



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 06:28 PM JST

PDB ID : 6KAC / pdb_00006kac
EMDB ID : EMD-9955
Title : Cryo-EM structure of the C2S2-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Sheng, X.; Li, A.J.; Song, D.F.; Liu, Z.F.
Deposited on : 2019-06-21
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

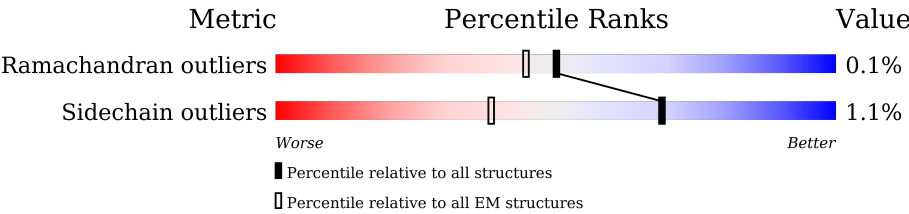
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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













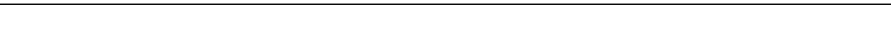
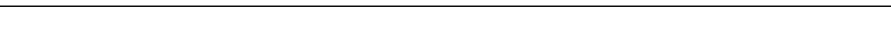
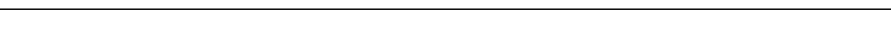
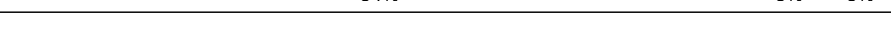
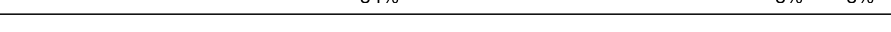








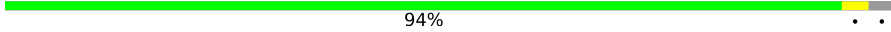
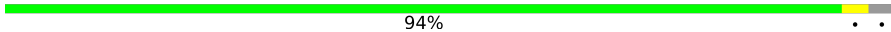
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	352	94% . 5%
1	a	352	94% . 5%
2	B	508	95% . .
2	b	508	95% . .
3	V	33	94% . .
3	v	33	94% . .
4	C	461	95% . .
4	c	461	96% . .
5	D	352	98% ..
5	d	352	98% ..




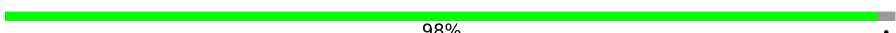
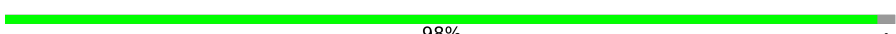









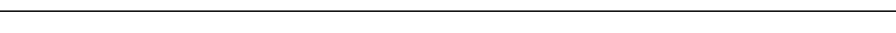
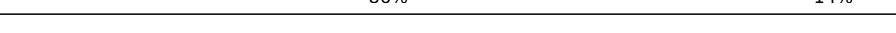


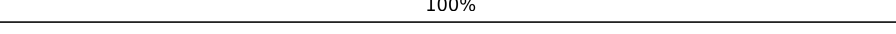
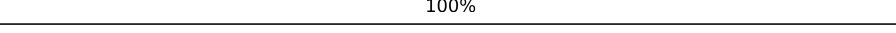
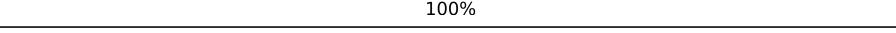
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Mol	Chain	Length	Quality of chain
6	E	82	 91% 7%
6	e	82	 91% 7%
7	F	44	 70% 30%
7	f	44	 70% 30%
8	H	88	 75% 23%
8	h	88	 75% 23%
9	I	37	 92% 5%
9	i	37	 92% 5%
10	J	42	 86% 14%
10	j	42	 86% 14%
11	K	46	 80% 20%
11	k	46	 80% 20%
12	L	38	 84% 8% 8%
12	l	38	 84% 8% 8%
13	M	34	 88% 12%
13	m	34	 88% 12%
14	O	291	 80% 18%
14	o	291	 80% 18%
15	P	245	 77% 23%
15	p	245	 76% 23%
16	Q	199	 73% 26%
16	q	199	 73% 26%
17	T	31	 94% . .
17	t	31	 94% . .
18	W	115	 48% 51%

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Mol	Chain	Length	Quality of chain
18	w	115	
19	X	101	
19	x	101	
20	Z	62	
20	z	62	
21	N	257	
21	n	257	
22	G	249	
22	g	249	
23	R	280	
23	r	280	
24	S	289	
24	s	289	
25	Y	256	
25	y	256	
26	U	178	
26	u	178	
27	0	25	
27	1	25	
28	3	25	
28	4	25	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	A	405	X	-	-	-
32	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	B	602	X	-	-	-
32	CLA	B	603	X	-	-	-
32	CLA	B	605	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-
32	CLA	B	609	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	612	X	-	-	-
32	CLA	B	613	X	-	-	-
32	CLA	B	614	X	-	-	-
32	CLA	B	615	X	-	-	-
32	CLA	B	616	X	-	-	-
32	CLA	B	617	X	-	-	-
32	CLA	C	501	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	504	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	D	402	X	-	-	-
32	CLA	G	602	X	-	-	-
32	CLA	G	603	X	-	-	-
32	CLA	G	604	X	-	-	-
32	CLA	G	610	X	-	-	-
32	CLA	G	611	X	-	-	-
32	CLA	G	612	X	-	-	-
32	CLA	G	614	X	-	-	-
32	CLA	N	602	X	-	-	-
32	CLA	N	603	X	-	-	-
32	CLA	N	604	X	-	-	-
32	CLA	N	610	X	-	-	-
32	CLA	N	611	X	-	-	-
32	CLA	N	612	X	-	-	-
32	CLA	N	614	X	-	-	-
32	CLA	R	602	X	-	-	-
32	CLA	R	603	X	-	-	-
32	CLA	R	604	X	-	-	-
32	CLA	R	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	R	610	X	-	-	-
32	CLA	S	602	X	-	-	-
32	CLA	S	603	X	-	-	-
32	CLA	S	604	X	-	-	-
32	CLA	S	605	X	-	-	-
32	CLA	S	609	X	-	-	-
32	CLA	S	610	X	-	-	-
32	CLA	S	611	X	-	-	-
32	CLA	S	612	X	-	-	-
32	CLA	S	614	X	-	-	-
32	CLA	Y	602	X	-	-	-
32	CLA	Y	603	X	-	-	-
32	CLA	Y	604	X	-	-	-
32	CLA	Y	610	X	-	-	-
32	CLA	Y	611	X	-	-	-
32	CLA	Y	612	X	-	-	-
32	CLA	Y	614	X	-	-	-
32	CLA	a	405	X	-	-	-
32	CLA	a	407	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-
32	CLA	b	616	X	-	-	-
32	CLA	b	617	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	d	402	X	-	-	-
32	CLA	g	602	X	-	-	-
32	CLA	g	603	X	-	-	-
32	CLA	g	604	X	-	-	-
32	CLA	g	610	X	-	-	-
32	CLA	g	611	X	-	-	-
32	CLA	g	612	X	-	-	-
32	CLA	g	614	X	-	-	-
32	CLA	n	602	X	-	-	-
32	CLA	n	603	X	-	-	-
32	CLA	n	604	X	-	-	-
32	CLA	n	610	X	-	-	-
32	CLA	n	611	X	-	-	-
32	CLA	n	612	X	-	-	-
32	CLA	n	614	X	-	-	-
32	CLA	r	602	X	-	-	-
32	CLA	r	603	X	-	-	-
32	CLA	r	604	X	-	-	-
32	CLA	r	609	X	-	-	-
32	CLA	r	610	X	-	-	-
32	CLA	s	602	X	-	-	-
32	CLA	s	603	X	-	-	-
32	CLA	s	604	X	-	-	-
32	CLA	s	605	X	-	-	-
32	CLA	s	609	X	-	-	-
32	CLA	s	610	X	-	-	-
32	CLA	s	611	X	-	-	-
32	CLA	s	612	X	-	-	-
32	CLA	s	614	X	-	-	-
32	CLA	y	602	X	-	-	-
32	CLA	y	603	X	-	-	-
32	CLA	y	604	X	-	-	-
32	CLA	y	610	X	-	-	-
32	CLA	y	611	X	-	-	-
32	CLA	y	612	X	-	-	-
32	CLA	y	614	X	-	-	-
43	CHL	G	601	X	-	-	-
43	CHL	G	605	X	-	-	-
43	CHL	G	606	X	-	-	-
43	CHL	G	607	X	-	-	-
43	CHL	G	608	X	-	-	-
43	CHL	G	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	CHL	N	601	X	-	-	-
43	CHL	N	605	X	-	-	-
43	CHL	N	606	X	-	-	-
43	CHL	N	607	X	-	-	-
43	CHL	N	608	X	-	-	-
43	CHL	N	609	X	-	-	-
43	CHL	R	606	X	-	-	-
43	CHL	R	607	X	-	-	-
43	CHL	R	608	X	-	-	-
43	CHL	S	601	X	-	-	-
43	CHL	S	606	X	-	-	-
43	CHL	S	607	X	-	-	-
43	CHL	S	608	X	-	-	-
43	CHL	Y	601	X	-	-	-
43	CHL	Y	605	X	-	-	-
43	CHL	Y	606	X	-	-	-
43	CHL	Y	607	X	-	-	-
43	CHL	Y	608	X	-	-	-
43	CHL	Y	609	X	-	-	-
43	CHL	g	601	X	-	-	-
43	CHL	g	605	X	-	-	-
43	CHL	g	606	X	-	-	-
43	CHL	g	607	X	-	-	-
43	CHL	g	608	X	-	-	-
43	CHL	g	609	X	-	-	-
43	CHL	n	601	X	-	-	-
43	CHL	n	605	X	-	-	-
43	CHL	n	606	X	-	-	-
43	CHL	n	607	X	-	-	-
43	CHL	n	608	X	-	-	-
43	CHL	n	609	X	-	-	-
43	CHL	r	606	X	-	-	-
43	CHL	r	607	X	-	-	-
43	CHL	r	608	X	-	-	-
43	CHL	s	601	X	-	-	-
43	CHL	s	606	X	-	-	-
43	CHL	s	607	X	-	-	-
43	CHL	s	608	X	-	-	-
43	CHL	y	601	X	-	-	-
43	CHL	y	605	X	-	-	-
43	CHL	y	606	X	-	-	-
43	CHL	y	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	CHL	y	608	X	-	-	-
43	CHL	y	609	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 77947 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
			2636	1719	434	468	15		
1	a	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		

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

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

- 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
			224	147	37	40		
3	v	32	Total	C	N	O	0	0
			224	147	37	40		

- 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
			3498	2288	584	609	17		
4	c	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		

- 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
			2771	1828	456	475	12		
5	d	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

- 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
			619	404	102	113			
6	e	76	Total	C	N	O	S	0	0
			619	404	102	113			

- 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
			251	171	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

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

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

- 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
			283	193	43	45	2		
9	i	35	Total	C	N	O	S	0	0
			283	193	43	45	2		

- 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
			262	178	40	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			262	178	40	44		

- 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	209	43	45		
11	k	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		
12	l	35	Total	C	N	O	0	0
			290	196	45	49		

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

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

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		
14	o	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		
15	p	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total	C	N	O	0	0
			1192	746	214	232		
16	q	148	Total	C	N	O	0	0
			1192	746	214	232		

- Molecule 17 is a protein called Photosystem II reaction center protein T.

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

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

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

- Molecule 19 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	35	Total	C	N	O	0	0
			242	159	39	44		
19	x	35	Total	C	N	O	0	0
			242	159	39	44		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
21	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
22	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		
23	r	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		
24	s	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
25	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

- Molecule 26 is a protein called Predicted protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	24	Total	C	N	O	0	0
			184	113	32	39		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	u	24	Total	C	N	O	0	0
			184	113	32	39		

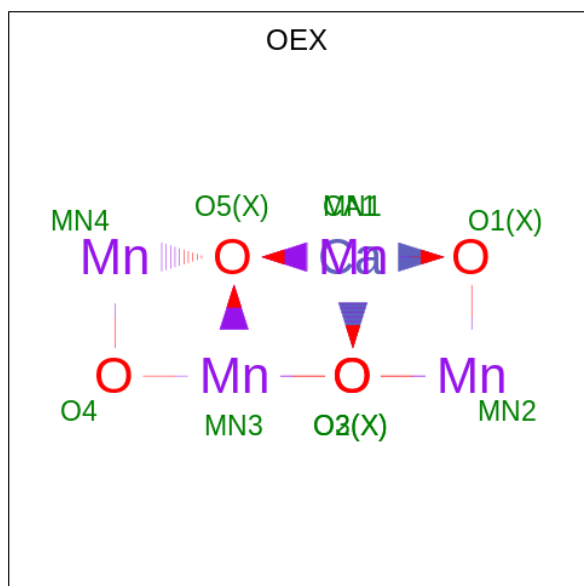
- Molecule 27 is a protein called 10 kDa photosystem II polypeptide PsbR (potential).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	25	Total	C	N	O	0	0
			121	71	25	25		
27	0	25	Total	C	N	O	0	0
			121	71	25	25		

- Molecule 28 is a protein called Unidentified Stromal Protein (USP).

Mol	Chain	Residues	Atoms				AltConf	Trace
28	4	25	Total	C	N	O	0	0
			169	109	29	31		
28	3	25	Total	C	N	O	0	0
			169	109	29	31		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

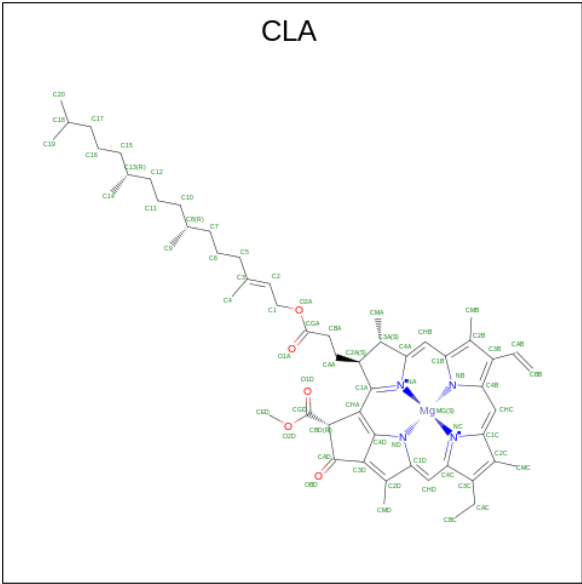
- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

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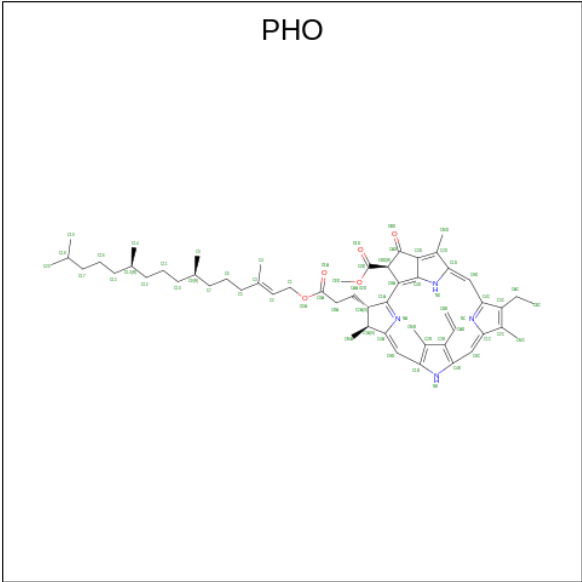
Mol	Chain	Residues	Atoms					AltConf
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	r	1	Total 41	C 33	Mg 1	N 4	O 3	0

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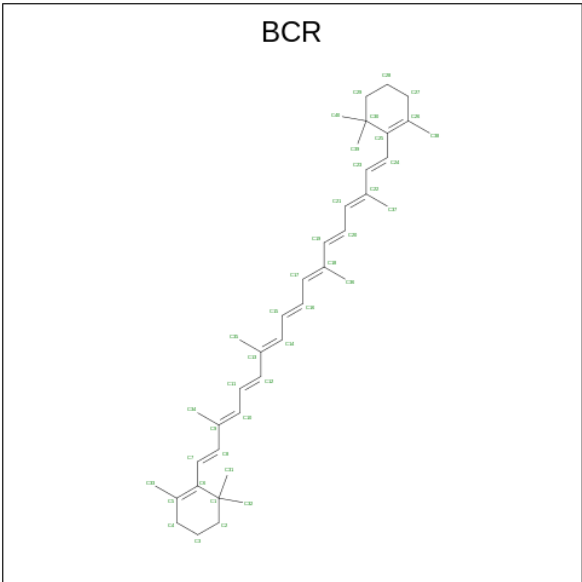
Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



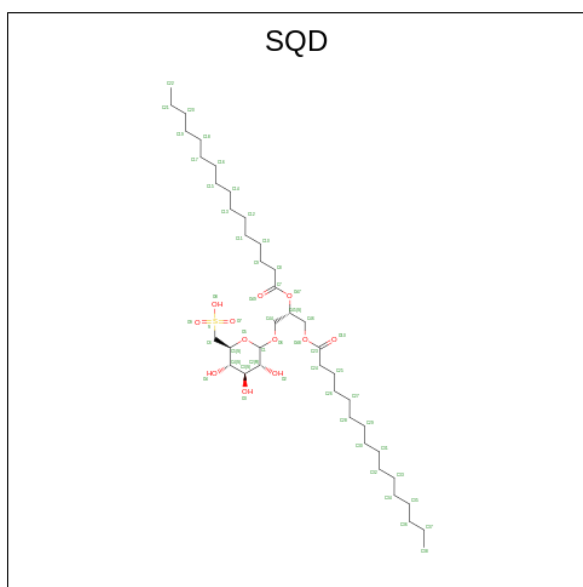
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



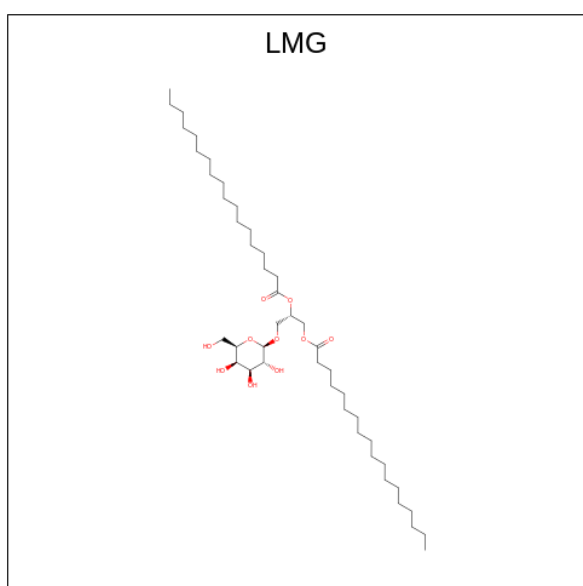
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	D	1	Total C 40 40	0
34	H	1	Total C 40 40	0
34	a	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	d	1	Total C 40 40	0
34	h	1	Total C 40 40	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



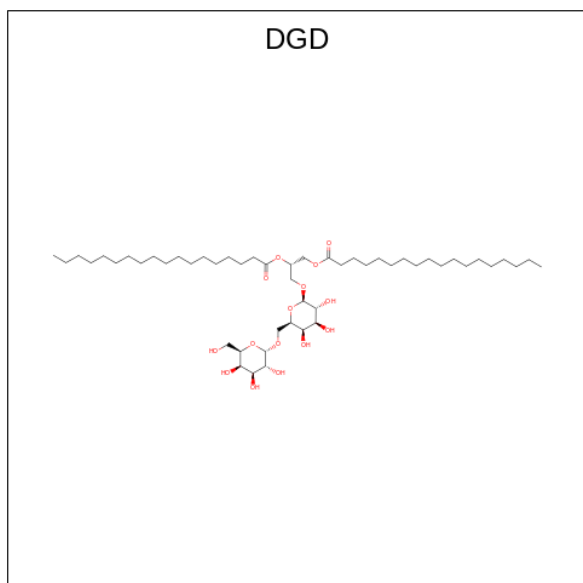
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			54	41	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	
35	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			48	38	10	
36	B	1	Total	C	O	0
			51	41	10	
36	C	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			46	36	10	
36	H	1	Total	C	O	0
			48	38	10	
36	a	1	Total	C	O	0
			48	38	10	
36	b	1	Total	C	O	0
			51	41	10	
36	c	1	Total	C	O	0
			51	41	10	
36	d	1	Total	C	O	0
			46	36	10	
36	h	1	Total	C	O	0
			48	38	10	

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



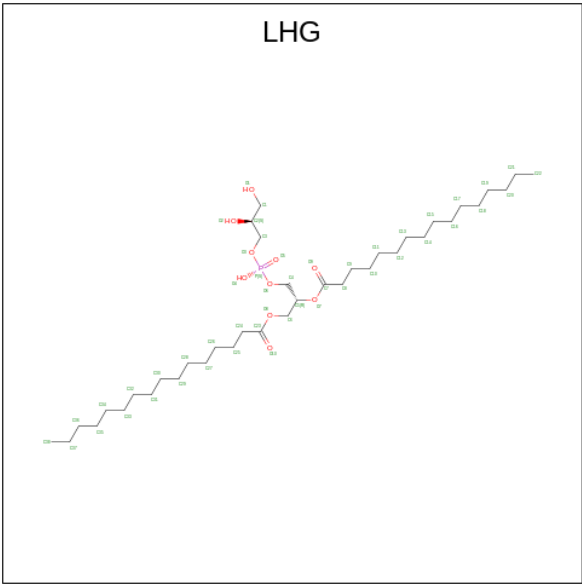
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			66	51	15	
37	C	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			62	47	15	
37	c	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			66	51	15	

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



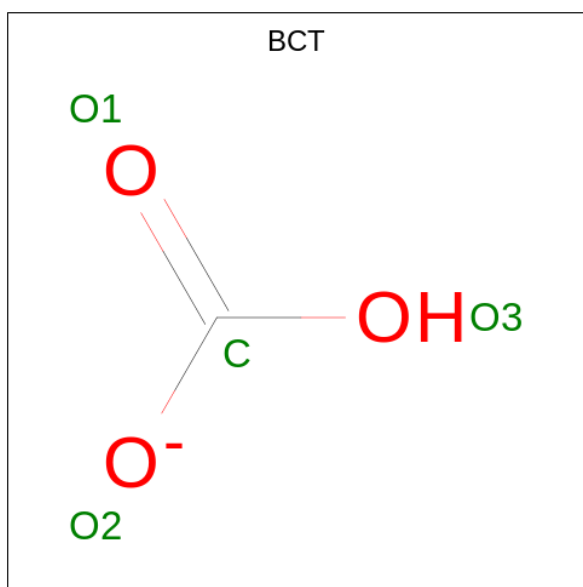
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	

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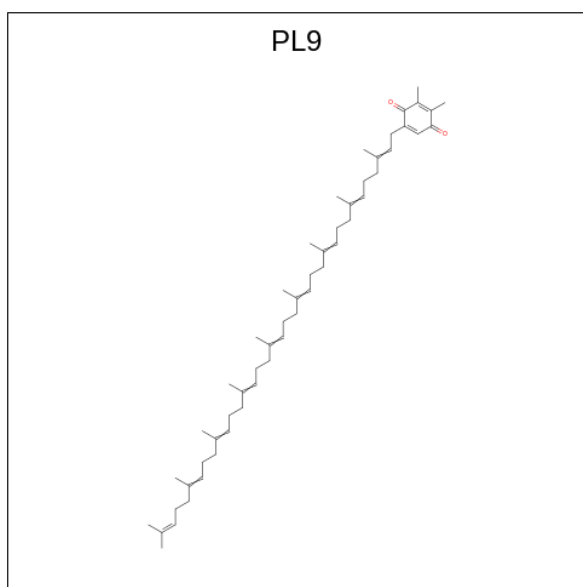
Mol	Chain	Residues	Atoms				AltConf
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			44	33	10	1	
38	d	1	Total	C	O	P	0
			49	38	10	1	
38	d	1	Total	C	O	P	0
			39	28	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	n	1	Total	C	O	P	0
			49	38	10	1	
38	g	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			45	34	10	1	
38	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 40 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



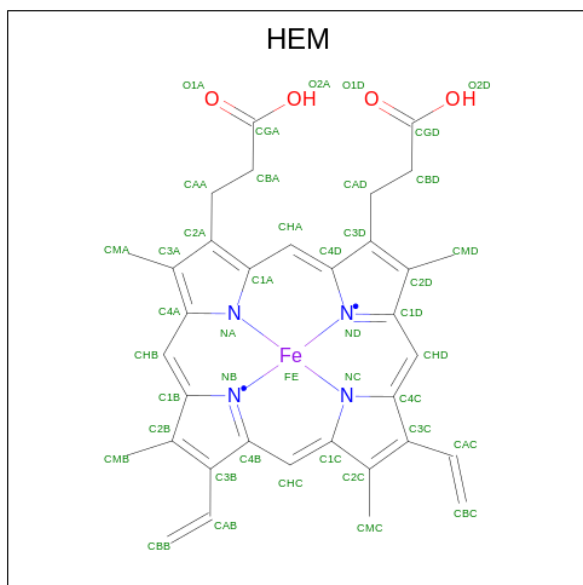
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			55	53	2	

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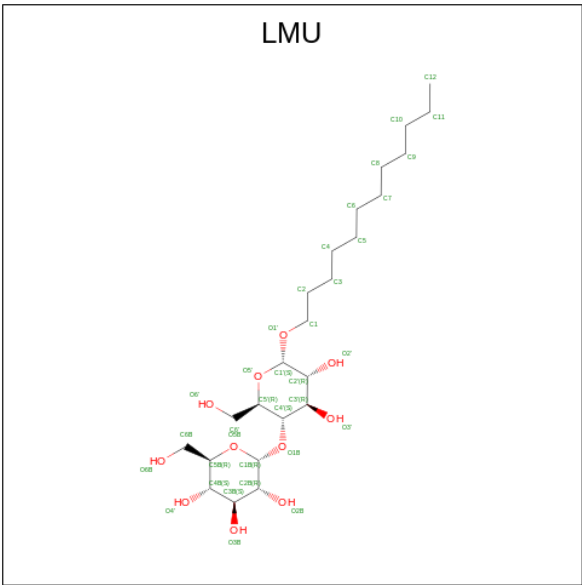
Mol	Chain	Residues	Atoms			AltConf
40	d	1	Total	C	O	0
			55	53	2	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



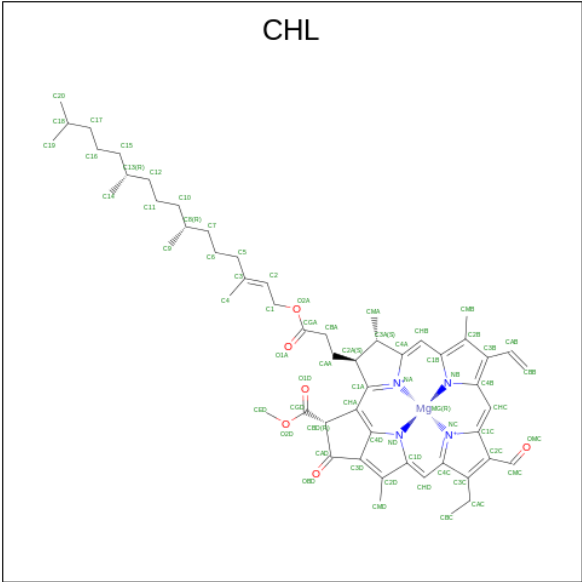
Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
42	Z	1	Total	C	O	0
			35	24	11	
42	Z	1	Total	C	O	0
			35	24	11	
42	Y	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	y	1	Total	C	O	0
			35	24	11	

- Molecule 43 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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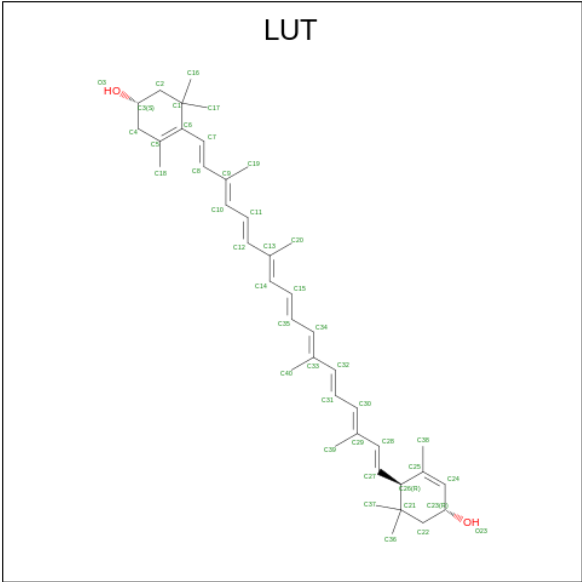
Mol	Chain	Residues	Atoms					AltConf
43	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
43	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
43	g	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
43	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
43	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
43	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
43	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
43	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
43	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
43	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
43	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
43	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 44 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



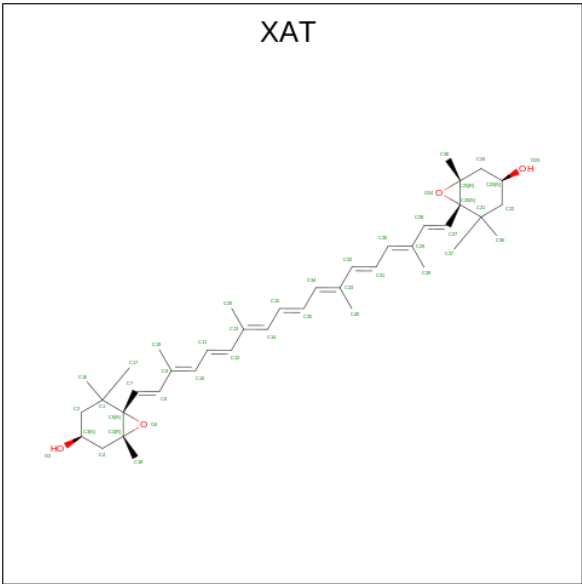
Mol	Chain	Residues	Atoms			AltConf
44	N	1	Total	C	O	0
			42	40	2	
44	N	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	n	1	Total	C	O	0
			42	40	2	
44	n	1	Total	C	O	0
			42	40	2	
44	g	1	Total	C	O	0
			42	40	2	
44	g	1	Total	C	O	0
			42	40	2	
44	s	1	Total	C	O	0
			42	40	2	
44	s	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
44	y	1	Total	C	O	0
			42	40	2	
44	y	1	Total	C	O	0
			42	40	2	

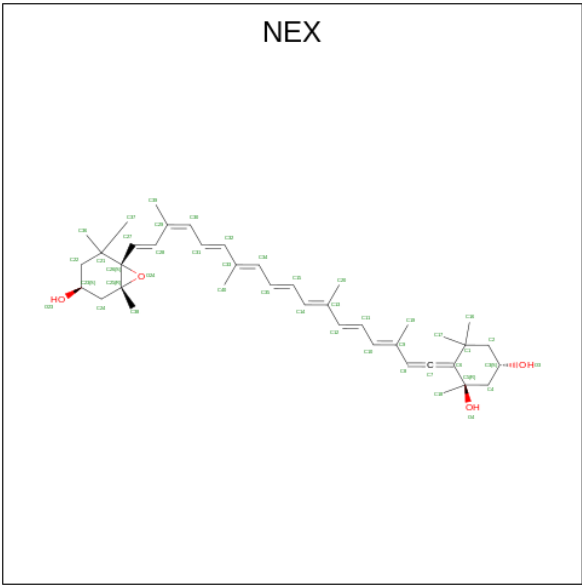
- Molecule 45 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



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

- Molecule 46 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2

,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA
DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,
3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



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

- Molecule 47 is water.

Mol	Chain	Residues	Atoms	AltConf
47	A	40	Total O 40 40	0
47	B	57	Total O 57 57	0
47	V	6	Total O 6 6	0
47	C	28	Total O 28 28	0
47	D	28	Total O 28 28	0
47	E	6	Total O 6 6	0
47	F	3	Total O 3 3	0
47	H	7	Total O 7 7	0
47	I	5	Total O 5 5	0
47	J	1	Total O 1 1	0
47	L	1	Total O 1 1	0
47	M	3	Total O 3 3	0
47	O	43	Total O 43 43	0
47	P	23	Total O 23 23	0
47	Q	20	Total O 20 20	0
47	T	3	Total O 3 3	0
47	W	3	Total O 3 3	0
47	X	1	Total O 1 1	0
47	Z	3	Total O 3 3	0
47	N	3	Total O 3 3	0
47	G	6	Total O 6 6	0
47	Y	8	Total O 8 8	0

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Mol	Chain	Residues	Atoms		AltConf
47	a	40	Total 40	O 40	0
47	b	57	Total 57	O 57	0
47	v	6	Total 6	O 6	0
47	c	28	Total 28	O 28	0
47	d	28	Total 28	O 28	0
47	e	6	Total 6	O 6	0
47	f	3	Total 3	O 3	0
47	h	7	Total 7	O 7	0
47	i	5	Total 5	O 5	0
47	j	1	Total 1	O 1	0
47	l	1	Total 1	O 1	0
47	m	2	Total 2	O 2	0
47	o	43	Total 43	O 43	0
47	p	23	Total 23	O 23	0
47	q	20	Total 20	O 20	0
47	t	3	Total 3	O 3	0
47	w	3	Total 3	O 3	0
47	x	1	Total 1	O 1	0
47	z	3	Total 3	O 3	0
47	n	3	Total 3	O 3	0
47	g	6	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
47	y	8	Total	O	0
			8	8	

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1

Chain A:  94% 5%



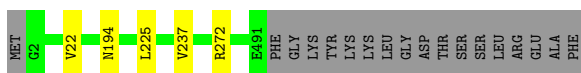
- Molecule 1: Photosystem II protein D1

Chain a:  94% 5%



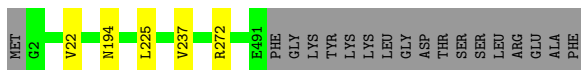
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  95%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  95%



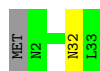
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  94%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  94%



- Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 95%



- Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 96%



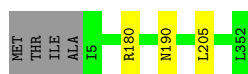
- Molecule 5: Photosystem II D2 protein

Chain D: 98%



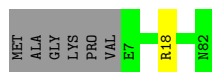
- Molecule 5: Photosystem II D2 protein

Chain d: 98%



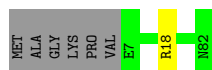
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 91% 7%



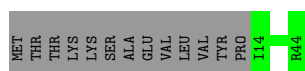
- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 91% 7%

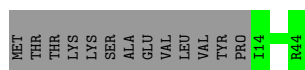


- Molecule 7: Cytochrome b559 subunit beta

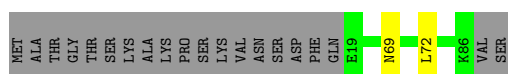
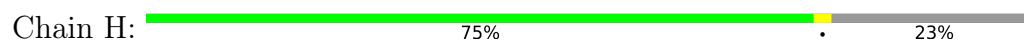
Chain F: 70% 30%



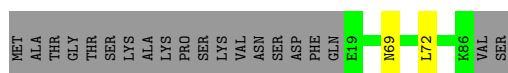
- Molecule 7: Cytochrome b559 subunit beta



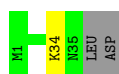
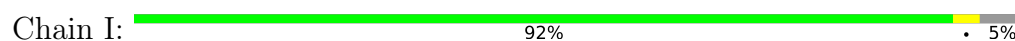
- Molecule 8: Photosystem II reaction center protein H



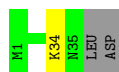
- Molecule 8: Photosystem II reaction center protein H



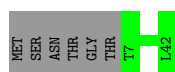
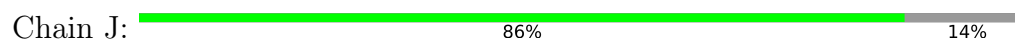
- Molecule 9: Photosystem II reaction center protein I



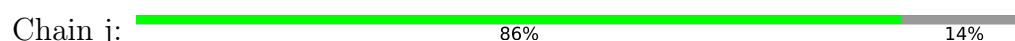
- Molecule 9: Photosystem II reaction center protein I

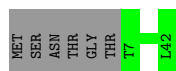


- Molecule 10: Photosystem II reaction center protein J

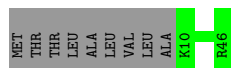


- Molecule 10: Photosystem II reaction center protein J

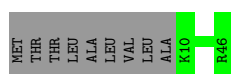
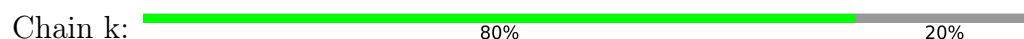




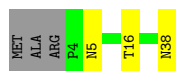
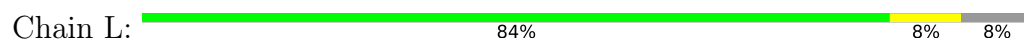
- Molecule 11: Photosystem II reaction center protein K



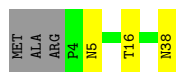
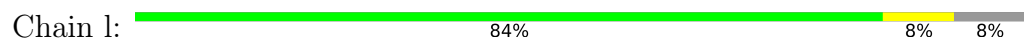
- Molecule 11: Photosystem II reaction center protein K



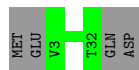
- Molecule 12: Photosystem II reaction center protein L



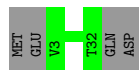
- Molecule 12: Photosystem II reaction center protein L



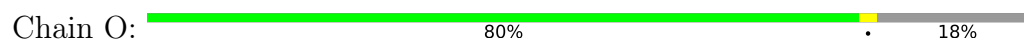
- Molecule 13: Photosystem II reaction center protein M

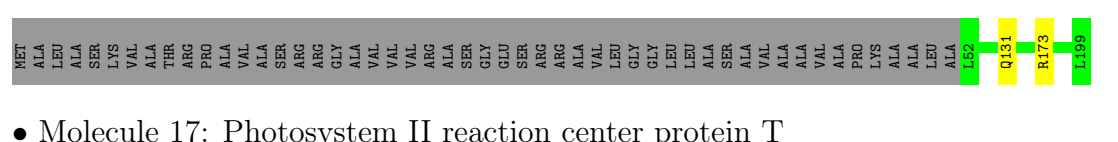
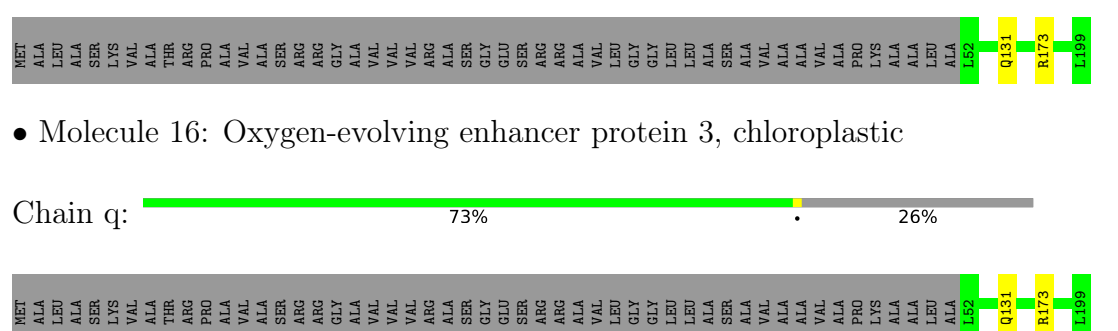
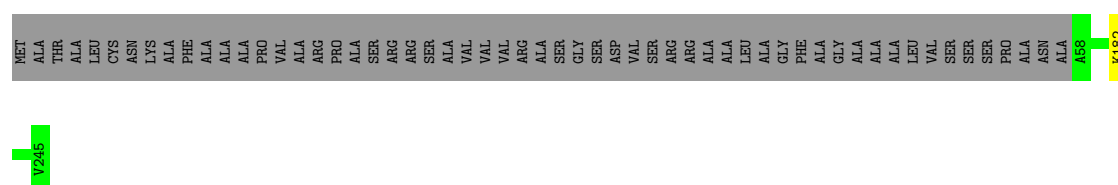
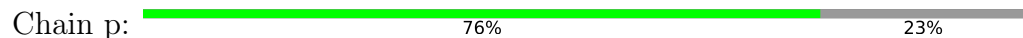
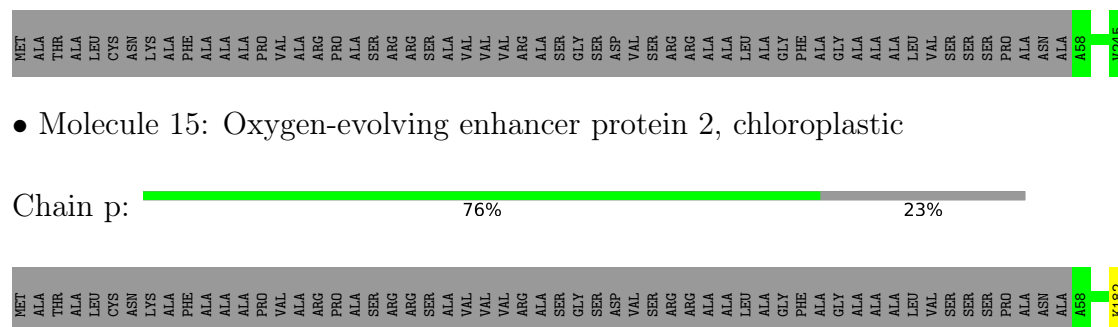
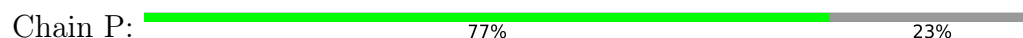
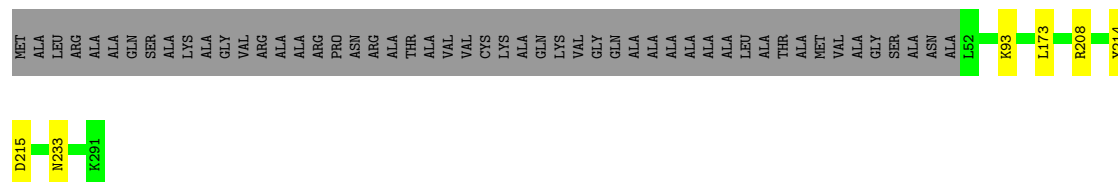
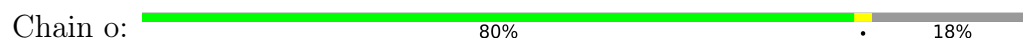
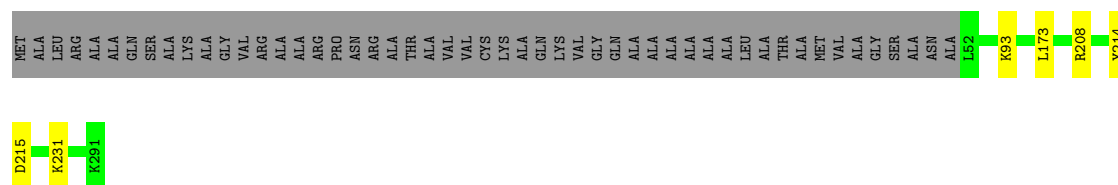


- Molecule 13: Photosystem II reaction center protein M



- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



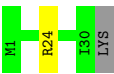


Chain T:  94%



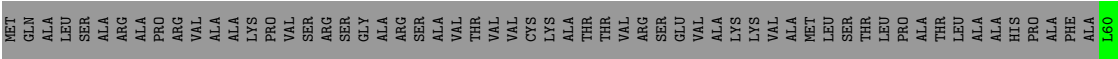
• Molecule 17: Photosystem II reaction center protein T

Chain t:  94%



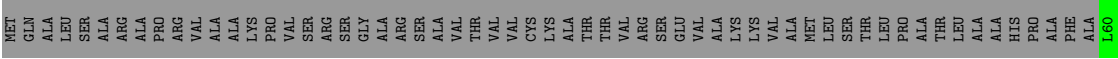
• Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain W:  48% 51%



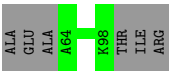
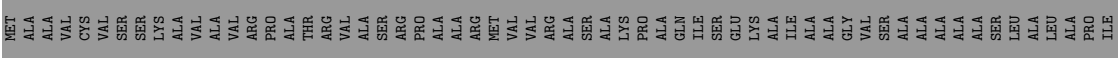
• Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain w:  48% 51%



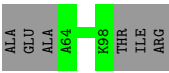
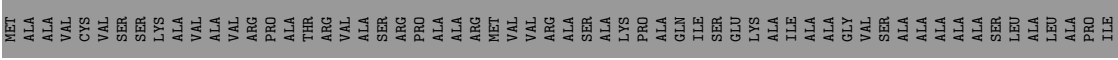
• Molecule 19: 4.1 kDa photosystem II subunit

Chain X:  35% 65%



• Molecule 19: 4.1 kDa photosystem II subunit

Chain x:  35% 65%



- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  98% .




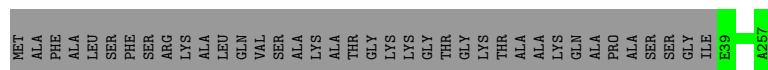
- Molecule 20: Photosystem II reaction center protein Z

Chain z:  98% .




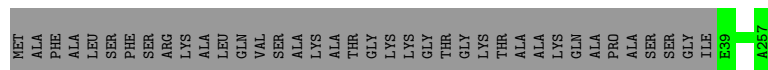
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain N:  85% 15%




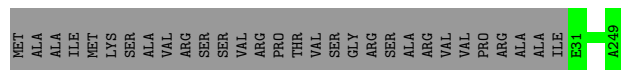
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain n:  85% 15%




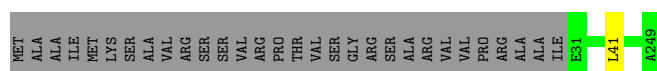
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain G:  88% 12%



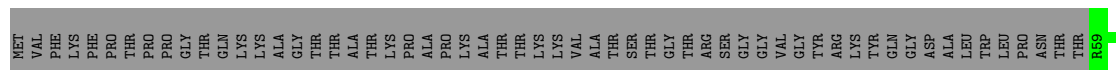
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

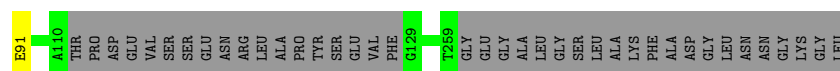
Chain g:  88% 12%



- Molecule 23: Chlorophyll a-b binding protein CP29

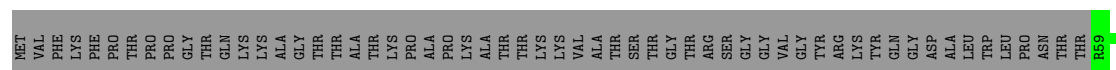
Chain R:  65% 35%





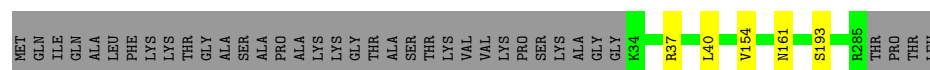
- Molecule 23: Chlorophyll a-b binding protein CP29

Chain r: 65% 35%



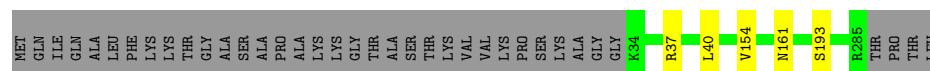
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain S: 85% 13%



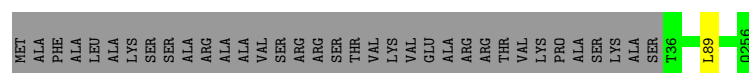
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain s: 85% 13%



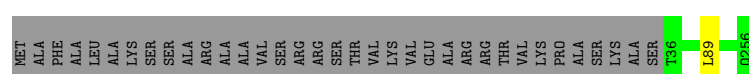
- Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain Y: 86% 14%



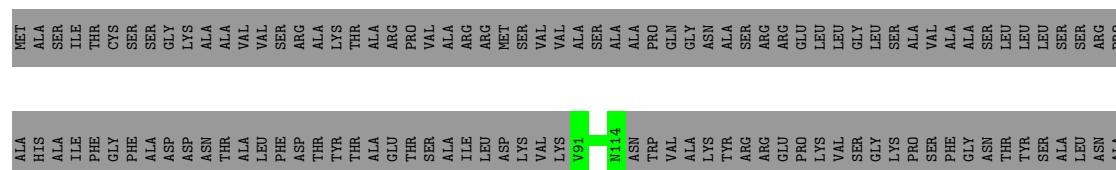
- Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain y: 86% 14%



- Molecule 26: Predicted protein

Chain U: 13% 87%



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

- Molecule 26: Predicted protein

Chain u:  13% 87%

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

ALA HIS ALA ILE PHE GLY PHE ALA ASP ASP ASN THR ALA VAL LEU PHE ASP THR TYR THR ALA GLU THR SER LYS ILE LEU ASP LYS VAL VAL LYS V91 V114 ASN TRP VAL ALA LYS TYR ARG GLU ARG PRO LYS VAL SER GLY LYS PRO SER PHE GLY ASN THR TYR SER ALA LEU SER ARG ALA

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

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 3:  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, C2	Depositor
Number of particles used	258242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.50	0/2718	0.60	0/3706
1	a	0.50	0/2718	0.60	0/3706
2	B	0.44	0/3964	0.57	1/5397 (0.0%)
2	b	0.44	0/3964	0.57	1/5397 (0.0%)
3	V	0.31	0/224	0.65	0/307
3	v	0.30	0/224	0.69	0/307
4	C	0.48	0/3619	0.57	1/4931 (0.0%)
4	c	0.48	0/3619	0.57	1/4931 (0.0%)
5	D	0.50	0/2866	0.62	1/3909 (0.0%)
5	d	0.49	0/2866	0.62	1/3909 (0.0%)
6	E	0.37	0/637	0.53	0/869
6	e	0.37	0/637	0.53	0/869
7	F	0.32	0/258	0.54	0/349
7	f	0.31	0/258	0.55	0/349
8	H	0.36	0/530	0.61	1/725 (0.1%)
8	h	0.36	0/530	0.61	1/725 (0.1%)
9	I	0.47	0/291	0.59	0/394
9	i	0.47	0/291	0.59	0/394
10	J	0.32	0/268	0.60	0/366
10	j	0.33	0/268	0.60	0/366
11	K	0.47	0/309	0.65	0/425
11	k	0.47	0/309	0.65	0/425
12	L	0.42	0/298	0.55	0/405
12	l	0.42	0/298	0.55	0/405
13	M	0.38	0/234	0.54	0/321
13	m	0.38	0/234	0.54	0/321
14	O	0.38	0/1839	0.64	3/2482 (0.1%)
14	o	0.38	0/1839	0.64	3/2482 (0.1%)
15	P	0.33	0/1473	0.57	0/1987
15	p	0.33	0/1473	0.56	0/1987
16	Q	0.30	0/1204	0.52	0/1616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	q	0.30	0/1204	0.52	0/1616
17	T	0.38	0/254	0.54	0/343
17	t	0.38	0/254	0.54	0/343
18	W	0.40	0/445	0.59	0/603
18	w	0.40	0/445	0.59	0/603
19	X	0.27	0/244	0.52	0/330
19	x	0.28	0/244	0.52	0/330
20	Z	0.31	0/469	0.55	0/644
20	z	0.32	0/469	0.55	0/644
21	N	0.35	0/1720	0.53	0/2341
21	n	0.35	0/1720	0.53	0/2341
22	G	0.33	0/1717	0.52	0/2337
22	g	0.33	0/1717	0.52	0/2337
23	R	0.32	0/1429	0.55	0/1934
23	r	0.32	0/1429	0.55	0/1934
24	S	0.36	0/1968	0.57	1/2679 (0.0%)
24	s	0.36	0/1968	0.57	1/2679 (0.0%)
25	Y	0.40	0/1746	0.56	1/2375 (0.0%)
25	y	0.40	0/1746	0.55	1/2375 (0.0%)
26	U	0.30	0/184	0.66	0/246
26	u	0.30	0/184	0.66	0/246
27	0	0.26	0/120	0.35	0/164
27	1	0.26	0/120	0.35	0/164
28	3	0.35	0/174	0.63	0/237
28	4	0.33	0/174	0.63	0/237
All	All	0.41	0/62404	0.57	18/84844 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	215	ASP	CB-CG-OD1	8.52	125.97	118.30
14	o	215	ASP	CB-CG-OD1	8.40	125.86	118.30
25	Y	89	LEU	CA-CB-CG	6.97	131.33	115.30
25	y	89	LEU	CA-CB-CG	6.96	131.30	115.30
4	C	368	LEU	CA-CB-CG	6.46	130.16	115.30
8	h	72	LEU	CA-CB-CG	6.38	129.96	115.30
8	H	72	LEU	CA-CB-CG	6.37	129.94	115.30
4	c	368	LEU	CA-CB-CG	6.36	129.94	115.30
14	o	173	LEU	CA-CB-CG	5.76	128.55	115.30
14	O	173	LEU	CA-CB-CG	5.75	128.52	115.30
14	o	214	TYR	C-N-CA	5.49	135.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	LEU	CA-CB-CG	5.49	127.92	115.30
2	b	225	LEU	CA-CB-CG	5.48	127.90	115.30
14	O	214	TYR	C-N-CA	5.46	135.35	121.70
24	s	40	LEU	CA-CB-CG	5.36	127.62	115.30
24	S	40	LEU	CA-CB-CG	5.34	127.58	115.30
5	D	205	LEU	CA-CB-CG	5.14	127.13	115.30
5	d	205	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
1	a	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
2	B	488/508 (96%)	477 (98%)	11 (2%)	0	100	100
2	b	488/508 (96%)	478 (98%)	10 (2%)	0	100	100
3	V	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
3	v	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
4	C	447/461 (97%)	421 (94%)	25 (6%)	1 (0%)	44	68
4	c	447/461 (97%)	422 (94%)	24 (5%)	1 (0%)	44	68
5	D	346/352 (98%)	334 (96%)	12 (4%)	0	100	100
5	d	346/352 (98%)	332 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
6	e	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
7	F	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
7	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
8	H	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
8	h	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
9	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
9	i	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
10	J	34/42 (81%)	34 (100%)	0	0	100	100
10	j	34/42 (81%)	34 (100%)	0	0	100	100
11	K	35/46 (76%)	35 (100%)	0	0	100	100
11	k	35/46 (76%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
12	l	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
13	M	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
13	m	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
14	O	238/291 (82%)	224 (94%)	14 (6%)	0	100	100
14	o	238/291 (82%)	221 (93%)	17 (7%)	0	100	100
15	P	186/245 (76%)	180 (97%)	6 (3%)	0	100	100
15	p	186/245 (76%)	179 (96%)	7 (4%)	0	100	100
16	Q	146/199 (73%)	139 (95%)	7 (5%)	0	100	100
16	q	146/199 (73%)	138 (94%)	8 (6%)	0	100	100
17	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
17	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
18	W	54/115 (47%)	50 (93%)	4 (7%)	0	100	100
18	w	54/115 (47%)	50 (93%)	4 (7%)	0	100	100
19	X	33/101 (33%)	31 (94%)	2 (6%)	0	100	100
19	x	33/101 (33%)	32 (97%)	1 (3%)	0	100	100
20	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
21	N	217/257 (84%)	202 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	n	217/257 (84%)	201 (93%)	16 (7%)	0	100	100
22	G	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
22	g	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
23	R	179/280 (64%)	169 (94%)	10 (6%)	0	100	100
23	r	179/280 (64%)	167 (93%)	12 (7%)	0	100	100
24	S	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	55
24	s	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	55
25	Y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
25	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
26	U	22/178 (12%)	19 (86%)	3 (14%)	0	100	100
26	u	22/178 (12%)	19 (86%)	3 (14%)	0	100	100
27	0	23/25 (92%)	23 (100%)	0	0	100	100
27	1	23/25 (92%)	23 (100%)	0	0	100	100
28	3	23/25 (92%)	17 (74%)	6 (26%)	0	100	100
28	4	23/25 (92%)	18 (78%)	5 (22%)	0	100	100
All	All	7742/9440 (82%)	7357 (95%)	381 (5%)	4 (0%)	50	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	211	TRP
4	c	211	TRP
24	S	193	SER
24	s	193	SER

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	274/289 (95%)	270 (98%)	4 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	274/289 (95%)	270 (98%)	4 (2%)	60	83
2	B	392/407 (96%)	388 (99%)	4 (1%)	73	89
2	b	392/407 (96%)	388 (99%)	4 (1%)	73	89
3	V	26/27 (96%)	25 (96%)	1 (4%)	28	56
3	v	26/27 (96%)	25 (96%)	1 (4%)	28	56
4	C	352/362 (97%)	345 (98%)	7 (2%)	50	78
4	c	352/362 (97%)	346 (98%)	6 (2%)	56	81
5	D	278/281 (99%)	276 (99%)	2 (1%)	81	93
5	d	278/281 (99%)	276 (99%)	2 (1%)	81	93
6	E	67/71 (94%)	66 (98%)	1 (2%)	60	83
6	e	67/71 (94%)	66 (98%)	1 (2%)	60	83
7	F	25/37 (68%)	25 (100%)	0	100	100
7	f	25/37 (68%)	25 (100%)	0	100	100
8	H	58/75 (77%)	57 (98%)	1 (2%)	56	81
8	h	58/75 (77%)	57 (98%)	1 (2%)	56	81
9	I	32/34 (94%)	31 (97%)	1 (3%)	35	64
9	i	32/34 (94%)	31 (97%)	1 (3%)	35	64
10	J	27/32 (84%)	27 (100%)	0	100	100
10	j	27/32 (84%)	27 (100%)	0	100	100
11	K	31/38 (82%)	31 (100%)	0	100	100
11	k	31/38 (82%)	31 (100%)	0	100	100
12	L	33/35 (94%)	30 (91%)	3 (9%)	7	19
12	l	33/35 (94%)	30 (91%)	3 (9%)	7	19
13	M	26/30 (87%)	26 (100%)	0	100	100
13	m	26/30 (87%)	26 (100%)	0	100	100
14	O	195/222 (88%)	192 (98%)	3 (2%)	60	83
14	o	195/222 (88%)	192 (98%)	3 (2%)	60	83
15	P	150/185 (81%)	150 (100%)	0	100	100
15	p	150/185 (81%)	149 (99%)	1 (1%)	81	93
16	Q	126/157 (80%)	124 (98%)	2 (2%)	58	82
16	q	126/157 (80%)	124 (98%)	2 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	T	27/28 (96%)	26 (96%)	1 (4%)	29	58
17	t	27/28 (96%)	26 (96%)	1 (4%)	29	58
18	W	44/87 (51%)	43 (98%)	1 (2%)	45	74
18	w	44/87 (51%)	43 (98%)	1 (2%)	45	74
19	X	25/67 (37%)	25 (100%)	0	100	100
19	x	25/67 (37%)	25 (100%)	0	100	100
20	Z	51/52 (98%)	51 (100%)	0	100	100
20	z	51/52 (98%)	51 (100%)	0	100	100
21	N	169/194 (87%)	169 (100%)	0	100	100
21	n	169/194 (87%)	169 (100%)	0	100	100
22	G	164/187 (88%)	164 (100%)	0	100	100
22	g	164/187 (88%)	163 (99%)	1 (1%)	84	94
23	R	144/218 (66%)	143 (99%)	1 (1%)	81	93
23	r	144/218 (66%)	143 (99%)	1 (1%)	81	93
24	S	190/217 (88%)	187 (98%)	3 (2%)	58	82
24	s	190/217 (88%)	187 (98%)	3 (2%)	58	82
25	Y	170/196 (87%)	170 (100%)	0	100	100
25	y	170/196 (87%)	170 (100%)	0	100	100
26	U	21/141 (15%)	21 (100%)	0	100	100
26	u	21/141 (15%)	21 (100%)	0	100	100
28	3	8/8 (100%)	8 (100%)	0	100	100
28	4	8/8 (100%)	8 (100%)	0	100	100
All	All	6210/7354 (84%)	6139 (99%)	71 (1%)	69	87

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	187	GLN
1	A	297	LEU
1	A	322	ASN
2	B	22	VAL
2	B	194	ASN
2	B	237	VAL

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Mol	Chain	Res	Type
2	B	272	ARG
3	V	32	ASN
4	C	30	LEU
4	C	128	LEU
4	C	143	ASN
4	C	147	ASN
4	C	193	ASN
4	C	365	LEU
4	C	389	LEU
5	D	180	ARG
5	D	190	ASN
6	E	18	ARG
8	H	69	ASN
9	I	34	LYS
12	L	5	ASN
12	L	16	THR
12	L	38	ASN
14	O	93	LYS
14	O	208	ARG
14	O	231	LYS
16	Q	131	GLN
16	Q	173	ARG
17	T	24	ARG
18	W	114	LYS
23	R	91	GLU
24	S	37	ARG
24	S	154	VAL
24	S	161	ASN
1	a	27	ARG
1	a	187	GLN
1	a	297	LEU
1	a	322	ASN
2	b	22	VAL
2	b	194	ASN
2	b	237	VAL
2	b	272	ARG
3	v	32	ASN
4	c	30	LEU
4	c	143	ASN
4	c	147	ASN
4	c	193	ASN
4	c	365	LEU

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Mol	Chain	Res	Type
4	c	389	LEU
5	d	180	ARG
5	d	190	ASN
6	e	18	ARG
8	h	69	ASN
9	i	34	LYS
12	l	5	ASN
12	l	16	THR
12	l	38	ASN
14	o	93	LYS
14	o	208	ARG
14	o	233	ASN
15	p	182	LYS
16	q	131	GLN
16	q	173	ARG
17	t	24	ARG
18	w	114	LYS
22	g	41	LEU
23	r	91	GLU
24	s	37	ARG
24	s	154	VAL
24	s	161	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	187	GLN
1	A	303	ASN
1	A	322	ASN
2	B	194	ASN
2	B	216	HIS
2	B	281	GLN
2	B	394	GLN
2	B	487	ASN
3	V	32	ASN
4	C	16	GLN
4	C	143	ASN
4	C	147	ASN
4	C	193	ASN
4	C	301	GLN
4	C	361	ASN

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Mol	Chain	Res	Type
4	C	403	ASN
5	D	83	ASN
5	D	137	ASN
5	D	190	ASN
5	D	220	ASN
12	L	5	ASN
12	L	38	ASN
14	O	266	GLN
15	P	121	GLN
15	P	213	ASN
15	P	221	GLN
16	Q	127	GLN
16	Q	131	GLN
18	W	100	GLN
21	N	147	GLN
21	N	222	GLN
22	G	120	GLN
22	G	214	GLN
22	G	225	ASN
23	R	99	ASN
24	S	161	ASN
25	Y	128	GLN
25	Y	233	ASN
25	Y	240	ASN
1	a	113	GLN
1	a	303	ASN
1	a	322	ASN
2	b	194	ASN
2	b	216	HIS
2	b	281	GLN
2	b	394	GLN
2	b	487	ASN
3	v	32	ASN
4	c	143	ASN
4	c	147	ASN
4	c	193	ASN
4	c	301	GLN
4	c	310	GLN
4	c	361	ASN
4	c	403	ASN
5	d	137	ASN
5	d	190	ASN

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Mol	Chain	Res	Type
5	d	220	ASN
12	l	5	ASN
12	l	38	ASN
14	o	233	ASN
14	o	266	GLN
15	p	121	GLN
15	p	213	ASN
15	p	221	GLN
16	q	127	GLN
16	q	131	GLN
18	w	100	GLN
21	n	222	GLN
22	g	120	GLN
22	g	214	GLN
22	g	225	ASN
24	s	161	ASN
25	y	128	GLN
25	y	233	ASN
25	y	240	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 318 ligands modelled in this entry, 6 are monoatomic - leaving 312 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	$\# Z > 2$
32	CLA	b	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.66	9 (11%)
32	CLA	N	602	21	65,73,73	1.48	7 (10%)	76,113,113	1.31	8 (10%)
36	LMG	H	102	-	48,48,55	0.92	2 (4%)	56,56,63	1.08	3 (5%)
43	CHL	G	608	-	44,52,74	2.17	13 (29%)	46,87,114	3.26	17 (36%)
32	CLA	B	604	-	65,73,73	1.51	9 (13%)	76,113,113	1.40	11 (14%)
34	BCR	D	404	-	41,41,41	0.72	0	56,56,56	1.92	21 (37%)
32	CLA	A	407	47	49,57,73	1.63	7 (14%)	55,93,113	1.71	8 (14%)
32	CLA	b	616	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
32	CLA	B	614	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	8 (10%)
32	CLA	B	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	7 (9%)
34	BCR	h	101	-	41,41,41	0.71	0	56,56,56	2.00	13 (23%)
32	CLA	G	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.39	8 (14%)
34	BCR	c	517	-	41,41,41	0.74	0	56,56,56	1.92	16 (28%)
43	CHL	g	609	22	66,74,74	1.85	14 (21%)	73,114,114	2.74	23 (31%)
42	LMU	Z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.14	4 (8%)
32	CLA	c	507	47	65,73,73	1.44	9 (13%)	76,113,113	1.54	10 (13%)
32	CLA	a	405	-	65,73,73	1.53	8 (12%)	76,113,113	1.57	10 (13%)
46	NEX	n	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.33	15 (30%)
32	CLA	y	611	38	65,73,73	1.46	9 (13%)	76,113,113	1.41	8 (10%)
44	LUT	N	1621	-	42,43,43	0.79	0	51,60,60	1.52	7 (13%)
32	CLA	Y	602	25	65,73,73	1.50	8 (12%)	76,113,113	1.34	9 (11%)
32	CLA	B	609	-	65,73,73	1.41	7 (10%)	76,113,113	1.47	7 (9%)
34	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.84	15 (26%)
43	CHL	y	605	25	46,54,74	2.23	15 (32%)	49,90,114	3.18	19 (38%)
32	CLA	n	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.34	7 (9%)
46	NEX	G	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.40	15 (30%)
42	LMU	y	2632	-	36,36,36	1.14	2 (5%)	47,47,47	1.13	5 (10%)
45	XAT	Y	1622	-	39,47,47	0.95	2 (5%)	54,74,74	4.34	24 (44%)
32	CLA	n	614	-	49,57,73	1.75	7 (14%)	55,93,113	1.41	8 (14%)
32	CLA	c	510	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	7 (9%)
32	CLA	b	617	-	65,73,73	1.43	8 (12%)	76,113,113	1.42	9 (11%)
32	CLA	g	602	22	65,73,73	1.51	8 (12%)	76,113,113	1.31	8 (10%)
32	CLA	C	508	-	65,73,73	1.41	7 (10%)	76,113,113	1.56	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	Y	609	25	66,74,74	1.82	13 (19%)	73,114,114	2.76	22 (30%)
32	CLA	G	610	22	65,73,73	1.44	8 (12%)	76,113,113	1.37	8 (10%)
43	CHL	n	606	-	46,54,74	2.22	14 (30%)	49,90,114	3.14	17 (34%)
35	SQD	b	621	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	5 (8%)
32	CLA	b	608	47	65,73,73	1.45	8 (12%)	76,113,113	1.42	7 (9%)
35	SQD	A	412	-	50,51,54	1.21	4 (8%)	59,62,65	3.80	9 (15%)
34	BCR	H	101	-	41,41,41	0.70	0	56,56,56	2.00	12 (21%)
43	CHL	N	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.79	22 (30%)
35	SQD	a	412	-	50,51,54	1.21	4 (8%)	59,62,65	3.79	9 (15%)
36	LMG	h	102	-	48,48,55	0.92	2 (4%)	56,56,63	1.10	3 (5%)
32	CLA	s	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.59	8 (14%)
32	CLA	a	406	47	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
43	CHL	S	601	24	46,54,74	2.26	14 (30%)	49,90,114	3.16	22 (44%)
46	NEX	r	625	-	38,46,46	0.99	2 (5%)	50,70,70	2.48	16 (32%)
32	CLA	B	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	11 (14%)
43	CHL	N	606	-	46,54,74	2.22	15 (32%)	49,90,114	3.14	17 (34%)
46	NEX	S	1623	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	17 (34%)
32	CLA	n	612	21	45,53,73	1.79	7 (15%)	52,89,113	1.51	10 (19%)
36	LMG	a	413	-	48,48,55	0.96	2 (4%)	56,56,63	1.06	4 (7%)
32	CLA	c	501	-	65,73,73	1.49	9 (13%)	76,113,113	1.29	11 (14%)
32	CLA	S	614	-	48,56,73	1.70	8 (16%)	55,92,113	1.38	8 (14%)
32	CLA	S	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.58	8 (14%)
32	CLA	C	505	-	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)
44	LUT	g	1621	-	42,43,43	0.81	0	51,60,60	1.56	11 (21%)
34	BCR	c	514	-	41,41,41	0.84	0	56,56,56	1.69	10 (17%)
32	CLA	b	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	7 (9%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.97	2 (2%)
34	BCR	C	516	-	41,41,41	0.83	0	56,56,56	1.89	18 (32%)
32	CLA	c	511	4	65,73,73	1.40	8 (12%)	76,113,113	1.48	8 (10%)
36	LMG	b	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	4 (6%)
32	CLA	Y	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	10 (13%)
32	CLA	n	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.37	6 (7%)
43	CHL	G	601	22	66,74,74	1.79	12 (18%)	73,114,114	2.70	23 (31%)
32	CLA	Y	613	25	65,73,73	1.48	10 (15%)	76,113,113	1.44	9 (11%)
43	CHL	Y	606	-	66,74,74	1.84	15 (22%)	73,114,114	2.65	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	XAT	g	1622	-	39,47,47	0.94	0	54,74,74	2.82	20 (37%)
32	CLA	s	609	24	41,49,73	1.89	7 (17%)	47,84,113	1.52	8 (17%)
38	LHG	D	410	-	38,38,48	1.00	2 (5%)	41,44,54	1.00	2 (4%)
32	CLA	G	602	22	65,73,73	1.51	7 (10%)	76,113,113	1.31	7 (9%)
38	LHG	y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.19	5 (9%)
34	BCR	B	619	-	41,41,41	0.72	0	56,56,56	1.94	13 (23%)
37	DGD	C	524	-	67,67,67	0.82	2 (2%)	81,81,81	1.00	4 (4%)
33	PHO	A	408	-	51,69,69	1.06	5 (9%)	47,99,99	1.33	8 (17%)
45	XAT	G	1622	-	39,47,47	0.93	0	54,74,74	2.83	20 (37%)
32	CLA	g	613	22	65,73,73	1.50	11 (16%)	76,113,113	1.51	6 (7%)
32	CLA	r	609	23	45,53,73	1.78	6 (13%)	52,89,113	1.62	9 (17%)
32	CLA	B	616	-	65,73,73	1.48	9 (13%)	76,113,113	1.36	10 (13%)
32	CLA	R	603	-	49,57,73	1.72	7 (14%)	55,93,113	1.55	10 (18%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	6 (8%)
38	LHG	D	409	-	48,48,48	0.88	3 (6%)	51,54,54	0.97	3 (5%)
32	CLA	C	506	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
34	BCR	B	620	-	41,41,41	0.73	0	56,56,56	1.75	13 (23%)
37	DGD	c	524	-	67,67,67	0.82	2 (2%)	81,81,81	1.00	4 (4%)
32	CLA	s	603	-	42,50,73	1.82	7 (16%)	48,85,113	1.68	10 (20%)
43	CHL	n	605	21	66,74,74	1.80	15 (22%)	73,114,114	2.85	24 (32%)
36	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
42	LMU	Z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.21	5 (10%)
35	SQD	B	621	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	5 (8%)
38	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	3 (5%)
38	LHG	C	2630	-	46,46,48	0.91	2 (4%)	49,52,54	1.03	3 (6%)
41	HEM	f	101	6,7	41,50,50	1.46	4 (9%)	45,82,82	1.35	5 (11%)
32	CLA	c	505	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	10 (13%)
29	OEX	A	401	4,1	0,15,15	-	-	-	-	-
46	NEX	s	1623	-	38,46,46	1.03	3 (7%)	50,70,70	2.38	17 (34%)
32	CLA	S	603	-	42,50,73	1.83	9 (21%)	48,85,113	1.70	10 (20%)
46	NEX	R	625	-	38,46,46	0.90	1 (2%)	50,70,70	2.45	17 (34%)
42	LMU	Y	2632	-	36,36,36	1.13	2 (5%)	47,47,47	1.12	5 (10%)
34	BCR	d	404	-	41,41,41	0.71	0	56,56,56	1.92	21 (37%)
32	CLA	d	403	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	9 (11%)
44	LUT	s	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.72	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	S	607	-	43,51,74	2.25	13 (30%)	45,86,114	3.22	16 (35%)
32	CLA	b	612	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	10 (13%)
32	CLA	B	603	-	65,73,73	1.42	7 (10%)	76,113,113	1.31	9 (11%)
32	CLA	s	611	38	49,57,73	1.63	7 (14%)	55,93,113	1.48	6 (10%)
43	CHL	s	607	-	43,51,74	2.25	13 (30%)	45,86,114	3.23	16 (35%)
32	CLA	n	603	-	65,73,73	1.52	9 (13%)	76,113,113	1.40	8 (10%)
32	CLA	N	614	-	49,57,73	1.74	7 (14%)	55,93,113	1.41	8 (14%)
32	CLA	n	610	21	65,73,73	1.44	7 (10%)	76,113,113	1.34	8 (10%)
39	BCT	d	401	30	2,3,3	1.29	0	2,3,3	4.18	2 (100%)
43	CHL	r	607	-	50,58,74	2.17	16 (32%)	52,94,114	3.09	21 (40%)
32	CLA	Y	604	-	65,73,73	1.50	9 (13%)	76,113,113	1.36	7 (9%)
32	CLA	b	615	-	65,73,73	1.45	8 (12%)	76,113,113	1.33	7 (9%)
43	CHL	R	607	-	50,58,74	2.17	16 (32%)	52,94,114	3.09	21 (40%)
32	CLA	S	611	38	49,57,73	1.64	7 (14%)	55,93,113	1.49	7 (12%)
45	XAT	y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.35	24 (44%)
32	CLA	n	602	21	65,73,73	1.48	7 (10%)	76,113,113	1.31	8 (10%)
45	XAT	r	624	-	39,47,47	0.88	2 (5%)	54,74,74	2.62	18 (33%)
32	CLA	G	613	22	65,73,73	1.50	10 (15%)	76,113,113	1.51	6 (7%)
46	NEX	N	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.37	15 (30%)
44	LUT	G	1621	-	42,43,43	0.82	0	51,60,60	1.56	10 (19%)
32	CLA	s	610	24	49,57,73	1.81	9 (18%)	55,93,113	1.33	9 (16%)
44	LUT	G	1620	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)
43	CHL	n	608	-	50,58,74	2.08	13 (26%)	52,94,114	3.22	18 (34%)
32	CLA	B	615	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	7 (9%)
32	CLA	C	501	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	11 (14%)
32	CLA	r	610	23	41,49,73	1.86	8 (19%)	47,84,113	1.48	7 (14%)
38	LHG	N	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
43	CHL	N	605	21	66,74,74	1.80	15 (22%)	73,114,114	2.85	24 (32%)
45	XAT	n	1622	-	39,47,47	0.98	1 (2%)	54,74,74	2.66	22 (40%)
32	CLA	g	603	-	65,73,73	1.50	8 (12%)	76,113,113	1.39	12 (15%)
40	PL9	D	405	-	55,55,55	2.01	14 (25%)	68,69,69	1.46	15 (22%)
32	CLA	R	610	23	41,49,73	1.86	8 (19%)	47,84,113	1.48	7 (14%)
43	CHL	G	606	-	50,58,74	2.14	14 (28%)	52,94,114	3.08	19 (36%)
32	CLA	s	602	24	49,57,73	1.66	7 (14%)	55,93,113	1.47	8 (14%)
46	NEX	Y	1623	-	38,46,46	0.97	2 (5%)	50,70,70	2.46	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	n	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
32	CLA	g	604	-	49,57,73	1.72	7 (14%)	55,93,113	1.53	6 (10%)
43	CHL	G	607	-	50,58,74	2.14	14 (28%)	52,94,114	3.09	22 (42%)
34	BCR	b	620	-	41,41,41	0.73	0	56,56,56	1.74	13 (23%)
44	LUT	Y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.71	10 (19%)
32	CLA	b	607	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	8 (10%)
44	LUT	Y	1620	-	42,43,43	0.93	3 (7%)	51,60,60	1.90	15 (29%)
32	CLA	S	602	24	49,57,73	1.67	7 (14%)	55,93,113	1.47	9 (16%)
32	CLA	N	603	-	65,73,73	1.52	10 (15%)	76,113,113	1.40	8 (10%)
32	CLA	y	603	-	65,73,73	1.49	10 (15%)	76,113,113	1.41	10 (13%)
32	CLA	G	611	38	45,53,73	1.76	7 (15%)	52,89,113	1.59	8 (15%)
32	CLA	C	503	-	65,73,73	1.51	8 (12%)	76,113,113	1.40	10 (13%)
34	BCR	C	515	-	41,41,41	0.85	1 (2%)	56,56,56	1.98	19 (33%)
43	CHL	Y	605	25	46,54,74	2.22	15 (32%)	49,90,114	3.18	19 (38%)
32	CLA	g	612	22	43,51,73	1.83	7 (16%)	49,86,113	1.59	9 (18%)
32	CLA	C	509	-	65,73,73	1.44	11 (16%)	76,113,113	1.58	10 (13%)
43	CHL	Y	607	-	66,74,74	1.81	14 (21%)	73,114,114	2.67	21 (28%)
32	CLA	A	406	47	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
33	PHO	a	409	-	51,69,69	1.04	4 (7%)	47,99,99	1.33	5 (10%)
32	CLA	c	504	47	65,73,73	1.50	10 (15%)	76,113,113	1.41	8 (10%)
32	CLA	B	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.67	9 (11%)
39	BCT	D	401	30	2,3,3	1.29	0	2,3,3	4.17	2 (100%)
42	LMU	z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.14	4 (8%)
32	CLA	b	603	-	65,73,73	1.43	7 (10%)	76,113,113	1.32	9 (11%)
32	CLA	r	603	-	49,57,73	1.73	7 (14%)	55,93,113	1.55	10 (18%)
32	CLA	s	614	-	48,56,73	1.69	8 (16%)	55,92,113	1.39	8 (14%)
38	LHG	Y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.19	5 (9%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
34	BCR	c	516	-	41,41,41	0.83	0	56,56,56	1.89	18 (32%)
38	LHG	S	2630	32	44,44,48	0.94	2 (4%)	47,50,54	1.00	2 (4%)
32	CLA	d	402	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	7 (9%)
45	XAT	N	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.66	23 (42%)
32	CLA	c	513	-	65,73,73	1.40	9 (13%)	76,113,113	1.44	9 (11%)
46	NEX	g	1623	-	38,46,46	0.92	1 (2%)	50,70,70	2.38	16 (32%)
32	CLA	R	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.50	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	G	609	22	66,74,74	1.85	13 (19%)	73,114,114	2.73	22 (30%)
32	CLA	b	614	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	8 (10%)
32	CLA	c	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	9 (11%)
32	CLA	b	604	-	65,73,73	1.51	9 (13%)	76,113,113	1.41	11 (14%)
32	CLA	A	405	-	65,73,73	1.53	8 (12%)	76,113,113	1.56	10 (13%)
32	CLA	c	508	-	65,73,73	1.42	7 (10%)	76,113,113	1.58	8 (10%)
34	BCR	a	411	-	41,41,41	0.76	0	56,56,56	1.70	14 (25%)
44	LUT	N	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.57	10 (19%)
38	LHG	D	408	-	43,43,48	0.95	2 (4%)	46,49,54	1.02	2 (4%)
32	CLA	G	604	-	49,57,73	1.72	8 (16%)	55,93,113	1.52	6 (10%)
32	CLA	g	611	38	45,53,73	1.77	7 (15%)	52,89,113	1.58	8 (15%)
43	CHL	s	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.22	19 (41%)
32	CLA	y	602	25	65,73,73	1.51	8 (12%)	76,113,113	1.34	9 (11%)
43	CHL	g	605	22	48,56,74	2.36	16 (33%)	51,92,114	3.05	19 (37%)
43	CHL	N	601	21	66,74,74	1.81	13 (19%)	73,114,114	2.68	20 (27%)
32	CLA	S	609	24	41,49,73	1.90	7 (17%)	47,84,113	1.52	8 (17%)
43	CHL	G	605	22	48,56,74	2.36	16 (33%)	51,92,114	3.05	19 (37%)
43	CHL	g	607	-	50,58,74	2.14	14 (28%)	52,94,114	3.09	22 (42%)
45	XAT	R	624	-	39,47,47	0.88	1 (2%)	54,74,74	2.61	17 (31%)
36	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
43	CHL	y	609	25	66,74,74	1.82	13 (19%)	73,114,114	2.76	22 (30%)
41	HEM	F	101	6,7	41,50,50	1.45	4 (9%)	45,82,82	1.35	6 (13%)
43	CHL	n	601	21	66,74,74	1.81	13 (19%)	73,114,114	2.67	20 (27%)
44	LUT	g	1620	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
32	CLA	G	612	22	43,51,73	1.83	8 (18%)	49,86,113	1.59	9 (18%)
32	CLA	S	605	24	50,58,73	1.70	7 (14%)	58,95,113	1.51	11 (18%)
32	CLA	B	608	47	65,73,73	1.45	8 (12%)	76,113,113	1.41	7 (9%)
43	CHL	s	608	-	49,57,74	2.18	15 (30%)	52,93,114	3.13	19 (36%)
32	CLA	b	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	11 (14%)
32	CLA	N	612	21	45,53,73	1.80	8 (17%)	52,89,113	1.50	10 (19%)
43	CHL	y	601	25	66,74,74	1.80	14 (21%)	73,114,114	2.67	26 (35%)
32	CLA	B	611	47	65,73,73	1.48	8 (12%)	76,113,113	1.55	11 (14%)
32	CLA	g	610	22	65,73,73	1.44	8 (12%)	76,113,113	1.37	8 (10%)
33	PHO	a	408	-	51,69,69	1.06	5 (9%)	47,99,99	1.32	8 (17%)
34	BCR	C	514	-	41,41,41	0.84	0	56,56,56	1.69	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	c	2630	-	46,46,48	0.92	2 (4%)	49,52,54	1.03	3 (6%)
32	CLA	B	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	8 (10%)
32	CLA	D	402	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
33	PHO	A	409	-	51,69,69	1.04	4 (7%)	47,99,99	1.34	6 (12%)
34	BCR	C	517	-	41,41,41	0.74	0	56,56,56	1.93	15 (26%)
36	LMG	D	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.15	4 (7%)
43	CHL	R	608	-	46,54,74	2.26	15 (32%)	49,90,114	3.10	20 (40%)
32	CLA	B	617	-	65,73,73	1.42	8 (12%)	76,113,113	1.41	9 (11%)
32	CLA	B	607	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	8 (10%)
37	DGD	C	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
32	CLA	c	509	-	65,73,73	1.44	11 (16%)	76,113,113	1.57	10 (13%)
36	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.16	4 (7%)
44	LUT	S	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.71	16 (31%)
32	CLA	Y	611	38	65,73,73	1.45	8 (12%)	76,113,113	1.42	8 (10%)
36	LMG	A	413	-	48,48,55	0.95	2 (4%)	56,56,63	1.07	4 (7%)
29	OEX	a	401	4,1	0,15,15	-	-	-	-	-
32	CLA	Y	610	25	65,73,73	1.46	9 (13%)	76,113,113	1.29	7 (9%)
43	CHL	N	608	-	50,58,74	2.08	13 (26%)	52,94,114	3.21	18 (34%)
37	DGD	C	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	5 (7%)
32	CLA	c	512	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	8 (10%)
32	CLA	C	502	-	65,73,73	1.46	11 (16%)	76,113,113	1.50	6 (7%)
32	CLA	R	609	23	45,53,73	1.78	6 (13%)	52,89,113	1.60	9 (17%)
32	CLA	Y	614	-	54,62,73	1.59	8 (14%)	62,99,113	1.36	8 (12%)
32	CLA	y	613	25	65,73,73	1.49	10 (15%)	76,113,113	1.44	9 (11%)
32	CLA	B	602	47	65,73,73	1.47	8 (12%)	76,113,113	1.38	8 (10%)
44	LUT	y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.71	10 (19%)
38	LHG	G	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.96	3 (5%)
32	CLA	S	610	24	49,57,73	1.80	9 (18%)	55,93,113	1.32	7 (12%)
32	CLA	b	611	47	65,73,73	1.48	8 (12%)	76,113,113	1.55	10 (13%)
32	CLA	s	605	24	50,58,73	1.69	7 (14%)	58,95,113	1.51	11 (18%)
42	LMU	z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.21	5 (10%)
32	CLA	c	502	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	6 (7%)
43	CHL	Y	608	-	50,58,74	2.10	14 (28%)	52,94,114	3.23	19 (36%)
46	NEX	y	1623	-	38,46,46	0.92	2 (5%)	50,70,70	2.45	17 (34%)
32	CLA	c	503	-	65,73,73	1.51	8 (12%)	76,113,113	1.39	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	d	409	-	48,48,48	0.89	3 (6%)	51,54,54	0.97	3 (5%)
43	CHL	g	608	-	44,52,74	2.18	14 (31%)	46,87,114	3.26	18 (39%)
43	CHL	y	608	-	50,58,74	2.10	14 (28%)	52,94,114	3.22	19 (36%)
32	CLA	a	407	47	49,57,73	1.64	7 (14%)	55,93,113	1.70	7 (12%)
32	CLA	C	510	-	65,73,73	1.42	9 (13%)	76,113,113	1.50	7 (9%)
32	CLA	C	513	-	65,73,73	1.40	9 (13%)	76,113,113	1.45	9 (11%)
32	CLA	D	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	9 (11%)
32	CLA	C	507	47	65,73,73	1.44	9 (13%)	76,113,113	1.54	10 (13%)
43	CHL	n	609	21	66,74,74	1.87	14 (21%)	73,114,114	2.66	20 (27%)
38	LHG	g	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.95	3 (5%)
32	CLA	y	610	25	65,73,73	1.46	9 (13%)	76,113,113	1.29	7 (9%)
43	CHL	y	607	-	66,74,74	1.81	14 (21%)	73,114,114	2.68	21 (28%)
32	CLA	g	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.40	8 (14%)
32	CLA	r	604	-	49,57,73	1.70	7 (14%)	55,93,113	1.50	7 (12%)
44	LUT	y	1620	-	42,43,43	0.92	3 (7%)	51,60,60	1.90	14 (27%)
43	CHL	R	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.27	20 (43%)
32	CLA	n	611	38	49,57,73	1.69	8 (16%)	55,93,113	1.45	8 (14%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.12	6 (7%)
32	CLA	R	602	23	60,68,73	1.61	8 (13%)	70,107,113	1.35	9 (12%)
32	CLA	G	603	-	65,73,73	1.50	9 (13%)	76,113,113	1.40	10 (13%)
34	BCR	b	619	-	41,41,41	0.72	0	56,56,56	1.95	13 (23%)
32	CLA	B	612	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	9 (11%)
32	CLA	N	613	21	65,73,73	1.53	10 (15%)	76,113,113	1.37	6 (7%)
43	CHL	s	601	24	46,54,74	2.25	14 (30%)	49,90,114	3.17	21 (42%)
32	CLA	b	602	47	65,73,73	1.47	8 (12%)	76,113,113	1.39	8 (10%)
32	CLA	r	602	23	60,68,73	1.61	8 (13%)	70,107,113	1.35	9 (12%)
32	CLA	A	410	-	60,68,73	1.47	9 (15%)	70,107,113	1.48	9 (12%)
32	CLA	b	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	8 (10%)
34	BCR	c	515	-	41,41,41	0.84	1 (2%)	56,56,56	1.98	18 (32%)
32	CLA	Y	612	25	65,73,73	1.47	10 (15%)	76,113,113	1.31	8 (10%)
38	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	3 (5%)
32	CLA	a	410	-	60,68,73	1.47	8 (13%)	70,107,113	1.46	9 (12%)
43	CHL	r	608	-	46,54,74	2.27	15 (32%)	49,90,114	3.09	19 (38%)
43	CHL	g	606	-	50,58,74	2.14	14 (28%)	52,94,114	3.08	18 (34%)
32	CLA	C	512	-	65,73,73	1.42	10 (15%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	d	410	-	38,38,48	1.00	2 (5%)	41,44,54	1.00	2 (4%)
34	BCR	b	618	-	41,41,41	0.76	0	56,56,56	1.84	15 (26%)
32	CLA	C	504	47	65,73,73	1.50	10 (15%)	76,113,113	1.41	8 (10%)
32	CLA	N	611	38	49,57,73	1.70	8 (16%)	55,93,113	1.44	8 (14%)
43	CHL	g	601	22	66,74,74	1.81	12 (18%)	73,114,114	2.71	23 (31%)
43	CHL	n	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.80	22 (30%)
32	CLA	y	604	-	65,73,73	1.50	8 (12%)	76,113,113	1.36	7 (9%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.13	6 (7%)
32	CLA	s	613	24	49,57,73	1.81	10 (20%)	55,93,113	1.45	6 (10%)
43	CHL	N	609	21	66,74,74	1.86	13 (19%)	73,114,114	2.67	20 (27%)
34	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.70	13 (23%)
44	LUT	n	1621	-	42,43,43	0.79	0	51,60,60	1.52	7 (13%)
38	LHG	d	408	-	43,43,48	0.95	2 (4%)	46,49,54	1.02	2 (4%)
44	LUT	n	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.56	10 (19%)
43	CHL	S	606	-	44,52,74	2.16	13 (29%)	46,87,114	3.24	19 (41%)
32	CLA	C	511	4	65,73,73	1.41	8 (12%)	76,113,113	1.49	8 (10%)
32	CLA	b	609	-	65,73,73	1.41	7 (10%)	76,113,113	1.48	7 (9%)
32	CLA	S	613	24	49,57,73	1.80	10 (20%)	55,93,113	1.44	6 (10%)
43	CHL	r	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.28	19 (41%)
32	CLA	s	612	24	45,53,73	1.75	10 (22%)	52,89,113	1.57	8 (15%)
43	CHL	Y	601	25	66,74,74	1.80	14 (21%)	73,114,114	2.67	26 (35%)
32	CLA	N	610	21	65,73,73	1.44	7 (10%)	76,113,113	1.35	8 (10%)
36	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	4 (6%)
40	PL9	d	405	-	55,55,55	2.02	13 (23%)	68,69,69	1.46	14 (20%)
37	DGD	C	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.97	2 (2%)
38	LHG	s	2630	32	44,44,48	0.94	2 (4%)	47,50,54	1.00	2 (4%)
43	CHL	S	608	-	49,57,74	2.19	15 (30%)	52,93,114	3.15	20 (38%)
32	CLA	S	612	24	45,53,73	1.75	10 (22%)	52,89,113	1.57	8 (15%)
44	LUT	s	1621	-	42,43,43	0.80	0	51,60,60	1.71	13 (25%)
32	CLA	y	614	-	54,62,73	1.59	8 (14%)	62,99,113	1.36	8 (12%)
32	CLA	y	612	25	65,73,73	1.46	9 (13%)	76,113,113	1.31	8 (10%)
32	CLA	N	604	-	65,73,73	1.48	8 (12%)	76,113,113	1.33	7 (9%)
44	LUT	S	1621	-	42,43,43	0.79	0	51,60,60	1.71	14 (27%)
43	CHL	y	606	-	66,74,74	1.84	15 (22%)	73,114,114	2.64	20 (27%)

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
32	CLA	b	613	-	1/1/15/20	9/37/115/115	-
32	CLA	N	602	21	1/1/15/20	12/37/115/115	-
36	LMG	H	102	-	-	14/43/63/70	0/1/1/1
43	CHL	G	608	-	3/3/15/26	7/13/111/137	-
32	CLA	B	604	-	-	12/37/115/115	-
34	BCR	D	404	-	-	2/29/63/63	0/2/2/2
32	CLA	A	407	47	1/1/11/20	2/18/96/115	-
32	CLA	b	616	-	1/1/15/20	13/37/115/115	-
32	CLA	B	614	-	1/1/15/20	10/37/115/115	-
32	CLA	B	606	-	1/1/15/20	9/37/115/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
32	CLA	G	614	-	1/1/11/20	11/18/96/115	-
34	BCR	c	517	-	-	1/29/63/63	0/2/2/2
43	CHL	g	609	22	3/3/20/26	21/39/137/137	-
42	LMU	Z	2635	-	-	10/21/61/61	0/2/2/2
32	CLA	c	507	47	1/1/15/20	11/37/115/115	-
32	CLA	a	405	-	1/1/15/20	15/37/115/115	-
46	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
32	CLA	y	611	38	1/1/15/20	11/37/115/115	-
44	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	Y	602	25	1/1/15/20	10/37/115/115	-
32	CLA	B	609	-	1/1/15/20	14/37/115/115	-
34	BCR	B	618	-	-	2/29/63/63	0/2/2/2
43	CHL	y	605	25	3/3/16/26	9/15/113/137	-
32	CLA	n	604	-	1/1/15/20	11/37/115/115	-
46	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
42	LMU	y	2632	-	-	9/21/61/61	0/2/2/2
45	XAT	Y	1622	-	-	4/31/93/93	0/4/4/4
32	CLA	n	614	-	1/1/11/20	8/18/96/115	-
32	CLA	c	510	-	1/1/15/20	17/37/115/115	-
32	CLA	b	617	-	1/1/15/20	16/37/115/115	-
32	CLA	g	602	22	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	C	508	-	1/1/15/20	13/37/115/115	-
43	CHL	Y	609	25	3/3/20/26	16/39/137/137	-
32	CLA	G	610	22	1/1/15/20	13/37/115/115	-
43	CHL	n	606	-	3/3/16/26	7/15/113/137	-
35	SQD	b	621	-	-	15/49/69/69	0/1/1/1
32	CLA	b	608	47	1/1/15/20	12/37/115/115	-
35	SQD	A	412	-	-	15/46/66/69	0/1/1/1
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
43	CHL	N	607	-	3/3/20/26	20/39/137/137	-
35	SQD	a	412	-	-	15/46/66/69	0/1/1/1
36	LMG	h	102	-	-	15/43/63/70	0/1/1/1
32	CLA	s	604	-	1/1/11/20	7/18/96/115	-
32	CLA	a	406	47	-	9/37/115/115	-
43	CHL	S	601	24	3/3/16/26	8/15/113/137	-
46	NEX	r	625	-	-	5/27/83/83	0/3/3/3
32	CLA	B	605	-	1/1/15/20	13/37/115/115	-
43	CHL	N	606	-	3/3/16/26	7/15/113/137	-
46	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
32	CLA	n	612	21	1/1/11/20	4/13/91/115	-
36	LMG	a	413	-	-	17/43/63/70	0/1/1/1
32	CLA	c	501	-	1/1/15/20	16/37/115/115	-
32	CLA	S	614	-	1/1/11/20	4/17/95/115	-
32	CLA	S	604	-	1/1/11/20	7/18/96/115	-
32	CLA	C	505	-	-	14/37/115/115	-
44	LUT	g	1621	-	-	5/29/67/67	0/2/2/2
34	BCR	c	514	-	-	2/29/63/63	0/2/2/2
32	CLA	b	606	-	1/1/15/20	9/37/115/115	-
37	DGD	c	520	-	-	14/48/88/95	0/2/2/2
34	BCR	C	516	-	-	8/29/63/63	0/2/2/2
32	CLA	c	511	4	-	12/37/115/115	-
36	LMG	b	622	-	-	4/46/66/70	0/1/1/1
32	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
32	CLA	n	613	21	-	12/37/115/115	-
43	CHL	G	601	22	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Y	613	25	-	13/37/115/115	-
43	CHL	Y	606	-	3/3/20/26	15/39/137/137	-
45	XAT	g	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	s	609	24	1/1/10/20	2/8/86/115	-
38	LHG	D	410	-	-	13/43/43/53	-
32	CLA	G	602	22	1/1/15/20	16/37/115/115	-
38	LHG	y	2630	32	-	18/53/53/53	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
37	DGD	C	524	-	-	10/55/95/95	0/2/2/2
33	PHO	A	408	-	-	12/37/103/103	0/5/6/6
45	XAT	G	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	g	613	22	-	16/37/115/115	-
32	CLA	r	609	23	1/1/11/20	8/13/91/115	-
32	CLA	B	616	-	1/1/15/20	14/37/115/115	-
32	CLA	C	506	-	-	4/37/115/115	-
37	DGD	c	518	-	-	10/44/84/95	0/2/2/2
38	LHG	D	409	-	-	20/53/53/53	-
32	CLA	R	603	-	1/1/11/20	11/18/96/115	-
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
37	DGD	c	524	-	-	10/55/95/95	0/2/2/2
32	CLA	s	603	-	1/1/10/20	5/10/88/115	-
43	CHL	n	605	21	3/3/20/26	17/39/137/137	-
36	LMG	c	521	-	-	5/46/66/70	0/1/1/1
42	LMU	Z	2634	-	-	9/21/61/61	0/2/2/2
35	SQD	B	621	-	-	16/49/69/69	0/1/1/1
38	LHG	L	101	-	-	20/53/53/53	-
38	LHG	C	2630	-	-	15/51/51/53	-
41	HEM	f	101	6,7	-	2/12/54/54	-
32	CLA	c	505	-	-	14/37/115/115	-
46	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
32	CLA	S	603	-	1/1/10/20	5/10/88/115	-
46	NEX	R	625	-	-	5/27/83/83	0/3/3/3
42	LMU	Y	2632	-	-	9/21/61/61	0/2/2/2
34	BCR	d	404	-	-	2/29/63/63	0/2/2/2
32	CLA	d	403	-	-	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	LUT	s	1620	-	-	4/29/67/67	0/2/2/2
43	CHL	S	607	-	3/3/15/26	4/12/110/137	-
32	CLA	b	612	-	1/1/15/20	11/37/115/115	-
32	CLA	B	603	-	1/1/15/20	14/37/115/115	-
32	CLA	s	611	38	1/1/11/20	7/18/96/115	-
43	CHL	s	607	-	3/3/15/26	3/12/110/137	-
32	CLA	n	603	-	1/1/15/20	14/37/115/115	-
32	CLA	N	614	-	1/1/11/20	7/18/96/115	-
32	CLA	n	610	21	1/1/15/20	3/37/115/115	-
43	CHL	r	607	-	3/3/16/26	7/20/118/137	-
32	CLA	Y	604	-	1/1/15/20	14/37/115/115	-
32	CLA	b	615	-	1/1/15/20	21/37/115/115	-
43	CHL	R	607	-	3/3/16/26	7/20/118/137	-
32	CLA	S	611	38	1/1/11/20	7/18/96/115	-
45	XAT	y	1622	-	-	4/31/93/93	0/4/4/4
32	CLA	n	602	21	1/1/15/20	13/37/115/115	-
45	XAT	r	624	-	-	1/31/93/93	0/4/4/4
32	CLA	G	613	22	-	16/37/115/115	-
46	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
44	LUT	G	1621	-	-	5/29/67/67	0/2/2/2
32	CLA	s	610	24	1/1/11/20	6/18/96/115	-
44	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	n	608	-	3/3/16/26	5/20/118/137	-
32	CLA	B	615	-	1/1/15/20	21/37/115/115	-
32	CLA	C	501	-	1/1/15/20	16/37/115/115	-
32	CLA	r	610	23	1/1/10/20	3/8/86/115	-
43	CHL	N	605	21	3/3/20/26	17/39/137/137	-
38	LHG	N	2630	32	-	12/53/53/53	-
45	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	g	603	-	1/1/15/20	14/37/115/115	-
40	PL9	D	405	-	-	14/53/73/73	0/1/1/1
32	CLA	R	610	23	1/1/10/20	3/8/86/115	-
43	CHL	G	606	-	3/3/16/26	8/20/118/137	-
32	CLA	s	602	24	1/1/11/20	8/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	NEX	Y	1623	-	-	8/27/83/83	0/3/3/3
38	LHG	n	2630	32	-	12/53/53/53	-
32	CLA	g	604	-	1/1/11/20	10/18/96/115	-
43	CHL	G	607	-	3/3/16/26	8/20/118/137	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
44	LUT	Y	1621	-	-	5/29/67/67	0/2/2/2
32	CLA	b	607	-	1/1/15/20	11/37/115/115	-
44	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	S	602	24	1/1/11/20	8/18/96/115	-
32	CLA	N	603	-	1/1/15/20	14/37/115/115	-
32	CLA	y	603	-	1/1/15/20	14/37/115/115	-
32	CLA	G	611	38	1/1/11/20	3/13/91/115	-
32	CLA	C	503	-	1/1/15/20	9/37/115/115	-
34	BCR	C	515	-	-	7/29/63/63	0/2/2/2
43	CHL	Y	605	25	3/3/16/26	9/15/113/137	-
32	CLA	g	612	22	1/1/10/20	4/11/89/115	-
32	CLA	C	509	-	1/1/15/20	10/37/115/115	-
43	CHL	Y	607	-	3/3/20/26	22/39/137/137	-
32	CLA	A	406	47	-	9/37/115/115	-
33	PHO	a	409	-	-	3/37/103/103	0/5/6/6
32	CLA	c	504	47	1/1/15/20	13/37/115/115	-
32	CLA	B	613	-	1/1/15/20	9/37/115/115	-
42	LMU	z	2635	-	-	10/21/61/61	0/2/2/2
32	CLA	b	603	-	1/1/15/20	14/37/115/115	-
32	CLA	r	603	-	1/1/11/20	11/18/96/115	-
32	CLA	s	614	-	1/1/11/20	4/17/95/115	-
38	LHG	Y	2630	32	-	18/53/53/53	-
37	DGD	c	523	-	-	15/55/95/95	0/2/2/2
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
38	LHG	S	2630	32	-	9/49/49/53	-
32	CLA	d	402	-	1/1/15/20	9/37/115/115	-
45	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	c	513	-	1/1/15/20	19/37/115/115	-
46	NEX	g	1623	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	R	604	-	1/1/11/20	7/18/96/115	-
43	CHL	G	609	22	3/3/20/26	21/39/137/137	-
32	CLA	b	614	-	1/1/15/20	10/37/115/115	-
32	CLA	c	506	-	-	4/37/115/115	-
32	CLA	b	604	-	-	12/37/115/115	-
32	CLA	A	405	-	1/1/15/20	15/37/115/115	-
32	CLA	c	508	-	1/1/15/20	13/37/115/115	-
34	BCR	a	411	-	-	5/29/63/63	0/2/2/2
44	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
38	LHG	D	408	-	-	17/48/48/53	-
32	CLA	G	604	-	1/1/11/20	10/18/96/115	-
32	CLA	g	611	38	1/1/11/20	3/13/91/115	-
43	CHL	s	606	-	3/3/15/26	5/13/111/137	-
32	CLA	y	602	25	1/1/15/20	10/37/115/115	-
43	CHL	g	605	22	3/3/16/26	4/18/116/137	-
43	CHL	N	601	21	3/3/20/26	17/39/137/137	-
32	CLA	S	609	24	1/1/10/20	3/8/86/115	-
43	CHL	G	605	22	3/3/16/26	4/18/116/137	-
43	CHL	g	607	-	3/3/16/26	8/20/118/137	-
45	XAT	R	624	-	-	1/31/93/93	0/4/4/4
43	CHL	y	609	25	3/3/20/26	17/39/137/137	-
36	LMG	C	521	-	-	5/46/66/70	0/1/1/1
41	HEM	F	101	6,7	-	2/12/54/54	-
43	CHL	n	601	21	3/3/20/26	17/39/137/137	-
44	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	G	612	22	1/1/10/20	4/11/89/115	-
32	CLA	S	605	24	1/1/12/20	6/19/97/115	-
32	CLA	B	608	47	1/1/15/20	12/37/115/115	-
43	CHL	s	608	-	3/3/16/26	10/19/117/137	-
32	CLA	b	605	-	1/1/15/20	13/37/115/115	-
32	CLA	N	612	21	1/1/11/20	4/13/91/115	-
43	CHL	y	601	25	3/3/20/26	19/39/137/137	-
32	CLA	B	611	47	1/1/15/20	7/37/115/115	-
32	CLA	g	610	22	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PHO	a	408	-	-	11/37/103/103	0/5/6/6
34	BCR	C	514	-	-	2/29/63/63	0/2/2/2
38	LHG	c	2630	-	-	15/51/51/53	-
32	CLA	D	402	-	1/1/15/20	9/37/115/115	-
32	CLA	B	610	-	-	15/37/115/115	-
33	PHO	A	409	-	-	1/37/103/103	0/5/6/6
34	BCR	C	517	-	-	1/29/63/63	0/2/2/2
36	LMG	D	411	-	-	10/41/61/70	0/1/1/1
43	CHL	R	608	-	3/3/16/26	5/15/113/137	-
32	CLA	B	617	-	1/1/15/20	16/37/115/115	-
32	CLA	B	607	-	1/1/15/20	11/37/115/115	-
37	DGD	C	523	-	-	15/55/95/95	0/2/2/2
32	CLA	c	509	-	1/1/15/20	10/37/115/115	-
36	LMG	d	411	-	-	10/41/61/70	0/1/1/1
44	LUT	S	1620	-	-	4/29/67/67	0/2/2/2
32	CLA	Y	611	38	1/1/15/20	11/37/115/115	-
36	LMG	A	413	-	-	17/43/63/70	0/1/1/1
32	CLA	Y	610	25	1/1/15/20	5/37/115/115	-
43	CHL	N	608	-	3/3/16/26	5/20/118/137	-
37	DGD	C	518	-	-	11/44/84/95	0/2/2/2
32	CLA	c	512	-	1/1/15/20	15/37/115/115	-
32	CLA	C	502	-	-	8/37/115/115	-
32	CLA	R	609	23	1/1/11/20	8/13/91/115	-
32	CLA	Y	614	-	1/1/12/20	6/24/102/115	-
32	CLA	y	613	25	-	13/37/115/115	-
32	CLA	B	602	47	1/1/15/20	12/37/115/115	-
44	LUT	y	1621	-	-	5/29/67/67	0/2/2/2
38	LHG	G	2630	32	-	17/53/53/53	-
32	CLA	S	610	24	1/1/11/20	6/18/96/115	-
32	CLA	b	611	47	1/1/15/20	7/37/115/115	-
32	CLA	s	605	24	1/1/12/20	6/19/97/115	-
42	LMU	z	2634	-	-	9/21/61/61	0/2/2/2
32	CLA	c	502	-	-	8/37/115/115	-
43	CHL	Y	608	-	3/3/16/26	4/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	NEX	y	1623	-	-	9/27/83/83	0/3/3/3
32	CLA	c	503	-	1/1/15/20	10/37/115/115	-
43	CHL	g	608	-	3/3/15/26	7/13/111/137	-
38	LHG	d	409	-	-	19/53/53/53	-
43	CHL	y	608	-	3/3/16/26	4/20/118/137	-
32	CLA	a	407	47	1/1/11/20	2/18/96/115	-
32	CLA	C	510	-	1/1/15/20	17/37/115/115	-
32	CLA	C	513	-	1/1/15/20	19/37/115/115	-
32	CLA	D	403	-	-	12/37/115/115	-
32	CLA	C	507	47	1/1/15/20	11/37/115/115	-
43	CHL	n	609	21	3/3/20/26	21/39/137/137	-
38	LHG	g	2630	32	-	17/53/53/53	-
32	CLA	y	610	25	1/1/15/20	5/37/115/115	-
43	CHL	y	607	-	3/3/20/26	22/39/137/137	-
32	CLA	g	614	-	1/1/11/20	11/18/96/115	-
32	CLA	r	604	-	1/1/11/20	7/18/96/115	-
44	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	R	606	-	3/3/15/26	5/13/111/137	-
32	CLA	n	611	38	1/1/11/20	12/18/96/115	-
37	DGD	C	519	-	-	11/51/91/95	0/2/2/2
32	CLA	R	602	23	1/1/14/20	5/31/109/115	-
32	CLA	G	603	-	1/1/15/20	14/37/115/115	-
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
32	CLA	B	612	-	1/1/15/20	11/37/115/115	-
32	CLA	N	613	21	-	12/37/115/115	-
43	CHL	s	601	24	3/3/16/26	8/15/113/137	-
32	CLA	b	602	47	1/1/15/20	12/37/115/115	-
32	CLA	r	602	23	1/1/14/20	5/31/109/115	-
32	CLA	A	410	-	-	4/31/109/115	-
32	CLA	b	610	-	-	15/37/115/115	-
34	BCR	c	515	-	-	7/29/63/63	0/2/2/2
32	CLA	Y	612	25	1/1/15/20	16/37/115/115	-
38	LHG	l	101	-	-	20/53/53/53	-
32	CLA	a	410	-	-	4/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CHL	r	608	-	3/3/16/26	5/15/113/137	-
43	CHL	g	606	-	3/3/16/26	8/20/118/137	-
32	CLA	C	512	-	1/1/15/20	15/37/115/115	-
38	LHG	d	410	-	-	13/43/43/53	-
34	BCR	b	618	-	-	2/29/63/63	0/2/2/2
32	CLA	C	504	47	1/1/15/20	13/37/115/115	-
32	CLA	N	611	38	1/1/11/20	12/18/96/115	-
43	CHL	g	601	22	3/3/20/26	14/39/137/137	-
43	CHL	n	607	-	3/3/20/26	20/39/137/137	-
32	CLA	y	604	-	1/1/15/20	13/37/115/115	-
37	DGD	c	519	-	-	13/51/91/95	0/2/2/2
32	CLA	s	613	24	-	8/18/96/115	-
43	CHL	N	609	21	3/3/20/26	21/39/137/137	-
34	BCR	A	411	-	-	5/29/63/63	0/2/2/2
44	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
38	LHG	d	408	-	-	18/48/48/53	-
44	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	S	606	-	3/3/15/26	5/13/111/137	-
32	CLA	C	511	4	-	12/37/115/115	-
32	CLA	b	609	-	1/1/15/20	14/37/115/115	-
32	CLA	S	613	24	-	8/18/96/115	-
43	CHL	r	606	-	3/3/15/26	5/13/111/137	-
32	CLA	s	612	24	1/1/11/20	4/13/91/115	-
43	CHL	Y	601	25	3/3/20/26	19/39/137/137	-
32	CLA	N	610	21	1/1/15/20	3/37/115/115	-
36	LMG	B	622	-	-	4/46/66/70	0/1/1/1
40	PL9	d	405	-	-	14/53/73/73	0/1/1/1
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
38	LHG	s	2630	32	-	9/49/49/53	-
43	CHL	S	608	-	3/3/16/26	10/19/117/137	-
32	CLA	S	612	24	1/1/11/20	4/13/91/115	-
44	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	y	614	-	1/1/12/20	6/24/102/115	-
32	CLA	y	612	25	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	N	604	-	1/1/15/20	12/37/115/115	-
44	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
43	CHL	y	606	-	3/3/20/26	15/39/137/137	-

