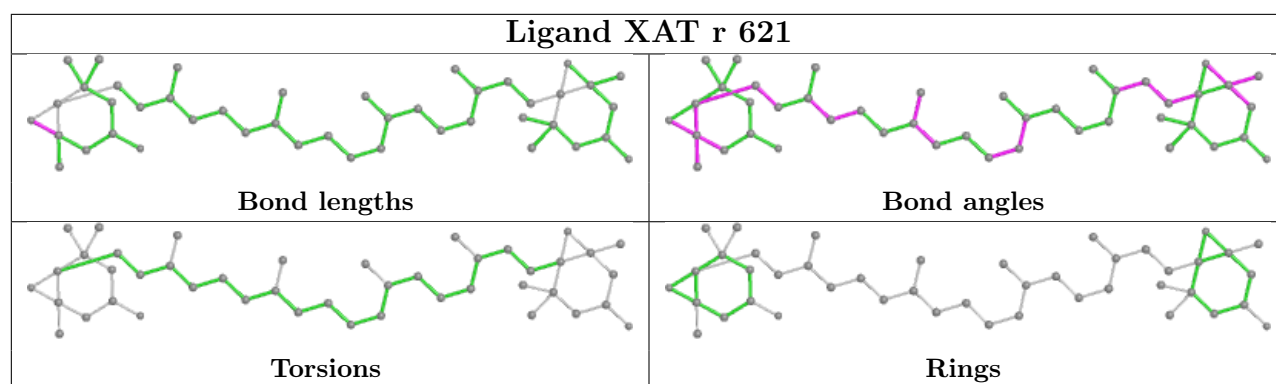


Ligand CLA d 403

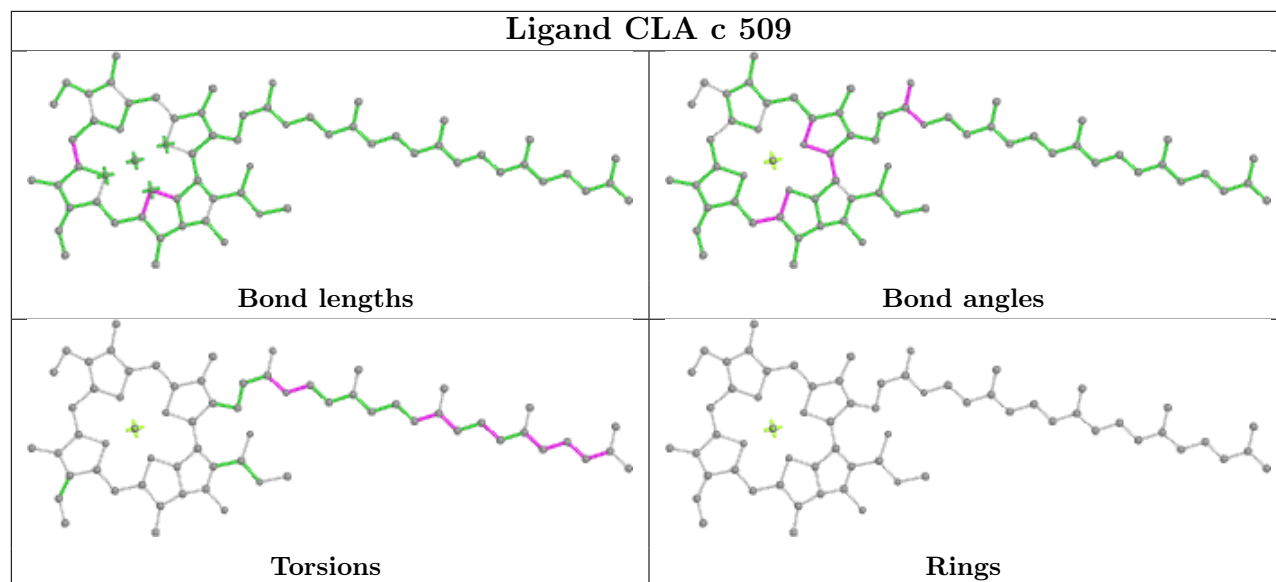


Ligand CLA a 407

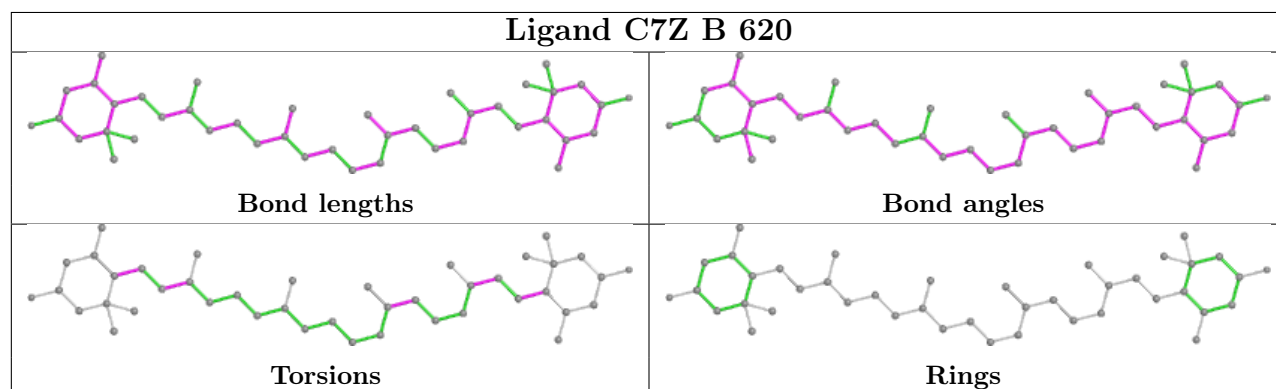




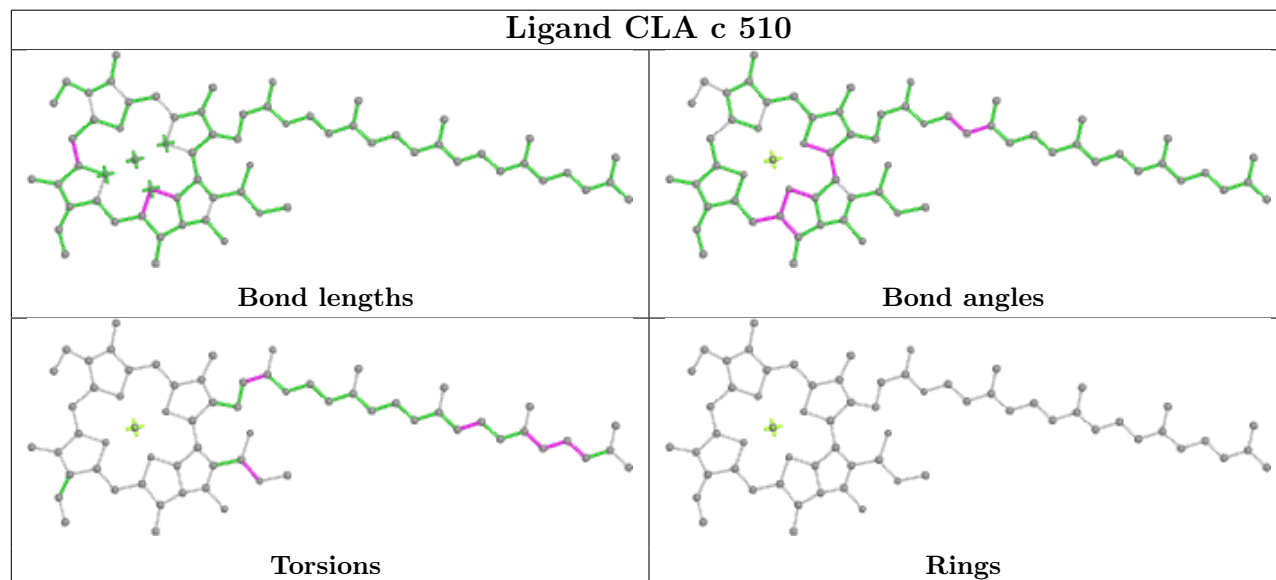
Ligand CLA c 509

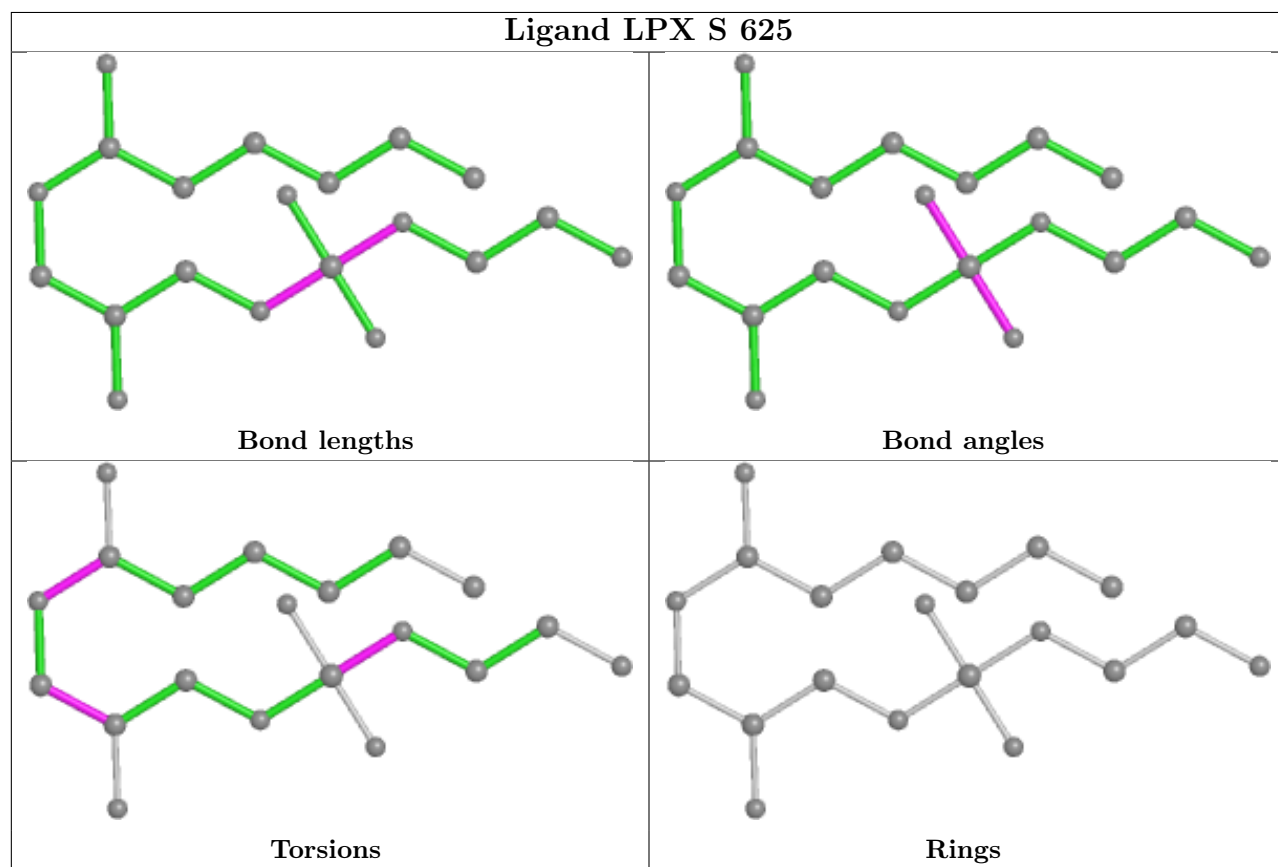
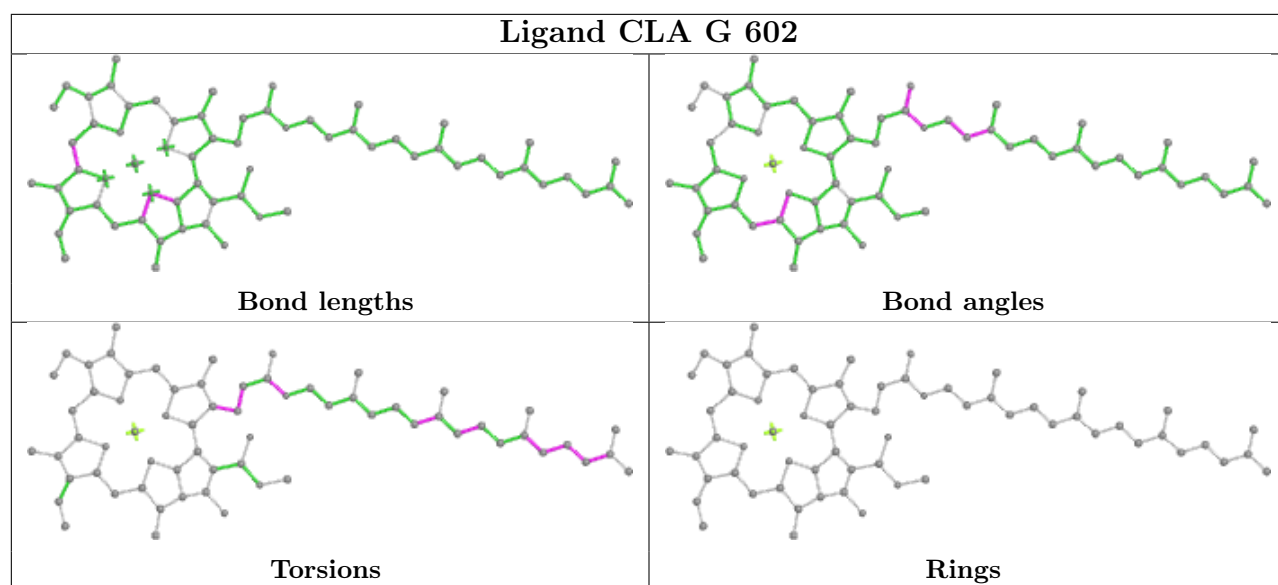


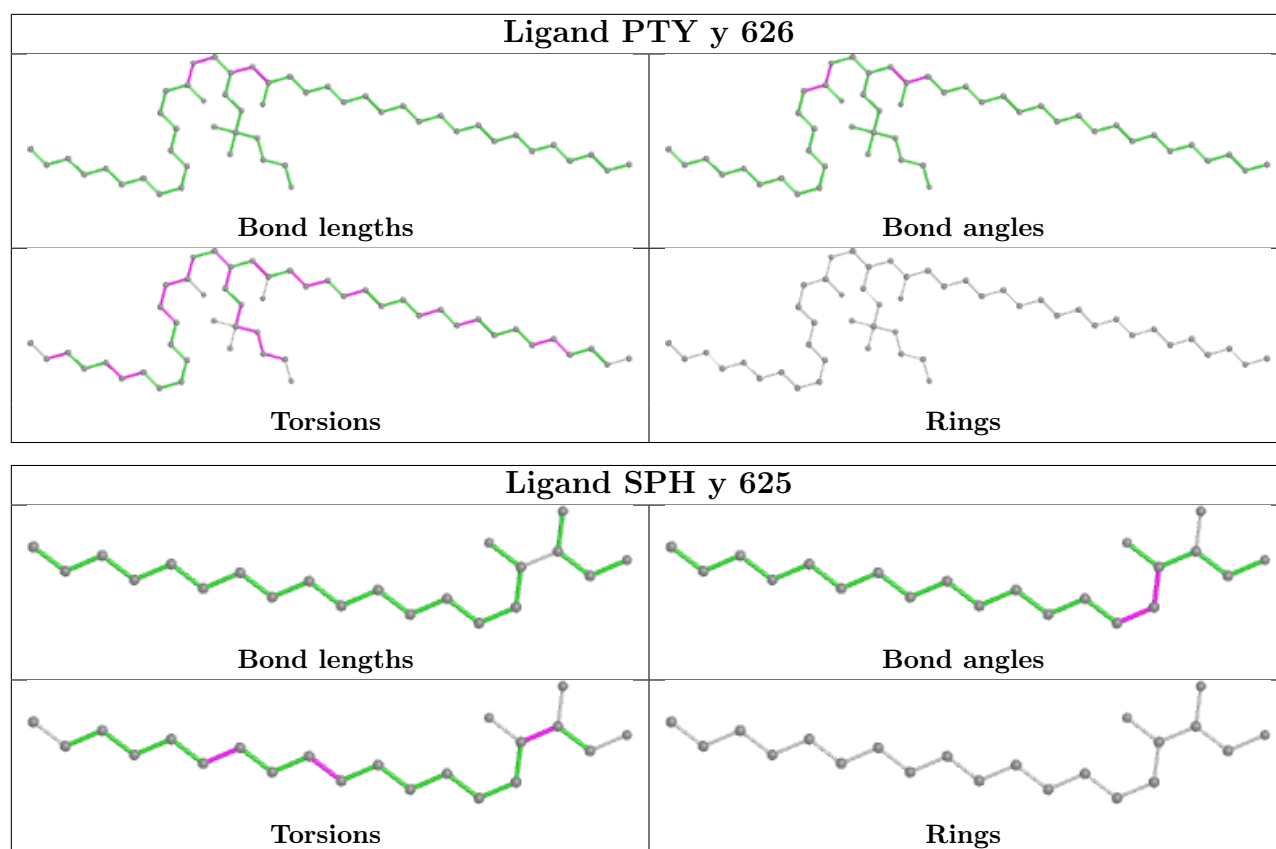
Ligand C7Z B 620

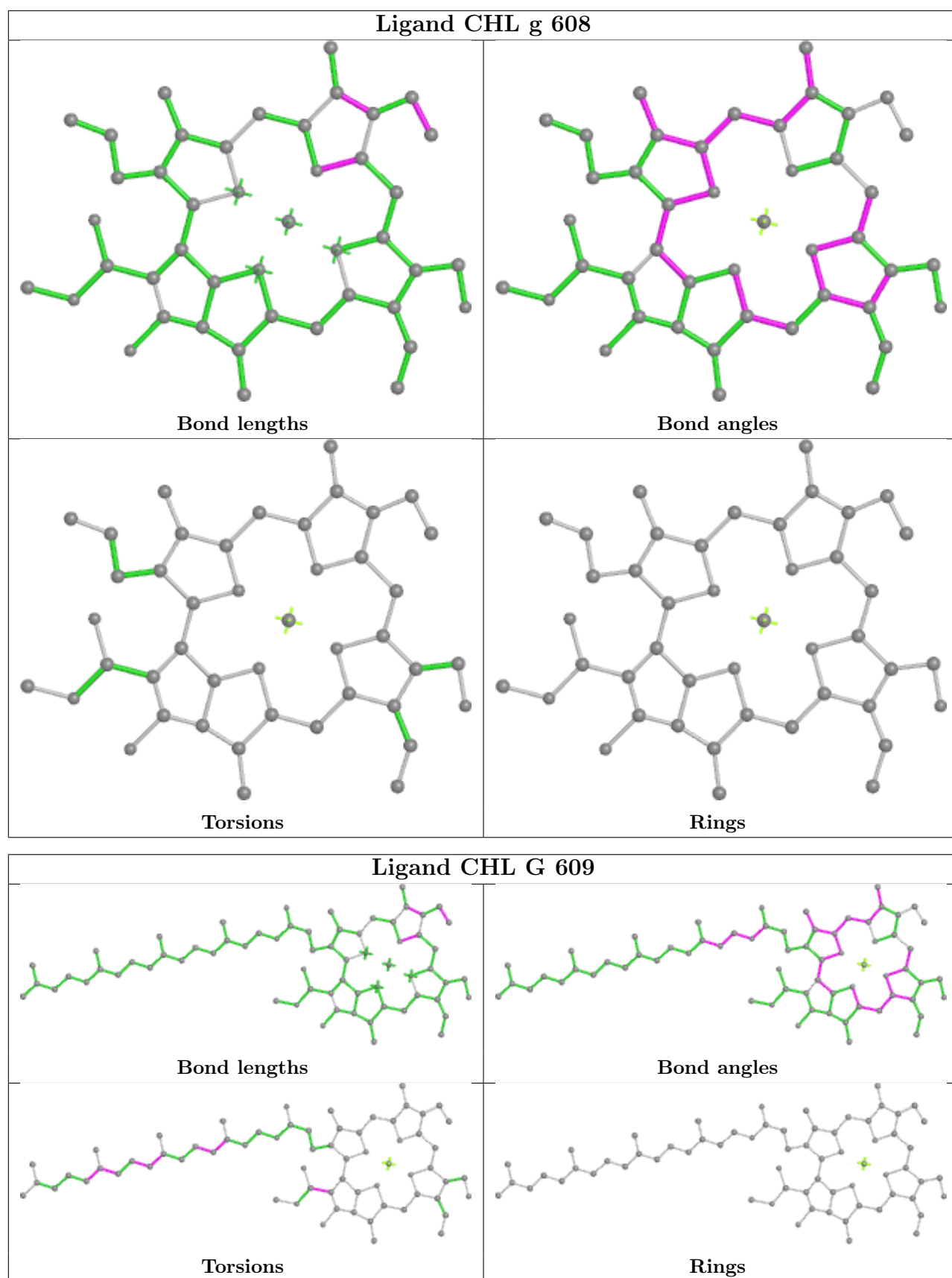


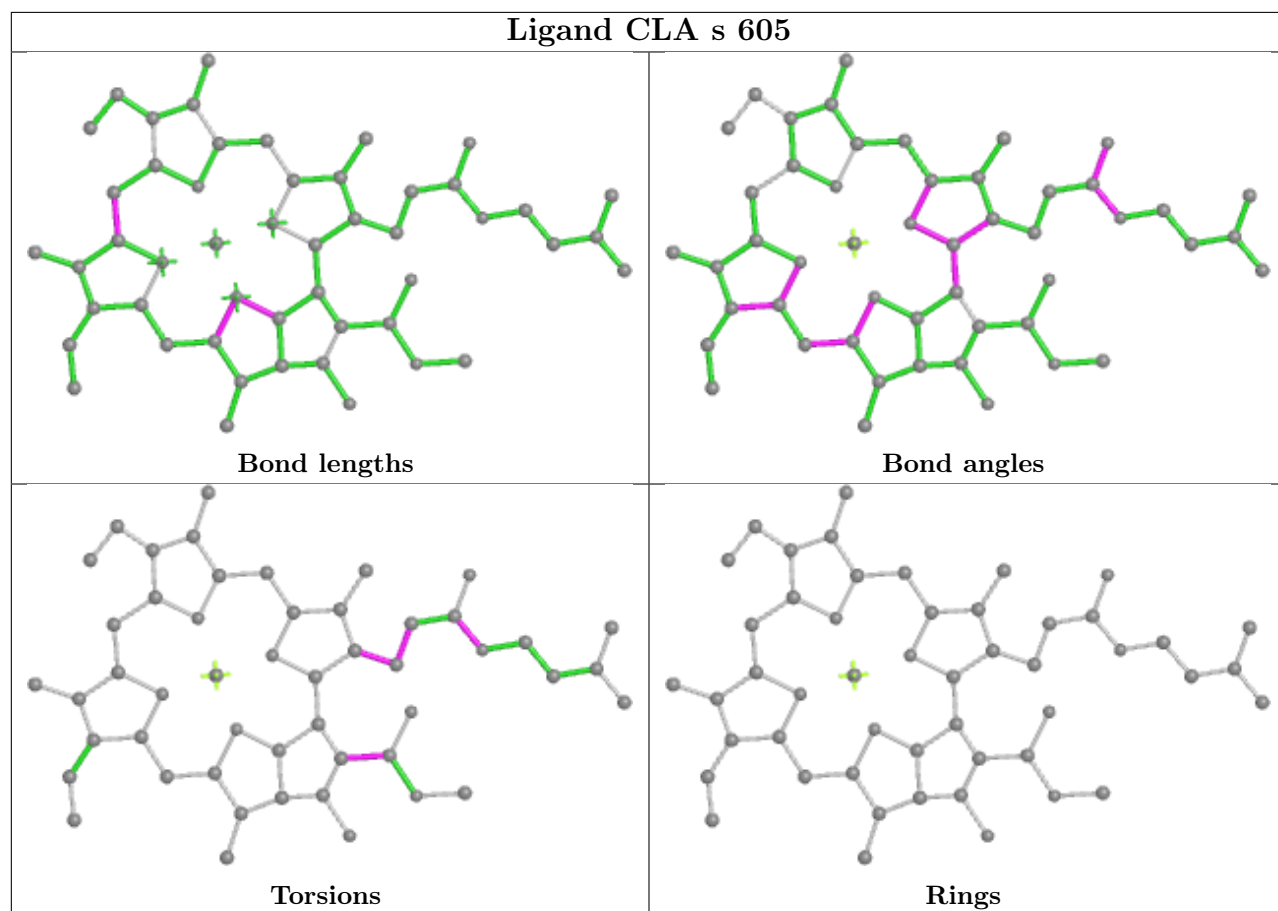
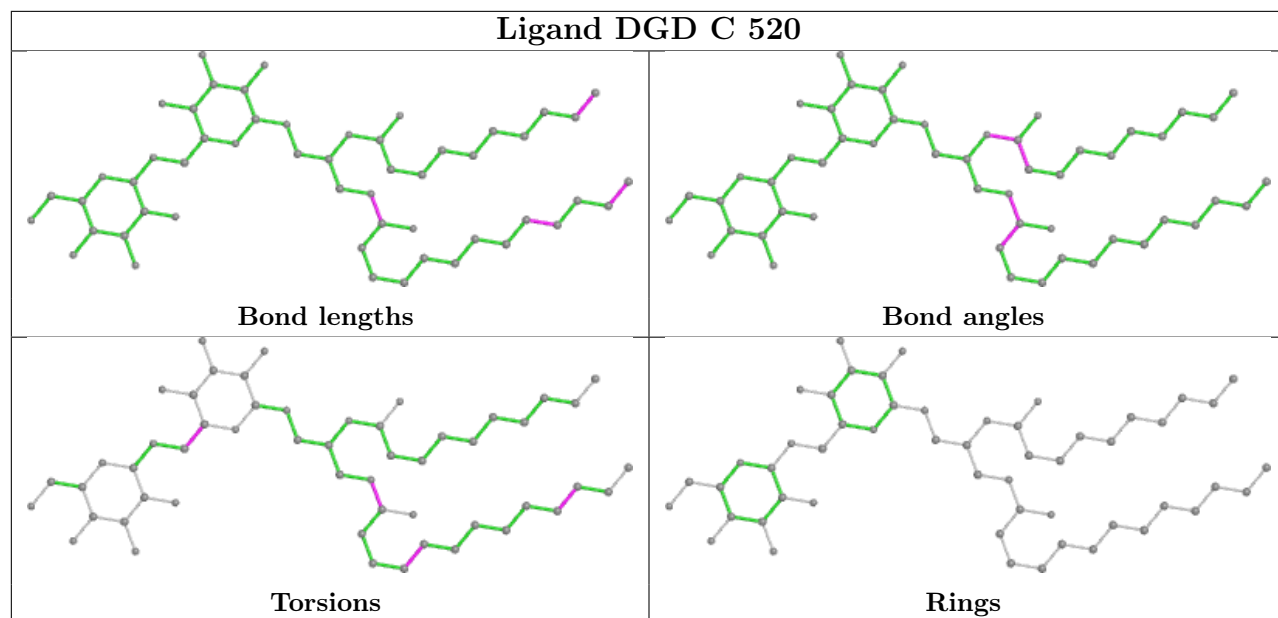
Ligand CLA c 510



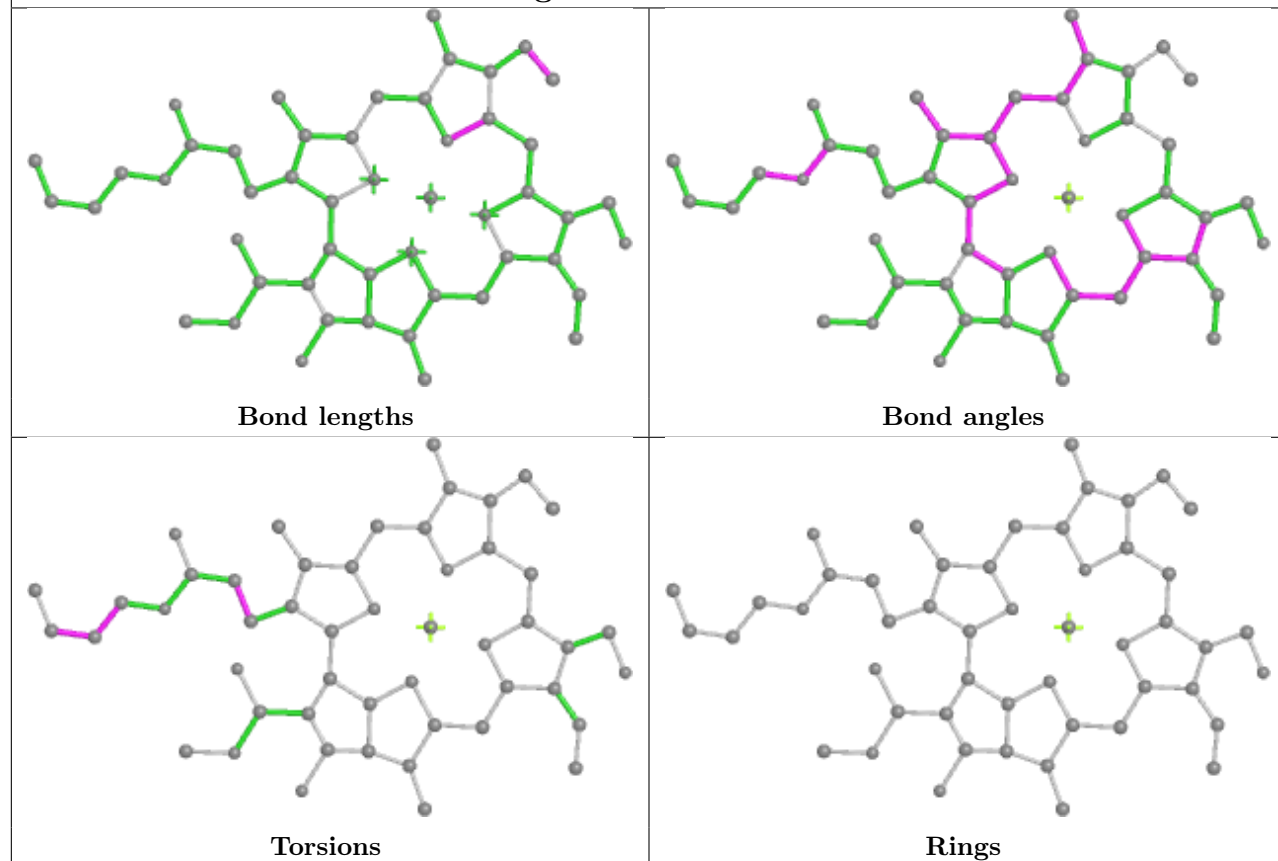




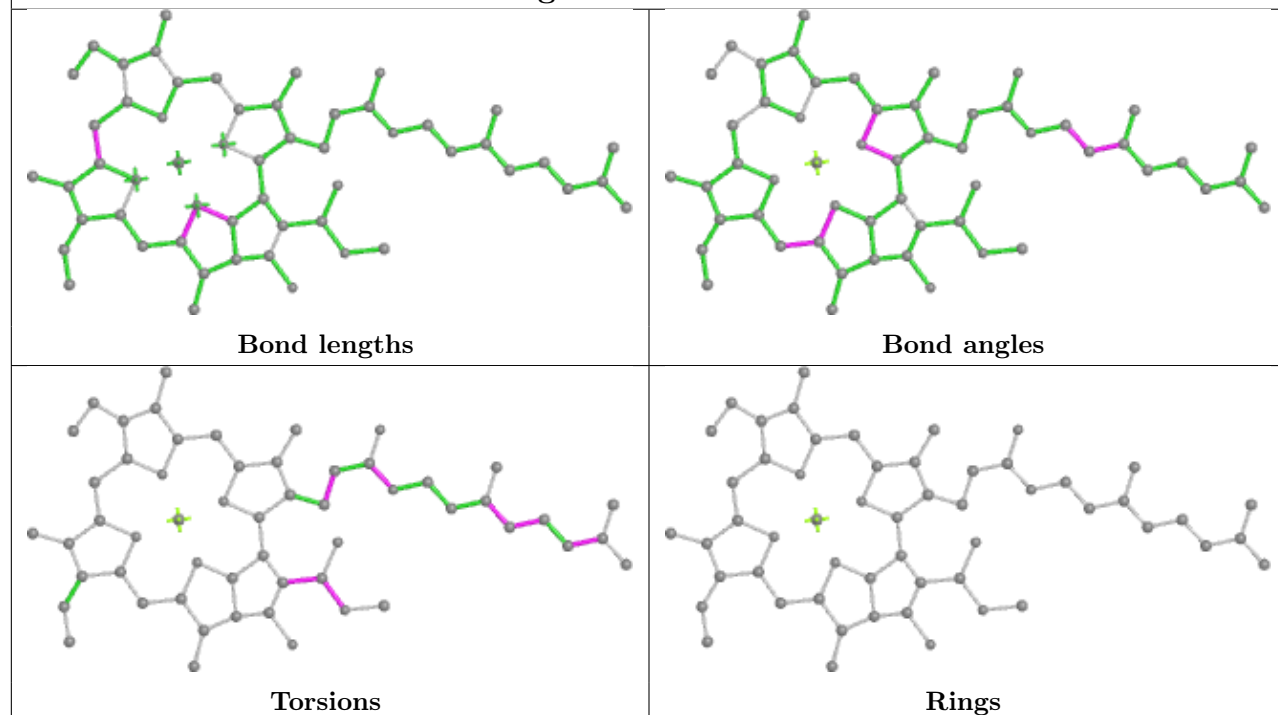


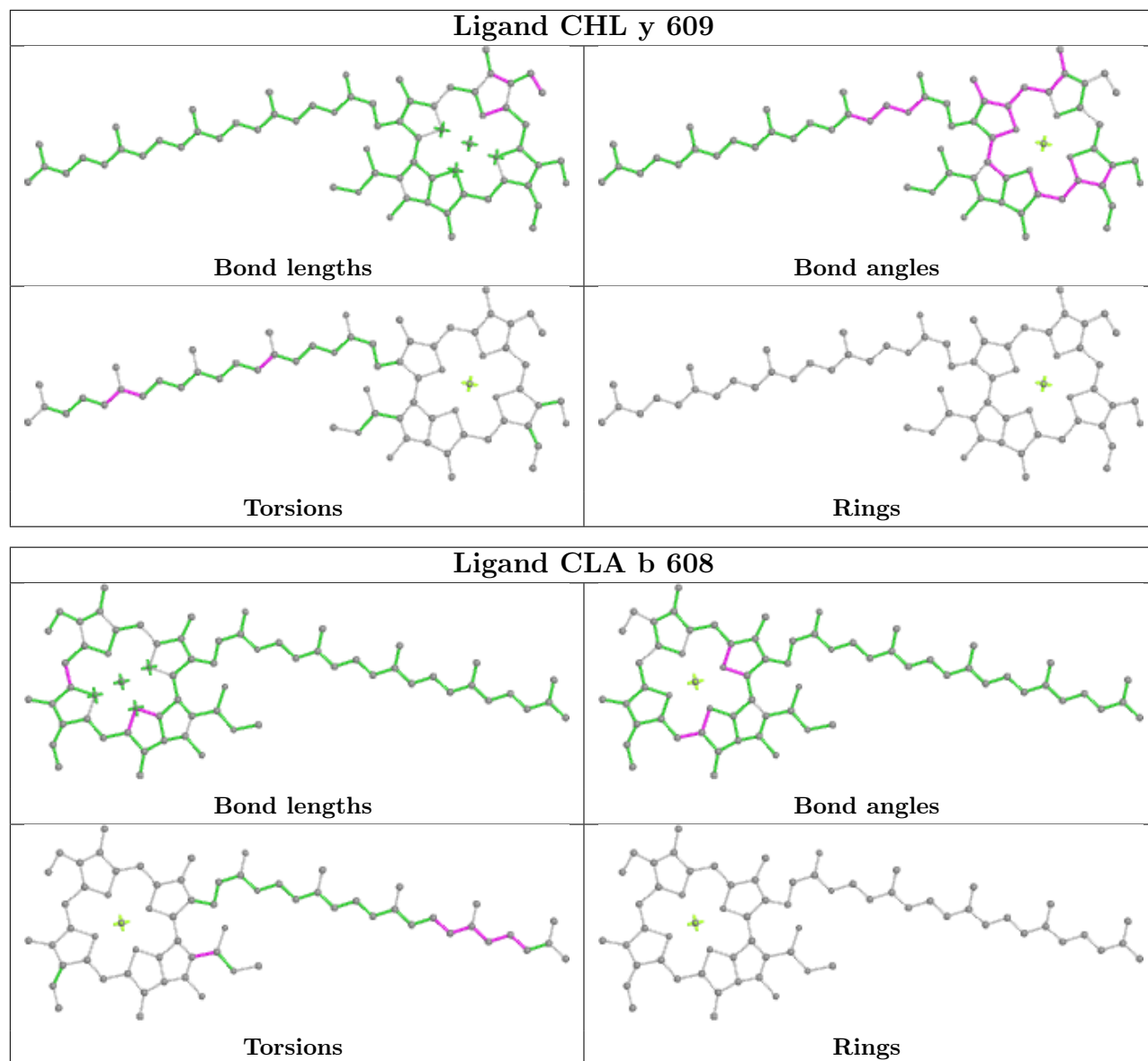


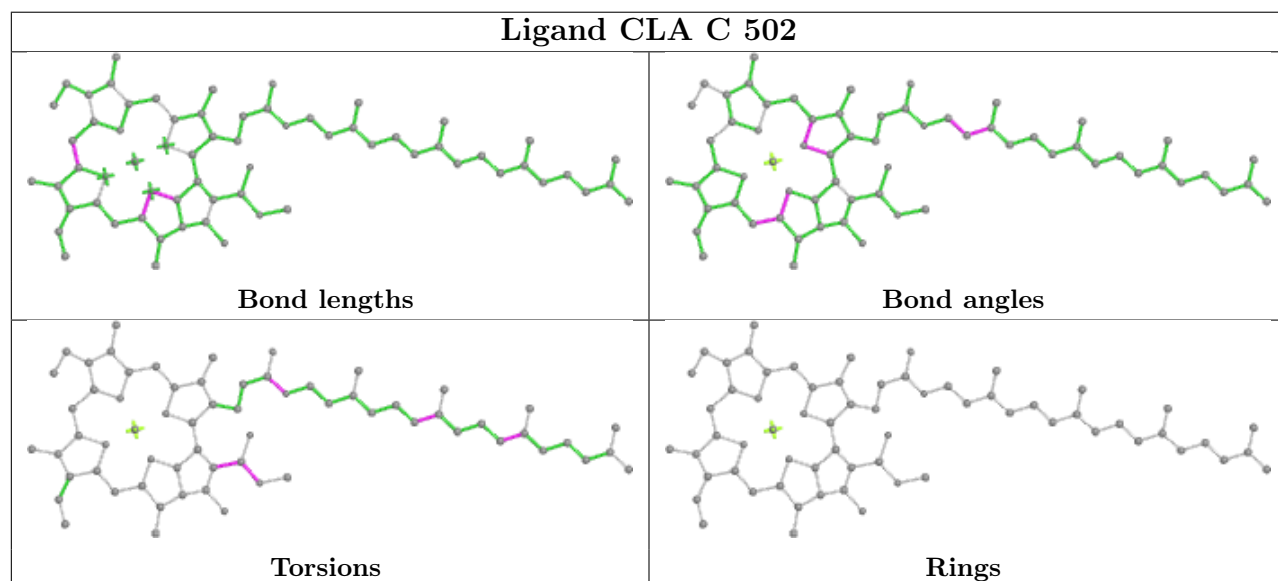
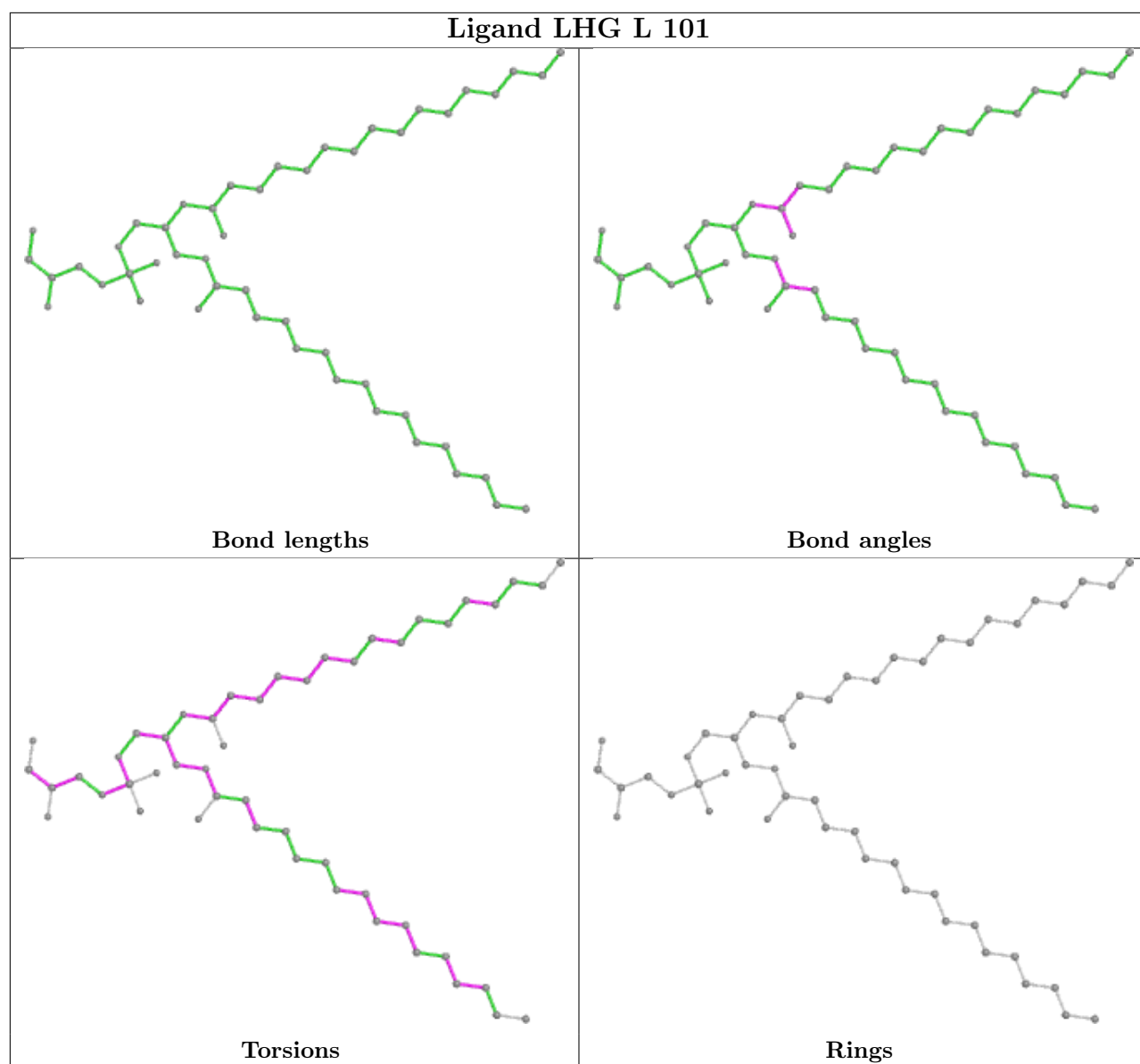
Ligand CHL n 608

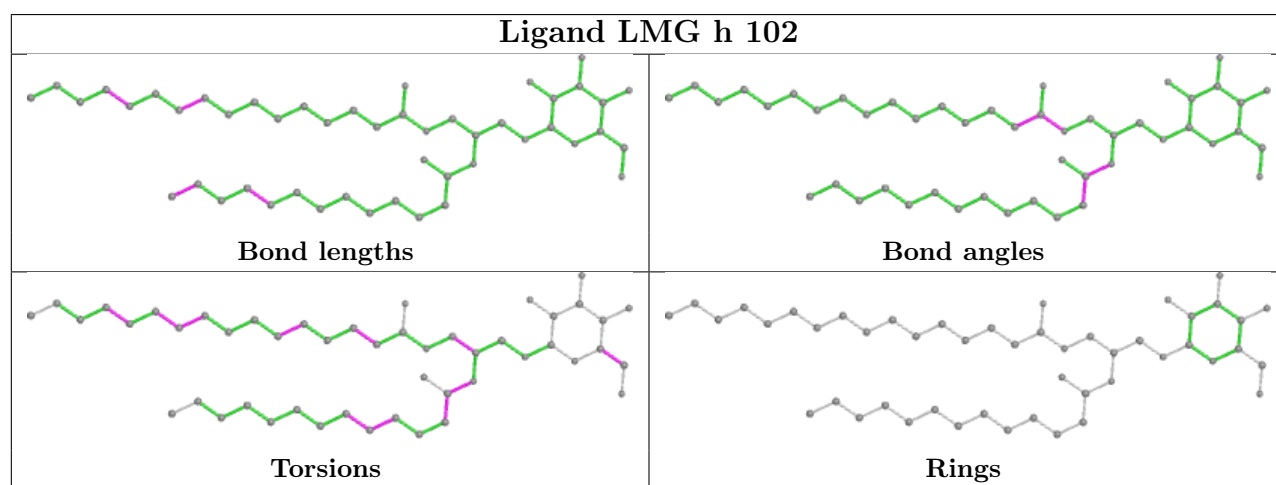
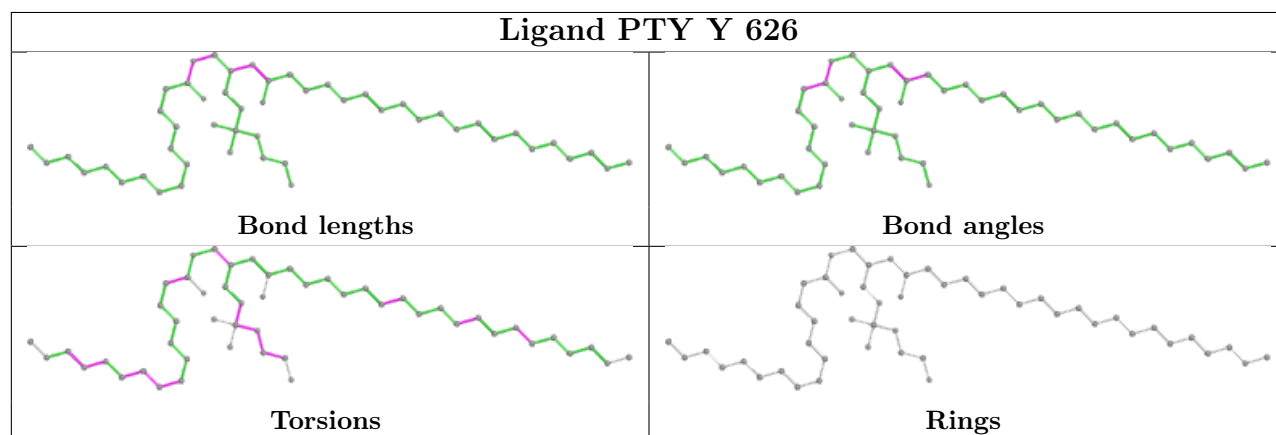
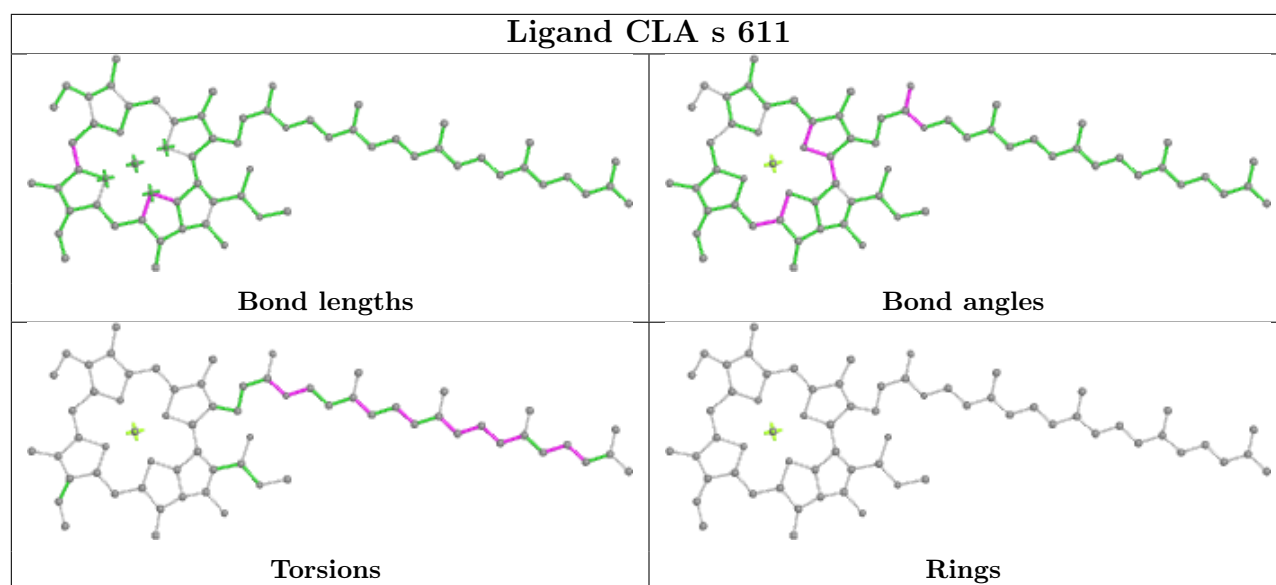


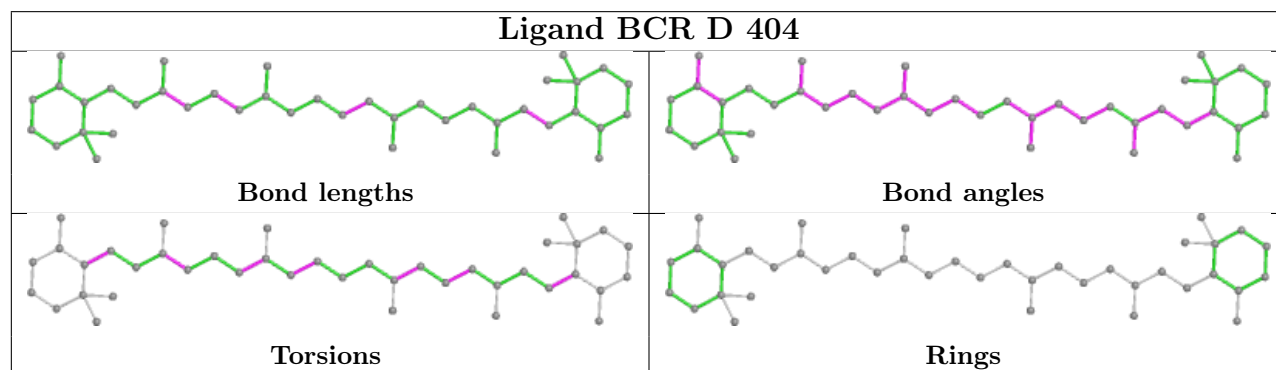
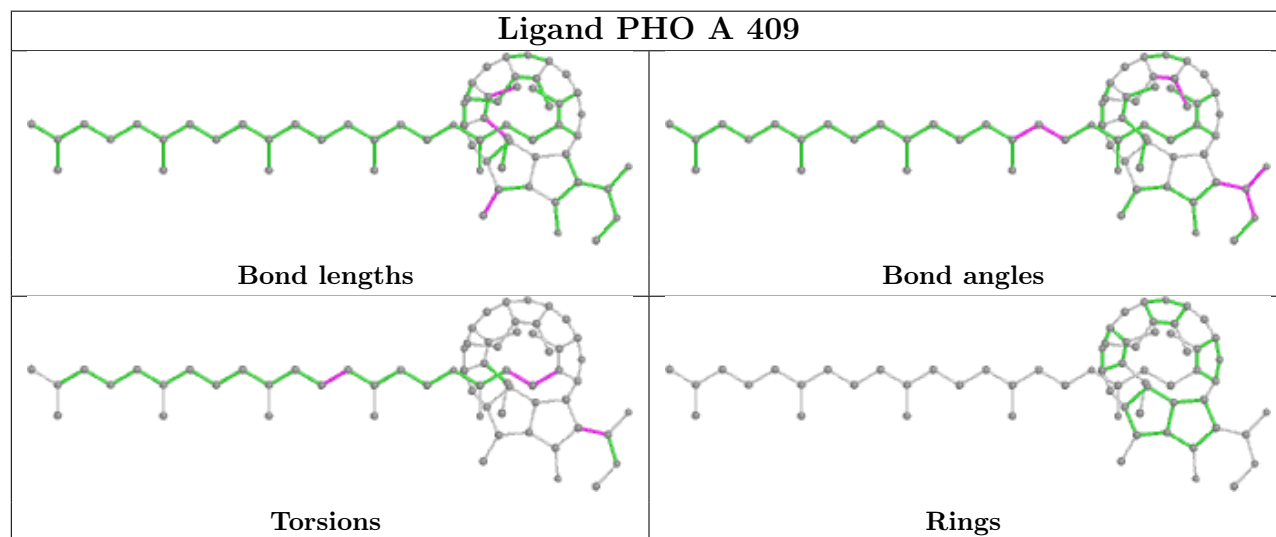
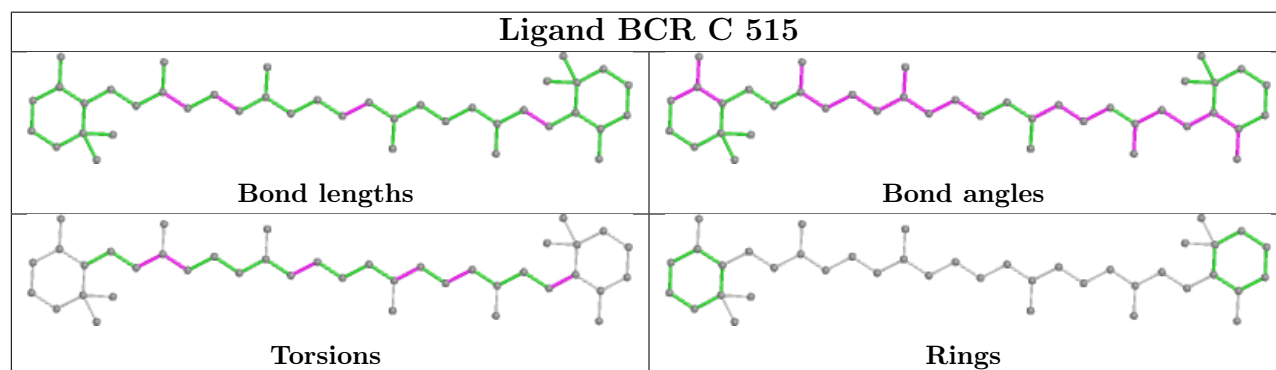
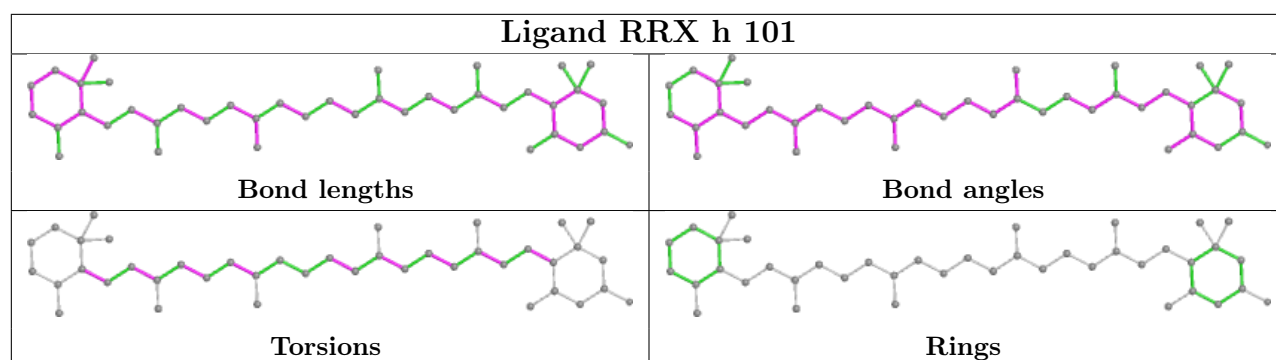
Ligand CLA s 604



