



Full wwPDB EM Validation Report ⓘ

Jun 11, 2025 – 04:40 PM JST

PDB ID : 9LK4 / pdb_00009lk4
EMDB ID : EMD-63167
Title : Cryo-EM structure of Lhcb4.1-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 : 3.10 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.dev118
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) : 2.43.1

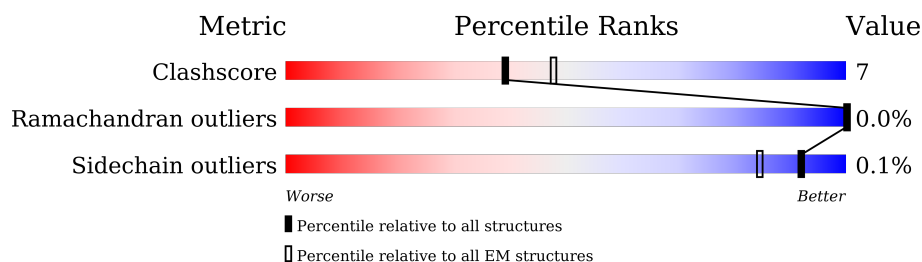
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



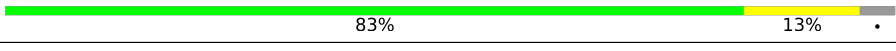

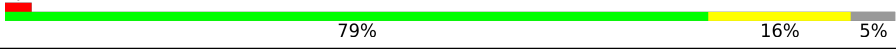



The reported resolution of this entry is 3.10 Å.

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.









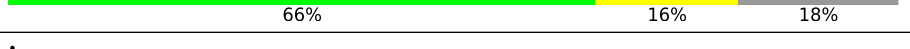
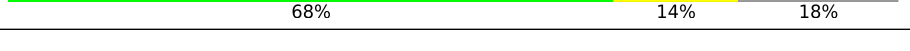
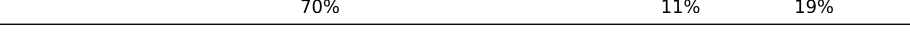
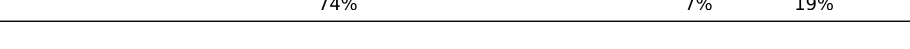
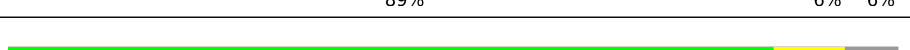

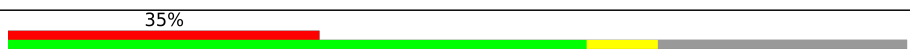
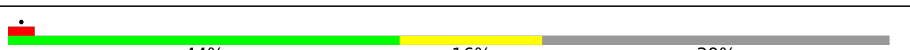
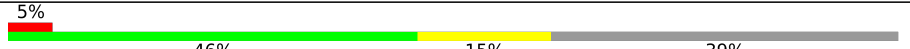
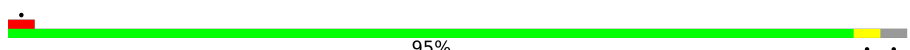





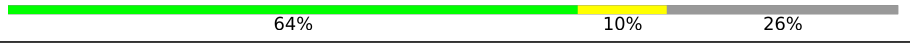



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	R	300	
15	r	300	
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	S	280	
22	s	280	