All (2131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	613	CLA	C4B-NB	7.90	1.42	1.35
32	s	613	CLA	C4B-NB	7.89	1.42	1.35
32	r	602	CLA	C4B-NB	7.82	1.42	1.35
32	s	610	CLA	C4B-NB	7.81	1.42	1.35
32	R	602	CLA	C4B-NB	7.80	1.42	1.35
32	S	609	CLA	C4B-NB	7.80	1.42	1.35
32	S	610	CLA	C4B-NB	7.76	1.42	1.35
32	n	614	CLA	C4B-NB	7.73	1.42	1.35
32	s	609	CLA	C4B-NB	7.70	1.42	1.35
32	N	614	CLA	C4B-NB	7.64	1.42	1.35
32	g	612	CLA	C4B-NB	7.58	1.42	1.35
32	g	602	CLA	C4B-NB	7.56	1.42	1.35
32	G	612	CLA	C4B-NB	7.54	1.41	1.35
32	G	602	CLA	C4B-NB	7.54	1.41	1.35
32	S	603	CLA	C4B-NB	7.53	1.41	1.35
32	C	504	CLA	C4B-NB	7.52	1.41	1.35
32	c	504	CLA	C4B-NB	7.52	1.41	1.35
32	N	613	CLA	C4B-NB	7.51	1.41	1.35
32	r	603	CLA	C4B-NB	7.51	1.41	1.35
32	G	604	CLA	C4B-NB	7.49	1.41	1.35
32	g	604	CLA	C4B-NB	7.49	1.41	1.35
32	R	604	CLA	C4B-NB	7.49	1.41	1.35
32	n	613	CLA	C4B-NB	7.49	1.41	1.35
32	r	610	CLA	C4B-NB	7.47	1.41	1.35
32	N	603	CLA	C4B-NB	7.47	1.41	1.35
32	g	614	CLA	C4B-NB	7.46	1.41	1.35
32	R	603	CLA	C4B-NB	7.43	1.41	1.35
32	R	610	CLA	C4B-NB	7.43	1.41	1.35
32	S	605	CLA	C4B-NB	7.43	1.41	1.35
32	g	613	CLA	C4B-NB	7.42	1.41	1.35
32	G	614	CLA	C4B-NB	7.42	1.41	1.35
32	n	603	CLA	C4B-NB	7.42	1.41	1.35
32	y	613	CLA	C4B-NB	7.42	1.41	1.35
32	N	612	CLA	C4B-NB	7.41	1.41	1.35
32	s	603	CLA	C4B-NB	7.41	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	603	CLA	C4B-NB	7.41	1.41	1.35
32	g	603	CLA	C4B-NB	7.41	1.41	1.35
32	r	604	CLA	C4B-NB	7.40	1.41	1.35
32	B	611	CLA	C4B-NB	7.40	1.41	1.35
32	b	611	CLA	C4B-NB	7.40	1.41	1.35
40	d	405	PL9	C7-C3	-7.39	1.43	1.51
40	D	405	PL9	C7-C3	-7.37	1.43	1.51
32	Y	602	CLA	C4B-NB	7.36	1.41	1.35
32	y	602	CLA	C4B-NB	7.36	1.41	1.35
32	S	604	CLA	C4B-NB	7.34	1.41	1.35
32	B	602	CLA	C4B-NB	7.34	1.41	1.35
32	G	613	CLA	C4B-NB	7.34	1.41	1.35
32	g	611	CLA	C4B-NB	7.34	1.41	1.35
32	s	604	CLA	C4B-NB	7.34	1.41	1.35
32	Y	613	CLA	C4B-NB	7.33	1.41	1.35
32	s	605	CLA	C4B-NB	7.32	1.41	1.35
32	G	611	CLA	C4B-NB	7.31	1.41	1.35
32	n	612	CLA	C4B-NB	7.31	1.41	1.35
32	b	607	CLA	C4B-NB	7.30	1.41	1.35
32	b	602	CLA	C4B-NB	7.27	1.41	1.35
32	R	609	CLA	C4B-NB	7.27	1.41	1.35
32	B	616	CLA	C4B-NB	7.27	1.41	1.35
32	r	609	CLA	C4B-NB	7.25	1.41	1.35
32	B	607	CLA	C4B-NB	7.22	1.41	1.35
32	B	604	CLA	C4B-NB	7.20	1.41	1.35
32	b	616	CLA	C4B-NB	7.20	1.41	1.35
32	N	602	CLA	C4B-NB	7.20	1.41	1.35
32	b	604	CLA	C4B-NB	7.19	1.41	1.35
32	B	612	CLA	C4B-NB	7.18	1.41	1.35
32	b	612	CLA	C4B-NB	7.18	1.41	1.35
32	n	602	CLA	C4B-NB	7.17	1.41	1.35
32	Y	604	CLA	C4B-NB	7.16	1.41	1.35
32	y	604	CLA	C4B-NB	7.16	1.41	1.35
32	y	603	CLA	C4B-NB	7.15	1.41	1.35
32	S	602	CLA	C4B-NB	7.15	1.41	1.35
32	B	615	CLA	C4B-NB	7.14	1.41	1.35
32	b	610	CLA	C4B-NB	7.14	1.41	1.35
32	B	610	CLA	C4B-NB	7.14	1.41	1.35
32	N	611	CLA	C4B-NB	7.13	1.41	1.35
32	s	602	CLA	C4B-NB	7.11	1.41	1.35
32	n	611	CLA	C4B-NB	7.11	1.41	1.35
32	S	614	CLA	C4B-NB	7.08	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	405	CLA	C4B-NB	7.07	1.41	1.35
32	a	405	CLA	C4B-NB	7.07	1.41	1.35
32	Y	603	CLA	C4B-NB	7.06	1.41	1.35
32	C	503	CLA	C4B-NB	7.06	1.41	1.35
32	D	402	CLA	C4B-NB	7.04	1.41	1.35
32	b	615	CLA	C4B-NB	7.03	1.41	1.35
32	c	503	CLA	C4B-NB	7.03	1.41	1.35
32	s	612	CLA	C4B-NB	7.03	1.41	1.35
32	S	612	CLA	C4B-NB	7.00	1.41	1.35
32	s	614	CLA	C4B-NB	7.00	1.41	1.35
32	C	501	CLA	C4B-NB	6.98	1.41	1.35
32	D	403	CLA	C4B-NB	6.98	1.41	1.35
32	b	606	CLA	C4B-NB	6.98	1.41	1.35
32	d	403	CLA	C4B-NB	6.96	1.41	1.35
32	B	606	CLA	C4B-NB	6.95	1.41	1.35
32	Y	612	CLA	C4B-NB	6.95	1.41	1.35
32	y	612	CLA	C4B-NB	6.95	1.41	1.35
32	d	402	CLA	C4B-NB	6.94	1.41	1.35
32	c	501	CLA	C4B-NB	6.91	1.41	1.35
32	b	603	CLA	C4B-NB	6.87	1.41	1.35
32	Y	610	CLA	C4B-NB	6.86	1.41	1.35
32	y	610	CLA	C4B-NB	6.86	1.41	1.35
32	N	604	CLA	C4B-NB	6.81	1.41	1.35
32	N	610	CLA	C4B-NB	6.79	1.41	1.35
32	n	610	CLA	C4B-NB	6.79	1.41	1.35
32	y	611	CLA	C4B-NB	6.79	1.41	1.35
32	G	610	CLA	C4B-NB	6.78	1.41	1.35
32	g	610	CLA	C4B-NB	6.77	1.41	1.35
40	d	405	PL9	C3-C4	-6.77	1.38	1.49
32	B	609	CLA	C4B-NB	6.76	1.41	1.35
32	b	609	CLA	C4B-NB	6.76	1.41	1.35
32	B	603	CLA	C4B-NB	6.75	1.41	1.35
32	Y	611	CLA	C4B-NB	6.72	1.41	1.35
32	B	608	CLA	C4B-NB	6.71	1.41	1.35
32	n	604	CLA	C4B-NB	6.71	1.41	1.35
40	D	405	PL9	C3-C4	-6.70	1.38	1.49
32	Y	614	CLA	C4B-NB	6.70	1.41	1.35
32	y	614	CLA	C4B-NB	6.70	1.41	1.35
32	a	407	CLA	C4B-NB	6.70	1.41	1.35
32	b	608	CLA	C4B-NB	6.69	1.41	1.35
32	S	611	CLA	C4B-NB	6.66	1.41	1.35
32	s	611	CLA	C4B-NB	6.66	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	507	CLA	C4B-NB	6.64	1.41	1.35
32	C	506	CLA	C4B-NB	6.63	1.41	1.35
32	C	505	CLA	C4B-NB	6.63	1.41	1.35
32	c	507	CLA	C4B-NB	6.60	1.41	1.35
32	A	407	CLA	C4B-NB	6.59	1.41	1.35
32	c	505	CLA	C4B-NB	6.59	1.41	1.35
32	b	617	CLA	C4B-NB	6.55	1.41	1.35
32	C	511	CLA	C4B-NB	6.54	1.41	1.35
32	B	617	CLA	C4B-NB	6.50	1.41	1.35
32	B	613	CLA	C4B-NB	6.49	1.41	1.35
32	b	613	CLA	C4B-NB	6.49	1.41	1.35
32	C	510	CLA	C4B-NB	6.49	1.41	1.35
32	c	506	CLA	C4B-NB	6.47	1.41	1.35
32	A	406	CLA	C4B-NB	6.46	1.41	1.35
32	c	511	CLA	C4B-NB	6.46	1.41	1.35
32	C	512	CLA	C4B-NB	6.45	1.41	1.35
32	c	510	CLA	C4B-NB	6.42	1.40	1.35
32	c	512	CLA	C4B-NB	6.42	1.40	1.35
32	a	406	CLA	C4B-NB	6.42	1.40	1.35
32	C	502	CLA	C4B-NB	6.42	1.40	1.35
32	a	410	CLA	C4B-NB	6.38	1.40	1.35
32	c	513	CLA	C4B-NB	6.37	1.40	1.35
32	C	513	CLA	C4B-NB	6.37	1.40	1.35
32	A	410	CLA	C4B-NB	6.35	1.40	1.35
32	B	614	CLA	C4B-NB	6.35	1.40	1.35
32	c	502	CLA	C4B-NB	6.32	1.40	1.35
32	b	614	CLA	C4B-NB	6.28	1.40	1.35
32	c	508	CLA	C4B-NB	6.26	1.40	1.35
32	C	508	CLA	C4B-NB	6.23	1.40	1.35
32	C	509	CLA	C4B-NB	6.19	1.40	1.35
32	c	509	CLA	C4B-NB	6.17	1.40	1.35
32	b	605	CLA	C4B-NB	5.88	1.40	1.35
32	B	605	CLA	C4B-NB	5.80	1.40	1.35
43	y	606	CHL	C3D-C4D	-5.68	1.31	1.44
43	Y	606	CHL	C3D-C4D	-5.68	1.31	1.44
43	y	601	CHL	C3D-C4D	-5.63	1.31	1.44
43	Y	601	CHL	C3D-C4D	-5.63	1.31	1.44
43	N	609	CHL	C3D-C4D	-5.51	1.31	1.44
43	n	609	CHL	C3D-C4D	-5.51	1.31	1.44
43	g	609	CHL	C3D-C4D	-5.51	1.31	1.44
43	G	609	CHL	C3D-C4D	-5.51	1.31	1.44
43	y	609	CHL	C3D-C4D	-5.43	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Y	609	CHL	C3D-C4D	-5.42	1.31	1.44
43	N	607	CHL	C3D-C4D	-5.33	1.32	1.44
43	n	607	CHL	C3D-C4D	-5.33	1.32	1.44
43	G	605	CHL	CHC-C1C	5.31	1.48	1.35
43	g	601	CHL	C3D-C4D	-5.30	1.32	1.44
43	s	601	CHL	C3D-C4D	-5.29	1.32	1.44
43	S	601	CHL	C3D-C4D	-5.29	1.32	1.44
43	g	605	CHL	CHC-C1C	5.29	1.48	1.35
43	Y	608	CHL	C3D-C4D	-5.27	1.32	1.44
43	y	607	CHL	C3D-C4D	-5.27	1.32	1.44
43	Y	607	CHL	C3D-C4D	-5.27	1.32	1.44
43	y	608	CHL	C3D-C4D	-5.25	1.32	1.44
43	r	607	CHL	O2D-CGD	5.21	1.45	1.33
43	R	607	CHL	O2D-CGD	5.19	1.45	1.33
43	G	601	CHL	C3D-C4D	-5.18	1.32	1.44
43	n	601	CHL	C3D-C4D	-5.15	1.32	1.44
43	S	607	CHL	O2D-CGD	5.15	1.45	1.33
43	N	601	CHL	C3D-C4D	-5.14	1.32	1.44
43	N	608	CHL	C3D-C4D	-5.14	1.32	1.44
43	N	605	CHL	C3D-C4D	-5.14	1.32	1.44
43	n	605	CHL	C3D-C4D	-5.14	1.32	1.44
43	g	605	CHL	O2D-CGD	5.14	1.45	1.33
43	N	606	CHL	C3D-C4D	-5.12	1.32	1.44
43	n	606	CHL	C3D-C4D	-5.12	1.32	1.44
43	n	608	CHL	C3D-C4D	-5.11	1.32	1.44
43	G	605	CHL	O2D-CGD	5.10	1.45	1.33
43	r	606	CHL	O2D-CGD	5.10	1.45	1.33
43	N	606	CHL	CHC-C1C	5.09	1.48	1.35
43	s	607	CHL	O2D-CGD	5.09	1.45	1.33
43	R	606	CHL	O2D-CGD	5.09	1.45	1.33
43	G	608	CHL	O2D-CGD	5.08	1.45	1.33
43	n	606	CHL	CHC-C1C	5.08	1.48	1.35
43	g	605	CHL	C3B-C2B	5.07	1.47	1.40
43	g	608	CHL	C3D-C4D	-5.07	1.32	1.44
43	g	608	CHL	O2D-CGD	5.07	1.45	1.33
43	g	607	CHL	O2D-CGD	5.05	1.45	1.33
43	s	608	CHL	CHC-C1C	5.05	1.47	1.35
43	G	605	CHL	C3B-C2B	5.05	1.47	1.40
43	g	606	CHL	CHC-C1C	5.05	1.47	1.35
43	g	605	CHL	C3D-C4D	-5.04	1.32	1.44
43	G	607	CHL	O2D-CGD	5.04	1.45	1.33
43	g	607	CHL	CHC-C1C	5.04	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	S	601	CHL	O2D-CGD	5.04	1.45	1.33
43	S	607	CHL	C3D-C4D	-5.03	1.32	1.44
43	s	607	CHL	C3D-C4D	-5.03	1.32	1.44
43	G	605	CHL	C3D-C4D	-5.03	1.32	1.44
43	G	608	CHL	C3D-C4D	-5.03	1.32	1.44
43	G	607	CHL	CHC-C1C	5.03	1.47	1.35
43	S	608	CHL	CHC-C1C	5.02	1.47	1.35
43	S	606	CHL	CHC-C1C	5.02	1.47	1.35
43	s	606	CHL	CHC-C1C	5.02	1.47	1.35
43	G	606	CHL	O2D-CGD	5.01	1.45	1.33
43	g	606	CHL	O2D-CGD	5.01	1.45	1.33
43	G	606	CHL	CHC-C1C	5.01	1.47	1.35
43	r	608	CHL	O2D-CGD	5.01	1.45	1.33
43	s	601	CHL	O2D-CGD	5.01	1.45	1.33
43	G	606	CHL	C3D-C4D	-5.00	1.32	1.44
43	n	606	CHL	O2D-CGD	4.98	1.45	1.33
43	R	608	CHL	O2D-CGD	4.98	1.45	1.33
43	r	608	CHL	C3D-C4D	-4.97	1.32	1.44
43	R	607	CHL	CHC-C1C	4.96	1.47	1.35
43	R	608	CHL	C3D-C4D	-4.96	1.33	1.44
43	r	608	CHL	CHC-C1C	4.96	1.47	1.35
43	g	606	CHL	C3D-C4D	-4.96	1.33	1.44
43	R	608	CHL	CHC-C1C	4.96	1.47	1.35
43	G	607	CHL	C3D-C4D	-4.96	1.33	1.44
43	N	606	CHL	O2D-CGD	4.95	1.45	1.33
43	s	606	CHL	O2D-CGD	4.95	1.45	1.33
43	g	607	CHL	C3D-C4D	-4.95	1.33	1.44
43	S	606	CHL	O2D-CGD	4.94	1.45	1.33
43	S	607	CHL	CHC-C1C	4.94	1.47	1.35
43	s	607	CHL	CHC-C1C	4.94	1.47	1.35
43	r	607	CHL	CHC-C1C	4.94	1.47	1.35
43	S	601	CHL	CHC-C1C	4.93	1.47	1.35
43	Y	607	CHL	O2D-CGD	4.93	1.45	1.33
43	s	601	CHL	CHC-C1C	4.92	1.47	1.35
43	n	608	CHL	CHC-C1C	4.91	1.47	1.35
43	Y	605	CHL	C3D-C4D	-4.91	1.33	1.44
43	y	605	CHL	C3D-C4D	-4.91	1.33	1.44
43	y	607	CHL	O2D-CGD	4.91	1.45	1.33
43	Y	605	CHL	O2D-CGD	4.91	1.45	1.33
43	y	605	CHL	O2D-CGD	4.91	1.45	1.33
43	N	608	CHL	CHC-C1C	4.91	1.47	1.35
43	N	601	CHL	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Y	606	CHL	CHC-C1C	4.89	1.47	1.35
43	n	601	CHL	O2D-CGD	4.88	1.45	1.33
43	y	606	CHL	CHC-C1C	4.87	1.47	1.35
43	S	608	CHL	C3D-C4D	-4.83	1.33	1.44
43	r	606	CHL	CHC-C1C	4.82	1.47	1.35
43	R	606	CHL	C3D-C4D	-4.81	1.33	1.44
43	r	606	CHL	C3D-C4D	-4.81	1.33	1.44
43	g	605	CHL	C2C-C3C	4.81	1.47	1.36
43	R	606	CHL	CHC-C1C	4.81	1.47	1.35
43	g	608	CHL	CHC-C1C	4.81	1.47	1.35
43	s	608	CHL	O2D-CGD	4.80	1.44	1.33
43	s	606	CHL	C3D-C4D	-4.80	1.33	1.44
43	S	608	CHL	O2D-CGD	4.80	1.44	1.33
43	Y	609	CHL	O2D-CGD	4.80	1.44	1.33
43	y	609	CHL	O2D-CGD	4.80	1.44	1.33
43	N	607	CHL	O2D-CGD	4.80	1.44	1.33
43	s	608	CHL	C3D-C4D	-4.79	1.33	1.44
35	A	412	SQD	O8-S	4.79	1.64	1.47
43	S	606	CHL	C3D-C4D	-4.78	1.33	1.44
43	Y	608	CHL	CHC-C1C	4.78	1.47	1.35
43	G	605	CHL	CHD-C1D	4.78	1.47	1.38
35	a	412	SQD	O8-S	4.78	1.64	1.47
43	y	606	CHL	O2D-CGD	4.78	1.44	1.33
43	g	605	CHL	CHD-C1D	4.78	1.47	1.38
43	N	608	CHL	O2D-CGD	4.77	1.44	1.33
43	G	605	CHL	C2C-C3C	4.77	1.47	1.36
43	G	608	CHL	CHC-C1C	4.77	1.47	1.35
43	y	608	CHL	CHC-C1C	4.77	1.47	1.35
43	G	609	CHL	O2D-CGD	4.76	1.44	1.33
43	n	607	CHL	O2D-CGD	4.76	1.44	1.33
43	Y	606	CHL	O2D-CGD	4.75	1.44	1.33
43	Y	605	CHL	CHC-C1C	4.75	1.47	1.35
43	y	605	CHL	CHC-C1C	4.74	1.47	1.35
43	n	608	CHL	O2D-CGD	4.74	1.44	1.33
43	Y	608	CHL	O2D-CGD	4.73	1.44	1.33
43	g	609	CHL	O2D-CGD	4.73	1.44	1.33
43	y	608	CHL	O2D-CGD	4.73	1.44	1.33
43	y	609	CHL	CHC-C1C	4.72	1.47	1.35
43	g	601	CHL	CHC-C1C	4.71	1.47	1.35
43	G	609	CHL	CHC-C1C	4.70	1.47	1.35
43	g	609	CHL	CHC-C1C	4.70	1.47	1.35
43	R	607	CHL	C3B-C2B	4.69	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	G	601	CHL	CHC-C1C	4.69	1.47	1.35
43	Y	609	CHL	CHC-C1C	4.69	1.47	1.35
43	g	601	CHL	O2D-CGD	4.69	1.44	1.33
43	r	607	CHL	C3D-C4D	-4.68	1.33	1.44
43	G	601	CHL	O2D-CGD	4.66	1.44	1.33
43	r	607	CHL	C3B-C2B	4.64	1.46	1.40
43	S	607	CHL	C3B-C2B	4.63	1.46	1.40
43	s	607	CHL	C3B-C2B	4.63	1.46	1.40
43	R	607	CHL	C3D-C4D	-4.62	1.33	1.44
35	B	621	SQD	O8-S	4.60	1.63	1.47
35	b	621	SQD	O8-S	4.60	1.63	1.47
43	n	609	CHL	O2A-CGA	4.59	1.46	1.33
43	N	609	CHL	O2A-CGA	4.58	1.46	1.33
43	s	608	CHL	C2C-C3C	4.56	1.46	1.36
43	n	609	CHL	O2D-CGD	4.55	1.44	1.33
43	Y	607	CHL	CHC-C1C	4.55	1.46	1.35
43	y	607	CHL	CHC-C1C	4.55	1.46	1.35
43	r	606	CHL	C3B-C2B	4.54	1.46	1.40
43	N	601	CHL	CHC-C1C	4.54	1.46	1.35
43	S	608	CHL	C2C-C3C	4.53	1.46	1.36
43	R	606	CHL	C3B-C2B	4.53	1.46	1.40
43	N	609	CHL	O2D-CGD	4.53	1.44	1.33
43	r	608	CHL	C2C-C3C	4.53	1.46	1.36
43	n	601	CHL	CHC-C1C	4.52	1.46	1.35
43	r	608	CHL	O2A-CGA	4.52	1.45	1.30
43	R	608	CHL	C3B-C2B	4.51	1.46	1.40
43	r	608	CHL	C3B-C2B	4.51	1.46	1.40
43	R	608	CHL	O2A-CGA	4.50	1.45	1.30
43	s	601	CHL	O2A-CGA	4.50	1.45	1.30
43	N	605	CHL	O2D-CGD	4.50	1.44	1.33
43	S	601	CHL	O2A-CGA	4.49	1.45	1.30
43	g	609	CHL	O2A-CGA	4.49	1.46	1.33
43	G	606	CHL	C3B-C2B	4.48	1.46	1.40
43	R	608	CHL	C2C-C3C	4.48	1.46	1.36
43	G	609	CHL	O2A-CGA	4.48	1.46	1.33
43	g	606	CHL	C3B-C2B	4.47	1.46	1.40
43	n	605	CHL	O2D-CGD	4.46	1.44	1.33
43	N	607	CHL	CHC-C1C	4.45	1.46	1.35
43	S	601	CHL	CHD-C1D	4.45	1.47	1.38
43	y	605	CHL	O2A-CGA	4.44	1.45	1.30
43	Y	605	CHL	O2A-CGA	4.44	1.45	1.30
43	n	607	CHL	CHC-C1C	4.43	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Y	605	CHL	C2C-C3C	4.43	1.46	1.36
43	S	608	CHL	C3B-C2B	4.43	1.46	1.40
43	N	608	CHL	C3B-C2B	4.43	1.46	1.40
43	y	605	CHL	C2C-C3C	4.42	1.46	1.36
43	S	607	CHL	C2C-C3C	4.40	1.46	1.36
43	n	606	CHL	O2A-CGA	4.40	1.45	1.30
43	N	606	CHL	O2A-CGA	4.40	1.45	1.30
43	n	608	CHL	C3B-C2B	4.40	1.46	1.40
43	s	601	CHL	CHD-C1D	4.39	1.46	1.38
43	s	607	CHL	C2C-C3C	4.36	1.46	1.36
43	Y	608	CHL	C3B-C2B	4.36	1.46	1.40
43	s	608	CHL	C3B-C2B	4.36	1.46	1.40
43	g	608	CHL	C2C-C3C	4.35	1.46	1.36
43	g	607	CHL	C2C-C3C	4.34	1.46	1.36
43	Y	601	CHL	O2D-CGD	4.34	1.43	1.33
43	y	601	CHL	O2D-CGD	4.34	1.43	1.33
43	R	607	CHL	O2A-CGA	4.34	1.46	1.33
43	r	607	CHL	O2A-CGA	4.34	1.46	1.33
43	y	608	CHL	C3B-C2B	4.34	1.46	1.40
43	g	606	CHL	O2A-CGA	4.34	1.46	1.33
43	G	607	CHL	C2C-C3C	4.33	1.46	1.36
43	G	608	CHL	C2C-C3C	4.33	1.46	1.36
43	Y	605	CHL	C3B-C2B	4.33	1.46	1.40
38	l	101	LHG	O8-C23	4.33	1.46	1.33
43	g	605	CHL	O2A-CGA	4.33	1.46	1.33
43	n	607	CHL	C2C-C3C	4.33	1.46	1.36
43	r	607	CHL	C2C-C3C	4.33	1.46	1.36
43	G	605	CHL	O2A-CGA	4.32	1.46	1.33
35	b	621	SQD	O47-C7	4.32	1.46	1.34
43	n	605	CHL	CHC-C1C	4.32	1.46	1.35
38	L	101	LHG	O8-C23	4.32	1.46	1.33
43	G	606	CHL	O2A-CGA	4.32	1.46	1.33
43	G	606	CHL	C2C-C3C	4.32	1.46	1.36
43	g	606	CHL	C2C-C3C	4.31	1.46	1.36
43	R	607	CHL	C2C-C3C	4.31	1.46	1.36
43	y	605	CHL	C3B-C2B	4.31	1.46	1.40
43	N	605	CHL	CHC-C1C	4.30	1.46	1.35
43	S	601	CHL	C3B-C2B	4.30	1.46	1.40
43	G	609	CHL	C2C-C3C	4.30	1.46	1.36
43	g	609	CHL	C2C-C3C	4.30	1.46	1.36
43	g	607	CHL	C3B-C2B	4.29	1.46	1.40
43	G	607	CHL	C3B-C2B	4.29	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	S	608	CHL	O2A-CGA	4.29	1.45	1.33
43	S	606	CHL	C3B-C2B	4.29	1.46	1.40
43	N	607	CHL	C2C-C3C	4.28	1.45	1.36
43	n	608	CHL	O2A-CGA	4.28	1.45	1.33
43	s	608	CHL	O2A-CGA	4.28	1.45	1.33
43	N	608	CHL	O2A-CGA	4.27	1.45	1.33
35	B	621	SQD	O47-C7	4.27	1.46	1.34
43	s	601	CHL	C3B-C2B	4.27	1.46	1.40
43	g	601	CHL	C3B-C2B	4.27	1.46	1.40
43	s	606	CHL	C3B-C2B	4.26	1.46	1.40
43	y	608	CHL	C2C-C3C	4.26	1.45	1.36
43	G	607	CHL	O2A-CGA	4.26	1.45	1.33
43	g	607	CHL	O2A-CGA	4.25	1.45	1.33
43	Y	601	CHL	CHC-C1C	4.25	1.45	1.35
43	y	601	CHL	CHC-C1C	4.25	1.45	1.35
43	S	601	CHL	C2C-C3C	4.25	1.45	1.36
43	s	601	CHL	C2C-C3C	4.25	1.45	1.36
43	Y	608	CHL	C2C-C3C	4.24	1.45	1.36
43	g	608	CHL	C3B-C2B	4.22	1.46	1.40
43	Y	606	CHL	O2A-CGA	4.22	1.45	1.33
43	N	601	CHL	C2C-C3C	4.21	1.45	1.36
43	n	601	CHL	C2C-C3C	4.21	1.45	1.36
43	y	606	CHL	O2A-CGA	4.20	1.45	1.33
43	Y	609	CHL	O2A-CGA	4.19	1.45	1.33
43	y	609	CHL	O2A-CGA	4.19	1.45	1.33
43	Y	608	CHL	O2A-CGA	4.19	1.45	1.33
43	G	608	CHL	C3B-C2B	4.19	1.46	1.40
43	y	608	CHL	O2A-CGA	4.19	1.45	1.33
43	r	608	CHL	CHD-C1D	4.18	1.46	1.38
43	N	605	CHL	C3B-C2B	4.18	1.46	1.40
38	G	2630	LHG	O8-C23	4.18	1.45	1.33
43	n	606	CHL	C2C-C3C	4.17	1.45	1.36
43	R	607	CHL	CHD-C1D	4.17	1.46	1.38
43	y	605	CHL	CHD-C1D	4.16	1.46	1.38
36	d	411	LMG	O8-C28	4.16	1.45	1.33
43	N	601	CHL	CHD-C1D	4.16	1.46	1.38
43	Y	605	CHL	CHD-C1D	4.16	1.46	1.38
38	g	2630	LHG	O8-C23	4.15	1.45	1.33
43	N	609	CHL	C2C-C3C	4.15	1.45	1.36
43	n	609	CHL	C2C-C3C	4.15	1.45	1.36
43	r	607	CHL	CHD-C1D	4.14	1.46	1.38
43	G	608	CHL	CHD-C1D	4.14	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	n	601	CHL	CHD-C1D	4.14	1.46	1.38
37	c	520	DGD	O1G-C1A	4.14	1.45	1.33
43	N	606	CHL	C2C-C3C	4.14	1.45	1.36
43	g	608	CHL	CHD-C1D	4.14	1.46	1.38
35	a	412	SQD	O47-C7	4.14	1.46	1.34
36	a	413	LMG	O7-C10	4.14	1.46	1.34
43	R	608	CHL	CHD-C1D	4.14	1.46	1.38
36	D	411	LMG	O8-C28	4.13	1.45	1.33
43	G	601	CHL	C3B-C2B	4.13	1.46	1.40
38	N	2630	LHG	O8-C23	4.13	1.45	1.33
38	n	2630	LHG	O8-C23	4.13	1.45	1.33
35	A	412	SQD	O47-C7	4.12	1.45	1.34
43	y	609	CHL	C2C-C3C	4.12	1.45	1.36
43	n	609	CHL	CHC-C1C	4.12	1.45	1.35
43	Y	609	CHL	C2C-C3C	4.12	1.45	1.36
43	n	607	CHL	O2A-CGA	4.12	1.45	1.33
37	C	520	DGD	O1G-C1A	4.12	1.45	1.33
43	N	607	CHL	O2A-CGA	4.12	1.45	1.33
43	S	608	CHL	CHD-C1D	4.11	1.46	1.38
35	b	621	SQD	O48-C23	4.11	1.45	1.33
37	C	524	DGD	O1G-C1A	4.11	1.45	1.33
43	n	605	CHL	C3B-C2B	4.11	1.46	1.40
43	y	609	CHL	C3B-C2B	4.10	1.46	1.40
36	A	413	LMG	O7-C10	4.10	1.45	1.34
43	s	607	CHL	CHD-C1D	4.10	1.46	1.38
43	n	605	CHL	O2A-CGA	4.10	1.45	1.33
43	N	609	CHL	CHC-C1C	4.10	1.45	1.35
35	B	621	SQD	O48-C23	4.09	1.45	1.33
37	c	524	DGD	O1G-C1A	4.09	1.45	1.33
37	C	518	DGD	O1G-C1A	4.09	1.45	1.33
43	S	607	CHL	CHD-C1D	4.08	1.46	1.38
43	n	608	CHL	C2C-C3C	4.08	1.45	1.36
37	C	520	DGD	O2G-C1B	4.08	1.45	1.34
37	c	520	DGD	O2G-C1B	4.08	1.45	1.34
37	c	518	DGD	O1G-C1A	4.08	1.45	1.33
36	H	102	LMG	O8-C28	4.08	1.45	1.33
43	G	601	CHL	O2A-CGA	4.07	1.45	1.33
36	C	521	LMG	O7-C10	4.07	1.45	1.34
43	g	601	CHL	O2A-CGA	4.07	1.45	1.33
43	N	605	CHL	O2A-CGA	4.06	1.45	1.33
36	c	521	LMG	O7-C10	4.06	1.45	1.34
43	s	608	CHL	CHD-C1D	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	519	DGD	O1G-C1A	4.06	1.45	1.33
36	B	622	LMG	O8-C28	4.06	1.45	1.33
36	b	622	LMG	O8-C28	4.06	1.45	1.33
36	h	102	LMG	O8-C28	4.06	1.45	1.33
37	C	519	DGD	O1G-C1A	4.05	1.45	1.33
43	Y	609	CHL	C3B-C2B	4.05	1.46	1.40
36	b	622	LMG	O7-C10	4.04	1.45	1.34
43	G	609	CHL	C3B-C2B	4.04	1.46	1.40
43	g	609	CHL	C3B-C2B	4.04	1.46	1.40
43	r	606	CHL	CHD-C1D	4.04	1.46	1.38
43	N	608	CHL	C2C-C3C	4.04	1.45	1.36
36	a	413	LMG	O8-C28	4.03	1.45	1.33
36	B	622	LMG	O7-C10	4.03	1.45	1.34
38	D	408	LHG	O8-C23	4.03	1.45	1.33
36	d	411	LMG	O7-C10	4.03	1.45	1.34
36	c	521	LMG	O8-C28	4.03	1.45	1.33
36	A	413	LMG	O8-C28	4.02	1.45	1.33
38	d	408	LHG	O8-C23	4.02	1.45	1.33
36	C	521	LMG	O8-C28	4.02	1.45	1.33
43	R	606	CHL	CHD-C1D	4.02	1.46	1.38
43	N	605	CHL	C2C-C3C	4.01	1.45	1.36
43	S	606	CHL	CHD-C1D	4.01	1.46	1.38
43	n	605	CHL	C2C-C3C	4.01	1.45	1.36
36	D	411	LMG	O7-C10	4.01	1.45	1.34
36	h	102	LMG	O7-C10	4.00	1.45	1.34
38	L	101	LHG	O7-C7	4.00	1.45	1.34
43	S	606	CHL	C2C-C3C	4.00	1.45	1.36
37	C	523	DGD	O2G-C1B	4.00	1.45	1.34
40	d	405	PL9	C6-C1	-3.99	1.41	1.48
36	H	102	LMG	O7-C10	3.99	1.45	1.34
43	G	605	CHL	CHD-C4C	3.99	1.48	1.39
43	Y	607	CHL	O2A-CGA	3.99	1.45	1.33
43	s	606	CHL	C2C-C3C	3.99	1.45	1.36
43	s	606	CHL	CHD-C1D	3.98	1.46	1.38
43	g	605	CHL	CHD-C4C	3.98	1.48	1.39
43	s	601	CHL	CHD-C4C	3.98	1.48	1.39
43	Y	601	CHL	O2A-CGA	3.98	1.45	1.33
43	y	601	CHL	O2A-CGA	3.98	1.45	1.33
38	l	101	LHG	O7-C7	3.98	1.45	1.34
35	a	412	SQD	O48-C23	3.97	1.44	1.33
37	c	523	DGD	O2G-C1B	3.97	1.45	1.34
38	c	2630	LHG	O8-C23	3.97	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	S	601	CHL	CHD-C4C	3.97	1.48	1.39
38	C	2630	LHG	O8-C23	3.96	1.44	1.33
40	D	405	PL9	C6-C1	-3.96	1.41	1.48
35	A	412	SQD	O48-C23	3.96	1.44	1.33
43	y	607	CHL	O2A-CGA	3.96	1.44	1.33
43	N	609	CHL	C3B-C2B	3.96	1.45	1.40
38	d	410	LHG	O8-C23	3.96	1.44	1.33
38	d	409	LHG	O8-C23	3.95	1.44	1.33
43	n	609	CHL	C3B-C2B	3.95	1.45	1.40
38	S	2630	LHG	O7-C7	3.94	1.45	1.34
38	s	2630	LHG	O7-C7	3.94	1.45	1.34
38	c	2630	LHG	O7-C7	3.93	1.45	1.34
38	D	410	LHG	O8-C23	3.93	1.44	1.33
37	c	519	DGD	O2G-C1B	3.93	1.45	1.34
43	N	606	CHL	C3B-C2B	3.92	1.45	1.40
32	a	406	CLA	C4D-ND	-3.92	1.32	1.37
38	g	2630	LHG	O7-C7	3.92	1.45	1.34
38	d	408	LHG	O7-C7	3.92	1.45	1.34
38	D	409	LHG	O8-C23	3.92	1.44	1.33
37	C	519	DGD	O2G-C1B	3.91	1.45	1.34
38	n	2630	LHG	O7-C7	3.91	1.45	1.34
43	N	601	CHL	O2A-CGA	3.91	1.44	1.33
43	Y	607	CHL	C3B-C2B	3.91	1.45	1.40
38	D	408	LHG	O7-C7	3.91	1.45	1.34
38	Y	2630	LHG	O8-C23	3.91	1.44	1.33
38	S	2630	LHG	O8-C23	3.90	1.44	1.33
38	N	2630	LHG	O7-C7	3.90	1.45	1.34
38	y	2630	LHG	O8-C23	3.90	1.44	1.33
32	r	609	CLA	C1D-ND	3.90	1.42	1.37
38	s	2630	LHG	O8-C23	3.90	1.44	1.33
37	C	518	DGD	O2G-C1B	3.90	1.45	1.34
38	C	2630	LHG	O7-C7	3.90	1.45	1.34
38	Y	2630	LHG	O7-C7	3.90	1.45	1.34
43	G	607	CHL	CHD-C1D	3.90	1.46	1.38
37	c	518	DGD	O2G-C1B	3.89	1.45	1.34
43	y	607	CHL	C3B-C2B	3.89	1.45	1.40
38	G	2630	LHG	O7-C7	3.89	1.45	1.34
41	F	101	HEM	C3C-CAC	3.89	1.55	1.47
43	n	606	CHL	C3B-C2B	3.89	1.45	1.40
43	n	601	CHL	O2A-CGA	3.88	1.44	1.33
37	c	523	DGD	O1G-C1A	3.88	1.44	1.33
37	C	524	DGD	O2G-C1B	3.88	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	f	101	HEM	C3C-CAC	3.88	1.55	1.47
32	c	508	CLA	C4D-ND	-3.88	1.32	1.37
37	C	523	DGD	O1G-C1A	3.87	1.44	1.33
42	Z	2635	LMU	O5B-C1B	3.87	1.51	1.41
38	y	2630	LHG	O7-C7	3.87	1.45	1.34
37	c	524	DGD	O2G-C1B	3.87	1.45	1.34
43	y	607	CHL	C2C-C3C	3.87	1.45	1.36
43	g	607	CHL	CHD-C1D	3.86	1.45	1.38
32	R	609	CLA	C1D-ND	3.86	1.42	1.37
42	z	2635	LMU	O5B-C1B	3.85	1.51	1.41
32	A	406	CLA	C4D-ND	-3.85	1.32	1.37
32	C	508	CLA	C4D-ND	-3.82	1.32	1.37
38	d	410	LHG	O7-C7	3.81	1.45	1.34
38	D	410	LHG	O7-C7	3.81	1.45	1.34
32	s	609	CLA	C1D-ND	3.81	1.42	1.37
32	B	612	CLA	C4D-ND	-3.81	1.32	1.37
43	Y	607	CHL	C2C-C3C	3.80	1.44	1.36
43	Y	601	CHL	C2C-C3C	3.79	1.44	1.36
43	y	601	CHL	C2C-C3C	3.79	1.44	1.36
43	y	608	CHL	CHD-C1D	3.79	1.45	1.38
32	R	610	CLA	C1D-ND	3.79	1.42	1.37
32	c	513	CLA	C4D-ND	-3.78	1.32	1.37
32	C	503	CLA	C4D-ND	-3.77	1.32	1.37
32	C	513	CLA	C4D-ND	-3.77	1.32	1.37
32	N	603	CLA	C1D-ND	3.77	1.42	1.37
32	g	610	CLA	C1D-ND	3.77	1.42	1.37
32	g	612	CLA	C1D-ND	3.76	1.42	1.37
32	g	614	CLA	C1D-ND	3.76	1.42	1.37
43	G	601	CHL	C2C-C3C	3.76	1.44	1.36
32	G	612	CLA	C1D-ND	3.76	1.42	1.37
43	Y	601	CHL	CHD-C1D	3.76	1.45	1.38
43	y	601	CHL	CHD-C1D	3.76	1.45	1.38
43	g	601	CHL	C2C-C3C	3.76	1.44	1.36
41	f	101	HEM	C3C-C2C	-3.76	1.35	1.40
32	Y	611	CLA	C4D-ND	-3.75	1.32	1.37
43	g	605	CHL	OBD-CAD	3.75	1.28	1.22
43	n	609	CHL	CHD-C1D	3.75	1.45	1.38
43	g	608	CHL	CHD-C4C	3.75	1.47	1.39
32	b	612	CLA	C4D-ND	-3.75	1.32	1.37
32	r	603	CLA	C1D-ND	3.75	1.42	1.37
32	S	609	CLA	C1D-ND	3.74	1.42	1.37
32	n	612	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	603	CLA	C1D-ND	3.74	1.42	1.37
32	G	610	CLA	C1D-ND	3.74	1.42	1.37
32	G	614	CLA	C1D-ND	3.74	1.42	1.37
43	Y	608	CHL	CHD-C1D	3.73	1.45	1.38
43	r	606	CHL	C2C-C3C	3.73	1.44	1.36
32	n	614	CLA	C1D-ND	3.73	1.42	1.37
43	G	608	CHL	CHD-C4C	3.73	1.47	1.39
32	c	503	CLA	C4D-ND	-3.73	1.32	1.37
43	n	606	CHL	CHD-C1D	3.73	1.45	1.38
43	S	608	CHL	CHD-C4C	3.72	1.47	1.39
43	N	607	CHL	CHD-C1D	3.72	1.45	1.38
32	r	602	CLA	C4D-ND	-3.72	1.32	1.37
43	R	608	CHL	CHD-C4C	3.71	1.47	1.39
43	N	606	CHL	CHD-C1D	3.71	1.45	1.38
43	N	609	CHL	CHD-C1D	3.71	1.45	1.38
41	F	101	HEM	C3C-C2C	-3.71	1.35	1.40
32	n	613	CLA	C4D-ND	-3.71	1.32	1.37
32	y	611	CLA	C4D-ND	-3.71	1.32	1.37
43	R	606	CHL	C2C-C3C	3.71	1.44	1.36
43	G	606	CHL	CHD-C1D	3.70	1.45	1.38
32	b	608	CLA	C4D-ND	-3.70	1.32	1.37
43	G	605	CHL	OBD-CAD	3.70	1.28	1.22
43	r	608	CHL	CHD-C4C	3.70	1.47	1.39
32	N	614	CLA	C1D-ND	3.70	1.42	1.37
43	n	607	CHL	CHD-C1D	3.70	1.45	1.38
43	g	609	CHL	CHD-C1D	3.69	1.45	1.38
32	R	603	CLA	C1D-ND	3.69	1.42	1.37
43	s	608	CHL	CHD-C4C	3.69	1.47	1.39
40	D	405	PL9	C52-C5	-3.69	1.43	1.50
32	N	612	CLA	C1D-ND	3.69	1.42	1.37
32	a	407	CLA	C4D-ND	-3.68	1.32	1.37
43	g	606	CHL	CHD-C1D	3.68	1.45	1.38
32	R	602	CLA	C1D-ND	3.67	1.42	1.37
32	R	602	CLA	C4D-ND	-3.66	1.32	1.37
32	N	611	CLA	C1D-ND	3.66	1.42	1.37
32	N	613	CLA	C4D-ND	-3.66	1.32	1.37
32	A	410	CLA	C4D-ND	-3.66	1.32	1.37
40	d	405	PL9	C52-C5	-3.66	1.43	1.50
32	n	604	CLA	C4D-ND	-3.65	1.32	1.37
32	r	610	CLA	C1D-ND	3.65	1.42	1.37
32	N	604	CLA	C4D-ND	-3.65	1.32	1.37
38	d	409	LHG	O7-C7	3.65	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	S	606	CHL	CHD-C4C	3.65	1.47	1.39
42	Z	2634	LMU	O5B-C1B	3.65	1.51	1.41
43	G	609	CHL	CHD-C1D	3.65	1.45	1.38
32	C	506	CLA	C4D-ND	-3.65	1.32	1.37
32	a	405	CLA	C1D-ND	3.65	1.42	1.37
42	z	2634	LMU	O5B-C1B	3.64	1.51	1.41
32	a	410	CLA	C4D-ND	-3.64	1.32	1.37
32	C	502	CLA	C4D-ND	-3.64	1.32	1.37
32	c	502	CLA	C4D-ND	-3.64	1.32	1.37
32	s	603	CLA	C1D-ND	3.64	1.42	1.37
32	D	402	CLA	C4D-ND	-3.64	1.32	1.37
32	d	402	CLA	C4D-ND	-3.64	1.32	1.37
43	s	606	CHL	CHD-C4C	3.64	1.47	1.39
32	B	608	CLA	C4D-ND	-3.63	1.32	1.37
43	N	605	CHL	CHD-C1D	3.63	1.45	1.38
32	A	405	CLA	C4D-ND	-3.63	1.32	1.37
32	a	405	CLA	C4D-ND	-3.63	1.32	1.37
43	Y	606	CHL	C2C-C3C	3.63	1.44	1.36
43	g	601	CHL	CHD-C1D	3.63	1.45	1.38
43	G	601	CHL	CHD-C1D	3.62	1.45	1.38
38	D	409	LHG	O7-C7	3.62	1.44	1.34
43	r	607	CHL	OBD-CAD	3.62	1.28	1.22
32	S	605	CLA	C1D-ND	3.62	1.42	1.37
32	s	605	CLA	C1D-ND	3.62	1.42	1.37
43	s	608	CHL	OBD-CAD	3.61	1.28	1.22
32	S	603	CLA	C1D-ND	3.61	1.42	1.37
32	A	407	CLA	C4D-ND	-3.61	1.32	1.37
43	n	601	CHL	CHD-C4C	3.61	1.47	1.39
43	s	607	CHL	CHD-C4C	3.61	1.47	1.39
32	r	602	CLA	C1D-ND	3.61	1.42	1.37
43	S	608	CHL	OBD-CAD	3.61	1.28	1.22
43	y	606	CHL	C2C-C3C	3.60	1.44	1.36
43	R	606	CHL	OBD-CAD	3.60	1.28	1.22
43	r	607	CHL	CHD-C4C	3.60	1.47	1.39
32	n	611	CLA	C1D-ND	3.60	1.42	1.37
43	N	601	CHL	CHD-C4C	3.59	1.47	1.39
32	G	613	CLA	C4D-ND	-3.59	1.32	1.37
32	c	506	CLA	C4D-ND	-3.59	1.32	1.37
43	n	605	CHL	CHD-C1D	3.58	1.45	1.38
32	A	405	CLA	C1D-ND	3.57	1.42	1.37
43	r	606	CHL	OBD-CAD	3.57	1.28	1.22
43	R	607	CHL	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	R	607	CHL	CHD-C4C	3.56	1.47	1.39
43	S	607	CHL	CHD-C4C	3.56	1.47	1.39
32	g	613	CLA	C4D-ND	-3.54	1.32	1.37
32	s	614	CLA	C1D-ND	3.54	1.42	1.37
43	Y	605	CHL	CHD-C4C	3.54	1.47	1.39
32	B	606	CLA	C4D-ND	-3.53	1.32	1.37
43	g	607	CHL	CHD-C4C	3.53	1.47	1.39
40	d	405	PL9	C7-C8	-3.53	1.45	1.50
32	B	606	CLA	C1D-ND	3.53	1.42	1.37
32	b	606	CLA	C1D-ND	3.53	1.42	1.37
43	y	605	CHL	CHD-C4C	3.53	1.47	1.39
43	r	606	CHL	CHD-C4C	3.52	1.47	1.39
32	S	611	CLA	C4D-ND	-3.52	1.32	1.37
32	s	611	CLA	C4D-ND	-3.52	1.32	1.37
43	G	607	CHL	CHD-C4C	3.52	1.47	1.39
43	g	606	CHL	OBD-CAD	3.52	1.28	1.22
43	Y	601	CHL	CHD-C4C	3.50	1.47	1.39
43	g	607	CHL	OBD-CAD	3.50	1.28	1.22
43	y	601	CHL	CHD-C4C	3.50	1.47	1.39
32	C	506	CLA	CMB-C2B	-3.50	1.44	1.51
32	b	610	CLA	C1D-ND	3.50	1.42	1.37
43	G	607	CHL	OBD-CAD	3.50	1.28	1.22
32	B	610	CLA	C1D-ND	3.50	1.42	1.37
32	c	503	CLA	C1D-ND	3.49	1.42	1.37
32	N	604	CLA	C1D-ND	3.49	1.42	1.37
43	R	608	CHL	OBD-CAD	3.49	1.28	1.22
32	n	610	CLA	C1D-ND	3.49	1.42	1.37
43	n	608	CHL	CHD-C1D	3.49	1.45	1.38
43	R	606	CHL	CHD-C4C	3.49	1.47	1.39
32	n	604	CLA	C1D-ND	3.49	1.42	1.37
43	N	601	CHL	OBD-CAD	3.48	1.28	1.22
43	n	601	CHL	OBD-CAD	3.48	1.28	1.22
42	z	2635	LMU	O5'-C1'	3.48	1.50	1.41
32	b	617	CLA	C1D-ND	3.48	1.42	1.37
32	C	509	CLA	C4D-ND	-3.48	1.32	1.37
40	D	405	PL9	C7-C8	-3.48	1.45	1.50
32	A	406	CLA	C1D-ND	3.47	1.42	1.37
32	y	613	CLA	C4D-ND	-3.47	1.32	1.37
43	y	605	CHL	OBD-CAD	3.47	1.28	1.22
43	n	601	CHL	C3B-C2B	3.47	1.45	1.40
43	G	606	CHL	OBD-CAD	3.47	1.28	1.22
32	b	606	CLA	C4D-ND	-3.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	406	CLA	C1D-ND	3.47	1.42	1.37
42	Z	2635	LMU	O5'-C1'	3.47	1.50	1.41
43	S	606	CHL	OBD-CAD	3.47	1.28	1.22
32	B	602	CLA	C1D-ND	3.47	1.42	1.37
32	b	602	CLA	C1D-ND	3.47	1.42	1.37
32	C	504	CLA	C4D-ND	-3.47	1.32	1.37
43	r	608	CHL	OBD-CAD	3.46	1.28	1.22
32	y	602	CLA	C4D-ND	-3.46	1.32	1.37
32	B	604	CLA	C4D-ND	-3.46	1.32	1.37
32	g	613	CLA	C1D-ND	3.46	1.42	1.37
43	y	607	CHL	CHD-C1D	3.46	1.45	1.38
32	c	506	CLA	CMB-C2B	-3.46	1.44	1.51
32	N	610	CLA	C1D-ND	3.46	1.42	1.37
43	N	608	CHL	CHD-C1D	3.46	1.45	1.38
43	N	606	CHL	OBD-CAD	3.46	1.28	1.22
32	S	614	CLA	C1D-ND	3.45	1.42	1.37
32	c	509	CLA	C4D-ND	-3.45	1.32	1.37
43	g	601	CHL	CHD-C4C	3.45	1.47	1.39
32	G	603	CLA	C1D-ND	3.45	1.42	1.37
32	G	613	CLA	C1D-ND	3.45	1.42	1.37
32	Y	613	CLA	C4D-ND	-3.45	1.33	1.37
32	g	603	CLA	C1D-ND	3.44	1.42	1.37
32	B	607	CLA	C1D-ND	3.44	1.42	1.37
32	B	617	CLA	C1D-ND	3.43	1.42	1.37
32	G	611	CLA	C1D-ND	3.43	1.42	1.37
43	Y	608	CHL	CHD-C4C	3.43	1.47	1.39
43	y	608	CHL	CHD-C4C	3.43	1.47	1.39
32	G	602	CLA	C4D-ND	-3.43	1.33	1.37
43	N	601	CHL	C3B-C2B	3.43	1.45	1.40
32	C	503	CLA	C1D-ND	3.43	1.42	1.37
32	R	604	CLA	C1D-ND	3.43	1.42	1.37
32	b	604	CLA	C4D-ND	-3.43	1.33	1.37
43	s	606	CHL	OBD-CAD	3.43	1.28	1.22
32	b	607	CLA	C1D-ND	3.43	1.42	1.37
43	Y	607	CHL	CHD-C1D	3.42	1.45	1.38
43	Y	605	CHL	OBD-CAD	3.42	1.28	1.22
32	g	611	CLA	C1D-ND	3.42	1.42	1.37
32	n	613	CLA	C1D-ND	3.42	1.42	1.37
32	N	613	CLA	C1D-ND	3.41	1.42	1.37
32	B	611	CLA	C1D-ND	3.41	1.42	1.37
32	G	602	CLA	C1D-ND	3.41	1.42	1.37
32	B	605	CLA	C4D-ND	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	504	CLA	C1D-ND	3.40	1.42	1.37
32	c	504	CLA	C1D-ND	3.40	1.42	1.37
32	s	613	CLA	C1D-ND	3.40	1.42	1.37
43	Y	606	CHL	CHD-C1D	3.40	1.45	1.38
32	c	504	CLA	C4D-ND	-3.40	1.33	1.37
32	y	610	CLA	C4D-ND	-3.40	1.33	1.37
32	g	602	CLA	C4D-ND	-3.40	1.33	1.37
32	d	403	CLA	C1D-ND	3.40	1.42	1.37
32	Y	604	CLA	C4D-ND	-3.40	1.33	1.37
32	y	604	CLA	C4D-ND	-3.40	1.33	1.37
32	g	602	CLA	C1D-ND	3.40	1.42	1.37
43	G	601	CHL	CHD-C4C	3.40	1.47	1.39
43	S	607	CHL	OBD-CAD	3.39	1.28	1.22
43	s	607	CHL	OBD-CAD	3.39	1.28	1.22
32	G	604	CLA	C1D-ND	3.39	1.42	1.37
32	g	604	CLA	C1D-ND	3.39	1.42	1.37
32	Y	602	CLA	C4D-ND	-3.39	1.33	1.37
32	Y	614	CLA	C1D-ND	3.39	1.42	1.37
32	y	614	CLA	C1D-ND	3.39	1.42	1.37
32	C	501	CLA	C1D-ND	3.39	1.42	1.37
43	n	606	CHL	OBD-CAD	3.39	1.28	1.22
32	b	611	CLA	C1D-ND	3.38	1.41	1.37
32	s	613	CLA	C4D-ND	-3.38	1.33	1.37
43	y	606	CHL	CHD-C1D	3.38	1.44	1.38
32	D	403	CLA	C1D-ND	3.38	1.41	1.37
32	c	507	CLA	C4D-ND	-3.37	1.33	1.37
32	r	604	CLA	C1D-ND	3.37	1.41	1.37
32	B	616	CLA	C4D-ND	-3.37	1.33	1.37
32	N	602	CLA	C4D-ND	-3.37	1.33	1.37
32	b	616	CLA	C4D-ND	-3.37	1.33	1.37
32	n	602	CLA	C4D-ND	-3.37	1.33	1.37
32	n	611	CLA	C4D-ND	-3.37	1.33	1.37
32	d	403	CLA	C4D-ND	-3.37	1.33	1.37
32	N	611	CLA	C4D-ND	-3.37	1.33	1.37
32	b	605	CLA	C4D-ND	-3.37	1.33	1.37
32	S	613	CLA	C4D-ND	-3.36	1.33	1.37
32	b	612	CLA	CMC-C2C	-3.36	1.43	1.50
32	A	407	CLA	C1D-ND	3.35	1.41	1.37
32	B	615	CLA	C1D-ND	3.35	1.41	1.37
32	b	615	CLA	C1D-ND	3.35	1.41	1.37
32	S	612	CLA	C4D-ND	-3.35	1.33	1.37
32	n	602	CLA	C1D-ND	3.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	609	CLA	C4D-ND	-3.35	1.33	1.37
32	b	609	CLA	C4D-ND	-3.35	1.33	1.37
32	b	617	CLA	C4D-ND	-3.35	1.33	1.37
32	s	610	CLA	C1D-ND	3.34	1.41	1.37
32	Y	610	CLA	C4D-ND	-3.34	1.33	1.37
42	y	2632	LMU	O5B-C1B	3.34	1.50	1.41
32	S	610	CLA	C1D-ND	3.34	1.41	1.37
32	S	604	CLA	C1D-ND	3.33	1.41	1.37
32	s	604	CLA	C1D-ND	3.33	1.41	1.37
32	n	603	CLA	C4D-ND	-3.33	1.33	1.37
32	C	507	CLA	C4D-ND	-3.33	1.33	1.37
32	D	403	CLA	C4D-ND	-3.33	1.33	1.37
32	B	612	CLA	CMC-C2C	-3.33	1.43	1.50
42	z	2634	LMU	O5'-C1'	3.33	1.50	1.41
32	s	604	CLA	C4D-ND	-3.33	1.33	1.37
32	C	508	CLA	C1D-ND	3.33	1.41	1.37
43	Y	609	CHL	CHD-C1D	3.32	1.44	1.38
32	N	602	CLA	C1D-ND	3.32	1.41	1.37
32	C	511	CLA	C1D-ND	3.32	1.41	1.37
32	S	604	CLA	C4D-ND	-3.32	1.33	1.37
32	C	502	CLA	C1D-ND	3.32	1.41	1.37
32	c	508	CLA	C1D-ND	3.32	1.41	1.37
32	b	607	CLA	C4D-ND	-3.31	1.33	1.37
32	S	613	CLA	C1D-ND	3.31	1.41	1.37
42	Z	2634	LMU	O5'-C1'	3.31	1.50	1.41
32	y	612	CLA	C4D-ND	-3.31	1.33	1.37
32	B	617	CLA	C4D-ND	-3.31	1.33	1.37
32	S	602	CLA	C4D-ND	-3.31	1.33	1.37
32	s	610	CLA	CHC-C1C	3.30	1.43	1.35
32	y	603	CLA	C1D-ND	3.30	1.41	1.37
32	a	407	CLA	C1D-ND	3.30	1.41	1.37
32	b	604	CLA	C1D-ND	3.30	1.41	1.37
32	n	610	CLA	C4D-ND	-3.30	1.33	1.37
42	Y	2632	LMU	O5B-C1B	3.30	1.50	1.41
32	y	610	CLA	C1D-ND	3.30	1.41	1.37
32	B	614	CLA	C4D-ND	-3.30	1.33	1.37
32	B	604	CLA	C1D-ND	3.30	1.41	1.37
32	Y	604	CLA	C1D-ND	3.29	1.41	1.37
32	y	604	CLA	C1D-ND	3.29	1.41	1.37
43	y	606	CHL	C3B-C2B	3.29	1.44	1.40
32	C	511	CLA	C4D-ND	-3.29	1.33	1.37
32	b	613	CLA	C4D-ND	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	511	CLA	C4D-ND	-3.29	1.33	1.37
32	s	602	CLA	C4D-ND	-3.29	1.33	1.37
32	s	612	CLA	C4D-ND	-3.29	1.33	1.37
43	G	606	CHL	CHD-C4C	3.28	1.46	1.39
32	b	614	CLA	C4D-ND	-3.28	1.33	1.37
43	y	609	CHL	CHD-C1D	3.28	1.44	1.38
32	c	501	CLA	C1D-ND	3.28	1.41	1.37
32	Y	603	CLA	C4D-ND	-3.28	1.33	1.37
43	N	606	CHL	CHD-C4C	3.28	1.46	1.39
43	g	606	CHL	CHD-C4C	3.28	1.46	1.39
43	g	609	CHL	OBD-CAD	3.28	1.28	1.22
32	c	501	CLA	C4D-ND	-3.28	1.33	1.37
32	c	502	CLA	C1D-ND	3.28	1.41	1.37
32	b	616	CLA	C1D-ND	3.27	1.41	1.37
32	N	603	CLA	C4D-ND	-3.27	1.33	1.37
32	Y	603	CLA	C1D-ND	3.27	1.41	1.37
32	S	610	CLA	CHC-C1C	3.27	1.43	1.35
32	s	610	CLA	C4D-ND	-3.27	1.33	1.37
32	B	616	CLA	C1D-ND	3.27	1.41	1.37
32	Y	604	CLA	CMB-C2B	-3.27	1.44	1.51
43	G	608	CHL	OBD-CAD	3.26	1.28	1.22
32	S	610	CLA	C4D-ND	-3.26	1.33	1.37
43	n	606	CHL	CHD-C4C	3.26	1.46	1.39
32	y	604	CLA	CMB-C2B	-3.26	1.44	1.51
32	Y	614	CLA	C4D-ND	-3.26	1.33	1.37
32	y	614	CLA	C4D-ND	-3.26	1.33	1.37
32	S	611	CLA	C1D-ND	3.26	1.41	1.37
32	Y	610	CLA	C1D-ND	3.26	1.41	1.37
32	s	614	CLA	C4D-ND	-3.25	1.33	1.37
32	B	607	CLA	C4D-ND	-3.25	1.33	1.37
32	B	613	CLA	C4D-ND	-3.25	1.33	1.37
32	S	614	CLA	C4D-ND	-3.25	1.33	1.37
32	Y	612	CLA	C4D-ND	-3.25	1.33	1.37
43	n	608	CHL	CHD-C4C	3.25	1.46	1.39
43	N	608	CHL	CHD-C4C	3.25	1.46	1.39
32	b	608	CLA	C1D-ND	3.25	1.41	1.37
32	s	610	CLA	C3B-C2B	-3.24	1.35	1.40
43	Y	607	CHL	OBD-CAD	3.24	1.28	1.22
46	s	1623	NEX	C7-C8	-3.24	1.26	1.32
32	N	610	CLA	C4D-ND	-3.24	1.33	1.37
32	y	603	CLA	C4D-ND	-3.24	1.33	1.37
32	Y	602	CLA	C1D-ND	3.23	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	511	CLA	C1D-ND	3.23	1.41	1.37
32	y	602	CLA	C1D-ND	3.23	1.41	1.37
43	G	609	CHL	OBD-CAD	3.23	1.28	1.22
32	Y	612	CLA	C1D-ND	3.23	1.41	1.37
32	c	512	CLA	C1D-ND	3.23	1.41	1.37
43	Y	609	CHL	OBD-CAD	3.23	1.28	1.22
43	y	607	CHL	CHD-C4C	3.23	1.46	1.39
43	y	609	CHL	OBD-CAD	3.22	1.28	1.22
32	B	602	CLA	C4D-ND	-3.22	1.33	1.37
43	G	601	CHL	OBD-CAD	3.22	1.28	1.22
32	c	510	CLA	C1D-ND	3.22	1.41	1.37
43	Y	607	CHL	CHD-C4C	3.22	1.46	1.39
32	B	611	CLA	C4D-ND	-3.22	1.33	1.37
43	S	601	CHL	OBD-CAD	3.21	1.28	1.22
43	s	601	CHL	OBD-CAD	3.21	1.28	1.22
32	S	610	CLA	C3B-C2B	-3.21	1.35	1.40
32	c	506	CLA	C1D-ND	3.20	1.41	1.37
43	N	608	CHL	OBD-CAD	3.20	1.28	1.22
32	S	602	CLA	C1D-ND	3.20	1.41	1.37
43	Y	606	CHL	C3B-C2B	3.20	1.44	1.40
32	g	604	CLA	C4D-ND	-3.19	1.33	1.37
43	g	608	CHL	OBD-CAD	3.19	1.28	1.22
43	y	607	CHL	OBD-CAD	3.19	1.28	1.22
43	g	609	CHL	CHD-C4C	3.19	1.46	1.39
32	C	506	CLA	C1D-ND	3.18	1.41	1.37
32	b	603	CLA	C1D-ND	3.18	1.41	1.37
43	N	609	CHL	CHD-C4C	3.18	1.46	1.39
43	n	609	CHL	CHD-C4C	3.18	1.46	1.39
32	C	512	CLA	C1D-ND	3.18	1.41	1.37
42	y	2632	LMU	O5'-C1'	3.18	1.49	1.41
32	y	611	CLA	C1D-ND	3.18	1.41	1.37
43	n	609	CHL	OBD-CAD	3.17	1.27	1.22
32	b	611	CLA	C4D-ND	-3.17	1.33	1.37
32	S	612	CLA	C1D-ND	3.17	1.41	1.37
32	s	612	CLA	C1D-ND	3.17	1.41	1.37
42	Y	2632	LMU	O5'-C1'	3.17	1.49	1.41
32	B	608	CLA	C1D-ND	3.17	1.41	1.37
43	N	609	CHL	OBD-CAD	3.17	1.27	1.22
46	G	1623	NEX	C7-C8	-3.16	1.26	1.32
32	b	610	CLA	C4D-ND	-3.16	1.33	1.37
32	S	605	CLA	C4D-ND	-3.16	1.33	1.37
43	G	609	CHL	CHD-C4C	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	501	CLA	C4D-ND	-3.16	1.33	1.37
32	b	602	CLA	C4D-ND	-3.16	1.33	1.37
32	s	605	CLA	C4D-ND	-3.16	1.33	1.37
32	R	603	CLA	C4D-ND	-3.16	1.33	1.37
32	r	603	CLA	C4D-ND	-3.16	1.33	1.37
32	A	405	CLA	CMC-C2C	-3.15	1.44	1.50
43	Y	601	CHL	C3B-C2B	3.15	1.44	1.40
43	y	601	CHL	C3B-C2B	3.15	1.44	1.40
32	s	611	CLA	C1D-ND	3.15	1.41	1.37
32	B	612	CLA	C1D-ND	3.15	1.41	1.37
32	s	602	CLA	C1D-ND	3.15	1.41	1.37
32	y	612	CLA	C1D-ND	3.15	1.41	1.37
43	N	607	CHL	CHD-C4C	3.15	1.46	1.39
32	B	603	CLA	C1D-ND	3.15	1.41	1.37
32	c	505	CLA	C4D-ND	-3.15	1.33	1.37
32	N	614	CLA	C4D-ND	-3.15	1.33	1.37
43	G	605	CHL	C1D-C2D	3.14	1.51	1.45
32	G	614	CLA	C4D-ND	-3.14	1.33	1.37
43	n	607	CHL	CHD-C4C	3.14	1.46	1.39
32	C	510	CLA	C1D-ND	3.14	1.41	1.37
43	g	601	CHL	OBD-CAD	3.14	1.27	1.22
32	B	610	CLA	C4D-ND	-3.14	1.33	1.37
32	R	604	CLA	C4D-ND	-3.14	1.33	1.37
32	r	604	CLA	C4D-ND	-3.14	1.33	1.37
32	Y	602	CLA	CHC-C1C	3.13	1.43	1.35
32	y	602	CLA	CHC-C1C	3.13	1.43	1.35
32	y	613	CLA	C1D-ND	3.13	1.41	1.37
32	S	604	CLA	CMB-C2B	-3.13	1.45	1.51
32	s	604	CLA	CMB-C2B	-3.13	1.45	1.51
43	n	608	CHL	OBD-CAD	3.13	1.27	1.22
32	a	405	CLA	CMC-C2C	-3.13	1.44	1.50
32	G	604	CLA	C4D-ND	-3.13	1.33	1.37
32	c	512	CLA	C4D-ND	-3.13	1.33	1.37
32	n	614	CLA	C4D-ND	-3.12	1.33	1.37
32	b	612	CLA	C1D-ND	3.12	1.41	1.37
32	c	510	CLA	C4D-ND	-3.12	1.33	1.37
32	C	512	CLA	C4D-ND	-3.11	1.33	1.37
32	g	611	CLA	C4D-ND	-3.10	1.33	1.37
32	B	609	CLA	C1D-ND	3.10	1.41	1.37
32	Y	611	CLA	C1D-ND	3.10	1.41	1.37
32	C	510	CLA	C4D-ND	-3.10	1.33	1.37
32	C	505	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	614	CLA	C1D-ND	3.09	1.41	1.37
32	r	609	CLA	C4D-ND	-3.09	1.33	1.37
32	b	609	CLA	C1D-ND	3.09	1.41	1.37
32	G	604	CLA	CMB-C2B	-3.08	1.45	1.51
43	N	605	CHL	OBD-CAD	3.08	1.27	1.22
43	n	605	CHL	OBD-CAD	3.08	1.27	1.22
43	g	605	CHL	C1D-C2D	3.07	1.51	1.45
43	Y	609	CHL	CHD-C4C	3.07	1.46	1.39
32	g	610	CLA	C4D-ND	-3.07	1.33	1.37
32	G	611	CLA	C4D-ND	-3.07	1.33	1.37
32	c	507	CLA	C1D-ND	3.06	1.41	1.37
40	d	405	PL9	C11-C9	-3.06	1.44	1.51
32	g	614	CLA	C4D-ND	-3.06	1.33	1.37
41	f	101	HEM	CAB-C3B	3.06	1.55	1.47
32	R	609	CLA	C4D-ND	-3.06	1.33	1.37
32	B	610	CLA	CMB-C2B	-3.06	1.45	1.51
32	b	610	CLA	CMB-C2B	-3.06	1.45	1.51
32	B	615	CLA	C4D-ND	-3.05	1.33	1.37
32	b	615	CLA	C4D-ND	-3.05	1.33	1.37
46	Y	1623	NEX	C7-C8	-3.05	1.26	1.32
43	N	607	CHL	OBD-CAD	3.05	1.27	1.22
43	y	609	CHL	CHD-C4C	3.05	1.46	1.39
43	N	607	CHL	MG-NA	-3.04	1.99	2.06
43	n	607	CHL	MG-NA	-3.04	1.99	2.06
32	b	613	CLA	CHC-C1C	3.04	1.42	1.35
43	n	607	CHL	OBD-CAD	3.04	1.27	1.22
32	Y	613	CLA	C1D-ND	3.04	1.41	1.37
32	b	603	CLA	CHC-C1C	3.03	1.42	1.35
46	r	625	NEX	C7-C8	-3.03	1.26	1.32
32	g	604	CLA	CMB-C2B	-3.03	1.45	1.51
41	F	101	HEM	CAB-C3B	3.03	1.55	1.47
40	D	405	PL9	C11-C9	-3.03	1.45	1.51
32	b	614	CLA	C1D-ND	3.02	1.41	1.37
32	G	602	CLA	CHC-C1C	3.02	1.42	1.35
32	B	613	CLA	CHC-C1C	3.01	1.42	1.35
32	B	603	CLA	CHC-C1C	3.01	1.42	1.35
32	c	502	CLA	CMB-C2B	-3.01	1.45	1.51
32	C	505	CLA	CMD-C2D	-3.01	1.44	1.50
46	S	1623	NEX	C7-C8	-3.01	1.27	1.32
32	g	603	CLA	C4D-ND	-3.01	1.33	1.37
43	n	609	CHL	C1B-NB	-3.00	1.32	1.35
32	B	605	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	602	CLA	CHC-C1C	3.00	1.42	1.35
32	G	603	CLA	C4D-ND	-3.00	1.33	1.37
32	a	405	CLA	CHC-C1C	2.99	1.42	1.35
32	G	612	CLA	C4D-ND	-2.99	1.33	1.37
32	C	503	CLA	CHC-C1C	2.99	1.42	1.35
32	c	503	CLA	CHC-C1C	2.99	1.42	1.35
32	C	507	CLA	C1D-ND	2.98	1.41	1.37
32	N	612	CLA	C4D-ND	-2.98	1.33	1.37
32	n	612	CLA	C4D-ND	-2.98	1.33	1.37
32	G	610	CLA	C4D-ND	-2.97	1.33	1.37
32	y	610	CLA	CHC-C1C	2.97	1.42	1.35
32	B	603	CLA	C4D-ND	-2.97	1.33	1.37
32	b	604	CLA	CHC-C1C	2.97	1.42	1.35
32	B	605	CLA	CMD-C2D	-2.97	1.44	1.50
32	A	405	CLA	CHC-C1C	2.97	1.42	1.35
32	a	410	CLA	C1D-ND	2.97	1.41	1.37
43	Y	606	CHL	OBD-CAD	2.96	1.27	1.22
43	y	606	CHL	OBD-CAD	2.96	1.27	1.22
32	c	505	CLA	CMD-C2D	-2.96	1.44	1.50
32	C	502	CLA	CMB-C2B	-2.96	1.45	1.51
32	b	603	CLA	C4D-ND	-2.96	1.33	1.37
32	B	604	CLA	CMB-C2B	-2.96	1.45	1.51
32	A	410	CLA	C1D-ND	2.96	1.41	1.37
46	N	1623	NEX	C7-C8	-2.96	1.27	1.32
32	b	605	CLA	CMD-C2D	-2.95	1.44	1.50
32	b	604	CLA	CMB-C2B	-2.95	1.45	1.51
32	b	605	CLA	C1D-ND	2.95	1.41	1.37
32	s	609	CLA	C4D-ND	-2.95	1.33	1.37
35	A	412	SQD	C6-S	-2.94	1.66	1.77
32	r	610	CLA	C4D-ND	-2.94	1.33	1.37
32	B	604	CLA	CHC-C1C	2.94	1.42	1.35
43	Y	606	CHL	CHD-C4C	2.94	1.45	1.39
43	y	606	CHL	CHD-C4C	2.94	1.45	1.39
32	R	603	CLA	CHC-C1C	2.94	1.42	1.35
32	B	615	CLA	CHC-C1C	2.94	1.42	1.35
32	b	615	CLA	CHC-C1C	2.94	1.42	1.35
32	n	602	CLA	CHC-C1C	2.93	1.42	1.35
43	Y	606	CHL	C1D-ND	-2.93	1.34	1.37
32	S	602	CLA	CHC-C1C	2.93	1.42	1.35
32	s	602	CLA	CHC-C1C	2.93	1.42	1.35
43	Y	608	CHL	OBD-CAD	2.93	1.27	1.22
32	r	603	CLA	CHC-C1C	2.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	N	609	CHL	C1B-NB	-2.93	1.32	1.35
35	a	412	SQD	C6-S	-2.93	1.66	1.77
43	y	608	CHL	OBD-CAD	2.92	1.27	1.22
32	Y	614	CLA	CHC-C1C	2.92	1.42	1.35
32	y	614	CLA	CHC-C1C	2.92	1.42	1.35
32	Y	610	CLA	CHC-C1C	2.92	1.42	1.35
32	R	602	CLA	CHC-C1C	2.92	1.42	1.35
32	C	505	CLA	C1D-ND	2.91	1.41	1.37
32	S	603	CLA	C4D-ND	-2.91	1.33	1.37
32	b	605	CLA	CMB-C2B	-2.90	1.45	1.51
32	s	603	CLA	C4D-ND	-2.90	1.33	1.37
32	c	509	CLA	C1D-ND	2.90	1.41	1.37
32	r	602	CLA	CHC-C1C	2.90	1.42	1.35
32	N	602	CLA	CHC-C1C	2.90	1.42	1.35
32	G	614	CLA	CHC-C1C	2.89	1.42	1.35
32	G	611	CLA	CHC-C1C	2.89	1.42	1.35
32	g	611	CLA	CHC-C1C	2.89	1.42	1.35
32	g	612	CLA	C4D-ND	-2.89	1.33	1.37
32	S	609	CLA	C4D-ND	-2.89	1.33	1.37
32	g	614	CLA	CHC-C1C	2.89	1.42	1.35
43	N	605	CHL	CHD-C4C	2.88	1.45	1.39
43	n	605	CHL	CHD-C4C	2.88	1.45	1.39
32	B	605	CLA	CMB-C2B	-2.88	1.45	1.51
32	R	610	CLA	C4D-ND	-2.88	1.33	1.37
32	n	614	CLA	CHC-C1C	2.88	1.42	1.35
32	S	611	CLA	CHC-C1C	2.87	1.42	1.35
32	R	604	CLA	CHC-C1C	2.86	1.42	1.35
35	B	621	SQD	C6-S	-2.86	1.66	1.77
46	n	1623	NEX	C7-C8	-2.86	1.27	1.32
43	y	606	CHL	C1D-ND	-2.86	1.34	1.37
32	R	610	CLA	CHC-C1C	2.86	1.42	1.35
35	b	621	SQD	C6-S	-2.86	1.66	1.77
32	C	509	CLA	C1D-ND	2.86	1.41	1.37
32	c	501	CLA	C3B-C2B	-2.85	1.36	1.40
43	Y	601	CHL	C1D-ND	-2.85	1.34	1.37
32	S	614	CLA	CHC-C1C	2.85	1.42	1.35
32	s	614	CLA	CHC-C1C	2.85	1.42	1.35
32	N	604	CLA	CHC-C1C	2.85	1.42	1.35
32	s	611	CLA	CHC-C1C	2.85	1.42	1.35
43	Y	601	CHL	OBD-CAD	2.85	1.27	1.22
43	y	601	CHL	OBD-CAD	2.85	1.27	1.22
32	N	614	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	604	CLA	CHC-C1C	2.84	1.42	1.35
32	r	609	CLA	CHC-C1C	2.84	1.42	1.35
32	c	505	CLA	C1D-ND	2.83	1.41	1.37
32	B	608	CLA	CMB-C2B	-2.83	1.45	1.51
32	D	403	CLA	CHC-C1C	2.83	1.42	1.35
32	N	612	CLA	CHC-C1C	2.83	1.42	1.35
32	d	403	CLA	CHC-C1C	2.83	1.42	1.35
32	g	612	CLA	CHC-C1C	2.82	1.42	1.35
32	C	508	CLA	CMB-C2B	-2.82	1.45	1.51
32	G	604	CLA	CHC-C1C	2.82	1.42	1.35
32	n	604	CLA	CHC-C1C	2.82	1.42	1.35
32	c	508	CLA	CMC-C2C	-2.82	1.44	1.50
43	G	605	CHL	MG-NA	-2.82	1.99	2.06
32	c	501	CLA	CHC-C1C	2.81	1.42	1.35
43	n	605	CHL	MG-NA	-2.81	1.99	2.06
32	C	501	CLA	C3B-C2B	-2.81	1.36	1.40
32	B	612	CLA	CHC-C1C	2.81	1.42	1.35
32	g	604	CLA	CHC-C1C	2.81	1.42	1.35
32	n	612	CLA	CHC-C1C	2.81	1.42	1.35
32	R	609	CLA	CHC-C1C	2.80	1.42	1.35
32	S	605	CLA	CHC-C1C	2.80	1.42	1.35
32	s	605	CLA	CHC-C1C	2.80	1.42	1.35
32	c	508	CLA	CHC-C1C	2.80	1.42	1.35
32	G	612	CLA	CHC-C1C	2.80	1.42	1.35
33	A	409	PHO	CMD-C2D	-2.80	1.44	1.51
32	b	612	CLA	CHC-C1C	2.80	1.42	1.35
32	C	508	CLA	CHC-C1C	2.79	1.42	1.35
32	r	610	CLA	CHC-C1C	2.79	1.42	1.35
32	N	604	CLA	CMB-C2B	-2.79	1.45	1.51
43	y	601	CHL	C1D-ND	-2.79	1.34	1.37
32	n	611	CLA	CHC-C1C	2.79	1.42	1.35
32	b	614	CLA	CHC-C1C	2.79	1.42	1.35
32	b	608	CLA	CMB-C2B	-2.79	1.45	1.51
32	B	614	CLA	CHC-C1C	2.78	1.42	1.35
32	N	610	CLA	CHC-C1C	2.78	1.42	1.35
32	n	610	CLA	CHC-C1C	2.78	1.42	1.35
43	g	605	CHL	MG-NA	-2.78	1.99	2.06
32	S	613	CLA	CMB-C2B	-2.78	1.45	1.51
32	y	603	CLA	CHC-C1C	2.78	1.42	1.35
32	Y	603	CLA	CHC-C1C	2.77	1.42	1.35
43	n	607	CHL	C3B-C2B	2.77	1.44	1.40
43	N	605	CHL	MG-NA	-2.77	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	508	CLA	CMB-C2B	-2.77	1.45	1.51
32	C	507	CLA	CMB-C2B	-2.77	1.45	1.51
32	c	507	CLA	CMB-C2B	-2.77	1.45	1.51
32	C	501	CLA	CHC-C1C	2.77	1.42	1.35
32	N	613	CLA	CHC-C1C	2.77	1.42	1.35
32	n	613	CLA	CHC-C1C	2.77	1.42	1.35
43	s	601	CHL	C1D-C2D	2.77	1.50	1.45
32	D	402	CLA	CMD-C2D	-2.76	1.44	1.50
32	S	613	CLA	C3B-C2B	-2.76	1.36	1.40
32	c	510	CLA	CMB-C2B	-2.76	1.45	1.51
32	Y	604	CLA	CHC-C1C	2.76	1.42	1.35
32	y	604	CLA	CHC-C1C	2.76	1.42	1.35
32	C	510	CLA	CMB-C2B	-2.76	1.45	1.51
32	n	604	CLA	CMB-C2B	-2.76	1.45	1.51
32	b	602	CLA	CHC-C1C	2.76	1.42	1.35
32	d	402	CLA	CMD-C2D	-2.75	1.45	1.50
32	C	508	CLA	CMC-C2C	-2.75	1.45	1.50
43	N	601	CHL	C1D-C2D	2.75	1.50	1.45
43	n	601	CHL	C1D-C2D	2.75	1.50	1.45
32	B	606	CLA	CHC-C1C	2.75	1.42	1.35
32	b	606	CLA	CHC-C1C	2.75	1.42	1.35
32	s	613	CLA	C3B-C2B	-2.75	1.36	1.40
32	c	513	CLA	CMD-C2D	-2.75	1.45	1.50
32	C	509	CLA	CHC-C1C	2.75	1.42	1.35
32	c	509	CLA	CHC-C1C	2.75	1.42	1.35
32	S	609	CLA	CHC-C1C	2.75	1.42	1.35
32	N	611	CLA	CHC-C1C	2.75	1.42	1.35
32	c	512	CLA	CHC-C1C	2.75	1.42	1.35
32	B	609	CLA	CMB-C2B	-2.75	1.45	1.51
33	a	409	PHO	CMD-C2D	-2.74	1.45	1.51
32	s	603	CLA	CHC-C1C	2.74	1.42	1.35
43	N	607	CHL	C3B-C2B	2.74	1.44	1.40
32	C	506	CLA	C3B-C2B	-2.73	1.36	1.40
33	a	408	PHO	CAC-C3C	-2.73	1.47	1.52
32	C	513	CLA	CMD-C2D	-2.73	1.45	1.50
32	Y	612	CLA	CHC-C1C	2.73	1.42	1.35
32	s	613	CLA	CMB-C2B	-2.73	1.46	1.51
32	B	607	CLA	CHC-C1C	2.73	1.42	1.35
32	b	609	CLA	CHC-C1C	2.73	1.42	1.35
32	d	402	CLA	CHC-C1C	2.73	1.42	1.35
32	B	609	CLA	CHC-C1C	2.73	1.42	1.35
33	A	408	PHO	CAC-C3C	-2.73	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	607	CLA	CHC-C1C	2.72	1.42	1.35
32	G	603	CLA	CMB-C2B	-2.72	1.46	1.51
32	g	603	CLA	CMB-C2B	-2.72	1.46	1.51
32	B	602	CLA	CHC-C1C	2.72	1.41	1.35
32	S	610	CLA	CMB-C2B	-2.72	1.46	1.51
32	s	610	CLA	CMB-C2B	-2.72	1.46	1.51
43	s	607	CHL	MG-NA	-2.72	1.99	2.06
32	C	512	CLA	CHC-C1C	2.72	1.41	1.35
32	b	613	CLA	CMD-C2D	-2.72	1.45	1.50
32	B	613	CLA	CMD-C2D	-2.72	1.45	1.50
32	n	603	CLA	CHC-C1C	2.72	1.41	1.35
32	A	406	CLA	CMB-C2B	-2.72	1.46	1.51
32	C	509	CLA	CMB-C2B	-2.71	1.46	1.51
32	c	509	CLA	CMB-C2B	-2.71	1.46	1.51
32	S	612	CLA	CHC-C1C	2.71	1.41	1.35
43	y	607	CHL	MG-NA	-2.71	1.99	2.06
32	B	610	CLA	CHC-C1C	2.71	1.41	1.35
32	a	406	CLA	CMB-C2B	-2.71	1.46	1.51
32	c	504	CLA	CMB-C2B	-2.71	1.46	1.51
32	S	603	CLA	CHC-C1C	2.71	1.41	1.35
32	b	609	CLA	CMB-C2B	-2.71	1.46	1.51
43	S	601	CHL	C1D-C2D	2.70	1.50	1.45
32	D	402	CLA	CHC-C1C	2.70	1.41	1.35
32	N	603	CLA	CMB-C2B	-2.70	1.46	1.51
32	n	603	CLA	CMB-C2B	-2.70	1.46	1.51
32	y	612	CLA	CHC-C1C	2.70	1.41	1.35
32	C	504	CLA	CMB-C2B	-2.69	1.46	1.51
32	B	613	CLA	C1D-ND	2.69	1.41	1.37
32	Y	611	CLA	CMB-C2B	-2.69	1.46	1.51
32	y	611	CLA	CMB-C2B	-2.69	1.46	1.51
32	s	612	CLA	CHC-C1C	2.69	1.41	1.35
43	S	607	CHL	MG-NA	-2.69	1.99	2.06
32	b	610	CLA	CHC-C1C	2.69	1.41	1.35
43	G	609	CHL	MG-NA	-2.69	1.99	2.06
32	b	608	CLA	CHC-C1C	2.69	1.41	1.35
43	Y	607	CHL	MG-NA	-2.69	1.99	2.06
43	Y	606	CHL	MG-NA	-2.69	1.99	2.06
32	B	608	CLA	CHC-C1C	2.69	1.41	1.35
32	B	611	CLA	CMB-C2B	-2.68	1.46	1.51
32	b	611	CLA	CMB-C2B	-2.68	1.46	1.51
32	c	510	CLA	CHC-C1C	2.68	1.41	1.35
32	Y	613	CLA	CHC-C1C	2.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	609	CLA	CHC-C1C	2.68	1.41	1.35
32	B	615	CLA	CMB-C2B	-2.67	1.46	1.51
32	b	615	CLA	CMB-C2B	-2.67	1.46	1.51
32	C	510	CLA	CHC-C1C	2.67	1.41	1.35
32	B	616	CLA	CMB-C2B	-2.67	1.46	1.51
43	y	606	CHL	MG-NA	-2.67	1.99	2.06
32	y	611	CLA	CMD-C2D	-2.67	1.45	1.50
32	b	611	CLA	CHC-C1C	2.67	1.41	1.35
32	b	604	CLA	CMD-C2D	-2.67	1.45	1.50
32	Y	611	CLA	CHC-C1C	2.66	1.41	1.35
32	b	614	CLA	CMB-C2B	-2.66	1.46	1.51
43	G	605	CHL	C3D-C2D	2.66	1.46	1.39
43	g	605	CHL	C3D-C2D	2.66	1.46	1.39
32	c	513	CLA	C1D-ND	2.66	1.41	1.37
32	D	403	CLA	CMB-C2B	-2.66	1.46	1.51
32	c	506	CLA	C3B-C2B	-2.66	1.36	1.40
32	b	616	CLA	CMB-C2B	-2.66	1.46	1.51
32	N	603	CLA	CHC-C1C	2.66	1.41	1.35
32	C	513	CLA	C1D-ND	2.65	1.41	1.37
32	n	613	CLA	CMB-C2B	-2.65	1.46	1.51
32	Y	614	CLA	CMB-C2B	-2.65	1.46	1.51
32	r	610	CLA	CMB-C2B	-2.65	1.46	1.51
32	y	614	CLA	CMB-C2B	-2.65	1.46	1.51
32	g	603	CLA	C3B-C2B	-2.65	1.36	1.40
32	d	402	CLA	CMB-C2B	-2.65	1.46	1.51
32	Y	611	CLA	CMD-C2D	-2.65	1.45	1.50
32	A	410	CLA	CMB-C2B	-2.65	1.46	1.51
32	b	613	CLA	C1D-ND	2.65	1.41	1.37
32	c	511	CLA	CHC-C1C	2.65	1.41	1.35
32	B	611	CLA	CHC-C1C	2.65	1.41	1.35
43	s	608	CHL	C1D-C2D	2.65	1.50	1.45
43	G	608	CHL	C1D-C2D	2.65	1.50	1.45
43	S	606	CHL	C1D-C2D	2.65	1.50	1.45
32	c	501	CLA	CMB-C2B	-2.65	1.46	1.51
32	C	501	CLA	CMB-C2B	-2.64	1.46	1.51
32	C	501	CLA	CMD-C2D	-2.64	1.45	1.50
32	y	613	CLA	CHC-C1C	2.64	1.41	1.35
32	S	613	CLA	CHC-C1C	2.64	1.41	1.35
32	s	613	CLA	CHC-C1C	2.64	1.41	1.35
32	y	611	CLA	CHC-C1C	2.64	1.41	1.35
32	a	410	CLA	CMB-C2B	-2.64	1.46	1.51
32	B	604	CLA	CMD-C2D	-2.64	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	614	CLA	CMB-C2B	-2.64	1.46	1.51
32	b	612	CLA	CMB-C2B	-2.64	1.46	1.51
43	g	609	CHL	MG-NA	-2.64	2.00	2.06
32	b	617	CLA	CMC-C2C	-2.63	1.45	1.50
32	N	613	CLA	CMB-C2B	-2.63	1.46	1.51
32	d	403	CLA	CMB-C2B	-2.63	1.46	1.51
32	B	612	CLA	CMB-C2B	-2.63	1.46	1.51
32	B	607	CLA	CMB-C2B	-2.63	1.46	1.51
32	b	607	CLA	CMB-C2B	-2.63	1.46	1.51
32	d	403	CLA	C3B-C2B	-2.63	1.36	1.40
32	b	606	CLA	CMB-C2B	-2.62	1.46	1.51
32	C	511	CLA	CHC-C1C	2.62	1.41	1.35
43	R	608	CHL	C1D-C2D	2.62	1.50	1.45
43	g	608	CHL	C1D-C2D	2.62	1.50	1.45
43	s	606	CHL	C1D-C2D	2.62	1.50	1.45
32	a	407	CLA	CMB-C2B	-2.62	1.46	1.51
32	C	503	CLA	CMB-C2B	-2.61	1.46	1.51
32	y	602	CLA	CMB-C2B	-2.61	1.46	1.51
32	D	403	CLA	C3B-C2B	-2.61	1.36	1.40
32	c	501	CLA	CMD-C2D	-2.61	1.45	1.50
32	G	603	CLA	C3B-C2B	-2.61	1.36	1.40
32	S	604	CLA	CHC-C1C	2.61	1.41	1.35
32	D	402	CLA	CMB-C2B	-2.61	1.46	1.51
32	Y	612	CLA	CMB-C2B	-2.61	1.46	1.51
32	c	513	CLA	CHC-C1C	2.60	1.41	1.35
32	B	606	CLA	CMB-C2B	-2.60	1.46	1.51
32	b	616	CLA	CHC-C1C	2.60	1.41	1.35
32	A	410	CLA	CHC-C1C	2.60	1.41	1.35
32	y	612	CLA	CMB-C2B	-2.60	1.46	1.51
43	S	608	CHL	C1D-C2D	2.60	1.50	1.45
32	G	613	CLA	CHC-C1C	2.60	1.41	1.35
43	s	607	CHL	C3D-C2D	2.60	1.46	1.39
32	b	617	CLA	CHC-C1C	2.60	1.41	1.35
33	A	409	PHO	CAC-C3C	-2.60	1.47	1.52
32	r	604	CLA	CMB-C2B	-2.60	1.46	1.51
32	B	602	CLA	CMB-C2B	-2.59	1.46	1.51
32	C	506	CLA	CHC-C1C	2.59	1.41	1.35
32	c	506	CLA	CHC-C1C	2.59	1.41	1.35
32	r	603	CLA	CMB-C2B	-2.59	1.46	1.51
32	a	410	CLA	CHC-C1C	2.59	1.41	1.35
32	c	504	CLA	CHC-C1C	2.59	1.41	1.35
32	C	504	CLA	CHC-C1C	2.59	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	602	CLA	CMB-C2B	-2.59	1.46	1.51
32	R	603	CLA	CMB-C2B	-2.59	1.46	1.51
32	B	617	CLA	CHC-C1C	2.59	1.41	1.35
32	C	510	CLA	CMD-C2D	-2.59	1.45	1.50
32	Y	602	CLA	CMB-C2B	-2.58	1.46	1.51
43	S	607	CHL	C3D-C2D	2.58	1.46	1.39
32	c	503	CLA	CMB-C2B	-2.58	1.46	1.51
32	B	617	CLA	CMC-C2C	-2.58	1.45	1.50
43	r	608	CHL	C1D-C2D	2.58	1.50	1.45
33	a	409	PHO	CAC-C3C	-2.58	1.47	1.52
32	Y	604	CLA	C3B-C2B	-2.58	1.36	1.40
32	y	604	CLA	C3B-C2B	-2.58	1.36	1.40
32	G	613	CLA	CMB-C2B	-2.58	1.46	1.51
32	g	613	CLA	CMB-C2B	-2.58	1.46	1.51
32	C	505	CLA	CHC-C1C	2.58	1.41	1.35
32	C	512	CLA	CMB-C2B	-2.58	1.46	1.51
46	R	625	NEX	C7-C8	-2.58	1.27	1.32
32	S	609	CLA	CMB-C2B	-2.57	1.46	1.51
32	s	604	CLA	CHC-C1C	2.57	1.41	1.35
43	r	607	CHL	C1D-C2D	2.57	1.50	1.45
32	G	610	CLA	CHC-C1C	2.57	1.41	1.35
32	c	505	CLA	CMB-C2B	-2.57	1.46	1.51
32	C	507	CLA	CHC-C1C	2.57	1.41	1.35
32	c	507	CLA	CHC-C1C	2.57	1.41	1.35
43	y	606	CHL	C4B-CHC	2.57	1.48	1.41
43	y	605	CHL	MG-NA	-2.57	2.00	2.06
32	b	604	CLA	C3B-C2B	-2.56	1.36	1.40
32	n	614	CLA	CMB-C2B	-2.56	1.46	1.51
32	g	613	CLA	CHC-C1C	2.56	1.41	1.35
43	y	605	CHL	C1D-C2D	2.56	1.50	1.45
32	N	611	CLA	CMB-C2B	-2.56	1.46	1.51
32	n	611	CLA	CMB-C2B	-2.56	1.46	1.51
32	C	513	CLA	CHC-C1C	2.56	1.41	1.35
32	c	512	CLA	CMB-C2B	-2.55	1.46	1.51
43	s	606	CHL	C3D-C2D	2.55	1.46	1.39
43	S	607	CHL	C1D-C2D	2.55	1.50	1.45
32	s	609	CLA	CMB-C2B	-2.55	1.46	1.51
43	Y	606	CHL	C4B-CHC	2.55	1.48	1.41
32	g	603	CLA	CHC-C1C	2.55	1.41	1.35
32	A	407	CLA	CMB-C2B	-2.55	1.46	1.51
32	D	402	CLA	C3B-C2B	-2.55	1.36	1.40
32	B	616	CLA	CHC-C1C	2.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	d	405	PL9	C53-C6	-2.55	1.45	1.50
32	g	610	CLA	CHC-C1C	2.55	1.41	1.35
32	d	402	CLA	C3B-C2B	-2.55	1.36	1.40
32	S	614	CLA	CMB-C2B	-2.55	1.46	1.51
32	Y	613	CLA	CMB-C2B	-2.55	1.46	1.51
32	s	614	CLA	CMB-C2B	-2.55	1.46	1.51
32	N	614	CLA	CMB-C2B	-2.55	1.46	1.51
46	y	1623	NEX	C7-C8	-2.54	1.27	1.32
32	R	604	CLA	CMB-C2B	-2.54	1.46	1.51
32	c	510	CLA	CMD-C2D	-2.54	1.45	1.50
43	y	601	CHL	MG-NA	-2.54	2.00	2.06
32	G	603	CLA	CHC-C1C	2.54	1.41	1.35
43	S	606	CHL	C3D-C2D	2.54	1.46	1.39
32	B	604	CLA	C3B-C2B	-2.54	1.36	1.40
32	y	613	CLA	CMB-C2B	-2.54	1.46	1.51
32	C	511	CLA	CMB-C2B	-2.54	1.46	1.51
43	R	607	CHL	C1D-C2D	2.54	1.50	1.45
32	c	505	CLA	CHC-C1C	2.54	1.41	1.35
32	N	613	CLA	CMD-C2D	-2.53	1.45	1.50
32	a	405	CLA	CMD-C2D	-2.53	1.45	1.50
32	s	602	CLA	CMB-C2B	-2.53	1.46	1.51
43	S	608	CHL	C3D-C2D	2.53	1.46	1.39
32	R	610	CLA	CMB-C2B	-2.53	1.46	1.51
32	c	511	CLA	CMB-C2B	-2.53	1.46	1.51
43	r	606	CHL	C3D-C2D	2.53	1.46	1.39
32	a	405	CLA	CMB-C2B	-2.53	1.46	1.51
43	Y	605	CHL	MG-NA	-2.53	2.00	2.06
32	G	612	CLA	CMB-C2B	-2.53	1.46	1.51
43	Y	601	CHL	MG-NA	-2.52	2.00	2.06
32	B	608	CLA	CMC-C2C	-2.52	1.45	1.50
32	b	608	CLA	CMC-C2C	-2.52	1.45	1.50
32	n	613	CLA	CMD-C2D	-2.52	1.45	1.50
43	N	606	CHL	C4B-CHC	2.52	1.48	1.41
32	Y	610	CLA	CMB-C2B	-2.52	1.46	1.51
43	s	607	CHL	C1D-C2D	2.52	1.50	1.45
32	g	612	CLA	CMB-C2B	-2.52	1.46	1.51
43	Y	605	CHL	C1D-C2D	2.51	1.50	1.45
32	d	402	CLA	CMC-C2C	-2.51	1.45	1.50
32	y	603	CLA	CMB-C2B	-2.51	1.46	1.51
43	n	606	CHL	C4B-CHC	2.51	1.48	1.41
43	s	608	CHL	C3D-C2D	2.51	1.46	1.39
32	G	611	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	405	CLA	CMD-C2D	-2.51	1.45	1.50
43	y	608	CHL	C1D-C2D	2.51	1.50	1.45
46	g	1623	NEX	C7-C8	-2.50	1.27	1.32
32	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
32	A	407	CLA	CHC-C1C	2.50	1.41	1.35
32	a	407	CLA	CHC-C1C	2.50	1.41	1.35
43	g	601	CHL	MG-NA	-2.50	2.00	2.06
32	G	614	CLA	CMB-C2B	-2.50	1.46	1.51
32	S	611	CLA	CMB-C2B	-2.50	1.46	1.51
32	s	603	CLA	CMB-C2B	-2.50	1.46	1.51
32	B	613	CLA	CMA-C3A	-2.50	1.47	1.53
32	b	613	CLA	CMA-C3A	-2.50	1.47	1.53
32	G	602	CLA	CMB-C2B	-2.50	1.46	1.51
43	r	606	CHL	C1D-C2D	2.50	1.50	1.45
43	R	606	CHL	C3D-C2D	2.50	1.45	1.39
32	R	609	CLA	CMB-C2B	-2.49	1.46	1.51
32	r	609	CLA	CMB-C2B	-2.49	1.46	1.51
43	R	606	CHL	MG-NA	-2.49	2.00	2.06
32	g	611	CLA	CMB-C2B	-2.49	1.46	1.51
43	y	605	CHL	C3D-C2D	2.49	1.45	1.39
43	Y	608	CHL	C1D-C2D	2.49	1.50	1.45
32	Y	603	CLA	CMB-C2B	-2.49	1.46	1.51
43	g	607	CHL	MG-NA	-2.49	2.00	2.06
40	D	405	PL9	C53-C6	-2.48	1.45	1.50
43	n	608	CHL	MG-NA	-2.48	2.00	2.06
32	A	405	CLA	CMB-C2B	-2.48	1.46	1.51
32	g	602	CLA	CMB-C2B	-2.48	1.46	1.51
32	G	613	CLA	CMD-C2D	-2.48	1.45	1.50
32	D	402	CLA	CMC-C2C	-2.48	1.45	1.50
43	R	606	CHL	C1D-C2D	2.48	1.50	1.45
32	n	610	CLA	CMB-C2B	-2.47	1.46	1.51
40	D	405	PL9	C31-C29	-2.47	1.46	1.51
40	d	405	PL9	C31-C29	-2.47	1.46	1.51
32	N	612	CLA	CMB-C2B	-2.47	1.46	1.51
32	n	602	CLA	CMB-C2B	-2.47	1.46	1.51
32	S	602	CLA	CMB-C2B	-2.47	1.46	1.51
32	n	612	CLA	CMB-C2B	-2.47	1.46	1.51
32	s	610	CLA	C3B-CAB	-2.47	1.42	1.47
32	C	513	CLA	CMB-C2B	-2.47	1.46	1.51
32	N	602	CLA	CMB-C2B	-2.47	1.46	1.51
43	N	608	CHL	MG-NA	-2.47	2.00	2.06
43	Y	608	CHL	MG-NA	-2.47	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	603	CLA	CMB-C2B	-2.46	1.46	1.51
43	r	608	CHL	MG-NA	-2.46	2.00	2.06
32	c	513	CLA	CMB-C2B	-2.46	1.46	1.51
43	G	607	CHL	MG-NA	-2.46	2.00	2.06
32	s	611	CLA	CMB-C2B	-2.46	1.46	1.51
43	R	608	CHL	MG-NA	-2.46	2.00	2.06
32	N	610	CLA	CMB-C2B	-2.46	1.46	1.51
32	r	602	CLA	CMB-C2B	-2.46	1.46	1.51
43	R	607	CHL	C3D-C2D	2.46	1.45	1.39
32	y	610	CLA	CMB-C2B	-2.46	1.46	1.51
32	s	605	CLA	CMB-C2B	-2.46	1.46	1.51
32	A	406	CLA	CHC-C1C	2.46	1.41	1.35
32	a	406	CLA	CHC-C1C	2.46	1.41	1.35
32	g	614	CLA	CMB-C2B	-2.46	1.46	1.51
43	r	608	CHL	C3D-C2D	2.45	1.45	1.39
32	R	602	CLA	CMB-C2B	-2.45	1.46	1.51
32	b	617	CLA	CMB-C2B	-2.45	1.46	1.51
32	C	502	CLA	CMD-C2D	-2.45	1.45	1.50
43	Y	605	CHL	C3D-C2D	2.45	1.45	1.39
32	b	603	CLA	CMB-C2B	-2.45	1.46	1.51
32	b	613	CLA	CMB-C2B	-2.45	1.46	1.51
32	S	610	CLA	C3B-CAB	-2.45	1.43	1.47
32	B	617	CLA	CMB-C2B	-2.45	1.46	1.51
32	b	615	CLA	CMD-C2D	-2.44	1.45	1.50
32	B	613	CLA	CMB-C2B	-2.44	1.46	1.51
32	C	504	CLA	C3B-C2B	-2.44	1.37	1.40
32	c	504	CLA	C3B-C2B	-2.44	1.37	1.40
32	B	615	CLA	CMD-C2D	-2.44	1.45	1.50
32	S	612	CLA	CMB-C2B	-2.44	1.46	1.51
43	r	607	CHL	C3D-C2D	2.44	1.45	1.39
32	c	502	CLA	CMD-C2D	-2.44	1.45	1.50
43	g	607	CHL	C1D-C2D	2.44	1.50	1.45
43	R	608	CHL	C3D-C2D	2.44	1.45	1.39
32	S	605	CLA	CMB-C2B	-2.44	1.46	1.51
32	b	605	CLA	CHC-C1C	2.43	1.41	1.35
32	B	603	CLA	CMB-C2B	-2.43	1.46	1.51
43	g	606	CHL	MG-NA	-2.43	2.00	2.06
32	g	613	CLA	CMD-C2D	-2.43	1.45	1.50
32	B	613	CLA	CMC-C2C	-2.43	1.45	1.50
32	b	613	CLA	CMC-C2C	-2.43	1.45	1.50
32	N	610	CLA	CMC-C2C	-2.43	1.45	1.50
32	n	612	CLA	C3B-C2B	-2.43	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	605	CLA	CHC-C1C	2.43	1.41	1.35
32	s	612	CLA	CMB-C2B	-2.42	1.46	1.51
43	y	608	CHL	MG-NA	-2.42	2.00	2.06
43	N	607	CHL	C1C-NC	-2.42	1.34	1.37
32	s	613	CLA	CMD-C2D	-2.42	1.45	1.50
43	n	607	CHL	C1C-NC	-2.42	1.34	1.37
32	B	614	CLA	CMD-C2D	-2.42	1.45	1.50
43	r	606	CHL	MG-NA	-2.42	2.00	2.06
32	n	610	CLA	CMC-C2C	-2.42	1.45	1.50
32	S	613	CLA	CMD-C2D	-2.41	1.45	1.50
43	G	605	CHL	C4B-CHC	2.41	1.47	1.41
32	b	607	CLA	CMC-C2C	-2.41	1.45	1.50
32	B	607	CLA	CMC-C2C	-2.41	1.45	1.50
43	Y	609	CHL	MG-NA	-2.41	2.00	2.06
32	G	610	CLA	CMB-C2B	-2.40	1.46	1.51
43	r	606	CHL	C4B-CHC	2.40	1.47	1.41
43	R	607	CHL	MG-NA	-2.40	2.00	2.06
43	r	607	CHL	MG-NA	-2.40	2.00	2.06
43	G	601	CHL	MG-NA	-2.40	2.00	2.06
32	s	611	CLA	CMD-C2D	-2.40	1.45	1.50
32	B	610	CLA	C3B-C2B	-2.40	1.37	1.40
32	b	610	CLA	C3B-C2B	-2.40	1.37	1.40
32	C	502	CLA	C4B-CHC	-2.40	1.34	1.41
43	g	607	CHL	C3D-C2D	2.39	1.45	1.39
43	g	605	CHL	C4B-CHC	2.39	1.47	1.41
43	N	606	CHL	C3D-C2D	2.39	1.45	1.39
43	n	606	CHL	C3D-C2D	2.39	1.45	1.39
43	g	606	CHL	C4B-CHC	2.39	1.47	1.41
43	G	607	CHL	C1D-C2D	2.39	1.50	1.45
43	N	606	CHL	MG-NA	-2.39	2.00	2.06
43	n	606	CHL	MG-NA	-2.39	2.00	2.06
43	G	606	CHL	C3D-C2D	2.39	1.45	1.39
43	y	609	CHL	MG-NA	-2.39	2.00	2.06
32	c	509	CLA	CMC-C2C	-2.39	1.45	1.50
32	Y	610	CLA	CMC-C2C	-2.39	1.45	1.50
32	c	509	CLA	CMD-C2D	-2.39	1.45	1.50
32	C	509	CLA	CMD-C2D	-2.39	1.45	1.50
43	g	606	CHL	C3D-C2D	2.39	1.45	1.39
32	C	509	CLA	CMC-C2C	-2.38	1.45	1.50
32	s	610	CLA	CMC-C2C	-2.38	1.45	1.50
32	c	505	CLA	MG-ND	-2.38	2.01	2.05
32	b	614	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	G	606	CHL	C4B-CHC	2.38	1.47	1.41
43	G	606	CHL	MG-NA	-2.38	2.00	2.06
32	N	612	CLA	C3B-C2B	-2.37	1.37	1.40
33	a	408	PHO	CMC-C2C	-2.37	1.45	1.51
43	g	605	CHL	C1B-CHB	2.37	1.47	1.41
32	c	507	CLA	CMD-C2D	-2.37	1.45	1.50
32	S	610	CLA	CMC-C2C	-2.37	1.45	1.50
32	S	611	CLA	CMD-C2D	-2.37	1.45	1.50
43	R	606	CHL	C4B-CHC	2.37	1.47	1.41
32	c	502	CLA	C4B-CHC	-2.37	1.34	1.41
32	y	610	CLA	CMC-C2C	-2.37	1.45	1.50
43	S	607	CHL	C4B-CHC	2.37	1.47	1.41
33	A	409	PHO	CMC-C2C	-2.37	1.45	1.51
32	b	616	CLA	C3B-C2B	-2.37	1.37	1.40
33	A	408	PHO	CMC-C2C	-2.36	1.45	1.51
43	G	605	CHL	C1B-CHB	2.36	1.47	1.41
32	C	505	CLA	MG-ND	-2.36	2.01	2.05
32	A	410	CLA	CMD-C2D	-2.36	1.45	1.50
40	d	405	PL9	C35-C34	-2.36	1.44	1.50
43	g	608	CHL	MG-NA	-2.36	2.00	2.06
33	a	409	PHO	CMC-C2C	-2.36	1.45	1.51
43	G	607	CHL	C3D-C2D	2.36	1.45	1.39
32	b	607	CLA	CMD-C2D	-2.35	1.45	1.50
32	C	507	CLA	CMD-C2D	-2.35	1.45	1.50
43	S	606	CHL	MG-NA	-2.35	2.00	2.06
43	s	606	CHL	MG-NA	-2.35	2.00	2.06
32	b	611	CLA	CMC-C2C	-2.35	1.45	1.50
32	a	410	CLA	CMD-C2D	-2.35	1.45	1.50
32	C	502	CLA	C3B-C2B	-2.35	1.37	1.40
32	B	616	CLA	C3B-C2B	-2.35	1.37	1.40
43	N	609	CHL	MG-NA	-2.35	2.00	2.06
32	B	607	CLA	CMD-C2D	-2.35	1.45	1.50
43	G	608	CHL	MG-NA	-2.35	2.00	2.06
32	B	605	CLA	CMC-C2C	-2.35	1.45	1.50
32	b	605	CLA	CMC-C2C	-2.35	1.45	1.50
43	n	606	CHL	C2C-C1C	2.34	1.49	1.44
32	g	610	CLA	CMB-C2B	-2.34	1.46	1.51
32	C	512	CLA	CMD-C2D	-2.34	1.45	1.50
43	N	606	CHL	C2C-C1C	2.34	1.49	1.44
43	S	608	CHL	C4C-C3C	2.34	1.49	1.45
32	c	512	CLA	CMD-C2D	-2.34	1.45	1.50
32	c	505	CLA	CMC-C2C	-2.33	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	502	CLA	CMC-C2C	-2.33	1.45	1.50
32	c	502	CLA	CMC-C2C	-2.33	1.45	1.50
32	g	604	CLA	CMD-C2D	-2.33	1.45	1.50
43	y	607	CHL	C1C-NC	-2.33	1.34	1.37
43	s	607	CHL	C4B-CHC	2.33	1.47	1.41
43	n	609	CHL	MG-NA	-2.33	2.00	2.06
32	Y	614	CLA	C3B-C2B	-2.33	1.37	1.40
32	y	614	CLA	C3B-C2B	-2.33	1.37	1.40
32	S	605	CLA	C3B-C2B	-2.33	1.37	1.40
32	s	605	CLA	C3B-C2B	-2.33	1.37	1.40
32	B	605	CLA	MG-ND	-2.33	2.01	2.05
32	b	605	CLA	MG-ND	-2.33	2.01	2.05
32	Y	603	CLA	C3B-C2B	-2.32	1.37	1.40
43	y	609	CHL	C3D-C2D	2.32	1.45	1.39
43	Y	607	CHL	C1C-NC	-2.32	1.34	1.37
32	C	509	CLA	CMA-C3A	-2.32	1.48	1.53
32	N	603	CLA	C3B-C2B	-2.32	1.37	1.40
32	n	603	CLA	C3B-C2B	-2.32	1.37	1.40
43	R	607	CHL	C4B-CHC	2.32	1.47	1.41
32	c	502	CLA	C3B-C2B	-2.32	1.37	1.40
32	C	504	CLA	CMD-C2D	-2.32	1.45	1.50
32	c	504	CLA	CMD-C2D	-2.32	1.45	1.50
43	s	608	CHL	C4C-C3C	2.32	1.49	1.45
45	y	1622	XAT	O24-C25	-2.32	1.42	1.46
43	Y	609	CHL	C3D-C2D	2.31	1.45	1.39
32	c	502	CLA	CHC-C1C	2.31	1.40	1.35
43	S	608	CHL	C4B-CHC	2.31	1.47	1.41
32	c	509	CLA	CMA-C3A	-2.31	1.48	1.53
40	D	405	PL9	C35-C34	-2.31	1.44	1.50
32	C	508	CLA	CMD-C2D	-2.30	1.45	1.50
32	G	604	CLA	CMD-C2D	-2.30	1.45	1.50
32	Y	612	CLA	CMD-C2D	-2.30	1.45	1.50
43	N	609	CHL	C1D-C2D	2.30	1.49	1.45
43	n	609	CHL	C1D-C2D	2.30	1.49	1.45
32	y	603	CLA	C3B-C2B	-2.30	1.37	1.40
34	C	515	BCR	C1-C6	-2.30	1.50	1.53
32	C	506	CLA	CMD-C2D	-2.30	1.45	1.50
32	c	506	CLA	CMD-C2D	-2.30	1.45	1.50
43	s	608	CHL	C4B-CHC	2.30	1.47	1.41
33	a	408	PHO	CMD-C2D	-2.30	1.46	1.51
43	Y	601	CHL	C1B-NB	-2.30	1.33	1.35
43	y	601	CHL	C1B-NB	-2.30	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	610	CLA	C3B-C2B	-2.30	1.37	1.40
43	r	607	CHL	C4B-CHC	2.30	1.47	1.41
32	y	612	CLA	CMD-C2D	-2.30	1.45	1.50
40	d	405	PL9	C46-C44	-2.30	1.46	1.51
32	A	407	CLA	CMD-C2D	-2.30	1.45	1.50
32	a	407	CLA	CMD-C2D	-2.30	1.45	1.50
32	c	508	CLA	CMD-C2D	-2.29	1.45	1.50
32	Y	602	CLA	CMC-C2C	-2.29	1.45	1.50
43	s	608	CHL	MG-NA	-2.29	2.00	2.06
32	B	611	CLA	CMC-C2C	-2.29	1.45	1.50
43	G	606	CHL	C2C-C1C	2.29	1.49	1.44
46	s	1623	NEX	C1-C6	-2.29	1.50	1.54
32	B	611	CLA	C3B-C2B	-2.29	1.37	1.40
32	Y	614	CLA	CMD-C2D	-2.29	1.46	1.50
32	y	614	CLA	CMD-C2D	-2.29	1.46	1.50
32	C	512	CLA	C3B-C2B	-2.28	1.37	1.40
32	C	505	CLA	CMC-C2C	-2.28	1.46	1.50
43	N	601	CHL	C3D-C2D	2.28	1.45	1.39
43	n	601	CHL	C3D-C2D	2.28	1.45	1.39
43	n	607	CHL	C3D-C2D	2.28	1.45	1.39
32	c	511	CLA	CMD-C2D	-2.28	1.46	1.50
32	y	602	CLA	CMC-C2C	-2.28	1.46	1.50
32	C	502	CLA	CHC-C1C	2.28	1.40	1.35
32	s	612	CLA	C3B-C2B	-2.28	1.37	1.40
32	n	611	CLA	CMD-C2D	-2.27	1.46	1.50
32	y	603	CLA	CMD-C2D	-2.27	1.46	1.50
43	g	606	CHL	C2C-C1C	2.27	1.49	1.44
32	C	506	CLA	CMC-C2C	-2.27	1.46	1.50
40	D	405	PL9	C46-C44	-2.27	1.46	1.51
45	Y	1622	XAT	O24-C25	-2.26	1.43	1.46
32	c	512	CLA	C3B-C2B	-2.26	1.37	1.40
43	Y	601	CHL	C1C-NC	-2.26	1.34	1.37
32	b	611	CLA	C3B-C2B	-2.26	1.37	1.40
32	r	602	CLA	C3B-C2B	-2.26	1.37	1.40
43	N	607	CHL	C3D-C2D	2.26	1.45	1.39
32	C	511	CLA	CMD-C2D	-2.26	1.46	1.50
32	Y	603	CLA	CMD-C2D	-2.26	1.46	1.50
32	C	510	CLA	CMC-C2C	-2.26	1.46	1.50
43	y	609	CHL	C4B-CHC	2.26	1.47	1.41
32	Y	610	CLA	C3B-C2B	-2.26	1.37	1.40
32	N	613	CLA	MG-ND	-2.26	2.01	2.05
32	G	614	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	602	CLA	CMD-C2D	-2.26	1.46	1.50
43	y	607	CHL	C3D-C2D	2.26	1.45	1.39
33	A	408	PHO	CMD-C2D	-2.25	1.46	1.51
43	Y	608	CHL	C3D-C2D	2.25	1.45	1.39
32	n	603	CLA	CMC-C2C	-2.25	1.46	1.50
32	N	611	CLA	C3B-C2B	-2.25	1.37	1.40
43	s	607	CHL	C1B-CHB	2.25	1.47	1.41
32	g	611	CLA	CMD-C2D	-2.25	1.46	1.50
43	n	608	CHL	C3D-C2D	2.25	1.45	1.39
32	n	613	CLA	MG-ND	-2.25	2.01	2.05
43	Y	607	CHL	C3D-C2D	2.25	1.45	1.39
32	s	613	CLA	CMC-C2C	-2.24	1.46	1.50
32	S	605	CLA	CMD-C2D	-2.24	1.46	1.50
32	A	406	CLA	C4B-CHC	-2.24	1.34	1.41
32	G	611	CLA	CMD-C2D	-2.24	1.46	1.50
43	y	608	CHL	C3D-C2D	2.24	1.45	1.39
43	Y	609	CHL	C4B-CHC	2.24	1.47	1.41
32	B	603	CLA	CMD-C2D	-2.24	1.46	1.50
32	b	603	CLA	CMD-C2D	-2.24	1.46	1.50
32	N	602	CLA	CMC-C2C	-2.24	1.46	1.50
32	N	603	CLA	CMD-C2D	-2.24	1.46	1.50
32	n	603	CLA	CMD-C2D	-2.24	1.46	1.50
32	n	614	CLA	C3B-C2B	-2.24	1.37	1.40
32	Y	611	CLA	CMC-C2C	-2.24	1.46	1.50
43	G	608	CHL	C3D-C2D	2.24	1.45	1.39
43	g	608	CHL	C3D-C2D	2.24	1.45	1.39
32	Y	613	CLA	CMD-C2D	-2.24	1.46	1.50
32	S	613	CLA	MG-ND	-2.24	2.01	2.05
32	s	613	CLA	MG-ND	-2.24	2.01	2.05
43	Y	605	CHL	C4B-CHC	2.24	1.47	1.41
32	d	403	CLA	CMD-C2D	-2.24	1.46	1.50
43	S	608	CHL	MG-NA	-2.24	2.01	2.06
32	c	504	CLA	CMC-C2C	-2.24	1.46	1.50
43	N	608	CHL	C3D-C2D	2.23	1.45	1.39
32	B	605	CLA	C4B-CHC	-2.23	1.34	1.41
32	b	605	CLA	C4B-CHC	-2.23	1.34	1.41
32	S	602	CLA	CMD-C2D	-2.23	1.46	1.50
32	b	606	CLA	CMD-C2D	-2.23	1.46	1.50
32	c	506	CLA	CMC-C2C	-2.23	1.46	1.50
32	D	402	CLA	C1D-ND	2.23	1.40	1.37
32	d	402	CLA	C1D-ND	2.23	1.40	1.37
32	Y	604	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	604	CLA	CMD-C2D	-2.23	1.46	1.50
32	C	509	CLA	C3B-CAB	-2.23	1.43	1.47
32	a	407	CLA	C4B-CHC	-2.23	1.34	1.41
43	N	609	CHL	C1D-ND	-2.23	1.35	1.37
43	n	605	CHL	C1C-NC	-2.23	1.34	1.37
43	S	607	CHL	C1B-CHB	2.23	1.47	1.41
32	B	608	CLA	CMD-C2D	-2.23	1.46	1.50
32	s	605	CLA	CMD-C2D	-2.23	1.46	1.50
32	N	613	CLA	MG-NC	2.23	2.11	2.06
32	n	613	CLA	MG-NC	2.23	2.11	2.06
32	R	610	CLA	C3B-C2B	-2.23	1.37	1.40
32	R	602	CLA	CMD-C2D	-2.23	1.46	1.50
32	S	614	CLA	CMD-C2D	-2.23	1.46	1.50
32	s	610	CLA	CMD-C2D	-2.23	1.46	1.50
32	c	510	CLA	CMC-C2C	-2.23	1.46	1.50
32	N	603	CLA	CMC-C2C	-2.23	1.46	1.50
43	N	605	CHL	C3D-C2D	2.23	1.45	1.39
43	n	605	CHL	C3D-C2D	2.23	1.45	1.39
32	G	603	CLA	CMD-C2D	-2.23	1.46	1.50
32	s	612	CLA	CMC-C2C	-2.23	1.46	1.50
32	Y	612	CLA	CMC-C2C	-2.23	1.46	1.50
40	D	405	PL9	C16-C14	-2.23	1.46	1.51
32	N	611	CLA	CMD-C2D	-2.23	1.46	1.50
32	n	602	CLA	CMC-C2C	-2.23	1.46	1.50
32	c	509	CLA	C3B-CAB	-2.22	1.43	1.47
32	B	609	CLA	CMD-C2D	-2.22	1.46	1.50
32	b	609	CLA	CMD-C2D	-2.22	1.46	1.50
32	C	507	CLA	C3B-C2B	-2.22	1.37	1.40
32	S	612	CLA	C3B-C2B	-2.22	1.37	1.40
32	c	507	CLA	C3B-C2B	-2.22	1.37	1.40
43	N	605	CHL	C1C-NC	-2.22	1.34	1.37
32	y	613	CLA	CMD-C2D	-2.22	1.46	1.50
34	c	515	BCR	C1-C6	-2.22	1.50	1.53
43	n	609	CHL	C1D-ND	-2.22	1.35	1.37
32	y	610	CLA	C3B-C2B	-2.22	1.37	1.40
43	y	605	CHL	C4B-CHC	2.22	1.47	1.41
32	R	610	CLA	CMD-C2D	-2.22	1.46	1.50
32	y	602	CLA	CMD-C2D	-2.22	1.46	1.50
32	Y	603	CLA	MG-ND	-2.22	2.01	2.05
32	C	504	CLA	CMC-C2C	-2.22	1.46	1.50
32	B	602	CLA	C3B-C2B	-2.21	1.37	1.40
32	b	602	CLA	C3B-C2B	-2.21	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	611	CLA	CMC-C2C	-2.21	1.46	1.50
32	s	602	CLA	CMD-C2D	-2.21	1.46	1.50
32	Y	612	CLA	C3B-C2B	-2.21	1.37	1.40
32	a	406	CLA	C4B-CHC	-2.21	1.34	1.41
32	s	612	CLA	CMD-C2D	-2.21	1.46	1.50
43	S	606	CHL	C4B-CHC	2.21	1.47	1.41
32	r	610	CLA	CMD-C2D	-2.21	1.46	1.50
32	g	614	CLA	CMD-C2D	-2.21	1.46	1.50
33	A	408	PHO	C1C-NC	-2.21	1.31	1.38
32	Y	602	CLA	C3B-C2B	-2.21	1.37	1.40
32	y	602	CLA	C3B-C2B	-2.21	1.37	1.40
32	N	602	CLA	CMD-C2D	-2.21	1.46	1.50
32	c	503	CLA	CMD-C2D	-2.20	1.46	1.50
32	B	616	CLA	CMD-C2D	-2.20	1.46	1.50
32	S	610	CLA	CMD-C2D	-2.20	1.46	1.50
32	s	614	CLA	CMD-C2D	-2.20	1.46	1.50
32	C	507	CLA	C4B-CHC	-2.20	1.34	1.41
32	b	616	CLA	CMD-C2D	-2.20	1.46	1.50
32	Y	614	CLA	C3B-CAB	-2.20	1.43	1.47
32	y	614	CLA	C3B-CAB	-2.20	1.43	1.47
32	A	407	CLA	C4B-CHC	-2.20	1.34	1.41
32	s	614	CLA	C3B-C2B	-2.20	1.37	1.40
32	C	503	CLA	CMD-C2D	-2.20	1.46	1.50
32	C	509	CLA	MG-ND	-2.20	2.01	2.05
43	s	606	CHL	C4B-CHC	2.20	1.47	1.41
32	R	602	CLA	C3B-C2B	-2.20	1.37	1.40
32	y	603	CLA	MG-ND	-2.20	2.01	2.05
43	Y	601	CHL	C3D-C2D	2.20	1.45	1.39
43	y	606	CHL	C2C-C1C	2.20	1.49	1.44
32	B	616	CLA	C4B-CHC	-2.20	1.34	1.41
32	b	616	CLA	C4B-CHC	-2.20	1.34	1.41
32	B	606	CLA	CMD-C2D	-2.19	1.46	1.50
32	S	613	CLA	CMC-C2C	-2.19	1.46	1.50
40	d	405	PL9	C16-C14	-2.19	1.46	1.51
32	D	402	CLA	MG-ND	-2.19	2.01	2.05
32	S	612	CLA	CMC-C2C	-2.19	1.46	1.50
43	G	606	CHL	C1B-CHB	2.19	1.47	1.41
43	g	606	CHL	C1B-CHB	2.19	1.47	1.41
32	n	611	CLA	C3B-C2B	-2.19	1.37	1.40
32	G	610	CLA	CMC-C2C	-2.19	1.46	1.50
32	g	610	CLA	CMC-C2C	-2.19	1.46	1.50
33	a	408	PHO	CMB-C2B	-2.19	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	N	601	CHL	MG-NA	-2.19	2.01	2.06
32	c	505	CLA	C4B-CHC	-2.19	1.34	1.41
33	A	408	PHO	CMB-C2B	-2.19	1.46	1.51
32	N	604	CLA	MG-ND	-2.19	2.01	2.05
32	n	604	CLA	MG-ND	-2.19	2.01	2.05
43	G	607	CHL	C4B-CHC	2.19	1.47	1.41
43	g	605	CHL	C4C-C3C	2.19	1.48	1.45
33	a	408	PHO	C1C-NC	-2.19	1.31	1.38
44	y	1620	LUT	C30-C29	-2.19	1.32	1.35
32	g	603	CLA	CMD-C2D	-2.19	1.46	1.50
32	D	403	CLA	CMD-C2D	-2.18	1.46	1.50
32	b	608	CLA	CMD-C2D	-2.18	1.46	1.50
32	A	406	CLA	CAC-C3C	-2.18	1.45	1.51
32	a	406	CLA	CAC-C3C	-2.18	1.45	1.51
32	N	614	CLA	C3B-C2B	-2.18	1.37	1.40
32	N	604	CLA	C3B-CAB	-2.18	1.43	1.47
32	n	604	CLA	C3B-CAB	-2.18	1.43	1.47
32	Y	602	CLA	CMD-C2D	-2.18	1.46	1.50
32	y	612	CLA	CMC-C2C	-2.18	1.46	1.50
43	y	601	CHL	C1C-NC	-2.18	1.34	1.37
32	c	507	CLA	C4B-CHC	-2.18	1.34	1.41
32	S	614	CLA	C3B-C2B	-2.18	1.37	1.40
32	c	509	CLA	MG-ND	-2.18	2.01	2.05
43	y	601	CHL	C3D-C2D	2.18	1.45	1.39
32	Y	610	CLA	CMD-C2D	-2.17	1.46	1.50
43	r	608	CHL	C4B-CHC	2.17	1.47	1.41
32	R	609	CLA	CMD-C2D	-2.17	1.46	1.50
43	n	601	CHL	MG-NA	-2.17	2.01	2.06
32	c	503	CLA	C3B-C2B	-2.17	1.37	1.40
32	R	604	CLA	CMD-C2D	-2.17	1.46	1.50
32	A	406	CLA	CMD-C2D	-2.17	1.46	1.50
32	B	617	CLA	CMD-C2D	-2.17	1.46	1.50
32	a	406	CLA	CMD-C2D	-2.17	1.46	1.50
32	b	614	CLA	CMC-C2C	-2.17	1.46	1.50
32	b	617	CLA	CMD-C2D	-2.17	1.46	1.50
32	r	604	CLA	CMD-C2D	-2.17	1.46	1.50
32	g	612	CLA	C3B-C2B	-2.17	1.37	1.40
32	C	505	CLA	C4B-CHC	-2.17	1.35	1.41
43	g	609	CHL	C4B-CHC	2.17	1.47	1.41
32	S	612	CLA	CMD-C2D	-2.17	1.46	1.50
43	g	607	CHL	C4B-CHC	2.17	1.47	1.41
32	d	402	CLA	MG-ND	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	612	CLA	CMD-C2D	-2.17	1.46	1.50
32	S	604	CLA	C3B-C2B	-2.17	1.37	1.40
43	G	609	CHL	C4B-CHC	2.17	1.47	1.41
43	S	601	CHL	MG-NA	-2.17	2.01	2.06
43	s	601	CHL	MG-NA	-2.17	2.01	2.06
32	n	602	CLA	CMD-C2D	-2.17	1.46	1.50
32	n	614	CLA	CMD-C2D	-2.17	1.46	1.50
43	n	608	CHL	C4B-CHC	2.17	1.47	1.41
32	g	610	CLA	CMD-C2D	-2.16	1.46	1.50
43	Y	606	CHL	C2C-C1C	2.16	1.49	1.44
32	B	614	CLA	CMC-C2C	-2.16	1.46	1.50
32	b	617	CLA	C4B-CHC	-2.16	1.35	1.41
32	B	602	CLA	CMD-C2D	-2.16	1.46	1.50
32	B	605	CLA	C3B-C2B	-2.16	1.37	1.40
32	B	612	CLA	CMD-C2D	-2.16	1.46	1.50
32	B	606	CLA	C3B-C2B	-2.16	1.37	1.40
43	N	608	CHL	C4B-CHC	2.16	1.47	1.41
32	B	610	CLA	CMD-C2D	-2.16	1.46	1.50
43	R	607	CHL	C4C-C3C	2.16	1.48	1.45
32	C	507	CLA	C3B-CAB	-2.15	1.43	1.47
32	b	611	CLA	CMD-C2D	-2.15	1.46	1.50
32	s	609	CLA	C3B-C2B	-2.15	1.37	1.40
32	A	410	CLA	MG-ND	-2.15	2.01	2.05
32	S	604	CLA	CMD-C2D	-2.15	1.46	1.50
43	S	601	CHL	C4C-C3C	2.15	1.48	1.45
43	s	601	CHL	C4C-C3C	2.15	1.48	1.45
43	G	609	CHL	C1D-C2D	2.15	1.49	1.45
43	g	609	CHL	C1D-C2D	2.15	1.49	1.45
32	n	604	CLA	CMD-C2D	-2.15	1.46	1.50
32	g	611	CLA	C3B-C2B	-2.15	1.37	1.40
32	B	606	CLA	CMC-C2C	-2.15	1.46	1.50
32	b	606	CLA	CMC-C2C	-2.15	1.46	1.50
43	G	609	CHL	C3D-C2D	2.15	1.45	1.39
43	R	608	CHL	C4B-CHC	2.15	1.47	1.41
32	G	602	CLA	CMC-C2C	-2.15	1.46	1.50
32	S	602	CLA	CMC-C2C	-2.15	1.46	1.50
32	b	602	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	512	CLA	CMC-C2C	-2.15	1.46	1.50
32	S	609	CLA	CMD-C2D	-2.15	1.46	1.50
32	s	609	CLA	CMD-C2D	-2.15	1.46	1.50
32	C	503	CLA	C3B-C2B	-2.15	1.37	1.40
43	N	608	CHL	C1D-C2D	2.15	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	g	609	CHL	C3D-C2D	2.14	1.45	1.39
43	n	607	CHL	C4B-NB	-2.14	1.33	1.35
32	a	410	CLA	MG-ND	-2.14	2.01	2.05
32	B	617	CLA	C4B-CHC	-2.14	1.35	1.41
32	G	610	CLA	C4B-CHC	-2.14	1.35	1.41
32	g	610	CLA	C4B-CHC	-2.14	1.35	1.41
32	G	610	CLA	CMD-C2D	-2.14	1.46	1.50
32	b	612	CLA	CMD-C2D	-2.14	1.46	1.50
32	N	613	CLA	C3B-C2B	-2.14	1.37	1.40
32	y	611	CLA	MG-ND	-2.14	2.01	2.05
32	y	610	CLA	CMD-C2D	-2.14	1.46	1.50
32	N	614	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	501	CLA	C3B-CAB	-2.14	1.43	1.47
32	B	604	CLA	CMC-C2C	-2.14	1.46	1.50
32	C	512	CLA	CMC-C2C	-2.13	1.46	1.50
43	s	601	CHL	C3D-C2D	2.13	1.44	1.39
32	C	501	CLA	CMC-C2C	-2.13	1.46	1.50
32	g	602	CLA	CMC-C2C	-2.13	1.46	1.50
33	a	409	PHO	C1C-NC	-2.13	1.31	1.38
32	r	609	CLA	CMD-C2D	-2.13	1.46	1.50
32	s	602	CLA	CMC-C2C	-2.13	1.46	1.50
32	C	501	CLA	C3B-CAB	-2.13	1.43	1.47
43	G	605	CHL	C4C-C3C	2.13	1.48	1.45
32	y	613	CLA	MG-ND	-2.13	2.01	2.05
32	B	616	CLA	CMC-C2C	-2.13	1.46	1.50
43	Y	607	CHL	C1D-ND	-2.13	1.35	1.37
43	y	607	CHL	C1D-ND	-2.13	1.35	1.37
32	b	610	CLA	CMD-C2D	-2.13	1.46	1.50
43	N	607	CHL	C4B-NB	-2.13	1.33	1.35
43	S	601	CHL	C3D-C2D	2.13	1.44	1.39
32	S	609	CLA	C3B-C2B	-2.12	1.37	1.40
32	b	606	CLA	C3B-C2B	-2.12	1.37	1.40
32	y	612	CLA	C3B-C2B	-2.12	1.37	1.40
32	S	613	CLA	C4B-CHC	-2.12	1.35	1.41
32	G	612	CLA	CMD-C2D	-2.12	1.46	1.50
32	y	613	CLA	CMC-C2C	-2.12	1.46	1.50
32	s	604	CLA	C3B-C2B	-2.12	1.37	1.40
32	S	612	CLA	C4B-CHC	-2.12	1.35	1.41
32	G	602	CLA	CMD-C2D	-2.12	1.46	1.50
44	Y	1620	LUT	C30-C29	-2.12	1.33	1.35
32	Y	603	CLA	C3B-CAB	-2.12	1.43	1.47
32	S	614	CLA	CMC-C2C	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	614	CLA	CMC-C2C	-2.12	1.46	1.50
33	A	409	PHO	C1C-NC	-2.12	1.32	1.38
32	B	615	CLA	CMC-C2C	-2.12	1.46	1.50
43	r	608	CHL	C4C-C3C	2.12	1.48	1.45
32	N	604	CLA	CMD-C2D	-2.12	1.46	1.50
32	b	604	CLA	CMC-C2C	-2.12	1.46	1.50
43	R	608	CHL	C4C-C3C	2.12	1.48	1.45
43	r	607	CHL	C4C-C3C	2.12	1.48	1.45
32	N	610	CLA	CMD-C2D	-2.12	1.46	1.50
32	Y	613	CLA	CMC-C2C	-2.12	1.46	1.50
32	n	610	CLA	CMD-C2D	-2.12	1.46	1.50
43	n	608	CHL	C1D-C2D	2.11	1.49	1.45
32	b	609	CLA	CMC-C2C	-2.11	1.46	1.50
43	G	608	CHL	C4C-C3C	2.11	1.48	1.45
43	S	608	CHL	C1B-CHB	2.11	1.46	1.41
43	N	601	CHL	C4C-C3C	2.11	1.48	1.45
43	S	606	CHL	C1B-CHB	2.11	1.46	1.41
32	S	612	CLA	MG-ND	-2.11	2.01	2.05
40	d	405	PL9	C26-C24	-2.11	1.46	1.51
43	N	605	CHL	C1D-C2D	2.11	1.49	1.45
43	n	605	CHL	C1D-C2D	2.11	1.49	1.45
32	B	611	CLA	CMD-C2D	-2.11	1.46	1.50
32	b	615	CLA	CMC-C2C	-2.11	1.46	1.50
32	s	612	CLA	MG-ND	-2.11	2.01	2.05
43	g	608	CHL	C4C-C3C	2.11	1.48	1.45
32	s	604	CLA	CMD-C2D	-2.11	1.46	1.50
32	r	610	CLA	CMC-C2C	-2.11	1.46	1.50
32	S	611	CLA	CMC-C2C	-2.11	1.46	1.50
32	s	611	CLA	CMC-C2C	-2.11	1.46	1.50
32	s	613	CLA	C4B-CHC	-2.11	1.35	1.41
32	G	614	CLA	C3B-C2B	-2.11	1.37	1.40
32	b	605	CLA	C3B-C2B	-2.11	1.37	1.40
32	B	603	CLA	CMC-C2C	-2.10	1.46	1.50
32	n	613	CLA	C3B-C2B	-2.10	1.37	1.40
32	C	503	CLA	CMC-C2C	-2.10	1.46	1.50
46	G	1623	NEX	C1-C6	-2.10	1.51	1.54
44	Y	1620	LUT	C14-C13	-2.10	1.33	1.35
45	n	1622	XAT	O4-C5	-2.10	1.43	1.46
43	Y	608	CHL	C4B-CHC	2.10	1.46	1.41
32	b	616	CLA	CMC-C2C	-2.10	1.46	1.50
32	y	603	CLA	C3B-CAB	-2.10	1.43	1.47
43	Y	606	CHL	MG-ND	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	603	CLA	CMC-C2C	-2.10	1.46	1.50
38	D	409	LHG	O7-C5	-2.10	1.41	1.46
43	Y	608	CHL	C1B-CHB	2.10	1.46	1.41
43	Y	605	CHL	C4C-C3C	2.10	1.48	1.45
43	y	605	CHL	C4C-C3C	2.10	1.48	1.45
32	c	501	CLA	CMC-C2C	-2.10	1.46	1.50
43	g	601	CHL	C1D-C2D	2.10	1.49	1.45
32	G	613	CLA	MG-NC	2.10	2.11	2.06
32	C	506	CLA	C4B-CHC	-2.09	1.35	1.41
32	c	507	CLA	C3B-CAB	-2.09	1.43	1.47
32	c	506	CLA	C4B-CHC	-2.09	1.35	1.41
32	B	613	CLA	MG-ND	-2.09	2.01	2.05
32	N	612	CLA	CMD-C2D	-2.09	1.46	1.50
32	b	604	CLA	C3B-CAB	-2.09	1.43	1.47
32	s	612	CLA	C4B-CHC	-2.09	1.35	1.41
32	B	602	CLA	CMC-C2C	-2.09	1.46	1.50
32	B	609	CLA	CMC-C2C	-2.09	1.46	1.50
32	B	615	CLA	C3B-C2B	-2.09	1.37	1.40
43	y	608	CHL	C1B-CHB	2.09	1.46	1.41
32	c	513	CLA	CMC-C2C	-2.09	1.46	1.50
43	Y	606	CHL	C1B-NB	-2.09	1.33	1.35
43	y	606	CHL	C1B-NB	-2.09	1.33	1.35
43	r	608	CHL	C2C-C1C	2.09	1.49	1.44
32	g	613	CLA	MG-NC	2.09	2.11	2.06
43	Y	607	CHL	C1B-NB	-2.09	1.33	1.35
43	y	607	CHL	C1B-NB	-2.09	1.33	1.35
32	Y	604	CLA	CMC-C2C	-2.09	1.46	1.50
32	y	604	CLA	CMC-C2C	-2.09	1.46	1.50
43	s	606	CHL	C1B-CHB	2.09	1.46	1.41
32	S	604	CLA	C4B-CHC	-2.09	1.35	1.41
43	n	601	CHL	C4C-C3C	2.09	1.48	1.45
32	Y	611	CLA	MG-ND	-2.09	2.01	2.05
32	A	406	CLA	CMC-C2C	-2.08	1.46	1.50
32	G	612	CLA	C3B-C2B	-2.08	1.37	1.40
32	C	513	CLA	CMC-C2C	-2.08	1.46	1.50
44	n	1620	LUT	C22-C21	-2.08	1.52	1.54
44	N	1620	LUT	C22-C21	-2.08	1.52	1.54
32	R	603	CLA	CMD-C2D	-2.08	1.46	1.50
43	R	608	CHL	C2C-C1C	2.08	1.49	1.44
44	y	1620	LUT	C14-C13	-2.08	1.33	1.35
32	c	506	CLA	MG-ND	-2.08	2.01	2.05
32	C	511	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	511	CLA	CMC-C2C	-2.08	1.46	1.50
32	B	610	CLA	C4B-CHC	-2.08	1.35	1.41
32	Y	613	CLA	MG-ND	-2.08	2.01	2.05
32	C	504	CLA	C4B-CHC	-2.08	1.35	1.41
32	R	602	CLA	CMC-C2C	-2.07	1.46	1.50
32	y	613	CLA	C4B-CHC	-2.07	1.35	1.41
40	D	405	PL9	C26-C24	-2.07	1.47	1.51
43	s	608	CHL	C1B-CHB	2.07	1.46	1.41
38	d	409	LHG	O7-C5	-2.07	1.41	1.46
32	r	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	a	406	CLA	CMC-C2C	-2.07	1.46	1.50
32	g	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	G	611	CLA	C3B-C2B	-2.07	1.37	1.40
32	b	602	CLA	CMC-C2C	-2.07	1.46	1.50
32	c	503	CLA	CMC-C2C	-2.07	1.46	1.50
32	g	602	CLA	C3B-C2B	-2.07	1.37	1.40
32	C	502	CLA	MG-ND	-2.07	2.01	2.05
32	c	502	CLA	MG-ND	-2.07	2.01	2.05
32	y	603	CLA	CMC-C2C	-2.07	1.46	1.50
46	Y	1623	NEX	O24-C25	-2.07	1.43	1.46
43	N	605	CHL	C1D-ND	-2.07	1.35	1.37
43	n	605	CHL	C1D-ND	-2.07	1.35	1.37
32	G	603	CLA	MG-ND	-2.07	2.01	2.05
32	A	410	CLA	C3B-CAB	-2.06	1.43	1.47
32	g	603	CLA	MG-ND	-2.06	2.01	2.05
32	g	613	CLA	C4B-CHC	-2.06	1.35	1.41
32	Y	613	CLA	C4B-CHC	-2.06	1.35	1.41
44	s	1620	LUT	C22-C21	-2.06	1.52	1.54
32	b	610	CLA	C4B-CHC	-2.06	1.35	1.41
32	s	604	CLA	C4B-CHC	-2.06	1.35	1.41
43	G	607	CHL	C2C-C1C	2.06	1.49	1.44
45	N	1622	XAT	O4-C5	-2.06	1.43	1.46
43	y	609	CHL	C1D-ND	-2.06	1.35	1.37
32	n	612	CLA	CMD-C2D	-2.06	1.46	1.50
44	Y	1620	LUT	C34-C33	-2.06	1.33	1.35
32	n	611	CLA	CMC-C2C	-2.06	1.46	1.50
43	r	607	CHL	C4D-CHA	2.05	1.45	1.38
32	C	509	CLA	C3B-C2B	-2.05	1.37	1.40
32	y	610	CLA	C3B-CAB	-2.05	1.43	1.47
43	R	607	CHL	C1B-CHB	2.05	1.46	1.41
32	N	603	CLA	CAC-C3C	-2.05	1.45	1.51
32	n	603	CLA	CAC-C3C	-2.05	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	605	CLA	C3B-CAB	-2.05	1.43	1.47
32	b	605	CLA	C3B-CAB	-2.05	1.43	1.47
43	g	608	CHL	C1B-CHB	2.05	1.46	1.41
43	y	608	CHL	C4B-CHC	2.05	1.46	1.41
32	g	614	CLA	C3B-C2B	-2.05	1.37	1.40
32	g	613	CLA	C3B-C2B	-2.05	1.37	1.40
43	y	606	CHL	MG-ND	-2.05	2.01	2.05
43	y	605	CHL	C1B-CHB	2.05	1.46	1.41
43	G	608	CHL	C1B-CHB	2.05	1.46	1.41
44	Y	1621	LUT	C22-C21	-2.05	1.52	1.54
44	y	1621	LUT	C22-C21	-2.05	1.52	1.54
32	a	405	CLA	CMA-C3A	-2.05	1.48	1.53
32	c	504	CLA	CAC-C3C	-2.05	1.45	1.51
32	B	607	CLA	C4B-CHC	-2.05	1.35	1.41
32	b	607	CLA	C4B-CHC	-2.05	1.35	1.41
43	n	605	CHL	C1B-CHB	2.05	1.46	1.41
32	b	613	CLA	MG-ND	-2.05	2.01	2.05
32	d	403	CLA	C3B-CAB	-2.05	1.43	1.47
32	B	604	CLA	C3B-CAB	-2.05	1.43	1.47
32	G	613	CLA	C3B-C2B	-2.04	1.37	1.40
32	B	614	CLA	MG-ND	-2.04	2.01	2.05
32	Y	610	CLA	C3B-CAB	-2.04	1.43	1.47
32	c	504	CLA	C4B-CHC	-2.04	1.35	1.41
32	A	406	CLA	C3B-C2B	-2.04	1.37	1.40
43	g	609	CHL	C1C-NC	-2.04	1.34	1.37
43	R	606	CHL	C1B-CHB	2.04	1.46	1.41
32	Y	613	CLA	C3B-C2B	-2.04	1.37	1.40
32	y	613	CLA	C3B-C2B	-2.04	1.37	1.40
45	r	624	XAT	O4-C5	-2.04	1.43	1.46
32	b	614	CLA	MG-ND	-2.04	2.01	2.05
32	s	603	CLA	MG-ND	-2.04	2.01	2.05
32	G	613	CLA	C4B-CHC	-2.04	1.35	1.41
32	D	403	CLA	C3B-CAB	-2.04	1.43	1.47
43	Y	609	CHL	C1D-ND	-2.04	1.35	1.37
32	C	512	CLA	MG-ND	-2.04	2.01	2.05
32	N	611	CLA	CMC-C2C	-2.04	1.46	1.50
43	R	607	CHL	C4D-CHA	2.04	1.45	1.38
32	C	513	CLA	MG-ND	-2.04	2.01	2.05
32	c	513	CLA	C4B-CHC	-2.04	1.35	1.41
43	r	607	CHL	C1B-CHB	2.04	1.46	1.41
40	d	405	PL9	C5-C4	-2.04	1.39	1.47
32	b	615	CLA	C3B-C2B	-2.04	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	502	CLA	CAC-C3C	-2.04	1.45	1.51
46	r	625	NEX	C1-C6	-2.04	1.51	1.54
32	C	506	CLA	MG-ND	-2.04	2.01	2.05
32	A	410	CLA	CMC-C2C	-2.04	1.46	1.50
32	A	405	CLA	CMA-C3A	-2.03	1.48	1.53
32	Y	603	CLA	CMC-C2C	-2.03	1.46	1.50
43	G	601	CHL	C3D-C2D	2.03	1.44	1.39
46	y	1623	NEX	O24-C25	-2.03	1.43	1.46
32	c	513	CLA	MG-ND	-2.03	2.01	2.05
43	N	605	CHL	C1B-CHB	2.03	1.46	1.41
32	Y	612	CLA	MG-ND	-2.03	2.01	2.05
32	C	505	CLA	C3B-C2B	-2.03	1.37	1.40
32	c	505	CLA	C3B-C2B	-2.03	1.37	1.40
32	R	603	CLA	MG-ND	-2.03	2.01	2.05
32	S	603	CLA	C3B-C2B	-2.03	1.37	1.40
32	C	513	CLA	C4B-CHC	-2.03	1.35	1.41
43	r	606	CHL	C1B-CHB	2.03	1.46	1.41
32	G	604	CLA	C3B-C2B	-2.03	1.37	1.40
32	g	604	CLA	C3B-C2B	-2.03	1.37	1.40
32	N	612	CLA	CMC-C2C	-2.03	1.46	1.50
32	S	603	CLA	CMD-C2D	-2.03	1.46	1.50
32	g	613	CLA	CMC-C2C	-2.03	1.46	1.50
32	R	610	CLA	CMC-C2C	-2.03	1.46	1.50
40	D	405	PL9	C5-C4	-2.03	1.40	1.47
44	S	1620	LUT	C22-C21	-2.03	1.52	1.54
32	a	406	CLA	C3B-CAB	-2.03	1.43	1.47
32	r	604	CLA	CMC-C2C	-2.03	1.46	1.50
32	s	603	CLA	CMD-C2D	-2.03	1.46	1.50
32	b	608	CLA	C4B-CHC	-2.03	1.35	1.41
45	Y	1622	XAT	O4-C5	-2.02	1.43	1.46
32	B	608	CLA	C4B-CHC	-2.02	1.35	1.41
43	s	601	CHL	C4B-CHC	2.02	1.46	1.41
32	r	602	CLA	CMC-C2C	-2.02	1.46	1.50
32	C	510	CLA	C4B-CHC	-2.02	1.35	1.41
32	G	604	CLA	CMC-C2C	-2.02	1.46	1.50
32	G	613	CLA	CMC-C2C	-2.02	1.46	1.50
43	S	601	CHL	C4B-CHC	2.02	1.46	1.41
32	C	504	CLA	CAC-C3C	-2.02	1.45	1.51
43	G	601	CHL	C1D-C2D	2.02	1.49	1.45
32	r	603	CLA	MG-ND	-2.02	2.01	2.05
32	c	502	CLA	CAC-C3C	-2.02	1.45	1.51
43	N	606	CHL	C1B-CHB	2.02	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	N	606	CHL	C1D-ND	-2.02	1.35	1.37
43	n	606	CHL	C1D-ND	-2.02	1.35	1.37
32	G	603	CLA	C4B-CHC	-2.02	1.35	1.41
43	G	605	CHL	C2C-C1C	2.02	1.48	1.44
43	n	609	CHL	C4B-NB	-2.02	1.33	1.35
32	a	410	CLA	CMC-C2C	-2.02	1.46	1.50
40	D	405	PL9	C36-C34	-2.02	1.47	1.51
32	N	603	CLA	MG-ND	-2.02	2.01	2.05
32	C	511	CLA	C4B-CHC	-2.02	1.35	1.41
32	C	512	CLA	C4B-CHC	-2.01	1.35	1.41
45	y	1622	XAT	O4-C5	-2.01	1.43	1.46
32	S	603	CLA	MG-ND	-2.01	2.01	2.05
45	R	624	XAT	O4-C5	-2.01	1.43	1.46
44	y	1620	LUT	C10-C9	-2.01	1.33	1.35
41	f	101	HEM	CMB-C2B	2.01	1.55	1.50
32	c	510	CLA	C4B-CHC	-2.01	1.35	1.41
46	s	1623	NEX	O24-C25	-2.01	1.43	1.46
32	N	613	CLA	C3B-CAB	-2.01	1.43	1.47
43	g	605	CHL	C2C-C1C	2.01	1.48	1.44
43	g	607	CHL	C2C-C1C	2.01	1.48	1.44
32	G	612	CLA	CMC-C2C	-2.01	1.46	1.50
41	F	101	HEM	CMB-C2B	2.01	1.55	1.50
32	c	511	CLA	C4B-CHC	-2.01	1.35	1.41
32	C	510	CLA	MG-ND	-2.01	2.01	2.05
32	g	613	CLA	MG-ND	-2.01	2.01	2.05
32	Y	604	CLA	MG-ND	-2.01	2.01	2.05
32	c	512	CLA	C4B-CHC	-2.01	1.35	1.41
46	n	1623	NEX	O24-C25	-2.01	1.43	1.46
43	Y	605	CHL	C1B-CHB	2.01	1.46	1.41
32	c	509	CLA	C3B-C2B	-2.01	1.37	1.40
32	Y	612	CLA	C4B-CHC	-2.01	1.35	1.41
32	y	612	CLA	C4B-CHC	-2.01	1.35	1.41
43	g	608	CHL	C4B-CHC	2.01	1.46	1.41
32	d	403	CLA	CMC-C2C	-2.01	1.46	1.50
43	g	601	CHL	C1D-ND	-2.01	1.35	1.37
32	y	611	CLA	C4B-CHC	-2.00	1.35	1.41
32	S	603	CLA	C4B-CHC	-2.00	1.35	1.41
45	r	624	XAT	O24-C25	-2.00	1.43	1.46