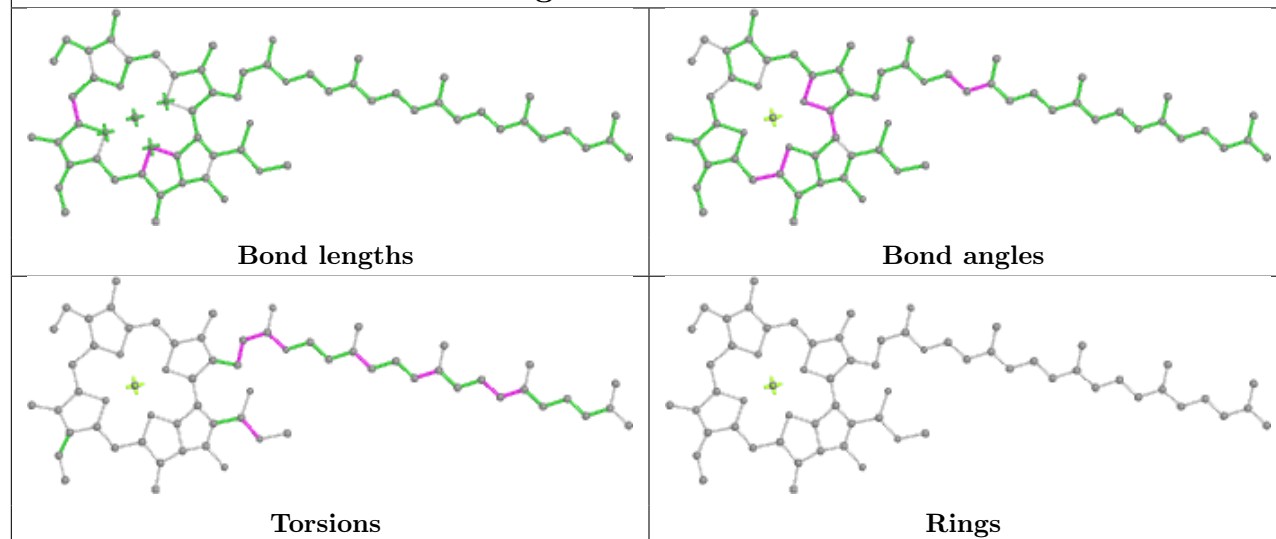




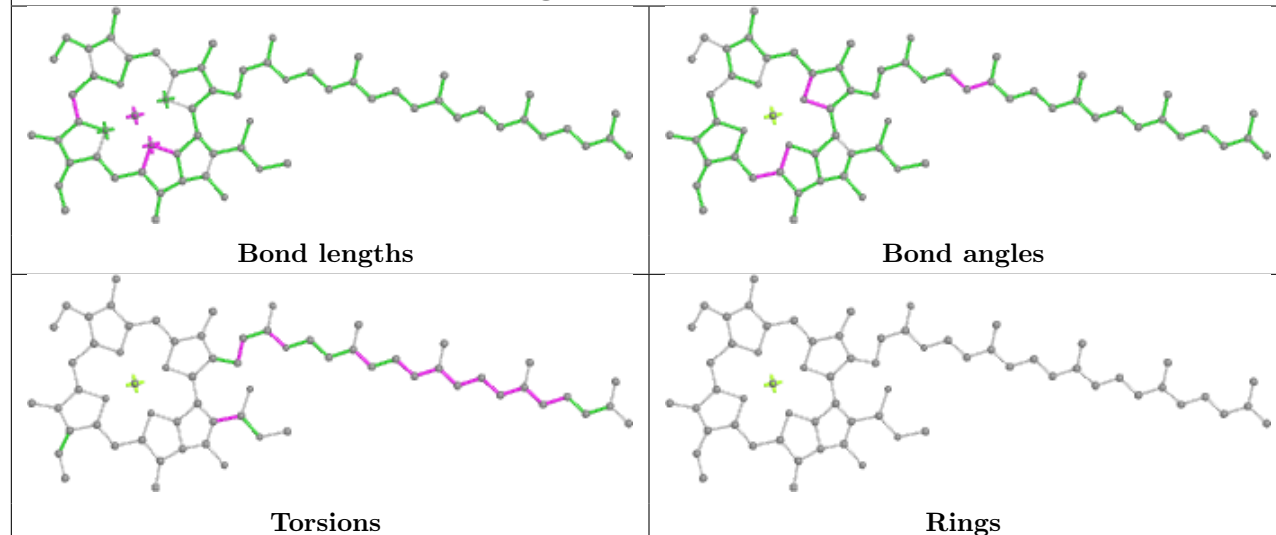




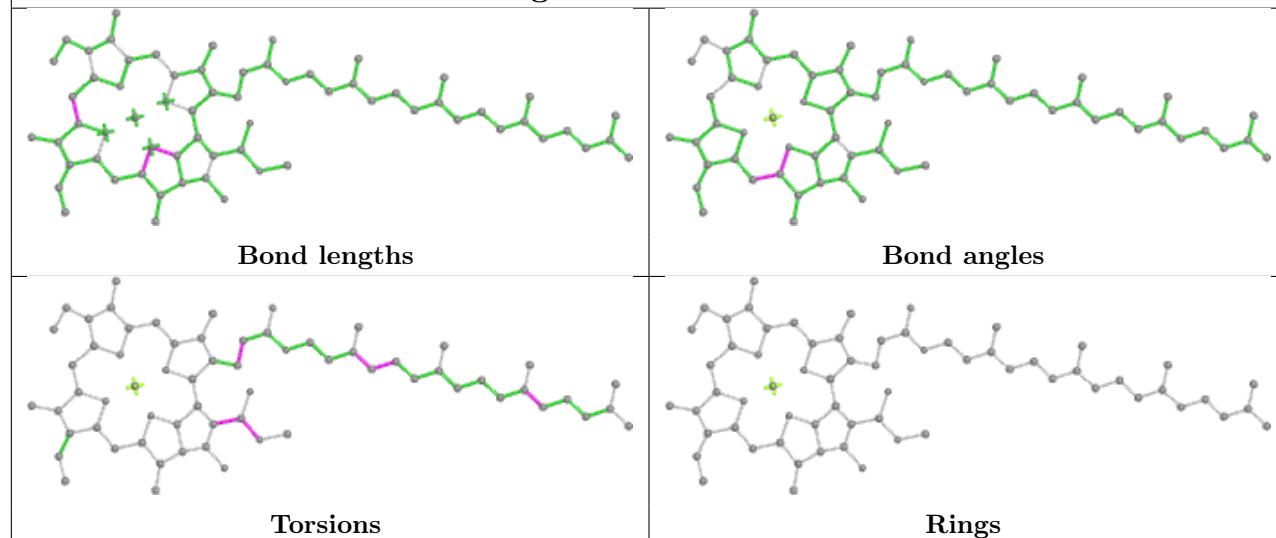
Ligand CLA b 615

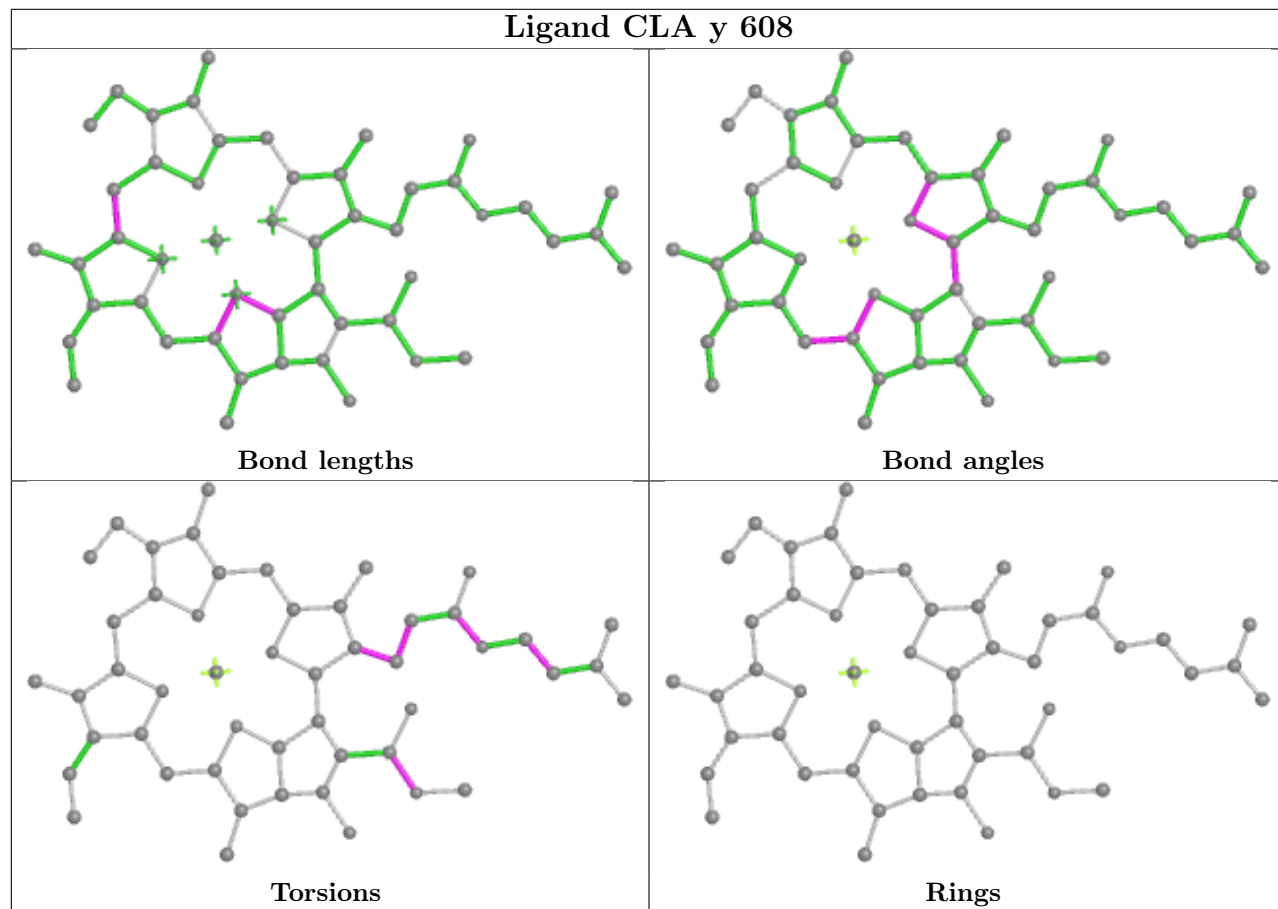
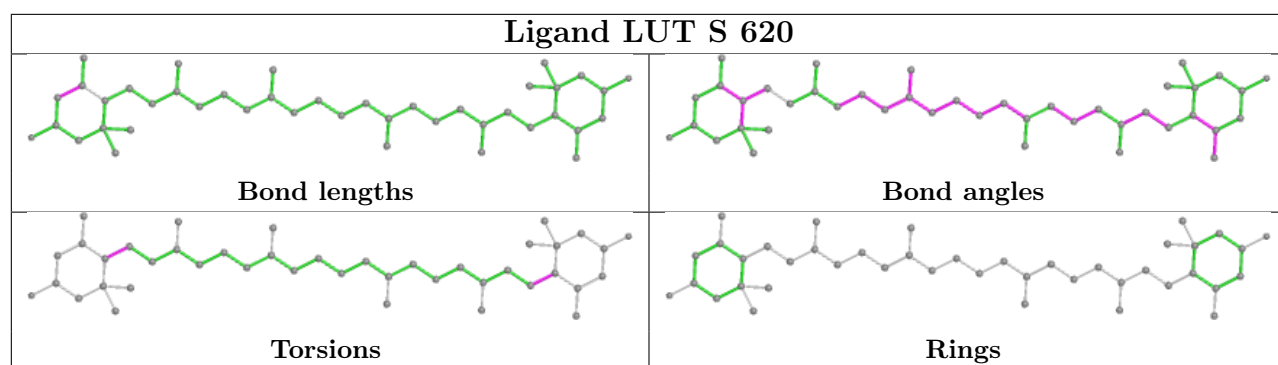


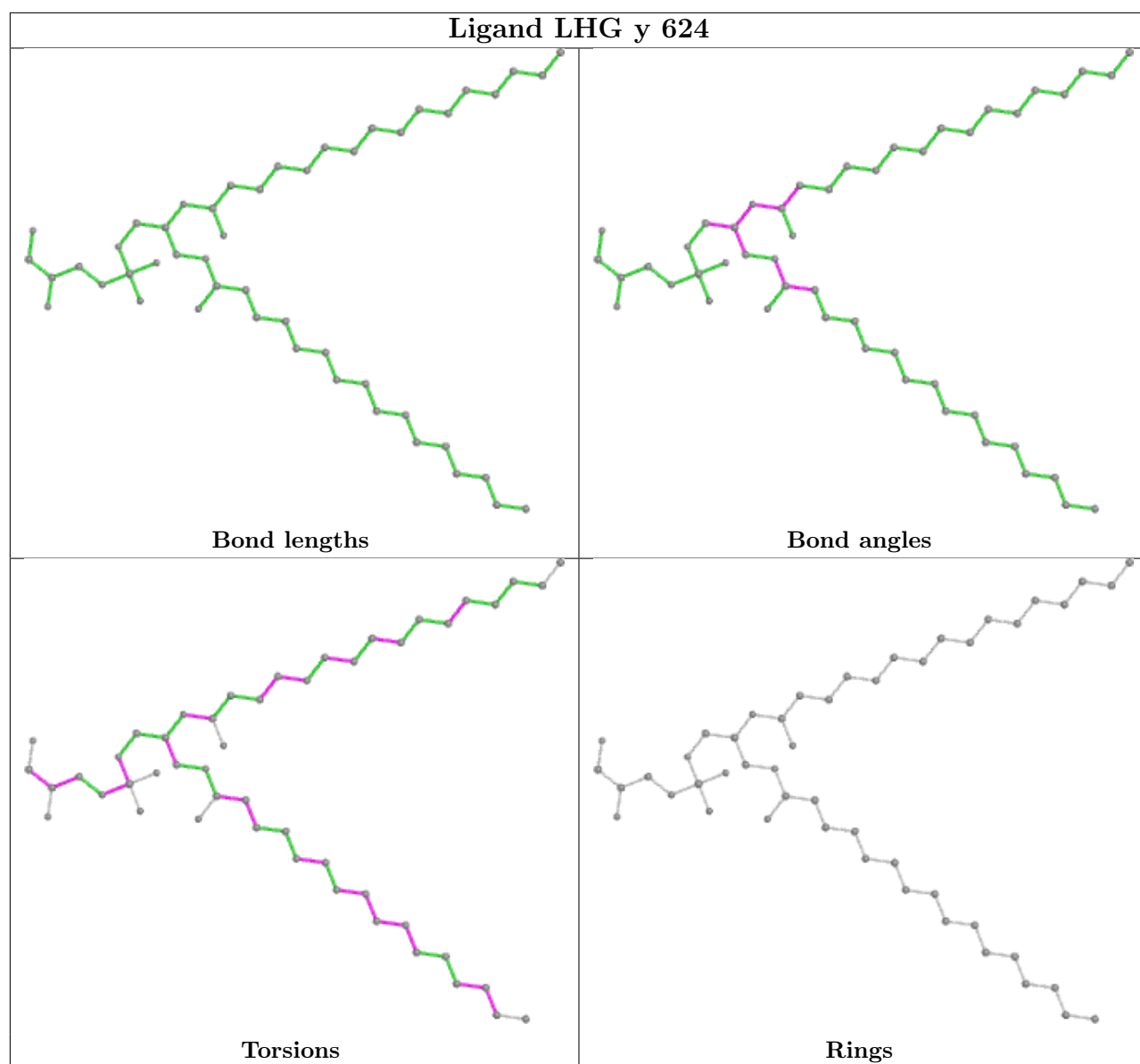
Ligand CLA c 505

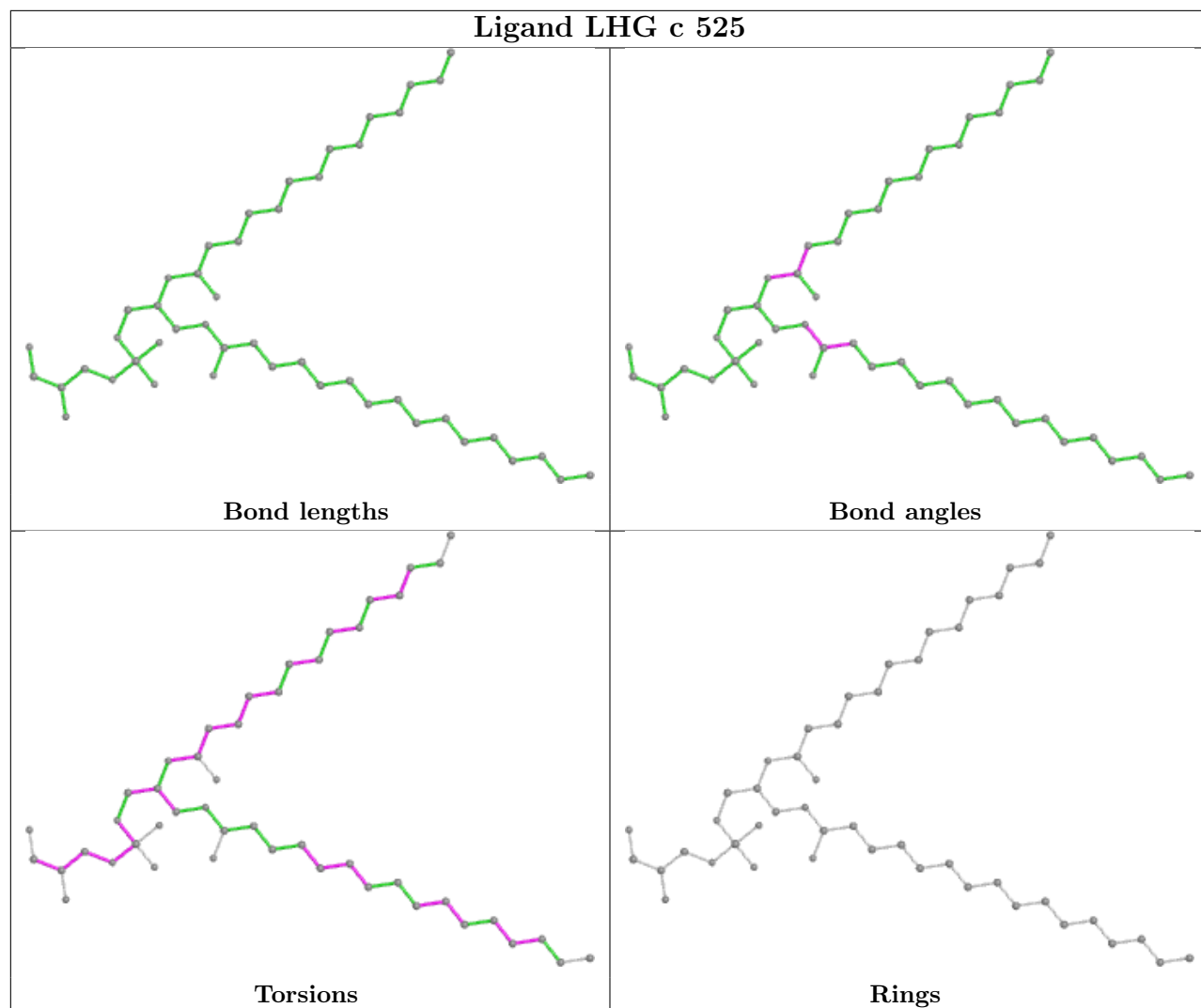
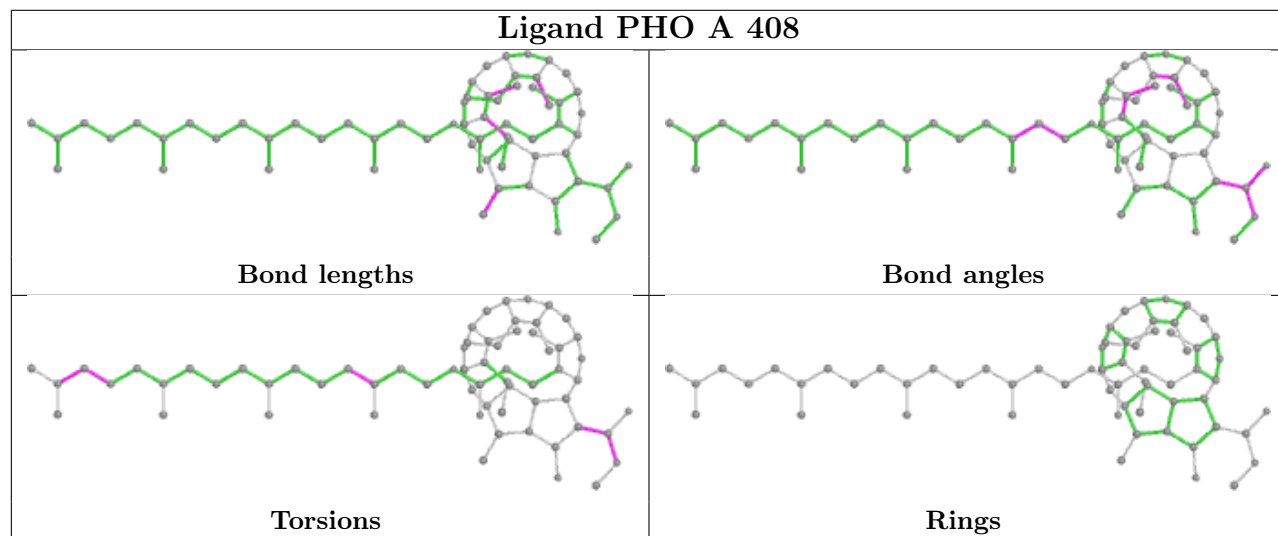


Ligand CLA G 613

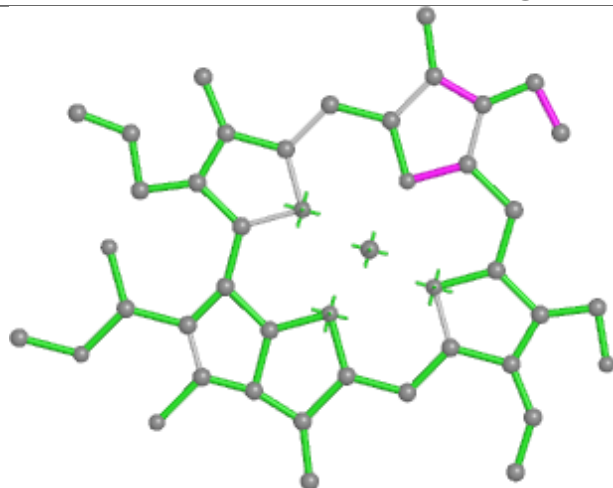




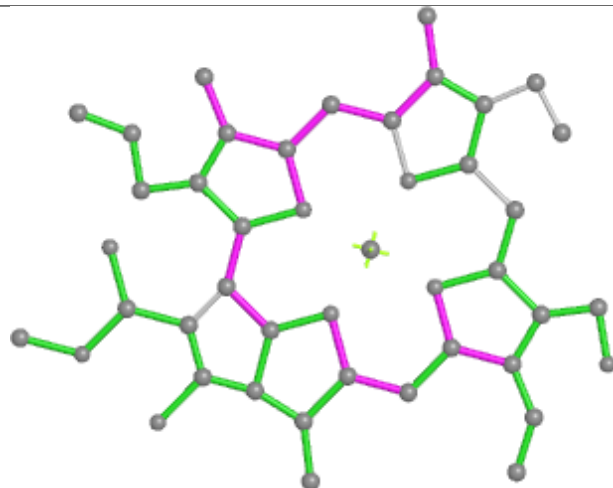


Ligand LHG c 525**Ligand PHO A 408**

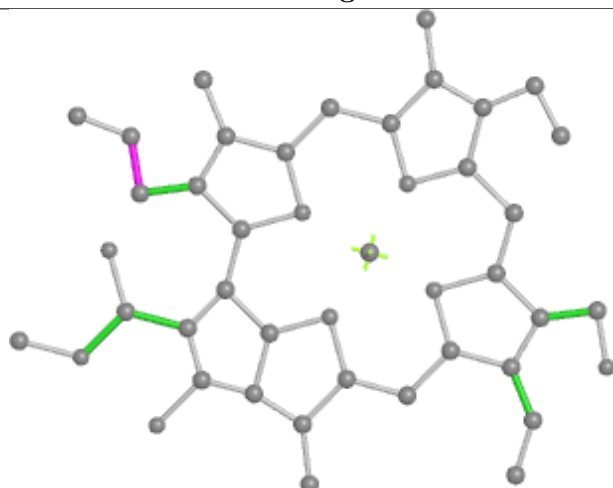
Ligand CHL S 606



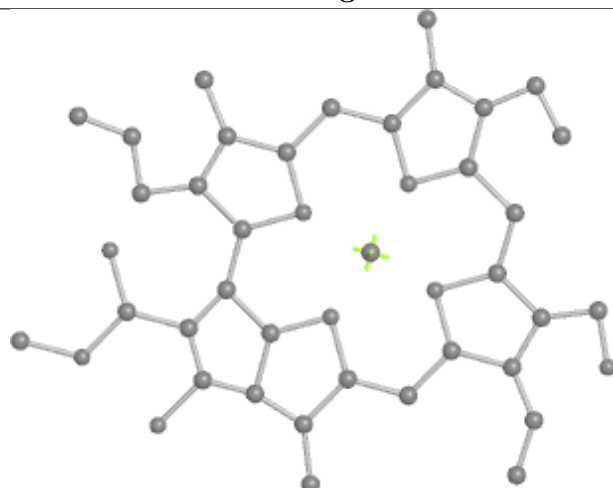
Bond lengths



Bond angles

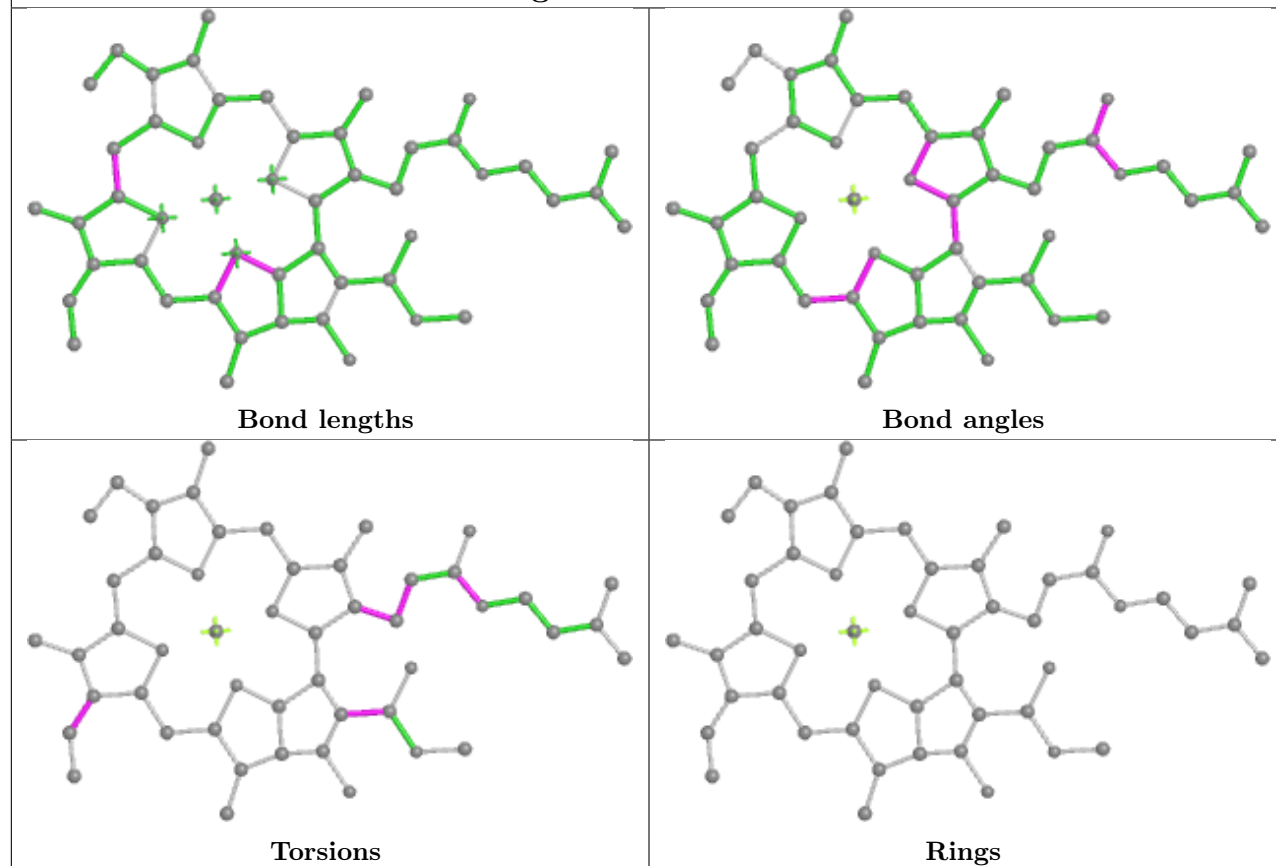


Torsions

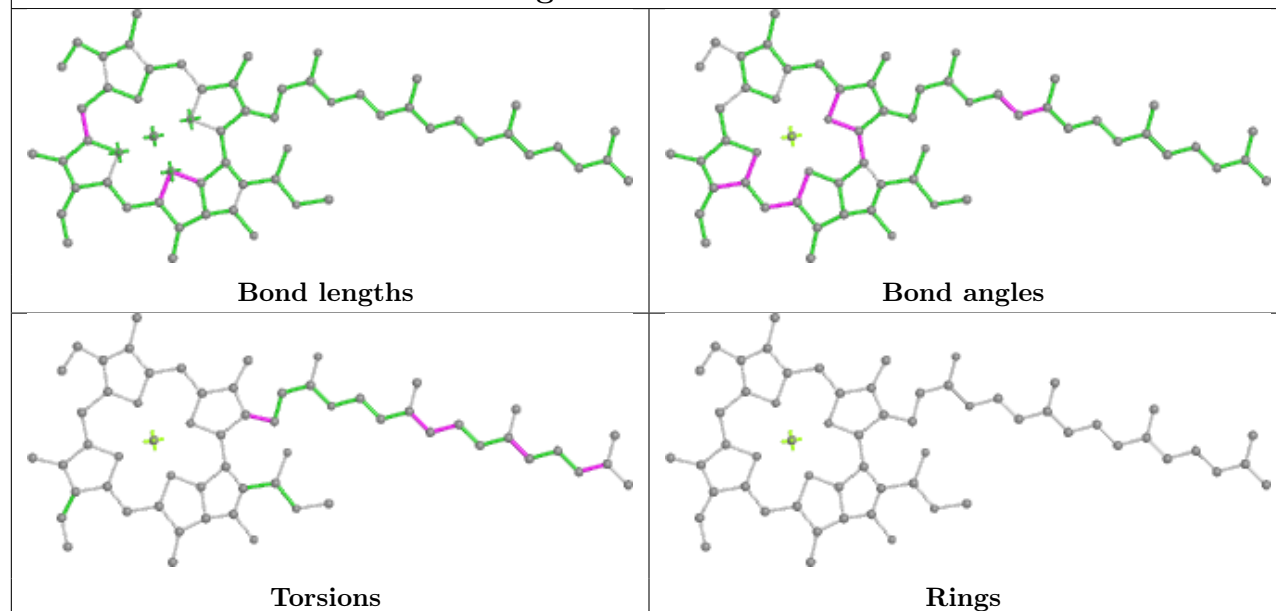


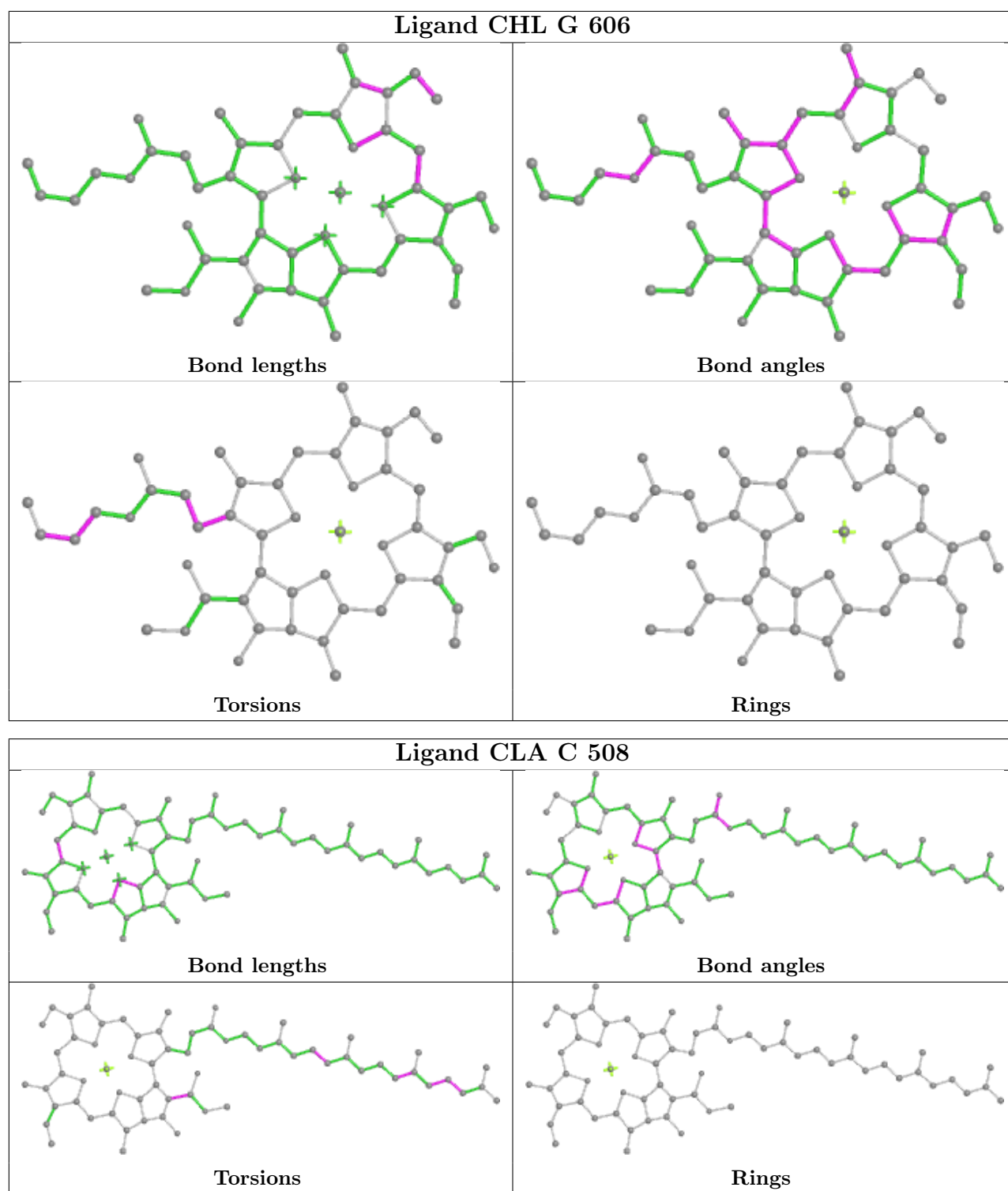
Rings

Ligand CLA A 407

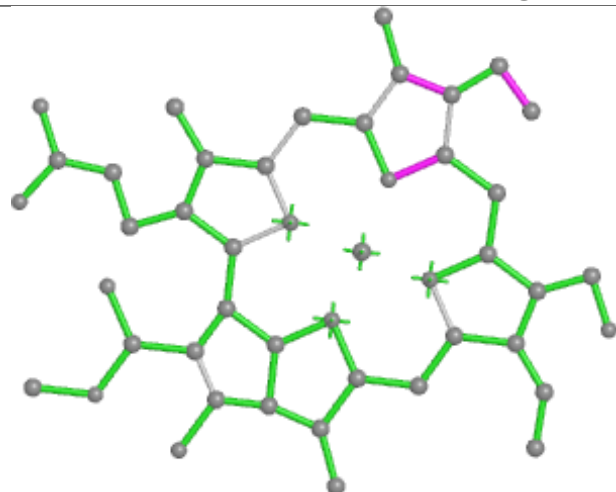


Ligand CLA a 410

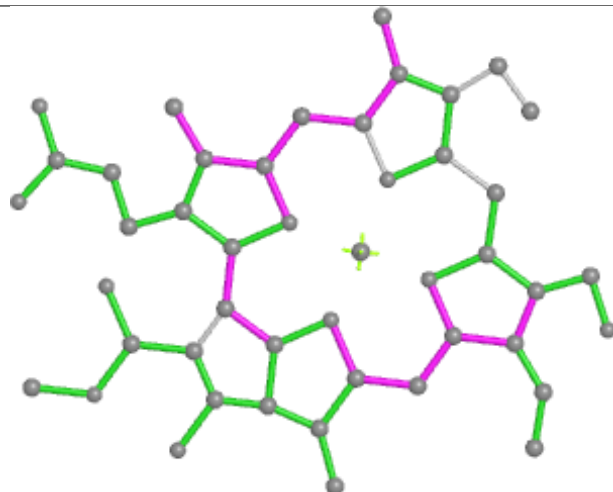




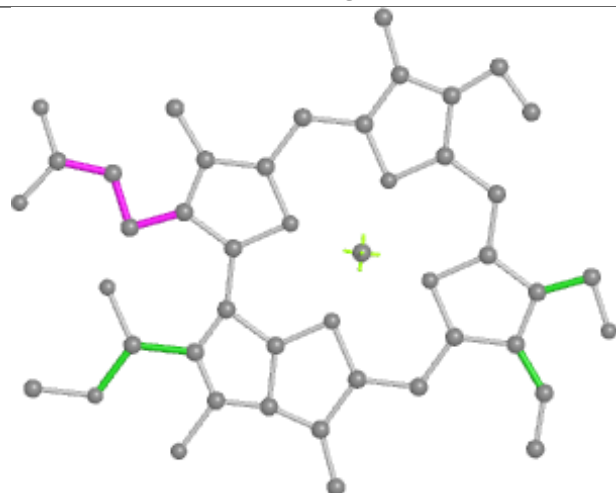
Ligand CHL Y 605



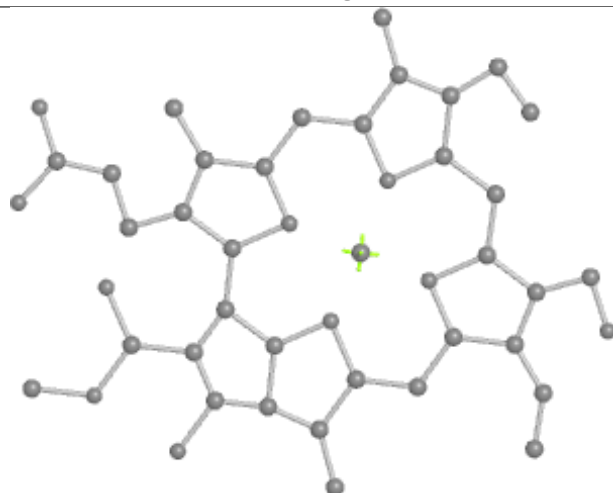
Bond lengths



Bond angles

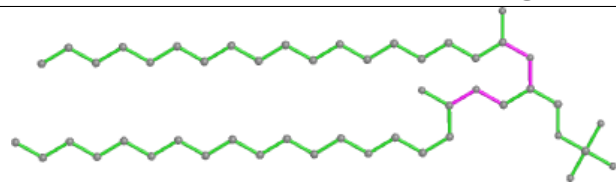


Torsions

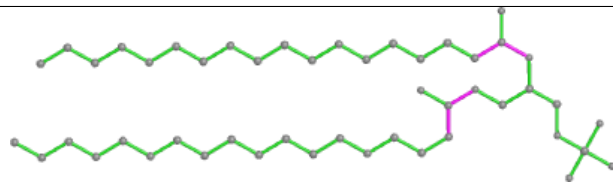


Rings

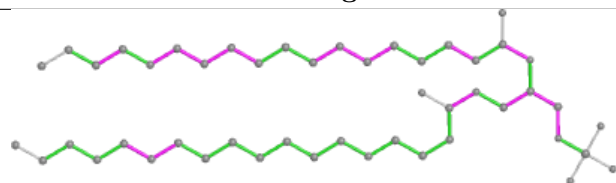
Ligand 3PH B 624



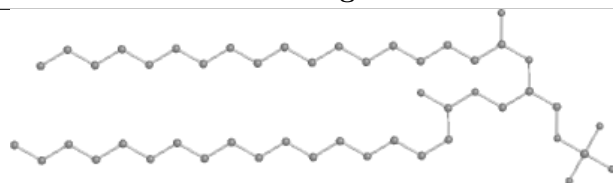
Bond lengths



Bond angles

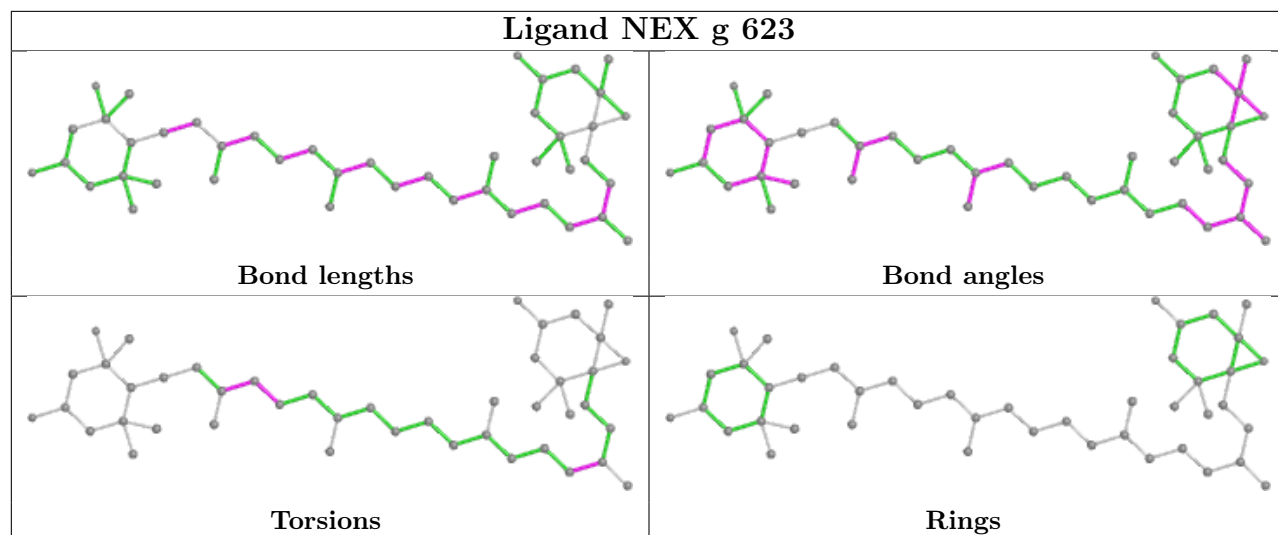


Torsions

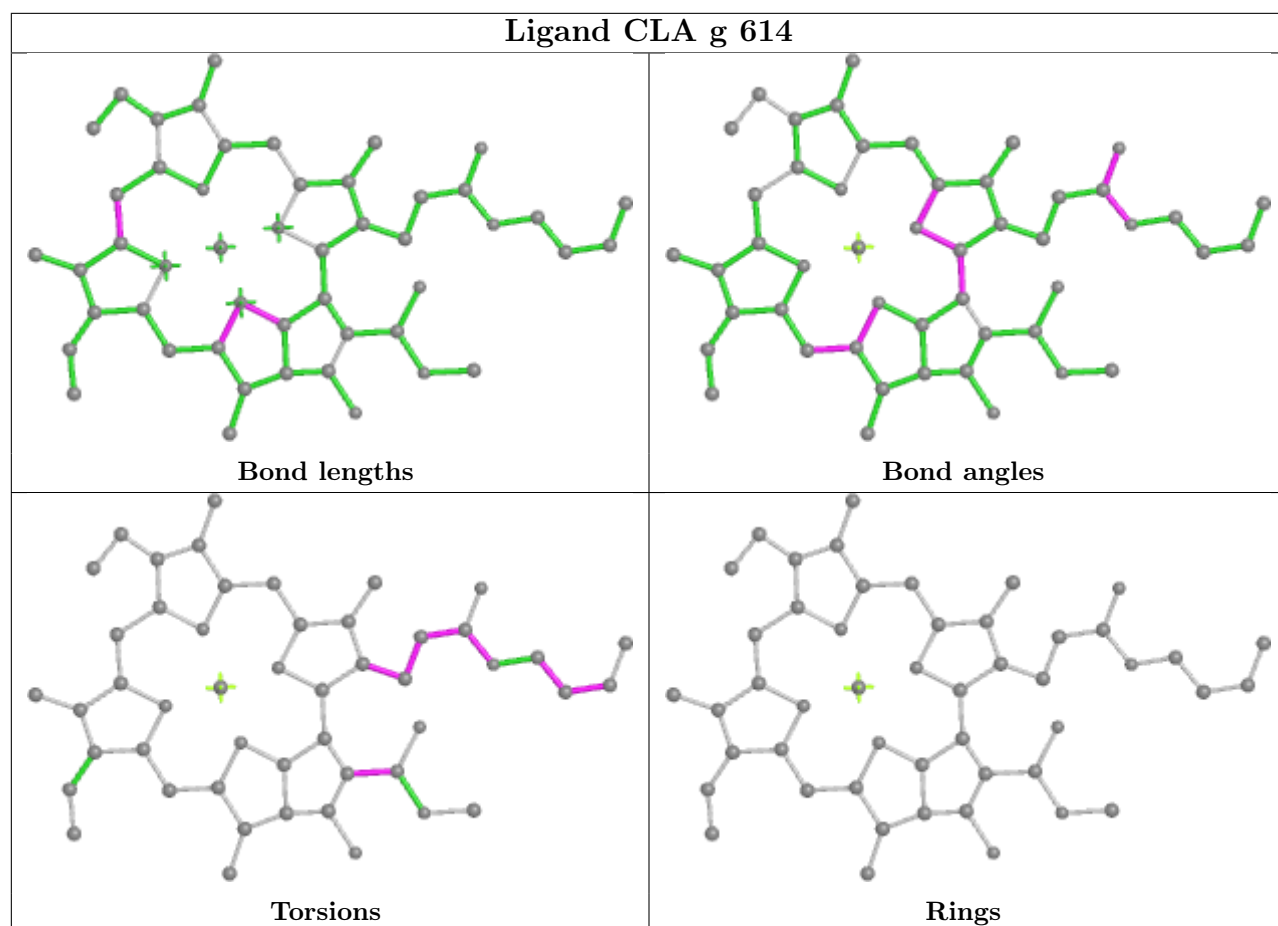


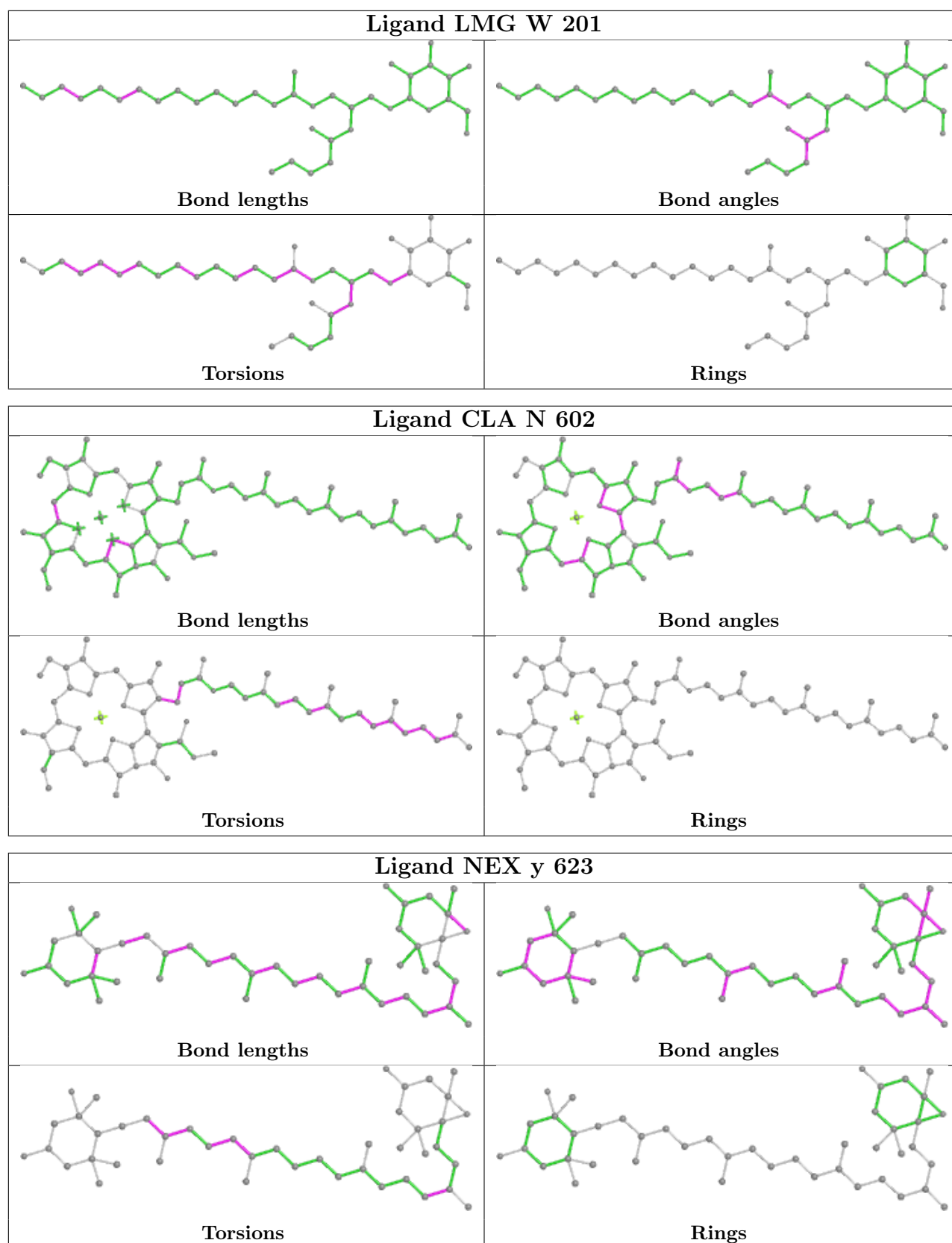
Rings

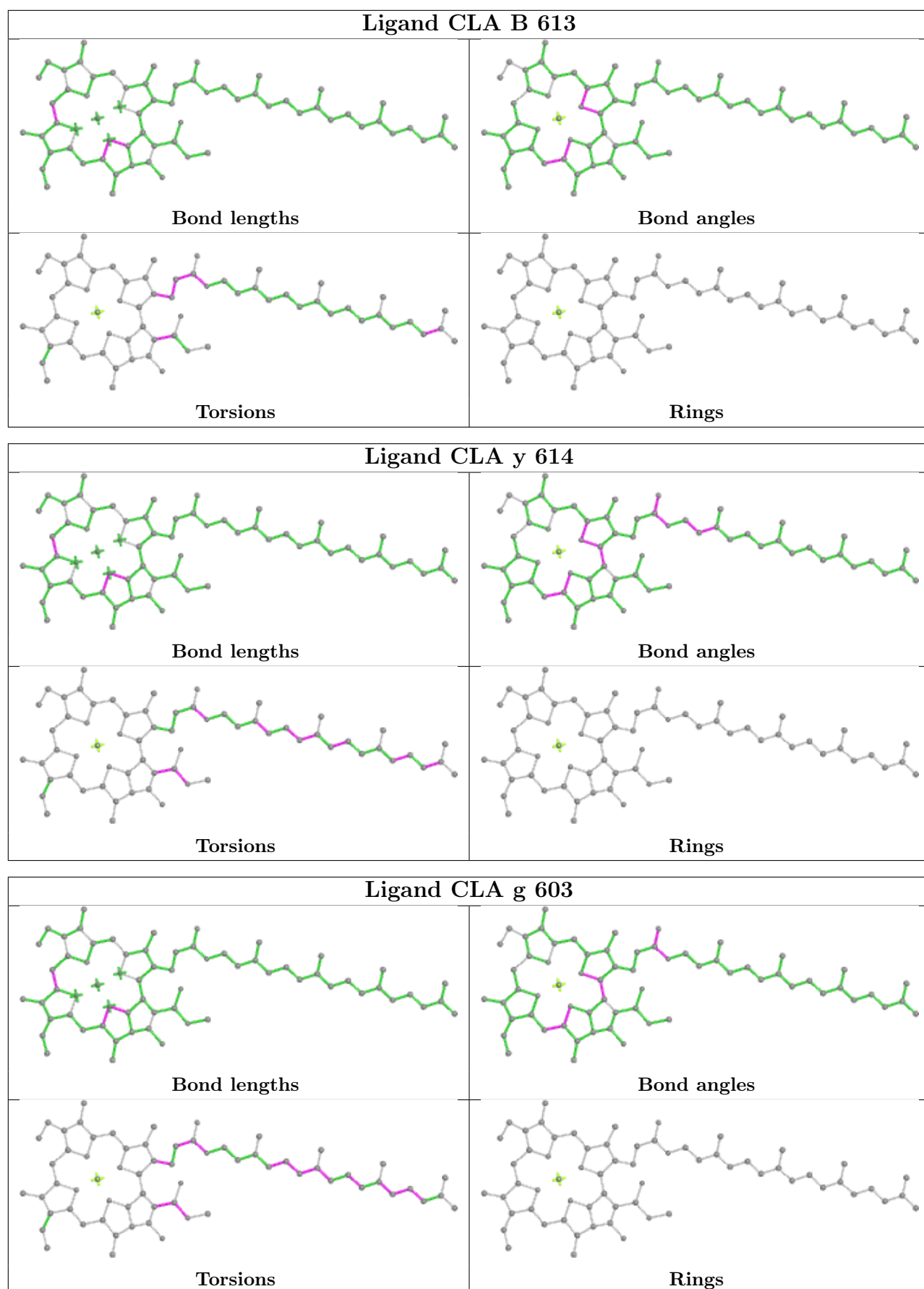
Ligand NEX g 623

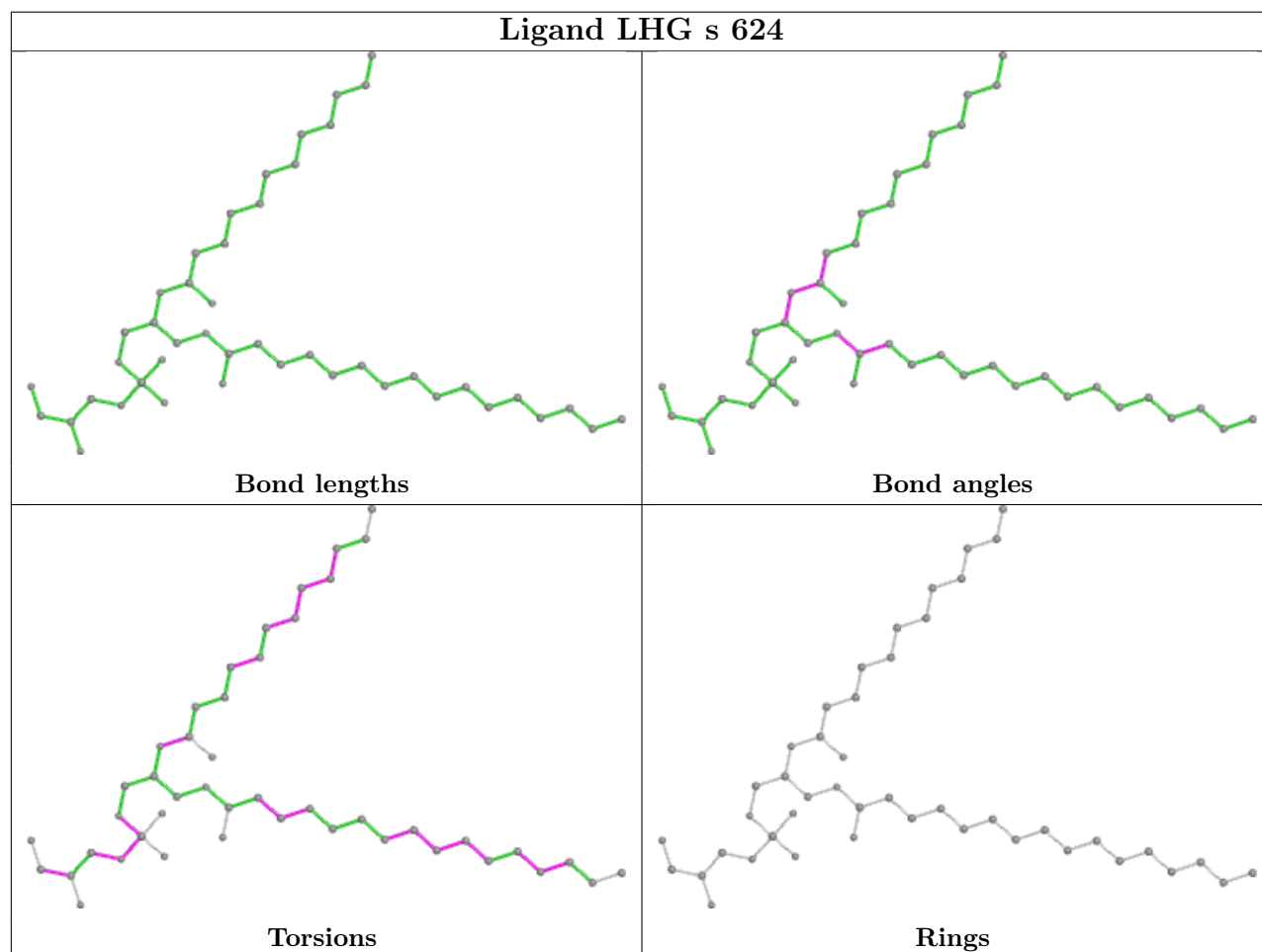
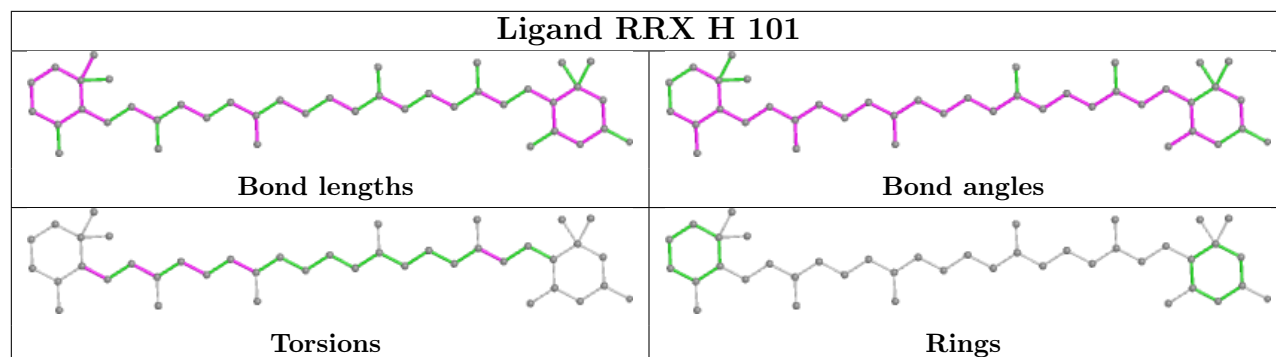