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	404	X	-	-	-
23	CLA	D	405	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	303	X	-	-	-
23	CLA	N	304	X	-	-	-
23	CLA	N	305	X	-	-	-
23	CLA	N	311	X	-	-	-
23	CLA	N	312	X	-	-	-
23	CLA	N	313	X	-	-	-
23	CLA	N	314	X	-	-	-
23	CLA	N	315	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	R	610	X	-	-	-
23	CLA	R	611	X	-	-	-
23	CLA	R	612	X	-	-	-
23	CLA	R	614	X	-	-	-
23	CLA	S	602	X	-	-	-
23	CLA	S	603	X	-	-	-
23	CLA	S	604	X	-	-	-
23	CLA	S	608	X	-	-	-
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	310	X	-	-	-
23	CLA	Y	311	X	-	-	-
23	CLA	Y	312	X	-	-	-
23	CLA	Y	313	X	-	-	-
23	CLA	Y	314	X	-	-	-
23	CLA	a	401	X	-	-	-
23	CLA	a	402	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	405	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	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	d	404	X	-	-	-
23	CLA	d	405	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	303	X	-	-	-
23	CLA	n	304	X	-	-	-
23	CLA	n	305	X	-	-	-
23	CLA	n	311	X	-	-	-
23	CLA	n	312	X	-	-	-
23	CLA	n	313	X	-	-	-
23	CLA	n	314	X	-	-	-
23	CLA	n	315	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	r	614	X	-	-	-
23	CLA	s	602	X	-	-	-
23	CLA	s	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	s	604	X	-	-	-
23	CLA	s	608	X	-	-	-
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	310	X	-	-	-
23	CLA	y	311	X	-	-	-
23	CLA	y	312	X	-	-	-
23	CLA	y	313	X	-	-	-
23	CLA	y	314	X	-	-	-
31	BCT	D	403	-	-	X	-
31	BCT	d	403	-	-	X	-
34	CHL	G	601	X	-	-	-
34	CHL	G	605	X	-	-	-
34	CHL	G	606	X	-	-	-
34	CHL	G	607	X	-	-	-
34	CHL	G	608	X	-	-	-
34	CHL	G	609	X	-	-	-
34	CHL	G	619	X	-	-	-
34	CHL	N	302	X	-	-	-
34	CHL	N	306	X	-	-	-
34	CHL	N	307	X	-	-	-
34	CHL	N	308	X	-	-	-
34	CHL	N	309	X	-	-	-
34	CHL	N	310	X	-	-	-
34	CHL	R	605	X	-	-	-
34	CHL	R	606	X	-	-	-
34	CHL	R	607	X	-	-	-
34	CHL	R	613	X	-	-	-
34	CHL	S	601	X	-	-	-
34	CHL	S	605	X	-	-	-
34	CHL	S	606	X	-	-	-
34	CHL	S	607	X	-	-	-
34	CHL	Y	302	X	-	-	-
34	CHL	Y	306	X	-	-	-
34	CHL	Y	307	X	-	-	-
34	CHL	Y	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	CHL	Y	309	X	-	-	-
34	CHL	g	601	X	-	-	-
34	CHL	g	605	X	-	-	-
34	CHL	g	606	X	-	-	-
34	CHL	g	607	X	-	-	-
34	CHL	g	608	X	-	-	-
34	CHL	g	609	X	-	-	-
34	CHL	g	619	X	-	-	-
34	CHL	n	302	X	-	-	-
34	CHL	n	306	X	-	-	-
34	CHL	n	307	X	-	-	-
34	CHL	n	308	X	-	-	-
34	CHL	n	309	X	-	-	-
34	CHL	n	310	X	-	-	-
34	CHL	r	605	X	-	-	-
34	CHL	r	606	X	-	-	-
34	CHL	r	607	X	-	-	-
34	CHL	r	613	X	-	-	-
34	CHL	s	601	X	-	-	-
34	CHL	s	605	X	-	-	-
34	CHL	s	606	X	-	-	-
34	CHL	s	607	X	-	-	-
34	CHL	y	302	X	-	-	-
34	CHL	y	306	X	-	-	-
34	CHL	y	307	X	-	-	-
34	CHL	y	308	X	-	-	-
34	CHL	y	309	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 70366 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	332	Total	C	N	O	S	0	0
			2599	1696	428	462	13		
1	a	332	Total	C	N	O	S	0	0
			2599	1696	428	462	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	66	Total	C	N	O	0	0
			540	354	88	98		
5	e	66	Total	C	N	O	0	0
			540	354	88	98		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			224	150	37	36	1		
6	f	29	Total	C	N	O	S	0	0
			224	150	37	36	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 CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	222	Total	C	N	O	S	0	0
			1724	1118	283	320	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	222	Total	C	N	O	S	0	0
			1724	1118	283	320	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	291	GLY	-	expression tag	UNP Q07473
R	292	GLY	-	expression tag	UNP Q07473
R	293	GLY	-	expression tag	UNP Q07473
R	294	GLY	-	expression tag	UNP Q07473
R	295	HIS	-	expression tag	UNP Q07473
R	296	HIS	-	expression tag	UNP Q07473
R	297	HIS	-	expression tag	UNP Q07473
R	298	HIS	-	expression tag	UNP Q07473
R	299	HIS	-	expression tag	UNP Q07473
R	300	HIS	-	expression tag	UNP Q07473
r	291	GLY	-	expression tag	UNP Q07473
r	292	GLY	-	expression tag	UNP Q07473
r	293	GLY	-	expression tag	UNP Q07473
r	294	GLY	-	expression tag	UNP Q07473
r	295	HIS	-	expression tag	UNP Q07473
r	296	HIS	-	expression tag	UNP Q07473
r	297	HIS	-	expression tag	UNP Q07473
r	298	HIS	-	expression tag	UNP Q07473
r	299	HIS	-	expression tag	UNP Q07473
r	300	HIS	-	expression tag	UNP Q07473

- 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		

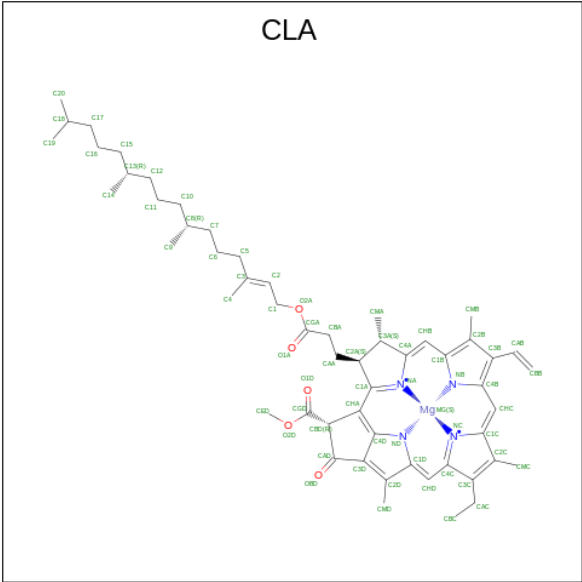
- Molecule 21 is a protein called Photosystem II reaction center protein Z.