All (3324) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	412	SQD	O9-S-C6	-20.28	82.84	106.94
35	a	412	SQD	O9-S-C6	-20.18	82.95	106.94
45	y	1622	XAT	C37-C21-C36	-17.09	82.16	107.37
45	Y	1622	XAT	C37-C21-C36	-17.08	82.17	107.37
45	y	1622	XAT	C37-C21-C22	-15.00	82.91	108.98
45	Y	1622	XAT	C37-C21-C22	-15.00	82.93	108.98
35	A	412	SQD	O8-S-O9	-12.13	81.63	111.27
35	a	412	SQD	O8-S-O9	-12.05	81.82	111.27
43	s	601	CHL	CMD-C2D-C1D	9.74	141.89	124.71
43	S	601	CHL	CMD-C2D-C1D	9.73	141.87	124.71
46	G	1623	NEX	O24-C25-C24	9.44	120.47	113.38
46	g	1623	NEX	O24-C25-C24	9.42	120.46	113.38
43	n	601	CHL	CMD-C2D-C1D	9.32	141.14	124.71
43	N	601	CHL	CMD-C2D-C1D	9.31	141.12	124.71
46	n	1623	NEX	O24-C25-C24	9.30	120.37	113.38
46	N	1623	NEX	O24-C25-C24	9.29	120.36	113.38
43	n	607	CHL	C2C-C3C-C4C	-9.26	99.89	106.49
35	a	412	SQD	O7-S-C6	9.20	117.88	106.94
43	N	607	CHL	C2C-C3C-C4C	-9.17	99.95	106.49
46	S	1623	NEX	O24-C25-C24	9.09	120.21	113.38
46	s	1623	NEX	O24-C25-C24	9.09	120.21	113.38
46	Y	1623	NEX	O24-C25-C24	9.08	120.20	113.38
43	g	601	CHL	CMD-C2D-C1D	9.02	140.61	124.71
43	g	608	CHL	CMD-C2D-C1D	9.01	140.59	124.71
43	G	608	CHL	CMD-C2D-C1D	9.00	140.57	124.71
46	r	625	NEX	O24-C25-C24	8.99	120.14	113.38
46	R	625	NEX	O24-C25-C24	8.98	120.13	113.38
46	y	1623	NEX	O24-C25-C24	8.97	120.12	113.38
43	G	605	CHL	CMD-C2D-C1D	8.92	140.43	124.71
43	g	605	CHL	CMD-C2D-C1D	8.92	140.43	124.71
35	A	412	SQD	O7-S-C6	8.90	117.52	106.94
43	N	609	CHL	CMD-C2D-C1D	8.88	140.37	124.71
43	n	609	CHL	CMD-C2D-C1D	8.87	140.35	124.71
43	y	608	CHL	CMD-C2D-C1D	8.86	140.33	124.71
43	Y	608	CHL	CMD-C2D-C1D	8.84	140.30	124.71
35	a	412	SQD	O9-S-O7	-8.77	83.61	113.95
43	Y	608	CHL	C1D-ND-C4D	-8.69	100.16	106.33
43	y	607	CHL	C2C-C3C-C4C	-8.69	100.30	106.49
35	A	412	SQD	O9-S-O7	-8.67	83.95	113.95
32	G	613	CLA	C4A-NA-C1A	8.67	110.60	106.71
32	g	613	CLA	C4A-NA-C1A	8.67	110.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	y	608	CHL	C1D-ND-C4D	-8.66	100.19	106.33
43	g	609	CHL	C2C-C3C-C4C	-8.63	100.33	106.49
43	Y	607	CHL	C2C-C3C-C4C	-8.63	100.34	106.49
43	R	608	CHL	CMD-C2D-C1D	8.63	139.92	124.71
43	r	608	CHL	CMD-C2D-C1D	8.60	139.86	124.71
43	G	609	CHL	C2C-C3C-C4C	-8.59	100.36	106.49
43	G	601	CHL	CMD-C2D-C1D	8.59	139.85	124.71
45	Y	1622	XAT	O24-C25-C24	8.52	119.78	113.38
43	n	608	CHL	C2C-C3C-C4C	-8.48	100.44	106.49
43	N	608	CHL	C2C-C3C-C4C	-8.44	100.47	106.49
43	R	606	CHL	C1D-ND-C4D	-8.44	100.34	106.33
45	y	1622	XAT	O24-C25-C24	8.44	119.72	113.38
43	n	608	CHL	C1D-ND-C4D	-8.43	100.34	106.33
43	r	606	CHL	C1D-ND-C4D	-8.43	100.34	106.33
43	N	608	CHL	C1D-ND-C4D	-8.40	100.37	106.33
43	G	601	CHL	C1D-ND-C4D	-8.39	100.37	106.33
43	s	606	CHL	C1D-ND-C4D	-8.37	100.39	106.33
43	S	606	CHL	C1D-ND-C4D	-8.37	100.39	106.33
43	y	605	CHL	CMD-C2D-C1D	8.35	139.43	124.71
43	S	608	CHL	CMD-C2D-C1D	8.35	139.43	124.71
43	N	605	CHL	CMD-C2D-C1D	8.35	139.42	124.71
43	n	605	CHL	CMD-C2D-C1D	8.35	139.42	124.71
43	n	605	CHL	C2C-C3C-C4C	-8.35	100.54	106.49
43	g	609	CHL	CMD-C2D-C1D	8.33	139.40	124.71
43	Y	605	CHL	CMD-C2D-C1D	8.33	139.40	124.71
43	s	608	CHL	CMD-C2D-C1D	8.33	139.40	124.71
43	g	606	CHL	C1D-ND-C4D	-8.31	100.43	106.33
43	G	609	CHL	CMD-C2D-C1D	8.30	139.34	124.71
43	n	608	CHL	CMD-C2D-C1D	8.29	139.33	124.71
43	N	605	CHL	C2C-C3C-C4C	-8.29	100.58	106.49
43	N	606	CHL	C1D-ND-C4D	-8.28	100.45	106.33
43	S	608	CHL	C1D-ND-C4D	-8.28	100.45	106.33
43	n	606	CHL	C1D-ND-C4D	-8.28	100.45	106.33
43	g	607	CHL	CMD-C2D-C1D	8.28	139.30	124.71
43	g	601	CHL	C1D-ND-C4D	-8.28	100.46	106.33
43	N	608	CHL	CMD-C2D-C1D	8.27	139.29	124.71
43	G	607	CHL	CMD-C2D-C1D	8.27	139.28	124.71
43	G	606	CHL	C1D-ND-C4D	-8.25	100.47	106.33
43	Y	609	CHL	C1D-ND-C4D	-8.23	100.49	106.33
43	R	607	CHL	CMD-C2D-C1D	8.19	139.15	124.71
43	s	608	CHL	C1D-ND-C4D	-8.19	100.52	106.33
43	y	609	CHL	C1D-ND-C4D	-8.17	100.53	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	607	CHL	CMD-C2D-C1D	8.16	139.09	124.71
43	G	606	CHL	C2C-C3C-C4C	-8.16	100.67	106.49
43	n	607	CHL	CMD-C2D-C1D	8.15	139.07	124.71
43	g	608	CHL	C1D-ND-C4D	-8.13	100.56	106.33
43	N	607	CHL	CMD-C2D-C1D	8.13	139.03	124.71
43	G	608	CHL	C1D-ND-C4D	-8.10	100.58	106.33
45	Y	1622	XAT	C36-C21-C22	8.09	123.04	108.98
43	g	606	CHL	C2C-C3C-C4C	-8.09	100.72	106.49
43	N	605	CHL	C1D-ND-C4D	-8.09	100.59	106.33
43	n	605	CHL	C1D-ND-C4D	-8.09	100.59	106.33
45	y	1622	XAT	C36-C21-C22	8.08	123.03	108.98
32	C	502	CLA	C4A-NA-C1A	8.08	110.34	106.71
43	g	609	CHL	C1D-ND-C4D	-8.08	100.60	106.33
43	s	606	CHL	CMD-C2D-C1D	8.07	138.93	124.71
43	G	607	CHL	C1D-ND-C4D	-8.06	100.61	106.33
43	S	606	CHL	CMD-C2D-C1D	8.06	138.92	124.71
43	Y	605	CHL	C2C-C3C-C4C	-8.05	100.75	106.49
43	r	607	CHL	C1D-ND-C4D	-8.04	100.62	106.33
43	y	605	CHL	C2C-C3C-C4C	-8.04	100.76	106.49
32	c	502	CLA	C4A-NA-C1A	8.04	110.32	106.71
43	y	601	CHL	C1D-ND-C4D	-8.03	100.63	106.33
43	Y	601	CHL	C1D-ND-C4D	-8.02	100.64	106.33
43	G	609	CHL	C1D-ND-C4D	-8.01	100.65	106.33
43	g	607	CHL	C1D-ND-C4D	-8.00	100.65	106.33
43	s	607	CHL	C1D-ND-C4D	-7.99	100.66	106.33
43	y	609	CHL	C2C-C3C-C4C	-7.99	100.79	106.49
43	S	607	CHL	C1D-ND-C4D	-7.98	100.66	106.33
43	R	607	CHL	C1D-ND-C4D	-7.97	100.67	106.33
43	Y	609	CHL	CMD-C2D-C1D	7.96	138.75	124.71
43	y	606	CHL	C2C-C3C-C4C	-7.96	100.82	106.49
43	S	608	CHL	C2C-C3C-C4C	-7.96	100.82	106.49
43	Y	601	CHL	CMD-C2D-C1D	7.96	138.74	124.71
43	y	601	CHL	CMD-C2D-C1D	7.96	138.74	124.71
43	y	609	CHL	CMD-C2D-C1D	7.95	138.73	124.71
43	Y	605	CHL	C1D-ND-C4D	-7.94	100.69	106.33
43	Y	608	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
43	y	605	CHL	C1D-ND-C4D	-7.92	100.71	106.33
43	s	608	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
43	Y	609	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
43	Y	606	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
35	A	412	SQD	O8-S-C6	7.89	118.31	105.74
32	B	611	CLA	C4A-NA-C1A	7.89	110.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	611	CLA	C4A-NA-C1A	7.89	110.25	106.71
43	s	607	CHL	C2C-C3C-C4C	-7.88	100.87	106.49
43	g	605	CHL	CHD-C1D-ND	-7.86	117.23	124.45
43	y	608	CHL	C2C-C3C-C4C	-7.86	100.89	106.49
43	s	607	CHL	CMD-C2D-C1D	7.85	138.56	124.71
43	S	607	CHL	C2C-C3C-C4C	-7.85	100.89	106.49
43	R	607	CHL	C2C-C3C-C4C	-7.85	100.90	106.49
43	r	606	CHL	C2C-C3C-C4C	-7.83	100.91	106.49
43	G	605	CHL	CHD-C1D-ND	-7.82	117.26	124.45
43	R	606	CHL	C2C-C3C-C4C	-7.82	100.92	106.49
43	S	607	CHL	CMD-C2D-C1D	7.81	138.48	124.71
43	r	607	CHL	C2C-C3C-C4C	-7.79	100.93	106.49
45	G	1622	XAT	O4-C5-C4	7.76	119.21	113.38
45	g	1622	XAT	O4-C5-C4	7.75	119.21	113.38
43	N	607	CHL	C1D-ND-C4D	-7.75	100.83	106.33
43	n	607	CHL	C1D-ND-C4D	-7.75	100.83	106.33
43	N	606	CHL	C2C-C3C-C4C	-7.73	100.98	106.49
43	Y	609	CHL	C2D-C1D-ND	7.73	115.80	110.10
43	N	609	CHL	C1D-ND-C4D	-7.72	100.85	106.33
43	n	606	CHL	C2C-C3C-C4C	-7.72	100.99	106.49
43	n	609	CHL	C1D-ND-C4D	-7.71	100.86	106.33
43	r	606	CHL	CMD-C2D-C1D	7.71	138.30	124.71
43	n	608	CHL	C2D-C1D-ND	7.70	115.78	110.10
43	R	606	CHL	CMD-C2D-C1D	7.69	138.27	124.71
43	y	609	CHL	C2D-C1D-ND	7.68	115.76	110.10
43	Y	606	CHL	C1D-ND-C4D	-7.67	100.89	106.33
43	g	607	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
35	a	412	SQD	O8-S-C6	7.63	117.90	105.74
43	G	607	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
43	R	608	CHL	C1D-ND-C4D	-7.63	100.92	106.33
43	y	606	CHL	C1D-ND-C4D	-7.63	100.92	106.33
43	y	607	CHL	C1D-ND-C4D	-7.63	100.92	106.33
43	N	608	CHL	C2D-C1D-ND	7.61	115.71	110.10
43	r	608	CHL	C1D-ND-C4D	-7.59	100.94	106.33
43	Y	608	CHL	C2D-C1D-ND	7.59	115.70	110.10
43	Y	607	CHL	C1D-ND-C4D	-7.57	100.95	106.33
43	y	608	CHL	C2D-C1D-ND	7.57	115.68	110.10
43	g	608	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
43	G	608	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
43	N	601	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
32	B	613	CLA	C4A-NA-C1A	7.52	110.09	106.71
32	b	613	CLA	C4A-NA-C1A	7.52	110.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	S	601	CHL	C1D-ND-C4D	-7.49	101.01	106.33
43	s	601	CHL	C1D-ND-C4D	-7.49	101.01	106.33
43	n	601	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
43	N	601	CHL	C1D-ND-C4D	-7.45	101.04	106.33
43	n	601	CHL	C1D-ND-C4D	-7.40	101.08	106.33
43	r	608	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
43	R	608	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
43	N	605	CHL	C2D-C1D-ND	7.38	115.54	110.10
43	n	605	CHL	C2D-C1D-ND	7.38	115.54	110.10
43	r	606	CHL	C2D-C1D-ND	7.30	115.48	110.10
43	N	606	CHL	CMD-C2D-C1D	7.29	137.55	124.71
43	n	606	CHL	CMD-C2D-C1D	7.29	137.55	124.71
43	y	607	CHL	CMD-C2D-C1D	7.28	137.54	124.71
43	S	606	CHL	C2C-C3C-C4C	-7.26	101.32	106.49
43	Y	607	CHL	CMD-C2D-C1D	7.24	137.47	124.71
43	g	605	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
43	R	606	CHL	C2D-C1D-ND	7.21	115.42	110.10
43	G	606	CHL	CMD-C2D-C1D	7.20	137.40	124.71
43	G	605	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
43	Y	606	CHL	CMD-C2D-C1D	7.18	137.37	124.71
43	g	606	CHL	CMD-C2D-C1D	7.18	137.37	124.71
43	y	606	CHL	CMD-C2D-C1D	7.16	137.34	124.71
43	s	606	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
45	N	1622	XAT	O24-C25-C24	7.15	118.75	113.38
45	n	1622	XAT	O24-C25-C24	7.15	118.75	113.38
32	c	510	CLA	C4A-NA-C1A	7.14	109.92	106.71
43	N	609	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
43	n	609	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
43	G	601	CHL	C2D-C1D-ND	7.11	115.34	110.10
43	S	606	CHL	C2D-C1D-ND	7.08	115.32	110.10
32	b	614	CLA	C4A-NA-C1A	7.07	109.89	106.71
43	S	608	CHL	C2D-C1D-ND	7.05	115.30	110.10
43	s	606	CHL	C2D-C1D-ND	7.04	115.29	110.10
32	n	613	CLA	C4A-NA-C1A	7.01	109.86	106.71
43	R	607	CHL	C2D-C1D-ND	7.00	115.26	110.10
43	s	608	CHL	C2D-C1D-ND	6.98	115.25	110.10
43	y	607	CHL	C2D-C1D-ND	6.98	115.25	110.10
32	N	613	CLA	C4A-NA-C1A	6.95	109.83	106.71
43	Y	607	CHL	C2D-C1D-ND	6.94	115.22	110.10
43	g	606	CHL	C2D-C1D-ND	6.93	115.21	110.10
43	r	607	CHL	C2D-C1D-ND	6.93	115.21	110.10
32	B	614	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	510	CLA	C4A-NA-C1A	6.90	109.81	106.71
43	G	607	CHL	C2D-C1D-ND	6.89	115.18	110.10
43	g	607	CHL	C2D-C1D-ND	6.87	115.17	110.10
43	g	601	CHL	C2D-C1D-ND	6.86	115.16	110.10
43	G	606	CHL	C2D-C1D-ND	6.85	115.15	110.10
43	N	606	CHL	C2D-C1D-ND	6.84	115.14	110.10
43	n	606	CHL	C2D-C1D-ND	6.84	115.14	110.10
32	b	602	CLA	C4A-NA-C1A	6.78	109.75	106.71
43	Y	606	CHL	C2D-C1D-ND	6.74	115.07	110.10
43	g	609	CHL	C2D-C1D-ND	6.72	115.06	110.10
43	n	607	CHL	C2D-C1D-ND	6.72	115.06	110.10
32	B	602	CLA	C4A-NA-C1A	6.70	109.72	106.71
43	N	607	CHL	C2D-C1D-ND	6.69	115.03	110.10
43	Y	601	CHL	C2D-C1D-ND	6.67	115.02	110.10
43	y	601	CHL	C2D-C1D-ND	6.65	115.01	110.10
43	y	606	CHL	C2D-C1D-ND	6.65	115.00	110.10
43	G	609	CHL	C2D-C1D-ND	6.64	115.00	110.10
45	y	1622	XAT	O4-C5-C4	6.63	118.37	113.38
43	S	601	CHL	C2C-C3C-C4C	-6.63	101.77	106.49
43	s	601	CHL	C2C-C3C-C4C	-6.63	101.77	106.49
43	S	608	CHL	CHD-C1D-ND	-6.61	118.38	124.45
43	Y	605	CHL	C2D-C1D-ND	6.59	114.96	110.10
43	s	608	CHL	CHD-C1D-ND	-6.58	118.41	124.45
43	y	605	CHL	C2D-C1D-ND	6.58	114.95	110.10
45	Y	1622	XAT	O4-C5-C4	6.57	118.32	113.38
43	s	607	CHL	C2D-C1D-ND	6.57	114.94	110.10
43	g	608	CHL	C2D-C1D-ND	6.56	114.94	110.10
43	G	608	CHL	C2D-C1D-ND	6.55	114.93	110.10
43	N	609	CHL	C2D-C1D-ND	6.55	114.93	110.10
43	Y	608	CHL	CHD-C1D-ND	-6.52	118.46	124.45
43	n	609	CHL	C2D-C1D-ND	6.51	114.90	110.10
43	S	607	CHL	C2D-C1D-ND	6.49	114.89	110.10
43	y	608	CHL	CHD-C1D-ND	-6.49	118.49	124.45
43	N	601	CHL	CHD-C1D-ND	-6.46	118.52	124.45
43	Y	601	CHL	CHD-C1D-ND	-6.45	118.52	124.45
32	A	410	CLA	C4A-NA-C1A	6.43	109.60	106.71
43	y	601	CHL	CHD-C1D-ND	-6.43	118.54	124.45
43	n	601	CHL	CHD-C1D-ND	-6.40	118.57	124.45
32	C	511	CLA	C4A-NA-C1A	6.40	109.58	106.71
32	a	406	CLA	C4A-NA-C1A	6.40	109.58	106.71
32	A	406	CLA	C4A-NA-C1A	6.39	109.58	106.71
32	c	511	CLA	C4A-NA-C1A	6.35	109.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	601	CHL	CHD-C1D-ND	-6.35	118.61	124.45
43	g	605	CHL	C1D-ND-C4D	-6.35	101.82	106.33
43	g	601	CHL	C2C-C3C-C4C	-6.33	101.98	106.49
43	Y	606	CHL	C3C-C4C-NC	6.32	117.66	110.57
43	y	606	CHL	C3C-C4C-NC	6.32	117.66	110.57
32	C	509	CLA	C4A-NA-C1A	6.32	109.55	106.71
43	S	601	CHL	CHD-C1D-ND	-6.30	118.66	124.45
43	N	609	CHL	CHD-C1D-ND	-6.30	118.66	124.45
32	a	410	CLA	C4A-NA-C1A	6.27	109.53	106.71
43	s	601	CHL	CHD-C1D-ND	-6.27	118.69	124.45
43	n	609	CHL	CHD-C1D-ND	-6.26	118.70	124.45
43	G	605	CHL	C1D-ND-C4D	-6.25	101.89	106.33
32	c	505	CLA	C4A-NA-C1A	6.25	109.52	106.71
43	r	608	CHL	C2D-C1D-ND	6.23	114.70	110.10
32	C	504	CLA	C4A-NA-C1A	6.23	109.51	106.71
43	n	605	CHL	CHD-C1D-ND	-6.22	118.74	124.45
32	c	504	CLA	C4A-NA-C1A	6.21	109.50	106.71
43	N	605	CHL	CHD-C1D-ND	-6.21	118.75	124.45
43	R	608	CHL	C2D-C1D-ND	6.21	114.68	110.10
43	S	607	CHL	CHD-C1D-ND	-6.19	118.76	124.45
32	c	509	CLA	C4A-NA-C1A	6.19	109.49	106.71
43	n	607	CHL	C3C-C4C-NC	6.18	117.50	110.57
43	N	607	CHL	C3C-C4C-NC	6.16	117.48	110.57
32	b	616	CLA	C4A-NA-C1A	6.16	109.47	106.71
43	s	607	CHL	CHD-C1D-ND	-6.16	118.79	124.45
43	N	601	CHL	C2D-C1D-ND	6.14	114.63	110.10
43	Y	605	CHL	CHD-C1D-ND	-6.14	118.81	124.45
32	c	508	CLA	C4A-NA-C1A	6.13	109.46	106.71
43	G	601	CHL	CHD-C1D-ND	-6.12	118.83	124.45
43	n	605	CHL	O2D-CGD-CBD	6.11	122.13	111.27
43	N	605	CHL	C3C-C4C-NC	6.11	117.42	110.57
43	n	601	CHL	C2D-C1D-ND	6.11	114.61	110.10
43	S	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
43	s	606	CHL	CHD-C1D-ND	-6.09	118.85	124.45
43	G	606	CHL	C3C-C4C-NC	6.09	117.41	110.57
43	y	605	CHL	CHD-C1D-ND	-6.09	118.86	124.45
43	n	605	CHL	C3C-C4C-NC	6.08	117.39	110.57
43	G	608	CHL	CHD-C1D-ND	-6.08	118.87	124.45
43	N	605	CHL	O2D-CGD-CBD	6.08	122.07	111.27
43	G	601	CHL	C2C-C3C-C4C	-6.06	102.17	106.49
45	R	624	XAT	O4-C5-C18	6.06	122.32	115.06
45	r	624	XAT	O4-C5-C18	6.06	122.32	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	402	CLA	C4A-NA-C1A	6.06	109.43	106.71
45	r	624	XAT	O4-C5-C4	6.05	117.93	113.38
43	g	606	CHL	C3C-C4C-NC	6.05	117.35	110.57
45	G	1622	XAT	C15-C14-C13	-6.04	118.69	127.31
32	B	616	CLA	C4A-NA-C1A	6.02	109.41	106.71
45	g	1622	XAT	C15-C14-C13	-6.02	118.72	127.31
45	n	1622	XAT	O4-C5-C4	6.02	117.90	113.38
45	R	624	XAT	C38-C25-C26	-6.02	112.18	122.26
43	n	606	CHL	C3C-C4C-NC	6.01	117.31	110.57
43	g	608	CHL	CHD-C1D-ND	-6.01	118.93	124.45
43	N	606	CHL	C3C-C4C-NC	6.00	117.30	110.57
45	r	624	XAT	C38-C25-C26	-5.99	112.22	122.26
32	C	505	CLA	C4A-NA-C1A	5.98	109.39	106.71
45	R	624	XAT	O4-C5-C4	5.96	117.86	113.38
45	y	1622	XAT	C15-C14-C13	-5.96	118.81	127.31
43	y	607	CHL	C3C-C4C-NC	5.95	117.25	110.57
32	Y	611	CLA	C4A-NA-C1A	5.95	109.38	106.71
45	N	1622	XAT	O4-C5-C4	5.94	117.84	113.38
43	Y	607	CHL	C3C-C4C-NC	5.94	117.23	110.57
32	D	402	CLA	C4A-NA-C1A	5.94	109.38	106.71
32	y	613	CLA	C4A-NA-C1A	5.90	109.36	106.71
43	N	608	CHL	C3C-C4C-NC	5.90	117.18	110.57
43	n	608	CHL	C3C-C4C-NC	5.89	117.18	110.57
43	Y	608	CHL	C3D-C2D-C1D	-5.89	97.79	105.83
32	C	507	CLA	C4A-NA-C1A	5.89	109.35	106.71
32	Y	613	CLA	C4A-NA-C1A	5.89	109.35	106.71
45	Y	1622	XAT	C15-C14-C13	-5.88	118.92	127.31
32	C	508	CLA	C4A-NA-C1A	5.87	109.34	106.71
43	G	609	CHL	C3C-C4C-NC	5.86	117.14	110.57
43	g	609	CHL	C3C-C4C-NC	5.86	117.14	110.57
43	Y	609	CHL	C3C-C4C-NC	5.85	117.14	110.57
43	y	609	CHL	C3C-C4C-NC	5.85	117.14	110.57
43	y	608	CHL	C3D-C2D-C1D	-5.85	97.84	105.83
32	B	612	CLA	C4A-NA-C1A	5.84	109.33	106.71
32	y	611	CLA	C4A-NA-C1A	5.84	109.33	106.71
32	c	507	CLA	C4A-NA-C1A	5.83	109.33	106.71
32	b	612	CLA	CMB-C2B-C1B	-5.82	119.51	128.46
32	Y	604	CLA	C4A-NA-C1A	5.82	109.32	106.71
32	b	612	CLA	C4A-NA-C1A	5.81	109.32	106.71
43	R	607	CHL	CHD-C1D-ND	-5.79	119.14	124.45
32	y	604	CLA	C4A-NA-C1A	5.79	109.31	106.71
32	B	612	CLA	CMB-C2B-C1B	-5.78	119.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	603	CLA	C4A-NA-C1A	5.78	109.31	106.71
32	G	611	CLA	C4A-NA-C1A	5.78	109.31	106.71
32	n	603	CLA	C4A-NA-C1A	5.78	109.31	106.71
43	R	606	CHL	CHD-C1D-ND	-5.77	119.15	124.45
32	B	613	CLA	CMB-C2B-C1B	-5.77	119.60	128.46
43	r	606	CHL	CHD-C1D-ND	-5.76	119.16	124.45
43	r	607	CHL	CHD-C1D-ND	-5.75	119.17	124.45
43	n	607	CHL	CHD-C1D-ND	-5.75	119.17	124.45
43	G	607	CHL	CHD-C1D-ND	-5.74	119.18	124.45
32	b	613	CLA	CMB-C2B-C1B	-5.74	119.65	128.46
32	g	611	CLA	C4A-NA-C1A	5.73	109.28	106.71
43	N	607	CHL	CHD-C1D-ND	-5.73	119.19	124.45
43	g	607	CHL	CHD-C1D-ND	-5.73	119.19	124.45
43	g	609	CHL	CHD-C1D-ND	-5.72	119.20	124.45
32	b	609	CLA	C4A-NA-C1A	5.71	109.28	106.71
32	b	608	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
43	y	609	CHL	C3D-C2D-C1D	-5.69	98.07	105.83
45	G	1622	XAT	O24-C25-C24	5.69	117.65	113.38
32	B	608	CLA	CMB-C2B-C1B	-5.68	119.73	128.46
43	Y	609	CHL	C3D-C2D-C1D	-5.68	98.08	105.83
43	Y	609	CHL	O2D-CGD-CBD	5.68	121.35	111.27
43	R	608	CHL	CHD-C1D-ND	-5.67	119.24	124.45
43	y	609	CHL	O2D-CGD-CBD	5.67	121.35	111.27
43	r	608	CHL	CHD-C1D-ND	-5.66	119.25	124.45
43	G	609	CHL	CHD-C1D-ND	-5.66	119.25	124.45
43	N	608	CHL	C3D-C2D-C1D	-5.65	98.12	105.83
32	a	405	CLA	C4A-NA-C1A	5.65	109.25	106.71
43	n	608	CHL	C3D-C2D-C1D	-5.65	98.12	105.83
43	n	608	CHL	CHD-C1D-ND	-5.65	119.26	124.45
45	g	1622	XAT	O24-C25-C24	5.65	117.62	113.38
32	B	609	CLA	C4A-NA-C1A	5.64	109.24	106.71
43	y	601	CHL	C2C-C3C-C4C	-5.64	102.47	106.49
32	b	609	CLA	CMB-C2B-C1B	-5.62	119.82	128.46
32	B	609	CLA	CMB-C2B-C1B	-5.61	119.83	128.46
43	y	606	CHL	CHD-C4C-C3C	-5.59	116.62	124.84
43	N	608	CHL	CHD-C1D-ND	-5.59	119.32	124.45
43	G	605	CHL	O2D-CGD-CBD	5.58	121.19	111.27
43	Y	601	CHL	C2C-C3C-C4C	-5.58	102.51	106.49
43	Y	606	CHL	CHD-C4C-C3C	-5.58	116.64	124.84
43	N	609	CHL	C3C-C4C-NC	5.58	116.83	110.57
43	n	609	CHL	C3C-C4C-NC	5.58	116.83	110.57
43	Y	605	CHL	C3C-C4C-NC	5.58	116.83	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	R	624	XAT	O24-C25-C38	5.56	121.72	115.06
45	r	624	XAT	C18-C5-C6	-5.55	112.95	122.26
45	r	624	XAT	O24-C25-C38	5.55	121.71	115.06
43	g	605	CHL	O2D-CGD-CBD	5.55	121.13	111.27
43	y	605	CHL	C3C-C4C-NC	5.54	116.79	110.57
45	G	1622	XAT	C38-C25-C26	-5.54	112.97	122.26
43	Y	609	CHL	CHD-C1D-ND	-5.54	119.36	124.45
45	R	624	XAT	C18-C5-C6	-5.53	112.99	122.26
43	N	605	CHL	C3D-C2D-C1D	-5.51	98.31	105.83
43	n	605	CHL	C3D-C2D-C1D	-5.51	98.31	105.83
45	g	1622	XAT	C38-C25-C26	-5.51	113.03	122.26
32	A	405	CLA	C4A-NA-C1A	5.50	109.18	106.71
43	y	609	CHL	CHD-C1D-ND	-5.48	119.42	124.45
46	r	625	NEX	C15-C14-C13	-5.48	119.50	127.31
43	n	606	CHL	CHD-C1D-ND	-5.47	119.43	124.45
43	N	606	CHL	CHD-C1D-ND	-5.46	119.44	124.45
46	R	625	NEX	C15-C14-C13	-5.46	119.52	127.31
43	g	607	CHL	C3C-C4C-NC	5.45	116.69	110.57
32	A	405	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
43	G	607	CHL	C3C-C4C-NC	5.43	116.67	110.57
46	g	1623	NEX	C15-C14-C13	-5.43	119.57	127.31
32	D	403	CLA	C4A-NA-C1A	5.42	109.14	106.71
32	a	405	CLA	CMB-C2B-C1B	-5.40	120.16	128.46
43	r	606	CHL	C3C-C4C-NC	5.39	116.61	110.57
43	n	609	CHL	C3D-C2D-C1D	-5.38	98.49	105.83
46	y	1623	NEX	C11-C10-C9	-5.38	119.63	127.31
43	N	609	CHL	C3D-C2D-C1D	-5.38	98.49	105.83
46	Y	1623	NEX	C11-C10-C9	-5.38	119.64	127.31
43	s	608	CHL	C3C-C4C-NC	5.37	116.59	110.57
43	G	606	CHL	O2D-CGD-CBD	5.37	120.81	111.27
43	g	606	CHL	O2D-CGD-CBD	5.37	120.81	111.27
43	S	608	CHL	C3C-C4C-NC	5.36	116.58	110.57
46	G	1623	NEX	C15-C14-C13	-5.35	119.67	127.31
34	C	516	BCR	C16-C17-C18	-5.35	119.68	127.31
32	c	512	CLA	C4A-NA-C1A	5.34	109.11	106.71
32	c	506	CLA	C4A-NA-C1A	5.34	109.11	106.71
46	S	1623	NEX	C15-C14-C13	-5.34	119.69	127.31
43	R	606	CHL	C3C-C4C-NC	5.33	116.55	110.57
43	g	609	CHL	C3D-C2D-C1D	-5.33	98.56	105.83
43	r	607	CHL	C3C-C4C-NC	5.32	116.53	110.57
32	n	614	CLA	C4A-NA-C1A	5.31	109.09	106.71
32	C	508	CLA	CMB-C2B-C1B	-5.31	120.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	508	CLA	CMB-C2B-C1B	-5.31	120.31	128.46
43	G	609	CHL	C3D-C2D-C1D	-5.30	98.59	105.83
32	B	610	CLA	C4A-NA-C1A	5.30	109.09	106.71
32	d	403	CLA	C4A-NA-C1A	5.30	109.09	106.71
43	R	607	CHL	C3C-C4C-NC	5.29	116.51	110.57
34	c	516	BCR	C16-C17-C18	-5.29	119.75	127.31
32	S	611	CLA	C4A-NA-C1A	5.28	109.08	106.71
43	Y	608	CHL	C3C-C4C-NC	5.26	116.47	110.57
39	d	401	BCT	O2-C-O1	5.26	133.19	119.55
39	D	401	BCT	O2-C-O1	5.26	133.19	119.55
43	S	606	CHL	C3C-C4C-NC	5.24	116.45	110.57
43	g	609	CHL	O2D-CGD-CBD	5.24	120.58	111.27
32	C	506	CLA	C4A-NA-C1A	5.23	109.06	106.71
32	b	617	CLA	C4A-NA-C1A	5.23	109.06	106.71
43	r	606	CHL	C3D-C2D-C1D	-5.23	98.70	105.83
43	G	609	CHL	O2D-CGD-CBD	5.22	120.55	111.27
43	y	608	CHL	C3C-C4C-NC	5.22	116.42	110.57
34	h	101	BCR	C11-C10-C9	-5.22	119.86	127.31
32	C	509	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
43	g	608	CHL	C3D-C2D-C1D	-5.21	98.72	105.83
32	b	610	CLA	C4A-NA-C1A	5.21	109.05	106.71
43	G	608	CHL	C3D-C2D-C1D	-5.20	98.73	105.83
45	r	624	XAT	O24-C25-C24	5.20	117.29	113.38
43	N	601	CHL	C3C-C4C-NC	5.20	116.40	110.57
43	n	607	CHL	C3D-C2D-C1D	-5.19	98.75	105.83
32	N	614	CLA	C4A-NA-C1A	5.19	109.04	106.71
32	c	509	CLA	CMB-C2B-C1B	-5.19	120.49	128.46
45	R	624	XAT	O24-C25-C24	5.19	117.28	113.38
34	H	101	BCR	C11-C10-C9	-5.19	119.91	127.31
43	R	606	CHL	C3D-C2D-C1D	-5.19	98.75	105.83
32	r	604	CLA	C4A-NA-C1A	5.18	109.04	106.71
43	N	601	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
43	n	601	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
43	s	608	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
43	g	601	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
43	s	606	CHL	C3C-C4C-NC	5.18	116.38	110.57
32	s	611	CLA	C4A-NA-C1A	5.18	109.03	106.71
43	S	608	CHL	C3D-C2D-C1D	-5.18	98.77	105.83
43	G	608	CHL	C3C-C4C-NC	5.18	116.38	110.57
43	G	601	CHL	C3D-C2D-C1D	-5.18	98.77	105.83
43	N	607	CHL	C3D-C2D-C1D	-5.17	98.78	105.83
32	B	617	CLA	C4A-NA-C1A	5.17	109.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	608	CHL	C3C-C4C-NC	5.17	116.36	110.57
32	B	607	CLA	C4A-NA-C1A	5.16	109.03	106.71
43	n	601	CHL	C3C-C4C-NC	5.16	116.36	110.57
43	R	608	CHL	C3C-C4C-NC	5.16	116.36	110.57
46	s	1623	NEX	C15-C14-C13	-5.16	119.95	127.31
32	R	604	CLA	C4A-NA-C1A	5.15	109.02	106.71
32	g	604	CLA	C4A-NA-C1A	5.15	109.02	106.71
43	r	608	CHL	C3C-C4C-NC	5.15	116.34	110.57
43	g	607	CHL	C3D-C2D-C1D	-5.14	98.82	105.83
45	n	1622	XAT	C15-C14-C13	-5.14	119.98	127.31
32	B	606	CLA	C4A-NA-C1A	5.14	109.02	106.71
32	b	606	CLA	C4A-NA-C1A	5.13	109.01	106.71
45	N	1622	XAT	C15-C14-C13	-5.13	119.98	127.31
43	Y	607	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
43	y	607	CHL	C3D-C2D-C1D	-5.13	98.84	105.83
45	Y	1622	XAT	O4-C5-C18	5.13	121.20	115.06
43	G	607	CHL	C3D-C2D-C1D	-5.12	98.84	105.83
32	B	613	CLA	CMB-C2B-C3B	5.12	134.26	124.68
43	s	607	CHL	C3C-C4C-NC	5.12	116.31	110.57
32	G	604	CLA	C4A-NA-C1A	5.11	109.00	106.71
32	b	607	CLA	C4A-NA-C1A	5.11	109.00	106.71
45	G	1622	XAT	O24-C25-C38	5.11	121.18	115.06
43	R	607	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
43	S	606	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
43	r	607	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
43	S	607	CHL	C3C-C4C-NC	5.09	116.28	110.57
45	g	1622	XAT	O24-C25-C38	5.09	121.16	115.06
32	c	513	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
46	G	1623	NEX	C11-C10-C9	-5.09	120.05	127.31
43	s	606	CHL	C3D-C2D-C1D	-5.08	98.89	105.83
43	Y	601	CHL	O2D-CGD-CBD	5.08	120.30	111.27
43	y	601	CHL	O2D-CGD-CBD	5.08	120.30	111.27
43	s	607	CHL	O2D-CGD-CBD	5.08	120.30	111.27
32	b	613	CLA	CMB-C2B-C3B	5.08	134.18	124.68
32	A	407	CLA	C4A-NA-C1A	5.08	108.99	106.71
32	C	512	CLA	C4A-NA-C1A	5.08	108.99	106.71
43	S	607	CHL	O2D-CGD-CBD	5.07	120.27	111.27
45	y	1622	XAT	O4-C5-C18	5.07	121.13	115.06
32	B	615	CLA	C4A-NA-C1A	5.06	108.98	106.71
32	S	603	CLA	C4A-NA-C1A	5.06	108.98	106.71
32	s	604	CLA	C4A-NA-C1A	5.06	108.98	106.71
32	C	513	CLA	CMB-C2B-C1B	-5.05	120.70	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	s	603	CLA	C4A-NA-C1A	5.04	108.97	106.71
32	s	613	CLA	C4A-NA-C1A	5.04	108.97	106.71
43	y	605	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
43	s	607	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
32	R	602	CLA	C4A-NA-C1A	5.04	108.97	106.71
43	S	607	CHL	C3D-C2D-C1D	-5.03	98.97	105.83
32	S	613	CLA	C4A-NA-C1A	5.03	108.97	106.71
43	Y	605	CHL	C3D-C2D-C1D	-5.03	98.97	105.83
43	S	601	CHL	C2D-C1D-ND	5.02	113.80	110.10
32	G	603	CLA	C4A-NA-C1A	5.02	108.96	106.71
45	y	1622	XAT	C38-C25-C26	-5.01	113.86	122.26
43	g	606	CHL	CHD-C1D-ND	-5.01	119.85	124.45
32	r	602	CLA	C4A-NA-C1A	5.00	108.95	106.71
43	g	605	CHL	C2D-C1D-ND	5.00	113.79	110.10
43	s	601	CHL	C2D-C1D-ND	5.00	113.79	110.10
45	Y	1622	XAT	C38-C25-C26	-4.99	113.89	122.26
43	N	606	CHL	C3D-C4D-ND	4.97	118.28	110.24
43	n	606	CHL	C3D-C4D-ND	4.97	118.28	110.24
32	b	615	CLA	C4A-NA-C1A	4.97	108.94	106.71
43	G	606	CHL	CHD-C1D-ND	-4.97	119.89	124.45
32	a	407	CLA	C4A-NA-C1A	4.97	108.94	106.71
45	n	1622	XAT	C31-C30-C29	-4.97	120.22	127.31
32	S	604	CLA	C4A-NA-C1A	4.96	108.94	106.71
32	g	603	CLA	C4A-NA-C1A	4.96	108.94	106.71
46	r	625	NEX	C27-C28-C29	-4.96	117.83	125.53
45	N	1622	XAT	C31-C30-C29	-4.95	120.24	127.31
46	R	625	NEX	C27-C28-C29	-4.95	117.86	125.53
43	r	608	CHL	C3D-C2D-C1D	-4.94	99.08	105.83
43	n	606	CHL	CHD-C4C-C3C	-4.94	117.57	124.84
43	R	608	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
43	N	606	CHL	CHD-C4C-C3C	-4.93	117.59	124.84
46	y	1623	NEX	C15-C14-C13	-4.93	120.27	127.31
43	S	607	CHL	C3D-C4D-ND	4.92	118.19	110.24
43	s	607	CHL	C3D-C4D-ND	4.92	118.19	110.24
43	G	605	CHL	C2D-C1D-ND	4.91	113.72	110.10
45	n	1622	XAT	C38-C25-C26	-4.91	114.03	122.26
32	n	604	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
46	n	1623	NEX	C38-C25-C26	-4.90	114.05	122.26
43	G	606	CHL	CHD-C4C-C3C	-4.90	117.64	124.84
43	n	608	CHL	O2D-CGD-CBD	4.90	119.97	111.27
32	N	604	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
44	Y	1621	LUT	C35-C34-C33	-4.90	120.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	y	1621	LUT	C35-C34-C33	-4.90	120.32	127.31
43	R	608	CHL	O2D-CGD-CBD	4.89	119.96	111.27
45	y	1622	XAT	C6-C7-C8	-4.89	115.66	125.99
45	N	1622	XAT	C38-C25-C26	-4.89	114.07	122.26
36	B	622	LMG	O7-C10-C11	4.88	122.03	111.50
36	b	622	LMG	O7-C10-C11	4.88	122.02	111.50
32	g	604	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
43	s	606	CHL	C3D-C4D-ND	4.88	118.13	110.24
44	S	1621	LUT	C35-C34-C33	-4.87	120.35	127.31
43	R	606	CHL	C3D-C4D-ND	4.87	118.11	110.24
46	N	1623	NEX	C38-C25-C26	-4.87	114.10	122.26
43	N	608	CHL	O2D-CGD-CBD	4.87	119.92	111.27
43	S	606	CHL	C3D-C4D-ND	4.87	118.11	110.24
43	g	606	CHL	CHD-C4C-C3C	-4.87	117.69	124.84
32	S	604	CLA	CMB-C2B-C1B	-4.87	120.99	128.46
32	s	604	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
32	r	603	CLA	C4A-NA-C1A	4.86	108.89	106.71
45	g	1622	XAT	C35-C15-C14	-4.86	113.52	123.47
45	G	1622	XAT	C35-C15-C14	-4.86	113.52	123.47
32	G	604	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
43	r	608	CHL	O2D-CGD-CBD	4.85	119.89	111.27
44	Y	1620	LUT	C15-C14-C13	-4.85	120.39	127.31
43	r	606	CHL	C3D-C4D-ND	4.85	118.08	110.24
43	s	601	CHL	C3D-C4D-ND	4.85	118.08	110.24
34	b	619	BCR	C11-C10-C9	-4.84	120.40	127.31
44	y	1620	LUT	C15-C14-C13	-4.84	120.40	127.31
44	s	1621	LUT	C35-C34-C33	-4.84	120.41	127.31
45	Y	1622	XAT	C6-C7-C8	-4.84	115.77	125.99
43	g	606	CHL	C3D-C4D-ND	4.83	118.05	110.24
43	G	601	CHL	C3C-C4C-NC	4.83	115.98	110.57
43	Y	606	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
43	y	601	CHL	C3D-C4D-ND	4.82	118.04	110.24
43	Y	601	CHL	C3D-C4D-ND	4.82	118.04	110.24
34	B	618	BCR	C15-C14-C13	-4.82	120.43	127.31
34	b	618	BCR	C15-C14-C13	-4.82	120.43	127.31
34	B	619	BCR	C11-C10-C9	-4.82	120.43	127.31
43	G	606	CHL	C3D-C4D-ND	4.82	118.04	110.24
43	S	601	CHL	C3D-C4D-ND	4.82	118.03	110.24
43	y	605	CHL	O2D-CGD-CBD	4.82	119.83	111.27
46	S	1623	NEX	C38-C25-C26	-4.81	114.20	122.26
43	Y	605	CHL	O2D-CGD-CBD	4.80	119.80	111.27
43	y	606	CHL	C3D-C2D-C1D	-4.80	99.28	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	s	1623	NEX	C38-C25-C26	-4.80	114.22	122.26
45	n	1622	XAT	O4-C5-C18	4.79	120.80	115.06
43	y	605	CHL	C3D-C4D-ND	4.79	117.98	110.24
43	n	608	CHL	CHD-C4C-C3C	-4.78	117.81	124.84
43	S	608	CHL	C3D-C4D-ND	4.78	117.97	110.24
32	b	604	CLA	C4A-NA-C1A	4.78	108.85	106.71
45	N	1622	XAT	O4-C5-C18	4.78	120.78	115.06
43	Y	605	CHL	C3D-C4D-ND	4.77	117.96	110.24
43	N	606	CHL	O2D-CGD-CBD	4.77	119.75	111.27
43	G	605	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
43	g	605	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
43	y	601	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
43	N	607	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
45	y	1622	XAT	C27-C28-C29	-4.76	118.14	125.53
43	Y	601	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
43	n	607	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
43	N	608	CHL	CHD-C4C-C3C	-4.76	117.85	124.84
43	N	606	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
43	n	606	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
32	b	612	CLA	CMB-C2B-C3B	4.76	133.57	124.68
33	a	409	PHO	CMB-C2B-C3B	4.75	133.57	124.68
43	g	601	CHL	O2D-CGD-CBD	4.75	119.71	111.27
33	A	409	PHO	CMB-C2B-C3B	4.75	133.56	124.68
46	Y	1623	NEX	C15-C14-C13	-4.75	120.53	127.31
43	Y	608	CHL	C3D-C4D-ND	4.75	117.92	110.24
32	R	603	CLA	C4A-NA-C1A	4.74	108.84	106.71
43	s	608	CHL	C3D-C4D-ND	4.74	117.91	110.24
43	g	609	CHL	C3D-C4D-ND	4.74	117.91	110.24
43	y	608	CHL	C3D-C4D-ND	4.74	117.91	110.24
43	G	601	CHL	O2D-CGD-CBD	4.74	119.69	111.27
32	n	611	CLA	C4A-NA-C1A	4.74	108.84	106.71
34	C	517	BCR	C28-C27-C26	-4.74	105.61	114.08
43	g	601	CHL	C3D-C4D-ND	4.74	117.90	110.24
43	n	606	CHL	O2D-CGD-CBD	4.74	119.68	111.27
44	Y	1621	LUT	C15-C14-C13	-4.73	120.56	127.31
44	y	1621	LUT	C15-C14-C13	-4.73	120.56	127.31
32	b	608	CLA	C4A-NA-C1A	4.73	108.83	106.71
43	Y	607	CHL	CHD-C1D-ND	-4.73	120.11	124.45
43	G	609	CHL	C3D-C4D-ND	4.72	117.88	110.24
32	A	407	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
43	r	606	CHL	CAC-C3C-C4C	4.72	130.93	124.81
32	B	612	CLA	CMB-C2B-C3B	4.71	133.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	517	BCR	C28-C27-C26	-4.71	105.66	114.08
43	Y	606	CHL	CAA-C2A-C3A	-4.71	99.88	112.78
43	S	608	CHL	O2D-CGD-CBD	4.71	119.64	111.27
46	y	1623	NEX	C27-C28-C29	-4.70	118.23	125.53
46	g	1623	NEX	C38-C25-C26	-4.70	114.38	122.26
45	y	1622	XAT	C37-C21-C26	-4.70	97.37	110.05
43	y	607	CHL	CHD-C1D-ND	-4.70	120.14	124.45
43	y	606	CHL	CAA-C2A-C3A	-4.69	99.93	112.78
46	Y	1623	NEX	C27-C28-C29	-4.69	118.25	125.53
32	a	407	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
43	N	601	CHL	O2D-CGD-CBD	4.69	119.60	111.27
32	N	611	CLA	C4A-NA-C1A	4.69	108.81	106.71
45	Y	1622	XAT	C37-C21-C26	-4.69	97.39	110.05
32	C	511	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
45	Y	1622	XAT	C18-C5-C6	-4.69	114.41	122.26
32	c	511	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
43	G	601	CHL	C3D-C4D-ND	4.69	117.82	110.24
43	s	608	CHL	O2D-CGD-CBD	4.68	119.59	111.27
45	y	1622	XAT	C18-C5-C6	-4.68	114.42	122.26
46	G	1623	NEX	C38-C25-C26	-4.68	114.42	122.26
34	a	411	BCR	C7-C8-C9	-4.68	119.17	126.23
43	R	606	CHL	CAC-C3C-C4C	4.68	130.88	124.81
43	r	607	CHL	O2D-CGD-CBD	4.67	119.57	111.27
43	R	607	CHL	O2D-CGD-CBD	4.67	119.57	111.27
43	n	601	CHL	O2D-CGD-CBD	4.67	119.57	111.27
43	g	608	CHL	C3D-C4D-ND	4.67	117.79	110.24
43	g	601	CHL	C3C-C4C-NC	4.67	115.81	110.57
43	G	608	CHL	C3D-C4D-ND	4.67	117.79	110.24
43	G	606	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
46	r	625	NEX	C11-C10-C9	-4.66	120.65	127.31
43	g	606	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
32	B	608	CLA	C4A-NA-C1A	4.66	108.80	106.71
32	B	608	CLA	CMB-C2B-C3B	4.65	133.38	124.68
43	G	605	CHL	C3C-C4C-NC	4.65	115.78	110.57
45	R	624	XAT	C6-C7-C8	-4.64	116.18	125.99
46	Y	1623	NEX	C38-C25-C26	-4.64	114.48	122.26
45	Y	1622	XAT	C27-C28-C29	-4.64	118.33	125.53
34	A	411	BCR	C7-C8-C9	-4.64	119.23	126.23
32	a	405	CLA	CMB-C2B-C3B	4.64	133.35	124.68
32	b	608	CLA	CMB-C2B-C3B	4.64	133.35	124.68
45	r	624	XAT	C6-C7-C8	-4.63	116.19	125.99
32	C	509	CLA	CMB-C2B-C3B	4.63	133.34	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	609	CLA	CMB-C2B-C3B	4.62	133.33	124.68
32	A	405	CLA	CMB-C2B-C3B	4.62	133.33	124.68
32	B	604	CLA	C4A-NA-C1A	4.62	108.78	106.71
46	y	1623	NEX	C38-C25-C26	-4.62	114.53	122.26
43	g	607	CHL	C3D-C4D-ND	4.61	117.70	110.24
43	R	608	CHL	C3D-C4D-ND	4.61	117.70	110.24
32	c	503	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
32	c	509	CLA	CMB-C2B-C3B	4.61	133.30	124.68
43	g	605	CHL	C3C-C4C-NC	4.61	115.74	110.57
43	N	607	CHL	C3D-C4D-ND	4.61	117.69	110.24
43	n	607	CHL	C3D-C4D-ND	4.61	117.69	110.24
32	b	609	CLA	CMB-C2B-C3B	4.60	133.28	124.68
43	G	607	CHL	C3D-C4D-ND	4.60	117.67	110.24
32	C	508	CLA	CMB-C2B-C3B	4.59	133.27	124.68
32	C	503	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
34	C	516	BCR	C33-C5-C6	-4.59	119.37	124.53
34	c	515	BCR	C15-C14-C13	-4.59	120.76	127.31
32	C	506	CLA	CMB-C2B-C1B	-4.59	121.42	128.46
32	s	602	CLA	C4A-NA-C1A	4.58	108.77	106.71
43	r	608	CHL	C3D-C4D-ND	4.58	117.65	110.24
43	n	605	CHL	CHD-C4C-C3C	-4.58	118.11	124.84
43	g	605	CHL	C3D-C4D-ND	4.58	117.65	110.24
43	N	605	CHL	CHD-C4C-C3C	-4.58	118.11	124.84
34	D	404	BCR	C7-C8-C9	4.58	133.15	126.23
32	c	508	CLA	CMB-C2B-C3B	4.58	133.24	124.68
34	B	619	BCR	C24-C23-C22	-4.57	119.32	126.23
34	c	516	BCR	C33-C5-C6	-4.57	119.39	124.53
43	S	601	CHL	C4A-NA-C1A	-4.57	104.65	106.71
43	y	606	CHL	CHD-C1D-ND	-4.57	120.26	124.45
34	d	404	BCR	C7-C8-C9	4.57	133.14	126.23
43	N	605	CHL	C3D-C4D-ND	4.57	117.63	110.24
43	n	605	CHL	C3D-C4D-ND	4.57	117.63	110.24
34	C	515	BCR	C15-C14-C13	-4.57	120.79	127.31
43	Y	608	CHL	O2D-CGD-CBD	4.57	119.38	111.27
43	Y	606	CHL	CHD-C1D-ND	-4.56	120.26	124.45
43	G	605	CHL	C3D-C4D-ND	4.56	117.62	110.24
44	G	1620	LUT	C35-C34-C33	-4.56	120.80	127.31
32	c	513	CLA	CMB-C2B-C3B	4.56	133.20	124.68
38	y	2630	LHG	O7-C7-C8	4.55	121.32	111.50
43	s	601	CHL	C4A-NA-C1A	-4.55	104.66	106.71
43	r	607	CHL	C3D-C4D-ND	4.55	117.60	110.24
44	g	1620	LUT	C35-C34-C33	-4.55	120.82	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	515	BCR	C7-C8-C9	-4.55	119.36	126.23
32	c	506	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
46	r	625	NEX	C38-C25-C26	-4.54	114.65	122.26
34	b	619	BCR	C15-C14-C13	-4.54	120.83	127.31
32	C	505	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
32	c	505	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
38	Y	2630	LHG	O7-C7-C8	4.54	121.29	111.50
32	B	614	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
46	R	625	NEX	C38-C25-C26	-4.54	114.66	122.26
34	c	515	BCR	C7-C8-C9	-4.54	119.38	126.23
32	N	602	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
32	b	614	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
43	n	601	CHL	C3D-C4D-ND	4.53	117.56	110.24
43	y	608	CHL	O2D-CGD-CBD	4.53	119.31	111.27
32	C	513	CLA	CMB-C2B-C3B	4.52	133.14	124.68
34	B	619	BCR	C15-C14-C13	-4.52	120.85	127.31
43	N	601	CHL	C3D-C4D-ND	4.52	117.55	110.24
32	n	602	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
34	b	619	BCR	C24-C23-C22	-4.52	119.41	126.23
32	c	512	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
45	G	1622	XAT	C18-C5-C6	-4.51	114.70	122.26
45	g	1622	XAT	C18-C5-C6	-4.51	114.70	122.26
44	y	1620	LUT	C35-C34-C33	-4.51	120.87	127.31
43	R	607	CHL	C3D-C4D-ND	4.51	117.54	110.24
32	S	602	CLA	C4A-NA-C1A	4.51	108.73	106.71
43	g	609	CHL	CHD-C4C-C3C	-4.51	118.22	124.84
36	a	413	LMG	O7-C10-C11	4.50	121.21	111.50
46	s	1623	NEX	C27-C28-C29	-4.50	118.54	125.53
34	c	514	BCR	C24-C23-C22	-4.49	119.44	126.23
34	C	514	BCR	C24-C23-C22	-4.49	119.45	126.23
34	b	619	BCR	C7-C8-C9	-4.49	119.45	126.23
43	n	609	CHL	C3D-C4D-ND	4.49	117.50	110.24
32	r	609	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
45	g	1622	XAT	C35-C34-C33	-4.48	120.92	127.31
32	C	510	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
43	N	609	CHL	C3D-C4D-ND	4.48	117.48	110.24
36	A	413	LMG	O7-C10-C11	4.48	121.15	111.50
43	y	609	CHL	CHD-C4C-C3C	-4.48	118.26	124.84
44	Y	1620	LUT	C35-C34-C33	-4.47	120.92	127.31
43	G	609	CHL	CHD-C4C-C3C	-4.47	118.26	124.84
34	B	619	BCR	C7-C8-C9	-4.47	119.48	126.23
32	C	507	CLA	CMB-C2B-C1B	-4.47	121.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	101	BCR	C7-C8-C9	-4.47	119.49	126.23
37	c	520	DGD	O2G-C1B-C2B	4.46	121.12	111.50
46	s	1623	NEX	C31-C30-C29	-4.46	120.94	127.31
43	N	608	CHL	C3D-C4D-ND	4.46	117.45	110.24
37	C	520	DGD	O2G-C1B-C2B	4.46	121.11	111.50
43	y	607	CHL	O2D-CGD-CBD	4.46	119.19	111.27
45	y	1622	XAT	C31-C30-C29	-4.46	120.95	127.31
46	S	1623	NEX	C27-C28-C29	-4.46	118.61	125.53
32	c	507	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
45	G	1622	XAT	C35-C34-C33	-4.46	120.95	127.31
43	n	608	CHL	C3D-C4D-ND	4.46	117.44	110.24
46	S	1623	NEX	C31-C30-C29	-4.45	120.95	127.31
43	Y	609	CHL	CHD-C4C-C3C	-4.45	118.29	124.84
45	n	1622	XAT	C6-C7-C8	-4.45	116.58	125.99
32	G	612	CLA	C4A-NA-C1A	4.45	108.71	106.71
45	N	1622	XAT	C6-C7-C8	-4.45	116.59	125.99
34	h	101	BCR	C7-C8-C9	-4.44	119.52	126.23
32	R	609	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
34	B	618	BCR	C16-C17-C18	-4.44	120.97	127.31
43	y	606	CHL	C3D-C4D-ND	4.44	117.42	110.24
43	Y	606	CHL	C3D-C4D-ND	4.44	117.41	110.24
32	C	512	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
32	g	602	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
43	Y	607	CHL	O2D-CGD-CBD	4.43	119.14	111.27
32	g	612	CLA	C4A-NA-C1A	4.42	108.69	106.71
32	n	604	CLA	C4A-NA-C1A	4.42	108.69	106.71
34	b	618	BCR	C16-C17-C18	-4.42	121.00	127.31
32	Y	611	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
32	G	602	CLA	C4A-NA-C1A	4.42	108.69	106.71
32	G	602	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
32	y	611	CLA	CMB-C2B-C1B	-4.42	121.68	128.46
34	H	101	BCR	C28-C27-C26	-4.41	106.20	114.08
34	h	101	BCR	C28-C27-C26	-4.41	106.21	114.08
43	r	606	CHL	O2D-CGD-CBD	4.40	119.09	111.27
43	R	606	CHL	O2D-CGD-CBD	4.40	119.09	111.27
37	c	524	DGD	O2G-C1B-C2B	4.40	120.98	111.50
43	y	609	CHL	C3D-C4D-ND	4.40	117.36	110.24
45	Y	1622	XAT	C31-C30-C29	-4.40	121.03	127.31
43	Y	609	CHL	C3D-C4D-ND	4.40	117.35	110.24
32	c	510	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
45	N	1622	XAT	C27-C28-C29	-4.39	118.72	125.53
32	Y	603	CLA	C4A-NA-C1A	4.38	108.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	524	DGD	O2G-C1B-C2B	4.38	120.94	111.50
43	G	608	CHL	O2D-CGD-CBD	4.37	119.03	111.27
34	H	101	BCR	C16-C17-C18	-4.37	121.08	127.31
34	h	101	BCR	C16-C17-C18	-4.36	121.08	127.31
43	s	601	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
32	b	617	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
45	n	1622	XAT	C27-C28-C29	-4.36	118.77	125.53
43	g	608	CHL	O2D-CGD-CBD	4.36	119.01	111.27
34	C	517	BCR	C11-C10-C9	-4.36	121.09	127.31
46	g	1623	NEX	C27-C28-C29	-4.36	118.77	125.53
43	S	601	CHL	C3C-C4C-NC	4.35	115.45	110.57
43	s	601	CHL	C3C-C4C-NC	4.35	115.45	110.57
46	G	1623	NEX	C27-C28-C29	-4.35	118.78	125.53
43	S	601	CHL	C3D-C2D-C1D	-4.35	99.90	105.83
43	y	607	CHL	C3D-C4D-ND	4.34	117.25	110.24
32	N	604	CLA	C4A-NA-C1A	4.33	108.65	106.71
32	y	610	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
43	y	607	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
34	c	517	BCR	C11-C10-C9	-4.33	121.13	127.31
32	B	617	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
46	R	625	NEX	C11-C10-C9	-4.33	121.14	127.31
32	Y	610	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
32	B	607	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
32	b	610	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
46	N	1623	NEX	C27-C28-C29	-4.31	118.83	125.53
43	g	607	CHL	O2D-CGD-CBD	4.31	118.94	111.27
45	N	1622	XAT	O24-C25-C38	4.31	120.22	115.06
45	n	1622	XAT	O24-C25-C38	4.31	120.22	115.06
43	Y	601	CHL	CBC-CAC-C3C	-4.31	100.54	112.43
43	y	601	CHL	CBC-CAC-C3C	-4.31	100.55	112.43
43	G	607	CHL	O2D-CGD-CBD	4.31	118.92	111.27
38	L	101	LHG	O7-C7-C8	4.31	120.78	111.50
43	Y	607	CHL	C3D-C4D-ND	4.31	117.21	110.24
32	b	607	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
45	g	1622	XAT	C26-C27-C28	-4.30	116.91	125.99
45	G	1622	XAT	C26-C27-C28	-4.30	116.91	125.99
32	b	604	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
32	B	605	CLA	C4A-NA-C1A	4.29	108.63	106.71
43	Y	607	CHL	CHD-C4C-C3C	-4.29	118.54	124.84
32	B	610	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
43	G	605	CHL	C1B-CHB-C4A	-4.28	121.64	130.12
32	B	604	CLA	CMB-C2B-C1B	-4.28	121.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	101	LHG	O7-C7-C8	4.28	120.73	111.50
43	g	605	CHL	C1B-CHB-C4A	-4.28	121.65	130.12
34	H	101	BCR	C3-C4-C5	-4.27	106.45	114.08
46	n	1623	NEX	C27-C28-C29	-4.27	118.90	125.53
32	g	602	CLA	C4A-NA-C1A	4.27	108.63	106.71
32	y	603	CLA	C4A-NA-C1A	4.27	108.63	106.71
43	S	606	CHL	CAC-C3C-C4C	4.27	130.35	124.81
32	c	501	CLA	C4A-NA-C1A	4.27	108.62	106.71
34	h	101	BCR	C3-C4-C5	-4.26	106.46	114.08
32	Y	604	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
32	s	611	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
45	G	1622	XAT	C31-C30-C29	-4.25	121.25	127.31
32	S	611	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
34	B	620	BCR	C24-C23-C22	-4.24	119.83	126.23
43	g	607	CHL	CHD-C4C-C3C	-4.24	118.61	124.84
43	G	607	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
32	y	613	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
32	G	610	CLA	C4A-NA-C1A	4.23	108.61	106.71
34	d	404	BCR	C34-C9-C8	4.23	124.74	118.08
32	y	604	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
43	N	609	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
43	n	609	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
34	b	620	BCR	C24-C23-C22	-4.22	119.85	126.23
45	g	1622	XAT	C31-C30-C29	-4.22	121.28	127.31
32	a	410	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
45	G	1622	XAT	C6-C7-C8	-4.22	117.07	125.99
32	N	612	CLA	C4A-NA-C1A	4.22	108.60	106.71
32	n	612	CLA	C4A-NA-C1A	4.22	108.60	106.71
43	s	606	CHL	CAC-C3C-C4C	4.21	130.27	124.81
43	S	601	CHL	O2D-CGD-CBD	4.21	118.75	111.27
32	r	604	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
45	g	1622	XAT	C6-C7-C8	-4.21	117.10	125.99
32	N	604	CLA	CMB-C2B-C3B	4.20	132.53	124.68
32	C	501	CLA	C4A-NA-C1A	4.20	108.59	106.71
43	s	601	CHL	O2D-CGD-CBD	4.19	118.72	111.27
32	A	410	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
32	A	406	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
32	r	609	CLA	C4A-NA-C1A	4.19	108.59	106.71
32	a	406	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
32	B	605	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
32	Y	613	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
32	b	605	CLA	C4A-NA-C1A	4.19	108.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	404	BCR	C34-C9-C8	4.19	124.67	118.08
43	S	606	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
32	s	612	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
43	r	606	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
32	g	610	CLA	C4A-NA-C1A	4.18	108.58	106.71
32	n	604	CLA	CMB-C2B-C3B	4.18	132.49	124.68
32	S	612	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
43	R	606	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
44	N	1621	LUT	C15-C14-C13	-4.17	121.36	127.31
32	R	604	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
32	b	605	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
45	N	1622	XAT	C18-C5-C6	-4.15	115.31	122.26
46	n	1623	NEX	C15-C14-C13	-4.15	121.39	127.31
32	S	603	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
45	R	624	XAT	C26-C27-C28	-4.13	117.25	125.99
32	N	610	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
45	r	624	XAT	C26-C27-C28	-4.13	117.25	125.99
43	s	606	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
45	n	1622	XAT	C18-C5-C6	-4.13	115.34	122.26
32	A	407	CLA	CMB-C2B-C3B	4.13	132.40	124.68
43	s	608	CHL	CAC-C3C-C4C	4.12	130.16	124.81
32	a	407	CLA	CMB-C2B-C3B	4.12	132.39	124.68
32	B	603	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
32	s	603	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
46	N	1623	NEX	C15-C14-C13	-4.12	121.44	127.31
44	n	1621	LUT	C15-C14-C13	-4.11	121.44	127.31
37	C	519	DGD	O2G-C1B-C2B	4.11	120.37	111.50
32	n	610	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
43	S	601	CHL	CAC-C3C-C4C	4.10	130.13	124.81
43	s	601	CHL	CAC-C3C-C4C	4.10	130.13	124.81
37	c	519	DGD	O2G-C1B-C2B	4.10	120.34	111.50
34	C	515	BCR	C1-C6-C5	-4.10	116.84	122.61
46	g	1623	NEX	C11-C10-C9	-4.10	121.46	127.31
43	S	608	CHL	CAC-C3C-C4C	4.09	130.12	124.81
45	G	1622	XAT	O4-C5-C18	4.09	119.95	115.06
45	r	624	XAT	C35-C34-C33	-4.08	121.48	127.31
43	S	601	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
43	s	601	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
32	b	603	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
43	N	607	CHL	O2D-CGD-CBD	4.08	118.51	111.27
34	c	515	BCR	C1-C6-C5	-4.07	116.88	122.61
43	Y	601	CHL	C3B-C4B-NB	4.07	114.47	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	y	601	CHL	C3B-C4B-NB	4.07	114.47	109.21
45	g	1622	XAT	O4-C5-C18	4.07	119.93	115.06
32	R	609	CLA	C4A-NA-C1A	4.07	108.54	106.71
32	C	503	CLA	C4A-NA-C1A	4.07	108.53	106.71
43	n	607	CHL	O2D-CGD-CBD	4.07	118.49	111.27
45	R	624	XAT	C35-C34-C33	-4.04	121.54	127.31
32	s	602	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
44	G	1621	LUT	C15-C14-C13	-4.04	121.54	127.31
44	g	1621	LUT	C15-C14-C13	-4.03	121.55	127.31
43	y	606	CHL	CAC-C3C-C4C	4.03	130.04	124.81
43	Y	606	CHL	CAC-C3C-C4C	4.03	130.04	124.81
32	S	602	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
43	N	601	CHL	CAC-C3C-C4C	4.03	130.04	124.81
32	B	614	CLA	CMB-C2B-C3B	4.02	132.20	124.68
32	B	615	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
35	A	412	SQD	O47-C7-C8	4.01	120.14	111.50
32	b	614	CLA	CMB-C2B-C3B	4.01	132.17	124.68
43	n	601	CHL	CAC-C3C-C4C	4.01	130.01	124.81
32	Y	602	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
35	a	412	SQD	O47-C7-C8	4.00	120.12	111.50
32	y	602	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
34	h	101	BCR	C20-C21-C22	-4.00	121.60	127.31
43	Y	608	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
34	c	517	BCR	C24-C23-C22	-3.99	120.21	126.23
32	b	615	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
34	C	517	BCR	C24-C23-C22	-3.98	120.22	126.23
43	s	606	CHL	O2D-CGD-CBD	3.98	118.33	111.27
43	S	606	CHL	O2D-CGD-CBD	3.98	118.33	111.27
32	c	511	CLA	CMB-C2B-C3B	3.96	132.09	124.68
34	H	101	BCR	C15-C14-C13	-3.96	121.66	127.31
34	H	101	BCR	C20-C21-C22	-3.96	121.66	127.31
32	C	508	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
43	r	607	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
34	c	515	BCR	C21-C20-C19	-3.95	110.88	123.22
32	c	508	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
34	C	515	BCR	C21-C20-C19	-3.95	110.88	123.22
32	C	511	CLA	CMB-C2B-C3B	3.95	132.07	124.68
43	y	608	CHL	CHD-C4C-C3C	-3.95	119.03	124.84
32	C	507	CLA	CMB-C2B-C3B	3.94	132.05	124.68
32	c	507	CLA	CMB-C2B-C3B	3.94	132.05	124.68
43	y	605	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
34	h	101	BCR	C15-C14-C13	-3.94	121.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	R	607	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
45	g	1622	XAT	C4-C3-C2	-3.94	103.17	110.77
32	C	513	CLA	C4A-NA-C1A	3.94	108.48	106.71
43	g	601	CHL	C1-C2-C3	-3.94	119.24	126.04
43	G	601	CHL	C1-C2-C3	-3.93	119.24	126.04
34	B	618	BCR	C28-C27-C26	-3.93	107.06	114.08
32	c	512	CLA	CMB-C2B-C3B	3.93	132.03	124.68
32	b	617	CLA	CMB-C2B-C3B	3.92	132.01	124.68
43	y	601	CHL	C3C-C4C-NC	3.92	114.96	110.57
45	G	1622	XAT	C4-C3-C2	-3.91	103.21	110.77
32	Y	610	CLA	CMB-C2B-C3B	3.91	132.00	124.68
34	b	618	BCR	C28-C27-C26	-3.91	107.09	114.08
34	C	514	BCR	C20-C21-C22	-3.91	121.73	127.31
32	B	617	CLA	CMB-C2B-C3B	3.90	131.97	124.68
43	r	607	CHL	CAC-C3C-C4C	3.90	129.87	124.81
36	H	102	LMG	O7-C10-C11	3.90	119.90	111.50
34	c	514	BCR	C20-C21-C22	-3.89	121.76	127.31
32	y	610	CLA	CMB-C2B-C3B	3.89	131.96	124.68
42	z	2634	LMU	O5B-C5B-C4B	3.89	116.76	109.69
32	b	602	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
43	R	608	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
32	N	610	CLA	C4A-NA-C1A	3.89	108.45	106.71
32	c	503	CLA	CMB-C2B-C3B	3.89	131.95	124.68
34	b	619	BCR	C20-C21-C22	-3.88	121.77	127.31
32	C	512	CLA	CMB-C2B-C3B	3.88	131.94	124.68
32	N	602	CLA	CMB-C2B-C3B	3.88	131.94	124.68
32	C	503	CLA	CMB-C2B-C3B	3.88	131.94	124.68
43	N	607	CHL	CHB-C4A-NA	3.88	129.88	124.51
43	Y	605	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
43	s	607	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
43	g	608	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
43	R	607	CHL	CAC-C3C-C4C	3.88	129.84	124.81
32	g	612	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
43	r	608	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
43	Y	601	CHL	C3C-C4C-NC	3.87	114.91	110.57
32	n	602	CLA	CMB-C2B-C3B	3.87	131.92	124.68
41	f	101	HEM	CMC-C2C-C3C	3.87	131.92	124.68
43	G	608	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
41	F	101	HEM	CMC-C2C-C3C	3.86	131.91	124.68
43	S	607	CHL	CHD-C4C-C3C	-3.86	119.16	124.84
42	Z	2634	LMU	O5B-C5B-C4B	3.86	116.70	109.69
34	C	517	BCR	C7-C8-C9	-3.85	120.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	N	605	CHL	C3B-C4B-NB	3.85	114.19	109.21
43	n	607	CHL	CHB-C4A-NA	3.85	129.83	124.51
32	G	612	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
43	N	609	CHL	O2D-CGD-CBD	3.85	118.10	111.27
32	B	602	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
43	n	609	CHL	O2D-CGD-CBD	3.84	118.09	111.27
43	G	601	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
34	C	514	BCR	C15-C14-C13	-3.84	121.84	127.31
34	c	514	BCR	C15-C14-C13	-3.84	121.84	127.31
34	c	517	BCR	C7-C8-C9	-3.83	120.44	126.23
34	B	619	BCR	C20-C21-C22	-3.83	121.85	127.31
35	B	621	SQD	O47-C7-C8	3.83	119.75	111.50
34	D	404	BCR	C16-C17-C18	-3.83	121.85	127.31
32	Y	610	CLA	C1B-CHB-C4A	-3.82	122.55	130.12
34	B	618	BCR	C11-C10-C9	-3.82	121.86	127.31
34	b	620	BCR	C7-C8-C9	-3.82	120.47	126.23
35	b	621	SQD	O47-C7-C8	3.82	119.73	111.50
34	d	404	BCR	C16-C17-C18	-3.81	121.87	127.31
32	r	609	CLA	CMB-C2B-C3B	3.80	131.79	124.68
43	n	605	CHL	C3B-C4B-NB	3.80	114.13	109.21
34	c	516	BCR	C15-C14-C13	-3.80	121.89	127.31
44	y	1620	LUT	C10-C11-C12	-3.80	111.36	123.22
43	y	607	CHL	CAC-C3C-C4C	3.80	129.74	124.81
36	h	102	LMG	O7-C10-C11	3.80	119.68	111.50
32	R	603	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
32	c	503	CLA	C4A-NA-C1A	3.79	108.41	106.71
34	c	515	BCR	C33-C5-C4	3.79	120.90	113.62
34	C	515	BCR	C33-C5-C4	3.79	120.89	113.62
34	B	620	BCR	C7-C8-C9	-3.79	120.51	126.23
34	b	618	BCR	C11-C10-C9	-3.79	121.91	127.31
32	y	610	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
32	r	603	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
34	C	516	BCR	C15-C14-C13	-3.78	121.91	127.31
44	Y	1620	LUT	C10-C11-C12	-3.78	111.41	123.22
32	R	609	CLA	CMB-C2B-C3B	3.78	131.75	124.68
32	n	610	CLA	C4A-NA-C1A	3.78	108.40	106.71
32	c	513	CLA	C4A-NA-C1A	3.77	108.40	106.71
32	g	610	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
43	y	607	CHL	C3B-C4B-NB	3.77	114.09	109.21
43	S	607	CHL	CAC-C3C-C4C	3.77	129.70	124.81
43	s	607	CHL	CAC-C3C-C4C	3.77	129.70	124.81
46	r	625	NEX	C35-C34-C33	-3.77	121.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	101	BCR	C24-C23-C22	-3.76	120.55	126.23
32	Y	603	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
34	c	514	BCR	C16-C17-C18	-3.76	121.94	127.31
43	Y	601	CHL	C1C-C2C-C3C	-3.76	104.13	107.11
43	Y	607	CHL	CAC-C3C-C4C	3.76	129.69	124.81
32	C	510	CLA	CMB-C2B-C3B	3.76	131.70	124.68
32	s	605	CLA	C1B-CHB-C4A	-3.75	122.68	130.12
46	R	625	NEX	C35-C34-C33	-3.75	121.95	127.31
32	Y	612	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
37	c	523	DGD	O2G-C1B-C2B	3.75	119.58	111.50
32	S	605	CLA	C1B-CHB-C4A	-3.75	122.69	130.12
43	Y	607	CHL	C3B-C4B-NB	3.75	114.06	109.21
37	C	518	DGD	O2G-C1B-C2B	3.75	119.58	111.50
37	C	523	DGD	O2G-C1B-C2B	3.75	119.58	111.50
32	S	611	CLA	CMB-C2B-C3B	3.75	131.69	124.68
32	G	610	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
45	Y	1622	XAT	C15-C35-C34	-3.75	115.80	123.47
32	y	603	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
32	G	602	CLA	CMB-C2B-C3B	3.74	131.68	124.68
32	S	603	CLA	CAA-C2A-C3A	-3.74	104.92	114.26
43	y	601	CHL	C1C-C2C-C3C	-3.74	104.15	107.11
32	C	505	CLA	CMB-C2B-C3B	3.73	131.66	124.68
32	s	611	CLA	CMB-C2B-C3B	3.73	131.66	124.68
43	S	601	CHL	C3B-C4B-NB	3.73	114.03	109.21
44	s	1620	LUT	C15-C14-C13	-3.73	121.99	127.31
37	c	518	DGD	O2G-C1B-C2B	3.73	119.53	111.50
43	n	609	CHL	C3B-C4B-NB	3.72	114.02	109.21
32	G	611	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
44	S	1620	LUT	C15-C14-C13	-3.72	122.00	127.31
43	s	601	CHL	C3B-C4B-NB	3.72	114.02	109.21
34	H	101	BCR	C24-C23-C22	-3.72	120.62	126.23
32	g	614	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
32	g	602	CLA	CMB-C2B-C3B	3.71	131.63	124.68
32	G	610	CLA	C1B-CHB-C4A	-3.71	122.76	130.12
32	g	610	CLA	C1B-CHB-C4A	-3.71	122.76	130.12
32	S	612	CLA	C4A-NA-C1A	3.71	108.38	106.71
43	y	608	CHL	CAC-C3C-C4C	3.71	129.63	124.81
43	N	601	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
32	G	614	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
46	y	1623	NEX	O24-C25-C38	3.71	119.50	115.06
46	Y	1623	NEX	O24-C25-C38	3.70	119.49	115.06
34	C	514	BCR	C16-C17-C18	-3.70	122.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	608	CHL	C3B-C4B-NB	3.70	114.00	109.21
43	Y	608	CHL	CAC-C3C-C4C	3.70	129.61	124.81
38	C	2630	LHG	O7-C7-C8	3.70	119.48	111.50
32	y	612	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
44	S	1620	LUT	C10-C11-C12	-3.69	111.70	123.22
32	S	604	CLA	CMB-C2B-C3B	3.69	131.58	124.68
32	s	605	CLA	C4A-NA-C1A	3.69	108.36	106.71
38	c	2630	LHG	O7-C7-C8	3.68	119.44	111.50
36	d	411	LMG	O7-C10-C11	3.68	119.44	111.50
44	s	1620	LUT	C10-C11-C12	-3.68	111.73	123.22
32	s	612	CLA	C4A-NA-C1A	3.68	108.36	106.71
43	N	609	CHL	C3B-C4B-NB	3.68	113.97	109.21
34	C	515	BCR	C16-C17-C18	-3.68	122.06	127.31
32	N	610	CLA	CMB-C2B-C3B	3.68	131.56	124.68
32	S	605	CLA	C4A-NA-C1A	3.68	108.36	106.71
32	c	510	CLA	CMB-C2B-C3B	3.68	131.56	124.68
32	s	604	CLA	CMB-C2B-C3B	3.68	131.55	124.68
43	Y	606	CHL	O2D-CGD-CBD	3.67	117.80	111.27
32	s	603	CLA	CAA-C2A-C3A	-3.67	105.09	114.26
46	N	1623	NEX	C39-C29-C30	-3.67	117.78	122.92
32	g	611	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
45	y	1622	XAT	C15-C35-C34	-3.67	115.96	123.47
36	D	411	LMG	O7-C10-C11	3.67	119.40	111.50
43	y	606	CHL	O2D-CGD-CBD	3.67	117.78	111.27
34	c	515	BCR	C16-C17-C18	-3.67	122.08	127.31
32	b	605	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
43	G	608	CHL	C3B-C4B-NB	3.66	113.94	109.21
32	c	505	CLA	CMB-C2B-C3B	3.66	131.53	124.68
46	n	1623	NEX	C39-C29-C30	-3.66	117.79	122.92
33	A	408	PHO	CMB-C2B-C3B	3.66	131.52	124.68
43	n	601	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
46	N	1623	NEX	C35-C34-C33	-3.66	122.09	127.31
32	n	610	CLA	CMB-C2B-C3B	3.66	131.52	124.68
32	B	605	CLA	CAA-C2A-C3A	-3.65	102.77	112.78
46	y	1623	NEX	C35-C34-C33	-3.65	122.10	127.31
43	g	607	CHL	CAC-C3C-C4C	3.65	129.54	124.81
43	G	607	CHL	CAC-C3C-C4C	3.64	129.53	124.81
46	n	1623	NEX	C35-C34-C33	-3.63	122.12	127.31
33	a	408	PHO	CMB-C2B-C3B	3.63	131.47	124.68
32	d	403	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
32	s	609	CLA	C4A-NA-C1A	3.63	108.34	106.71
43	y	605	CHL	CAC-C3C-C4C	3.63	129.52	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	613	CLA	CHB-C4A-NA	3.63	129.53	124.51
32	Y	614	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
34	C	517	BCR	C15-C14-C13	-3.62	122.14	127.31
46	Y	1623	NEX	C35-C34-C33	-3.62	122.14	127.31
32	B	603	CLA	CMB-C2B-C3B	3.62	131.45	124.68
32	S	609	CLA	CMA-C3A-C2A	-3.62	107.65	116.10
32	b	613	CLA	CHB-C4A-NA	3.62	129.51	124.51
32	D	403	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
34	c	517	BCR	C15-C14-C13	-3.61	122.15	127.31
32	A	410	CLA	CMB-C2B-C3B	3.61	131.43	124.68
36	c	521	LMG	O7-C10-C11	3.61	119.28	111.50
32	n	612	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
43	Y	605	CHL	CAC-C3C-C4C	3.60	129.49	124.81
43	r	608	CHL	CAC-C3C-C4C	3.60	129.48	124.81
32	c	504	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
43	n	609	CHL	C1C-C2C-C3C	-3.60	104.26	107.11
32	y	614	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
36	C	521	LMG	O7-C10-C11	3.60	119.25	111.50
32	b	603	CLA	CMB-C2B-C3B	3.59	131.40	124.68
32	s	612	CLA	CMB-C2B-C3B	3.59	131.40	124.68
32	N	610	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
43	R	608	CHL	CAC-C3C-C4C	3.59	129.47	124.81
44	N	1620	LUT	C35-C34-C33	-3.59	122.19	127.31
38	S	2630	LHG	O7-C7-C8	3.58	119.23	111.50
38	s	2630	LHG	O7-C7-C8	3.58	119.23	111.50
32	S	612	CLA	CMB-C2B-C3B	3.58	131.38	124.68
34	C	516	BCR	C24-C23-C22	-3.58	120.82	126.23
32	R	610	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
43	N	609	CHL	C1C-C2C-C3C	-3.58	104.27	107.11
32	n	610	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
32	s	610	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
32	N	613	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
32	a	410	CLA	CMB-C2B-C3B	3.57	131.36	124.68
32	N	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
34	A	411	BCR	C24-C23-C22	-3.57	120.84	126.23
32	A	406	CLA	CMB-C2B-C3B	3.57	131.35	124.68
32	C	504	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
34	a	411	BCR	C24-C23-C22	-3.56	120.85	126.23
34	c	517	BCR	C10-C11-C12	-3.56	112.12	123.22
45	y	1622	XAT	O24-C25-C38	3.55	119.31	115.06
32	r	604	CLA	CMB-C2B-C3B	3.55	131.32	124.68
34	C	517	BCR	C10-C11-C12	-3.55	112.14	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	n	1620	LUT	C35-C34-C33	-3.55	122.24	127.31
46	N	1623	NEX	C11-C10-C9	-3.55	122.24	127.31
43	Y	608	CHL	C3B-C4B-NB	3.55	113.80	109.21
43	Y	606	CHL	C4A-NA-C1A	-3.55	105.11	106.71
32	n	613	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
32	s	614	CLA	C4A-NA-C1A	3.54	108.30	106.71
32	a	406	CLA	CMB-C2B-C3B	3.54	131.30	124.68
43	G	606	CHL	CAC-C3C-C4C	3.54	129.40	124.81
32	B	611	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
32	b	611	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
32	S	610	CLA	C1B-CHB-C4A	-3.54	123.11	130.12
43	N	608	CHL	C3B-C4B-NB	3.53	113.78	109.21
32	y	613	CLA	CMB-C2B-C3B	3.53	131.29	124.68
44	g	1620	LUT	C15-C14-C13	-3.53	122.27	127.31
32	C	502	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
34	C	517	BCR	C20-C21-C22	-3.53	122.27	127.31
34	c	516	BCR	C24-C23-C22	-3.53	120.90	126.23
46	g	1623	NEX	O24-C25-C38	3.53	119.28	115.06
32	c	502	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
32	Y	613	CLA	CMB-C2B-C3B	3.53	131.27	124.68
32	s	603	CLA	CMB-C2B-C3B	3.52	131.27	124.68
43	y	608	CHL	C3B-C4B-NB	3.52	113.76	109.21
34	c	517	BCR	C20-C21-C22	-3.52	122.28	127.31
32	G	604	CLA	CMB-C2B-C3B	3.52	131.26	124.68
32	s	613	CLA	C1B-CHB-C4A	-3.52	123.15	130.12
32	g	604	CLA	CMB-C2B-C3B	3.52	131.26	124.68
43	G	601	CHL	C3B-C4B-NB	3.52	113.76	109.21
32	r	610	CLA	C4A-NA-C1A	3.52	108.29	106.71
32	B	605	CLA	CMB-C2B-C3B	3.52	131.26	124.68
32	Y	614	CLA	C4A-NA-C1A	3.51	108.29	106.71
32	y	614	CLA	C4A-NA-C1A	3.51	108.29	106.71
32	S	603	CLA	CMB-C2B-C3B	3.51	131.25	124.68
32	B	607	CLA	CMB-C2B-C3B	3.51	131.25	124.68
32	b	607	CLA	CMB-C2B-C3B	3.51	131.25	124.68
43	N	607	CHL	CAA-CBA-CGA	-3.51	103.00	113.25
43	g	601	CHL	C3B-C4B-NB	3.51	113.75	109.21
44	G	1620	LUT	C15-C14-C13	-3.51	122.30	127.31
43	g	601	CHL	CAC-C3C-C4C	3.51	129.36	124.81
32	S	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
32	b	605	CLA	CMB-C2B-C3B	3.51	131.24	124.68
32	Y	611	CLA	CMB-C2B-C3B	3.50	131.23	124.68
32	y	611	CLA	CMB-C2B-C3B	3.50	131.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	408	LHG	O7-C7-C8	3.50	119.05	111.50
32	S	609	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
44	n	1621	LUT	C35-C34-C33	-3.50	122.31	127.31
32	B	604	CLA	CMB-C2B-C3B	3.50	131.22	124.68
43	g	606	CHL	CAC-C3C-C4C	3.50	129.35	124.81
46	Y	1623	NEX	C11-C12-C13	-3.49	116.60	126.42
43	N	605	CHL	CGD-CBD-CAD	-3.49	99.42	110.73
43	n	608	CHL	C3B-C4B-NB	3.49	113.72	109.21
32	s	609	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
46	G	1623	NEX	O24-C25-C38	3.49	119.24	115.06
34	d	404	BCR	C38-C26-C25	-3.49	120.61	124.53
32	R	604	CLA	CMB-C2B-C3B	3.49	131.20	124.68
32	Y	614	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
32	y	614	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
43	g	601	CHL	CHD-C4C-C3C	-3.49	119.72	124.84
32	b	603	CLA	C4A-NA-C1A	3.48	108.27	106.71
43	n	607	CHL	CAA-CBA-CGA	-3.48	103.08	113.25
32	R	610	CLA	C4A-NA-C1A	3.48	108.27	106.71
32	b	615	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
43	n	606	CHL	CAC-C3C-C4C	3.48	129.32	124.81
32	b	604	CLA	CMB-C2B-C3B	3.48	131.18	124.68
32	s	602	CLA	CMB-C2B-C3B	3.48	131.18	124.68
32	r	610	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
32	S	614	CLA	C4A-NA-C1A	3.47	108.27	106.71
43	n	605	CHL	CGD-CBD-CAD	-3.47	99.49	110.73
38	d	408	LHG	O7-C7-C8	3.47	118.97	111.50
43	S	608	CHL	CHD-C4C-C3C	-3.47	119.75	124.84
32	B	615	CLA	O2D-CGD-O1D	-3.46	117.06	123.84
32	R	610	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
43	N	606	CHL	CAC-C3C-C4C	3.46	129.30	124.81
44	N	1621	LUT	C35-C34-C33	-3.46	122.38	127.31
32	A	410	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
40	D	405	PL9	C7-C8-C9	-3.46	121.04	126.79
40	d	405	PL9	C7-C8-C9	-3.45	121.04	126.79
43	y	606	CHL	C4A-NA-C1A	-3.45	105.15	106.71
45	N	1622	XAT	C4-C3-C2	-3.45	104.11	110.77
43	n	601	CHL	C3B-C4B-NB	3.45	113.67	109.21
43	Y	607	CHL	CHB-C4A-NA	3.45	129.28	124.51
45	n	1622	XAT	C4-C3-C2	-3.45	104.11	110.77
34	B	619	BCR	C16-C17-C18	-3.45	122.39	127.31
34	b	619	BCR	C16-C17-C18	-3.45	122.39	127.31
32	B	606	CLA	CMB-C2B-C1B	-3.44	123.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	s	608	CHL	CHD-C4C-C3C	-3.44	119.78	124.84
43	N	601	CHL	C3B-C4B-NB	3.44	113.66	109.21
32	g	614	CLA	C4A-NA-C1A	3.44	108.25	106.71
34	D	404	BCR	C38-C26-C25	-3.44	120.66	124.53
32	b	605	CLA	CAA-CBA-CGA	-3.44	103.20	113.25
34	c	515	BCR	C8-C7-C6	-3.44	117.55	127.20
32	S	602	CLA	CMB-C2B-C3B	3.44	131.11	124.68
34	C	515	BCR	C8-C7-C6	-3.44	117.55	127.20
32	C	512	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
32	S	605	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
32	s	605	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
32	C	506	CLA	C1B-CHB-C4A	-3.43	123.32	130.12
43	y	601	CHL	CHB-C4A-NA	3.43	129.25	124.51
43	y	607	CHL	CHB-C4A-NA	3.43	129.25	124.51
32	B	605	CLA	CAA-CBA-CGA	-3.43	103.23	113.25
32	n	602	CLA	C4A-NA-C1A	3.43	108.25	106.71
43	Y	601	CHL	CHB-C4A-NA	3.42	129.25	124.51
45	Y	1622	XAT	O24-C25-C38	3.42	119.16	115.06
32	C	509	CLA	CHB-C4A-NA	3.42	129.24	124.51
32	B	604	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
32	c	501	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
32	c	506	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
32	b	604	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
32	N	602	CLA	C4A-NA-C1A	3.41	108.24	106.71
32	c	512	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
43	G	601	CHL	C1C-C2C-C3C	-3.41	104.41	107.11
32	R	602	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
43	G	608	CHL	CAC-C3C-C4C	3.40	129.23	124.81
34	A	411	BCR	C11-C10-C9	-3.40	122.45	127.31
43	n	607	CHL	C3B-C4B-NB	3.40	113.61	109.21
32	r	602	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
32	G	610	CLA	CMB-C2B-C3B	3.40	131.04	124.68
32	c	509	CLA	CHB-C4A-NA	3.40	129.21	124.51
32	b	606	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
38	n	2630	LHG	O7-C7-C8	3.40	118.82	111.50
35	a	412	SQD	O8-S-O7	3.40	119.57	111.27
43	g	608	CHL	CAC-C3C-C4C	3.39	129.21	124.81
32	C	501	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
32	R	602	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
38	D	410	LHG	O7-C7-C8	3.39	118.81	111.50
38	d	410	LHG	O7-C7-C8	3.39	118.81	111.50
32	c	508	CLA	C1B-CHB-C4A	-3.39	123.41	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	613	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
38	N	2630	LHG	O7-C7-C8	3.39	118.80	111.50
34	a	411	BCR	C11-C10-C9	-3.39	122.48	127.31
32	a	410	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
46	n	1623	NEX	C11-C10-C9	-3.38	122.48	127.31
45	R	624	XAT	C10-C11-C12	-3.38	112.66	123.22
32	C	508	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
35	A	412	SQD	O8-S-O7	3.38	119.53	111.27
45	r	624	XAT	C10-C11-C12	-3.37	112.69	123.22
32	G	612	CLA	CMB-C2B-C3B	3.37	130.99	124.68
32	g	612	CLA	CMB-C2B-C3B	3.37	130.99	124.68
42	Z	2634	LMU	C1B-O5B-C5B	3.37	120.30	113.69
32	g	613	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
45	r	624	XAT	C35-C15-C14	-3.37	116.58	123.47
32	B	604	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
32	y	604	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
32	g	610	CLA	CMB-C2B-C3B	3.36	130.97	124.68
32	r	602	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
45	R	624	XAT	C35-C15-C14	-3.36	116.59	123.47
46	y	1623	NEX	C11-C12-C13	-3.36	116.98	126.42
43	n	608	CHL	CAC-C3C-C4C	3.36	129.16	124.81
34	b	618	BCR	C20-C21-C22	-3.35	122.52	127.31
34	B	620	BCR	C11-C10-C9	-3.35	122.52	127.31
32	s	610	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
44	y	1621	LUT	C10-C11-C12	-3.35	112.76	123.22
42	z	2634	LMU	C1B-O5B-C5B	3.35	120.27	113.69
32	N	611	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
44	Y	1621	LUT	C10-C11-C12	-3.35	112.77	123.22
43	Y	605	CHL	C3B-C4B-NB	3.35	113.54	109.21
43	y	605	CHL	C3B-C4B-NB	3.35	113.54	109.21
32	r	610	CLA	C1B-CHB-C4A	-3.34	123.49	130.12
32	Y	602	CLA	CMB-C2B-C3B	3.34	130.93	124.68
32	y	602	CLA	CMB-C2B-C3B	3.34	130.93	124.68
34	D	404	BCR	C23-C24-C25	-3.34	117.81	127.20
32	G	603	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
34	b	620	BCR	C11-C10-C9	-3.34	122.55	127.31
32	Y	602	CLA	C4A-NA-C1A	3.33	108.20	106.71
32	y	602	CLA	C4A-NA-C1A	3.33	108.20	106.71
34	B	618	BCR	C20-C21-C22	-3.33	122.55	127.31
32	Y	604	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
43	n	607	CHL	C6-C5-C3	-3.33	104.73	113.45
32	S	610	CLA	CMB-C2B-C1B	-3.33	123.35	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Y	1622	XAT	C35-C34-C33	-3.33	122.56	127.31
43	N	607	CHL	C3B-C4B-NB	3.33	113.51	109.21
32	s	605	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
32	G	614	CLA	C4A-NA-C1A	3.32	108.20	106.71
45	y	1622	XAT	C35-C34-C33	-3.32	122.57	127.31
34	d	404	BCR	C23-C24-C25	-3.32	117.88	127.20
32	S	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
32	s	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
32	G	603	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
32	b	604	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
32	S	605	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
44	g	1621	LUT	C35-C34-C33	-3.31	122.58	127.31
43	N	608	CHL	CAC-C3C-C4C	3.31	129.11	124.81
32	n	611	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
34	C	517	BCR	C21-C20-C19	-3.31	112.89	123.22
32	D	403	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
34	c	517	BCR	C21-C20-C19	-3.31	112.90	123.22
32	B	608	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
32	b	608	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
43	y	601	CHL	CAC-C3C-C4C	3.30	129.09	124.81
43	N	607	CHL	C6-C5-C3	-3.30	104.80	113.45
43	G	601	CHL	CHB-C4A-NA	3.30	129.08	124.51
34	c	515	BCR	C11-C10-C9	-3.30	122.60	127.31
34	c	515	BCR	C4-C5-C6	-3.30	117.94	122.73
44	Y	1620	LUT	C35-C15-C14	-3.30	116.72	123.47
44	y	1620	LUT	C35-C15-C14	-3.30	116.72	123.47
43	Y	601	CHL	CAC-C3C-C4C	3.30	129.09	124.81
32	A	406	CLA	CHD-C1D-ND	-3.29	121.43	124.45
44	G	1621	LUT	C35-C34-C33	-3.29	122.61	127.31
43	r	608	CHL	C3B-C4B-NB	3.29	113.46	109.21
32	Y	603	CLA	CMB-C2B-C3B	3.29	130.83	124.68
32	r	609	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
43	N	607	CHL	C4-C3-C5	3.28	120.80	115.27
32	y	603	CLA	CMB-C2B-C3B	3.28	130.82	124.68
32	r	603	CLA	CMB-C2B-C3B	3.28	130.82	124.68
32	R	603	CLA	CMB-C2B-C3B	3.28	130.82	124.68
32	d	403	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
34	A	411	BCR	C21-C20-C19	-3.28	112.98	123.22
34	C	515	BCR	C4-C5-C6	-3.28	117.97	122.73
46	n	1623	NEX	O24-C25-C38	3.28	118.98	115.06
34	a	411	BCR	C21-C20-C19	-3.27	113.00	123.22
34	C	515	BCR	C11-C10-C9	-3.27	122.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	R	608	CHL	C3B-C4B-NB	3.27	113.44	109.21
32	g	611	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
43	n	601	CHL	CMD-C2D-C3D	-3.27	120.09	127.61
44	s	1620	LUT	C7-C8-C9	-3.27	121.30	126.23
32	R	609	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
32	c	513	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
32	g	603	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
43	N	601	CHL	CMD-C2D-C3D	-3.26	120.11	127.61
43	n	607	CHL	C4-C3-C5	3.26	120.76	115.27
32	c	505	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
32	G	611	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
32	R	603	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
32	C	506	CLA	CMB-C2B-C3B	3.26	130.78	124.68
44	S	1620	LUT	C7-C8-C9	-3.26	121.31	126.23
45	g	1622	XAT	C11-C10-C9	-3.25	122.67	127.31
32	a	406	CLA	CHD-C1D-ND	-3.25	121.46	124.45
32	s	609	CLA	CMA-C3A-C2A	-3.25	108.51	116.10
32	s	614	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
32	S	614	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
43	S	606	CHL	C3B-C4B-NB	3.25	113.41	109.21
46	N	1623	NEX	O24-C25-C38	3.25	118.95	115.06
43	G	607	CHL	C3B-C4B-NB	3.25	113.41	109.21
32	C	505	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
45	Y	1622	XAT	C10-C11-C12	-3.25	113.08	123.22
43	y	609	CHL	C3B-C4B-NB	3.25	113.41	109.21
34	b	620	BCR	C15-C14-C13	-3.24	122.68	127.31
43	G	607	CHL	CHB-C4A-NA	3.24	129.00	124.51
43	N	609	CHL	C1-O2A-CGA	3.24	124.94	116.44
43	y	609	CHL	CAC-C3C-C4C	3.24	129.01	124.81
32	B	603	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
45	G	1622	XAT	C27-C28-C29	-3.24	120.51	125.53
32	B	603	CLA	C4A-NA-C1A	3.23	108.16	106.71
46	R	625	NEX	C15-C35-C34	-3.23	116.85	123.47
43	g	607	CHL	C3B-C4B-NB	3.23	113.39	109.21
32	G	602	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
32	r	603	CLA	CAA-C2A-C3A	-3.23	103.94	112.78
46	g	1623	NEX	C15-C35-C34	-3.23	116.86	123.47
32	Y	612	CLA	CMB-C2B-C3B	3.22	130.71	124.68
45	g	1622	XAT	C27-C28-C29	-3.22	120.53	125.53
45	G	1622	XAT	C11-C10-C9	-3.22	122.72	127.31
32	b	603	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
32	C	505	CLA	O2D-CGD-O1D	-3.22	117.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	N	1622	XAT	C35-C34-C33	-3.22	122.72	127.31
45	n	1622	XAT	C35-C34-C33	-3.22	122.72	127.31
32	c	509	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
43	S	608	CHL	C3B-C4B-NB	3.21	113.37	109.21
43	G	605	CHL	CAC-C3C-C4C	3.21	128.98	124.81
43	g	605	CHL	CAC-C3C-C4C	3.21	128.98	124.81
43	g	601	CHL	CHB-C4A-NA	3.21	128.95	124.51
32	C	509	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
32	c	505	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
43	s	606	CHL	C3B-C4B-NB	3.21	113.36	109.21
32	D	403	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
32	c	506	CLA	CMB-C2B-C3B	3.21	130.68	124.68
34	B	620	BCR	C15-C14-C13	-3.21	122.73	127.31
32	N	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
32	n	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
32	B	615	CLA	CMB-C2B-C3B	3.21	130.68	124.68
46	S	1623	NEX	C35-C34-C33	-3.21	122.73	127.31
32	g	602	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
32	d	403	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
32	y	612	CLA	CMB-C2B-C3B	3.20	130.67	124.68
32	B	612	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
43	Y	609	CHL	CAC-C3C-C4C	3.20	128.96	124.81
43	g	605	CHL	CMD-C2D-C3D	-3.20	120.25	127.61
32	y	612	CLA	C4A-NA-C1A	3.20	108.14	106.71
43	G	605	CHL	CMD-C2D-C3D	-3.20	120.26	127.61
32	B	610	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
32	b	610	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
43	g	607	CHL	CHB-C4A-NA	3.20	128.93	124.51
46	G	1623	NEX	C15-C35-C34	-3.19	116.94	123.47
32	S	613	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
32	g	603	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
32	b	612	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
43	n	609	CHL	C1-O2A-CGA	3.18	124.79	116.44
32	a	406	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
45	Y	1622	XAT	C4-C3-C2	-3.18	104.63	110.77
43	N	609	CHL	CMB-C2B-C3B	3.18	130.62	124.68
32	s	613	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
32	S	602	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
45	y	1622	XAT	C4-C3-C2	-3.18	104.64	110.77
32	b	602	CLA	CMB-C2B-C1B	-3.17	123.58	128.46
45	y	1622	XAT	C10-C11-C12	-3.17	113.31	123.22
43	y	601	CHL	O2D-CGD-O1D	-3.17	117.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	602	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
32	c	512	CLA	CHB-C4A-NA	3.17	128.90	124.51
32	b	610	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
45	r	624	XAT	C15-C14-C13	-3.17	122.78	127.31
43	Y	609	CHL	C3B-C4B-NB	3.17	113.31	109.21
34	D	404	BCR	C24-C23-C22	-3.17	121.44	126.23
32	n	614	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
32	b	615	CLA	CMB-C2B-C3B	3.17	130.61	124.68
32	G	614	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
43	Y	601	CHL	O2D-CGD-O1D	-3.17	117.65	123.84
32	C	513	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
32	g	614	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
43	n	609	CHL	CMB-C2B-C3B	3.16	130.59	124.68
32	A	407	CLA	O2D-CGD-CBD	3.16	116.89	111.27
32	c	511	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
32	N	614	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
43	s	608	CHL	C3B-C4B-NB	3.16	113.29	109.21
43	R	607	CHL	C3B-C4B-NB	3.16	113.29	109.21
43	r	607	CHL	C3B-C4B-NB	3.16	113.29	109.21
32	y	611	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
45	R	624	XAT	C15-C14-C13	-3.15	122.81	127.31
32	s	602	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
43	S	607	CHL	C3B-C4B-NB	3.15	113.28	109.21
34	d	404	BCR	C38-C26-C27	3.15	119.67	113.62
34	b	620	BCR	C28-C27-C26	-3.15	108.45	114.08
34	D	404	BCR	C38-C26-C27	3.15	119.66	113.62
34	c	516	BCR	C20-C21-C22	-3.15	122.82	127.31
32	A	406	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
32	a	407	CLA	O2D-CGD-CBD	3.15	116.86	111.27
32	C	513	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
32	B	610	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
32	Y	612	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
32	C	512	CLA	CHB-C4A-NA	3.14	128.86	124.51
32	y	612	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
32	S	609	CLA	C4A-NA-C1A	3.14	108.12	106.71
32	n	604	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
34	d	404	BCR	C24-C23-C22	-3.14	121.49	126.23
32	C	512	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
32	C	511	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
32	d	403	CLA	CMB-C2B-C3B	3.13	130.54	124.68
46	S	1623	NEX	O24-C25-C38	3.13	118.81	115.06
32	c	513	CLA	C1B-CHB-C4A	-3.13	123.91	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	403	CLA	CMB-C2B-C3B	3.13	130.54	124.68
34	B	620	BCR	C28-C27-C26	-3.13	108.48	114.08
46	S	1623	NEX	C11-C10-C9	-3.13	122.84	127.31
32	Y	611	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
34	b	619	BCR	C38-C26-C25	-3.13	121.02	124.53
46	s	1623	NEX	C35-C34-C33	-3.13	122.85	127.31
32	S	605	CLA	CHB-C4A-NA	3.12	128.83	124.51
32	Y	613	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
32	N	604	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
34	B	620	BCR	C33-C5-C6	-3.12	121.03	124.53
43	S	601	CHL	CHD-C4C-C3C	-3.12	120.26	124.84
34	C	516	BCR	C20-C21-C22	-3.12	122.86	127.31
32	y	613	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
32	s	605	CLA	CHB-C4A-NA	3.11	128.82	124.51
43	g	609	CHL	CMB-C2B-C3B	3.11	130.50	124.68
38	D	409	LHG	O7-C7-C8	3.11	118.21	111.50
32	Y	612	CLA	C4A-NA-C1A	3.11	108.11	106.71
34	A	411	BCR	C33-C5-C6	-3.11	121.03	124.53
32	S	609	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
34	a	411	BCR	C33-C5-C6	-3.11	121.04	124.53
43	n	606	CHL	CMB-C2B-C3B	3.11	130.50	124.68
32	N	613	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
32	N	611	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
32	n	611	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
32	s	609	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
46	s	1623	NEX	O24-C25-C38	3.10	118.78	115.06
32	D	403	CLA	CHB-C4A-NA	3.10	128.80	124.51
34	b	620	BCR	C33-C5-C6	-3.10	121.04	124.53
32	B	610	CLA	CMB-C2B-C3B	3.10	130.48	124.68
32	b	610	CLA	CMB-C2B-C3B	3.10	130.48	124.68
43	s	607	CHL	C3B-C4B-NB	3.10	113.22	109.21
32	n	613	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
32	c	504	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
32	A	407	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
43	y	609	CHL	O2D-CGD-O1D	-3.09	117.79	123.84
38	d	409	LHG	O7-C7-C8	3.09	118.17	111.50
43	N	606	CHL	CMB-C2B-C3B	3.09	130.47	124.68
43	s	601	CHL	CHD-C4C-C3C	-3.09	120.29	124.84
43	G	609	CHL	CMB-C2B-C3B	3.09	130.47	124.68
43	Y	609	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
32	C	504	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
46	r	625	NEX	C15-C35-C34	-3.09	117.15	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	s	604	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
43	y	601	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
43	n	605	CHL	O1D-CGD-CBD	-3.08	118.18	124.48
32	a	407	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
32	G	614	CLA	CMB-C2B-C3B	3.08	130.44	124.68
32	Y	614	CLA	CMB-C2B-C3B	3.08	130.44	124.68
32	y	614	CLA	CMB-C2B-C3B	3.08	130.44	124.68
32	c	504	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
43	n	605	CHL	CAC-C3C-C4C	3.08	128.80	124.81
32	c	512	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
43	N	605	CHL	CAC-C3C-C4C	3.07	128.80	124.81
43	N	608	CHL	CHB-C4A-NA	3.07	128.76	124.51
43	G	609	CHL	C3B-C4B-NB	3.07	113.18	109.21
43	g	609	CHL	C3B-C4B-NB	3.07	113.18	109.21
32	Y	604	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
32	d	403	CLA	CHB-C4A-NA	3.07	128.76	124.51
43	R	606	CHL	C3B-C4B-NB	3.07	113.18	109.21
43	r	606	CHL	C3B-C4B-NB	3.07	113.18	109.21
32	b	607	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
34	B	619	BCR	C38-C26-C25	-3.07	121.08	124.53
43	G	601	CHL	CAC-C3C-C4C	3.07	128.79	124.81
32	g	614	CLA	CMB-C2B-C3B	3.07	130.41	124.68
32	y	604	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
34	C	514	BCR	C7-C8-C9	-3.06	121.61	126.23
32	a	405	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
34	c	517	BCR	C16-C17-C18	-3.06	122.94	127.31
32	C	504	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
32	S	604	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
43	n	608	CHL	CHB-C4A-NA	3.06	128.75	124.51
32	B	603	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
32	Y	604	CLA	CMB-C2B-C3B	3.06	130.40	124.68
32	s	612	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
34	c	514	BCR	C7-C8-C9	-3.06	121.62	126.23
32	b	609	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
44	y	1620	LUT	C30-C31-C32	-3.06	113.68	123.22
32	B	607	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
32	g	612	CLA	CHB-C4A-NA	3.05	128.73	124.51
32	A	405	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
32	n	612	CLA	CMB-C2B-C3B	3.05	130.39	124.68
43	Y	601	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
34	C	517	BCR	C16-C17-C18	-3.05	122.96	127.31
44	Y	1620	LUT	C30-C31-C32	-3.05	113.70	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	601	CHL	C1C-C2C-C3C	-3.05	104.69	107.11
34	B	618	BCR	C7-C8-C9	-3.05	121.63	126.23
32	c	507	CLA	C2A-C1A-CHA	3.05	129.19	123.86
43	N	605	CHL	O1D-CGD-CBD	-3.05	118.25	124.48
43	g	601	CHL	CMD-C2D-C3D	-3.04	120.61	127.61
46	G	1623	NEX	C39-C29-C30	-3.04	118.66	122.92
36	h	102	LMG	O8-C28-C29	3.04	121.45	111.91
32	Y	602	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
32	y	602	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
32	c	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
32	g	604	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
34	d	404	BCR	C20-C21-C22	-3.04	122.97	127.31
32	b	603	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
32	y	604	CLA	CMB-C2B-C3B	3.04	130.36	124.68
40	D	405	PL9	C7-C3-C4	3.04	119.35	116.88
32	B	609	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
32	G	612	CLA	CHB-C4A-NA	3.04	128.71	124.51
32	Y	603	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
34	b	618	BCR	C7-C8-C9	-3.04	121.65	126.23
32	G	614	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
46	Y	1623	NEX	C16-C1-C6	3.03	113.19	110.47
32	g	614	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
32	S	612	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
32	C	506	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
34	C	515	BCR	C33-C5-C6	-3.03	121.13	124.53
32	G	612	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
44	y	1620	LUT	C8-C9-C10	-3.02	114.30	118.94
32	y	603	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
32	y	602	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
32	N	612	CLA	CMB-C2B-C3B	3.02	130.33	124.68
32	G	604	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
32	C	512	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
32	s	614	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
34	D	404	BCR	C20-C21-C22	-3.01	123.01	127.31
46	R	625	NEX	C26-C27-C28	-3.01	119.62	125.99
43	n	605	CHL	C4-C3-C5	3.01	120.34	115.27
43	g	608	CHL	CMD-C2D-C3D	-3.01	120.68	127.61
36	H	102	LMG	O8-C28-C29	3.01	121.36	111.91
32	g	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
32	C	507	CLA	C2A-C1A-CHA	3.01	129.12	123.86
32	S	614	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
32	g	603	CLA	CHB-C4A-NA	3.01	128.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	602	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
43	G	608	CHL	CMD-C2D-C3D	-3.01	120.70	127.61
46	g	1623	NEX	C39-C29-C30	-3.00	118.71	122.92
45	Y	1622	XAT	C36-C21-C26	3.00	118.16	110.05
34	c	515	BCR	C33-C5-C6	-3.00	121.16	124.53
43	N	605	CHL	C4-C3-C5	3.00	120.32	115.27
32	s	612	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
32	G	603	CLA	CHB-C4A-NA	3.00	128.66	124.51
32	S	611	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
32	s	611	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
46	r	625	NEX	C26-C27-C28	-3.00	119.65	125.99
46	y	1623	NEX	C31-C30-C29	-3.00	123.03	127.31
43	n	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
43	N	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
34	c	514	BCR	C15-C16-C17	-3.00	117.34	123.47
32	Y	602	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
32	a	407	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
44	y	1620	LUT	C38-C25-C24	-2.99	117.15	123.56
44	Y	1620	LUT	C8-C9-C10	-2.99	114.35	118.94
32	R	610	CLA	CMB-C2B-C3B	2.99	130.28	124.68
32	s	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
32	s	602	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
32	A	407	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
45	y	1622	XAT	C36-C21-C26	2.99	118.11	110.05
32	N	612	CLA	CHB-C4A-NA	2.99	128.64	124.51
32	n	612	CLA	CHB-C4A-NA	2.99	128.64	124.51
32	S	612	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
43	n	607	CHL	CAA-C2A-C3A	-2.98	104.61	112.78
32	A	410	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
43	y	608	CHL	O2A-CGA-CBA	2.98	121.26	111.91
32	N	613	CLA	CMB-C2B-C3B	2.98	130.25	124.68
43	N	607	CHL	CAA-C2A-C3A	-2.98	104.62	112.78
32	b	616	CLA	CHB-C4A-NA	2.98	128.63	124.51
43	y	609	CHL	CMB-C2B-C3B	2.98	130.25	124.68
43	n	607	CHL	CAC-C3C-C4C	2.97	128.67	124.81
34	C	514	BCR	C15-C16-C17	-2.97	117.38	123.47
43	r	608	CHL	CMB-C2B-C3B	2.97	130.24	124.68
43	R	608	CHL	CMB-C2B-C3B	2.97	130.24	124.68
32	B	616	CLA	CHB-C4A-NA	2.97	128.62	124.51
44	g	1620	LUT	C35-C15-C14	-2.97	117.38	123.47
42	y	2632	LMU	O5B-C5B-C4B	2.97	115.09	109.69
44	Y	1620	LUT	C38-C25-C24	-2.97	117.20	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	r	624	XAT	C24-C23-C22	-2.97	105.04	110.77
32	c	510	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
43	Y	608	CHL	O2A-CGA-CBA	2.97	121.23	111.91
32	S	612	CLA	CHB-C4A-NA	2.97	128.62	124.51
45	R	624	XAT	C24-C23-C22	-2.97	105.04	110.77
32	n	613	CLA	CMB-C2B-C3B	2.97	130.23	124.68
38	y	2630	LHG	C6-C5-C4	-2.96	104.78	111.79
38	Y	2630	LHG	C6-C5-C4	-2.96	104.78	111.79
44	G	1620	LUT	C35-C15-C14	-2.96	117.40	123.47
32	a	410	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
32	s	610	CLA	CMB-C2B-C3B	2.96	130.22	124.68
43	Y	609	CHL	CMB-C2B-C3B	2.96	130.22	124.68
32	b	607	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
32	C	511	CLA	CHB-C4A-NA	2.96	128.60	124.51
32	c	507	CLA	CHB-C4A-NA	2.96	128.60	124.51
40	d	405	PL9	C7-C3-C4	2.96	119.28	116.88
32	Y	614	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
43	N	607	CHL	CMB-C2B-C1B	2.96	133.01	128.46
38	y	2630	LHG	O8-C23-C24	2.96	121.18	111.91
38	Y	2630	LHG	O8-C23-C24	2.95	121.17	111.91
32	N	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
32	g	611	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
32	y	614	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
32	c	512	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
43	g	609	CHL	C1-O2A-CGA	2.94	124.17	116.44
32	G	612	CLA	C1B-CHB-C4A	-2.94	124.28	130.12
43	n	607	CHL	CMB-C2B-C1B	2.94	132.99	128.46
32	B	611	CLA	CHB-C4A-NA	2.94	128.58	124.51
32	b	611	CLA	CHB-C4A-NA	2.94	128.58	124.51
32	C	510	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
32	c	508	CLA	CHB-C4A-NA	2.94	128.58	124.51
32	S	610	CLA	CMB-C2B-C3B	2.94	130.18	124.68
32	B	607	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
43	g	609	CHL	C4-C3-C5	2.94	120.22	115.27
45	g	1622	XAT	C7-C8-C9	-2.94	120.97	125.53
38	G	2630	LHG	O7-C7-C8	2.94	117.84	111.50
32	n	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
44	s	1621	LUT	C15-C14-C13	-2.94	123.12	127.31
38	g	2630	LHG	O7-C7-C8	2.94	117.83	111.50
43	G	609	CHL	C1-O2A-CGA	2.94	124.15	116.44
42	Y	2632	LMU	O5B-C5B-C4B	2.94	115.03	109.69
32	N	610	CLA	CHB-C4A-NA	2.94	128.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	n	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
43	N	607	CHL	CAC-C3C-C4C	2.93	128.62	124.81
43	G	609	CHL	C4-C3-C5	2.93	120.21	115.27
32	c	503	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
45	G	1622	XAT	C7-C8-C9	-2.93	120.98	125.53
44	S	1621	LUT	C15-C14-C13	-2.93	123.13	127.31
32	c	511	CLA	CHB-C4A-NA	2.93	128.56	124.51
32	S	605	CLA	CMB-C2B-C3B	2.93	130.16	124.68
32	y	603	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
36	B	622	LMG	C8-O7-C10	-2.93	110.58	117.79
33	A	408	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
44	s	1620	LUT	C15-C35-C34	-2.93	117.48	123.47
32	g	612	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
43	N	605	CHL	C1C-C2C-C3C	-2.93	104.79	107.11
44	S	1620	LUT	C15-C35-C34	-2.92	117.48	123.47
32	C	507	CLA	CHB-C4A-NA	2.92	128.56	124.51
32	s	605	CLA	CMB-C2B-C3B	2.92	130.15	124.68
44	S	1621	LUT	C35-C15-C14	-2.92	117.49	123.47
36	b	622	LMG	C8-O7-C10	-2.92	110.60	117.79
32	G	611	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
32	B	611	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
32	N	604	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
32	n	610	CLA	CHB-C4A-NA	2.92	128.55	124.51
34	B	620	BCR	C20-C21-C22	-2.92	123.14	127.31
32	Y	603	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
46	r	625	NEX	C31-C30-C29	-2.92	123.15	127.31
36	c	521	LMG	O8-C28-C29	2.92	121.06	111.91
44	g	1620	LUT	C11-C10-C9	-2.92	123.15	127.31
36	C	521	LMG	O8-C28-C29	2.92	121.06	111.91
37	C	519	DGD	O1G-C1A-C2A	2.91	121.03	111.91
33	a	408	PHO	O2D-CGD-O1D	-2.91	118.15	123.84
32	C	508	CLA	CHB-C4A-NA	2.91	128.53	124.51
32	C	507	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
32	B	605	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
46	s	1623	NEX	C2-C1-C6	2.90	112.03	109.21
32	C	503	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
45	r	624	XAT	C31-C30-C29	-2.90	123.17	127.31
32	C	501	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
37	c	519	DGD	O1G-C1A-C2A	2.90	121.01	111.91
36	d	411	LMG	O8-C28-C29	2.90	121.00	111.91
32	b	611	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
32	b	605	CLA	C1B-CHB-C4A	-2.90	124.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	501	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
44	s	1621	LUT	C35-C15-C14	-2.90	117.54	123.47
32	C	503	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
46	r	625	NEX	C24-C23-C22	-2.90	105.18	110.77
32	C	502	CLA	CHB-C4A-NA	2.90	128.52	124.51
32	G	613	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
32	D	402	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
38	L	101	LHG	C5-O7-C7	-2.89	110.67	117.79
32	B	615	CLA	CHB-C4A-NA	2.89	128.51	124.51
46	R	625	NEX	C24-C23-C22	-2.89	105.19	110.77
32	c	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	c	502	CLA	CHB-C4A-NA	2.89	128.51	124.51
32	r	602	CLA	CMB-C2B-C3B	2.89	130.08	124.68
34	A	411	BCR	C15-C14-C13	-2.89	123.19	127.31
32	C	513	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
45	r	624	XAT	C4-C3-C2	-2.89	105.20	110.77
36	D	411	LMG	O8-C28-C29	2.89	120.97	111.91
32	b	606	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
45	R	624	XAT	C31-C30-C29	-2.88	123.19	127.31
32	G	610	CLA	CHB-C4A-NA	2.88	128.50	124.51
32	c	502	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
45	R	624	XAT	C4-C3-C2	-2.88	105.21	110.77
44	S	1621	LUT	C39-C29-C28	2.88	122.62	118.08
32	b	606	CLA	CMB-C2B-C3B	2.88	130.07	124.68
34	b	620	BCR	C20-C21-C22	-2.88	123.20	127.31
32	B	606	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
32	R	602	CLA	CMB-C2B-C3B	2.88	130.07	124.68
38	l	101	LHG	C5-O7-C7	-2.88	110.70	117.79
43	R	608	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
34	c	516	BCR	C16-C15-C14	-2.88	117.58	123.47
43	Y	609	CHL	CHB-C4A-NA	2.88	128.49	124.51
32	B	606	CLA	CMB-C2B-C3B	2.88	130.06	124.68
32	Y	613	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
32	c	503	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
44	N	1621	LUT	C10-C11-C12	-2.87	114.25	123.22
32	g	610	CLA	CHB-C4A-NA	2.87	128.49	124.51
32	C	502	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
46	Y	1623	NEX	C31-C30-C29	-2.87	123.21	127.31
32	c	507	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
32	r	604	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
32	B	607	CLA	CHB-C4A-NA	2.87	128.48	124.51
32	g	613	CLA	O2D-CGD-O1D	-2.87	118.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	613	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	s	603	CLA	CHB-C4A-NA	2.87	128.48	124.51
43	S	608	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
43	s	601	CHL	CMB-C2B-C3B	2.86	130.04	124.68
43	y	609	CHL	CHB-C4A-NA	2.86	128.47	124.51
32	R	603	CLA	CHB-C4A-NA	2.86	128.47	124.51
32	R	604	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
44	Y	1621	LUT	C30-C31-C32	-2.86	114.28	123.22
44	y	1621	LUT	C30-C31-C32	-2.86	114.28	123.22
32	S	613	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
32	c	513	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
44	n	1621	LUT	C10-C11-C12	-2.86	114.29	123.22
43	n	605	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
32	S	603	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
43	G	605	CHL	CHD-C4C-C3C	-2.86	120.64	124.84
32	b	607	CLA	CHB-C4A-NA	2.86	128.47	124.51
32	s	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
46	r	625	NEX	C39-C29-C30	-2.86	118.92	122.92
34	b	619	BCR	C33-C5-C6	-2.86	121.32	124.53
32	d	402	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
44	s	1621	LUT	C39-C29-C28	2.85	122.57	118.08
43	g	605	CHL	CHD-C4C-C3C	-2.85	120.64	124.84
32	R	609	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	g	613	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
43	r	608	CHL	CMD-C2D-C3D	-2.85	121.05	127.61
32	s	603	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
32	S	603	CLA	CHB-C4A-NA	2.85	128.45	124.51
32	G	613	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
32	G	611	CLA	O2D-CGD-CBD	2.85	116.33	111.27
34	C	516	BCR	C16-C15-C14	-2.85	117.64	123.47
44	G	1620	LUT	C11-C10-C9	-2.85	123.25	127.31
34	B	619	BCR	C33-C5-C6	-2.85	121.33	124.53
43	Y	607	CHL	C11-C12-C13	-2.85	106.72	115.92
42	Z	2635	LMU	O5B-C5B-C4B	2.85	114.86	109.69
32	b	615	CLA	CHB-C4A-NA	2.85	128.45	124.51
34	a	411	BCR	C15-C14-C13	-2.85	123.25	127.31
43	y	609	CHL	C1-O2A-CGA	2.84	123.91	116.44
43	n	605	CHL	CHB-C4A-NA	2.84	128.44	124.51
32	N	611	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
32	g	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
32	r	609	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
32	b	616	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	n	611	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
46	r	625	NEX	O24-C25-C38	2.84	118.46	115.06
32	r	603	CLA	CHB-C4A-NA	2.84	128.44	124.51
46	y	1623	NEX	C16-C1-C6	2.84	113.01	110.47
46	R	625	NEX	O24-C25-C38	2.84	118.46	115.06
45	g	1622	XAT	C30-C31-C32	-2.84	114.37	123.22
44	N	1621	LUT	C19-C9-C8	2.84	122.54	118.08
43	y	607	CHL	C11-C12-C13	-2.83	106.76	115.92
32	B	614	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
34	D	404	BCR	C8-C7-C6	2.83	135.15	127.20
34	C	517	BCR	C29-C30-C25	2.83	114.84	110.48
32	C	507	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
45	G	1622	XAT	C30-C31-C32	-2.83	114.39	123.22
37	c	524	DGD	O1G-C1A-C2A	2.83	120.78	111.91
37	C	524	DGD	O1G-C1A-C2A	2.82	120.77	111.91
43	S	601	CHL	CMB-C2B-C3B	2.82	129.96	124.68
34	d	404	BCR	C8-C7-C6	2.82	135.13	127.20
32	s	614	CLA	CMB-C2B-C3B	2.82	129.96	124.68
32	B	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
42	z	2635	LMU	O5B-C5B-C4B	2.82	114.81	109.69
34	c	517	BCR	C29-C30-C25	2.82	114.82	110.48
32	c	504	CLA	CMB-C2B-C3B	2.82	129.95	124.68
43	N	609	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
32	N	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68
43	s	608	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
32	G	602	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
43	N	605	CHL	CHB-C4A-NA	2.81	128.40	124.51
32	b	602	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
38	l	101	LHG	O8-C23-C24	2.81	120.72	111.91
32	n	611	CLA	CMB-C2B-C3B	2.81	129.93	124.68
34	C	514	BCR	C11-C10-C9	-2.81	123.30	127.31
32	B	616	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
34	C	514	BCR	C21-C20-C19	-2.81	114.46	123.22
32	s	604	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
32	S	611	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
32	N	614	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
43	n	609	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
32	g	611	CLA	O2D-CGD-CBD	2.80	116.25	111.27
32	g	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
32	b	614	CLA	CHB-C4A-NA	2.80	128.38	124.51
32	S	614	CLA	CMB-C2B-C3B	2.80	129.92	124.68
32	G	613	CLA	CHB-C4A-NA	2.80	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	406	CLA	CHB-C4A-NA	2.80	128.38	124.51
32	s	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
32	n	612	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
32	s	609	CLA	CMB-C2B-C3B	2.80	129.91	124.68
32	G	610	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	b	614	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	S	609	CLA	CMB-C2B-C3B	2.80	129.91	124.68
32	Y	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
32	N	603	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
32	n	603	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
34	d	404	BCR	C30-C25-C26	-2.79	118.68	122.61
38	L	101	LHG	O8-C23-C24	2.79	120.67	111.91
44	G	1621	LUT	C10-C11-C12	-2.79	114.50	123.22
43	Y	609	CHL	C1-O2A-CGA	2.79	123.77	116.44
45	n	1622	XAT	C35-C15-C14	-2.79	117.75	123.47
32	d	402	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	y	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	C	504	CLA	CMB-C2B-C3B	2.79	129.90	124.68
32	A	410	CLA	CHB-C4A-NA	2.79	128.37	124.51
34	C	517	BCR	C3-C4-C5	-2.79	109.09	114.08
34	c	514	BCR	C21-C20-C19	-2.79	114.51	123.22
44	g	1621	LUT	C10-C11-C12	-2.79	114.51	123.22
32	y	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
32	B	613	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
32	b	611	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
44	n	1621	LUT	C19-C9-C8	2.79	122.47	118.08
32	N	612	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
32	B	602	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
32	b	613	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
32	Y	612	CLA	CHB-C4A-NA	2.79	128.36	124.51
34	D	404	BCR	C30-C25-C26	-2.78	118.69	122.61
32	S	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
43	n	608	CHL	CMB-C2B-C3B	2.78	129.88	124.68
38	g	2630	LHG	O8-C23-C24	2.78	120.63	111.91
43	y	607	CHL	CAA-C2A-C3A	-2.78	105.17	112.78
32	g	613	CLA	CHB-C4A-NA	2.78	128.35	124.51
32	n	614	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
32	B	609	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
43	N	608	CHL	CMB-C2B-C3B	2.78	129.87	124.68
43	G	605	CHL	C3B-C4B-NB	2.78	112.80	109.21
45	N	1622	XAT	C35-C15-C14	-2.78	117.79	123.47
32	r	610	CLA	O2D-CGD-O1D	-2.78	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	402	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
32	B	615	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
32	g	611	CLA	CHB-C4A-NA	2.77	128.35	124.51
32	b	616	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
32	b	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
33	A	409	PHO	O2D-CGD-O1D	-2.77	118.42	123.84
34	C	515	BCR	C3-C4-C5	-2.77	109.13	114.08
46	R	625	NEX	C31-C30-C29	-2.77	123.36	127.31
32	b	615	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
44	N	1620	LUT	C35-C15-C14	-2.77	117.80	123.47
32	b	609	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
34	c	517	BCR	C3-C4-C5	-2.77	109.14	114.08
34	b	619	BCR	C33-C5-C4	2.77	118.93	113.62
32	r	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
32	C	504	CLA	CHD-C1D-ND	-2.76	121.91	124.45
32	y	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
46	R	625	NEX	C39-C29-C30	-2.76	119.06	122.92
35	A	412	SQD	O48-C23-C24	2.76	120.57	111.91
43	g	605	CHL	C3B-C4B-NB	2.76	112.78	109.21
32	n	610	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
38	G	2630	LHG	O8-C23-C24	2.76	120.56	111.91
32	B	614	CLA	CHB-C4A-NA	2.76	128.32	124.51
32	Y	613	CLA	CHB-C4A-NA	2.76	128.32	124.51
32	G	611	CLA	CHB-C4A-NA	2.76	128.32	124.51
45	n	1622	XAT	C26-C27-C28	-2.76	120.17	125.99
32	y	604	CLA	CHB-C4A-NA	2.76	128.32	124.51
32	n	602	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
43	Y	607	CHL	CAA-C2A-C3A	-2.75	105.24	112.78
43	Y	601	CHL	C4-C3-C5	2.75	119.90	115.27
35	a	412	SQD	O48-C23-C24	2.75	120.54	111.91
45	N	1622	XAT	C26-C27-C28	-2.75	120.17	125.99
32	Y	612	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
32	A	410	CLA	C1-C2-C3	-2.75	121.29	126.04
44	n	1620	LUT	C35-C15-C14	-2.75	117.84	123.47
32	s	610	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
46	s	1623	NEX	C11-C10-C9	-2.75	123.39	127.31
34	c	515	BCR	C3-C4-C5	-2.75	109.17	114.08
44	Y	1621	LUT	C16-C1-C6	-2.74	105.85	110.30
32	a	410	CLA	CHB-C4A-NA	2.74	128.31	124.51
42	z	2635	LMU	C1B-O5B-C5B	2.74	119.07	113.69
32	G	603	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
32	N	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	609	CLA	CHB-C4A-NA	2.74	128.30	124.51
43	y	601	CHL	C4-C3-C5	2.74	119.88	115.27
32	r	610	CLA	CMB-C2B-C3B	2.74	129.80	124.68
34	c	516	BCR	C30-C25-C26	-2.74	118.76	122.61
32	Y	611	CLA	CHB-C4A-NA	2.74	128.30	124.51
46	G	1623	NEX	C24-C23-C22	-2.74	105.49	110.77
33	A	408	PHO	CBA-CAA-C2A	-2.74	105.82	113.81
32	y	612	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
32	R	610	CLA	CHB-C4A-NA	2.73	128.29	124.51
32	B	616	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
32	Y	603	CLA	CHB-C4A-NA	2.73	128.29	124.51
32	g	611	CLA	CMB-C2B-C3B	2.73	129.79	124.68
43	g	606	CHL	C3B-C4B-NB	2.73	112.74	109.21
32	c	504	CLA	CHD-C1D-ND	-2.73	121.94	124.45
32	Y	604	CLA	CHB-C4A-NA	2.73	128.29	124.51
34	c	514	BCR	C11-C10-C9	-2.73	123.42	127.31
42	Z	2635	LMU	C1B-O5B-C5B	2.73	119.04	113.69
43	G	607	CHL	CAA-C2A-C3A	-2.73	105.31	112.78
45	n	1622	XAT	C11-C10-C9	-2.73	123.42	127.31
32	A	405	CLA	CAC-C3C-C4C	2.73	128.35	124.81
32	B	612	CLA	CHB-C4A-NA	2.73	128.28	124.51
46	g	1623	NEX	C24-C23-C22	-2.72	105.51	110.77
32	A	406	CLA	CHB-C4A-NA	2.72	128.28	124.51
32	N	602	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
40	D	405	PL9	O1-C4-C3	-2.72	117.72	120.72
32	y	603	CLA	CHB-C4A-NA	2.72	128.28	124.51
34	B	619	BCR	C33-C5-C4	2.72	118.84	113.62
32	b	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
32	G	611	CLA	CMB-C2B-C3B	2.72	129.77	124.68
46	N	1623	NEX	C16-C1-C6	2.72	112.91	110.47
32	N	614	CLA	CHB-C4A-NA	2.72	128.27	124.51
32	Y	610	CLA	CHB-C4A-NA	2.72	128.27	124.51
32	y	611	CLA	CHB-C4A-NA	2.72	128.27	124.51
40	d	405	PL9	C31-C32-C33	-2.72	102.94	111.88
32	y	610	CLA	CHB-C4A-NA	2.72	128.27	124.51
32	g	603	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
43	G	601	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
32	R	603	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	b	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
32	a	410	CLA	C1-C2-C3	-2.72	121.34	126.04
46	n	1623	NEX	C24-C23-C22	-2.72	105.53	110.77
44	y	1621	LUT	C16-C1-C6	-2.72	105.89	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	521	LMG	C4-C3-C2	2.71	115.56	110.82
46	N	1623	NEX	C24-C23-C22	-2.71	105.53	110.77
44	Y	1620	LUT	C8-C7-C6	-2.71	119.58	127.20
44	y	1620	LUT	C8-C7-C6	-2.71	119.58	127.20
46	y	1623	NEX	C24-C23-C22	-2.71	105.53	110.77
46	Y	1623	NEX	C24-C23-C22	-2.71	105.54	110.77
32	c	504	CLA	CHB-C4A-NA	2.71	128.26	124.51
32	C	509	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
43	y	607	CHL	O2A-CGA-CBA	2.71	120.41	111.91
43	n	605	CHL	CMB-C2B-C3B	2.71	129.75	124.68
44	N	1620	LUT	C15-C14-C13	-2.71	123.44	127.31
44	n	1620	LUT	C15-C14-C13	-2.71	123.44	127.31
32	r	603	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	R	609	CLA	CHB-C4A-NA	2.71	128.26	124.51
43	G	606	CHL	C3B-C4B-NB	2.71	112.71	109.21
40	D	405	PL9	C31-C32-C33	-2.71	102.98	111.88
32	c	509	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	s	612	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
32	a	405	CLA	CAC-C3C-C4C	2.70	128.32	124.81
43	g	601	CHL	C4-C3-C5	2.70	119.82	115.27
32	S	612	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
32	N	603	CLA	CHB-C4A-NA	2.70	128.25	124.51
32	n	603	CLA	CHB-C4A-NA	2.70	128.25	124.51
40	d	405	PL9	C36-C34-C33	-2.70	115.65	121.12
32	b	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
43	g	609	CHL	CAC-C3C-C4C	2.70	128.31	124.81
43	g	607	CHL	CAA-C2A-C3A	-2.70	105.39	112.78
43	Y	607	CHL	O2A-CGA-CBA	2.70	120.38	111.91
32	C	510	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
32	g	613	CLA	CMB-C2B-C3B	2.70	129.73	124.68
45	G	1622	XAT	C24-C23-C22	-2.70	105.56	110.77
43	Y	601	CHL	C4D-CHA-C1A	-2.70	117.97	121.25
43	y	601	CHL	C4D-CHA-C1A	-2.70	117.97	121.25
32	B	608	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
37	c	519	DGD	C4E-C3E-C2E	2.70	115.53	110.82
43	Y	601	CHL	CBA-CAA-C2A	2.69	121.82	113.86
44	N	1621	LUT	C8-C9-C10	-2.69	114.81	118.94
32	B	617	CLA	CHB-C4A-NA	2.69	128.24	124.51
32	b	617	CLA	CHB-C4A-NA	2.69	128.24	124.51
32	G	613	CLA	CMB-C2B-C3B	2.69	129.71	124.68
32	b	614	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
32	n	614	CLA	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
44	S	1621	LUT	C19-C9-C8	2.69	122.31	118.08
43	N	605	CHL	CMB-C2B-C3B	2.69	129.71	124.68
32	N	614	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	R	604	CLA	CHB-C4A-NA	2.69	128.23	124.51
32	b	605	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
32	B	605	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
38	d	409	LHG	O8-C23-C24	2.69	120.34	111.91
32	c	502	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
43	g	606	CHL	CMB-C2B-C3B	2.68	129.70	124.68
46	s	1623	NEX	C26-C27-C28	-2.68	120.32	125.99
39	d	401	BCT	O3-C-O1	-2.68	112.59	119.55
32	S	610	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
39	D	401	BCT	O3-C-O1	-2.68	112.59	119.55
32	C	504	CLA	CHB-C4A-NA	2.68	128.22	124.51
36	C	521	LMG	C4-C3-C2	2.68	115.50	110.82
32	B	603	CLA	O2D-CGD-CBD	2.68	116.03	111.27
43	s	607	CHL	CMB-C2B-C3B	2.68	129.69	124.68
32	B	605	CLA	C2D-C1D-ND	-2.68	108.13	110.10
43	G	609	CHL	CAC-C3C-C4C	2.68	128.28	124.81
32	b	606	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	C	502	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	B	606	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
32	B	602	CLA	CHB-C4A-NA	2.68	128.21	124.51
32	C	508	CLA	O2D-CGD-CBD	2.68	116.02	111.27
37	C	519	DGD	C4E-C3E-C2E	2.67	115.49	110.82
38	C	2630	LHG	O8-C23-C24	2.67	120.30	111.91
32	B	617	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
46	r	625	NEX	C2-C1-C6	2.67	111.81	109.21
44	n	1620	LUT	C38-C25-C24	-2.67	117.84	123.56
32	b	603	CLA	O2D-CGD-CBD	2.67	116.02	111.27
45	g	1622	XAT	C24-C23-C22	-2.67	105.61	110.77
32	B	617	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
43	S	607	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
32	b	617	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
32	b	617	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
32	r	602	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
40	D	405	PL9	C36-C34-C33	-2.67	115.71	121.12
34	C	516	BCR	C30-C25-C26	-2.67	118.85	122.61
43	s	608	CHL	CHB-C4A-NA	2.67	128.20	124.51
45	Y	1622	XAT	C7-C8-C9	-2.67	121.39	125.53
46	S	1623	NEX	C2-C1-C6	2.67	111.80	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	611	CLA	CMB-C2B-C3B	2.67	129.67	124.68
32	y	610	CLA	C4A-NA-C1A	2.67	107.91	106.71
32	b	613	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
43	y	601	CHL	CBA-CAA-C2A	2.67	121.73	113.86
33	a	409	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
43	n	609	CHL	CHB-C4A-NA	2.67	128.20	124.51
32	B	614	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
32	G	612	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
32	n	613	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	B	611	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
32	b	611	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
38	D	409	LHG	O8-C23-C24	2.66	120.26	111.91
44	s	1621	LUT	C38-C25-C24	-2.66	117.87	123.56
38	c	2630	LHG	O8-C23-C24	2.66	120.26	111.91
43	G	606	CHL	CMB-C2B-C3B	2.66	129.65	124.68
43	S	607	CHL	CMB-C2B-C3B	2.66	129.65	124.68
34	B	618	BCR	C33-C5-C6	-2.66	121.54	124.53
32	n	613	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
32	G	604	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
46	Y	1623	NEX	C15-C35-C34	-2.66	118.03	123.47
43	Y	609	CHL	C4D-CHA-C1A	-2.66	118.02	121.25
44	N	1620	LUT	C38-C25-C24	-2.66	117.87	123.56
32	N	603	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
43	G	605	CHL	O2A-CGA-CBA	2.66	120.24	111.91
40	d	405	PL9	O1-C4-C3	-2.66	117.80	120.72
44	s	1621	LUT	C19-C9-C8	2.65	122.26	118.08
36	A	413	LMG	C8-O7-C10	-2.65	111.26	117.79
32	r	604	CLA	CHB-C4A-NA	2.65	128.18	124.51
34	A	411	BCR	C38-C26-C25	-2.65	121.55	124.53
46	S	1623	NEX	C26-C27-C28	-2.65	120.38	125.99
38	N	2630	LHG	O8-C23-C24	2.65	120.23	111.91
32	s	610	CLA	CHB-C4A-NA	2.65	128.18	124.51
43	S	608	CHL	CHB-C4A-NA	2.65	128.18	124.51
32	N	613	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
34	b	619	BCR	C15-C16-C17	-2.65	118.05	123.47
44	S	1621	LUT	C38-C25-C24	-2.65	117.89	123.56
43	r	608	CHL	C1B-CHB-C4A	-2.65	124.87	130.12
32	b	611	CLA	CMB-C2B-C3B	2.65	129.63	124.68
45	N	1622	XAT	C11-C10-C9	-2.65	123.53	127.31
32	c	508	CLA	O2D-CGD-CBD	2.64	115.97	111.27
34	b	618	BCR	C33-C5-C6	-2.64	121.56	124.53
32	B	613	CLA	C1B-CHB-C4A	-2.64	124.88	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	N	609	CHL	CHB-C4A-NA	2.64	128.17	124.51
43	y	609	CHL	C4D-CHA-C1A	-2.64	118.03	121.25
32	R	603	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
32	b	613	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
32	g	612	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
43	G	609	CHL	OMC-CMC-C2C	-2.64	119.71	125.69
43	G	601	CHL	O2A-CGA-CBA	2.64	120.20	111.91
32	Y	610	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
34	a	411	BCR	C38-C26-C25	-2.64	121.56	124.53
38	n	2630	LHG	O8-C23-C24	2.64	120.20	111.91
45	y	1622	XAT	C7-C8-C9	-2.64	121.43	125.53
32	y	610	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
32	G	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
37	c	519	DGD	C2G-O2G-C1B	-2.64	111.29	117.79
43	g	605	CHL	O2A-CGA-CBA	2.64	120.19	111.91
32	b	605	CLA	C2D-C1D-ND	-2.64	108.16	110.10
32	b	603	CLA	CHB-C4A-NA	2.64	128.16	124.51
32	r	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
44	n	1621	LUT	C8-C9-C10	-2.64	114.90	118.94
46	g	1623	NEX	C11-C12-C13	-2.64	119.01	126.42
43	s	607	CHL	O2D-CGD-O1D	-2.64	118.69	123.84
32	g	604	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
34	B	619	BCR	C15-C16-C17	-2.63	118.08	123.47
44	Y	1620	LUT	C31-C30-C29	-2.63	123.55	127.31
32	y	612	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
46	r	625	NEX	C28-C29-C30	2.63	122.98	118.94
43	y	601	CHL	C4A-NA-C1A	-2.63	105.52	106.71
32	c	510	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
43	s	601	CHL	CHB-C4A-NA	2.63	128.15	124.51
44	s	1621	LUT	C10-C11-C12	-2.63	115.01	123.22
32	n	603	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
32	g	603	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
32	R	602	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
32	n	614	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
32	B	613	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
34	C	514	BCR	C10-C11-C12	-2.62	115.03	123.22
32	Y	610	CLA	C4A-NA-C1A	2.62	107.89	106.71
43	n	601	CHL	O2A-CGA-CBA	2.62	120.14	111.91
32	G	602	CLA	CHB-C4A-NA	2.62	128.14	124.51
32	c	505	CLA	O2D-CGD-CBD	2.62	115.93	111.27
43	G	607	CHL	CMB-C2B-C3B	2.62	129.58	124.68
43	N	601	CHL	O2A-CGA-CBA	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	n	1620	LUT	C10-C11-C12	-2.62	115.04	123.22
32	Y	612	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
43	g	607	CHL	CMB-C2B-C3B	2.62	129.58	124.68
44	S	1621	LUT	C10-C11-C12	-2.62	115.04	123.22
46	R	625	NEX	C28-C29-C30	2.62	122.96	118.94
43	r	607	CHL	O2A-CGA-CBA	2.62	120.13	111.91
32	S	609	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
37	C	519	DGD	C2G-O2G-C1B	-2.62	111.34	117.79
43	y	606	CHL	CMB-C2B-C3B	2.62	129.58	124.68
36	a	413	LMG	C8-O7-C10	-2.62	111.35	117.79
43	R	608	CHL	C1B-CHB-C4A	-2.61	124.94	130.12
32	S	610	CLA	CHB-C4A-NA	2.61	128.13	124.51
42	Y	2632	LMU	C3B-C4B-C5B	2.61	114.90	110.24
44	N	1620	LUT	C10-C11-C12	-2.61	115.06	123.22
44	y	1620	LUT	C31-C30-C29	-2.61	123.58	127.31
43	N	605	CHL	OMC-CMC-C2C	-2.61	119.79	125.69
43	y	605	CHL	CMD-C2D-C3D	-2.61	121.61	127.61
44	s	1620	LUT	C38-C25-C24	-2.61	117.98	123.56
34	b	620	BCR	C16-C17-C18	-2.61	123.59	127.31
44	S	1620	LUT	C38-C25-C24	-2.61	117.98	123.56
43	G	601	CHL	CMB-C2B-C3B	2.61	129.55	124.68
37	C	518	DGD	O3G-C3G-C2G	-2.60	104.61	110.90
43	Y	607	CHL	CAA-CBA-CGA	-2.60	105.64	113.25
32	S	604	CLA	CHD-C1D-ND	-2.60	122.06	124.45
32	s	604	CLA	CHD-C1D-ND	-2.60	122.06	124.45
34	B	620	BCR	C16-C17-C18	-2.60	123.60	127.31
37	c	518	DGD	O3G-C3G-C2G	-2.60	104.62	110.90
43	g	601	CHL	CMB-C2B-C3B	2.60	129.55	124.68
43	R	607	CHL	O2A-CGA-CBA	2.60	120.07	111.91
43	Y	605	CHL	CMD-C2D-C3D	-2.60	121.63	127.61
32	B	610	CLA	CHB-C4A-NA	2.60	128.11	124.51
32	D	402	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
46	s	1623	NEX	C24-C23-C22	-2.60	105.75	110.77
43	y	607	CHL	CAA-CBA-CGA	-2.60	105.65	113.25
42	y	2632	LMU	C3B-C4B-C5B	2.60	114.88	110.24
43	y	607	CHL	CMB-C2B-C3B	2.60	129.54	124.68
43	Y	606	CHL	CMB-C2B-C3B	2.60	129.54	124.68
46	G	1623	NEX	C11-C12-C13	-2.60	119.12	126.42
43	n	605	CHL	OMC-CMC-C2C	-2.59	119.82	125.69
32	C	513	CLA	CHB-C4A-NA	2.59	128.10	124.51
46	s	1623	NEX	C15-C35-C34	-2.59	118.16	123.47
34	c	514	BCR	C10-C11-C12	-2.59	115.12	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	S	601	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
43	s	601	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
43	g	609	CHL	OMC-CMC-C2C	-2.59	119.83	125.69
45	n	1622	XAT	C10-C11-C12	-2.59	115.14	123.22
43	S	601	CHL	CHB-C4A-NA	2.59	128.09	124.51
32	S	603	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
45	N	1622	XAT	C10-C11-C12	-2.58	115.15	123.22
32	b	608	CLA	CHB-C4A-NA	2.58	128.08	124.51
43	R	606	CHL	OMC-CMC-C2C	-2.58	119.85	125.69
32	n	614	CLA	CMB-C2B-C3B	2.58	129.51	124.68
32	b	610	CLA	CHB-C4A-NA	2.58	128.08	124.51
32	g	602	CLA	CHB-C4A-NA	2.58	128.07	124.51
43	Y	607	CHL	CMB-C2B-C3B	2.58	129.50	124.68
46	S	1623	NEX	C24-C23-C22	-2.58	105.80	110.77
32	c	501	CLA	CHB-C4A-NA	2.58	128.07	124.51
43	Y	606	CHL	CED-O2D-CGD	2.57	121.76	115.94
32	g	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
32	b	614	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
43	Y	609	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
43	y	609	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
32	d	402	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
32	N	612	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
46	n	1623	NEX	C31-C30-C29	-2.57	123.64	127.31
32	R	602	CLA	CHB-C4A-NA	2.57	128.07	124.51
46	y	1623	NEX	C39-C29-C30	-2.57	119.32	122.92
32	C	505	CLA	O2D-CGD-CBD	2.57	115.83	111.27
37	c	520	DGD	O1G-C1A-C2A	2.57	119.97	111.91
37	C	520	DGD	O1G-C1A-C2A	2.57	119.96	111.91
44	G	1621	LUT	C38-C25-C24	-2.57	118.07	123.56
43	r	606	CHL	OMC-CMC-C2C	-2.57	119.89	125.69
32	A	407	CLA	CHB-C4A-NA	2.57	128.06	124.51
32	N	614	CLA	CMB-C2B-C3B	2.56	129.48	124.68
43	G	601	CHL	C4-C3-C5	2.56	119.58	115.27
43	y	606	CHL	CED-O2D-CGD	2.56	121.74	115.94
44	Y	1620	LUT	C39-C29-C28	2.56	122.12	118.08
32	G	604	CLA	CHB-C4A-NA	2.56	128.06	124.51
35	B	621	SQD	O8-S-C6	2.56	109.82	105.74
32	B	614	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
32	r	602	CLA	CHB-C4A-NA	2.56	128.06	124.51
32	C	501	CLA	CHB-C4A-NA	2.56	128.05	124.51
32	R	610	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
32	s	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	621	SQD	O8-S-C6	2.56	109.81	105.74
34	a	411	BCR	C15-C16-C17	-2.56	118.24	123.47
46	y	1623	NEX	C26-C27-C28	-2.56	120.59	125.99
41	F	101	HEM	C4B-CHC-C1C	2.55	125.93	122.56
44	g	1620	LUT	C10-C11-C12	-2.55	115.25	123.22
32	Y	613	CLA	O2D-CGD-CBD	2.55	115.81	111.27
43	g	601	CHL	O2A-CGA-CBA	2.55	119.92	111.91
43	Y	609	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
32	b	602	CLA	O2D-CGD-CBD	2.55	115.80	111.27
43	Y	601	CHL	C4A-NA-C1A	-2.55	105.56	106.71
32	s	609	CLA	CHB-C4A-NA	2.55	128.04	124.51
46	y	1623	NEX	C15-C35-C34	-2.55	118.25	123.47
32	B	603	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	B	608	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	D	403	CLA	CHD-C1D-ND	-2.55	122.11	124.45
32	C	510	CLA	CHB-C4A-NA	2.55	128.03	124.51
32	n	612	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
44	G	1620	LUT	C10-C11-C12	-2.55	115.27	123.22
34	A	411	BCR	C15-C16-C17	-2.55	118.26	123.47
46	N	1623	NEX	C31-C30-C29	-2.54	123.68	127.31
32	c	510	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	y	613	CLA	O2D-CGD-CBD	2.54	115.79	111.27
32	S	609	CLA	CAA-C2A-C3A	-2.54	110.17	116.10
34	a	411	BCR	C35-C13-C12	2.54	122.08	118.08
43	r	608	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
43	s	608	CHL	CMB-C2B-C3B	2.54	129.43	124.68
32	d	403	CLA	CHD-C1D-ND	-2.54	122.12	124.45
46	Y	1623	NEX	C39-C29-C30	-2.53	119.37	122.92
32	s	609	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
32	a	405	CLA	CHB-C4A-NA	2.53	128.02	124.51
34	H	101	BCR	C29-C30-C25	2.53	114.38	110.48
45	r	624	XAT	C19-C9-C8	2.53	122.07	118.08
37	c	518	DGD	C2G-O2G-C1B	-2.53	111.56	117.79
46	Y	1623	NEX	C26-C27-C28	-2.53	120.64	125.99
32	n	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	B	616	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
44	s	1620	LUT	C1-C2-C3	2.53	119.36	113.64
32	a	407	CLA	CHB-C4A-NA	2.53	128.01	124.51
45	N	1622	XAT	C30-C31-C32	-2.53	115.33	123.22
32	B	602	CLA	O2D-CGD-CBD	2.53	115.76	111.27
44	S	1621	LUT	C28-C29-C30	-2.53	115.07	118.94
43	S	608	CHL	CMD-C2D-C3D	-2.53	121.81	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	518	DGD	O1G-C1A-C2A	2.52	119.83	111.91
44	y	1620	LUT	C39-C29-C28	2.52	122.05	118.08
44	n	1621	LUT	C38-C25-C24	-2.52	118.16	123.56
46	s	1623	NEX	C4-C3-C2	-2.52	105.90	110.77
37	c	523	DGD	O6D-C5D-C6D	2.52	111.75	106.67
32	r	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
34	c	517	BCR	C27-C26-C25	-2.52	119.07	122.73
32	c	507	CLA	CHA-C1A-NA	-2.52	120.63	126.40
46	r	625	NEX	C11-C12-C13	-2.52	119.34	126.42
32	s	609	CLA	CAA-C2A-C3A	-2.52	110.22	116.10
37	C	518	DGD	O1G-C1A-C2A	2.52	119.81	111.91
43	y	608	CHL	CMD-C2D-C3D	-2.52	121.82	127.61
44	g	1621	LUT	C38-C25-C24	-2.52	118.17	123.56
41	f	101	HEM	C4B-CHC-C1C	2.52	125.88	122.56
34	A	411	BCR	C35-C13-C12	2.52	122.04	118.08
43	S	606	CHL	CHB-C4A-NA	2.52	127.99	124.51
32	c	502	CLA	CMB-C2B-C3B	2.52	129.39	124.68
37	C	523	DGD	O6D-C5D-C6D	2.52	111.74	106.67
32	n	612	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
43	G	606	CHL	O2A-CGA-CBA	2.51	119.80	111.91
43	s	601	CHL	C4D-CHA-C1A	-2.51	118.19	121.25
44	Y	1621	LUT	C7-C8-C9	-2.51	122.44	126.23
44	y	1621	LUT	C7-C8-C9	-2.51	122.44	126.23
32	s	602	CLA	CHB-C4A-NA	2.51	127.99	124.51
43	S	608	CHL	CMB-C2B-C3B	2.51	129.38	124.68
45	N	1622	XAT	C24-C23-C22	-2.51	105.92	110.77
45	n	1622	XAT	C24-C23-C22	-2.51	105.92	110.77
32	c	513	CLA	CHB-C4A-NA	2.51	127.99	124.51
32	N	612	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
44	S	1620	LUT	C1-C2-C3	2.51	119.31	113.64
43	g	606	CHL	O2A-CGA-CBA	2.51	119.79	111.91
32	C	502	CLA	CMB-C2B-C3B	2.51	129.38	124.68
43	s	606	CHL	CHB-C4A-NA	2.51	127.98	124.51
32	R	604	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
43	S	601	CHL	C4D-CHA-C1A	-2.51	118.20	121.25
43	s	608	CHL	CMD-C2D-C3D	-2.51	121.85	127.61
32	b	616	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
32	Y	602	CLA	C6-C7-C8	-2.51	107.82	115.92
32	c	501	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
34	C	517	BCR	C27-C26-C25	-2.51	119.09	122.73
34	h	101	BCR	C29-C30-C25	2.51	114.34	110.48
43	Y	605	CHL	C1C-C2C-C3C	-2.50	105.13	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	518	DGD	C2G-O2G-C1B	-2.50	111.63	117.79
45	n	1622	XAT	C30-C31-C32	-2.50	115.41	123.22
45	R	624	XAT	C19-C9-C8	2.50	122.02	118.08
32	y	602	CLA	C6-C7-C8	-2.50	107.83	115.92
32	S	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
32	C	509	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
45	g	1622	XAT	C11-C12-C13	-2.50	119.39	126.42
43	n	608	CHL	O2A-CGA-CBA	2.50	119.75	111.91
37	C	524	DGD	C2G-O2G-C1B	-2.50	111.64	117.79
44	N	1621	LUT	C38-C25-C24	-2.50	118.21	123.56
44	G	1621	LUT	C31-C30-C29	-2.50	123.74	127.31
44	S	1620	LUT	C8-C7-C6	-2.50	120.19	127.20
44	s	1621	LUT	C28-C29-C30	-2.50	115.11	118.94
32	S	613	CLA	CMB-C2B-C3B	2.50	129.35	124.68
43	r	608	CHL	O2D-CGD-O1D	-2.50	118.96	123.84
43	R	608	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
43	G	607	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
32	g	614	CLA	CHB-C4A-NA	2.49	127.96	124.51
32	N	603	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
32	S	605	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
43	g	607	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
43	y	609	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
32	b	605	CLA	C1-C2-C3	-2.49	121.73	126.04
44	s	1620	LUT	C8-C7-C6	-2.49	120.20	127.20
32	C	507	CLA	CHA-C1A-NA	-2.49	120.69	126.40
32	s	614	CLA	CHD-C1D-ND	-2.49	122.17	124.45
34	C	517	BCR	C15-C16-C17	-2.49	118.37	123.47
32	D	402	CLA	CHB-C4A-NA	2.49	127.95	124.51
46	g	1623	NEX	C26-C27-C28	-2.49	120.73	125.99
32	n	603	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
44	G	1621	LUT	C19-C9-C8	2.49	122.00	118.08
32	s	605	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
45	G	1622	XAT	C11-C12-C13	-2.49	119.43	126.42
32	N	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
43	G	608	CHL	CHB-C4A-NA	2.49	127.95	124.51
43	N	608	CHL	O2A-CGA-CBA	2.49	119.71	111.91
43	G	607	CHL	CAA-CBA-CGA	-2.49	105.99	113.25
32	c	509	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
34	c	516	BCR	C31-C1-C6	-2.49	106.27	110.30
43	Y	601	CHL	CMD-C2D-C3D	-2.49	121.90	127.61
34	c	517	BCR	C15-C16-C17	-2.48	118.39	123.47
32	r	610	CLA	CAA-C2A-C3A	-2.48	110.30	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	405	CLA	CHB-C4A-NA	2.48	127.94	124.51
43	y	601	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
46	R	625	NEX	C11-C12-C13	-2.48	119.45	126.42
32	B	606	CLA	CHB-C4A-NA	2.48	127.94	124.51
43	Y	608	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
34	h	101	BCR	C2-C1-C6	2.48	114.30	110.48
45	y	1622	XAT	C31-C32-C33	-2.48	119.45	126.42
34	H	101	BCR	C2-C1-C6	2.48	114.30	110.48
38	d	410	LHG	O8-C23-C24	2.48	119.68	111.91
43	g	608	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
38	D	410	LHG	O8-C23-C24	2.48	119.68	111.91
32	b	606	CLA	CHB-C4A-NA	2.48	127.94	124.51
44	S	1621	LUT	C18-C5-C6	-2.48	121.75	124.53
44	s	1621	LUT	C18-C5-C6	-2.48	121.75	124.53
32	S	614	CLA	CHD-C1D-ND	-2.48	122.18	124.45
43	R	608	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
43	y	605	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
37	c	524	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
43	y	609	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
32	c	501	CLA	C2D-C1D-ND	-2.47	108.28	110.10
32	d	402	CLA	CHB-C4A-NA	2.47	127.93	124.51
32	N	603	CLA	CMB-C2B-C3B	2.47	129.30	124.68
32	n	603	CLA	CMB-C2B-C3B	2.47	129.30	124.68
32	B	605	CLA	C1-C2-C3	-2.47	121.77	126.04
46	G	1623	NEX	C26-C27-C28	-2.47	120.77	125.99
44	g	1621	LUT	C19-C9-C8	2.47	121.97	118.08
32	s	613	CLA	CMB-C2B-C3B	2.47	129.29	124.68
32	c	506	CLA	O1D-CGD-CBD	2.47	129.53	124.48
44	N	1620	LUT	C30-C31-C32	-2.46	115.53	123.22
43	G	608	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
32	C	501	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
32	G	614	CLA	CHB-C4A-NA	2.46	127.92	124.51
34	c	516	BCR	C10-C11-C12	-2.46	115.53	123.22
44	n	1620	LUT	C30-C31-C32	-2.46	115.53	123.22
40	D	405	PL9	C7-C3-C2	-2.46	120.06	123.30
43	g	607	CHL	CAA-CBA-CGA	-2.46	106.06	113.25
32	B	605	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
43	n	606	CHL	C4A-NA-C1A	-2.46	105.60	106.71
36	D	411	LMG	C1-C2-C3	-2.46	104.87	110.00
32	b	605	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
33	a	409	PHO	O1D-CGD-CBD	2.46	128.83	124.74
44	G	1620	LUT	C30-C31-C32	-2.46	115.55	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	608	CHL	CHB-C4A-NA	2.45	127.91	124.51
46	Y	1623	NEX	C19-C9-C10	-2.45	119.49	122.92
43	g	605	CHL	CMB-C2B-C3B	2.45	129.27	124.68
32	C	506	CLA	O1D-CGD-CBD	2.45	129.50	124.48
32	b	602	CLA	CMB-C2B-C3B	2.45	129.26	124.68
43	Y	609	CHL	C2A-C1A-CHA	-2.45	119.57	123.86
44	g	1621	LUT	C31-C30-C29	-2.45	123.81	127.31
43	G	605	CHL	CMB-C2B-C3B	2.45	129.26	124.68
34	C	516	BCR	C10-C11-C12	-2.45	115.58	123.22
33	a	408	PHO	CBA-CAA-C2A	-2.45	106.66	113.81
32	B	602	CLA	CMB-C2B-C3B	2.45	129.26	124.68
43	s	608	CHL	O2A-CGA-CBA	2.45	119.59	111.91
34	B	620	BCR	C29-C30-C25	2.45	114.25	110.48
35	B	621	SQD	O48-C23-C24	2.45	119.59	111.91
43	R	607	CHL	CMD-C2D-C3D	-2.45	121.99	127.61
32	G	603	CLA	O1D-CGD-CBD	2.45	129.49	124.48
36	d	411	LMG	C1-C2-C3	-2.44	104.91	110.00
43	S	608	CHL	O2A-CGA-CBA	2.44	119.58	111.91
43	G	609	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
32	S	609	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	b	621	SQD	O48-C23-C24	2.44	119.57	111.91
32	C	513	CLA	CBA-CAA-C2A	2.44	121.07	113.86
43	g	609	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
44	g	1620	LUT	C30-C31-C32	-2.44	115.60	123.22
34	C	516	BCR	C31-C1-C6	-2.44	106.34	110.30
46	S	1623	NEX	C15-C35-C34	-2.44	118.48	123.47
34	H	101	BCR	C11-C12-C13	-2.44	119.57	126.42
34	c	515	BCR	C37-C22-C23	2.44	121.92	118.08
32	y	610	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
34	C	515	BCR	C37-C22-C23	2.44	121.91	118.08
44	s	1620	LUT	C30-C31-C32	-2.43	115.62	123.22
32	S	602	CLA	O2D-CGD-CBD	2.43	115.59	111.27
32	g	603	CLA	O1D-CGD-CBD	2.43	129.46	124.48
40	d	405	PL9	C7-C3-C2	-2.43	120.10	123.30
40	D	405	PL9	C37-C38-C39	-2.43	121.81	127.66
34	h	101	BCR	C11-C12-C13	-2.43	119.59	126.42
43	r	607	CHL	CED-O2D-CGD	2.43	121.43	115.94
32	B	617	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
43	R	606	CHL	CMB-C2B-C3B	2.43	129.22	124.68
32	c	505	CLA	CHB-C4A-NA	2.43	127.87	124.51
43	r	607	CHL	CMD-C2D-C3D	-2.43	122.03	127.61
43	N	606	CHL	C4A-NA-C1A	-2.42	105.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	1623	NEX	C19-C9-C10	-2.42	119.53	122.92
43	g	609	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
43	G	601	CHL	CBC-CAC-C3C	-2.42	105.75	112.43
33	A	409	PHO	O1D-CGD-CBD	2.42	128.77	124.74
44	S	1620	LUT	C30-C31-C32	-2.42	115.66	123.22
40	d	405	PL9	C37-C38-C39	-2.42	121.83	127.66
32	B	612	CLA	C1-C2-C3	-2.42	121.86	126.04
32	b	617	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
45	n	1622	XAT	C7-C8-C9	-2.42	121.78	125.53
44	G	1620	LUT	C7-C8-C9	-2.42	122.58	126.23
32	B	612	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
46	N	1623	NEX	C26-C27-C28	-2.42	120.88	125.99
43	r	607	CHL	CHB-C4A-NA	2.42	127.85	124.51
43	g	609	CHL	CHB-C4A-NA	2.41	127.85	124.51
32	b	616	CLA	C2A-C1A-CHA	2.41	128.08	123.86
43	G	609	CHL	CMD-C2D-C3D	-2.41	122.06	127.61
32	r	610	CLA	CHB-C4A-NA	2.41	127.85	124.51
32	C	505	CLA	CHB-C4A-NA	2.41	127.85	124.51
34	d	404	BCR	C16-C15-C14	-2.41	118.54	123.47
43	G	601	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
43	g	609	CHL	O1D-CGD-CBD	-2.41	119.55	124.48
32	G	612	CLA	O2D-CGD-CBD	2.41	115.55	111.27
34	b	620	BCR	C29-C30-C25	2.41	114.19	110.48
44	N	1620	LUT	C18-C5-C6	-2.41	121.82	124.53
43	R	607	CHL	CHB-C4A-NA	2.41	127.84	124.51
32	b	612	CLA	CAC-C3C-C4C	2.41	127.93	124.81
32	s	604	CLA	CHB-C4A-NA	2.40	127.83	124.51
41	f	101	HEM	C4D-ND-C1D	2.40	107.56	105.07
34	D	404	BCR	C16-C15-C14	-2.40	118.56	123.47
43	r	606	CHL	CMB-C2B-C3B	2.40	129.17	124.68
43	y	606	CHL	C4-C3-C5	2.40	119.31	115.27
45	Y	1622	XAT	C31-C32-C33	-2.40	119.67	126.42
43	y	605	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
43	Y	605	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
32	Y	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
32	B	616	CLA	C2A-C1A-CHA	2.40	128.05	123.86
34	B	618	BCR	C29-C30-C25	2.40	114.17	110.48
43	G	609	CHL	O1D-CGD-CBD	-2.40	119.58	124.48
32	S	611	CLA	CHB-C4A-NA	2.40	127.82	124.51
32	g	612	CLA	O2D-CGD-CBD	2.40	115.52	111.27
32	b	612	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
43	y	608	CHL	CHB-C4A-NA	2.39	127.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	1623	NEX	C19-C9-C10	-2.39	119.57	122.92
43	G	605	CHL	O1D-CGD-CBD	-2.39	119.59	124.48
32	G	603	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
44	g	1620	LUT	C7-C8-C9	-2.39	122.62	126.23
33	A	408	PHO	CMC-C2C-C3C	2.39	129.44	124.94
32	s	611	CLA	CHB-C4A-NA	2.39	127.81	124.51
46	s	1623	NEX	C19-C9-C10	-2.39	119.58	122.92
43	N	608	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
43	R	607	CHL	CED-O2D-CGD	2.39	121.33	115.94
46	n	1623	NEX	C26-C27-C28	-2.39	120.95	125.99
32	b	612	CLA	C1-C2-C3	-2.39	121.92	126.04
32	g	603	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
43	Y	606	CHL	C1-C2-C3	-2.38	121.92	126.04
32	c	511	CLA	O2D-CGD-CBD	2.38	115.50	111.27
32	C	503	CLA	CHB-C4A-NA	2.38	127.81	124.51
43	g	606	CHL	C4D-CHA-C1A	-2.38	118.35	121.25
32	s	602	CLA	O2D-CGD-CBD	2.38	115.50	111.27
32	Y	611	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
34	b	618	BCR	C29-C30-C25	2.38	114.14	110.48
43	n	608	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
43	G	606	CHL	C4D-CHA-C1A	-2.38	118.35	121.25
32	c	513	CLA	CBA-CAA-C2A	2.38	120.88	113.86
43	Y	608	CHL	CHB-C4A-NA	2.38	127.80	124.51
43	R	607	CHL	CMB-C2B-C3B	2.38	129.13	124.68
43	s	601	CHL	C4D-C3D-CAD	2.38	110.90	108.10
44	s	1620	LUT	C31-C30-C29	-2.38	123.92	127.31
44	S	1620	LUT	C31-C30-C29	-2.38	123.92	127.31
43	G	609	CHL	CHB-C4A-NA	2.38	127.80	124.51
45	N	1622	XAT	C7-C8-C9	-2.37	121.84	125.53
41	F	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
43	G	605	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
34	C	515	BCR	C23-C22-C21	-2.37	115.31	118.94
44	y	1620	LUT	C15-C35-C34	-2.37	118.62	123.47
32	y	603	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
43	g	601	CHL	C11-C10-C8	-2.37	108.27	115.92
43	g	605	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
46	S	1623	NEX	C31-C32-C33	-2.37	119.77	126.42
33	a	408	PHO	CMC-C2C-C3C	2.37	129.40	124.94
32	y	611	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
43	g	605	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
32	c	503	CLA	CHB-C4A-NA	2.37	127.78	124.51
43	n	607	CHL	CMD-C2D-C3D	-2.36	122.17	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	603	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	c	519	DGD	C3E-C4E-C5E	2.36	114.45	110.24
43	s	606	CHL	CMD-C2D-C3D	-2.36	122.18	127.61
32	c	509	CLA	CMA-C3A-C4A	-2.36	105.43	111.77
32	S	604	CLA	CHB-C4A-NA	2.36	127.78	124.51
43	N	607	CHL	CMD-C2D-C3D	-2.36	122.18	127.61
36	b	622	LMG	O8-C28-C29	2.36	119.31	111.91
43	N	609	CHL	CAC-C3C-C4C	2.36	127.87	124.81
43	n	609	CHL	CAC-C3C-C4C	2.36	127.87	124.81
32	C	511	CLA	O2D-CGD-CBD	2.36	115.46	111.27
43	G	601	CHL	C11-C10-C8	-2.36	108.30	115.92
34	C	515	BCR	C1-C6-C7	2.36	122.45	115.78
32	B	612	CLA	CAC-C3C-C4C	2.36	127.87	124.81
32	A	405	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
32	a	405	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
32	S	603	CLA	C2A-C1A-CHA	2.36	127.98	123.86
32	N	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
32	n	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
32	a	405	CLA	CBA-CAA-C2A	-2.36	106.91	113.86
43	N	605	CHL	O2A-CGA-CBA	2.35	119.30	111.91
43	r	607	CHL	CMB-C2B-C3B	2.35	129.08	124.68
43	s	601	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
38	d	408	LHG	O8-C23-C24	2.35	119.29	111.91
38	D	408	LHG	O8-C23-C24	2.35	119.28	111.91
32	s	603	CLA	C2A-C1A-CHA	2.35	127.97	123.86
43	S	606	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
36	B	622	LMG	O8-C28-C29	2.35	119.28	111.91
43	n	607	CHL	CED-O2D-CGD	2.35	121.25	115.94
32	c	503	CLA	CAA-CBA-CGA	-2.35	106.39	113.25
34	d	404	BCR	C8-C9-C10	-2.35	115.34	118.94
32	b	616	CLA	CMB-C2B-C3B	2.35	129.07	124.68
43	S	601	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
32	s	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
44	n	1620	LUT	C18-C5-C6	-2.35	121.89	124.53
46	s	1623	NEX	C31-C32-C33	-2.35	119.82	126.42
43	N	607	CHL	CED-O2D-CGD	2.35	121.24	115.94
45	r	624	XAT	C38-C25-C24	2.35	116.92	114.28
43	g	608	CHL	CMB-C2B-C3B	2.35	129.07	124.68
43	s	606	CHL	CAA-C2A-C3A	-2.35	106.36	112.78
32	A	405	CLA	CBA-CAA-C2A	-2.34	106.95	113.86
44	Y	1620	LUT	C15-C35-C34	-2.34	118.67	123.47
45	R	624	XAT	C38-C25-C24	2.34	116.92	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	503	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
32	N	610	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
37	C	523	DGD	O1G-C1A-C2A	2.34	119.26	111.91
43	n	605	CHL	O2A-CGA-CBA	2.34	119.26	111.91
43	g	601	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
43	S	601	CHL	C4D-C3D-CAD	2.34	110.85	108.10
32	c	506	CLA	CHB-C4A-NA	2.34	127.74	124.51
32	y	614	CLA	CHB-C4A-NA	2.33	127.74	124.51
37	C	519	DGD	C3E-C4E-C5E	2.33	114.40	110.24
32	d	402	CLA	CAC-C3C-C4C	2.33	127.83	124.81
43	g	607	CHL	O2A-CGA-CBA	2.33	119.22	111.91
37	c	523	DGD	O1G-C1A-C2A	2.33	119.22	111.91
32	C	509	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
43	g	606	CHL	O1D-CGD-CBD	-2.33	119.72	124.48
33	a	409	PHO	C1-C2-C3	-2.33	122.02	126.04
34	c	515	BCR	C1-C6-C7	2.33	122.36	115.78
32	Y	614	CLA	CHB-C4A-NA	2.33	127.73	124.51
33	A	409	PHO	C1-C2-C3	-2.33	122.02	126.04
43	N	605	CHL	CMD-C2D-C3D	-2.33	122.26	127.61
43	n	605	CHL	CMD-C2D-C3D	-2.33	122.26	127.61
43	S	606	CHL	CAA-C2A-C3A	-2.33	106.41	112.78
32	B	606	CLA	CHD-C1D-ND	-2.33	122.32	124.45
32	c	504	CLA	O2D-CGD-CBD	2.32	115.40	111.27
43	G	607	CHL	O2A-CGA-CBA	2.32	119.20	111.91
32	b	606	CLA	CHD-C1D-ND	-2.32	122.32	124.45
43	G	606	CHL	O1D-CGD-CBD	-2.32	119.73	124.48
32	D	402	CLA	CAC-C3C-C4C	2.32	127.82	124.81
32	N	602	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	S	613	CLA	CHB-C4A-NA	2.32	127.72	124.51
32	n	610	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
32	B	616	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
34	c	515	BCR	C23-C22-C21	-2.32	115.38	118.94
43	Y	606	CHL	C4D-CHA-C1A	-2.32	118.43	121.25
35	b	621	SQD	O9-S-C6	2.32	109.69	106.94
32	C	513	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
32	C	506	CLA	CHB-C4A-NA	2.31	127.71	124.51
43	N	606	CHL	C3B-C4B-NB	2.31	112.20	109.21
34	D	404	BCR	C8-C9-C10	-2.31	115.39	118.94
35	B	621	SQD	O9-S-C6	2.31	109.69	106.94
32	B	604	CLA	CAA-CBA-CGA	-2.31	106.50	113.25
32	b	616	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
32	B	616	CLA	CMB-C2B-C3B	2.31	129.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	S	606	CHL	CMB-C2B-C3B	2.31	129.00	124.68
44	Y	1621	LUT	C15-C35-C34	-2.31	118.75	123.47
44	y	1621	LUT	C15-C35-C34	-2.31	118.75	123.47
34	c	516	BCR	C38-C26-C25	-2.31	121.94	124.53
32	b	604	CLA	CAA-CBA-CGA	-2.31	106.52	113.25
43	r	607	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
43	Y	608	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
43	G	608	CHL	CMB-C2B-C3B	2.30	128.99	124.68
43	R	607	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
44	G	1621	LUT	C30-C31-C32	-2.30	116.03	123.22
44	G	1621	LUT	C16-C1-C6	-2.30	106.57	110.30
34	c	516	BCR	C7-C8-C9	-2.30	122.76	126.23
44	N	1620	LUT	C39-C29-C28	2.30	121.70	118.08
32	r	603	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
44	n	1620	LUT	C39-C29-C28	2.30	121.70	118.08
43	N	601	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
32	b	604	CLA	O2D-CGD-CBD	2.30	115.35	111.27
32	c	501	CLA	C1-C2-C3	-2.30	122.07	126.04
34	B	620	BCR	C33-C5-C4	2.30	118.03	113.62
46	G	1623	NEX	C4-C3-C2	-2.29	106.34	110.77
42	z	2635	LMU	C2'-C3'-C4'	2.29	114.92	109.68
44	s	1621	LUT	C30-C31-C32	-2.29	116.06	123.22
32	c	513	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
34	A	411	BCR	C20-C21-C22	-2.29	124.04	127.31
34	a	411	BCR	C20-C21-C22	-2.29	124.04	127.31
32	c	507	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
33	a	408	PHO	O2D-CGD-CBD	2.29	113.90	111.00
32	B	607	CLA	C1-C2-C3	-2.29	122.08	126.04
32	C	507	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
32	r	609	CLA	C2A-C1A-CHA	2.29	127.86	123.86
43	n	601	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
38	d	409	LHG	O8-C23-O10	-2.29	117.82	123.59
32	C	501	CLA	C1-C2-C3	-2.29	122.09	126.04
34	c	516	BCR	C34-C9-C8	2.29	121.68	118.08
44	g	1621	LUT	C30-C31-C32	-2.29	116.08	123.22
42	Z	2635	LMU	C2'-C3'-C4'	2.29	114.90	109.68
32	R	603	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
32	d	403	CLA	O2D-CGD-CBD	2.29	115.33	111.27
34	b	618	BCR	C21-C20-C19	-2.28	116.09	123.22
43	s	606	CHL	CMB-C2B-C3B	2.28	128.95	124.68
34	d	404	BCR	C3-C4-C5	-2.28	110.00	114.08
43	y	606	CHL	C4D-CHA-C1A	-2.28	118.47	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	604	CLA	O2D-CGD-CBD	2.28	115.32	111.27
34	C	516	BCR	C38-C26-C25	-2.28	121.97	124.53
40	d	405	PL9	C11-C12-C13	-2.28	104.39	111.88
46	g	1623	NEX	C31-C30-C29	-2.28	124.06	127.31
40	D	405	PL9	C40-C39-C41	2.28	119.11	115.27
44	S	1621	LUT	C30-C31-C32	-2.28	116.11	123.22
32	a	405	CLA	CHC-C1C-NC	2.28	127.66	124.20
34	a	411	BCR	C10-C11-C12	-2.28	116.11	123.22
34	B	620	BCR	C1-C6-C5	-2.28	119.41	122.61
32	b	607	CLA	C1-C2-C3	-2.28	122.10	126.04
43	N	609	CHL	CED-O2D-CGD	2.28	121.09	115.94
32	Y	602	CLA	CHB-C4A-NA	2.28	127.66	124.51
32	y	602	CLA	CHB-C4A-NA	2.28	127.66	124.51
43	y	601	CHL	CMB-C2B-C3B	2.27	128.93	124.68
33	A	408	PHO	O2D-CGD-CBD	2.27	113.88	111.00
44	S	1620	LUT	C21-C26-C27	-2.27	109.83	112.70
34	C	516	BCR	C7-C8-C9	-2.27	122.80	126.23
34	B	618	BCR	C21-C20-C19	-2.27	116.13	123.22
42	Y	2632	LMU	C6B-C5B-C4B	-2.27	107.68	113.00
32	C	501	CLA	C2D-C1D-ND	-2.27	108.43	110.10
43	G	606	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
43	G	601	CHL	C4D-CHA-C1A	-2.27	118.49	121.25
34	C	516	BCR	C34-C9-C8	2.27	121.65	118.08
32	b	611	CLA	C3A-C2A-C1A	2.27	104.74	101.34
44	s	1620	LUT	C21-C26-C27	-2.27	109.83	112.70
42	y	2632	LMU	C6B-C5B-C4B	-2.27	107.69	113.00
34	d	404	BCR	C28-C27-C26	-2.27	110.03	114.08
35	B	621	SQD	O7-S-C6	2.27	109.63	106.94
34	C	517	BCR	C16-C15-C14	-2.27	118.83	123.47
46	G	1623	NEX	C31-C30-C29	-2.27	124.07	127.31
43	Y	605	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
43	y	605	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
40	D	405	PL9	C11-C12-C13	-2.27	104.43	111.88
40	d	405	PL9	C40-C39-C41	2.27	119.08	115.27
34	b	620	BCR	C33-C5-C4	2.27	117.97	113.62
44	Y	1620	LUT	C19-C9-C8	2.27	121.65	118.08
43	y	608	CHL	CMB-C2B-C3B	2.27	128.92	124.68
32	Y	614	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
34	A	411	BCR	C10-C11-C12	-2.27	116.15	123.22
43	Y	601	CHL	CMB-C2B-C3B	2.27	128.92	124.68
43	y	608	CHL	C2A-C1A-CHA	-2.26	119.90	123.86
32	C	510	CLA	C1B-CHB-C4A	-2.26	125.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Z	2634	LMU	C3B-C4B-C5B	2.26	114.28	110.24
43	n	609	CHL	CED-O2D-CGD	2.26	121.06	115.94
34	D	404	BCR	C3-C4-C5	-2.26	110.03	114.08
32	C	504	CLA	O2D-CGD-CBD	2.26	115.29	111.27
32	G	614	CLA	CHD-C1D-ND	-2.26	122.37	124.45
43	Y	606	CHL	C4-C3-C5	2.26	119.08	115.27
32	c	510	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
32	c	505	CLA	CMC-C2C-C1C	-2.26	121.59	125.04
43	g	606	CHL	O2D-CGD-O1D	-2.26	119.41	123.84
32	n	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
43	n	606	CHL	C3B-C4B-NB	2.26	112.13	109.21
43	Y	608	CHL	CMB-C2B-C3B	2.26	128.91	124.68
44	g	1621	LUT	C16-C1-C6	-2.26	106.63	110.30
34	B	618	BCR	C29-C28-C27	-2.26	106.33	111.38
32	D	403	CLA	O2D-CGD-CBD	2.26	115.28	111.27
33	a	408	PHO	CMD-C2D-C3D	2.26	128.90	124.68
32	A	410	CLA	O2D-CGD-CBD	2.26	115.28	111.27
44	g	1621	LUT	C39-C29-C28	2.26	121.64	118.08
43	y	606	CHL	C1-C2-C3	-2.26	122.14	126.04
32	b	603	CLA	CHD-C1D-ND	-2.26	122.38	124.45
32	R	603	CLA	C2A-C1A-CHA	2.26	127.80	123.86
34	D	404	BCR	C28-C27-C26	-2.25	110.05	114.08
43	Y	605	CHL	CMB-C2B-C3B	2.25	128.90	124.68
32	g	614	CLA	CHD-C1D-ND	-2.25	122.38	124.45
43	g	601	CHL	C4D-CHA-C1A	-2.25	118.51	121.25
32	c	507	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
44	y	1620	LUT	C19-C9-C8	2.25	121.62	118.08
43	y	605	CHL	CMB-C2B-C3B	2.25	128.89	124.68
32	a	410	CLA	O2D-CGD-CBD	2.25	115.27	111.27
40	d	405	PL9	C22-C23-C24	-2.25	122.24	127.66
43	n	601	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
32	R	603	CLA	CHA-C1A-NA	-2.25	121.25	126.40
33	A	408	PHO	CMD-C2D-C3D	2.25	128.88	124.68
34	b	620	BCR	C16-C15-C14	-2.25	118.87	123.47
43	S	607	CHL	CHB-C4A-NA	2.25	127.62	124.51
43	G	605	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
32	N	602	CLA	CHD-C1D-ND	-2.25	122.39	124.45
43	N	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
34	A	411	BCR	C16-C15-C14	-2.25	118.87	123.47
43	Y	605	CHL	OMC-CMC-C2C	-2.25	120.61	125.69
32	y	614	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
32	s	614	CLA	CHB-C4A-NA	2.24	127.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	618	BCR	C23-C24-C25	-2.24	120.90	127.20
32	R	609	CLA	C2A-C1A-CHA	2.24	127.78	123.86
34	B	619	BCR	C39-C30-C25	-2.24	106.66	110.30
34	b	618	BCR	C29-C28-C27	-2.24	106.37	111.38
32	C	507	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
34	b	618	BCR	C23-C24-C25	-2.24	120.91	127.20
34	a	411	BCR	C16-C15-C14	-2.24	118.88	123.47
42	z	2634	LMU	O5B-C1B-C2B	2.24	115.09	110.35
43	y	605	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
43	n	601	CHL	C4D-C3D-CAD	2.24	110.74	108.10
34	c	517	BCR	C16-C15-C14	-2.24	118.89	123.47
43	s	607	CHL	CHB-C4A-NA	2.24	127.61	124.51
43	N	606	CHL	O2D-CGD-O1D	-2.24	119.47	123.84
34	b	619	BCR	C39-C30-C25	-2.24	106.67	110.30
32	A	405	CLA	CHC-C1C-NC	2.24	127.59	124.20
32	C	505	CLA	CMC-C2C-C1C	-2.23	121.64	125.04
43	n	607	CHL	O2A-CGA-CBA	2.23	118.92	111.91
32	r	603	CLA	C2A-C1A-CHA	2.23	127.77	123.86
43	G	606	CHL	CHB-C4A-NA	2.23	127.60	124.51
45	y	1622	XAT	C11-C10-C9	-2.23	124.12	127.31
32	Y	613	CLA	C16-C15-C13	-2.23	108.70	115.92
32	y	613	CLA	C16-C15-C13	-2.23	108.70	115.92
43	Y	601	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
43	y	601	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
43	N	607	CHL	O2A-CGA-CBA	2.23	118.91	111.91
43	S	606	CHL	CBA-CAA-C2A	-2.23	109.31	114.02
44	Y	1620	LUT	C21-C26-C27	-2.23	109.88	112.70
34	C	516	BCR	C28-C27-C26	-2.23	110.10	114.08
44	G	1621	LUT	C39-C29-C28	2.23	121.59	118.08
43	s	607	CHL	CMD-C2D-C3D	-2.23	122.49	127.61
43	g	606	CHL	CHB-C4A-NA	2.23	127.59	124.51
42	z	2634	LMU	C3B-C4B-C5B	2.23	114.21	110.24
32	B	611	CLA	C3A-C2A-C1A	2.23	104.67	101.34
42	Z	2634	LMU	O5B-C1B-C2B	2.23	115.06	110.35
32	N	614	CLA	CHD-C1D-ND	-2.22	122.41	124.45
32	y	603	CLA	C3C-C4C-NC	-2.22	108.08	110.57
32	C	511	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
38	D	409	LHG	O8-C23-O10	-2.22	117.98	123.59
35	b	621	SQD	O7-S-C6	2.22	109.58	106.94
46	y	1623	NEX	C30-C31-C32	-2.22	116.29	123.22
43	N	601	CHL	C4D-C3D-CAD	2.22	110.71	108.10
34	b	618	BCR	C3-C4-C5	-2.22	110.11	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
43	y	609	CHL	O2A-CGA-CBA	2.22	118.87	111.91
32	c	506	CLA	CHD-C1D-ND	-2.22	122.42	124.45
32	n	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
46	S	1623	NEX	C39-C29-C30	-2.22	119.82	122.92
32	B	605	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	c	516	BCR	C28-C27-C26	-2.22	110.12	114.08
32	b	604	CLA	CHD-C1D-ND	-2.22	122.42	124.45
34	B	618	BCR	C3-C4-C5	-2.21	110.12	114.08
44	N	1620	LUT	C19-C9-C8	2.21	121.57	118.08
34	c	515	BCR	C15-C16-C17	-2.21	118.94	123.47
32	a	410	CLA	CAA-CBA-CGA	-2.21	106.78	113.25
46	S	1623	NEX	C17-C1-C6	-2.21	108.49	110.47
34	b	620	BCR	C1-C6-C5	-2.21	119.50	122.61
32	c	511	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
40	D	405	PL9	C22-C23-C24	-2.21	122.33	127.66
43	s	601	CHL	CED-O2D-CGD	2.21	120.94	115.94
32	S	605	CLA	CHD-C1D-ND	-2.21	122.42	124.45
32	c	506	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
34	D	404	BCR	C1-C6-C5	-2.21	119.50	122.61
43	y	601	CHL	C11-C10-C8	-2.21	108.77	115.92
32	S	614	CLA	CHB-C4A-NA	2.21	127.57	124.51
44	n	1620	LUT	C11-C10-C9	-2.21	124.15	127.31
34	B	619	BCR	C1-C6-C5	-2.21	119.50	122.61
33	a	408	PHO	C1B-NB-C4B	2.21	111.63	107.09
45	Y	1622	XAT	C11-C10-C9	-2.21	124.16	127.31
46	Y	1623	NEX	C30-C31-C32	-2.21	116.32	123.22
46	y	1623	NEX	O24-C25-C26	-2.21	57.13	58.96
43	G	607	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
43	g	605	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
32	n	614	CLA	CHD-C1D-ND	-2.21	122.42	124.45
44	y	1620	LUT	C21-C26-C27	-2.21	109.91	112.70
43	N	605	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
34	d	404	BCR	C1-C6-C5	-2.21	119.50	122.61
43	R	606	CHL	CHB-C4A-NA	2.21	127.56	124.51
45	N	1622	XAT	C18-C5-C4	2.20	116.76	114.28
34	C	515	BCR	C15-C16-C17	-2.20	118.96	123.47
32	Y	611	CLA	O2D-CGD-CBD	2.20	115.18	111.27
32	y	611	CLA	O2D-CGD-CBD	2.20	115.18	111.27
34	B	620	BCR	C16-C15-C14	-2.20	118.96	123.47
32	s	604	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
36	h	102	LMG	O8-C28-O10	-2.20	118.03	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	n	606	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
43	Y	609	CHL	O2A-CGA-CBA	2.20	118.82	111.91
43	S	601	CHL	CED-O2D-CGD	2.20	120.92	115.94
32	A	410	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
34	c	516	BCR	C21-C20-C19	-2.20	116.35	123.22
44	N	1620	LUT	C11-C10-C9	-2.20	124.17	127.31
43	S	607	CHL	CMD-C2D-C3D	-2.20	122.55	127.61
43	n	608	CHL	CMD-C2D-C3D	-2.20	122.55	127.61
43	s	606	CHL	CBA-CAA-C2A	-2.20	109.38	114.02
43	n	605	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
32	B	612	CLA	CHC-C1C-NC	2.20	127.54	124.20
34	C	516	BCR	C21-C20-C19	-2.20	116.36	123.22
32	r	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
43	n	605	CHL	C1-C2-C3	-2.20	122.24	126.04
37	c	519	DGD	O1G-C1A-O1A	-2.20	118.05	123.59
33	A	408	PHO	C1B-NB-C4B	2.20	111.60	107.09
32	b	612	CLA	CHC-C1C-NC	2.20	127.53	124.20
44	G	1620	LUT	C21-C26-C27	-2.20	109.92	112.70
32	B	603	CLA	CHD-C1D-ND	-2.20	122.44	124.45
45	N	1622	XAT	C40-C33-C32	2.19	121.53	118.08
32	B	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	Y	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
32	y	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
34	h	101	BCR	C31-C1-C6	-2.19	106.74	110.30
32	c	505	CLA	C2D-C1D-ND	-2.19	108.49	110.10
44	y	1621	LUT	C38-C25-C24	-2.19	118.87	123.56
34	b	619	BCR	C1-C6-C5	-2.19	119.53	122.61
43	r	606	CHL	CHB-C4A-NA	2.19	127.54	124.51
37	C	518	DGD	C6E-C5E-C4E	-2.19	107.87	113.00
34	B	618	BCR	C37-C22-C23	2.19	121.53	118.08
34	b	618	BCR	C37-C22-C23	2.19	121.53	118.08
44	n	1620	LUT	C19-C9-C8	2.19	121.53	118.08
46	R	625	NEX	C19-C9-C10	-2.19	119.85	122.92
37	c	518	DGD	C6E-C5E-C4E	-2.19	107.88	113.00
32	C	505	CLA	C7-C6-C5	-2.19	107.42	113.36
33	a	408	PHO	OBD-CAD-CBD	-2.19	122.61	125.82
32	c	509	CLA	C2A-C1A-CHA	2.19	127.68	123.86
32	N	612	CLA	CHA-C1A-NA	-2.19	121.39	126.40
32	S	604	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
43	Y	601	CHL	C11-C10-C8	-2.19	108.85	115.92
44	g	1620	LUT	C21-C26-C27	-2.19	109.94	112.70
32	B	615	CLA	O2D-CGD-CBD	2.19	115.15	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	603	CLA	CHD-C1D-ND	-2.19	122.45	124.45
43	n	606	CHL	C2A-C1A-CHA	-2.18	120.04	123.86
45	n	1622	XAT	C40-C33-C32	2.18	121.52	118.08
42	y	2632	LMU	C2'-C3'-C4'	2.18	114.67	109.68
43	N	608	CHL	CMD-C2D-C3D	-2.18	122.59	127.61
32	b	604	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	n	611	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
34	C	515	BCR	C24-C23-C22	-2.18	122.94	126.23
32	b	605	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	c	501	CLA	CMB-C2B-C3B	2.18	128.76	124.68
32	c	505	CLA	C7-C6-C5	-2.18	107.44	113.36
34	d	404	BCR	C10-C11-C12	-2.18	116.42	123.22
46	n	1623	NEX	C30-C31-C32	-2.18	116.42	123.22
36	H	102	LMG	O8-C28-O10	-2.18	118.10	123.59
32	n	612	CLA	CHA-C1A-NA	-2.18	121.41	126.40
32	s	605	CLA	CHD-C1D-ND	-2.18	122.45	124.45
44	s	1620	LUT	C8-C9-C10	-2.18	115.60	118.94
43	G	609	CHL	C4D-CHA-C1A	-2.18	118.60	121.25
32	Y	603	CLA	C3C-C4C-NC	-2.18	108.13	110.57
32	B	604	CLA	CHB-C4A-NA	2.17	127.52	124.51
44	Y	1621	LUT	C38-C25-C24	-2.17	118.91	123.56
32	C	506	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
32	G	603	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
32	n	612	CLA	C2A-C1A-CHA	2.17	127.66	123.86
32	Y	603	CLA	CHD-C1D-ND	-2.17	122.46	124.45
37	C	519	DGD	O1G-C1A-O1A	-2.17	118.11	123.59
32	C	509	CLA	C2A-C1A-CHA	2.17	127.65	123.86
43	N	605	CHL	C1-C2-C3	-2.17	122.29	126.04
44	G	1621	LUT	C8-C9-C10	-2.17	115.61	118.94
37	c	524	DGD	O2G-C1B-O1B	-2.17	118.46	123.70
32	N	612	CLA	C2A-C1A-CHA	2.17	127.65	123.86
32	N	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
34	D	404	BCR	C10-C11-C12	-2.17	116.45	123.22
34	B	618	BCR	C15-C16-C17	-2.17	119.03	123.47
34	H	101	BCR	C31-C1-C6	-2.17	106.79	110.30
38	Y	2630	LHG	C5-O7-C7	-2.16	112.46	117.79
34	c	515	BCR	C24-C23-C22	-2.16	122.96	126.23
32	b	615	CLA	O2D-CGD-CBD	2.16	115.11	111.27
46	s	1623	NEX	C39-C29-C30	-2.16	119.89	122.92
44	g	1621	LUT	C8-C9-C10	-2.16	115.62	118.94
46	S	1623	NEX	C11-C12-C13	-2.16	120.34	126.42
43	y	601	CHL	C1-C2-C3	-2.16	122.31	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	412	SQD	O48-C23-O10	-2.16	118.14	123.59
46	N	1623	NEX	C30-C31-C32	-2.16	116.48	123.22
42	Y	2632	LMU	C2'-C3'-C4'	2.16	114.61	109.68
37	C	524	DGD	O2G-C1B-O1B	-2.16	118.48	123.70
34	d	404	BCR	C34-C9-C10	-2.16	119.90	122.92
32	G	610	CLA	C1-C2-C3	-2.16	122.31	126.04
34	C	514	BCR	C16-C15-C14	-2.16	119.05	123.47
34	b	618	BCR	C15-C16-C17	-2.16	119.05	123.47
32	a	405	CLA	C16-C15-C13	-2.16	108.94	115.92
35	a	412	SQD	O48-C23-O10	-2.16	118.15	123.59
34	D	404	BCR	C34-C9-C10	-2.16	119.90	122.92
32	g	603	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
34	c	514	BCR	C16-C15-C14	-2.15	119.06	123.47
43	R	608	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
44	S	1620	LUT	C8-C9-C10	-2.15	115.64	118.94
32	B	613	CLA	C2A-C3A-C4A	2.15	105.34	101.87
42	z	2635	LMU	O5B-C1B-C2B	2.15	114.90	110.35
45	n	1622	XAT	C15-C35-C34	-2.15	119.07	123.47
32	C	506	CLA	CHD-C1D-ND	-2.15	122.48	124.45
44	Y	1621	LUT	C19-C9-C8	2.15	121.46	118.08
43	s	608	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
44	G	1620	LUT	C39-C29-C28	2.15	121.46	118.08
38	y	2630	LHG	C5-O7-C7	-2.15	112.50	117.79
32	Y	612	CLA	O2D-CGD-CBD	2.15	115.08	111.27
46	Y	1623	NEX	O24-C25-C26	-2.15	57.18	58.96
32	A	405	CLA	C16-C15-C13	-2.14	108.99	115.92
43	Y	601	CHL	C1-C2-C3	-2.14	122.33	126.04
32	c	501	CLA	C16-C15-C13	-2.14	108.99	115.92
38	Y	2630	LHG	O8-C23-O10	-2.14	118.19	123.59
42	Z	2635	LMU	O5B-C1B-C2B	2.14	114.88	110.35
45	N	1622	XAT	C15-C35-C34	-2.14	119.09	123.47
44	g	1620	LUT	C39-C29-C28	2.14	121.45	118.08
43	y	608	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
32	Y	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
32	y	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
44	y	1621	LUT	C19-C9-C8	2.14	121.45	118.08
33	A	408	PHO	C1-C2-C3	-2.14	122.34	126.04
43	g	609	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
32	B	607	CLA	CAC-C3C-C4C	2.14	127.58	124.81
43	N	606	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
43	g	607	CHL	C1C-C2C-C3C	-2.14	105.42	107.11
46	S	1623	NEX	C4-C3-C2	-2.14	106.65	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	Y	608	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
43	s	606	CHL	C1C-C2C-C3C	-2.14	105.42	107.11
46	g	1623	NEX	C4-C3-C2	-2.13	106.65	110.77
32	C	501	CLA	C16-C15-C13	-2.13	109.03	115.92
32	C	501	CLA	CMB-C2B-C3B	2.13	128.67	124.68
32	b	613	CLA	C2A-C3A-C4A	2.13	105.31	101.87
32	s	610	CLA	C4A-NA-C1A	2.13	107.66	106.71
32	C	511	CLA	C2A-C1A-CHA	2.13	127.58	123.86
32	b	617	CLA	CHC-C1C-NC	2.13	127.43	124.20
40	D	405	PL9	C50-C49-C48	-2.13	116.49	122.65
32	S	610	CLA	C4A-NA-C1A	2.13	107.66	106.71
32	b	611	CLA	C2A-C1A-CHA	2.13	127.58	123.86
46	n	1623	NEX	C11-C12-C13	-2.13	120.44	126.42
38	y	2630	LHG	O8-C23-O10	-2.12	118.23	123.59
38	g	2630	LHG	C6-C5-C4	-2.12	106.77	111.79
43	y	607	CHL	CED-O2D-CGD	2.12	120.74	115.94
43	n	609	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
38	s	2630	LHG	O8-C23-C24	2.12	118.56	111.91
34	D	404	BCR	C27-C26-C25	-2.12	119.65	122.73
32	B	617	CLA	CHC-C1C-NC	2.12	127.42	124.20
34	C	515	BCR	C23-C24-C25	-2.12	121.25	127.20
32	s	603	CLA	CHA-C1A-NA	-2.12	121.54	126.40
32	C	505	CLA	C2D-C1D-ND	-2.12	108.54	110.10
32	b	604	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
32	R	602	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
32	B	609	CLA	CHD-C1D-ND	-2.12	122.51	124.45
43	y	607	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
32	g	610	CLA	C1-C2-C3	-2.12	122.39	126.04
43	Y	601	CHL	O2A-CGA-CBA	2.11	118.54	111.91
32	B	604	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
45	n	1622	XAT	C18-C5-C4	2.11	116.66	114.28
43	g	608	CHL	CED-O2D-CGD	2.11	120.72	115.94
34	c	515	BCR	C23-C24-C25	-2.11	121.27	127.20
32	y	612	CLA	O2D-CGD-CBD	2.11	115.02	111.27
43	r	607	CHL	C1B-CHB-C4A	-2.11	125.93	130.12
43	G	607	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
38	G	2630	LHG	C6-C5-C4	-2.11	106.79	111.79
32	r	602	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
43	r	608	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
40	d	405	PL9	C50-C49-C48	-2.11	116.55	122.65
32	B	603	CLA	C4-C3-C5	2.11	118.82	115.27
34	c	516	BCR	C8-C9-C10	-2.11	115.70	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	603	CLA	C4-C3-C5	2.11	118.82	115.27
43	n	606	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
43	S	608	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
43	G	608	CHL	CED-O2D-CGD	2.11	120.71	115.94
44	s	1621	LUT	C21-C26-C27	-2.11	110.04	112.70
32	b	617	CLA	CMC-C2C-C1C	-2.11	121.83	125.04
32	C	509	CLA	C11-C12-C13	-2.11	109.11	115.92
34	B	620	BCR	C39-C30-C25	-2.11	106.88	110.30
34	b	620	BCR	C39-C30-C25	-2.11	106.88	110.30
32	B	613	CLA	O2D-CGD-CBD	2.10	115.01	111.27
32	c	511	CLA	C2A-C1A-CHA	2.10	127.54	123.86
43	Y	606	CHL	C2A-C3A-C4A	-2.10	98.47	101.87
32	g	602	CLA	CHD-C1D-ND	-2.10	122.52	124.45
32	B	604	CLA	C2D-C1D-ND	-2.10	108.55	110.10
34	C	516	BCR	C8-C9-C10	-2.10	115.71	118.94
43	y	601	CHL	O2A-CGA-CBA	2.10	118.51	111.91
46	r	625	NEX	C30-C31-C32	-2.10	116.66	123.22
32	G	610	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
43	Y	607	CHL	C11-C10-C8	-2.10	109.13	115.92
32	g	610	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
32	B	616	CLA	CHA-C1A-NA	-2.10	121.59	126.40
32	D	402	CLA	CMB-C2B-C3B	2.10	128.61	124.68
32	b	609	CLA	CHD-C1D-ND	-2.10	122.53	124.45
44	s	1621	LUT	C20-C13-C12	2.10	121.38	118.08
46	R	625	NEX	C30-C31-C32	-2.10	116.67	123.22
32	B	611	CLA	C2A-C1A-CHA	2.10	127.53	123.86
36	C	521	LMG	O8-C28-O10	-2.10	118.30	123.59
32	c	509	CLA	C11-C12-C13	-2.10	109.14	115.92
43	Y	607	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
43	Y	607	CHL	CED-O2D-CGD	2.10	120.68	115.94
43	R	607	CHL	C4D-CHA-C1A	-2.10	118.70	121.25
38	S	2630	LHG	O8-C23-C24	2.10	118.48	111.91
32	g	611	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
43	y	606	CHL	C2A-C3A-C4A	-2.09	98.49	101.87
42	y	2632	LMU	C1B-O1B-C4'	-2.09	112.78	117.96
43	N	601	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
43	N	609	CHL	O2D-CGD-O1D	-2.09	119.74	123.84
32	r	602	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	s	602	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	G	603	CLA	CMB-C2B-C3B	2.09	128.60	124.68
43	y	607	CHL	C11-C10-C8	-2.09	109.15	115.92
32	b	604	CLA	C2D-C1D-ND	-2.09	108.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	N	609	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
43	G	607	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
36	c	521	LMG	O8-C28-O10	-2.09	118.31	123.59
43	s	606	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
43	s	608	CHL	C1C-C2C-C3C	-2.09	105.45	107.11
32	S	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
43	n	609	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
32	b	613	CLA	O2D-CGD-CBD	2.09	114.98	111.27
42	Y	2632	LMU	C1B-O1B-C4'	-2.09	112.79	117.96
44	G	1620	LUT	C38-C25-C24	-2.09	119.09	123.56
34	B	618	BCR	C10-C11-C12	-2.09	116.70	123.22
43	S	606	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
32	n	602	CLA	C1-C2-C3	-2.09	122.43	126.04
32	c	501	CLA	O2D-CGD-CBD	2.09	114.98	111.27
32	s	610	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
32	b	607	CLA	CAC-C3C-C4C	2.09	127.52	124.81
32	R	610	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
32	N	602	CLA	C1-C2-C3	-2.09	122.43	126.04
32	b	616	CLA	CHA-C1A-NA	-2.09	121.62	126.40
32	d	402	CLA	CMB-C2B-C3B	2.09	128.58	124.68
34	d	404	BCR	C27-C26-C25	-2.09	119.70	122.73
40	d	405	PL9	C27-C28-C29	-2.08	122.64	127.66
32	c	503	CLA	O1D-CGD-CBD	2.08	128.75	124.48
43	R	607	CHL	C1B-CHB-C4A	-2.08	125.99	130.12
44	s	1620	LUT	C2-C3-C4	2.08	113.16	110.30
32	A	406	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
43	S	606	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
34	c	515	BCR	C16-C15-C14	-2.08	119.21	123.47
32	n	612	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
44	Y	1620	LUT	C7-C8-C9	-2.08	123.09	126.23
44	y	1620	LUT	C7-C8-C9	-2.08	123.09	126.23
32	G	611	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
34	d	404	BCR	C35-C13-C12	2.08	121.36	118.08
43	r	607	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
32	r	609	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
44	S	1621	LUT	C16-C1-C6	-2.08	106.92	110.30
32	S	602	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
34	b	618	BCR	C10-C11-C12	-2.08	116.73	123.22
44	S	1621	LUT	C20-C13-C12	2.08	121.35	118.08
41	f	101	HEM	CMB-C2B-C1B	-2.08	121.87	125.04
32	N	612	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
32	B	610	CLA	CAC-C3C-C4C	2.08	127.51	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	603	CLA	CMB-C2B-C3B	2.08	128.56	124.68
46	s	1623	NEX	C11-C12-C13	-2.08	120.58	126.42
34	D	404	BCR	C15-C14-C13	-2.08	124.35	127.31
43	n	601	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
32	S	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
43	G	607	CHL	CED-O2D-CGD	2.07	120.63	115.94
40	D	405	PL9	C27-C28-C29	-2.07	122.66	127.66
32	N	610	CLA	CHD-C1D-ND	-2.07	122.55	124.45
44	g	1620	LUT	C38-C25-C24	-2.07	119.12	123.56
43	n	605	CHL	CAA-C2A-C3A	-2.07	107.10	112.78
43	g	607	CHL	CED-O2D-CGD	2.07	120.62	115.94
32	G	614	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
45	y	1622	XAT	C39-C29-C30	-2.07	120.02	122.92
43	Y	609	CHL	OBD-CAD-C3D	-2.07	123.54	128.52
32	b	610	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
43	N	601	CHL	CMB-C2B-C3B	2.07	128.55	124.68
32	g	614	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
34	b	619	BCR	C4-C5-C6	-2.07	119.73	122.73
44	S	1620	LUT	C2-C3-C4	2.07	113.14	110.30
34	D	404	BCR	C35-C13-C12	2.07	121.34	118.08
45	Y	1622	XAT	C40-C33-C32	2.07	121.34	118.08
43	R	606	CHL	C4D-CHA-C1A	-2.07	118.73	121.25
43	S	608	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
44	S	1621	LUT	C21-C26-C27	-2.07	110.09	112.70
41	F	101	HEM	CAD-CBD-CGD	-2.07	109.16	113.60
43	N	605	CHL	CAA-C2A-C3A	-2.07	107.12	112.78
34	d	404	BCR	C15-C14-C13	-2.07	124.36	127.31
34	D	404	BCR	C21-C20-C19	-2.07	116.77	123.22
32	r	602	CLA	C1-C2-C3	-2.07	122.47	126.04
32	r	604	CLA	CAA-C2A-C1A	2.06	118.74	111.97
32	C	503	CLA	O1D-CGD-CBD	2.06	128.71	124.48
43	g	607	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
32	Y	614	CLA	O2D-CGD-CBD	2.06	114.93	111.27
34	C	515	BCR	C16-C15-C14	-2.06	119.25	123.47
32	N	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
32	n	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
43	N	606	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
32	a	406	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
32	B	610	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
46	R	625	NEX	C5-C4-C3	-2.06	109.31	111.75
43	N	607	CHL	C1B-CHB-C4A	-2.06	126.03	130.12
41	F	101	HEM	CMB-C2B-C1B	-2.06	121.90	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	Y	606	CHL	O2A-CGA-CBA	2.06	118.37	111.91
44	s	1620	LUT	C35-C15-C14	-2.06	119.25	123.47
46	G	1623	NEX	C28-C29-C30	2.06	122.10	118.94
38	C	2630	LHG	O8-C23-O10	-2.06	118.39	123.59
34	C	516	BCR	C38-C26-C27	2.06	117.57	113.62
32	r	609	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
43	y	606	CHL	O2A-CGA-CBA	2.06	118.36	111.91
43	g	601	CHL	C4D-C3D-CAD	2.06	110.52	108.10
32	c	512	CLA	O2D-CGD-CBD	2.06	114.92	111.27
44	s	1620	LUT	C16-C1-C6	-2.06	106.96	110.30
46	n	1623	NEX	C28-C29-C30	2.06	122.10	118.94
43	r	606	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
34	d	404	BCR	C21-C20-C19	-2.06	116.80	123.22
32	R	609	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
32	R	609	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
34	c	516	BCR	C38-C26-C27	2.06	117.56	113.62
43	R	606	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
36	a	413	LMG	O7-C10-O9	-2.05	118.74	123.70
44	S	1620	LUT	C16-C1-C6	-2.05	106.97	110.30
43	Y	605	CHL	O2A-CGA-CBA	2.05	120.63	114.03
32	B	614	CLA	O1D-CGD-CBD	2.05	128.69	124.48
43	r	606	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
32	n	604	CLA	CHA-C4D-ND	2.05	136.79	132.50
32	n	614	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
32	B	616	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
32	y	603	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
32	B	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
32	s	612	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	C	501	CLA	O2D-CGD-CBD	2.05	114.91	111.27
32	Y	603	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
32	B	617	CLA	CMC-C2C-C1C	-2.05	121.92	125.04
43	R	608	CHL	CHB-C4A-NA	2.05	127.34	124.51
32	b	610	CLA	CAC-C3C-C4C	2.05	127.47	124.81
43	n	601	CHL	CMB-C2B-C3B	2.05	128.51	124.68
34	c	516	BCR	C33-C5-C4	2.05	117.55	113.62
46	N	1623	NEX	C28-C29-C30	2.05	122.08	118.94
36	A	413	LMG	O8-C28-C29	2.05	118.33	111.91
33	A	409	PHO	CMC-C2C-C3C	2.05	128.80	124.94
43	g	609	CHL	CED-O2D-CGD	2.05	120.57	115.94
32	S	605	CLA	CBA-CAA-C2A	2.05	119.90	113.86
32	s	605	CLA	CBA-CAA-C2A	2.05	119.90	113.86
32	N	614	CLA	O2A-CGA-O1A	-2.05	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	y	609	CHL	OBD-CAD-C3D	-2.05	123.60	128.52
43	y	605	CHL	O2A-CGA-CBA	2.05	120.60	114.03
43	R	606	CHL	CBC-CAC-C3C	-2.05	106.79	112.43
32	S	605	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
32	N	604	CLA	CHA-C4D-ND	2.05	136.78	132.50
32	R	602	CLA	C1-C2-C3	-2.05	122.51	126.04
42	Z	2634	LMU	C1B-O1B-C4'	-2.04	112.91	117.96
43	r	608	CHL	C4D-C3D-CAD	2.04	110.50	108.10
36	b	622	LMG	O7-C10-O9	-2.04	118.77	123.70
33	a	409	PHO	CMC-C2C-C3C	2.04	128.79	124.94
46	N	1623	NEX	C11-C12-C13	-2.04	120.68	126.42
32	R	604	CLA	CAA-C2A-C1A	2.04	118.67	111.97
44	s	1620	LUT	C40-C33-C32	2.04	121.29	118.08
32	S	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	S	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
32	s	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
32	y	614	CLA	O2D-CGD-CBD	2.04	114.89	111.27
40	D	405	PL9	O2-C1-C6	2.04	124.12	120.59
32	N	611	CLA	O2D-CGD-CBD	2.04	114.89	111.27
34	A	411	BCR	C16-C17-C18	-2.04	124.40	127.31
46	g	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
32	b	616	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
36	d	411	LMG	O8-C28-O10	-2.04	118.45	123.59
46	g	1623	NEX	C28-C29-C30	2.04	122.07	118.94
32	s	610	CLA	O2D-CGD-CBD	2.04	114.89	111.27
32	b	612	CLA	CHD-C1D-ND	-2.04	122.58	124.45
34	C	516	BCR	C33-C5-C4	2.04	117.53	113.62
43	R	608	CHL	C4D-C3D-CAD	2.04	110.50	108.10
44	Y	1620	LUT	C28-C29-C30	-2.04	115.82	118.94
44	s	1621	LUT	C16-C1-C6	-2.04	107.00	110.30
43	R	607	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
36	C	521	LMG	C3-C4-C5	2.04	113.87	110.24
32	s	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
38	c	2630	LHG	O8-C23-O10	-2.04	118.45	123.59
45	y	1622	XAT	C40-C33-C32	2.03	121.28	118.08
44	s	1620	LUT	C36-C21-C26	2.03	112.63	109.55
44	n	1621	LUT	C15-C35-C34	-2.03	119.31	123.47
32	n	611	CLA	O2D-CGD-CBD	2.03	114.88	111.27
32	Y	613	CLA	CHD-C1D-ND	-2.03	122.58	124.45
43	n	607	CHL	C1B-CHB-C4A	-2.03	126.09	130.12
36	B	622	LMG	O7-C10-O9	-2.03	118.79	123.70
43	r	607	CHL	C1C-C2C-C3C	-2.03	105.50	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	n	1623	NEX	C35-C15-C14	-2.03	119.31	123.47
45	G	1622	XAT	C40-C33-C32	2.03	121.28	118.08
32	b	602	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
43	G	609	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
43	g	609	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
36	D	411	LMG	O8-C28-O10	-2.03	118.47	123.59
43	r	606	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
40	D	405	PL9	C8-C7-C3	2.03	117.72	111.98
32	G	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
40	d	405	PL9	C8-C7-C3	2.03	117.71	111.98
46	G	1623	NEX	O24-C25-C26	-2.03	57.28	58.96
32	C	503	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	n	610	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	S	605	CLA	O2D-CGD-CBD	2.03	114.87	111.27
32	s	605	CLA	O2D-CGD-CBD	2.03	114.87	111.27
41	f	101	HEM	CAA-CBA-CGA	-2.03	108.07	113.76
32	c	503	CLA	CHA-C1A-NA	-2.03	121.75	126.40
44	S	1620	LUT	C35-C15-C14	-2.03	119.32	123.47
37	c	518	DGD	C3E-C4E-C5E	2.03	113.86	110.24
41	F	101	HEM	CAA-CBA-CGA	-2.03	108.08	113.76
32	R	602	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
32	c	501	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
36	A	413	LMG	O7-C10-O9	-2.03	118.81	123.70
42	z	2634	LMU	C1B-O1B-C4'	-2.02	112.95	117.96
32	B	602	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
32	D	403	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
32	g	612	CLA	C2A-C1A-CHA	2.02	127.40	123.86
34	C	516	BCR	C37-C22-C21	-2.02	120.09	122.92
40	d	405	PL9	C20-C19-C21	2.02	118.67	115.27
32	b	608	CLA	CHD-C1D-ND	-2.02	122.59	124.45
32	b	611	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
45	Y	1622	XAT	C39-C29-C30	-2.02	120.09	122.92
43	y	608	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
32	C	512	CLA	O2D-CGD-CBD	2.02	114.86	111.27
32	b	614	CLA	O1D-CGD-CBD	2.02	128.62	124.48
32	y	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
32	B	611	CLA	O1D-CGD-CBD	2.02	128.62	124.48
36	c	521	LMG	C3-C4-C5	2.02	113.84	110.24
32	B	611	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
32	C	501	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
44	g	1620	LUT	C1-C2-C3	2.02	118.20	113.64
43	R	606	CHL	CMD-C2D-C3D	-2.02	122.97	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	603	CLA	C3A-C2A-C1A	2.02	104.36	101.34
34	c	517	BCR	C2-C3-C4	-2.02	106.87	111.38
44	G	1620	LUT	C1-C2-C3	2.02	118.20	113.64
32	s	603	CLA	CHD-C1D-ND	-2.02	122.60	124.45
32	s	610	CLA	CHD-C1D-ND	-2.02	122.60	124.45
43	S	601	CHL	O2A-CGA-O1A	-2.02	118.27	123.30
43	N	608	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
34	B	619	BCR	C4-C5-C6	-2.02	119.80	122.73
44	N	1621	LUT	C15-C35-C34	-2.02	119.34	123.47
32	S	602	CLA	CHD-C1D-ND	-2.02	122.60	124.45
43	G	606	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
44	S	1620	LUT	C36-C21-C26	2.01	112.60	109.55
45	r	624	XAT	O4-C5-C6	-2.01	57.29	58.96
32	Y	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
43	R	606	CHL	CED-O2D-CGD	2.01	120.49	115.94
32	A	407	CLA	CHD-C1D-ND	-2.01	122.60	124.45
36	a	413	LMG	O8-C28-C29	2.01	118.23	111.91
34	C	515	BCR	C36-C18-C19	2.01	121.25	118.08
45	N	1622	XAT	O24-C25-C26	-2.01	57.29	58.96
32	d	403	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
34	a	411	BCR	C37-C22-C23	2.01	121.25	118.08
32	g	603	CLA	C2A-C1A-CHA	2.01	127.38	123.86
33	A	409	PHO	C1B-NB-C4B	2.01	111.22	107.09
44	S	1621	LUT	C8-C7-C6	-2.01	121.55	127.20
32	g	602	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
32	C	503	CLA	CHA-C1A-NA	-2.01	121.79	126.40
44	G	1620	LUT	C8-C7-C6	-2.01	121.56	127.20
43	g	608	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
32	g	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
34	a	411	BCR	C16-C17-C18	-2.01	124.44	127.31
32	G	612	CLA	C2A-C1A-CHA	2.01	127.37	123.86
44	g	1621	LUT	C35-C15-C14	-2.01	119.36	123.47
40	D	405	PL9	C20-C19-C21	2.01	118.65	115.27
43	Y	608	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
32	C	508	CLA	C1-C2-C3	-2.01	122.57	126.04
32	S	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
34	h	101	BCR	C4-C5-C6	-2.01	119.82	122.73
34	c	517	BCR	C2-C1-C6	2.01	113.57	110.48
43	r	606	CHL	CMD-C2D-C3D	-2.01	123.00	127.61
34	C	517	BCR	C2-C1-C6	2.00	113.57	110.48
45	g	1622	XAT	C40-C33-C32	2.00	121.23	118.08
44	Y	1621	LUT	C36-C21-C26	2.00	112.58	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	y	1621	LUT	C36-C21-C26	2.00	112.58	109.55
32	y	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
34	c	516	BCR	C37-C22-C21	-2.00	120.12	122.92
44	S	1620	LUT	C40-C33-C32	2.00	121.23	118.08
43	n	608	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
32	c	508	CLA	C1-C2-C3	-2.00	122.58	126.04
43	S	608	CHL	C2A-C1A-CHA	-2.00	120.36	123.86

All (272) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	407	CLA	ND
32	B	602	CLA	ND
32	B	603	CLA	ND
32	B	605	CLA	ND
32	B	606	CLA	ND
32	B	607	CLA	ND
32	B	608	CLA	ND
32	B	609	CLA	ND
32	B	611	CLA	ND
32	B	612	CLA	ND
32	B	613	CLA	ND
32	B	614	CLA	ND
32	B	615	CLA	ND
32	B	616	CLA	ND
32	B	617	CLA	ND
32	C	501	CLA	ND
32	C	503	CLA	ND
32	C	504	CLA	ND
32	C	507	CLA	ND
32	C	508	CLA	ND
32	C	509	CLA	ND
32	C	510	CLA	ND
32	C	512	CLA	ND
32	C	513	CLA	ND
32	D	402	CLA	ND
32	N	602	CLA	ND
32	N	603	CLA	ND
32	N	604	CLA	ND
32	N	610	CLA	ND
32	N	611	CLA	ND

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Mol	Chain	Res	Type	Atom
32	N	612	CLA	ND
32	N	614	CLA	ND
32	G	602	CLA	ND
32	G	603	CLA	ND
32	G	604	CLA	ND
32	G	610	CLA	ND
32	G	611	CLA	ND
32	G	612	CLA	ND
32	G	614	CLA	ND
32	R	602	CLA	ND
32	R	603	CLA	ND
32	R	604	CLA	ND
32	R	609	CLA	ND
32	R	610	CLA	ND
32	S	602	CLA	ND
32	S	603	CLA	ND
32	S	604	CLA	ND
32	S	605	CLA	ND
32	S	609	CLA	ND
32	S	610	CLA	ND
32	S	611	CLA	ND
32	S	612	CLA	ND
32	S	614	CLA	ND
32	Y	602	CLA	ND
32	Y	603	CLA	ND
32	Y	604	CLA	ND
32	Y	610	CLA	ND
32	Y	611	CLA	ND
32	Y	612	CLA	ND
32	Y	614	CLA	ND
32	a	405	CLA	ND
32	a	407	CLA	ND
32	b	602	CLA	ND
32	b	603	CLA	ND
32	b	605	CLA	ND
32	b	606	CLA	ND
32	b	607	CLA	ND
32	b	608	CLA	ND
32	b	609	CLA	ND
32	b	611	CLA	ND
32	b	612	CLA	ND
32	b	613	CLA	ND

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Mol	Chain	Res	Type	Atom
32	b	614	CLA	ND
32	b	615	CLA	ND
32	b	616	CLA	ND
32	b	617	CLA	ND
32	c	501	CLA	ND
32	c	503	CLA	ND
32	c	504	CLA	ND
32	c	507	CLA	ND
32	c	508	CLA	ND
32	c	509	CLA	ND
32	c	510	CLA	ND
32	c	512	CLA	ND
32	c	513	CLA	ND
32	d	402	CLA	ND
32	n	602	CLA	ND
32	n	603	CLA	ND
32	n	604	CLA	ND
32	n	610	CLA	ND
32	n	611	CLA	ND
32	n	612	CLA	ND
32	n	614	CLA	ND
32	g	602	CLA	ND
32	g	603	CLA	ND
32	g	604	CLA	ND
32	g	610	CLA	ND
32	g	611	CLA	ND
32	g	612	CLA	ND
32	g	614	CLA	ND
32	r	602	CLA	ND
32	r	603	CLA	ND
32	r	604	CLA	ND
32	r	609	CLA	ND
32	r	610	CLA	ND
32	s	602	CLA	ND
32	s	603	CLA	ND
32	s	604	CLA	ND
32	s	605	CLA	ND
32	s	609	CLA	ND
32	s	610	CLA	ND
32	s	611	CLA	ND
32	s	612	CLA	ND
32	s	614	CLA	ND

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Mol	Chain	Res	Type	Atom
32	y	602	CLA	ND
32	y	603	CLA	ND
32	y	604	CLA	ND
32	y	610	CLA	ND
32	y	611	CLA	ND
32	y	612	CLA	ND
32	y	614	CLA	ND
43	N	601	CHL	ND
43	N	601	CHL	NA
43	N	601	CHL	NC
43	N	605	CHL	ND
43	N	605	CHL	NA
43	N	605	CHL	NC
43	N	606	CHL	ND
43	N	606	CHL	NA
43	N	606	CHL	NC
43	N	607	CHL	ND
43	N	607	CHL	NA
43	N	607	CHL	NC
43	N	608	CHL	ND
43	N	608	CHL	NA
43	N	608	CHL	NC
43	N	609	CHL	ND
43	N	609	CHL	NA
43	N	609	CHL	NC
43	G	601	CHL	ND
43	G	601	CHL	NA
43	G	601	CHL	NC
43	G	605	CHL	ND
43	G	605	CHL	NA
43	G	605	CHL	NC
43	G	606	CHL	ND
43	G	606	CHL	NA
43	G	606	CHL	NC
43	G	607	CHL	ND
43	G	607	CHL	NA
43	G	607	CHL	NC
43	G	608	CHL	ND
43	G	608	CHL	NA
43	G	608	CHL	NC
43	G	609	CHL	ND
43	G	609	CHL	NA