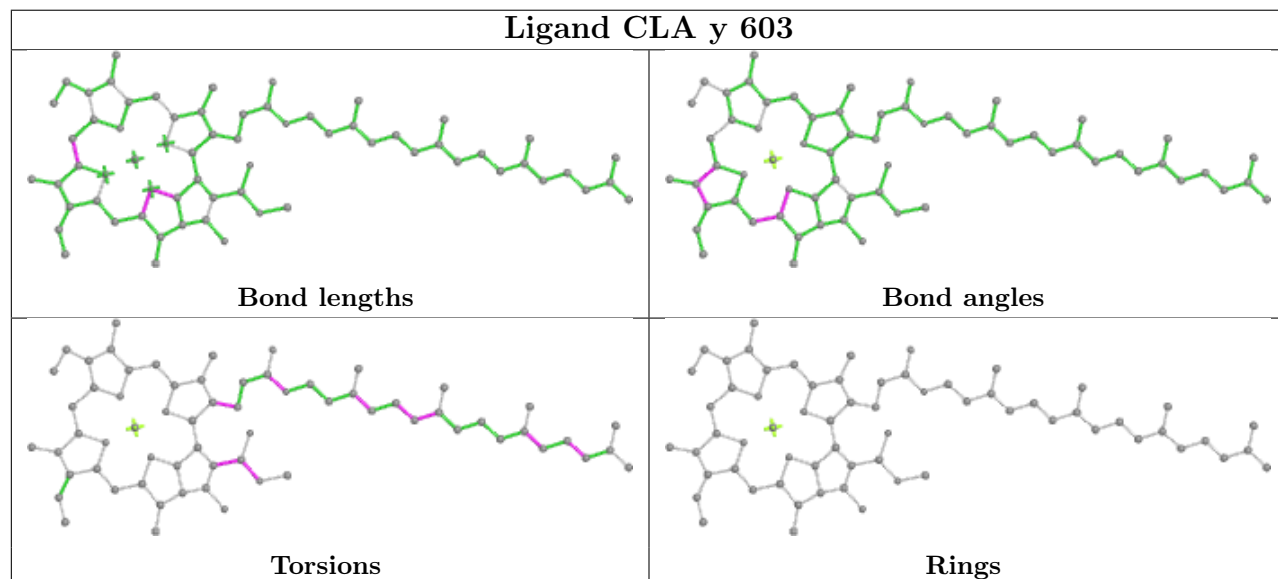
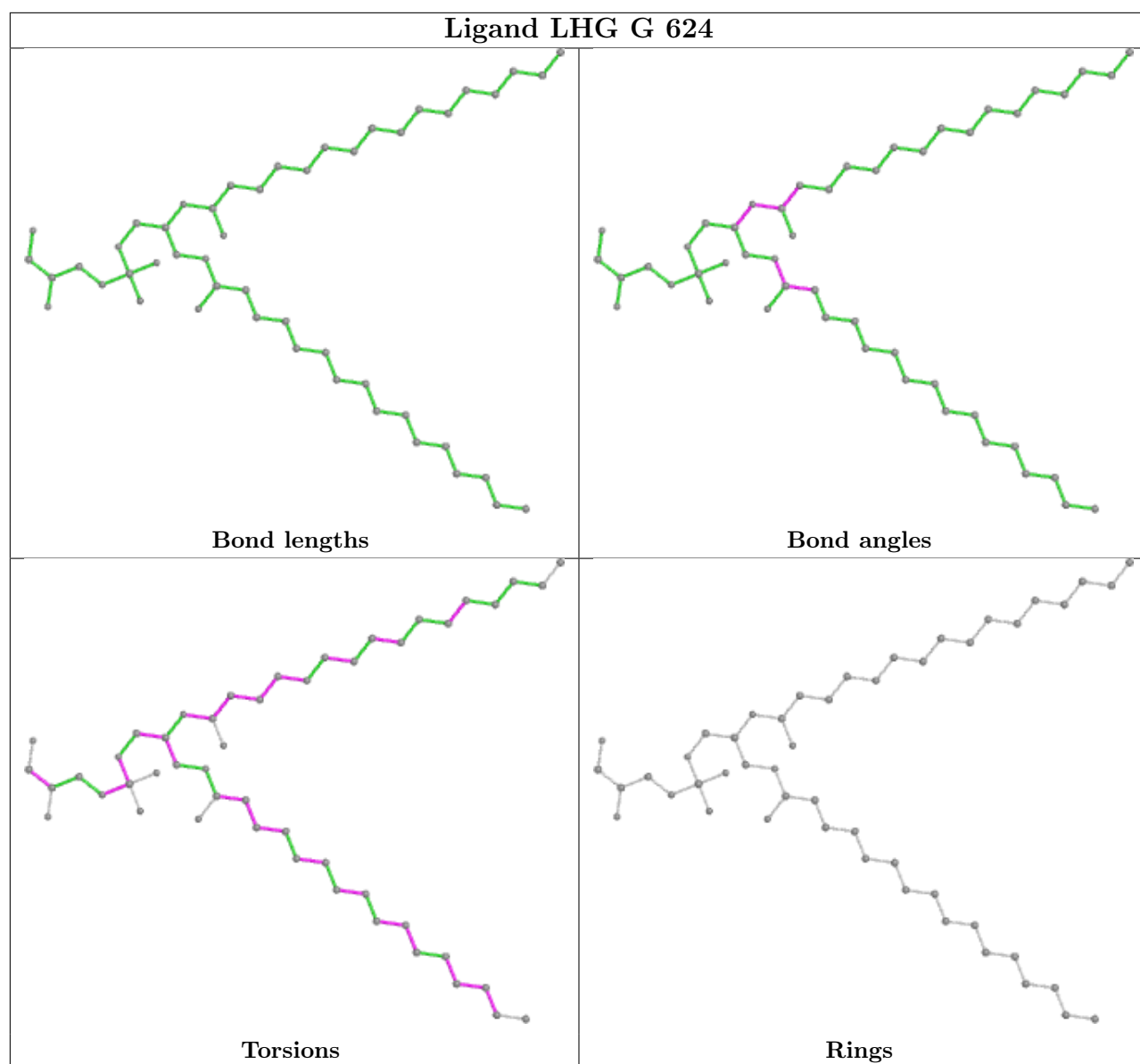
Ligand CLA g 614

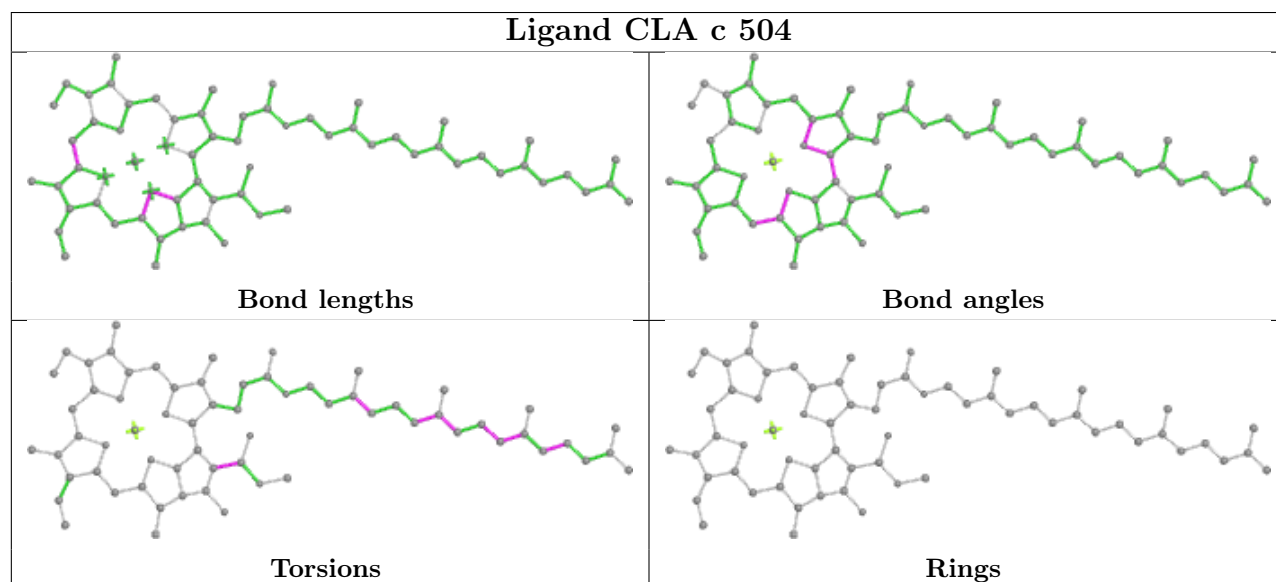
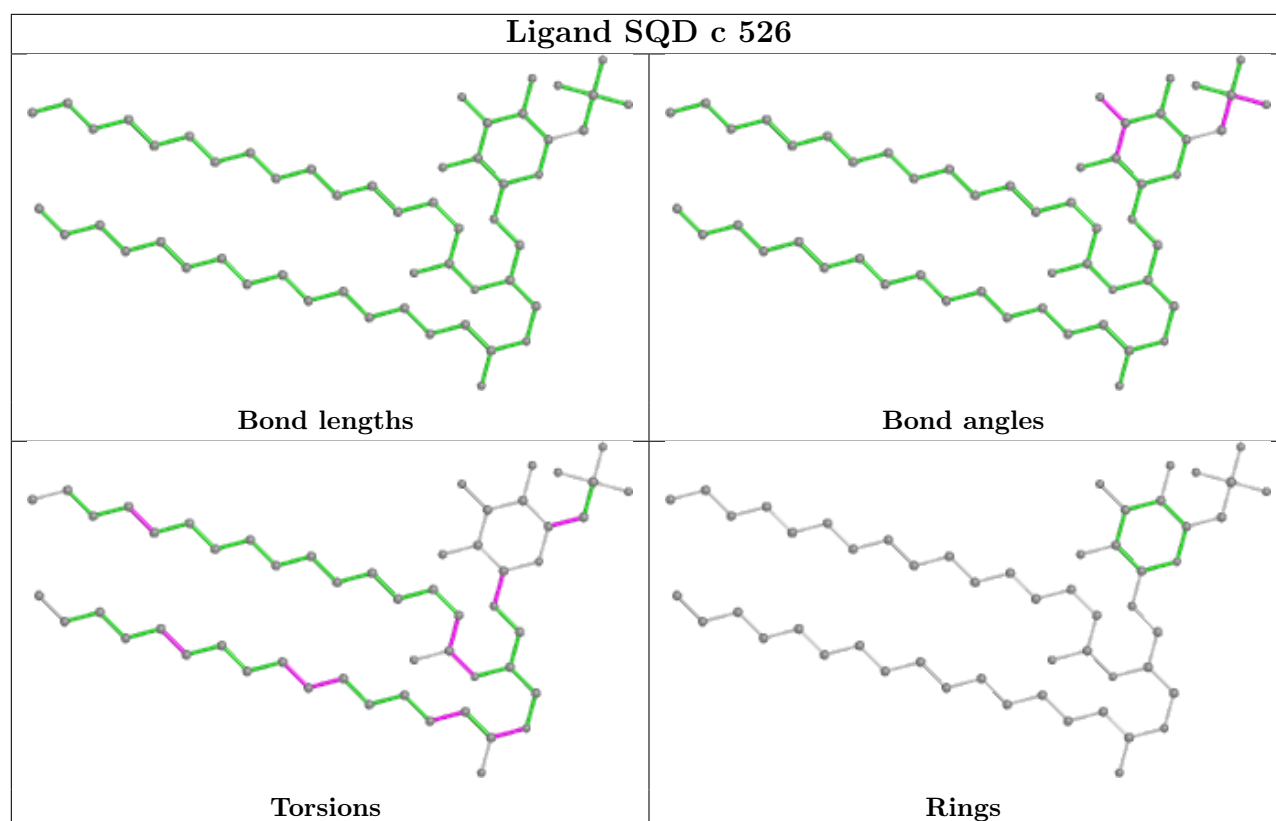


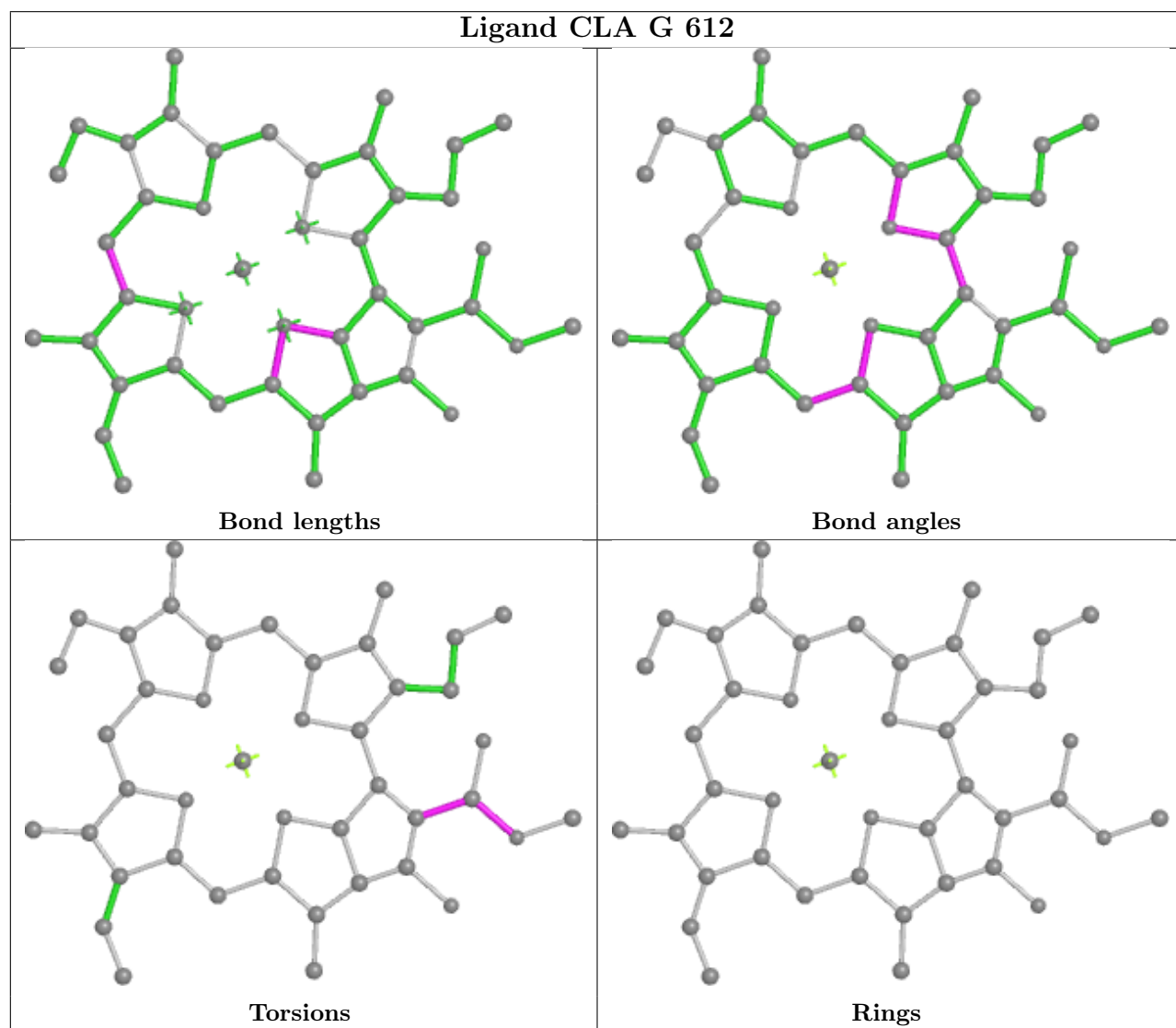
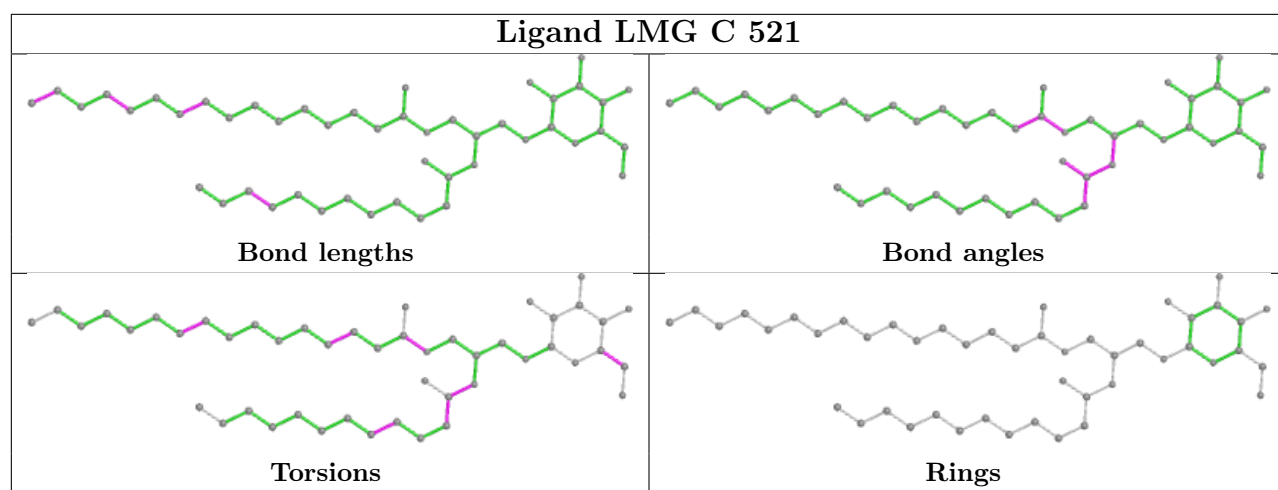


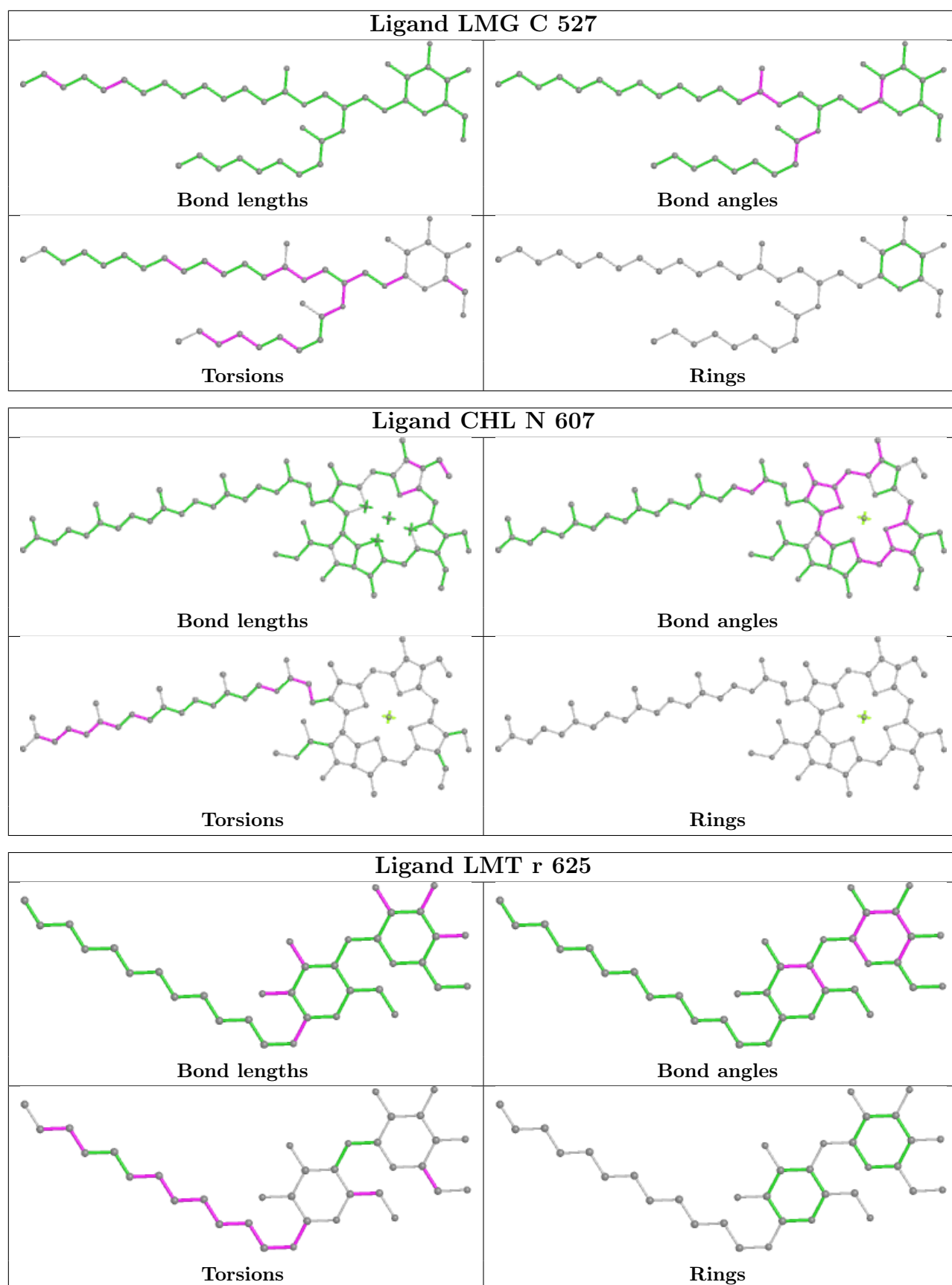


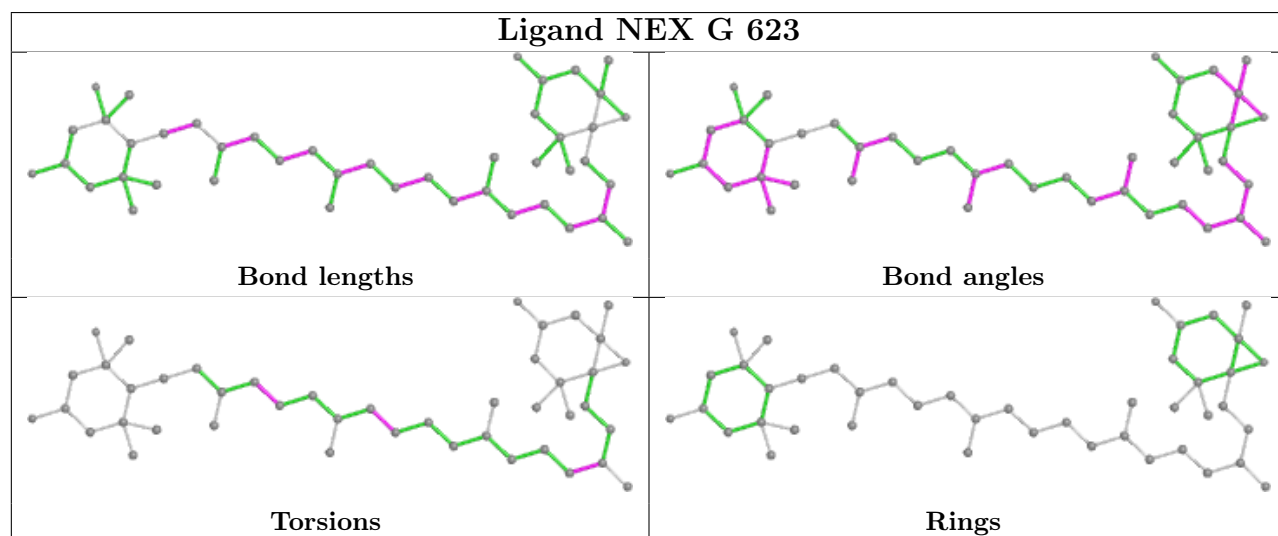
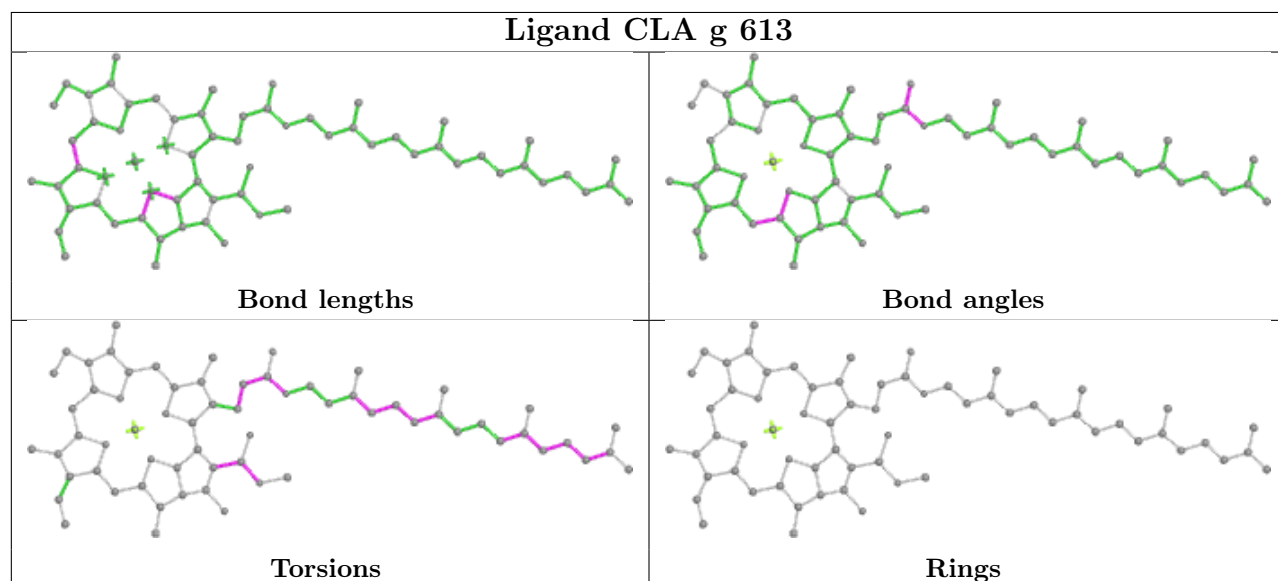
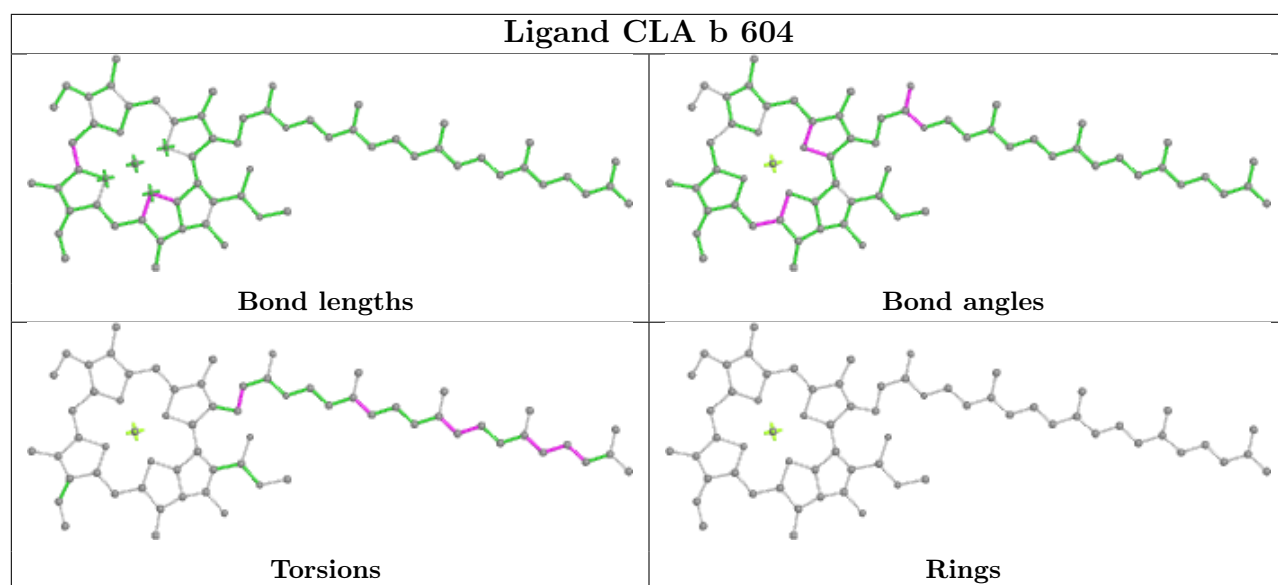


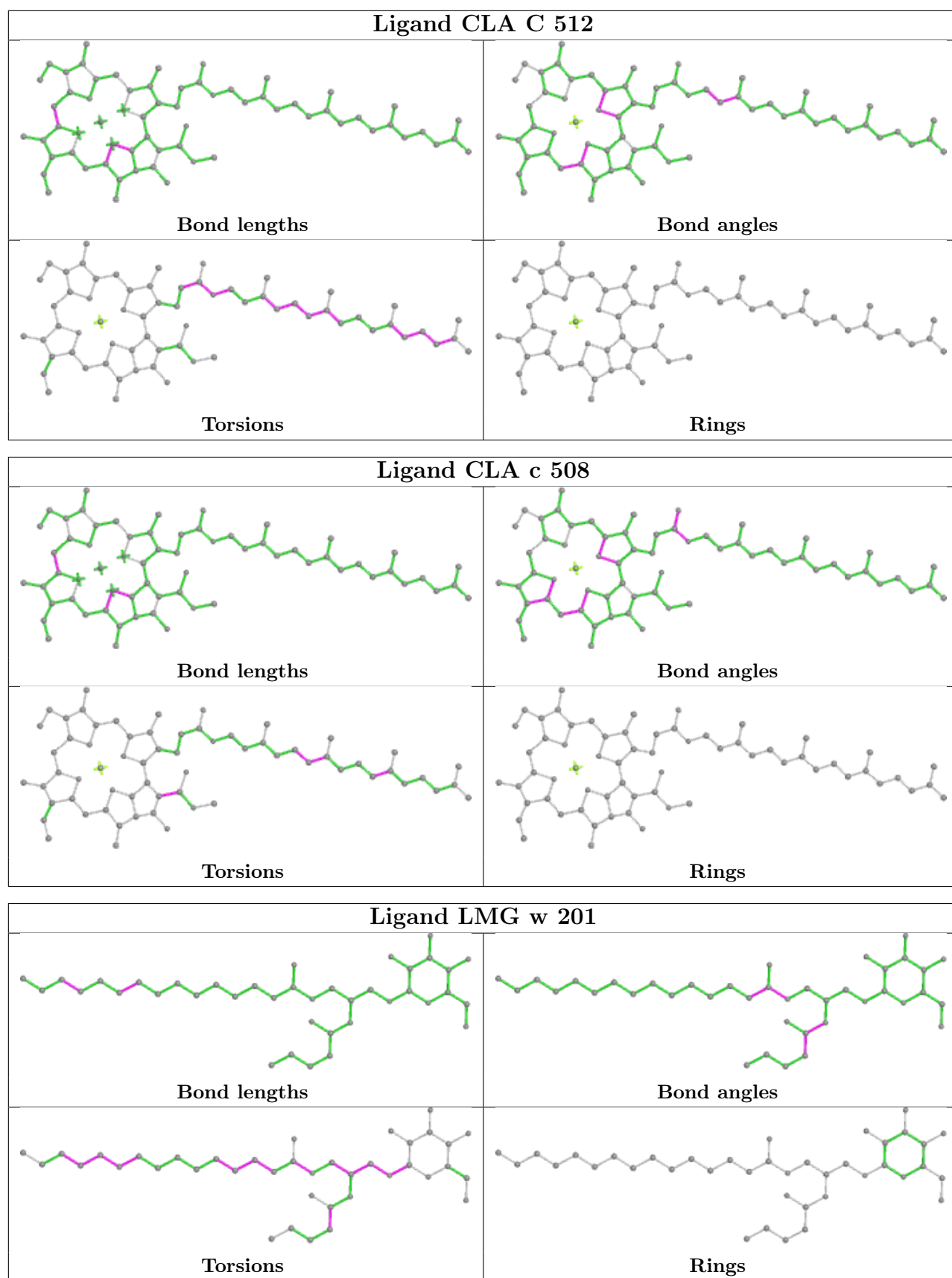


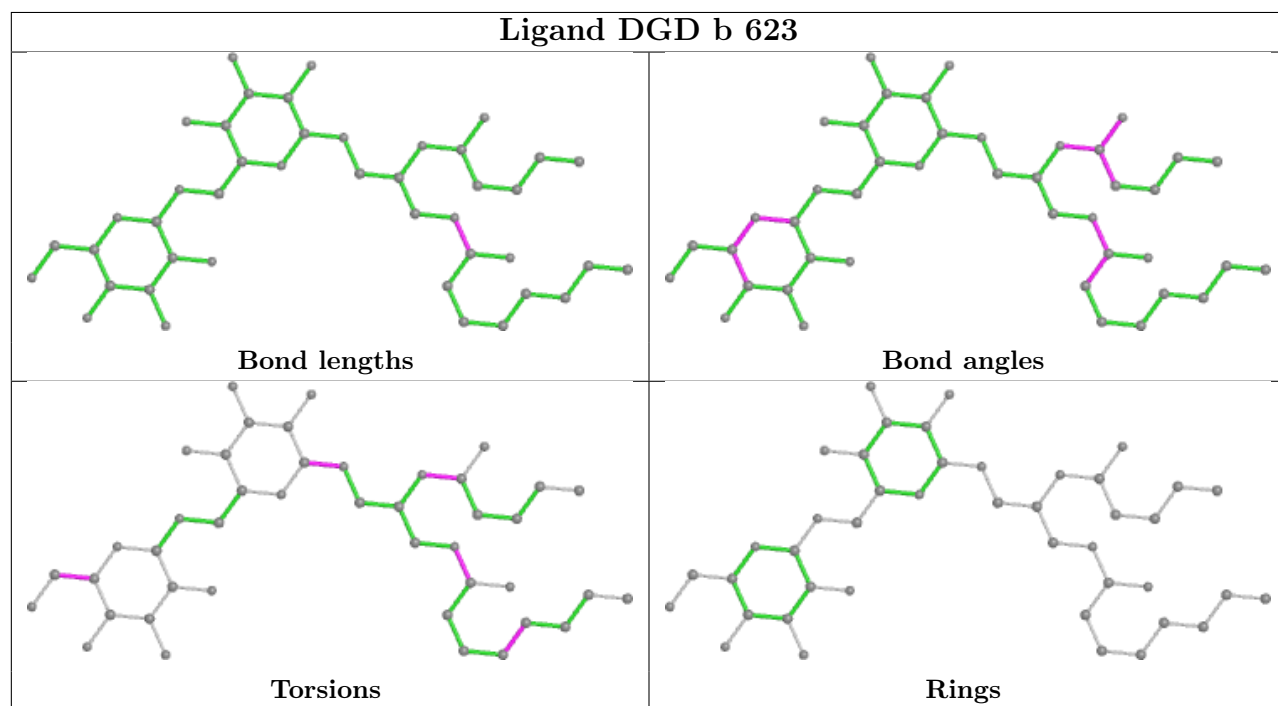
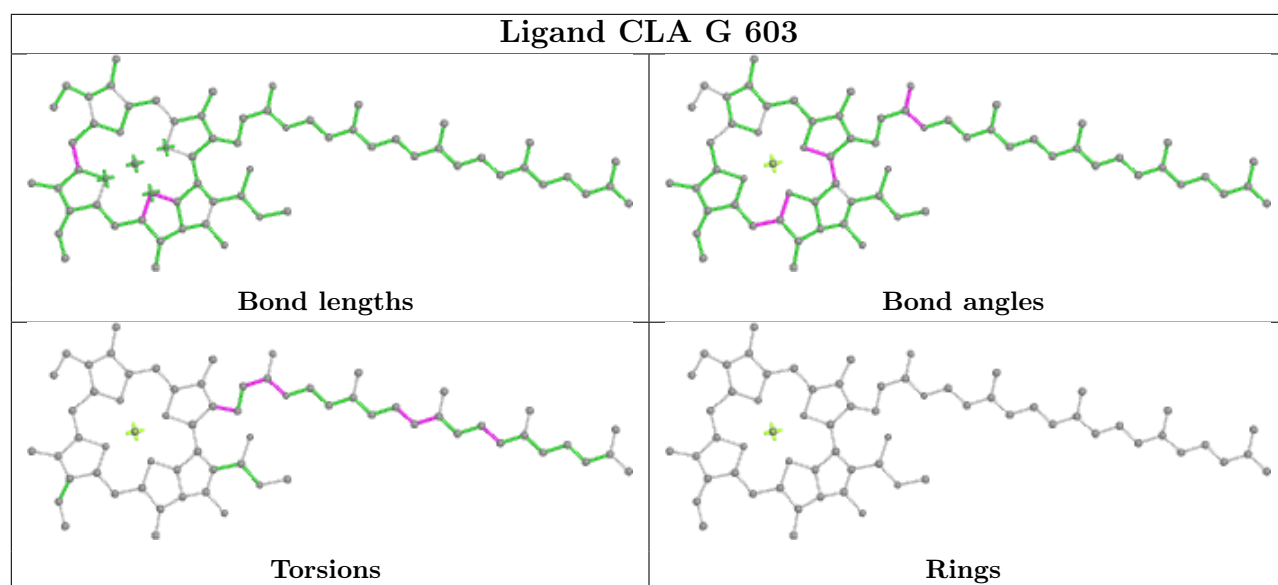


