



Full wwPDB EM Validation Report ⓘ

Aug 3, 2025 – 12:56 AM JST

PDB ID : 9LK5 / pdb_00009lk5
EMDB ID : EMD-63168
Title : The structure of Lhcb8-C2S2 PSII-LHCII supercomplex from Arabidopsis thaliana
Authors : Zhou, Q.; Caferri, R.; Shan, J.Y.; Amelii, A.; Bassi, R.; Liu, Z.F.
Deposited on : 2025-01-16
Resolution : 3.00 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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

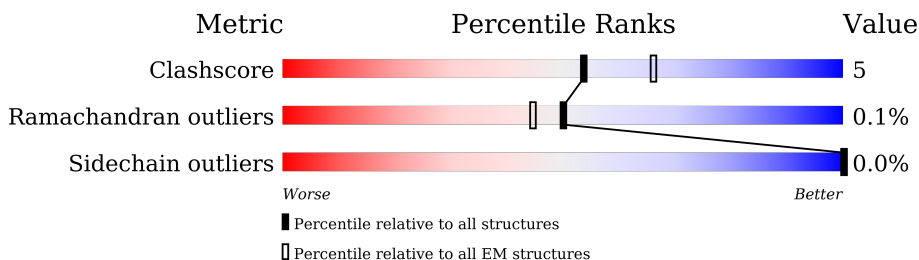
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.





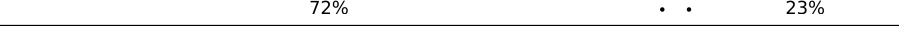
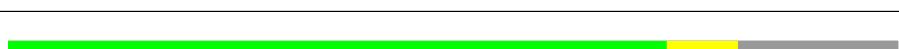



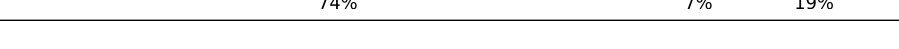



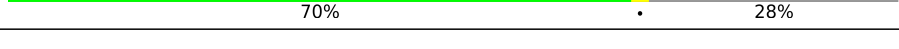

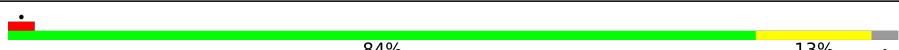


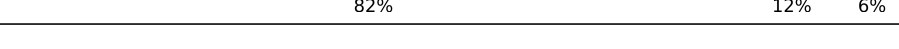







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	
1	a	353	
2	B	508	
2	b	508	
3	C	473	
3	c	473	
4	D	353	
4	d	353	





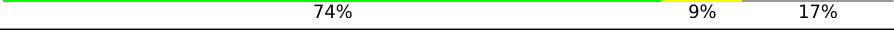
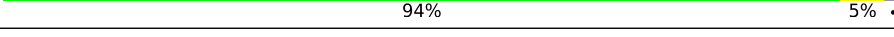

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Mol	Chain	Length	Quality of chain
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	g	267	
7	n	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	61	
11	k	61	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	
14	o	332	
15	S	280	
15	s	280	
16	T	33	

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Mol	Chain	Length	Quality of chain
16	t	33	
17	U	103	
17	u	103	
18	W	133	
18	w	133	
19	X	116	
19	x	116	
20	Y	265	
20	y	265	
21	Z	62	
21	z	62	
22	R	286	
22	r	286	

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
23	CLA	A	401	X	-	-	-
23	CLA	A	402	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	G	602	X	-	-	-
23	CLA	G	603	X	-	-	-
23	CLA	G	604	X	-	-	-
23	CLA	G	610	X	-	-	-
23	CLA	G	611	X	-	-	-
23	CLA	G	612	X	-	-	-
23	CLA	G	613	X	-	-	-
23	CLA	G	614	X	-	-	-
23	CLA	N	602	X	-	-	-
23	CLA	N	603	X	-	-	-
23	CLA	N	604	X	-	-	-
23	CLA	N	610	X	-	-	-
23	CLA	N	611	X	-	-	-
23	CLA	N	612	X	-	-	-
23	CLA	N	613	X	-	-	-
23	CLA	N	614	X	-	-	-
23	CLA	R	302	X	-	-	-
23	CLA	R	303	X	-	-	-
23	CLA	R	304	X	-	-	-
23	CLA	R	305	X	-	-	-
23	CLA	R	309	X	-	-	-
23	CLA	R	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	R	311	X	-	-	-
23	CLA	R	312	X	-	-	-
23	CLA	R	313	X	-	-	-
23	CLA	S	303	X	-	-	-
23	CLA	S	304	X	-	-	-
23	CLA	S	305	X	-	-	-
23	CLA	S	309	X	-	-	-
23	CLA	S	310	X	-	-	-
23	CLA	S	311	X	-	-	-
23	CLA	S	312	X	-	-	-
23	CLA	S	313	X	-	-	-
23	CLA	S	314	X	-	-	-
23	CLA	Y	303	X	-	-	-
23	CLA	Y	304	X	-	-	-
23	CLA	Y	305	X	-	-	-
23	CLA	Y	311	X	-	-	-
23	CLA	Y	312	X	-	-	-
23	CLA	Y	313	X	-	-	-
23	CLA	Y	314	X	-	-	-
23	CLA	Y	315	X	-	-	-
23	CLA	a	401	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	g	602	X	-	-	-
23	CLA	g	603	X	-	-	-
23	CLA	g	604	X	-	-	-
23	CLA	g	610	X	-	-	-
23	CLA	g	611	X	-	-	-
23	CLA	g	612	X	-	-	-
23	CLA	g	613	X	-	-	-
23	CLA	g	614	X	-	-	-
23	CLA	n	602	X	-	-	-
23	CLA	n	603	X	-	-	-
23	CLA	n	604	X	-	-	-
23	CLA	n	610	X	-	-	-
23	CLA	n	611	X	-	-	-
23	CLA	n	612	X	-	-	-
23	CLA	n	613	X	-	-	-
23	CLA	n	614	X	-	-	-
23	CLA	r	601	X	-	-	-
23	CLA	r	602	X	-	-	-
23	CLA	r	603	X	-	-	-
23	CLA	r	604	X	-	-	-
23	CLA	r	608	X	-	-	-
23	CLA	r	609	X	-	-	-
23	CLA	r	610	X	-	-	-
23	CLA	r	611	X	-	-	-
23	CLA	r	612	X	-	-	-
23	CLA	s	602	X	-	-	-
23	CLA	s	603	X	-	-	-
23	CLA	s	604	X	-	-	-
23	CLA	s	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	s	609	X	-	-	-
23	CLA	s	610	X	-	-	-
23	CLA	s	611	X	-	-	-
23	CLA	s	612	X	-	-	-
23	CLA	s	613	X	-	-	-
23	CLA	y	303	X	-	-	-
23	CLA	y	304	X	-	-	-
23	CLA	y	305	X	-	-	-
23	CLA	y	311	X	-	-	-
23	CLA	y	312	X	-	-	-
23	CLA	y	313	X	-	-	-
23	CLA	y	314	X	-	-	-
23	CLA	y	315	X	-	-	-
27	BCT	A	407	-	-	X	-
27	BCT	a	408	-	-	X	-
33	PL9	D	406	-	X	-	-
33	PL9	d	406	-	X	-	-
35	CHL	G	601	X	-	-	-
35	CHL	G	605	X	-	-	-
35	CHL	G	606	X	-	-	-
35	CHL	G	607	X	-	-	-
35	CHL	G	608	X	-	-	-
35	CHL	G	609	X	-	-	-
35	CHL	N	601	X	-	-	-
35	CHL	N	605	X	-	-	-
35	CHL	N	606	X	-	-	-
35	CHL	N	607	X	-	-	-
35	CHL	N	608	X	-	-	-
35	CHL	N	609	X	-	-	-
35	CHL	R	306	X	-	-	-
35	CHL	R	307	X	-	-	-
35	CHL	R	308	X	-	-	-
35	CHL	S	302	X	-	-	-
35	CHL	S	306	X	-	-	-
35	CHL	S	307	X	-	-	-
35	CHL	S	308	X	-	-	-
35	CHL	Y	302	X	-	-	-
35	CHL	Y	306	X	-	-	-
35	CHL	Y	307	X	-	-	-
35	CHL	Y	308	X	-	-	-
35	CHL	Y	309	X	-	-	-
35	CHL	Y	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CHL	g	601	X	-	-	-
35	CHL	g	605	X	-	-	-
35	CHL	g	606	X	-	-	-
35	CHL	g	607	X	-	-	-
35	CHL	g	608	X	-	-	-
35	CHL	g	609	X	-	-	-
35	CHL	n	601	X	-	-	-
35	CHL	n	605	X	-	-	-
35	CHL	n	606	X	-	-	-
35	CHL	n	607	X	-	-	-
35	CHL	n	608	X	-	-	-
35	CHL	n	609	X	-	-	-
35	CHL	r	605	X	-	-	-
35	CHL	r	606	X	-	-	-
35	CHL	r	607	X	-	-	-
35	CHL	s	601	X	-	-	-
35	CHL	s	605	X	-	-	-
35	CHL	s	606	X	-	-	-
35	CHL	s	607	X	-	-	-
35	CHL	y	302	X	-	-	-
35	CHL	y	306	X	-	-	-
35	CHL	y	307	X	-	-	-
35	CHL	y	308	X	-	-	-
35	CHL	y	309	X	-	-	-
35	CHL	y	310	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 71232 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	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		
1	a	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		
2	b	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		
3	c	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		
4	d	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	71	Total	C	N	O	0	0
			576	377	93	106		
5	e	71	Total	C	N	O	0	0
			576	377	93	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			235	156	41	37	1		
6	f	30	Total	C	N	O	S	0	0
			235	156	41	37	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
8	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			277	190	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	29	Total	C	N	O	0	0
			219	152	33	34		
10	j	29	Total	C	N	O	0	0
			219	152	33	34		

- 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	S	0	0
			301	211	44	45	1		
11	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			309	204	48	57		
12	l	37	Total	C	N	O	0	0
			309	204	48	57		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			250	172	36	42		
13	m	32	Total	C	N	O	0	0
			250	172	36	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		
14	o	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	23	Total	C	N	O	S	0	0
			179	114	31	31	3		
17	u	23	Total	C	N	O	S	0	0
			179	114	31	31	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
18	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 19 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	38	Total	C	N	O	0	0
			267	176	42	49		
19	x	38	Total	C	N	O	0	0
			267	176	42	49		

- Molecule 20 is a protein called Chlorophyll a-b binding protein 2.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		
20	y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
21	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

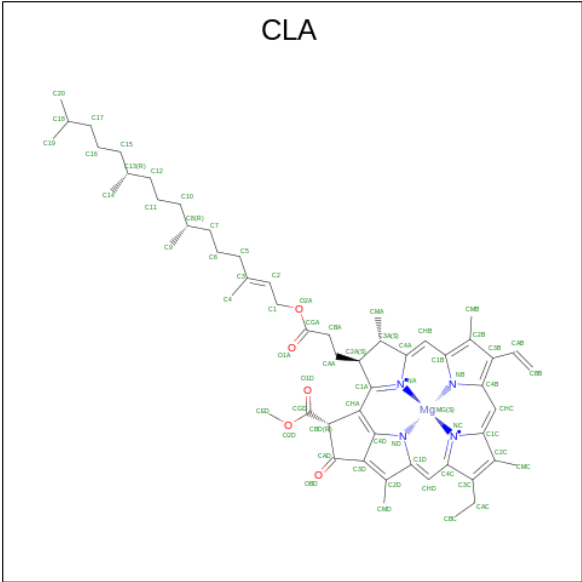
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		
22	R	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	277	GLY	-	expression tag	UNP Q9S7W1
r	278	GLY	-	expression tag	UNP Q9S7W1
r	279	GLY	-	expression tag	UNP Q9S7W1
r	280	GLY	-	expression tag	UNP Q9S7W1
r	281	HIS	-	expression tag	UNP Q9S7W1
r	282	HIS	-	expression tag	UNP Q9S7W1
r	283	HIS	-	expression tag	UNP Q9S7W1
r	284	HIS	-	expression tag	UNP Q9S7W1
r	285	HIS	-	expression tag	UNP Q9S7W1
r	286	HIS	-	expression tag	UNP Q9S7W1
R	277	GLY	-	expression tag	UNP Q9S7W1
R	278	GLY	-	expression tag	UNP Q9S7W1
R	279	GLY	-	expression tag	UNP Q9S7W1
R	280	GLY	-	expression tag	UNP Q9S7W1
R	281	HIS	-	expression tag	UNP Q9S7W1
R	282	HIS	-	expression tag	UNP Q9S7W1
R	283	HIS	-	expression tag	UNP Q9S7W1
R	284	HIS	-	expression tag	UNP Q9S7W1
R	285	HIS	-	expression tag	UNP Q9S7W1
R	286	HIS	-	expression tag	UNP Q9S7W1

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	C	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	N	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	Y	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	g	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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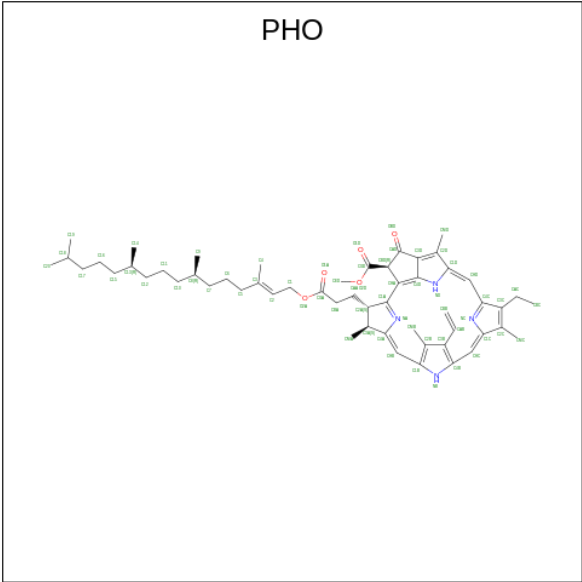
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	n	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	y	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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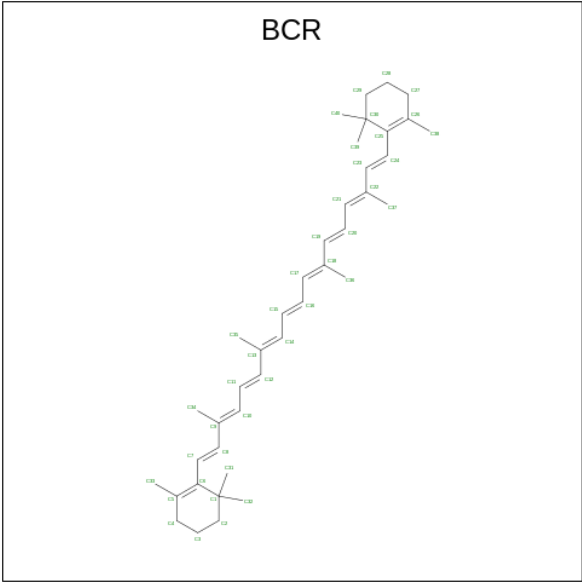
Mol	Chain	Residues	Atoms					AltConf
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



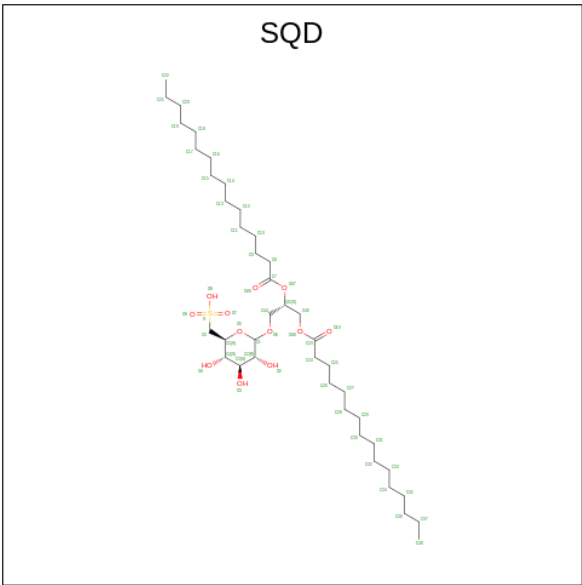
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



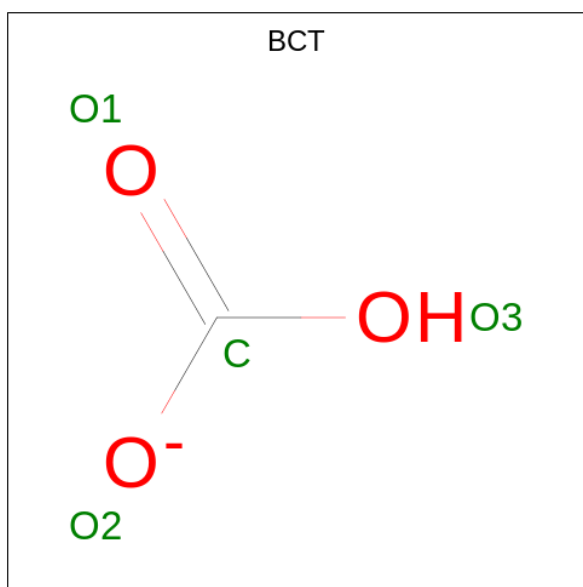
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



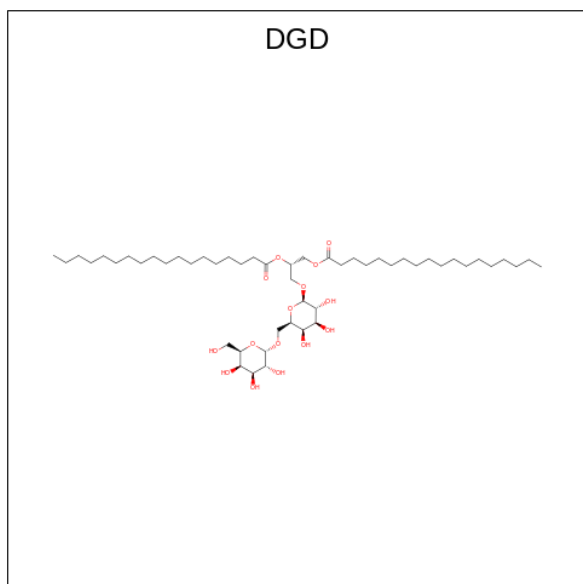
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	C	1	Total	C	O	S	0
			45	32	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			50	37	12	1	
26	b	1	Total	C	O	S	0
			54	41	12	1	
26	c	1	Total	C	O	S	0
			45	32	12	1	
26	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			4	1	3	
27	a	1	Total	C	O	0
			4	1	3	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			59	44	15	

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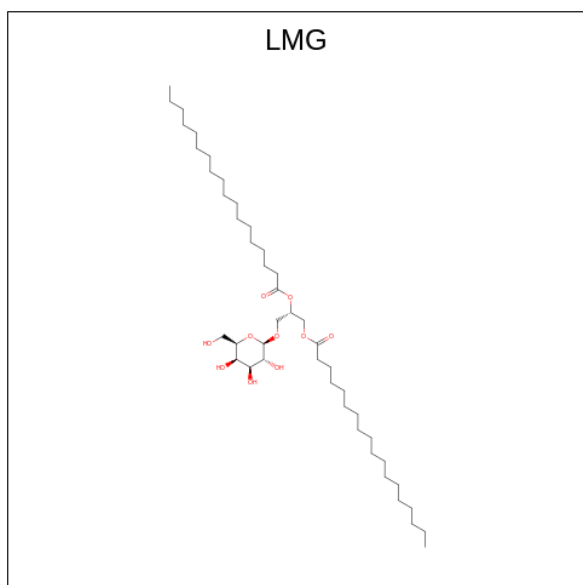
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Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			59	44	15	
28	B	1	Total	C	O	0
			56	41	15	
28	C	1	Total	C	O	0
			55	40	15	
28	D	1	Total	C	O	0
			62	47	15	
28	b	1	Total	C	O	0
			56	41	15	
28	c	1	Total	C	O	0
			55	40	15	
28	d	1	Total	C	O	0
			62	47	15	

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

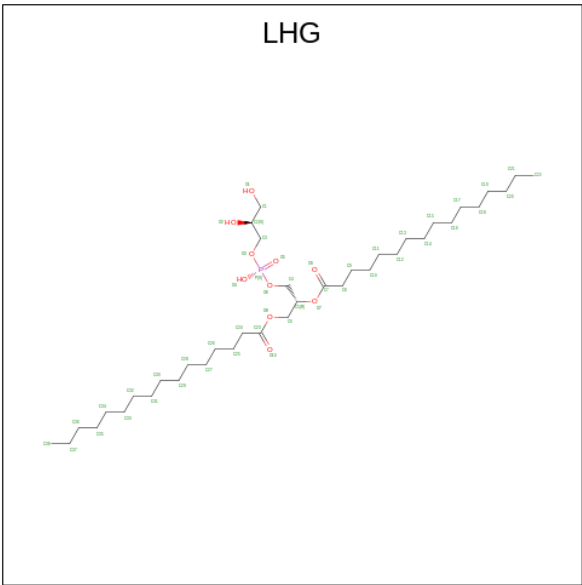
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Fe	0
			1	1	
29	a	1	Total	Fe	0
			1	1	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	B	1	Total	C	O	0
			40	30	10	
30	C	1	Total	C	O	0
			48	38	10	
30	C	1	Total	C	O	0
			50	40	10	
30	D	1	Total	C	O	0
			46	36	10	
30	S	1	Total	C	O	0
			55	45	10	
30	W	1	Total	C	O	0
			51	41	10	
30	a	1	Total	C	O	0
			48	38	10	
30	b	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			50	40	10	
30	d	1	Total	C	O	0
			46	36	10	
30	s	1	Total	C	O	0
			55	45	10	
30	w	1	Total	C	O	0
			51	41	10	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



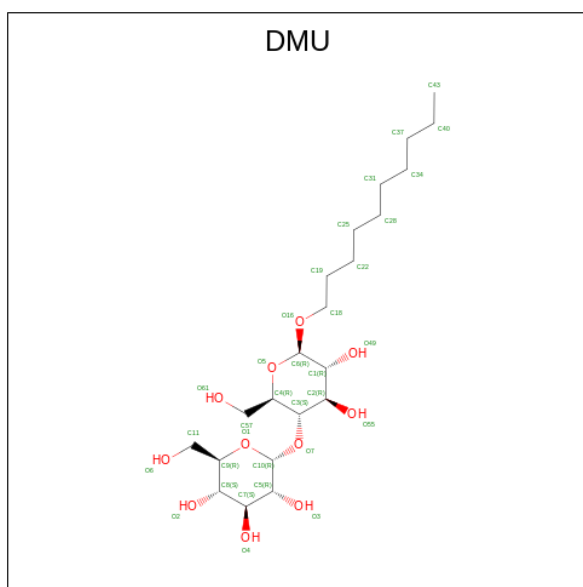
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	P	0
			49	38	10	1	
31	B	1	Total	C	O	P	0
			46	35	10	1	
31	B	1	Total	C	O	P	0
			40	29	10	1	
31	C	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	G	1	Total	C	O	P	0
			46	35	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	N	1	Total	C	O	P	0
			49	38	10	1	
31	S	1	Total	C	O	P	0
			49	38	10	1	
31	W	1	Total	C	O	P	0
			49	38	10	1	
31	Y	1	Total	C	O	P	0
			49	38	10	1	
31	b	1	Total	C	O	P	0
			49	38	10	1	

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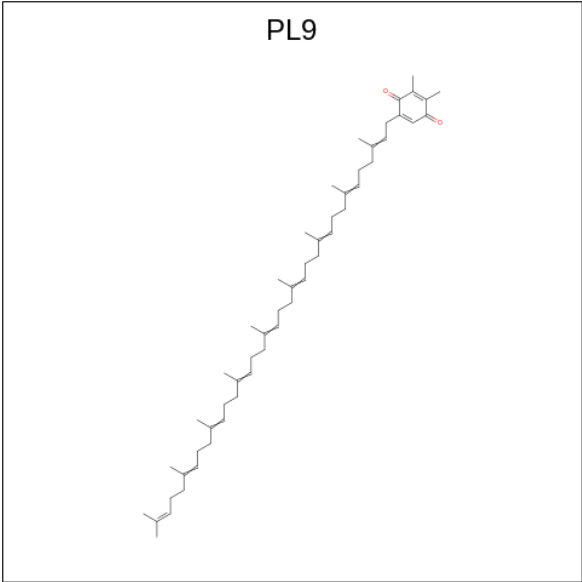
Mol	Chain	Residues	Atoms				AltConf
31	b	1	Total	C	O	P	0
			46	35	10	1	
31	b	1	Total	C	O	P	0
			40	29	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	g	1	Total	C	O	P	0
			46	35	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	r	1	Total	C	O	P	0
			42	31	10	1	
31	s	1	Total	C	O	P	0
			49	38	10	1	
31	n	1	Total	C	O	P	0
			49	38	10	1	
31	y	1	Total	C	O	P	0
			49	38	10	1	
31	R	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 32 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



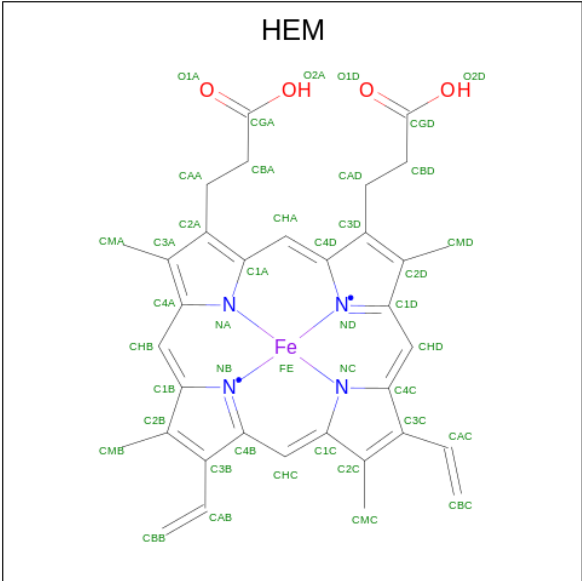
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			33	22	11	
32	C	1	Total	C	O	0
			33	22	11	
32	S	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	s	1	Total	C	O	0
			33	22	11	

- Molecule 33 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
33	D	1	Total	C	O	0
			55	53	2	
33	d	1	Total	C	O	0
			55	53	2	

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



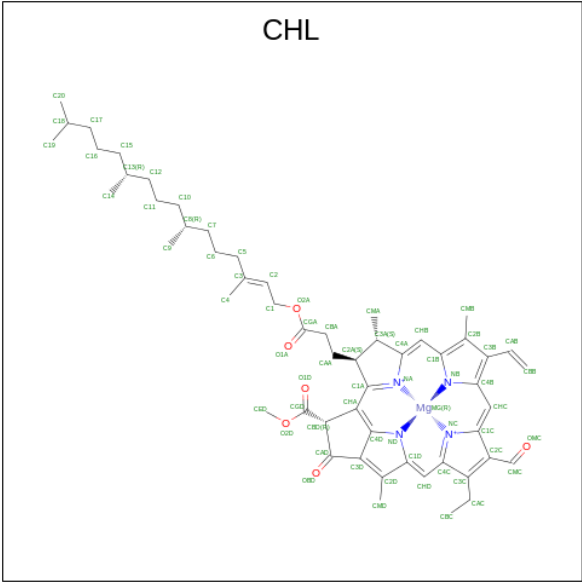
Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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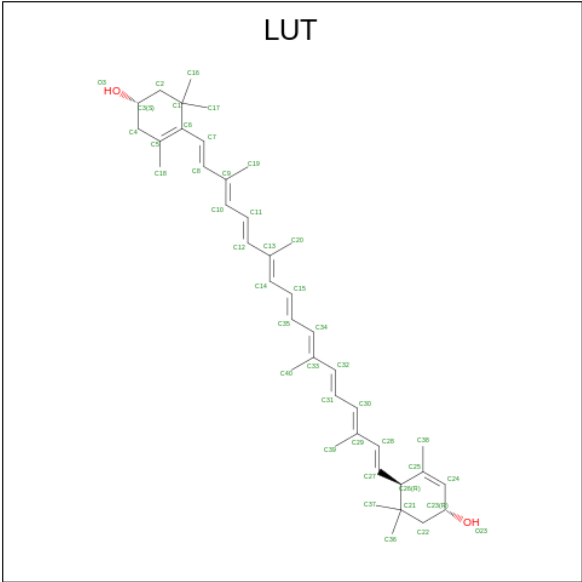
Mol	Chain	Residues	Atoms					AltConf
35	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
35	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
35	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	r	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
35	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



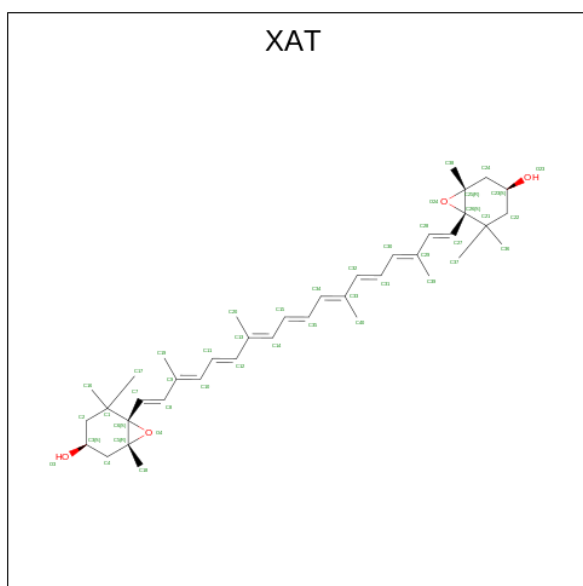
Mol	Chain	Residues	Atoms			AltConf
36	G	1	Total	C	O	0
			42	40	2	
36	G	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
36	n	1	Total	C	O	0
			42	40	2	
36	y	1	Total	C	O	0
			42	40	2	
36	y	1	Total	C	O	0
			42	40	2	
36	R	1	Total	C	O	0
			42	40	2	

- Molecule 37 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) (labeled as "Ligand of Interest" by depositor).



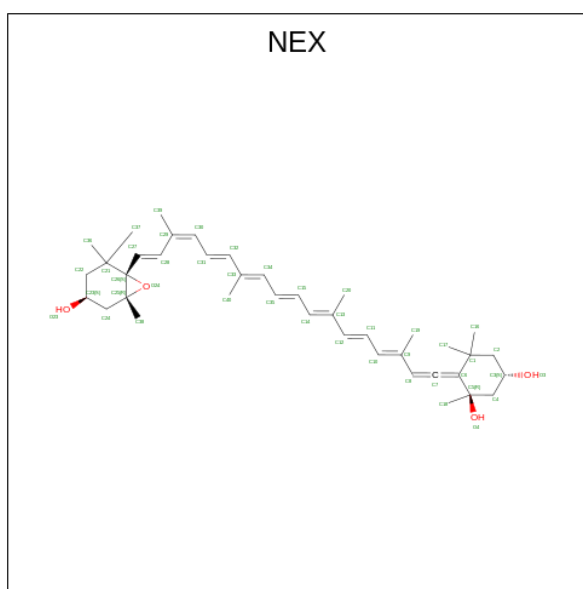
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	40	4	
37	G	1	Total	C	O	0
			44	40	4	
37	Y	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
37	y	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	

- Molecule 38 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-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



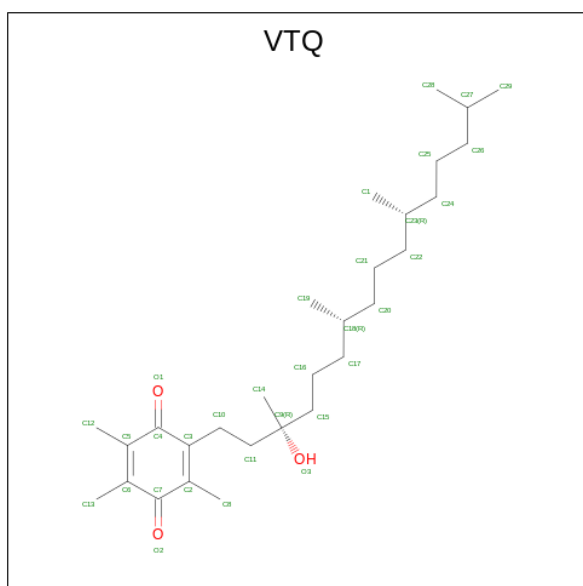
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			44	40	4	
38	N	1	Total	C	O	0
			44	40	4	
38	S	1	Total	C	O	0
			44	40	4	
38	Y	1	Total	C	O	0
			44	40	4	
38	g	1	Total	C	O	0
			44	40	4	
38	r	1	Total	C	O	0
			44	40	4	
38	s	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
38	n	1	Total	C	O	0
			44	40	4	
38	R	1	Total	C	O	0
			44	40	4	
38	R	1	Total	C	O	0
			44	40	4	

- Molecule 39 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula: $C_{29}H_{50}O_3$).

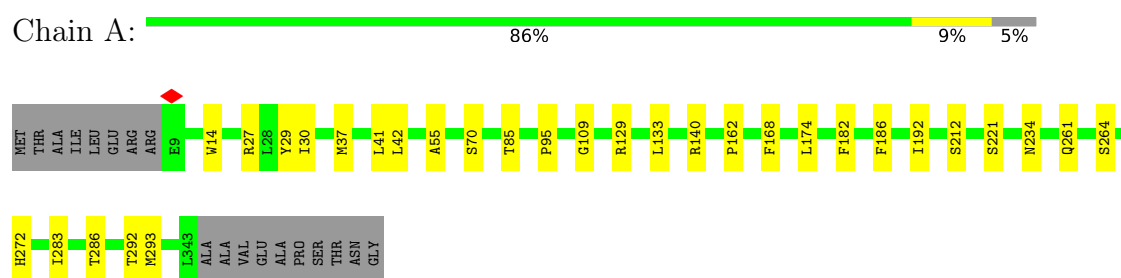


Mol	Chain	Residues	Atoms			AltConf
39	W	1	Total	C	O	0
			32	29	3	
39	w	1	Total	C	O	0
			32	29	3	

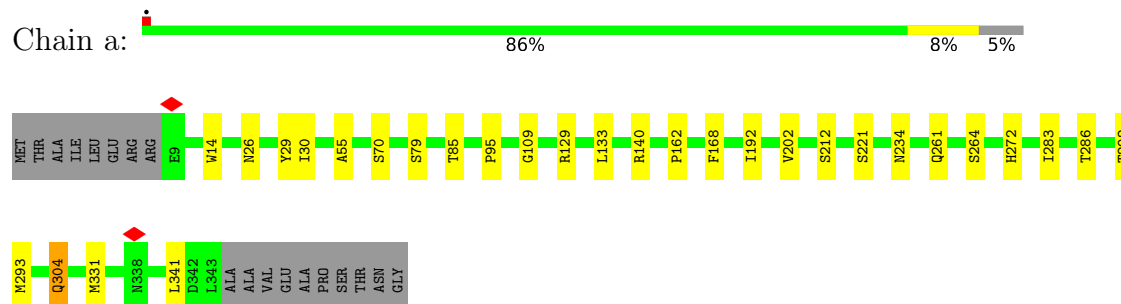
3 Residue-property plots

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

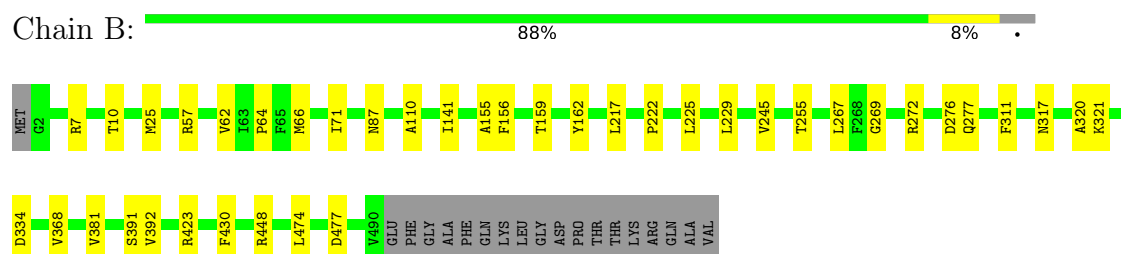
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

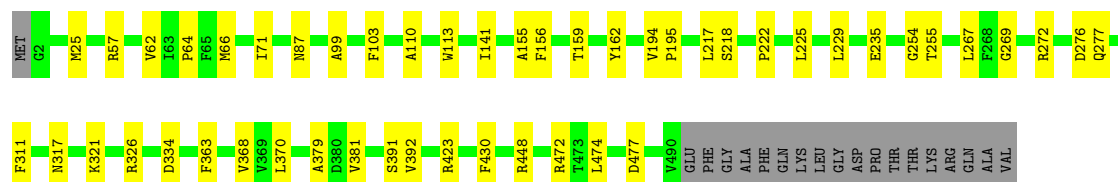


- Molecule 2: Photosystem II CP47 reaction center protein



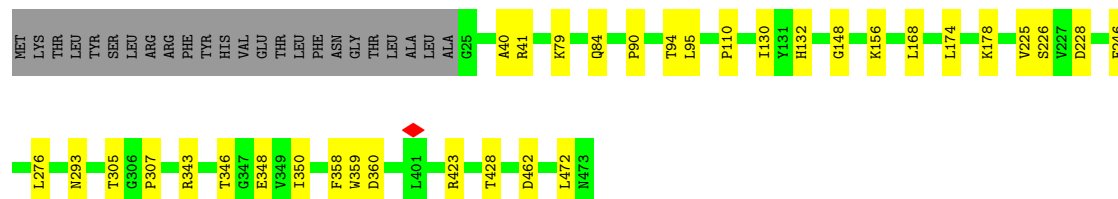
- Molecule 2: Photosystem II CP47 reaction center protein





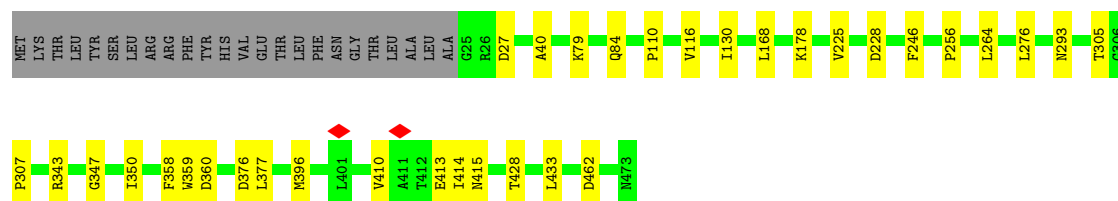
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 7% 5%



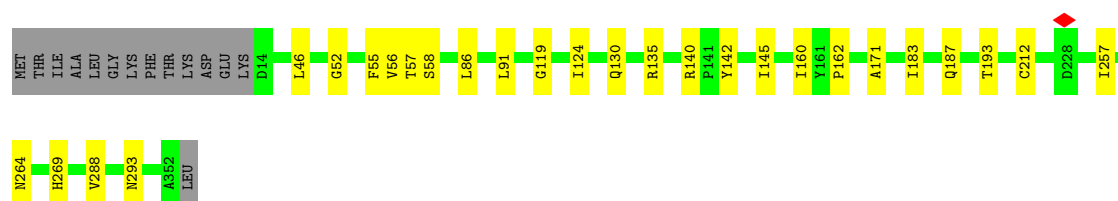
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 7% 5%



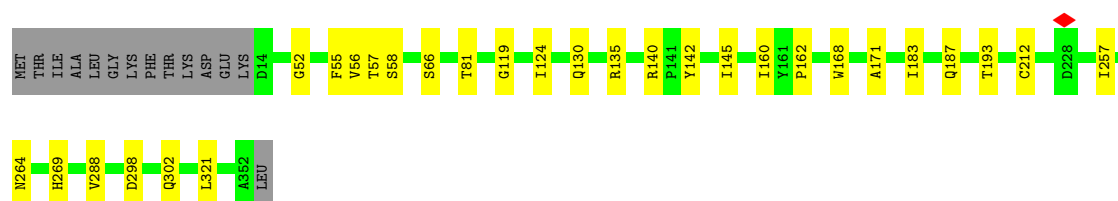
- Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .

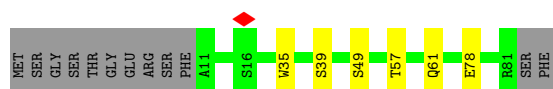
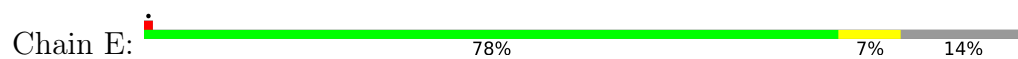


- Molecule 4: Photosystem II D2 protein

Chain d: 88% 8% .



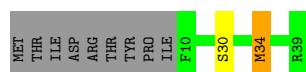
- Molecule 5: Cytochrome b559 subunit alpha



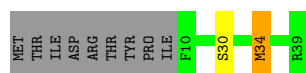
- Molecule 5: Cytochrome b559 subunit alpha



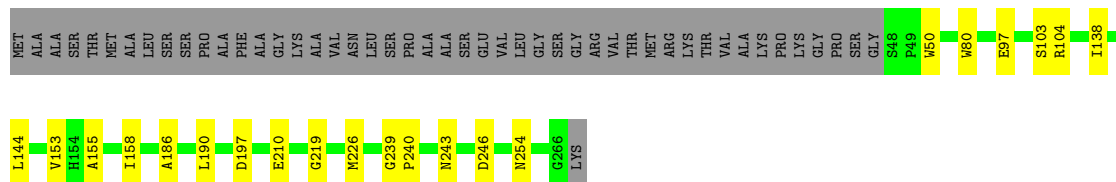
- Molecule 6: Cytochrome b559 subunit beta



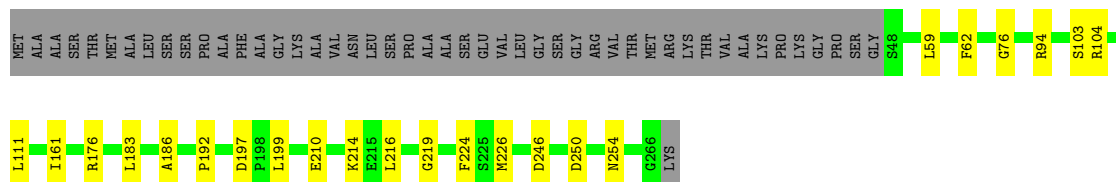
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

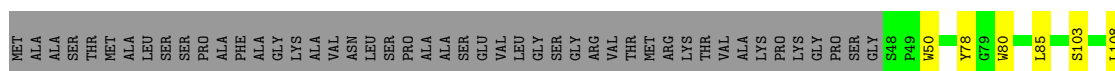


- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic



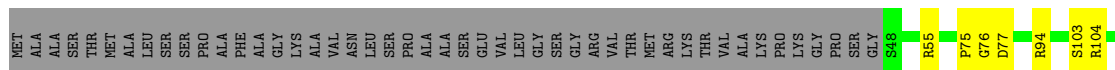
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic





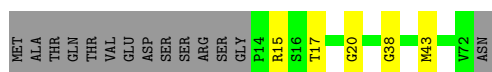
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain n: 73% 9% 18%



- Molecule 8: Photosystem II reaction center protein H

Chain H: 74% 7% 19%



- Molecule 8: Photosystem II reaction center protein H

Chain h: 67% 14% 19%



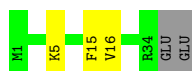
- Molecule 9: Photosystem II reaction center protein I

Chain I: 86% 8% 6%



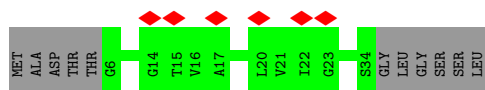
- Molecule 9: Photosystem II reaction center protein I

Chain i: 86% 8% 6%

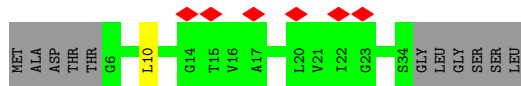


- Molecule 10: Photosystem II reaction center protein J

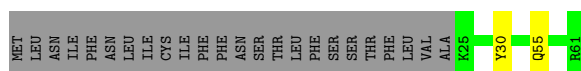
Chain J: 15% 72% 28%



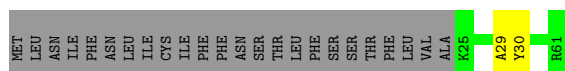
- Molecule 10: Photosystem II reaction center protein J



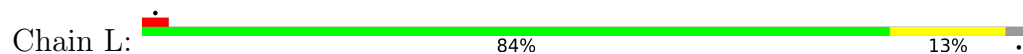
- Molecule 11: Photosystem II reaction center protein K



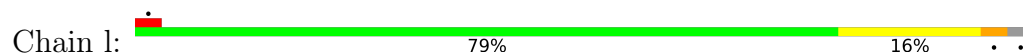
- Molecule 11: Photosystem II reaction center protein K



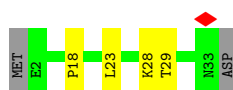
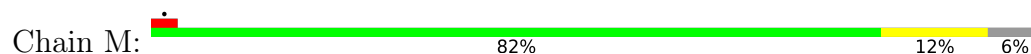
- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein M



- Molecule 13: Photosystem II reaction center protein M

Diagram illustrating the structure of the E2 domain of the E2F1 protein. The residues shown are MET, E2, P18, V27, K28, T29, N33, and ASP.

- Chain O:  53% 6% 40%

[illegible]

- Chain o:

[illegible]

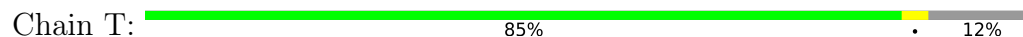
- Chain S:

- Chain s: 1% 71% 8% 21%

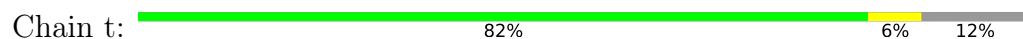
[illegible]



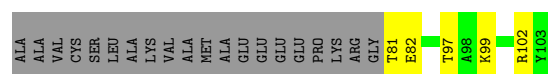
- Molecule 16: Photosystem II reaction center protein T



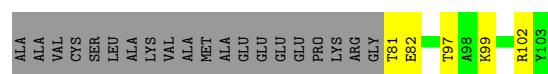
- Molecule 16: Photosystem II reaction center protein T



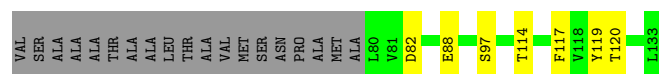
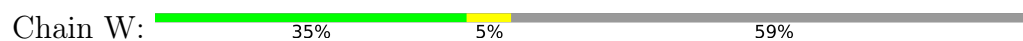
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic



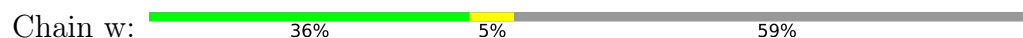
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic

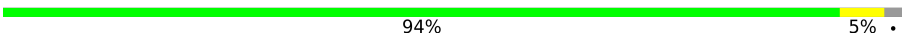


- Molecule 18: Photosystem II reaction center W protein, chloroplastic



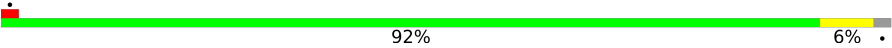
- Molecule 18: Photosystem II reaction center W protein, chloroplastic

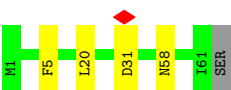


Chain Z:  94% 5% .



• Molecule 21: Photosystem II reaction center protein Z

Chain z:  92% 6% .



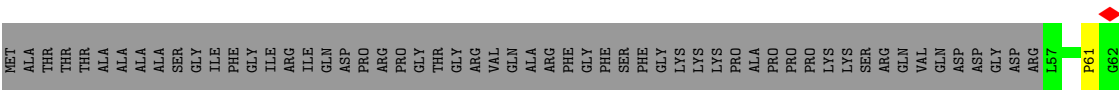
• Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain r:  72% 5% 23%



• Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain R:  71% 6% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.356	Depositor
Minimum map value	-16.319	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	3	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/2704	0.54	0/3687
1	a	0.27	0/2704	0.56	1/3687 (0.0%)
2	B	0.22	0/3959	0.44	0/5394
2	b	0.22	0/3959	0.46	0/5394
3	C	0.23	0/3595	0.49	0/4899
3	c	0.23	0/3595	0.49	0/4899
4	D	0.24	0/2789	0.51	0/3803
4	d	0.24	0/2789	0.49	0/3803
5	E	0.30	0/593	0.79	1/808 (0.1%)
5	e	0.30	0/593	0.84	4/808 (0.5%)
6	F	0.31	0/241	0.78	2/327 (0.6%)
6	f	0.32	0/241	0.81	1/327 (0.3%)
7	G	0.23	0/1716	0.47	1/2336 (0.0%)
7	N	0.23	0/1716	0.47	0/2336
7	g	0.25	0/1716	0.55	1/2336 (0.0%)
7	n	0.22	0/1716	0.44	0/2336
8	H	0.29	0/447	0.52	0/608
8	h	0.30	0/447	0.58	0/608
9	I	0.28	0/285	0.58	0/385
9	i	0.28	0/285	0.56	0/385
10	J	0.23	0/225	0.43	0/306
10	j	0.23	0/225	0.42	0/306
11	K	0.47	0/312	0.86	0/428
11	k	0.44	0/312	0.89	0/428
12	L	0.23	0/317	0.52	0/431
12	l	0.29	0/317	0.62	0/431
13	M	0.41	0/254	0.69	0/348
13	m	0.35	0/254	0.71	0/348
14	O	0.23	0/1556	0.62	4/2104 (0.2%)
14	o	0.26	0/1556	0.66	4/2104 (0.2%)
15	S	0.26	0/1750	0.57	0/2376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	s	0.25	0/1750	0.54	0/2376
16	T	0.23	0/246	0.53	0/333
16	t	0.29	0/246	0.65	0/333
17	U	0.13	0/181	0.39	0/242
17	u	0.12	0/181	0.40	0/242
18	W	0.24	0/438	0.54	0/594
18	w	0.22	0/438	0.47	0/594
19	X	0.25	0/270	0.48	0/367
19	x	0.25	0/270	0.49	0/367
20	Y	0.23	0/1753	0.51	0/2385
20	y	0.23	0/1753	0.51	0/2385
21	Z	0.30	0/468	0.64	0/641
21	z	0.33	0/468	0.71	0/641
22	R	0.25	0/1766	0.58	0/2403
22	r	0.23	0/1766	0.52	0/2403
All	All	0.25	0/55162	0.54	19/75082 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	34	MET	CB-CG-SD	-6.43	93.41	112.70
14	O	311	THR	CA-C-N	6.36	133.69	121.54
14	O	311	THR	C-N-CA	6.36	133.69	121.54
14	o	311	THR	CA-C-N	6.21	133.40	121.54
14	o	311	THR	C-N-CA	6.21	133.40	121.54
7	g	173	GLU	CA-CB-CG	6.12	126.34	114.10
5	e	78	GLU	N-CA-CB	6.09	119.77	110.44
5	e	78	GLU	CA-CB-CG	5.96	126.01	114.10
5	E	78	GLU	N-CA-CB	5.93	120.08	110.40
7	G	197	ASP	CB-CA-C	5.85	120.27	111.14
6	F	34	MET	CA-CB-CG	5.71	125.52	114.10
5	e	77	ASP	CA-C-N	-5.62	112.21	122.38
5	e	77	ASP	C-N-CA	-5.62	112.21	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	218	LEU	CA-C-N	5.59	132.21	121.54
14	O	218	LEU	C-N-CA	5.59	132.21	121.54
14	o	218	LEU	CA-C-N	5.50	132.06	121.54
14	o	218	LEU	C-N-CA	5.50	132.06	121.54
1	a	304	GLN	CA-CB-CG	5.47	125.05	114.10
6	F	34	MET	CB-CG-SD	-5.05	97.54	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	413	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2527	22	0
1	a	2623	0	2527	24	0
2	B	3829	0	3707	30	0
2	b	3829	0	3707	36	0
3	C	3480	0	3409	27	0
3	c	3480	0	3409	28	0
4	D	2696	0	2585	22	0
4	d	2696	0	2585	25	0
5	E	576	0	559	3	0
5	e	576	0	559	4	0
6	F	235	0	242	1	0
6	f	235	0	242	1	0
7	G	1666	0	1593	12	0
7	N	1666	0	1593	19	0
7	g	1666	0	1593	12	0
7	n	1666	0	1593	18	0
8	H	438	0	465	4	0
8	h	438	0	465	8	0
9	I	277	0	289	3	0
9	i	277	0	289	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	219	0	231	0	0
10	j	219	0	231	1	0
11	K	301	0	313	2	0
11	k	301	0	313	2	0
12	L	309	0	298	5	0
12	l	309	0	298	6	0
13	M	250	0	273	5	0
13	m	250	0	273	4	0
14	O	1523	0	1504	11	0
14	o	1523	0	1504	12	0
15	S	1705	0	1681	14	0
15	s	1705	0	1681	15	0
16	T	239	0	255	1	0
16	t	239	0	255	2	0
17	U	179	0	190	3	0
17	u	179	0	190	3	0
18	W	427	0	405	6	0
18	w	427	0	405	5	0
19	X	267	0	292	0	0
19	x	267	0	292	1	0
20	Y	1699	0	1630	17	0
20	y	1699	0	1630	17	0
21	Z	458	0	490	2	0
21	z	458	0	490	4	0
22	R	1718	0	1691	13	0
22	r	1718	0	1691	11	0
23	A	175	0	170	6	0
23	B	1040	0	1152	23	0
23	C	810	0	854	21	0
23	D	195	0	216	9	0
23	G	448	0	429	9	0
23	N	435	0	396	7	0
23	R	511	0	493	11	0
23	S	415	0	313	8	0
23	Y	466	0	454	15	0
23	a	125	0	131	5	0
23	b	1040	0	1152	22	0
23	c	810	0	854	16	0
23	d	245	0	255	8	0
23	g	448	0	429	9	0
23	n	435	0	396	8	0
23	r	511	0	493	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	s	415	0	313	6	0
23	y	466	0	454	12	0
24	A	64	0	74	3	0
24	D	64	0	74	5	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	120	0	168	10	0
25	D	40	0	56	1	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	a	40	0	56	4	0
25	b	120	0	168	11	0
25	c	80	0	112	6	0
25	d	40	0	56	1	0
25	h	40	0	56	2	0
25	k	40	0	56	3	0
25	z	40	0	56	2	0
26	A	50	0	67	0	0
26	B	54	0	78	3	0
26	C	45	0	54	2	0
26	L	54	0	78	1	0
26	a	50	0	67	2	0
26	b	54	0	78	3	0
26	c	45	0	54	1	0
26	l	54	0	78	4	0
27	A	4	0	0	2	0
27	a	4	0	0	2	0
28	A	59	0	76	1	0
28	B	115	0	146	4	0
28	C	55	0	68	2	0
28	D	62	0	82	3	0
28	b	56	0	70	0	0
28	c	55	0	68	2	0
28	d	62	0	82	5	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	91	0	122	6	0
30	C	98	0	139	2	0
30	D	46	0	62	1	0
30	S	55	0	86	0	0
30	W	51	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	48	0	66	0	0
30	b	91	0	122	6	0
30	c	50	0	73	0	0
30	d	46	0	62	0	0
30	s	55	0	86	0	0
30	w	51	0	75	0	0
31	B	135	0	192	3	0
31	C	49	0	74	2	0
31	D	98	0	148	4	0
31	G	46	0	65	2	0
31	L	98	0	148	4	0
31	N	49	0	74	2	0
31	R	42	0	57	1	0
31	S	49	0	74	3	0
31	W	49	0	74	1	0
31	Y	49	0	74	3	0
31	b	135	0	192	3	0
31	c	98	0	148	2	0
31	d	98	0	148	7	0
31	g	46	0	65	4	0
31	l	98	0	148	3	0
31	n	49	0	74	1	0
31	r	42	0	57	1	0
31	s	49	0	74	2	0
31	y	49	0	74	3	0
32	C	66	0	84	2	0
32	S	33	0	42	1	0
32	c	66	0	84	2	0
32	s	33	0	42	1	0
33	D	55	0	80	2	0
33	d	55	0	80	0	0
34	F	43	0	30	1	0
34	f	43	0	30	1	0
35	G	325	0	286	7	0
35	N	338	0	305	9	0
35	R	153	0	119	2	0
35	S	184	0	125	5	0
35	Y	365	0	354	13	0
35	g	325	0	286	8	0
35	n	338	0	305	11	0
35	r	153	0	119	2	0
35	s	184	0	125	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	y	365	0	354	15	0
36	G	84	0	112	6	0
36	N	84	0	112	9	0
36	R	42	0	56	4	0
36	S	84	0	112	6	0
36	Y	84	0	112	7	0
36	g	84	0	112	5	0
36	n	84	0	112	7	0
36	r	42	0	56	3	0
36	s	84	0	112	4	0
36	y	84	0	112	7	0
37	G	88	0	112	4	0
37	R	44	0	56	1	0
37	Y	44	0	56	5	0
37	g	88	0	112	6	0
37	r	44	0	56	2	0
37	y	44	0	56	6	0
38	G	44	0	56	1	0
38	N	44	0	56	3	0
38	R	88	0	112	6	0
38	S	44	0	56	1	0
38	Y	44	0	56	1	0
38	g	44	0	56	1	0
38	n	44	0	56	1	0
38	r	44	0	56	1	0
38	s	44	0	56	1	0
39	W	32	0	50	0	0
39	w	32	0	50	0	0
All	All	71232	0	71854	714	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:311:CLA:HAB	36:Y:316:LUT:H32	1.62	0.80
3:c:276:LEU:HD21	23:c:508:CLA:HAB	1.69	0.75
23:s:609:CLA:HAB	36:s:614:LUT:H32	1.70	0.74
3:C:276:LEU:HD21	23:C:509:CLA:HAB	1.69	0.74
23:n:602:CLA:HAB	36:n:616:LUT:H32	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:514:CLA:HBB1	25:C:515:BCR:H24C	1.70	0.73
23:n:610:CLA:HAB	36:n:615:LUT:H32	1.69	0.73
35:G:601:CHL:H52	35:Y:310:CHL:HBB1	1.69	0.73
7:n:226:MET:HE2	36:n:616:LUT:H10	1.70	0.73
23:y:311:CLA:HAB	36:y:316:LUT:H32	1.71	0.72
15:S:236:MET:HE1	36:S:316:LUT:H10	1.72	0.72
23:c:513:CLA:HBB1	25:z:101:BCR:H24C	1.71	0.72
23:G:610:CLA:HAB	36:G:615:LUT:H32	1.72	0.70
23:S:310:CLA:HAB	36:S:315:LUT:H32	1.75	0.68
20:y:213:GLU:OE1	23:y:311:CLA:NB	2.27	0.68
22:R:61:PRO:HG3	23:R:302:CLA:H3A	1.76	0.68
20:Y:213:GLU:OE1	23:Y:311:CLA:NB	2.27	0.67
6:F:30:SER:O	6:F:34:MET:HB3	1.95	0.67
2:b:254:GLY:HA3	28:d:410:DGD:HB51	1.77	0.66
23:A:402:CLA:HAB	23:D:403:CLA:H72	1.78	0.66
35:g:601:CHL:H52	35:y:310:CHL:HBB1	1.79	0.65
7:n:183:LEU:HD13	35:n:608:CHL:HAB	1.79	0.64
7:N:183:LEU:HD13	35:N:608:CHL:HAB	1.79	0.63
20:Y:224:MET:HE2	36:Y:317:LUT:H10	1.80	0.62
23:g:610:CLA:HAB	36:g:615:LUT:H32	1.80	0.62
22:r:61:PRO:HG3	23:r:601:CLA:H3A	1.82	0.61
1:A:272:HIS:CE1	27:A:407:BCT:O3	2.52	0.61
2:B:277:GLN:HB3	17:U:99:LYS:HG3	1.82	0.61
3:c:178:LYS:HB2	23:c:502:CLA:H172	1.83	0.61
37:Y:301:XAT:H32	31:Y:319:LHG:H191	1.82	0.60
2:b:225:LEU:O	2:b:229:LEU:HB2	2.01	0.60
1:a:272:HIS:CE1	27:a:408:BCT:O3	2.53	0.60
12:L:13:LEU:H	13:M:29:THR:HG21	1.67	0.60
20:y:224:MET:HE2	36:y:317:LUT:H10	1.84	0.59
1:a:331:MET:HE2	4:d:321:LEU:HB3	1.83	0.59
8:h:29:GLU:HB2	8:h:32:LYS:HG3	1.85	0.59
1:a:304:GLN:NE2	3:c:415:ASN:OD1	2.35	0.59
37:y:301:XAT:H32	31:y:318:LHG:H191	1.85	0.59
4:D:119:GLY:HA3	24:D:402:PHO:H92	1.85	0.58
7:G:144:LEU:HB3	7:G:155:ALA:HB3	1.85	0.58
7:G:226:MET:HG2	36:G:616:LUT:H12	1.85	0.58
23:N:610:CLA:HAB	36:N:615:LUT:H32	1.84	0.58
23:g:602:CLA:H102	23:y:304:CLA:H41	1.86	0.58
37:G:617:XAT:H222	35:N:601:CHL:HMC	1.86	0.58
31:D:407:LHG:H291	16:T:17:ILE:HG23	1.86	0.57
7:N:226:MET:HG2	36:N:616:LUT:H12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:y:137:ILE:HG21	20:y:157:ILE:HD13	1.86	0.57
23:b:614:CLA:H8	23:b:615:CLA:HAB	1.87	0.57
24:a:403:PHO:H92	4:d:119:GLY:HA3	1.87	0.57
7:n:76:GLY:HA3	7:n:216:LEU:HD23	1.87	0.57
27:a:408:BCT:O2	4:d:269:HIS:CE1	2.57	0.57
2:b:391:SER:OG	2:b:392:VAL:N	2.38	0.57
15:s:236:MET:HG2	36:s:615:LUT:H14	1.87	0.57
23:B:612:CLA:H8	23:B:613:CLA:HAB	1.87	0.56
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.88	0.56
23:c:513:CLA:H101	25:z:101:BCR:H23C	1.87	0.56
1:A:212:SER:HB2	4:D:212:CYS:HB2	1.87	0.56
31:d:407:LHG:H311	16:t:21:ILE:HD11	1.85	0.56
35:G:601:CHL:HMC	37:G:620:XAT:H242	1.88	0.56
27:A:407:BCT:O2	4:D:269:HIS:CE1	2.57	0.56
35:g:601:CHL:HMC	37:g:620:XAT:H242	1.88	0.56
3:C:178:LYS:HB2	23:C:503:CLA:H172	1.86	0.56
7:N:246:ASP:O	7:N:254:ASN:ND2	2.38	0.56
23:C:514:CLA:H101	25:C:515:BCR:H23C	1.88	0.56
7:G:239:GLY:O	7:G:243:ASN:ND2	2.39	0.56
23:B:608:CLA:HAB	4:D:124:ILE:HG23	1.87	0.55
2:B:141:ILE:HG13	2:B:217:LEU:HD21	1.89	0.55
37:g:617:XAT:H222	35:n:601:CHL:HMC	1.88	0.55
14:o:146:LYS:HE3	14:o:320:ASP:H	1.72	0.55
7:n:246:ASP:O	7:n:254:ASN:ND2	2.38	0.55
2:b:269:GLY:O	2:b:448:ARG:NH1	2.40	0.55
31:d:407:LHG:H291	16:t:17:ILE:HG23	1.87	0.55
23:A:404:CLA:H3A	30:C:501:LMG:H122	1.88	0.55
8:H:17:THR:HG23	8:H:20:GLY:H	1.70	0.55
22:R:208:ASN:HA	22:R:216:ARG:HE	1.71	0.55
1:a:212:SER:HB2	4:d:212:CYS:HB2	1.88	0.55
7:G:103:SER:HB2	7:G:219:GLY:HA3	1.89	0.55
26:L:103:SQD:H441	26:L:103:SQD:H102	1.88	0.55
3:c:305:THR:HG22	3:c:307:PRO:HD2	1.88	0.54
23:b:609:CLA:H161	23:b:615:CLA:H171	1.89	0.54
31:L:101:LHG:H331	13:M:18:PRO:HB3	1.89	0.54
7:n:55:ARG:NH1	7:n:77:ASP:OD2	2.41	0.54
24:D:402:PHO:HHC	23:D:403:CLA:H11	1.88	0.54
14:O:281:SER:HB2	14:O:308:PRO:HG3	1.90	0.54
37:Y:301:XAT:H30	31:Y:319:LHG:H211	1.89	0.54
23:b:615:CLA:H12	23:b:615:CLA:H2A	1.90	0.54
23:B:610:CLA:H43	23:B:612:CLA:H51	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:17:THR:HG23	8:h:20:GLY:H	1.72	0.54
2:B:391:SER:OG	2:B:392:VAL:N	2.40	0.54
2:b:222:PRO:HB3	8:h:38:GLY:H	1.73	0.54
23:b:609:CLA:H12	30:b:622:LMG:H121	1.90	0.54
2:B:269:GLY:O	2:B:448:ARG:NH1	2.41	0.53
23:B:607:CLA:H12	30:B:620:LMG:H121	1.90	0.53
14:O:166:ARG:NH2	18:W:88:GLU:OE1	2.41	0.53
20:y:132:LYS:HA	35:y:308:CHL:HED3	1.91	0.53
23:n:603:CLA:HBB1	35:n:609:CHL:H161	1.91	0.53
23:b:612:CLA:H43	23:b:614:CLA:H51	1.90	0.53
23:B:613:CLA:H12	23:B:613:CLA:H2A	1.89	0.53
7:N:76:GLY:HA3	7:N:216:LEU:HD23	1.90	0.53
2:b:272:ARG:NH1	2:b:276:ASP:OD2	2.41	0.53
9:i:5:LYS:NZ	18:w:97:SER:OG	2.42	0.53
2:B:311:PHE:O	2:B:317:ASN:ND2	2.42	0.53
2:B:222:PRO:HB3	8:H:38:GLY:H	1.72	0.53
2:B:255:THR:HG21	23:B:602:CLA:HED1	1.91	0.53
2:b:25:MET:HE3	25:b:619:BCR:H23C	1.91	0.53
23:Y:304:CLA:H91	35:Y:310:CHL:H121	1.90	0.53
23:R:309:CLA:H43	23:R:313:CLA:H122	1.91	0.52
2:b:311:PHE:O	2:b:317:ASN:ND2	2.42	0.52
23:r:608:CLA:H43	23:r:612:CLA:H122	1.91	0.52
1:A:192:ILE:HA	1:A:293:MET:HE1	1.91	0.52
7:G:138:ILE:HG21	7:G:158:ILE:HD13	1.91	0.52
2:b:141:ILE:HG13	2:b:217:LEU:HD21	1.92	0.52
23:b:606:CLA:HBB1	23:b:615:CLA:HBC2	1.92	0.52
23:C:512:CLA:HBC2	11:K:55:GLN:HG3	1.91	0.52
4:D:130:GLN:NE2	24:D:402:PHO:OBD	2.43	0.52
7:N:210:GLU:HG2	7:N:214:LYS:HE2	1.91	0.52
7:n:250:ASP:OD1	7:n:254:ASN:ND2	2.43	0.52
7:n:103:SER:HB3	7:n:219:GLY:HA3	1.90	0.52
14:O:311:THR:HB	14:O:318:PRO:HG3	1.91	0.52
26:C:521:SQD:H112	23:S:311:CLA:HBB1	1.91	0.51
2:b:235:GLU:OE2	2:b:472:ARG:NH1	2.40	0.51
3:c:27:ASP:N	3:c:27:ASP:OD1	2.43	0.51
15:s:194:LEU:HB2	35:s:607:CHL:HMC	1.91	0.51
23:B:604:CLA:HBB1	23:B:613:CLA:HBC2	1.93	0.51
11:k:30:TYR:OH	21:z:58:ASN:ND2	2.42	0.51
31:n:618:LHG:H311	31:n:618:LHG:H122	1.93	0.51
23:B:607:CLA:H161	23:B:613:CLA:H171	1.92	0.51
25:C:515:BCR:HC42	25:C:519:BCR:HC42	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:10:SER:OG	13:m:28:LYS:NZ	2.43	0.51
31:l:102:LHG:H331	13:m:18:PRO:HB3	1.92	0.51
23:g:602:CLA:H92	23:g:603:CLA:H9B	1.91	0.51
24:a:403:PHO:OBD	4:d:130:GLN:NE2	2.43	0.51
22:r:145:GLY:HA3	22:r:246:SER:HB2	1.93	0.51
20:y:113:THR:HG23	20:y:239:ILE:HD11	1.93	0.51
2:B:71:ILE:HD11	23:B:606:CLA:H2A	1.93	0.51
1:a:304:GLN:HE22	3:c:414:ILE:HG12	1.75	0.51
23:B:602:CLA:H42	28:D:410:DGD:HB22	1.92	0.51
14:o:281:SER:HB2	14:o:308:PRO:HG3	1.92	0.51
28:B:624:DGD:HB91	28:B:624:DGD:HA91	1.93	0.51
2:b:477:ASP:OD1	2:b:477:ASP:N	2.44	0.51
7:N:161:ILE:HG12	35:N:605:CHL:HBC2	1.93	0.50
20:Y:175:ARG:NH2	35:Y:310:CHL:O1D	2.45	0.50
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.44	0.50
20:Y:132:LYS:HA	35:Y:308:CHL:HED3	1.93	0.50
2:b:64:PRO:HB3	2:b:267:LEU:HB3	1.94	0.50
7:g:103:SER:HB2	7:g:219:GLY:HA3	1.94	0.50
12:l:27:VAL:HG11	31:l:102:LHG:H201	1.92	0.50
4:d:52:GLY:HA2	4:d:56:VAL:HB	1.94	0.50
22:R:145:GLY:HA3	22:R:246:SER:HB2	1.93	0.50
2:B:474:LEU:O	4:D:135:ARG:NH1	2.44	0.50
3:c:130:ILE:HD11	25:c:518:BCR:H21C	1.94	0.50
1:A:29:TYR:O	1:A:129:ARG:NH1	2.45	0.50
28:B:624:DGD:O3D	14:o:162:LYS:NZ	2.43	0.50
4:D:124:ILE:HD11	28:D:410:DGD:HAH2	1.94	0.50
1:a:85:THR:HA	1:a:109:GLY:HA3	1.94	0.50
12:l:12:GLU:HB2	13:m:29:THR:HG23	1.94	0.50
1:a:95:PRO:HA	23:a:404:CLA:HED3	1.93	0.49
7:g:85:LEU:HD11	23:y:304:CLA:H12	1.94	0.49
8:h:67:LEU:HD21	19:x:322:LEU:HD13	1.93	0.49
23:A:401:CLA:H192	23:D:401:CLA:H161	1.93	0.49
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.45	0.49
25:B:617:BCR:H383	31:l:103:LHG:H291	1.94	0.49
9:I:5:LYS:NZ	18:W:97:SER:OG	2.45	0.49
13:M:28:LYS:HB2	13:m:27:VAL:HG12	1.94	0.49
3:c:343:ARG:NH1	3:c:347:GLY:O	2.45	0.49
7:g:138:ILE:HG21	7:g:158:ILE:HD13	1.93	0.49
24:a:403:PHO:H152	23:d:402:CLA:HMB2	1.94	0.49
20:y:102:SER:HB3	20:y:217:GLY:HA3	1.94	0.49
37:y:301:XAT:H30	31:y:318:LHG:H211	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R:308:CHL:H101	35:R:308:CHL:HAB	1.95	0.49
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.94	0.49
2:B:25:MET:HE3	25:B:617:BCR:H23C	1.94	0.49
7:G:240:PRO:HB3	36:G:615:LUT:H41	1.94	0.49
17:U:81:THR:OG1	17:U:82:GLU:N	2.45	0.49
7:g:240:PRO:HB3	36:g:615:LUT:H41	1.92	0.49
20:y:175:ARG:NH2	35:y:310:CHL:O1D	2.45	0.49
22:R:146:ARG:NE	22:R:242:GLU:OE2	2.45	0.49
3:C:225:VAL:O	3:C:293:ASN:ND2	2.44	0.49
4:D:55:PHE:O	5:E:49:SER:OG	2.31	0.49
2:b:87:ASN:ND2	30:b:601:LMG:O4	2.43	0.49
2:b:255:THR:HG21	23:b:604:CLA:HED1	1.94	0.49
3:c:228:ASP:OD1	3:c:228:ASP:N	2.45	0.49
22:r:151:GLY:HA2	37:r:614:XAT:H181	1.93	0.49
2:B:156:PHE:HB3	2:B:162:TYR:HB3	1.94	0.49
15:S:194:LEU:HB2	35:S:308:CHL:HMC	1.94	0.49
2:b:113:TRP:NE1	26:b:602:SQD:O3	2.45	0.49
23:A:404:CLA:H92	9:I:16:VAL:HG11	1.94	0.49
20:Y:102:SER:HB3	20:Y:217:GLY:HA3	1.93	0.49
2:b:57:ARG:NH1	2:b:317:ASN:OD1	2.44	0.49
15:s:190:ILE:HG23	15:s:191:THR:HG23	1.95	0.49
3:C:79:LYS:HD2	3:C:84:GLN:HG2	1.95	0.49
31:D:408:LHG:H342	31:D:408:LHG:H131	1.94	0.49
5:E:35:TRP:O	5:E:39:SER:HB3	2.12	0.49
15:S:117:HIS:HD2	36:S:316:LUT:H15	1.78	0.49
14:o:166:ARG:NH2	18:w:88:GLU:OE2	2.45	0.49
1:A:292:THR:HG22	3:C:428:THR:HG23	1.94	0.49
23:A:401:CLA:H152	23:D:401:CLA:H102	1.95	0.49
15:S:68:ARG:NH1	31:S:318:LHG:O1	2.45	0.49
23:b:610:CLA:H172	23:b:611:CLA:H18	1.95	0.49
1:A:27:ARG:HA	3:C:472:LEU:HD11	1.95	0.49
1:A:85:THR:HA	1:A:109:GLY:HA3	1.95	0.49
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.45	0.49
12:L:10:SER:OG	13:M:28:LYS:NZ	2.42	0.49
23:a:404:CLA:H92	9:i:16:VAL:HG11	1.94	0.49
35:s:607:CHL:H12	36:s:614:LUT:H383	1.95	0.49
2:B:87:ASN:ND2	30:B:623:LMG:O4	2.42	0.48
7:N:59:LEU:HB3	7:N:62:PHE:HB2	1.95	0.48
7:N:176:ARG:NH2	35:N:609:CHL:O1D	2.46	0.48
15:S:160:LEU:HD22	23:S:305:CLA:HED1	1.95	0.48
4:d:55:PHE:O	5:e:49:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:118:ALA:HB1	15:S:229:GLY:HA3	1.95	0.48
20:Y:218:ARG:HA	20:Y:221:MET:HG3	1.95	0.48
1:A:95:PRO:HA	23:A:404:CLA:HED3	1.95	0.48
3:C:40:ALA:HB2	23:C:509:CLA:H2A	1.94	0.48
11:K:30:TYR:OH	21:Z:58:ASN:ND2	2.47	0.48
15:S:89:VAL:HG21	15:S:107:PHE:HE2	1.77	0.48
20:Y:230:GLN:O	20:Y:234:THR:OG1	2.29	0.48
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.47	0.48
23:b:610:CLA:HAB	4:d:124:ILE:HG23	1.96	0.48
4:D:160:ILE:HG21	4:D:288:VAL:HG22	1.95	0.48
23:S:303:CLA:H3A	23:S:303:CLA:HBA2	1.61	0.48
2:b:474:LEU:O	4:d:135:ARG:NH1	2.46	0.48
31:d:408:LHG:H342	31:d:408:LHG:H131	1.95	0.48
23:y:304:CLA:H91	35:y:310:CHL:H121	1.94	0.48
31:C:518:LHG:H242	23:Y:312:CLA:H43	1.96	0.48
23:N:602:CLA:HAB	36:N:616:LUT:H32	1.95	0.48
3:c:462:ASP:OD1	3:c:462:ASP:N	2.47	0.48
4:d:193:THR:HG23	23:d:403:CLA:HBC2	1.95	0.48
5:e:35:TRP:O	5:e:39:SER:HB3	2.13	0.48
26:l:101:SQD:H102	26:l:101:SQD:H441	1.94	0.48
15:s:186:GLU:HA	15:s:189:ARG:HG2	1.94	0.48
7:n:210:GLU:HG2	7:n:214:LYS:HE2	1.96	0.48
3:C:148:GLY:O	3:C:156:LYS:NZ	2.45	0.48
12:l:2:THR:OG1	12:l:3:GLN:N	2.47	0.48
2:b:71:ILE:HD11	23:b:608:CLA:H2A	1.95	0.48
3:c:225:VAL:O	3:c:293:ASN:ND2	2.45	0.48
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.95	0.48
1:A:140:ARG:NH2	31:D:408:LHG:O5	2.47	0.48
23:S:310:CLA:HBA2	23:S:310:CLA:H3A	1.51	0.48
15:s:176:VAL:HA	15:s:179:VAL:HG12	1.95	0.48
23:g:613:CLA:H12	23:g:614:CLA:HED2	1.95	0.47
2:B:64:PRO:HB3	2:B:267:LEU:HB3	1.96	0.47
7:G:246:ASP:OD1	7:G:254:ASN:ND2	2.47	0.47
15:S:110:TYR:HB3	23:S:303:CLA:HHB	1.95	0.47
1:a:133:LEU:HD23	4:d:257:ILE:HG12	1.96	0.47
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.96	0.47
3:C:462:ASP:OD1	3:C:462:ASP:N	2.47	0.47
24:D:402:PHO:H41	24:D:402:PHO:H61	1.60	0.47
4:d:81:THR:OG1	4:d:168:TRP:O	2.30	0.47
28:d:410:DGD:HG11	8:h:62:ASN:ND2	2.29	0.47
7:g:108:LEU:HB3	23:g:604:CLA:HBB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:251:VAL:HG21	31:R:317:LHG:H261	1.96	0.47
35:S:306:CHL:HMC	35:S:307:CHL:C4C	2.45	0.47
1:a:261:GLN:HE22	1:a:264:SER:H	1.62	0.47
2:b:321:LYS:NZ	2:b:363:PHE:O	2.48	0.47
35:N:607:CHL:HAA2	37:Y:301:XAT:H241	1.95	0.47
23:Y:303:CLA:HBA2	23:Y:303:CLA:H3A	1.51	0.47
1:a:140:ARG:NH2	31:d:408:LHG:O5	2.47	0.47
7:n:176:ARG:NH2	35:n:609:CHL:O1D	2.47	0.47
20:y:107:LEU:HB3	23:y:305:CLA:HBB2	1.96	0.47
2:B:7:ARG:NH2	31:B:622:LHG:O5	2.48	0.47
23:B:614:CLA:H8	23:B:614:CLA:H52	1.71	0.47
3:C:130:ILE:HD11	25:C:519:BCR:H21C	1.97	0.47
31:b:624:LHG:O4	4:d:142:TYR:OH	2.33	0.47
35:r:607:CHL:H101	35:r:607:CHL:HAB	1.97	0.47
15:s:231:LEU:HD21	23:s:611:CLA:HBC2	1.96	0.47
38:R:301:NEX:H15	38:R:301:NEX:H201	1.78	0.47
23:C:507:CLA:HBB2	23:C:508:CLA:H62	1.97	0.47
4:D:52:GLY:HA2	4:D:56:VAL:HB	1.96	0.47
2:b:156:PHE:HB3	2:b:162:TYR:HB3	1.95	0.47
25:b:619:BCR:H322	30:b:622:LMG:H111	1.97	0.47
4:d:124:ILE:HD11	28:d:410:DGD:HAH2	1.97	0.47
23:s:609:CLA:HED2	23:s:609:CLA:H2A	1.96	0.47
3:c:168:LEU:HD13	23:c:507:CLA:H43	1.97	0.47
22:R:151:GLY:HA2	37:R:315:XAT:H181	1.96	0.47
2:B:320:ALA:HB1	4:D:293:ASN:HD22	1.80	0.47
4:D:162:PRO:HB3	4:D:171:ALA:HB2	1.96	0.47
4:d:162:PRO:HB3	4:d:171:ALA:HB2	1.97	0.47
23:s:602:CLA:HBA2	23:s:602:CLA:H3A	1.61	0.47
18:w:117:PHE:HA	18:w:120:THR:HG22	1.97	0.47
35:n:601:CHL:H61	35:n:601:CHL:H41	1.79	0.47
3:C:168:LEU:HD13	23:C:508:CLA:H43	1.97	0.47
3:c:79:LYS:HD2	3:c:84:GLN:HG2	1.96	0.47
7:N:250:ASP:OD1	7:N:254:ASN:ND2	2.48	0.46
18:W:117:PHE:HA	18:W:120:THR:HG22	1.97	0.46
15:s:68:ARG:NH1	31:s:617:LHG:O1	2.47	0.46
25:c:518:BCR:H24C	25:c:518:BCR:H371	1.75	0.46
2:B:477:ASP:OD1	2:B:477:ASP:N	2.49	0.46
23:Y:311:CLA:H52	36:Y:316:LUT:H30	1.97	0.46
1:a:341:LEU:HD21	3:c:410:VAL:HG11	1.97	0.46
22:R:218:TYR:HB3	23:R:310:CLA:HED2	1.97	0.46
7:G:186:ALA:HB2	35:G:608:CHL:HBC1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:94:ARG:HH21	20:Y:66:PRO:HG3	1.80	0.46
14:O:232:LEU:HA	14:O:282:VAL:HA	1.97	0.46
17:U:97:THR:HA	17:U:102:ARG:HH21	1.80	0.46
31:Y:319:LHG:HC91	31:Y:319:LHG:H321	1.96	0.46
23:G:613:CLA:H12	23:G:614:CLA:HED2	1.97	0.46
23:r:609:CLA:H52	36:r:613:LUT:H30	1.98	0.46
20:y:135:SER:HB3	35:y:308:CHL:HED2	1.97	0.46
23:N:610:CLA:H3A	23:N:610:CLA:HBA2	1.65	0.46
1:a:292:THR:HG22	3:c:428:THR:HG23	1.98	0.46
23:R:303:CLA:HBA2	23:R:303:CLA:H3A	1.57	0.46
23:S:304:CLA:H2A	23:S:304:CLA:HED2	1.98	0.46
1:a:29:TYR:O	1:a:129:ARG:NH1	2.45	0.46
7:g:186:ALA:HB2	35:g:608:CHL:HBC1	1.97	0.46
7:N:186:ALA:HA	7:N:192:PRO:HB3	1.98	0.46
4:d:160:ILE:HG21	4:d:288:VAL:HG22	1.98	0.46
7:g:50:TRP:NE1	7:g:210:GLU:OE2	2.49	0.46
14:o:136:PHE:HB2	14:o:174:ILE:HB	1.98	0.46
2:b:368:VAL:HB	2:b:381:VAL:HB	1.98	0.46
3:c:40:ALA:HB2	23:c:508:CLA:H2A	1.96	0.46
3:c:116:VAL:HG22	25:c:518:BCR:H323	1.98	0.46
3:c:396:MET:HE3	3:c:396:MET:HB3	1.83	0.46
35:y:310:CHL:HBA2	35:y:310:CHL:H3A	1.62	0.46
2:b:370:LEU:HD12	2:b:379:ALA:HB3	1.98	0.45
23:B:601:CLA:HAC1	25:H:101:BCR:H383	1.98	0.45
4:D:193:THR:HG23	23:D:403:CLA:HBC2	1.97	0.45
28:D:410:DGD:O5D	28:D:410:DGD:O4D	2.31	0.45
12:L:27:VAL:HG11	31:L:101:LHG:H201	1.98	0.45
31:L:102:LHG:H291	25:b:619:BCR:H383	1.98	0.45
11:k:29:ALA:HB1	21:z:5:PHE:HE2	1.80	0.45
7:n:94:ARG:HH21	20:y:66:PRO:HG3	1.80	0.45
3:C:174:LEU:HG	23:C:503:CLA:H171	1.98	0.45
23:b:609:CLA:HBB1	30:b:622:LMG:H191	1.99	0.45
7:g:149:ASN:OD1	7:g:151:SER:OG	2.33	0.45
14:O:146:LYS:HE3	14:O:320:ASP:H	1.82	0.45
23:r:610:CLA:H2A	23:r:610:CLA:HED3	1.98	0.45
22:R:244:LYS:NZ	23:R:311:CLA:O1D	2.46	0.45
38:N:617:NEX:H15	38:N:617:NEX:H201	1.81	0.45
25:a:405:BCR:H11C	25:a:405:BCR:H341	1.84	0.45
26:C:521:SQD:H442	31:S:318:LHG:HC12	1.99	0.45
38:Y:318:NEX:H15	38:Y:318:NEX:H201	1.78	0.45
23:c:507:CLA:HMA1	23:c:507:CLA:H2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:n:610:CLA:HBA2	23:n:610:CLA:H3A	1.65	0.45
38:n:617:NEX:H11	38:n:617:NEX:H191	1.82	0.45
31:y:318:LHG:HC91	31:y:318:LHG:H321	1.98	0.45
15:S:64:GLY:H	15:S:87:GLY:HA3	1.81	0.45
1:a:283:ILE:HA	1:a:286:THR:HG22	1.98	0.45
23:a:401:CLA:H192	23:d:401:CLA:H161	1.97	0.45
23:r:603:CLA:H62	23:r:603:CLA:H41	1.72	0.45
20:y:120:LYS:HE2	20:y:120:LYS:HB2	1.78	0.45
14:O:136:PHE:HB2	14:O:174:ILE:HB	1.99	0.45
23:b:618:CLA:H93	23:b:618:CLA:H41	1.99	0.45
3:c:246:PHE:HD2	32:c:522:DMU:H23	1.81	0.45
28:d:410:DGD:HG11	8:h:62:ASN:HD22	1.82	0.45
36:g:615:LUT:H35	36:g:615:LUT:H401	1.81	0.45
35:y:308:CHL:H3A	35:y:308:CHL:HBA1	1.71	0.45
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.99	0.45
23:c:510:CLA:H41	31:d:408:LHG:H151	1.99	0.45
22:R:73:MET:HE1	22:R:134:ILE:HG12	1.99	0.45
25:H:101:BCR:H20C	25:H:101:BCR:H361	1.84	0.45
3:C:246:PHE:HD2	32:C:523:DMU:H23	1.82	0.44
23:a:401:CLA:H152	23:d:401:CLA:H102	1.98	0.44
2:b:277:GLN:HB3	17:u:99:LYS:HG3	1.99	0.44
37:g:620:XAT:H15	37:g:620:XAT:H201	1.80	0.44
38:s:616:NEX:H15	38:s:616:NEX:H201	1.80	0.44
1:A:283:ILE:HA	1:A:286:THR:HG22	1.98	0.44
3:C:110:PRO:HB3	32:C:520:DMU:H1	1.99	0.44
25:b:620:BCR:H24C	25:b:620:BCR:H371	1.82	0.44
20:y:195:ASP:OD1	36:y:316:LUT:O23	2.35	0.44
23:C:504:CLA:H202	23:C:504:CLA:H162	1.87	0.44
38:N:617:NEX:H11	38:N:617:NEX:H191	1.86	0.44
2:b:62:VAL:HG12	2:b:66:MET:HE2	2.00	0.44
25:b:620:BCR:H15C	25:b:620:BCR:H351	1.82	0.44
4:d:187:GLN:HB2	23:d:403:CLA:HBC1	1.99	0.44
1:A:261:GLN:HE22	1:A:264:SER:H	1.66	0.44
25:A:405:BCR:H15C	25:A:405:BCR:H351	1.87	0.44
26:B:625:SQD:O8	8:H:15:ARG:NH1	2.46	0.44
31:C:518:LHG:H321	31:C:518:LHG:H352	1.81	0.44
23:G:603:CLA:H93	23:Y:304:CLA:H102	2.00	0.44
1:a:202:VAL:HG23	23:a:401:CLA:HMB2	1.99	0.44
2:b:334:ASP:OD1	2:b:334:ASP:N	2.50	0.44
7:n:104:ARG:NH1	35:n:608:CHL:OBD	2.48	0.44
23:G:602:CLA:H102	23:Y:304:CLA:H41	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:111:LEU:HG	23:N:604:CLA:HBC2	1.99	0.44
14:O:180:VAL:HA	14:O:186:VAL:HG12	1.99	0.44
20:Y:96:GLU:HA	20:Y:188:LEU:HD21	2.00	0.44
2:b:423:ARG:NH2	2:b:430:PHE:O	2.51	0.44
23:b:617:CLA:H71	31:b:623:LHG:H362	1.99	0.44
31:b:624:LHG:H271	31:b:624:LHG:H242	1.85	0.44
36:n:616:LUT:H15	36:n:616:LUT:H201	1.86	0.44
2:B:423:ARG:NH2	2:B:430:PHE:O	2.50	0.44
30:C:501:LMG:H381	28:C:517:DGD:HB51	1.99	0.44
23:c:511:CLA:H171	21:z:20:LEU:HD12	2.00	0.44
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	2.00	0.44
7:g:80:TRP:HZ3	23:g:602:CLA:HBC2	1.83	0.44
7:n:111:LEU:HG	23:n:604:CLA:HBC2	1.99	0.44
35:y:302:CHL:H143	35:y:302:CHL:H161	1.89	0.44
2:B:368:VAL:HB	2:B:381:VAL:HB	2.00	0.44
30:B:620:LMG:H341	30:B:620:LMG:H372	1.84	0.44
31:B:627:LHG:H151	31:B:627:LHG:H121	1.85	0.44
20:Y:136:GLN:HE22	23:Y:305:CLA:HED2	1.82	0.44
1:a:14:TRP:HB3	18:w:119:TYR:HB2	2.00	0.44
20:y:96:GLU:HA	20:y:188:LEU:HD21	2.00	0.44
20:y:136:GLN:HE22	23:y:305:CLA:HED2	1.82	0.44
3:C:307:PRO:HB3	3:C:358:PHE:HB3	1.99	0.44
23:C:508:CLA:HMA1	23:C:508:CLA:H2	1.99	0.44
38:G:618:NEX:H15	38:G:618:NEX:H201	1.70	0.44
12:L:2:THR:OG1	12:L:3:GLN:N	2.51	0.44
35:Y:302:CHL:H143	35:Y:302:CHL:H161	1.89	0.44
35:Y:308:CHL:H3A	35:Y:308:CHL:HBA1	1.72	0.44
3:c:307:PRO:HB3	3:c:358:PHE:HB3	1.99	0.44
12:l:34:ASN:ND2	12:l:34:ASN:H	2.15	0.44
35:n:607:CHL:HAA2	37:y:301:XAT:H241	1.99	0.44
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.86	0.44
14:o:116:THR:OG1	14:o:117:ILE:N	2.51	0.44
35:r:607:CHL:H92	35:r:607:CHL:H61	1.87	0.44
3:C:90:PRO:O	3:C:94:THR:OG1	2.36	0.43
7:N:199:LEU:HD12	36:N:615:LUT:H222	2.00	0.43
35:N:601:CHL:HBA1	35:N:601:CHL:H3A	1.78	0.43
2:b:326:ARG:NH2	4:d:298:ASP:OD2	2.48	0.43
15:s:118:ALA:HB1	15:s:229:GLY:HA3	1.99	0.43
23:y:312:CLA:H92	23:y:312:CLA:H61	1.85	0.43
2:B:25:MET:HG2	25:B:617:BCR:H23C	2.00	0.43
23:B:603:CLA:H3A	23:B:603:CLA:HBA2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:403:CLA:H192	30:D:409:LMG:H222	2.00	0.43
33:D:406:PL9:H38	12:L:27:VAL:HG13	2.00	0.43
15:S:67:ARG:NH2	15:S:85:LEU:O	2.46	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.80	0.43
37:g:620:XAT:H31	37:g:620:XAT:H391	1.85	0.43
38:R:316:NEX:H35	38:R:316:NEX:H401	1.91	0.43
25:B:619:BCR:H11C	25:B:619:BCR:H341	1.85	0.43
23:C:511:CLA:HBA1	23:C:511:CLA:H3A	1.78	0.43
35:Y:308:CHL:H93	35:Y:308:CHL:H61	1.85	0.43
23:b:605:CLA:H61	23:b:605:CLA:H41	1.77	0.43
7:n:197:ASP:OD1	36:n:615:LUT:O23	2.36	0.43
25:K:101:BCR:H15C	25:K:101:BCR:H351	1.87	0.43
23:N:611:CLA:HBA1	23:N:611:CLA:H3A	1.72	0.43
25:a:405:BCR:H24C	25:a:405:BCR:H371	1.86	0.43
26:b:602:SQD:H462	25:b:621:BCR:H393	2.00	0.43
23:r:602:CLA:H3A	23:r:602:CLA:HBA2	1.57	0.43
15:s:162:TYR:HB3	15:s:165:LYS:HE2	1.99	0.43
37:y:301:XAT:H31	37:y:301:XAT:H391	1.90	0.43
2:B:225:LEU:O	2:B:229:LEU:HB2	2.18	0.43
4:D:142:TYR:HA	4:D:145:ILE:HD12	2.00	0.43
7:G:80:TRP:HZ3	23:G:602:CLA:HBC2	1.84	0.43
23:G:610:CLA:HBA2	23:G:610:CLA:H3A	1.72	0.43
35:S:306:CHL:HBA1	35:S:306:CHL:HED3	2.01	0.43
22:r:251:VAL:HG21	31:r:616:LHG:H261	2.00	0.43
23:R:310:CLA:H52	36:R:314:LUT:H30	2.00	0.43
20:Y:85:SER:O	20:Y:85:SER:OG	2.33	0.43
21:Z:18:ILE:HA	21:Z:21:ILE:HG22	2.01	0.43
3:c:360:ASP:O	28:c:515:DGD:O2E	2.34	0.43
38:R:316:NEX:H191	38:R:316:NEX:H11	1.76	0.43
1:A:14:TRP:HB3	18:W:119:TYR:HB2	2.00	0.43
1:A:182:PHE:O	1:A:186:PHE:HB2	2.19	0.43
24:A:403:PHO:H8	24:A:403:PHO:H122	1.82	0.43
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.91	0.43
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	2.00	0.43
36:G:615:LUT:H15	36:G:615:LUT:H201	1.91	0.43
36:N:616:LUT:H15	36:N:616:LUT:H201	1.87	0.43
23:b:616:CLA:H52	26:l:101:SQD:H281	2.00	0.43
3:c:264:LEU:HD21	25:c:514:BCR:H322	1.99	0.43
3:c:377:LEU:HB2	14:o:173:GLU:HG3	2.01	0.43
36:r:613:LUT:H11	36:r:613:LUT:H191	1.86	0.43
36:r:613:LUT:H31	36:r:613:LUT:H391	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:R:314:LUT:H15	36:R:314:LUT:H201	1.86	0.43
2:B:155:ALA:O	2:B:159:THR:OG1	2.37	0.43
36:s:615:LUT:H35	36:s:615:LUT:H401	1.86	0.43
2:B:10:THR:O	22:R:100:GLN:NE2	2.52	0.43
37:G:620:XAT:H31	37:G:620:XAT:H391	1.85	0.43
23:Y:304:CLA:HAB	35:Y:310:CHL:H162	2.00	0.43
2:b:103:PHE:HB2	23:b:608:CLA:H61	1.99	0.43
15:s:159:THR:OG1	15:s:167:ILE:O	2.36	0.43
2:B:334:ASP:OD1	2:B:334:ASP:N	2.49	0.43
23:B:607:CLA:HBB1	30:B:620:LMG:H191	2.00	0.43
7:N:104:ARG:NH1	35:N:608:CHL:OBD	2.46	0.43
35:S:306:CHL:HBC2	35:S:307:CHL:HHD	2.01	0.43
25:a:405:BCR:H15C	25:a:405:BCR:H351	1.86	0.43
8:h:63:SER:HB3	8:h:72:VAL:HG12	2.01	0.43
21:z:31:ASP:OD1	21:z:31:ASP:N	2.51	0.43
20:Y:107:LEU:HB3	23:Y:305:CLA:HBB2	2.01	0.42
23:b:618:CLA:H61	23:b:618:CLA:H102	1.61	0.42
4:d:58:SER:OG	4:d:66:SER:OG	2.32	0.42
14:o:180:VAL:HA	14:o:186:VAL:HG12	2.00	0.42
22:r:207:ARG:NH2	23:r:608:CLA:O1D	2.48	0.42
35:n:608:CHL:H51	35:n:608:CHL:H11	1.84	0.42
24:A:403:PHO:H152	24:A:403:PHO:H111	1.90	0.42
2:B:321:LYS:HE3	2:B:321:LYS:HB3	1.85	0.42
23:B:611:CLA:HAB	23:B:613:CLA:HMA3	2.01	0.42
23:C:510:CLA:H3A	23:C:510:CLA:HBA1	1.61	0.42
4:D:183:ILE:HG23	23:D:403:CLA:HAC1	2.00	0.42
23:D:401:CLA:H61	23:D:401:CLA:H2	1.75	0.42
5:E:57:THR:O	5:E:61:GLN:NE2	2.46	0.42
7:N:216:LEU:HD12	7:N:216:LEU:HA	1.91	0.42
14:O:116:THR:OG1	14:O:117:ILE:N	2.52	0.42
20:Y:195:ASP:OD1	36:Y:316:LUT:O23	2.36	0.42
23:s:603:CLA:H2A	23:s:603:CLA:HED2	2.01	0.42
7:n:186:ALA:HA	7:n:192:PRO:HB3	2.00	0.42
3:C:343:ARG:HB3	14:O:168:THR:HB	2.01	0.42
7:G:97:GLU:HG2	7:G:190:LEU:HD13	2.01	0.42
1:a:55:ALA:HB3	1:a:70:SER:HB2	2.02	0.42
25:b:621:BCR:H351	25:b:621:BCR:H15C	1.83	0.42
35:g:601:CHL:HBA1	35:g:601:CHL:H3A	1.78	0.42
37:r:614:XAT:H35	37:r:614:XAT:H401	1.85	0.42
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.83	0.42
35:N:601:CHL:HED3	31:N:618:LHG:H142	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:265:ASN:HD21	32:S:319:DMU:H14	1.84	0.42
37:Y:301:XAT:H31	37:Y:301:XAT:H391	1.90	0.42
1:a:79:SER:OG	4:d:302:GLN:NE2	2.49	0.42
2:b:155:ALA:O	2:b:159:THR:OG1	2.36	0.42
6:f:30:SER:O	6:f:34:MET:HB2	2.19	0.42
23:g:602:CLA:H141	23:g:602:CLA:H162	1.84	0.42
38:r:615:NEX:H191	38:r:615:NEX:H11	1.75	0.42
23:B:611:CLA:H202	23:B:611:CLA:H162	1.93	0.42
7:G:50:TRP:NE1	7:G:210:GLU:OE2	2.52	0.42
7:N:111:LEU:HD13	23:N:612:CLA:HBB2	2.02	0.42
3:c:256:PRO:HA	23:c:506:CLA:HED3	2.01	0.42
23:c:509:CLA:H11	23:c:509:CLA:H51	1.89	0.42
28:c:515:DGD:HBE1	28:c:515:DGD:HB82	1.88	0.42
23:d:401:CLA:H2	23:d:401:CLA:H61	1.72	0.42
14:o:131:TYR:HB3	14:o:331:LEU:HD12	2.02	0.42
22:r:142:LEU:HD23	22:r:142:LEU:HA	1.82	0.42
17:u:97:THR:HA	17:u:102:ARG:HH21	1.85	0.42
3:C:293:ASN:O	3:C:423:ARG:NH1	2.50	0.42
33:D:406:PL9:H212	31:L:101:LHG:H222	2.02	0.42
23:g:602:CLA:H42	36:g:616:LUT:H373	2.01	0.42
35:g:609:CHL:H43	35:n:601:CHL:H12	2.02	0.42
23:y:311:CLA:H52	36:y:316:LUT:H30	2.02	0.42
25:B:617:BCR:H322	30:B:620:LMG:H111	2.02	0.42
3:C:226:SER:O	3:C:226:SER:OG	2.32	0.42
25:H:101:BCR:H15C	25:H:101:BCR:H351	1.90	0.42
35:Y:309:CHL:H122	35:Y:309:CHL:HBA1	2.02	0.42
2:b:99:ALA:HB1	23:b:608:CLA:H72	2.02	0.42
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.01	0.42
3:c:376:ASP:OD1	3:c:376:ASP:N	2.47	0.42
14:o:310:ASP:H	14:o:318:PRO:HB3	1.85	0.42
15:s:89:VAL:HG21	15:s:107:PHE:HE2	1.84	0.42
15:s:265:ASN:HD21	32:s:618:DMU:H14	1.85	0.42
36:y:317:LUT:H11	36:y:317:LUT:H191	1.89	0.42
4:D:187:GLN:HB2	23:D:403:CLA:HBC1	2.02	0.42
7:N:197:ASP:OD1	36:N:615:LUT:O23	2.38	0.42
20:Y:135:SER:HB3	35:Y:308:CHL:HED2	2.01	0.42
37:Y:301:XAT:H11	37:Y:301:XAT:H191	1.84	0.42
24:a:403:PHO:H143	23:d:403:CLA:H162	2.02	0.42
31:c:516:LHG:H152	31:c:516:LHG:H122	1.86	0.42
25:d:405:BCR:H351	25:d:405:BCR:H15C	1.82	0.42
23:n:612:CLA:HBB1	36:n:615:LUT:C14	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:y:316:LUT:H35	36:y:316:LUT:H401	1.86	0.42
8:H:43:MET:HE2	8:H:43:MET:HB3	1.84	0.42
23:S:314:CLA:HBC1	36:S:315:LUT:H162	2.01	0.42
35:Y:310:CHL:H3A	35:Y:310:CHL:HBA2	1.62	0.42
23:c:502:CLA:H142	23:c:503:CLA:H3A	2.02	0.42
4:d:183:ILE:HG23	23:d:403:CLA:HAC1	2.01	0.42
14:o:232:LEU:HA	14:o:282:VAL:HA	2.01	0.42
22:r:92:GLN:HG3	22:r:111:ILE:HD11	2.02	0.42
17:u:81:THR:OG1	17:u:82:GLU:N	2.45	0.42
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.86	0.42
26:B:625:SQD:H81	1:a:26:ASN:HB3	2.01	0.42
15:S:199:LYS:HA	35:S:308:CHL:HBC1	2.02	0.42
3:c:433:LEU:HD22	23:c:502:CLA:HMC3	2.02	0.42
23:c:503:CLA:H142	23:c:509:CLA:H42	2.02	0.42
4:d:142:TYR:HA	4:d:145:ILE:HD12	2.02	0.42
18:w:114:THR:HG23	23:y:313:CLA:H61	2.02	0.42
7:n:111:LEU:HD13	23:n:612:CLA:HBB2	2.01	0.42
35:y:308:CHL:H61	35:y:308:CHL:H93	1.84	0.42
22:R:153:LEU:HG	23:R:305:CLA:HBC2	2.00	0.42
23:R:311:CLA:H2A	23:R:311:CLA:HED3	2.02	0.42
23:B:606:CLA:H122	28:B:624:DGD:HAW2	2.02	0.41
3:C:132:HIS:HE1	23:C:514:CLA:HMA3	1.85	0.41
4:D:57:THR:OG1	4:D:58:SER:N	2.52	0.41
23:G:602:CLA:H91	23:G:602:CLA:H112	1.82	0.41
25:b:621:BCR:H11C	25:b:621:BCR:H341	1.87	0.41
14:o:165:THR:HG21	14:o:199:VAL:HG22	2.02	0.41
22:r:60:PHE:HB3	22:r:62:GLY:H	1.85	0.41
22:r:69:LEU:HD11	22:r:80:ASP:HB2	2.01	0.41
37:y:301:XAT:H15	37:y:301:XAT:H201	1.89	0.41
23:C:503:CLA:H142	23:C:504:CLA:H3A	2.02	0.41
13:M:23:LEU:HD13	26:l:101:SQD:H162	2.01	0.41
18:W:82:ASP:OD1	18:W:82:ASP:N	2.53	0.41
2:b:218:SER:HB2	22:r:131:VAL:HG21	2.02	0.41
26:l:101:SQD:H112	26:l:101:SQD:H81	1.87	0.41
7:n:75:PRO:HG3	7:n:212:LYS:HD3	2.02	0.41
20:y:110:LEU:HD13	23:y:313:CLA:HBB2	2.02	0.41
35:y:302:CHL:HBA1	35:y:302:CHL:H3A	1.77	0.41
35:y:308:CHL:H142	35:y:308:CHL:H111	1.89	0.41
22:R:265:LYS:HE3	22:R:270:PHE:HD1	1.85	0.41
28:A:408:DGD:HBT1	30:b:601:LMG:H362	2.01	0.41
31:B:621:LHG:H312	31:B:621:LHG:H281	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:625:SQD:H91	1:a:30:ILE:HD11	2.02	0.41
23:N:612:CLA:HBB1	36:N:615:LUT:C14	2.50	0.41
35:Y:302:CHL:HBA1	35:Y:302:CHL:H3A	1.79	0.41
2:b:194:VAL:HA	2:b:195:PRO:HD3	1.92	0.41
15:s:59:LEU:HD21	15:s:216:GLU:HG3	2.00	0.41
36:R:314:LUT:H11	36:R:314:LUT:H191	1.91	0.41
3:C:360:ASP:O	28:C:517:DGD:O2E	2.35	0.41
20:Y:110:LEU:HD13	23:Y:313:CLA:HBB2	2.03	0.41
23:b:608:CLA:H143	23:b:608:CLA:H111	1.90	0.41
3:c:110:PRO:HB3	32:c:519:DMU:H1	2.01	0.41
5:e:57:THR:O	5:e:61:GLN:NE2	2.49	0.41
1:A:37:MET:HE3	1:A:41:LEU:HD12	2.01	0.41
23:B:614:CLA:H93	23:B:614:CLA:H111	1.93	0.41
23:C:511:CLA:H93	23:C:511:CLA:H61	1.94	0.41
4:D:86:LEU:HD13	4:D:91:LEU:HD11	2.03	0.41
35:G:601:CHL:HBC1	31:G:619:LHG:HC11	2.03	0.41
31:S:318:LHG:H112	31:S:318:LHG:HC81	1.91	0.41
20:Y:218:ARG:HB3	23:Y:303:CLA:HBC3	2.02	0.41
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.03	0.41
31:g:619:LHG:H302	31:g:619:LHG:H271	1.91	0.41
35:n:606:CHL:HMC	35:n:607:CHL:C4C	2.50	0.41
20:y:230:GLN:O	20:y:234:THR:OG1	2.34	0.41
23:R:303:CLA:H41	23:R:303:CLA:H61	1.83	0.41
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.01	0.41
23:C:514:CLA:HBB1	25:C:515:BCR:H371	2.03	0.41
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.82	0.41
7:G:104:ARG:NH1	35:G:608:CHL:OBD	2.54	0.41
23:G:602:CLA:H141	23:G:602:CLA:H162	1.85	0.41
36:S:316:LUT:H15	36:S:316:LUT:H201	1.86	0.41
36:S:316:LUT:H35	36:S:316:LUT:H401	1.92	0.41
35:Y:309:CHL:H121	35:Y:309:CHL:H162	1.92	0.41
23:b:616:CLA:H93	23:b:616:CLA:H111	1.92	0.41
35:g:601:CHL:H41	35:g:601:CHL:H61	1.87	0.41
38:g:618:NEX:H35	38:g:618:NEX:H401	1.88	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.89	0.41
2:B:245:VAL:HG22	23:B:612:CLA:H201	2.01	0.41
23:B:614:CLA:H141	23:B:614:CLA:H162	1.92	0.41
28:B:624:DGD:HBF2	28:B:624:DGD:HBE1	1.96	0.41
23:C:502:CLA:H92	23:C:502:CLA:H62	1.91	0.41
25:D:405:BCR:H15C	25:D:405:BCR:H351	1.82	0.41
36:N:615:LUT:H35	36:N:615:LUT:H401	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:131:TYR:HB3	14:O:331:LEU:HD12	2.02	0.41
31:W:201:LHG:H122	31:W:201:LHG:H152	1.86	0.41
25:a:405:BCR:HC41	9:i:15:PHE:HE1	1.86	0.41
2:b:25:MET:HG2	25:b:619:BCR:H23C	2.03	0.41
28:d:410:DGD:HBN1	28:d:410:DGD:HBW2	1.87	0.41
8:h:47:MET:HG2	25:h:101:BCR:H312	2.02	0.41
25:h:101:BCR:H371	25:h:101:BCR:H24C	1.77	0.41
25:k:101:BCR:H371	25:k:101:BCR:H24C	1.89	0.41
20:y:160:ILE:HG12	35:y:306:CHL:HAC1	2.03	0.41
35:y:309:CHL:HBA1	35:y:309:CHL:H122	2.03	0.41
22:R:224:ASP:OD1	36:R:314:LUT:O23	2.37	0.41
38:R:301:NEX:H191	38:R:301:NEX:H11	1.83	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.93	0.41
23:B:612:CLA:H93	23:B:612:CLA:H62	1.87	0.41
38:N:617:NEX:H35	38:N:617:NEX:H401	1.89	0.41
26:a:406:SQD:H292	31:d:408:LHG:H383	2.03	0.41
38:R:316:NEX:H15	38:R:316:NEX:H201	1.77	0.41
2:B:110:ALA:HB2	25:B:619:BCR:H17C	2.01	0.41
23:B:604:CLA:H12	23:B:604:CLA:H51	1.85	0.41
30:B:620:LMG:H312	30:B:620:LMG:H342	1.92	0.41
3:C:95:LEU:HD12	3:C:178:LYS:HG2	2.02	0.41
23:C:511:CLA:H41	31:D:408:LHG:H151	2.03	0.41
23:G:613:CLA:H93	31:G:619:LHG:H132	2.03	0.41
7:N:103:SER:HB3	7:N:219:GLY:HA3	2.01	0.41
36:N:616:LUT:H35	36:N:616:LUT:H401	1.96	0.41
38:S:317:NEX:H35	38:S:317:NEX:H401	1.86	0.41
1:a:234:ASN:HB2	4:d:264:ASN:HD22	1.86	0.41
7:g:161:ILE:HG12	35:g:605:CHL:HAC1	2.02	0.41
31:g:619:LHG:H362	37:g:620:XAT:H371	2.01	0.41
15:s:230:ARG:HB3	23:s:602:CLA:HBC3	2.03	0.41
36:y:317:LUT:H15	36:y:317:LUT:H201	1.86	0.41
1:A:30:ILE:HD11	26:b:602:SQD:H91	2.02	0.41
1:A:221:SER:HA	4:D:140:ARG:HB2	2.03	0.41
36:G:615:LUT:H11	36:G:615:LUT:H191	1.94	0.41
1:a:221:SER:HA	4:d:140:ARG:HB2	2.03	0.41
23:b:616:CLA:H52	23:b:616:CLA:H8	1.84	0.41
23:c:509:CLA:H3A	23:c:509:CLA:HBA1	1.61	0.41
23:c:513:CLA:H93	23:c:513:CLA:H61	1.93	0.41
31:c:516:LHG:O3	31:c:516:LHG:O1	2.39	0.41
26:c:520:SQD:H442	31:s:617:LHG:HC12	2.03	0.41
4:d:57:THR:OG1	4:d:58:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:78:TYR:OH	7:g:217:LYS:NZ	2.44	0.41
31:g:619:LHG:H382	37:g:620:XAT:H28	2.02	0.41
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.96	0.41
15:s:199:LYS:HA	35:s:607:CHL:HBC1	2.03	0.41
23:n:611:CLA:H3A	23:n:611:CLA:HBA1	1.72	0.41
35:R:307:CHL:HAB	23:R:313:CLA:H191	2.03	0.41
1:A:234:ASN:HB3	4:D:264:ASN:HD22	1.86	0.40
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.89	0.40
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.80	0.40
4:D:46:LEU:HD23	4:D:46:LEU:HA	1.97	0.40
37:G:617:XAT:H31	37:G:617:XAT:H391	1.85	0.40
35:N:608:CHL:H51	35:N:608:CHL:H11	1.85	0.40
36:Y:316:LUT:H15	36:Y:316:LUT:H201	1.92	0.40
23:g:603:CLA:H93	23:y:304:CLA:H102	2.03	0.40
7:n:198:PRO:HD2	36:n:615:LUT:H23	2.03	0.40
3:C:228:ASP:OD1	3:C:228:ASP:N	2.54	0.40
25:C:519:BCR:H15C	25:C:519:BCR:H351	1.84	0.40
36:G:616:LUT:H35	36:G:616:LUT:H401	1.91	0.40
15:S:71:LEU:HB2	15:S:76:LEU:HD22	2.04	0.40
2:b:110:ALA:HB2	25:b:621:BCR:H17C	2.02	0.40
30:b:622:LMG:H352	30:b:622:LMG:H382	1.93	0.40
12:l:14:ASN:OD1	12:l:14:ASN:N	2.54	0.40
22:r:153:LEU:HG	23:r:604:CLA:HBC2	2.03	0.40
37:y:301:XAT:H22	35:y:302:CHL:HMC	2.02	0.40
35:y:307:CHL:H42	38:R:301:NEX:H35	2.03	0.40
1:A:55:ALA:HB3	1:A:70:SER:HB2	2.02	0.40
1:A:174:LEU:HD22	24:A:403:PHO:H151	2.02	0.40
23:C:509:CLA:H141	23:C:509:CLA:H161	1.91	0.40
24:D:402:PHO:HBA2	24:D:402:PHO:H3A	1.79	0.40
9:I:13:ILE:HD12	9:I:13:ILE:HA	1.93	0.40
36:Y:316:LUT:H35	36:Y:316:LUT:H401	1.86	0.40
36:Y:317:LUT:H35	36:Y:317:LUT:H401	1.84	0.40
5:e:14:ILE:HD13	10:j:10:LEU:HB2	2.03	0.40
36:g:616:LUT:H31	36:g:616:LUT:H391	1.99	0.40
7:n:133:LYS:HE3	7:n:133:LYS:HB2	1.80	0.40
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.32	0.40
35:G:601:CHL:H3A	35:G:601:CHL:HBA1	1.77	0.40
15:S:162:TYR:HB3	15:S:165:LYS:HE2	2.03	0.40
18:W:114:THR:HG23	23:Y:313:CLA:H61	2.04	0.40
20:Y:209:LEU:HB3	23:Y:311:CLA:H3A	2.04	0.40
26:a:406:SQD:H151	31:d:408:LHG:H352	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:321:LYS:HE3	2:b:321:LYS:HB3	1.88	0.40
7:g:187:GLU:H	7:g:187:GLU:HG2	1.75	0.40
35:n:601:CHL:HBA1	35:n:601:CHL:H3A	1.81	0.40
23:R:310:CLA:H151	23:R:310:CLA:H111	1.98	0.40
23:B:616:CLA:H141	23:B:616:CLA:H162	1.93	0.40
3:C:41:ARG:NH1	23:C:512:CLA:OBD	2.54	0.40
35:G:601:CHL:H61	35:G:601:CHL:H41	1.86	0.40
7:N:224:PHE:HZ	31:N:618:LHG:H172	1.85	0.40
14:O:290:THR:HG22	14:O:291:LYS:H	1.86	0.40
23:b:610:CLA:H41	23:b:610:CLA:H62	1.80	0.40
25:c:518:BCR:H11C	25:c:518:BCR:H341	1.89	0.40
35:g:601:CHL:HBC1	31:g:619:LHG:HC11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/353 (94%)	314 (94%)	19 (6%)	0	100	100
1	a	333/353 (94%)	315 (95%)	18 (5%)	0	100	100
2	B	487/508 (96%)	467 (96%)	20 (4%)	0	100	100
2	b	487/508 (96%)	469 (96%)	18 (4%)	0	100	100
3	C	447/473 (94%)	432 (97%)	15 (3%)	0	100	100
3	c	447/473 (94%)	434 (97%)	13 (3%)	0	100	100
4	D	337/353 (96%)	327 (97%)	10 (3%)	0	100	100
4	d	337/353 (96%)	329 (98%)	8 (2%)	0	100	100
5	E	69/83 (83%)	65 (94%)	4 (6%)	0	100	100
5	e	69/83 (83%)	63 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	28/39 (72%)	26 (93%)	2 (7%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	0	100	100
7	G	217/267 (81%)	206 (95%)	10 (5%)	1 (0%)	25	61
7	N	217/267 (81%)	207 (95%)	10 (5%)	0	100	100
7	g	217/267 (81%)	208 (96%)	8 (4%)	1 (0%)	25	61
7	n	217/267 (81%)	204 (94%)	13 (6%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	32/36 (89%)	32 (100%)	0	0	100	100
9	i	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
10	J	27/40 (68%)	27 (100%)	0	0	100	100
10	j	27/40 (68%)	27 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
13	m	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
14	O	194/332 (58%)	180 (93%)	14 (7%)	0	100	100
14	o	194/332 (58%)	176 (91%)	17 (9%)	1 (0%)	25	61
15	S	219/280 (78%)	200 (91%)	19 (9%)	0	100	100
15	s	219/280 (78%)	206 (94%)	13 (6%)	0	100	100
16	T	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
16	t	27/33 (82%)	27 (100%)	0	0	100	100
17	U	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
17	u	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
18	W	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
18	w	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
19	X	36/116 (31%)	36 (100%)	0	0	100	100
19	x	36/116 (31%)	36 (100%)	0	0	100	100
20	Y	218/265 (82%)	211 (97%)	6 (3%)	1 (0%)	25	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	y	218/265 (82%)	209 (96%)	8 (4%)	1 (0%)	25	61
21	Z	59/62 (95%)	59 (100%)	0	0	100	100
21	z	59/62 (95%)	59 (100%)	0	0	100	100
22	R	218/286 (76%)	210 (96%)	8 (4%)	0	100	100
22	r	218/286 (76%)	209 (96%)	9 (4%)	0	100	100
All	All	6790/8470 (80%)	6501 (96%)	284 (4%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	o	312	ASP
20	y	152	ILE
20	Y	152	ILE
7	g	153	VAL
7	G	153	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/285 (95%)	272 (100%)	0	100	100
1	a	272/285 (95%)	272 (100%)	0	100	100
2	B	387/402 (96%)	387 (100%)	0	100	100
2	b	387/402 (96%)	387 (100%)	0	100	100
3	C	352/373 (94%)	352 (100%)	0	100	100
3	c	352/373 (94%)	352 (100%)	0	100	100
4	D	271/283 (96%)	271 (100%)	0	100	100
4	d	271/283 (96%)	271 (100%)	0	100	100
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	167/201 (83%)	167 (100%)	0	100	100
7	N	167/201 (83%)	167 (100%)	0	100	100
7	g	167/201 (83%)	167 (100%)	0	100	100
7	n	167/201 (83%)	167 (100%)	0	100	100
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	31/33 (94%)	31 (100%)	0	100	100
9	i	31/33 (94%)	31 (100%)	0	100	100
10	J	22/30 (73%)	22 (100%)	0	100	100
10	j	22/30 (73%)	22 (100%)	0	100	100
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	34 (97%)	1 (3%)	37	70
13	M	28/30 (93%)	28 (100%)	0	100	100
13	m	28/30 (93%)	28 (100%)	0	100	100
14	O	170/268 (63%)	170 (100%)	0	100	100
14	o	170/268 (63%)	170 (100%)	0	100	100
15	S	172/219 (78%)	172 (100%)	0	100	100
15	s	172/219 (78%)	172 (100%)	0	100	100
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	U	19/82 (23%)	19 (100%)	0	100	100
17	u	19/82 (23%)	19 (100%)	0	100	100
18	W	47/102 (46%)	47 (100%)	0	100	100
18	w	47/102 (46%)	47 (100%)	0	100	100
19	X	32/92 (35%)	32 (100%)	0	100	100
19	x	32/92 (35%)	32 (100%)	0	100	100
20	Y	173/209 (83%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	y	173/209 (83%)	173 (100%)	0	100	100
21	Z	53/54 (98%)	53 (100%)	0	100	100
21	z	53/54 (98%)	53 (100%)	0	100	100
22	R	178/226 (79%)	178 (100%)	0	100	100
22	r	178/226 (79%)	178 (100%)	0	100	100
All	All	5542/6758 (82%)	5541 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
12	l	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	108	ASN
1	A	181	ASN
1	A	187	GLN
1	A	261	GLN
1	A	325	ASN
1	A	335	ASN
2	B	182	ASN
3	C	418	ASN
4	D	187	GLN
4	D	251	ASN
5	E	53	ASN
7	G	102	HIS
7	N	262	ASN
14	O	113	GLN
15	S	265	ASN
20	Y	164	GLN
21	Z	58	ASN
1	a	75	ASN
1	a	181	ASN
1	a	304	GLN
2	b	182	ASN
4	d	187	GLN
4	d	251	ASN

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Mol	Chain	Res	Type
4	d	264	ASN
5	e	53	ASN
7	g	154	HIS
7	g	156	GLN
7	g	243	ASN
14	o	307	GLN
22	r	126	GLN
21	z	58	ASN
7	n	165	GLN
7	n	218	ASN
7	n	262	ASN
20	y	164	GLN
20	y	198	ASN
22	R	126	GLN

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 338 ligands modelled in this entry, 2 are monoatomic - leaving 336 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
27	BCT	A	407	29	2,3,3	0.87	0	2,3,3	3.25	2 (100%)
25	BCR	k	101	-	41,41,41	0.65	0	56,56,56	1.84	15 (26%)
31	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
31	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	Y	313	20	60,68,73	1.54	7 (11%)	70,107,113	1.44	9 (12%)
23	CLA	c	504	-	60,68,73	1.57	6 (10%)	70,107,113	1.36	6 (8%)
23	CLA	c	512	3	56,64,73	1.60	6 (10%)	65,102,113	1.53	7 (10%)
23	CLA	b	615	2	65,73,73	1.52	8 (12%)	76,113,113	1.34	7 (9%)
35	CHL	r	606	-	46,54,74	1.74	6 (13%)	49,90,114	1.52	8 (16%)
23	CLA	c	505	3	58,66,73	1.59	6 (10%)	67,104,113	1.43	8 (11%)
35	CHL	s	605	-	46,54,74	1.77	6 (13%)	49,90,114	1.63	7 (14%)
31	LHG	N	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.05	4 (7%)
23	CLA	b	618	2	65,73,73	1.47	7 (10%)	76,113,113	1.46	9 (11%)
31	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
23	CLA	R	302	22	49,57,73	1.77	6 (12%)	55,93,113	1.49	8 (14%)
23	CLA	B	602	2	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
23	CLA	R	309	22	58,66,73	1.59	6 (10%)	67,104,113	1.35	7 (10%)
31	LHG	n	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
30	LMG	s	619	-	55,55,55	0.90	2 (3%)	63,63,63	0.98	4 (6%)
35	CHL	N	601	7	66,74,74	1.41	6 (9%)	73,114,114	1.49	9 (12%)
23	CLA	B	612	2	65,73,73	1.44	7 (10%)	76,113,113	1.55	7 (9%)
23	CLA	s	602	15	46,54,73	1.79	6 (13%)	53,90,113	1.47	7 (13%)
23	CLA	Y	314	20	65,73,73	1.52	6 (9%)	76,113,113	1.35	7 (9%)
23	CLA	Y	304	20	65,73,73	1.53	7 (10%)	76,113,113	1.38	8 (10%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	B	608	2	65,73,73	1.51	7 (10%)	76,113,113	1.33	7 (9%)
23	CLA	A	402	-	50,58,73	1.74	7 (14%)	58,95,113	1.58	9 (15%)
23	CLA	B	611	2	65,73,73	1.49	7 (10%)	76,113,113	1.32	6 (7%)
23	CLA	b	612	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	7 (9%)
31	LHG	Y	319	23	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
36	LUT	n	615	-	42,43,43	0.72	0	51,60,60	1.53	11 (21%)
28	DGD	A	408	-	60,60,67	0.91	2 (3%)	74,74,81	0.96	3 (4%)
39	VTQ	W	202	-	30,32,32	0.42	0	39,44,44	0.50	0
28	DGD	d	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.94	2 (2%)
23	CLA	r	603	22	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	CHL	y	310	20	66,74,74	1.51	7 (10%)	73,114,114	1.53	10 (13%)
23	CLA	r	604	-	48,56,73	1.76	7 (14%)	55,92,113	1.54	8 (14%)
23	CLA	C	502	3	65,73,73	1.53	7 (10%)	76,113,113	1.24	7 (9%)
37	XAT	g	617	-	39,47,47	0.89	0	54,74,74	2.51	16 (29%)
37	XAT	g	620	-	39,47,47	0.92	0	54,74,74	2.47	18 (33%)
35	CHL	G	606	-	43,51,74	1.80	6 (13%)	45,86,114	1.71	10 (22%)
30	LMG	S	301	-	55,55,55	0.90	2 (3%)	63,63,63	0.97	4 (6%)
23	CLA	s	610	31	42,50,73	1.85	6 (14%)	48,85,113	1.53	7 (14%)
23	CLA	R	305	-	48,56,73	1.76	6 (12%)	55,92,113	1.54	8 (14%)
31	LHG	s	617	23	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
25	BCR	B	619	-	41,41,41	0.68	0	56,56,56	1.73	11 (19%)
23	CLA	r	611	22	65,73,73	1.52	6 (9%)	76,113,113	1.35	7 (9%)
35	CHL	N	607	-	46,54,74	1.74	6 (13%)	49,90,114	1.74	10 (20%)
23	CLA	g	604	-	49,57,73	1.73	6 (12%)	55,93,113	1.48	6 (10%)
23	CLA	S	312	15	45,53,73	1.76	6 (13%)	52,89,113	1.72	8 (15%)
25	BCR	A	405	-	41,41,41	0.68	0	56,56,56	1.69	12 (21%)
27	BCT	a	408	29	2,3,3	0.87	0	2,3,3	3.26	2 (100%)
28	DGD	D	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.92	2 (2%)
36	LUT	g	616	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
35	CHL	n	606	-	46,54,74	1.75	6 (13%)	49,90,114	1.62	9 (18%)
35	CHL	n	608	-	66,74,74	1.47	6 (9%)	73,114,114	1.30	7 (9%)
35	CHL	s	607	-	49,57,74	1.71	5 (10%)	52,93,114	1.53	10 (19%)
23	CLA	b	608	2	65,73,73	1.50	8 (12%)	76,113,113	1.33	7 (9%)
24	PHO	a	403	-	51,69,69	0.65	0	47,99,99	0.90	3 (6%)
32	DMU	c	519	-	34,34,34	0.54	0	45,45,45	1.50	5 (11%)
36	LUT	r	613	-	42,43,43	0.73	0	51,60,60	1.67	11 (21%)
30	LMG	w	202	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
23	CLA	s	613	15	41,49,73	1.85	6 (14%)	47,84,113	1.63	9 (19%)
35	CHL	g	607	-	43,51,74	1.78	6 (13%)	45,86,114	1.72	9 (20%)
26	SQD	A	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
35	CHL	n	605	7	48,56,74	1.65	5 (10%)	51,92,114	1.82	10 (19%)
23	CLA	b	611	2	65,73,73	1.53	7 (10%)	76,113,113	1.28	7 (9%)
23	CLA	B	604	2	65,73,73	1.52	7 (10%)	76,113,113	1.45	8 (10%)
23	CLA	b	617	2	65,73,73	1.49	7 (10%)	76,113,113	1.44	10 (13%)
35	CHL	Y	309	-	66,74,74	1.47	6 (9%)	73,114,114	1.34	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	614	2	65,73,73	1.50	6 (9%)	76,113,113	1.32	9 (11%)
38	NEX	G	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.34	16 (32%)
31	LHG	B	622	-	45,45,48	0.96	2 (4%)	48,51,54	0.99	3 (6%)
25	BCR	d	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
35	CHL	R	306	-	46,54,74	1.75	5 (10%)	49,90,114	1.63	8 (16%)
23	CLA	a	401	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	6 (7%)
23	CLA	S	303	15	46,54,73	1.78	6 (13%)	53,90,113	1.49	6 (11%)
35	CHL	G	607	-	43,51,74	1.79	6 (13%)	45,86,114	1.68	8 (17%)
37	XAT	R	315	-	39,47,47	0.88	0	54,74,74	2.51	19 (35%)
23	CLA	C	507	3	51,59,73	1.62	6 (11%)	59,96,113	1.78	8 (13%)
23	CLA	R	312	22	65,73,73	1.51	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	R	310	22	65,73,73	1.50	6 (9%)	76,113,113	1.31	6 (7%)
35	CHL	s	606	-	43,51,74	1.78	5 (11%)	45,86,114	1.77	10 (22%)
23	CLA	B	616	2	65,73,73	1.47	7 (10%)	76,113,113	1.46	9 (11%)
23	CLA	G	612	7	45,53,73	1.80	6 (13%)	52,89,113	1.53	9 (17%)
35	CHL	Y	306	20	51,59,74	1.68	6 (11%)	55,96,114	1.49	10 (18%)
23	CLA	b	614	2	65,73,73	1.46	7 (10%)	76,113,113	1.54	7 (9%)
38	NEX	R	301	-	38,46,46	0.91	1 (2%)	50,70,70	4.00	18 (36%)
23	CLA	B	609	2	65,73,73	1.52	7 (10%)	76,113,113	1.28	7 (9%)
35	CHL	r	607	-	61,69,74	1.52	6 (9%)	67,108,114	1.40	10 (14%)
23	CLA	B	606	2	65,73,73	1.50	8 (12%)	76,113,113	1.34	7 (9%)
28	DGD	b	625	-	57,57,67	0.95	2 (3%)	71,71,81	1.06	4 (5%)
31	LHG	L	102	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	2 (3%)
23	CLA	b	606	2	65,73,73	1.51	8 (12%)	76,113,113	1.46	9 (11%)
35	CHL	N	609	7	66,74,74	1.46	6 (9%)	73,114,114	1.59	11 (15%)
23	CLA	n	610	7	59,67,73	1.52	6 (10%)	68,105,113	1.38	7 (10%)
35	CHL	S	306	-	46,54,74	1.80	5 (10%)	49,90,114	1.65	10 (20%)
23	CLA	r	612	22	65,73,73	1.52	6 (9%)	76,113,113	1.37	8 (10%)
31	LHG	B	627	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)
30	LMG	d	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.98	2 (3%)
23	CLA	n	602	7	61,69,73	1.51	7 (11%)	71,108,113	1.51	7 (9%)
23	CLA	C	506	3	58,66,73	1.58	6 (10%)	67,104,113	1.46	8 (11%)
32	DMU	s	618	-	34,34,34	0.54	0	45,45,45	0.98	1 (2%)
35	CHL	r	605	-	46,54,74	1.75	5 (10%)	49,90,114	1.62	8 (16%)
36	LUT	g	615	-	42,43,43	0.73	0	51,60,60	1.53	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	NEX	R	316	-	38,46,46	0.86	1 (2%)	50,70,70	2.30	16 (32%)
23	CLA	s	612	15	55,63,73	1.65	6 (10%)	64,101,113	1.43	6 (9%)
31	LHG	R	317	23	41,41,48	1.01	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	B	607	-	65,73,73	1.52	7 (10%)	76,113,113	1.32	6 (7%)
31	LHG	l	103	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	3 (5%)
23	CLA	c	508	3	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
32	DMU	C	523	-	34,34,34	0.59	0	45,45,45	0.81	1 (2%)
36	LUT	s	615	-	42,43,43	0.73	0	51,60,60	1.47	8 (15%)
30	LMG	a	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.01	3 (5%)
23	CLA	c	502	3	65,73,73	1.50	7 (10%)	76,113,113	1.44	8 (10%)
25	BCR	z	101	-	41,41,41	0.71	0	56,56,56	1.63	9 (16%)
23	CLA	s	609	15	45,53,73	1.78	6 (13%)	52,89,113	1.64	8 (15%)
38	NEX	n	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	16 (32%)
35	CHL	y	308	-	66,74,74	1.44	7 (10%)	73,114,114	1.50	11 (15%)
23	CLA	c	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
38	NEX	r	615	-	38,46,46	0.90	1 (2%)	50,70,70	2.31	18 (36%)
23	CLA	S	310	15	45,53,73	1.79	6 (13%)	52,89,113	1.52	7 (13%)
31	LHG	D	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.94	2 (3%)
26	SQD	L	103	-	53,54,54	1.18	4 (7%)	62,65,65	1.10	6 (9%)
23	CLA	r	601	22	49,57,73	1.79	6 (12%)	55,93,113	1.49	8 (14%)
23	CLA	D	401	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
23	CLA	b	603	-	65,73,73	1.53	7 (10%)	76,113,113	1.34	9 (11%)
23	CLA	R	304	22	60,68,73	1.56	6 (10%)	70,107,113	1.42	7 (10%)
35	CHL	y	306	20	51,59,74	1.68	6 (11%)	55,96,114	1.50	10 (18%)
36	LUT	Y	317	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
23	CLA	Y	311	20	60,68,73	1.48	6 (10%)	70,107,113	1.40	6 (8%)
30	LMG	b	601	-	40,40,55	1.06	2 (5%)	48,48,63	1.00	2 (4%)
30	LMG	c	521	-	50,50,55	0.97	2 (4%)	58,58,63	1.07	4 (6%)
31	LHG	b	626	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)
23	CLA	G	614	7	42,50,73	1.83	6 (14%)	48,85,113	1.49	8 (16%)
23	CLA	g	611	31	60,68,73	1.57	6 (10%)	70,107,113	1.35	6 (8%)
26	SQD	b	602	-	53,54,54	1.20	4 (7%)	62,65,65	3.65	8 (12%)
23	CLA	b	607	2	65,73,73	1.50	8 (12%)	76,113,113	1.50	10 (13%)
23	CLA	c	510	3	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	C	513	3	56,64,73	1.60	5 (8%)	65,102,113	1.51	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	CHL	g	605	7	46,54,74	1.79	6 (13%)	49,90,114	1.50	9 (18%)
23	CLA	B	610	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	7 (9%)
37	XAT	y	301	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
30	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
35	CHL	g	601	7	66,74,74	1.45	8 (12%)	73,114,114	1.41	11 (15%)
23	CLA	B	603	2	65,73,73	1.49	7 (10%)	76,113,113	1.31	7 (9%)
23	CLA	N	603	7	59,67,73	1.62	7 (11%)	68,105,113	1.47	8 (11%)
23	CLA	R	303	22	60,68,73	1.58	7 (11%)	70,107,113	1.30	7 (10%)
23	CLA	A	401	1	65,73,73	1.50	7 (10%)	76,113,113	1.31	6 (7%)
23	CLA	a	404	1	60,68,73	1.53	6 (10%)	70,107,113	1.41	7 (10%)
23	CLA	y	305	-	50,58,73	1.72	7 (14%)	58,95,113	1.52	6 (10%)
23	CLA	B	601	-	65,73,73	1.53	7 (10%)	76,113,113	1.34	9 (11%)
36	LUT	y	317	-	42,43,43	0.74	0	51,60,60	1.50	10 (19%)
23	CLA	g	603	7	65,73,73	1.53	7 (10%)	76,113,113	1.34	10 (13%)
23	CLA	n	614	7	41,49,73	1.86	6 (14%)	47,84,113	1.51	7 (14%)
23	CLA	S	314	15	41,49,73	1.87	6 (14%)	47,84,113	1.66	10 (21%)
35	CHL	y	309	-	66,74,74	1.47	6 (9%)	73,114,114	1.34	9 (12%)
23	CLA	S	311	31	42,50,73	1.85	6 (14%)	48,85,113	1.48	7 (14%)
36	LUT	y	316	-	42,43,43	0.72	0	51,60,60	1.52	10 (19%)
28	DGD	c	515	-	56,56,67	0.92	2 (3%)	70,70,81	1.01	3 (4%)
23	CLA	n	612	7	45,53,73	1.84	7 (15%)	52,89,113	1.58	8 (15%)
35	CHL	n	601	7	66,74,74	1.43	6 (9%)	73,114,114	1.51	8 (10%)
31	LHG	g	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.04	3 (6%)
31	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)
23	CLA	g	613	7	58,66,73	1.61	6 (10%)	67,104,113	1.40	7 (10%)
23	CLA	c	513	3	65,73,73	1.51	7 (10%)	76,113,113	1.34	9 (11%)
35	CHL	Y	307	-	50,58,74	1.66	6 (12%)	52,94,114	1.69	8 (15%)
23	CLA	S	304	15	45,53,73	1.81	6 (13%)	52,89,113	1.58	7 (13%)
35	CHL	Y	308	-	66,74,74	1.45	7 (10%)	73,114,114	1.49	11 (15%)
35	CHL	g	609	7	61,69,74	1.58	8 (13%)	67,108,114	1.37	8 (11%)
23	CLA	B	613	2	65,73,73	1.51	8 (12%)	76,113,113	1.34	7 (9%)
23	CLA	S	309	15	45,53,73	1.88	6 (13%)	52,89,113	1.50	7 (13%)
23	CLA	D	403	4	65,73,73	1.54	7 (10%)	76,113,113	1.30	7 (9%)
23	CLA	R	313	22	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)
35	CHL	G	608	-	66,74,74	1.46	6 (9%)	73,114,114	1.28	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	N	604	-	50,58,73	1.71	6 (12%)	58,95,113	1.53	6 (10%)
23	CLA	r	610	31	41,49,73	1.87	6 (14%)	47,84,113	1.60	7 (14%)
23	CLA	b	613	2	65,73,73	1.48	7 (10%)	76,113,113	1.32	6 (7%)
26	SQD	C	521	-	44,45,54	1.31	4 (9%)	53,56,65	3.96	8 (15%)
25	BCR	b	621	-	41,41,41	0.68	0	56,56,56	1.72	10 (17%)
24	PHO	a	402	-	51,69,69	0.69	1 (1%)	47,99,99	0.87	3 (6%)
31	LHG	y	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
32	DMU	C	520	-	34,34,34	0.54	0	45,45,45	1.48	5 (11%)
23	CLA	D	404	4	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
23	CLA	S	313	15	55,63,73	1.65	6 (10%)	64,101,113	1.44	6 (9%)
23	CLA	g	610	7	64,72,73	1.44	6 (9%)	74,111,113	1.30	6 (8%)
31	LHG	b	624	-	45,45,48	0.96	2 (4%)	48,51,54	0.98	2 (4%)
30	LMG	W	203	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	3 (5%)
23	CLA	b	616	2	65,73,73	1.51	6 (9%)	76,113,113	1.33	9 (11%)
23	CLA	C	512	3	65,73,73	1.52	5 (7%)	76,113,113	1.41	8 (10%)
25	BCR	b	619	-	41,41,41	0.70	0	56,56,56	1.68	12 (21%)
23	CLA	A	404	1	60,68,73	1.52	6 (10%)	70,107,113	1.41	7 (10%)
28	DGD	C	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.02	3 (4%)
23	CLA	c	501	3	65,73,73	1.53	8 (12%)	76,113,113	1.26	7 (9%)
36	LUT	G	615	-	42,43,43	0.73	0	51,60,60	1.54	10 (19%)
23	CLA	c	509	3	65,73,73	1.52	6 (9%)	76,113,113	1.33	7 (9%)
25	BCR	b	620	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
35	CHL	n	607	-	46,54,74	1.72	6 (13%)	49,90,114	1.79	11 (22%)
37	XAT	G	617	-	39,47,47	0.87	0	54,74,74	2.51	16 (29%)
35	CHL	n	609	7	66,74,74	1.46	6 (9%)	73,114,114	1.57	11 (15%)
23	CLA	S	305	-	50,58,73	1.75	7 (14%)	58,95,113	1.53	7 (12%)
35	CHL	Y	310	20	66,74,74	1.51	7 (10%)	73,114,114	1.53	9 (12%)
36	LUT	s	614	-	42,43,43	0.74	0	51,60,60	1.59	11 (21%)
23	CLA	G	603	7	65,73,73	1.51	6 (9%)	76,113,113	1.36	10 (13%)
31	LHG	b	623	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	511	3	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
24	PHO	D	402	-	51,69,69	0.64	0	47,99,99	0.96	3 (6%)
23	CLA	n	604	-	50,58,73	1.70	6 (12%)	58,95,113	1.48	6 (10%)
30	LMG	B	623	-	40,40,55	1.06	2 (5%)	48,48,63	0.99	2 (4%)
26	SQD	c	520	-	44,45,54	1.31	4 (9%)	53,56,65	3.95	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	615	2	65,73,73	1.49	7 (10%)	76,113,113	1.43	11 (14%)
23	CLA	b	604	2	65,73,73	1.50	6 (9%)	76,113,113	1.27	8 (10%)
36	LUT	R	314	-	42,43,43	0.73	0	51,60,60	1.60	10 (19%)
23	CLA	C	510	3	65,73,73	1.53	7 (10%)	76,113,113	1.33	7 (9%)
31	LHG	c	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
24	PHO	A	403	-	51,69,69	0.69	1 (1%)	47,99,99	0.87	3 (6%)
23	CLA	r	609	22	65,73,73	1.49	7 (10%)	76,113,113	1.30	7 (9%)
23	CLA	N	612	7	45,53,73	1.84	7 (15%)	52,89,113	1.60	8 (15%)
38	NEX	N	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	15 (30%)
31	LHG	l	102	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
31	LHG	W	201	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
30	LMG	b	622	-	51,51,55	0.94	2 (3%)	59,59,63	0.99	3 (5%)
23	CLA	y	312	31	60,68,73	1.55	6 (10%)	70,107,113	1.38	7 (10%)
36	LUT	S	315	-	42,43,43	0.74	0	51,60,60	1.60	11 (21%)
38	NEX	Y	318	-	38,46,46	0.92	1 (2%)	50,70,70	3.98	18 (36%)
31	LHG	C	518	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
37	XAT	r	614	-	39,47,47	0.89	0	54,74,74	2.49	17 (31%)
35	CHL	N	606	-	46,54,74	1.75	6 (13%)	49,90,114	1.63	11 (22%)
23	CLA	y	313	20	60,68,73	1.56	7 (11%)	70,107,113	1.42	10 (14%)
30	LMG	C	501	-	48,48,55	0.95	2 (4%)	56,56,63	1.06	4 (7%)
23	CLA	r	608	22	58,66,73	1.58	6 (10%)	67,104,113	1.36	7 (10%)
25	BCR	H	101	-	41,41,41	0.71	0	56,56,56	1.56	7 (12%)
35	CHL	N	608	-	66,74,74	1.47	6 (9%)	73,114,114	1.33	8 (10%)
23	CLA	g	602	7	65,73,73	1.46	7 (10%)	76,113,113	1.26	7 (9%)
25	BCR	a	405	-	41,41,41	0.69	0	56,56,56	1.70	11 (19%)
39	VTQ	w	201	-	30,32,32	0.42	0	39,44,44	0.50	0
23	CLA	C	509	3	65,73,73	1.50	7 (10%)	76,113,113	1.40	7 (9%)
35	CHL	g	606	-	43,51,74	1.74	6 (13%)	45,86,114	1.70	8 (17%)
23	CLA	G	613	7	58,66,73	1.62	6 (10%)	67,104,113	1.39	7 (10%)
38	NEX	s	616	-	38,46,46	0.89	1 (2%)	50,70,70	2.35	20 (40%)
36	LUT	n	616	-	42,43,43	0.76	0	51,60,60	1.54	13 (25%)
23	CLA	C	503	3	65,73,73	1.51	7 (10%)	76,113,113	1.44	8 (10%)
36	LUT	G	616	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
23	CLA	C	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
36	LUT	N	615	-	42,43,43	0.72	0	51,60,60	1.48	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	S	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
28	DGD	B	624	-	60,60,67	0.89	2 (3%)	74,74,81	0.91	2 (2%)
25	BCR	B	617	-	41,41,41	0.70	0	56,56,56	1.66	12 (21%)
23	CLA	C	505	-	60,68,73	1.57	6 (10%)	70,107,113	1.37	7 (10%)
35	CHL	y	302	20	66,74,74	1.44	6 (9%)	73,114,114	1.38	9 (12%)
25	BCR	D	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
23	CLA	b	609	-	65,73,73	1.51	7 (10%)	76,113,113	1.31	6 (7%)
23	CLA	N	611	31	60,68,73	1.56	6 (10%)	70,107,113	1.45	8 (11%)
31	LHG	c	517	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
28	DGD	B	626	-	57,57,67	0.96	2 (3%)	71,71,81	1.04	4 (5%)
23	CLA	s	611	15	45,53,73	1.85	7 (15%)	52,89,113	1.56	10 (19%)
26	SQD	l	101	-	53,54,54	1.19	4 (7%)	62,65,65	1.09	4 (6%)
34	HEM	f	101	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.62	8 (17%)
23	CLA	b	610	2	65,73,73	1.50	7 (10%)	76,113,113	1.32	7 (9%)
23	CLA	Y	312	31	60,68,73	1.55	6 (10%)	70,107,113	1.39	7 (10%)
23	CLA	Y	305	-	50,58,73	1.73	7 (14%)	58,95,113	1.55	6 (10%)
23	CLA	C	514	3	65,73,73	1.51	7 (10%)	76,113,113	1.36	9 (11%)
38	NEX	g	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.45	16 (32%)
30	LMG	C	522	-	50,50,55	0.96	2 (4%)	58,58,63	1.08	4 (6%)
36	LUT	S	316	-	42,43,43	0.77	0	51,60,60	1.48	8 (15%)
23	CLA	G	611	31	60,68,73	1.55	6 (10%)	70,107,113	1.35	7 (10%)
35	CHL	G	609	7	61,69,74	1.54	7 (11%)	67,108,114	1.68	10 (14%)
23	CLA	y	315	20	45,53,73	1.80	6 (13%)	52,89,113	1.47	6 (11%)
23	CLA	d	403	4	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
23	CLA	s	608	15	45,53,73	1.83	6 (13%)	52,89,113	1.52	9 (17%)
23	CLA	d	401	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	G	604	-	49,57,73	1.72	6 (12%)	55,93,113	1.50	6 (10%)
35	CHL	G	601	7	66,74,74	1.46	8 (12%)	73,114,114	1.42	10 (13%)
23	CLA	Y	303	20	61,69,73	1.53	6 (9%)	71,108,113	1.37	6 (8%)
23	CLA	g	614	7	42,50,73	1.84	6 (14%)	48,85,113	1.47	8 (16%)
35	CHL	N	605	7	48,56,74	1.64	6 (12%)	51,92,114	1.85	11 (21%)
37	XAT	G	620	-	39,47,47	0.91	0	54,74,74	2.47	17 (31%)
23	CLA	N	602	7	61,69,73	1.52	7 (11%)	71,108,113	1.49	8 (11%)
23	CLA	s	604	-	50,58,73	1.73	7 (14%)	58,95,113	1.53	6 (10%)
31	LHG	G	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	y	311	20	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
23	CLA	c	506	3	51,59,73	1.67	6 (11%)	59,96,113	1.53	7 (11%)
35	CHL	y	307	-	50,58,74	1.66	6 (12%)	52,94,114	1.68	8 (15%)
38	NEX	S	317	-	38,46,46	0.86	1 (2%)	50,70,70	2.26	17 (34%)
23	CLA	y	314	20	65,73,73	1.51	6 (9%)	76,113,113	1.35	7 (9%)
35	CHL	S	307	-	43,51,74	1.77	5 (11%)	45,86,114	1.72	9 (20%)
23	CLA	R	311	31	41,49,73	1.89	6 (14%)	47,84,113	1.59	7 (14%)
23	CLA	g	612	7	45,53,73	1.80	7 (15%)	52,89,113	1.52	7 (13%)
36	LUT	N	616	-	42,43,43	0.75	0	51,60,60	1.49	11 (21%)
23	CLA	B	605	2	65,73,73	1.50	7 (10%)	76,113,113	1.49	10 (13%)
25	BCR	B	618	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
23	CLA	N	610	7	59,67,73	1.51	6 (10%)	68,105,113	1.45	7 (10%)
31	LHG	r	616	23	41,41,48	1.00	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	c	503	3	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
23	CLA	n	613	7	60,68,73	1.57	6 (10%)	70,107,113	1.45	10 (14%)
35	CHL	S	308	-	49,57,74	1.70	5 (10%)	52,93,114	1.66	10 (19%)
30	LMG	D	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.97	2 (3%)
35	CHL	R	308	-	61,69,74	1.53	6 (9%)	67,108,114	1.43	10 (14%)
37	XAT	Y	301	-	39,47,47	0.91	0	54,74,74	2.56	18 (33%)
23	CLA	n	611	31	60,68,73	1.57	6 (10%)	70,107,113	1.45	8 (11%)
23	CLA	y	303	20	61,69,73	1.53	6 (9%)	71,108,113	1.36	6 (8%)
35	CHL	S	302	15	46,54,74	1.73	6 (13%)	49,90,114	1.70	8 (16%)
35	CHL	Y	302	20	66,74,74	1.44	6 (9%)	73,114,114	1.38	9 (12%)
36	LUT	Y	316	-	42,43,43	0.71	0	51,60,60	1.48	9 (17%)
25	BCR	C	519	-	41,41,41	0.67	0	56,56,56	1.96	15 (26%)
32	DMU	c	522	-	34,34,34	0.58	0	45,45,45	0.81	1 (2%)
35	CHL	g	608	-	66,74,74	1.46	6 (9%)	73,114,114	1.28	7 (9%)
26	SQD	a	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
34	HEM	F	101	6,5	41,50,50	1.51	5 (12%)	45,82,82	1.63	8 (17%)
23	CLA	y	304	20	65,73,73	1.56	7 (10%)	76,113,113	1.40	9 (11%)
25	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.61	9 (16%)
33	PL9	D	406	-	55,55,55	4.31	22 (40%)	68,69,69	3.66	33 (48%)
35	CHL	s	601	15	46,54,74	1.73	6 (13%)	49,90,114	1.69	7 (14%)
32	DMU	S	319	-	34,34,34	0.53	0	45,45,45	0.97	2 (4%)
25	BCR	h	101	-	41,41,41	0.70	0	56,56,56	1.59	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	Y	315	20	45,53,73	1.80	6 (13%)	52,89,113	1.48	6 (11%)
23	CLA	C	504	3	65,73,73	1.50	6 (9%)	76,113,113	1.31	6 (7%)
25	BCR	c	518	-	41,41,41	0.67	0	56,56,56	1.82	13 (23%)
26	SQD	B	625	-	53,54,54	1.20	4 (7%)	62,65,65	3.67	8 (12%)
35	CHL	G	605	7	46,54,74	1.79	6 (13%)	49,90,114	1.50	9 (18%)
23	CLA	b	605	2	65,73,73	1.49	8 (12%)	76,113,113	1.31	7 (9%)
25	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.72	14 (25%)
35	CHL	R	307	-	46,54,74	1.77	6 (13%)	49,90,114	1.52	8 (16%)
23	CLA	n	603	7	59,67,73	1.60	7 (11%)	68,105,113	1.42	9 (13%)
23	CLA	N	613	7	60,68,73	1.58	6 (10%)	70,107,113	1.44	10 (14%)
23	CLA	c	511	3	65,73,73	1.52	7 (10%)	76,113,113	1.36	7 (9%)
23	CLA	r	602	22	60,68,73	1.56	6 (10%)	70,107,113	1.29	8 (11%)
23	CLA	s	603	15	45,53,73	1.83	7 (15%)	52,89,113	1.59	8 (15%)
25	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.71	13 (23%)
23	CLA	N	614	7	41,49,73	1.88	5 (12%)	47,84,113	1.50	7 (14%)
25	BCR	K	101	-	41,41,41	0.65	0	56,56,56	1.80	16 (28%)
23	CLA	d	404	4	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	G	610	7	64,72,73	1.49	6 (9%)	74,111,113	1.33	7 (9%)
23	CLA	d	402	-	50,58,73	1.77	7 (14%)	58,95,113	1.52	8 (13%)
33	PL9	d	406	-	55,55,55	4.32	23 (41%)	68,69,69	3.64	33 (48%)
23	CLA	G	602	7	65,73,73	1.48	8 (12%)	76,113,113	1.25	7 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
31	LHG	D	408	-	-	7/53/53/53	-
31	LHG	B	621	-	-	11/53/53/53	-
23	CLA	Y	313	20	1/1/14/20	9/31/109/115	-
23	CLA	c	504	-	1/1/14/20	3/31/109/115	-
23	CLA	c	512	3	1/1/13/20	8/27/105/115	-
23	CLA	b	615	2	1/1/15/20	13/37/115/115	-
35	CHL	r	606	-	3/3/16/26	5/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	505	3	1/1/13/20	13/29/107/115	-
35	CHL	s	605	-	3/3/16/26	6/15/113/137	-
31	LHG	N	618	23	-	9/53/53/53	-
23	CLA	b	618	2	1/1/15/20	12/37/115/115	-
31	LHG	d	408	-	-	9/53/53/53	-
23	CLA	R	302	22	1/1/11/20	10/18/96/115	-
23	CLA	B	602	2	1/1/15/20	13/37/115/115	-
23	CLA	R	309	22	1/1/13/20	5/29/107/115	-
31	LHG	n	618	23	-	10/53/53/53	-
30	LMG	s	619	-	-	5/50/70/70	0/1/1/1
35	CHL	N	601	7	3/3/20/26	11/39/137/137	-
23	CLA	B	612	2	1/1/15/20	18/37/115/115	-
23	CLA	s	602	15	1/1/11/20	8/15/93/115	-
23	CLA	Y	314	20	1/1/15/20	11/37/115/115	-
23	CLA	Y	304	20	1/1/15/20	11/37/115/115	-
31	LHG	L	101	-	-	8/53/53/53	-
23	CLA	B	608	2	1/1/15/20	12/37/115/115	-
23	CLA	A	402	-	1/1/12/20	5/19/97/115	-
23	CLA	B	611	2	1/1/15/20	9/37/115/115	-
23	CLA	b	612	-	1/1/15/20	11/37/115/115	-
31	LHG	Y	319	23	-	12/53/53/53	-
36	LUT	n	615	-	-	3/29/67/67	0/2/2/2
28	DGD	A	408	-	-	8/48/88/95	0/2/2/2
39	VTQ	W	202	-	-	3/25/49/49	0/1/1/1
28	DGD	d	410	-	-	9/51/91/95	0/2/2/2
23	CLA	r	603	22	1/1/14/20	6/31/109/115	-
35	CHL	y	310	20	3/3/20/26	19/39/137/137	-
23	CLA	r	604	-	1/1/11/20	8/17/95/115	-
23	CLA	C	502	3	1/1/15/20	13/37/115/115	-
37	XAT	g	617	-	-	2/31/93/93	0/4/4/4
37	XAT	g	620	-	-	0/31/93/93	0/4/4/4
35	CHL	G	606	-	3/3/15/26	8/12/110/137	-
30	LMG	S	301	-	-	5/50/70/70	0/1/1/1
23	CLA	s	610	31	1/1/10/20	4/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	R	305	-	1/1/11/20	8/17/95/115	-
31	LHG	s	617	23	-	9/53/53/53	-
25	BCR	B	619	-	-	6/29/63/63	0/2/2/2
23	CLA	r	611	22	1/1/15/20	10/37/115/115	-
35	CHL	N	607	-	3/3/16/26	9/15/113/137	-
23	CLA	g	604	-	1/1/11/20	7/18/96/115	-
23	CLA	S	312	15	1/1/11/20	6/13/91/115	-
25	BCR	A	405	-	-	2/29/63/63	0/2/2/2
28	DGD	D	410	-	-	4/51/91/95	0/2/2/2
36	LUT	g	616	-	-	0/29/67/67	0/2/2/2
35	CHL	n	606	-	3/3/16/26	7/15/113/137	-
35	CHL	n	608	-	3/3/20/26	8/39/137/137	-
35	CHL	s	607	-	3/3/16/26	12/19/117/137	-
23	CLA	b	608	2	1/1/15/20	10/37/115/115	-
24	PHO	a	403	-	-	7/37/103/103	0/5/6/6
32	DMU	c	519	-	-	6/19/59/59	0/2/2/2
36	LUT	r	613	-	-	2/29/67/67	0/2/2/2
30	LMG	w	202	-	-	7/46/66/70	0/1/1/1
23	CLA	s	613	15	1/1/10/20	6/8/86/115	-
35	CHL	g	607	-	3/3/15/26	5/12/110/137	-
26	SQD	A	406	-	-	5/45/65/69	0/1/1/1
35	CHL	n	605	7	3/3/16/26	12/18/116/137	-
23	CLA	b	611	2	1/1/15/20	11/37/115/115	-
23	CLA	B	604	2	1/1/15/20	9/37/115/115	-
23	CLA	b	617	2	1/1/15/20	18/37/115/115	-
35	CHL	Y	309	-	3/3/20/26	12/39/137/137	-
23	CLA	B	614	2	1/1/15/20	21/37/115/115	-
38	NEX	G	618	-	-	3/27/83/83	0/3/3/3
31	LHG	B	622	-	-	11/50/50/53	-
25	BCR	d	405	-	-	7/29/63/63	0/2/2/2
35	CHL	R	306	-	3/3/16/26	7/15/113/137	-
23	CLA	a	401	1	1/1/15/20	8/37/115/115	-
23	CLA	S	303	15	1/1/11/20	6/15/93/115	-
35	CHL	G	607	-	3/3/15/26	4/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	XAT	R	315	-	-	1/31/93/93	0/4/4/4
23	CLA	C	507	3	1/1/12/20	5/21/99/115	-
23	CLA	R	312	22	1/1/15/20	12/37/115/115	-
23	CLA	R	310	22	1/1/15/20	9/37/115/115	-
35	CHL	s	606	-	3/3/15/26	4/12/110/137	-
23	CLA	B	616	2	1/1/15/20	10/37/115/115	-
23	CLA	G	612	7	1/1/11/20	7/13/91/115	-
35	CHL	Y	306	20	3/3/17/26	11/21/119/137	-
23	CLA	b	614	2	1/1/15/20	18/37/115/115	-
38	NEX	R	301	-	-	4/27/83/83	0/3/3/3
23	CLA	B	609	2	1/1/15/20	12/37/115/115	-
35	CHL	r	607	-	3/3/19/26	11/33/131/137	-
23	CLA	B	606	2	1/1/15/20	7/37/115/115	-
28	DGD	b	625	-	-	12/45/85/95	0/2/2/2
31	LHG	L	102	-	-	18/53/53/53	-
23	CLA	b	606	2	1/1/15/20	9/37/115/115	-
35	CHL	N	609	7	3/3/20/26	14/39/137/137	-
23	CLA	n	610	7	1/1/13/20	10/30/108/115	-
35	CHL	S	306	-	3/3/16/26	8/15/113/137	-
23	CLA	r	612	22	1/1/15/20	9/37/115/115	-
31	LHG	B	627	-	-	13/44/44/53	-
30	LMG	d	409	-	-	3/41/61/70	0/1/1/1
23	CLA	n	602	7	1/1/14/20	10/33/111/115	-
23	CLA	C	506	3	1/1/13/20	13/29/107/115	-
35	CHL	r	605	-	3/3/16/26	7/15/113/137	-
32	DMU	s	618	-	-	5/19/59/59	0/2/2/2
36	LUT	g	615	-	-	3/29/67/67	0/2/2/2
38	NEX	R	316	-	-	5/27/83/83	0/3/3/3
23	CLA	s	612	15	1/1/13/20	9/25/103/115	-
31	LHG	R	317	23	-	8/46/46/53	-
23	CLA	B	607	-	1/1/15/20	13/37/115/115	-
31	LHG	l	103	-	-	18/53/53/53	-
23	CLA	c	508	3	1/1/15/20	11/37/115/115	-
32	DMU	C	523	-	-	6/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	s	615	-	-	3/29/67/67	0/2/2/2
30	LMG	a	407	-	-	2/43/63/70	0/1/1/1
23	CLA	c	502	3	1/1/15/20	11/37/115/115	-
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
23	CLA	s	609	15	1/1/11/20	6/13/91/115	-
38	NEX	n	617	-	-	5/27/83/83	0/3/3/3
35	CHL	y	308	-	3/3/20/26	20/39/137/137	-
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
38	NEX	r	615	-	-	5/27/83/83	0/3/3/3
23	CLA	S	310	15	1/1/11/20	9/13/91/115	-
31	LHG	D	407	-	-	11/53/53/53	-
26	SQD	L	103	-	-	15/49/69/69	0/1/1/1
23	CLA	r	601	22	1/1/11/20	11/18/96/115	-
23	CLA	D	401	-	1/1/15/20	14/37/115/115	-
23	CLA	b	603	-	1/1/15/20	13/37/115/115	-
23	CLA	R	304	22	1/1/14/20	7/31/109/115	-
35	CHL	y	306	20	3/3/17/26	11/21/119/137	-
36	LUT	Y	317	-	-	1/29/67/67	0/2/2/2
23	CLA	Y	311	20	1/1/14/20	8/31/109/115	-
30	LMG	b	601	-	-	3/35/55/70	0/1/1/1
30	LMG	c	521	-	-	9/45/65/70	0/1/1/1
31	LHG	b	626	-	-	13/44/44/53	-
23	CLA	G	614	7	1/1/10/20	5/10/88/115	-
23	CLA	g	611	31	1/1/14/20	4/31/109/115	-
26	SQD	b	602	-	-	20/49/69/69	0/1/1/1
23	CLA	b	607	2	1/1/15/20	11/37/115/115	-
23	CLA	c	510	3	1/1/15/20	13/37/115/115	-
23	CLA	C	513	3	1/1/13/20	8/27/105/115	-
35	CHL	g	605	7	3/3/16/26	10/15/113/137	-
23	CLA	B	610	-	1/1/15/20	11/37/115/115	-
37	XAT	y	301	-	-	0/31/93/93	0/4/4/4
30	LMG	B	620	-	-	9/46/66/70	0/1/1/1
35	CHL	g	601	7	3/3/20/26	17/39/137/137	-
23	CLA	B	603	2	1/1/15/20	17/37/115/115	-
23	CLA	N	603	7	1/1/13/20	11/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	R	303	22	1/1/14/20	13/31/109/115	-
23	CLA	A	401	1	1/1/15/20	8/37/115/115	-
23	CLA	a	404	1	1/1/14/20	12/31/109/115	-
23	CLA	y	305	-	1/1/12/20	7/19/97/115	-
23	CLA	B	601	-	1/1/15/20	13/37/115/115	-
36	LUT	y	317	-	-	1/29/67/67	0/2/2/2
23	CLA	g	603	7	1/1/15/20	6/37/115/115	-
23	CLA	n	614	7	1/1/10/20	3/8/86/115	-
23	CLA	S	314	15	1/1/10/20	6/8/86/115	-
35	CHL	y	309	-	3/3/20/26	11/39/137/137	-
23	CLA	S	311	31	1/1/10/20	4/10/88/115	-
36	LUT	y	316	-	-	2/29/67/67	0/2/2/2
28	DGD	c	515	-	-	4/44/84/95	0/2/2/2
23	CLA	n	612	7	1/1/11/20	8/13/91/115	-
35	CHL	n	601	7	3/3/20/26	14/39/137/137	-
31	LHG	g	619	23	-	10/50/50/53	-
31	LHG	d	407	-	-	12/53/53/53	-
23	CLA	g	613	7	1/1/13/20	11/29/107/115	-
23	CLA	c	513	3	1/1/15/20	7/37/115/115	-
35	CHL	Y	307	-	3/3/16/26	10/20/118/137	-
23	CLA	S	304	15	1/1/11/20	5/13/91/115	-
35	CHL	Y	308	-	3/3/20/26	22/39/137/137	-
35	CHL	g	609	7	3/3/19/26	12/33/131/137	-
23	CLA	B	613	2	1/1/15/20	13/37/115/115	-
23	CLA	S	309	15	1/1/11/20	8/13/91/115	-
23	CLA	D	403	4	1/1/15/20	5/37/115/115	-
23	CLA	R	313	22	1/1/15/20	9/37/115/115	-
35	CHL	G	608	-	3/3/20/26	15/39/137/137	-
23	CLA	N	604	-	1/1/12/20	5/19/97/115	-
23	CLA	r	610	31	1/1/10/20	4/8/86/115	-
23	CLA	b	613	2	1/1/15/20	10/37/115/115	-
26	SQD	C	521	-	-	2/40/60/69	0/1/1/1
25	BCR	b	621	-	-	4/29/63/63	0/2/2/2
24	PHO	a	402	-	-	14/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	y	318	23	-	12/53/53/53	-
32	DMU	C	520	-	-	7/19/59/59	0/2/2/2
23	CLA	D	404	4	1/1/15/20	16/37/115/115	-
23	CLA	S	313	15	1/1/13/20	9/25/103/115	-
23	CLA	g	610	7	1/1/14/20	13/36/114/115	-
31	LHG	b	624	-	-	9/50/50/53	-
30	LMG	W	203	-	-	7/46/66/70	0/1/1/1
23	CLA	b	616	2	1/1/15/20	16/37/115/115	-
23	CLA	C	512	3	1/1/15/20	14/37/115/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	A	404	1	1/1/14/20	12/31/109/115	-
28	DGD	C	517	-	-	4/44/84/95	0/2/2/2
23	CLA	c	501	3	1/1/15/20	12/37/115/115	-
36	LUT	G	615	-	-	2/29/67/67	0/2/2/2
23	CLA	c	509	3	1/1/15/20	9/37/115/115	-
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
35	CHL	n	607	-	3/3/16/26	9/15/113/137	-
37	XAT	G	617	-	-	1/31/93/93	0/4/4/4
35	CHL	n	609	7	3/3/20/26	13/39/137/137	-
23	CLA	S	305	-	1/1/12/20	5/19/97/115	-
35	CHL	Y	310	20	3/3/20/26	18/39/137/137	-
36	LUT	s	614	-	-	2/29/67/67	0/2/2/2
23	CLA	G	603	7	1/1/15/20	7/37/115/115	-
31	LHG	b	623	-	-	11/53/53/53	-
23	CLA	C	511	3	1/1/15/20	13/37/115/115	-
24	PHO	D	402	-	-	6/37/103/103	0/5/6/6
23	CLA	n	604	-	1/1/12/20	4/19/97/115	-
30	LMG	B	623	-	-	3/35/55/70	0/1/1/1
26	SQD	c	520	-	-	2/40/60/69	0/1/1/1
23	CLA	B	615	2	1/1/15/20	14/37/115/115	-
23	CLA	b	604	2	1/1/15/20	10/37/115/115	-
36	LUT	R	314	-	-	2/29/67/67	0/2/2/2
23	CLA	C	510	3	1/1/15/20	9/37/115/115	-
31	LHG	c	516	-	-	9/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	403	-	-	13/37/103/103	0/5/6/6
23	CLA	r	609	22	1/1/15/20	10/37/115/115	-
23	CLA	N	612	7	1/1/11/20	7/13/91/115	-
38	NEX	N	617	-	-	4/27/83/83	0/3/3/3
31	LHG	l	102	-	-	9/53/53/53	-
31	LHG	W	201	-	-	9/53/53/53	-
30	LMG	b	622	-	-	7/46/66/70	0/1/1/1
23	CLA	y	312	31	1/1/14/20	8/31/109/115	-
36	LUT	S	315	-	-	2/29/67/67	0/2/2/2
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
31	LHG	C	518	-	-	11/53/53/53	-
37	XAT	r	614	-	-	1/31/93/93	0/4/4/4
35	CHL	N	606	-	3/3/16/26	9/15/113/137	-
23	CLA	y	313	20	1/1/14/20	9/31/109/115	-
30	LMG	C	501	-	-	5/43/63/70	0/1/1/1
23	CLA	r	608	22	1/1/13/20	7/29/107/115	-
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
35	CHL	N	608	-	3/3/20/26	8/39/137/137	-
23	CLA	g	602	7	1/1/15/20	14/37/115/115	-
25	BCR	a	405	-	-	2/29/63/63	0/2/2/2
39	VTQ	w	201	-	-	3/25/49/49	0/1/1/1
23	CLA	C	509	3	1/1/15/20	11/37/115/115	-
35	CHL	g	606	-	3/3/15/26	4/12/110/137	-
23	CLA	G	613	7	1/1/13/20	12/29/107/115	-
38	NEX	s	616	-	-	2/27/83/83	0/3/3/3
36	LUT	n	616	-	-	1/29/67/67	0/2/2/2
23	CLA	C	503	3	1/1/15/20	11/37/115/115	-
36	LUT	G	616	-	-	1/29/67/67	0/2/2/2
23	CLA	C	508	-	1/1/15/20	10/37/115/115	-
36	LUT	N	615	-	-	2/29/67/67	0/2/2/2
31	LHG	S	318	23	-	10/53/53/53	-
28	DGD	B	624	-	-	7/48/88/95	0/2/2/2
25	BCR	B	617	-	-	6/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/14/20	5/31/109/115	-
35	CHL	y	302	20	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	D	405	-	-	7/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	14/37/115/115	-
23	CLA	N	611	31	1/1/14/20	9/31/109/115	-
31	LHG	c	517	-	-	12/53/53/53	-
28	DGD	B	626	-	-	13/45/85/95	0/2/2/2
23	CLA	s	611	15	1/1/11/20	2/13/91/115	-
26	SQD	l	101	-	-	17/49/69/69	0/1/1/1
34	HEM	f	101	6,5	-	5/12/54/54	-
23	CLA	b	610	2	1/1/15/20	16/37/115/115	-
23	CLA	Y	312	31	1/1/14/20	9/31/109/115	-
23	CLA	Y	305	-	1/1/12/20	7/19/97/115	-
23	CLA	C	514	3	1/1/15/20	5/37/115/115	-
38	NEX	g	618	-	-	2/27/83/83	0/3/3/3
30	LMG	C	522	-	-	9/45/65/70	0/1/1/1
36	LUT	S	316	-	-	2/29/67/67	0/2/2/2
23	CLA	G	611	31	1/1/14/20	3/31/109/115	-
35	CHL	G	609	7	3/3/19/26	10/33/131/137	-
23	CLA	y	315	20	1/1/11/20	4/13/91/115	-
23	CLA	d	403	4	1/1/15/20	11/37/115/115	-
23	CLA	s	608	15	1/1/11/20	4/13/91/115	-
23	CLA	d	401	-	1/1/15/20	12/37/115/115	-
23	CLA	G	604	-	1/1/11/20	9/18/96/115	-
35	CHL	G	601	7	3/3/20/26	18/39/137/137	-
23	CLA	Y	303	20	1/1/14/20	16/33/111/115	-
23	CLA	g	614	7	1/1/10/20	5/10/88/115	-
35	CHL	N	605	7	3/3/16/26	12/18/116/137	-
37	XAT	G	620	-	-	0/31/93/93	0/4/4/4
23	CLA	N	602	7	1/1/14/20	11/33/111/115	-
23	CLA	s	604	-	1/1/12/20	3/19/97/115	-
31	LHG	G	619	23	-	11/50/50/53	-
23	CLA	y	311	20	1/1/14/20	8/31/109/115	-
23	CLA	c	506	3	1/1/12/20	8/21/99/115	-
35	CHL	y	307	-	3/3/16/26	10/20/118/137	-
38	NEX	S	317	-	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	y	314	20	1/1/15/20	13/37/115/115	-
35	CHL	S	307	-	3/3/15/26	5/12/110/137	-
23	CLA	R	311	31	1/1/10/20	5/8/86/115	-
23	CLA	g	612	7	1/1/11/20	7/13/91/115	-
36	LUT	N	616	-	-	1/29/67/67	0/2/2/2
23	CLA	B	605	2	1/1/15/20	11/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	N	610	7	1/1/13/20	9/30/108/115	-
31	LHG	r	616	23	-	6/46/46/53	-
23	CLA	c	503	3	1/1/15/20	16/37/115/115	-
23	CLA	n	613	7	1/1/14/20	12/31/109/115	-
35	CHL	S	308	-	3/3/16/26	12/19/117/137	-
30	LMG	D	409	-	-	3/41/61/70	0/1/1/1
35	CHL	R	308	-	3/3/19/26	11/33/131/137	-
37	XAT	Y	301	-	-	0/31/93/93	0/4/4/4
23	CLA	n	611	31	1/1/14/20	9/31/109/115	-
23	CLA	y	303	20	1/1/14/20	16/33/111/115	-
35	CHL	S	302	15	3/3/16/26	7/15/113/137	-
35	CHL	Y	302	20	3/3/20/26	15/39/137/137	-
36	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
25	BCR	C	519	-	-	0/29/63/63	0/2/2/2
32	DMU	c	522	-	-	5/19/59/59	0/2/2/2
35	CHL	g	608	-	3/3/20/26	16/39/137/137	-
26	SQD	a	406	-	-	8/45/65/69	0/1/1/1
34	HEM	F	101	6,5	-	5/12/54/54	-
23	CLA	y	304	20	1/1/15/20	13/37/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	CHL	s	601	15	3/3/16/26	6/15/113/137	-
33	PL9	D	406	-	-	26/53/73/73	0/1/1/1
32	DMU	S	319	-	-	4/19/59/59	0/2/2/2
25	BCR	h	101	-	-	7/29/63/63	0/2/2/2
23	CLA	Y	315	20	1/1/11/20	4/13/91/115	-
23	CLA	C	504	3	1/1/15/20	17/37/115/115	-
25	BCR	c	518	-	-	2/29/63/63	0/2/2/2
26	SQD	B	625	-	-	19/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CHL	G	605	7	3/3/16/26	10/15/113/137	-
23	CLA	b	605	2	1/1/15/20	14/37/115/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
35	CHL	R	307	-	3/3/16/26	5/15/113/137	-
23	CLA	n	603	7	1/1/13/20	10/30/108/115	-
23	CLA	N	613	7	1/1/14/20	12/31/109/115	-
23	CLA	c	511	3	1/1/15/20	11/37/115/115	-
23	CLA	r	602	22	1/1/14/20	16/31/109/115	-
23	CLA	s	603	15	1/1/11/20	5/13/91/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	N	614	7	1/1/10/20	3/8/86/115	-
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
23	CLA	d	404	4	1/1/15/20	15/37/115/115	-
23	CLA	G	610	7	1/1/14/20	11/36/114/115	-
23	CLA	d	402	-	1/1/12/20	10/19/97/115	-
33	PL9	d	406	-	-	25/53/73/73	0/1/1/1
23	CLA	G	602	7	1/1/15/20	18/37/115/115	-