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

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

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

All (2937) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	406	CLA	CHA-CBD-CGD-O1D
32	A	406	CLA	CHA-CBD-CGD-O2D
32	B	603	CLA	C2-C3-C5-C6
32	B	603	CLA	C4-C3-C5-C6
32	B	604	CLA	C2-C3-C5-C6
32	B	604	CLA	C4-C3-C5-C6
32	B	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	B	605	CLA	CHA-CBD-CGD-O1D
32	B	605	CLA	CHA-CBD-CGD-O2D
32	B	605	CLA	CAD-CBD-CGD-O1D
32	B	610	CLA	C1A-C2A-CAA-CBA
32	B	610	CLA	CHA-CBD-CGD-O1D
32	B	610	CLA	CHA-CBD-CGD-O2D
32	B	610	CLA	CAD-CBD-CGD-O1D
32	B	615	CLA	CHA-CBD-CGD-O1D
32	B	615	CLA	CHA-CBD-CGD-O2D
32	B	615	CLA	CAD-CBD-CGD-O1D
32	B	617	CLA	C2A-CAA-CBA-CGA
32	C	504	CLA	CHA-CBD-CGD-O1D
32	C	504	CLA	CHA-CBD-CGD-O2D
32	C	504	CLA	CAD-CBD-CGD-O1D
32	C	504	CLA	CAD-CBD-CGD-O2D
32	C	512	CLA	CHA-CBD-CGD-O1D
32	C	512	CLA	CHA-CBD-CGD-O2D
32	C	513	CLA	C2-C3-C5-C6
32	C	513	CLA	C4-C3-C5-C6
32	D	402	CLA	C1A-C2A-CAA-CBA
32	D	403	CLA	C1A-C2A-CAA-CBA
32	D	403	CLA	C3A-C2A-CAA-CBA
32	N	604	CLA	CHA-CBD-CGD-O1D
32	N	604	CLA	CHA-CBD-CGD-O2D
32	N	604	CLA	CAD-CBD-CGD-O1D
32	N	611	CLA	CHA-CBD-CGD-O1D
32	N	611	CLA	CHA-CBD-CGD-O2D
32	N	614	CLA	CBD-CGD-O2D-CED
32	G	604	CLA	C1A-C2A-CAA-CBA
32	G	604	CLA	C3A-C2A-CAA-CBA
32	G	612	CLA	CBD-CGD-O2D-CED
32	G	613	CLA	C6-C7-C8-C10
32	R	603	CLA	C1A-C2A-CAA-CBA
32	R	604	CLA	C1A-C2A-CAA-CBA
32	R	609	CLA	C1A-C2A-CAA-CBA
32	R	609	CLA	C3A-C2A-CAA-CBA
32	S	602	CLA	CHA-CBD-CGD-O1D
32	S	602	CLA	CHA-CBD-CGD-O2D
32	S	603	CLA	C1A-C2A-CAA-CBA
32	S	603	CLA	C3A-C2A-CAA-CBA
32	S	604	CLA	CBD-CGD-O2D-CED
32	S	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	S	605	CLA	CHA-CBD-CGD-O1D
32	S	605	CLA	CHA-CBD-CGD-O2D
32	S	610	CLA	CHA-CBD-CGD-O1D
32	S	613	CLA	CBD-CGD-O2D-CED
32	Y	613	CLA	CHA-CBD-CGD-O1D
32	Y	613	CLA	CHA-CBD-CGD-O2D
32	a	406	CLA	CHA-CBD-CGD-O1D
32	a	406	CLA	CHA-CBD-CGD-O2D
32	b	603	CLA	C2-C3-C5-C6
32	b	603	CLA	C4-C3-C5-C6
32	b	604	CLA	C2-C3-C5-C6
32	b	604	CLA	C4-C3-C5-C6
32	b	605	CLA	C1A-C2A-CAA-CBA
32	b	605	CLA	CHA-CBD-CGD-O1D
32	b	605	CLA	CHA-CBD-CGD-O2D
32	b	605	CLA	CAD-CBD-CGD-O1D
32	b	610	CLA	C1A-C2A-CAA-CBA
32	b	610	CLA	CHA-CBD-CGD-O1D
32	b	610	CLA	CHA-CBD-CGD-O2D
32	b	610	CLA	CAD-CBD-CGD-O1D
32	b	615	CLA	CHA-CBD-CGD-O1D
32	b	615	CLA	CHA-CBD-CGD-O2D
32	b	615	CLA	CAD-CBD-CGD-O1D
32	b	617	CLA	C2A-CAA-CBA-CGA
32	c	504	CLA	CHA-CBD-CGD-O1D
32	c	504	CLA	CHA-CBD-CGD-O2D
32	c	504	CLA	CAD-CBD-CGD-O1D
32	c	504	CLA	CAD-CBD-CGD-O2D
32	c	512	CLA	CHA-CBD-CGD-O1D
32	c	512	CLA	CHA-CBD-CGD-O2D
32	c	513	CLA	C2-C3-C5-C6
32	c	513	CLA	C4-C3-C5-C6
32	d	402	CLA	C1A-C2A-CAA-CBA
32	d	403	CLA	C1A-C2A-CAA-CBA
32	d	403	CLA	C3A-C2A-CAA-CBA
32	n	604	CLA	CHA-CBD-CGD-O1D
32	n	604	CLA	CHA-CBD-CGD-O2D
32	n	604	CLA	CAD-CBD-CGD-O1D
32	n	611	CLA	CHA-CBD-CGD-O1D
32	n	611	CLA	CHA-CBD-CGD-O2D
32	n	614	CLA	CBD-CGD-O2D-CED
32	g	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	g	604	CLA	C3A-C2A-CAA-CBA
32	g	612	CLA	CBD-CGD-O2D-CED
32	g	613	CLA	C6-C7-C8-C10
32	r	603	CLA	C1A-C2A-CAA-CBA
32	r	604	CLA	C1A-C2A-CAA-CBA
32	r	609	CLA	C1A-C2A-CAA-CBA
32	r	609	CLA	C3A-C2A-CAA-CBA
32	r	610	CLA	CBD-CGD-O2D-CED
32	s	602	CLA	CHA-CBD-CGD-O1D
32	s	602	CLA	CHA-CBD-CGD-O2D
32	s	603	CLA	C1A-C2A-CAA-CBA
32	s	603	CLA	C3A-C2A-CAA-CBA
32	s	604	CLA	CBD-CGD-O2D-CED
32	s	605	CLA	C1A-C2A-CAA-CBA
32	s	605	CLA	CHA-CBD-CGD-O1D
32	s	605	CLA	CHA-CBD-CGD-O2D
32	s	609	CLA	CBD-CGD-O2D-CED
32	s	610	CLA	CHA-CBD-CGD-O1D
32	s	610	CLA	CHA-CBD-CGD-O2D
32	s	613	CLA	CBD-CGD-O2D-CED
32	y	613	CLA	CHA-CBD-CGD-O1D
32	y	613	CLA	CHA-CBD-CGD-O2D
34	A	411	BCR	C23-C24-C25-C30
34	B	620	BCR	C7-C8-C9-C10
34	B	620	BCR	C7-C8-C9-C34
34	C	515	BCR	C7-C8-C9-C34
34	C	515	BCR	C11-C12-C13-C35
34	C	516	BCR	C1-C6-C7-C8
34	C	516	BCR	C7-C8-C9-C10
34	C	516	BCR	C7-C8-C9-C34
34	D	404	BCR	C7-C8-C9-C10
34	D	404	BCR	C7-C8-C9-C34
34	H	101	BCR	C7-C8-C9-C10
34	H	101	BCR	C7-C8-C9-C34
34	a	411	BCR	C23-C24-C25-C30
34	b	620	BCR	C7-C8-C9-C10
34	b	620	BCR	C7-C8-C9-C34
34	c	515	BCR	C7-C8-C9-C34
34	c	515	BCR	C11-C12-C13-C35
34	c	516	BCR	C1-C6-C7-C8
34	c	516	BCR	C7-C8-C9-C10
34	c	516	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
34	d	404	BCR	C7-C8-C9-C10
34	d	404	BCR	C7-C8-C9-C34
34	h	101	BCR	C7-C8-C9-C10
34	h	101	BCR	C7-C8-C9-C34
34	h	101	BCR	C23-C24-C25-C30
35	A	412	SQD	C5-C6-S-O8
35	A	412	SQD	C5-C6-S-O9
35	a	412	SQD	C5-C6-S-O8
36	A	413	LMG	O6-C1-O1-C7
36	H	102	LMG	O7-C8-C9-O8
36	a	413	LMG	O6-C1-O1-C7
36	h	102	LMG	O7-C8-C9-O8
37	C	519	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	O1G-C1G-C2G-O2G
38	C	2630	LHG	C3-O3-P-O4
38	C	2630	LHG	C4-O6-P-O5
38	D	408	LHG	C1-C2-C3-O3
38	D	408	LHG	C3-O3-P-O6
38	D	408	LHG	C4-O6-P-O3
38	D	408	LHG	C4-O6-P-O4
38	D	408	LHG	C4-O6-P-O5
38	D	409	LHG	C4-O6-P-O4
38	D	409	LHG	C4-O6-P-O5
38	D	410	LHG	C1-C2-C3-O3
38	D	410	LHG	C3-O3-P-O5
38	D	410	LHG	C4-O6-P-O4
38	D	410	LHG	C4-O6-P-O5
38	L	101	LHG	C3-O3-P-O4
38	L	101	LHG	C3-O3-P-O5
38	N	2630	LHG	C4-O6-P-O3
38	N	2630	LHG	C4-O6-P-O4
38	N	2630	LHG	C4-O6-P-O5
38	G	2630	LHG	C3-O3-P-O4
38	G	2630	LHG	C4-O6-P-O3
38	G	2630	LHG	C4-O6-P-O4
38	G	2630	LHG	C4-O6-P-O5
38	Y	2630	LHG	C1-C2-C3-O3
38	Y	2630	LHG	C4-O6-P-O3
38	Y	2630	LHG	C4-O6-P-O4
38	Y	2630	LHG	C4-O6-P-O5
38	c	2630	LHG	C3-O3-P-O4
38	c	2630	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
38	d	408	LHG	C1-C2-C3-O3
38	d	408	LHG	C4-O6-P-O3
38	d	408	LHG	C4-O6-P-O4
38	d	408	LHG	C4-O6-P-O5
38	d	409	LHG	C4-O6-P-O4
38	d	409	LHG	C4-O6-P-O5
38	d	410	LHG	C1-C2-C3-O3
38	d	410	LHG	C3-O3-P-O5
38	d	410	LHG	C4-O6-P-O5
38	l	101	LHG	C3-O3-P-O4
38	l	101	LHG	C3-O3-P-O5
38	n	2630	LHG	C4-O6-P-O3
38	n	2630	LHG	C4-O6-P-O4
38	n	2630	LHG	C4-O6-P-O5
38	g	2630	LHG	C3-O3-P-O4
38	g	2630	LHG	C4-O6-P-O3
38	g	2630	LHG	C4-O6-P-O4
38	g	2630	LHG	C4-O6-P-O5
38	y	2630	LHG	C1-C2-C3-O3
38	y	2630	LHG	C4-O6-P-O3
38	y	2630	LHG	C4-O6-P-O4
38	y	2630	LHG	C4-O6-P-O5
40	D	405	PL9	C37-C38-C39-C40
40	d	405	PL9	C37-C38-C39-C40
42	Z	2635	LMU	O5B-C1B-O1B-C4'
42	z	2635	LMU	O5B-C1B-O1B-C4'
43	N	601	CHL	C1C-C2C-CMC-OMC
43	N	601	CHL	C3C-C2C-CMC-OMC
43	N	601	CHL	CHA-CBD-CGD-O1D
43	N	601	CHL	CHA-CBD-CGD-O2D
43	N	605	CHL	C1C-C2C-CMC-OMC
43	N	605	CHL	C3C-C2C-CMC-OMC
43	N	606	CHL	C1A-C2A-CAA-CBA
43	N	606	CHL	CBD-CGD-O2D-CED
43	N	607	CHL	C3C-C2C-CMC-OMC
43	N	607	CHL	C11-C10-C8-C7
43	N	609	CHL	C3C-C2C-CMC-OMC
43	G	601	CHL	C1A-C2A-CAA-CBA
43	G	601	CHL	C3A-C2A-CAA-CBA
43	G	608	CHL	C3C-C2C-CMC-OMC
43	G	609	CHL	C1C-C2C-CMC-OMC
43	G	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
43	R	606	CHL	C1C-C2C-CMC-OMC
43	R	606	CHL	C3C-C2C-CMC-OMC
43	R	607	CHL	C1C-C2C-CMC-OMC
43	R	607	CHL	C3C-C2C-CMC-OMC
43	S	601	CHL	C2A-CAA-CBA-CGA
43	S	601	CHL	C3C-C2C-CMC-OMC
43	S	606	CHL	CBD-CGD-O2D-CED
43	S	607	CHL	C3C-C2C-CMC-OMC
43	S	608	CHL	C1C-C2C-CMC-OMC
43	S	608	CHL	C3C-C2C-CMC-OMC
43	S	608	CHL	CHA-CBD-CGD-O1D
43	S	608	CHL	CHA-CBD-CGD-O2D
43	S	608	CHL	CAD-CBD-CGD-O1D
43	S	608	CHL	CAD-CBD-CGD-O2D
43	S	608	CHL	CBD-CGD-O2D-CED
43	Y	605	CHL	C1C-C2C-CMC-OMC
43	Y	605	CHL	C3C-C2C-CMC-OMC
43	Y	606	CHL	C1A-C2A-CAA-CBA
43	Y	608	CHL	CBD-CGD-O2D-CED
43	Y	609	CHL	C1C-C2C-CMC-OMC
43	Y	609	CHL	C3C-C2C-CMC-OMC
43	Y	609	CHL	C11-C10-C8-C9
43	n	601	CHL	C1C-C2C-CMC-OMC
43	n	601	CHL	C3C-C2C-CMC-OMC
43	n	601	CHL	CHA-CBD-CGD-O1D
43	n	601	CHL	CHA-CBD-CGD-O2D
43	n	605	CHL	C1C-C2C-CMC-OMC
43	n	605	CHL	C3C-C2C-CMC-OMC
43	n	606	CHL	C1A-C2A-CAA-CBA
43	n	606	CHL	CBD-CGD-O2D-CED
43	n	607	CHL	C3C-C2C-CMC-OMC
43	n	607	CHL	C11-C10-C8-C7
43	n	609	CHL	C3C-C2C-CMC-OMC
43	g	608	CHL	C3C-C2C-CMC-OMC
43	g	609	CHL	C1C-C2C-CMC-OMC
43	g	609	CHL	C3C-C2C-CMC-OMC
43	r	606	CHL	C1C-C2C-CMC-OMC
43	r	606	CHL	C3C-C2C-CMC-OMC
43	r	607	CHL	C1C-C2C-CMC-OMC
43	r	607	CHL	C3C-C2C-CMC-OMC
43	s	601	CHL	C2A-CAA-CBA-CGA
43	s	601	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
43	s	606	CHL	CBD-CGD-O2D-CED
43	s	607	CHL	C3C-C2C-CMC-OMC
43	s	608	CHL	C1C-C2C-CMC-OMC
43	s	608	CHL	C3C-C2C-CMC-OMC
43	s	608	CHL	CHA-CBD-CGD-O1D
43	s	608	CHL	CHA-CBD-CGD-O2D
43	s	608	CHL	CAD-CBD-CGD-O1D
43	s	608	CHL	CAD-CBD-CGD-O2D
43	s	608	CHL	CBD-CGD-O2D-CED
43	y	605	CHL	C1C-C2C-CMC-OMC
43	y	605	CHL	C3C-C2C-CMC-OMC
43	y	606	CHL	C1A-C2A-CAA-CBA
43	y	608	CHL	CBD-CGD-O2D-CED
43	y	609	CHL	C1C-C2C-CMC-OMC
43	y	609	CHL	C3C-C2C-CMC-OMC
43	y	609	CHL	C11-C10-C8-C9
44	N	1620	LUT	C1-C6-C7-C8
44	G	1620	LUT	C1-C6-C7-C8
44	S	1620	LUT	C27-C28-C29-C30
44	S	1620	LUT	C27-C28-C29-C39
44	g	1620	LUT	C1-C6-C7-C8
44	s	1620	LUT	C27-C28-C29-C30
44	s	1620	LUT	C27-C28-C29-C39
45	Y	1622	XAT	C11-C12-C13-C14
45	Y	1622	XAT	C11-C12-C13-C20
45	y	1622	XAT	C11-C12-C13-C14
45	y	1622	XAT	C11-C12-C13-C20
45	y	1622	XAT	C31-C32-C33-C34
45	y	1622	XAT	C31-C32-C33-C40
46	S	1623	NEX	C31-C32-C33-C40
46	Y	1623	NEX	C31-C32-C33-C34
46	Y	1623	NEX	C31-C32-C33-C40
46	y	1623	NEX	C31-C32-C33-C34
46	y	1623	NEX	C31-C32-C33-C40
32	S	613	CLA	O1D-CGD-O2D-CED
43	S	606	CHL	O1D-CGD-O2D-CED
43	s	606	CHL	O1D-CGD-O2D-CED
32	A	405	CLA	O1D-CGD-O2D-CED
32	N	612	CLA	O1D-CGD-O2D-CED
32	R	603	CLA	O1D-CGD-O2D-CED
32	R	609	CLA	O1D-CGD-O2D-CED
32	S	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	Y	612	CLA	O1D-CGD-O2D-CED
32	a	405	CLA	O1D-CGD-O2D-CED
32	n	612	CLA	O1D-CGD-O2D-CED
32	r	602	CLA	O1D-CGD-O2D-CED
32	r	603	CLA	O1D-CGD-O2D-CED
32	r	609	CLA	O1D-CGD-O2D-CED
32	s	611	CLA	O1D-CGD-O2D-CED
32	s	613	CLA	O1D-CGD-O2D-CED
32	y	612	CLA	O1D-CGD-O2D-CED
32	A	405	CLA	CBD-CGD-O2D-CED
32	B	610	CLA	CBD-CGD-O2D-CED
32	B	615	CLA	CBD-CGD-O2D-CED
32	C	501	CLA	CBD-CGD-O2D-CED
32	C	503	CLA	CBD-CGD-O2D-CED
32	C	508	CLA	CBD-CGD-O2D-CED
32	D	403	CLA	CBD-CGD-O2D-CED
32	N	612	CLA	CBD-CGD-O2D-CED
32	G	614	CLA	CBD-CGD-O2D-CED
32	R	602	CLA	CBD-CGD-O2D-CED
32	R	603	CLA	CBD-CGD-O2D-CED
32	R	609	CLA	CBD-CGD-O2D-CED
32	S	609	CLA	CBD-CGD-O2D-CED
32	S	611	CLA	CBD-CGD-O2D-CED
32	Y	612	CLA	CBD-CGD-O2D-CED
32	Y	614	CLA	CBD-CGD-O2D-CED
32	a	405	CLA	CBD-CGD-O2D-CED
32	b	610	CLA	CBD-CGD-O2D-CED
32	b	615	CLA	CBD-CGD-O2D-CED
32	c	501	CLA	CBD-CGD-O2D-CED
32	c	503	CLA	CBD-CGD-O2D-CED
32	c	508	CLA	CBD-CGD-O2D-CED
32	d	403	CLA	CBD-CGD-O2D-CED
32	n	612	CLA	CBD-CGD-O2D-CED
32	g	614	CLA	CBD-CGD-O2D-CED
32	r	602	CLA	CBD-CGD-O2D-CED
32	r	603	CLA	CBD-CGD-O2D-CED
32	r	609	CLA	CBD-CGD-O2D-CED
32	s	611	CLA	CBD-CGD-O2D-CED
32	y	612	CLA	CBD-CGD-O2D-CED
32	y	614	CLA	CBD-CGD-O2D-CED
43	N	608	CHL	CBD-CGD-O2D-CED
43	G	601	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
43	G	608	CHL	CBD-CGD-O2D-CED
43	R	608	CHL	CBD-CGD-O2D-CED
43	S	601	CHL	CBD-CGD-O2D-CED
43	n	608	CHL	CBD-CGD-O2D-CED
43	g	601	CHL	CBD-CGD-O2D-CED
43	g	608	CHL	CBD-CGD-O2D-CED
43	r	608	CHL	CBD-CGD-O2D-CED
43	s	601	CHL	CBD-CGD-O2D-CED
32	B	614	CLA	O1A-CGA-O2A-C1
32	S	613	CLA	O1A-CGA-O2A-C1
32	b	614	CLA	O1A-CGA-O2A-C1
32	s	613	CLA	O1A-CGA-O2A-C1
43	Y	608	CHL	O1D-CGD-O2D-CED
32	G	612	CLA	O1D-CGD-O2D-CED
32	R	602	CLA	O1D-CGD-O2D-CED
32	S	604	CLA	O1D-CGD-O2D-CED
32	g	612	CLA	O1D-CGD-O2D-CED
32	s	604	CLA	O1D-CGD-O2D-CED
32	s	609	CLA	O1D-CGD-O2D-CED
43	S	608	CHL	O1D-CGD-O2D-CED
43	s	608	CHL	O1D-CGD-O2D-CED
43	y	608	CHL	O1D-CGD-O2D-CED
32	B	614	CLA	CBA-CGA-O2A-C1
32	D	403	CLA	CBA-CGA-O2A-C1
32	S	613	CLA	CBA-CGA-O2A-C1
32	b	614	CLA	CBA-CGA-O2A-C1
32	d	403	CLA	CBA-CGA-O2A-C1
32	s	613	CLA	CBA-CGA-O2A-C1
32	B	606	CLA	CBD-CGD-O2D-CED
32	C	506	CLA	CBD-CGD-O2D-CED
32	C	512	CLA	CBD-CGD-O2D-CED
32	G	604	CLA	CBD-CGD-O2D-CED
32	G	613	CLA	CBD-CGD-O2D-CED
32	R	610	CLA	CBD-CGD-O2D-CED
32	S	603	CLA	CBD-CGD-O2D-CED
32	Y	604	CLA	CBD-CGD-O2D-CED
32	Y	613	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	CBD-CGD-O2D-CED
32	c	506	CLA	CBD-CGD-O2D-CED
32	c	512	CLA	CBD-CGD-O2D-CED
32	g	604	CLA	CBD-CGD-O2D-CED
32	g	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	s	603	CLA	CBD-CGD-O2D-CED
32	y	604	CLA	CBD-CGD-O2D-CED
32	y	613	CLA	CBD-CGD-O2D-CED
43	G	607	CHL	CBD-CGD-O2D-CED
43	Y	605	CHL	CBD-CGD-O2D-CED
43	g	607	CHL	CBD-CGD-O2D-CED
43	y	605	CHL	CBD-CGD-O2D-CED
32	A	405	CLA	O1A-CGA-O2A-C1
32	C	510	CLA	O1A-CGA-O2A-C1
32	D	403	CLA	O1A-CGA-O2A-C1
32	N	614	CLA	O1A-CGA-O2A-C1
32	G	614	CLA	O1A-CGA-O2A-C1
32	a	405	CLA	O1A-CGA-O2A-C1
32	c	510	CLA	O1A-CGA-O2A-C1
32	d	403	CLA	O1A-CGA-O2A-C1
32	n	614	CLA	O1A-CGA-O2A-C1
32	g	614	CLA	O1A-CGA-O2A-C1
32	r	610	CLA	O1D-CGD-O2D-CED
43	N	606	CHL	O1D-CGD-O2D-CED
43	n	606	CHL	O1D-CGD-O2D-CED
32	N	614	CLA	O1D-CGD-O2D-CED
32	S	609	CLA	O1D-CGD-O2D-CED
32	c	503	CLA	O1D-CGD-O2D-CED
32	n	614	CLA	O1D-CGD-O2D-CED
32	B	614	CLA	CBD-CGD-O2D-CED
32	G	603	CLA	CBD-CGD-O2D-CED
32	b	614	CLA	CBD-CGD-O2D-CED
43	r	607	CHL	CBD-CGD-O2D-CED
32	C	503	CLA	O1D-CGD-O2D-CED
32	B	617	CLA	O1A-CGA-O2A-C1
32	S	611	CLA	O1A-CGA-O2A-C1
32	b	617	CLA	O1A-CGA-O2A-C1
32	s	611	CLA	O1A-CGA-O2A-C1
32	A	410	CLA	C3-C5-C6-C7
32	B	615	CLA	C3-C5-C6-C7
32	B	617	CLA	C3-C5-C6-C7
32	a	410	CLA	C3-C5-C6-C7
32	b	615	CLA	C3-C5-C6-C7
32	b	617	CLA	C3-C5-C6-C7
33	A	409	PHO	C3-C5-C6-C7
33	a	409	PHO	C3-C5-C6-C7
43	Y	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
43	Y	607	CHL	C3-C5-C6-C7
43	y	601	CHL	C3-C5-C6-C7
43	y	607	CHL	C3-C5-C6-C7
32	C	510	CLA	CBA-CGA-O2A-C1
32	C	513	CLA	CBA-CGA-O2A-C1
32	N	614	CLA	CBA-CGA-O2A-C1
32	G	614	CLA	CBA-CGA-O2A-C1
32	n	614	CLA	CBA-CGA-O2A-C1
32	g	614	CLA	CBA-CGA-O2A-C1
32	G	614	CLA	O1D-CGD-O2D-CED
32	g	614	CLA	O1D-CGD-O2D-CED
43	N	608	CHL	O1D-CGD-O2D-CED
43	n	608	CHL	O1D-CGD-O2D-CED
43	g	601	CHL	O1D-CGD-O2D-CED
32	B	604	CLA	CBD-CGD-O2D-CED
32	S	602	CLA	CBD-CGD-O2D-CED
32	b	604	CLA	CBD-CGD-O2D-CED
32	s	602	CLA	CBD-CGD-O2D-CED
43	R	607	CHL	CBD-CGD-O2D-CED
32	B	611	CLA	CBD-CGD-O2D-CED
43	Y	601	CHL	CBD-CGD-O2D-CED
43	y	601	CHL	CBD-CGD-O2D-CED
32	B	607	CLA	C2A-CAA-CBA-CGA
32	B	614	CLA	C2A-CAA-CBA-CGA
32	N	614	CLA	C2A-CAA-CBA-CGA
32	G	614	CLA	C2A-CAA-CBA-CGA
32	R	609	CLA	C2A-CAA-CBA-CGA
32	b	607	CLA	C2A-CAA-CBA-CGA
32	b	614	CLA	C2A-CAA-CBA-CGA
32	n	614	CLA	C2A-CAA-CBA-CGA
32	g	614	CLA	C2A-CAA-CBA-CGA
32	r	609	CLA	C2A-CAA-CBA-CGA
43	N	608	CHL	C2A-CAA-CBA-CGA
43	Y	601	CHL	C2A-CAA-CBA-CGA
43	Y	607	CHL	C2A-CAA-CBA-CGA
43	n	608	CHL	C2A-CAA-CBA-CGA
43	y	601	CHL	C2A-CAA-CBA-CGA
43	y	607	CHL	C2A-CAA-CBA-CGA
32	C	507	CLA	C3-C5-C6-C7
32	c	507	CLA	C3-C5-C6-C7
32	A	405	CLA	CBA-CGA-O2A-C1
32	B	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	S	611	CLA	CBA-CGA-O2A-C1
32	a	405	CLA	CBA-CGA-O2A-C1
32	b	617	CLA	CBA-CGA-O2A-C1
32	c	510	CLA	CBA-CGA-O2A-C1
32	c	513	CLA	CBA-CGA-O2A-C1
32	s	611	CLA	CBA-CGA-O2A-C1
43	G	601	CHL	O1D-CGD-O2D-CED
43	S	601	CHL	O1D-CGD-O2D-CED
43	s	601	CHL	O1D-CGD-O2D-CED
32	B	617	CLA	CBD-CGD-O2D-CED
32	C	511	CLA	CBD-CGD-O2D-CED
32	b	611	CLA	CBD-CGD-O2D-CED
32	b	617	CLA	CBD-CGD-O2D-CED
32	c	511	CLA	CBD-CGD-O2D-CED
32	g	603	CLA	CBD-CGD-O2D-CED
32	B	610	CLA	O1D-CGD-O2D-CED
32	Y	614	CLA	O1D-CGD-O2D-CED
32	b	610	CLA	O1D-CGD-O2D-CED
32	c	501	CLA	O1D-CGD-O2D-CED
32	y	614	CLA	O1D-CGD-O2D-CED
43	R	608	CHL	O1D-CGD-O2D-CED
43	r	608	CHL	O1D-CGD-O2D-CED
37	C	523	DGD	C4E-C5E-C6E-O5E
37	c	523	DGD	C4E-C5E-C6E-O5E
42	Z	2635	LMU	C4'-C5'-C6'-O6'
42	z	2635	LMU	C4'-C5'-C6'-O6'
32	C	501	CLA	O1D-CGD-O2D-CED
42	Z	2635	LMU	O5B-C5B-C6B-O6B
42	z	2635	LMU	O5B-C5B-C6B-O6B
32	C	510	CLA	CBD-CGD-O2D-CED
32	N	602	CLA	CBD-CGD-O2D-CED
32	c	510	CLA	CBD-CGD-O2D-CED
32	n	602	CLA	CBD-CGD-O2D-CED
43	N	605	CHL	CBD-CGD-O2D-CED
43	G	606	CHL	CBD-CGD-O2D-CED
43	n	605	CHL	CBD-CGD-O2D-CED
43	g	606	CHL	CBD-CGD-O2D-CED
38	D	408	LHG	O2-C2-C3-O3
38	Y	2630	LHG	O2-C2-C3-O3
38	d	408	LHG	O2-C2-C3-O3
38	y	2630	LHG	O2-C2-C3-O3
32	G	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	Y	612	CLA	C3-C5-C6-C7
32	Y	613	CLA	C3-C5-C6-C7
32	g	613	CLA	C3-C5-C6-C7
32	y	612	CLA	C3-C5-C6-C7
32	y	613	CLA	C3-C5-C6-C7
32	Y	611	CLA	CBA-CGA-O2A-C1
32	y	611	CLA	CBA-CGA-O2A-C1
32	C	513	CLA	O1A-CGA-O2A-C1
32	c	513	CLA	O1A-CGA-O2A-C1
32	c	508	CLA	O1D-CGD-O2D-CED
32	B	616	CLA	CBD-CGD-O2D-CED
32	b	616	CLA	CBD-CGD-O2D-CED
42	Z	2634	LMU	C4'-C5'-C6'-O6'
42	z	2634	LMU	C4'-C5'-C6'-O6'
32	C	508	CLA	O1D-CGD-O2D-CED
36	D	411	LMG	O6-C5-C6-O5
36	d	411	LMG	O6-C5-C6-O5
32	N	613	CLA	C3-C5-C6-C7
32	Y	603	CLA	C3-C5-C6-C7
32	n	613	CLA	C3-C5-C6-C7
32	y	603	CLA	C3-C5-C6-C7
32	Y	611	CLA	O1A-CGA-O2A-C1
32	y	611	CLA	O1A-CGA-O2A-C1
32	r	603	CLA	C2A-CAA-CBA-CGA
43	N	605	CHL	C2A-CAA-CBA-CGA
43	R	608	CHL	C2A-CAA-CBA-CGA
43	n	605	CHL	C2A-CAA-CBA-CGA
43	r	608	CHL	C2A-CAA-CBA-CGA
32	d	403	CLA	O1D-CGD-O2D-CED
37	C	523	DGD	O6E-C5E-C6E-O5E
37	c	523	DGD	O6E-C5E-C6E-O5E
42	Y	2632	LMU	O5B-C5B-C6B-O6B
42	y	2632	LMU	O5B-C5B-C6B-O6B
43	g	608	CHL	O1D-CGD-O2D-CED
43	G	608	CHL	O1D-CGD-O2D-CED
32	B	615	CLA	O1D-CGD-O2D-CED
32	C	506	CLA	O1D-CGD-O2D-CED
32	C	512	CLA	O1D-CGD-O2D-CED
32	D	403	CLA	O1D-CGD-O2D-CED
32	b	615	CLA	O1D-CGD-O2D-CED
32	c	506	CLA	O1D-CGD-O2D-CED
37	C	524	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
37	c	524	DGD	C4D-C5D-C6D-O5D
40	D	405	PL9	C47-C48-C49-C51
40	d	405	PL9	C47-C48-C49-C51
32	B	606	CLA	O1D-CGD-O2D-CED
32	G	604	CLA	O1D-CGD-O2D-CED
32	G	613	CLA	O1D-CGD-O2D-CED
32	Y	604	CLA	O1D-CGD-O2D-CED
32	b	606	CLA	O1D-CGD-O2D-CED
32	c	512	CLA	O1D-CGD-O2D-CED
32	g	604	CLA	O1D-CGD-O2D-CED
32	y	604	CLA	O1D-CGD-O2D-CED
32	B	607	CLA	CBD-CGD-O2D-CED
32	g	613	CLA	O1D-CGD-O2D-CED
38	L	101	LHG	C1-C2-C3-O3
38	l	101	LHG	C1-C2-C3-O3
32	B	609	CLA	C3-C5-C6-C7
32	Y	611	CLA	C3-C5-C6-C7
32	b	609	CLA	C3-C5-C6-C7
32	y	611	CLA	C3-C5-C6-C7
43	y	606	CHL	C3-C5-C6-C7
43	Y	605	CHL	O1D-CGD-O2D-CED
32	C	505	CLA	CBA-CGA-O2A-C1
32	R	604	CLA	CBA-CGA-O2A-C1
32	c	505	CLA	CBA-CGA-O2A-C1
32	g	603	CLA	CBA-CGA-O2A-C1
32	r	604	CLA	CBA-CGA-O2A-C1
32	b	602	CLA	CBD-CGD-O2D-CED
32	b	607	CLA	CBD-CGD-O2D-CED
43	G	609	CHL	CBD-CGD-O2D-CED
43	g	609	CHL	CBD-CGD-O2D-CED
32	A	405	CLA	C13-C15-C16-C17
32	a	405	CLA	C13-C15-C16-C17
43	y	605	CHL	O1D-CGD-O2D-CED
42	Z	2634	LMU	O5'-C5'-C6'-O6'
42	z	2634	LMU	O5'-C5'-C6'-O6'
32	B	610	CLA	C13-C15-C16-C17
32	b	608	CLA	C13-C15-C16-C17
32	b	610	CLA	C13-C15-C16-C17
43	N	609	CHL	C8-C10-C11-C12
43	G	609	CHL	C15-C16-C17-C18
43	n	609	CHL	C8-C10-C11-C12
43	g	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	D	410	LHG	O2-C2-C3-O3
38	L	101	LHG	O2-C2-C3-O3
38	d	410	LHG	O2-C2-C3-O3
38	l	101	LHG	O2-C2-C3-O3
38	G	2630	LHG	O7-C5-C6-O8
38	g	2630	LHG	O7-C5-C6-O8
42	Z	2635	LMU	O5'-C5'-C6'-O6'
42	z	2635	LMU	O5'-C5'-C6'-O6'
32	B	602	CLA	C14-C13-C15-C16
32	B	603	CLA	C14-C13-C15-C16
32	B	605	CLA	C6-C7-C8-C9
32	B	607	CLA	C6-C7-C8-C9
32	B	615	CLA	C11-C10-C8-C9
32	C	509	CLA	C6-C7-C8-C9
32	G	610	CLA	C11-C10-C8-C9
32	b	602	CLA	C14-C13-C15-C16
32	b	603	CLA	C14-C13-C15-C16
32	b	605	CLA	C6-C7-C8-C9
32	b	607	CLA	C6-C7-C8-C9
32	b	615	CLA	C11-C10-C8-C9
32	c	509	CLA	C6-C7-C8-C9
32	g	610	CLA	C11-C10-C8-C9
43	N	607	CHL	C11-C12-C13-C14
43	G	609	CHL	C11-C10-C8-C9
43	Y	606	CHL	C6-C7-C8-C9
43	Y	607	CHL	C6-C7-C8-C9
43	n	607	CHL	C11-C12-C13-C14
43	g	609	CHL	C11-C10-C8-C9
43	y	606	CHL	C6-C7-C8-C9
43	y	607	CHL	C6-C7-C8-C9
32	Y	613	CLA	O1D-CGD-O2D-CED
32	y	613	CLA	O1D-CGD-O2D-CED
32	S	612	CLA	CBD-CGD-O2D-CED
32	s	612	CLA	CBD-CGD-O2D-CED
32	B	608	CLA	C13-C15-C16-C17
43	y	609	CHL	C13-C15-C16-C17
44	Y	1621	LUT	C7-C8-C9-C19
44	y	1621	LUT	C7-C8-C9-C19
45	Y	1622	XAT	C31-C32-C33-C40
46	s	1623	NEX	C31-C32-C33-C40
38	D	409	LHG	C23-C24-C25-C26
32	C	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	c	505	CLA	O1A-CGA-O2A-C1
32	B	615	CLA	C8-C10-C11-C12
32	N	602	CLA	C8-C10-C11-C12
32	b	615	CLA	C8-C10-C11-C12
32	n	602	CLA	C8-C10-C11-C12
43	N	609	CHL	C15-C16-C17-C18
43	G	609	CHL	C5-C6-C7-C8
43	Y	609	CHL	C13-C15-C16-C17
42	Z	2635	LMU	C4B-C5B-C6B-O6B
42	z	2635	LMU	C4B-C5B-C6B-O6B
32	b	603	CLA	C3-C5-C6-C7
43	G	608	CHL	C2A-CAA-CBA-CGA
43	g	608	CHL	C2A-CAA-CBA-CGA
32	B	605	CLA	CBA-CGA-O2A-C1
32	G	603	CLA	CBA-CGA-O2A-C1
32	b	605	CLA	CBA-CGA-O2A-C1
32	B	612	CLA	C10-C11-C12-C13
32	B	615	CLA	C5-C6-C7-C8
32	D	403	CLA	C8-C10-C11-C12
32	Y	602	CLA	C10-C11-C12-C13
32	b	602	CLA	C15-C16-C17-C18
32	b	612	CLA	C10-C11-C12-C13
32	b	615	CLA	C5-C6-C7-C8
32	d	403	CLA	C8-C10-C11-C12
32	y	602	CLA	C10-C11-C12-C13
43	G	609	CHL	C13-C15-C16-C17
43	n	609	CHL	C15-C16-C17-C18
43	y	606	CHL	C15-C16-C17-C18
37	C	518	DGD	C1B-C2B-C3B-C4B
37	C	520	DGD	C1A-C2A-C3A-C4A
37	c	518	DGD	C1B-C2B-C3B-C4B
37	c	520	DGD	C1A-C2A-C3A-C4A
38	d	409	LHG	C23-C24-C25-C26
32	R	610	CLA	O1D-CGD-O2D-CED
32	S	603	CLA	O1D-CGD-O2D-CED
32	B	602	CLA	C15-C16-C17-C18
32	B	608	CLA	C8-C10-C11-C12
32	B	609	CLA	C10-C11-C12-C13
32	B	609	CLA	C13-C15-C16-C17
32	C	504	CLA	C10-C11-C12-C13
32	G	603	CLA	C10-C11-C12-C13
32	G	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	Y	610	CLA	C8-C10-C11-C12
32	Y	611	CLA	C10-C11-C12-C13
32	b	608	CLA	C8-C10-C11-C12
32	b	609	CLA	C10-C11-C12-C13
32	b	609	CLA	C13-C15-C16-C17
32	c	504	CLA	C10-C11-C12-C13
32	g	603	CLA	C10-C11-C12-C13
32	g	603	CLA	C15-C16-C17-C18
32	y	610	CLA	C8-C10-C11-C12
32	y	611	CLA	C10-C11-C12-C13
43	N	601	CHL	C13-C15-C16-C17
43	N	607	CHL	C13-C15-C16-C17
43	G	609	CHL	C10-C11-C12-C13
43	Y	601	CHL	C13-C15-C16-C17
43	Y	606	CHL	C15-C16-C17-C18
43	Y	607	CHL	C8-C10-C11-C12
43	Y	607	CHL	C15-C16-C17-C18
43	n	601	CHL	C13-C15-C16-C17
43	n	607	CHL	C13-C15-C16-C17
43	g	601	CHL	C13-C15-C16-C17
43	g	609	CHL	C5-C6-C7-C8
43	g	609	CHL	C10-C11-C12-C13
43	g	609	CHL	C13-C15-C16-C17
43	y	601	CHL	C13-C15-C16-C17
43	y	607	CHL	C8-C10-C11-C12
32	s	603	CLA	O1D-CGD-O2D-CED
43	G	607	CHL	O1D-CGD-O2D-CED
35	A	412	SQD	C7-C8-C9-C10
35	a	412	SQD	C7-C8-C9-C10
36	H	102	LMG	O6-C5-C6-O5
32	B	612	CLA	CBD-CGD-O2D-CED
43	g	607	CHL	O1D-CGD-O2D-CED
32	B	608	CLA	C15-C16-C17-C18
32	B	614	CLA	C10-C11-C12-C13
32	B	617	CLA	C8-C10-C11-C12
32	C	501	CLA	C15-C16-C17-C18
32	Y	602	CLA	C8-C10-C11-C12
32	b	614	CLA	C10-C11-C12-C13
32	b	617	CLA	C8-C10-C11-C12
32	c	501	CLA	C15-C16-C17-C18
32	y	602	CLA	C8-C10-C11-C12
43	G	601	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
43	Y	606	CHL	C13-C15-C16-C17
43	y	606	CHL	C13-C15-C16-C17
32	B	603	CLA	C3-C5-C6-C7
32	B	612	CLA	C13-C15-C16-C17
32	C	505	CLA	C15-C16-C17-C18
32	C	510	CLA	C8-C10-C11-C12
32	D	402	CLA	C13-C15-C16-C17
32	G	610	CLA	C13-C15-C16-C17
32	Y	604	CLA	C8-C10-C11-C12
32	b	608	CLA	C15-C16-C17-C18
32	b	612	CLA	C13-C15-C16-C17
32	d	402	CLA	C10-C11-C12-C13
32	d	402	CLA	C13-C15-C16-C17
32	y	604	CLA	C8-C10-C11-C12
43	y	607	CHL	C15-C16-C17-C18
32	N	604	CLA	CBD-CGD-O2D-CED
32	n	604	CLA	CBD-CGD-O2D-CED
43	S	606	CHL	C2A-CAA-CBA-CGA
43	s	606	CHL	C2A-CAA-CBA-CGA
32	D	402	CLA	C10-C11-C12-C13
32	b	615	CLA	C13-C15-C16-C17
32	c	505	CLA	C15-C16-C17-C18
32	c	507	CLA	C5-C6-C7-C8
32	c	510	CLA	C8-C10-C11-C12
32	g	610	CLA	C13-C15-C16-C17
32	G	603	CLA	O1D-CGD-O2D-CED
32	B	602	CLA	C12-C13-C15-C16
32	C	501	CLA	C11-C10-C8-C7
32	G	602	CLA	C6-C7-C8-C10
32	G	602	CLA	C11-C10-C8-C7
32	b	602	CLA	C12-C13-C15-C16
32	c	501	CLA	C11-C10-C8-C7
32	g	602	CLA	C6-C7-C8-C10
32	g	602	CLA	C11-C10-C8-C7
43	Y	601	CHL	C6-C7-C8-C10
43	Y	606	CHL	C11-C12-C13-C15
43	y	601	CHL	C6-C7-C8-C10
43	y	606	CHL	C11-C12-C13-C15
32	R	604	CLA	O1A-CGA-O2A-C1
32	r	604	CLA	O1A-CGA-O2A-C1
32	N	611	CLA	CBD-CGD-O2D-CED
32	n	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	B	611	CLA	C2A-CAA-CBA-CGA
32	R	603	CLA	C2A-CAA-CBA-CGA
32	b	611	CLA	C2A-CAA-CBA-CGA
43	R	607	CHL	C2A-CAA-CBA-CGA
43	Y	605	CHL	C2A-CAA-CBA-CGA
43	r	607	CHL	C2A-CAA-CBA-CGA
43	y	605	CHL	C2A-CAA-CBA-CGA
32	B	614	CLA	O1D-CGD-O2D-CED
32	b	614	CLA	O1D-CGD-O2D-CED
43	R	607	CHL	O1D-CGD-O2D-CED
43	r	607	CHL	O1D-CGD-O2D-CED
32	B	617	CLA	C15-C16-C17-C18
32	C	507	CLA	C5-C6-C7-C8
32	G	613	CLA	C15-C16-C17-C18
32	b	605	CLA	C8-C10-C11-C12
32	b	617	CLA	C15-C16-C17-C18
32	c	503	CLA	C15-C16-C17-C18
32	c	505	CLA	C10-C11-C12-C13
32	g	603	CLA	C13-C15-C16-C17
32	g	613	CLA	C15-C16-C17-C18
43	y	601	CHL	C5-C6-C7-C8
37	C	523	DGD	O6D-C1D-O3G-C3G
37	c	523	DGD	O6D-C1D-O3G-C3G
32	B	605	CLA	C8-C10-C11-C12
32	B	615	CLA	C13-C15-C16-C17
32	C	505	CLA	C10-C11-C12-C13
32	C	503	CLA	C15-C16-C17-C18
32	G	603	CLA	C13-C15-C16-C17
32	Y	604	CLA	C10-C11-C12-C13
32	y	604	CLA	C10-C11-C12-C13
43	N	601	CHL	C5-C6-C7-C8
43	N	607	CHL	C15-C16-C17-C18
43	Y	601	CHL	C5-C6-C7-C8
43	n	601	CHL	C5-C6-C7-C8
43	n	607	CHL	C15-C16-C17-C18
32	C	512	CLA	CBA-CGA-O2A-C1
32	c	512	CLA	CBA-CGA-O2A-C1
32	C	510	CLA	C13-C15-C16-C17
32	C	510	CLA	C15-C16-C17-C18
32	N	602	CLA	C10-C11-C12-C13
32	G	602	CLA	C10-C11-C12-C13
32	c	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	c	510	CLA	C15-C16-C17-C18
32	n	602	CLA	C10-C11-C12-C13
32	g	602	CLA	C10-C11-C12-C13
43	N	605	CHL	C8-C10-C11-C12
43	N	605	CHL	C13-C15-C16-C17
43	N	607	CHL	C8-C10-C11-C12
43	n	605	CHL	C13-C15-C16-C17
43	n	607	CHL	C8-C10-C11-C12
43	g	601	CHL	C5-C6-C7-C8
43	Y	601	CHL	O1D-CGD-O2D-CED
43	y	601	CHL	O1D-CGD-O2D-CED
32	g	603	CLA	O1A-CGA-O2A-C1
32	B	603	CLA	C10-C11-C12-C13
32	N	603	CLA	C15-C16-C17-C18
32	b	603	CLA	C10-C11-C12-C13
32	n	603	CLA	C15-C16-C17-C18
43	N	601	CHL	C15-C16-C17-C18
43	G	601	CHL	C5-C6-C7-C8
43	Y	609	CHL	C8-C10-C11-C12
43	n	601	CHL	C15-C16-C17-C18
43	n	605	CHL	C8-C10-C11-C12
43	y	609	CHL	C8-C10-C11-C12
38	C	2630	LHG	C3-O3-P-O6
38	C	2630	LHG	C4-O6-P-O3
38	D	409	LHG	C4-O6-P-O3
38	D	410	LHG	C4-O6-P-O3
38	L	101	LHG	C3-O3-P-O6
38	G	2630	LHG	C3-O3-P-O6
38	c	2630	LHG	C3-O3-P-O6
38	c	2630	LHG	C4-O6-P-O3
38	d	408	LHG	C3-O3-P-O6
38	d	409	LHG	C4-O6-P-O3
38	d	410	LHG	C4-O6-P-O3
38	l	101	LHG	C3-O3-P-O6
38	g	2630	LHG	C3-O3-P-O6
37	c	519	DGD	O6E-C5E-C6E-O5E
32	A	405	CLA	C3-C5-C6-C7
32	a	405	CLA	C3-C5-C6-C7
43	Y	606	CHL	C3-C5-C6-C7
32	s	602	CLA	CBA-CGA-O2A-C1
32	b	604	CLA	O1D-CGD-O2D-CED
43	N	609	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
43	n	609	CHL	C5-C6-C7-C8
43	S	608	CHL	O2A-C1-C2-C3
43	s	608	CHL	O2A-C1-C2-C3
32	B	604	CLA	O1D-CGD-O2D-CED
37	C	518	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	O6E-C5E-C6E-O5E
32	Y	603	CLA	C4-C3-C5-C6
32	y	603	CLA	C4-C3-C5-C6
32	B	611	CLA	O1D-CGD-O2D-CED
32	G	603	CLA	C3-C5-C6-C7
32	B	602	CLA	CBA-CGA-O2A-C1
32	S	602	CLA	CBA-CGA-O2A-C1
32	b	602	CLA	CBA-CGA-O2A-C1
37	C	519	DGD	C2A-C1A-O1G-C1G
37	c	519	DGD	C2A-C1A-O1G-C1G
43	N	607	CHL	CBA-CGA-O2A-C1
43	n	607	CHL	CBA-CGA-O2A-C1
43	y	601	CHL	CBA-CGA-O2A-C1
36	h	102	LMG	C30-C31-C32-C33
32	c	510	CLA	O1D-CGD-O2D-CED
36	H	102	LMG	C30-C31-C32-C33
38	C	2630	LHG	C33-C34-C35-C36
38	c	2630	LHG	C33-C34-C35-C36
42	Z	2634	LMU	C5-C6-C7-C8
42	Z	2635	LMU	O1'-C1-C2-C3
42	z	2634	LMU	C5-C6-C7-C8
42	z	2635	LMU	O1'-C1-C2-C3
42	Y	2632	LMU	C4B-C5B-C6B-O6B
42	y	2632	LMU	C4B-C5B-C6B-O6B
32	g	603	CLA	O1D-CGD-O2D-CED
32	B	617	CLA	C16-C17-C18-C19
32	N	602	CLA	C16-C17-C18-C20
32	b	617	CLA	C16-C17-C18-C19
32	n	602	CLA	C16-C17-C18-C20
43	N	605	CHL	C16-C17-C18-C19
43	G	609	CHL	C16-C17-C18-C20
43	Y	606	CHL	C16-C17-C18-C19
43	n	605	CHL	C16-C17-C18-C19
43	g	609	CHL	C16-C17-C18-C20
43	y	606	CHL	C16-C17-C18-C19
32	N	611	CLA	CBA-CGA-O2A-C1
32	n	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
43	Y	601	CHL	CBA-CGA-O2A-C1
38	D	409	LHG	C14-C15-C16-C17
38	N	2630	LHG	C17-C18-C19-C20
32	B	617	CLA	O1D-CGD-O2D-CED
32	C	510	CLA	O1D-CGD-O2D-CED
32	b	611	CLA	O1D-CGD-O2D-CED
32	b	617	CLA	O1D-CGD-O2D-CED
32	n	610	CLA	C5-C6-C7-C8
43	N	605	CHL	C15-C16-C17-C18
32	G	602	CLA	CBD-CGD-O2D-CED
43	R	606	CHL	CBD-CGD-O2D-CED
38	d	409	LHG	C14-C15-C16-C17
38	n	2630	LHG	C17-C18-C19-C20
32	B	605	CLA	O1A-CGA-O2A-C1
32	b	605	CLA	O1A-CGA-O2A-C1
36	H	102	LMG	C15-C16-C17-C18
37	C	520	DGD	C6B-C7B-C8B-C9B
37	C	523	DGD	CCA-CDA-CEA-CFA
37	c	520	DGD	C6B-C7B-C8B-C9B
37	c	523	DGD	CCA-CDA-CEA-CFA
32	c	511	CLA	O1D-CGD-O2D-CED
32	s	602	CLA	O1D-CGD-O2D-CED
32	N	610	CLA	C5-C6-C7-C8
43	n	605	CHL	C15-C16-C17-C18
36	h	102	LMG	C15-C16-C17-C18
42	z	2635	LMU	C2-C3-C4-C5
32	g	603	CLA	C3-C5-C6-C7
36	c	521	LMG	C28-C29-C30-C31
32	S	602	CLA	O1D-CGD-O2D-CED
42	Y	2632	LMU	C2'-C1'-O1'-C1
42	y	2632	LMU	C2'-C1'-O1'-C1
42	Z	2635	LMU	C2-C3-C4-C5
32	g	602	CLA	C15-C16-C17-C18
43	G	609	CHL	C8-C10-C11-C12
43	Y	601	CHL	C15-C16-C17-C18
43	g	609	CHL	C8-C10-C11-C12
43	y	601	CHL	C15-C16-C17-C18
32	G	603	CLA	O1A-CGA-O2A-C1
37	C	519	DGD	O1A-C1A-O1G-C1G
37	c	519	DGD	O1A-C1A-O1G-C1G
43	N	607	CHL	O1A-CGA-O2A-C1
43	n	607	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	A	406	CLA	C16-C17-C18-C20
32	A	410	CLA	C11-C12-C13-C15
32	B	610	CLA	C16-C17-C18-C20
32	B	615	CLA	C16-C17-C18-C20
32	B	616	CLA	C16-C17-C18-C20
32	a	406	CLA	C16-C17-C18-C20
32	a	410	CLA	C11-C12-C13-C15
32	b	610	CLA	C16-C17-C18-C20
32	b	615	CLA	C16-C17-C18-C20
32	b	616	CLA	C16-C17-C18-C20
43	N	601	CHL	C16-C17-C18-C19
43	n	601	CHL	C16-C17-C18-C19
32	C	511	CLA	O1D-CGD-O2D-CED
32	n	602	CLA	O1D-CGD-O2D-CED
37	C	519	DGD	O6E-C5E-C6E-O5E
32	N	613	CLA	C4-C3-C5-C6
32	n	613	CLA	C4-C3-C5-C6
33	a	408	PHO	C4-C3-C5-C6
40	D	405	PL9	C15-C14-C16-C17
40	d	405	PL9	C15-C14-C16-C17
36	D	411	LMG	C12-C13-C14-C15
36	d	411	LMG	C12-C13-C14-C15
38	D	409	LHG	C33-C34-C35-C36
32	Y	603	CLA	C2-C3-C5-C6
32	y	603	CLA	C2-C3-C5-C6
32	C	501	CLA	C11-C10-C8-C9
32	C	504	CLA	C11-C12-C13-C14
32	C	513	CLA	C6-C7-C8-C9
32	a	406	CLA	C11-C12-C13-C14
32	c	501	CLA	C11-C10-C8-C9
32	c	504	CLA	C11-C12-C13-C14
32	c	513	CLA	C6-C7-C8-C9
43	Y	607	CHL	C11-C10-C8-C9
43	y	607	CHL	C11-C10-C8-C9
32	N	602	CLA	O1D-CGD-O2D-CED
32	B	602	CLA	CBD-CGD-O2D-CED
32	b	612	CLA	CBD-CGD-O2D-CED
37	C	524	DGD	O6D-C5D-C6D-O5D
37	c	524	DGD	O6D-C5D-C6D-O5D
38	g	2630	LHG	C14-C15-C16-C17
32	B	612	CLA	C8-C10-C11-C12
32	b	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
43	n	609	CHL	C10-C11-C12-C13
32	C	501	CLA	C2A-CAA-CBA-CGA
32	S	613	CLA	C2A-CAA-CBA-CGA
32	c	501	CLA	C2A-CAA-CBA-CGA
32	s	613	CLA	C2A-CAA-CBA-CGA
43	Y	606	CHL	C2A-CAA-CBA-CGA
32	C	512	CLA	O1A-CGA-O2A-C1
32	c	512	CLA	O1A-CGA-O2A-C1
38	D	409	LHG	O1-C1-C2-C3
38	d	409	LHG	O1-C1-C2-C3
45	Y	1622	XAT	C31-C32-C33-C34
32	C	501	CLA	C10-C11-C12-C13
32	c	501	CLA	C10-C11-C12-C13
43	N	609	CHL	C10-C11-C12-C13
43	Y	609	CHL	C10-C11-C12-C13
43	y	609	CHL	C10-C11-C12-C13
32	A	406	CLA	C16-C17-C18-C19
32	C	507	CLA	C16-C17-C18-C20
32	a	406	CLA	C16-C17-C18-C19
32	c	507	CLA	C16-C17-C18-C20
43	N	609	CHL	C16-C17-C18-C20
43	n	609	CHL	C16-C17-C18-C20
43	y	606	CHL	C16-C17-C18-C20
32	B	603	CLA	C13-C15-C16-C17
32	G	602	CLA	C15-C16-C17-C18
32	c	508	CLA	C15-C16-C17-C18
38	D	409	LHG	C12-C13-C14-C15
38	d	409	LHG	C12-C13-C14-C15
38	S	2630	LHG	C23-C24-C25-C26
38	s	2630	LHG	C23-C24-C25-C26
32	C	508	CLA	C15-C16-C17-C18
37	c	520	DGD	C2A-C3A-C4A-C5A
38	N	2630	LHG	C14-C15-C16-C17
32	Y	612	CLA	CBA-CGA-O2A-C1
32	y	612	CLA	CBA-CGA-O2A-C1
38	C	2630	LHG	C9-C10-C11-C12
38	c	2630	LHG	C9-C10-C11-C12
32	A	405	CLA	C3A-C2A-CAA-CBA
32	C	513	CLA	C3A-C2A-CAA-CBA
32	D	402	CLA	C3A-C2A-CAA-CBA
32	N	603	CLA	C3A-C2A-CAA-CBA
32	N	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	G	603	CLA	C3A-C2A-CAA-CBA
32	G	611	CLA	C3A-C2A-CAA-CBA
32	R	603	CLA	C3A-C2A-CAA-CBA
32	R	604	CLA	C3A-C2A-CAA-CBA
32	S	605	CLA	C3A-C2A-CAA-CBA
32	Y	603	CLA	C3A-C2A-CAA-CBA
32	a	405	CLA	C3A-C2A-CAA-CBA
32	c	513	CLA	C3A-C2A-CAA-CBA
32	d	402	CLA	C3A-C2A-CAA-CBA
32	n	603	CLA	C3A-C2A-CAA-CBA
32	n	611	CLA	C3A-C2A-CAA-CBA
32	g	603	CLA	C3A-C2A-CAA-CBA
32	g	611	CLA	C3A-C2A-CAA-CBA
32	r	603	CLA	C3A-C2A-CAA-CBA
32	r	604	CLA	C3A-C2A-CAA-CBA
32	s	605	CLA	C3A-C2A-CAA-CBA
32	y	603	CLA	C3A-C2A-CAA-CBA
43	N	606	CHL	C3A-C2A-CAA-CBA
43	N	607	CHL	C3A-C2A-CAA-CBA
43	G	606	CHL	C3A-C2A-CAA-CBA
43	G	607	CHL	C3A-C2A-CAA-CBA
43	n	606	CHL	C3A-C2A-CAA-CBA
43	n	607	CHL	C3A-C2A-CAA-CBA
43	g	606	CHL	C3A-C2A-CAA-CBA
43	g	607	CHL	C3A-C2A-CAA-CBA
32	C	507	CLA	C13-C15-C16-C17
32	c	507	CLA	C13-C15-C16-C17
35	b	621	SQD	C34-C35-C36-C37
38	D	408	LHG	C30-C31-C32-C33
38	d	408	LHG	C30-C31-C32-C33
38	n	2630	LHG	C14-C15-C16-C17
32	B	616	CLA	C16-C17-C18-C19
32	C	507	CLA	C16-C17-C18-C19
32	b	616	CLA	C16-C17-C18-C19
32	c	507	CLA	C16-C17-C18-C19
43	N	605	CHL	C16-C17-C18-C20
43	N	609	CHL	C16-C17-C18-C19
43	Y	606	CHL	C16-C17-C18-C20
43	n	605	CHL	C16-C17-C18-C20
43	n	609	CHL	C16-C17-C18-C19
32	g	602	CLA	CBD-CGD-O2D-CED
43	n	609	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
43	r	606	CHL	CBD-CGD-O2D-CED
38	N	2630	LHG	C27-C28-C29-C30
32	B	616	CLA	O1D-CGD-O2D-CED
36	C	521	LMG	C28-C29-C30-C31
38	n	2630	LHG	C27-C28-C29-C30
32	s	602	CLA	O1A-CGA-O2A-C1
32	Y	614	CLA	CBA-CGA-O2A-C1
32	y	614	CLA	CBA-CGA-O2A-C1
32	N	613	CLA	C2-C3-C5-C6
32	Y	611	CLA	C2-C3-C5-C6
32	n	613	CLA	C2-C3-C5-C6
32	y	611	CLA	C2-C3-C5-C6
33	A	408	PHO	C2-C3-C5-C6
40	D	405	PL9	C13-C14-C16-C17
32	b	616	CLA	O1D-CGD-O2D-CED
43	N	609	CHL	CBD-CGD-O2D-CED
37	C	520	DGD	C2A-C3A-C4A-C5A
36	h	102	LMG	O6-C5-C6-O5
36	D	411	LMG	C4-C5-C6-O5
36	d	411	LMG	C4-C5-C6-O5
32	Y	604	CLA	C2A-CAA-CBA-CGA
43	y	606	CHL	C2A-CAA-CBA-CGA
32	B	606	CLA	C5-C6-C7-C8
38	C	2630	LHG	C32-C33-C34-C35
43	R	606	CHL	C2A-CAA-CBA-CGA
43	r	606	CHL	C2A-CAA-CBA-CGA
32	S	602	CLA	O1A-CGA-O2A-C1
32	b	602	CLA	O1A-CGA-O2A-C1
43	Y	601	CHL	O1A-CGA-O2A-C1
43	y	601	CHL	O1A-CGA-O2A-C1
32	N	602	CLA	C16-C17-C18-C19
32	n	602	CLA	C16-C17-C18-C19
38	c	2630	LHG	C32-C33-C34-C35
32	b	606	CLA	C5-C6-C7-C8
42	Z	2634	LMU	C3-C4-C5-C6
42	Z	2634	LMU	C6-C7-C8-C9
32	B	602	CLA	O1A-CGA-O2A-C1
38	D	409	LHG	C7-C8-C9-C10
38	d	409	LHG	C7-C8-C9-C10
38	D	408	LHG	C26-C27-C28-C29
38	d	408	LHG	C26-C27-C28-C29
42	z	2634	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
38	G	2630	LHG	C26-C27-C28-C29
42	Y	2632	LMU	C3-C4-C5-C6
42	z	2634	LMU	C3-C4-C5-C6
42	y	2632	LMU	C3-C4-C5-C6
32	C	512	CLA	C13-C15-C16-C17
32	C	512	CLA	C15-C16-C17-C18
32	R	602	CLA	C10-C11-C12-C13
32	c	501	CLA	C8-C10-C11-C12
32	c	512	CLA	C13-C15-C16-C17
32	c	512	CLA	C15-C16-C17-C18
32	r	602	CLA	C10-C11-C12-C13
32	A	410	CLA	C11-C12-C13-C14
32	B	615	CLA	C16-C17-C18-C19
32	a	410	CLA	C11-C12-C13-C14
32	b	615	CLA	C16-C17-C18-C19
38	N	2630	LHG	C23-C24-C25-C26
38	n	2630	LHG	C23-C24-C25-C26
34	A	411	BCR	C23-C24-C25-C26
34	B	618	BCR	C1-C6-C7-C8
34	B	618	BCR	C5-C6-C7-C8
34	C	516	BCR	C5-C6-C7-C8
34	C	516	BCR	C23-C24-C25-C26
34	C	516	BCR	C23-C24-C25-C30
34	H	101	BCR	C23-C24-C25-C26
34	H	101	BCR	C23-C24-C25-C30
34	a	411	BCR	C23-C24-C25-C26
34	b	618	BCR	C1-C6-C7-C8
34	b	618	BCR	C5-C6-C7-C8
34	c	516	BCR	C5-C6-C7-C8
34	c	516	BCR	C23-C24-C25-C26
34	c	516	BCR	C23-C24-C25-C30
34	h	101	BCR	C23-C24-C25-C26
44	N	1620	LUT	C5-C6-C7-C8
44	G	1620	LUT	C5-C6-C7-C8
44	S	1621	LUT	C1-C6-C7-C8
44	S	1621	LUT	C5-C6-C7-C8
44	Y	1620	LUT	C1-C6-C7-C8
44	Y	1620	LUT	C5-C6-C7-C8
44	n	1620	LUT	C1-C6-C7-C8
44	n	1620	LUT	C5-C6-C7-C8
44	g	1620	LUT	C5-C6-C7-C8
44	s	1621	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
44	s	1621	LUT	C5-C6-C7-C8
44	y	1620	LUT	C1-C6-C7-C8
44	y	1620	LUT	C5-C6-C7-C8
35	A	412	SQD	C29-C30-C31-C32
35	B	621	SQD	C34-C35-C36-C37
35	a	412	SQD	C29-C30-C31-C32
37	C	523	DGD	C7A-C8A-C9A-CAA
37	c	519	DGD	C5A-C6A-C7A-C8A
38	g	2630	LHG	C26-C27-C28-C29
36	a	413	LMG	C29-C28-O8-C9
43	G	609	CHL	CBA-CGA-O2A-C1
43	g	609	CHL	CBA-CGA-O2A-C1
32	G	602	CLA	C13-C15-C16-C17
32	Y	603	CLA	C13-C15-C16-C17
32	b	614	CLA	C15-C16-C17-C18
32	g	602	CLA	C13-C15-C16-C17
32	y	603	CLA	C13-C15-C16-C17
43	N	609	CHL	C13-C15-C16-C17
43	n	609	CHL	C13-C15-C16-C17
37	c	523	DGD	C7A-C8A-C9A-CAA
32	N	611	CLA	O1A-CGA-O2A-C1
32	Y	612	CLA	O1A-CGA-O2A-C1
32	n	611	CLA	O1A-CGA-O2A-C1
32	y	612	CLA	O1A-CGA-O2A-C1
38	y	2630	LHG	C26-C27-C28-C29
32	B	614	CLA	C15-C16-C17-C18
32	C	501	CLA	C8-C10-C11-C12
32	G	610	CLA	C8-C10-C11-C12
38	Y	2630	LHG	C26-C27-C28-C29
32	Y	611	CLA	C4-C3-C5-C6
32	y	611	CLA	C4-C3-C5-C6
33	A	408	PHO	C4-C3-C5-C6
32	B	603	CLA	C12-C13-C15-C16
32	B	612	CLA	C6-C7-C8-C10
32	C	504	CLA	C11-C12-C13-C15
32	C	508	CLA	C11-C12-C13-C15
32	C	513	CLA	C6-C7-C8-C10
32	N	613	CLA	C6-C7-C8-C10
32	a	406	CLA	C11-C12-C13-C15
32	b	603	CLA	C12-C13-C15-C16
32	b	612	CLA	C6-C7-C8-C10
32	c	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	c	508	CLA	C11-C12-C13-C15
32	c	513	CLA	C6-C7-C8-C10
32	n	613	CLA	C6-C7-C8-C10
33	a	408	PHO	C2-C3-C5-C6
40	d	405	PL9	C13-C14-C16-C17
40	d	405	PL9	C43-C44-C46-C47
43	N	601	CHL	C11-C10-C8-C7
43	N	607	CHL	C11-C12-C13-C15
43	Y	607	CHL	C6-C7-C8-C10
43	n	601	CHL	C11-C10-C8-C7
43	n	607	CHL	C11-C12-C13-C15
43	y	607	CHL	C6-C7-C8-C10
32	Y	614	CLA	O1A-CGA-O2A-C1
32	y	614	CLA	O1A-CGA-O2A-C1
32	B	603	CLA	C5-C6-C7-C8
32	B	617	CLA	C13-C15-C16-C17
32	b	617	CLA	C13-C15-C16-C17
43	Y	601	CHL	C10-C11-C12-C13
34	C	517	BCR	C9-C10-C11-C12
34	c	517	BCR	C9-C10-C11-C12
45	G	1622	XAT	C13-C14-C15-C35
45	g	1622	XAT	C13-C14-C15-C35
43	Y	606	CHL	CBD-CGD-O2D-CED
43	y	606	CHL	CBD-CGD-O2D-CED
32	b	610	CLA	C16-C17-C18-C19
32	g	602	CLA	C16-C17-C18-C19
33	A	408	PHO	C16-C17-C18-C20
33	a	408	PHO	C16-C17-C18-C20
43	N	601	CHL	C16-C17-C18-C20
43	n	601	CHL	C16-C17-C18-C20
36	A	413	LMG	C29-C28-O8-C9
42	Y	2632	LMU	C2-C3-C4-C5
32	G	613	CLA	C2A-CAA-CBA-CGA
32	g	613	CLA	C2A-CAA-CBA-CGA
32	y	604	CLA	C2A-CAA-CBA-CGA
43	N	606	CHL	C2A-CAA-CBA-CGA
43	G	605	CHL	C2A-CAA-CBA-CGA
43	n	606	CHL	C2A-CAA-CBA-CGA
43	g	605	CHL	C2A-CAA-CBA-CGA
32	B	602	CLA	C5-C6-C7-C8
32	b	615	CLA	C15-C16-C17-C18
42	y	2632	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
38	d	408	LHG	C29-C30-C31-C32
42	Z	2634	LMU	C4-C5-C6-C7
42	z	2634	LMU	C4-C5-C6-C7
32	B	615	CLA	C15-C16-C17-C18
32	N	610	CLA	C15-C16-C17-C18
32	b	602	CLA	C5-C6-C7-C8
32	b	603	CLA	C5-C6-C7-C8
32	n	610	CLA	C15-C16-C17-C18
43	y	601	CHL	C10-C11-C12-C13
38	D	408	LHG	C29-C30-C31-C32
38	d	409	LHG	C33-C34-C35-C36
32	B	610	CLA	C16-C17-C18-C19
32	G	602	CLA	C16-C17-C18-C19
43	Y	607	CHL	C16-C17-C18-C20
43	y	607	CHL	C16-C17-C18-C20
32	b	603	CLA	C13-C15-C16-C17
32	g	610	CLA	C8-C10-C11-C12
37	C	519	DGD	C5A-C6A-C7A-C8A
43	G	609	CHL	C2C-C3C-CAC-CBC
32	Y	613	CLA	C8-C10-C11-C12
32	y	613	CLA	C8-C10-C11-C12
32	C	502	CLA	CBD-CGD-O2D-CED
32	c	502	CLA	CBD-CGD-O2D-CED
32	b	605	CLA	C3-C5-C6-C7
43	g	609	CHL	C2C-C3C-CAC-CBC
43	g	609	CHL	C16-C17-C18-C19
32	B	608	CLA	C10-C11-C12-C13
32	C	507	CLA	C4-C3-C5-C6
40	D	405	PL9	C43-C44-C46-C47
32	B	609	CLA	C11-C12-C13-C14
32	B	612	CLA	C6-C7-C8-C9
32	B	616	CLA	C11-C12-C13-C14
32	C	508	CLA	C11-C12-C13-C14
32	G	602	CLA	C6-C7-C8-C9
32	b	609	CLA	C11-C12-C13-C14
32	b	612	CLA	C6-C7-C8-C9
32	b	616	CLA	C11-C12-C13-C14
32	c	508	CLA	C11-C12-C13-C14
32	g	602	CLA	C6-C7-C8-C9
43	N	601	CHL	C11-C10-C8-C9
43	Y	606	CHL	C11-C12-C13-C14
43	n	601	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
43	y	606	CHL	C11-C12-C13-C14
36	h	102	LMG	C35-C36-C37-C38
32	B	605	CLA	C3-C5-C6-C7
32	B	604	CLA	C2A-CAA-CBA-CGA
32	C	505	CLA	C2A-CAA-CBA-CGA
32	S	610	CLA	C2A-CAA-CBA-CGA
32	Y	602	CLA	C2A-CAA-CBA-CGA
32	Y	610	CLA	C2A-CAA-CBA-CGA
32	b	604	CLA	C2A-CAA-CBA-CGA
32	c	505	CLA	C2A-CAA-CBA-CGA
32	s	610	CLA	C2A-CAA-CBA-CGA
32	y	602	CLA	C2A-CAA-CBA-CGA
32	y	610	CLA	C2A-CAA-CBA-CGA
36	H	102	LMG	C35-C36-C37-C38
35	a	412	SQD	C23-C24-C25-C26
32	b	608	CLA	C10-C11-C12-C13
46	S	1623	NEX	C31-C32-C33-C34
43	G	609	CHL	O1A-CGA-O2A-C1
43	g	609	CHL	O1A-CGA-O2A-C1
32	A	405	CLA	C1A-C2A-CAA-CBA
32	A	406	CLA	C1A-C2A-CAA-CBA
32	A	407	CLA	C1A-C2A-CAA-CBA
32	C	504	CLA	C1A-C2A-CAA-CBA
32	C	508	CLA	C1A-C2A-CAA-CBA
32	C	513	CLA	C1A-C2A-CAA-CBA
32	N	603	CLA	C1A-C2A-CAA-CBA
32	N	611	CLA	C1A-C2A-CAA-CBA
32	G	603	CLA	C1A-C2A-CAA-CBA
32	G	610	CLA	C1A-C2A-CAA-CBA
32	G	611	CLA	C1A-C2A-CAA-CBA
32	G	614	CLA	C1A-C2A-CAA-CBA
32	S	604	CLA	C1A-C2A-CAA-CBA
32	S	610	CLA	C1A-C2A-CAA-CBA
32	S	611	CLA	C1A-C2A-CAA-CBA
32	S	613	CLA	C1A-C2A-CAA-CBA
32	Y	603	CLA	C1A-C2A-CAA-CBA
32	Y	610	CLA	C1A-C2A-CAA-CBA
32	a	405	CLA	C1A-C2A-CAA-CBA
32	a	406	CLA	C1A-C2A-CAA-CBA
32	a	407	CLA	C1A-C2A-CAA-CBA
32	c	504	CLA	C1A-C2A-CAA-CBA
32	c	508	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	c	513	CLA	C1A-C2A-CAA-CBA
32	n	603	CLA	C1A-C2A-CAA-CBA
32	n	611	CLA	C1A-C2A-CAA-CBA
32	g	603	CLA	C1A-C2A-CAA-CBA
32	g	610	CLA	C1A-C2A-CAA-CBA
32	g	611	CLA	C1A-C2A-CAA-CBA
32	g	614	CLA	C1A-C2A-CAA-CBA
32	s	604	CLA	C1A-C2A-CAA-CBA
32	s	610	CLA	C1A-C2A-CAA-CBA
32	s	611	CLA	C1A-C2A-CAA-CBA
32	s	613	CLA	C1A-C2A-CAA-CBA
32	y	603	CLA	C1A-C2A-CAA-CBA
32	y	610	CLA	C1A-C2A-CAA-CBA
43	N	607	CHL	C1A-C2A-CAA-CBA
43	G	606	CHL	C1A-C2A-CAA-CBA
43	G	607	CHL	C1A-C2A-CAA-CBA
43	G	608	CHL	C1A-C2A-CAA-CBA
43	G	609	CHL	C1A-C2A-CAA-CBA
43	S	608	CHL	C1A-C2A-CAA-CBA
43	Y	605	CHL	C1A-C2A-CAA-CBA
43	Y	609	CHL	C1A-C2A-CAA-CBA
43	n	607	CHL	C1A-C2A-CAA-CBA
43	g	601	CHL	C1A-C2A-CAA-CBA
43	g	606	CHL	C1A-C2A-CAA-CBA
43	g	607	CHL	C1A-C2A-CAA-CBA
43	g	608	CHL	C1A-C2A-CAA-CBA
43	g	609	CHL	C1A-C2A-CAA-CBA
43	s	608	CHL	C1A-C2A-CAA-CBA
43	y	605	CHL	C1A-C2A-CAA-CBA
43	y	609	CHL	C1A-C2A-CAA-CBA
43	G	609	CHL	C16-C17-C18-C19
43	Y	607	CHL	C16-C17-C18-C19
43	y	607	CHL	C16-C17-C18-C19
35	A	412	SQD	C9-C10-C11-C12
37	C	524	DGD	C5A-C6A-C7A-C8A
37	c	524	DGD	C5A-C6A-C7A-C8A
38	D	409	LHG	C11-C12-C13-C14
38	d	409	LHG	C11-C12-C13-C14
32	A	405	CLA	C15-C16-C17-C18
32	A	406	CLA	C15-C16-C17-C18
38	D	410	LHG	C3-O3-P-O6
38	S	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
38	s	2630	LHG	C3-O3-P-O6
35	a	412	SQD	C9-C10-C11-C12
35	A	412	SQD	C23-C24-C25-C26
43	G	609	CHL	C3-C5-C6-C7
43	g	609	CHL	C3-C5-C6-C7
32	D	403	CLA	C10-C11-C12-C13
38	D	409	LHG	O6-C4-C5-C6
38	d	409	LHG	O6-C4-C5-C6
43	g	609	CHL	O1D-CGD-O2D-CED
37	C	520	DGD	C4B-C5B-C6B-C7B
32	B	612	CLA	O1D-CGD-O2D-CED
32	b	602	CLA	O1D-CGD-O2D-CED
32	B	606	CLA	C8-C10-C11-C12
32	d	403	CLA	C10-C11-C12-C13
37	c	520	DGD	C4B-C5B-C6B-C7B
32	C	506	CLA	C3-C5-C6-C7
32	c	506	CLA	C3-C5-C6-C7
32	D	403	CLA	C5-C6-C7-C8
32	a	405	CLA	C8-C10-C11-C12
32	b	606	CLA	C8-C10-C11-C12
32	c	507	CLA	C4-C3-C5-C6
38	G	2630	LHG	C14-C15-C16-C17
32	A	405	CLA	C8-C10-C11-C12
32	a	405	CLA	C15-C16-C17-C18
32	d	403	CLA	C5-C6-C7-C8
36	a	413	LMG	O10-C28-O8-C9
38	D	410	LHG	C30-C31-C32-C33
38	d	410	LHG	C30-C31-C32-C33
32	C	503	CLA	C2A-CAA-CBA-CGA
32	S	602	CLA	C2A-CAA-CBA-CGA
32	s	602	CLA	C2A-CAA-CBA-CGA
32	B	617	CLA	C16-C17-C18-C20
32	C	508	CLA	C16-C17-C18-C19
32	N	603	CLA	C16-C17-C18-C20
32	b	602	CLA	C16-C17-C18-C20
32	b	617	CLA	C16-C17-C18-C20
32	c	508	CLA	C16-C17-C18-C19
32	n	603	CLA	C16-C17-C18-C20
43	G	601	CHL	C16-C17-C18-C19
43	g	601	CHL	C16-C17-C18-C19
43	G	609	CHL	O1D-CGD-O2D-CED
43	G	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	B	621	SQD	O6-C44-C45-C46
35	b	621	SQD	O6-C44-C45-C46
36	A	413	LMG	O1-C7-C8-C9
36	a	413	LMG	O1-C7-C8-C9
37	C	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	O1G-C1G-C2G-C3G
38	d	408	LHG	C11-C12-C13-C14
36	A	413	LMG	O10-C28-O8-C9
32	B	607	CLA	O1D-CGD-O2D-CED
32	b	607	CLA	O1D-CGD-O2D-CED
38	D	408	LHG	C11-C12-C13-C14
43	G	606	CHL	O1D-CGD-O2D-CED
43	g	606	CHL	O1D-CGD-O2D-CED
32	a	406	CLA	C15-C16-C17-C18
38	C	2630	LHG	C34-C35-C36-C37
38	g	2630	LHG	O8-C23-C24-C25
43	N	605	CHL	O1D-CGD-O2D-CED
43	n	605	CHL	O1D-CGD-O2D-CED
32	B	602	CLA	C16-C17-C18-C20
32	G	602	CLA	C16-C17-C18-C20
42	y	2632	LMU	O5'-C1'-O1'-C1
43	g	601	CHL	C15-C16-C17-C18
38	D	408	LHG	C33-C34-C35-C36
38	d	408	LHG	C33-C34-C35-C36
32	G	602	CLA	C8-C10-C11-C12
32	g	602	CLA	C8-C10-C11-C12
38	c	2630	LHG	C34-C35-C36-C37
32	C	508	CLA	C10-C11-C12-C13
32	c	508	CLA	C10-C11-C12-C13
32	y	611	CLA	C8-C10-C11-C12
33	a	408	PHO	C10-C11-C12-C13
43	G	601	CHL	C16-C17-C18-C20
37	C	524	DGD	C2A-C1A-O1G-C1G
37	c	524	DGD	C2A-C1A-O1G-C1G
37	C	520	DGD	C9B-CAB-CBB-CCB
32	B	605	CLA	C5-C6-C7-C8
32	Y	611	CLA	C8-C10-C11-C12
32	b	605	CLA	C5-C6-C7-C8
32	c	503	CLA	C2A-CAA-CBA-CGA
32	c	505	CLA	C8-C10-C11-C12
43	Y	609	CHL	C5-C6-C7-C8
43	y	609	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	c	523	DGD	C5B-C6B-C7B-C8B
38	n	2630	LHG	C26-C27-C28-C29
32	S	612	CLA	O1D-CGD-O2D-CED
32	s	612	CLA	O1D-CGD-O2D-CED
43	R	606	CHL	O1D-CGD-O2D-CED
37	C	523	DGD	C5B-C6B-C7B-C8B
38	N	2630	LHG	C26-C27-C28-C29
32	S	614	CLA	CBA-CGA-O2A-C1
32	s	614	CLA	CBA-CGA-O2A-C1
38	l	101	LHG	O6-C4-C5-O7
32	N	603	CLA	C16-C17-C18-C19
32	b	602	CLA	C16-C17-C18-C19
32	n	603	CLA	C16-C17-C18-C19
32	g	602	CLA	C16-C17-C18-C20
43	g	601	CHL	C16-C17-C18-C20
32	g	610	CLA	C5-C6-C7-C8
43	Y	606	CHL	O1D-CGD-O2D-CED
43	n	609	CHL	O1D-CGD-O2D-CED
43	y	606	CHL	O1D-CGD-O2D-CED
32	C	504	CLA	C13-C15-C16-C17
32	G	610	CLA	C5-C6-C7-C8
32	c	504	CLA	C13-C15-C16-C17
43	G	601	CHL	C15-C16-C17-C18
38	G	2630	LHG	O8-C23-C24-C25
36	A	413	LMG	O1-C7-C8-O7
36	a	413	LMG	O1-C7-C8-O7
32	b	612	CLA	O1D-CGD-O2D-CED
37	c	520	DGD	C9B-CAB-CBB-CCB
32	C	505	CLA	C8-C10-C11-C12
32	B	602	CLA	C16-C17-C18-C19
43	N	609	CHL	O1D-CGD-O2D-CED
36	A	413	LMG	C12-C13-C14-C15
36	a	413	LMG	C12-C13-C14-C15
40	D	405	PL9	C40-C39-C41-C42
40	D	405	PL9	C45-C44-C46-C47
40	d	405	PL9	C40-C39-C41-C42
40	d	405	PL9	C45-C44-C46-C47
43	Y	607	CHL	C4-C3-C5-C6
43	y	607	CHL	C4-C3-C5-C6
38	D	409	LHG	C35-C36-C37-C38
38	c	2630	LHG	C14-C15-C16-C17
32	A	405	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	B	604	CLA	C6-C7-C8-C10
32	B	606	CLA	C11-C10-C8-C7
32	B	615	CLA	C6-C7-C8-C10
32	B	616	CLA	C11-C12-C13-C15
32	B	617	CLA	C6-C7-C8-C10
32	B	617	CLA	C11-C12-C13-C15
32	C	509	CLA	C11-C10-C8-C7
32	C	510	CLA	C12-C13-C15-C16
32	C	511	CLA	C6-C7-C8-C10
32	D	402	CLA	C11-C12-C13-C15
32	N	602	CLA	C6-C7-C8-C10
32	N	603	CLA	C6-C7-C8-C10
32	N	603	CLA	C12-C13-C15-C16
32	G	610	CLA	C12-C13-C15-C16
32	Y	611	CLA	C12-C13-C15-C16
32	a	405	CLA	C11-C12-C13-C15
32	b	604	CLA	C6-C7-C8-C10
32	b	606	CLA	C11-C10-C8-C7
32	b	615	CLA	C6-C7-C8-C10
32	b	616	CLA	C11-C12-C13-C15
32	b	617	CLA	C6-C7-C8-C10
32	b	617	CLA	C11-C12-C13-C15
32	c	509	CLA	C11-C10-C8-C7
32	c	510	CLA	C12-C13-C15-C16
32	c	511	CLA	C6-C7-C8-C10
32	d	402	CLA	C11-C12-C13-C15
32	n	602	CLA	C6-C7-C8-C10
32	n	603	CLA	C6-C7-C8-C10
32	n	603	CLA	C12-C13-C15-C16
32	g	610	CLA	C12-C13-C15-C16
32	y	611	CLA	C12-C13-C15-C16
43	N	601	CHL	C6-C7-C8-C10
43	G	601	CHL	C11-C10-C8-C7
43	G	609	CHL	C12-C13-C15-C16
43	Y	601	CHL	C11-C12-C13-C15
43	Y	607	CHL	C2-C3-C5-C6
43	Y	607	CHL	C11-C12-C13-C15
43	Y	609	CHL	C11-C10-C8-C7
43	n	601	CHL	C6-C7-C8-C10
43	g	601	CHL	C11-C10-C8-C7
43	g	609	CHL	C12-C13-C15-C16
43	y	601	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
43	y	601	CHL	C11-C12-C13-C15
43	y	607	CHL	C2-C3-C5-C6
43	y	607	CHL	C11-C12-C13-C15
43	y	609	CHL	C11-C10-C8-C7
32	A	405	CLA	C11-C12-C13-C14
32	B	607	CLA	C14-C13-C15-C16
32	B	615	CLA	C6-C7-C8-C9
32	B	617	CLA	C6-C7-C8-C9
32	B	617	CLA	C11-C12-C13-C14
32	D	402	CLA	C11-C12-C13-C14
32	N	602	CLA	C6-C7-C8-C9
32	G	610	CLA	C14-C13-C15-C16
32	Y	610	CLA	C14-C13-C15-C16
32	Y	611	CLA	C14-C13-C15-C16
32	Y	612	CLA	C11-C10-C8-C9
32	Y	613	CLA	C14-C13-C15-C16
32	a	405	CLA	C11-C12-C13-C14
32	b	607	CLA	C14-C13-C15-C16
32	b	615	CLA	C6-C7-C8-C9
32	b	617	CLA	C6-C7-C8-C9
32	b	617	CLA	C11-C12-C13-C14
32	c	511	CLA	C6-C7-C8-C9
32	d	402	CLA	C11-C12-C13-C14
32	n	602	CLA	C6-C7-C8-C9
32	g	610	CLA	C14-C13-C15-C16
32	y	610	CLA	C14-C13-C15-C16
32	y	611	CLA	C14-C13-C15-C16
32	y	612	CLA	C11-C10-C8-C9
32	y	613	CLA	C14-C13-C15-C16
43	G	601	CHL	C11-C10-C8-C9
43	G	609	CHL	C14-C13-C15-C16
43	g	601	CHL	C11-C10-C8-C9
43	g	609	CHL	C14-C13-C15-C16
43	Y	609	CHL	CBA-CGA-O2A-C1
43	y	609	CHL	CBA-CGA-O2A-C1
32	C	503	CLA	C8-C10-C11-C12
32	c	503	CLA	C8-C10-C11-C12
32	c	513	CLA	C2A-CAA-CBA-CGA
38	C	2630	LHG	C14-C15-C16-C17
43	r	606	CHL	O1D-CGD-O2D-CED
34	C	516	BCR	C37-C22-C23-C24
34	c	516	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
46	Y	1623	NEX	C11-C12-C13-C20
46	r	625	NEX	C11-C12-C13-C20
32	y	603	CLA	C16-C17-C18-C19
35	B	621	SQD	C10-C11-C12-C13
44	y	1621	LUT	C7-C8-C9-C10
37	C	520	DGD	O6D-C5D-C6D-O5D
32	n	604	CLA	O1D-CGD-O2D-CED
32	n	611	CLA	O1D-CGD-O2D-CED
32	C	513	CLA	C15-C16-C17-C18
37	C	520	DGD	C2B-C1B-O2G-C2G
37	c	520	DGD	C2B-C1B-O2G-C2G
35	b	621	SQD	C10-C11-C12-C13
42	Y	2632	LMU	C9-C10-C11-C12
42	y	2632	LMU	C9-C10-C11-C12
37	C	524	DGD	C1B-C2B-C3B-C4B
37	c	524	DGD	C1B-C2B-C3B-C4B
33	A	408	PHO	C10-C11-C12-C13
43	Y	607	CHL	C10-C11-C12-C13
43	y	607	CHL	C10-C11-C12-C13
32	N	611	CLA	O1D-CGD-O2D-CED
37	c	520	DGD	O6D-C5D-C6D-O5D
32	N	613	CLA	CBD-CGD-O2D-CED
32	C	508	CLA	C16-C17-C18-C20
32	c	508	CLA	C16-C17-C18-C20
42	Y	2632	LMU	O5'-C1'-O1'-C1
32	c	513	CLA	C15-C16-C17-C18
32	N	604	CLA	O1D-CGD-O2D-CED
38	D	408	LHG	C10-C11-C12-C13
38	d	408	LHG	C10-C11-C12-C13
32	G	602	CLA	O1D-CGD-O2D-CED
37	C	524	DGD	O1A-C1A-O1G-C1G
37	c	524	DGD	O1A-C1A-O1G-C1G
35	b	621	SQD	C24-C25-C26-C27
32	C	513	CLA	C3-C5-C6-C7
32	Y	603	CLA	C16-C17-C18-C19
38	Y	2630	LHG	C17-C18-C19-C20
43	G	607	CHL	CBA-CGA-O2A-C1
43	g	607	CHL	CBA-CGA-O2A-C1
32	B	610	CLA	C3A-C2A-CAA-CBA
32	b	610	CLA	C3A-C2A-CAA-CBA
43	g	601	CHL	C3A-C2A-CAA-CBA
35	B	621	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
32	B	602	CLA	O1D-CGD-O2D-CED
44	Y	1621	LUT	C29-C30-C31-C32
44	y	1621	LUT	C29-C30-C31-C32
32	c	513	CLA	C3-C5-C6-C7
33	a	408	PHO	C16-C17-C18-C19
32	C	508	CLA	CBA-CGA-O2A-C1
32	c	508	CLA	CBA-CGA-O2A-C1
37	c	524	DGD	C9A-CAA-CBA-CCA
32	B	604	CLA	C10-C11-C12-C13
32	C	510	CLA	C10-C11-C12-C13
32	b	604	CLA	C10-C11-C12-C13
36	h	102	LMG	C7-C8-C9-O8
38	Y	2630	LHG	C4-C5-C6-O8
38	g	2630	LHG	C4-C5-C6-O8
38	y	2630	LHG	C4-C5-C6-O8
32	S	605	CLA	CBD-CGD-O2D-CED
32	s	605	CLA	CBD-CGD-O2D-CED
38	d	410	LHG	C11-C10-C9-C8
32	g	602	CLA	O1D-CGD-O2D-CED
43	g	601	CHL	C3-C5-C6-C7
38	D	410	LHG	C11-C10-C9-C8
33	A	408	PHO	C16-C17-C18-C19
40	D	405	PL9	C28-C29-C31-C32
40	d	405	PL9	C28-C29-C31-C32
38	g	2630	LHG	C11-C10-C9-C8
38	c	2630	LHG	C29-C30-C31-C32
43	G	605	CHL	C3C-C2C-CMC-OMC
43	Y	601	CHL	C3C-C2C-CMC-OMC
43	Y	607	CHL	C3C-C2C-CMC-OMC
43	g	605	CHL	C3C-C2C-CMC-OMC
43	y	601	CHL	C3C-C2C-CMC-OMC
43	y	607	CHL	C3C-C2C-CMC-OMC
32	C	507	CLA	C15-C16-C17-C18
32	Y	612	CLA	C10-C11-C12-C13
32	c	507	CLA	C15-C16-C17-C18
32	c	510	CLA	C10-C11-C12-C13
32	y	612	CLA	C10-C11-C12-C13
37	C	524	DGD	C9A-CAA-CBA-CCA
38	l	101	LHG	C25-C26-C27-C28
38	y	2630	LHG	C17-C18-C19-C20
38	L	101	LHG	O6-C4-C5-O7
38	C	2630	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	C4A-C5A-C6A-C7A
35	B	621	SQD	O47-C7-C8-C9
35	b	621	SQD	O47-C7-C8-C9
32	S	614	CLA	O1A-CGA-O2A-C1
32	s	614	CLA	O1A-CGA-O2A-C1
43	G	607	CHL	O1A-CGA-O2A-C1
43	g	607	CHL	O1A-CGA-O2A-C1
32	S	614	CLA	O2A-C1-C2-C3
32	s	614	CLA	O2A-C1-C2-C3
37	c	518	DGD	C4A-C5A-C6A-C7A
35	B	621	SQD	O6-C44-C45-O47
35	b	621	SQD	O6-C44-C45-O47
36	D	411	LMG	O1-C7-C8-O7
36	d	411	LMG	O1-C7-C8-O7
38	Y	2630	LHG	O7-C5-C6-O8
38	y	2630	LHG	O7-C5-C6-O8
38	d	409	LHG	C35-C36-C37-C38
32	Y	603	CLA	C10-C11-C12-C13
38	G	2630	LHG	C11-C10-C9-C8
32	B	614	CLA	C2-C1-O2A-CGA
32	b	614	CLA	C2-C1-O2A-CGA
36	a	413	LMG	C11-C12-C13-C14
32	B	609	CLA	C14-C13-C15-C16
32	B	612	CLA	C14-C13-C15-C16
32	C	510	CLA	C14-C13-C15-C16
32	C	511	CLA	C6-C7-C8-C9
32	b	609	CLA	C14-C13-C15-C16
32	b	612	CLA	C14-C13-C15-C16
32	c	510	CLA	C14-C13-C15-C16
32	y	604	CLA	C6-C7-C8-C9
43	Y	607	CHL	C11-C12-C13-C14
43	y	607	CHL	C11-C12-C13-C14
32	n	613	CLA	CBD-CGD-O2D-CED
36	A	413	LMG	C33-C34-C35-C36
42	z	2634	LMU	C7-C8-C9-C10
32	y	603	CLA	C10-C11-C12-C13
37	C	519	DGD	C7B-C8B-C9B-CAB
37	C	523	DGD	CBB-CCB-CDB-CEB
37	c	519	DGD	C7B-C8B-C9B-CAB
37	c	523	DGD	CBB-CCB-CDB-CEB
42	Z	2634	LMU	C7-C8-C9-C10
32	B	615	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	b	615	CLA	C2A-CAA-CBA-CGA
32	y	603	CLA	C16-C17-C18-C20
43	N	607	CHL	C16-C17-C18-C20
34	B	620	BCR	C23-C24-C25-C26
34	C	514	BCR	C5-C6-C7-C8
34	C	515	BCR	C23-C24-C25-C26
34	b	620	BCR	C23-C24-C25-C26
34	c	514	BCR	C5-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C26
44	N	1621	LUT	C1-C6-C7-C8
44	N	1621	LUT	C5-C6-C7-C8
44	G	1621	LUT	C5-C6-C7-C8
44	Y	1621	LUT	C5-C6-C7-C8
44	n	1621	LUT	C1-C6-C7-C8
44	n	1621	LUT	C5-C6-C7-C8
44	y	1621	LUT	C5-C6-C7-C8
32	B	615	CLA	C10-C11-C12-C13
32	C	502	CLA	C8-C10-C11-C12
32	C	511	CLA	C5-C6-C7-C8
36	A	413	LMG	C11-C12-C13-C14
36	a	413	LMG	C33-C34-C35-C36
38	s	2630	LHG	C30-C31-C32-C33
46	y	1623	NEX	C11-C12-C13-C20
38	S	2630	LHG	C30-C31-C32-C33
32	C	502	CLA	O1D-CGD-O2D-CED
34	C	515	BCR	C7-C8-C9-C10
34	C	515	BCR	C11-C12-C13-C14
34	c	515	BCR	C7-C8-C9-C10
34	c	515	BCR	C11-C12-C13-C14
44	Y	1621	LUT	C7-C8-C9-C10
46	s	1623	NEX	C31-C32-C33-C34
32	B	616	CLA	C5-C6-C7-C8
32	N	602	CLA	C13-C15-C16-C17
32	b	615	CLA	C10-C11-C12-C13
32	c	502	CLA	C8-C10-C11-C12
32	n	602	CLA	C13-C15-C16-C17
32	c	502	CLA	O1D-CGD-O2D-CED
37	c	520	DGD	O1B-C1B-O2G-C2G
32	Y	603	CLA	C16-C17-C18-C20
43	n	607	CHL	C16-C17-C18-C20
38	L	101	LHG	C25-C26-C27-C28
32	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
38	l	101	LHG	O6-C4-C5-C6
32	B	607	CLA	C12-C13-C15-C16
32	B	609	CLA	C12-C13-C15-C16
32	B	612	CLA	C11-C12-C13-C15
32	B	612	CLA	C12-C13-C15-C16
32	C	504	CLA	C12-C13-C15-C16
32	C	509	CLA	C6-C7-C8-C10
32	D	403	CLA	C11-C12-C13-C15
32	N	603	CLA	C11-C10-C8-C7
32	Y	604	CLA	C6-C7-C8-C10
32	Y	610	CLA	C12-C13-C15-C16
32	Y	612	CLA	C11-C10-C8-C7
32	Y	613	CLA	C12-C13-C15-C16
32	b	607	CLA	C12-C13-C15-C16
32	b	609	CLA	C12-C13-C15-C16
32	b	612	CLA	C11-C12-C13-C15
32	b	612	CLA	C12-C13-C15-C16
32	c	504	CLA	C12-C13-C15-C16
32	c	509	CLA	C6-C7-C8-C10
32	d	403	CLA	C11-C12-C13-C15
32	n	603	CLA	C11-C10-C8-C7
32	y	604	CLA	C6-C7-C8-C10
32	y	610	CLA	C12-C13-C15-C16
32	y	612	CLA	C11-C10-C8-C7
32	y	613	CLA	C12-C13-C15-C16
43	N	605	CHL	C11-C12-C13-C15
43	G	609	CHL	C11-C10-C8-C7
43	Y	601	CHL	C11-C10-C8-C7
43	n	605	CHL	C11-C12-C13-C15
43	g	609	CHL	C11-C10-C8-C7
44	N	1621	LUT	C29-C30-C31-C32
44	G	1621	LUT	C29-C30-C31-C32
44	n	1621	LUT	C29-C30-C31-C32
44	g	1621	LUT	C29-C30-C31-C32
37	C	520	DGD	O1B-C1B-O2G-C2G
38	c	2630	LHG	O9-C7-O7-C5
32	B	608	CLA	C2A-CAA-CBA-CGA
38	C	2630	LHG	C8-C7-O7-C5
38	c	2630	LHG	C8-C7-O7-C5
42	Y	2632	LMU	C4-C5-C6-C7
42	y	2632	LMU	C4-C5-C6-C7
35	a	412	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	R	603	CLA	CBA-CGA-O2A-C1
32	r	603	CLA	CBA-CGA-O2A-C1
43	g	606	CHL	CBA-CGA-O2A-C1
35	A	412	SQD	C32-C33-C34-C35
32	B	610	CLA	CAD-CBD-CGD-O2D
32	B	613	CLA	CAD-CBD-CGD-O2D
32	B	615	CLA	CAD-CBD-CGD-O2D
32	C	503	CLA	CAD-CBD-CGD-O2D
32	C	510	CLA	CAD-CBD-CGD-O2D
32	D	403	CLA	CAD-CBD-CGD-O2D
32	N	602	CLA	CAD-CBD-CGD-O2D
32	N	614	CLA	CAD-CBD-CGD-O2D
32	G	614	CLA	CAD-CBD-CGD-O2D
32	Y	614	CLA	CAD-CBD-CGD-O2D
32	b	610	CLA	CAD-CBD-CGD-O2D
32	b	613	CLA	CAD-CBD-CGD-O2D
32	b	615	CLA	CAD-CBD-CGD-O2D
32	c	510	CLA	CAD-CBD-CGD-O2D
32	d	403	CLA	CAD-CBD-CGD-O2D
32	n	602	CLA	CAD-CBD-CGD-O2D
32	n	614	CLA	CAD-CBD-CGD-O2D
32	g	614	CLA	CAD-CBD-CGD-O2D
32	y	614	CLA	CAD-CBD-CGD-O2D
43	N	607	CHL	CAD-CBD-CGD-O2D
43	G	608	CHL	CAD-CBD-CGD-O2D
43	Y	605	CHL	CAD-CBD-CGD-O2D
43	n	607	CHL	CAD-CBD-CGD-O2D
43	g	608	CHL	CAD-CBD-CGD-O2D
43	y	605	CHL	CAD-CBD-CGD-O2D
38	C	2630	LHG	O9-C7-O7-C5
32	G	602	CLA	CBA-CGA-O2A-C1
43	G	606	CHL	CBA-CGA-O2A-C1
37	c	523	DGD	C9B-CAB-CBB-CCB
36	H	102	LMG	C7-C8-C9-O8
38	C	2630	LHG	C4-C5-C6-O8
38	G	2630	LHG	C4-C5-C6-O8
38	c	2630	LHG	C4-C5-C6-O8
32	C	513	CLA	CBD-CGD-O2D-CED
43	y	609	CHL	O1A-CGA-O2A-C1
33	a	408	PHO	C15-C16-C17-C18
32	S	611	CLA	O2A-C1-C2-C3
32	S	613	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	s	611	CLA	O2A-C1-C2-C3
32	s	613	CLA	O2A-C1-C2-C3
38	l	101	LHG	C27-C28-C29-C30
32	C	513	CLA	C2A-CAA-CBA-CGA
32	b	608	CLA	C2A-CAA-CBA-CGA
37	C	523	DGD	C9B-CAB-CBB-CCB
38	D	409	LHG	C10-C11-C12-C13
38	d	409	LHG	C10-C11-C12-C13
32	B	608	CLA	CHA-CBD-CGD-O1D
32	B	608	CLA	CHA-CBD-CGD-O2D
32	C	501	CLA	CHA-CBD-CGD-O1D
32	C	501	CLA	CHA-CBD-CGD-O2D
32	C	505	CLA	CHA-CBD-CGD-O1D
32	C	505	CLA	CHA-CBD-CGD-O2D
32	G	603	CLA	CHA-CBD-CGD-O1D
32	G	603	CLA	CHA-CBD-CGD-O2D
32	G	612	CLA	CHA-CBD-CGD-O1D
32	G	612	CLA	CHA-CBD-CGD-O2D
32	G	613	CLA	CHA-CBD-CGD-O1D
32	G	613	CLA	CHA-CBD-CGD-O2D
32	S	604	CLA	CHA-CBD-CGD-O1D
32	S	604	CLA	CHA-CBD-CGD-O2D
32	S	610	CLA	CHA-CBD-CGD-O2D
32	Y	604	CLA	CHA-CBD-CGD-O1D
32	Y	604	CLA	CHA-CBD-CGD-O2D
32	b	608	CLA	CHA-CBD-CGD-O1D
32	b	608	CLA	CHA-CBD-CGD-O2D
32	c	501	CLA	CHA-CBD-CGD-O1D
32	c	501	CLA	CHA-CBD-CGD-O2D
32	c	503	CLA	CHA-CBD-CGD-O1D
32	c	505	CLA	CHA-CBD-CGD-O1D
32	c	505	CLA	CHA-CBD-CGD-O2D
32	g	603	CLA	CHA-CBD-CGD-O1D
32	g	612	CLA	CHA-CBD-CGD-O1D
32	g	612	CLA	CHA-CBD-CGD-O2D
32	g	613	CLA	CHA-CBD-CGD-O1D
32	g	613	CLA	CHA-CBD-CGD-O2D
32	s	604	CLA	CHA-CBD-CGD-O1D
32	s	604	CLA	CHA-CBD-CGD-O2D
32	y	604	CLA	CHA-CBD-CGD-O1D
32	y	604	CLA	CHA-CBD-CGD-O2D
43	S	606	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
43	S	606	CHL	CHA-CBD-CGD-O2D
43	s	606	CHL	CHA-CBD-CGD-O1D
43	s	606	CHL	CHA-CBD-CGD-O2D
44	S	1621	LUT	C29-C30-C31-C32
33	A	408	PHO	C3-C5-C6-C7
32	C	508	CLA	O1A-CGA-O2A-C1
32	c	508	CLA	O1A-CGA-O2A-C1
43	Y	609	CHL	O1A-CGA-O2A-C1
37	C	523	DGD	O2G-C2G-C3G-O3G
37	c	523	DGD	O2G-C2G-C3G-O3G
38	C	2630	LHG	O7-C5-C6-O8
38	c	2630	LHG	O7-C5-C6-O8
35	b	621	SQD	C13-C14-C15-C16
36	D	411	LMG	C19-C20-C21-C22
36	D	411	LMG	C20-C21-C22-C23
36	d	411	LMG	C19-C20-C21-C22
43	n	607	CHL	O1D-CGD-O2D-CED
36	d	411	LMG	C20-C21-C22-C23
32	B	609	CLA	C16-C17-C18-C20
35	B	621	SQD	C15-C16-C17-C18
38	l	101	LHG	C26-C27-C28-C29
32	c	511	CLA	C5-C6-C7-C8
37	c	523	DGD	CBA-CCA-CDA-CEA
36	c	521	LMG	C4-C5-C6-O5
43	N	607	CHL	O1D-CGD-O2D-CED
40	D	405	PL9	C4-C3-C7-C8
40	d	405	PL9	C4-C3-C7-C8
35	B	621	SQD	C13-C14-C15-C16
32	B	610	CLA	C14-C13-C15-C16
32	B	612	CLA	C11-C12-C13-C14
32	C	512	CLA	C14-C13-C15-C16
32	D	403	CLA	C11-C12-C13-C14
32	N	613	CLA	C14-C13-C15-C16
32	G	602	CLA	C11-C10-C8-C9
32	G	613	CLA	C6-C7-C8-C9
32	Y	604	CLA	C6-C7-C8-C9
32	Y	613	CLA	C11-C10-C8-C9
32	b	612	CLA	C11-C12-C13-C14
32	c	512	CLA	C14-C13-C15-C16
32	d	403	CLA	C11-C12-C13-C14
32	n	613	CLA	C14-C13-C15-C16
32	g	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	g	613	CLA	C6-C7-C8-C9
32	y	613	CLA	C11-C10-C8-C9
43	N	605	CHL	C11-C12-C13-C14
43	N	607	CHL	C11-C10-C8-C9
43	n	605	CHL	C11-C12-C13-C14
43	n	607	CHL	C11-C10-C8-C9
35	b	621	SQD	C15-C16-C17-C18
36	H	102	LMG	C34-C35-C36-C37
38	L	101	LHG	C27-C28-C29-C30
32	R	603	CLA	O1A-CGA-O2A-C1
32	r	603	CLA	O1A-CGA-O2A-C1
32	G	602	CLA	C2A-CAA-CBA-CGA
32	Y	613	CLA	C2A-CAA-CBA-CGA
32	y	613	CLA	C2A-CAA-CBA-CGA
32	c	513	CLA	CBD-CGD-O2D-CED
46	R	625	NEX	C11-C12-C13-C20
37	C	523	DGD	CBA-CCA-CDA-CEA
34	C	516	BCR	C21-C22-C23-C24
34	c	516	BCR	C21-C22-C23-C24
32	B	604	CLA	C1A-C2A-CAA-CBA
32	C	501	CLA	C1A-C2A-CAA-CBA
32	N	610	CLA	C1A-C2A-CAA-CBA
32	Y	611	CLA	C1A-C2A-CAA-CBA
32	b	604	CLA	C1A-C2A-CAA-CBA
32	c	501	CLA	C1A-C2A-CAA-CBA
32	n	610	CLA	C1A-C2A-CAA-CBA
32	y	611	CLA	C1A-C2A-CAA-CBA
32	b	606	CLA	C13-C15-C16-C17
36	B	622	LMG	C16-C17-C18-C19
36	b	622	LMG	C16-C17-C18-C19
32	g	602	CLA	CBA-CGA-O2A-C1
38	L	101	LHG	C26-C27-C28-C29
44	s	1621	LUT	C29-C30-C31-C32
38	d	410	LHG	C3-O3-P-O6
32	C	507	CLA	C2-C3-C5-C6
40	D	405	PL9	C18-C19-C21-C22
40	d	405	PL9	C18-C19-C21-C22
38	g	2630	LHG	C17-C18-C19-C20
38	C	2630	LHG	C4-O6-P-O4
38	D	408	LHG	C3-O3-P-O4
38	D	410	LHG	C3-O3-P-O4
38	S	2630	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
38	c	2630	LHG	C4-O6-P-O4
38	d	408	LHG	C3-O3-P-O4
38	d	410	LHG	C4-O6-P-O4
32	c	511	CLA	C16-C17-C18-C20
38	g	2630	LHG	C23-C24-C25-C26
36	h	102	LMG	C34-C35-C36-C37
32	B	606	CLA	C13-C15-C16-C17
33	A	408	PHO	C15-C16-C17-C18
43	N	605	CHL	C10-C11-C12-C13
43	n	605	CHL	C10-C11-C12-C13
38	L	101	LHG	O6-C4-C5-C6
37	c	518	DGD	C2B-C3B-C4B-C5B
33	A	408	PHO	C2A-CAA-CBA-CGA
43	g	606	CHL	O1A-CGA-O2A-C1
32	b	609	CLA	C16-C17-C18-C20
35	B	621	SQD	C11-C12-C13-C14
37	C	518	DGD	C2B-C3B-C4B-C5B
32	B	602	CLA	CAD-CBD-CGD-O1D
32	B	604	CLA	CAD-CBD-CGD-O1D
32	B	608	CLA	CAD-CBD-CGD-O1D
32	C	501	CLA	CAD-CBD-CGD-O1D
32	C	505	CLA	CAD-CBD-CGD-O1D
32	C	512	CLA	CAD-CBD-CGD-O1D
32	N	611	CLA	CAD-CBD-CGD-O1D
32	G	603	CLA	CAD-CBD-CGD-O1D
32	S	604	CLA	CAD-CBD-CGD-O1D
32	b	602	CLA	CAD-CBD-CGD-O1D
32	b	604	CLA	CAD-CBD-CGD-O1D
32	b	608	CLA	CAD-CBD-CGD-O1D
32	c	501	CLA	CAD-CBD-CGD-O1D
32	c	505	CLA	CAD-CBD-CGD-O1D
32	c	512	CLA	CAD-CBD-CGD-O1D
32	n	611	CLA	CAD-CBD-CGD-O1D
32	g	603	CLA	CAD-CBD-CGD-O1D
32	s	604	CLA	CAD-CBD-CGD-O1D
35	B	621	SQD	C5-C6-S-O7
35	a	412	SQD	C5-C6-S-O9
35	b	621	SQD	C5-C6-S-O7
32	B	607	CLA	C15-C16-C17-C18
32	b	607	CLA	C15-C16-C17-C18
37	c	518	DGD	O6D-C5D-C6D-O5D
35	b	621	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	G	602	CLA	O1A-CGA-O2A-C1
38	l	101	LHG	C30-C31-C32-C33
36	h	102	LMG	C31-C32-C33-C34
38	L	101	LHG	C30-C31-C32-C33
38	S	2630	LHG	C7-C8-C9-C10
38	s	2630	LHG	C7-C8-C9-C10
36	C	521	LMG	C4-C5-C6-O5
37	C	518	DGD	O6D-C5D-C6D-O5D
32	C	511	CLA	C16-C17-C18-C20
32	B	609	CLA	C11-C10-C8-C7
32	B	613	CLA	C11-C10-C8-C7
32	C	505	CLA	C11-C10-C8-C7
32	C	510	CLA	C11-C10-C8-C7
32	C	512	CLA	C12-C13-C15-C16
32	N	604	CLA	C6-C7-C8-C10
32	N	613	CLA	C12-C13-C15-C16
32	G	610	CLA	C11-C10-C8-C7
32	Y	603	CLA	C11-C12-C13-C15
32	Y	612	CLA	C6-C7-C8-C10
32	b	609	CLA	C11-C10-C8-C7
32	b	610	CLA	C11-C12-C13-C15
32	b	613	CLA	C11-C10-C8-C7
32	c	507	CLA	C2-C3-C5-C6
32	c	510	CLA	C11-C10-C8-C7
32	c	512	CLA	C12-C13-C15-C16
32	n	604	CLA	C6-C7-C8-C10
32	n	613	CLA	C12-C13-C15-C16
32	g	610	CLA	C11-C10-C8-C7
32	y	603	CLA	C11-C12-C13-C15
32	y	612	CLA	C6-C7-C8-C10
38	D	409	LHG	O6-C4-C5-O7
38	d	409	LHG	O6-C4-C5-O7
43	N	609	CHL	C6-C7-C8-C10
43	N	609	CHL	C11-C12-C13-C15
43	n	609	CHL	C6-C7-C8-C10
43	n	609	CHL	C11-C12-C13-C15
37	c	519	DGD	CBA-CCA-CDA-CEA
32	C	502	CLA	O1A-CGA-O2A-C1
32	c	502	CLA	O1A-CGA-O2A-C1
43	G	606	CHL	O1A-CGA-O2A-C1
32	g	602	CLA	C2A-CAA-CBA-CGA
36	h	102	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
38	G	2630	LHG	C23-C24-C25-C26
37	C	523	DGD	C1G-C2G-C3G-O3G
37	c	523	DGD	C1G-C2G-C3G-O3G
38	d	409	LHG	C31-C32-C33-C34
43	N	607	CHL	C1C-C2C-CMC-OMC
43	N	609	CHL	C1C-C2C-CMC-OMC
43	G	605	CHL	C1C-C2C-CMC-OMC
43	G	608	CHL	C1C-C2C-CMC-OMC
43	S	601	CHL	C1C-C2C-CMC-OMC
43	S	607	CHL	C1C-C2C-CMC-OMC
43	Y	601	CHL	C1C-C2C-CMC-OMC
43	Y	607	CHL	C1C-C2C-CMC-OMC
43	n	607	CHL	C1C-C2C-CMC-OMC
43	n	609	CHL	C1C-C2C-CMC-OMC
43	g	605	CHL	C1C-C2C-CMC-OMC
43	g	608	CHL	C1C-C2C-CMC-OMC
43	s	601	CHL	C1C-C2C-CMC-OMC
43	s	607	CHL	C1C-C2C-CMC-OMC
43	y	601	CHL	C1C-C2C-CMC-OMC
43	y	607	CHL	C1C-C2C-CMC-OMC
37	C	519	DGD	CBA-CCA-CDA-CEA
38	G	2630	LHG	C17-C18-C19-C20
32	N	613	CLA	O1D-CGD-O2D-CED
36	b	622	LMG	C37-C38-C39-C40
43	G	609	CHL	C4C-C3C-CAC-CBC
32	g	602	CLA	O1A-CGA-O2A-C1
32	b	610	CLA	C4-C3-C5-C6
40	D	405	PL9	C30-C29-C31-C32
40	d	405	PL9	C30-C29-C31-C32
36	B	622	LMG	C37-C38-C39-C40
36	h	102	LMG	C11-C10-O7-C8
32	N	604	CLA	C10-C11-C12-C13
32	n	604	CLA	C10-C11-C12-C13
32	A	406	CLA	C11-C12-C13-C14
32	B	604	CLA	C6-C7-C8-C9
32	B	606	CLA	C11-C10-C8-C9
32	C	504	CLA	C14-C13-C15-C16
32	C	507	CLA	C14-C13-C15-C16
32	C	510	CLA	C11-C10-C8-C9
32	C	513	CLA	C14-C13-C15-C16
32	N	603	CLA	C6-C7-C8-C9
32	N	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	N	604	CLA	C6-C7-C8-C9
32	b	604	CLA	C6-C7-C8-C9
32	b	606	CLA	C11-C10-C8-C9
32	b	610	CLA	C14-C13-C15-C16
32	c	504	CLA	C14-C13-C15-C16
32	c	507	CLA	C14-C13-C15-C16
32	c	510	CLA	C11-C10-C8-C9
32	c	513	CLA	C14-C13-C15-C16
32	n	603	CLA	C6-C7-C8-C9
32	n	603	CLA	C11-C10-C8-C9
32	n	604	CLA	C6-C7-C8-C9
43	n	609	CHL	C6-C7-C8-C9
40	D	405	PL9	C47-C48-C49-C50
40	d	405	PL9	C47-C48-C49-C50
32	B	609	CLA	C16-C17-C18-C19
46	r	625	NEX	C11-C12-C13-C14
38	S	2630	LHG	C33-C34-C35-C36
38	s	2630	LHG	C33-C34-C35-C36
43	g	609	CHL	C4C-C3C-CAC-CBC
36	H	102	LMG	C31-C32-C33-C34
32	B	611	CLA	C15-C16-C17-C18
32	B	610	CLA	C4-C3-C5-C6
32	G	613	CLA	C4-C3-C5-C6
32	g	613	CLA	C4-C3-C5-C6
43	N	609	CHL	C4-C3-C5-C6
43	n	609	CHL	C4-C3-C5-C6
32	n	613	CLA	O1D-CGD-O2D-CED
32	B	609	CLA	C15-C16-C17-C18
32	a	410	CLA	C5-C6-C7-C8
32	b	609	CLA	C15-C16-C17-C18
32	b	611	CLA	C15-C16-C17-C18
43	n	607	CHL	C16-C17-C18-C19
32	A	410	CLA	C5-C6-C7-C8
32	N	611	CLA	C1-C2-C3-C4
32	N	614	CLA	C1-C2-C3-C4
32	G	604	CLA	C1-C2-C3-C4
32	G	614	CLA	C1-C2-C3-C4
32	R	603	CLA	C1-C2-C3-C4
32	R	604	CLA	C1-C2-C3-C4
32	S	602	CLA	C1-C2-C3-C4
32	S	604	CLA	C1-C2-C3-C4
32	S	610	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	S	611	CLA	C1-C2-C3-C4
32	S	613	CLA	C1-C2-C3-C4
32	n	611	CLA	C1-C2-C3-C4
32	n	614	CLA	C1-C2-C3-C4
32	g	604	CLA	C1-C2-C3-C4
32	g	614	CLA	C1-C2-C3-C4
32	r	603	CLA	C1-C2-C3-C4
32	r	604	CLA	C1-C2-C3-C4
32	s	602	CLA	C1-C2-C3-C4
32	s	604	CLA	C1-C2-C3-C4
32	s	610	CLA	C1-C2-C3-C4
32	s	611	CLA	C1-C2-C3-C4
32	s	613	CLA	C1-C2-C3-C4
43	N	608	CHL	C1-C2-C3-C4
43	G	606	CHL	C1-C2-C3-C4
43	G	607	CHL	C1-C2-C3-C4
43	R	607	CHL	C1-C2-C3-C4
43	Y	608	CHL	C1-C2-C3-C4
43	n	608	CHL	C1-C2-C3-C4
43	g	606	CHL	C1-C2-C3-C4
43	g	607	CHL	C1-C2-C3-C4
43	r	607	CHL	C1-C2-C3-C4
43	y	608	CHL	C1-C2-C3-C4
37	C	523	DGD	O6D-C5D-C6D-O5D
37	c	523	DGD	O6D-C5D-C6D-O5D
37	c	518	DGD	C4D-C5D-C6D-O5D
38	Y	2630	LHG	C9-C10-C11-C12
37	c	518	DGD	O1G-C1A-C2A-C3A
42	Y	2632	LMU	C6-C7-C8-C9
42	y	2632	LMU	C6-C7-C8-C9
38	G	2630	LHG	O6-C4-C5-C6
38	g	2630	LHG	O6-C4-C5-C6
32	B	611	CLA	C2-C1-O2A-CGA
32	C	513	CLA	C2-C1-O2A-CGA
32	D	402	CLA	C2-C1-O2A-CGA
32	b	611	CLA	C2-C1-O2A-CGA
32	c	513	CLA	C2-C1-O2A-CGA
32	d	402	CLA	C2-C1-O2A-CGA
43	N	605	CHL	C2-C1-O2A-CGA
43	n	605	CHL	C2-C1-O2A-CGA
37	C	520	DGD	C2B-C3B-C4B-C5B
32	b	609	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	O1G-C1A-C2A-C3A
43	R	607	CHL	CAA-CBA-CGA-O2A
43	r	607	CHL	CAA-CBA-CGA-O2A
32	G	613	CLA	C10-C11-C12-C13
37	C	518	DGD	C4D-C5D-C6D-O5D
32	C	502	CLA	CBA-CGA-O2A-C1
32	Y	603	CLA	CBA-CGA-O2A-C1
32	c	502	CLA	CBA-CGA-O2A-C1
38	d	410	LHG	O6-C4-C5-O7
35	A	412	SQD	C25-C26-C27-C28
35	a	412	SQD	C25-C26-C27-C28
43	N	607	CHL	C16-C17-C18-C19
32	B	607	CLA	C5-C6-C7-C8
32	a	406	CLA	C8-C10-C11-C12
32	g	613	CLA	C10-C11-C12-C13
38	y	2630	LHG	C9-C10-C11-C12
34	A	411	BCR	C5-C6-C7-C8
34	C	514	BCR	C1-C6-C7-C8
34	C	515	BCR	C23-C24-C25-C30
34	a	411	BCR	C5-C6-C7-C8
34	c	514	BCR	C1-C6-C7-C8
34	c	515	BCR	C23-C24-C25-C30
44	G	1621	LUT	C1-C6-C7-C8
44	S	1620	LUT	C1-C6-C7-C8
44	S	1620	LUT	C5-C6-C7-C8
44	Y	1621	LUT	C1-C6-C7-C8
44	g	1621	LUT	C1-C6-C7-C8
44	g	1621	LUT	C5-C6-C7-C8
44	s	1620	LUT	C1-C6-C7-C8
44	s	1620	LUT	C5-C6-C7-C8
44	y	1621	LUT	C1-C6-C7-C8
32	C	501	CLA	O1A-CGA-O2A-C1
32	c	501	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	C2B-C3B-C4B-C5B
38	S	2630	LHG	C32-C33-C34-C35
38	s	2630	LHG	C32-C33-C34-C35
32	y	603	CLA	CBA-CGA-O2A-C1
32	b	607	CLA	C5-C6-C7-C8
32	n	613	CLA	C13-C15-C16-C17
42	Z	2635	LMU	C2'-C1'-O1'-C1
42	z	2635	LMU	C2'-C1'-O1'-C1
36	h	102	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
38	D	409	LHG	C3-O3-P-O6
38	N	2630	LHG	C3-O3-P-O6
38	Y	2630	LHG	C3-O3-P-O6
38	d	409	LHG	C3-O3-P-O6
38	n	2630	LHG	C3-O3-P-O6
38	y	2630	LHG	C3-O3-P-O6
43	Y	607	CHL	C13-C15-C16-C17
32	B	604	CLA	C15-C16-C17-C18
32	b	604	CLA	C15-C16-C17-C18
32	C	511	CLA	CBA-CGA-O2A-C1
32	c	501	CLA	CBA-CGA-O2A-C1
36	A	413	LMG	C7-C8-C9-O8
36	D	411	LMG	O1-C7-C8-C9
36	d	411	LMG	O1-C7-C8-C9
32	A	405	CLA	C12-C13-C15-C16
32	A	406	CLA	C11-C12-C13-C15
32	B	610	CLA	C11-C12-C13-C15
32	Y	604	CLA	C11-C12-C13-C15
32	Y	613	CLA	C11-C10-C8-C7
32	a	405	CLA	C12-C13-C15-C16
32	c	505	CLA	C11-C10-C8-C7
32	c	510	CLA	C6-C7-C8-C10
32	y	604	CLA	C11-C12-C13-C15
32	y	613	CLA	C11-C10-C8-C7
43	N	605	CHL	C12-C13-C15-C16
43	n	605	CHL	C12-C13-C15-C16
43	y	609	CHL	C11-C12-C13-C15
36	C	521	LMG	C30-C31-C32-C33
33	a	408	PHO	C3-C5-C6-C7
32	B	609	CLA	C11-C10-C8-C9
32	B	613	CLA	C11-C10-C8-C9
32	N	603	CLA	C14-C13-C15-C16
32	N	613	CLA	C6-C7-C8-C9
32	Y	603	CLA	C11-C12-C13-C14
32	b	609	CLA	C11-C10-C8-C9
32	b	613	CLA	C11-C10-C8-C9
32	n	603	CLA	C14-C13-C15-C16
32	n	613	CLA	C6-C7-C8-C9
32	y	603	CLA	C11-C12-C13-C14
43	N	609	CHL	C6-C7-C8-C9
43	N	609	CHL	C11-C12-C13-C14
43	Y	601	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
43	Y	601	CHL	C11-C10-C8-C9
43	Y	601	CHL	C11-C12-C13-C14
43	n	609	CHL	C11-C12-C13-C14
43	y	601	CHL	C6-C7-C8-C9
43	y	601	CHL	C11-C10-C8-C9
43	y	601	CHL	C11-C12-C13-C14
32	B	613	CLA	C16-C17-C18-C19
32	b	613	CLA	C16-C17-C18-C19
32	C	513	CLA	O1D-CGD-O2D-CED
36	h	102	LMG	C18-C19-C20-C21
32	C	501	CLA	CBA-CGA-O2A-C1
32	g	613	CLA	CBA-CGA-O2A-C1
36	B	622	LMG	C12-C13-C14-C15
32	N	613	CLA	C13-C15-C16-C17
36	b	622	LMG	C12-C13-C14-C15
32	C	511	CLA	O1A-CGA-O2A-C1
32	Y	603	CLA	O1A-CGA-O2A-C1
33	A	408	PHO	O1A-CGA-O2A-C1
43	y	607	CHL	C13-C15-C16-C17
32	B	607	CLA	C16-C17-C18-C19
32	c	511	CLA	CBA-CGA-O2A-C1
32	N	604	CLA	C3-C5-C6-C7
32	G	614	CLA	O2A-C1-C2-C3
32	g	614	CLA	O2A-C1-C2-C3
32	B	615	CLA	C4-C3-C5-C6
32	b	615	CLA	C4-C3-C5-C6
32	b	610	CLA	C2-C3-C5-C6
32	b	607	CLA	C16-C17-C18-C19
33	A	408	PHO	CBA-CGA-O2A-C1
32	g	613	CLA	O1A-CGA-O2A-C1
32	y	603	CLA	O1A-CGA-O2A-C1
36	c	521	LMG	C30-C31-C32-C33
38	Y	2630	LHG	C16-C17-C18-C19
32	G	613	CLA	CBA-CGA-O2A-C1
32	N	602	CLA	C2A-CAA-CBA-CGA
32	N	603	CLA	C2A-CAA-CBA-CGA
32	R	604	CLA	C2A-CAA-CBA-CGA
32	n	602	CLA	C2A-CAA-CBA-CGA
32	n	603	CLA	C2A-CAA-CBA-CGA
41	F	101	HEM	CAA-CBA-CGA-O1A
34	A	411	BCR	C19-C20-C21-C22
34	a	411	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
45	N	1622	XAT	C29-C30-C31-C32
45	n	1622	XAT	C29-C30-C31-C32
46	s	1623	NEX	C9-C10-C11-C12
32	n	604	CLA	C3-C5-C6-C7
41	f	101	HEM	CAA-CBA-CGA-O1A
32	G	613	CLA	O1A-CGA-O2A-C1
36	A	413	LMG	C17-C18-C19-C20
32	B	613	CLA	C10-C11-C12-C13
32	B	610	CLA	C2-C3-C5-C6
32	B	615	CLA	C2-C3-C5-C6
32	b	615	CLA	C2-C3-C5-C6
32	b	613	CLA	C10-C11-C12-C13
43	Y	606	CHL	C2-C1-O2A-CGA
36	a	413	LMG	C17-C18-C19-C20
38	s	2630	LHG	C34-C35-C36-C37
32	N	613	CLA	C2A-CAA-CBA-CGA
32	n	613	CLA	C2A-CAA-CBA-CGA
32	g	603	CLA	C2A-CAA-CBA-CGA
32	r	604	CLA	C2A-CAA-CBA-CGA
32	c	504	CLA	C15-C16-C17-C18
38	S	2630	LHG	C34-C35-C36-C37
38	g	2630	LHG	O10-C23-C24-C25
37	c	520	DGD	CCB-CDB-CEB-CFB
32	B	605	CLA	C3A-C2A-CAA-CBA
32	b	605	CLA	C3A-C2A-CAA-CBA
33	A	408	PHO	C3A-C2A-CAA-CBA
32	c	513	CLA	O1D-CGD-O2D-CED
38	D	408	LHG	C25-C26-C27-C28
38	d	408	LHG	C25-C26-C27-C28
36	h	102	LMG	O9-C10-O7-C8
38	L	101	LHG	C11-C10-C9-C8
38	l	101	LHG	C32-C33-C34-C35
38	y	2630	LHG	C16-C17-C18-C19
40	D	405	PL9	C38-C39-C41-C42
40	d	405	PL9	C38-C39-C41-C42
37	C	523	DGD	O1G-C1A-C2A-C3A
32	Y	611	CLA	C6-C7-C8-C9
32	c	509	CLA	C11-C10-C8-C9
32	y	611	CLA	C6-C7-C8-C9
32	C	505	CLA	C16-C17-C18-C20
32	c	505	CLA	C16-C17-C18-C20
35	A	412	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C32-C33-C34-C35
38	y	2630	LHG	C27-C28-C29-C30
32	C	504	CLA	C15-C16-C17-C18
37	C	520	DGD	CCB-CDB-CEB-CFB
38	l	101	LHG	C11-C10-C9-C8
35	a	412	SQD	C27-C28-C29-C30
36	h	102	LMG	C39-C40-C41-C42
38	D	409	LHG	C31-C32-C33-C34
38	Y	2630	LHG	C27-C28-C29-C30
36	a	413	LMG	C7-C8-C9-O8
46	N	1623	NEX	C39-C29-C30-C31
46	G	1623	NEX	C39-C29-C30-C31
46	R	625	NEX	C39-C29-C30-C31
46	S	1623	NEX	C39-C29-C30-C31
46	Y	1623	NEX	C39-C29-C30-C31
46	n	1623	NEX	C39-C29-C30-C31
46	g	1623	NEX	C39-C29-C30-C31
46	r	625	NEX	C39-C29-C30-C31
46	s	1623	NEX	C39-C29-C30-C31
46	y	1623	NEX	C39-C29-C30-C31
37	c	523	DGD	O1G-C1A-C2A-C3A
33	a	408	PHO	C2A-CAA-CBA-CGA
35	B	621	SQD	C32-C33-C34-C35
32	c	511	CLA	O1A-CGA-O2A-C1
42	Z	2635	LMU	O5'-C1'-O1'-C1
42	z	2635	LMU	O5'-C1'-O1'-C1
44	G	1621	LUT	C7-C8-C9-C19
44	g	1621	LUT	C7-C8-C9-C19
36	H	102	LMG	C39-C40-C41-C42
46	R	625	NEX	C11-C12-C13-C14
32	C	503	CLA	C1A-C2A-CAA-CBA
32	C	506	CLA	C1A-C2A-CAA-CBA
32	c	503	CLA	C1A-C2A-CAA-CBA
32	c	506	CLA	C1A-C2A-CAA-CBA
43	N	609	CHL	C1A-C2A-CAA-CBA
43	n	609	CHL	C1A-C2A-CAA-CBA
43	n	607	CHL	CBD-CGD-O2D-CED
32	B	605	CLA	C6-C7-C8-C10
32	B	608	CLA	C11-C12-C13-C15
32	B	609	CLA	C6-C7-C8-C10
32	C	508	CLA	C6-C7-C8-C10
32	C	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
32	N	604	CLA	C12-C13-C15-C16
32	b	605	CLA	C6-C7-C8-C10
32	b	608	CLA	C11-C12-C13-C15
32	b	609	CLA	C6-C7-C8-C10
32	c	508	CLA	C6-C7-C8-C10
32	n	604	CLA	C12-C13-C15-C16
43	Y	609	CHL	C11-C12-C13-C15
32	S	612	CLA	CAA-CBA-CGA-O1A
38	G	2630	LHG	O10-C23-C24-C25
37	C	519	DGD	C8B-C9B-CAB-CBB
32	s	612	CLA	CAA-CBA-CGA-O1A
43	Y	609	CHL	C15-C16-C17-C18
32	G	610	CLA	C16-C17-C18-C20
36	D	411	LMG	C21-C22-C23-C24
36	H	102	LMG	C18-C19-C20-C21
36	d	411	LMG	C21-C22-C23-C24
32	S	605	CLA	O1D-CGD-O2D-CED
32	s	605	CLA	O1D-CGD-O2D-CED
32	N	604	CLA	C8-C10-C11-C12
32	n	604	CLA	C8-C10-C11-C12
43	y	609	CHL	C15-C16-C17-C18
35	a	412	SQD	C34-C35-C36-C37
38	D	410	LHG	O6-C4-C5-O7
36	A	413	LMG	O9-C10-O7-C8
43	Y	608	CHL	O2A-C1-C2-C3
43	y	608	CHL	O2A-C1-C2-C3
38	D	409	LHG	C24-C23-O8-C6
37	c	519	DGD	C8B-C9B-CAB-CBB
35	A	412	SQD	C34-C35-C36-C37
36	H	102	LMG	C19-C20-C21-C22
32	g	610	CLA	C16-C17-C18-C20
32	Y	604	CLA	C4-C3-C5-C6
32	c	505	CLA	C4-C3-C5-C6
32	y	604	CLA	C4-C3-C5-C6
43	Y	609	CHL	C4-C3-C5-C6
43	y	609	CHL	C4-C3-C5-C6
32	S	612	CLA	CAA-CBA-CGA-O2A
32	s	612	CLA	CAA-CBA-CGA-O2A
37	c	520	DGD	CAA-CBA-CCA-CDA
36	a	413	LMG	O9-C10-O7-C8
46	N	1623	NEX	C28-C29-C30-C31
46	G	1623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
46	R	625	NEX	C28-C29-C30-C31
46	S	1623	NEX	C28-C29-C30-C31
46	Y	1623	NEX	C28-C29-C30-C31
46	n	1623	NEX	C28-C29-C30-C31
46	g	1623	NEX	C28-C29-C30-C31
46	r	625	NEX	C28-C29-C30-C31
46	s	1623	NEX	C28-C29-C30-C31
46	y	1623	NEX	C28-C29-C30-C31
34	H	101	BCR	C9-C10-C11-C12
34	c	515	BCR	C19-C20-C21-C22
34	h	101	BCR	C9-C10-C11-C12
46	N	1623	NEX	C9-C10-C11-C12
46	S	1623	NEX	C9-C10-C11-C12
46	Y	1623	NEX	C33-C34-C35-C15
46	y	1623	NEX	C33-C34-C35-C15
41	F	101	HEM	CAA-CBA-CGA-O2A
41	f	101	HEM	CAA-CBA-CGA-O2A
37	C	524	DGD	C9B-CAB-CBB-CCB
37	c	524	DGD	C9B-CAB-CBB-CCB
43	Y	605	CHL	CAA-CBA-CGA-O2A
43	S	607	CHL	O1D-CGD-O2D-CED
43	s	607	CHL	O1D-CGD-O2D-CED
32	C	505	CLA	C4-C3-C5-C6
32	B	603	CLA	C2-C1-O2A-CGA
32	b	603	CLA	C2-C1-O2A-CGA
43	y	606	CHL	C2-C1-O2A-CGA
43	y	605	CHL	CAA-CBA-CGA-O2A
32	B	616	CLA	C14-C13-C15-C16
32	C	502	CLA	C6-C7-C8-C9
32	C	509	CLA	C11-C10-C8-C9
32	C	510	CLA	C6-C7-C8-C9
32	b	616	CLA	C14-C13-C15-C16
38	y	2630	LHG	C30-C31-C32-C33
38	Y	2630	LHG	C30-C31-C32-C33
32	r	604	CLA	O2A-C1-C2-C3
34	A	411	BCR	C1-C6-C7-C8
34	B	620	BCR	C23-C24-C25-C30
34	a	411	BCR	C1-C6-C7-C8
34	b	620	BCR	C23-C24-C25-C30
32	g	610	CLA	O1D-CGD-O2D-CED
43	N	607	CHL	CBD-CGD-O2D-CED
38	L	101	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	l	101	LHG	O1-C1-C2-C3
37	C	520	DGD	O1A-C1A-O1G-C1G
46	n	1623	NEX	C9-C10-C11-C12
38	l	101	LHG	C24-C23-O8-C6
32	G	613	CLA	C2-C3-C5-C6
32	g	613	CLA	C2-C3-C5-C6
43	N	609	CHL	C2-C3-C5-C6
43	n	609	CHL	C2-C3-C5-C6
43	s	601	CHL	CAA-CBA-CGA-O2A
32	A	406	CLA	C8-C10-C11-C12
43	S	601	CHL	CAA-CBA-CGA-O2A
32	B	607	CLA	C16-C17-C18-C20
32	b	607	CLA	C16-C17-C18-C20
32	N	612	CLA	CAA-CBA-CGA-O2A
32	Y	602	CLA	CBD-CGD-O2D-CED
37	C	520	DGD	C2A-C1A-O1G-C1G
38	L	101	LHG	C24-C23-O8-C6
43	Y	607	CHL	CBA-CGA-O2A-C1
43	y	607	CHL	CBA-CGA-O2A-C1
38	D	408	LHG	C28-C29-C30-C31
38	d	408	LHG	C28-C29-C30-C31
43	G	605	CHL	C2-C1-O2A-CGA
43	g	605	CHL	C2-C1-O2A-CGA
32	G	610	CLA	O1D-CGD-O2D-CED
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O1A-C1A-O1G-C1G
32	C	511	CLA	C4-C3-C5-C6
43	N	601	CHL	C4-C3-C5-C6
43	n	601	CHL	C4-C3-C5-C6
38	D	408	LHG	C11-C10-C9-C8
32	B	616	CLA	C12-C13-C15-C16
32	C	505	CLA	C2-C3-C5-C6
32	C	507	CLA	C12-C13-C15-C16
32	b	616	CLA	C12-C13-C15-C16
32	c	507	CLA	C12-C13-C15-C16
43	Y	607	CHL	C11-C10-C8-C7
43	y	607	CHL	C11-C10-C8-C7
32	n	612	CLA	CAA-CBA-CGA-O2A
38	d	409	LHG	C24-C23-O8-C6
37	c	523	DGD	CAA-CBA-CCA-CDA
38	L	101	LHG	O1-C1-C2-O2
38	l	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
42	z	2634	LMU	C1-C2-C3-C4
43	N	609	CHL	C2C-C3C-CAC-CBC
34	C	515	BCR	C19-C20-C21-C22
32	y	602	CLA	CBD-CGD-O2D-CED
32	b	613	CLA	C16-C17-C18-C20
37	C	520	DGD	CAA-CBA-CCA-CDA
42	Z	2634	LMU	C1-C2-C3-C4
43	n	609	CHL	C2C-C3C-CAC-CBC
37	c	520	DGD	C2A-C1A-O1G-C1G
37	C	523	DGD	CAA-CBA-CCA-CDA
35	A	412	SQD	C10-C11-C12-C13
38	d	408	LHG	C11-C10-C9-C8
32	R	604	CLA	O2A-C1-C2-C3
43	N	608	CHL	O2A-C1-C2-C3
43	n	608	CHL	O2A-C1-C2-C3
35	B	621	SQD	C14-C15-C16-C17
32	C	507	CLA	C2A-CAA-CBA-CGA
32	c	507	CLA	C2A-CAA-CBA-CGA
32	B	613	CLA	C16-C17-C18-C20
32	R	609	CLA	CAA-CBA-CGA-O2A
32	r	609	CLA	CAA-CBA-CGA-O2A
43	Y	605	CHL	CAA-CBA-CGA-O1A
43	y	605	CHL	CAA-CBA-CGA-O1A
32	c	503	CLA	CBA-CGA-O2A-C1
35	a	412	SQD	C10-C11-C12-C13
38	L	101	LHG	C28-C29-C30-C31
35	b	621	SQD	C7-C8-C9-C10
32	R	603	CLA	CAA-CBA-CGA-O2A
32	d	402	CLA	CAA-CBA-CGA-O2A
32	r	603	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	O7-C7-C8-C9
38	l	101	LHG	O7-C7-C8-C9
32	C	504	CLA	C4-C3-C5-C6
35	b	621	SQD	C14-C15-C16-C17
43	N	606	CHL	CAA-CBA-CGA-O2A
43	n	606	CHL	CAA-CBA-CGA-O2A
32	c	505	CLA	C2-C3-C5-C6
32	y	604	CLA	C2-C3-C5-C6
43	Y	609	CHL	C2-C3-C5-C6
43	y	609	CHL	C2-C3-C5-C6
32	A	405	CLA	C14-C13-C15-C16
32	B	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	a	405	CLA	C14-C13-C15-C16
32	b	609	CLA	C6-C7-C8-C9
32	c	502	CLA	C6-C7-C8-C9
43	N	601	CHL	C6-C7-C8-C9
43	N	605	CHL	C14-C13-C15-C16
43	n	601	CHL	C6-C7-C8-C9
43	n	605	CHL	C14-C13-C15-C16
35	B	621	SQD	C7-C8-C9-C10
32	B	608	CLA	C3A-C2A-CAA-CBA
32	G	613	CLA	C3A-C2A-CAA-CBA
32	b	608	CLA	C3A-C2A-CAA-CBA
32	g	613	CLA	C3A-C2A-CAA-CBA
33	a	408	PHO	C3A-C2A-CAA-CBA
43	N	601	CHL	C3A-C2A-CAA-CBA
43	n	601	CHL	C3A-C2A-CAA-CBA
32	c	503	CLA	O1A-CGA-O2A-C1
32	D	402	CLA	CAA-CBA-CGA-O2A
32	A	407	CLA	CAD-CBD-CGD-O2D
32	B	605	CLA	CAD-CBD-CGD-O2D
32	B	606	CLA	CAD-CBD-CGD-O2D
32	B	607	CLA	CAD-CBD-CGD-O2D
32	C	509	CLA	CAD-CBD-CGD-O2D
32	C	513	CLA	CAD-CBD-CGD-O2D
32	G	610	CLA	CAD-CBD-CGD-O2D
32	R	609	CLA	CAD-CBD-CGD-O2D
32	R	610	CLA	CAD-CBD-CGD-O2D
32	S	603	CLA	CAD-CBD-CGD-O2D
32	S	609	CLA	CAD-CBD-CGD-O2D
32	S	614	CLA	CAD-CBD-CGD-O2D
32	Y	603	CLA	CAD-CBD-CGD-O2D
32	a	407	CLA	CAD-CBD-CGD-O2D
32	b	605	CLA	CAD-CBD-CGD-O2D
32	b	606	CLA	CAD-CBD-CGD-O2D
32	b	607	CLA	CAD-CBD-CGD-O2D
32	c	503	CLA	CAD-CBD-CGD-O2D
32	c	509	CLA	CAD-CBD-CGD-O2D
32	c	513	CLA	CAD-CBD-CGD-O2D
32	g	610	CLA	CAD-CBD-CGD-O2D
32	r	609	CLA	CAD-CBD-CGD-O2D
32	r	610	CLA	CAD-CBD-CGD-O2D
32	s	603	CLA	CAD-CBD-CGD-O2D
32	s	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	y	603	CLA	CAD-CBD-CGD-O2D
43	S	601	CHL	CAD-CBD-CGD-O2D
43	s	601	CHL	CAD-CBD-CGD-O2D
32	G	603	CLA	C2A-CAA-CBA-CGA
35	A	412	SQD	O49-C7-O47-C45
35	a	412	SQD	O49-C7-O47-C45
43	N	606	CHL	CAA-CBA-CGA-O1A
43	R	608	CHL	CAA-CBA-CGA-O2A
43	n	606	CHL	CAA-CBA-CGA-O1A
43	r	608	CHL	CAA-CBA-CGA-O2A
37	c	524	DGD	CEA-CFA-CGA-CHA
38	l	101	LHG	C28-C29-C30-C31
32	B	603	CLA	CAA-CBA-CGA-O2A
35	A	412	SQD	O47-C7-C8-C9
37	c	518	DGD	O2G-C1B-C2B-C3B
36	H	102	LMG	C13-C14-C15-C16
37	C	524	DGD	CEA-CFA-CGA-CHA
32	c	504	CLA	C4-C3-C5-C6
43	n	607	CHL	C4-C3-C5-C6
32	B	609	CLA	C5-C6-C7-C8
32	Y	604	CLA	C2-C3-C5-C6
32	C	513	CLA	CAA-CBA-CGA-O2A
32	b	603	CLA	CAA-CBA-CGA-O2A
32	c	501	CLA	CAA-CBA-CGA-O2A
44	G	1621	LUT	C7-C8-C9-C10
44	g	1621	LUT	C7-C8-C9-C10
46	Y	1623	NEX	C11-C12-C13-C14
46	y	1623	NEX	C11-C12-C13-C14
45	R	624	XAT	O24-C26-C27-C28
45	r	624	XAT	O24-C26-C27-C28
46	N	1623	NEX	O24-C26-C27-C28
46	R	625	NEX	O24-C26-C27-C28
46	Y	1623	NEX	O24-C26-C27-C28
46	n	1623	NEX	O24-C26-C27-C28
46	r	625	NEX	O24-C26-C27-C28
46	y	1623	NEX	O24-C26-C27-C28
35	B	621	SQD	O49-C7-C8-C9
32	b	609	CLA	C5-C6-C7-C8
32	c	513	CLA	CAA-CBA-CGA-O2A
32	y	612	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	O2G-C1B-C2B-C3B
43	G	606	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
43	g	606	CHL	O2A-C1-C2-C3
32	R	609	CLA	CAA-CBA-CGA-O1A
32	r	609	CLA	CAA-CBA-CGA-O1A
43	S	601	CHL	CAA-CBA-CGA-O1A
43	s	601	CHL	CAA-CBA-CGA-O1A
43	N	601	CHL	O2A-C1-C2-C3
43	N	609	CHL	O2A-C1-C2-C3
43	Y	601	CHL	O2A-C1-C2-C3
43	Y	607	CHL	O2A-C1-C2-C3
43	n	601	CHL	O2A-C1-C2-C3
43	n	609	CHL	O2A-C1-C2-C3
43	y	601	CHL	O2A-C1-C2-C3
43	y	607	CHL	O2A-C1-C2-C3
43	y	609	CHL	O2A-C1-C2-C3
32	C	503	CLA	CBA-CGA-O2A-C1
32	B	613	CLA	CAA-CBA-CGA-O2A
32	Y	612	CLA	CAA-CBA-CGA-O2A
35	a	412	SQD	O47-C7-C8-C9
35	b	621	SQD	O49-C7-C8-C9
32	G	604	CLA	O1A-CGA-O2A-C1
32	g	604	CLA	O1A-CGA-O2A-C1
43	r	608	CHL	CAA-CBA-CGA-O1A
36	a	413	LMG	C29-C30-C31-C32
40	d	405	PL9	C32-C33-C34-C35
32	y	614	CLA	C5-C6-C7-C8
37	C	523	DGD	CAB-CBB-CCB-CDB
37	c	523	DGD	CAB-CBB-CCB-CDB
43	Y	607	CHL	O1A-CGA-O2A-C1
32	B	611	CLA	CHA-CBD-CGD-O2D
32	B	616	CLA	CHA-CBD-CGD-O1D
32	B	616	CLA	CHA-CBD-CGD-O2D
32	C	502	CLA	CHA-CBD-CGD-O1D
32	C	509	CLA	CHA-CBD-CGD-O1D
32	C	511	CLA	CHA-CBD-CGD-O1D
32	C	511	CLA	CHA-CBD-CGD-O2D
32	G	602	CLA	CHA-CBD-CGD-O1D
32	G	604	CLA	CHA-CBD-CGD-O1D
32	R	603	CLA	CHA-CBD-CGD-O1D
32	Y	602	CLA	CHA-CBD-CGD-O1D
32	Y	602	CLA	CHA-CBD-CGD-O2D
32	Y	612	CLA	CHA-CBD-CGD-O1D
32	Y	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	b	611	CLA	CHA-CBD-CGD-O2D
32	b	616	CLA	CHA-CBD-CGD-O1D
32	b	616	CLA	CHA-CBD-CGD-O2D
32	c	502	CLA	CHA-CBD-CGD-O1D
32	c	509	CLA	CHA-CBD-CGD-O1D
32	c	511	CLA	CHA-CBD-CGD-O1D
32	c	511	CLA	CHA-CBD-CGD-O2D
32	n	602	CLA	CHA-CBD-CGD-O2D
32	g	602	CLA	CHA-CBD-CGD-O1D
32	g	603	CLA	CHA-CBD-CGD-O2D
32	g	604	CLA	CHA-CBD-CGD-O1D
32	r	603	CLA	CHA-CBD-CGD-O1D
32	y	602	CLA	CHA-CBD-CGD-O1D
32	y	602	CLA	CHA-CBD-CGD-O2D
32	y	612	CLA	CHA-CBD-CGD-O1D
32	y	612	CLA	CHA-CBD-CGD-O2D
43	G	601	CHL	CHA-CBD-CGD-O1D
43	G	601	CHL	CHA-CBD-CGD-O2D
43	g	601	CHL	CHA-CBD-CGD-O1D
43	g	601	CHL	CHA-CBD-CGD-O2D
43	N	607	CHL	C4-C3-C5-C6
32	b	613	CLA	CAA-CBA-CGA-O2A
38	d	410	LHG	O8-C23-C24-C25
32	Y	614	CLA	C5-C6-C7-C8
43	R	608	CHL	CAA-CBA-CGA-O1A
36	A	413	LMG	C29-C30-C31-C32
32	C	509	CLA	C8-C10-C11-C12
32	C	512	CLA	CAA-CBA-CGA-O2A
32	c	512	CLA	CAA-CBA-CGA-O2A
32	C	503	CLA	O1A-CGA-O2A-C1
32	Y	612	CLA	C15-C16-C17-C18
32	c	509	CLA	C8-C10-C11-C12
32	y	612	CLA	C15-C16-C17-C18
43	y	607	CHL	O1A-CGA-O2A-C1
32	B	614	CLA	CAA-CBA-CGA-O2A
32	b	614	CLA	CAA-CBA-CGA-O2A
32	n	603	CLA	CAA-CBA-CGA-O2A
36	D	411	LMG	O7-C10-C11-C12
36	c	521	LMG	O7-C10-C11-C12
36	d	411	LMG	O7-C10-C11-C12
38	D	410	LHG	O8-C23-C24-C25
43	y	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	C	524	DGD	CDA-CEA-CFA-CGA
32	A	405	CLA	C2A-CAA-CBA-CGA
32	a	405	CLA	C2A-CAA-CBA-CGA
33	a	409	PHO	CHA-CBD-CGD-O1D
33	a	409	PHO	CHA-CBD-CGD-O2D
36	A	413	LMG	C14-C15-C16-C17
38	Y	2630	LHG	C29-C30-C31-C32
35	A	412	SQD	C8-C7-O47-C45
32	C	501	CLA	CAA-CBA-CGA-O2A
32	N	603	CLA	CAA-CBA-CGA-O2A
32	g	614	CLA	CAA-CBA-CGA-O2A
36	C	521	LMG	O7-C10-C11-C12
38	Y	2630	LHG	O8-C23-C24-C25
38	y	2630	LHG	O8-C23-C24-C25
36	h	102	LMG	C36-C37-C38-C39
40	D	405	PL9	C32-C33-C34-C35
32	C	513	CLA	C12-C13-C15-C16
32	c	513	CLA	C12-C13-C15-C16
32	G	610	CLA	C16-C17-C18-C19
36	H	102	LMG	C36-C37-C38-C39
38	y	2630	LHG	C29-C30-C31-C32
32	Y	602	CLA	O1D-CGD-O2D-CED
32	B	603	CLA	C15-C16-C17-C18
32	G	614	CLA	CAA-CBA-CGA-O2A
37	c	518	DGD	C3B-C4B-C5B-C6B
32	C	508	CLA	C6-C7-C8-C9
32	Y	612	CLA	C6-C7-C8-C9
32	b	603	CLA	C6-C7-C8-C9
32	c	508	CLA	C6-C7-C8-C9
32	c	510	CLA	C6-C7-C8-C9
32	y	612	CLA	C6-C7-C8-C9
38	l	101	LHG	O9-C7-C8-C9
32	c	509	CLA	C13-C15-C16-C17
32	G	604	CLA	CBA-CGA-O2A-C1
32	g	604	CLA	CBA-CGA-O2A-C1
32	C	509	CLA	C13-C15-C16-C17
43	Y	606	CHL	CAA-CBA-CGA-O2A
35	B	621	SQD	C5-C6-S-O8
35	b	621	SQD	C5-C6-S-O8
32	g	610	CLA	C16-C17-C18-C19
35	a	412	SQD	C8-C7-O47-C45
36	A	413	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
36	a	413	LMG	C11-C10-O7-C8
32	N	612	CLA	CAA-CBA-CGA-O1A
32	n	612	CLA	CAA-CBA-CGA-O1A
32	C	513	CLA	CAA-CBA-CGA-O1A
32	y	602	CLA	O1D-CGD-O2D-CED
37	C	518	DGD	C3B-C4B-C5B-C6B
36	a	413	LMG	C14-C15-C16-C17
37	c	524	DGD	CDA-CEA-CFA-CGA
32	d	402	CLA	CAA-CBA-CGA-O1A
33	a	408	PHO	C8-C10-C11-C12
38	l	101	LHG	O10-C23-O8-C6
42	z	2635	LMU	C1-C2-C3-C4
32	c	513	CLA	CAA-CBA-CGA-O1A
38	L	101	LHG	O9-C7-C8-C9
32	B	606	CLA	C1A-C2A-CAA-CBA
32	B	608	CLA	C1A-C2A-CAA-CBA
32	C	512	CLA	C1A-C2A-CAA-CBA
32	N	604	CLA	C1A-C2A-CAA-CBA
32	G	613	CLA	C1A-C2A-CAA-CBA
32	R	602	CLA	C1A-C2A-CAA-CBA
32	Y	602	CLA	C1A-C2A-CAA-CBA
32	b	606	CLA	C1A-C2A-CAA-CBA
32	b	608	CLA	C1A-C2A-CAA-CBA
32	c	512	CLA	C1A-C2A-CAA-CBA
32	g	613	CLA	C1A-C2A-CAA-CBA
32	r	602	CLA	C1A-C2A-CAA-CBA
32	y	602	CLA	C1A-C2A-CAA-CBA
43	N	601	CHL	C1A-C2A-CAA-CBA
43	Y	607	CHL	C1A-C2A-CAA-CBA
43	n	601	CHL	C1A-C2A-CAA-CBA
43	y	607	CHL	C1A-C2A-CAA-CBA
32	r	603	CLA	CAA-CBA-CGA-O1A
38	L	101	LHG	O10-C23-O8-C6
38	y	2630	LHG	C18-C19-C20-C21
32	D	402	CLA	CAA-CBA-CGA-O1A
32	R	603	CLA	CAA-CBA-CGA-O1A
32	b	603	CLA	CAA-CBA-CGA-O1A
38	g	2630	LHG	C18-C19-C20-C21
32	G	610	CLA	C2A-CAA-CBA-CGA
32	g	610	CLA	C2A-CAA-CBA-CGA
36	A	413	LMG	C35-C36-C37-C38
35	a	412	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	B	616	CLA	C10-C11-C12-C13
32	y	612	CLA	C8-C10-C11-C12
32	Y	612	CLA	C8-C10-C11-C12
32	C	501	CLA	CAA-CBA-CGA-O1A
36	A	413	LMG	C2-C1-O1-C7
36	a	413	LMG	C2-C1-O1-C7
38	N	2630	LHG	C3-O3-P-O5
38	d	410	LHG	C3-O3-P-O4
38	n	2630	LHG	C3-O3-P-O5
38	s	2630	LHG	C3-O3-P-O4
32	B	603	CLA	CAA-CBA-CGA-O1A
32	Y	612	CLA	CAA-CBA-CGA-O1A
32	y	612	CLA	CAA-CBA-CGA-O1A
35	A	412	SQD	O49-C7-C8-C9
32	G	604	CLA	O2A-C1-C2-C3
32	S	610	CLA	O2A-C1-C2-C3
32	g	604	CLA	O2A-C1-C2-C3
32	s	610	CLA	O2A-C1-C2-C3
43	G	607	CHL	O2A-C1-C2-C3
37	c	519	DGD	O6E-C1E-O5D-C6D
38	N	2630	LHG	O6-C4-C5-C6
38	n	2630	LHG	O6-C4-C5-C6
36	a	413	LMG	C35-C36-C37-C38
37	C	518	DGD	C5A-C6A-C7A-C8A
32	b	616	CLA	C3-C5-C6-C7
42	Z	2635	LMU	C1-C2-C3-C4
32	B	614	CLA	CAA-CBA-CGA-O1A
32	c	501	CLA	CAA-CBA-CGA-O1A
32	c	512	CLA	CAA-CBA-CGA-O1A
38	D	410	LHG	O10-C23-C24-C25
38	d	410	LHG	O10-C23-C24-C25
32	C	510	CLA	CAA-CBA-CGA-O2A
32	c	510	CLA	CAA-CBA-CGA-O2A
43	N	605	CHL	CAA-CBA-CGA-O2A
43	n	605	CHL	CAA-CBA-CGA-O2A
43	y	609	CHL	C2C-C3C-CAC-CBC
32	b	616	CLA	C10-C11-C12-C13
32	R	602	CLA	C2A-CAA-CBA-CGA
32	r	602	CLA	C2A-CAA-CBA-CGA
32	C	512	CLA	CAA-CBA-CGA-O1A
32	b	614	CLA	CAA-CBA-CGA-O1A
32	B	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	b	603	CLA	C15-C16-C17-C18
32	n	613	CLA	C8-C10-C11-C12
33	A	408	PHO	C8-C10-C11-C12
32	C	505	CLA	C4C-C3C-CAC-CBC
38	d	409	LHG	O8-C23-C24-C25
32	B	617	CLA	C5-C6-C7-C8
32	N	613	CLA	C8-C10-C11-C12
32	b	604	CLA	C13-C15-C16-C17
32	b	617	CLA	C5-C6-C7-C8
37	c	518	DGD	O1B-C1B-C2B-C3B
38	Y	2630	LHG	O10-C23-C24-C25
38	y	2630	LHG	O10-C23-C24-C25
38	G	2630	LHG	C18-C19-C20-C21
32	B	616	CLA	CAD-CBD-CGD-O1D
32	C	502	CLA	CAD-CBD-CGD-O1D
32	C	509	CLA	CAD-CBD-CGD-O1D
32	C	511	CLA	CAD-CBD-CGD-O1D
32	G	604	CLA	CAD-CBD-CGD-O1D
32	G	611	CLA	CAD-CBD-CGD-O1D
32	c	502	CLA	CAD-CBD-CGD-O1D
32	c	509	CLA	CAD-CBD-CGD-O1D
32	c	511	CLA	CAD-CBD-CGD-O1D
32	g	604	CLA	CAD-CBD-CGD-O1D
32	g	611	CLA	CAD-CBD-CGD-O1D
32	N	603	CLA	CAA-CBA-CGA-O1A
32	G	614	CLA	CAA-CBA-CGA-O1A
32	n	603	CLA	CAA-CBA-CGA-O1A
36	C	521	LMG	O9-C10-C11-C12
36	c	521	LMG	O9-C10-C11-C12
37	C	518	DGD	O1B-C1B-C2B-C3B
32	B	603	CLA	C6-C7-C8-C9
32	Y	604	CLA	C11-C12-C13-C14
32	Y	604	CLA	C14-C13-C15-C16
32	y	604	CLA	C14-C13-C15-C16
33	a	408	PHO	C11-C10-C8-C9
32	c	505	CLA	C4C-C3C-CAC-CBC
32	g	614	CLA	CAA-CBA-CGA-O1A
43	Y	609	CHL	C2C-C3C-CAC-CBC
32	B	616	CLA	C3-C5-C6-C7
32	B	602	CLA	CAA-CBA-CGA-O2A
32	b	602	CLA	CAA-CBA-CGA-O2A
32	y	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	H	102	LMG	C14-C15-C16-C17
37	c	519	DGD	C5B-C6B-C7B-C8B
38	Y	2630	LHG	C18-C19-C20-C21
32	B	611	CLA	CAA-CBA-CGA-O2A
32	Y	602	CLA	CAA-CBA-CGA-O2A
32	b	611	CLA	CAA-CBA-CGA-O2A
37	C	520	DGD	O1G-C1A-C2A-C3A
37	c	520	DGD	O1G-C1A-C2A-C3A
38	D	409	LHG	O8-C23-C24-C25
38	D	409	LHG	O10-C23-O8-C6
37	C	519	DGD	C5B-C6B-C7B-C8B
38	d	408	LHG	C27-C28-C29-C30
32	b	613	CLA	CAA-CBA-CGA-O1A
36	A	413	LMG	C13-C14-C15-C16
32	Y	613	CLA	C4-C3-C5-C6
32	c	511	CLA	C4-C3-C5-C6
32	y	613	CLA	C4-C3-C5-C6
43	n	607	CHL	C10-C11-C12-C13
32	B	603	CLA	C6-C7-C8-C10
32	B	608	CLA	C12-C13-C15-C16
32	C	509	CLA	C11-C12-C13-C15
32	C	512	CLA	C3A-C2A-CAA-CBA
32	b	603	CLA	C6-C7-C8-C10
32	b	608	CLA	C12-C13-C15-C16
32	c	509	CLA	C11-C12-C13-C15
32	c	512	CLA	C3A-C2A-CAA-CBA
38	G	2630	LHG	O6-C4-C5-O7
38	g	2630	LHG	O6-C4-C5-O7
43	N	609	CHL	C11-C10-C8-C7
43	n	609	CHL	C11-C10-C8-C7
32	B	613	CLA	CAA-CBA-CGA-O1A
36	D	411	LMG	O9-C10-C11-C12
36	d	411	LMG	O9-C10-C11-C12
38	D	408	LHG	C27-C28-C29-C30
32	N	602	CLA	CAA-CBA-CGA-O2A
32	N	611	CLA	CAA-CBA-CGA-O2A
32	Y	613	CLA	CAA-CBA-CGA-O2A
32	n	611	CLA	CAA-CBA-CGA-O2A
32	y	613	CLA	CAA-CBA-CGA-O2A
43	S	607	CHL	CBD-CGD-O2D-CED
43	g	607	CHL	O2A-C1-C2-C3
35	B	621	SQD	C11-C10-C9-C8

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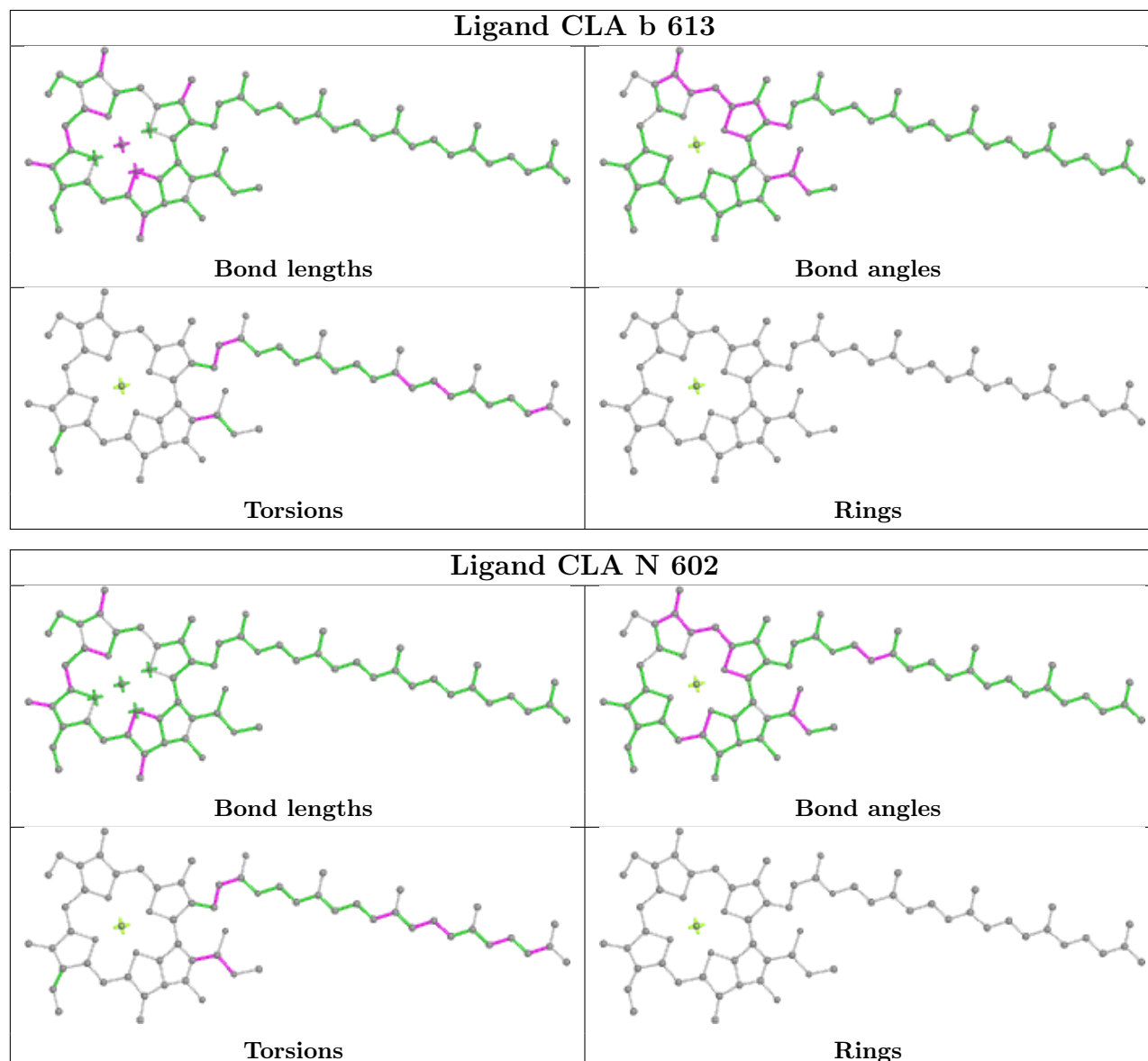
Mol	Chain	Res	Type	Atoms
32	C	510	CLA	CAA-CBA-CGA-O1A
32	n	611	CLA	CAA-CBA-CGA-O1A
38	d	409	LHG	O10-C23-C24-C25
46	G	1623	NEX	C13-C14-C15-C35
46	y	1623	NEX	C9-C10-C11-C12
42	Z	2634	LMU	C2-C1-O1'-C1'
42	z	2634	LMU	C2-C1-O1'-C1'
38	S	2630	LHG	C10-C11-C12-C13
43	N	607	CHL	C10-C11-C12-C13
32	Y	602	CLA	CAA-CBA-CGA-O1A
32	c	510	CLA	CAA-CBA-CGA-O1A
38	D	409	LHG	O10-C23-C24-C25
32	b	615	CLA	CBA-CGA-O2A-C1
36	B	622	LMG	C29-C28-O8-C9
36	b	622	LMG	C29-C28-O8-C9
36	a	413	LMG	C13-C14-C15-C16
37	c	519	DGD	C4A-C5A-C6A-C7A
38	s	2630	LHG	C10-C11-C12-C13
38	N	2630	LHG	O8-C23-C24-C25
32	N	611	CLA	CAA-CBA-CGA-O1A
32	y	602	CLA	CAA-CBA-CGA-O1A
43	Y	606	CHL	CAA-CBA-CGA-O1A
43	y	606	CHL	CAA-CBA-CGA-O1A
32	B	613	CLA	C2A-CAA-CBA-CGA
32	b	613	CLA	C2A-CAA-CBA-CGA
35	b	621	SQD	C11-C10-C9-C8
37	c	519	DGD	C2A-C3A-C4A-C5A
32	B	615	CLA	CBA-CGA-O2A-C1
32	n	602	CLA	CAA-CBA-CGA-O2A
32	n	614	CLA	CAA-CBA-CGA-O2A
38	d	408	LHG	O8-C23-C24-C25
38	n	2630	LHG	O8-C23-C24-C25

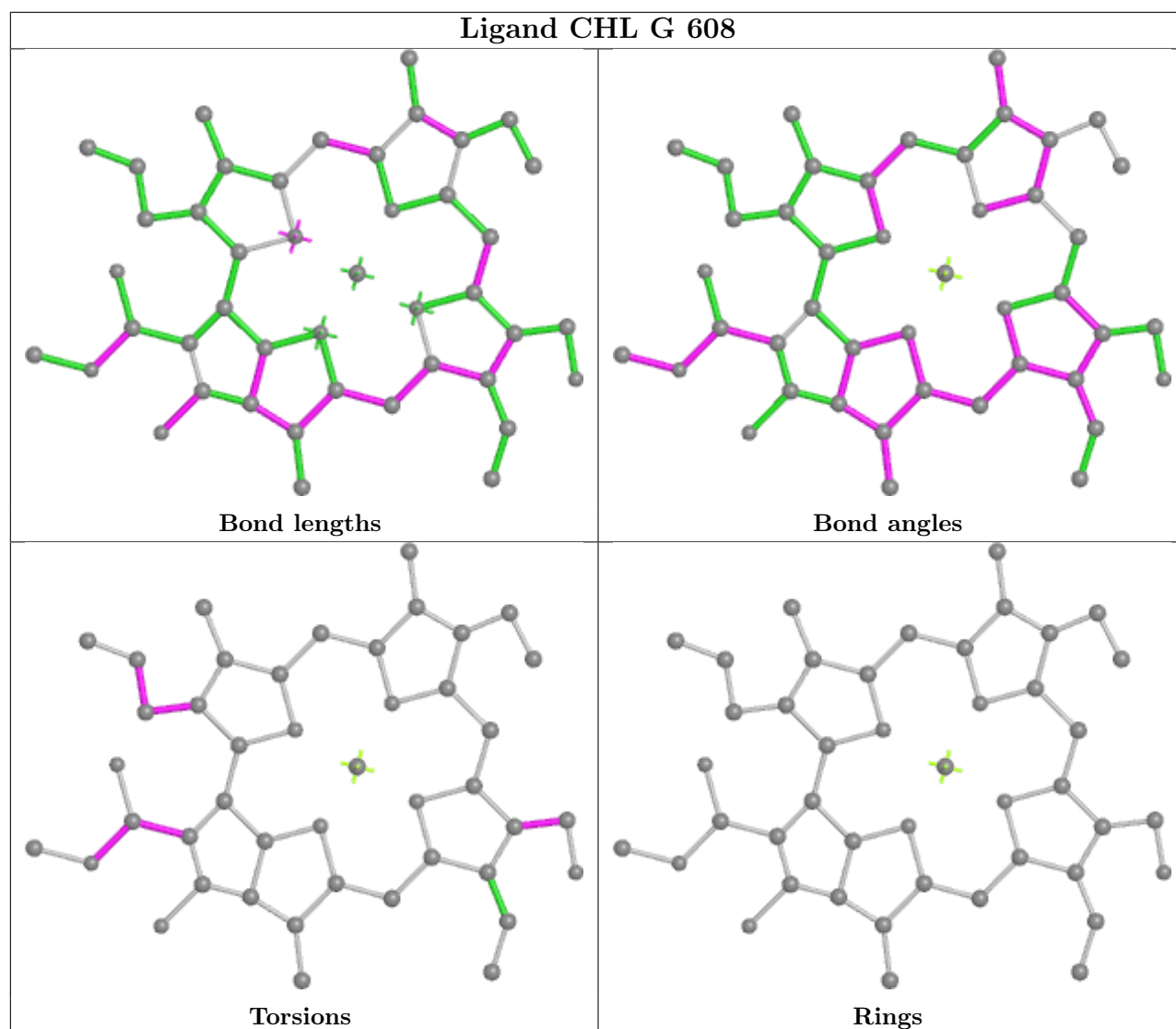
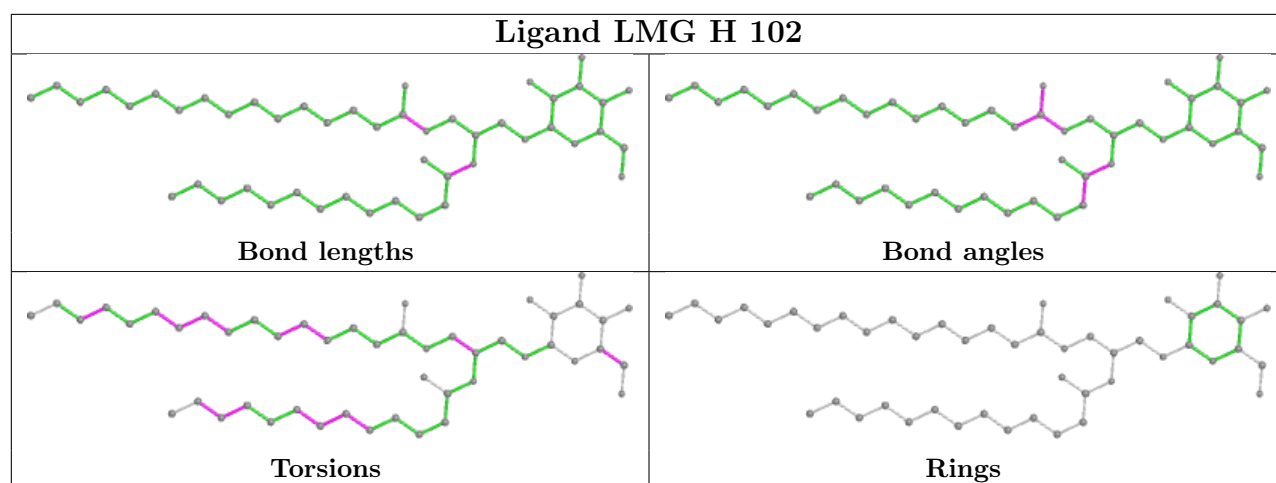
There are no ring outliers.

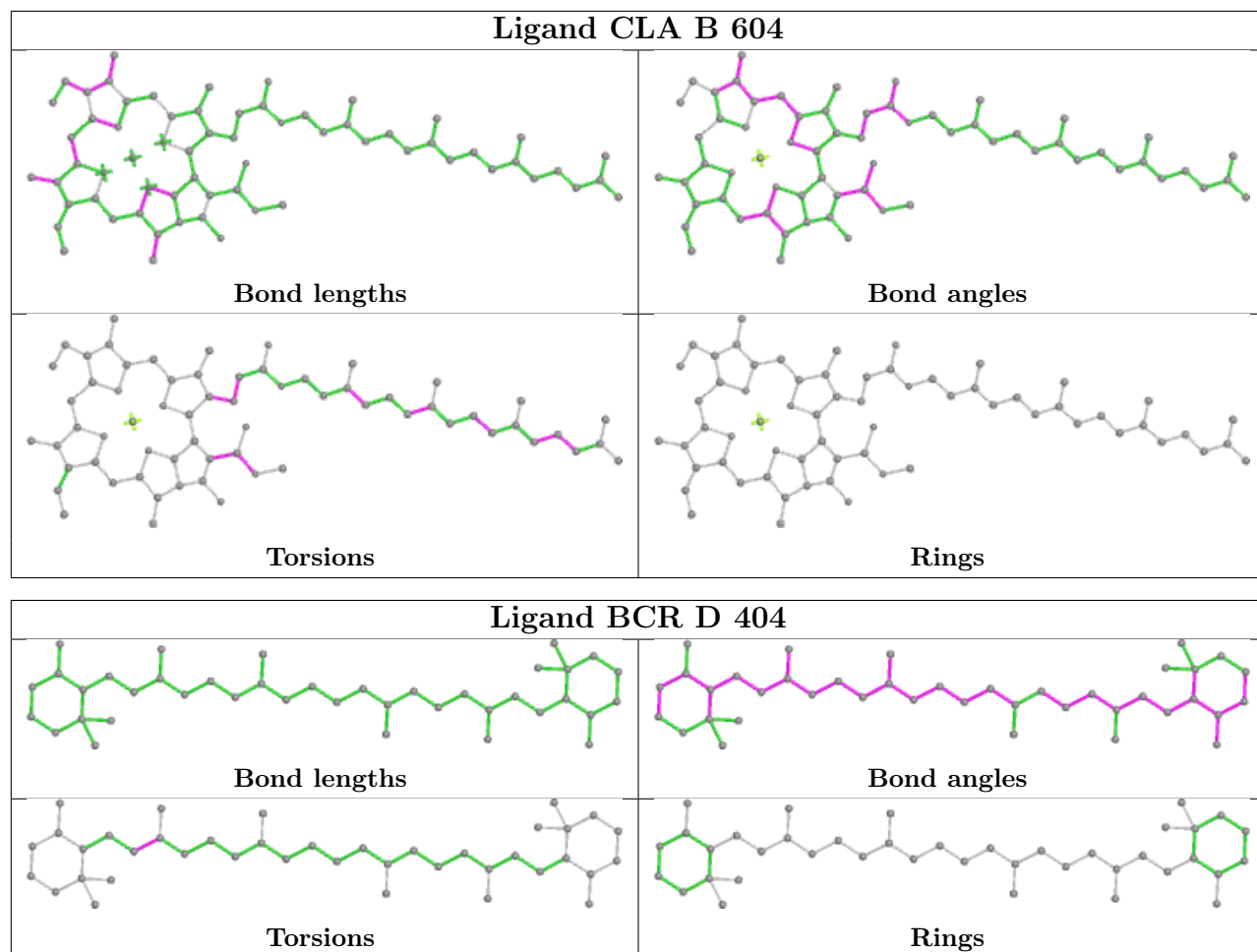
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

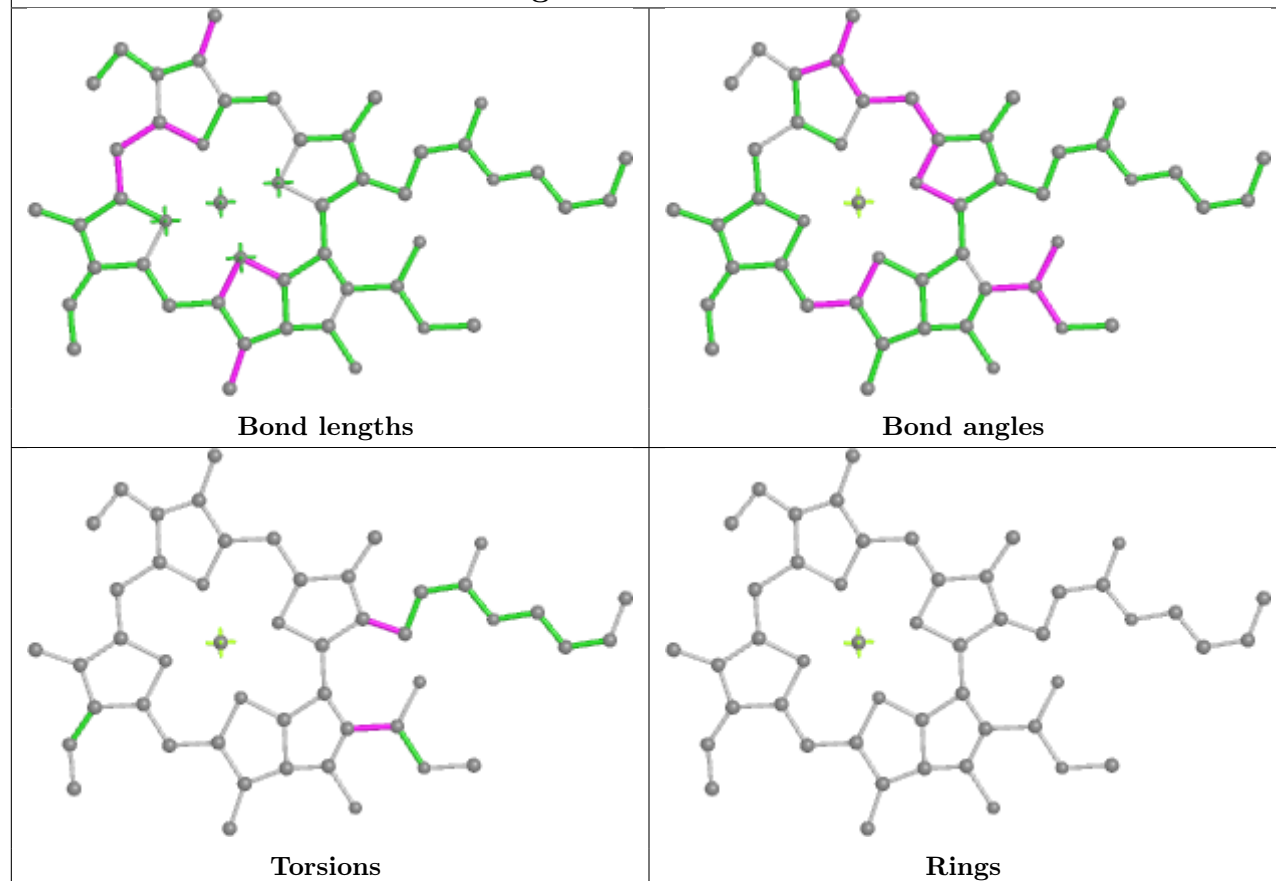
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



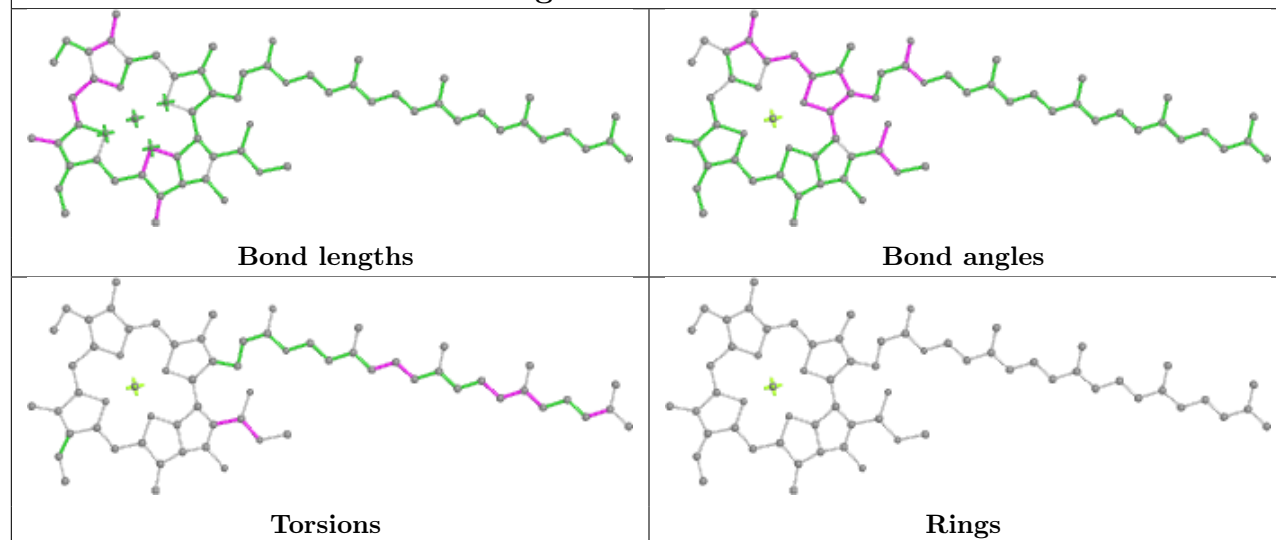




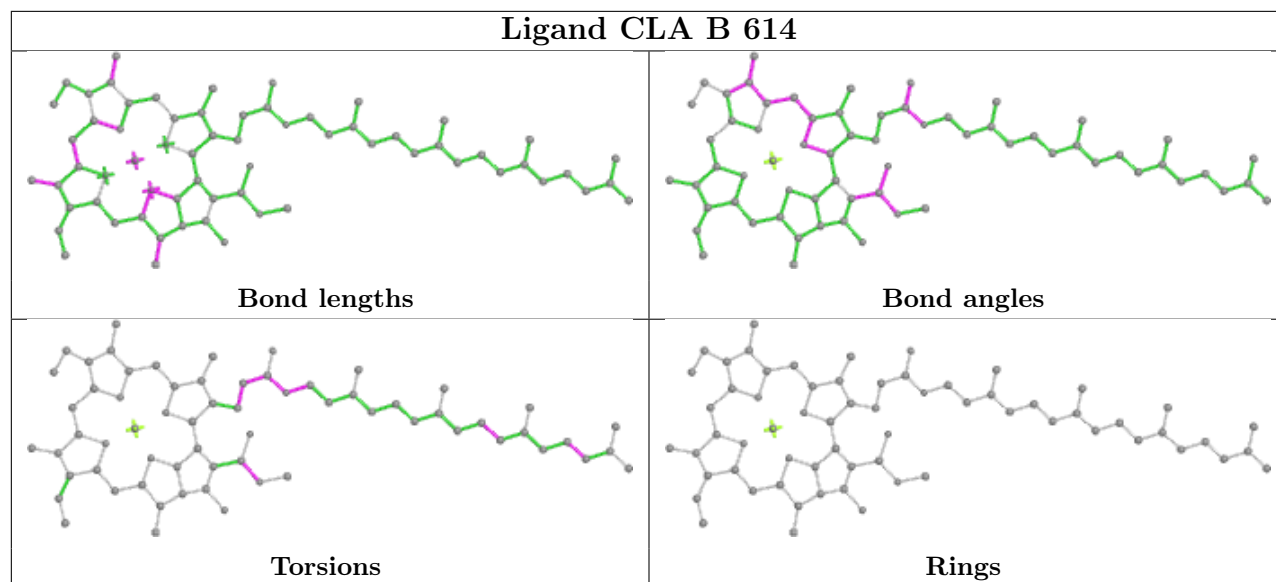
Ligand CLA A 407



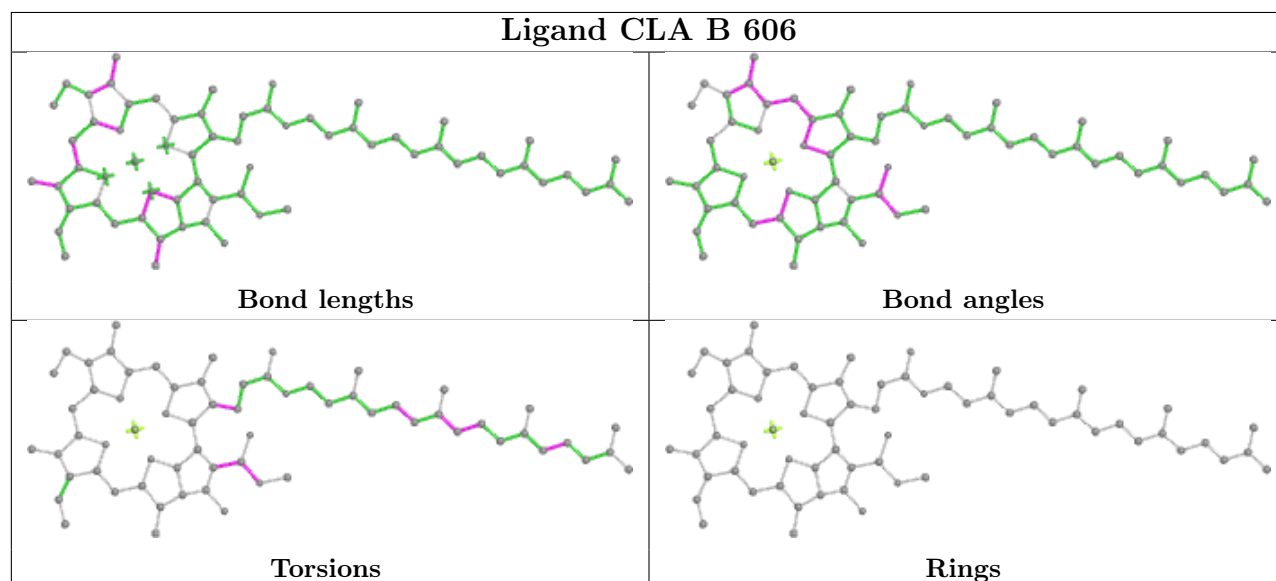
Ligand CLA b 616



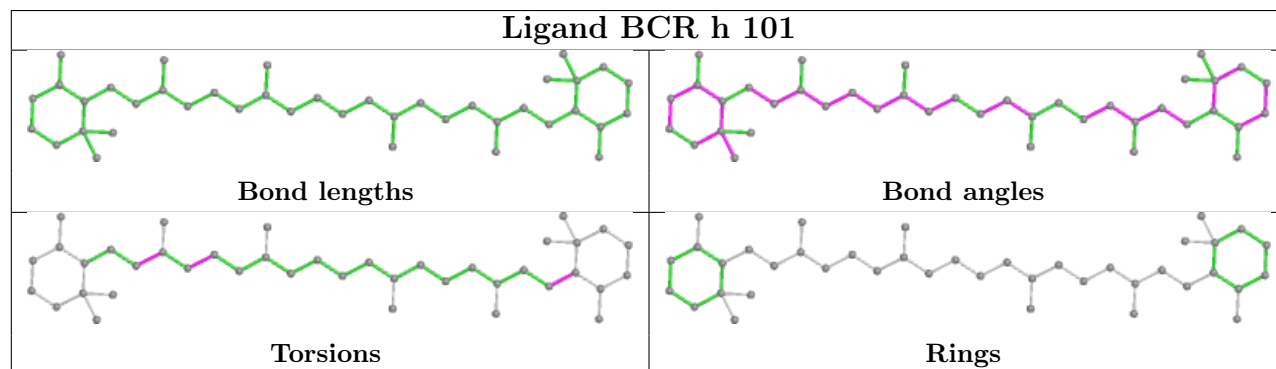
Ligand CLA B 614

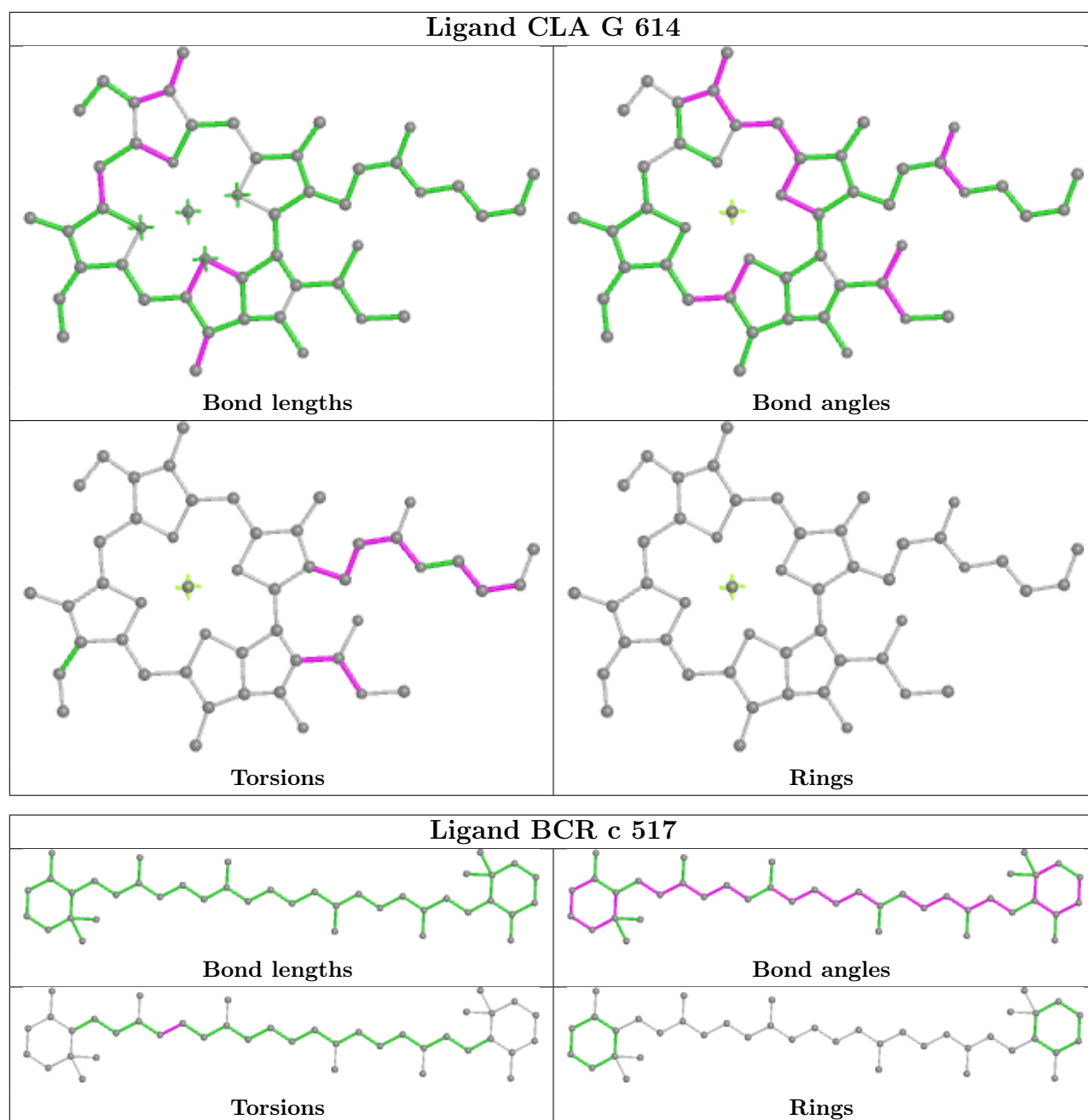


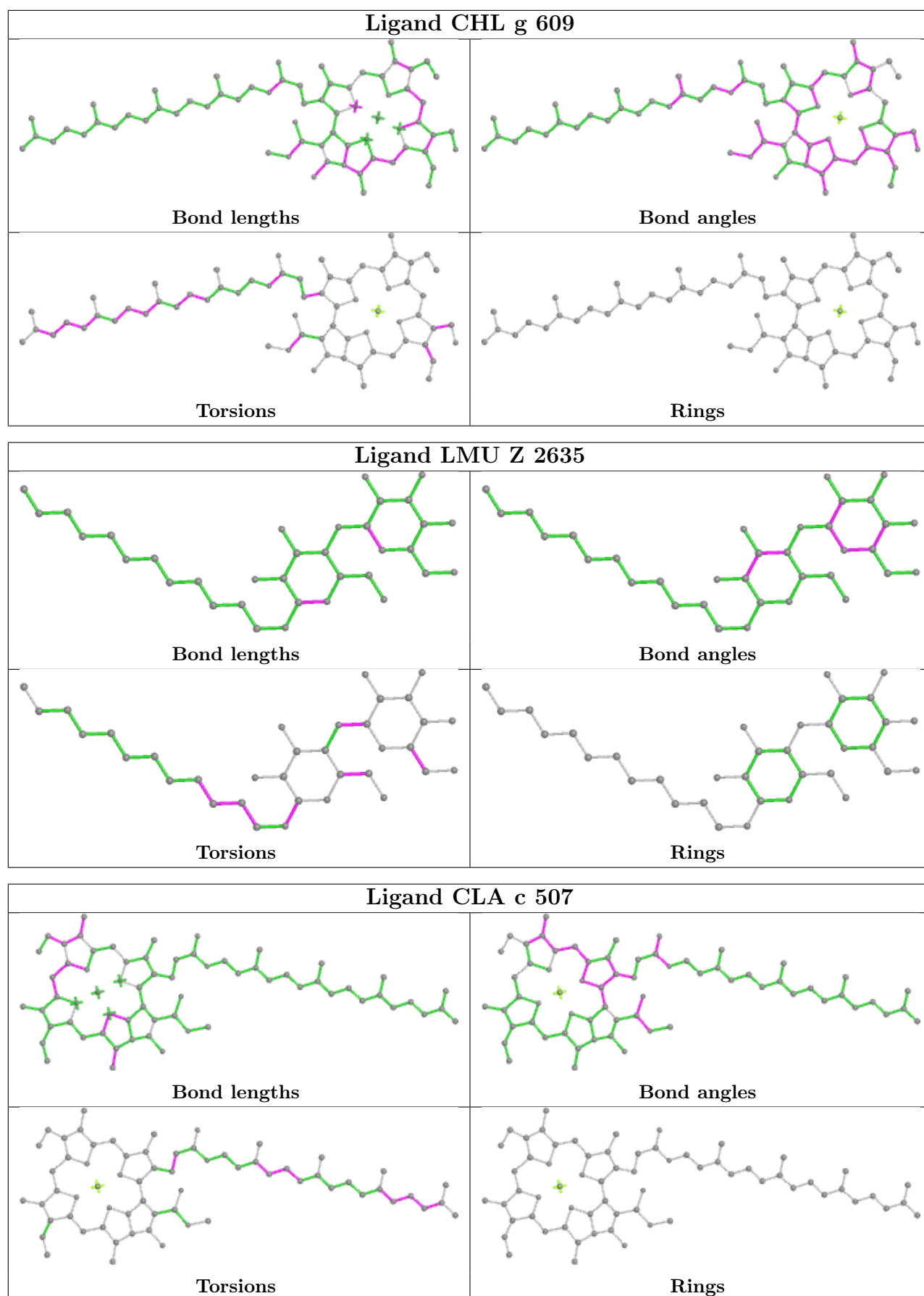
Ligand CLA B 606



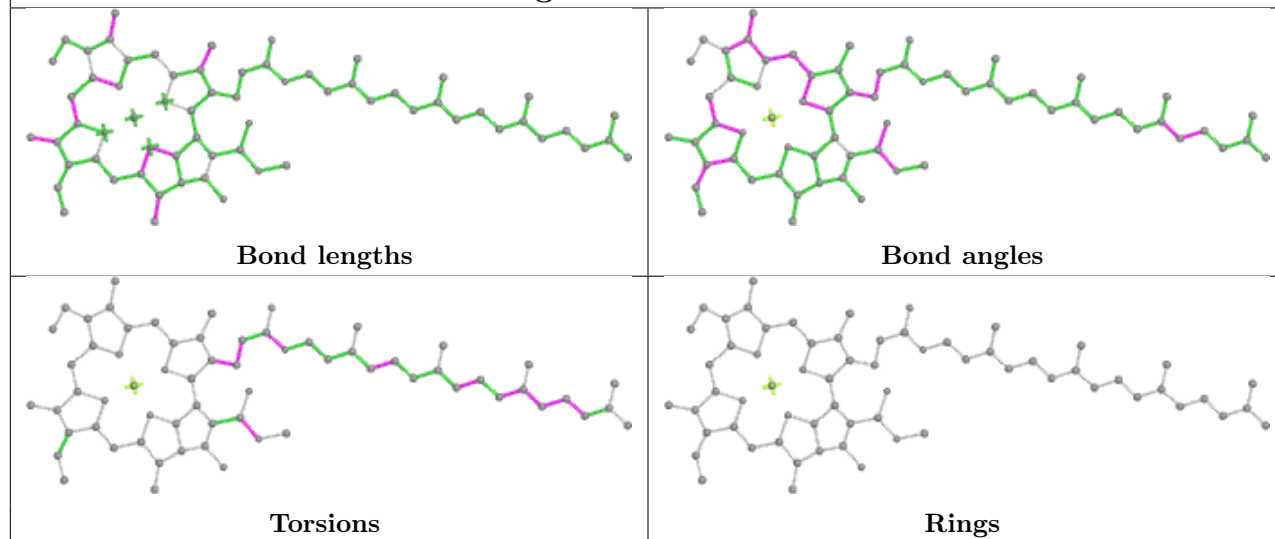
Ligand BCR h 101



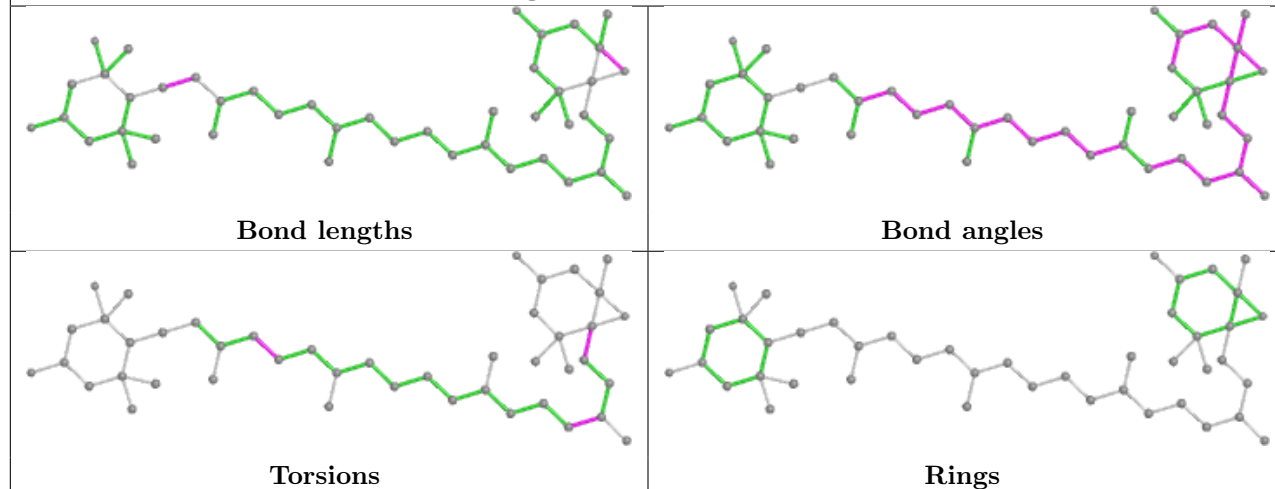




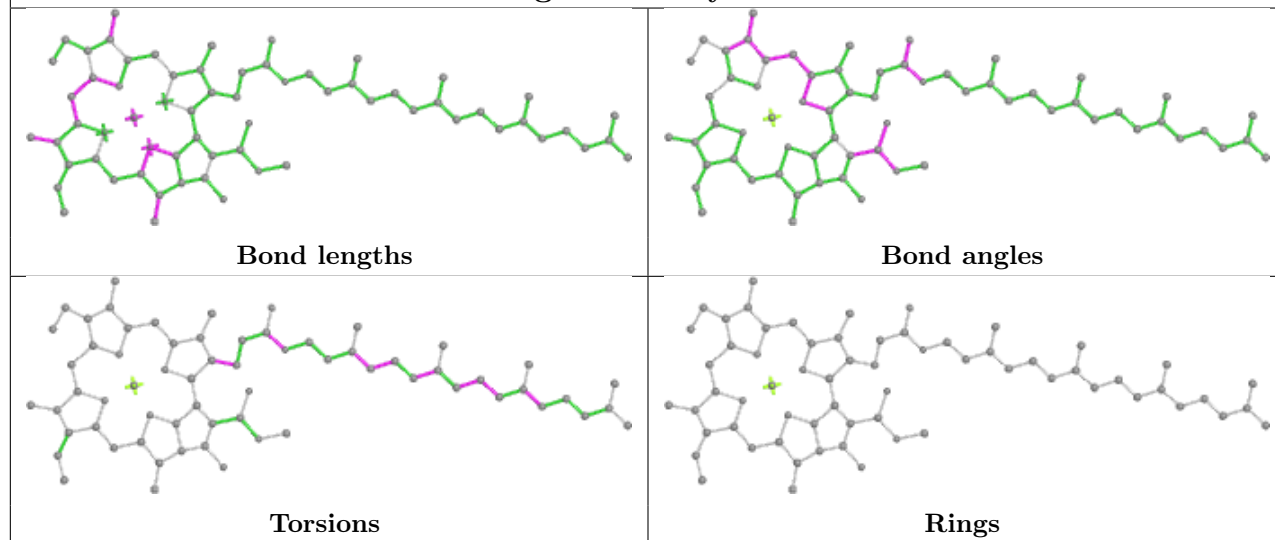
Ligand CLA a 405

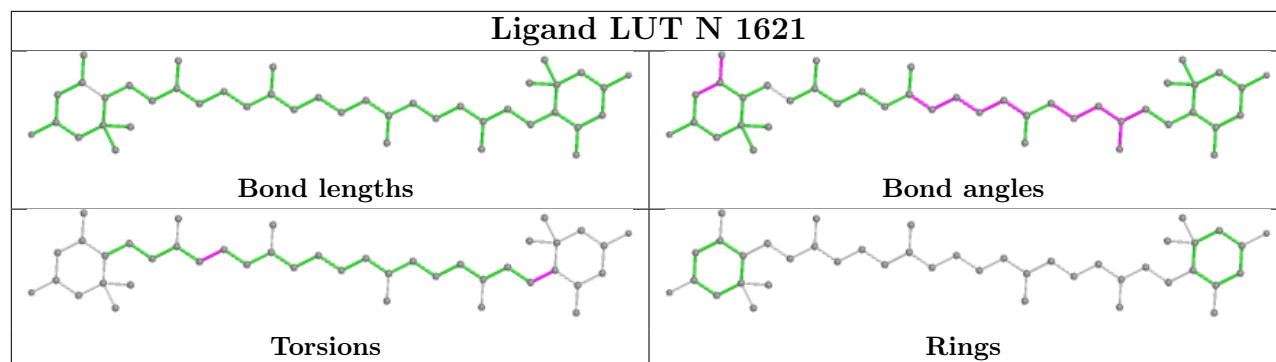
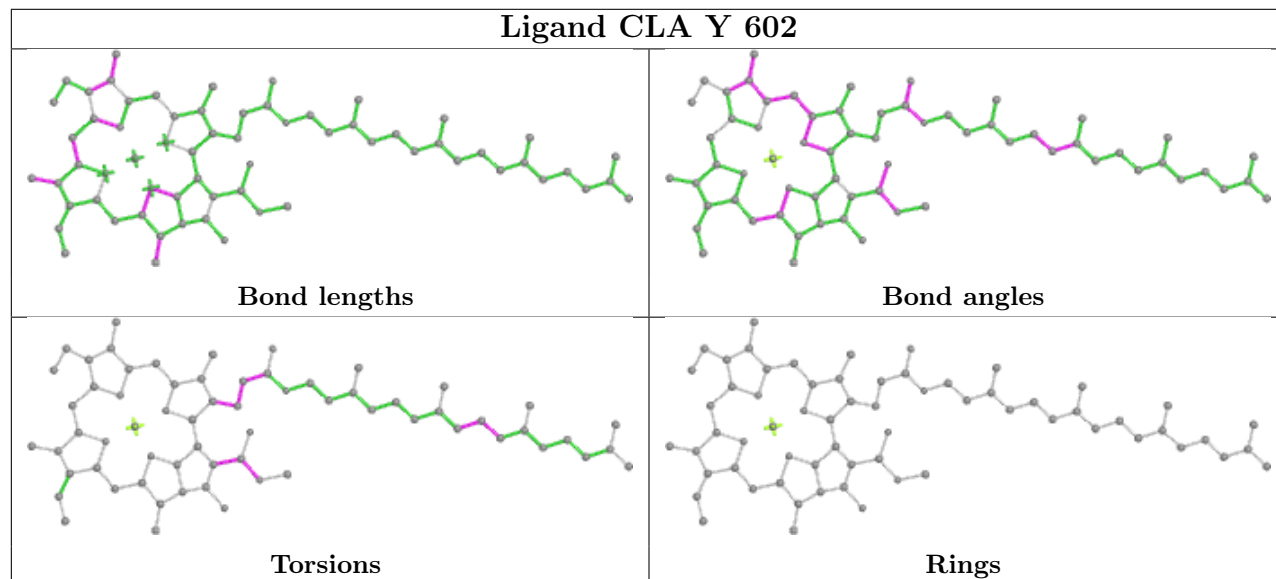
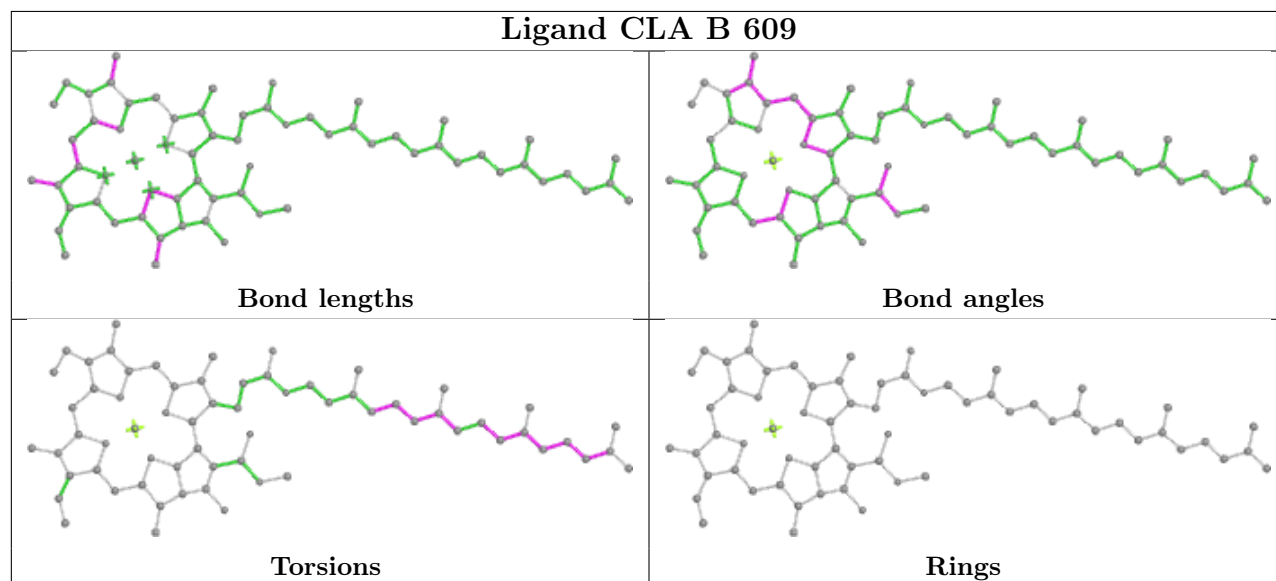