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 CP26, chloroplastic.

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

- 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	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

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Mol	Chain	Residues	Atoms					AltConf
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	R	1	Total 45	C 35	Mg 1	N 4	O 5	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 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 50	C 40	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

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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	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
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

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

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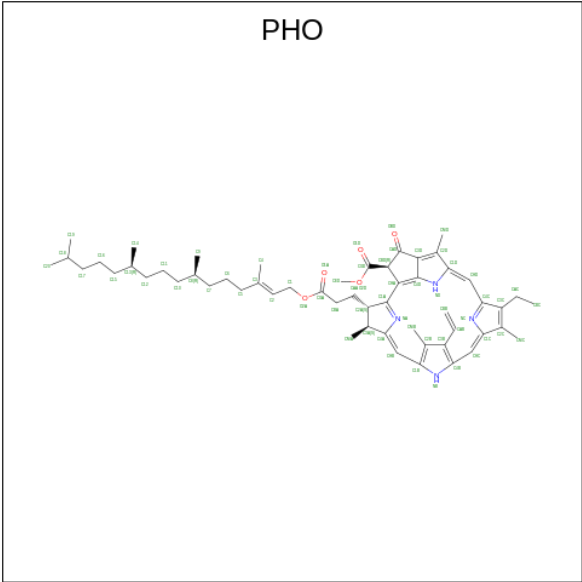
Mol	Chain	Residues	Atoms					AltConf
23	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	r	1	Total 45	C 35	Mg 1	N 4	O 5	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	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

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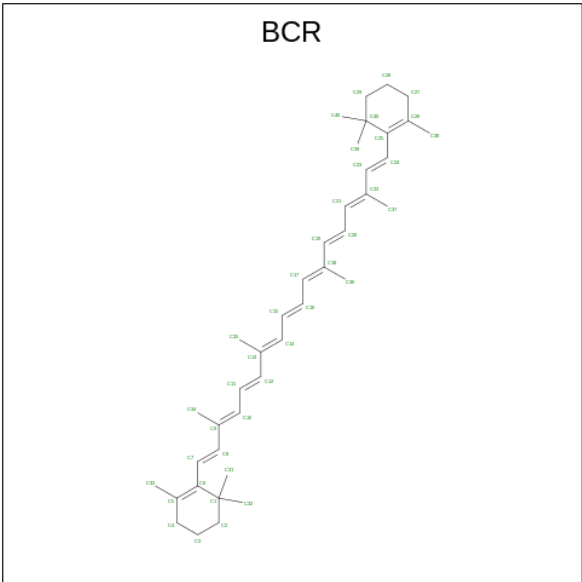
Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	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
			45	35	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	

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



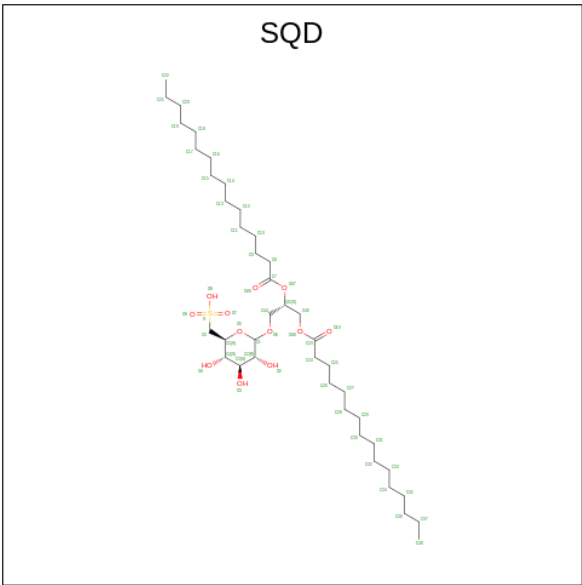
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