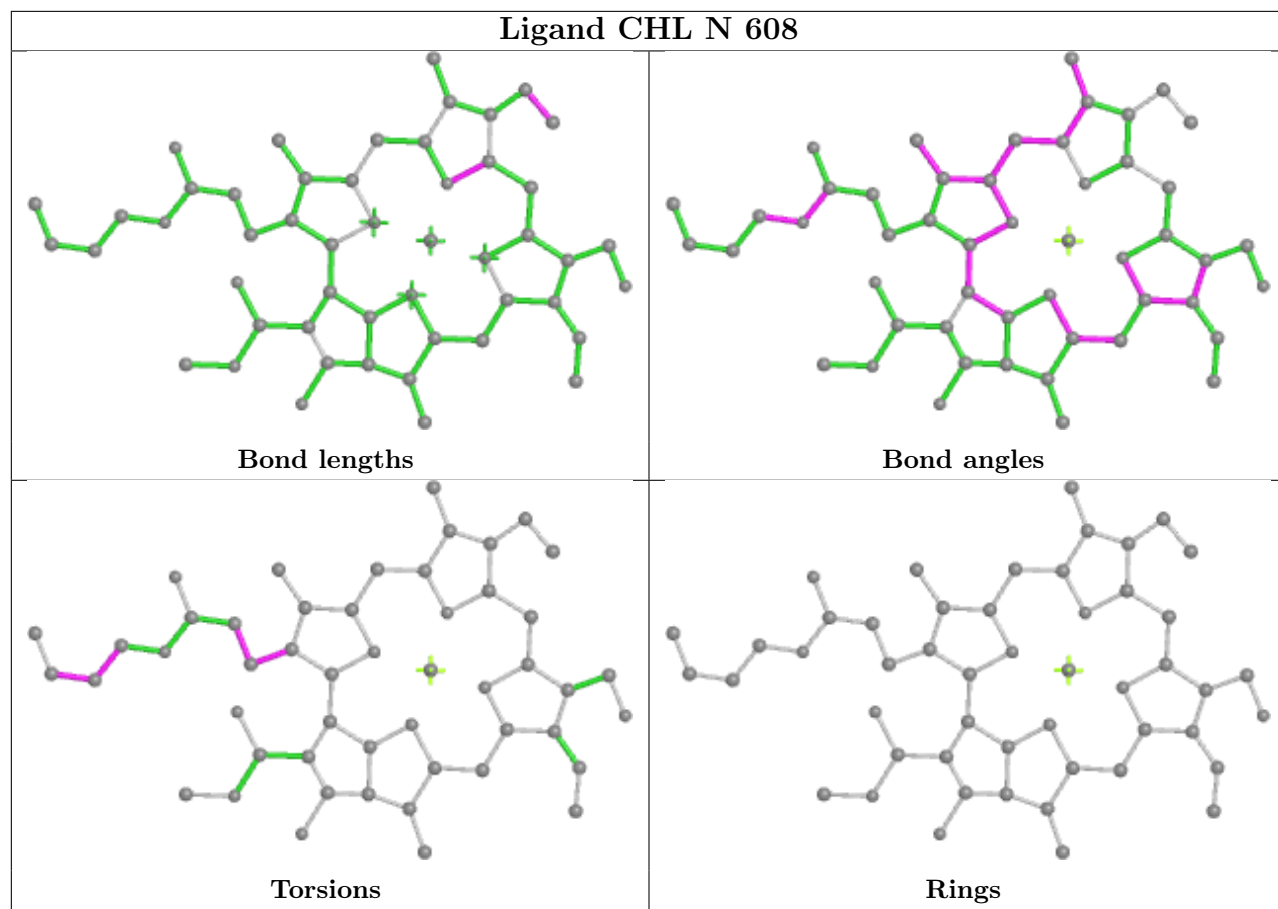




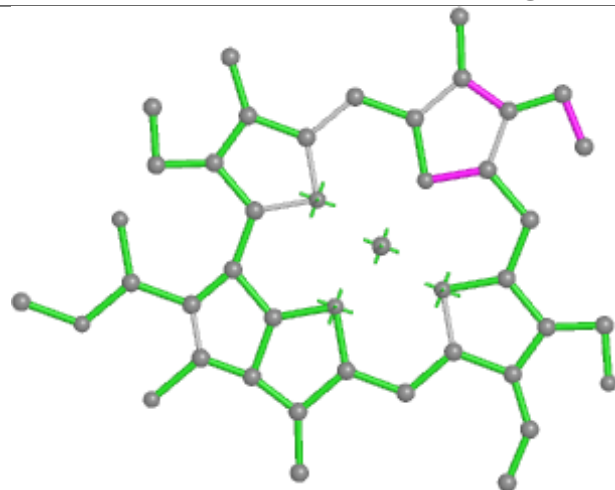




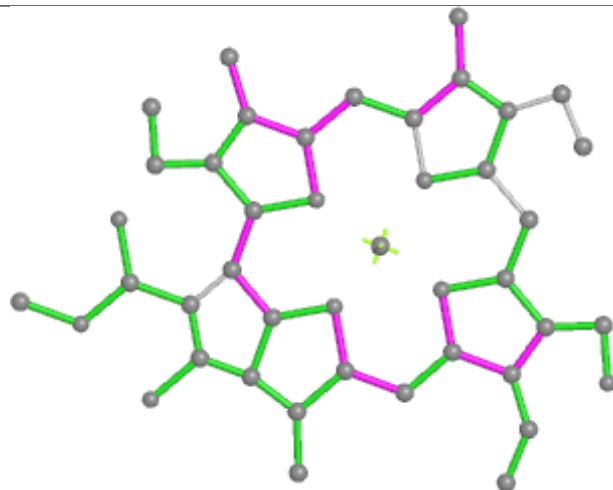




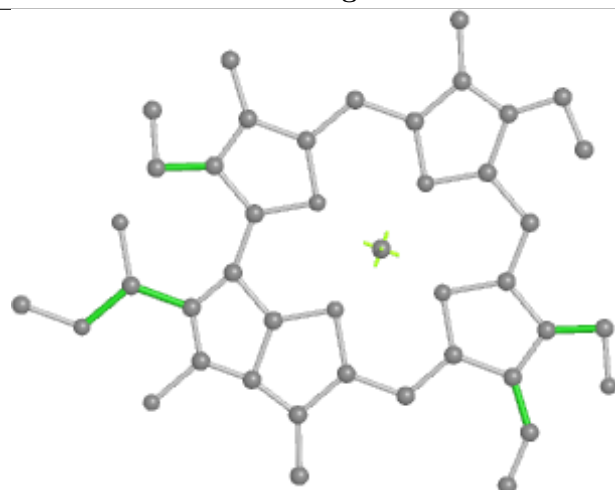
Ligand CHL s 607



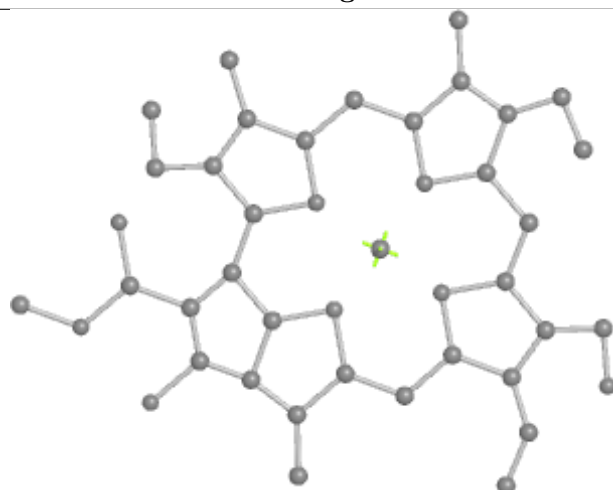
Bond lengths



Bond angles

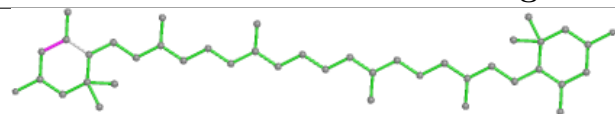


Torsions

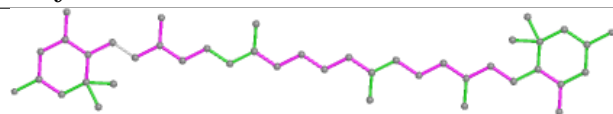


Rings

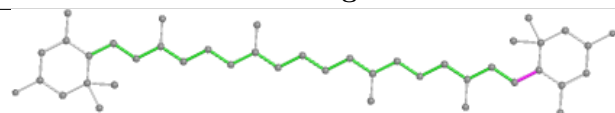
Ligand LUT y 620



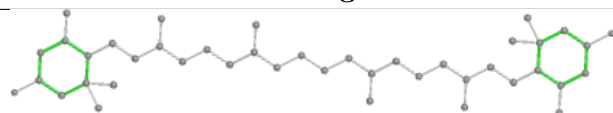
Bond lengths



Bond angles

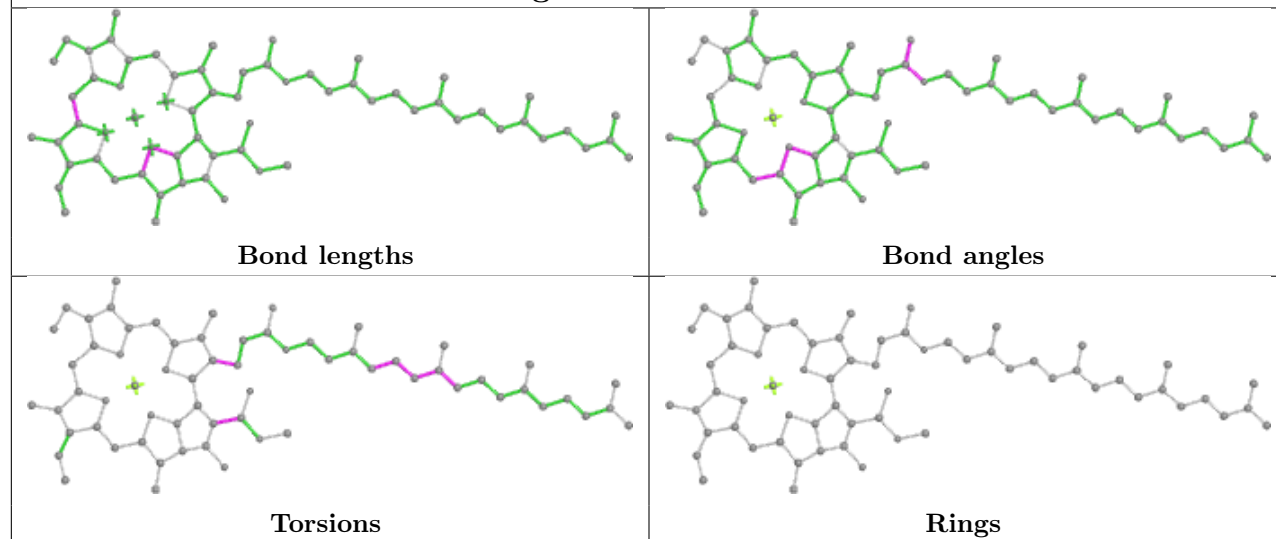


Torsions

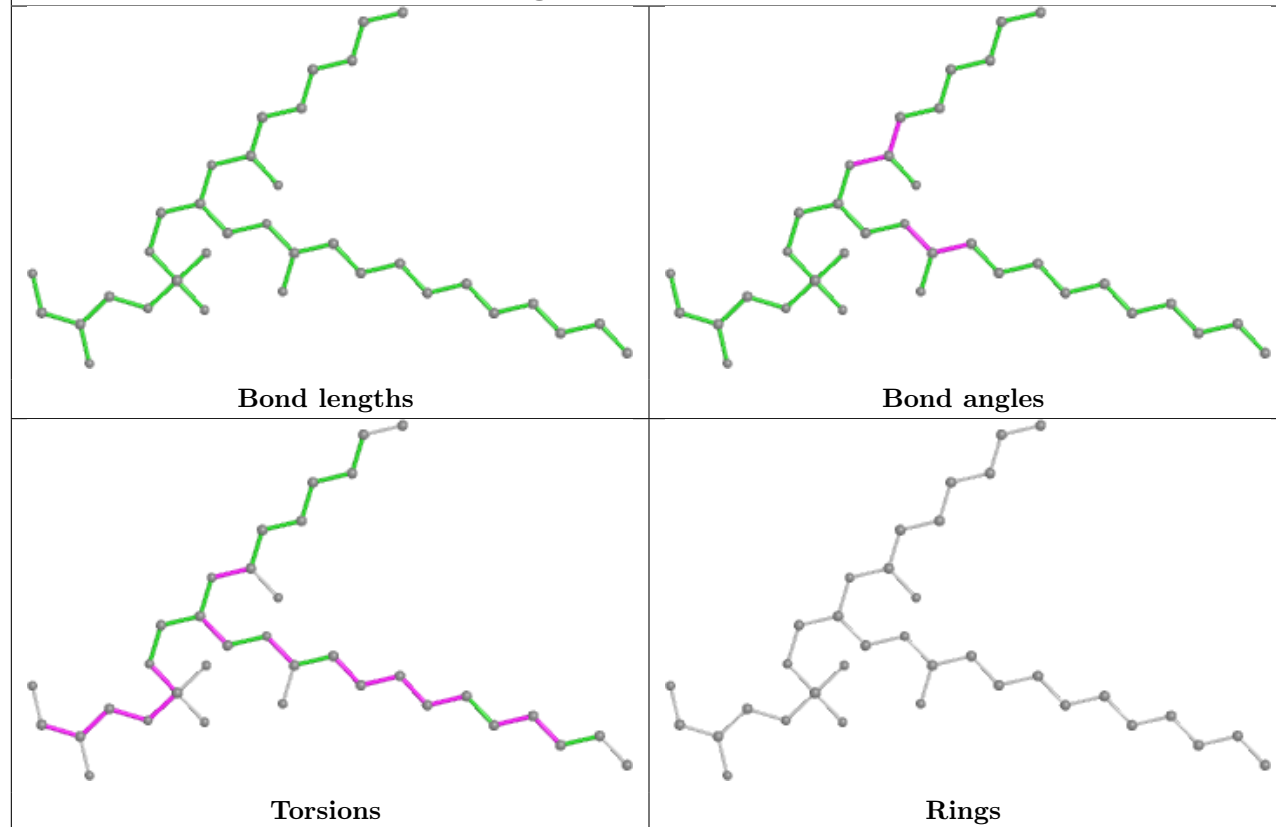


Rings

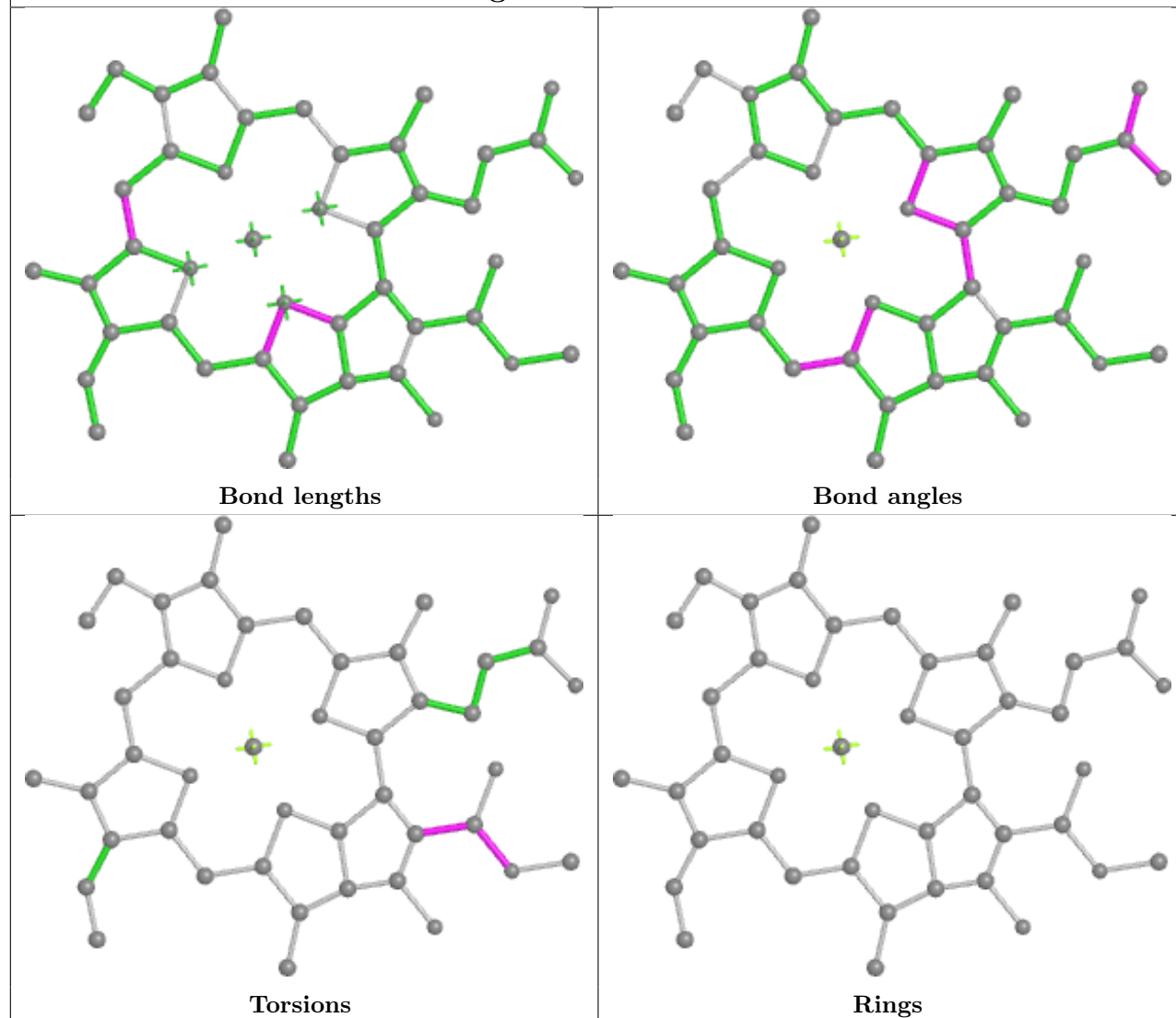
Ligand CLA C 506



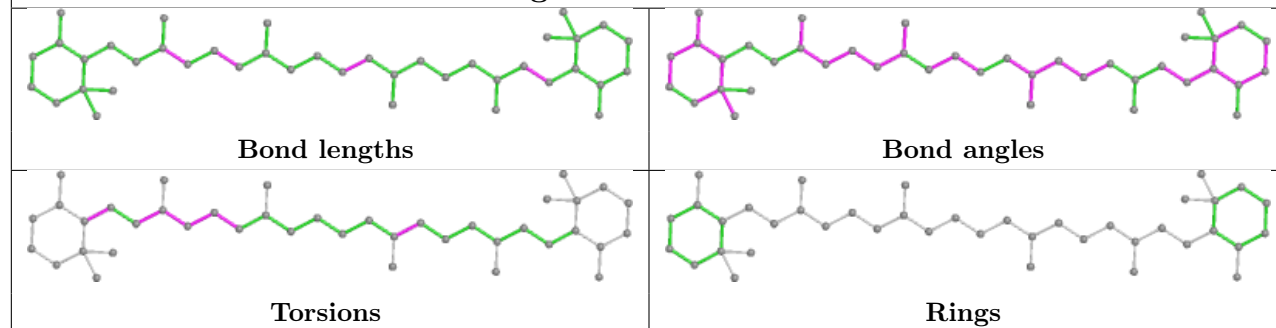
Ligand LHG C 525

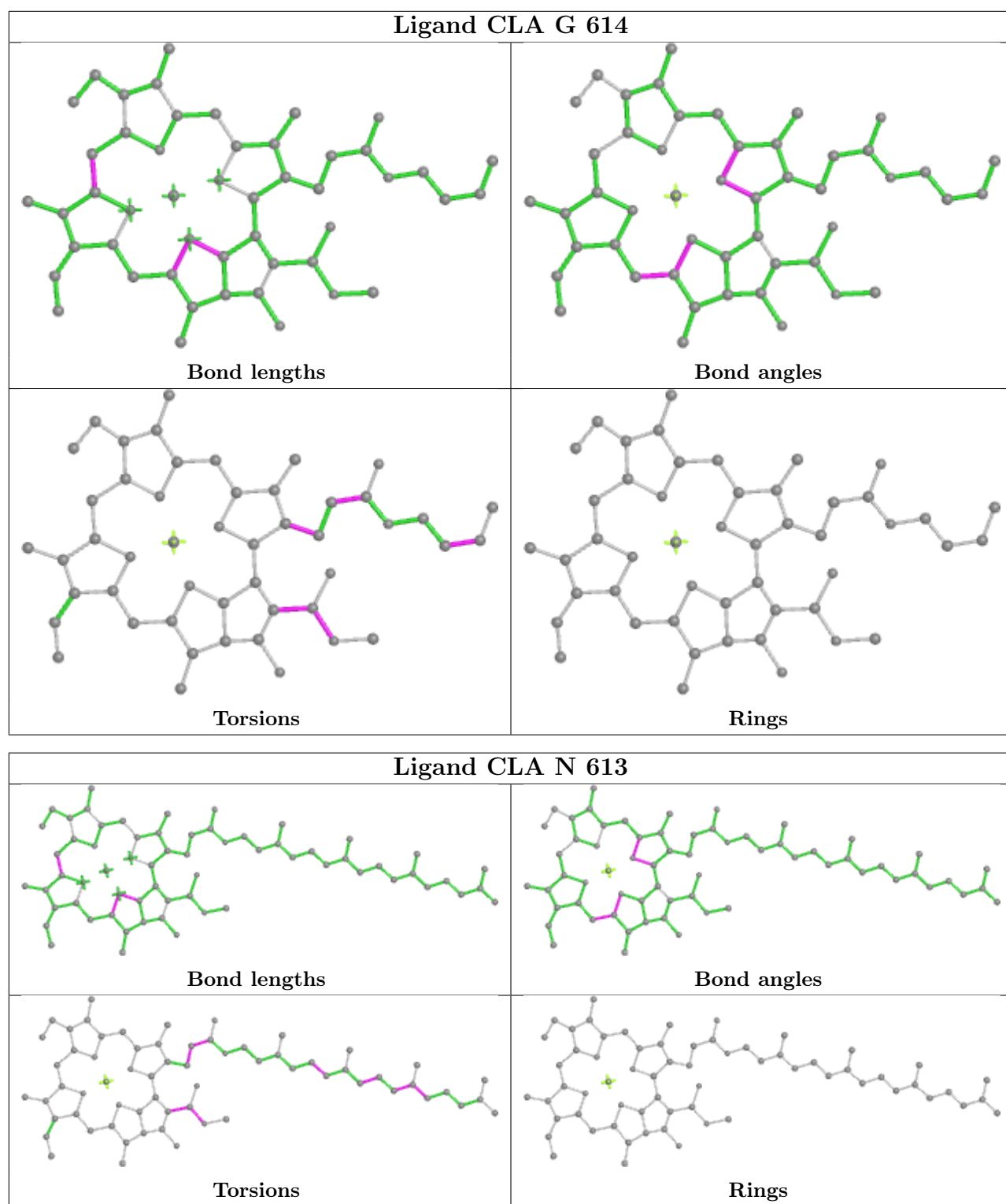


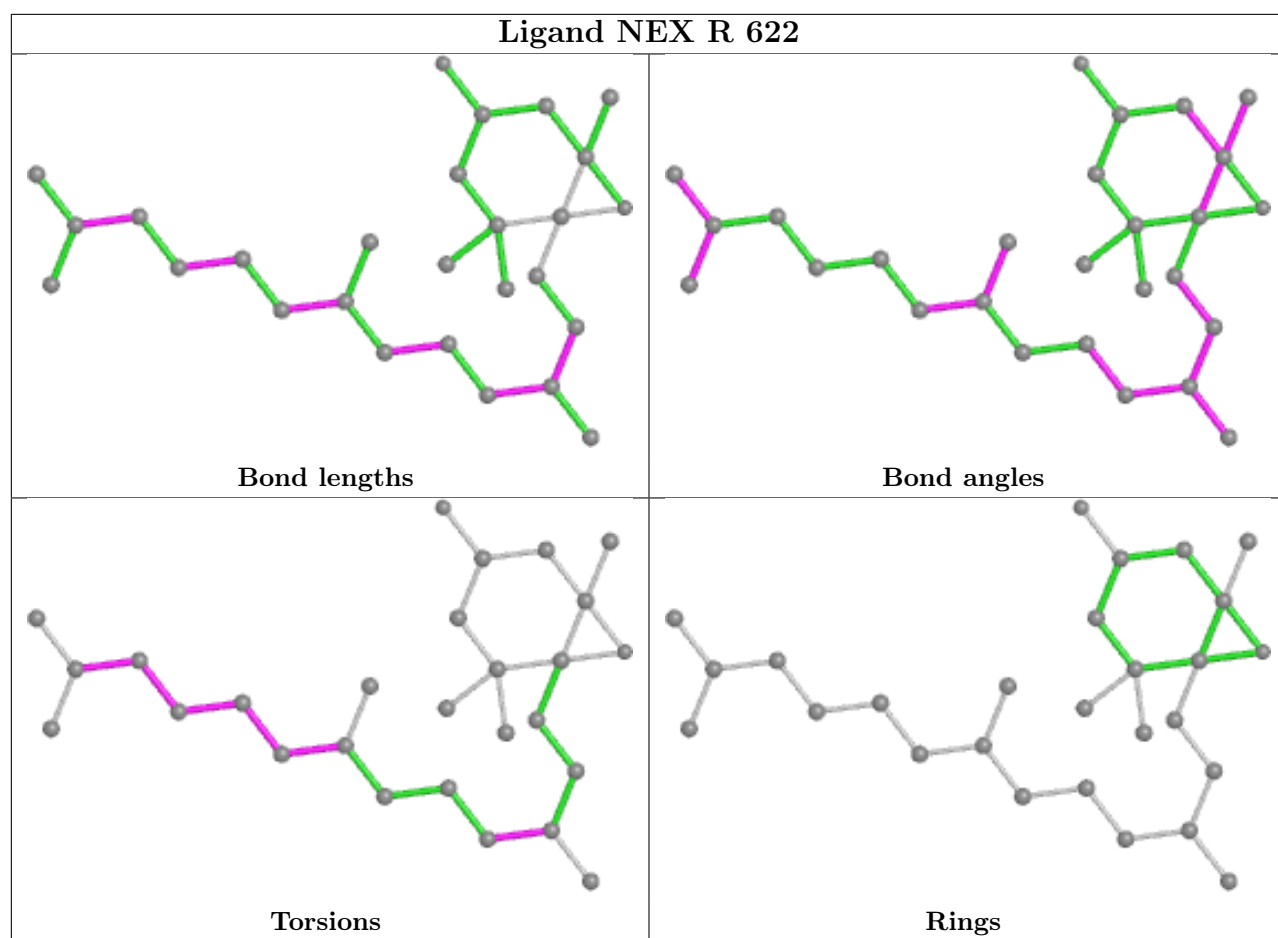
Ligand CLA N 612



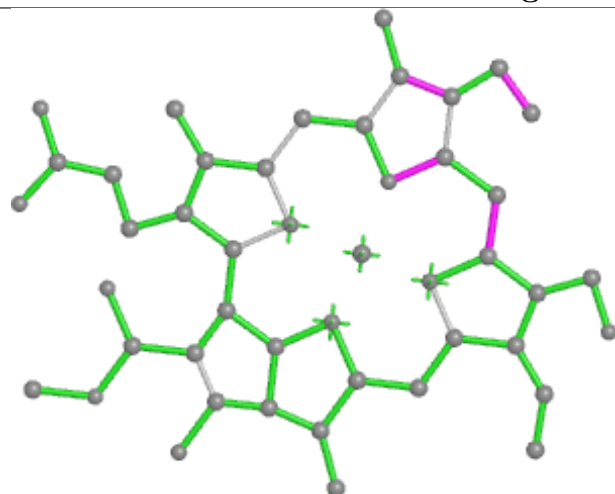
Ligand BCR C 517



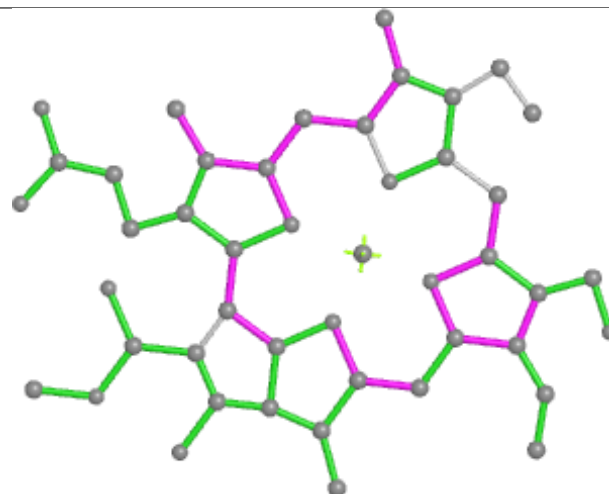




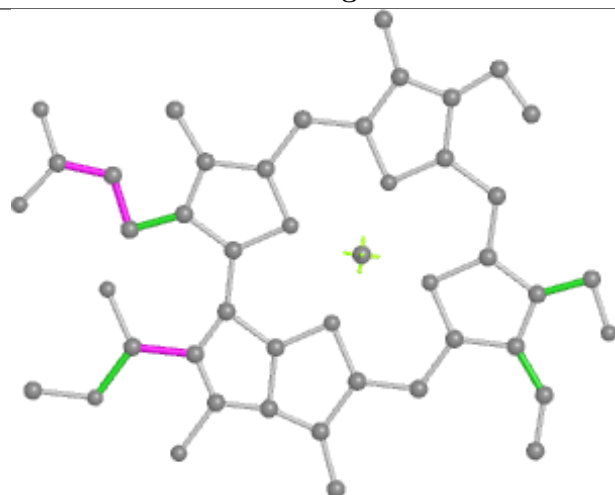
Ligand CHL s 601



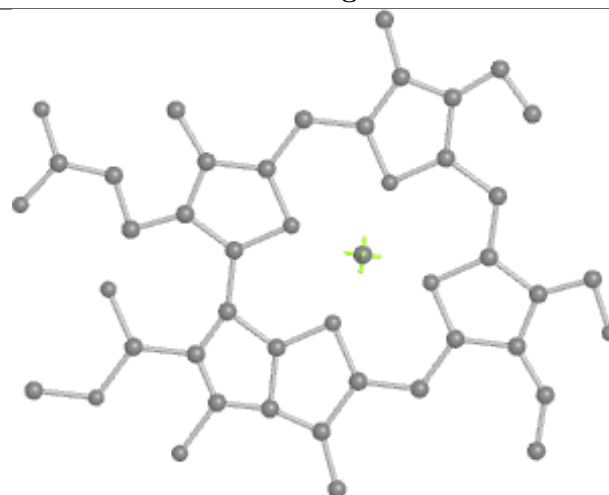
Bond lengths



Bond angles

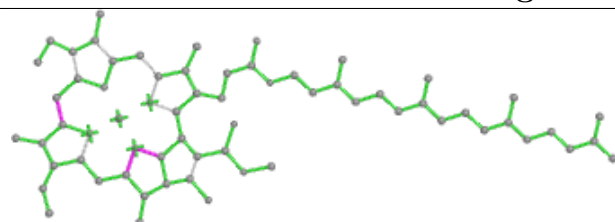


Torsions

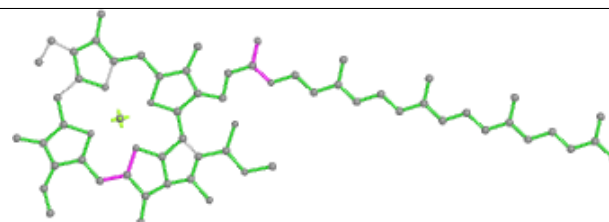


Rings

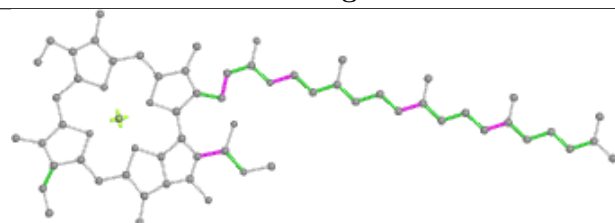
Ligand CLA B 609



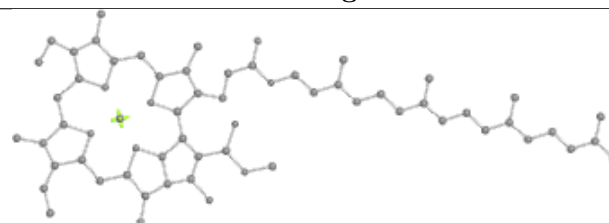
Bond lengths



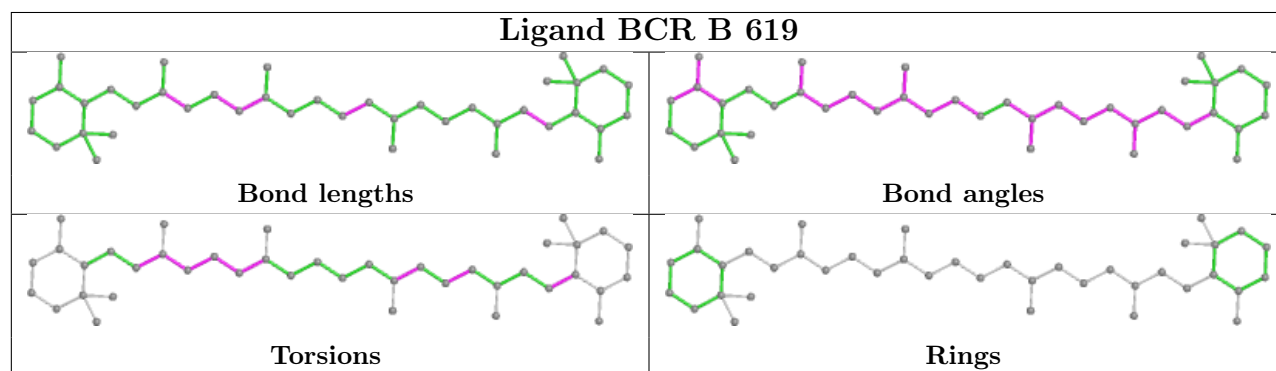
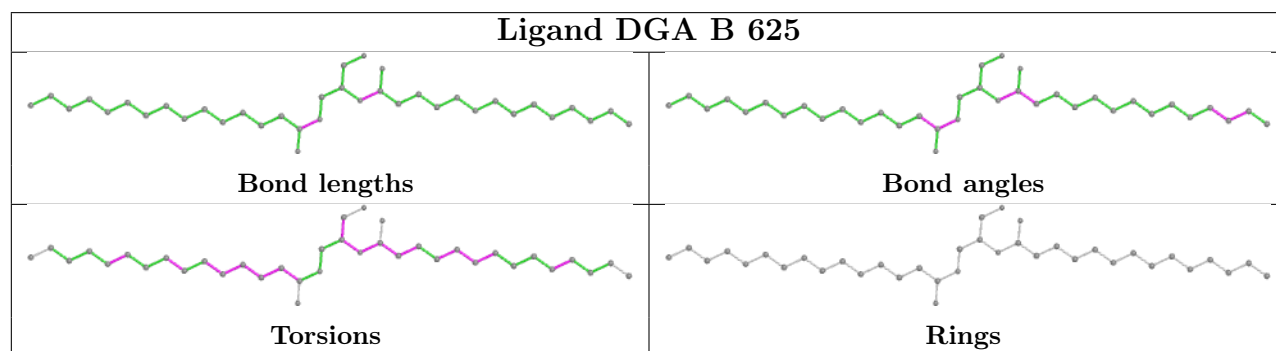
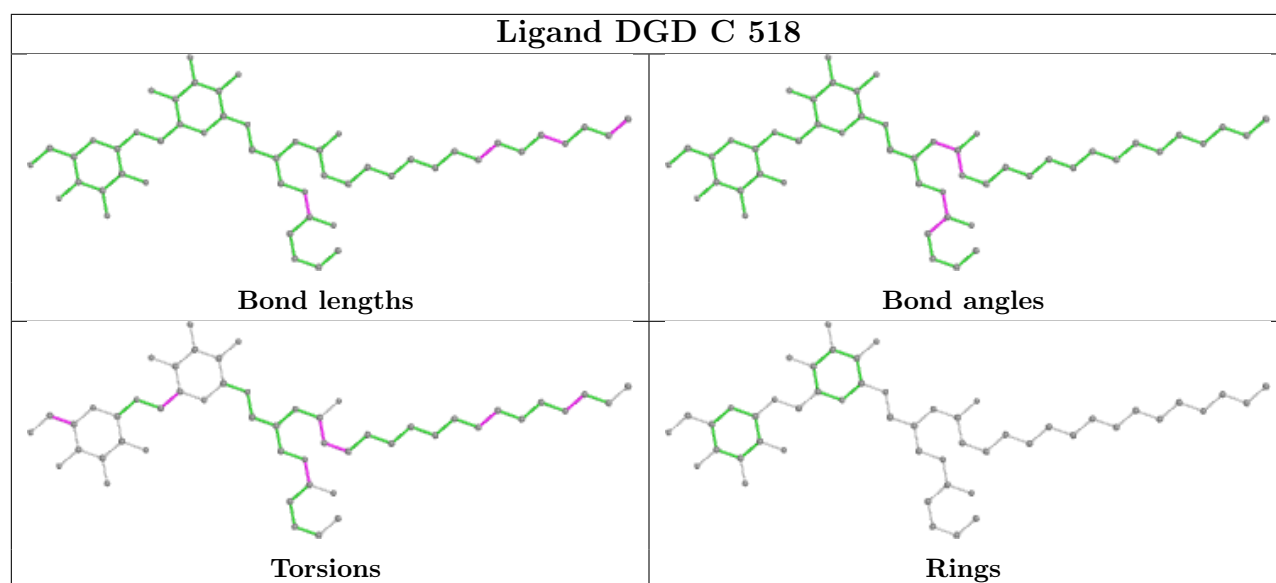
Bond angles

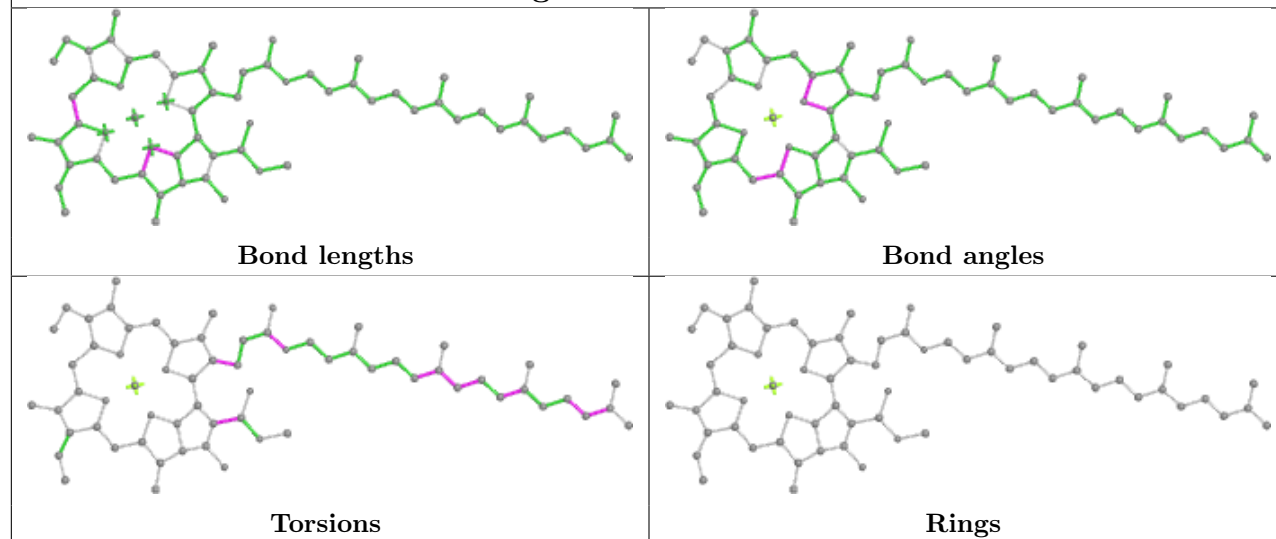
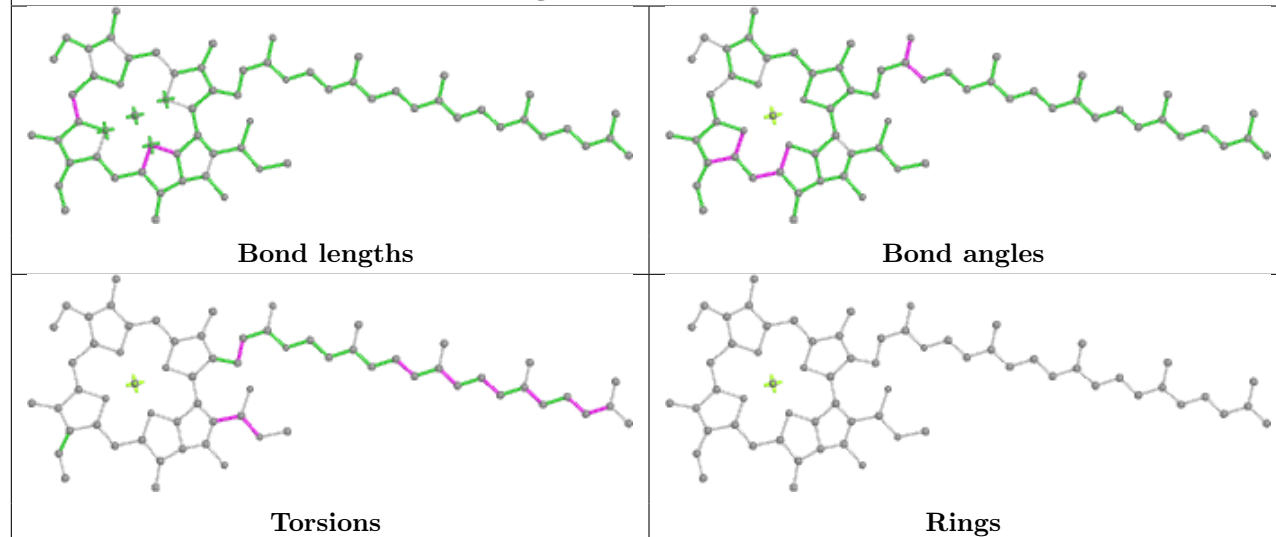


Torsions

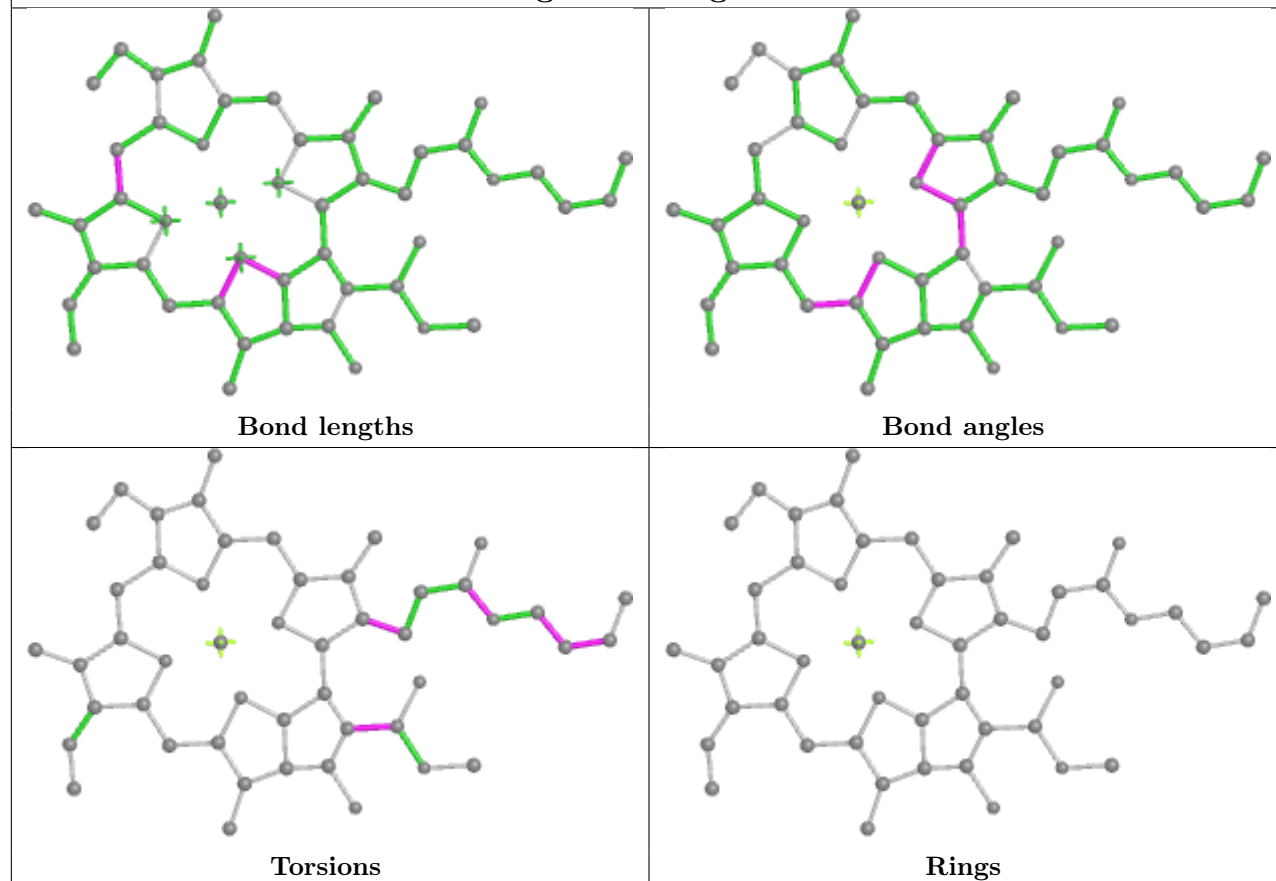


Rings

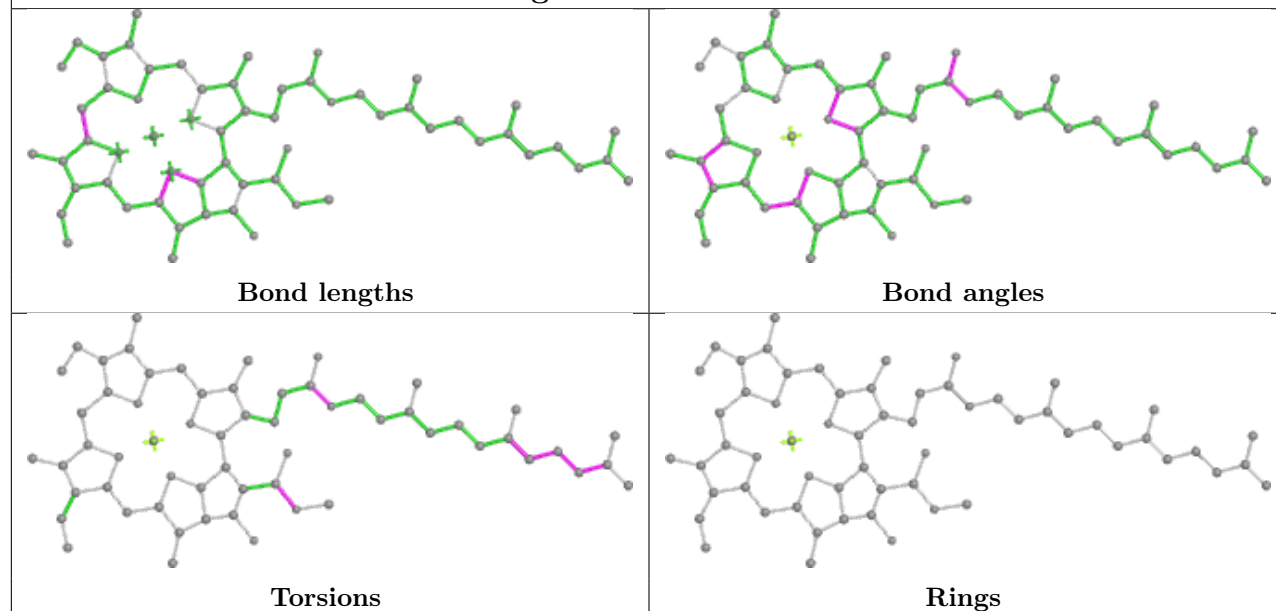


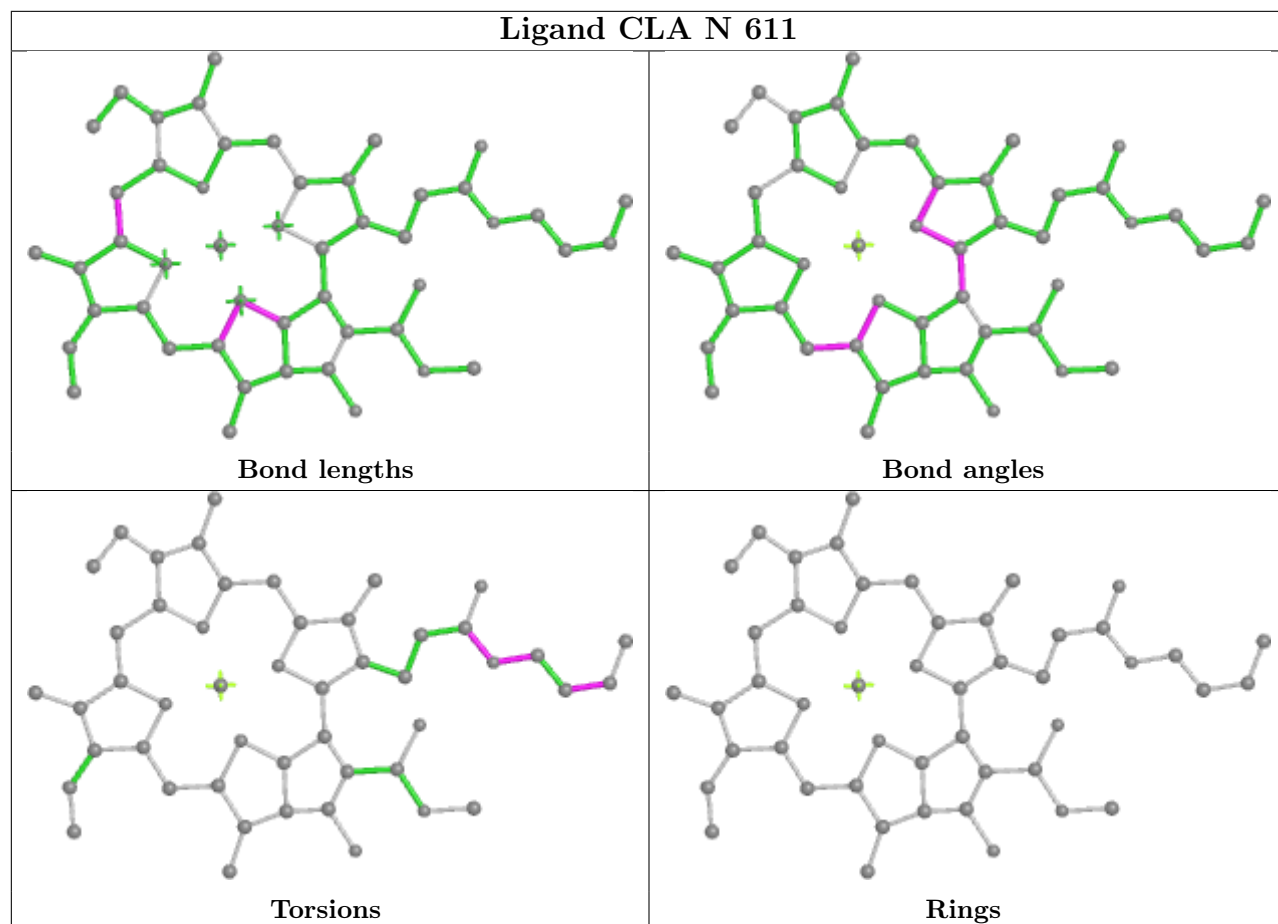
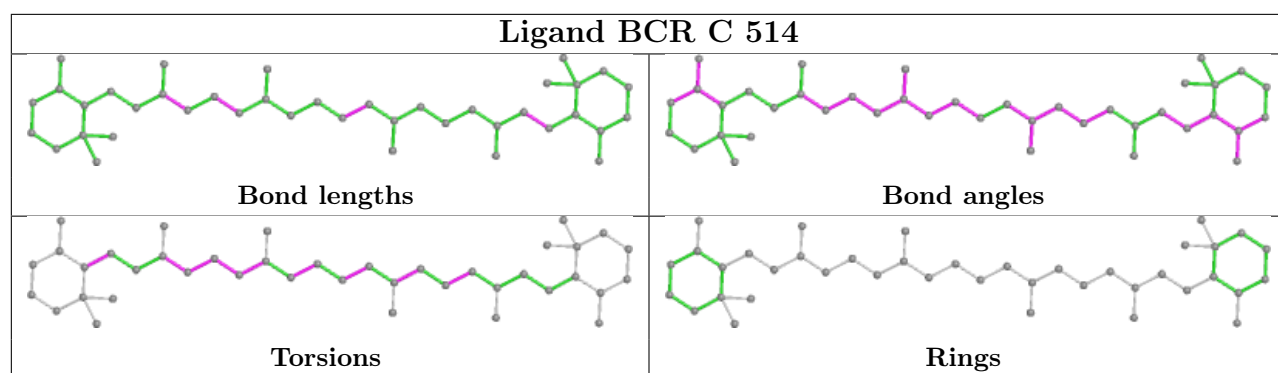
Ligand CLA C 513**Ligand CLA C 503**

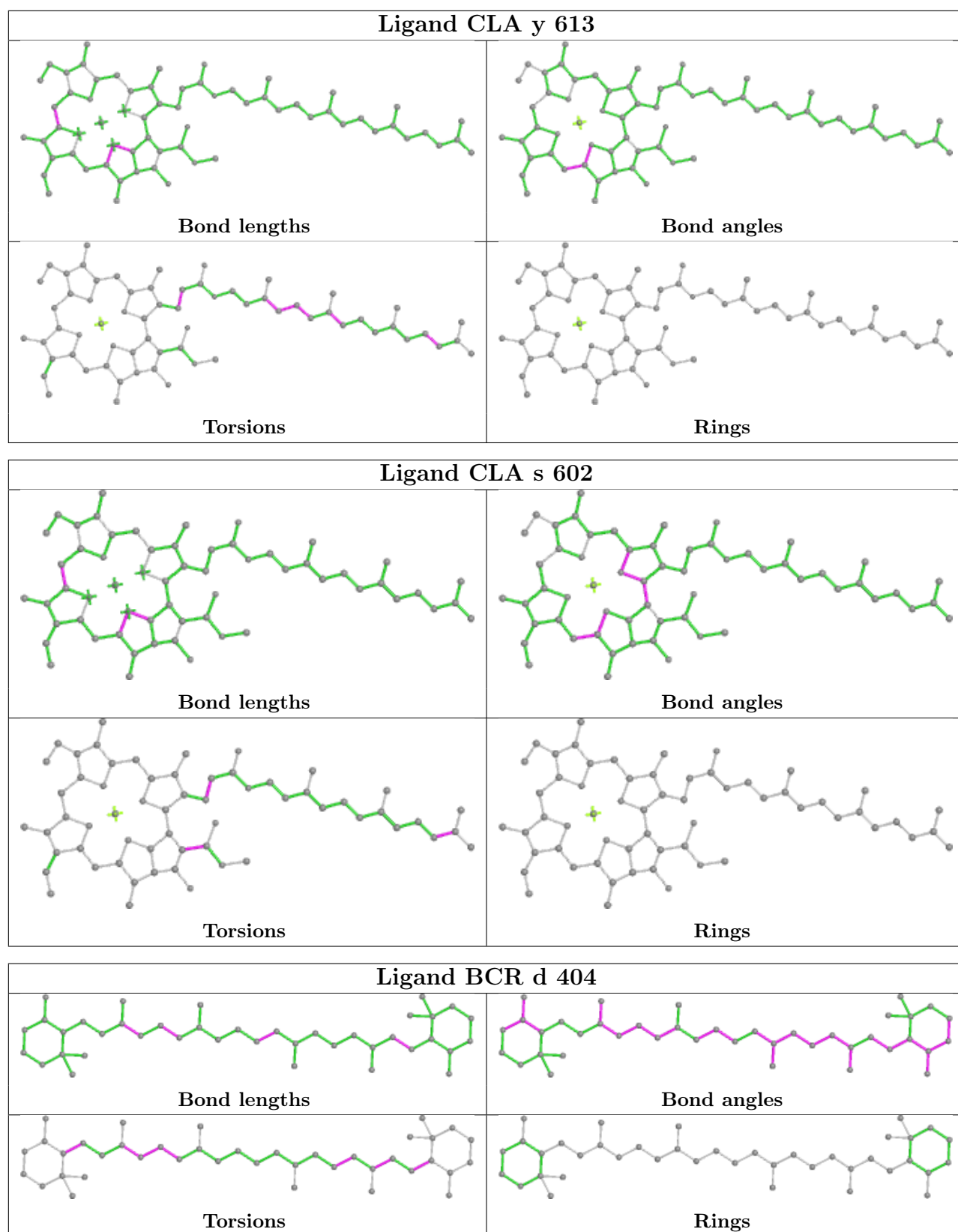
Ligand CLA g 604

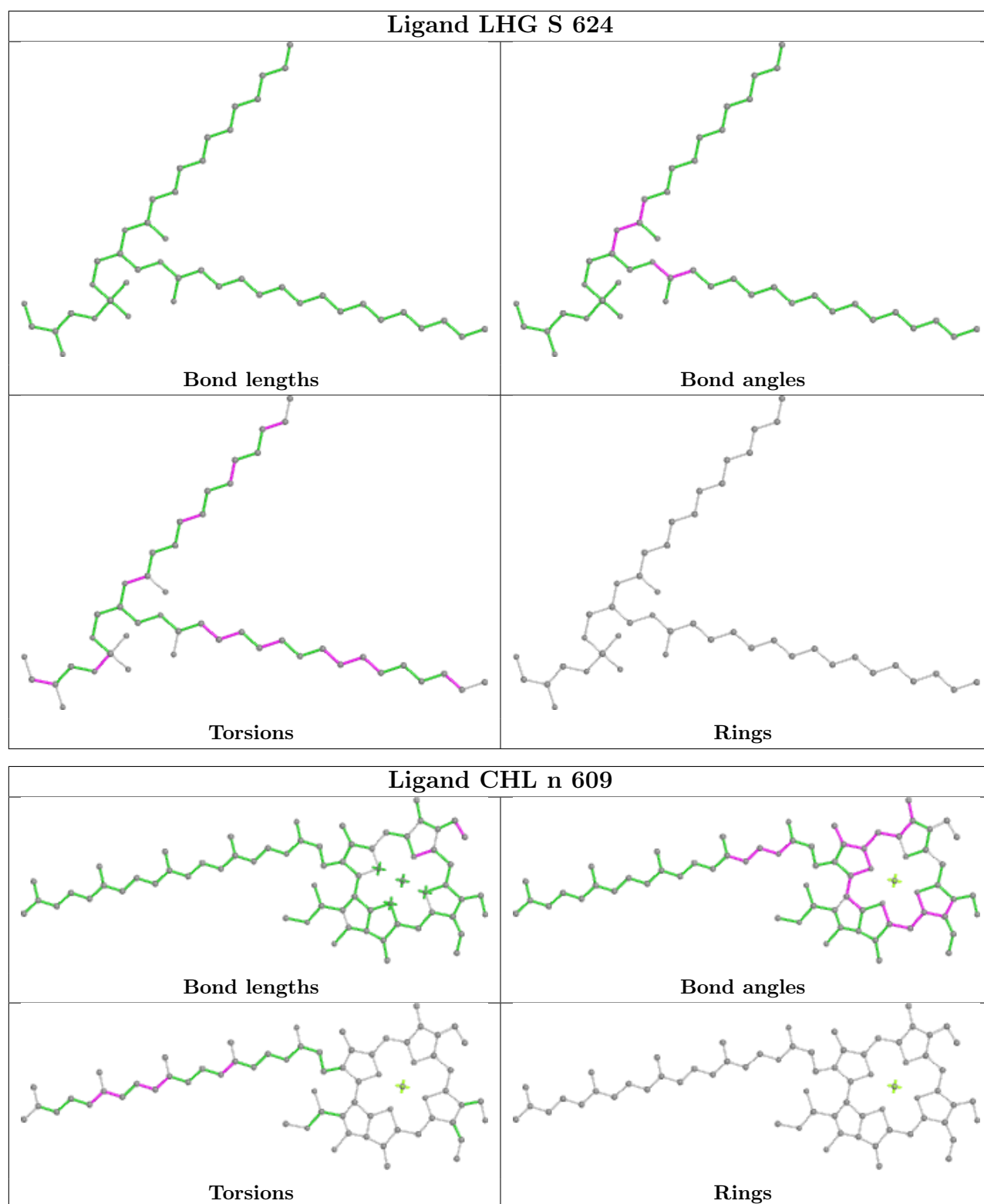


Ligand CLA D 403

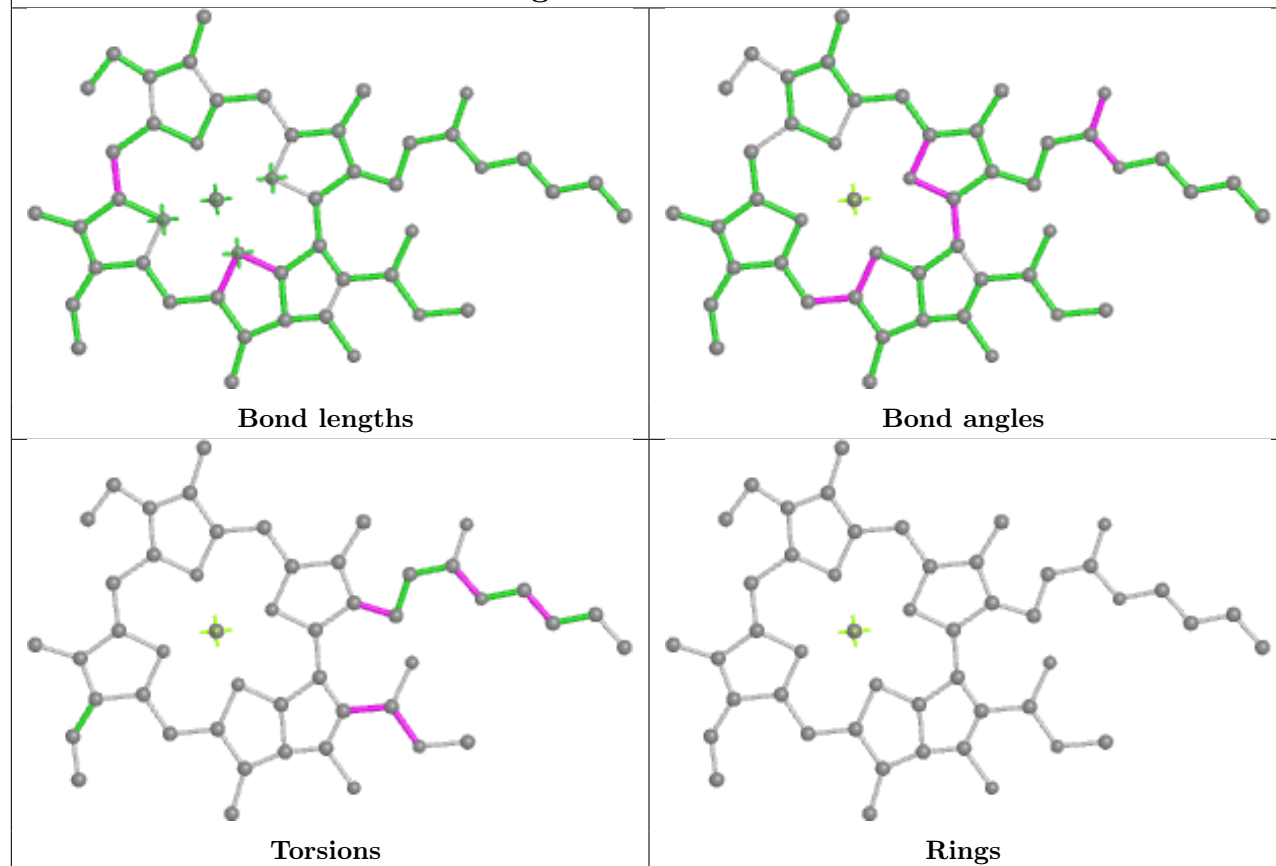




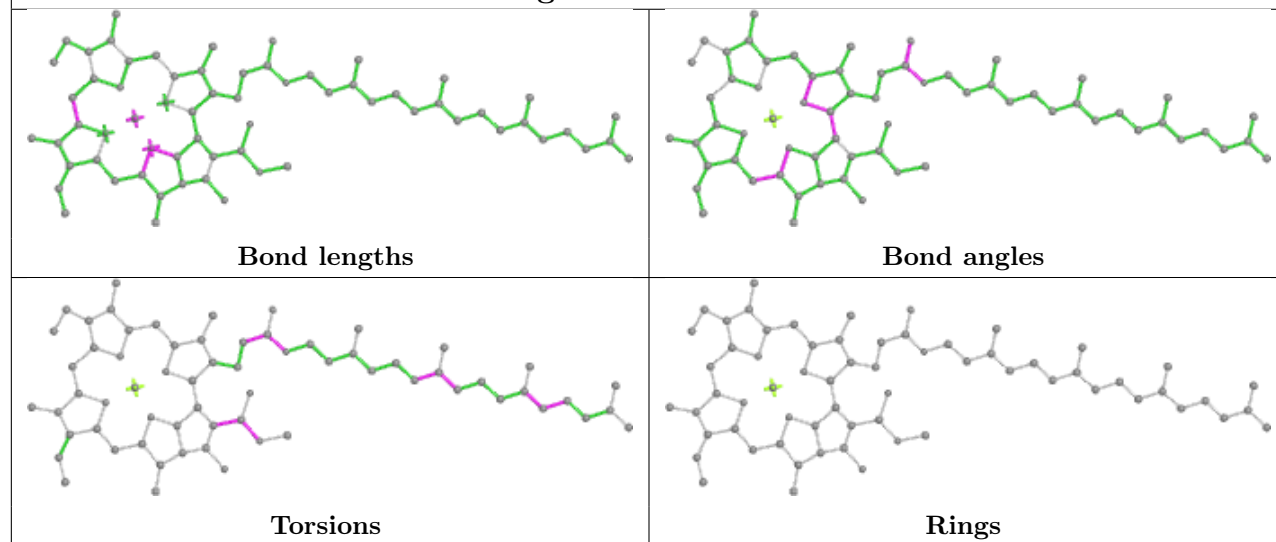


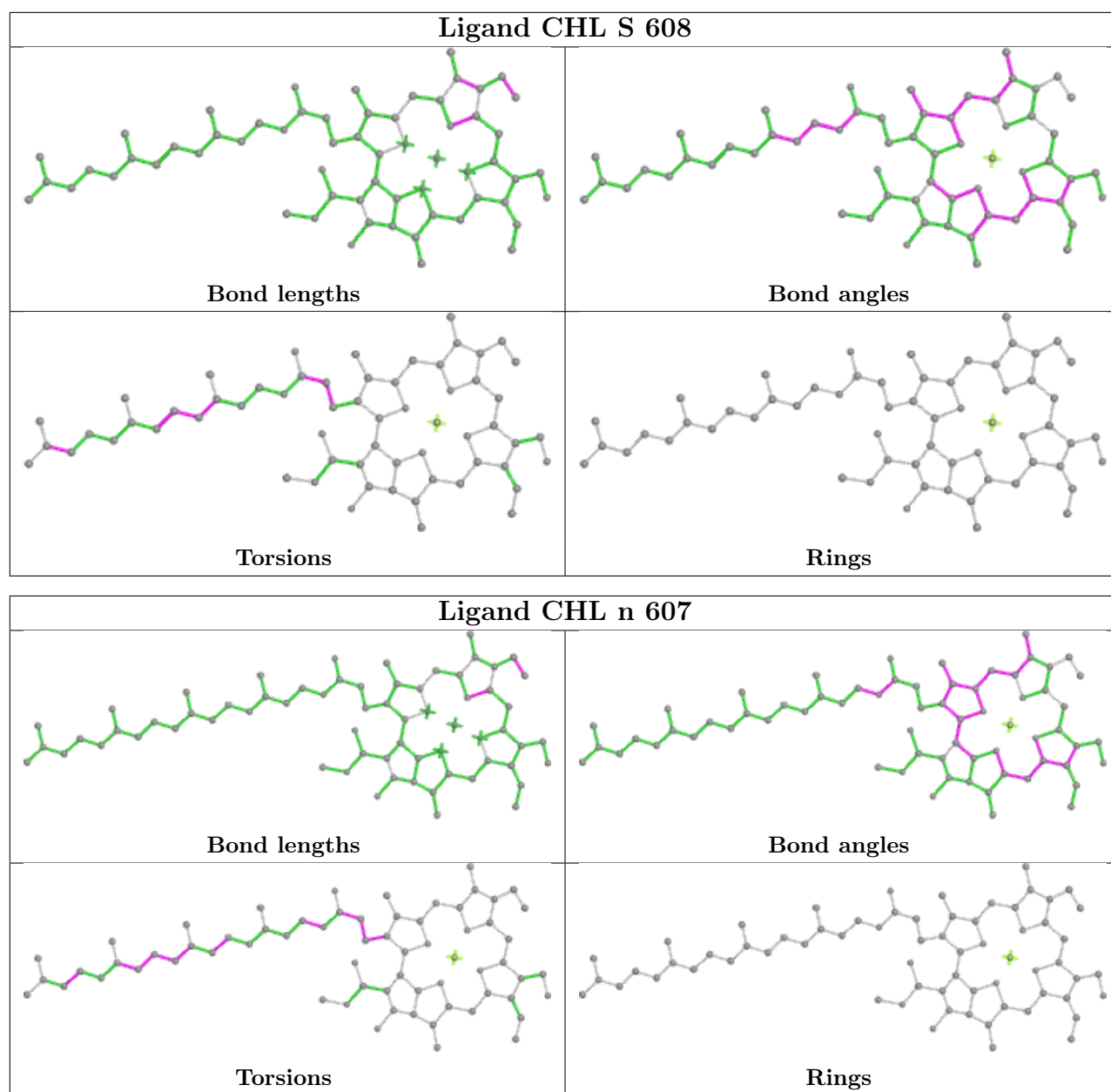


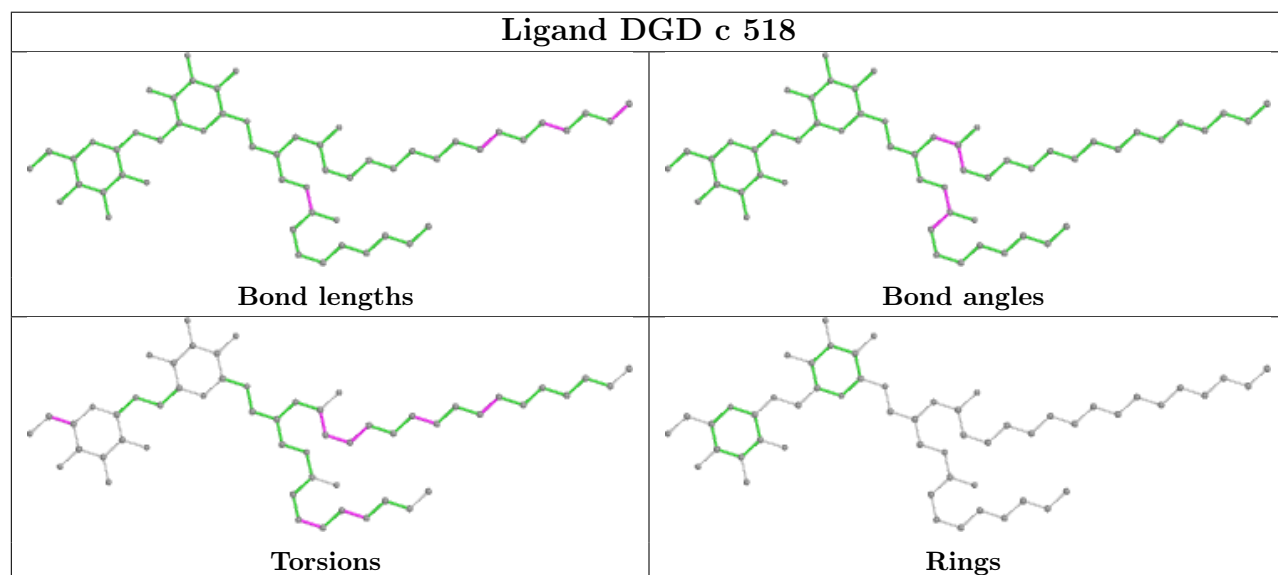
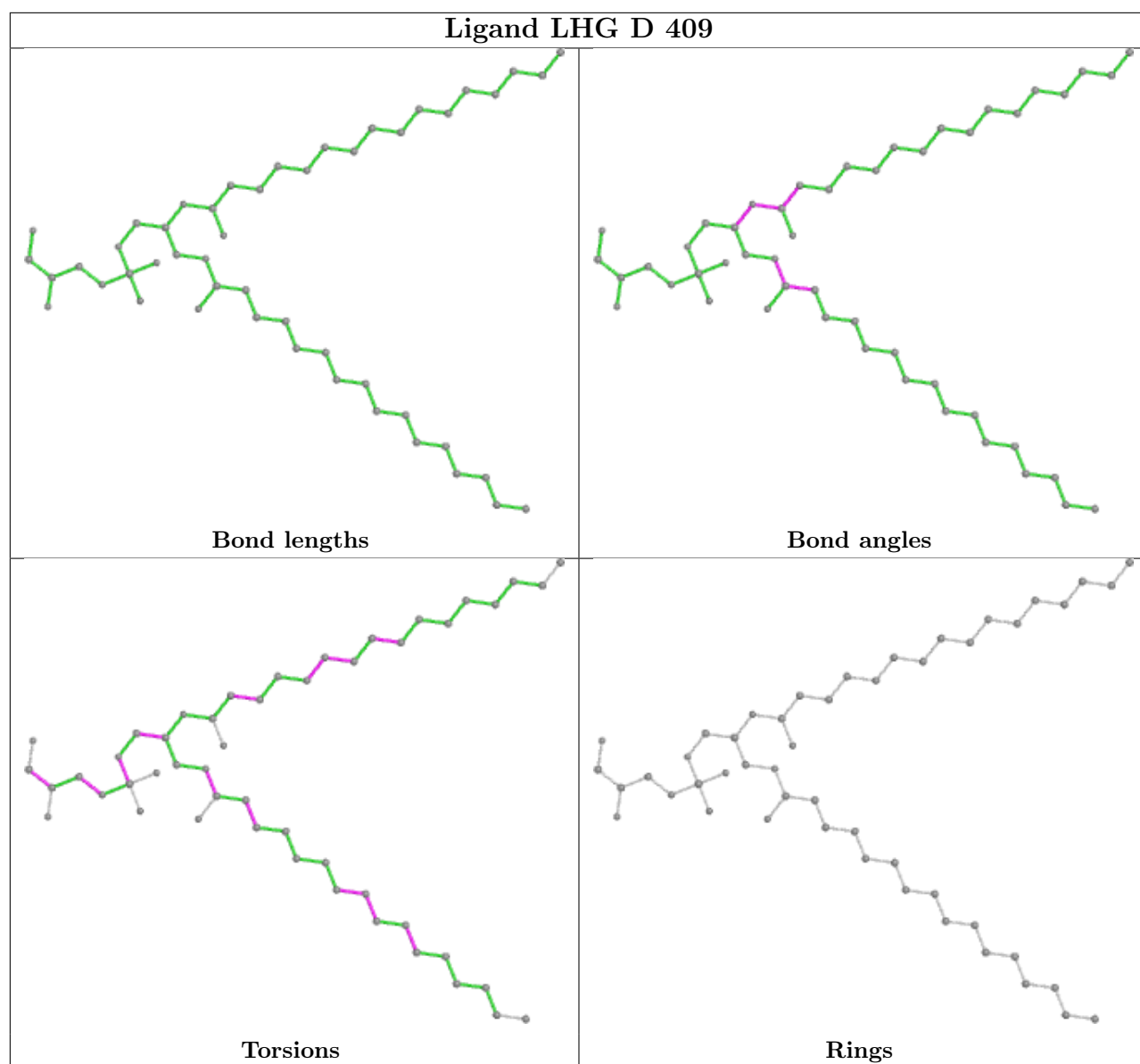
Ligand CLA N 614

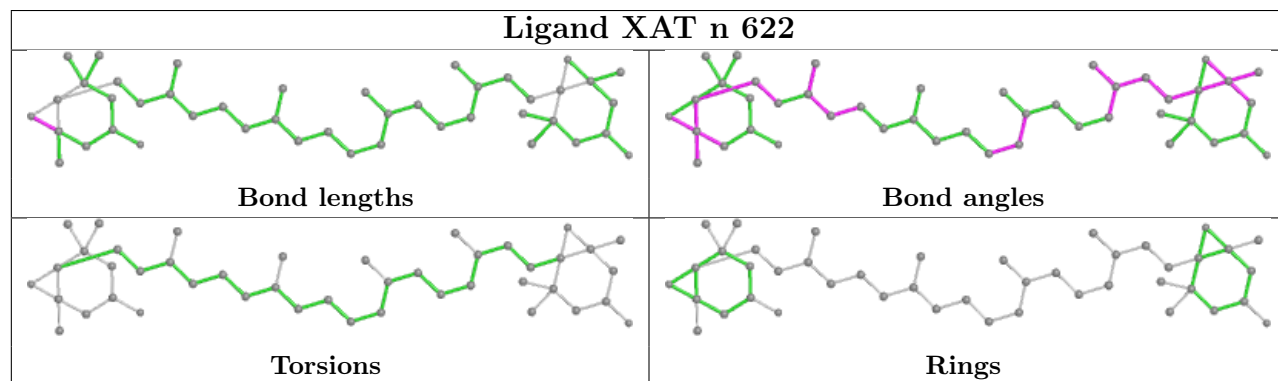
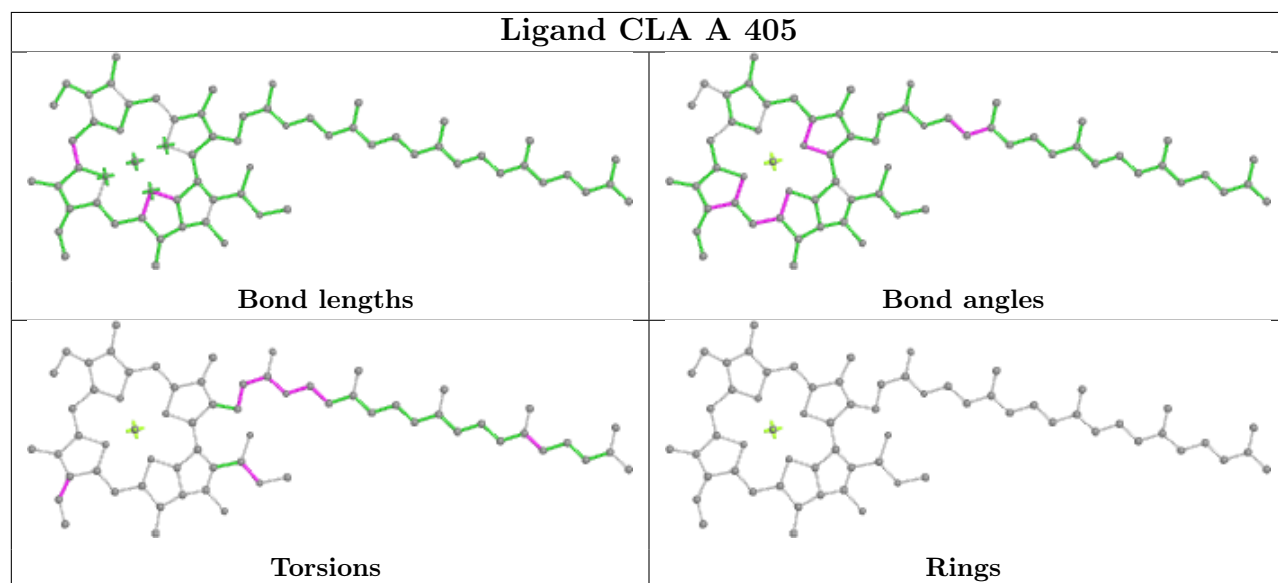
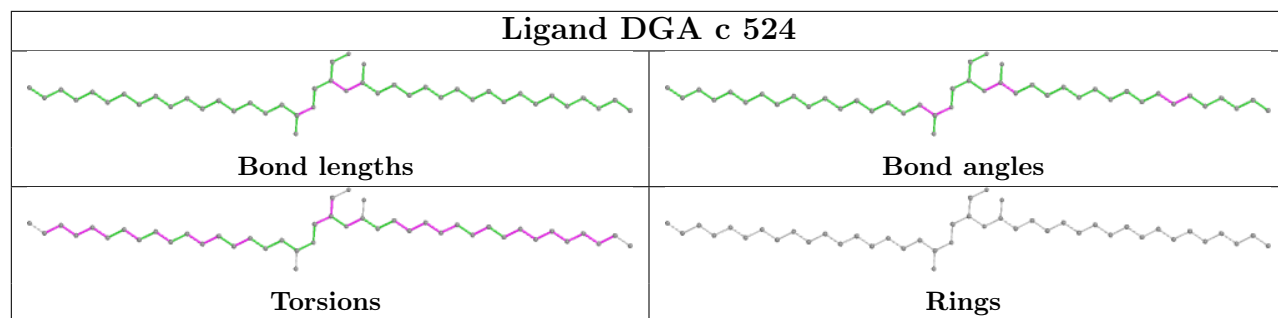