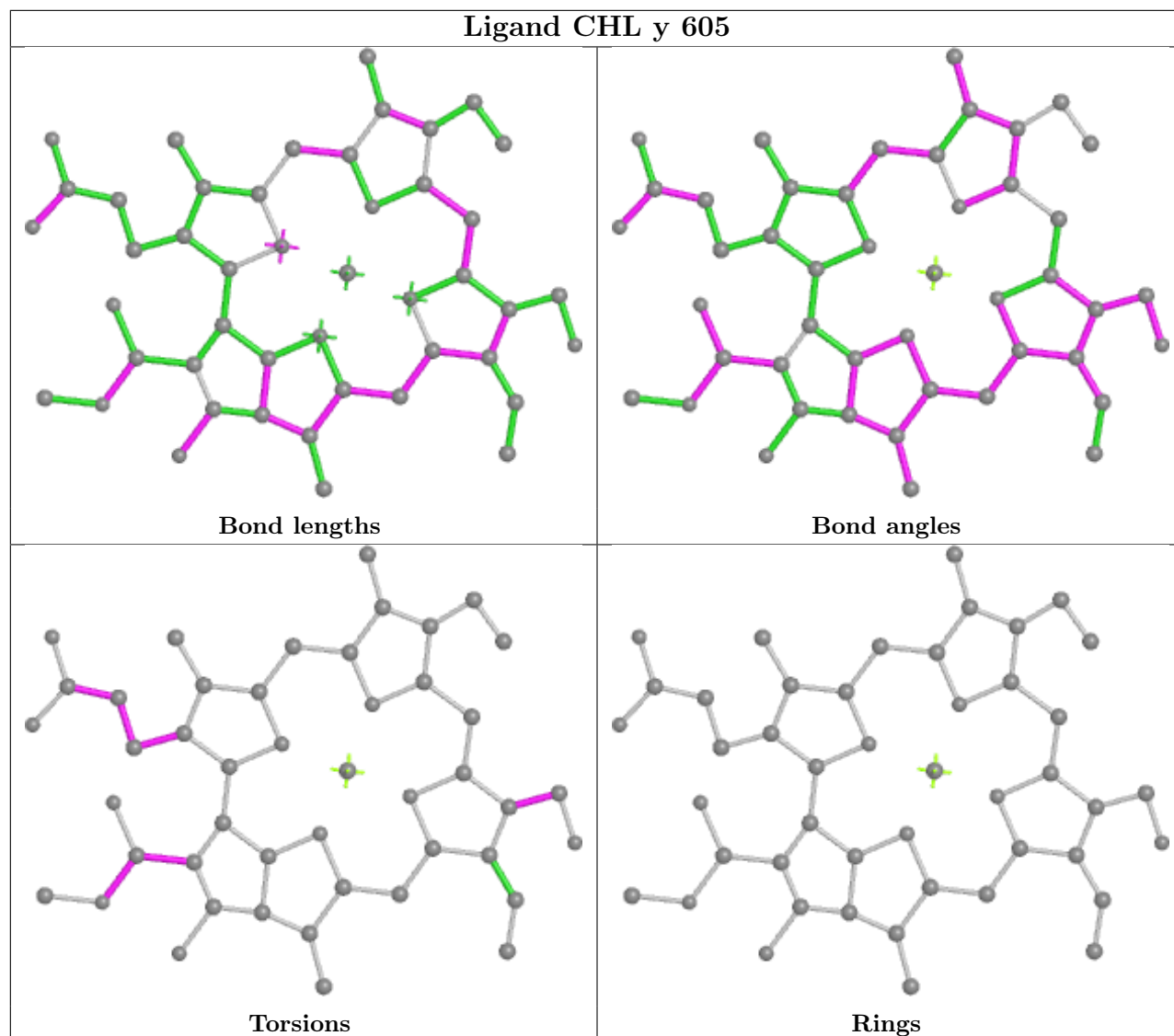
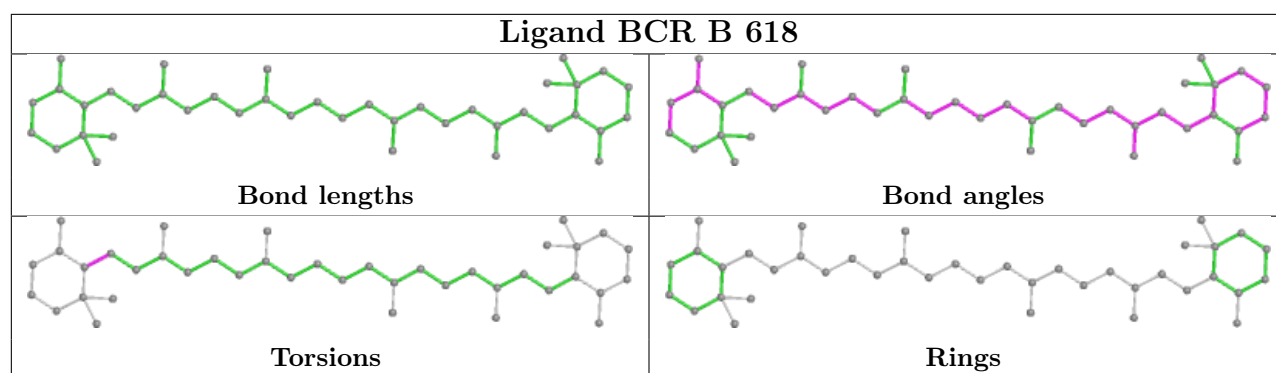
Ligand NEX n 1623

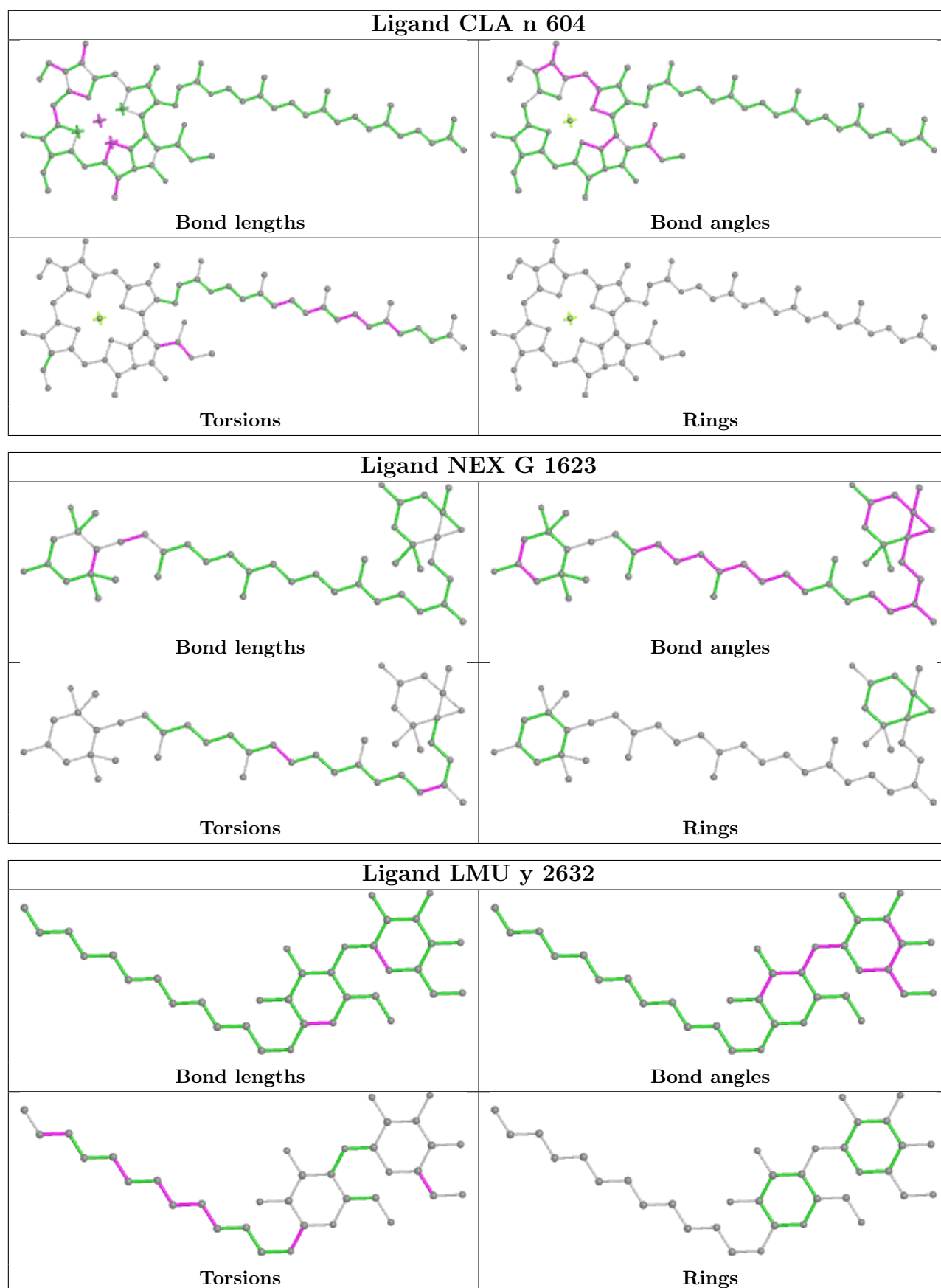


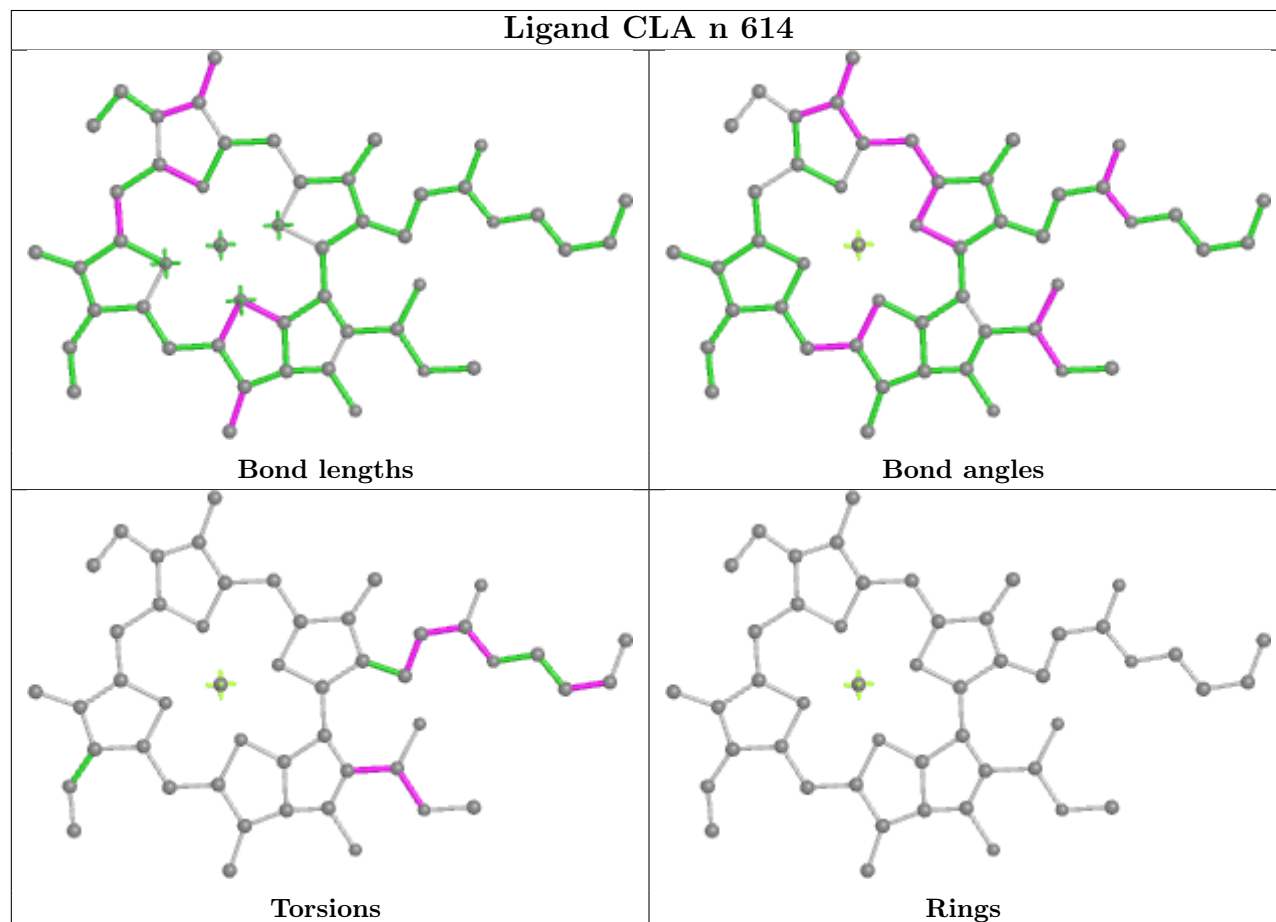
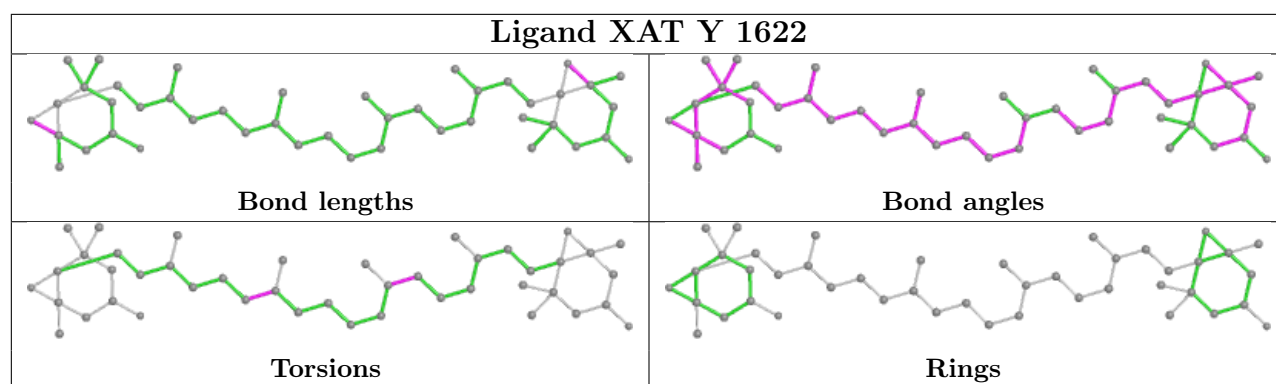
Ligand CLA y 611



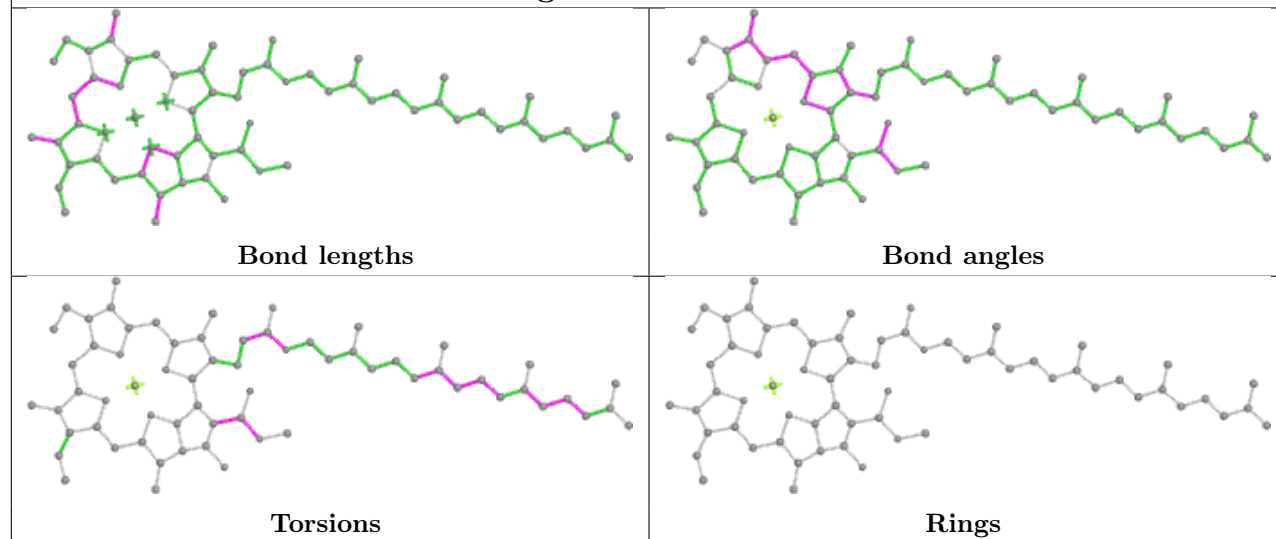
Ligand LUT N 1621**Ligand CLA Y 602****Ligand CLA B 609**



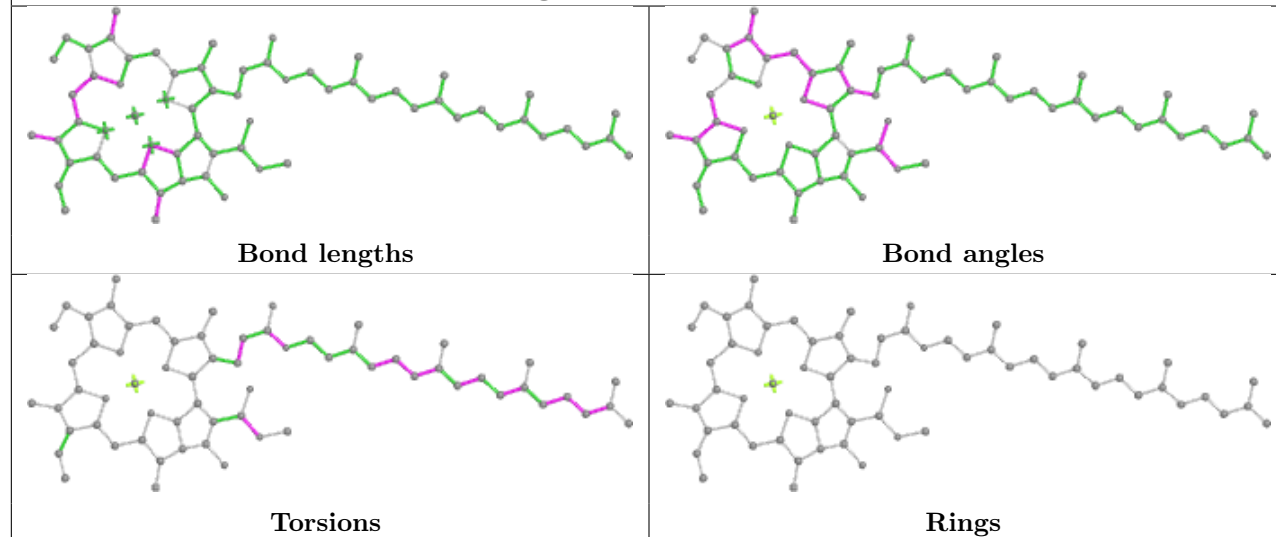




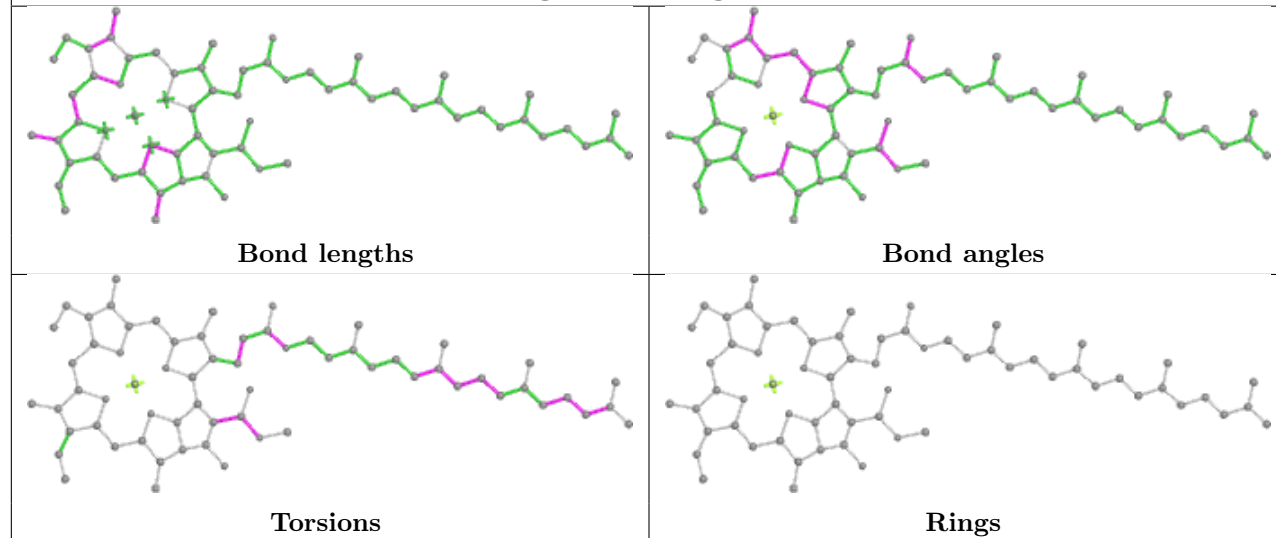
Ligand CLA c 510



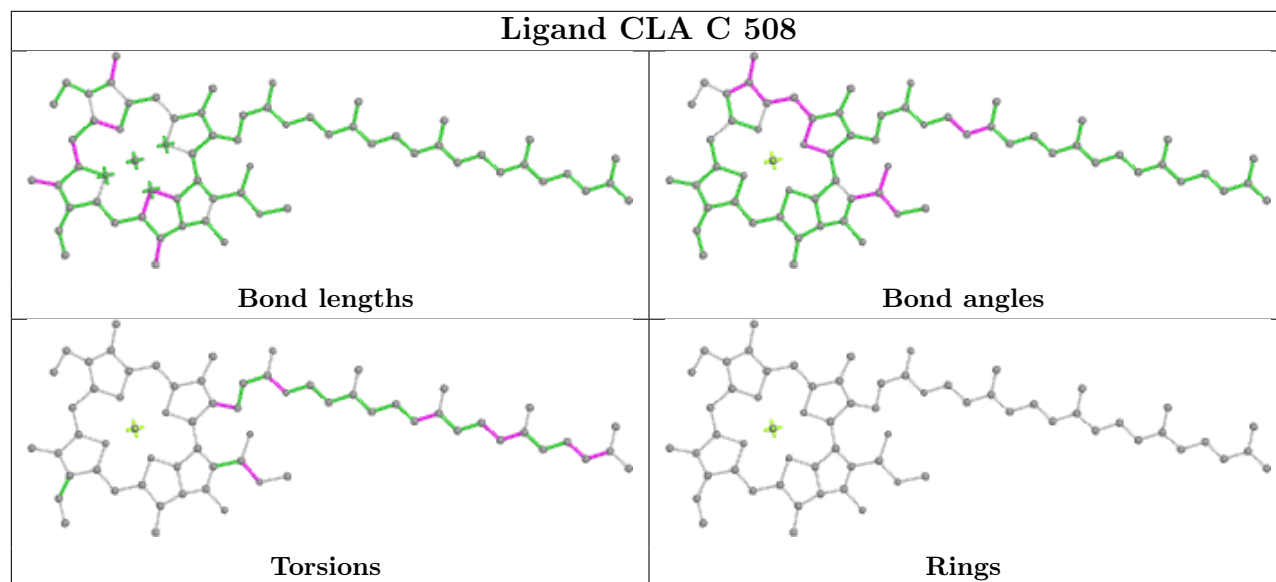
Ligand CLA b 617



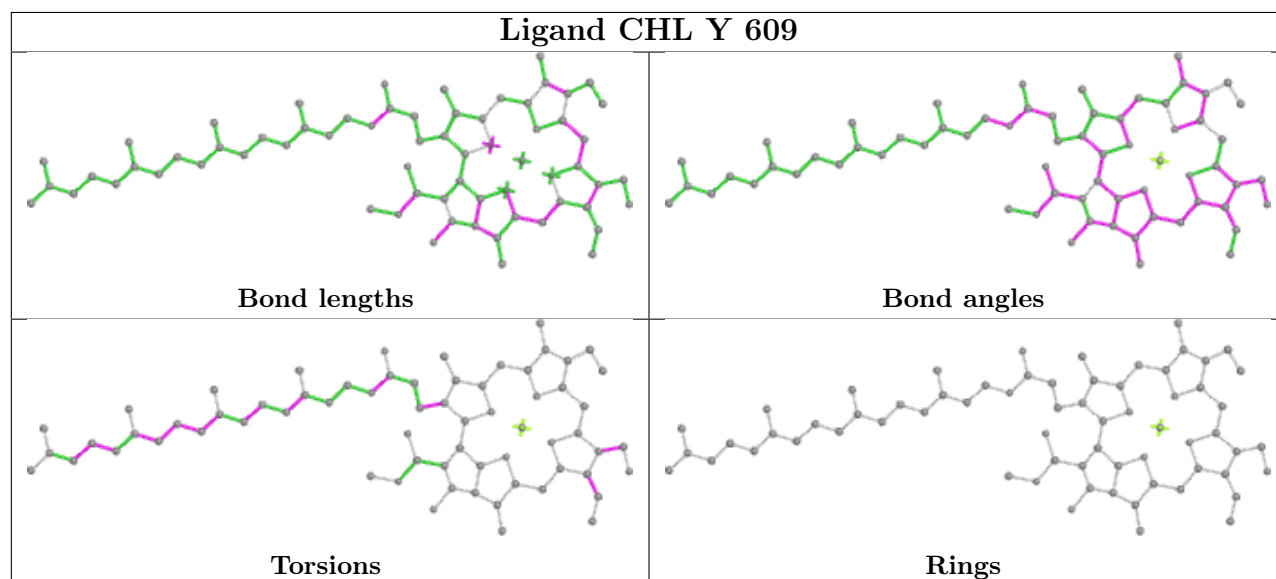
Ligand CLA g 602



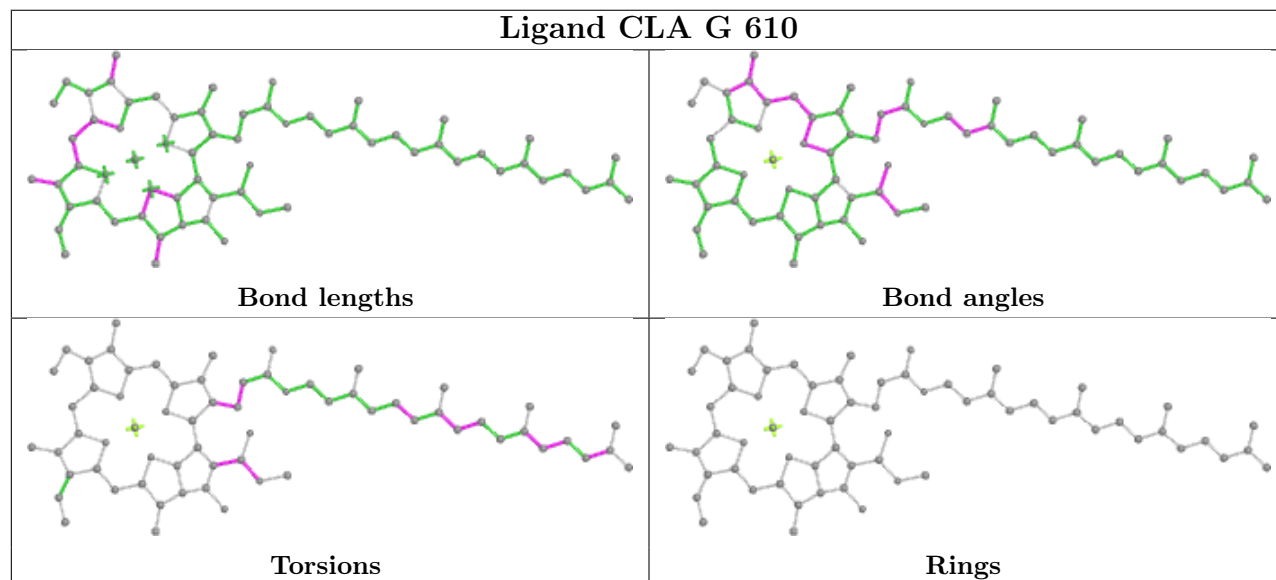
Ligand CLA C 508



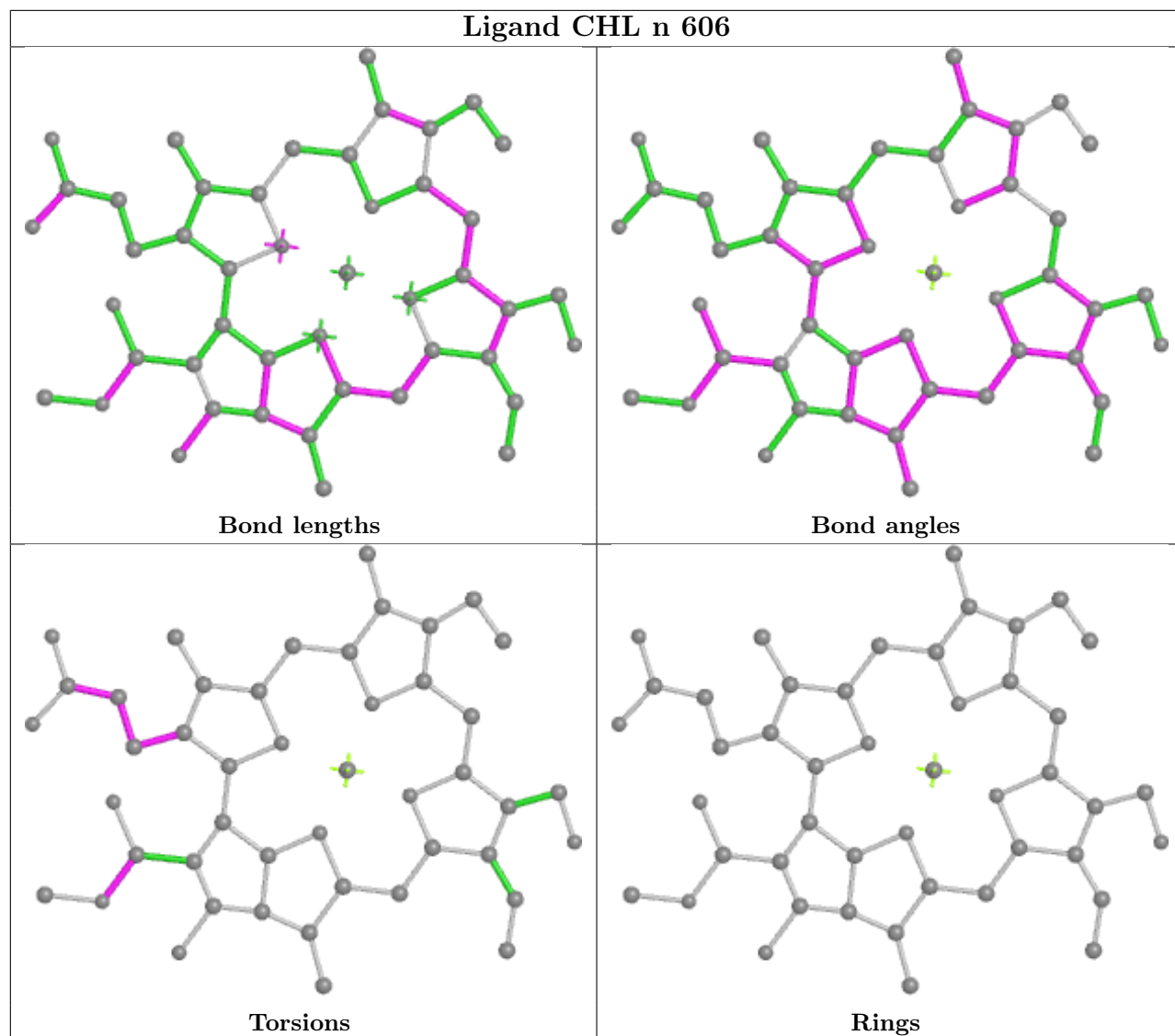
Ligand CHL Y 609

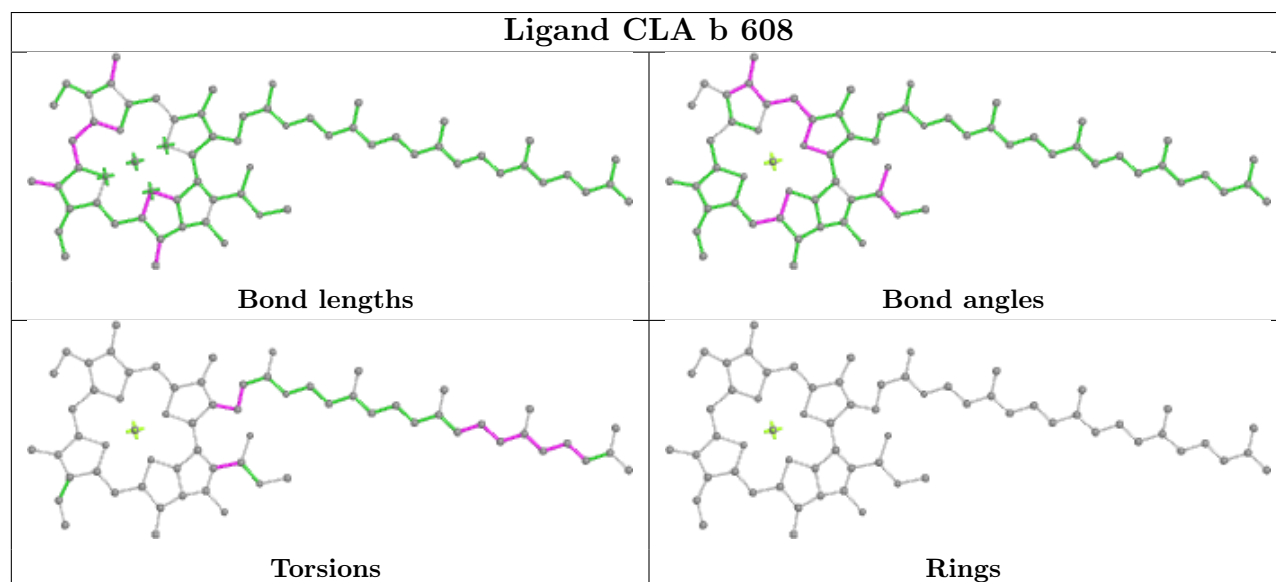
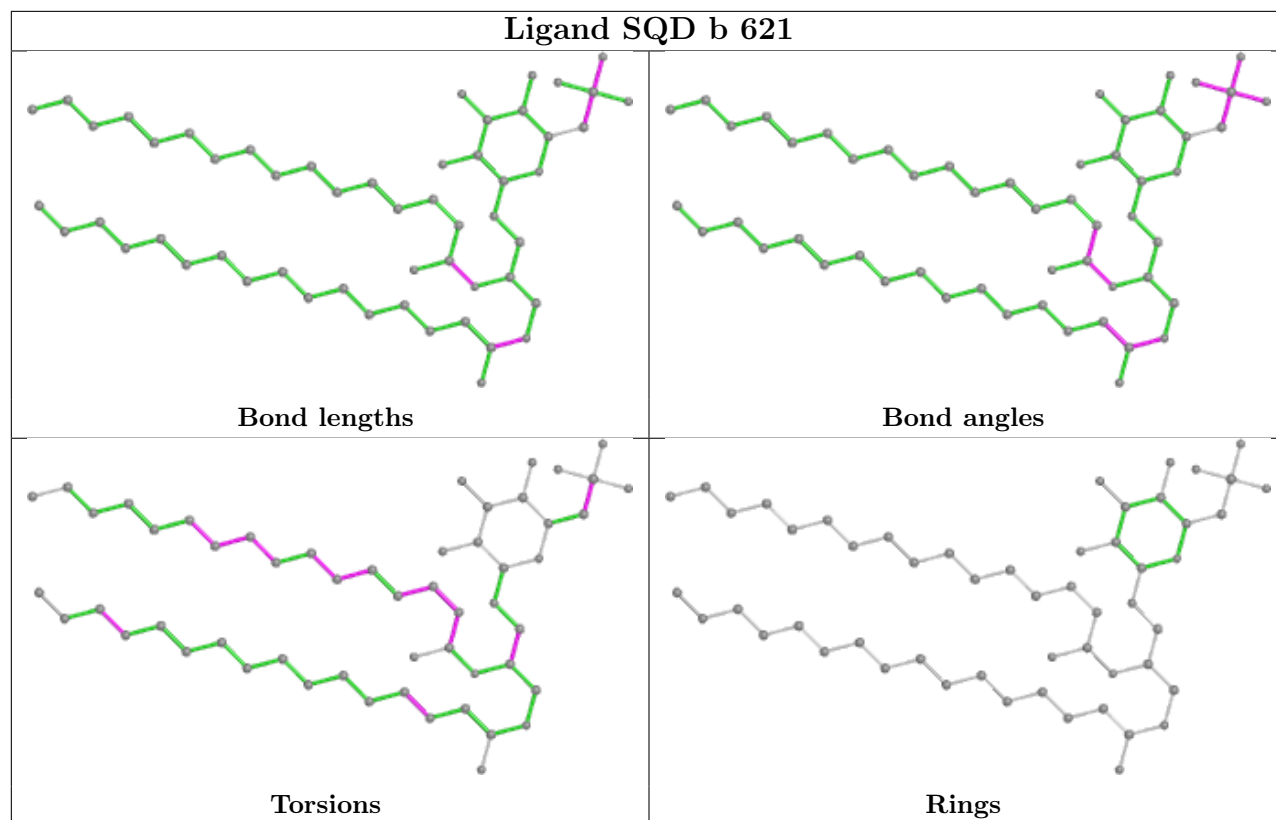


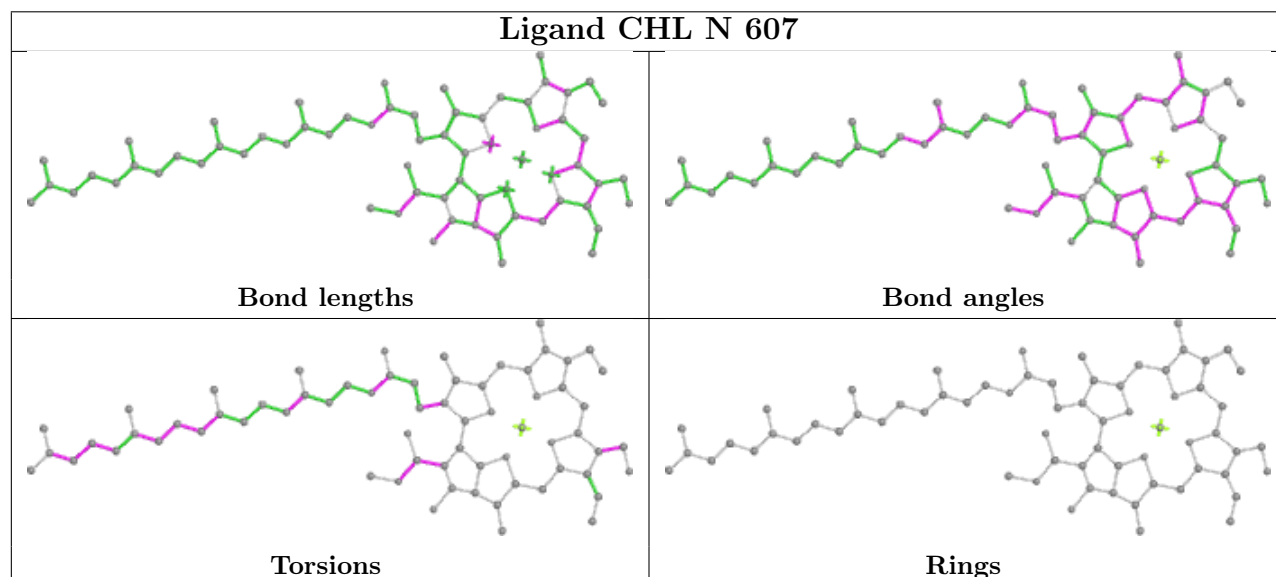
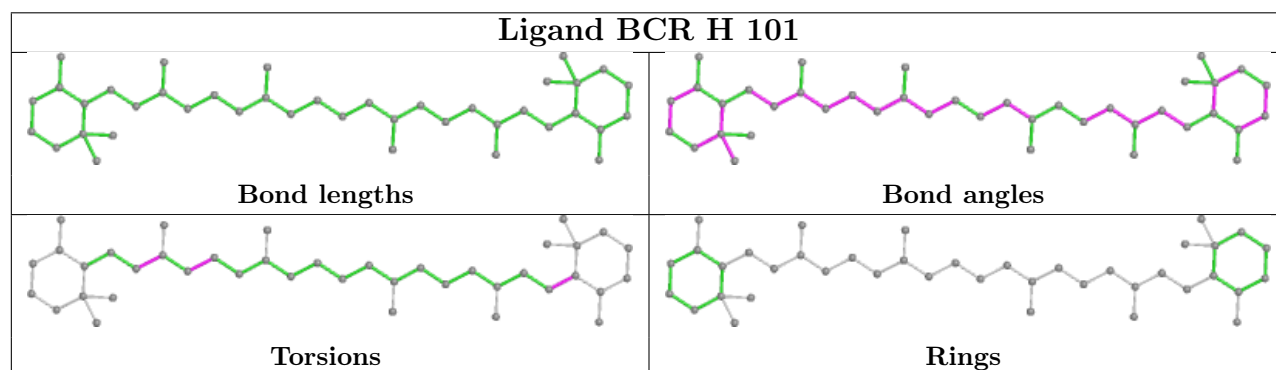
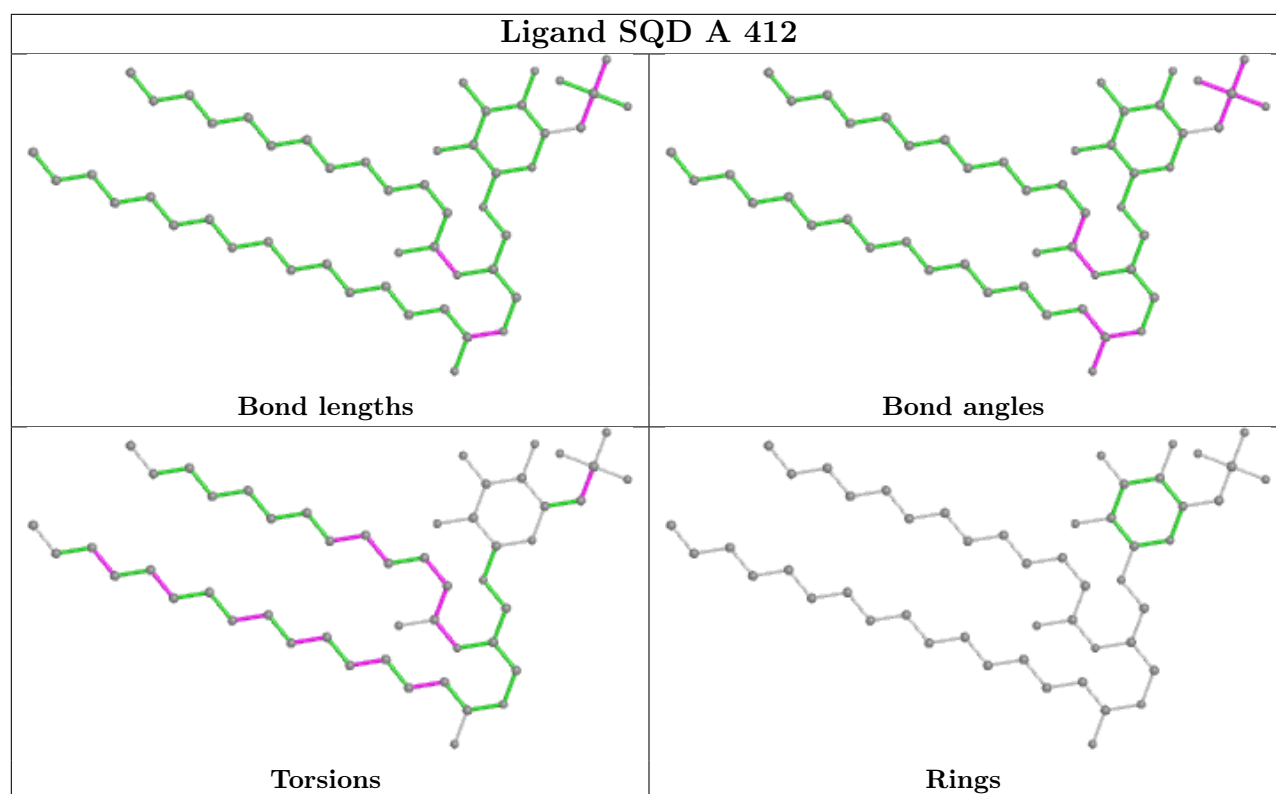
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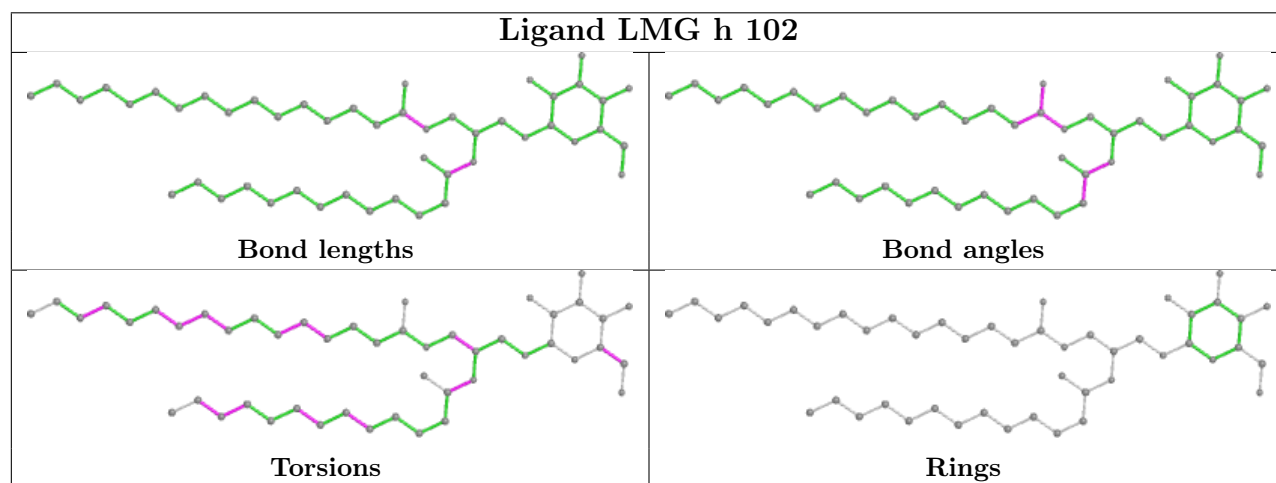
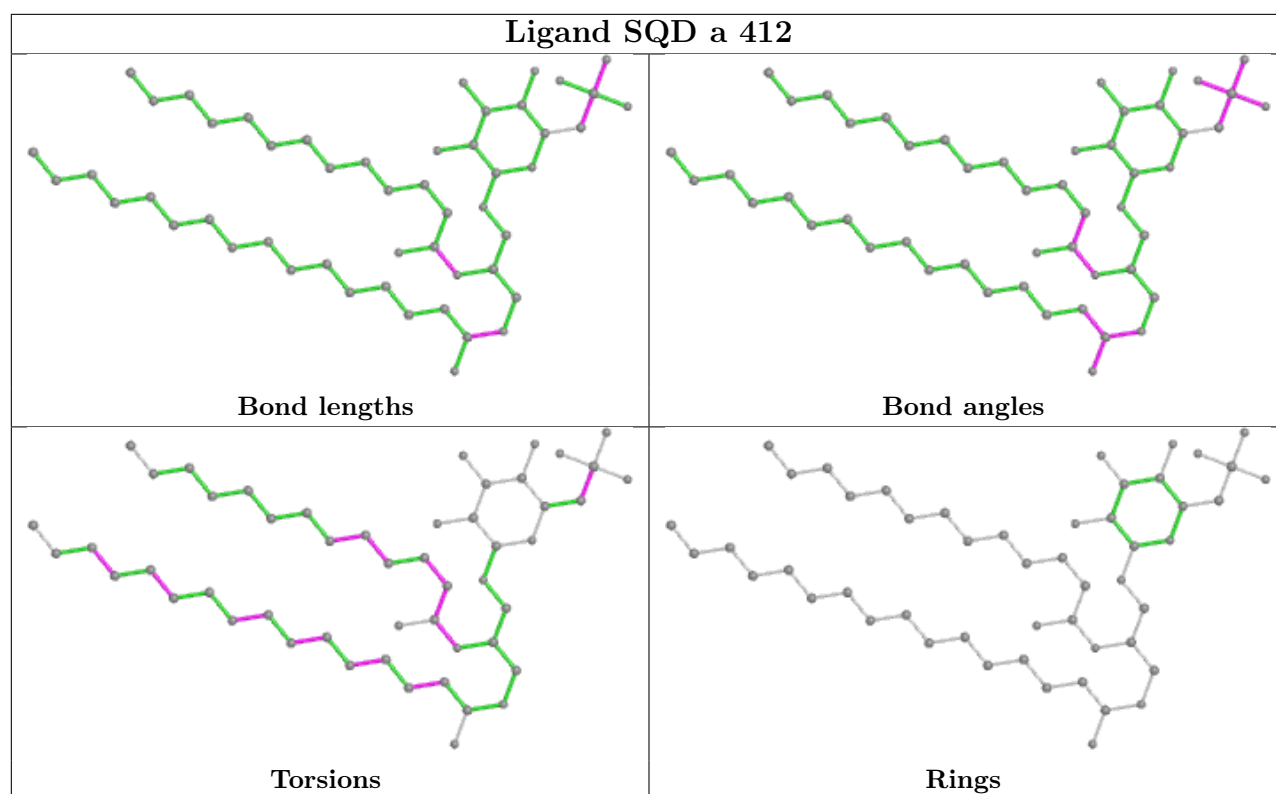


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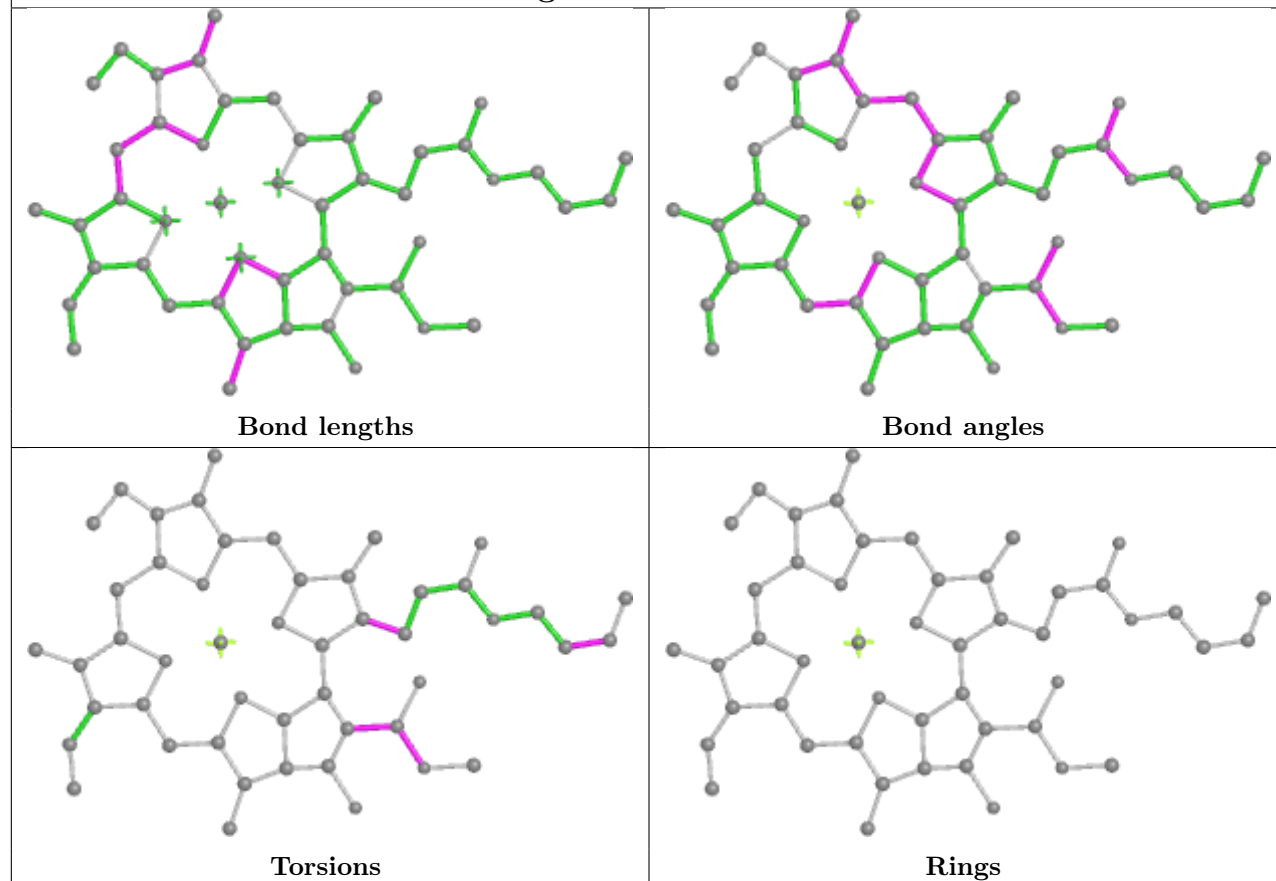




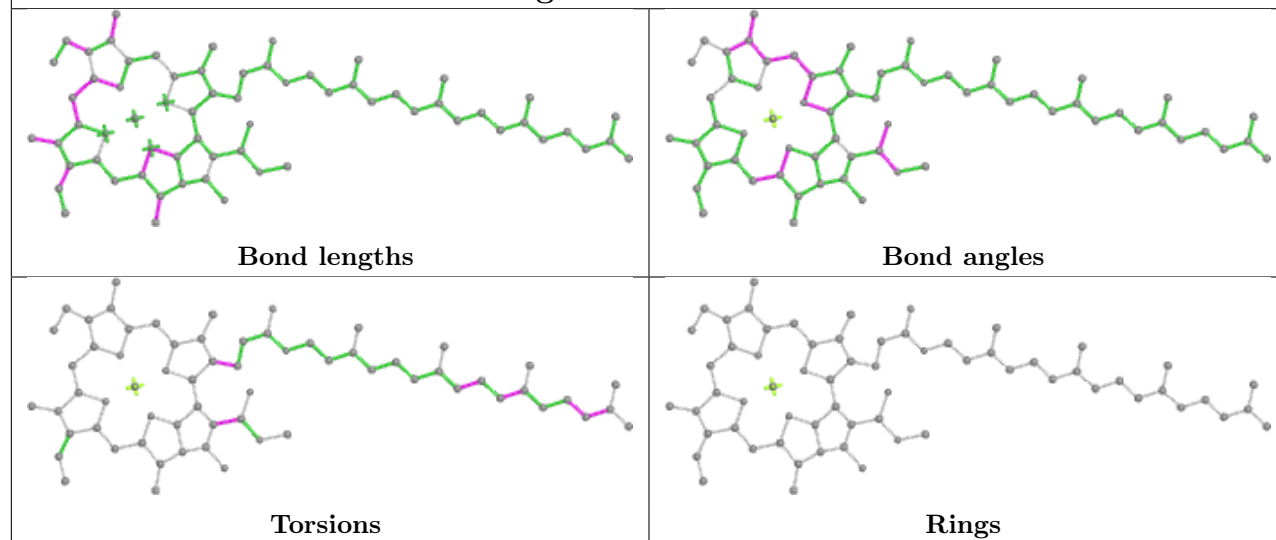




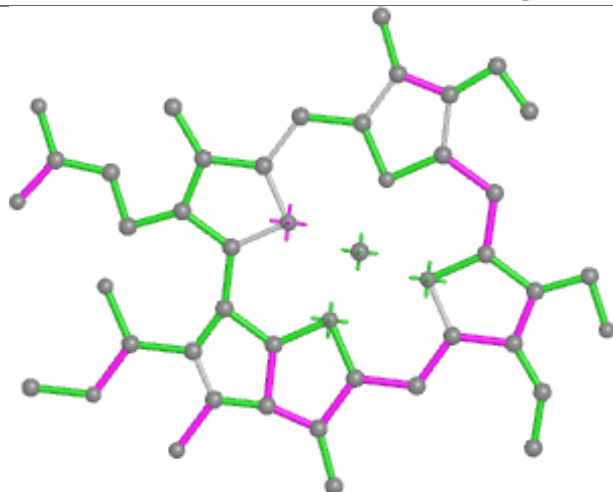
Ligand CLA s 604



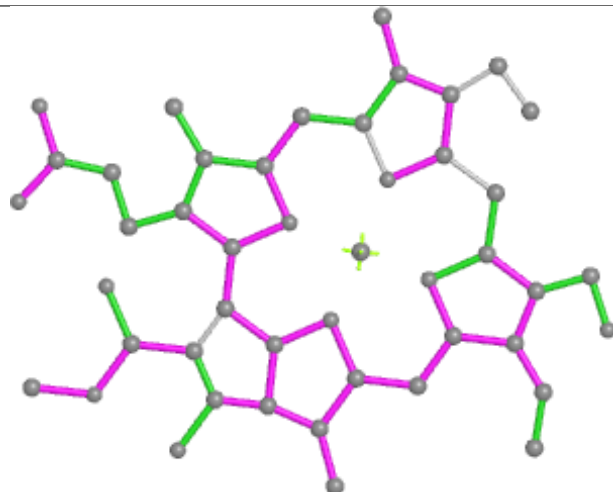
Ligand CLA a 406



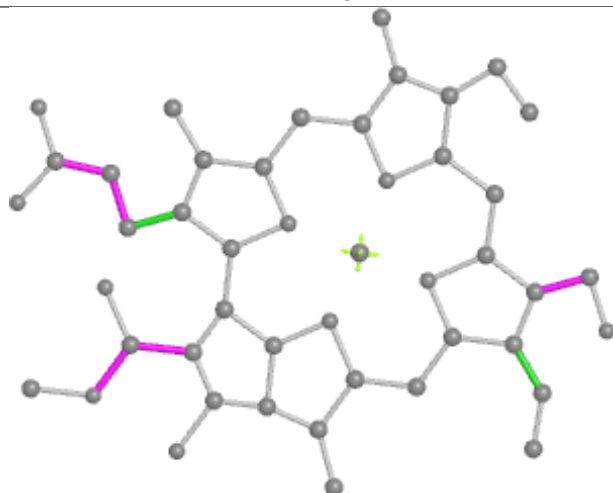
Ligand CHL S 601



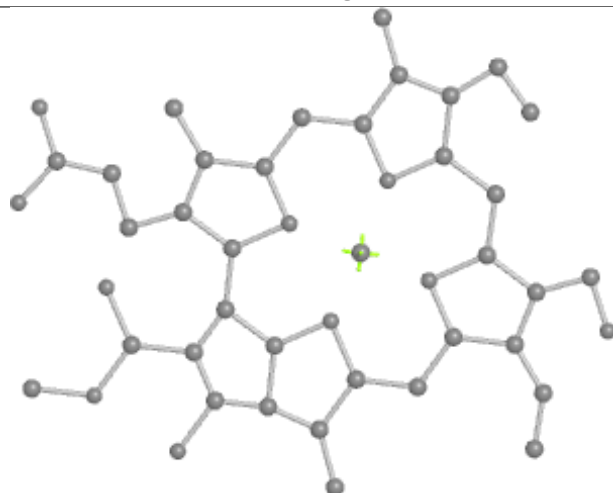
Bond lengths



Bond angles

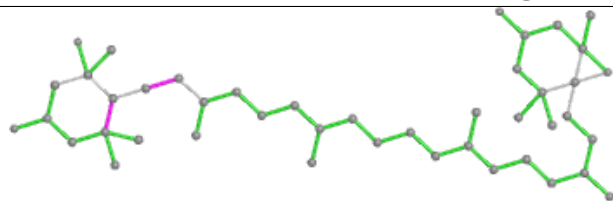


Torsions

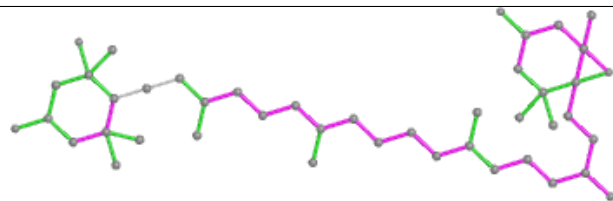


Rings

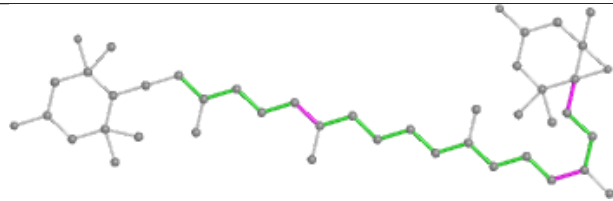
Ligand NEX r 625



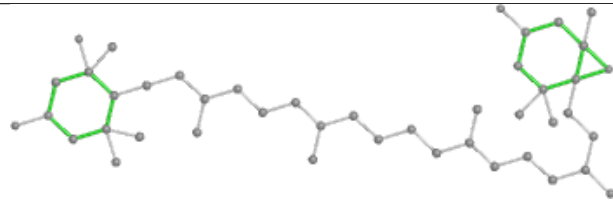
Bond lengths



Bond angles

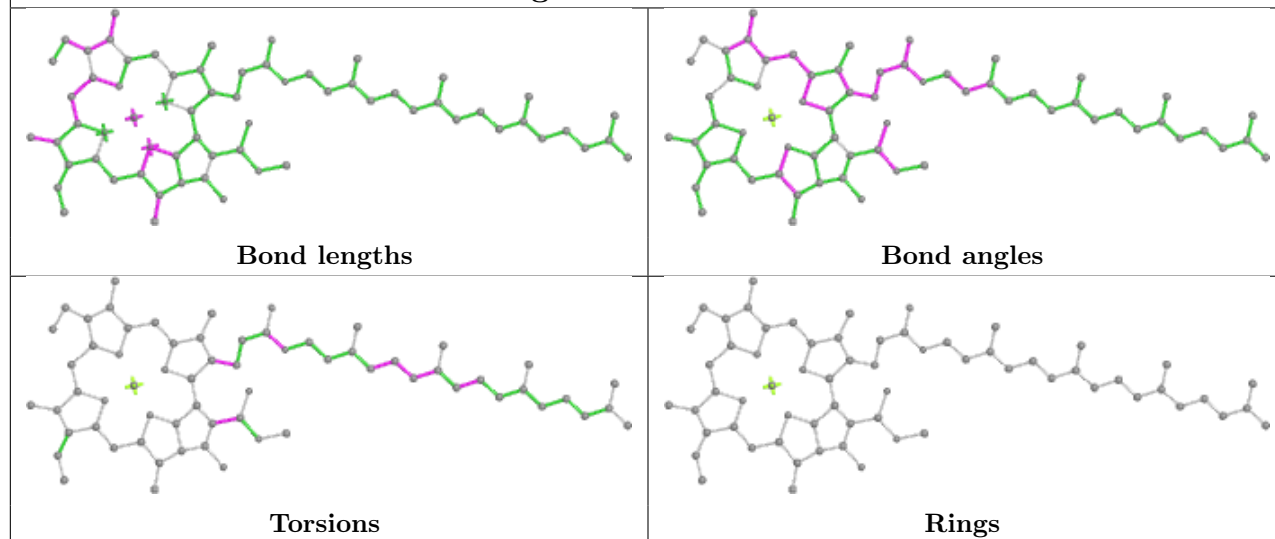


Torsions

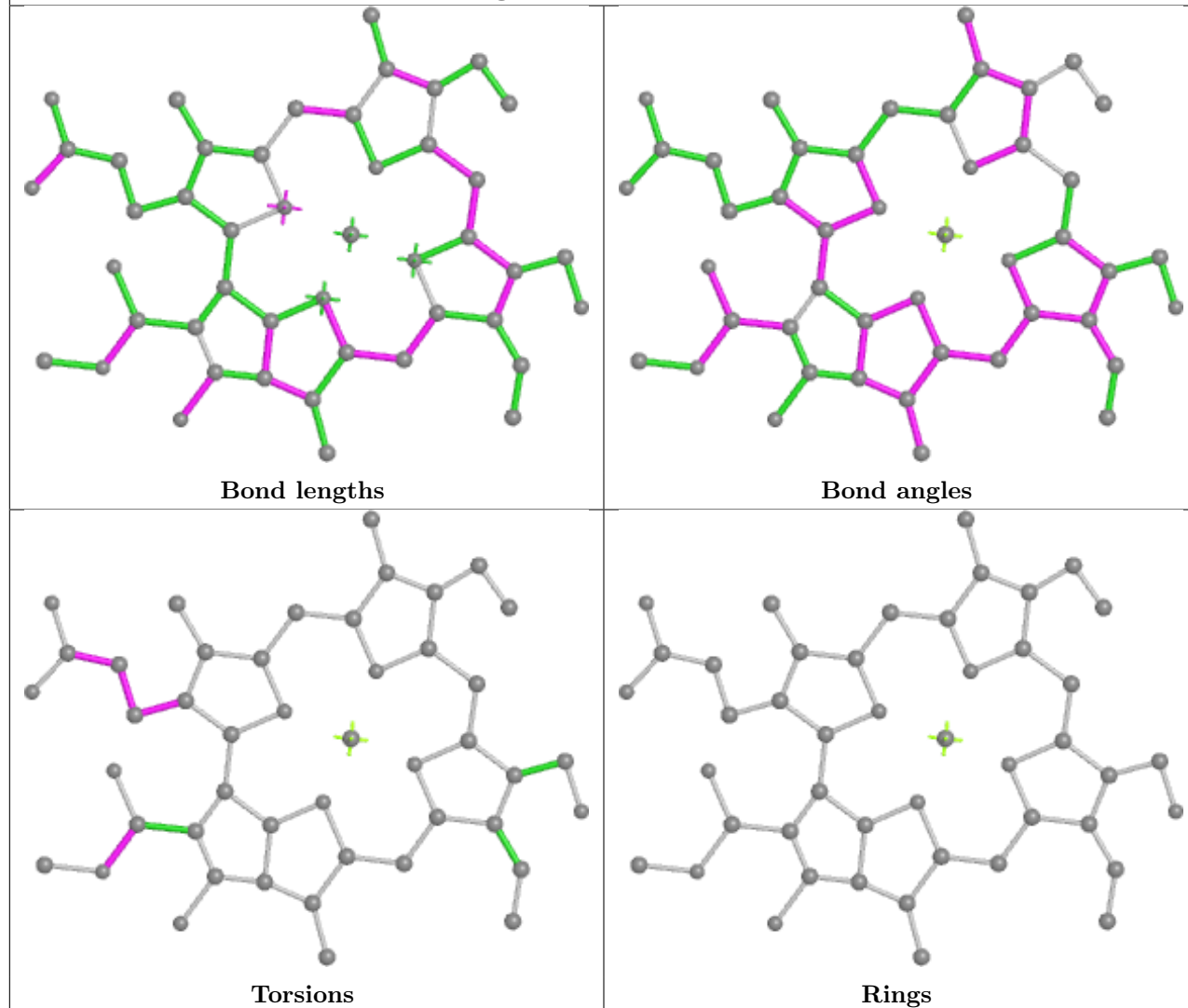


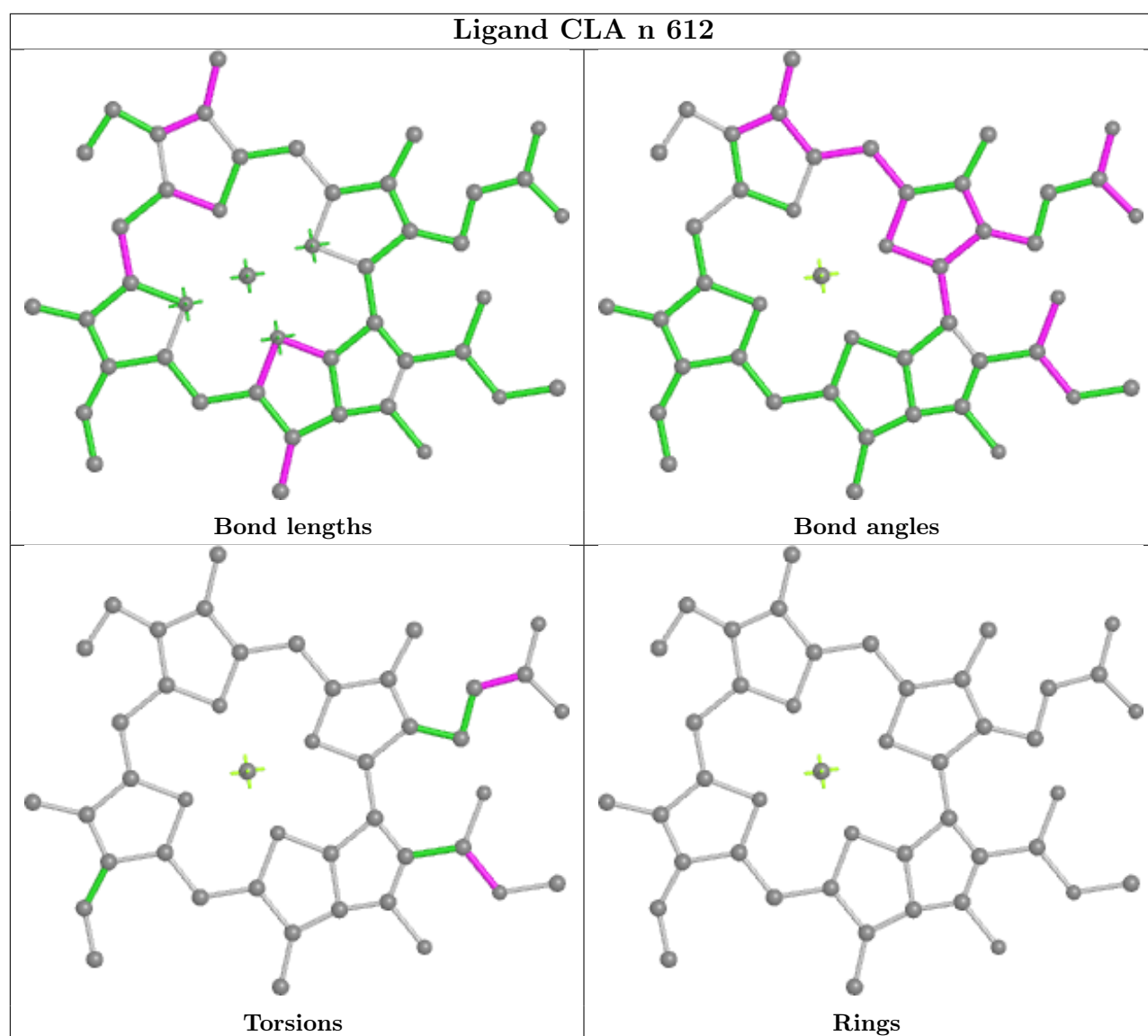
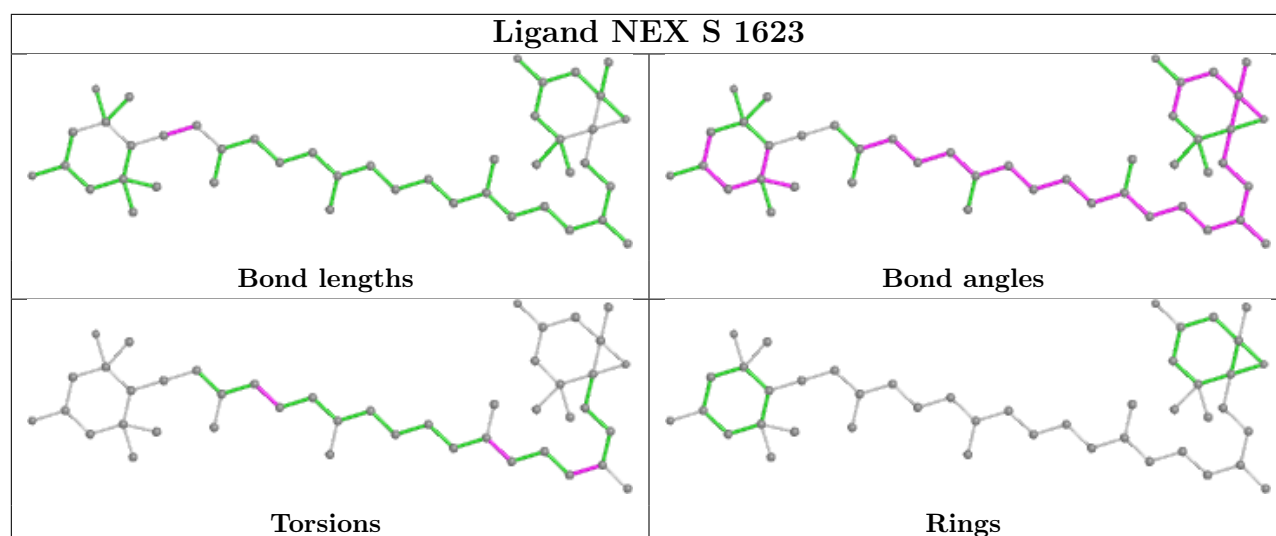
Rings

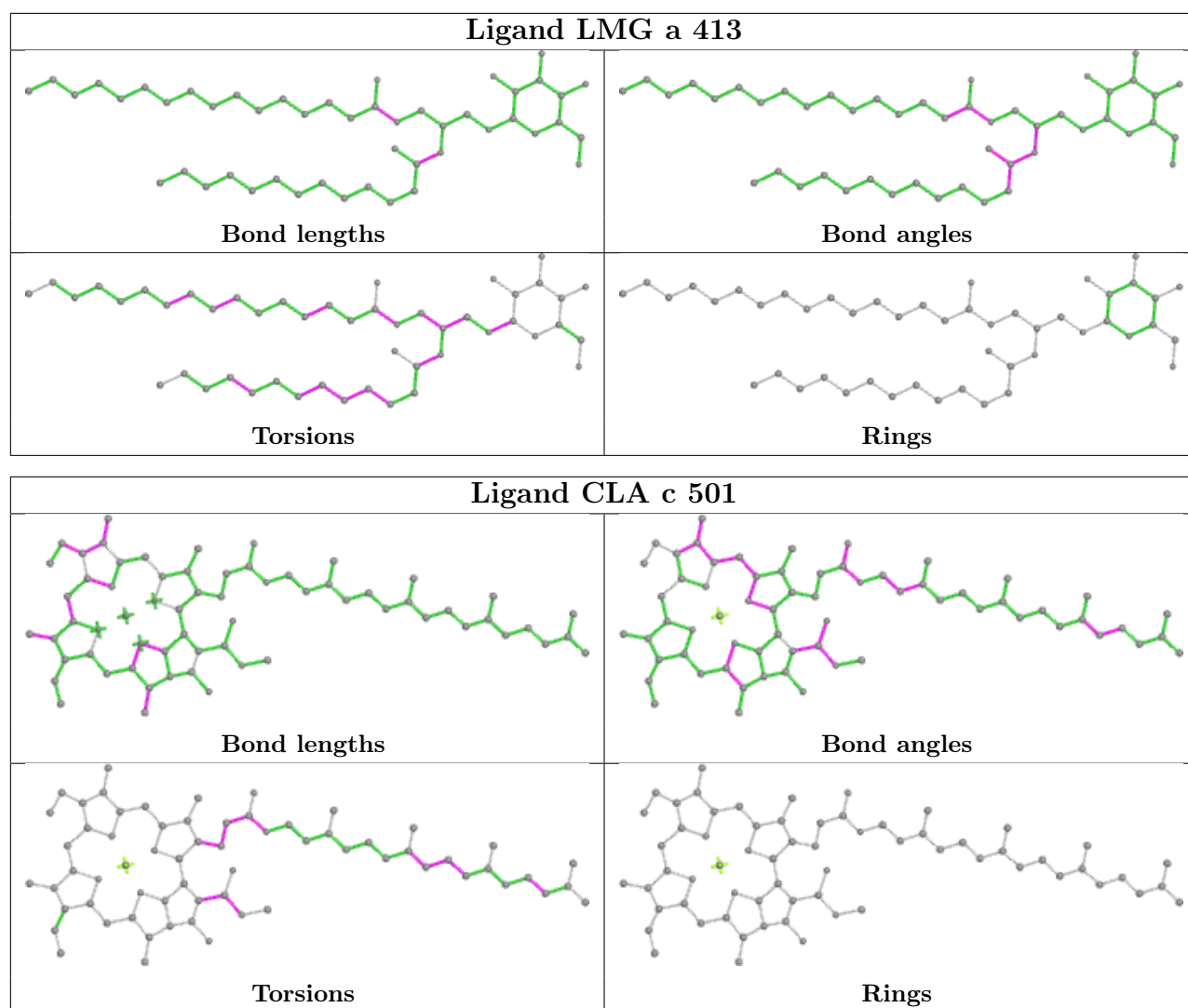
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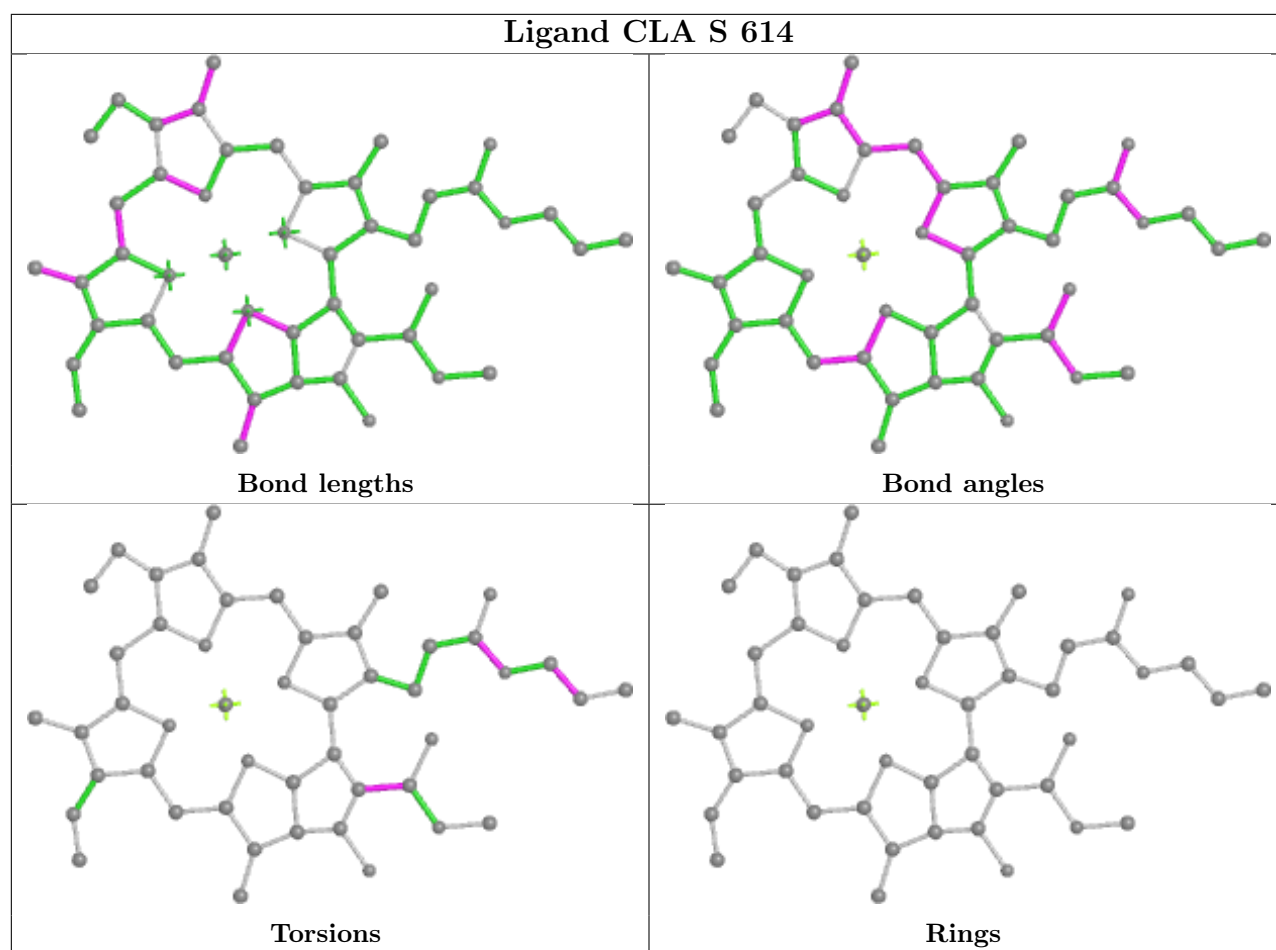


Ligand CHL N 606

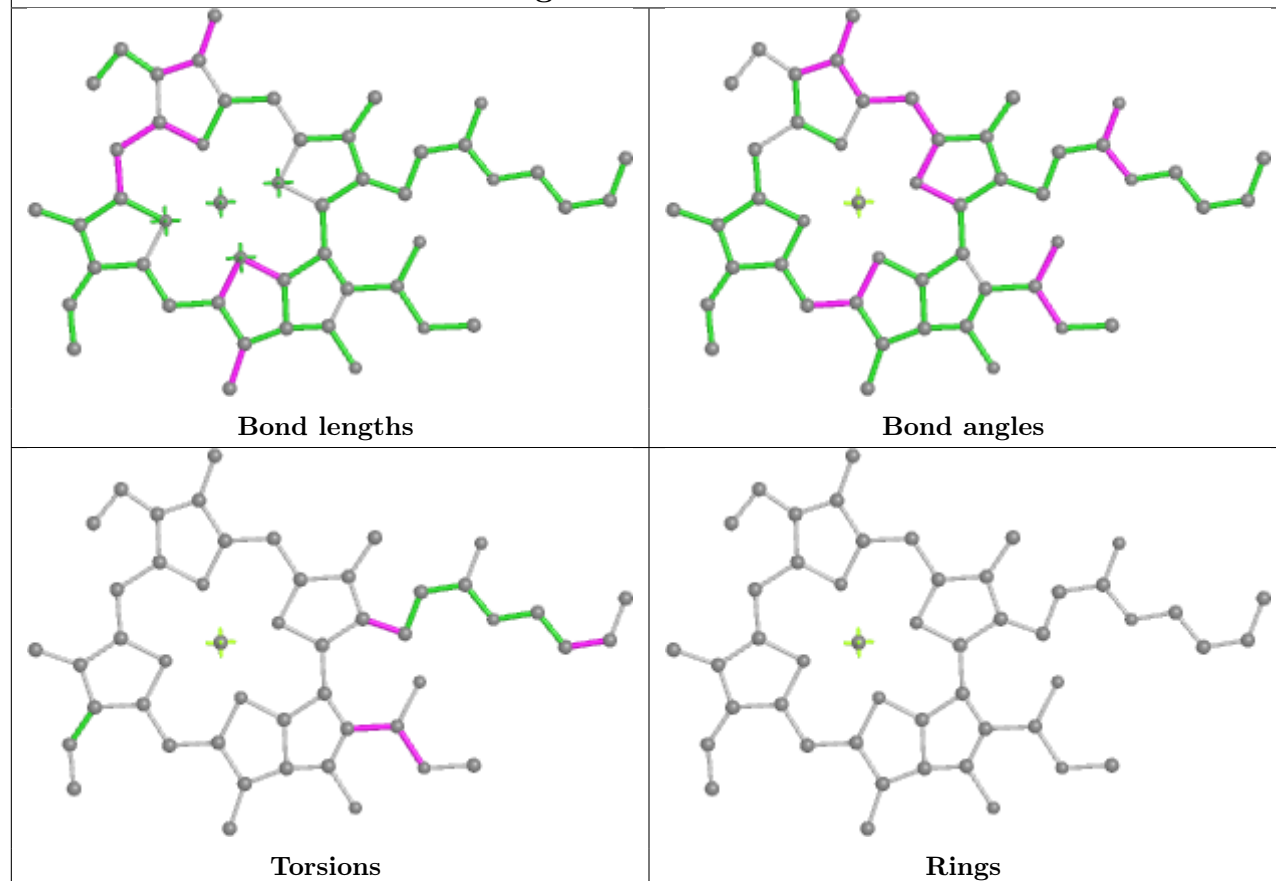




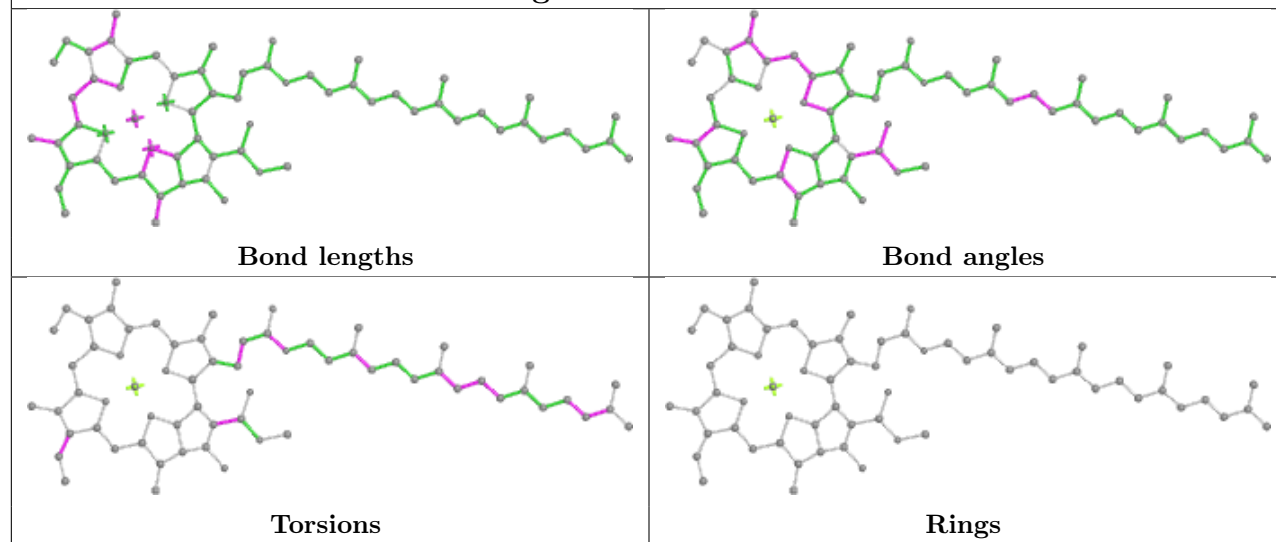


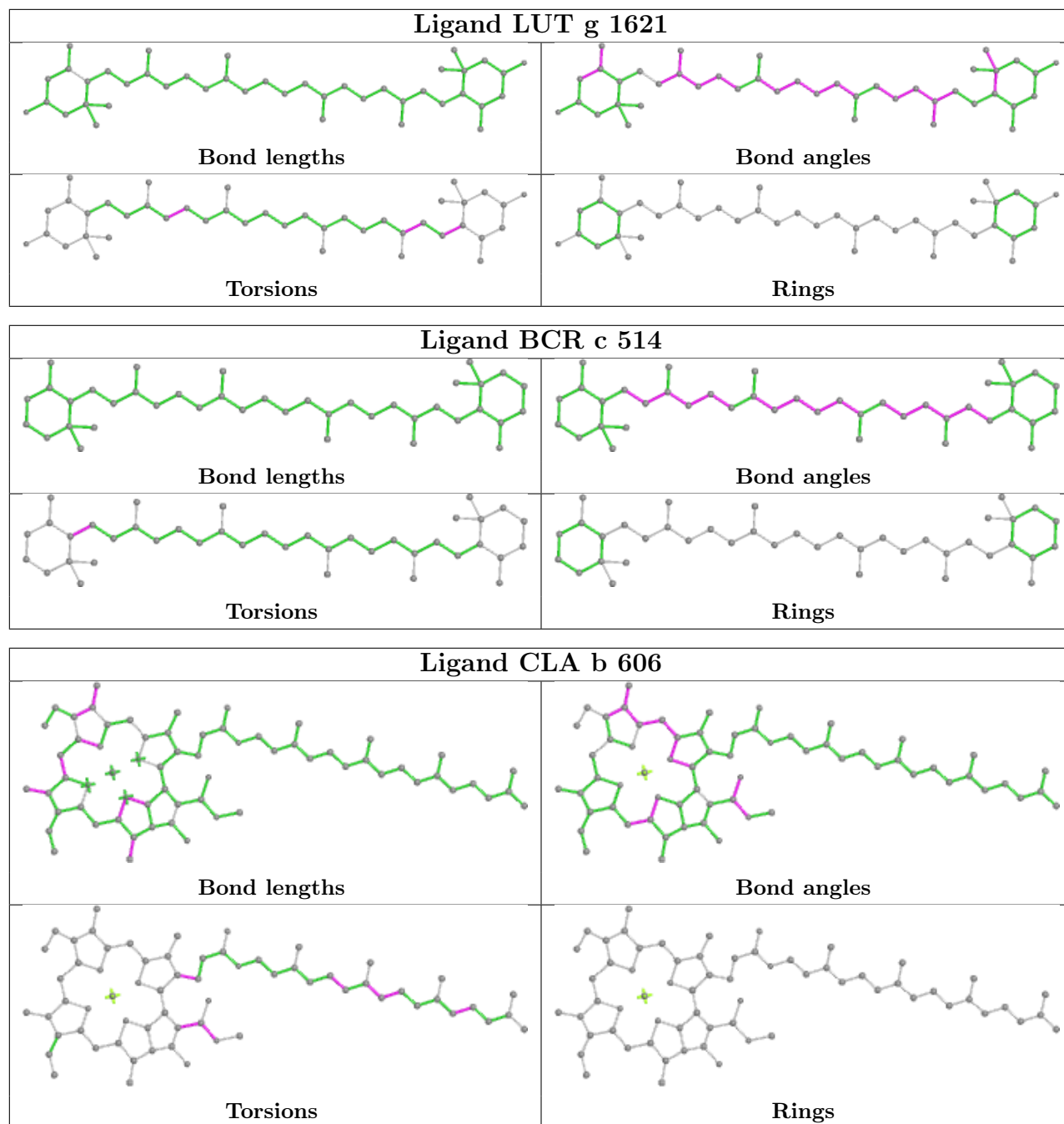


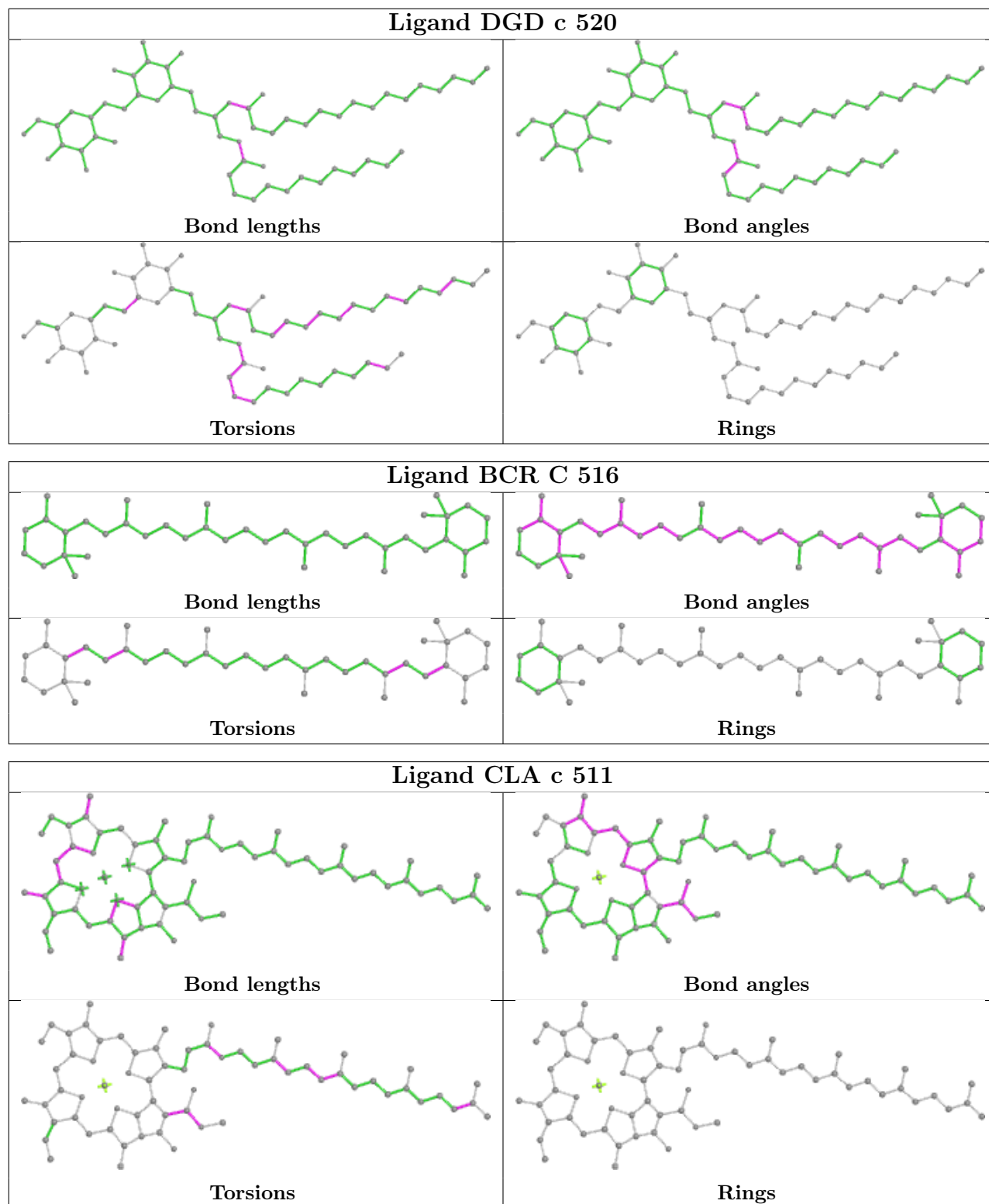
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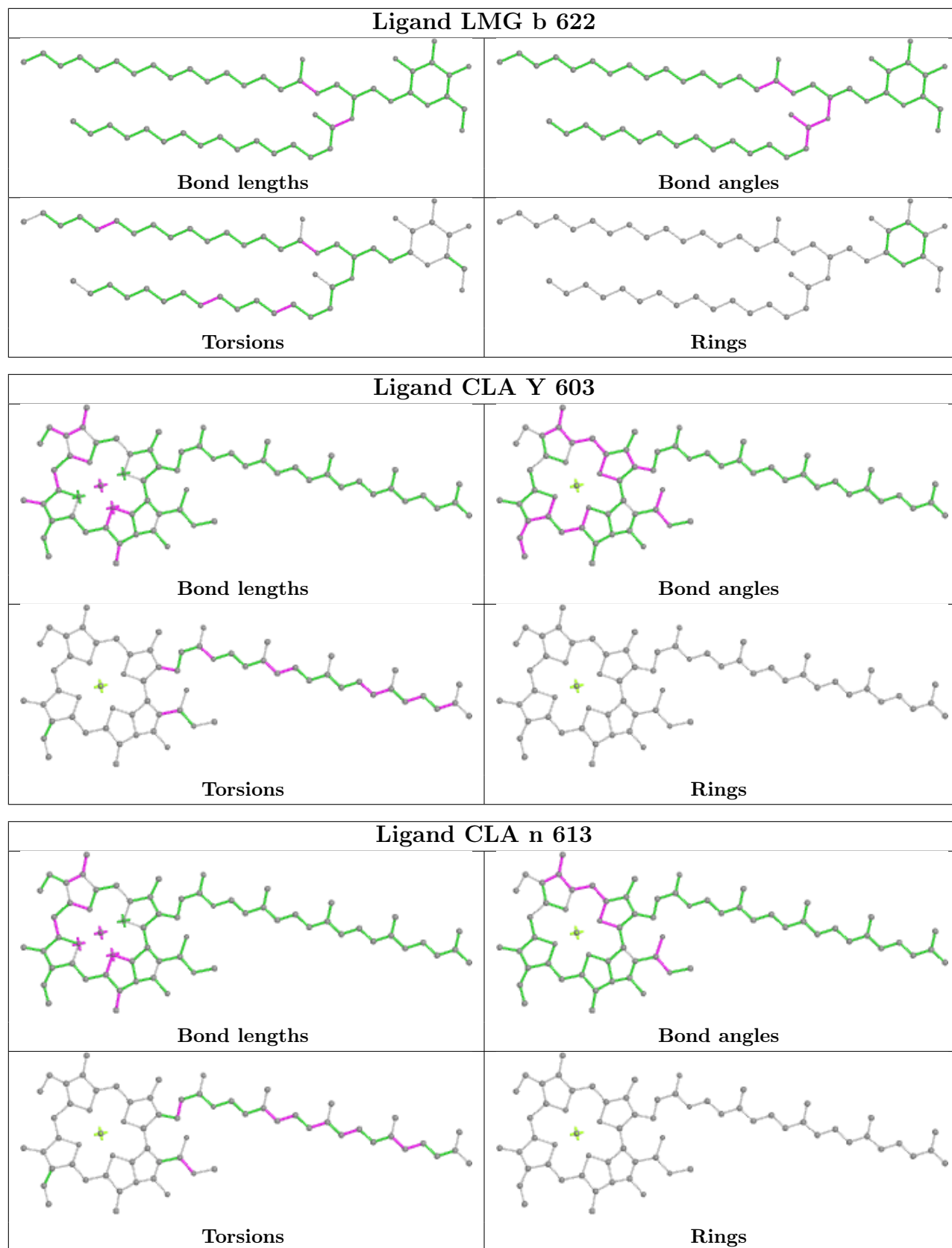


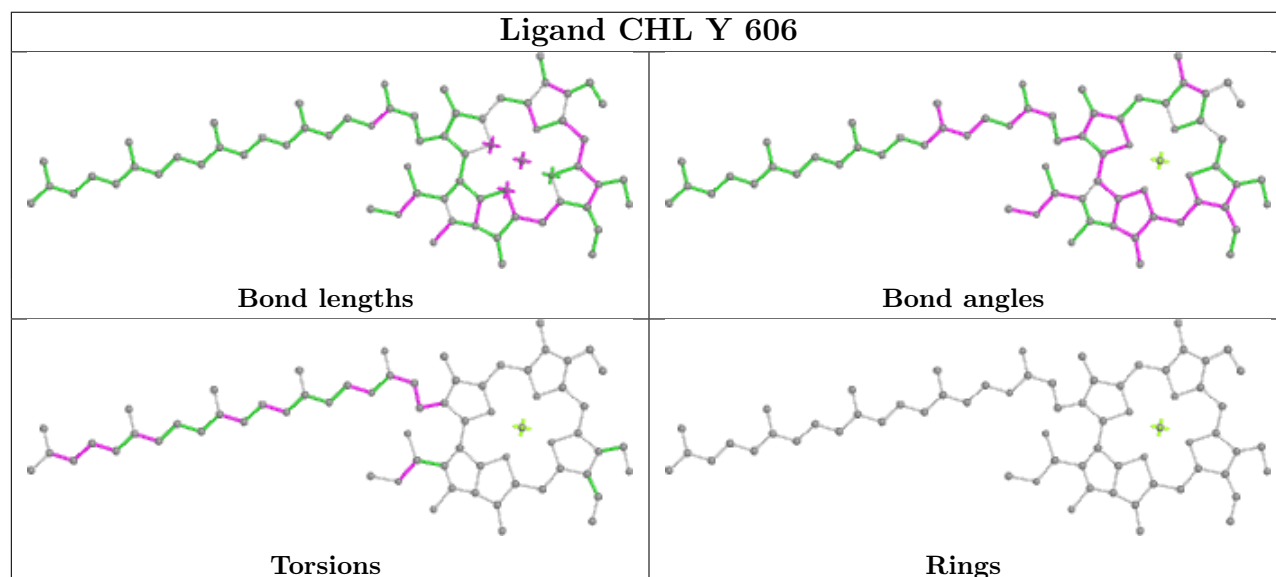
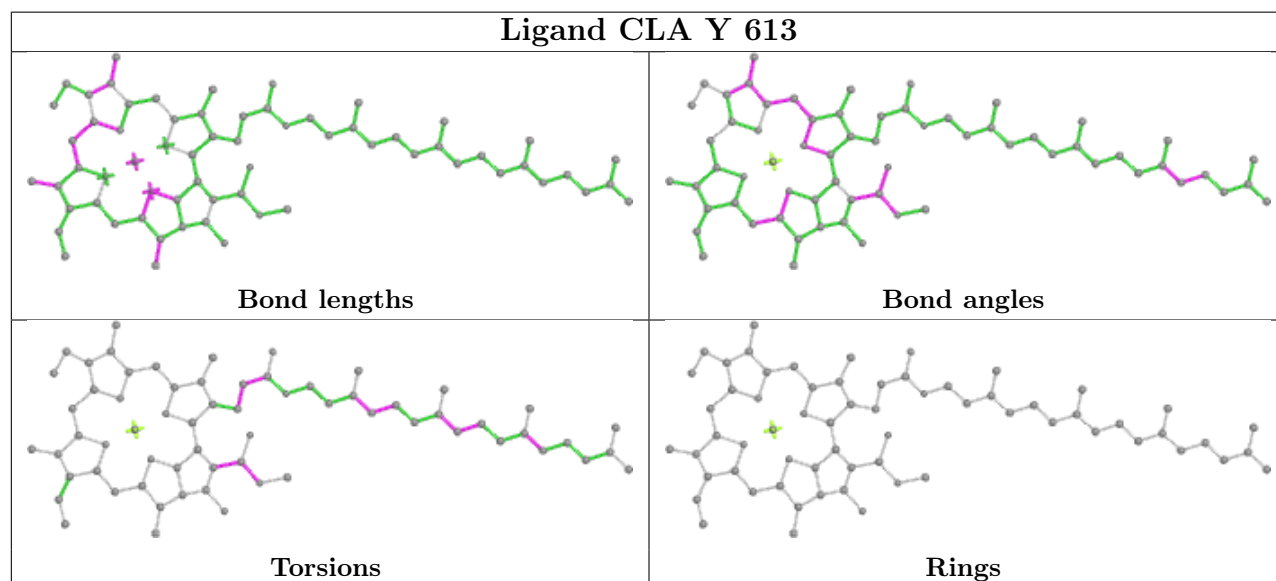
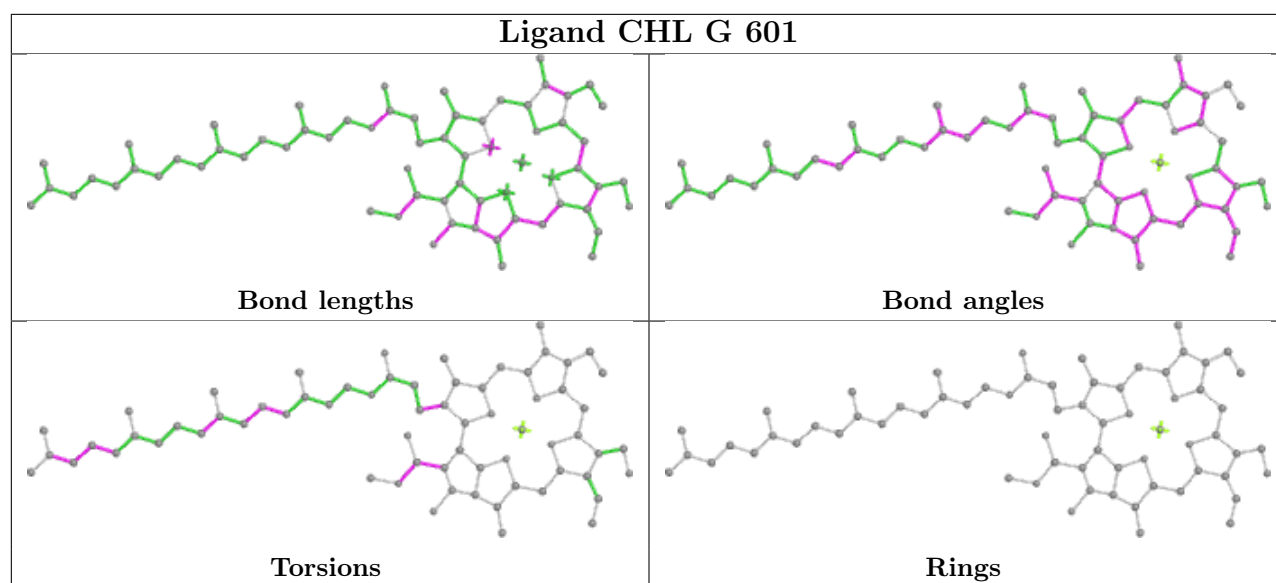
Ligand CLA C 505

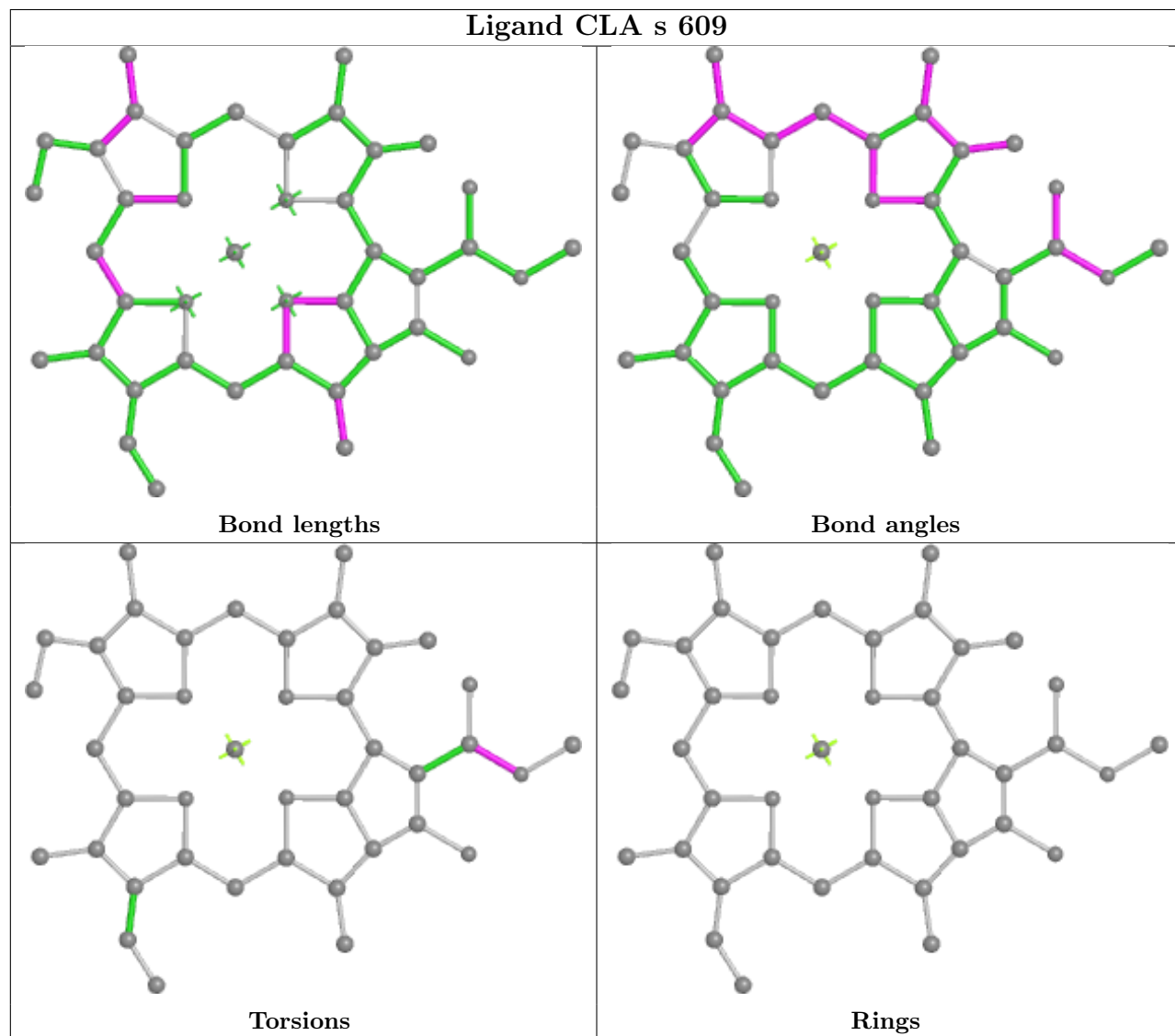
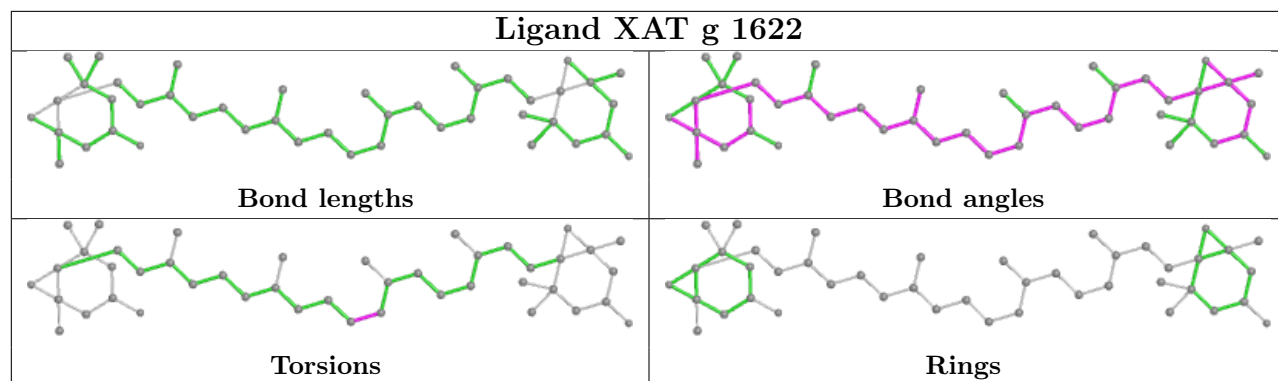


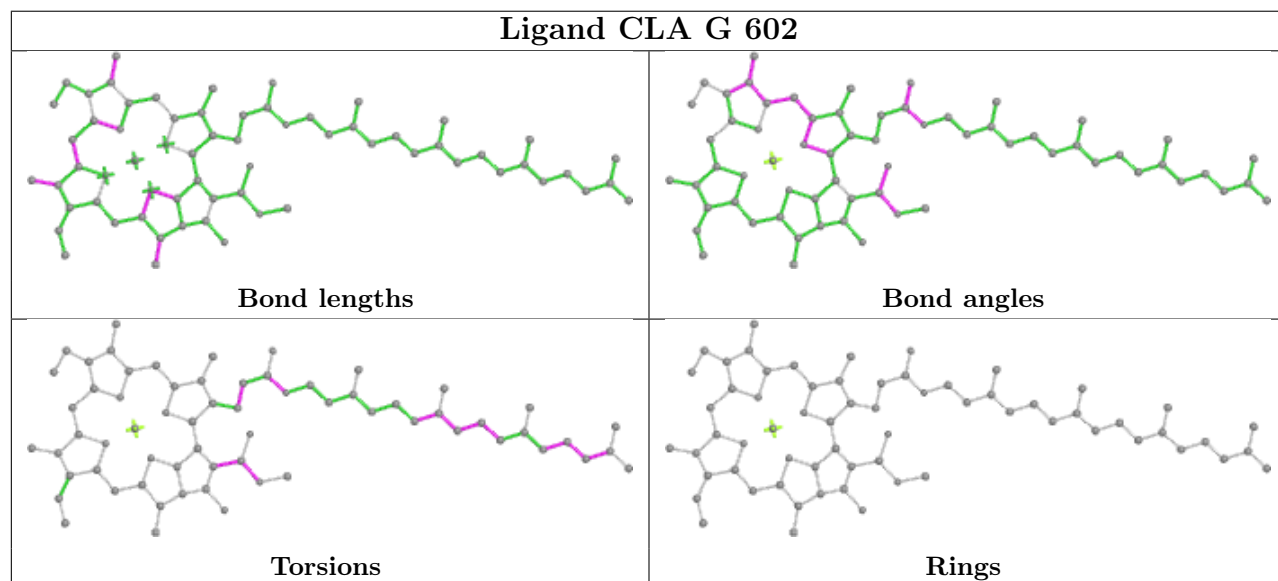
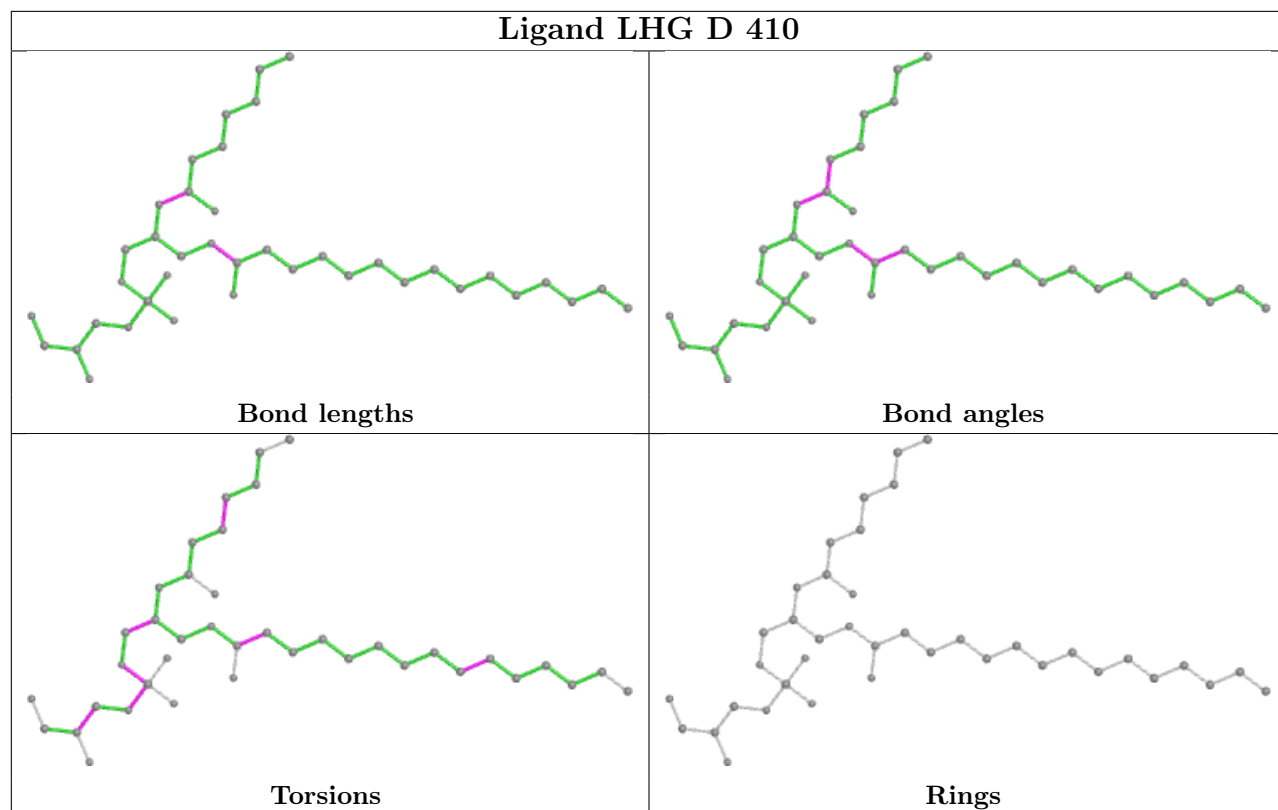


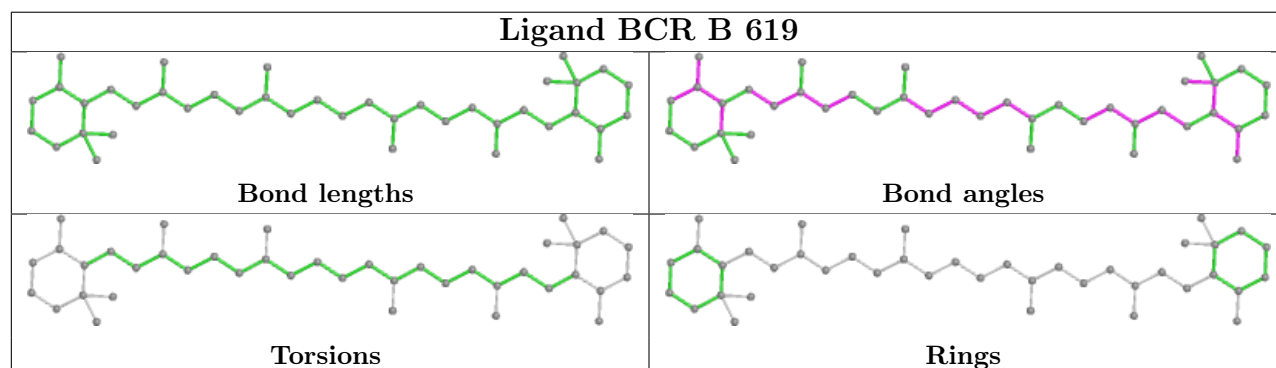
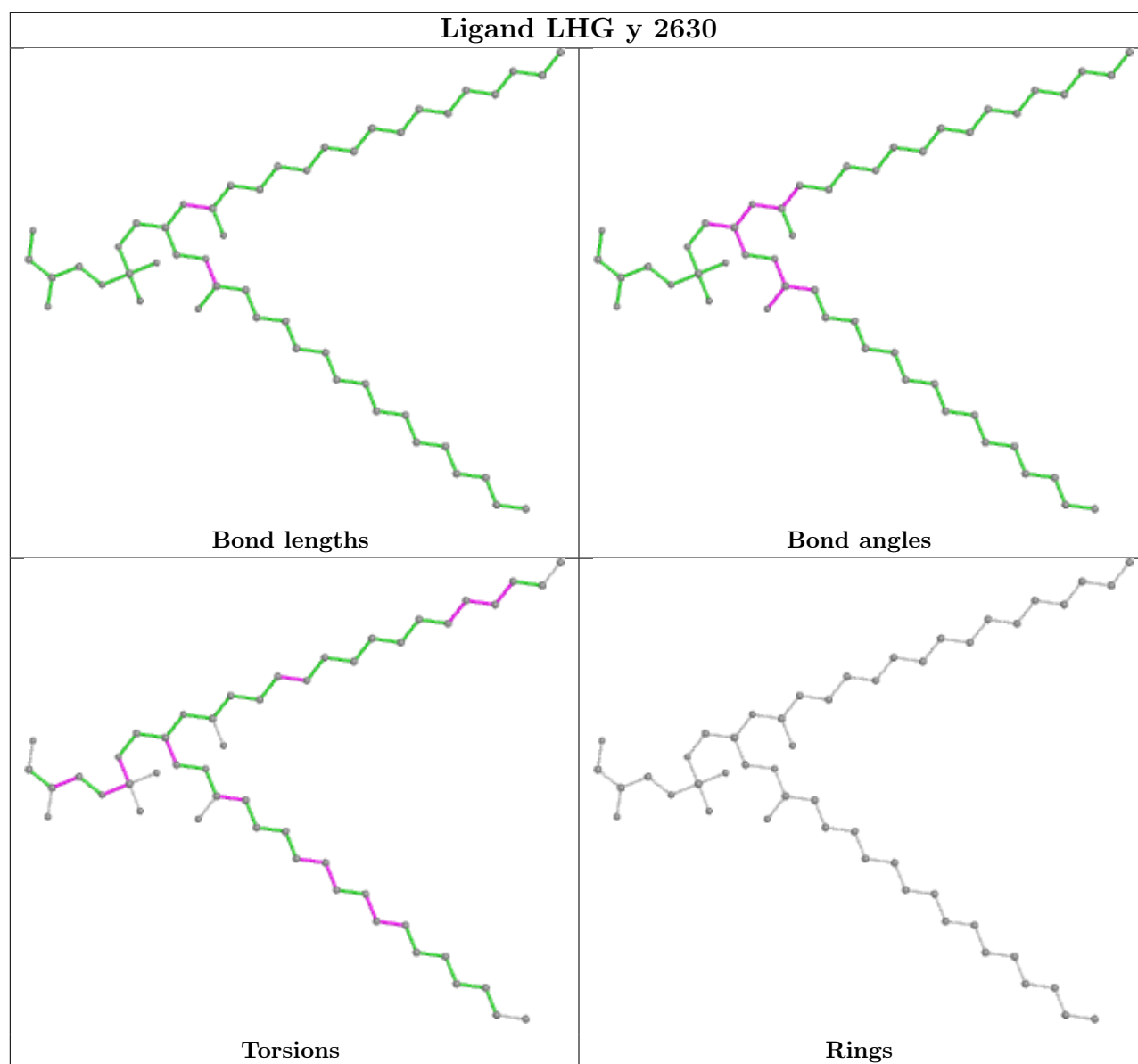


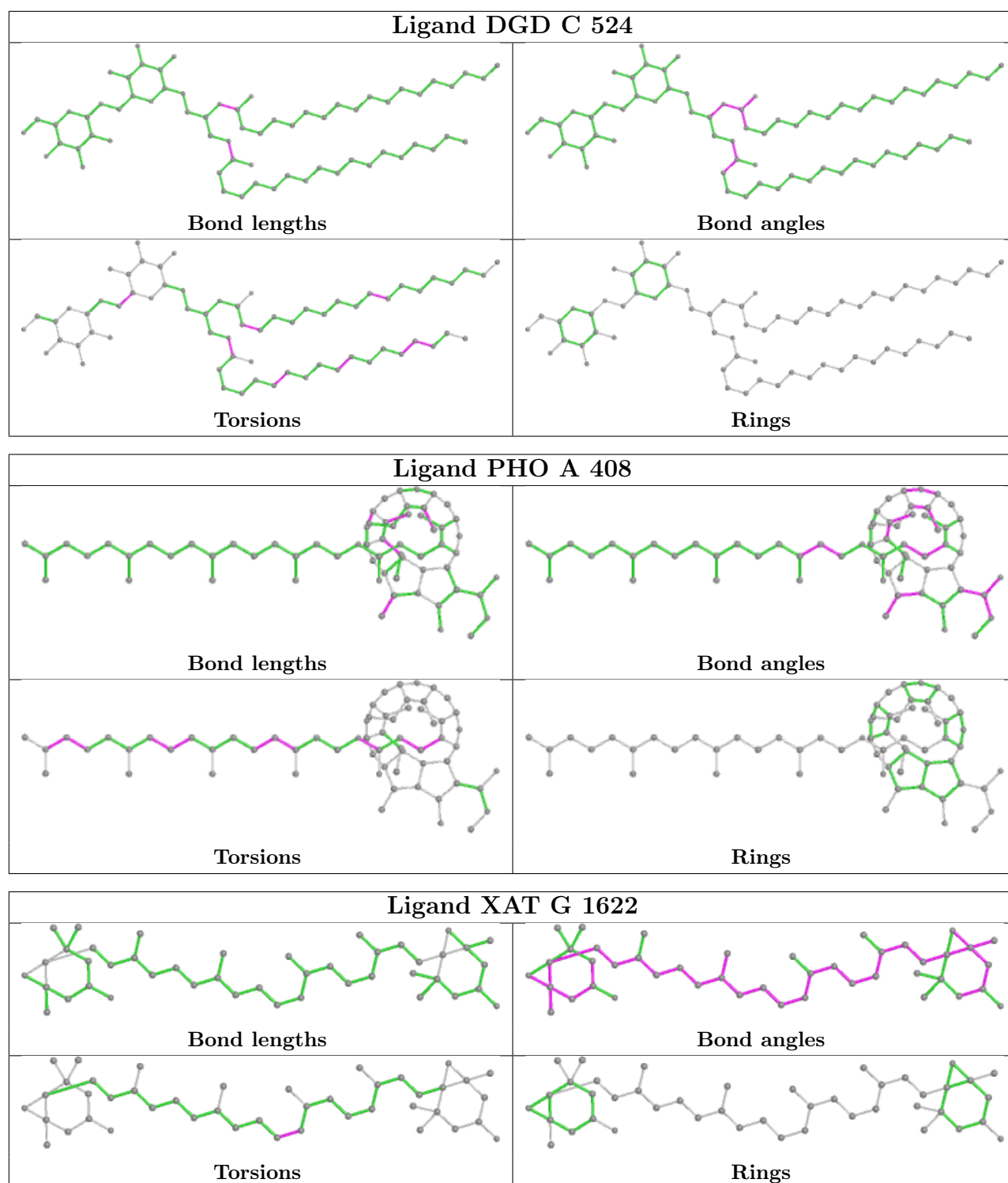




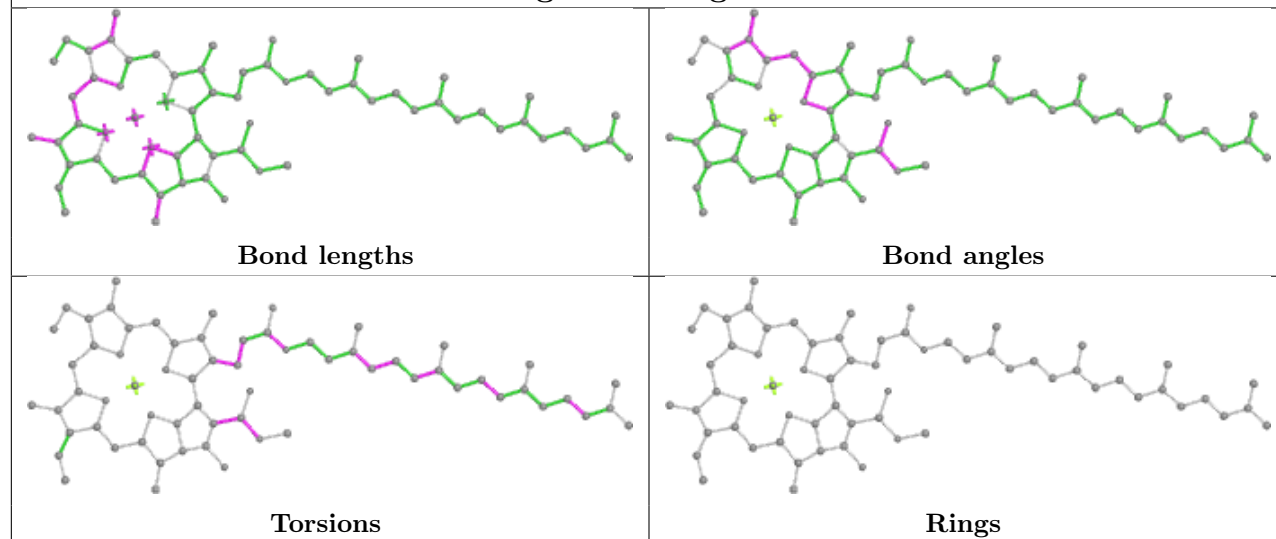




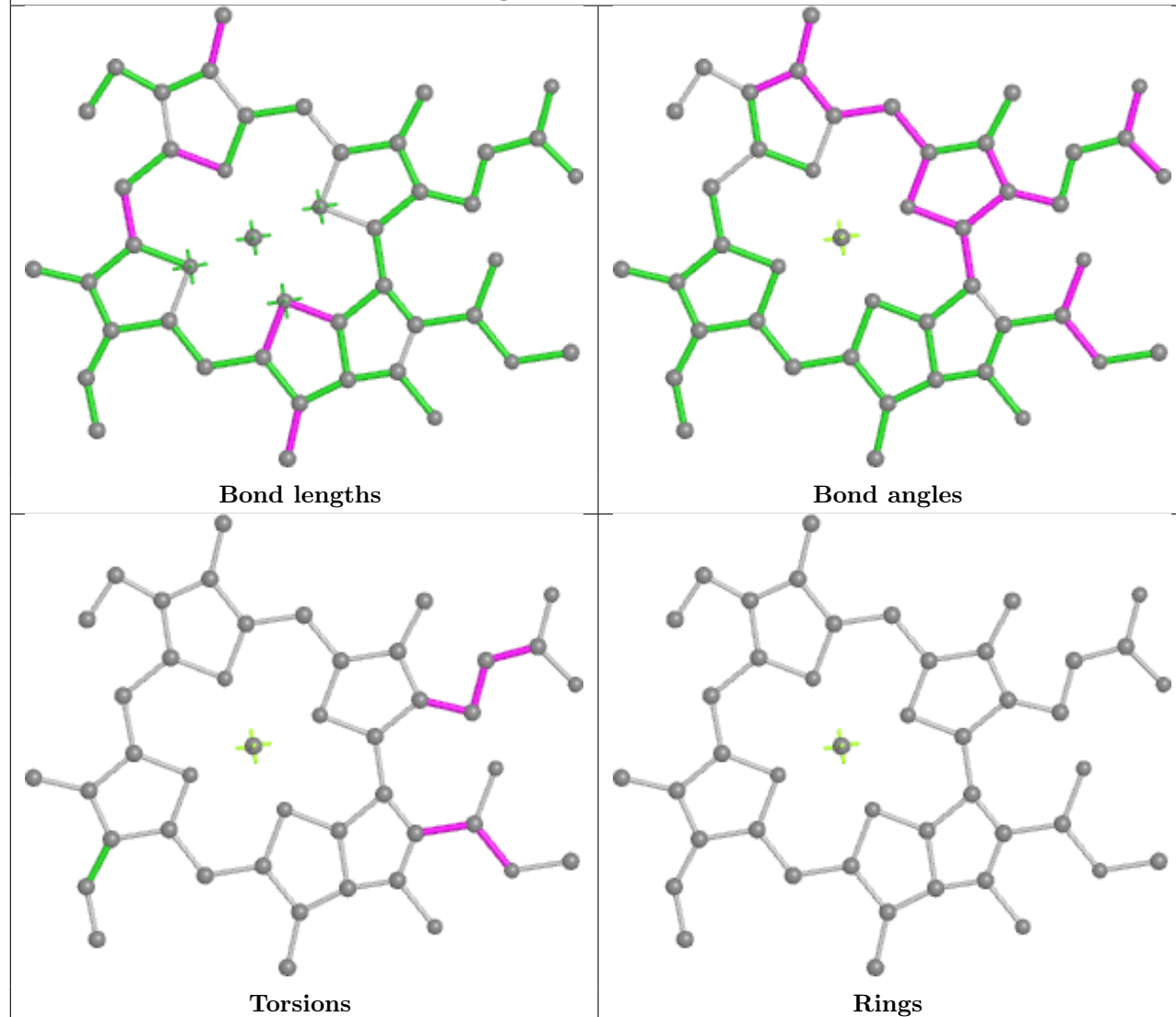




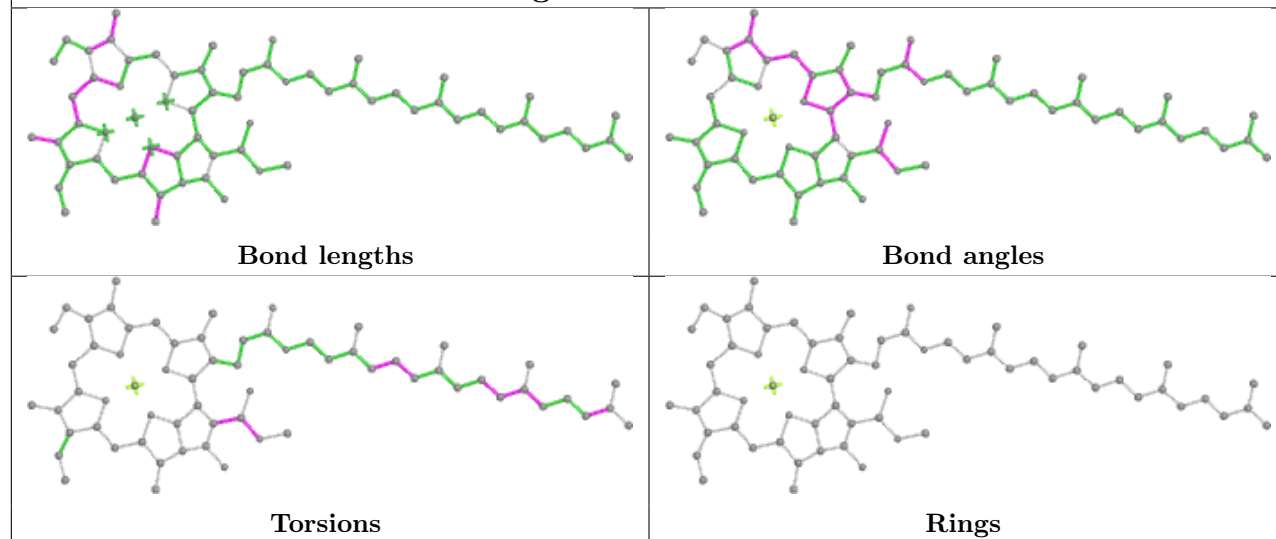
Ligand CLA g 613



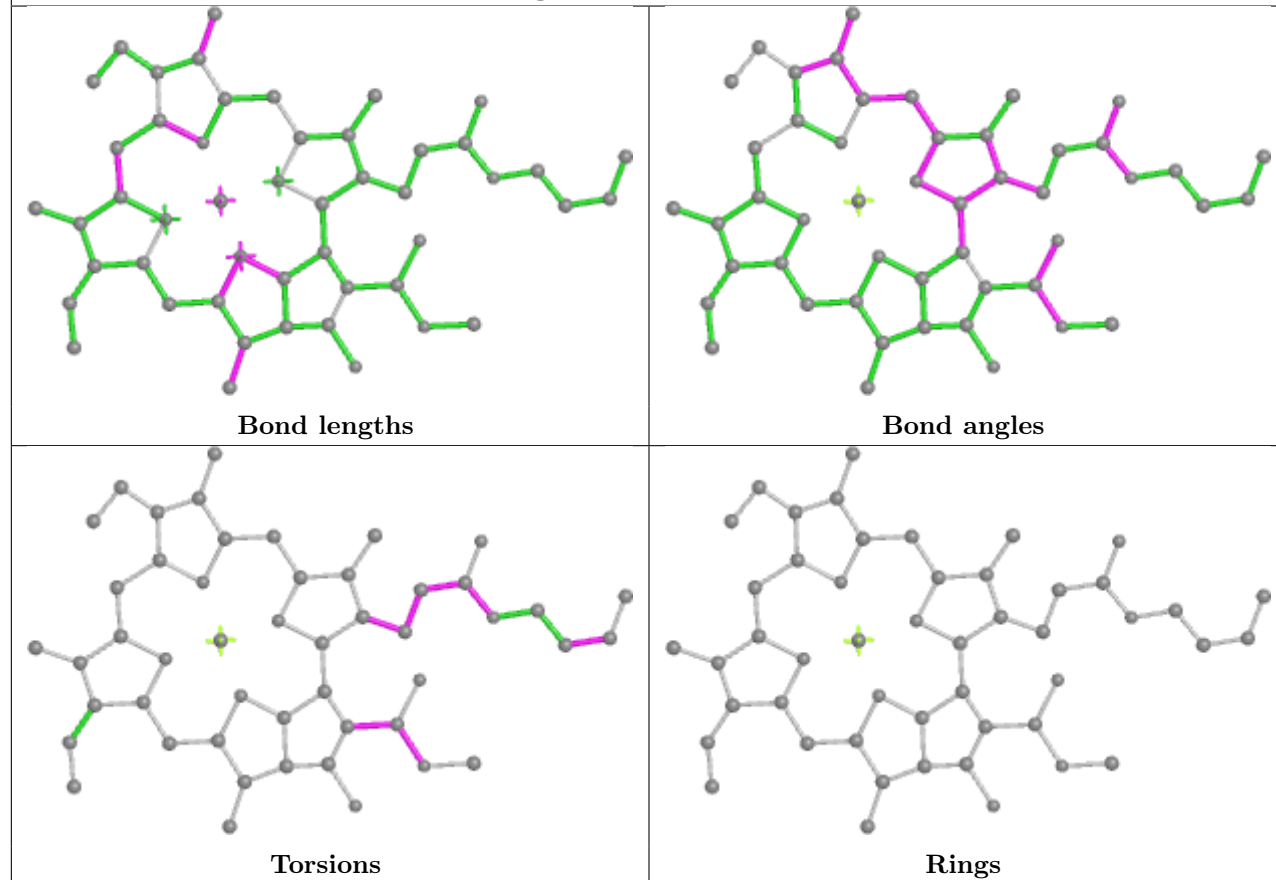
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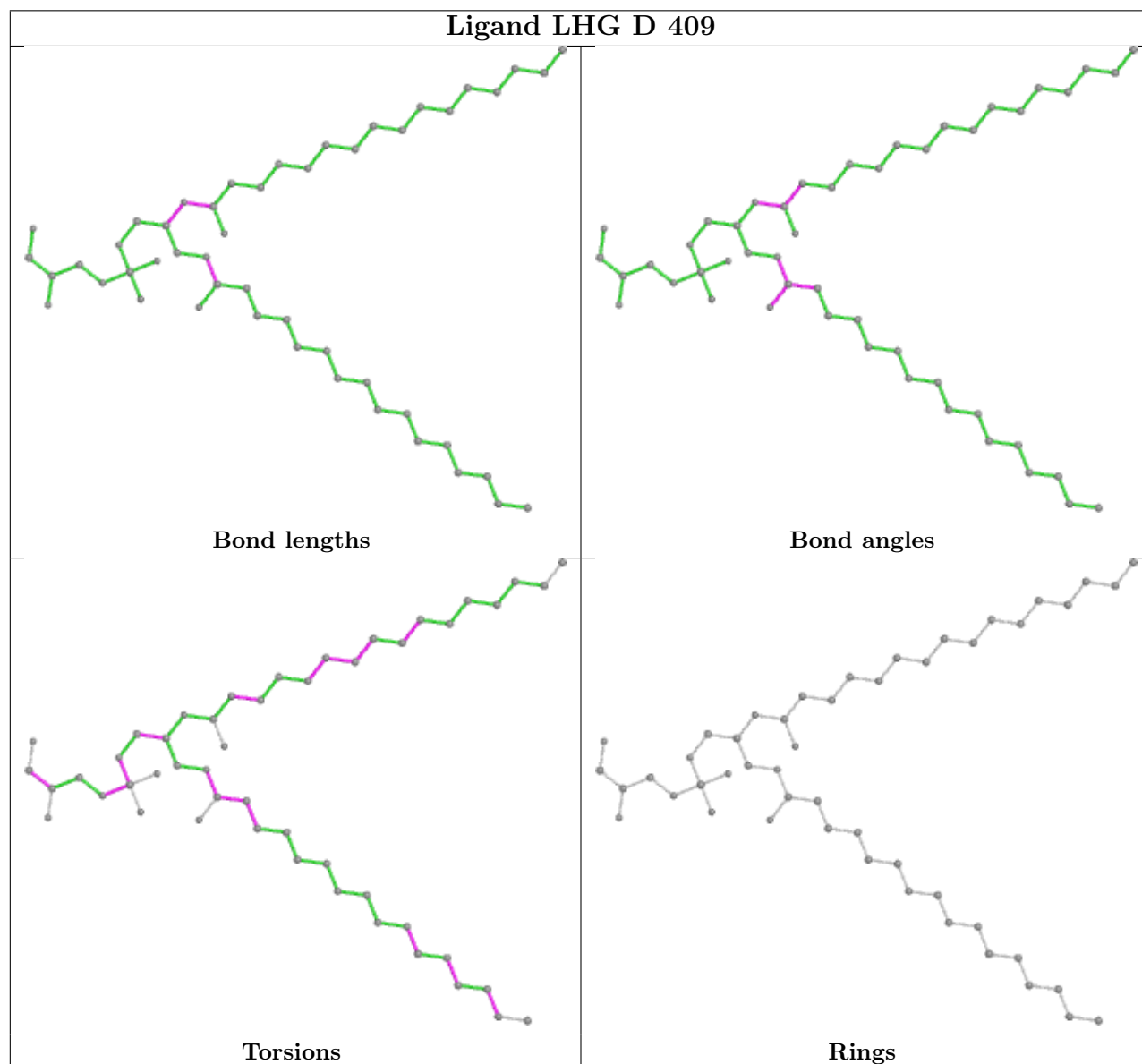
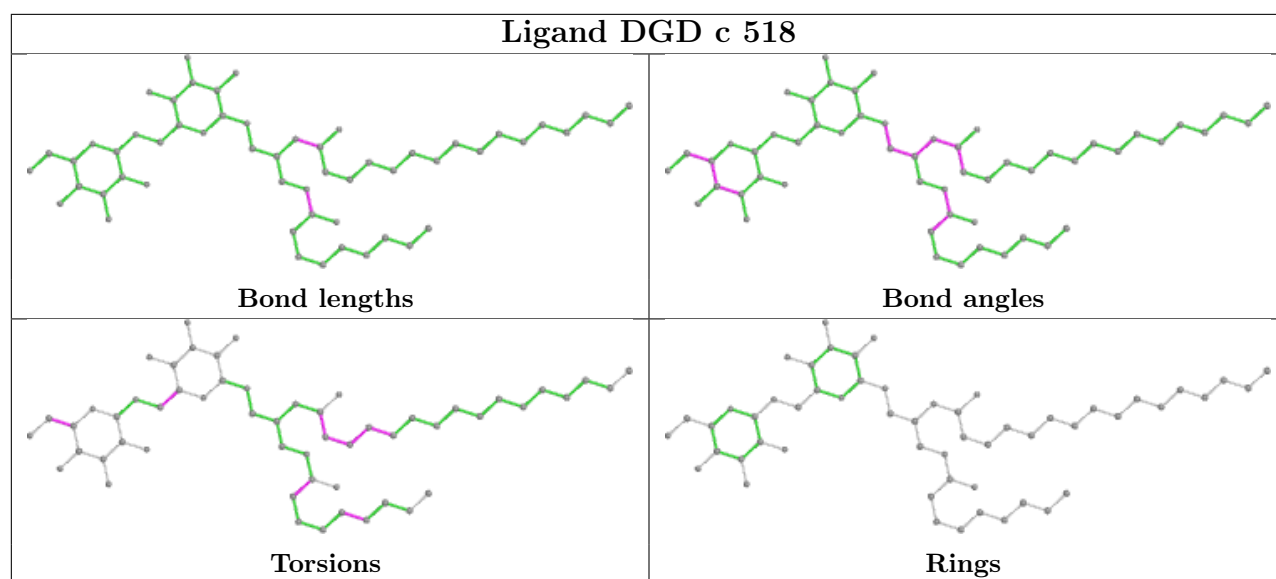


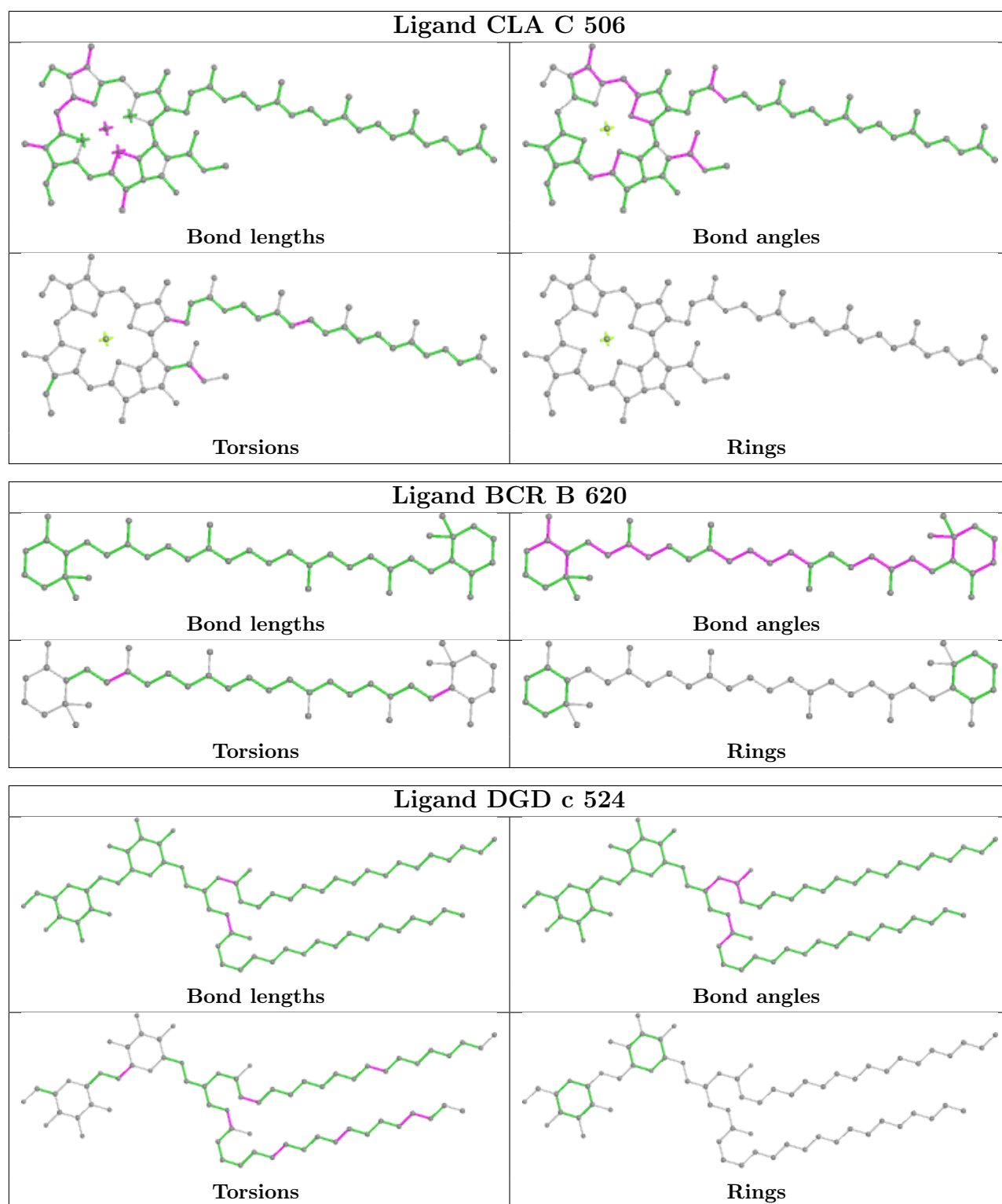
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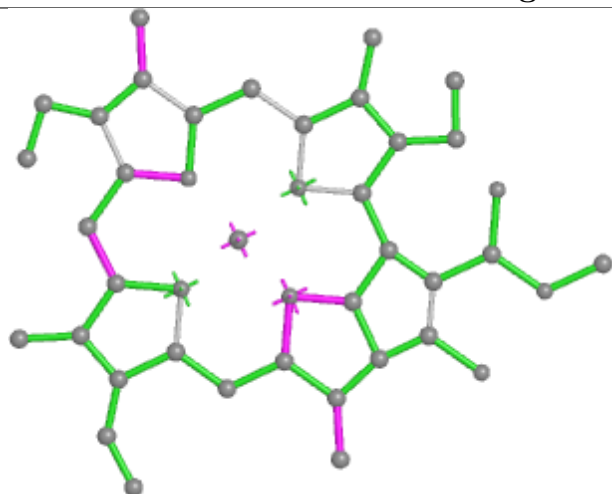
Ligand CLA R 603



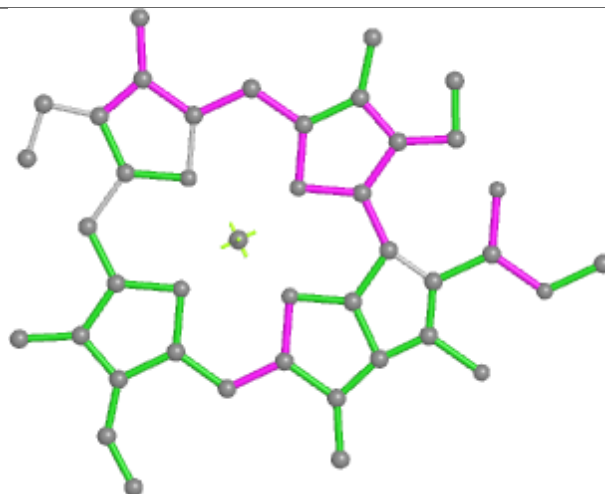




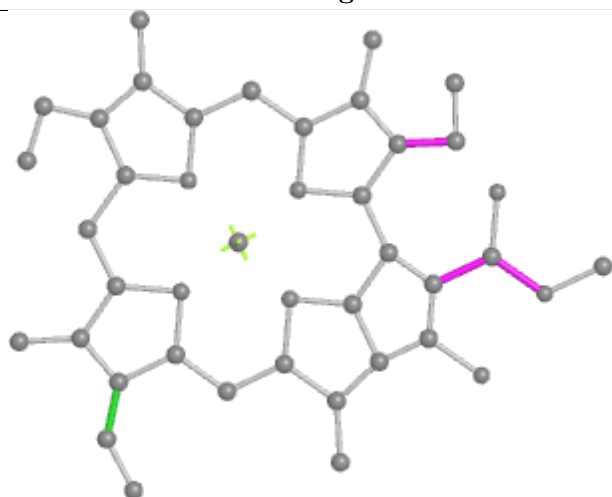
Ligand CLA s 603



Bond lengths



Bond angles

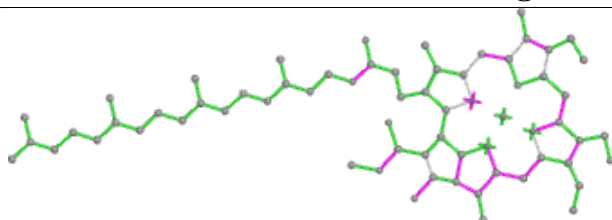


Torsions

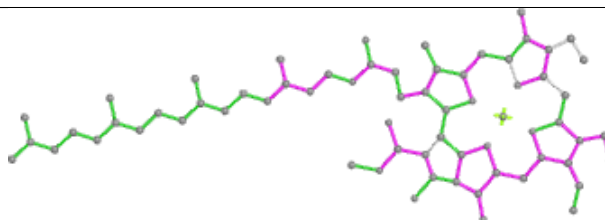


Rings

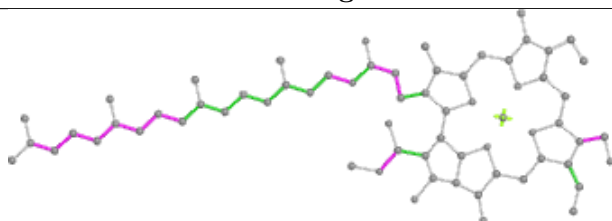
Ligand CHL n 605



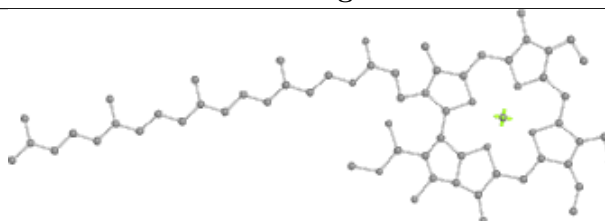
Bond lengths



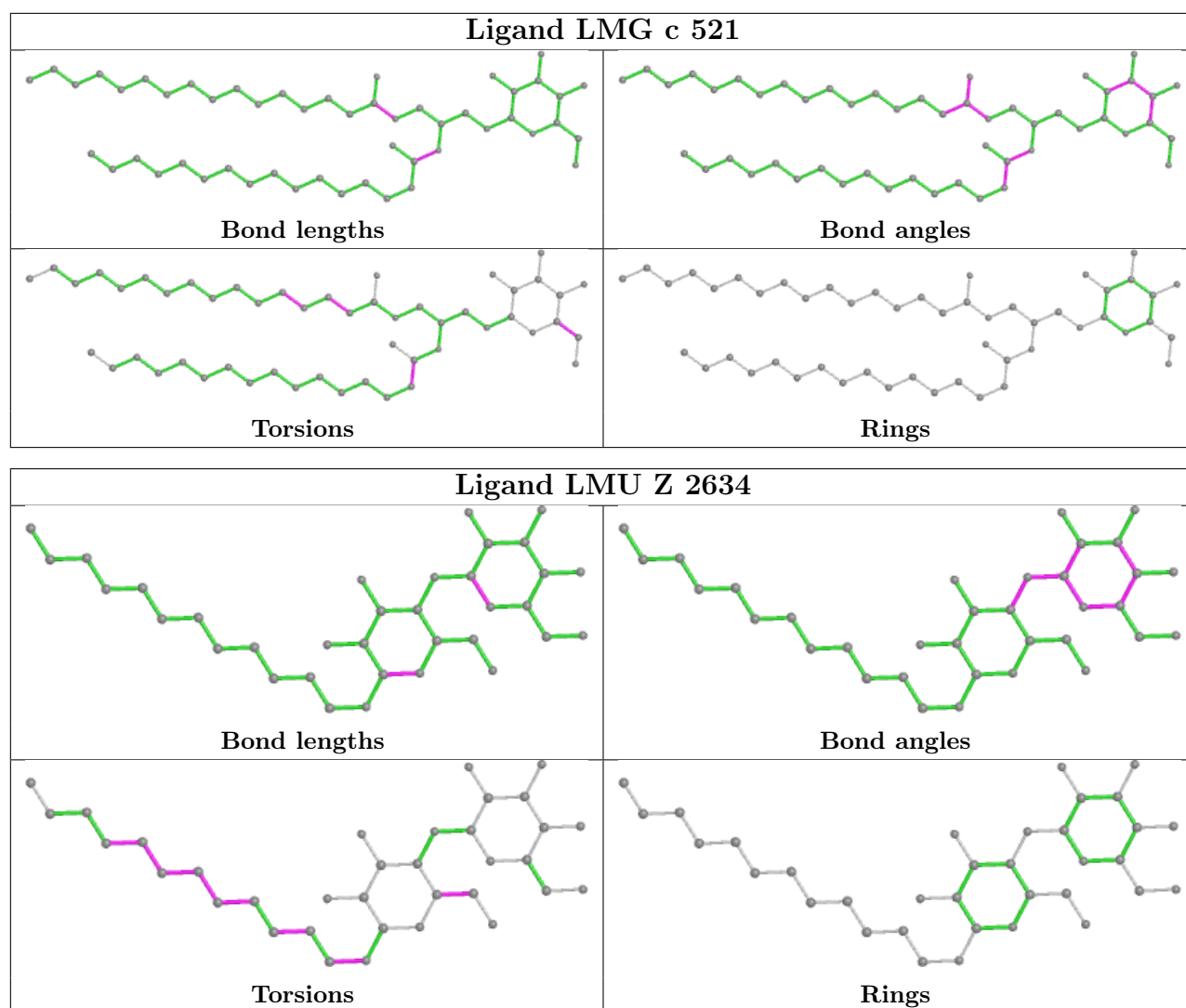
Bond angles

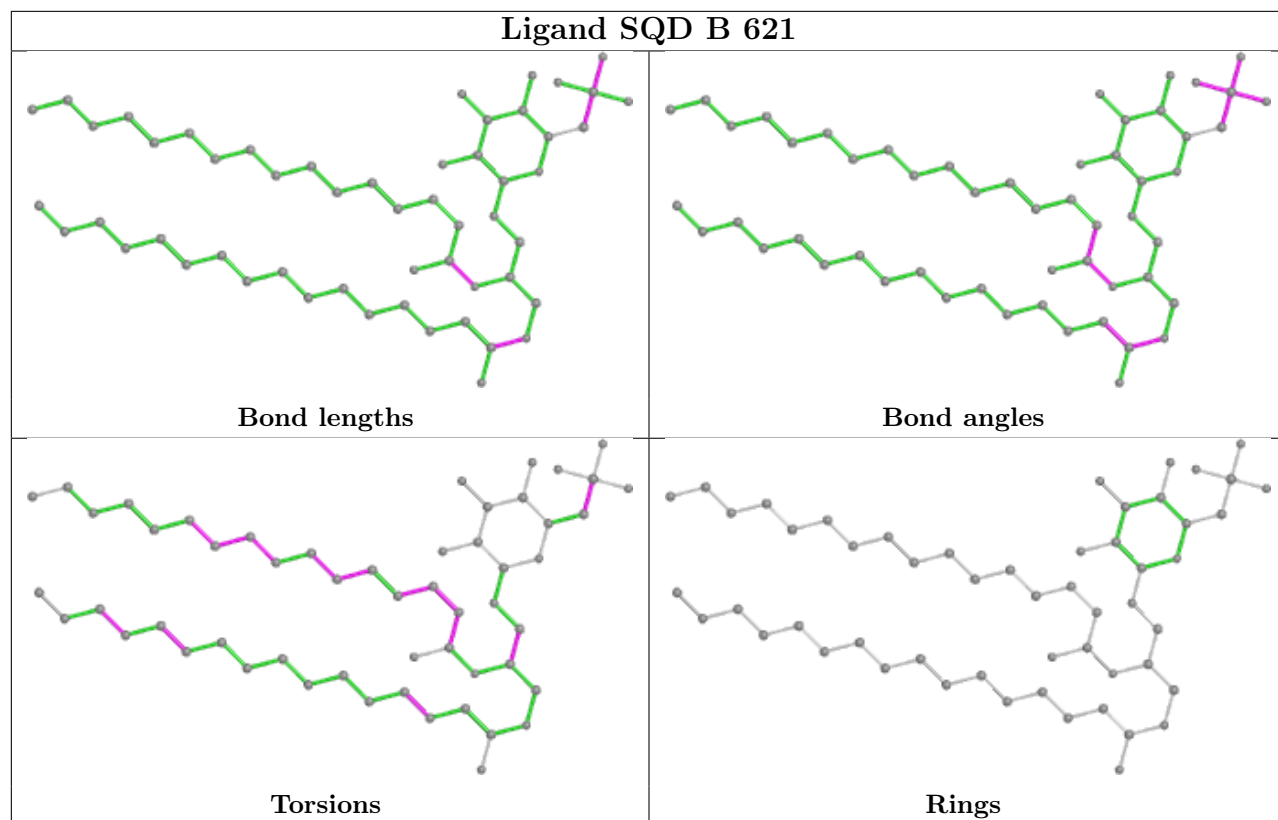


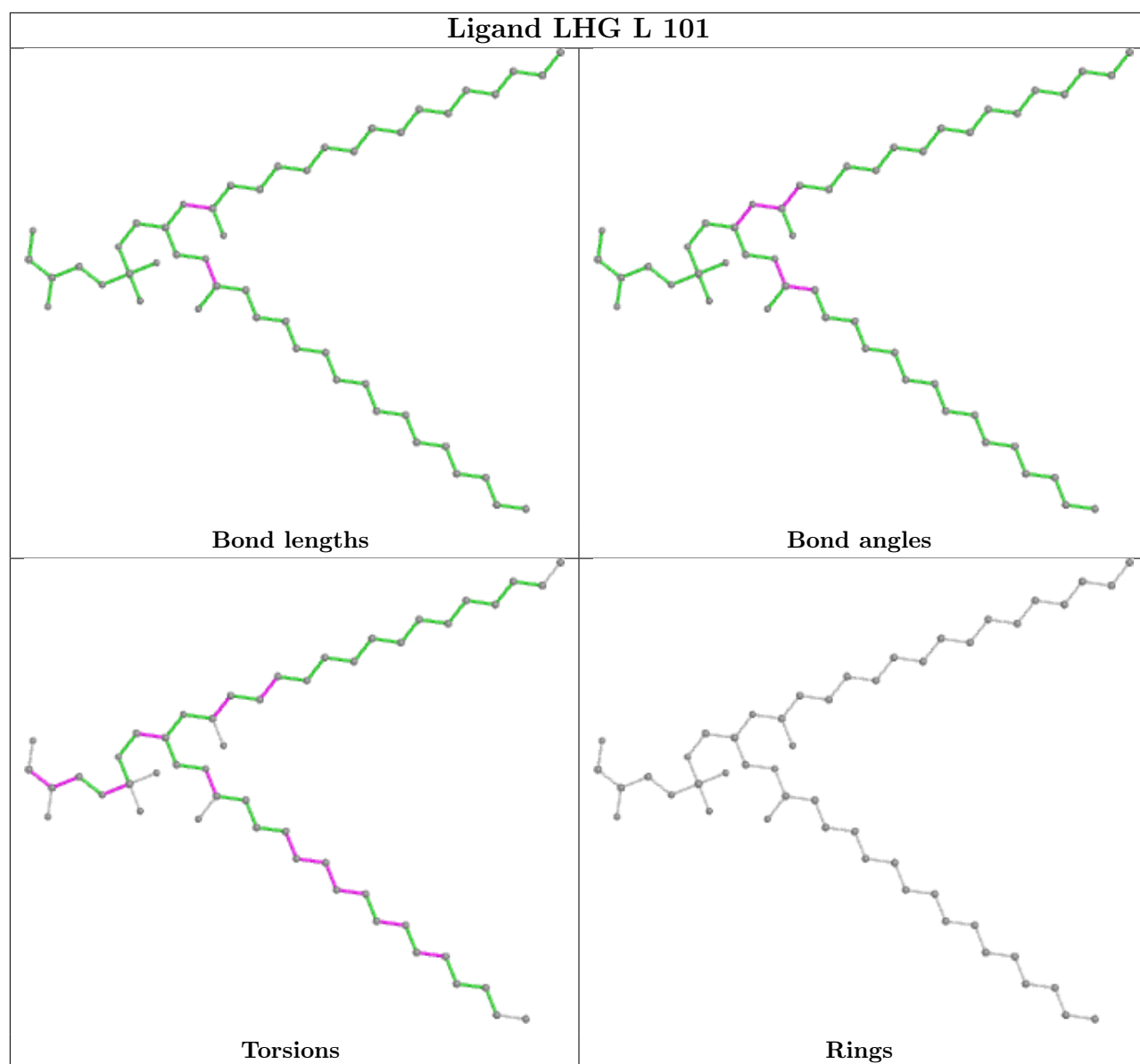
Torsions

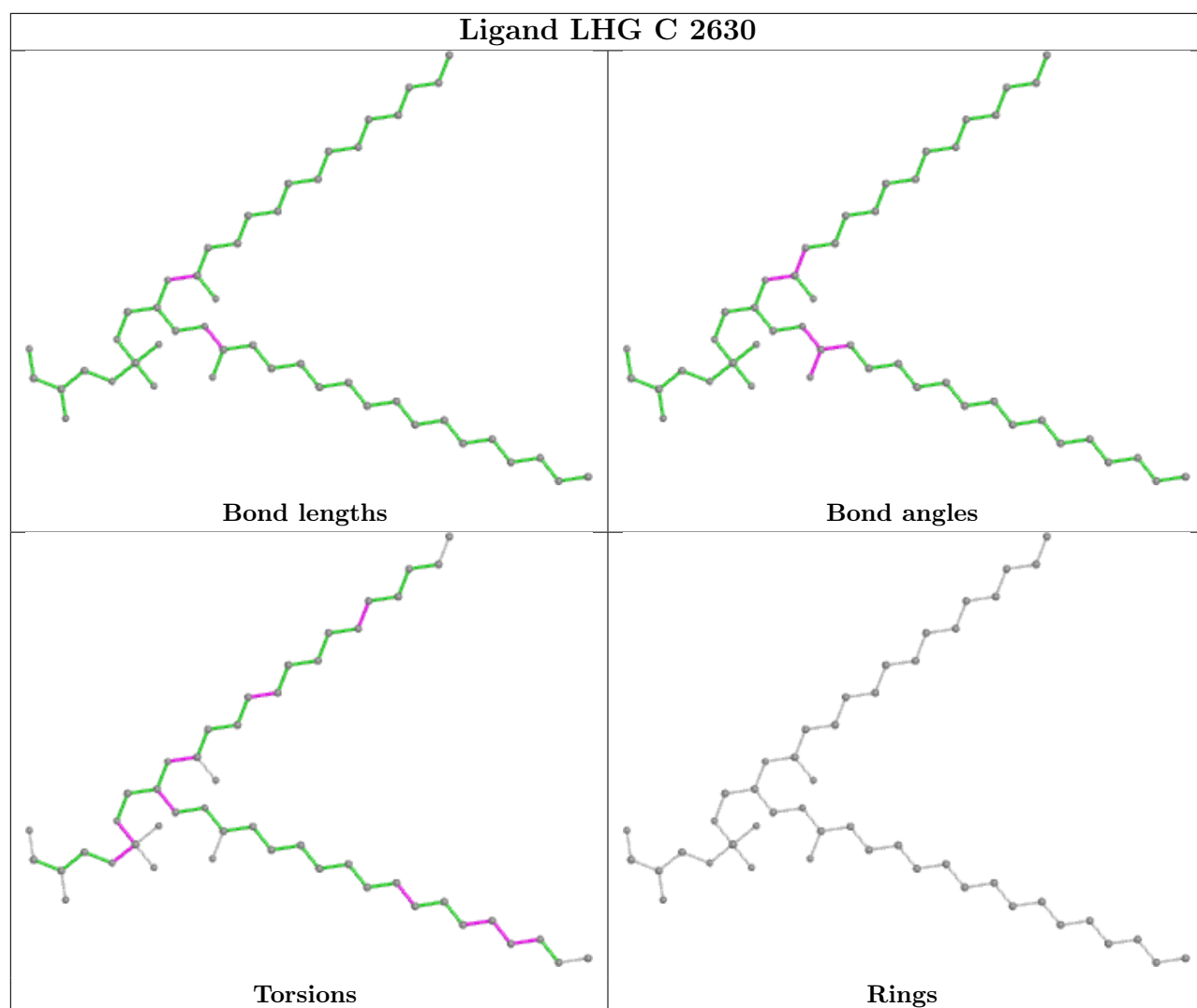


Rings

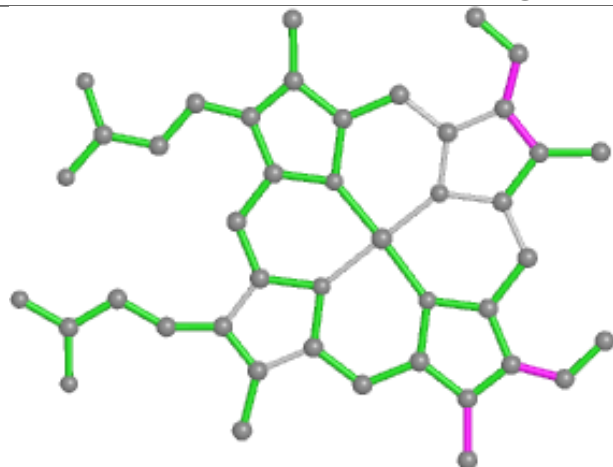




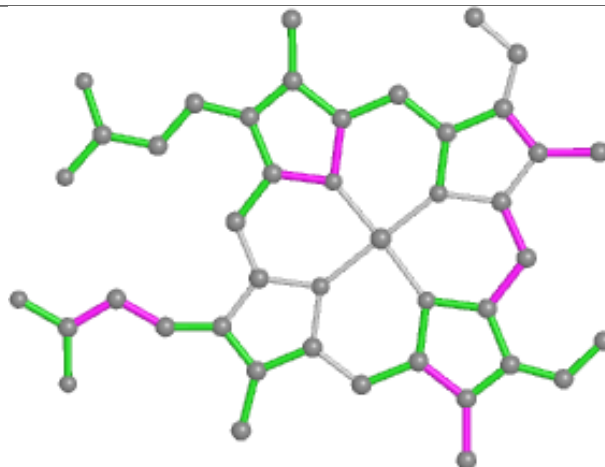




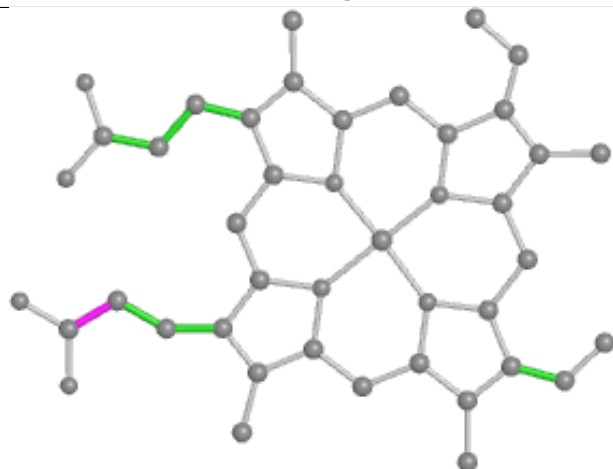
Ligand HEM f 101



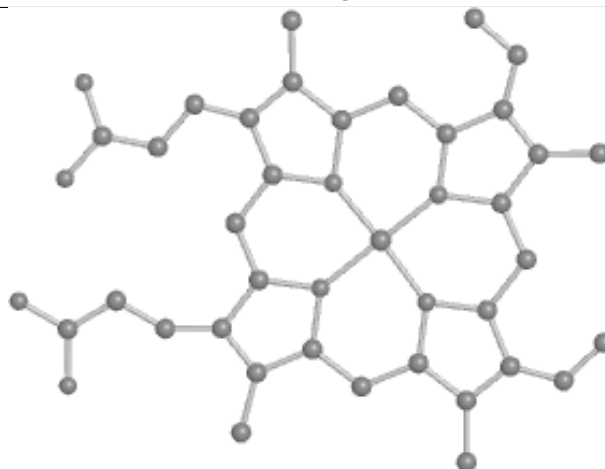
Bond lengths



Bond angles

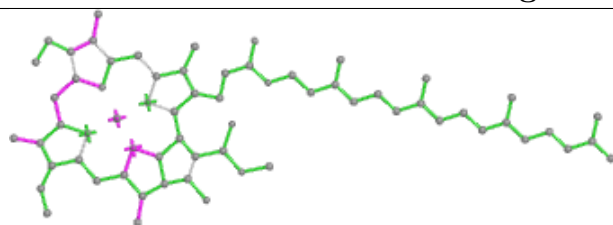


Torsions

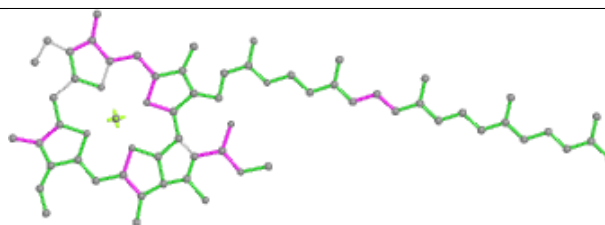


Rings

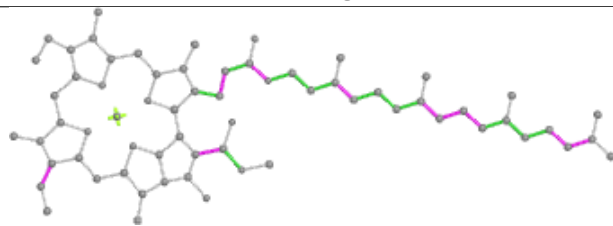
Ligand CLA c 505



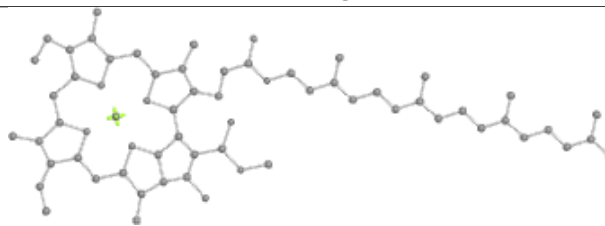
Bond lengths



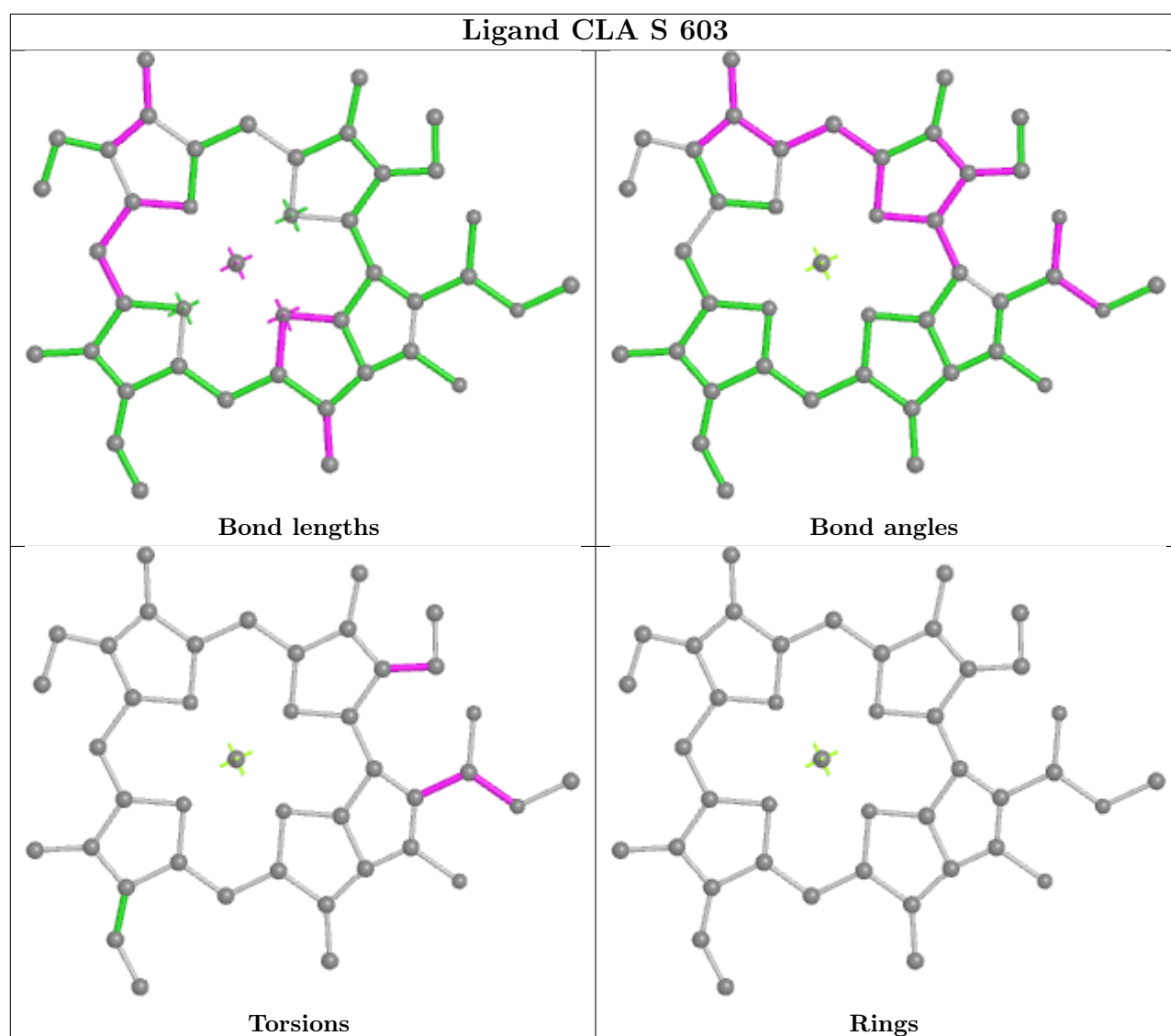
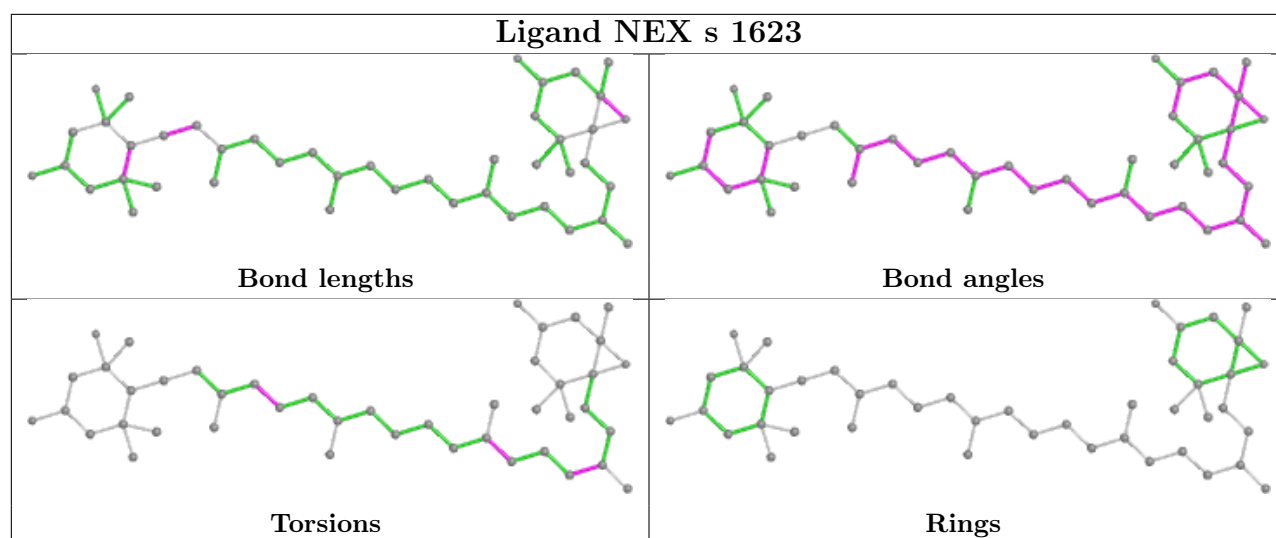
Bond angles