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



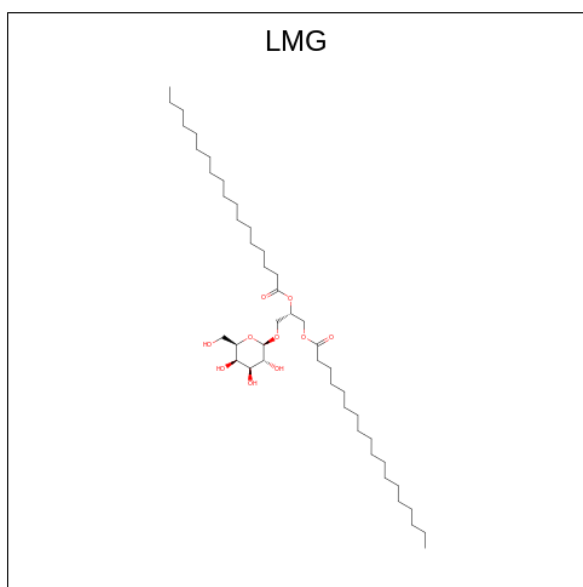
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



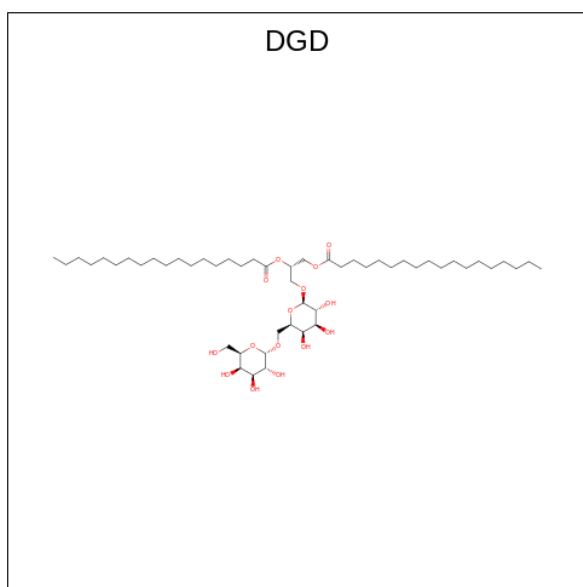
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	M	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			54	41	12	1	
26	d	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			40	30	10	
27	B	1	Total	C	O	0
			51	41	10	
27	B	1	Total	C	O	0
			40	30	10	
27	C	1	Total	C	O	0
			48	38	10	
27	D	1	Total	C	O	0
			46	36	10	
27	a	1	Total	C	O	0
			48	38	10	
27	b	1	Total	C	O	0
			51	41	10	
27	d	1	Total	C	O	0
			46	36	10	

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

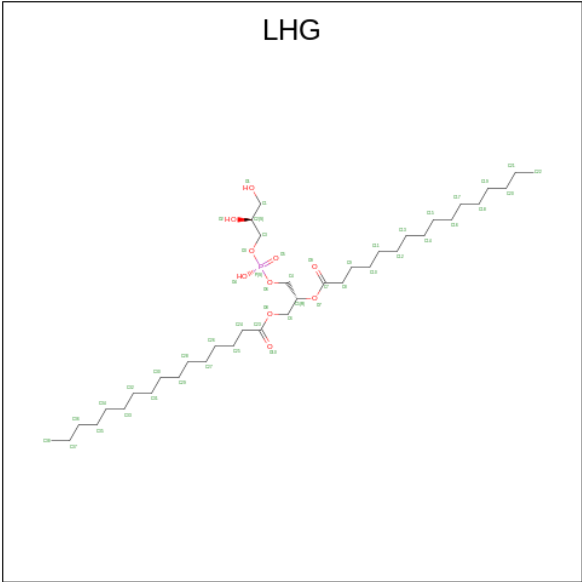


Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			59	44	15	
28	C	1	Total	C	O	0
			55	40	15	
28	H	1	Total	C	O	0
			62	47	15	
28	a	1	Total	C	O	0
			59	44	15	
28	c	1	Total	C	O	0
			55	40	15	
28	d	1	Total	C	O	0
			62	47	15	

- 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-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



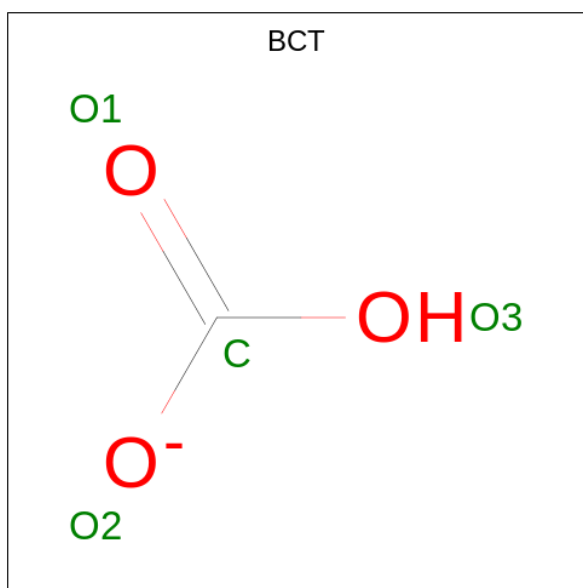
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			46	35	10	1	
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	G	1	Total	C	O	P	0
			46	35	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	T	1	Total	C	O	P	0
			49	38	10	1	
30	W	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			46	35	10	1	