All (1498) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	406	PL9	C23-C24	10.33	1.57	1.33
33	D	406	PL9	C23-C24	10.29	1.57	1.33
33	d	406	PL9	C38-C39	10.14	1.57	1.33
33	D	406	PL9	C38-C39	10.02	1.57	1.33
33	d	406	PL9	C18-C19	9.68	1.56	1.33
33	D	406	PL9	C18-C19	9.67	1.56	1.33
33	D	406	PL9	C28-C29	9.55	1.55	1.33
33	d	406	PL9	C28-C29	9.53	1.55	1.33
33	D	406	PL9	C33-C34	9.09	1.54	1.33
33	d	406	PL9	C43-C44	9.06	1.54	1.33
33	d	406	PL9	C33-C34	9.04	1.54	1.33
33	D	406	PL9	C43-C44	9.02	1.54	1.33
33	D	406	PL9	C8-C9	8.80	1.54	1.33
33	d	406	PL9	C8-C9	8.78	1.54	1.33
23	y	304	CLA	C4B-NB	8.23	1.42	1.35
23	S	309	CLA	C4B-NB	8.13	1.42	1.35
23	r	601	CLA	C4B-NB	8.06	1.42	1.35
23	Y	304	CLA	C4B-NB	8.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	406	PL9	C13-C14	7.99	1.52	1.33
23	s	611	CLA	C4B-NB	7.99	1.42	1.35
33	d	406	PL9	C13-C14	7.97	1.52	1.33
23	N	603	CLA	C4B-NB	7.95	1.42	1.35
23	C	510	CLA	C4B-NB	7.95	1.42	1.35
23	C	502	CLA	C4B-NB	7.95	1.42	1.35
23	D	403	CLA	C4B-NB	7.94	1.42	1.35
23	d	402	CLA	C4B-NB	7.94	1.42	1.35
23	n	612	CLA	C4B-NB	7.92	1.42	1.35
23	S	305	CLA	C4B-NB	7.87	1.42	1.35
23	N	612	CLA	C4B-NB	7.86	1.42	1.35
23	c	509	CLA	C4B-NB	7.86	1.42	1.35
23	G	613	CLA	C4B-NB	7.86	1.42	1.35
23	R	311	CLA	C4B-NB	7.84	1.42	1.35
35	S	308	CHL	C4B-NB	7.84	1.42	1.35
23	c	501	CLA	C4B-NB	7.82	1.42	1.35
23	C	514	CLA	C4B-NB	7.81	1.42	1.35
23	g	613	CLA	C4B-NB	7.81	1.42	1.35
23	N	613	CLA	C4B-NB	7.81	1.42	1.35
23	s	604	CLA	C4B-NB	7.80	1.42	1.35
35	g	605	CHL	C4B-NB	7.79	1.42	1.35
23	g	603	CLA	C4B-NB	7.79	1.42	1.35
23	b	611	CLA	C4B-NB	7.79	1.42	1.35
23	s	608	CLA	C4B-NB	7.79	1.42	1.35
35	S	306	CHL	C4B-NB	7.77	1.42	1.35
23	n	613	CLA	C4B-NB	7.77	1.42	1.35
23	S	313	CLA	C4B-NB	7.76	1.42	1.35
23	r	604	CLA	C4B-NB	7.76	1.42	1.35
23	B	609	CLA	C4B-NB	7.76	1.42	1.35
23	r	611	CLA	C4B-NB	7.76	1.42	1.35
23	s	612	CLA	C4B-NB	7.75	1.42	1.35
23	R	305	CLA	C4B-NB	7.75	1.42	1.35
35	s	607	CHL	C4B-NB	7.75	1.42	1.35
23	B	607	CLA	C4B-NB	7.74	1.42	1.35
23	B	601	CLA	C4B-NB	7.74	1.42	1.35
23	R	302	CLA	C4B-NB	7.73	1.42	1.35
23	G	603	CLA	C4B-NB	7.72	1.42	1.35
35	G	606	CHL	C4B-NB	7.72	1.42	1.35
23	b	603	CLA	C4B-NB	7.72	1.42	1.35
23	n	603	CLA	C4B-NB	7.71	1.42	1.35
23	Y	314	CLA	C4B-NB	7.71	1.42	1.35
35	R	306	CHL	C4B-NB	7.71	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C4B-NB	7.70	1.42	1.35
35	y	306	CHL	C4B-NB	7.70	1.42	1.35
23	r	610	CLA	C4B-NB	7.70	1.42	1.35
35	G	605	CHL	C4B-NB	7.70	1.42	1.35
35	s	605	CHL	C4B-NB	7.69	1.42	1.35
23	c	513	CLA	C4B-NB	7.69	1.42	1.35
35	Y	309	CHL	C4B-NB	7.69	1.42	1.35
23	s	610	CLA	C4B-NB	7.68	1.42	1.35
23	R	313	CLA	C4B-NB	7.68	1.42	1.35
23	N	614	CLA	C4B-NB	7.68	1.42	1.35
23	r	612	CLA	C4B-NB	7.68	1.42	1.35
35	R	307	CHL	C4B-NB	7.68	1.42	1.35
23	c	511	CLA	C4B-NB	7.67	1.42	1.35
23	s	603	CLA	C4B-NB	7.67	1.42	1.35
23	R	303	CLA	C4B-NB	7.67	1.42	1.35
35	y	309	CHL	C4B-NB	7.67	1.42	1.35
23	S	311	CLA	C4B-NB	7.67	1.42	1.35
23	n	611	CLA	C4B-NB	7.67	1.42	1.35
23	A	402	CLA	C4B-NB	7.66	1.42	1.35
35	n	606	CHL	C4B-NB	7.66	1.42	1.35
35	Y	306	CHL	C4B-NB	7.66	1.42	1.35
23	y	305	CLA	C4B-NB	7.66	1.42	1.35
35	N	606	CHL	C4B-NB	7.66	1.42	1.35
23	y	314	CLA	C4B-NB	7.65	1.42	1.35
23	s	602	CLA	C4B-NB	7.65	1.42	1.35
23	S	310	CLA	C4B-NB	7.63	1.42	1.35
23	R	304	CLA	C4B-NB	7.63	1.42	1.35
23	B	608	CLA	C4B-NB	7.63	1.42	1.35
35	r	605	CHL	C4B-NB	7.62	1.42	1.35
23	S	314	CLA	C4B-NB	7.62	1.42	1.35
23	d	404	CLA	C4B-NB	7.62	1.42	1.35
23	r	603	CLA	C4B-NB	7.62	1.42	1.35
23	b	609	CLA	C4B-NB	7.62	1.42	1.35
23	c	505	CLA	C4B-NB	7.62	1.42	1.35
23	C	512	CLA	C4B-NB	7.61	1.42	1.35
23	g	611	CLA	C4B-NB	7.61	1.42	1.35
23	Y	305	CLA	C4B-NB	7.61	1.42	1.35
23	G	612	CLA	C4B-NB	7.61	1.42	1.35
23	S	304	CLA	C4B-NB	7.61	1.42	1.35
23	c	504	CLA	C4B-NB	7.60	1.42	1.35
23	B	606	CLA	C4B-NB	7.60	1.42	1.35
23	N	604	CLA	C4B-NB	7.60	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4B-NB	7.60	1.42	1.35
23	R	312	CLA	C4B-NB	7.60	1.42	1.35
23	g	612	CLA	C4B-NB	7.59	1.42	1.35
23	C	506	CLA	C4B-NB	7.59	1.42	1.35
23	G	604	CLA	C4B-NB	7.59	1.42	1.35
23	n	614	CLA	C4B-NB	7.59	1.42	1.35
23	b	610	CLA	C4B-NB	7.58	1.42	1.35
23	C	505	CLA	C4B-NB	7.58	1.42	1.35
23	Y	315	CLA	C4B-NB	7.58	1.42	1.35
35	Y	310	CHL	C4B-NB	7.58	1.42	1.35
23	g	604	CLA	C4B-NB	7.58	1.42	1.35
23	y	315	CLA	C4B-NB	7.58	1.42	1.35
23	g	614	CLA	C4B-NB	7.57	1.42	1.35
33	d	406	PL9	C48-C49	7.57	1.54	1.32
23	s	609	CLA	C4B-NB	7.57	1.42	1.35
33	D	406	PL9	C48-C49	7.57	1.54	1.32
23	G	614	CLA	C4B-NB	7.57	1.42	1.35
23	C	503	CLA	C4B-NB	7.56	1.42	1.35
35	g	608	CHL	C4B-NB	7.56	1.42	1.35
23	C	513	CLA	C4B-NB	7.56	1.42	1.35
35	G	609	CHL	C4B-NB	7.55	1.41	1.35
23	c	503	CLA	C4B-NB	7.54	1.41	1.35
23	C	509	CLA	C4B-NB	7.54	1.41	1.35
23	R	309	CLA	C4B-NB	7.54	1.41	1.35
23	N	611	CLA	C4B-NB	7.54	1.41	1.35
23	s	613	CLA	C4B-NB	7.54	1.41	1.35
23	b	617	CLA	C4B-NB	7.53	1.41	1.35
35	g	609	CHL	C4B-NB	7.53	1.41	1.35
23	B	611	CLA	C4B-NB	7.53	1.41	1.35
23	S	303	CLA	C4B-NB	7.53	1.41	1.35
23	c	512	CLA	C4B-NB	7.53	1.41	1.35
23	c	508	CLA	C4B-NB	7.52	1.41	1.35
35	y	307	CHL	C4B-NB	7.52	1.41	1.35
23	B	605	CLA	C4B-NB	7.52	1.41	1.35
35	r	607	CHL	C4B-NB	7.51	1.41	1.35
23	c	502	CLA	C4B-NB	7.50	1.41	1.35
23	B	602	CLA	C4B-NB	7.49	1.41	1.35
23	C	504	CLA	C4B-NB	7.49	1.41	1.35
23	b	607	CLA	C4B-NB	7.49	1.41	1.35
23	B	613	CLA	C4B-NB	7.49	1.41	1.35
35	N	608	CHL	C4B-NB	7.49	1.41	1.35
23	B	604	CLA	C4B-NB	7.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4B-NB	7.48	1.41	1.35
23	c	510	CLA	C4B-NB	7.48	1.41	1.35
23	r	608	CLA	C4B-NB	7.48	1.41	1.35
23	b	616	CLA	C4B-NB	7.48	1.41	1.35
33	D	406	PL9	O1-C4	7.48	1.39	1.23
23	C	511	CLA	C4B-NB	7.48	1.41	1.35
23	G	611	CLA	C4B-NB	7.48	1.41	1.35
35	R	308	CHL	C4B-NB	7.48	1.41	1.35
33	d	406	PL9	O1-C4	7.48	1.39	1.23
35	G	608	CHL	C4B-NB	7.47	1.41	1.35
35	Y	307	CHL	C4B-NB	7.47	1.41	1.35
23	r	602	CLA	C4B-NB	7.47	1.41	1.35
35	n	608	CHL	C4B-NB	7.47	1.41	1.35
23	b	615	CLA	C4B-NB	7.46	1.41	1.35
23	S	312	CLA	C4B-NB	7.46	1.41	1.35
23	b	604	CLA	C4B-NB	7.46	1.41	1.35
23	b	605	CLA	C4B-NB	7.45	1.41	1.35
23	y	312	CLA	C4B-NB	7.45	1.41	1.35
35	S	307	CHL	C4B-NB	7.45	1.41	1.35
23	n	604	CLA	C4B-NB	7.45	1.41	1.35
23	y	313	CLA	C4B-NB	7.44	1.41	1.35
23	B	615	CLA	C4B-NB	7.44	1.41	1.35
23	B	603	CLA	C4B-NB	7.43	1.41	1.35
23	b	613	CLA	C4B-NB	7.43	1.41	1.35
23	R	310	CLA	C4B-NB	7.43	1.41	1.35
35	y	310	CHL	C4B-NB	7.42	1.41	1.35
23	d	403	CLA	C4B-NB	7.42	1.41	1.35
35	S	302	CHL	C4B-NB	7.41	1.41	1.35
23	y	303	CLA	C4B-NB	7.41	1.41	1.35
23	Y	312	CLA	C4B-NB	7.40	1.41	1.35
35	n	605	CHL	C4B-NB	7.40	1.41	1.35
23	N	602	CLA	C4B-NB	7.40	1.41	1.35
23	a	404	CLA	C4B-NB	7.37	1.41	1.35
23	b	614	CLA	C4B-NB	7.37	1.41	1.35
35	y	302	CHL	C4B-NB	7.37	1.41	1.35
23	Y	313	CLA	C4B-NB	7.37	1.41	1.35
23	b	606	CLA	C4B-NB	7.37	1.41	1.35
23	c	506	CLA	C4B-NB	7.37	1.41	1.35
23	D	401	CLA	C4B-NB	7.36	1.41	1.35
23	r	609	CLA	C4B-NB	7.35	1.41	1.35
35	g	606	CHL	C4B-NB	7.34	1.41	1.35
35	r	606	CHL	C4B-NB	7.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	607	CHL	C4B-NB	7.34	1.41	1.35
35	n	601	CHL	C4B-NB	7.33	1.41	1.35
23	a	401	CLA	C4B-NB	7.33	1.41	1.35
35	s	601	CHL	C4B-NB	7.32	1.41	1.35
35	G	607	CHL	C4B-NB	7.32	1.41	1.35
35	s	606	CHL	C4B-NB	7.32	1.41	1.35
23	A	404	CLA	C4B-NB	7.31	1.41	1.35
35	Y	302	CHL	C4B-NB	7.31	1.41	1.35
35	N	607	CHL	C4B-NB	7.30	1.41	1.35
23	A	401	CLA	C4B-NB	7.29	1.41	1.35
23	G	610	CLA	C4B-NB	7.28	1.41	1.35
23	Y	303	CLA	C4B-NB	7.28	1.41	1.35
23	B	612	CLA	C4B-NB	7.27	1.41	1.35
23	n	602	CLA	C4B-NB	7.27	1.41	1.35
23	b	618	CLA	C4B-NB	7.27	1.41	1.35
35	Y	308	CHL	C4B-NB	7.26	1.41	1.35
35	N	609	CHL	C4B-NB	7.26	1.41	1.35
23	d	401	CLA	C4B-NB	7.25	1.41	1.35
35	y	308	CHL	C4B-NB	7.25	1.41	1.35
35	n	609	CHL	C4B-NB	7.24	1.41	1.35
23	B	616	CLA	C4B-NB	7.23	1.41	1.35
35	N	605	CHL	C4B-NB	7.20	1.41	1.35
35	N	601	CHL	C4B-NB	7.18	1.41	1.35
35	n	607	CHL	C4B-NB	7.17	1.41	1.35
23	b	612	CLA	C4B-NB	7.16	1.41	1.35
35	g	601	CHL	C4B-NB	7.14	1.41	1.35
23	B	610	CLA	C4B-NB	7.13	1.41	1.35
23	C	507	CLA	C4B-NB	7.11	1.41	1.35
23	N	610	CLA	C4B-NB	7.08	1.41	1.35
23	y	311	CLA	C4B-NB	7.08	1.41	1.35
23	n	610	CLA	C4B-NB	7.06	1.41	1.35
35	G	601	CHL	C4B-NB	7.05	1.41	1.35
23	C	508	CLA	C4B-NB	6.98	1.41	1.35
23	c	507	CLA	C4B-NB	6.95	1.41	1.35
23	G	602	CLA	C4B-NB	6.94	1.41	1.35
23	g	602	CLA	C4B-NB	6.90	1.41	1.35
23	g	610	CLA	C4B-NB	6.63	1.41	1.35
23	Y	311	CLA	C4B-NB	6.40	1.40	1.35
33	d	406	PL9	C3-C4	-6.34	1.39	1.49
33	D	406	PL9	C3-C4	-6.34	1.39	1.49
33	D	406	PL9	O2-C1	5.71	1.39	1.24
33	d	406	PL9	O2-C1	5.70	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	406	PL9	C6-C1	-5.50	1.38	1.48
33	d	406	PL9	C6-C1	-5.49	1.38	1.48
26	b	602	SQD	O8-S	5.00	1.65	1.47
26	C	521	SQD	O8-S	4.98	1.65	1.47
26	c	520	SQD	O8-S	4.98	1.65	1.47
26	B	625	SQD	O8-S	4.97	1.65	1.47
26	L	103	SQD	O8-S	4.62	1.63	1.47
26	a	406	SQD	O8-S	4.61	1.63	1.47
26	A	406	SQD	O8-S	4.60	1.63	1.47
26	l	101	SQD	O8-S	4.60	1.63	1.47
23	R	302	CLA	C1D-ND	4.53	1.43	1.37
31	L	102	LHG	O7-C7	4.50	1.47	1.34
31	l	103	LHG	O7-C7	4.50	1.47	1.34
28	d	410	DGD	O1G-C1A	4.32	1.46	1.33
23	S	309	CLA	C1D-ND	4.29	1.43	1.37
33	d	406	PL9	C7-C3	4.27	1.55	1.51
28	C	517	DGD	O2G-C1B	4.27	1.46	1.34
31	L	102	LHG	O8-C23	4.27	1.45	1.33
30	C	522	LMG	O8-C28	4.27	1.45	1.33
30	b	601	LMG	O8-C28	4.27	1.45	1.33
30	B	623	LMG	O8-C28	4.27	1.45	1.33
28	b	625	DGD	O2G-C1B	4.26	1.46	1.34
26	l	101	SQD	O48-C23	4.26	1.45	1.33
28	d	410	DGD	O2G-C1B	4.26	1.46	1.34
31	B	627	LHG	O8-C23	4.26	1.45	1.33
30	c	521	LMG	O8-C28	4.25	1.45	1.33
28	B	626	DGD	O2G-C1B	4.25	1.46	1.34
26	B	625	SQD	O48-C23	4.25	1.45	1.33
31	l	103	LHG	O8-C23	4.25	1.45	1.33
28	D	410	DGD	O1G-C1A	4.24	1.45	1.33
31	D	408	LHG	O7-C7	4.24	1.46	1.34
31	b	626	LHG	O8-C23	4.23	1.45	1.33
26	a	406	SQD	O48-C23	4.23	1.45	1.33
28	c	515	DGD	O2G-C1B	4.23	1.46	1.34
30	b	622	LMG	O8-C28	4.22	1.45	1.33
30	S	301	LMG	O8-C28	4.22	1.45	1.33
30	w	202	LMG	O8-C28	4.22	1.45	1.33
30	B	620	LMG	O8-C28	4.22	1.45	1.33
23	Y	311	CLA	C1D-ND	4.22	1.43	1.37
31	D	407	LHG	O8-C23	4.22	1.45	1.33
30	W	203	LMG	O8-C28	4.21	1.45	1.33
26	A	406	SQD	O47-C7	4.21	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	619	LMG	O8-C28	4.21	1.45	1.33
31	d	408	LHG	O8-C23	4.21	1.45	1.33
31	d	408	LHG	O7-C7	4.21	1.46	1.34
26	C	521	SQD	O48-C23	4.21	1.45	1.33
26	b	602	SQD	O48-C23	4.21	1.45	1.33
28	A	408	DGD	O1G-C1A	4.21	1.45	1.33
26	c	520	SQD	O48-C23	4.20	1.45	1.33
28	C	517	DGD	O1G-C1A	4.20	1.45	1.33
31	R	317	LHG	O8-C23	4.20	1.45	1.33
30	D	409	LMG	O8-C28	4.20	1.45	1.33
26	A	406	SQD	O48-C23	4.20	1.45	1.33
31	d	407	LHG	O8-C23	4.20	1.45	1.33
26	a	406	SQD	O47-C7	4.20	1.46	1.34
31	D	408	LHG	O8-C23	4.20	1.45	1.33
26	C	521	SQD	O47-C7	4.19	1.46	1.34
28	b	625	DGD	O1G-C1A	4.19	1.45	1.33
31	g	619	LHG	O7-C7	4.19	1.46	1.34
28	B	624	DGD	O1G-C1A	4.19	1.45	1.33
28	D	410	DGD	O2G-C1B	4.19	1.46	1.34
31	C	518	LHG	O8-C23	4.18	1.45	1.33
33	D	406	PL9	C7-C3	4.18	1.55	1.51
26	c	520	SQD	O47-C7	4.18	1.46	1.34
31	r	616	LHG	O8-C23	4.18	1.45	1.33
30	d	409	LMG	O8-C28	4.18	1.45	1.33
30	b	601	LMG	O7-C10	4.18	1.46	1.34
28	c	515	DGD	O1G-C1A	4.18	1.45	1.33
31	W	201	LHG	O8-C23	4.18	1.45	1.33
28	B	626	DGD	O1G-C1A	4.17	1.45	1.33
23	r	601	CLA	C1D-ND	4.17	1.42	1.37
31	c	516	LHG	O8-C23	4.17	1.45	1.33
30	a	407	LMG	O8-C28	4.17	1.45	1.33
30	D	409	LMG	O7-C10	4.17	1.46	1.34
30	d	409	LMG	O7-C10	4.17	1.46	1.34
26	B	625	SQD	O47-C7	4.17	1.46	1.34
23	y	311	CLA	C1D-ND	4.17	1.42	1.37
30	B	623	LMG	O7-C10	4.16	1.46	1.34
31	b	623	LHG	O7-C7	4.16	1.46	1.34
34	f	101	HEM	C3C-CAC	4.16	1.56	1.47
34	F	101	HEM	C3C-CAC	4.16	1.56	1.47
30	c	521	LMG	O7-C10	4.15	1.46	1.34
31	c	517	LHG	O8-C23	4.14	1.45	1.33
31	B	621	LHG	O7-C7	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	516	LHG	O7-C7	4.14	1.46	1.34
31	s	617	LHG	O7-C7	4.14	1.46	1.34
31	Y	319	LHG	O8-C23	4.14	1.45	1.33
26	b	602	SQD	O47-C7	4.14	1.46	1.34
26	L	103	SQD	O48-C23	4.14	1.45	1.33
30	a	407	LMG	O7-C10	4.14	1.46	1.34
31	b	624	LHG	O7-C7	4.13	1.46	1.34
30	b	622	LMG	O7-C10	4.13	1.46	1.34
31	B	622	LHG	O7-C7	4.13	1.46	1.34
31	b	624	LHG	O8-C23	4.13	1.45	1.33
31	s	617	LHG	O8-C23	4.13	1.45	1.33
31	y	318	LHG	O8-C23	4.13	1.45	1.33
30	C	501	LMG	O8-C28	4.13	1.45	1.33
31	N	618	LHG	O8-C23	4.12	1.45	1.33
31	G	619	LHG	O7-C7	4.12	1.45	1.34
31	b	623	LHG	O8-C23	4.12	1.45	1.33
30	W	203	LMG	O7-C10	4.12	1.45	1.34
31	S	318	LHG	O8-C23	4.12	1.45	1.33
31	B	622	LHG	O8-C23	4.12	1.45	1.33
31	n	618	LHG	O8-C23	4.11	1.45	1.33
28	A	408	DGD	O2G-C1B	4.11	1.45	1.34
31	B	621	LHG	O8-C23	4.11	1.45	1.33
31	G	619	LHG	O8-C23	4.11	1.45	1.33
31	W	201	LHG	O7-C7	4.11	1.45	1.34
30	C	522	LMG	O7-C10	4.11	1.45	1.34
26	l	101	SQD	O47-C7	4.10	1.45	1.34
30	w	202	LMG	O7-C10	4.10	1.45	1.34
31	r	616	LHG	O7-C7	4.10	1.45	1.34
31	S	318	LHG	O7-C7	4.10	1.45	1.34
31	R	317	LHG	O7-C7	4.09	1.45	1.34
30	B	620	LMG	O7-C10	4.09	1.45	1.34
30	C	501	LMG	O7-C10	4.08	1.45	1.34
31	y	318	LHG	O7-C7	4.08	1.45	1.34
31	Y	319	LHG	O7-C7	4.08	1.45	1.34
23	s	611	CLA	C1D-ND	4.08	1.42	1.37
23	C	512	CLA	C1D-ND	4.07	1.42	1.37
23	R	310	CLA	C1D-ND	4.07	1.42	1.37
31	g	619	LHG	O8-C23	4.07	1.45	1.33
31	d	407	LHG	O7-C7	4.07	1.45	1.34
31	D	407	LHG	O7-C7	4.07	1.45	1.34
31	L	101	LHG	O8-C23	4.07	1.45	1.33
30	s	619	LMG	O7-C10	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S	301	LMG	O7-C10	4.06	1.45	1.34
28	B	624	DGD	O2G-C1B	4.06	1.45	1.34
23	N	612	CLA	C1D-ND	4.06	1.42	1.37
23	r	602	CLA	C1D-ND	4.06	1.42	1.37
31	l	102	LHG	O7-C7	4.05	1.45	1.34
31	L	101	LHG	O7-C7	4.04	1.45	1.34
31	l	102	LHG	O8-C23	4.03	1.45	1.33
31	N	618	LHG	O7-C7	4.03	1.45	1.34
31	c	517	LHG	O7-C7	4.02	1.45	1.34
23	Y	303	CLA	C1D-ND	4.00	1.42	1.37
31	B	627	LHG	O7-C7	4.00	1.45	1.34
35	G	606	CHL	C1D-ND	3.99	1.42	1.37
31	b	626	LHG	O7-C7	3.99	1.45	1.34
31	n	618	LHG	O7-C7	3.99	1.45	1.34
23	S	303	CLA	C1D-ND	3.98	1.42	1.37
31	C	518	LHG	O7-C7	3.98	1.45	1.34
26	L	103	SQD	O47-C7	3.98	1.45	1.34
23	Y	313	CLA	C1D-ND	3.98	1.42	1.37
23	R	312	CLA	C1D-ND	3.97	1.42	1.37
23	R	303	CLA	C1D-ND	3.97	1.42	1.37
23	n	612	CLA	C1D-ND	3.96	1.42	1.37
23	N	614	CLA	C1D-ND	3.95	1.42	1.37
23	y	313	CLA	C1D-ND	3.95	1.42	1.37
35	G	605	CHL	C1D-ND	3.95	1.42	1.37
23	r	609	CLA	C1D-ND	3.94	1.42	1.37
23	N	610	CLA	C1D-ND	3.94	1.42	1.37
23	G	614	CLA	C1D-ND	3.93	1.42	1.37
23	R	309	CLA	C1D-ND	3.93	1.42	1.37
23	g	610	CLA	C1D-ND	3.93	1.42	1.37
23	n	610	CLA	C1D-ND	3.93	1.42	1.37
23	s	608	CLA	C1D-ND	3.93	1.42	1.37
23	s	603	CLA	C1D-ND	3.92	1.42	1.37
35	g	606	CHL	C1D-ND	3.92	1.42	1.37
23	n	614	CLA	C1D-ND	3.92	1.42	1.37
35	N	605	CHL	C1D-ND	3.92	1.42	1.37
23	n	602	CLA	C1D-ND	3.91	1.42	1.37
23	C	505	CLA	C1D-ND	3.91	1.42	1.37
23	y	303	CLA	C1D-ND	3.91	1.42	1.37
23	Y	312	CLA	C1D-ND	3.91	1.42	1.37
23	S	312	CLA	C1D-ND	3.90	1.42	1.37
23	g	614	CLA	C1D-ND	3.90	1.42	1.37
35	N	601	CHL	C1D-ND	3.90	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	612	CLA	C1D-ND	3.89	1.42	1.37
23	s	602	CLA	C1D-ND	3.88	1.42	1.37
23	C	508	CLA	C1D-ND	3.88	1.42	1.37
23	r	610	CLA	C1D-ND	3.88	1.42	1.37
23	G	613	CLA	C1D-ND	3.88	1.42	1.37
23	N	602	CLA	C1D-ND	3.88	1.42	1.37
23	c	504	CLA	C1D-ND	3.87	1.42	1.37
23	A	402	CLA	C1D-ND	3.87	1.42	1.37
23	c	503	CLA	C1D-ND	3.87	1.42	1.37
23	G	603	CLA	C1D-ND	3.86	1.42	1.37
23	c	509	CLA	C1D-ND	3.86	1.42	1.37
23	G	602	CLA	C1D-ND	3.86	1.42	1.37
23	G	611	CLA	C1D-ND	3.86	1.42	1.37
35	y	308	CHL	C1D-ND	3.86	1.42	1.37
23	b	606	CLA	C1D-ND	3.86	1.42	1.37
23	R	311	CLA	C1D-ND	3.85	1.42	1.37
23	b	607	CLA	C1D-ND	3.85	1.42	1.37
23	c	501	CLA	C1D-ND	3.85	1.42	1.37
23	g	611	CLA	C1D-ND	3.85	1.42	1.37
23	G	612	CLA	C1D-ND	3.85	1.42	1.37
23	r	608	CLA	C1D-ND	3.85	1.42	1.37
23	S	304	CLA	C1D-ND	3.85	1.42	1.37
23	B	601	CLA	C1D-ND	3.84	1.42	1.37
23	Y	315	CLA	C1D-ND	3.84	1.42	1.37
23	C	510	CLA	C1D-ND	3.84	1.42	1.37
23	g	602	CLA	C1D-ND	3.84	1.42	1.37
23	y	312	CLA	C1D-ND	3.84	1.42	1.37
23	C	513	CLA	C1D-ND	3.84	1.42	1.37
23	r	611	CLA	C1D-ND	3.84	1.42	1.37
23	A	401	CLA	C1D-ND	3.84	1.42	1.37
23	g	613	CLA	C1D-ND	3.84	1.42	1.37
23	B	604	CLA	C1D-ND	3.83	1.42	1.37
23	S	314	CLA	C1D-ND	3.83	1.42	1.37
35	s	601	CHL	C1D-ND	3.83	1.42	1.37
23	n	611	CLA	C1D-ND	3.83	1.42	1.37
23	b	603	CLA	C1D-ND	3.83	1.42	1.37
23	a	401	CLA	C1D-ND	3.83	1.42	1.37
35	Y	302	CHL	C1D-ND	3.83	1.42	1.37
23	G	610	CLA	C1D-ND	3.83	1.42	1.37
35	Y	307	CHL	C1D-ND	3.82	1.42	1.37
23	s	612	CLA	C1D-ND	3.82	1.42	1.37
23	c	511	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	606	CHL	C1D-ND	3.82	1.42	1.37
23	N	603	CLA	C1D-ND	3.82	1.42	1.37
23	c	507	CLA	C1D-ND	3.82	1.42	1.37
23	C	509	CLA	C1D-ND	3.82	1.42	1.37
23	s	610	CLA	C1D-ND	3.82	1.42	1.37
23	y	315	CLA	C1D-ND	3.82	1.42	1.37
23	B	615	CLA	C1D-ND	3.82	1.42	1.37
23	B	605	CLA	C1D-ND	3.81	1.42	1.37
35	s	605	CHL	C1D-ND	3.81	1.42	1.37
23	c	512	CLA	C1D-ND	3.81	1.42	1.37
35	G	601	CHL	C1D-ND	3.81	1.42	1.37
23	n	613	CLA	C1D-ND	3.80	1.42	1.37
23	C	502	CLA	C1D-ND	3.80	1.42	1.37
23	y	305	CLA	C1D-ND	3.80	1.42	1.37
23	d	401	CLA	C1D-ND	3.80	1.42	1.37
23	d	402	CLA	C1D-ND	3.80	1.42	1.37
35	s	606	CHL	C1D-ND	3.80	1.42	1.37
23	n	603	CLA	C1D-ND	3.80	1.42	1.37
35	N	609	CHL	C1D-ND	3.80	1.42	1.37
35	S	302	CHL	C1D-ND	3.79	1.42	1.37
23	s	613	CLA	C1D-ND	3.79	1.42	1.37
23	D	404	CLA	C1D-ND	3.79	1.42	1.37
23	a	404	CLA	C1D-ND	3.79	1.42	1.37
23	C	504	CLA	C1D-ND	3.79	1.42	1.37
23	c	502	CLA	C1D-ND	3.79	1.42	1.37
23	S	310	CLA	C1D-ND	3.78	1.42	1.37
23	b	611	CLA	C1D-ND	3.78	1.42	1.37
23	r	612	CLA	C1D-ND	3.78	1.42	1.37
35	G	607	CHL	C1D-ND	3.78	1.42	1.37
23	S	311	CLA	C1D-ND	3.78	1.42	1.37
23	N	613	CLA	C1D-ND	3.78	1.42	1.37
23	Y	304	CLA	C1D-ND	3.78	1.42	1.37
23	N	604	CLA	C1D-ND	3.78	1.42	1.37
23	G	604	CLA	C1D-ND	3.78	1.42	1.37
23	Y	305	CLA	C1D-ND	3.78	1.42	1.37
23	b	615	CLA	C1D-ND	3.77	1.42	1.37
35	g	607	CHL	C1D-ND	3.77	1.42	1.37
23	s	609	CLA	C1D-ND	3.77	1.42	1.37
23	y	314	CLA	C1D-ND	3.77	1.42	1.37
35	G	609	CHL	C1D-ND	3.77	1.42	1.37
23	r	604	CLA	C1D-ND	3.77	1.42	1.37
23	d	404	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	608	CHL	C1D-ND	3.76	1.42	1.37
23	B	607	CLA	C1D-ND	3.76	1.42	1.37
23	g	604	CLA	C1D-ND	3.76	1.42	1.37
23	S	313	CLA	C1D-ND	3.76	1.42	1.37
35	N	606	CHL	C1D-ND	3.76	1.42	1.37
35	N	608	CHL	C1D-ND	3.76	1.42	1.37
35	Y	308	CHL	C1D-ND	3.76	1.42	1.37
23	Y	314	CLA	C1D-ND	3.76	1.42	1.37
35	S	308	CHL	C1D-ND	3.76	1.42	1.37
23	b	617	CLA	C1D-ND	3.75	1.42	1.37
23	C	514	CLA	C1D-ND	3.75	1.42	1.37
23	B	614	CLA	C1D-ND	3.75	1.42	1.37
23	N	611	CLA	C1D-ND	3.75	1.42	1.37
35	Y	310	CHL	C1D-ND	3.75	1.42	1.37
23	y	304	CLA	C1D-ND	3.75	1.42	1.37
35	n	607	CHL	C1D-ND	3.75	1.42	1.37
35	n	608	CHL	C1D-ND	3.75	1.42	1.37
23	s	604	CLA	C1D-ND	3.75	1.42	1.37
23	c	513	CLA	C1D-ND	3.74	1.42	1.37
23	B	616	CLA	C1D-ND	3.74	1.42	1.37
23	c	508	CLA	C1D-ND	3.74	1.42	1.37
23	n	604	CLA	C1D-ND	3.74	1.42	1.37
23	A	404	CLA	C1D-ND	3.74	1.42	1.37
35	r	605	CHL	C1D-ND	3.73	1.42	1.37
35	s	607	CHL	C1D-ND	3.73	1.42	1.37
23	b	618	CLA	C1D-ND	3.73	1.42	1.37
35	R	307	CHL	C1D-ND	3.73	1.42	1.37
35	n	609	CHL	C1D-ND	3.73	1.42	1.37
23	C	503	CLA	C1D-ND	3.73	1.42	1.37
35	g	609	CHL	C1D-ND	3.73	1.42	1.37
23	R	305	CLA	C1D-ND	3.73	1.42	1.37
23	B	613	CLA	C1D-ND	3.72	1.42	1.37
35	y	302	CHL	C1D-ND	3.72	1.42	1.37
35	Y	306	CHL	C1D-ND	3.72	1.42	1.37
23	B	609	CLA	C1D-ND	3.72	1.42	1.37
35	n	601	CHL	C1D-ND	3.72	1.42	1.37
35	Y	309	CHL	C1D-ND	3.72	1.42	1.37
35	N	607	CHL	C1D-ND	3.71	1.42	1.37
35	R	306	CHL	C1D-ND	3.71	1.42	1.37
35	S	306	CHL	C1D-ND	3.71	1.42	1.37
35	y	306	CHL	C1D-ND	3.71	1.42	1.37
23	D	401	CLA	C1D-ND	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	605	CHL	C1D-ND	3.71	1.42	1.37
35	y	309	CHL	C1D-ND	3.71	1.42	1.37
35	S	307	CHL	C1D-ND	3.70	1.42	1.37
23	b	609	CLA	C1D-ND	3.70	1.42	1.37
23	c	506	CLA	C1D-ND	3.70	1.42	1.37
35	g	601	CHL	C1D-ND	3.70	1.42	1.37
23	B	611	CLA	C1D-ND	3.70	1.42	1.37
35	r	606	CHL	C1D-ND	3.69	1.42	1.37
35	R	308	CHL	C1D-ND	3.69	1.42	1.37
23	b	616	CLA	C1D-ND	3.68	1.42	1.37
23	b	612	CLA	C1D-ND	3.68	1.42	1.37
35	y	310	CHL	C1D-ND	3.68	1.42	1.37
23	B	610	CLA	C1D-ND	3.67	1.42	1.37
23	b	608	CLA	C1D-ND	3.67	1.42	1.37
35	y	307	CHL	C1D-ND	3.67	1.42	1.37
23	B	603	CLA	C1D-ND	3.67	1.42	1.37
23	B	606	CLA	C1D-ND	3.67	1.42	1.37
35	g	608	CHL	C1D-ND	3.66	1.42	1.37
23	g	603	CLA	C1D-ND	3.66	1.42	1.37
23	b	604	CLA	C1D-ND	3.66	1.42	1.37
23	C	506	CLA	C1D-ND	3.65	1.42	1.37
23	S	305	CLA	C1D-ND	3.64	1.42	1.37
23	b	613	CLA	C1D-ND	3.64	1.42	1.37
35	n	605	CHL	C1D-ND	3.64	1.42	1.37
23	r	603	CLA	C1D-ND	3.64	1.42	1.37
23	C	507	CLA	C1D-ND	3.64	1.42	1.37
23	c	505	CLA	C1D-ND	3.64	1.42	1.37
23	B	602	CLA	C1D-ND	3.64	1.42	1.37
23	R	304	CLA	C1D-ND	3.63	1.42	1.37
35	r	607	CHL	C1D-ND	3.62	1.42	1.37
23	R	313	CLA	C1D-ND	3.62	1.42	1.37
23	b	605	CLA	C1D-ND	3.61	1.42	1.37
23	c	510	CLA	C1D-ND	3.61	1.42	1.37
23	b	610	CLA	C1D-ND	3.57	1.42	1.37
23	C	511	CLA	C1D-ND	3.56	1.42	1.37
23	B	608	CLA	C1D-ND	3.46	1.42	1.37
23	B	612	CLA	C1D-ND	3.46	1.42	1.37
23	d	403	CLA	C1D-ND	3.40	1.42	1.37
23	b	614	CLA	C1D-ND	3.36	1.41	1.37
23	D	403	CLA	C1D-ND	3.34	1.41	1.37
23	A	402	CLA	C4D-ND	-3.31	1.33	1.37
23	d	402	CLA	C4D-ND	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	310	CLA	CHC-C1C	3.25	1.43	1.35
23	D	403	CLA	CHC-C1C	3.24	1.43	1.35
23	N	602	CLA	CHC-C1C	3.23	1.43	1.35
34	F	101	HEM	C3C-C2C	-3.20	1.35	1.40
34	f	101	HEM	C3C-C2C	-3.20	1.35	1.40
23	Y	303	CLA	C4D-ND	-3.19	1.33	1.37
23	C	509	CLA	C4D-ND	-3.19	1.33	1.37
23	s	609	CLA	CHC-C1C	3.19	1.43	1.35
35	y	310	CHL	CMB-C2B	-3.19	1.45	1.51
23	G	602	CLA	C4D-ND	-3.18	1.33	1.37
23	d	403	CLA	CHC-C1C	3.16	1.43	1.35
23	c	508	CLA	C4D-ND	-3.16	1.33	1.37
23	b	612	CLA	C4D-ND	-3.15	1.33	1.37
34	f	101	HEM	CAB-C3B	3.15	1.56	1.47
35	N	601	CHL	CHC-C1C	3.15	1.43	1.35
34	F	101	HEM	CAB-C3B	3.14	1.56	1.47
23	s	602	CLA	C4D-ND	-3.14	1.33	1.37
23	B	610	CLA	C4D-ND	-3.14	1.33	1.37
35	Y	309	CHL	CHC-C1C	3.14	1.43	1.35
35	s	607	CHL	CHC-C1C	3.14	1.43	1.35
23	S	303	CLA	C4D-ND	-3.14	1.33	1.37
23	y	311	CLA	CHC-C1C	3.13	1.43	1.35
23	B	616	CLA	CHC-C1C	3.13	1.43	1.35
23	S	305	CLA	C4D-ND	-3.13	1.33	1.37
35	Y	310	CHL	CMB-C2B	-3.13	1.45	1.51
23	N	613	CLA	C4D-ND	-3.13	1.33	1.37
35	y	309	CHL	CHC-C1C	3.13	1.43	1.35
23	b	614	CLA	CHC-C1C	3.12	1.43	1.35
35	n	601	CHL	CHC-C1C	3.12	1.43	1.35
35	S	306	CHL	C4D-ND	-3.11	1.33	1.37
23	b	604	CLA	CHC-C1C	3.11	1.42	1.35
23	r	602	CLA	CHC-C1C	3.11	1.42	1.35
23	b	603	CLA	C4D-ND	-3.11	1.33	1.37
35	S	308	CHL	CHC-C1C	3.11	1.42	1.35
23	n	613	CLA	C4D-ND	-3.11	1.33	1.37
23	y	303	CLA	C4D-ND	-3.11	1.33	1.37
23	B	606	CLA	C4D-ND	-3.10	1.33	1.37
23	b	608	CLA	C4D-ND	-3.10	1.33	1.37
23	c	504	CLA	C4D-ND	-3.10	1.33	1.37
23	G	604	CLA	CHC-C1C	3.10	1.42	1.35
35	N	608	CHL	CHC-C1C	3.10	1.42	1.35
35	n	606	CHL	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	309	CLA	CHC-C1C	3.09	1.42	1.35
23	b	618	CLA	CHC-C1C	3.09	1.42	1.35
35	n	608	CHL	CHC-C1C	3.09	1.42	1.35
23	B	605	CLA	C4D-ND	-3.09	1.33	1.37
23	R	303	CLA	CHC-C1C	3.09	1.42	1.35
23	B	612	CLA	CHC-C1C	3.09	1.42	1.35
35	G	607	CHL	CHC-C1C	3.08	1.42	1.35
35	g	609	CHL	CMB-C2B	-3.08	1.45	1.51
23	S	310	CLA	C4D-ND	-3.08	1.33	1.37
23	B	602	CLA	CHC-C1C	3.08	1.42	1.35
23	c	513	CLA	CHC-C1C	3.08	1.42	1.35
35	s	601	CHL	CHC-C1C	3.08	1.42	1.35
23	n	602	CLA	CHC-C1C	3.08	1.42	1.35
23	s	604	CLA	C4D-ND	-3.07	1.33	1.37
23	s	608	CLA	CHC-C1C	3.07	1.42	1.35
35	g	608	CHL	CHC-C1C	3.07	1.42	1.35
23	B	608	CLA	C4D-ND	-3.07	1.33	1.37
35	G	606	CHL	CHC-C1C	3.07	1.42	1.35
23	b	613	CLA	C4D-ND	-3.07	1.33	1.37
23	C	514	CLA	C4D-ND	-3.07	1.33	1.37
35	N	606	CHL	CHC-C1C	3.07	1.42	1.35
35	G	608	CHL	CHC-C1C	3.07	1.42	1.35
23	A	404	CLA	CHC-C1C	3.07	1.42	1.35
23	G	611	CLA	CHC-C1C	3.07	1.42	1.35
35	N	607	CHL	CHC-C1C	3.07	1.42	1.35
35	r	605	CHL	CHC-C1C	3.06	1.42	1.35
23	y	312	CLA	C4D-ND	-3.06	1.33	1.37
23	c	513	CLA	C4D-ND	-3.06	1.33	1.37
23	N	603	CLA	C4D-ND	-3.06	1.33	1.37
23	y	312	CLA	CHC-C1C	3.06	1.42	1.35
23	C	505	CLA	C4D-ND	-3.06	1.33	1.37
35	r	606	CHL	CHC-C1C	3.06	1.42	1.35
38	Y	318	NEX	C7-C8	-3.06	1.26	1.32
23	b	616	CLA	CHC-C1C	3.06	1.42	1.35
23	g	603	CLA	C4D-ND	-3.06	1.33	1.37
23	g	613	CLA	C4D-ND	-3.06	1.33	1.37
23	d	402	CLA	CHC-C1C	3.06	1.42	1.35
35	y	302	CHL	CHC-C1C	3.06	1.42	1.35
35	N	605	CHL	CHC-C1C	3.06	1.42	1.35
35	R	306	CHL	CHC-C1C	3.06	1.42	1.35
23	c	510	CLA	CHC-C1C	3.06	1.42	1.35
23	Y	312	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	314	CLA	C4D-ND	-3.05	1.33	1.37
35	y	306	CHL	CHC-C1C	3.05	1.42	1.35
23	C	503	CLA	C4D-ND	-3.05	1.33	1.37
23	D	404	CLA	C4D-ND	-3.05	1.33	1.37
23	C	507	CLA	C4D-ND	-3.05	1.33	1.37
23	N	610	CLA	CHC-C1C	3.05	1.42	1.35
23	g	611	CLA	CHC-C1C	3.05	1.42	1.35
23	c	506	CLA	C4D-ND	-3.05	1.33	1.37
23	d	403	CLA	C4D-ND	-3.05	1.33	1.37
35	n	607	CHL	CHC-C1C	3.05	1.42	1.35
35	S	302	CHL	CHC-C1C	3.05	1.42	1.35
23	r	612	CLA	C4D-ND	-3.05	1.33	1.37
23	y	314	CLA	C4D-ND	-3.05	1.33	1.37
23	B	614	CLA	C4D-ND	-3.04	1.33	1.37
35	Y	302	CHL	CHC-C1C	3.04	1.42	1.35
23	B	607	CLA	C4D-ND	-3.04	1.33	1.37
23	B	611	CLA	C4D-ND	-3.04	1.33	1.37
35	s	605	CHL	CHC-C1C	3.04	1.42	1.35
23	g	602	CLA	C4D-ND	-3.04	1.33	1.37
35	R	308	CHL	CHC-C1C	3.04	1.42	1.35
23	r	608	CLA	CHC-C1C	3.04	1.42	1.35
23	R	311	CLA	CHC-C1C	3.04	1.42	1.35
23	B	614	CLA	CHC-C1C	3.04	1.42	1.35
23	D	401	CLA	C4D-ND	-3.04	1.33	1.37
23	G	613	CLA	C4D-ND	-3.04	1.33	1.37
23	B	601	CLA	C4D-ND	-3.04	1.33	1.37
23	G	614	CLA	CHC-C1C	3.04	1.42	1.35
35	R	307	CHL	CHC-C1C	3.04	1.42	1.35
23	r	609	CLA	CHC-C1C	3.04	1.42	1.35
23	r	611	CLA	CHC-C1C	3.04	1.42	1.35
23	R	312	CLA	CHC-C1C	3.04	1.42	1.35
23	r	610	CLA	CHC-C1C	3.04	1.42	1.35
23	c	501	CLA	CHC-C1C	3.03	1.42	1.35
23	a	404	CLA	C4D-ND	-3.03	1.33	1.37
23	N	604	CLA	CHC-C1C	3.03	1.42	1.35
23	b	609	CLA	CHC-C1C	3.03	1.42	1.35
23	a	404	CLA	CHC-C1C	3.03	1.42	1.35
23	b	607	CLA	C4D-ND	-3.03	1.33	1.37
35	G	609	CHL	C4D-ND	-3.03	1.33	1.37
35	y	307	CHL	CHC-C1C	3.03	1.42	1.35
23	S	305	CLA	CHC-C1C	3.02	1.42	1.35
35	y	309	CHL	C4D-ND	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHC-C1C	3.02	1.42	1.35
35	r	607	CHL	CHC-C1C	3.02	1.42	1.35
35	Y	308	CHL	CHC-C1C	3.02	1.42	1.35
23	D	403	CLA	C4D-ND	-3.02	1.33	1.37
23	r	603	CLA	CHC-C1C	3.02	1.42	1.35
23	g	604	CLA	CHC-C1C	3.02	1.42	1.35
35	S	307	CHL	CHC-C1C	3.02	1.42	1.35
23	y	315	CLA	CHC-C1C	3.02	1.42	1.35
23	R	302	CLA	CHC-C1C	3.02	1.42	1.35
23	b	611	CLA	C4D-ND	-3.02	1.33	1.37
23	g	614	CLA	CHC-C1C	3.02	1.42	1.35
23	r	609	CLA	C4D-ND	-3.02	1.33	1.37
23	C	511	CLA	CHC-C1C	3.01	1.42	1.35
35	Y	307	CHL	CHC-C1C	3.01	1.42	1.35
23	c	501	CLA	C4D-ND	-3.01	1.33	1.37
23	s	609	CLA	C4D-ND	-3.01	1.33	1.37
23	b	610	CLA	C4D-ND	-3.01	1.33	1.37
35	Y	306	CHL	CHC-C1C	3.01	1.42	1.35
35	y	310	CHL	CHC-C1C	3.01	1.42	1.35
23	S	305	CLA	CMB-C2B	-3.01	1.45	1.51
23	B	601	CLA	CHC-C1C	3.01	1.42	1.35
23	C	502	CLA	CHC-C1C	3.01	1.42	1.35
35	Y	310	CHL	CHC-C1C	3.01	1.42	1.35
35	y	308	CHL	CHC-C1C	3.01	1.42	1.35
23	g	610	CLA	C4D-ND	-3.01	1.33	1.37
23	a	401	CLA	C4D-ND	-3.00	1.33	1.37
23	Y	312	CLA	C4D-ND	-3.00	1.33	1.37
23	b	609	CLA	C4D-ND	-3.00	1.33	1.37
23	A	401	CLA	C4D-ND	-3.00	1.33	1.37
23	S	311	CLA	C4D-ND	-3.00	1.33	1.37
35	g	607	CHL	C4D-ND	-3.00	1.33	1.37
23	C	509	CLA	CHC-C1C	3.00	1.42	1.35
23	r	601	CLA	CHC-C1C	3.00	1.42	1.35
23	b	615	CLA	CHC-C1C	3.00	1.42	1.35
23	y	303	CLA	CHC-C1C	3.00	1.42	1.35
23	y	315	CLA	C4D-ND	-3.00	1.33	1.37
23	r	612	CLA	CHC-C1C	3.00	1.42	1.35
35	G	605	CHL	CHC-C1C	3.00	1.42	1.35
23	n	604	CLA	CHC-C1C	3.00	1.42	1.35
23	A	404	CLA	C4D-ND	-3.00	1.33	1.37
23	B	607	CLA	CHC-C1C	3.00	1.42	1.35
23	B	609	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	s	606	CHL	CHC-C1C	2.99	1.42	1.35
23	R	313	CLA	C4D-ND	-2.99	1.33	1.37
23	b	603	CLA	CHC-C1C	2.99	1.42	1.35
23	S	311	CLA	CHC-C1C	2.99	1.42	1.35
23	G	602	CLA	CHC-C1C	2.99	1.42	1.35
23	c	512	CLA	C4D-ND	-2.99	1.33	1.37
23	c	502	CLA	C4D-ND	-2.99	1.33	1.37
23	s	603	CLA	CHC-C1C	2.99	1.42	1.35
23	S	312	CLA	CHC-C1C	2.99	1.42	1.35
23	N	611	CLA	C4D-ND	-2.99	1.33	1.37
23	s	604	CLA	CHC-C1C	2.99	1.42	1.35
23	s	602	CLA	CHC-C1C	2.99	1.42	1.35
23	r	608	CLA	C4D-ND	-2.99	1.33	1.37
23	Y	305	CLA	CHC-C1C	2.99	1.42	1.35
23	C	507	CLA	CHC-C1C	2.99	1.42	1.35
35	Y	309	CHL	C4D-ND	-2.99	1.33	1.37
23	R	305	CLA	C4D-ND	-2.98	1.33	1.37
23	s	613	CLA	CHC-C1C	2.98	1.42	1.35
23	n	614	CLA	CHC-C1C	2.98	1.42	1.35
35	N	609	CHL	C4D-ND	-2.98	1.33	1.37
23	B	611	CLA	CHC-C1C	2.98	1.42	1.35
23	d	404	CLA	C4D-ND	-2.98	1.33	1.37
23	n	604	CLA	C4D-ND	-2.98	1.33	1.37
23	y	305	CLA	CHC-C1C	2.98	1.42	1.35
23	d	401	CLA	C4D-ND	-2.98	1.33	1.37
23	S	309	CLA	CHC-C1C	2.98	1.42	1.35
23	N	614	CLA	CHC-C1C	2.98	1.42	1.35
23	S	303	CLA	CHC-C1C	2.98	1.42	1.35
23	c	508	CLA	CHC-C1C	2.98	1.42	1.35
35	g	605	CHL	CHC-C1C	2.98	1.42	1.35
23	C	510	CLA	CHC-C1C	2.98	1.42	1.35
23	R	305	CLA	CHC-C1C	2.98	1.42	1.35
23	R	304	CLA	CHC-C1C	2.98	1.42	1.35
23	n	610	CLA	CHC-C1C	2.98	1.42	1.35
23	Y	305	CLA	C4D-ND	-2.98	1.33	1.37
35	r	607	CHL	C4D-ND	-2.98	1.33	1.37
23	g	612	CLA	CHC-C1C	2.98	1.42	1.35
35	n	605	CHL	CHC-C1C	2.97	1.42	1.35
23	S	314	CLA	CHC-C1C	2.97	1.42	1.35
23	s	610	CLA	CHC-C1C	2.97	1.42	1.35
23	N	604	CLA	C4D-ND	-2.97	1.33	1.37
23	b	613	CLA	CHC-C1C	2.97	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHC-C1C	2.97	1.42	1.35
23	Y	313	CLA	C4D-ND	-2.97	1.33	1.37
23	r	604	CLA	C4D-ND	-2.97	1.33	1.37
23	C	512	CLA	CHC-C1C	2.97	1.42	1.35
23	c	509	CLA	CHC-C1C	2.97	1.42	1.35
26	A	406	SQD	C6-S	-2.97	1.66	1.77
26	a	406	SQD	C6-S	-2.97	1.66	1.77
23	C	504	CLA	CHC-C1C	2.97	1.42	1.35
23	Y	305	CLA	CMB-C2B	-2.97	1.45	1.51
23	D	401	CLA	CHC-C1C	2.97	1.42	1.35
23	N	614	CLA	C4D-ND	-2.97	1.33	1.37
23	Y	311	CLA	CHC-C1C	2.96	1.42	1.35
23	B	613	CLA	CHC-C1C	2.96	1.42	1.35
23	c	511	CLA	CHC-C1C	2.96	1.42	1.35
23	b	610	CLA	CHC-C1C	2.96	1.42	1.35
23	Y	315	CLA	C4D-ND	-2.96	1.33	1.37
23	c	503	CLA	C4D-ND	-2.96	1.33	1.37
23	C	502	CLA	C4D-ND	-2.96	1.33	1.37
23	c	503	CLA	CHC-C1C	2.96	1.42	1.35
23	R	303	CLA	C4D-ND	-2.96	1.33	1.37
23	Y	315	CLA	CHC-C1C	2.96	1.42	1.35
23	S	314	CLA	C4D-ND	-2.96	1.33	1.37
23	b	616	CLA	C4D-ND	-2.96	1.33	1.37
23	c	506	CLA	CHC-C1C	2.96	1.42	1.35
23	B	609	CLA	CHC-C1C	2.95	1.42	1.35
23	b	611	CLA	CHC-C1C	2.95	1.42	1.35
23	B	606	CLA	CHC-C1C	2.95	1.42	1.35
23	g	602	CLA	CHC-C1C	2.95	1.42	1.35
23	b	605	CLA	CHC-C1C	2.95	1.42	1.35
35	g	606	CHL	CHC-C1C	2.95	1.42	1.35
35	Y	306	CHL	C4D-ND	-2.95	1.33	1.37
35	N	608	CHL	C4D-ND	-2.95	1.33	1.37
26	L	103	SQD	C6-S	-2.94	1.66	1.77
23	C	504	CLA	C4D-ND	-2.94	1.33	1.37
23	y	305	CLA	C4D-ND	-2.94	1.33	1.37
23	B	603	CLA	CHC-C1C	2.94	1.42	1.35
23	y	313	CLA	CHC-C1C	2.94	1.42	1.35
23	r	604	CLA	CHC-C1C	2.94	1.42	1.35
35	g	607	CHL	CHC-C1C	2.94	1.42	1.35
35	G	607	CHL	C4D-ND	-2.94	1.33	1.37
35	n	609	CHL	C4D-ND	-2.94	1.33	1.37
23	Y	311	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C4D-ND	-2.94	1.33	1.37
23	c	510	CLA	C4D-ND	-2.94	1.33	1.37
23	n	602	CLA	C4D-ND	-2.94	1.33	1.37
23	R	310	CLA	C4D-ND	-2.94	1.33	1.37
23	b	615	CLA	C4D-ND	-2.93	1.33	1.37
35	N	606	CHL	C4D-ND	-2.93	1.33	1.37
23	c	505	CLA	C4D-ND	-2.93	1.33	1.37
23	b	606	CLA	C4D-ND	-2.93	1.33	1.37
23	C	506	CLA	CHC-C1C	2.93	1.42	1.35
35	n	606	CHL	C4D-ND	-2.93	1.33	1.37
23	A	402	CLA	CHC-C1C	2.93	1.42	1.35
23	B	604	CLA	C4D-ND	-2.93	1.33	1.37
23	Y	303	CLA	CHC-C1C	2.93	1.42	1.35
23	S	313	CLA	C4D-ND	-2.92	1.33	1.37
23	R	309	CLA	C4D-ND	-2.92	1.33	1.37
23	n	613	CLA	CHC-C1C	2.92	1.42	1.35
23	c	504	CLA	CHC-C1C	2.92	1.42	1.35
35	G	608	CHL	C4D-ND	-2.92	1.33	1.37
35	n	609	CHL	CHC-C1C	2.92	1.42	1.35
35	y	306	CHL	C4D-ND	-2.92	1.33	1.37
23	n	610	CLA	C4D-ND	-2.92	1.33	1.37
23	g	604	CLA	C4D-ND	-2.92	1.33	1.37
23	N	613	CLA	CHC-C1C	2.92	1.42	1.35
23	n	614	CLA	C4D-ND	-2.92	1.33	1.37
35	s	606	CHL	C4D-ND	-2.92	1.33	1.37
23	A	401	CLA	CHC-C1C	2.92	1.42	1.35
23	G	612	CLA	CHC-C1C	2.92	1.42	1.35
23	B	603	CLA	C4D-ND	-2.92	1.33	1.37
23	N	610	CLA	C4D-ND	-2.92	1.33	1.37
23	b	614	CLA	C4D-ND	-2.92	1.33	1.37
26	l	101	SQD	C6-S	-2.92	1.66	1.77
23	n	603	CLA	C4D-ND	-2.92	1.33	1.37
23	b	608	CLA	CHC-C1C	2.92	1.42	1.35
23	N	611	CLA	CHC-C1C	2.91	1.42	1.35
23	y	313	CLA	C4D-ND	-2.91	1.33	1.37
35	g	605	CHL	C4D-ND	-2.91	1.33	1.37
23	C	506	CLA	C4D-ND	-2.91	1.33	1.37
23	n	612	CLA	CHC-C1C	2.91	1.42	1.35
23	b	617	CLA	CHC-C1C	2.91	1.42	1.35
23	c	511	CLA	C4D-ND	-2.91	1.33	1.37
23	B	608	CLA	CHC-C1C	2.91	1.42	1.35
23	G	604	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	609	CHL	CHC-C1C	2.91	1.42	1.35
23	C	513	CLA	C4D-ND	-2.91	1.33	1.37
23	R	311	CLA	C4D-ND	-2.91	1.33	1.37
23	s	612	CLA	CHC-C1C	2.91	1.42	1.35
35	n	608	CHL	C4D-ND	-2.91	1.33	1.37
23	S	304	CLA	CHC-C1C	2.91	1.42	1.35
23	r	610	CLA	C4D-ND	-2.91	1.33	1.37
23	s	611	CLA	CHC-C1C	2.90	1.42	1.35
23	n	611	CLA	CHC-C1C	2.90	1.42	1.35
23	B	616	CLA	C4D-ND	-2.90	1.33	1.37
23	C	510	CLA	C4D-ND	-2.90	1.33	1.37
23	y	305	CLA	CMB-C2B	-2.90	1.45	1.51
23	Y	314	CLA	CHC-C1C	2.90	1.42	1.35
23	c	509	CLA	C4D-ND	-2.90	1.33	1.37
23	s	603	CLA	C4D-ND	-2.90	1.33	1.37
38	R	301	NEX	C7-C8	-2.90	1.27	1.32
23	C	511	CLA	C4D-ND	-2.90	1.33	1.37
23	G	603	CLA	C4D-ND	-2.89	1.33	1.37
23	s	613	CLA	C4D-ND	-2.89	1.33	1.37
23	g	613	CLA	CHC-C1C	2.89	1.42	1.35
23	y	314	CLA	CHC-C1C	2.89	1.42	1.35
23	G	611	CLA	C4D-ND	-2.89	1.33	1.37
35	y	307	CHL	C4D-ND	-2.89	1.33	1.37
35	R	307	CHL	C4D-ND	-2.89	1.33	1.37
23	G	610	CLA	C4D-ND	-2.89	1.33	1.37
23	g	614	CLA	C4D-ND	-2.89	1.33	1.37
35	n	607	CHL	C4D-ND	-2.89	1.33	1.37
23	n	611	CLA	C4D-ND	-2.89	1.33	1.37
23	G	603	CLA	CHC-C1C	2.89	1.42	1.35
23	C	505	CLA	CHC-C1C	2.89	1.42	1.35
23	c	507	CLA	CHC-C1C	2.89	1.42	1.35
23	B	615	CLA	CHC-C1C	2.89	1.42	1.35
23	G	613	CLA	CHC-C1C	2.89	1.42	1.35
35	S	306	CHL	CHC-C1C	2.88	1.42	1.35
35	Y	307	CHL	C4D-ND	-2.88	1.33	1.37
23	R	310	CLA	CHC-C1C	2.88	1.42	1.35
23	G	610	CLA	CHC-C1C	2.88	1.42	1.35
23	g	610	CLA	CHC-C1C	2.88	1.42	1.35
35	R	306	CHL	C4D-ND	-2.88	1.33	1.37
23	N	612	CLA	CHC-C1C	2.88	1.42	1.35
23	r	602	CLA	C4D-ND	-2.88	1.33	1.37
23	y	304	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHC-C1C	2.88	1.42	1.35
23	d	401	CLA	CHC-C1C	2.88	1.42	1.35
23	d	404	CLA	CHC-C1C	2.87	1.42	1.35
23	B	602	CLA	C4D-ND	-2.87	1.33	1.37
23	s	612	CLA	C4D-ND	-2.87	1.33	1.37
23	D	404	CLA	CHC-C1C	2.87	1.42	1.35
23	R	313	CLA	CHC-C1C	2.87	1.42	1.35
23	B	613	CLA	C4D-ND	-2.87	1.33	1.37
35	R	308	CHL	C4D-ND	-2.87	1.33	1.37
23	C	513	CLA	CHC-C1C	2.87	1.42	1.35
23	a	401	CLA	CHC-C1C	2.87	1.42	1.35
23	s	610	CLA	C4D-ND	-2.86	1.33	1.37
23	N	602	CLA	C4D-ND	-2.86	1.33	1.37
23	b	618	CLA	C4D-ND	-2.86	1.33	1.37
23	Y	313	CLA	CHC-C1C	2.86	1.42	1.35
23	C	503	CLA	CHC-C1C	2.85	1.42	1.35
23	y	311	CLA	C4D-ND	-2.85	1.33	1.37
35	Y	310	CHL	C4D-ND	-2.85	1.33	1.37
23	B	612	CLA	C4D-ND	-2.85	1.33	1.37
35	N	607	CHL	C4D-ND	-2.85	1.33	1.37
23	G	614	CLA	C4D-ND	-2.85	1.33	1.37
35	r	606	CHL	C4D-ND	-2.85	1.33	1.37
23	R	313	CLA	CMB-C2B	-2.85	1.45	1.51
35	s	605	CHL	C4D-ND	-2.85	1.33	1.37
23	c	512	CLA	CHC-C1C	2.84	1.42	1.35
35	G	605	CHL	C4D-ND	-2.84	1.33	1.37
23	c	502	CLA	CHC-C1C	2.84	1.42	1.35
23	b	604	CLA	C4D-ND	-2.84	1.33	1.37
23	c	507	CLA	C4D-ND	-2.83	1.33	1.37
33	d	406	PL9	C36-C34	2.83	1.57	1.51
23	S	304	CLA	C4D-ND	-2.83	1.33	1.37
23	r	611	CLA	C4D-ND	-2.83	1.33	1.37
35	S	307	CHL	C4D-ND	-2.83	1.33	1.37
23	C	508	CLA	C4D-ND	-2.83	1.33	1.37
35	r	605	CHL	C4D-ND	-2.83	1.33	1.37
23	b	606	CLA	CMB-C2B	-2.83	1.45	1.51
23	g	611	CLA	C4D-ND	-2.83	1.33	1.37
23	n	603	CLA	CHC-C1C	2.83	1.42	1.35
35	s	601	CHL	C4D-ND	-2.82	1.33	1.37
23	n	604	CLA	CMB-C2B	-2.82	1.45	1.51
23	b	612	CLA	CHC-C1C	2.82	1.42	1.35
35	N	609	CHL	CHC-C1C	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	406	PL9	C36-C34	2.82	1.57	1.51
23	Y	304	CLA	CHC-C1C	2.81	1.42	1.35
23	N	612	CLA	C4D-ND	-2.81	1.33	1.37
23	S	313	CLA	CHC-C1C	2.81	1.42	1.35
35	S	308	CHL	C4D-ND	-2.81	1.33	1.37
35	G	609	CHL	CHC-C1C	2.81	1.42	1.35
23	R	304	CLA	C4D-ND	-2.81	1.33	1.37
35	s	607	CHL	C4D-ND	-2.81	1.33	1.37
23	B	608	CLA	CMB-C2B	-2.81	1.45	1.51
23	B	605	CLA	CHC-C1C	2.81	1.42	1.35
23	r	603	CLA	C4D-ND	-2.81	1.33	1.37
35	y	308	CHL	C4D-ND	-2.80	1.33	1.37
35	y	310	CHL	C4D-ND	-2.80	1.33	1.37
23	g	604	CLA	CMB-C2B	-2.80	1.45	1.51
23	B	610	CLA	CHC-C1C	2.79	1.42	1.35
23	C	512	CLA	C4D-ND	-2.79	1.33	1.37
23	R	312	CLA	C4D-ND	-2.79	1.33	1.37
35	g	606	CHL	C4D-ND	-2.79	1.33	1.37
23	n	612	CLA	C4D-ND	-2.79	1.33	1.37
23	s	608	CLA	C4D-ND	-2.79	1.33	1.37
35	g	608	CHL	C4D-ND	-2.78	1.33	1.37
23	B	604	CLA	CMB-C2B	-2.77	1.45	1.51
23	s	611	CLA	C4D-ND	-2.77	1.33	1.37
38	r	615	NEX	C7-C8	-2.77	1.27	1.32
23	c	506	CLA	CMB-C2B	-2.77	1.45	1.51
35	G	601	CHL	C4D-ND	-2.77	1.33	1.37
23	g	603	CLA	CHC-C1C	2.76	1.42	1.35
23	y	304	CLA	CHC-C1C	2.76	1.42	1.35
23	b	609	CLA	CMB-C2B	-2.76	1.45	1.51
33	d	406	PL9	C41-C39	2.75	1.57	1.51
23	g	612	CLA	C4D-ND	-2.74	1.33	1.37
35	g	601	CHL	CHC-C1C	2.74	1.42	1.35
23	N	604	CLA	CMB-C2B	-2.74	1.45	1.51
23	c	510	CLA	CMD-C2D	-2.74	1.45	1.50
23	N	603	CLA	CHC-C1C	2.74	1.42	1.35
23	B	607	CLA	CMB-C2B	-2.74	1.45	1.51
23	r	601	CLA	C4D-ND	-2.74	1.33	1.37
23	R	302	CLA	C4D-ND	-2.73	1.33	1.37
35	g	601	CHL	C4D-ND	-2.73	1.33	1.37
35	G	606	CHL	C4D-ND	-2.73	1.33	1.37
23	b	607	CLA	CHC-C1C	2.73	1.42	1.35
35	G	601	CHL	CHC-C1C	2.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	s	616	NEX	C7-C8	-2.73	1.27	1.32
23	G	612	CLA	C4D-ND	-2.73	1.33	1.37
23	S	309	CLA	C4D-ND	-2.73	1.33	1.37
23	Y	304	CLA	C4D-ND	-2.72	1.33	1.37
35	G	609	CHL	CMB-C2B	-2.72	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.72	1.46	1.51
33	D	406	PL9	C41-C39	2.71	1.56	1.51
35	n	605	CHL	C4D-ND	-2.71	1.34	1.37
35	n	601	CHL	C4D-ND	-2.70	1.34	1.37
23	r	604	CLA	CMB-C2B	-2.70	1.46	1.51
23	S	312	CLA	C4D-ND	-2.70	1.34	1.37
23	r	612	CLA	CMB-C2B	-2.70	1.46	1.51
23	d	402	CLA	CMB-C2B	-2.69	1.46	1.51
35	S	302	CHL	C4D-ND	-2.69	1.34	1.37
38	G	618	NEX	C7-C8	-2.69	1.27	1.32
35	Y	302	CHL	C4D-ND	-2.68	1.34	1.37
23	R	305	CLA	CMB-C2B	-2.68	1.46	1.51
23	B	604	CLA	CHC-C1C	2.68	1.41	1.35
35	Y	308	CHL	C4D-ND	-2.68	1.34	1.37
23	B	615	CLA	C4D-ND	-2.66	1.34	1.37
23	c	508	CLA	CMB-C2B	-2.66	1.46	1.51
23	b	605	CLA	CMB-C2B	-2.66	1.46	1.51
23	b	617	CLA	C4D-ND	-2.66	1.34	1.37
23	b	606	CLA	CHC-C1C	2.65	1.41	1.35
23	C	509	CLA	CMB-C2B	-2.65	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.65	1.46	1.51
35	n	609	CHL	CMB-C2B	-2.64	1.46	1.51
23	c	502	CLA	CMB-C2B	-2.64	1.46	1.51
23	G	604	CLA	CMB-C2B	-2.63	1.46	1.51
35	N	609	CHL	CMB-C2B	-2.63	1.46	1.51
23	s	604	CLA	CMB-C2B	-2.62	1.46	1.51
23	C	503	CLA	CMB-C2B	-2.62	1.46	1.51
33	d	406	PL9	C21-C19	2.61	1.56	1.51
35	y	302	CHL	C4D-ND	-2.61	1.34	1.37
23	b	610	CLA	CMB-C2B	-2.60	1.46	1.51
26	b	602	SQD	C6-S	-2.59	1.67	1.77
23	b	616	CLA	CMB-C2B	-2.59	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.59	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.59	1.46	1.51
33	D	406	PL9	C21-C19	2.59	1.56	1.51
35	R	308	CHL	CMB-C2B	-2.58	1.46	1.51
23	R	310	CLA	CMB-C2B	-2.58	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	608	CHL	CMB-C2B	-2.58	1.46	1.51
23	g	603	CLA	CMB-C2B	-2.57	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.57	1.46	1.51
26	B	625	SQD	C6-S	-2.57	1.67	1.77
38	g	618	NEX	C7-C8	-2.57	1.27	1.32
26	c	520	SQD	C6-S	-2.57	1.67	1.77
23	A	402	CLA	CMB-C2B	-2.56	1.46	1.51
23	S	313	CLA	CMB-C2B	-2.56	1.46	1.51
23	b	615	CLA	CMB-C2B	-2.56	1.46	1.51
23	d	401	CLA	CMB-C2B	-2.55	1.46	1.51
35	N	601	CHL	C4D-ND	-2.55	1.34	1.37
23	S	314	CLA	CMB-C2B	-2.55	1.46	1.51
35	g	601	CHL	CMB-C2B	-2.55	1.46	1.51
23	B	606	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	613	CLA	CMB-C2B	-2.55	1.46	1.51
26	C	521	SQD	C6-S	-2.54	1.68	1.77
38	R	316	NEX	C7-C8	-2.54	1.27	1.32
23	c	505	CLA	CMB-C2B	-2.54	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.54	1.46	1.51
35	N	608	CHL	CMB-C2B	-2.53	1.46	1.51
35	S	306	CHL	CMB-C2B	-2.53	1.46	1.51
23	s	602	CLA	CMB-C2B	-2.53	1.46	1.51
23	C	511	CLA	CMD-C2D	-2.53	1.45	1.50
23	c	501	CLA	CMB-C2B	-2.53	1.46	1.51
35	N	605	CHL	C4D-ND	-2.53	1.34	1.37
23	s	613	CLA	CMB-C2B	-2.53	1.46	1.51
35	Y	308	CHL	CMB-C2B	-2.53	1.46	1.51
23	b	615	CLA	C3B-C2B	-2.53	1.36	1.40
35	g	609	CHL	C4D-ND	-2.52	1.34	1.37
23	D	401	CLA	CMB-C2B	-2.52	1.46	1.51
23	R	303	CLA	CMB-C2B	-2.52	1.46	1.51
23	n	603	CLA	CMB-C2B	-2.52	1.46	1.51
23	c	509	CLA	CMB-C2B	-2.51	1.46	1.51
23	S	303	CLA	CMB-C2B	-2.51	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.51	1.46	1.51
23	C	512	CLA	CMB-C2B	-2.51	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.51	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.51	1.46	1.51
35	Y	309	CHL	CMB-C2B	-2.51	1.46	1.51
23	y	304	CLA	CMB-C2B	-2.51	1.46	1.51
35	y	308	CHL	CMB-C2B	-2.51	1.46	1.51
23	B	602	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	CMB-C2B	-2.51	1.46	1.51
23	B	611	CLA	CMB-C2B	-2.50	1.46	1.51
23	C	510	CLA	CMB-C2B	-2.50	1.46	1.51
23	R	304	CLA	CMB-C2B	-2.50	1.46	1.51
23	S	304	CLA	CMB-C2B	-2.50	1.46	1.51
23	s	612	CLA	CMB-C2B	-2.49	1.46	1.51
23	N	603	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	601	CLA	CMB-C2B	-2.49	1.46	1.51
23	C	502	CLA	CMB-C2B	-2.49	1.46	1.51
23	r	602	CLA	CMB-C2B	-2.49	1.46	1.51
35	G	601	CHL	CMB-C2B	-2.49	1.46	1.51
23	a	401	CLA	CMB-C2B	-2.49	1.46	1.51
23	Y	304	CLA	CMB-C2B	-2.49	1.46	1.51
23	y	314	CLA	CMB-C2B	-2.49	1.46	1.51
35	y	309	CHL	CMB-C2B	-2.48	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.48	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.48	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.48	1.46	1.51
35	y	302	CHL	CMB-C2B	-2.48	1.46	1.51
23	A	401	CLA	CMB-C2B	-2.48	1.46	1.51
23	r	603	CLA	CMB-C2B	-2.48	1.46	1.51
23	y	315	CLA	CMB-C2B	-2.48	1.46	1.51
33	D	406	PL9	C7-C8	2.47	1.54	1.50
23	b	604	CLA	CMB-C2B	-2.47	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.47	1.46	1.51
23	c	504	CLA	CMB-C2B	-2.47	1.46	1.51
23	D	403	CLA	CMC-C2C	-2.47	1.45	1.50
23	s	610	CLA	CMB-C2B	-2.47	1.46	1.51
35	Y	302	CHL	CMB-C2B	-2.46	1.46	1.51
23	Y	311	CLA	CMB-C2B	-2.46	1.46	1.51
23	y	311	CLA	CMB-C2B	-2.46	1.46	1.51
35	G	605	CHL	CMB-C2B	-2.46	1.46	1.51
35	g	605	CHL	CMB-C2B	-2.46	1.46	1.51
23	G	610	CLA	CMB-C2B	-2.46	1.46	1.51
23	b	617	CLA	CMB-C2B	-2.46	1.46	1.51
23	s	609	CLA	CMB-C2B	-2.46	1.46	1.51
23	G	613	CLA	CMB-C2B	-2.46	1.46	1.51
38	S	317	NEX	C7-C8	-2.45	1.27	1.32
23	Y	314	CLA	CMB-C2B	-2.45	1.46	1.51
23	G	602	CLA	CMB-C2B	-2.45	1.46	1.51
35	g	607	CHL	CMB-C2B	-2.45	1.46	1.51
23	N	612	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	s	605	CHL	CMB-C2B	-2.45	1.46	1.51
23	r	611	CLA	CMB-C2B	-2.45	1.46	1.51
23	n	612	CLA	CMB-C2B	-2.45	1.46	1.51
35	g	608	CHL	CMB-C2B	-2.45	1.46	1.51
23	G	611	CLA	CMB-C2B	-2.44	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.44	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.44	1.46	1.51
23	s	611	CLA	CMB-C2B	-2.44	1.46	1.51
35	N	606	CHL	CMB-C2B	-2.44	1.46	1.51
33	d	406	PL9	C7-C8	2.44	1.54	1.50
23	d	403	CLA	CMC-C2C	-2.44	1.45	1.50
35	G	607	CHL	CMB-C2B	-2.44	1.46	1.51
23	G	603	CLA	CMB-C2B	-2.44	1.46	1.51
23	S	311	CLA	CMB-C2B	-2.44	1.46	1.51
35	g	609	CHL	C3B-C2B	-2.44	1.37	1.40
23	g	613	CLA	CMB-C2B	-2.44	1.46	1.51
23	n	614	CLA	CMB-C2B	-2.44	1.46	1.51
23	g	611	CLA	CMB-C2B	-2.44	1.46	1.51
35	r	607	CHL	CMB-C2B	-2.44	1.46	1.51
23	Y	315	CLA	CMB-C2B	-2.44	1.46	1.51
23	R	312	CLA	CMB-C2B	-2.43	1.46	1.51
23	R	302	CLA	CMB-C2B	-2.43	1.46	1.51
23	C	508	CLA	CMB-C2B	-2.43	1.46	1.51
23	N	614	CLA	CMB-C2B	-2.43	1.46	1.51
23	g	610	CLA	CMB-C2B	-2.43	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.43	1.46	1.51
35	s	606	CHL	CMB-C2B	-2.43	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.43	1.46	1.51
23	N	613	CLA	CMB-C2B	-2.43	1.46	1.51
23	B	613	CLA	C3B-C2B	-2.43	1.37	1.40
23	y	303	CLA	CMB-C2B	-2.43	1.46	1.51
35	N	607	CHL	CMB-C2B	-2.43	1.46	1.51
23	g	612	CLA	CMB-C2B	-2.43	1.46	1.51
35	n	607	CHL	CMB-C2B	-2.43	1.46	1.51
23	D	404	CLA	CMB-C2B	-2.42	1.46	1.51
23	C	514	CLA	CMB-C2B	-2.42	1.46	1.51
23	d	404	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	612	CLA	CMB-C2B	-2.42	1.46	1.51
23	a	401	CLA	CMC-C2C	-2.42	1.45	1.50
23	N	611	CLA	CMB-C2B	-2.42	1.46	1.51
23	R	309	CLA	CMB-C2B	-2.42	1.46	1.51
23	r	608	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	602	CLA	CMB-C2B	-2.42	1.46	1.51
35	G	606	CHL	CMB-C2B	-2.42	1.46	1.51
23	b	618	CLA	CMB-C2B	-2.42	1.46	1.51
23	R	311	CLA	CMB-C2B	-2.42	1.46	1.51
35	S	307	CHL	CMB-C2B	-2.42	1.46	1.51
23	Y	312	CLA	CMB-C2B	-2.42	1.46	1.51
35	r	606	CHL	CMB-C2B	-2.41	1.46	1.51
38	n	617	NEX	C7-C8	-2.41	1.27	1.32
35	n	606	CHL	CMB-C2B	-2.41	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.41	1.46	1.51
23	C	505	CLA	CMB-C2B	-2.41	1.46	1.51
23	s	603	CLA	CMB-C2B	-2.41	1.46	1.51
23	n	613	CLA	CMB-C2B	-2.41	1.46	1.51
35	s	601	CHL	CMB-C2B	-2.41	1.46	1.51
35	y	307	CHL	CMB-C2B	-2.40	1.46	1.51
23	r	601	CLA	CMB-C2B	-2.40	1.46	1.51
23	A	401	CLA	CMC-C2C	-2.40	1.45	1.50
35	Y	307	CHL	CMB-C2B	-2.40	1.46	1.51
35	Y	306	CHL	CMB-C2B	-2.40	1.46	1.51
23	r	610	CLA	CMB-C2B	-2.40	1.46	1.51
23	A	404	CLA	CMB-C2B	-2.40	1.46	1.51
23	Y	303	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	610	CLA	CMB-C2B	-2.39	1.46	1.51
23	C	511	CLA	CMB-C2B	-2.39	1.46	1.51
23	s	608	CLA	CMB-C2B	-2.39	1.46	1.51
23	c	512	CLA	CMB-C2B	-2.39	1.46	1.51
35	G	608	CHL	CMB-C2B	-2.39	1.46	1.51
23	g	614	CLA	CMB-C2B	-2.39	1.46	1.51
23	G	614	CLA	CMB-C2B	-2.39	1.46	1.51
35	S	302	CHL	CMB-C2B	-2.39	1.46	1.51
23	G	612	CLA	CMB-C2B	-2.39	1.46	1.51
35	s	607	CHL	CMB-C2B	-2.39	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.38	1.46	1.51
35	R	307	CHL	CMB-C2B	-2.38	1.46	1.51
23	c	510	CLA	CMB-C2B	-2.38	1.46	1.51
35	y	306	CHL	CMB-C2B	-2.38	1.46	1.51
23	r	609	CLA	CMB-C2B	-2.38	1.46	1.51
23	y	313	CLA	CMB-C2B	-2.38	1.46	1.51
38	N	617	NEX	C7-C8	-2.38	1.28	1.32
23	n	611	CLA	CMB-C2B	-2.37	1.46	1.51
23	S	309	CLA	CMB-C2B	-2.37	1.46	1.51
23	y	312	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	601	CHL	CMB-C2B	-2.37	1.46	1.51
35	N	601	CHL	CMB-C2B	-2.37	1.46	1.51
23	a	404	CLA	CMB-C2B	-2.37	1.46	1.51
35	g	606	CHL	CMB-C2B	-2.37	1.46	1.51
23	y	304	CLA	C3B-C2B	-2.36	1.37	1.40
23	n	610	CLA	CMB-C2B	-2.35	1.46	1.51
23	D	403	CLA	CMD-C2D	-2.35	1.45	1.50
23	n	602	CLA	CMB-C2B	-2.34	1.46	1.51
23	C	506	CLA	CMD-C2D	-2.34	1.45	1.50
23	d	402	CLA	C3B-C2B	-2.34	1.37	1.40
35	r	607	CHL	CMD-C2D	-2.34	1.45	1.50
35	R	306	CHL	CMB-C2B	-2.34	1.46	1.51
23	S	310	CLA	CMB-C2B	-2.33	1.46	1.51
23	c	505	CLA	CMD-C2D	-2.32	1.45	1.50
23	B	615	CLA	C3B-C2B	-2.32	1.37	1.40
23	Y	313	CLA	CMB-C2B	-2.32	1.46	1.51
23	S	312	CLA	CMB-C2B	-2.31	1.46	1.51
23	b	617	CLA	C3B-C2B	-2.30	1.37	1.40
23	b	609	CLA	C3B-C2B	-2.30	1.37	1.40
35	r	605	CHL	CMB-C2B	-2.30	1.46	1.51
23	B	605	CLA	CMD-C2D	-2.30	1.45	1.50
35	N	605	CHL	CMB-C2B	-2.30	1.46	1.51
35	Y	310	CHL	C3B-C2B	-2.29	1.37	1.40
23	d	403	CLA	CMD-C2D	-2.29	1.45	1.50
23	b	614	CLA	CMB-C2B	-2.29	1.46	1.51
35	n	605	CHL	CMB-C2B	-2.29	1.46	1.51
23	d	403	CLA	CMB-C2B	-2.28	1.46	1.51
23	B	612	CLA	CMB-C2B	-2.28	1.46	1.51
23	b	614	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	612	CLA	CMD-C2D	-2.27	1.46	1.50
23	N	602	CLA	CMB-C2B	-2.27	1.46	1.51
23	N	610	CLA	CMB-C2B	-2.27	1.46	1.51
35	S	308	CHL	CMB-C2B	-2.26	1.46	1.51
23	b	618	CLA	CMC-C2C	-2.25	1.46	1.50
23	B	604	CLA	CMD-C2D	-2.25	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.24	1.46	1.50
23	B	603	CLA	CMD-C2D	-2.24	1.46	1.50
23	a	401	CLA	CMD-C2D	-2.23	1.46	1.50
23	b	614	CLA	CMC-C2C	-2.23	1.46	1.50
23	b	610	CLA	CMD-C2D	-2.23	1.46	1.50
33	D	406	PL9	C5-C4	-2.23	1.39	1.47
23	b	607	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	406	PL9	C5-C4	-2.22	1.39	1.47
23	B	616	CLA	CMC-C2C	-2.22	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.21	1.46	1.50
33	D	406	PL9	C26-C24	2.21	1.55	1.51
33	d	406	PL9	C26-C24	2.21	1.55	1.51
23	c	501	CLA	CMD-C2D	-2.21	1.46	1.50
23	A	401	CLA	CMD-C2D	-2.20	1.46	1.50
23	N	603	CLA	C3B-C2B	-2.20	1.37	1.40
35	y	310	CHL	C3B-C2B	-2.20	1.37	1.40
23	N	611	CLA	CMD-C2D	-2.20	1.46	1.50
23	C	502	CLA	CMD-C2D	-2.20	1.46	1.50
35	Y	307	CHL	CMD-C2D	-2.20	1.46	1.50
35	g	609	CHL	MG-NA	2.20	2.11	2.06
35	R	308	CHL	CMD-C2D	-2.20	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.19	1.46	1.50
23	B	608	CLA	C3B-C2B	-2.19	1.37	1.40
23	B	607	CLA	C3B-C2B	-2.19	1.37	1.40
23	n	603	CLA	C3B-C2B	-2.19	1.37	1.40
35	G	601	CHL	C3B-C2B	-2.19	1.37	1.40
23	B	613	CLA	C3B-CAB	-2.18	1.43	1.47
23	B	612	CLA	CMC-C2C	-2.18	1.46	1.50
23	b	616	CLA	CMD-C2D	-2.17	1.46	1.50
35	g	601	CHL	C3B-C2B	-2.17	1.37	1.40
23	B	601	CLA	CMD-C2D	-2.17	1.46	1.50
23	Y	304	CLA	C3B-C2B	-2.17	1.37	1.40
23	b	615	CLA	C3B-CAB	-2.16	1.43	1.47
23	D	401	CLA	CMD-C2D	-2.16	1.46	1.50
23	n	611	CLA	CMD-C2D	-2.16	1.46	1.50
35	y	307	CHL	CMD-C2D	-2.16	1.46	1.50
35	Y	310	CHL	CMD-C2D	-2.16	1.46	1.50
23	B	606	CLA	CMC-C2C	-2.15	1.46	1.50
23	g	603	CLA	C3B-C2B	-2.15	1.37	1.40
35	g	608	CHL	CMD-C2D	-2.15	1.46	1.50
23	b	608	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	613	CLA	CMC-C2C	-2.15	1.46	1.50
23	y	304	CLA	CMD-C2D	-2.14	1.46	1.50
23	N	612	CLA	C3B-C2B	-2.13	1.37	1.40
35	G	601	CHL	CMD-C2D	-2.13	1.46	1.50
23	b	612	CLA	CMC-C2C	-2.13	1.46	1.50
23	B	606	CLA	CMD-C2D	-2.13	1.46	1.50
35	N	606	CHL	CMD-C2D	-2.13	1.46	1.50
35	G	608	CHL	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C3B-C2B	-2.13	1.37	1.40
23	S	314	CLA	CMD-C2D	-2.13	1.46	1.50
23	B	607	CLA	CMD-C2D	-2.13	1.46	1.50
35	Y	308	CHL	CMD-C2D	-2.13	1.46	1.50
23	c	501	CLA	C3B-C2B	-2.12	1.37	1.40
23	B	611	CLA	CMC-C2C	-2.12	1.46	1.50
23	b	603	CLA	CMD-C2D	-2.12	1.46	1.50
23	B	610	CLA	CMC-C2C	-2.12	1.46	1.50
23	b	618	CLA	CMD-C2D	-2.12	1.46	1.50
23	Y	304	CLA	CMD-C2D	-2.11	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.11	1.46	1.50
23	N	610	CLA	CMD-C2D	-2.11	1.46	1.50
23	n	612	CLA	C3B-C2B	-2.11	1.37	1.40
23	R	303	CLA	CMC-C2C	-2.11	1.46	1.50
23	c	503	CLA	CMD-C2D	-2.11	1.46	1.50
23	C	510	CLA	CMD-C2D	-2.11	1.46	1.50
23	r	603	CLA	CMD-C2D	-2.11	1.46	1.50
35	y	308	CHL	CMD-C2D	-2.11	1.46	1.50
23	A	402	CLA	C3B-C2B	-2.11	1.37	1.40
23	R	304	CLA	CMD-C2D	-2.10	1.46	1.50
23	C	514	CLA	CMD-C2D	-2.10	1.46	1.50
35	N	601	CHL	CMD-C2D	-2.10	1.46	1.50
23	b	609	CLA	CMD-C2D	-2.10	1.46	1.50
35	g	601	CHL	CMD-C2D	-2.10	1.46	1.50
23	Y	315	CLA	CMD-C2D	-2.10	1.46	1.50
23	R	302	CLA	CMD-C2D	-2.10	1.46	1.50
23	y	315	CLA	CMD-C2D	-2.10	1.46	1.50
35	n	608	CHL	CMD-C2D	-2.10	1.46	1.50
23	G	612	CLA	CMD-C2D	-2.10	1.46	1.50
35	y	310	CHL	CMD-C2D	-2.10	1.46	1.50
23	B	603	CLA	C3B-C2B	-2.10	1.37	1.40
35	Y	302	CHL	CMD-C2D	-2.09	1.46	1.50
23	d	402	CLA	CMD-C2D	-2.09	1.46	1.50
23	g	602	CLA	CMD-C2D	-2.09	1.46	1.50
23	c	506	CLA	CMD-C2D	-2.09	1.46	1.50
35	n	601	CHL	CMD-C2D	-2.09	1.46	1.50
23	b	607	CLA	C3B-C2B	-2.09	1.37	1.40
23	B	616	CLA	CMD-C2D	-2.09	1.46	1.50
23	G	610	CLA	CMD-C2D	-2.09	1.46	1.50
23	s	608	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	611	CLA	CMD-C2D	-2.09	1.46	1.50
35	n	606	CHL	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	CMD-C2D	-2.09	1.46	1.50
23	y	311	CLA	CMD-C2D	-2.09	1.46	1.50
23	Y	303	CLA	CMC-C2C	-2.09	1.46	1.50
23	G	611	CLA	CMD-C2D	-2.09	1.46	1.50
23	S	309	CLA	CMD-C2D	-2.09	1.46	1.50
23	c	508	CLA	CMC-C2C	-2.09	1.46	1.50
23	d	401	CLA	CMD-C2D	-2.09	1.46	1.50
23	G	613	CLA	CMD-C2D	-2.08	1.46	1.50
23	n	610	CLA	CMD-C2D	-2.08	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	511	CLA	C3B-C2B	-2.08	1.37	1.40
23	Y	305	CLA	CMD-C2D	-2.08	1.46	1.50
23	G	602	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	513	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	608	CLA	CMD-C2D	-2.08	1.46	1.50
35	N	609	CHL	CMD-C2D	-2.08	1.46	1.50
35	Y	308	CHL	C3B-C2B	-2.08	1.37	1.40
23	C	503	CLA	C3B-C2B	-2.08	1.37	1.40
23	c	502	CLA	C3B-C2B	-2.08	1.37	1.40
23	s	613	CLA	CMD-C2D	-2.08	1.46	1.50
23	R	303	CLA	CMD-C2D	-2.08	1.46	1.50
35	y	302	CHL	CMD-C2D	-2.08	1.46	1.50
23	Y	313	CLA	CMD-C2D	-2.08	1.46	1.50
23	s	612	CLA	CMD-C2D	-2.08	1.46	1.50
23	g	611	CLA	CMD-C2D	-2.08	1.46	1.50
23	g	614	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	613	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	610	CLA	C3B-C2B	-2.07	1.37	1.40
35	G	601	CHL	C4B-CHC	-2.07	1.35	1.41
23	S	305	CLA	C3B-C2B	-2.07	1.37	1.40
35	N	608	CHL	CMD-C2D	-2.07	1.46	1.50
35	G	605	CHL	CMD-C2D	-2.07	1.46	1.50
23	b	603	CLA	C3B-C2B	-2.07	1.37	1.40
35	n	609	CHL	CMD-C2D	-2.07	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.07	1.46	1.50
23	R	309	CLA	CMD-C2D	-2.07	1.46	1.50
35	s	601	CHL	CMD-C2D	-2.07	1.46	1.50
23	b	611	CLA	C3B-C2B	-2.07	1.37	1.40
35	Y	309	CHL	CMD-C2D	-2.07	1.46	1.50
23	y	313	CLA	CMD-C2D	-2.07	1.46	1.50
23	C	502	CLA	C3B-C2B	-2.07	1.37	1.40
23	B	613	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CMC-C2C	-2.07	1.46	1.50
23	b	612	CLA	CMD-C2D	-2.06	1.46	1.50
23	g	613	CLA	CMD-C2D	-2.06	1.46	1.50
23	n	603	CLA	CMD-C2D	-2.06	1.46	1.50
23	y	305	CLA	CMC-C2C	-2.06	1.46	1.50
23	G	614	CLA	CMD-C2D	-2.06	1.46	1.50
23	R	305	CLA	CMD-C2D	-2.06	1.46	1.50
23	s	609	CLA	CMD-C2D	-2.06	1.46	1.50
23	S	313	CLA	CMD-C2D	-2.06	1.46	1.50
35	y	309	CHL	CMD-C2D	-2.06	1.46	1.50
23	N	604	CLA	CMD-C2D	-2.06	1.46	1.50
23	c	509	CLA	CMD-C2D	-2.06	1.46	1.50
23	r	608	CLA	CMD-C2D	-2.06	1.46	1.50
23	Y	312	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	605	CLA	C3B-C2B	-2.06	1.37	1.40
23	B	614	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	503	CLA	CMD-C2D	-2.06	1.46	1.50
23	Y	313	CLA	CMC-C2C	-2.06	1.46	1.50
35	G	607	CHL	CMD-C2D	-2.06	1.46	1.50
33	d	406	PL9	C31-C29	2.06	1.55	1.51
23	R	313	CLA	CMD-C2D	-2.06	1.46	1.50
23	B	610	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	609	CLA	CMD-C2D	-2.05	1.46	1.50
35	S	302	CHL	CMD-C2D	-2.05	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.05	1.46	1.50
23	A	404	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	404	CLA	CMD-C2D	-2.05	1.46	1.50
35	g	606	CHL	CMD-C2D	-2.05	1.46	1.50
23	n	602	CLA	CMD-C2D	-2.05	1.46	1.50
23	R	310	CLA	CMD-C2D	-2.05	1.46	1.50
23	g	603	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	612	CLA	CMD-C2D	-2.05	1.46	1.50
35	r	606	CHL	CMD-C2D	-2.05	1.46	1.50
35	y	306	CHL	CMD-C2D	-2.05	1.46	1.50
23	c	507	CLA	CMD-C2D	-2.05	1.46	1.50
23	Y	314	CLA	CMD-C2D	-2.05	1.46	1.50
35	g	607	CHL	CMD-C2D	-2.05	1.46	1.50
33	D	406	PL9	C31-C29	2.05	1.55	1.51
23	b	606	CLA	C3B-C2B	-2.05	1.37	1.40
23	g	610	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	602	CLA	CMC-C2C	-2.05	1.46	1.50
35	N	607	CHL	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	603	CLA	C3B-C2B	-2.05	1.37	1.40
23	G	603	CLA	CMD-C2D	-2.05	1.46	1.50
23	n	604	CLA	CMD-C2D	-2.05	1.46	1.50
23	y	314	CLA	CMD-C2D	-2.04	1.46	1.50
23	D	404	CLA	CMD-C2D	-2.04	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.04	1.46	1.50
33	d	406	PL9	C37-C38	2.04	1.57	1.50
23	b	608	CLA	C3B-C2B	-2.04	1.37	1.40
35	G	606	CHL	CMD-C2D	-2.04	1.46	1.50
23	G	602	CLA	CMC-C2C	-2.04	1.46	1.50
35	n	607	CHL	CMD-C2D	-2.04	1.46	1.50
23	g	612	CLA	CMD-C2D	-2.04	1.46	1.50
23	G	602	CLA	C3B-C2B	-2.04	1.37	1.40
23	N	602	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	601	CLA	CMD-C2D	-2.04	1.46	1.50
23	n	613	CLA	CMD-C2D	-2.04	1.46	1.50
24	a	402	PHO	C3B-C2B	-2.04	1.37	1.40
23	c	502	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	610	CLA	CMD-C2D	-2.04	1.46	1.50
23	n	602	CLA	CMC-C2C	-2.04	1.46	1.50
23	Y	305	CLA	CMC-C2C	-2.04	1.46	1.50
23	s	602	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	509	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	604	CLA	CMD-C2D	-2.04	1.46	1.50
23	s	603	CLA	CMD-C2D	-2.03	1.46	1.50
35	g	609	CHL	CMD-C2D	-2.03	1.46	1.50
23	C	510	CLA	CMC-C2C	-2.03	1.46	1.50
23	N	603	CLA	CMD-C2D	-2.03	1.46	1.50
23	A	402	CLA	CMD-C2D	-2.03	1.46	1.50
23	S	303	CLA	CMD-C2D	-2.03	1.46	1.50
23	r	609	CLA	CMC-C2C	-2.03	1.46	1.50
23	s	610	CLA	CMD-C2D	-2.03	1.46	1.50
34	F	101	HEM	FE-NB	2.03	2.06	1.96
23	b	604	CLA	CMD-C2D	-2.03	1.46	1.50
23	N	612	CLA	CMD-C2D	-2.03	1.46	1.50
35	N	605	CHL	CMD-C2D	-2.03	1.46	1.50
35	G	609	CHL	C3B-C2B	-2.03	1.37	1.40
23	b	617	CLA	CMD-C2D	-2.03	1.46	1.50
23	B	602	CLA	CMD-C2D	-2.03	1.46	1.50
23	N	602	CLA	CMC-C2C	-2.03	1.46	1.50
23	B	611	CLA	CMD-C2D	-2.03	1.46	1.50
23	c	504	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C4B-CHC	-2.03	1.35	1.41
34	f	101	HEM	FE-ND	2.02	2.06	1.96
23	g	602	CLA	CMC-C2C	-2.02	1.46	1.50
24	A	403	PHO	C3B-C2B	-2.02	1.37	1.40
23	Y	311	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	501	CLA	CMC-C2C	-2.02	1.46	1.50
23	y	303	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	611	CLA	C3B-C2B	-2.02	1.37	1.40
23	c	513	CLA	CMC-C2C	-2.02	1.46	1.50
35	G	609	CHL	CMD-C2D	-2.02	1.46	1.50
35	g	601	CHL	C4B-CHC	-2.02	1.35	1.41
23	y	312	CLA	CMD-C2D	-2.02	1.46	1.50
35	s	605	CHL	CMD-C2D	-2.02	1.46	1.50
34	f	101	HEM	FE-NB	2.02	2.06	1.96
23	N	613	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	611	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	601	CLA	C3B-C2B	-2.02	1.37	1.40
23	B	605	CLA	C3B-C2B	-2.02	1.37	1.40
23	c	511	CLA	CMD-C2D	-2.02	1.46	1.50
23	r	611	CLA	C3B-C2B	-2.02	1.37	1.40
23	C	505	CLA	CMD-C2D	-2.02	1.46	1.50
23	y	313	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	604	CLA	C4B-CHC	-2.01	1.35	1.41
23	S	312	CLA	CMD-C2D	-2.01	1.46	1.50
23	r	604	CLA	C3B-C2B	-2.01	1.37	1.40
23	S	311	CLA	CMD-C2D	-2.01	1.46	1.50
35	Y	306	CHL	CMD-C2D	-2.01	1.46	1.50
35	g	605	CHL	CMD-C2D	-2.01	1.46	1.50
23	S	310	CLA	CMC-C2C	-2.01	1.46	1.50
35	R	307	CHL	CMD-C2D	-2.01	1.46	1.50
34	F	101	HEM	FE-ND	2.01	2.06	1.96
23	y	305	CLA	CMD-C2D	-2.01	1.46	1.50
33	d	406	PL9	C42-C43	2.01	1.57	1.50
23	d	404	CLA	CMD-C2D	-2.01	1.46	1.50
23	S	305	CLA	CMD-C2D	-2.01	1.46	1.50
23	g	612	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	606	CLA	C3B-C2B	-2.01	1.37	1.40
23	S	304	CLA	C3B-C2B	-2.01	1.37	1.40
23	C	514	CLA	CMC-C2C	-2.01	1.46	1.50
35	y	308	CHL	C3B-C2B	-2.01	1.37	1.40
23	b	606	CLA	C4B-CHC	-2.01	1.35	1.41
23	G	604	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
23	s	604	CLA	CMD-C2D	-2.00	1.46	1.50
23	R	311	CLA	CMD-C2D	-2.00	1.46	1.50
23	n	614	CLA	CMD-C2D	-2.00	1.46	1.50
23	R	312	CLA	CMD-C2D	-2.00	1.46	1.50
33	D	406	PL9	C42-C43	2.00	1.56	1.50
23	s	604	CLA	CMC-C2C	-2.00	1.46	1.50
23	b	605	CLA	CMC-C2C	-2.00	1.46	1.50
23	g	604	CLA	CMD-C2D	-2.00	1.46	1.50
23	n	612	CLA	CMD-C2D	-2.00	1.46	1.50

All (2661) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	625	SQD	O9-S-C6	-20.17	82.96	106.94
26	C	521	SQD	O9-S-C6	-20.02	83.14	106.94
26	c	520	SQD	O9-S-C6	-19.99	83.18	106.94
26	b	602	SQD	O9-S-C6	-19.91	83.27	106.94
38	R	301	NEX	C17-C1-C6	-17.45	94.86	110.47
38	Y	318	NEX	C17-C1-C6	-17.35	94.94	110.47
26	C	521	SQD	O8-S-O9	-11.90	82.21	111.27
26	c	520	SQD	O8-S-O9	-11.86	82.29	111.27
26	b	602	SQD	O8-S-O9	-11.63	82.86	111.27
26	B	625	SQD	O8-S-O9	-11.52	83.12	111.27
26	B	625	SQD	O7-S-C6	9.73	118.51	106.94
38	R	301	NEX	C16-C1-C6	9.72	119.17	110.47
26	b	602	SQD	O7-S-C6	9.63	118.38	106.94
26	C	521	SQD	O7-S-C6	9.53	118.27	106.94
26	c	520	SQD	O7-S-C6	9.52	118.25	106.94
38	Y	318	NEX	C16-C1-C6	9.38	118.87	110.47
38	g	618	NEX	O24-C25-C24	9.28	120.36	113.38
38	s	616	NEX	O24-C25-C24	9.27	120.35	113.38
33	D	406	PL9	C7-C8-C9	-9.19	111.50	126.79
33	d	406	PL9	C7-C8-C9	-9.16	111.55	126.79
26	B	625	SQD	O9-S-O7	-8.98	82.88	113.95
38	N	617	NEX	O24-C25-C24	8.93	120.09	113.38
26	b	602	SQD	O9-S-O7	-8.91	83.12	113.95
38	Y	318	NEX	C17-C1-C16	-8.76	81.63	108.53
26	C	521	SQD	O9-S-O7	-8.76	83.64	113.95
38	R	301	NEX	C17-C1-C16	-8.76	81.65	108.53
26	c	520	SQD	O9-S-O7	-8.75	83.68	113.95
38	n	617	NEX	O24-C25-C24	8.73	119.94	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	G	618	NEX	O24-C25-C24	8.68	119.90	113.38
38	R	316	NEX	O24-C25-C24	8.62	119.86	113.38
38	Y	318	NEX	O24-C25-C24	8.45	119.73	113.38
38	r	615	NEX	O24-C25-C24	8.40	119.69	113.38
38	R	301	NEX	O24-C25-C24	8.38	119.68	113.38
26	c	520	SQD	O8-S-C6	8.19	118.80	105.74
38	S	317	NEX	O24-C25-C24	8.19	119.53	113.38
26	C	521	SQD	O8-S-C6	8.18	118.77	105.74
37	y	301	XAT	O24-C25-C24	8.09	119.46	113.38
26	b	602	SQD	O8-S-C6	8.08	118.61	105.74
26	B	625	SQD	O8-S-C6	8.02	118.52	105.74
37	Y	301	XAT	O24-C25-C24	7.86	119.29	113.38
37	Y	301	XAT	O4-C5-C4	7.85	119.28	113.38
37	y	301	XAT	O4-C5-C4	7.84	119.27	113.38
37	g	617	XAT	O24-C25-C24	7.70	119.17	113.38
37	G	617	XAT	O24-C25-C24	7.67	119.14	113.38
35	G	609	CHL	C4A-NA-C1A	7.65	110.14	106.71
23	b	618	CLA	C4A-NA-C1A	7.64	110.14	106.71
23	B	616	CLA	C4A-NA-C1A	7.27	109.97	106.71
37	R	315	XAT	O4-C5-C4	7.22	118.81	113.38
35	Y	310	CHL	C4A-NA-C1A	7.22	109.95	106.71
35	N	609	CHL	C4A-NA-C1A	7.14	109.92	106.71
37	G	617	XAT	O4-C5-C4	7.09	118.71	113.38
37	r	614	XAT	O24-C25-C24	7.09	118.71	113.38
35	y	310	CHL	C4A-NA-C1A	7.07	109.89	106.71
23	b	614	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	B	612	CLA	C4A-NA-C1A	7.05	109.88	106.71
37	g	620	XAT	O24-C25-C24	7.02	118.66	113.38
23	C	503	CLA	C4A-NA-C1A	7.00	109.85	106.71
37	G	620	XAT	O24-C25-C24	6.99	118.64	113.38
23	c	502	CLA	C4A-NA-C1A	6.98	109.84	106.71
37	r	614	XAT	O4-C5-C4	6.96	118.61	113.38
23	b	607	CLA	C4A-NA-C1A	6.95	109.83	106.71
38	Y	318	NEX	C2-C1-C6	6.93	115.95	109.21
33	D	406	PL9	C17-C18-C19	-6.87	111.12	127.66
37	g	617	XAT	O4-C5-C4	6.86	118.54	113.38
33	d	406	PL9	C17-C18-C19	-6.84	111.19	127.66
35	n	609	CHL	C4A-NA-C1A	6.83	109.78	106.71
23	C	508	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	n	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
35	n	607	CHL	C4A-NA-C1A	6.72	109.73	106.71
23	c	507	CLA	C4A-NA-C1A	6.72	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	N	611	CLA	C4A-NA-C1A	6.71	109.72	106.71
38	R	301	NEX	C2-C1-C6	6.68	115.71	109.21
37	R	315	XAT	O24-C25-C24	6.66	118.39	113.38
23	B	605	CLA	C4A-NA-C1A	6.64	109.69	106.71
35	y	308	CHL	C4A-NA-C1A	6.55	109.65	106.71
23	s	612	CLA	C4A-NA-C1A	6.51	109.63	106.71
35	Y	308	CHL	C4A-NA-C1A	6.47	109.62	106.71
35	N	607	CHL	C4A-NA-C1A	6.45	109.61	106.71
23	S	313	CLA	C4A-NA-C1A	6.42	109.59	106.71
23	b	606	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	r	611	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	C	511	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	d	401	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	B	604	CLA	C4A-NA-C1A	6.27	109.52	106.71
33	D	406	PL9	C15-C14-C13	-6.24	107.66	123.68
33	d	406	PL9	C15-C14-C13	-6.24	107.67	123.68
23	R	310	CLA	C4A-NA-C1A	6.23	109.51	106.71
33	D	406	PL9	C12-C13-C14	-6.23	112.66	127.66
35	s	606	CHL	C4A-NA-C1A	6.21	109.50	106.71
33	D	406	PL9	C11-C9-C8	-6.20	108.56	121.12
33	d	406	PL9	C22-C23-C24	-6.20	112.74	127.66
23	D	401	CLA	C4A-NA-C1A	6.19	109.49	106.71
33	d	406	PL9	C12-C13-C14	-6.19	112.75	127.66
33	d	406	PL9	C11-C9-C8	-6.18	108.62	121.12
23	G	613	CLA	C4A-NA-C1A	6.17	109.48	106.71
33	D	406	PL9	C22-C23-C24	-6.17	112.81	127.66
23	G	611	CLA	C4A-NA-C1A	6.16	109.47	106.71
23	C	507	CLA	C4A-NA-C1A	6.15	109.47	106.71
23	g	611	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	C	505	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	C	510	CLA	C4A-NA-C1A	6.07	109.44	106.71
33	D	406	PL9	C27-C28-C29	-6.07	113.06	127.66
23	c	504	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	g	613	CLA	C4A-NA-C1A	6.06	109.43	106.71
33	d	406	PL9	C27-C28-C29	-6.05	113.10	127.66
23	b	617	CLA	C4A-NA-C1A	6.05	109.42	106.71
23	b	615	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	c	512	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	y	314	CLA	C4A-NA-C1A	6.03	109.42	106.71
23	c	509	CLA	C4A-NA-C1A	6.03	109.42	106.71
35	g	607	CHL	C4A-NA-C1A	6.02	109.41	106.71
23	Y	312	CLA	C4A-NA-C1A	6.01	109.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	c	511	CLA	C4A-NA-C1A	5.98	109.40	106.71
23	Y	314	CLA	C4A-NA-C1A	5.98	109.39	106.71
23	B	613	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	y	312	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	R	312	CLA	C4A-NA-C1A	5.97	109.39	106.71
33	d	406	PL9	C32-C33-C34	-5.96	113.30	127.66
23	d	404	CLA	C4A-NA-C1A	5.96	109.39	106.71
23	c	506	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	s	604	CLA	C4A-NA-C1A	5.94	109.38	106.71
23	R	304	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	B	615	CLA	C4A-NA-C1A	5.93	109.37	106.71
33	d	406	PL9	C37-C38-C39	-5.92	113.40	127.66
23	B	609	CLA	C4A-NA-C1A	5.92	109.37	106.71
33	D	406	PL9	C32-C33-C34	-5.92	113.42	127.66
33	D	406	PL9	C37-C38-C39	-5.91	113.42	127.66
23	r	604	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	C	512	CLA	C4A-NA-C1A	5.90	109.36	106.71
23	D	404	CLA	C4A-NA-C1A	5.89	109.35	106.71
23	R	305	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	b	612	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	b	611	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	n	613	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	C	507	CLA	CMB-C2B-C1B	-5.80	119.55	128.46
23	B	607	CLA	C4A-NA-C1A	5.80	109.31	106.71
35	Y	307	CHL	C4A-NA-C1A	5.79	109.31	106.71
35	n	605	CHL	C4A-NA-C1A	5.79	109.31	106.71
35	S	307	CHL	C4A-NA-C1A	5.78	109.30	106.71
35	n	601	CHL	C4A-NA-C1A	5.77	109.30	106.71
23	N	612	CLA	C4A-NA-C1A	5.77	109.30	106.71
33	d	406	PL9	C42-C43-C44	-5.76	113.78	127.66
37	g	620	XAT	O4-C5-C4	5.76	117.71	113.38
23	N	613	CLA	C4A-NA-C1A	5.75	109.29	106.71
23	b	608	CLA	C4A-NA-C1A	5.74	109.29	106.71
23	r	601	CLA	C4A-NA-C1A	5.74	109.29	106.71
35	s	601	CHL	C4A-NA-C1A	5.73	109.28	106.71
33	D	406	PL9	C42-C43-C44	-5.73	113.87	127.66
35	N	601	CHL	C4A-NA-C1A	5.71	109.27	106.71
35	s	605	CHL	C4A-NA-C1A	5.71	109.27	106.71
23	r	608	CLA	C4A-NA-C1A	5.71	109.27	106.71
35	S	302	CHL	C4A-NA-C1A	5.70	109.27	106.71
23	s	610	CLA	C4A-NA-C1A	5.69	109.26	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C4A-NA-C1A	5.67	109.26	106.71
23	B	606	CLA	C4A-NA-C1A	5.66	109.25	106.71
23	Y	304	CLA	C4A-NA-C1A	5.66	109.25	106.71
23	d	403	CLA	C4A-NA-C1A	5.66	109.25	106.71
35	y	307	CHL	C4A-NA-C1A	5.66	109.25	106.71
23	S	312	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	D	403	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	C	513	CLA	C4A-NA-C1A	5.61	109.23	106.71
23	a	404	CLA	C4A-NA-C1A	5.61	109.23	106.71
23	A	404	CLA	C4A-NA-C1A	5.61	109.23	106.71
38	g	618	NEX	C11-C10-C9	-5.58	119.35	127.31
33	D	406	PL9	C36-C34-C33	-5.58	109.83	121.12
35	N	605	CHL	C4A-NA-C1A	5.57	109.21	106.71
23	r	610	CLA	C4A-NA-C1A	5.57	109.21	106.71
33	D	406	PL9	C16-C14-C13	-5.56	109.86	121.12
23	b	613	CLA	C4A-NA-C1A	5.55	109.20	106.71
35	G	607	CHL	C4A-NA-C1A	5.55	109.20	106.71
35	R	308	CHL	C4A-NA-C1A	5.55	109.20	106.71
23	B	611	CLA	C4A-NA-C1A	5.54	109.20	106.71
37	G	620	XAT	O4-C5-C4	5.54	117.55	113.38
23	B	610	CLA	C4A-NA-C1A	5.54	109.20	106.71
23	R	309	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	C	504	CLA	C4A-NA-C1A	5.52	109.19	106.71
33	d	406	PL9	C16-C14-C13	-5.52	109.95	121.12
23	N	603	CLA	C4A-NA-C1A	5.49	109.17	106.71
23	R	302	CLA	C4A-NA-C1A	5.49	109.17	106.71
23	R	311	CLA	C4A-NA-C1A	5.48	109.17	106.71
33	d	406	PL9	C10-C9-C8	-5.47	109.64	123.68
23	s	603	CLA	C4A-NA-C1A	5.47	109.17	106.71
33	D	406	PL9	C10-C9-C8	-5.46	109.67	123.68
23	N	604	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	S	303	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	r	603	CLA	C4A-NA-C1A	5.44	109.15	106.71
32	C	520	DMU	O7-C10-C5	5.44	122.19	108.10
38	R	301	NEX	C17-C1-C2	-5.43	84.65	109.05
33	D	406	PL9	C46-C44-C43	-5.43	110.13	121.12
38	Y	318	NEX	C17-C1-C2	-5.43	84.67	109.05
23	n	612	CLA	C4A-NA-C1A	5.43	109.15	106.71
23	G	604	CLA	C4A-NA-C1A	5.42	109.14	106.71
23	r	612	CLA	C4A-NA-C1A	5.41	109.14	106.71
33	d	406	PL9	C36-C34-C33	-5.40	110.18	121.12
23	B	612	CLA	CMB-C2B-C1B	-5.39	120.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C4A-NA-C1A	5.38	109.13	106.71
33	d	406	PL9	C46-C44-C43	-5.38	110.23	121.12
35	g	606	CHL	CMB-C2B-C1B	-5.37	120.21	128.46
23	y	311	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
23	R	303	CLA	C4A-NA-C1A	5.36	109.12	106.71
35	g	601	CHL	C4A-NA-C1A	5.35	109.11	106.71
35	Y	302	CHL	C4A-NA-C1A	5.34	109.11	106.71
23	c	503	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	y	304	CLA	C4A-NA-C1A	5.32	109.10	106.71
23	N	610	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
23	A	402	CLA	C4A-NA-C1A	5.30	109.09	106.71
32	C	520	DMU	C10-O7-C3	5.29	131.05	117.96
23	r	602	CLA	C4A-NA-C1A	5.28	109.08	106.71
23	b	610	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	D	405	BCR	C28-C27-C26	-5.26	104.69	114.08
23	a	401	CLA	C4A-NA-C1A	5.25	109.07	106.71
25	d	405	BCR	C28-C27-C26	-5.25	104.70	114.08
23	s	608	CLA	C4A-NA-C1A	5.25	109.07	106.71
33	d	406	PL9	C35-C34-C33	-5.25	110.21	123.68
23	S	311	CLA	C4A-NA-C1A	5.24	109.06	106.71
35	G	601	CHL	C4A-NA-C1A	5.24	109.06	106.71
35	y	302	CHL	C4A-NA-C1A	5.23	109.06	106.71
23	B	610	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
23	n	602	CLA	C4A-NA-C1A	5.22	109.06	106.71
23	C	509	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
23	A	401	CLA	C4A-NA-C1A	5.22	109.05	106.71
23	S	305	CLA	C4A-NA-C1A	5.20	109.05	106.71
35	Y	309	CHL	C4A-NA-C1A	5.20	109.05	106.71
33	D	406	PL9	C35-C34-C33	-5.20	110.34	123.68
23	Y	313	CLA	C4A-NA-C1A	5.20	109.04	106.71
23	b	612	CLA	CMB-C2B-C1B	-5.20	120.48	128.46
23	n	603	CLA	C4A-NA-C1A	5.19	109.04	106.71
35	r	607	CHL	C4A-NA-C1A	5.19	109.04	106.71
23	b	614	CLA	CMB-C2B-C1B	-5.19	120.48	128.46
25	k	101	BCR	C3-C4-C5	-5.19	104.82	114.08
23	S	304	CLA	C4A-NA-C1A	5.17	109.03	106.71
23	d	403	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
38	g	618	NEX	C15-C14-C13	-5.16	119.94	127.31
33	D	406	PL9	C41-C39-C38	-5.16	110.67	121.12
32	c	519	DMU	C10-O7-C3	5.16	130.73	117.96
23	y	303	CLA	C4A-NA-C1A	5.15	109.02	106.71
23	g	602	CLA	C4A-NA-C1A	5.14	109.02	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	s	609	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
38	G	618	NEX	C15-C14-C13	-5.11	120.02	127.31
23	g	604	CLA	C4A-NA-C1A	5.11	109.00	106.71
23	n	604	CLA	C4A-NA-C1A	5.10	109.00	106.71
23	c	501	CLA	C4A-NA-C1A	5.08	108.99	106.71
37	G	620	XAT	C38-C25-C26	-5.08	113.74	122.26
35	y	309	CHL	C4A-NA-C1A	5.08	108.99	106.71
23	Y	311	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
23	Y	303	CLA	C4A-NA-C1A	5.07	108.98	106.71
33	d	406	PL9	C45-C44-C43	-5.06	110.69	123.68
23	G	612	CLA	C4A-NA-C1A	5.06	108.98	106.71
23	y	305	CLA	C4A-NA-C1A	5.06	108.98	106.71
23	Y	305	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
37	G	620	XAT	C18-C5-C6	-5.06	113.78	122.26
33	D	406	PL9	C45-C44-C43	-5.04	110.75	123.68
23	R	313	CLA	C4A-NA-C1A	5.04	108.97	106.71
35	S	308	CHL	CMB-C2B-C1B	-5.03	120.73	128.46
37	g	620	XAT	C38-C25-C26	-5.03	113.83	122.26
23	g	612	CLA	C4A-NA-C1A	5.03	108.97	106.71
23	Y	305	CLA	C4A-NA-C1A	5.02	108.97	106.71
23	g	603	CLA	C4A-NA-C1A	5.02	108.96	106.71
37	R	315	XAT	C38-C25-C26	-5.01	113.86	122.26
37	g	620	XAT	C18-C5-C6	-5.01	113.86	122.26
23	S	314	CLA	C4A-NA-C1A	5.01	108.96	106.71
23	c	508	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
32	c	519	DMU	O7-C10-C5	5.01	121.08	108.10
23	s	602	CLA	C4A-NA-C1A	4.98	108.95	106.71
23	S	312	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
33	d	406	PL9	C41-C39-C38	-4.98	111.04	121.12
23	s	609	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	s	613	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	b	605	CLA	C4A-NA-C1A	4.96	108.94	106.71
38	S	317	NEX	C11-C10-C9	-4.96	120.24	127.31
35	n	605	CHL	CMB-C2B-C1B	-4.95	120.86	128.46
23	B	603	CLA	C4A-NA-C1A	4.94	108.93	106.71
35	N	608	CHL	C4A-NA-C1A	4.94	108.93	106.71
35	G	606	CHL	CMB-C2B-C1B	-4.94	120.88	128.46
23	S	305	CLA	CMB-C2B-C1B	-4.93	120.88	128.46
23	s	611	CLA	C4A-NA-C1A	4.93	108.92	106.71
37	G	620	XAT	O4-C5-C18	4.92	120.95	115.06
25	K	101	BCR	C3-C4-C5	-4.90	105.32	114.08
23	y	315	CLA	C4A-NA-C1A	4.89	108.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	609	CLA	C4A-NA-C1A	4.89	108.91	106.71
33	D	406	PL9	C40-C39-C38	-4.89	111.14	123.68
35	S	306	CHL	C4A-NA-C1A	4.88	108.90	106.71
23	Y	315	CLA	C4A-NA-C1A	4.87	108.90	106.71
35	r	605	CHL	CMB-C2B-C1B	-4.87	120.99	128.46
23	G	602	CLA	C4A-NA-C1A	4.86	108.89	106.71
37	G	617	XAT	C38-C25-C26	-4.85	114.13	122.26
37	g	620	XAT	O4-C5-C18	4.85	120.86	115.06
23	y	313	CLA	C4A-NA-C1A	4.84	108.88	106.71
35	R	306	CHL	CMB-C2B-C1B	-4.84	121.02	128.46
37	R	315	XAT	C6-C7-C8	-4.83	115.77	125.99
37	g	617	XAT	C38-C25-C26	-4.82	114.19	122.26
37	r	614	XAT	C18-C5-C6	-4.80	114.22	122.26
38	G	618	NEX	C11-C10-C9	-4.80	120.46	127.31
25	D	405	BCR	C7-C8-C9	-4.79	118.99	126.23
23	G	610	CLA	C4A-NA-C1A	4.78	108.86	106.71
35	N	605	CHL	CMB-C2B-C1B	-4.77	121.13	128.46
37	r	614	XAT	C38-C25-C26	-4.77	114.26	122.26
25	C	519	BCR	C7-C8-C9	-4.76	119.05	126.23
37	r	614	XAT	O4-C5-C18	4.75	120.75	115.06
23	B	608	CLA	C4A-NA-C1A	4.75	108.84	106.71
25	d	405	BCR	C7-C8-C9	-4.75	119.06	126.23
23	B	612	CLA	CMB-C2B-C3B	4.73	133.53	124.68
37	r	614	XAT	C6-C7-C8	-4.73	115.99	125.99
37	g	617	XAT	C18-C5-C6	-4.73	114.34	122.26
33	d	406	PL9	C40-C39-C38	-4.72	111.56	123.68
23	y	305	CLA	CMB-C2B-C1B	-4.72	121.20	128.46
23	c	508	CLA	C4A-NA-C1A	4.72	108.83	106.71
23	N	602	CLA	C4A-NA-C1A	4.71	108.82	106.71
38	r	615	NEX	C11-C10-C9	-4.70	120.60	127.31
37	R	315	XAT	O24-C25-C38	4.70	120.69	115.06
35	N	605	CHL	O2D-CGD-O1D	-4.70	114.65	123.84
37	R	315	XAT	C18-C5-C6	-4.69	114.39	122.26
33	D	406	PL9	C21-C19-C18	-4.69	111.62	121.12
23	C	502	CLA	C4A-NA-C1A	4.68	108.81	106.71
23	S	309	CLA	C4A-NA-C1A	4.67	108.81	106.71
23	C	509	CLA	C4A-NA-C1A	4.67	108.81	106.71
23	n	602	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
23	g	610	CLA	C4A-NA-C1A	4.65	108.80	106.71
35	n	606	CHL	CMB-C2B-C1B	-4.65	121.32	128.46
23	C	507	CLA	CMB-C2B-C3B	4.65	133.37	124.68
31	D	408	LHG	O7-C7-C8	4.65	121.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	y	301	XAT	C18-C5-C6	-4.64	114.48	122.26
33	D	406	PL9	C20-C19-C18	-4.64	111.77	123.68
23	b	603	CLA	C4A-NA-C1A	4.64	108.79	106.71
35	y	307	CHL	CMB-C2B-C1B	-4.64	121.33	128.46
31	d	408	LHG	O7-C7-C8	4.64	121.50	111.50
37	Y	301	XAT	C18-C5-C6	-4.64	114.49	122.26
35	G	606	CHL	C4A-NA-C1A	4.64	108.79	106.71
33	d	406	PL9	C20-C19-C18	-4.63	111.79	123.68
33	d	406	PL9	C21-C19-C18	-4.63	111.74	121.12
35	N	606	CHL	CMB-C2B-C1B	-4.63	121.35	128.46
33	D	406	PL9	C30-C29-C28	-4.63	111.81	123.68
23	S	310	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
35	Y	307	CHL	CMB-C2B-C1B	-4.62	121.36	128.46
23	N	604	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
23	N	602	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
33	d	406	PL9	C30-C29-C28	-4.61	111.84	123.68
37	G	617	XAT	C18-C5-C6	-4.61	114.53	122.26
35	G	608	CHL	C4A-NA-C1A	4.61	108.78	106.71
23	N	610	CLA	CMB-C2B-C3B	4.60	133.29	124.68
35	R	306	CHL	C4A-NA-C1A	4.60	108.77	106.71
23	B	601	CLA	C4A-NA-C1A	4.60	108.77	106.71
33	d	406	PL9	C31-C29-C28	-4.59	111.82	121.12
37	R	315	XAT	O4-C5-C18	4.59	120.55	115.06
35	G	609	CHL	C1B-CHB-C4A	-4.58	121.06	130.12
23	b	614	CLA	CMB-C2B-C3B	4.57	133.22	124.68
23	c	506	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
35	n	608	CHL	C4A-NA-C1A	4.56	108.75	106.71
37	Y	301	XAT	C38-C25-C26	-4.55	114.63	122.26
33	D	406	PL9	C47-C48-C49	-4.55	112.20	127.75
23	B	610	CLA	CMB-C2B-C3B	4.53	133.15	124.68
37	y	301	XAT	C38-C25-C26	-4.52	114.68	122.26
23	y	311	CLA	CMB-C2B-C3B	4.52	133.14	124.68
35	r	605	CHL	C4A-NA-C1A	4.52	108.74	106.71
35	N	601	CHL	CMB-C2B-C1B	-4.50	121.56	128.46
33	d	406	PL9	C47-C48-C49	-4.49	112.41	127.75
38	n	617	NEX	C38-C25-C26	-4.49	114.74	122.26
23	s	604	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
33	D	406	PL9	C26-C24-C23	-4.49	112.04	121.12
23	C	514	CLA	C4A-NA-C1A	4.48	108.72	106.71
23	b	612	CLA	CMB-C2B-C3B	4.47	133.04	124.68
33	D	406	PL9	C45-C44-C46	-4.47	107.75	115.27
23	C	507	CLA	O2D-CGD-O1D	-4.47	115.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	R	316	NEX	C11-C10-C9	-4.47	120.94	127.31
38	r	615	NEX	C38-C25-C26	-4.47	114.78	122.26
33	d	406	PL9	C45-C44-C46	-4.46	107.76	115.27
38	S	317	NEX	C38-C25-C26	-4.46	114.78	122.26
38	Y	318	NEX	C38-C25-C26	-4.46	114.78	122.26
37	G	620	XAT	O24-C25-C38	4.46	120.40	115.06
35	g	606	CHL	CMB-C2B-C3B	4.46	133.02	124.68
33	d	406	PL9	C26-C24-C23	-4.46	112.10	121.12
37	g	620	XAT	O24-C25-C38	4.46	120.39	115.06
25	c	518	BCR	C28-C27-C26	-4.45	106.13	114.08
38	R	316	NEX	C15-C14-C13	-4.45	120.96	127.31
23	n	604	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
25	C	519	BCR	C28-C27-C26	-4.44	106.15	114.08
23	G	603	CLA	C4A-NA-C1A	4.43	108.70	106.71
23	C	513	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
23	n	610	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
23	d	403	CLA	CMB-C2B-C3B	4.42	132.95	124.68
33	D	406	PL9	C31-C29-C28	-4.42	112.18	121.12
23	n	614	CLA	C4A-NA-C1A	4.42	108.69	106.71
38	R	316	NEX	C38-C25-C26	-4.41	114.86	122.26
38	R	301	NEX	C38-C25-C26	-4.41	114.87	122.26
23	Y	303	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
38	N	617	NEX	C38-C25-C26	-4.37	114.94	122.26
35	n	601	CHL	C1B-CHB-C4A	-4.37	121.47	130.12
33	d	406	PL9	C25-C24-C23	-4.36	112.49	123.68
31	n	618	LHG	O7-C7-C8	4.35	120.89	111.50
23	N	614	CLA	C4A-NA-C1A	4.35	108.66	106.71
23	g	614	CLA	C4A-NA-C1A	4.35	108.66	106.71
23	Y	313	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
33	D	406	PL9	C25-C24-C23	-4.35	112.53	123.68
38	s	616	NEX	C27-C28-C29	-4.34	118.79	125.53
37	G	617	XAT	O24-C25-C38	4.34	120.26	115.06
23	c	513	CLA	C4A-NA-C1A	4.34	108.66	106.71
35	r	606	CHL	C4A-NA-C1A	4.33	108.65	106.71
23	S	310	CLA	C4A-NA-C1A	4.33	108.65	106.71
38	g	618	NEX	C38-C25-C26	-4.33	115.01	122.26
37	g	617	XAT	O24-C25-C38	4.32	120.23	115.06
38	r	615	NEX	C15-C14-C13	-4.31	121.16	127.31
37	g	617	XAT	O4-C5-C18	4.30	120.21	115.06
23	c	505	CLA	C4A-NA-C1A	4.30	108.64	106.71
23	Y	311	CLA	CMB-C2B-C3B	4.30	132.72	124.68
23	S	312	CLA	CMB-C2B-C3B	4.28	132.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	313	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
38	s	616	NEX	C38-C25-C26	-4.27	115.10	122.26
23	D	401	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
37	r	614	XAT	C26-C27-C28	-4.26	116.98	125.99
35	n	605	CHL	CMB-C2B-C3B	4.26	132.65	124.68
28	C	517	DGD	O2G-C1B-C2B	4.26	120.67	111.50
23	C	509	CLA	CMB-C2B-C3B	4.25	132.63	124.68
23	n	610	CLA	C4A-NA-C1A	4.24	108.61	106.71
23	c	512	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
23	C	506	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
37	g	617	XAT	C15-C14-C13	-4.24	121.27	127.31
35	N	606	CHL	C4A-NA-C1A	4.24	108.61	106.71
31	N	618	LHG	O7-C7-C8	4.23	120.61	111.50
23	d	401	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
23	s	609	CLA	CMB-C2B-C3B	4.22	132.57	124.68
35	R	307	CHL	C4A-NA-C1A	4.22	108.60	106.71
38	G	618	NEX	C38-C25-C26	-4.20	115.21	122.26
38	s	616	NEX	C11-C10-C9	-4.20	121.31	127.31
23	r	612	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
23	y	303	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
25	C	519	BCR	C24-C23-C22	-4.19	119.90	126.23
35	g	605	CHL	C4A-NA-C1A	4.19	108.59	106.71
35	S	308	CHL	CMB-C2B-C3B	4.19	132.51	124.68
37	G	620	XAT	C15-C14-C13	-4.18	121.34	127.31
23	A	404	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
23	G	604	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
37	y	301	XAT	O4-C5-C18	4.18	120.06	115.06
25	c	518	BCR	C24-C23-C22	-4.17	119.93	126.23
23	g	604	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
23	R	313	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
23	C	506	CLA	C4A-NA-C1A	4.17	108.58	106.71
36	r	613	LUT	C7-C8-C9	-4.17	119.94	126.23
38	Y	318	NEX	C15-C14-C13	-4.16	121.37	127.31
23	n	602	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
35	y	310	CHL	CMB-C2B-C1B	-4.16	122.08	128.46
28	b	625	DGD	O2G-C1B-C2B	4.14	120.43	111.50
23	a	404	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
38	R	301	NEX	C15-C14-C13	-4.14	121.40	127.31
35	N	605	CHL	CMB-C2B-C3B	4.14	132.42	124.68
37	Y	301	XAT	O4-C5-C18	4.14	120.01	115.06
37	R	315	XAT	C26-C27-C28	-4.13	117.25	125.99
23	n	602	CLA	CMB-C2B-C3B	4.13	132.41	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	519	DMU	C10-O1-C9	4.13	121.80	113.69
35	n	605	CHL	O2D-CGD-O1D	-4.13	115.77	123.84
37	G	617	XAT	O4-C5-C18	4.13	120.00	115.06
23	G	614	CLA	C4A-NA-C1A	4.13	108.56	106.71
28	c	515	DGD	O2G-C1B-C2B	4.12	120.39	111.50
25	H	101	BCR	C16-C17-C18	-4.12	121.43	127.31
35	g	608	CHL	C4A-NA-C1A	4.11	108.56	106.71
38	s	616	NEX	C15-C14-C13	-4.11	121.45	127.31
25	C	516	BCR	C15-C14-C13	-4.10	121.45	127.31
31	g	619	LHG	O7-C7-C8	4.10	120.34	111.50
23	N	610	CLA	C4A-NA-C1A	4.10	108.55	106.71
25	h	101	BCR	C16-C17-C18	-4.10	121.46	127.31
25	c	514	BCR	C15-C14-C13	-4.10	121.46	127.31
37	g	620	XAT	C15-C14-C13	-4.10	121.46	127.31
23	c	508	CLA	CMB-C2B-C3B	4.09	132.32	124.68
31	G	619	LHG	O7-C7-C8	4.08	120.30	111.50
37	r	614	XAT	O24-C25-C38	4.08	119.95	115.06
26	l	101	SQD	O47-C7-C8	4.08	120.29	111.50
23	N	602	CLA	O2D-CGD-CBD	4.08	118.51	111.27
23	N	602	CLA	CMB-C2B-C3B	4.07	132.29	124.68
35	R	306	CHL	CMB-C2B-C3B	4.07	132.29	124.68
33	d	406	PL9	C51-C49-C48	-4.07	110.89	122.65
35	r	605	CHL	CMB-C2B-C3B	4.06	132.28	124.68
35	G	606	CHL	CMB-C2B-C3B	4.06	132.27	124.68
35	Y	310	CHL	CMB-C2B-C1B	-4.06	122.23	128.46
36	g	615	LUT	C35-C34-C33	-4.05	121.53	127.31
38	R	301	NEX	O24-C25-C38	4.04	119.90	115.06
25	B	618	BCR	C15-C14-C13	-4.04	121.55	127.31
23	r	609	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
28	A	408	DGD	O2G-C1B-C2B	4.03	120.20	111.50
23	b	613	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
33	D	406	PL9	C51-C49-C48	-4.03	110.99	122.65
37	G	617	XAT	C15-C14-C13	-4.03	121.56	127.31
37	Y	301	XAT	C35-C34-C33	-4.03	121.56	127.31
35	y	306	CHL	C4A-NA-C1A	4.03	108.52	106.71
35	N	609	CHL	CMB-C2B-C1B	-4.02	122.28	128.46
27	a	408	BCT	O2-C-O1	4.02	129.98	119.55
23	c	513	CLA	CAA-C2A-C3A	-4.02	101.77	112.78
23	R	305	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
25	b	620	BCR	C15-C14-C13	-4.02	121.58	127.31
27	A	407	BCT	O2-C-O1	4.02	129.97	119.55
23	B	614	CLA	CMB-C2B-C1B	-4.02	122.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	317	NEX	C27-C28-C29	-4.02	119.30	125.53
28	B	626	DGD	O2G-C1B-C2B	4.01	120.14	111.50
35	s	607	CHL	CMB-C2B-C1B	-4.01	122.31	128.46
23	b	616	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
35	n	601	CHL	CMB-C2B-C1B	-4.00	122.32	128.46
23	r	604	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
37	y	301	XAT	C26-C27-C28	-3.99	117.56	125.99
33	d	406	PL9	C50-C49-C48	-3.99	111.13	122.65
30	W	203	LMG	O7-C10-C11	3.98	120.09	111.50
33	D	406	PL9	C50-C49-C48	-3.98	111.13	122.65
23	N	602	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
25	k	101	BCR	C16-C17-C18	-3.98	121.63	127.31
30	C	522	LMG	O7-C10-C11	3.98	120.08	111.50
35	n	606	CHL	C4A-NA-C1A	3.98	108.49	106.71
37	g	617	XAT	C6-C7-C8	-3.98	117.58	125.99
23	B	611	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
35	g	606	CHL	C4A-NA-C1A	3.97	108.49	106.71
38	Y	318	NEX	O24-C25-C38	3.97	119.81	115.06
23	b	616	CLA	C4A-NA-C1A	3.97	108.49	106.71
25	h	101	BCR	C20-C21-C22	-3.97	121.65	127.31
26	a	406	SQD	O47-C7-C8	3.96	120.03	111.50
30	w	202	LMG	O7-C10-C11	3.96	120.03	111.50
23	S	310	CLA	CMB-C2B-C3B	3.96	132.08	124.68
25	H	101	BCR	C20-C21-C22	-3.95	121.67	127.31
38	n	617	NEX	C15-C14-C13	-3.95	121.67	127.31
38	N	617	NEX	C35-C34-C33	-3.95	121.68	127.31
38	N	617	NEX	C27-C28-C29	-3.94	119.41	125.53
23	Y	311	CLA	C1B-CHB-C4A	-3.94	122.31	130.12
23	G	603	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
37	y	301	XAT	C35-C34-C33	-3.94	121.68	127.31
35	y	307	CHL	CMB-C2B-C3B	3.94	132.05	124.68
38	r	615	NEX	C27-C28-C29	-3.94	119.42	125.53
23	n	610	CLA	CMB-C2B-C3B	3.93	132.04	124.68
37	g	620	XAT	C6-C7-C8	-3.93	117.68	125.99
31	r	616	LHG	O7-C7-C8	3.93	119.98	111.50
30	c	521	LMG	O7-C10-C11	3.93	119.97	111.50
37	G	620	XAT	C6-C7-C8	-3.93	117.69	125.99
25	D	405	BCR	C11-C10-C9	-3.92	121.71	127.31
35	Y	307	CHL	CMB-C2B-C3B	3.92	132.01	124.68
38	S	317	NEX	O24-C25-C38	3.92	119.75	115.06
37	Y	301	XAT	C26-C27-C28	-3.91	117.72	125.99
25	h	101	BCR	C24-C23-C22	-3.91	120.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C24-C23-C22	-3.91	120.33	126.23
25	b	619	BCR	C15-C14-C13	-3.91	121.73	127.31
25	K	101	BCR	C16-C17-C18	-3.91	121.73	127.31
23	c	510	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
38	R	301	NEX	C15-C35-C34	-3.90	115.48	123.47
37	G	617	XAT	C6-C7-C8	-3.90	117.75	125.99
23	C	513	CLA	CMB-C2B-C3B	3.90	131.97	124.68
26	A	406	SQD	O47-C7-C8	3.90	119.90	111.50
35	Y	306	CHL	C4A-NA-C1A	3.89	108.46	106.71
35	n	609	CHL	CMB-C2B-C1B	-3.89	122.48	128.46
31	W	201	LHG	O7-C7-C8	3.89	119.89	111.50
23	B	616	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	C	506	CLA	C1B-CHB-C4A	-3.89	122.41	130.12
25	B	617	BCR	C15-C14-C13	-3.89	121.76	127.31
25	d	405	BCR	C15-C14-C13	-3.89	121.76	127.31
23	G	614	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
25	D	405	BCR	C15-C14-C13	-3.89	121.77	127.31
23	n	602	CLA	O2D-CGD-CBD	3.89	118.17	111.27
35	N	601	CHL	CMB-C2B-C3B	3.88	131.94	124.68
38	R	316	NEX	C27-C28-C29	-3.88	119.51	125.53
25	d	405	BCR	C11-C10-C9	-3.88	121.77	127.31
35	N	608	CHL	CMB-C2B-C1B	-3.87	122.51	128.46
35	G	605	CHL	C4A-NA-C1A	3.87	108.45	106.71
23	Y	303	CLA	CMB-C2B-C3B	3.87	131.91	124.68
37	G	620	XAT	C26-C27-C28	-3.87	117.82	125.99
25	C	515	BCR	C7-C8-C9	-3.86	120.40	126.23
35	n	609	CHL	C1B-CHB-C4A	-3.86	122.47	130.12
23	C	511	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
30	b	622	LMG	O7-C10-C11	3.86	119.82	111.50
23	B	608	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
35	g	609	CHL	CMB-C2B-C1B	-3.86	122.53	128.46
23	b	609	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
35	n	608	CHL	CMB-C2B-C1B	-3.86	122.53	128.46
23	b	603	CLA	CAA-C2A-C3A	-3.86	102.22	112.78
23	B	607	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
25	C	519	BCR	C15-C14-C13	-3.85	121.81	127.31
23	b	608	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
31	R	317	LHG	O7-C7-C8	3.85	119.80	111.50
25	C	519	BCR	C20-C21-C22	-3.85	121.82	127.31
38	r	615	NEX	O24-C25-C38	3.85	119.67	115.06
25	d	405	BCR	C24-C23-C22	-3.85	120.42	126.23
23	B	606	CLA	CMB-C2B-C1B	-3.85	122.55	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	n	615	LUT	C35-C34-C33	-3.85	121.82	127.31
38	R	301	NEX	C11-C10-C9	-3.84	121.82	127.31
23	B	601	CLA	CAA-C2A-C3A	-3.84	102.26	112.78
31	c	516	LHG	O7-C7-C8	3.84	119.78	111.50
36	R	314	LUT	C7-C8-C9	-3.84	120.43	126.23
23	g	610	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
35	n	606	CHL	CMB-C2B-C3B	3.84	131.85	124.68
35	s	605	CHL	CMB-C2B-C1B	-3.84	122.57	128.46
28	d	410	DGD	O2G-C1B-C2B	3.83	119.76	111.50
31	B	622	LHG	O7-C7-C8	3.83	119.76	111.50
25	z	101	BCR	C7-C8-C9	-3.83	120.45	126.23
30	B	620	LMG	O7-C10-C11	3.83	119.75	111.50
38	g	618	NEX	C31-C30-C29	-3.83	121.85	127.31
23	Y	313	CLA	CMB-C2B-C3B	3.83	131.84	124.68
38	N	617	NEX	C15-C14-C13	-3.82	121.86	127.31
25	B	617	BCR	C3-C4-C5	-3.82	107.25	114.08
23	B	603	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
31	b	624	LHG	O7-C7-C8	3.82	119.73	111.50
23	C	514	CLA	CAA-C2A-C3A	-3.82	102.32	112.78
23	b	618	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	y	312	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
38	n	617	NEX	C35-C34-C33	-3.81	121.87	127.31
35	s	601	CHL	C1B-CHB-C4A	-3.81	122.57	130.12
35	S	302	CHL	CMB-C2B-C1B	-3.80	122.62	128.46
30	D	409	LMG	O7-C10-C11	3.80	119.70	111.50
23	s	602	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
30	d	409	LMG	O7-C10-C11	3.80	119.69	111.50
26	L	103	SQD	O47-C7-C8	3.80	119.69	111.50
25	b	619	BCR	C3-C4-C5	-3.80	107.30	114.08
35	y	310	CHL	C1B-CHB-C4A	-3.80	122.60	130.12
31	y	318	LHG	O7-C7-C8	3.80	119.68	111.50
23	d	402	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
23	G	610	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
36	s	614	LUT	C35-C34-C33	-3.78	121.91	127.31
23	Y	305	CLA	CMB-C2B-C3B	3.78	131.76	124.68
36	G	615	LUT	C35-C34-C33	-3.78	121.91	127.31
35	N	606	CHL	CMB-C2B-C3B	3.78	131.75	124.68
23	B	614	CLA	C4A-NA-C1A	3.78	108.40	106.71
23	b	605	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
38	N	617	NEX	O24-C25-C38	3.77	119.58	115.06
35	y	309	CHL	CMB-C2B-C1B	-3.77	122.67	128.46
31	Y	319	LHG	O7-C7-C8	3.77	119.63	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	R	316	NEX	O24-C25-C38	3.77	119.57	115.06
23	c	505	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	y	313	CLA	CMB-C2B-C3B	3.77	131.73	124.68
23	n	613	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
26	c	520	SQD	O47-C7-C8	3.76	119.61	111.50
25	D	405	BCR	C24-C23-C22	-3.76	120.55	126.23
37	g	620	XAT	C26-C27-C28	-3.76	118.04	125.99
38	Y	318	NEX	C15-C35-C34	-3.76	115.77	123.47
23	C	514	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	y	311	CLA	C1B-CHB-C4A	-3.75	122.69	130.12
30	C	501	LMG	O7-C10-C11	3.75	119.58	111.50
35	Y	310	CHL	C1B-CHB-C4A	-3.75	122.69	130.12
25	z	101	BCR	C15-C14-C13	-3.75	121.96	127.31
23	Y	311	CLA	C4A-NA-C1A	3.75	108.39	106.71
38	n	617	NEX	O24-C25-C38	3.74	119.54	115.06
23	S	305	CLA	CMB-C2B-C3B	3.74	131.67	124.68
25	c	514	BCR	C11-C10-C9	-3.73	121.98	127.31
23	c	512	CLA	CMB-C2B-C3B	3.73	131.66	124.68
35	Y	309	CHL	CMB-C2B-C1B	-3.73	122.73	128.46
25	C	516	BCR	C11-C10-C9	-3.72	122.00	127.31
23	S	303	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
23	Y	312	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
23	N	611	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
23	S	314	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
23	C	507	CLA	O2D-CGD-CBD	3.71	117.85	111.27
31	c	517	LHG	O7-C7-C8	3.70	119.48	111.50
23	B	604	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
23	r	603	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	b	621	BCR	C33-C5-C6	-3.69	120.39	124.53
38	R	301	NEX	C27-C28-C29	-3.68	119.81	125.53
38	S	317	NEX	C15-C14-C13	-3.68	122.06	127.31
25	d	405	BCR	C27-C26-C25	-3.68	117.39	122.73
31	b	623	LHG	O7-C7-C8	3.68	119.43	111.50
23	b	606	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	K	101	BCR	C15-C14-C13	-3.68	122.06	127.31
31	B	621	LHG	O7-C7-C8	3.68	119.42	111.50
23	n	611	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
30	b	601	LMG	O7-C10-C11	3.67	119.42	111.50
23	N	604	CLA	CMB-C2B-C3B	3.67	131.55	124.68
25	k	101	BCR	C15-C14-C13	-3.67	122.07	127.31
35	S	307	CHL	CMB-C2B-C1B	-3.67	122.83	128.46
23	Y	315	CLA	CMB-C2B-C1B	-3.66	122.83	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
35	g	609	CHL	C1B-CHB-C4A	-3.66	122.86	130.12
25	C	515	BCR	C15-C14-C13	-3.66	122.08	127.31
36	n	616	LUT	C35-C34-C33	-3.66	122.09	127.31
26	C	521	SQD	O47-C7-C8	3.66	119.39	111.50
36	r	613	LUT	C35-C34-C33	-3.66	122.09	127.31
38	Y	318	NEX	C27-C28-C29	-3.66	119.86	125.53
35	S	302	CHL	C1B-CHB-C4A	-3.66	122.88	130.12
25	B	619	BCR	C33-C5-C6	-3.66	120.42	124.53
25	B	619	BCR	C16-C17-C18	-3.66	122.09	127.31
23	N	613	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
35	N	607	CHL	CMB-C2B-C1B	-3.65	122.85	128.46
25	c	514	BCR	C7-C8-C9	-3.65	120.71	126.23
25	D	405	BCR	C27-C26-C25	-3.65	117.43	122.73
23	R	304	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
23	S	314	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
31	s	617	LHG	O7-C7-C8	3.65	119.36	111.50
23	y	315	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
23	y	314	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	y	303	CLA	CMB-C2B-C3B	3.64	131.48	124.68
23	s	613	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
30	a	407	LMG	O7-C10-C11	3.63	119.33	111.50
35	s	601	CHL	CMB-C2B-C1B	-3.63	122.88	128.46
36	Y	316	LUT	C35-C34-C33	-3.63	122.13	127.31
28	D	410	DGD	O2G-C1B-C2B	3.63	119.32	111.50
35	N	609	CHL	C1B-CHB-C4A	-3.63	122.93	130.12
36	N	615	LUT	C35-C34-C33	-3.63	122.13	127.31
25	c	518	BCR	C7-C8-C9	-3.62	120.76	126.23
30	B	623	LMG	O7-C10-C11	3.62	119.31	111.50
23	c	505	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
23	c	513	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
23	A	404	CLA	CMB-C2B-C3B	3.62	131.45	124.68
23	G	610	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
25	A	405	BCR	C16-C17-C18	-3.61	122.15	127.31
25	b	619	BCR	C16-C17-C18	-3.61	122.15	127.31
23	g	612	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
23	D	401	CLA	CMB-C2B-C3B	3.61	131.44	124.68
23	s	604	CLA	CMB-C2B-C3B	3.61	131.43	124.68
37	Y	301	XAT	O24-C25-C38	3.61	119.38	115.06
23	c	511	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
25	C	516	BCR	C7-C8-C9	-3.60	120.79	126.23
23	R	309	CLA	CMB-C2B-C1B	-3.60	122.92	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	g	616	LUT	C15-C14-C13	-3.60	122.17	127.31
23	A	402	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	C	502	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	G	612	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	N	610	CLA	C1B-CHB-C4A	-3.60	122.99	130.12
23	Y	314	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	c	506	CLA	CMB-C2B-C3B	3.59	131.40	124.68
35	n	607	CHL	CMB-C2B-C1B	-3.59	122.94	128.46
25	c	518	BCR	C15-C14-C13	-3.59	122.19	127.31
25	B	618	BCR	C24-C23-C22	-3.59	120.81	126.23
37	G	617	XAT	C26-C27-C28	-3.59	118.41	125.99
25	a	405	BCR	C16-C17-C18	-3.59	122.19	127.31
35	g	607	CHL	C1B-CHB-C4A	-3.58	123.03	130.12
25	A	405	BCR	C15-C14-C13	-3.58	122.20	127.31
38	g	618	NEX	C15-C35-C34	-3.58	116.14	123.47
37	Y	301	XAT	C11-C10-C9	-3.58	122.20	127.31
38	G	618	NEX	C27-C28-C29	-3.57	119.99	125.53
31	l	102	LHG	O7-C7-C8	3.57	119.19	111.50
25	a	405	BCR	C7-C8-C9	-3.57	120.84	126.23
37	y	301	XAT	C11-C10-C9	-3.57	122.22	127.31
25	A	405	BCR	C7-C8-C9	-3.57	120.85	126.23
25	b	621	BCR	C15-C14-C13	-3.56	122.22	127.31
23	a	404	CLA	CMB-C2B-C3B	3.56	131.34	124.68
25	B	617	BCR	C16-C17-C18	-3.56	122.23	127.31
25	C	519	BCR	C11-C10-C9	-3.56	122.23	127.31
37	y	301	XAT	O24-C25-C38	3.56	119.32	115.06
23	y	305	CLA	CMB-C2B-C3B	3.56	131.34	124.68
23	s	611	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
35	r	607	CHL	CMB-C2B-C1B	-3.56	123.00	128.46
36	R	314	LUT	C35-C34-C33	-3.56	122.23	127.31
35	R	308	CHL	CMB-C2B-C1B	-3.56	123.00	128.46
23	r	609	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
36	S	316	LUT	C10-C11-C12	-3.55	112.12	123.22
23	d	404	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
34	f	101	HEM	C3B-C2B-C1B	3.55	109.12	106.49
36	y	316	LUT	C35-C34-C33	-3.55	122.24	127.31
25	a	405	BCR	C15-C14-C13	-3.55	122.24	127.31
23	s	613	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
38	g	618	NEX	C27-C28-C29	-3.55	120.02	125.53
23	g	613	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
31	S	318	LHG	O7-C7-C8	3.55	119.14	111.50
25	b	620	BCR	C24-C23-C22	-3.54	120.88	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	611	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	b	616	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
23	d	401	CLA	CMB-C2B-C3B	3.54	131.30	124.68
23	b	604	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
35	G	607	CHL	C1B-CHB-C4A	-3.54	123.11	130.12
38	g	618	NEX	O24-C25-C38	3.54	119.29	115.06
35	R	307	CHL	CMB-C2B-C1B	-3.53	123.03	128.46
38	G	618	NEX	O24-C25-C38	3.53	119.29	115.06
31	L	101	LHG	O7-C7-C8	3.53	119.11	111.50
23	D	404	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
35	y	306	CHL	CMB-C2B-C1B	-3.53	123.04	128.46
36	S	315	LUT	C35-C34-C33	-3.53	122.28	127.31
23	R	303	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	B	619	BCR	C15-C14-C13	-3.52	122.28	127.31
23	B	602	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
35	Y	308	CHL	C1B-CHB-C4A	-3.52	123.14	130.12
35	y	308	CHL	C1B-CHB-C4A	-3.52	123.14	130.12
25	c	518	BCR	C20-C21-C22	-3.52	122.28	127.31
28	B	624	DGD	O2G-C1B-C2B	3.52	119.09	111.50
31	d	407	LHG	O7-C7-C8	3.52	119.08	111.50
31	D	407	LHG	O7-C7-C8	3.52	119.08	111.50
25	b	621	BCR	C16-C17-C18	-3.52	122.29	127.31
23	g	614	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
35	s	607	CHL	C1B-CHB-C4A	-3.51	123.16	130.12
23	r	608	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
35	S	306	CHL	CMB-C2B-C1B	-3.51	123.07	128.46
23	G	611	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
23	B	602	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
23	B	614	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
23	r	610	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
34	F	101	HEM	C3B-C2B-C1B	3.50	109.08	106.49
35	Y	306	CHL	CMB-C2B-C1B	-3.50	123.09	128.46
37	g	617	XAT	C31-C30-C29	-3.50	122.32	127.31
25	b	620	BCR	C3-C4-C5	-3.50	107.84	114.08
25	B	618	BCR	C3-C4-C5	-3.49	107.84	114.08
23	c	501	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
38	s	616	NEX	O24-C25-C38	3.49	119.24	115.06
23	G	613	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
35	S	308	CHL	C1B-CHB-C4A	-3.49	123.20	130.12
25	B	619	BCR	C24-C23-C22	-3.49	120.96	126.23
32	C	520	DMU	O3-C5-C10	3.49	118.52	110.05
23	n	604	CLA	CMB-C2B-C3B	3.49	131.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	401	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	c	505	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
36	S	316	LUT	C15-C14-C13	-3.48	122.35	127.31
25	C	519	BCR	C16-C17-C18	-3.48	122.35	127.31
23	c	503	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
38	S	317	NEX	C39-C29-C30	-3.47	118.06	122.92
23	b	604	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
38	s	616	NEX	C39-C29-C30	-3.47	118.06	122.92
23	C	510	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
23	S	304	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
23	G	602	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	c	510	CLA	CMB-C2B-C3B	3.46	131.16	124.68
36	s	615	LUT	C35-C34-C33	-3.46	122.37	127.31
23	C	506	CLA	CMB-C2B-C3B	3.46	131.16	124.68
23	b	604	CLA	C4A-NA-C1A	3.46	108.26	106.71
23	y	304	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
35	g	608	CHL	CMB-C2B-C1B	-3.46	123.14	128.46
23	s	603	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	a	405	BCR	C11-C10-C9	-3.45	122.38	127.31
23	C	504	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	b	617	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
23	g	602	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
37	g	617	XAT	C11-C10-C9	-3.45	122.39	127.31
37	y	301	XAT	C35-C15-C14	-3.44	116.42	123.47
23	D	404	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	g	610	CLA	CMB-C2B-C3B	3.44	131.11	124.68
23	G	603	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
35	r	606	CHL	CMB-C2B-C1B	-3.44	123.18	128.46
38	s	616	NEX	C35-C34-C33	-3.43	122.41	127.31
23	d	404	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
23	C	508	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	R	310	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	b	619	BCR	C20-C21-C22	-3.43	122.41	127.31
23	c	509	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
35	G	608	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
23	c	507	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	S	301	LMG	O7-C10-C11	3.43	118.89	111.50
23	r	609	CLA	CMB-C2B-C3B	3.43	131.09	124.68
35	G	609	CHL	CMB-C2B-C1B	-3.43	123.20	128.46
23	n	614	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
37	Y	301	XAT	C35-C15-C14	-3.42	116.47	123.47
23	R	311	CLA	CMB-C2B-C1B	-3.42	123.21	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	n	601	CHL	CMB-C2B-C3B	3.41	131.06	124.68
30	s	619	LMG	O7-C10-C11	3.41	118.85	111.50
23	Y	304	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	R	312	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
25	b	619	BCR	C11-C10-C9	-3.41	122.45	127.31
23	G	604	CLA	CMB-C2B-C3B	3.41	131.05	124.68
23	S	313	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
36	s	614	LUT	C35-C15-C14	-3.40	116.51	123.47
23	D	403	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
37	g	620	XAT	C11-C10-C9	-3.39	122.47	127.31
23	a	404	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
23	B	605	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
38	Y	318	NEX	C16-C1-C2	3.39	124.28	109.05
35	s	607	CHL	CMB-C2B-C3B	3.39	131.03	124.68
23	C	505	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
36	g	616	LUT	C35-C34-C33	-3.39	122.47	127.31
23	C	511	CLA	CMB-C2B-C3B	3.39	131.02	124.68
25	A	405	BCR	C11-C10-C9	-3.39	122.47	127.31
25	b	621	BCR	C24-C23-C22	-3.39	121.11	126.23
35	Y	306	CHL	C1B-CHB-C4A	-3.39	123.41	130.12
23	S	311	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
25	C	516	BCR	C3-C4-C5	-3.39	108.03	114.08
23	n	612	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
35	y	302	CHL	CMB-C2B-C1B	-3.39	123.26	128.46
25	z	101	BCR	C16-C17-C18	-3.38	122.48	127.31
23	B	615	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
25	c	514	BCR	C3-C4-C5	-3.38	108.04	114.08
36	R	314	LUT	C15-C14-C13	-3.38	122.48	127.31
32	c	519	DMU	O3-C5-C10	3.38	118.25	110.05
23	s	602	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
38	n	617	NEX	C27-C28-C29	-3.38	120.29	125.53
23	g	610	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
31	C	518	LHG	O7-C7-C8	3.38	118.78	111.50
23	s	612	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
38	R	301	NEX	C16-C1-C2	3.38	124.21	109.05
35	y	306	CHL	C1B-CHB-C4A	-3.38	123.43	130.12
25	A	405	BCR	C3-C4-C5	-3.37	108.05	114.08
23	b	607	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	B	605	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
25	c	518	BCR	C16-C17-C18	-3.37	122.50	127.31
36	Y	317	LUT	C35-C34-C33	-3.37	122.50	127.31
35	N	609	CHL	CMB-C2B-C3B	3.37	130.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	102	LHG	O7-C7-C8	3.37	118.76	111.50
23	b	613	CLA	CMB-C2B-C3B	3.37	130.97	124.68
25	b	620	BCR	C28-C27-C26	-3.36	108.07	114.08
37	G	617	XAT	C31-C30-C29	-3.36	122.51	127.31
37	G	620	XAT	C11-C10-C9	-3.36	122.51	127.31
23	r	602	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	c	504	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
35	G	605	CHL	CMB-C2B-C1B	-3.36	123.31	128.46
25	a	405	BCR	C3-C4-C5	-3.36	108.09	114.08
35	G	607	CHL	CMB-C2B-C1B	-3.35	123.31	128.46
25	C	515	BCR	C11-C10-C9	-3.35	122.53	127.31
35	g	605	CHL	CMB-C2B-C1B	-3.35	123.31	128.46
23	s	608	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	N	614	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
23	s	611	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	A	404	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	G	603	CLA	CMB-C2B-C3B	3.35	130.94	124.68
25	B	617	BCR	C11-C10-C9	-3.35	122.54	127.31
23	n	610	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
34	f	101	HEM	CMC-C2C-C3C	3.34	130.93	124.68
23	N	612	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	B	618	BCR	C28-C27-C26	-3.34	108.12	114.08
25	B	617	BCR	C20-C21-C22	-3.33	122.55	127.31
23	s	608	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
23	r	612	CLA	CMB-C2B-C3B	3.33	130.91	124.68
35	Y	302	CHL	CMB-C2B-C1B	-3.33	123.35	128.46
25	C	515	BCR	C16-C17-C18	-3.33	122.56	127.31
31	l	103	LHG	O7-C7-C8	3.32	118.66	111.50
36	G	616	LUT	C15-C14-C13	-3.32	122.57	127.31
35	s	606	CHL	CMB-C2B-C1B	-3.32	123.36	128.46
35	N	601	CHL	C1B-CHB-C4A	-3.32	123.54	130.12
23	B	611	CLA	CMB-C2B-C3B	3.32	130.89	124.68
37	g	620	XAT	C31-C30-C29	-3.32	122.57	127.31
23	b	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
25	z	101	BCR	C11-C10-C9	-3.32	122.57	127.31
33	d	406	PL9	C10-C9-C11	-3.32	109.69	115.27
23	G	610	CLA	CMB-C2B-C3B	3.32	130.88	124.68
25	d	405	BCR	C38-C26-C27	3.32	119.99	113.62
34	f	101	HEM	C4B-CHC-C1C	3.32	126.93	122.56
23	s	609	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	B	602	CLA	C4A-NA-C1A	3.31	108.19	106.71
35	G	601	CHL	C1B-CHB-C4A	-3.31	123.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CMB-C2B-C3B	3.31	130.87	124.68
25	B	619	BCR	C28-C27-C26	-3.31	108.17	114.08
35	S	302	CHL	CMB-C2B-C3B	3.30	130.86	124.68
23	G	614	CLA	CMB-C2B-C3B	3.30	130.86	124.68
35	n	609	CHL	CMB-C2B-C3B	3.30	130.85	124.68
23	y	311	CLA	C4A-NA-C1A	3.30	108.19	106.71
37	g	617	XAT	C26-C27-C28	-3.30	119.02	125.99
23	b	603	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
32	S	319	DMU	C10-O1-C9	3.30	120.16	113.69
23	R	305	CLA	CMB-C2B-C3B	3.30	130.85	124.68
25	D	405	BCR	C38-C26-C27	3.29	119.94	113.62
25	k	101	BCR	C11-C10-C9	-3.29	122.61	127.31
34	F	101	HEM	C4B-CHC-C1C	3.29	126.90	122.56
35	y	302	CHL	C1B-CHB-C4A	-3.29	123.60	130.12
23	s	610	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	b	619	BCR	C7-C8-C9	-3.29	121.26	126.23
35	N	605	CHL	C1B-CHB-C4A	-3.29	123.60	130.12
23	B	601	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
34	F	101	HEM	CMC-C2C-C3C	3.29	130.83	124.68
37	G	620	XAT	C31-C30-C29	-3.28	122.62	127.31
25	b	620	BCR	C20-C21-C22	-3.28	122.63	127.31
38	G	618	NEX	C31-C30-C29	-3.28	122.63	127.31
37	Y	301	XAT	C24-C23-C22	-3.28	104.44	110.77
23	B	614	CLA	CMB-C2B-C3B	3.28	130.81	124.68
37	R	315	XAT	C35-C34-C33	-3.28	122.63	127.31
33	D	406	PL9	C10-C9-C11	-3.28	109.76	115.27
23	r	611	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
38	Y	318	NEX	C11-C10-C9	-3.28	122.63	127.31
23	S	309	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
32	s	618	DMU	C10-O1-C9	3.27	120.11	113.69
36	r	613	LUT	C15-C14-C13	-3.27	122.64	127.31
23	C	506	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
23	n	613	CLA	CBA-CAA-C2A	3.27	123.50	113.86
23	R	313	CLA	CMB-C2B-C3B	3.26	130.78	124.68
37	R	315	XAT	C15-C14-C13	-3.26	122.66	127.31
25	b	621	BCR	C28-C27-C26	-3.26	108.26	114.08
23	R	302	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
23	r	601	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	B	618	BCR	C20-C21-C22	-3.25	122.68	127.31
23	b	617	CLA	CHB-C4A-NA	3.24	129.00	124.51
23	N	613	CLA	CBA-CAA-C2A	3.24	123.44	113.86
23	b	617	CLA	CMB-C2B-C1B	-3.24	123.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	618	CLA	CMB-C2B-C3B	3.24	130.74	124.68
35	S	308	CHL	O2D-CGD-O1D	-3.24	117.51	123.84
23	S	310	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
23	g	604	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	b	616	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	C	512	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
38	S	317	NEX	C35-C34-C33	-3.23	122.70	127.31
23	y	312	CLA	CMB-C2B-C3B	3.23	130.71	124.68
38	n	617	NEX	C11-C10-C9	-3.23	122.71	127.31
23	S	309	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
31	b	626	LHG	O7-C7-C8	3.22	118.45	111.50
23	A	401	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
35	s	606	CHL	C1B-CHB-C4A	-3.22	123.74	130.12
37	R	315	XAT	C24-C23-C22	-3.22	104.55	110.77
23	N	603	CLA	CAA-C2A-C3A	-3.22	103.96	112.78
35	g	607	CHL	CMB-C2B-C1B	-3.22	123.52	128.46
25	h	101	BCR	C10-C11-C12	-3.22	113.18	123.22
25	d	405	BCR	C16-C17-C18	-3.22	122.72	127.31
23	S	303	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
36	N	615	LUT	C35-C15-C14	-3.21	116.89	123.47
25	B	619	BCR	C7-C8-C9	-3.21	121.38	126.23
23	B	606	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	H	101	BCR	C10-C11-C12	-3.21	113.20	123.22
23	B	615	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
36	Y	317	LUT	C15-C14-C13	-3.21	122.73	127.31
23	N	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
35	Y	302	CHL	O2D-CGD-O1D	-3.21	117.57	123.84
35	N	607	CHL	CMB-C2B-C3B	3.21	130.68	124.68
23	r	608	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
23	r	604	CLA	CMB-C2B-C3B	3.21	130.68	124.68
35	N	608	CHL	CMB-C2B-C3B	3.20	130.67	124.68
37	r	614	XAT	C15-C14-C13	-3.20	122.74	127.31
23	R	309	CLA	CMB-C2B-C3B	3.20	130.66	124.68
37	r	614	XAT	C24-C23-C22	-3.20	104.60	110.77
23	B	615	CLA	CHB-C4A-NA	3.19	128.93	124.51
35	y	302	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
23	R	311	CLA	CAA-C2A-C3A	-3.19	108.66	116.10
35	g	601	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
36	n	616	LUT	C15-C14-C13	-3.19	122.76	127.31
23	n	603	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
37	r	614	XAT	C35-C34-C33	-3.18	122.77	127.31
35	y	309	CHL	CMB-C2B-C3B	3.18	130.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C7-C8-C9	-3.18	121.42	126.23
36	r	613	LUT	C11-C10-C9	-3.18	122.77	127.31
23	b	608	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	s	602	CLA	CMB-C2B-C3B	3.18	130.63	124.68
32	C	520	DMU	C10-O1-C9	3.18	119.93	113.69
37	G	617	XAT	C11-C10-C9	-3.18	122.78	127.31
38	G	618	NEX	C15-C35-C34	-3.18	116.97	123.47
35	r	606	CHL	C1B-CHB-C4A	-3.17	123.83	130.12
23	n	613	CLA	CMB-C2B-C3B	3.17	130.62	124.68
23	B	602	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
35	s	605	CHL	CMB-C2B-C3B	3.17	130.61	124.68
36	r	613	LUT	C18-C5-C6	-3.17	120.97	124.53
25	D	405	BCR	C16-C17-C18	-3.16	122.80	127.31
23	R	312	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
35	s	601	CHL	CMB-C2B-C3B	3.16	130.60	124.68
35	n	608	CHL	CMB-C2B-C3B	3.16	130.60	124.68
31	B	627	LHG	O7-C7-C8	3.16	118.32	111.50
23	N	602	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
38	N	617	NEX	C39-C29-C30	-3.16	118.50	122.92
25	C	515	BCR	C20-C21-C22	-3.16	122.80	127.31
25	B	619	BCR	C11-C10-C9	-3.16	122.80	127.31
23	C	512	CLA	CMB-C2B-C3B	3.16	130.58	124.68
35	n	605	CHL	C1B-CHB-C4A	-3.16	123.87	130.12
35	S	307	CHL	CMB-C2B-C3B	3.15	130.58	124.68
35	n	607	CHL	CMB-C2B-C3B	3.15	130.58	124.68
37	y	301	XAT	C24-C23-C22	-3.15	104.69	110.77
23	r	603	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	b	620	BCR	C11-C10-C9	-3.15	122.81	127.31
23	Y	312	CLA	CMB-C2B-C3B	3.15	130.57	124.68
35	R	307	CHL	C1B-CHB-C4A	-3.15	123.89	130.12
23	s	609	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
23	B	603	CLA	CMB-C2B-C3B	3.14	130.55	124.68
36	y	317	LUT	C35-C34-C33	-3.14	122.83	127.31
23	b	604	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
38	Y	318	NEX	C31-C30-C29	-3.13	122.84	127.31
23	y	303	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
23	B	605	CLA	CGD-CBD-CAD	-3.13	100.59	110.73
23	Y	303	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
23	R	309	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
25	z	101	BCR	C20-C21-C22	-3.13	122.84	127.31
23	D	404	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	b	621	BCR	C20-C21-C22	-3.13	122.84	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	O2D-CGD-CBD	3.13	116.83	111.27
36	n	615	LUT	C35-C15-C14	-3.13	117.07	123.47
25	B	617	BCR	C7-C8-C9	-3.13	121.51	126.23
36	G	616	LUT	C10-C11-C12	-3.13	113.46	123.22
23	G	612	CLA	CMB-C2B-C3B	3.13	130.53	124.68
23	C	503	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
23	d	404	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	a	401	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
35	R	306	CHL	C1B-CHB-C4A	-3.12	123.93	130.12
35	Y	309	CHL	CMB-C2B-C3B	3.12	130.52	124.68
23	Y	305	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
23	C	509	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	g	612	CLA	CMB-C2B-C3B	3.12	130.51	124.68
23	Y	315	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
35	G	607	CHL	CHD-C1D-ND	-3.12	121.59	124.45
34	F	101	HEM	C1B-NB-C4B	3.12	108.29	105.07
23	r	610	CLA	CAA-C2A-C3A	-3.12	108.82	116.10
24	D	402	PHO	CMB-C2B-C3B	3.11	130.50	124.68
23	A	401	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
25	B	618	BCR	C11-C10-C9	-3.11	122.87	127.31
37	y	301	XAT	C7-C8-C9	-3.11	120.71	125.53
35	G	605	CHL	C1B-CHB-C4A	-3.11	123.97	130.12
23	c	502	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
23	B	614	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
23	Y	315	CLA	CMB-C2B-C3B	3.10	130.48	124.68
35	G	609	CHL	CHD-C1D-ND	-3.10	121.60	124.45
23	C	509	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
23	c	507	CLA	CMB-C2B-C3B	3.10	130.48	124.68
23	c	508	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	c	508	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
23	c	511	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	g	614	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
35	y	308	CHL	CMB-C2B-C1B	-3.09	123.72	128.46
23	g	602	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
35	g	605	CHL	C1B-CHB-C4A	-3.09	124.00	130.12
23	b	616	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
35	Y	302	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
23	N	611	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	C	508	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	N	613	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	g	602	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	C	508	CLA	CHB-C4A-NA	3.07	128.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	314	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	N	614	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	G	602	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	b	605	CLA	CMB-C2B-C3B	3.07	130.43	124.68
37	g	620	XAT	C35-C34-C33	-3.07	122.93	127.31
23	y	315	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	G	602	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
38	r	615	NEX	C39-C29-C30	-3.07	118.62	122.92
23	R	304	CLA	CMB-C2B-C3B	3.07	130.42	124.68
36	S	315	LUT	C35-C15-C14	-3.07	117.19	123.47
23	n	614	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	c	507	CLA	CHB-C4A-NA	3.06	128.75	124.51
37	Y	301	XAT	C7-C8-C9	-3.06	120.78	125.53
23	y	305	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
35	g	608	CHL	C1B-CHB-C4A	-3.06	124.05	130.12
23	s	603	CLA	CMB-C2B-C3B	3.06	130.41	124.68
35	Y	307	CHL	C1B-CHB-C4A	-3.06	124.06	130.12
23	B	607	CLA	CMB-C2B-C3B	3.06	130.40	124.68
35	N	608	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
23	G	614	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	S	303	CLA	CMB-C2B-C3B	3.06	130.40	124.68
23	r	611	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
35	N	607	CHL	CHB-C4A-NA	3.05	128.74	124.51
36	Y	316	LUT	C35-C15-C14	-3.05	117.22	123.47
35	y	307	CHL	C1B-CHB-C4A	-3.05	124.07	130.12
34	f	101	HEM	C1B-NB-C4B	3.05	108.22	105.07
36	Y	317	LUT	C7-C8-C9	-3.05	121.63	126.23
37	G	620	XAT	C35-C34-C33	-3.05	122.96	127.31
33	D	406	PL9	C35-C34-C36	-3.05	110.14	115.27
26	b	602	SQD	O8-S-O7	3.05	118.72	111.27
23	A	402	CLA	CMB-C2B-C3B	3.05	130.38	124.68
23	r	608	CLA	CMB-C2B-C3B	3.05	130.38	124.68
35	n	607	CHL	C1B-CHB-C4A	-3.05	124.09	130.12
33	D	406	PL9	C30-C29-C31	-3.04	110.15	115.27
25	B	619	BCR	C20-C21-C22	-3.04	122.97	127.31
35	n	608	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
23	C	514	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	R	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	S	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	S	305	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
23	b	603	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
23	g	613	CLA	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-CBD	3.04	116.67	111.27
23	n	611	CLA	CMB-C2B-C3B	3.04	130.36	124.68
23	b	609	CLA	CMB-C2B-C3B	3.03	130.35	124.68
35	r	607	CHL	CMB-C2B-C3B	3.03	130.35	124.68
35	Y	308	CHL	CMB-C2B-C1B	-3.03	123.81	128.46
36	G	616	LUT	C7-C8-C9	-3.03	121.66	126.23
37	G	617	XAT	C4-C3-C2	-3.03	104.92	110.77
35	N	609	CHL	CAA-C2A-C3A	-3.03	104.49	112.78
23	c	505	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	d	402	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	R	302	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
37	R	315	XAT	C10-C11-C12	-3.02	113.78	123.22
35	y	309	CHL	O2D-CGD-O1D	-3.02	117.93	123.84
23	g	603	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
35	R	308	CHL	CMB-C2B-C3B	3.02	130.33	124.68
35	n	609	CHL	CAA-C2A-C3A	-3.02	104.51	112.78
38	R	301	NEX	C31-C30-C29	-3.02	123.00	127.31
23	b	615	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	S	312	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
23	n	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
23	c	511	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	B	609	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
33	d	406	PL9	C30-C29-C31	-3.02	110.20	115.27
35	G	607	CHL	CMB-C2B-C3B	3.01	130.32	124.68
23	B	601	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
23	b	611	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
23	y	315	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
36	N	616	LUT	C15-C14-C13	-3.01	123.01	127.31
23	b	616	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
35	g	609	CHL	C4A-NA-C1A	3.01	108.06	106.71
23	b	615	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
35	r	605	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
23	N	610	CLA	CHB-C4A-NA	3.01	128.67	124.51
25	b	620	BCR	C7-C8-C9	-3.01	121.69	126.23
26	c	520	SQD	O8-S-O7	3.01	118.62	111.27
23	Y	304	CLA	CHB-C4A-NA	3.01	128.67	124.51
35	N	608	CHL	C1B-CHB-C4A	-3.00	124.17	130.12
36	y	317	LUT	C7-C8-C9	-3.00	121.70	126.23
25	D	405	BCR	C20-C21-C22	-3.00	123.02	127.31
23	G	613	CLA	CMB-C2B-C3B	3.00	130.29	124.68
23	Y	314	CLA	CMB-C2B-C3B	3.00	130.29	124.68
35	n	607	CHL	CHB-C4A-NA	3.00	128.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C7-C8-C9	-3.00	121.70	126.23
23	c	503	CLA	CMB-C2B-C3B	3.00	130.29	124.68
23	B	614	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	G	610	CLA	CHB-C4A-NA	3.00	128.65	124.51
36	y	316	LUT	C35-C15-C14	-2.99	117.34	123.47
23	s	613	CLA	CMB-C2B-C3B	2.99	130.28	124.68
23	b	614	CLA	CHB-C4A-NA	2.99	128.65	124.51
23	S	314	CLA	CMB-C2B-C3B	2.99	130.28	124.68
35	y	310	CHL	CMB-C2B-C3B	2.99	130.28	124.68
23	b	607	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
23	B	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
23	S	304	CLA	CMB-C2B-C3B	2.99	130.28	124.68
25	d	405	BCR	C20-C21-C22	-2.99	123.04	127.31
23	g	614	CLA	CMB-C2B-C3B	2.99	130.28	124.68
23	B	613	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
37	y	301	XAT	C15-C14-C13	-2.99	123.05	127.31
37	y	301	XAT	C6-C7-C8	-2.99	119.68	125.99
31	L	101	LHG	O8-C23-C24	2.99	121.28	111.91
36	n	615	LUT	C11-C10-C9	-2.99	123.05	127.31
23	y	304	CLA	CHB-C4A-NA	2.99	128.64	124.51
35	s	606	CHL	CAA-C2A-C3A	-2.99	106.80	114.26
23	A	404	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
35	Y	309	CHL	O2D-CGD-O1D	-2.99	118.00	123.84
26	B	625	SQD	O8-S-O7	2.98	118.57	111.27
35	g	606	CHL	C1B-CHB-C4A	-2.98	124.21	130.12
26	C	521	SQD	O8-S-O7	2.98	118.56	111.27
35	n	606	CHL	C1B-CHB-C4A	-2.98	124.21	130.12
23	N	612	CLA	CHB-C4A-NA	2.98	128.64	124.51
35	y	306	CHL	CMB-C2B-C3B	2.98	130.26	124.68
23	c	513	CLA	CMB-C2B-C3B	2.98	130.26	124.68
23	a	404	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
25	b	620	BCR	C16-C17-C18	-2.98	123.06	127.31
23	n	603	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
25	c	518	BCR	C11-C10-C9	-2.98	123.06	127.31
38	R	316	NEX	C39-C29-C30	-2.98	118.75	122.92
36	S	315	LUT	C30-C31-C32	-2.97	113.93	123.22
35	Y	306	CHL	CMB-C2B-C3B	2.97	130.24	124.68
23	A	402	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
23	B	602	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	B	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
35	r	607	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
23	C	506	CLA	CHB-C4A-NA	2.97	128.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
23	r	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	A	402	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
37	Y	301	XAT	C6-C7-C8	-2.97	119.71	125.99
25	b	621	BCR	C11-C10-C9	-2.97	123.07	127.31
35	N	605	CHL	O2D-CGD-CBD	2.97	116.54	111.27
23	r	610	CLA	CMB-C2B-C3B	2.97	130.23	124.68
25	H	101	BCR	C15-C14-C13	-2.97	123.07	127.31
25	c	514	BCR	C15-C16-C17	-2.97	117.40	123.47
23	C	504	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	r	604	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
35	g	609	CHL	CHB-C4A-NA	2.96	128.61	124.51
37	r	614	XAT	C4-C3-C2	-2.96	105.05	110.77
25	h	101	BCR	C15-C14-C13	-2.96	123.08	127.31
35	y	302	CHL	CMB-C2B-C3B	2.96	130.22	124.68
36	y	317	LUT	C15-C14-C13	-2.96	123.08	127.31
23	s	608	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
23	g	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	b	604	CLA	CMB-C2B-C3B	2.96	130.22	124.68
35	g	609	CHL	CHD-C1D-ND	-2.96	121.73	124.45
35	s	607	CHL	O2D-CGD-O1D	-2.96	118.05	123.84
23	B	607	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
23	B	611	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
23	d	401	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
35	R	307	CHL	CMB-C2B-C3B	2.96	130.21	124.68
37	r	614	XAT	C10-C11-C12	-2.96	113.99	123.22
23	R	305	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	b	607	CLA	CGD-CBD-CAD	-2.96	101.16	110.73
35	s	606	CHL	CMB-C2B-C3B	2.96	130.21	124.68
23	S	304	CLA	CHB-C4A-NA	2.95	128.59	124.51
35	s	605	CHL	C1B-CHB-C4A	-2.95	124.28	130.12
23	R	311	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	n	614	CLA	CAA-C2A-C3A	-2.95	109.22	116.10
23	b	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
35	G	608	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
23	n	614	CLA	CMB-C2B-C3B	2.95	130.19	124.68
38	g	618	NEX	C35-C34-C33	-2.95	123.10	127.31
35	N	609	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
23	g	613	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
35	n	608	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
23	S	312	CLA	CHB-C4A-NA	2.94	128.58	124.51
35	r	606	CHL	CMB-C2B-C3B	2.94	130.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	601	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
35	S	308	CHL	CHD-C1D-ND	-2.94	121.75	124.45
35	g	608	CHL	O2D-CGD-O1D	-2.94	118.09	123.84
35	g	607	CHL	CHD-C1D-ND	-2.94	121.75	124.45
23	G	611	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	a	401	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	n	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
23	b	613	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
35	G	608	CHL	C1B-CHB-C4A	-2.94	124.30	130.12
25	C	516	BCR	C15-C16-C17	-2.94	117.46	123.47
34	F	101	HEM	CHC-C4B-C3B	2.94	129.06	124.57
23	c	505	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	s	603	CLA	CHB-C4A-NA	2.94	128.57	124.51
35	Y	306	CHL	O2D-CGD-O1D	-2.94	118.10	123.84
23	N	614	CLA	CAA-C2A-C3A	-2.93	109.25	116.10
23	R	303	CLA	CMB-C2B-C3B	2.93	130.17	124.68
35	R	307	CHL	CHD-C1D-ND	-2.93	121.76	124.45
23	s	604	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
23	n	604	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
37	g	617	XAT	C35-C34-C33	-2.93	123.12	127.31
23	c	506	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	S	315	LUT	C10-C11-C12	-2.93	114.08	123.22
37	G	620	XAT	C4-C3-C2	-2.93	105.12	110.77
23	b	609	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
35	y	306	CHL	O2D-CGD-O1D	-2.92	118.12	123.84
25	B	618	BCR	C16-C17-C18	-2.92	123.14	127.31
23	y	313	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
35	y	308	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
38	r	615	NEX	C11-C12-C13	-2.92	118.21	126.42
23	D	404	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
35	n	609	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
23	B	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
31	b	623	LHG	O8-C23-C24	2.92	121.06	111.91
23	R	313	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
34	f	101	HEM	CHC-C4B-C3B	2.91	129.03	124.57
38	G	618	NEX	C39-C29-C30	-2.91	118.84	122.92
37	Y	301	XAT	C15-C14-C13	-2.91	123.15	127.31
23	R	305	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
31	B	621	LHG	O8-C23-C24	2.91	121.05	111.91
23	B	608	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	D	401	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
35	S	306	CHL	CHB-C4A-NA	2.91	128.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	d	404	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	y	311	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	B	603	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
31	l	102	LHG	O8-C23-C24	2.91	121.04	111.91
23	s	613	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
23	C	511	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	C	513	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
38	R	316	NEX	C24-C23-C22	-2.91	105.16	110.77
23	g	610	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	N	604	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
23	r	604	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
23	n	612	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	N	610	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
35	Y	308	CHL	O2D-CGD-O1D	-2.90	118.16	123.84
36	N	616	LUT	C10-C11-C12	-2.90	114.16	123.22
35	g	608	CHL	CMB-C2B-C3B	2.90	130.11	124.68
37	g	617	XAT	C4-C3-C2	-2.90	105.17	110.77
24	A	403	PHO	C1B-NB-C4B	2.90	113.05	107.09
23	B	606	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
23	S	309	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	S	313	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	S	314	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
35	R	308	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
35	Y	310	CHL	CMB-C2B-C3B	2.90	130.10	124.68
23	s	612	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	s	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	N	603	CLA	CHB-C4A-NA	2.90	128.52	124.51
35	N	607	CHL	C1B-CHB-C4A	-2.90	124.38	130.12
23	b	605	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
23	b	610	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
38	n	617	NEX	C26-C27-C28	-2.89	119.88	125.99
23	y	303	CLA	CHB-C4A-NA	2.89	128.51	124.51
23	Y	315	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
23	R	302	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	a	402	PHO	C1B-NB-C4B	2.89	113.03	107.09
35	Y	302	CHL	CMB-C2B-C3B	2.89	130.09	124.68
23	c	509	CLA	CHB-C4A-NA	2.89	128.51	124.51
35	S	306	CHL	CMB-C2B-C3B	2.89	130.09	124.68
23	C	505	CLA	CMB-C2B-C3B	2.89	130.08	124.68
23	g	614	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
23	g	603	CLA	CHB-C4A-NA	2.89	128.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	G	607	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
23	S	304	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	S	310	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	b	619	BCR	C1-C6-C5	-2.89	118.55	122.61
23	b	612	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
23	b	606	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	c	513	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	R	302	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
23	C	502	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
23	Y	313	CLA	CHB-C4A-NA	2.88	128.49	124.51
35	y	306	CHL	CHD-C1D-ND	-2.88	121.81	124.45
36	g	615	LUT	C7-C8-C9	-2.88	121.89	126.23
23	b	603	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	N	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	R	312	CLA	CMB-C2B-C3B	2.87	130.06	124.68
38	r	615	NEX	C24-C23-C22	-2.87	105.22	110.77
23	B	601	CLA	CMB-C2B-C3B	2.87	130.06	124.68
23	B	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	y	315	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
23	r	604	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	N	614	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
35	G	606	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
23	C	508	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	b	608	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
35	g	607	CHL	CMB-C2B-C3B	2.87	130.04	124.68
23	n	610	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	B	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	a	405	BCR	C20-C21-C22	-2.87	123.22	127.31
35	N	606	CHL	C1B-CHB-C4A	-2.87	124.44	130.12
35	Y	306	CHL	CHD-C1D-ND	-2.87	121.82	124.45
35	G	601	CHL	CMB-C2B-C1B	-2.86	124.06	128.46
23	c	504	CLA	CMB-C2B-C3B	2.86	130.04	124.68
36	R	314	LUT	C11-C10-C9	-2.86	123.22	127.31
35	R	308	CHL	C1B-CHB-C4A	-2.86	124.45	130.12
23	G	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	B	608	CLA	CMB-C2B-C3B	2.86	130.03	124.68
36	s	614	LUT	C30-C31-C32	-2.86	114.29	123.22
35	G	609	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
23	B	615	CLA	CMB-C2B-C3B	2.86	130.03	124.68
33	d	406	PL9	C35-C34-C36	-2.86	110.46	115.27
37	g	620	XAT	C4-C3-C2	-2.86	105.25	110.77
23	d	402	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
23	C	514	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
23	r	601	CLA	CMB-C2B-C3B	2.86	130.02	124.68
37	R	315	XAT	C4-C3-C2	-2.86	105.25	110.77
23	B	605	CLA	CHB-C4A-NA	2.86	128.46	124.51
23	n	614	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
35	g	609	CHL	CMB-C2B-C3B	2.86	130.02	124.68
23	b	605	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
23	c	513	CLA	C1B-CHB-C4A	-2.85	124.46	130.12
23	Y	311	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	B	613	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
23	d	401	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	b	617	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	g	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	S	303	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	n	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	C	510	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	B	617	BCR	C1-C6-C5	-2.85	118.60	122.61
23	y	313	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	C	504	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	y	316	LUT	C38-C25-C24	-2.85	117.47	123.56
23	c	503	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	G	614	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
23	C	503	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	g	615	LUT	C15-C14-C13	-2.85	123.25	127.31
35	G	608	CHL	CMB-C2B-C3B	2.85	130.00	124.68
23	c	502	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	C	514	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	c	510	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	c	512	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
23	Y	313	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	R	312	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	k	101	BCR	C24-C23-C22	-2.84	121.94	126.23
23	N	614	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	Y	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	519	BCR	C3-C4-C5	-2.84	109.01	114.08
35	r	607	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
36	s	615	LUT	C38-C25-C24	-2.84	117.48	123.56
36	g	615	LUT	C35-C15-C14	-2.84	117.67	123.47
23	n	612	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
36	N	616	LUT	C38-C25-C24	-2.83	117.49	123.56
23	N	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	s	607	CHL	CHD-C1D-ND	-2.83	121.85	124.45
23	c	501	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
23	C	513	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	s	611	CLA	CHB-C4A-NA	2.83	128.43	124.51
38	n	617	NEX	C39-C29-C30	-2.83	118.96	122.92
23	s	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	h	101	BCR	C38-C26-C25	-2.83	121.35	124.53
23	S	313	CLA	CMB-C2B-C3B	2.83	129.97	124.68
36	S	316	LUT	C38-C25-C24	-2.83	117.51	123.56
23	b	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
35	g	609	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
23	r	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	y	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
36	g	616	LUT	C38-C25-C24	-2.82	117.52	123.56
23	c	506	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
23	B	606	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	Y	303	CLA	CHB-C4A-NA	2.82	128.41	124.51
35	S	307	CHL	CHB-C4A-NA	2.82	128.41	124.51
23	n	613	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
23	n	612	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
36	G	616	LUT	C38-C25-C24	-2.82	117.53	123.56
23	G	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	C	503	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	n	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	R	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	b	612	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	C	516	BCR	C21-C20-C19	-2.81	114.44	123.22
23	C	502	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	c	501	CLA	CMB-C2B-C3B	2.81	129.94	124.68
35	n	607	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
23	Y	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	r	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	c	512	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	N	613	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
23	R	310	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	g	613	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
23	b	615	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
36	g	615	LUT	C11-C10-C9	-2.80	123.31	127.31
23	R	310	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
23	R	304	CLA	CHB-C4A-NA	2.80	128.39	124.51
36	Y	316	LUT	C38-C25-C24	-2.80	117.56	123.56
35	r	605	CHL	CHD-C1D-ND	-2.80	121.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	615	LUT	C35-C15-C14	-2.80	117.73	123.47
23	b	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	R	309	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	G	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	g	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
35	S	307	CHL	C1B-CHB-C4A	-2.80	124.57	130.12
23	y	303	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	r	609	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	S	311	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	B	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	G	605	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
23	s	611	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	b	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	Y	310	CHL	C2A-C1A-CHA	2.80	128.75	123.86
23	G	610	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	g	601	CHL	CMB-C2B-C1B	-2.80	124.17	128.46
35	g	605	CHL	CMB-C2B-C3B	2.79	129.91	124.68
35	N	606	CHL	O2D-CGD-O1D	-2.79	118.38	123.84
23	B	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
37	Y	301	XAT	C31-C30-C29	-2.79	123.32	127.31
25	z	101	BCR	C24-C23-C22	-2.79	122.01	126.23
23	G	613	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
23	G	603	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	r	602	CLA	CMB-C2B-C3B	2.79	129.90	124.68
35	S	306	CHL	O2D-CGD-O1D	-2.79	118.38	123.84
35	y	310	CHL	C2A-C1A-CHA	2.79	128.74	123.86
25	c	514	BCR	C21-C20-C19	-2.79	114.51	123.22
23	D	401	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	R	311	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	r	601	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
35	s	606	CHL	OMC-CMC-C2C	-2.79	119.38	125.69
25	C	516	BCR	C16-C17-C18	-2.79	123.33	127.31
23	N	611	CLA	CHB-C4A-NA	2.79	128.37	124.51
38	G	618	NEX	C35-C34-C33	-2.79	123.33	127.31
36	s	614	LUT	C38-C25-C24	-2.79	117.60	123.56
35	n	609	CHL	CHD-C1D-ND	-2.78	121.89	124.45
23	s	612	CLA	CMB-C2B-C3B	2.78	129.89	124.68
23	S	309	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
23	R	303	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	c	514	BCR	C16-C17-C18	-2.78	123.34	127.31
38	R	301	NEX	C26-C27-C28	-2.78	120.11	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	306	CHL	CHD-C1D-ND	-2.78	121.90	124.45
37	G	617	XAT	C15-C35-C34	-2.78	117.78	123.47
23	r	610	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
36	s	614	LUT	C10-C11-C12	-2.78	114.54	123.22
37	y	301	XAT	C31-C30-C29	-2.78	123.34	127.31
23	s	608	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	B	613	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	y	314	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
23	R	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
35	S	308	CHL	C2A-C1A-CHA	2.78	128.72	123.86
23	R	311	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
24	D	402	PHO	C1B-NB-C4B	2.78	112.79	107.09
23	b	609	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
38	G	618	NEX	C11-C12-C13	-2.78	118.62	126.42
36	r	613	LUT	C31-C30-C29	-2.78	123.35	127.31
23	c	502	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	r	603	CLA	CHB-C4A-NA	2.77	128.35	124.51
35	y	310	CHL	O2D-CGD-O1D	-2.77	118.41	123.84
23	r	612	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
23	B	605	CLA	CMB-C2B-C3B	2.77	129.87	124.68
23	d	401	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	b	615	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	512	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	B	615	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
38	g	618	NEX	C24-C23-C22	-2.77	105.42	110.77
23	s	610	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	S	304	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
23	C	505	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
35	S	307	CHL	O2D-CGD-O1D	-2.77	118.43	123.84
25	k	101	BCR	C7-C8-C9	-2.76	122.06	126.23
35	G	605	CHL	CMB-C2B-C3B	2.76	129.85	124.68
23	Y	311	CLA	CHB-C4A-NA	2.76	128.34	124.51
23	b	618	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	d	403	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
23	B	608	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b	618	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	G	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	N	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
23	D	403	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	Y	314	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
35	g	605	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
23	N	612	CLA	C1B-CHB-C4A	-2.76	124.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
23	n	603	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	n	604	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	A	401	CLA	CMB-C2B-C3B	2.76	129.83	124.68
23	s	613	CLA	CAA-C2A-C3A	-2.75	109.67	116.10
23	n	612	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	r	611	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
36	S	316	LUT	C19-C9-C8	2.75	122.42	118.08
23	B	607	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	g	604	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
36	y	316	LUT	C30-C31-C32	-2.75	114.63	123.22
35	s	606	CHL	CHB-C4A-NA	2.75	128.32	124.51
23	b	617	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
35	S	302	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
23	n	611	CLA	CHB-C4A-NA	2.75	128.31	124.51
35	n	605	CHL	OMC-CMC-C2C	-2.75	119.47	125.69
23	Y	303	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	g	603	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	G	604	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
23	s	603	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
37	g	617	XAT	C24-C23-C22	-2.75	105.47	110.77
35	G	606	CHL	C1B-CHB-C4A	-2.74	124.68	130.12
25	A	405	BCR	C20-C21-C22	-2.74	123.39	127.31
23	y	304	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
23	b	604	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	C	506	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	r	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
36	G	615	LUT	C7-C8-C9	-2.74	122.09	126.23
23	b	607	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
23	c	509	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	a	403	PHO	CMB-C2B-C3B	2.74	129.80	124.68
35	y	309	CHL	C1B-CHB-C4A	-2.74	124.70	130.12
23	r	602	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
36	N	616	LUT	C7-C8-C9	-2.73	122.11	126.23
23	n	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	a	401	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
36	G	615	LUT	C15-C14-C13	-2.73	123.41	127.31
35	Y	309	CHL	C1B-CHB-C4A	-2.73	124.70	130.12
35	N	607	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
23	n	603	CLA	CMB-C2B-C3B	2.73	129.79	124.68
38	Y	318	NEX	C26-C27-C28	-2.73	120.22	125.99
36	y	317	LUT	C38-C25-C24	-2.73	117.72	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	N	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	N	612	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
23	S	311	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
36	g	615	LUT	C38-C25-C24	-2.73	117.72	123.56
23	D	401	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
35	Y	310	CHL	O2D-CGD-O1D	-2.73	118.51	123.84
23	N	612	CLA	CMB-C2B-C3B	2.72	129.78	124.68
35	N	605	CHL	OMC-CMC-C2C	-2.72	119.53	125.69
23	b	610	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	A	405	BCR	C33-C5-C6	-2.72	121.47	124.53
38	R	316	NEX	C11-C12-C13	-2.72	118.78	126.42
35	Y	308	CHL	CHB-C4A-NA	2.72	128.27	124.51
23	C	510	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
30	C	522	LMG	O8-C28-C29	2.72	120.44	111.91
23	d	404	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	n	603	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
23	G	613	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	s	610	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
38	R	316	NEX	C31-C30-C29	-2.71	123.44	127.31
23	D	404	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	b	610	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	c	521	LMG	O8-C28-C29	2.71	120.42	111.91
37	G	617	XAT	C35-C34-C33	-2.71	123.44	127.31
23	B	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	c	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	Y	317	LUT	C38-C25-C24	-2.71	117.76	123.56
24	a	403	PHO	C1B-NB-C4B	2.71	112.65	107.09
25	C	515	BCR	C24-C23-C22	-2.71	122.14	126.23
38	R	316	NEX	C15-C35-C34	-2.71	117.93	123.47
35	G	601	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
23	B	605	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
37	r	614	XAT	C31-C30-C29	-2.71	123.45	127.31
23	C	504	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
38	G	618	NEX	C24-C23-C22	-2.70	105.55	110.77
23	C	510	CLA	CMB-C2B-C3B	2.70	129.74	124.68
36	r	613	LUT	C38-C25-C24	-2.70	117.77	123.56
23	D	403	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
23	s	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	c	503	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
23	S	314	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
23	c	509	CLA	CMB-C2B-C3B	2.70	129.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	604	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	G	611	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	y	304	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
26	B	625	SQD	O47-C7-C8	2.70	117.31	111.50
35	r	606	CHL	CHD-C1D-ND	-2.70	121.98	124.45
25	H	101	BCR	C38-C26-C25	-2.70	121.50	124.53
23	S	303	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	b	602	SQD	O48-C23-C24	2.69	120.36	111.91
36	G	615	LUT	C38-C25-C24	-2.69	117.80	123.56
23	C	505	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
35	g	601	CHL	O2D-CGD-O1D	-2.69	118.57	123.84
23	A	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	r	602	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
38	s	616	NEX	C17-C1-C6	-2.69	108.06	110.47
35	s	607	CHL	C2A-C1A-CHA	2.69	128.56	123.86
36	n	616	LUT	C38-C25-C24	-2.69	117.81	123.56
23	C	513	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	s	608	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	n	615	LUT	C38-C25-C24	-2.69	117.81	123.56
23	B	612	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	C	512	CLA	CHB-C4A-NA	2.68	128.22	124.51
35	n	601	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
23	N	611	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
25	K	101	BCR	C30-C25-C26	-2.68	118.84	122.61
25	c	514	BCR	C33-C5-C6	-2.68	121.52	124.53
23	A	402	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	R	301	NEX	C24-C23-C22	-2.68	105.60	110.77
23	A	401	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
36	N	615	LUT	C30-C31-C32	-2.68	114.86	123.22
25	a	405	BCR	C33-C5-C6	-2.68	121.52	124.53
23	b	609	CLA	CHB-C4A-NA	2.68	128.21	124.51
30	C	522	LMG	C8-O7-C10	-2.67	111.21	117.79
35	n	606	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
23	G	602	CLA	CHB-C4A-NA	2.67	128.21	124.51
35	N	606	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
38	S	317	NEX	C24-C23-C22	-2.67	105.61	110.77
33	d	406	PL9	C7-C3-C4	2.67	119.05	116.88
23	N	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
36	N	615	LUT	C38-C25-C24	-2.67	117.84	123.56
25	K	101	BCR	C11-C10-C9	-2.67	123.50	127.31
38	Y	318	NEX	C39-C29-C30	-2.67	119.18	122.92
23	g	602	CLA	CHB-C4A-NA	2.67	128.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	102	LHG	O8-C23-C24	2.67	120.28	111.91
23	B	613	CLA	CMB-C2B-C3B	2.67	129.67	124.68
35	G	609	CHL	CMB-C2B-C3B	2.67	129.67	124.68
23	n	611	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	b	614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
35	s	606	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
36	n	615	LUT	C30-C31-C32	-2.67	114.89	123.22
23	A	404	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	y	311	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	r	603	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
23	b	612	CLA	CHB-C4A-NA	2.66	128.20	124.51
36	R	314	LUT	C38-C25-C24	-2.66	117.86	123.56
23	r	608	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
23	c	507	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
25	C	516	BCR	C33-C5-C6	-2.66	121.54	124.53
31	l	103	LHG	O8-C23-C24	2.66	120.27	111.91
23	c	507	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
23	B	616	CLA	CHB-C4A-NA	2.66	128.19	124.51
35	g	606	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
38	g	618	NEX	C39-C29-C30	-2.66	119.20	122.92
35	y	308	CHL	CHB-C4A-NA	2.66	128.19	124.51
35	n	605	CHL	CHD-C1D-ND	-2.66	122.01	124.45
23	s	610	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
23	y	312	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
23	g	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	C	504	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	g	610	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	B	610	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	A	402	CLA	CBA-CAA-C2A	2.66	121.70	113.86
23	B	616	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
38	n	617	NEX	C16-C1-C6	2.65	112.85	110.47
26	B	625	SQD	O48-C23-C24	2.65	120.24	111.91
23	R	312	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	k	101	BCR	C16-C15-C14	-2.65	118.04	123.47
23	s	613	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	B	606	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	C	514	CLA	CHB-C4A-NA	2.65	128.18	124.51
35	s	601	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
23	R	304	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
23	s	603	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
38	Y	318	NEX	C24-C23-C22	-2.65	105.66	110.77
38	n	617	NEX	C31-C30-C29	-2.65	123.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
35	S	306	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
36	G	615	LUT	C11-C10-C9	-2.65	123.53	127.31
23	b	606	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	c	518	BCR	C29-C30-C25	2.65	114.55	110.48
38	R	301	NEX	C39-C29-C30	-2.64	119.22	122.92
23	g	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
35	y	307	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
23	c	513	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	B	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	b	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	B	604	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	g	611	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
31	W	201	LHG	C5-O7-C7	-2.64	111.30	117.79
23	a	404	CLA	CHB-C4A-NA	2.64	128.16	124.51
38	r	615	NEX	C35-C34-C33	-2.64	123.55	127.31
23	S	314	CLA	CMA-C3A-C2A	-2.64	109.94	116.10
25	C	519	BCR	C15-C16-C17	-2.64	118.07	123.47
38	r	615	NEX	C16-C1-C6	2.64	112.83	110.47
23	G	612	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
23	Y	304	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
30	a	407	LMG	O8-C28-C29	2.64	120.18	111.91
23	N	611	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
23	S	314	CLA	CHB-C4A-NA	2.63	128.16	124.51
23	g	612	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
23	y	313	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
23	G	611	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
23	C	514	CLA	CBA-CAA-C2A	2.63	121.63	113.86
23	c	511	CLA	CHB-C4A-NA	2.63	128.15	124.51
35	n	601	CHL	CHD-C1D-ND	-2.63	122.03	124.45
35	g	607	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
36	Y	316	LUT	C30-C31-C32	-2.63	115.00	123.22
35	g	605	CHL	CHD-C1D-ND	-2.63	122.04	124.45
35	Y	307	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
35	n	605	CHL	CHB-C4A-NA	2.63	128.15	124.51
31	c	516	LHG	C5-O7-C7	-2.63	111.32	117.79
23	C	505	CLA	CHB-C4A-NA	2.63	128.14	124.51
38	R	316	NEX	C35-C34-C33	-2.63	123.56	127.31
23	n	611	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
26	b	602	SQD	O47-C7-C8	2.62	117.16	111.50
23	N	603	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
25	a	405	BCR	C24-C23-C22	-2.62	122.27	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	405	BCR	C29-C30-C25	2.62	114.52	110.48
31	c	516	LHG	O8-C23-C24	2.62	120.14	111.91
23	C	502	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	y	304	CLA	CMB-C2B-C3B	2.62	129.59	124.68
35	Y	307	CHL	CHD-C1D-ND	-2.62	122.04	124.45
23	g	603	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
23	R	304	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
30	s	619	LMG	C7-O1-C1	-2.62	108.62	113.74
23	B	609	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	Y	304	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
23	B	604	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
35	S	307	CHL	CAA-C2A-C3A	-2.62	107.71	114.26
23	S	313	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
36	g	616	LUT	C7-C8-C9	-2.62	122.28	126.23
23	c	504	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	b	614	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
23	y	312	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
35	N	601	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
23	D	403	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
36	g	616	LUT	C10-C11-C12	-2.62	115.05	123.22
25	b	620	BCR	C15-C16-C17	-2.62	118.12	123.47
23	n	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	S	304	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
25	B	618	BCR	C15-C16-C17	-2.61	118.12	123.47
35	S	307	CHL	OMC-CMC-C2C	-2.61	119.78	125.69
37	G	620	XAT	C15-C35-C34	-2.61	118.12	123.47
35	Y	310	CHL	CHD-C1D-ND	-2.61	122.05	124.45
23	b	606	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
35	n	606	CHL	CHD-C1D-ND	-2.61	122.05	124.45
23	C	508	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
30	B	620	LMG	O8-C28-C29	2.61	120.10	111.91
35	G	609	CHL	CAA-C2A-C3A	-2.61	105.63	112.78
26	l	101	SQD	O7-S-C6	2.61	110.04	106.94
35	y	308	CHL	CMB-C2B-C3B	2.61	129.56	124.68
23	d	403	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	R	309	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	Y	304	CLA	CMB-C2B-C3B	2.61	129.55	124.68
23	s	610	CLA	CAA-C2A-C3A	-2.60	107.75	114.26
23	B	604	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	B	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	K	101	BCR	C38-C26-C27	2.60	118.62	113.62
31	W	201	LHG	O8-C23-C24	2.60	120.07	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	101	SQD	O48-C23-C24	2.60	120.07	111.91
23	b	615	CLA	CMB-C2B-C3B	2.60	129.54	124.68
23	b	615	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
25	D	405	BCR	C29-C30-C25	2.60	114.48	110.48
23	R	303	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	g	612	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
35	s	601	CHL	OMC-CMC-C2C	-2.60	119.81	125.69
23	r	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	b	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
35	N	609	CHL	CHD-C1D-ND	-2.60	122.07	124.45
38	n	617	NEX	C24-C23-C22	-2.60	105.76	110.77
23	G	603	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
31	s	617	LHG	O8-C23-C24	2.59	120.05	111.91
23	S	312	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
38	r	615	NEX	C31-C30-C29	-2.59	123.61	127.31
23	n	613	CLA	CHB-C4A-NA	2.59	128.10	124.51
23	c	503	CLA	CHB-C4A-NA	2.59	128.09	124.51
35	s	606	CHL	CHD-C1D-ND	-2.59	122.07	124.45
36	Y	316	LUT	C15-C14-C13	-2.59	123.61	127.31
23	r	601	CLA	CHB-C4A-NA	2.59	128.09	124.51
38	g	618	NEX	C26-C27-C28	-2.59	120.52	125.99
35	G	609	CHL	C2A-C1A-CHA	2.59	128.38	123.86
23	b	606	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	G	612	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
35	G	601	CHL	CHD-C1D-ND	-2.59	122.08	124.45
23	Y	312	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
35	s	605	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
25	c	514	BCR	C24-C23-C22	-2.59	122.33	126.23
23	C	511	CLA	CHB-C4A-NA	2.59	128.09	124.51
33	D	406	PL9	C7-C3-C4	2.59	118.98	116.88
35	g	605	CHL	OMC-CMC-C2C	-2.59	119.84	125.69
23	S	305	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	N	603	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	Y	313	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
23	s	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
23	n	613	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
37	g	620	XAT	C15-C35-C34	-2.58	118.18	123.47
23	B	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
35	G	601	CHL	CMB-C2B-C3B	2.58	129.51	124.68
24	D	402	PHO	C6-C5-C3	2.58	120.22	113.45
35	R	308	CHL	CHB-C4A-NA	2.58	128.08	124.51
31	D	408	LHG	O8-C23-C24	2.58	120.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	y	316	LUT	C10-C11-C12	-2.58	115.16	123.22
25	k	101	BCR	C38-C26-C27	2.58	118.57	113.62
28	B	626	DGD	C1D-O6D-C5D	2.58	118.75	113.69
35	r	606	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
23	C	512	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
35	y	307	CHL	CHD-C1D-ND	-2.58	122.08	124.45
35	G	605	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
23	b	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	s	609	CLA	O2D-CGD-CBD	2.58	115.85	111.27
23	B	609	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
23	Y	304	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	b	610	CLA	CHB-C4A-NA	2.58	128.07	124.51
34	F	101	HEM	C4D-ND-C1D	2.57	107.73	105.07
30	C	501	LMG	O8-C28-C29	2.57	119.98	111.91
23	c	501	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
28	A	408	DGD	O1G-C1A-C2A	2.57	119.98	111.91
25	k	101	BCR	C30-C25-C26	-2.57	118.99	122.61
23	R	311	CLA	CHB-C4A-NA	2.57	128.06	124.51
35	R	306	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
35	Y	308	CHL	CMB-C2B-C3B	2.57	129.48	124.68
35	G	605	CHL	CHD-C1D-ND	-2.57	122.09	124.45
31	d	408	LHG	O8-C23-C24	2.57	119.97	111.91
35	n	605	CHL	O2D-CGD-CBD	2.57	115.83	111.27
23	b	611	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
35	s	605	CHL	CHD-C1D-ND	-2.56	122.10	124.45
35	N	609	CHL	O2D-CGD-CBD	2.56	115.83	111.27
23	N	604	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	a	403	PHO	C6-C5-C3	2.56	120.18	113.45
23	s	604	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
35	S	302	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
36	S	315	LUT	C38-C25-C24	-2.56	118.08	123.56
23	c	507	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
35	N	605	CHL	CHB-C4A-NA	2.56	128.05	124.51
36	R	314	LUT	C31-C30-C29	-2.56	123.66	127.31
25	c	518	BCR	C1-C6-C5	-2.56	119.01	122.61
30	W	203	LMG	O8-C28-C29	2.56	119.94	111.91
23	Y	312	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	Y	315	CLA	CHB-C4A-NA	2.56	128.05	124.51
35	Y	308	CHL	OMC-CMC-C2C	-2.56	119.90	125.69
23	B	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	Y	314	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	c	510	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	s	611	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
25	k	101	BCR	C38-C26-C25	-2.56	121.66	124.53
23	b	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	D	405	BCR	C3-C4-C5	-2.55	109.52	114.08
35	G	606	CHL	OMC-CMC-C2C	-2.55	119.91	125.69
30	D	409	LMG	O8-C28-C29	2.55	119.92	111.91
23	s	613	CLA	CMA-C3A-C2A	-2.55	110.14	116.10
35	g	606	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
23	C	508	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
38	N	617	NEX	C24-C23-C22	-2.55	105.85	110.77
23	B	615	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
23	c	504	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
35	r	606	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
35	R	307	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
23	c	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	d	409	LMG	O8-C28-C29	2.55	119.90	111.91
23	C	513	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
25	d	405	BCR	C3-C4-C5	-2.55	109.53	114.08
35	g	601	CHL	CMB-C2B-C3B	2.55	129.44	124.68
23	C	509	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	G	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	S	310	CLA	CHB-C4A-NA	2.54	128.03	124.51
34	f	101	HEM	C4D-ND-C1D	2.54	107.70	105.07
30	w	202	LMG	O8-C28-C29	2.54	119.89	111.91
23	c	512	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	y	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	c	521	LMG	C8-O7-C10	-2.54	111.53	117.79
23	c	508	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	C	503	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
35	y	310	CHL	CHD-C1D-ND	-2.54	122.12	124.45
23	y	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	N	613	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
35	g	601	CHL	OMC-CMC-C2C	-2.54	119.95	125.69
23	s	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
28	c	515	DGD	O1G-C1A-C2A	2.54	119.87	111.91
35	r	605	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
23	g	603	CLA	CMB-C2B-C3B	2.54	129.42	124.68
23	g	611	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	y	314	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	B	611	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
36	y	316	LUT	C7-C8-C9	-2.53	122.41	126.23
35	g	606	CHL	CHD-C1D-ND	-2.53	122.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	N	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
38	g	618	NEX	C11-C12-C13	-2.53	119.31	126.42
36	g	616	LUT	C11-C10-C9	-2.53	123.70	127.31
23	c	510	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
28	C	517	DGD	O1G-C1A-C2A	2.53	119.83	111.91
37	R	315	XAT	C19-C9-C8	2.52	122.06	118.08
35	g	601	CHL	CHD-C1D-ND	-2.52	122.13	124.45
37	R	315	XAT	C31-C30-C29	-2.52	123.71	127.31
31	S	318	LHG	O8-C23-C24	2.52	119.83	111.91
25	A	405	BCR	C24-C23-C22	-2.52	122.42	126.23
23	r	603	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
35	N	609	CHL	CHB-C4A-NA	2.52	128.00	124.51
38	S	317	NEX	C16-C1-C6	2.52	112.73	110.47
23	r	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
35	G	601	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
23	c	502	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	b	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
38	r	615	NEX	C2-C1-C6	2.52	111.66	109.21
23	C	503	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	c	511	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
36	Y	317	LUT	C36-C21-C26	2.51	113.35	109.55
23	y	304	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
23	S	313	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	a	401	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	R	304	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	b	617	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	r	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
35	y	308	CHL	OMC-CMC-C2C	-2.51	120.02	125.69
35	y	302	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
36	S	315	LUT	C15-C14-C13	-2.50	123.74	127.31
25	b	620	BCR	C33-C5-C4	2.50	118.42	113.62
36	N	616	LUT	C11-C10-C9	-2.50	123.74	127.31
38	s	616	NEX	C24-C23-C22	-2.50	105.94	110.77
30	b	601	LMG	O8-C28-C29	2.50	119.76	111.91
30	b	622	LMG	O8-C28-C29	2.50	119.76	111.91
25	k	101	BCR	C10-C11-C12	-2.50	115.41	123.22
23	Y	313	CLA	C2A-C1A-CHA	2.50	128.23	123.86
25	z	101	BCR	C33-C5-C6	-2.50	121.72	124.53
35	S	307	CHL	CHD-C1D-ND	-2.50	122.16	124.45
23	R	302	CLA	CHB-C4A-NA	2.50	127.97	124.51
35	S	306	CHL	C1B-CHB-C4A	-2.50	125.17	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	623	LMG	O8-C28-C29	2.50	119.74	111.91
23	B	614	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	c	509	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
23	s	604	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	g	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	G	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
35	r	607	CHL	CHB-C4A-NA	2.49	127.96	124.51
36	y	317	LUT	C11-C10-C9	-2.49	123.75	127.31
23	d	403	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	s	609	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	c	514	BCR	C33-C5-C4	2.49	118.40	113.62
23	b	616	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	C	516	BCR	C33-C5-C4	2.49	118.40	113.62
35	Y	302	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
23	n	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	c	506	CLA	CHB-C4A-NA	2.49	127.95	124.51
36	G	615	LUT	C10-C11-C12	-2.49	115.46	123.22
35	N	601	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
23	S	311	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
23	D	403	CLA	CHB-C4A-NA	2.48	127.95	124.51
36	N	615	LUT	C11-C10-C9	-2.48	123.77	127.31
25	K	101	BCR	C24-C23-C22	-2.48	122.49	126.23
28	b	625	DGD	C1D-O6D-C5D	2.48	118.55	113.69
30	S	301	LMG	C7-O1-C1	-2.48	108.90	113.74
23	y	304	CLA	C2A-C1A-CHA	2.48	128.19	123.86
28	B	626	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	N	612	CLA	C2A-C1A-CHA	2.47	128.19	123.86
25	b	620	BCR	C38-C26-C25	-2.47	121.75	124.53
35	y	307	CHL	OMC-CMC-C2C	-2.47	120.09	125.69
38	N	617	NEX	C11-C10-C9	-2.47	123.78	127.31
23	R	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	c	502	CLA	CMB-C2B-C3B	2.47	129.30	124.68
25	C	519	BCR	C29-C30-C25	2.47	114.29	110.48
23	y	313	CLA	C2A-C1A-CHA	2.47	128.18	123.86
25	K	101	BCR	C2-C1-C6	2.47	114.28	110.48
31	G	619	LHG	O8-C23-C24	2.47	119.66	111.91
23	Y	312	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	C	502	CLA	CHB-C4A-NA	2.47	127.92	124.51
35	s	601	CHL	CHD-C1D-ND	-2.47	122.19	124.45
36	s	615	LUT	C15-C14-C13	-2.47	123.79	127.31
25	a	405	BCR	C33-C5-C4	2.47	118.35	113.62
23	R	310	CLA	CHB-C4A-NA	2.47	127.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	401	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	B	618	BCR	C33-C5-C4	2.46	118.35	113.62
23	C	510	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
36	s	615	LUT	C10-C11-C12	-2.46	115.53	123.22
25	B	618	BCR	C38-C26-C25	-2.46	121.76	124.53
38	r	615	NEX	C17-C1-C6	-2.46	108.27	110.47
23	g	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	R	313	CLA	O2D-CGD-CBD	2.46	115.64	111.27
26	A	406	SQD	O48-C23-C24	2.46	119.62	111.91
35	Y	307	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
23	S	309	CLA	CMB-C2B-C3B	2.46	129.28	124.68
36	g	616	LUT	C31-C30-C29	-2.46	123.80	127.31
35	S	308	CHL	CAA-C2A-C3A	-2.46	106.05	112.78
23	b	611	CLA	CMB-C2B-C3B	2.46	129.27	124.68
23	S	309	CLA	O2D-CGD-CBD	2.45	115.63	111.27
36	N	615	LUT	C15-C14-C13	-2.45	123.81	127.31
25	A	405	BCR	C33-C5-C4	2.45	118.33	113.62
23	N	614	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	h	101	BCR	C16-C15-C14	-2.45	118.45	123.47
25	K	101	BCR	C23-C24-C25	-2.45	120.32	127.20
23	b	607	CLA	CMB-C2B-C3B	2.45	129.26	124.68
30	s	619	LMG	O8-C28-C29	2.45	119.58	111.91
23	n	614	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	B	609	CLA	CMB-C2B-C3B	2.44	129.25	124.68
35	Y	302	CHL	CHB-C4A-NA	2.44	127.89	124.51
23	B	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	y	306	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
23	b	612	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
23	G	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	D	405	BCR	C30-C25-C26	-2.44	119.18	122.61
36	s	614	LUT	C15-C14-C13	-2.44	123.83	127.31
37	r	614	XAT	C19-C9-C8	2.44	121.92	118.08
31	g	619	LHG	O8-C23-C24	2.44	119.56	111.91
23	r	612	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	G	603	CLA	O2D-CGD-CBD	2.44	115.60	111.27
35	N	608	CHL	CHD-C1D-ND	-2.44	122.21	124.45
30	C	501	LMG	C8-O7-C10	-2.44	111.79	117.79
38	R	316	NEX	C26-C27-C28	-2.44	120.84	125.99
38	S	317	NEX	C11-C12-C13	-2.44	119.57	126.42
36	g	616	LUT	C3-C4-C5	-2.43	107.01	111.85
23	r	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	n	612	CLA	C2A-C1A-CHA	2.43	128.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	s	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
35	s	607	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
35	Y	306	CHL	CHB-C4A-NA	2.43	127.87	124.51
28	d	410	DGD	O1G-C1A-C2A	2.43	119.53	111.91
25	C	519	BCR	C27-C26-C25	-2.43	119.21	122.73
25	H	101	BCR	C16-C15-C14	-2.43	118.50	123.47
35	y	306	CHL	CHB-C4A-NA	2.43	127.87	124.51
25	d	405	BCR	C30-C25-C26	-2.42	119.20	122.61
36	Y	317	LUT	C11-C10-C9	-2.42	123.85	127.31
25	C	516	BCR	C24-C23-C22	-2.42	122.58	126.23
23	Y	312	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
35	n	607	CHL	CAA-C2A-C3A	-2.42	106.15	112.78
35	n	601	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
35	N	606	CHL	CHD-C1D-ND	-2.42	122.23	124.45
36	y	316	LUT	C15-C14-C13	-2.42	123.86	127.31
30	S	301	LMG	O8-C28-C29	2.42	119.50	111.91
36	G	616	LUT	C15-C35-C34	-2.42	118.52	123.47
36	Y	316	LUT	C7-C8-C9	-2.42	122.58	126.23
25	K	101	BCR	C16-C15-C14	-2.42	118.53	123.47
23	c	505	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
35	r	607	CHL	CHD-C1D-ND	-2.41	122.24	124.45
25	b	621	BCR	C33-C5-C4	2.41	118.25	113.62
36	Y	316	LUT	C10-C11-C12	-2.41	115.69	123.22
23	d	402	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	b	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
35	S	302	CHL	CHD-C1D-ND	-2.41	122.24	124.45
23	c	507	CLA	C2A-C1A-CHA	2.41	128.07	123.86
36	n	616	LUT	C10-C11-C12	-2.41	115.70	123.22
23	R	310	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
36	R	314	LUT	C18-C5-C6	-2.41	121.82	124.53
26	L	103	SQD	O48-C23-C24	2.41	119.46	111.91
23	r	601	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
23	y	305	CLA	CHB-C4A-NA	2.40	127.84	124.51
26	L	103	SQD	C1-O5-C5	2.40	118.41	113.69
23	C	508	CLA	C2A-C1A-CHA	2.40	128.06	123.86
38	s	616	NEX	C2-C1-C6	2.40	111.55	109.21
23	B	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	s	611	CLA	C2A-C1A-CHA	2.40	128.06	123.86
36	N	616	LUT	C31-C30-C29	-2.40	123.89	127.31
38	S	317	NEX	C26-C27-C28	-2.40	120.92	125.99
31	n	618	LHG	C5-O7-C7	-2.40	111.88	117.79
35	s	607	CHL	C2A-C3A-C4A	-2.40	97.99	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	616	LUT	C35-C34-C33	-2.40	123.89	127.31
23	b	605	CLA	CHB-C4A-NA	2.40	127.83	124.51
35	n	608	CHL	CHD-C1D-ND	-2.40	122.25	124.45
35	n	609	CHL	O2D-CGD-CBD	2.40	115.53	111.27
25	B	619	BCR	C33-C5-C4	2.40	118.22	113.62
26	a	406	SQD	O48-C23-C24	2.40	119.43	111.91
32	c	522	DMU	C1-C2-C3	2.40	115.15	109.68
23	B	615	CLA	O2D-CGD-CBD	2.40	115.53	111.27
28	B	624	DGD	O1G-C1A-C2A	2.40	119.42	111.91
23	c	510	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
35	g	609	CHL	O2D-CGD-CBD	2.39	115.52	111.27
25	b	620	BCR	C38-C26-C27	2.39	118.21	113.62
31	c	517	LHG	O8-C23-C24	2.39	119.42	111.91
31	C	518	LHG	O8-C23-C24	2.39	119.41	111.91
35	n	606	CHL	CHB-C4A-NA	2.39	127.82	124.51
31	R	317	LHG	O8-C23-C24	2.39	119.41	111.91
35	Y	306	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
23	b	617	CLA	O2D-CGD-CBD	2.39	115.51	111.27
36	S	316	LUT	C8-C9-C10	-2.39	115.28	118.94
35	y	302	CHL	CHB-C4A-NA	2.38	127.81	124.51
37	g	617	XAT	C15-C35-C34	-2.38	118.59	123.47
23	Y	305	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	B	608	CLA	CBA-CAA-C2A	2.38	120.89	113.86
32	C	523	DMU	C1-C2-C3	2.38	115.11	109.68
25	B	618	BCR	C38-C26-C27	2.38	118.18	113.62
23	b	610	CLA	CBA-CAA-C2A	2.38	120.88	113.86
23	B	608	CLA	CHB-C4A-NA	2.38	127.80	124.51
31	b	626	LHG	O8-C23-C24	2.38	119.36	111.91
38	r	615	NEX	C26-C27-C28	-2.37	120.98	125.99
23	S	311	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	G	608	CHL	CHB-C4A-NA	2.37	127.79	124.51
36	n	616	LUT	C7-C8-C9	-2.37	122.65	126.23
23	R	303	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	r	606	CHL	CHB-C4A-NA	2.37	127.79	124.51
31	N	618	LHG	C5-O7-C7	-2.37	111.96	117.79
30	W	203	LMG	C8-O7-C10	-2.37	111.97	117.79
36	Y	317	LUT	C3-C4-C5	-2.37	107.14	111.85
35	g	607	CHL	CAA-C2A-C3A	-2.37	108.35	114.26
23	G	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	b	620	BCR	C33-C5-C6	-2.36	121.87	124.53
23	r	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	C	506	CLA	O2A-CGA-O1A	-2.36	117.63	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	617	XAT	C24-C23-C22	-2.36	106.22	110.77
35	N	605	CHL	CHD-C1D-ND	-2.36	122.29	124.45
25	c	518	BCR	C15-C16-C17	-2.36	118.64	123.47
35	n	606	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
36	g	616	LUT	C15-C35-C34	-2.36	118.64	123.47
25	k	101	BCR	C21-C20-C19	-2.36	115.86	123.22
23	S	314	CLA	O2D-CGD-CBD	2.35	115.45	111.27
23	r	612	CLA	O2D-CGD-CBD	2.35	115.44	111.27
23	C	511	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
38	N	617	NEX	C26-C27-C28	-2.35	121.03	125.99
35	N	608	CHL	CHB-C4A-NA	2.35	127.76	124.51
35	S	306	CHL	CHD-C1D-ND	-2.35	122.30	124.45
31	r	616	LHG	O8-C23-C24	2.35	119.28	111.91
25	b	620	BCR	C30-C25-C26	-2.35	119.31	122.61
35	G	601	CHL	CHC-C1C-NC	2.34	127.76	124.20
23	C	511	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	B	618	BCR	C30-C25-C26	-2.34	119.31	122.61
23	g	604	CLA	CHB-C4A-NA	2.34	127.75	124.51
35	g	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
25	K	101	BCR	C38-C26-C25	-2.34	121.90	124.53
38	N	617	NEX	C16-C1-C6	2.34	112.56	110.47
31	R	317	LHG	C5-O7-C7	-2.34	112.04	117.79
35	Y	308	CHL	CAA-CBA-CGA	-2.34	106.42	113.25
28	D	410	DGD	O1G-C1A-C2A	2.34	119.24	111.91
25	k	101	BCR	C2-C1-C6	2.34	114.08	110.48
30	w	202	LMG	C8-O7-C10	-2.34	112.04	117.79
36	n	615	LUT	C7-C8-C9	-2.33	122.71	126.23
23	S	311	CLA	CAA-C2A-C3A	-2.33	108.43	114.26
25	c	518	BCR	C21-C20-C19	-2.33	115.94	123.22
25	K	101	BCR	C21-C20-C19	-2.33	115.95	123.22
35	g	607	CHL	CHB-C4A-NA	2.33	127.73	124.51
35	n	608	CHL	CHB-C4A-NA	2.32	127.72	124.51
36	S	315	LUT	C39-C29-C28	2.32	121.74	118.08
35	S	306	CHL	C3C-C4C-NC	-2.32	107.97	110.57
34	F	101	HEM	C4C-CHD-C1D	2.32	125.62	122.56
35	S	308	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
36	s	614	LUT	C39-C29-C28	2.32	121.73	118.08
38	r	615	NEX	C15-C35-C34	-2.32	118.72	123.47
35	N	609	CHL	C2A-C1A-CHA	2.32	127.91	123.86
35	n	607	CHL	C2A-C1A-CHA	2.32	127.91	123.86
25	c	518	BCR	C27-C26-C25	-2.32	119.37	122.73
35	y	309	CHL	OMC-CMC-C2C	-2.31	120.46	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Y	307	CHL	CHB-C4A-NA	2.31	127.71	124.51
26	L	103	SQD	O7-S-C6	2.31	109.69	106.94
35	G	606	CHL	CHB-C4A-NA	2.31	127.71	124.51
23	R	302	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
35	r	607	CHL	O2A-CGA-O1A	-2.31	117.76	123.59
37	g	617	XAT	C27-C28-C29	-2.31	121.95	125.53
36	y	317	LUT	C36-C21-C26	2.31	113.04	109.55
35	g	605	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	y	309	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	R	306	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	S	308	CHL	C2A-C3A-C4A	-2.31	98.14	101.87
28	b	625	DGD	C2G-O2G-C1B	-2.31	112.12	117.79
35	n	609	CHL	C2A-C1A-CHA	2.30	127.89	123.86
23	s	603	CLA	C2A-C1A-CHA	2.30	127.89	123.86
25	B	618	BCR	C33-C5-C6	-2.30	121.94	124.53
36	n	616	LUT	C30-C31-C32	-2.30	116.03	123.22
38	s	616	NEX	C15-C35-C34	-2.30	118.76	123.47
23	Y	313	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
35	n	607	CHL	O2D-CGD-CBD	2.30	115.36	111.27
23	n	610	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
38	R	316	NEX	C4-C3-C2	-2.30	106.33	110.77
23	S	305	CLA	CHB-C4A-NA	2.30	127.69	124.51
35	N	601	CHL	CHD-C1D-ND	-2.30	122.34	124.45
35	n	601	CHL	CHB-C4A-NA	2.30	127.69	124.51
31	d	407	LHG	O8-C23-C24	2.30	119.11	111.91
23	R	313	CLA	CHD-C1D-ND	-2.29	122.34	124.45
35	Y	309	CHL	CHB-C4A-NA	2.29	127.68	124.51
35	R	308	CHL	CHD-C1D-ND	-2.29	122.35	124.45
36	s	615	LUT	C35-C15-C14	-2.29	118.78	123.47
35	G	608	CHL	CHD-C1D-ND	-2.29	122.35	124.45
25	B	619	BCR	C29-C30-C25	2.29	114.01	110.48
36	G	616	LUT	C3-C4-C5	-2.29	107.29	111.85
31	B	627	LHG	O8-C23-C24	2.29	119.10	111.91
36	G	616	LUT	C11-C10-C9	-2.29	124.04	127.31
35	g	601	CHL	CHC-C1C-NC	2.29	127.68	124.20
36	s	614	LUT	C20-C13-C12	2.29	121.69	118.08
35	G	601	CHL	C2A-C1A-CHA	2.29	127.86	123.86
37	Y	301	XAT	C30-C31-C32	-2.29	116.08	123.22
35	y	308	CHL	CHD-C1D-ND	-2.29	122.35	124.45
23	N	603	CLA	C2A-C1A-CHA	2.29	127.86	123.86
36	N	616	LUT	C15-C35-C34	-2.29	118.79	123.47
35	G	606	CHL	CHD-C1D-ND	-2.29	122.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	408	DGD	C2G-O2G-C1B	-2.28	112.17	117.79
35	N	607	CHL	C2A-C1A-CHA	2.28	127.85	123.86
23	S	312	CLA	C2A-C1A-CHA	2.28	127.85	123.86
35	g	601	CHL	C2A-C1A-CHA	2.28	127.85	123.86
23	b	617	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
25	K	101	BCR	C7-C8-C9	-2.28	122.79	126.23
35	n	609	CHL	CHB-C4A-NA	2.28	127.67	124.51
31	D	407	LHG	O8-C23-C24	2.28	119.06	111.91
38	G	618	NEX	C26-C27-C28	-2.28	121.17	125.99
25	a	405	BCR	C1-C6-C5	-2.28	119.40	122.61
36	n	616	LUT	C16-C1-C6	-2.28	106.60	110.30
36	g	616	LUT	C16-C1-C6	-2.28	106.61	110.30
35	n	606	CHL	C2A-C1A-CHA	2.28	127.84	123.86
38	S	317	NEX	C28-C29-C30	2.28	122.43	118.94
35	g	608	CHL	CHD-C1D-ND	-2.28	122.36	124.45
23	B	616	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
38	s	616	NEX	C11-C12-C13	-2.27	120.03	126.42
25	K	101	BCR	C27-C26-C25	-2.27	119.43	122.73
32	C	520	DMU	C1-C2-C3	2.27	114.87	109.68
23	Y	304	CLA	C2A-C1A-CHA	2.27	127.83	123.86
25	A	405	BCR	C1-C6-C5	-2.27	119.41	122.61
35	R	307	CHL	CHB-C4A-NA	2.27	127.65	124.51
35	s	605	CHL	CHB-C4A-NA	2.27	127.65	124.51
25	C	519	BCR	C21-C20-C19	-2.27	116.14	123.22
36	n	616	LUT	C36-C21-C26	2.27	112.98	109.55
25	d	405	BCR	C15-C16-C17	-2.27	118.83	123.47
23	g	614	CLA	CAA-C2A-C3A	-2.27	108.60	114.26
36	r	613	LUT	C1-C6-C5	-2.27	119.42	122.61
25	C	519	BCR	C31-C1-C6	-2.27	106.62	110.30
34	f	101	HEM	C4C-CHD-C1D	2.26	125.55	122.56
25	b	619	BCR	C24-C23-C22	-2.26	122.82	126.23
23	N	610	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
25	B	617	BCR	C24-C23-C22	-2.26	122.82	126.23
36	r	613	LUT	C35-C15-C14	-2.26	118.84	123.47
35	y	307	CHL	CHB-C4A-NA	2.26	127.64	124.51
36	y	316	LUT	C20-C13-C12	2.26	121.64	118.08
37	G	620	XAT	C7-C8-C9	-2.26	122.03	125.53
23	g	603	CLA	C2A-C1A-CHA	2.26	127.81	123.86
35	N	606	CHL	CHB-C4A-NA	2.26	127.63	124.51
36	S	315	LUT	C11-C10-C9	-2.26	124.09	127.31
35	r	605	CHL	CHB-C4A-NA	2.25	127.62	124.51
34	F	101	HEM	CAB-C3B-C2B	-2.25	121.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	312	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
27	a	408	BCT	O3-C-O1	-2.25	113.71	119.55
23	g	602	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
36	S	315	LUT	C20-C13-C12	2.25	121.62	118.08
35	G	607	CHL	CHB-C4A-NA	2.25	127.62	124.51
25	b	621	BCR	C29-C30-C25	2.25	113.94	110.48
25	d	405	BCR	C33-C5-C6	-2.24	122.01	124.53
35	N	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
35	y	302	CHL	CHD-C1D-ND	-2.24	122.39	124.45
23	y	313	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	L	101	LHG	O8-C23-O10	-2.24	117.93	123.59
34	f	101	HEM	CAB-C3B-C2B	-2.24	121.21	128.60
32	c	519	DMU	C1-C2-C3	2.24	114.80	109.68
35	n	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
31	y	318	LHG	O8-C23-C24	2.24	118.94	111.91
26	L	103	SQD	O8-S-C6	2.24	109.31	105.74
25	k	101	BCR	C23-C24-C25	-2.24	120.92	127.20
23	r	602	CLA	O2D-CGD-CBD	2.24	115.24	111.27
26	a	406	SQD	O8-S-C6	2.24	109.31	105.74
25	c	514	BCR	C1-C6-C5	-2.24	119.46	122.61
36	n	615	LUT	C20-C13-C12	2.24	121.60	118.08
30	a	407	LMG	C8-O7-C10	-2.24	112.29	117.79
23	Y	313	CLA	CHA-C1A-NA	-2.23	121.28	126.40
25	c	518	BCR	C10-C11-C12	-2.23	116.25	123.22
23	G	603	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
26	A	406	SQD	O8-S-C6	2.23	109.30	105.74
25	C	516	BCR	C1-C6-C5	-2.23	119.47	122.61
27	A	407	BCT	O3-C-O1	-2.23	113.77	119.55
23	d	403	CLA	O2D-CGD-CBD	2.23	115.22	111.27
23	B	615	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	y	313	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
36	G	615	LUT	C30-C31-C32	-2.22	116.28	123.22
25	b	620	BCR	C1-C6-C5	-2.22	119.48	122.61
36	S	316	LUT	C15-C35-C34	-2.22	118.92	123.47
35	G	601	CHL	C2D-C1D-ND	-2.22	108.47	110.10
23	B	605	CLA	CHD-C1D-ND	-2.22	122.41	124.45
36	G	616	LUT	C16-C1-C6	-2.22	106.70	110.30
23	D	401	CLA	O2D-CGD-CBD	2.22	115.21	111.27
38	s	616	NEX	C31-C30-C29	-2.22	124.14	127.31
23	s	613	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	D	405	BCR	C33-C5-C6	-2.22	122.04	124.53
23	R	305	CLA	O2D-CGD-CBD	2.21	115.20	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	n	615	LUT	C10-C11-C12	-2.21	116.31	123.22
23	G	603	CLA	C2A-C1A-CHA	2.21	127.73	123.86
23	B	616	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
23	b	618	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
26	c	520	SQD	O48-C23-C24	2.21	118.85	111.91
35	G	605	CHL	CHB-C4A-NA	2.21	127.57	124.51
23	G	614	CLA	CAA-C2A-C3A	-2.21	108.74	114.26
36	s	614	LUT	C11-C10-C9	-2.21	124.16	127.31
25	D	405	BCR	C15-C16-C17	-2.21	118.95	123.47
38	S	317	NEX	C4-C3-C2	-2.21	106.51	110.77
36	n	615	LUT	C39-C29-C28	2.21	121.55	118.08
31	Y	319	LHG	O8-C23-C24	2.20	118.83	111.91
36	N	616	LUT	C16-C1-C6	-2.20	106.72	110.30
25	C	515	BCR	C33-C5-C6	-2.20	122.05	124.53
38	s	616	NEX	C16-C1-C6	2.20	112.44	110.47
36	n	616	LUT	C3-C4-C5	-2.20	107.47	111.85
35	Y	302	CHL	CHD-C1D-ND	-2.20	122.43	124.45
31	N	618	LHG	O8-C23-C24	2.20	118.81	111.91
25	B	618	BCR	C1-C6-C5	-2.20	119.52	122.61
23	G	612	CLA	C2A-C1A-CHA	2.20	127.70	123.86
23	d	401	CLA	O2D-CGD-CBD	2.20	115.17	111.27
35	Y	308	CHL	CAA-C2A-C1A	-2.20	104.78	111.97
25	B	617	BCR	C33-C5-C4	2.19	117.83	113.62
26	a	406	SQD	O9-S-C6	2.19	109.55	106.94
35	Y	308	CHL	CHD-C1D-ND	-2.19	122.44	124.45
36	r	613	LUT	C18-C5-C4	2.19	118.42	114.36
35	y	308	CHL	CAA-CBA-CGA	-2.19	106.85	113.25
36	Y	317	LUT	C35-C15-C14	-2.19	118.99	123.47
36	N	615	LUT	C7-C8-C9	-2.19	122.93	126.23
36	S	315	LUT	C19-C9-C8	2.19	121.53	118.08
23	B	614	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
35	Y	309	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
35	Y	306	CHL	O2A-CGA-O1A	-2.19	118.07	123.59
35	r	607	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
31	l	102	LHG	O8-C23-O10	-2.19	118.08	123.59
26	C	521	SQD	O48-C23-C24	2.19	118.77	111.91
35	n	607	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
23	N	613	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	l	101	SQD	O8-S-C6	2.18	109.22	105.74
25	C	515	BCR	C1-C6-C5	-2.18	119.54	122.61
36	N	615	LUT	C39-C29-C28	2.18	121.51	118.08
36	s	615	LUT	C11-C10-C9	-2.18	124.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	307	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
31	n	618	LHG	O8-C23-C24	2.18	118.75	111.91
38	r	615	NEX	C4-C3-C2	-2.18	106.56	110.77
38	s	616	NEX	C30-C31-C32	-2.18	116.42	123.22
36	N	615	LUT	C10-C11-C12	-2.18	116.42	123.22
23	r	604	CLA	O2D-CGD-CBD	2.18	115.13	111.27
25	b	619	BCR	C15-C16-C17	-2.17	119.02	123.47
26	A	406	SQD	O9-S-C6	2.17	109.52	106.94
36	g	615	LUT	C10-C11-C12	-2.17	116.43	123.22
36	n	615	LUT	C15-C14-C13	-2.17	124.21	127.31
23	C	511	CLA	O2D-CGD-CBD	2.17	115.13	111.27
38	G	618	NEX	C17-C1-C6	-2.17	108.53	110.47
23	b	618	CLA	C2A-C1A-CHA	2.17	127.66	123.86
23	c	502	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
35	N	607	CHL	CAA-C2A-C3A	-2.17	106.83	112.78
35	y	308	CHL	CAA-C2A-C1A	-2.17	104.86	111.97
25	b	619	BCR	C33-C5-C4	2.17	117.79	113.62
38	N	617	NEX	C31-C30-C29	-2.17	124.21	127.31
23	s	608	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
35	G	609	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
23	s	611	CLA	CHA-C1A-NA	-2.17	121.43	126.40
36	s	614	LUT	C7-C8-C9	-2.17	122.96	126.23
23	A	402	CLA	CAA-C2A-C1A	2.17	119.08	111.97
36	G	616	LUT	C20-C13-C12	2.17	121.49	118.08
38	n	617	NEX	C30-C31-C32	-2.17	116.45	123.22
23	r	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
35	G	607	CHL	CAA-C2A-C3A	-2.17	108.84	114.26
35	R	308	CHL	O2D-CGD-CBD	2.17	115.12	111.27
36	y	317	LUT	C35-C15-C14	-2.16	119.04	123.47
23	g	613	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	z	101	BCR	C30-C25-C26	-2.16	119.57	122.61
23	C	503	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
37	G	617	XAT	C27-C28-C29	-2.16	122.18	125.53
23	b	607	CLA	CHD-C1D-ND	-2.16	122.47	124.45
35	y	306	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	513	CLA	CBA-CAA-C2A	2.16	120.23	113.86
23	C	512	CLA	C2A-C1A-CHA	2.15	127.63	123.86
35	s	607	CHL	CHB-C4A-NA	2.15	127.49	124.51
35	y	310	CHL	CHB-C4A-NA	2.15	127.49	124.51
25	b	620	BCR	C8-C7-C6	-2.15	121.15	127.20
23	B	614	CLA	C2A-C1A-CHA	2.15	127.62	123.86
23	b	616	CLA	C2A-C1A-CHA	2.15	127.62	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	C2A-C1A-CHA	2.15	127.62	123.86
35	y	306	CHL	C2A-C1A-CHA	2.15	127.62	123.86
25	B	618	BCR	C8-C7-C6	-2.15	121.16	127.20
24	a	402	PHO	CMB-C2B-C3B	2.15	128.70	124.68
38	N	617	NEX	C2-C1-C6	2.15	111.30	109.21
23	g	603	CLA	CHA-C1A-NA	-2.15	121.47	126.40
26	L	103	SQD	O9-S-C6	2.15	109.50	106.94
36	G	616	LUT	C30-C31-C32	-2.15	116.51	123.22
38	R	316	NEX	C2-C1-C6	2.15	111.30	109.21
36	N	616	LUT	C20-C13-C12	2.15	121.46	118.08
36	g	615	LUT	C30-C31-C32	-2.15	116.51	123.22
38	g	618	NEX	C17-C1-C6	-2.15	108.55	110.47
23	b	616	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
35	g	606	CHL	CHB-C4A-NA	2.15	127.48	124.51
36	y	317	LUT	C1-C2-C3	2.15	118.49	113.64
28	C	517	DGD	C2G-O2G-C1B	-2.14	112.51	117.79
37	y	301	XAT	C30-C31-C32	-2.14	116.53	123.22
23	b	606	CLA	C2A-C1A-CHA	2.14	127.61	123.86
25	B	617	BCR	C15-C16-C17	-2.14	119.09	123.47
23	n	613	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	y	304	CLA	CHA-C1A-NA	-2.14	121.49	126.40
23	b	611	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	B	615	CLA	C2A-C1A-CHA	2.14	127.60	123.86
25	z	101	BCR	C1-C6-C5	-2.14	119.60	122.61
23	c	510	CLA	O2D-CGD-CBD	2.14	115.07	111.27
37	R	315	XAT	C15-C35-C34	-2.14	119.09	123.47
37	g	620	XAT	C7-C8-C9	-2.14	122.21	125.53
35	Y	310	CHL	CHB-C4A-NA	2.14	127.47	124.51
33	D	406	PL9	C53-C6-C1	2.14	119.36	114.99
31	r	616	LHG	C5-O7-C7	-2.14	112.53	117.79
35	g	607	CHL	C2A-C1A-CHA	2.14	127.59	123.86
23	C	512	CLA	CHD-C1D-ND	-2.14	122.49	124.45
36	Y	317	LUT	C16-C1-C6	-2.14	106.83	110.30
38	s	616	NEX	C26-C27-C28	-2.13	121.48	125.99
36	r	613	LUT	C30-C31-C32	-2.13	116.56	123.22
37	Y	301	XAT	C27-C28-C29	-2.13	122.22	125.53
35	Y	306	CHL	C2A-C1A-CHA	2.13	127.59	123.86
23	B	604	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
31	n	618	LHG	O7-C7-O9	-2.13	118.55	123.70
36	Y	316	LUT	C39-C29-C28	2.13	121.44	118.08
35	S	306	CHL	C2D-C1D-ND	-2.13	108.53	110.10
30	B	620	LMG	C8-O7-C10	-2.13	112.54	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	622	LHG	O8-C23-C24	2.13	118.59	111.91
25	C	516	BCR	C37-C22-C23	2.13	121.43	118.08
38	s	616	NEX	C28-C29-C30	2.13	122.21	118.94
36	R	314	LUT	C10-C11-C12	-2.13	116.57	123.22
23	D	403	CLA	O2D-CGD-CBD	2.13	115.05	111.27
25	C	519	BCR	C1-C6-C5	-2.13	119.62	122.61
24	A	403	PHO	CMB-C2B-C3B	2.13	128.66	124.68
35	s	606	CHL	C2A-C1A-CHA	2.13	127.58	123.86
36	G	615	LUT	C20-C13-C12	2.12	121.42	118.08
36	y	316	LUT	C39-C29-C28	2.12	121.42	118.08
25	c	514	BCR	C20-C21-C22	-2.12	124.28	127.31
35	y	310	CHL	CHA-C1A-NA	-2.12	121.54	126.40
36	n	616	LUT	C11-C10-C9	-2.12	124.28	127.31
25	b	619	BCR	C4-C5-C6	-2.12	119.65	122.73
23	s	611	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
23	B	616	CLA	C2A-C1A-CHA	2.12	127.57	123.86
30	S	301	LMG	O1-C1-C2	2.12	111.61	108.30
25	K	101	BCR	C10-C11-C12	-2.12	116.60	123.22
35	y	309	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
23	R	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	G	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
35	S	302	CHL	CHB-C4A-NA	2.12	127.44	124.51
33	d	406	PL9	C53-C6-C1	2.12	119.31	114.99
38	G	618	NEX	O24-C25-C26	-2.11	57.21	58.96
36	n	616	LUT	C35-C15-C14	-2.11	119.14	123.47
36	R	314	LUT	C16-C1-C6	-2.11	106.87	110.30
23	B	604	CLA	C2A-C1A-CHA	2.11	127.55	123.86
35	N	605	CHL	O1D-CGD-CBD	2.11	128.80	124.48
25	B	617	BCR	C4-C5-C6	-2.11	119.67	122.73
23	r	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	b	620	BCR	C4-C5-C6	-2.11	119.67	122.73
31	b	624	LHG	O8-C23-C24	2.11	118.53	111.91
23	s	608	CLA	O2D-CGD-CBD	2.11	115.02	111.27
38	S	317	NEX	O24-C25-C26	-2.11	57.21	58.96
35	y	309	CHL	CHD-C1D-ND	-2.11	122.52	124.45
30	s	619	LMG	O1-C1-C2	2.11	111.59	108.30
23	D	404	CLA	O2D-CGD-CBD	2.11	115.01	111.27
23	r	612	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	B	618	BCR	C4-C5-C6	-2.10	119.67	122.73
23	B	609	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	y	314	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	d	402	CLA	CHD-C1D-ND	-2.10	122.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	317	NEX	C30-C31-C32	-2.10	116.65	123.22
37	G	620	XAT	O24-C25-C26	-2.10	57.22	58.96
23	b	606	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
23	c	502	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	C	522	LMG	C4-C3-C2	2.10	114.49	110.82
31	B	621	LHG	O8-C23-O10	-2.10	118.29	123.59
25	K	101	BCR	C37-C22-C23	2.10	121.39	118.08
30	b	622	LMG	C8-O7-C10	-2.10	112.62	117.79
23	G	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
35	Y	310	CHL	CHA-C1A-NA	-2.10	121.59	126.40
23	G	614	CLA	CHD-C1D-ND	-2.10	122.53	124.45
35	N	606	CHL	C2A-C1A-CHA	2.10	127.53	123.86
23	B	615	CLA	C3A-C2A-C1A	2.10	104.48	101.34
35	Y	309	CHL	CHD-C1D-ND	-2.10	122.53	124.45
26	A	406	SQD	O7-S-C6	2.10	109.43	106.94
23	b	605	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	618	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
23	B	603	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	G	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
35	n	609	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
36	g	616	LUT	C30-C31-C32	-2.09	116.69	123.22
23	C	510	CLA	C2A-C1A-CHA	2.09	127.51	123.86
35	R	308	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
31	b	623	LHG	O8-C23-O10	-2.09	118.32	123.59
38	g	618	NEX	C2-C1-C6	2.09	111.24	109.21
38	N	617	NEX	C19-C9-C10	-2.09	120.00	122.92
25	C	515	BCR	C30-C25-C26	-2.08	119.68	122.61
23	d	404	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	n	611	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
35	r	607	CHL	O2D-CGD-CBD	2.08	114.97	111.27
35	g	601	CHL	CHB-C4A-NA	2.08	127.39	124.51
38	n	617	NEX	O24-C25-C26	-2.08	57.24	58.96
38	Y	318	NEX	O24-C25-C26	-2.08	57.24	58.96
23	C	514	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
31	B	622	LHG	C5-O7-C7	-2.08	112.67	117.79
35	G	606	CHL	C2A-C1A-CHA	2.08	127.50	123.86
37	g	620	XAT	O24-C25-C26	-2.08	57.24	58.96
25	c	514	BCR	C37-C22-C23	2.08	121.35	118.08
35	Y	309	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
23	B	606	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
38	R	316	NEX	C17-C1-C6	-2.07	108.62	110.47
26	a	406	SQD	O7-S-C6	2.07	109.40	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	y	316	LUT	C11-C10-C9	-2.07	124.35	127.31
36	N	616	LUT	C35-C15-C14	-2.07	119.23	123.47
25	k	101	BCR	C27-C26-C25	-2.07	119.72	122.73
36	n	616	LUT	C19-C9-C8	2.07	121.34	118.08
38	N	617	NEX	O24-C25-C26	-2.07	57.25	58.96
32	S	319	DMU	C1-C2-C3	2.07	114.41	109.68
36	Y	317	LUT	C31-C30-C29	-2.07	124.36	127.31
35	N	601	CHL	CHB-C4A-NA	2.07	127.37	124.51
38	s	616	NEX	O24-C25-C26	-2.07	57.25	58.96
23	C	503	CLA	C2A-C1A-CHA	2.07	127.47	123.86
23	d	402	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
36	R	314	LUT	C30-C31-C32	-2.07	116.77	123.22
23	N	602	CLA	CHD-C1D-ND	-2.07	122.56	124.45
37	r	614	XAT	O24-C25-C26	-2.07	57.25	58.96
35	N	607	CHL	OMC-CMC-C2C	-2.06	121.02	125.69
31	G	619	LHG	C5-O7-C7	-2.06	112.71	117.79
37	R	315	XAT	C8-C9-C10	-2.06	115.78	118.94
25	B	619	BCR	C16-C15-C14	-2.06	119.25	123.47
38	g	618	NEX	C20-C13-C14	-2.06	120.03	122.92
25	h	101	BCR	C34-C9-C8	2.06	121.33	118.08
25	A	405	BCR	C16-C15-C14	-2.06	119.25	123.47
23	s	611	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
23	S	305	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	S	310	CLA	O2D-CGD-CBD	2.06	114.92	111.27
36	G	615	LUT	C31-C30-C29	-2.06	124.37	127.31
23	g	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	D	405	BCR	C10-C11-C12	-2.06	116.80	123.22
35	R	306	CHL	O2A-CGA-O1A	-2.06	118.17	123.30
23	g	603	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	g	603	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
35	s	607	CHL	C4A-NA-C1A	2.06	107.63	106.71
23	c	511	CLA	C2A-C1A-CHA	2.05	127.45	123.86
23	c	509	CLA	C2A-C1A-CHA	2.05	127.45	123.86
36	S	316	LUT	C18-C5-C6	-2.05	122.22	124.53
35	g	605	CHL	O2A-CGA-O1A	-2.05	118.18	123.30
23	n	603	CLA	C2A-C1A-CHA	2.05	127.45	123.86
35	N	609	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
23	c	513	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
38	R	301	NEX	O24-C25-C26	-2.05	57.26	58.96
36	y	317	LUT	C16-C1-C6	-2.05	106.97	110.30
23	Y	314	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	d	404	CLA	O2D-CGD-CBD	2.05	114.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	s	609	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
36	n	616	LUT	C31-C30-C29	-2.05	124.39	127.31
23	b	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	r	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	y	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
36	g	615	LUT	C39-C29-C28	2.05	121.30	118.08
35	y	308	CHL	C2A-C1A-CHA	2.05	127.44	123.86
23	r	604	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
36	S	316	LUT	C11-C10-C9	2.05	130.23	127.31
23	B	601	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	a	404	CLA	O2D-CGD-CBD	2.05	114.90	111.27
35	G	606	CHL	O2D-CGD-CBD	2.04	114.90	111.27
25	C	519	BCR	C38-C26-C27	2.04	117.54	113.62
35	y	302	CHL	O2D-CGD-CBD	2.04	114.90	111.27
37	R	315	XAT	O24-C25-C26	-2.04	57.27	58.96
38	n	617	NEX	C15-C35-C34	-2.04	119.29	123.47
25	d	405	BCR	C10-C11-C12	-2.04	116.84	123.22
23	N	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	Y	308	CHL	C2A-C1A-CHA	2.04	127.43	123.86
23	c	501	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	y	310	CHL	CBA-CAA-C2A	2.04	119.88	113.86
23	B	601	CLA	CBA-CAA-C2A	2.04	119.88	113.86
23	s	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	n	611	CLA	C2A-C1A-CHA	2.04	127.42	123.86
25	h	101	BCR	C20-C19-C18	-2.04	120.69	126.42
36	N	616	LUT	C3-C4-C5	-2.04	107.80	111.85
35	G	605	CHL	O2A-CGA-O1A	-2.04	118.22	123.30
38	G	618	NEX	C2-C1-C6	2.04	111.19	109.21
35	G	609	CHL	C1D-CHD-C4C	-2.04	121.67	126.06
35	Y	302	CHL	O2D-CGD-CBD	2.03	114.88	111.27
37	G	620	XAT	O4-C5-C6	-2.03	57.28	58.96
36	s	615	LUT	C30-C31-C32	-2.03	116.87	123.22
23	b	608	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
35	N	605	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
38	r	615	NEX	O24-C25-C26	-2.03	57.28	58.96
30	C	501	LMG	C7-O1-C1	-2.03	109.77	113.74
31	g	619	LHG	C5-O7-C7	-2.03	112.79	117.79
38	S	317	NEX	C15-C35-C34	-2.03	119.31	123.47
35	S	308	CHL	CHB-C4A-NA	2.03	127.32	124.51
23	r	601	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
31	l	103	LHG	O8-C23-O10	-2.03	118.47	123.59
23	B	612	CLA	C2A-C1A-CHA	2.03	127.41	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	s	614	LUT	C19-C9-C8	2.03	121.28	118.08
36	Y	317	LUT	C1-C2-C3	2.03	118.23	113.64
30	c	521	LMG	C4-C3-C2	2.03	114.36	110.82
23	C	509	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	b	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
23	N	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
38	n	617	NEX	C19-C9-C10	-2.03	120.08	122.92
23	G	603	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	c	515	DGD	C2G-O2G-C1B	-2.03	112.80	117.79
28	b	625	DGD	O1G-C1A-C2A	2.03	118.27	111.91
23	C	502	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	b	619	BCR	C21-C20-C19	-2.03	116.89	123.22
25	B	617	BCR	C21-C20-C19	-2.03	116.90	123.22
23	G	612	CLA	CHA-C1A-NA	-2.02	121.76	126.40
24	A	403	PHO	CMC-C2C-C3C	2.02	128.76	124.94
37	R	315	XAT	O4-C5-C6	-2.02	57.28	58.96
23	N	611	CLA	C2A-C1A-CHA	2.02	127.40	123.86
28	B	626	DGD	O1G-C1A-C2A	2.02	118.25	111.91
36	n	615	LUT	C1-C2-C3	2.02	118.21	113.64
23	n	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	C	507	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
36	Y	316	LUT	C20-C13-C12	2.02	121.26	118.08
23	n	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
35	N	606	CHL	CAA-C2A-C3A	-2.02	107.25	112.78
23	y	313	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
37	g	620	XAT	O4-C5-C6	-2.02	57.29	58.96
23	b	607	CLA	C11-C12-C13	-2.02	109.39	115.92
25	C	516	BCR	C20-C21-C22	-2.02	124.43	127.31
35	R	308	CHL	CAA-C2A-C3A	-2.02	107.25	112.78
23	S	314	CLA	CHD-C1D-ND	-2.02	122.60	124.45
38	s	616	NEX	C4-C3-C2	-2.02	106.88	110.77
37	g	620	XAT	C27-C28-C29	-2.02	122.40	125.53
23	c	506	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
36	y	317	LUT	C31-C30-C29	-2.02	124.43	127.31
23	R	313	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	n	605	CHL	O2A-CGA-O1A	-2.02	118.50	123.59
23	G	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
24	a	402	PHO	CMC-C2C-C3C	2.01	128.74	124.94
23	B	602	CLA	C2A-C1A-CHA	2.01	127.38	123.86
23	A	404	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	b	618	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C36-C18-C19	2.01	121.25	118.08
23	c	503	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
37	Y	301	XAT	C4-C3-C2	-2.01	106.89	110.77
31	N	618	LHG	O7-C7-O9	-2.01	118.84	123.70
35	r	605	CHL	O2A-CGA-O1A	-2.01	118.29	123.30
23	R	305	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
35	N	606	CHL	O2A-CGA-O1A	-2.01	118.29	123.30
25	a	405	BCR	C16-C15-C14	-2.01	119.36	123.47
23	s	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	R	303	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	B	605	CLA	C11-C12-C13	-2.01	109.43	115.92
23	C	505	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
35	N	601	CHL	C3C-C4C-NC	-2.01	108.32	110.57
35	g	601	CHL	C2D-C1D-ND	-2.01	108.62	110.10
25	A	405	BCR	C21-C20-C19	-2.01	116.95	123.22
23	R	302	CLA	O2D-CGD-CBD	2.01	114.83	111.27
37	r	614	XAT	O4-C5-C6	-2.01	57.30	58.96
36	G	616	LUT	C31-C30-C29	-2.01	124.45	127.31
35	N	608	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
36	s	615	LUT	C19-C9-C8	2.01	121.24	118.08
37	y	301	XAT	C27-C28-C29	-2.00	122.42	125.53
23	b	603	CLA	CBA-CAA-C2A	2.00	119.78	113.86
23	B	616	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	c	508	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
36	S	315	LUT	C7-C8-C9	-2.00	123.21	126.23
23	b	606	CLA	CBC-CAC-C3C	2.00	117.95	112.43
23	d	401	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	R	309	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	r	609	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (304) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	401	CLA	ND
23	A	402	CLA	ND
23	A	404	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	401	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	G	602	CLA	ND
23	G	603	CLA	ND
23	G	604	CLA	ND
23	G	610	CLA	ND
23	G	611	CLA	ND
23	G	612	CLA	ND
23	G	613	CLA	ND
23	G	614	CLA	ND
23	N	602	CLA	ND
23	N	603	CLA	ND
23	N	604	CLA	ND
23	N	610	CLA	ND
23	N	611	CLA	ND
23	N	612	CLA	ND
23	N	613	CLA	ND
23	N	614	CLA	ND