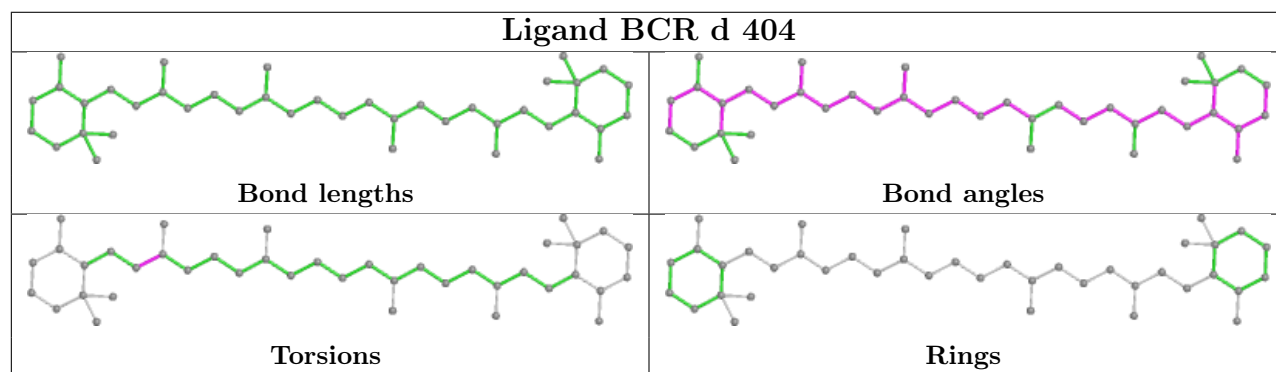
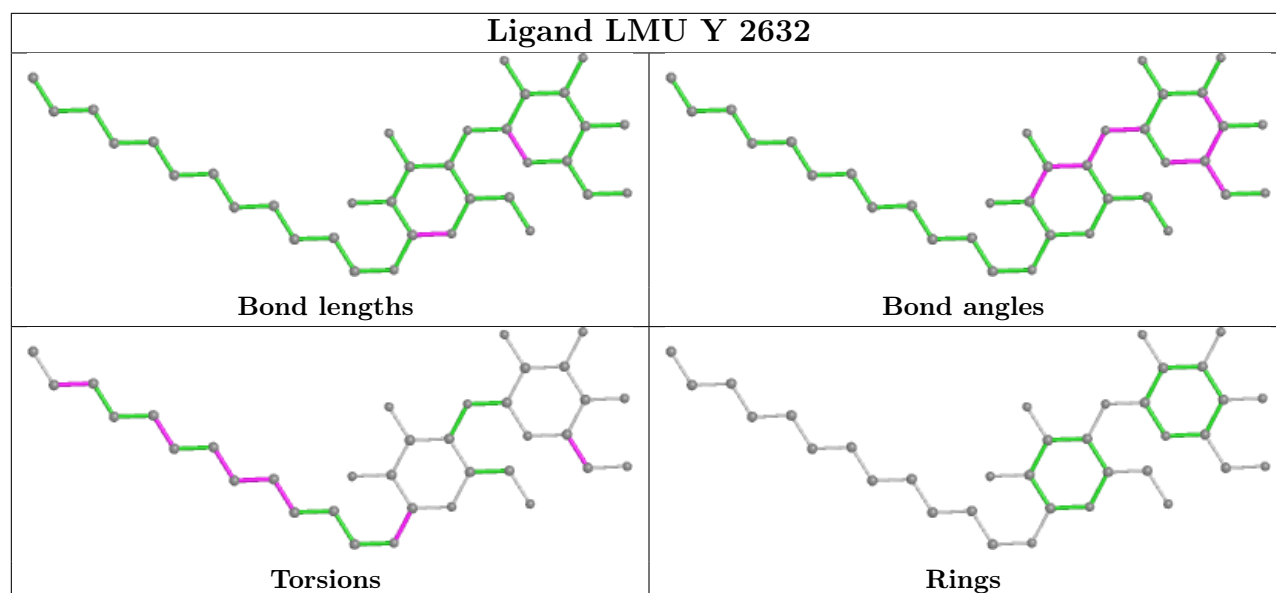
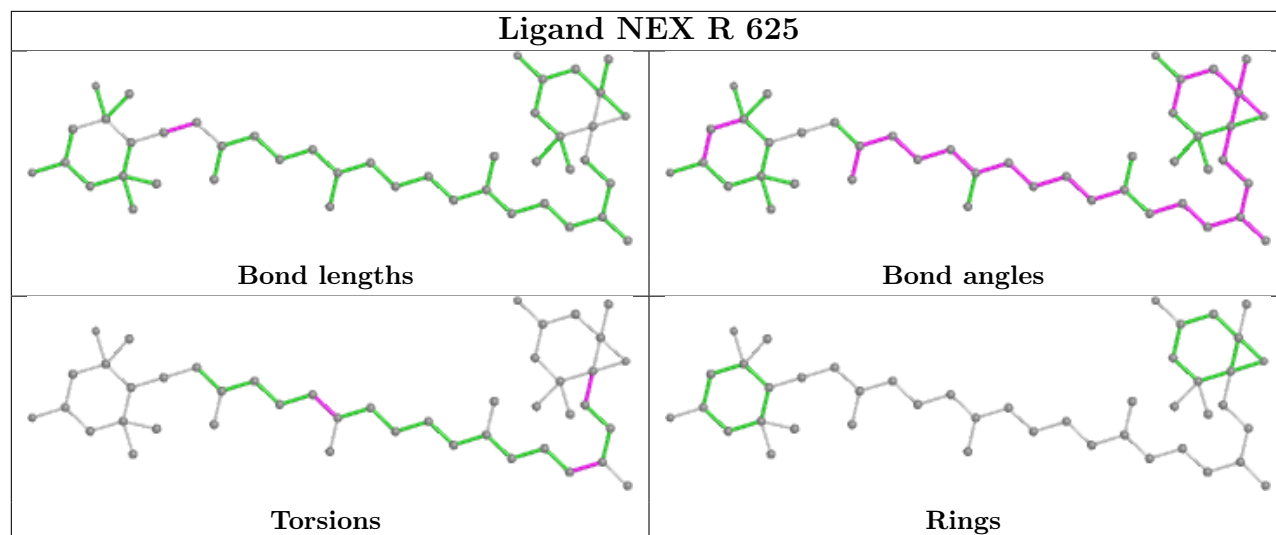


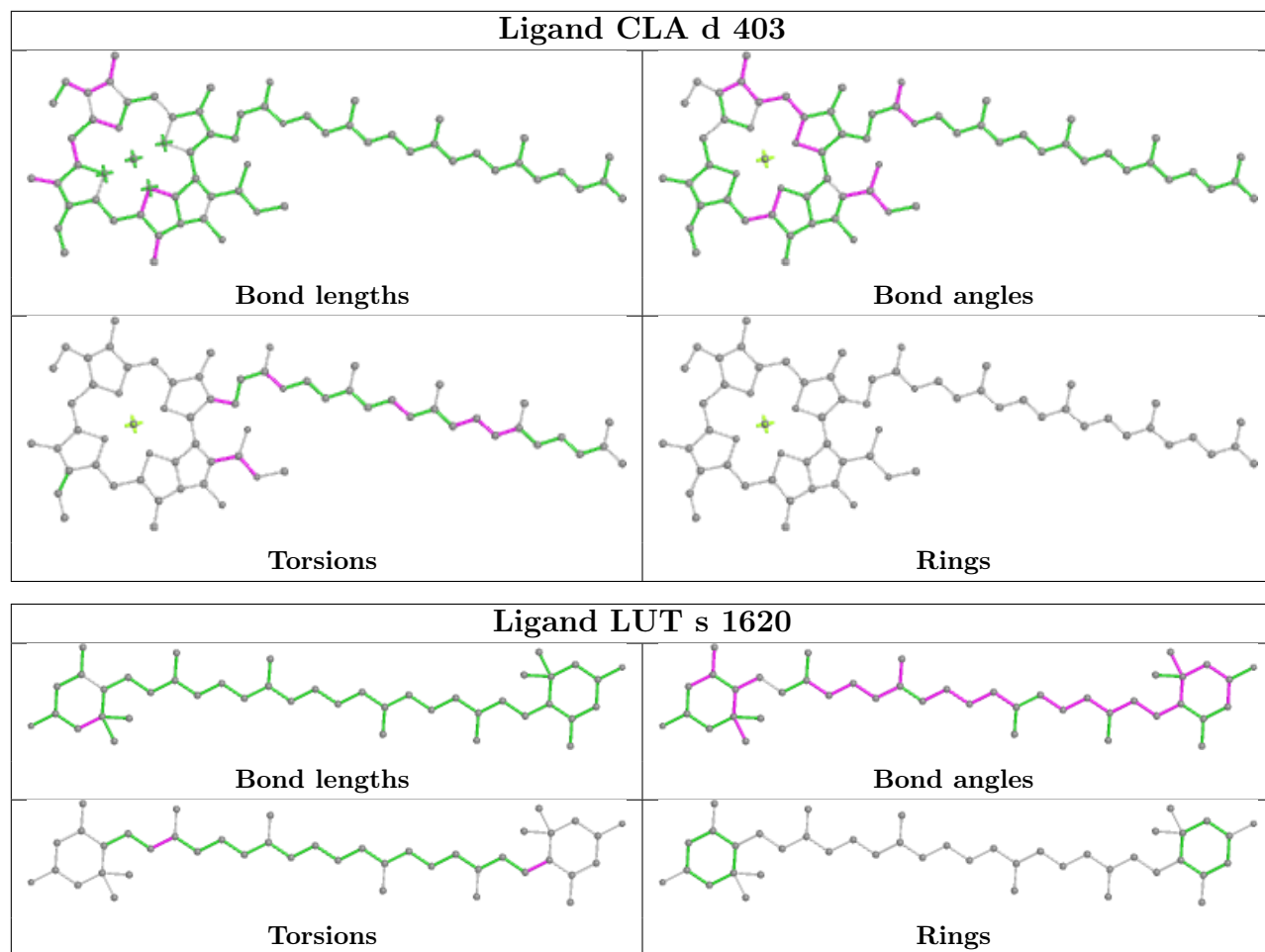
Torsions



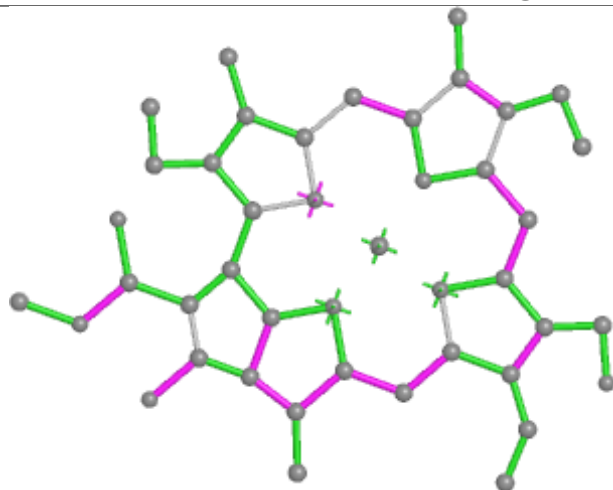
Rings



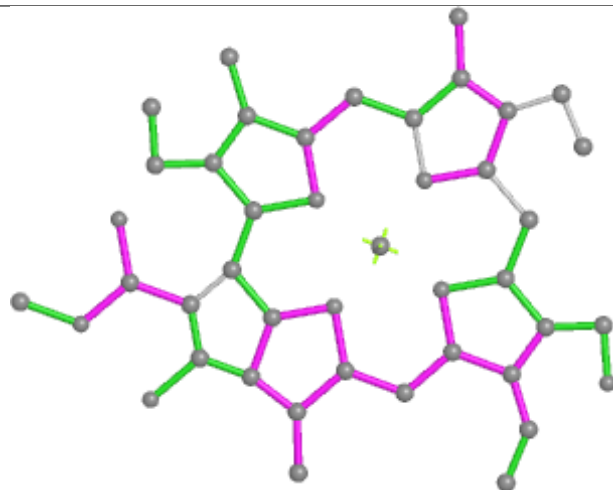




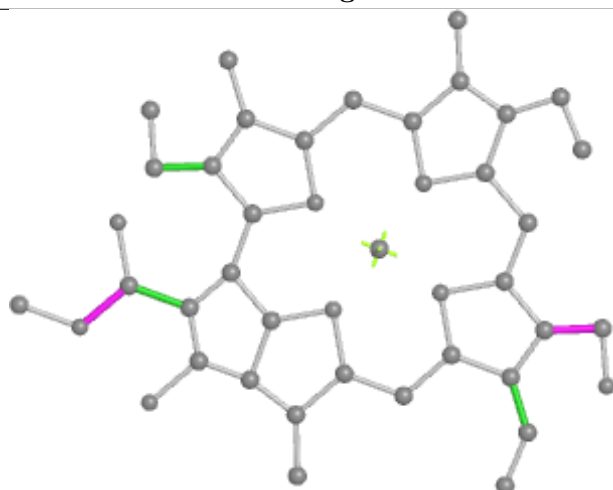
Ligand CHL S 607



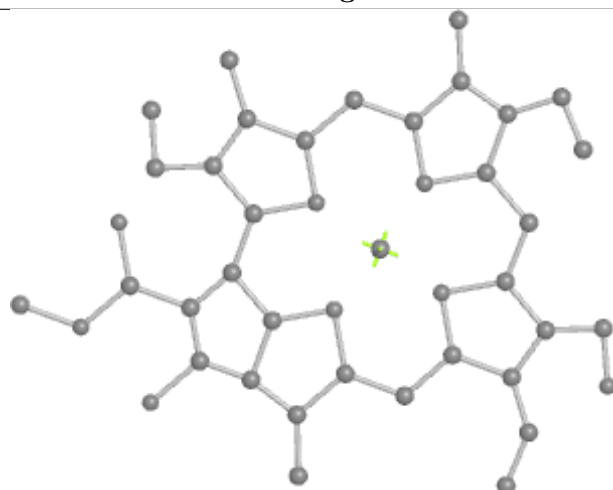
Bond lengths



Bond angles

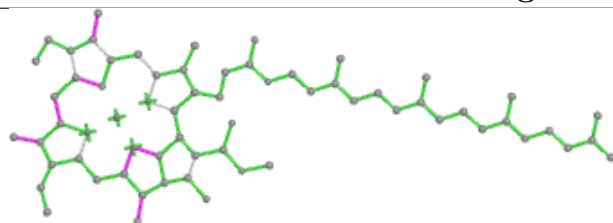


Torsions

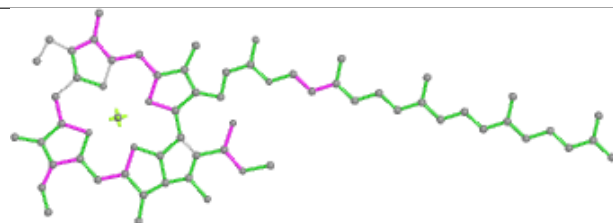


Rings

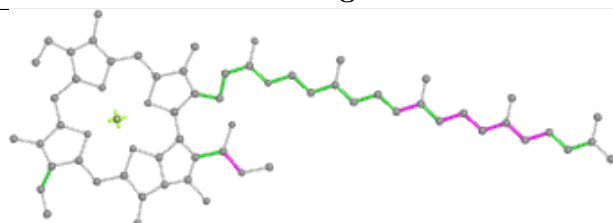
Ligand CLA b 612



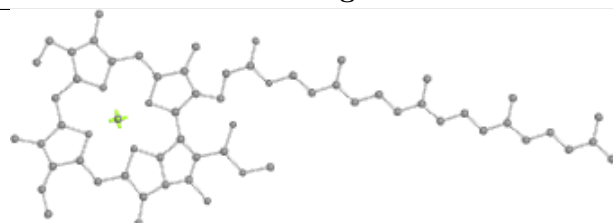
Bond lengths



Bond angles

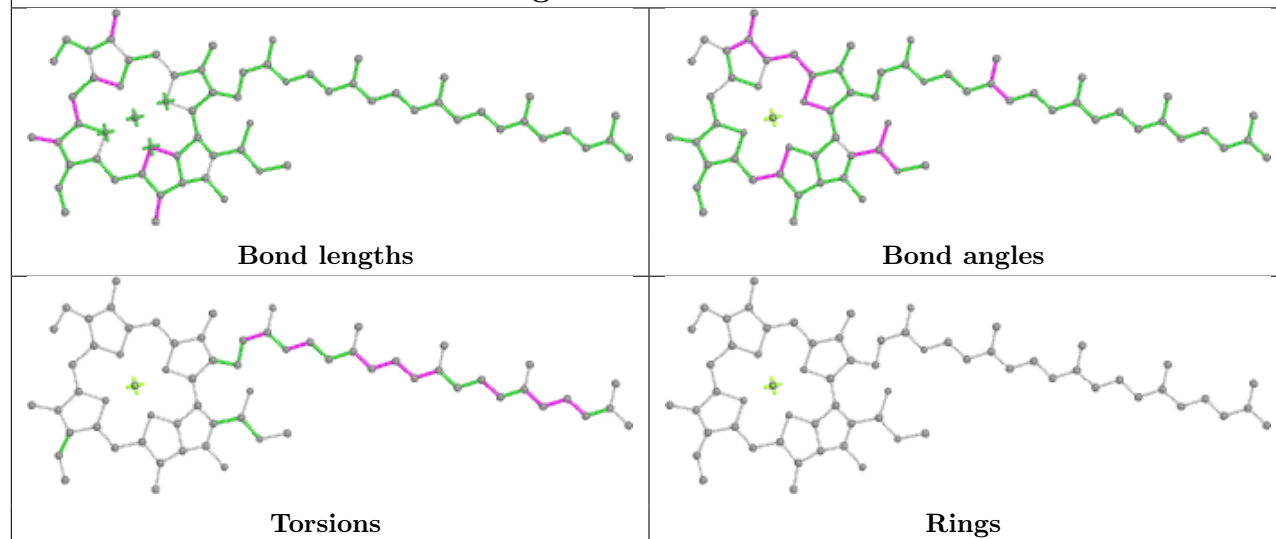


Torsions

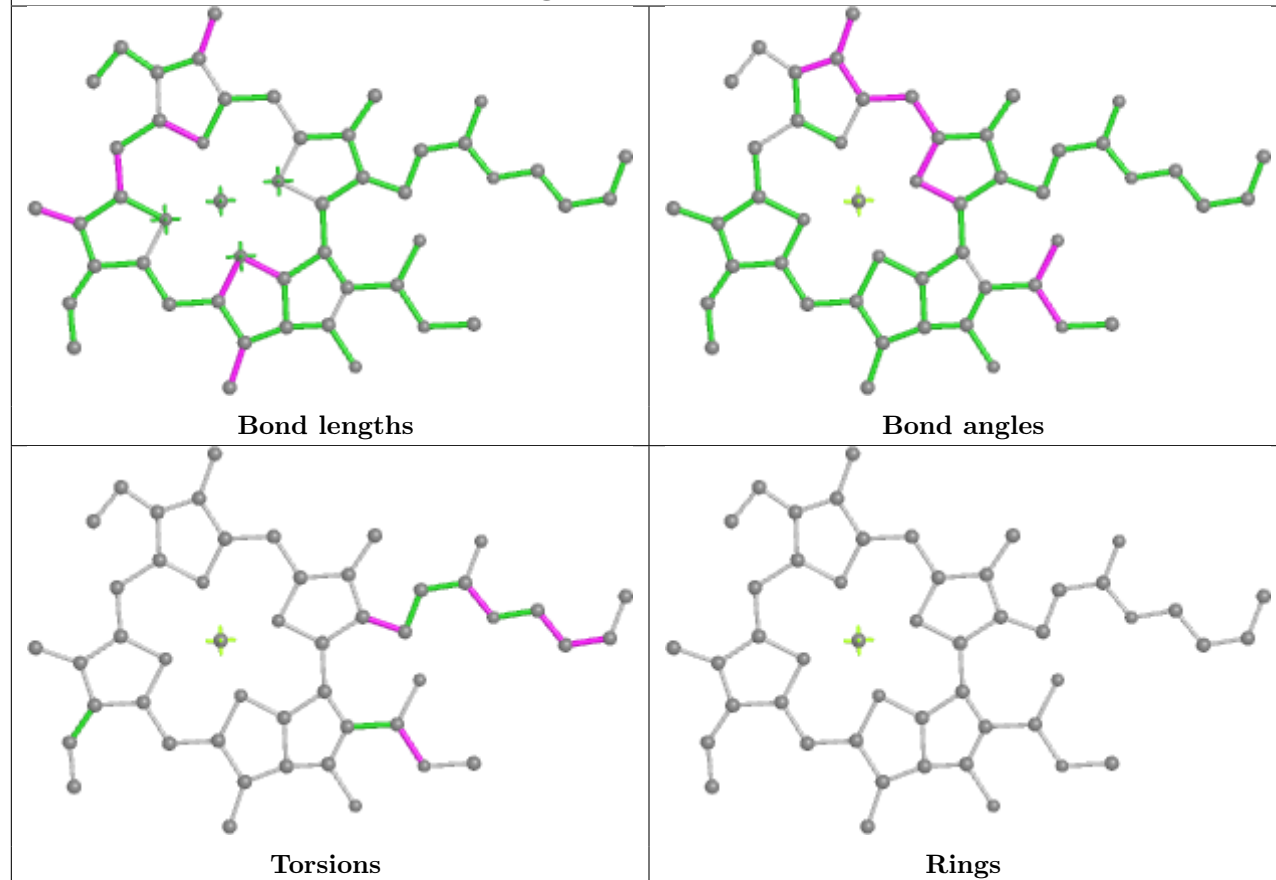


Rings

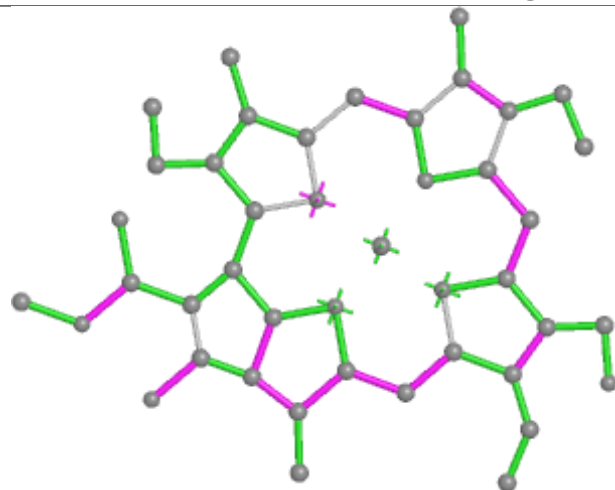
Ligand CLA B 603



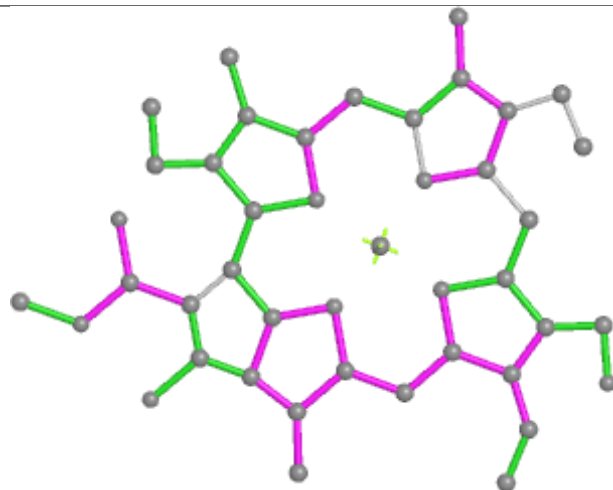
Ligand CLA s 611



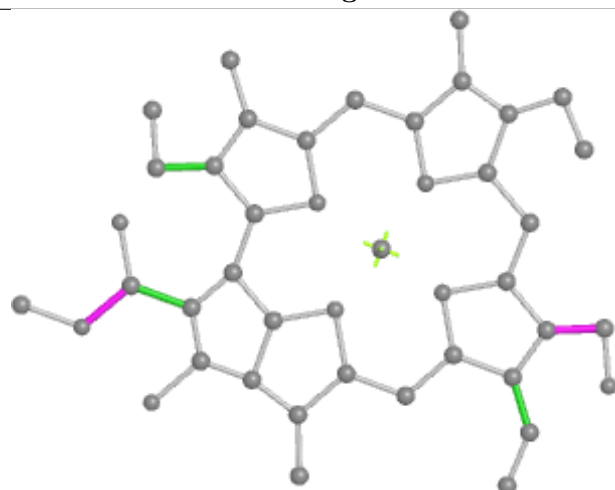
Ligand CHL s 607



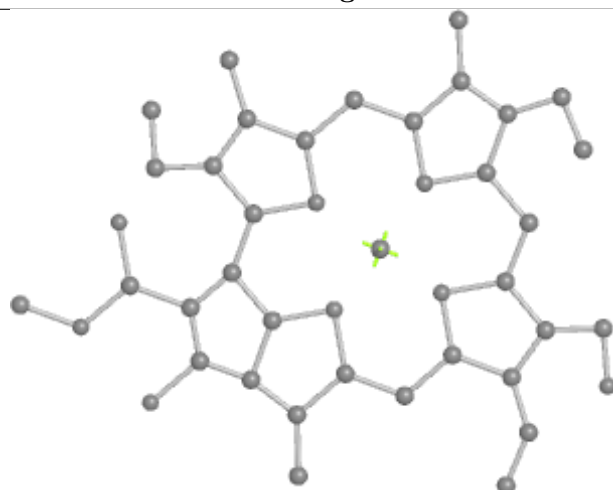
Bond lengths



Bond angles

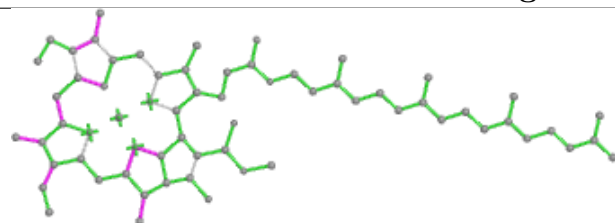


Torsions

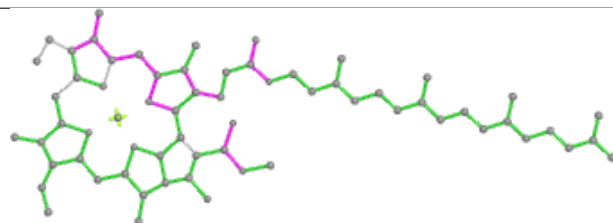


Rings

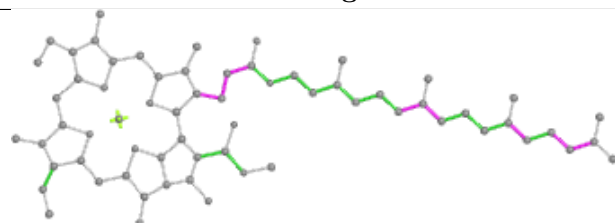
Ligand CLA n 603



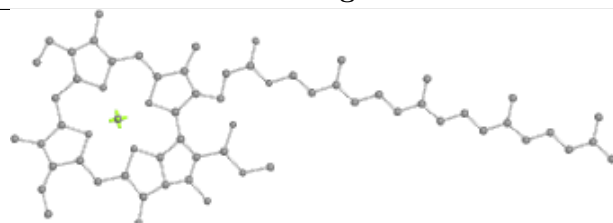
Bond lengths



Bond angles

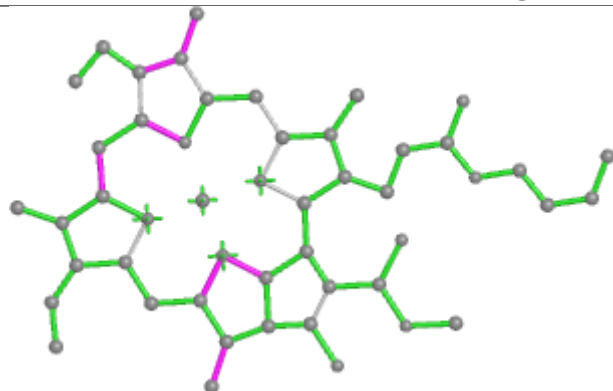


Torsions

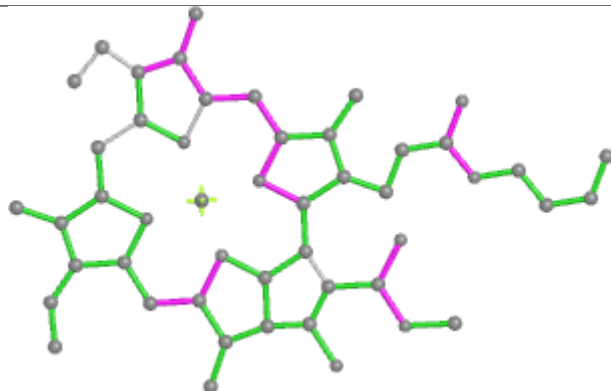


Rings

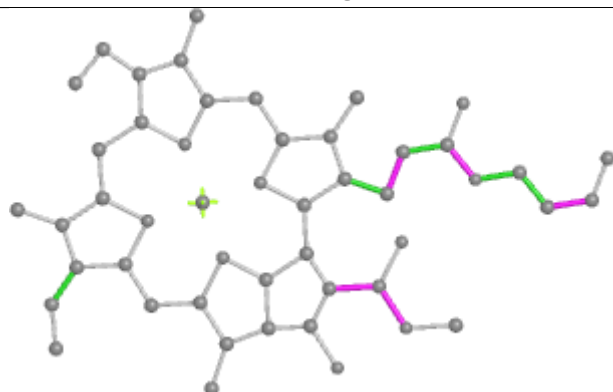
Ligand CLA N 614



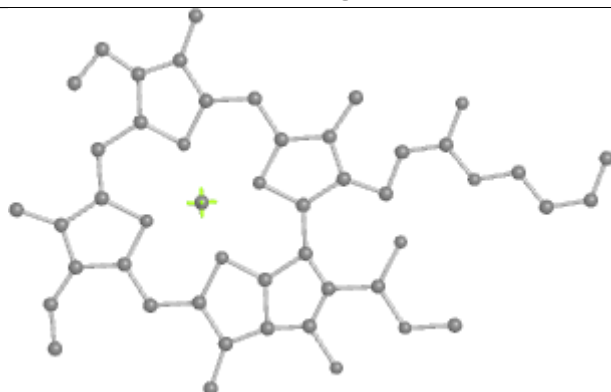
Bond lengths



Bond angles

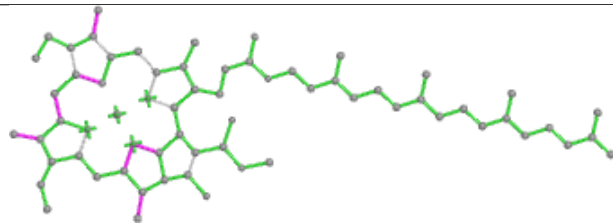


Torsions

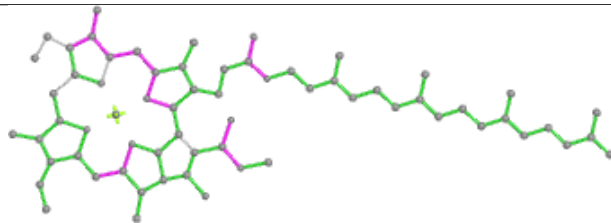


Rings

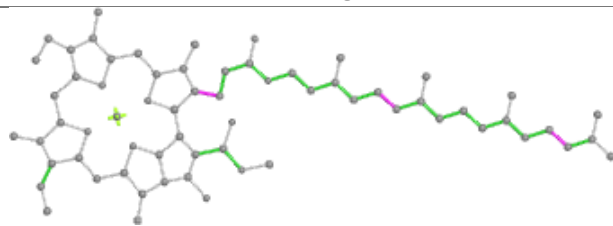
Ligand CLA n 610



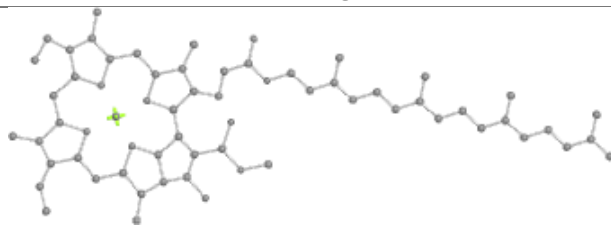
Bond lengths



Bond angles

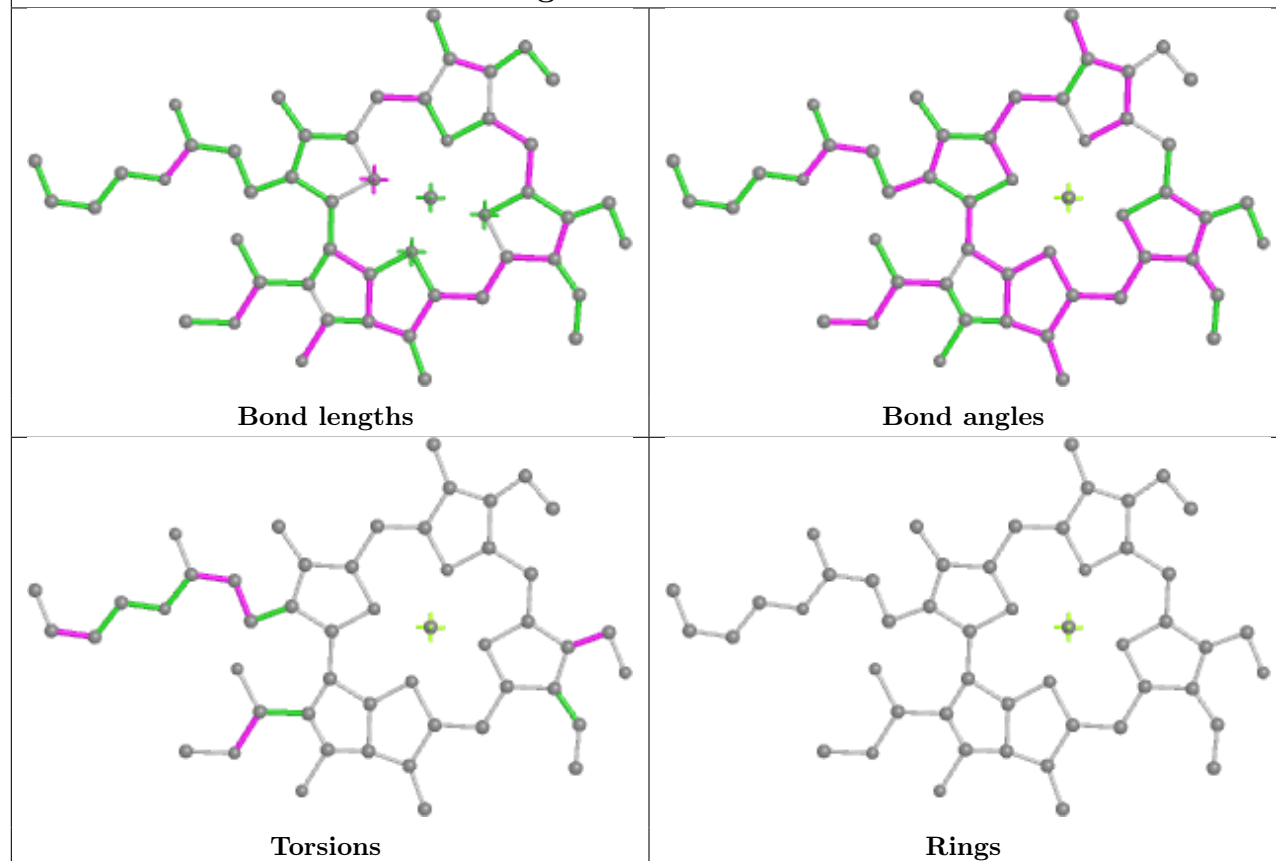


Torsions

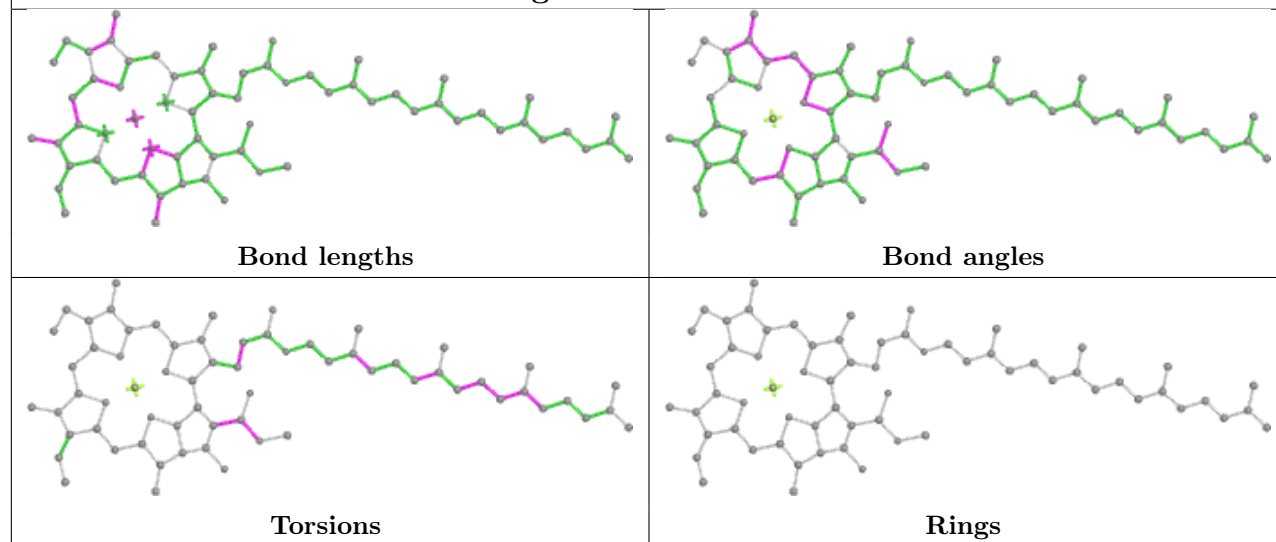


Rings

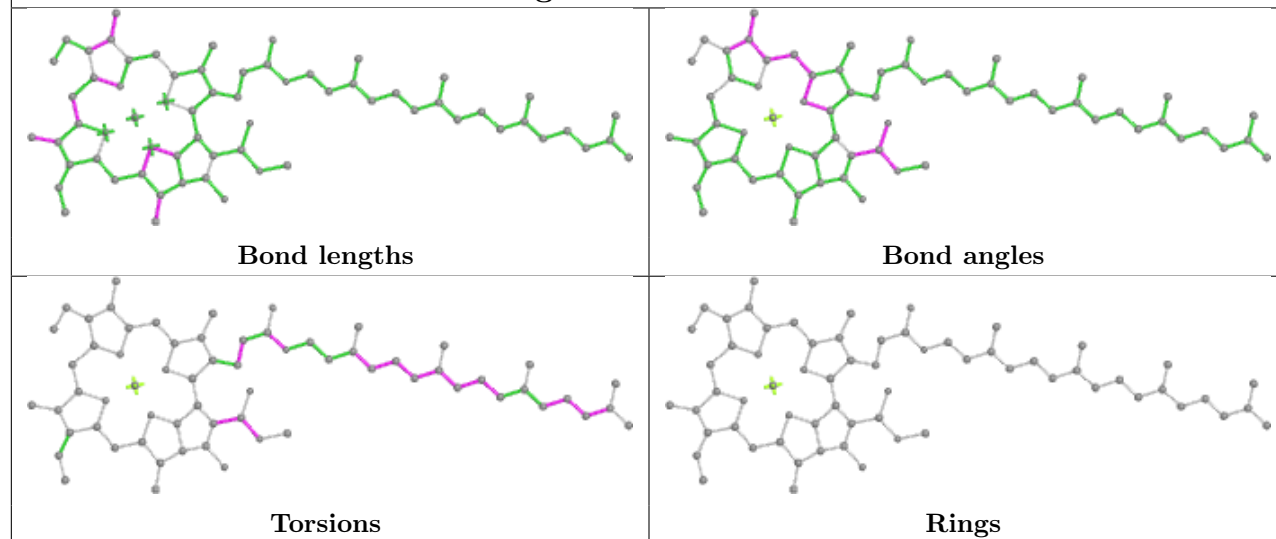
Ligand CHL r 607



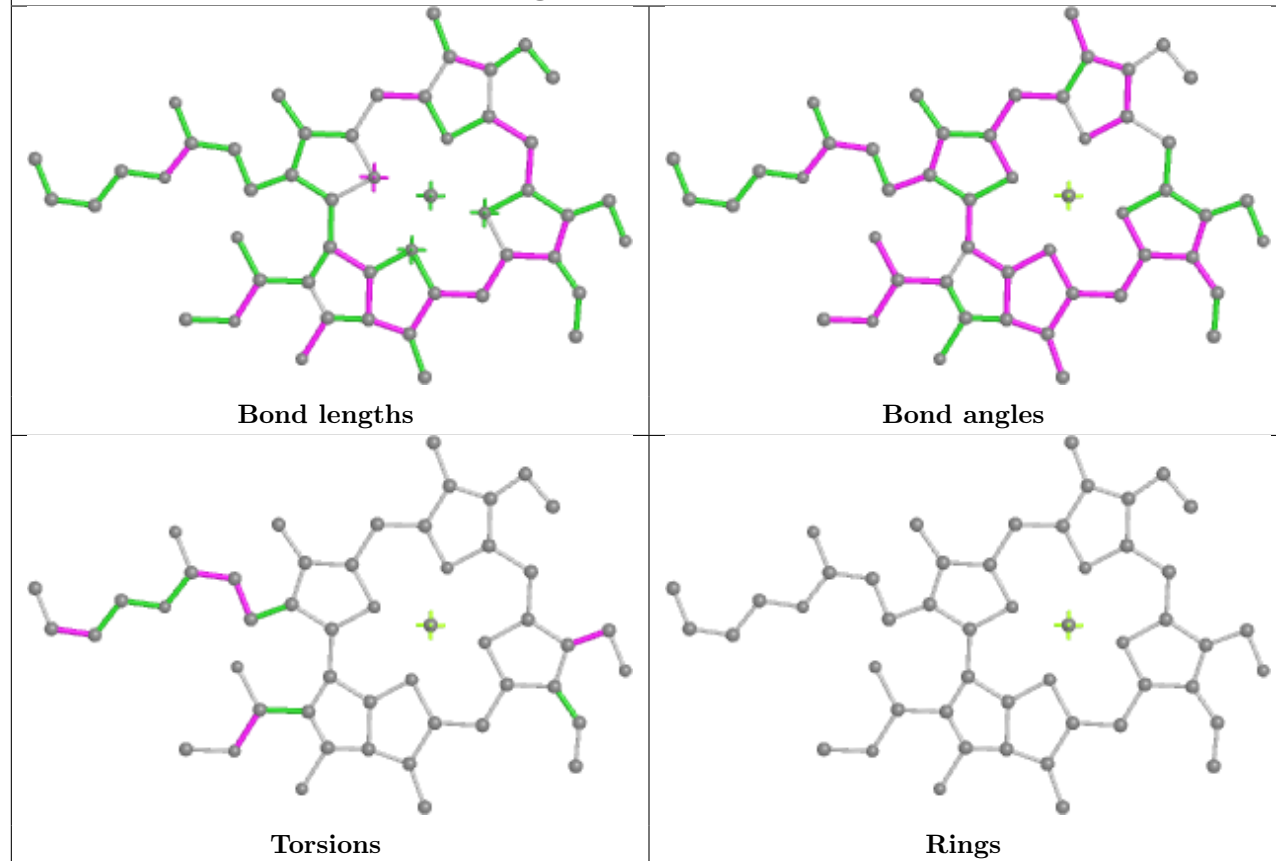
Ligand CLA Y 604



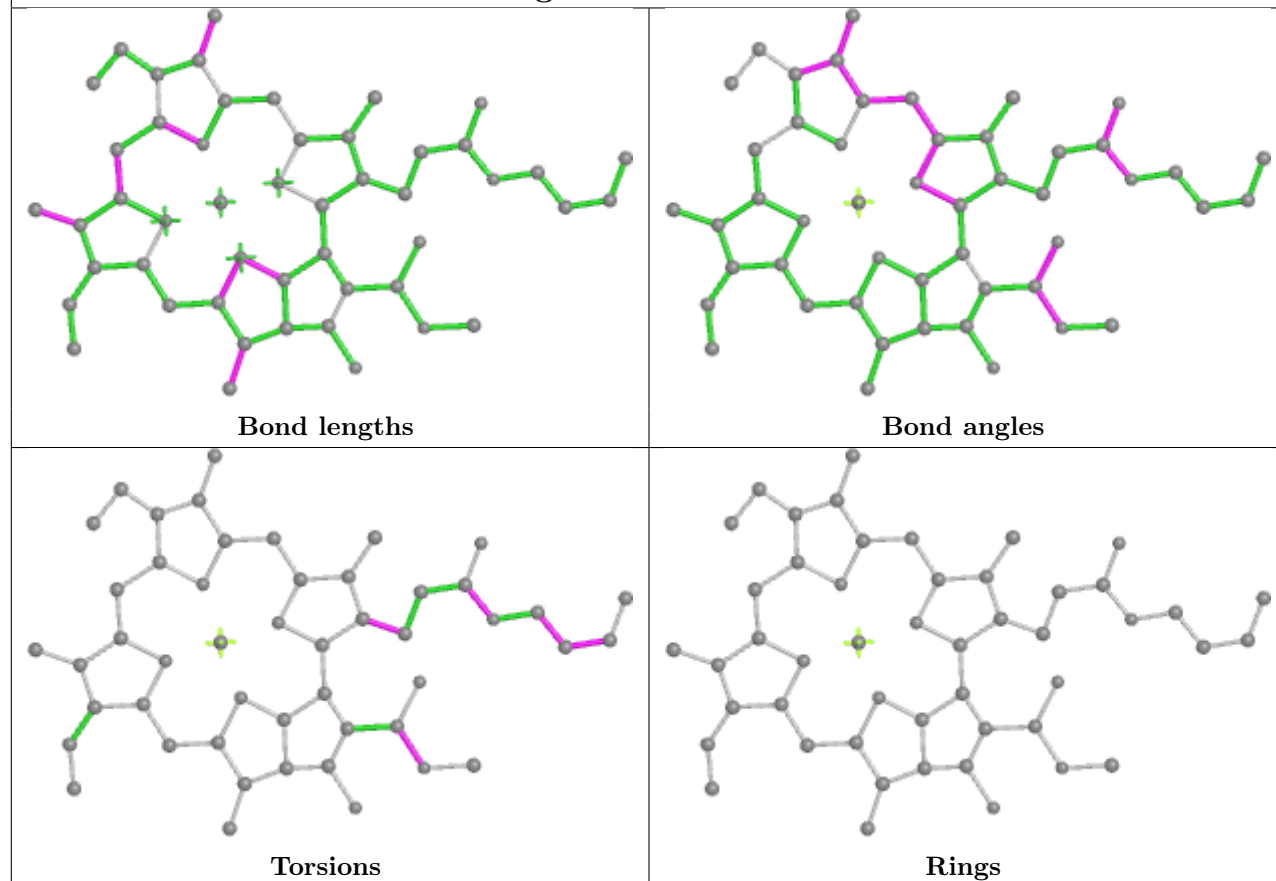
Ligand CLA b 615



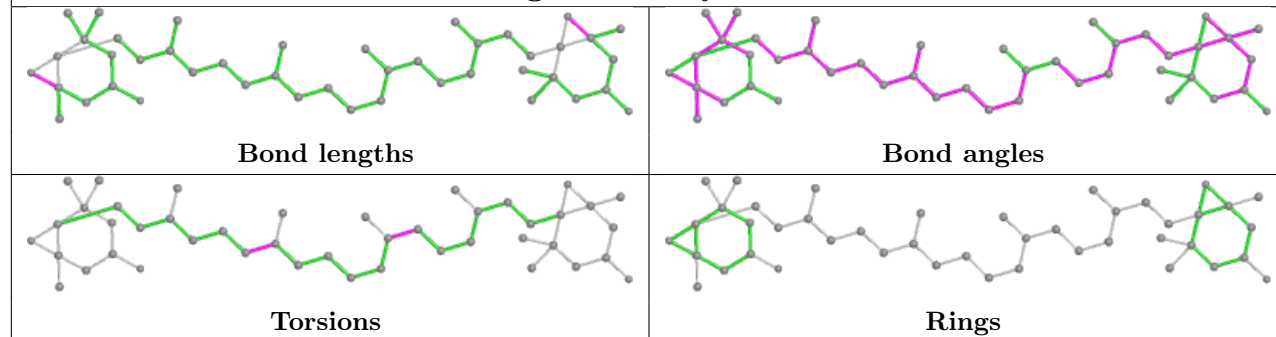
Ligand CHL R 607



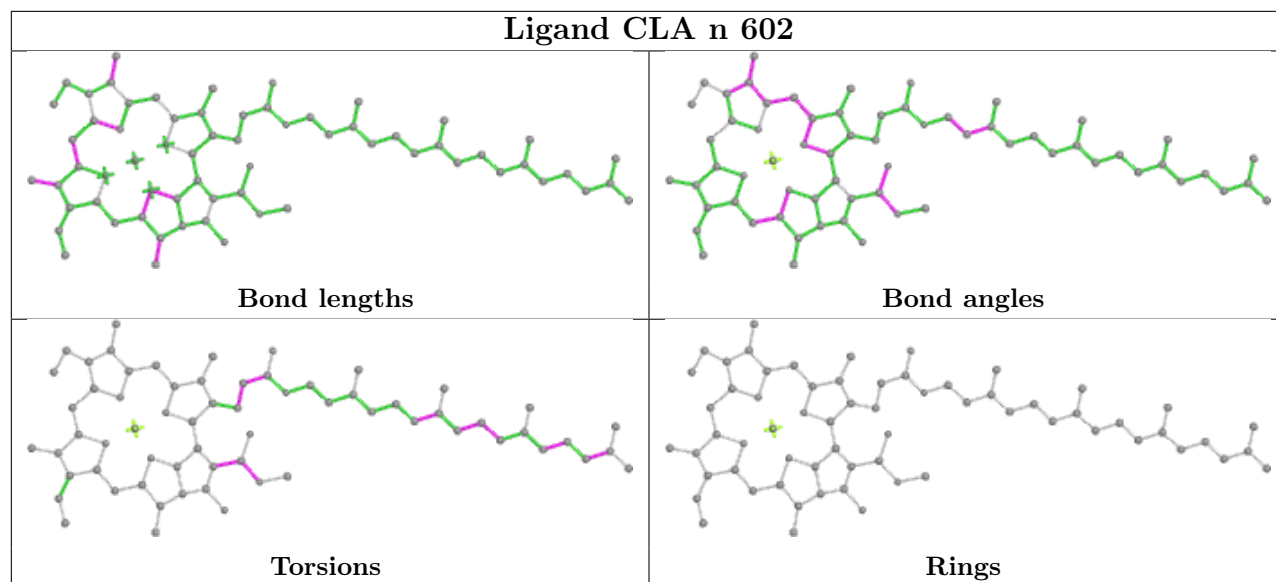
Ligand CLA S 611



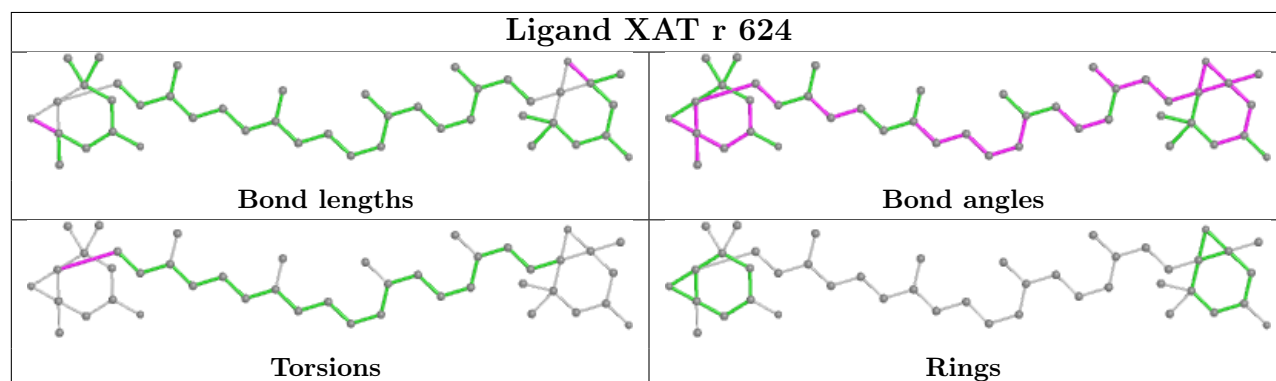
Ligand XAT y 1622



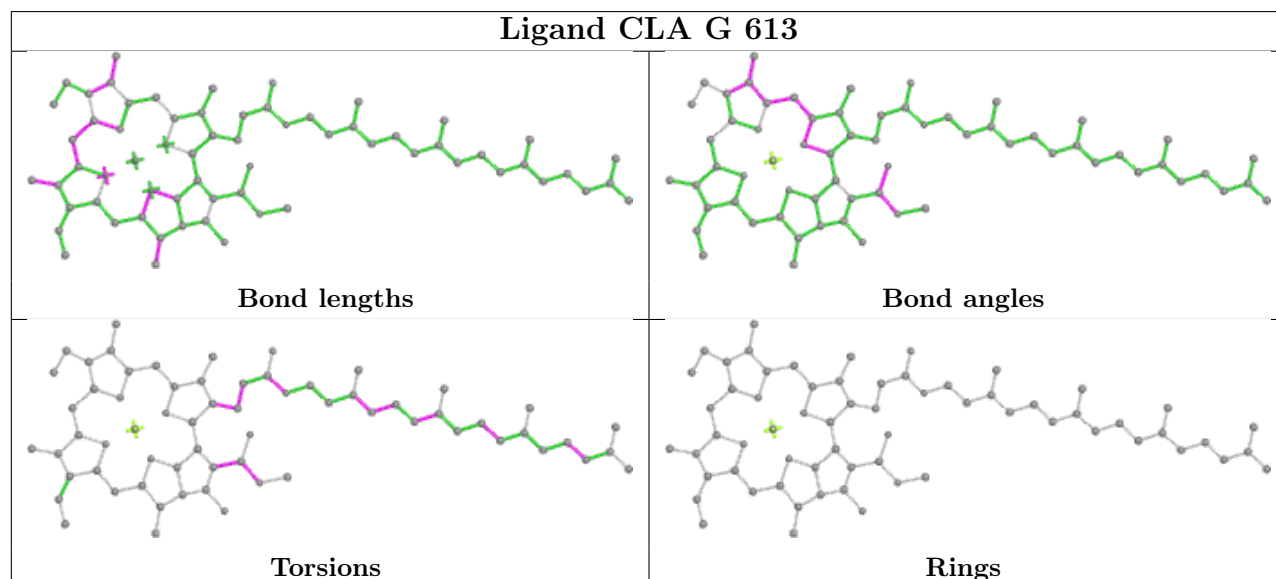
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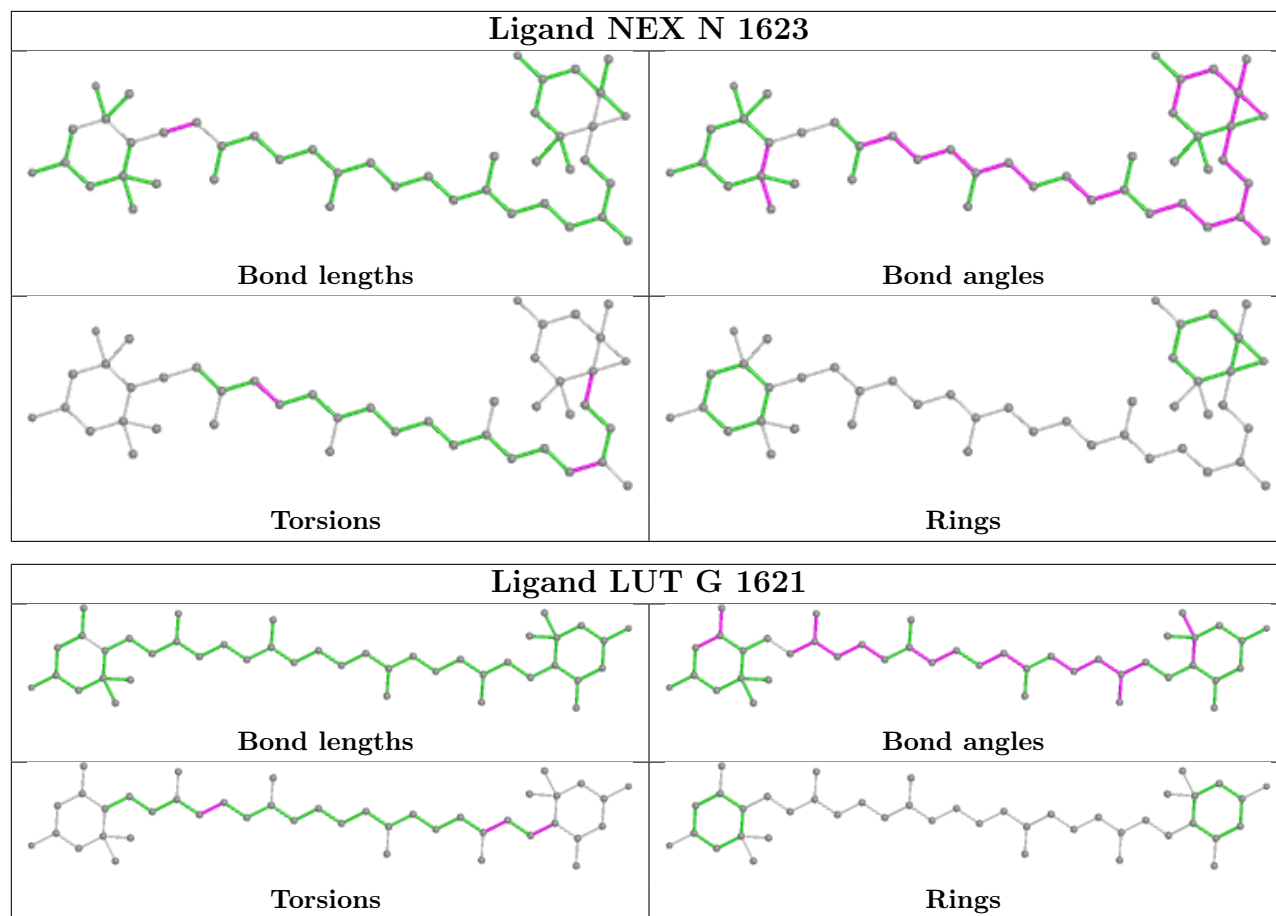


Ligand XAT r 624

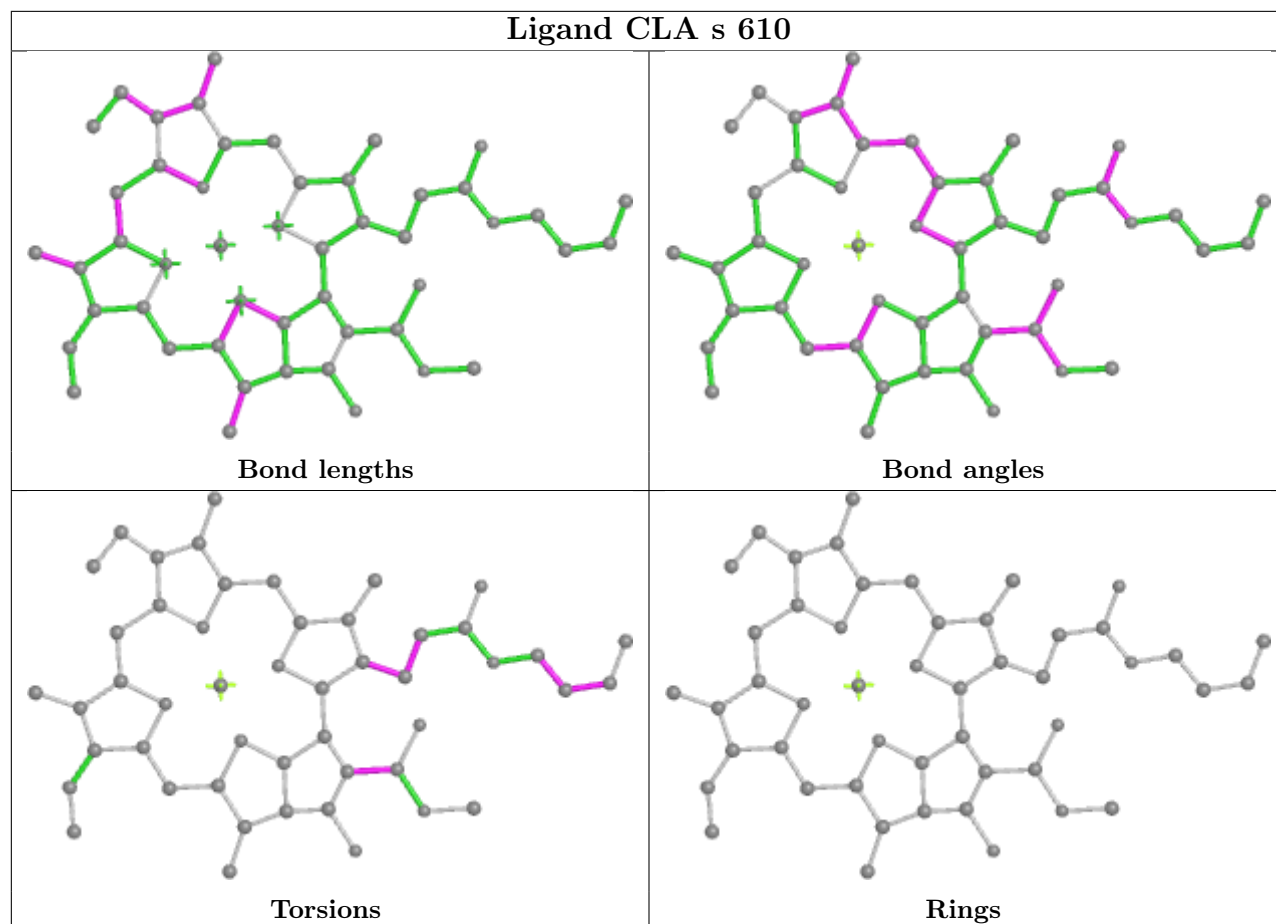


Ligand CLA G 613

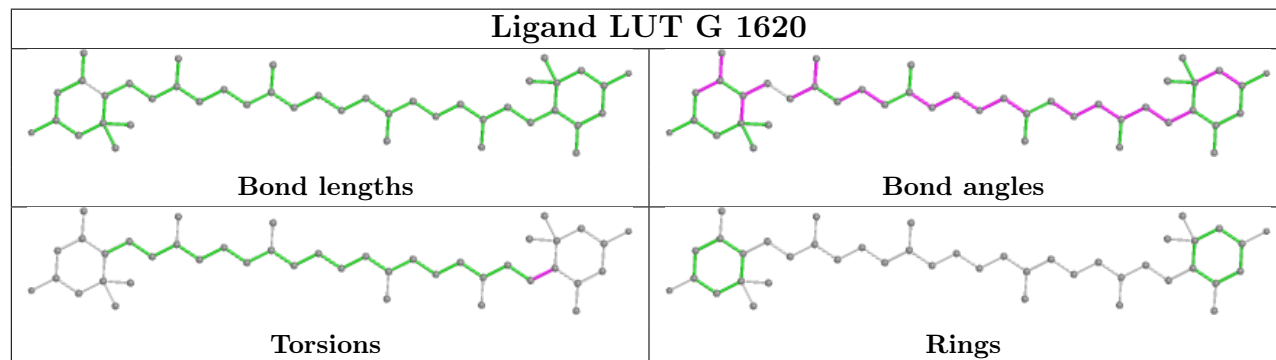




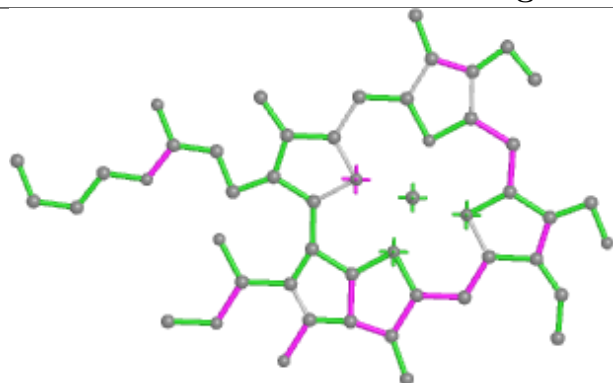
Ligand CLA s 610



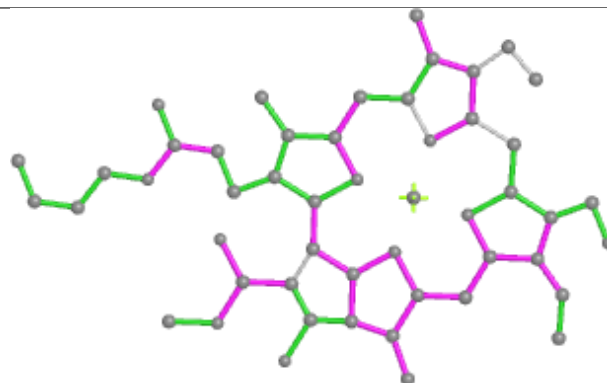
Ligand LUT G 1620



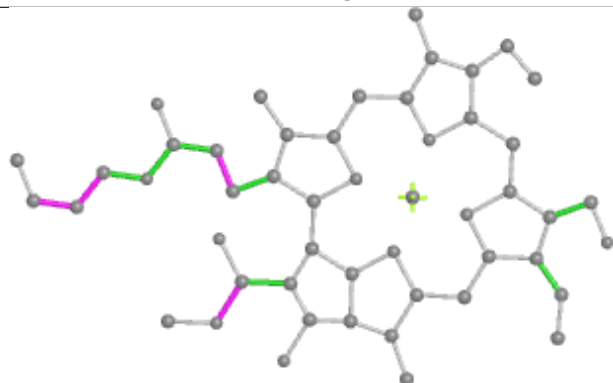
Ligand CHL n 608



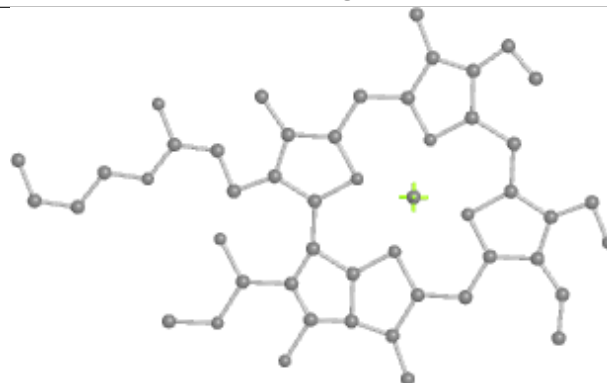
Bond lengths



Bond angles

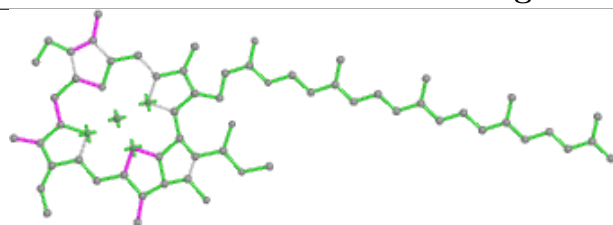


Torsions

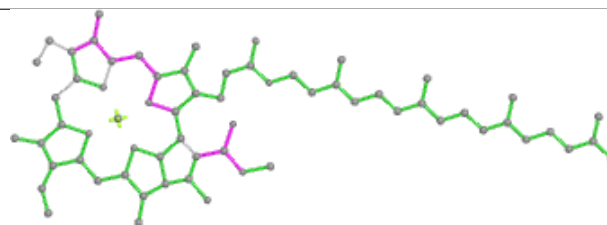


Rings

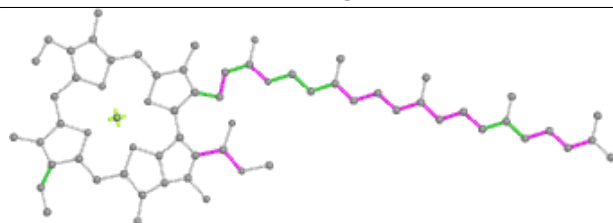
Ligand CLA B 615



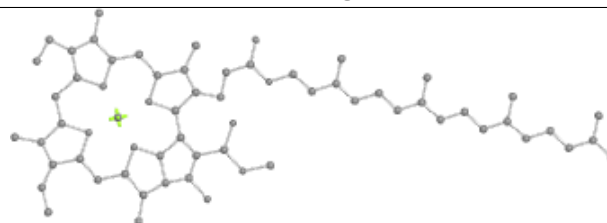
Bond lengths



Bond angles

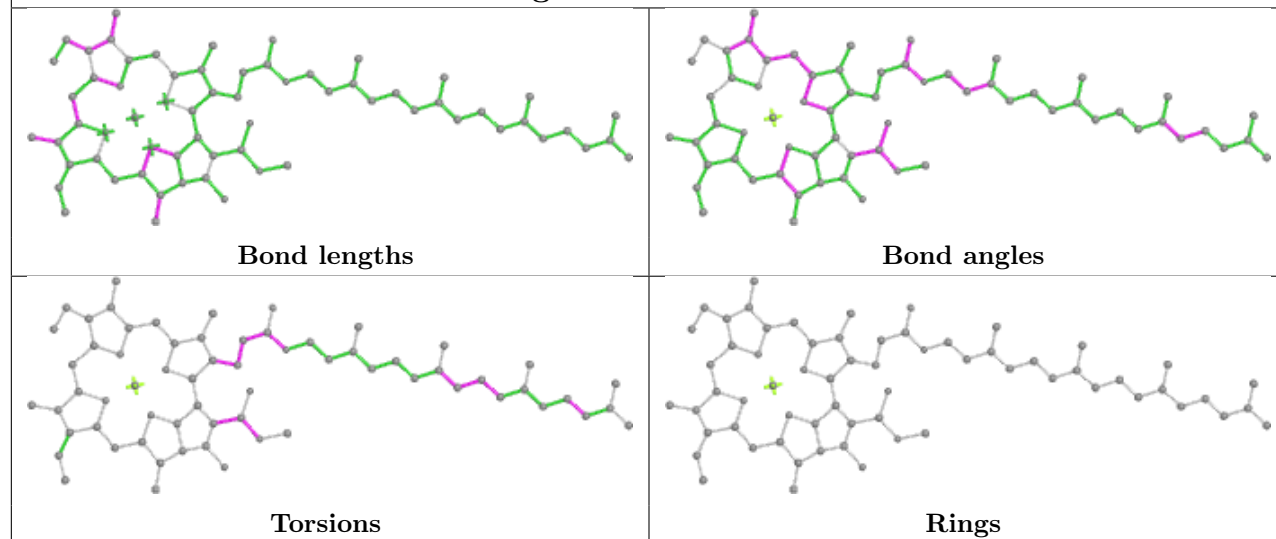


Torsions

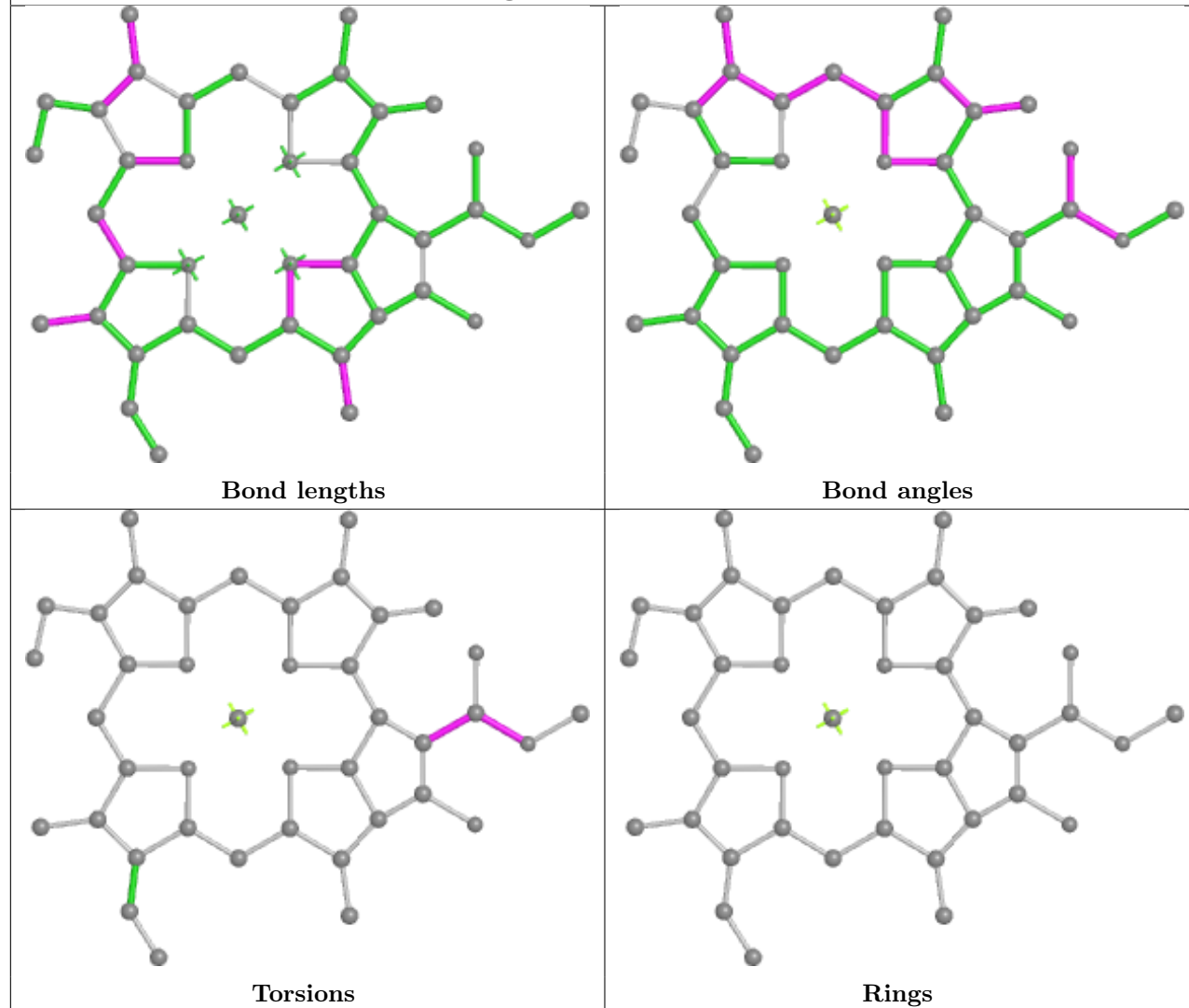


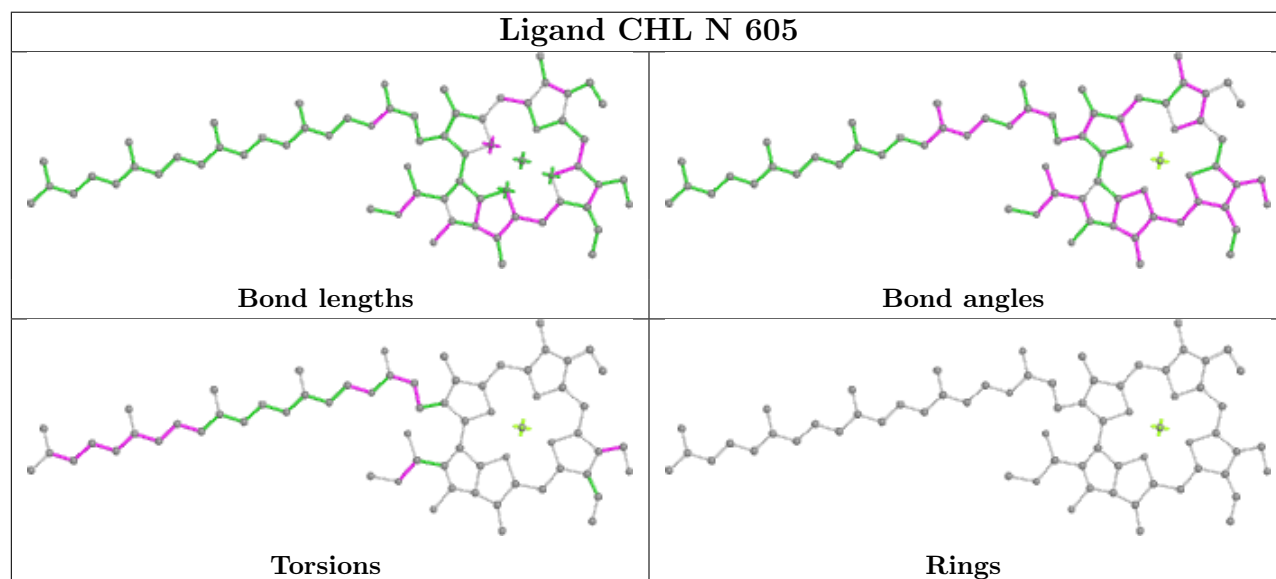
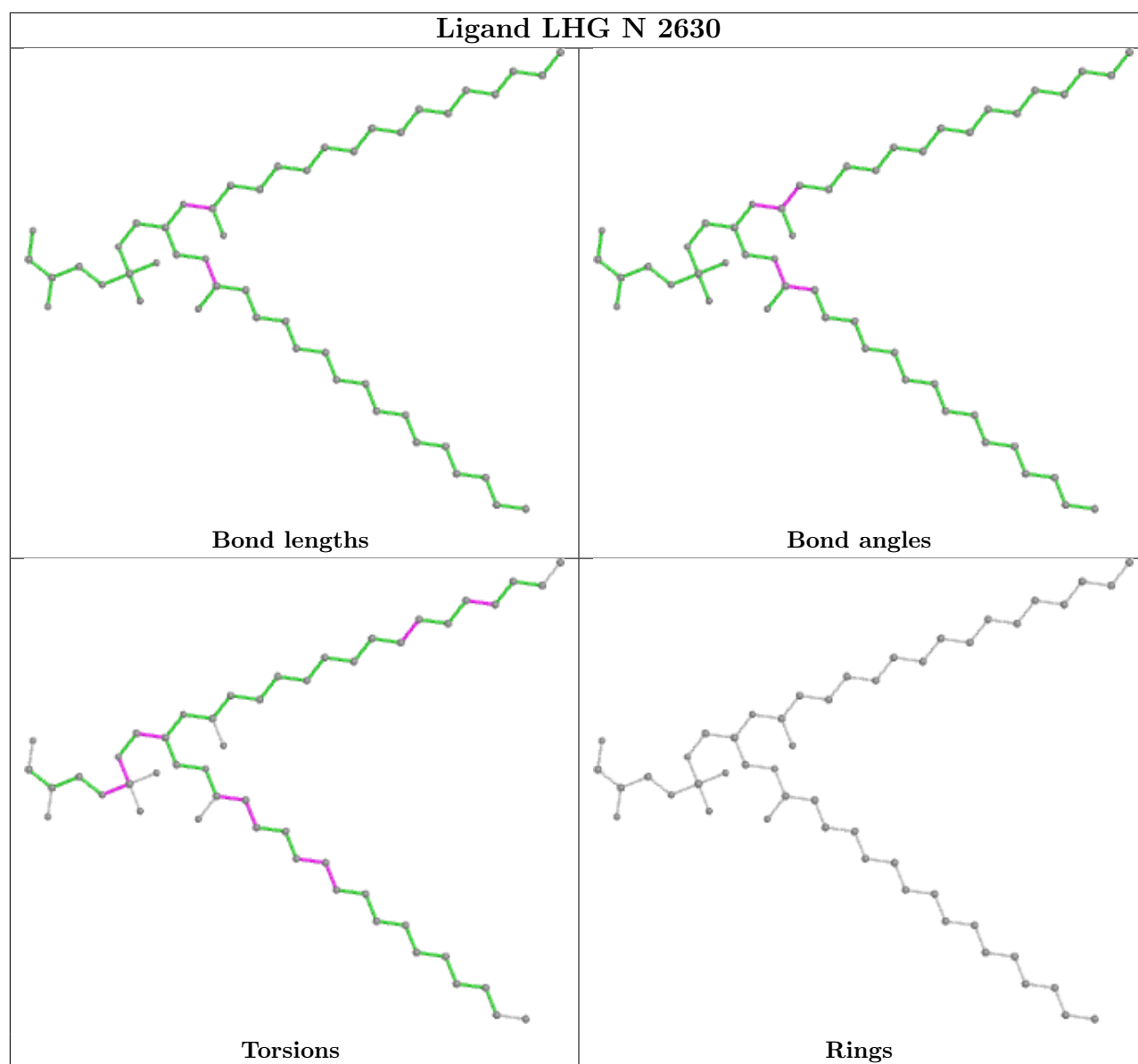
Rings

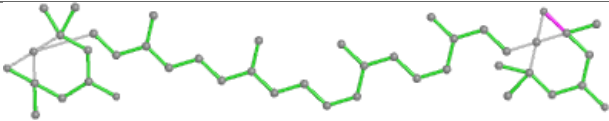
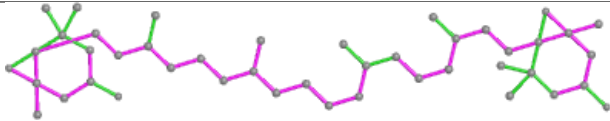
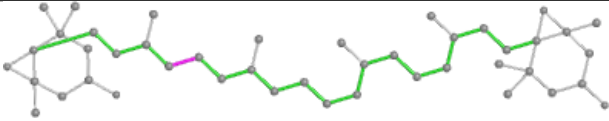
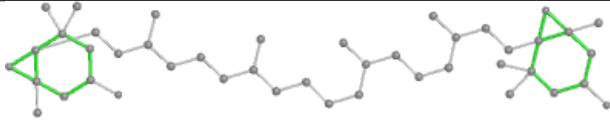
Ligand CLA C 501

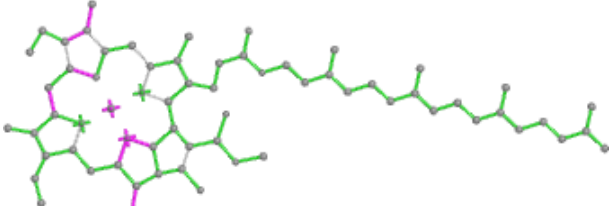
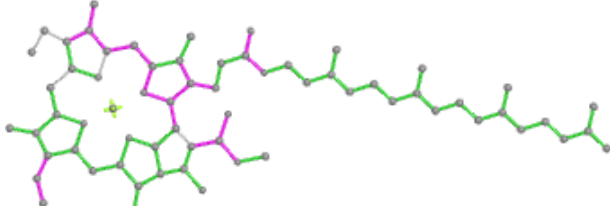
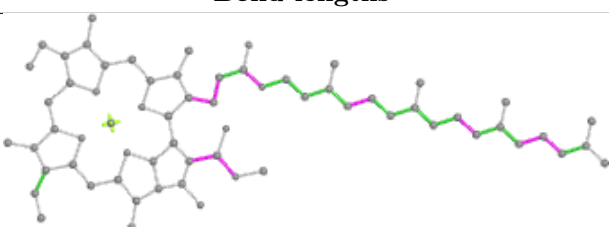
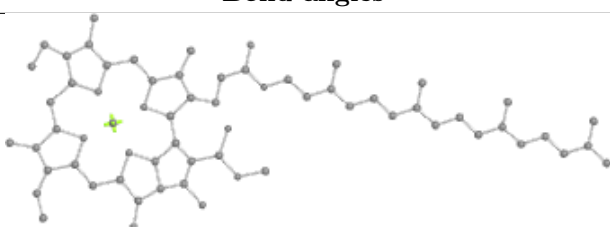


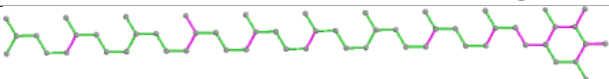
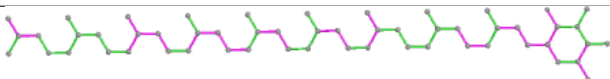
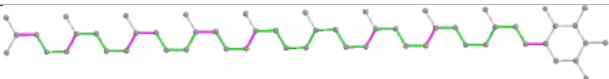
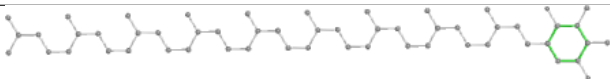
Ligand CLA r 610



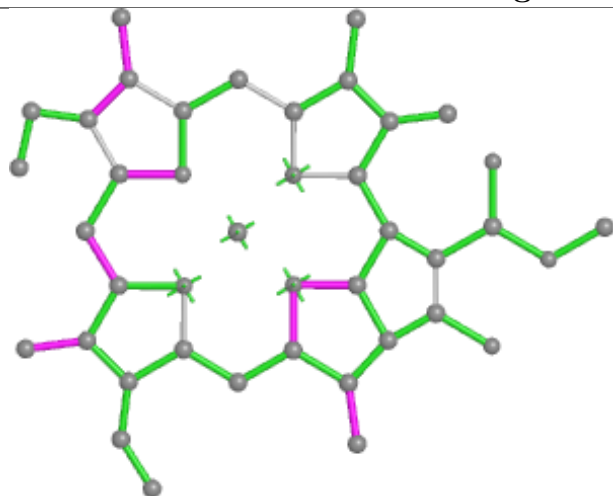


Ligand XAT n 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

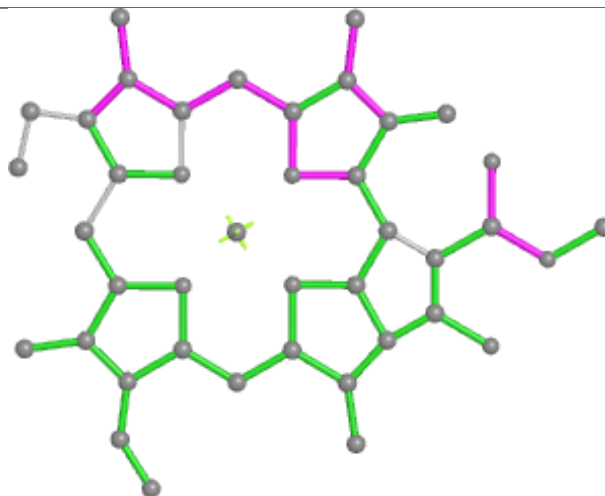
Ligand CLA g 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

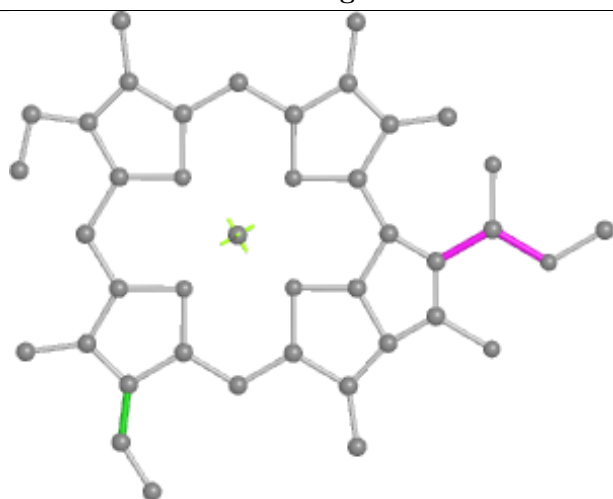
Ligand CLA R 610



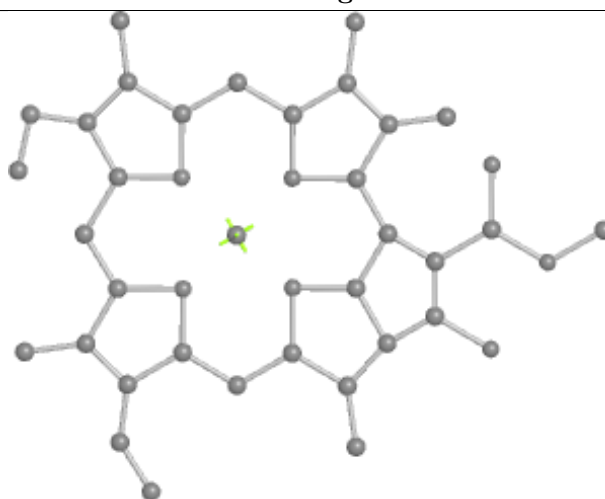
Bond lengths



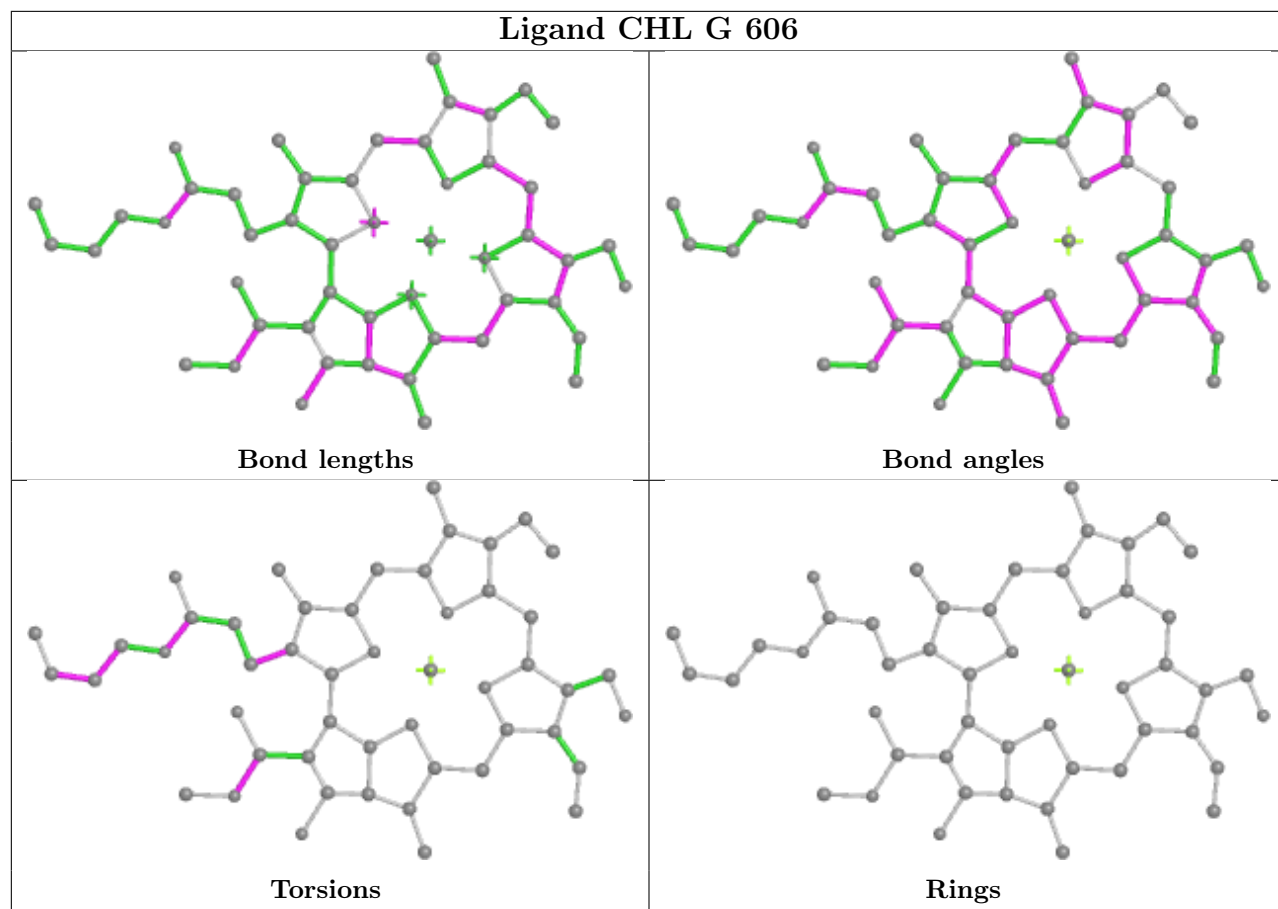
Bond angles



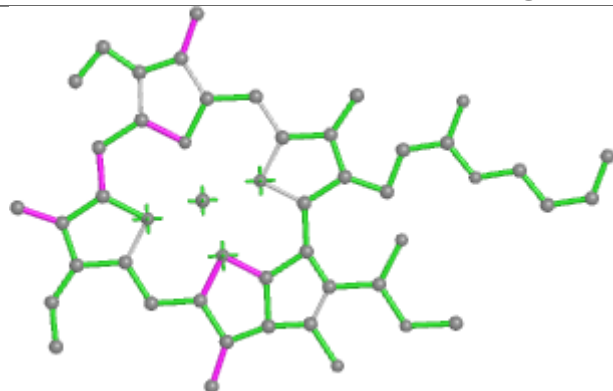
Torsions



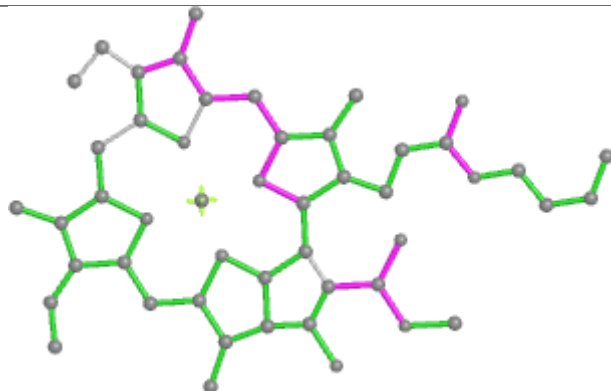
Rings



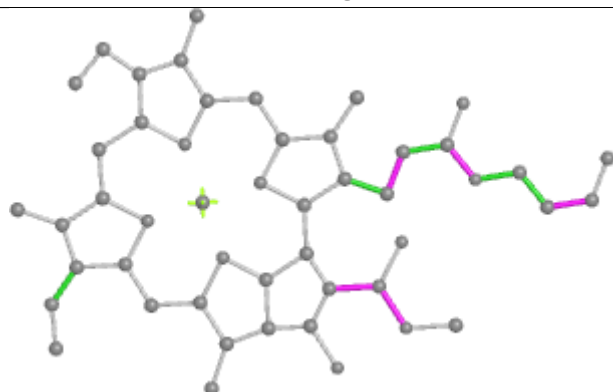
Ligand CLA s 602



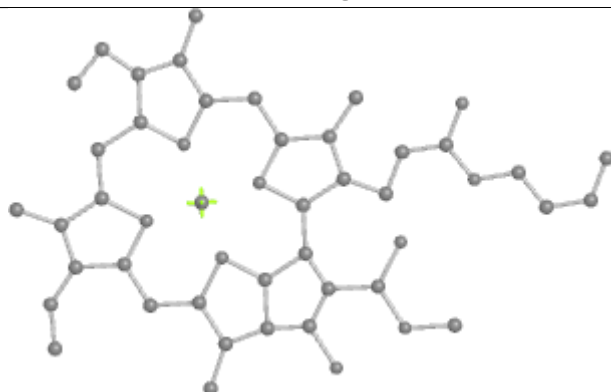
Bond lengths



Bond angles

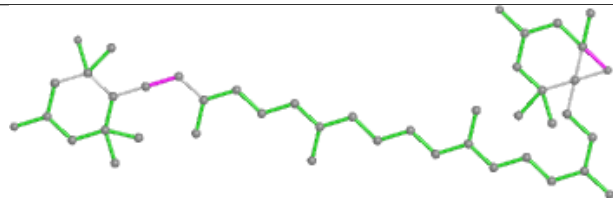


Torsions

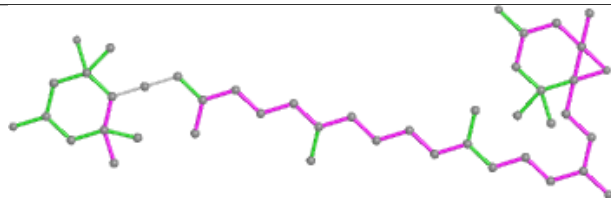


Rings

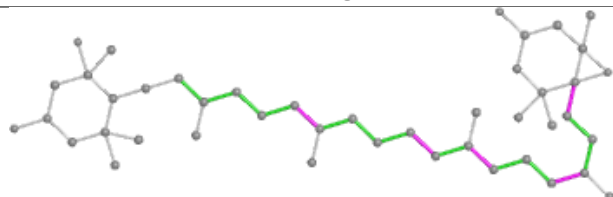
Ligand NEX Y 1623



Bond lengths



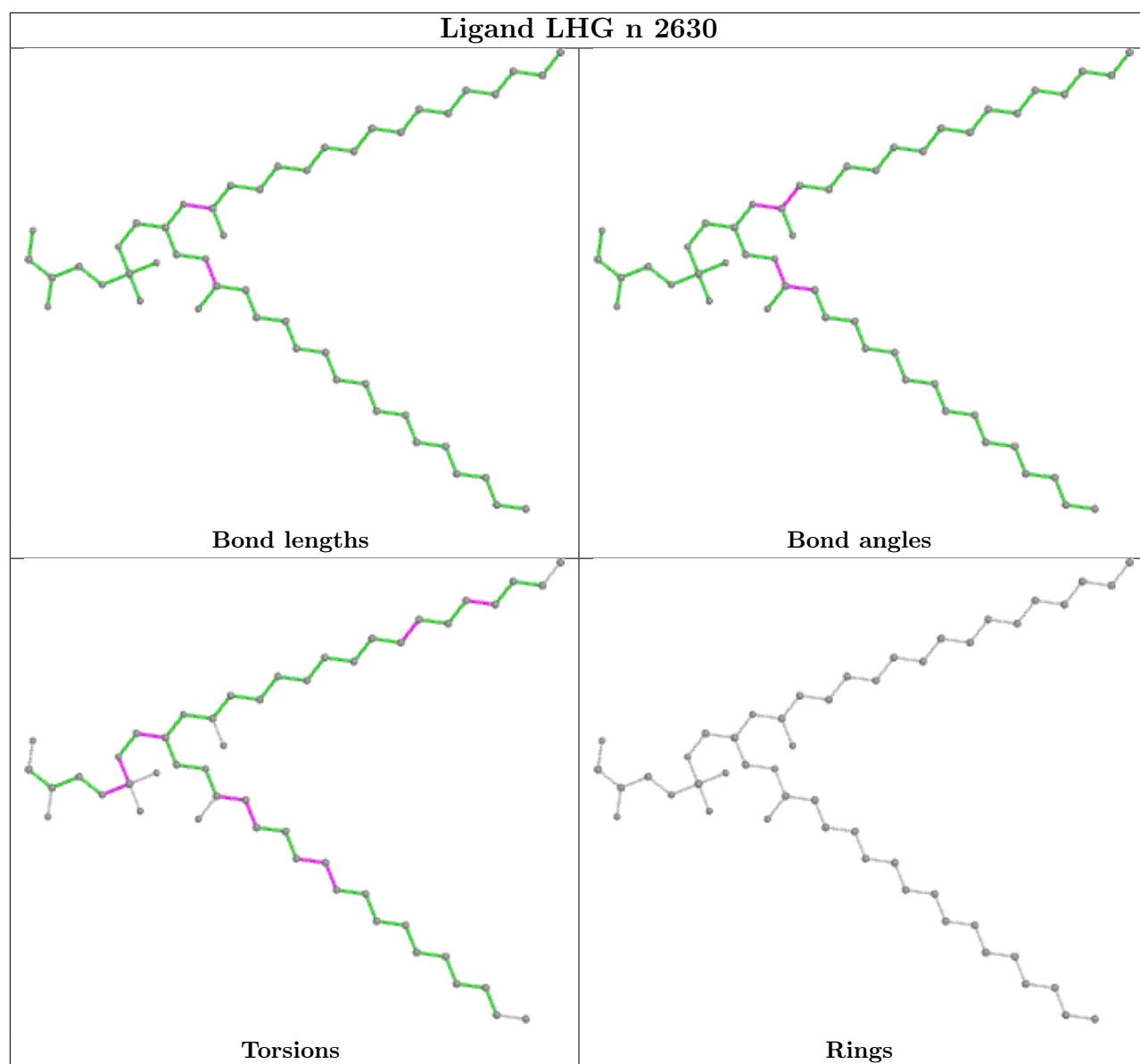
Bond angles

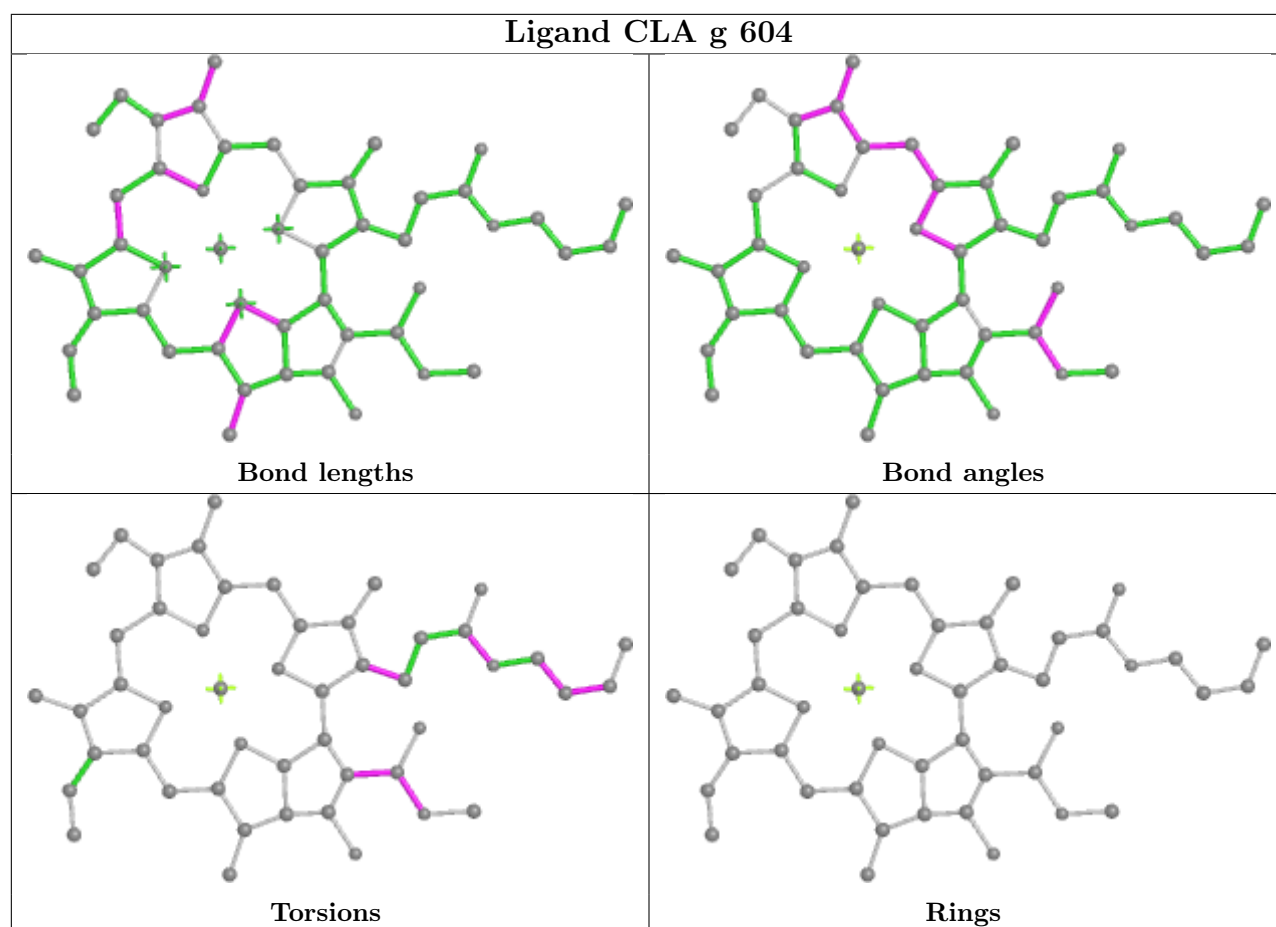


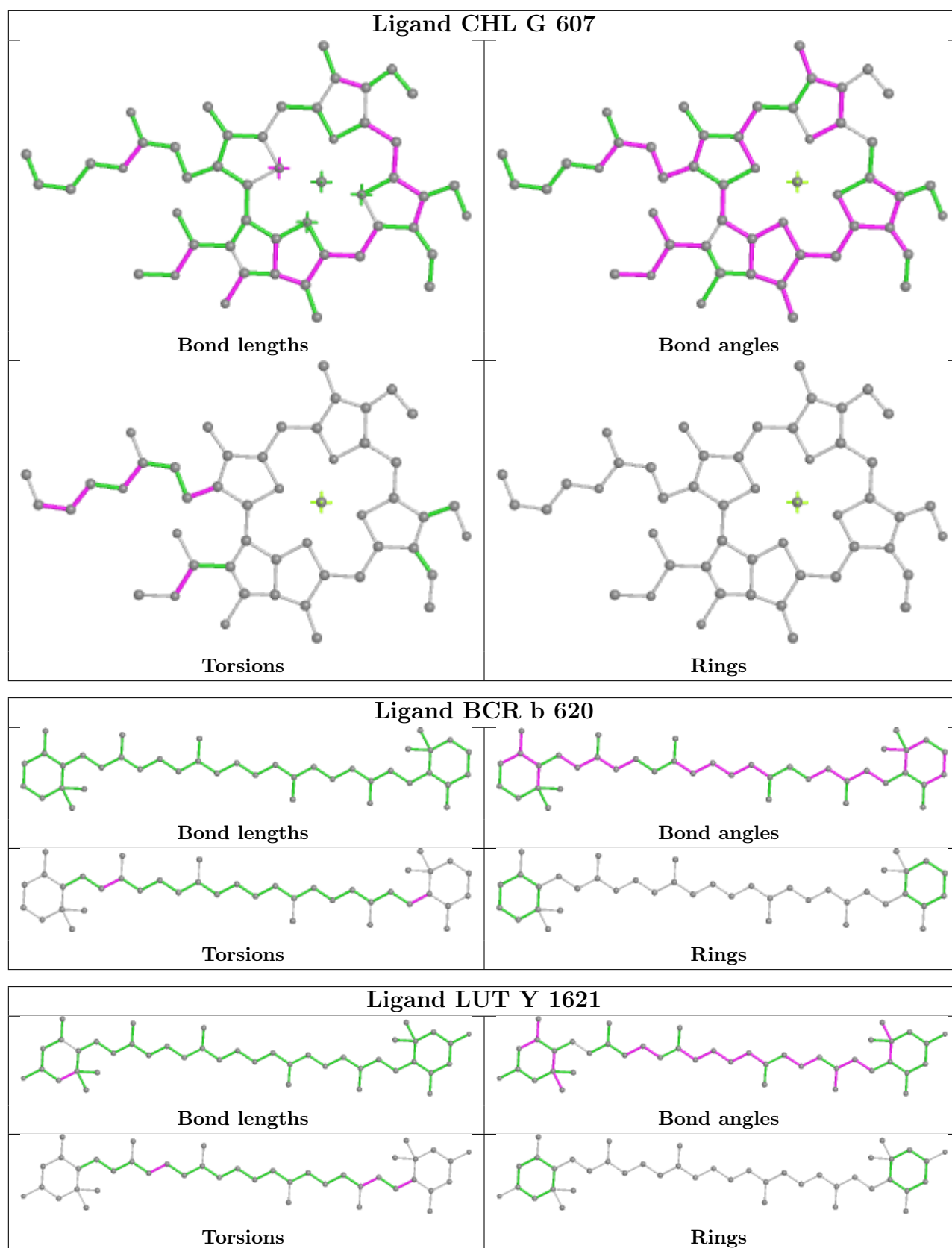
Torsions

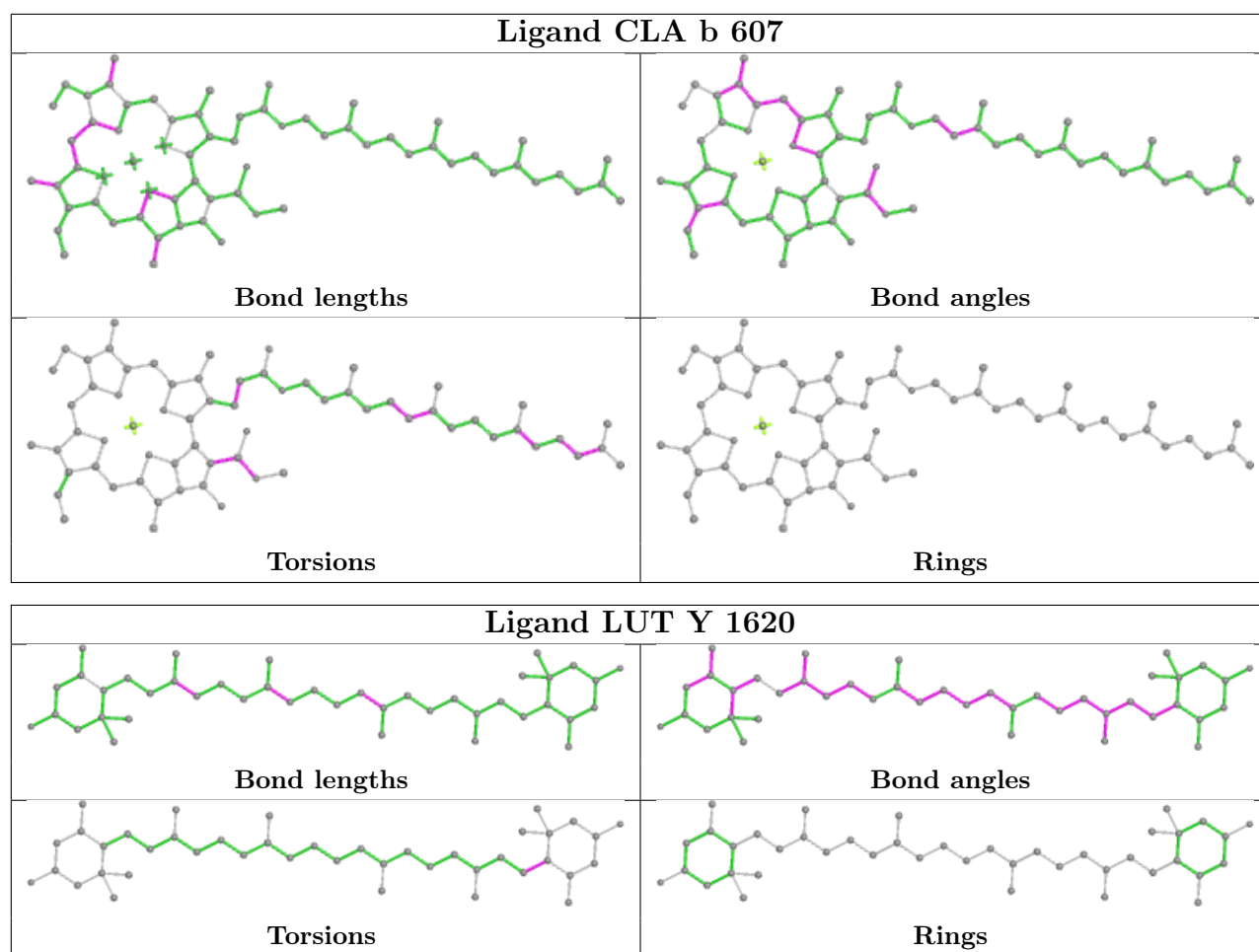


Rings

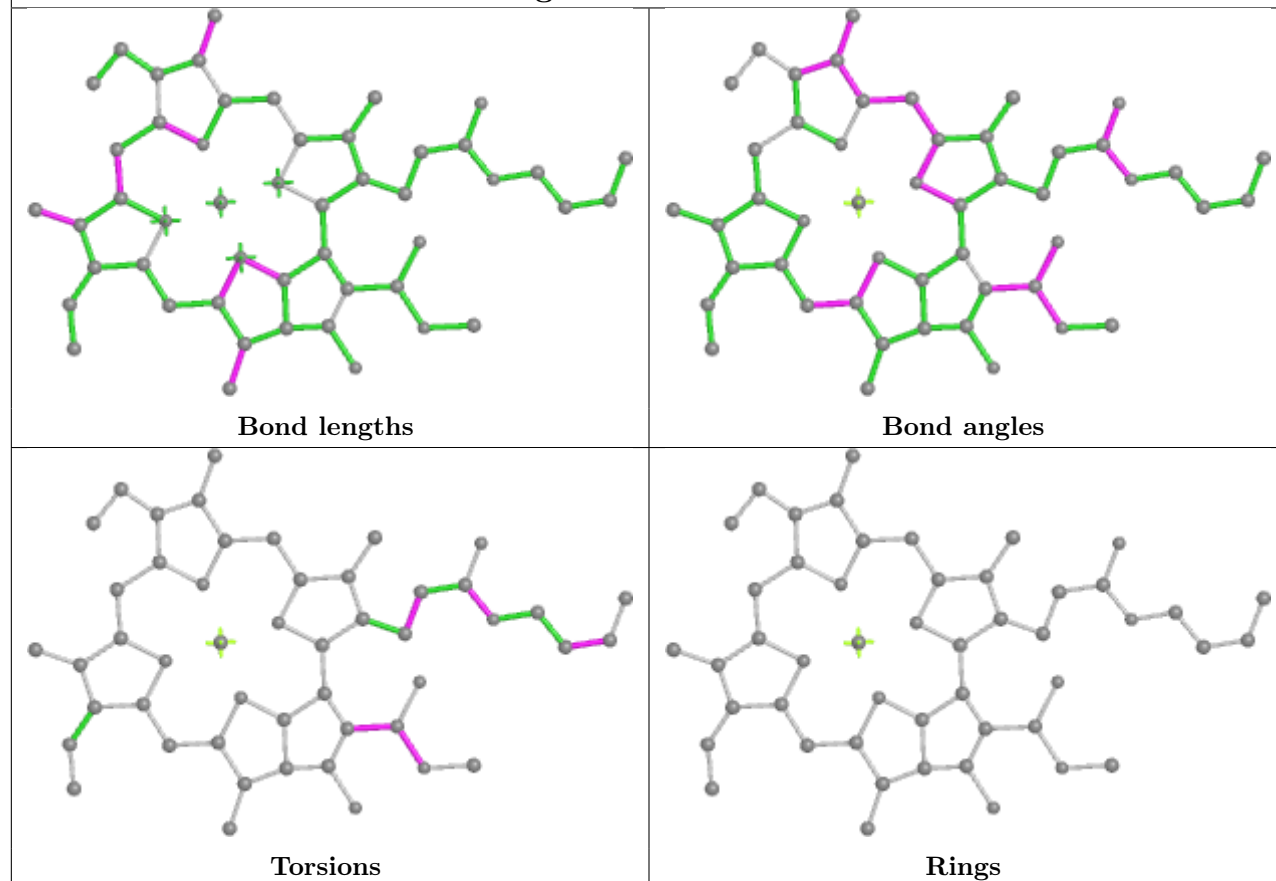




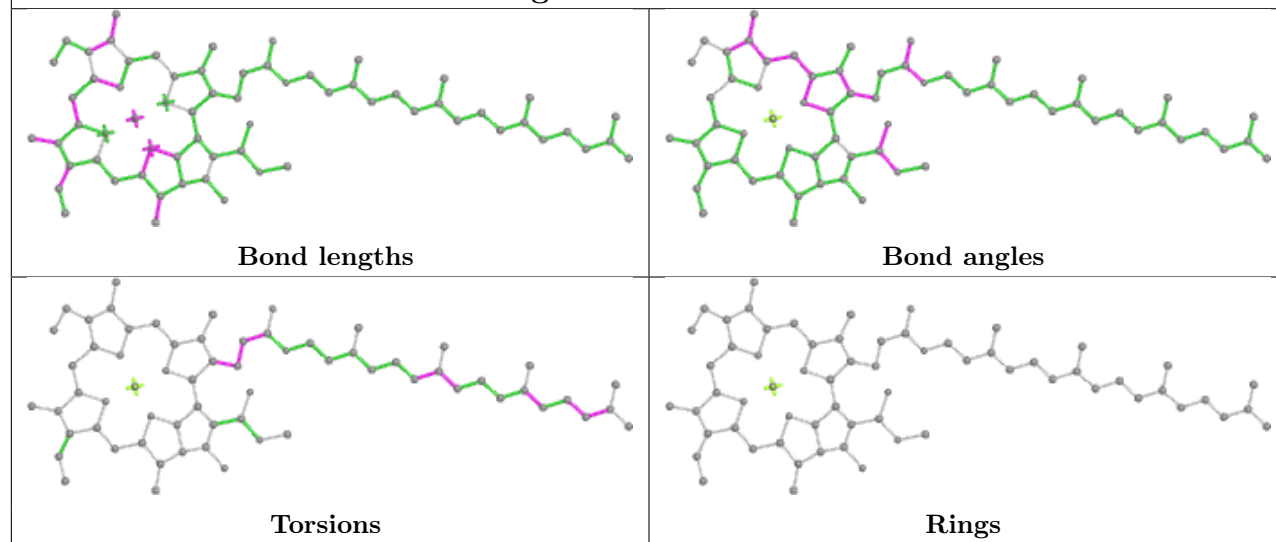




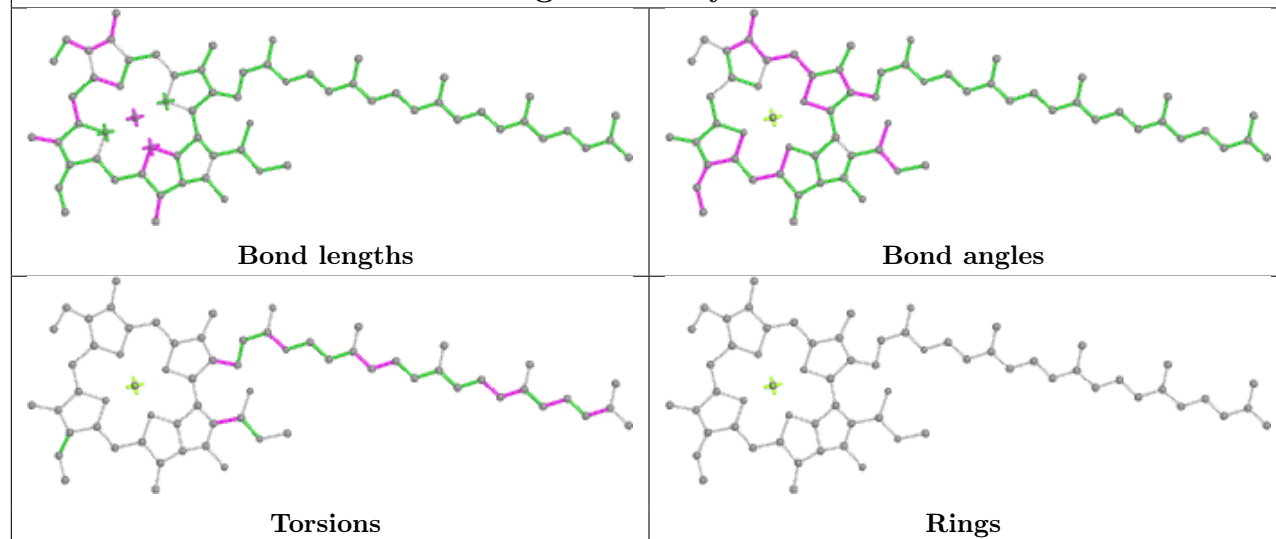
Ligand CLA S 602



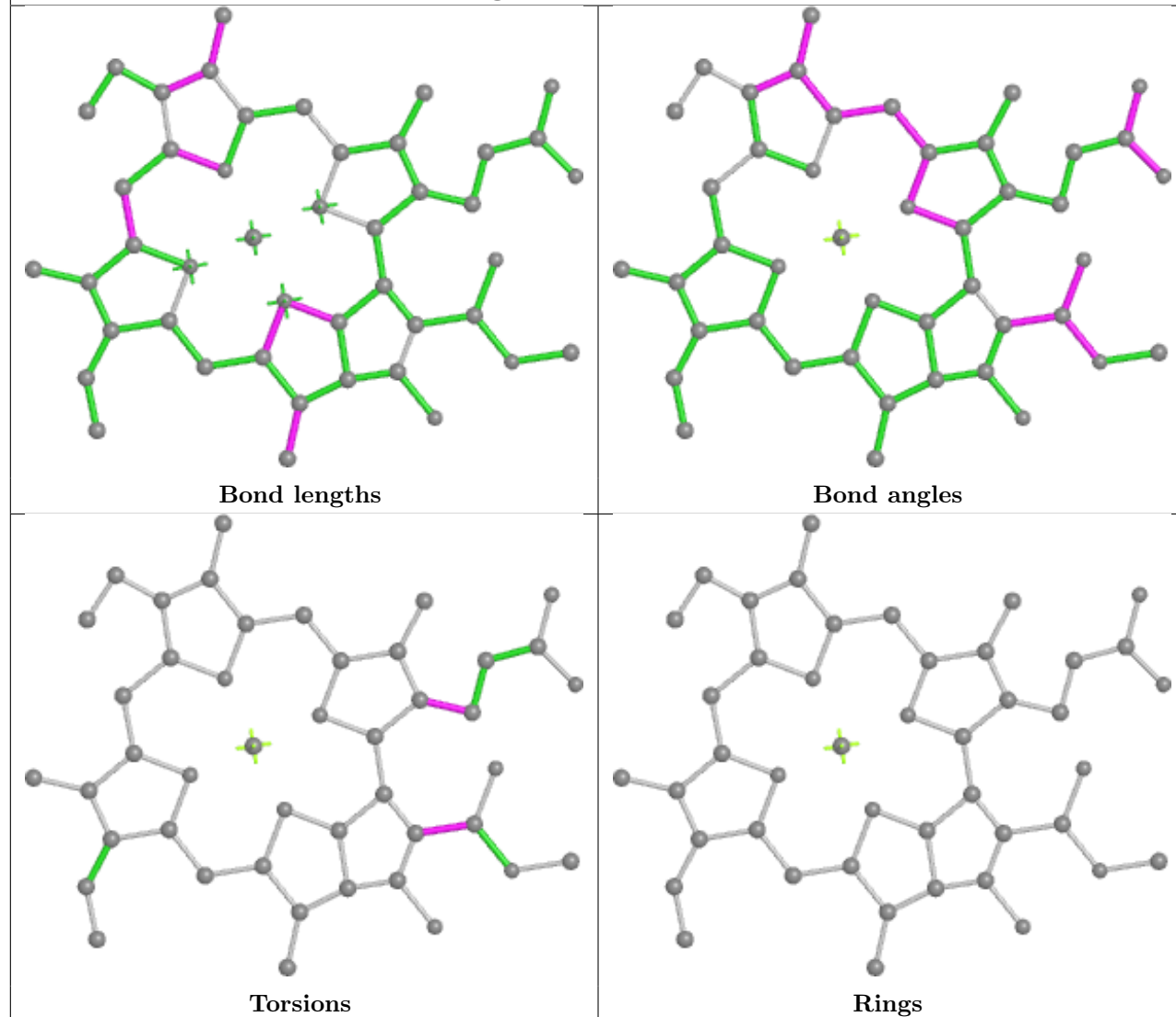
Ligand CLA N 603

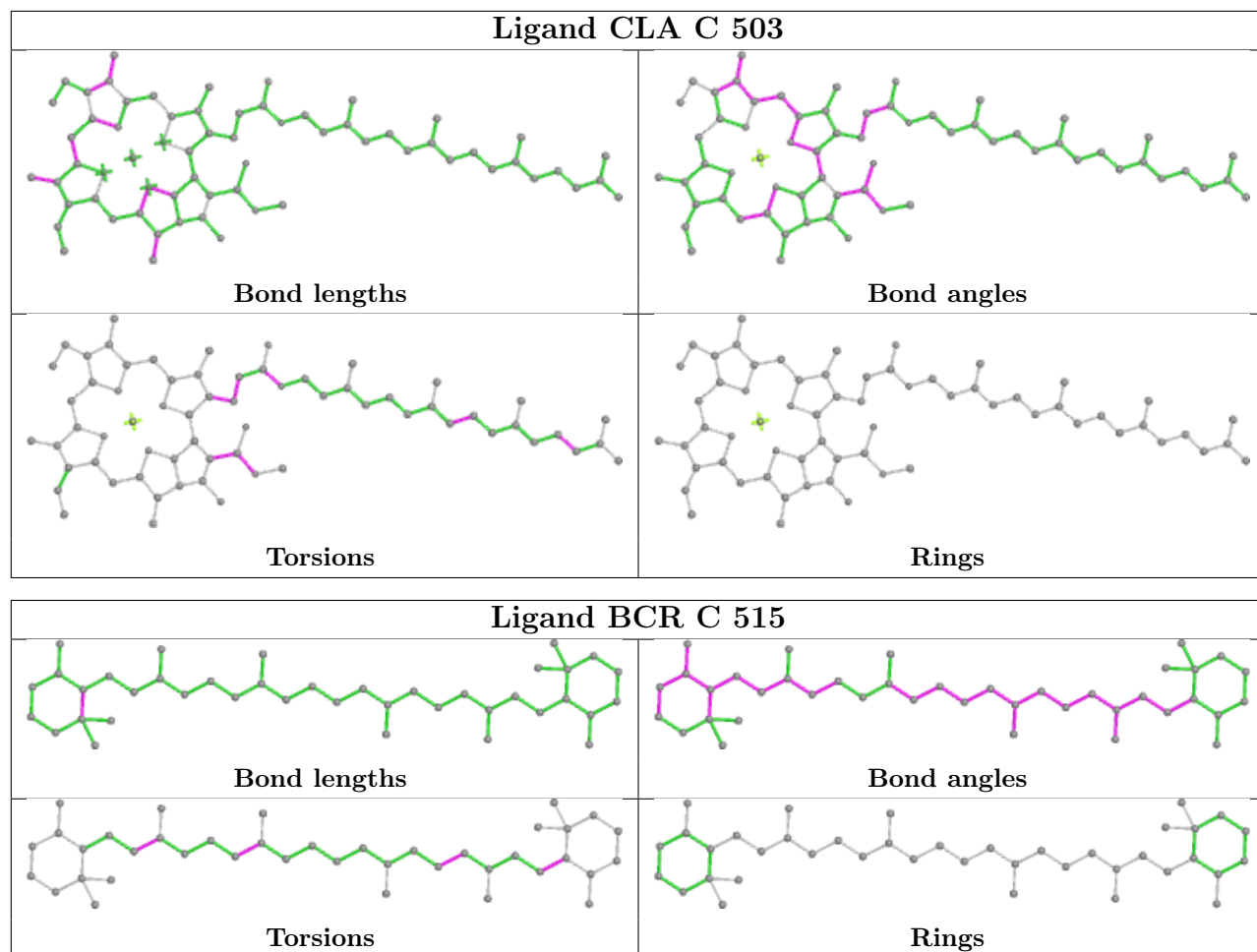


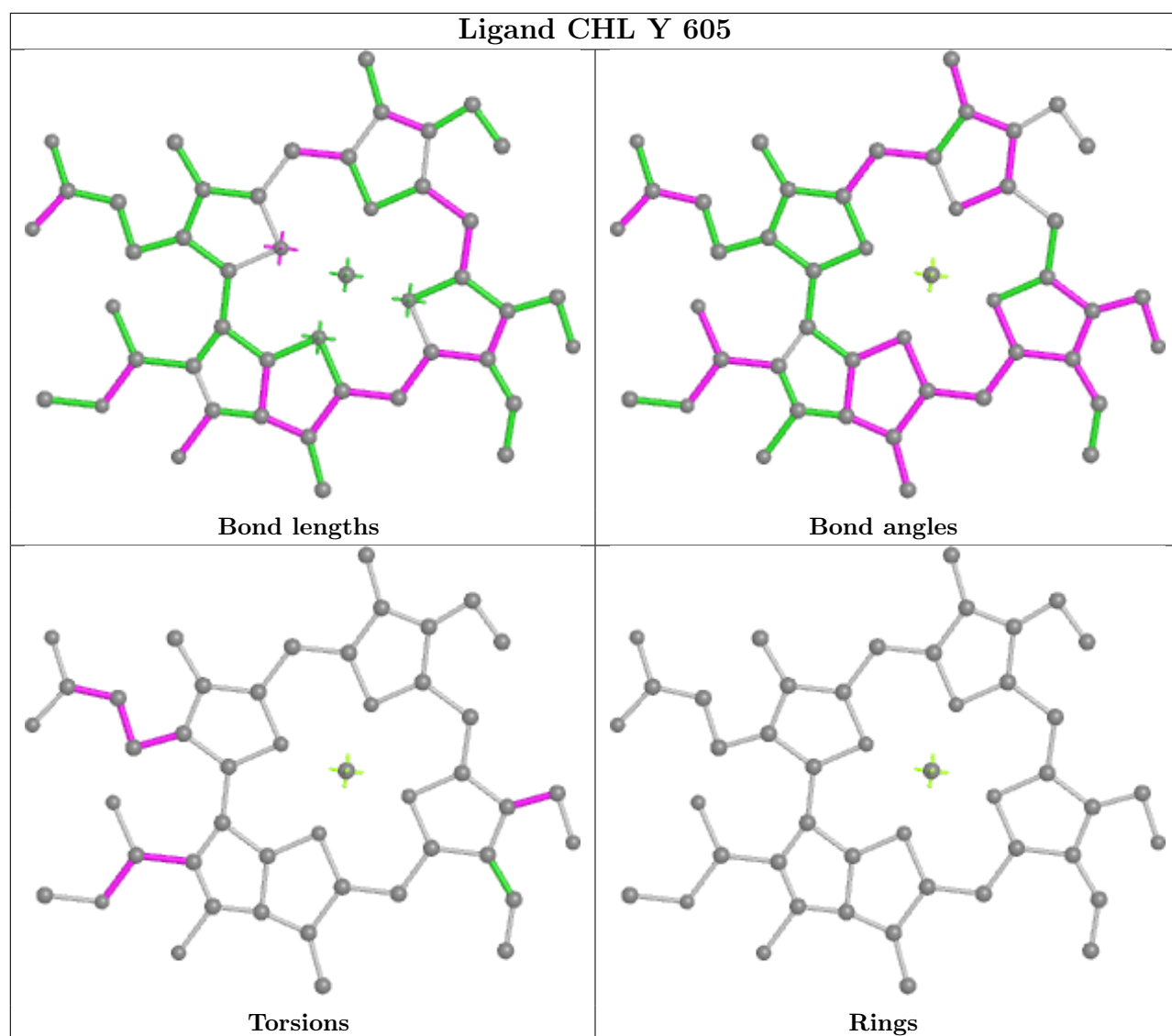
Ligand CLA y 603



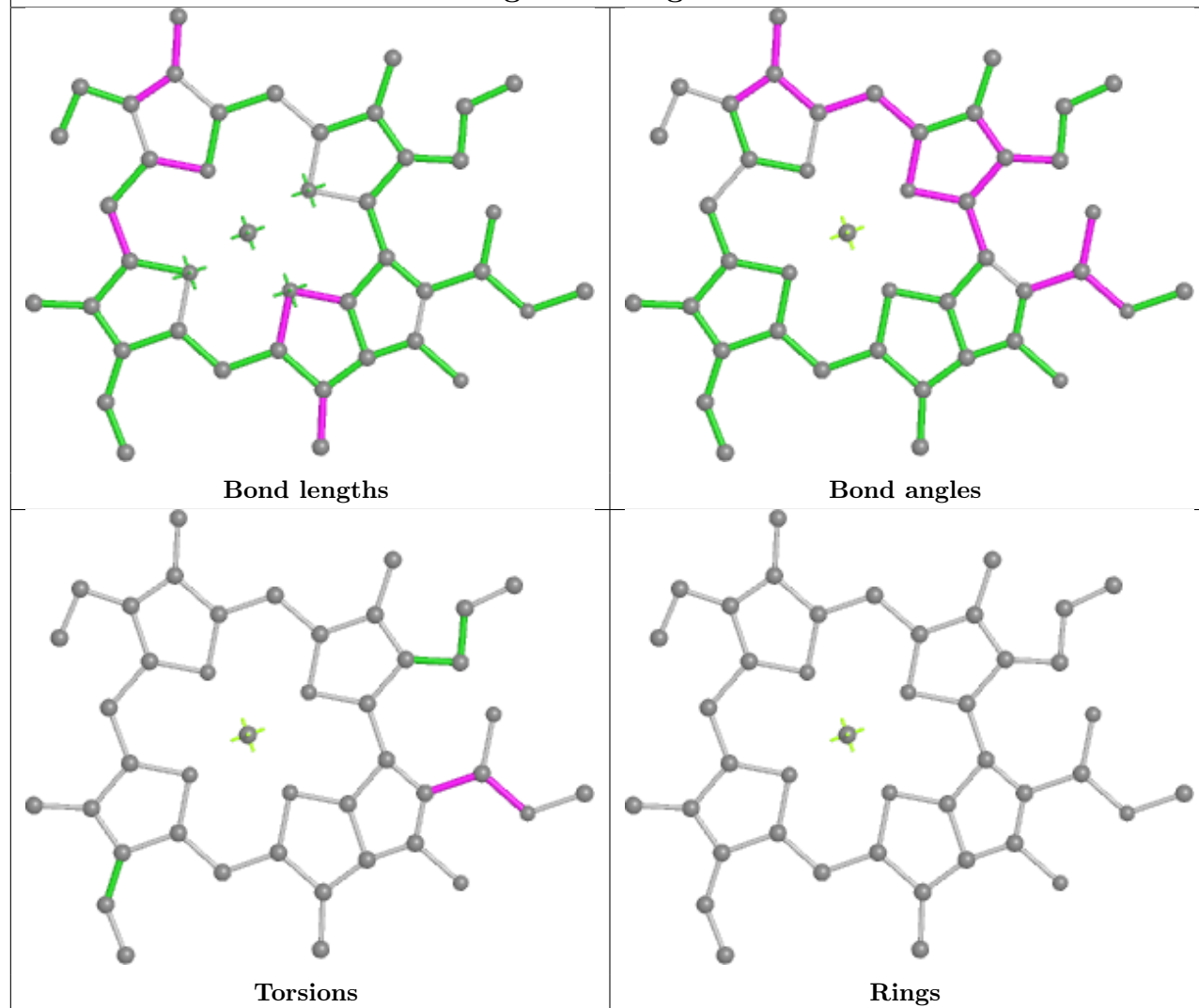
Ligand CLA G 611



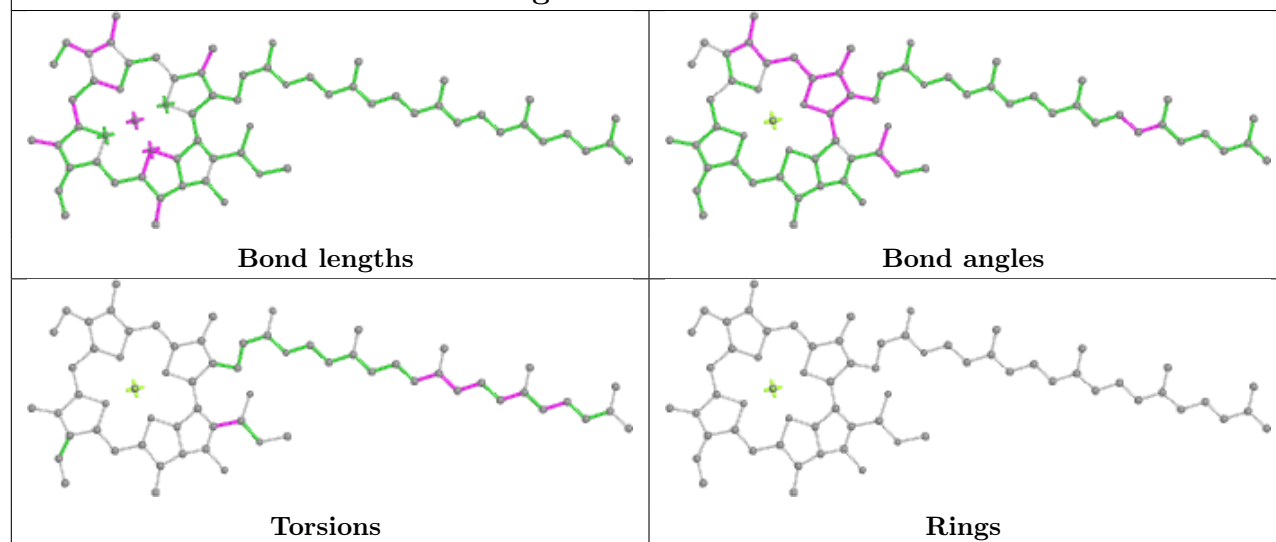


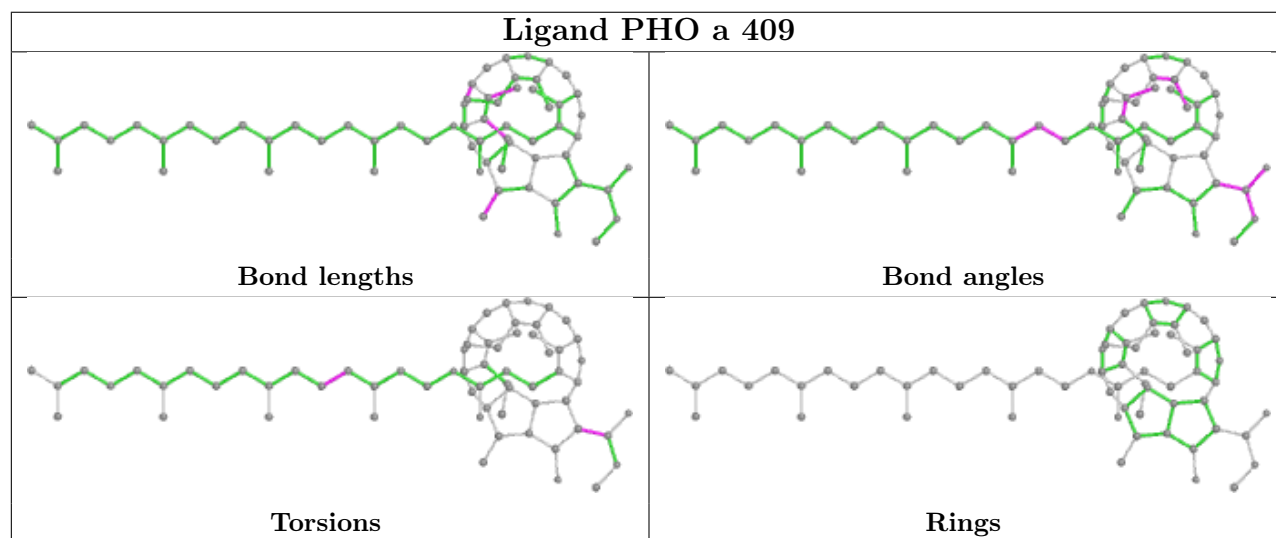
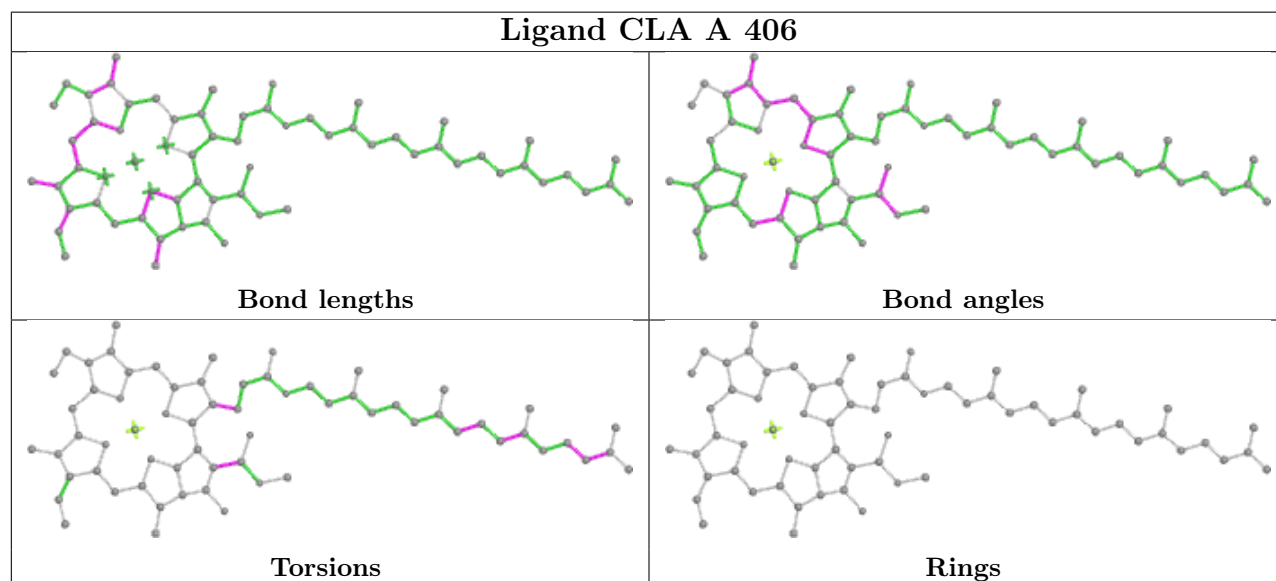
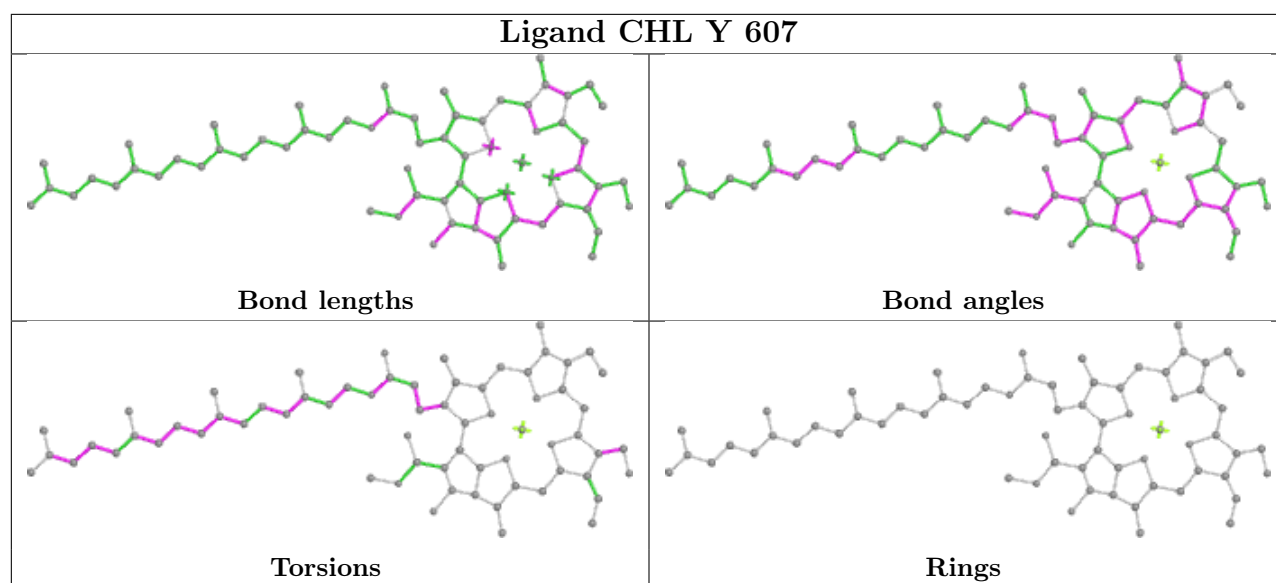


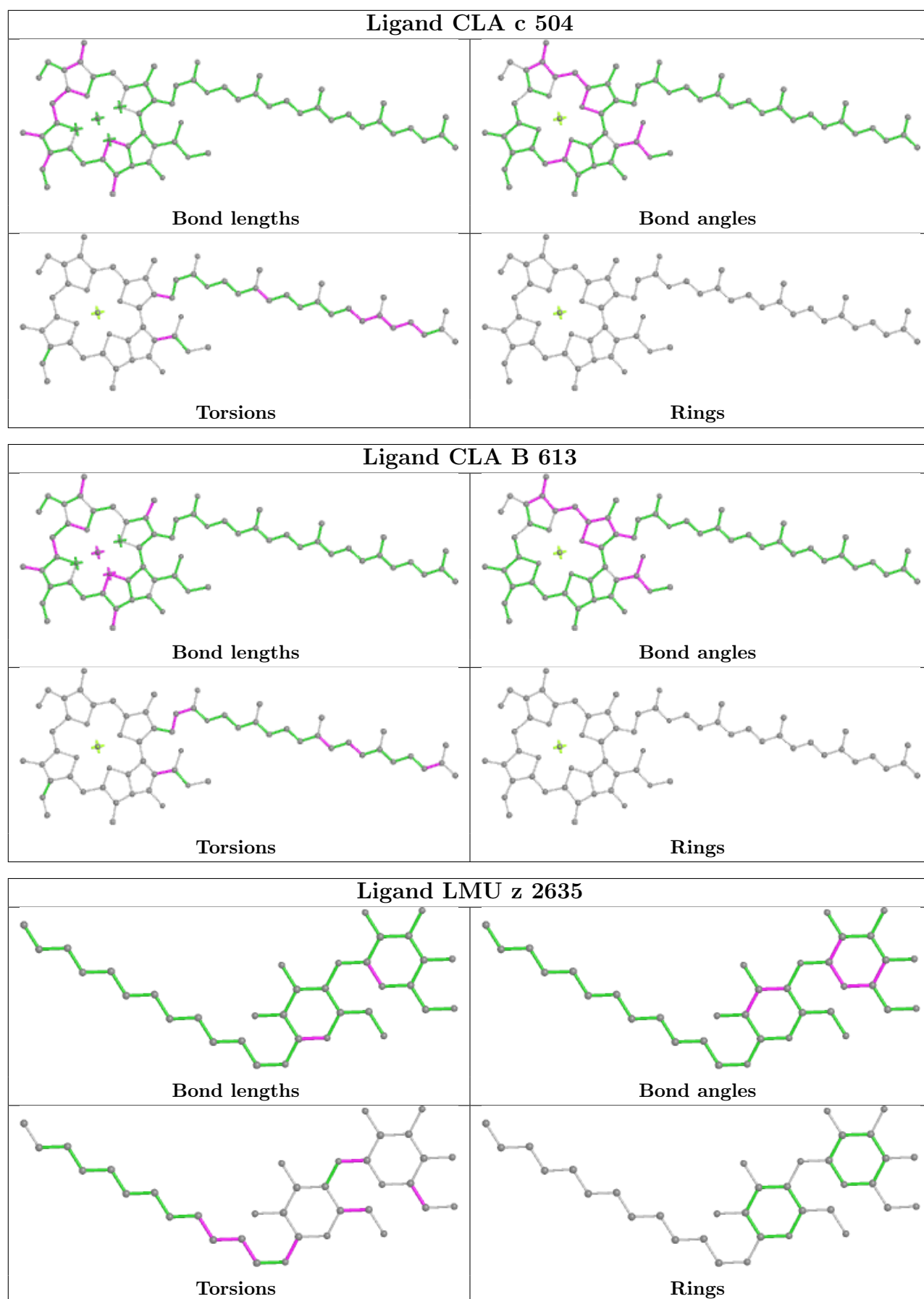
Ligand CLA g 612



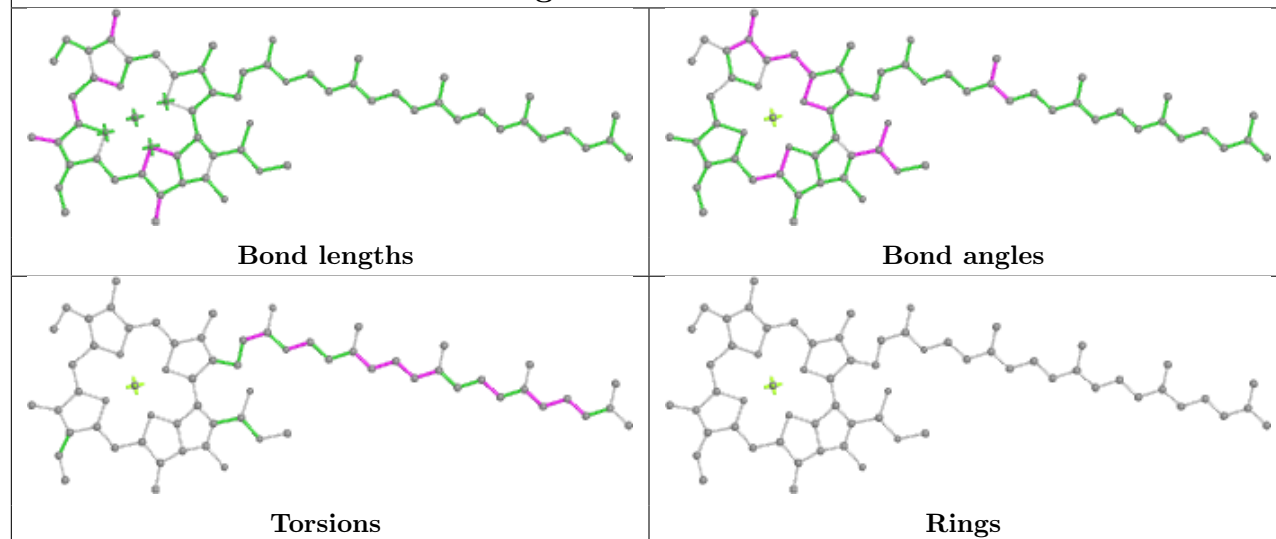
Ligand CLA C 509



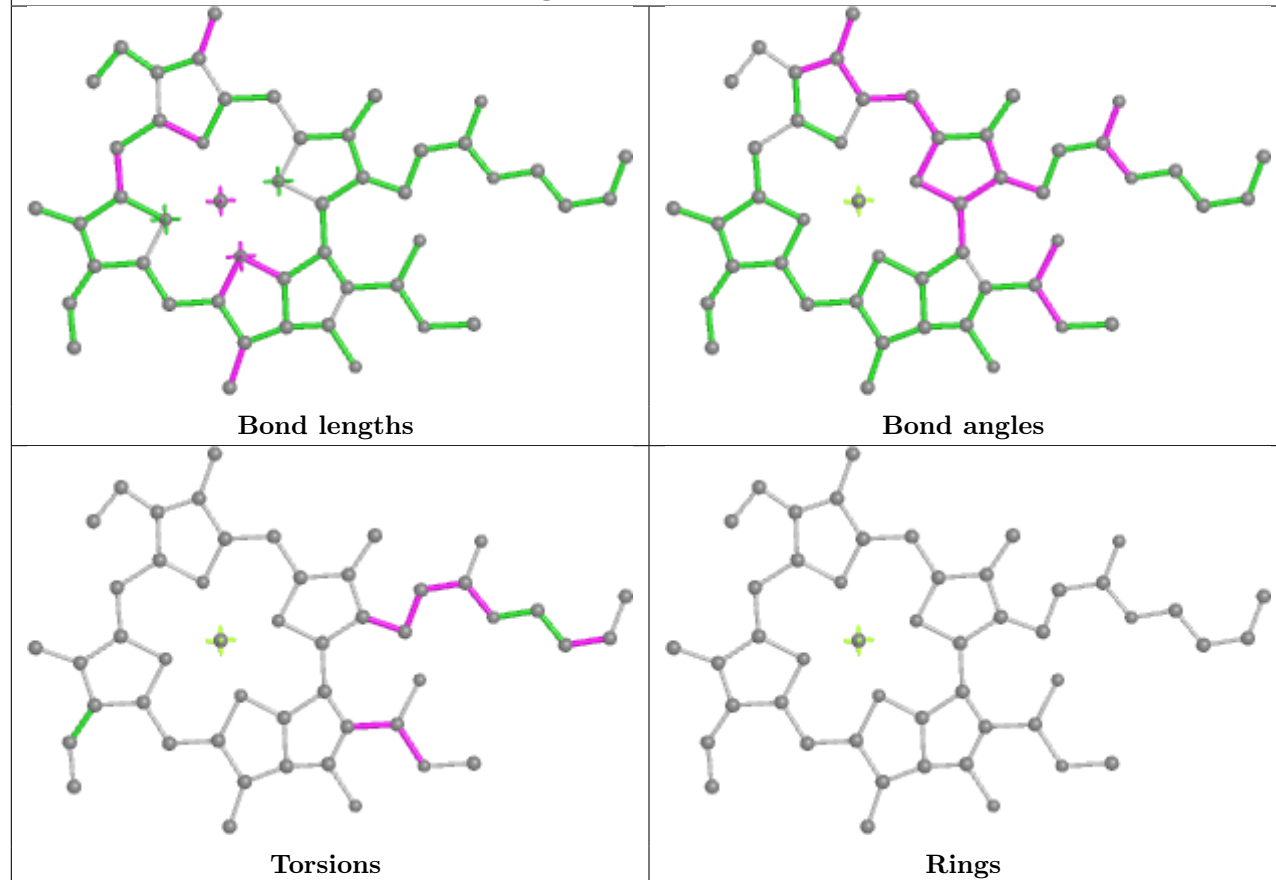


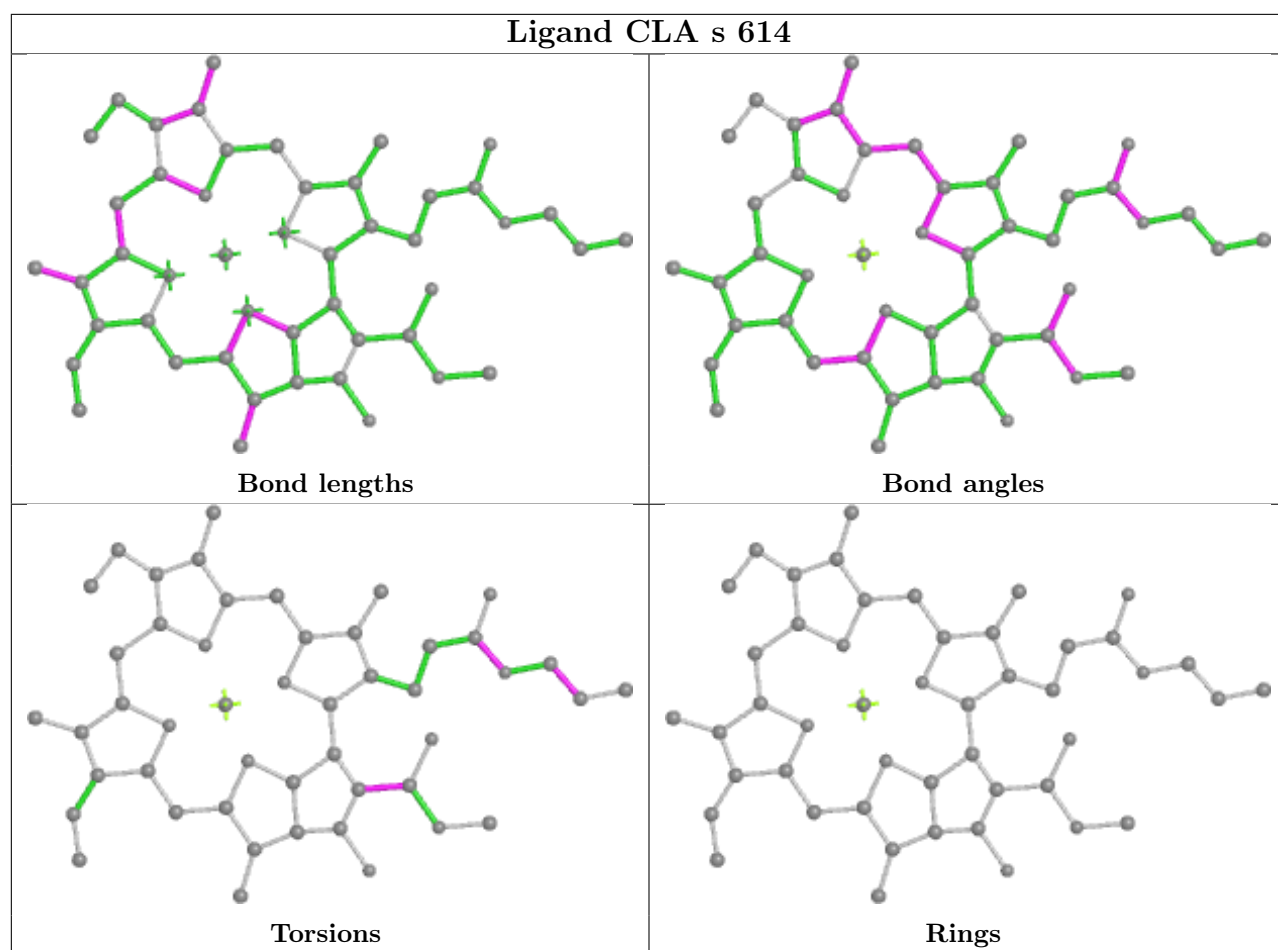


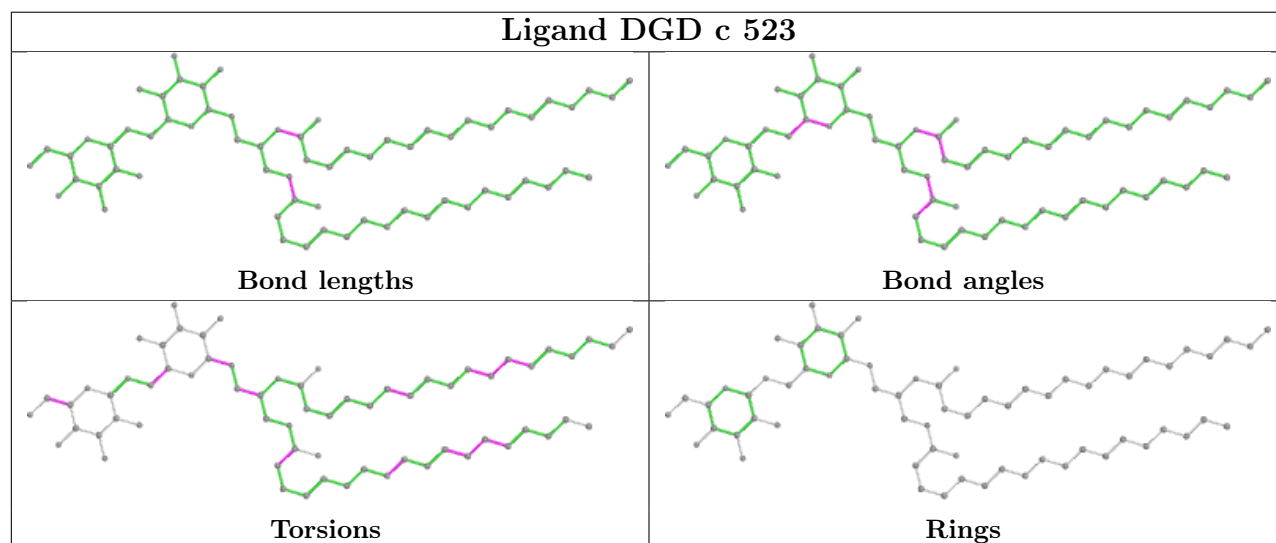
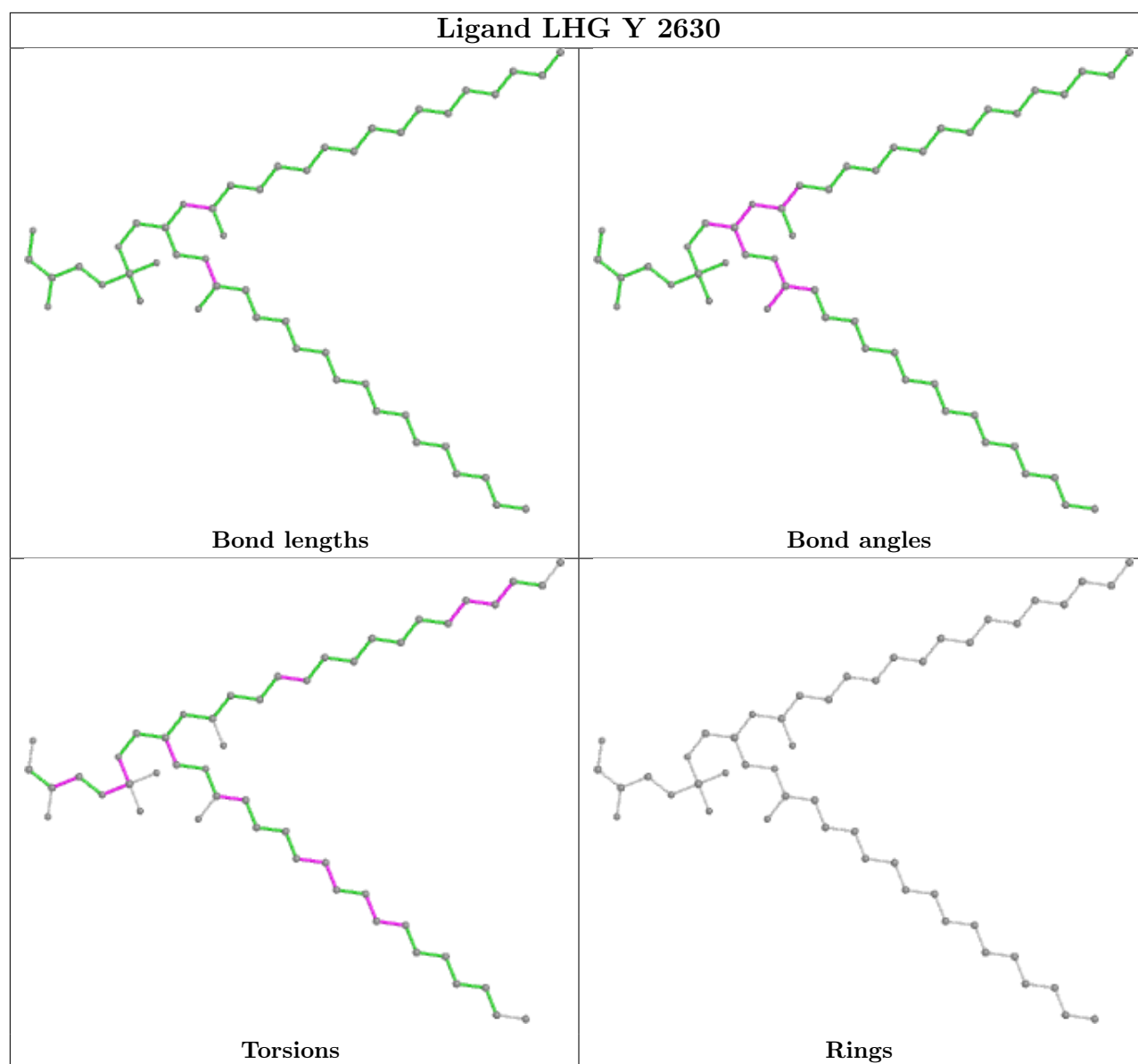
Ligand CLA b 603

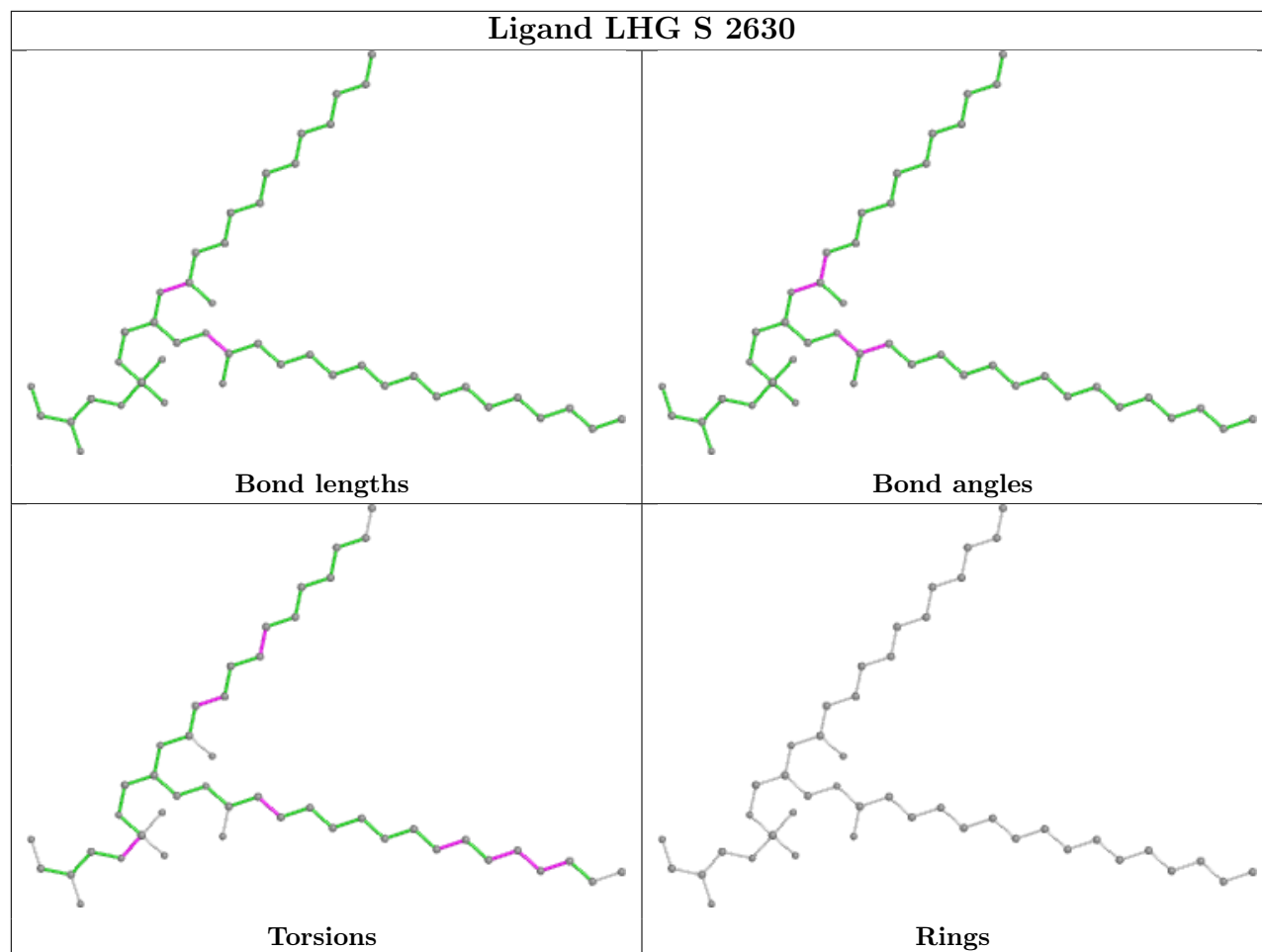
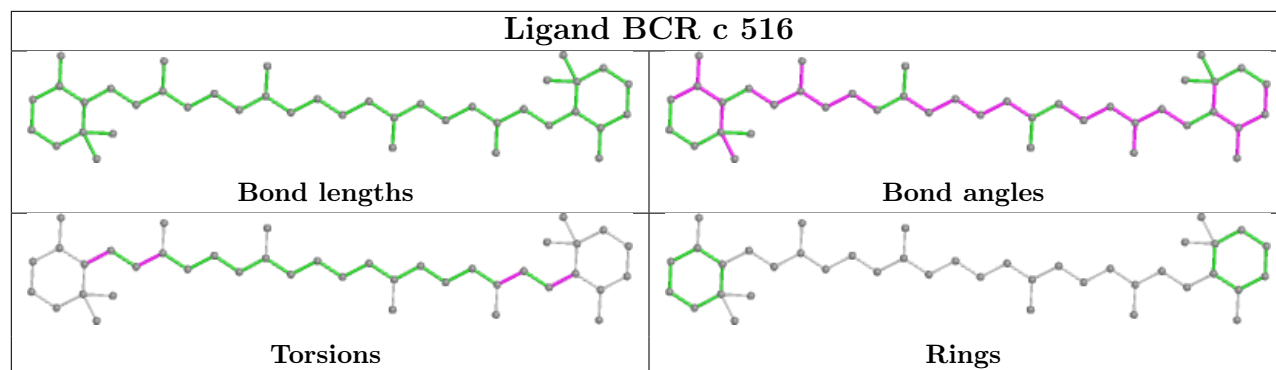