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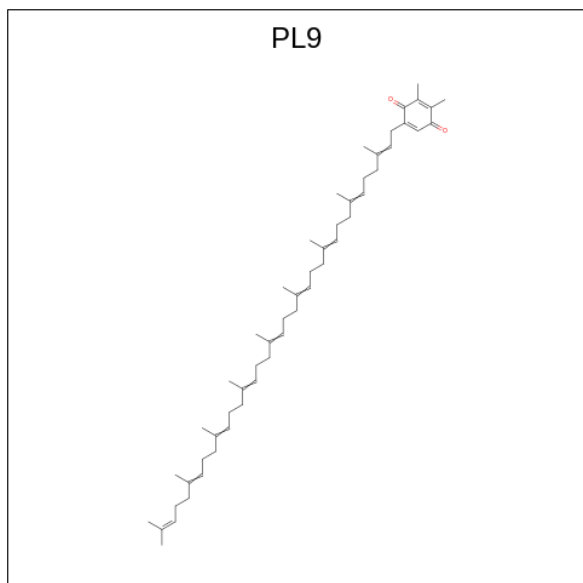
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	g	1	Total	C	O	P	0
			46	35	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	w	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



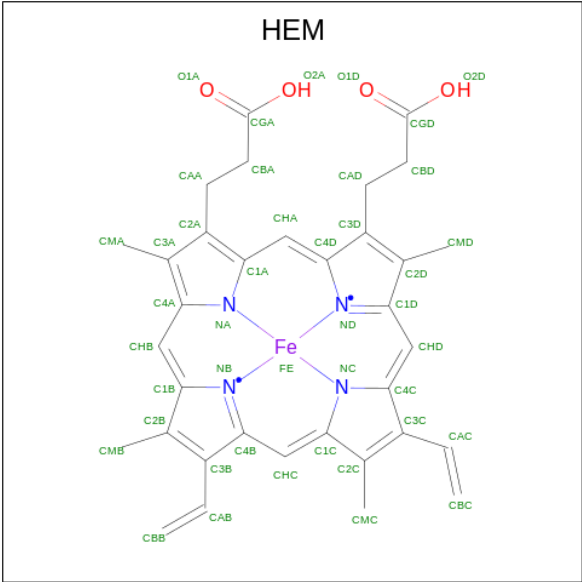
Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	0
			4	1	3	
31	d	1	Total	C	O	0
			4	1	3	

- Molecule 32 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: $C_{53}H_{80}O_2$).



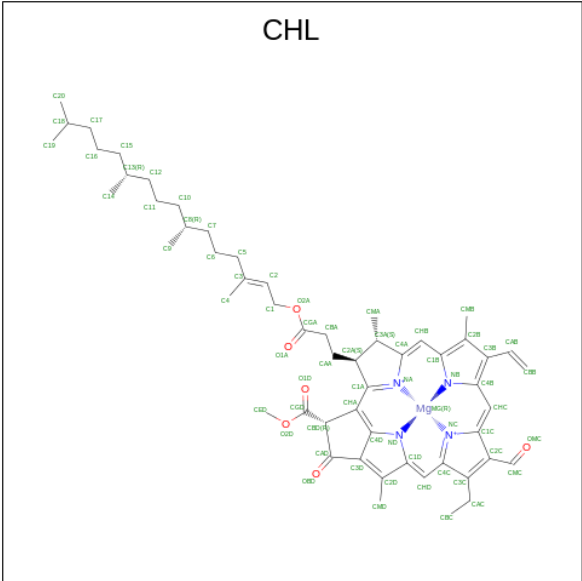
Mol	Chain	Residues	Atoms			AltConf
32	D	1	Total	C	O	0
			55	53	2	
32	d	1	Total	C	O	0
			55	53	2	

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
33	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 34 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
34	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
34	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
34	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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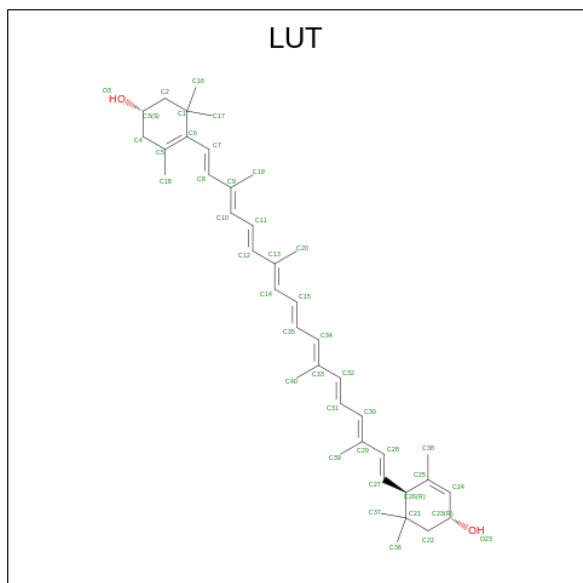
Mol	Chain	Residues	Atoms					AltConf
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
34	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	r	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	r	1	Total 42	C 33	Mg 1	N 4	O 4	0
34	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	y	1	Total 51	C 40	Mg 1	N 4	O 6	0
34	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
34	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