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Mol	Chain	Res	Type	Atom
23	S	303	CLA	ND
23	S	304	CLA	ND
23	S	305	CLA	ND
23	S	309	CLA	ND
23	S	310	CLA	ND
23	S	311	CLA	ND
23	S	312	CLA	ND
23	S	313	CLA	ND
23	S	314	CLA	ND
23	Y	303	CLA	ND
23	Y	304	CLA	ND
23	Y	305	CLA	ND
23	Y	311	CLA	ND
23	Y	312	CLA	ND
23	Y	313	CLA	ND
23	Y	314	CLA	ND
23	Y	315	CLA	ND
23	a	401	CLA	ND
23	a	404	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	b	618	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	401	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND
23	d	404	CLA	ND
23	g	602	CLA	ND
23	g	603	CLA	ND
23	g	604	CLA	ND
23	g	610	CLA	ND
23	g	611	CLA	ND
23	g	612	CLA	ND
23	g	613	CLA	ND
23	g	614	CLA	ND
23	r	601	CLA	ND
23	r	602	CLA	ND
23	r	603	CLA	ND
23	r	604	CLA	ND
23	r	608	CLA	ND
23	r	609	CLA	ND
23	r	610	CLA	ND
23	r	611	CLA	ND
23	r	612	CLA	ND
23	s	602	CLA	ND
23	s	603	CLA	ND
23	s	604	CLA	ND
23	s	608	CLA	ND
23	s	609	CLA	ND
23	s	610	CLA	ND
23	s	611	CLA	ND
23	s	612	CLA	ND
23	s	613	CLA	ND
23	n	602	CLA	ND
23	n	603	CLA	ND
23	n	604	CLA	ND
23	n	610	CLA	ND
23	n	611	CLA	ND
23	n	612	CLA	ND

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Mol	Chain	Res	Type	Atom
23	n	613	CLA	ND
23	n	614	CLA	ND
23	y	303	CLA	ND
23	y	304	CLA	ND
23	y	305	CLA	ND
23	y	311	CLA	ND
23	y	312	CLA	ND
23	y	313	CLA	ND
23	y	314	CLA	ND
23	y	315	CLA	ND
23	R	302	CLA	ND
23	R	303	CLA	ND
23	R	304	CLA	ND
23	R	305	CLA	ND
23	R	309	CLA	ND
23	R	310	CLA	ND
23	R	311	CLA	ND
23	R	312	CLA	ND
23	R	313	CLA	ND
35	G	601	CHL	NA
35	G	601	CHL	NC
35	G	601	CHL	ND
35	G	605	CHL	NA
35	G	605	CHL	NC
35	G	605	CHL	ND
35	G	606	CHL	NA
35	G	606	CHL	NC
35	G	606	CHL	ND
35	G	607	CHL	NA
35	G	607	CHL	NC
35	G	607	CHL	ND
35	G	608	CHL	NA
35	G	608	CHL	NC
35	G	608	CHL	ND
35	G	609	CHL	NA
35	G	609	CHL	NC
35	G	609	CHL	ND
35	N	601	CHL	NA
35	N	601	CHL	NC
35	N	601	CHL	ND
35	N	605	CHL	NA
35	N	605	CHL	NC

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Mol	Chain	Res	Type	Atom
35	N	605	CHL	ND
35	N	606	CHL	NA
35	N	606	CHL	NC
35	N	606	CHL	ND
35	N	607	CHL	NA
35	N	607	CHL	NC
35	N	607	CHL	ND
35	N	608	CHL	NA
35	N	608	CHL	NC
35	N	608	CHL	ND
35	N	609	CHL	NA
35	N	609	CHL	NC
35	N	609	CHL	ND
35	S	302	CHL	NA
35	S	302	CHL	NC
35	S	302	CHL	ND
35	S	306	CHL	NA
35	S	306	CHL	NC
35	S	306	CHL	ND
35	S	307	CHL	NA
35	S	307	CHL	NC
35	S	307	CHL	ND
35	S	308	CHL	NA
35	S	308	CHL	NC
35	S	308	CHL	ND
35	Y	302	CHL	NA
35	Y	302	CHL	NC
35	Y	302	CHL	ND
35	Y	306	CHL	NA
35	Y	306	CHL	NC
35	Y	306	CHL	ND
35	Y	307	CHL	NA
35	Y	307	CHL	NC
35	Y	307	CHL	ND
35	Y	308	CHL	NA
35	Y	308	CHL	NC
35	Y	308	CHL	ND
35	Y	309	CHL	NA
35	Y	309	CHL	NC
35	Y	309	CHL	ND
35	Y	310	CHL	NA
35	Y	310	CHL	NC

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Mol	Chain	Res	Type	Atom
35	Y	310	CHL	ND
35	g	601	CHL	NA
35	g	601	CHL	NC
35	g	601	CHL	ND
35	g	605	CHL	NA
35	g	605	CHL	NC
35	g	605	CHL	ND
35	g	606	CHL	NA
35	g	606	CHL	NC
35	g	606	CHL	ND
35	g	607	CHL	NA
35	g	607	CHL	NC
35	g	607	CHL	ND
35	g	608	CHL	NA
35	g	608	CHL	NC
35	g	608	CHL	ND
35	g	609	CHL	NA
35	g	609	CHL	NC
35	g	609	CHL	ND
35	r	605	CHL	NA
35	r	605	CHL	NC
35	r	605	CHL	ND
35	r	606	CHL	NA
35	r	606	CHL	NC
35	r	606	CHL	ND
35	r	607	CHL	NA
35	r	607	CHL	NC
35	r	607	CHL	ND
35	s	601	CHL	NA
35	s	601	CHL	NC
35	s	601	CHL	ND
35	s	605	CHL	NA
35	s	605	CHL	NC
35	s	605	CHL	ND
35	s	606	CHL	NA
35	s	606	CHL	NC
35	s	606	CHL	ND
35	s	607	CHL	NA
35	s	607	CHL	NC
35	s	607	CHL	ND
35	n	601	CHL	NA
35	n	601	CHL	NC

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Mol	Chain	Res	Type	Atom
35	n	601	CHL	ND
35	n	605	CHL	NA
35	n	605	CHL	NC
35	n	605	CHL	ND
35	n	606	CHL	NA
35	n	606	CHL	NC
35	n	606	CHL	ND
35	n	607	CHL	NA
35	n	607	CHL	NC
35	n	607	CHL	ND
35	n	608	CHL	NA
35	n	608	CHL	NC
35	n	608	CHL	ND
35	n	609	CHL	NA
35	n	609	CHL	NC
35	n	609	CHL	ND
35	y	302	CHL	NA
35	y	302	CHL	NC
35	y	302	CHL	ND
35	y	306	CHL	NA
35	y	306	CHL	NC
35	y	306	CHL	ND
35	y	307	CHL	NA
35	y	307	CHL	NC
35	y	307	CHL	ND
35	y	308	CHL	NA
35	y	308	CHL	NC
35	y	308	CHL	ND
35	y	309	CHL	NA
35	y	309	CHL	NC
35	y	309	CHL	ND
35	y	310	CHL	NA
35	y	310	CHL	NC
35	y	310	CHL	ND
35	R	306	CHL	NA
35	R	306	CHL	NC
35	R	306	CHL	ND
35	R	307	CHL	NA
35	R	307	CHL	NC
35	R	307	CHL	ND
35	R	308	CHL	NA
35	R	308	CHL	NC

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Mol	Chain	Res	Type	Atom
35	R	308	CHL	ND

All (2827) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	401	CLA	CBD-CGD-O2D-CED
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	402	CLA	CHA-CBD-CGD-O1D
23	A	402	CLA	CHA-CBD-CGD-O2D
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	A	404	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C2-C3-C5-C6
23	B	602	CLA	C4-C3-C5-C6
23	B	603	CLA	C3A-C2A-CAA-CBA
23	B	604	CLA	CHA-CBD-CGD-O1D
23	B	604	CLA	CHA-CBD-CGD-O2D
23	B	605	CLA	C11-C10-C8-C9
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	D	401	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	D	401	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	CHA-CBD-CGD-O1D
23	D	404	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O1D
23	G	610	CLA	C1A-C2A-CAA-CBA
23	G	610	CLA	C3A-C2A-CAA-CBA
23	G	613	CLA	CHA-CBD-CGD-O1D
23	G	613	CLA	CHA-CBD-CGD-O2D
23	G	614	CLA	C1A-C2A-CAA-CBA
23	G	614	CLA	C3A-C2A-CAA-CBA
23	N	610	CLA	C3A-C2A-CAA-CBA
23	N	611	CLA	C1A-C2A-CAA-CBA
23	N	613	CLA	C1A-C2A-CAA-CBA
23	N	613	CLA	CHA-CBD-CGD-O1D
23	N	613	CLA	CHA-CBD-CGD-O2D
23	S	303	CLA	C3A-C2A-CAA-CBA
23	S	305	CLA	CHA-CBD-CGD-O1D
23	S	305	CLA	CHA-CBD-CGD-O2D
23	S	309	CLA	CHA-CBD-CGD-O1D
23	S	309	CLA	CHA-CBD-CGD-O2D
23	S	309	CLA	CAD-CBD-CGD-O1D
23	S	310	CLA	C1A-C2A-CAA-CBA
23	S	310	CLA	C3A-C2A-CAA-CBA
23	S	310	CLA	C2A-CAA-CBA-CGA
23	S	311	CLA	CHA-CBD-CGD-O1D
23	S	311	CLA	CHA-CBD-CGD-O2D
23	S	312	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	CHA-CBD-CGD-O1D
23	S	313	CLA	CHA-CBD-CGD-O2D
23	S	314	CLA	CHA-CBD-CGD-O1D
23	S	314	CLA	CHA-CBD-CGD-O2D
23	S	314	CLA	CAD-CBD-CGD-O1D
23	S	314	CLA	CAD-CBD-CGD-O2D
23	Y	303	CLA	C1A-C2A-CAA-CBA
23	Y	303	CLA	C3A-C2A-CAA-CBA
23	Y	311	CLA	CBD-CGD-O2D-CED
23	Y	313	CLA	CBD-CGD-O2D-CED
23	Y	314	CLA	C6-C7-C8-C9
23	a	401	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CHA-CBD-CGD-O1D
23	a	404	CLA	CHA-CBD-CGD-O2D
23	a	404	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C1A-C2A-CAA-CBA
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C1A-C2A-CAA-CBA
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C3A-C2A-CAA-CBA
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	C11-C10-C8-C9
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
23	b	611	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	CHA-CBD-CGD-O1D
23	b	616	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O2D
23	d	401	CLA	CHA-CBD-CGD-O1D
23	d	401	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	C1A-C2A-CAA-CBA
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
23	d	404	CLA	CHA-CBD-CGD-O1D
23	d	404	CLA	CHA-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	g	610	CLA	C3A-C2A-CAA-CBA
23	g	613	CLA	CHA-CBD-CGD-O1D
23	g	613	CLA	CHA-CBD-CGD-O2D
23	g	614	CLA	C1A-C2A-CAA-CBA
23	g	614	CLA	C3A-C2A-CAA-CBA
23	g	614	CLA	CBD-CGD-O2D-CED
23	r	601	CLA	C1A-C2A-CAA-CBA
23	r	601	CLA	C3A-C2A-CAA-CBA
23	r	601	CLA	CHA-CBD-CGD-O1D
23	r	601	CLA	CHA-CBD-CGD-O2D
23	r	602	CLA	C1A-C2A-CAA-CBA
23	r	602	CLA	C3A-C2A-CAA-CBA
23	r	602	CLA	CHA-CBD-CGD-O1D
23	r	602	CLA	CHA-CBD-CGD-O2D
23	r	611	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	CHA-CBD-CGD-O1D
23	r	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	C3A-C2A-CAA-CBA
23	s	604	CLA	CHA-CBD-CGD-O1D
23	s	604	CLA	CHA-CBD-CGD-O2D
23	s	610	CLA	CHA-CBD-CGD-O1D
23	s	610	CLA	CHA-CBD-CGD-O2D
23	s	611	CLA	CBD-CGD-O2D-CED
23	s	612	CLA	CHA-CBD-CGD-O1D
23	s	612	CLA	CHA-CBD-CGD-O2D
23	s	613	CLA	CHA-CBD-CGD-O1D
23	s	613	CLA	CHA-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O1D
23	n	610	CLA	C3A-C2A-CAA-CBA
23	n	611	CLA	C1A-C2A-CAA-CBA
23	n	613	CLA	C1A-C2A-CAA-CBA
23	n	613	CLA	CHA-CBD-CGD-O1D
23	n	613	CLA	CHA-CBD-CGD-O2D
23	y	303	CLA	C1A-C2A-CAA-CBA
23	y	303	CLA	C3A-C2A-CAA-CBA
23	y	311	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	CBD-CGD-O2D-CED
23	R	302	CLA	C1A-C2A-CAA-CBA
23	R	302	CLA	C3A-C2A-CAA-CBA
23	R	302	CLA	CHA-CBD-CGD-O1D
23	R	303	CLA	C1A-C2A-CAA-CBA
23	R	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	R	303	CLA	CHA-CBD-CGD-O1D
23	R	303	CLA	CHA-CBD-CGD-O2D
23	R	312	CLA	CBD-CGD-O2D-CED
23	R	313	CLA	CHA-CBD-CGD-O1D
23	R	313	CLA	CHA-CBD-CGD-O2D
25	B	617	BCR	C21-C22-C23-C24
25	B	617	BCR	C37-C22-C23-C24
25	D	405	BCR	C5-C6-C7-C8
25	D	405	BCR	C7-C8-C9-C34
25	H	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C1-C6-C7-C8
25	b	619	BCR	C21-C22-C23-C24
25	b	619	BCR	C37-C22-C23-C24
25	b	619	BCR	C23-C24-C25-C30
25	d	405	BCR	C5-C6-C7-C8
25	d	405	BCR	C7-C8-C9-C34
25	h	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C7-C8-C9-C10
25	k	101	BCR	C7-C8-C9-C34
26	B	625	SQD	C5-C6-S-O7
26	C	521	SQD	C5-C6-S-O9
26	L	103	SQD	O5-C5-C6-S
26	b	602	SQD	C5-C6-S-O8
26	c	520	SQD	C5-C6-S-O9
26	l	101	SQD	C2-C1-O6-C44
26	l	101	SQD	O5-C5-C6-S
28	A	408	DGD	C2B-C1B-O2G-C2G
28	A	408	DGD	O1B-C1B-O2G-C2G
28	B	626	DGD	O1B-C1B-O2G-C2G
28	b	625	DGD	O1B-C1B-O2G-C2G
30	C	522	LMG	C11-C10-O7-C8
30	c	521	LMG	C11-C10-O7-C8
31	B	621	LHG	C4-O6-P-O4
31	B	627	LHG	C3-O3-P-O5
31	B	627	LHG	C4-O6-P-O3
31	B	627	LHG	C4-O6-P-O4
31	B	627	LHG	C4-O6-P-O5
31	C	518	LHG	C3-O3-P-O5
31	C	518	LHG	C4-O6-P-O5
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C4-O6-P-O4
31	G	619	LHG	O2-C2-C3-O3
31	G	619	LHG	C3-O3-P-O5
31	G	619	LHG	C4-O6-P-O4
31	L	101	LHG	C3-O3-P-O4
31	L	102	LHG	C4-O6-P-O3
31	L	102	LHG	C4-O6-P-O4
31	L	102	LHG	C4-O6-P-O5
31	L	102	LHG	O6-C4-C5-O7
31	N	618	LHG	C4-O6-P-O4
31	S	318	LHG	C3-O3-P-O5
31	S	318	LHG	C4-O6-P-O4
31	S	318	LHG	C4-O6-P-O5
31	Y	319	LHG	C3-O3-P-O4
31	Y	319	LHG	C4-O6-P-O4
31	b	623	LHG	C4-O6-P-O4
31	b	624	LHG	C3-O3-P-O6
31	b	624	LHG	C4-O6-P-O4
31	b	626	LHG	C4-O6-P-O4
31	b	626	LHG	C4-O6-P-O5
31	c	517	LHG	C3-O3-P-O5
31	c	517	LHG	C4-O6-P-O3
31	c	517	LHG	C4-O6-P-O5
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	g	619	LHG	O2-C2-C3-O3
31	g	619	LHG	C3-O3-P-O5
31	g	619	LHG	C4-O6-P-O4
31	l	102	LHG	C3-O3-P-O4
31	l	103	LHG	C3-O3-P-O5
31	l	103	LHG	C4-O6-P-O3
31	l	103	LHG	C4-O6-P-O4
31	l	103	LHG	C4-O6-P-O5
31	l	103	LHG	O6-C4-C5-O7
31	r	616	LHG	C3-O3-P-O6
31	r	616	LHG	C4-O6-P-O3
31	s	617	LHG	C3-O3-P-O5
31	s	617	LHG	C4-O6-P-O4
31	s	617	LHG	C4-O6-P-O5
31	n	618	LHG	C4-O6-P-O4
31	y	318	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
31	y	318	LHG	C4-O6-P-O4
32	C	520	DMU	C1-C6-O16-C18
32	C	520	DMU	O5-C6-O16-C18
32	C	520	DMU	C5-C10-O7-C3
32	c	519	DMU	C5-C10-O7-C3
33	D	406	PL9	C12-C11-C9-C8
33	D	406	PL9	C9-C11-C12-C13
33	D	406	PL9	C12-C13-C14-C16
33	D	406	PL9	C13-C14-C16-C17
33	D	406	PL9	C17-C18-C19-C20
33	D	406	PL9	C17-C18-C19-C21
33	D	406	PL9	C22-C23-C24-C25
33	D	406	PL9	C27-C28-C29-C30
33	D	406	PL9	C32-C33-C34-C35
33	D	406	PL9	C34-C36-C37-C38
33	D	406	PL9	C37-C38-C39-C40
33	D	406	PL9	C37-C38-C39-C41
33	D	406	PL9	C42-C43-C44-C45
33	d	406	PL9	C12-C11-C9-C8
33	d	406	PL9	C9-C11-C12-C13
33	d	406	PL9	C12-C13-C14-C16
33	d	406	PL9	C13-C14-C16-C17
33	d	406	PL9	C17-C18-C19-C20
33	d	406	PL9	C17-C18-C19-C21
33	d	406	PL9	C22-C23-C24-C25
33	d	406	PL9	C27-C28-C29-C30
33	d	406	PL9	C32-C33-C34-C35
33	d	406	PL9	C37-C38-C39-C40
33	d	406	PL9	C37-C38-C39-C41
33	d	406	PL9	C42-C43-C44-C45
35	G	601	CHL	C1C-C2C-CMC-OMC
35	G	601	CHL	C3C-C2C-CMC-OMC
35	G	601	CHL	CHA-CBD-CGD-O1D
35	G	601	CHL	CHA-CBD-CGD-O2D
35	G	605	CHL	C1A-C2A-CAA-CBA
35	G	605	CHL	C3A-C2A-CAA-CBA
35	G	605	CHL	C1C-C2C-CMC-OMC
35	G	605	CHL	C3C-C2C-CMC-OMC
35	G	605	CHL	CHA-CBD-CGD-O1D
35	G	605	CHL	CHA-CBD-CGD-O2D
35	G	606	CHL	C1A-C2A-CAA-CBA
35	G	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
35	G	606	CHL	C3C-C2C-CMC-OMC
35	G	606	CHL	CHA-CBD-CGD-O1D
35	G	606	CHL	CHA-CBD-CGD-O2D
35	G	607	CHL	C1C-C2C-CMC-OMC
35	G	607	CHL	C3C-C2C-CMC-OMC
35	G	607	CHL	CBD-CGD-O2D-CED
35	G	608	CHL	C1A-C2A-CAA-CBA
35	G	608	CHL	C1C-C2C-CMC-OMC
35	G	608	CHL	C3C-C2C-CMC-OMC
35	G	608	CHL	CBD-CGD-O2D-CED
35	G	609	CHL	C1C-C2C-CMC-OMC
35	G	609	CHL	C3C-C2C-CMC-OMC
35	N	601	CHL	C1C-C2C-CMC-OMC
35	N	601	CHL	C3C-C2C-CMC-OMC
35	N	601	CHL	CHA-CBD-CGD-O1D
35	N	601	CHL	CHA-CBD-CGD-O2D
35	N	605	CHL	C1C-C2C-CMC-OMC
35	N	605	CHL	C3C-C2C-CMC-OMC
35	N	605	CHL	CAD-CBD-CGD-O1D
35	N	605	CHL	CAD-CBD-CGD-O2D
35	N	606	CHL	C1A-C2A-CAA-CBA
35	N	606	CHL	C1C-C2C-CMC-OMC
35	N	606	CHL	C3C-C2C-CMC-OMC
35	N	607	CHL	C1A-C2A-CAA-CBA
35	N	607	CHL	C1C-C2C-CMC-OMC
35	N	607	CHL	C3C-C2C-CMC-OMC
35	N	608	CHL	C1C-C2C-CMC-OMC
35	N	608	CHL	C3C-C2C-CMC-OMC
35	N	609	CHL	C1C-C2C-CMC-OMC
35	N	609	CHL	C3C-C2C-CMC-OMC
35	S	302	CHL	C1C-C2C-CMC-OMC
35	S	302	CHL	C3C-C2C-CMC-OMC
35	S	306	CHL	C1C-C2C-CMC-OMC
35	S	306	CHL	C3C-C2C-CMC-OMC
35	S	307	CHL	C1A-C2A-CAA-CBA
35	S	307	CHL	C3A-C2A-CAA-CBA
35	S	307	CHL	C1C-C2C-CMC-OMC
35	S	307	CHL	C3C-C2C-CMC-OMC
35	S	308	CHL	C1C-C2C-CMC-OMC
35	S	308	CHL	C3C-C2C-CMC-OMC
35	S	308	CHL	CHA-CBD-CGD-O1D
35	S	308	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
35	S	308	CHL	CAD-CBD-CGD-O1D
35	S	308	CHL	CBD-CGD-O2D-CED
35	Y	302	CHL	C1C-C2C-CMC-OMC
35	Y	302	CHL	C3C-C2C-CMC-OMC
35	Y	302	CHL	CHA-CBD-CGD-O1D
35	Y	302	CHL	CHA-CBD-CGD-O2D
35	Y	306	CHL	C1A-C2A-CAA-CBA
35	Y	306	CHL	C2A-CAA-CBA-CGA
35	Y	306	CHL	C1C-C2C-CMC-OMC
35	Y	306	CHL	C3C-C2C-CMC-OMC
35	Y	307	CHL	C1A-C2A-CAA-CBA
35	Y	307	CHL	C1C-C2C-CMC-OMC
35	Y	307	CHL	C3C-C2C-CMC-OMC
35	Y	308	CHL	O1A-CGA-O2A-C1
35	Y	308	CHL	C1C-C2C-CMC-OMC
35	Y	308	CHL	C3C-C2C-CMC-OMC
35	Y	309	CHL	C1C-C2C-CMC-OMC
35	Y	309	CHL	C3C-C2C-CMC-OMC
35	Y	310	CHL	C1A-C2A-CAA-CBA
35	Y	310	CHL	C3A-C2A-CAA-CBA
35	Y	310	CHL	C1C-C2C-CMC-OMC
35	Y	310	CHL	C3C-C2C-CMC-OMC
35	g	601	CHL	C1C-C2C-CMC-OMC
35	g	601	CHL	C3C-C2C-CMC-OMC
35	g	601	CHL	CHA-CBD-CGD-O1D
35	g	601	CHL	CHA-CBD-CGD-O2D
35	g	605	CHL	C1A-C2A-CAA-CBA
35	g	605	CHL	C3A-C2A-CAA-CBA
35	g	605	CHL	C1C-C2C-CMC-OMC
35	g	605	CHL	C3C-C2C-CMC-OMC
35	g	605	CHL	CHA-CBD-CGD-O1D
35	g	605	CHL	CHA-CBD-CGD-O2D
35	g	606	CHL	C1A-C2A-CAA-CBA
35	g	606	CHL	C1C-C2C-CMC-OMC
35	g	606	CHL	C3C-C2C-CMC-OMC
35	g	607	CHL	C1C-C2C-CMC-OMC
35	g	607	CHL	C3C-C2C-CMC-OMC
35	g	608	CHL	C1A-C2A-CAA-CBA
35	g	608	CHL	C1C-C2C-CMC-OMC
35	g	608	CHL	C3C-C2C-CMC-OMC
35	g	608	CHL	CBD-CGD-O2D-CED
35	g	609	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
35	g	609	CHL	C3C-C2C-CMC-OMC
35	r	605	CHL	C1C-C2C-CMC-OMC
35	r	606	CHL	C1C-C2C-CMC-OMC
35	r	606	CHL	C3C-C2C-CMC-OMC
35	r	607	CHL	C1C-C2C-CMC-OMC
35	r	607	CHL	C3C-C2C-CMC-OMC
35	s	601	CHL	C1C-C2C-CMC-OMC
35	s	601	CHL	C3C-C2C-CMC-OMC
35	s	605	CHL	C1C-C2C-CMC-OMC
35	s	606	CHL	C1A-C2A-CAA-CBA
35	s	606	CHL	C3A-C2A-CAA-CBA
35	s	606	CHL	C1C-C2C-CMC-OMC
35	s	606	CHL	C3C-C2C-CMC-OMC
35	s	607	CHL	C1A-C2A-CAA-CBA
35	s	607	CHL	C1C-C2C-CMC-OMC
35	s	607	CHL	C3C-C2C-CMC-OMC
35	n	601	CHL	C1C-C2C-CMC-OMC
35	n	601	CHL	C3C-C2C-CMC-OMC
35	n	601	CHL	CHA-CBD-CGD-O1D
35	n	601	CHL	CHA-CBD-CGD-O2D
35	n	605	CHL	C1C-C2C-CMC-OMC
35	n	605	CHL	C3C-C2C-CMC-OMC
35	n	605	CHL	CHA-CBD-CGD-O1D
35	n	605	CHL	CAD-CBD-CGD-O1D
35	n	605	CHL	CAD-CBD-CGD-O2D
35	n	606	CHL	C1A-C2A-CAA-CBA
35	n	606	CHL	C1C-C2C-CMC-OMC
35	n	606	CHL	C3C-C2C-CMC-OMC
35	n	607	CHL	C1A-C2A-CAA-CBA
35	n	607	CHL	C1C-C2C-CMC-OMC
35	n	607	CHL	C3C-C2C-CMC-OMC
35	n	608	CHL	C1C-C2C-CMC-OMC
35	n	608	CHL	C3C-C2C-CMC-OMC
35	n	609	CHL	C1C-C2C-CMC-OMC
35	n	609	CHL	C3C-C2C-CMC-OMC
35	y	302	CHL	C1C-C2C-CMC-OMC
35	y	302	CHL	C3C-C2C-CMC-OMC
35	y	302	CHL	CHA-CBD-CGD-O1D
35	y	302	CHL	CHA-CBD-CGD-O2D
35	y	306	CHL	C1A-C2A-CAA-CBA
35	y	306	CHL	C1C-C2C-CMC-OMC
35	y	306	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
35	y	307	CHL	C1A-C2A-CAA-CBA
35	y	307	CHL	C1C-C2C-CMC-OMC
35	y	307	CHL	C3C-C2C-CMC-OMC
35	y	308	CHL	O1A-CGA-O2A-C1
35	y	308	CHL	C1C-C2C-CMC-OMC
35	y	308	CHL	C3C-C2C-CMC-OMC
35	y	309	CHL	C1C-C2C-CMC-OMC
35	y	309	CHL	C3C-C2C-CMC-OMC
35	y	310	CHL	C1A-C2A-CAA-CBA
35	y	310	CHL	C3A-C2A-CAA-CBA
35	y	310	CHL	C1C-C2C-CMC-OMC
35	y	310	CHL	C3C-C2C-CMC-OMC
35	R	306	CHL	C1C-C2C-CMC-OMC
35	R	307	CHL	C1C-C2C-CMC-OMC
35	R	307	CHL	C3C-C2C-CMC-OMC
35	R	308	CHL	C1C-C2C-CMC-OMC
35	R	308	CHL	C3C-C2C-CMC-OMC
36	N	615	LUT	C1-C6-C7-C8
36	Y	316	LUT	C1-C6-C7-C8
36	r	613	LUT	C7-C8-C9-C10
36	r	613	LUT	C7-C8-C9-C19
36	s	614	LUT	C1-C6-C7-C8
36	n	615	LUT	C1-C6-C7-C8
36	y	316	LUT	C1-C6-C7-C8
36	R	314	LUT	C7-C8-C9-C19
38	S	317	NEX	C11-C12-C13-C20
38	r	615	NEX	C11-C12-C13-C20
38	n	617	NEX	C31-C32-C33-C40
23	A	401	CLA	O1D-CGD-O2D-CED
23	g	603	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1D-CGD-O2D-CED
23	R	312	CLA	O1D-CGD-O2D-CED
23	Y	313	CLA	O1D-CGD-O2D-CED
23	a	401	CLA	O1D-CGD-O2D-CED
23	g	610	CLA	O1D-CGD-O2D-CED
23	y	313	CLA	O1D-CGD-O2D-CED
35	s	607	CHL	O1D-CGD-O2D-CED
23	A	404	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	CBD-CGD-O2D-CED
23	G	614	CLA	CBD-CGD-O2D-CED
23	N	602	CLA	CBD-CGD-O2D-CED
23	N	610	CLA	CBD-CGD-O2D-CED
23	S	303	CLA	CBD-CGD-O2D-CED
23	S	304	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	CBD-CGD-O2D-CED
23	S	314	CLA	CBD-CGD-O2D-CED
23	Y	315	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	g	603	CLA	CBD-CGD-O2D-CED
23	g	610	CLA	CBD-CGD-O2D-CED
23	g	613	CLA	CBD-CGD-O2D-CED
23	s	612	CLA	CBD-CGD-O2D-CED
23	s	613	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	CBD-CGD-O2D-CED
23	n	610	CLA	CBD-CGD-O2D-CED
23	y	315	CLA	CBD-CGD-O2D-CED
35	N	608	CHL	CBD-CGD-O2D-CED
35	S	306	CHL	CBD-CGD-O2D-CED
35	Y	302	CHL	CBD-CGD-O2D-CED
35	Y	308	CHL	CBD-CGD-O2D-CED
35	Y	309	CHL	CBD-CGD-O2D-CED
35	s	607	CHL	CBD-CGD-O2D-CED
35	y	302	CHL	CBD-CGD-O2D-CED
35	y	308	CHL	CBD-CGD-O2D-CED
35	y	309	CHL	CBD-CGD-O2D-CED
23	Y	312	CLA	O1A-CGA-O2A-C1
23	g	611	CLA	O1A-CGA-O2A-C1
23	R	309	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	O1D-CGD-O2D-CED
23	G	610	CLA	O1D-CGD-O2D-CED
23	N	610	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	O1D-CGD-O2D-CED
35	S	306	CHL	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	S	312	CLA	O1D-CGD-O2D-CED
23	Y	311	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	s	611	CLA	O1D-CGD-O2D-CED
35	G	607	CHL	O1D-CGD-O2D-CED
35	g	608	CHL	O1D-CGD-O2D-CED
32	C	520	DMU	O6-C11-C9-C8
33	D	406	PL9	C47-C48-C49-C50
33	D	406	PL9	C47-C48-C49-C51
33	d	406	PL9	C47-C48-C49-C50
33	d	406	PL9	C47-C48-C49-C51
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	D	404	CLA	CBD-CGD-O2D-CED
23	G	603	CLA	CBD-CGD-O2D-CED
23	G	613	CLA	CBD-CGD-O2D-CED
23	N	604	CLA	CBD-CGD-O2D-CED
23	N	612	CLA	CBD-CGD-O2D-CED
23	N	614	CLA	CBD-CGD-O2D-CED
23	Y	305	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	d	404	CLA	CBD-CGD-O2D-CED
23	r	608	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	CBD-CGD-O2D-CED
23	s	602	CLA	CBD-CGD-O2D-CED
23	s	603	CLA	CBD-CGD-O2D-CED
23	s	609	CLA	CBD-CGD-O2D-CED
23	n	614	CLA	CBD-CGD-O2D-CED
23	y	305	CLA	CBD-CGD-O2D-CED
23	R	302	CLA	CBD-CGD-O2D-CED
23	R	311	CLA	CBD-CGD-O2D-CED
35	N	605	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	Y	306	CHL	CBD-CGD-O2D-CED
35	n	608	CHL	CBD-CGD-O2D-CED
35	y	306	CHL	CBD-CGD-O2D-CED
23	B	607	CLA	O1A-CGA-O2A-C1
23	B	613	CLA	O1A-CGA-O2A-C1
23	G	604	CLA	O1A-CGA-O2A-C1
23	G	611	CLA	O1A-CGA-O2A-C1
23	N	603	CLA	O1A-CGA-O2A-C1
23	N	611	CLA	O1A-CGA-O2A-C1
23	Y	313	CLA	O1A-CGA-O2A-C1
23	b	609	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
23	g	602	CLA	O1A-CGA-O2A-C1
23	g	604	CLA	O1A-CGA-O2A-C1
23	r	608	CLA	O1A-CGA-O2A-C1
23	n	603	CLA	O1A-CGA-O2A-C1
23	n	611	CLA	O1A-CGA-O2A-C1
23	y	312	CLA	O1A-CGA-O2A-C1
24	A	403	PHO	O1A-CGA-O2A-C1
24	a	402	PHO	O1A-CGA-O2A-C1
35	S	308	CHL	O1A-CGA-O2A-C1
35	Y	307	CHL	O1A-CGA-O2A-C1
35	r	607	CHL	O1A-CGA-O2A-C1
35	y	307	CHL	O1A-CGA-O2A-C1
35	R	308	CHL	O1A-CGA-O2A-C1
23	C	507	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	g	614	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	O1D-CGD-O2D-CED
35	G	608	CHL	O1D-CGD-O2D-CED
35	S	308	CHL	O1D-CGD-O2D-CED
23	S	310	CLA	CBD-CGD-O2D-CED
23	b	618	CLA	CBD-CGD-O2D-CED
23	r	601	CLA	CBD-CGD-O2D-CED
23	S	303	CLA	O1D-CGD-O2D-CED
30	C	522	LMG	O9-C10-O7-C8
30	c	521	LMG	O9-C10-O7-C8
23	G	610	CLA	O1A-CGA-O2A-C1
23	n	610	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C3-C5-C6-C7
23	C	512	CLA	C3-C5-C6-C7
23	D	401	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
23	b	618	CLA	C3-C5-C6-C7
23	c	507	CLA	C3-C5-C6-C7
23	c	511	CLA	C3-C5-C6-C7
23	d	401	CLA	C3-C5-C6-C7
23	g	602	CLA	C3-C5-C6-C7
23	r	609	CLA	C3-C5-C6-C7
23	R	310	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
24	a	403	PHO	C3-C5-C6-C7
35	G	609	CHL	C3-C5-C6-C7
35	Y	308	CHL	C3-C5-C6-C7
35	g	609	CHL	C3-C5-C6-C7
35	r	607	CHL	C3-C5-C6-C7
35	n	609	CHL	C3-C5-C6-C7
35	y	308	CHL	C3-C5-C6-C7
23	B	607	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	CBA-CGA-O2A-C1
23	C	503	CLA	CBA-CGA-O2A-C1
23	G	604	CLA	CBA-CGA-O2A-C1
23	N	603	CLA	CBA-CGA-O2A-C1
23	Y	312	CLA	CBA-CGA-O2A-C1
23	b	609	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
23	g	602	CLA	CBA-CGA-O2A-C1
23	g	604	CLA	CBA-CGA-O2A-C1
23	g	611	CLA	CBA-CGA-O2A-C1
23	n	613	CLA	CBA-CGA-O2A-C1
23	y	312	CLA	CBA-CGA-O2A-C1
23	y	313	CLA	CBA-CGA-O2A-C1
23	R	309	CLA	CBA-CGA-O2A-C1
24	A	403	PHO	CBA-CGA-O2A-C1
24	a	402	PHO	CBA-CGA-O2A-C1
35	Y	307	CHL	CBA-CGA-O2A-C1
35	r	607	CHL	CBA-CGA-O2A-C1
35	y	307	CHL	CBA-CGA-O2A-C1
35	y	308	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	R	308	CHL	CBA-CGA-O2A-C1
28	B	626	DGD	C2B-C1B-O2G-C2G
28	b	625	DGD	C2B-C1B-O2G-C2G
23	A	404	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	r	603	CLA	C4-C3-C5-C6
23	R	304	CLA	C4-C3-C5-C6
33	D	406	PL9	C25-C24-C26-C27
33	d	406	PL9	C25-C24-C26-C27
35	n	601	CHL	C4-C3-C5-C6
32	c	519	DMU	O6-C11-C9-C8
23	r	603	CLA	C2-C3-C5-C6
35	n	601	CHL	C2-C3-C5-C6
23	n	604	CLA	CBD-CGD-O2D-CED
35	G	605	CHL	CBD-CGD-O2D-CED
35	g	605	CHL	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	608	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C2A-CAA-CBA-CGA
23	g	602	CLA	C2A-CAA-CBA-CGA
23	g	604	CLA	C2A-CAA-CBA-CGA
23	r	602	CLA	C2A-CAA-CBA-CGA
35	S	308	CHL	C2A-CAA-CBA-CGA
35	Y	307	CHL	C2A-CAA-CBA-CGA
35	y	307	CHL	C2A-CAA-CBA-CGA
23	g	613	CLA	O1D-CGD-O2D-CED
35	y	308	CHL	O1D-CGD-O2D-CED
23	B	604	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
23	c	502	CLA	C3-C5-C6-C7
35	N	609	CHL	C3-C5-C6-C7
35	Y	310	CHL	C3-C5-C6-C7
35	y	310	CHL	C3-C5-C6-C7
35	R	308	CHL	C3-C5-C6-C7
23	G	610	CLA	CBA-CGA-O2A-C1
23	G	611	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	S	305	CLA	CBA-CGA-O2A-C1
23	Y	313	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
23	r	608	CLA	CBA-CGA-O2A-C1
23	n	603	CLA	CBA-CGA-O2A-C1
23	n	611	CLA	CBA-CGA-O2A-C1
35	S	308	CHL	CBA-CGA-O2A-C1
35	Y	308	CHL	CBA-CGA-O2A-C1
35	s	607	CHL	CBA-CGA-O2A-C1
32	C	520	DMU	O6-C11-C9-O1
23	B	614	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
23	Y	315	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
33	D	406	PL9	C7-C8-C9-C10
33	d	406	PL9	C7-C8-C9-C10
23	b	605	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
23	C	510	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
23	s	613	CLA	O1D-CGD-O2D-CED
35	N	608	CHL	O1D-CGD-O2D-CED
35	Y	308	CHL	O1D-CGD-O2D-CED
32	C	523	DMU	O6-C11-C9-C8
32	c	522	DMU	O6-C11-C9-C8
23	C	503	CLA	O1A-CGA-O2A-C1
23	C	505	CLA	O1A-CGA-O2A-C1
23	G	602	CLA	O1A-CGA-O2A-C1
23	S	305	CLA	O1A-CGA-O2A-C1
23	Y	303	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
23	n	613	CLA	O1A-CGA-O2A-C1
23	y	313	CLA	O1A-CGA-O2A-C1
35	s	607	CHL	O1A-CGA-O2A-C1
23	G	614	CLA	O1D-CGD-O2D-CED
23	s	612	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	G	602	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	s	610	CLA	CBD-CGD-O2D-CED
23	n	612	CLA	CBD-CGD-O2D-CED
35	S	302	CHL	CBD-CGD-O2D-CED
35	n	605	CHL	CBD-CGD-O2D-CED
23	B	605	CLA	O1D-CGD-O2D-CED
23	N	602	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C3-C5-C6-C7
23	C	508	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
23	C	505	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
35	G	608	CHL	CBA-CGA-O2A-C1
35	g	608	CHL	CBA-CGA-O2A-C1
35	n	605	CHL	CBA-CGA-O2A-C1
23	c	502	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	O1A-CGA-O2A-C1
23	y	303	CLA	O1A-CGA-O2A-C1
23	S	313	CLA	O1D-CGD-O2D-CED
26	B	625	SQD	C8-C7-O47-C45
23	S	314	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	CBD-CGD-O2D-CED
23	b	603	CLA	CBD-CGD-O2D-CED
32	c	519	DMU	O6-C11-C9-O1
35	G	608	CHL	O1A-CGA-O2A-C1
23	c	509	CLA	O1D-CGD-O2D-CED
35	y	309	CHL	O1D-CGD-O2D-CED
23	d	403	CLA	C3-C5-C6-C7
23	G	602	CLA	CBA-CGA-O2A-C1
23	Y	303	CLA	CBA-CGA-O2A-C1
23	y	303	CLA	CBA-CGA-O2A-C1
23	S	304	CLA	O1D-CGD-O2D-CED
23	N	613	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	C4-C3-C5-C6
24	a	403	PHO	C4-C3-C5-C6
33	D	406	PL9	C40-C39-C41-C42
33	d	406	PL9	C40-C39-C41-C42
23	R	304	CLA	C2-C3-C5-C6
24	D	402	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	a	403	PHO	C2-C3-C5-C6
35	R	308	CHL	CBD-CGD-O2D-CED
23	G	604	CLA	C2A-CAA-CBA-CGA
23	N	603	CLA	C2A-CAA-CBA-CGA
23	Y	313	CLA	C2A-CAA-CBA-CGA
23	R	303	CLA	C2A-CAA-CBA-CGA
32	s	618	DMU	C4-C3-O7-C10
32	C	523	DMU	O6-C11-C9-O1
32	c	522	DMU	O6-C11-C9-O1
35	g	608	CHL	O1A-CGA-O2A-C1
30	C	522	LMG	O6-C1-O1-C7
30	W	203	LMG	O6-C1-O1-C7
30	c	521	LMG	O6-C1-O1-C7
30	w	202	LMG	O6-C1-O1-C7
35	Y	309	CHL	O1D-CGD-O2D-CED
33	d	406	PL9	C34-C36-C37-C38
23	C	506	CLA	CBA-CGA-O2A-C1
23	y	305	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	O1D-CGD-O2D-CED
23	N	614	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
23	n	614	CLA	O1D-CGD-O2D-CED
35	Y	302	CHL	O1D-CGD-O2D-CED
35	y	302	CHL	O1D-CGD-O2D-CED
35	n	605	CHL	O1A-CGA-O2A-C1
26	b	602	SQD	C8-C7-O47-C45
23	G	603	CLA	O1D-CGD-O2D-CED
23	N	604	CLA	O1D-CGD-O2D-CED
23	s	602	CLA	O1D-CGD-O2D-CED
23	y	305	CLA	O1D-CGD-O2D-CED
31	G	619	LHG	C1-C2-C3-O3
31	g	619	LHG	C1-C2-C3-O3
32	S	319	DMU	C4-C3-O7-C10
23	B	605	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
23	r	610	CLA	O1D-CGD-O2D-CED
23	s	603	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	CBA-CGA-O2A-C1
23	G	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	Y	305	CLA	CBA-CGA-O2A-C1
23	b	604	CLA	CBA-CGA-O2A-C1
23	b	605	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
23	g	613	CLA	CBA-CGA-O2A-C1
35	N	605	CHL	CBA-CGA-O2A-C1
23	Y	314	CLA	CBD-CGD-O2D-CED
35	s	601	CHL	CBD-CGD-O2D-CED
31	b	623	LHG	C7-C8-C9-C10
23	R	310	CLA	C10-C11-C12-C13
24	a	403	PHO	C15-C16-C17-C18
35	Y	310	CHL	C13-C15-C16-C17
35	n	608	CHL	C15-C16-C17-C18
35	y	310	CHL	C13-C15-C16-C17
28	d	410	DGD	O1G-C1G-C2G-O2G
23	B	616	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	G	602	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	g	602	CLA	C6-C7-C8-C9
23	y	314	CLA	C6-C7-C8-C9
35	Y	309	CHL	C11-C10-C8-C9
35	y	309	CHL	C11-C10-C8-C9
23	D	404	CLA	O1D-CGD-O2D-CED
23	G	613	CLA	O1D-CGD-O2D-CED
23	d	404	CLA	O1D-CGD-O2D-CED
23	r	608	CLA	O1D-CGD-O2D-CED
23	R	302	CLA	O1D-CGD-O2D-CED
23	y	303	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	C2A-CAA-CBA-CGA
23	r	604	CLA	C2A-CAA-CBA-CGA
23	R	305	CLA	C2A-CAA-CBA-CGA
25	B	619	BCR	C37-C22-C23-C24
25	K	101	BCR	C7-C8-C9-C34
25	b	621	BCR	C37-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
35	n	608	CHL	O1D-CGD-O2D-CED
23	B	603	CLA	O1A-CGA-O2A-C1
23	b	605	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C5-C6-C7-C8
23	B	608	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13
23	c	508	CLA	C5-C6-C7-C8
23	r	609	CLA	C10-C11-C12-C13
35	N	608	CHL	C15-C16-C17-C18
35	g	601	CHL	C13-C15-C16-C17
35	g	608	CHL	C15-C16-C17-C18
35	r	607	CHL	C10-C11-C12-C13
23	R	311	CLA	O1D-CGD-O2D-CED
23	Y	314	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
23	y	314	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	510	CLA	C13-C15-C16-C17
23	D	404	CLA	C13-C15-C16-C17
23	Y	303	CLA	C10-C11-C12-C13
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
24	D	402	PHO	C15-C16-C17-C18
35	G	608	CHL	C15-C16-C17-C18
28	B	624	DGD	C1B-C2B-C3B-C4B
30	b	622	LMG	C28-C29-C30-C31
31	B	621	LHG	C7-C8-C9-C10
31	G	619	LHG	C23-C24-C25-C26
23	N	612	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	C10-C11-C12-C13
23	C	504	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
23	b	604	CLA	C5-C6-C7-C8
23	b	610	CLA	C5-C6-C7-C8
23	b	614	CLA	C10-C11-C12-C13
23	c	503	CLA	C10-C11-C12-C13
23	c	509	CLA	C13-C15-C16-C17
23	d	403	CLA	C10-C11-C12-C13
35	G	601	CHL	C13-C15-C16-C17
35	R	308	CHL	C5-C6-C7-C8
39	W	202	VTQ	C15-C16-C17-C18
39	W	202	VTQ	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
39	w	201	VTQ	C23-C24-C25-C26
31	d	408	LHG	C7-C8-C9-C10
35	Y	306	CHL	O1D-CGD-O2D-CED
23	y	311	CLA	C5-C6-C7-C8
24	A	403	PHO	C15-C16-C17-C18
35	Y	302	CHL	C13-C15-C16-C17
23	b	617	CLA	O1D-CGD-O2D-CED
35	N	605	CHL	O1D-CGD-O2D-CED
35	y	306	CHL	O1D-CGD-O2D-CED
26	B	625	SQD	O49-C7-O47-C45
26	b	602	SQD	O49-C7-O47-C45
23	Y	312	CLA	C8-C10-C11-C12
35	G	601	CHL	C5-C6-C7-C8
23	Y	305	CLA	O1D-CGD-O2D-CED
30	B	620	LMG	C28-C29-C30-C31
23	B	616	CLA	CBD-CGD-O2D-CED
23	G	604	CLA	CBD-CGD-O2D-CED
23	S	309	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	n	611	CLA	CBD-CGD-O2D-CED
35	s	607	CHL	O2A-C1-C2-C3
23	B	612	CLA	C5-C6-C7-C8
24	a	402	PHO	C10-C11-C12-C13
24	a	402	PHO	C15-C16-C17-C18
35	g	601	CHL	C5-C6-C7-C8
35	y	302	CHL	C13-C15-C16-C17
23	b	618	CLA	C6-C7-C8-C10
23	r	611	CLA	C6-C7-C8-C10
35	Y	310	CHL	C11-C12-C13-C15
23	B	602	CLA	O1A-CGA-O2A-C1
23	G	613	CLA	O1A-CGA-O2A-C1
23	Y	314	CLA	O1A-CGA-O2A-C1
23	Y	303	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
23	n	610	CLA	C2A-CAA-CBA-CGA
23	y	313	CLA	C2A-CAA-CBA-CGA
35	y	306	CHL	C2A-CAA-CBA-CGA
23	s	609	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C5-C6-C7-C8
23	B	611	CLA	C13-C15-C16-C17
23	Y	311	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C5-C6-C7-C8
23	b	613	CLA	C13-C15-C16-C17
23	b	614	CLA	C5-C6-C7-C8
23	c	509	CLA	C10-C11-C12-C13
23	d	404	CLA	C5-C6-C7-C8
23	r	609	CLA	C15-C16-C17-C18
23	y	312	CLA	C8-C10-C11-C12
24	A	403	PHO	C10-C11-C12-C13
24	a	403	PHO	C13-C15-C16-C17
35	Y	308	CHL	C13-C15-C16-C17
35	y	308	CHL	C13-C15-C16-C17
39	w	201	VTQ	C15-C16-C17-C18
23	C	506	CLA	O1A-CGA-O2A-C1
23	Y	305	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	O1A-CGA-O2A-C1
35	N	605	CHL	O1A-CGA-O2A-C1
26	l	101	SQD	O5-C1-O6-C44
32	c	519	DMU	O5-C6-O16-C18
24	D	402	PHO	C13-C15-C16-C17
23	B	615	CLA	O1D-CGD-O2D-CED
23	S	310	CLA	O1D-CGD-O2D-CED
33	D	406	PL9	C39-C41-C42-C43
33	d	406	PL9	C39-C41-C42-C43
31	B	622	LHG	C23-C24-C25-C26
35	N	601	CHL	C15-C16-C17-C18
35	n	609	CHL	C5-C6-C7-C8
23	D	404	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	O1A-CGA-O2A-C1
23	y	314	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	C13-C15-C16-C17
23	C	511	CLA	C15-C16-C17-C18
23	Y	313	CLA	C10-C11-C12-C13
23	r	611	CLA	C5-C6-C7-C8
23	y	303	CLA	C10-C11-C12-C13
23	y	313	CLA	C10-C11-C12-C13
35	Y	308	CHL	C8-C10-C11-C12
35	Y	310	CHL	C5-C6-C7-C8
35	r	607	CHL	C5-C6-C7-C8
35	n	601	CHL	C15-C16-C17-C18
23	C	508	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	618	CLA	O1D-CGD-O2D-CED
23	r	601	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C8-C10-C11-C12
23	b	608	CLA	C8-C10-C11-C12
23	c	503	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
35	N	609	CHL	C5-C6-C7-C8
35	y	308	CHL	C8-C10-C11-C12
35	y	310	CHL	C5-C6-C7-C8
35	R	308	CHL	C10-C11-C12-C13
31	B	621	LHG	C3-O3-P-O6
31	B	621	LHG	C4-O6-P-O3
31	B	622	LHG	C3-O3-P-O6
31	D	407	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	G	619	LHG	C4-O6-P-O3
31	L	101	LHG	C3-O3-P-O6
31	N	618	LHG	C4-O6-P-O3
31	S	318	LHG	C4-O6-P-O3
31	W	201	LHG	C4-O6-P-O3
31	Y	319	LHG	C3-O3-P-O6
31	Y	319	LHG	C4-O6-P-O3
31	b	623	LHG	C3-O3-P-O6
31	b	623	LHG	C4-O6-P-O3
31	b	624	LHG	C4-O6-P-O3
31	b	626	LHG	C4-O6-P-O3
31	c	516	LHG	C4-O6-P-O3
31	d	407	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O3
31	g	619	LHG	C4-O6-P-O3
31	l	102	LHG	C3-O3-P-O6
31	s	617	LHG	C4-O6-P-O3
31	n	618	LHG	C4-O6-P-O3
31	y	318	LHG	C3-O3-P-O6
31	y	318	LHG	C4-O6-P-O3
31	D	408	LHG	C7-C8-C9-C10
23	C	509	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C5-C6-C7-C8
23	b	615	CLA	C8-C10-C11-C12
23	c	508	CLA	C8-C10-C11-C12
23	n	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	g	603	CLA	C4-C3-C5-C6
23	R	309	CLA	C5-C6-C7-C8
23	R	312	CLA	C8-C10-C11-C12
35	g	609	CHL	C5-C6-C7-C8
35	G	605	CHL	O1D-CGD-O2D-CED
23	C	502	CLA	C2A-CAA-CBA-CGA
23	y	303	CLA	C2A-CAA-CBA-CGA
35	Y	308	CHL	C2A-CAA-CBA-CGA
23	B	605	CLA	C16-C17-C18-C19
23	B	608	CLA	C16-C17-C18-C19
23	y	311	CLA	C11-C12-C13-C15
35	g	605	CHL	O1D-CGD-O2D-CED
23	A	401	CLA	CBA-CGA-O2A-C1
23	a	401	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	C8-C10-C11-C12
35	Y	310	CHL	C15-C16-C17-C18
31	g	619	LHG	C23-C24-C25-C26
31	n	618	LHG	C11-C12-C13-C14
23	n	603	CLA	CBD-CGD-O2D-CED
28	d	410	DGD	C4B-C5B-C6B-C7B
31	B	621	LHG	C15-C16-C17-C18
35	g	601	CHL	C2C-C3C-CAC-CBC
23	B	602	CLA	C16-C17-C18-C20
23	D	401	CLA	C16-C17-C18-C19
23	G	602	CLA	C16-C17-C18-C19
23	b	604	CLA	C16-C17-C18-C20
23	d	401	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
23	r	602	CLA	C11-C12-C13-C14
35	Y	308	CHL	C16-C17-C18-C20
23	r	602	CLA	CBA-CGA-O2A-C1
23	R	303	CLA	CBA-CGA-O2A-C1
31	D	407	LHG	C30-C31-C32-C33
31	b	623	LHG	C15-C16-C17-C18
31	L	102	LHG	O9-C7-O7-C5
31	l	103	LHG	O9-C7-O7-C5
31	D	408	LHG	C11-C12-C13-C14
31	d	408	LHG	C11-C12-C13-C14
35	G	601	CHL	C2C-C3C-CAC-CBC
31	B	622	LHG	O2-C2-C3-O3
26	l	101	SQD	C17-C18-C19-C20
23	C	511	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C3-C5-C6-C7
23	b	605	CLA	O1D-CGD-O2D-CED
35	S	302	CHL	O1D-CGD-O2D-CED
26	B	625	SQD	C2-C1-O6-C44
26	L	103	SQD	C2-C1-O6-C44
26	b	602	SQD	C2-C1-O6-C44
32	c	519	DMU	C1-C6-O16-C18
23	N	610	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C16-C17-C18-C19
23	D	401	CLA	C16-C17-C18-C20
23	Y	311	CLA	C11-C12-C13-C15
23	b	607	CLA	C16-C17-C18-C19
35	Y	310	CHL	C16-C17-C18-C20
35	y	308	CHL	C16-C17-C18-C20
35	y	310	CHL	C16-C17-C18-C20
23	B	603	CLA	O1D-CGD-O2D-CED
23	s	610	CLA	O1D-CGD-O2D-CED
23	B	611	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	N	611	CLA	C4-C3-C5-C6
23	b	613	CLA	C4-C3-C5-C6
23	n	611	CLA	C4-C3-C5-C6
23	B	611	CLA	C2-C3-C5-C6
23	g	603	CLA	C2-C3-C5-C6
23	B	609	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	B	613	CLA	C6-C7-C8-C9
23	B	614	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	611	CLA	C11-C12-C13-C14
23	b	618	CLA	C11-C10-C8-C9
23	y	304	CLA	C6-C7-C8-C9
23	R	312	CLA	C14-C13-C15-C16
35	y	310	CHL	C11-C12-C13-C14
23	G	602	CLA	O1D-CGD-O2D-CED
23	n	612	CLA	O1D-CGD-O2D-CED
30	d	409	LMG	C28-C29-C30-C31
26	c	520	SQD	C10-C11-C12-C13
31	N	618	LHG	C11-C12-C13-C14
23	B	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C8-C10-C11-C12
23	A	401	CLA	C2A-CAA-CBA-CGA
23	C	506	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C2A-CAA-CBA-CGA
23	a	401	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
23	n	603	CLA	C2A-CAA-CBA-CGA
35	N	608	CHL	C2A-CAA-CBA-CGA
35	n	607	CHL	C2A-CAA-CBA-CGA
31	D	407	LHG	O1-C1-C2-C3
31	d	407	LHG	O1-C1-C2-C3
25	D	405	BCR	C7-C8-C9-C10
38	S	317	NEX	C11-C12-C13-C14
23	b	610	CLA	C3-C5-C6-C7
23	B	601	CLA	C8-C10-C11-C12
31	L	102	LHG	C8-C7-O7-C5
31	l	103	LHG	C8-C7-O7-C5
30	c	521	LMG	C13-C14-C15-C16
31	L	102	LHG	C24-C25-C26-C27
31	l	103	LHG	C24-C25-C26-C27
28	A	408	DGD	C1B-C2B-C3B-C4B
30	s	619	LMG	C19-C20-C21-C22
31	L	102	LHG	C28-C29-C30-C31
31	l	103	LHG	C28-C29-C30-C31
23	C	511	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
23	d	401	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
23	g	602	CLA	C16-C17-C18-C19
23	g	602	CLA	C16-C17-C18-C20
23	y	311	CLA	C11-C12-C13-C14
23	R	303	CLA	C11-C12-C13-C14
26	B	625	SQD	O5-C1-O6-C44
26	b	602	SQD	O5-C1-O6-C44
23	A	404	CLA	C5-C6-C7-C8
23	b	618	CLA	C5-C6-C7-C8
23	y	312	CLA	C5-C6-C7-C8
23	R	312	CLA	C5-C6-C7-C8
35	G	606	CHL	CBD-CGD-O2D-CED
23	C	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	O1D-CGD-O2D-CED
30	S	301	LMG	C19-C20-C21-C22
31	C	518	LHG	C14-C15-C16-C17
23	G	602	CLA	C13-C15-C16-C17
23	r	608	CLA	C5-C6-C7-C8
24	A	403	PHO	C5-C6-C7-C8
24	a	402	PHO	C5-C6-C7-C8
35	G	609	CHL	C5-C6-C7-C8
23	g	610	CLA	C15-C16-C17-C18
31	c	517	LHG	C14-C15-C16-C17
23	B	614	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	n	610	CLA	CBA-CGA-O2A-C1
28	B	626	DGD	C2A-C1A-O1G-C1G
28	b	625	DGD	C2A-C1A-O1G-C1G
23	A	402	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	C3A-C2A-CAA-CBA
23	C	508	CLA	C3A-C2A-CAA-CBA
23	D	403	CLA	C3A-C2A-CAA-CBA
23	N	603	CLA	C3A-C2A-CAA-CBA
23	N	612	CLA	C3A-C2A-CAA-CBA
23	N	613	CLA	C3A-C2A-CAA-CBA
23	S	312	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	615	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	d	403	CLA	C3A-C2A-CAA-CBA
23	r	611	CLA	C3A-C2A-CAA-CBA
23	s	608	CLA	C3A-C2A-CAA-CBA
23	n	603	CLA	C3A-C2A-CAA-CBA
23	n	612	CLA	C3A-C2A-CAA-CBA
23	n	613	CLA	C3A-C2A-CAA-CBA
23	R	312	CLA	C3A-C2A-CAA-CBA
35	N	607	CHL	C3A-C2A-CAA-CBA
35	Y	306	CHL	C3A-C2A-CAA-CBA
35	Y	307	CHL	C3A-C2A-CAA-CBA
35	r	605	CHL	C3A-C2A-CAA-CBA
35	n	607	CHL	C3A-C2A-CAA-CBA
35	y	306	CHL	C3A-C2A-CAA-CBA
35	y	307	CHL	C3A-C2A-CAA-CBA
35	R	306	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	Y	302	CHL	C10-C11-C12-C13
32	C	523	DMU	C19-C18-O16-C6
31	Y	319	LHG	C30-C31-C32-C33
23	D	404	CLA	O1A-CGA-O2A-C1
23	C	511	CLA	C16-C17-C18-C19
23	G	602	CLA	C16-C17-C18-C20
23	r	602	CLA	C11-C12-C13-C15
23	R	303	CLA	C11-C12-C13-C15
35	y	310	CHL	C16-C17-C18-C19
26	B	625	SQD	C9-C10-C11-C12
28	C	517	DGD	C3B-C4B-C5B-C6B
26	l	101	SQD	O6-C44-C45-C46
32	S	319	DMU	C18-C19-C22-C25
32	s	618	DMU	C18-C19-C22-C25
23	g	612	CLA	CBD-CGD-O2D-CED
23	r	604	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C3-C5-C6-C7
23	Y	304	CLA	C3-C5-C6-C7
23	C	513	CLA	C4-C3-C5-C6
23	N	613	CLA	C4-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
23	C	513	CLA	C2-C3-C5-C6
23	N	613	CLA	C2-C3-C5-C6
23	b	613	CLA	C2-C3-C5-C6
23	r	612	CLA	C2-C3-C5-C6
23	R	313	CLA	C2-C3-C5-C6
35	n	605	CHL	O1D-CGD-O2D-CED
23	C	511	CLA	O1D-CGD-O2D-CED
30	C	522	LMG	C30-C31-C32-C33
31	b	624	LHG	C28-C29-C30-C31
23	a	401	CLA	O1A-CGA-O2A-C1
23	Y	311	CLA	C11-C12-C13-C14
23	G	602	CLA	C8-C10-C11-C12
30	C	522	LMG	C14-C15-C16-C17
31	c	517	LHG	C26-C27-C28-C29
23	B	601	CLA	O1D-CGD-O2D-CED
30	C	501	LMG	C37-C38-C39-C40
31	y	318	LHG	C30-C31-C32-C33
23	A	401	CLA	O1A-CGA-O2A-C1
23	r	602	CLA	O1A-CGA-O2A-C1
23	R	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	g	610	CLA	C10-C11-C12-C13
30	b	622	LMG	C36-C37-C38-C39
30	B	620	LMG	C32-C33-C34-C35
23	B	603	CLA	C8-C10-C11-C12
23	b	603	CLA	C8-C10-C11-C12
35	n	609	CHL	C8-C10-C11-C12
23	N	610	CLA	O1A-CGA-O2A-C1
28	B	626	DGD	O1A-C1A-O1G-C1G
28	b	625	DGD	O1A-C1A-O1G-C1G
30	C	522	LMG	C13-C14-C15-C16
31	L	102	LHG	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C30
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C26
25	B	617	BCR	C23-C24-C25-C30
25	B	619	BCR	C23-C24-C25-C26
25	B	619	BCR	C23-C24-C25-C30
25	D	405	BCR	C1-C6-C7-C8
25	H	101	BCR	C1-C6-C7-C8
25	H	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	a	405	BCR	C23-C24-C25-C26
25	a	405	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
25	b	621	BCR	C23-C24-C25-C26
25	b	621	BCR	C23-C24-C25-C30
25	c	518	BCR	C1-C6-C7-C8
25	c	518	BCR	C5-C6-C7-C8
25	d	405	BCR	C1-C6-C7-C8
25	h	101	BCR	C1-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
36	N	615	LUT	C5-C6-C7-C8
36	S	315	LUT	C1-C6-C7-C8
36	S	315	LUT	C5-C6-C7-C8
36	S	316	LUT	C1-C6-C7-C8
36	S	316	LUT	C5-C6-C7-C8
36	Y	316	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	s	614	LUT	C5-C6-C7-C8
36	n	615	LUT	C5-C6-C7-C8
36	y	316	LUT	C5-C6-C7-C8
30	c	521	LMG	C30-C31-C32-C33
23	C	514	CLA	CBA-CGA-O2A-C1
23	g	610	CLA	CBA-CGA-O2A-C1
23	C	503	CLA	C15-C16-C17-C18
23	R	310	CLA	C15-C16-C17-C18
35	N	609	CHL	C8-C10-C11-C12
35	y	310	CHL	C15-C16-C17-C18
31	N	618	LHG	C8-C7-O7-C5
23	r	604	CLA	O2A-C1-C2-C3
23	B	608	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	C4-C3-C5-C6
23	b	603	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C6-C7-C8-C10
23	B	607	CLA	C11-C10-C8-C7
23	B	609	CLA	C11-C12-C13-C15
23	B	613	CLA	C6-C7-C8-C10
23	Y	304	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	b	611	CLA	C11-C12-C13-C15
23	b	617	CLA	C11-C12-C13-C15
23	b	617	CLA	C12-C13-C15-C16
23	c	512	CLA	C2-C3-C5-C6
23	g	602	CLA	C6-C7-C8-C10
23	n	611	CLA	C2-C3-C5-C6
23	y	304	CLA	C6-C7-C8-C10
23	R	312	CLA	C6-C7-C8-C10
23	R	312	CLA	C12-C13-C15-C16
35	y	310	CHL	C11-C12-C13-C15
23	B	614	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
23	n	610	CLA	O1A-CGA-O2A-C1
23	B	616	CLA	C5-C6-C7-C8
23	a	404	CLA	C5-C6-C7-C8
39	w	201	VTQ	C18-C20-C21-C22
23	b	607	CLA	C16-C17-C18-C20
31	b	626	LHG	O9-C7-O7-C5
31	n	618	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
23	y	304	CLA	CBA-CGA-O2A-C1
31	Y	319	LHG	C24-C23-O8-C6
26	L	103	SQD	C26-C27-C28-C29
23	A	402	CLA	C2A-CAA-CBA-CGA
23	N	602	CLA	C2A-CAA-CBA-CGA
23	Y	314	CLA	C2A-CAA-CBA-CGA
23	n	602	CLA	C2A-CAA-CBA-CGA
23	y	314	CLA	C2A-CAA-CBA-CGA
35	N	607	CHL	C2A-CAA-CBA-CGA
23	B	615	CLA	C15-C16-C17-C18
23	G	611	CLA	C10-C11-C12-C13
23	Y	303	CLA	CBD-CGD-O2D-CED
23	R	313	CLA	C15-C16-C17-C18
35	y	302	CHL	C10-C11-C12-C13
26	B	625	SQD	C31-C32-C33-C34
31	D	407	LHG	C10-C11-C12-C13
23	g	610	CLA	O1A-CGA-O2A-C1
23	Y	304	CLA	CBA-CGA-O2A-C1
23	R	312	CLA	CBA-CGA-O2A-C1
23	Y	313	CLA	C11-C12-C13-C14
26	L	103	SQD	O5-C1-O6-C44
26	L	103	SQD	C15-C16-C17-C18
31	G	619	LHG	C11-C10-C9-C8
26	a	406	SQD	C23-C24-C25-C26
31	l	103	LHG	C23-C24-C25-C26
26	l	101	SQD	C8-C7-O47-C45
31	B	627	LHG	C8-C7-O7-C5
31	b	626	LHG	C8-C7-O7-C5
31	n	618	LHG	C8-C7-O7-C5
23	B	607	CLA	C8-C10-C11-C12
23	r	602	CLA	CBD-CGD-O2D-CED
26	l	101	SQD	O49-C7-O47-C45
31	B	627	LHG	O9-C7-O7-C5
31	N	618	LHG	O9-C7-O7-C5
35	Y	309	CHL	C3-C5-C6-C7
23	d	404	CLA	C15-C16-C17-C18
26	B	625	SQD	O47-C45-C46-O48
26	b	602	SQD	O47-C45-C46-O48
28	B	624	DGD	O1G-C1G-C2G-O2G
28	D	410	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
30	b	601	LMG	O7-C8-C9-O8
31	N	618	LHG	O7-C5-C6-O8
31	Y	319	LHG	O7-C5-C6-O8
31	y	318	LHG	O7-C5-C6-O8
23	b	608	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	C11-C12-C13-C14
35	y	308	CHL	C16-C17-C18-C19
23	D	401	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
23	n	613	CLA	C4-C3-C5-C6
23	R	303	CLA	C4-C3-C5-C6
23	R	313	CLA	C4-C3-C5-C6
23	N	611	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
31	d	407	LHG	C10-C11-C12-C13
23	Y	304	CLA	C6-C7-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C12-C13-C14
23	b	617	CLA	C14-C13-C15-C16
23	r	611	CLA	C6-C7-C8-C9
23	R	312	CLA	C6-C7-C8-C9
35	Y	310	CHL	C11-C12-C13-C14
35	R	308	CHL	O1D-CGD-O2D-CED
23	N	611	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	C3-C5-C6-C7
35	y	309	CHL	C3-C5-C6-C7
23	G	613	CLA	C2A-CAA-CBA-CGA
23	N	604	CLA	C2A-CAA-CBA-CGA
23	g	613	CLA	C2A-CAA-CBA-CGA
35	r	606	CHL	C2A-CAA-CBA-CGA
35	n	606	CHL	C2A-CAA-CBA-CGA
35	n	608	CHL	C2A-CAA-CBA-CGA
35	y	308	CHL	C2A-CAA-CBA-CGA
26	l	101	SQD	C25-C26-C27-C28
28	c	515	DGD	C3B-C4B-C5B-C6B
31	g	619	LHG	C11-C10-C9-C8
23	r	611	CLA	CBA-CGA-O2A-C1
35	G	601	CHL	C8-C10-C11-C12
26	l	101	SQD	C26-C27-C28-C29
25	d	405	BCR	C7-C8-C9-C10
38	r	615	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	n	617	NEX	C31-C32-C33-C34
23	C	514	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	503	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C1A-C2A-CAA-CBA
23	C	509	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C1A-C2A-CAA-CBA
23	D	403	CLA	C1A-C2A-CAA-CBA
23	D	404	CLA	C1A-C2A-CAA-CBA
23	G	604	CLA	C1A-C2A-CAA-CBA
23	N	603	CLA	C1A-C2A-CAA-CBA
23	N	610	CLA	C1A-C2A-CAA-CBA
23	N	612	CLA	C1A-C2A-CAA-CBA
23	S	303	CLA	C1A-C2A-CAA-CBA
23	S	305	CLA	C1A-C2A-CAA-CBA
23	S	312	CLA	C1A-C2A-CAA-CBA
23	Y	311	CLA	C1A-C2A-CAA-CBA
23	Y	312	CLA	C1A-C2A-CAA-CBA
23	Y	315	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
23	b	615	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	502	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	d	401	CLA	C1A-C2A-CAA-CBA
23	d	403	CLA	C1A-C2A-CAA-CBA
23	g	604	CLA	C1A-C2A-CAA-CBA
23	g	610	CLA	C1A-C2A-CAA-CBA
23	r	608	CLA	C1A-C2A-CAA-CBA
23	r	609	CLA	C1A-C2A-CAA-CBA
23	r	611	CLA	C1A-C2A-CAA-CBA
23	r	612	CLA	C1A-C2A-CAA-CBA
23	s	602	CLA	C1A-C2A-CAA-CBA
23	s	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	s	608	CLA	C1A-C2A-CAA-CBA
23	s	609	CLA	C1A-C2A-CAA-CBA
23	n	603	CLA	C1A-C2A-CAA-CBA
23	n	610	CLA	C1A-C2A-CAA-CBA
23	n	612	CLA	C1A-C2A-CAA-CBA
23	y	311	CLA	C1A-C2A-CAA-CBA
23	y	312	CLA	C1A-C2A-CAA-CBA
23	y	315	CLA	C1A-C2A-CAA-CBA
23	R	309	CLA	C1A-C2A-CAA-CBA
23	R	310	CLA	C1A-C2A-CAA-CBA
23	R	312	CLA	C1A-C2A-CAA-CBA
23	R	313	CLA	C1A-C2A-CAA-CBA
28	B	624	DGD	O6E-C5E-C6E-O5E
35	r	605	CHL	C1A-C2A-CAA-CBA
35	r	607	CHL	C1A-C2A-CAA-CBA
35	n	608	CHL	C1A-C2A-CAA-CBA
35	R	306	CHL	C1A-C2A-CAA-CBA
35	R	308	CHL	C1A-C2A-CAA-CBA
23	B	605	CLA	C16-C17-C18-C20
23	B	608	CLA	C16-C17-C18-C20
23	Y	313	CLA	C11-C12-C13-C15
23	c	511	CLA	C16-C17-C18-C19
35	Y	310	CHL	C16-C17-C18-C19
23	G	610	CLA	C15-C16-C17-C18
38	R	301	NEX	C33-C34-C35-C15
23	Y	314	CLA	O1D-CGD-O2D-CED
23	G	610	CLA	C10-C11-C12-C13
23	b	609	CLA	C8-C10-C11-C12
35	g	601	CHL	C8-C10-C11-C12
35	n	609	CHL	C10-C11-C12-C13
31	R	317	LHG	C3-O3-P-O6
35	s	601	CHL	O1D-CGD-O2D-CED
23	Y	312	CLA	C5-C6-C7-C8
23	B	608	CLA	CBA-CGA-O2A-C1
31	B	627	LHG	O6-C4-C5-C6
31	C	518	LHG	O6-C4-C5-C6
31	L	102	LHG	O6-C4-C5-C6
31	c	517	LHG	O6-C4-C5-C6
31	l	103	LHG	O6-C4-C5-C6
30	D	409	LMG	C28-C29-C30-C31
30	b	601	LMG	O6-C5-C6-O5
35	Y	308	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	B	623	LMG	O6-C5-C6-O5
31	B	622	LHG	C11-C10-C9-C8
31	y	318	LHG	C24-C23-O8-C6
23	S	311	CLA	C3A-C2A-CAA-CBA
35	g	606	CHL	C3A-C2A-CAA-CBA
35	Y	302	CHL	C8-C10-C11-C12
32	C	520	DMU	C18-C19-C22-C25
30	w	202	LMG	C11-C10-O7-C8
23	c	506	CLA	O1A-CGA-O2A-C1
23	y	304	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C8-C10-C11-C12
23	n	604	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C16-C17-C18-C19
26	B	625	SQD	C44-C45-C46-O48
26	L	103	SQD	O6-C44-C45-C46
26	l	101	SQD	C11-C10-C9-C8
31	N	618	LHG	C4-C5-C6-O8
31	S	318	LHG	C4-C5-C6-O8
31	b	626	LHG	C4-C5-C6-O8
31	n	618	LHG	C4-C5-C6-O8
31	b	624	LHG	C11-C10-C9-C8
23	C	507	CLA	O1A-CGA-O2A-C1
30	C	522	LMG	C8-C7-O1-C1
30	c	521	LMG	C8-C7-O1-C1
35	g	601	CHL	C4C-C3C-CAC-CBC
23	c	502	CLA	C15-C16-C17-C18
23	g	611	CLA	C10-C11-C12-C13
28	b	625	DGD	C1A-C2A-C3A-C4A
23	y	303	CLA	O1D-CGD-O2D-CED
26	b	602	SQD	C12-C13-C14-C15
30	c	521	LMG	C14-C15-C16-C17
30	D	409	LMG	O6-C5-C6-O5
35	S	308	CHL	O2A-C1-C2-C3
23	B	610	CLA	C15-C16-C17-C18
30	W	203	LMG	C11-C10-O7-C8
31	W	201	LHG	C8-C7-O7-C5
28	B	626	DGD	O6E-C5E-C6E-O5E
28	b	625	DGD	O6E-C5E-C6E-O5E
30	d	409	LMG	O6-C5-C6-O5
23	b	616	CLA	C4-C3-C5-C6
30	B	620	LMG	C17-C18-C19-C20
31	b	623	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	S	319	DMU	C2-C3-O7-C10
23	R	312	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	CBA-CGA-O2A-C1
23	c	501	CLA	CBA-CGA-O2A-C1
23	R	313	CLA	CBA-CGA-O2A-C1
35	N	601	CHL	CBA-CGA-O2A-C1
35	G	601	CHL	C4C-C3C-CAC-CBC
23	r	609	CLA	CBD-CGD-O2D-CED
23	g	602	CLA	C8-C10-C11-C12
31	c	516	LHG	C13-C14-C15-C16
30	C	522	LMG	O6-C5-C6-O5
30	c	521	LMG	O6-C5-C6-O5
23	B	608	CLA	O1A-CGA-O2A-C1
23	c	503	CLA	C15-C16-C17-C18
35	G	601	CHL	C2-C1-O2A-CGA
35	y	308	CHL	C2-C1-O2A-CGA
32	s	618	DMU	C2-C3-O7-C10
32	s	618	DMU	C3-C4-C57-O61
23	G	604	CLA	O1D-CGD-O2D-CED
31	C	518	LHG	C10-C11-C12-C13
23	n	611	CLA	O1D-CGD-O2D-CED
30	b	622	LMG	C17-C18-C19-C20
31	G	619	LHG	C30-C31-C32-C33
23	A	404	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
31	b	623	LHG	C24-C23-O8-C6
31	c	517	LHG	C24-C23-O8-C6
23	Y	304	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	C16-C17-C18-C19
23	G	612	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1A-CGA-O2A-C1
23	d	402	CLA	CBD-CGD-O2D-CED
28	B	626	DGD	C1A-C2A-C3A-C4A
23	b	613	CLA	C10-C11-C12-C13
30	B	623	LMG	O7-C8-C9-O8
31	n	618	LHG	O7-C5-C6-O8
23	B	616	CLA	O1D-CGD-O2D-CED
28	d	410	DGD	CBB-CCB-CDB-CEB
31	Y	319	LHG	O10-C23-O8-C6
23	y	313	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	B	609	CLA	C12-C13-C15-C16
23	B	611	CLA	C12-C13-C15-C16
23	B	612	CLA	C6-C7-C8-C10
23	B	616	CLA	C11-C10-C8-C7
23	C	502	CLA	C11-C10-C8-C7
23	C	504	CLA	C12-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C10
23	C	510	CLA	C12-C13-C15-C16
23	C	512	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	G	603	CLA	C12-C13-C15-C16
23	N	602	CLA	C6-C7-C8-C10
23	Y	304	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	611	CLA	C12-C13-C15-C16
23	b	613	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	b	616	CLA	C2-C3-C5-C6
23	b	618	CLA	C11-C10-C8-C7
23	c	507	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
23	n	602	CLA	C6-C7-C8-C10
23	y	303	CLA	C11-C12-C13-C15
33	D	406	PL9	C28-C29-C31-C32
33	d	406	PL9	C28-C29-C31-C32
35	G	608	CHL	C12-C13-C15-C16
35	N	609	CHL	C6-C7-C8-C10
35	Y	309	CHL	C11-C10-C8-C7
35	g	608	CHL	C12-C13-C15-C16
35	y	309	CHL	C11-C10-C8-C7
31	W	201	LHG	C13-C14-C15-C16
23	B	601	CLA	C11-C12-C13-C14
23	B	603	CLA	C11-C10-C8-C9
23	B	606	CLA	C11-C12-C13-C14
23	B	607	CLA	C11-C10-C8-C9
23	B	609	CLA	C14-C13-C15-C16
23	B	611	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C9
23	B	612	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C10-C8-C9
23	C	504	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C6-C7-C8-C9
23	C	512	CLA	C6-C7-C8-C9
23	N	602	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C9
23	c	503	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	r	609	CLA	C6-C7-C8-C9
23	n	602	CLA	C6-C7-C8-C9
23	y	304	CLA	C11-C12-C13-C14
23	R	310	CLA	C6-C7-C8-C9
35	G	608	CHL	C14-C13-C15-C16
35	g	608	CHL	C14-C13-C15-C16
23	b	610	CLA	CBA-CGA-O2A-C1
23	d	402	CLA	CBA-CGA-O2A-C1
31	B	621	LHG	C24-C23-O8-C6
35	y	306	CHL	CBA-CGA-O2A-C1
35	y	309	CHL	C2A-CAA-CBA-CGA
35	N	601	CHL	O1A-CGA-O2A-C1
26	b	602	SQD	C9-C10-C11-C12
25	B	619	BCR	C21-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C10
36	R	314	LUT	C7-C8-C9-C10
23	B	614	CLA	C3-C5-C6-C7
23	S	309	CLA	O1D-CGD-O2D-CED
35	N	609	CHL	C10-C11-C12-C13
30	C	501	LMG	C11-C10-O7-C8
23	R	304	CLA	CBA-CGA-O2A-C1
31	C	518	LHG	C24-C23-O8-C6
35	Y	310	CHL	CBA-CGA-O2A-C1
35	n	601	CHL	CBA-CGA-O2A-C1
23	C	505	CLA	CBD-CGD-O2D-CED
35	r	607	CHL	CBD-CGD-O2D-CED
23	C	512	CLA	C16-C17-C18-C20
28	A	408	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
23	b	617	CLA	C5-C6-C7-C8
31	B	622	LHG	O6-C4-C5-C6
23	B	608	CLA	C3-C5-C6-C7
23	b	609	CLA	C3-C5-C6-C7
33	D	406	PL9	C24-C26-C27-C28
33	d	406	PL9	C24-C26-C27-C28
26	B	625	SQD	C23-C24-C25-C26
23	b	618	CLA	CBA-CGA-O2A-C1
35	Y	306	CHL	CBA-CGA-O2A-C1
24	a	402	PHO	CBD-CGD-O2D-CED
23	b	605	CLA	C8-C10-C11-C12
23	D	401	CLA	C2-C3-C5-C6
23	n	613	CLA	C2-C3-C5-C6
23	C	502	CLA	C10-C11-C12-C13
23	b	614	CLA	C3-C5-C6-C7
35	Y	308	CHL	C10-C11-C12-C13
23	r	612	CLA	CBA-CGA-O2A-C1
23	g	612	CLA	O1D-CGD-O2D-CED
23	n	603	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C3A-C2A-CAA-CBA
23	C	510	CLA	C3A-C2A-CAA-CBA
23	N	611	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	c	509	CLA	C3A-C2A-CAA-CBA
23	d	402	CLA	C3A-C2A-CAA-CBA
23	n	611	CLA	C3A-C2A-CAA-CBA
35	Y	308	CHL	C3A-C2A-CAA-CBA
35	g	608	CHL	C3A-C2A-CAA-CBA
35	n	601	CHL	C3A-C2A-CAA-CBA
32	S	319	DMU	C19-C18-O16-C6
32	c	522	DMU	C19-C18-O16-C6
32	s	618	DMU	C19-C18-O16-C6
23	r	603	CLA	C3-C5-C6-C7
23	B	604	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
35	y	308	CHL	C5-C6-C7-C8
23	c	510	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	C15-C16-C17-C18
26	b	602	SQD	C44-C45-C46-O48
28	B	624	DGD	O1G-C1G-C2G-C3G
28	C	517	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
28	D	410	DGD	O1G-C1G-C2G-C3G
28	d	410	DGD	O1G-C1G-C2G-C3G
30	b	601	LMG	C7-C8-C9-O8
31	y	318	LHG	C4-C5-C6-O8
23	C	502	CLA	O1A-CGA-O2A-C1
30	C	501	LMG	C13-C14-C15-C16
23	d	404	CLA	C3-C5-C6-C7
23	R	313	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	C15-C16-C17-C18
23	g	602	CLA	C13-C15-C16-C17
23	c	505	CLA	C4-C3-C5-C6
23	n	603	CLA	C4-C3-C5-C6
23	r	603	CLA	CBA-CGA-O2A-C1
30	W	203	LMG	C38-C39-C40-C41
28	B	626	DGD	C3A-C4A-C5A-C6A
31	B	621	LHG	C27-C28-C29-C30
23	r	604	CLA	O1D-CGD-O2D-CED
35	y	302	CHL	C8-C10-C11-C12
31	l	102	LHG	C4-O6-P-O3
35	r	605	CHL	C3C-C2C-CMC-OMC
35	s	605	CHL	C3C-C2C-CMC-OMC
35	R	306	CHL	C3C-C2C-CMC-OMC
23	c	501	CLA	O1A-CGA-O2A-C1
31	c	517	LHG	O10-C23-O8-C6
31	y	318	LHG	O10-C23-O8-C6
31	L	102	LHG	C11-C10-C9-C8
23	R	304	CLA	C3-C5-C6-C7
23	S	312	CLA	C2A-CAA-CBA-CGA
23	R	302	CLA	C2A-CAA-CBA-CGA
31	B	621	LHG	O6-C4-C5-O7
31	b	626	LHG	O6-C4-C5-O7
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	O1A-CGA-O2A-C1
23	C	509	CLA	C16-C17-C18-C20
30	w	202	LMG	C38-C39-C40-C41
31	L	102	LHG	C33-C34-C35-C36
23	C	506	CLA	CAA-CBA-CGA-O2A
23	c	505	CLA	CAA-CBA-CGA-O2A
23	B	607	CLA	C3-C5-C6-C7
26	b	602	SQD	C23-C24-C25-C26
26	l	101	SQD	O47-C45-C46-O48
30	W	203	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
30	w	202	LMG	O1-C7-C8-O7
31	b	626	LHG	O7-C5-C6-O8
35	G	606	CHL	O1D-CGD-O2D-CED
23	n	610	CLA	C11-C12-C13-C14
26	L	103	SQD	C8-C7-O47-C45
30	s	619	LMG	C11-C10-O7-C8
23	B	605	CLA	C8-C10-C11-C12
23	b	607	CLA	C8-C10-C11-C12
26	L	103	SQD	O49-C7-O47-C45
30	W	203	LMG	O9-C10-O7-C8
30	w	202	LMG	O9-C10-O7-C8
31	W	201	LHG	O9-C7-O7-C5
23	N	603	CLA	C4-C3-C5-C6
35	N	609	CHL	C2-C1-O2A-CGA
35	g	601	CHL	C2-C1-O2A-CGA
35	G	601	CHL	C10-C11-C12-C13
23	B	614	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C9
23	C	503	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	D	401	CLA	C11-C12-C13-C14
23	N	613	CLA	C6-C7-C8-C9
23	Y	304	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C10-C8-C9
23	b	617	CLA	C6-C7-C8-C9
23	c	501	CLA	C11-C10-C8-C9
23	c	502	CLA	C6-C7-C8-C9
23	d	401	CLA	C11-C12-C13-C14
23	n	613	CLA	C6-C7-C8-C9
31	l	103	LHG	C33-C34-C35-C36
31	b	623	LHG	O10-C23-O8-C6
35	Y	310	CHL	O1A-CGA-O2A-C1
23	s	602	CLA	C2A-CAA-CBA-CGA
35	Y	309	CHL	C2A-CAA-CBA-CGA
35	R	307	CHL	C2A-CAA-CBA-CGA
23	c	508	CLA	C16-C17-C18-C20
35	Y	307	CHL	O2A-C1-C2-C3
35	y	307	CHL	O2A-C1-C2-C3
25	H	101	BCR	C23-C24-C25-C26
36	G	615	LUT	C1-C6-C7-C8
36	g	615	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	s	615	LUT	C1-C6-C7-C8
36	s	615	LUT	C5-C6-C7-C8
23	B	611	CLA	C10-C11-C12-C13
31	b	624	LHG	C31-C32-C33-C34
23	d	402	CLA	O1A-CGA-O2A-C1
35	y	306	CHL	O1A-CGA-O2A-C1
23	r	604	CLA	CBA-CGA-O2A-C1
23	S	311	CLA	C1A-C2A-CAA-CBA
25	b	621	BCR	C21-C22-C23-C24
25	h	101	BCR	C7-C8-C9-C10
23	d	403	CLA	C15-C16-C17-C18
26	B	625	SQD	C15-C16-C17-C18
23	B	608	CLA	O1D-CGD-O2D-CED
30	C	501	LMG	O9-C10-O7-C8
30	s	619	LMG	O9-C10-O7-C8
26	l	101	SQD	C32-C33-C34-C35
23	n	613	CLA	C8-C10-C11-C12
31	b	623	LHG	O6-C4-C5-C6
31	b	626	LHG	O6-C4-C5-C6
23	A	401	CLA	C11-C12-C13-C15
23	B	601	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C10-C8-C7
23	B	610	CLA	C12-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C7
23	B	612	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C12-C13-C15
23	D	401	CLA	C11-C12-C13-C15
23	D	404	CLA	C11-C12-C13-C15
23	N	603	CLA	C2-C3-C5-C6
23	N	613	CLA	C6-C7-C8-C10
23	Y	303	CLA	C6-C7-C8-C10
23	a	401	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C10-C8-C7
23	b	612	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C10
23	b	617	CLA	C6-C7-C8-C10
23	c	501	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C6-C7-C8-C10
23	c	503	CLA	C12-C13-C15-C16
23	d	401	CLA	C11-C12-C13-C15
23	r	609	CLA	C6-C7-C8-C10
23	n	603	CLA	C2-C3-C5-C6
23	n	613	CLA	C6-C7-C8-C10
23	y	303	CLA	C6-C7-C8-C10
23	y	304	CLA	C11-C12-C13-C15
23	R	310	CLA	C6-C7-C8-C10
33	D	406	PL9	C43-C44-C46-C47
33	d	406	PL9	C43-C44-C46-C47
35	G	601	CHL	C11-C12-C13-C15
35	G	609	CHL	C6-C7-C8-C10
35	Y	302	CHL	C11-C12-C13-C15
35	Y	308	CHL	C11-C10-C8-C7
35	g	601	CHL	C11-C12-C13-C15
35	g	609	CHL	C6-C7-C8-C10
35	n	609	CHL	C6-C7-C8-C10
23	c	501	CLA	C10-C11-C12-C13
36	Y	317	LUT	C29-C30-C31-C32
36	y	317	LUT	C29-C30-C31-C32
37	r	614	XAT	C29-C30-C31-C32
37	R	315	XAT	C29-C30-C31-C32
28	b	625	DGD	C3A-C4A-C5A-C6A
31	S	318	LHG	C27-C28-C29-C30
23	a	404	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	C5-C6-C7-C8
31	l	103	LHG	C11-C10-C9-C8
23	B	612	CLA	C3-C5-C6-C7
23	C	509	CLA	C16-C17-C18-C19
23	B	614	CLA	C5-C6-C7-C8
39	W	202	VTQ	C18-C20-C21-C22
23	B	601	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	C8-C10-C11-C12
35	g	601	CHL	C10-C11-C12-C13
31	c	517	LHG	C10-C11-C12-C13
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
23	G	614	CLA	CAD-CBD-CGD-O2D
23	N	610	CLA	CAD-CBD-CGD-O2D
23	N	614	CLA	CAD-CBD-CGD-O2D
23	Y	315	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
23	g	610	CLA	CAD-CBD-CGD-O2D
23	g	614	CLA	CAD-CBD-CGD-O2D
23	r	609	CLA	CAD-CBD-CGD-O2D
23	r	611	CLA	CAD-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O2D
23	n	602	CLA	CAD-CBD-CGD-O2D
23	n	610	CLA	CAD-CBD-CGD-O2D
23	n	614	CLA	CAD-CBD-CGD-O2D
23	y	305	CLA	CAD-CBD-CGD-O2D
23	y	315	CLA	CAD-CBD-CGD-O2D
23	R	309	CLA	CAD-CBD-CGD-O2D
23	R	310	CLA	CAD-CBD-CGD-O2D
35	S	302	CHL	CAD-CBD-CGD-O2D
35	r	605	CHL	CAD-CBD-CGD-O2D
35	R	306	CHL	CAD-CBD-CGD-O2D
23	Y	303	CLA	O1D-CGD-O2D-CED
30	B	620	LMG	C35-C36-C37-C38
23	b	617	CLA	C10-C11-C12-C13
26	B	625	SQD	C11-C10-C9-C8
32	c	519	DMU	C18-C19-C22-C25
31	B	621	LHG	O10-C23-O8-C6
23	b	606	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBA-CGA-O2A-C1
23	C	506	CLA	C4-C3-C5-C6
23	G	602	CLA	C4-C3-C5-C6
30	B	620	LMG	O6-C1-O1-C7
30	b	622	LMG	O6-C1-O1-C7
28	c	515	DGD	O1G-C1G-C2G-C3G
30	W	203	LMG	O1-C7-C8-C9
31	B	627	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
31	Y	319	LHG	C4-C5-C6-O8
31	s	617	LHG	C4-C5-C6-O8
23	b	618	CLA	O1A-CGA-O2A-C1
31	c	516	LHG	C8-C7-O7-C5
31	B	622	LHG	O6-C4-C5-O7
31	B	627	LHG	O6-C4-C5-O7
31	C	518	LHG	O6-C4-C5-O7
23	B	601	CLA	C10-C11-C12-C13
23	g	604	CLA	O2A-C1-C2-C3
23	d	402	CLA	O1D-CGD-O2D-CED
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
23	B	604	CLA	CBD-CGD-O2D-CED
23	r	604	CLA	O1A-CGA-O2A-C1
23	G	612	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	G	603	CLA	CHA-CBD-CGD-O1D
23	G	612	CLA	CHA-CBD-CGD-O1D
23	N	602	CLA	CHA-CBD-CGD-O1D
23	Y	314	CLA	CHA-CBD-CGD-O1D
23	Y	314	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	g	612	CLA	CHA-CBD-CGD-O1D
23	g	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	CHA-CBD-CGD-O1D
23	s	602	CLA	CHA-CBD-CGD-O2D
23	R	302	CLA	CHA-CBD-CGD-O2D
35	s	607	CHL	CHA-CBD-CGD-O1D
35	s	607	CHL	CHA-CBD-CGD-O2D
35	n	605	CHL	CHA-CBD-CGD-O2D
23	y	304	CLA	C3-C5-C6-C7
23	a	404	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
23	R	304	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	C	518	LHG	O10-C23-O8-C6
35	Y	306	CHL	O1A-CGA-O2A-C1
35	n	601	CHL	O1A-CGA-O2A-C1
23	R	305	CLA	O2A-C1-C2-C3
35	y	308	CHL	C10-C11-C12-C13
26	a	406	SQD	O6-C44-C45-O47
26	l	101	SQD	O6-C44-C45-O47
30	B	620	LMG	O7-C8-C9-O8
30	b	622	LMG	O7-C8-C9-O8
31	B	627	LHG	O7-C5-C6-O8
23	y	304	CLA	CBD-CGD-O2D-CED
23	r	603	CLA	O1A-CGA-O2A-C1
31	l	102	LHG	C13-C14-C15-C16
23	r	602	CLA	O1D-CGD-O2D-CED
31	Y	319	LHG	C17-C18-C19-C20
23	r	612	CLA	O1A-CGA-O2A-C1
23	G	602	CLA	C2-C3-C5-C6
31	c	516	LHG	O9-C7-O7-C5
23	B	610	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C9
23	b	612	CLA	C14-C13-C15-C16
35	G	601	CHL	C11-C12-C13-C14
35	Y	308	CHL	C11-C10-C8-C9
35	g	601	CHL	C11-C12-C13-C14
35	y	308	CHL	C11-C10-C8-C9
35	r	607	CHL	O1D-CGD-O2D-CED
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	r	609	CLA	O1D-CGD-O2D-CED
28	D	410	DGD	C4B-C5B-C6B-C7B
31	L	101	LHG	C13-C14-C15-C16
23	Y	314	CLA	C5-C6-C7-C8
26	l	101	SQD	C4-C5-C6-S
23	c	508	CLA	C16-C17-C18-C19
35	N	606	CHL	C2A-CAA-CBA-CGA
23	b	613	CLA	O1A-CGA-O2A-C1
25	D	405	BCR	C37-C22-C23-C24
38	R	316	NEX	C11-C12-C13-C20
30	a	407	LMG	O6-C5-C6-O5
25	d	405	BCR	C21-C22-C23-C24
31	L	101	LHG	C30-C31-C32-C33
23	B	607	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C1A-C2A-CAA-CBA
23	G	602	CLA	C1A-C2A-CAA-CBA
23	N	602	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C1A-C2A-CAA-CBA
23	c	504	CLA	C1A-C2A-CAA-CBA
23	c	506	CLA	C1A-C2A-CAA-CBA
23	g	602	CLA	C1A-C2A-CAA-CBA
23	n	602	CLA	C1A-C2A-CAA-CBA
35	N	605	CHL	C1A-C2A-CAA-CBA
35	Y	308	CHL	C1A-C2A-CAA-CBA
35	n	601	CHL	C1A-C2A-CAA-CBA
35	n	605	CHL	C1A-C2A-CAA-CBA
23	B	611	CLA	CBA-CGA-O2A-C1
31	C	518	LHG	C4-O6-P-O3
31	G	619	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	c	517	LHG	C3-O3-P-O6
31	R	317	LHG	C4-O6-P-O3
23	C	505	CLA	O1D-CGD-O2D-CED
23	r	602	CLA	C4-C3-C5-C6
23	Y	312	CLA	C3-C5-C6-C7
23	d	403	CLA	C2-C3-C5-C6
23	R	303	CLA	C2-C3-C5-C6
31	B	621	LHG	C3-O3-P-O4
31	B	622	LHG	C3-O3-P-O5
31	D	407	LHG	C4-O6-P-O4
31	G	619	LHG	C4-O6-P-O5
31	W	201	LHG	C4-O6-P-O5
31	b	623	LHG	C3-O3-P-O4
31	b	624	LHG	C3-O3-P-O4
31	c	516	LHG	C4-O6-P-O5
31	d	407	LHG	C4-O6-P-O4
31	g	619	LHG	C4-O6-P-O5
31	l	102	LHG	C4-O6-P-O4
31	r	616	LHG	C3-O3-P-O4
31	r	616	LHG	C4-O6-P-O4
31	R	317	LHG	C3-O3-P-O4
23	b	610	CLA	C16-C17-C18-C19
23	R	302	CLA	O2A-C1-C2-C3
35	G	608	CHL	C5-C6-C7-C8
23	c	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	y	310	CHL	CBA-CGA-O2A-C1
24	A	403	PHO	CBD-CGD-O2D-CED
31	W	201	LHG	O6-C4-C5-C6
30	c	521	LMG	C12-C13-C14-C15
23	r	609	CLA	C2A-CAA-CBA-CGA
23	Y	303	CLA	C3-C5-C6-C7
23	c	501	CLA	C3-C5-C6-C7
28	d	410	DGD	C3B-C4B-C5B-C6B
31	b	624	LHG	C32-C33-C34-C35
23	B	614	CLA	C16-C17-C18-C20
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	604	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	b	603	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	611	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	616	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	g	612	CLA	CAD-CBD-CGD-O1D
23	s	602	CLA	CAD-CBD-CGD-O1D
26	B	625	SQD	C5-C6-S-O9
26	b	602	SQD	C5-C6-S-O9
35	G	606	CHL	CAD-CBD-CGD-O1D
35	Y	302	CHL	CAD-CBD-CGD-O1D
35	s	607	CHL	CAD-CBD-CGD-O1D
35	y	302	CHL	CAD-CBD-CGD-O1D
35	g	608	CHL	C13-C15-C16-C17
23	s	612	CLA	C3-C5-C6-C7
23	y	303	CLA	C3-C5-C6-C7
23	b	606	CLA	C15-C16-C17-C18
23	y	312	CLA	C10-C11-C12-C13
32	c	522	DMU	C22-C25-C28-C31
31	B	622	LHG	C1-C2-C3-O3
23	Y	312	CLA	C10-C11-C12-C13
31	g	619	LHG	C24-C25-C26-C27
23	B	603	CLA	C16-C17-C18-C19
23	B	607	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C6-C7-C8-C10
23	D	403	CLA	C11-C12-C13-C15
23	D	404	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C10-C8-C7
23	Y	303	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16
23	b	612	CLA	C11-C10-C8-C7
23	g	610	CLA	C6-C7-C8-C10
24	A	403	PHO	C6-C7-C8-C10
24	a	402	PHO	C6-C7-C8-C10
31	L	101	LHG	O6-C4-C5-O7
31	W	201	LHG	O6-C4-C5-O7
31	b	623	LHG	O6-C4-C5-O7
31	c	516	LHG	O6-C4-C5-O7
31	c	517	LHG	O6-C4-C5-O7
35	y	302	CHL	C11-C12-C13-C15
35	y	308	CHL	C11-C10-C8-C7
31	b	626	LHG	C10-C11-C12-C13
26	B	625	SQD	C7-C8-C9-C10
31	d	407	LHG	C9-C10-C11-C12
23	g	610	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C11-C12-C13-C14
30	B	623	LMG	C7-C8-C9-O8
26	B	625	SQD	O6-C44-C45-O47
26	L	103	SQD	O6-C44-C45-O47
26	b	602	SQD	O6-C44-C45-O47
28	B	626	DGD	O1G-C1G-C2G-O2G
28	b	625	DGD	O1G-C1G-C2G-O2G
31	S	318	LHG	O7-C5-C6-O8
23	B	611	CLA	O1A-CGA-O2A-C1
23	c	503	CLA	O1A-CGA-O2A-C1
23	D	401	CLA	C13-C15-C16-C17
23	b	617	CLA	C8-C10-C11-C12
31	l	102	LHG	C30-C31-C32-C33
35	y	310	CHL	O1A-CGA-O2A-C1
23	d	401	CLA	C4-C3-C5-C6
35	g	609	CHL	C4-C3-C5-C6
23	C	513	CLA	CBA-CGA-O2A-C1
31	c	516	LHG	C14-C15-C16-C17
23	D	401	CLA	C14-C13-C15-C16
23	D	404	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	G	602	CLA	C11-C10-C8-C9
23	G	603	CLA	C14-C13-C15-C16
23	Y	303	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C10-C8-C9
23	c	503	CLA	C14-C13-C15-C16
23	y	303	CLA	C6-C7-C8-C9
23	y	303	CLA	C11-C12-C13-C14
24	D	402	PHO	C11-C12-C13-C14
35	G	609	CHL	C6-C7-C8-C9
35	Y	302	CHL	C11-C12-C13-C14
35	y	302	CHL	C11-C12-C13-C14
23	C	513	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	C2A-CAA-CBA-CGA
31	d	407	LHG	O1-C1-C2-O2
31	D	408	LHG	C23-C24-C25-C26
26	b	602	SQD	C29-C30-C31-C32
23	y	304	CLA	O1D-CGD-O2D-CED
23	y	314	CLA	C5-C6-C7-C8
26	l	101	SQD	C10-C11-C12-C13
31	L	102	LHG	O2-C2-C3-O3
35	G	601	CHL	C4-C3-C5-C6
31	d	407	LHG	C28-C29-C30-C31
23	G	604	CLA	C1-C2-C3-C4
23	g	604	CLA	C1-C2-C3-C4
23	r	601	CLA	C1-C2-C3-C4
23	R	302	CLA	C1-C2-C3-C4
35	Y	307	CHL	C1-C2-C3-C4
35	y	307	CHL	C1-C2-C3-C4
23	N	603	CLA	C3-C5-C6-C7
26	B	625	SQD	C44-C45-O47-C7
26	b	602	SQD	C44-C45-O47-C7
31	L	102	LHG	C6-C5-O7-C7
31	l	103	LHG	C6-C5-O7-C7
31	B	621	LHG	O6-C4-C5-C6
31	c	516	LHG	O6-C4-C5-C6
23	N	612	CLA	C2A-CAA-CBA-CGA
23	s	609	CLA	C2A-CAA-CBA-CGA
35	Y	310	CHL	C2A-CAA-CBA-CGA
35	y	310	CHL	C2A-CAA-CBA-CGA
26	L	103	SQD	C11-C10-C9-C8
31	d	407	LHG	C30-C31-C32-C33
30	S	301	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	g	607	CHL	O1D-CGD-O2D-CED
23	a	404	CLA	C10-C11-C12-C13
23	G	613	CLA	C2-C1-O2A-CGA
23	g	613	CLA	C2-C1-O2A-CGA
35	Y	308	CHL	C2-C1-O2A-CGA
35	r	607	CHL	C2-C1-O2A-CGA
28	B	626	DGD	C4D-C5D-C6D-O5D
28	b	625	DGD	C4D-C5D-C6D-O5D
26	L	103	SQD	C32-C33-C34-C35
23	C	504	CLA	O1A-CGA-O2A-C1
25	H	101	BCR	C23-C24-C25-C30
36	G	615	LUT	C5-C6-C7-C8
36	g	615	LUT	C1-C6-C7-C8
23	C	504	CLA	CBA-CGA-O2A-C1
30	S	301	LMG	C11-C10-O7-C8
23	b	609	CLA	C5-C6-C7-C8
28	A	408	DGD	O2G-C2G-C3G-O3G
30	C	522	LMG	C12-C13-C14-C15
31	B	622	LHG	C4-O6-P-O3
31	B	627	LHG	C3-O3-P-O6
31	C	518	LHG	C3-O3-P-O6
31	D	408	LHG	C3-O3-P-O6
31	L	102	LHG	C3-O3-P-O6
31	N	618	LHG	C3-O3-P-O6
31	S	318	LHG	C3-O3-P-O6
31	W	201	LHG	C3-O3-P-O6
31	b	626	LHG	C3-O3-P-O6
31	c	516	LHG	C3-O3-P-O6
31	d	408	LHG	C3-O3-P-O6
31	g	619	LHG	C3-O3-P-O6
31	l	103	LHG	C3-O3-P-O6
31	s	617	LHG	C3-O3-P-O6
31	n	618	LHG	C3-O3-P-O6
24	a	402	PHO	O1D-CGD-O2D-CED
26	b	602	SQD	C11-C10-C9-C8
23	B	614	CLA	C16-C17-C18-C19
35	g	607	CHL	CBD-CGD-O2D-CED
31	d	408	LHG	C23-C24-C25-C26
26	a	406	SQD	O6-C44-C45-C46
28	A	408	DGD	C1G-C2G-C3G-O3G
30	B	620	LMG	C7-C8-C9-O8
30	b	622	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
30	w	202	LMG	O1-C7-C8-C9
31	l	102	LHG	C10-C11-C12-C13
23	B	614	CLA	C6-C7-C8-C10
23	c	505	CLA	C2-C3-C5-C6
23	c	507	CLA	C11-C12-C13-C15
23	A	401	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	a	401	CLA	C11-C12-C13-C14
23	b	618	CLA	C6-C7-C8-C9
23	c	509	CLA	C14-C13-C15-C16
35	N	609	CHL	C6-C7-C8-C9
35	g	609	CHL	C6-C7-C8-C9
35	n	609	CHL	C6-C7-C8-C9
23	b	603	CLA	C10-C11-C12-C13
23	b	606	CLA	O1D-CGD-O2D-CED
25	D	405	BCR	C9-C10-C11-C12
25	H	101	BCR	C9-C10-C11-C12
25	d	405	BCR	C9-C10-C11-C12
38	Y	318	NEX	C33-C34-C35-C15
23	B	603	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C20
23	B	604	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C10-C11-C12-C13
31	B	627	LHG	C14-C15-C16-C17
35	g	608	CHL	C16-C17-C18-C20
23	b	611	CLA	CBA-CGA-O2A-C1
23	R	305	CLA	CBA-CGA-O2A-C1
25	K	101	BCR	C7-C8-C9-C10
23	G	604	CLA	O2A-C1-C2-C3
31	D	407	LHG	C9-C10-C11-C12
31	y	318	LHG	C17-C18-C19-C20
30	C	501	LMG	O6-C5-C6-O5
23	b	611	CLA	O1A-CGA-O2A-C1
28	B	626	DGD	O6D-C5D-C6D-O5D
23	R	305	CLA	O1A-CGA-O2A-C1
35	n	609	CHL	CBA-CGA-O2A-C1
23	y	312	CLA	C11-C12-C13-C15
25	h	101	BCR	C9-C10-C11-C12
36	g	615	LUT	C29-C30-C31-C32
36	s	615	LUT	C29-C30-C31-C32
23	C	502	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	S	306	CHL	CAA-CBA-CGA-O2A
23	B	606	CLA	CBD-CGD-O2D-CED
28	c	515	DGD	C4B-C5B-C6B-C7B
31	W	201	LHG	C14-C15-C16-C17
32	C	523	DMU	C22-C25-C28-C31
23	d	404	CLA	C8-C10-C11-C12
23	C	506	CLA	C2-C3-C5-C6
23	d	401	CLA	C2-C3-C5-C6
23	B	616	CLA	C8-C10-C11-C12
23	C	503	CLA	C2-C1-O2A-CGA
23	c	502	CLA	C2-C1-O2A-CGA
35	n	609	CHL	C2-C1-O2A-CGA
35	R	308	CHL	C2-C1-O2A-CGA
31	R	317	LHG	C11-C12-C13-C14
32	C	523	DMU	O5-C4-C57-O61
23	B	601	CLA	C2A-CAA-CBA-CGA
23	S	303	CLA	C2A-CAA-CBA-CGA
23	Y	305	CLA	C2A-CAA-CBA-CGA
23	s	612	CLA	C2A-CAA-CBA-CGA
23	n	612	CLA	C2A-CAA-CBA-CGA
23	R	313	CLA	C2A-CAA-CBA-CGA
28	d	410	DGD	CAB-CBB-CCB-CDB
23	B	612	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
23	b	614	CLA	C3A-C2A-CAA-CBA
23	c	505	CLA	C3A-C2A-CAA-CBA
35	G	601	CHL	C3A-C2A-CAA-CBA
35	N	606	CHL	C3A-C2A-CAA-CBA
35	S	308	CHL	C3A-C2A-CAA-CBA
35	Y	302	CHL	C3A-C2A-CAA-CBA
35	n	606	CHL	C3A-C2A-CAA-CBA
35	y	302	CHL	C3A-C2A-CAA-CBA
35	y	308	CHL	C3A-C2A-CAA-CBA
23	Y	312	CLA	C11-C12-C13-C15
26	b	602	SQD	C24-C25-C26-C27
35	n	606	CHL	CAA-CBA-CGA-O1A
35	g	609	CHL	C2-C3-C5-C6
23	n	613	CLA	C3-C5-C6-C7
31	D	408	LHG	C12-C13-C14-C15
28	D	410	DGD	O2G-C1B-C2B-C3B
31	D	407	LHG	O7-C7-C8-C9
23	B	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	Y	303	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
23	y	314	CLA	C11-C10-C8-C9
35	Y	302	CHL	C14-C13-C15-C16
38	G	618	NEX	C39-C29-C30-C31
38	N	617	NEX	C39-C29-C30-C31
38	S	317	NEX	C39-C29-C30-C31
38	Y	318	NEX	C39-C29-C30-C31
38	g	618	NEX	C39-C29-C30-C31
38	r	615	NEX	C39-C29-C30-C31
38	s	616	NEX	C39-C29-C30-C31
38	n	617	NEX	C39-C29-C30-C31
38	R	301	NEX	C39-C29-C30-C31
38	R	316	NEX	C39-C29-C30-C31
28	b	625	DGD	O6D-C5D-C6D-O5D
23	B	606	CLA	C3-C5-C6-C7
23	S	309	CLA	CAA-CBA-CGA-O1A
35	S	306	CHL	C2A-CAA-CBA-CGA
23	b	616	CLA	C16-C17-C18-C20
35	g	608	CHL	C16-C17-C18-C19
31	B	627	LHG	C10-C11-C12-C13
23	D	403	CLA	C15-C16-C17-C18
23	b	610	CLA	CBD-CGD-O2D-CED
23	g	612	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	C1A-C2A-CAA-CBA
23	C	510	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C1A-C2A-CAA-CBA
23	b	618	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA
23	g	611	CLA	C1A-C2A-CAA-CBA
35	G	601	CHL	C1A-C2A-CAA-CBA
35	N	608	CHL	C1A-C2A-CAA-CBA
35	S	306	CHL	C1A-C2A-CAA-CBA
35	Y	302	CHL	C1A-C2A-CAA-CBA
35	y	302	CHL	C1A-C2A-CAA-CBA
35	y	308	CHL	C1A-C2A-CAA-CBA
32	C	520	DMU	O16-C18-C19-C22
23	Y	314	CLA	C6-C7-C8-C10
23	c	501	CLA	C15-C16-C17-C18
35	n	609	CHL	O1A-CGA-O2A-C1
36	n	616	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	O1D-CGD-O2D-CED
28	B	626	DGD	O1G-C1A-C2A-C3A
35	N	606	CHL	CAA-CBA-CGA-O1A
35	G	601	CHL	C3-C5-C6-C7
23	S	313	CLA	C2A-CAA-CBA-CGA
23	R	310	CLA	C2A-CAA-CBA-CGA
31	D	407	LHG	O1-C1-C2-O2
23	N	613	CLA	C8-C10-C11-C12
35	N	607	CHL	CAA-CBA-CGA-O2A
30	B	620	LMG	O9-C10-O7-C8
23	r	601	CLA	O2A-C1-C2-C3
35	N	609	CHL	CBA-CGA-O2A-C1
26	a	406	SQD	C15-C16-C17-C18
35	G	605	CHL	CAA-CBA-CGA-O1A
35	N	607	CHL	CAA-CBA-CGA-O1A
23	C	511	CLA	C4-C3-C5-C6
35	G	609	CHL	C4-C3-C5-C6
35	g	601	CHL	C4-C3-C5-C6
23	g	612	CLA	CAA-CBA-CGA-O2A
35	G	605	CHL	CAA-CBA-CGA-O2A
31	b	624	LHG	C27-C28-C29-C30
23	B	612	CLA	C8-C10-C11-C12
26	b	602	SQD	C7-C8-C9-C10
30	w	202	LMG	C10-C11-C12-C13
31	R	317	LHG	O9-C7-O7-C5
38	G	618	NEX	C28-C29-C30-C31
38	N	617	NEX	C28-C29-C30-C31
38	S	317	NEX	C28-C29-C30-C31
38	Y	318	NEX	C28-C29-C30-C31
38	g	618	NEX	C28-C29-C30-C31
38	r	615	NEX	C28-C29-C30-C31
38	s	616	NEX	C28-C29-C30-C31
38	n	617	NEX	C28-C29-C30-C31
38	R	301	NEX	C28-C29-C30-C31
38	R	316	NEX	C28-C29-C30-C31
31	s	617	LHG	O7-C5-C6-O8
31	d	407	LHG	O7-C7-C8-C9
23	G	612	CLA	CAA-CBA-CGA-O1A
35	S	306	CHL	CAA-CBA-CGA-O1A
35	g	605	CHL	CAA-CBA-CGA-O1A
24	A	403	PHO	C8-C10-C11-C12
23	b	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	C5-C6-C7-C8
23	b	614	CLA	C13-C15-C16-C17
23	B	612	CLA	C13-C15-C16-C17
23	c	502	CLA	C5-C6-C7-C8
24	A	403	PHO	O1D-CGD-O2D-CED
23	c	503	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
23	B	613	CLA	C2-C1-O2A-CGA
23	G	603	CLA	C2-C1-O2A-CGA
23	N	611	CLA	C2-C1-O2A-CGA
23	Y	314	CLA	C2-C1-O2A-CGA
23	b	609	CLA	C2-C1-O2A-CGA
23	b	615	CLA	C2-C1-O2A-CGA
23	r	602	CLA	C2-C1-O2A-CGA
23	s	604	CLA	C2-C1-O2A-CGA
23	n	611	CLA	C2-C1-O2A-CGA
23	y	314	CLA	C2-C1-O2A-CGA
23	S	309	CLA	CAA-CBA-CGA-O2A
35	n	606	CHL	CAA-CBA-CGA-O2A
35	n	607	CHL	CAA-CBA-CGA-O2A
23	y	314	CLA	O1D-CGD-O2D-CED
23	r	601	CLA	CAA-CBA-CGA-O2A
23	R	302	CLA	CAA-CBA-CGA-O2A
28	b	625	DGD	O1G-C1A-C2A-C3A
24	a	402	PHO	C8-C10-C11-C12
35	N	606	CHL	CAA-CBA-CGA-O2A
35	n	607	CHL	CAA-CBA-CGA-O1A
26	B	625	SQD	O47-C7-C8-C9
23	r	612	CLA	C2A-CAA-CBA-CGA
23	G	612	CLA	CAA-CBA-CGA-O2A
34	F	101	HEM	CAD-CBD-CGD-O2D
31	d	407	LHG	C23-C24-C25-C26
30	a	407	LMG	C33-C34-C35-C36
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
36	G	616	LUT	C1-C6-C7-C8
36	N	616	LUT	C1-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
26	L	103	SQD	C25-C26-C27-C28
34	f	101	HEM	CAA-CBA-CGA-O2A
23	C	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C10-C11-C12-C13
30	D	409	LMG	C21-C22-C23-C24
36	Y	316	LUT	C29-C30-C31-C32
38	R	301	NEX	C29-C30-C31-C32
23	C	504	CLA	C4-C3-C5-C6
35	N	609	CHL	C4-C3-C5-C6
25	D	405	BCR	C21-C22-C23-C24
38	R	316	NEX	C11-C12-C13-C14
35	Y	308	CHL	C5-C6-C7-C8
28	A	408	DGD	O2G-C1B-C2B-C3B
23	G	613	CLA	C3-C5-C6-C7
23	g	613	CLA	C3-C5-C6-C7
23	S	304	CLA	CAA-CBA-CGA-O2A
35	R	307	CHL	CAA-CBA-CGA-O2A
35	s	605	CHL	O1D-CGD-O2D-CED
35	N	609	CHL	O1A-CGA-O2A-C1
35	G	608	CHL	C13-C15-C16-C17
35	n	601	CHL	C13-C15-C16-C17
31	d	408	LHG	C12-C13-C14-C15
26	b	602	SQD	O47-C7-C8-C9
23	B	608	CLA	C15-C16-C17-C18
23	a	401	CLA	C10-C11-C12-C13
35	Y	308	CHL	C15-C16-C17-C18
31	l	102	LHG	O6-C4-C5-O7
23	S	310	CLA	CAA-CBA-CGA-O2A
34	F	101	HEM	CAA-CBA-CGA-O2A
34	f	101	HEM	CAD-CBD-CGD-O2D
35	g	605	CHL	CAA-CBA-CGA-O2A
35	r	606	CHL	CAA-CBA-CGA-O2A
23	r	601	CLA	O1A-CGA-O2A-C1
31	B	622	LHG	C28-C29-C30-C31
35	S	302	CHL	CAA-CBA-CGA-O2A
23	G	610	CLA	C16-C17-C18-C19
23	b	606	CLA	C13-C15-C16-C17
31	Y	319	LHG	O6-C4-C5-C6
31	y	318	LHG	O6-C4-C5-C6
23	B	608	CLA	C4-C3-C5-C6
23	s	608	CLA	O1D-CGD-O2D-CED
33	d	406	PL9	C44-C46-C47-C48
23	B	614	CLA	C11-C10-C8-C7
23	D	401	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	S	301	LMG	C29-C28-O8-C9
30	s	619	LMG	C29-C28-O8-C9
23	B	604	CLA	C13-C15-C16-C17
35	y	308	CHL	C15-C16-C17-C18
38	n	617	NEX	C33-C34-C35-C15
35	s	601	CHL	CAA-CBA-CGA-O2A
23	B	607	CLA	C10-C11-C12-C13
26	A	406	SQD	O6-C44-C45-O47
28	B	624	DGD	O2G-C2G-C3G-O3G
23	c	501	CLA	C5-C6-C7-C8
23	N	604	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	C5-C6-C7-C8
23	d	401	CLA	C13-C15-C16-C17
31	n	618	LHG	C13-C14-C15-C16
35	r	605	CHL	CAA-CBA-CGA-O2A
23	r	601	CLA	CBA-CGA-O2A-C1
23	R	303	CLA	CAA-CBA-CGA-O2A
33	D	406	PL9	C35-C34-C36-C37
35	n	609	CHL	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
23	r	602	CLA	C2-C3-C5-C6
35	G	601	CHL	C2-C3-C5-C6
35	N	609	CHL	C2-C3-C5-C6
23	y	312	CLA	C11-C12-C13-C14
23	D	401	CLA	C5-C6-C7-C8
23	N	604	CLA	CBA-CGA-O2A-C1
31	L	102	LHG	O7-C7-C8-C9
31	C	518	LHG	C11-C12-C13-C14
23	C	508	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	g	610	CLA	C6-C7-C8-C9
24	A	403	PHO	C6-C7-C8-C9
24	a	402	PHO	C6-C7-C8-C9
24	a	403	PHO	C6-C7-C8-C9
24	a	403	PHO	C11-C12-C13-C14
23	n	612	CLA	CAA-CBA-CGA-O2A
23	C	506	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
35	G	608	CHL	C3A-C2A-CAA-CBA
35	N	601	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	g	601	CHL	C3A-C2A-CAA-CBA
31	l	103	LHG	O2-C2-C3-O3
23	b	614	CLA	CAA-CBA-CGA-O2A
23	g	602	CLA	CAA-CBA-CGA-O2A
35	S	302	CHL	CAA-CBA-CGA-O1A
23	A	404	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	G	604	CLA	CAD-CBD-CGD-O2D
23	G	610	CLA	CAD-CBD-CGD-O2D
23	N	602	CLA	CAD-CBD-CGD-O2D
23	S	303	CLA	CAD-CBD-CGD-O2D
23	S	309	CLA	CAD-CBD-CGD-O2D
23	S	310	CLA	CAD-CBD-CGD-O2D
23	S	312	CLA	CAD-CBD-CGD-O2D
23	Y	303	CLA	CAD-CBD-CGD-O2D
23	Y	305	CLA	CAD-CBD-CGD-O2D
23	Y	311	CLA	CAD-CBD-CGD-O2D
23	Y	313	CLA	CAD-CBD-CGD-O2D
23	a	404	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	g	602	CLA	CAD-CBD-CGD-O2D
23	g	604	CLA	CAD-CBD-CGD-O2D
23	r	608	CLA	CAD-CBD-CGD-O2D
23	s	608	CLA	CAD-CBD-CGD-O2D
23	y	303	CLA	CAD-CBD-CGD-O2D
23	y	311	CLA	CAD-CBD-CGD-O2D
23	y	313	CLA	CAD-CBD-CGD-O2D
24	a	402	PHO	CAD-CBD-CGD-O2D
35	G	609	CHL	CAD-CBD-CGD-O2D
35	Y	306	CHL	CAD-CBD-CGD-O2D
35	Y	307	CHL	CAD-CBD-CGD-O2D
35	g	607	CHL	CAD-CBD-CGD-O2D
35	y	306	CHL	CAD-CBD-CGD-O2D
35	y	307	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	C16-C17-C18-C19
35	y	310	CHL	C10-C11-C12-C13
30	b	622	LMG	O9-C10-O7-C8
31	d	408	LHG	C13-C14-C15-C16
23	s	609	CLA	CAA-CBA-CGA-O2A
35	R	306	CHL	CAA-CBA-CGA-O2A
23	B	615	CLA	CAA-CBA-CGA-O2A
23	r	602	CLA	CAA-CBA-CGA-O2A
26	A	406	SQD	O47-C7-C8-C9
23	C	502	CLA	C3-C5-C6-C7
23	S	304	CLA	CAA-CBA-CGA-O1A
23	S	310	CLA	CAA-CBA-CGA-O1A
35	r	605	CHL	CAA-CBA-CGA-O1A
35	G	609	CHL	C2-C3-C5-C6
28	B	624	DGD	O1G-C1A-C2A-C3A
31	N	618	LHG	C24-C25-C26-C27
37	G	617	XAT	C31-C32-C33-C34
37	g	617	XAT	C31-C32-C33-C34
31	b	626	LHG	C14-C15-C16-C17
23	C	509	CLA	C13-C15-C16-C17
26	l	101	SQD	C44-C45-C46-O48
28	B	624	DGD	C1G-C2G-C3G-O3G
28	B	626	DGD	O1G-C1G-C2G-C3G
28	b	625	DGD	O1G-C1G-C2G-C3G
38	G	618	NEX	O24-C26-C27-C28
38	N	617	NEX	O24-C26-C27-C28
38	r	615	NEX	O24-C26-C27-C28
38	R	316	NEX	O24-C26-C27-C28
35	s	601	CHL	CAA-CBA-CGA-O1A
35	R	307	CHL	CAA-CBA-CGA-O1A
23	s	612	CLA	CBA-CGA-O2A-C1
35	s	605	CHL	CBD-CGD-O2D-CED
35	S	307	CHL	O1D-CGD-O2D-CED
31	Y	319	LHG	O6-C4-C5-O7
31	y	318	LHG	O6-C4-C5-O7
23	G	602	CLA	C5-C6-C7-C8
23	G	602	CLA	CAA-CBA-CGA-O2A
23	b	617	CLA	CAA-CBA-CGA-O2A
23	d	402	CLA	CAA-CBA-CGA-O2A
31	s	617	LHG	O8-C23-C24-C25
34	F	101	HEM	CAD-CBD-CGD-O1D
34	f	101	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
35	R	306	CHL	CAA-CBA-CGA-O1A
31	d	408	LHG	C32-C33-C34-C35
23	b	615	CLA	C5-C6-C7-C8
23	B	602	CLA	O2A-C1-C2-C3
23	C	506	CLA	O2A-C1-C2-C3
23	G	602	CLA	O2A-C1-C2-C3
23	c	505	CLA	O2A-C1-C2-C3
23	S	313	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	C5-C6-C7-C8
31	D	407	LHG	C23-C24-C25-C26
23	g	603	CLA	CAA-CBA-CGA-O2A
35	r	606	CHL	CAA-CBA-CGA-O1A
23	g	610	CLA	C16-C17-C18-C19
23	b	616	CLA	C13-C15-C16-C17
23	Y	312	CLA	C11-C12-C13-C14
31	l	102	LHG	C27-C28-C29-C30
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	G	603	CLA	CHA-CBD-CGD-O2D
23	G	612	CLA	CHA-CBD-CGD-O2D
23	N	602	CLA	CHA-CBD-CGD-O2D
23	N	603	CLA	CHA-CBD-CGD-O1D
23	S	304	CLA	CHA-CBD-CGD-O2D
23	S	310	CLA	CHA-CBD-CGD-O2D
23	Y	304	CLA	CHA-CBD-CGD-O1D
23	Y	304	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	r	604	CLA	CHA-CBD-CGD-O1D
23	r	604	CLA	CHA-CBD-CGD-O2D
23	r	610	CLA	CHA-CBD-CGD-O1D
23	r	610	CLA	CHA-CBD-CGD-O2D
23	s	603	CLA	CHA-CBD-CGD-O1D
23	s	603	CLA	CHA-CBD-CGD-O2D
23	n	603	CLA	CHA-CBD-CGD-O2D
23	n	612	CLA	CHA-CBD-CGD-O2D
23	y	304	CLA	CHA-CBD-CGD-O1D
23	y	314	CLA	CHA-CBD-CGD-O1D
23	y	314	CLA	CHA-CBD-CGD-O2D
23	R	305	CLA	CHA-CBD-CGD-O1D
23	R	305	CLA	CHA-CBD-CGD-O2D
23	R	311	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	R	311	CLA	CHA-CBD-CGD-O2D
35	N	605	CHL	CHA-CBD-CGD-O1D
35	N	605	CHL	CHA-CBD-CGD-O2D
35	N	607	CHL	CHA-CBD-CGD-O1D
35	N	607	CHL	CHA-CBD-CGD-O2D
35	Y	308	CHL	CHA-CBD-CGD-O1D
35	Y	308	CHL	CHA-CBD-CGD-O2D
35	g	609	CHL	CHA-CBD-CGD-O1D
35	g	609	CHL	CHA-CBD-CGD-O2D
35	n	607	CHL	CHA-CBD-CGD-O1D
35	n	607	CHL	CHA-CBD-CGD-O2D
23	s	609	CLA	CAA-CBA-CGA-O1A
35	s	605	CHL	CAA-CBA-CGA-O1A
23	y	303	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	C4B-C5B-C6B-C7B
31	R	317	LHG	C10-C11-C12-C13
23	b	613	CLA	C3-C5-C6-C7
34	F	101	HEM	CAA-CBA-CGA-O1A
23	C	502	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A
26	L	103	SQD	O47-C7-C8-C9
26	a	406	SQD	O47-C7-C8-C9
23	B	602	CLA	C10-C11-C12-C13
35	Y	309	CHL	C13-C15-C16-C17
23	N	603	CLA	CAA-CBA-CGA-O2A
31	S	318	LHG	O8-C23-C24-C25
31	l	103	LHG	O7-C7-C8-C9
35	N	601	CHL	CAA-CBA-CGA-O2A
23	y	311	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C5-C6-C7-C8
23	n	610	CLA	C5-C6-C7-C8
23	B	609	CLA	CBA-CGA-O2A-C1
23	B	609	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	CAA-CBA-CGA-O2A
26	C	521	SQD	O47-C7-C8-C9
34	f	101	HEM	CAD-CBD-CGD-O1D
23	B	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	609	CLA	C12-C13-C15-C16
35	Y	310	CHL	C6-C7-C8-C10
35	n	609	CHL	C2-C3-C5-C6
35	y	310	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	G	619	LHG	C34-C35-C36-C37
23	Y	303	CLA	CAA-CBA-CGA-O2A
23	d	404	CLA	CAA-CBA-CGA-O2A
23	B	607	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	d	401	CLA	C14-C13-C15-C16
24	A	403	PHO	C11-C10-C8-C9
24	a	402	PHO	C11-C10-C8-C9
35	Y	309	CHL	O1A-CGA-O2A-C1
35	Y	309	CHL	CBA-CGA-O2A-C1
35	g	608	CHL	CAA-CBA-CGA-O2A
26	A	406	SQD	C5-C6-S-O8
26	L	103	SQD	C4-C5-C6-S
26	a	406	SQD	C5-C6-S-O8
23	s	612	CLA	O1A-CGA-O2A-C1
30	S	301	LMG	O10-C28-O8-C9
31	R	317	LHG	C8-C7-O7-C5
23	B	603	CLA	C2A-CAA-CBA-CGA
23	G	610	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	C2A-CAA-CBA-CGA
23	G	602	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	CAA-CBA-CGA-O2A
35	n	605	CHL	CAA-CBA-CGA-O2A
23	n	612	CLA	CAA-CBA-CGA-O1A
37	g	617	XAT	C31-C32-C33-C40
23	c	513	CLA	C16-C17-C18-C19
33	d	406	PL9	C20-C19-C21-C22
23	S	313	CLA	O1A-CGA-O2A-C1
28	d	410	DGD	O1A-C1A-O1G-C1G
23	b	617	CLA	CAA-CBA-CGA-O1A
23	d	402	CLA	CAA-CBA-CGA-O1A
28	d	410	DGD	C2A-C1A-O1G-C1G
35	N	606	CHL	O1D-CGD-O2D-CED
23	R	310	CLA	C8-C10-C11-C12
35	g	609	CHL	C10-C11-C12-C13
23	B	609	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	Y	305	CLA	C1A-C2A-CAA-CBA
23	y	305	CLA	C1A-C2A-CAA-CBA
23	R	305	CLA	C1A-C2A-CAA-CBA
35	N	601	CHL	C1A-C2A-CAA-CBA
35	g	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	g	602	CLA	CAA-CBA-CGA-O1A
23	R	303	CLA	CAA-CBA-CGA-O1A
35	s	605	CHL	CAA-CBA-CGA-O2A
30	B	620	LMG	C11-C10-O7-C8
30	s	619	LMG	O10-C28-O8-C9
23	Y	304	CLA	C2-C1-O2A-CGA
23	y	304	CLA	C2-C1-O2A-CGA
23	r	602	CLA	CAA-CBA-CGA-O1A
23	N	612	CLA	CAA-CBA-CGA-O2A
26	B	625	SQD	O6-C44-C45-C46
26	b	602	SQD	O6-C44-C45-C46
23	n	602	CLA	CAA-CBA-CGA-O2A
35	G	608	CHL	CAA-CBA-CGA-O2A
32	c	522	DMU	C25-C28-C31-C34
23	Y	311	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	CAA-CBA-CGA-O1A
23	Y	303	CLA	CAA-CBA-CGA-O1A
23	b	614	CLA	CAA-CBA-CGA-O1A
23	c	505	CLA	CAA-CBA-CGA-O1A
23	G	613	CLA	CAA-CBA-CGA-O2A
23	C	504	CLA	C5-C6-C7-C8
23	b	603	CLA	C5-C6-C7-C8
23	c	508	CLA	C13-C15-C16-C17
24	a	402	PHO	C13-C15-C16-C17
31	c	517	LHG	C11-C12-C13-C14
31	L	102	LHG	C3-O3-P-O5
31	b	626	LHG	C3-O3-P-O5
23	B	615	CLA	CAA-CBA-CGA-O1A
23	d	404	CLA	CAA-CBA-CGA-O1A
23	y	303	CLA	CAA-CBA-CGA-O1A
31	L	102	LHG	O9-C7-C8-C9
31	S	318	LHG	O10-C23-C24-C25
25	h	101	BCR	C23-C24-C25-C26
23	c	501	CLA	CAA-CBA-CGA-O1A
26	A	406	SQD	O49-C7-C8-C9
26	a	406	SQD	O49-C7-C8-C9
31	s	617	LHG	O10-C23-C24-C25
26	B	625	SQD	C16-C17-C18-C19
23	Y	304	CLA	CAA-CBA-CGA-O2A
23	r	603	CLA	CAA-CBA-CGA-O2A
31	B	622	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	CAA-CBA-CGA-O1A
23	C	506	CLA	CAA-CBA-CGA-O1A
23	g	603	CLA	CAA-CBA-CGA-O1A
23	G	613	CLA	C5-C6-C7-C8
35	Y	310	CHL	C10-C11-C12-C13
31	R	317	LHG	C11-C10-C9-C8
23	b	610	CLA	C8-C10-C11-C12
23	y	314	CLA	CBD-CGD-O2D-CED
32	C	523	DMU	C25-C28-C31-C34
30	W	203	LMG	O6-C5-C6-O5
35	N	601	CHL	CAA-CBA-CGA-O1A
33	D	406	PL9	C30-C29-C31-C32
33	d	406	PL9	C35-C34-C36-C37
23	R	305	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	G	612	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	n	602	CLA	CAD-CBD-CGD-O1D
23	R	311	CLA	CAD-CBD-CGD-O1D
26	A	406	SQD	C5-C6-S-O7
26	a	406	SQD	C5-C6-S-O7
26	l	101	SQD	C46-C45-O47-C7
35	g	609	CHL	CAD-CBD-CGD-O1D
35	N	606	CHL	CBD-CGD-O2D-CED
23	b	606	CLA	O1A-CGA-O2A-C1
23	N	603	CLA	CAA-CBA-CGA-O1A
23	g	613	CLA	CAA-CBA-CGA-O1A
23	N	602	CLA	CAA-CBA-CGA-O2A
23	B	602	CLA	C15-C16-C17-C18
23	b	609	CLA	C14-C13-C15-C16
35	N	609	CHL	C11-C12-C13-C14
28	B	626	DGD	C2B-C3B-C4B-C5B
28	d	410	DGD	C5A-C6A-C7A-C8A
23	B	604	CLA	O1A-CGA-O2A-C1
23	y	304	CLA	CAA-CBA-CGA-O2A
35	y	306	CHL	CAA-CBA-CGA-O2A
35	y	310	CHL	CAA-CBA-CGA-O2A
28	A	408	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
31	r	616	LHG	C11-C10-C9-C8
23	C	504	CLA	C8-C10-C11-C12
23	S	313	CLA	C5-C6-C7-C8
35	G	609	CHL	O1D-CGD-O2D-CED
23	b	603	CLA	O1A-CGA-O2A-C1
23	n	604	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	C2A-CAA-CBA-CGA
26	b	602	SQD	C16-C17-C18-C19
23	A	404	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
35	N	608	CHL	CAA-CBA-CGA-O2A
23	s	612	CLA	C5-C6-C7-C8
24	A	403	PHO	C13-C15-C16-C17
31	r	616	LHG	C11-C12-C13-C14
30	d	409	LMG	C10-C11-C12-C13
33	D	406	PL9	C20-C19-C21-C22
23	A	401	CLA	C10-C11-C12-C13
23	B	610	CLA	C11-C10-C8-C7
23	c	503	CLA	C2-C3-C5-C6
23	y	314	CLA	C6-C7-C8-C10
23	y	314	CLA	C11-C10-C8-C7
24	A	403	PHO	C11-C10-C8-C7
24	a	402	PHO	C11-C10-C8-C7
35	g	601	CHL	C2-C3-C5-C6
35	s	607	CHL	C3A-C2A-CAA-CBA
23	N	602	CLA	CAA-CBA-CGA-O1A
23	n	602	CLA	CAA-CBA-CGA-O1A
23	N	612	CLA	CAA-CBA-CGA-O1A
31	n	618	LHG	C29-C30-C31-C32
23	R	304	CLA	CAA-CBA-CGA-O2A
35	Y	306	CHL	CAA-CBA-CGA-O2A
35	Y	309	CHL	CAA-CBA-CGA-O2A
35	Y	310	CHL	CAA-CBA-CGA-O2A
35	n	608	CHL	CAA-CBA-CGA-O2A
35	y	309	CHL	CAA-CBA-CGA-O2A
23	r	612	CLA	C15-C16-C17-C18
36	n	615	LUT	C11-C12-C13-C14
23	A	404	CLA	CAA-CBA-CGA-O1A
23	y	304	CLA	CAA-CBA-CGA-O1A
31	l	103	LHG	O9-C7-C8-C9
35	g	608	CHL	CAA-CBA-CGA-O1A
35	y	309	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
35	y	310	CHL	CAA-CBA-CGA-O1A
38	N	617	NEX	C33-C34-C35-C15
23	a	404	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	O1G-C1A-C2A-C3A
35	N	605	CHL	CAA-CBA-CGA-O2A
35	n	601	CHL	CAA-CBA-CGA-O2A
26	L	103	SQD	O49-C7-C8-C9
33	D	406	PL9	C44-C46-C47-C48
23	B	614	CLA	CAA-CBA-CGA-O2A
23	G	613	CLA	CAA-CBA-CGA-O1A
35	G	608	CHL	CAA-CBA-CGA-O1A
23	c	513	CLA	C16-C17-C18-C20
31	L	101	LHG	C27-C28-C29-C30
35	y	309	CHL	C13-C15-C16-C17
23	R	304	CLA	CAA-CBA-CGA-O1A
35	n	601	CHL	CAA-CBA-CGA-O1A
28	c	515	DGD	O1G-C1A-C2A-C3A