Ligand CLA r 603

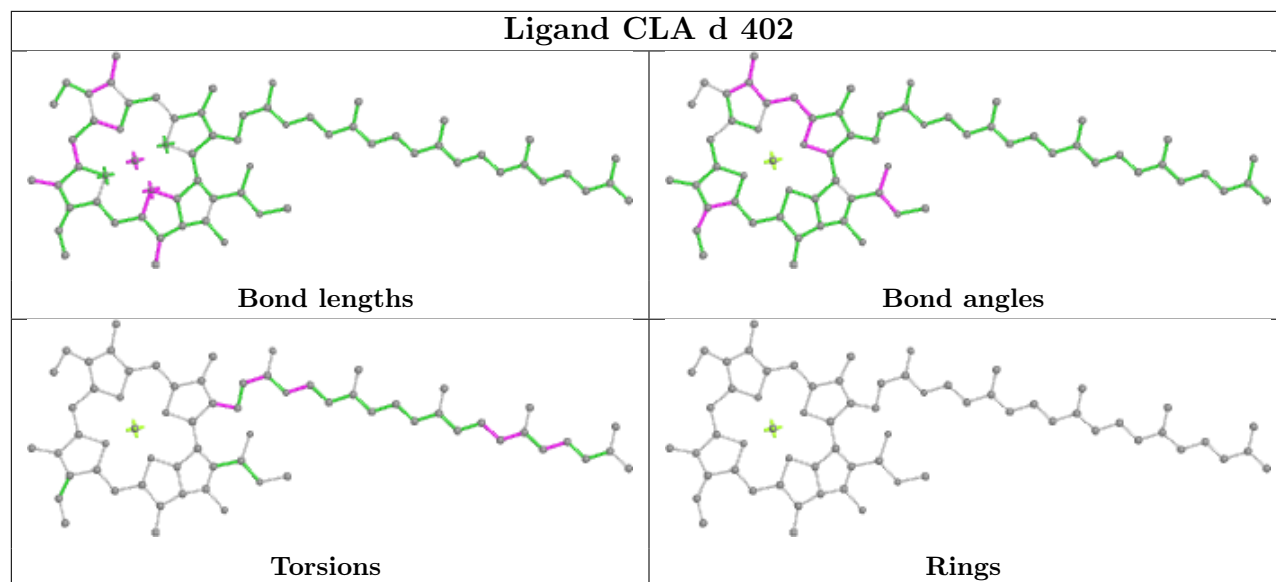




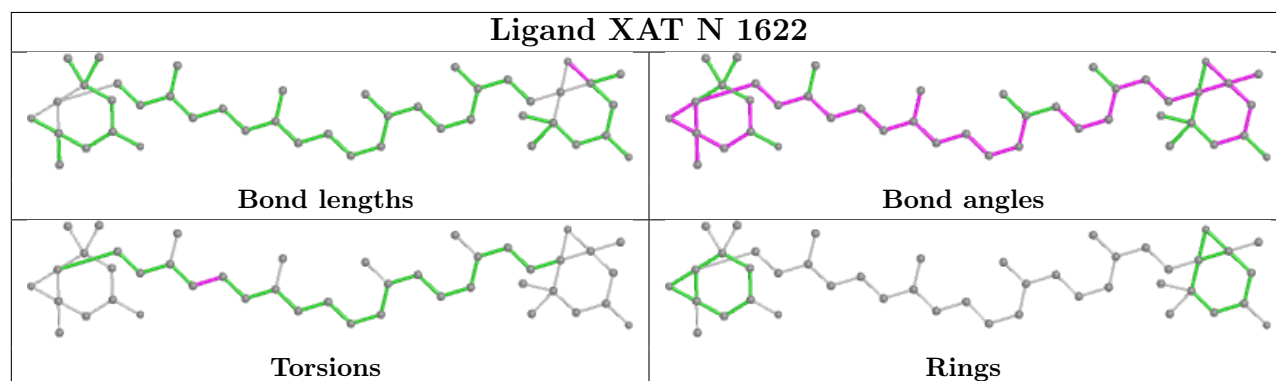




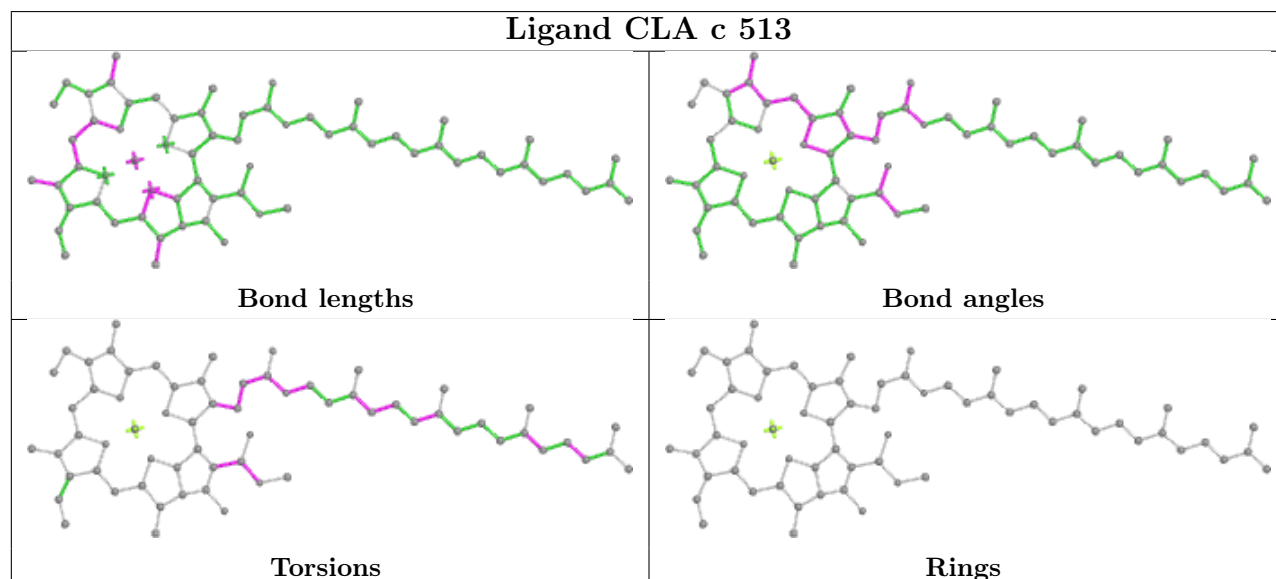
Ligand CLA d 402

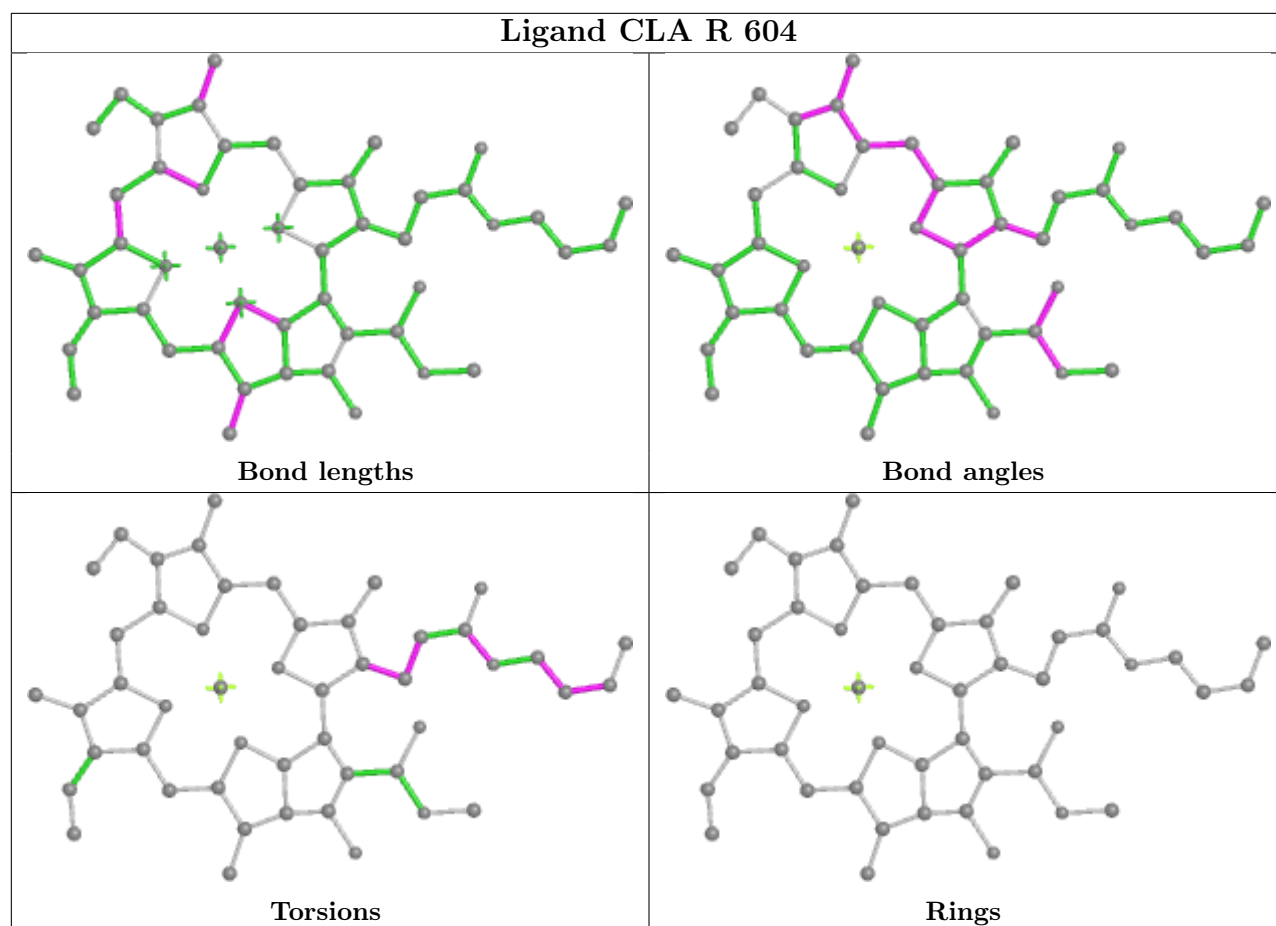
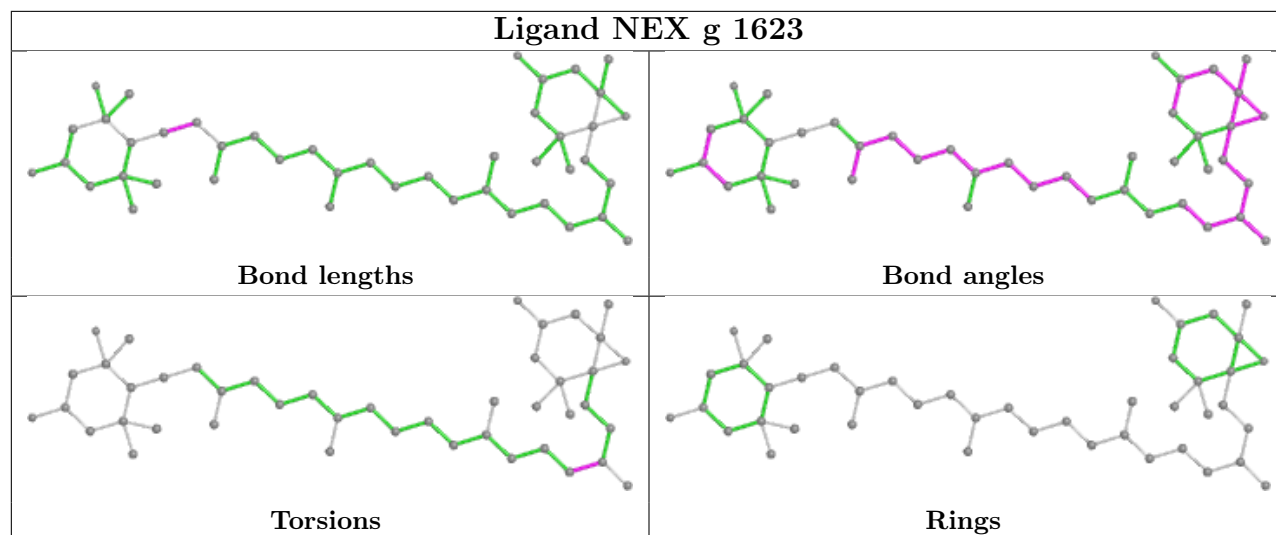


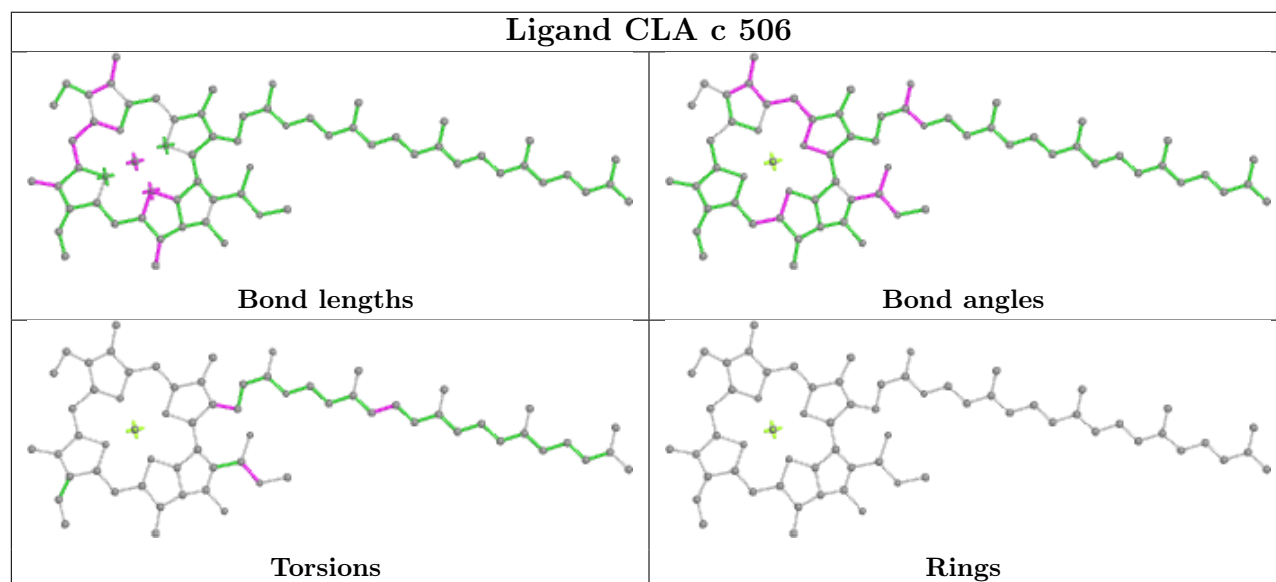
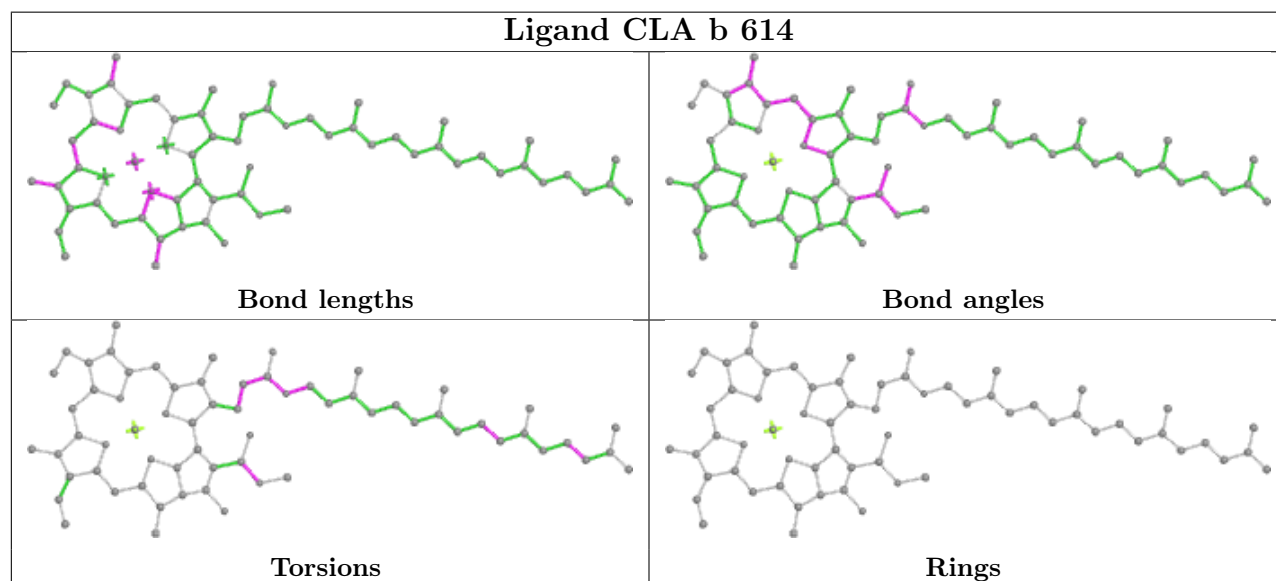
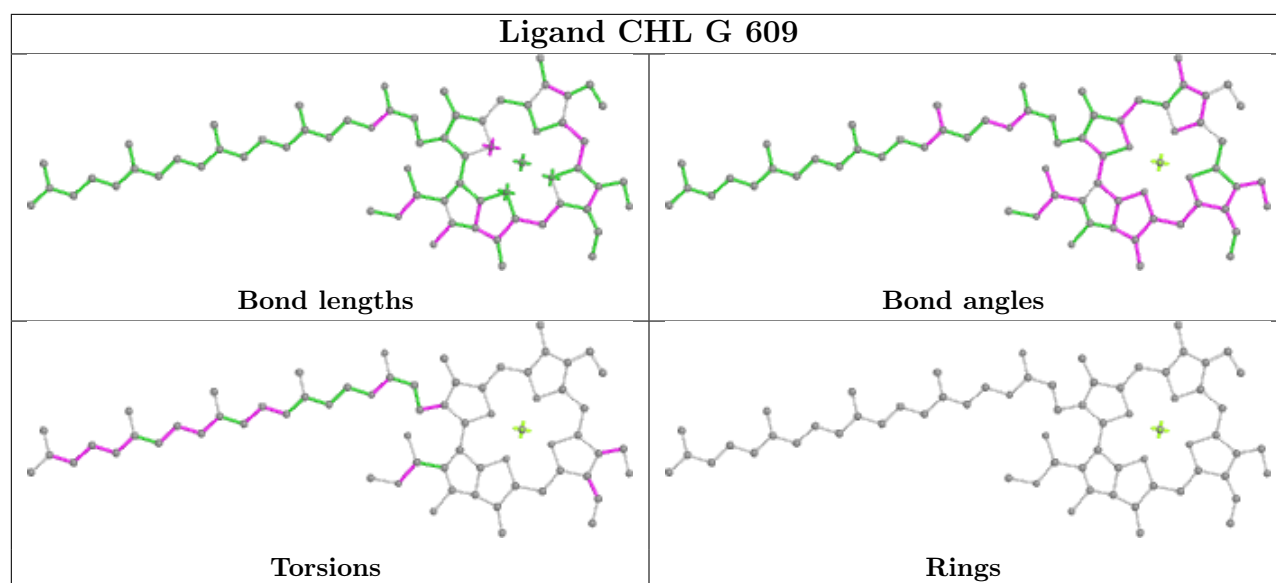
Ligand XAT N 1622



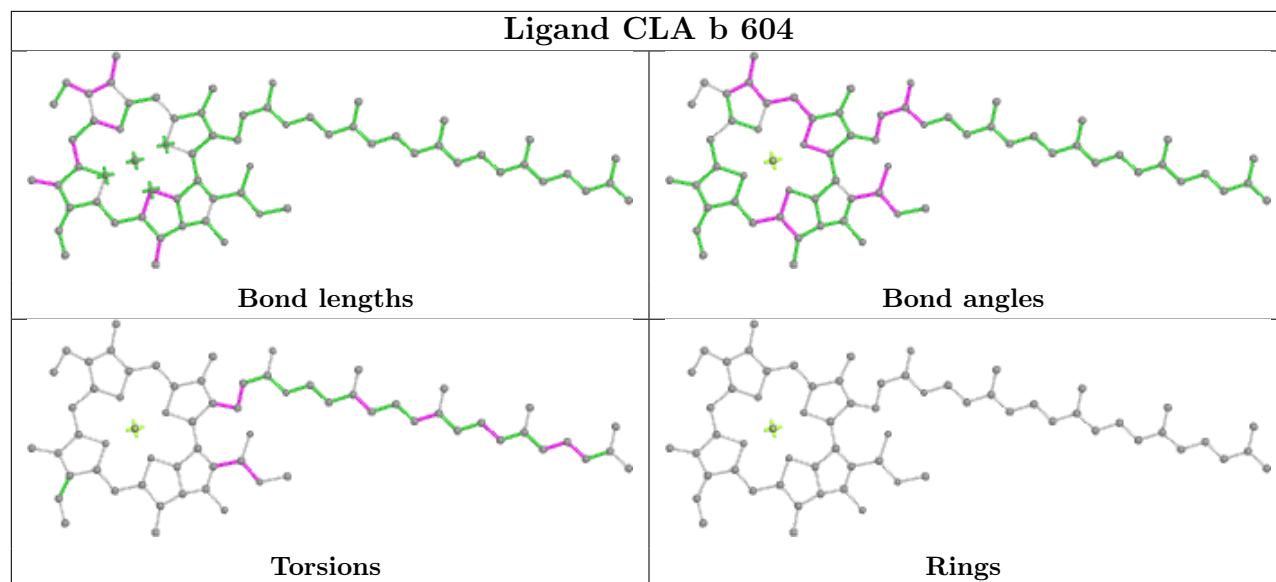
Ligand CLA c 513



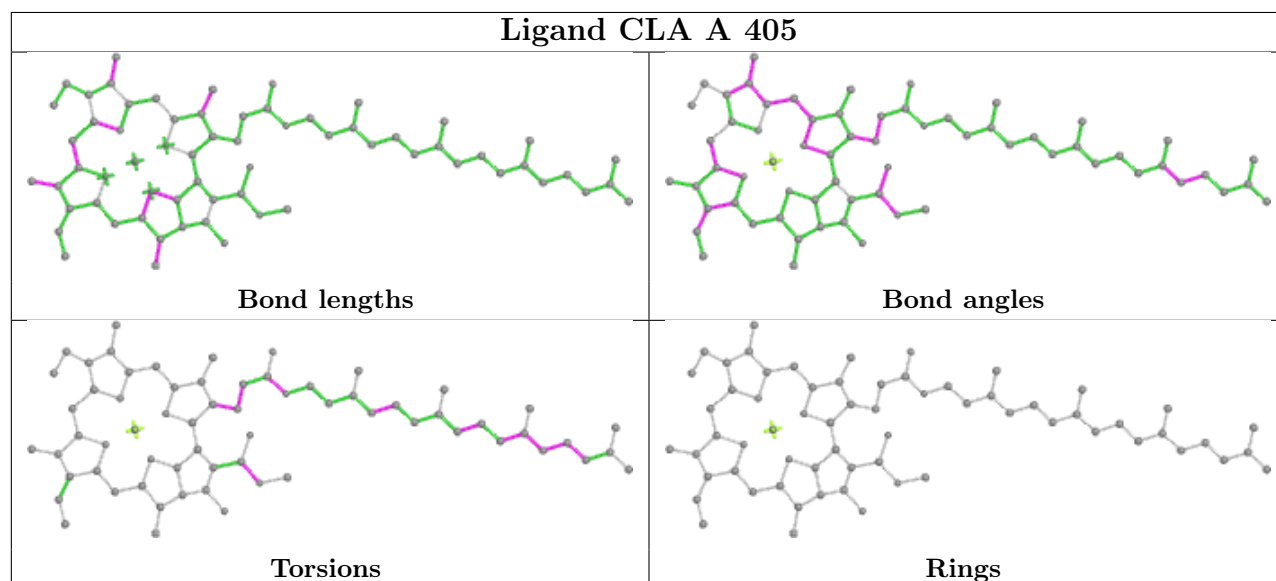




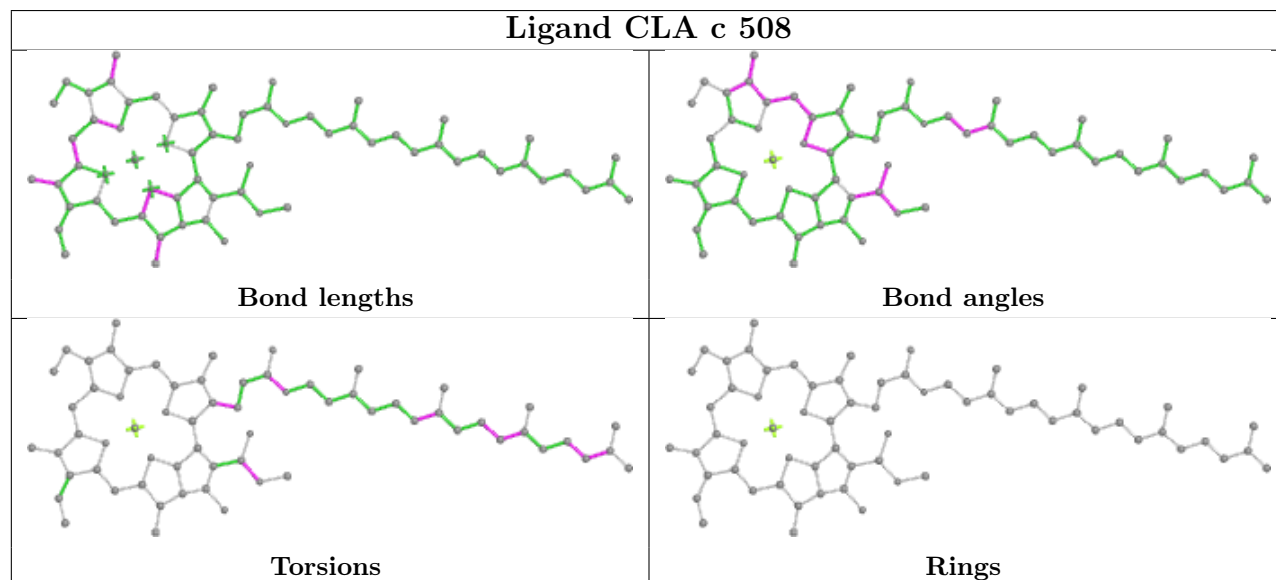
Ligand CLA b 604

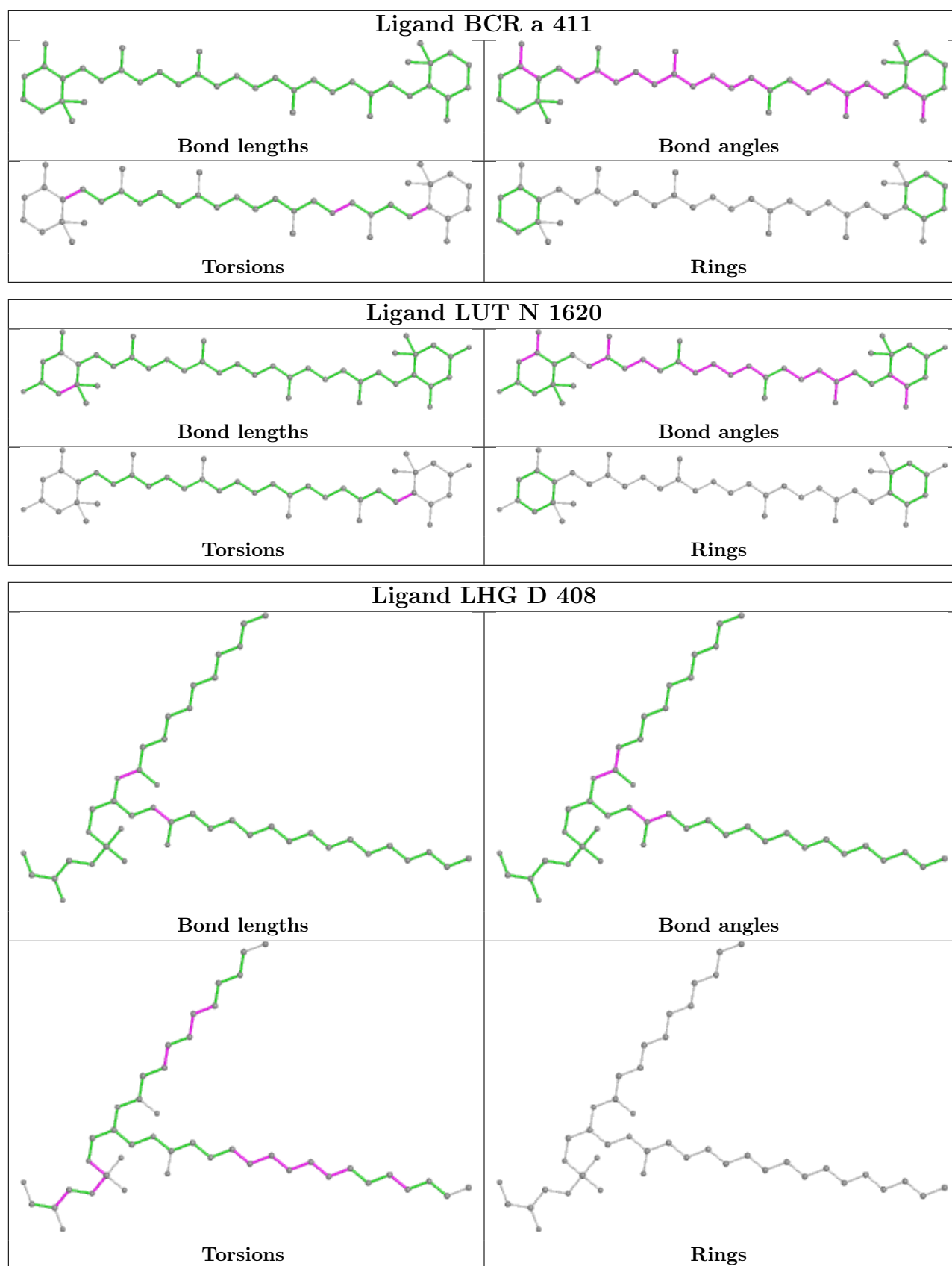


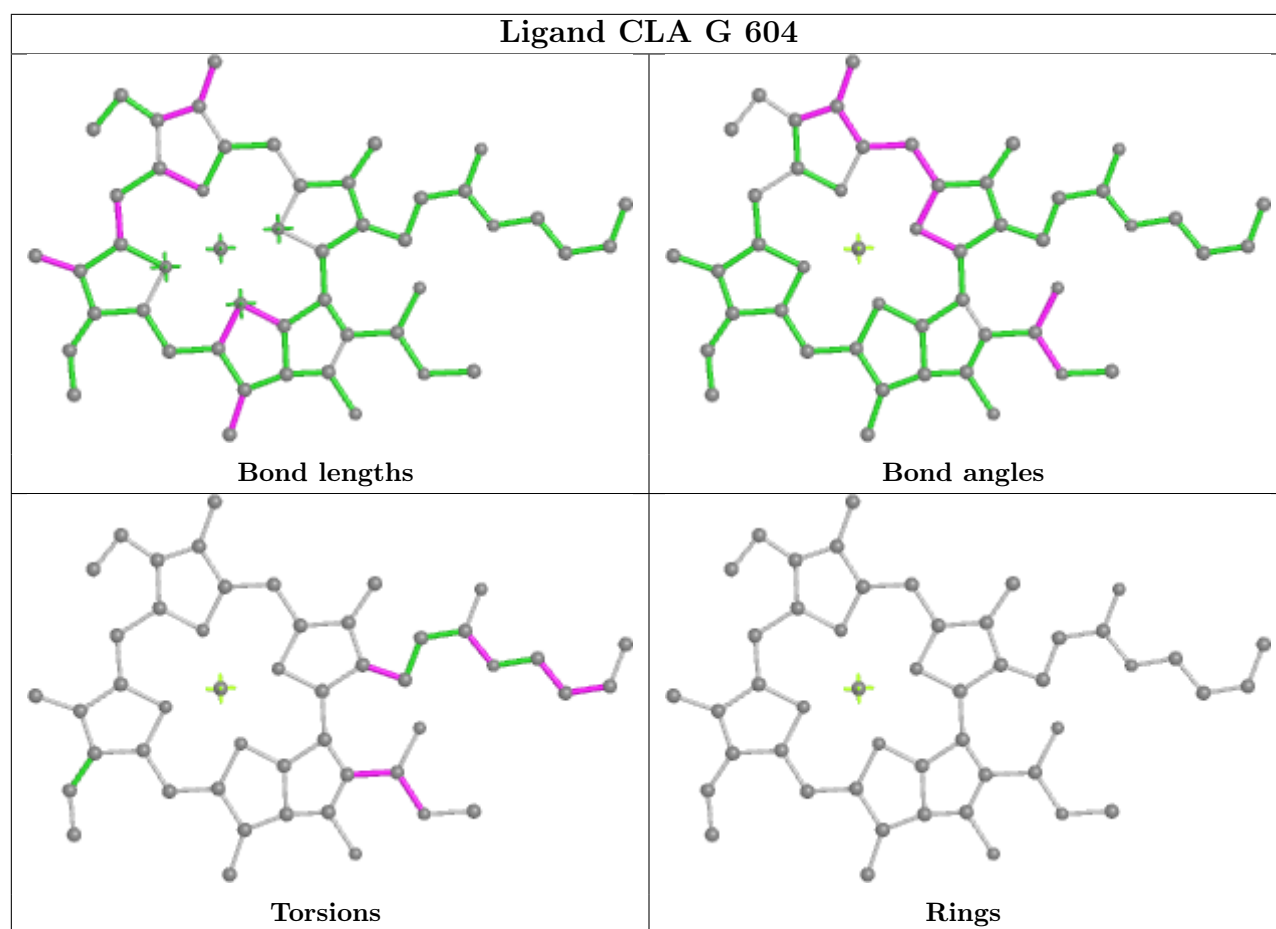
Ligand CLA A 405



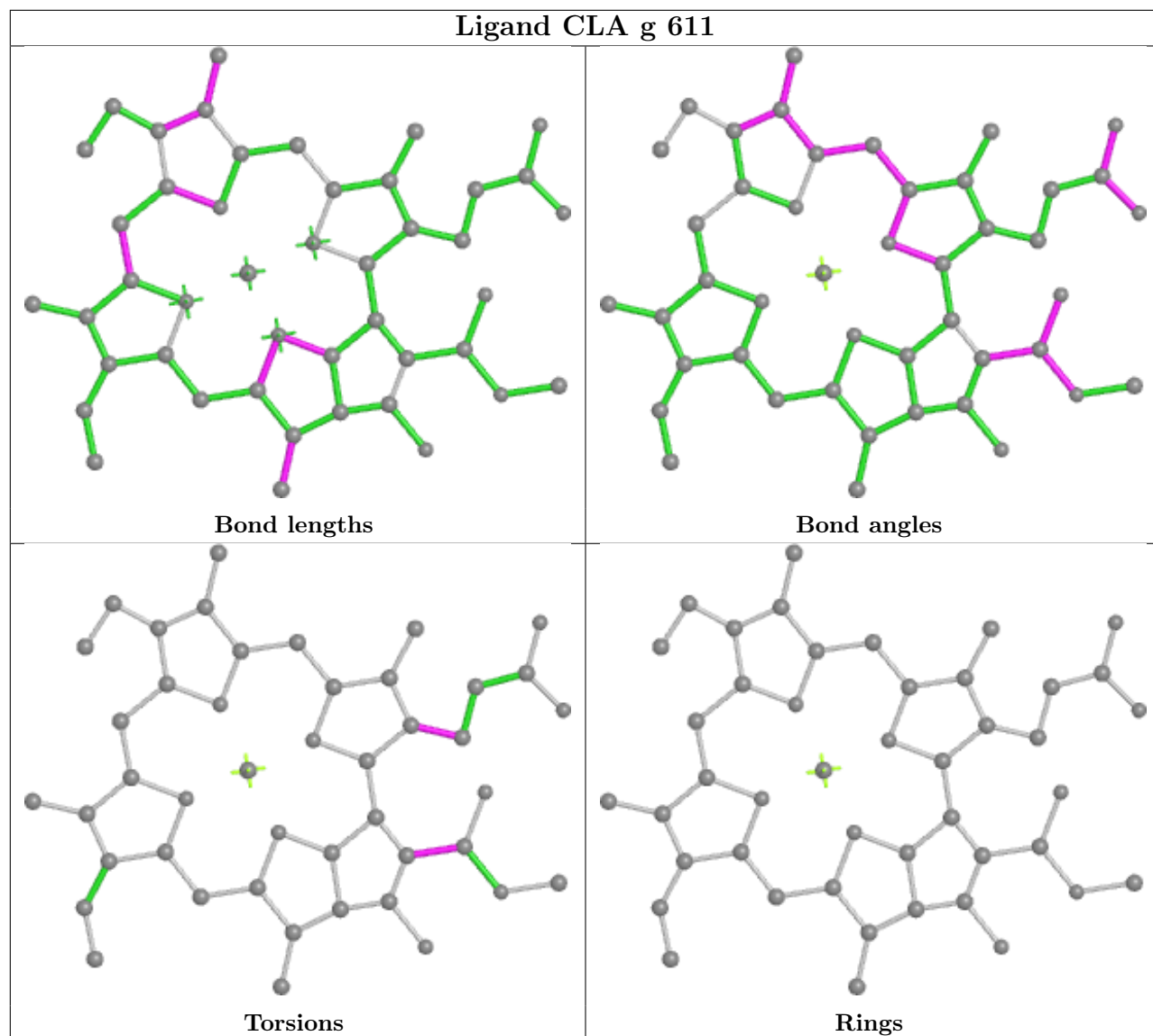
Ligand CLA c 508



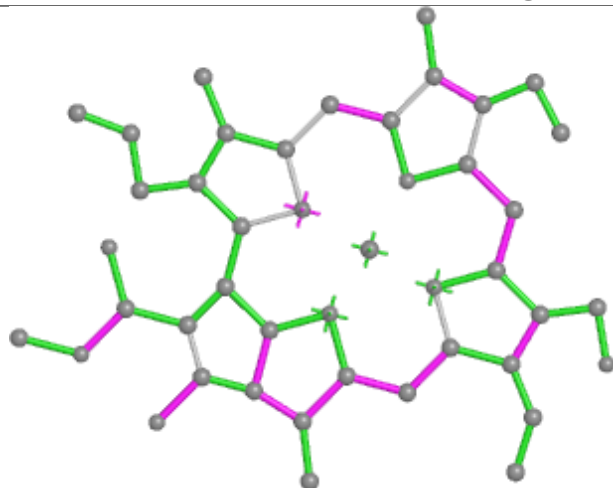




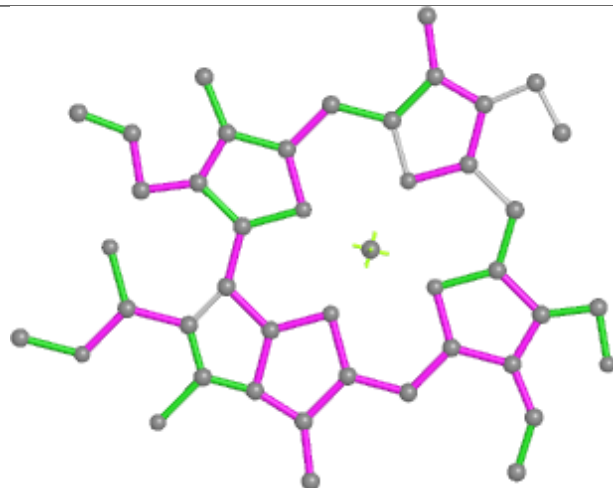
Ligand CLA g 611



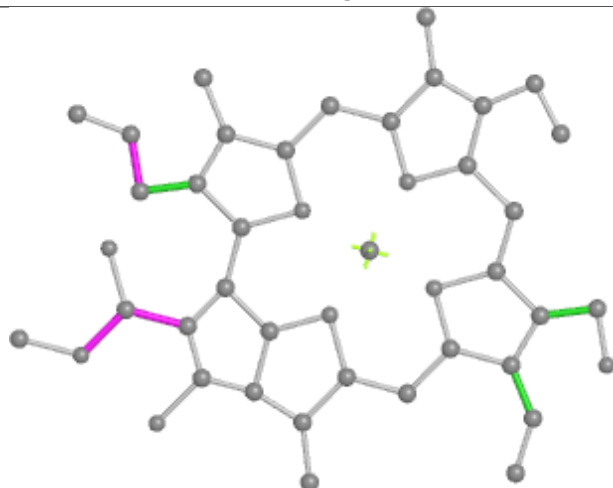
Ligand CHL s 606



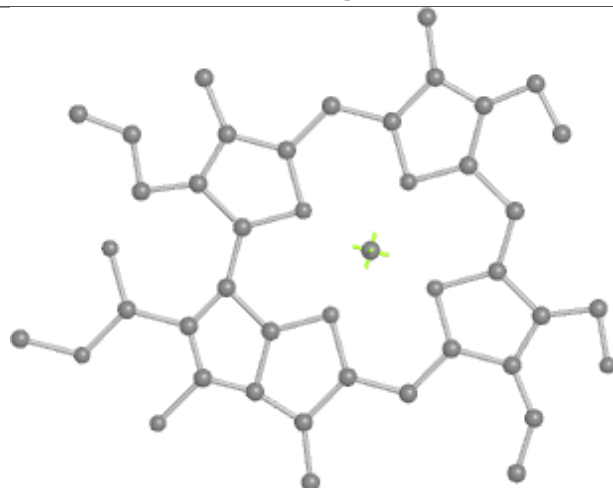
Bond lengths



Bond angles

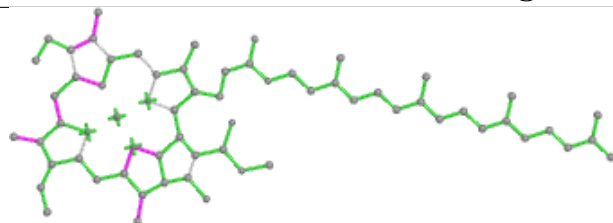


Torsions

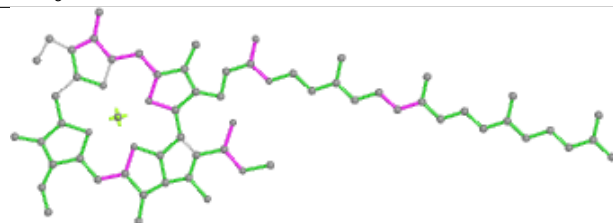


Rings

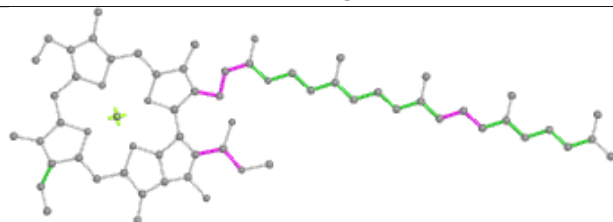
Ligand CLA y 602



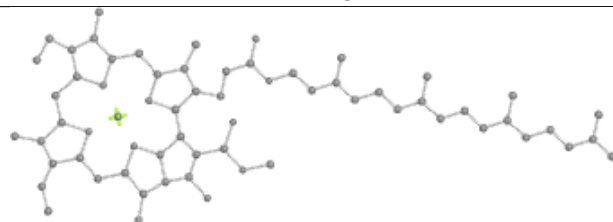
Bond lengths



Bond angles

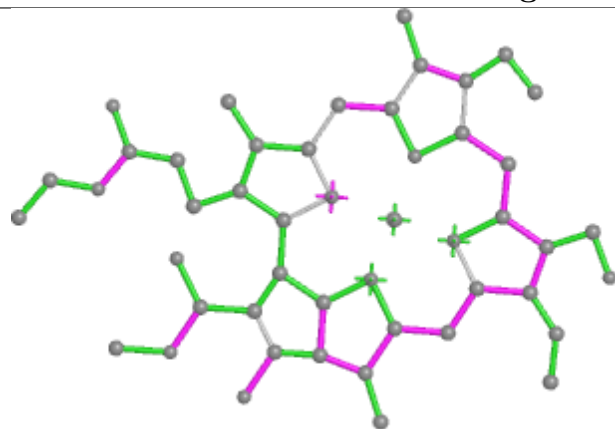


Torsions

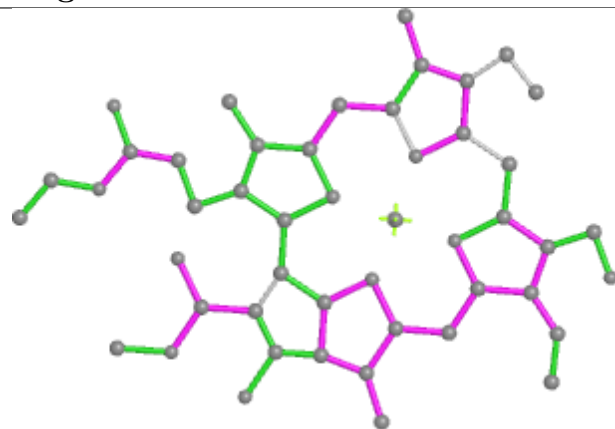


Rings

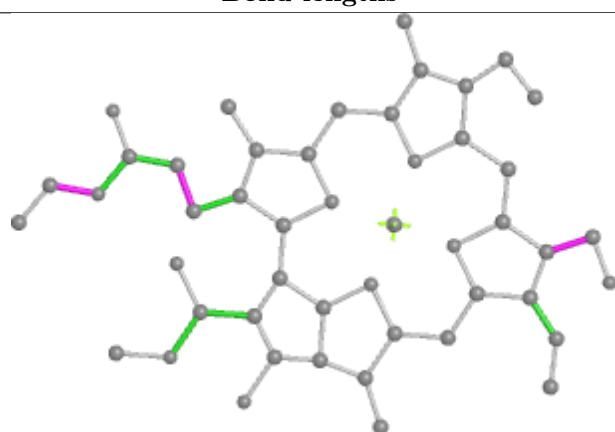
Ligand CHL g 605



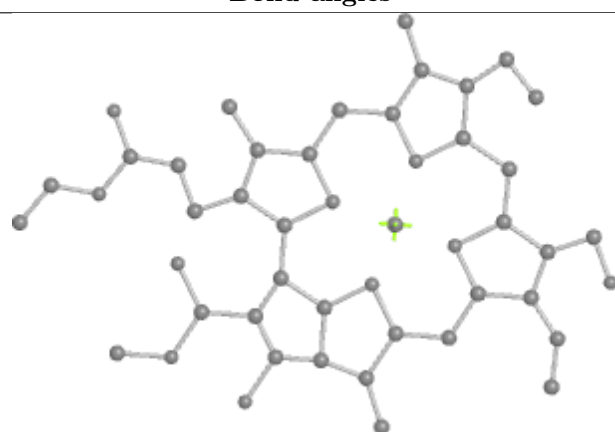
Bond lengths



Bond angles

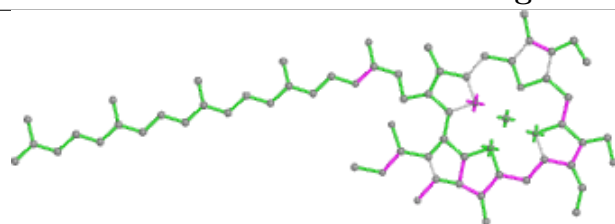


Torsions

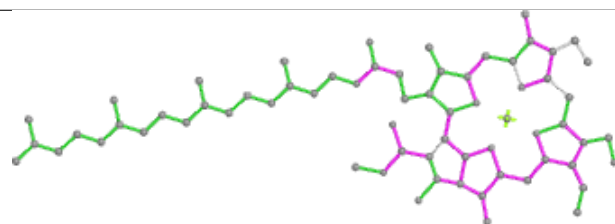


Rings

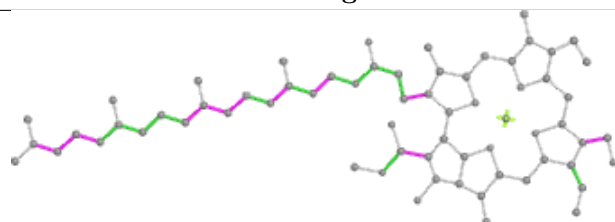
Ligand CHL N 601



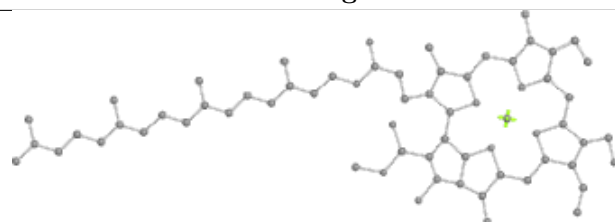
Bond lengths



Bond angles

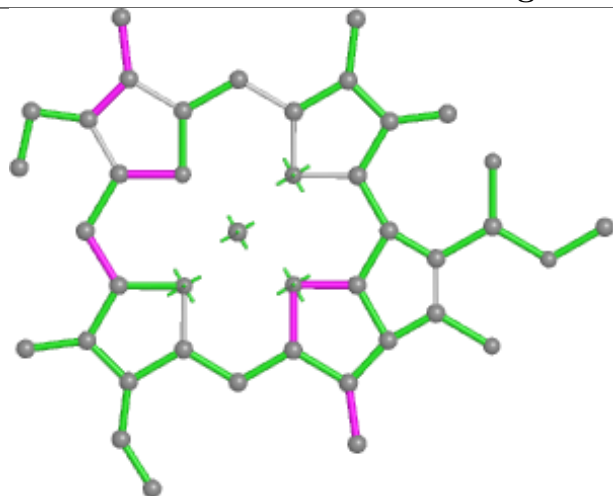


Torsions

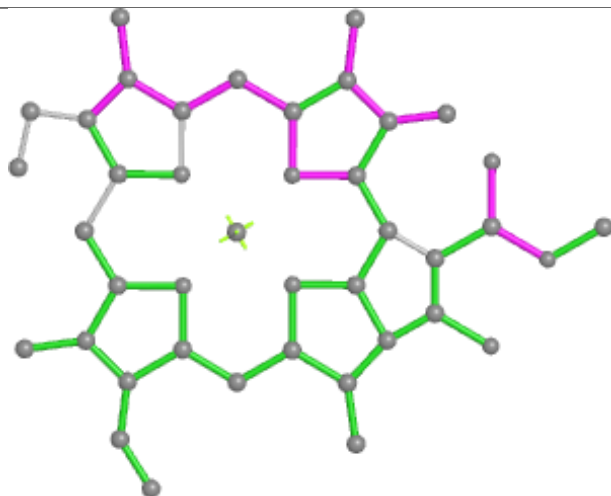


Rings

Ligand CLA S 609



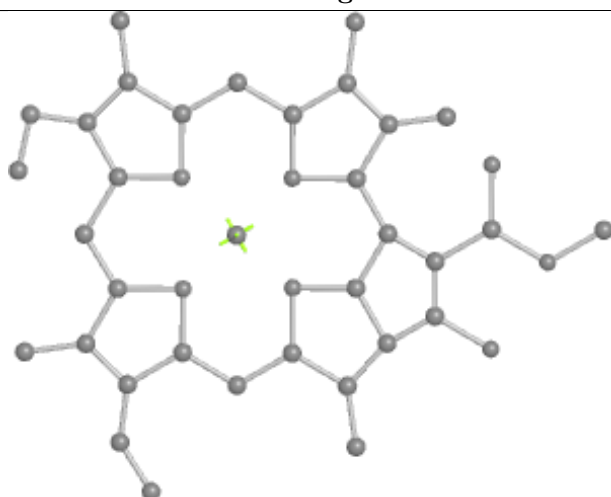
Bond lengths



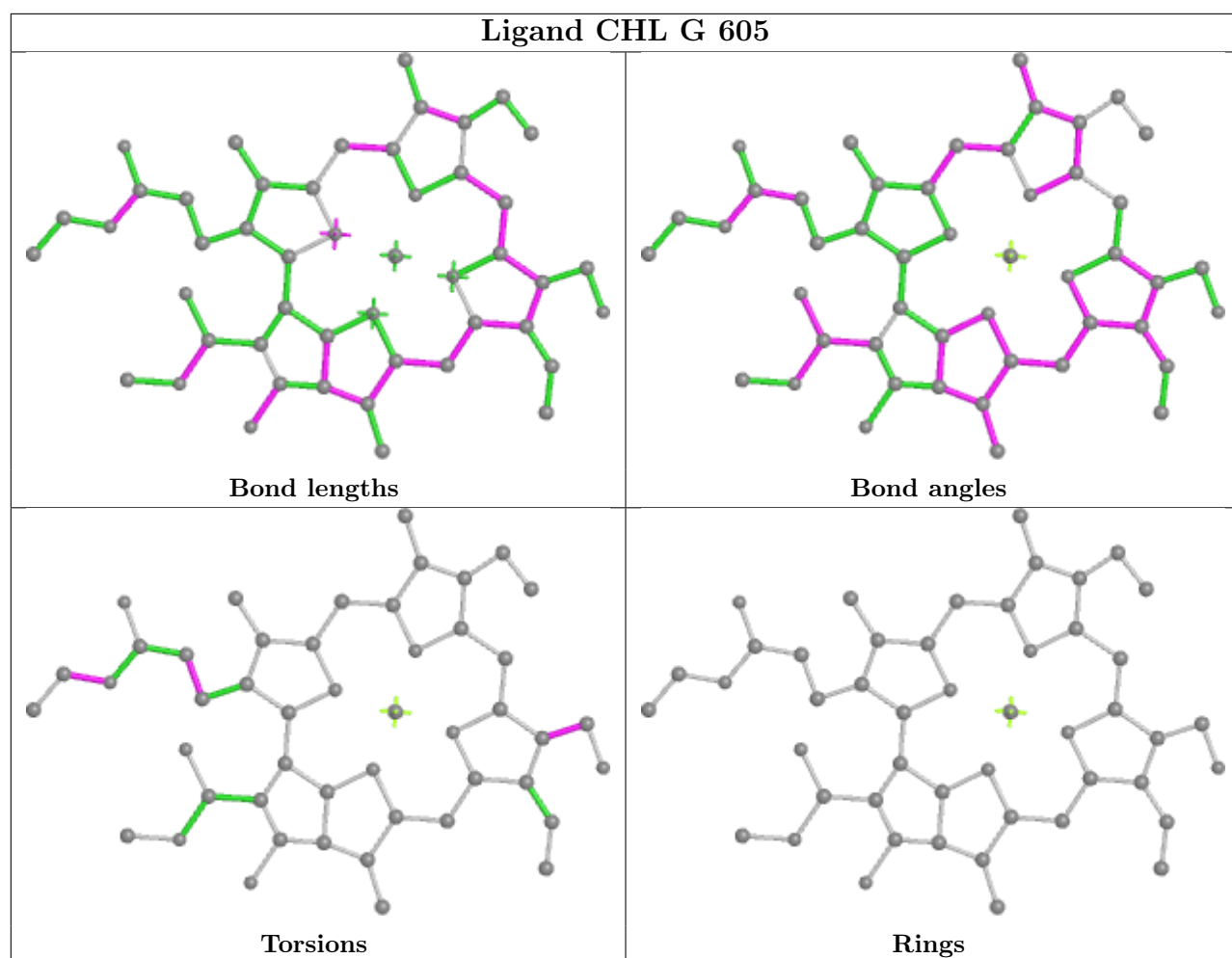
Bond angles

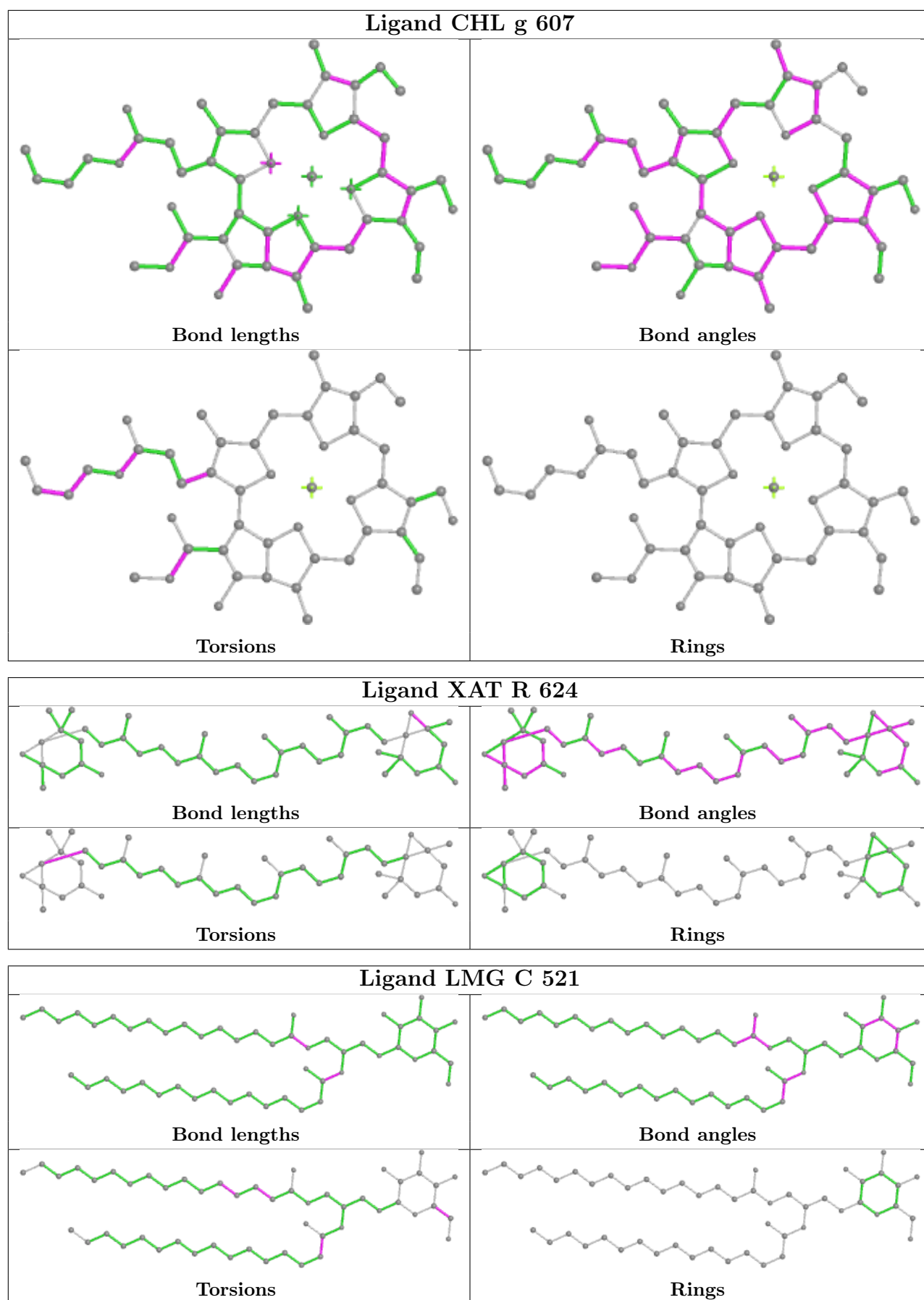


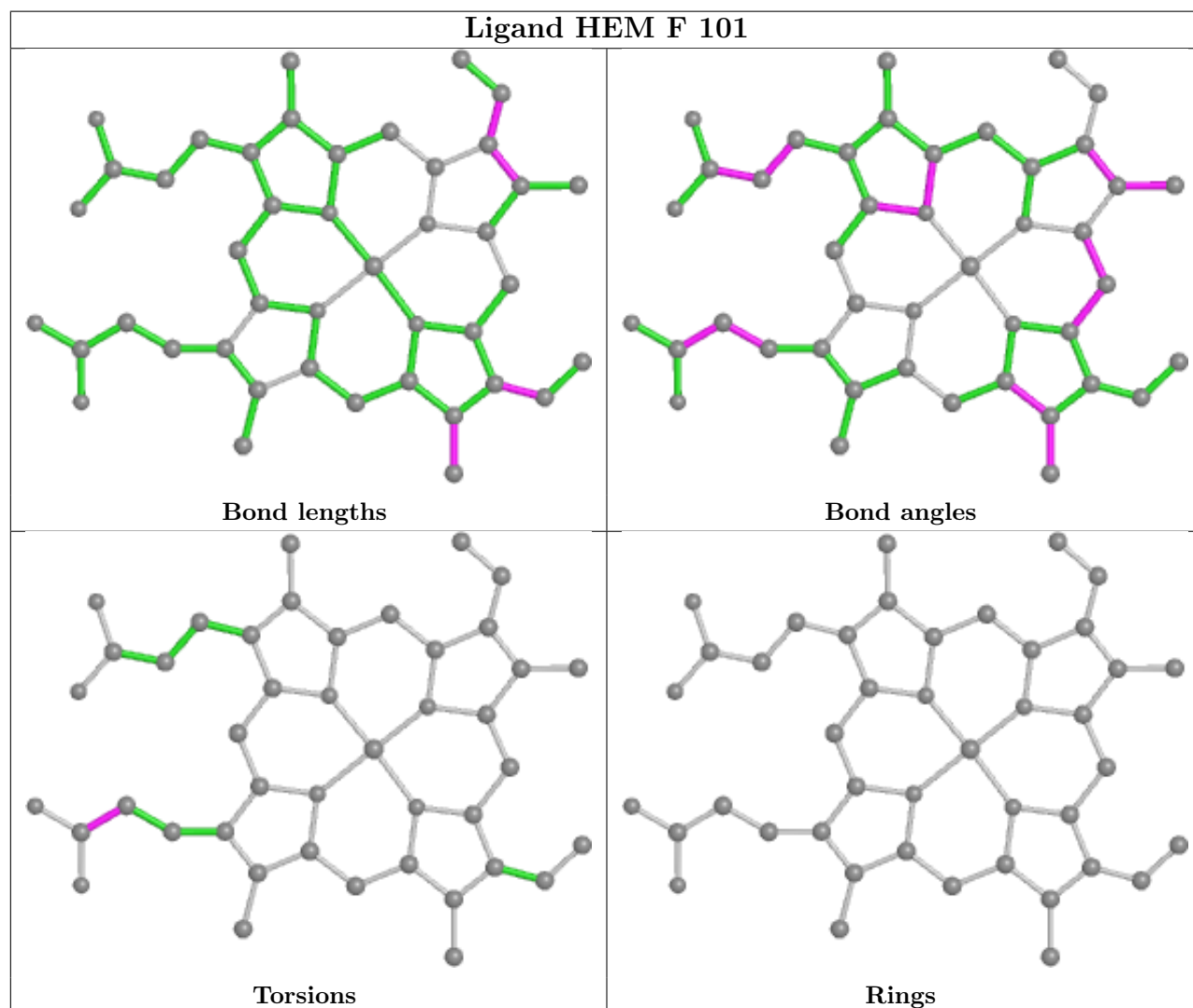
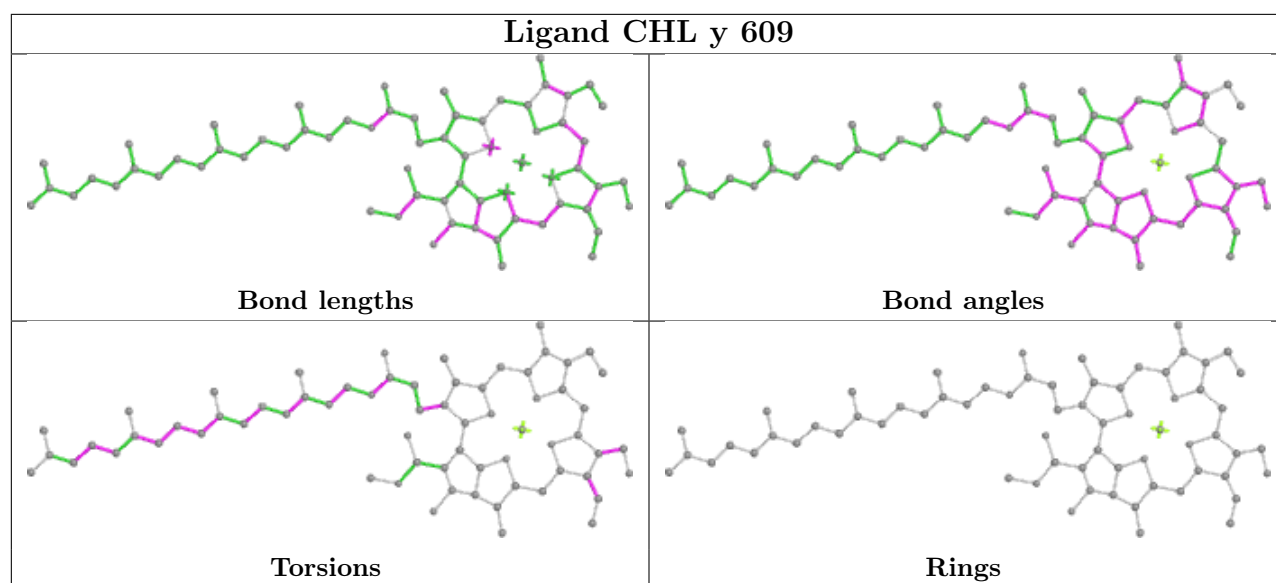
Torsions

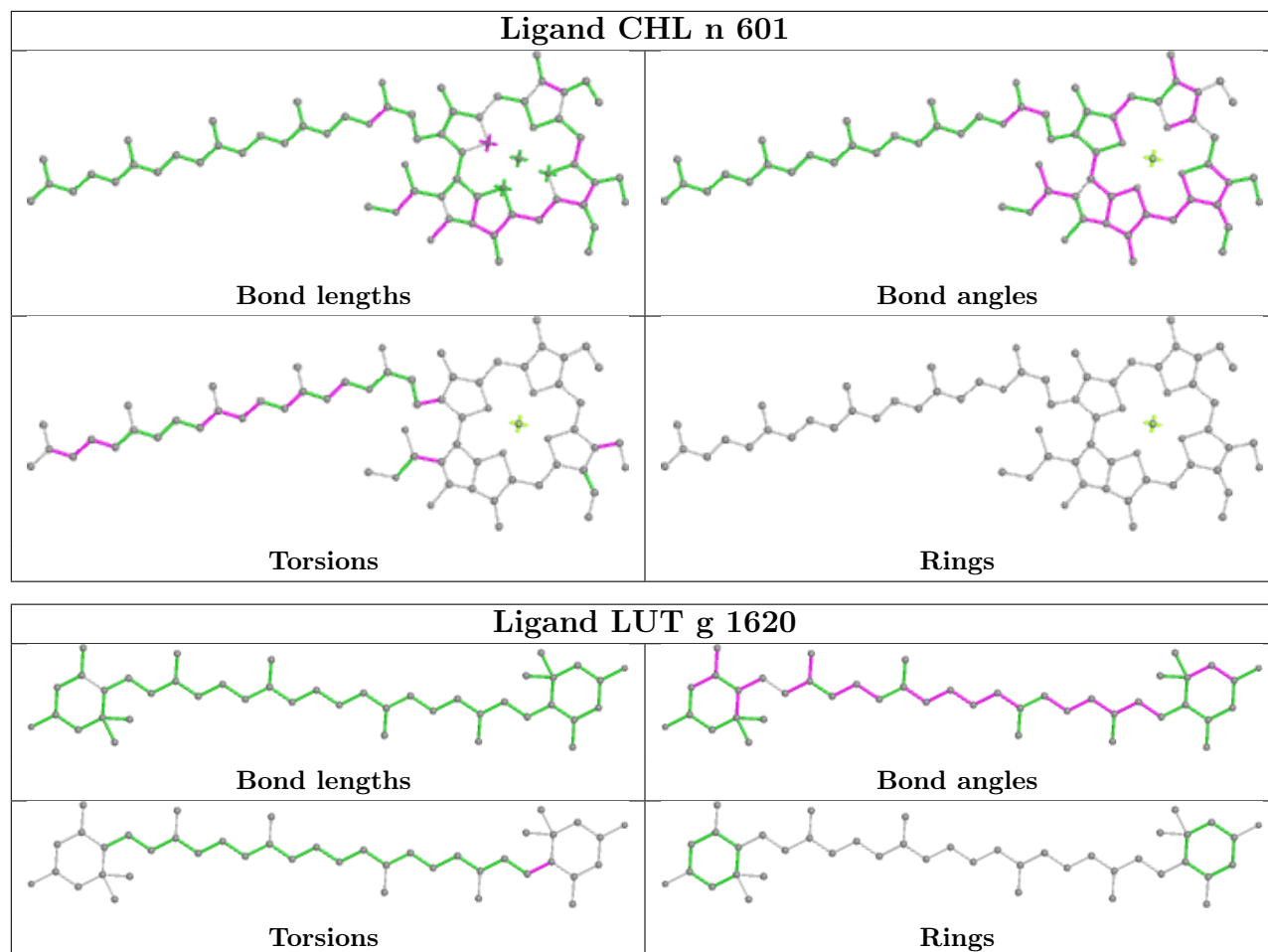


Rings

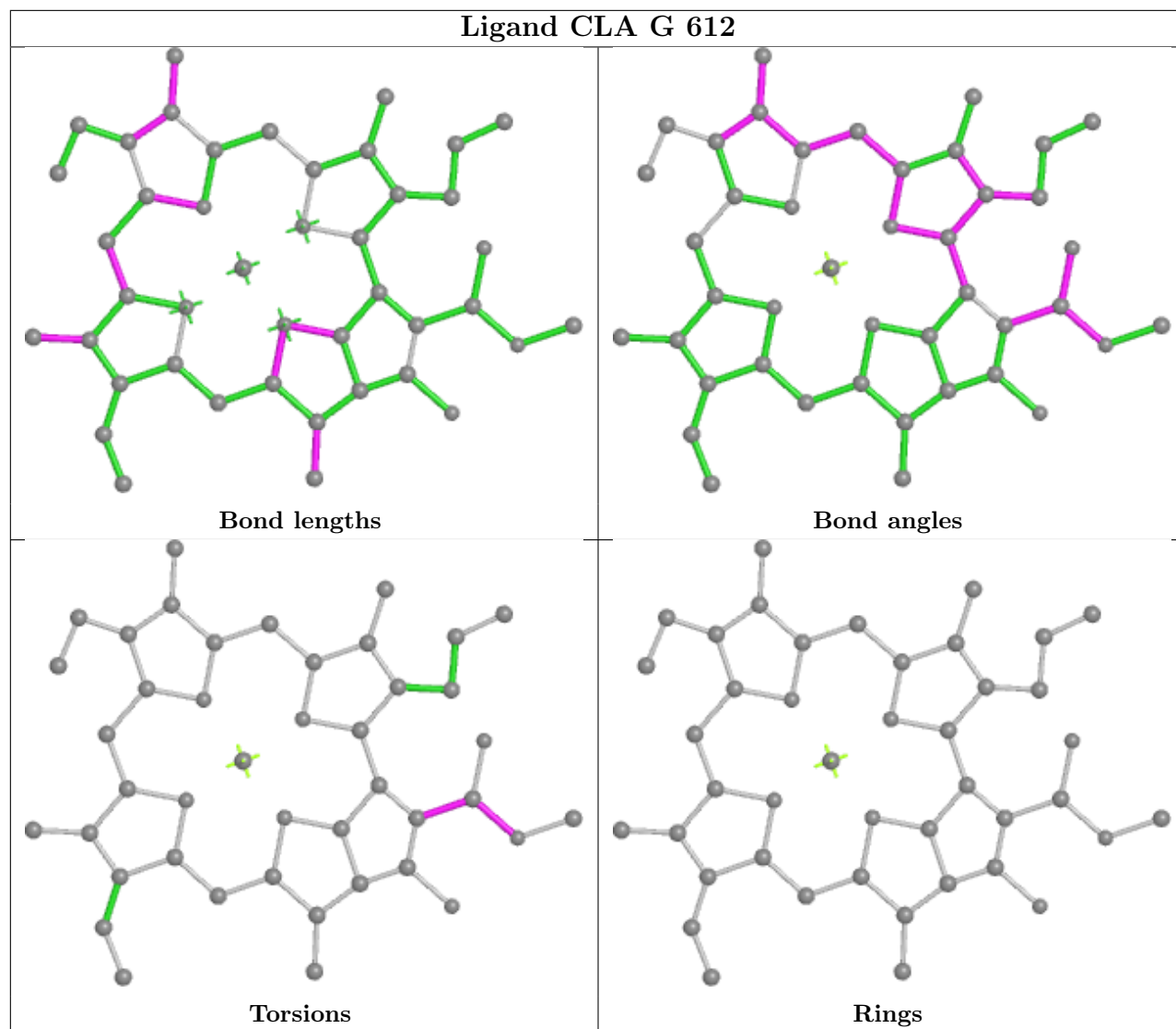




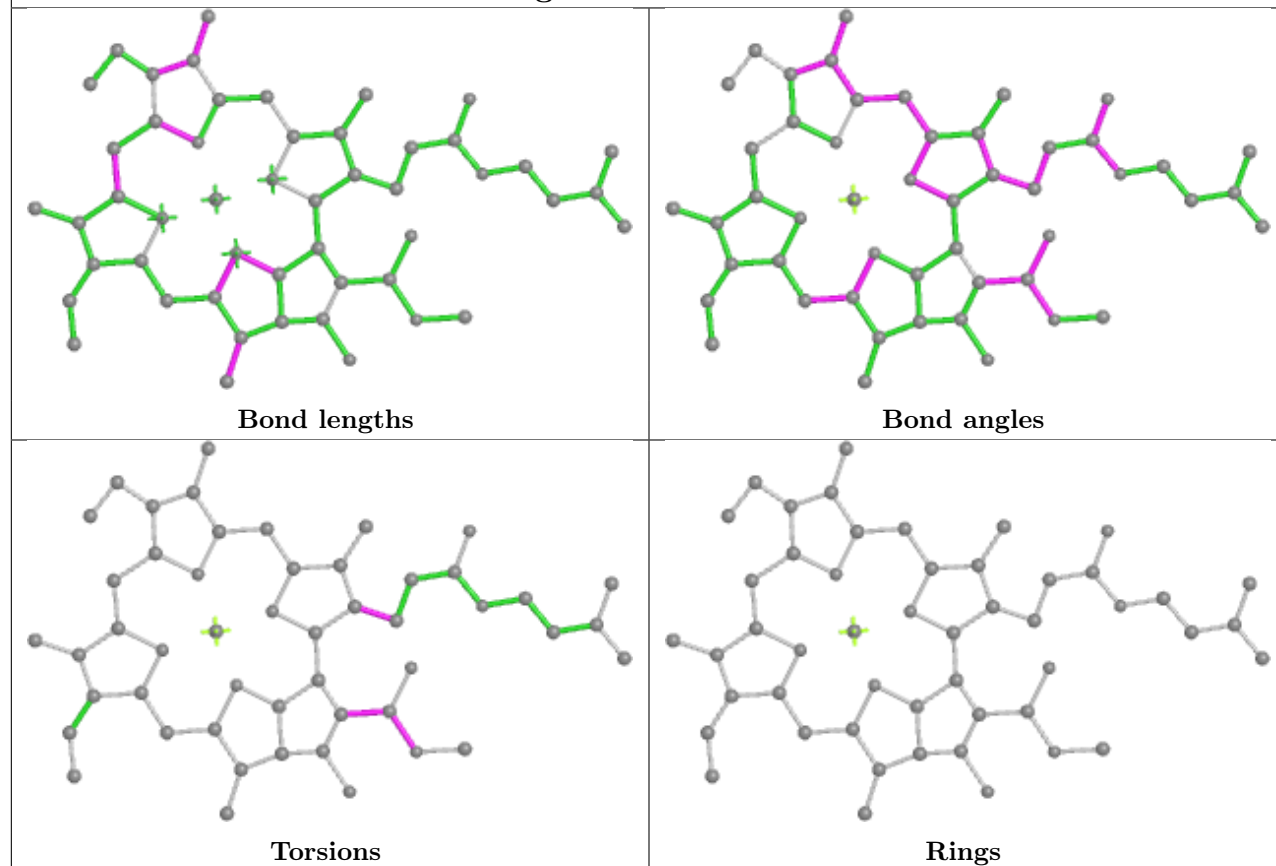




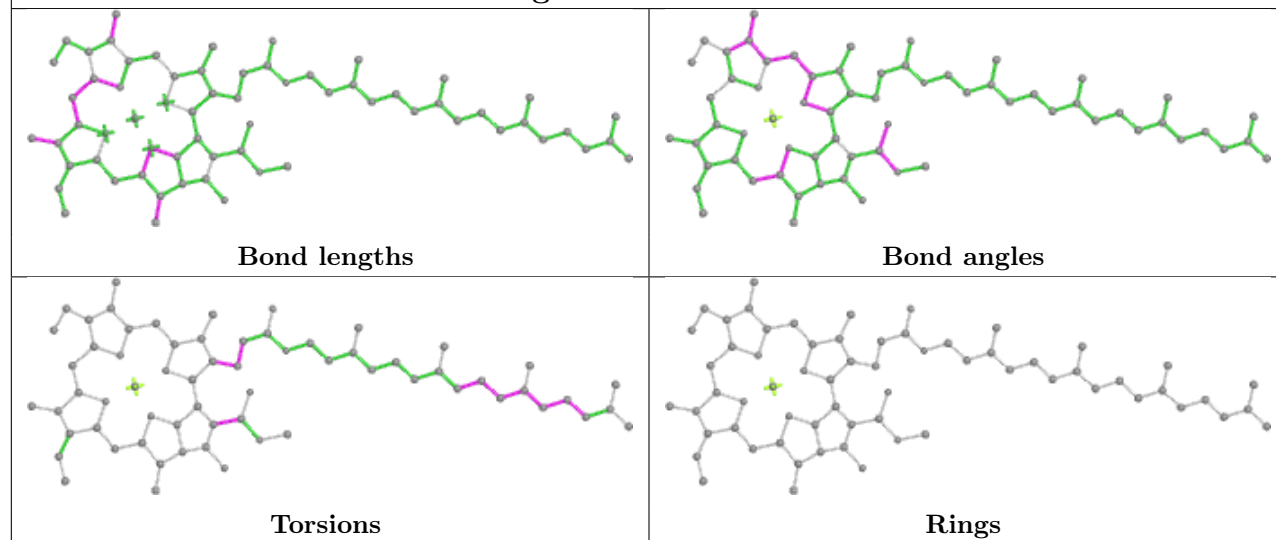
Ligand CLA G 612



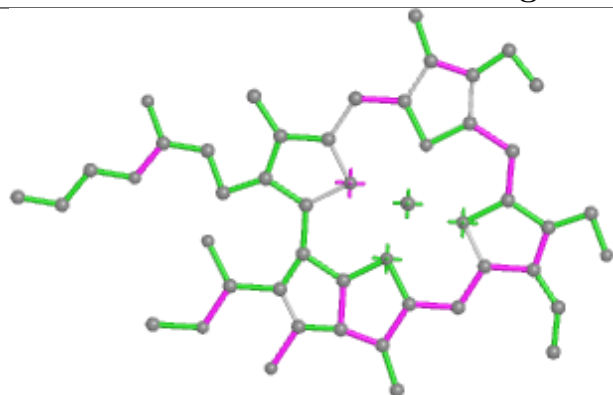
Ligand CLA S 605



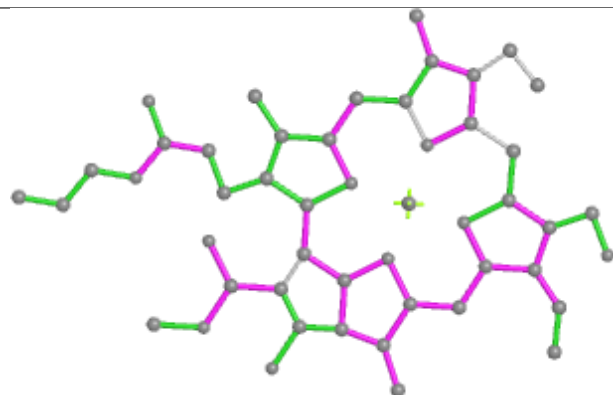
Ligand CLA B 608



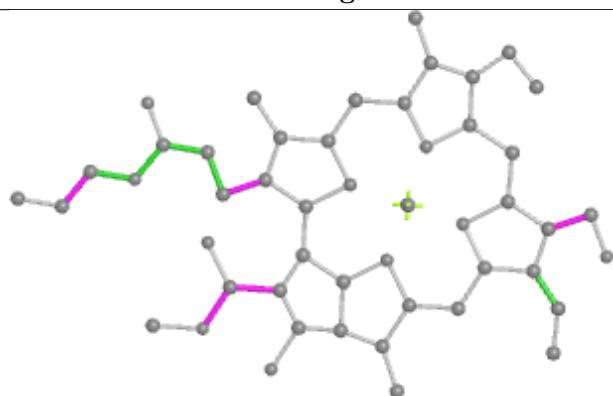
Ligand CHL s 608



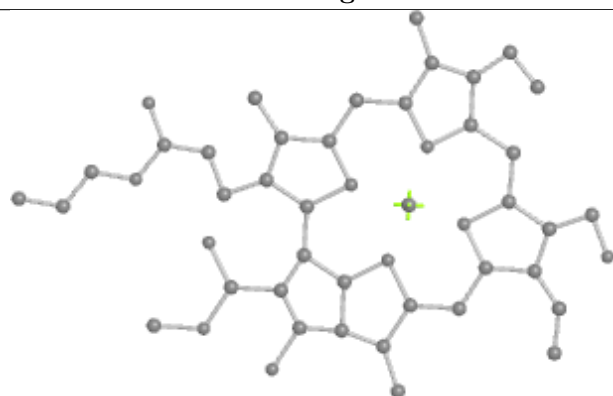
Bond lengths



Bond angles

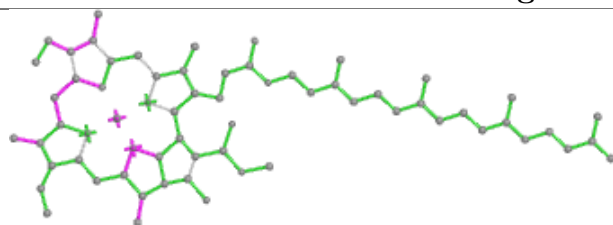


Torsions

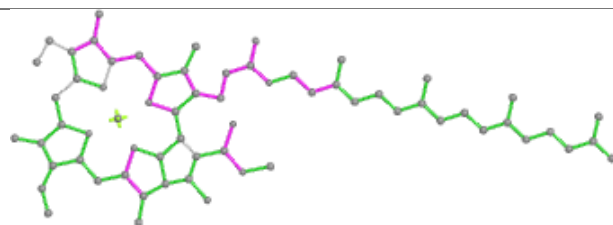


Rings

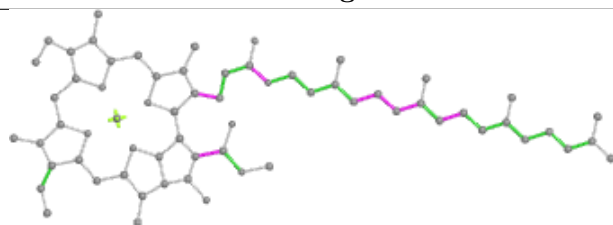
Ligand CLA b 605



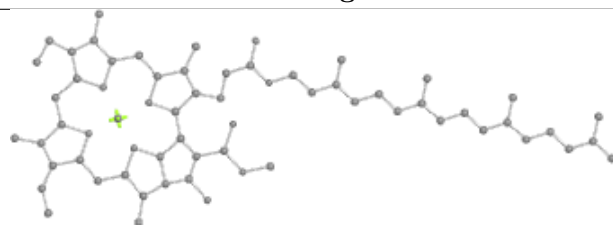
Bond lengths



Bond angles

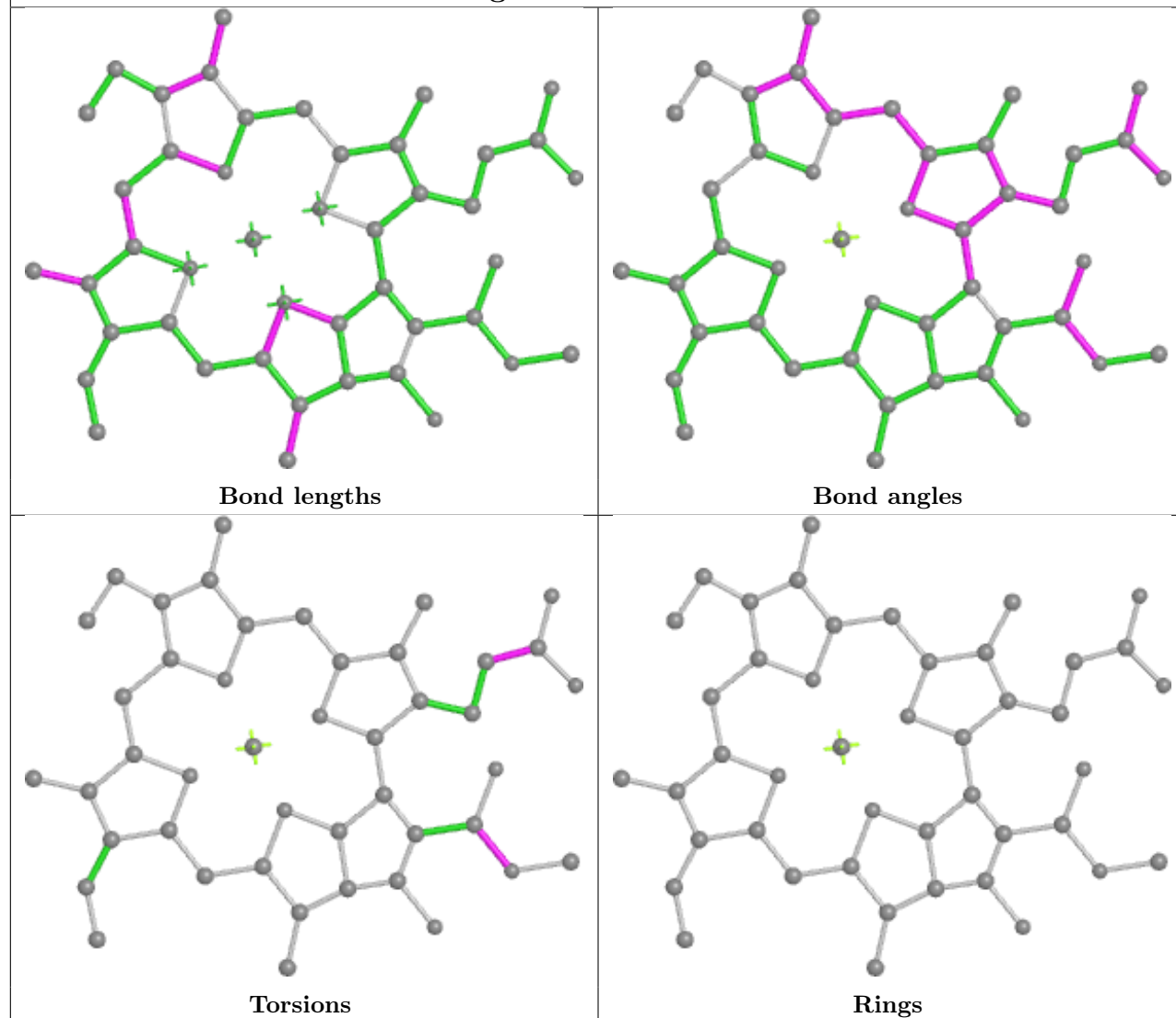


Torsions

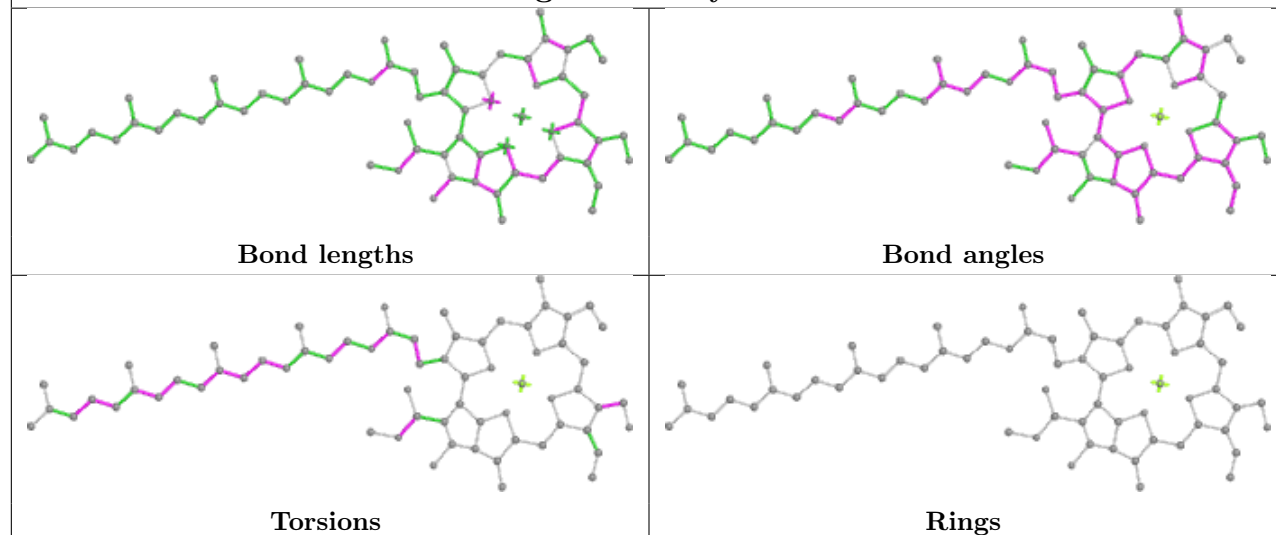


Rings

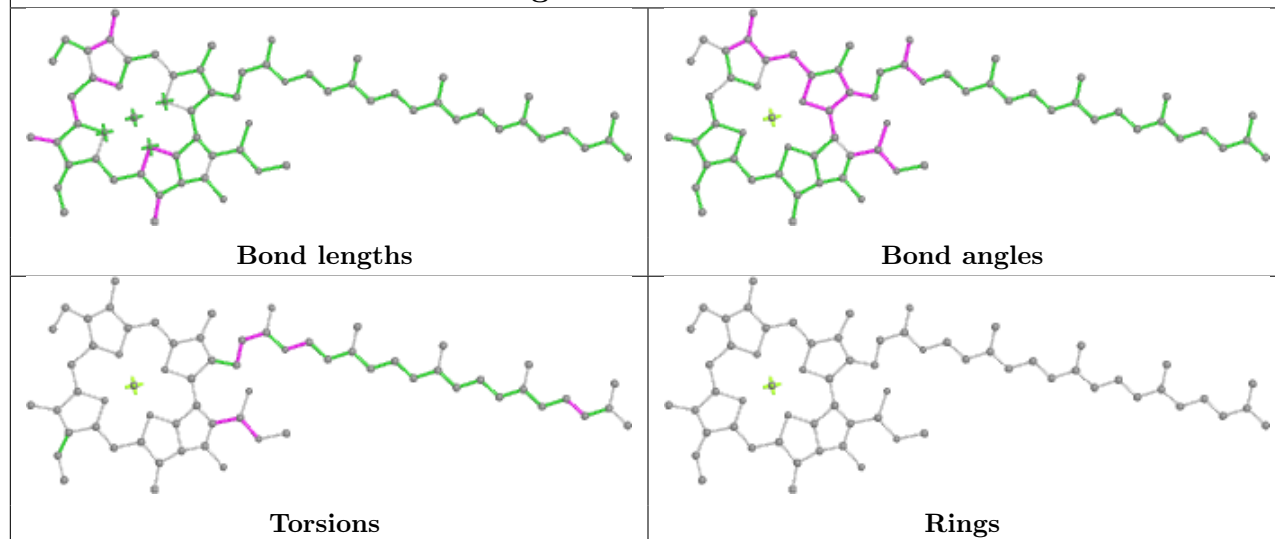
Ligand CLA N 612



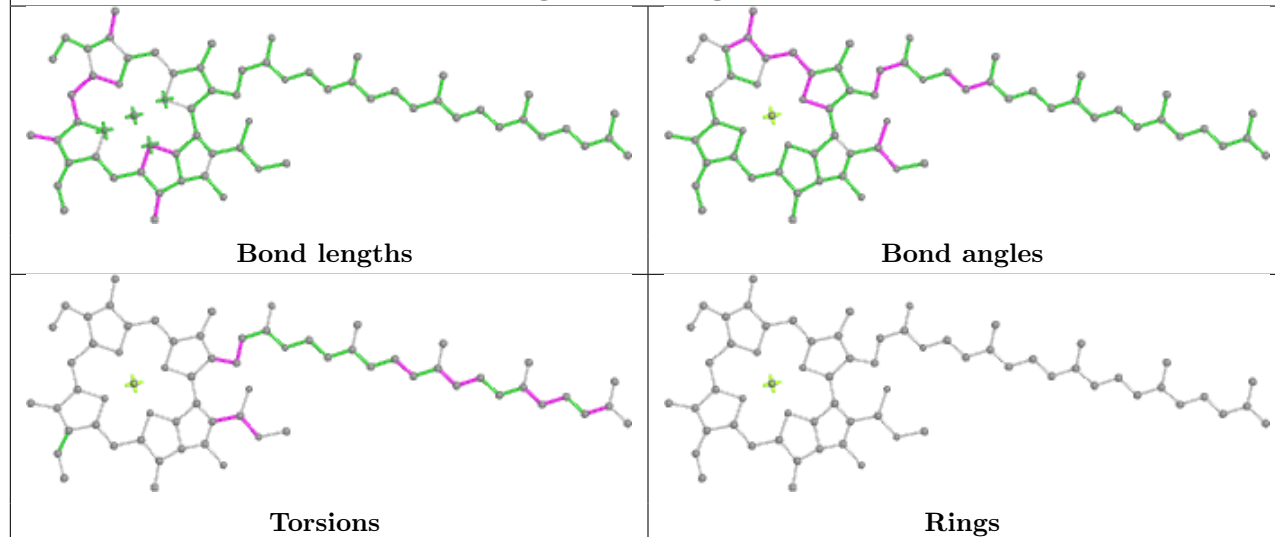
Ligand CHL y 601



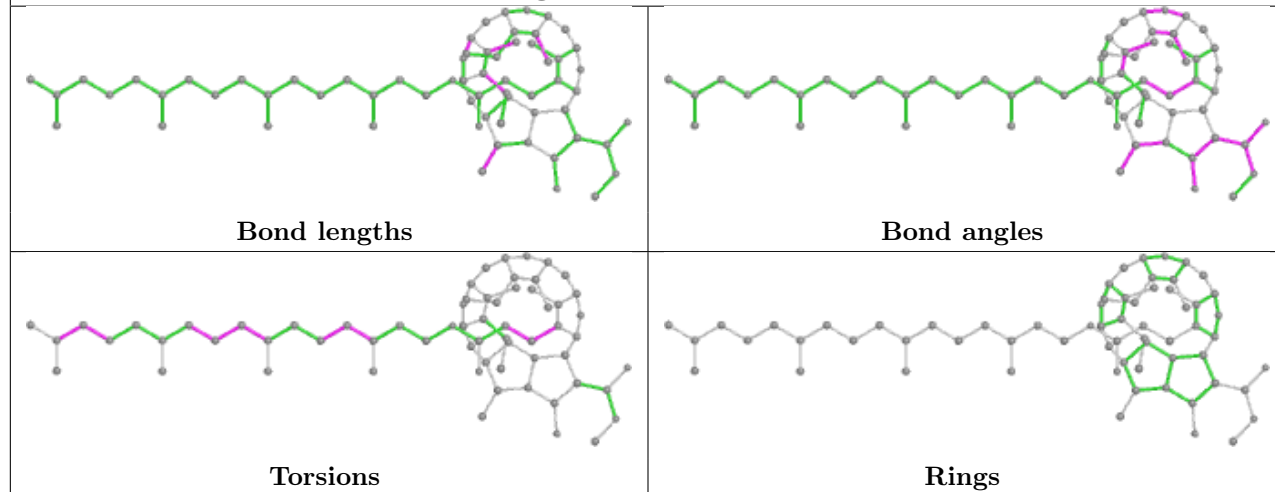
Ligand CLA B 611

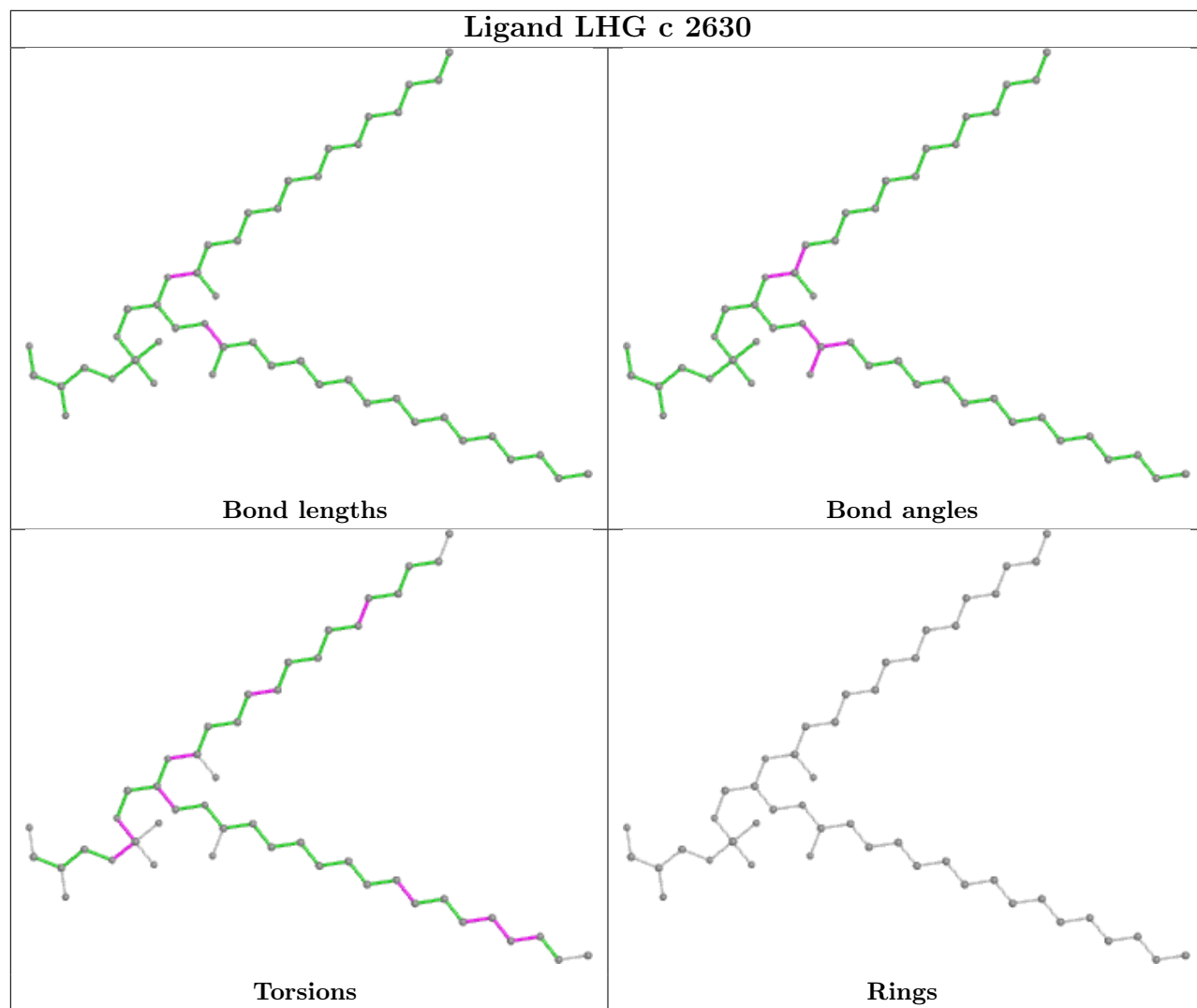
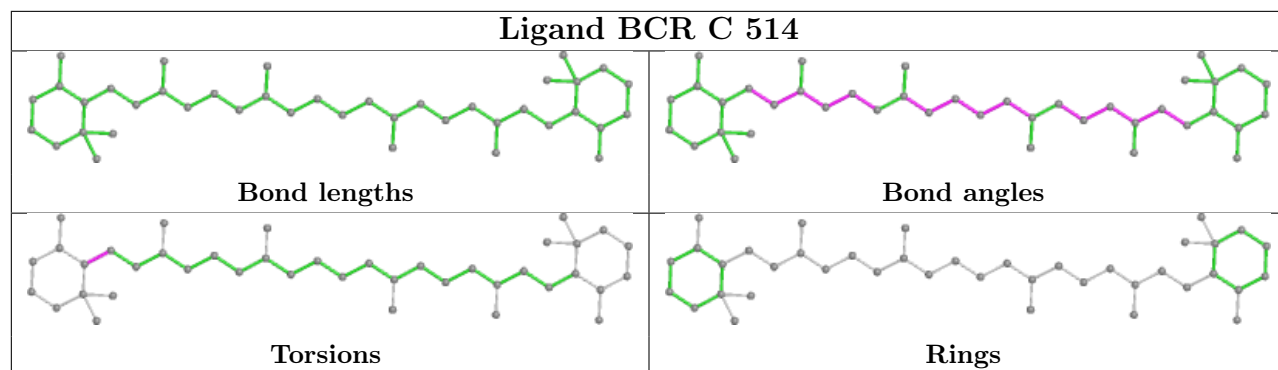


Ligand CLA g 610

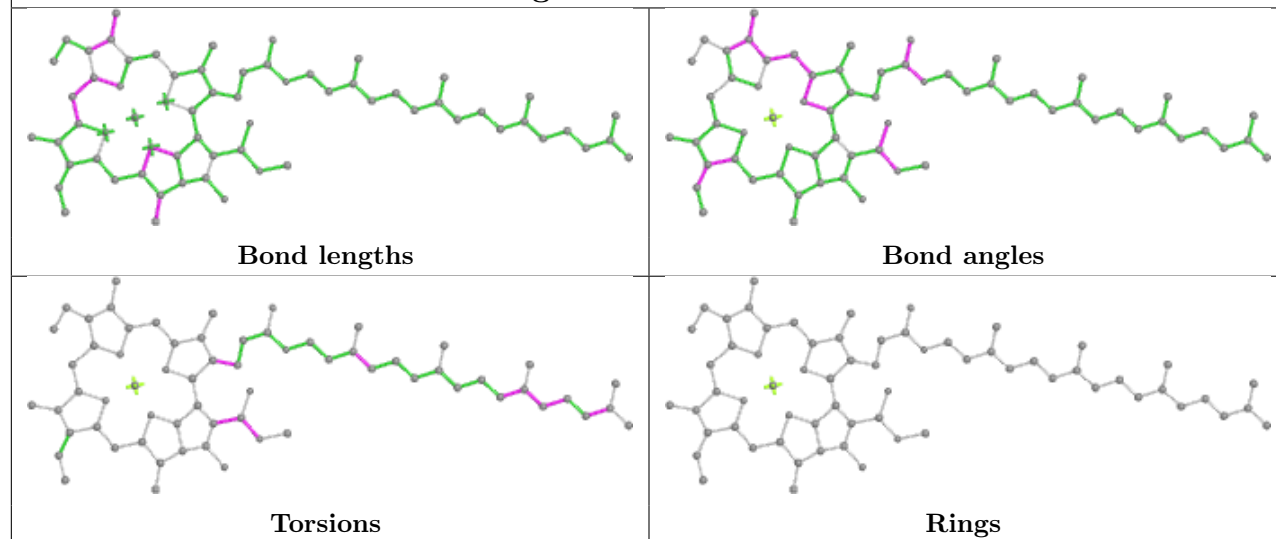


Ligand PHO a 408

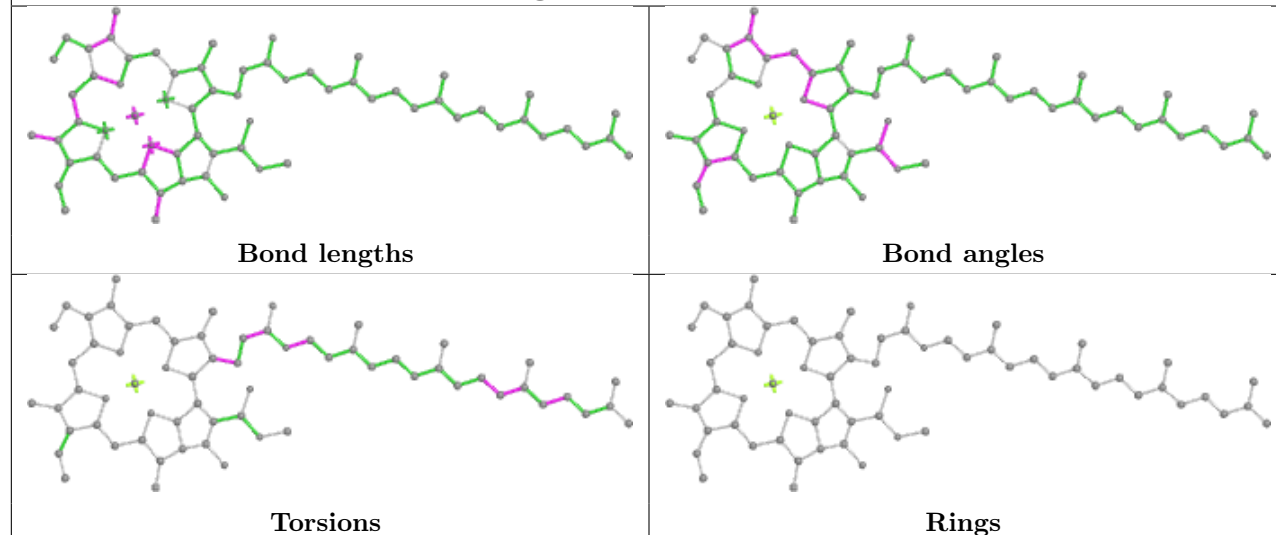




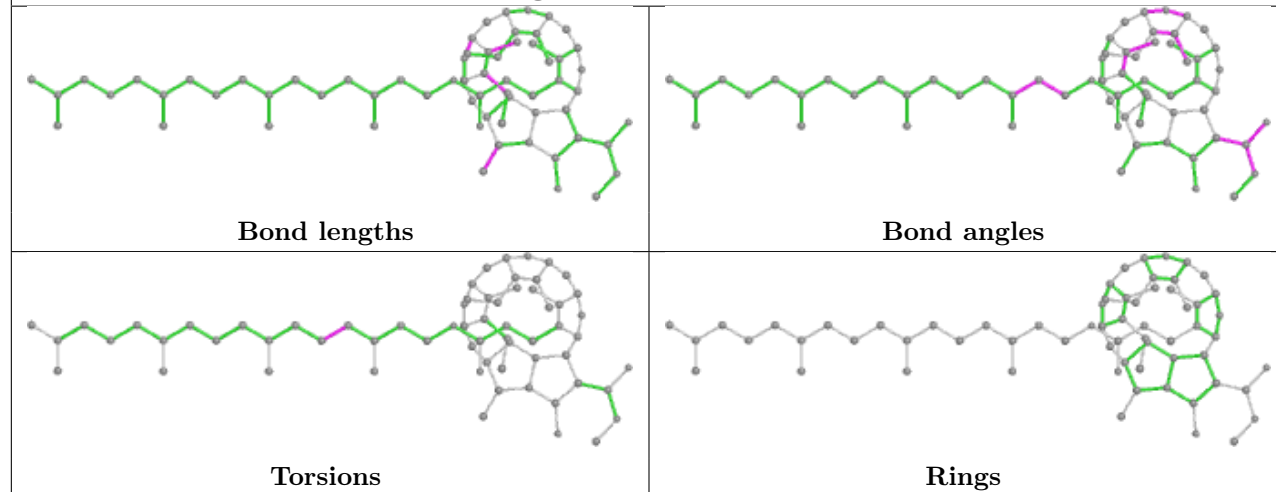
Ligand CLA B 610

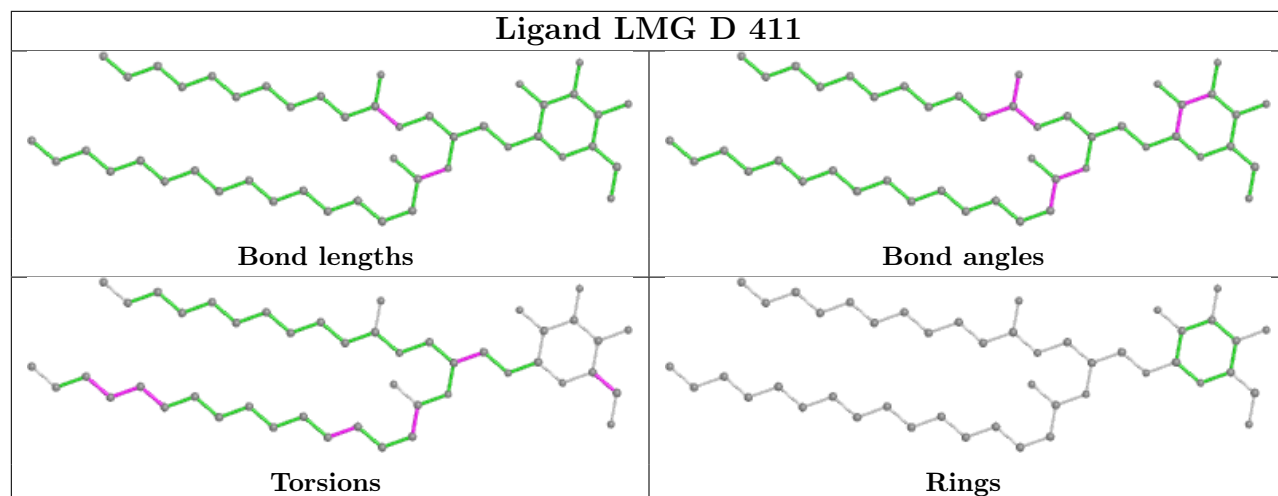
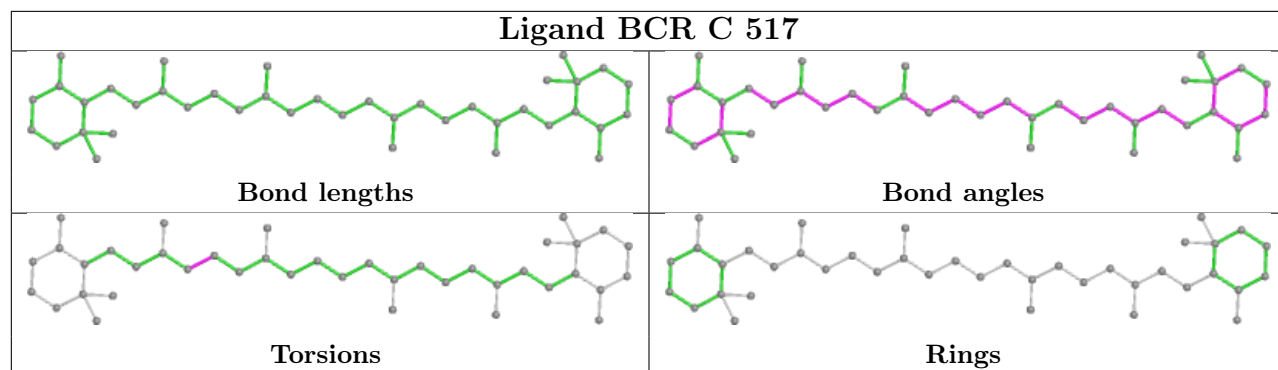


Ligand CLA D 402

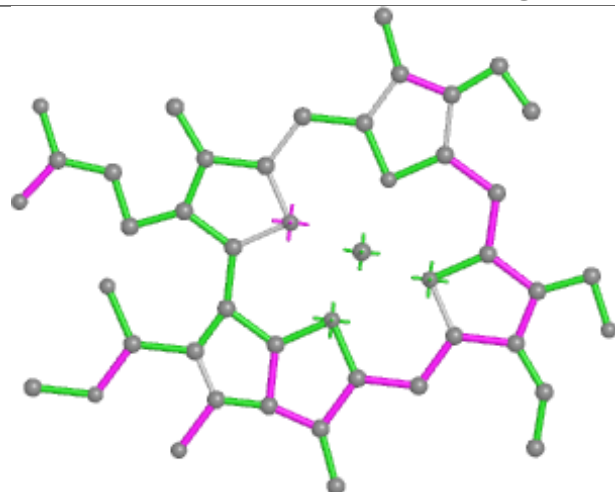


Ligand PHO A 409

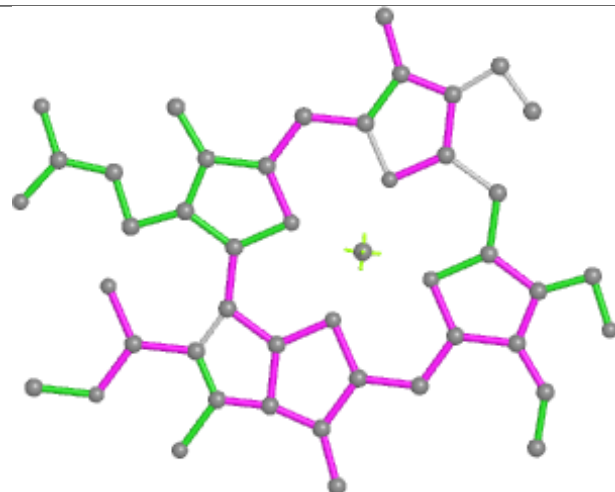




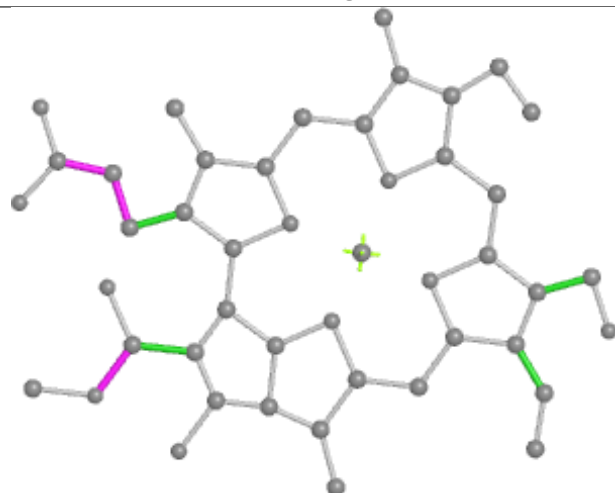
Ligand CHL R 608



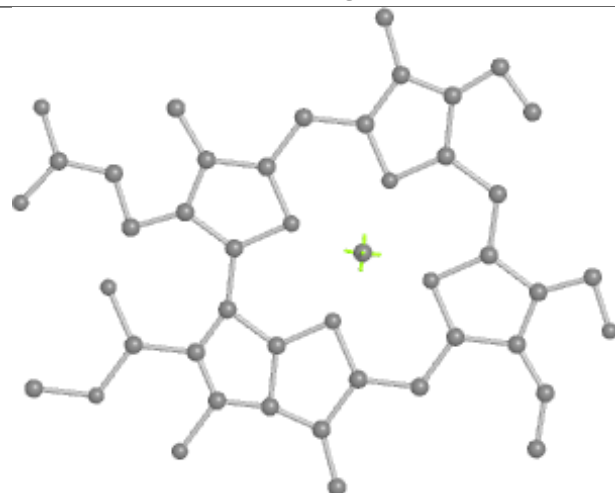
Bond lengths



Bond angles

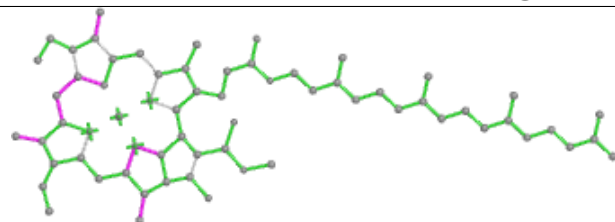


Torsions

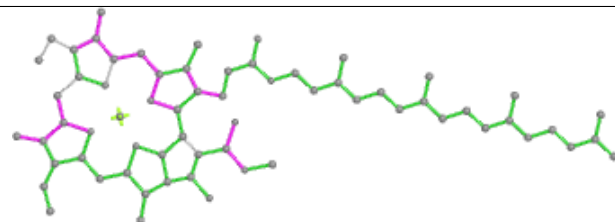


Rings

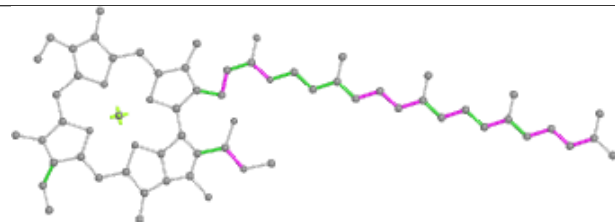
Ligand CLA B 617



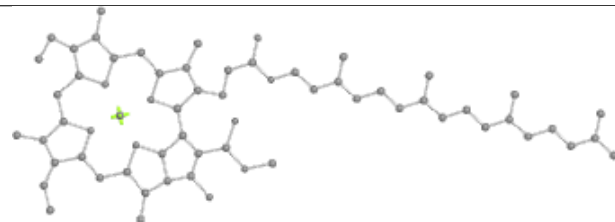
Bond lengths



Bond angles

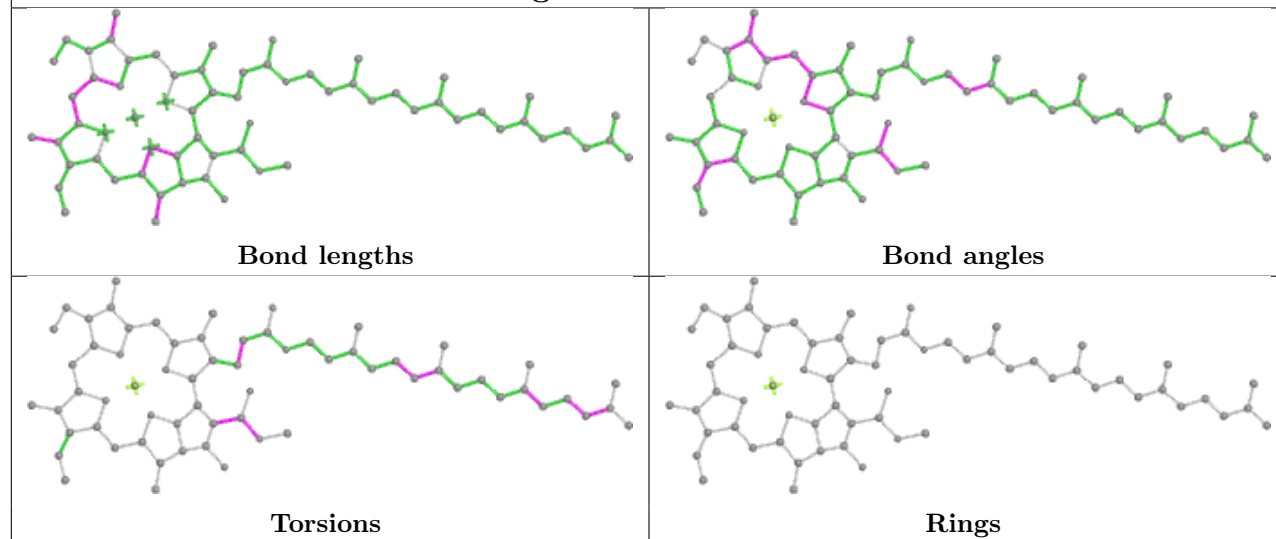


Torsions

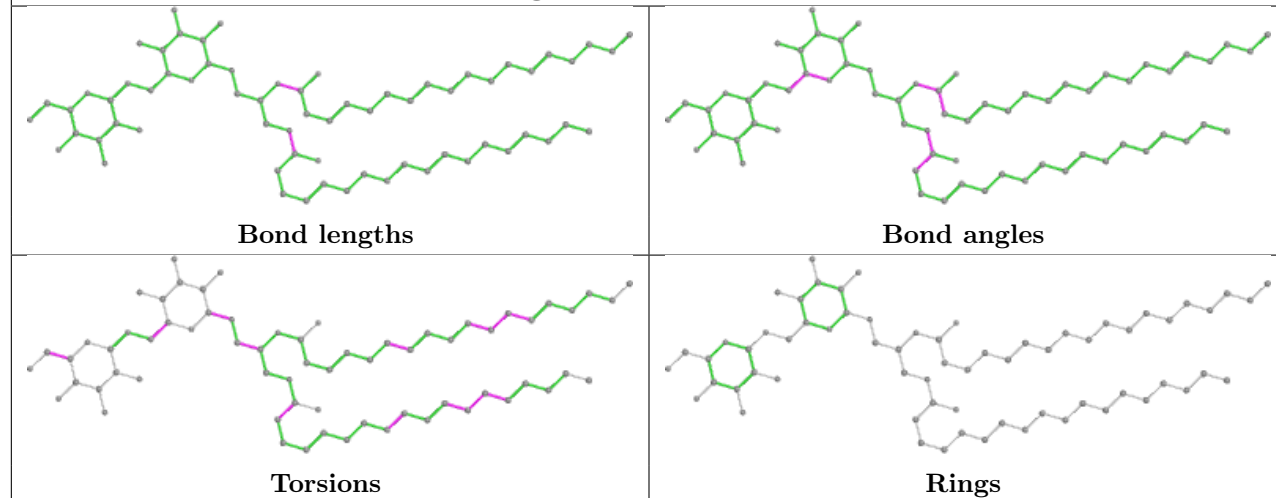


Rings

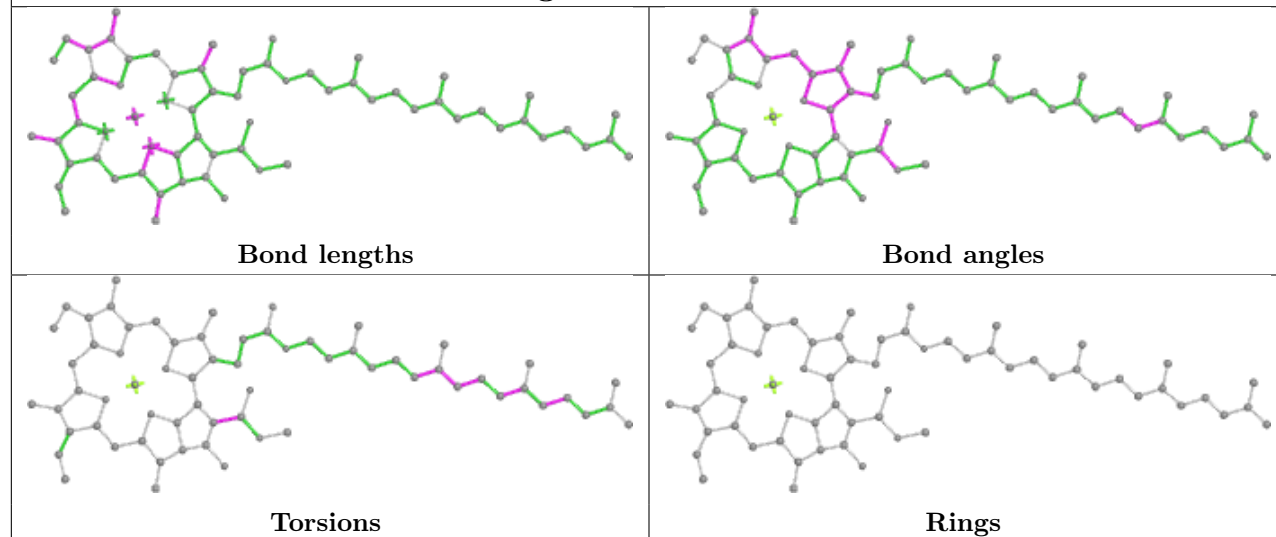
Ligand CLA B 607

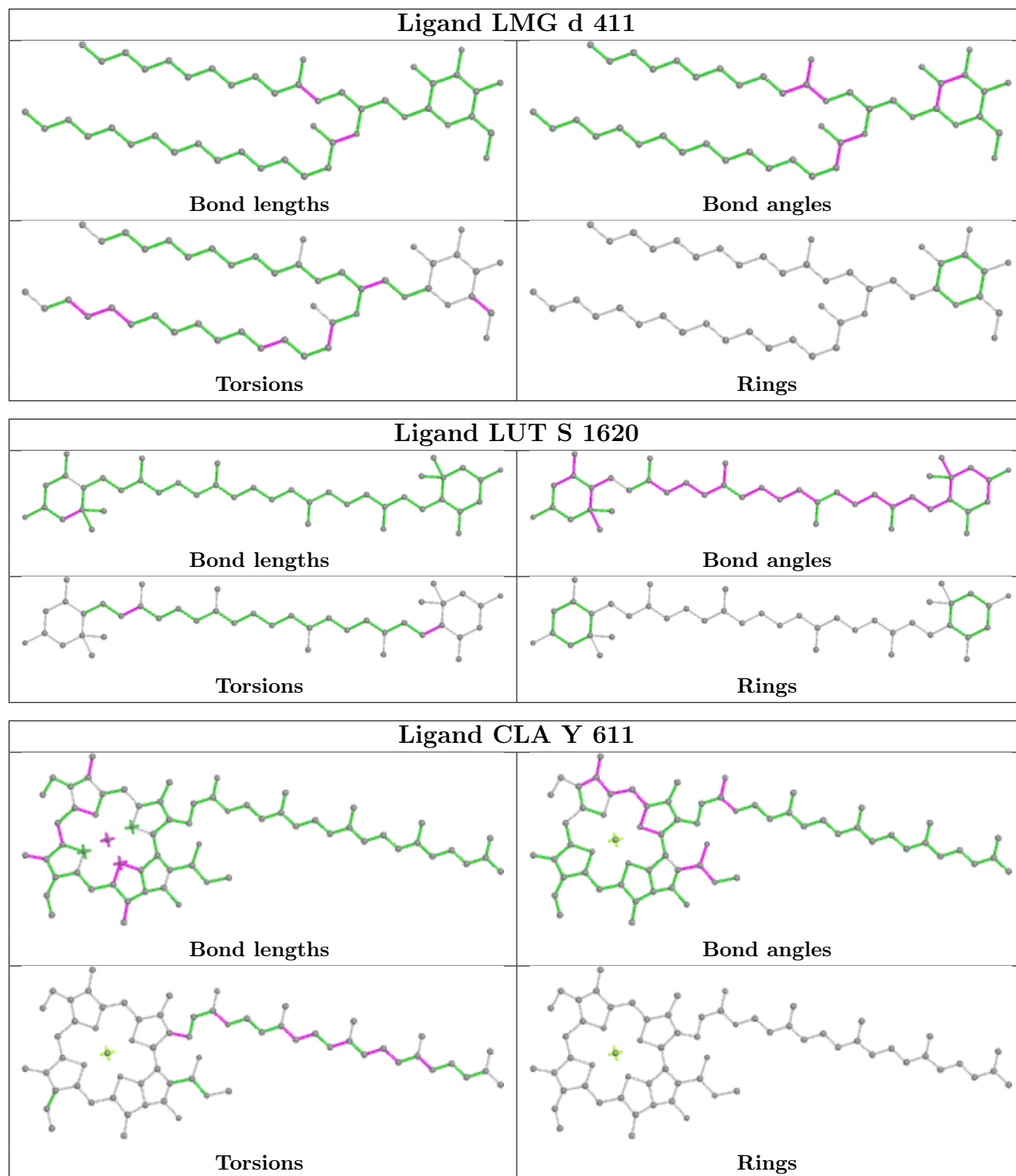


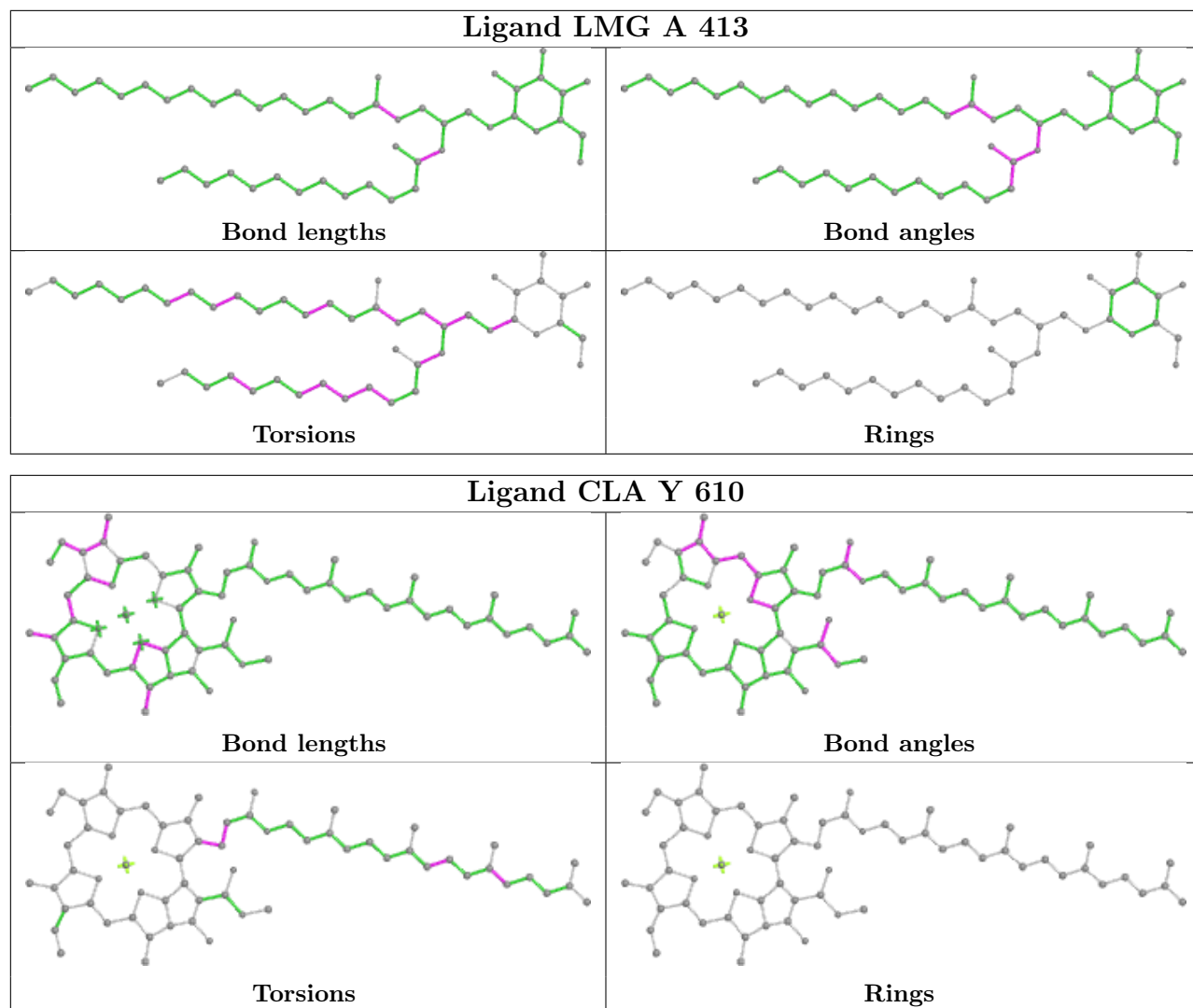
Ligand DGD C 523

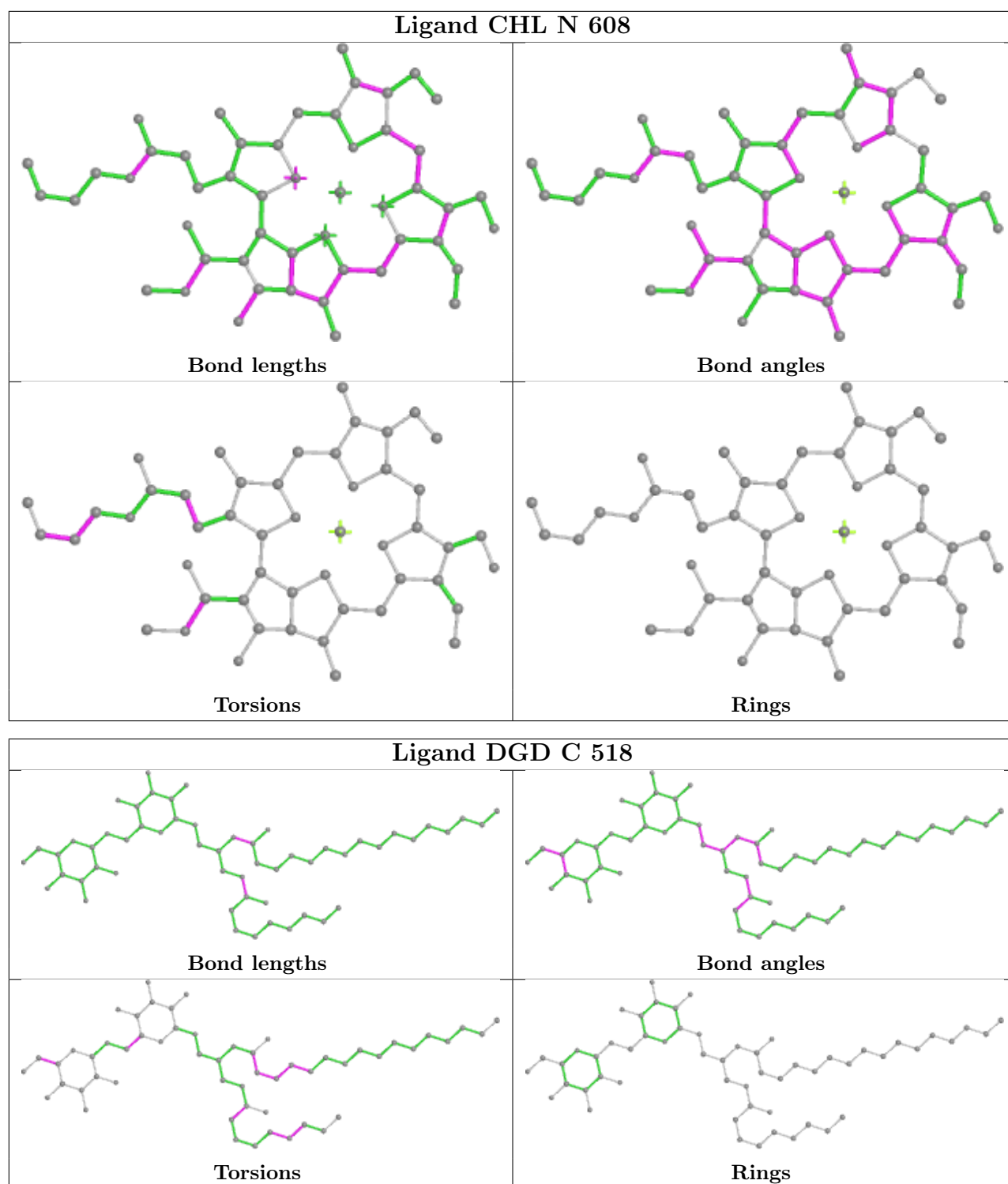


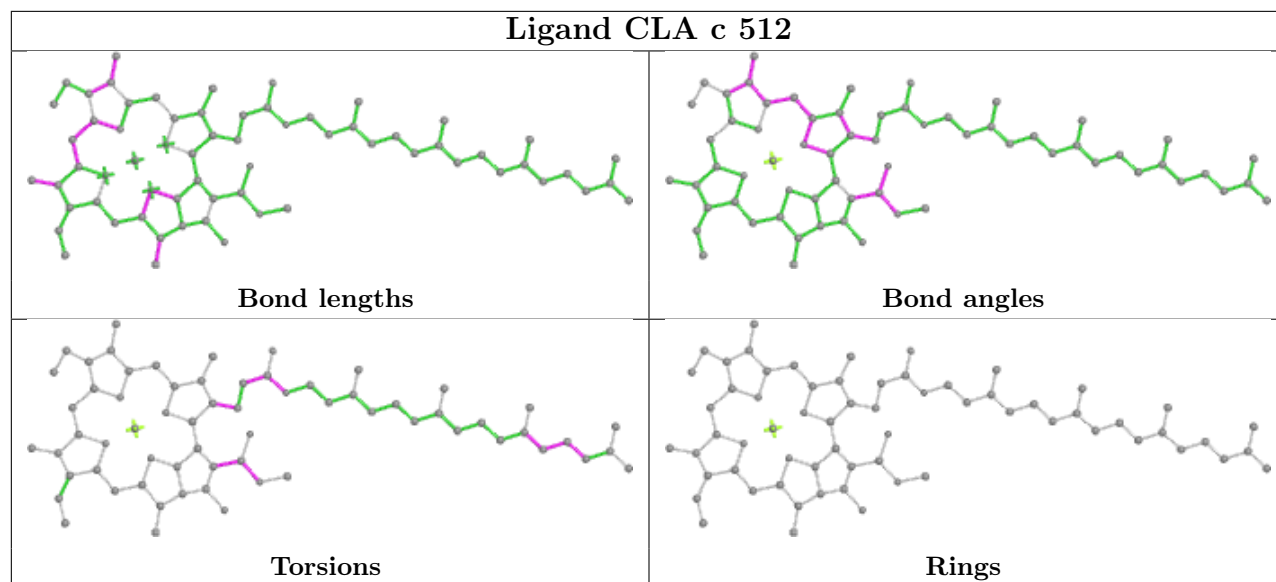
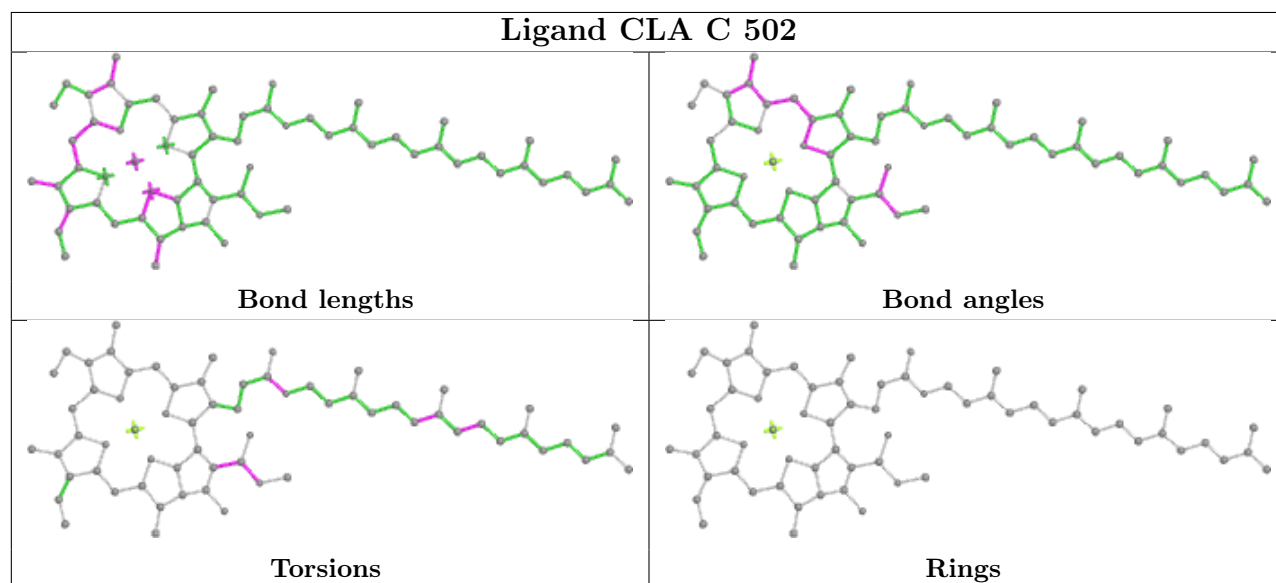
Ligand CLA c 509



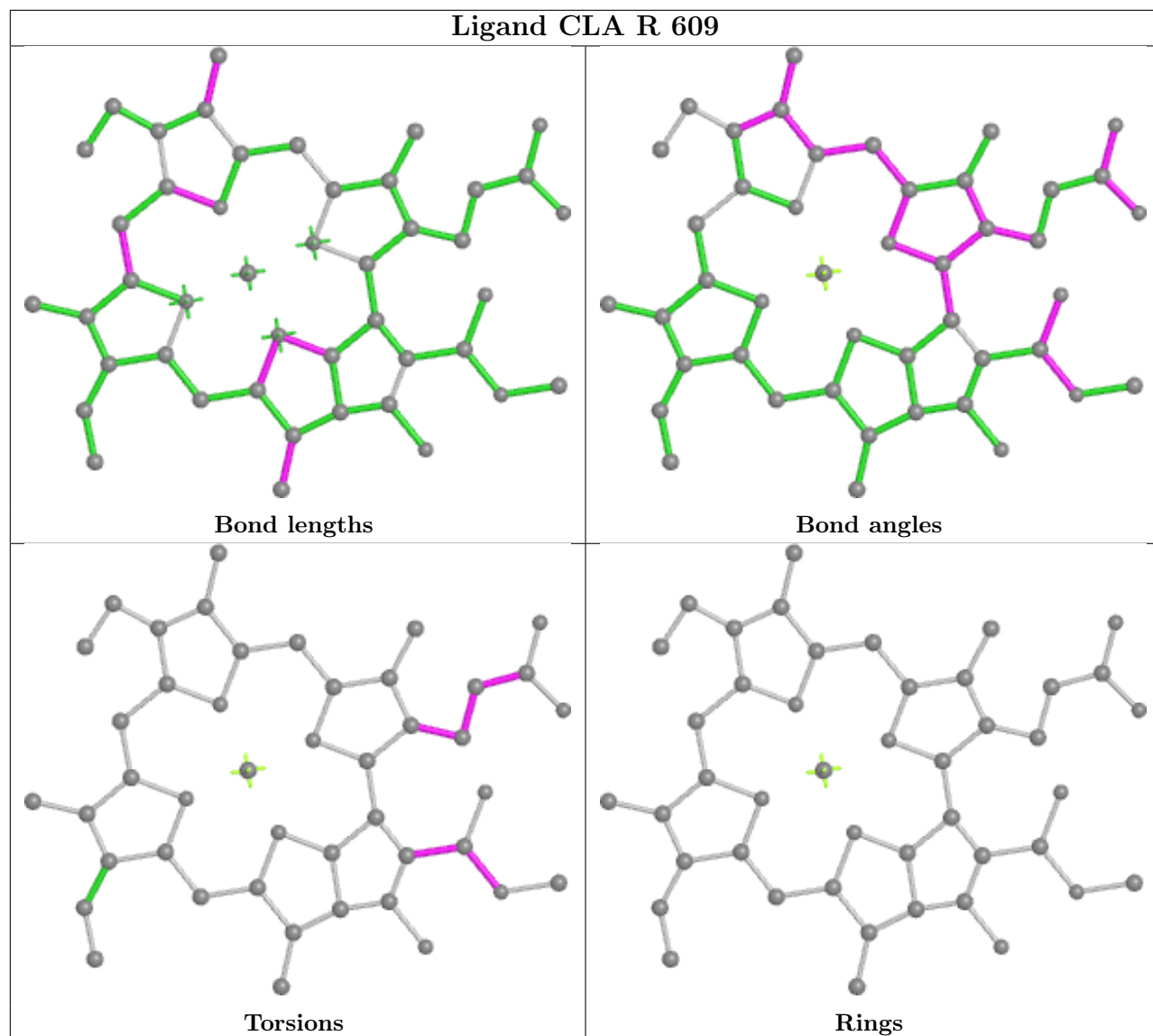




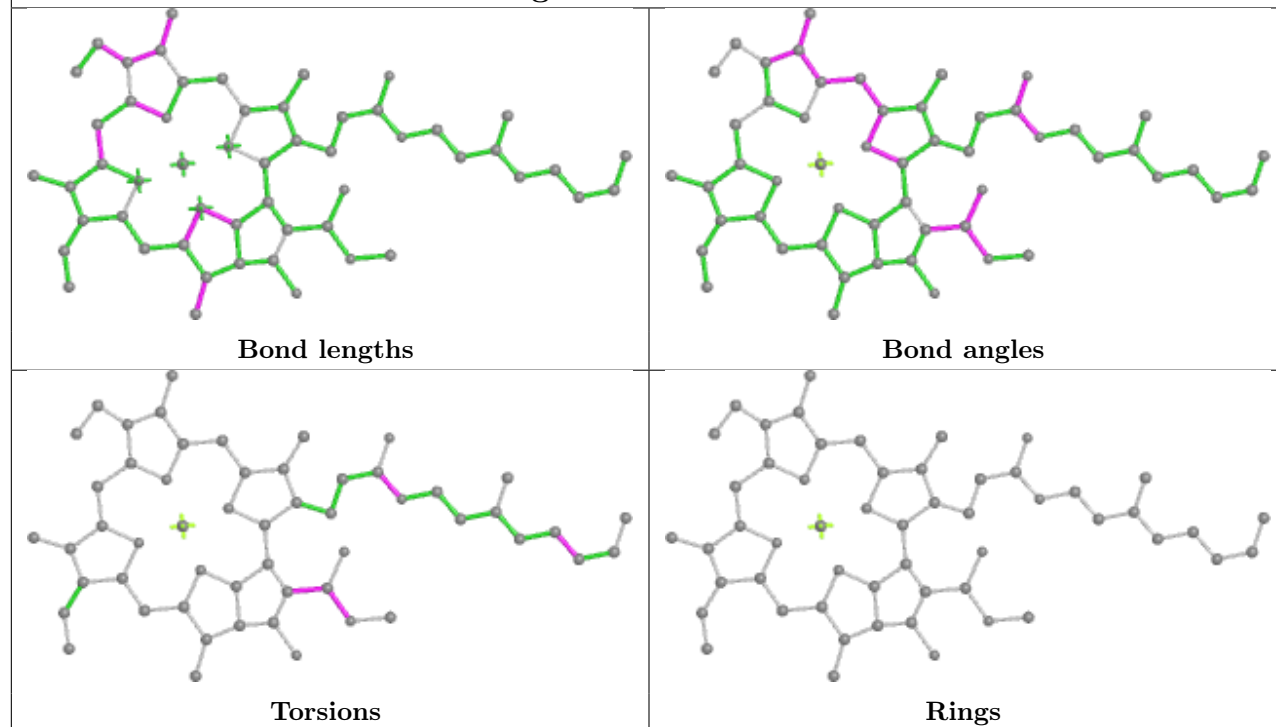


Ligand CLA c 512**Ligand CLA C 502**

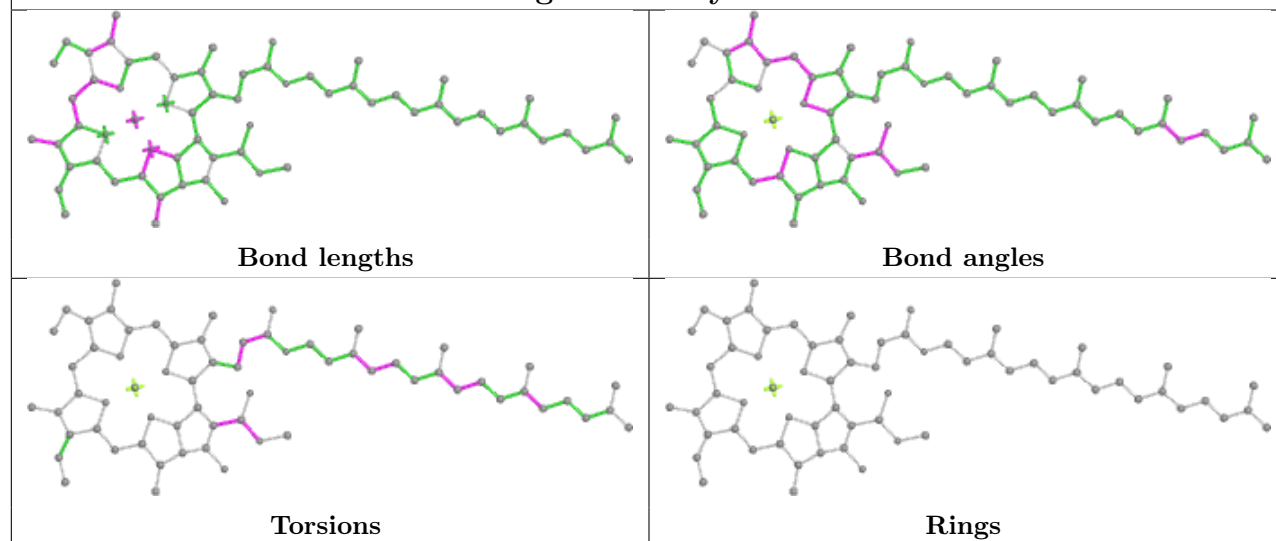
Ligand CLA R 609

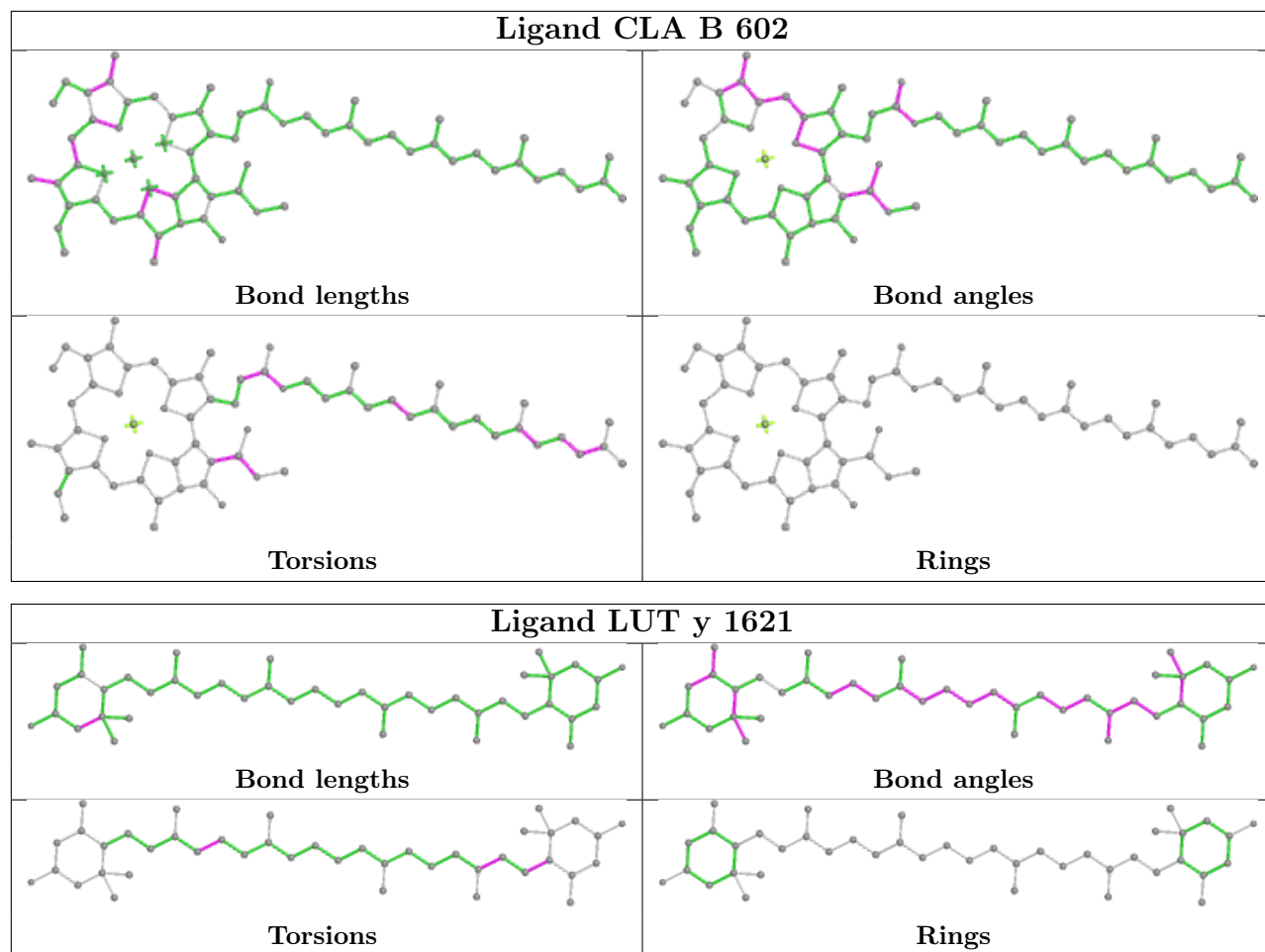


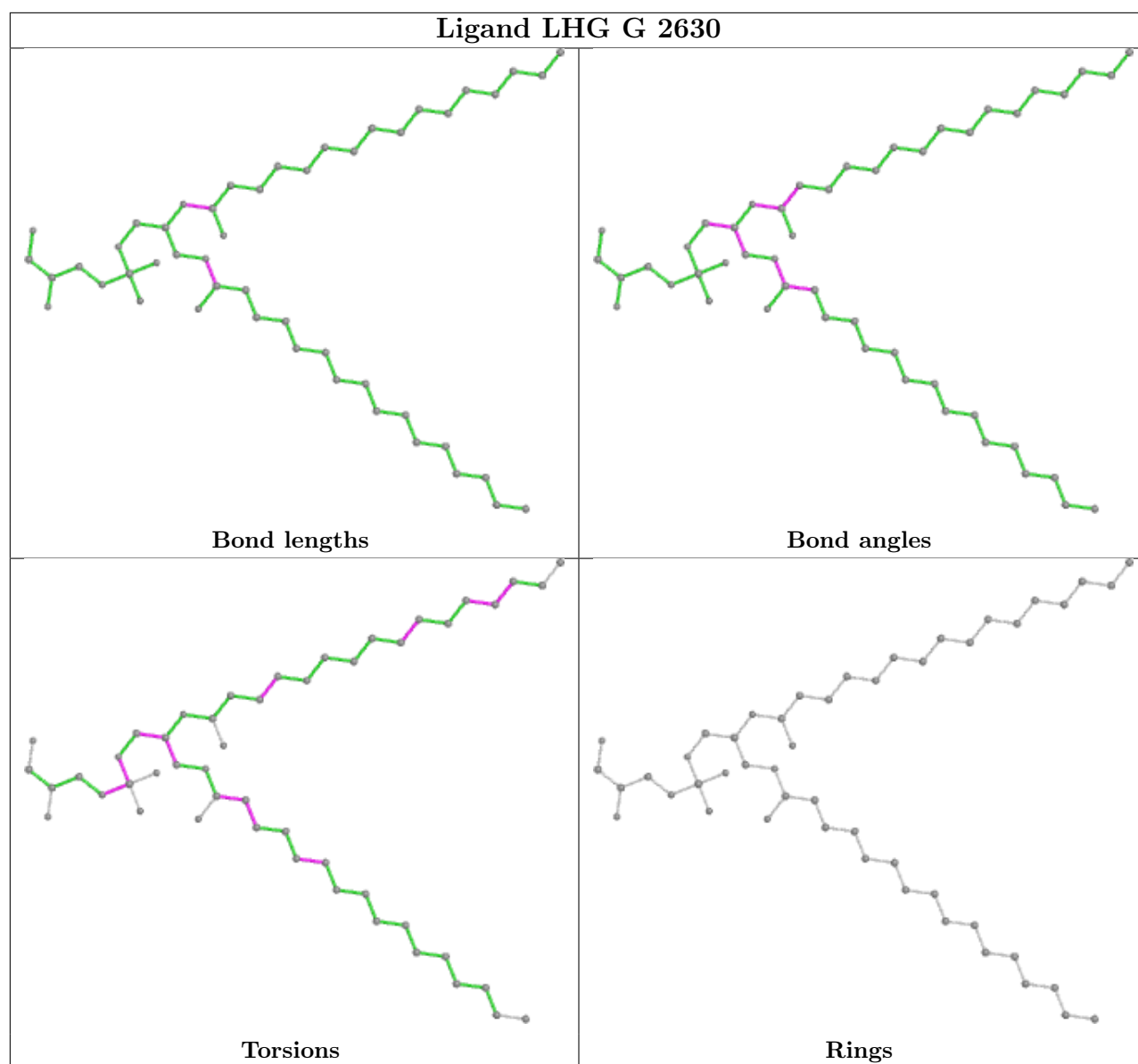
Ligand CLA Y 614



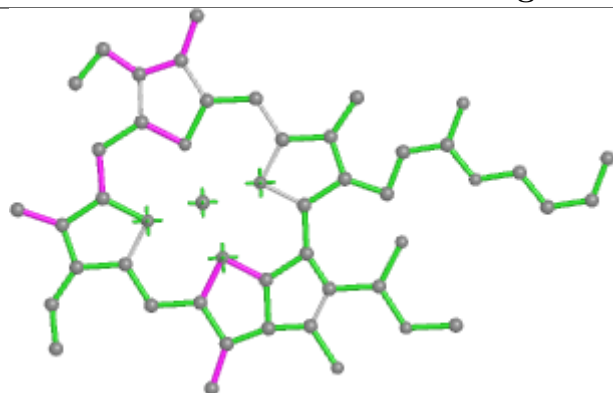
Ligand CLA y 613



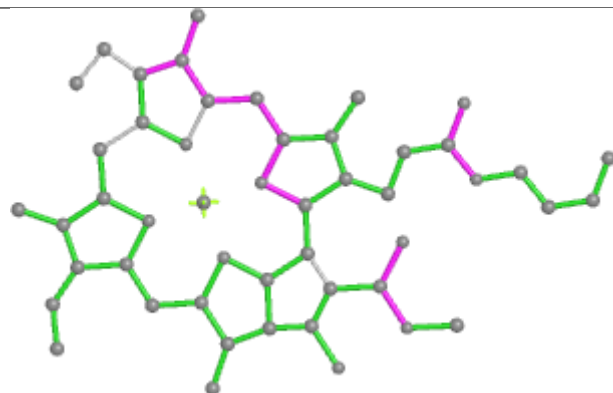




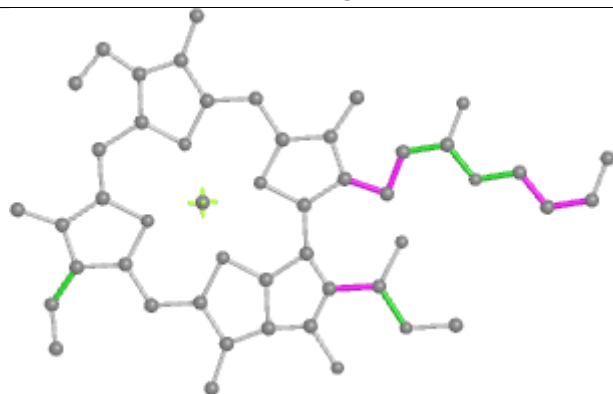
Ligand CLA S 610



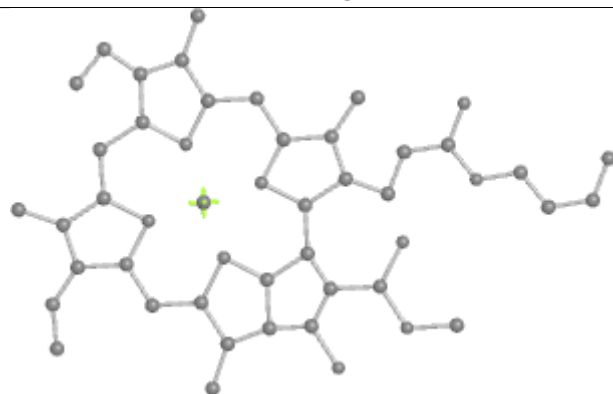
Bond lengths



Bond angles

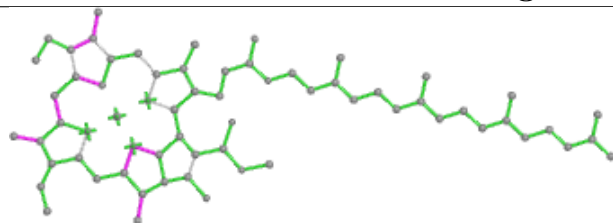


Torsions

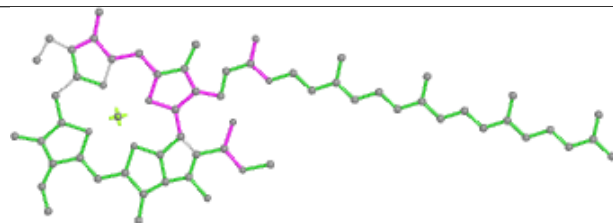


Rings

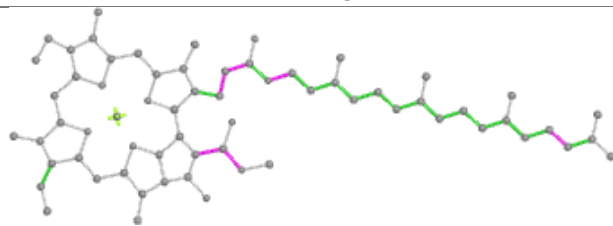
Ligand CLA b 611



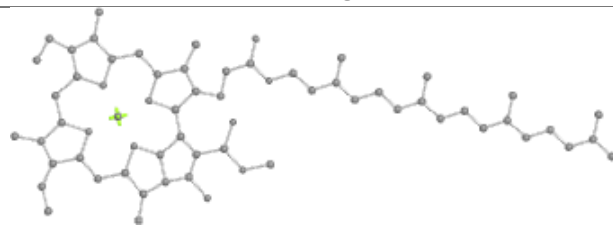
Bond lengths



Bond angles

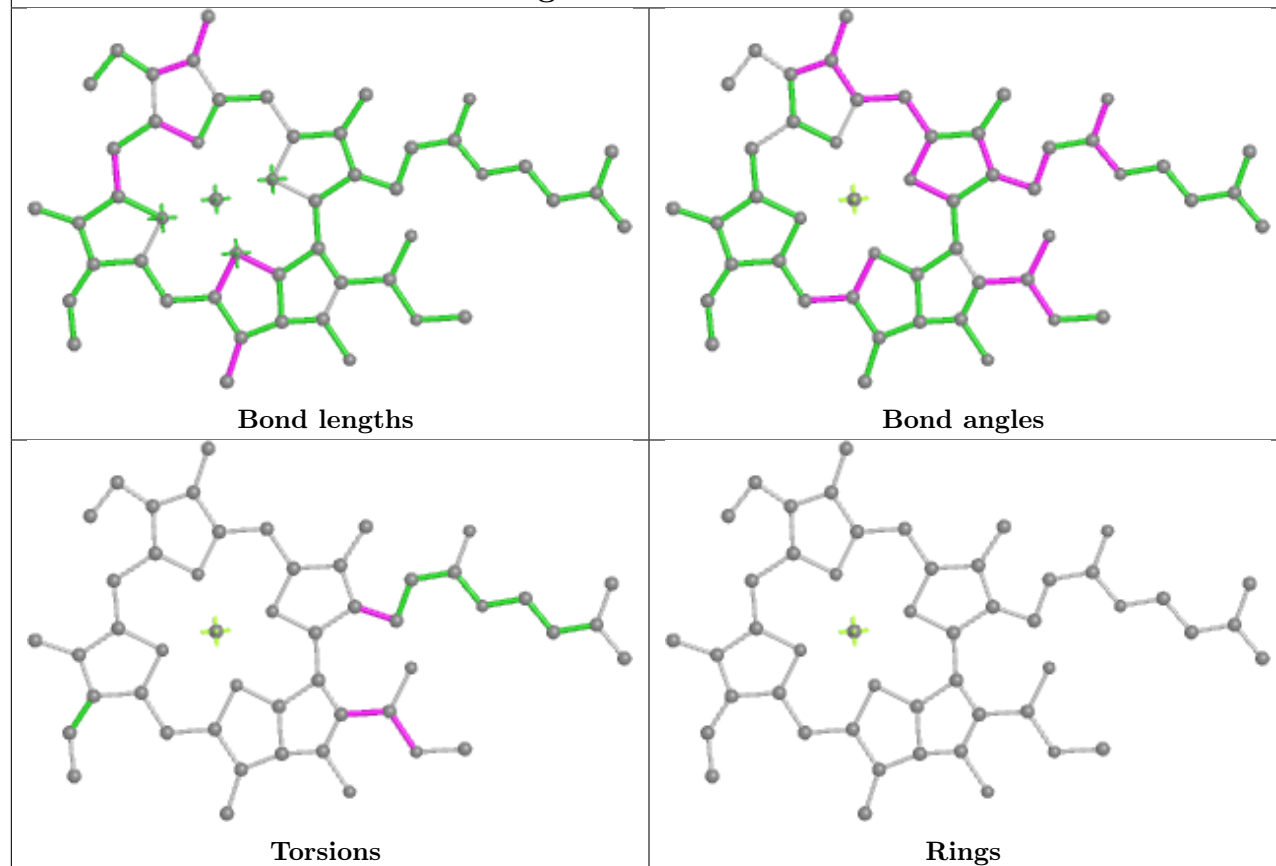


Torsions

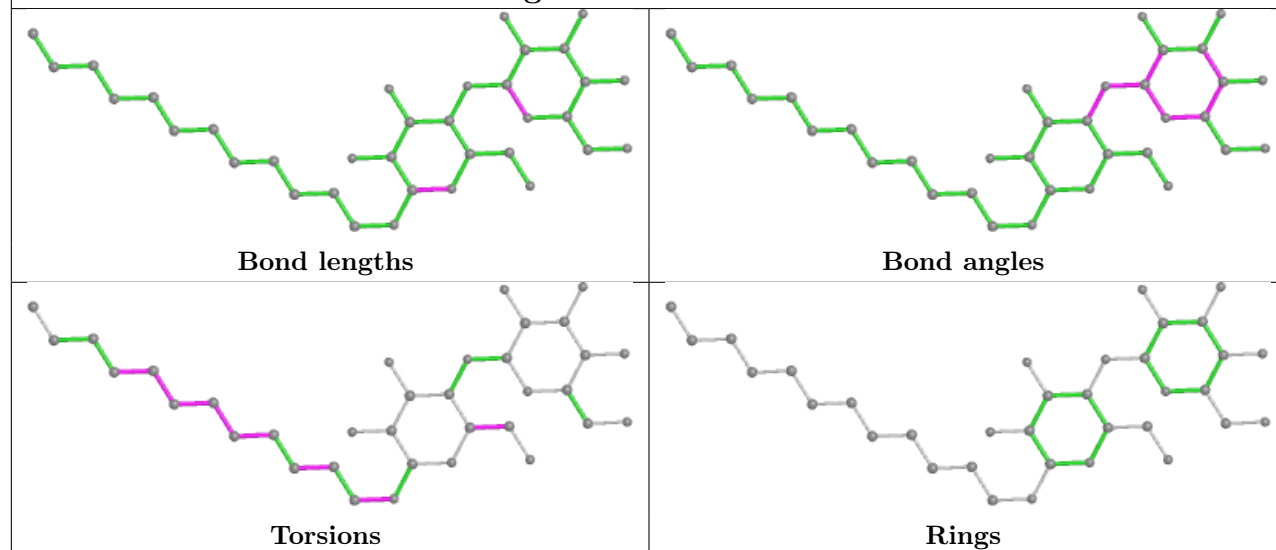


Rings

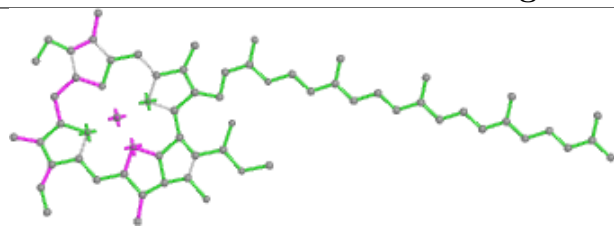
Ligand CLA s 605



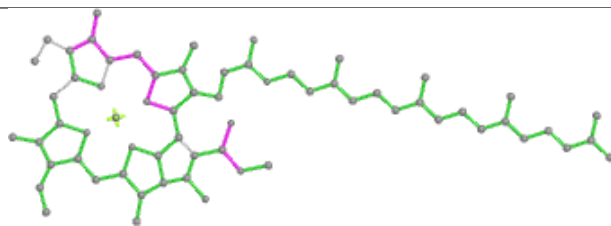
Ligand LMU z 2634



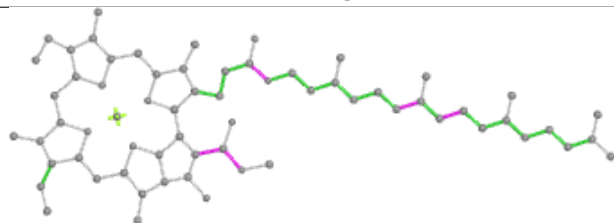
Ligand CLA c 502



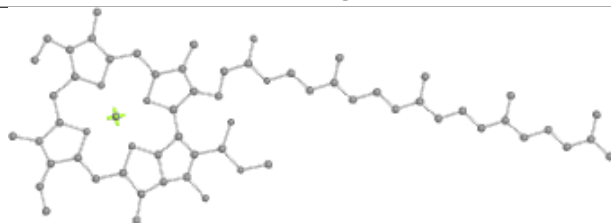
Bond lengths



Bond angles

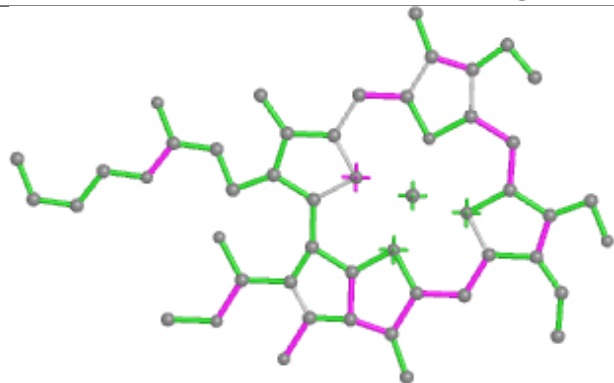


Torsions

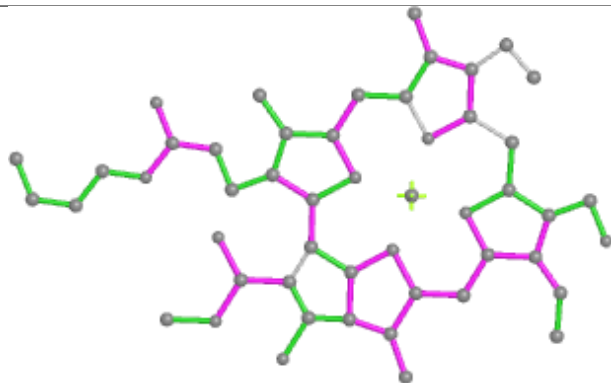


Rings

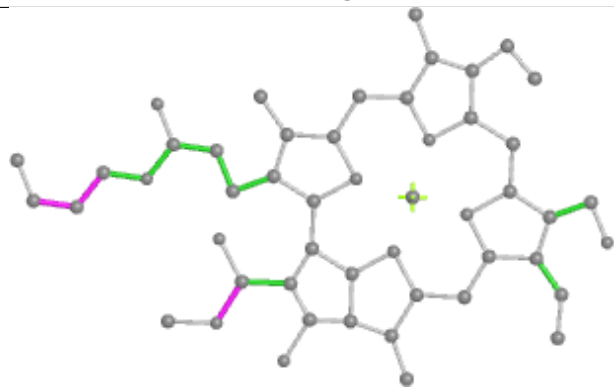
Ligand CHL Y 608



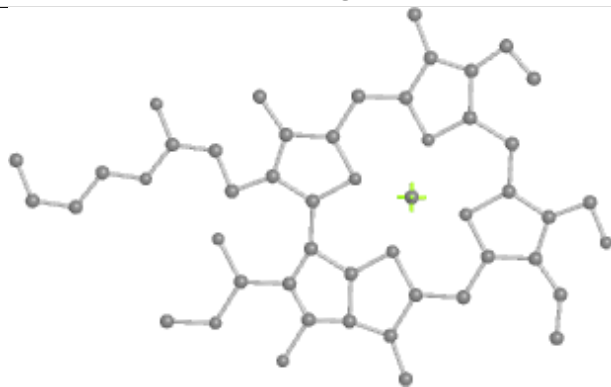
Bond lengths



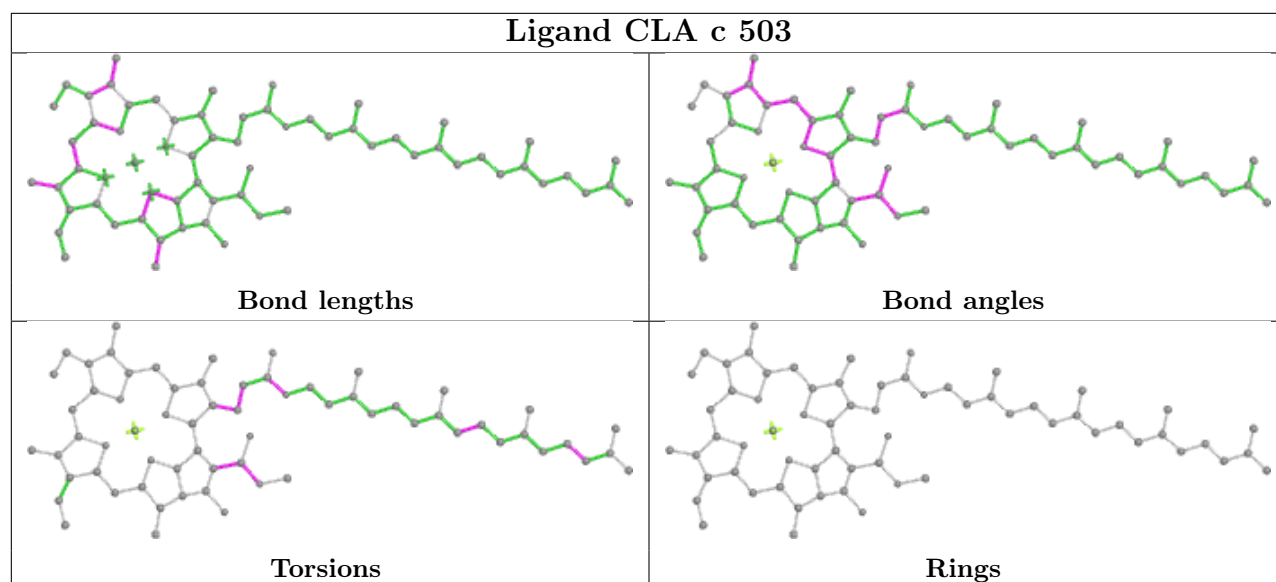
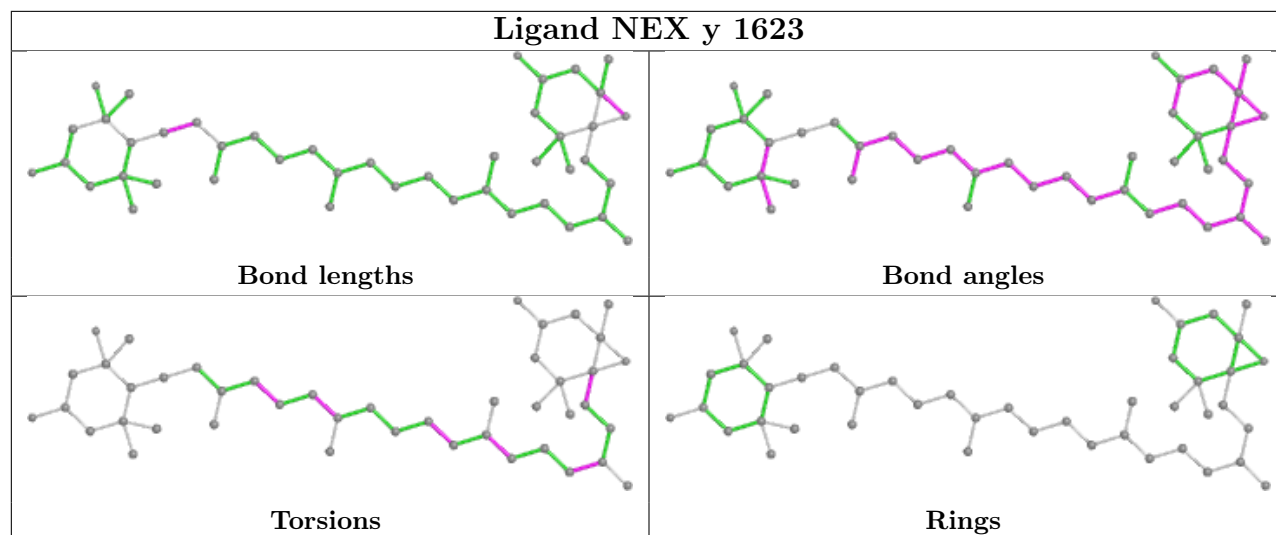
Bond angles