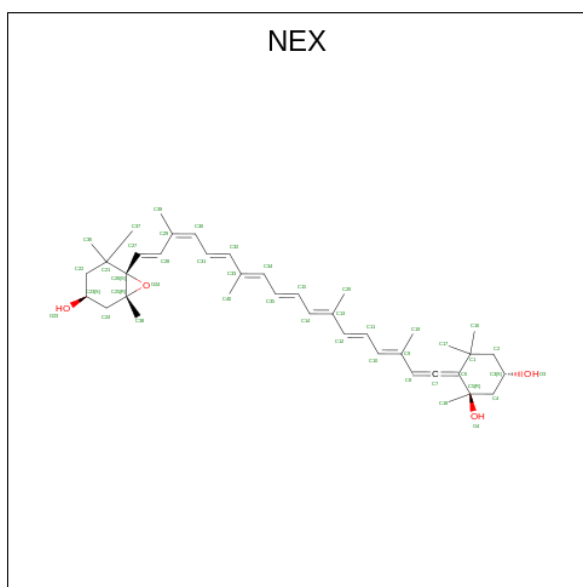
Mol	Chain	Residues	Atoms				AltConf
35	G	1	Total	C	O		0
			42	40	2		

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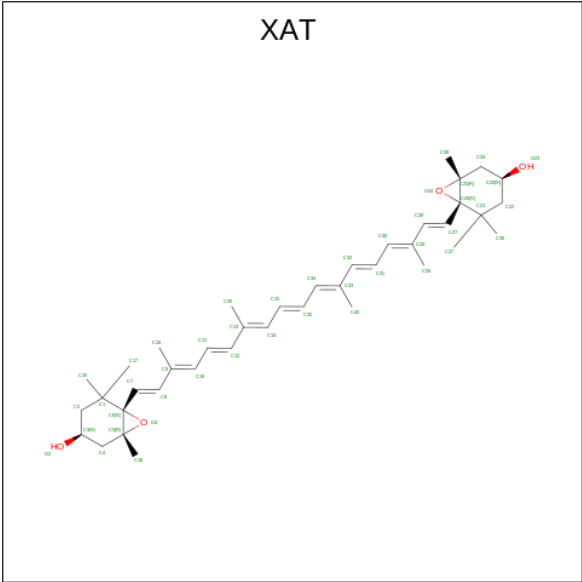
Mol	Chain	Residues	Atoms			AltConf
35	G	1	Total	C	O	0
			42	40	2	
35	N	1	Total	C	O	0
			42	40	2	
35	N	1	Total	C	O	0
			42	40	2	
35	R	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	g	1	Total	C	O	0
			42	40	2	
35	g	1	Total	C	O	0
			42	40	2	
35	n	1	Total	C	O	0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

- Molecule 36 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
36	G	1	Total	C	O	0
			44	40	4	
36	N	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	g	1	Total	C	O	0
			44	40	4	
36	n	1	Total	C	O	0
			44	40	4	
36	r	1	Total	C	O	0
			44	40	4	
36	y	1	Total	C	O	0
			44	40	4	
36	S	1	Total	C	O	0
			44	40	4	
36	s	1	Total	C	O	0
			44	40	4	

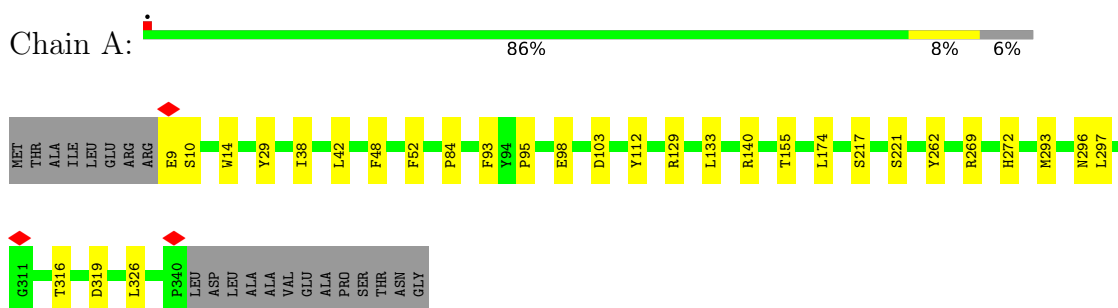
- Molecule 37 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