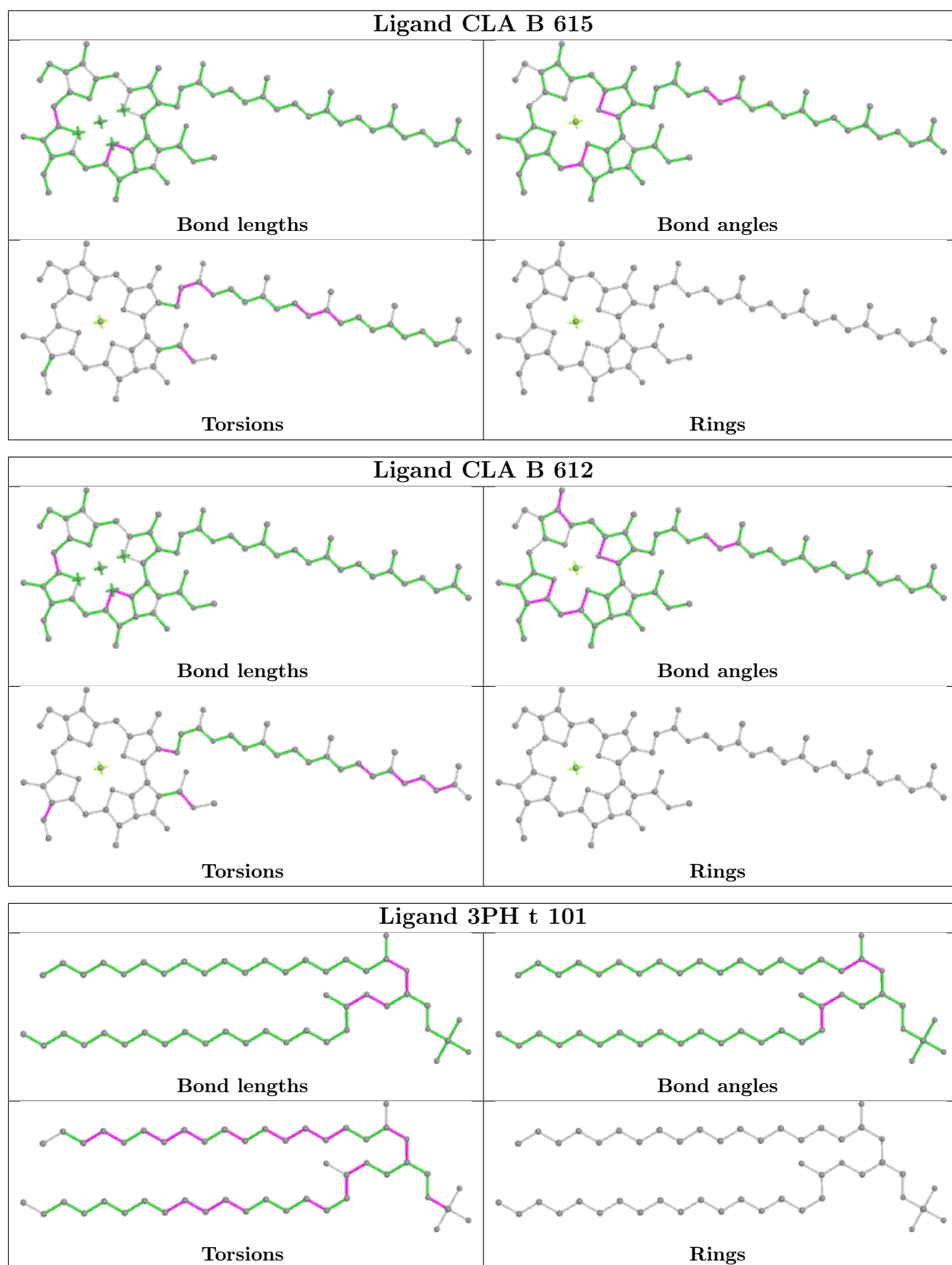
Ligand CLA c 507

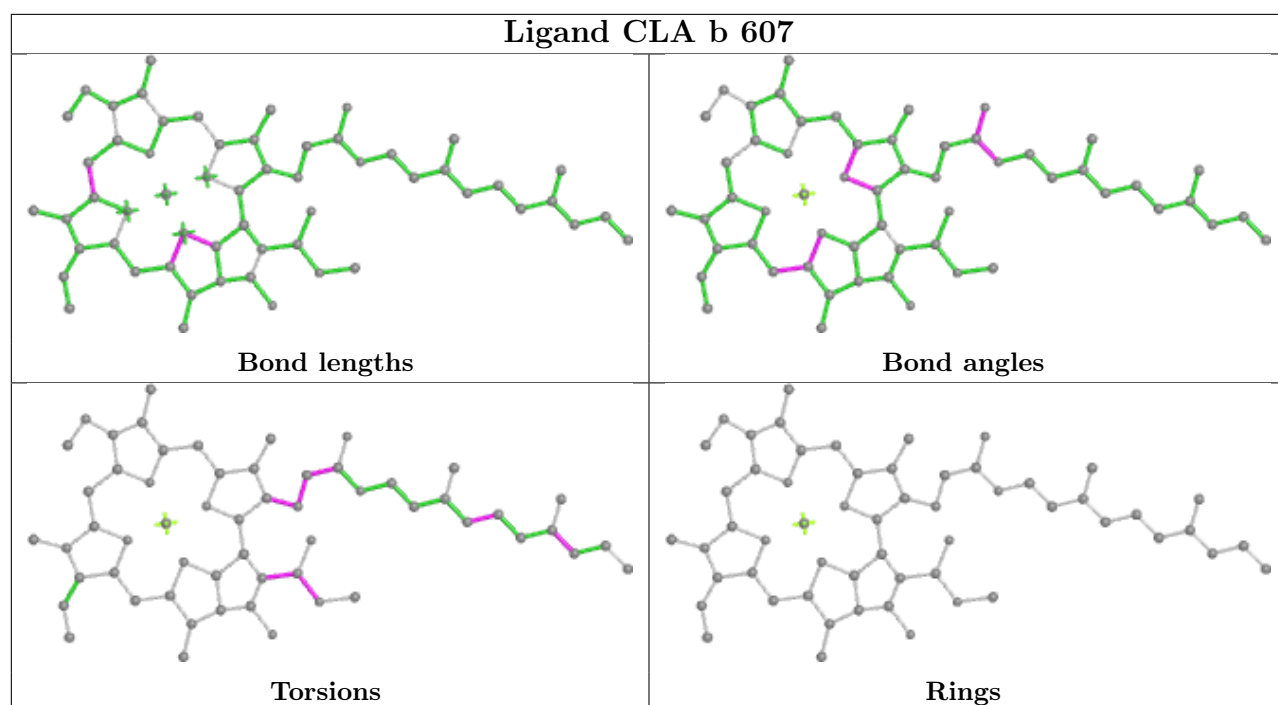




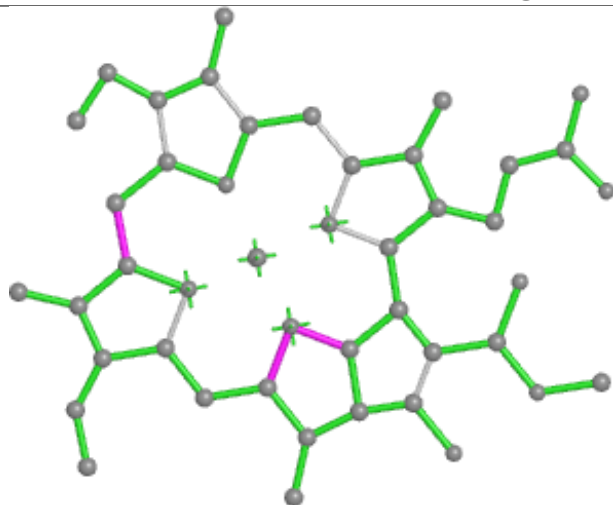




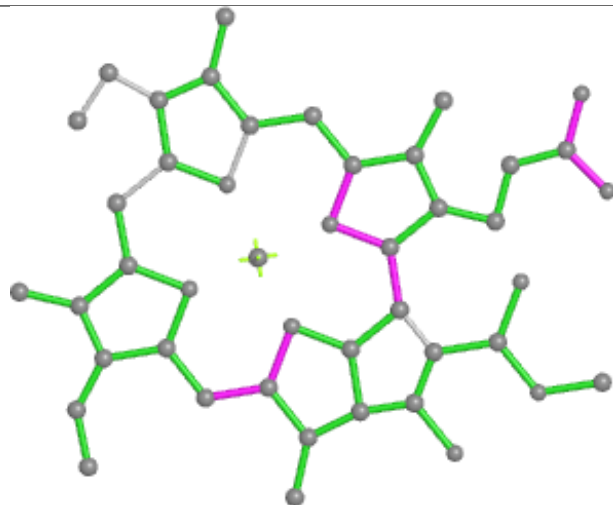




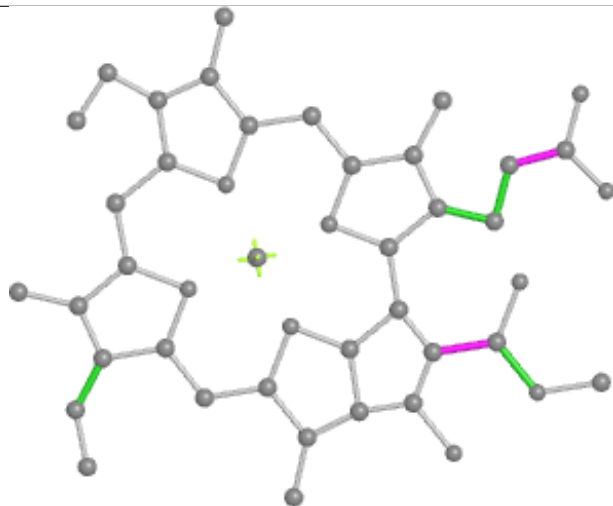
Ligand CLA S 612



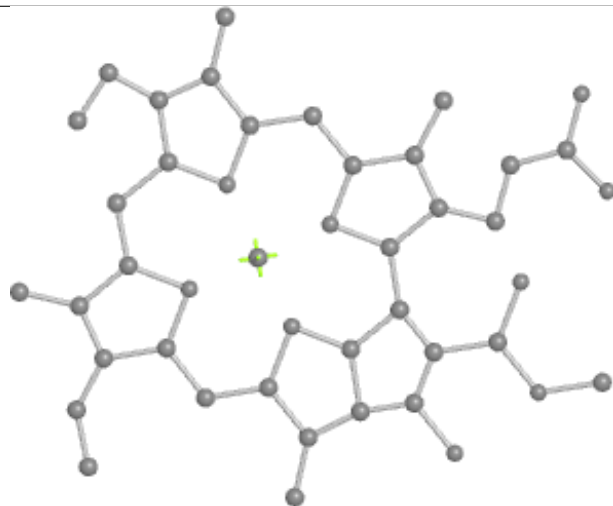
Bond lengths



Bond angles

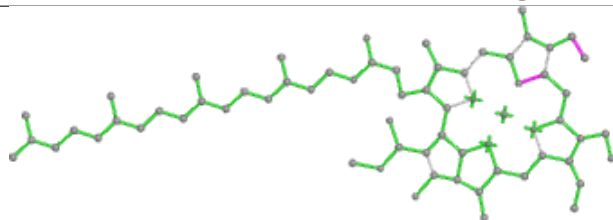


Torsions

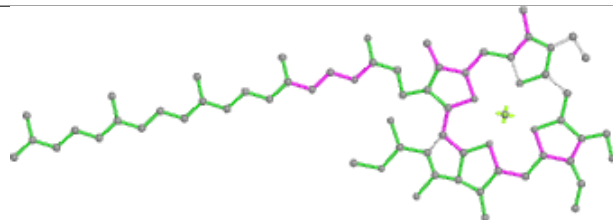


Rings

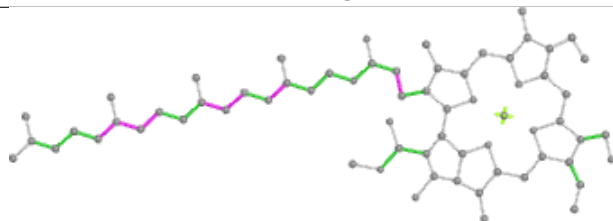
Ligand CHL Y 607



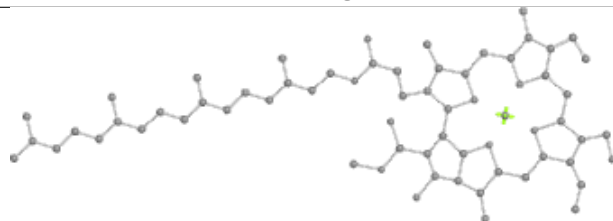
Bond lengths



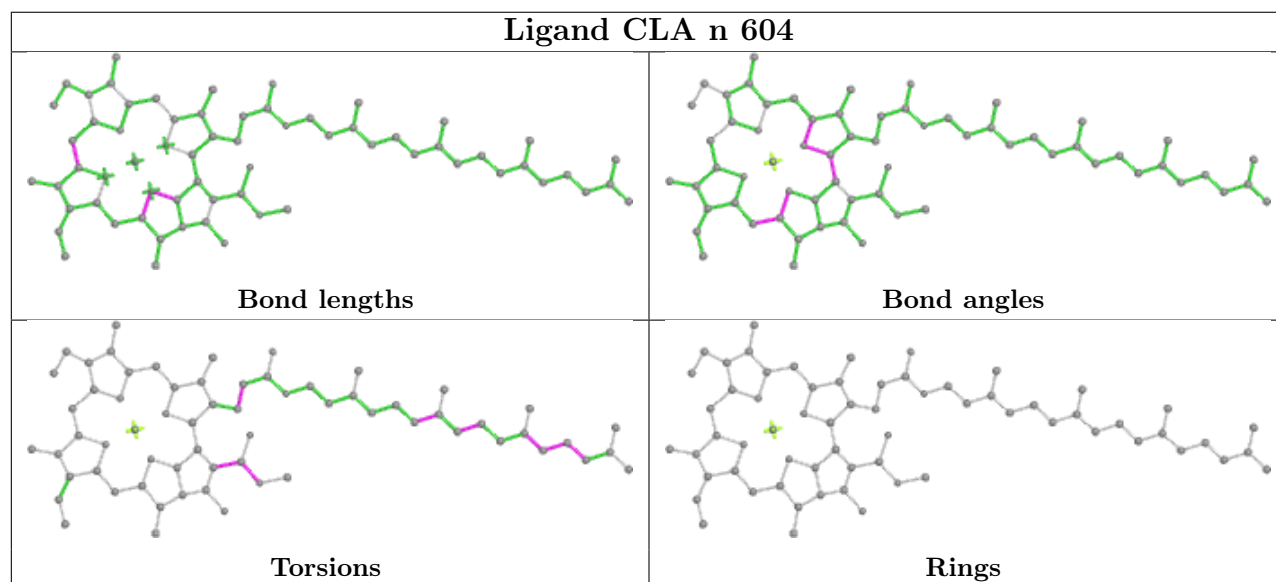
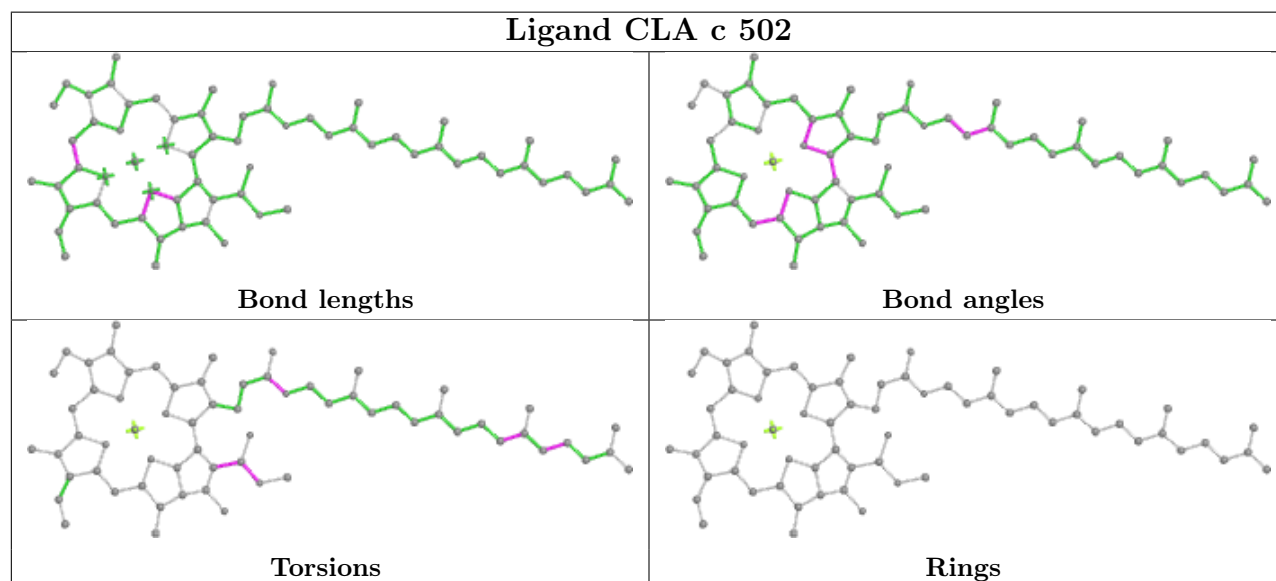
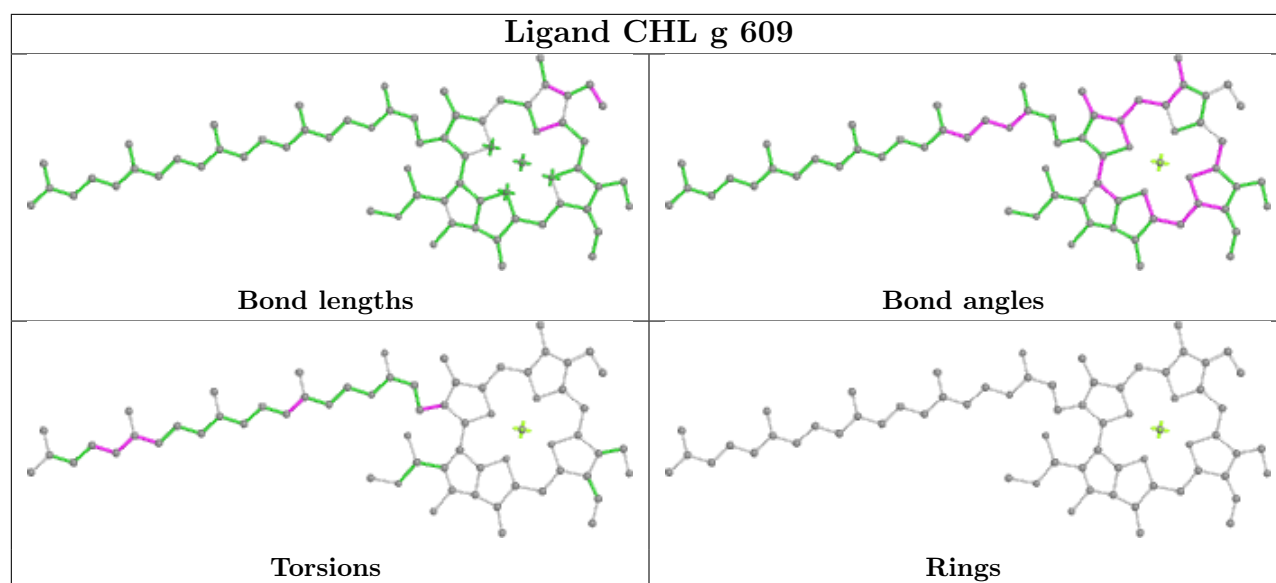
Bond angles

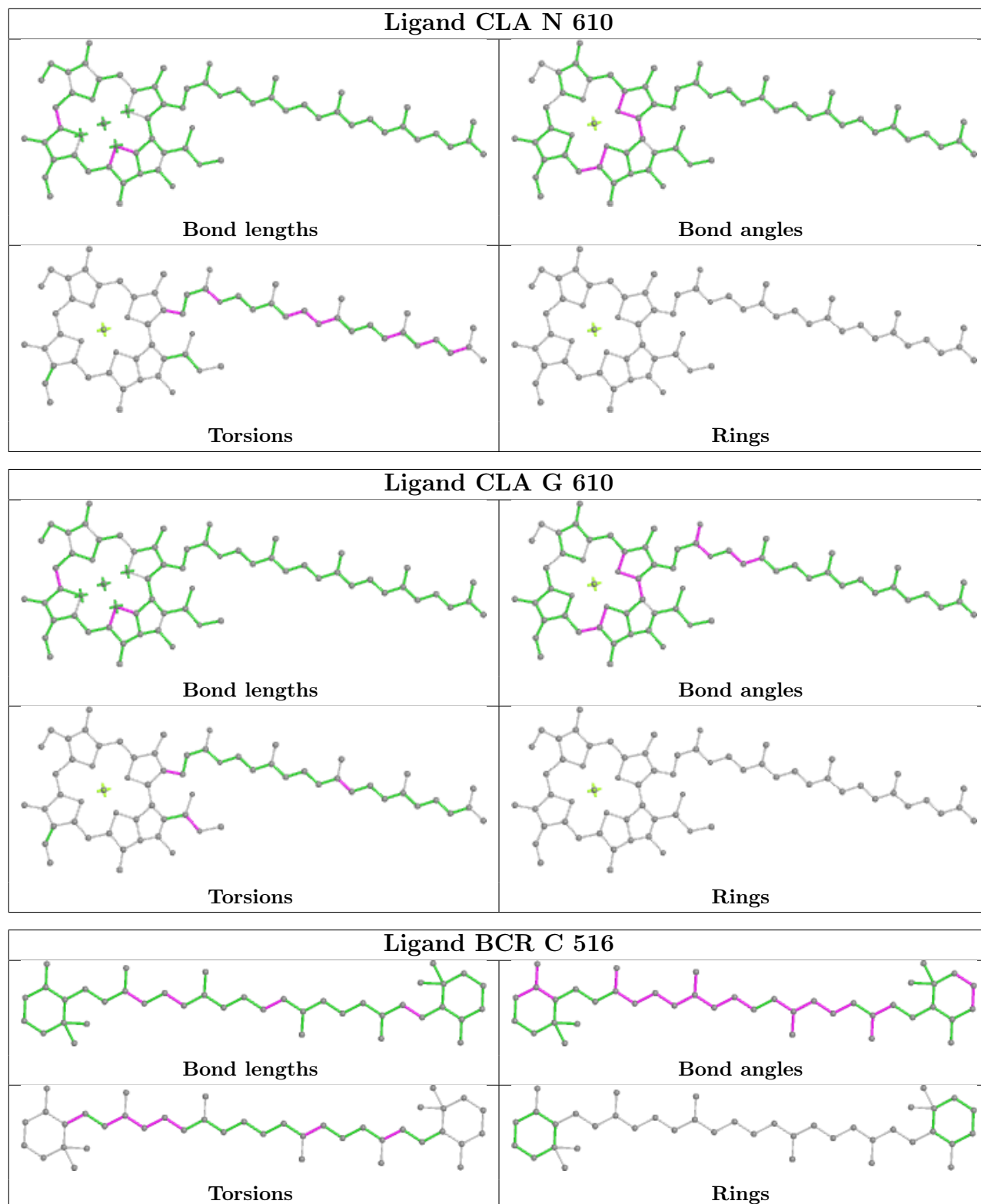


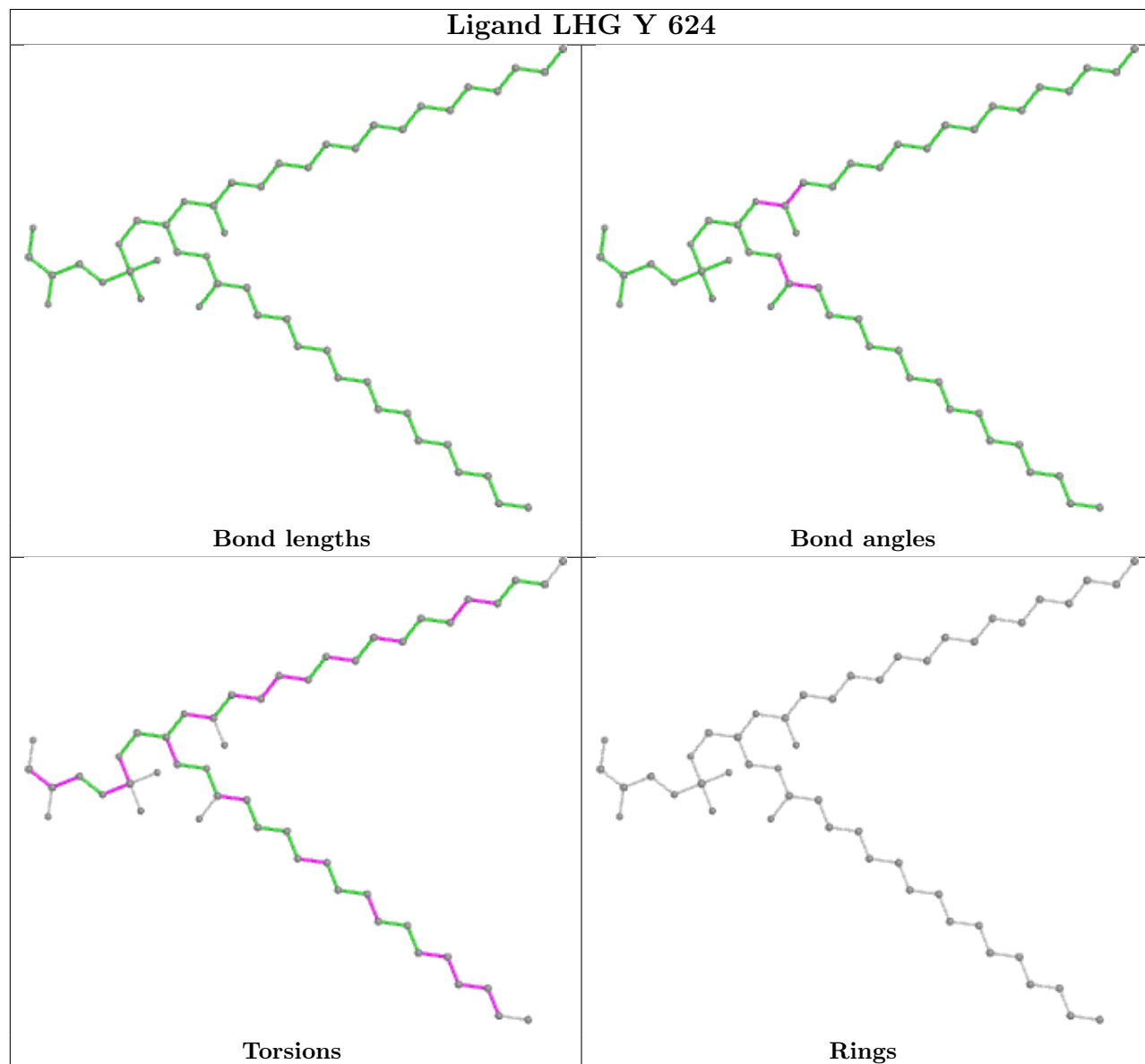
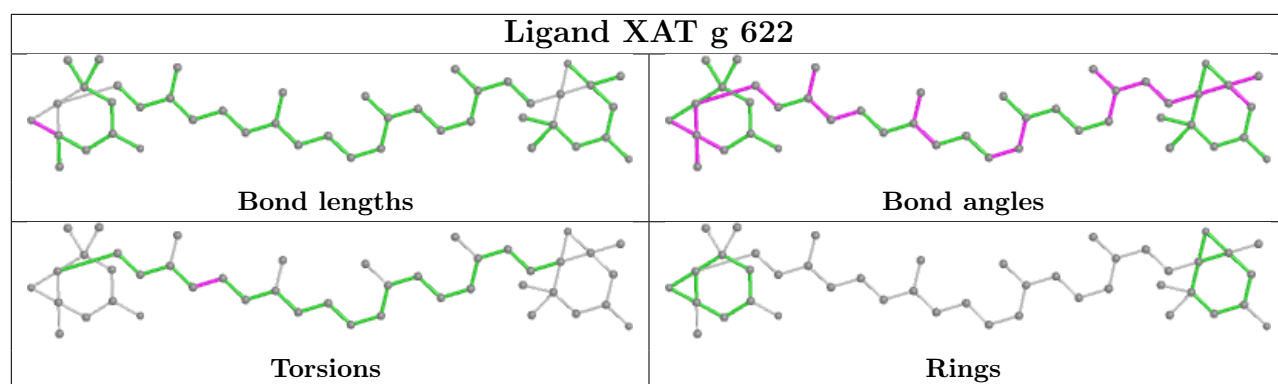
Torsions



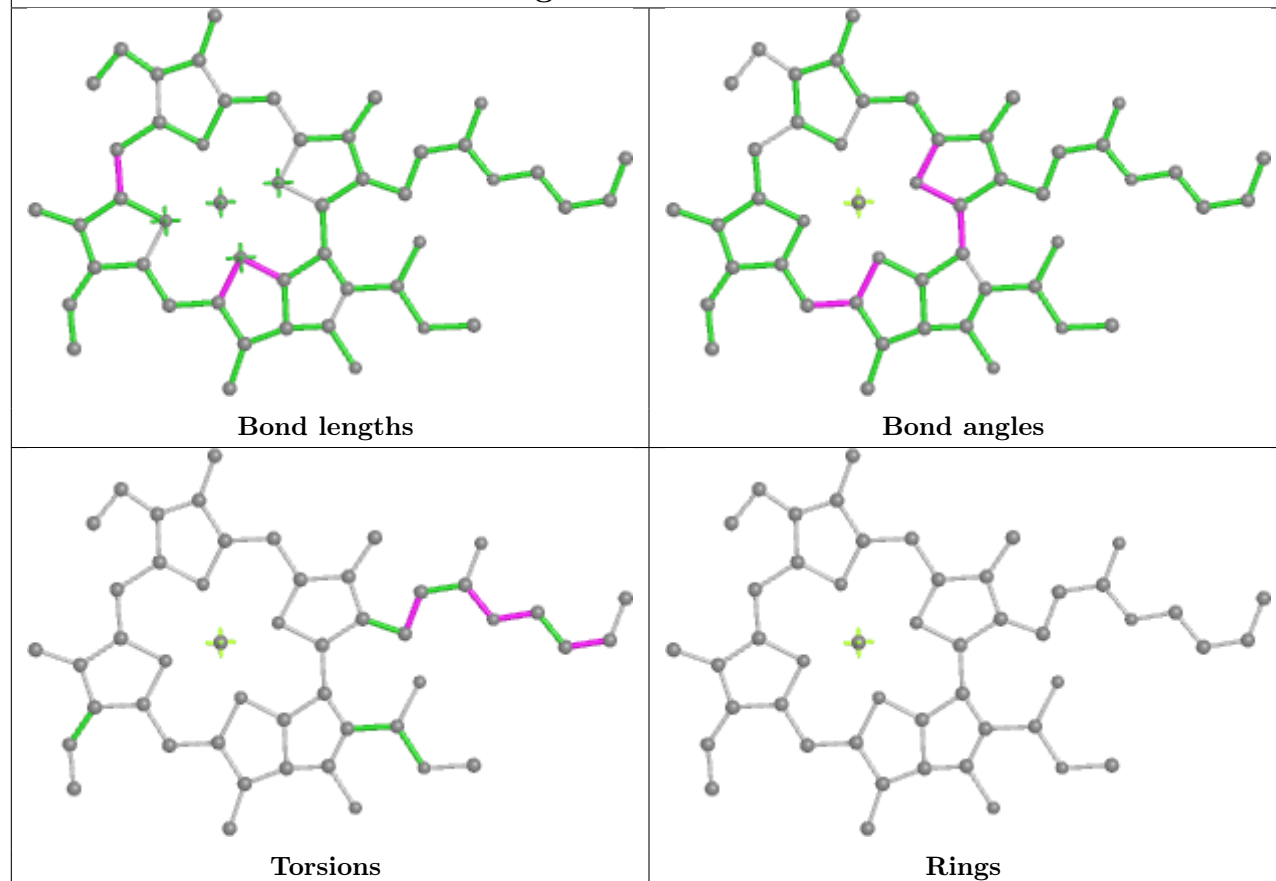
Rings



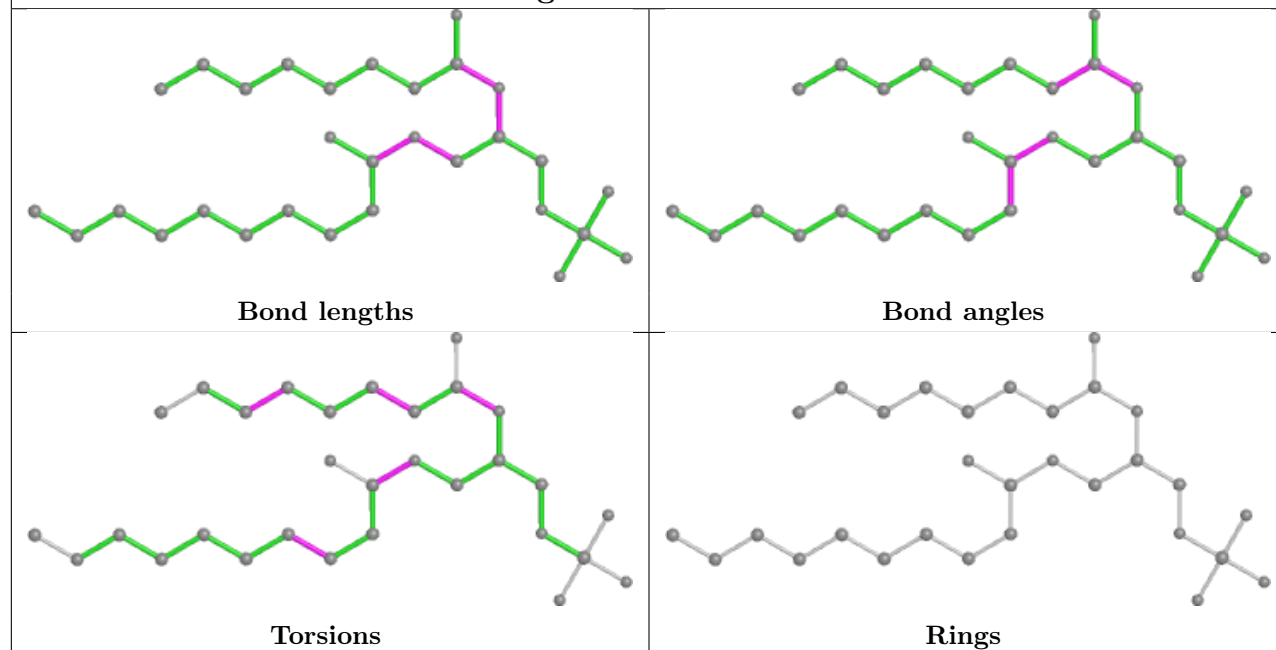


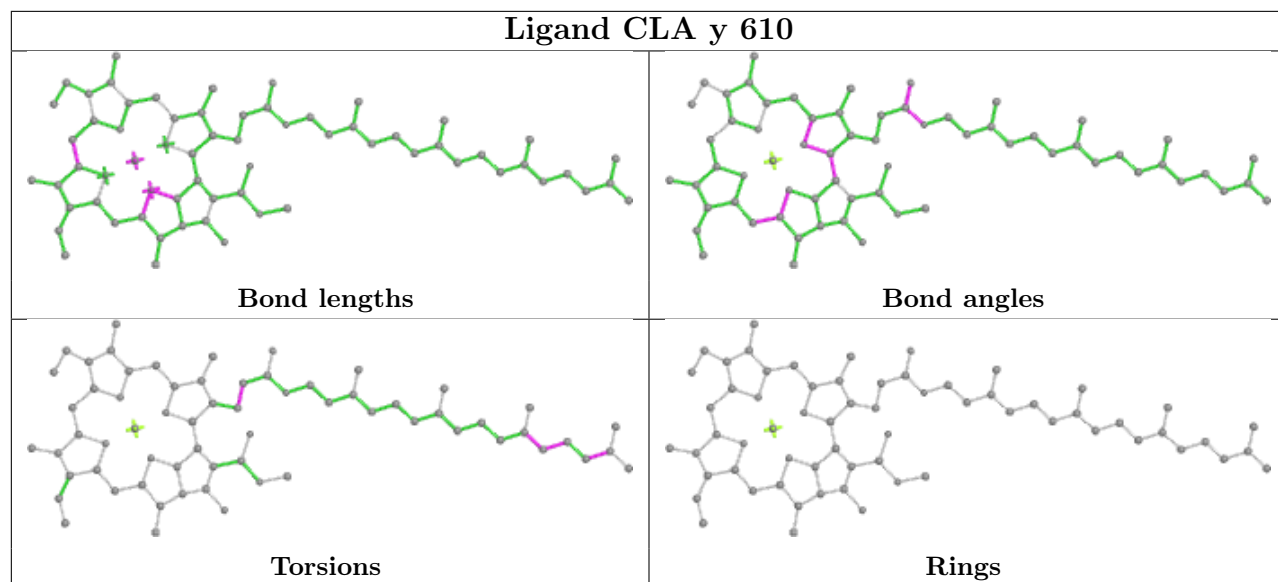
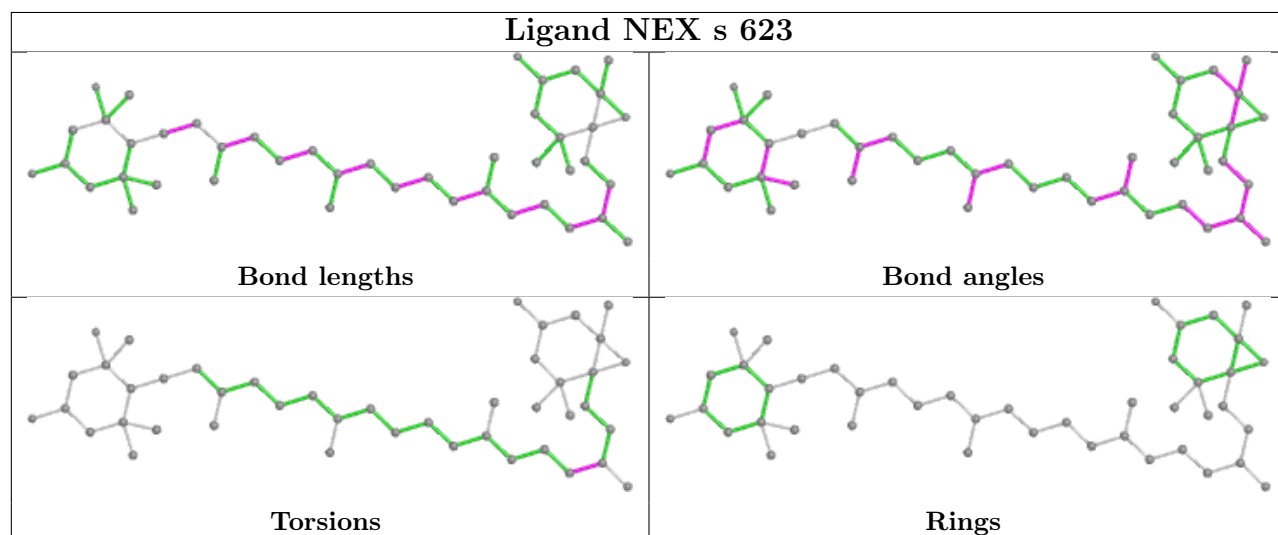


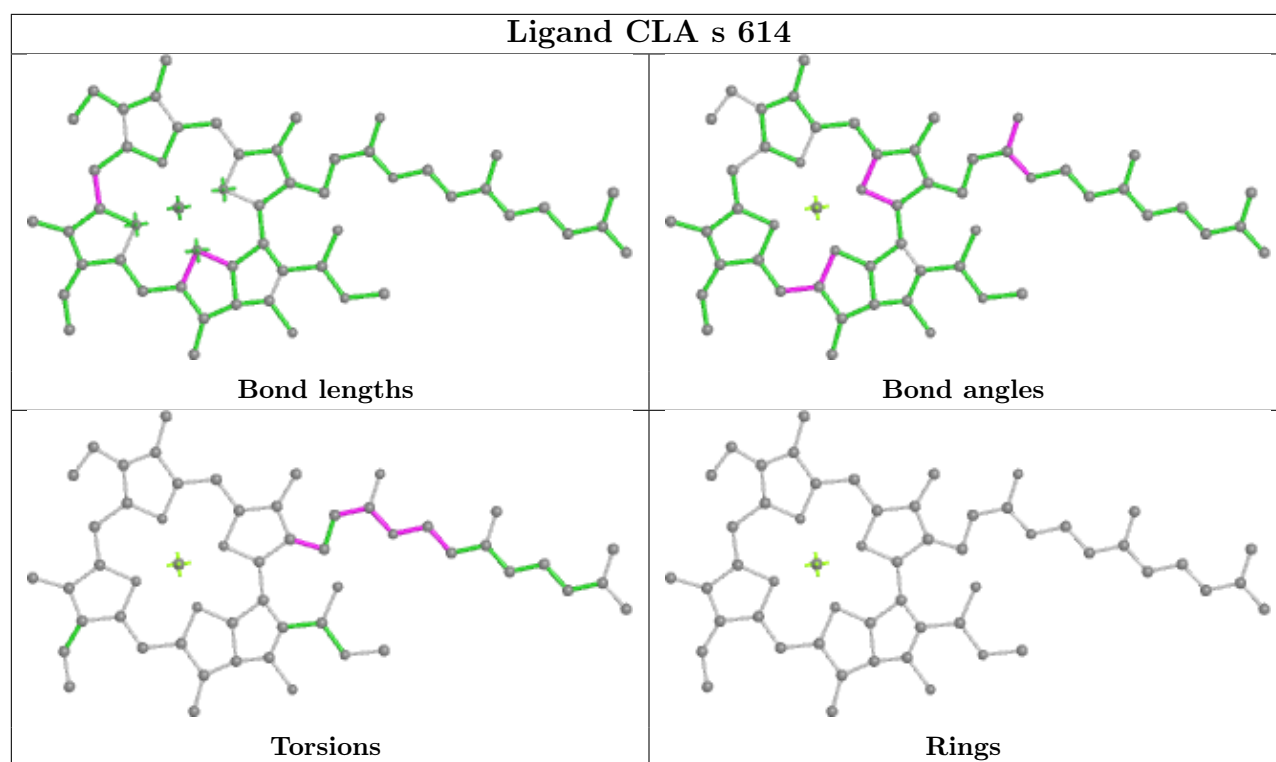
Ligand CLA n 611

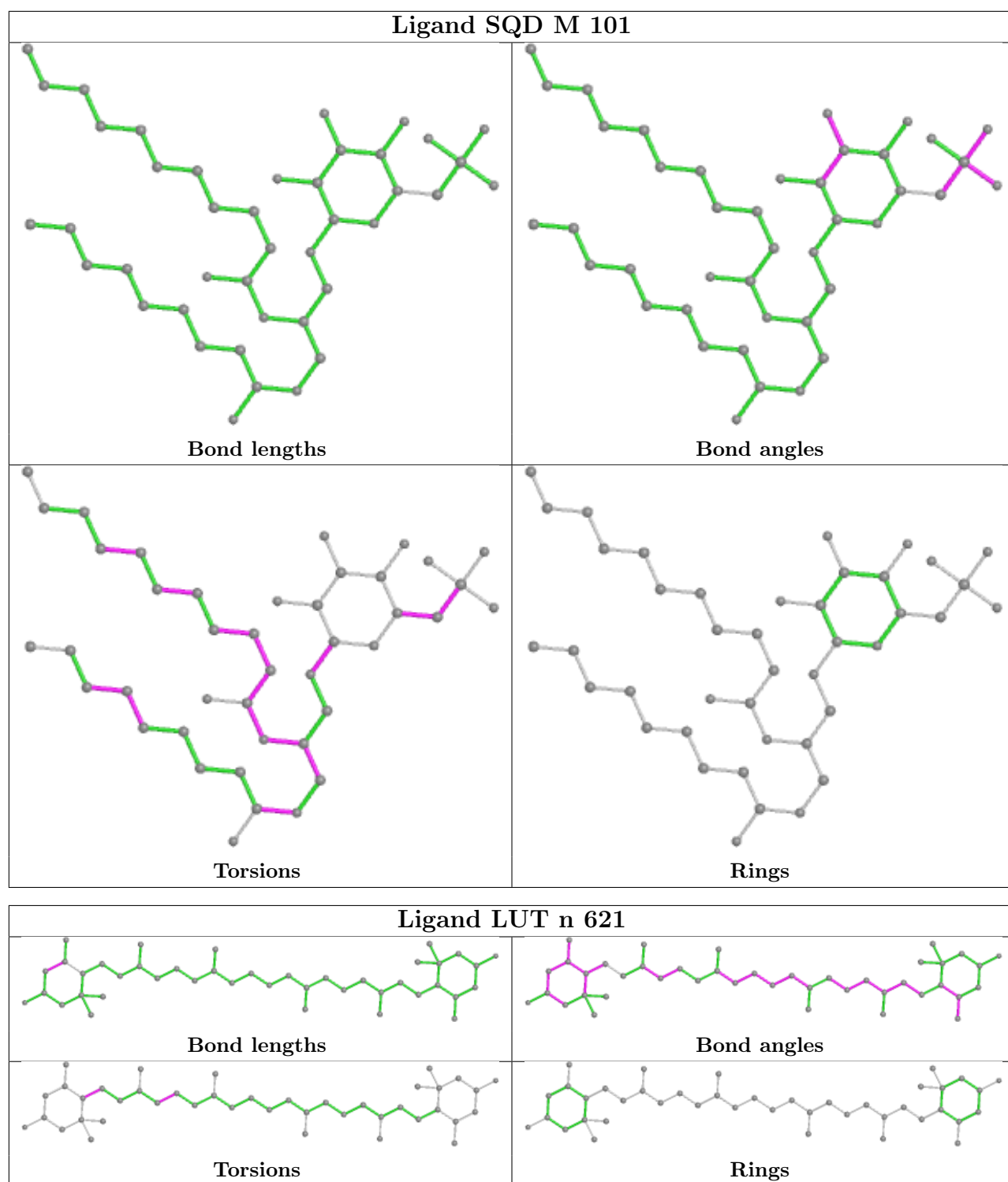


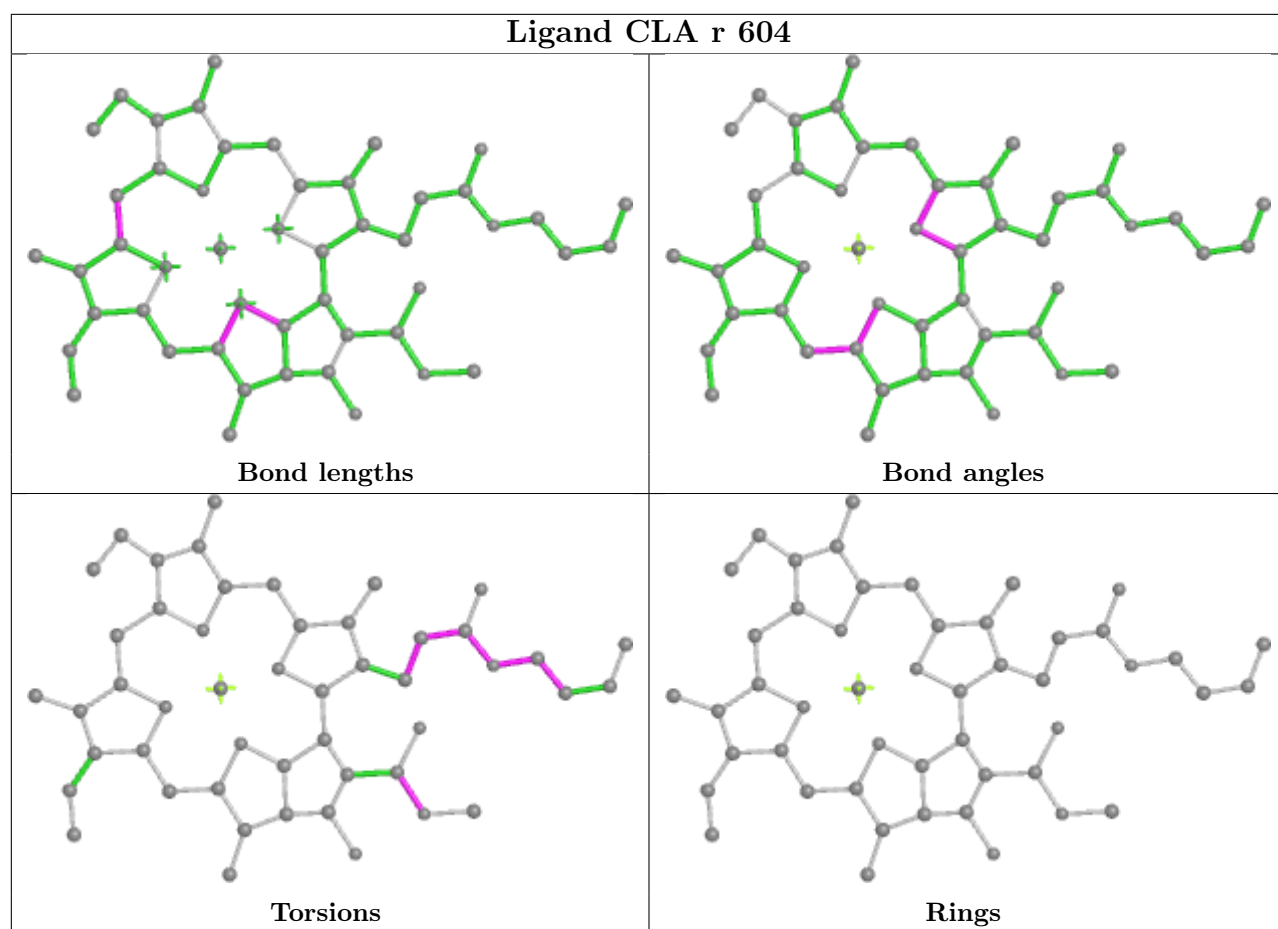
Ligand 3PH S 626

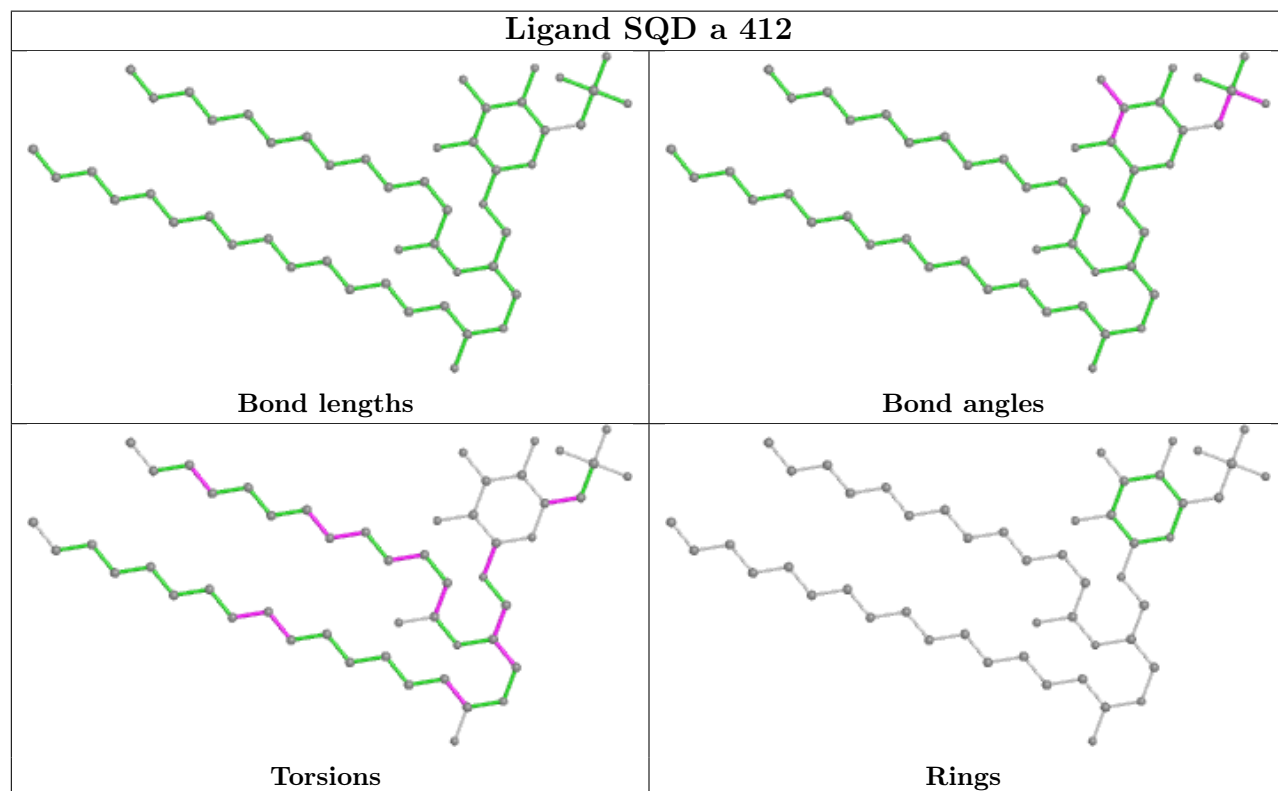
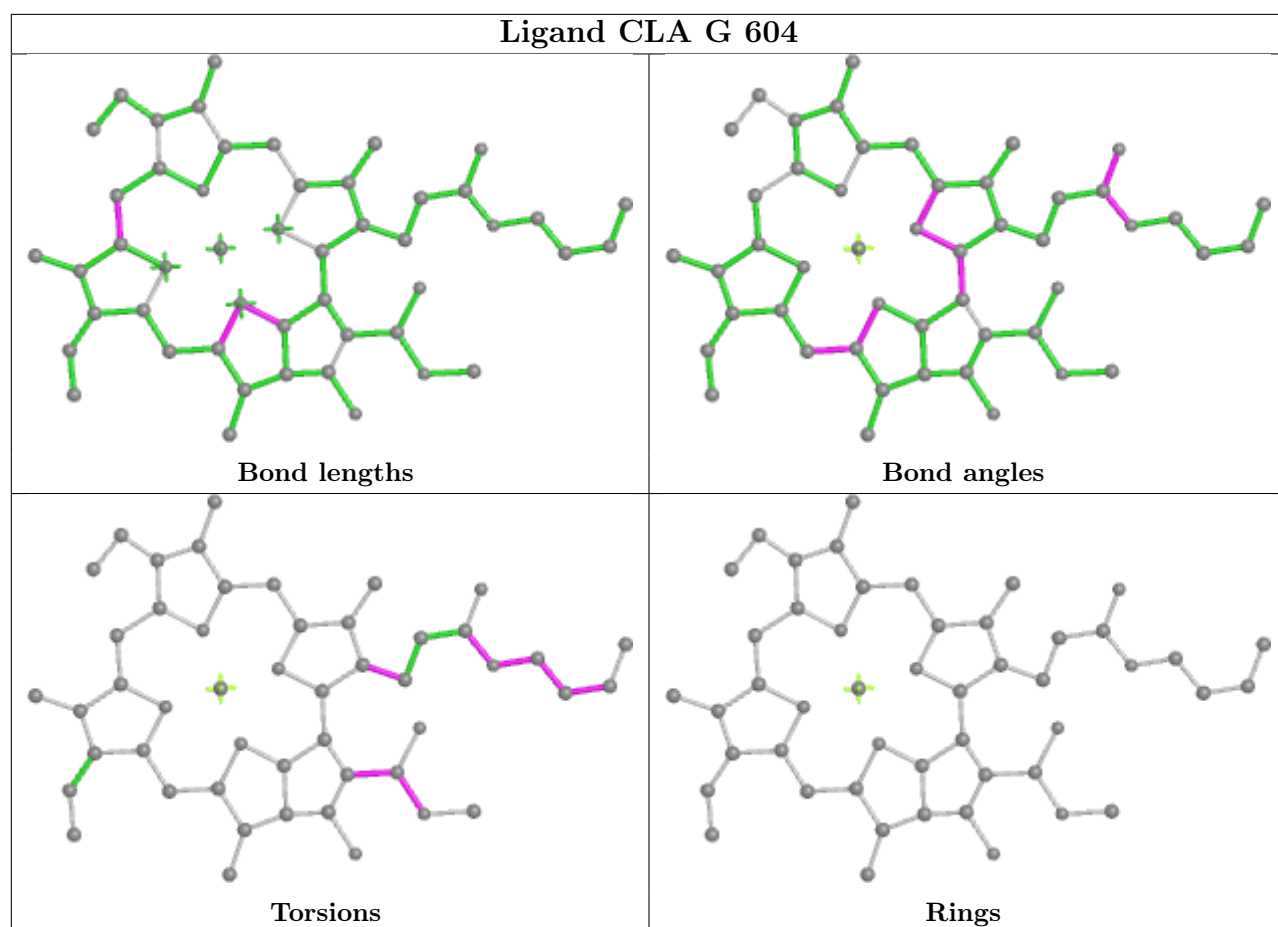