There are no ring outliers.

260 monomers are involved in 465 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	407	BCT	2	0
25	k	101	BCR	3	0
31	D	408	LHG	3	0
31	B	621	LHG	1	0
23	Y	313	CLA	2	0
23	b	615	CLA	4	0
31	N	618	LHG	2	0
23	b	618	CLA	2	0
31	d	408	LHG	5	0
23	R	302	CLA	1	0
23	B	602	CLA	2	0
23	R	309	CLA	1	0
31	n	618	LHG	1	0
35	N	601	CHL	3	0
23	B	612	CLA	4	0
23	s	602	CLA	2	0
23	Y	304	CLA	4	0
31	L	101	LHG	3	0
23	B	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	402	CLA	1	0
23	B	611	CLA	2	0
23	b	612	CLA	1	0
31	Y	319	LHG	3	0
36	n	615	LUT	4	0
28	A	408	DGD	1	0
28	d	410	DGD	5	0
23	r	603	CLA	1	0
35	y	310	CHL	4	0
23	r	604	CLA	1	0
23	C	502	CLA	1	0
37	g	617	XAT	1	0
37	g	620	XAT	5	0
23	R	305	CLA	1	0
31	s	617	LHG	2	0
25	B	619	BCR	4	0
35	N	607	CHL	1	0
23	g	604	CLA	1	0
25	A	405	BCR	1	0
27	a	408	BCT	2	0
28	D	410	DGD	3	0
36	g	616	LUT	2	0
35	n	606	CHL	1	0
35	n	608	CHL	3	0
35	s	607	CHL	3	0
23	b	608	CLA	4	0
24	a	403	PHO	4	0
32	c	519	DMU	1	0
36	r	613	LUT	3	0
23	b	611	CLA	1	0
23	B	604	CLA	2	0
23	b	617	CLA	1	0
35	Y	309	CHL	2	0
23	B	614	CLA	3	0
38	G	618	NEX	1	0
31	B	622	LHG	1	0
25	d	405	BCR	1	0
23	a	401	CLA	3	0
23	S	303	CLA	2	0
37	R	315	XAT	1	0
23	C	507	CLA	1	0
23	R	310	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	616	CLA	1	0
23	b	614	CLA	2	0
38	R	301	NEX	3	0
35	r	607	CHL	2	0
23	B	606	CLA	2	0
31	L	102	LHG	1	0
23	b	606	CLA	1	0
35	N	609	CHL	1	0
23	n	610	CLA	2	0
35	S	306	CHL	3	0
23	r	612	CLA	1	0
31	B	627	LHG	1	0
23	n	602	CLA	1	0
32	s	618	DMU	1	0
36	g	615	LUT	3	0
38	R	316	NEX	3	0
31	R	317	LHG	1	0
23	B	607	CLA	3	0
31	l	103	LHG	1	0
23	c	508	CLA	2	0
32	C	523	DMU	1	0
36	s	615	LUT	2	0
23	c	502	CLA	3	0
25	z	101	BCR	2	0
23	s	609	CLA	2	0
38	n	617	NEX	1	0
35	y	308	CHL	5	0
23	c	507	CLA	2	0
38	r	615	NEX	1	0
23	S	310	CLA	2	0
31	D	407	LHG	1	0
26	L	103	SQD	1	0
23	r	601	CLA	1	0
23	D	401	CLA	3	0
35	y	306	CHL	1	0
36	Y	317	LUT	2	0
23	Y	311	CLA	4	0
30	b	601	LMG	2	0
23	G	614	CLA	1	0
26	b	602	SQD	3	0
23	c	510	CLA	1	0
35	g	605	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	610	CLA	1	0
37	y	301	XAT	6	0
30	B	620	LMG	5	0
35	g	601	CHL	5	0
23	B	603	CLA	1	0
23	R	303	CLA	2	0
23	A	401	CLA	2	0
23	a	404	CLA	2	0
23	y	305	CLA	2	0
23	B	601	CLA	1	0
36	y	317	LUT	3	0
23	g	603	CLA	2	0
23	S	314	CLA	1	0
35	y	309	CHL	1	0
23	S	311	CLA	1	0
36	y	316	LUT	4	0
28	c	515	DGD	2	0
23	n	612	CLA	2	0
35	n	601	CHL	4	0
31	g	619	LHG	4	0
31	d	407	LHG	2	0
23	g	613	CLA	1	0
23	c	513	CLA	3	0
23	S	304	CLA	1	0
35	Y	308	CHL	4	0
35	g	609	CHL	1	0
23	B	613	CLA	5	0
23	D	403	CLA	6	0
23	R	313	CLA	2	0
35	G	608	CHL	2	0
23	N	604	CLA	1	0
23	r	610	CLA	1	0
26	C	521	SQD	2	0
25	b	621	BCR	4	0
31	y	318	LHG	3	0
32	C	520	DMU	1	0
23	g	610	CLA	1	0
31	b	624	LHG	2	0
23	b	616	CLA	3	0
23	C	512	CLA	2	0
25	b	619	BCR	5	0
23	A	404	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	517	DGD	2	0
36	G	615	LUT	4	0
23	c	509	CLA	3	0
25	b	620	BCR	2	0
35	n	607	CHL	2	0
37	G	617	XAT	2	0
35	n	609	CHL	2	0
23	S	305	CLA	1	0
35	Y	310	CHL	5	0
36	s	614	LUT	2	0
23	G	603	CLA	1	0
31	b	623	LHG	1	0
23	C	511	CLA	3	0
24	D	402	PHO	5	0
23	n	604	CLA	1	0
30	B	623	LMG	1	0
26	c	520	SQD	1	0
23	b	604	CLA	1	0
36	R	314	LUT	4	0
23	C	510	CLA	1	0
31	c	516	LHG	2	0
24	A	403	PHO	3	0
23	r	609	CLA	1	0
23	N	612	CLA	2	0
38	N	617	NEX	3	0
31	l	102	LHG	2	0
31	W	201	LHG	1	0
30	b	622	LMG	4	0
23	y	312	CLA	1	0
36	S	315	LUT	2	0
38	Y	318	NEX	1	0
31	C	518	LHG	2	0
37	r	614	XAT	2	0
23	y	313	CLA	2	0
30	C	501	LMG	2	0
23	r	608	CLA	2	0
25	H	101	BCR	3	0
35	N	608	CHL	3	0
23	g	602	CLA	5	0
25	a	405	BCR	4	0
23	C	509	CLA	3	0
23	G	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	s	616	NEX	1	0
36	n	616	LUT	3	0
23	C	503	CLA	3	0
36	G	616	LUT	2	0
23	C	508	CLA	3	0
36	N	615	LUT	5	0
31	S	318	LHG	3	0
28	B	624	DGD	4	0
25	B	617	BCR	4	0
35	y	302	CHL	3	0
25	D	405	BCR	1	0
23	b	609	CLA	3	0
23	N	611	CLA	1	0
23	s	611	CLA	1	0
26	l	101	SQD	4	0
34	f	101	HEM	1	0
23	b	610	CLA	3	0
23	Y	312	CLA	1	0
23	Y	305	CLA	2	0
23	C	514	CLA	4	0
38	g	618	NEX	1	0
36	S	316	LUT	4	0
23	d	403	CLA	4	0
23	d	401	CLA	3	0
35	G	601	CHL	5	0
23	Y	303	CLA	2	0
23	g	614	CLA	1	0
35	N	605	CHL	1	0
37	G	620	XAT	2	0
23	N	602	CLA	1	0
31	G	619	LHG	2	0
23	y	311	CLA	3	0
23	c	506	CLA	1	0
35	y	307	CHL	1	0
38	S	317	NEX	1	0
35	S	307	CHL	2	0
23	R	311	CLA	2	0
36	N	616	LUT	4	0
23	N	610	CLA	2	0
31	r	616	LHG	1	0
23	c	503	CLA	2	0
35	S	308	CHL	2	0

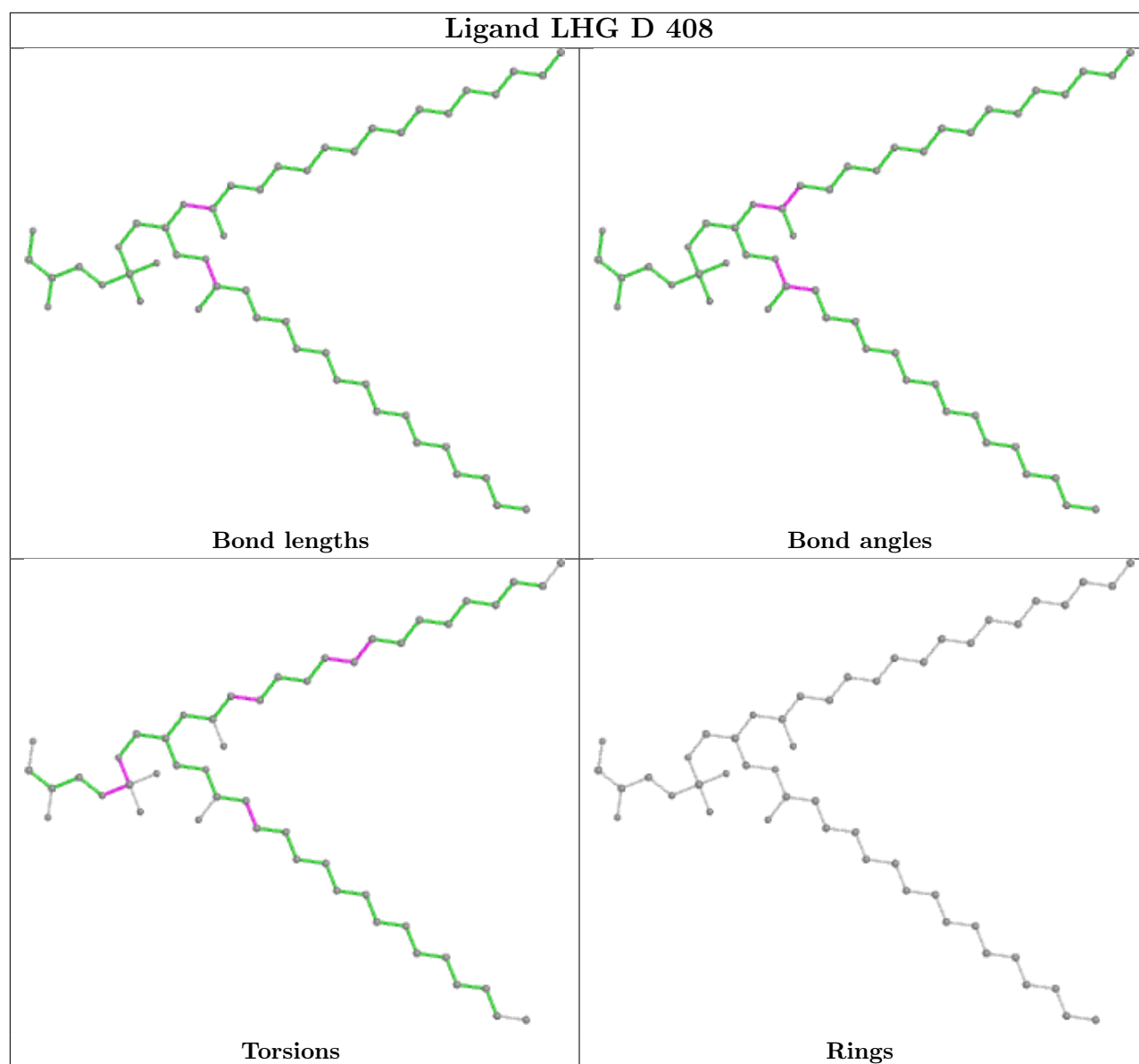
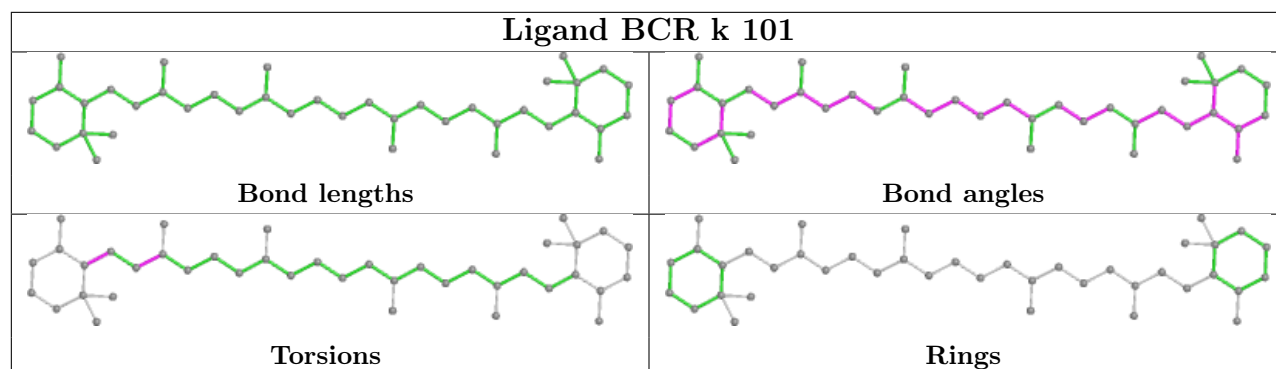
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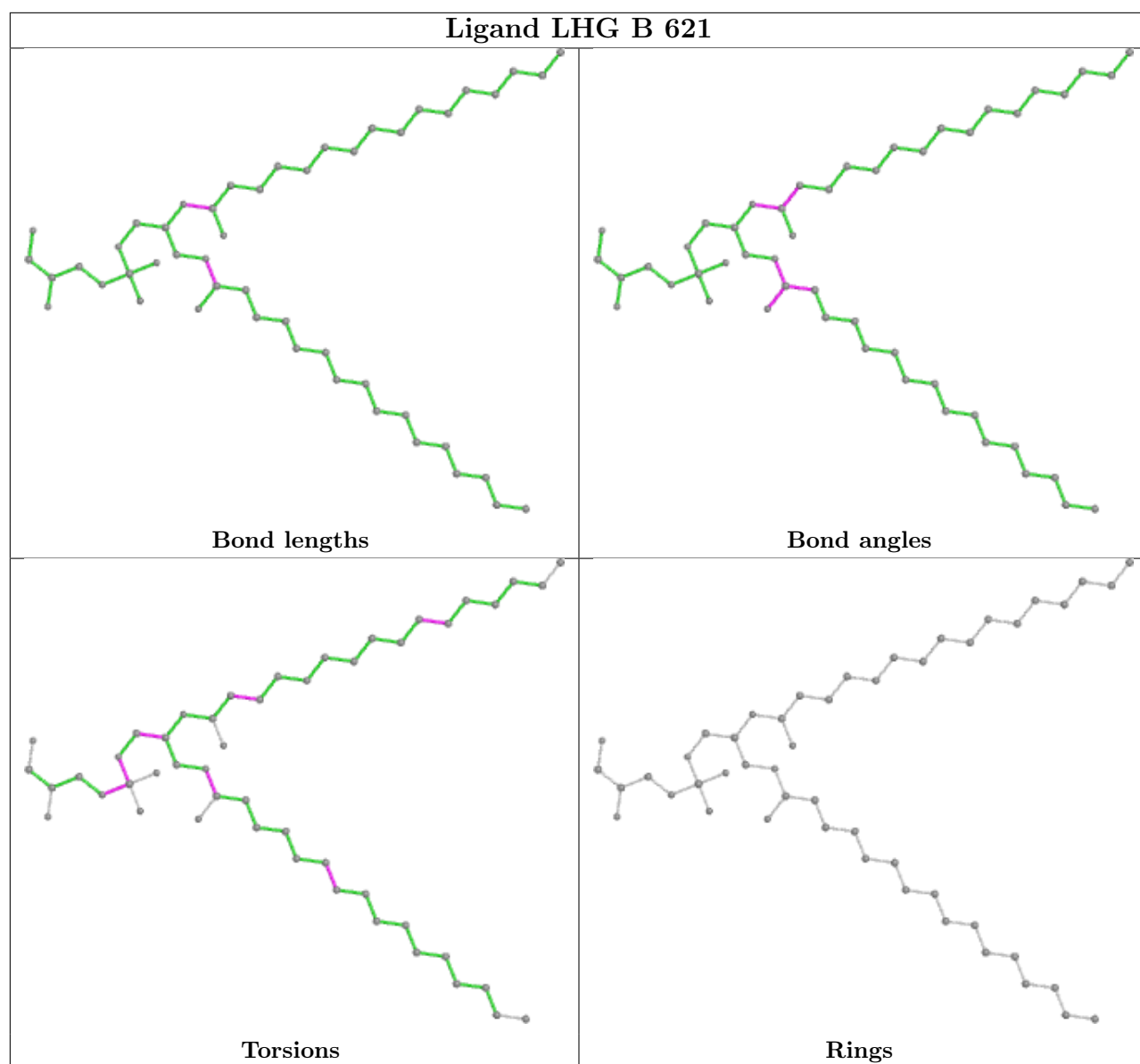
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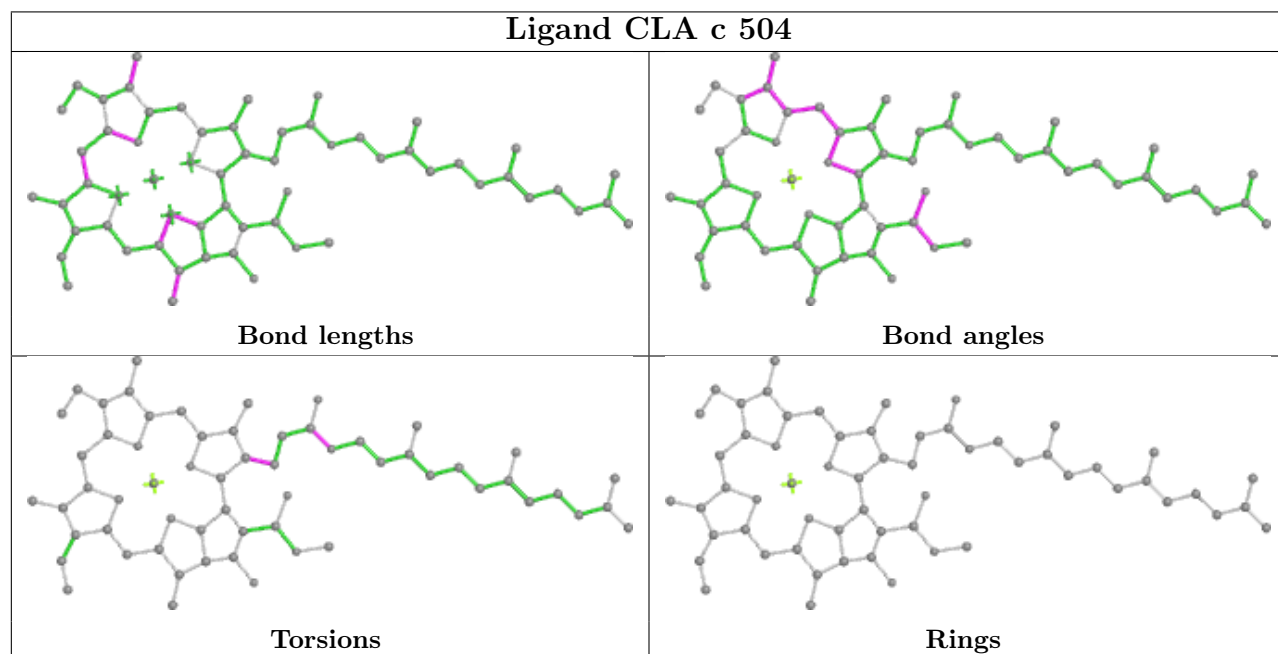
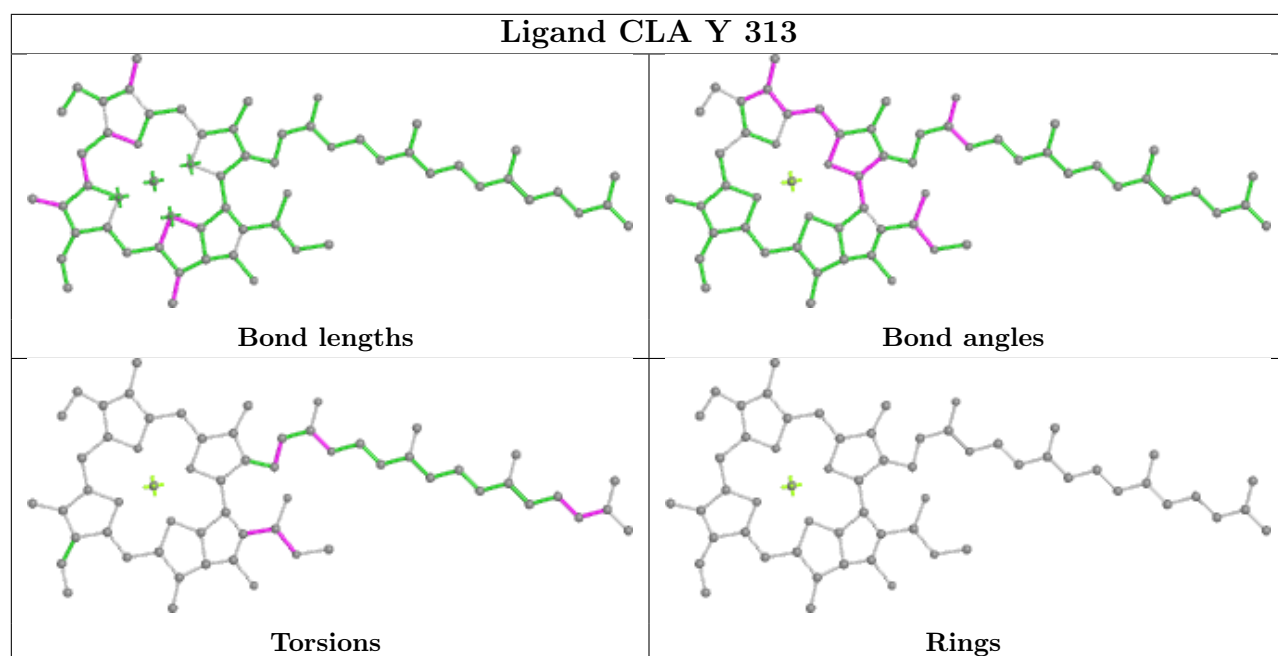
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	409	LMG	1	0
35	R	308	CHL	1	0
37	Y	301	XAT	5	0
23	n	611	CLA	1	0
35	Y	302	CHL	2	0
36	Y	316	LUT	5	0
25	C	519	BCR	3	0
32	c	522	DMU	1	0
35	g	608	CHL	1	0
26	a	406	SQD	2	0
34	F	101	HEM	1	0
23	y	304	CLA	4	0
25	C	515	BCR	7	0
33	D	406	PL9	2	0
32	S	319	DMU	1	0
25	h	101	BCR	2	0
23	C	504	CLA	2	0
25	c	518	BCR	4	0
26	B	625	SQD	3	0
23	b	605	CLA	1	0
25	c	514	BCR	2	0
35	R	307	CHL	1	0
23	n	603	CLA	1	0
23	c	511	CLA	1	0
23	r	602	CLA	1	0
23	s	603	CLA	1	0
25	C	516	BCR	1	0
25	K	101	BCR	1	0
23	G	610	CLA	2	0
23	d	402	CLA	1	0
23	G	602	CLA	4	0

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

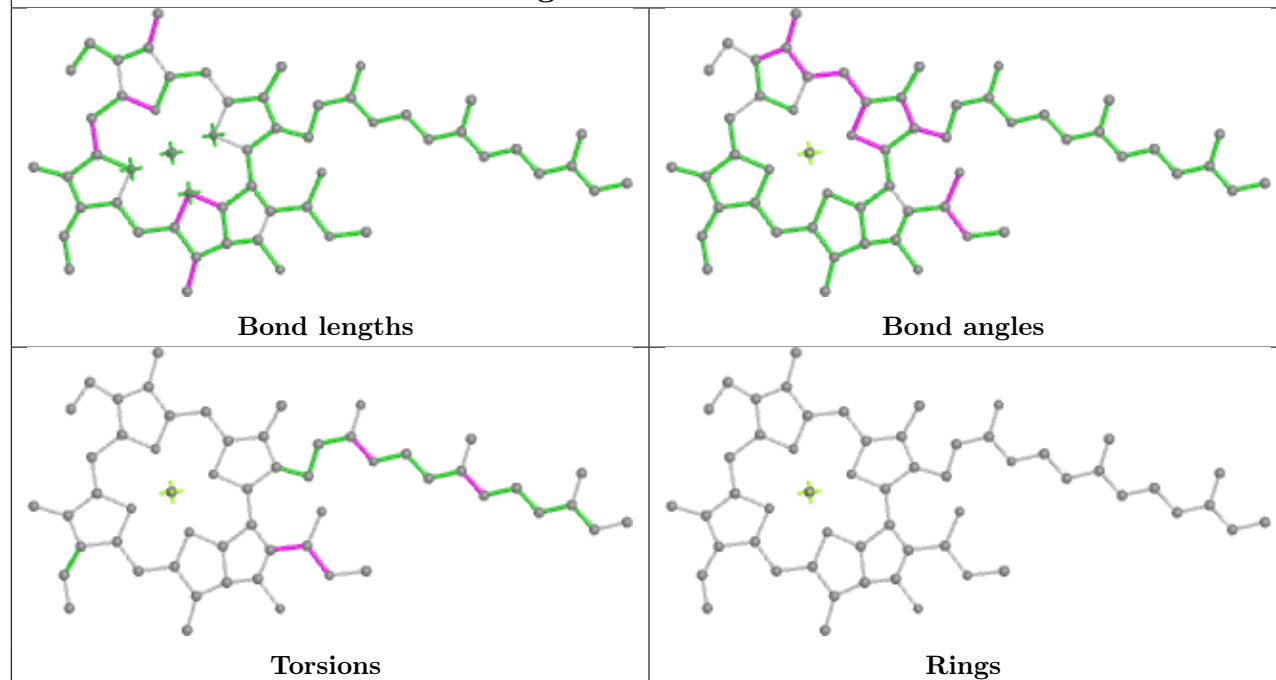
equivalents in the CSD to analyse the geometry.



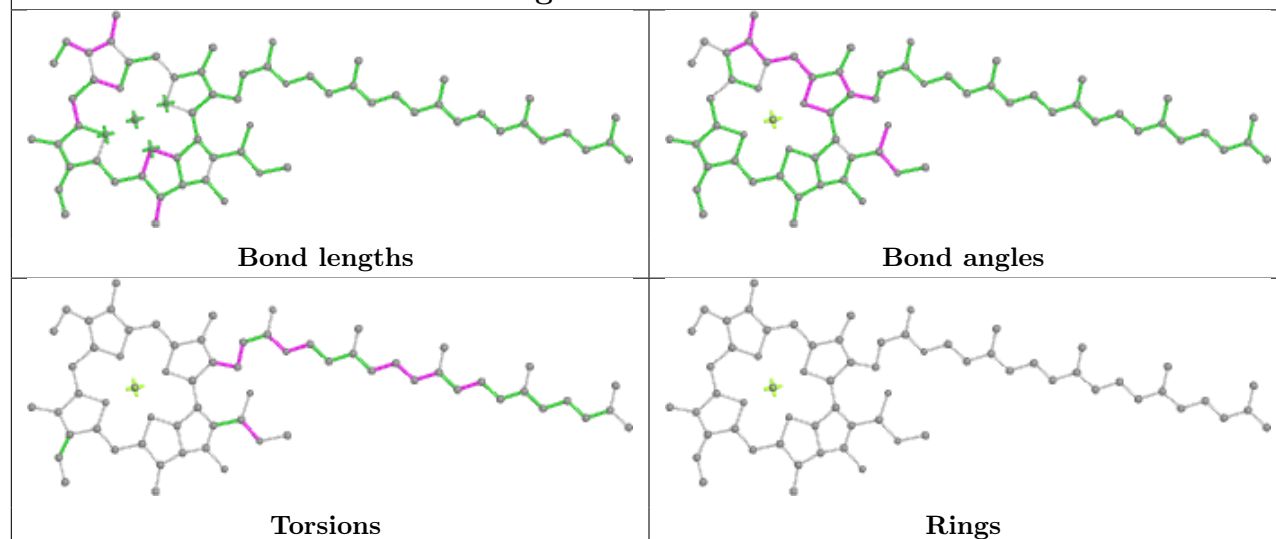




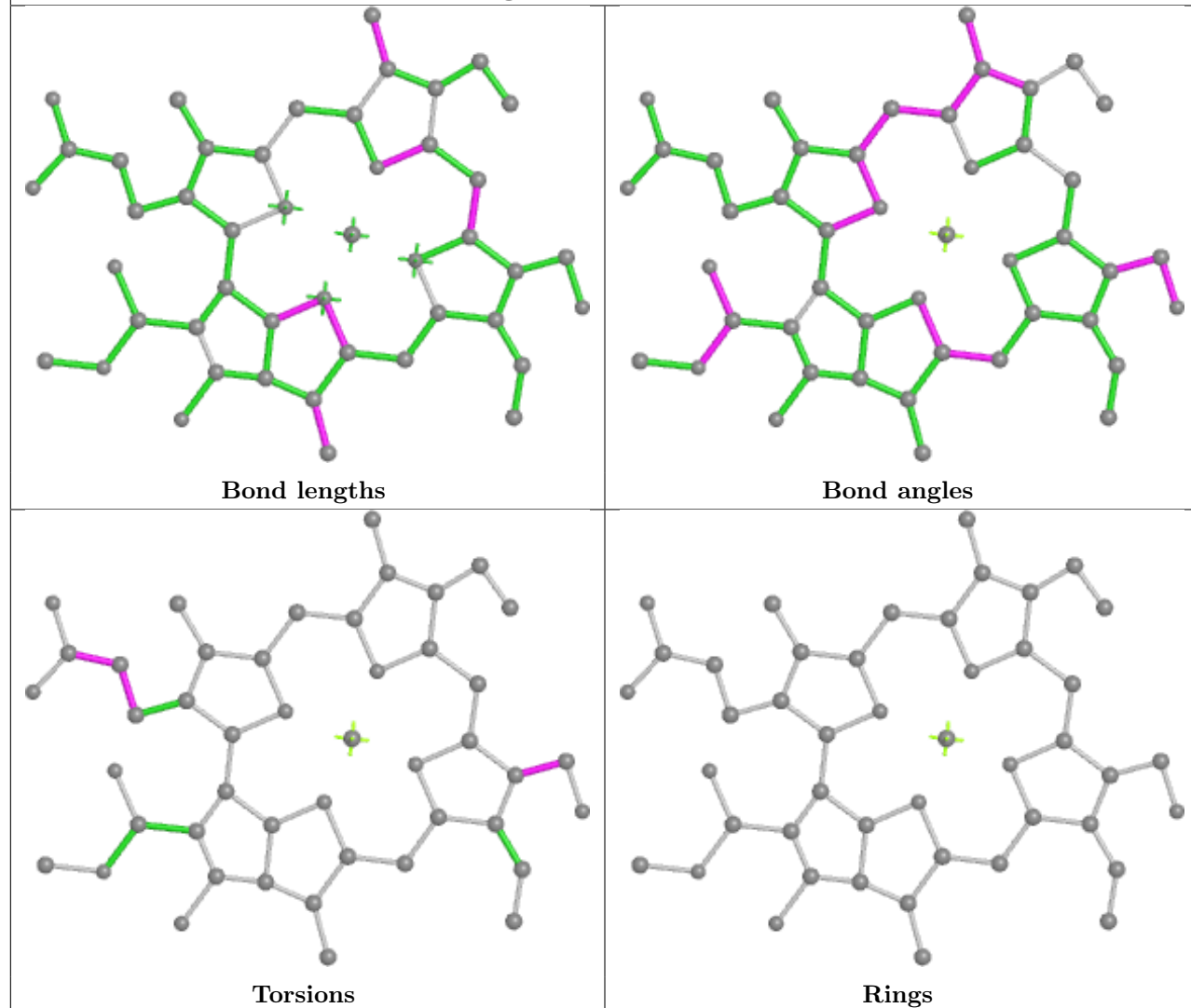
Ligand CLA c 512

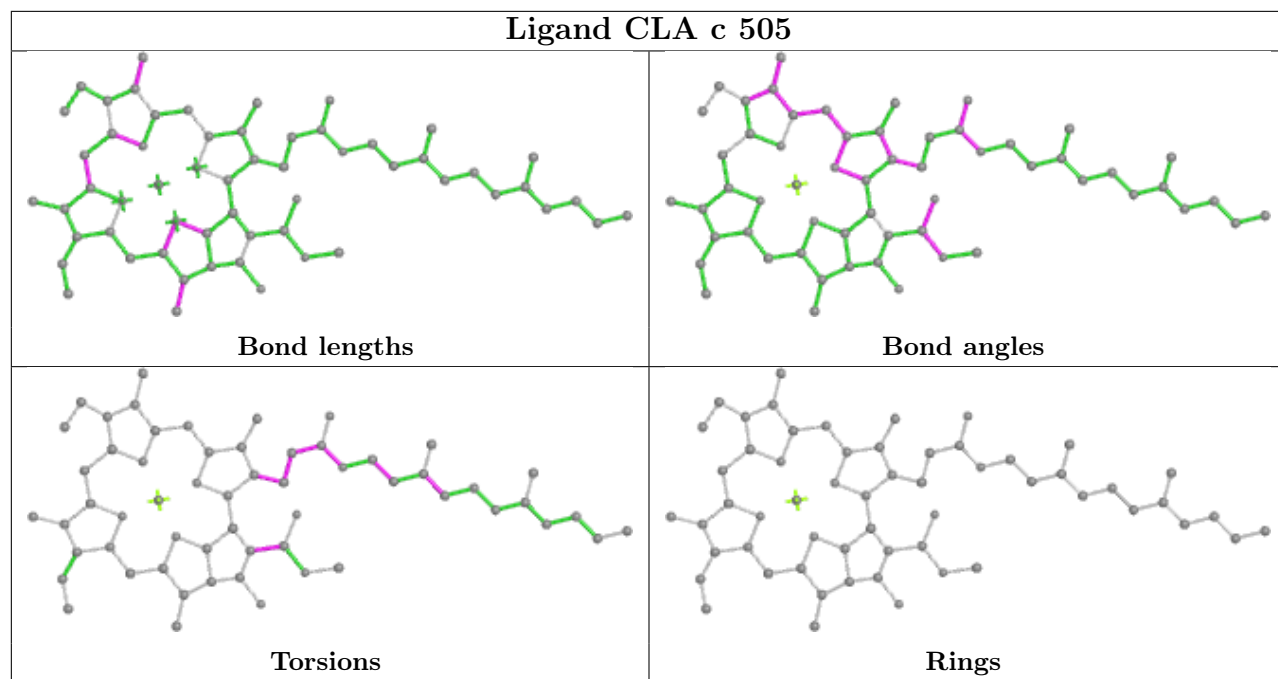


Ligand CLA b 615

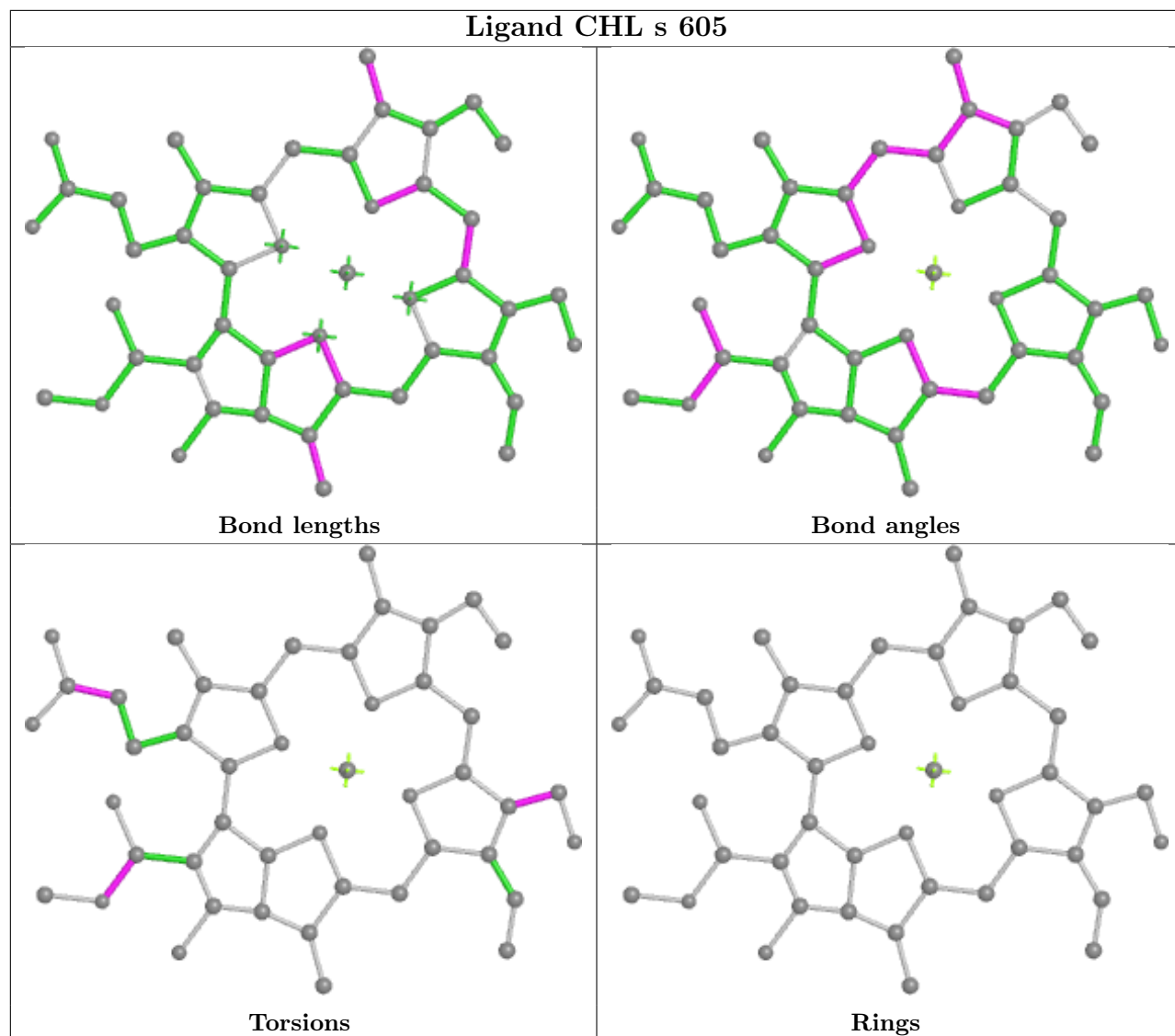


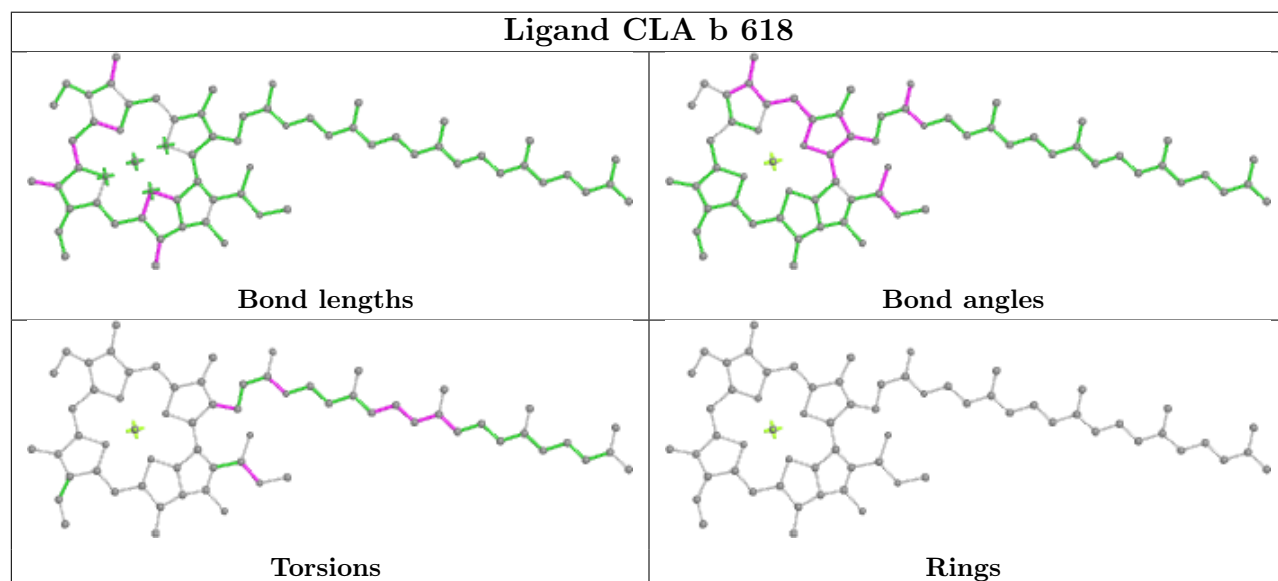
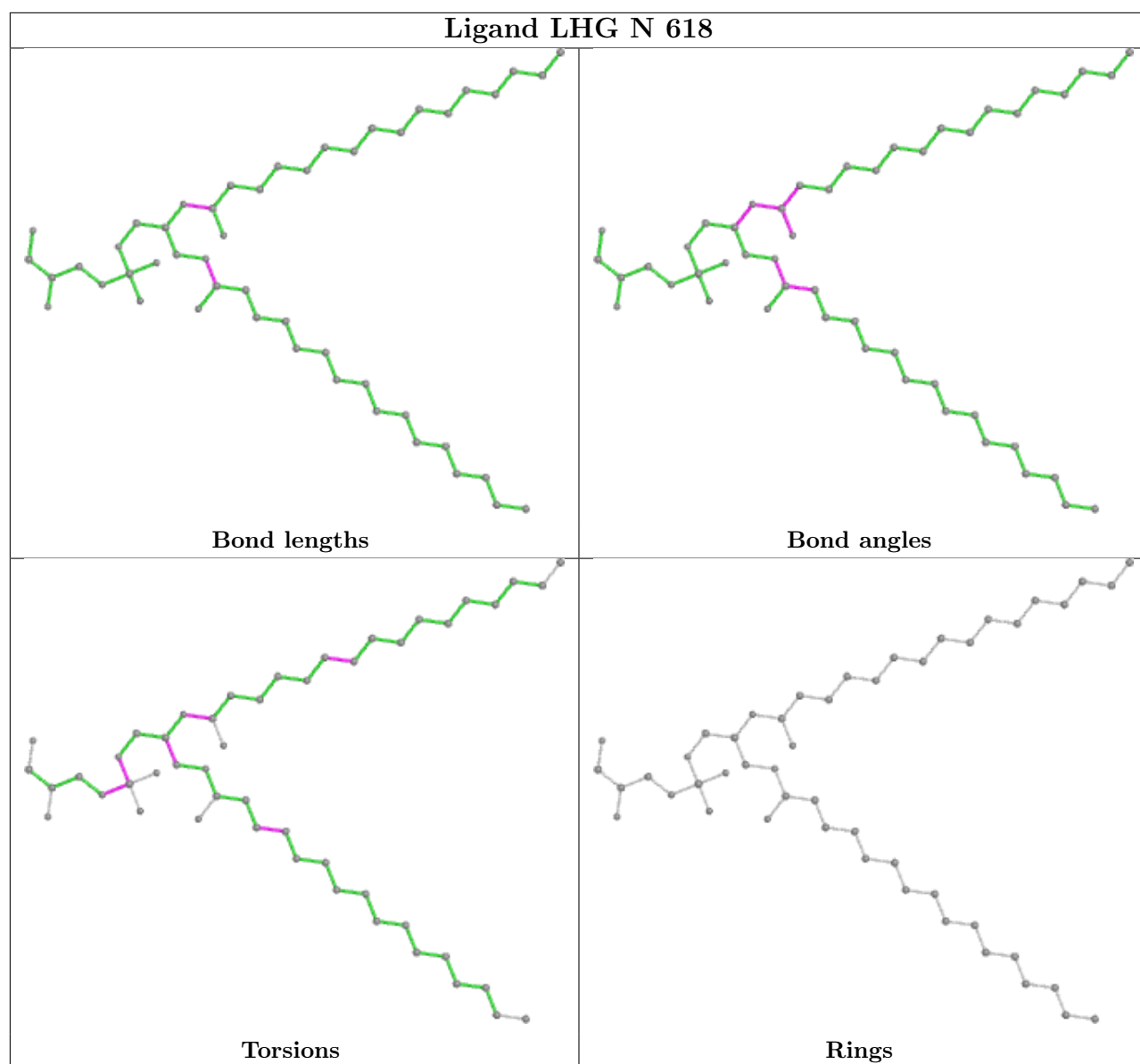
Ligand CHL r 606

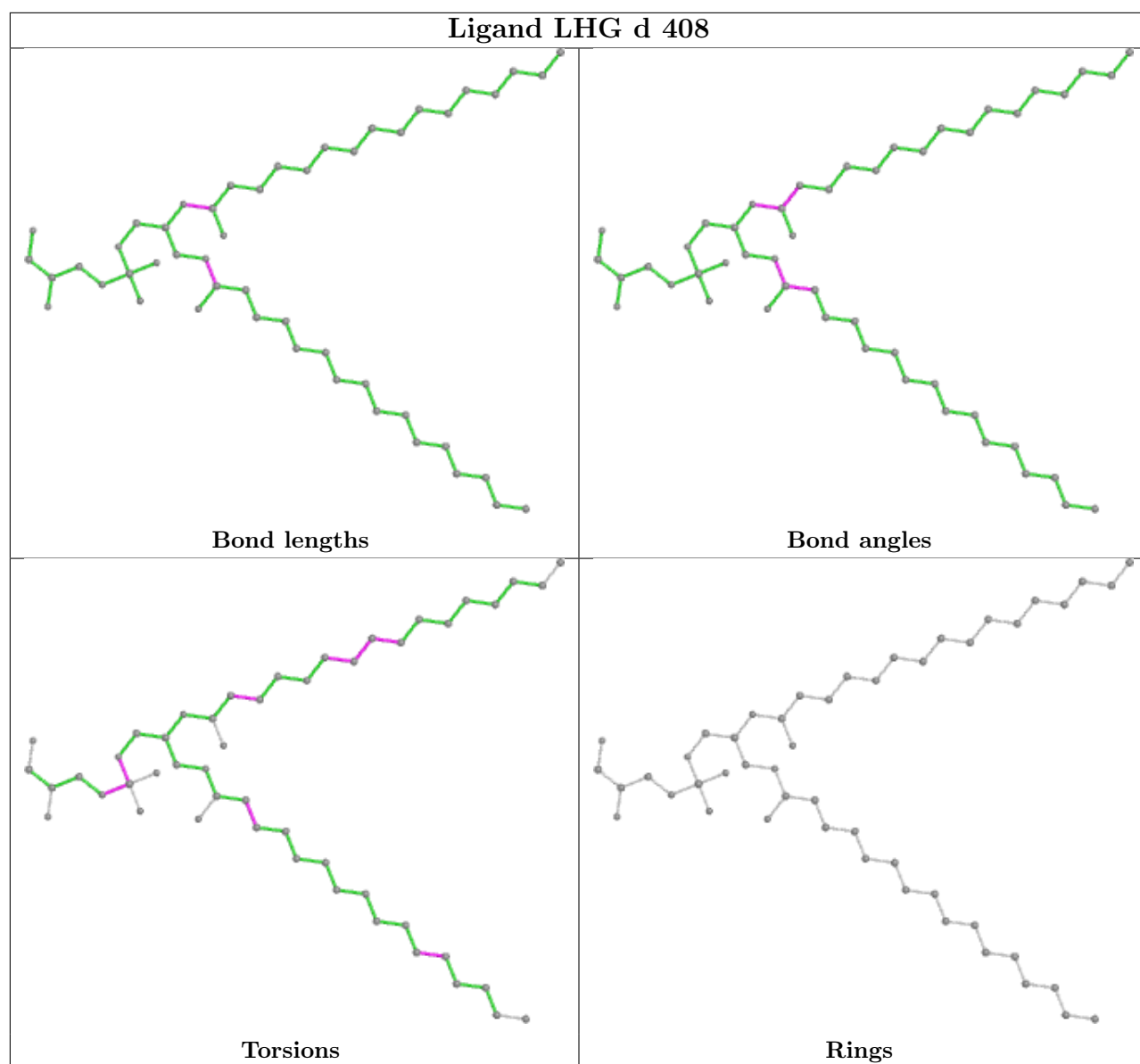




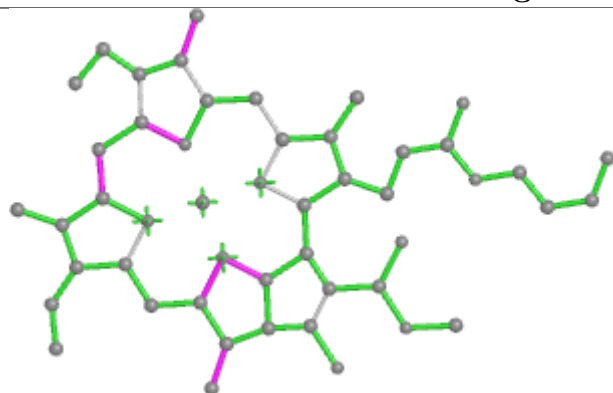
Ligand CHL s 605



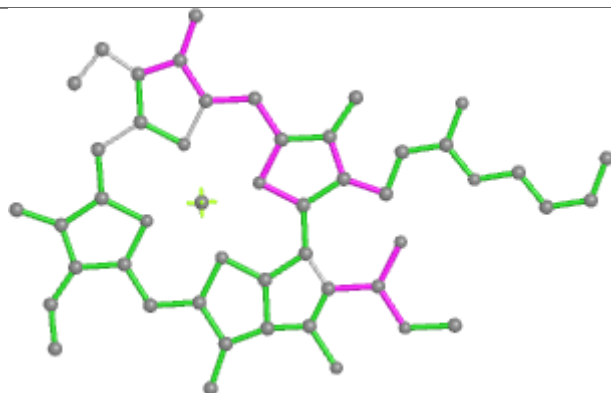




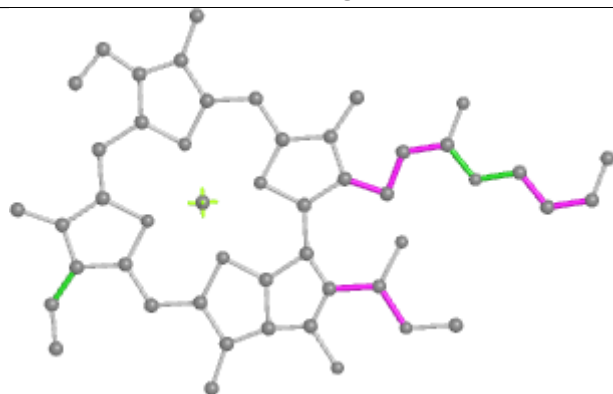
Ligand CLA R 302



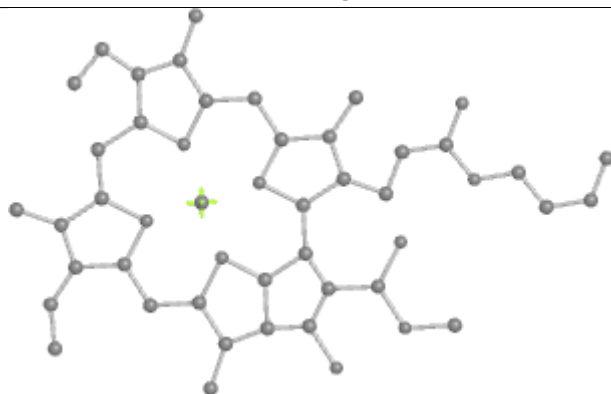
Bond lengths



Bond angles

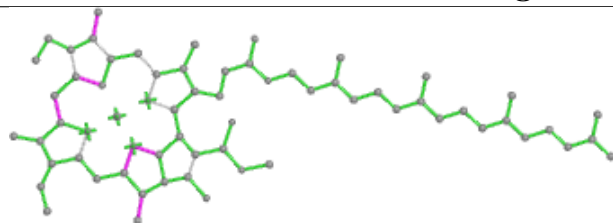


Torsions

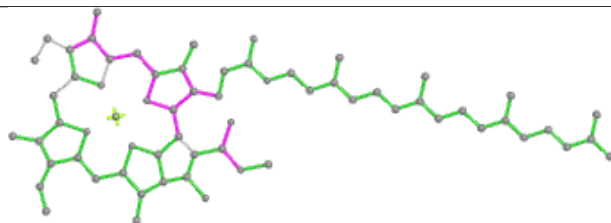


Rings

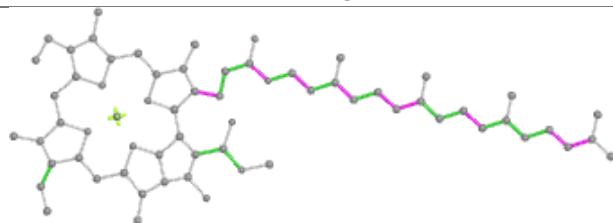
Ligand CLA B 602



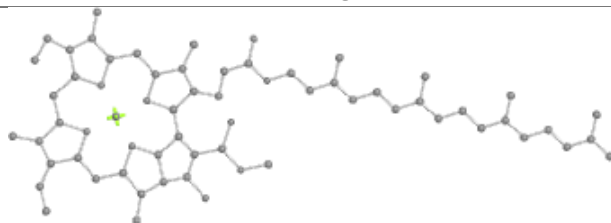
Bond lengths



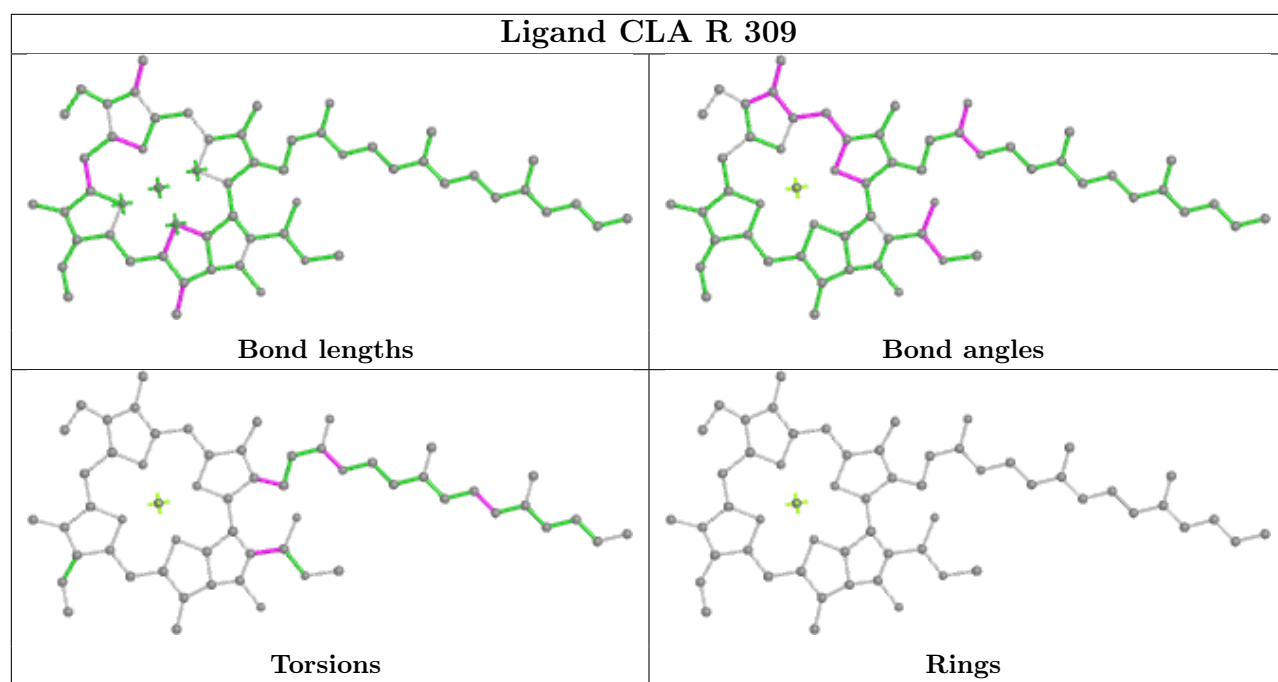
Bond angles

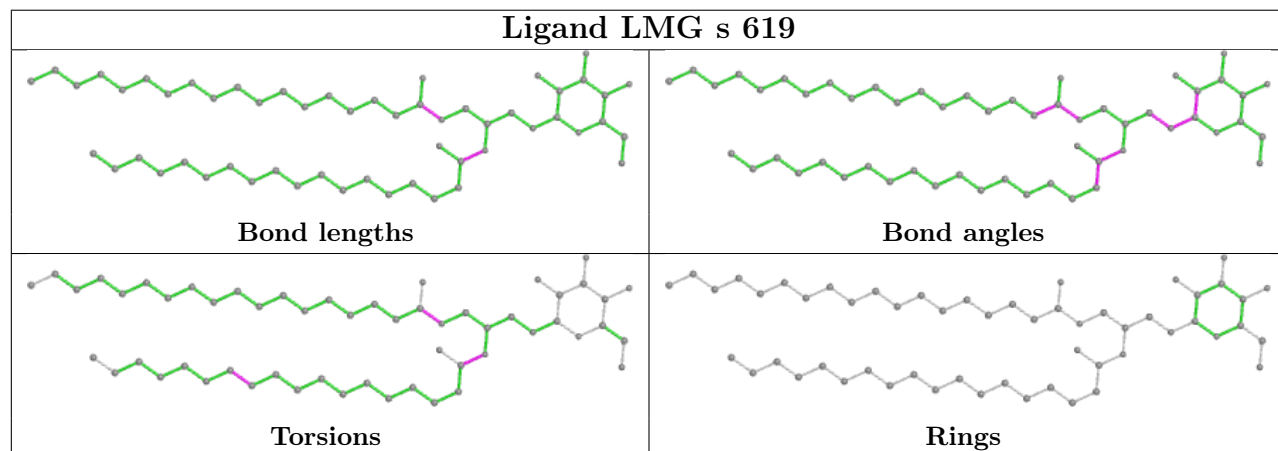
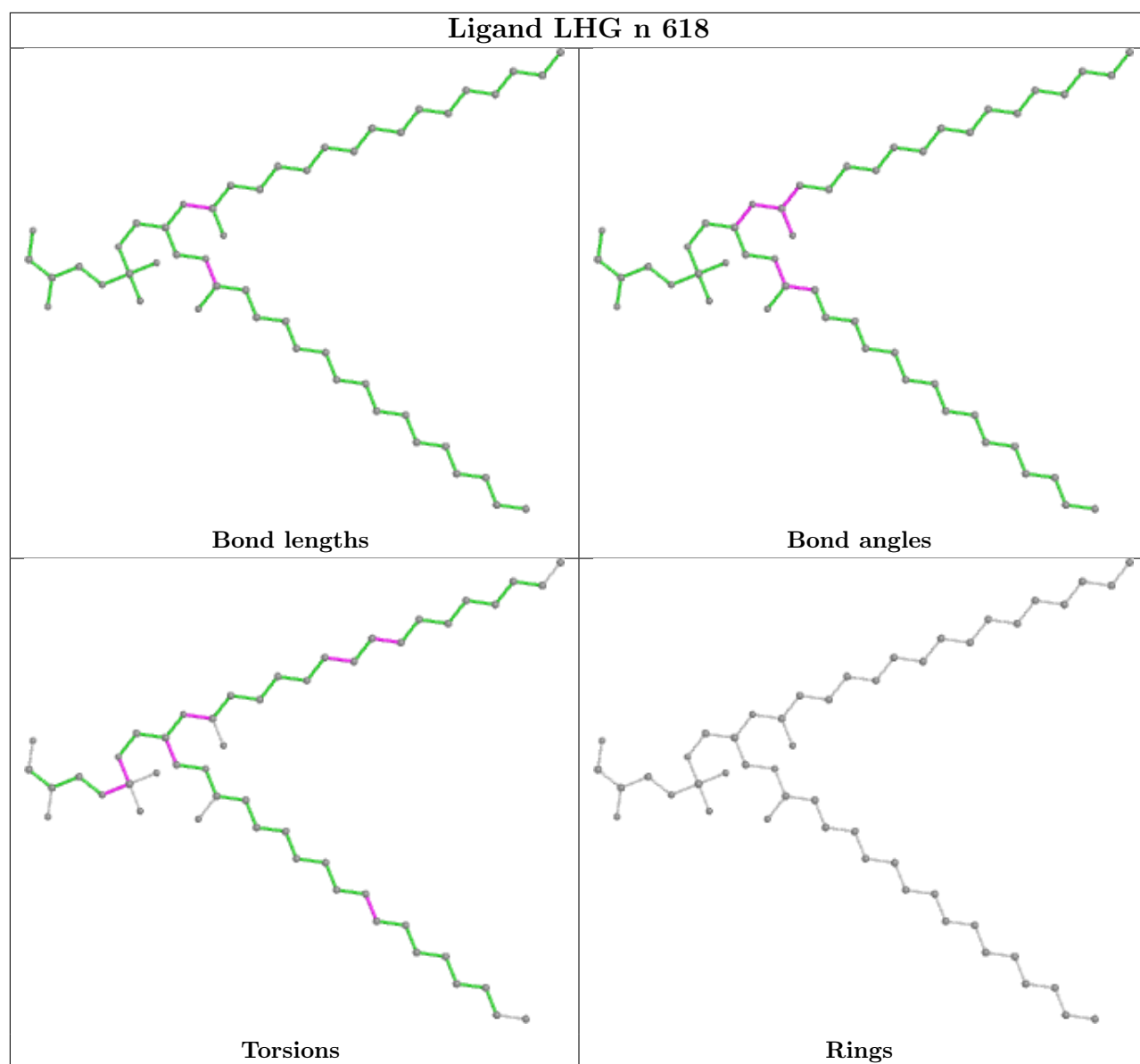


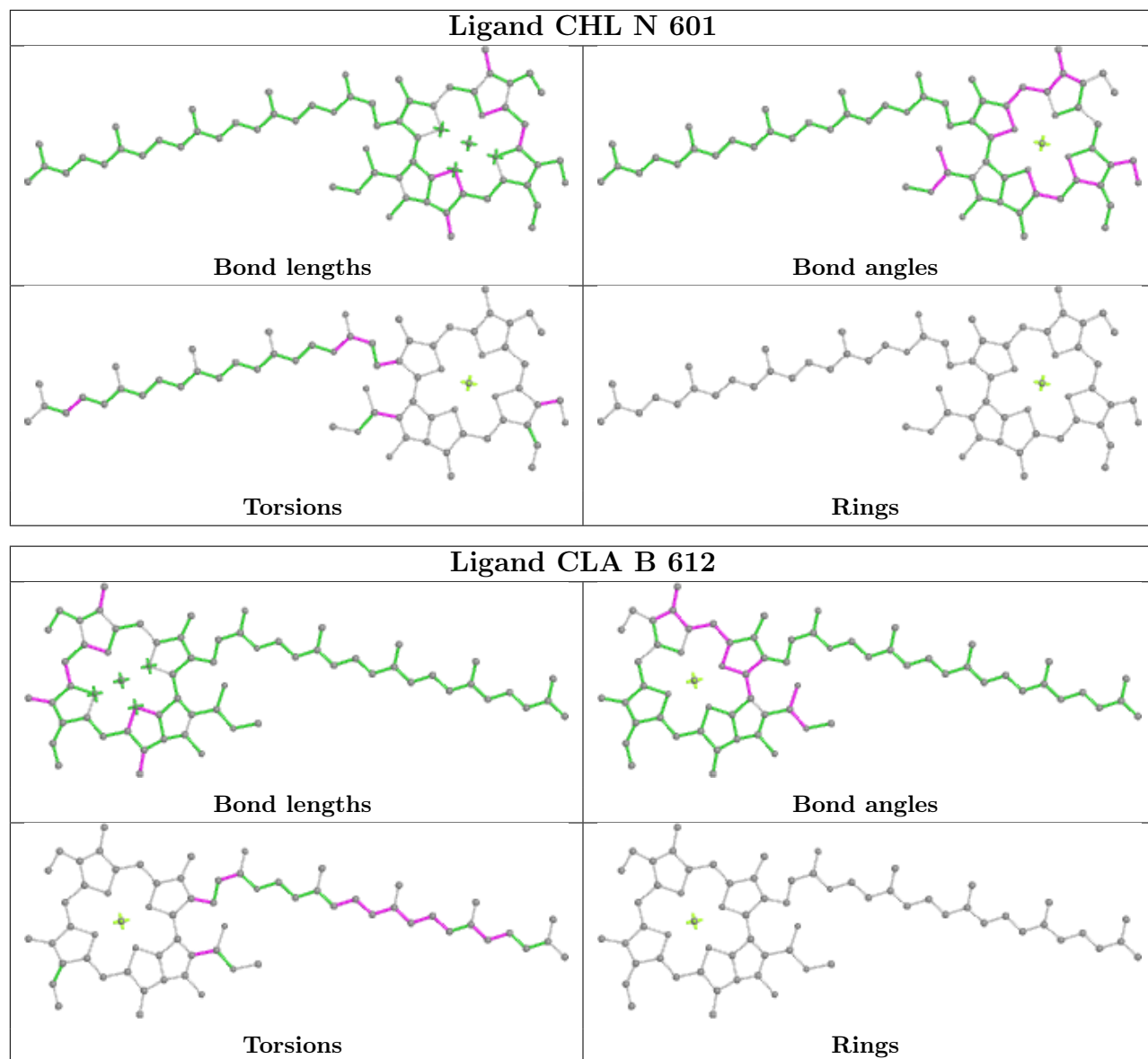
Torsions



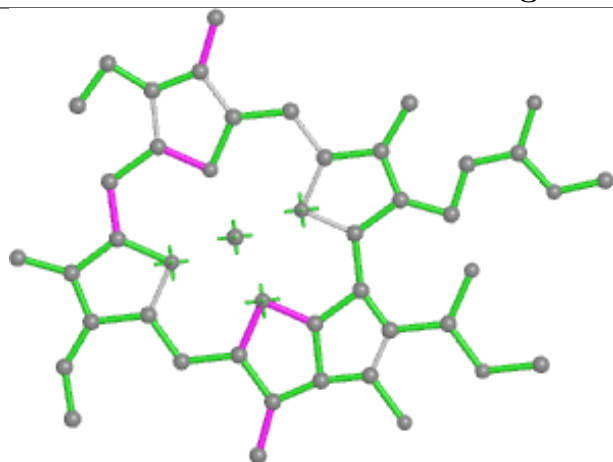
Rings



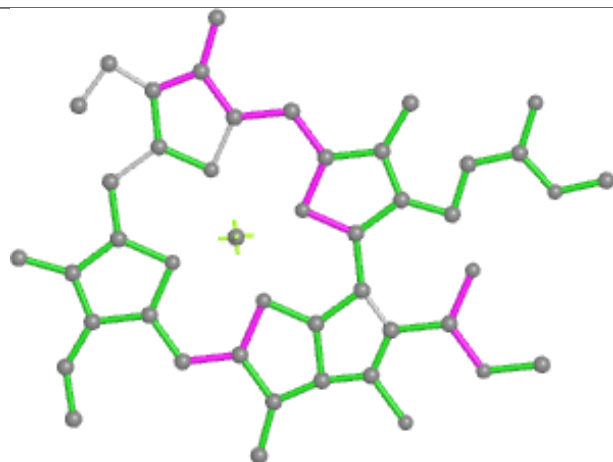




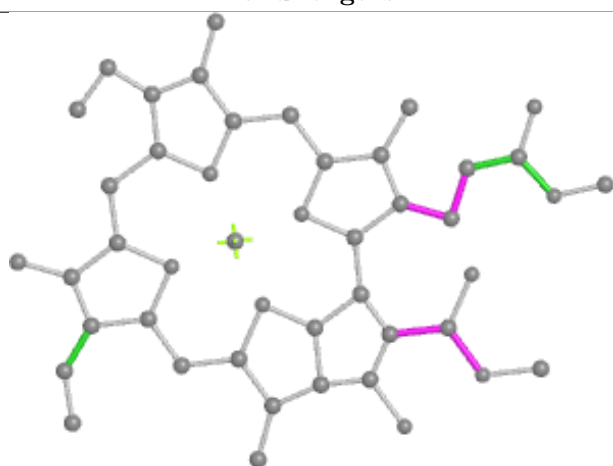
Ligand CLA s 602



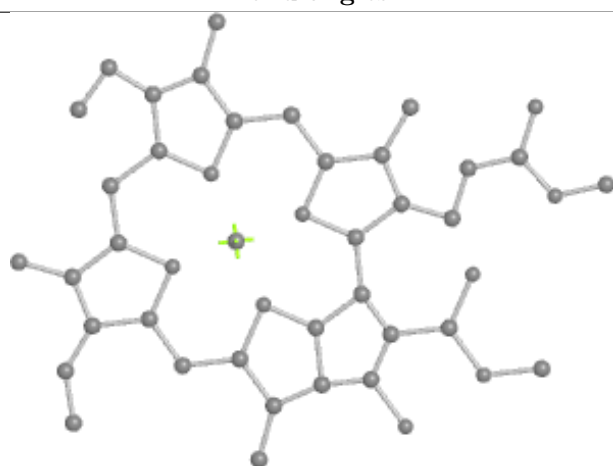
Bond lengths



Bond angles

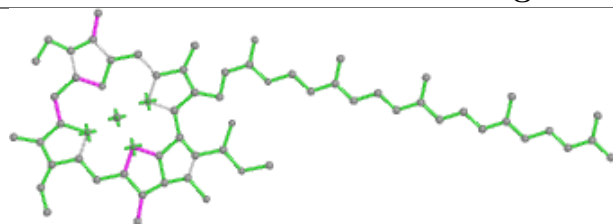


Torsions

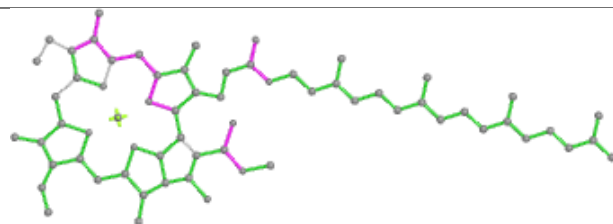


Rings

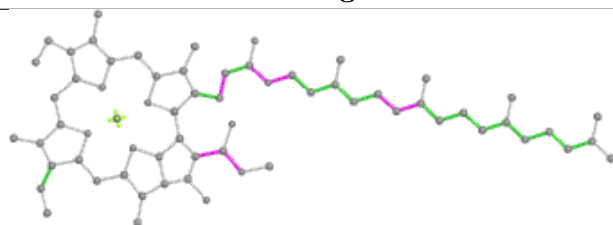
Ligand CLA Y 314



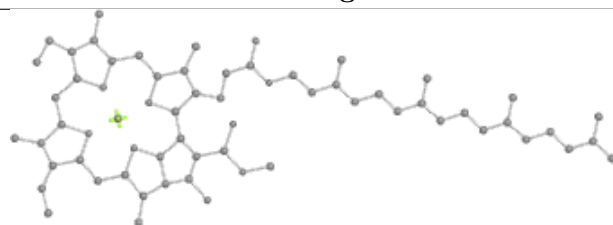
Bond lengths



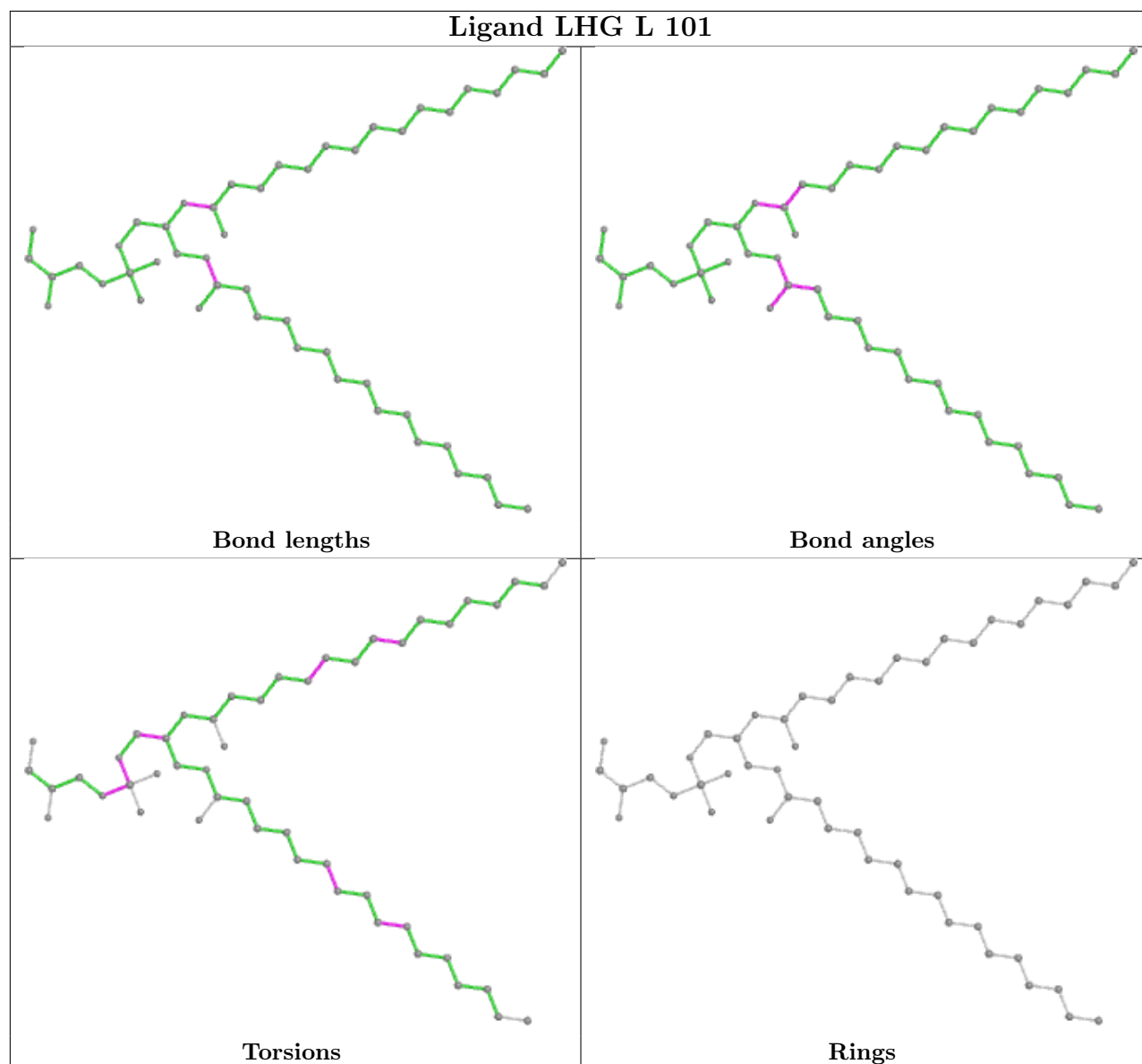
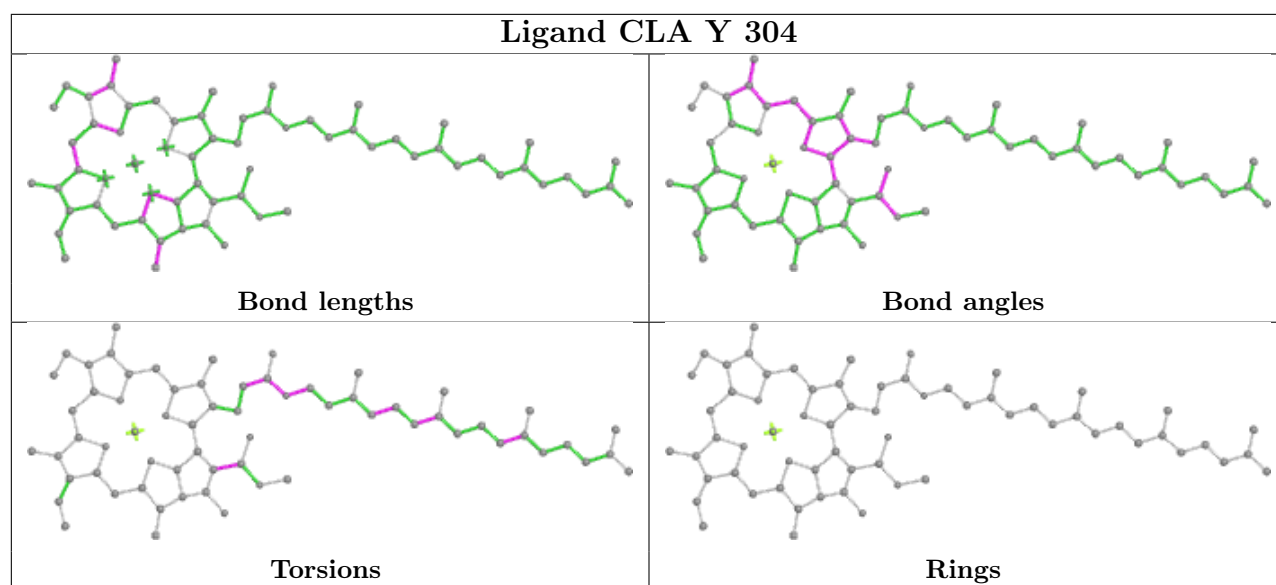
Bond angles



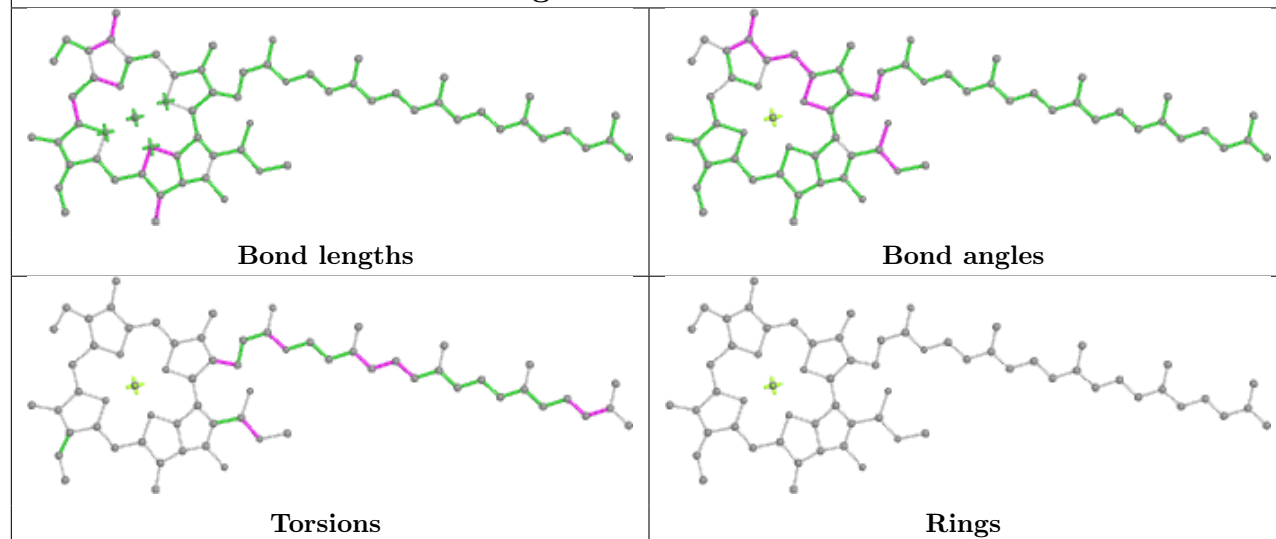
Torsions



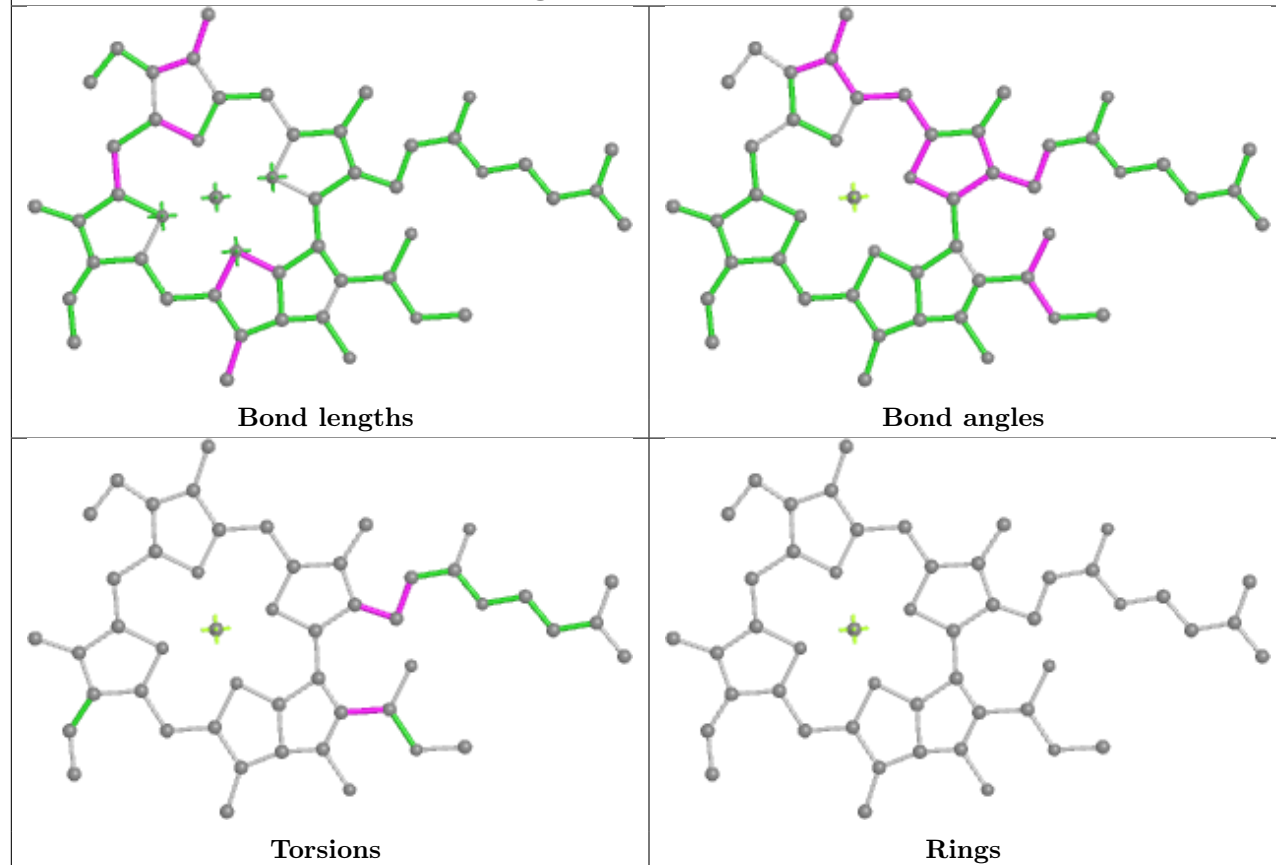
Rings

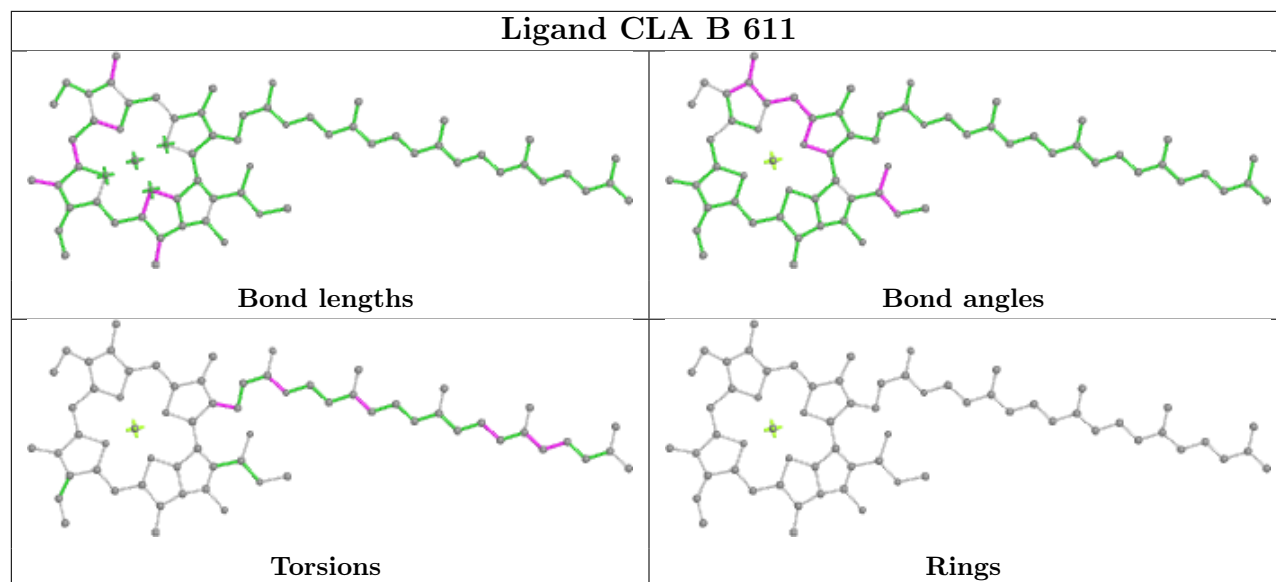
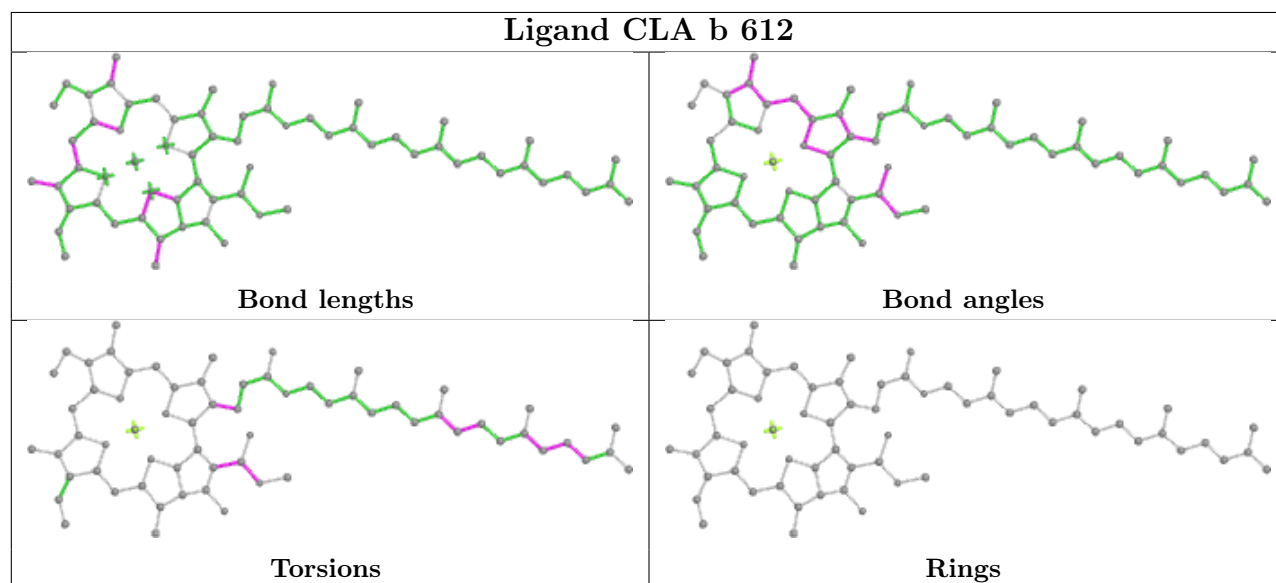


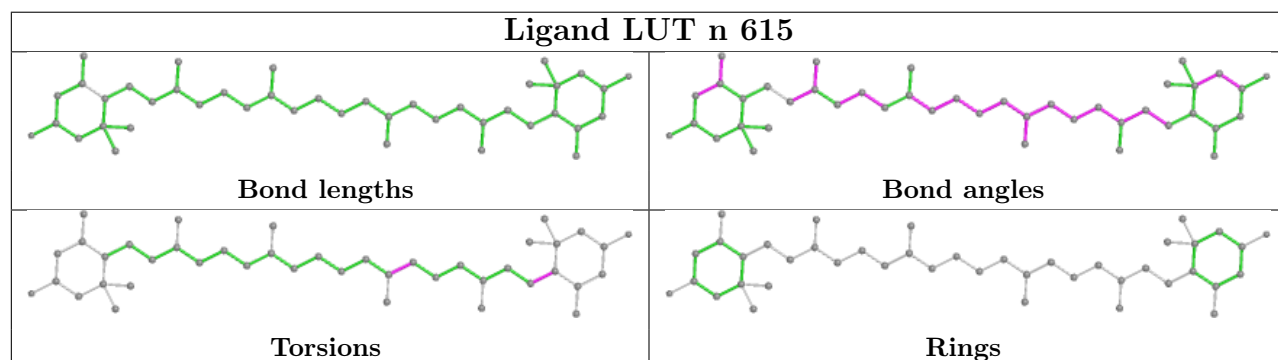
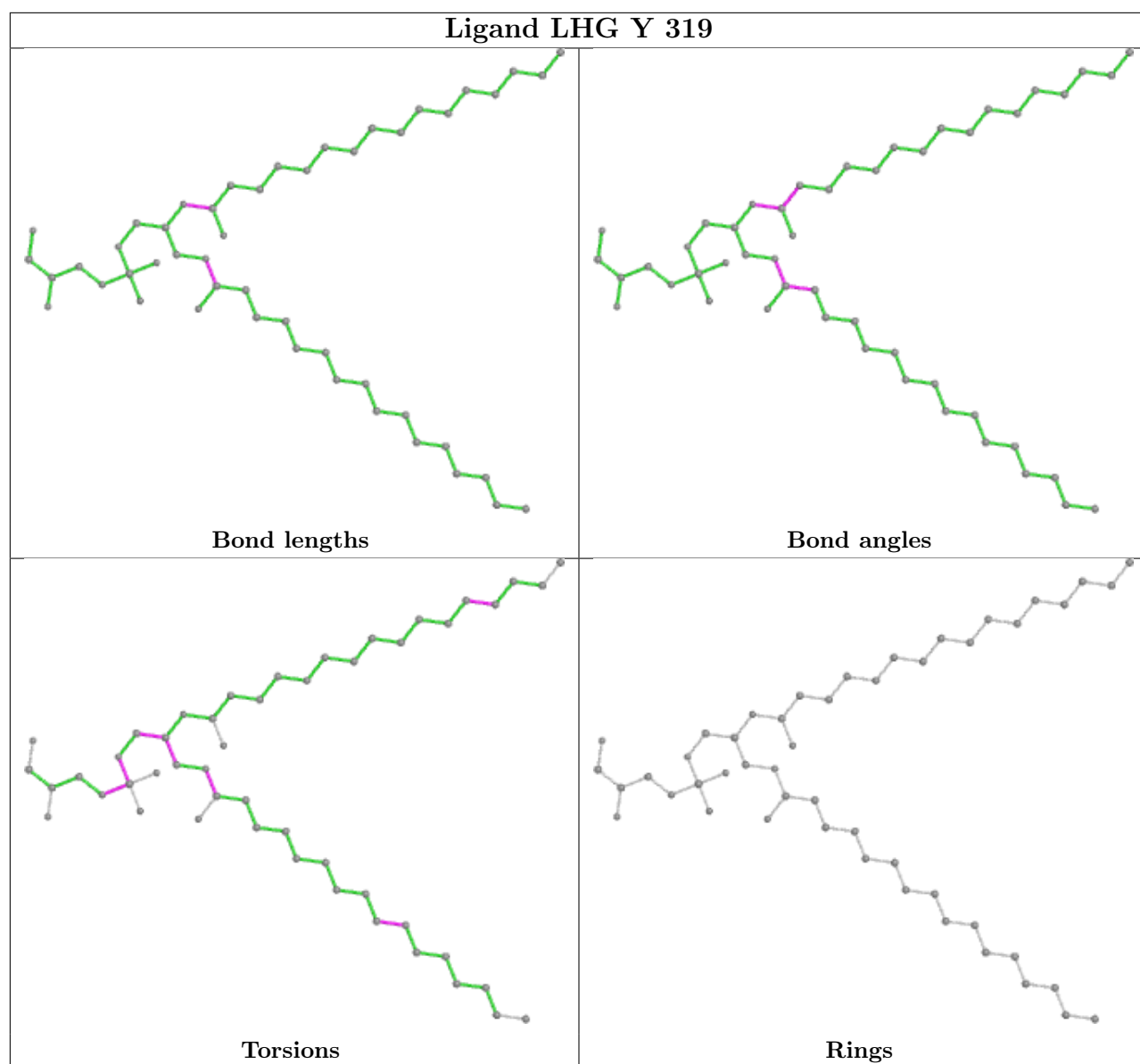
Ligand CLA B 608

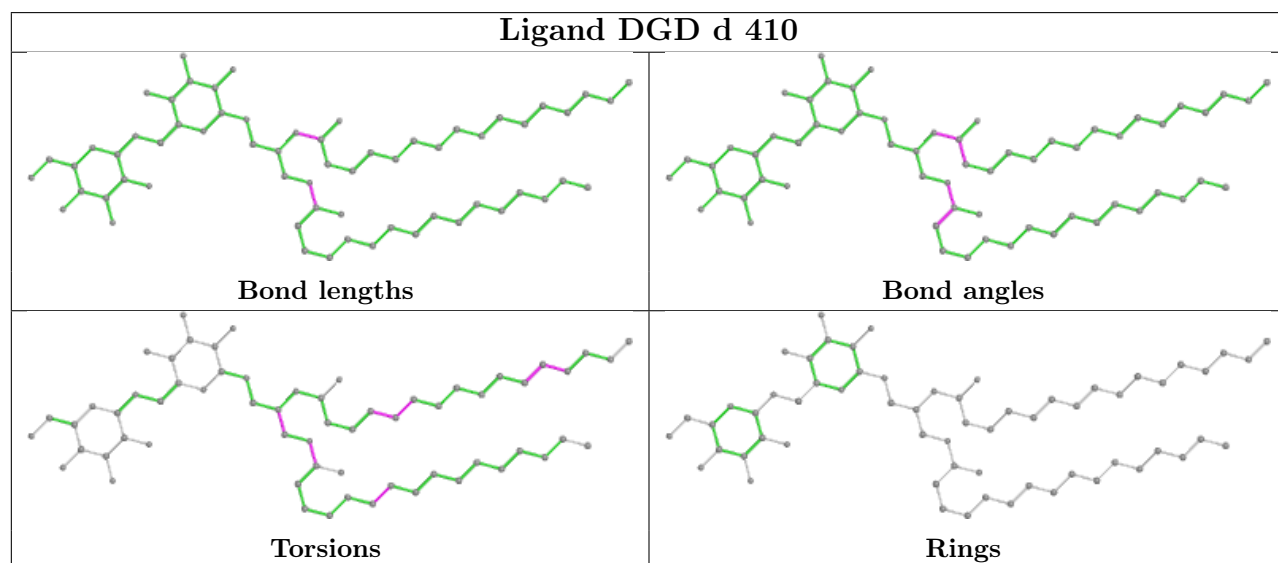
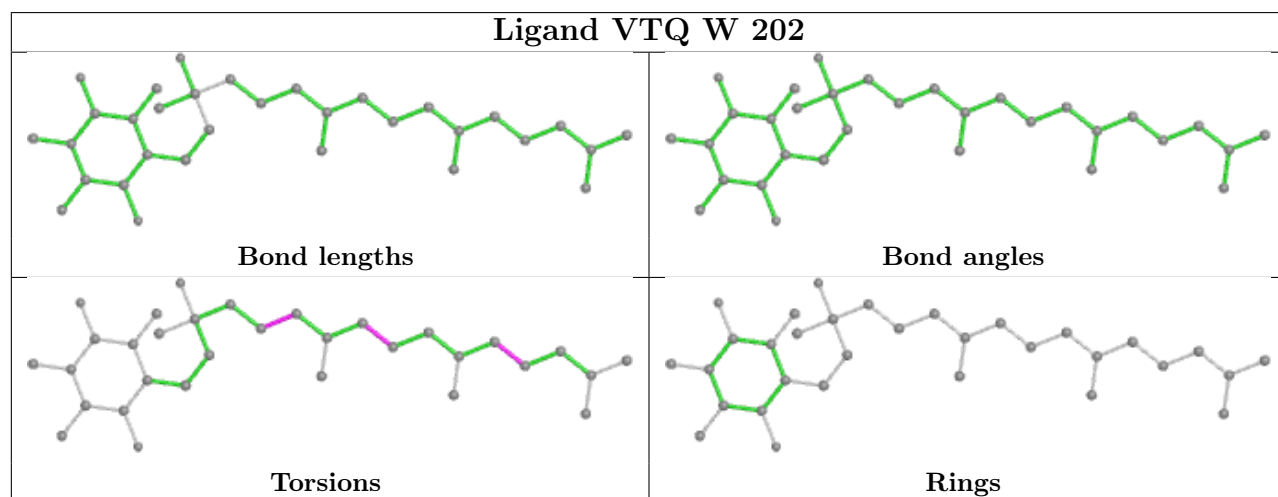
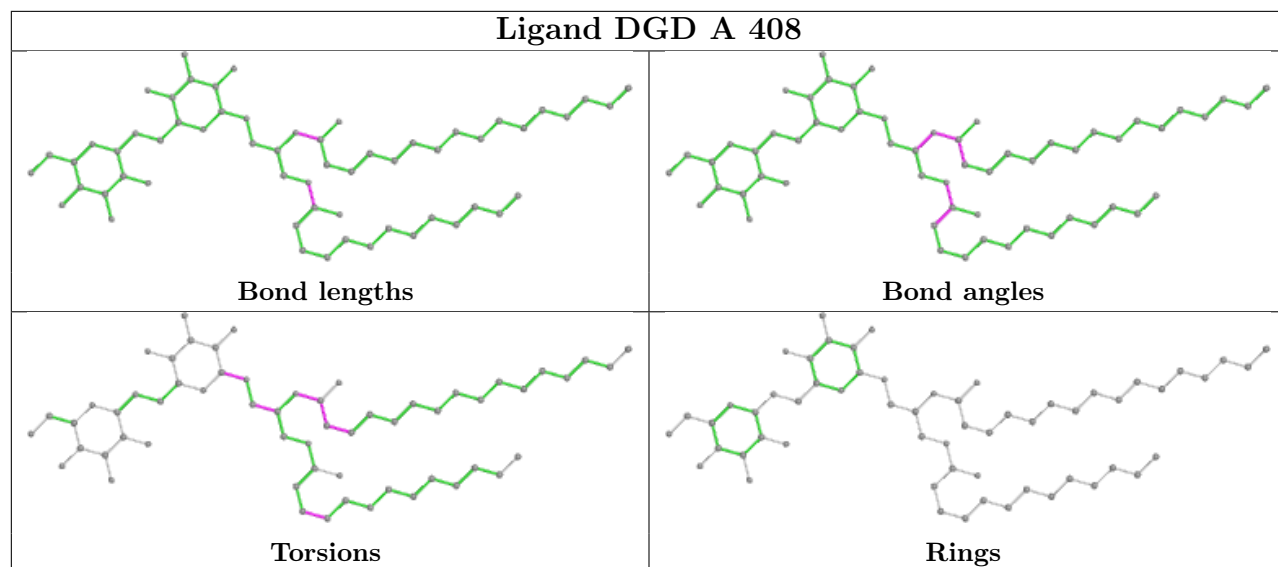


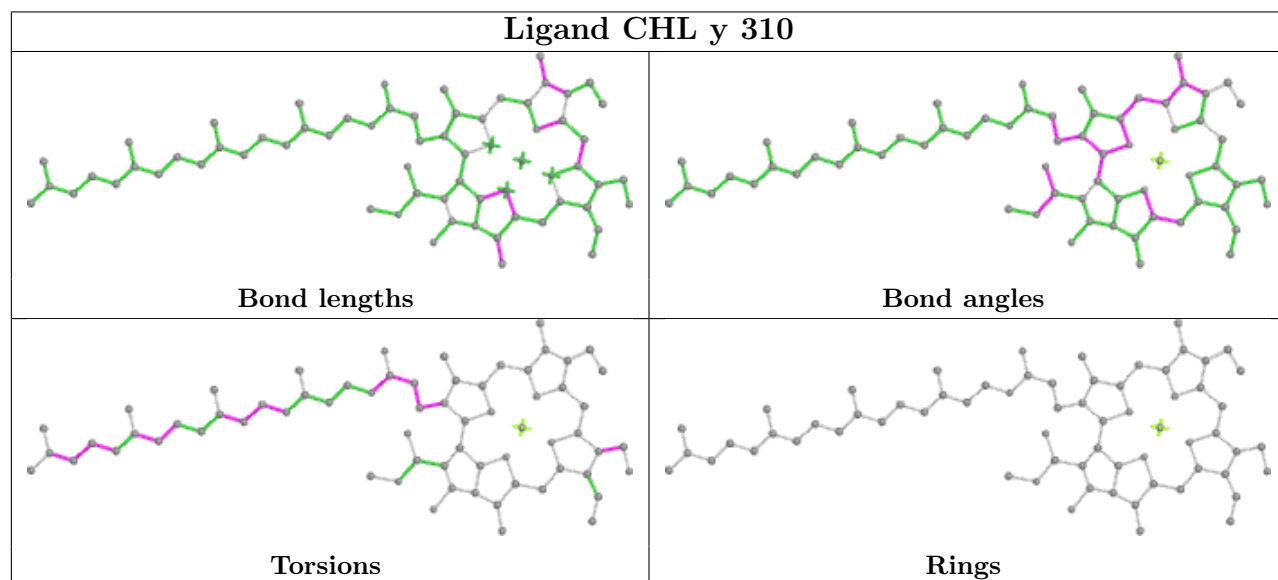
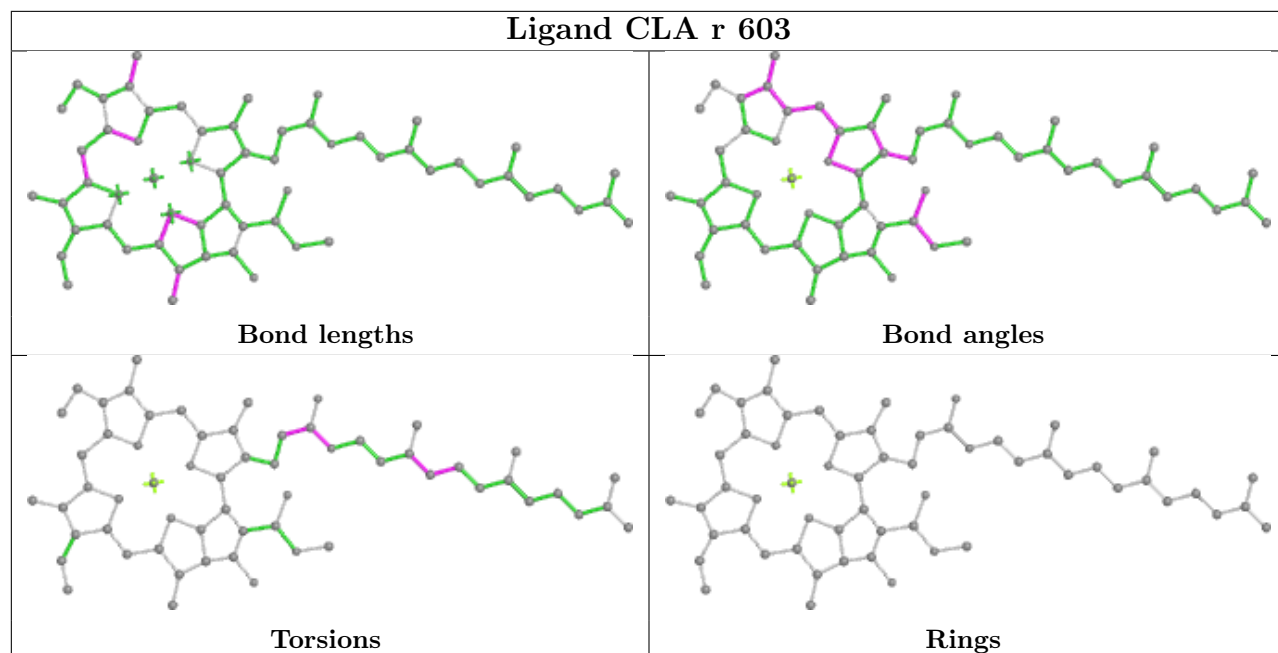
Ligand CLA A 402



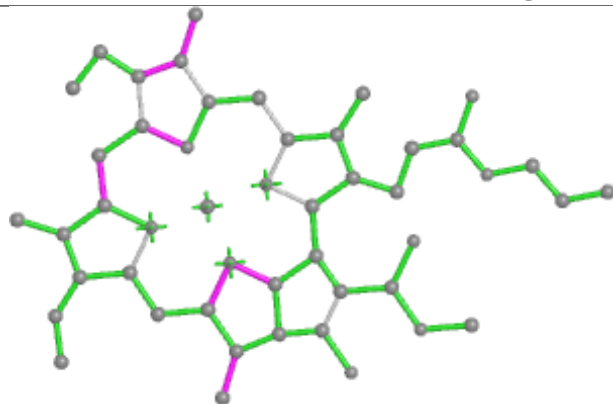
Ligand CLA B 611**Ligand CLA b 612**



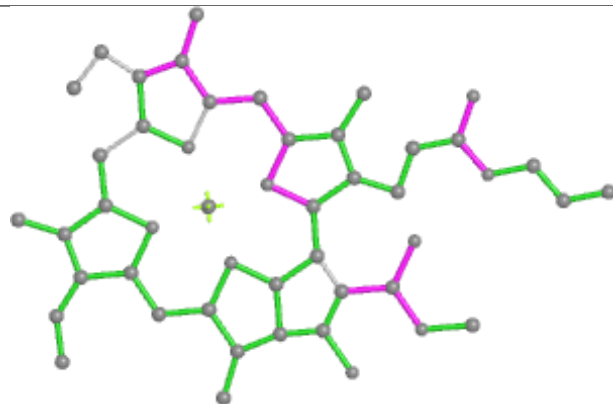




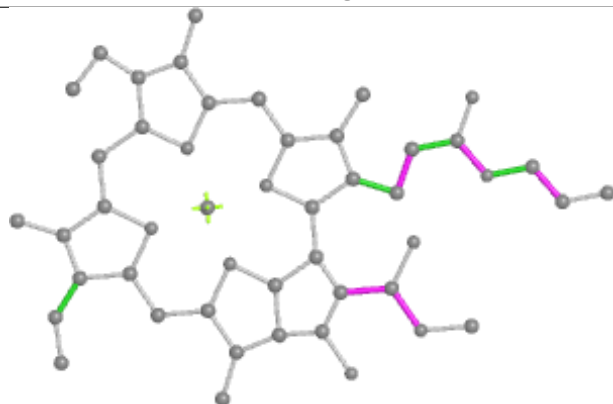
Ligand CLA r 604



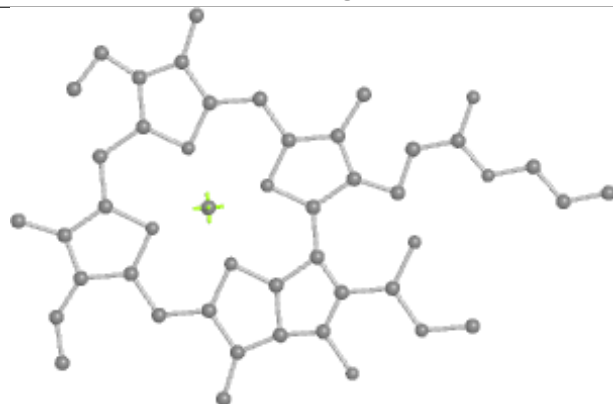
Bond lengths



Bond angles

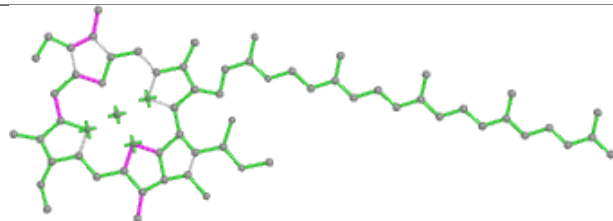


Torsions

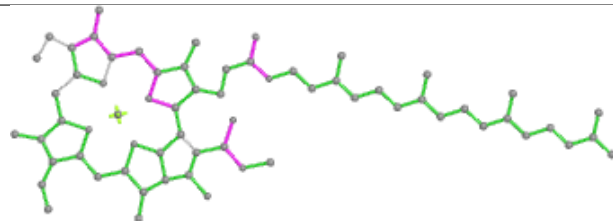


Rings

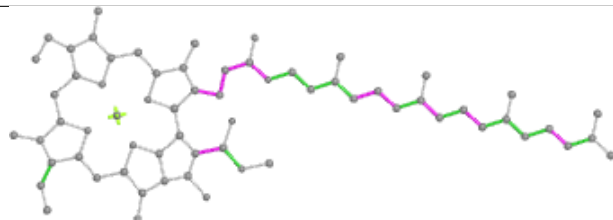
Ligand CLA C 502



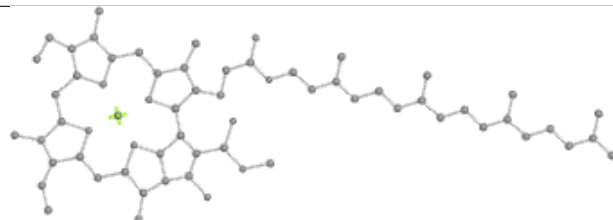
Bond lengths



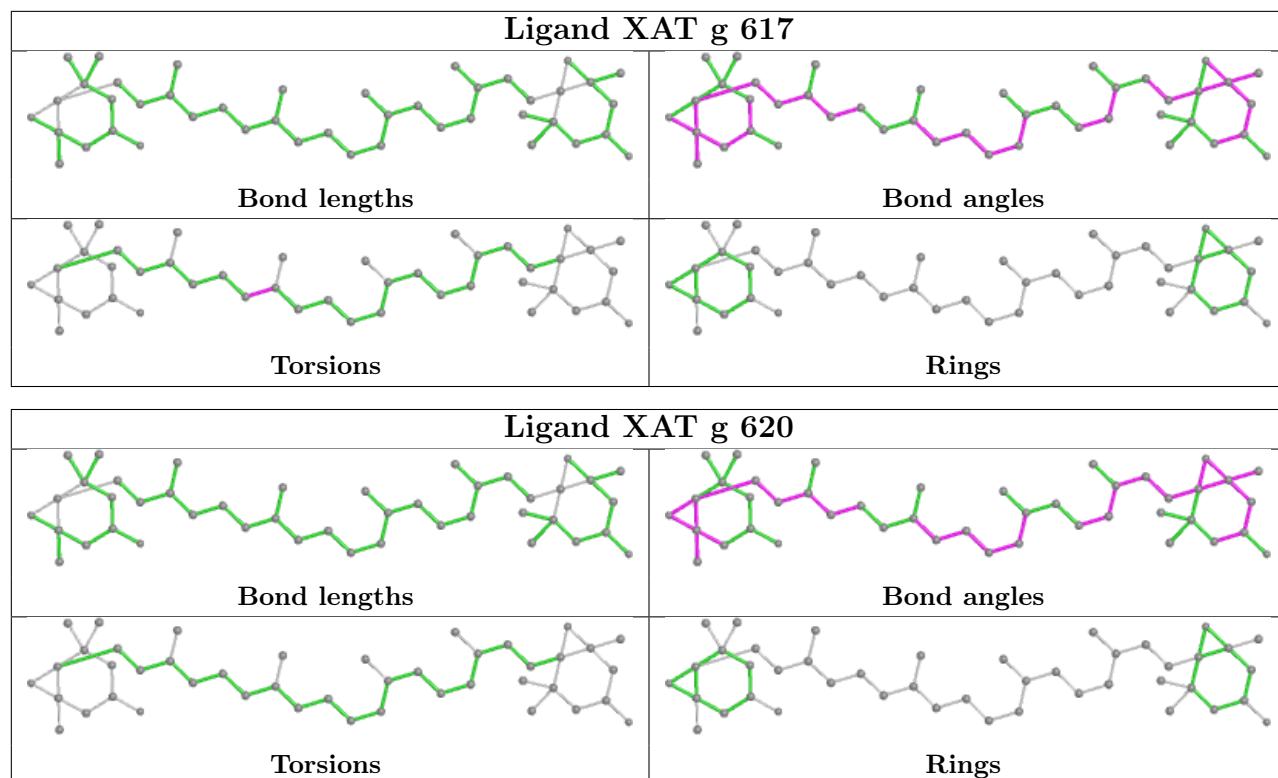
Bond angles



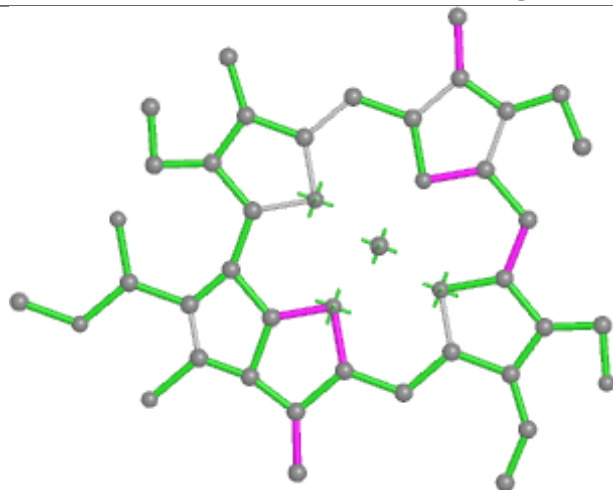
Torsions



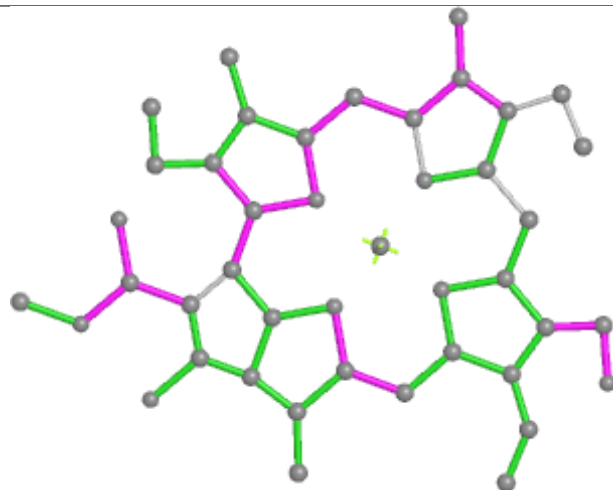
Rings



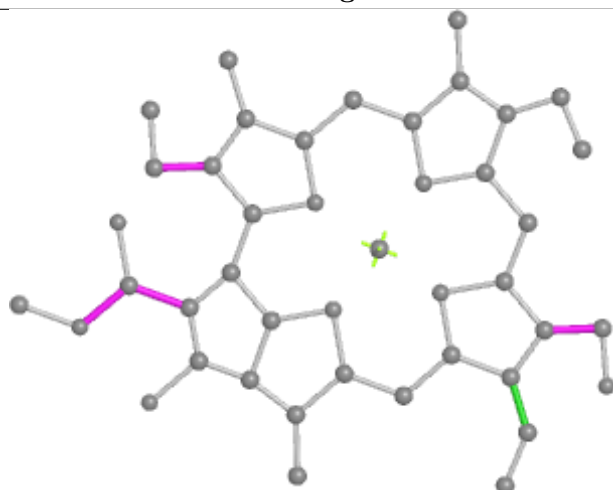
Ligand CHL G 606



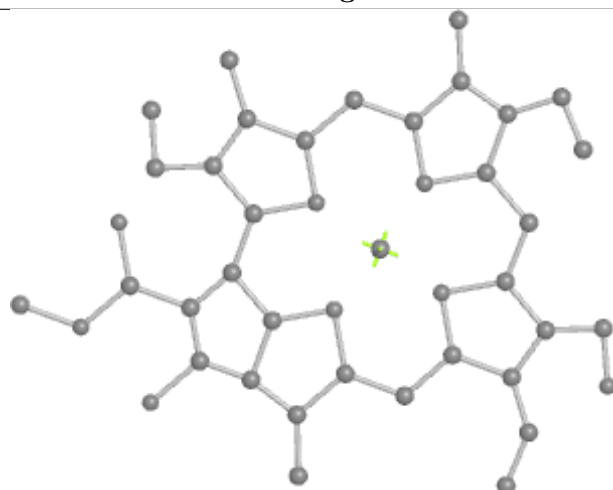
Bond lengths



Bond angles

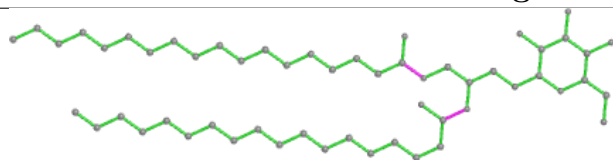


Torsions

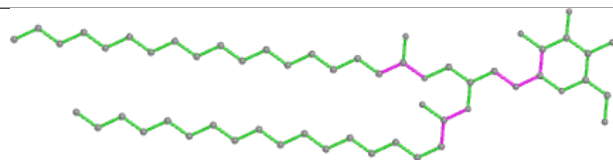


Rings

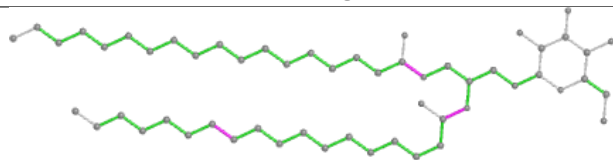
Ligand LMG S 301



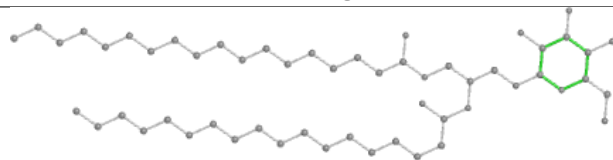
Bond lengths



Bond angles

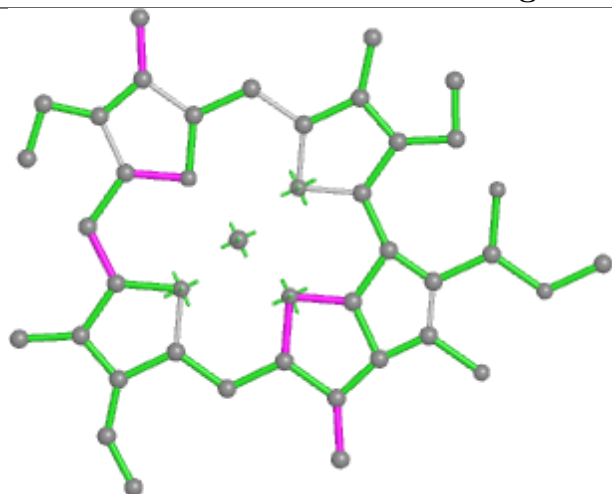


Torsions

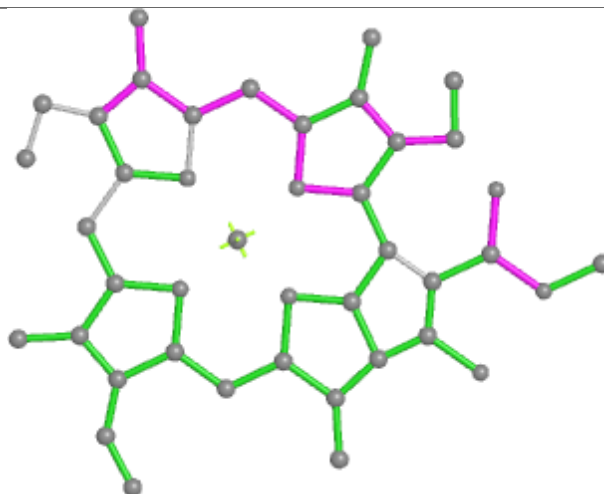


Rings

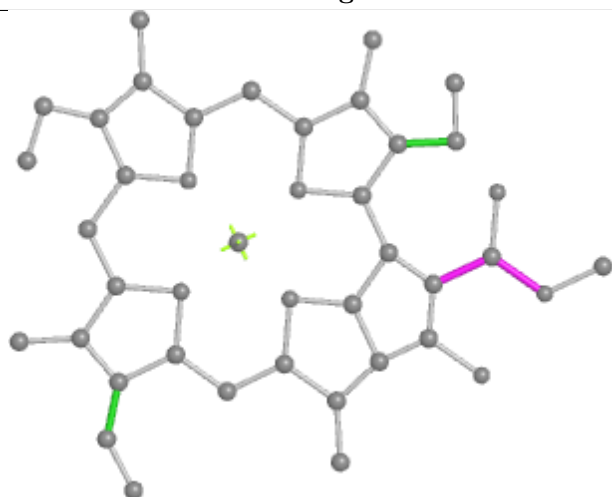
Ligand CLA s 610



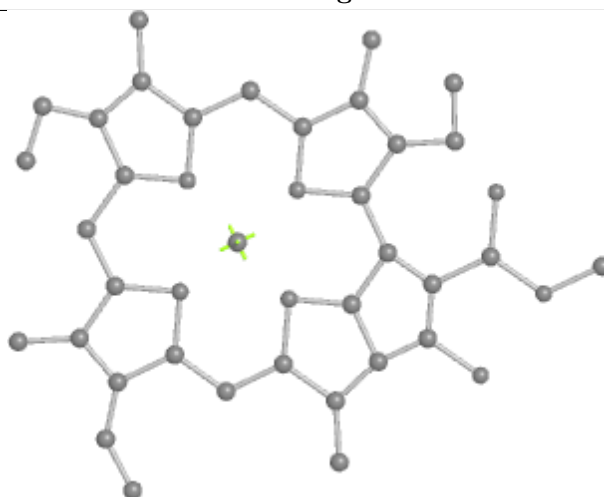
Bond lengths



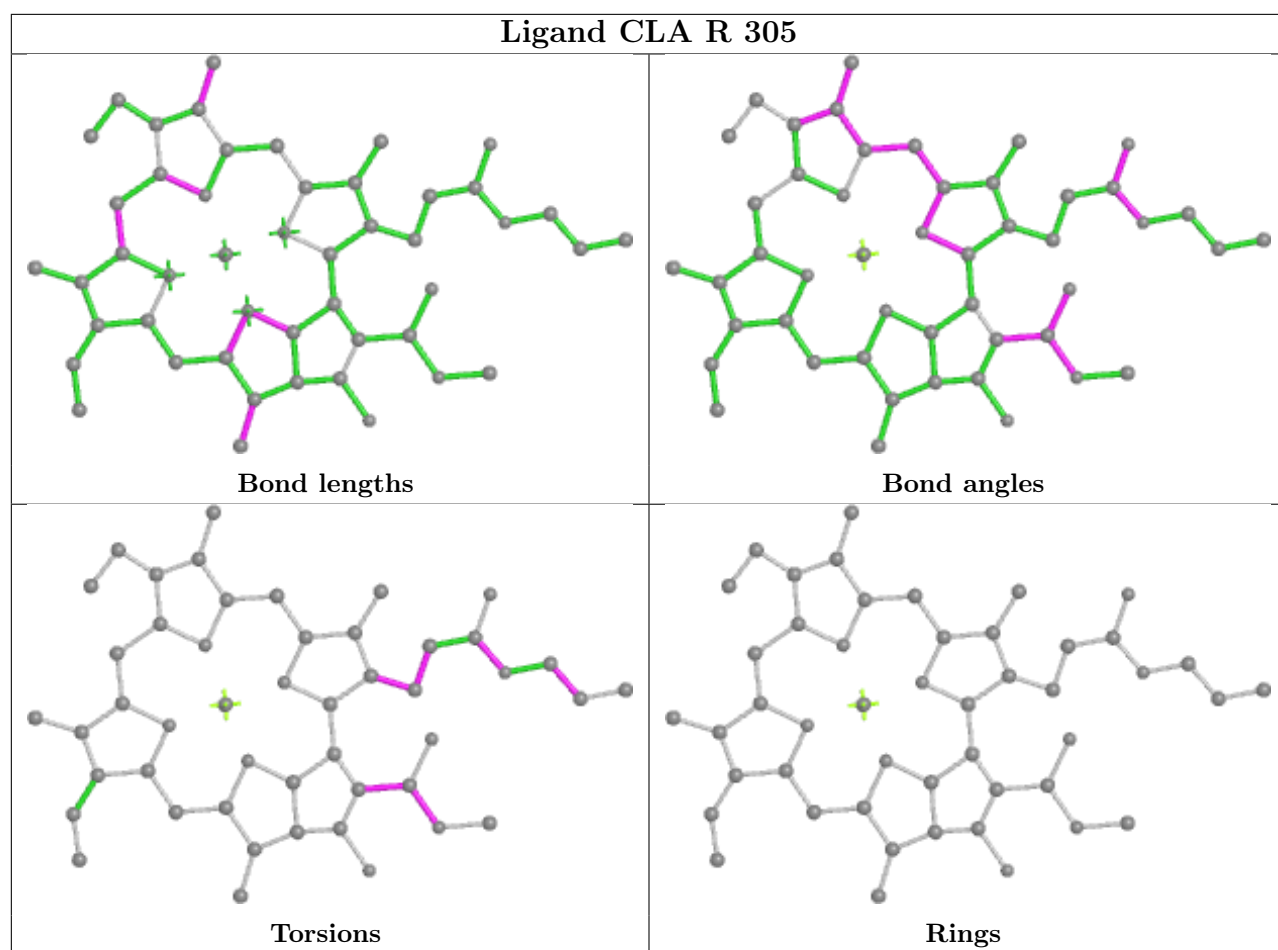
Bond angles

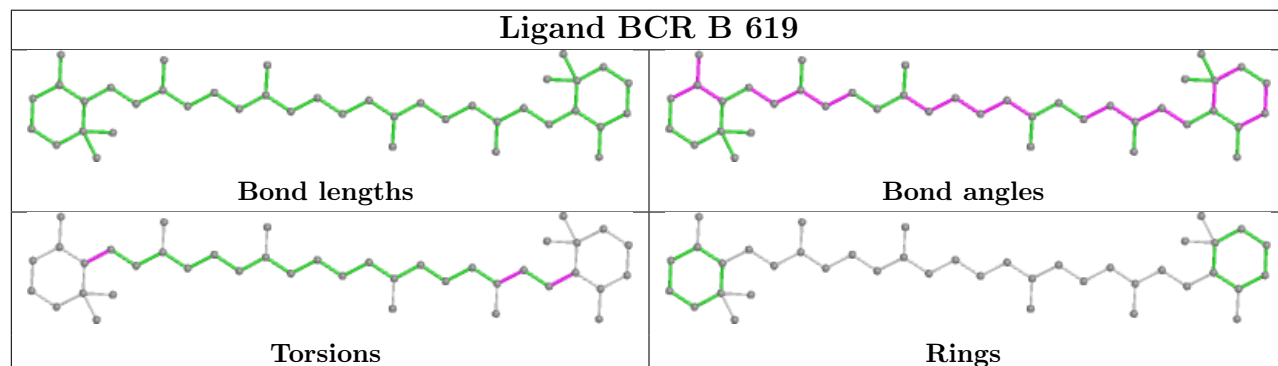
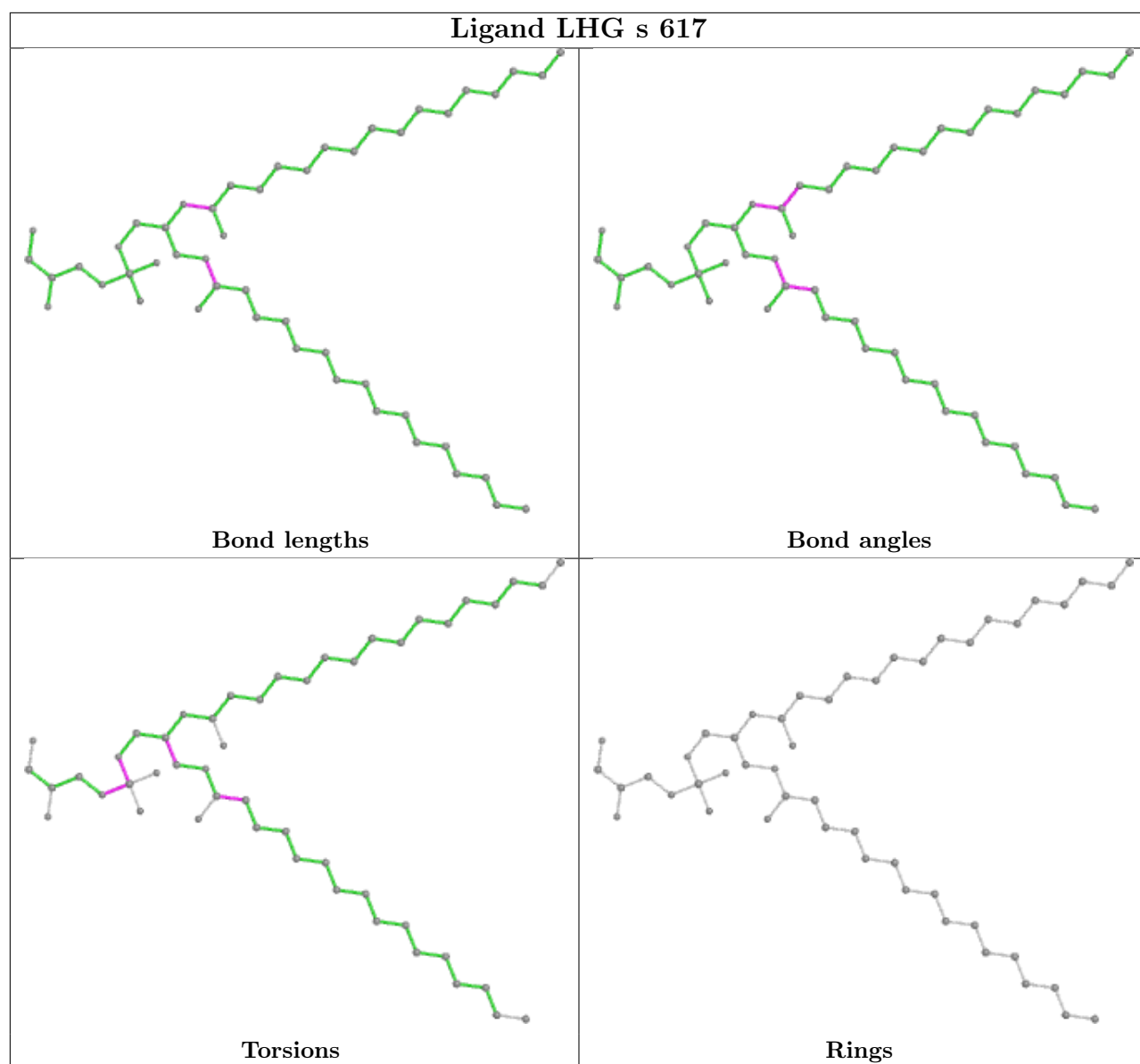