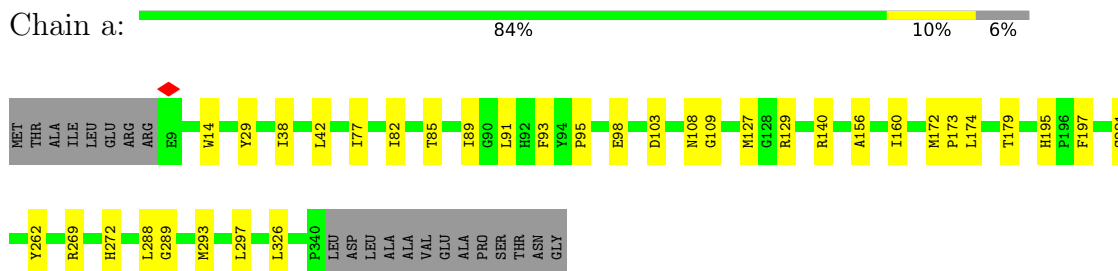
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

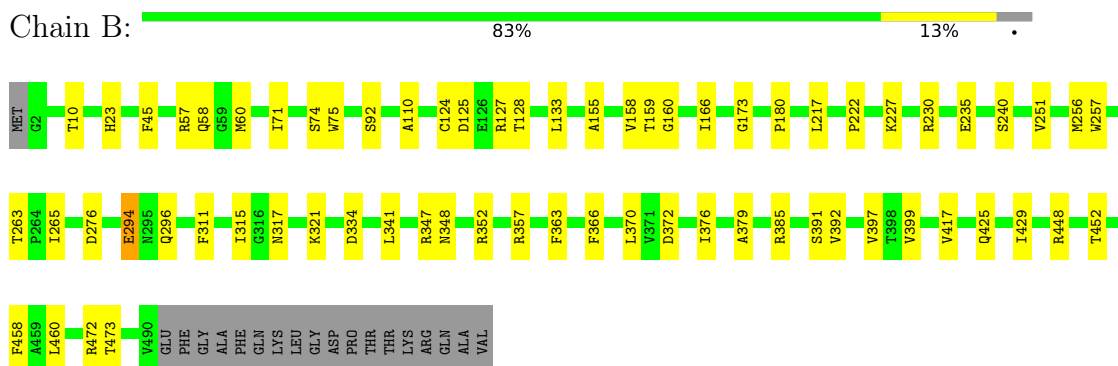
- Molecule 1: Photosystem II protein D1




- Molecule 1: Photosystem II protein D1

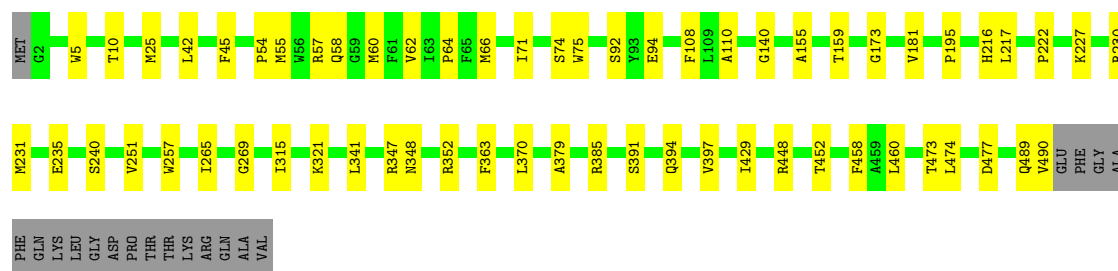


- Molecule 2: Photosystem II CP47 reaction center protein




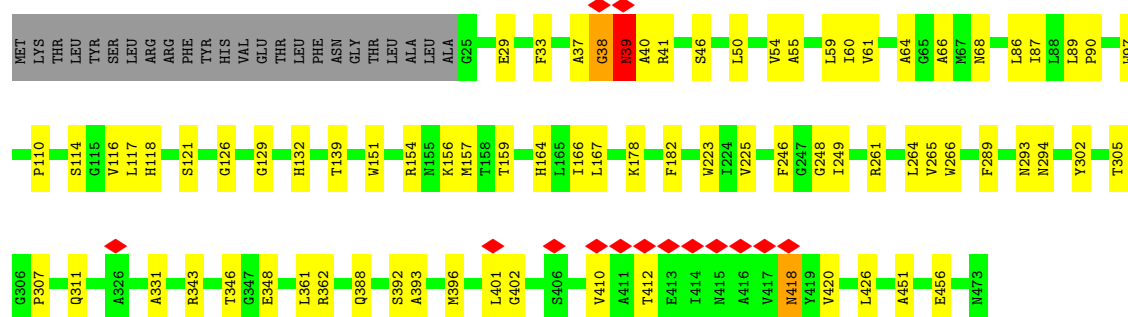
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  84% 12%