Ligand CLA y 610**Ligand NEX s 623**

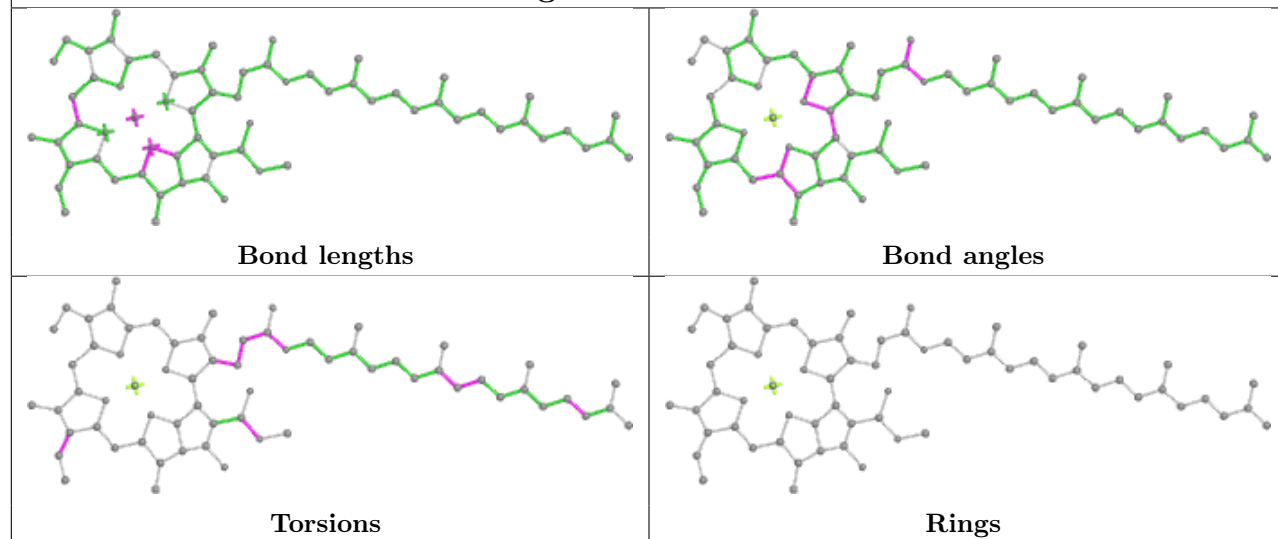




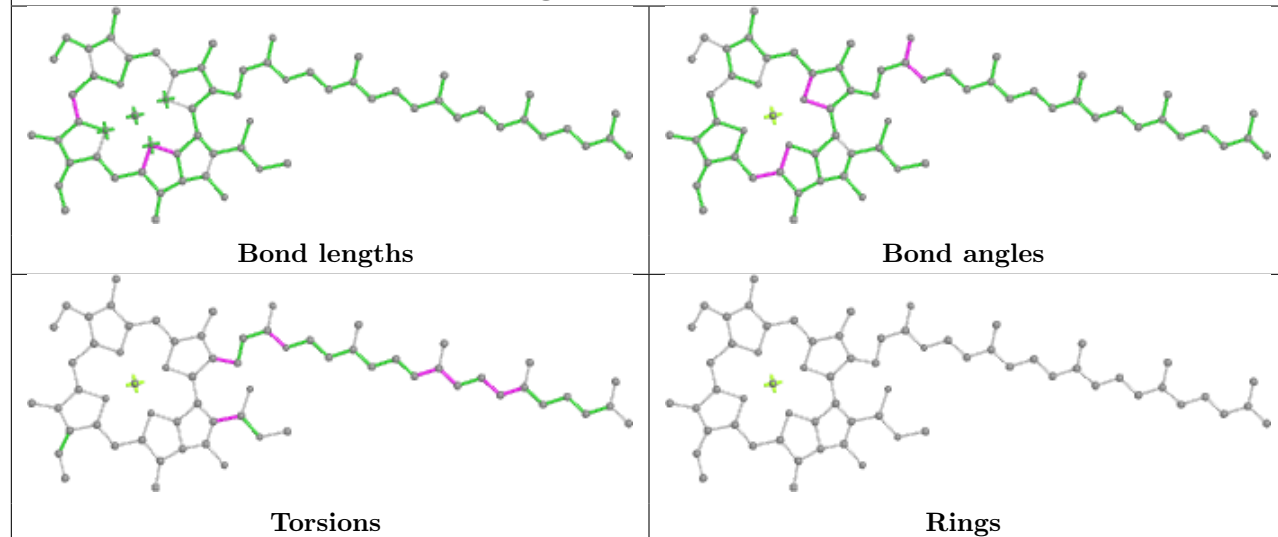




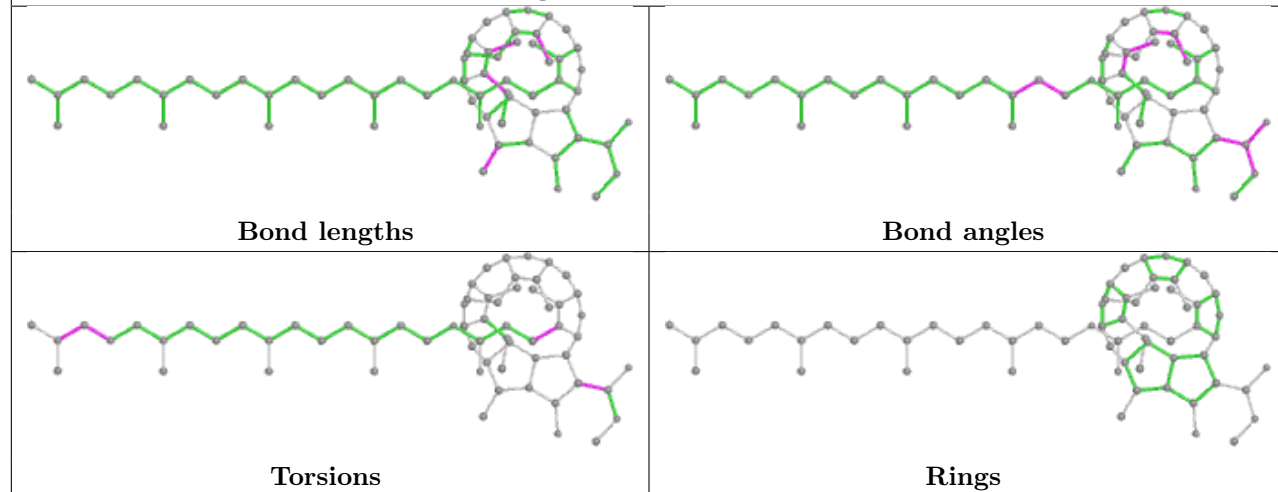
Ligand CLA s 603

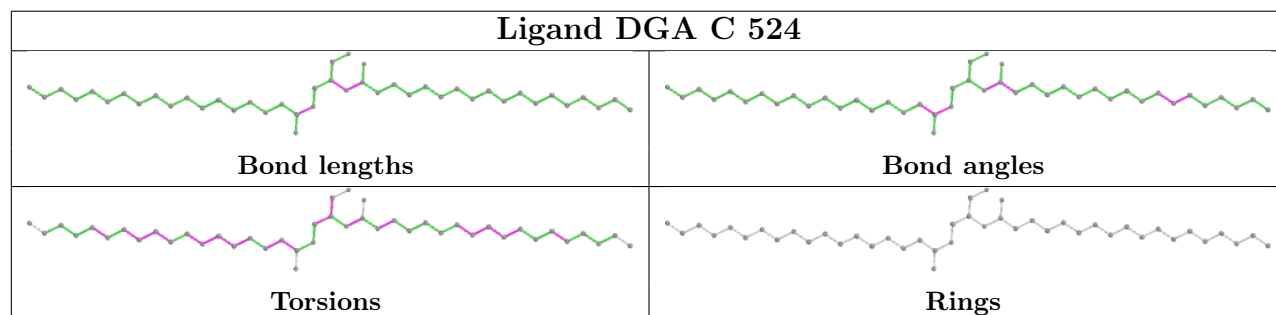
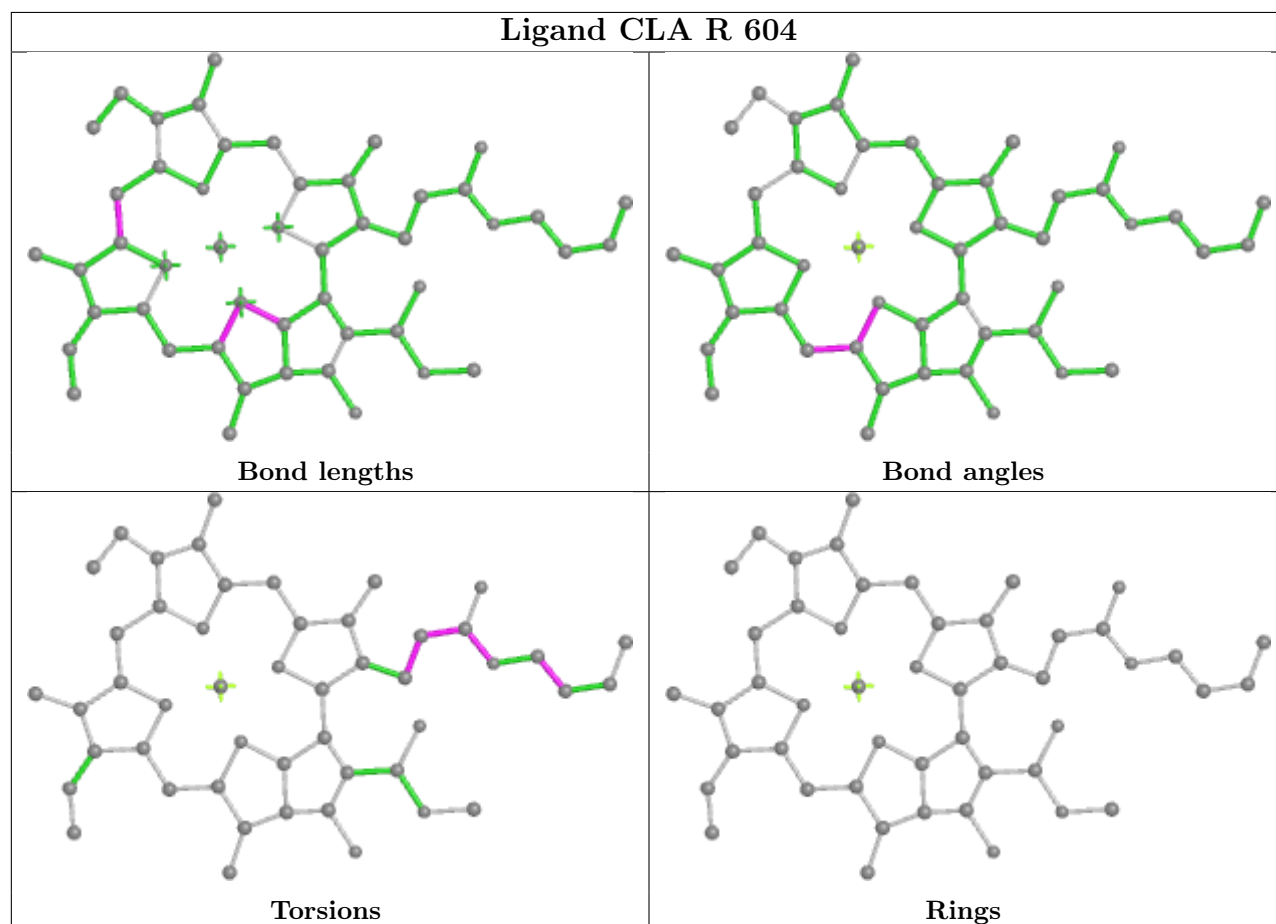
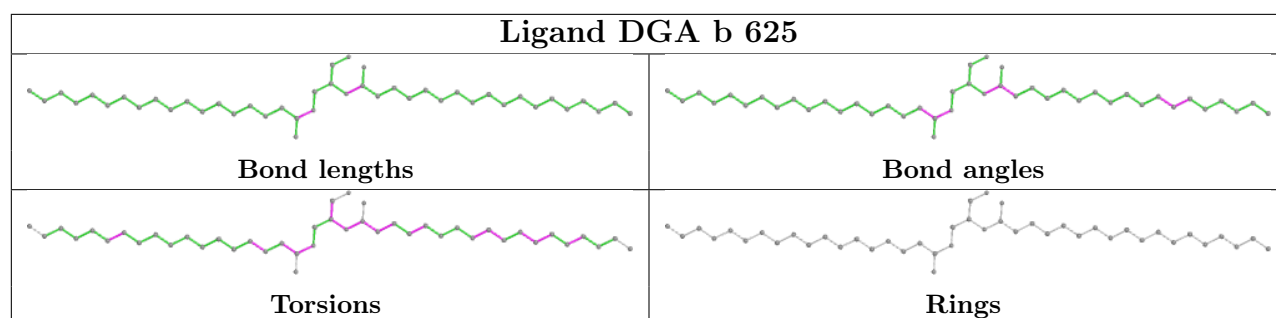


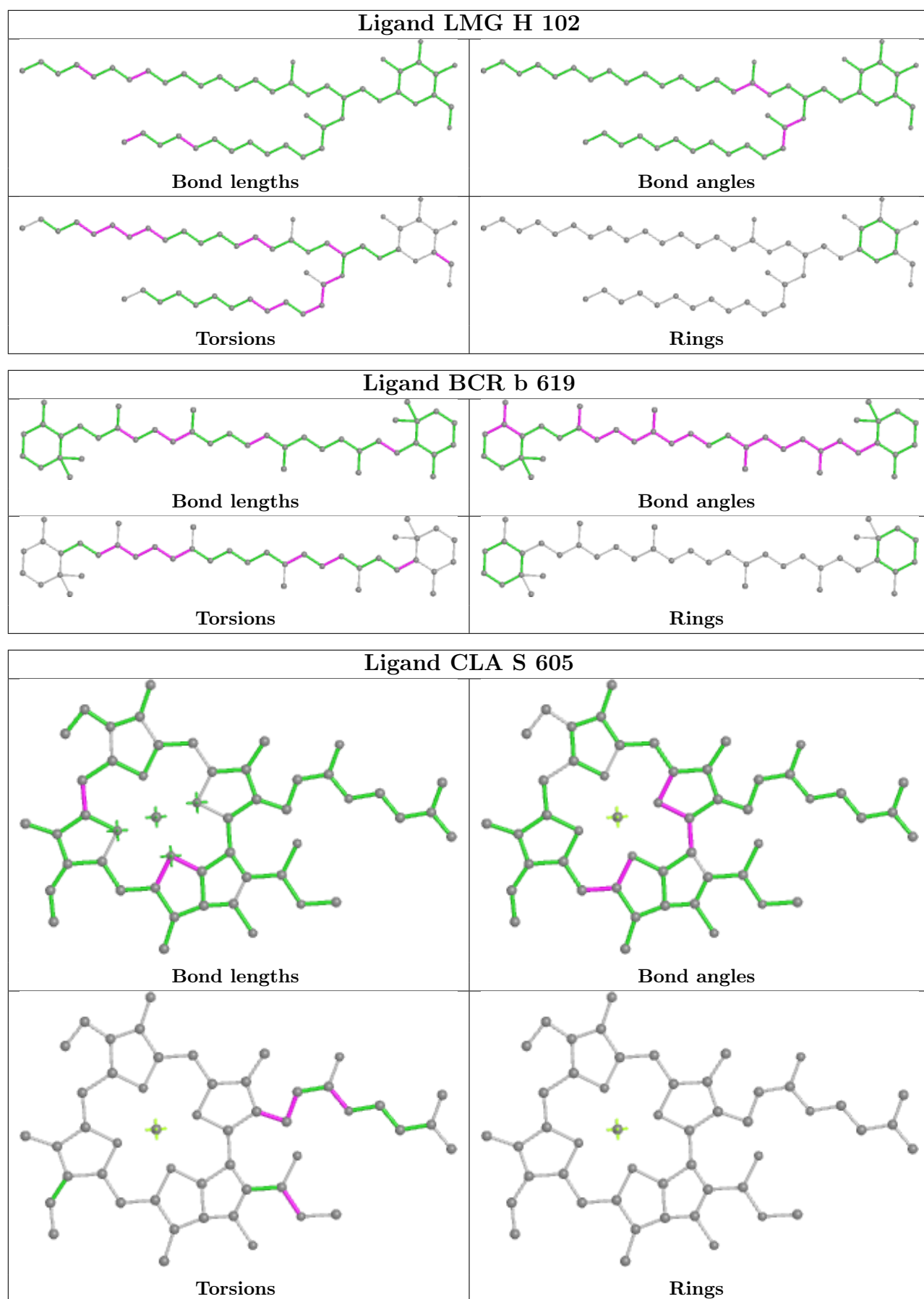
Ligand CLA c 513

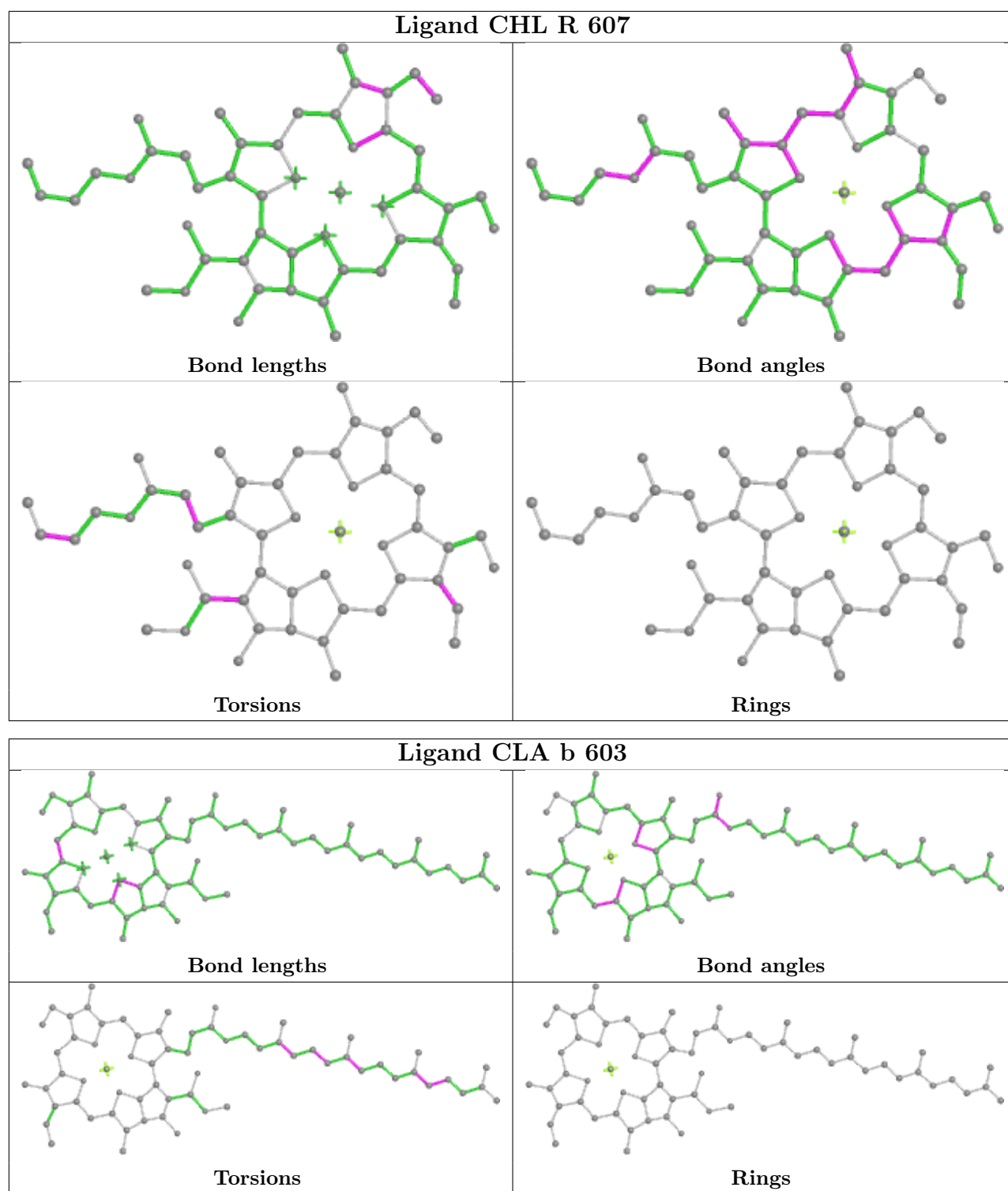


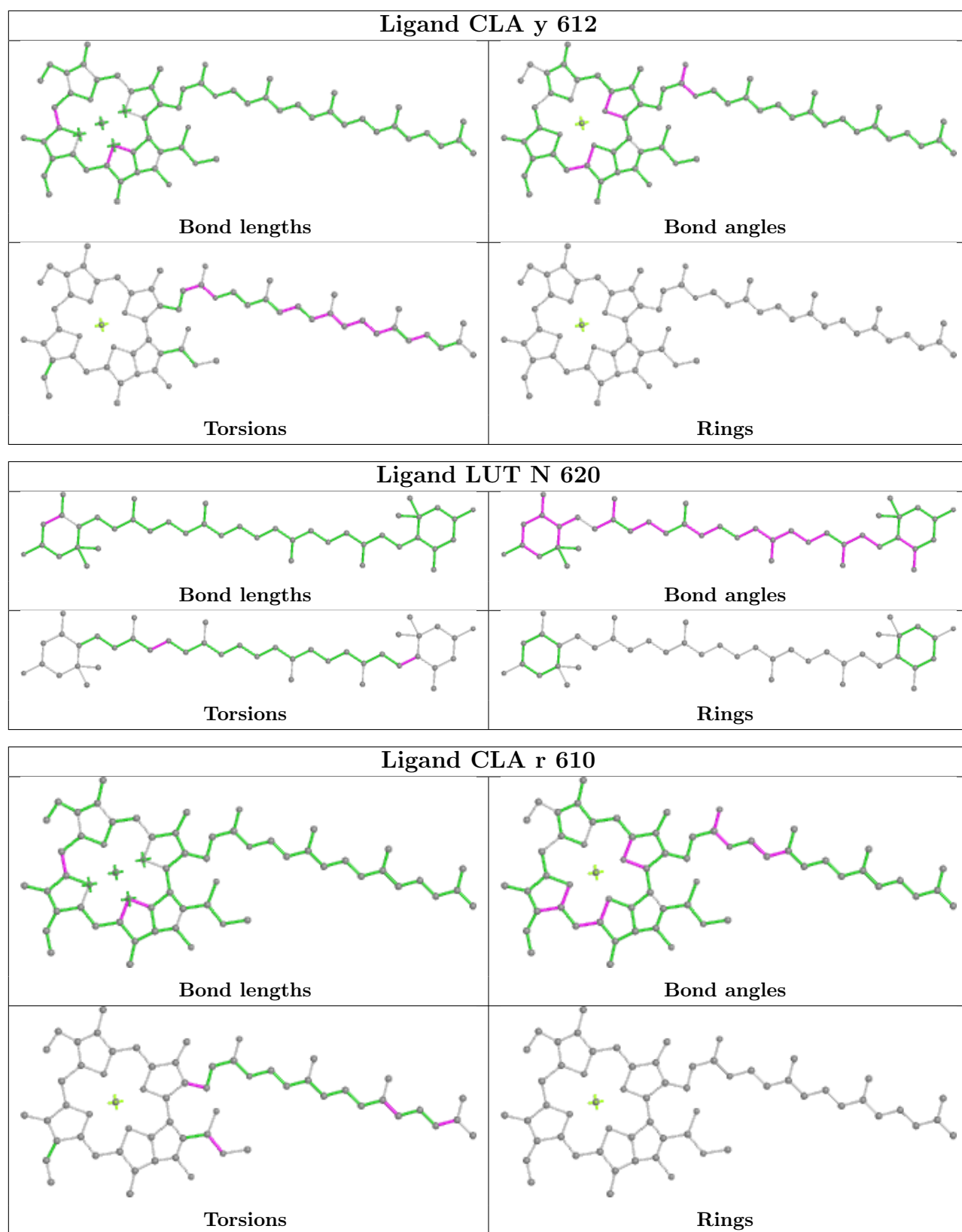
Ligand PHO a 408



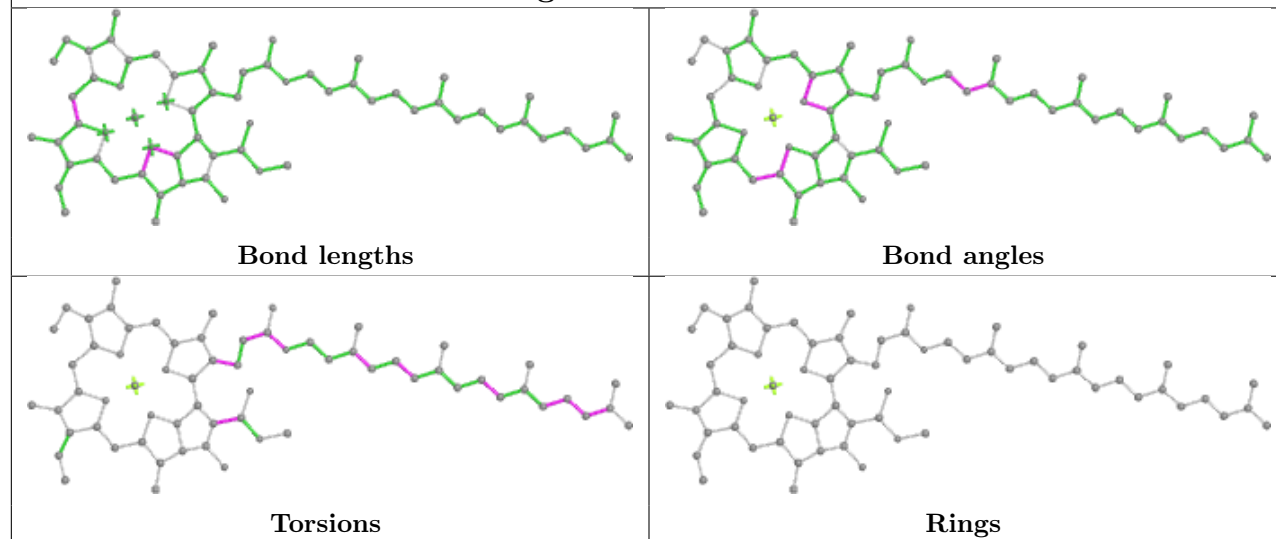




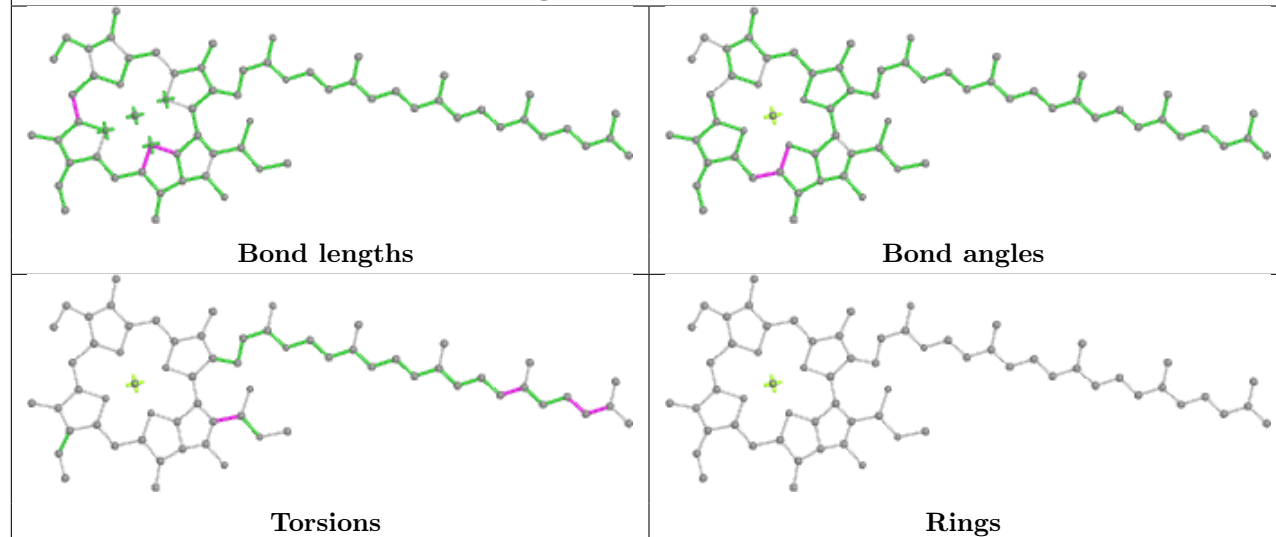




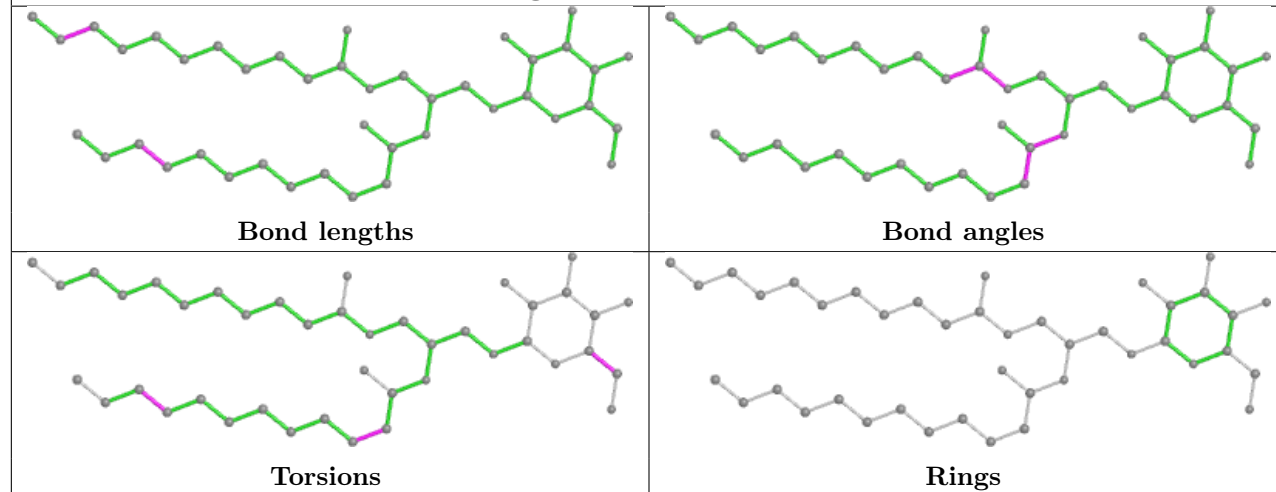
Ligand CLA c 512



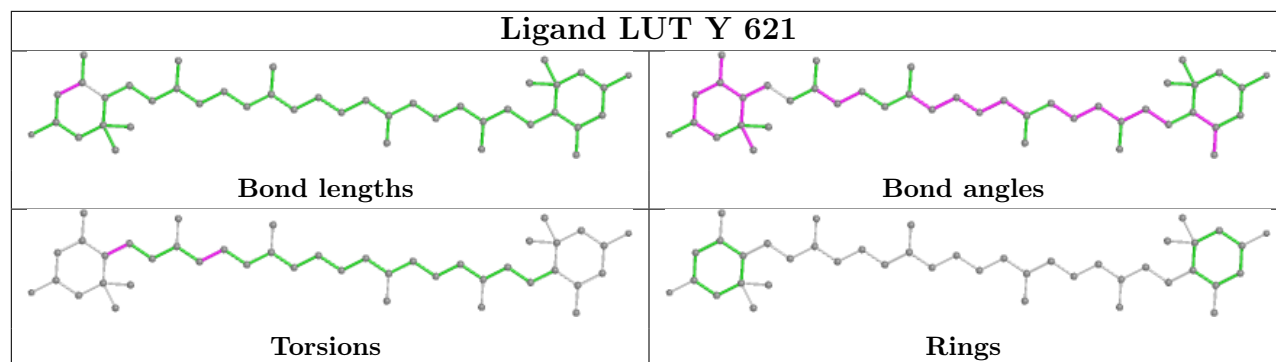
Ligand CLA b 611



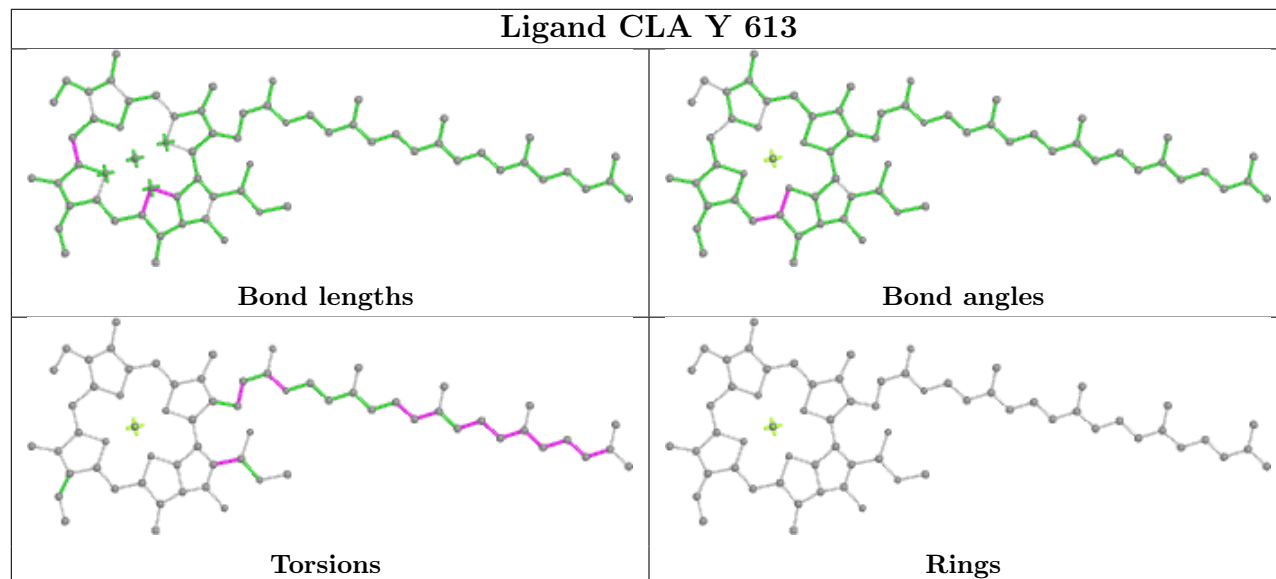
Ligand LMG D 411



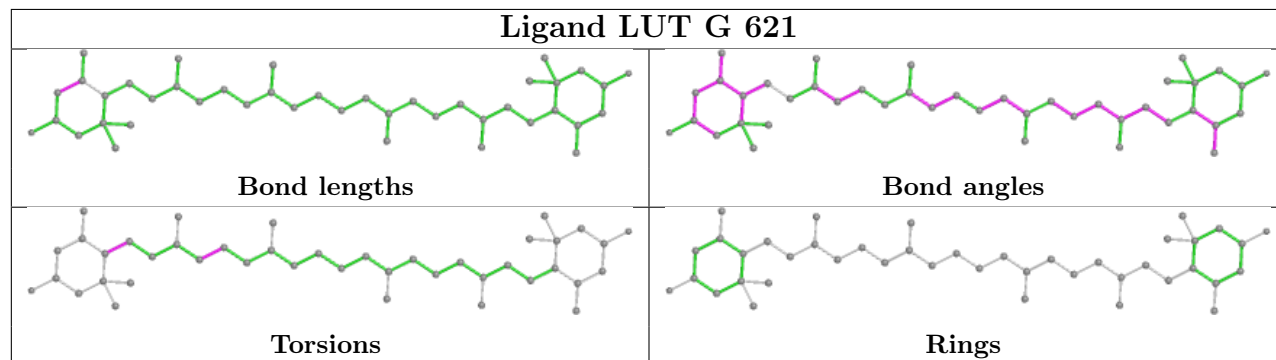
Ligand LUT Y 621



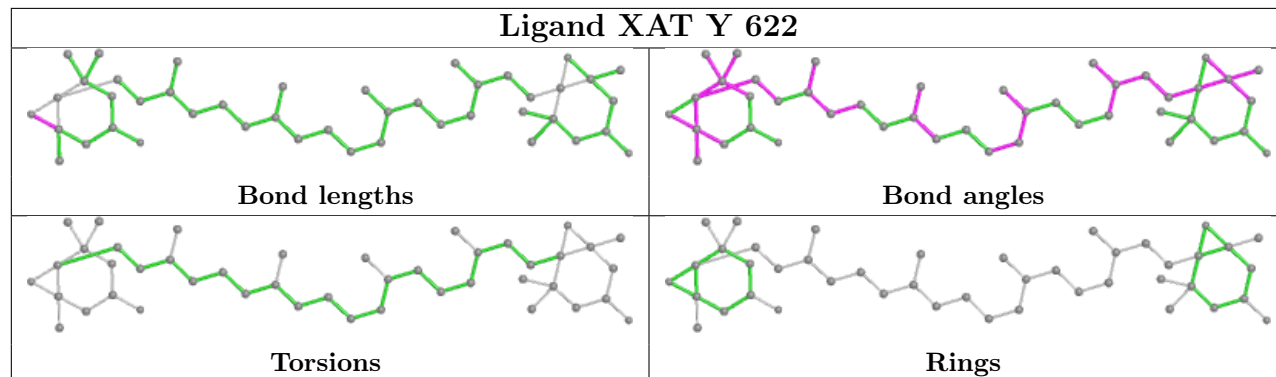
Ligand CLA Y 613

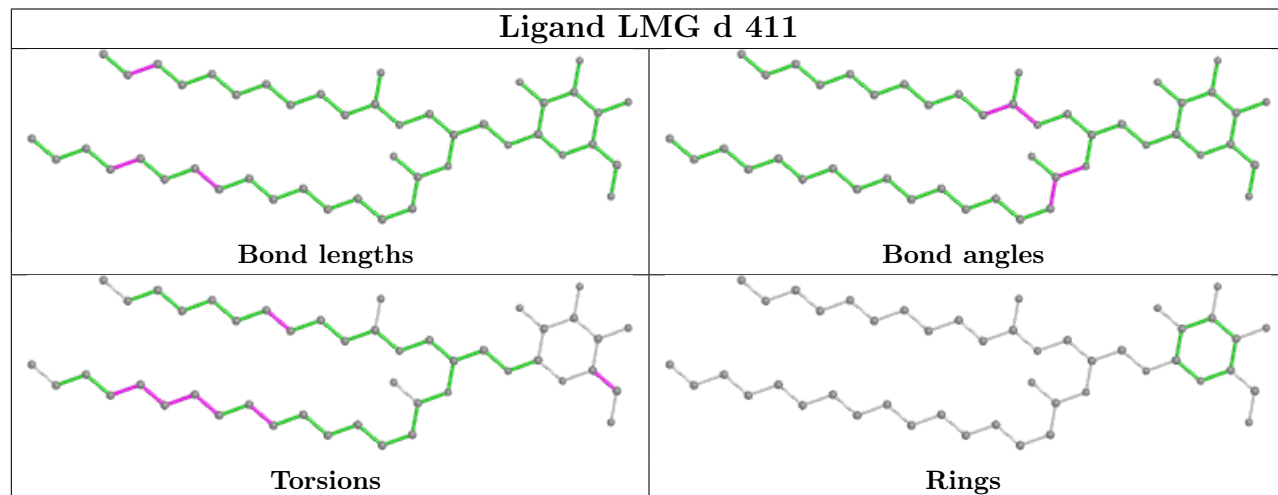
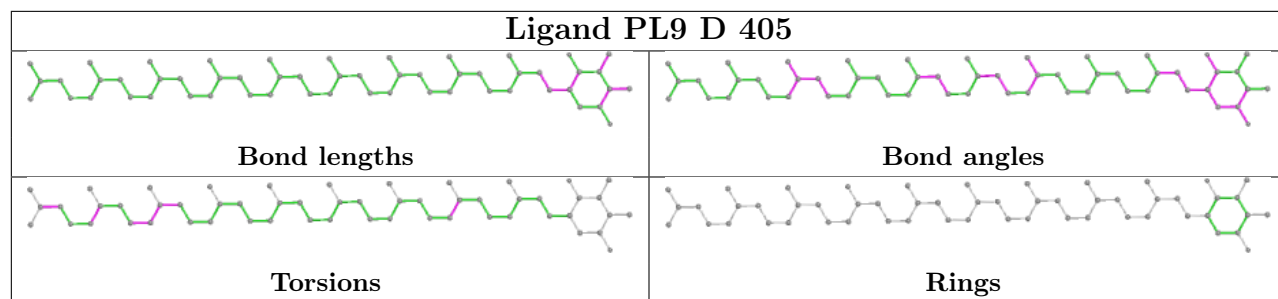


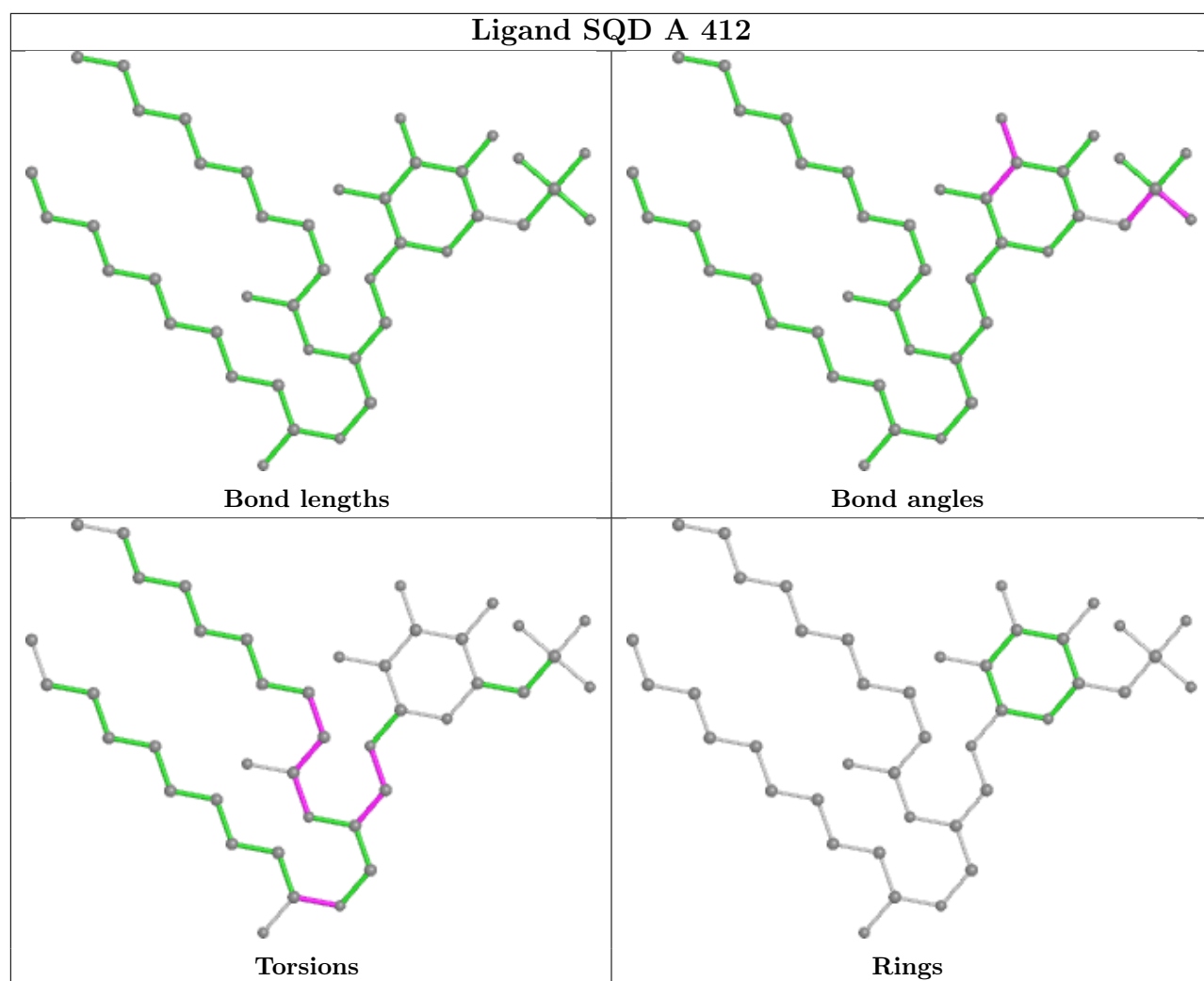
Ligand LUT G 621

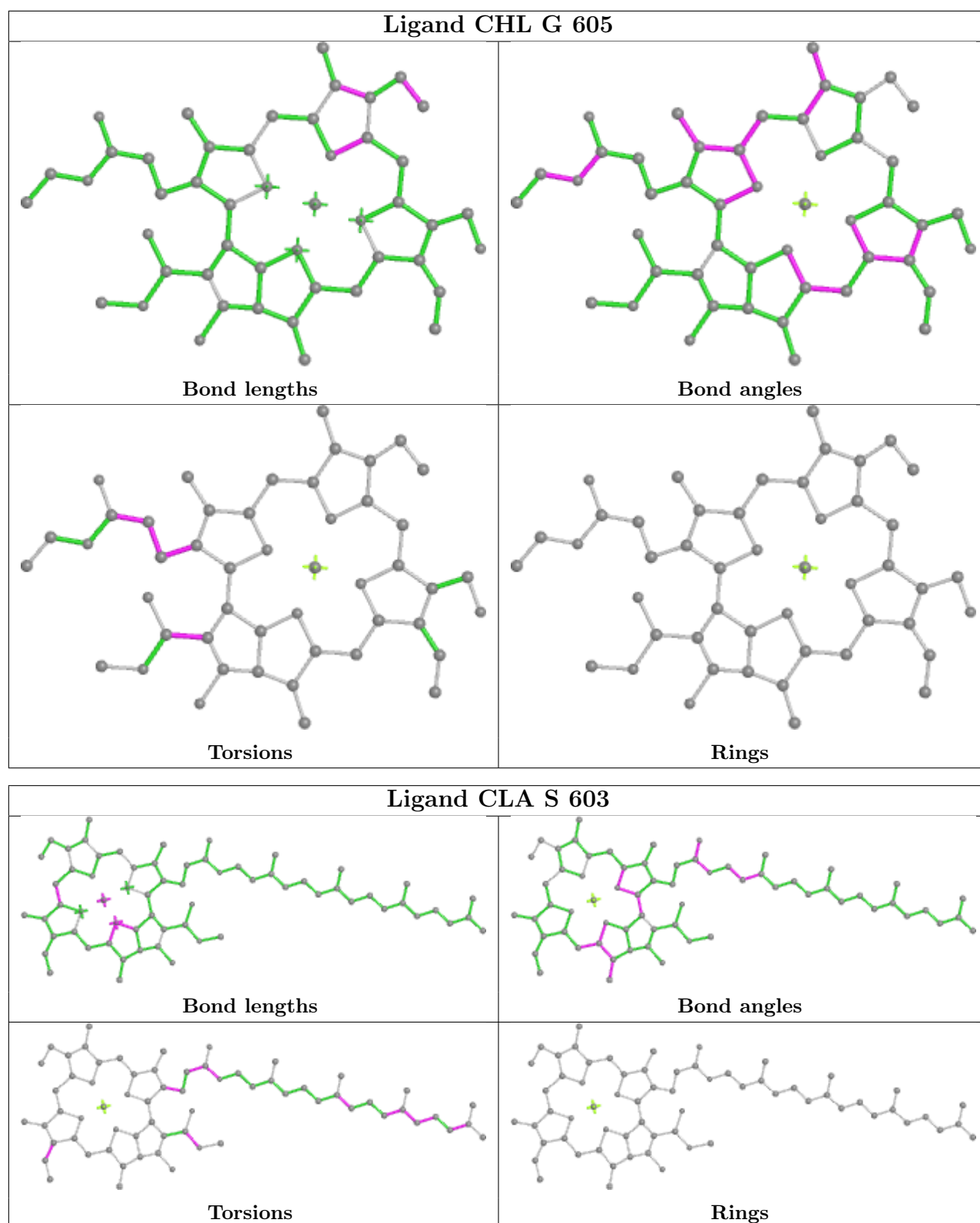


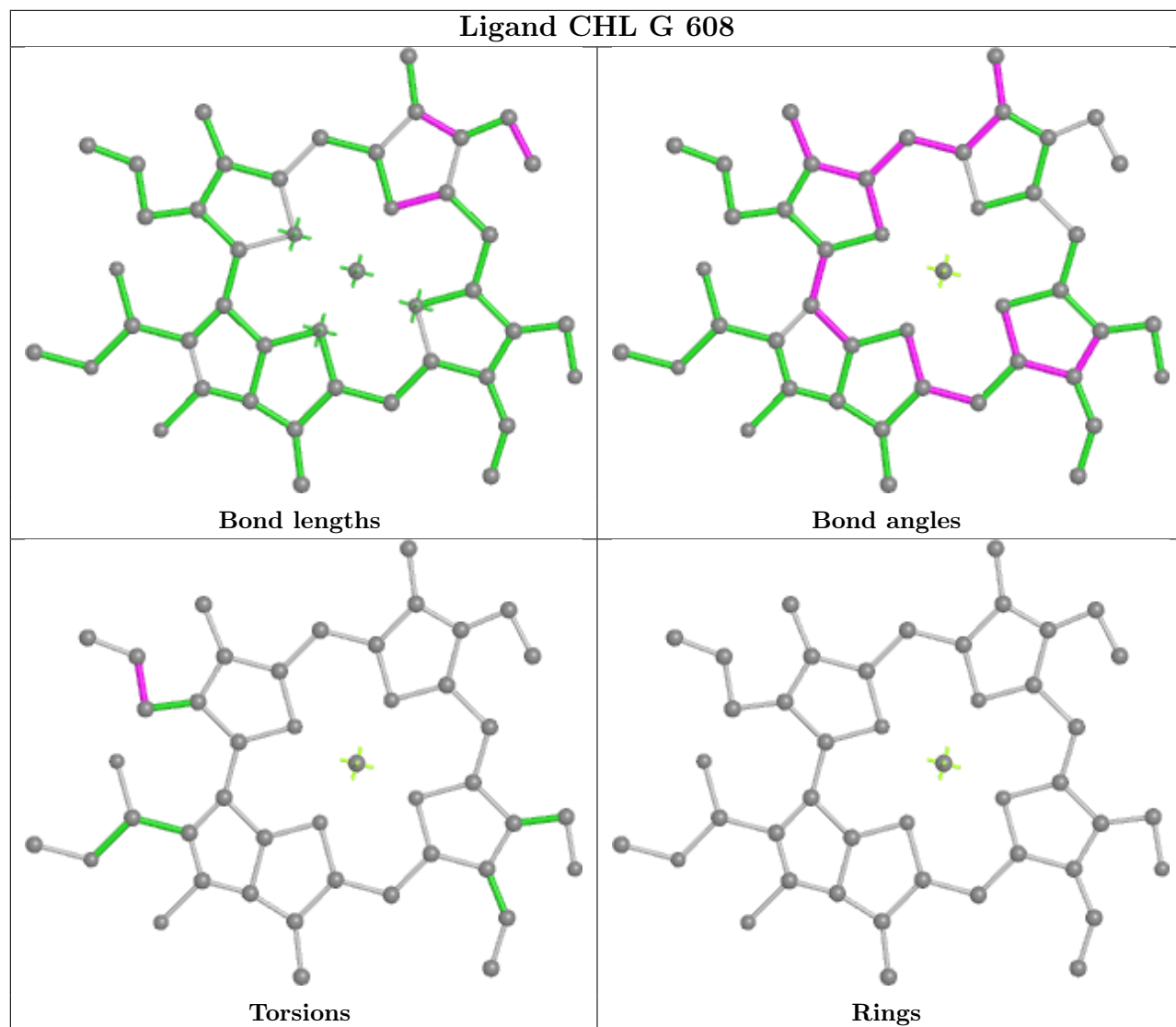
Ligand XAT Y 622

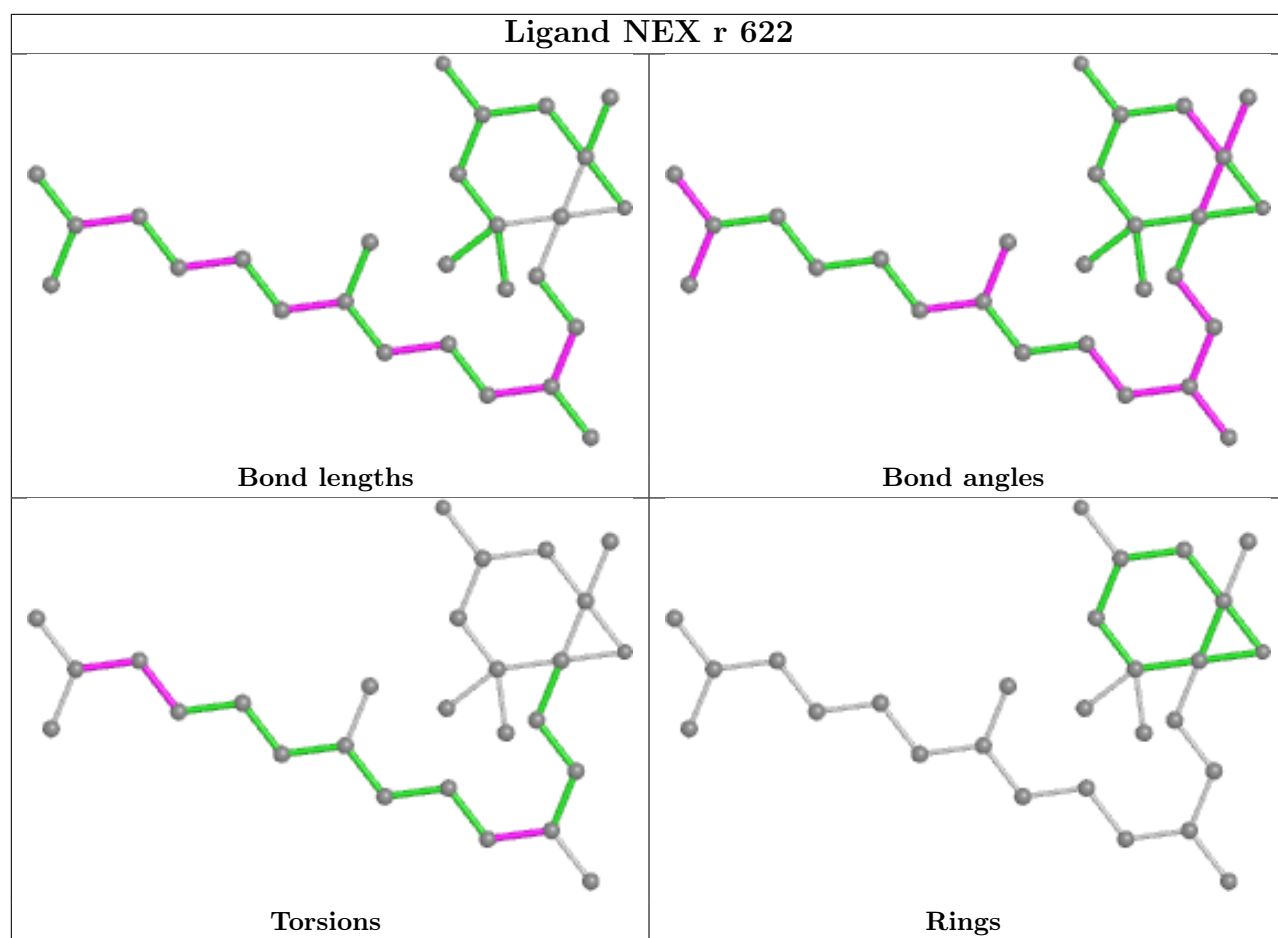




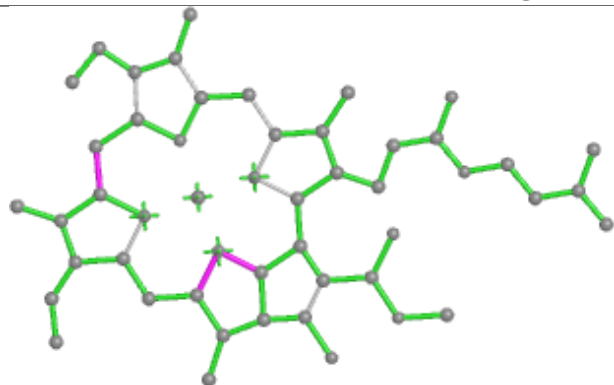




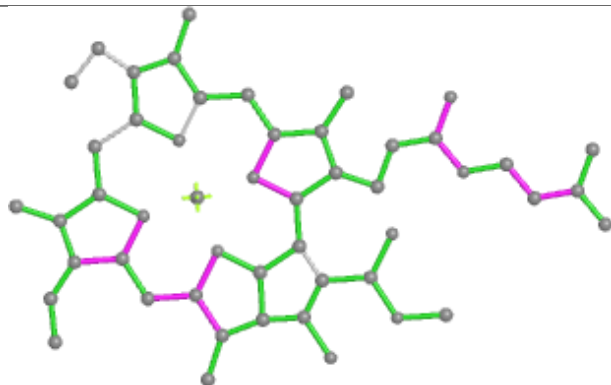




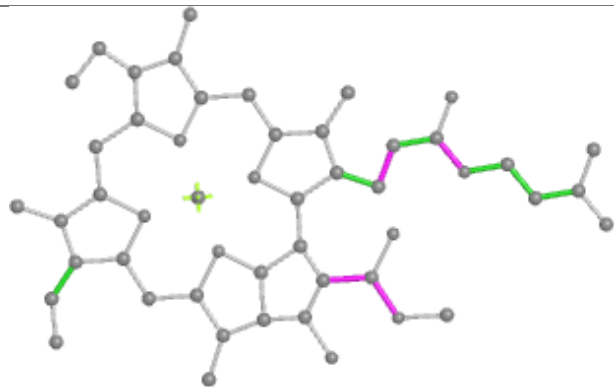
Ligand CLA S 617



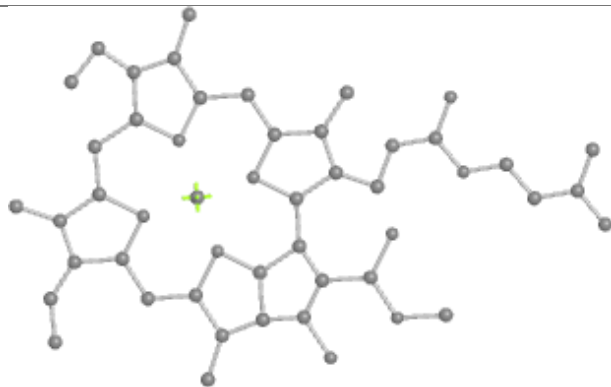
Bond lengths



Bond angles

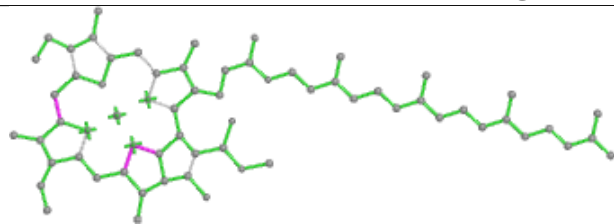


Torsions

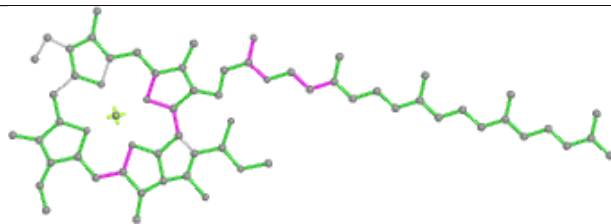


Rings

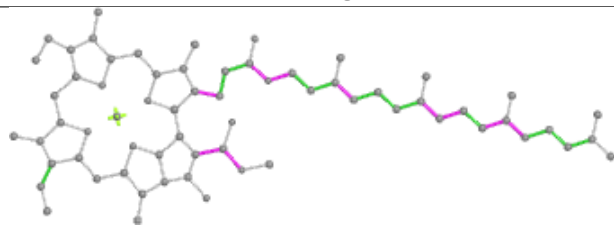
Ligand CLA Y 604



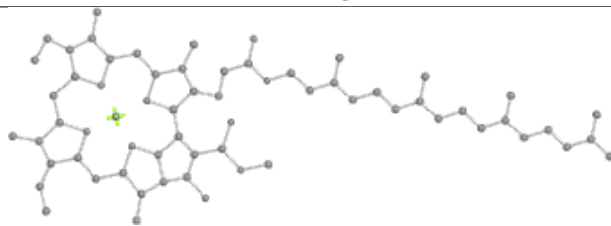
Bond lengths



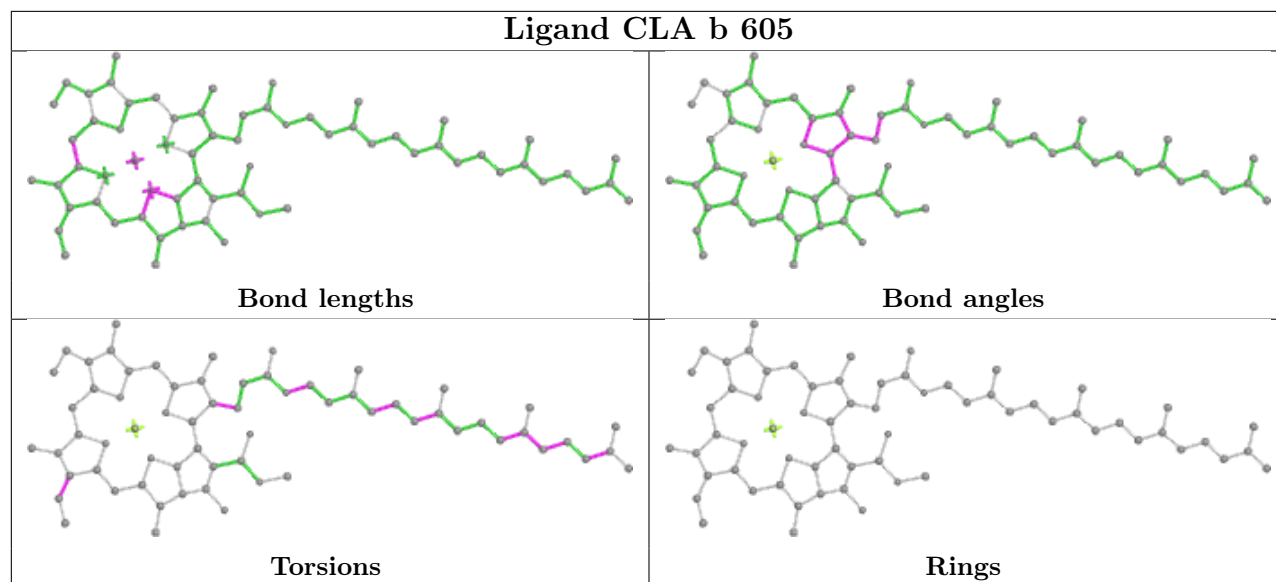
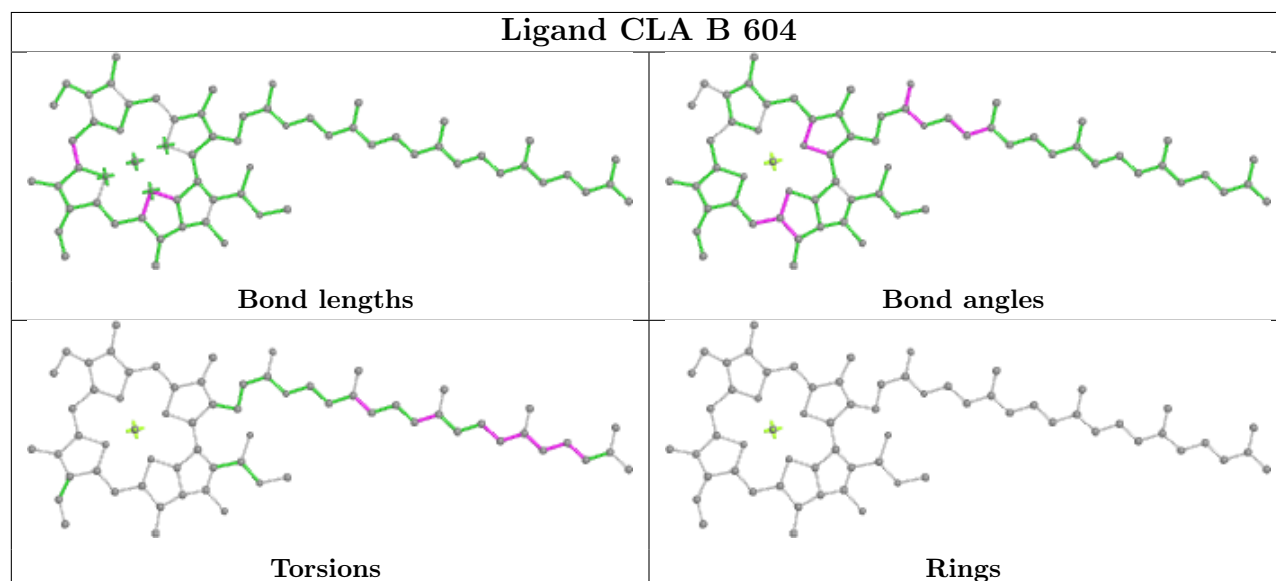
Bond angles