Torsions

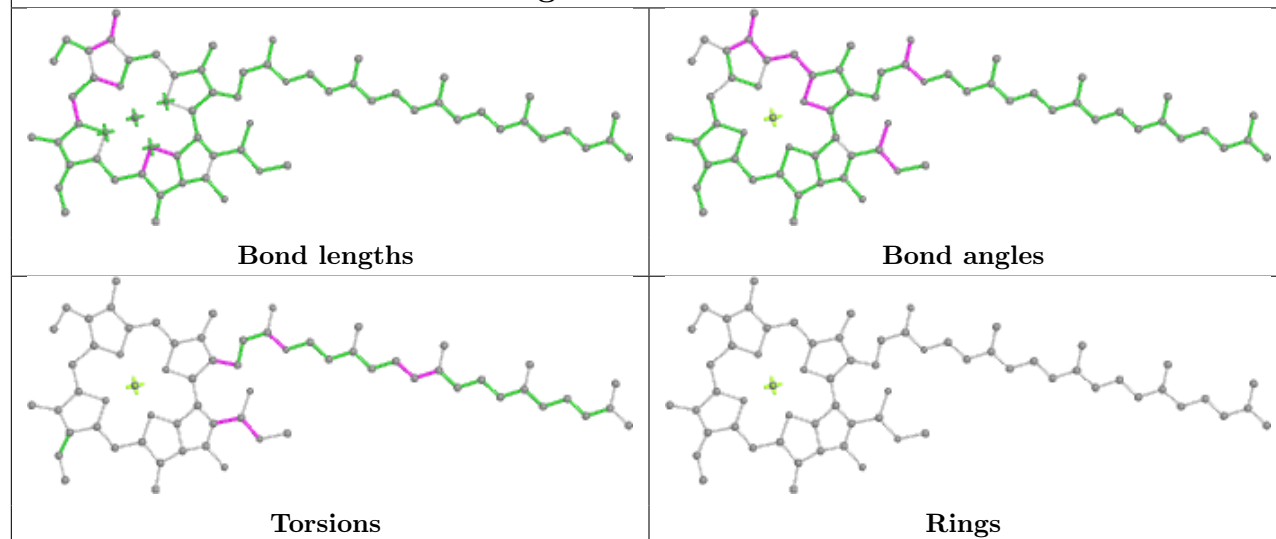


Rings

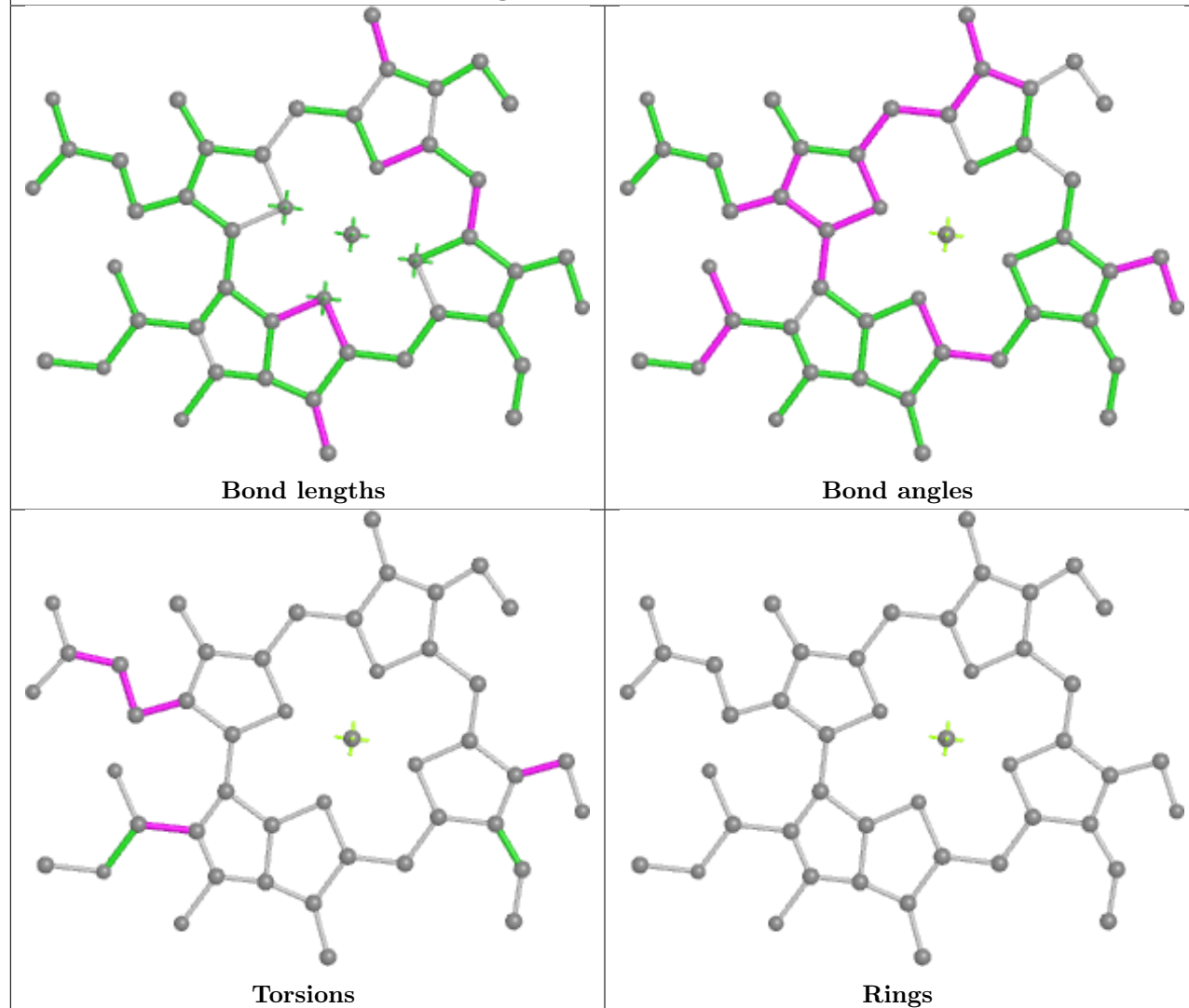


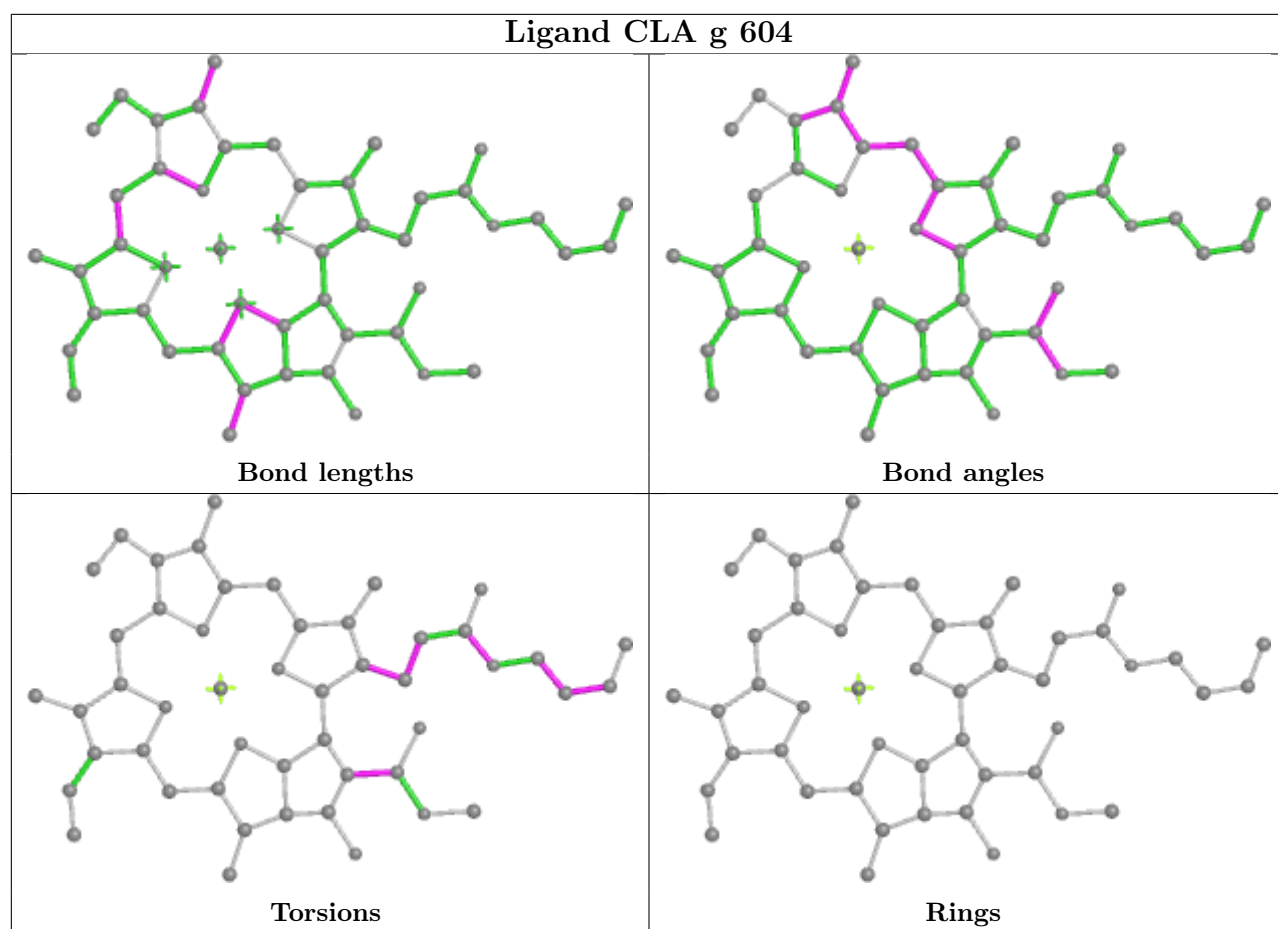


Ligand CLA r 611

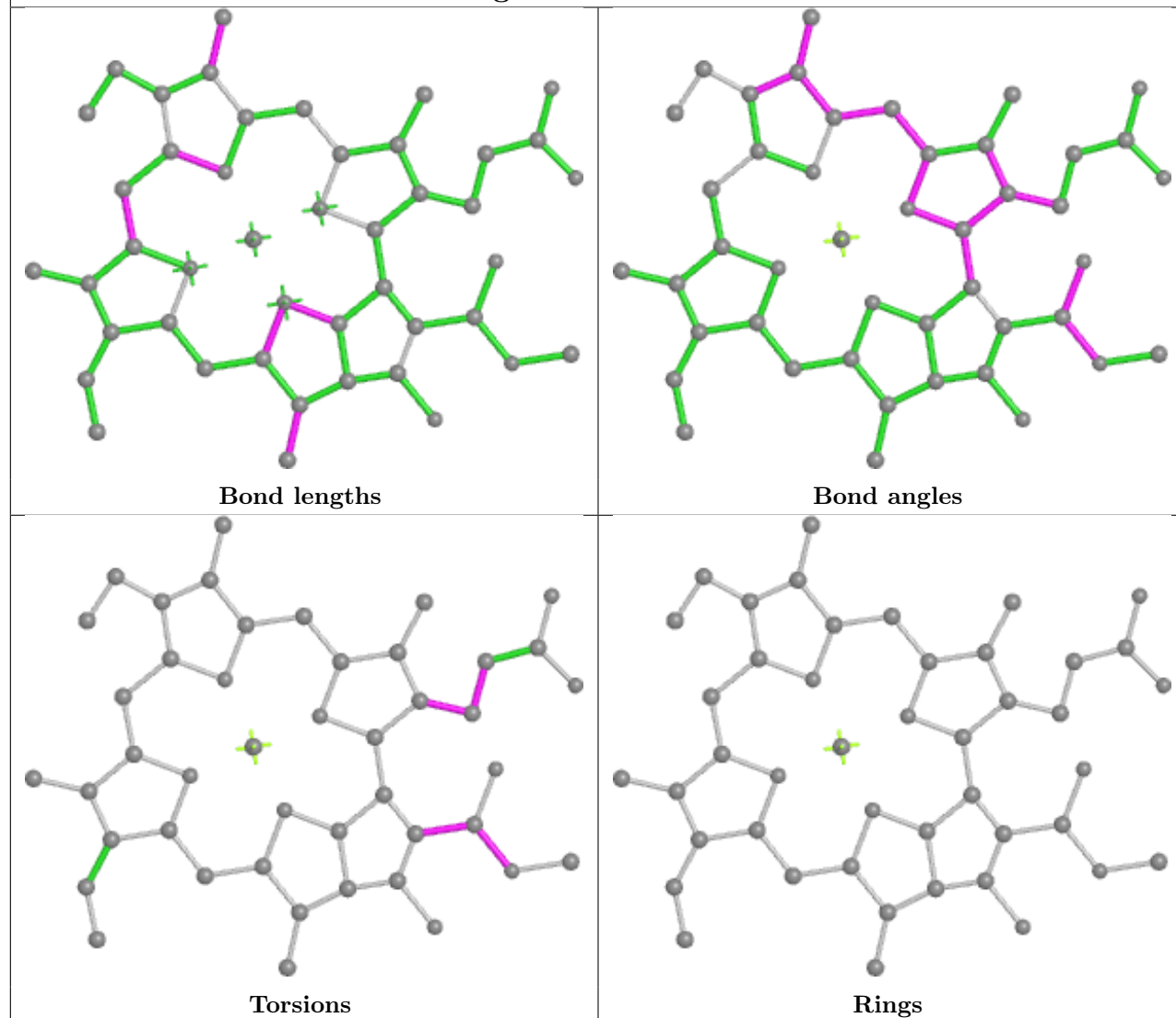


Ligand CHL N 607

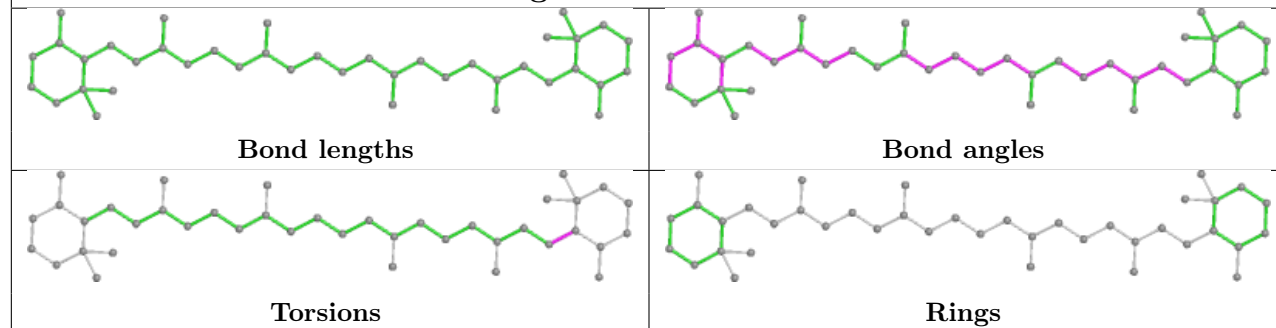


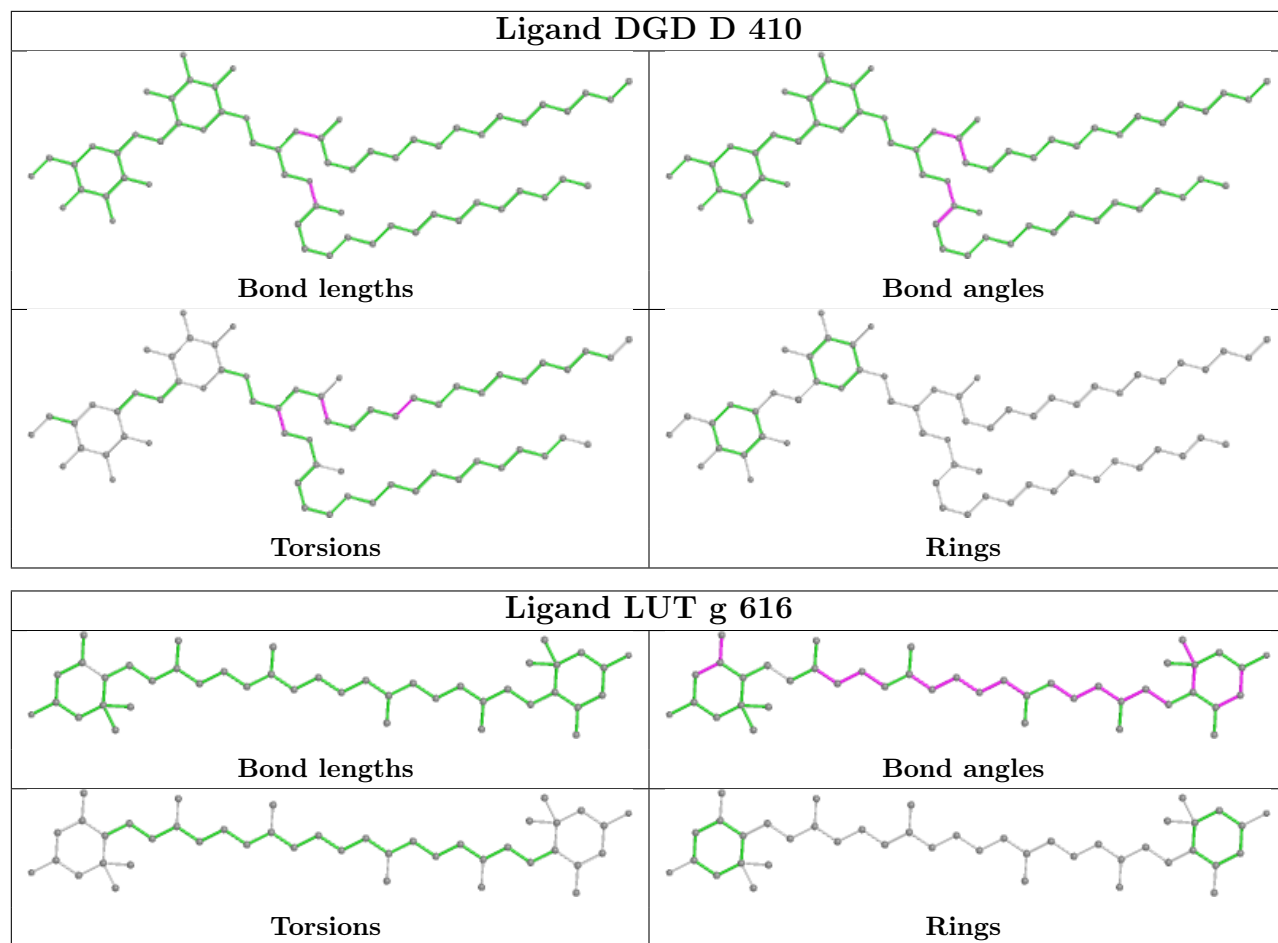


Ligand CLA S 312

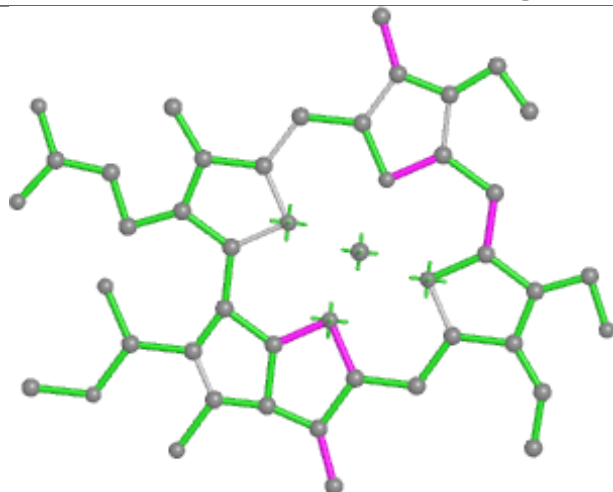


Ligand BCR A 405

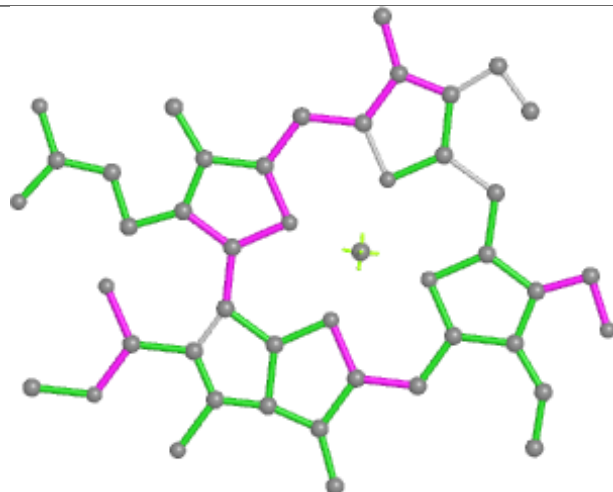




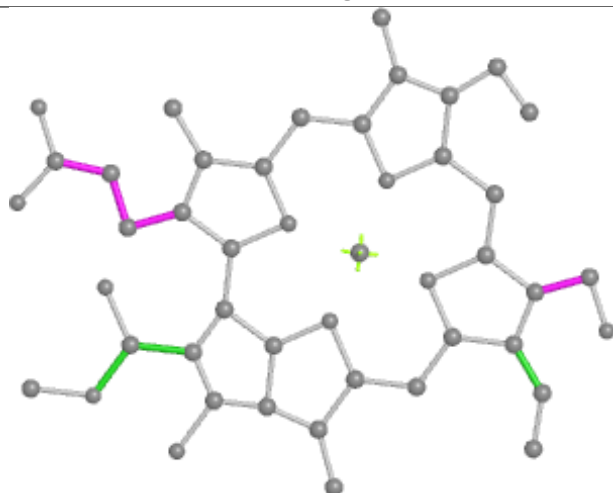
Ligand CHL n 606



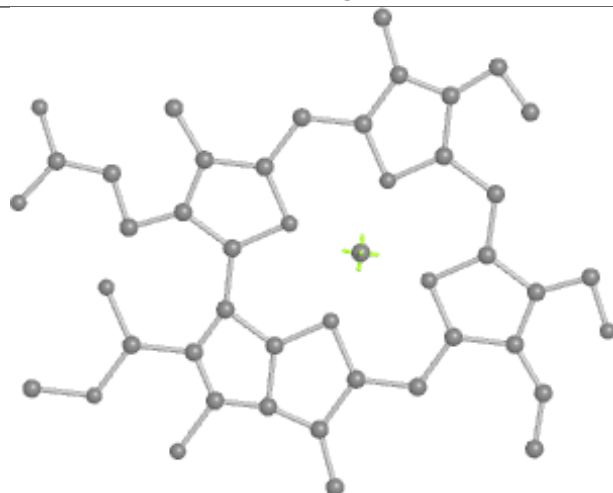
Bond lengths



Bond angles

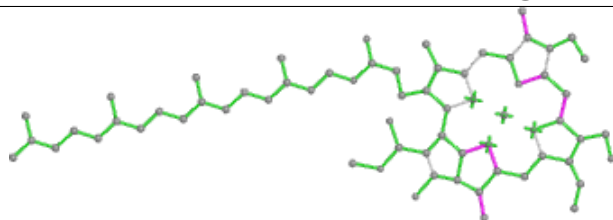


Torsions

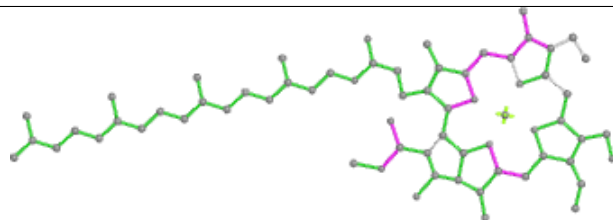


Rings

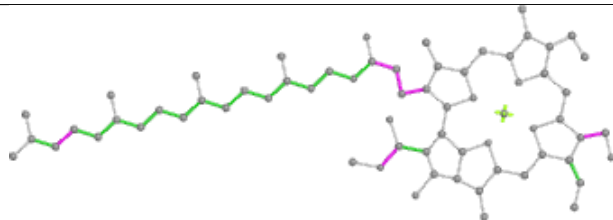
Ligand CHL n 608



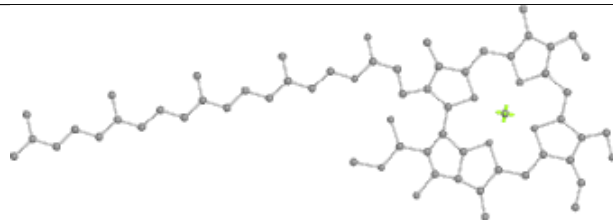
Bond lengths



Bond angles

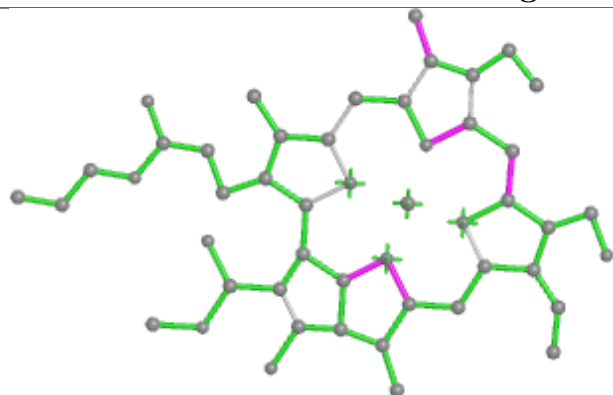


Torsions

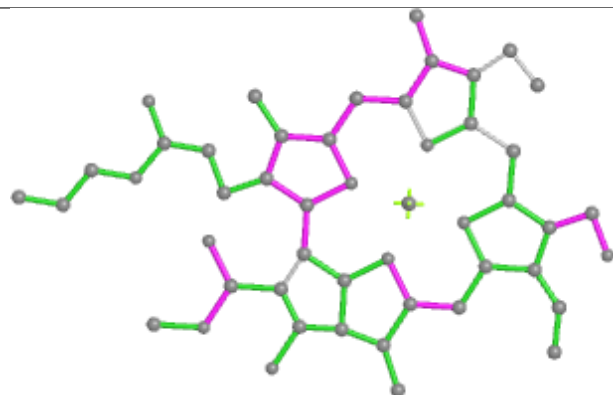


Rings

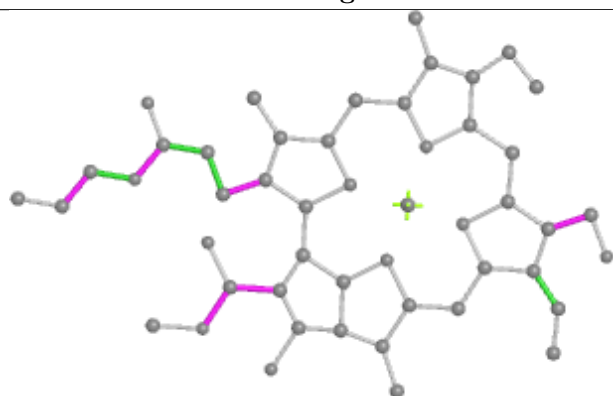
Ligand CHL s 607



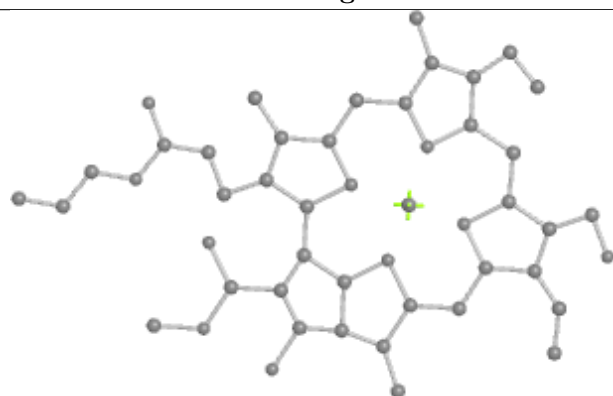
Bond lengths



Bond angles

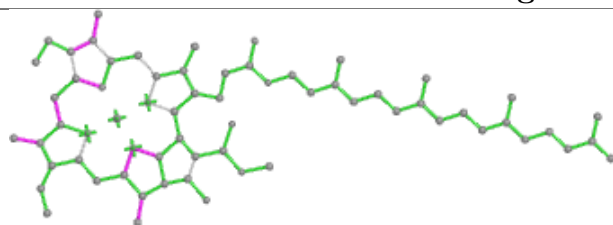


Torsions

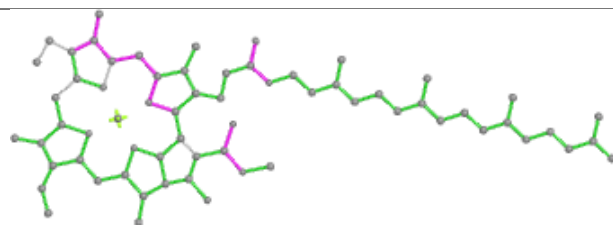


Rings

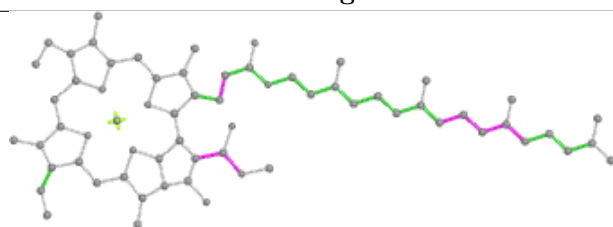
Ligand CLA b 608



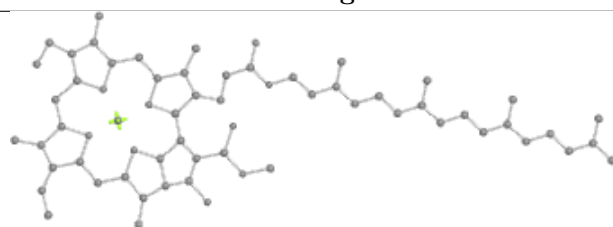
Bond lengths



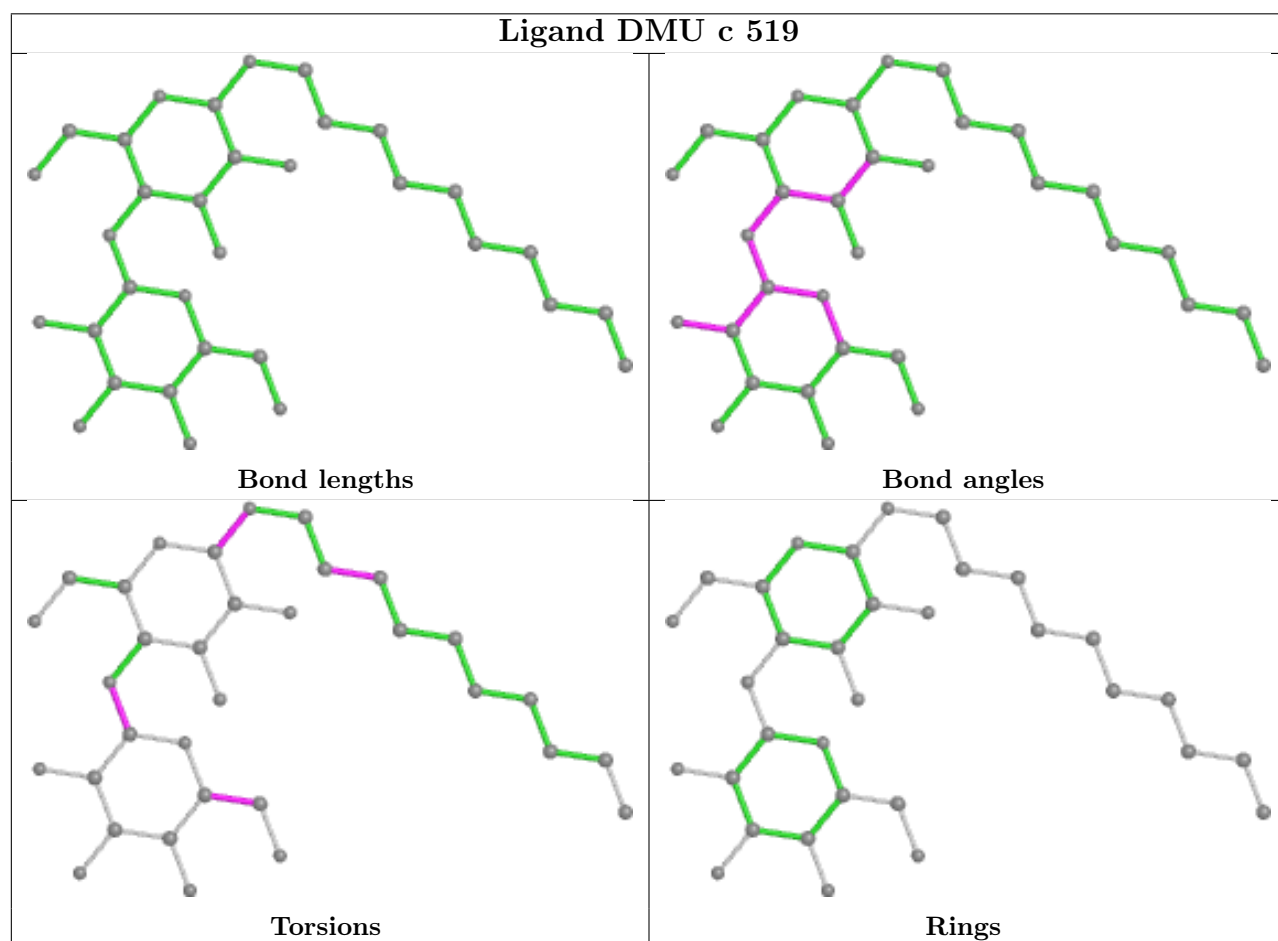
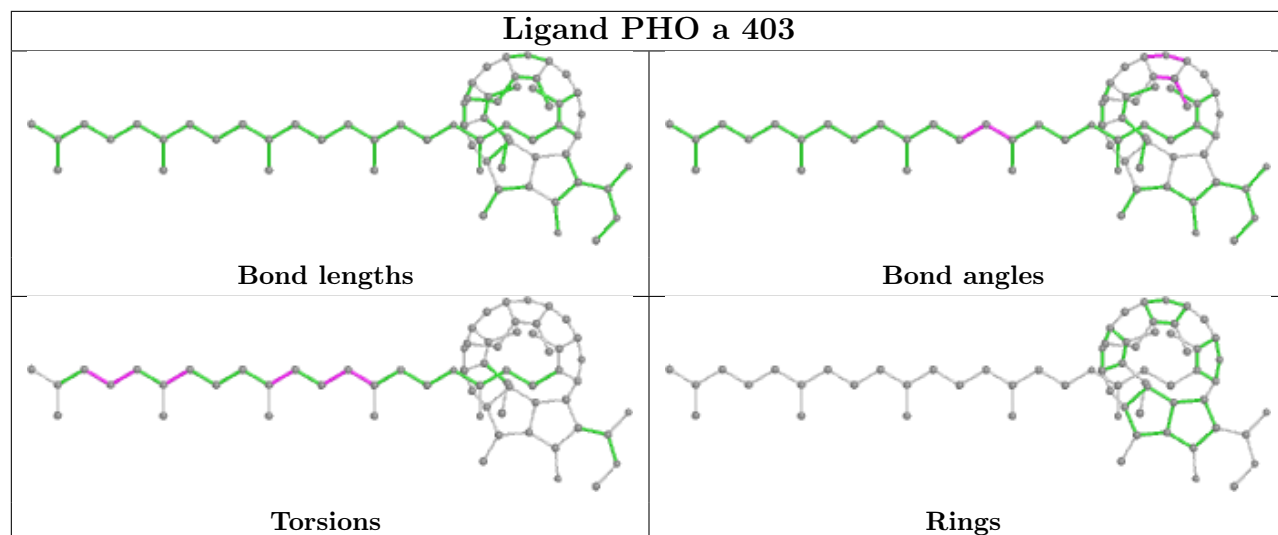
Bond angles

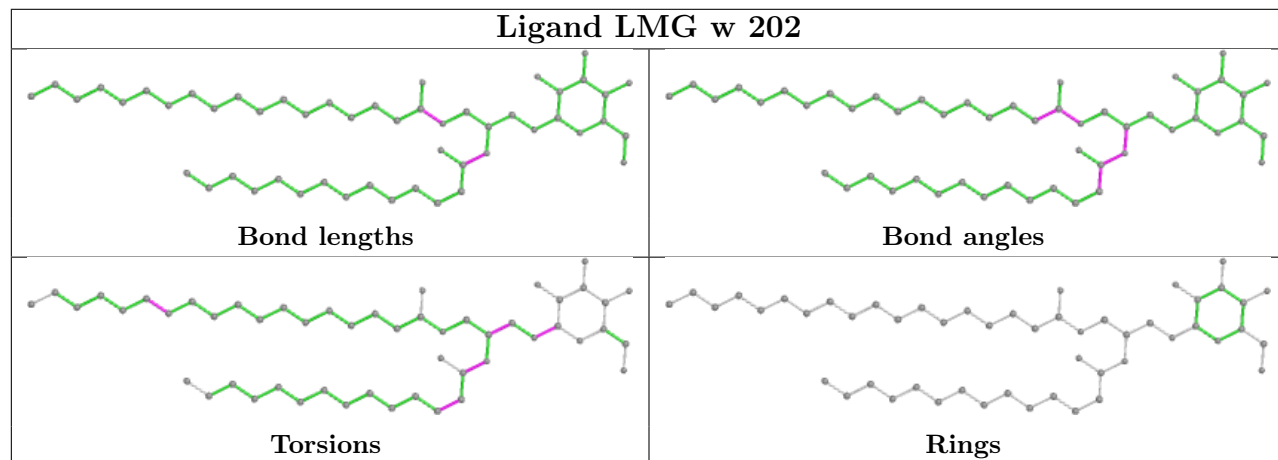
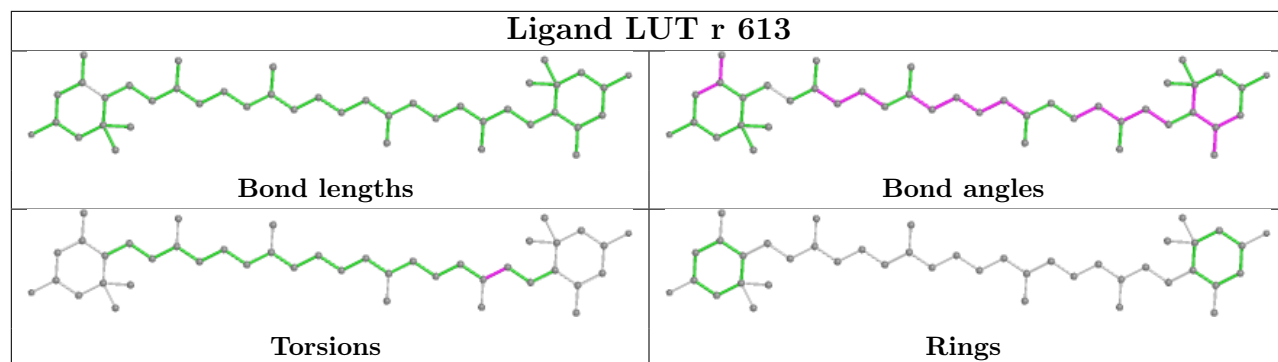


Torsions

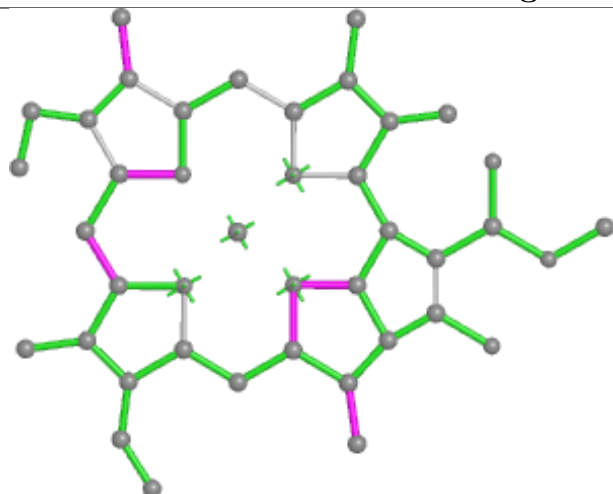


Rings

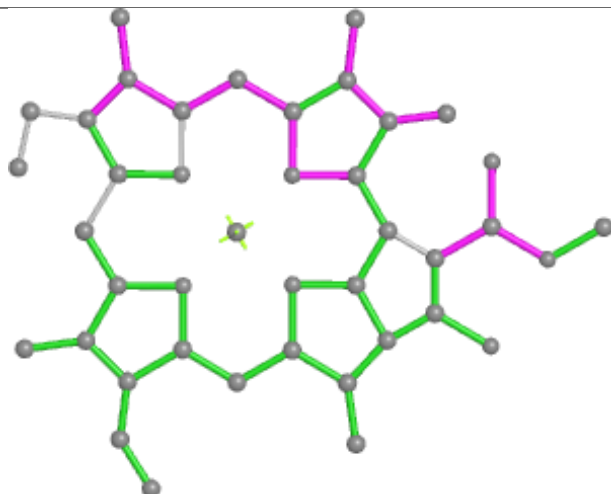




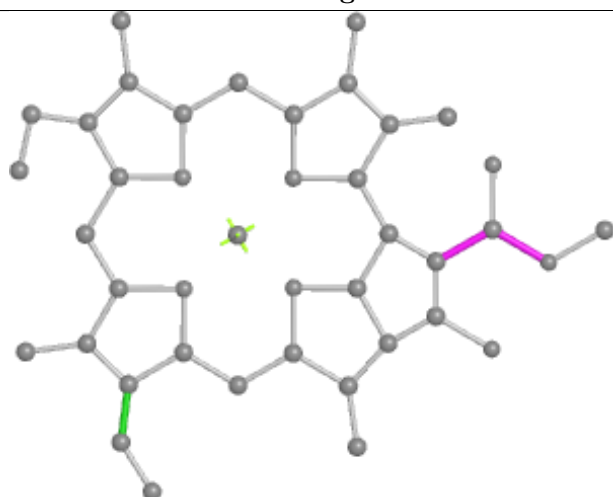
Ligand CLA s 613



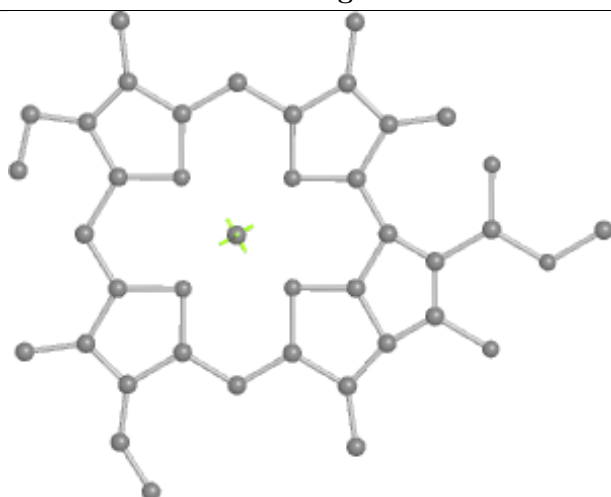
Bond lengths



Bond angles

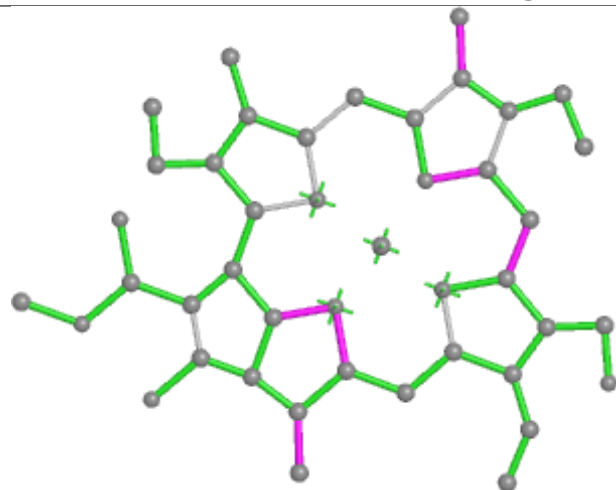


Torsions

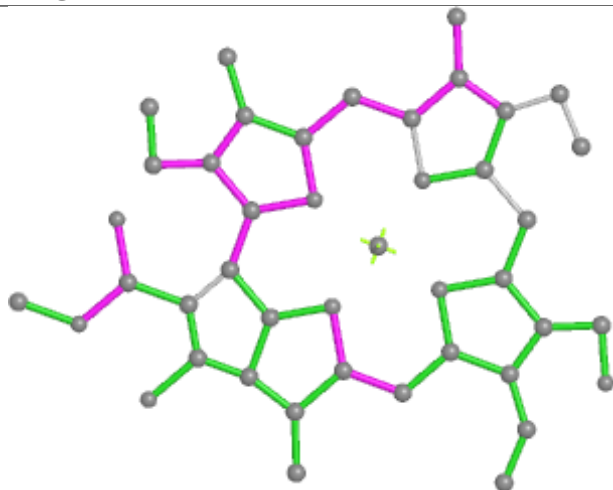


Rings

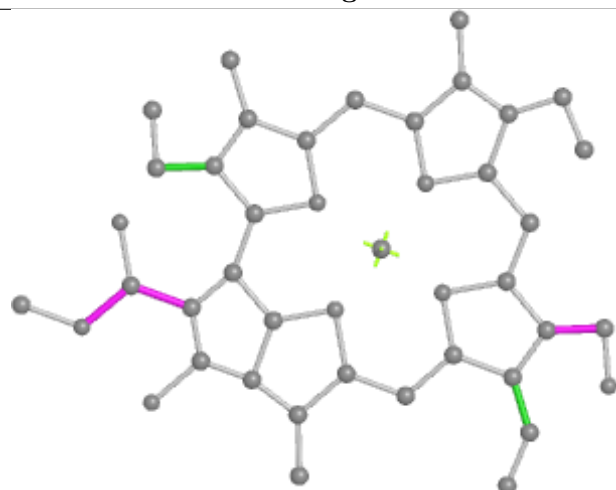
Ligand CHL g 607



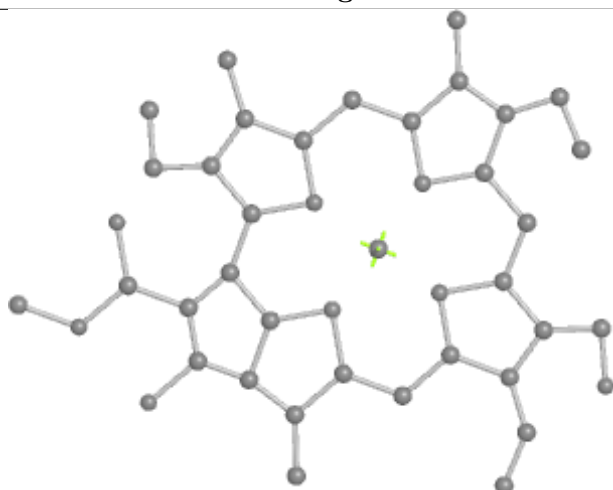
Bond lengths



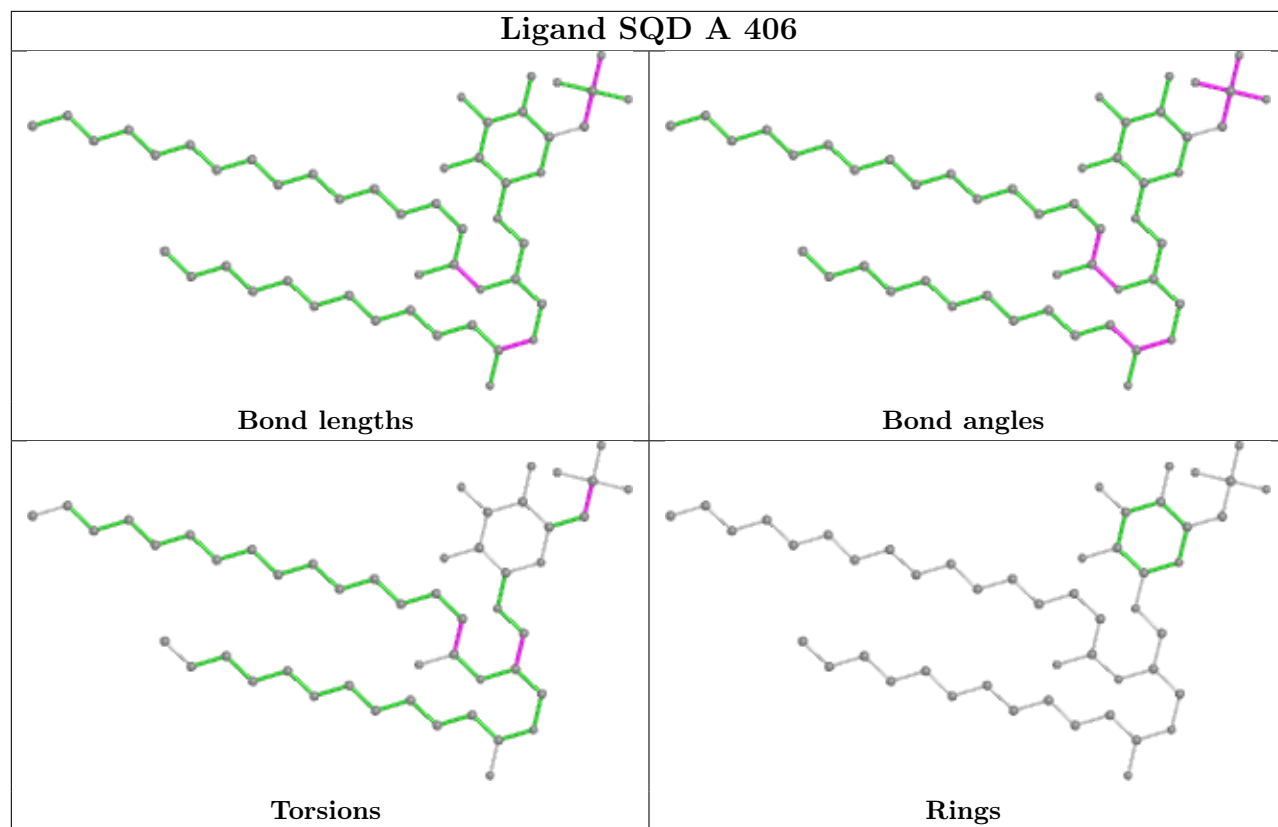
Bond angles



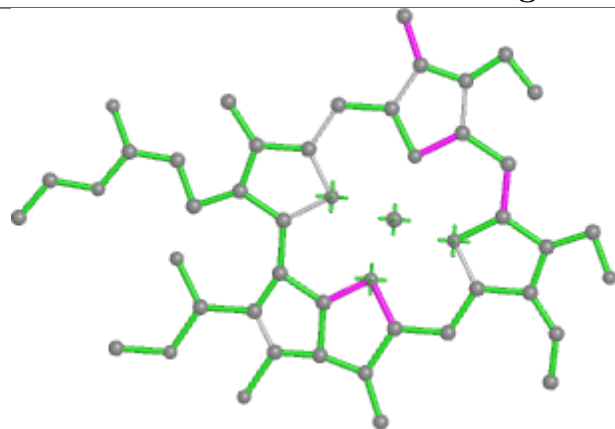
Torsions



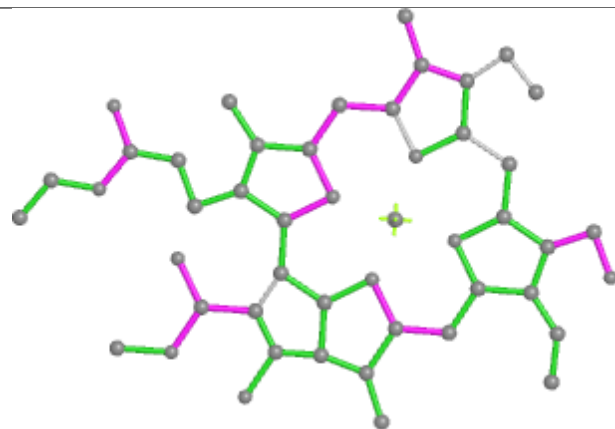
Rings



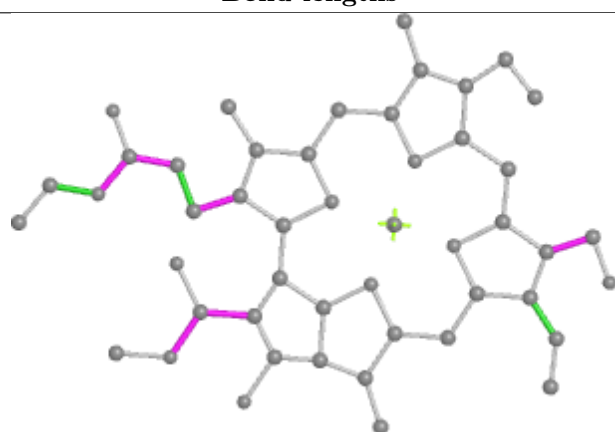
Ligand CHL n 605



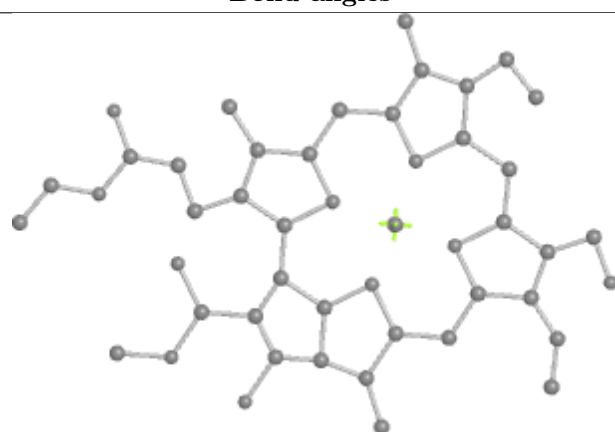
Bond lengths



Bond angles

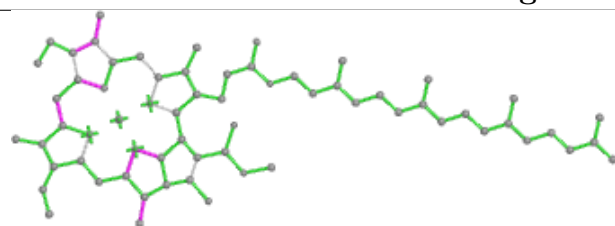


Torsions

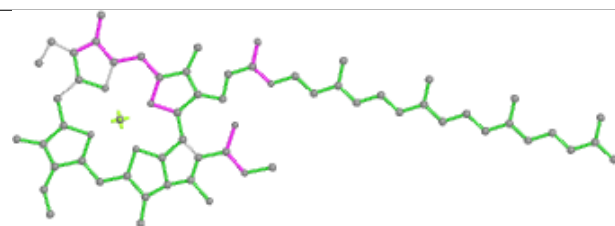


Rings

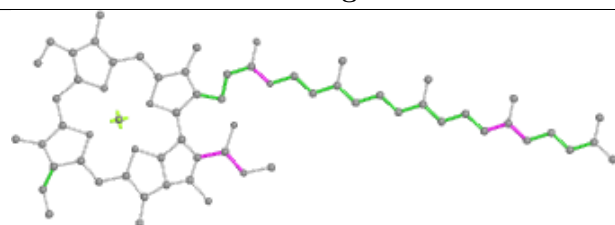
Ligand CLA b 611



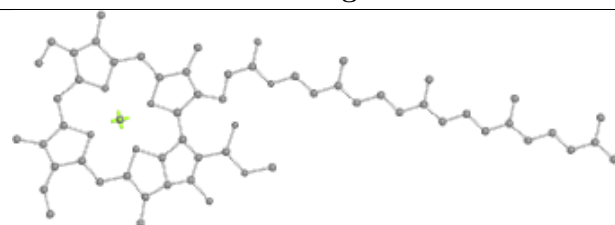
Bond lengths



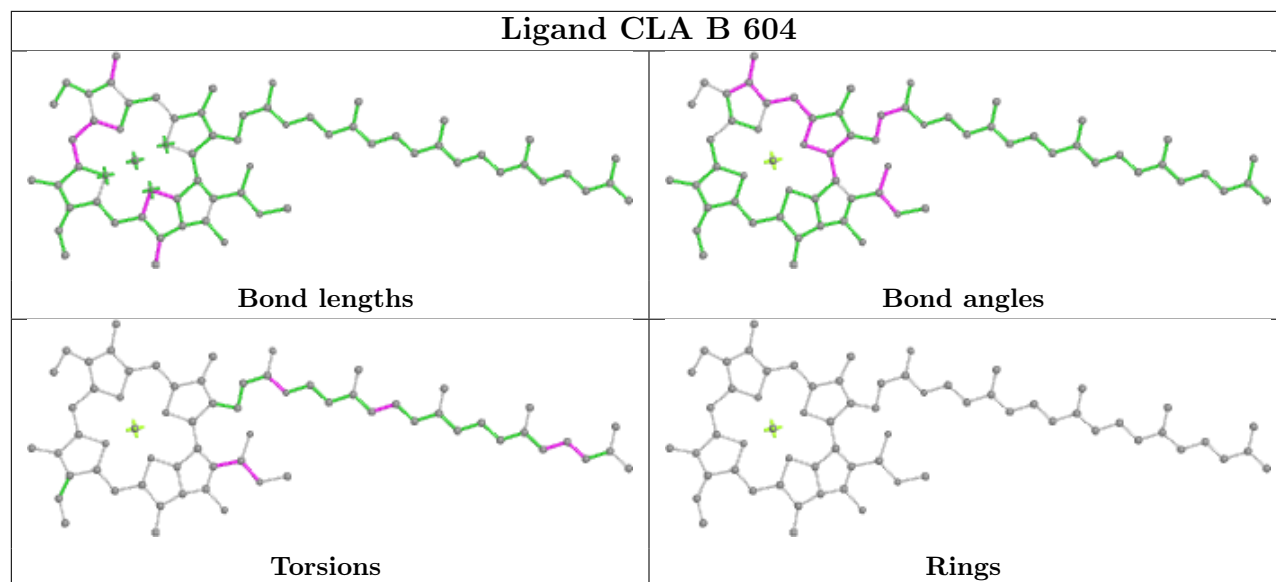
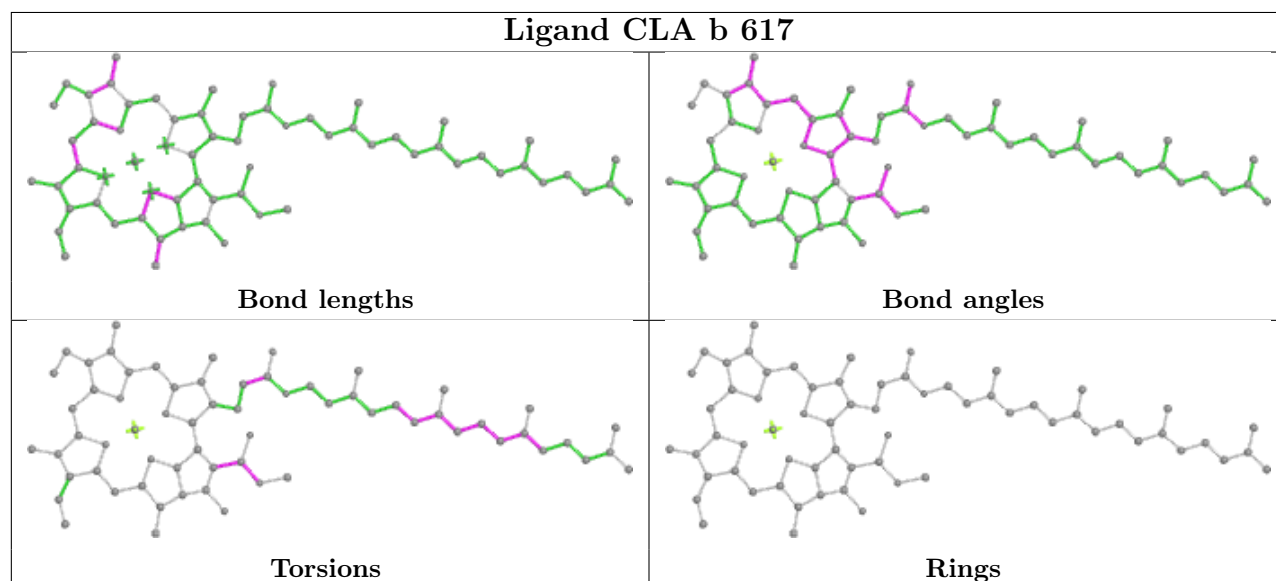
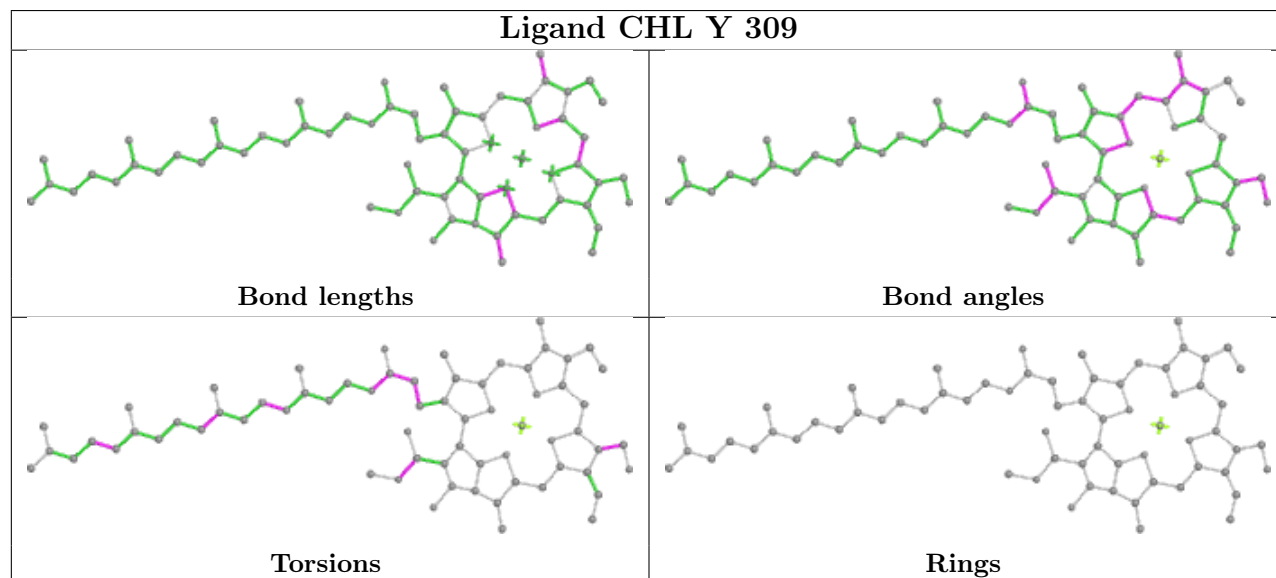
Bond angles

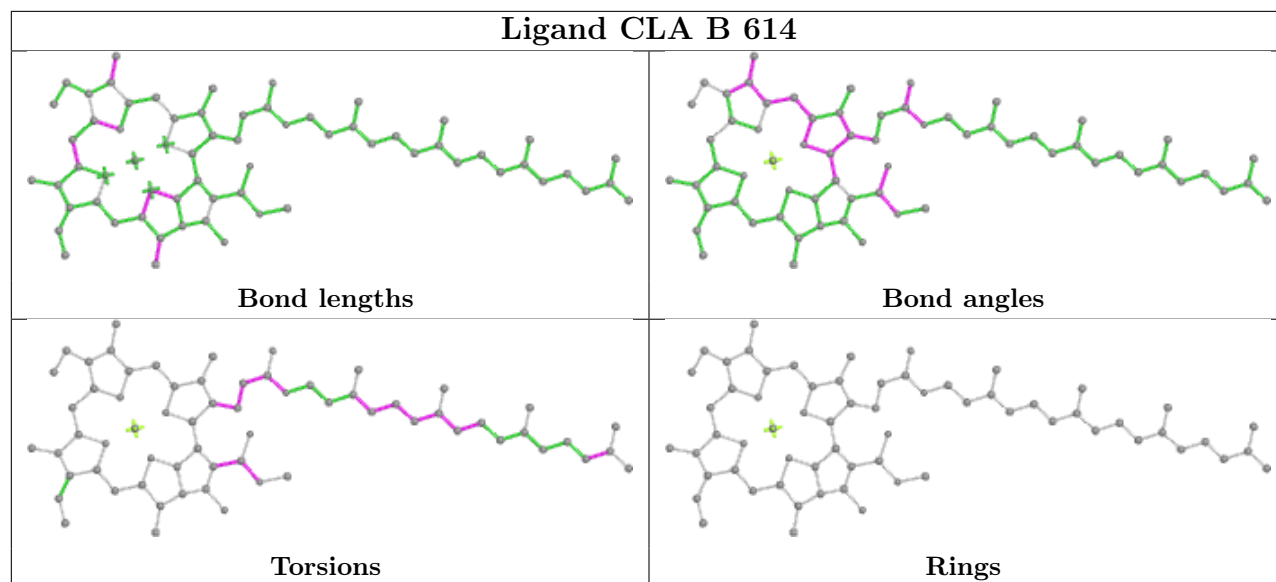
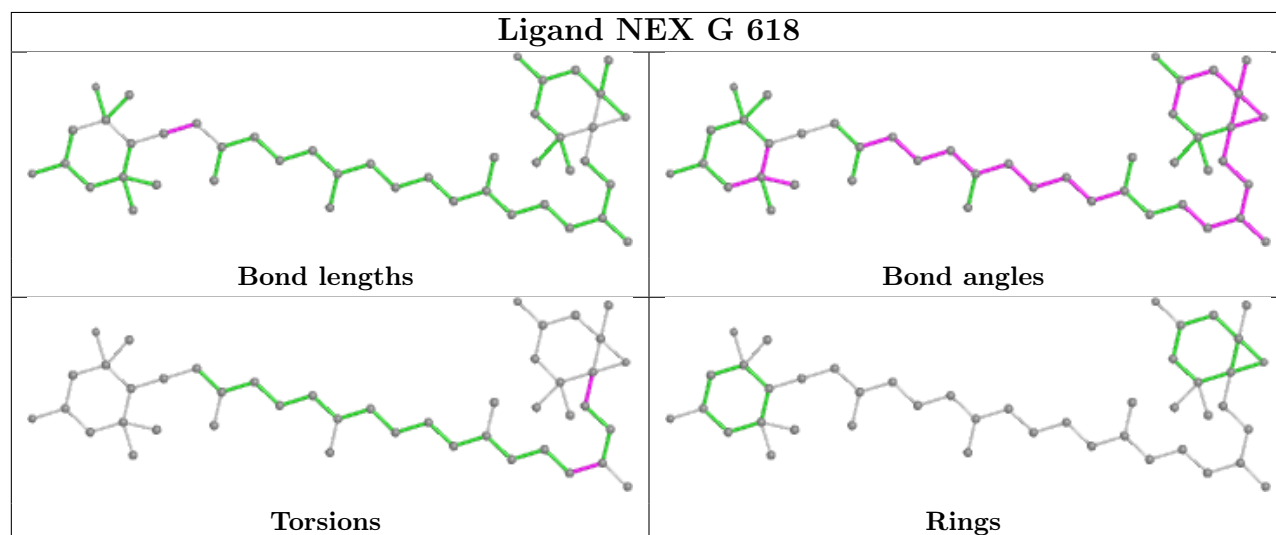


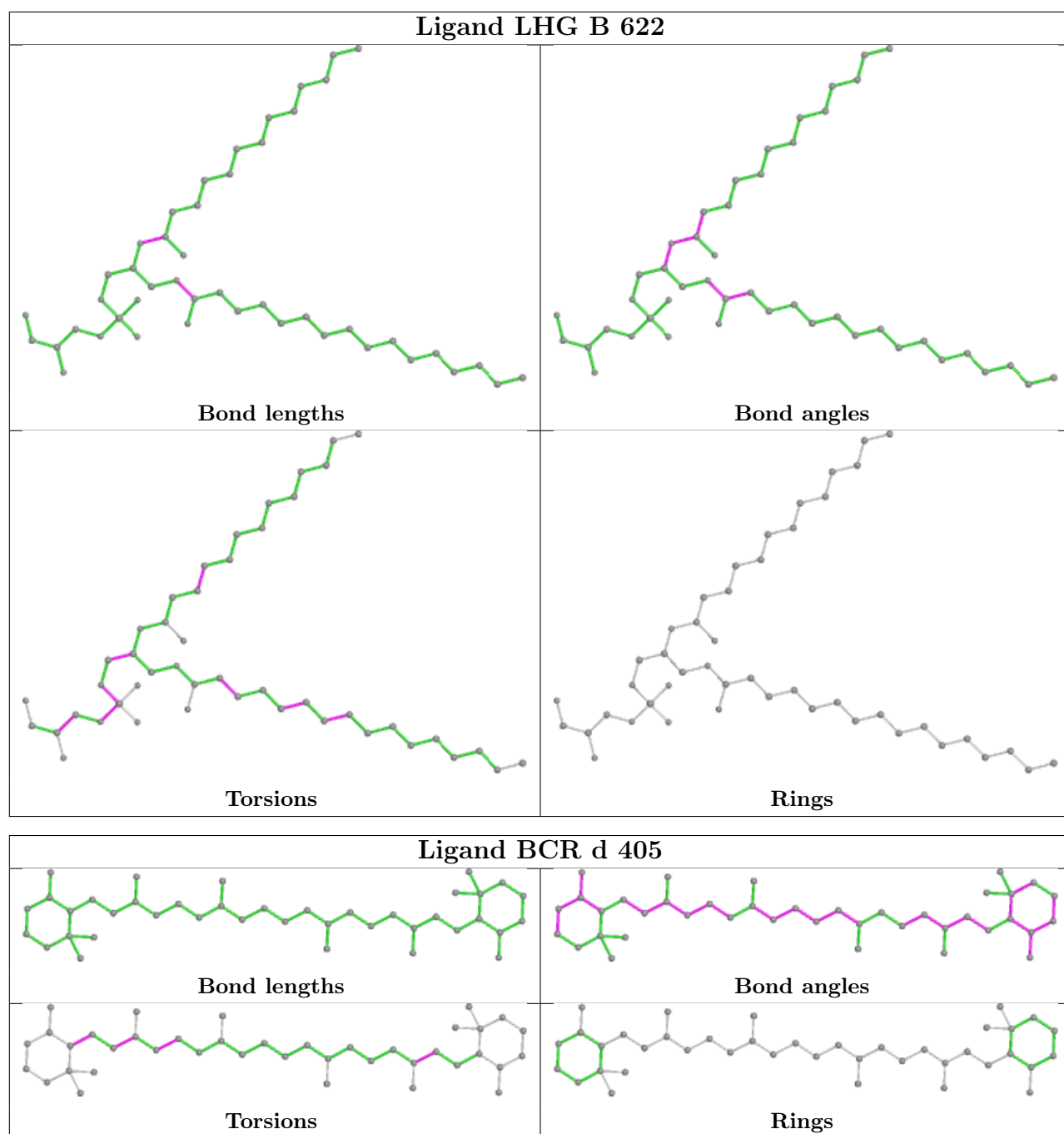
Torsions



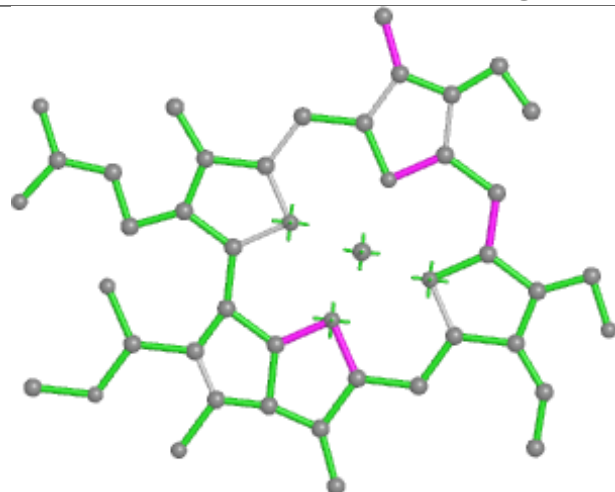
Rings

Ligand CLA B 604**Ligand CLA b 617****Ligand CHL Y 309**

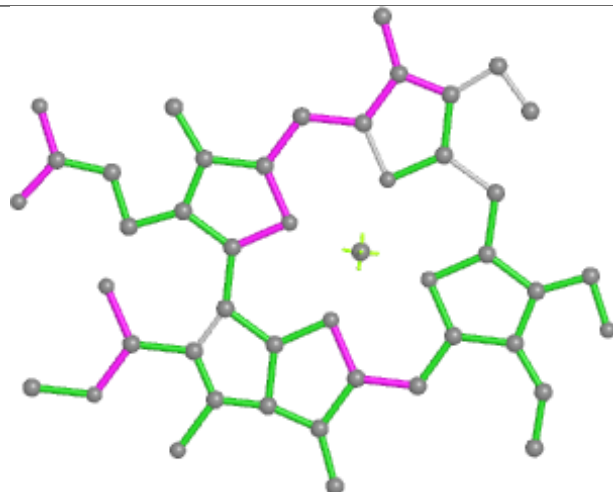
Ligand CLA B 614**Ligand NEX G 618**



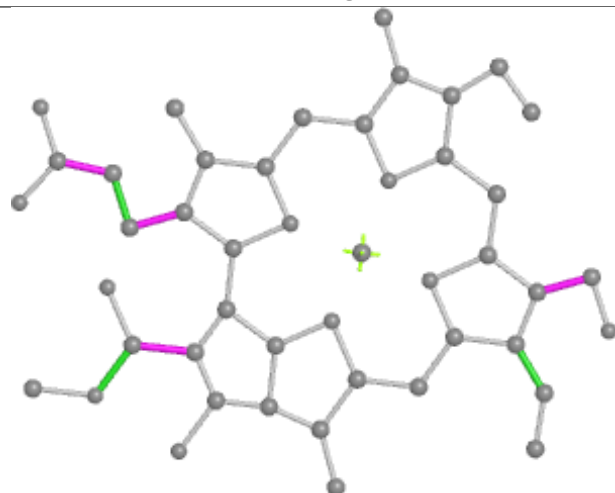
Ligand CHL R 306



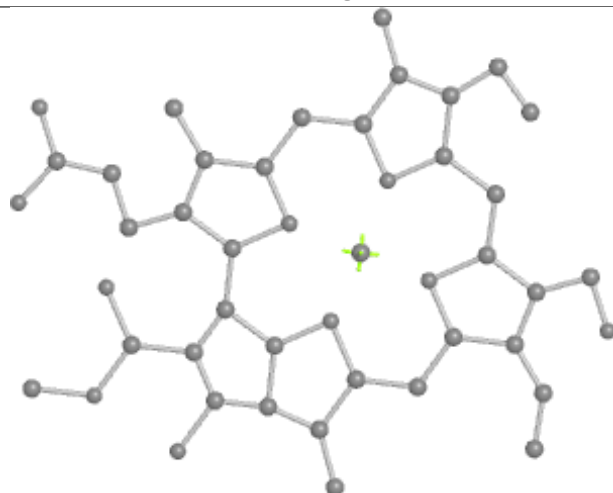
Bond lengths



Bond angles

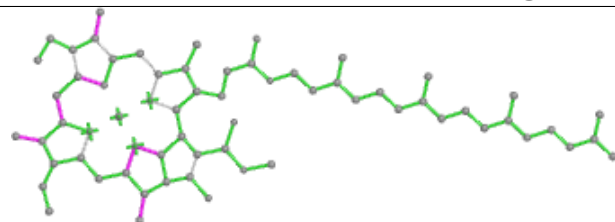


Torsions

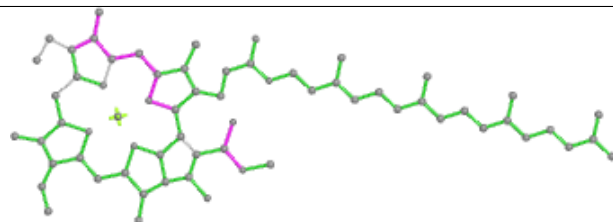


Rings

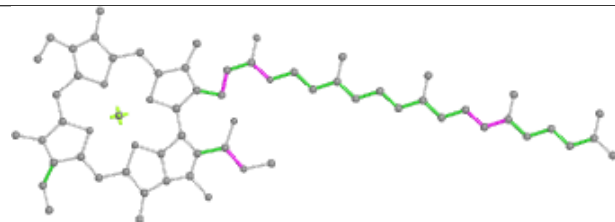
Ligand CLA a 401



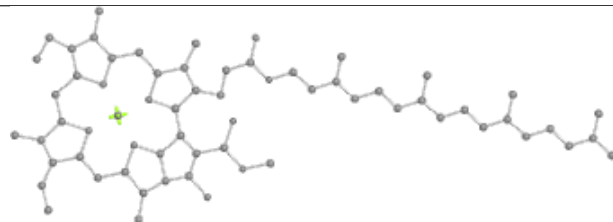
Bond lengths



Bond angles

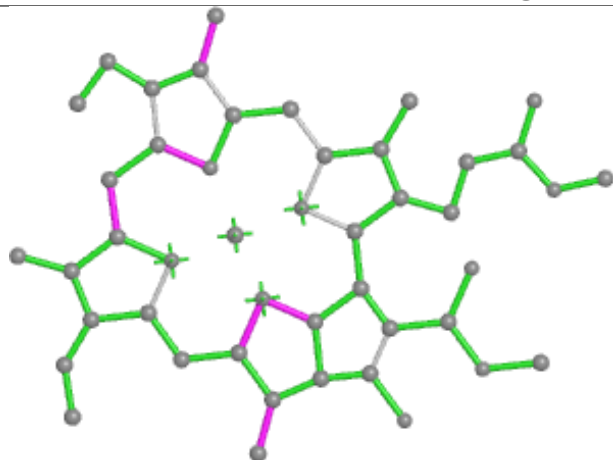


Torsions

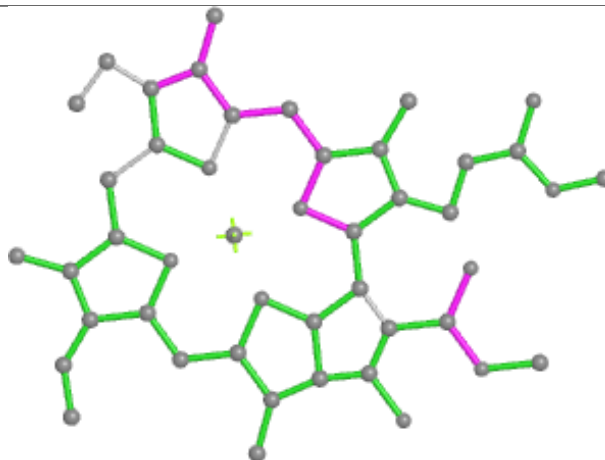


Rings

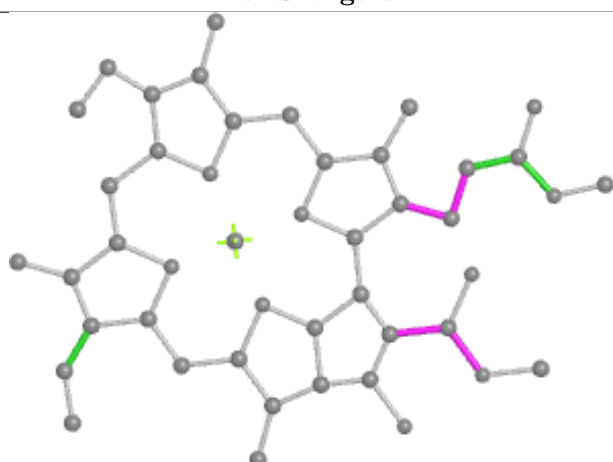
Ligand CLA S 303



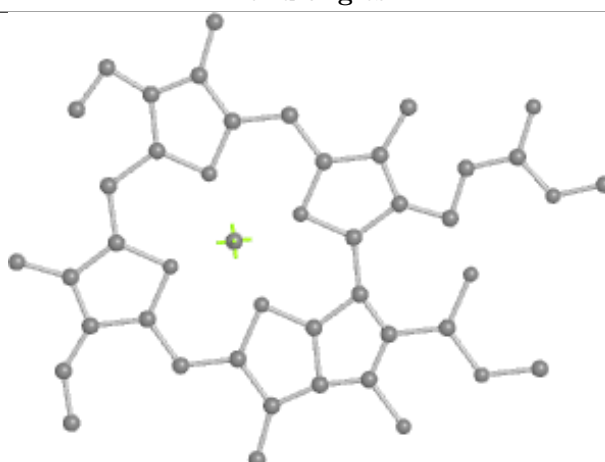
Bond lengths



Bond angles

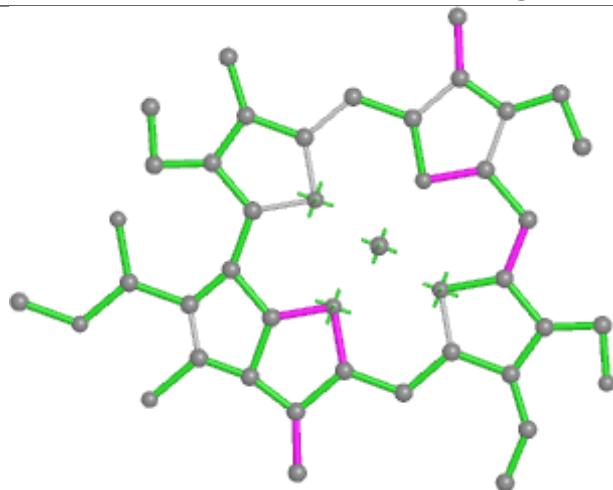


Torsions

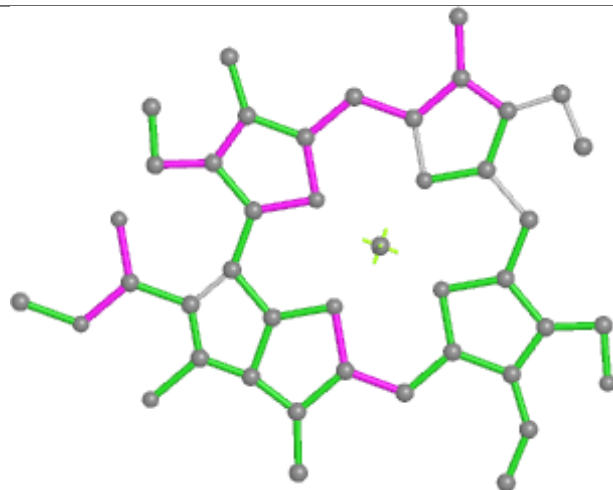


Rings

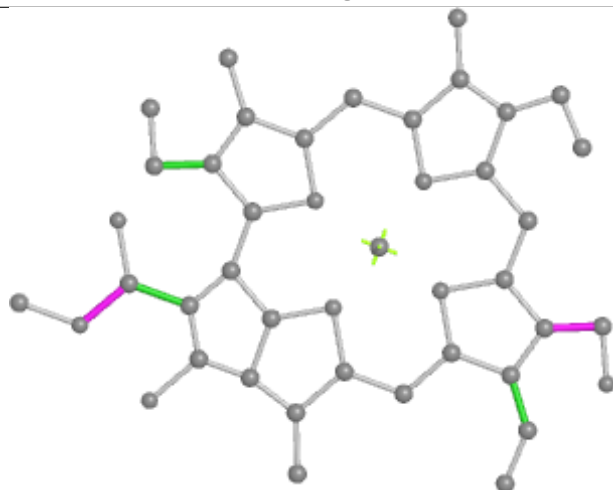
Ligand CHL G 607



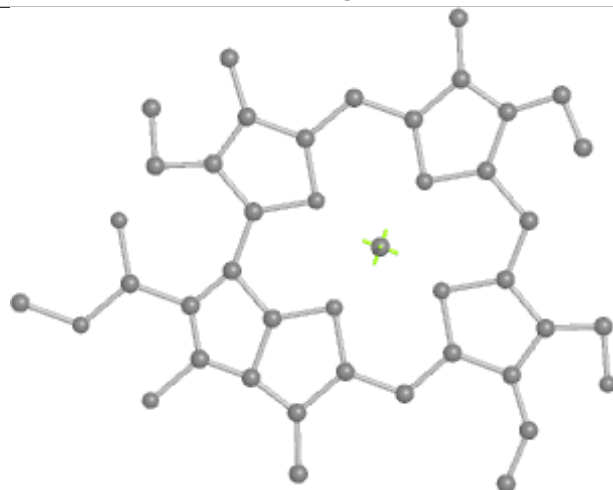
Bond lengths



Bond angles

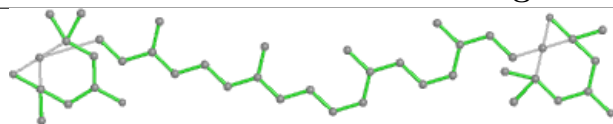


Torsions

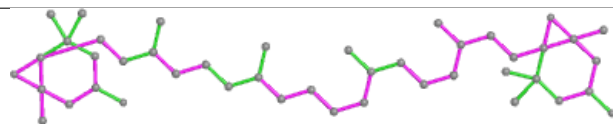


Rings

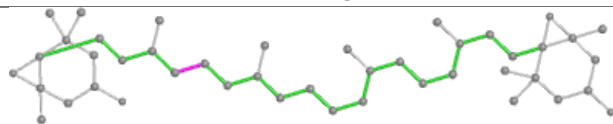
Ligand XAT R 315



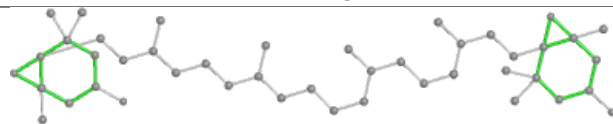
Bond lengths



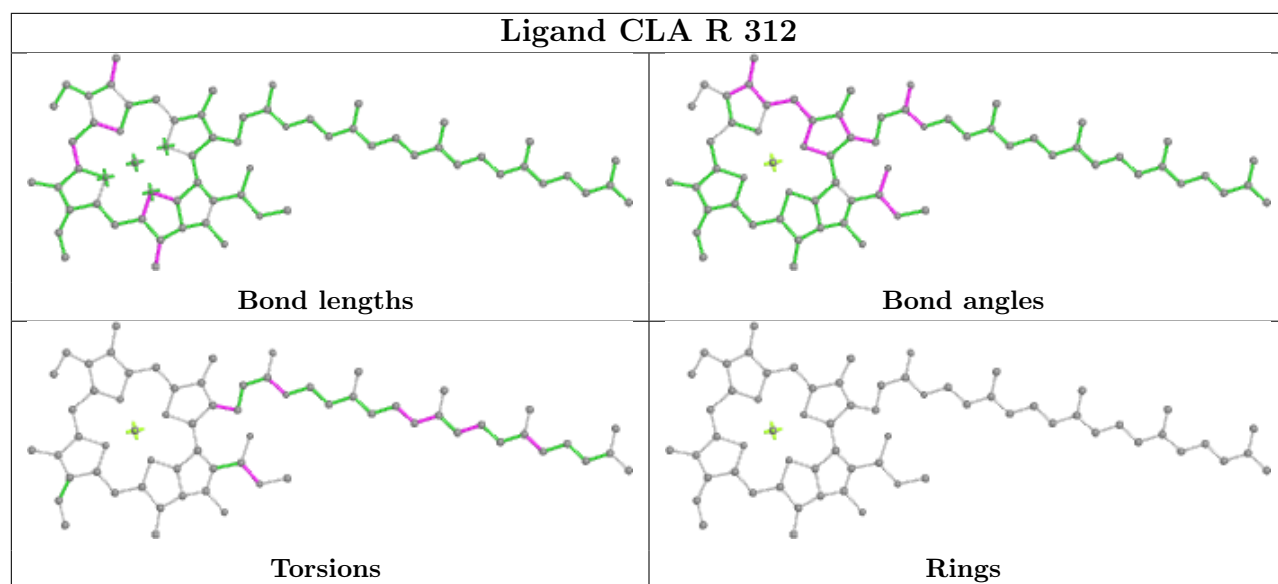
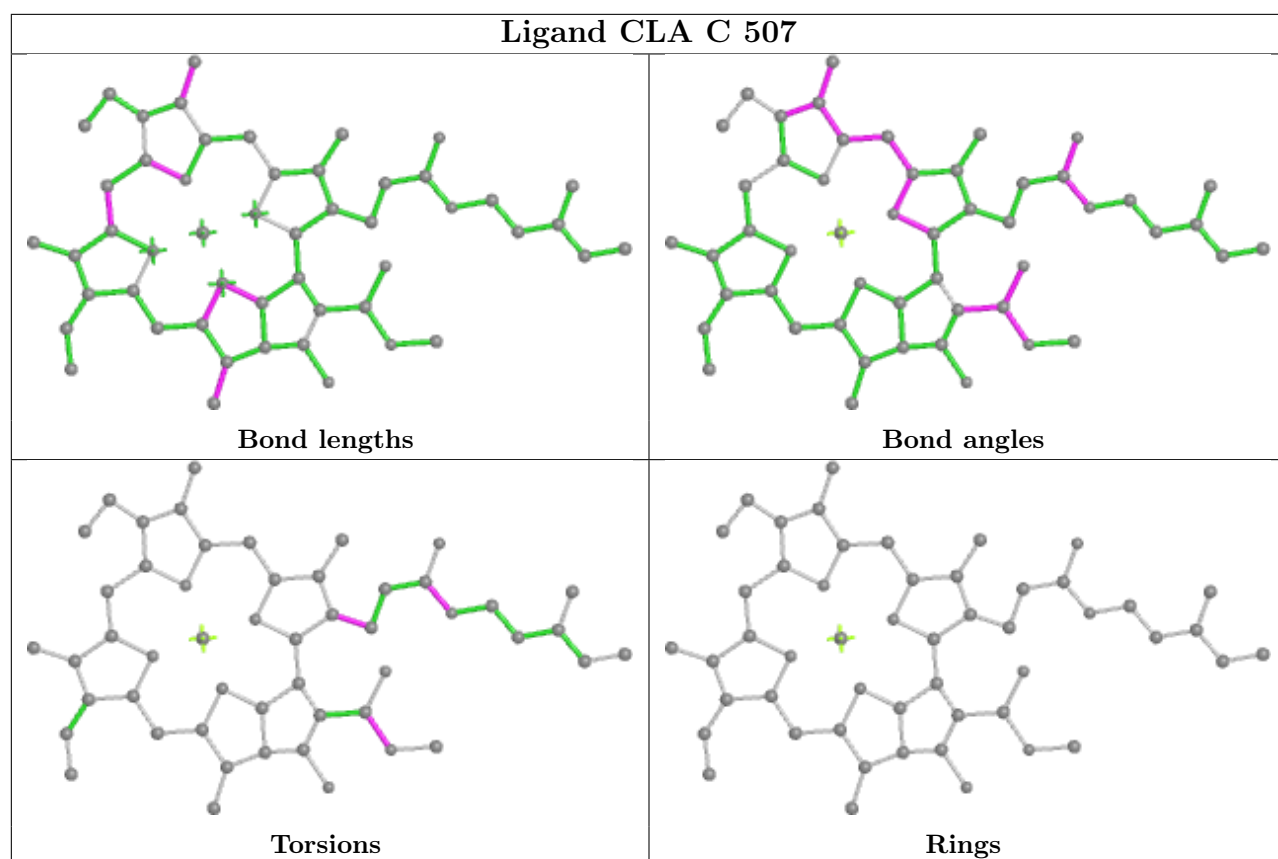
Bond angles



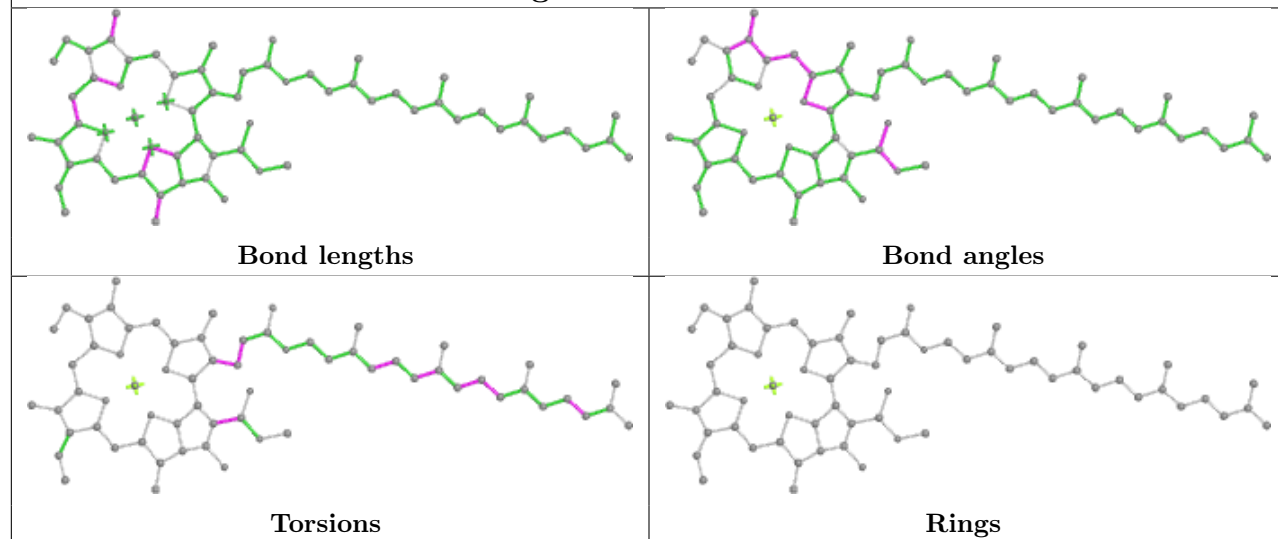
Torsions



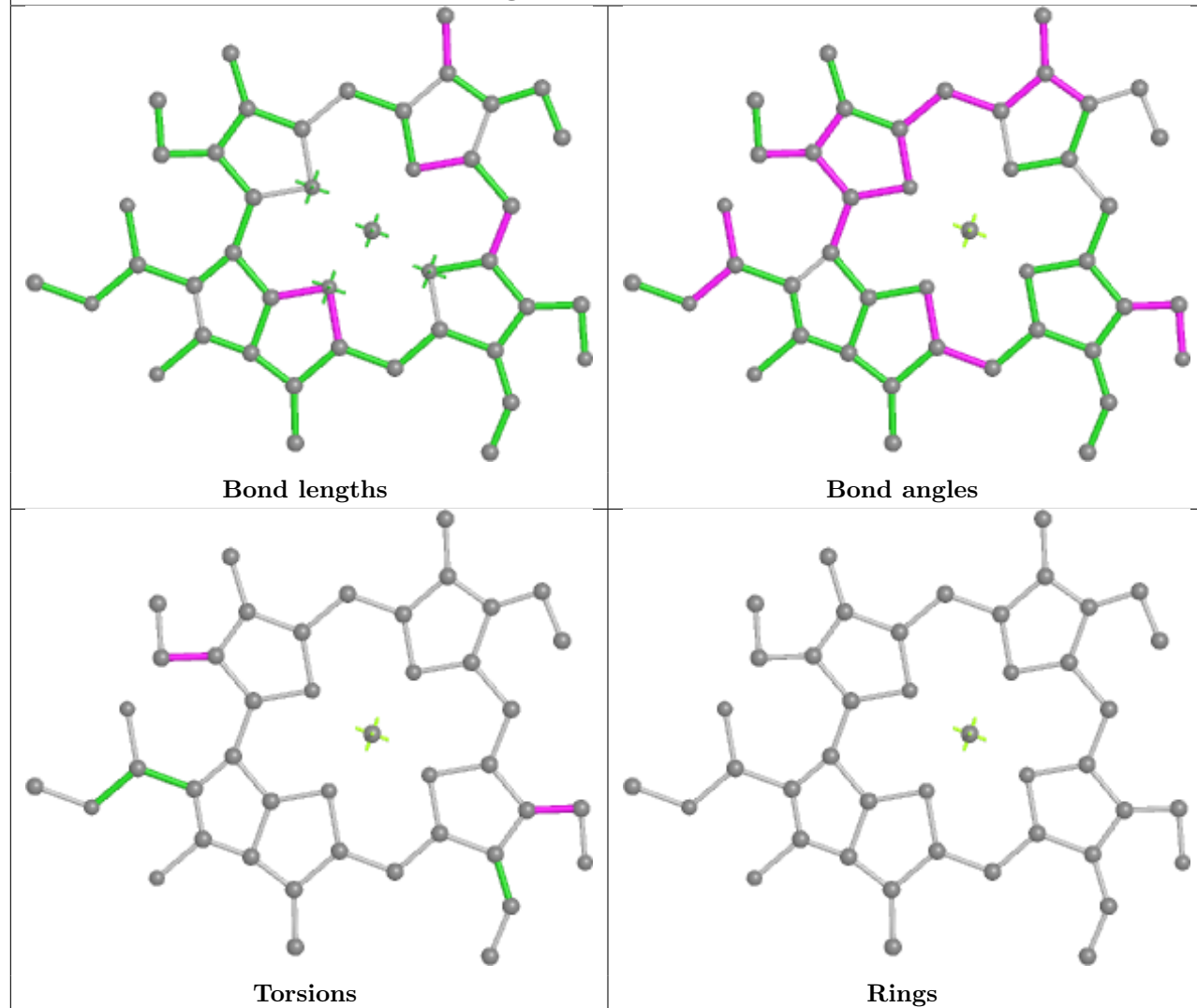
Rings



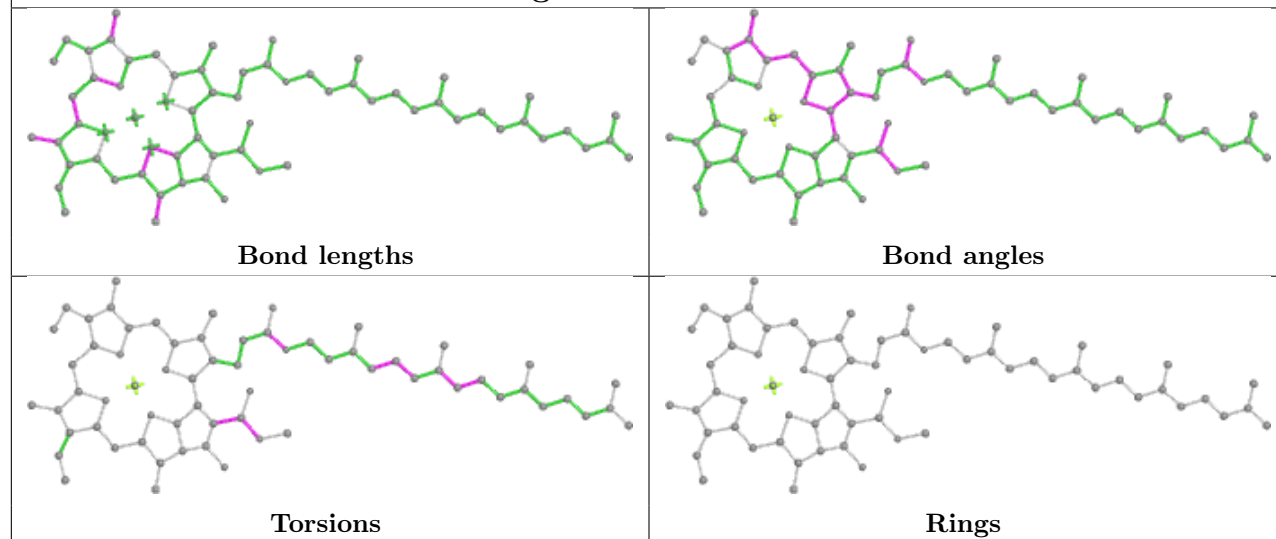
Ligand CLA R 310



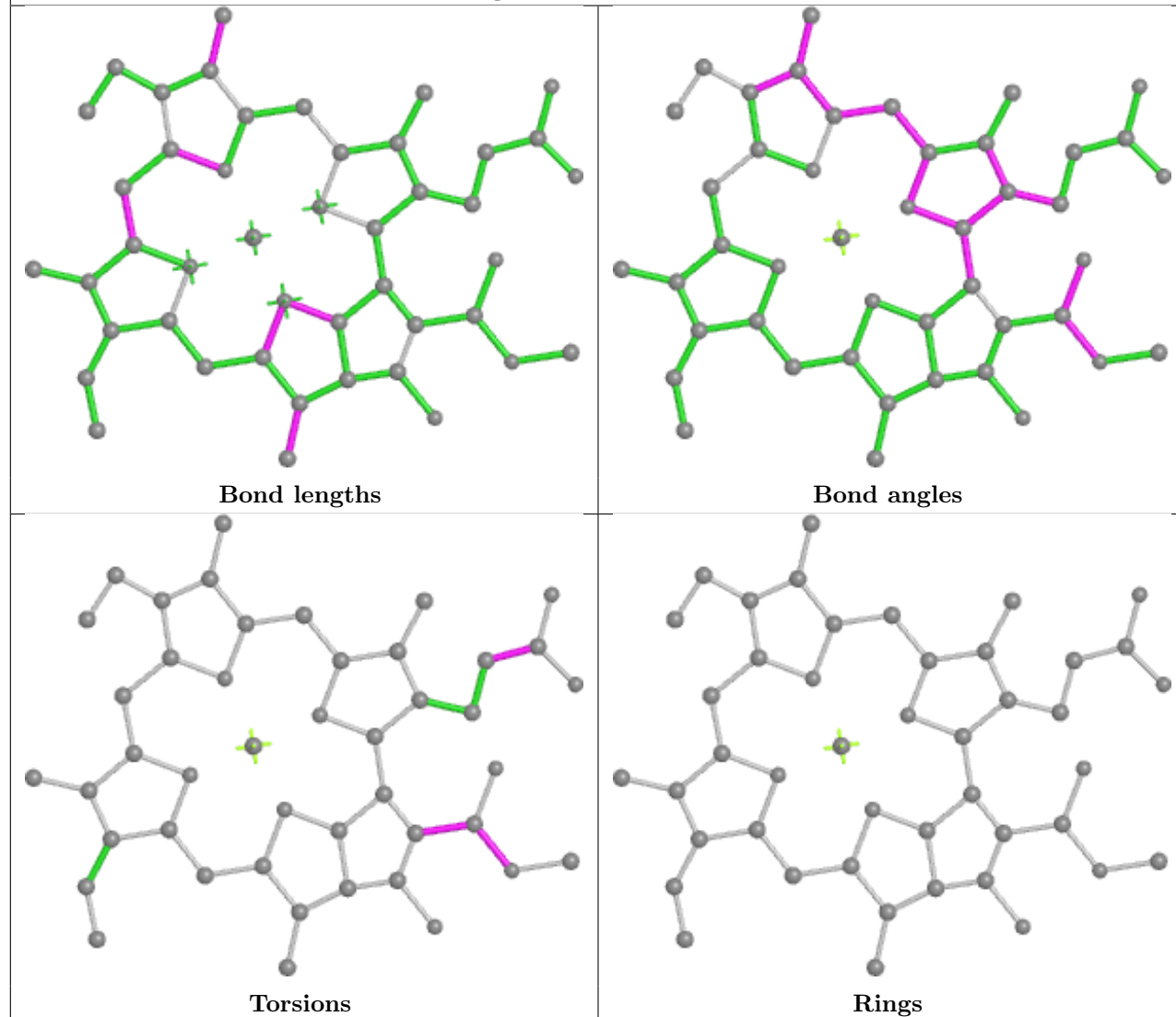
Ligand CHL s 606



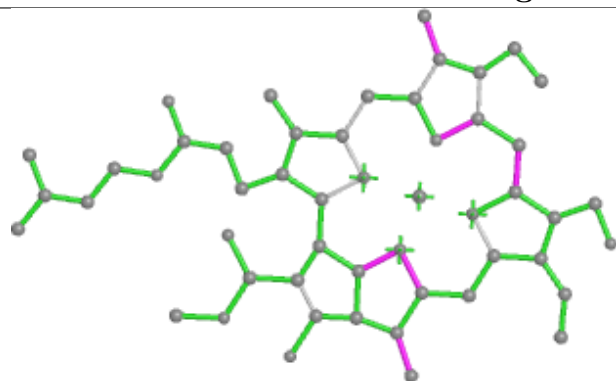
Ligand CLA B 616



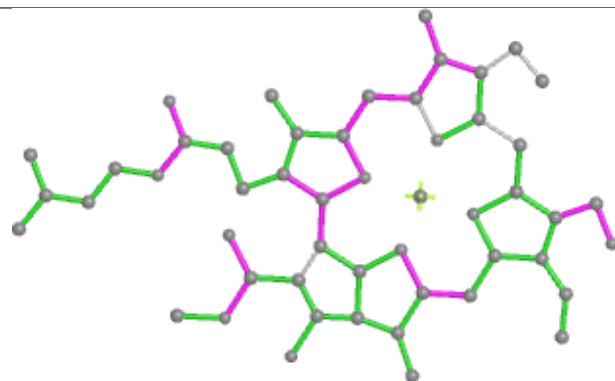
Ligand CLA G 612



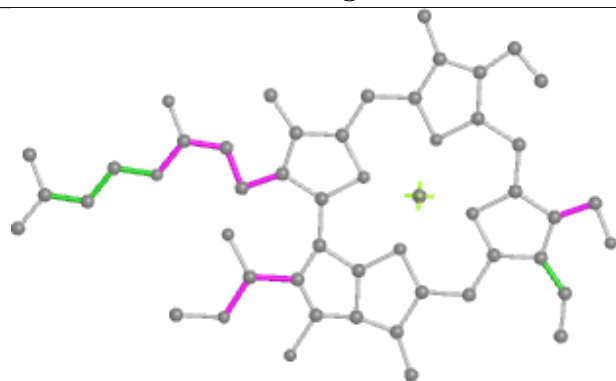
Ligand CHL Y 306



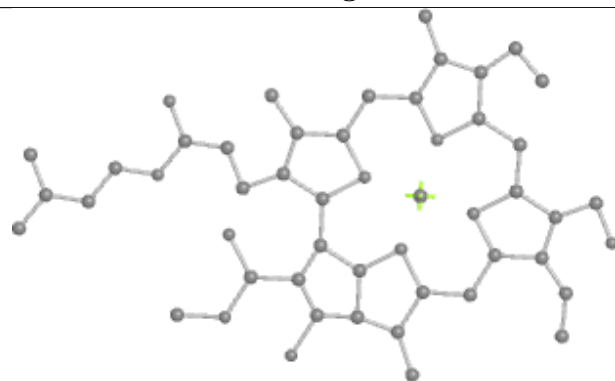
Bond lengths



Bond angles

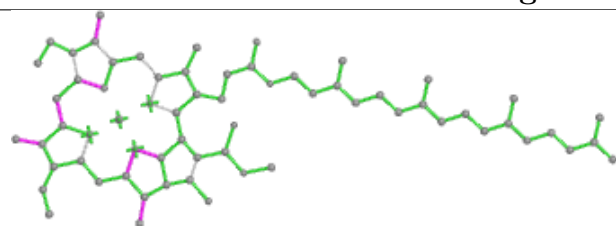


Torsions

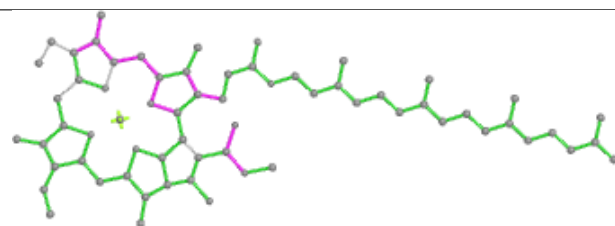


Rings

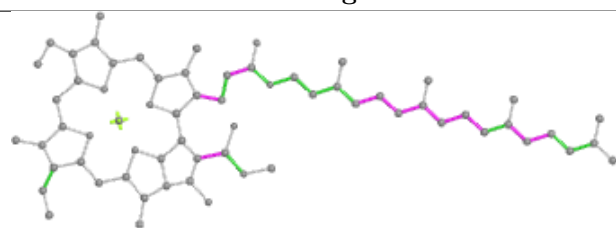
Ligand CLA b 614



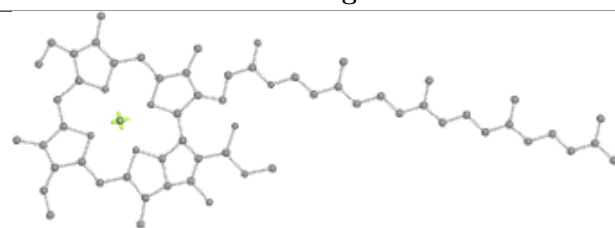
Bond lengths



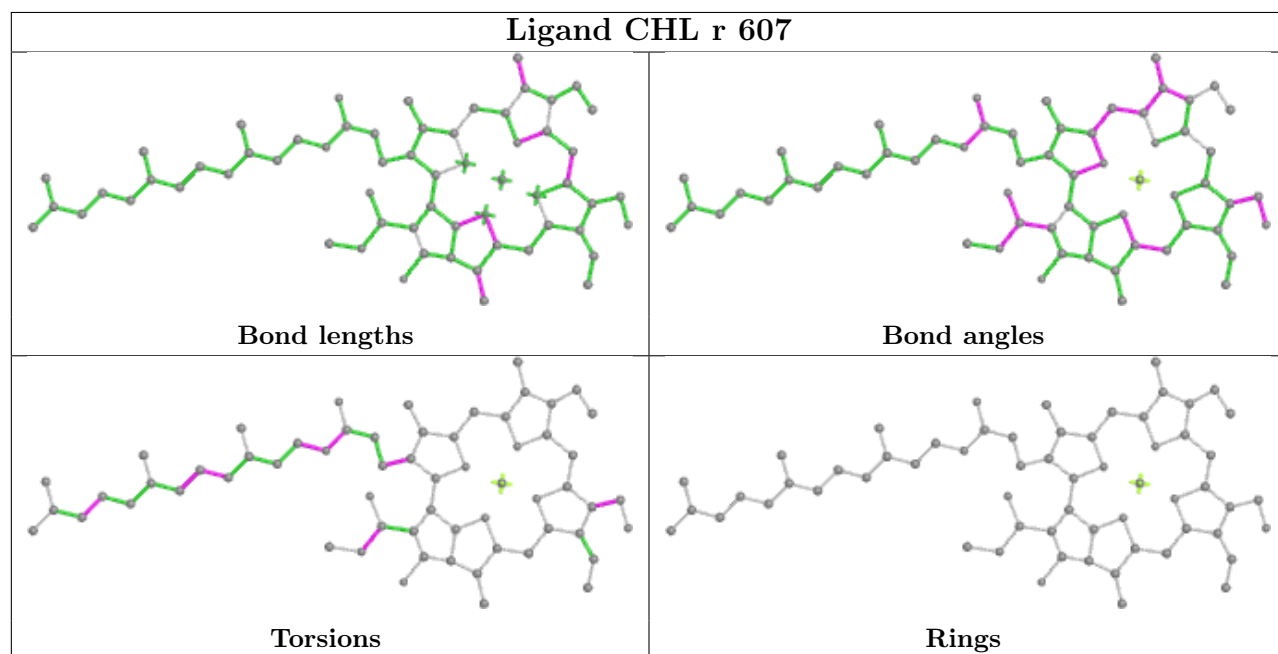
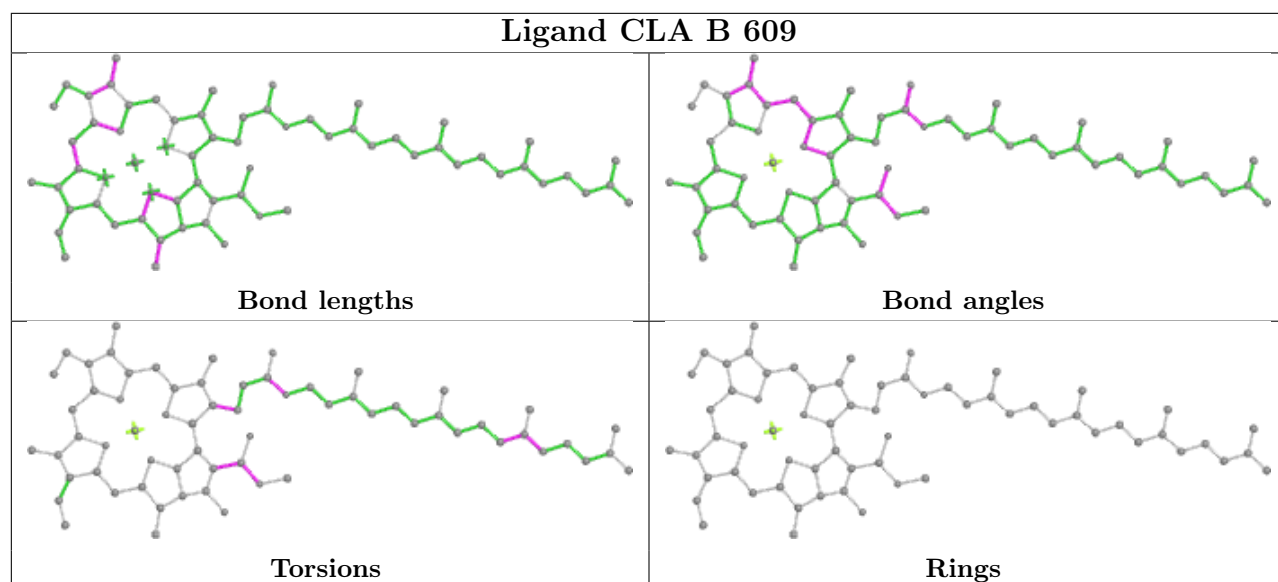
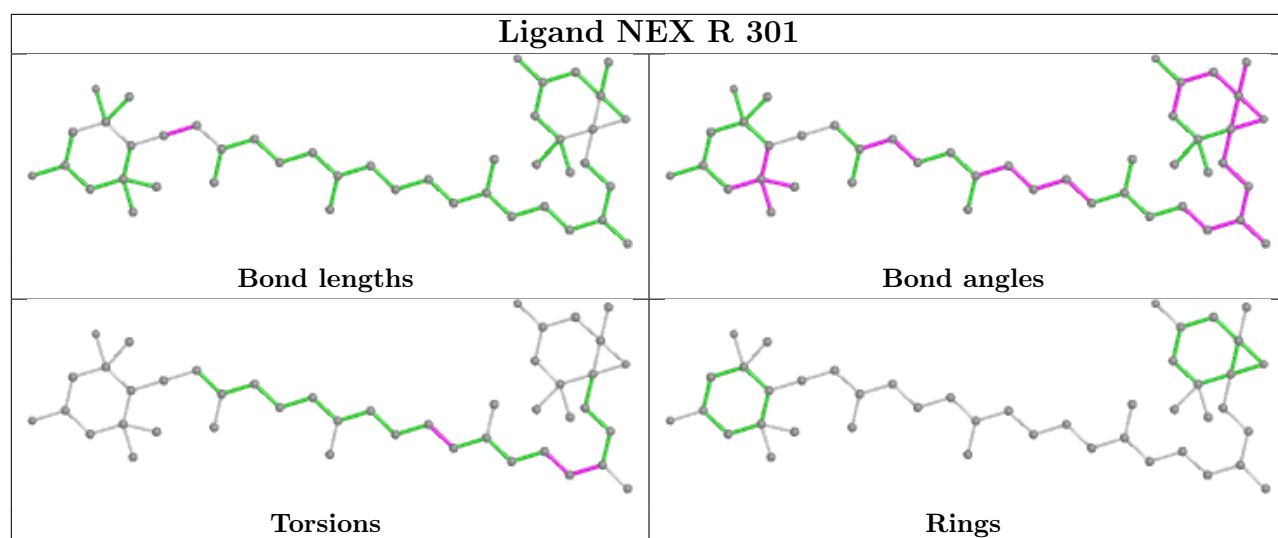
Bond angles

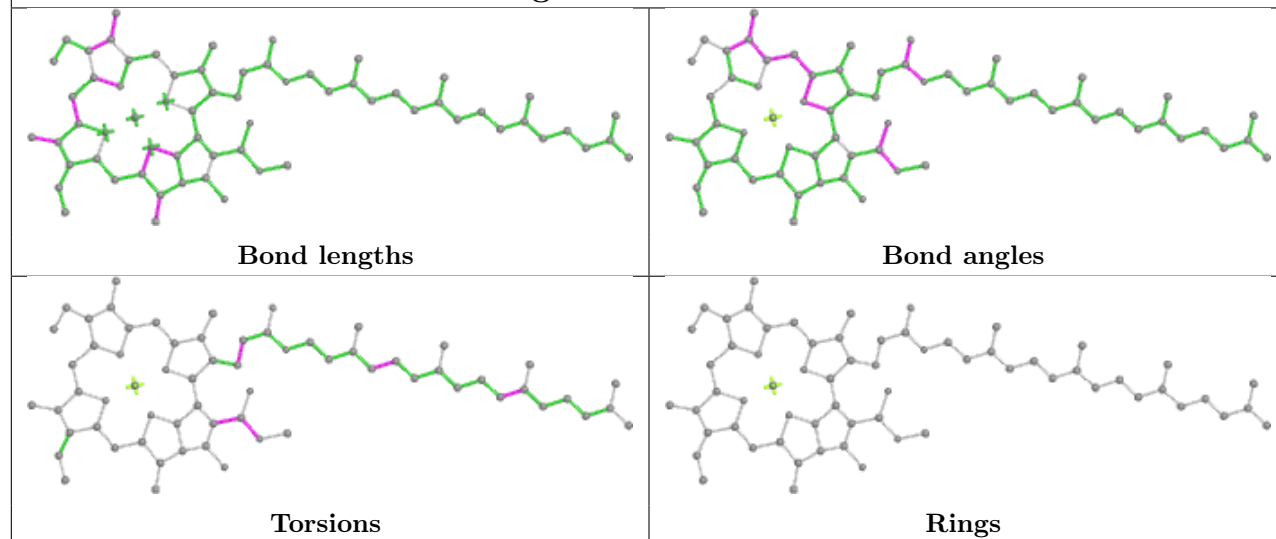
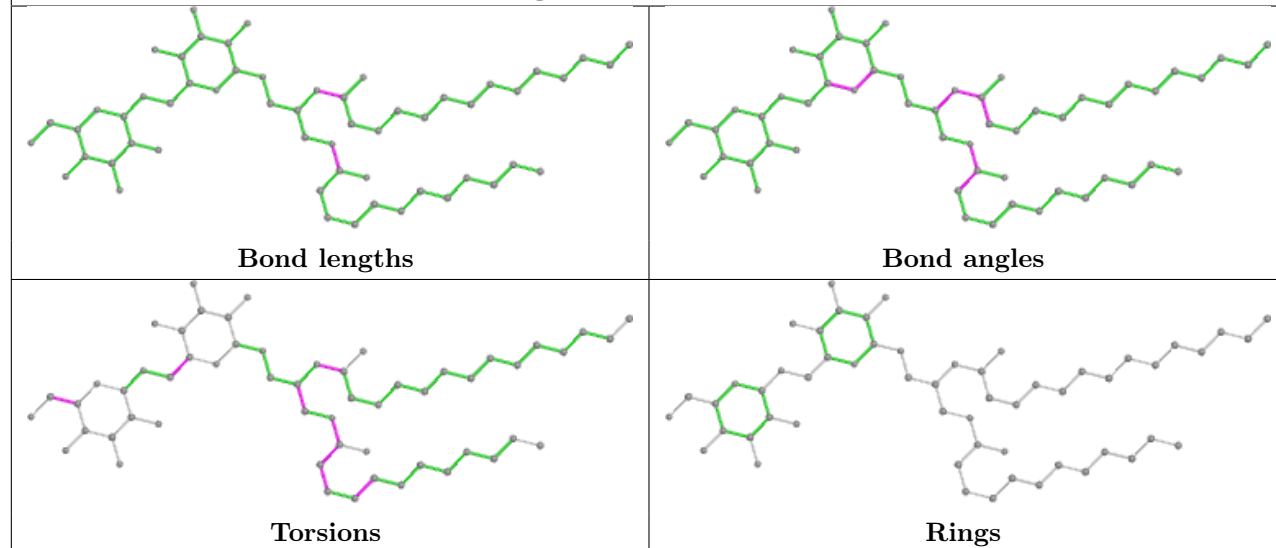


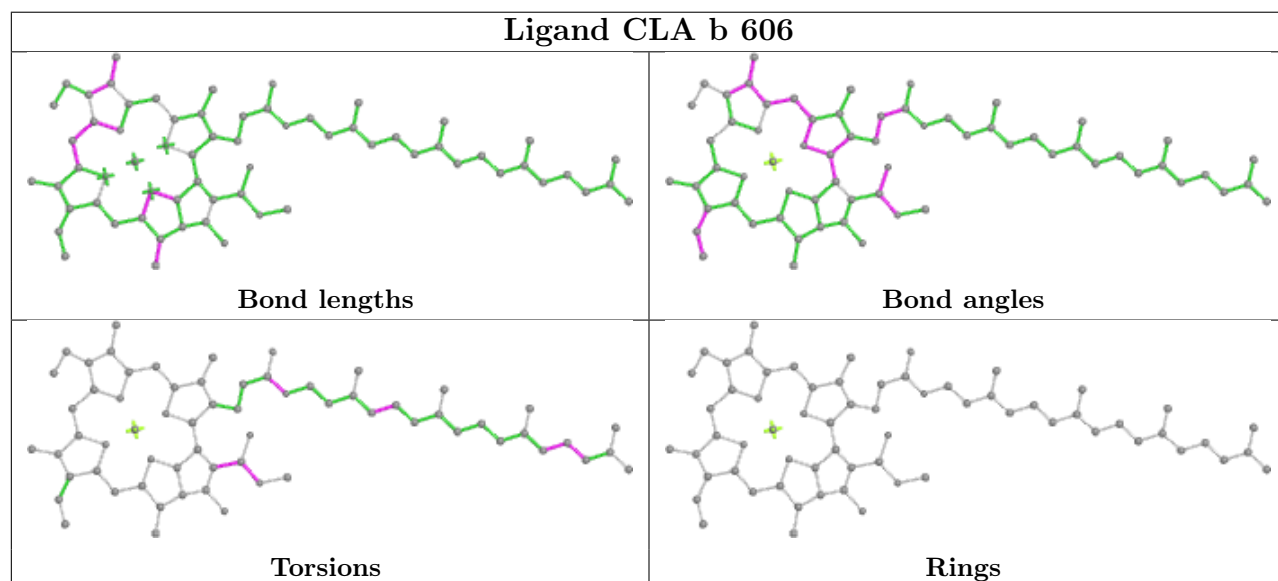
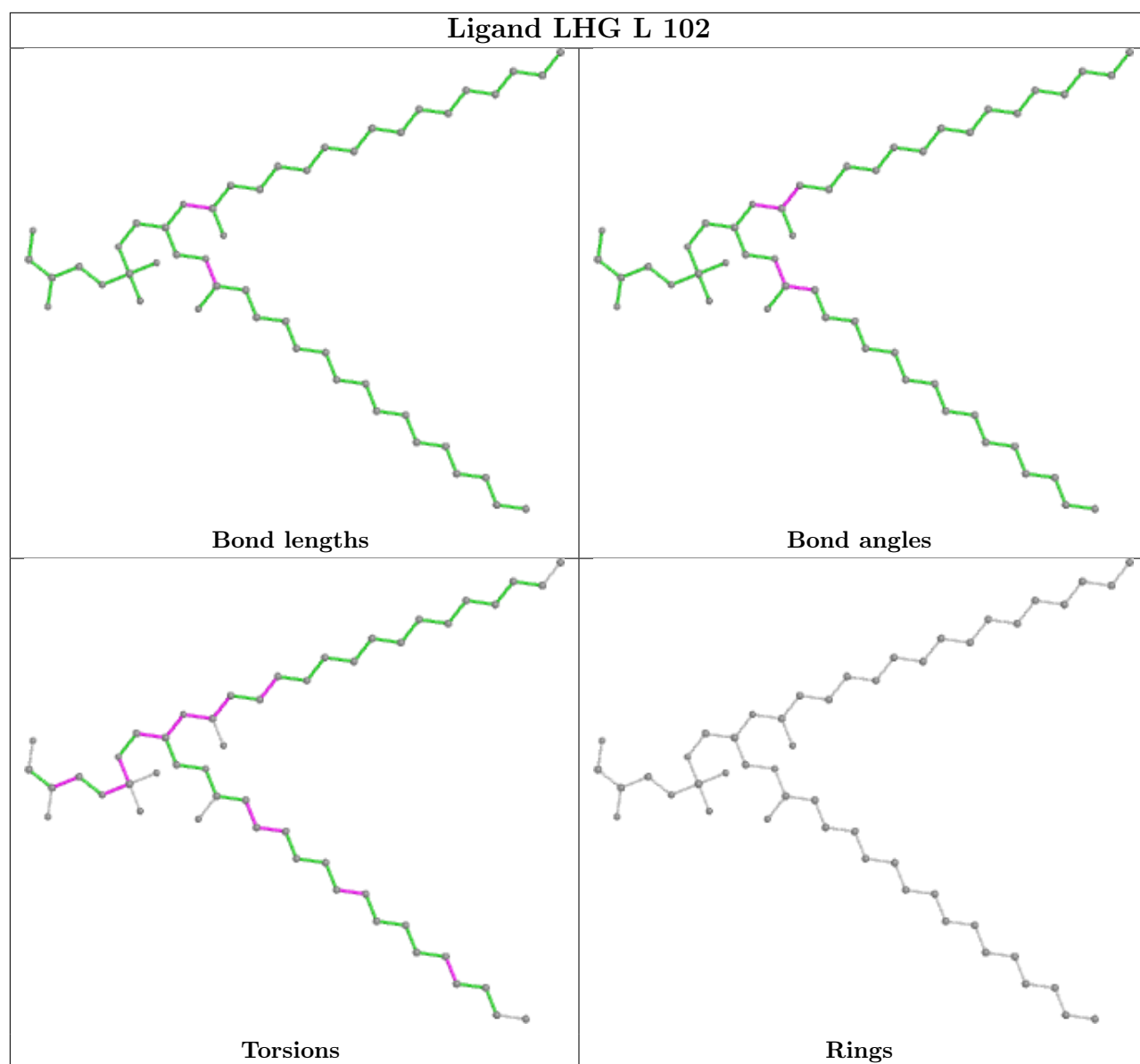
Torsions

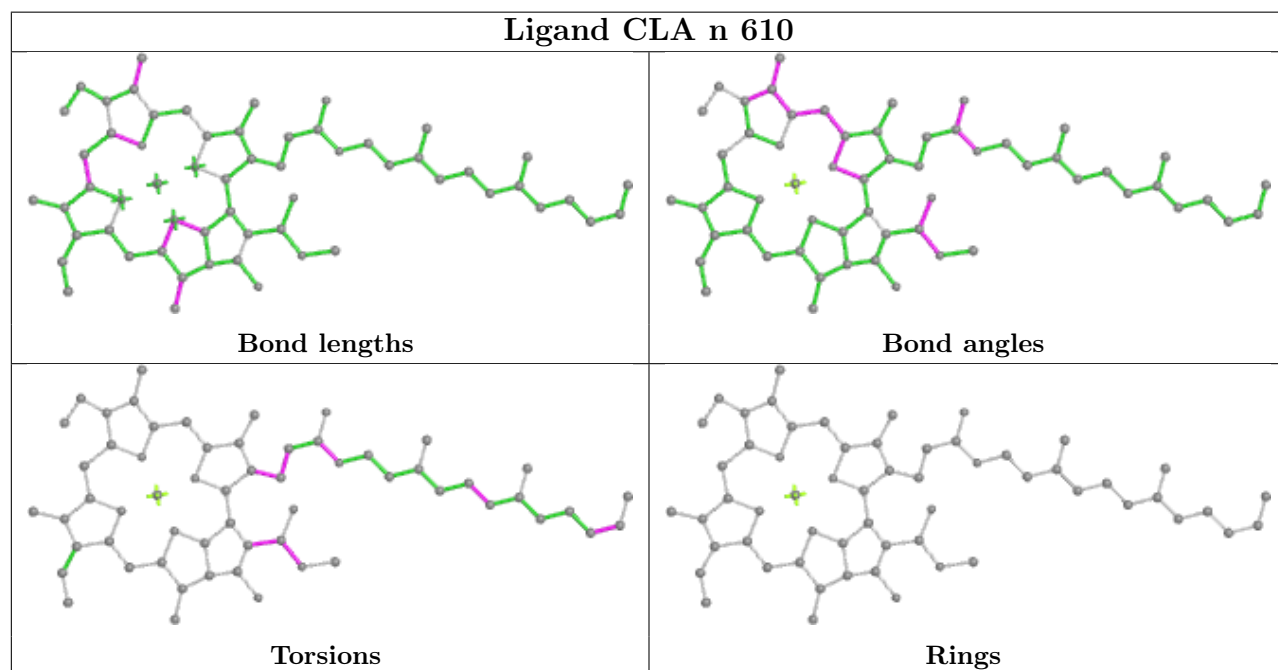
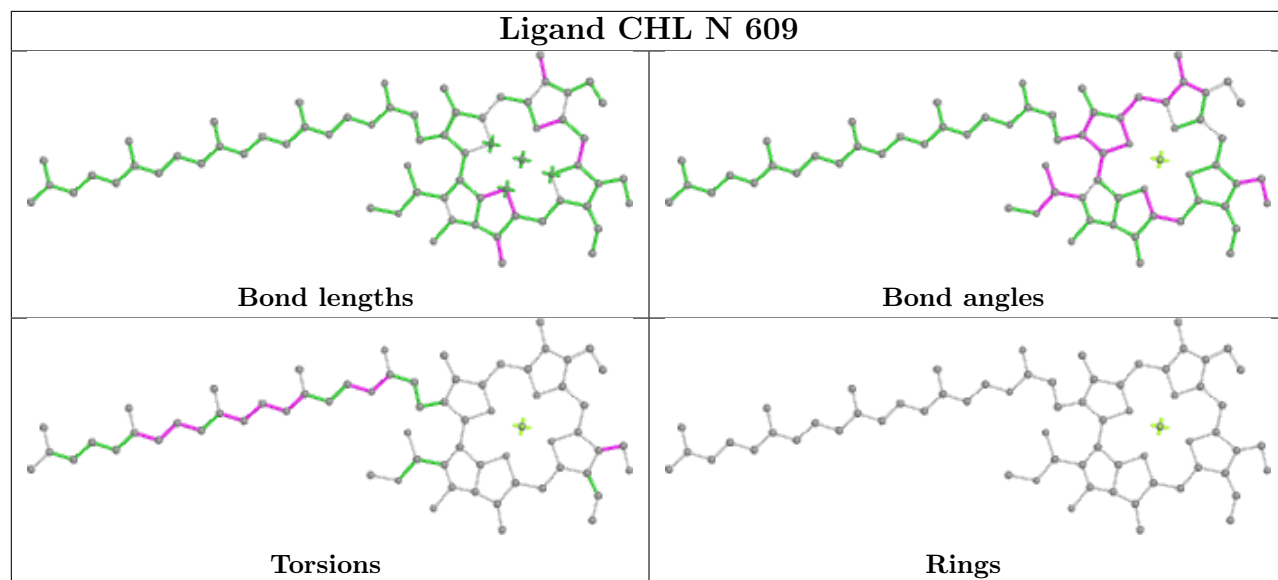


Rings

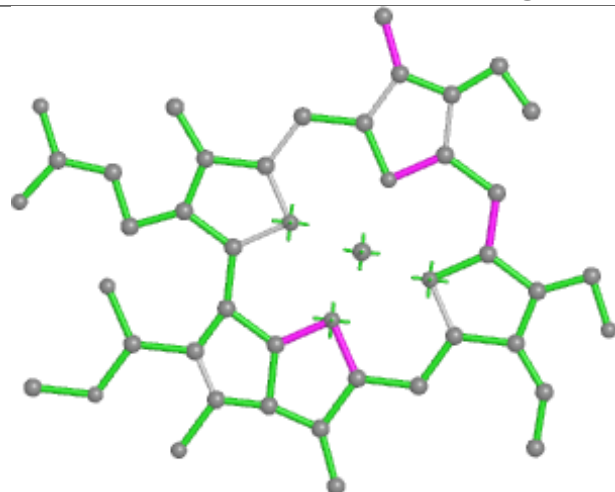


Ligand CLA B 606**Ligand DGD b 625**

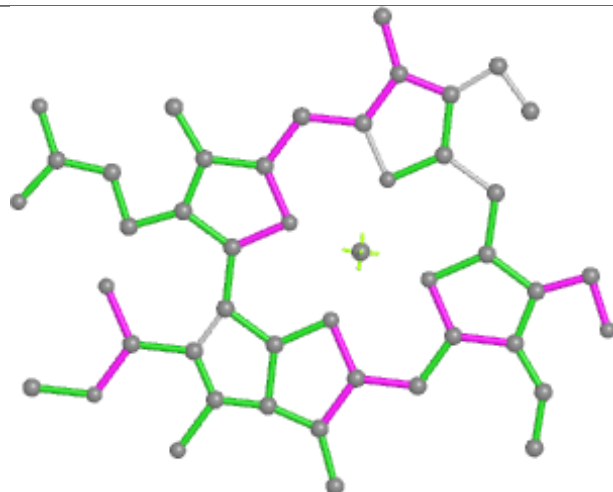




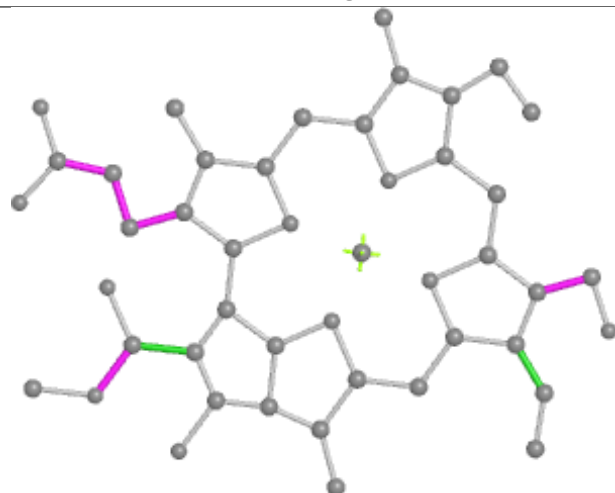
Ligand CHL S 306



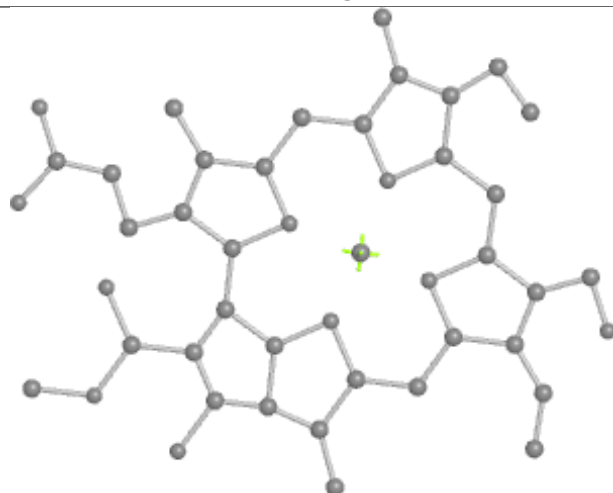
Bond lengths



Bond angles

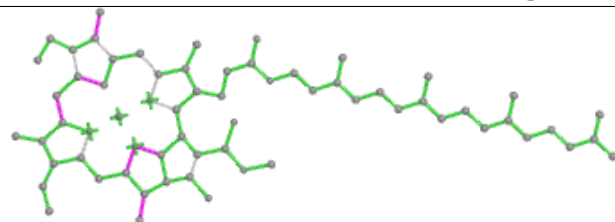


Torsions

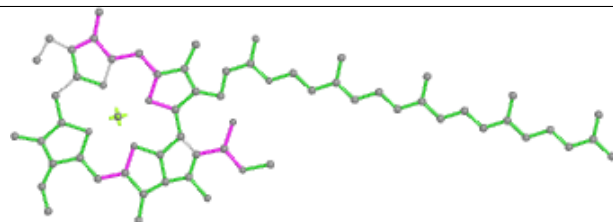


Rings

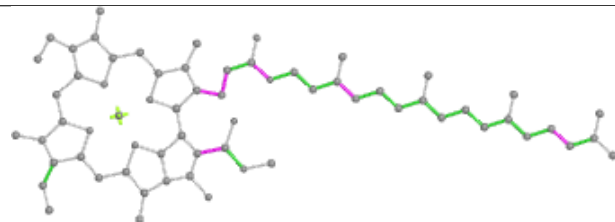
Ligand CLA r 612



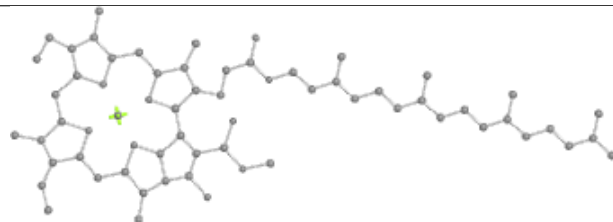
Bond lengths



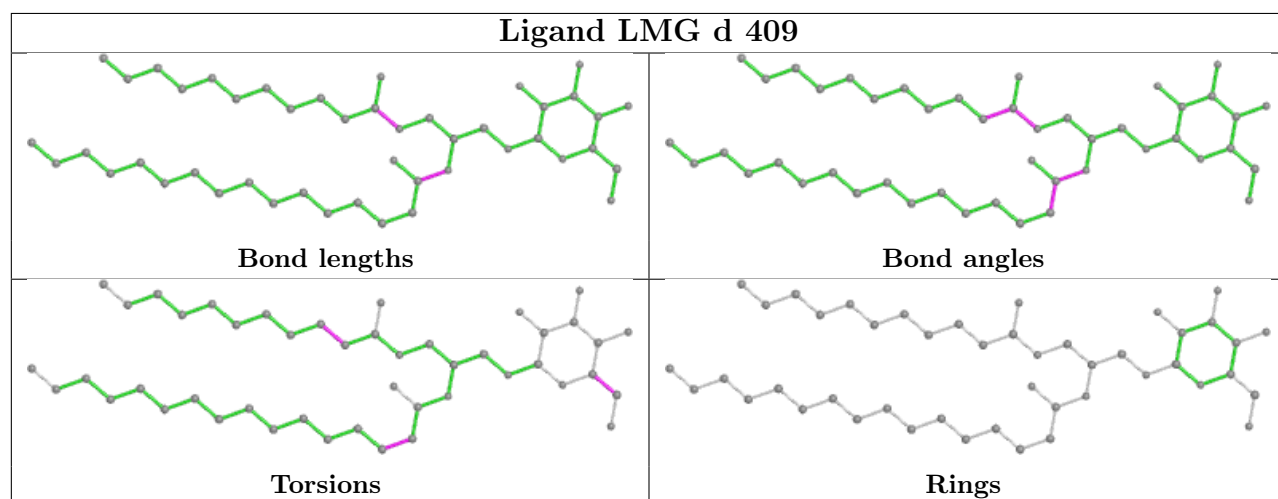
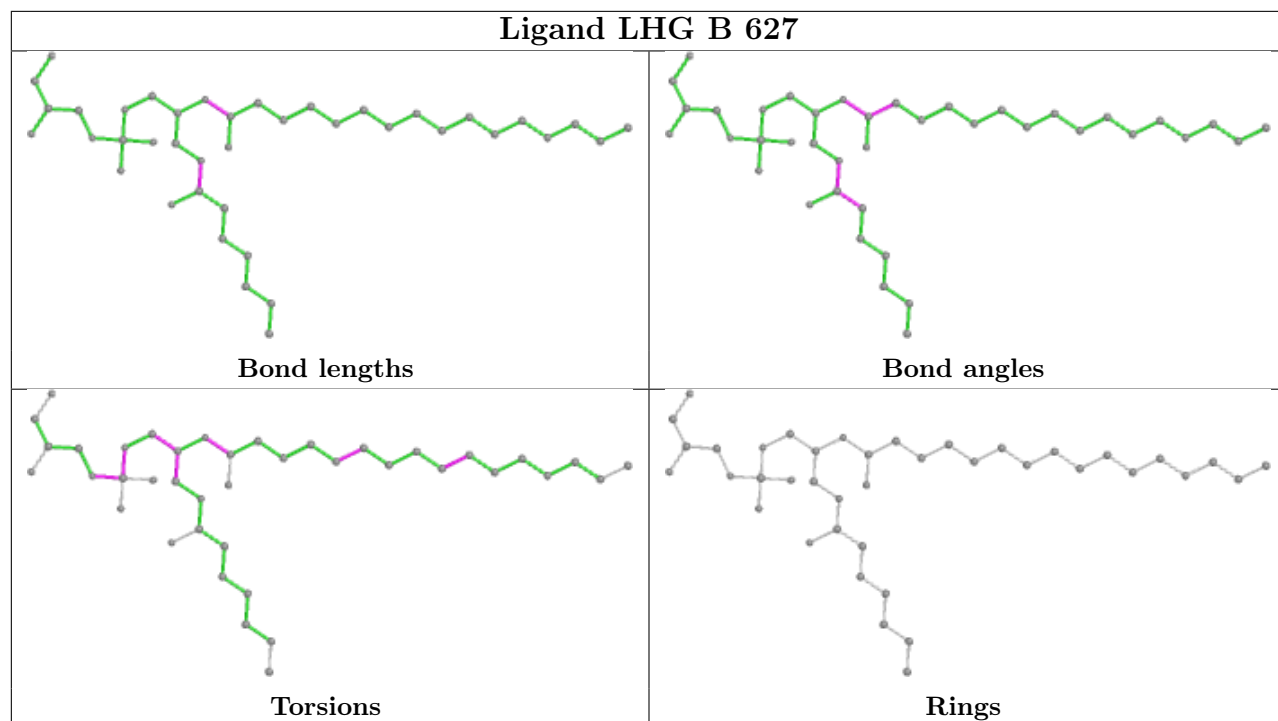
Bond angles

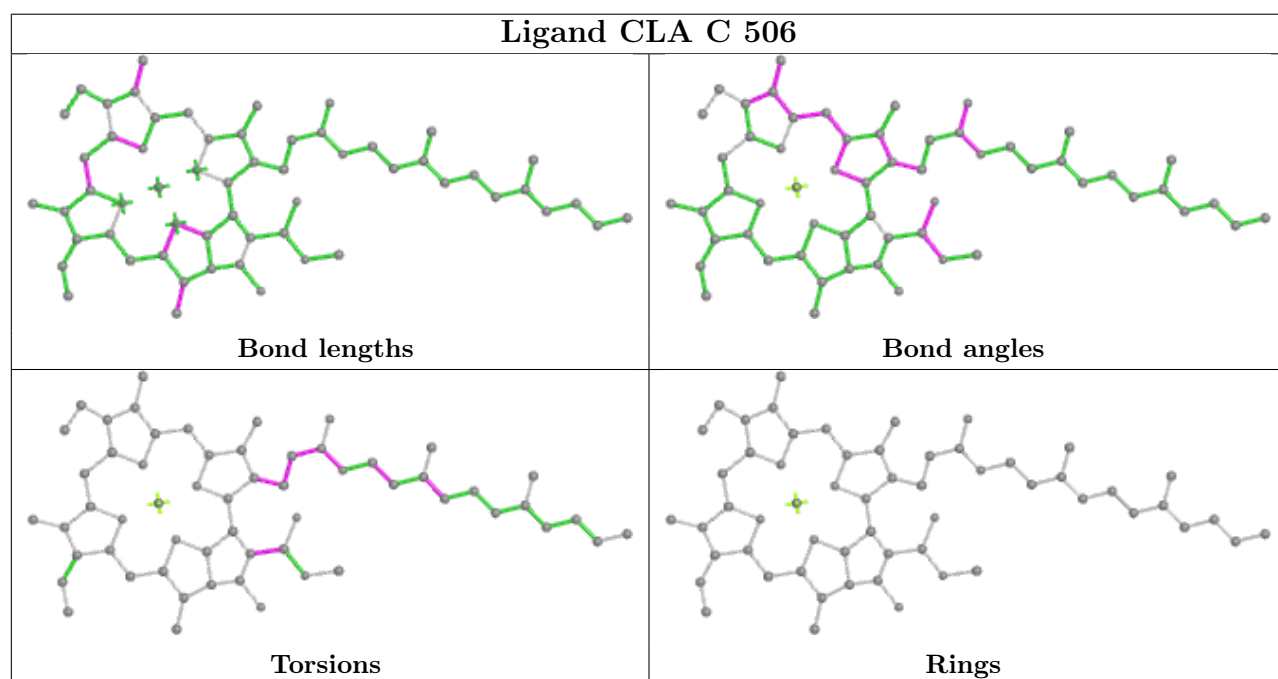
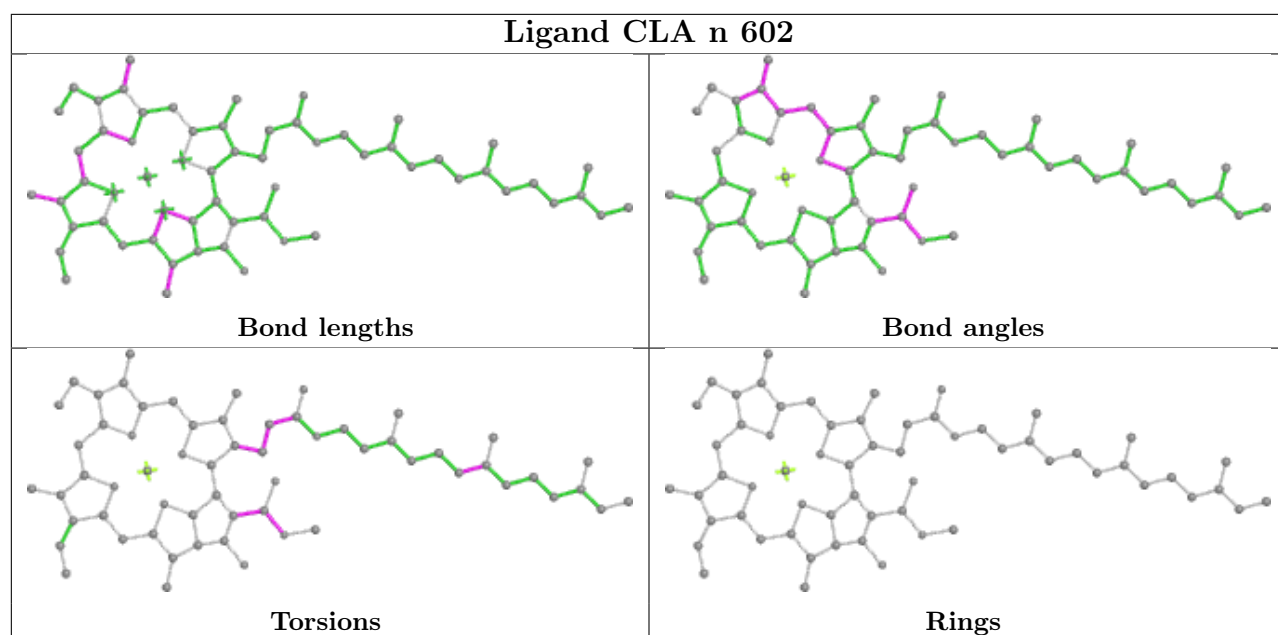


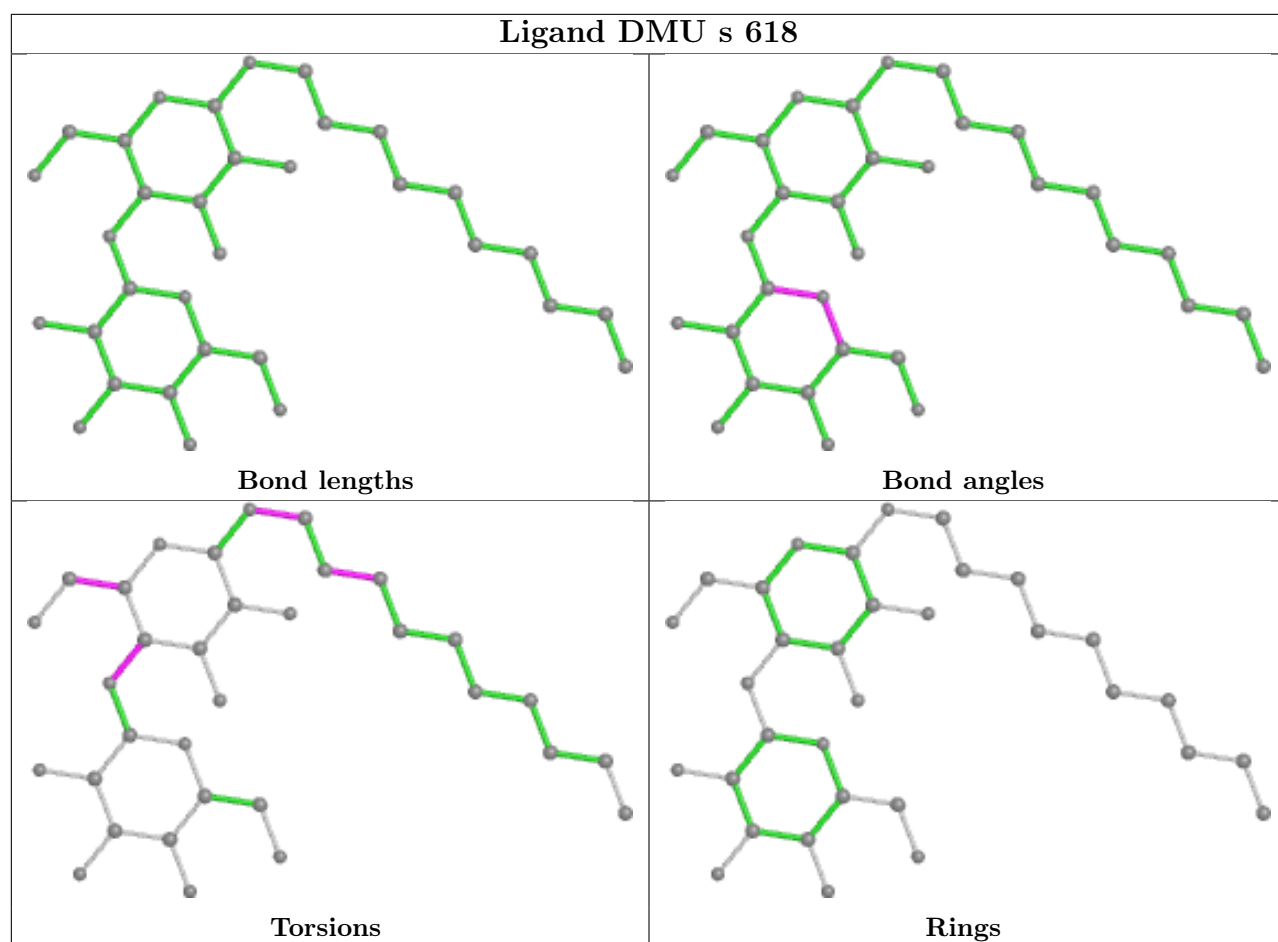
Torsions



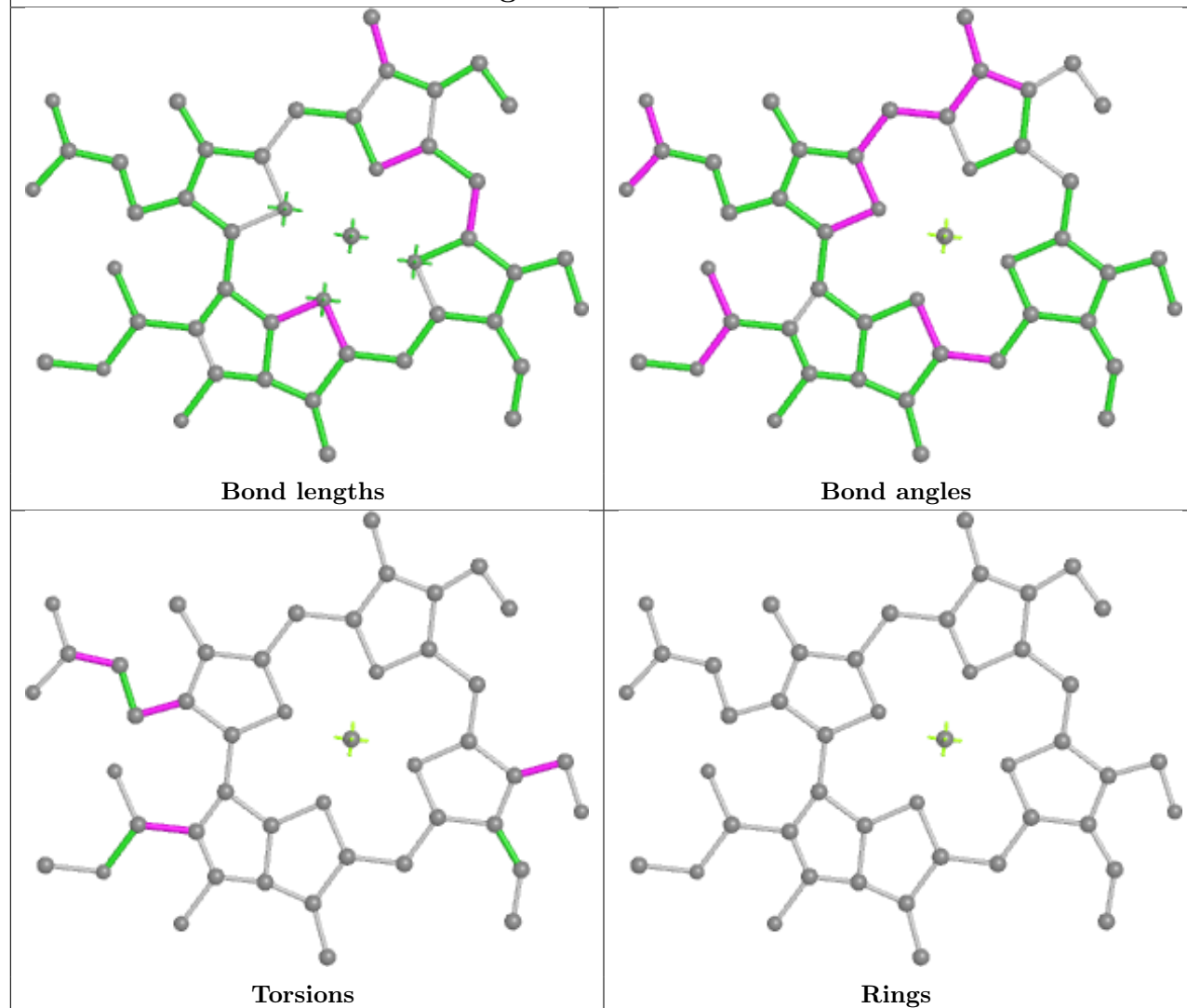
Rings



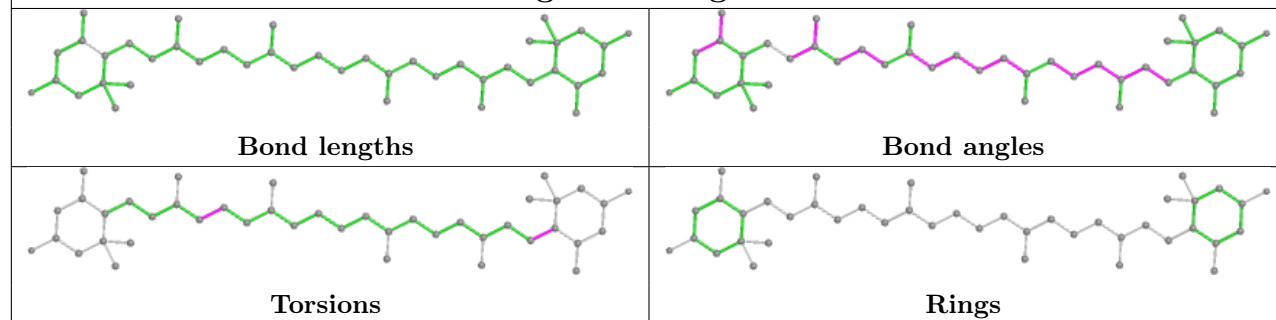


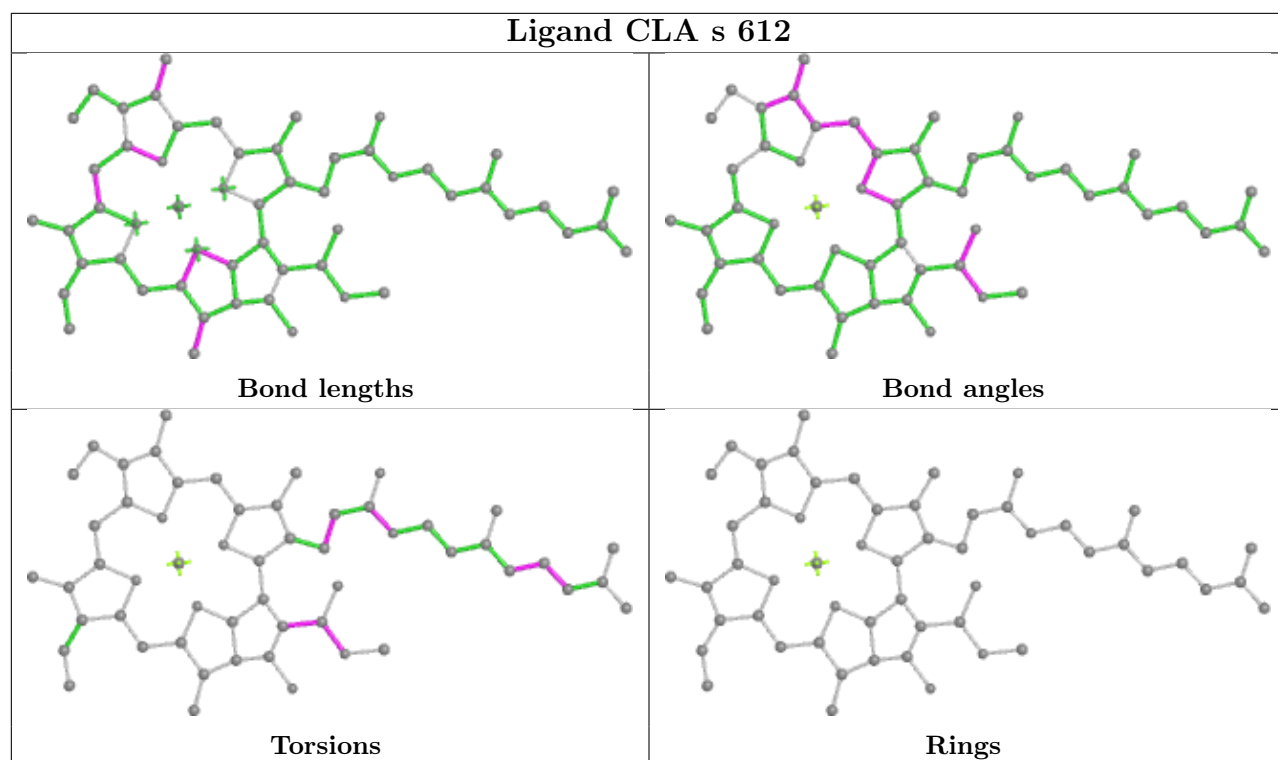
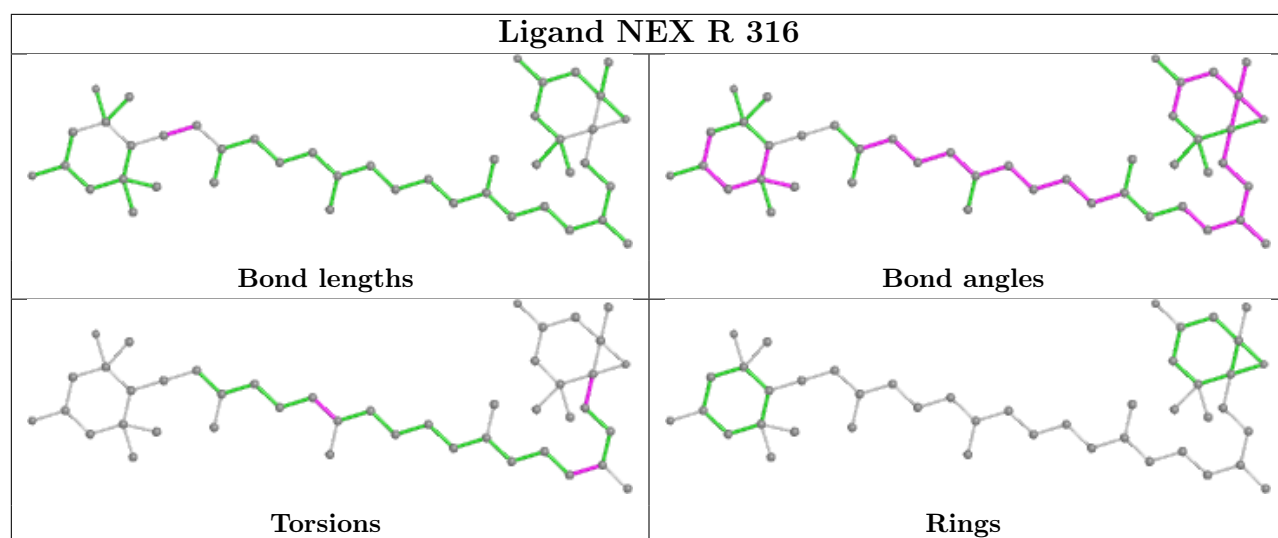


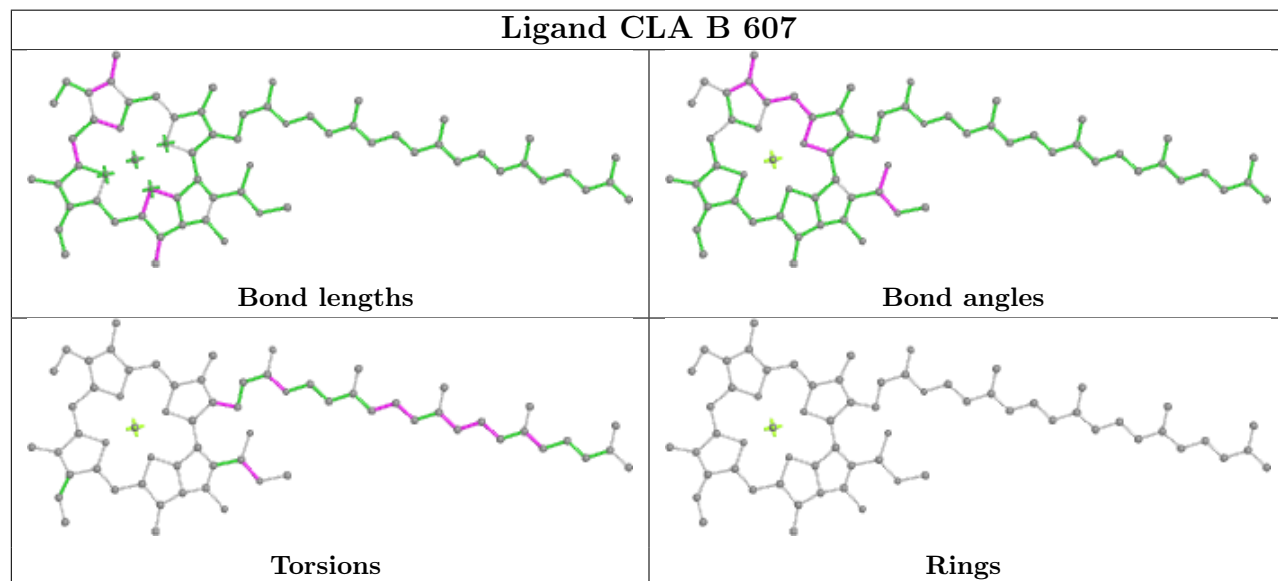
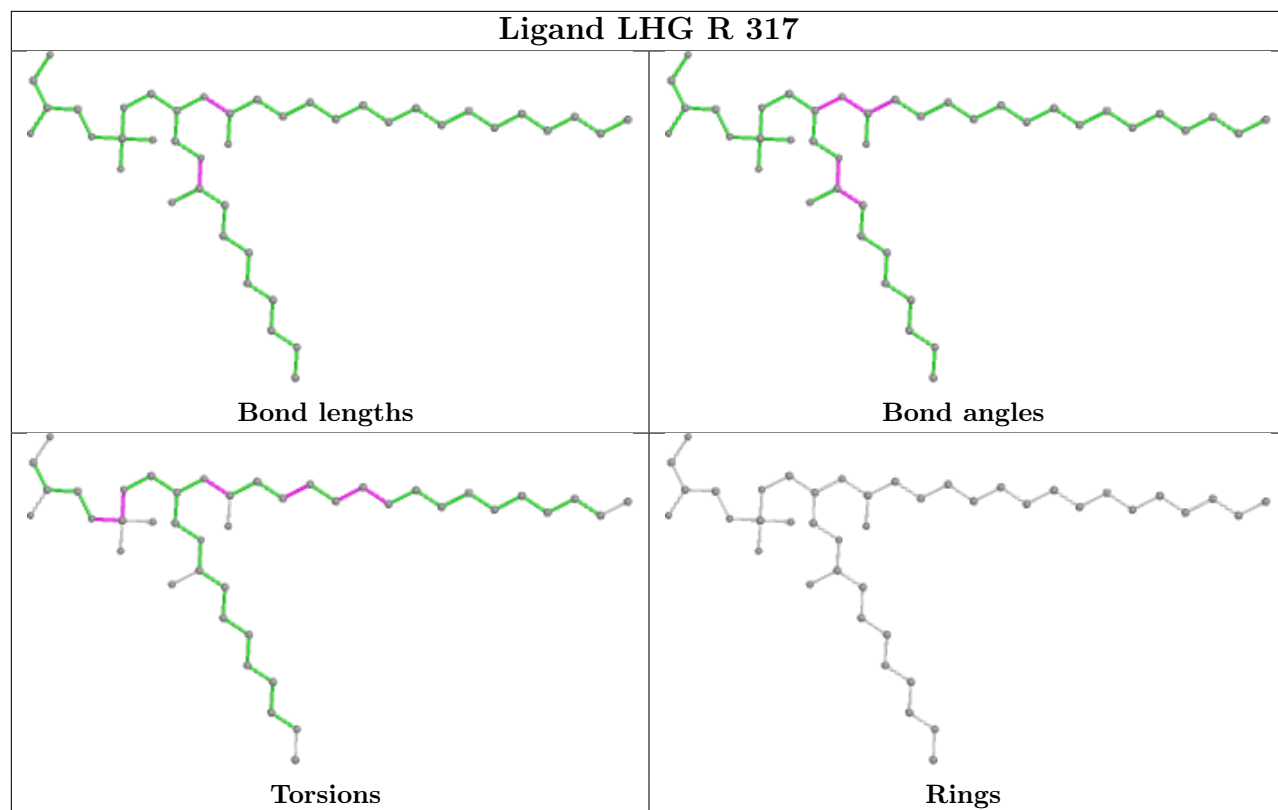
Ligand CHL r 605

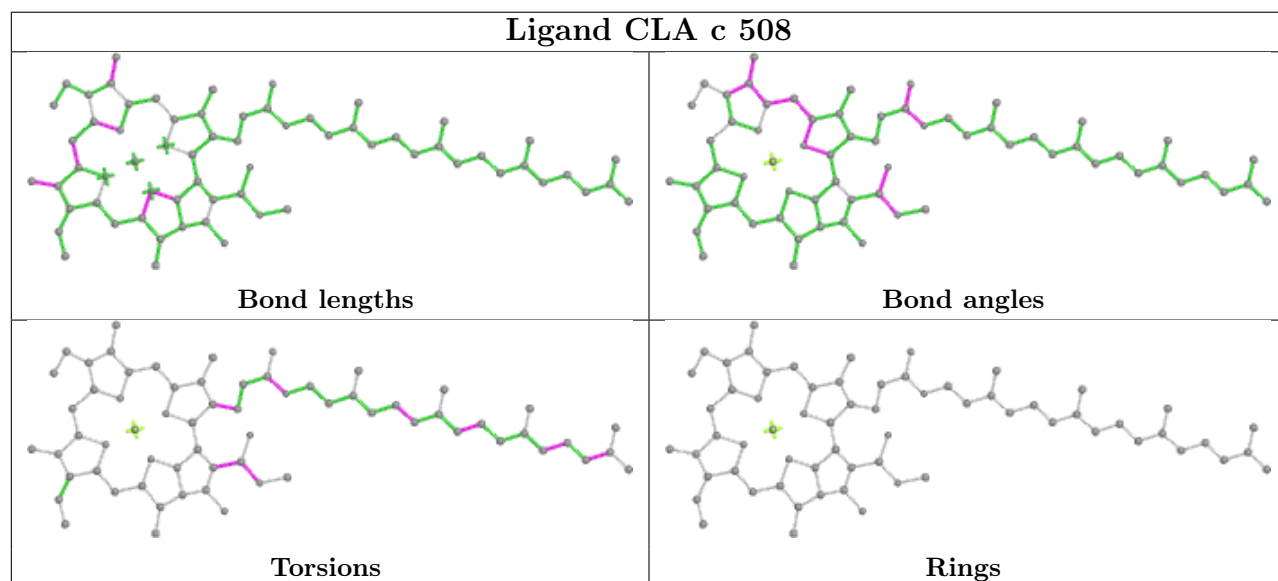
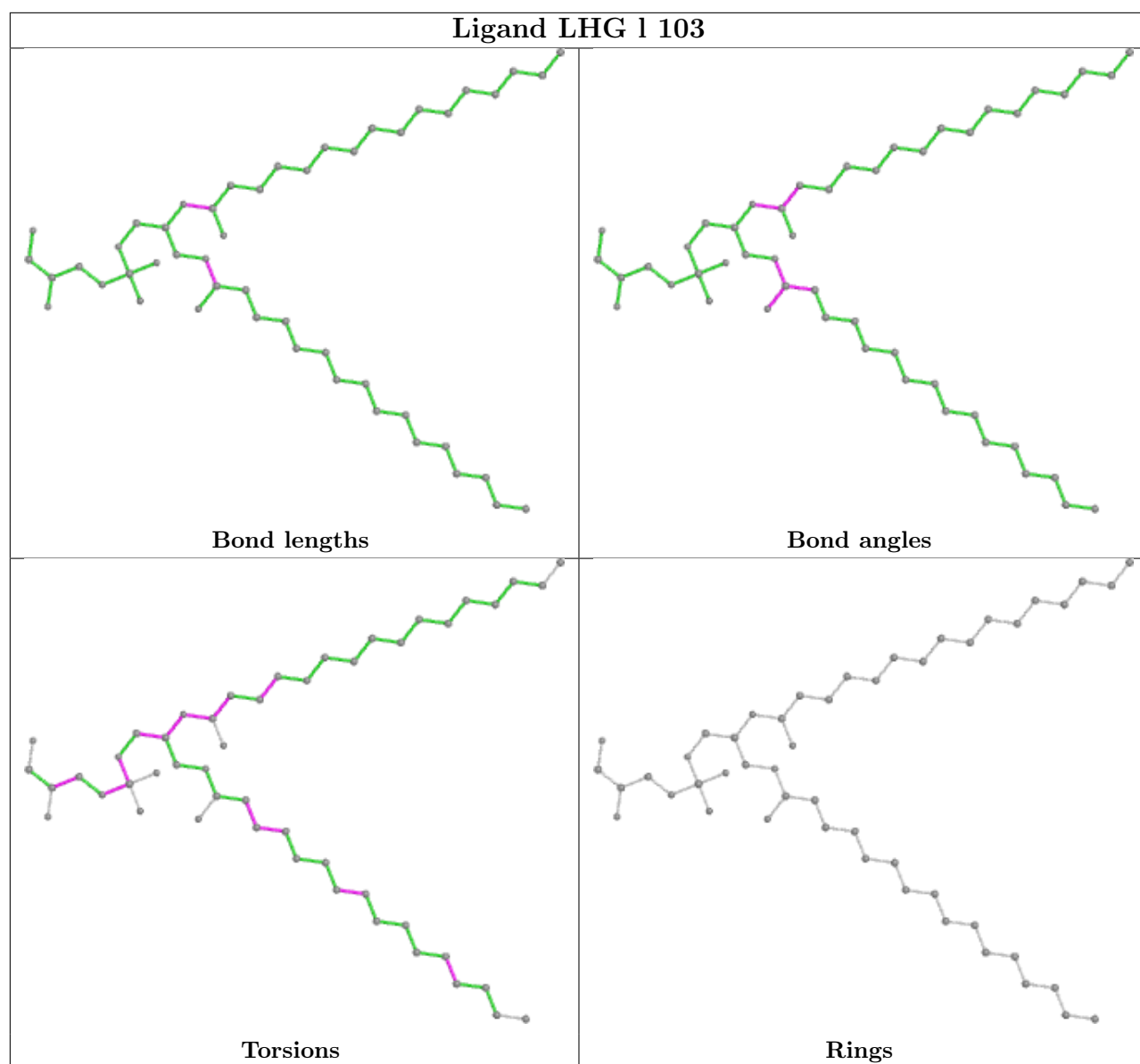


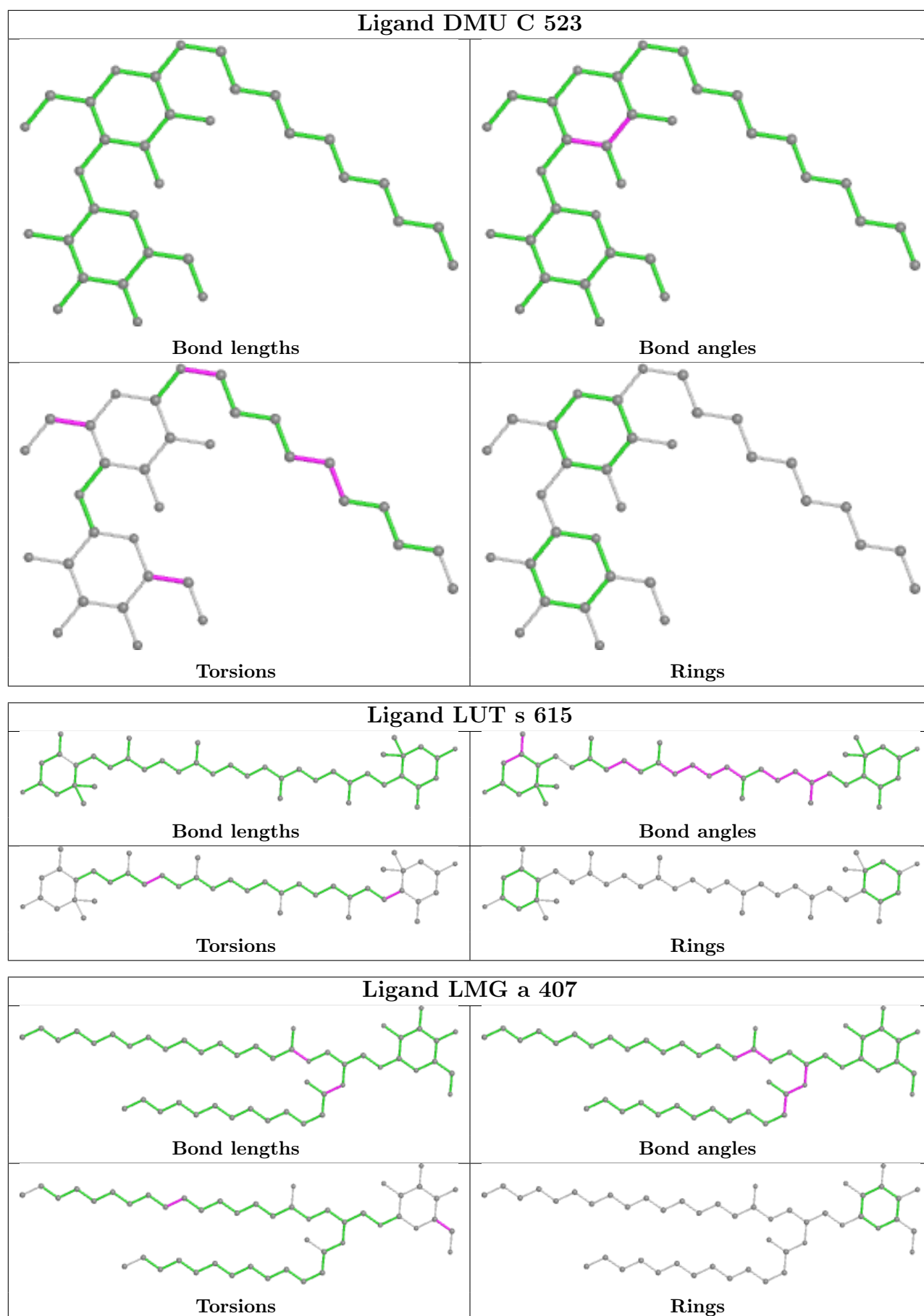
Ligand LUT g 615

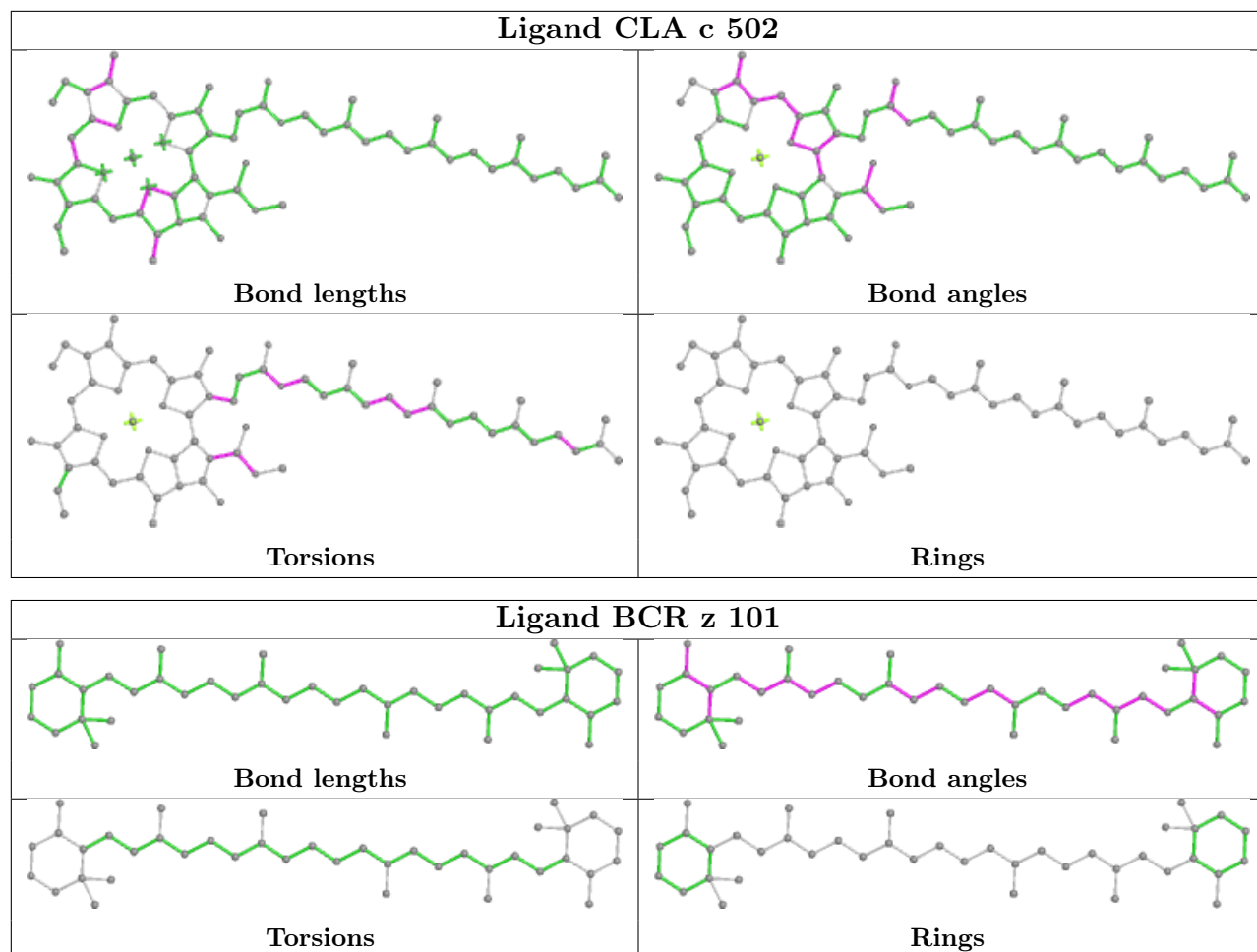




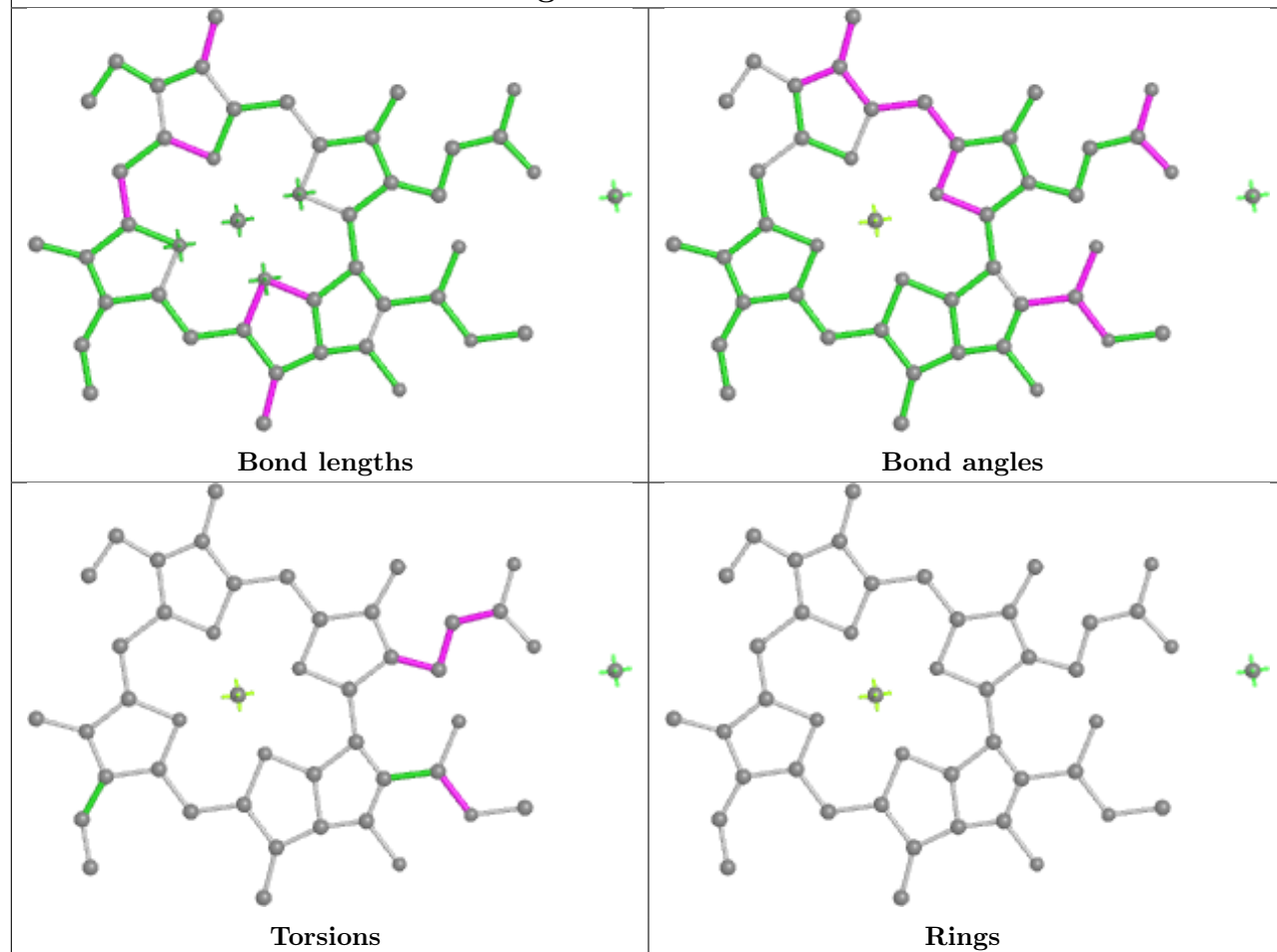




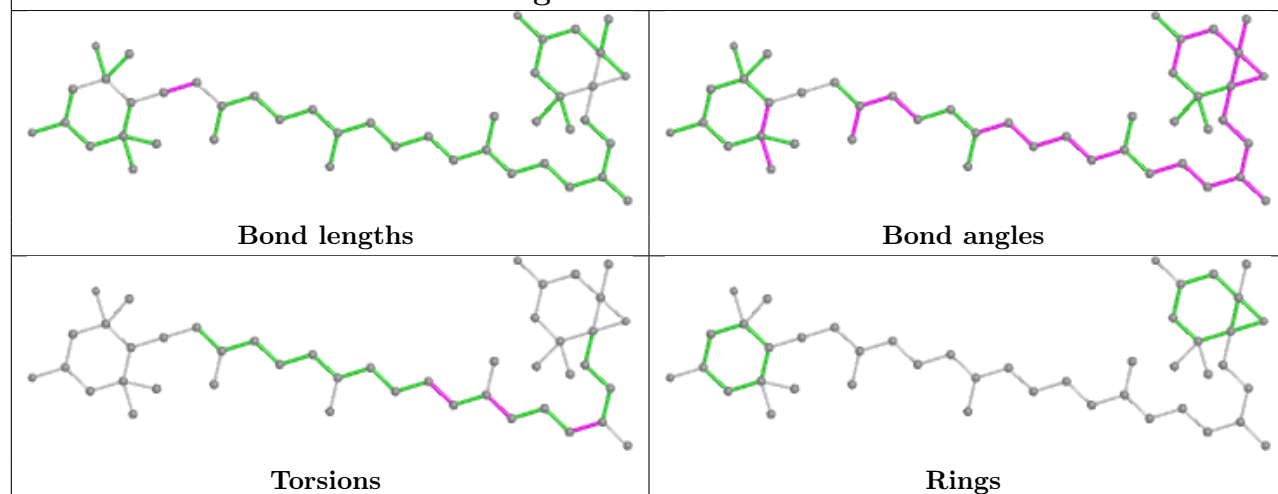


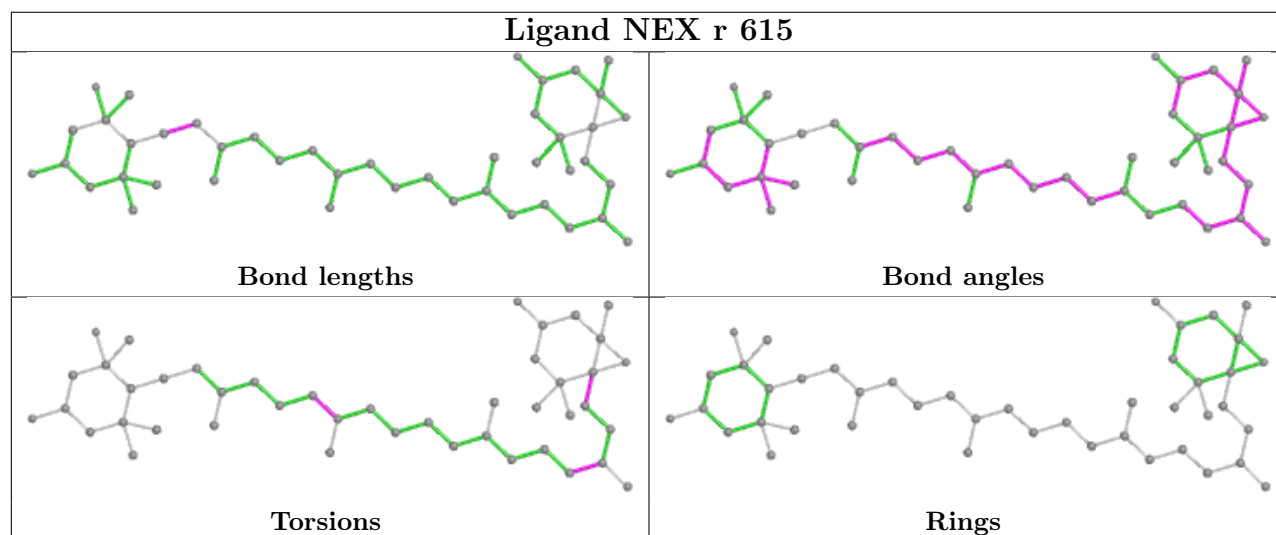
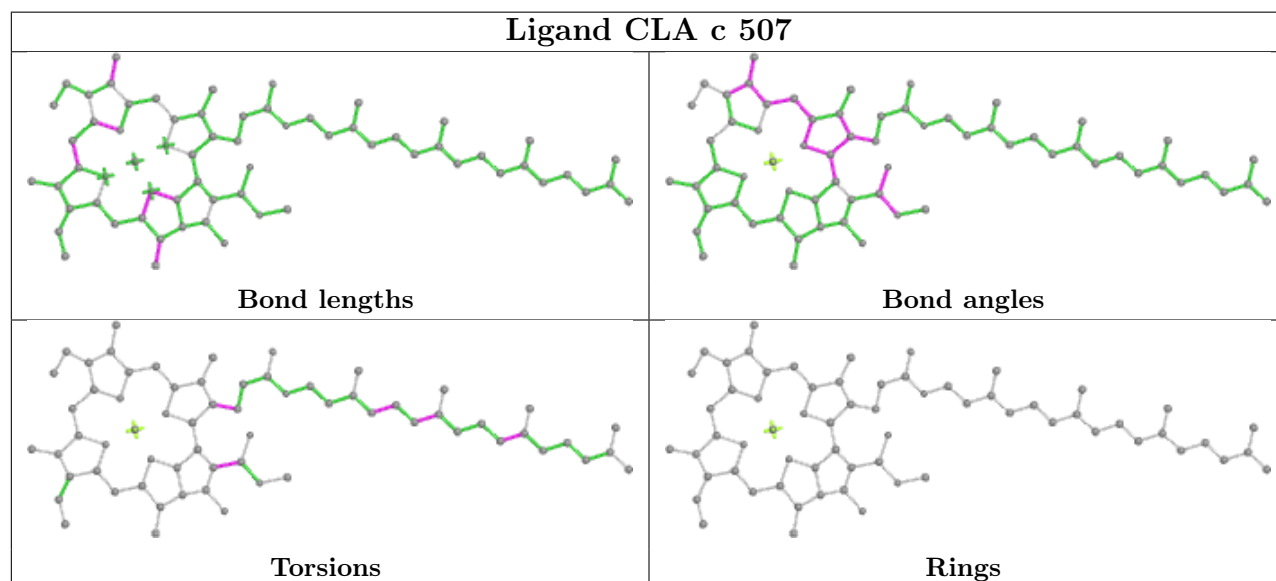
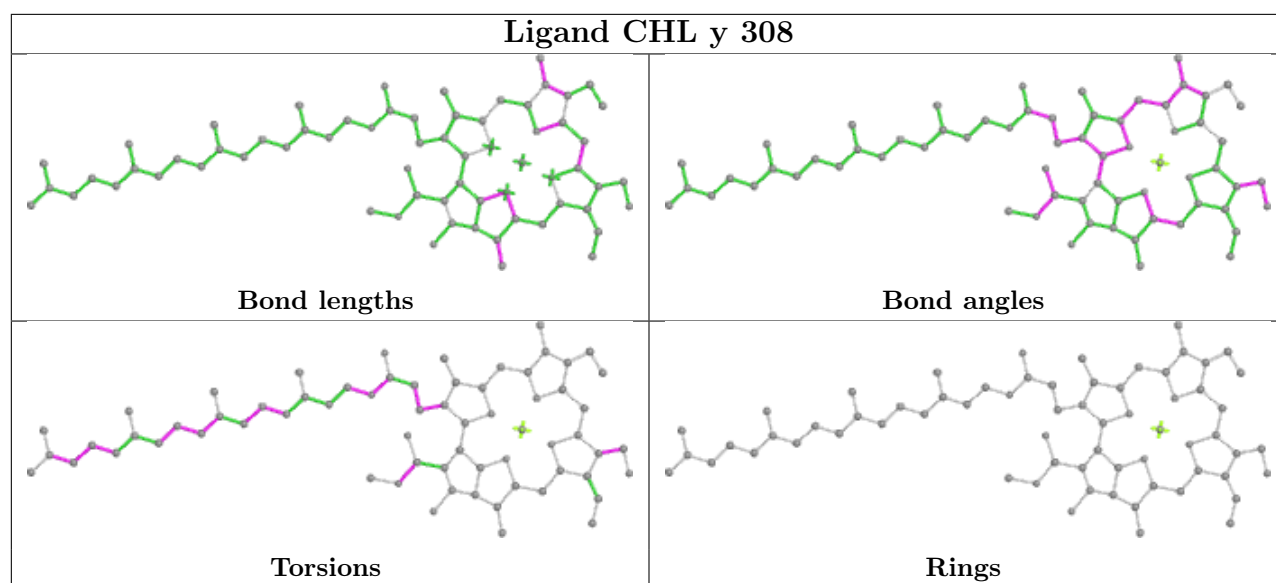