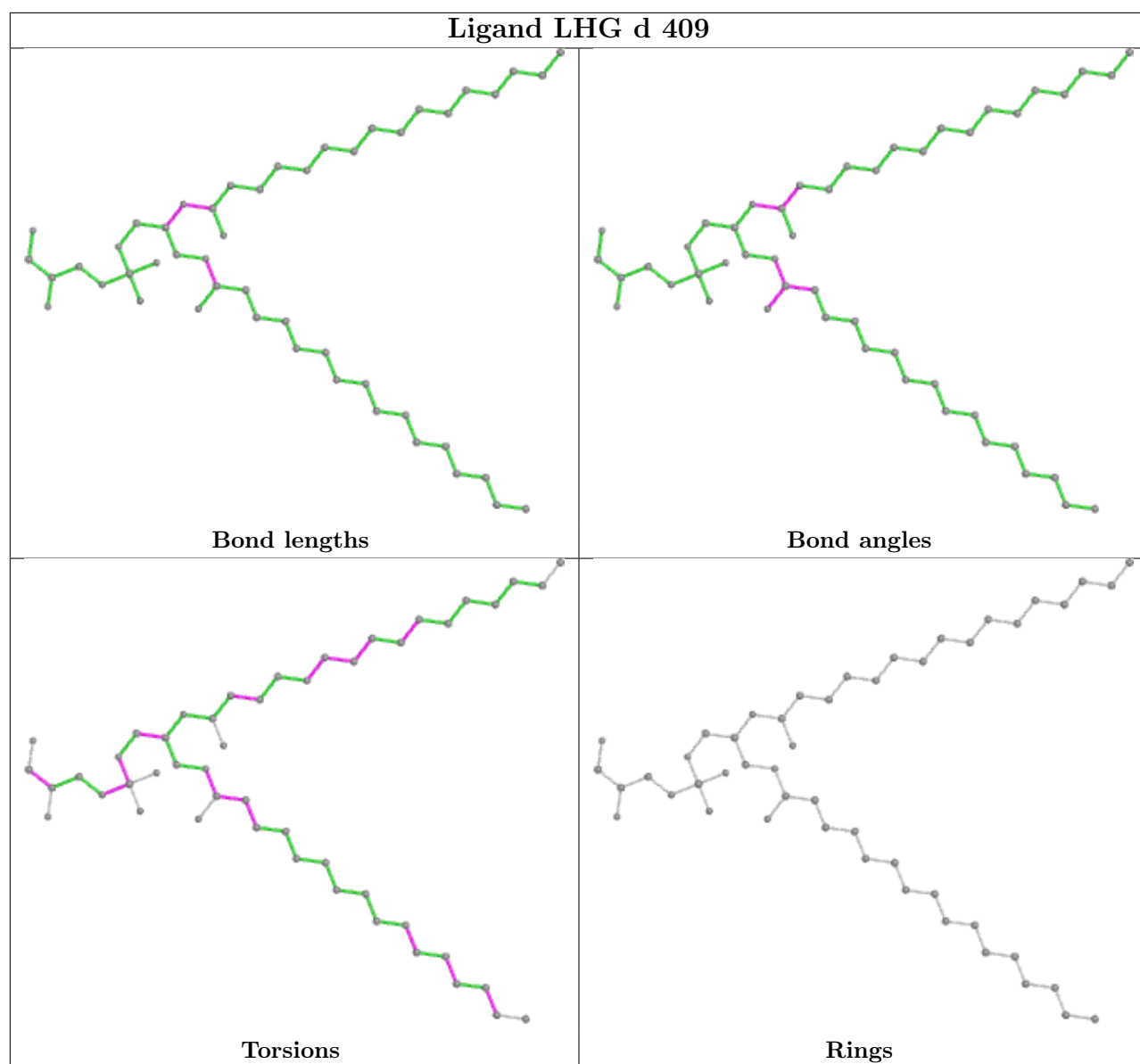


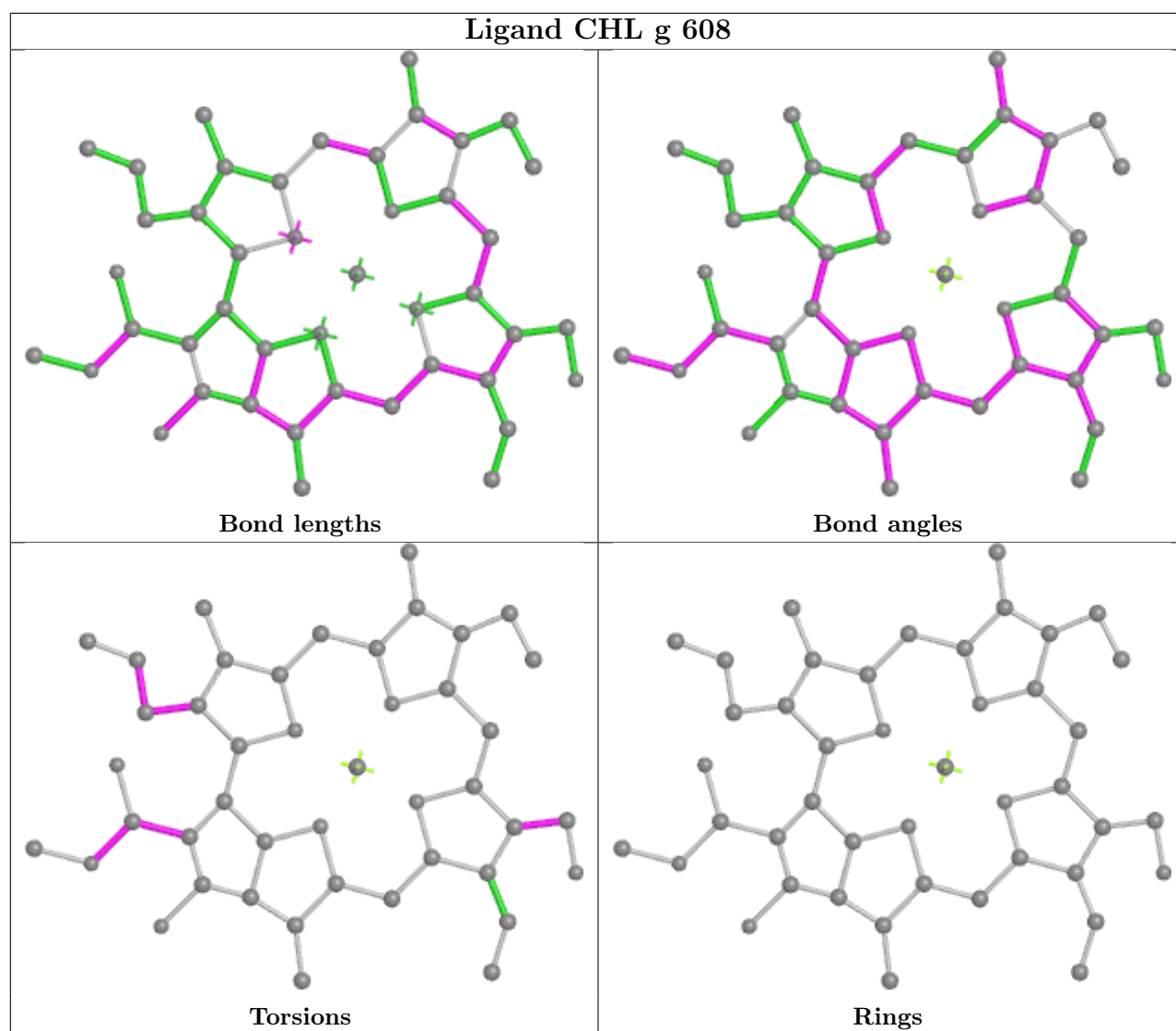
Torsions

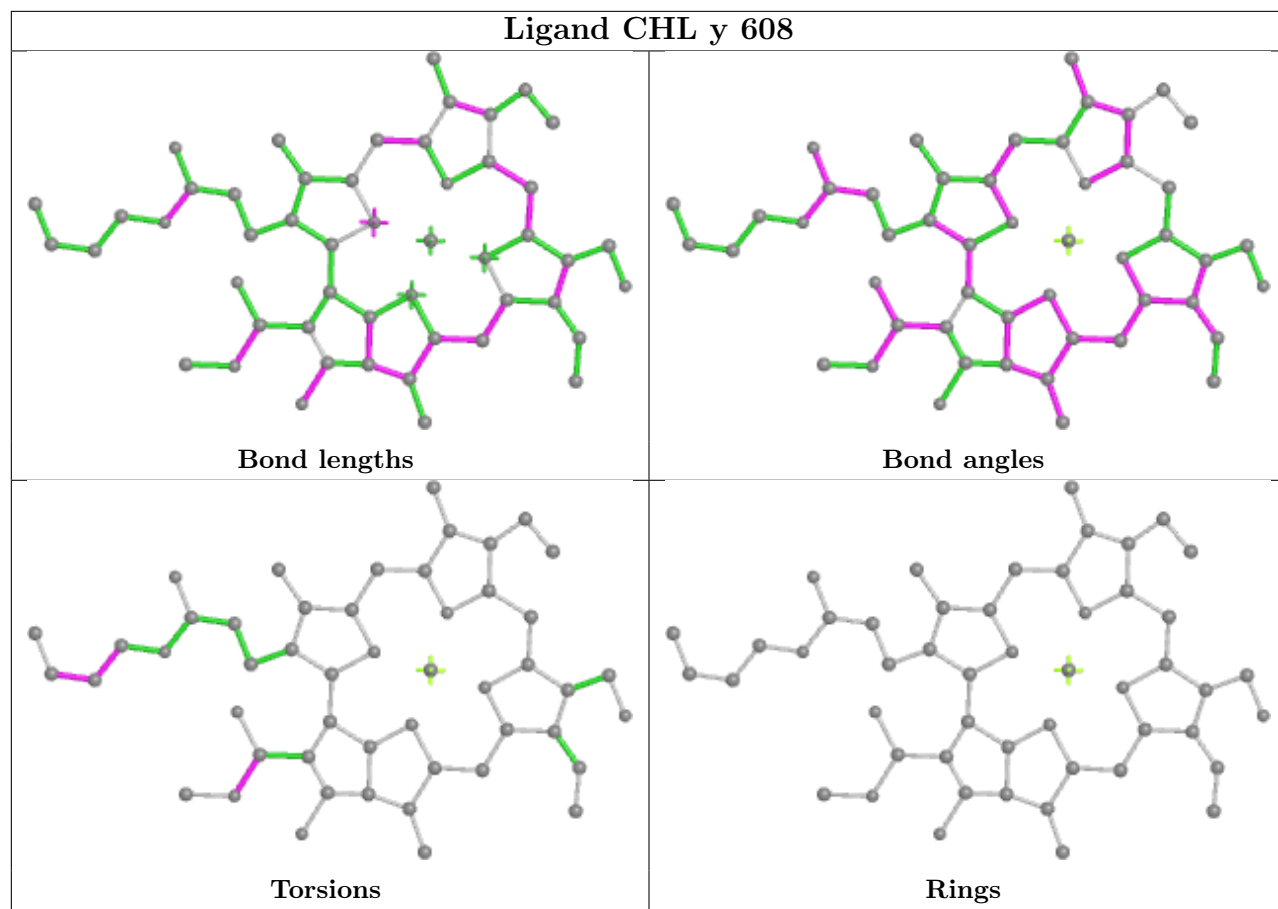


Rings

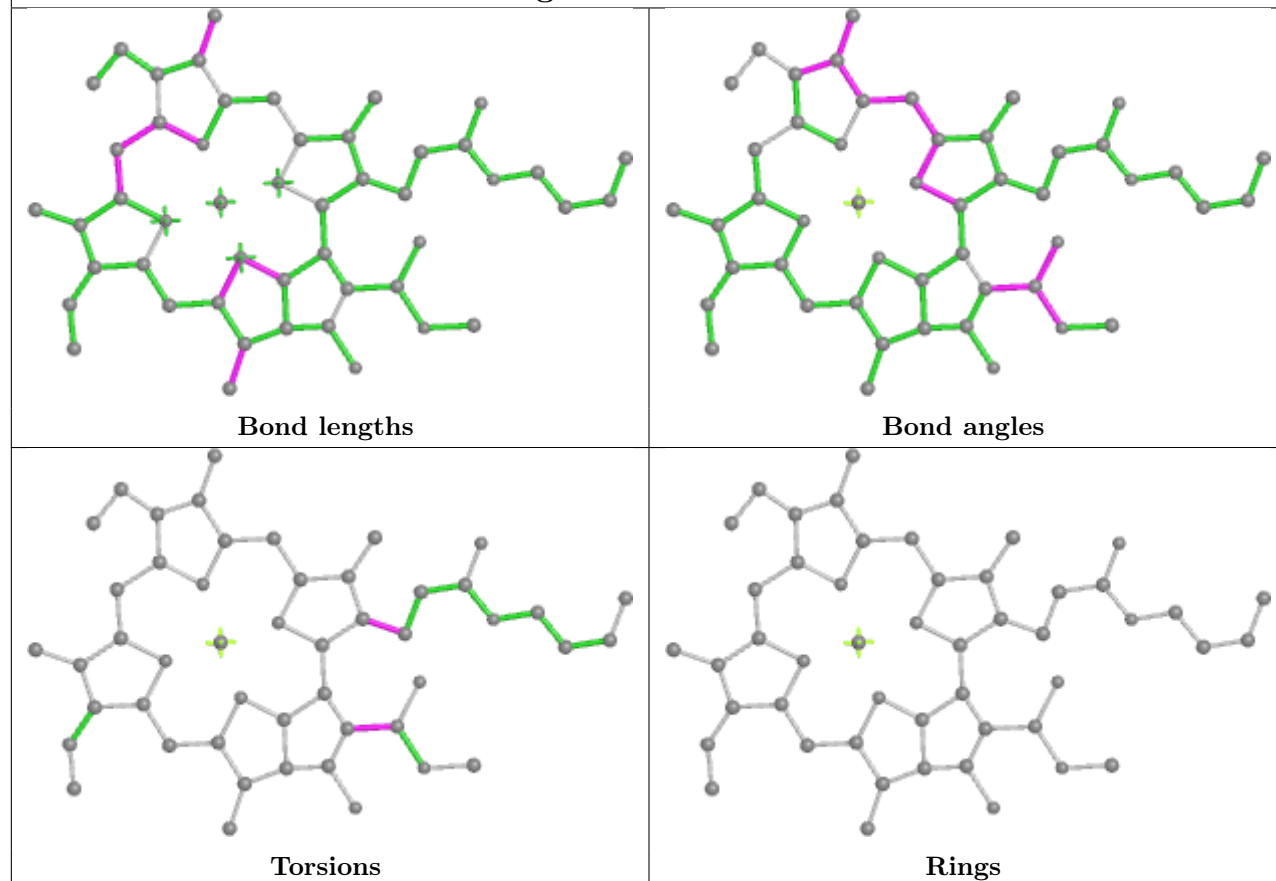




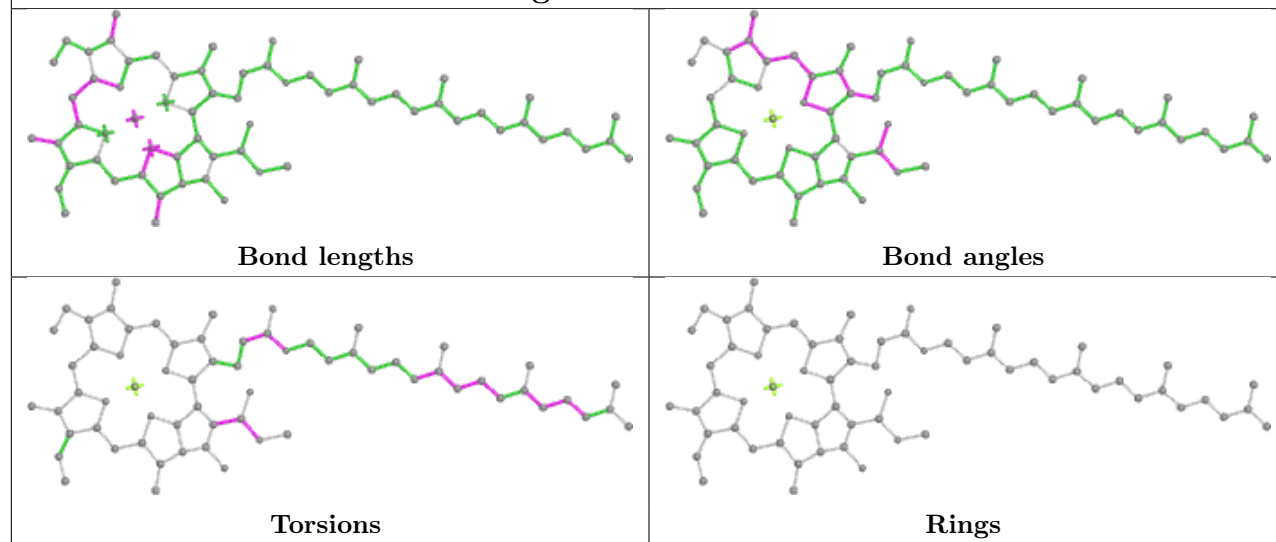


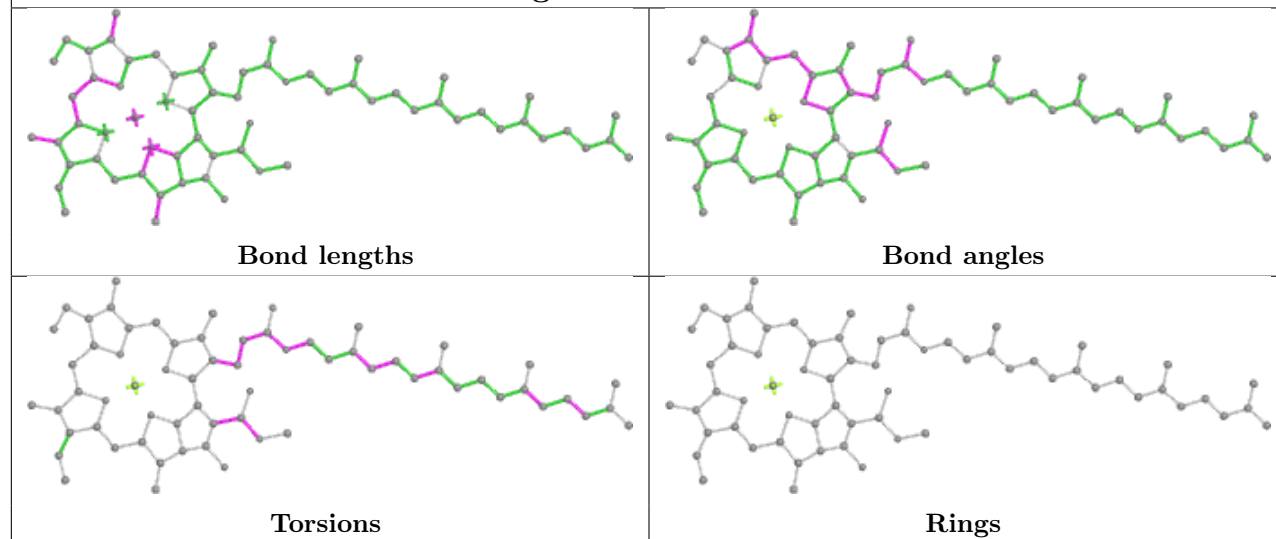
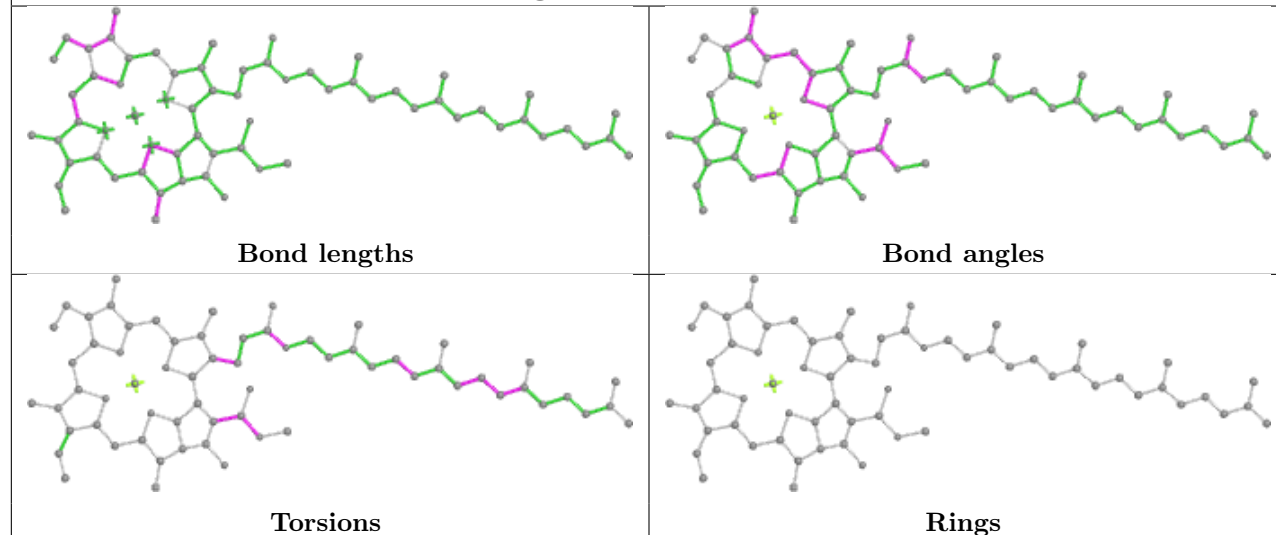
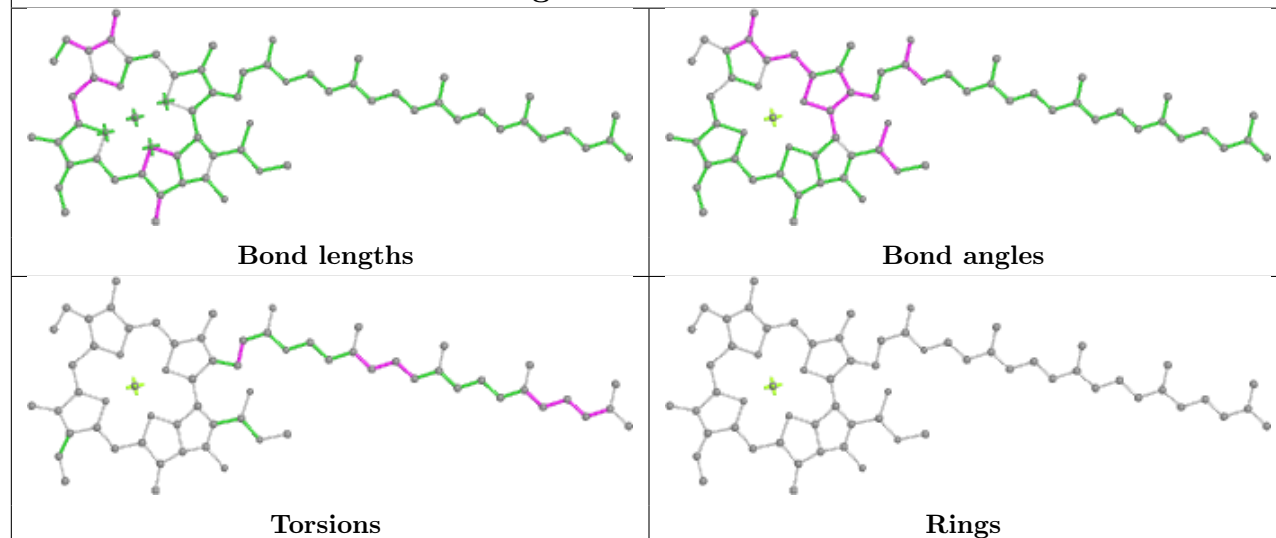


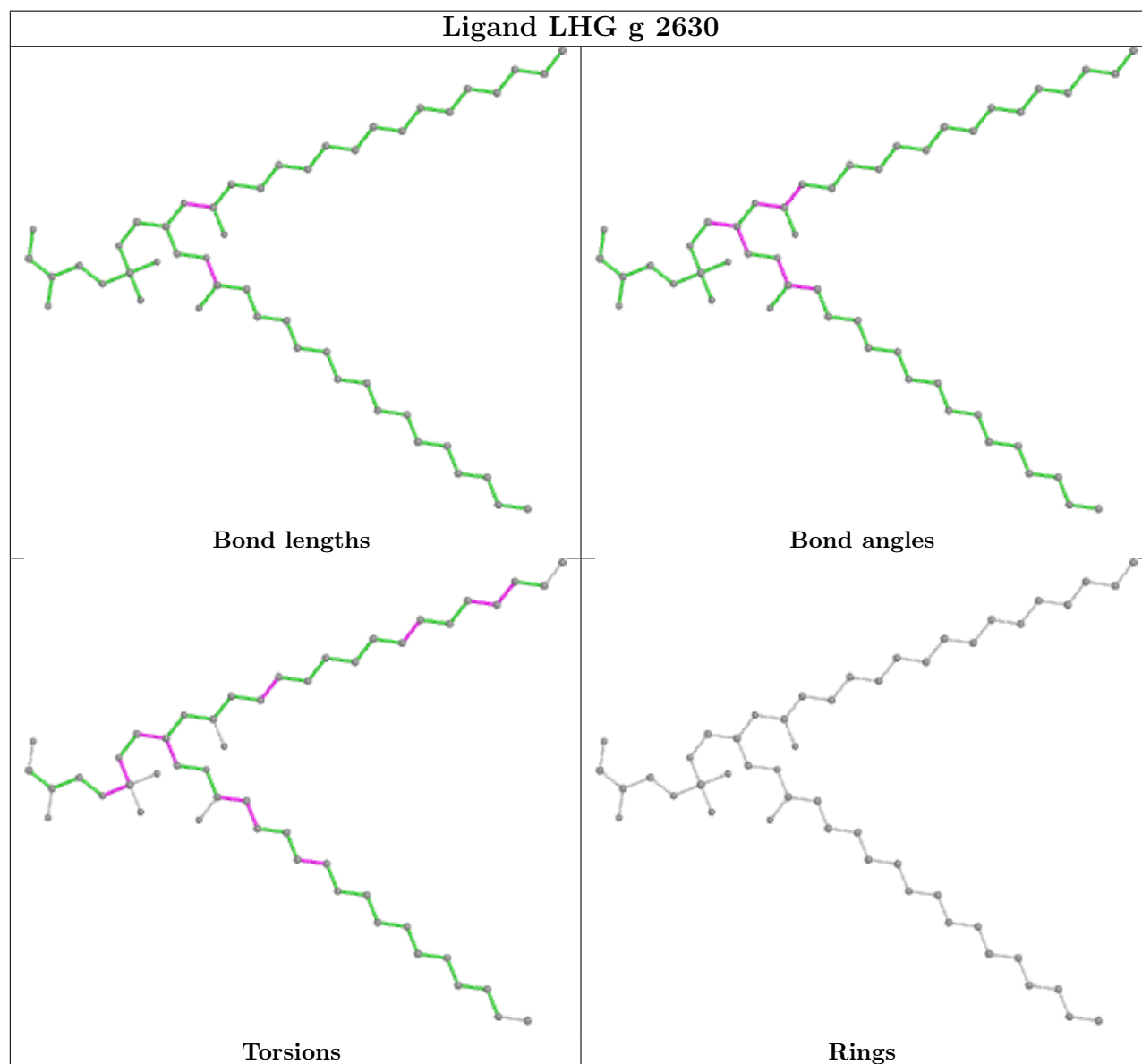
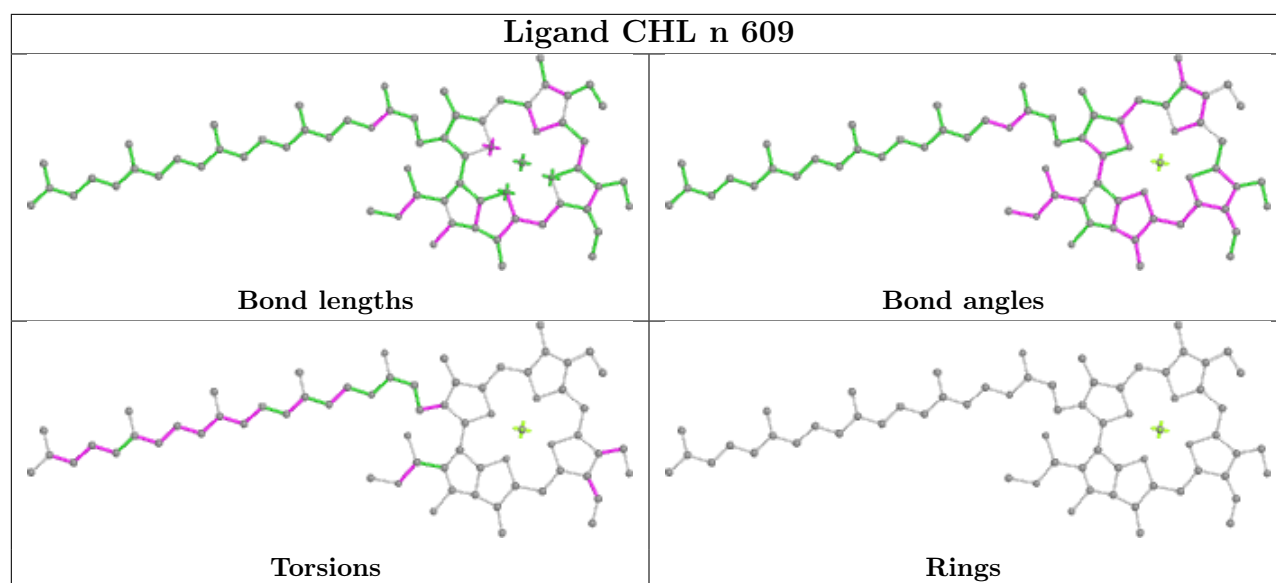
Ligand CLA a 407

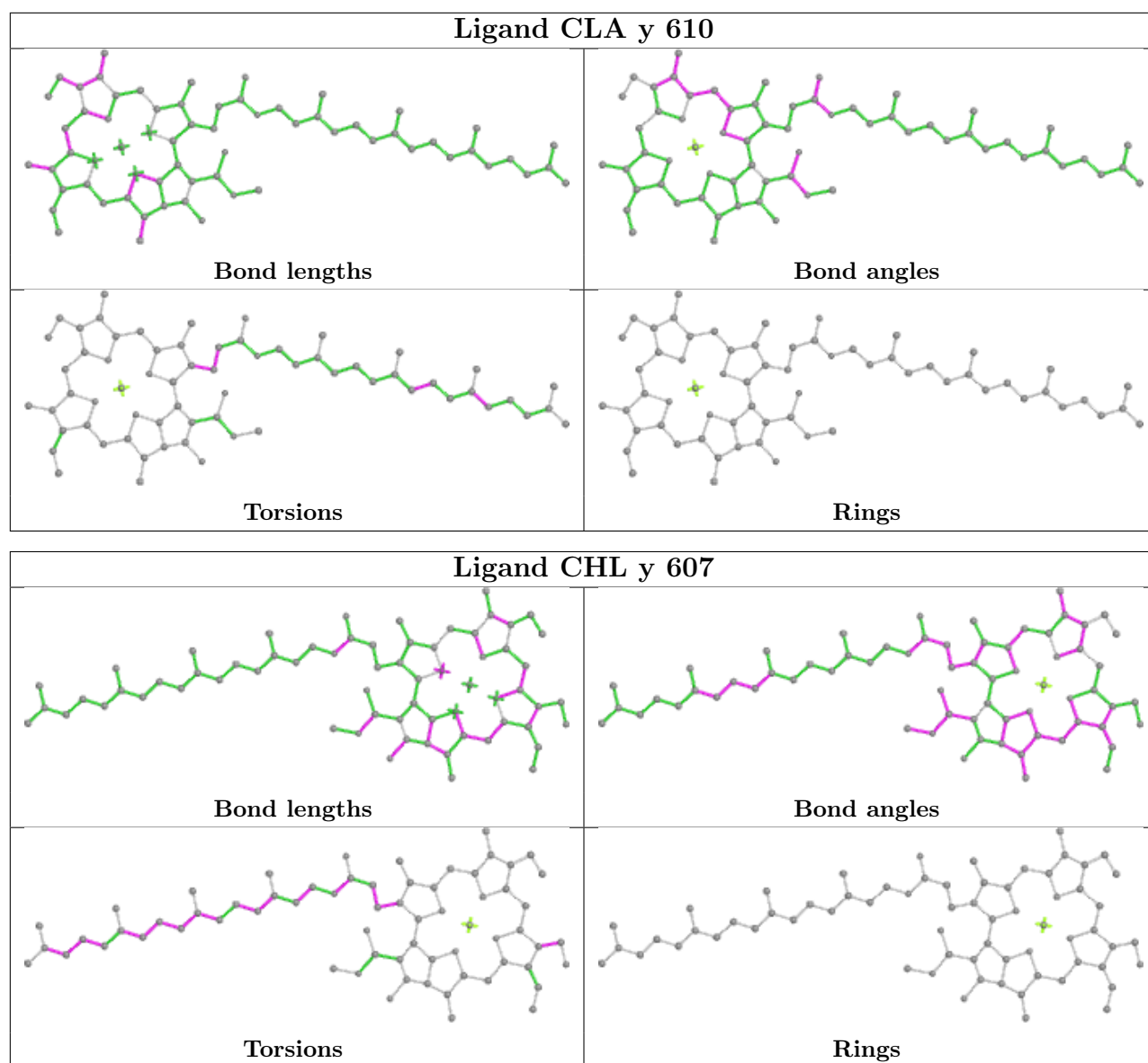


Ligand CLA C 510

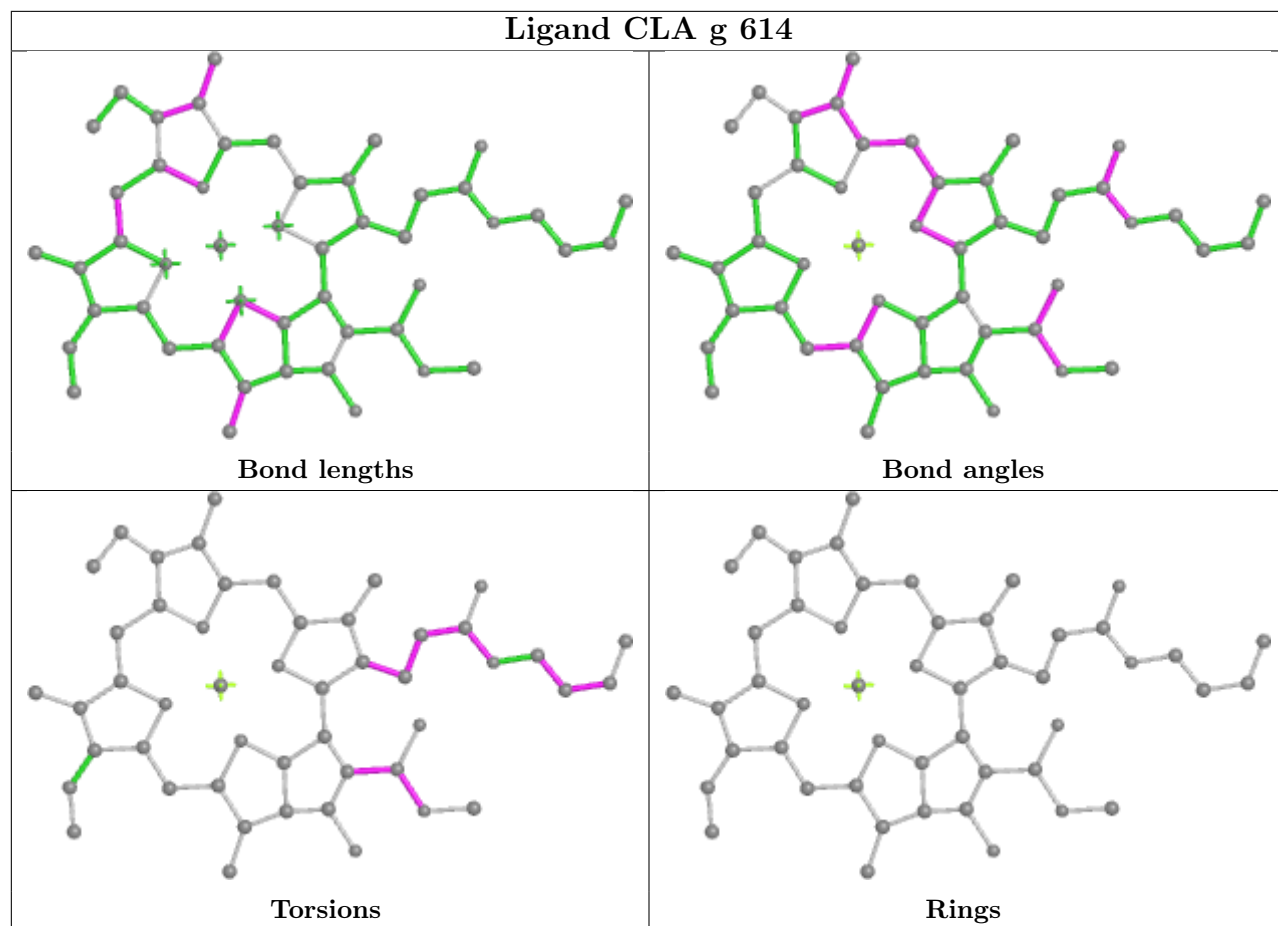


Ligand CLA C 513**Ligand CLA D 403****Ligand CLA C 507**

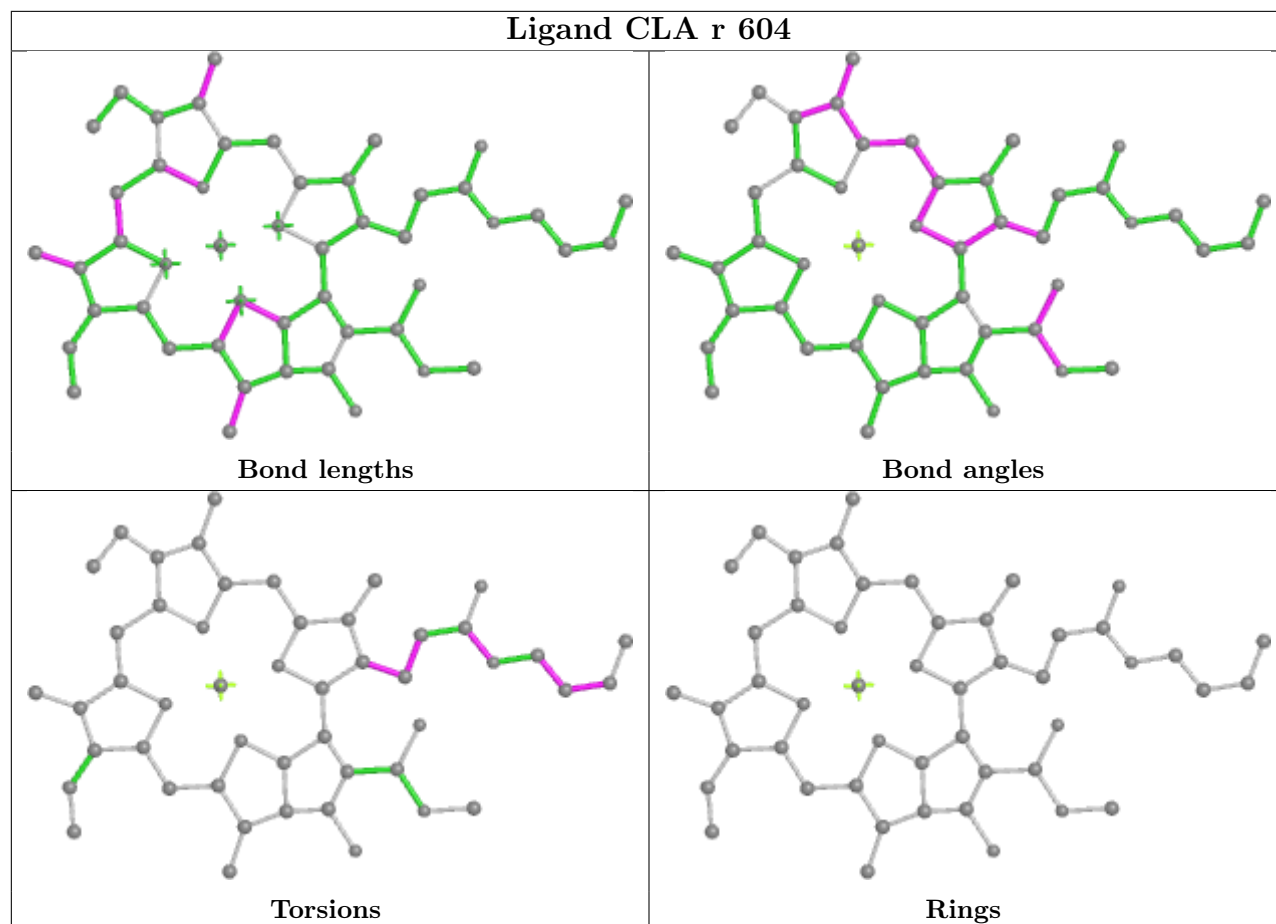




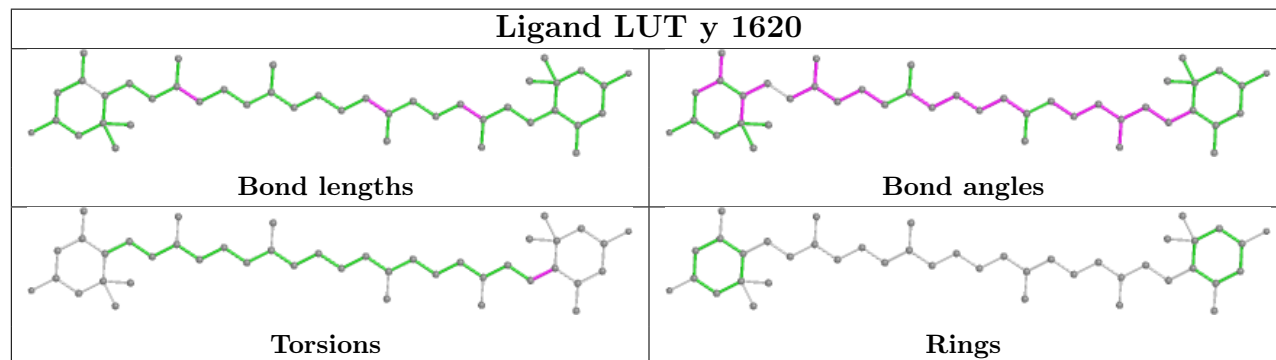
Ligand CLA g 614

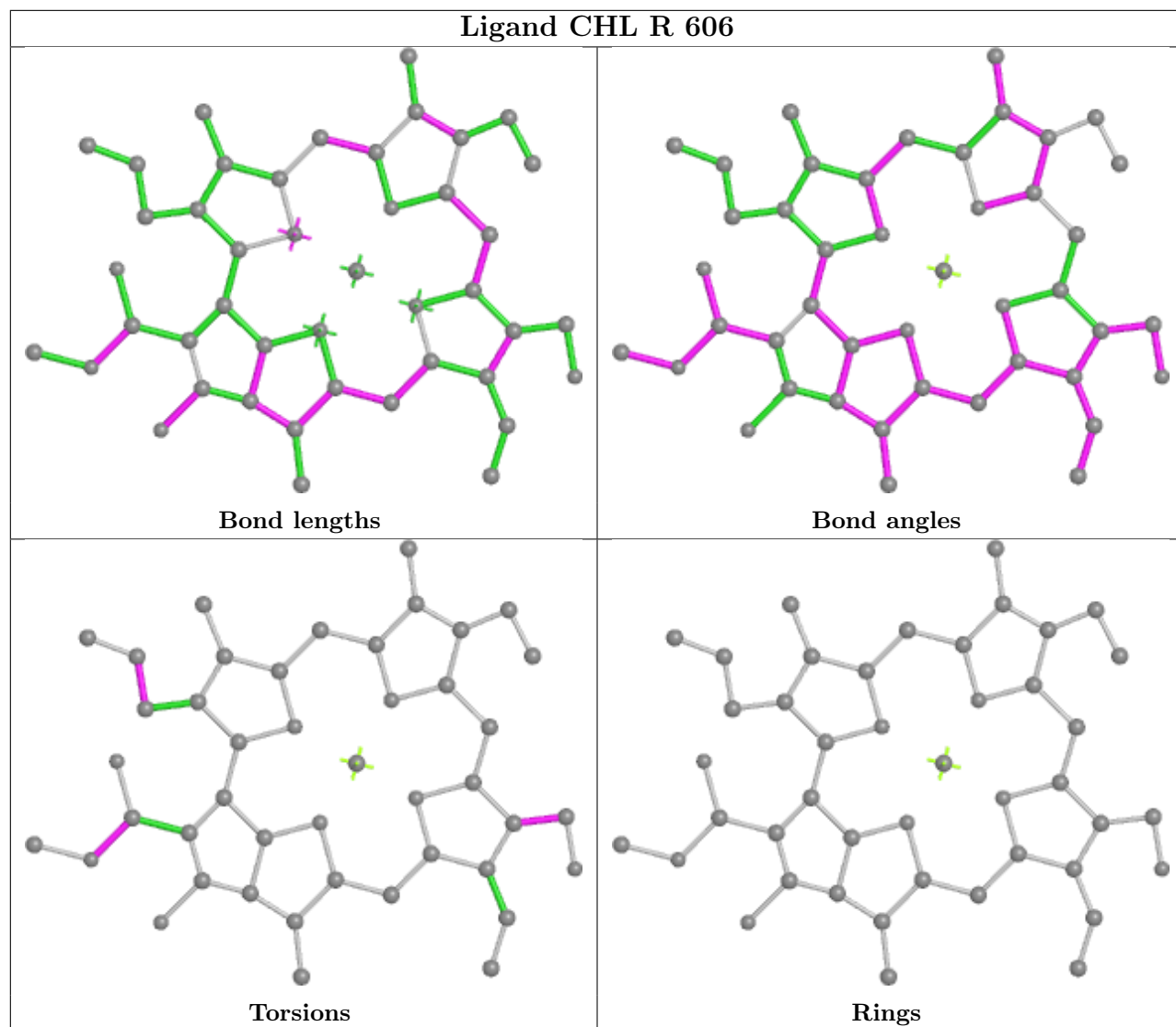


Ligand CLA r 604

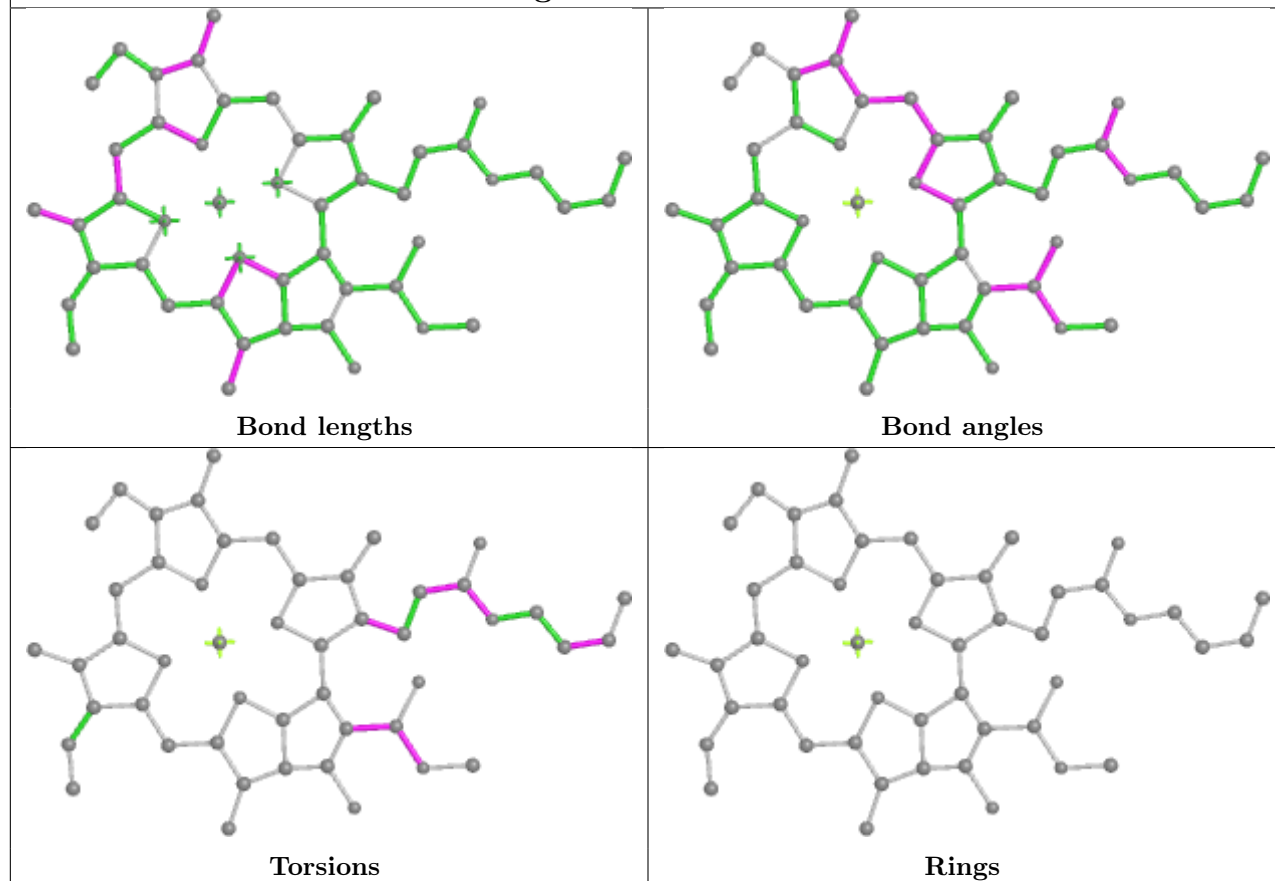


Ligand LUT y 1620

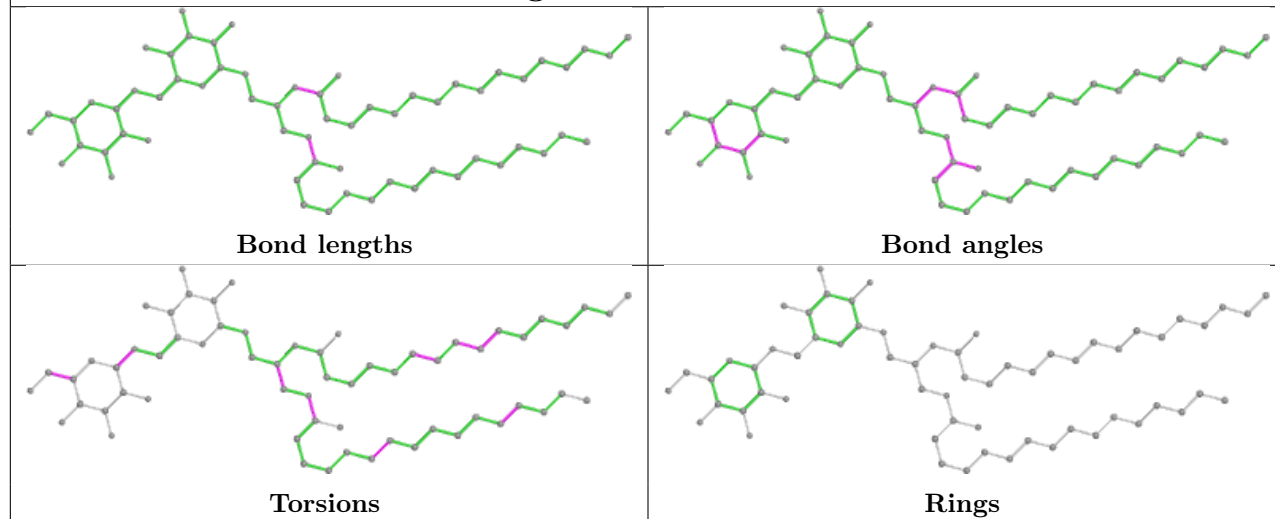


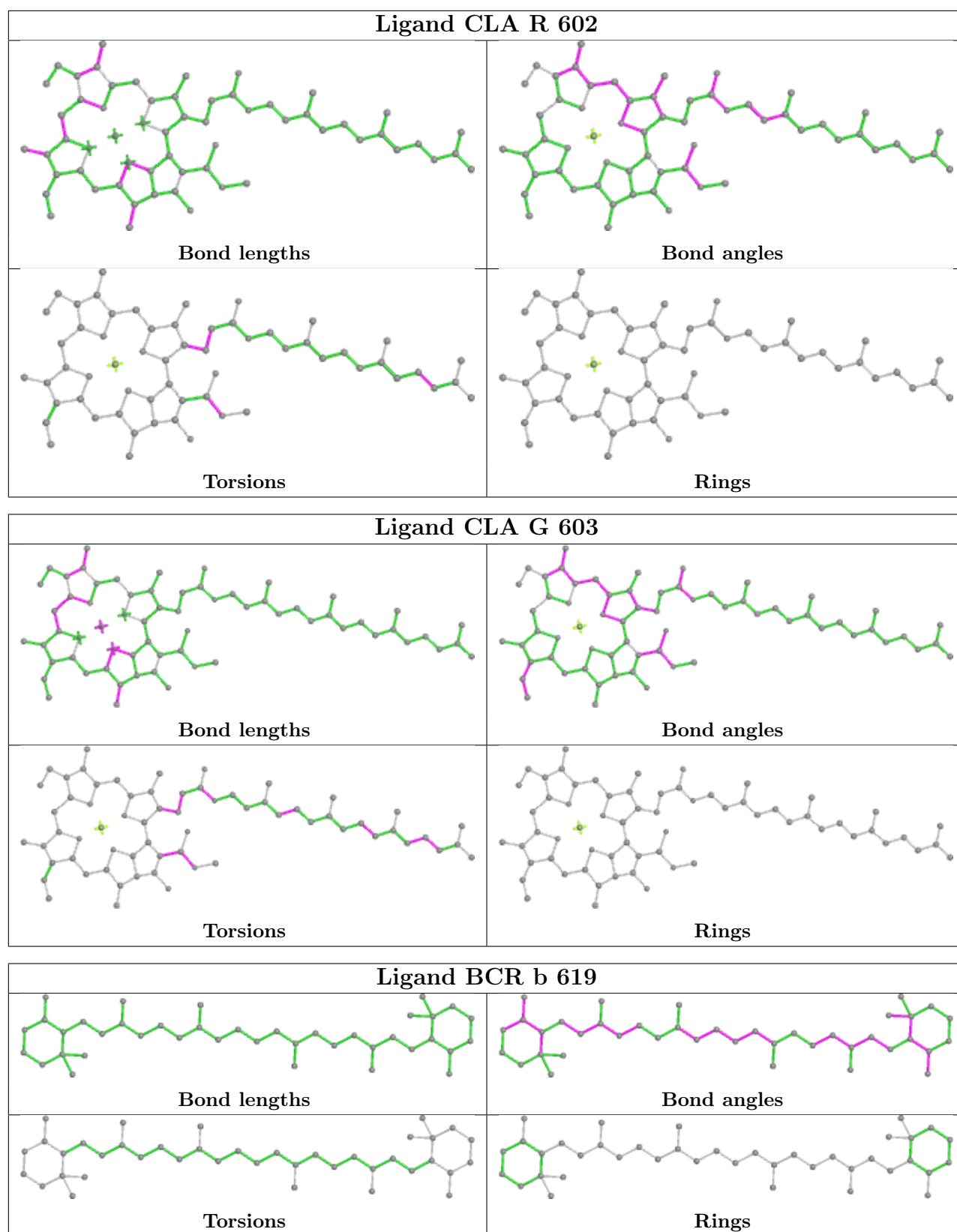


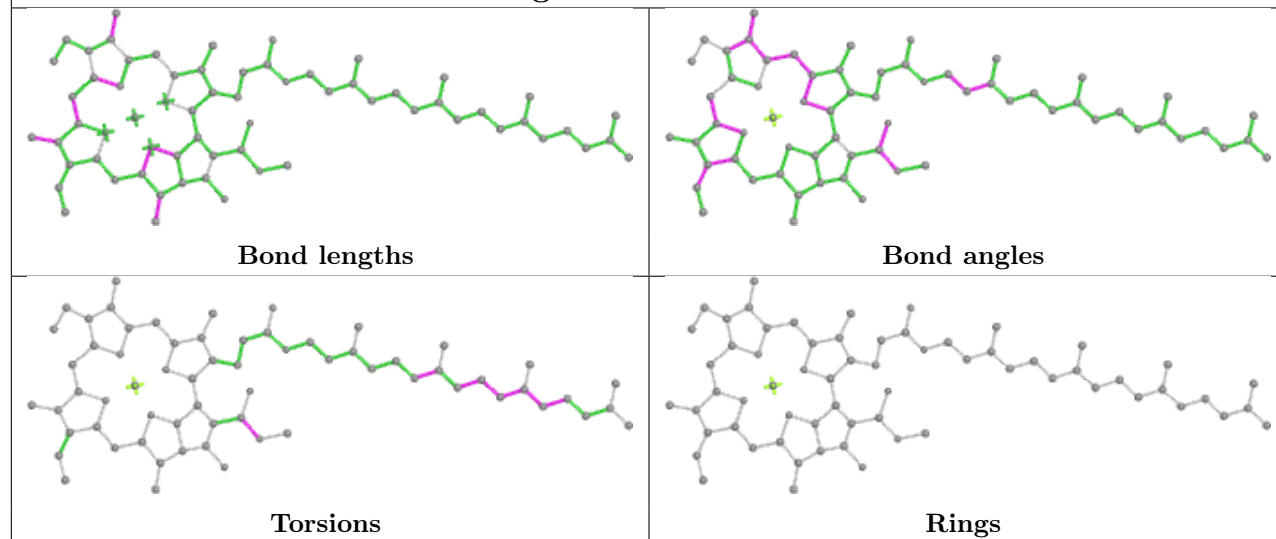
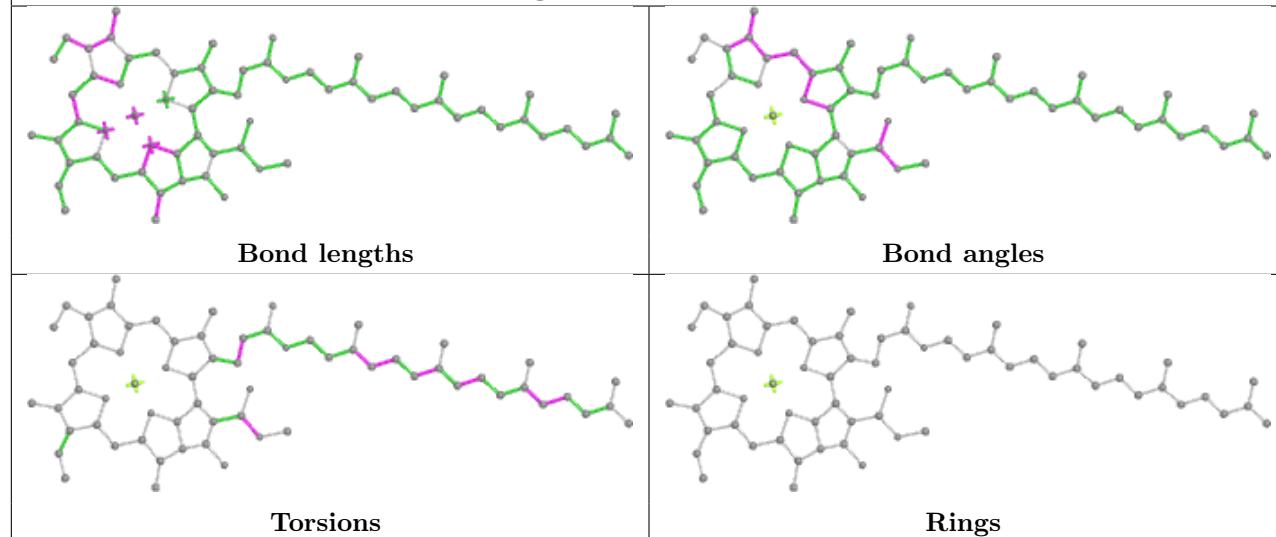
Ligand CLA n 611



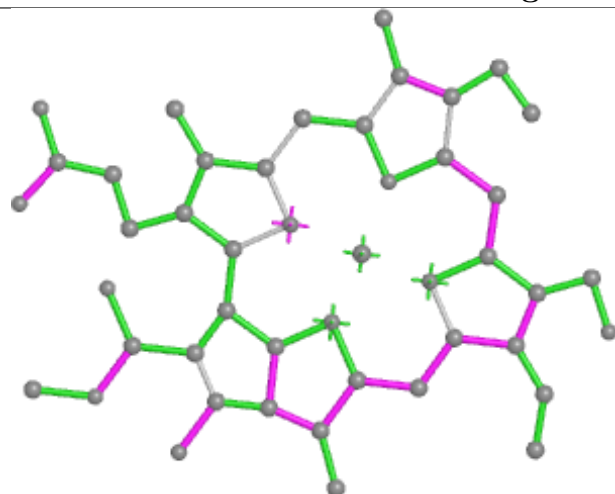
Ligand DGD C 519



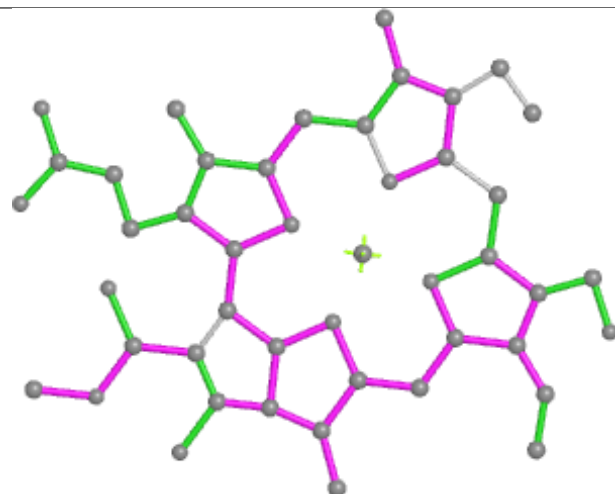


Ligand CLA B 612**Ligand CLA N 613**

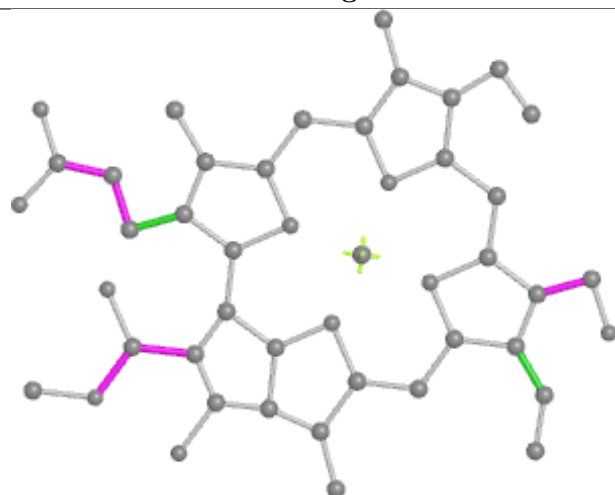
Ligand CHL s 601



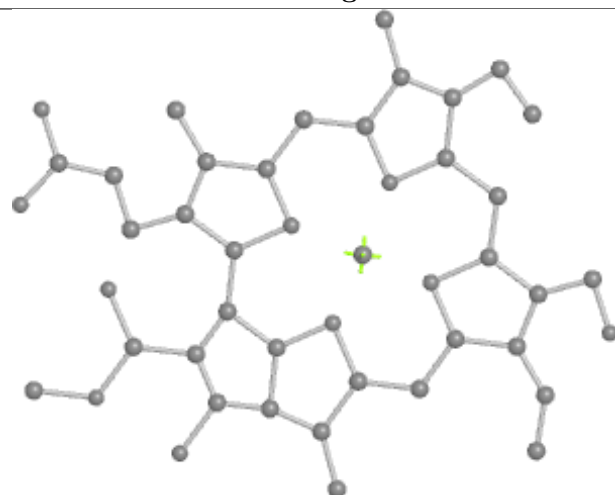
Bond lengths



Bond angles

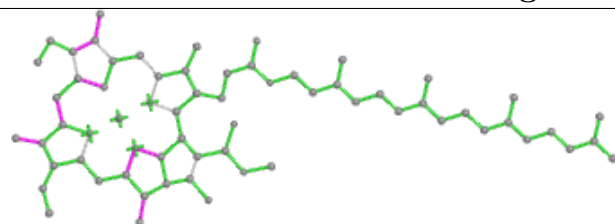


Torsions

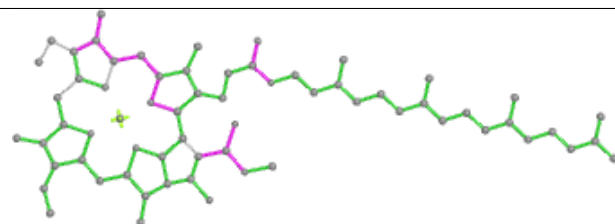


Rings

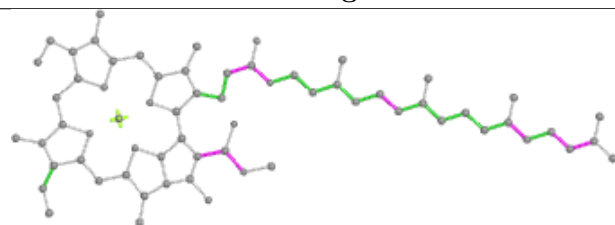
Ligand CLA b 602



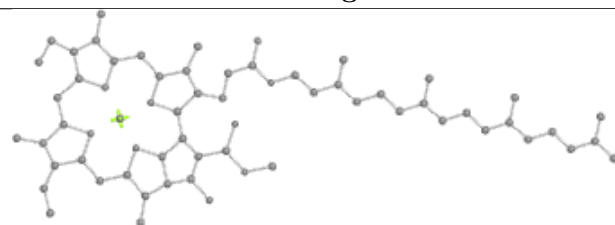
Bond lengths



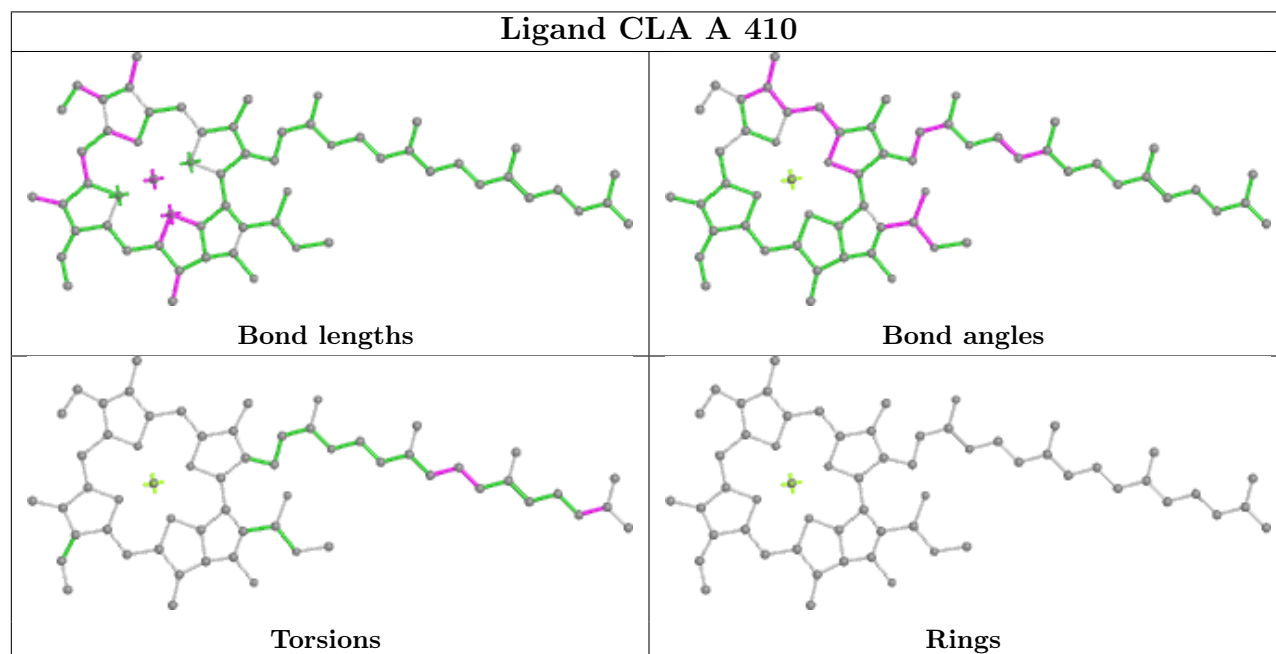
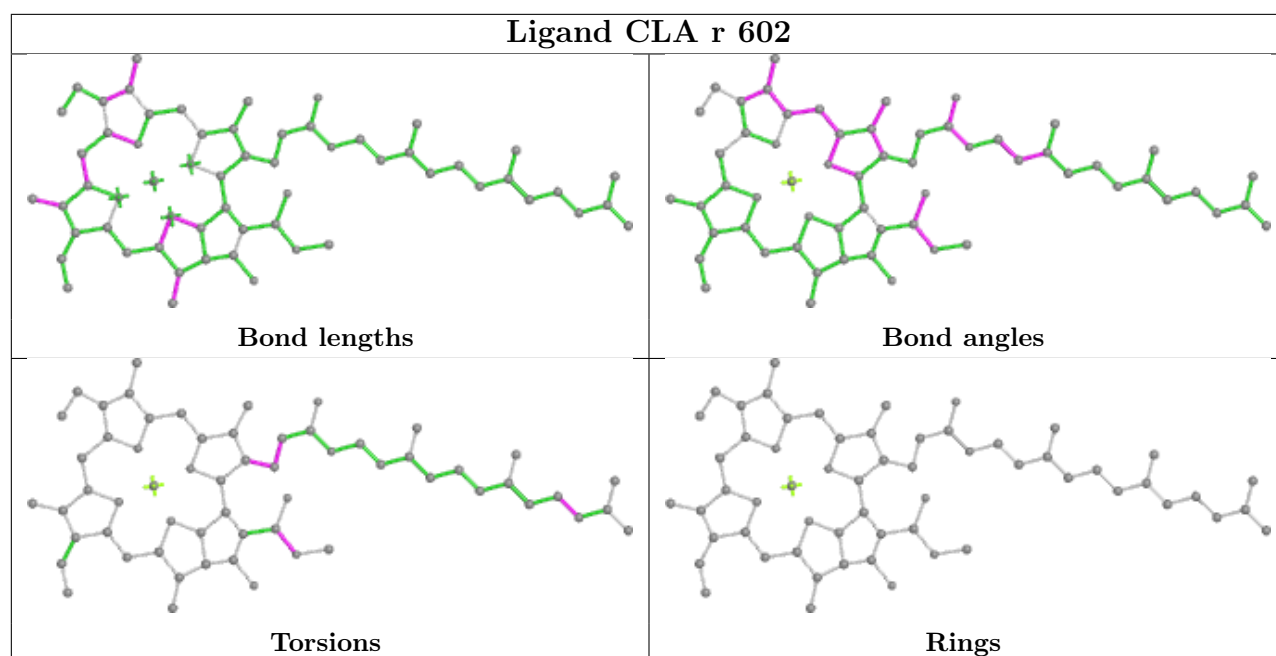
Bond angles



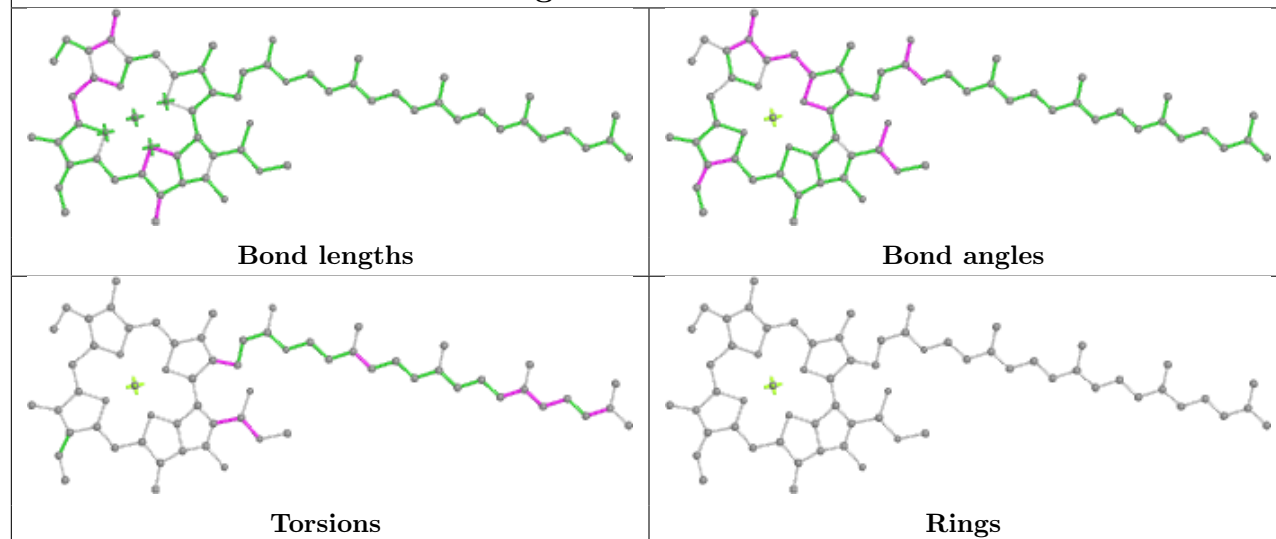
Torsions



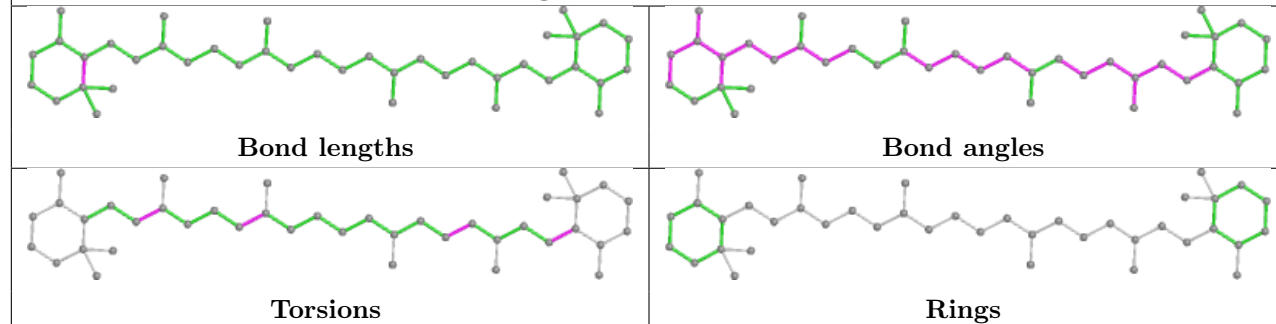
Rings



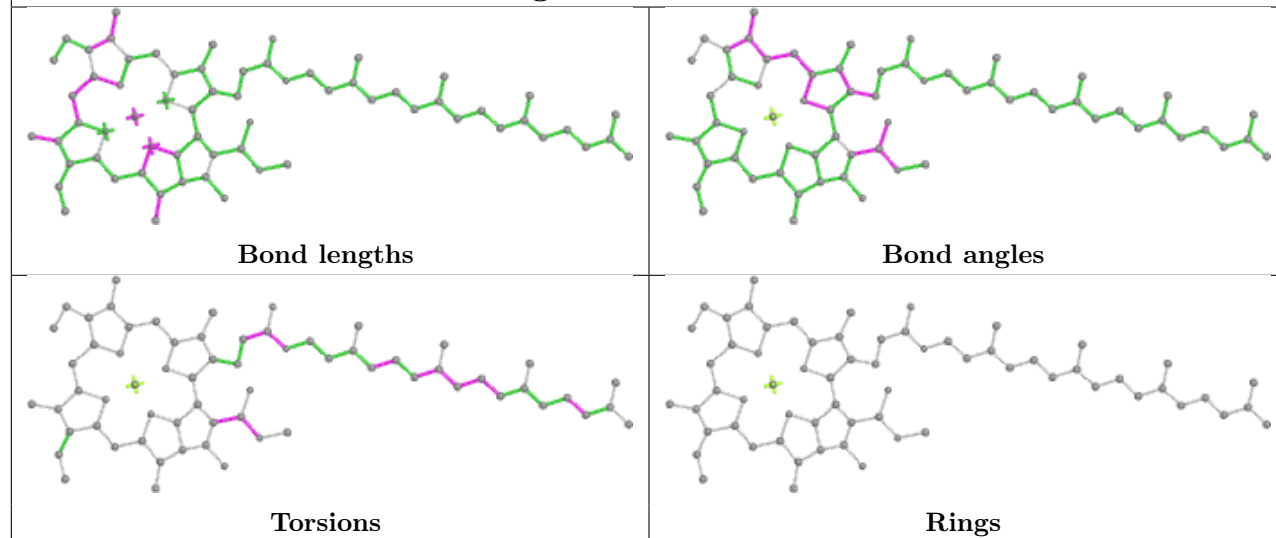
Ligand CLA b 610

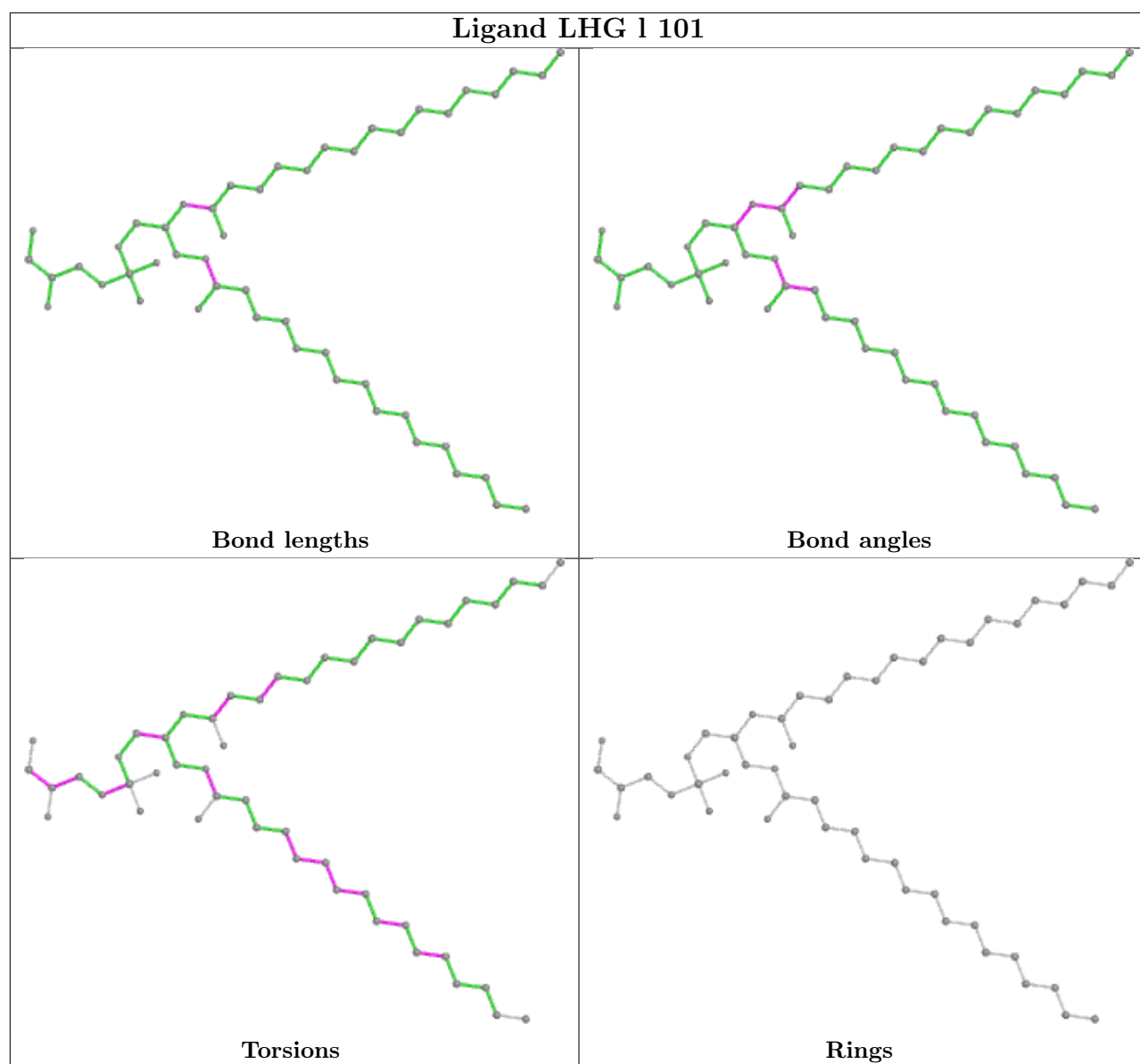


Ligand BCR c 515

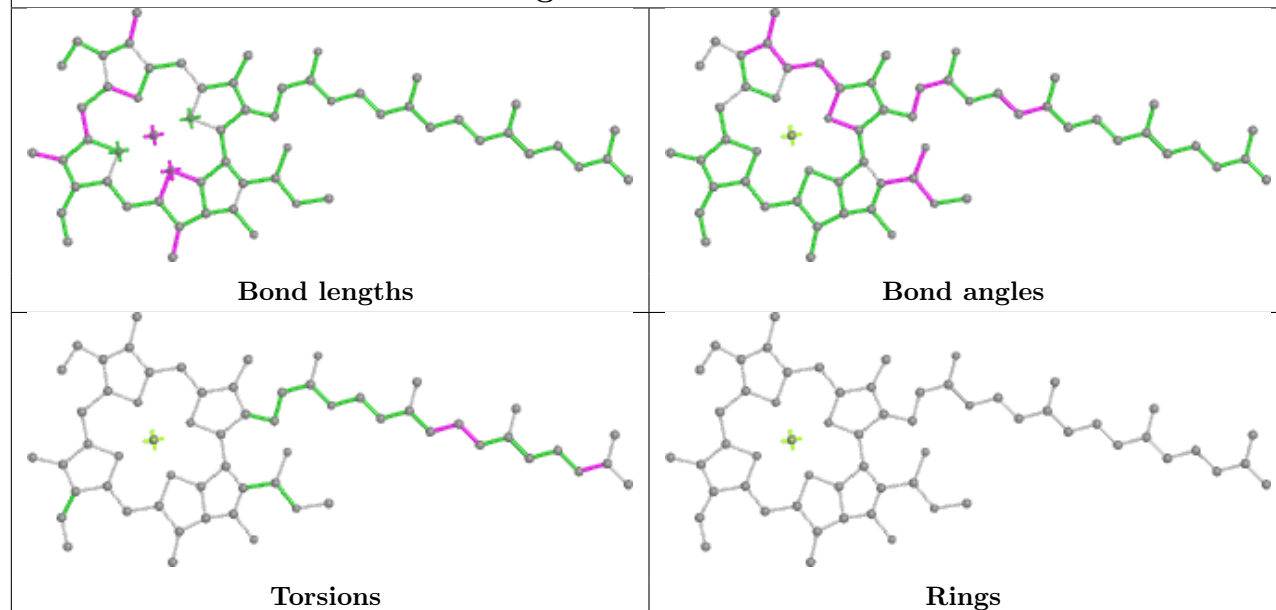


Ligand CLA Y 612

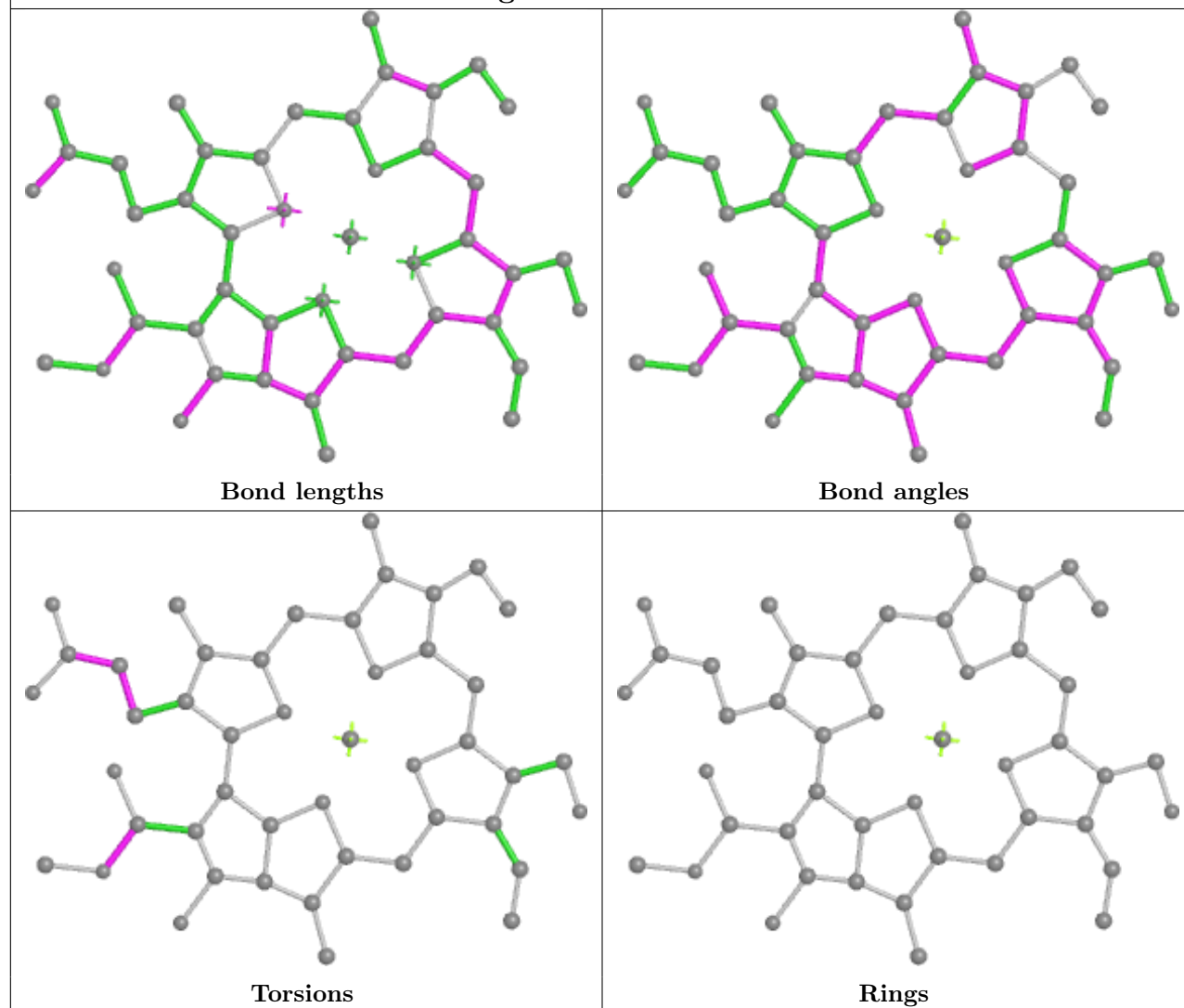


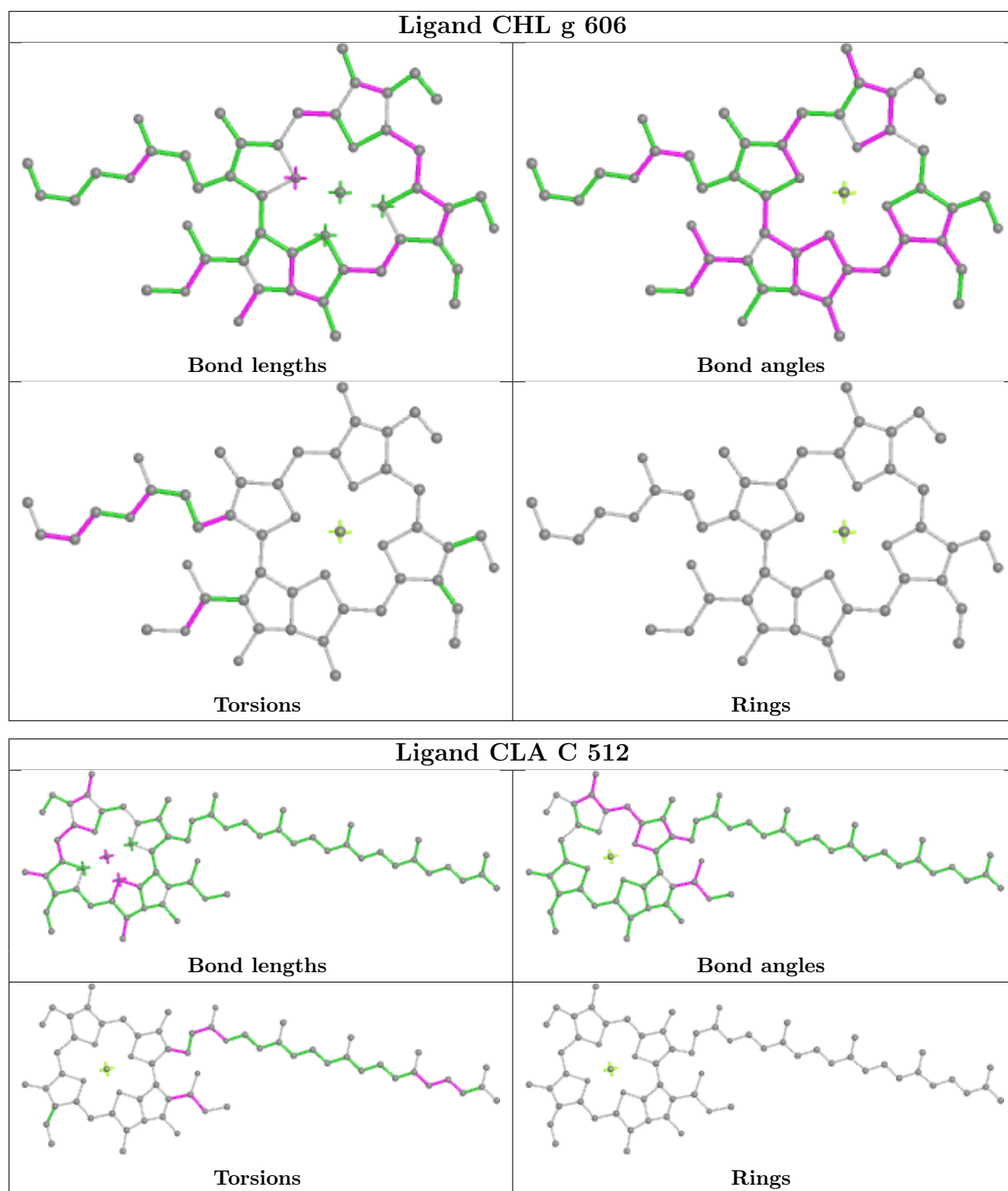


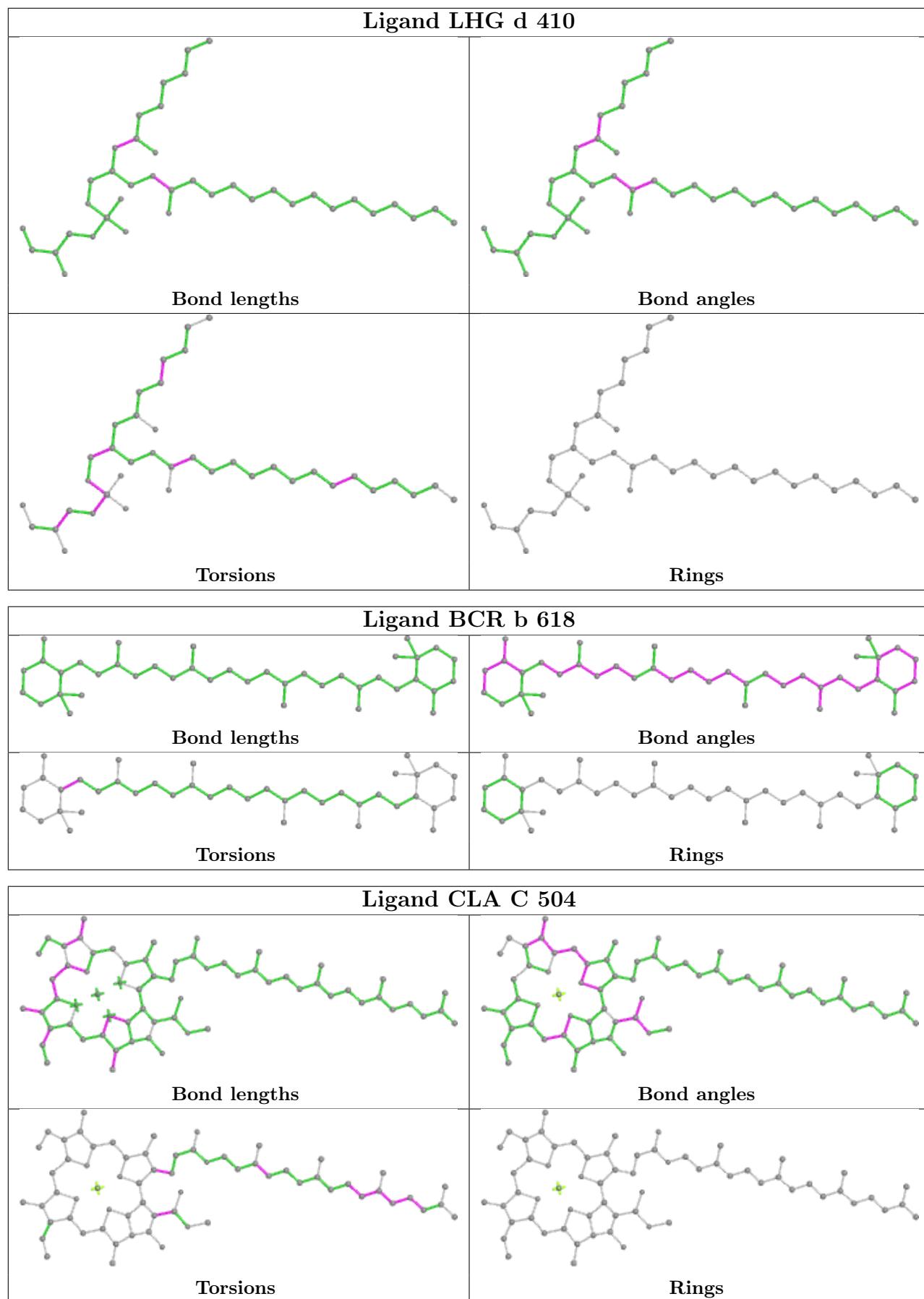
Ligand CLA a 410



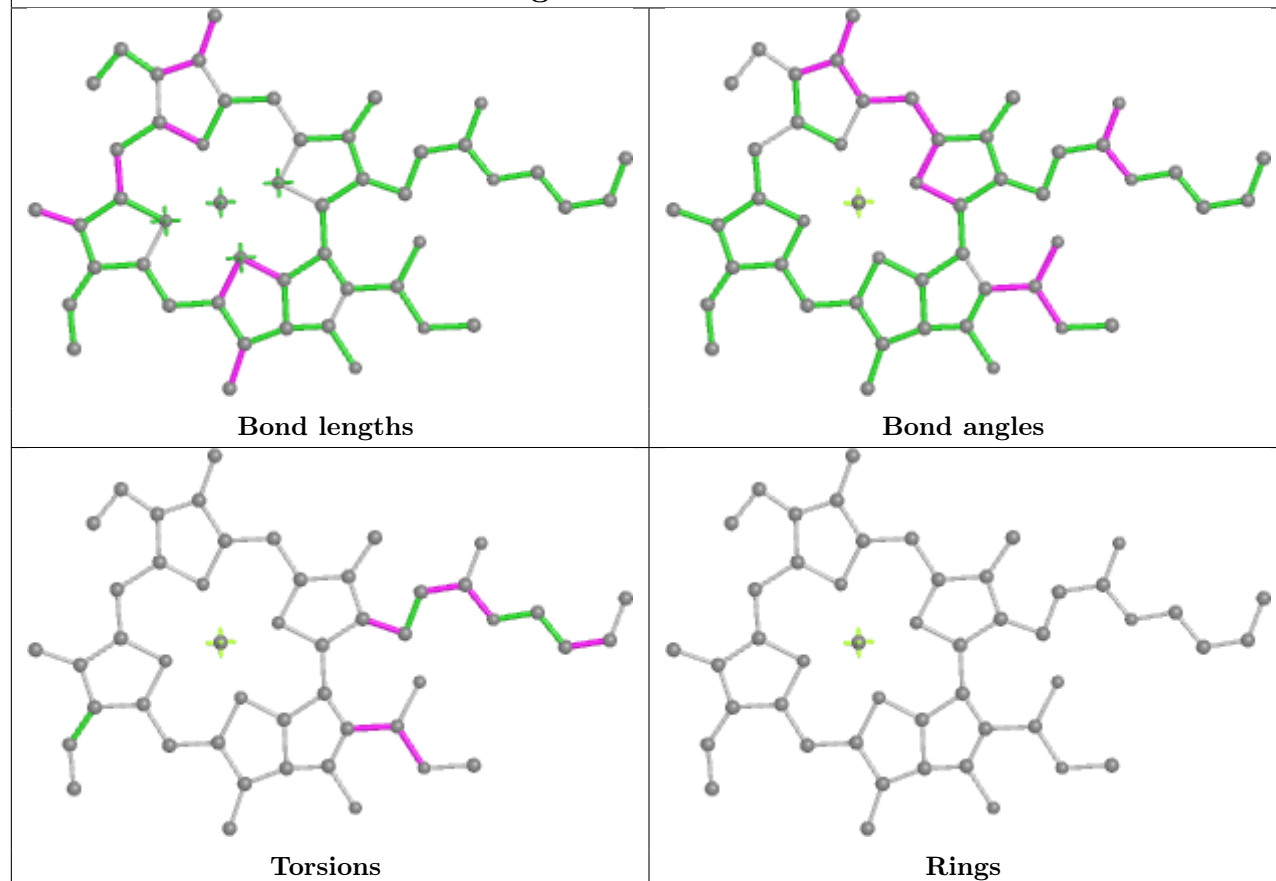
Ligand CHL r 608



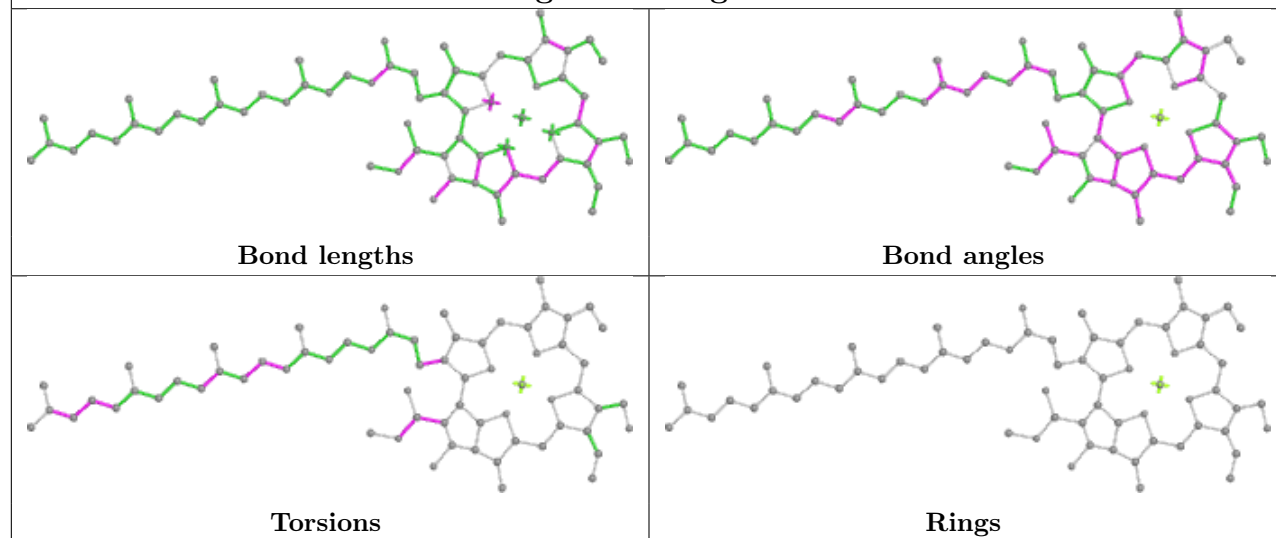


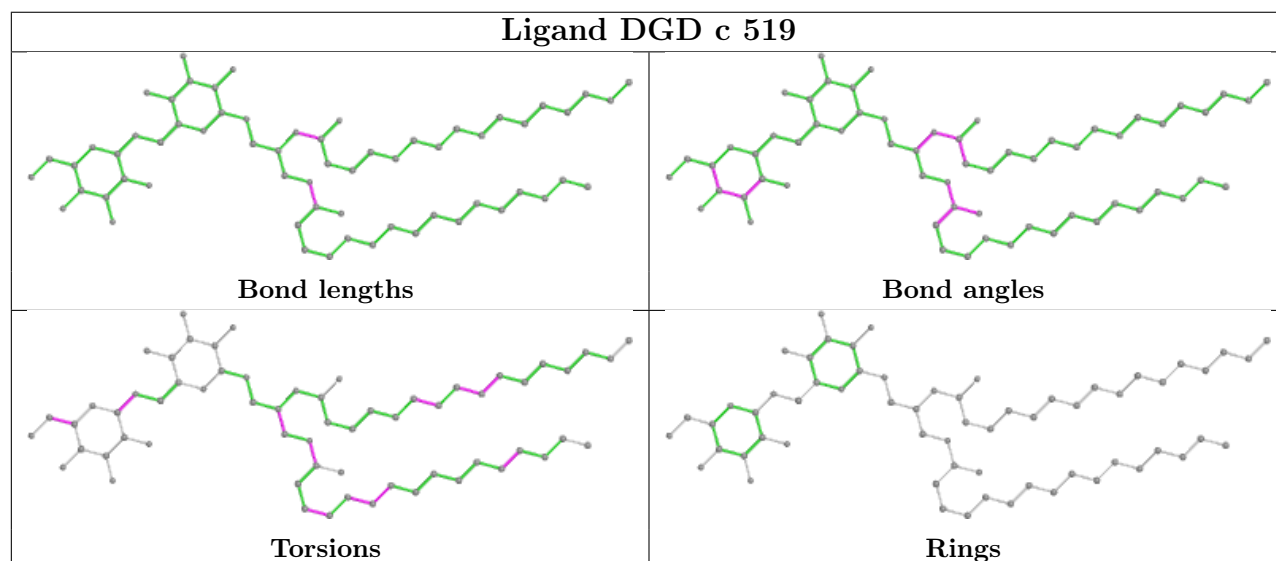
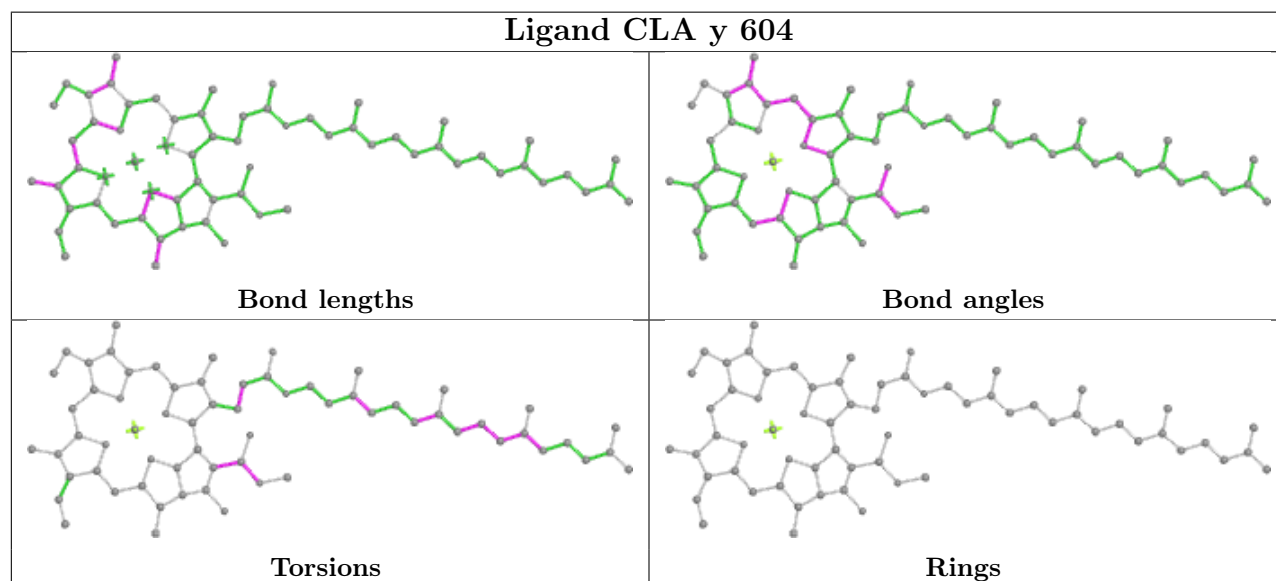
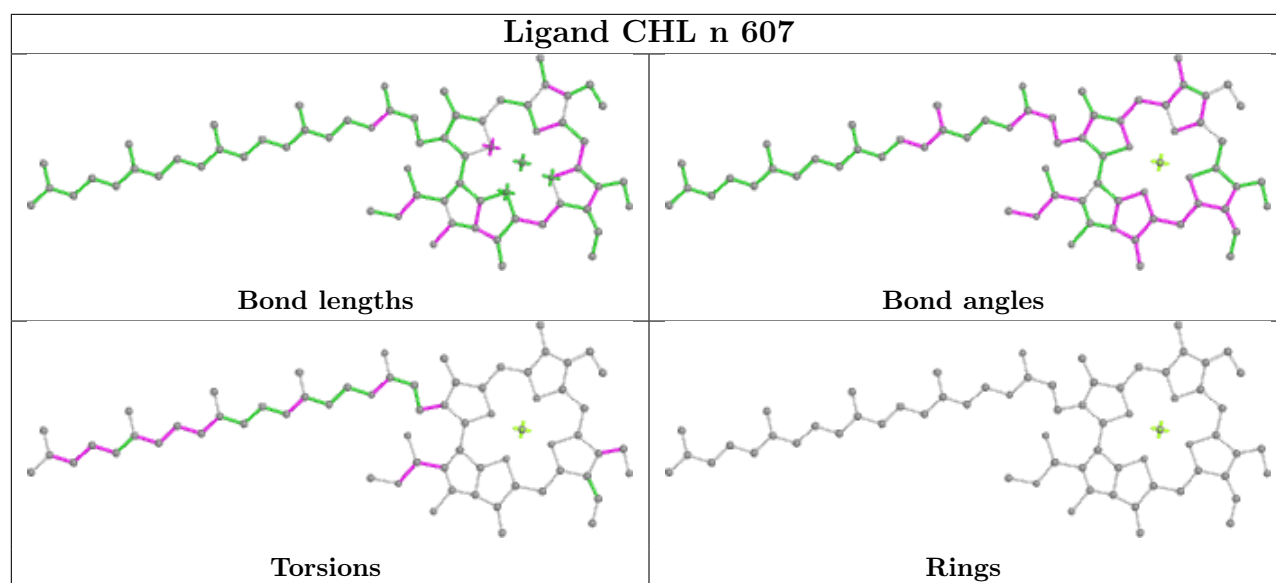


Ligand CLA N 611

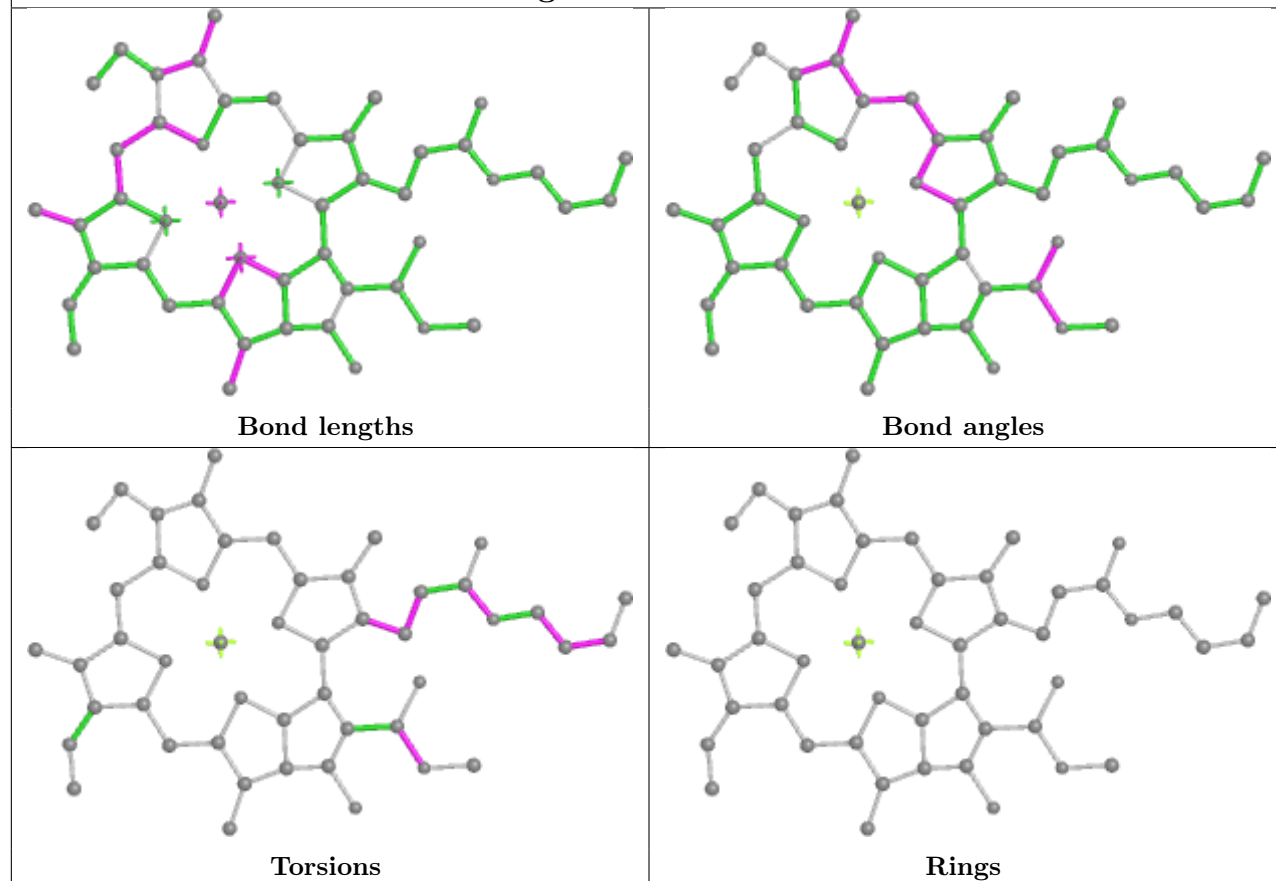


Ligand CHL g 601

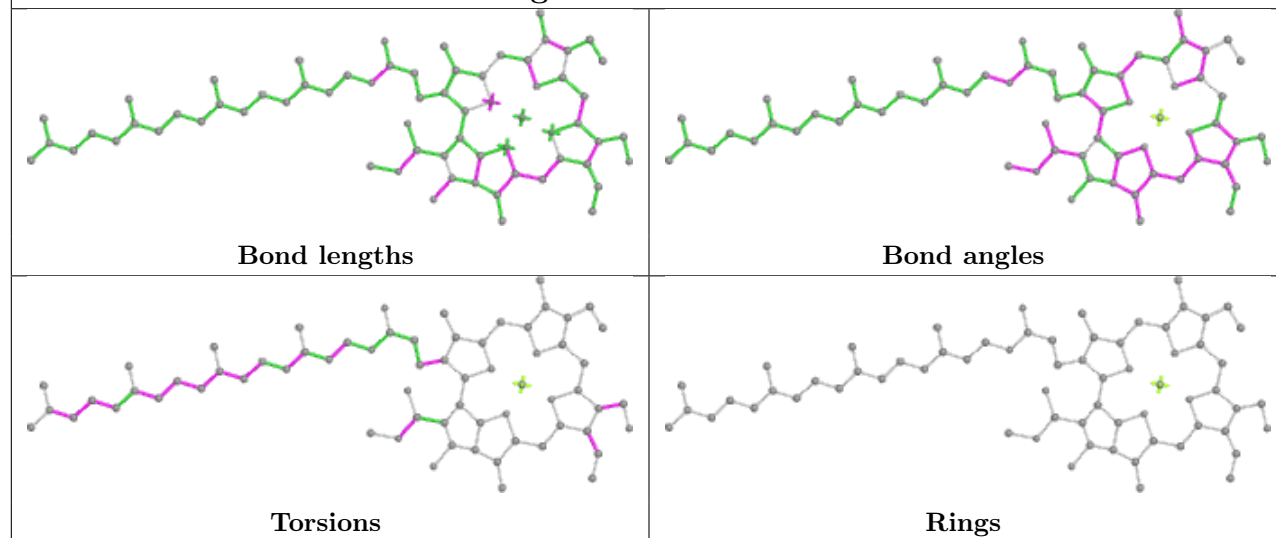


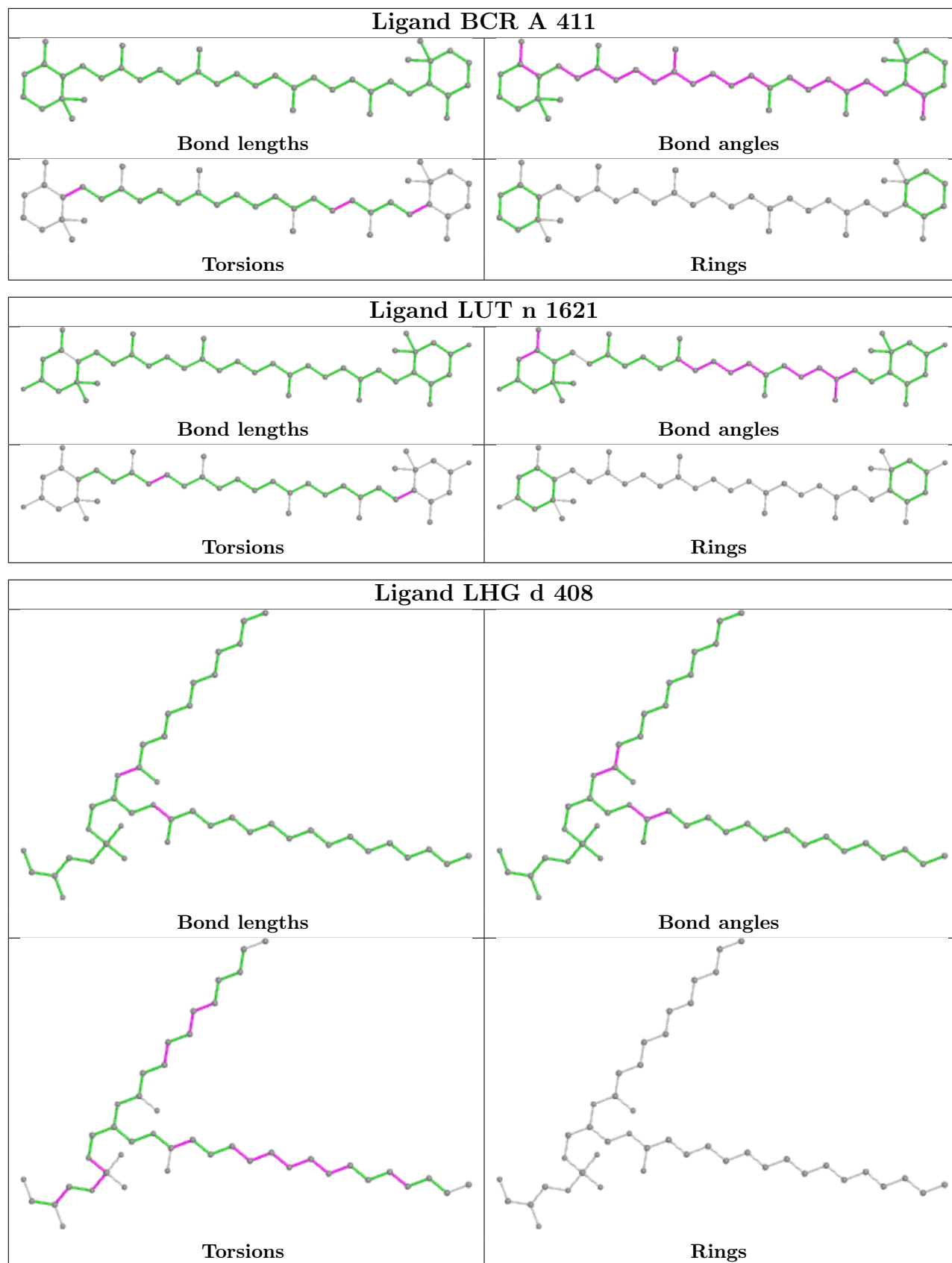


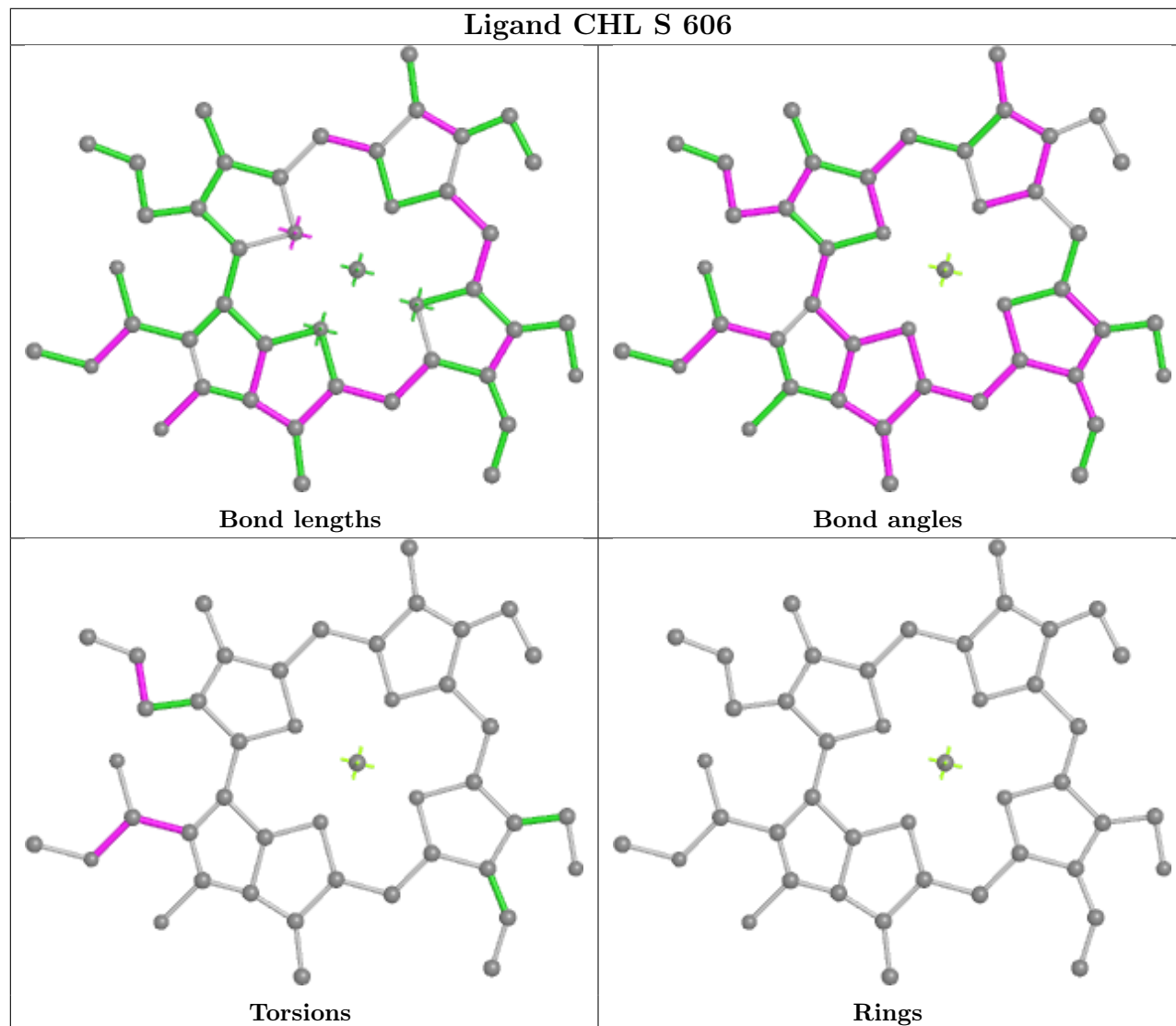
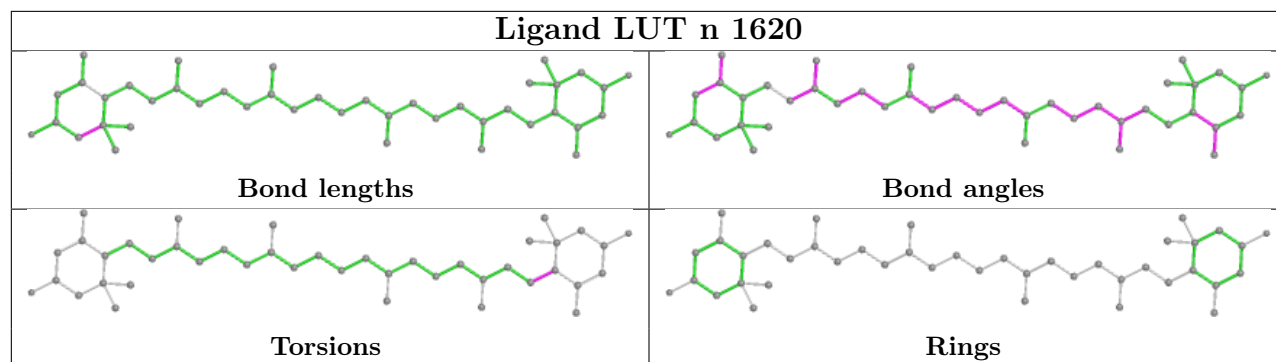
Ligand CLA s 613

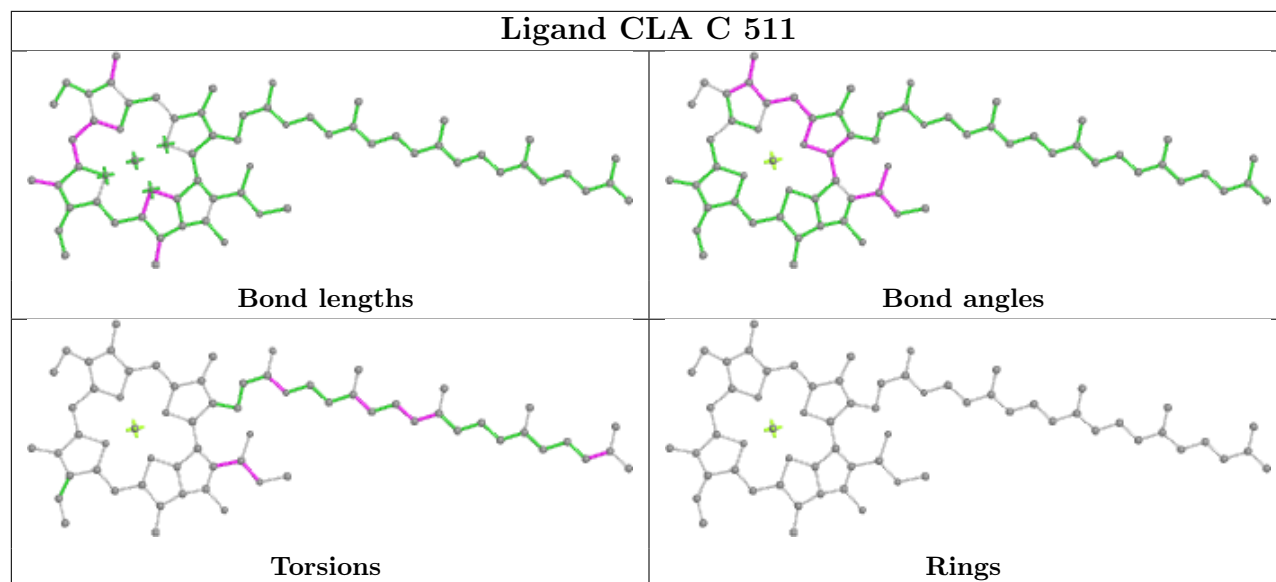
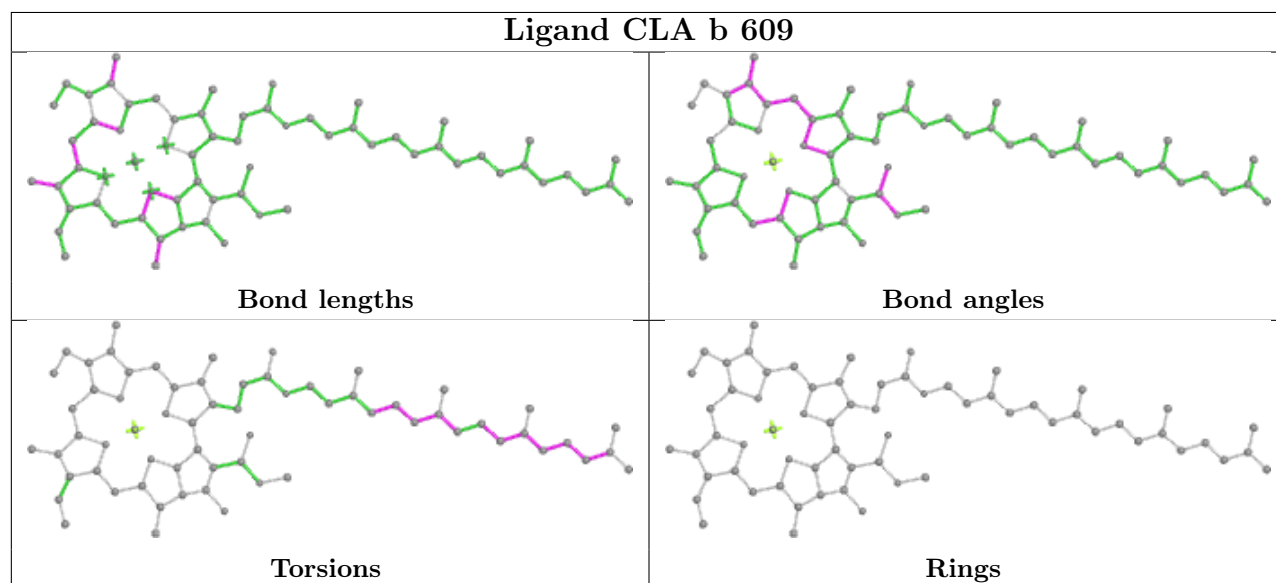


Ligand CHL N 609

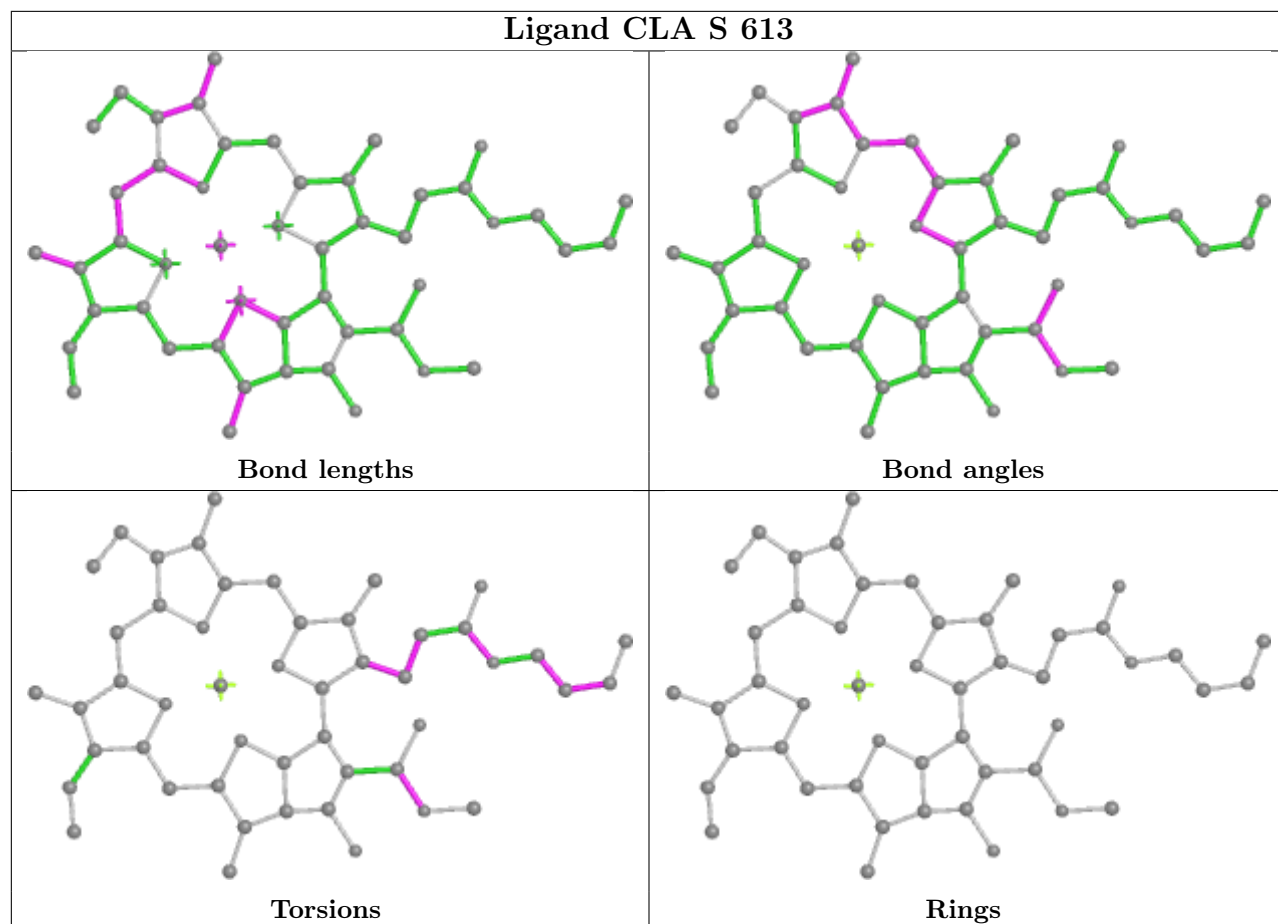




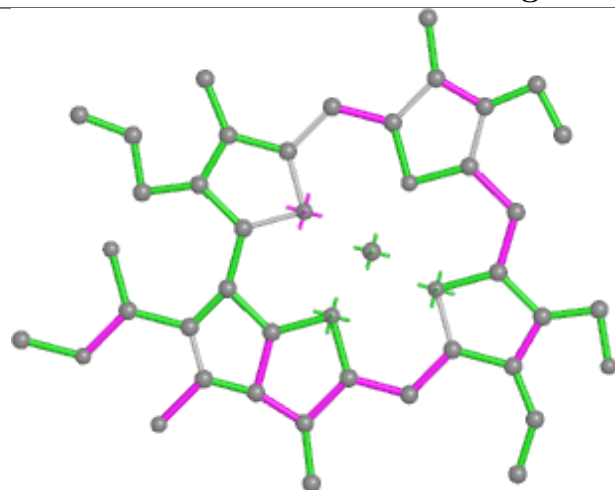


Ligand CLA C 511**Ligand CLA b 609**

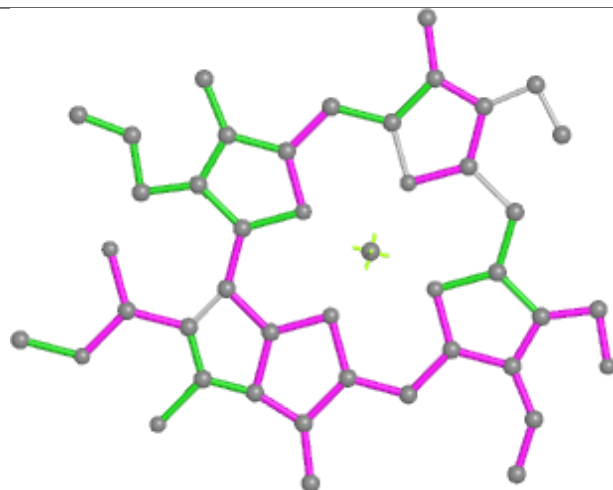
Ligand CLA S 613



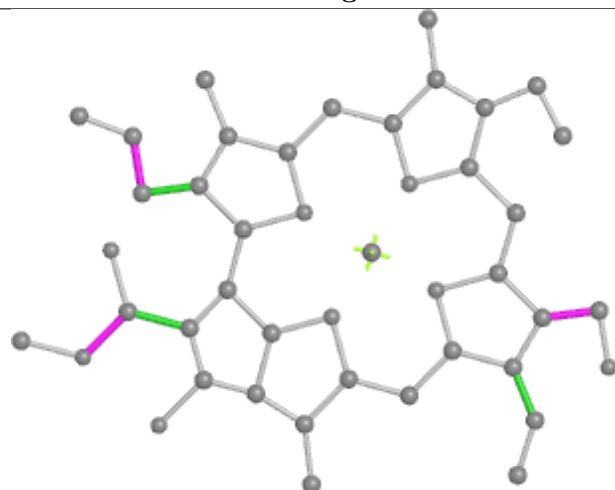
Ligand CHL r 606



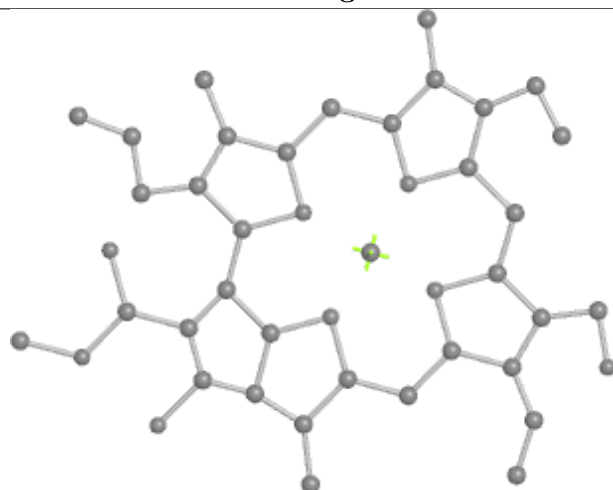
Bond lengths



Bond angles

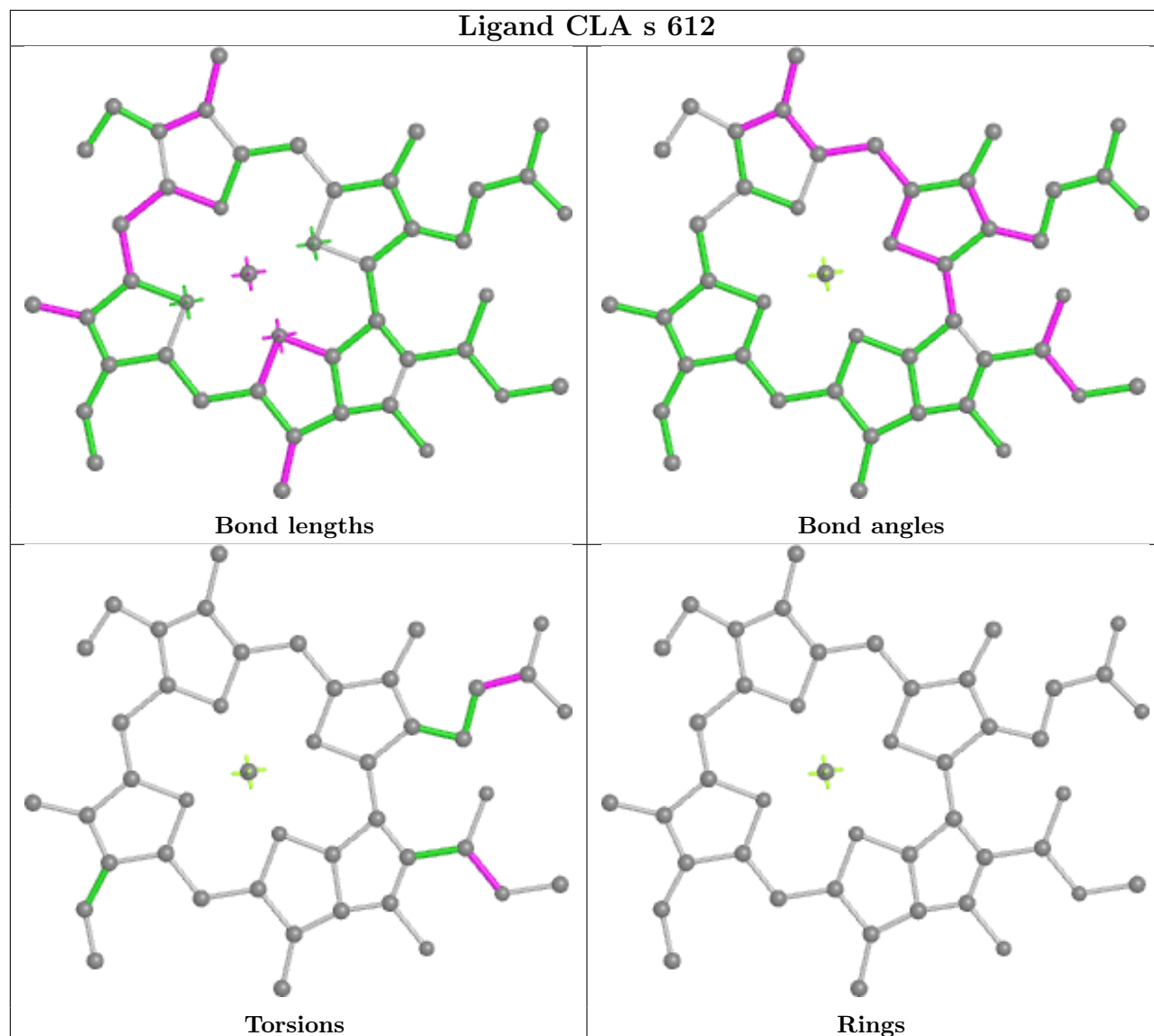


Torsions

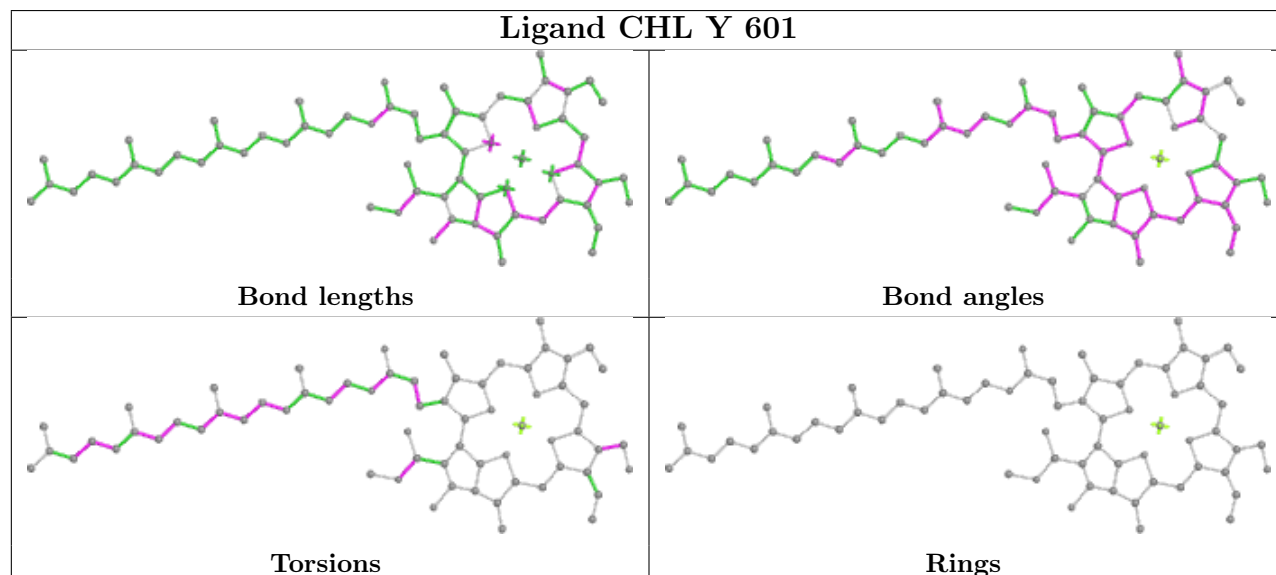


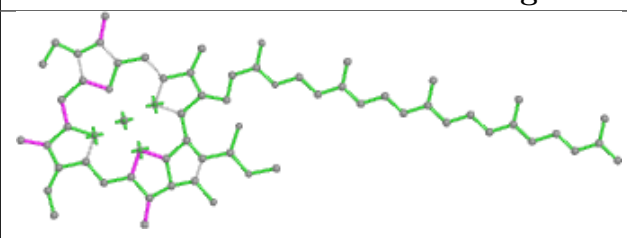
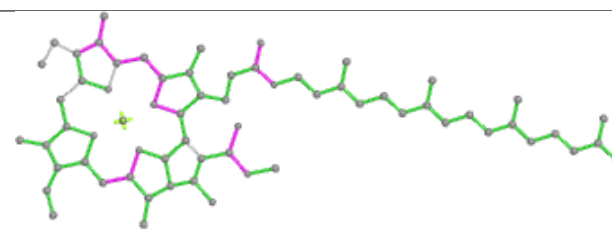
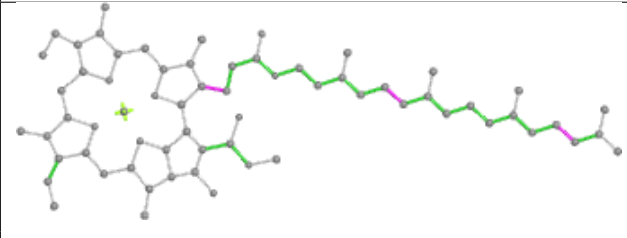
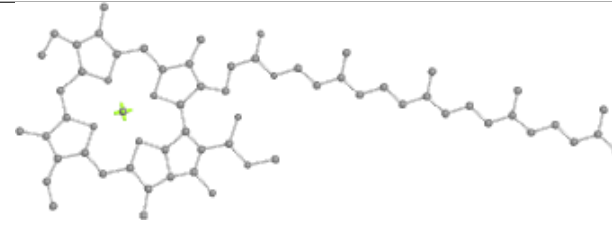
Rings

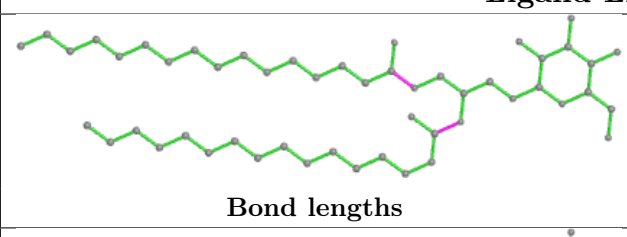
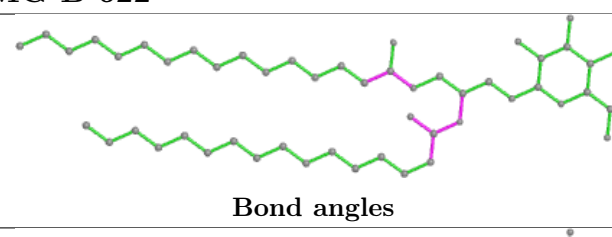
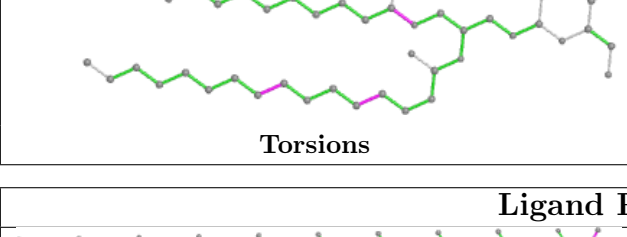

Ligand CLA s 612

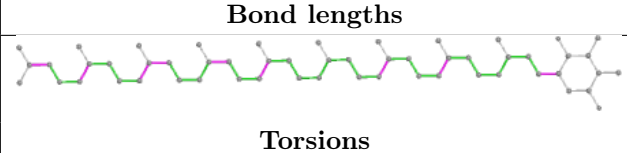
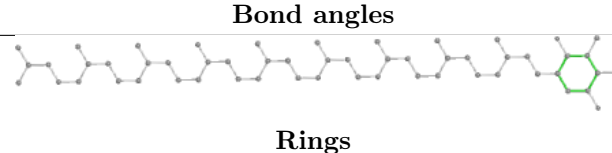




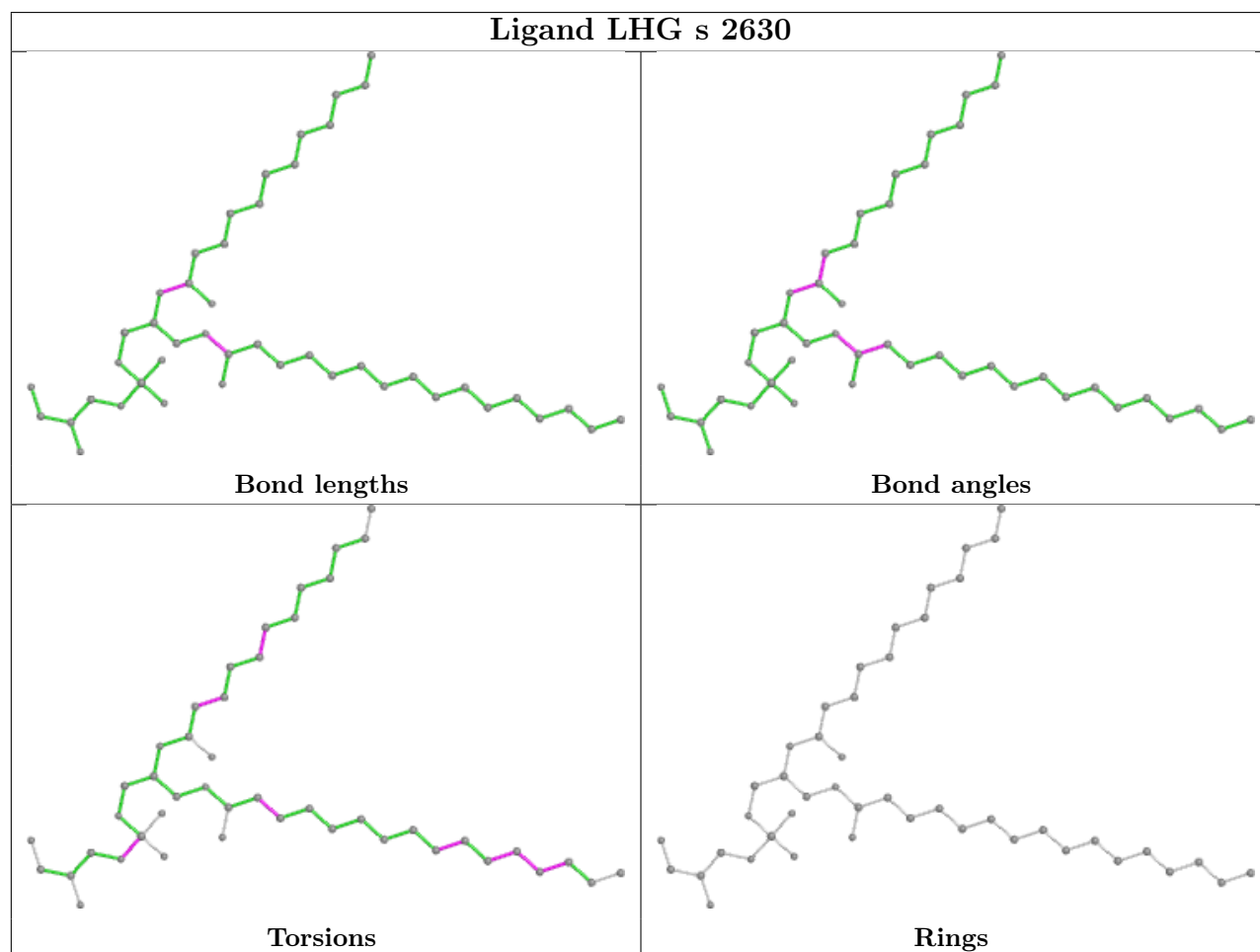
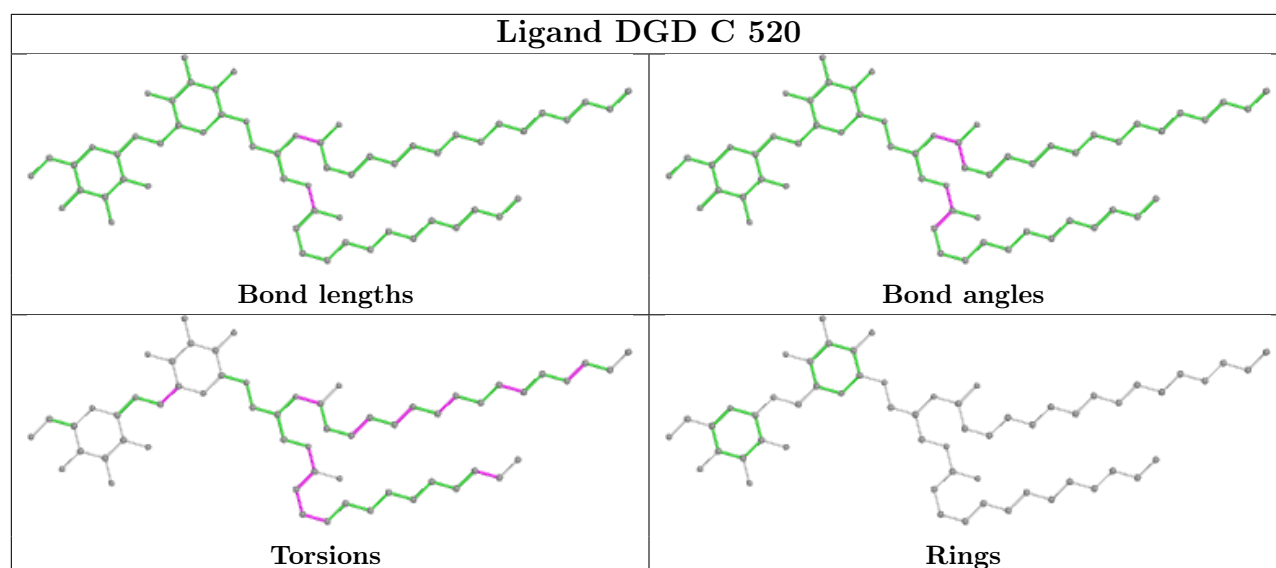
Ligand CHL Y 601

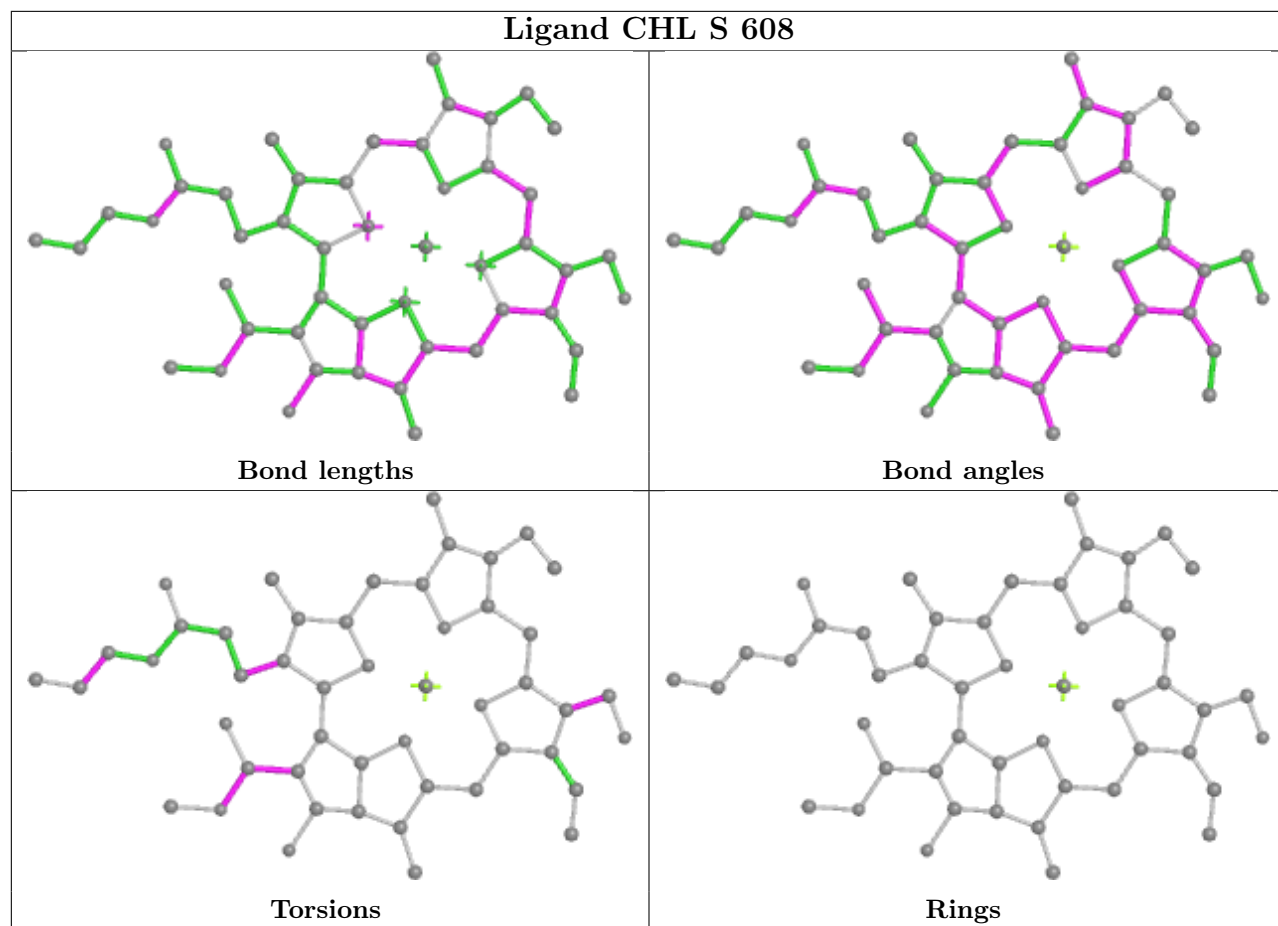


Ligand CLA N 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

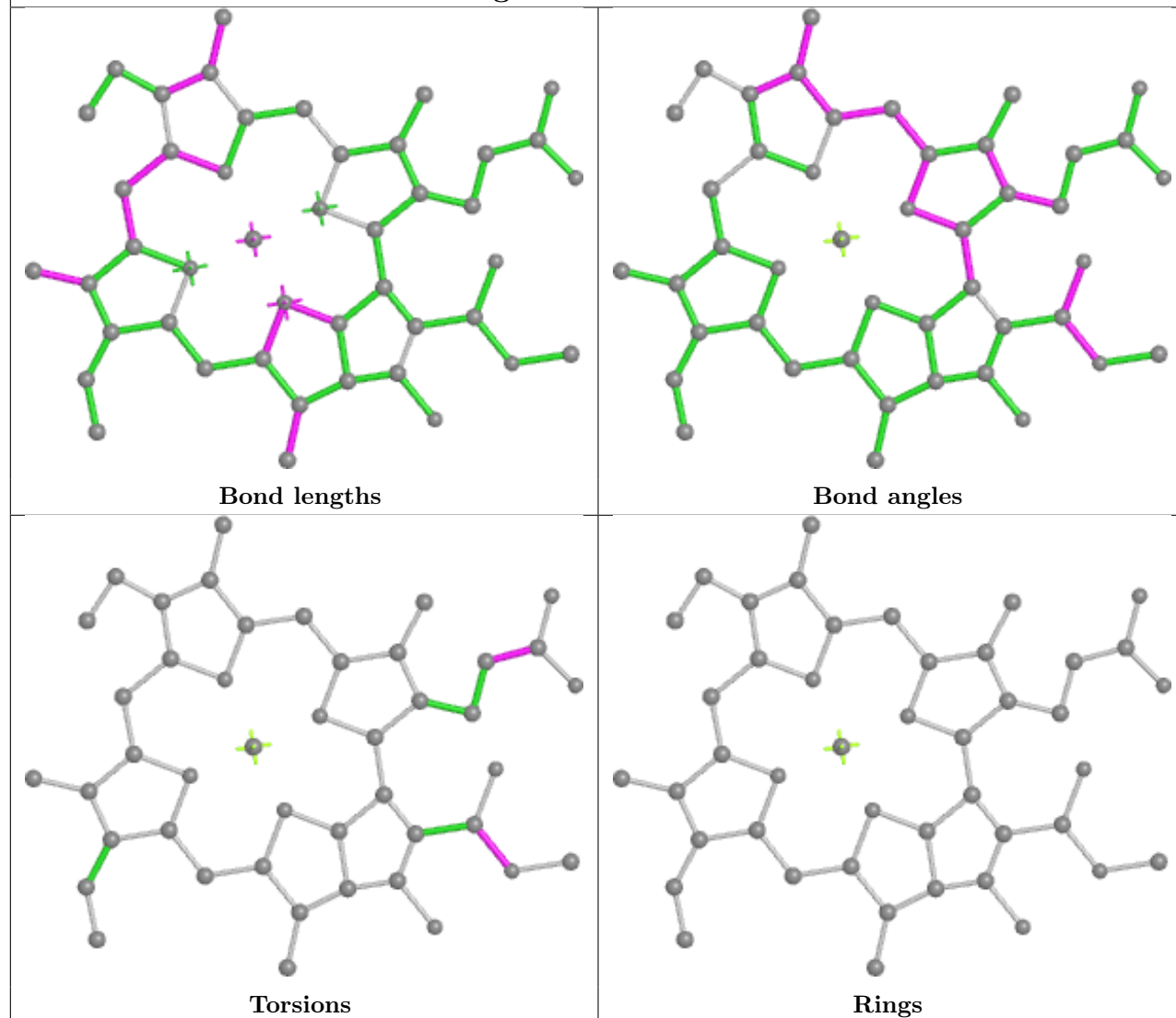
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

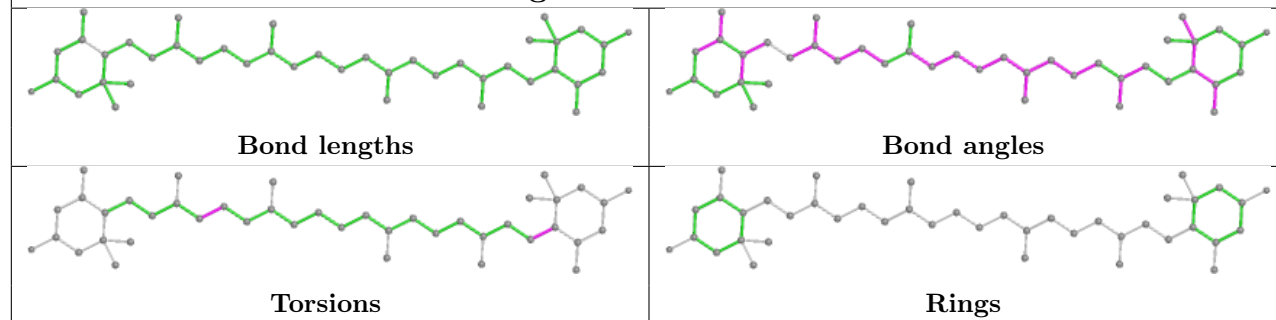




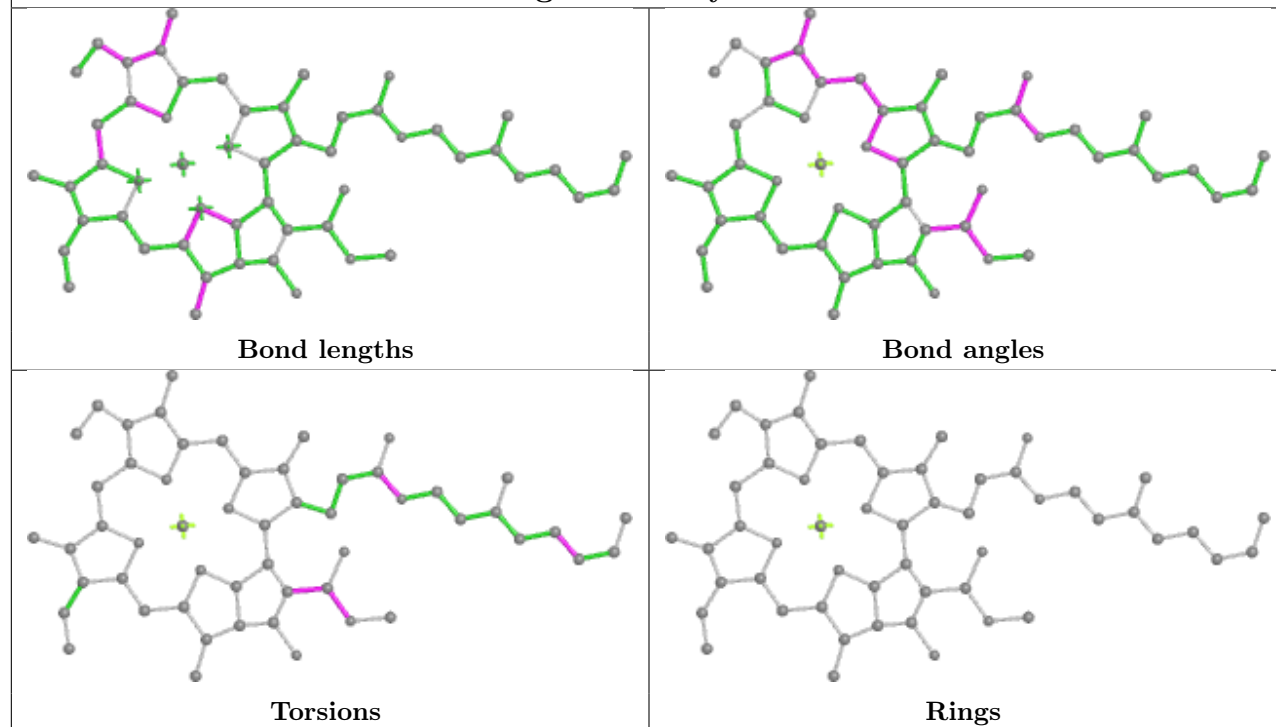
Ligand CLA S 612



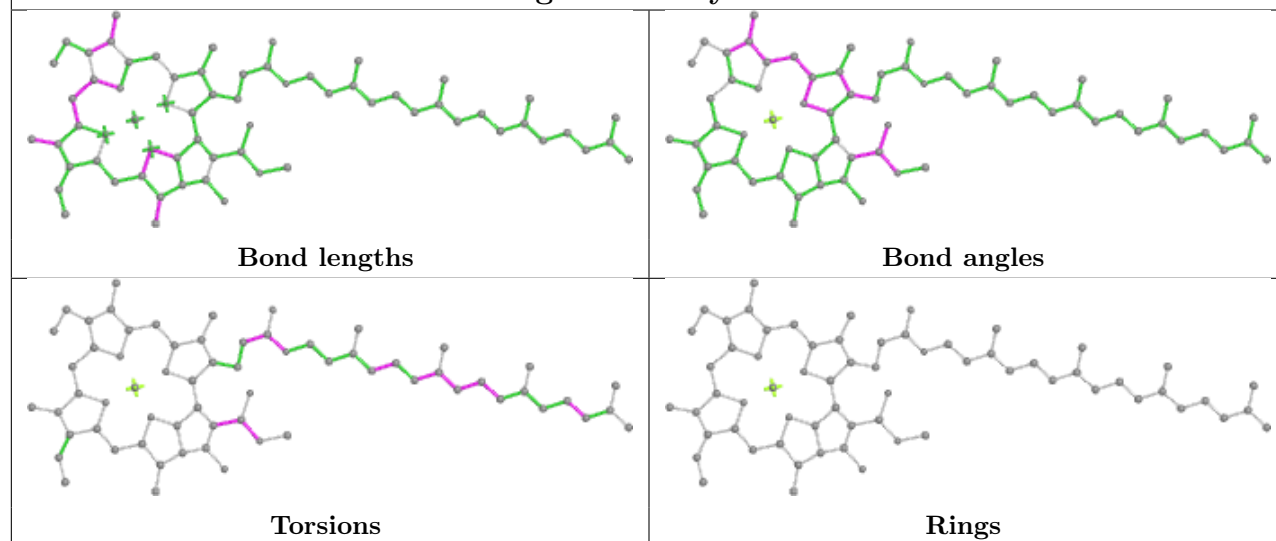
Ligand LUT s 1621

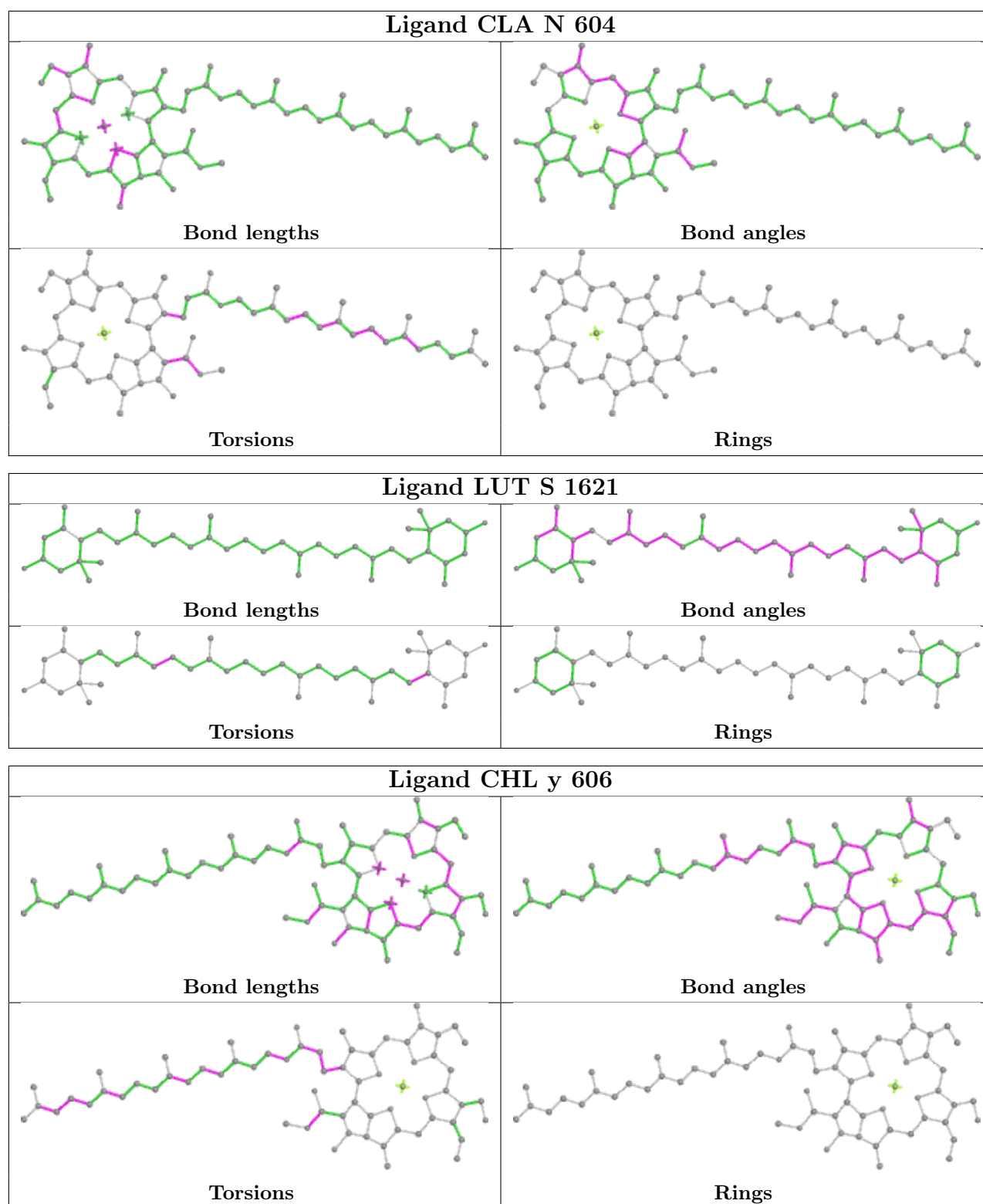


Ligand CLA y 614



Ligand CLA y 612





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9955. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.