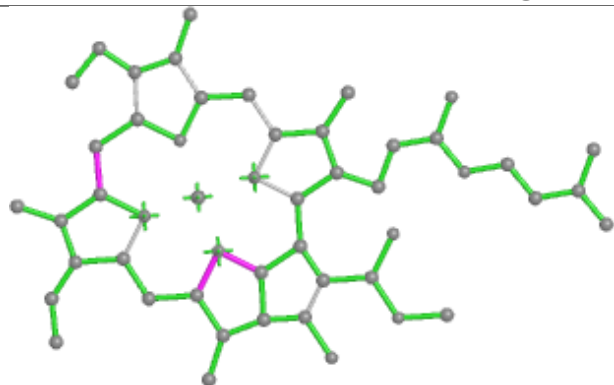
Torsions



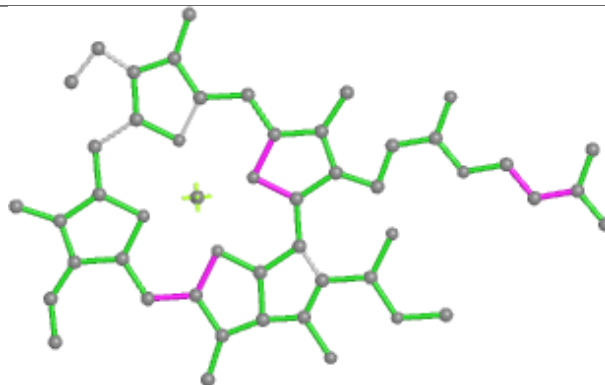
Rings

Ligand CLA b 605**Ligand CLA B 604**

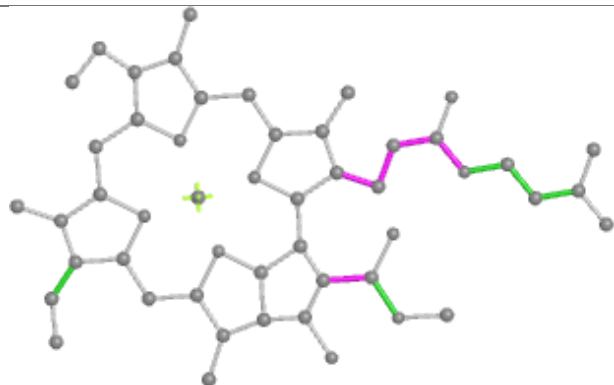
Ligand CLA S 614



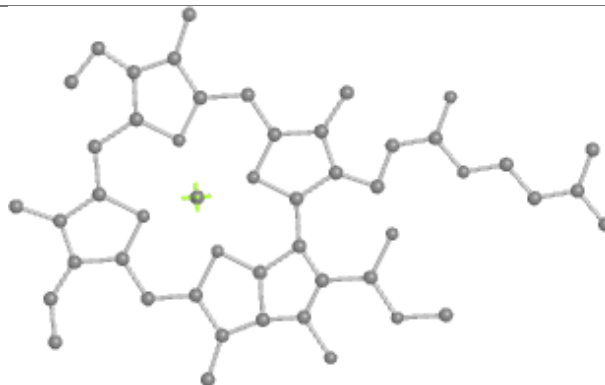
Bond lengths



Bond angles

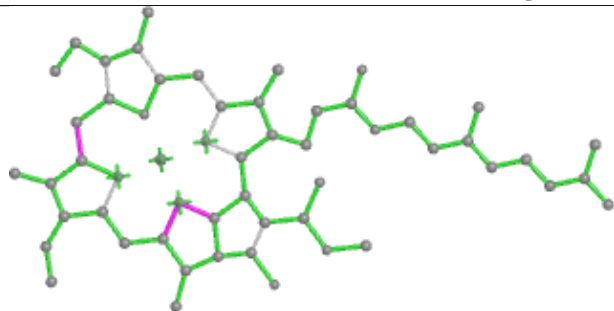


Torsions

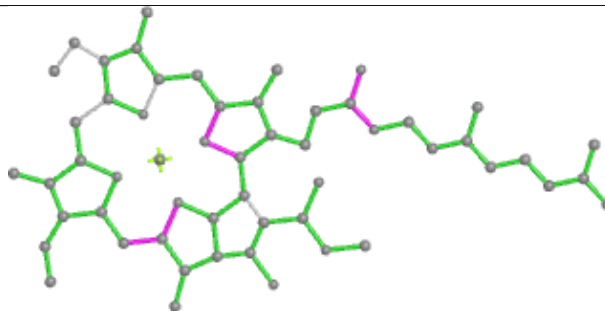


Rings

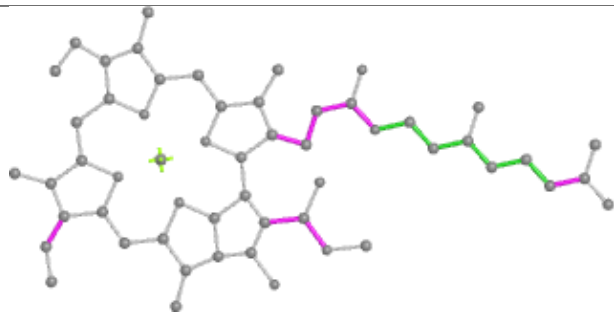
Ligand CLA s 613



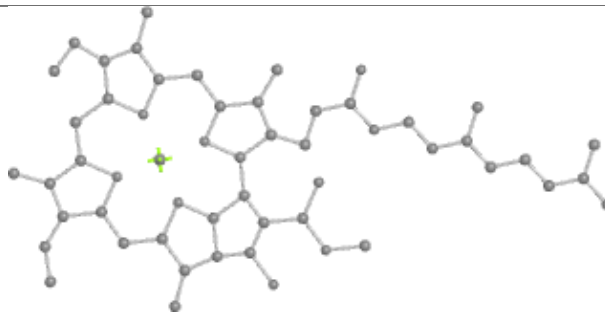
Bond lengths



Bond angles

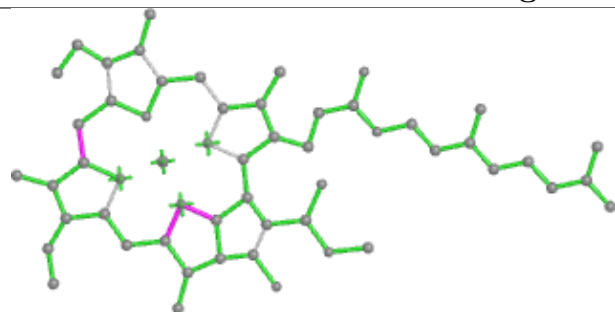


Torsions

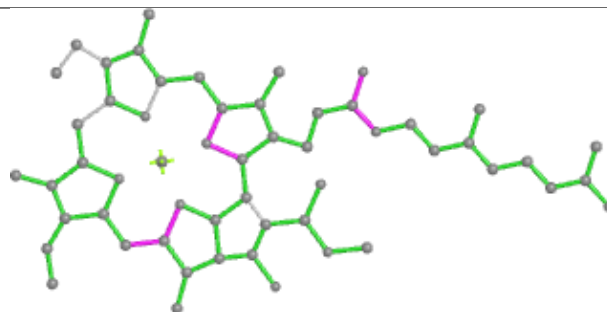


Rings

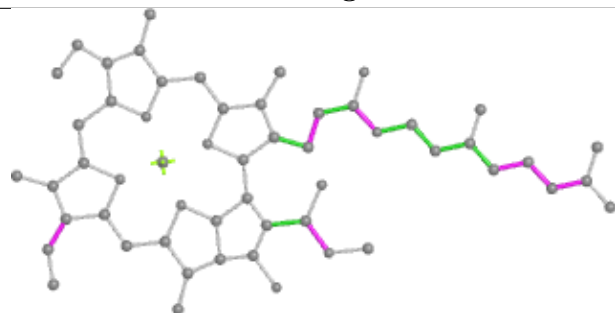
Ligand CLA S 613



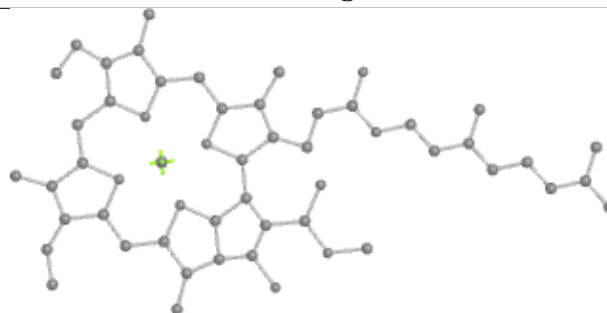
Bond lengths



Bond angles

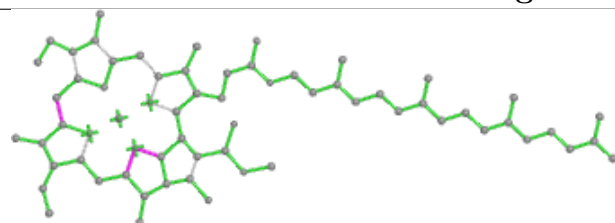


Torsions

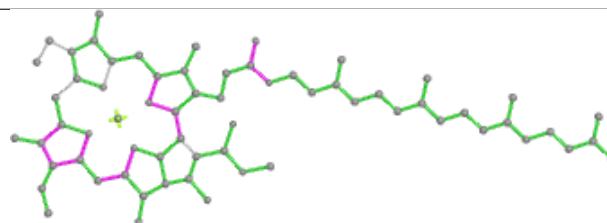


Rings

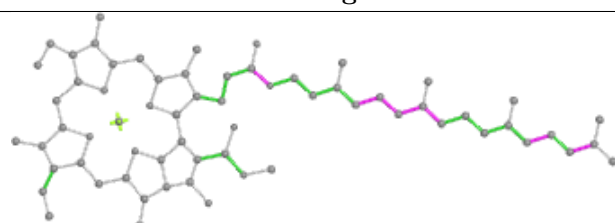
Ligand CLA Y 611



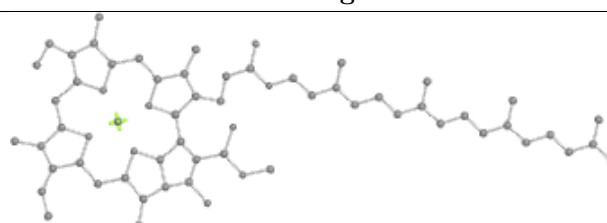
Bond lengths



Bond angles

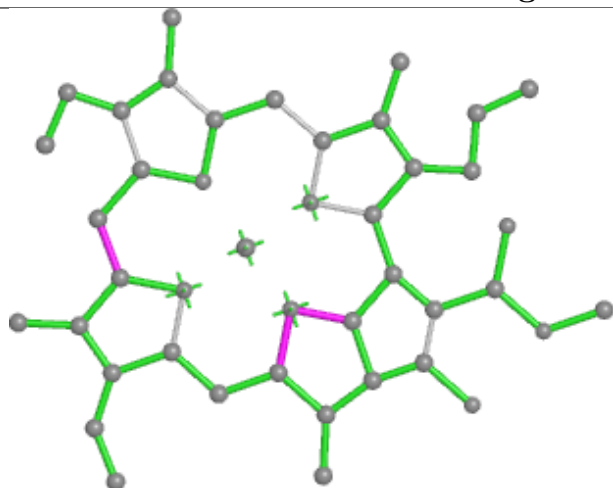


Torsions

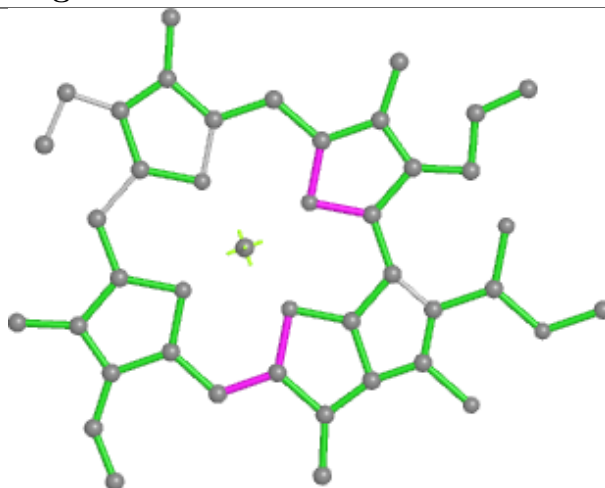


Rings

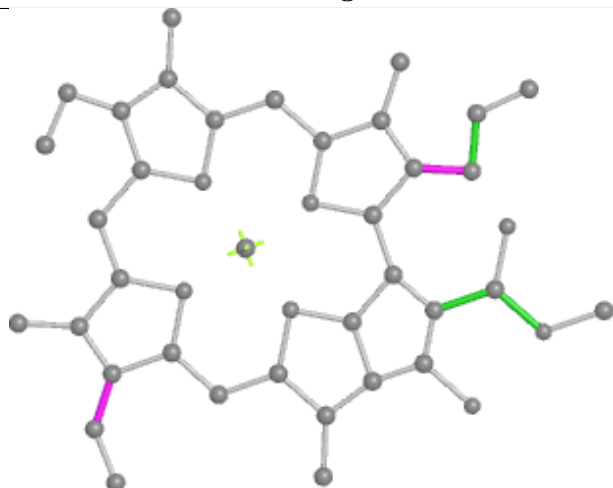
Ligand CLA g 612



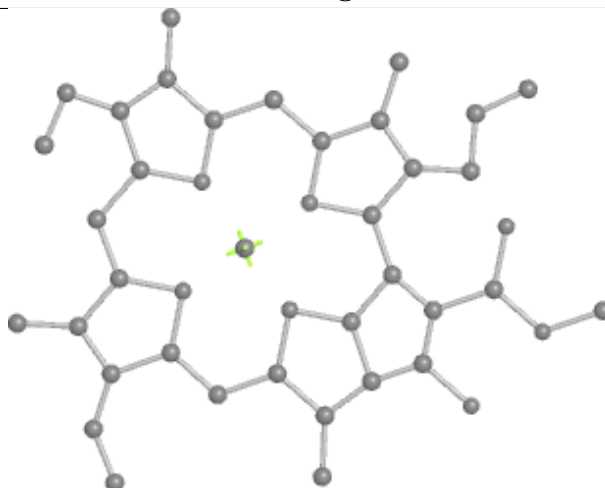
Bond lengths



Bond angles

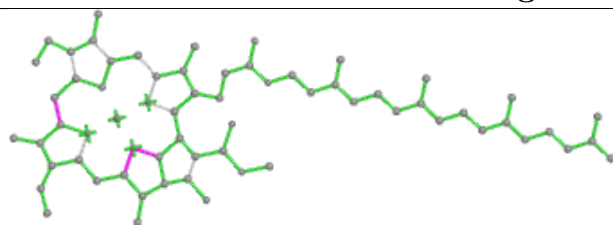


Torsions

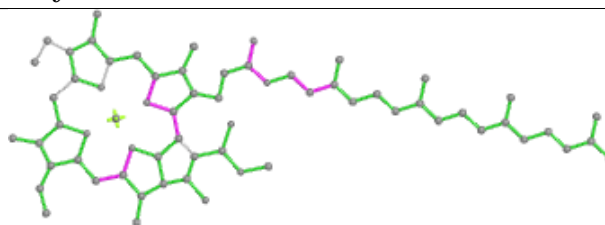


Rings

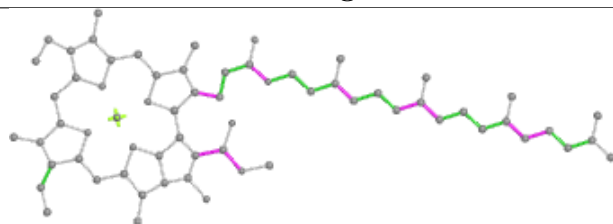
Ligand CLA y 604



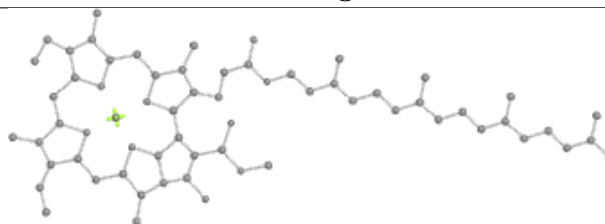
Bond lengths



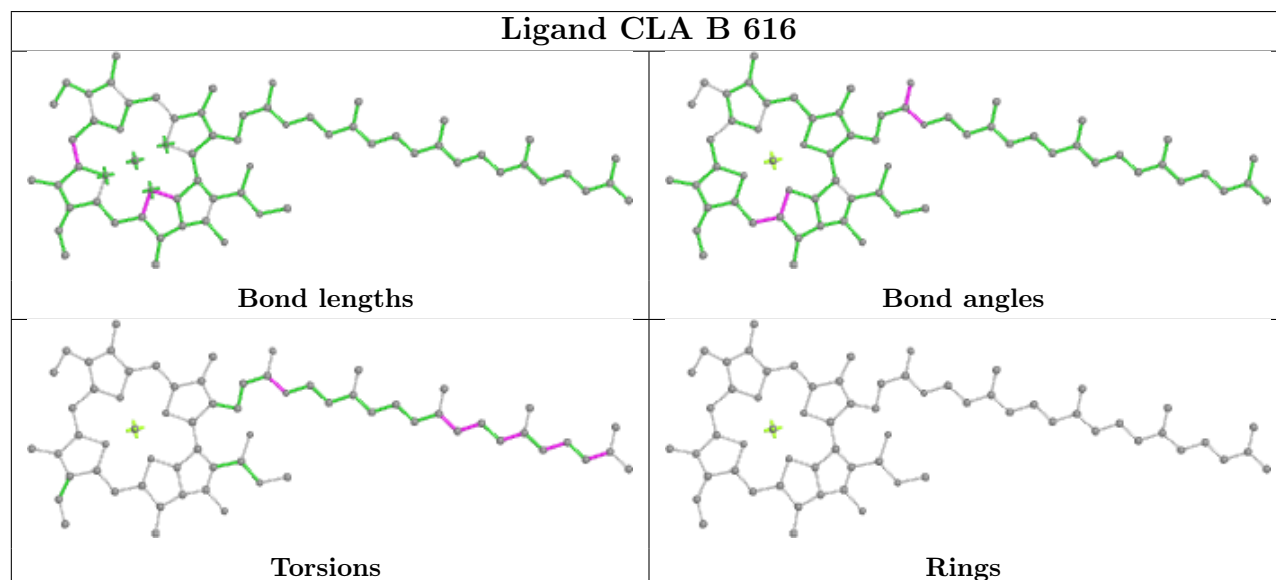
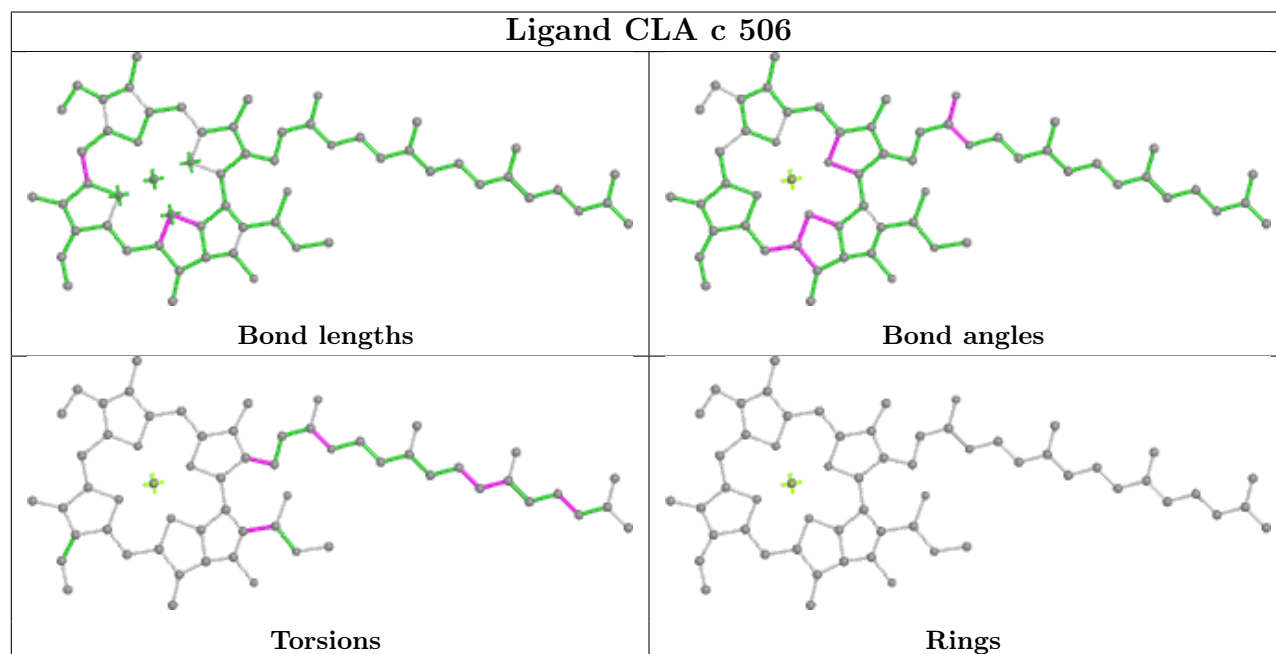
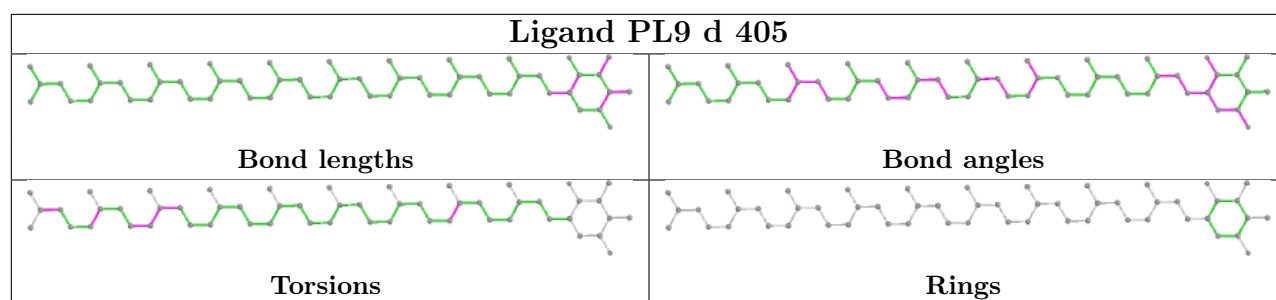
Bond angles

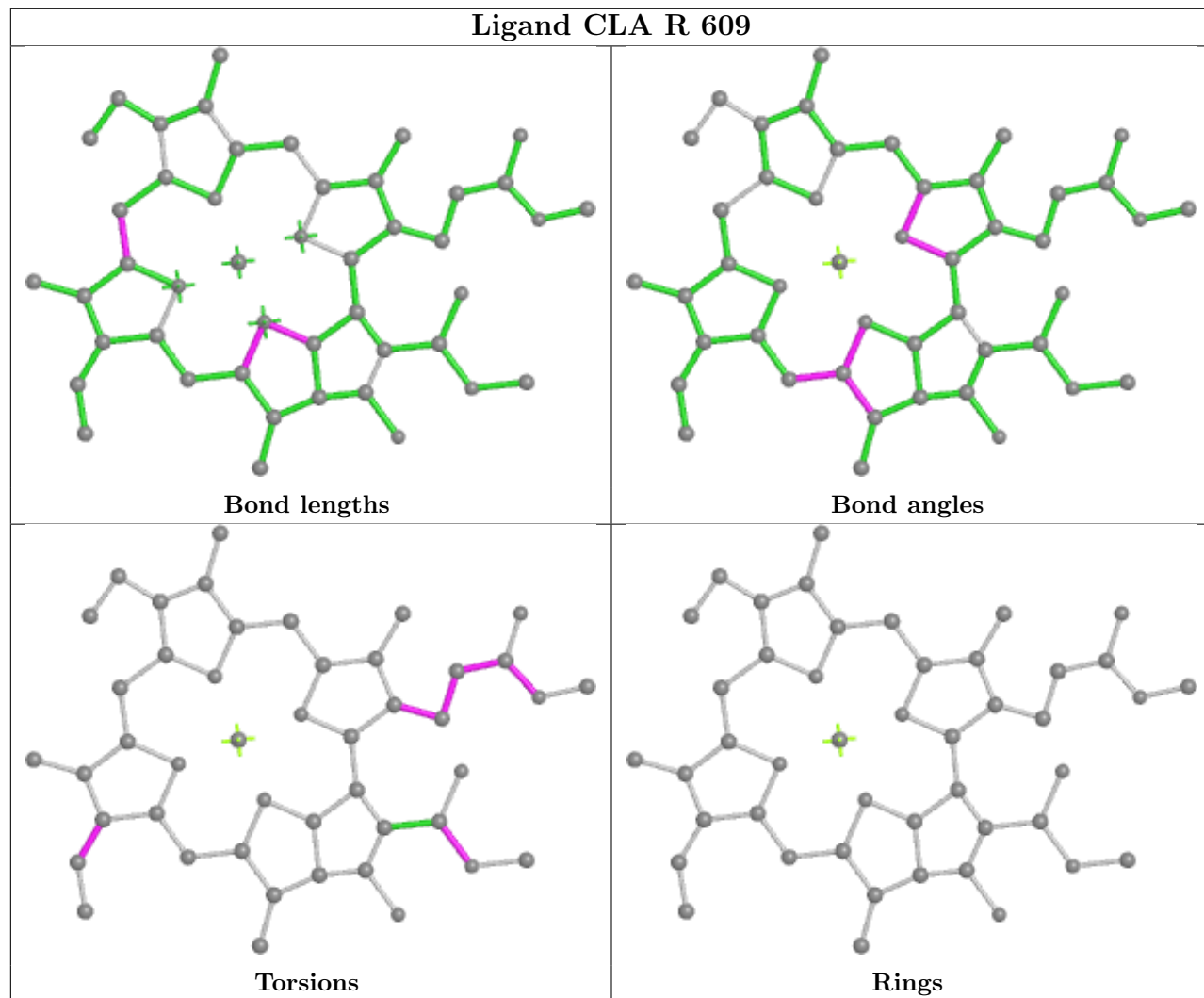
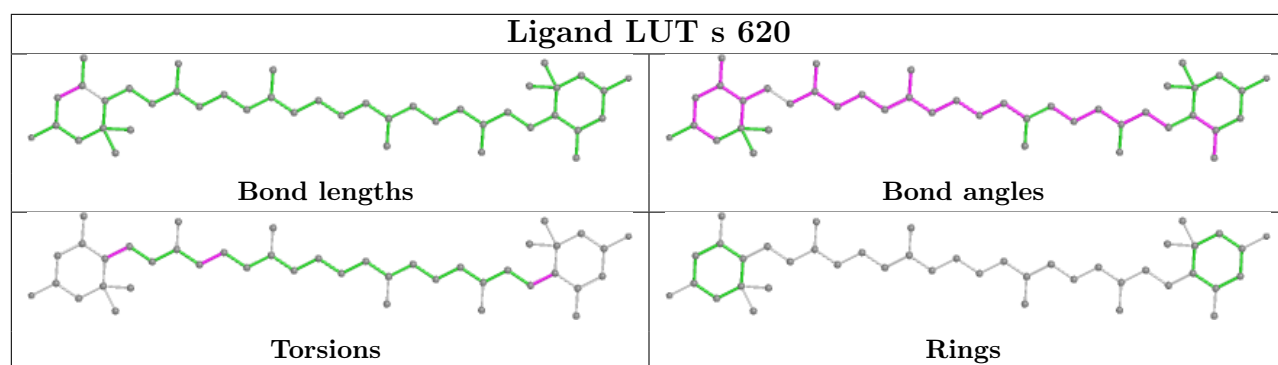


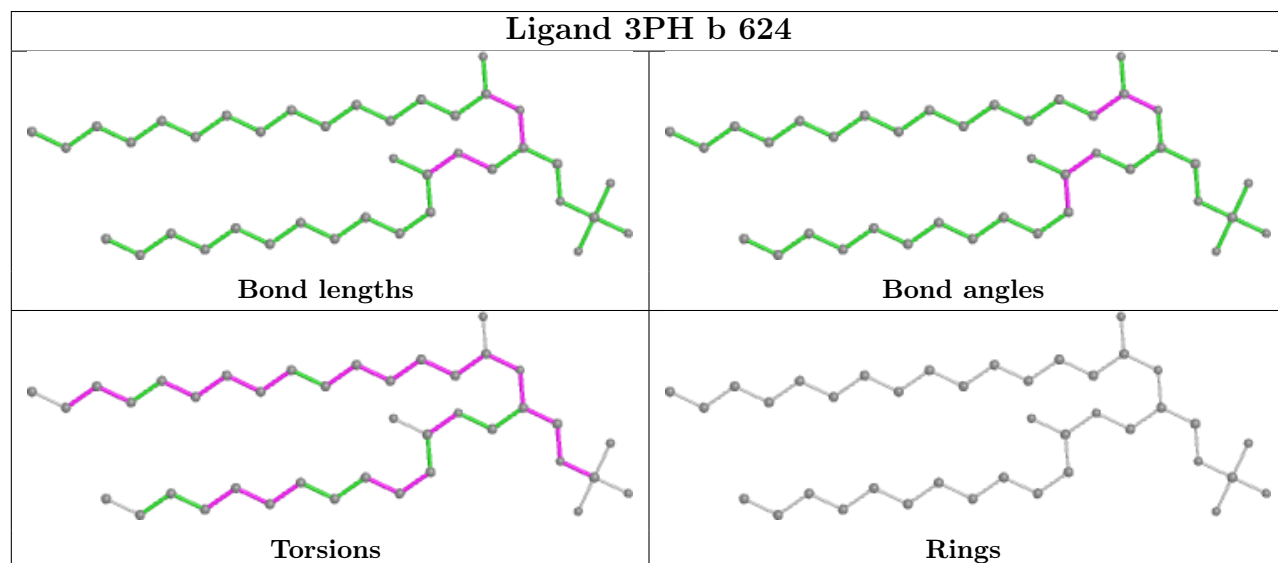
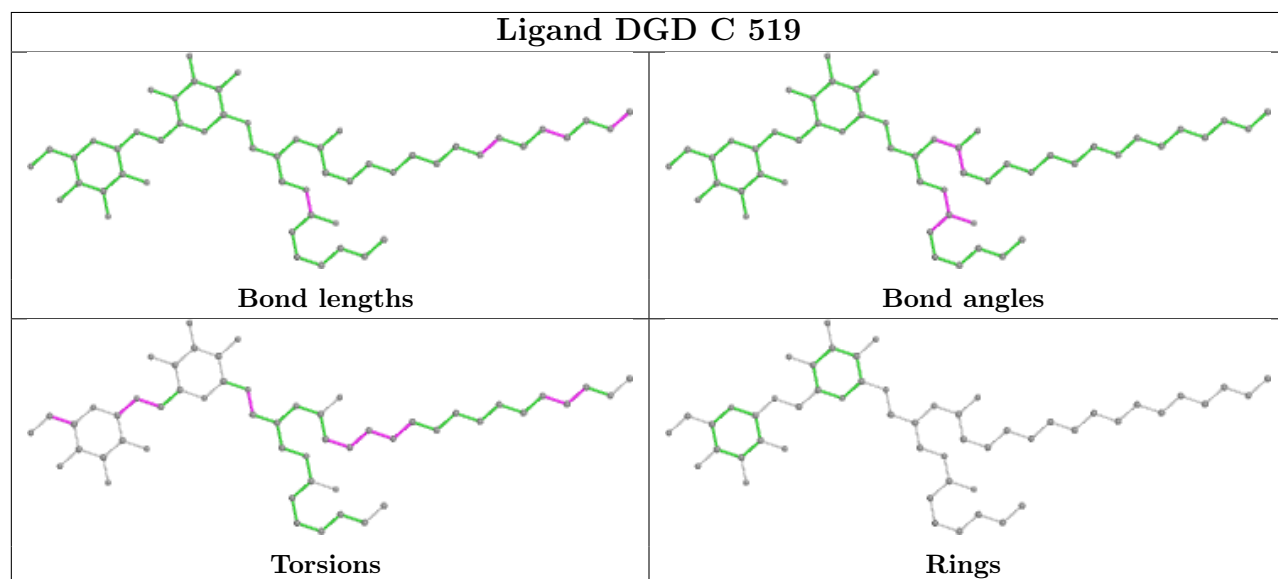
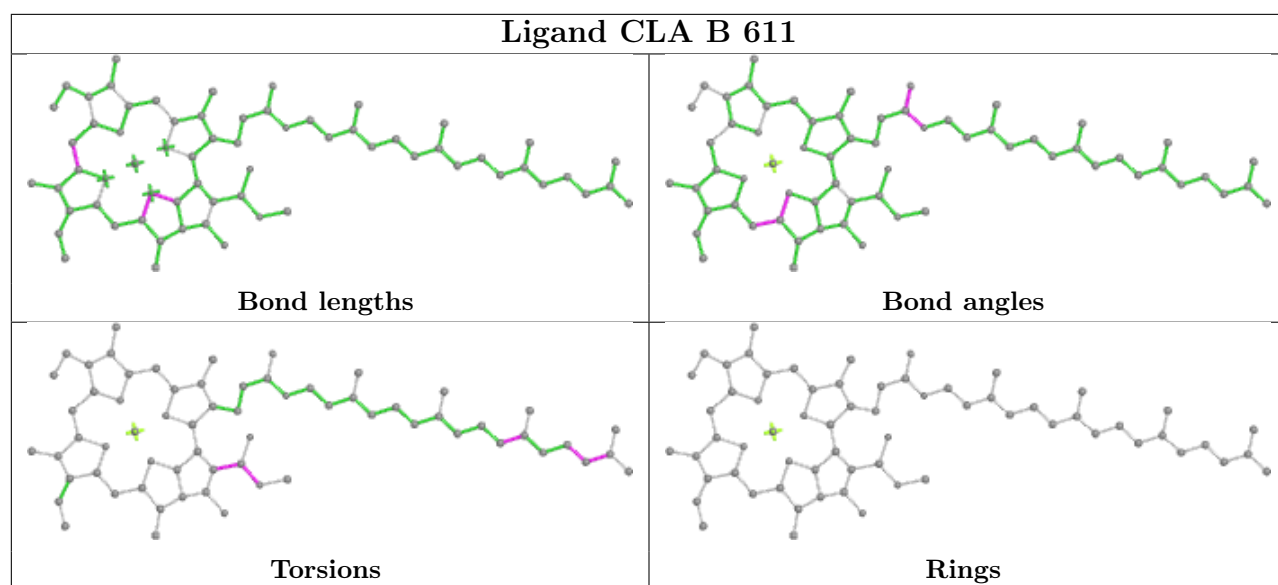
Torsions



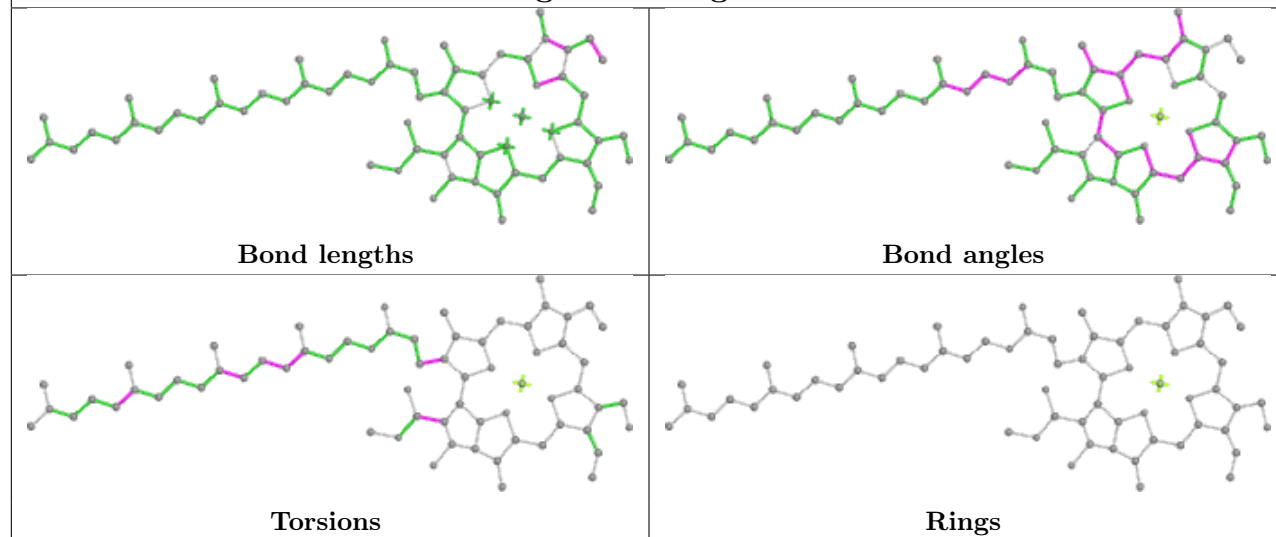
Rings



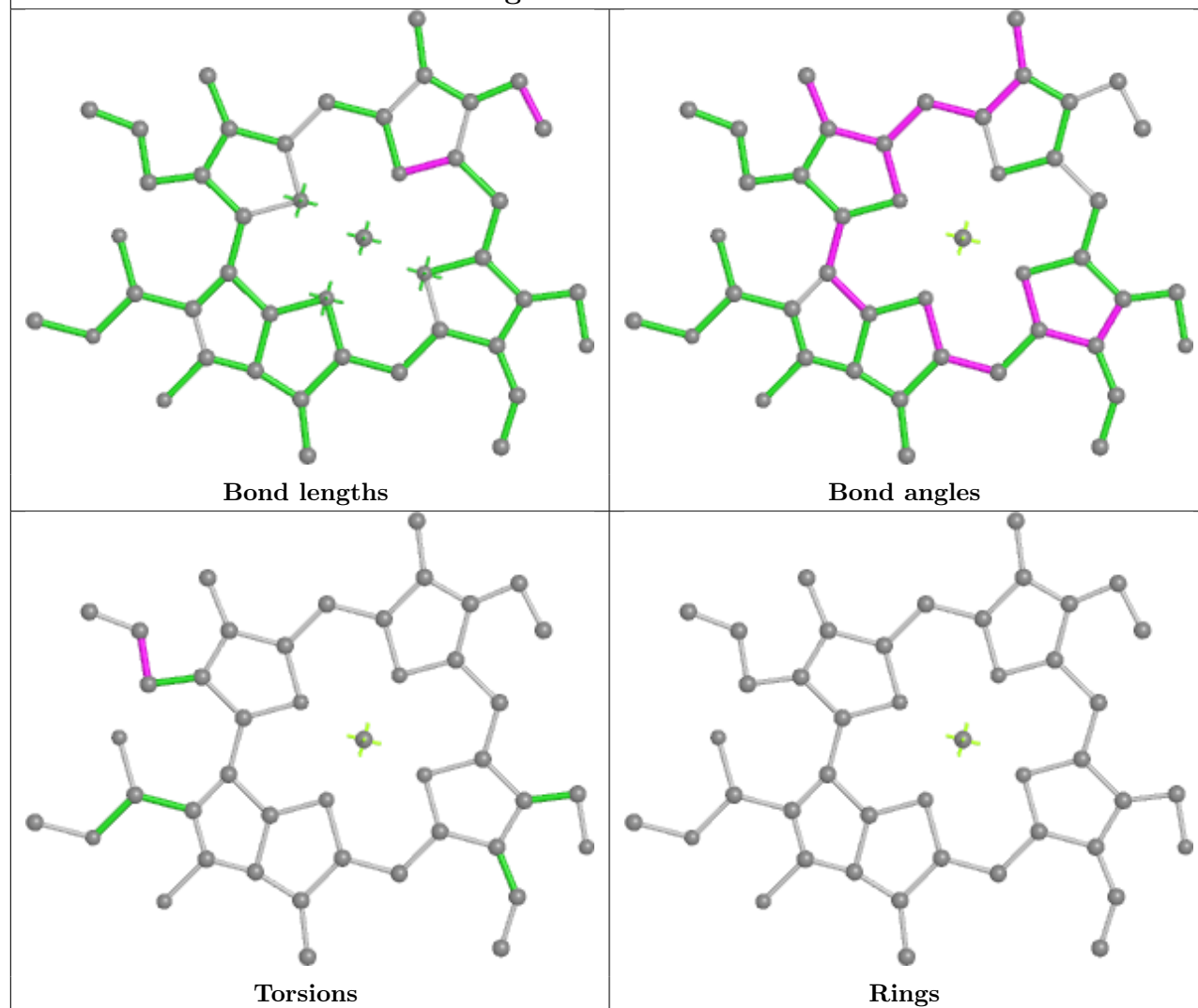


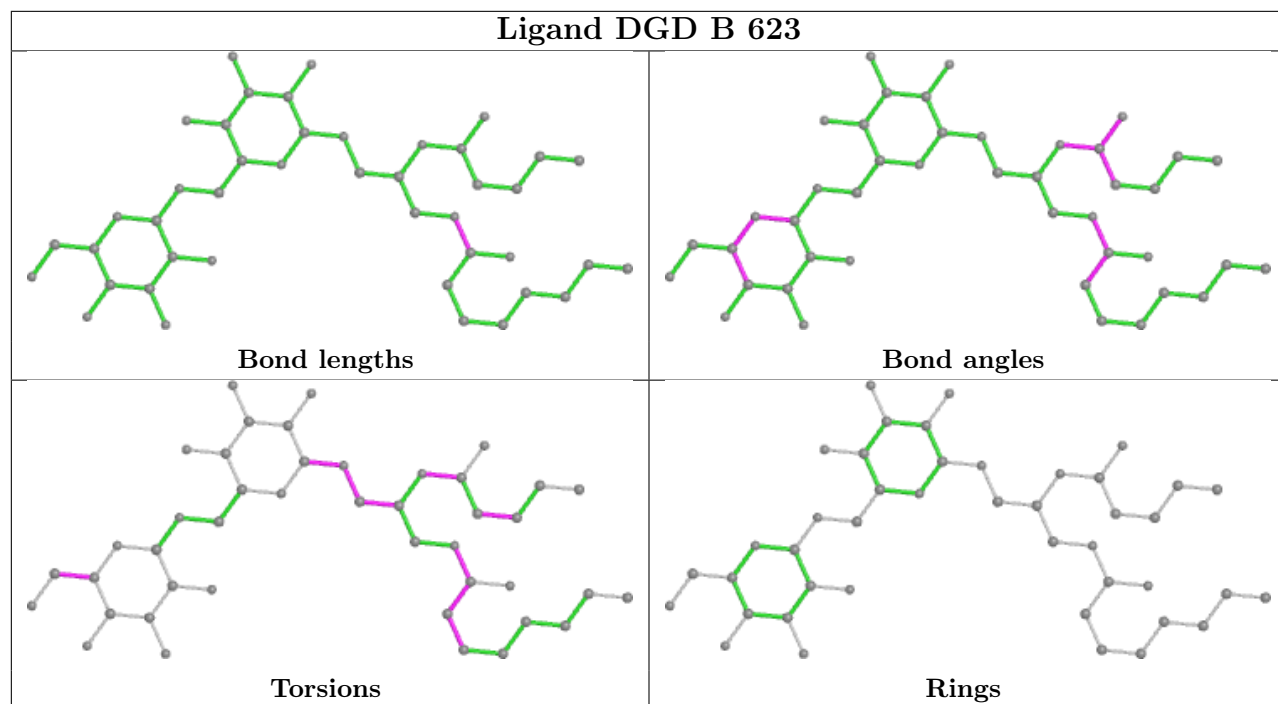
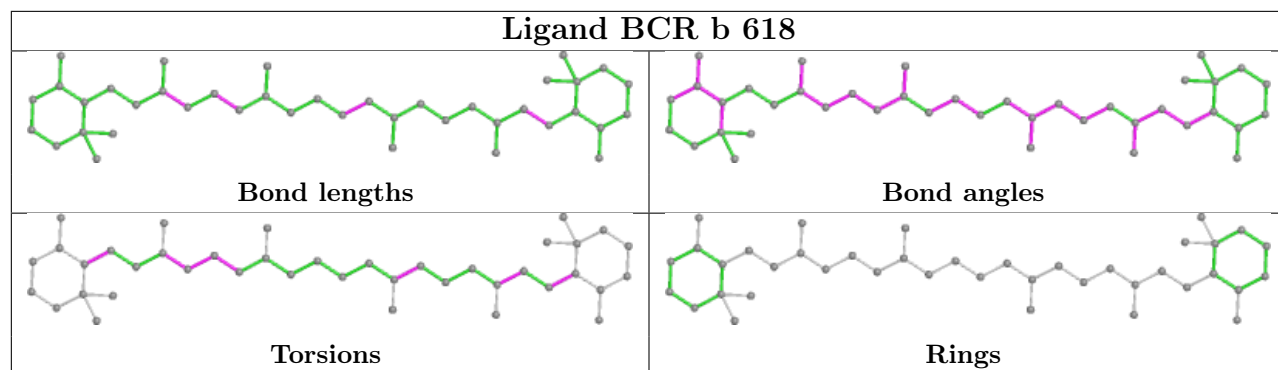


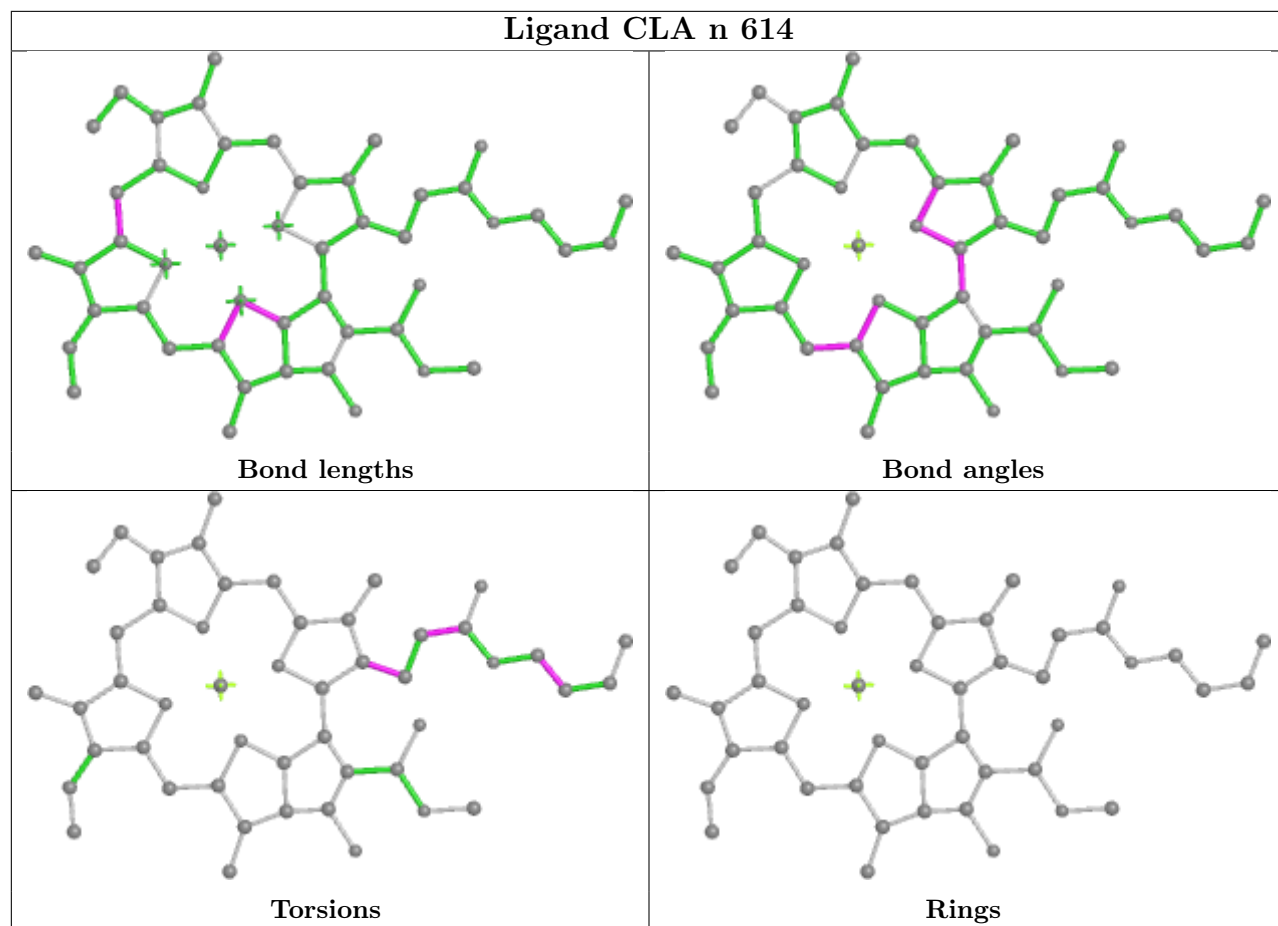
Ligand CHL g 601

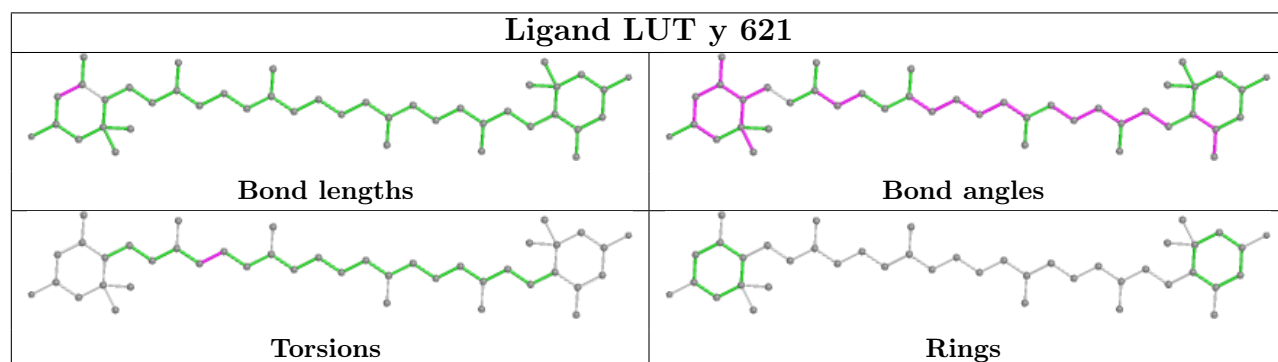
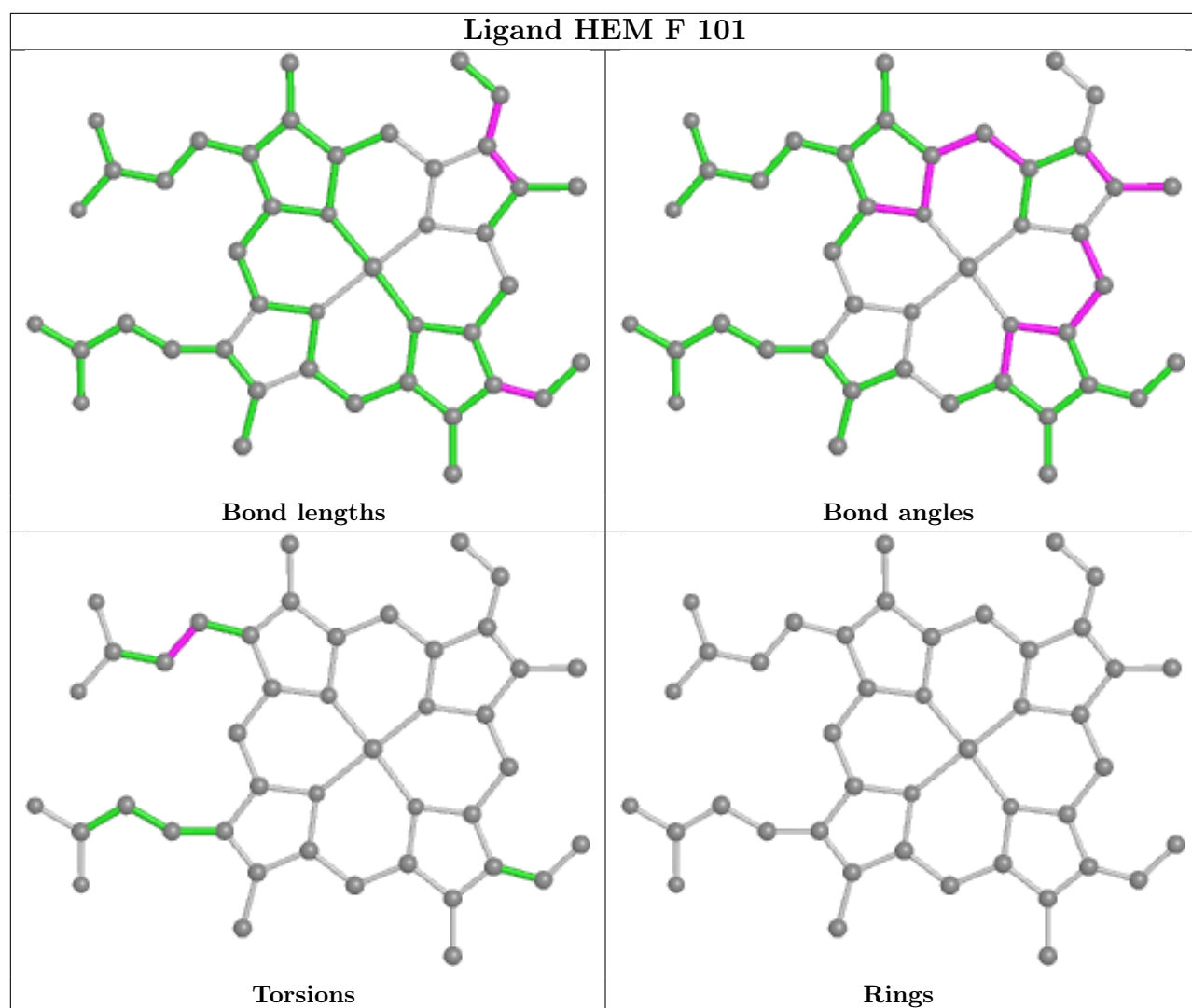