Ligand CLA s 609

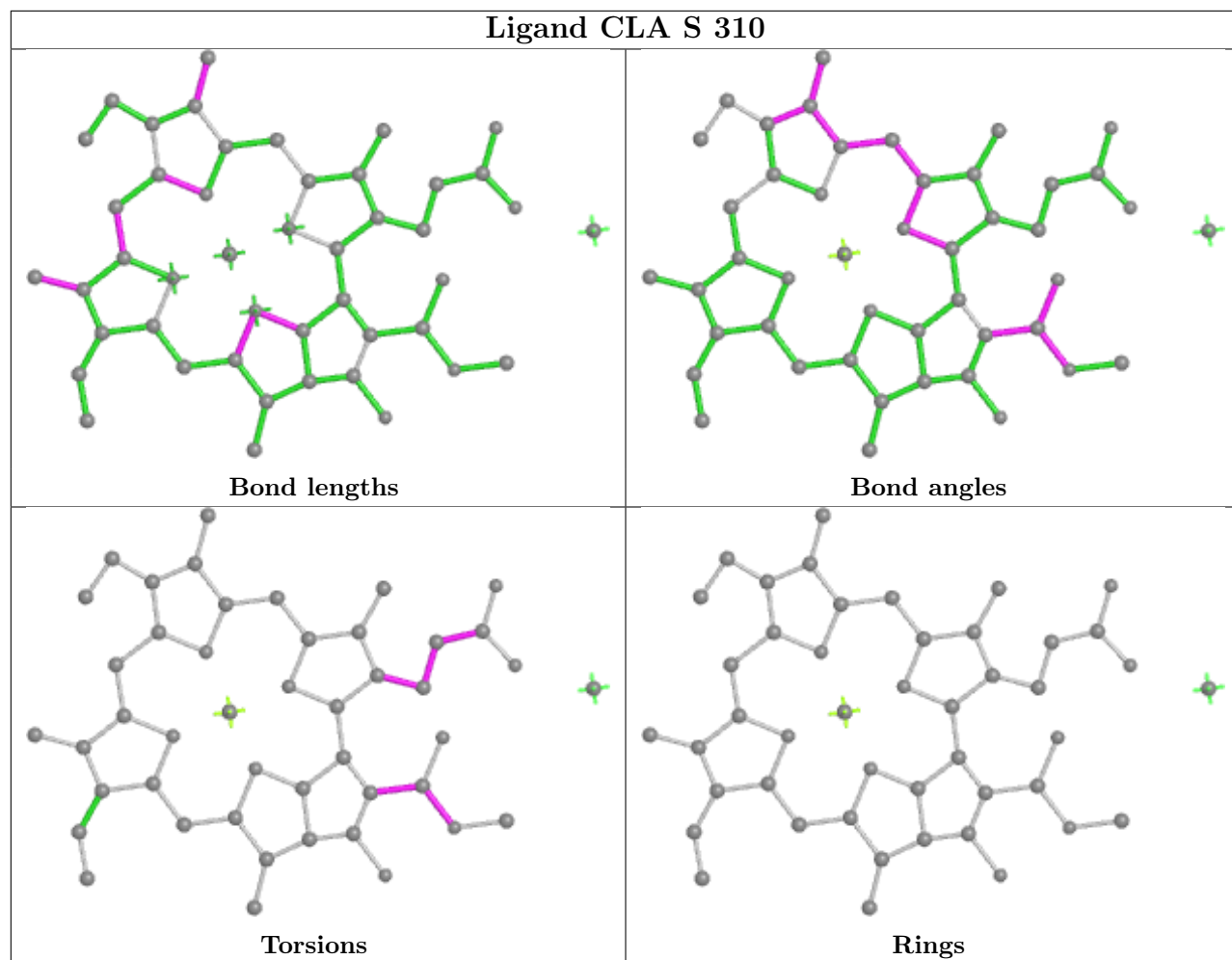


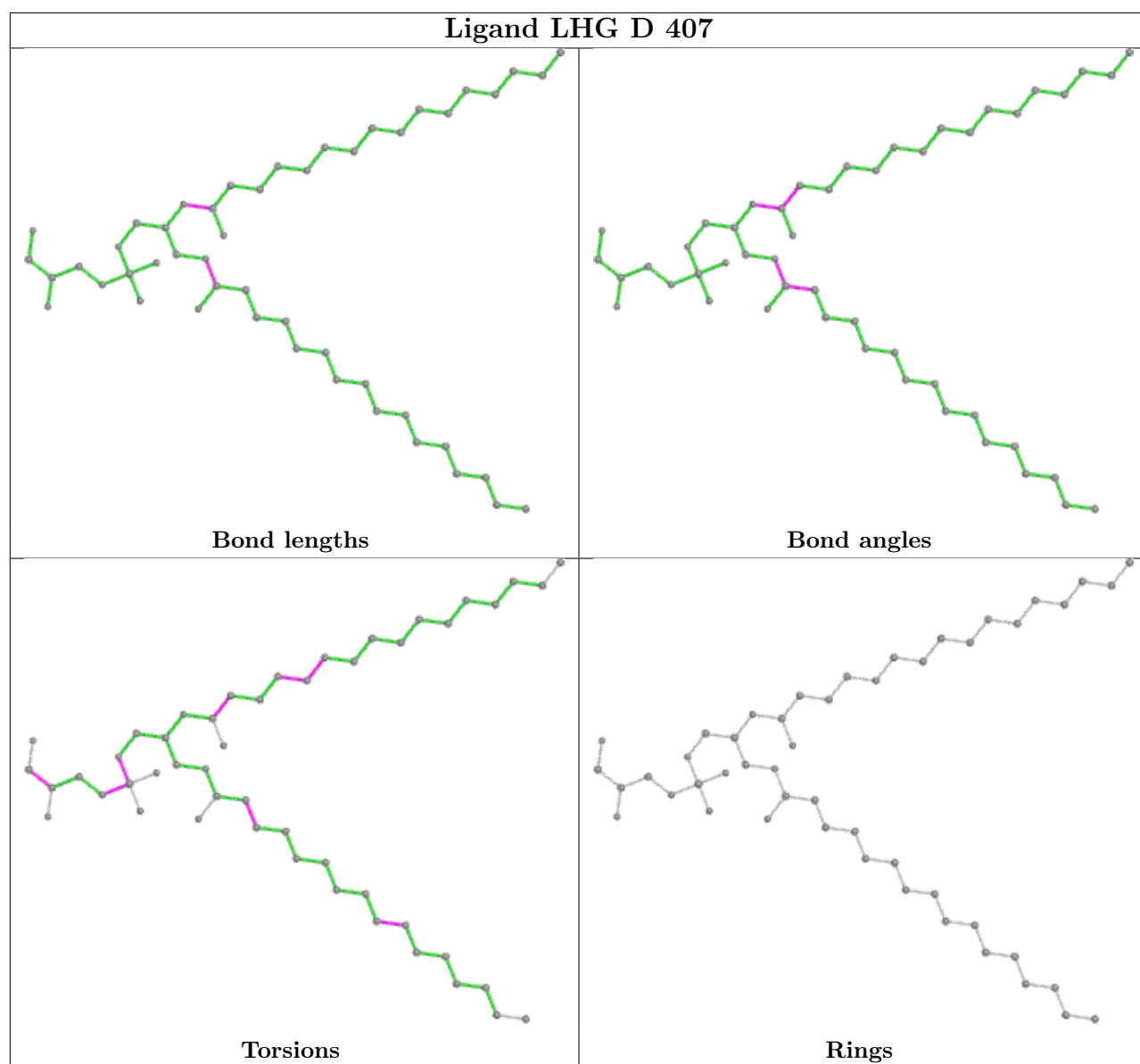
Ligand NEX n 617

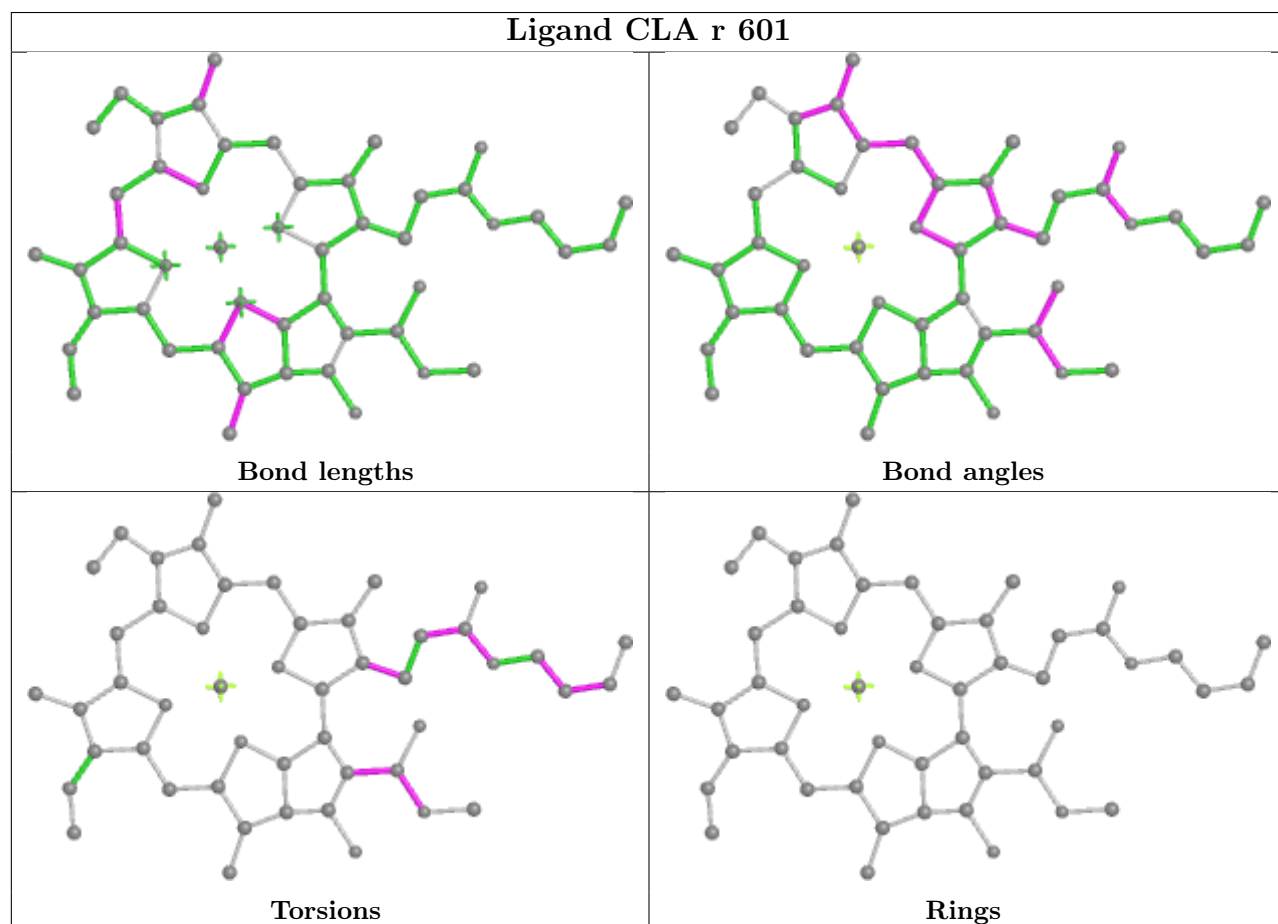
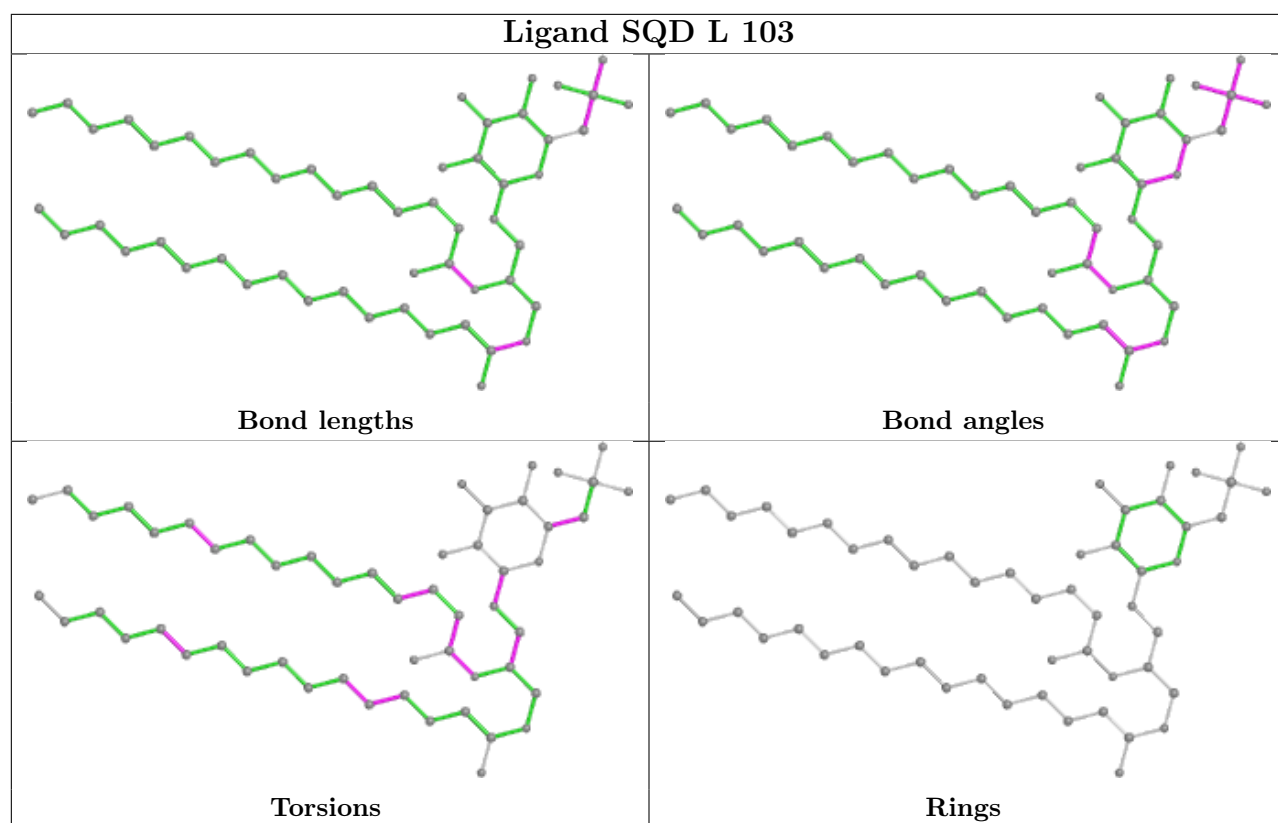


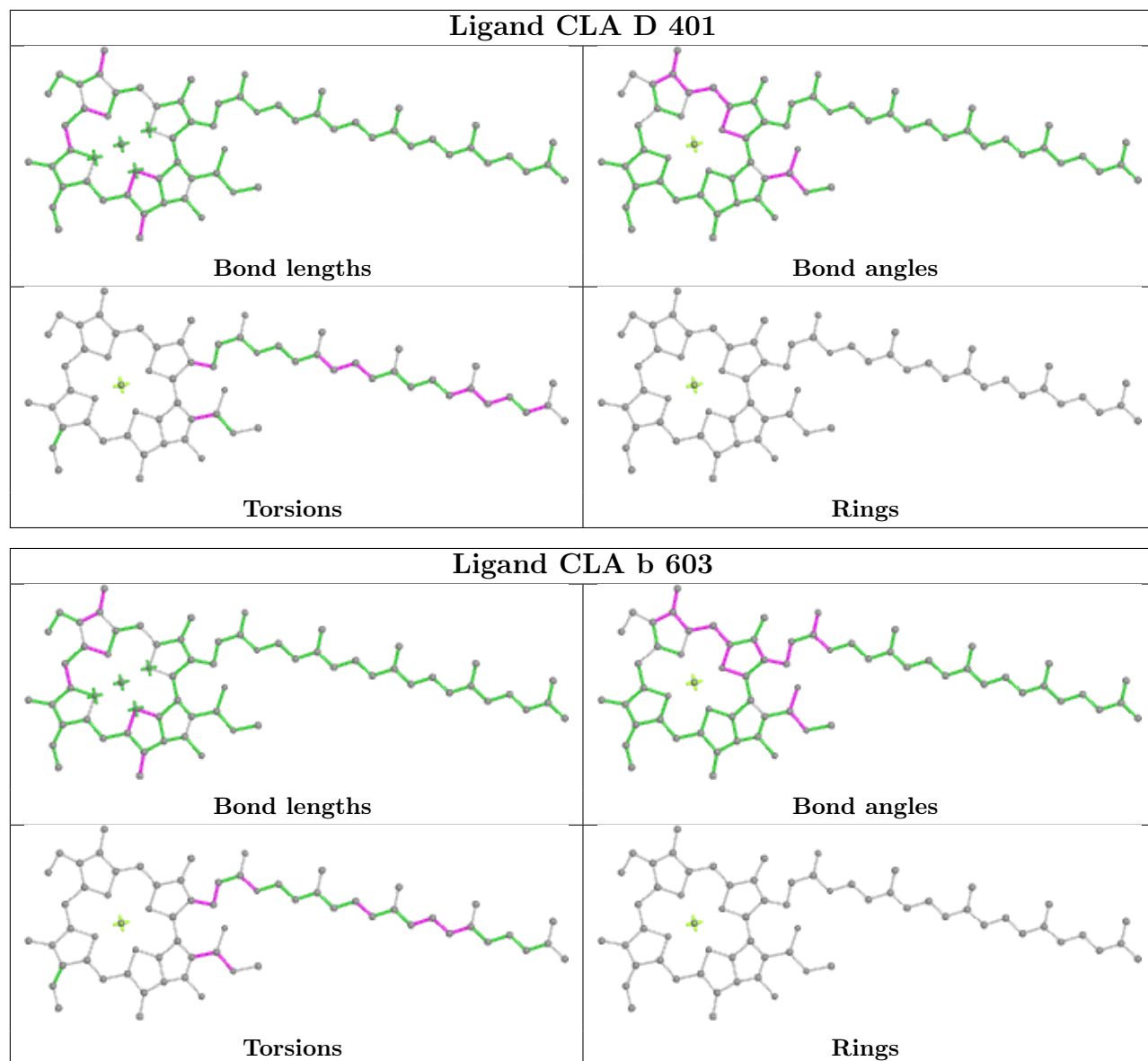


Ligand CLA S 310

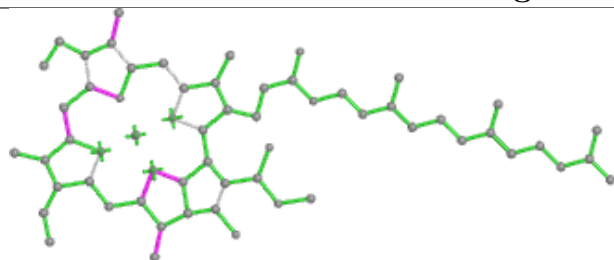




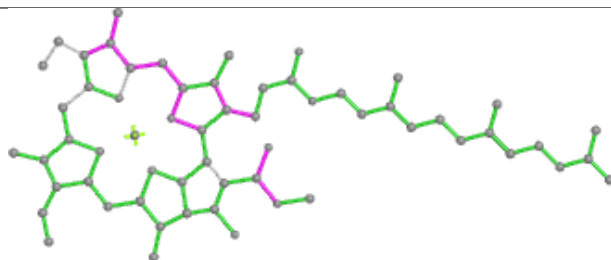




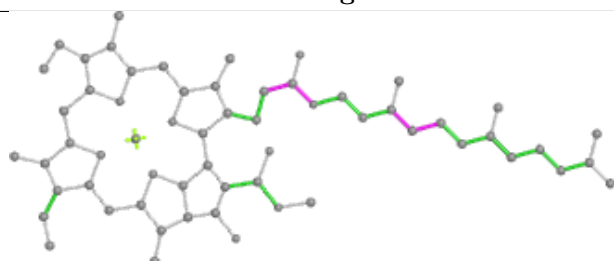
Ligand CLA R 304



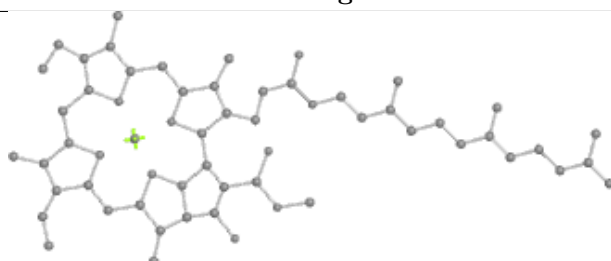
Bond lengths



Bond angles

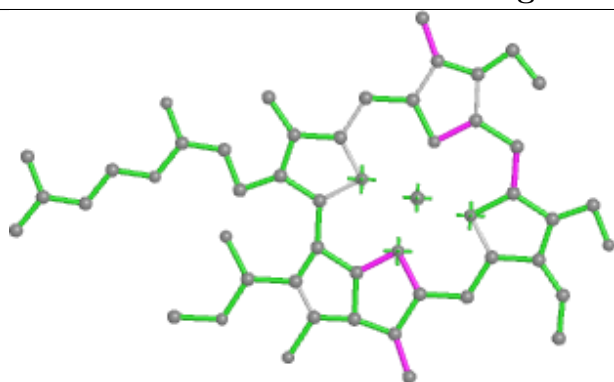


Torsions

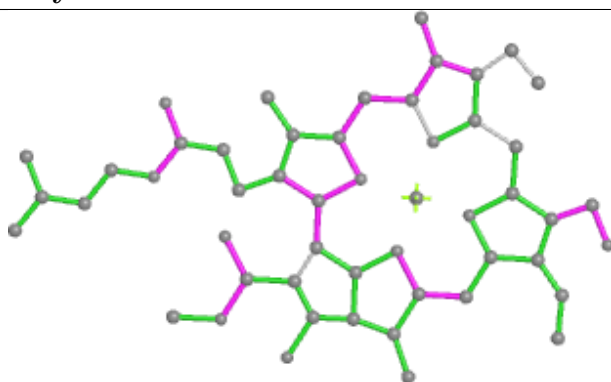


Rings

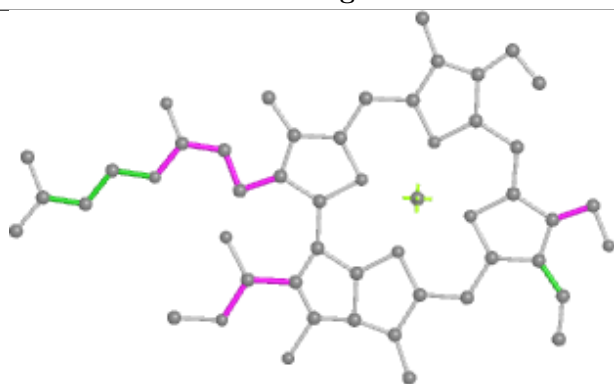
Ligand CHL y 306



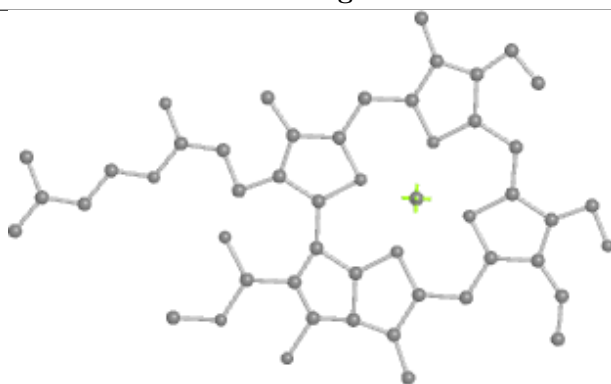
Bond lengths



Bond angles

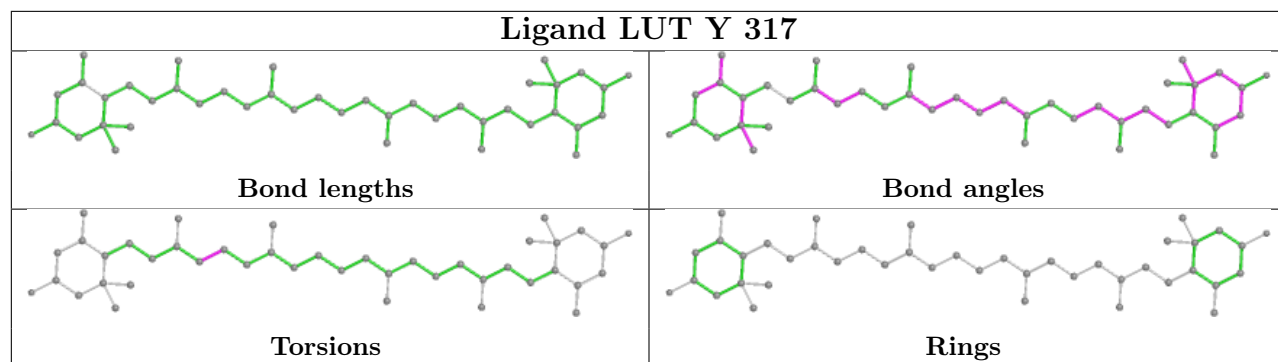


Torsions

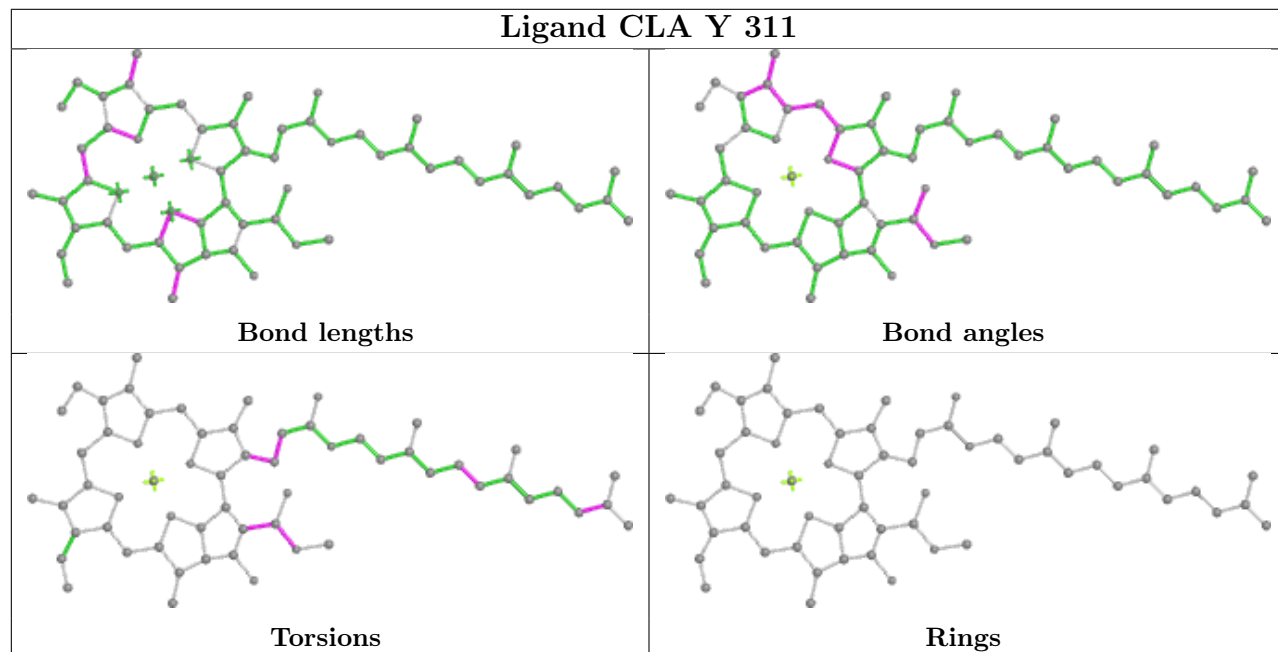


Rings

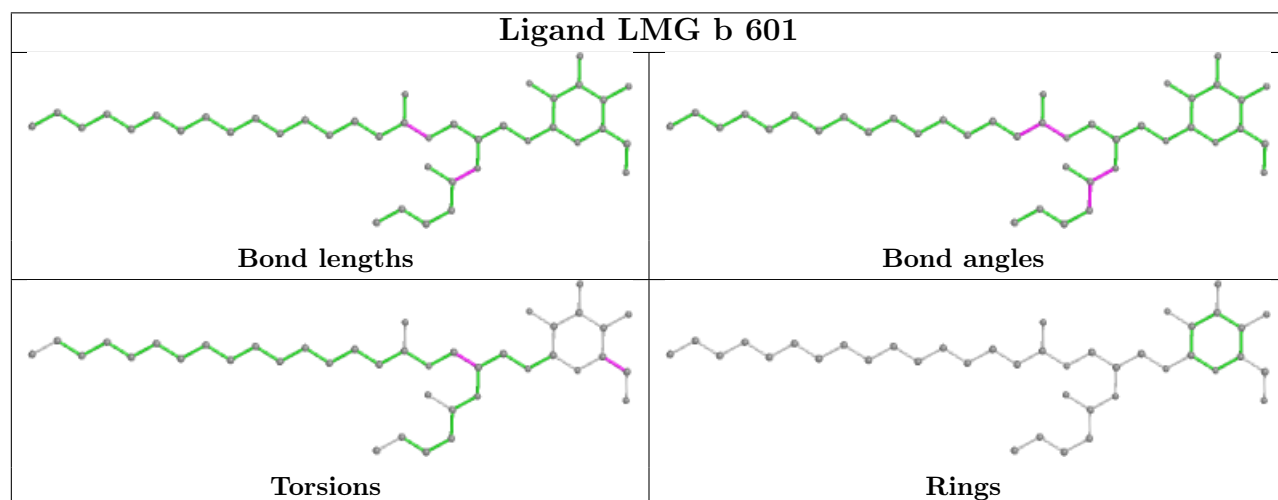
Ligand LUT Y 317

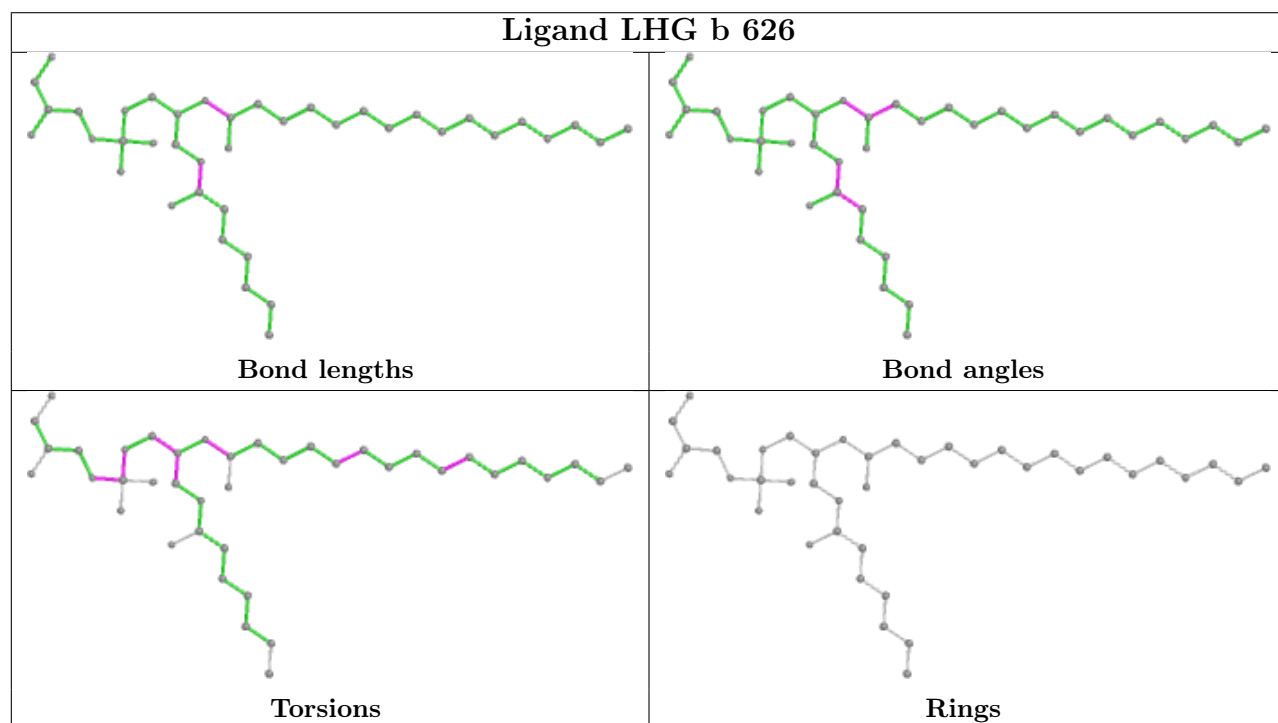
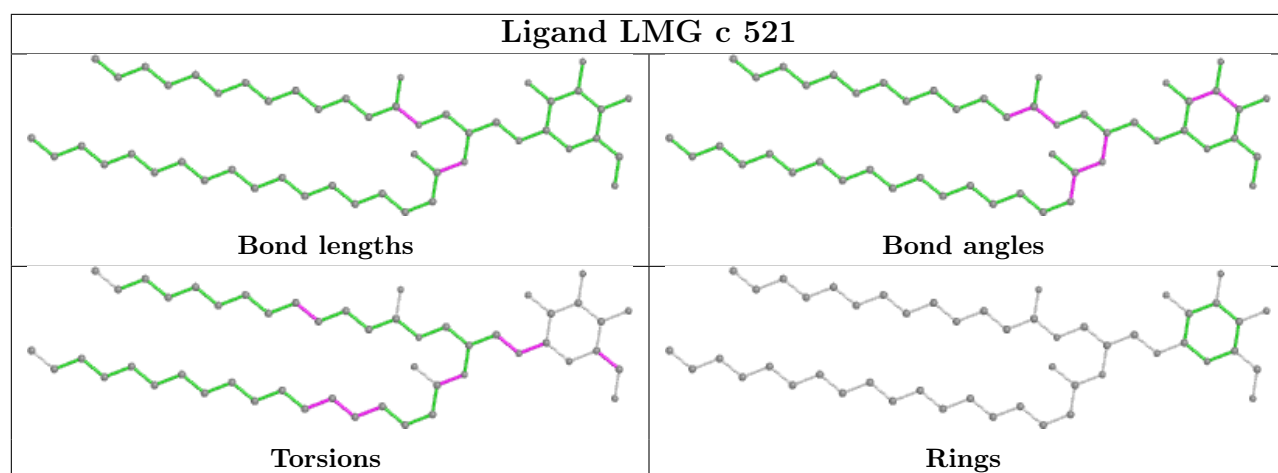


Ligand CLA Y 311

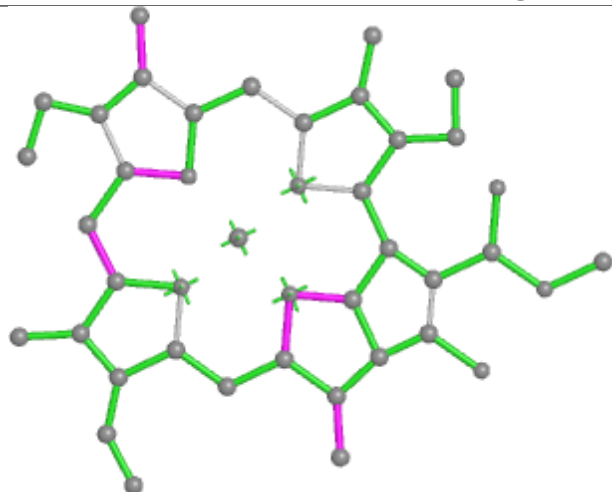


Ligand LMG b 601

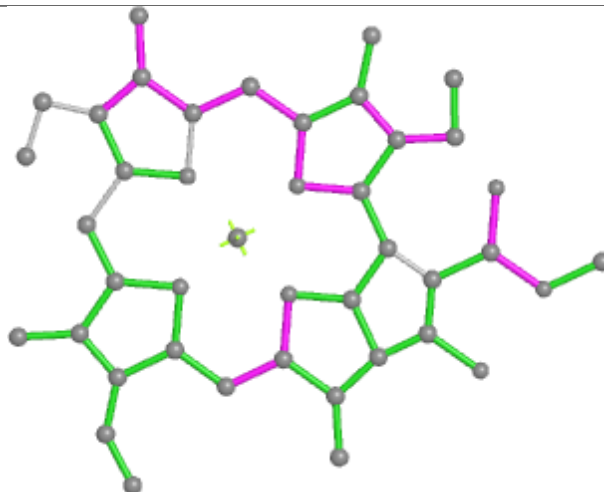




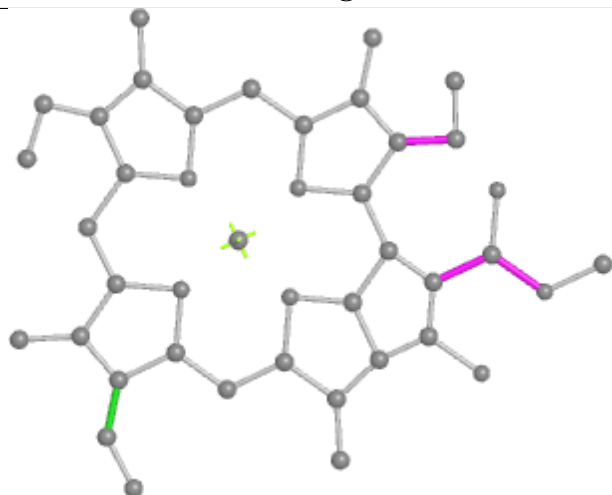
Ligand CLA G 614



Bond lengths



Bond angles

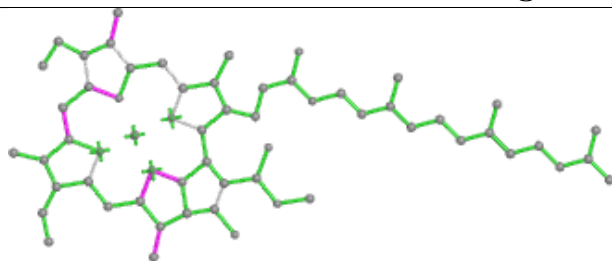


Torsions

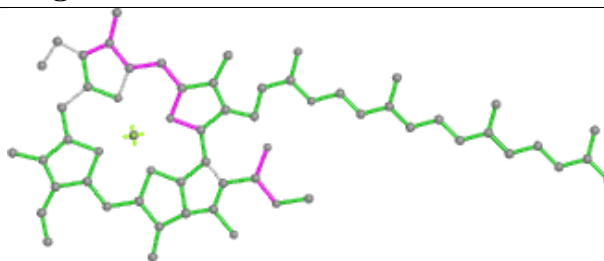


Rings

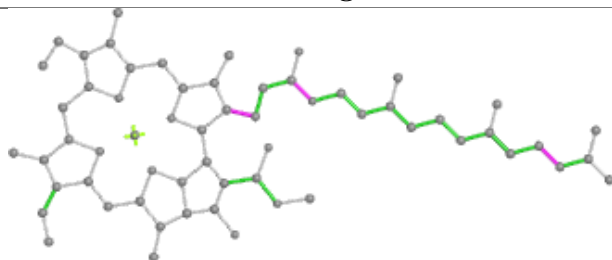
Ligand CLA g 611



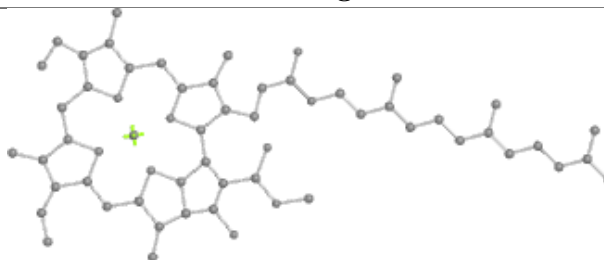
Bond lengths



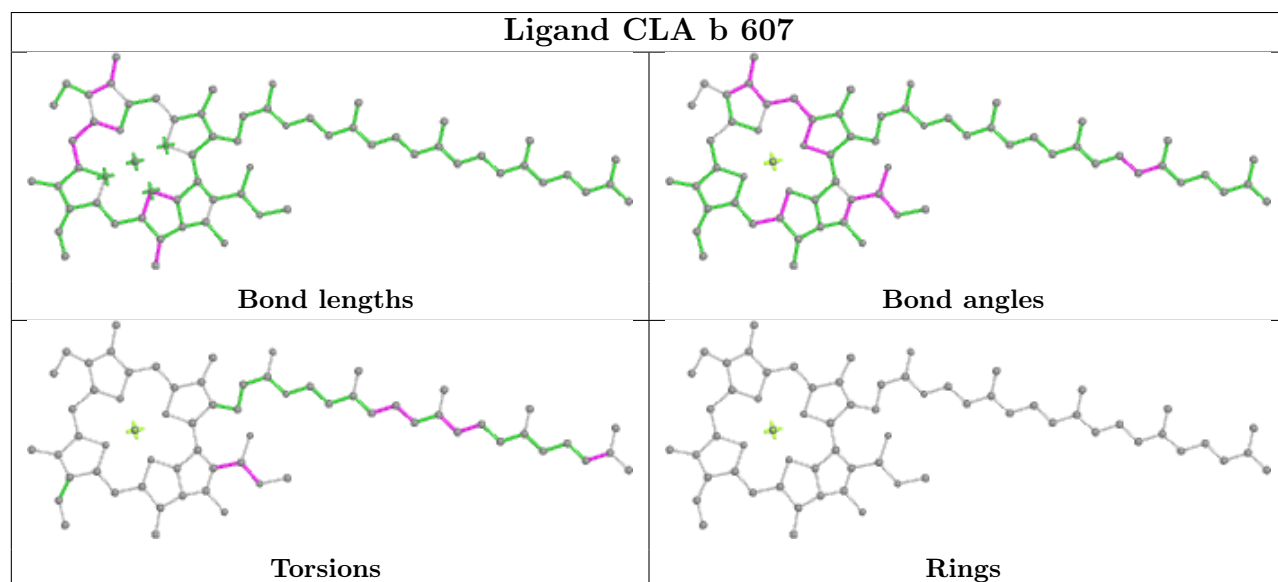
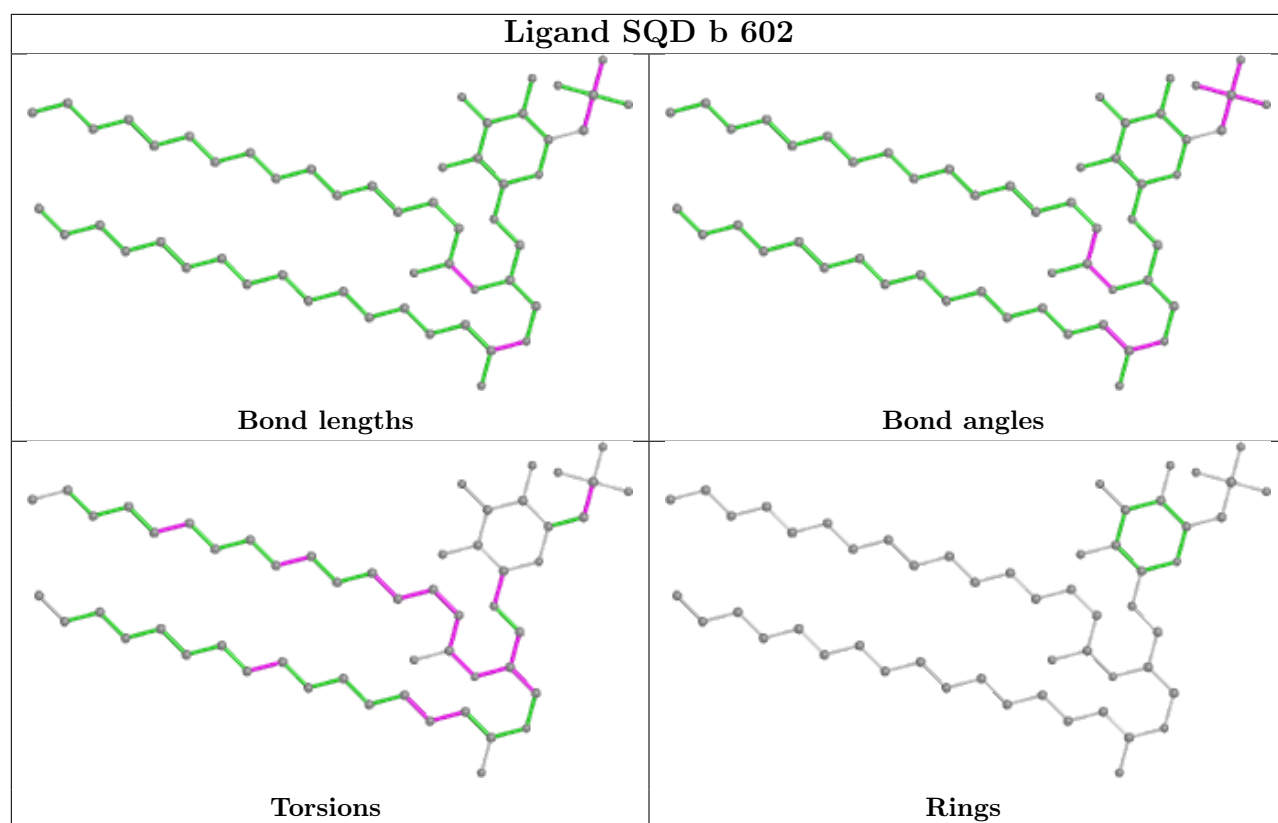
Bond angles



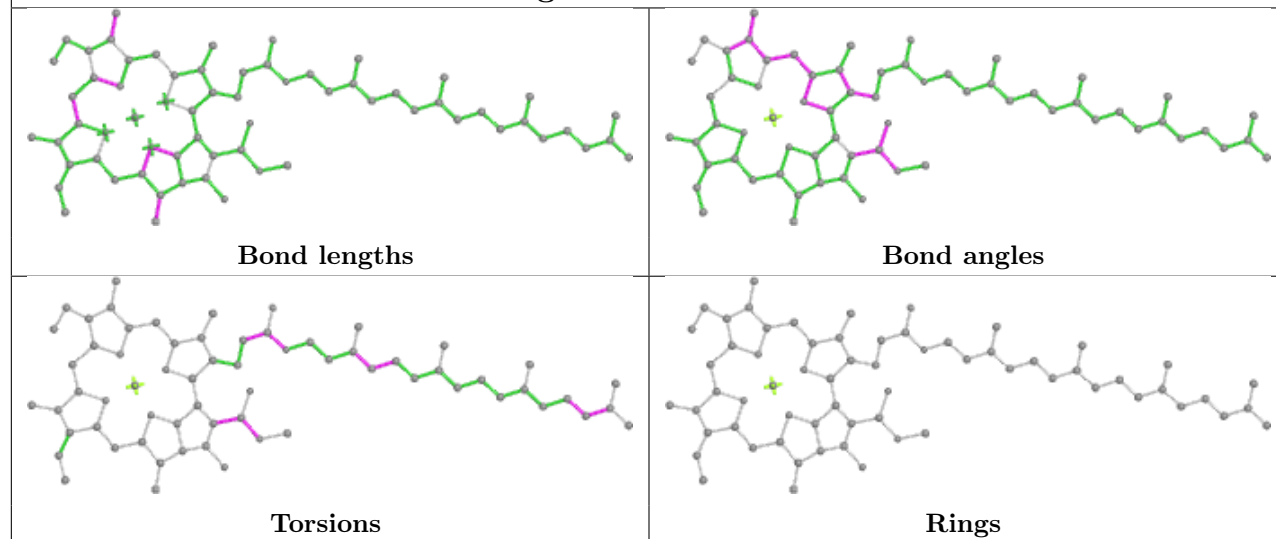
Torsions



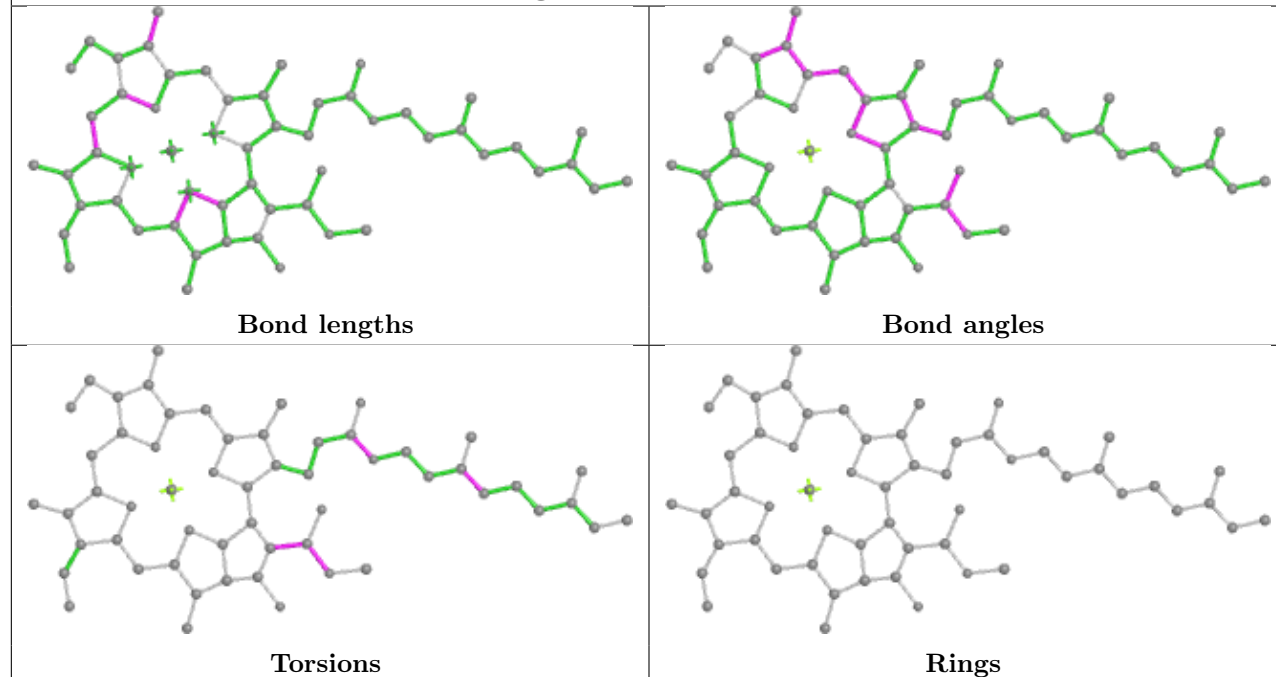
Rings



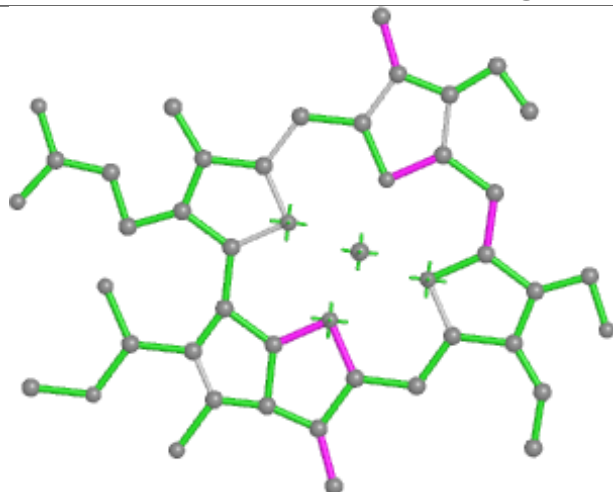
Ligand CLA c 510



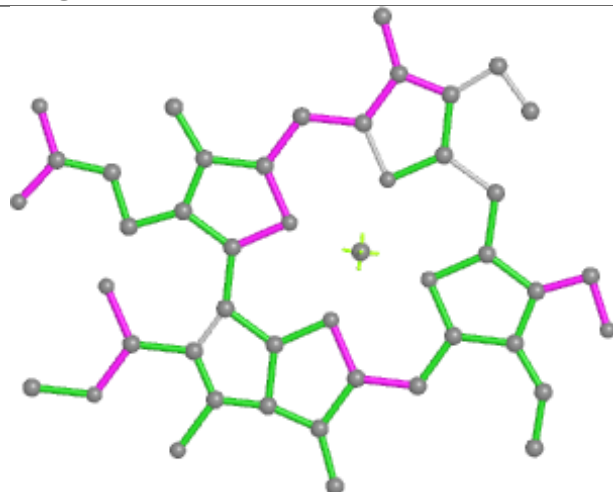
Ligand CLA C 513



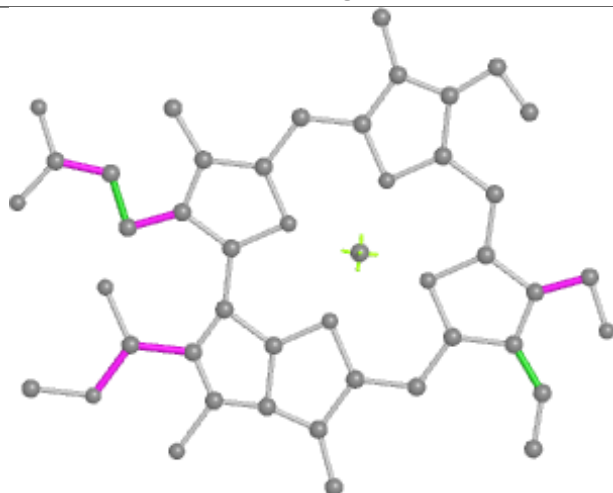
Ligand CHL g 605



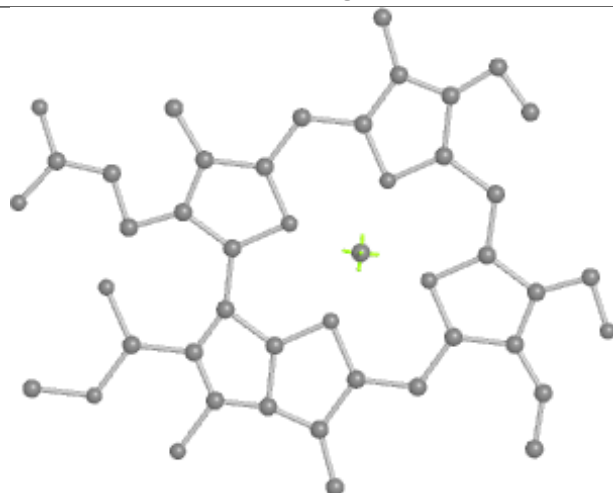
Bond lengths



Bond angles

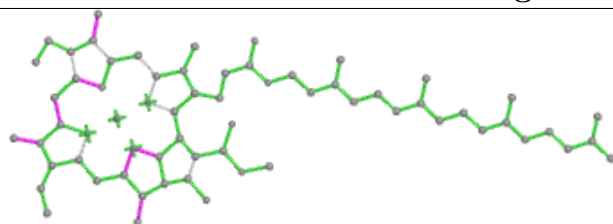


Torsions

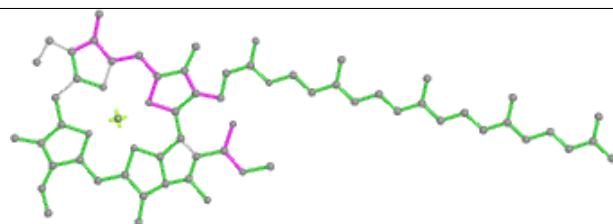


Rings

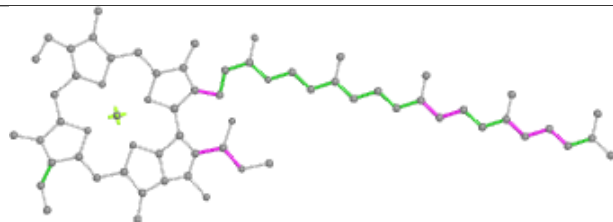
Ligand CLA B 610



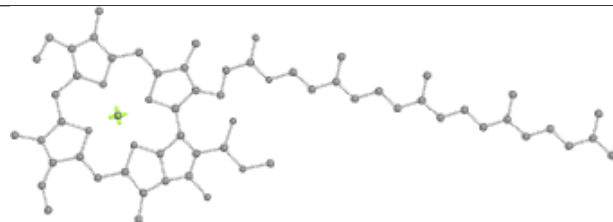
Bond lengths



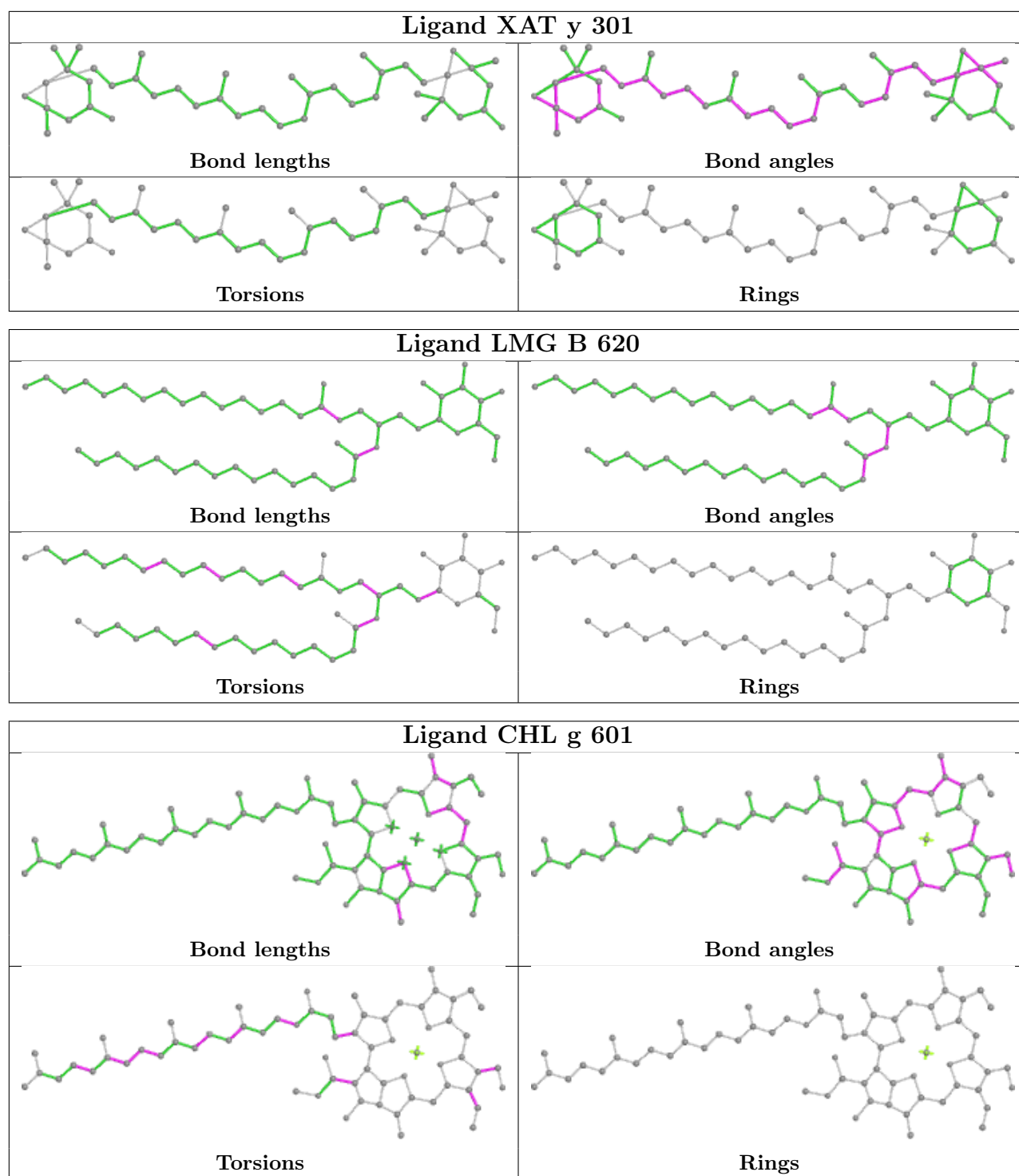
Bond angles

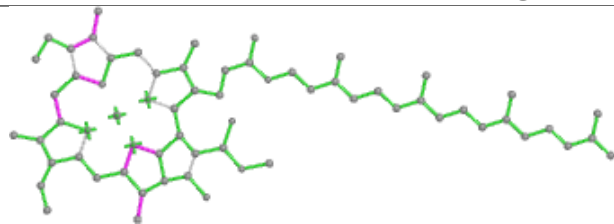
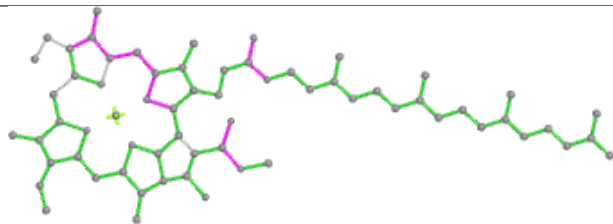
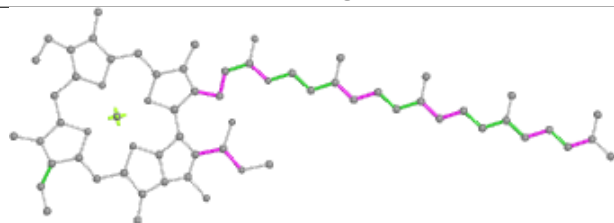
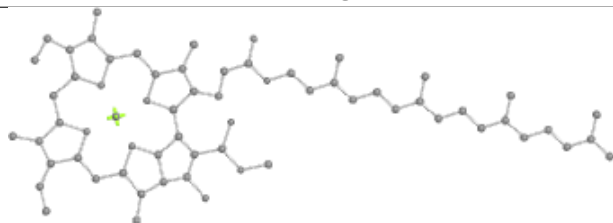
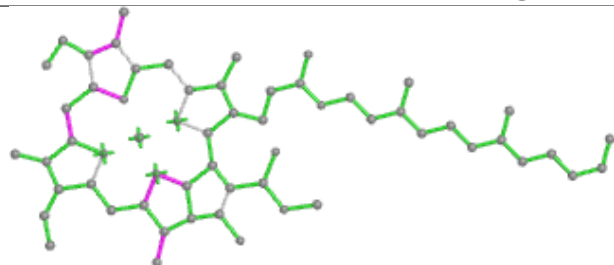
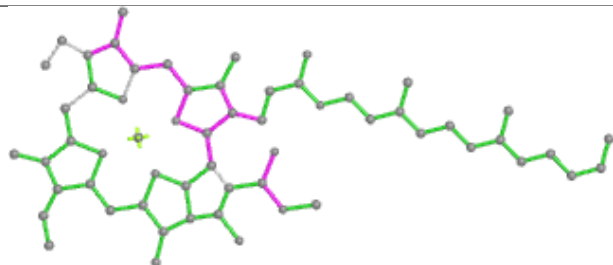
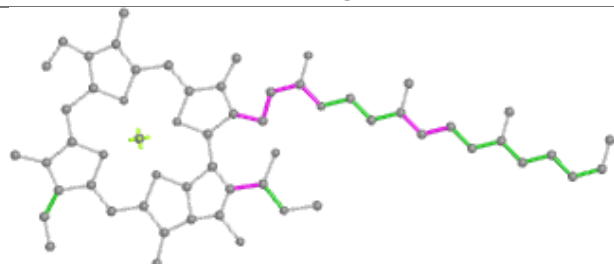
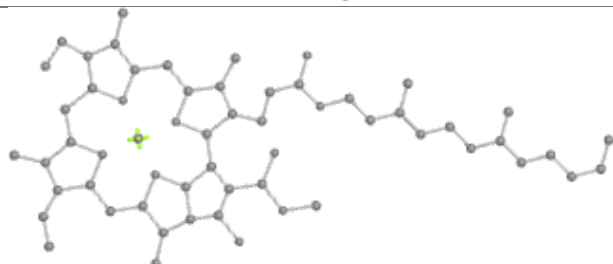


Torsions

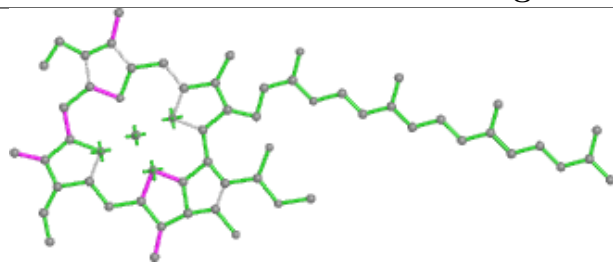


Rings

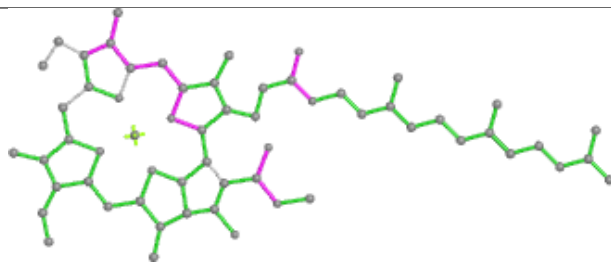


Ligand CLA B 603**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA N 603****Bond lengths****Bond angles****Torsions****Rings**

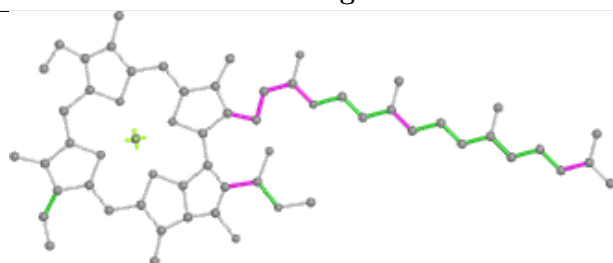
Ligand CLA R 303



Bond lengths



Bond angles

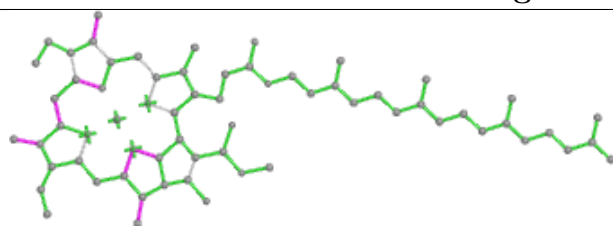


Torsions

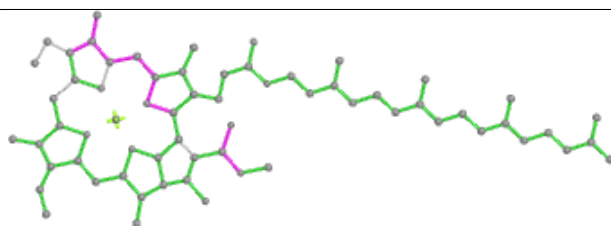


Rings

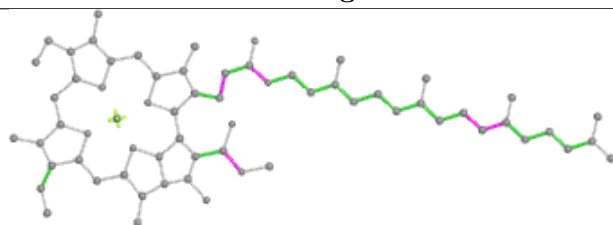
Ligand CLA A 401



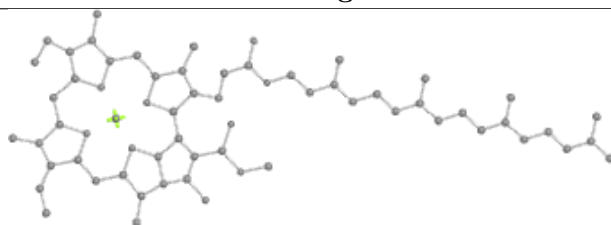
Bond lengths



Bond angles

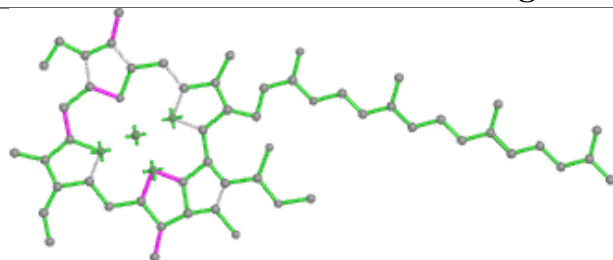


Torsions

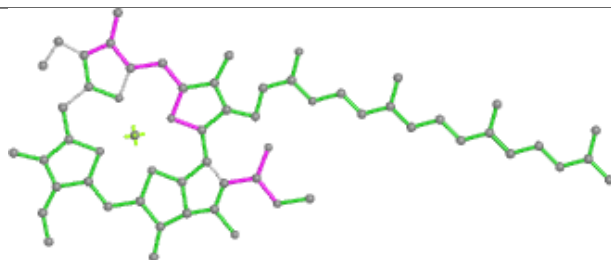


Rings

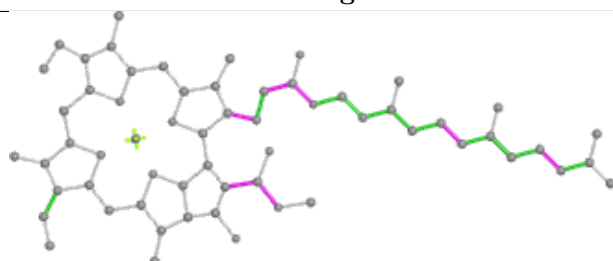
Ligand CLA a 404



Bond lengths



Bond angles

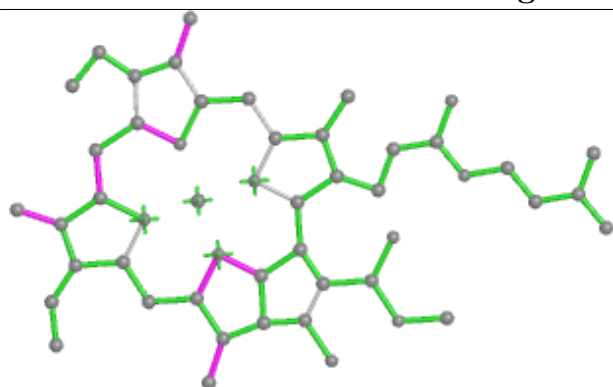


Torsions

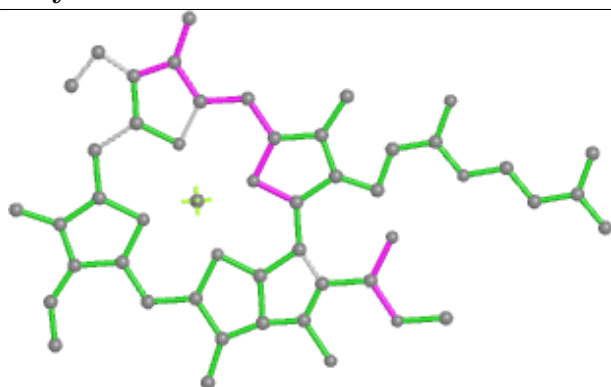


Rings

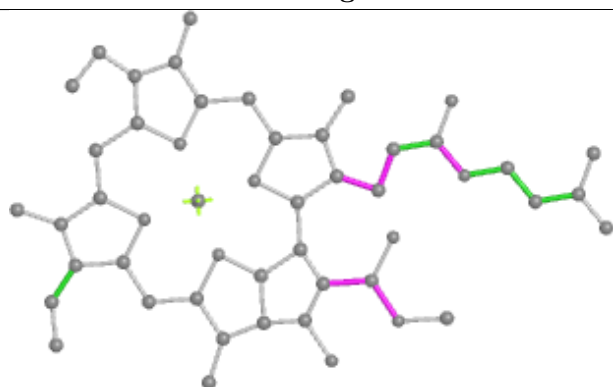
Ligand CLA y 305



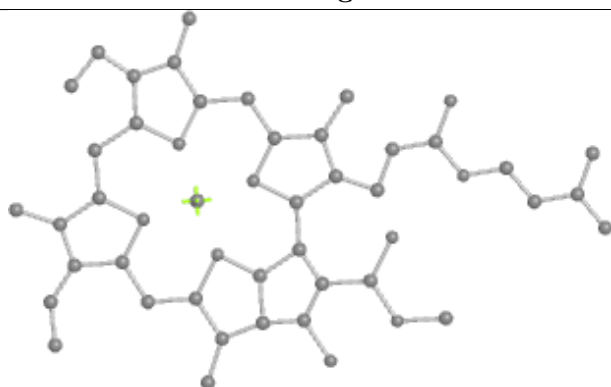
Bond lengths



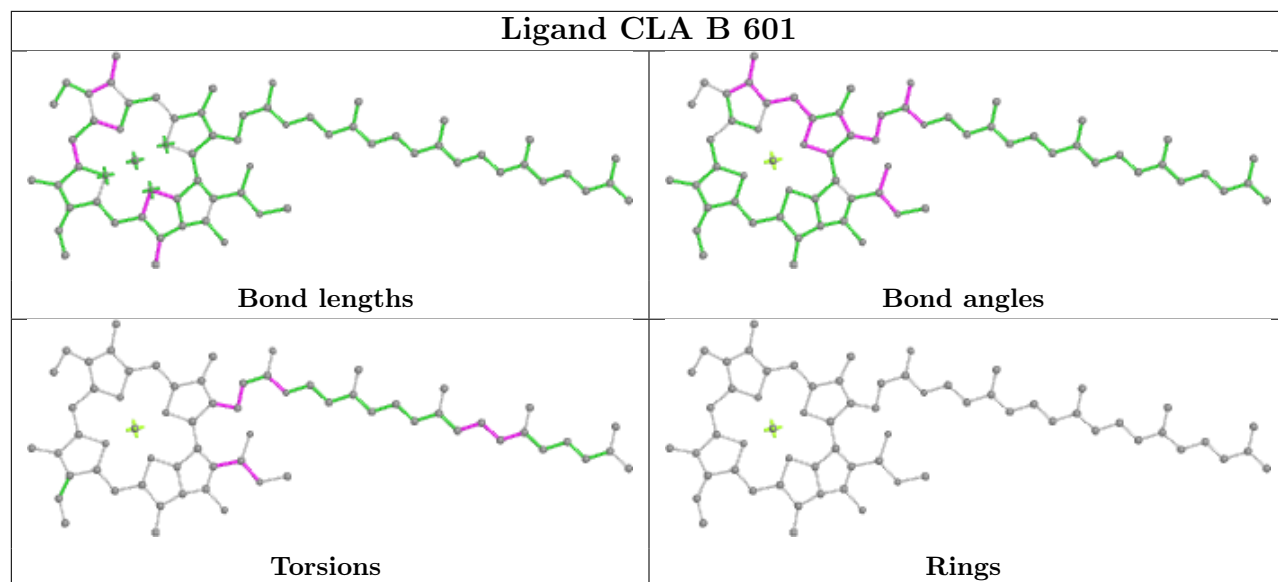
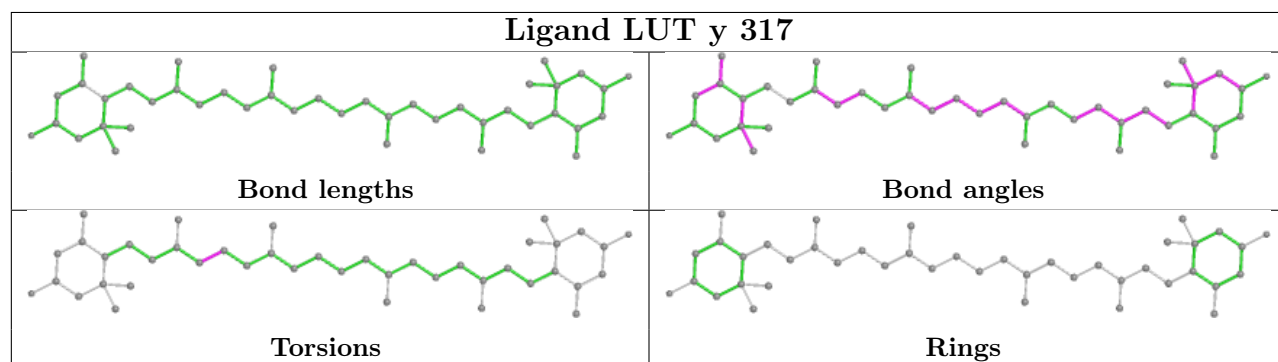
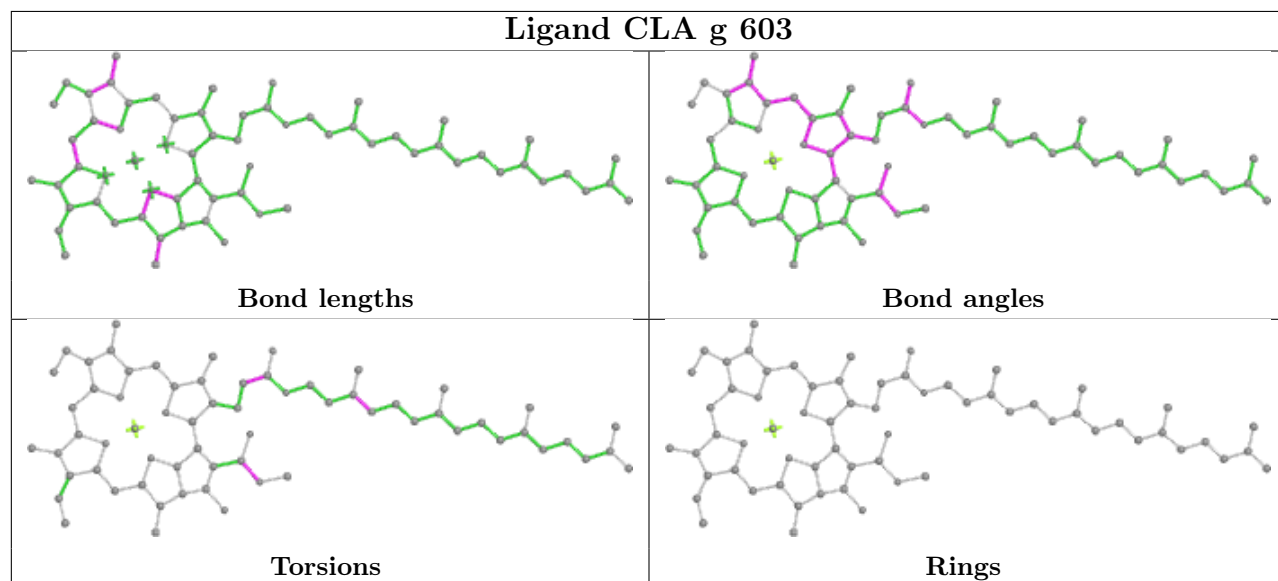
Bond angles



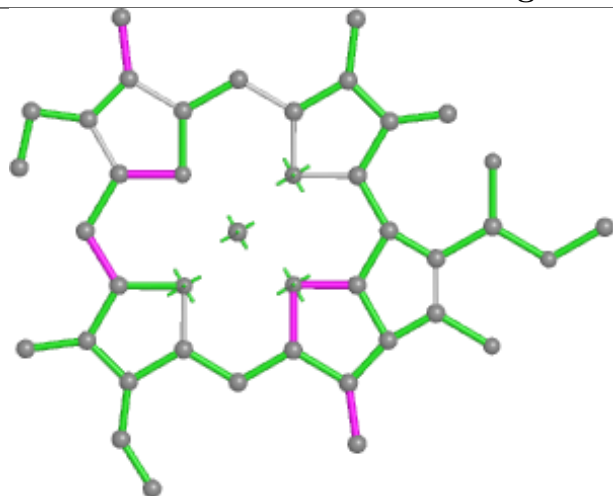
Torsions



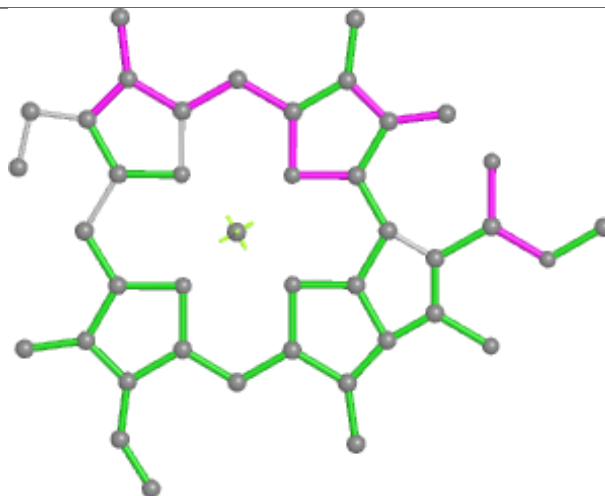
Rings

Ligand CLA B 601**Ligand LUT y 317****Ligand CLA g 603**

Ligand CLA n 614



Bond lengths



Bond angles

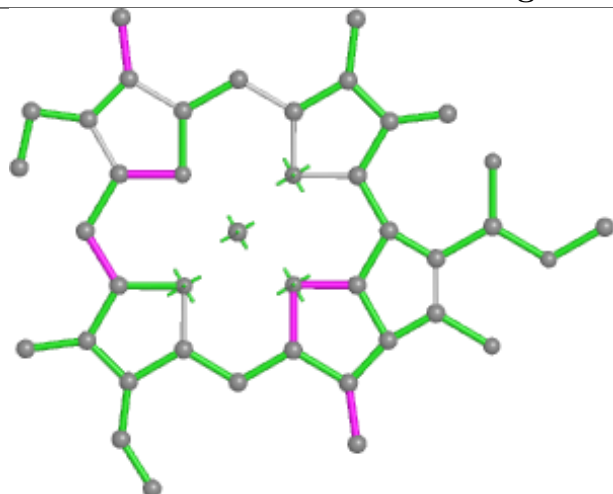


Torsions

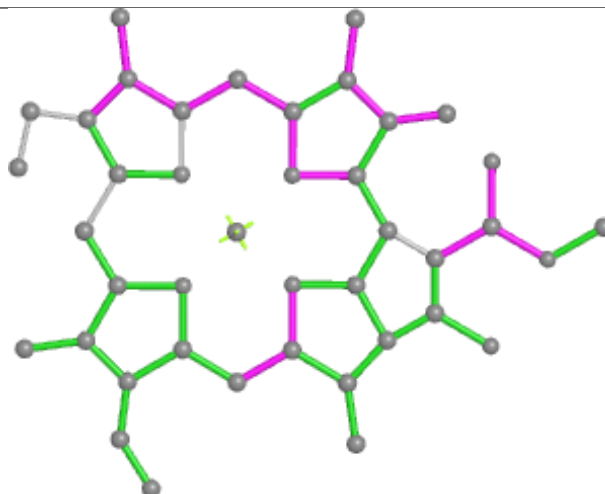


Rings

Ligand CLA S 314



Bond lengths



Bond angles

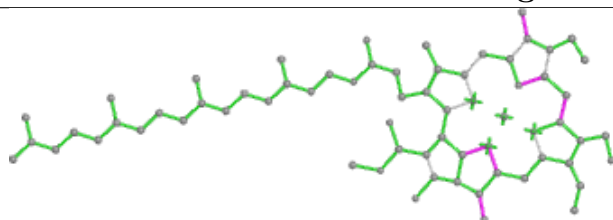


Torsions

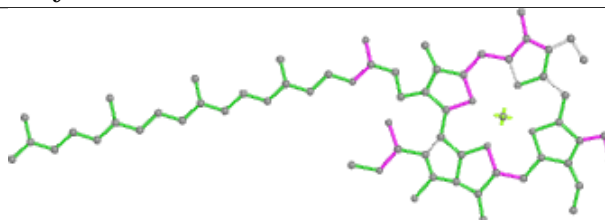


Rings

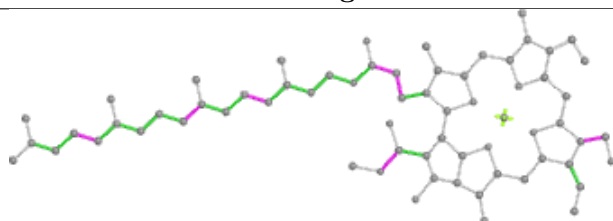
Ligand CHL y 309



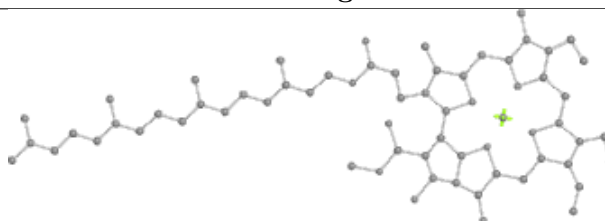
Bond lengths



Bond angles

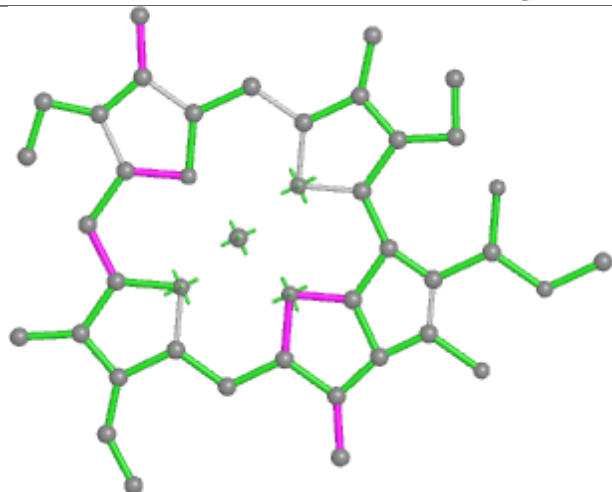


Torsions

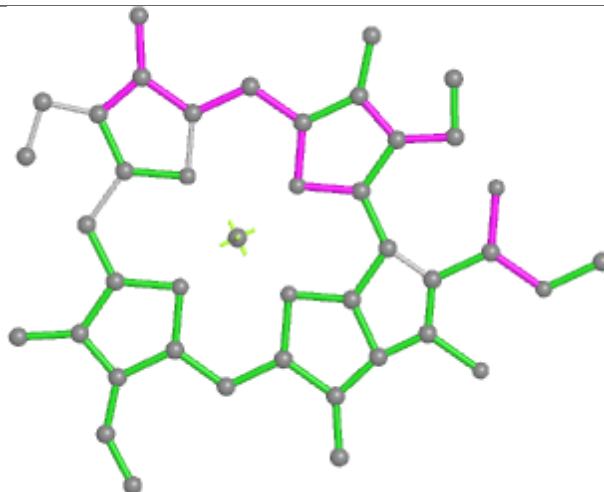


Rings

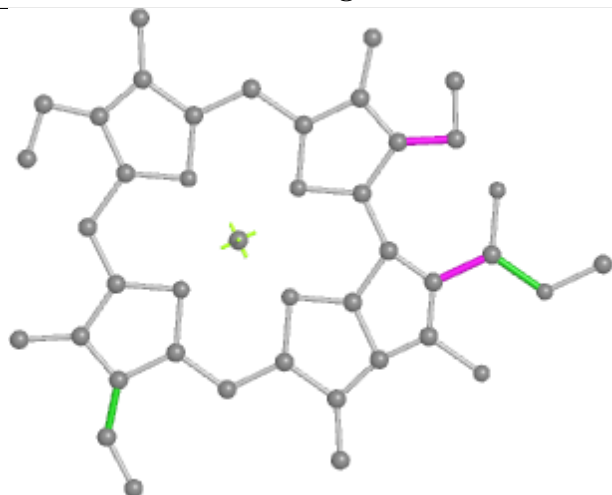
Ligand CLA S 311



Bond lengths



Bond angles

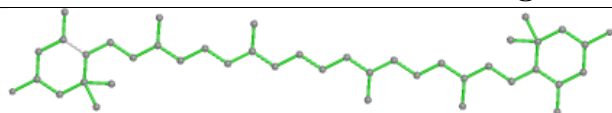


Torsions

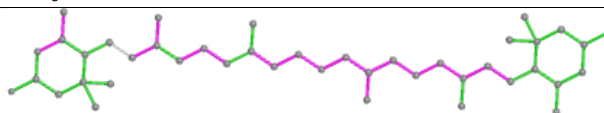


Rings

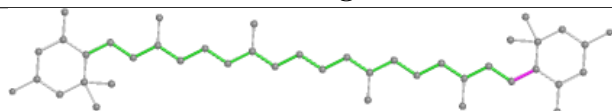
Ligand LUT y 316



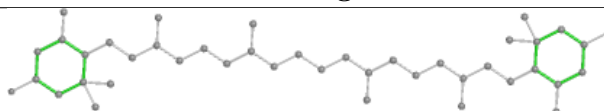
Bond lengths



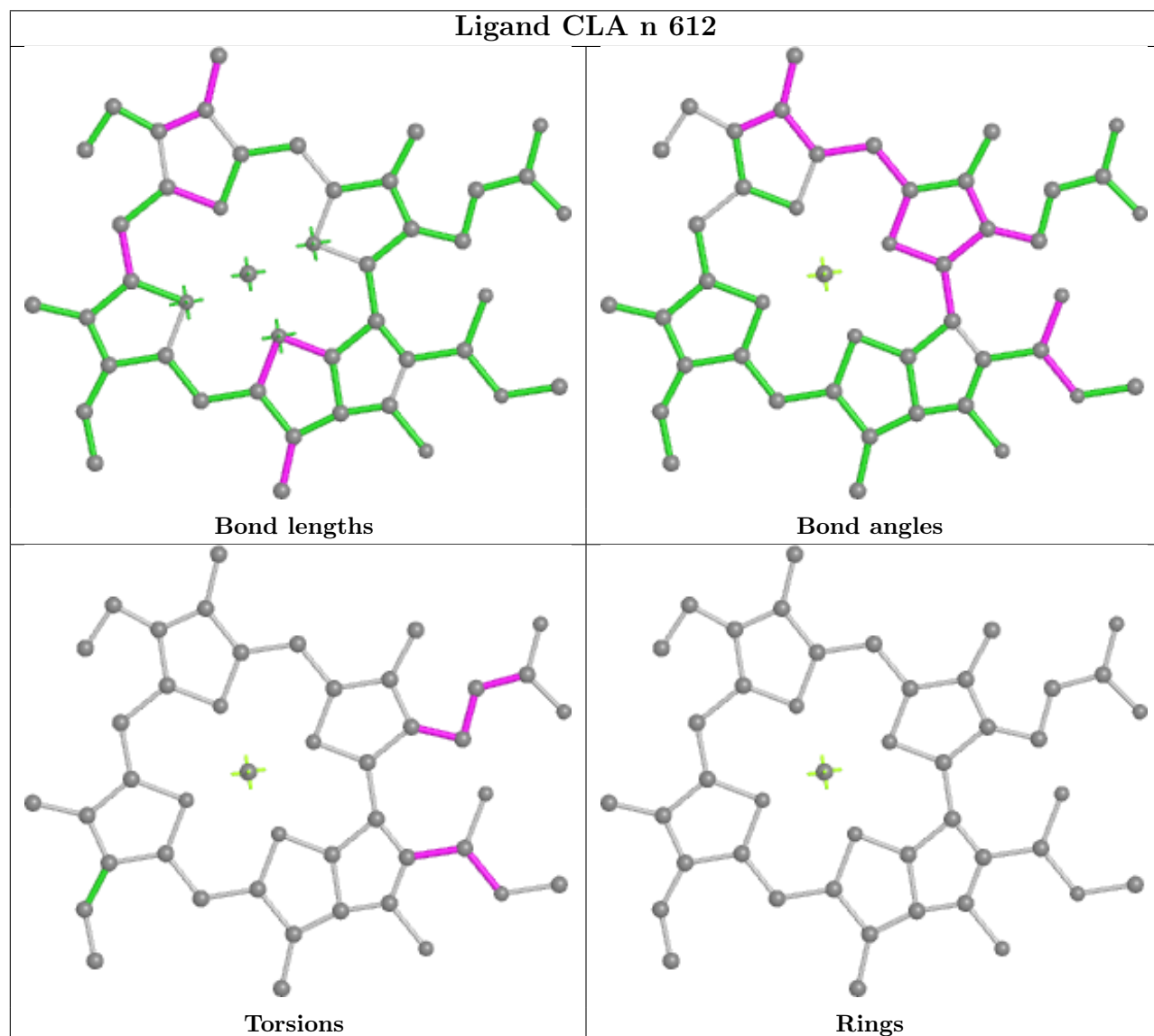
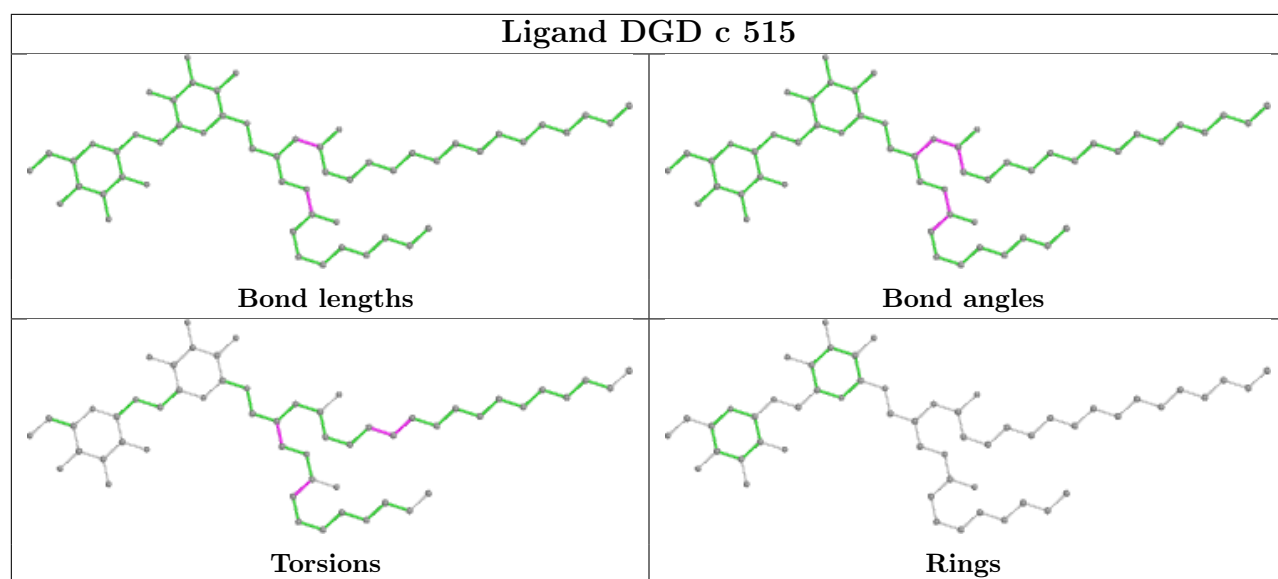
Bond angles

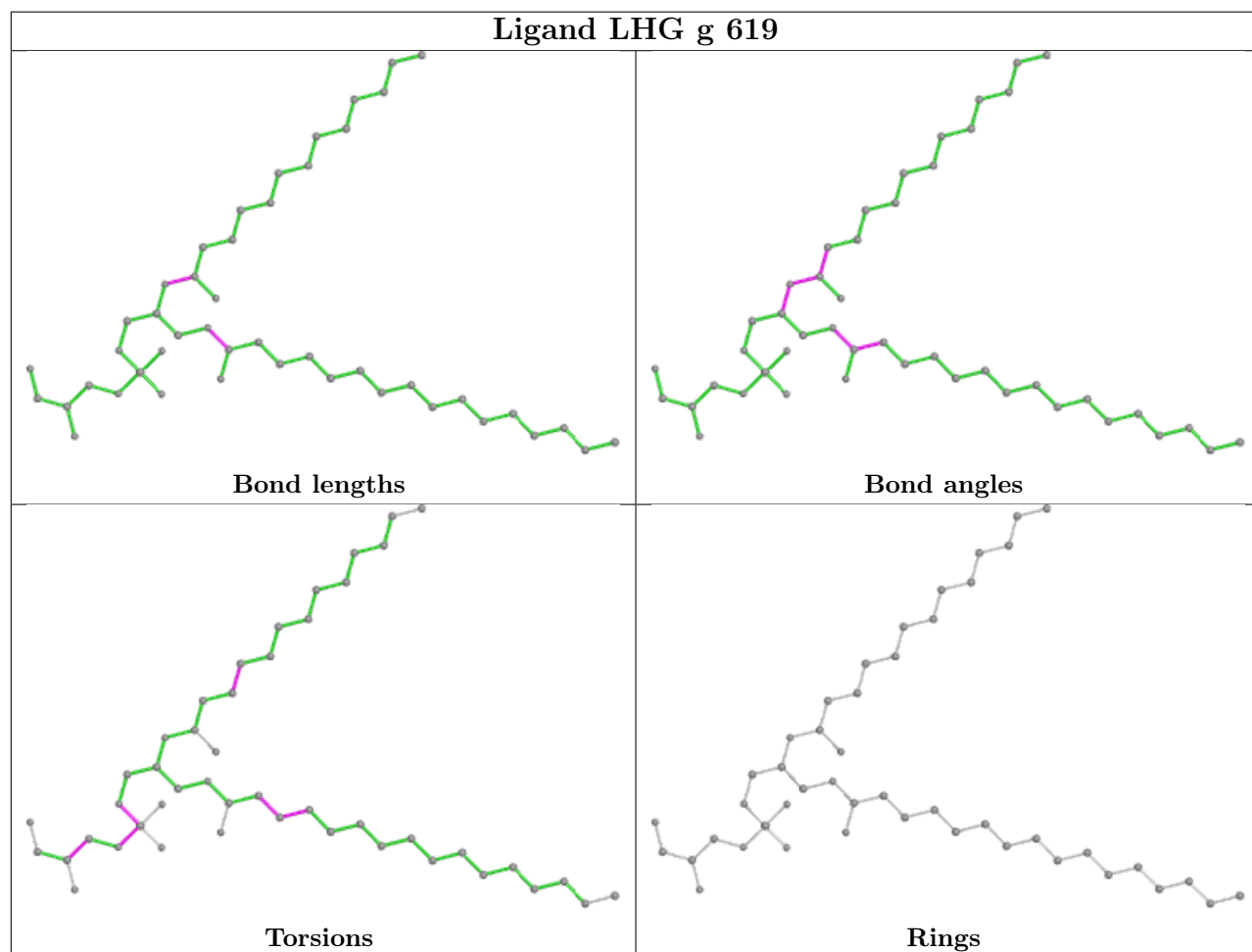
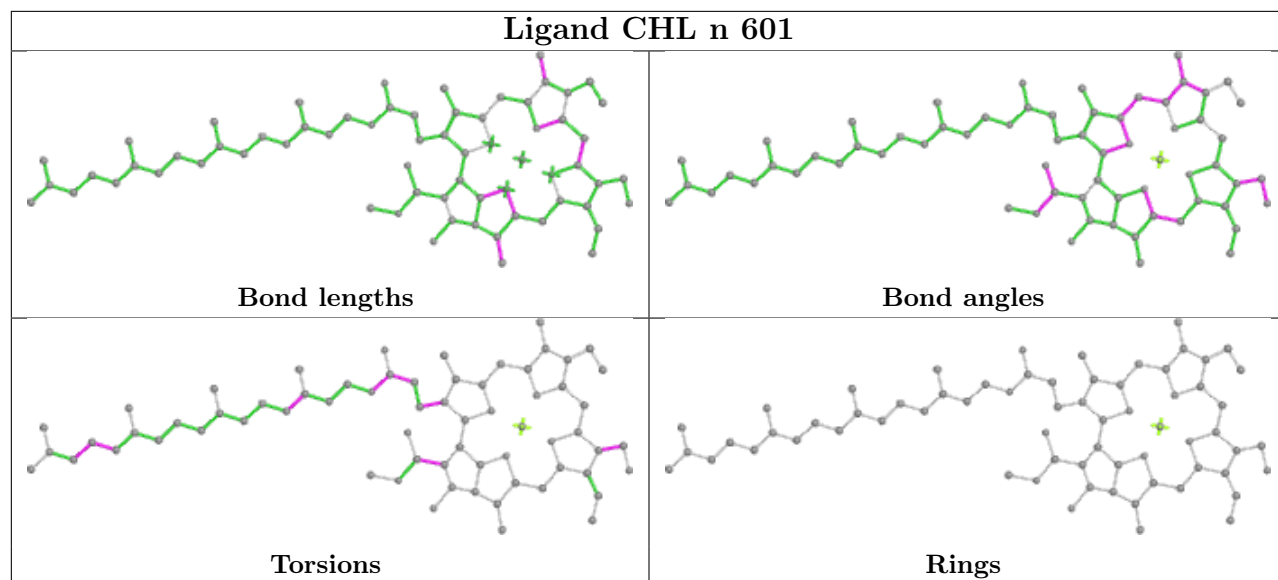


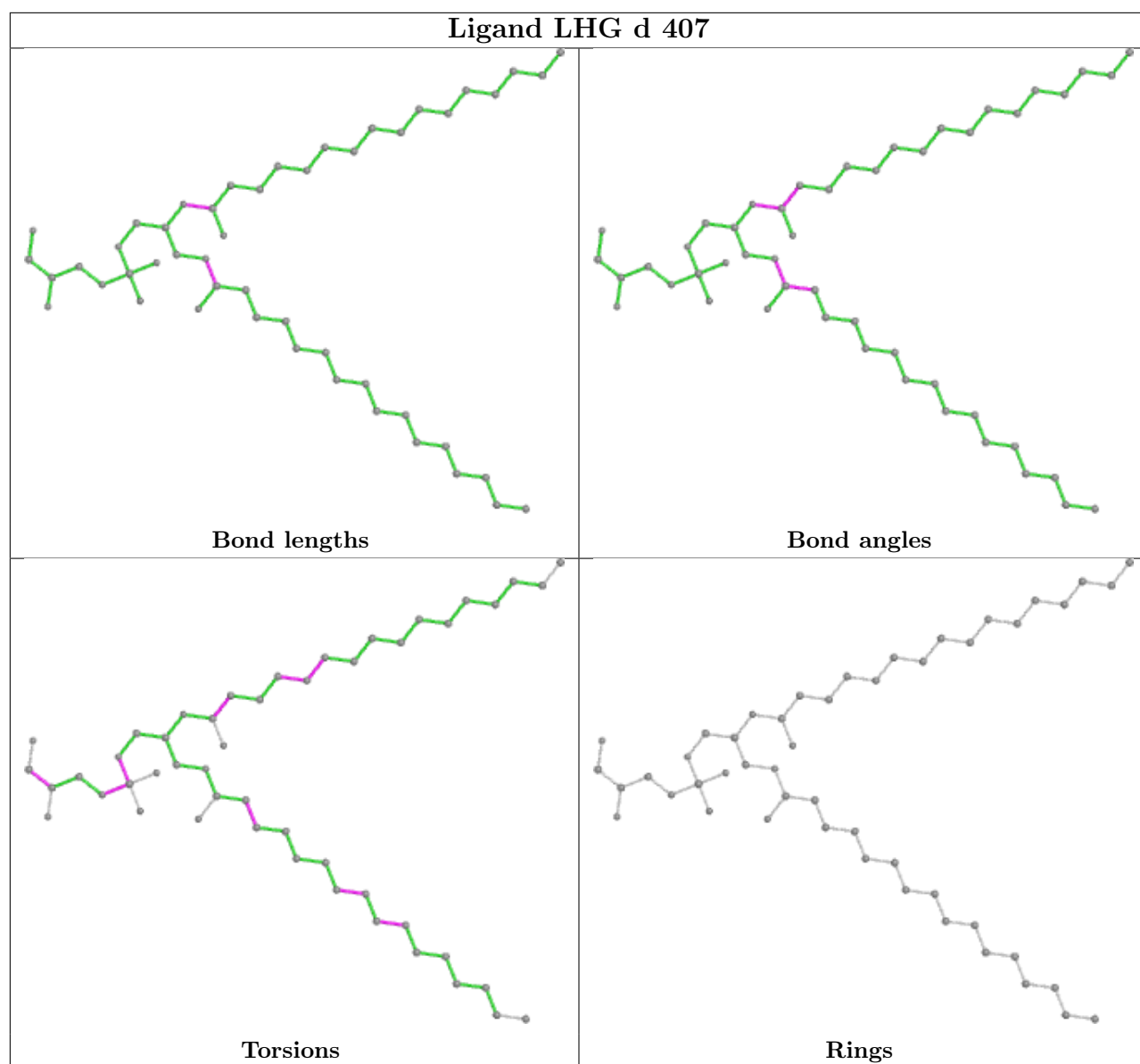
Torsions

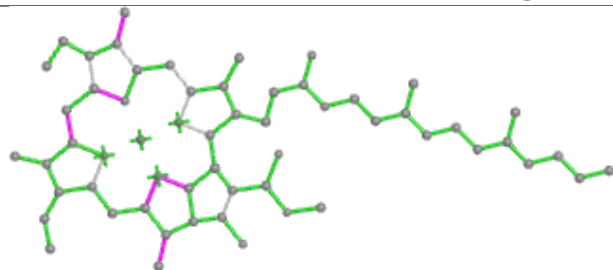


Rings

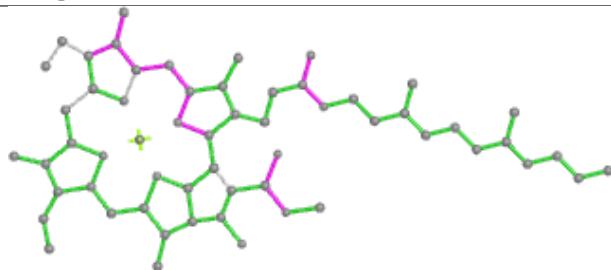




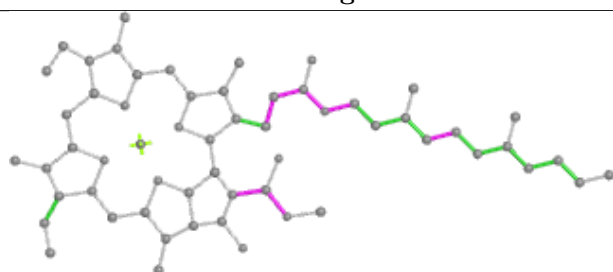


Ligand CLA g 613

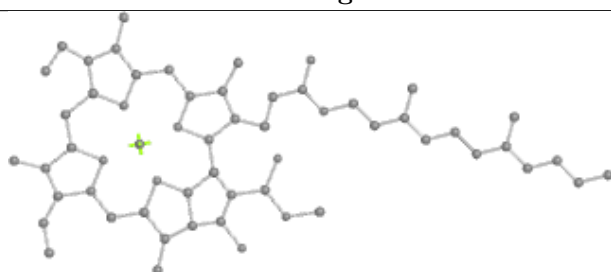
Bond lengths



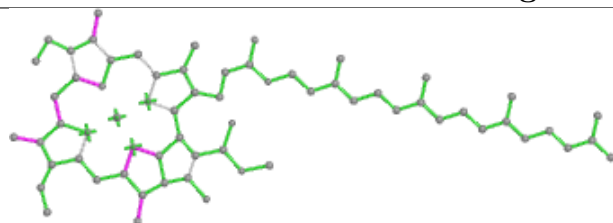
Bond angles



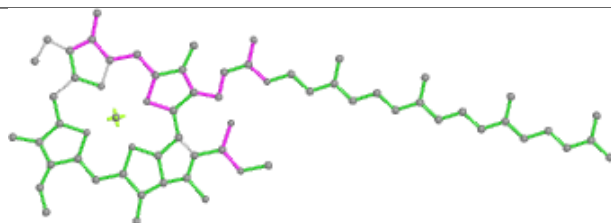
Torsions



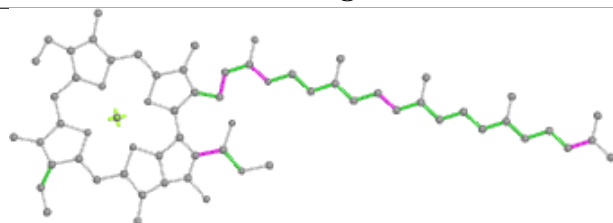
Rings

Ligand CLA c 513

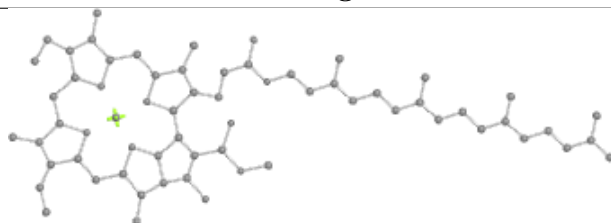
Bond lengths



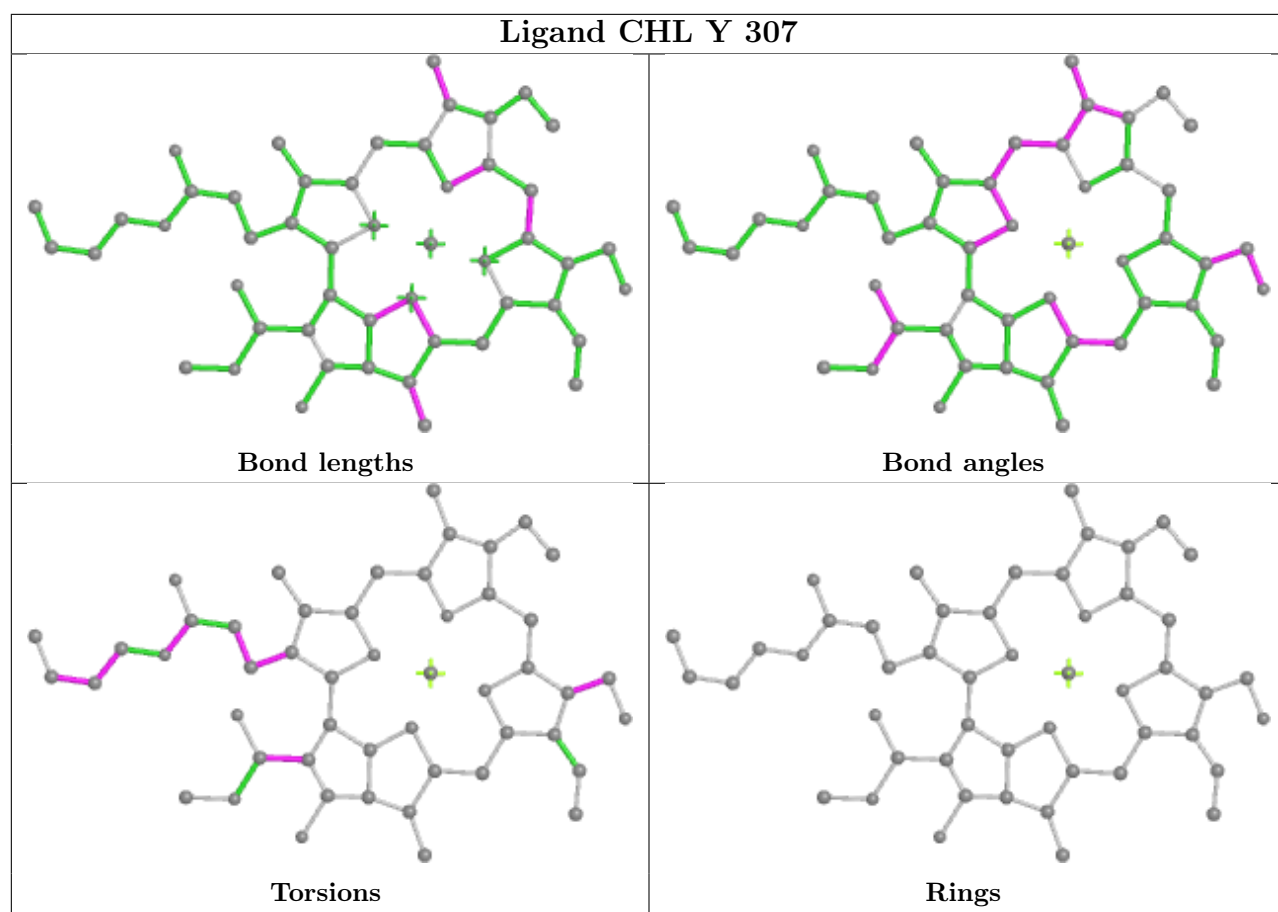
Bond angles



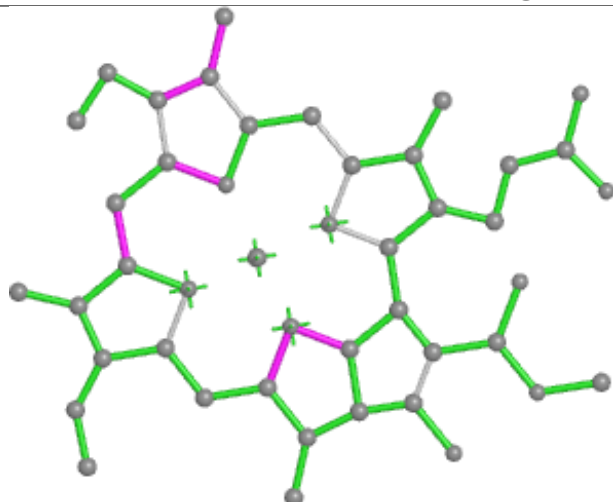
Torsions



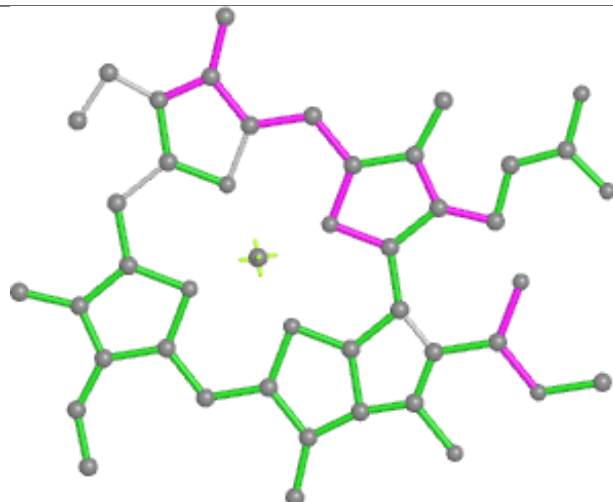
Rings



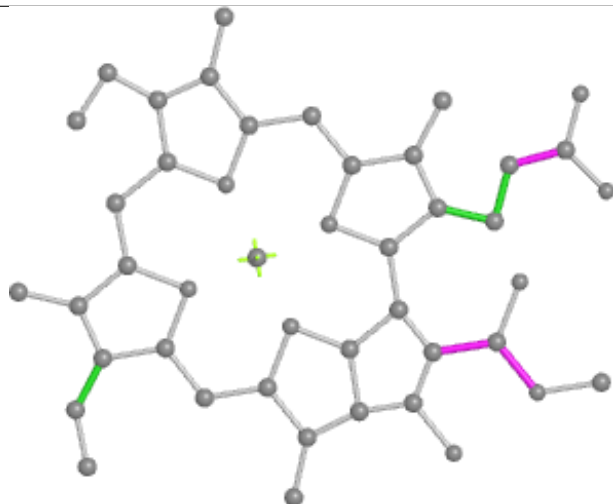
Ligand CLA S 304



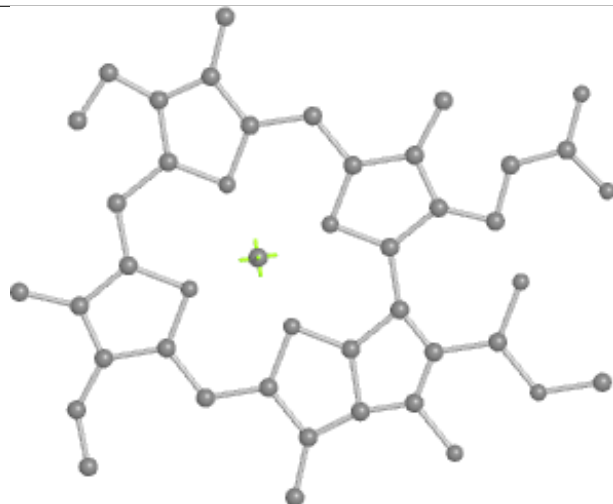
Bond lengths



Bond angles

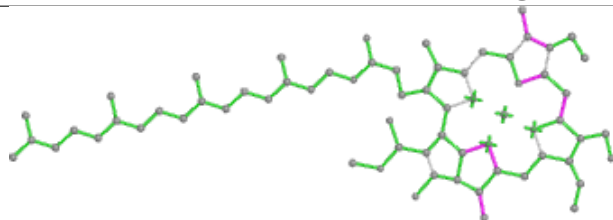


Torsions

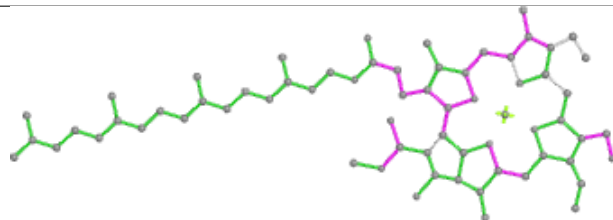


Rings

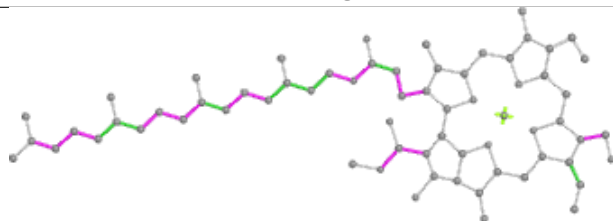
Ligand CHL Y 308



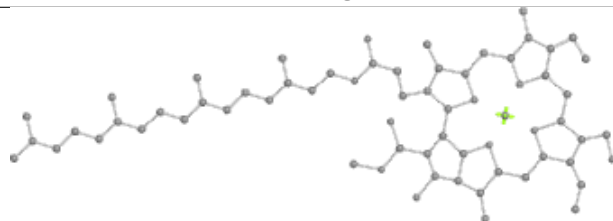
Bond lengths



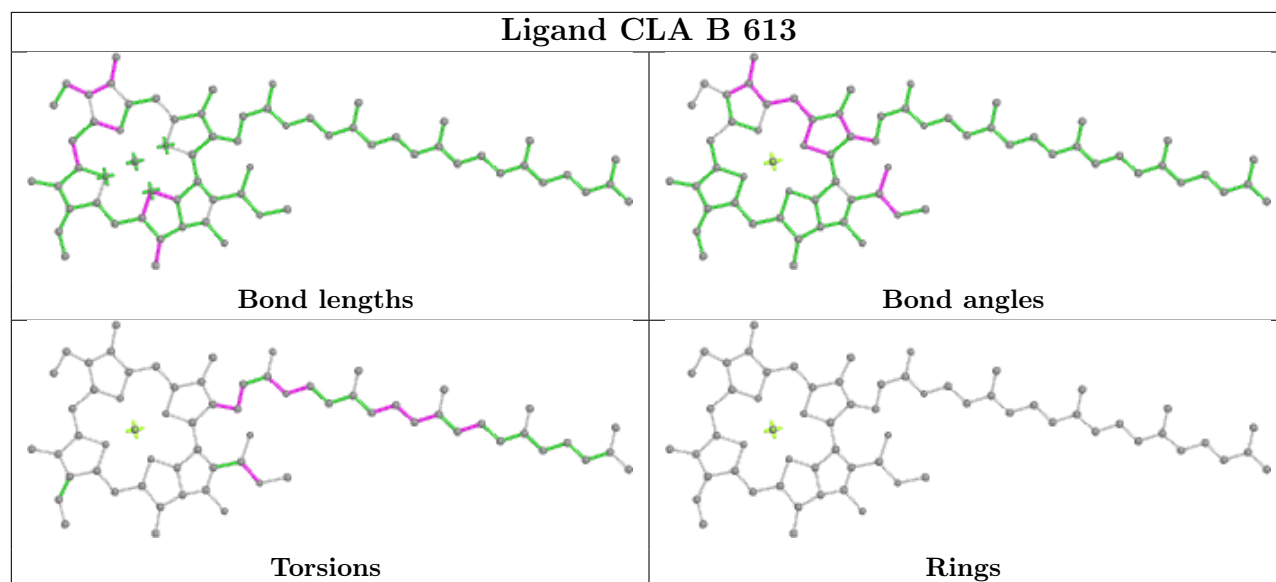
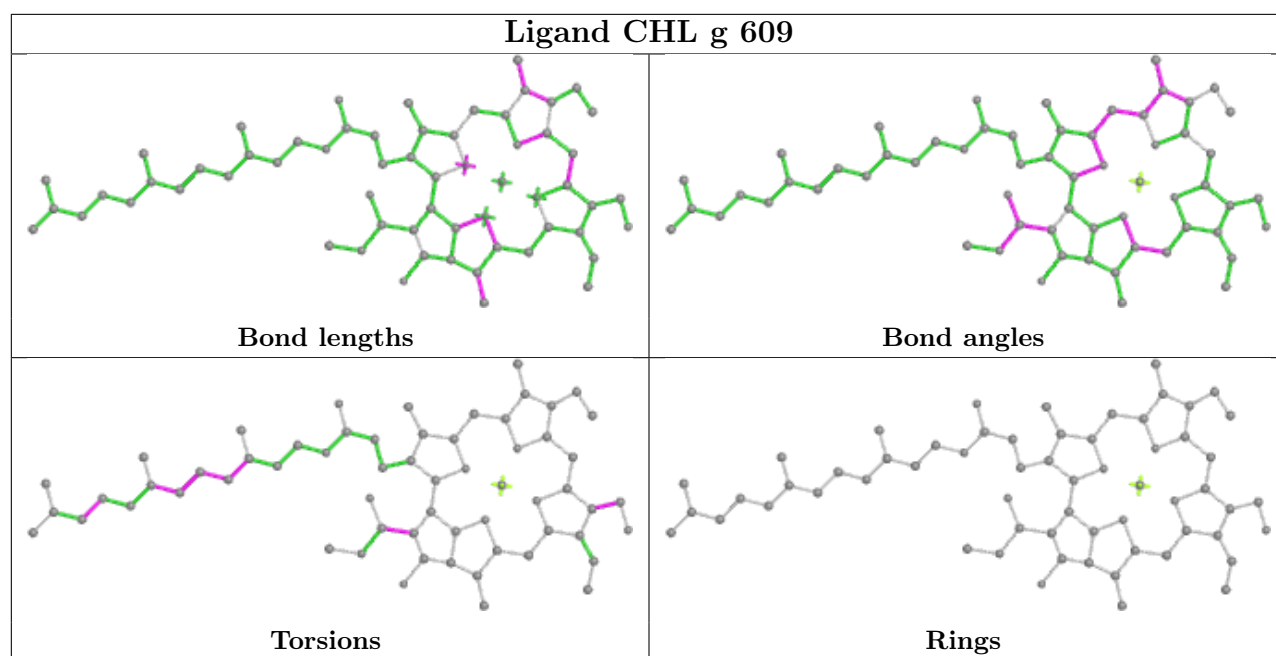
Bond angles



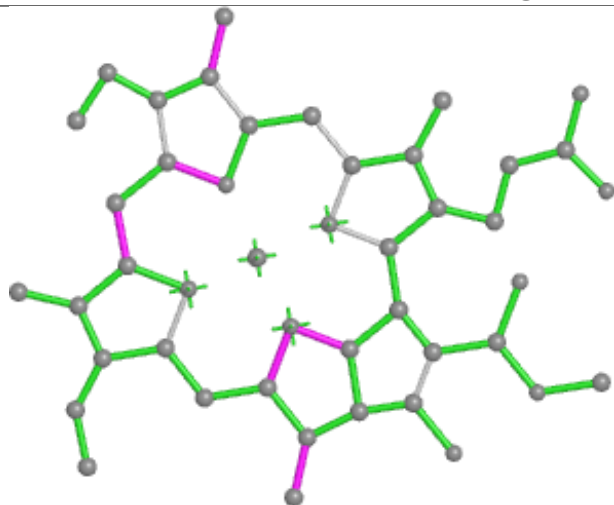
Torsions



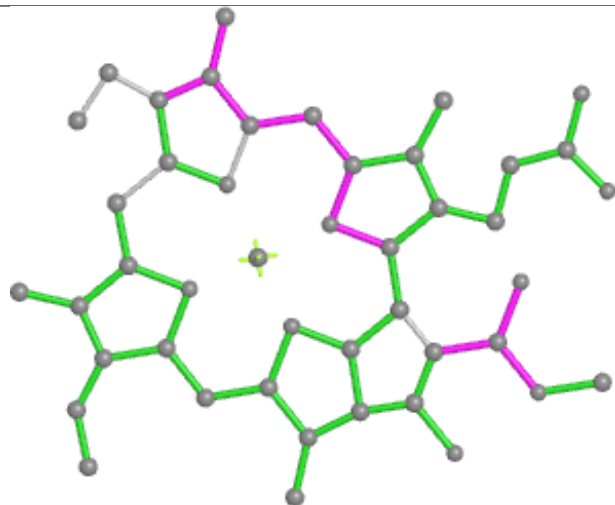
Rings



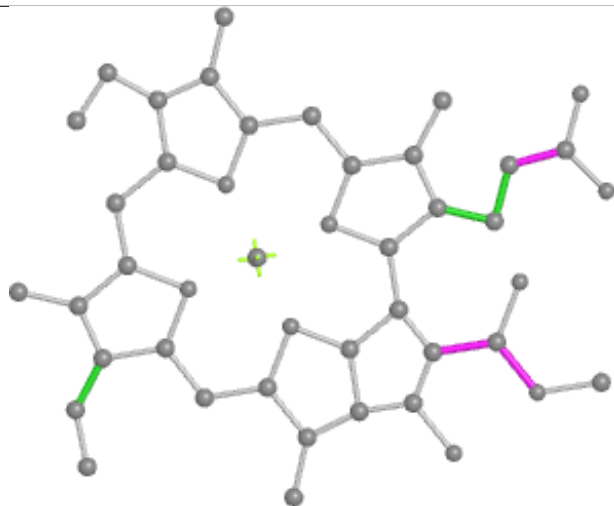
Ligand CLA S 309



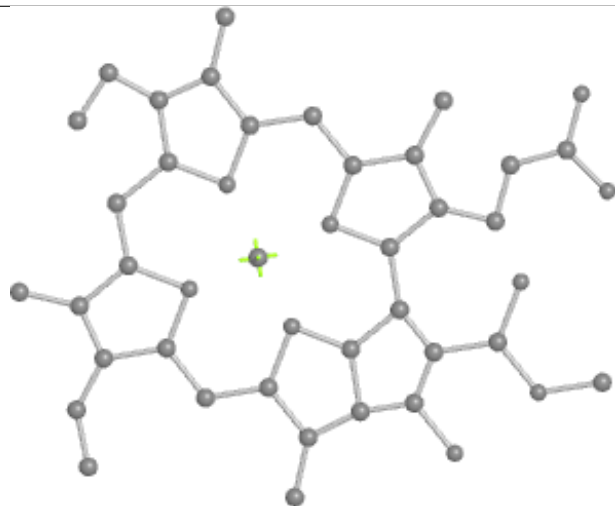
Bond lengths



Bond angles

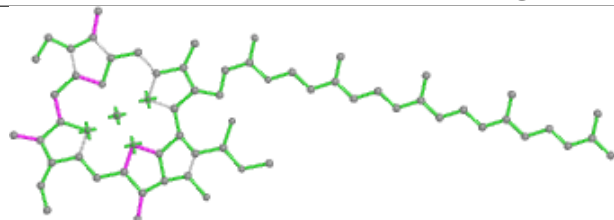


Torsions

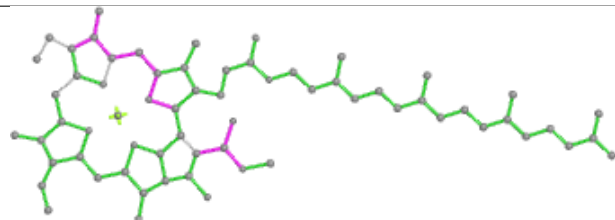


Rings

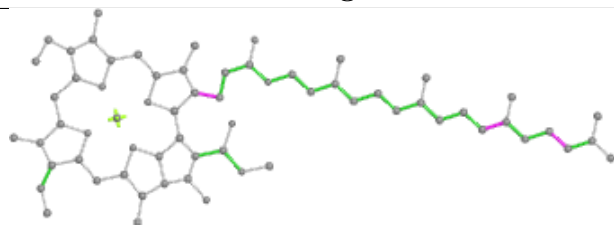
Ligand CLA D 403



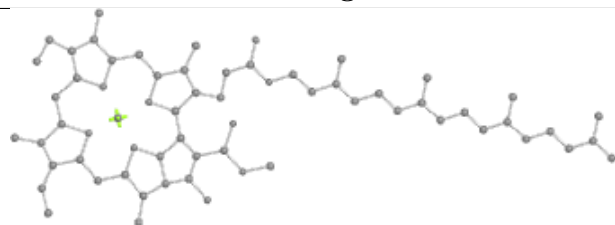
Bond lengths



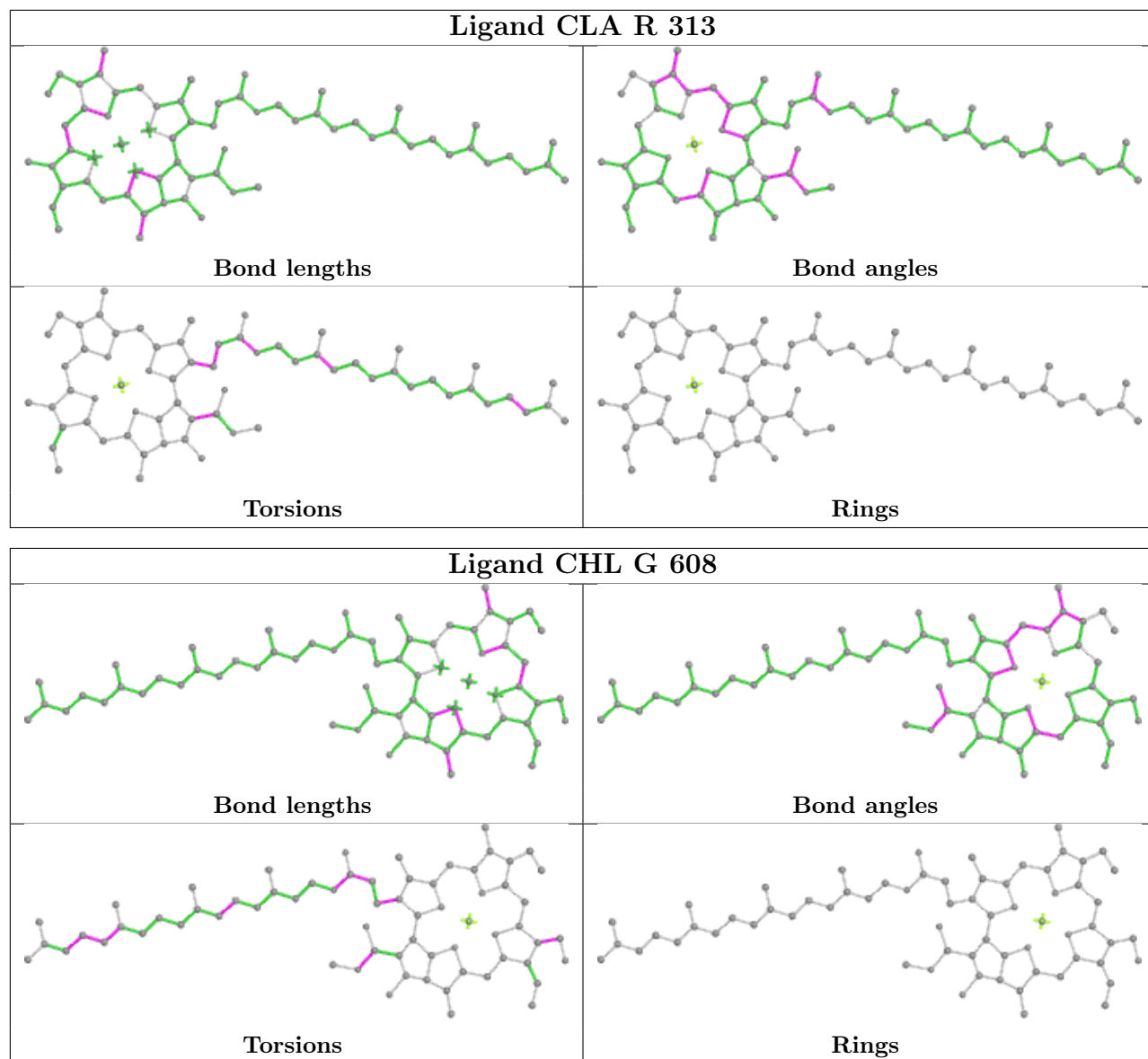
Bond angles

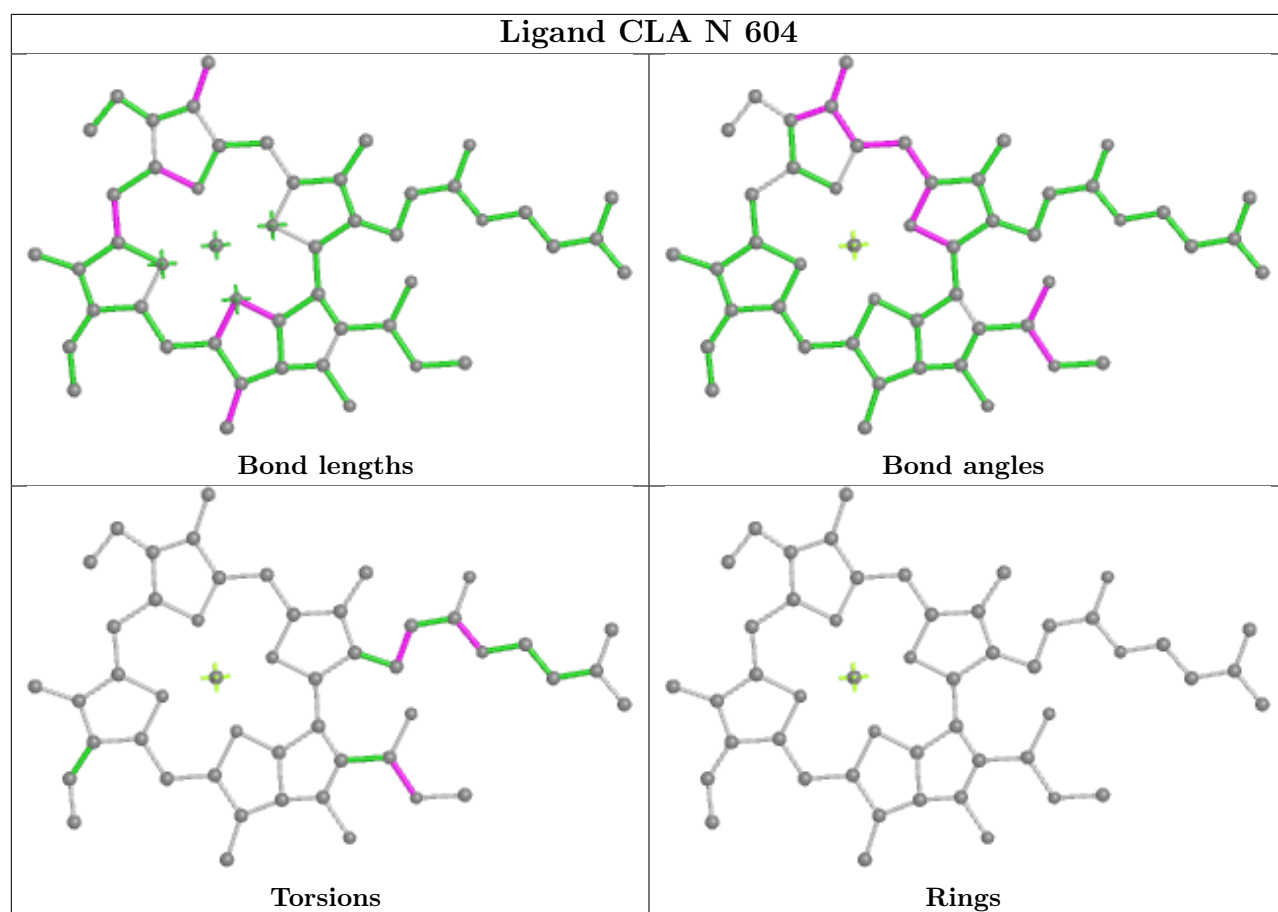


Torsions

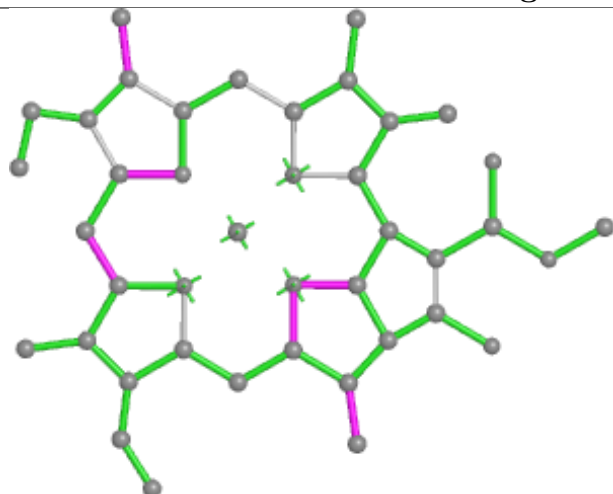


Rings

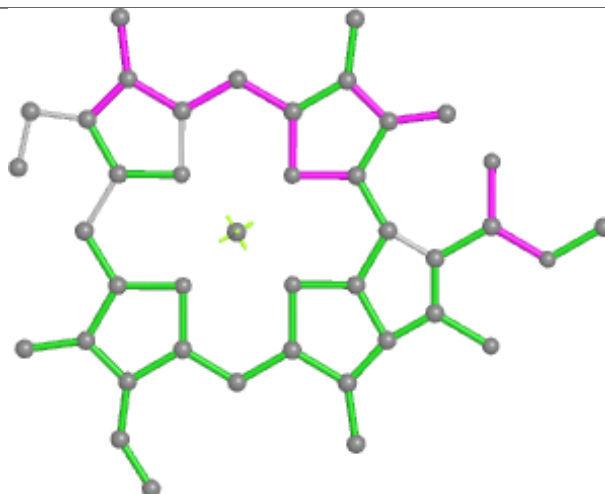




Ligand CLA r 610



Bond lengths



Bond angles

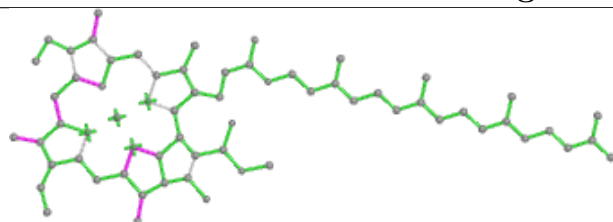


Torsions

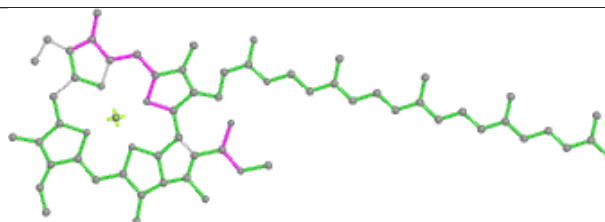


Rings

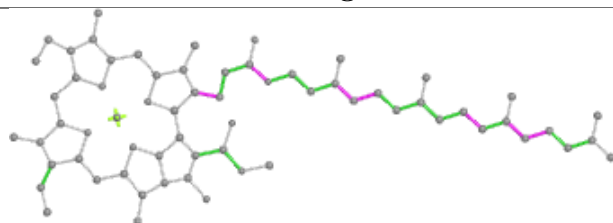
Ligand CLA b 613



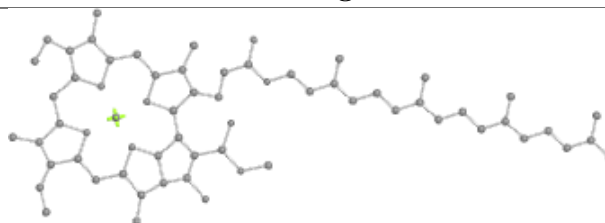
Bond lengths



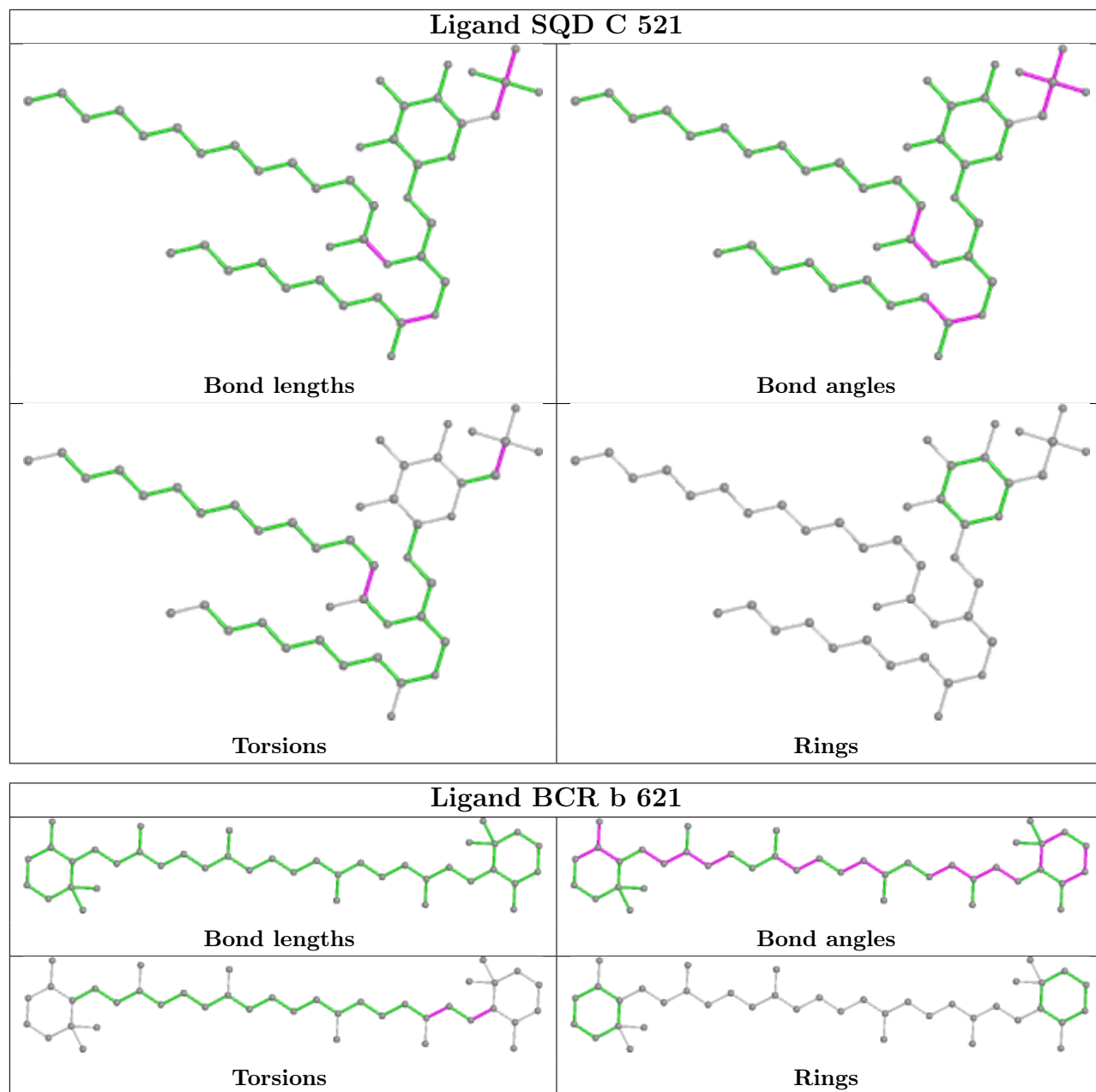
Bond angles

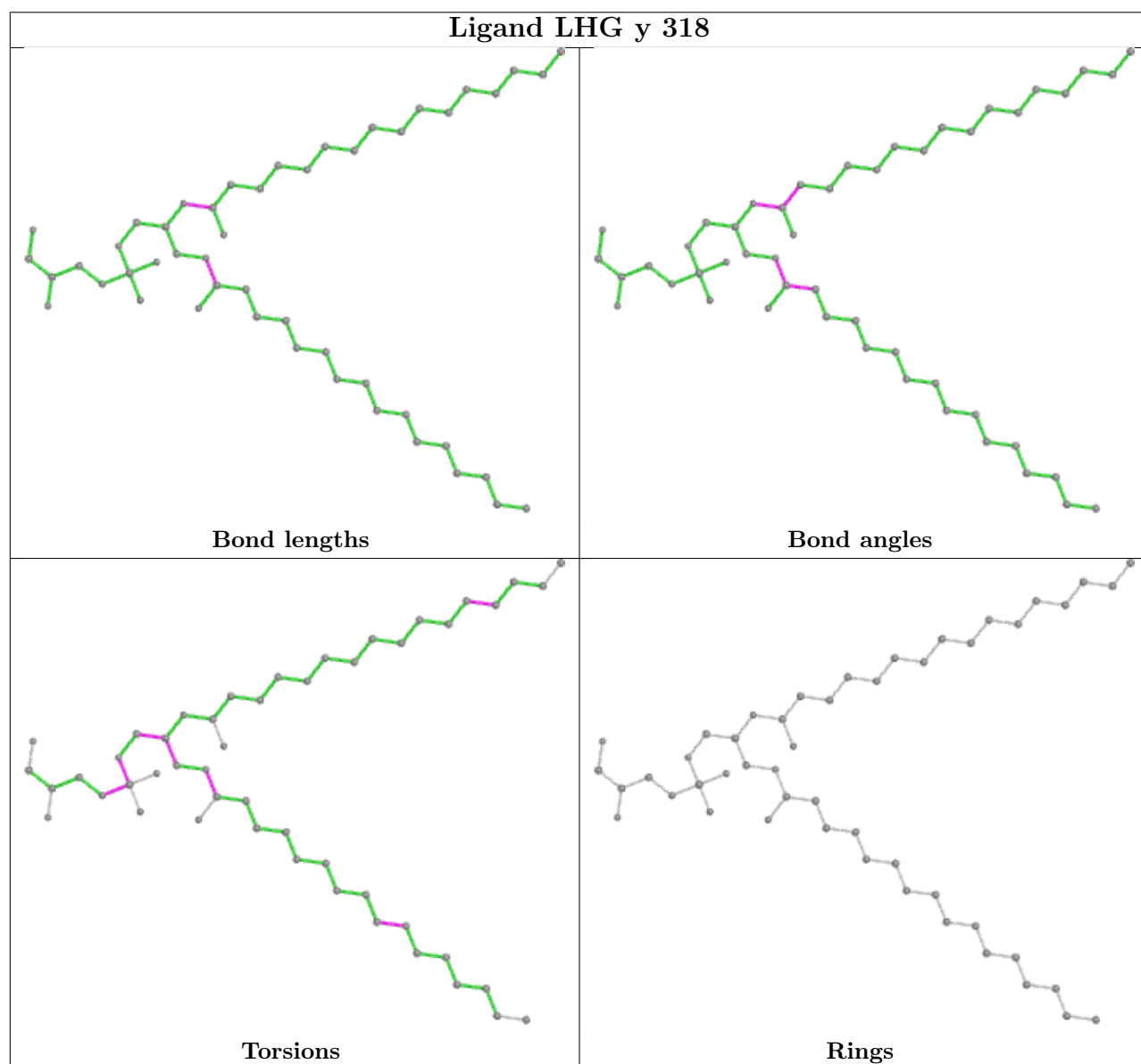
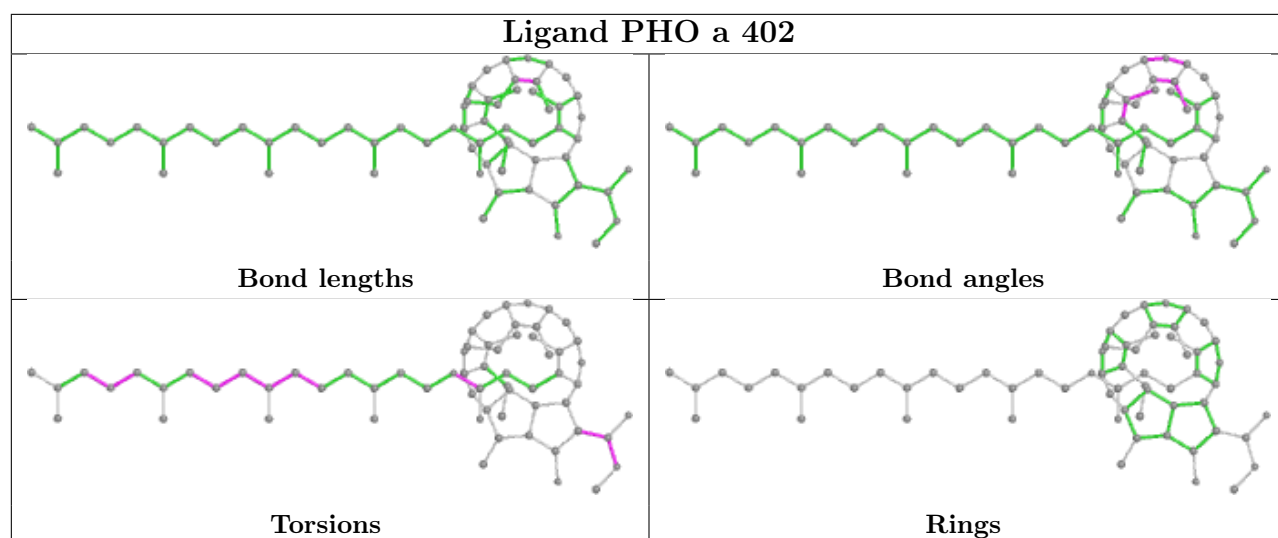


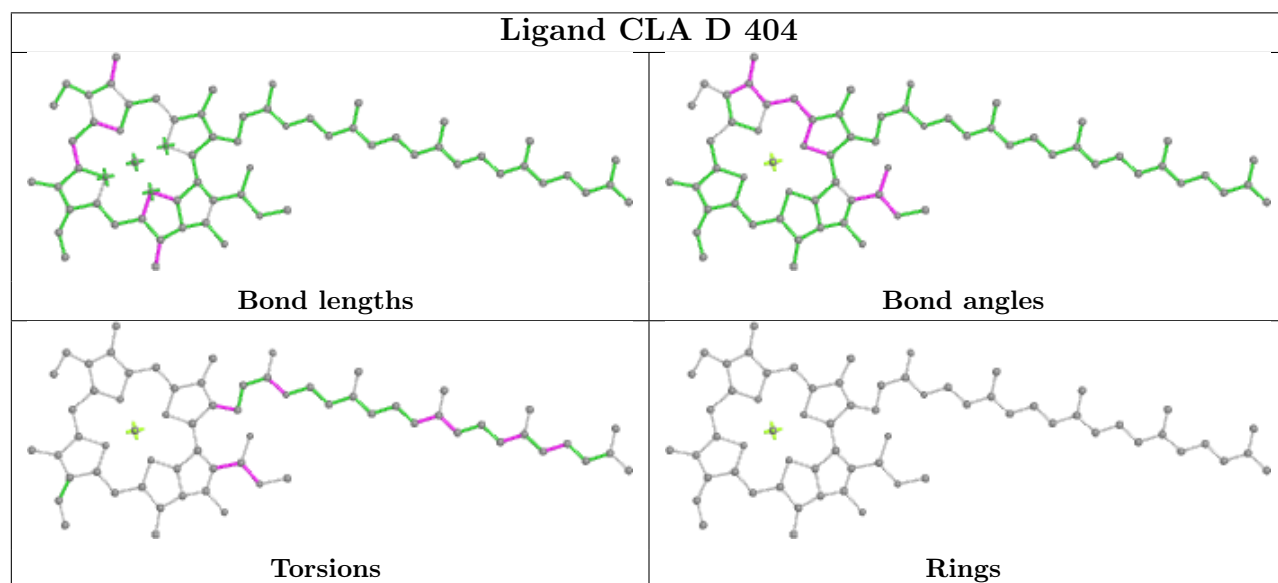
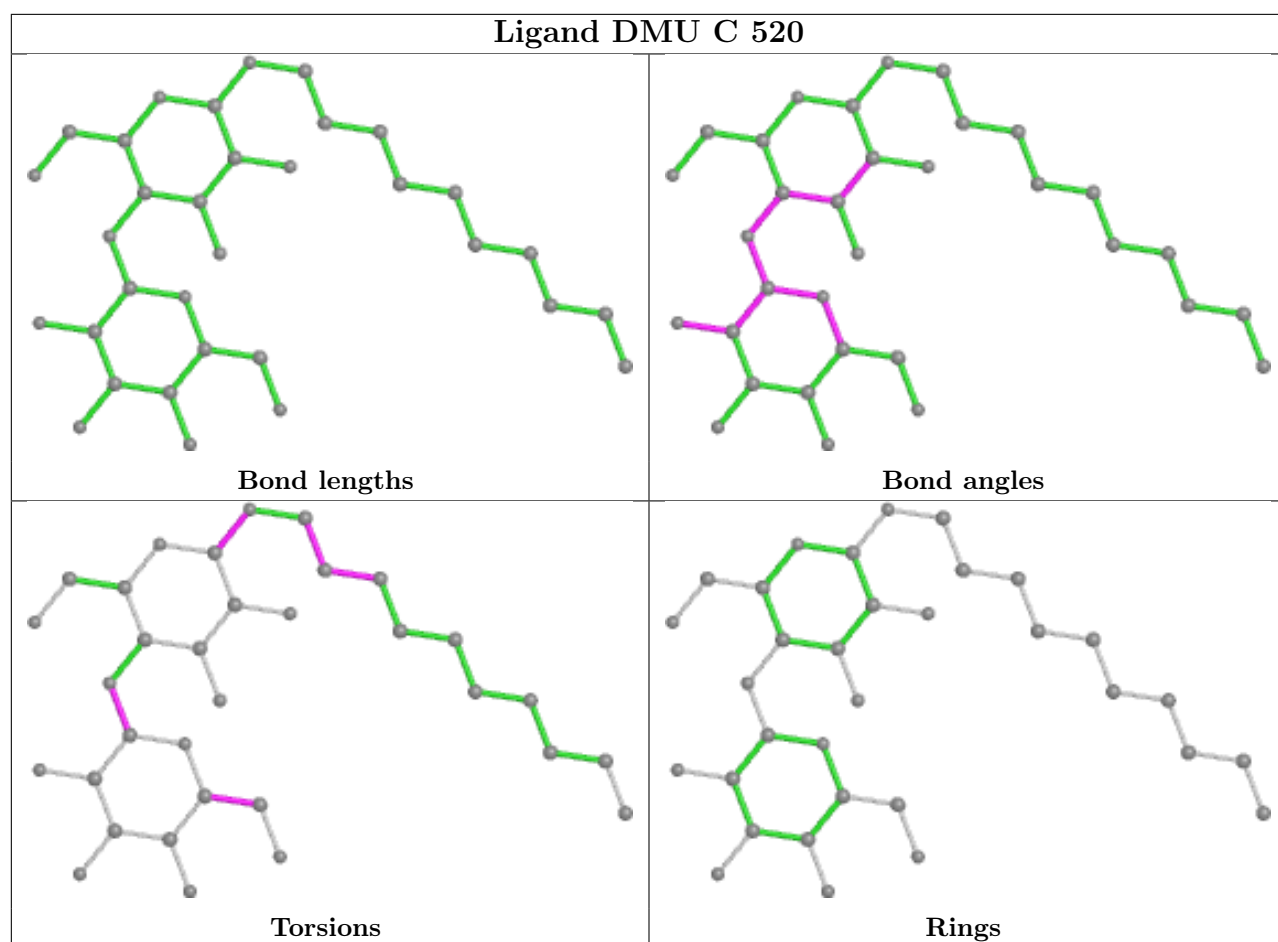
Torsions



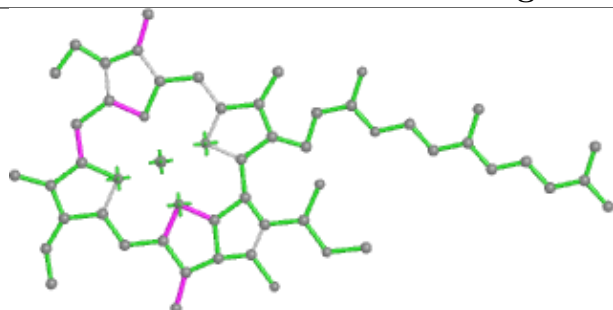
Rings



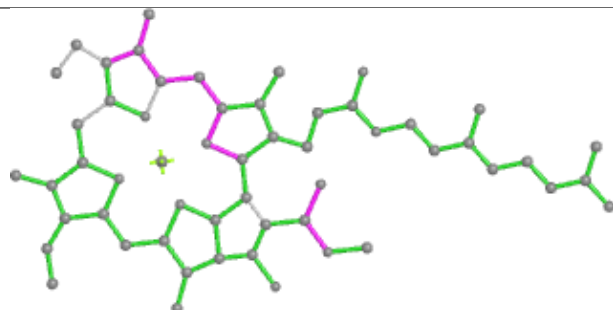




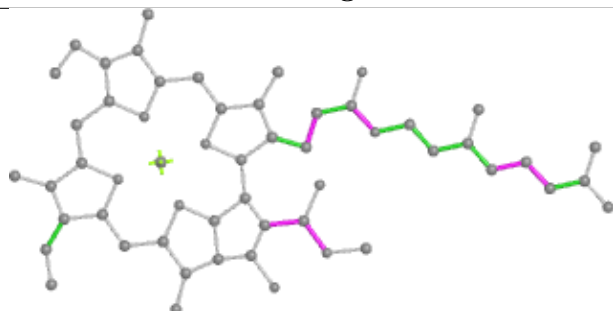
Ligand CLA S 313



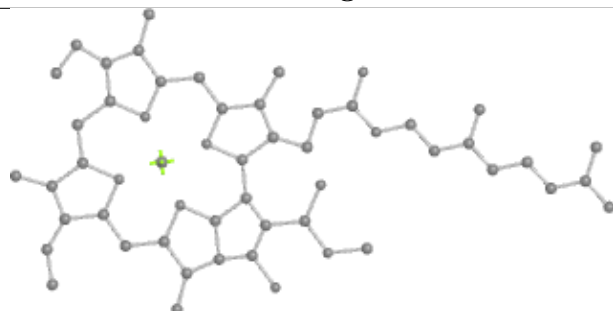
Bond lengths



Bond angles

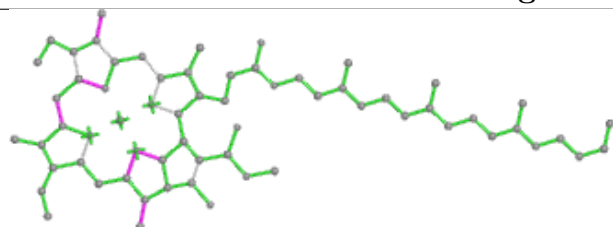


Torsions

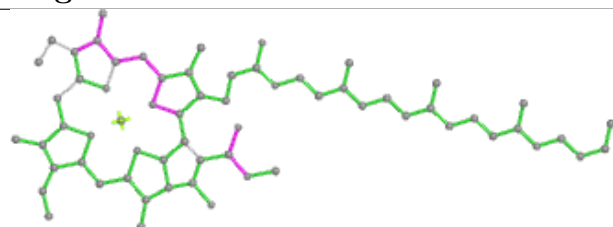


Rings

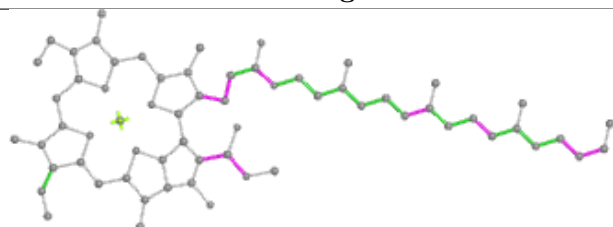
Ligand CLA g 610



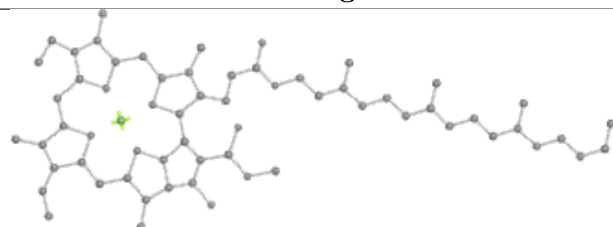
Bond lengths



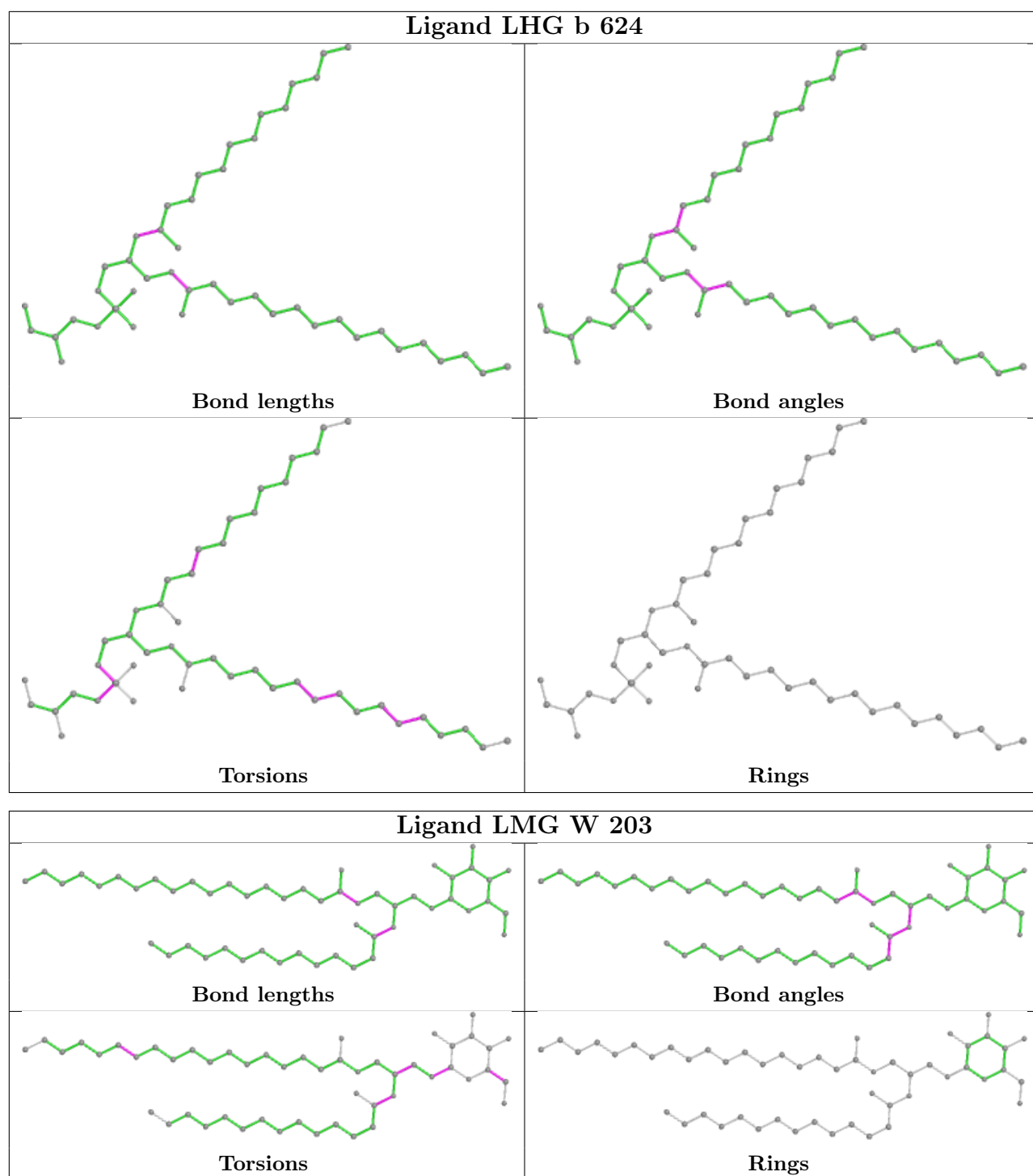
Bond angles



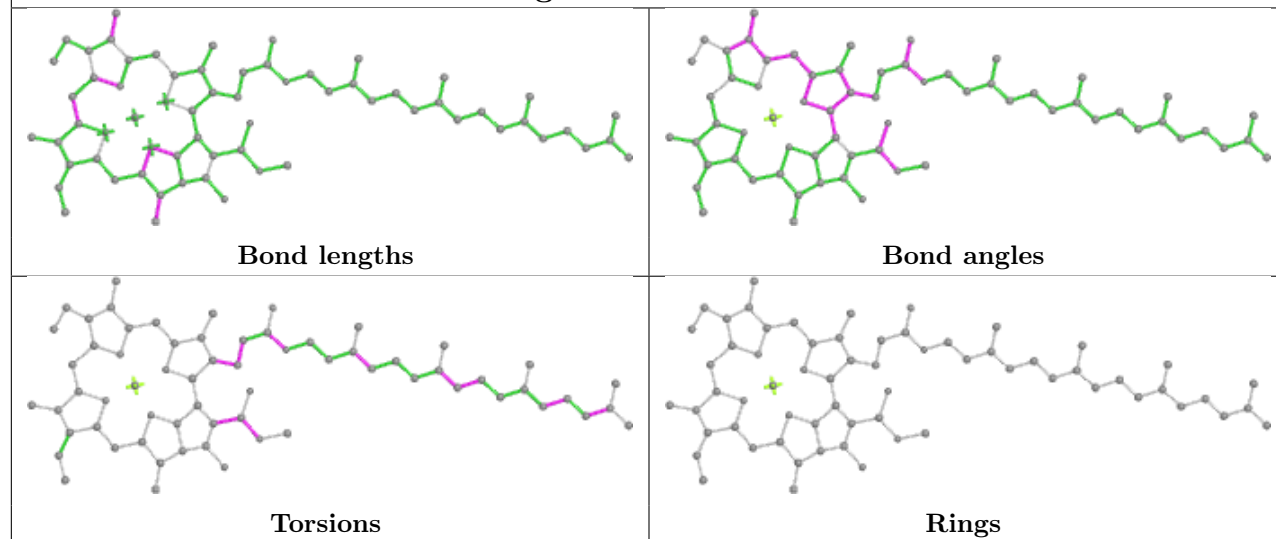
Torsions



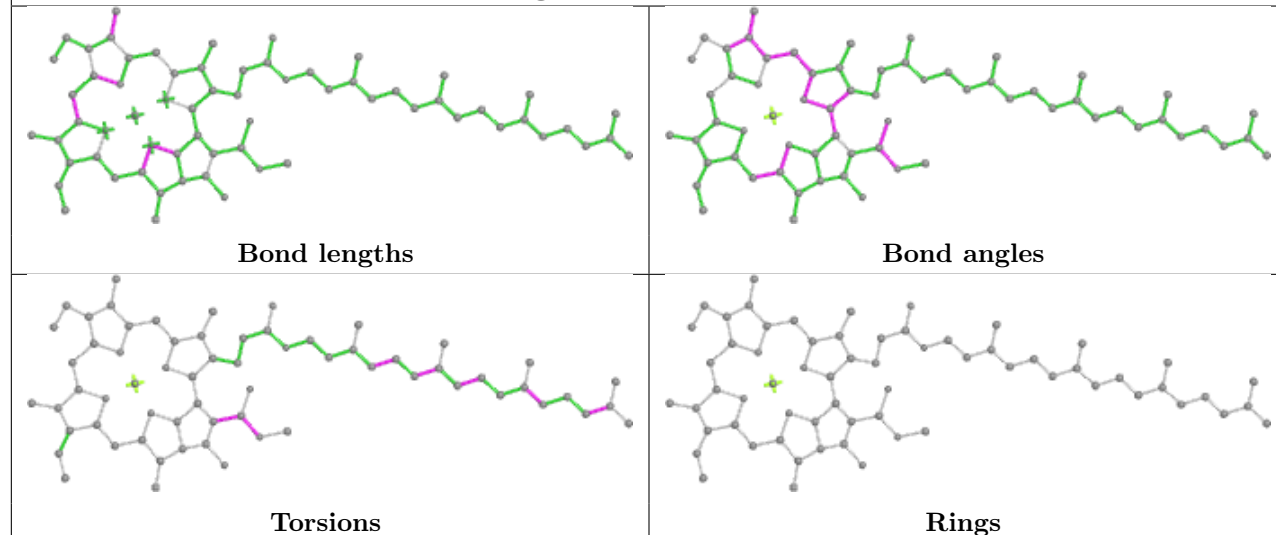
Rings



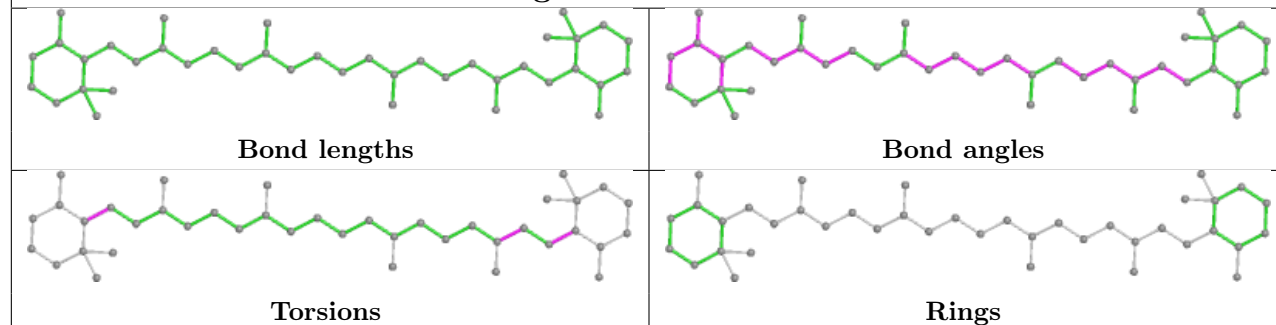
Ligand CLA b 616

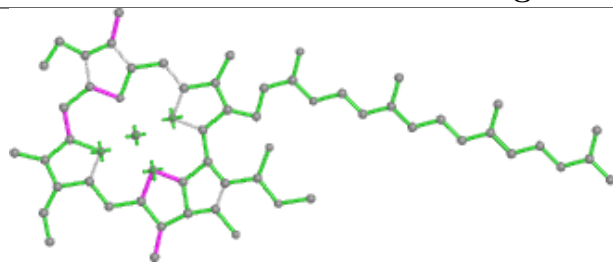
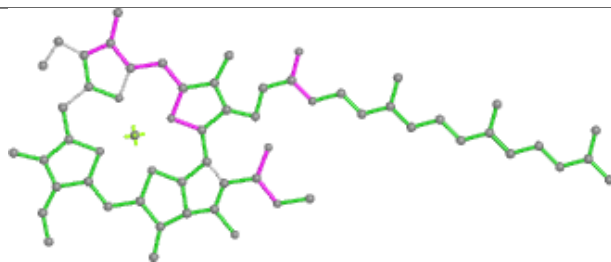
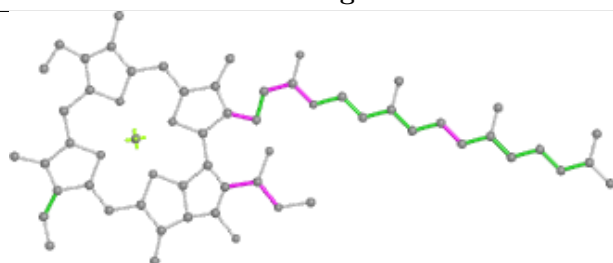
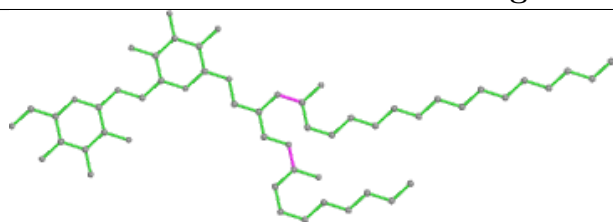
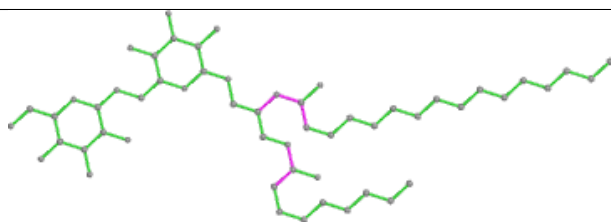
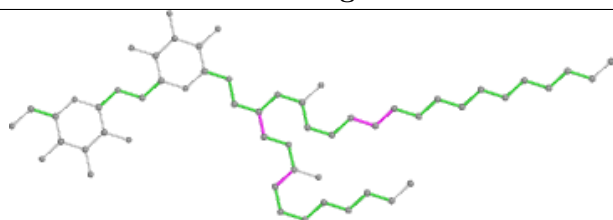
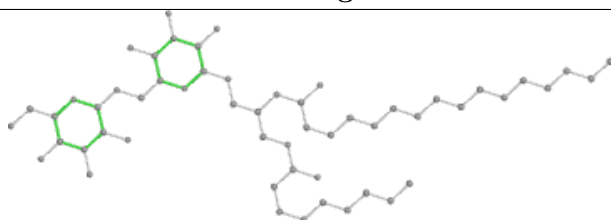


Ligand CLA C 512

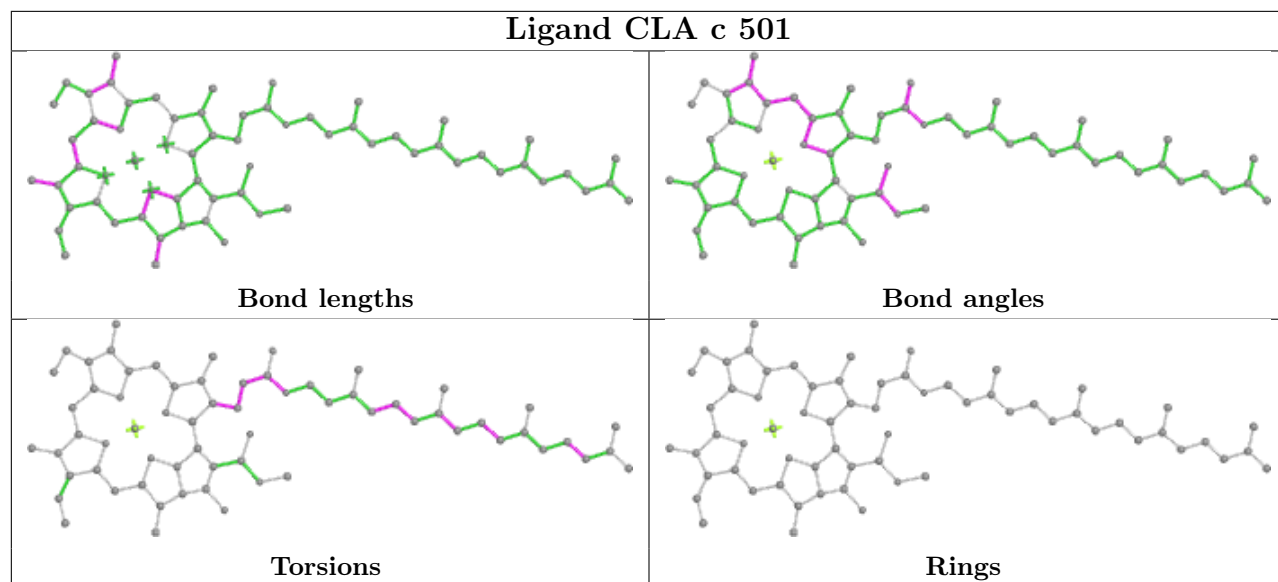


Ligand BCR b 619

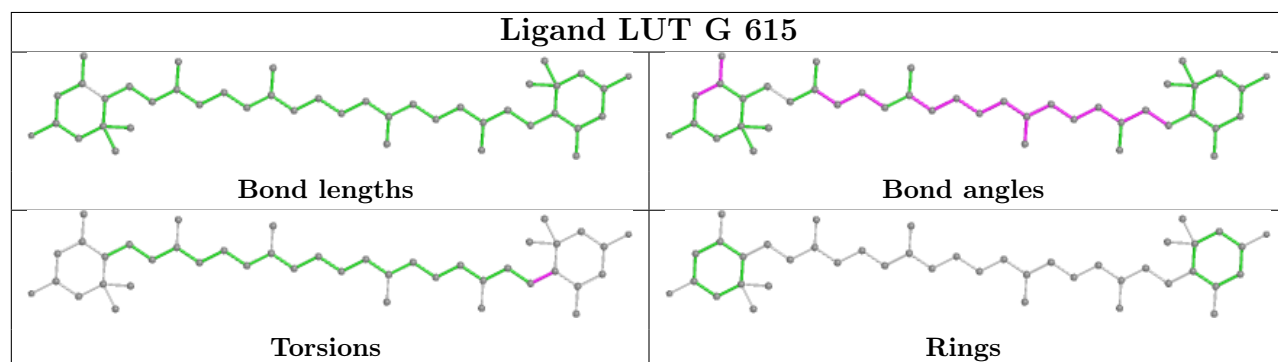


Ligand CLA A 404**Bond lengths****Bond angles****Torsions****Rings****Ligand DGD C 517****Bond lengths****Bond angles****Torsions****Rings**