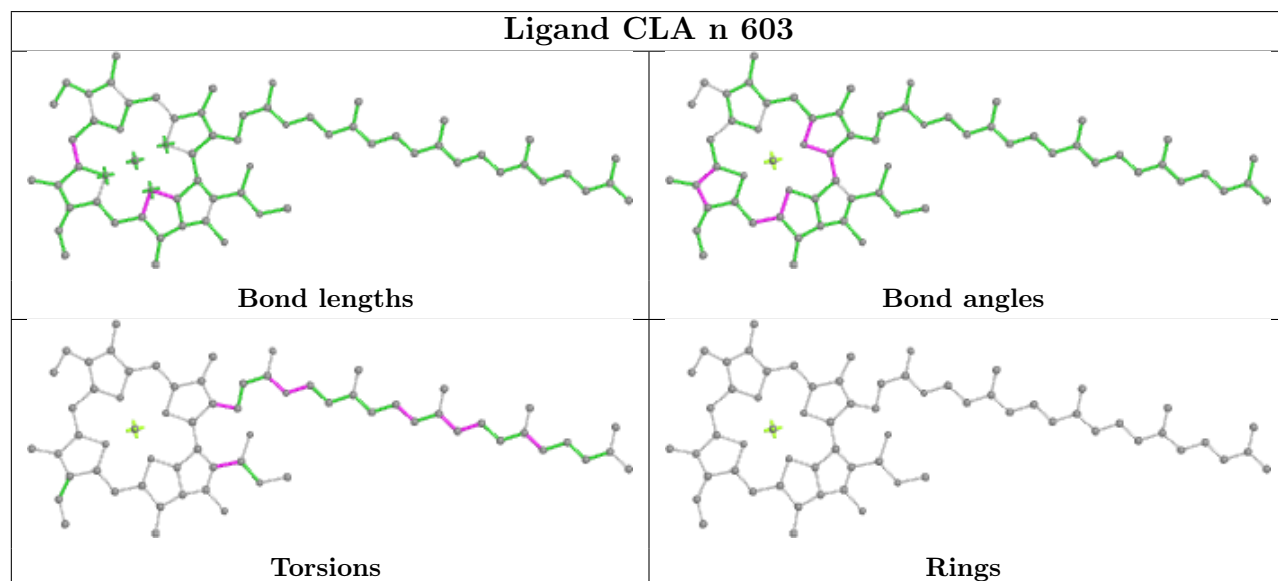
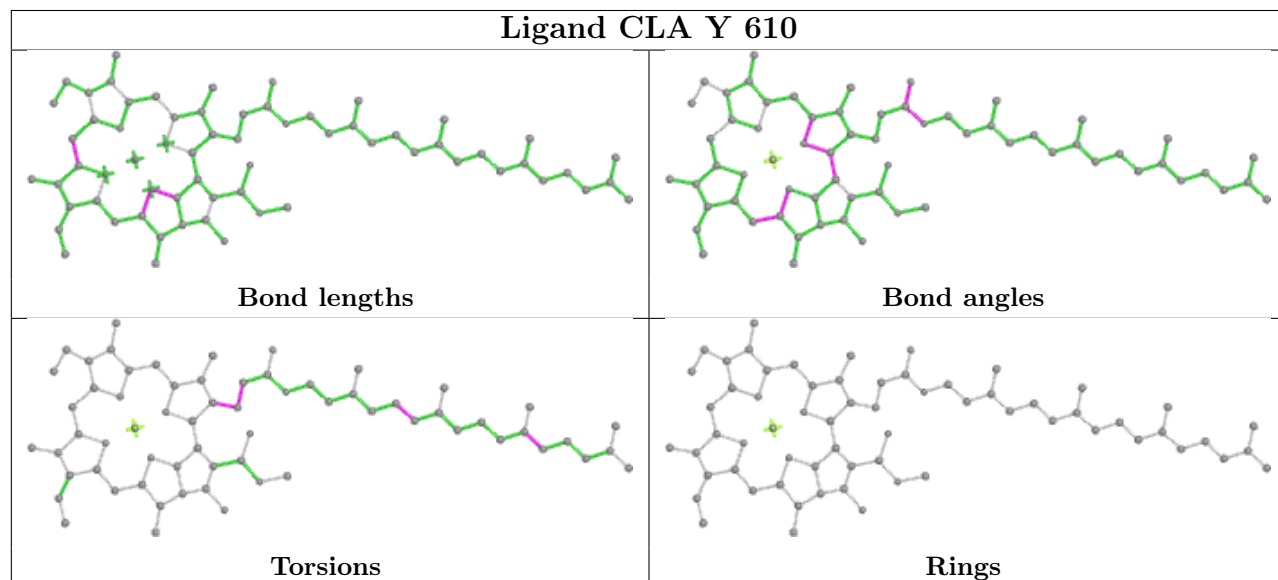
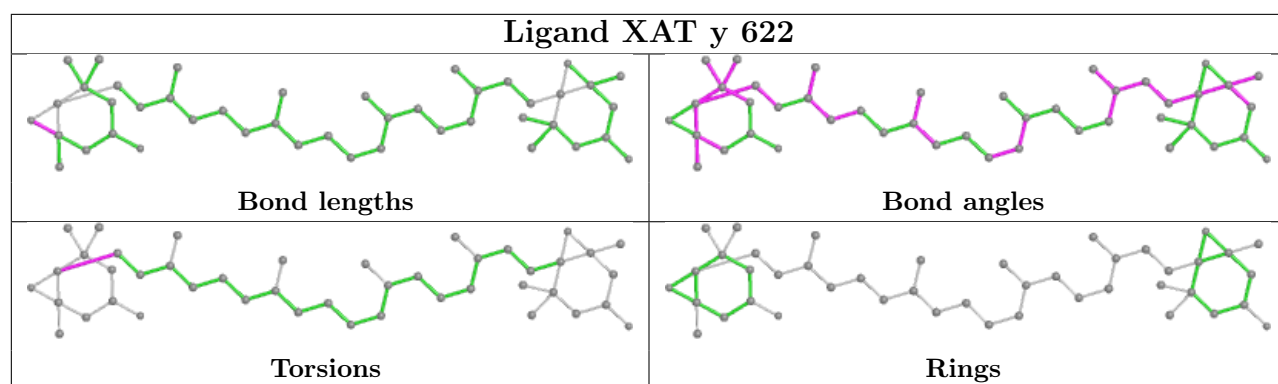
Ligand CHL s 606

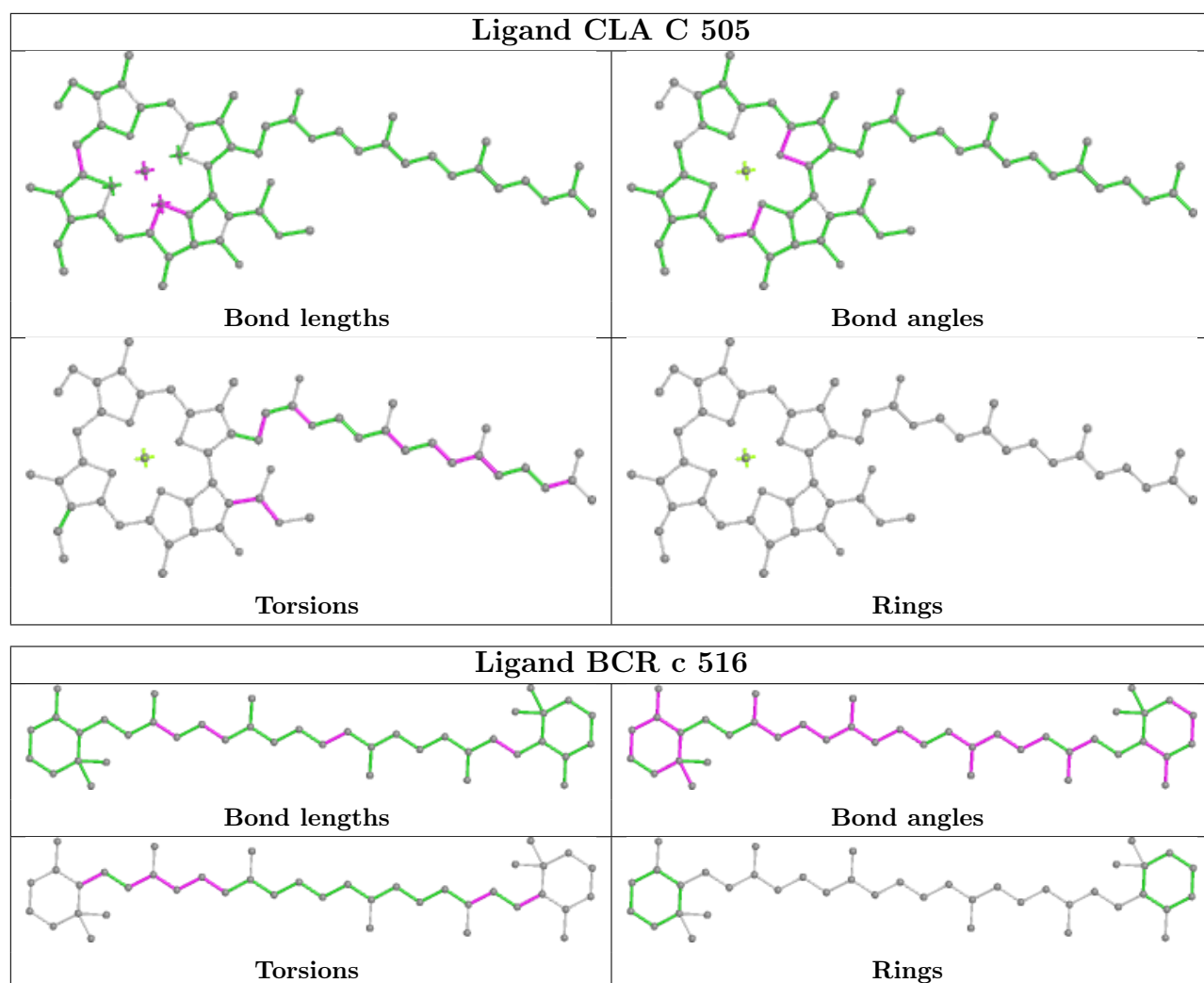


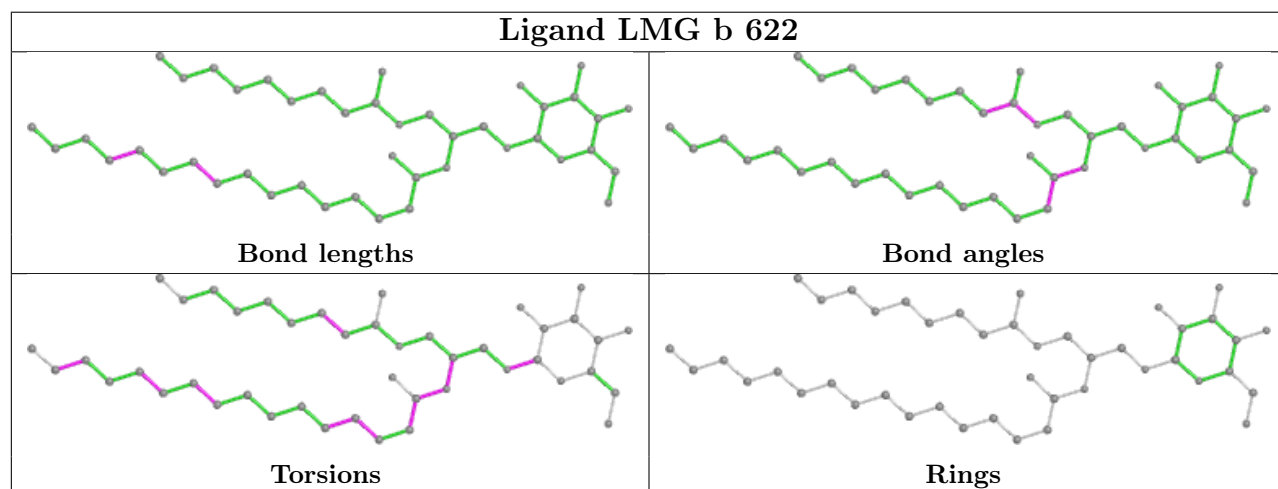
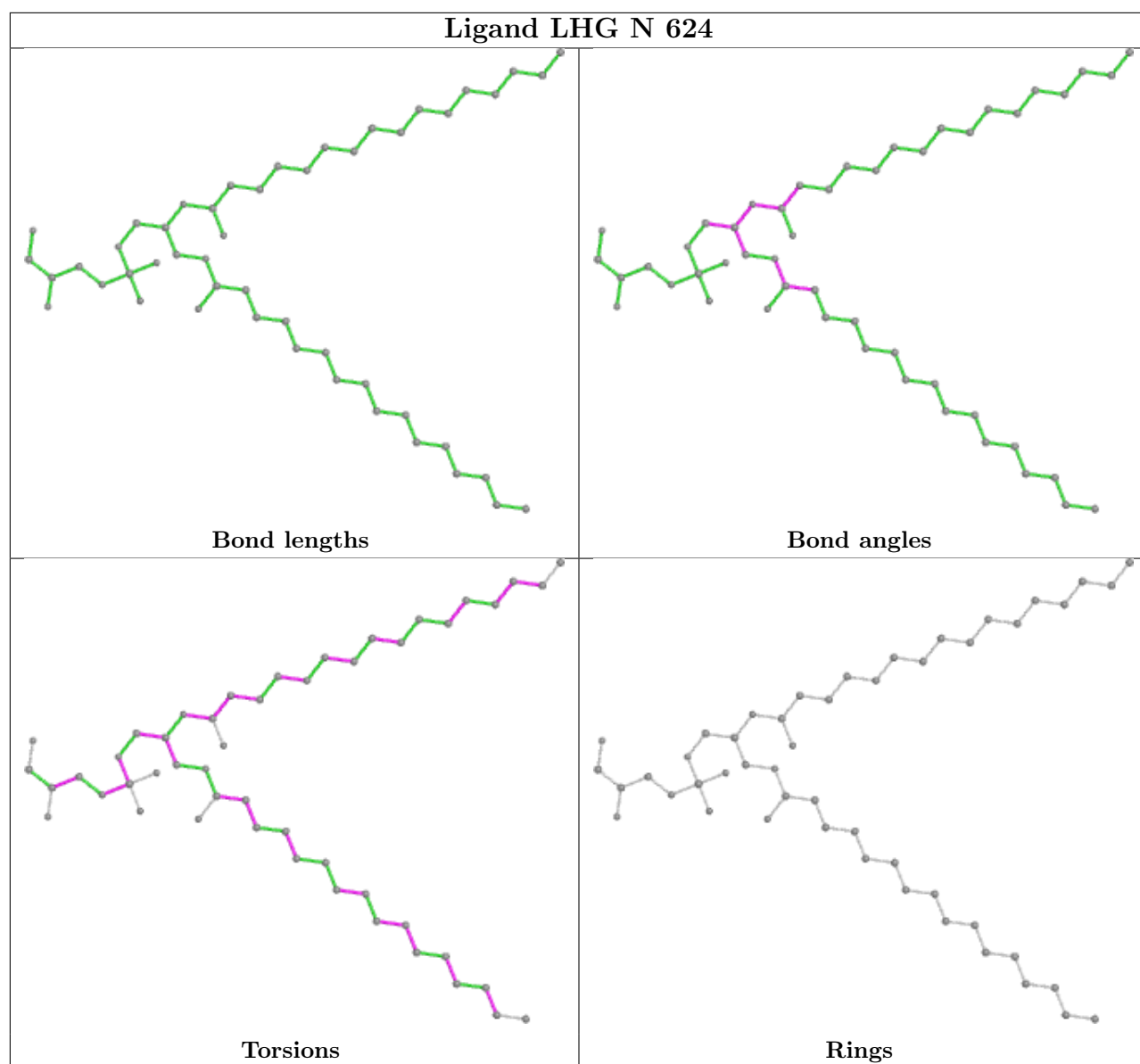




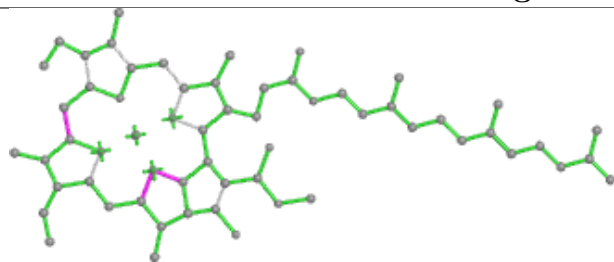




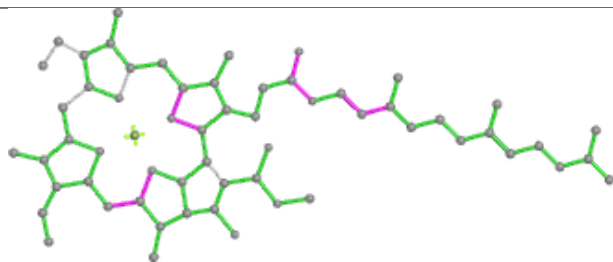




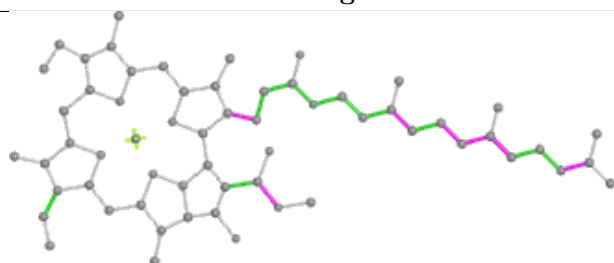
Ligand CLA R 610



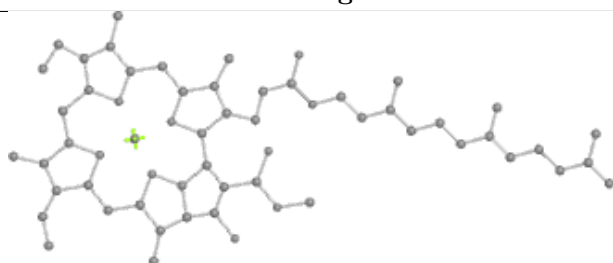
Bond lengths



Bond angles

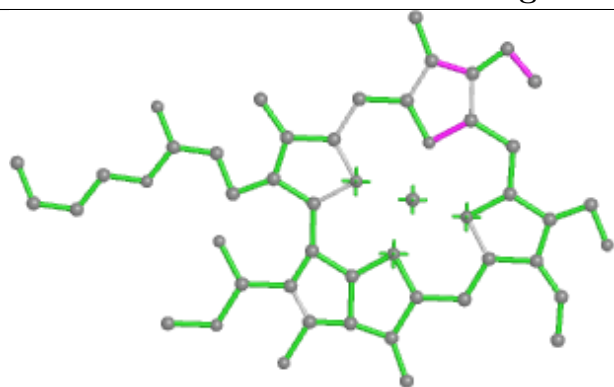


Torsions

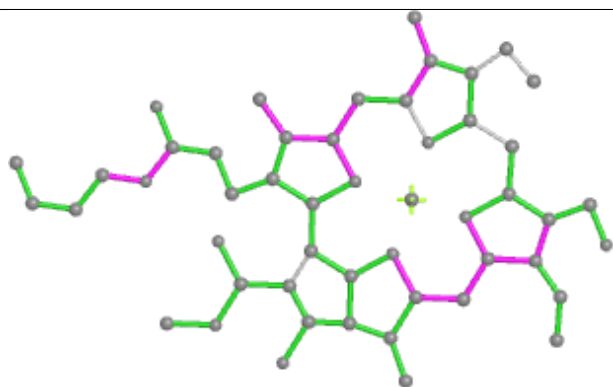


Rings

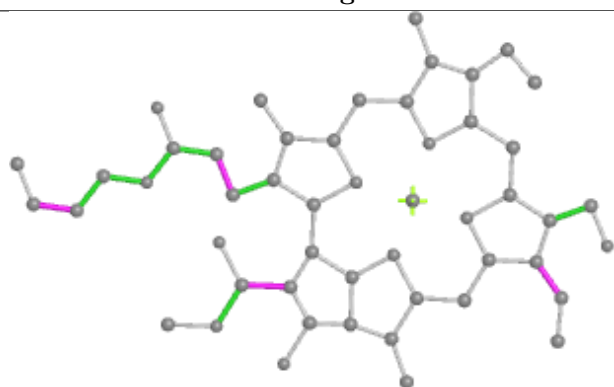
Ligand CHL r 607



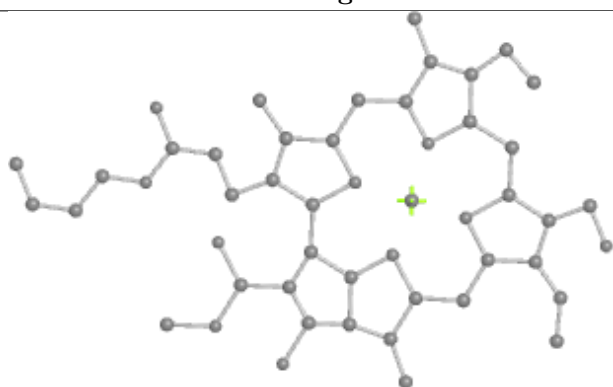
Bond lengths



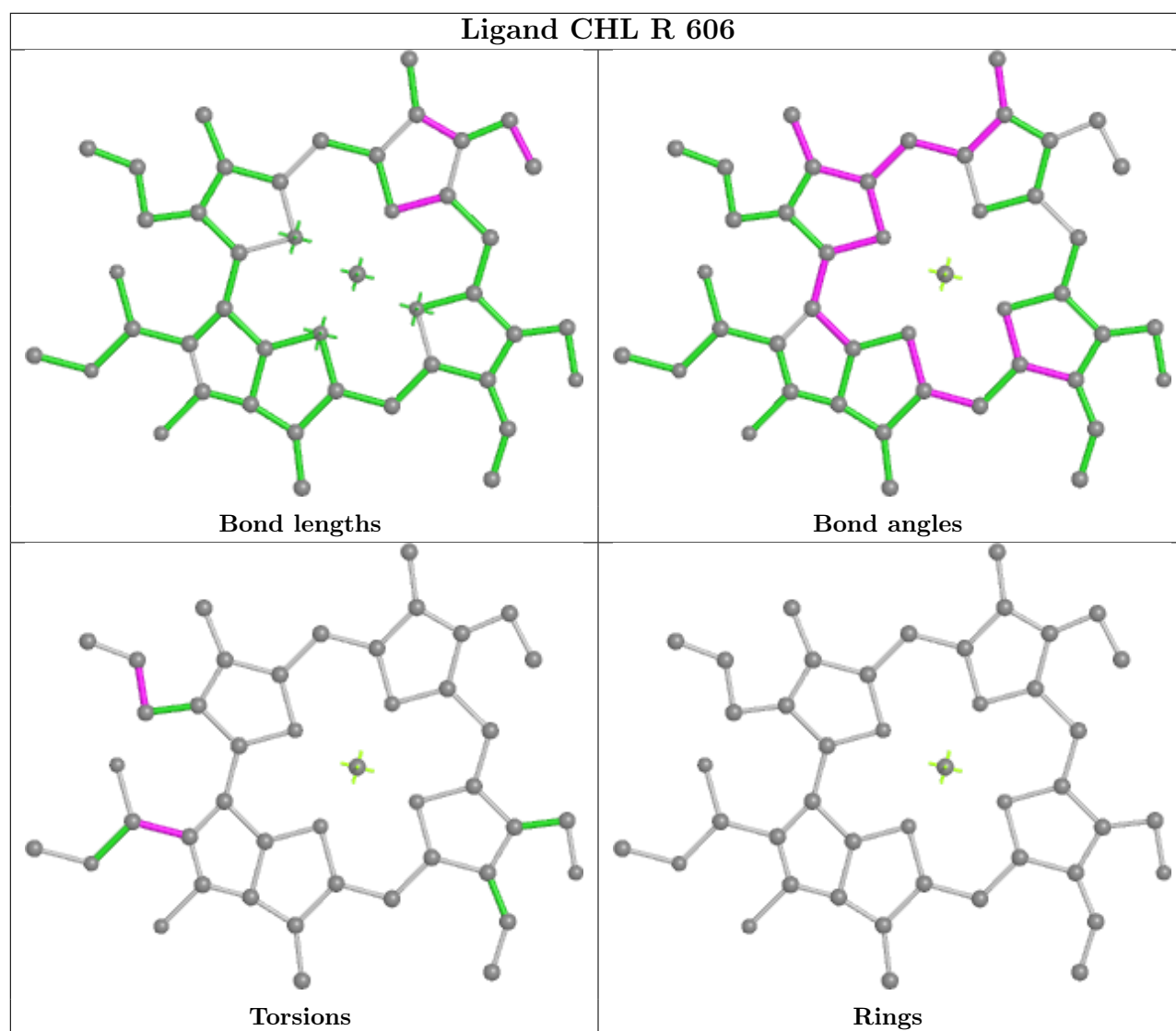
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.60
1	R	110:PRO	C	126:GLU	N	12.92

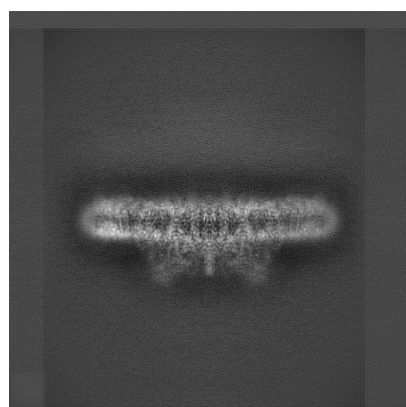
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13429. These allow visual inspection of the internal detail of the map and identification of artifacts.

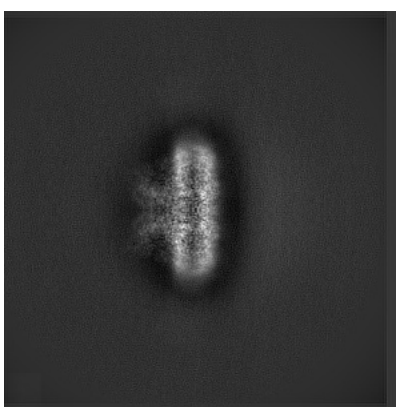
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

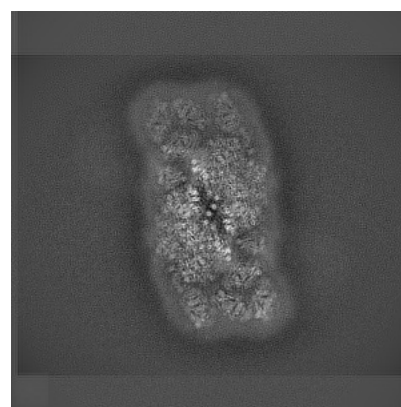
6.1.1 Primary map



X



Y

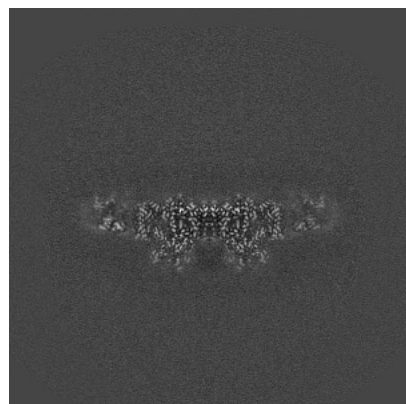


Z

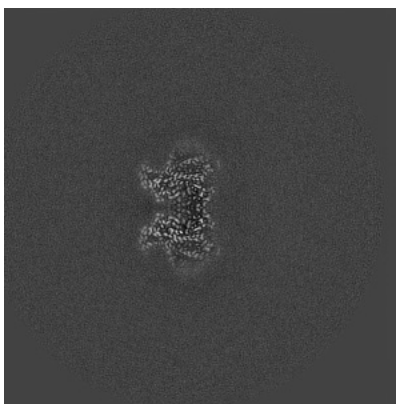
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

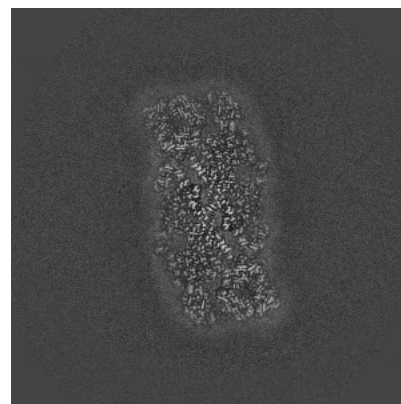
6.2.1 Primary map



X Index: 250



Y Index: 250

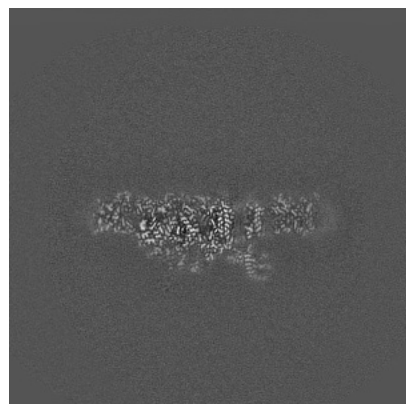


Z Index: 250

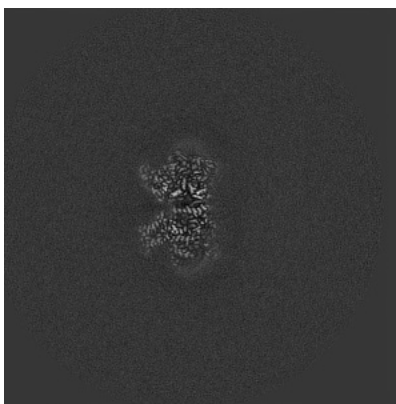
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

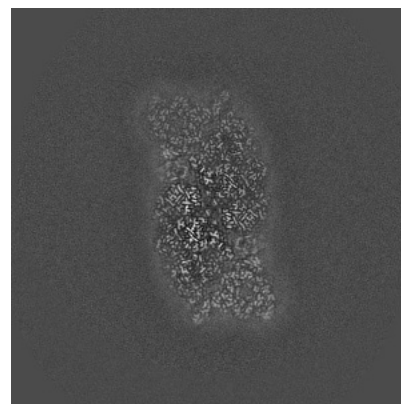
6.3.1 Primary map



X Index: 229



Y Index: 247



Z Index: 221

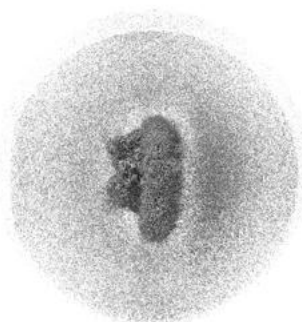
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

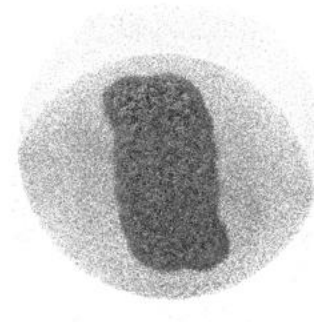
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

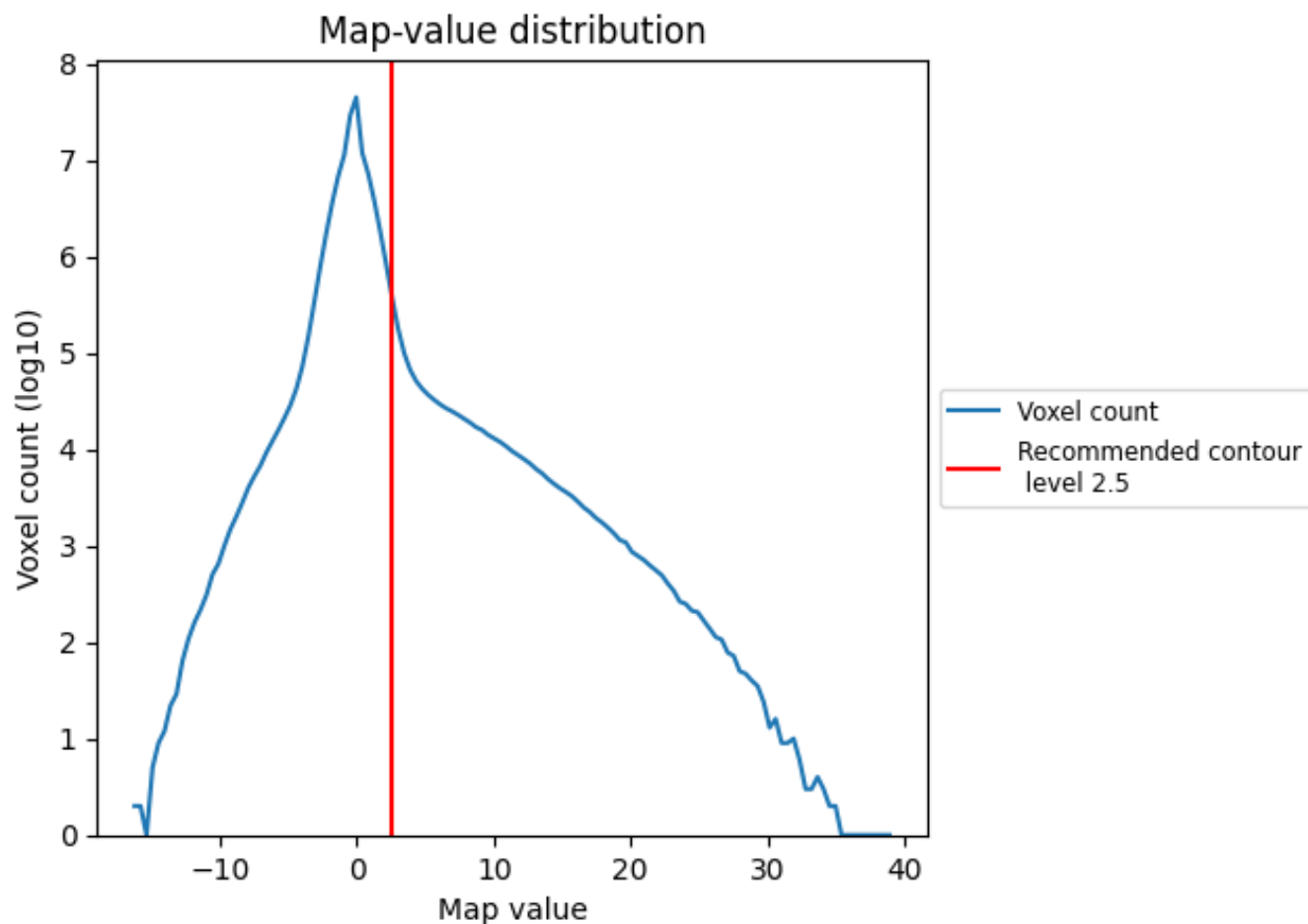
6.5 Mask visualisation

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

7 Map analysis [i](#)

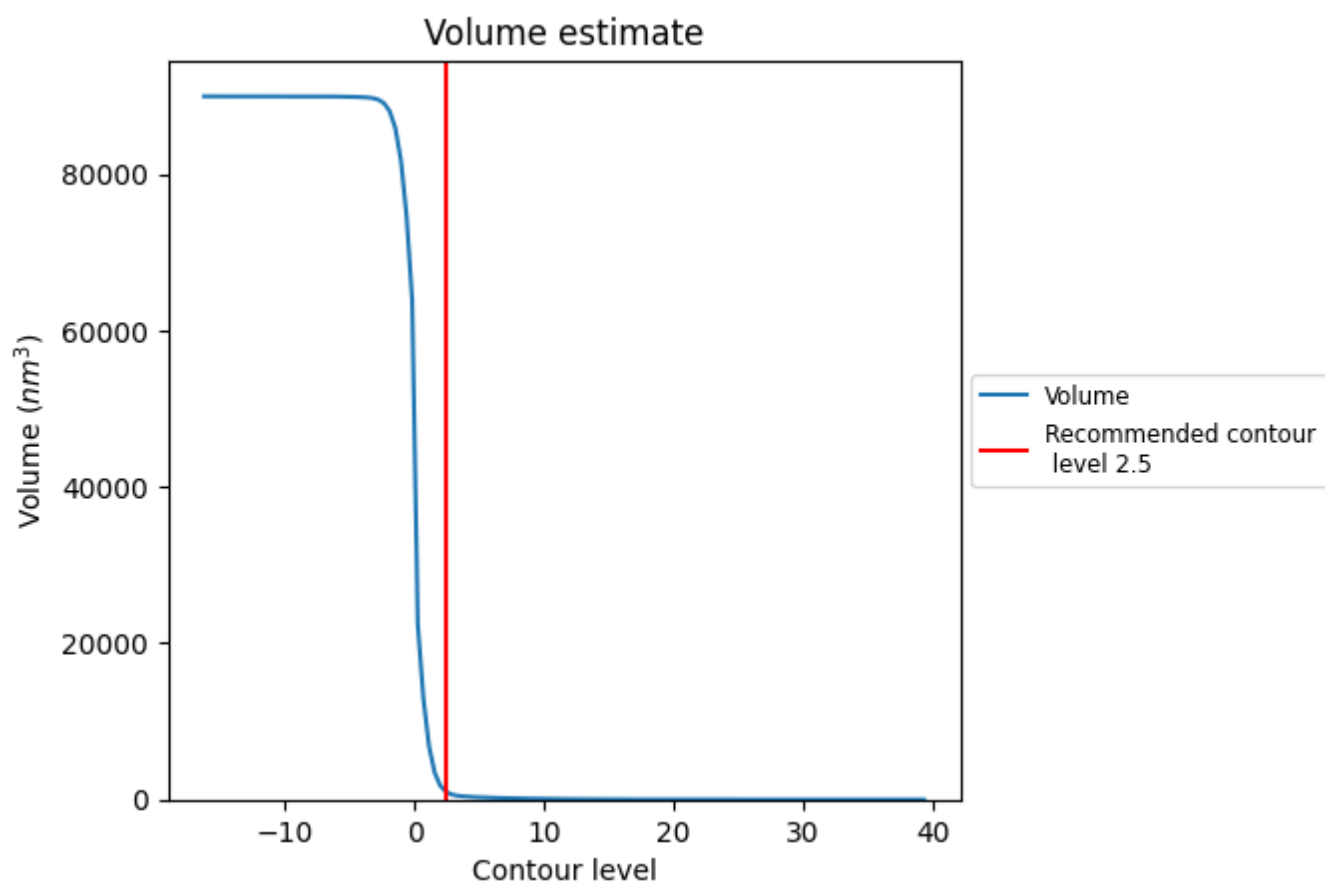
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

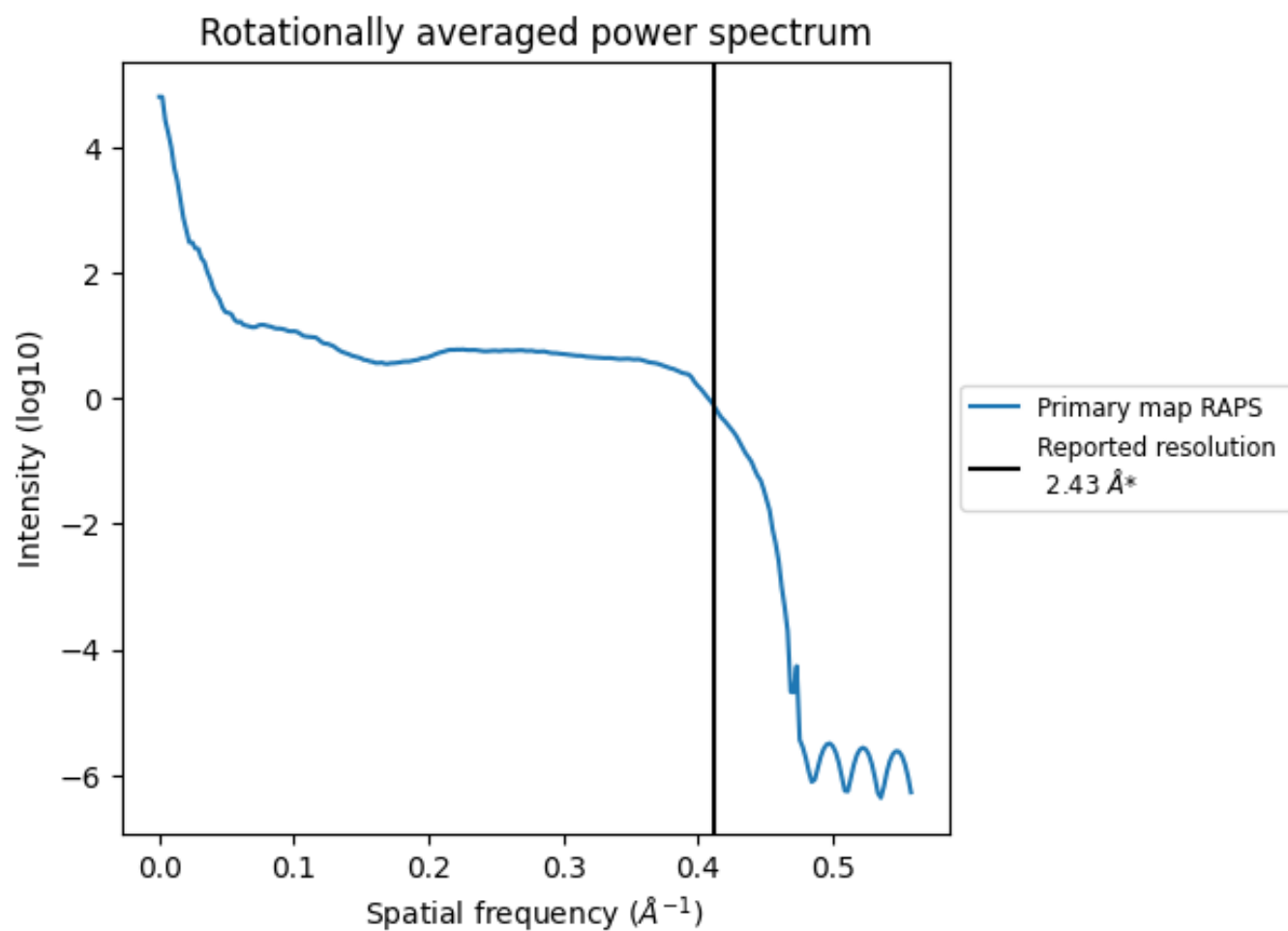
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm^3 ; this corresponds to an approximate mass of 856 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

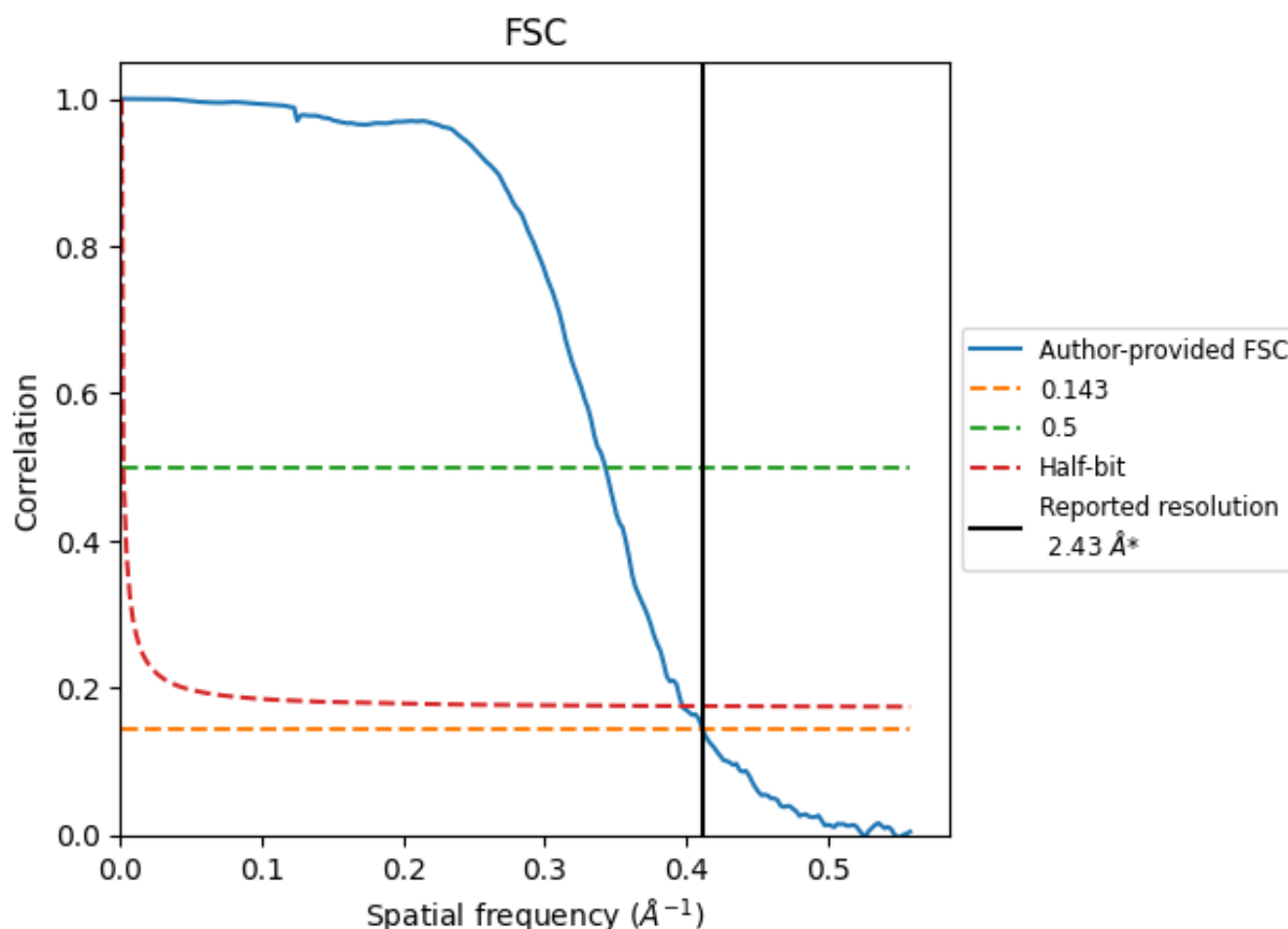


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

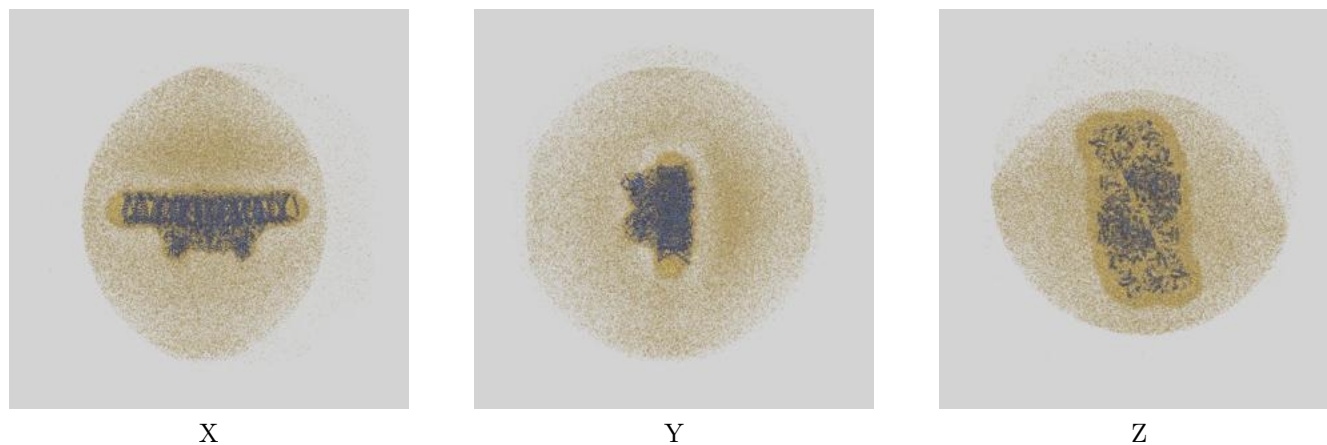
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

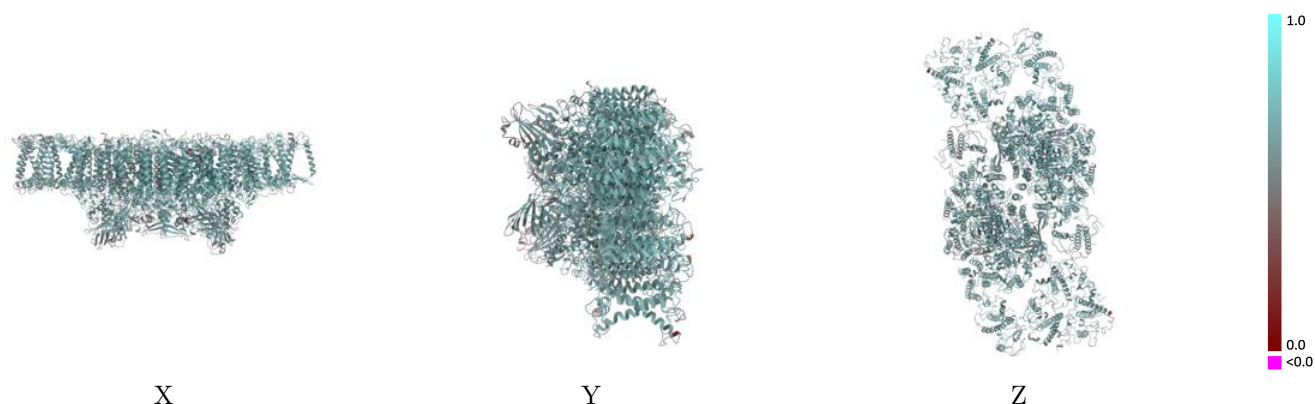
This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in section 3 on page 61.

9.1 Map-model overlay [i](#)



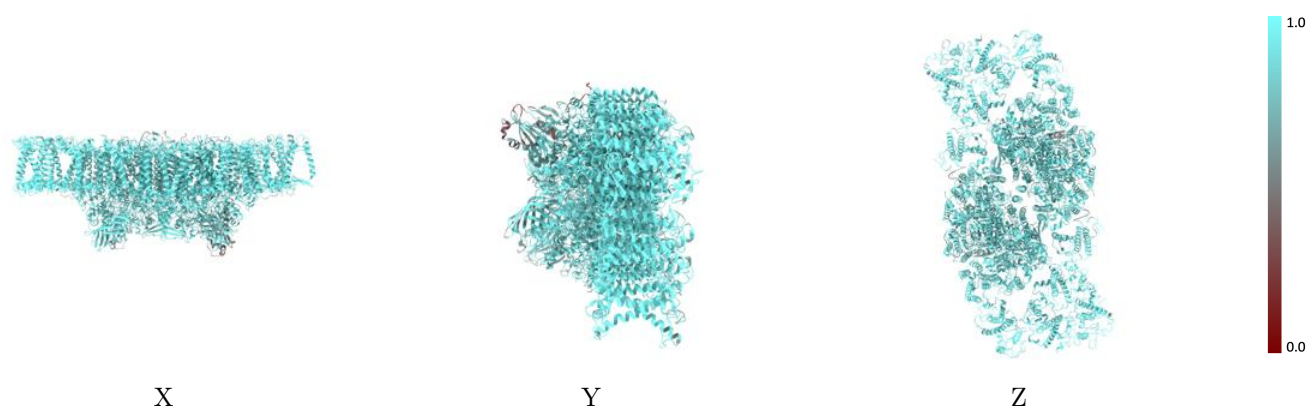
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



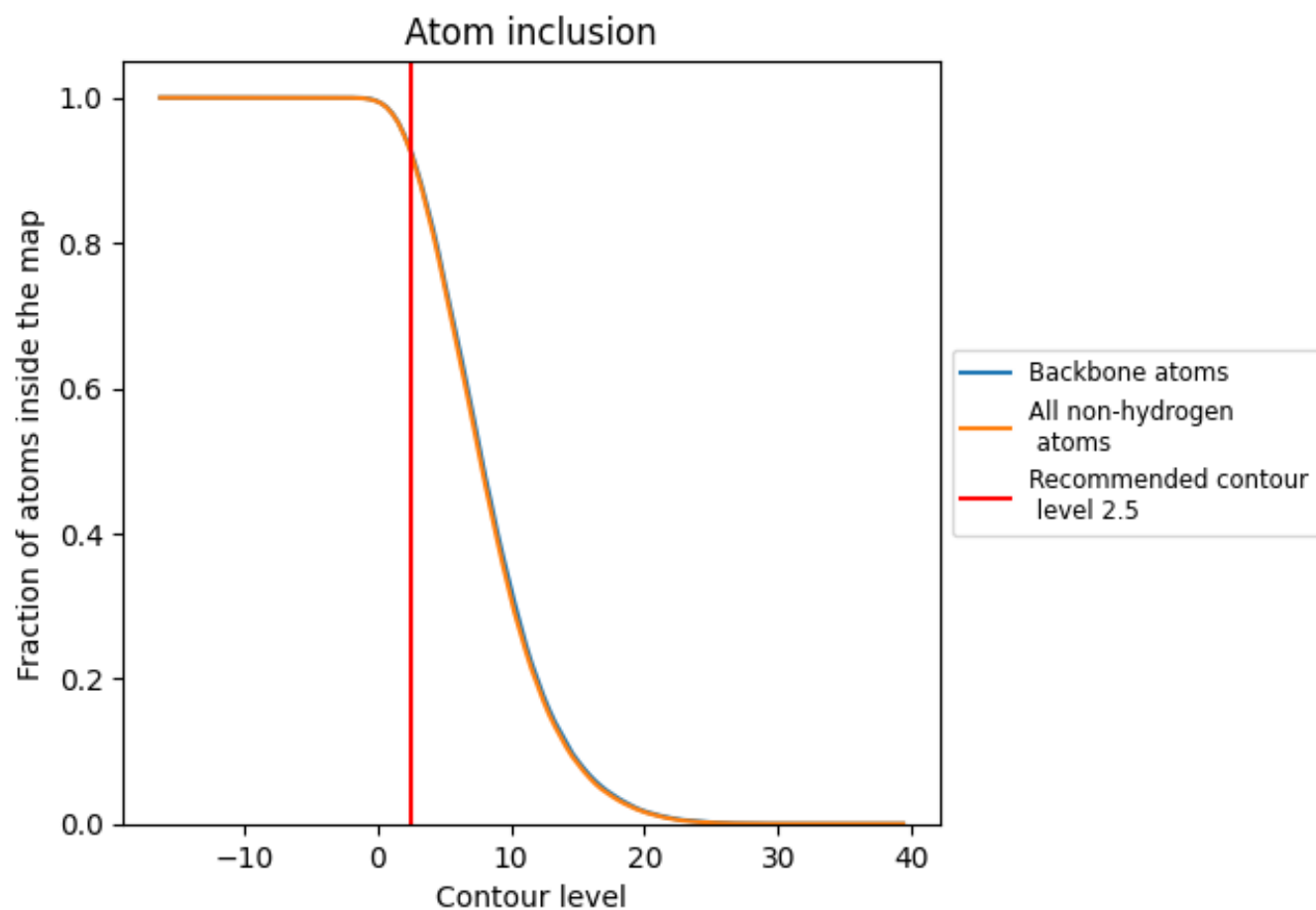
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6230
A	 0.9692	 0.6720
B	 0.9579	 0.6590
C	 0.9473	 0.6640
D	 0.9646	 0.6740
E	 0.9439	 0.6310
F	 0.9476	 0.6320
G	 0.8999	 0.6030
H	 0.9574	 0.6470
I	 0.9601	 0.6560
J	 0.9207	 0.6230
K	 0.9522	 0.6600
L	 0.9521	 0.6430
M	 0.9382	 0.6120
N	 0.9127	 0.6210
O	 0.8919	 0.5830
P	 0.6077	 0.5280
R	 0.8975	 0.5670
S	 0.9138	 0.6190
T	 0.9062	 0.6210
U	 0.8303	 0.5380
V	 0.9289	 0.6250
W	 0.9208	 0.5970
X	 0.8955	 0.5910
Y	 0.9183	 0.6310
Z	 0.9582	 0.6380
a	 0.9604	 0.6570
b	 0.9562	 0.6440
c	 0.9403	 0.6430
d	 0.9560	 0.6510
e	 0.9389	 0.5970
f	 0.9196	 0.5960
g	 0.9365	 0.5760
h	 0.9574	 0.6240
i	 0.9601	 0.6560



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.9069	 0.6080
k	 0.9556	 0.6300
l	 0.9662	 0.6480
m	 0.9491	 0.6110
n	 0.9434	 0.6050
o	 0.8975	 0.5620
p	 0.7120	 0.5100
r	 0.9079	 0.5520
s	 0.9204	 0.5880
t	 0.9097	 0.6220
u	 0.7936	 0.5120
v	 0.9156	 0.5980
w	 0.9071	 0.5810
x	 0.8856	 0.5720
y	 0.9345	 0.6200
z	 0.9538	 0.6090