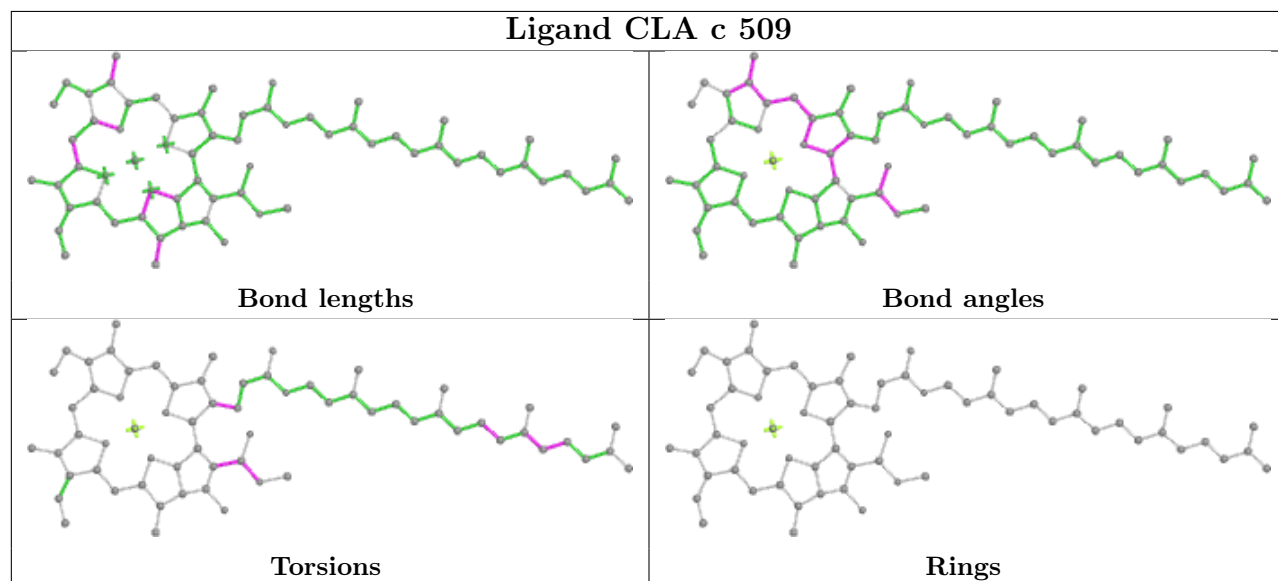
Ligand CLA c 501

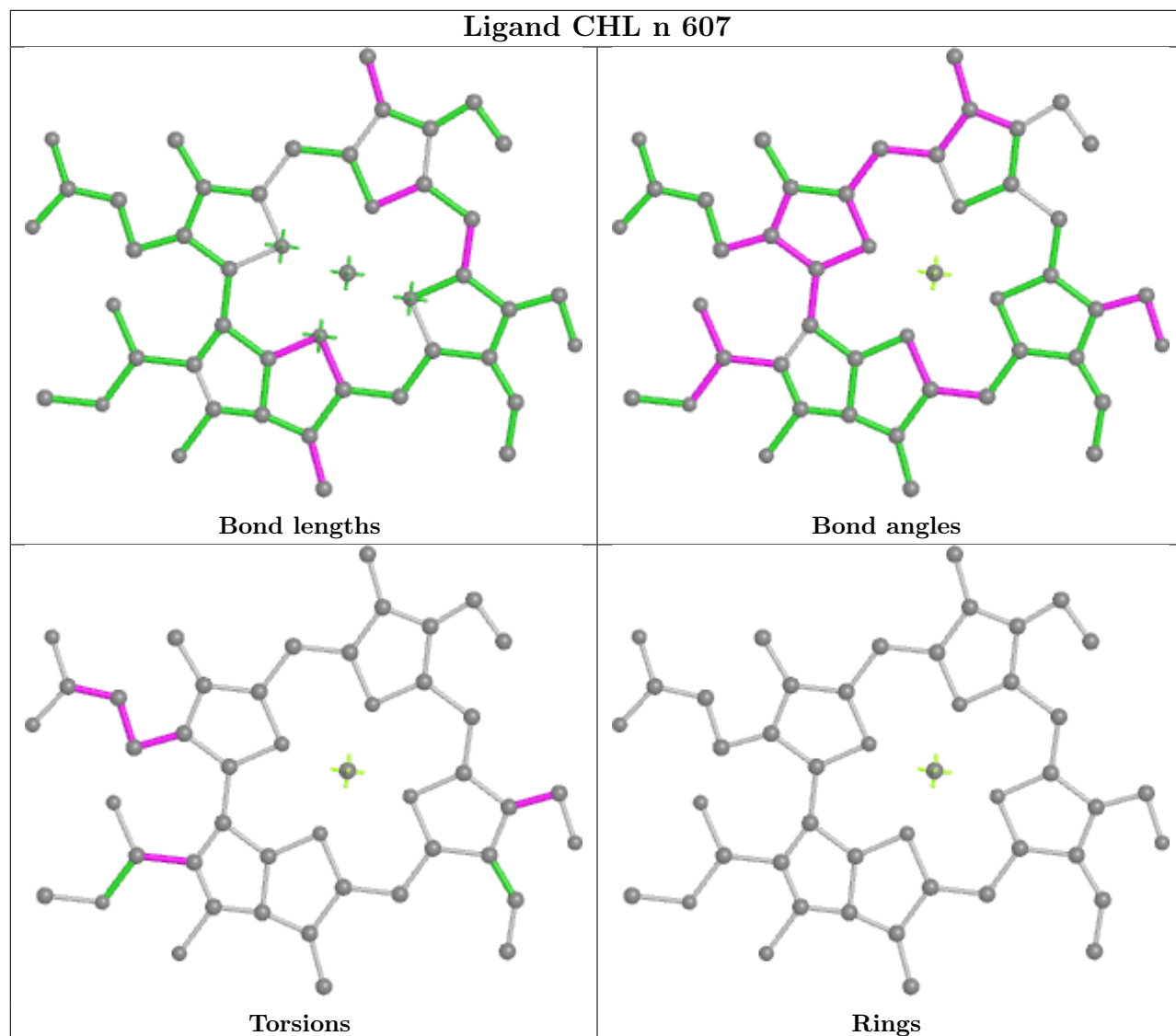
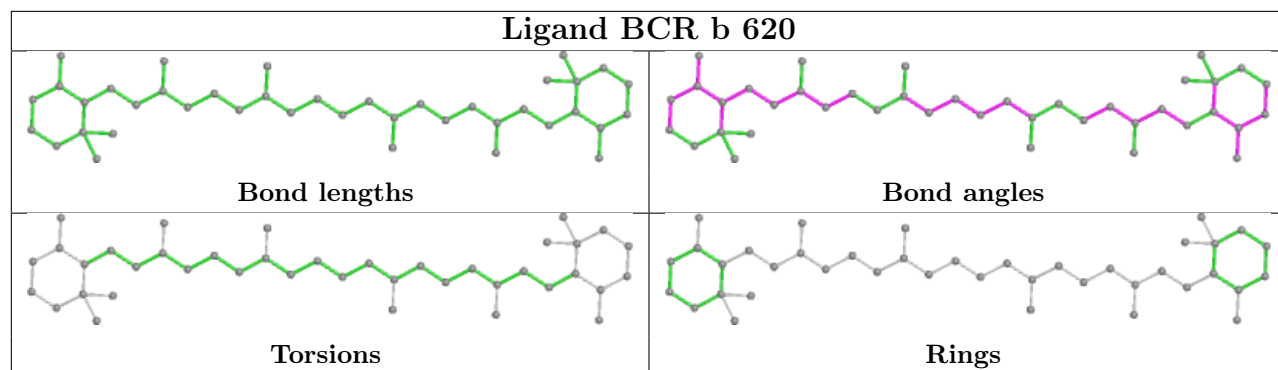


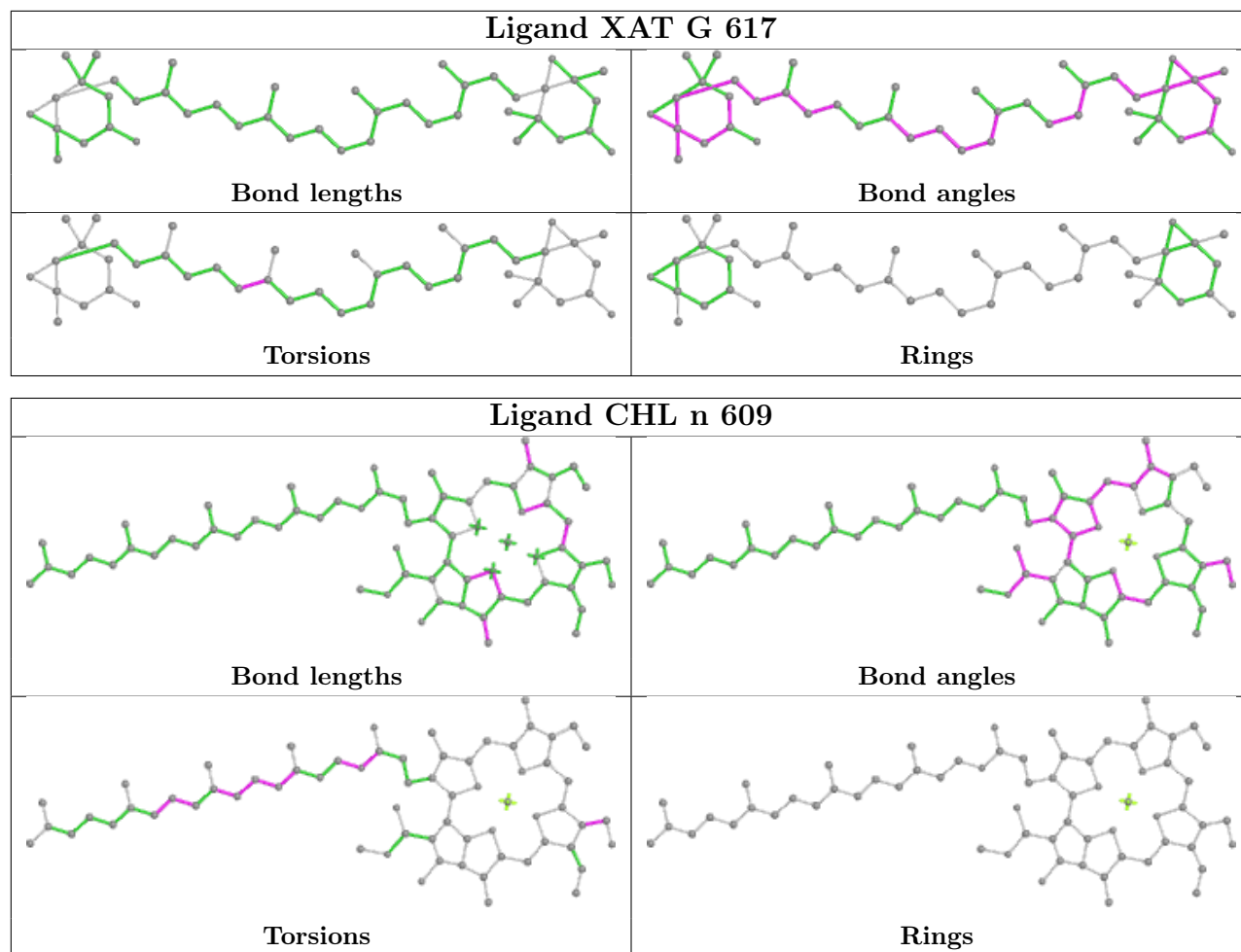
Ligand LUT G 615



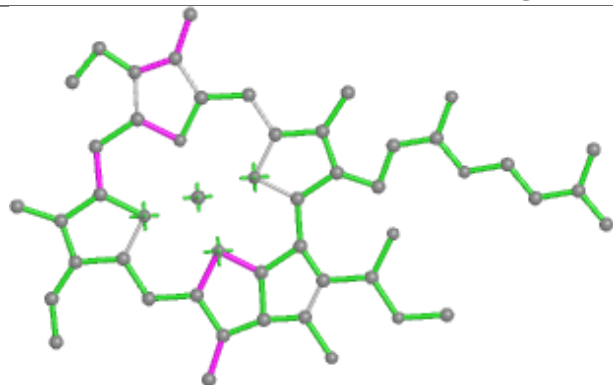
Ligand CLA c 509



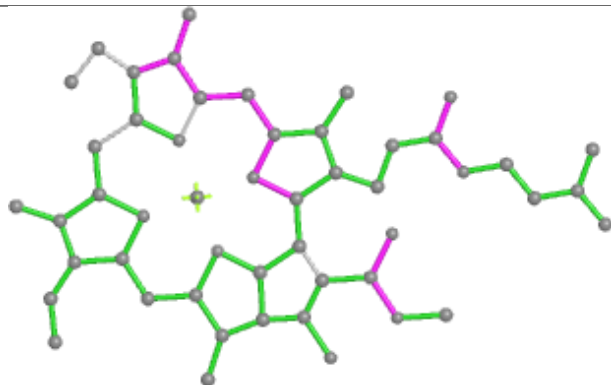




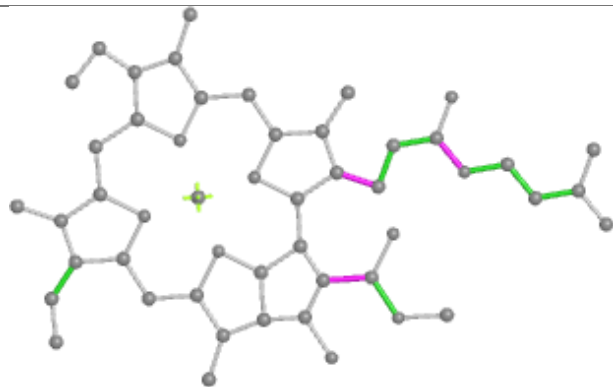
Ligand CLA S 305



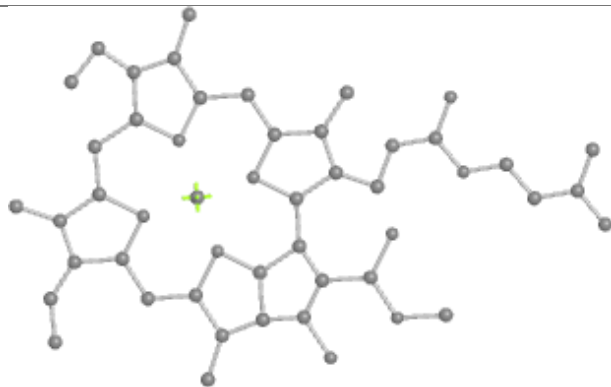
Bond lengths



Bond angles

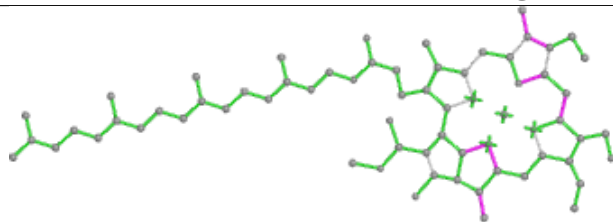


Torsions

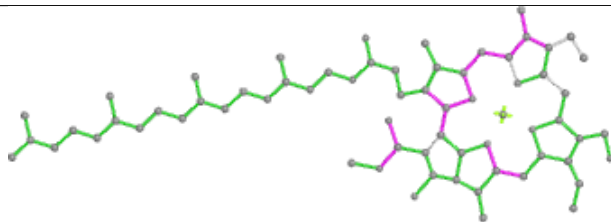


Rings

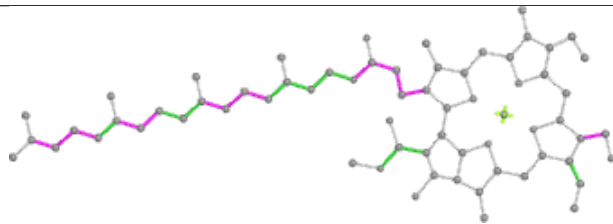
Ligand CHL Y 310



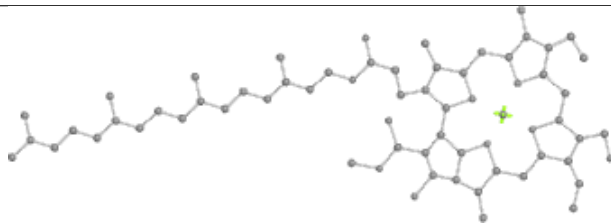
Bond lengths



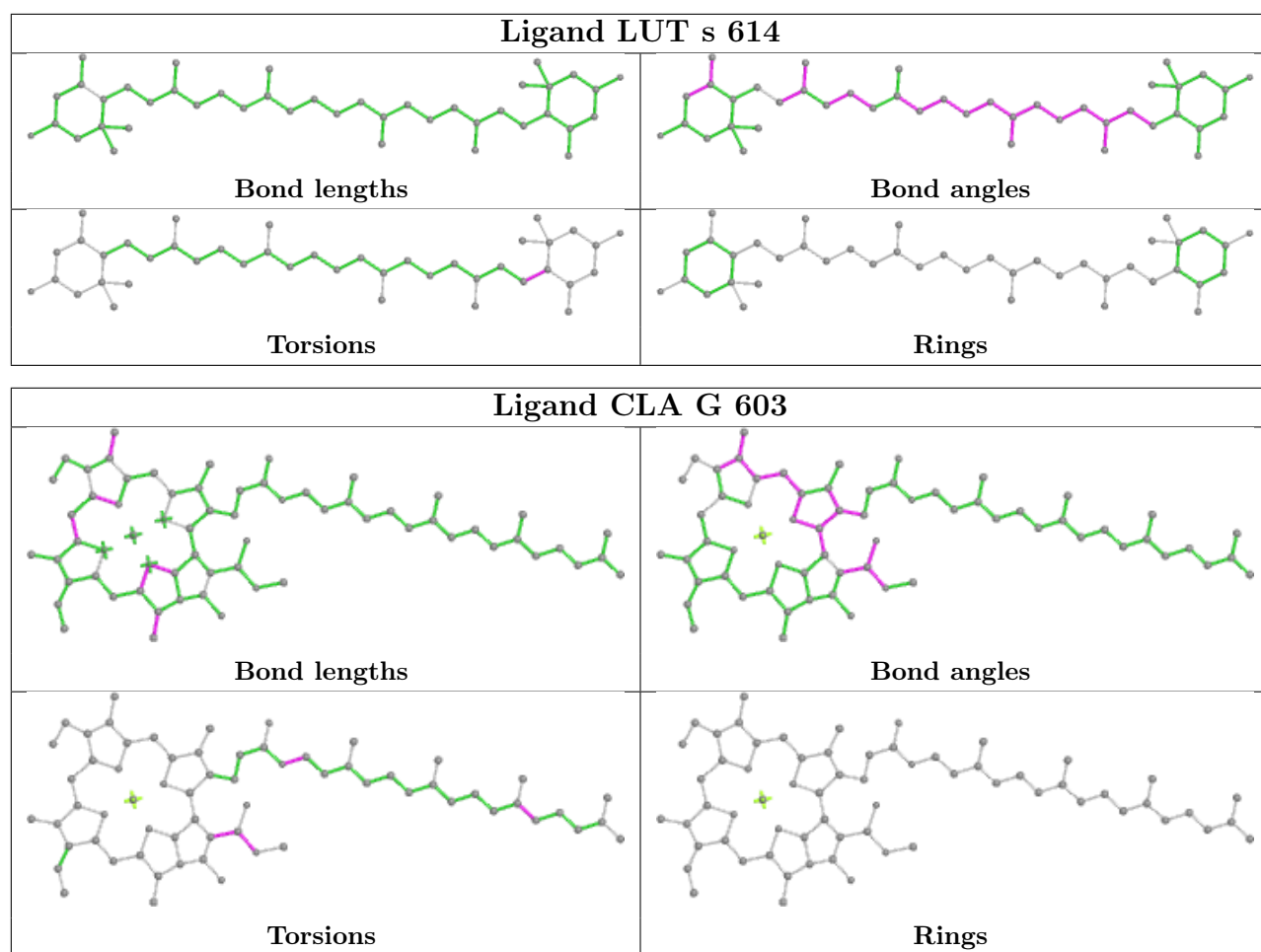
Bond angles

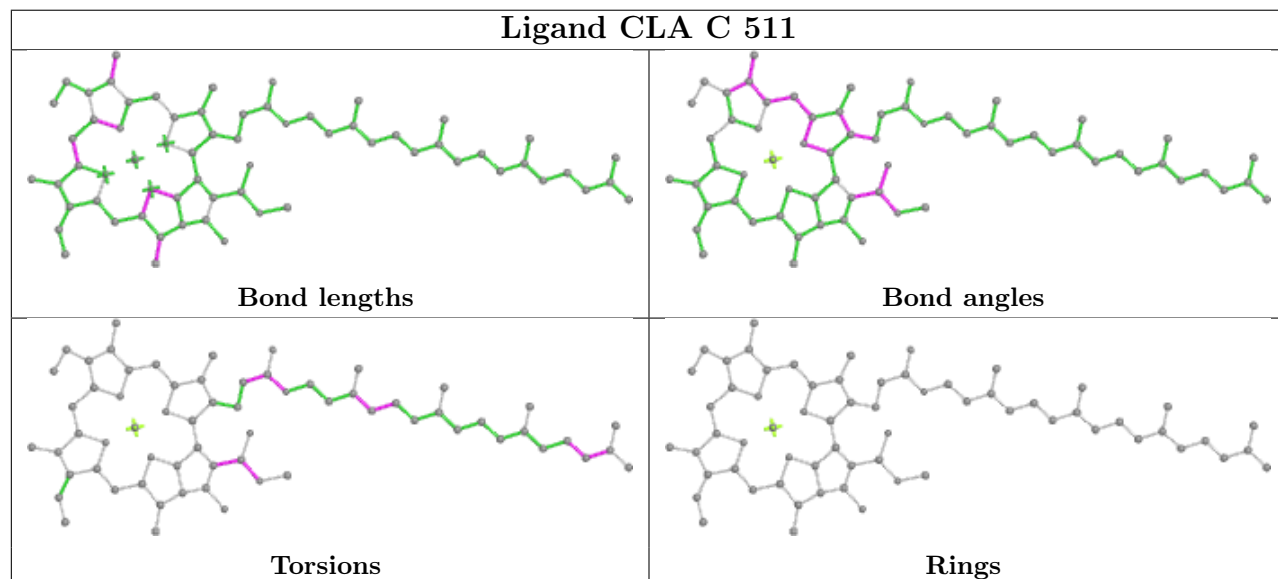
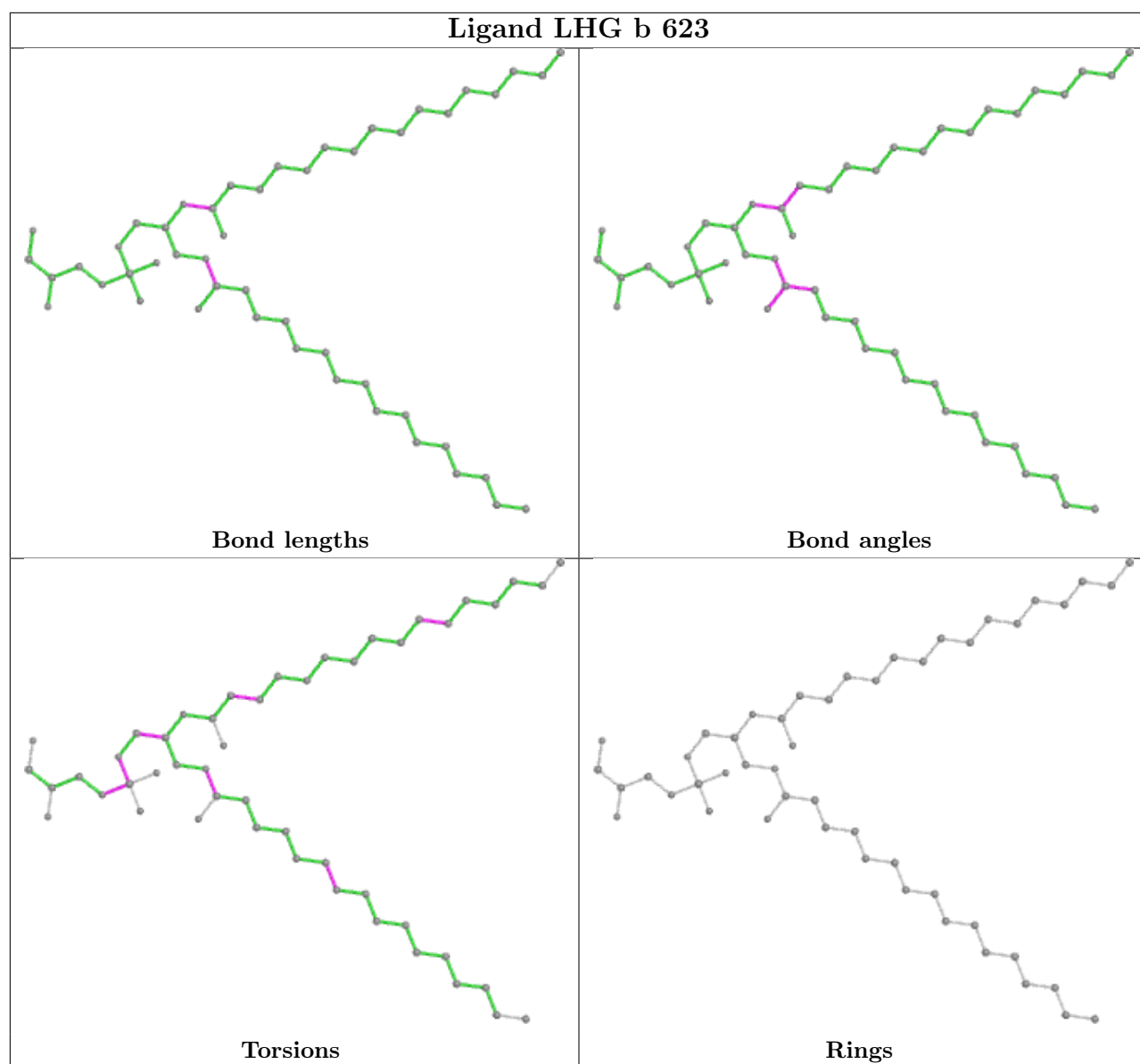


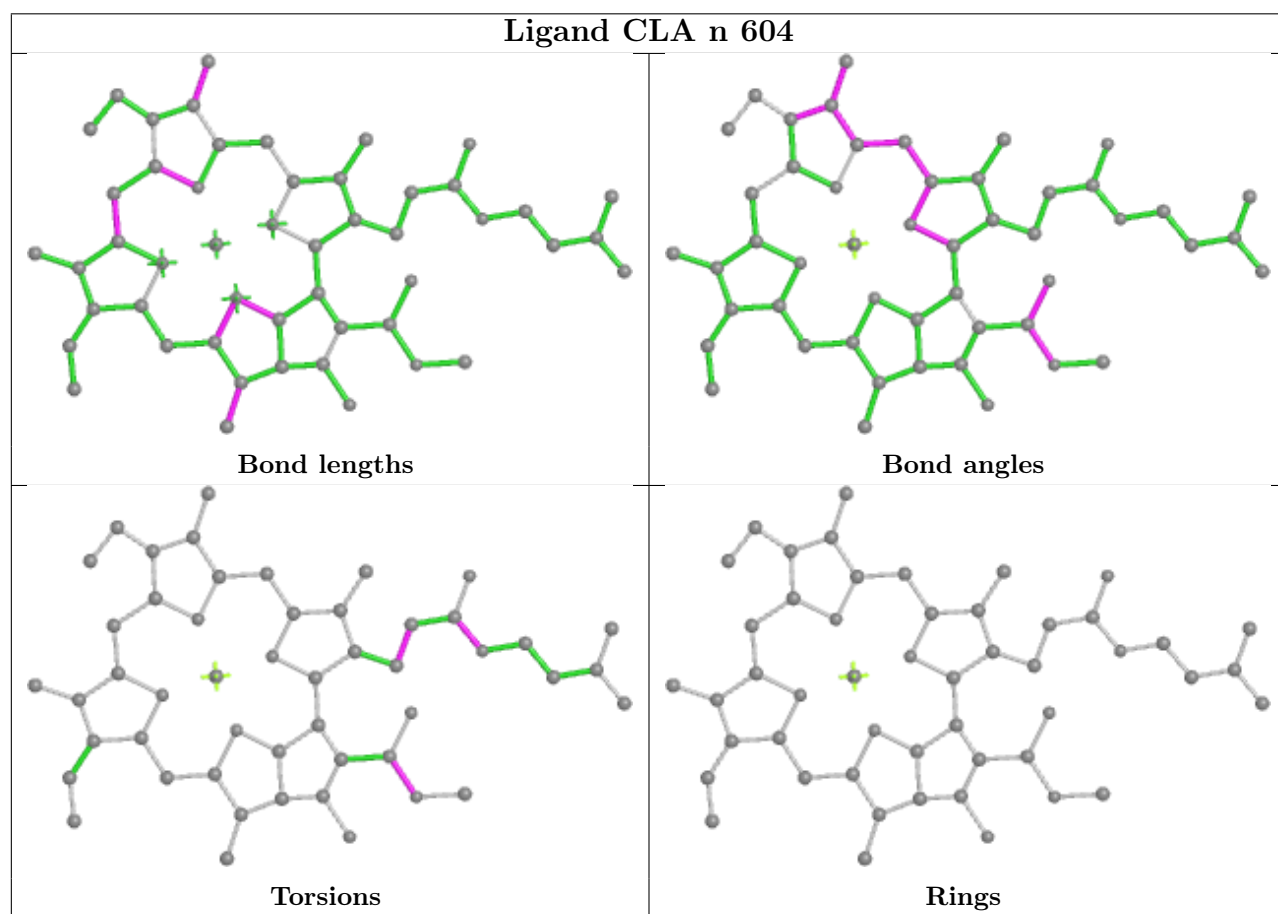
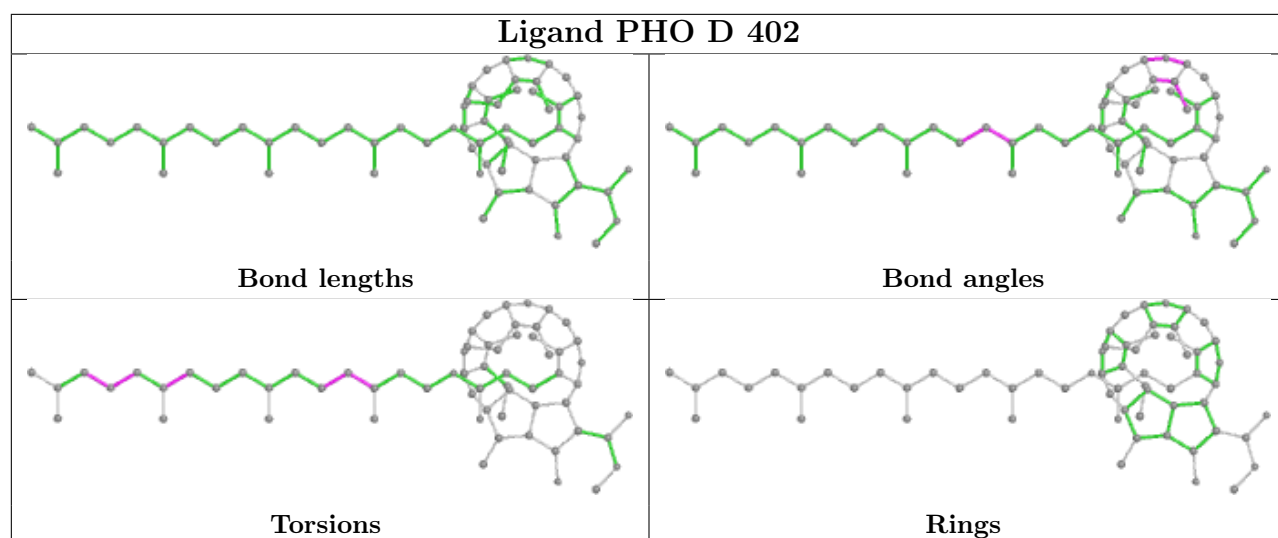
Torsions

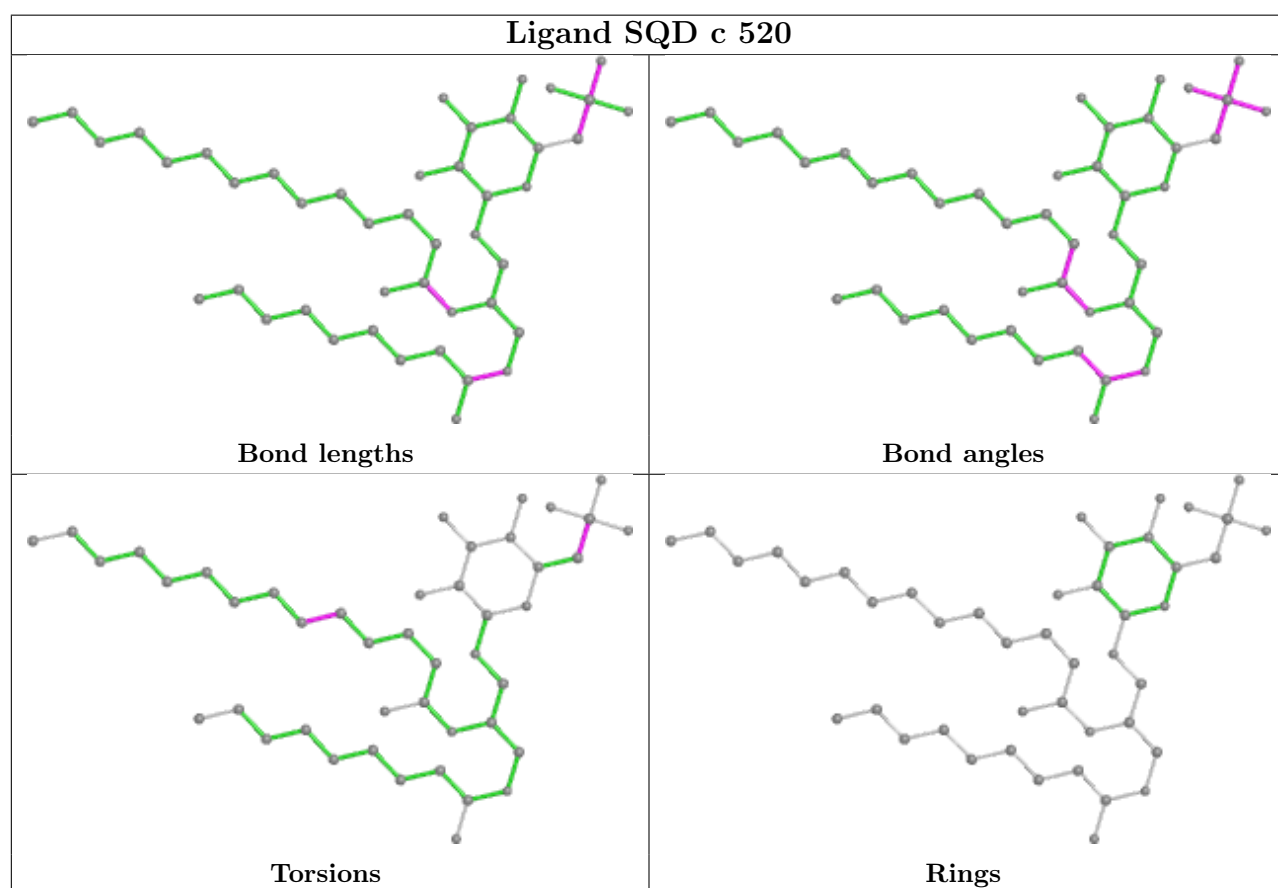
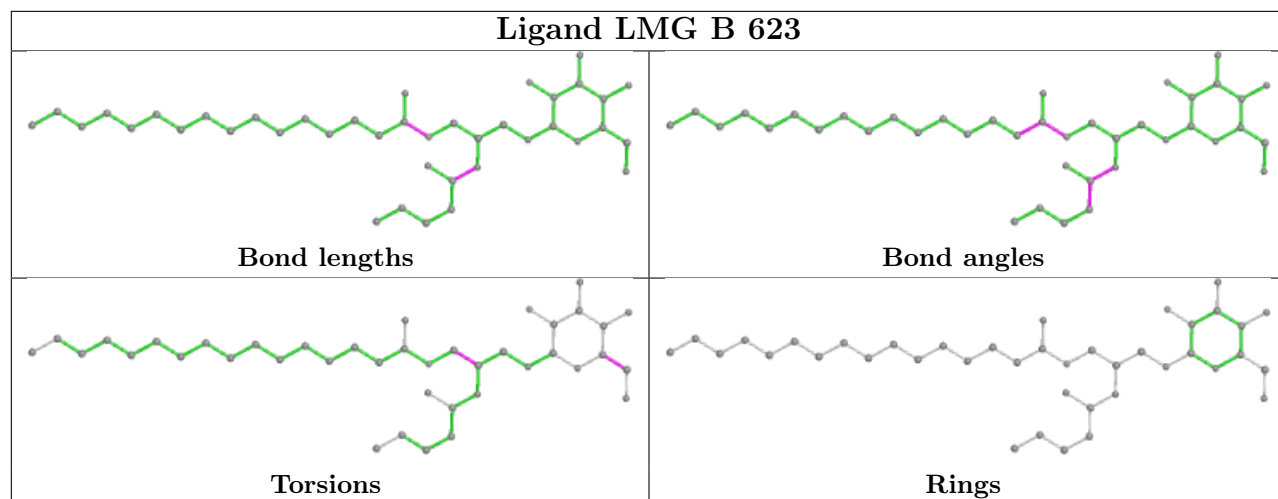


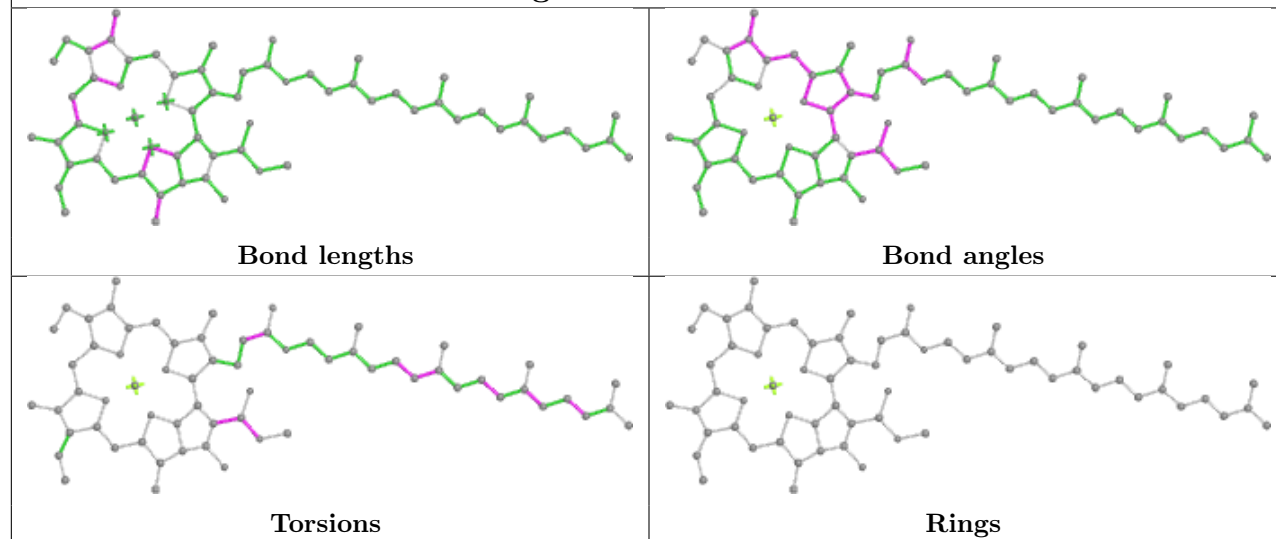
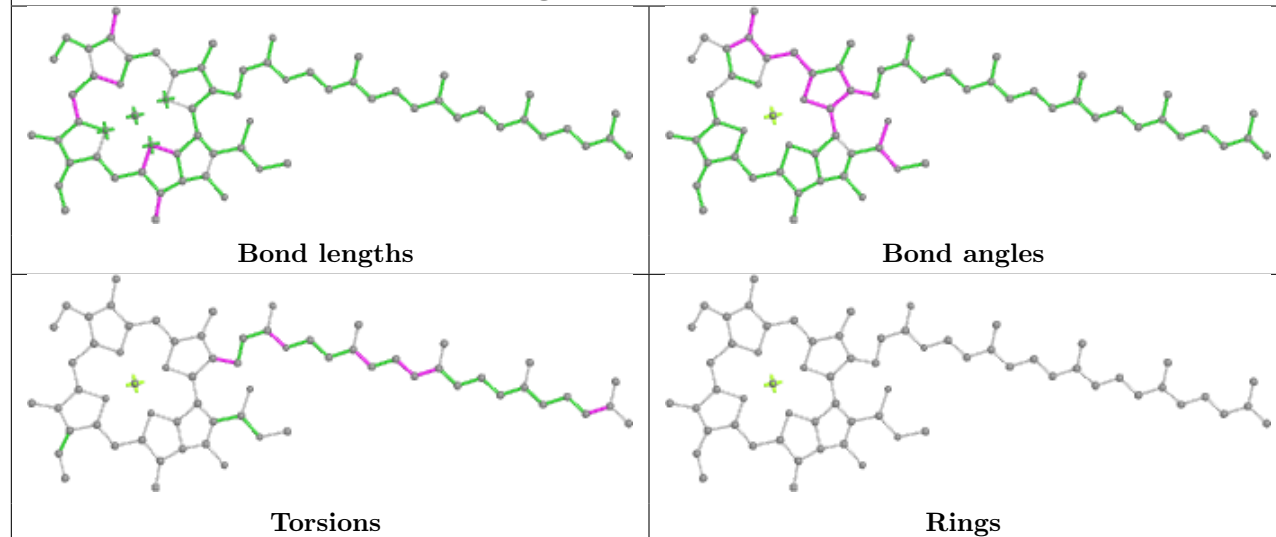
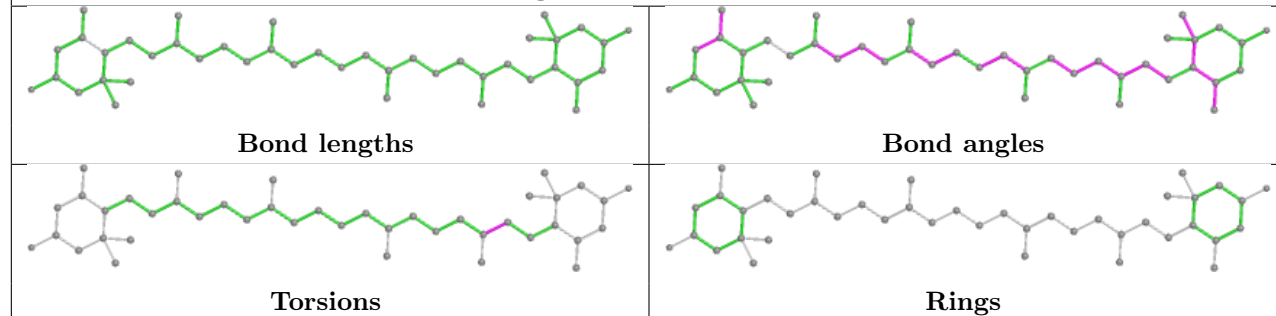
Rings

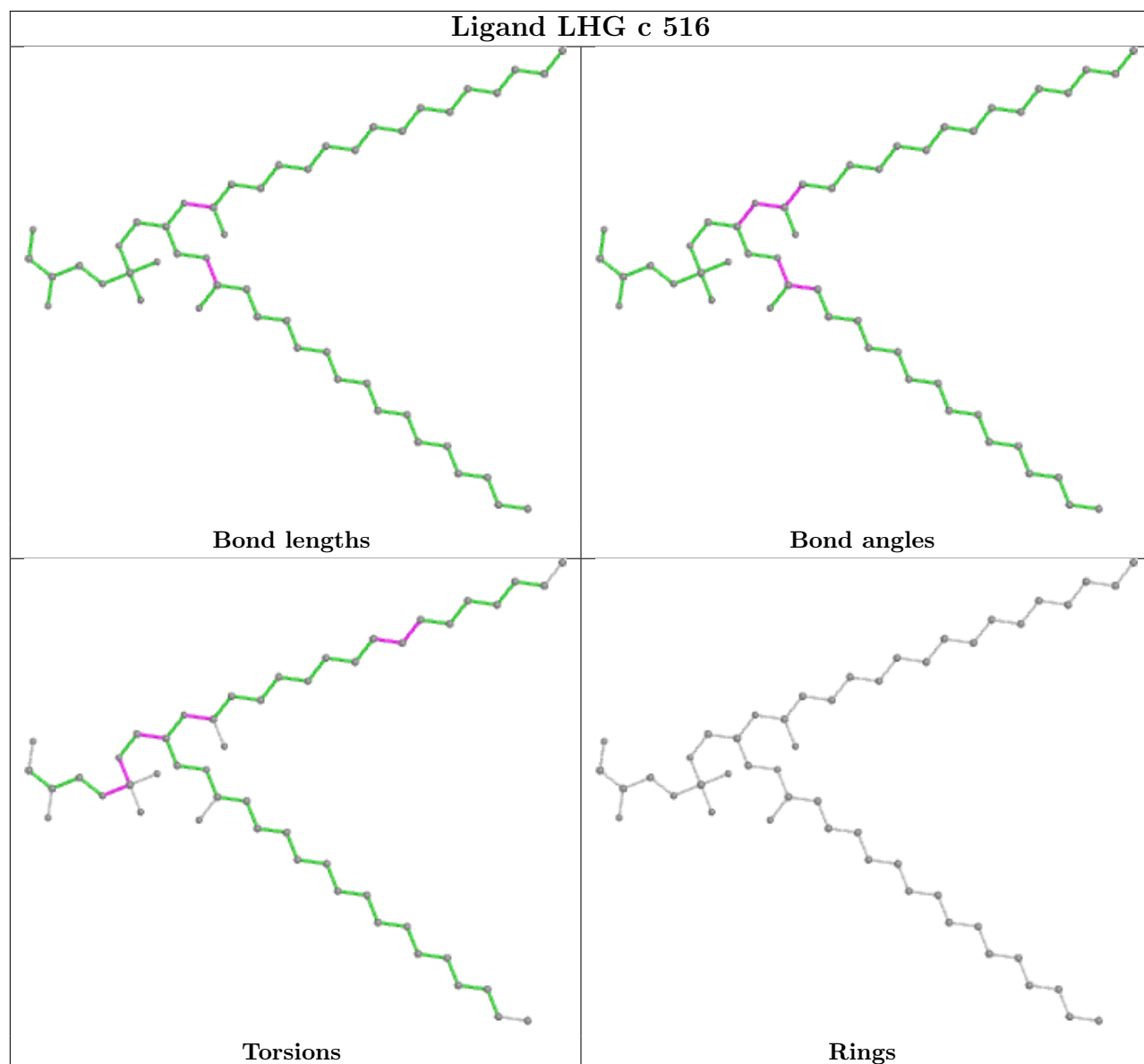
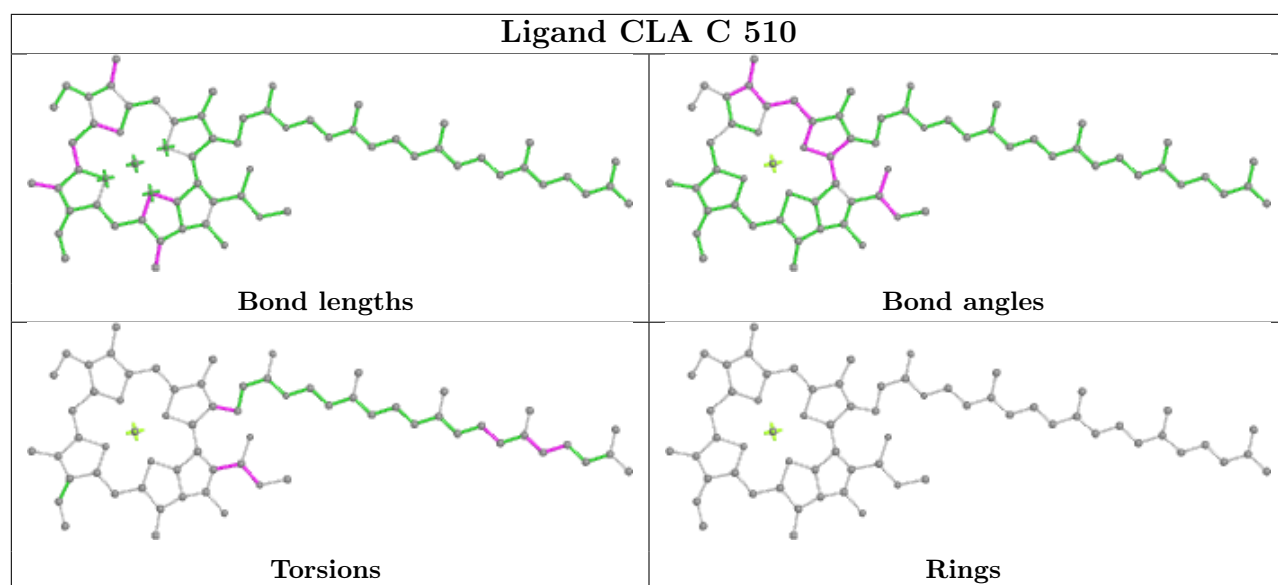


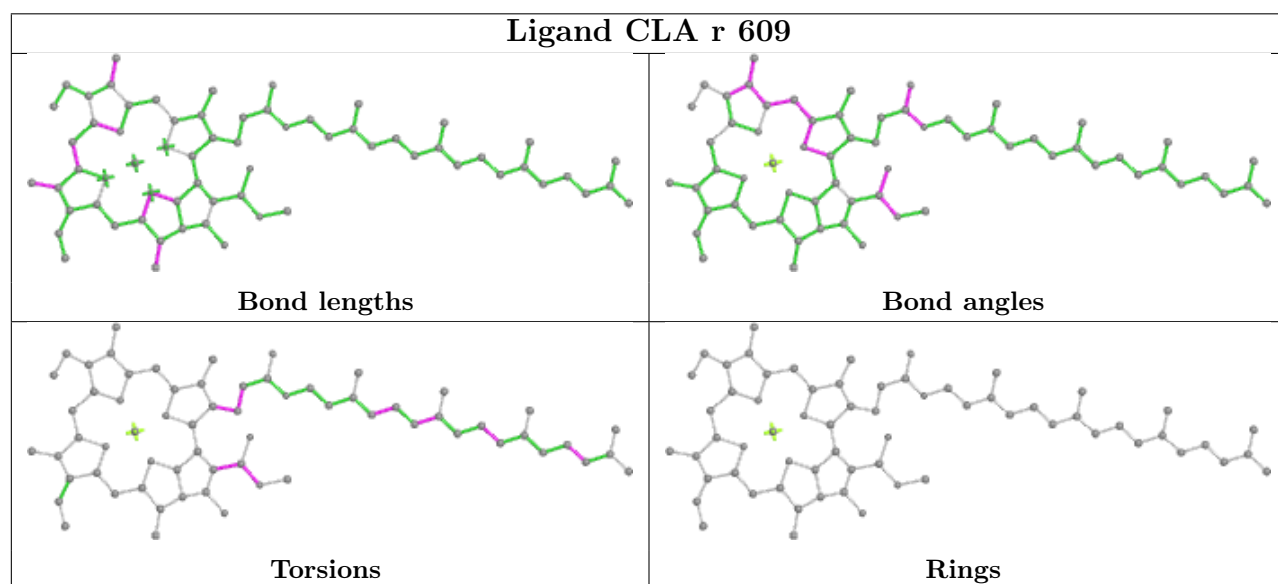
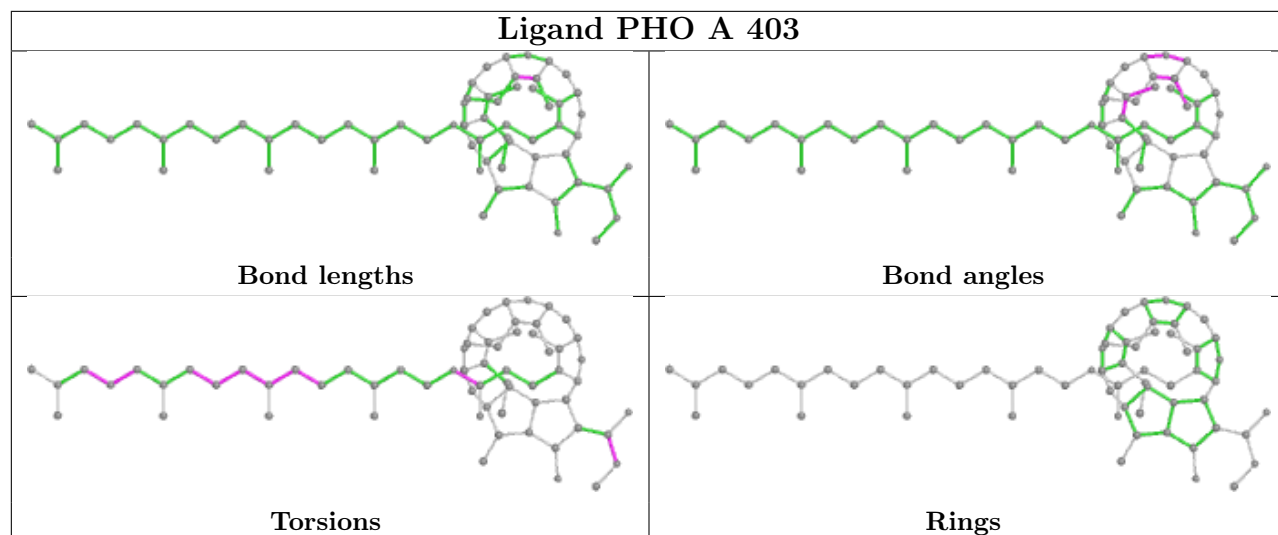




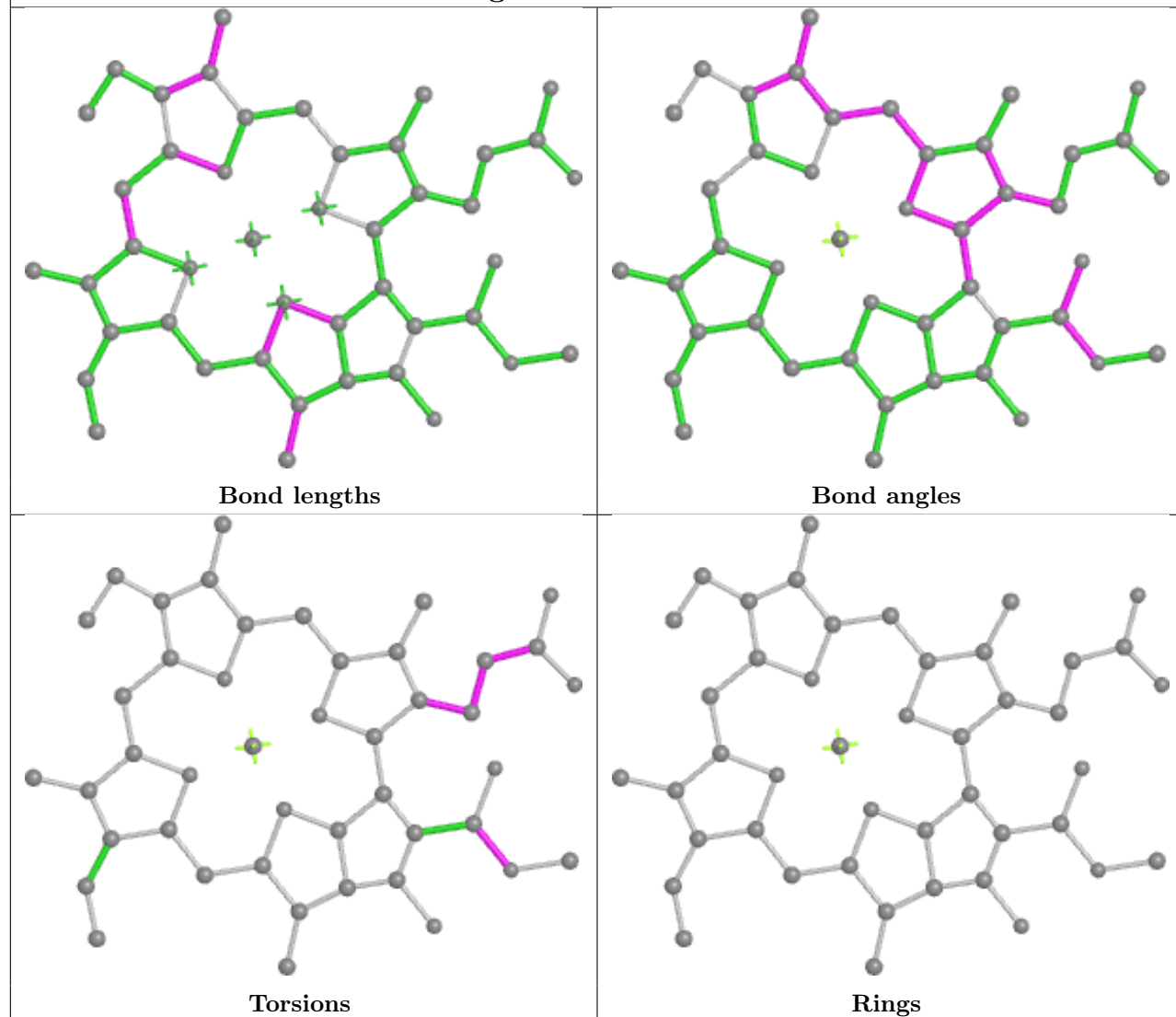


Ligand CLA B 615**Ligand CLA b 604****Ligand LUT R 314**

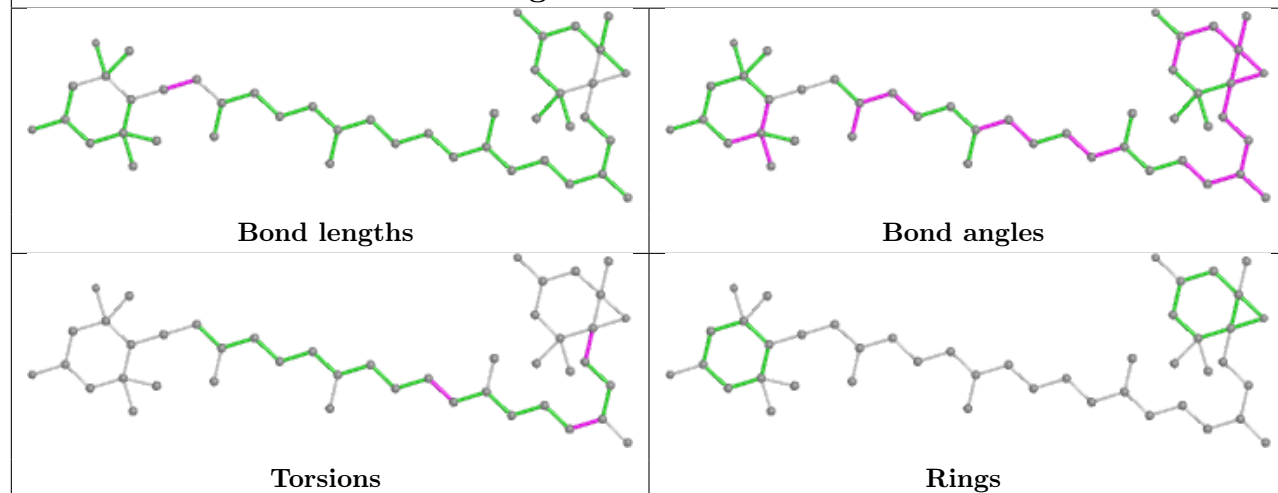


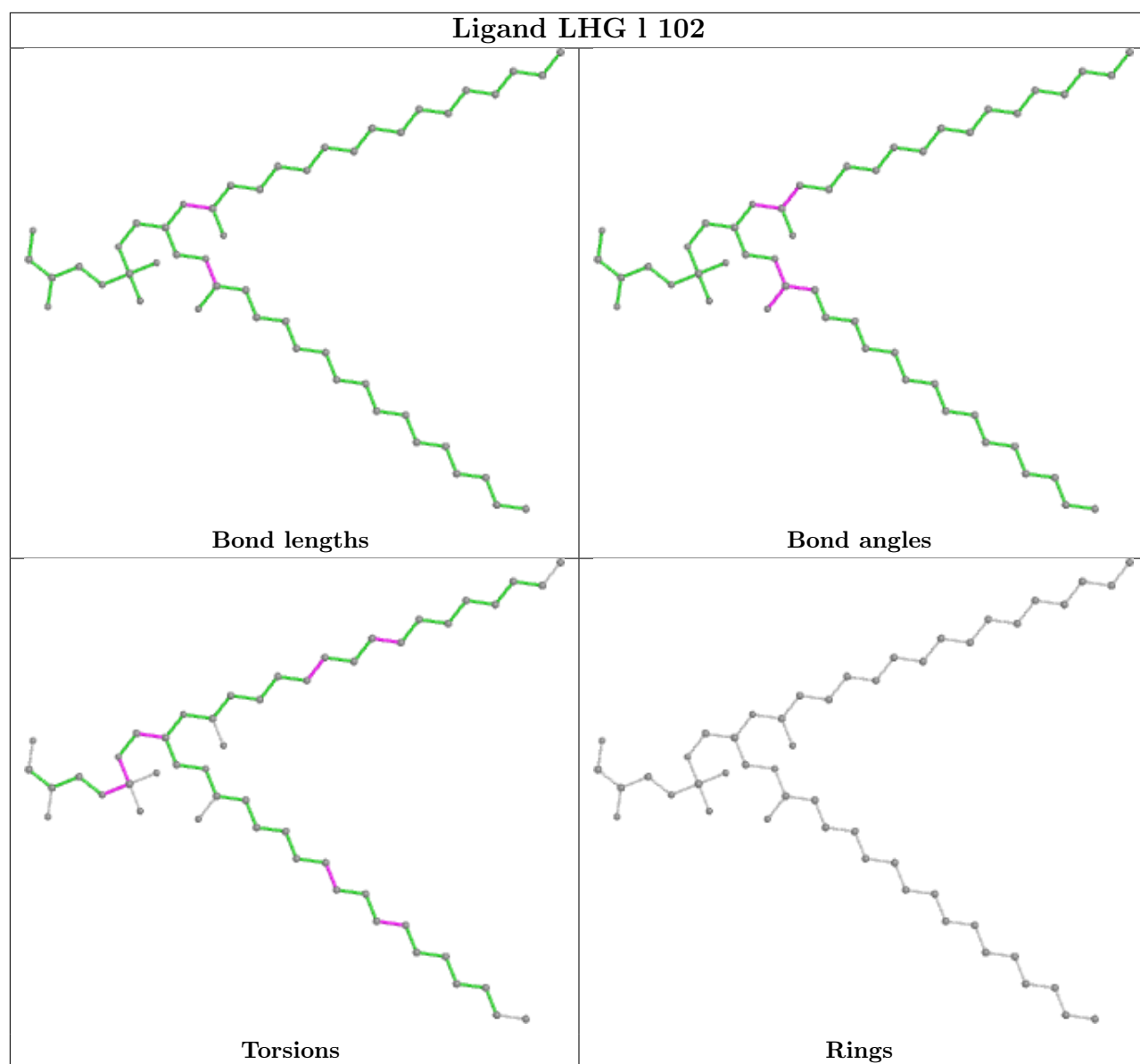


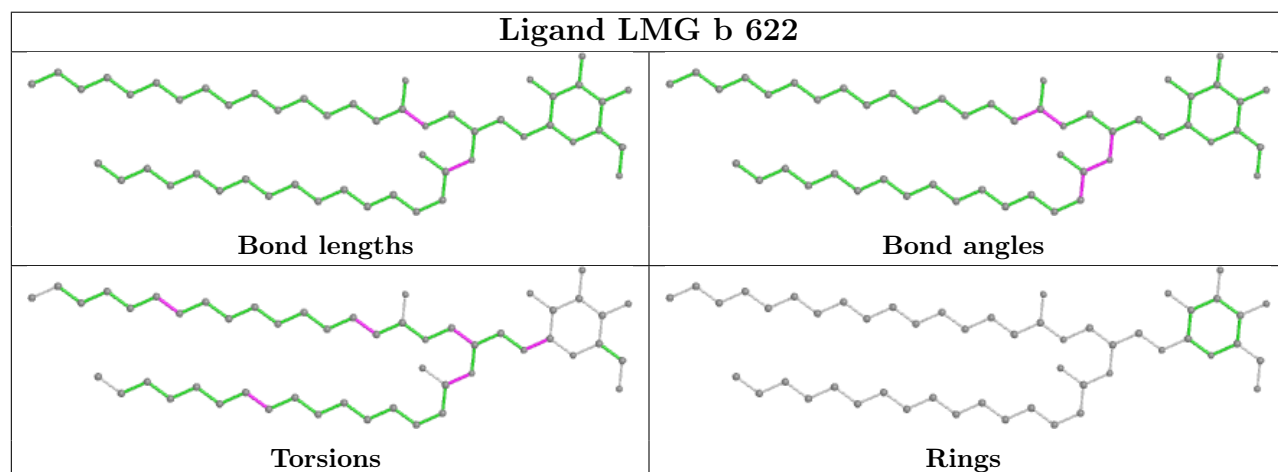
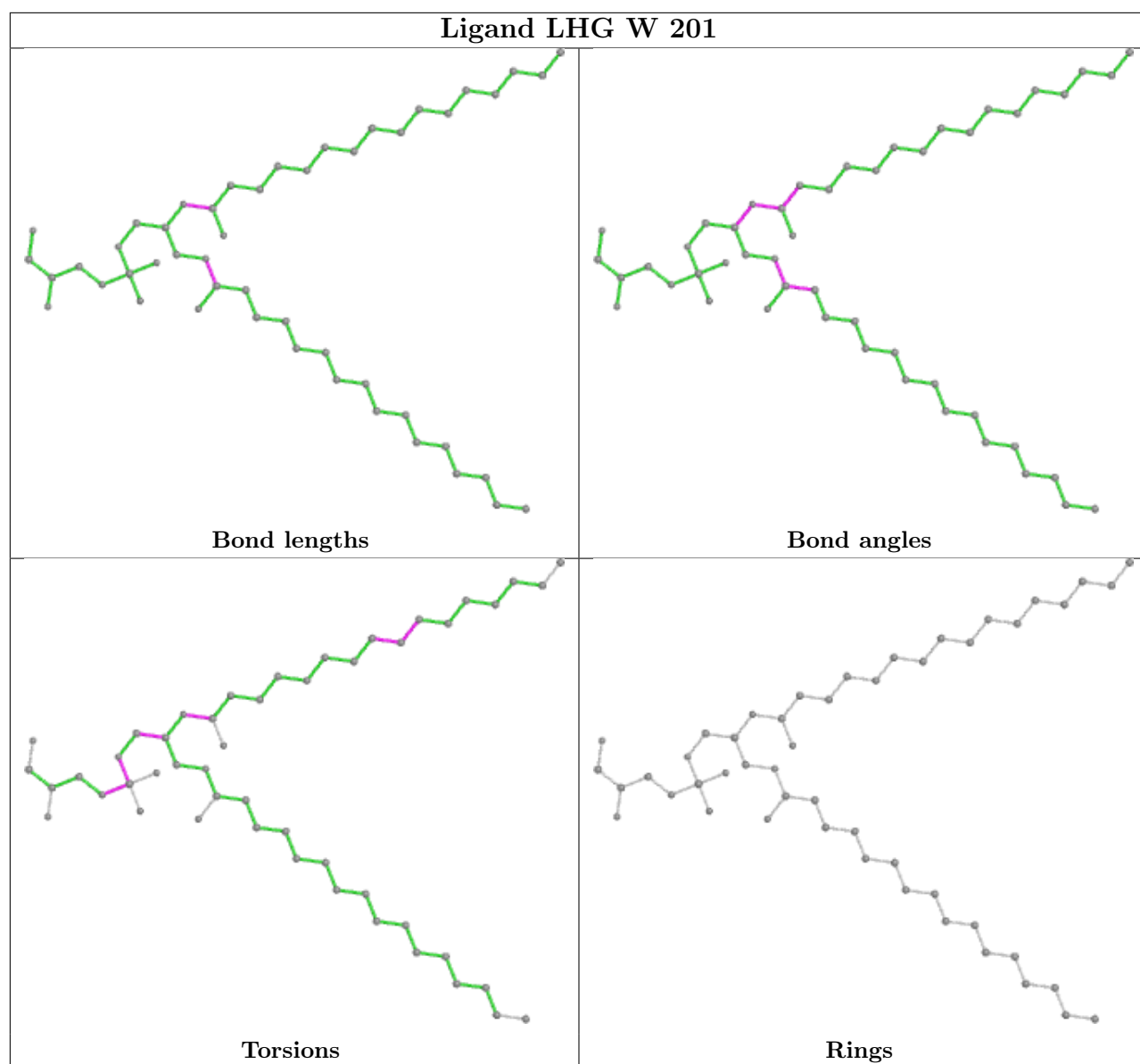
Ligand CLA N 612

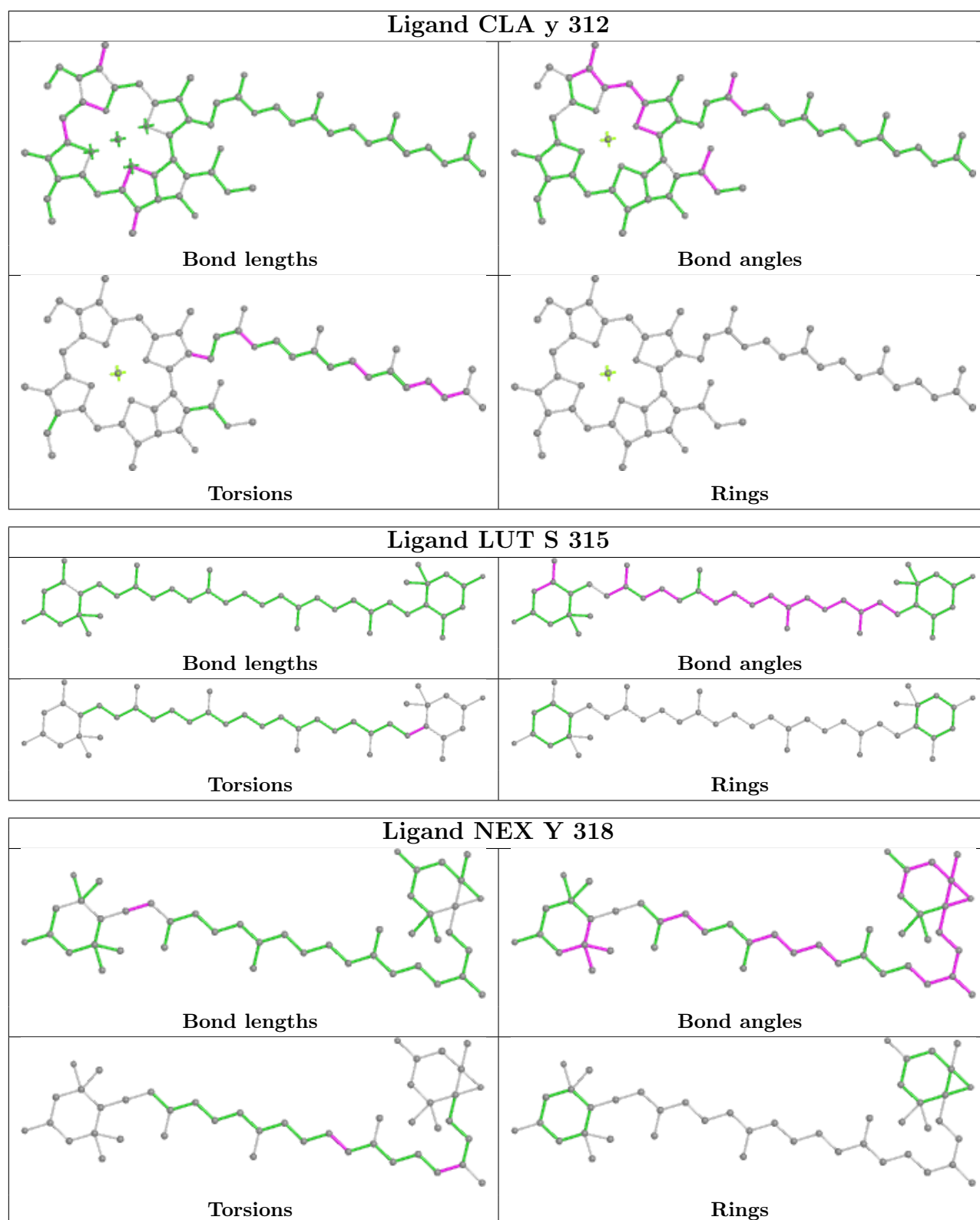


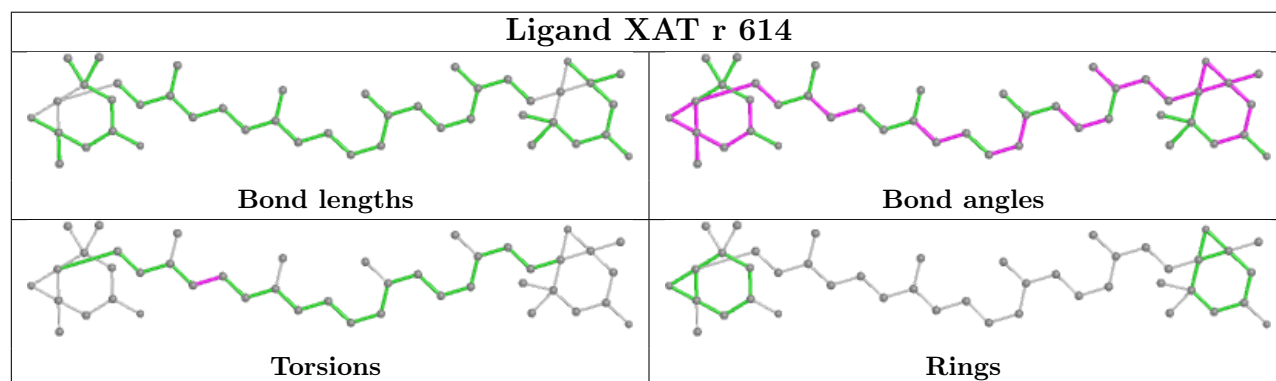
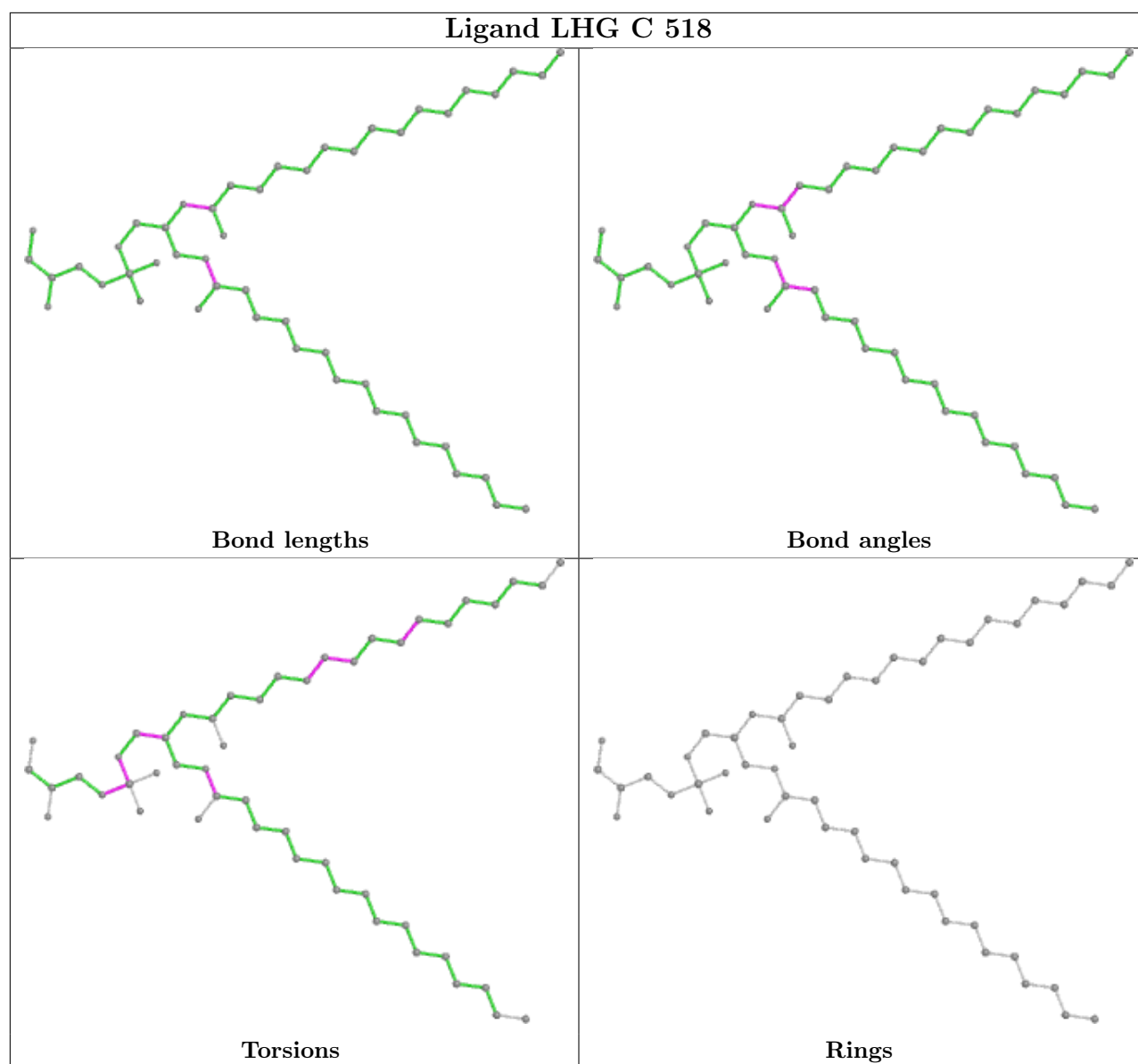
Ligand NEX N 617



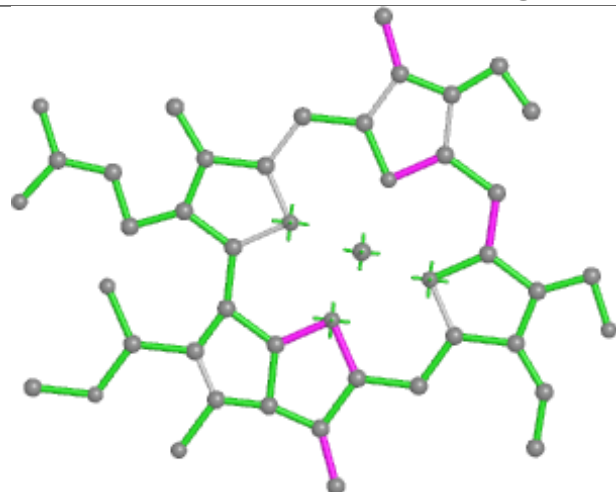




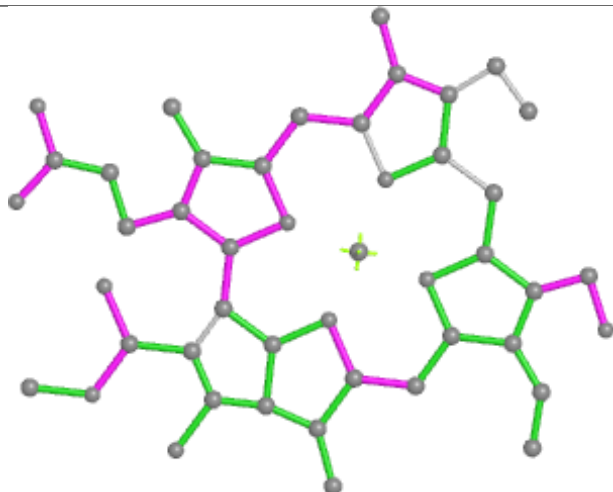




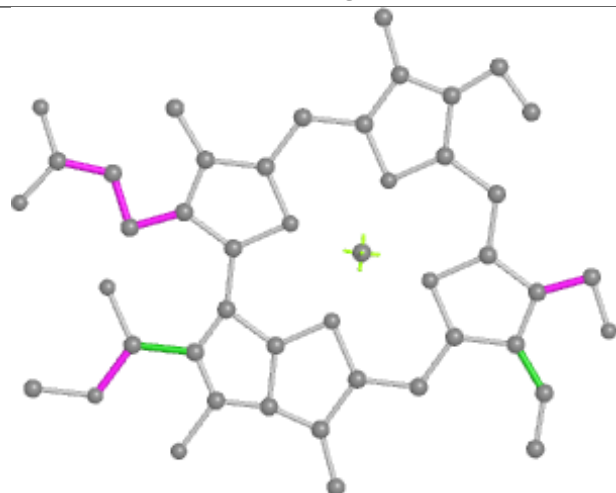
Ligand CHL N 606



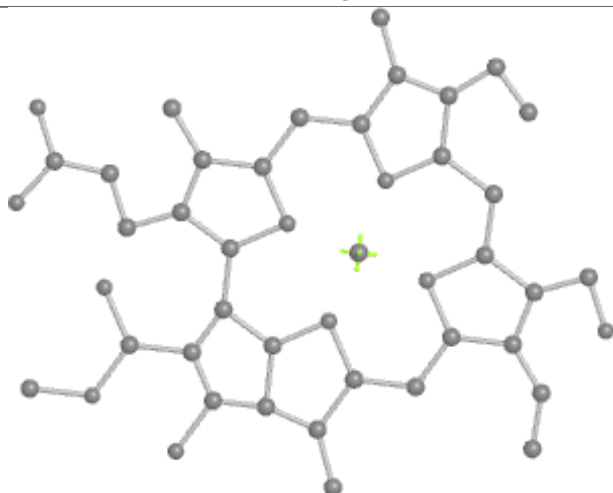
Bond lengths



Bond angles

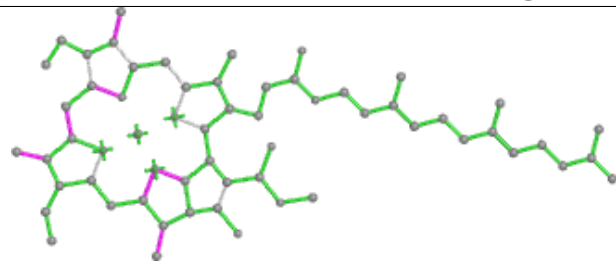


Torsions

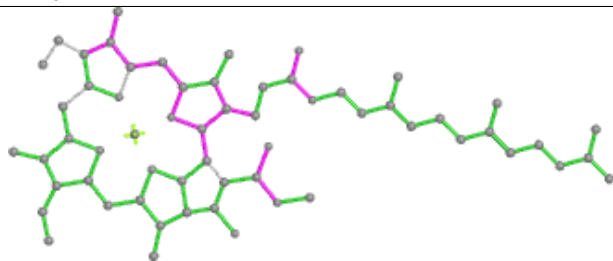


Rings

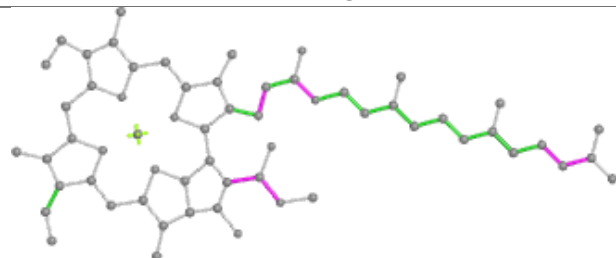
Ligand CLA y 313



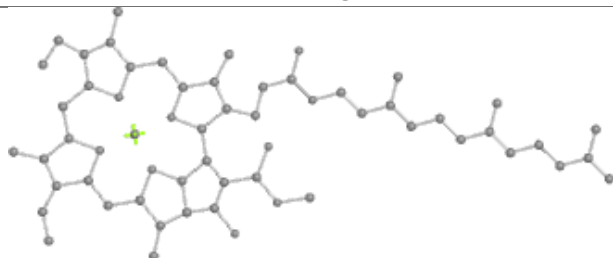
Bond lengths



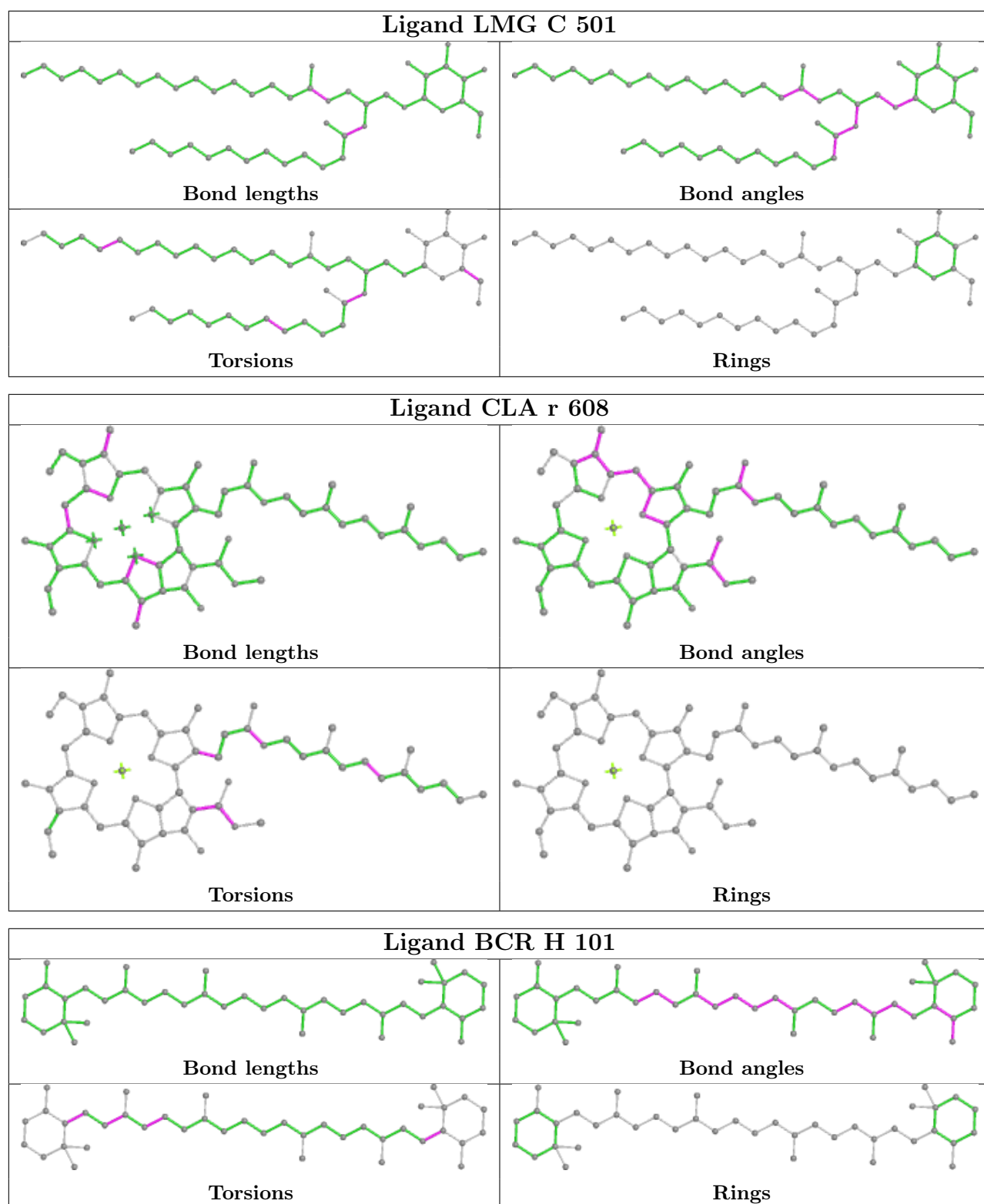
Bond angles

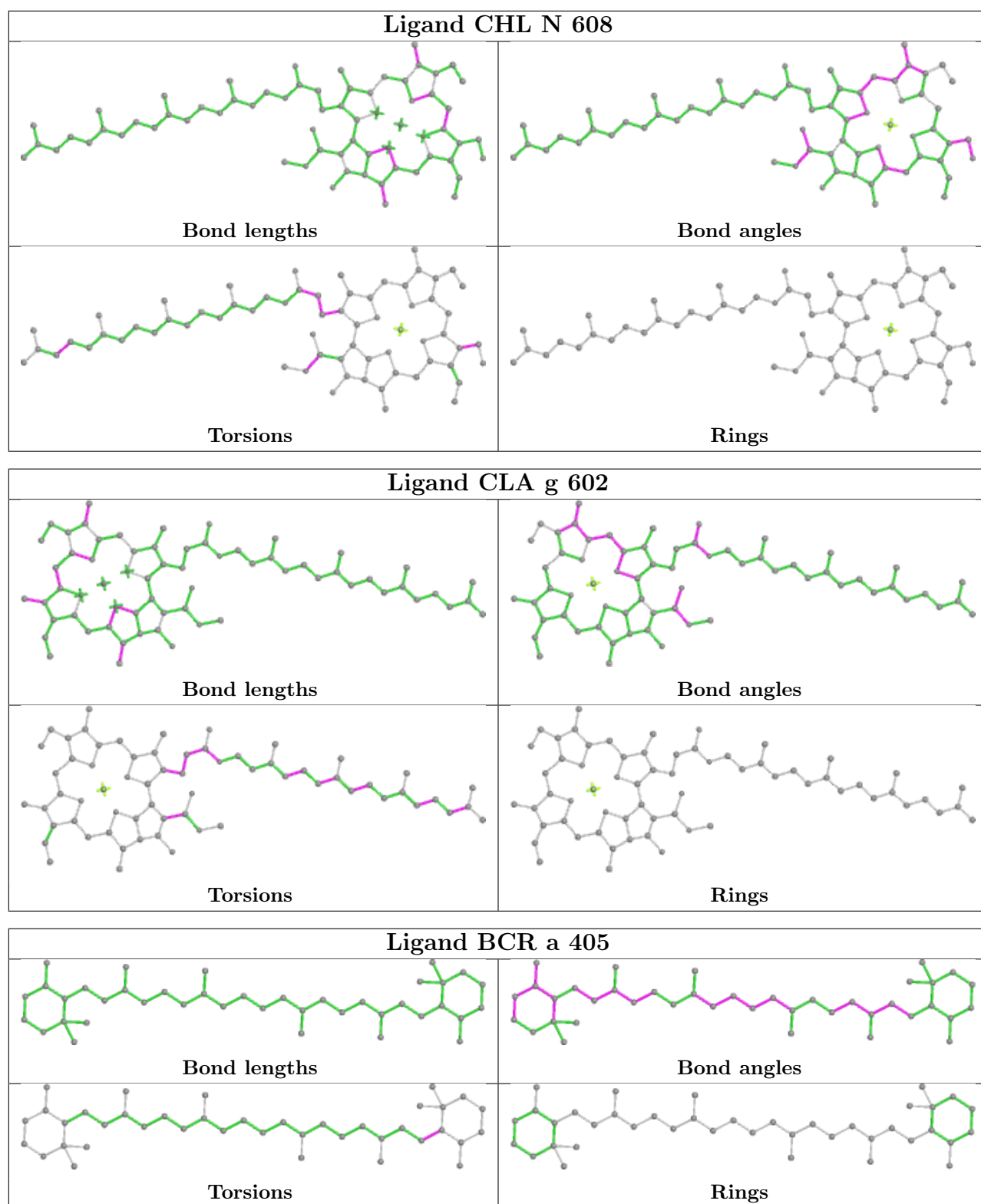


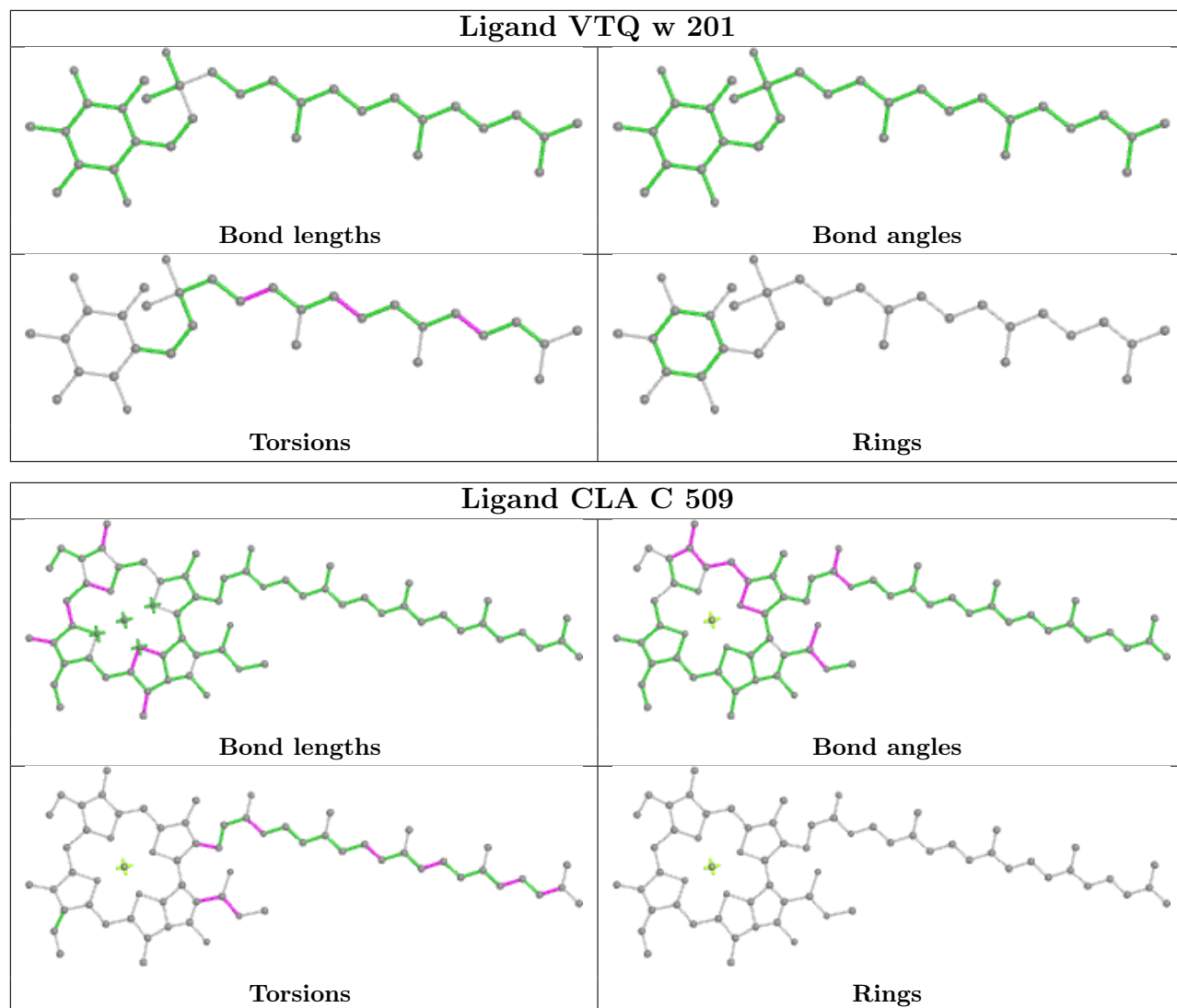
Torsions



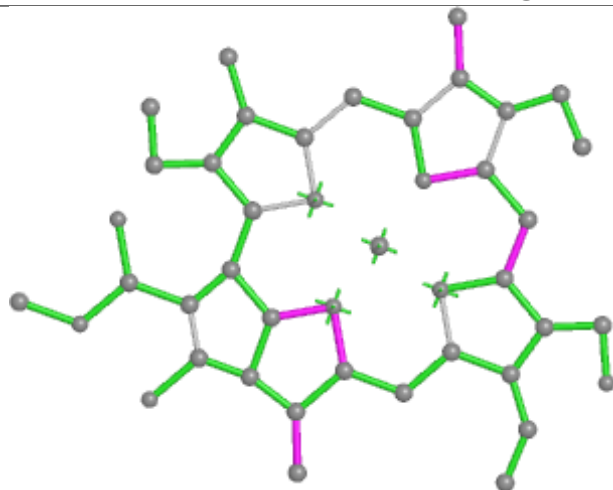
Rings



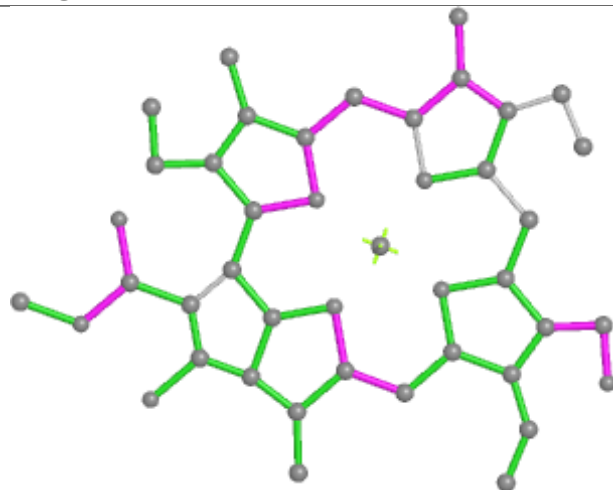




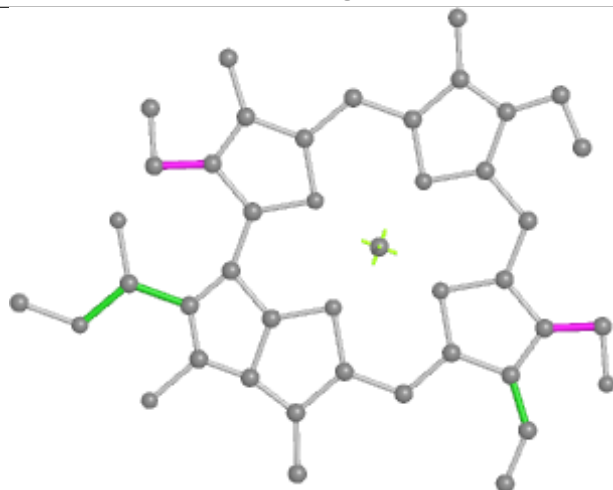
Ligand CHL g 606



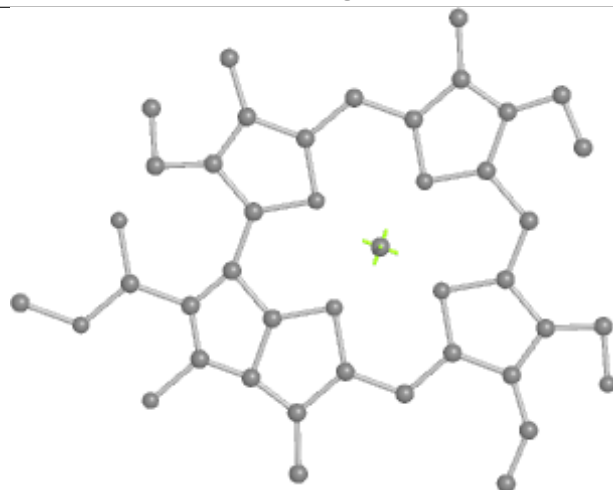
Bond lengths



Bond angles

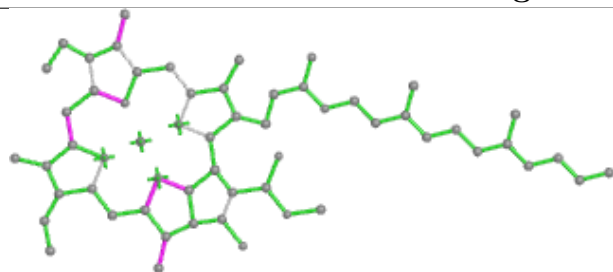


Torsions

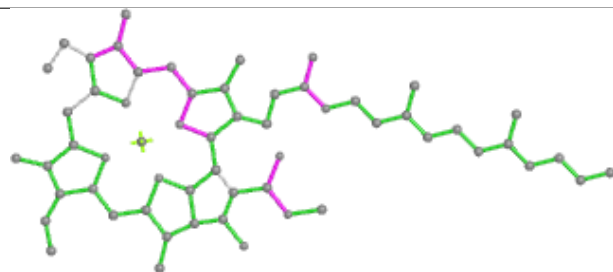


Rings

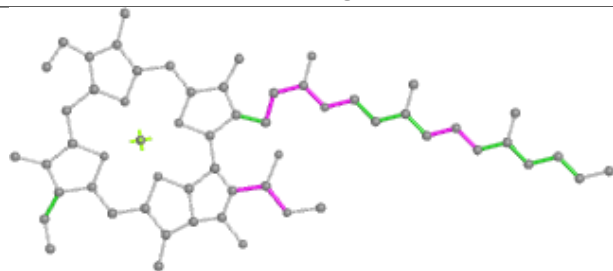
Ligand CLA G 613



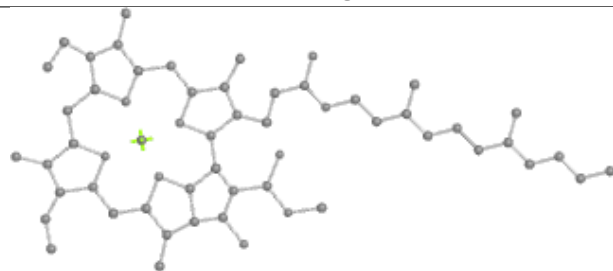
Bond lengths



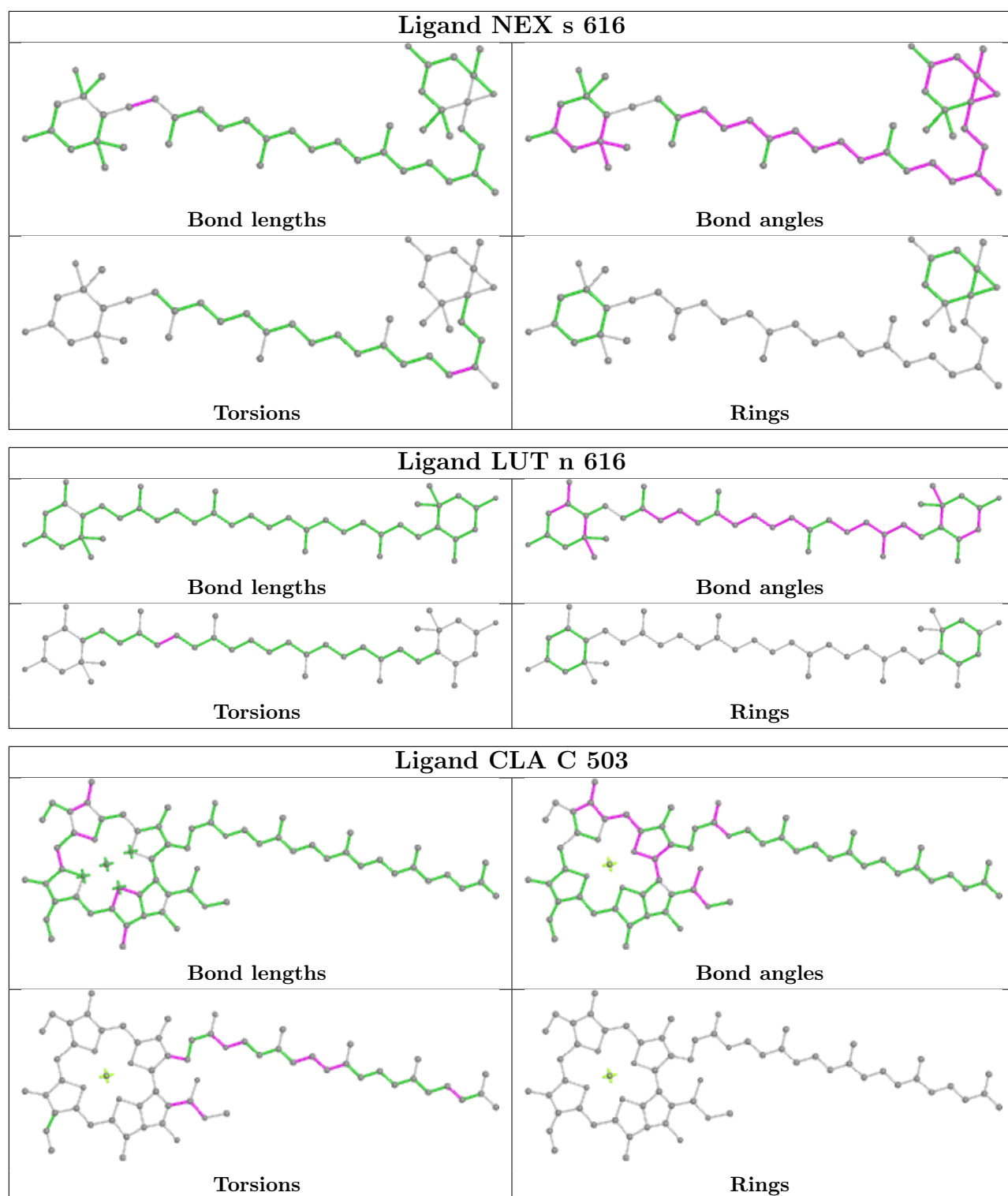
Bond angles

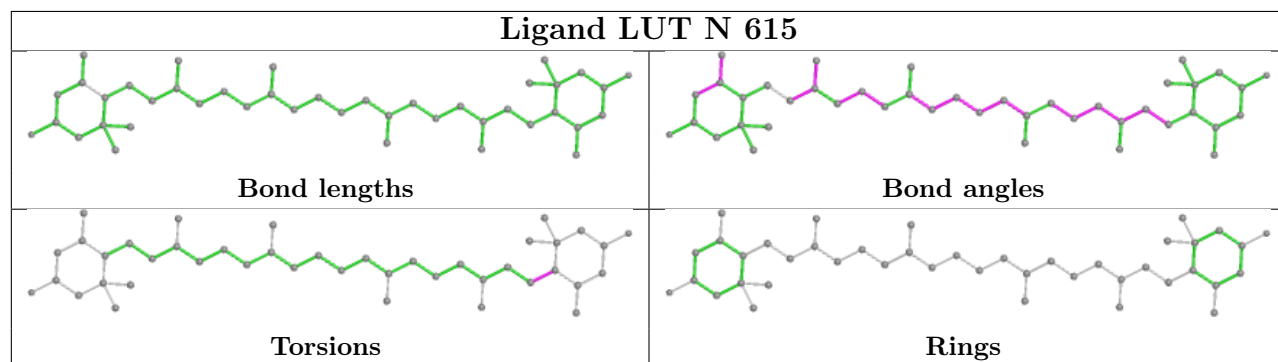
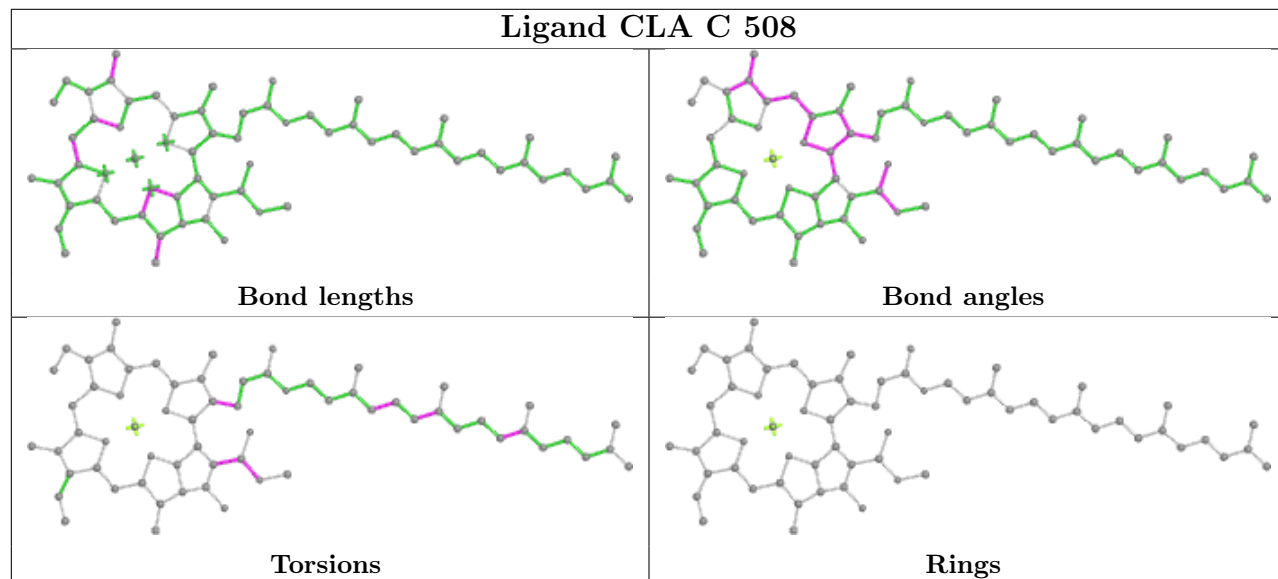
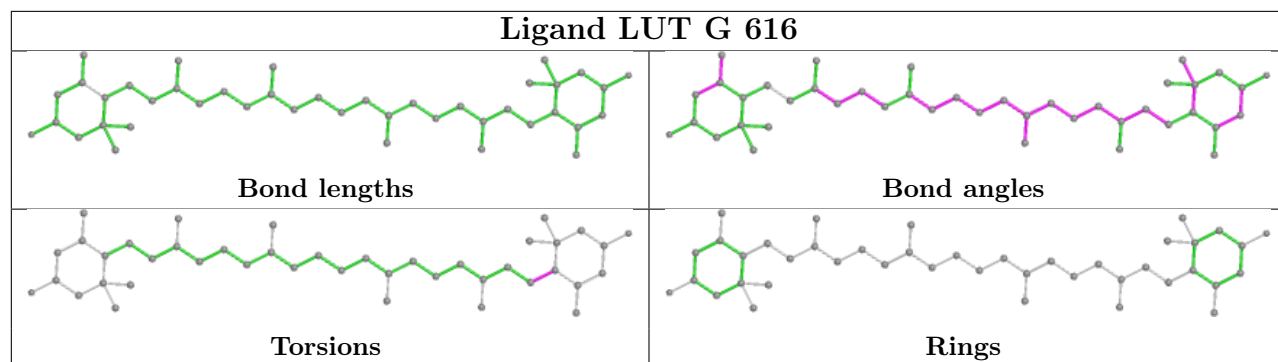


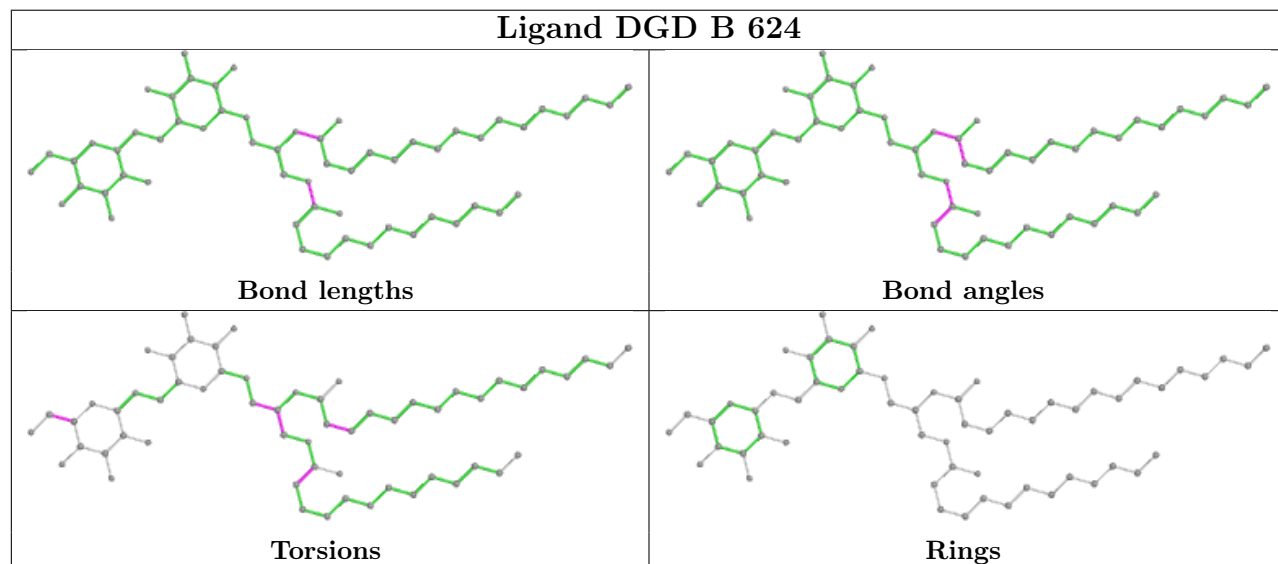
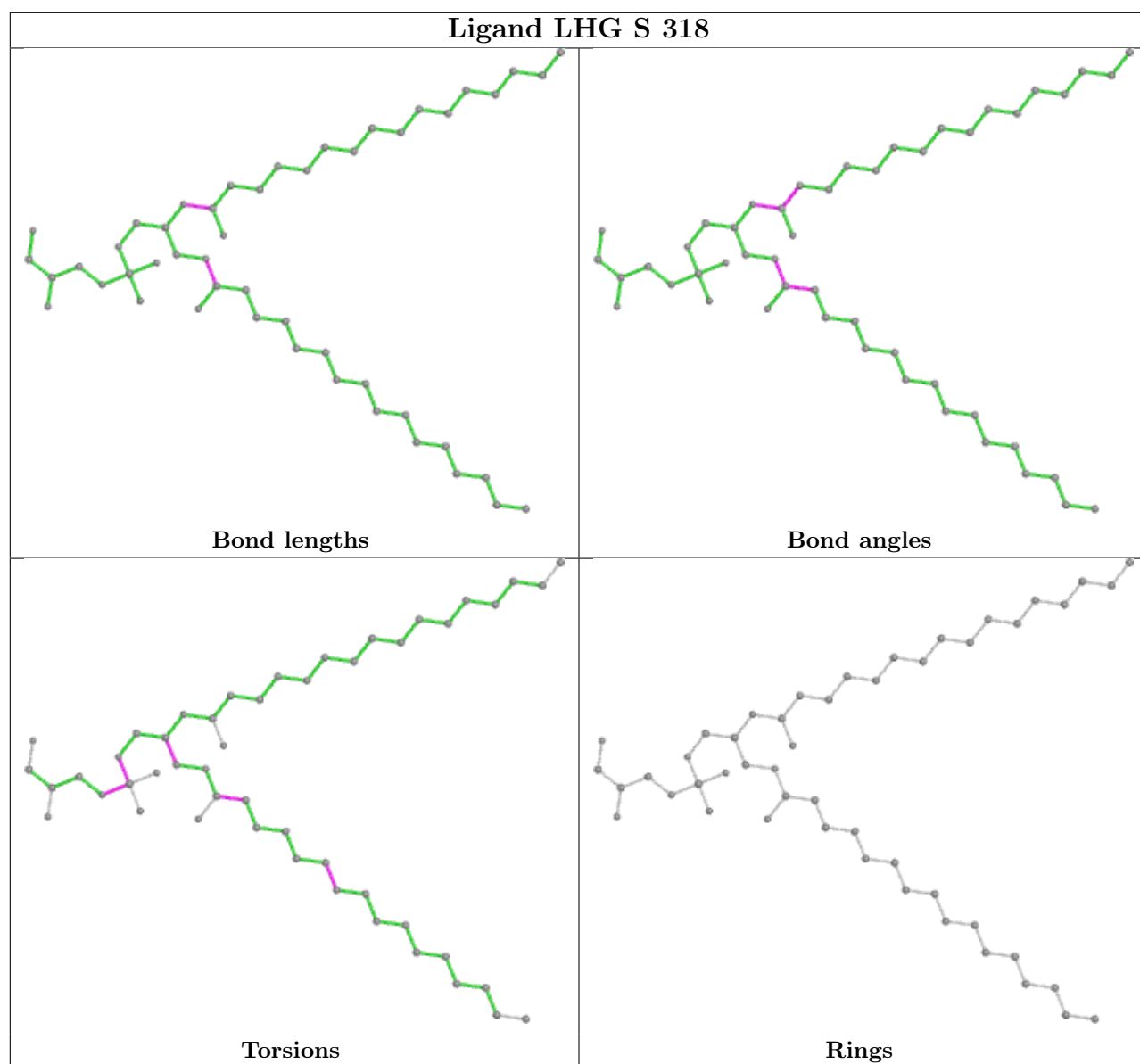
Torsions

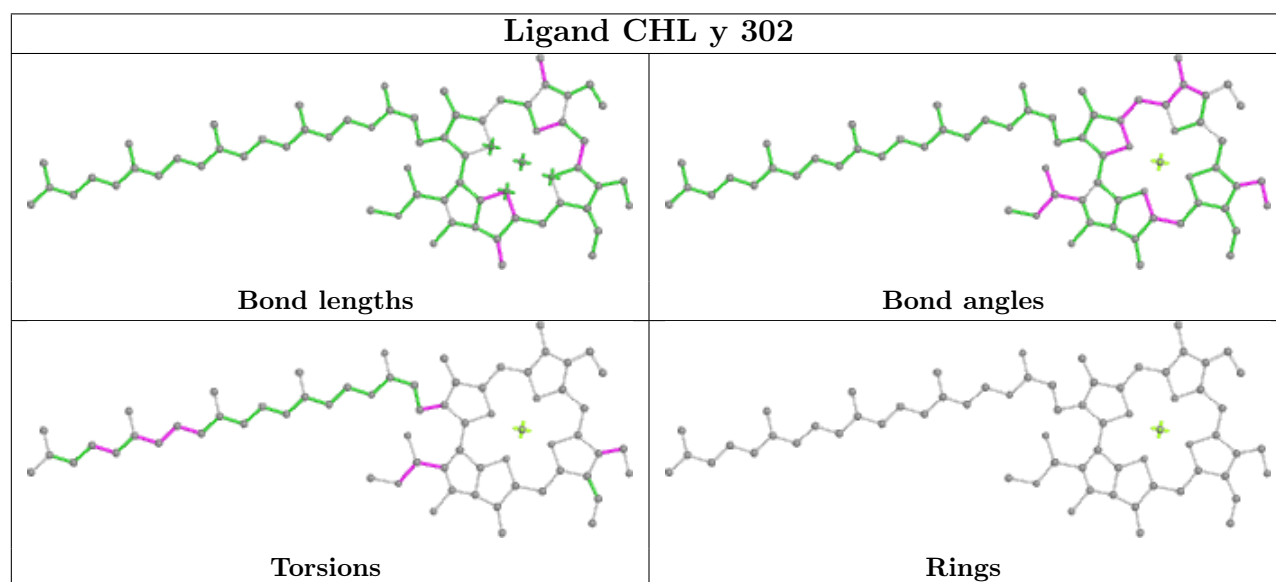
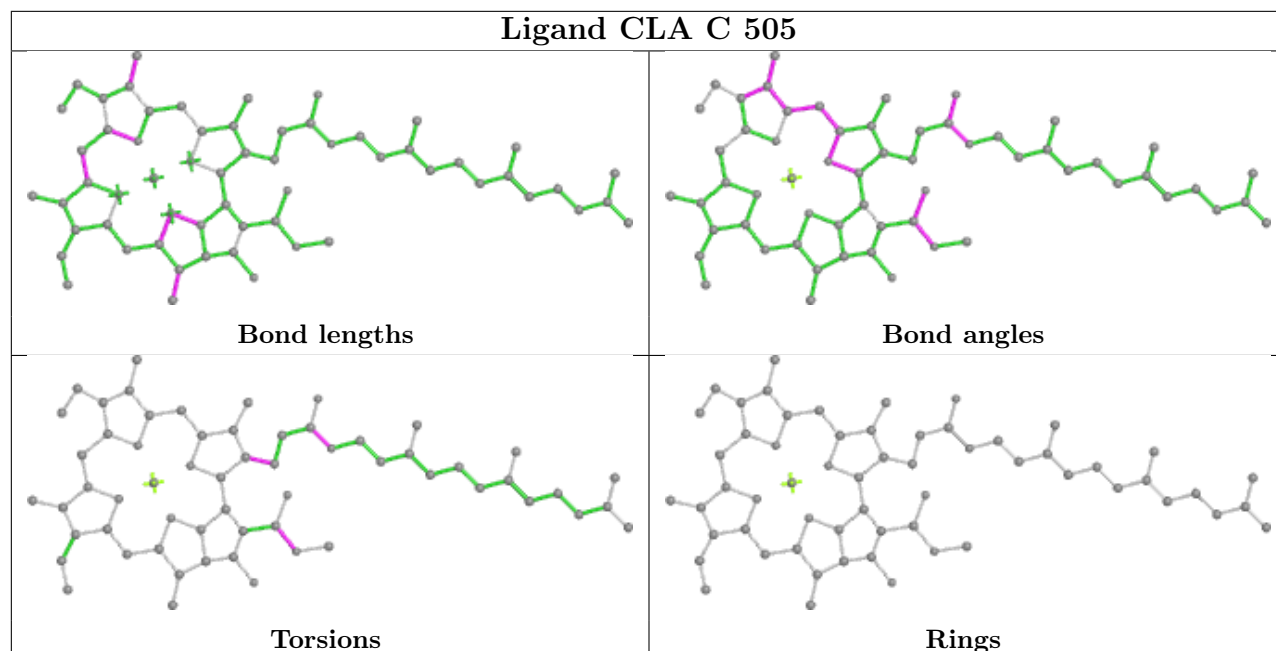
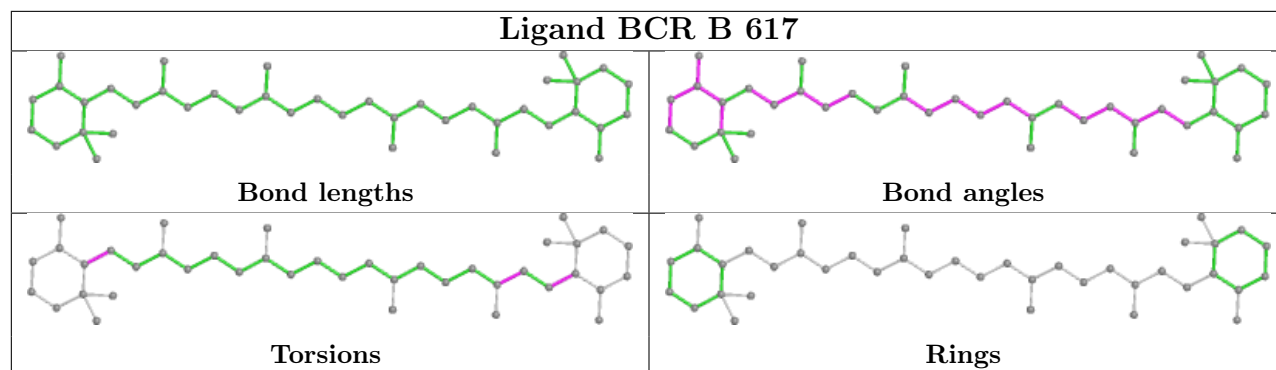


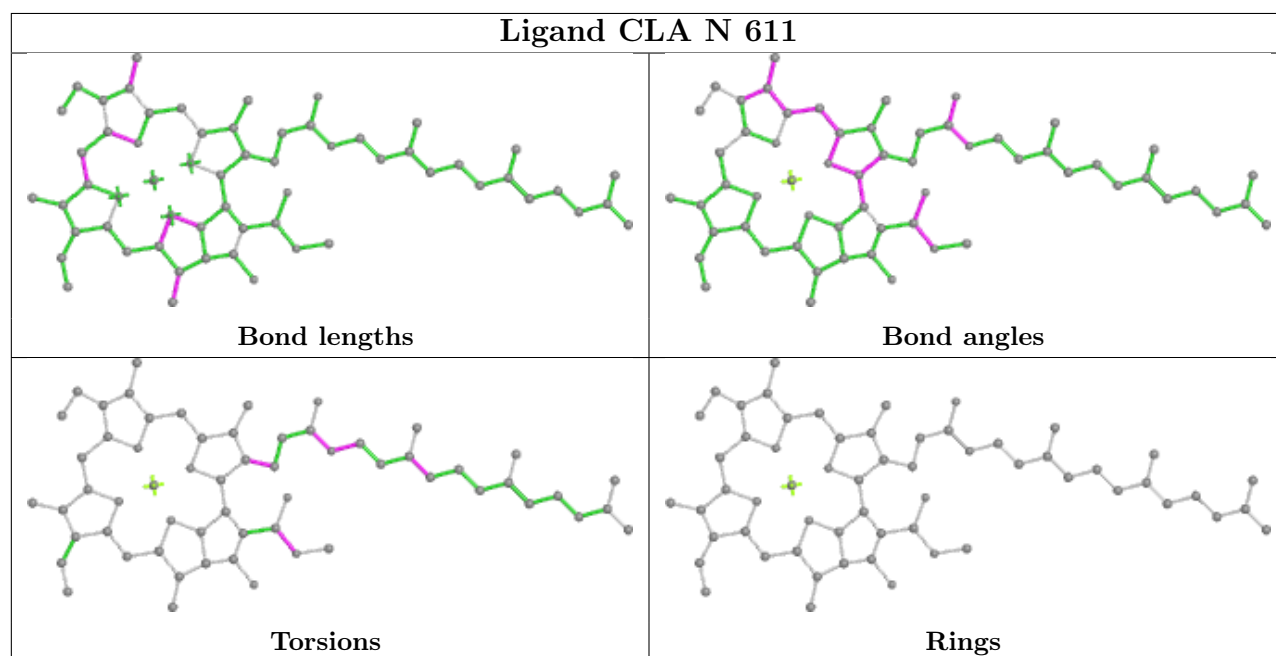
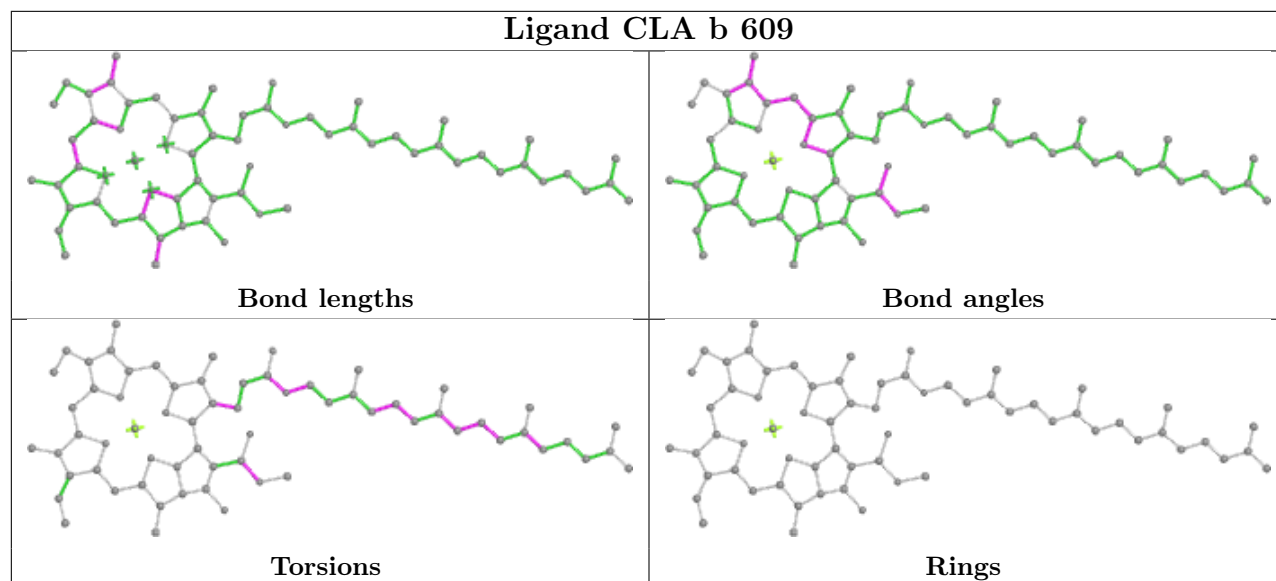
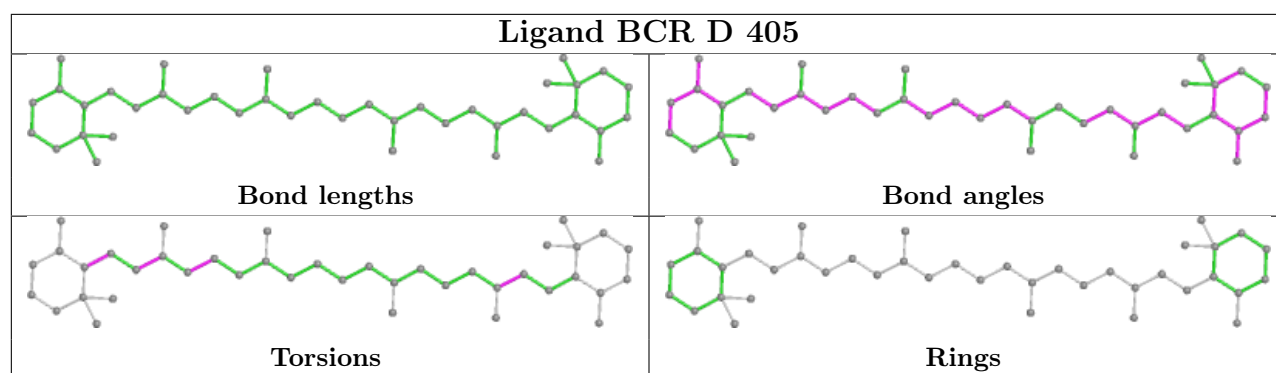
Rings

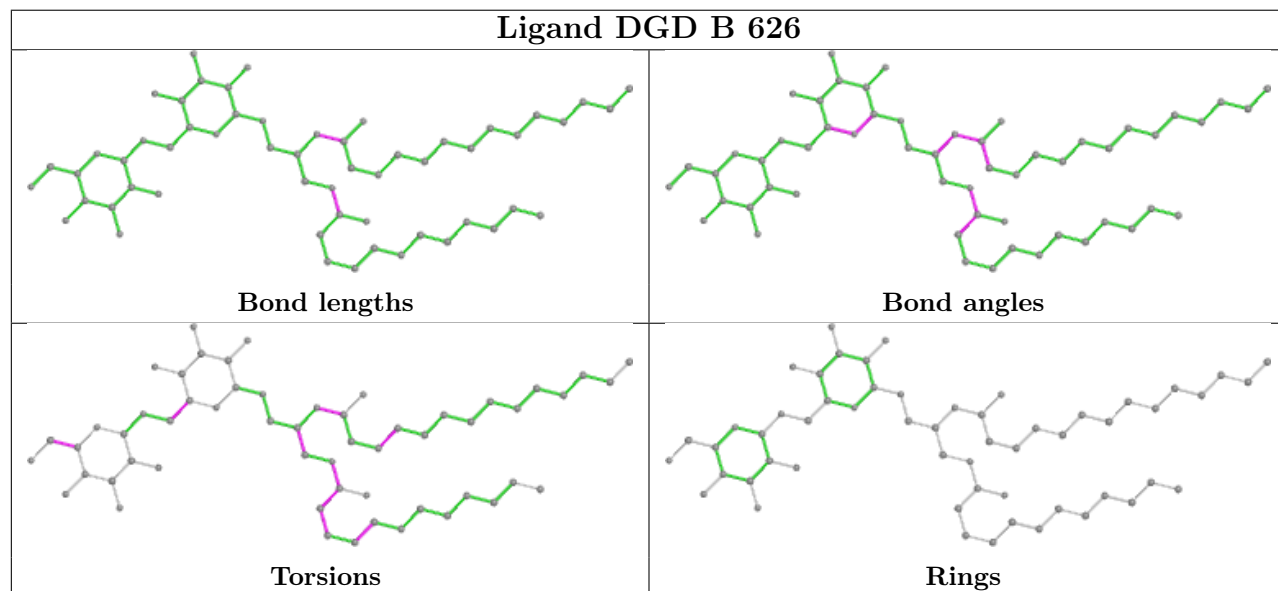
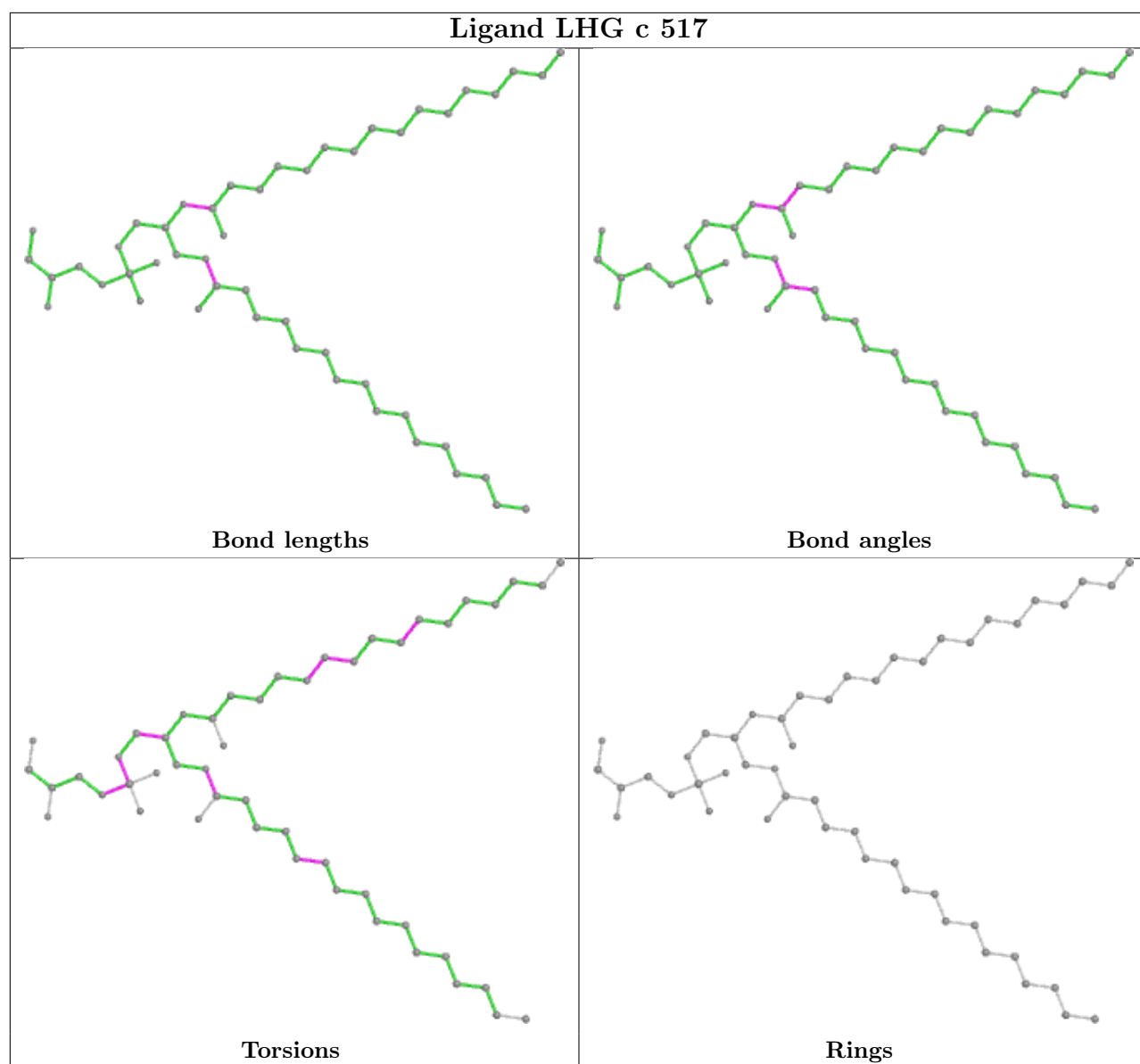




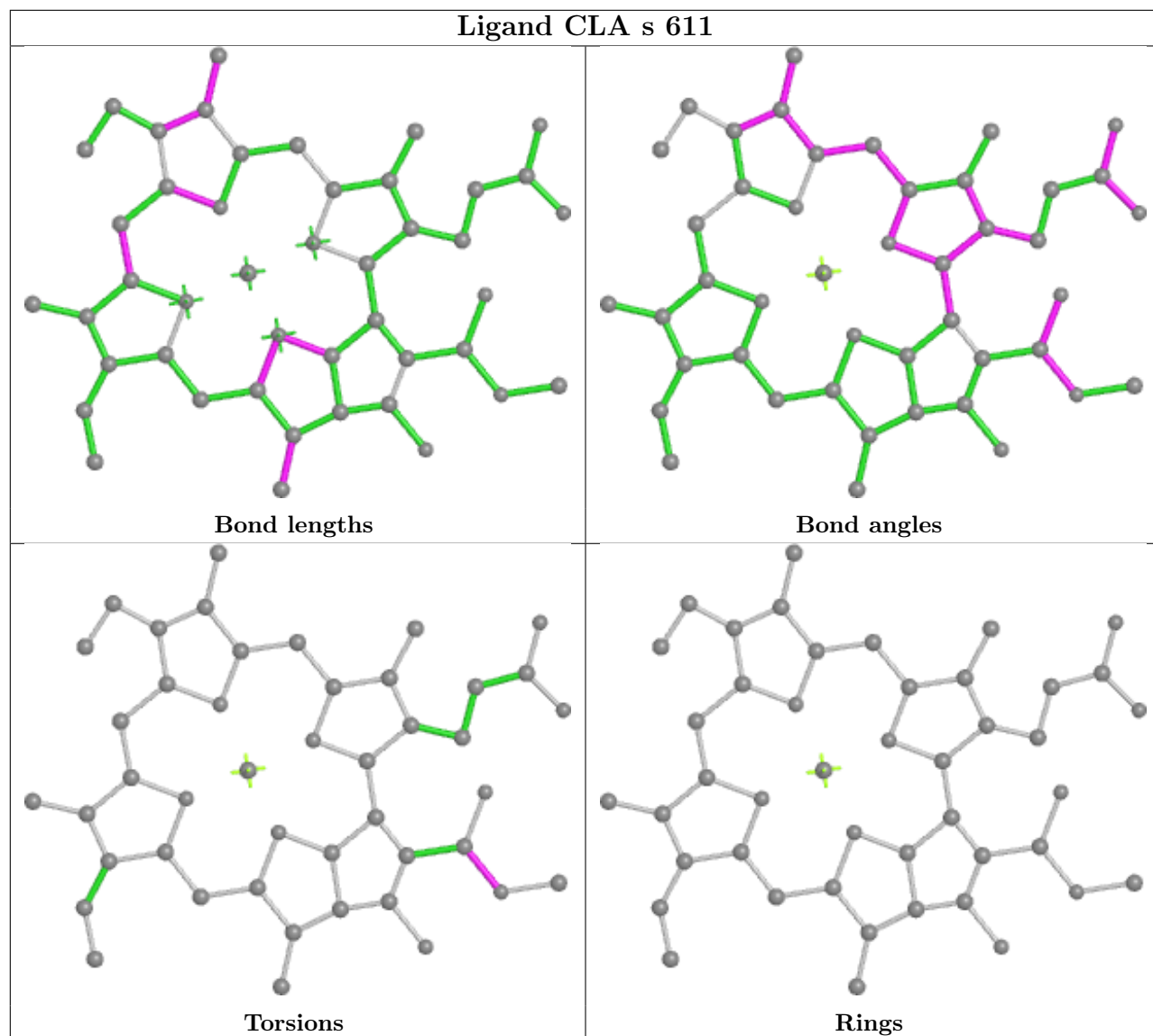


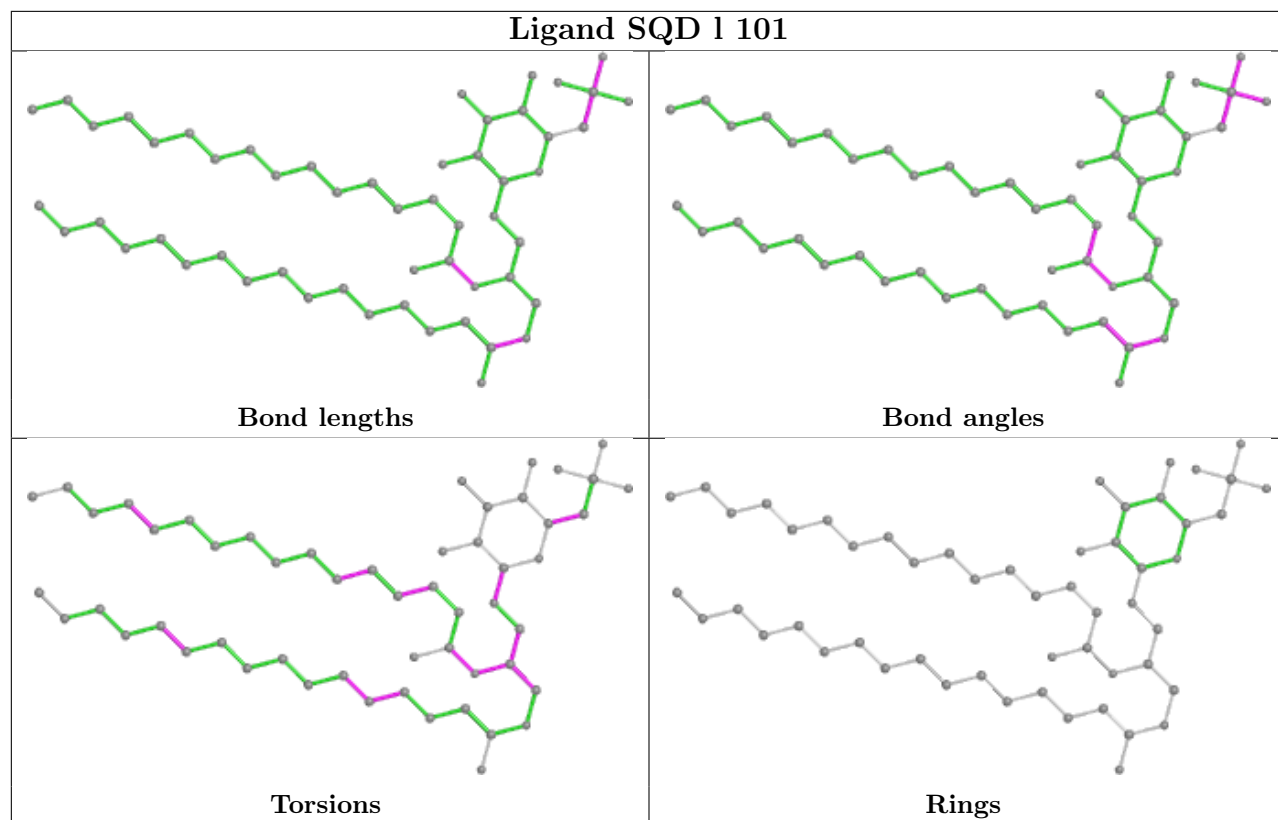




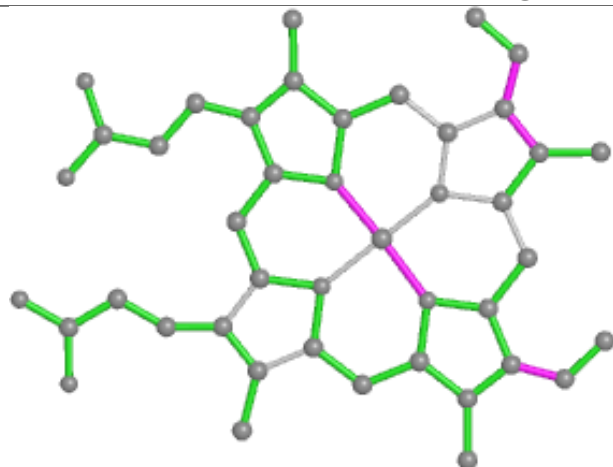


Ligand CLA s 611

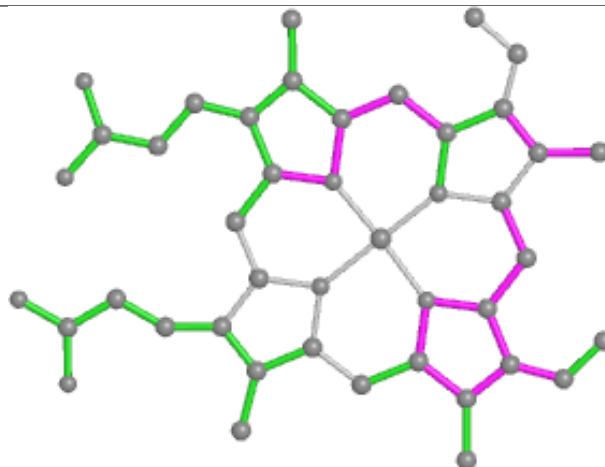




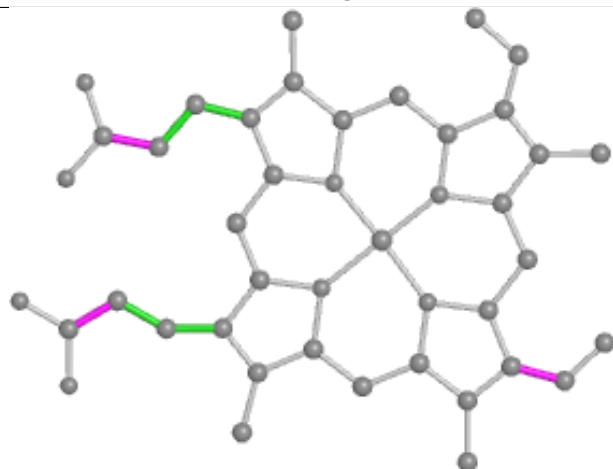
Ligand HEM f 101



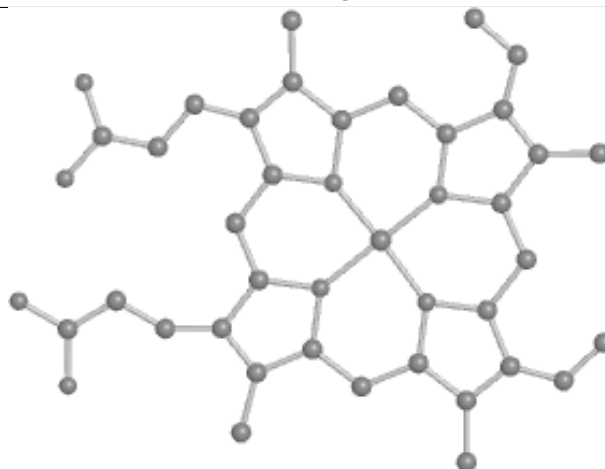
Bond lengths



Bond angles

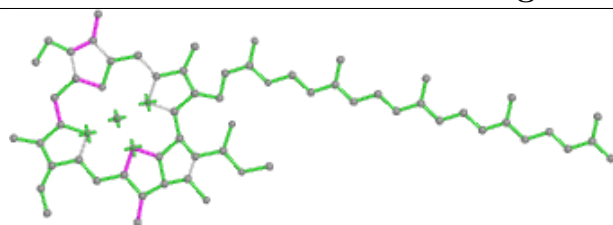


Torsions

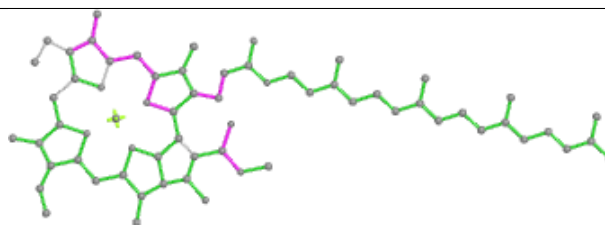


Rings

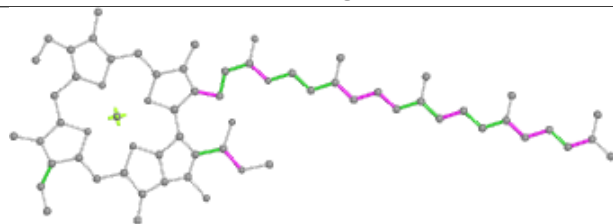
Ligand CLA b 610



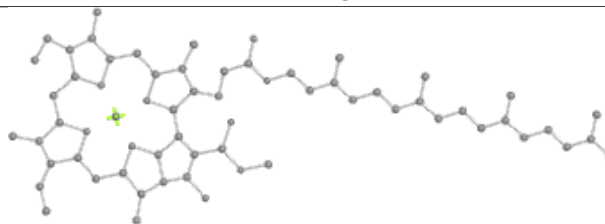
Bond lengths



Bond angles

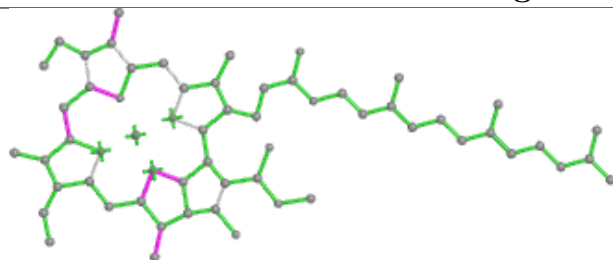


Torsions

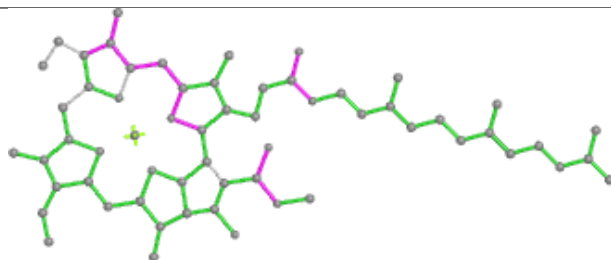


Rings

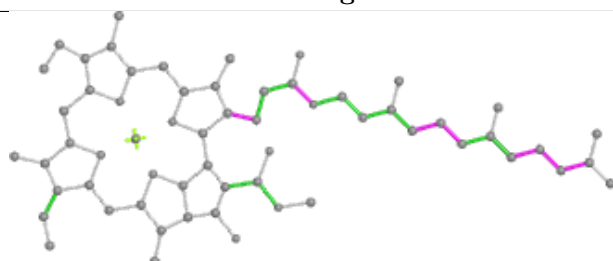
Ligand CLA Y 312



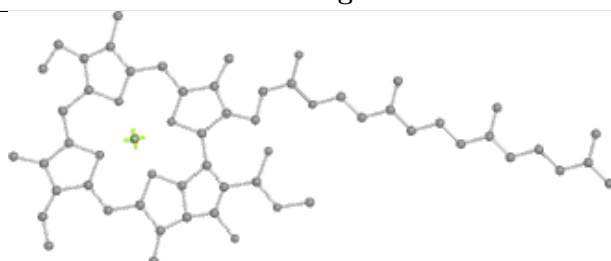
Bond lengths



Bond angles

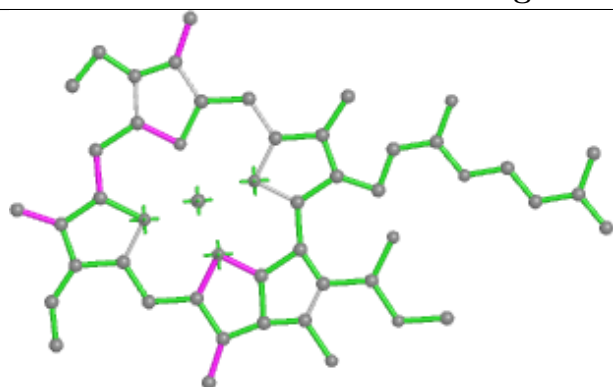


Torsions

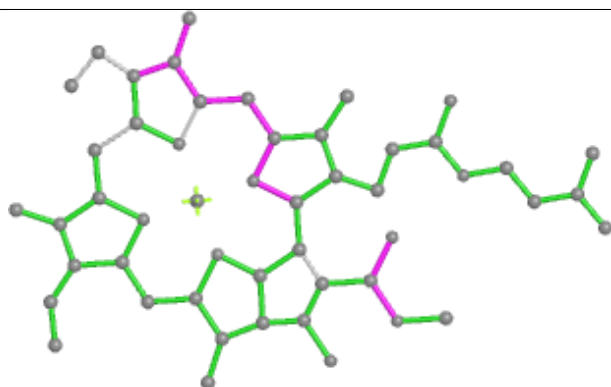


Rings

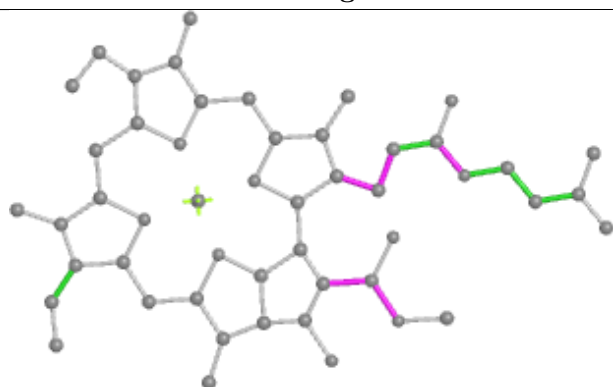
Ligand CLA Y 305



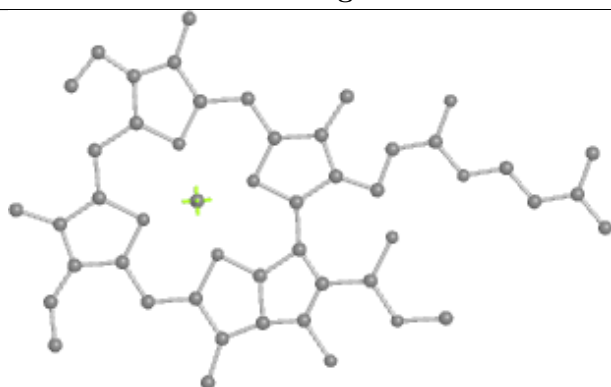
Bond lengths



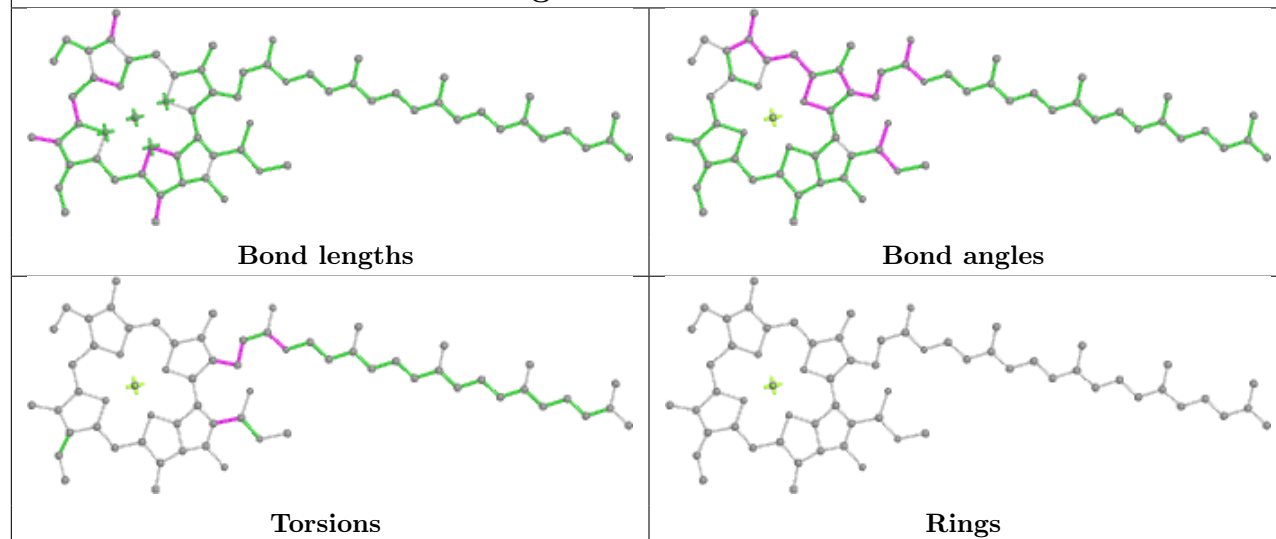
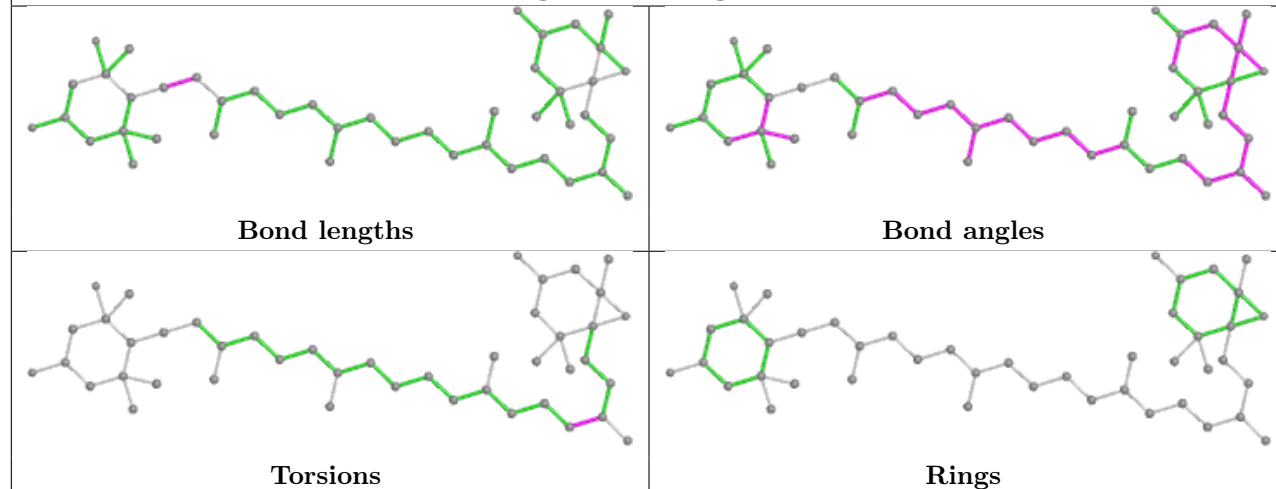
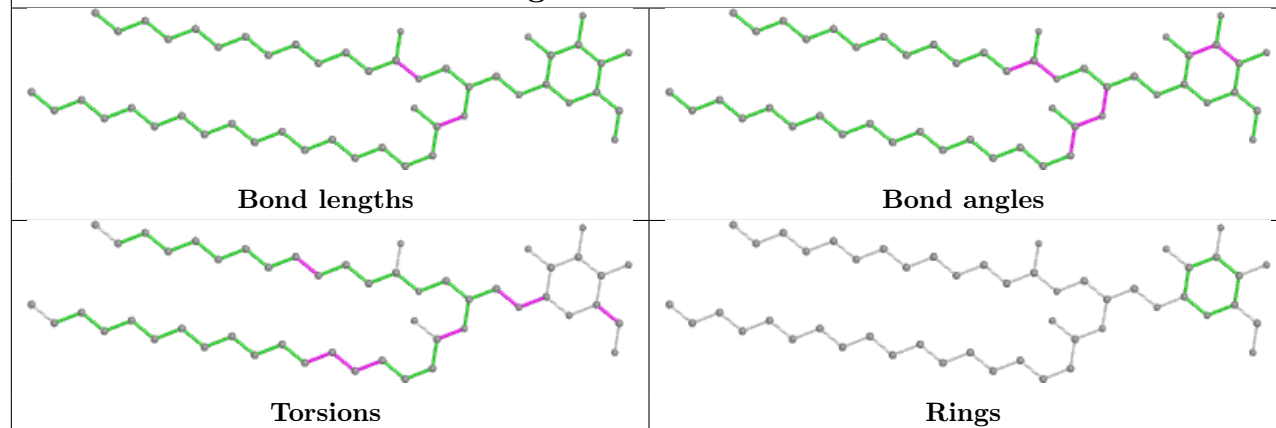
Bond angles

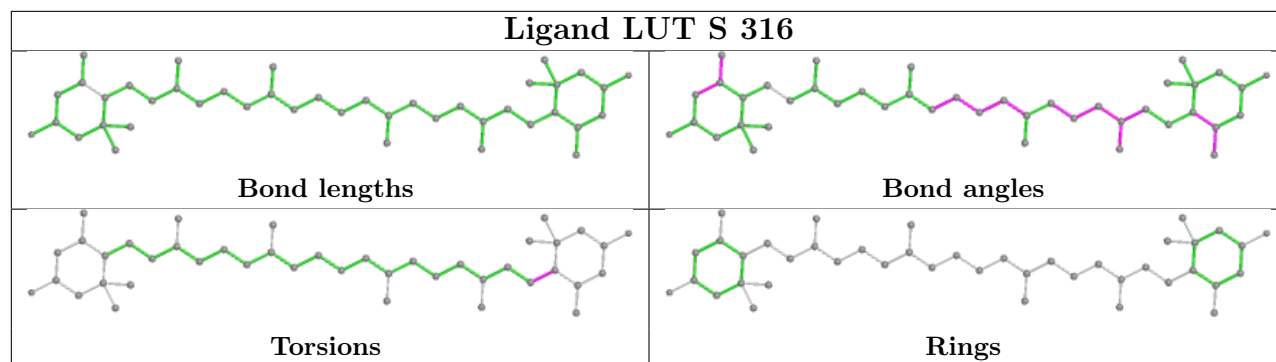
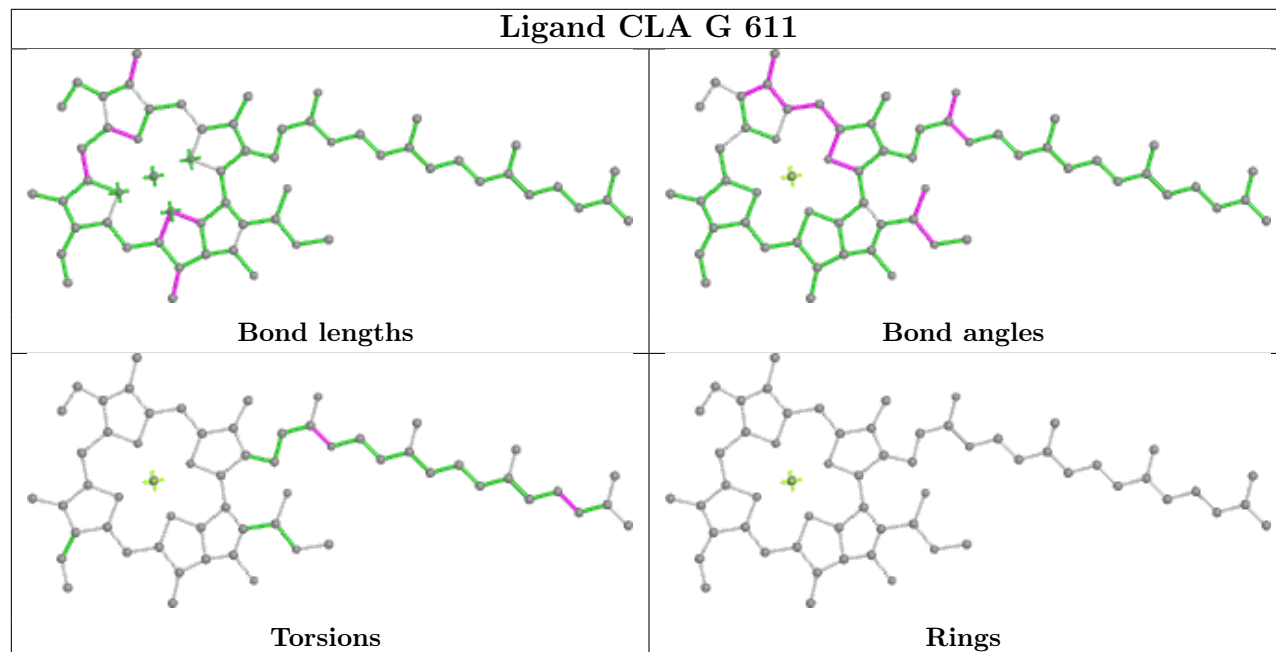
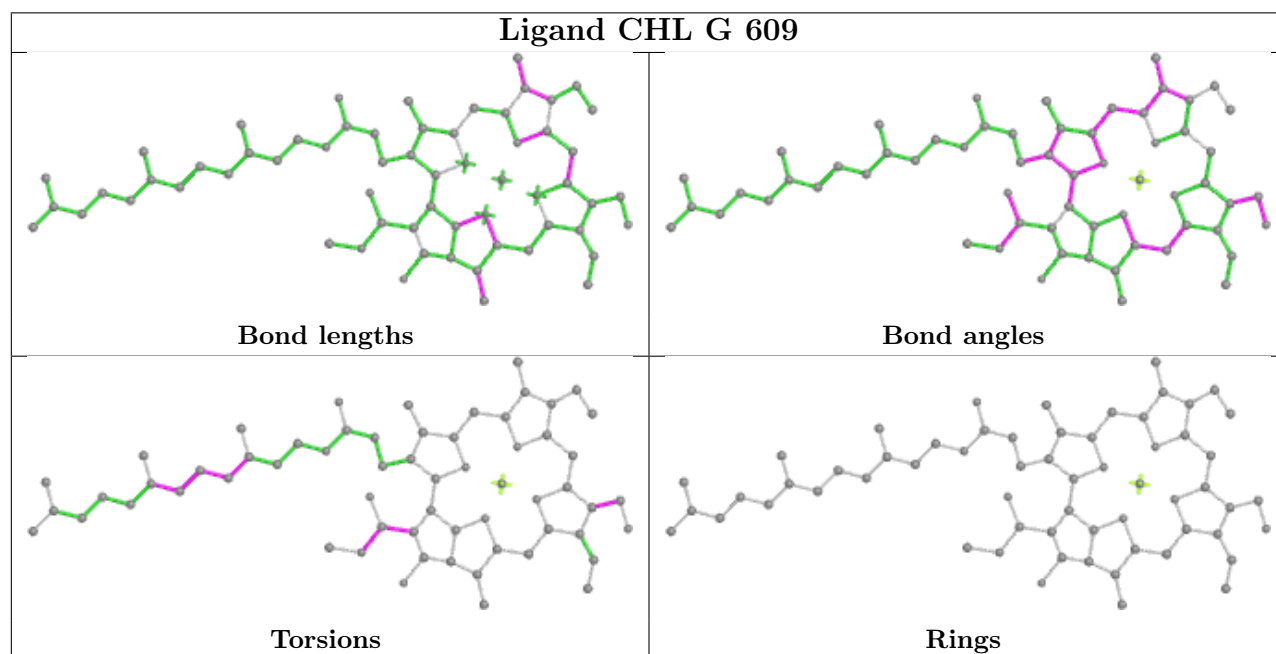


Torsions

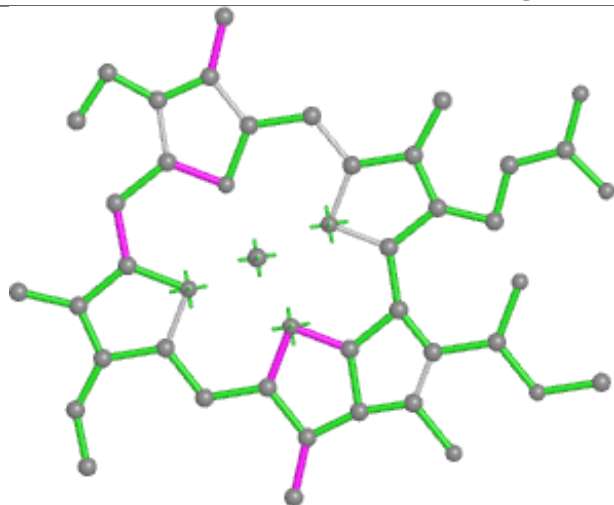


Rings

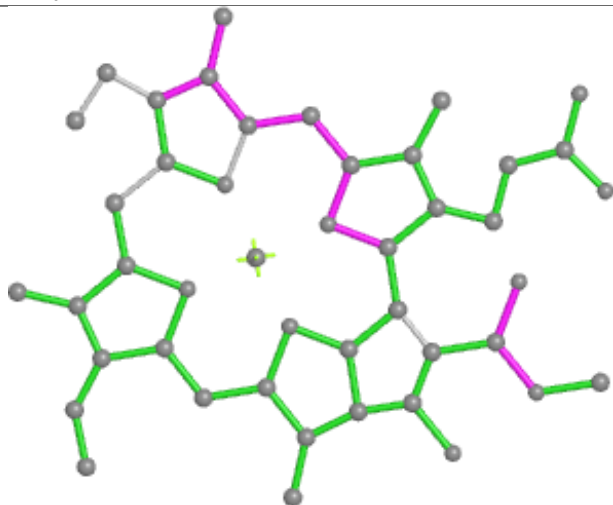
Ligand CLA C 514**Ligand NEX g 618****Ligand LMG C 522**

Ligand LUT S 316**Ligand CLA G 611****Ligand CHL G 609**

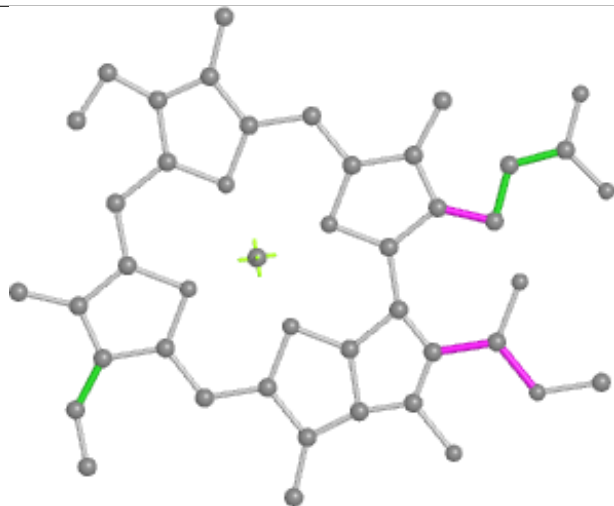
Ligand CLA y 315



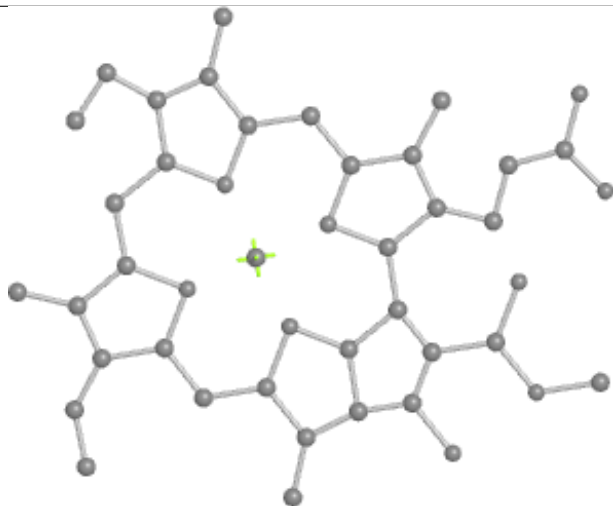
Bond lengths



Bond angles

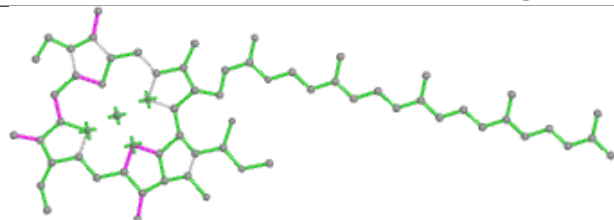


Torsions

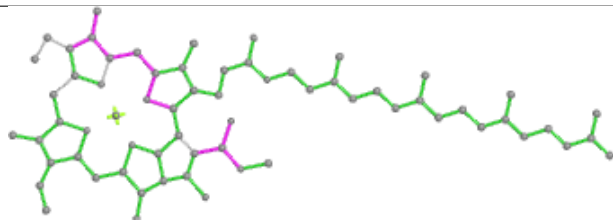


Rings

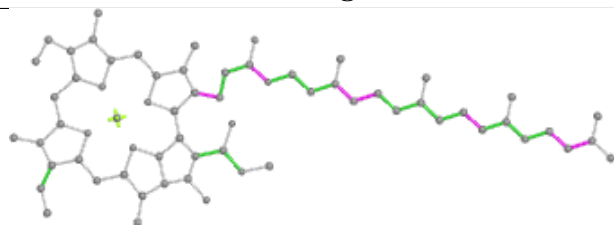
Ligand CLA d 403



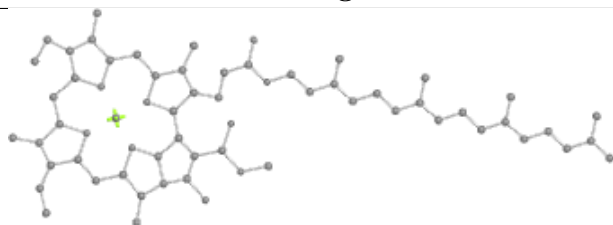
Bond lengths



Bond angles

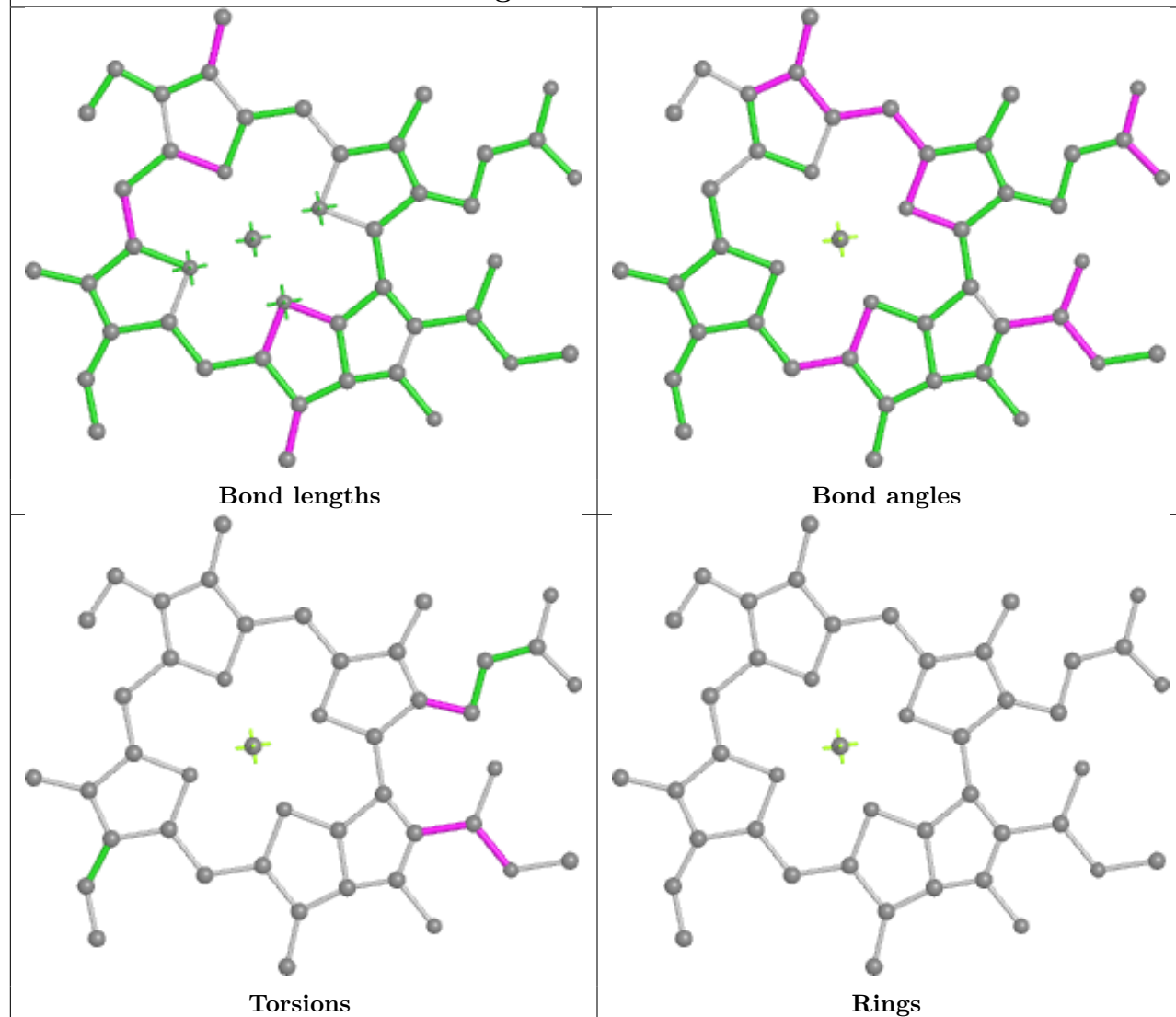


Torsions

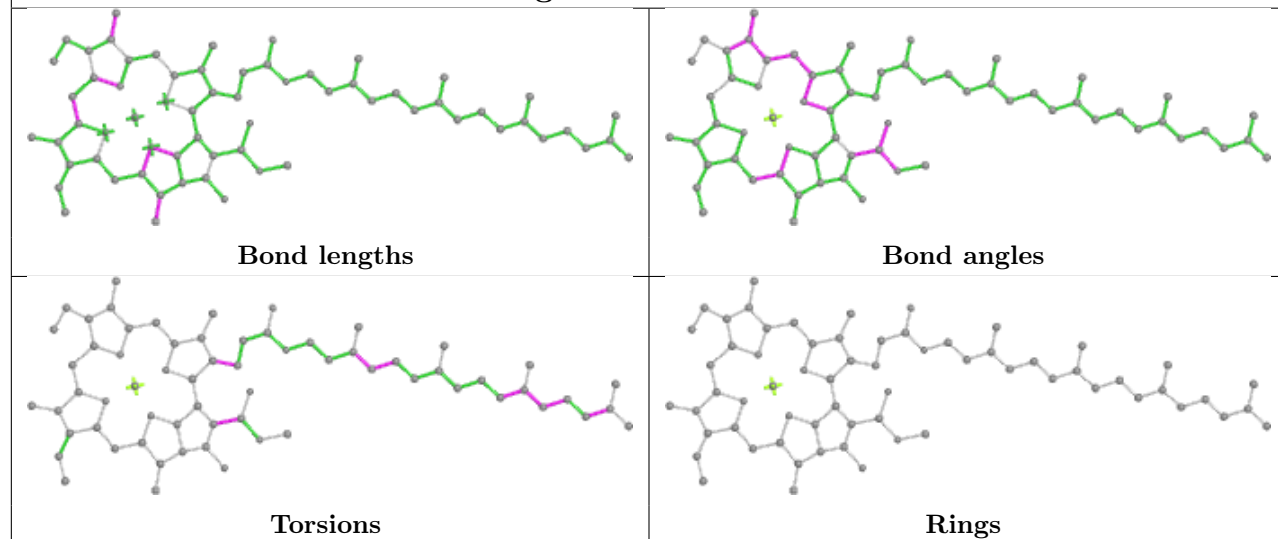


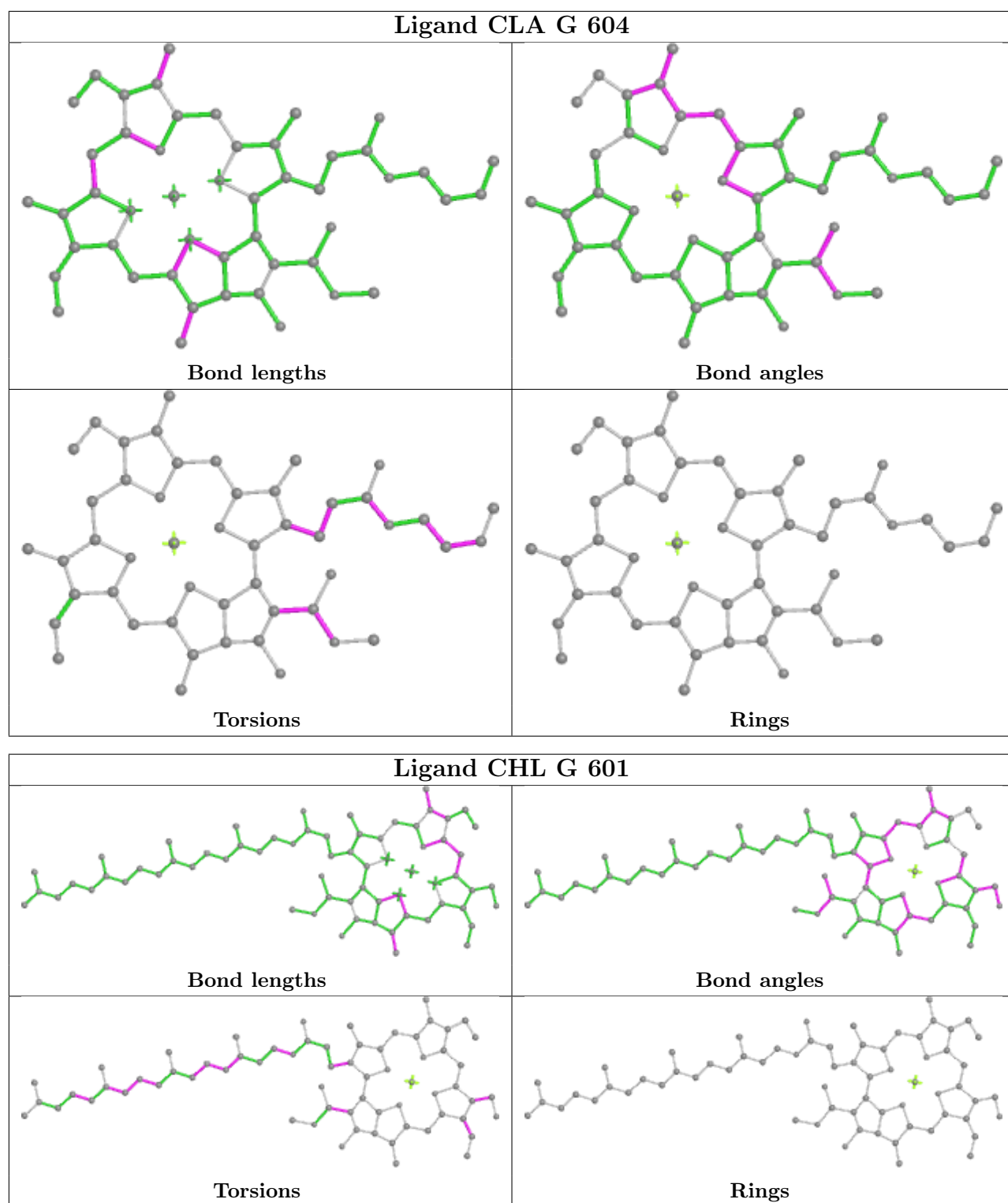
Rings

Ligand CLA s 608

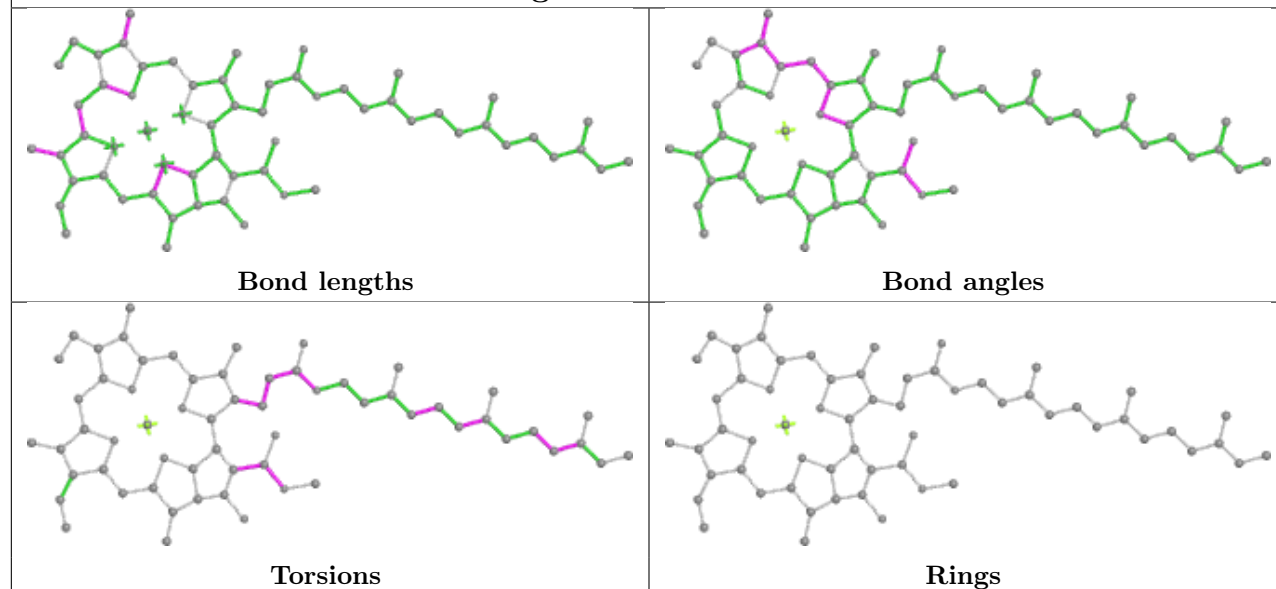


Ligand CLA d 401

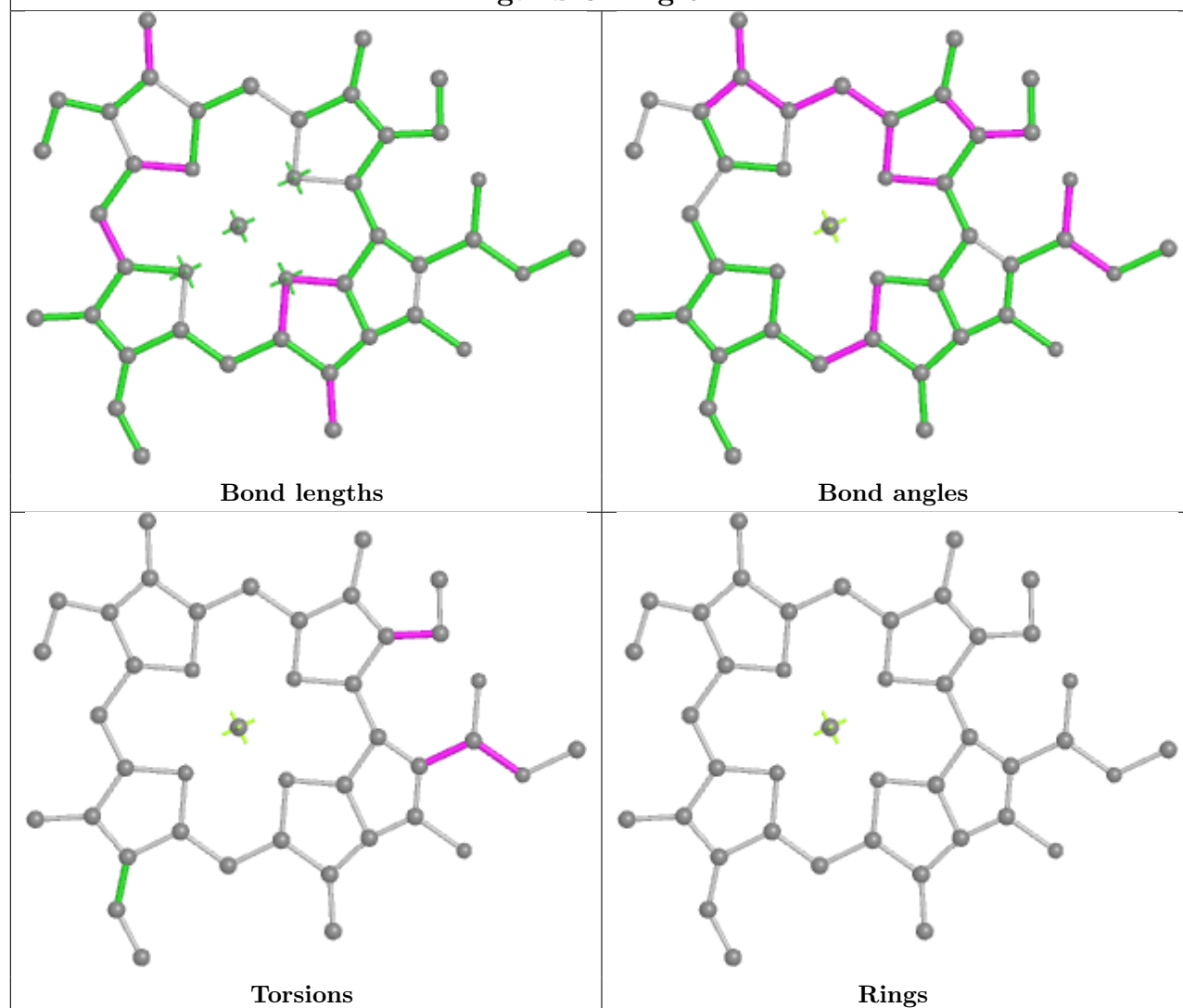


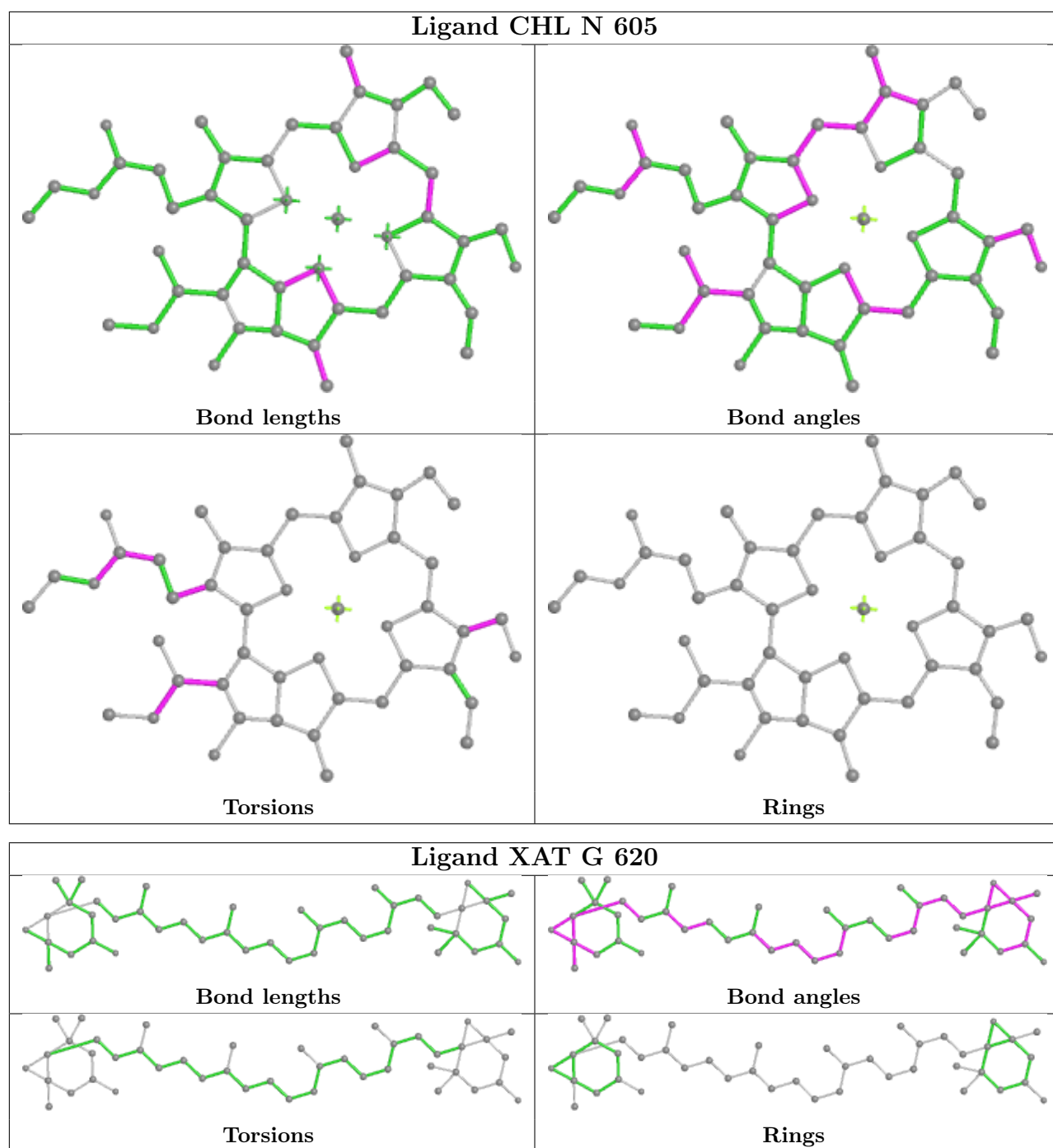


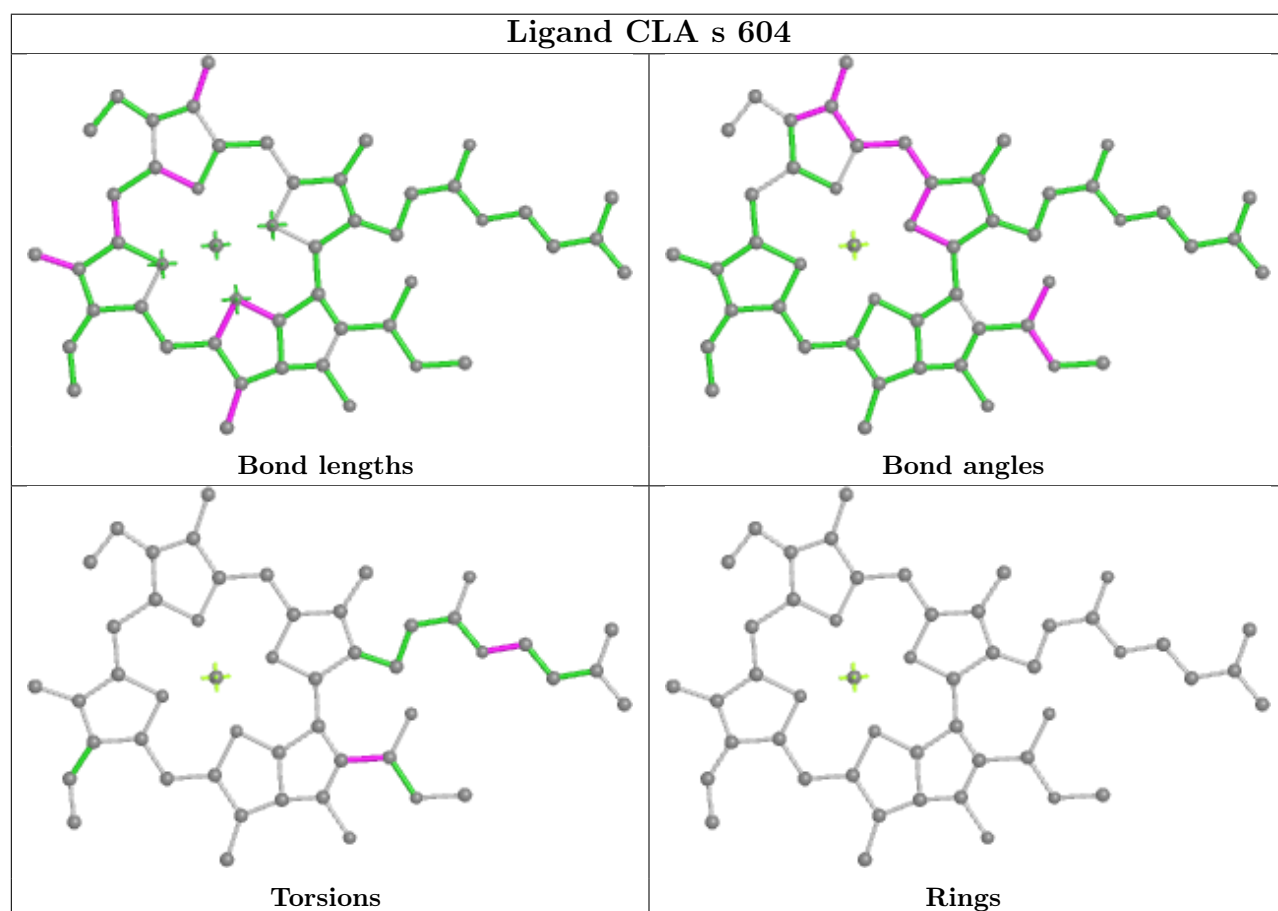
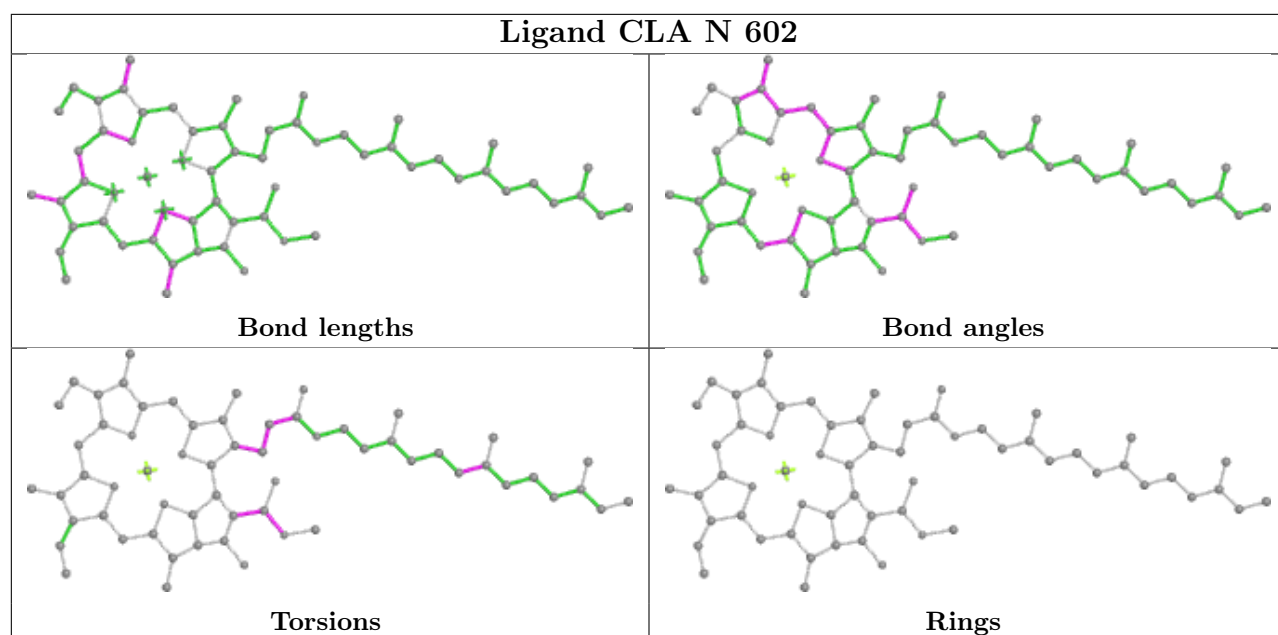
Ligand CLA Y 303

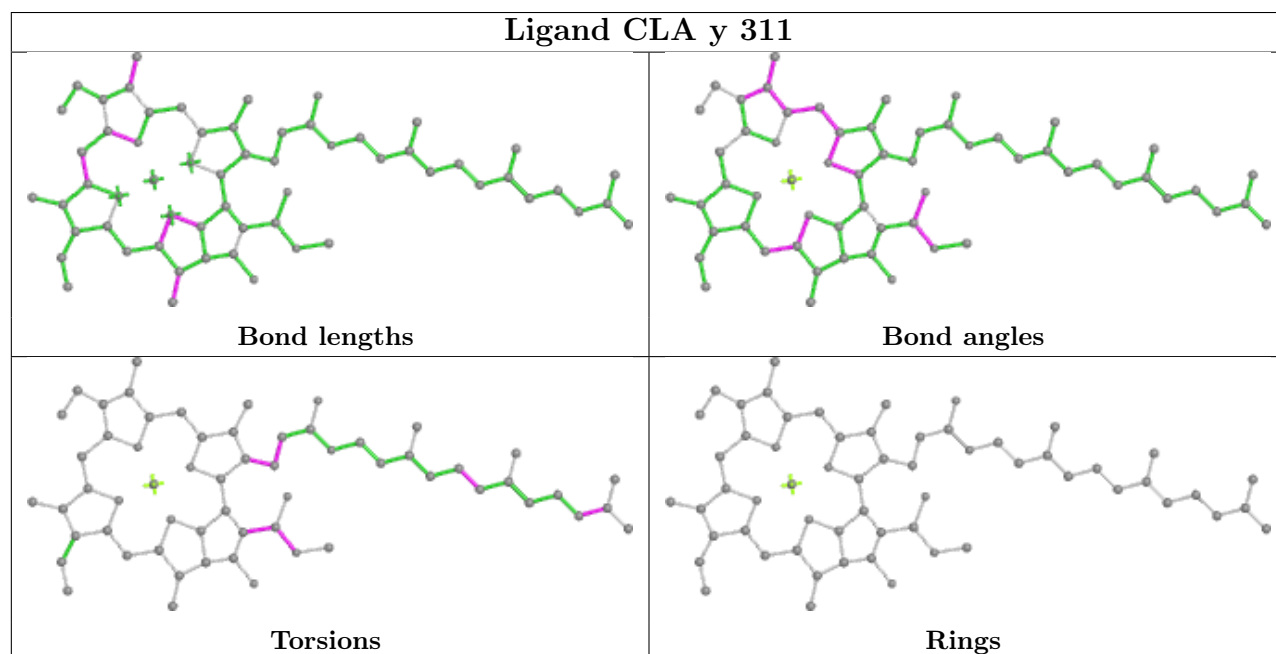
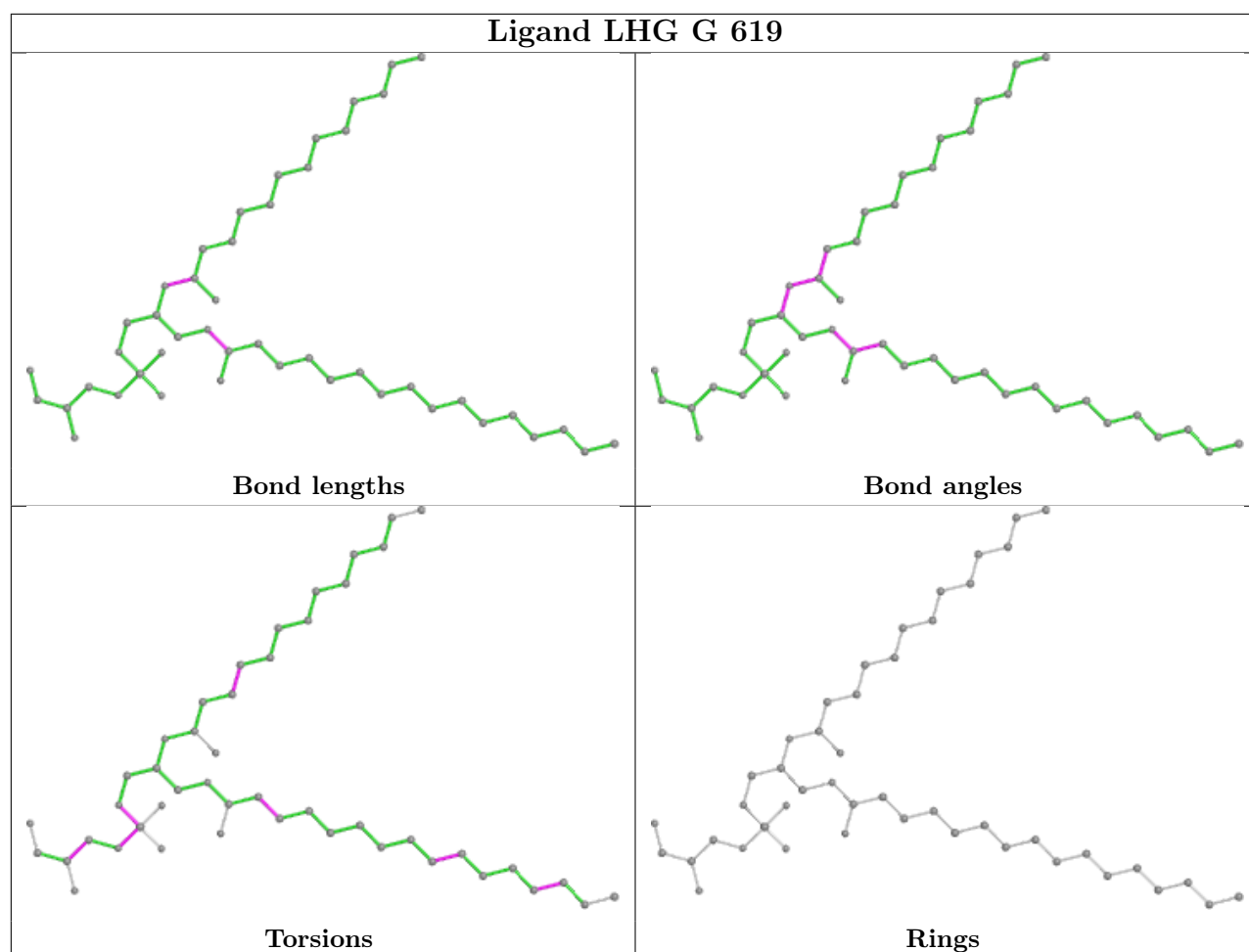


Ligand CLA g 614

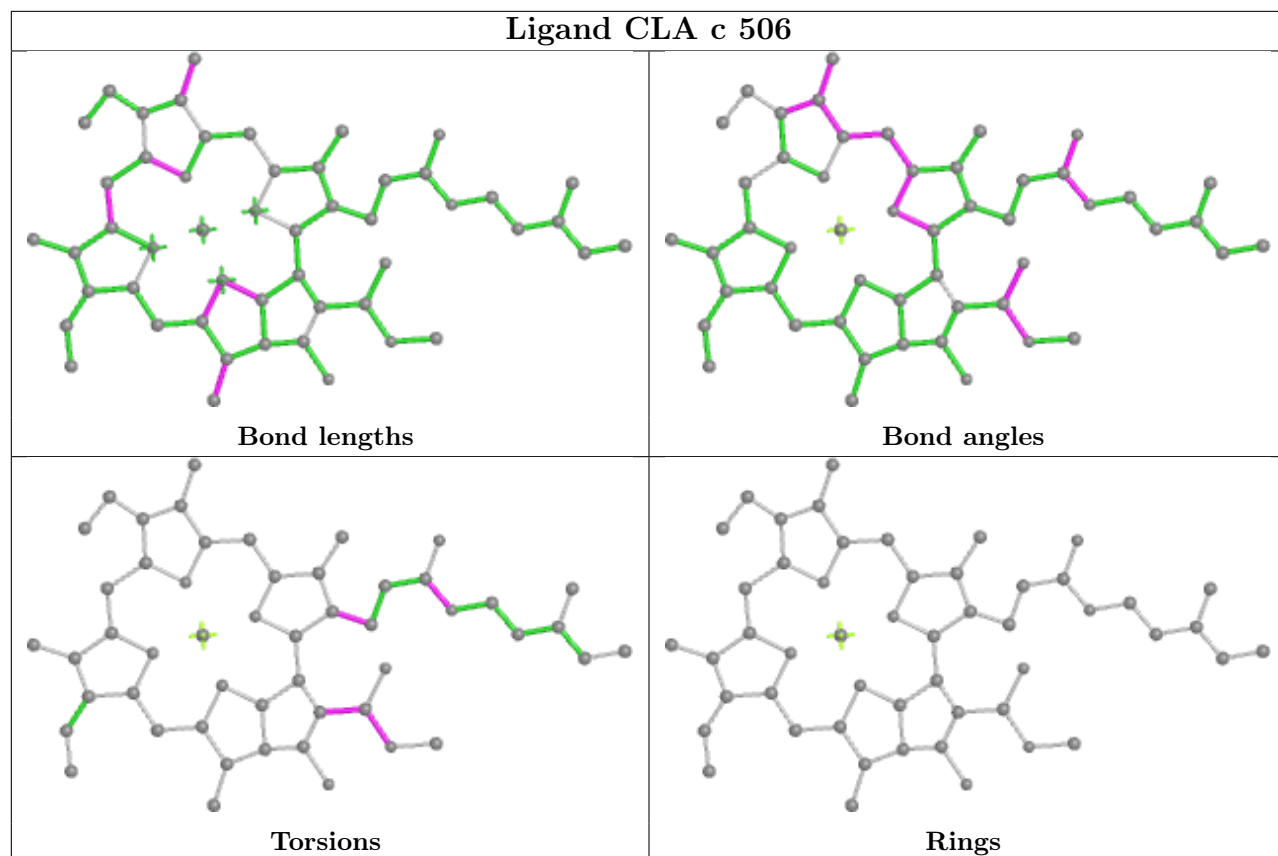




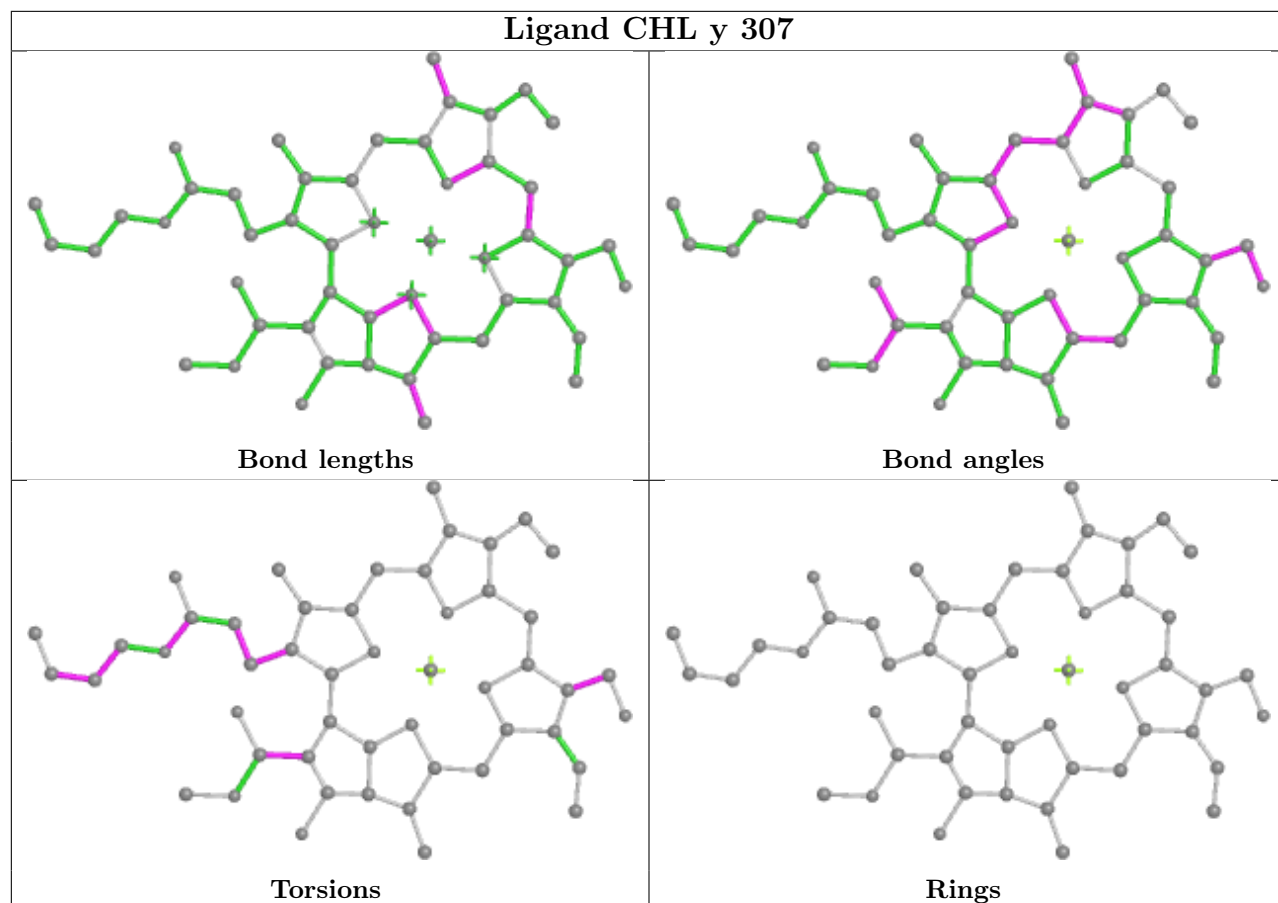


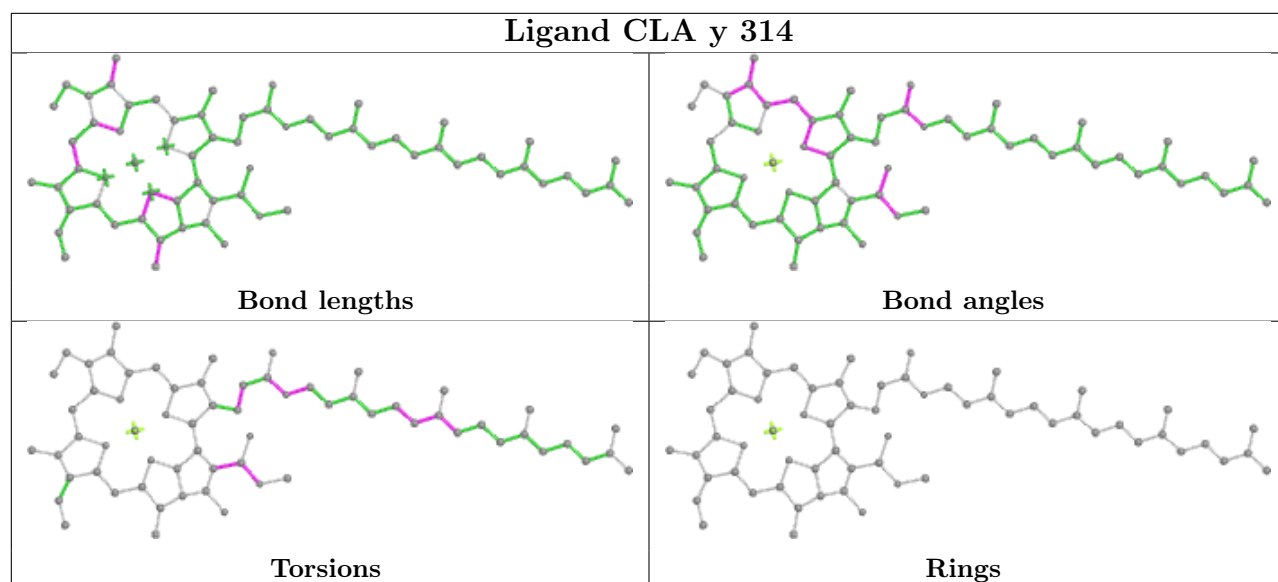
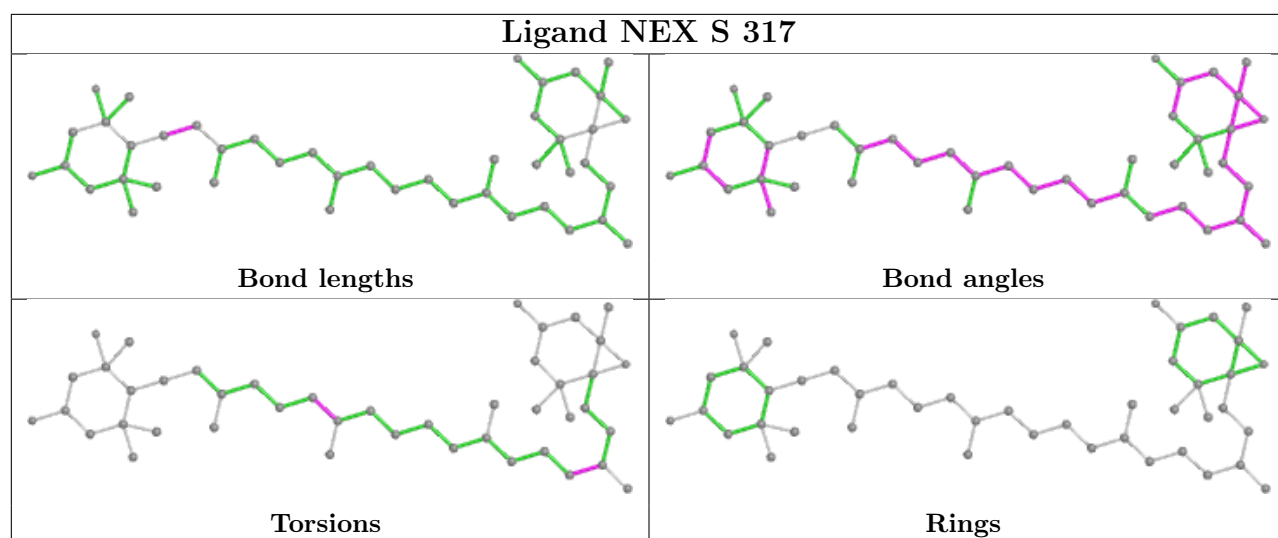


Ligand CLA c 506

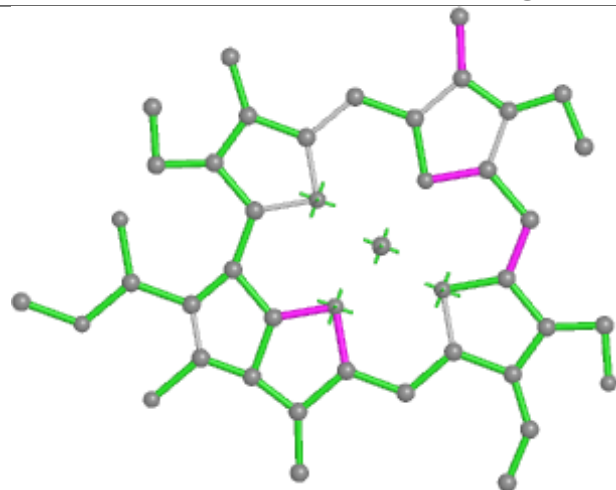


Ligand CHL y 307

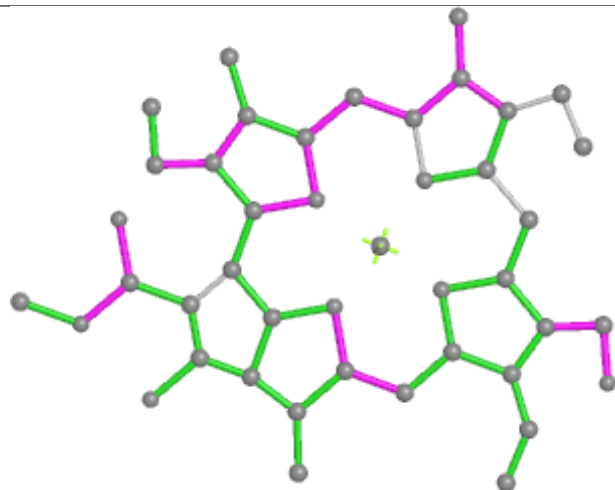




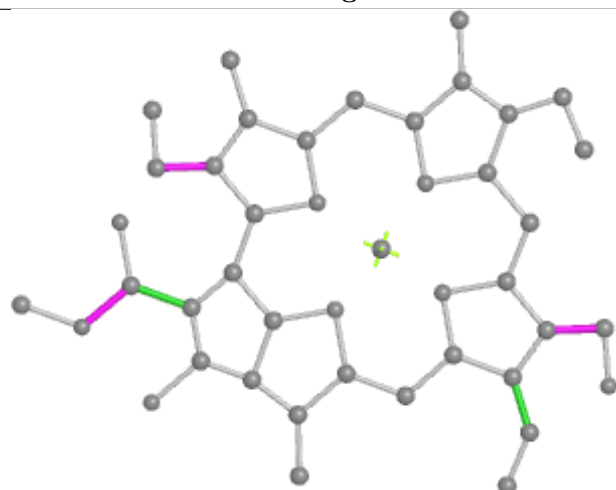
Ligand CHL S 307



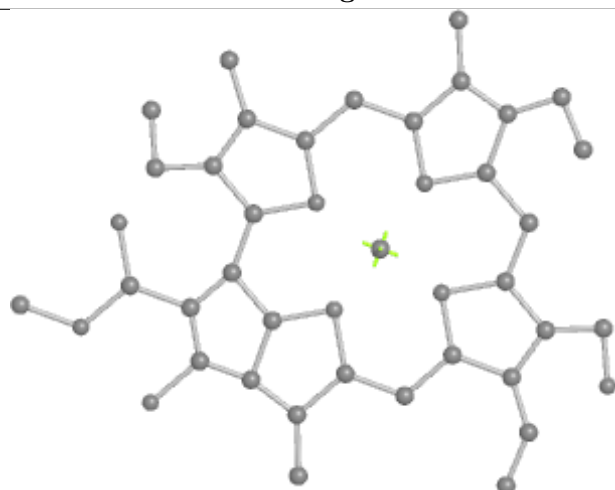
Bond lengths



Bond angles

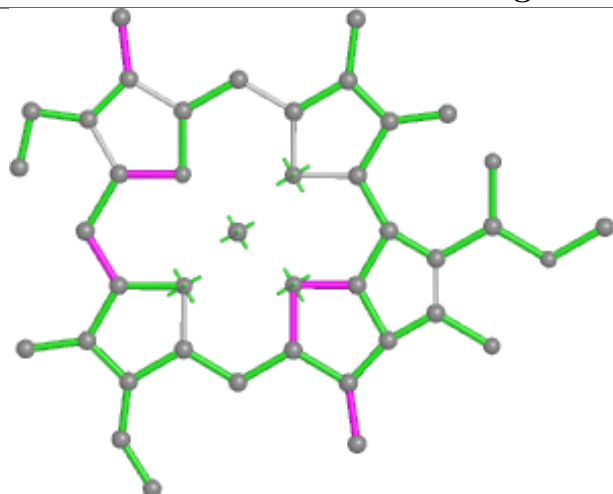


Torsions

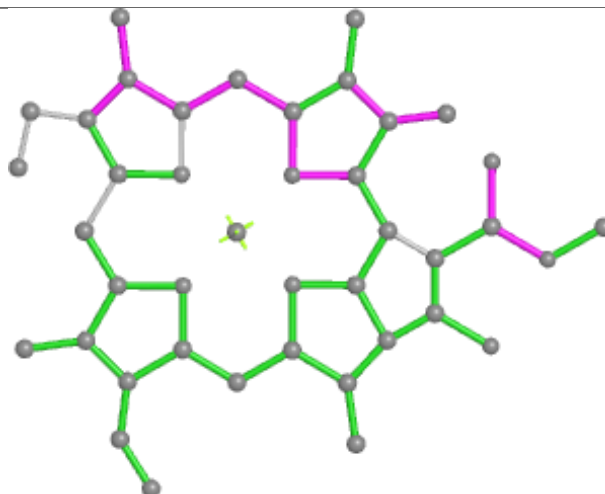


Rings

Ligand CLA R 311



Bond lengths



Bond angles

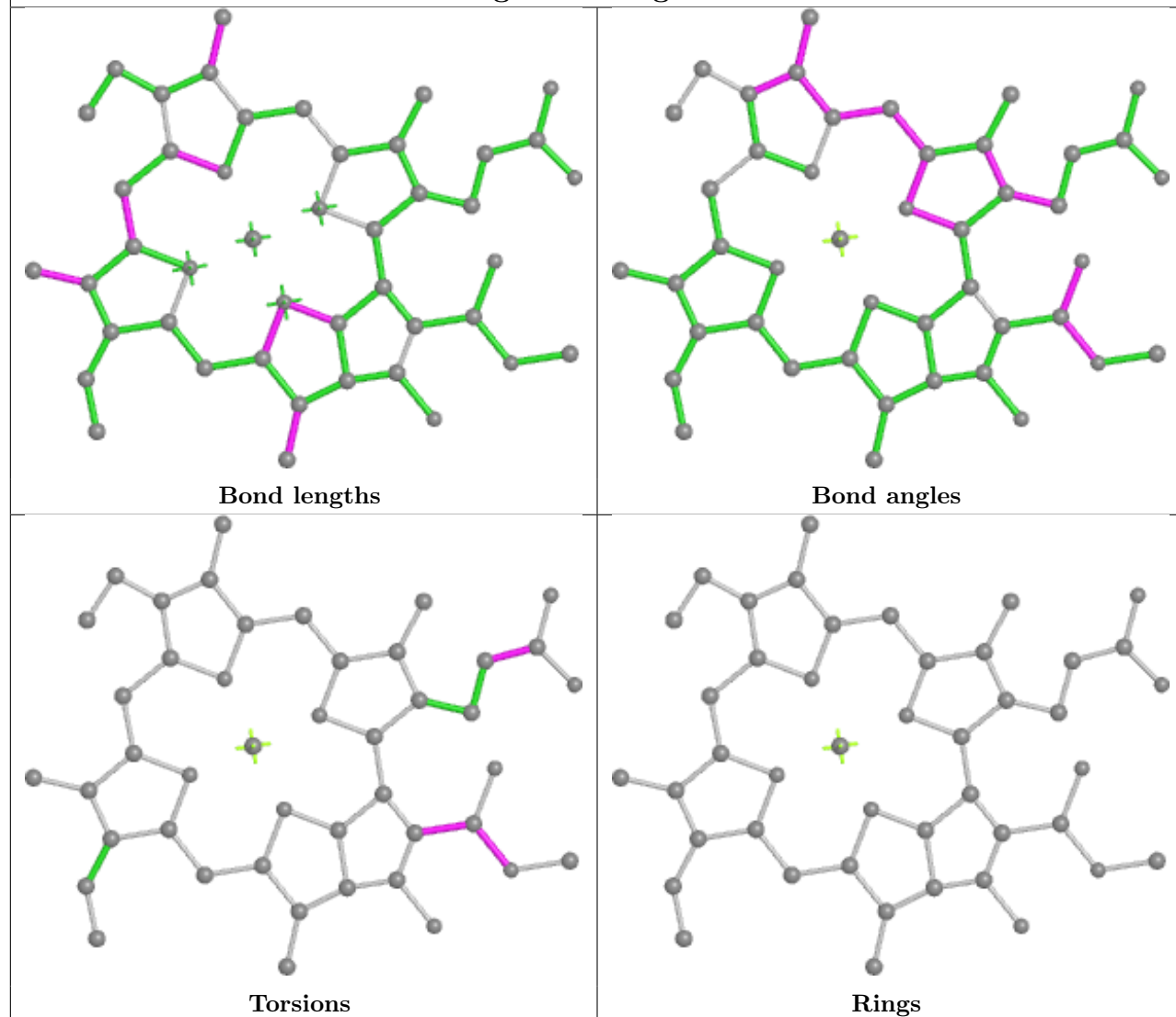


Torsions

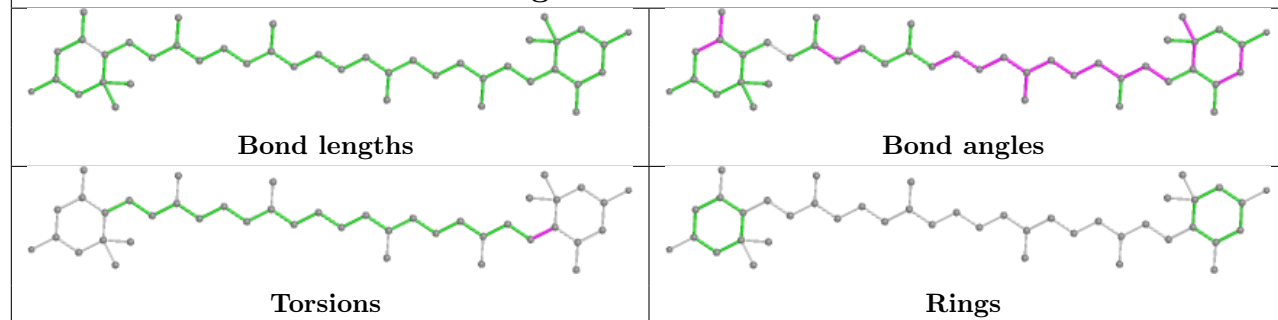


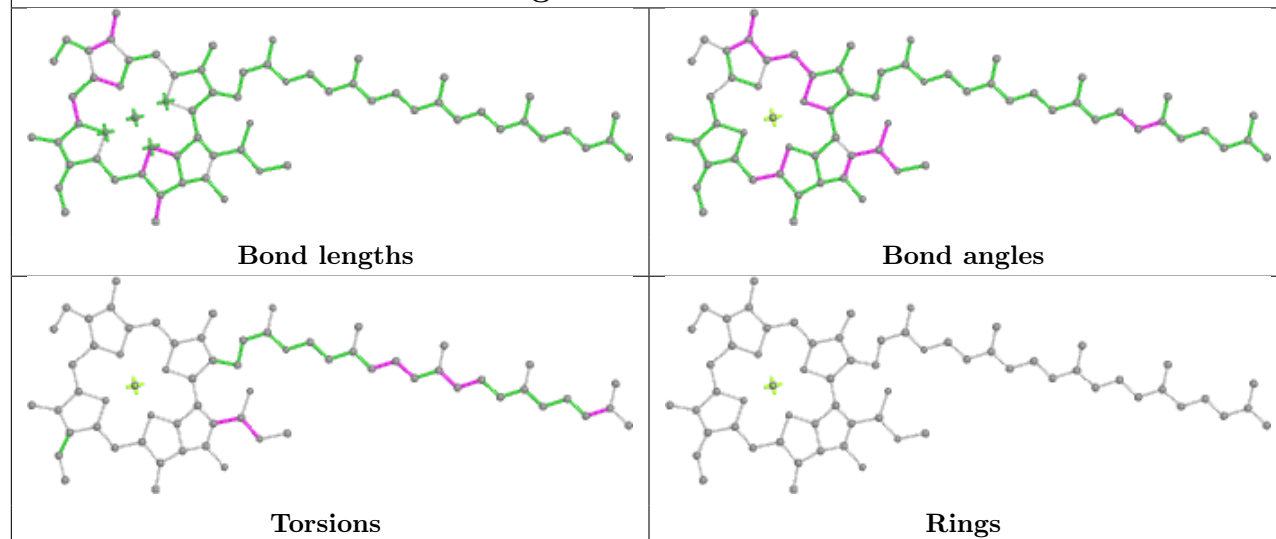
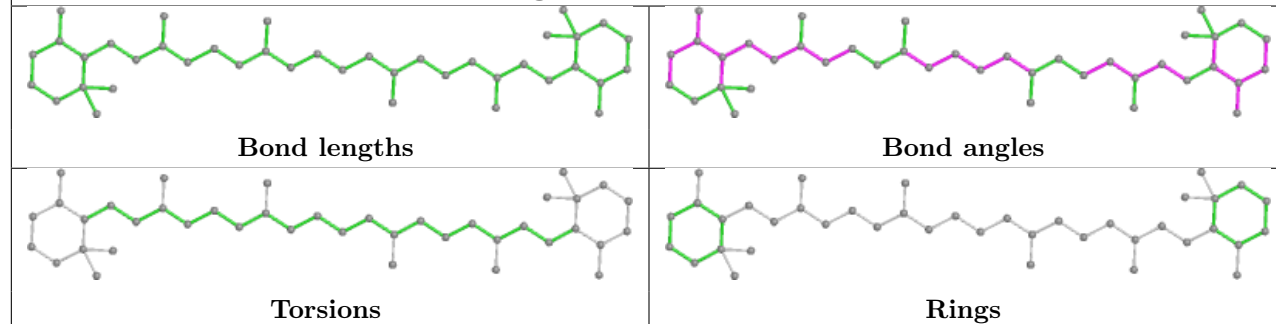
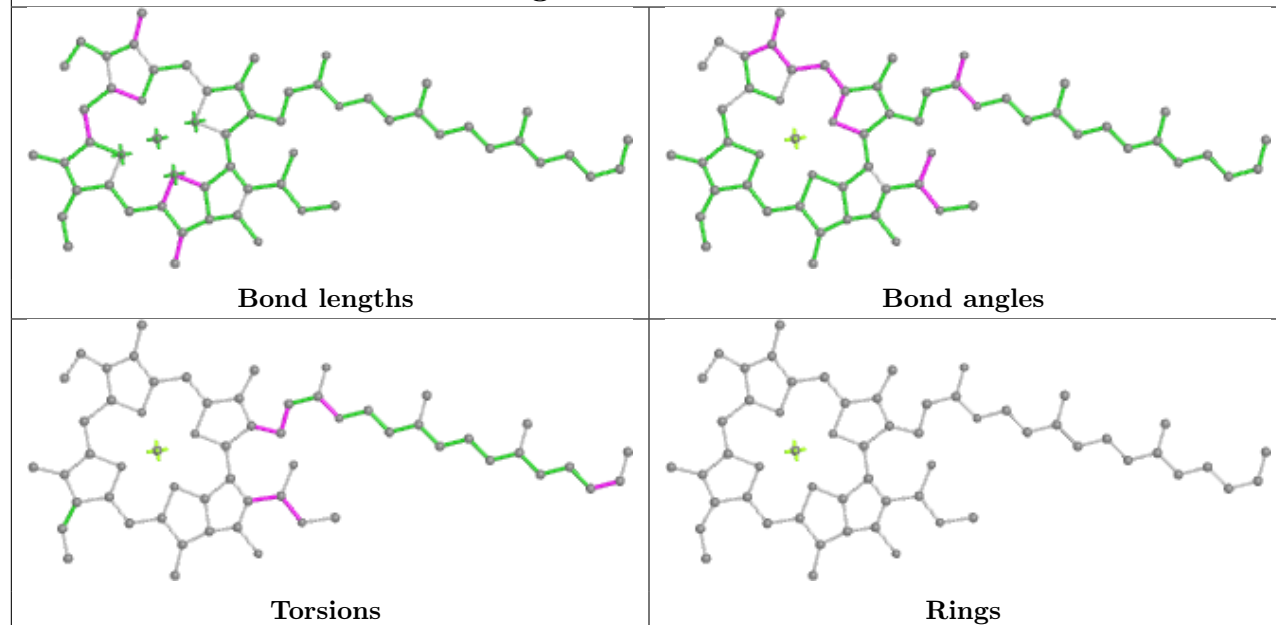
Rings

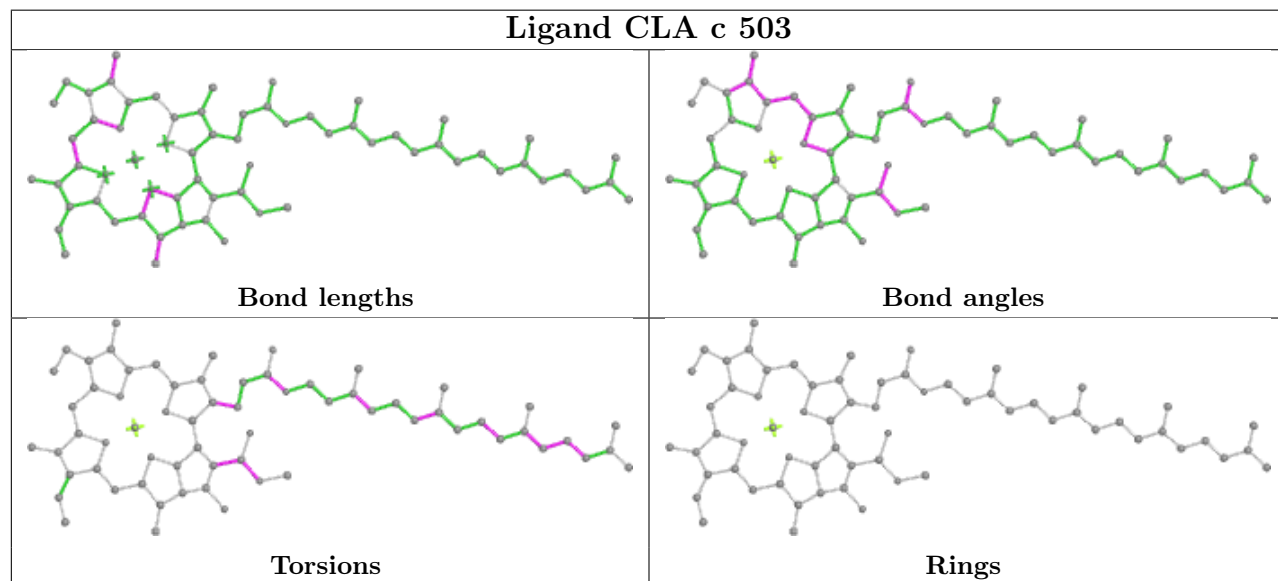
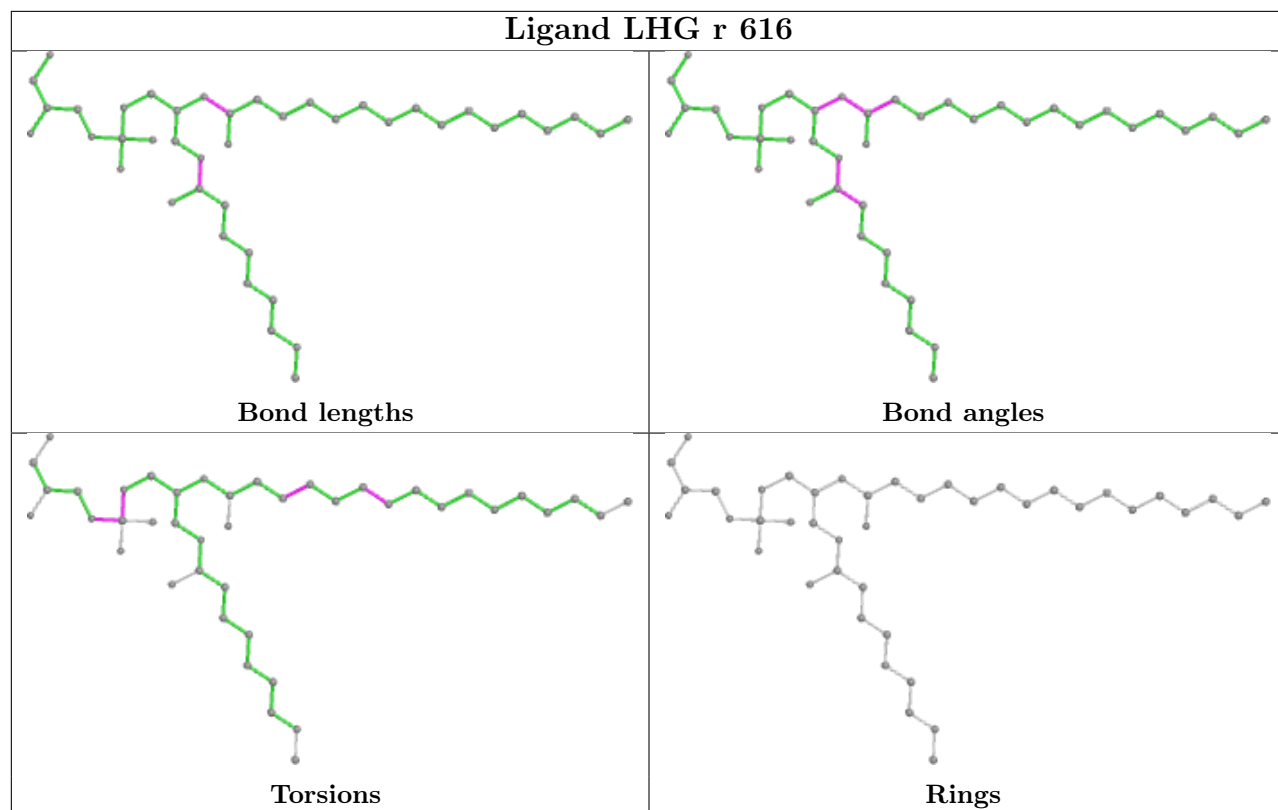
Ligand CLA g 612



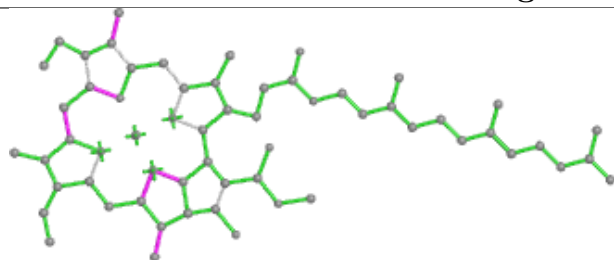
Ligand LUT N 616



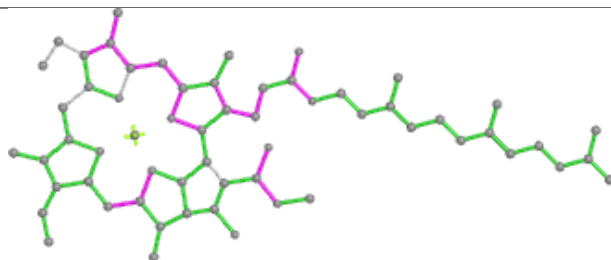
Ligand CLA B 605**Ligand BCR B 618****Ligand CLA N 610**



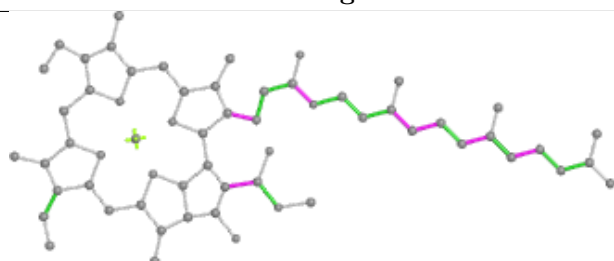
Ligand CLA n 613



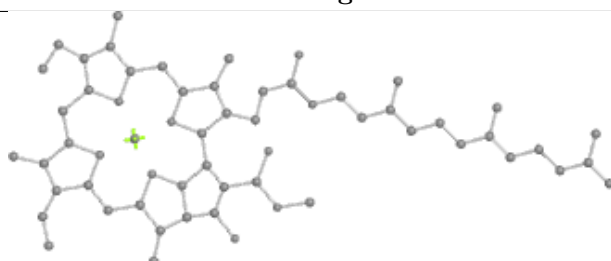
Bond lengths



Bond angles

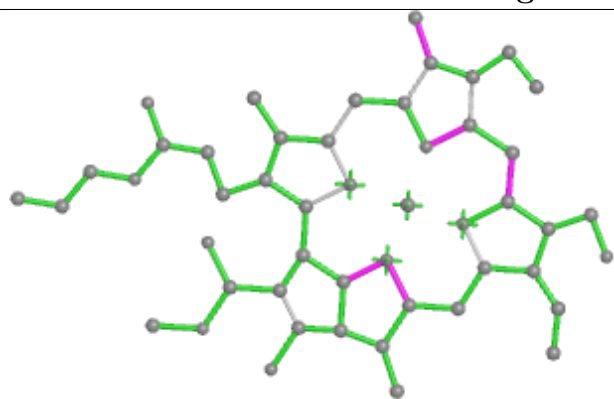


Torsions

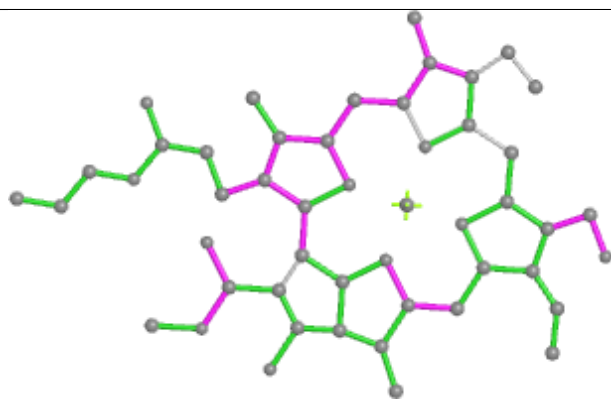


Rings

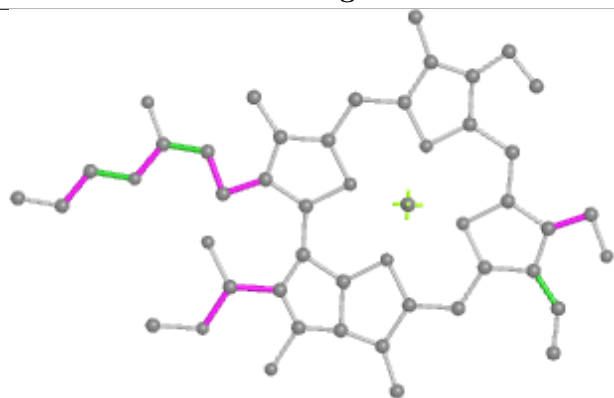
Ligand CHL S 308



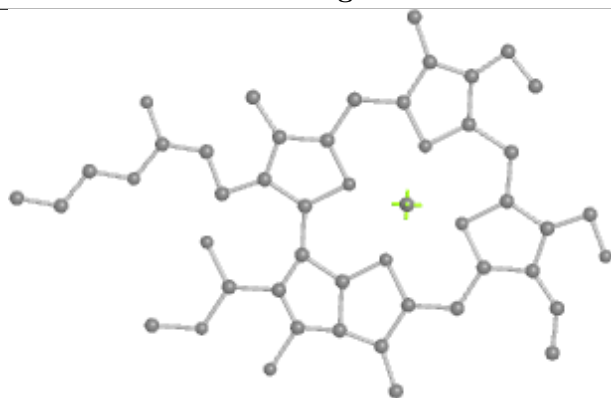
Bond lengths



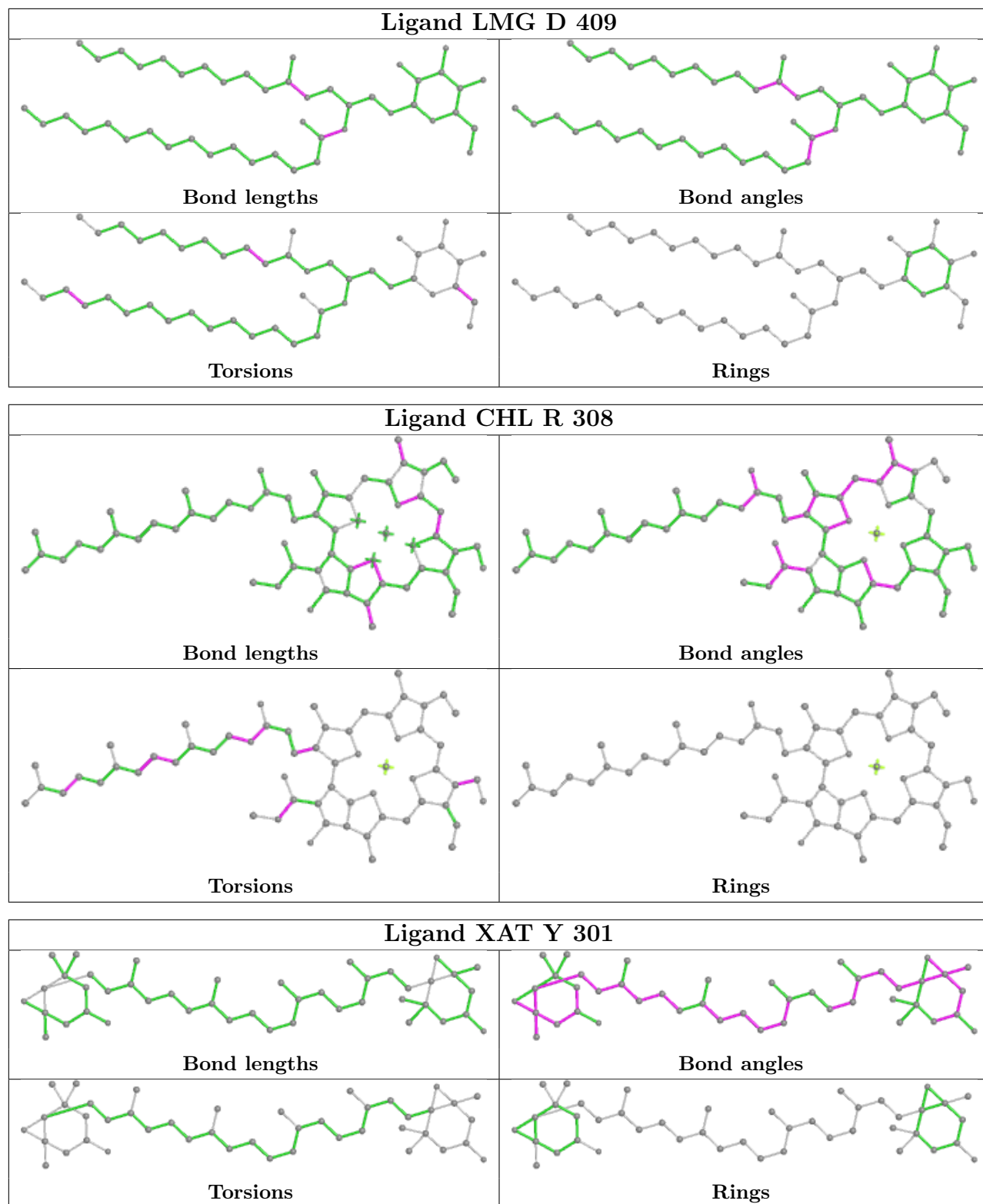
Bond angles

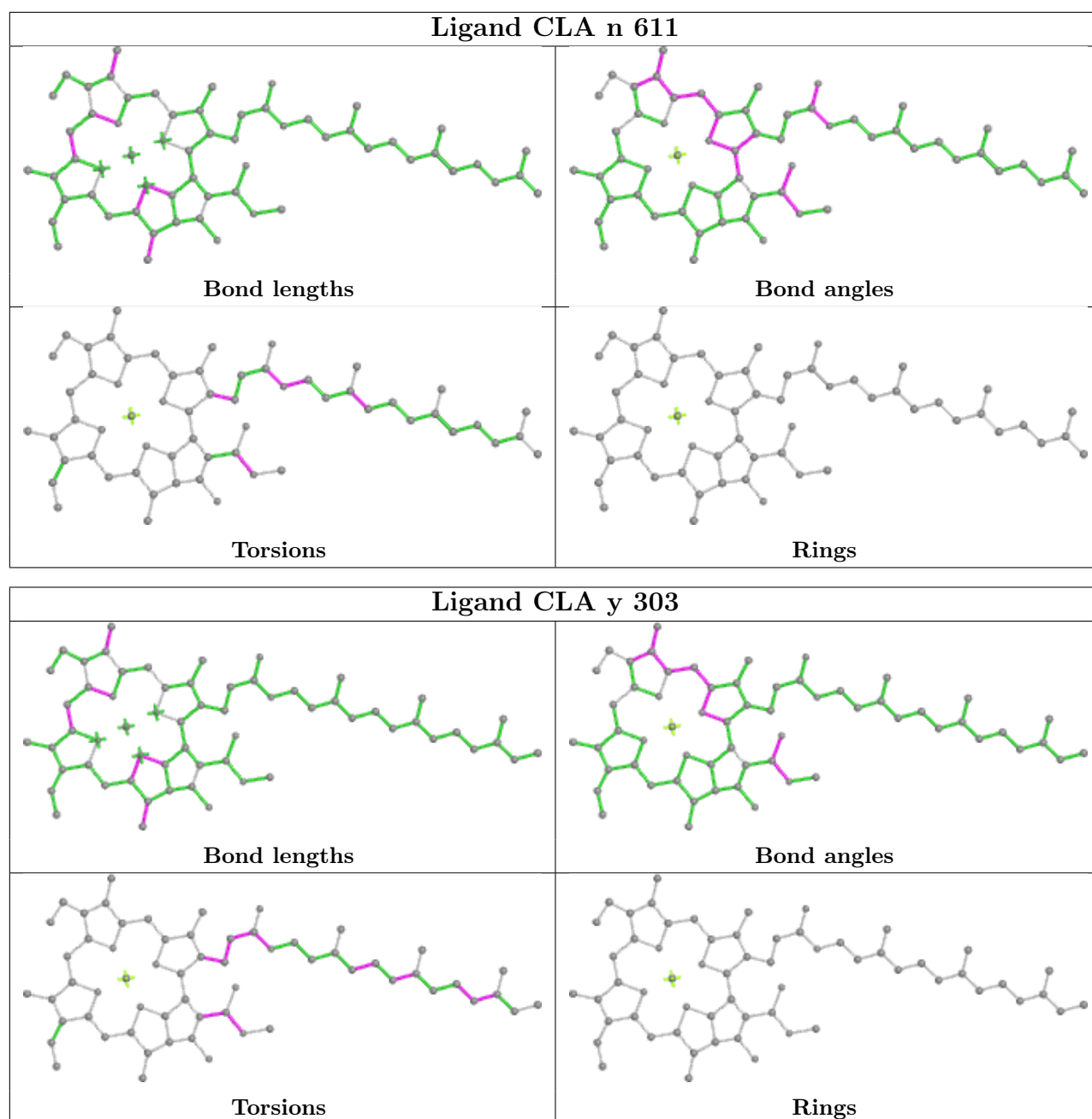


Torsions

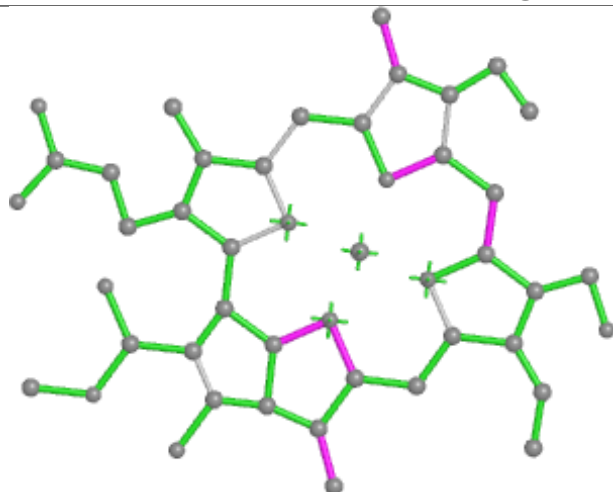


Rings

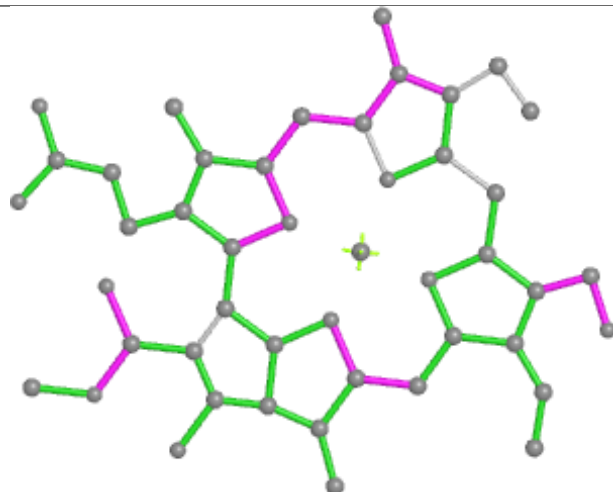




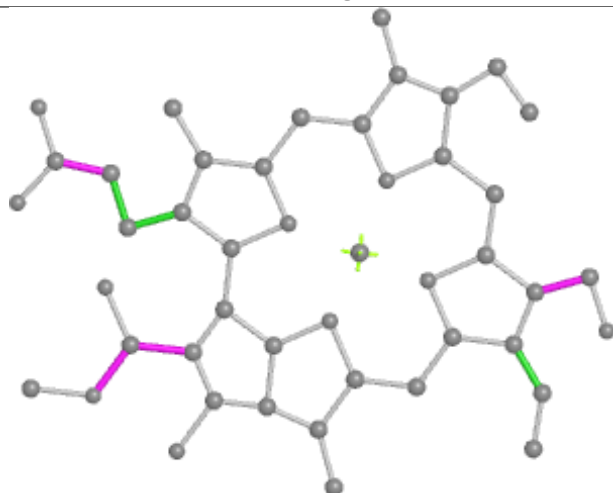
Ligand CHL S 302



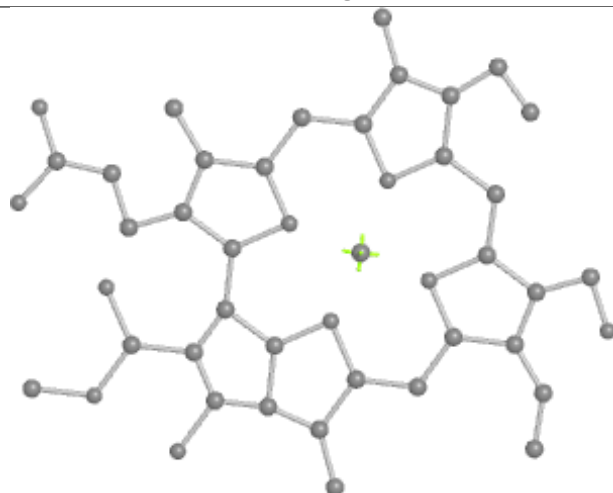
Bond lengths



Bond angles

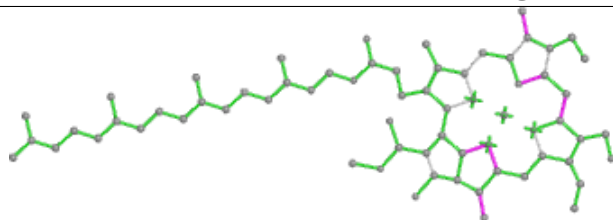


Torsions

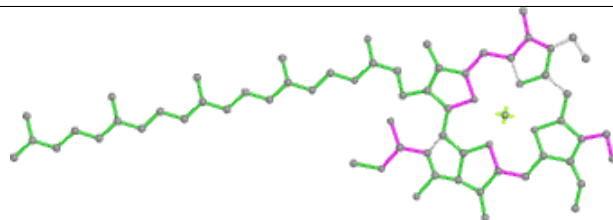


Rings

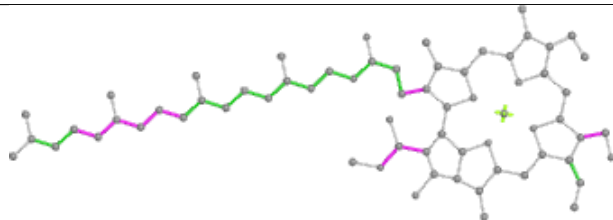
Ligand CHL Y 302



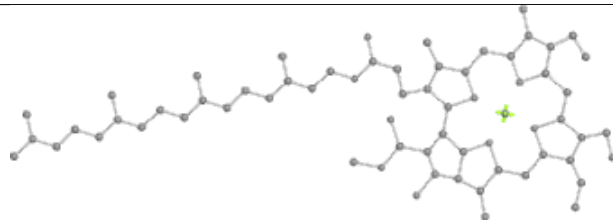
Bond lengths



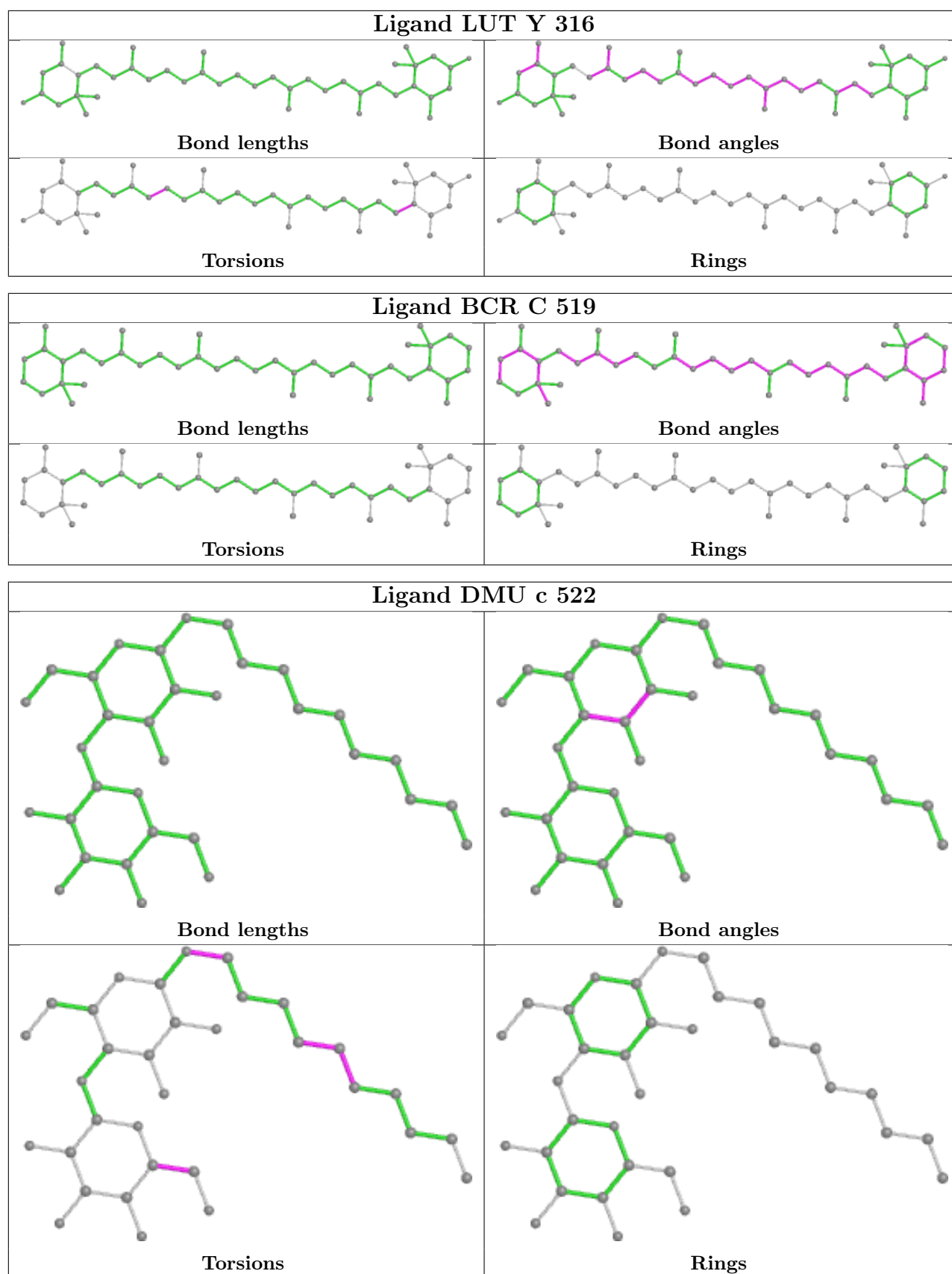
Bond angles

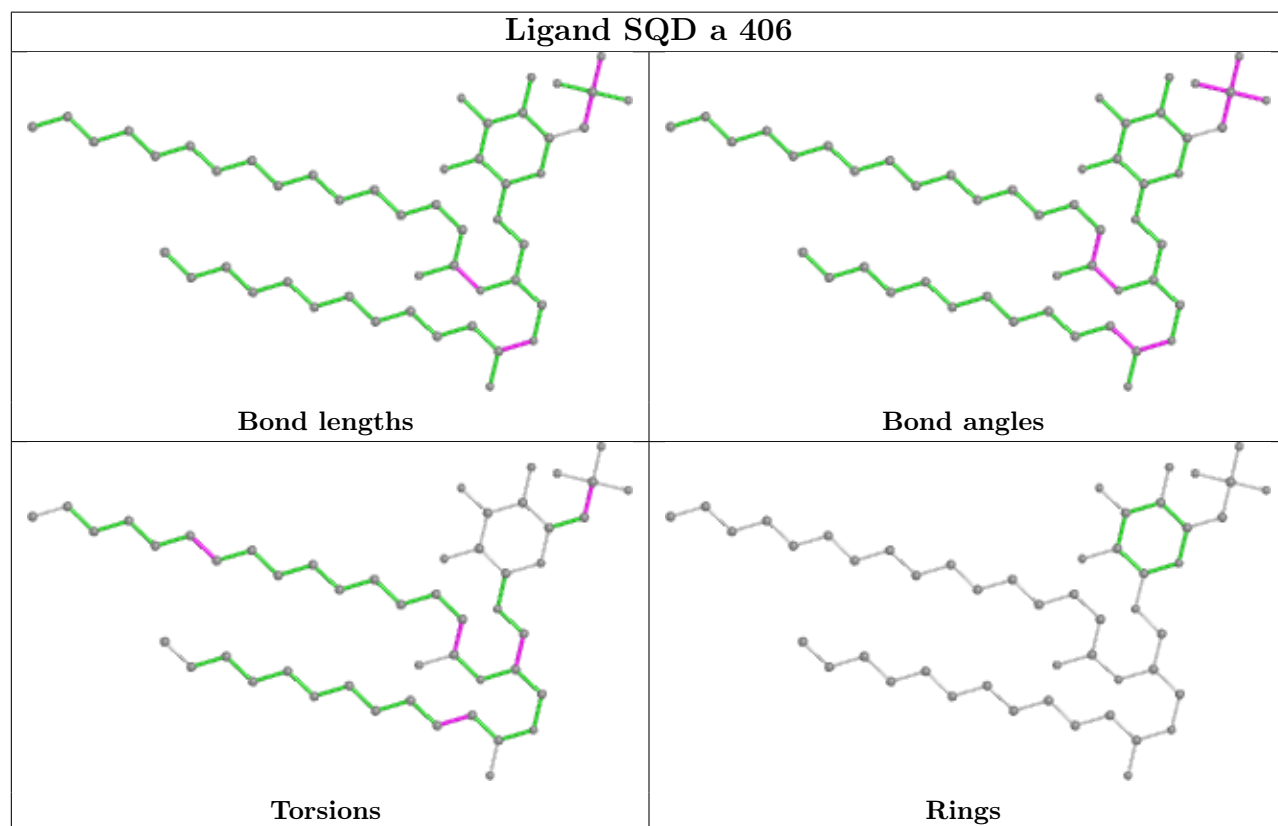
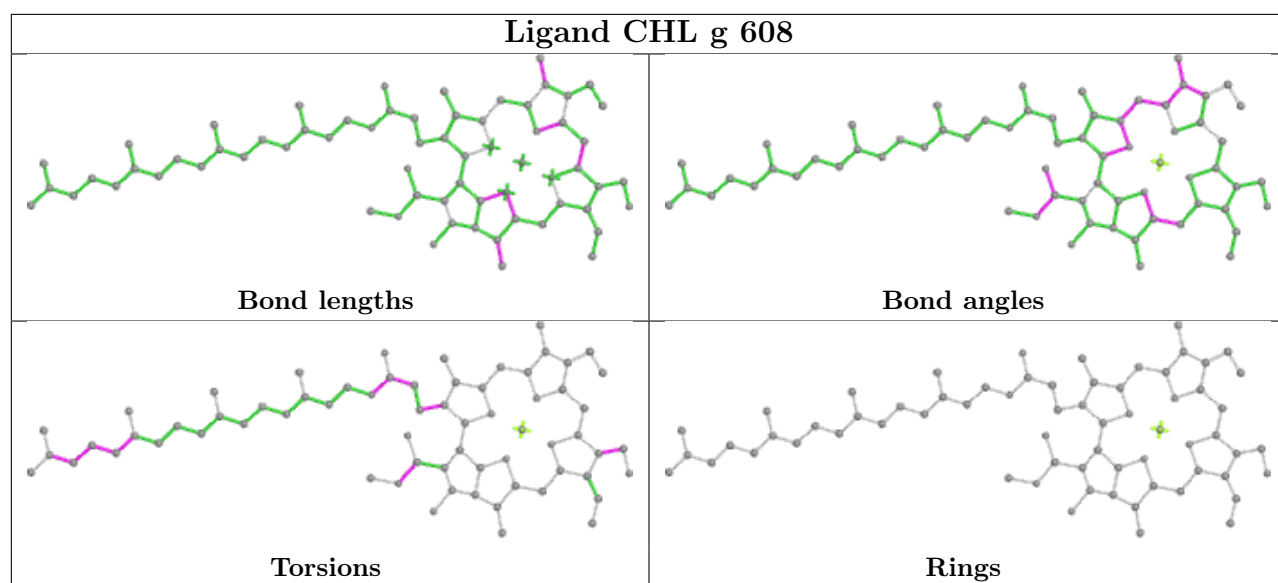


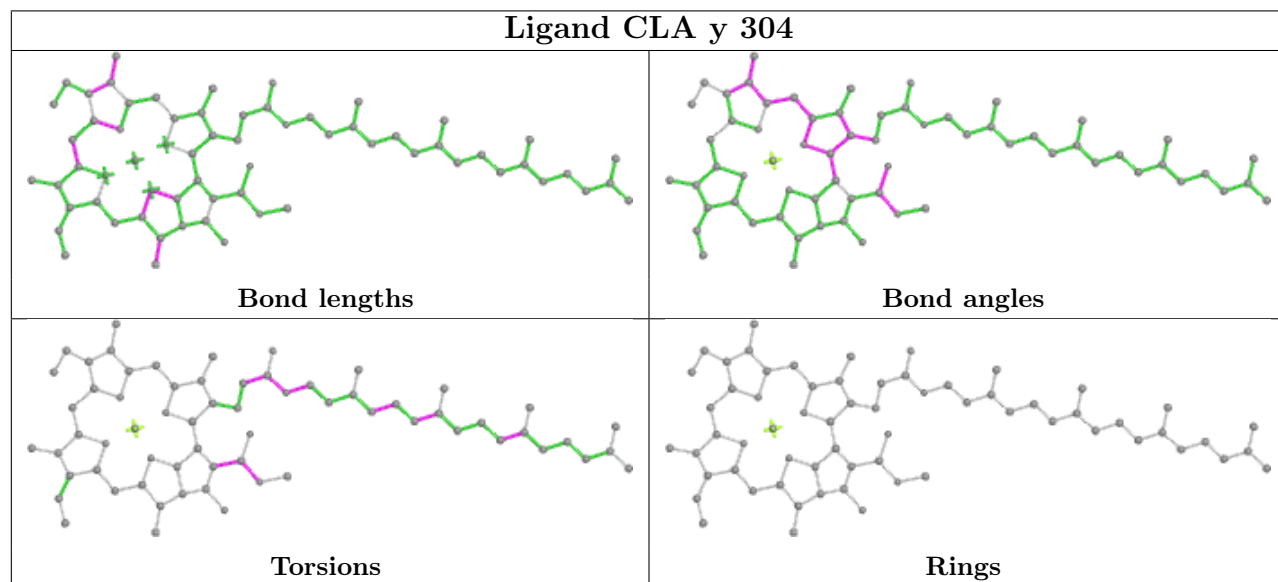
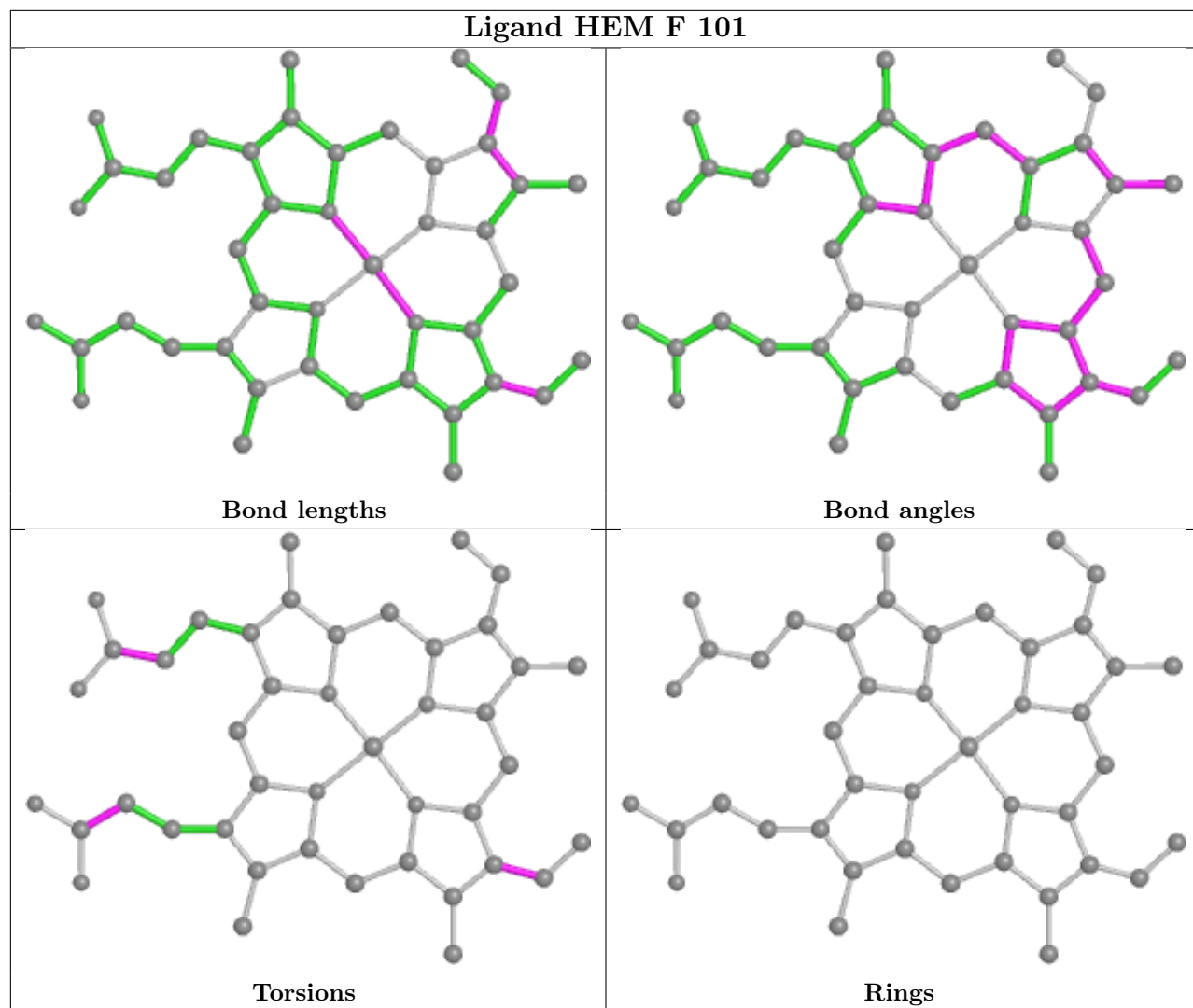
Torsions

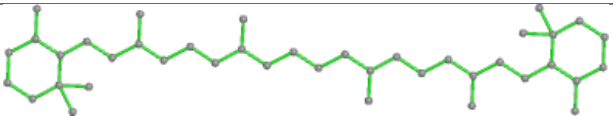
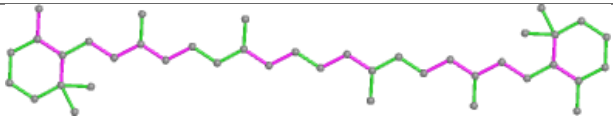
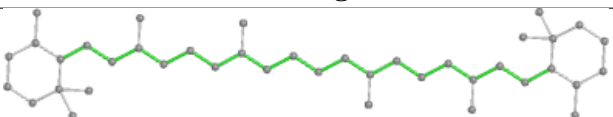
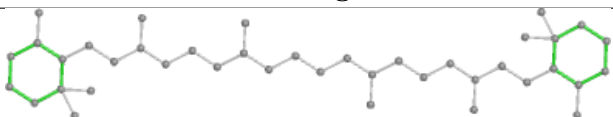


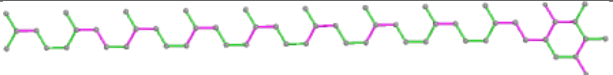
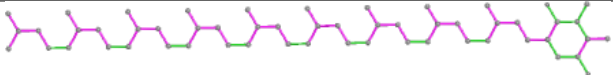
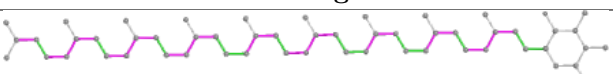
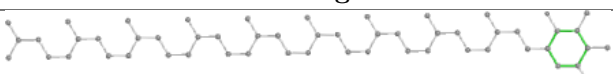
Rings



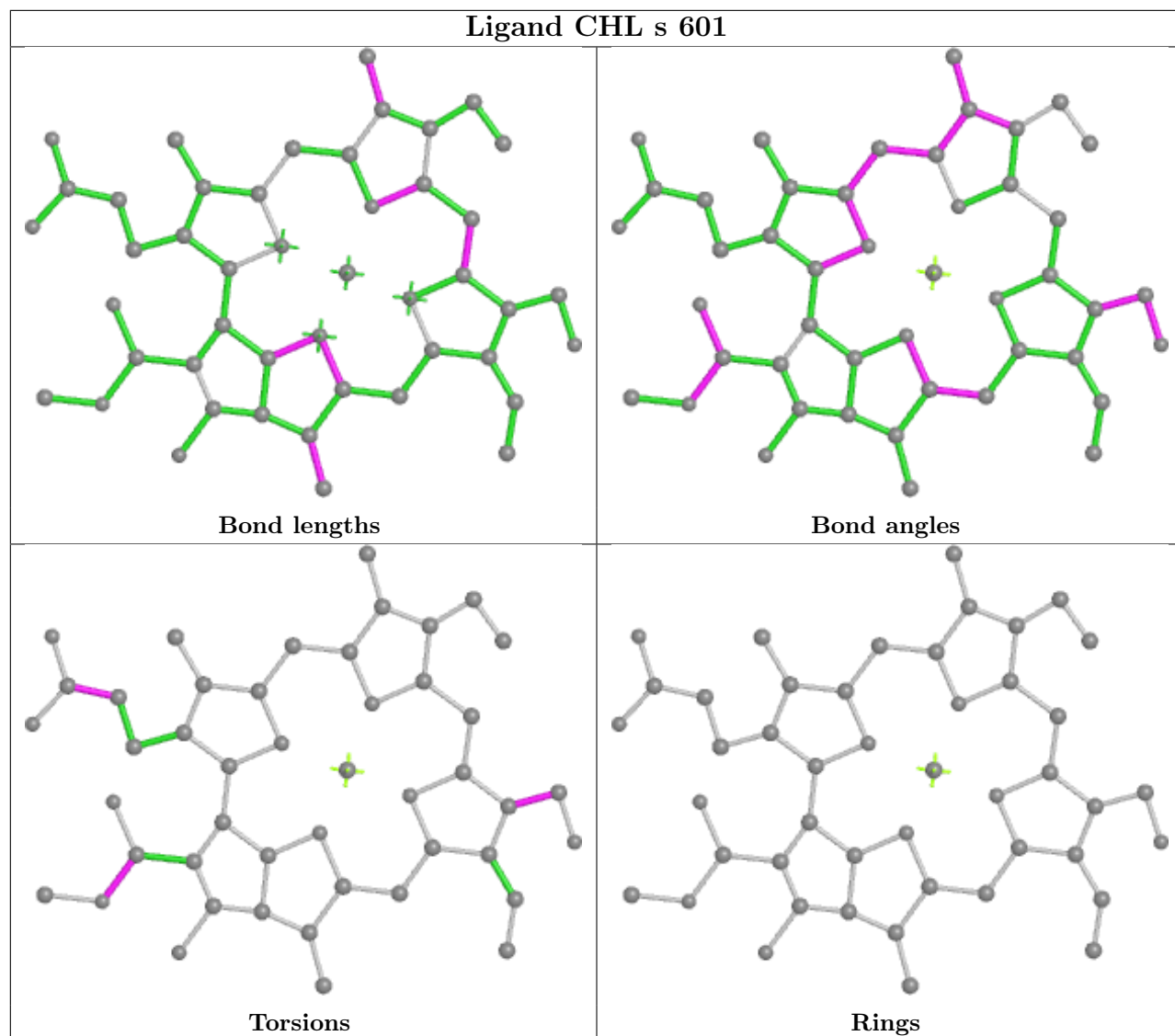


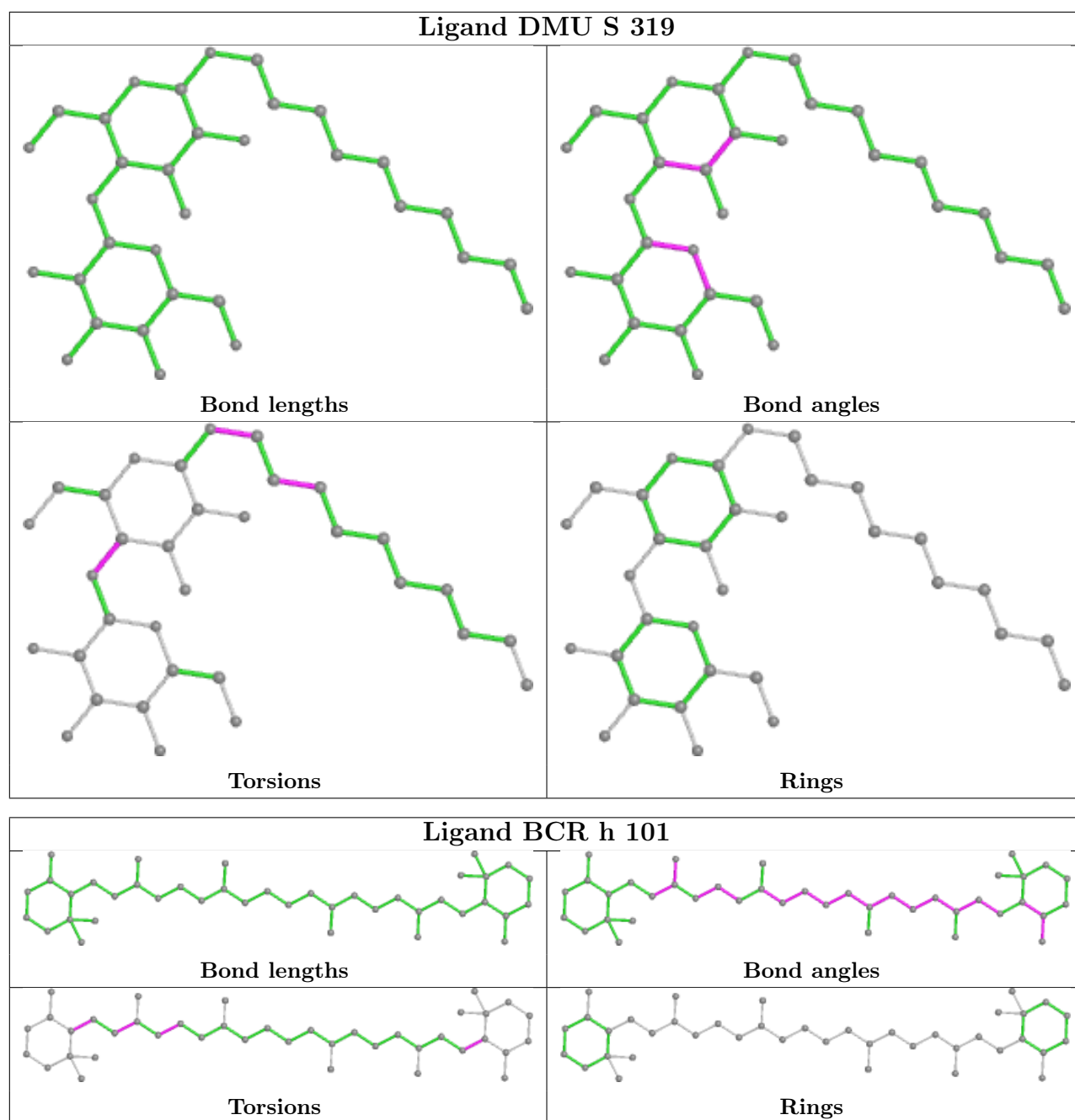


Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

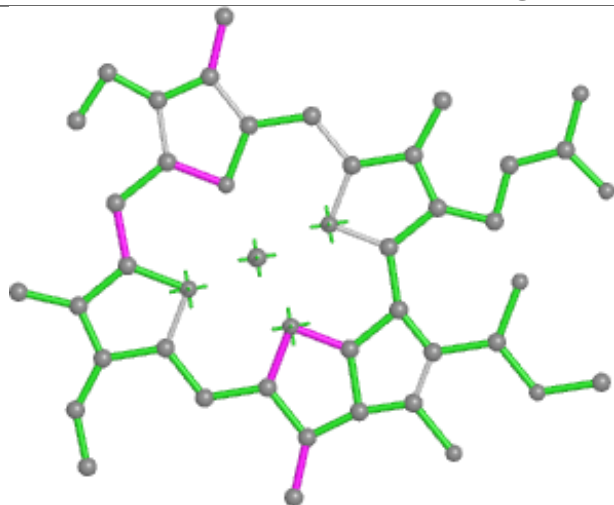
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL s 601

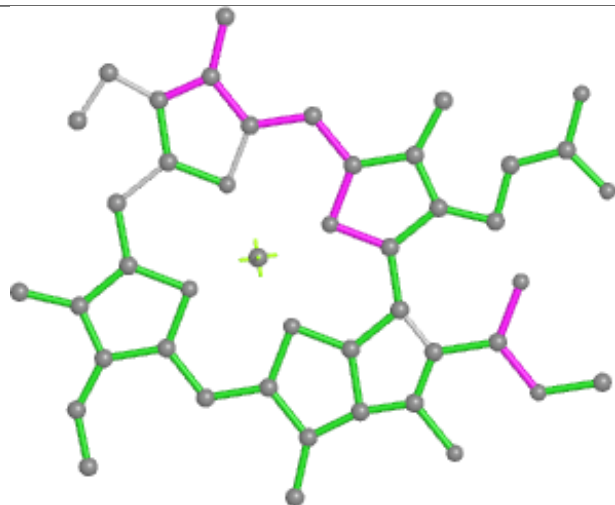




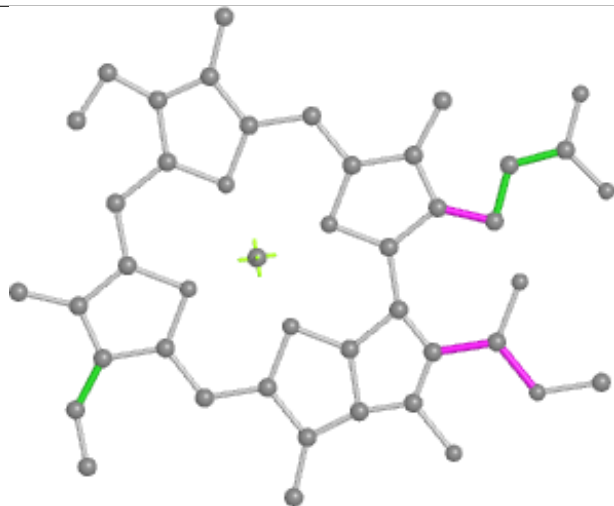
Ligand CLA Y 315



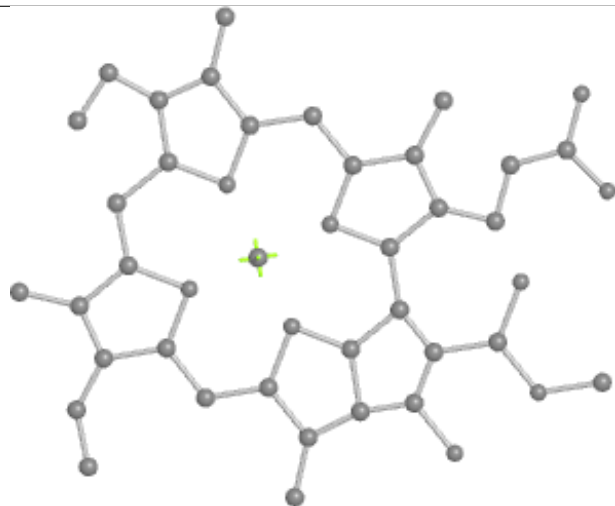
Bond lengths



Bond angles

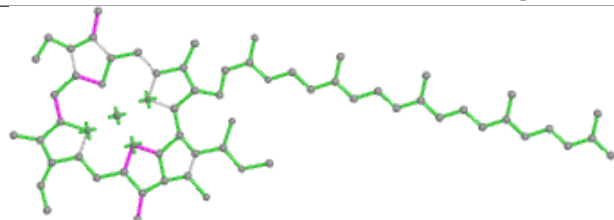


Torsions

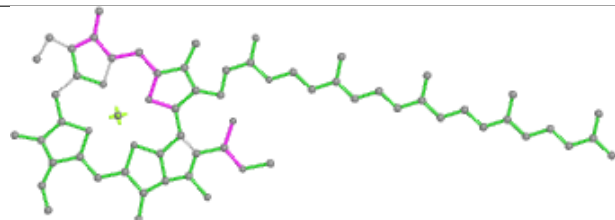


Rings

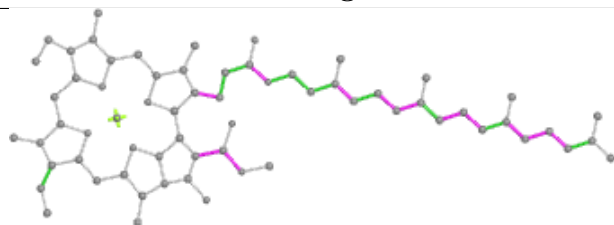
Ligand CLA C 504



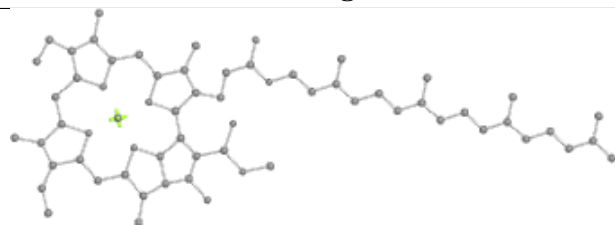
Bond lengths



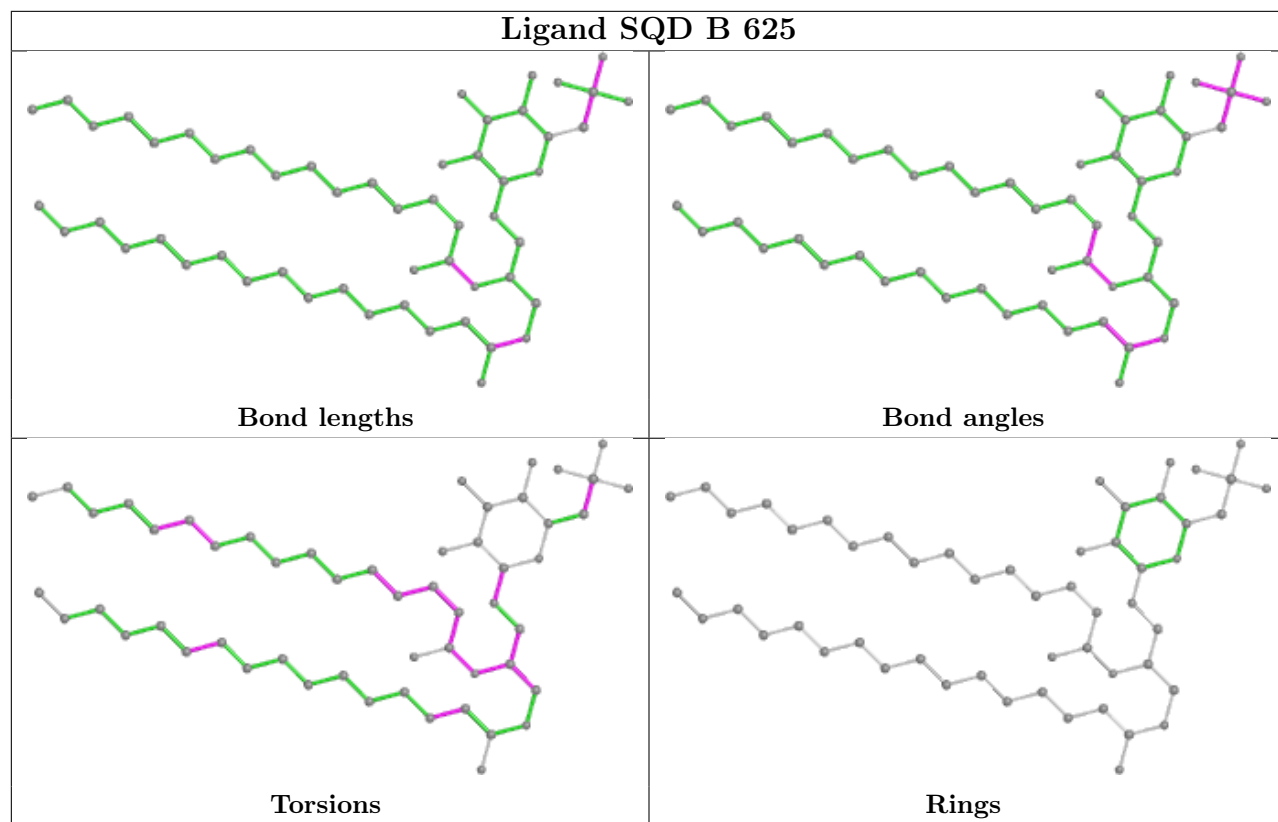
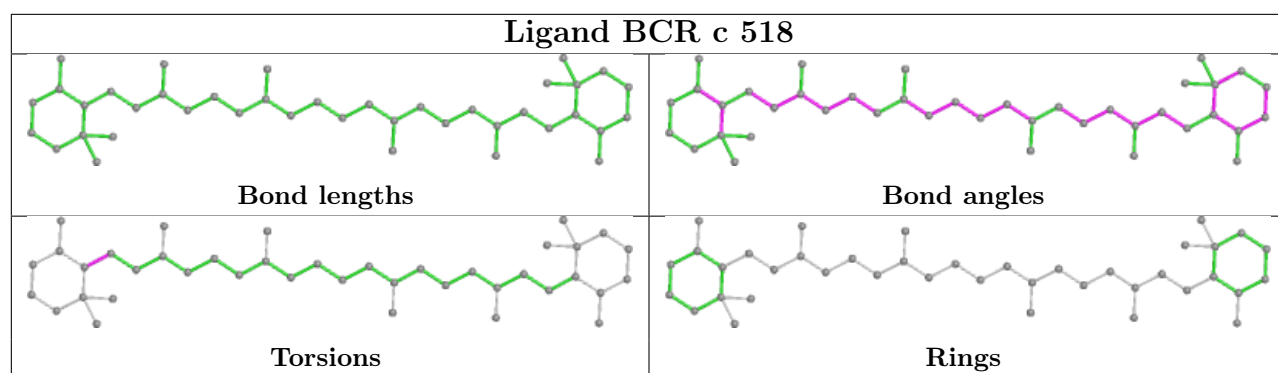
Bond angles

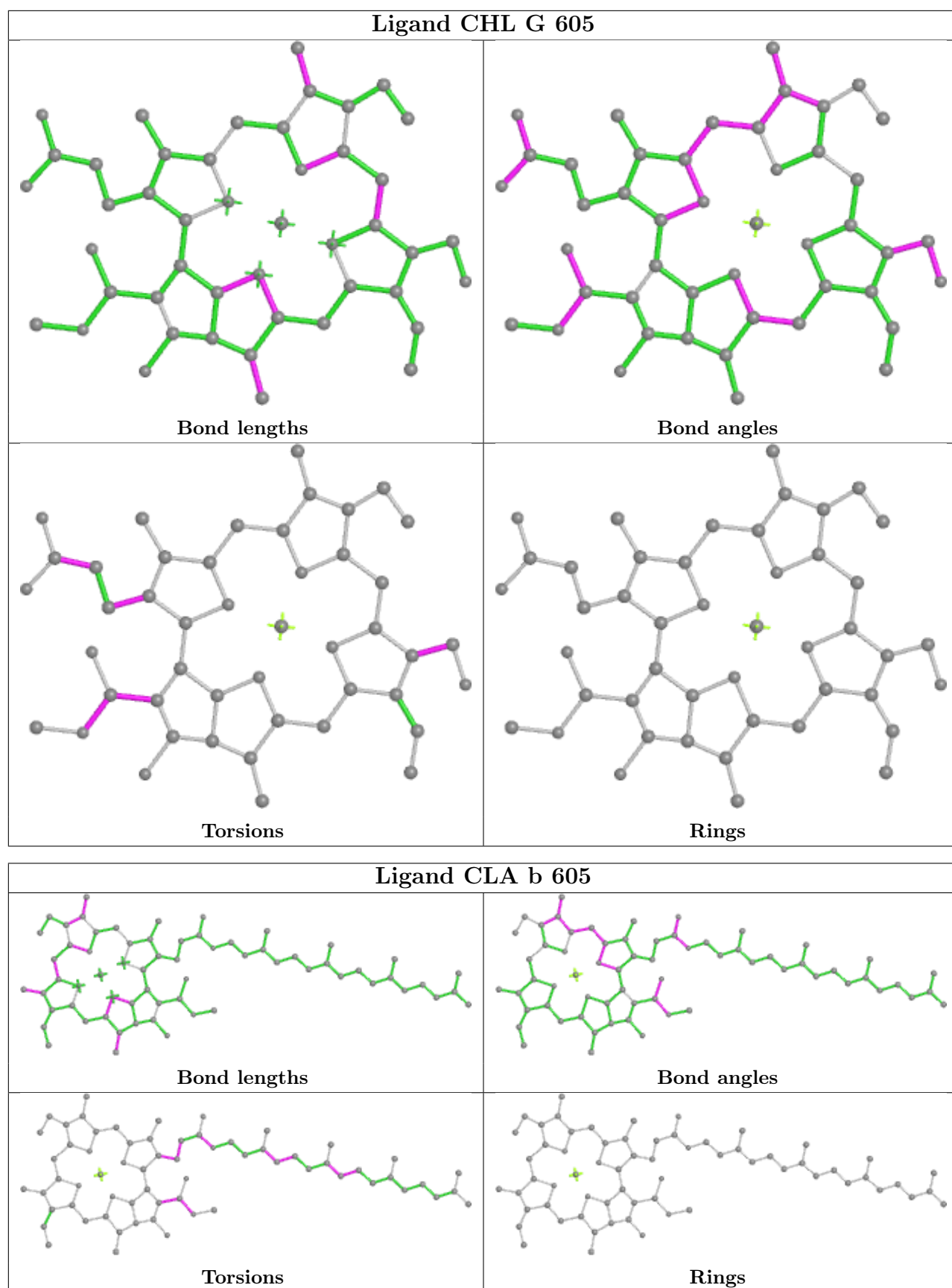


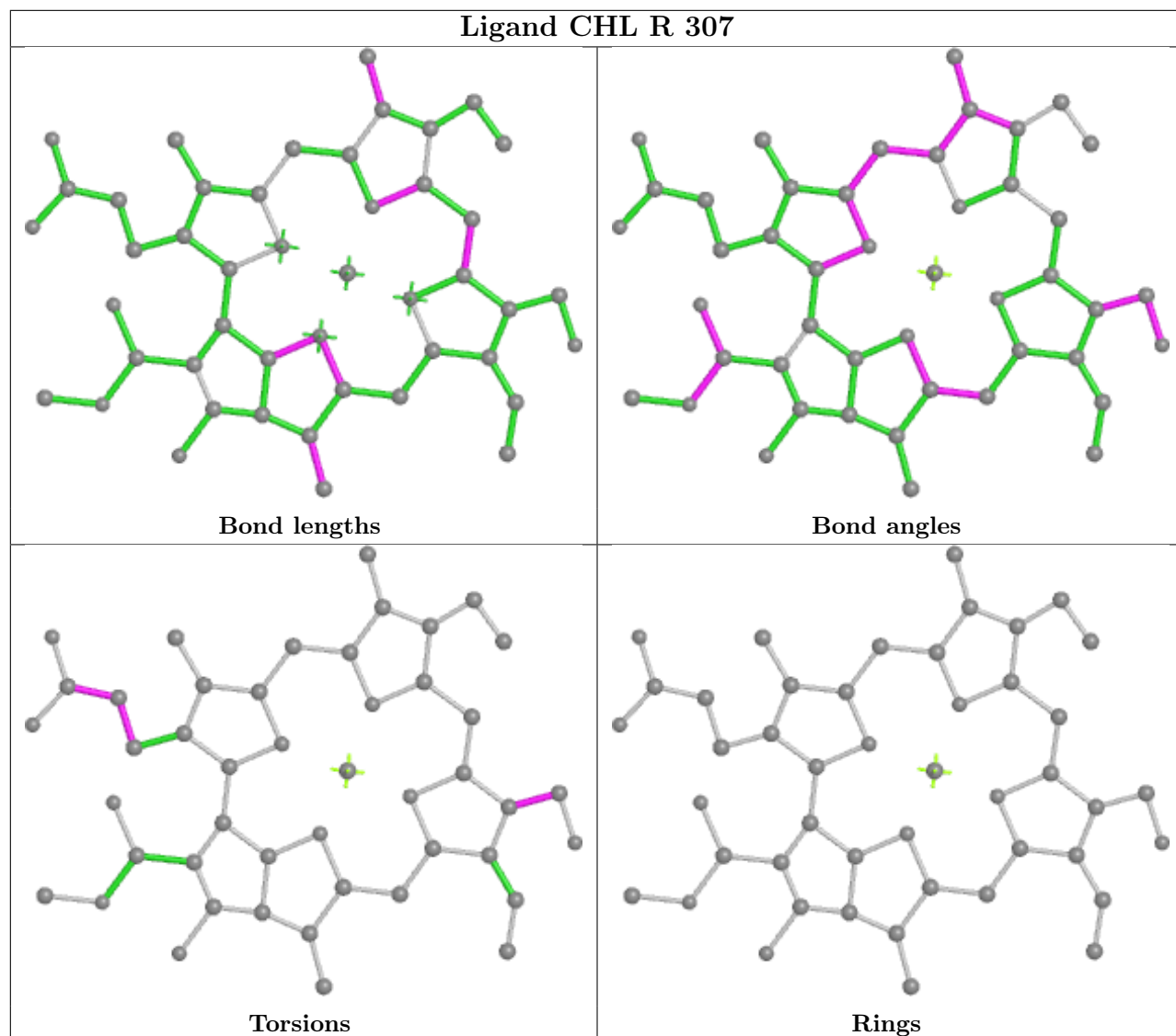
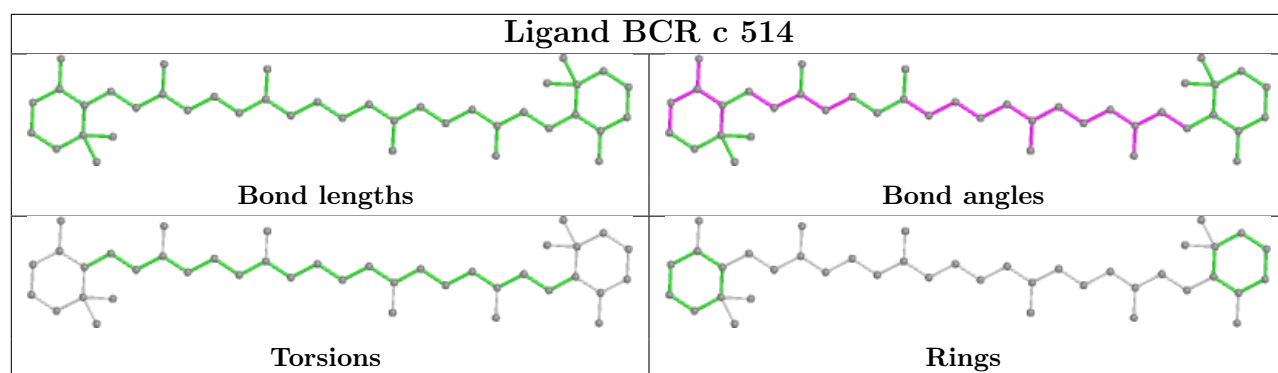
Torsions

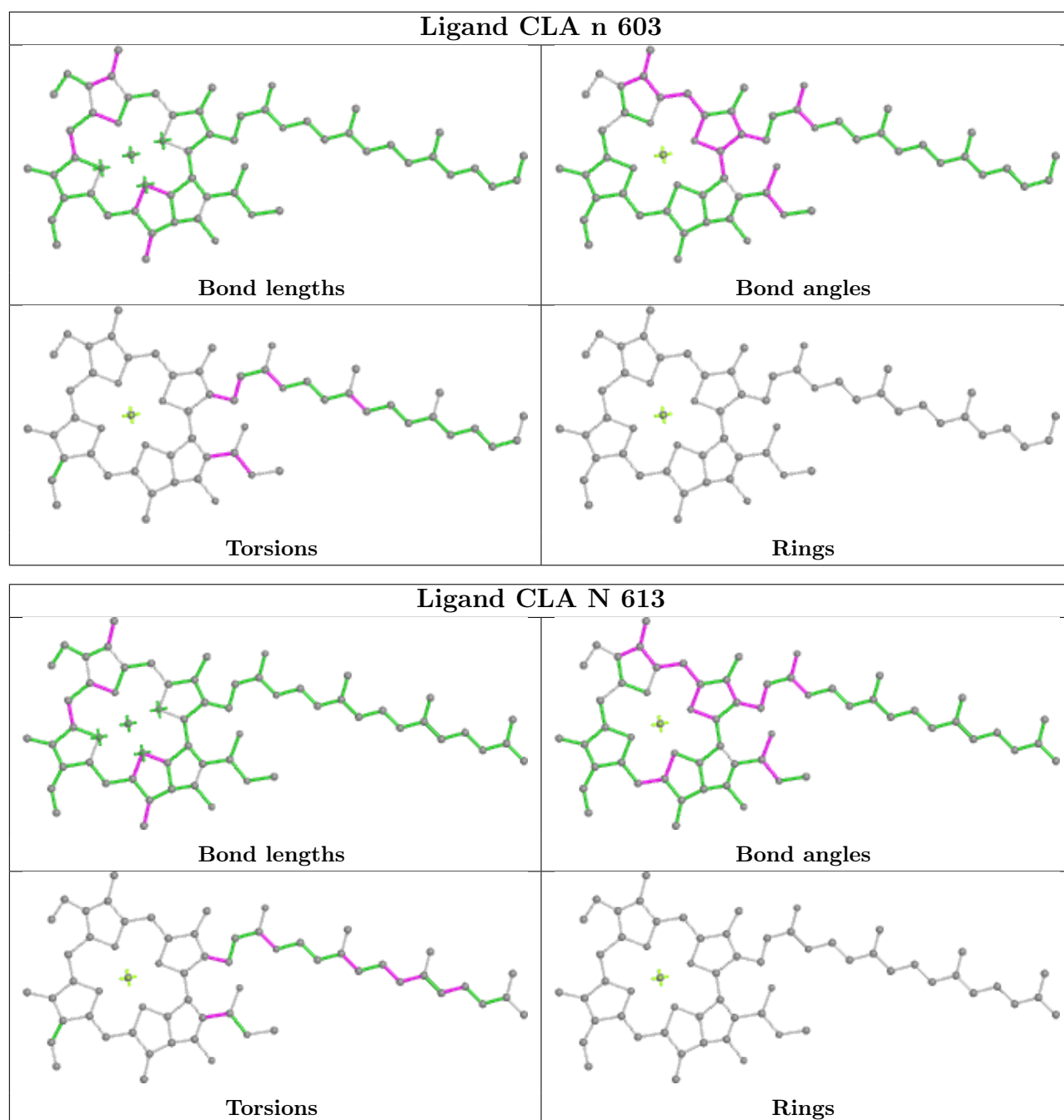


Rings

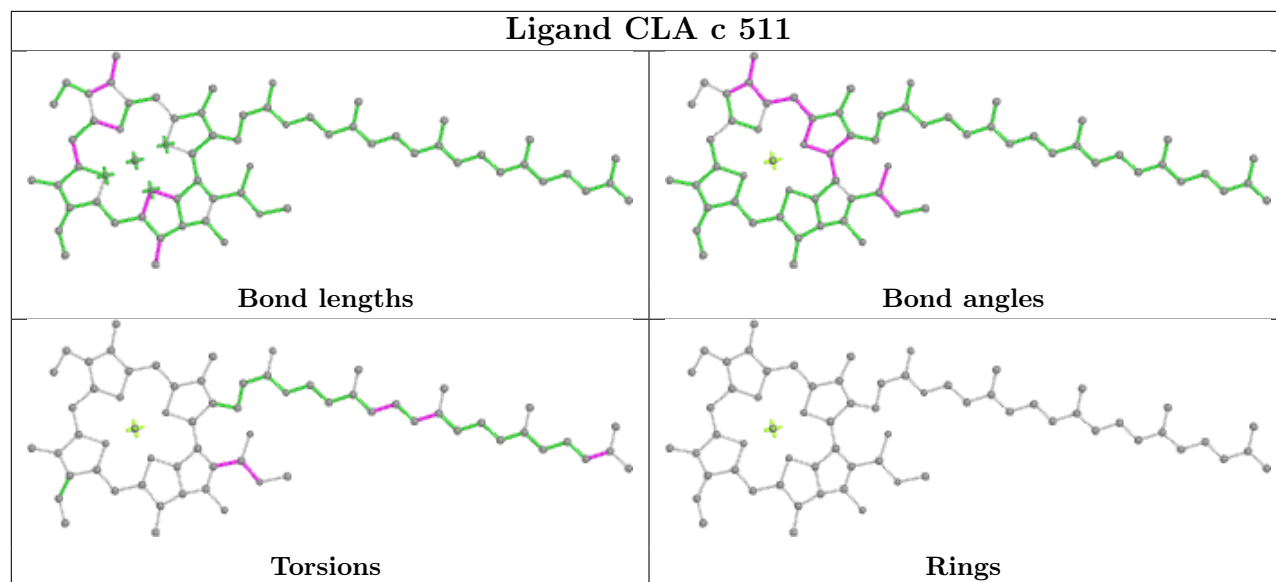




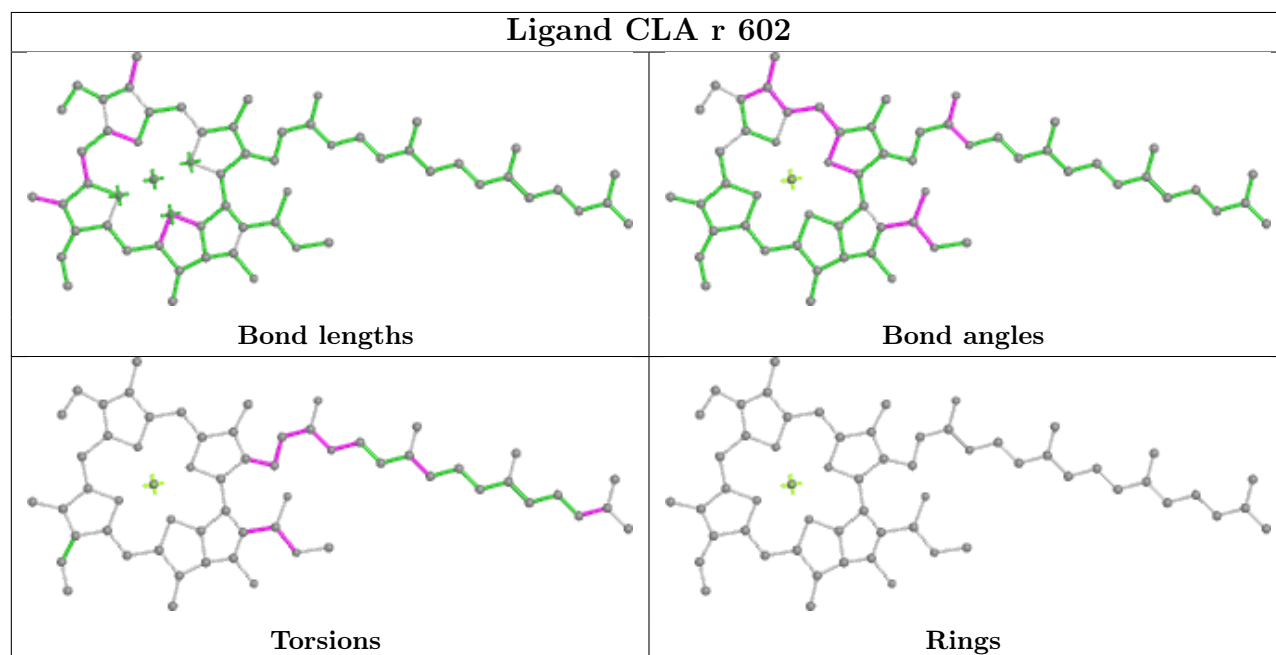




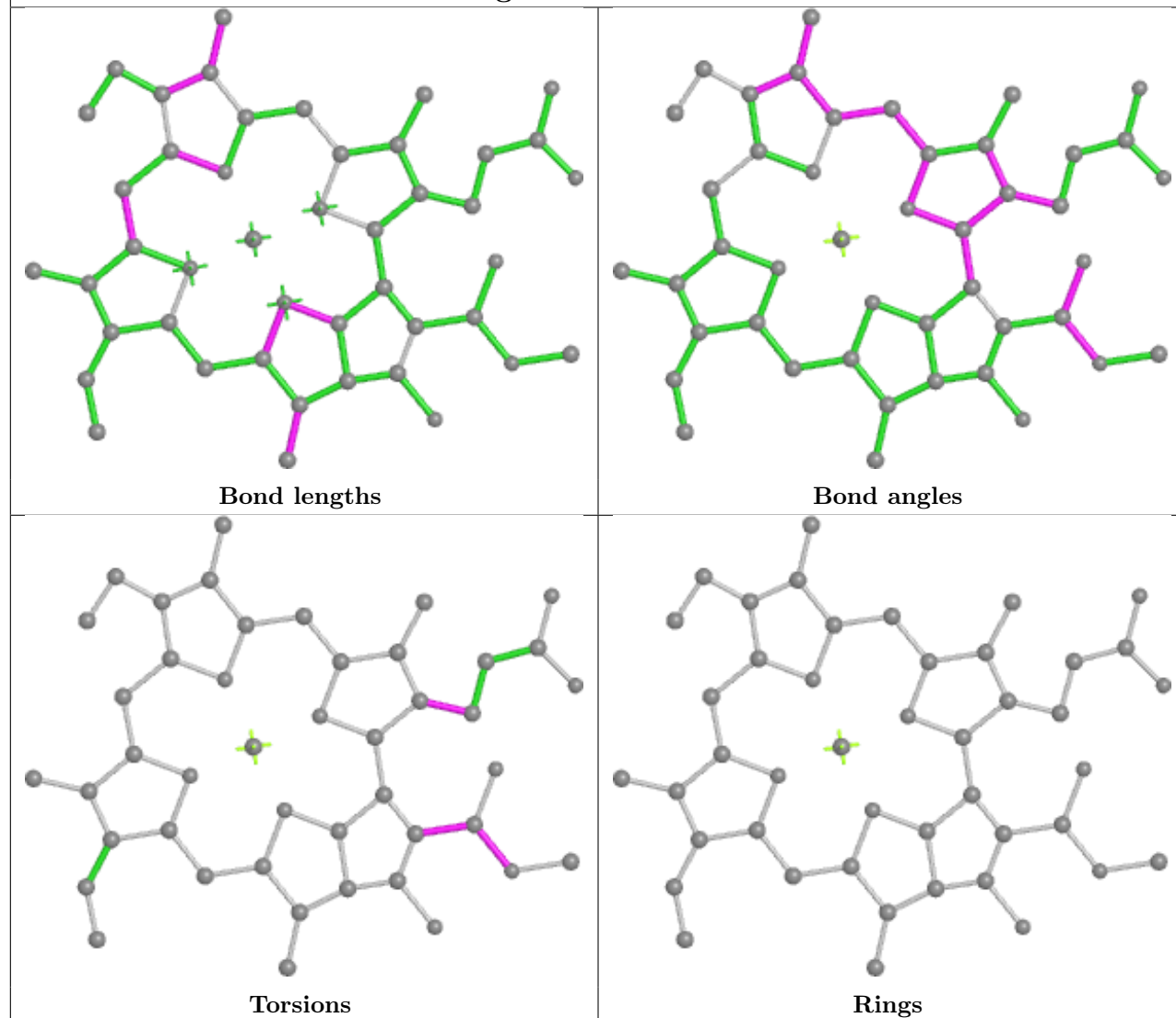
Ligand CLA c 511



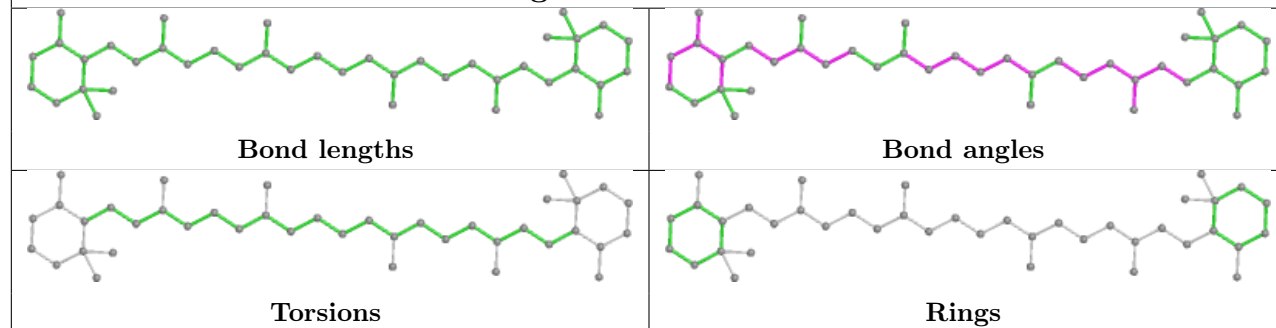
Ligand CLA r 602



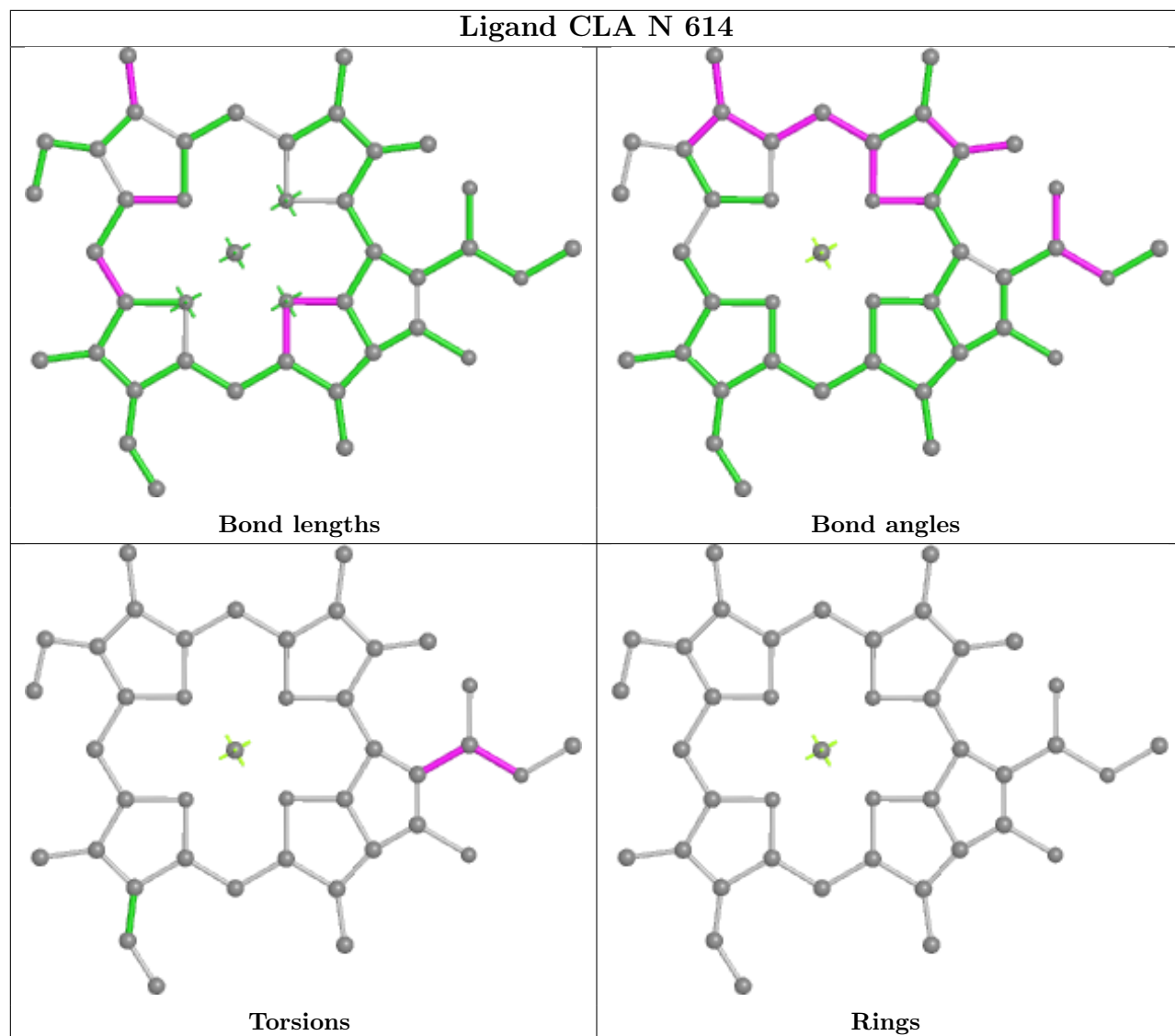
Ligand CLA s 603



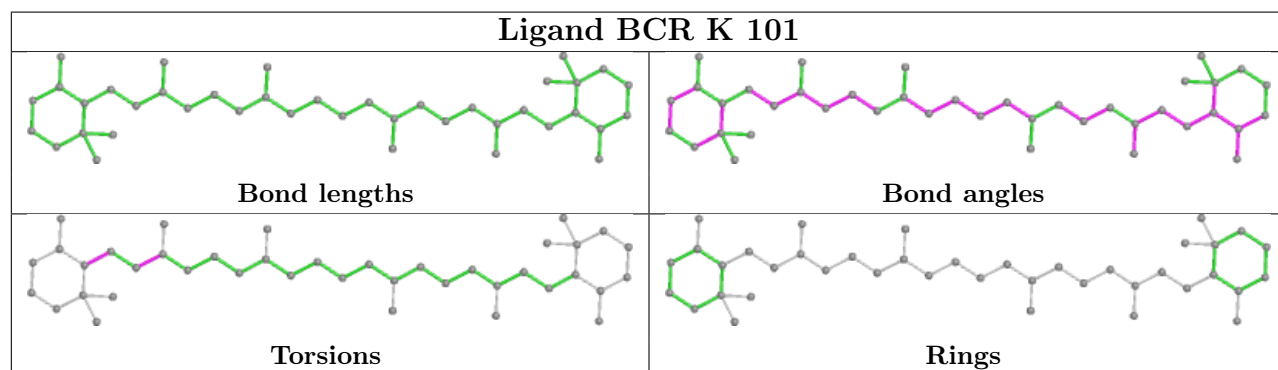
Ligand BCR C 516



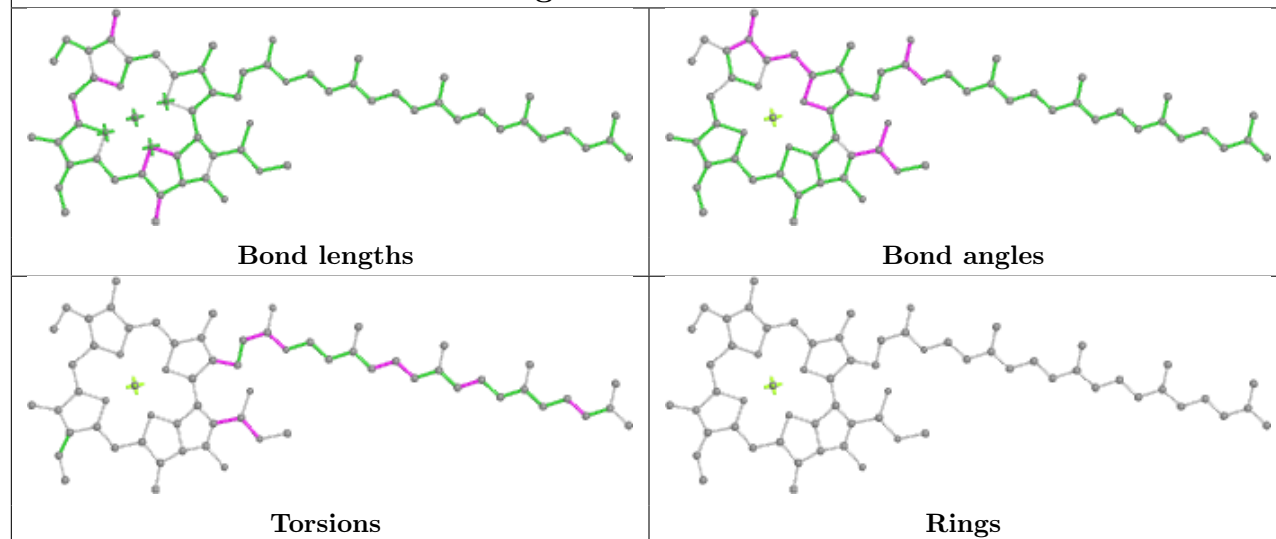
Ligand CLA N 614



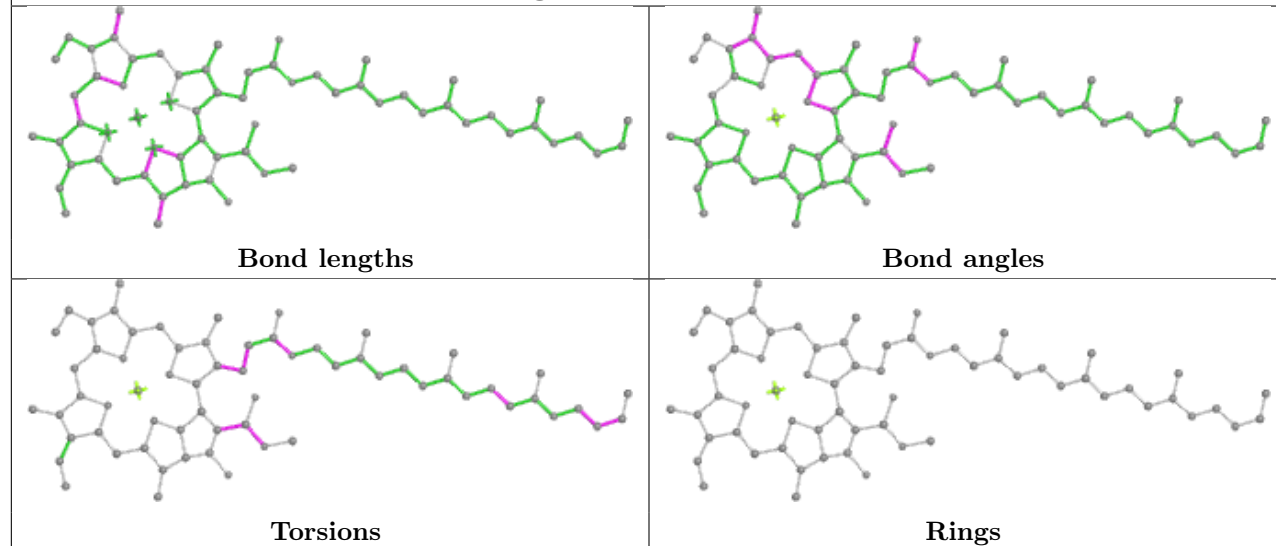
Ligand BCR K 101

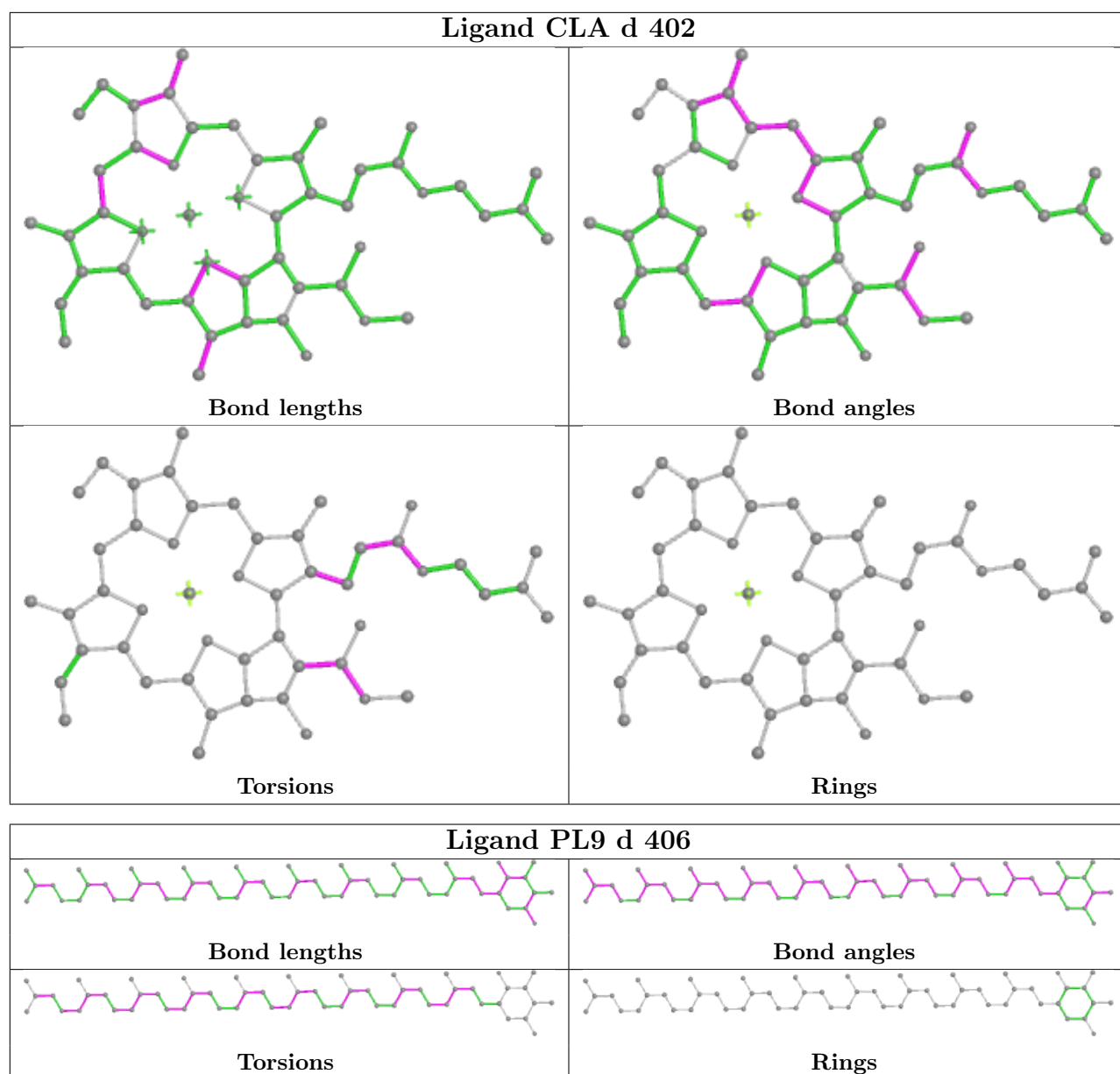


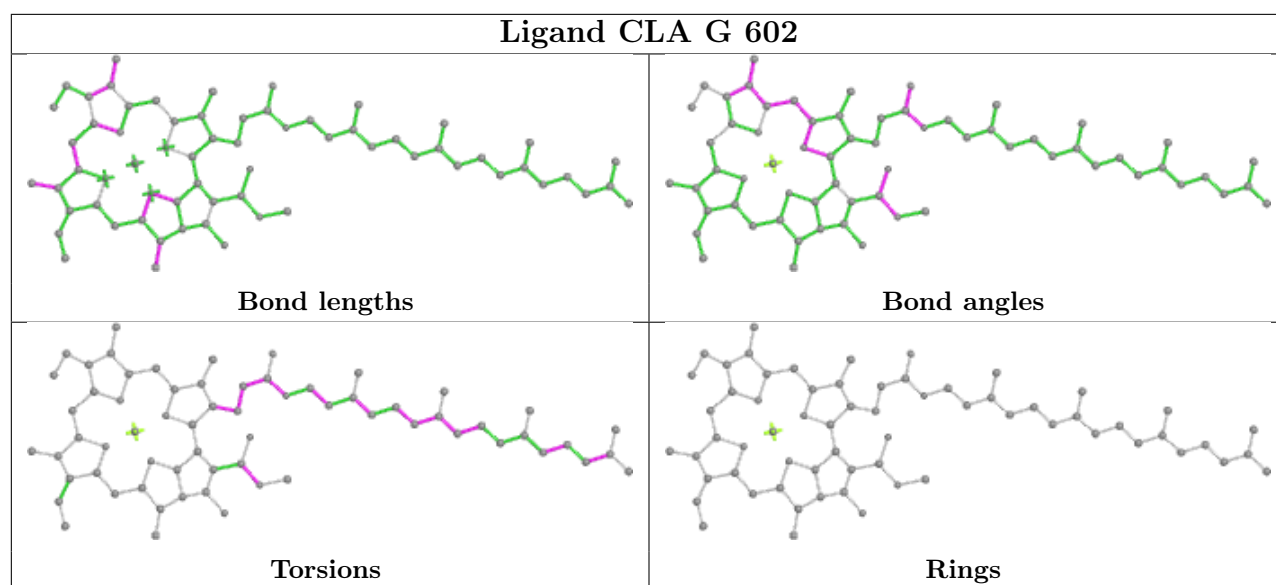
Ligand CLA d 404



Ligand CLA G 610







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

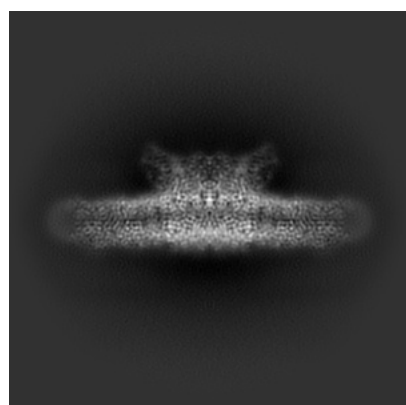
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63168. These allow visual inspection of the internal detail of the map and identification of artifacts.

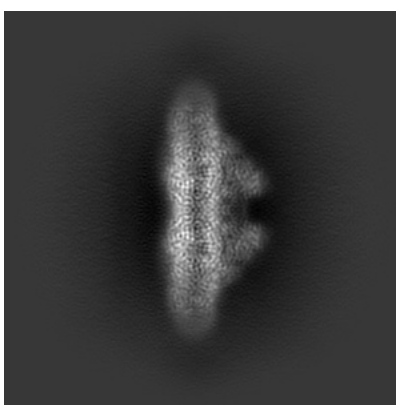
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

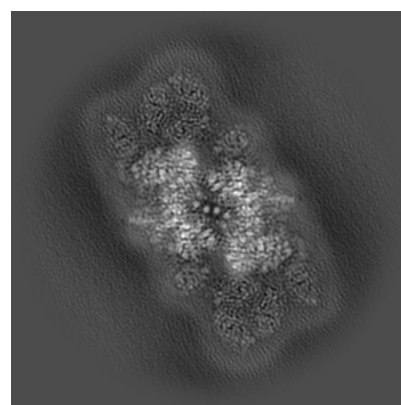
6.1.1 Primary map



X



Y

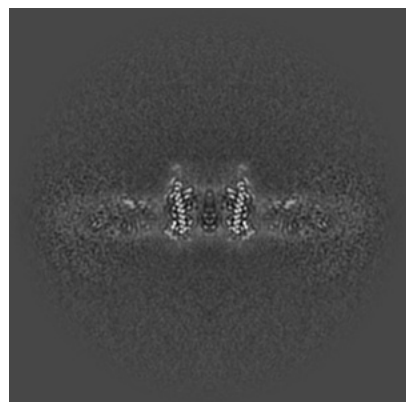


Z

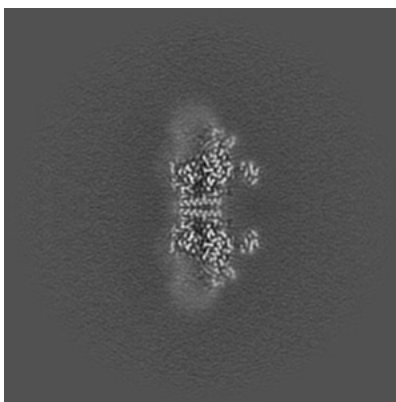
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

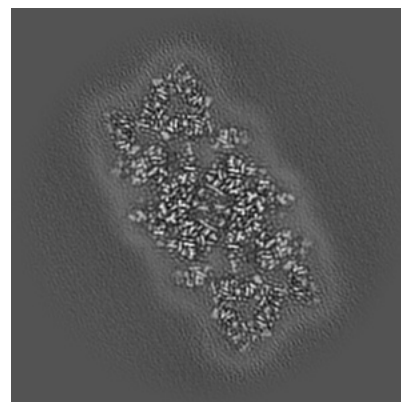
6.2.1 Primary map



X Index: 180



Y Index: 180

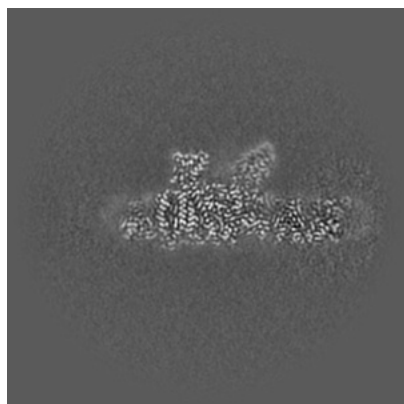


Z Index: 180

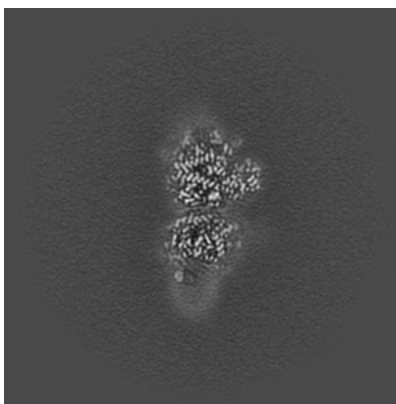
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

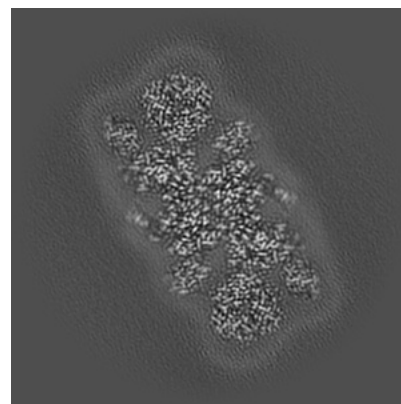
6.3.1 Primary map



X Index: 155



Y Index: 194

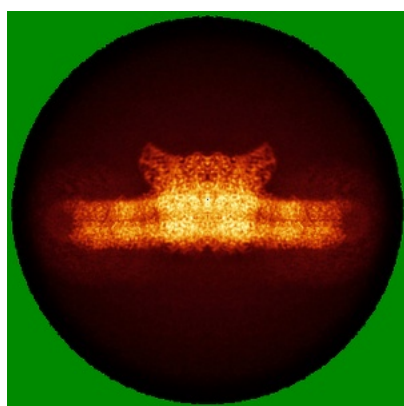


Z Index: 164

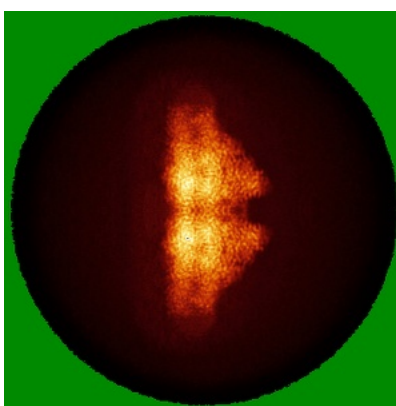
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

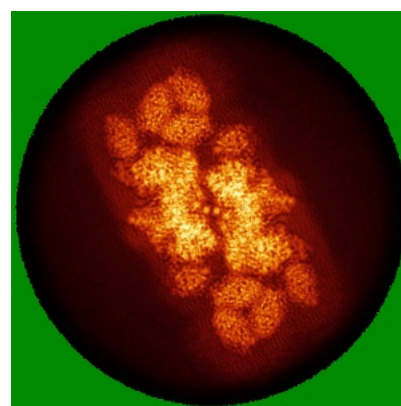
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

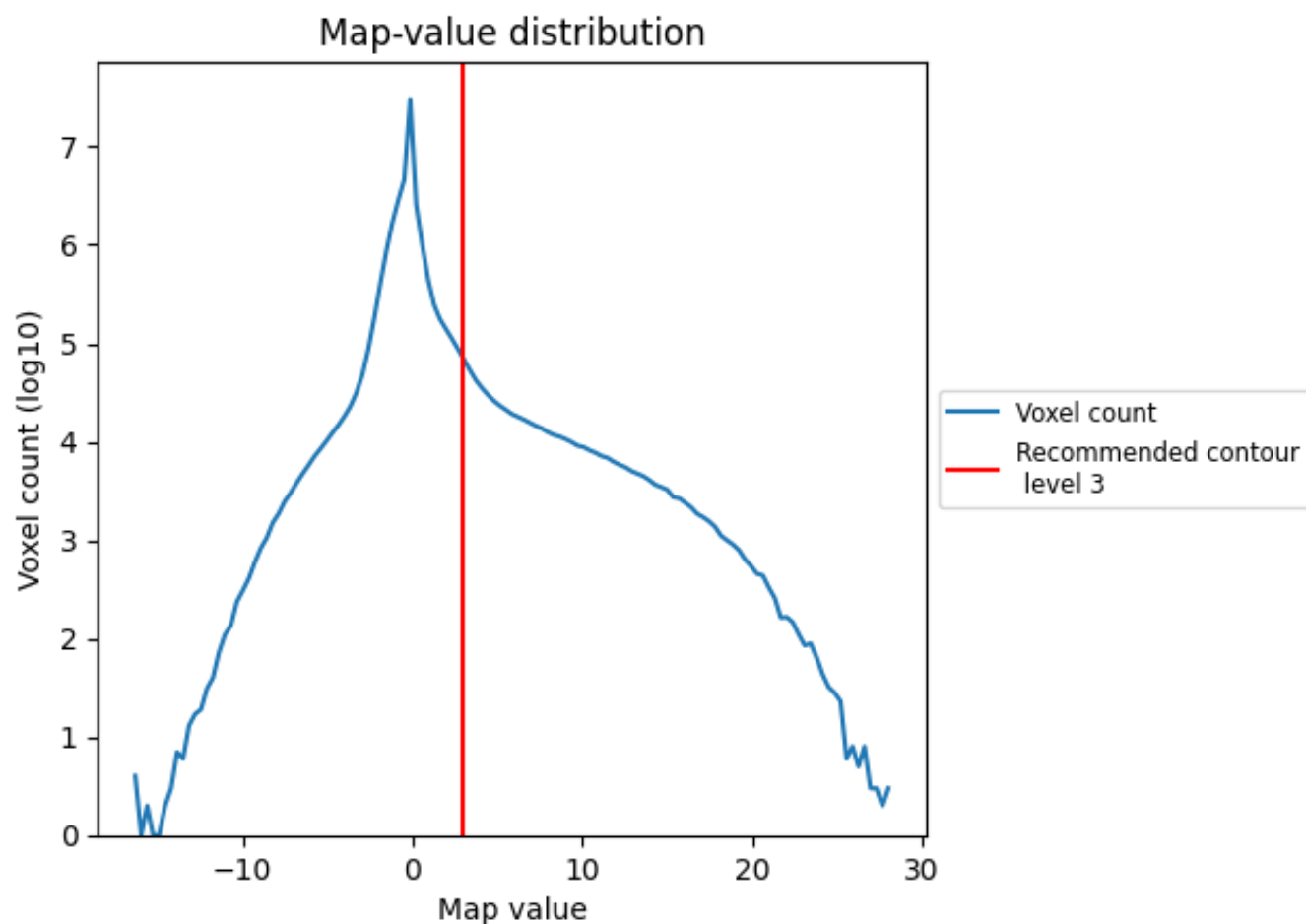
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

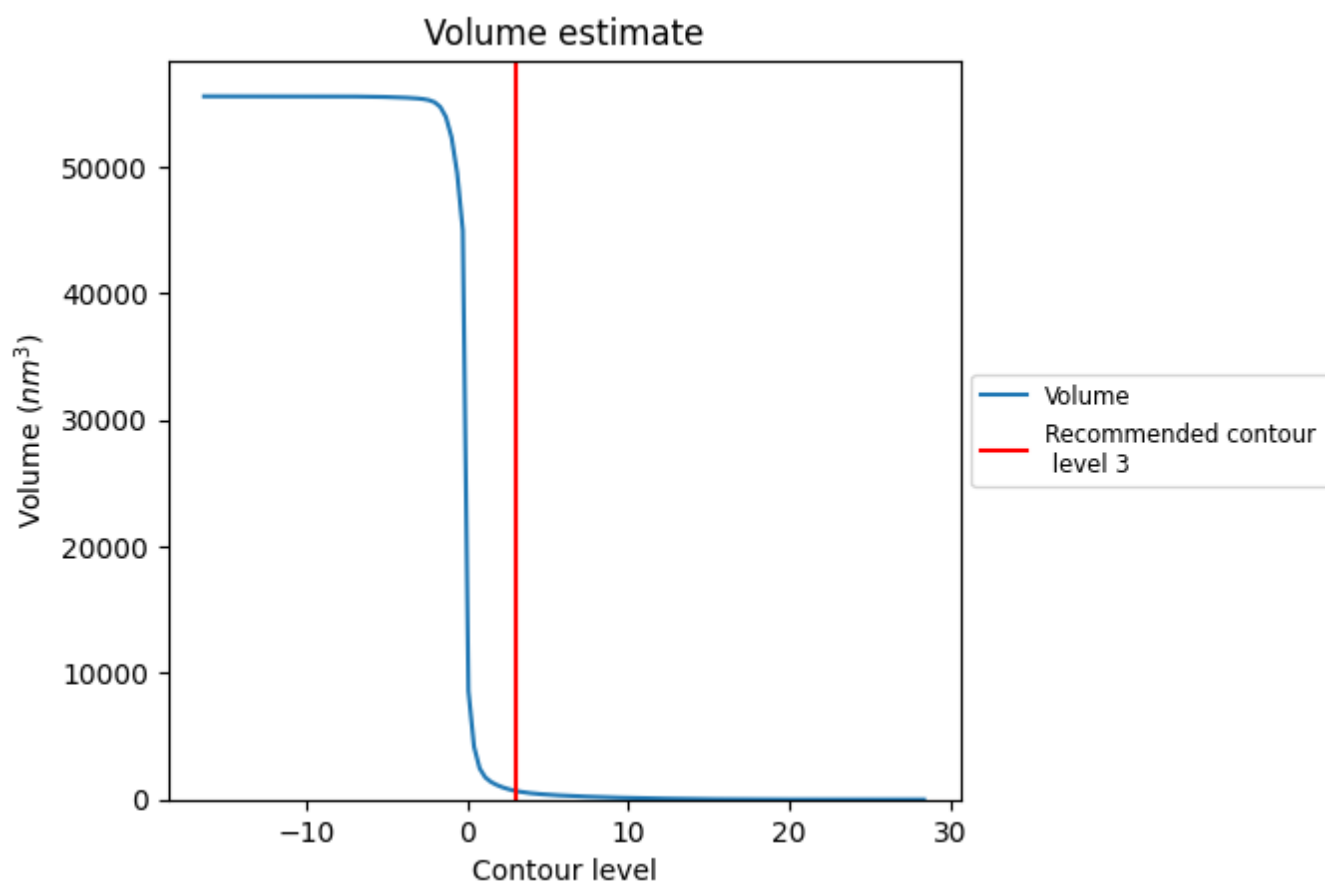
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

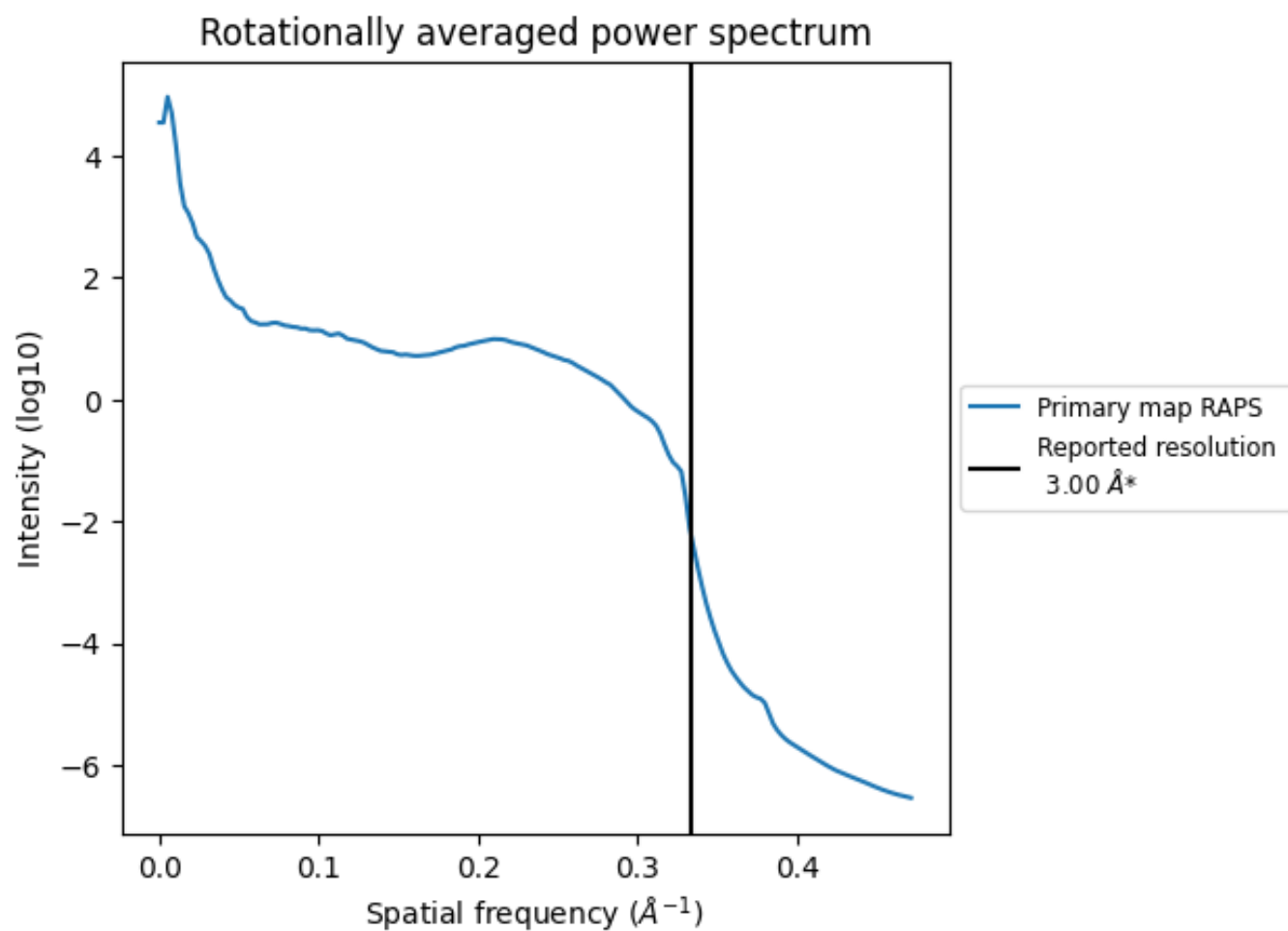
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 690 nm³; this corresponds to an approximate mass of 624 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

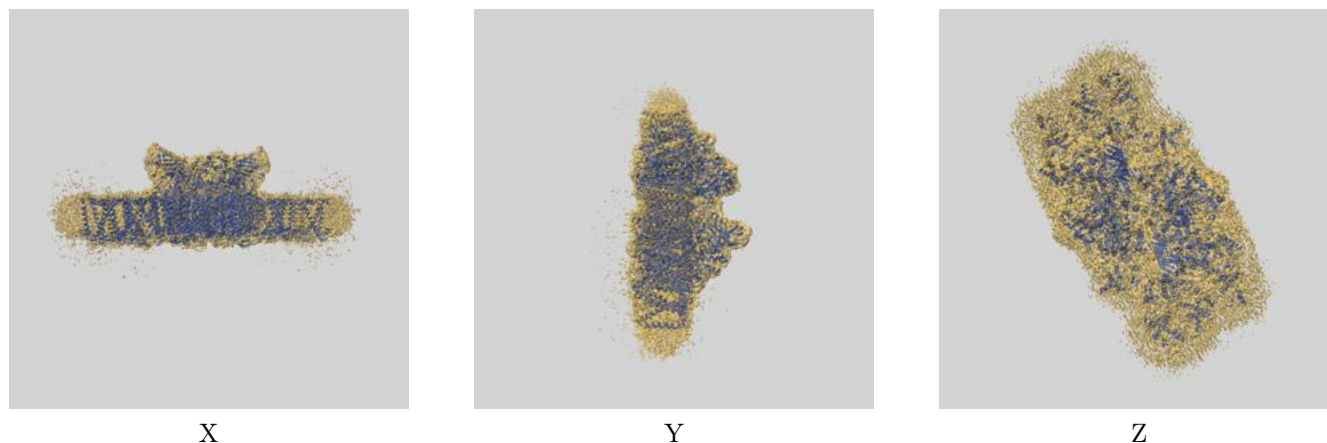
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

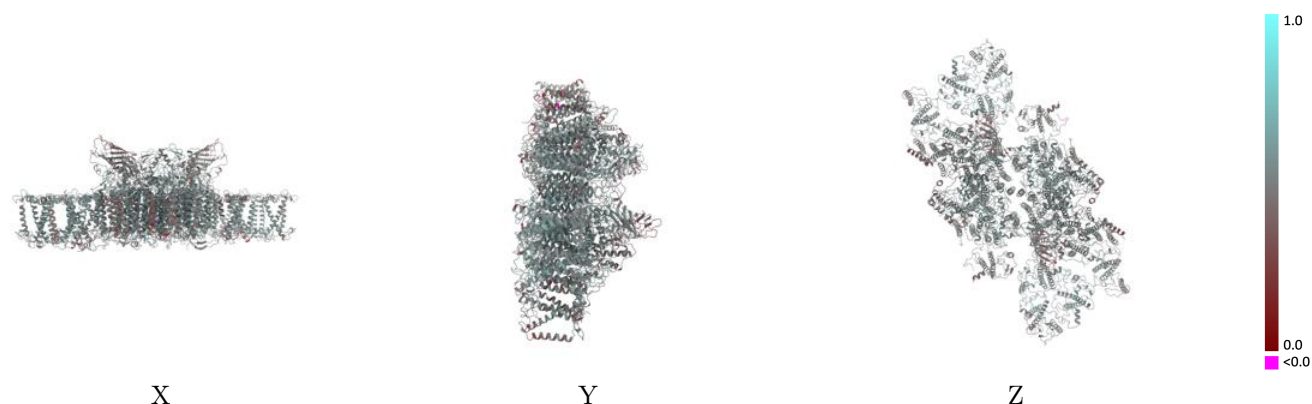
This section contains information regarding the fit between EMDB map EMD-63168 and PDB model 9LK5. Per-residue inclusion information can be found in section [3](#) on page [40](#).

9.1 Map-model overlay [i](#)



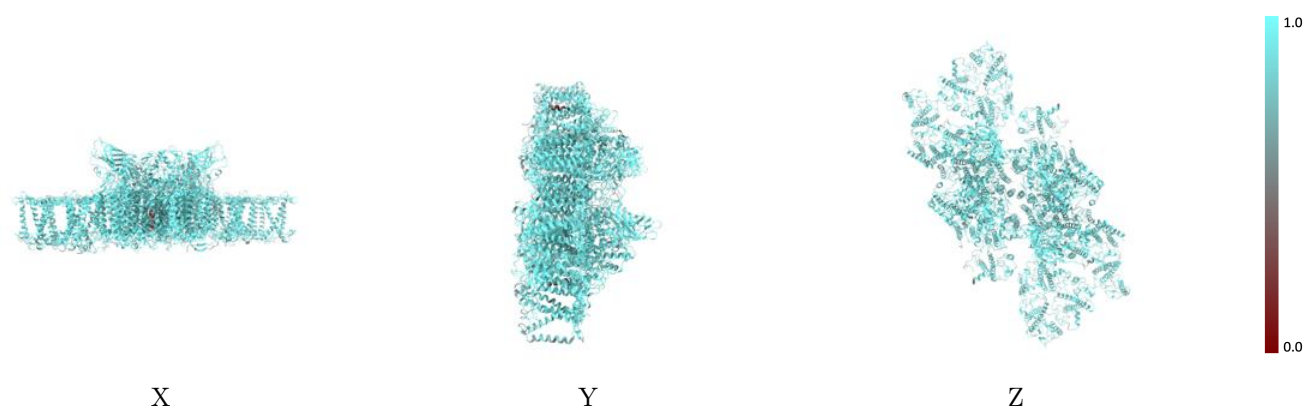
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



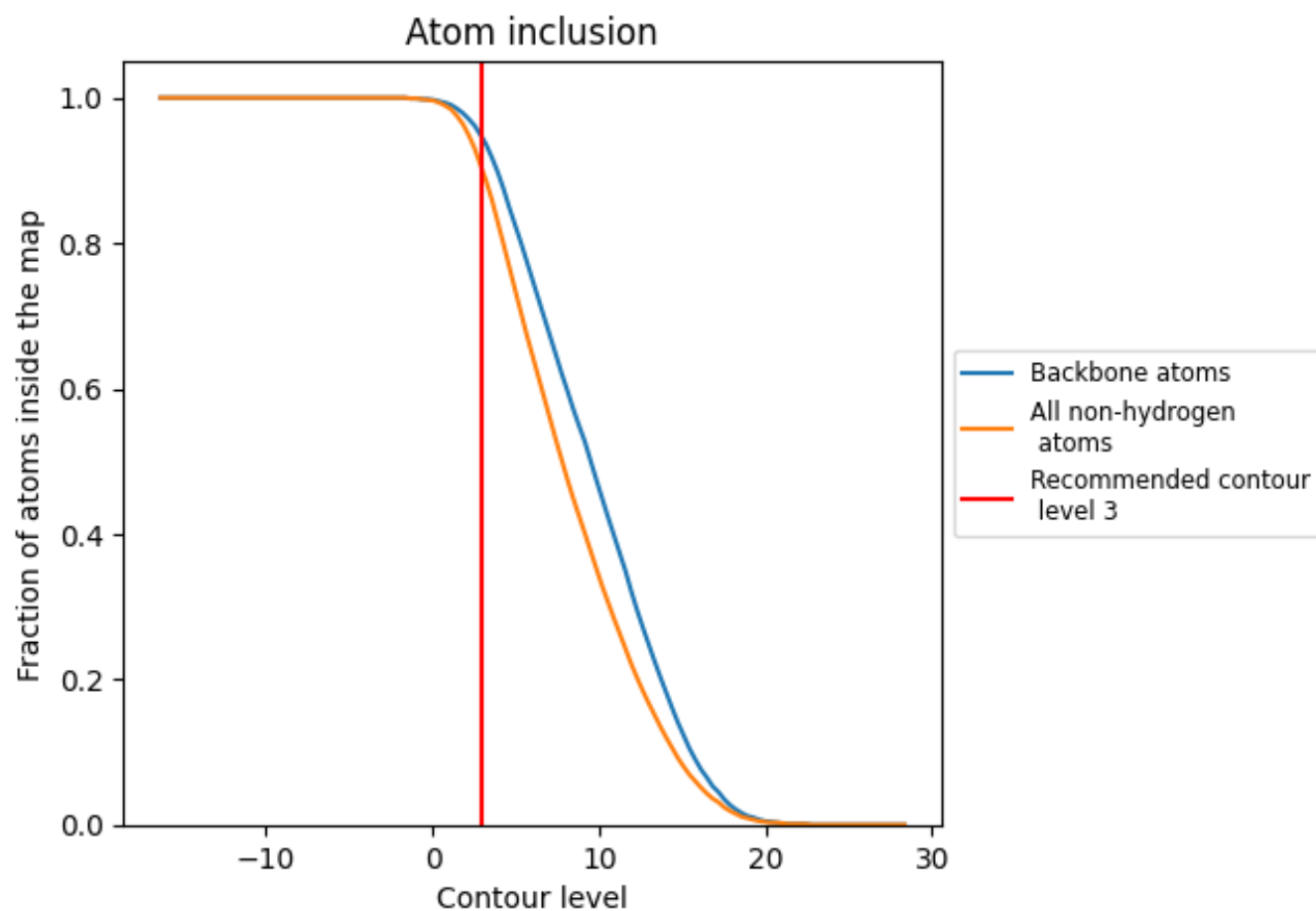
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

























The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5180
A	 0.9390	 0.5340
B	 0.9400	 0.5440
C	 0.9310	 0.5240
D	 0.9470	 0.5450
E	 0.9160	 0.4170
F	 0.9070	 0.4570
G	 0.8560	 0.5250
H	 0.9390	 0.5300
I	 0.9670	 0.5430
J	 0.6820	 0.3290
K	 0.8690	 0.4710
L	 0.8900	 0.5250
M	 0.8830	 0.4970
N	 0.8900	 0.5430
O	 0.8950	 0.4240
R	 0.8310	 0.4860
S	 0.8270	 0.4920
T	 0.9240	 0.5250
U	 0.7090	 0.4720
W	 0.8520	 0.5190
X	 0.8500	 0.4700
Y	 0.9070	 0.5580
Z	 0.8640	 0.4290
a	 0.9420	 0.5360
b	 0.9430	 0.5440
c	 0.9300	 0.5240
d	 0.9470	 0.5440
e	 0.9220	 0.4190
f	 0.9140	 0.4560
g	 0.8530	 0.5240
h	 0.9390	 0.5280
i	 0.9670	 0.5490
j	 0.6820	 0.3310
k	 0.8750	 0.4720



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Chain	Atom inclusion	Q-score
l	 0.8920	 0.5270
m	 0.8680	 0.4860
n	 0.8810	 0.5410
o	 0.8980	 0.4230
r	 0.8400	 0.4830
s	 0.8210	 0.4920
t	 0.9150	 0.5270
u	 0.7200	 0.4620
w	 0.8730	 0.5140
x	 0.8350	 0.4650
y	 0.9060	 0.5560
z	 0.8690	 0.4320