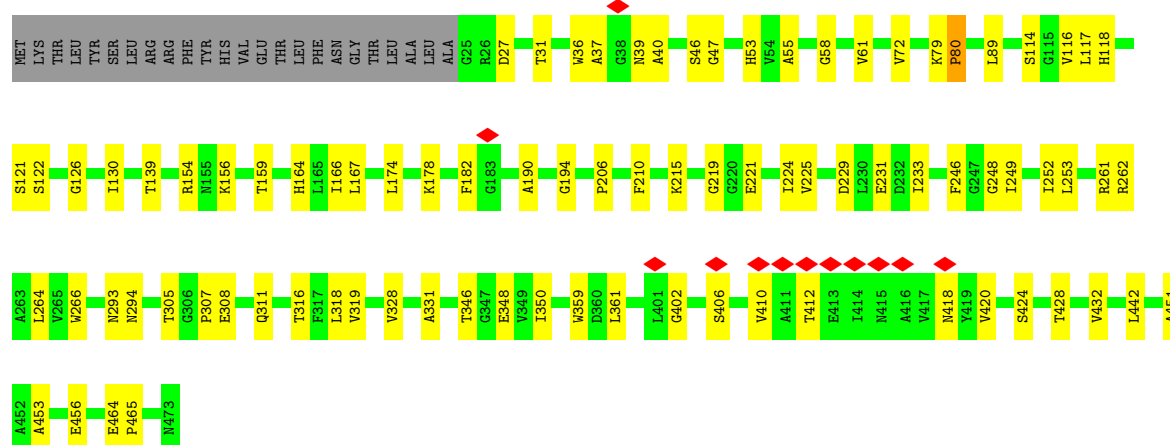
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  79% 16% 5%




• Molecule 3: Photosystem II CP43 reaction center protein

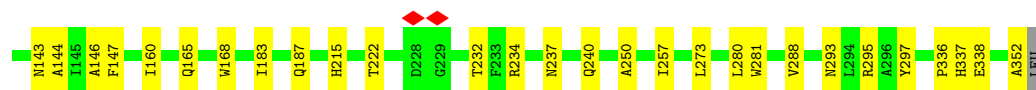
Chain c:  77% 18% 5%



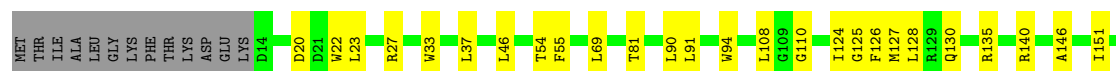
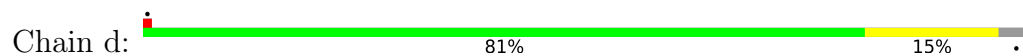
• Molecule 4: Photosystem II D2 protein

Chain D:  81% 15%

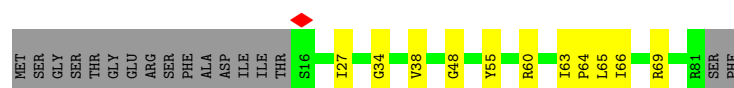




• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



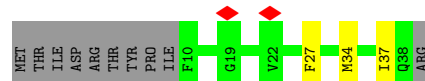
• Molecule 5: Cytochrome b559 subunit alpha



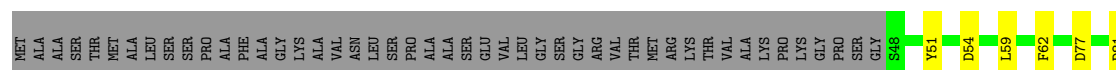
• Molecule 6: Cytochrome b559 subunit beta

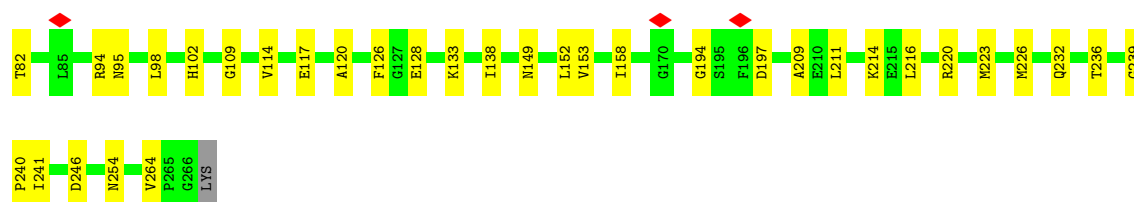


• Molecule 6: Cytochrome b559 subunit beta



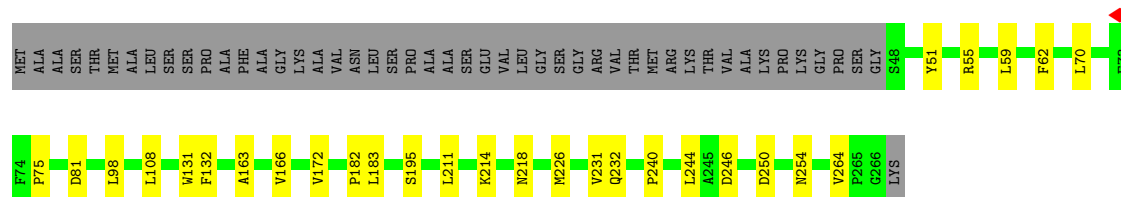
• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic





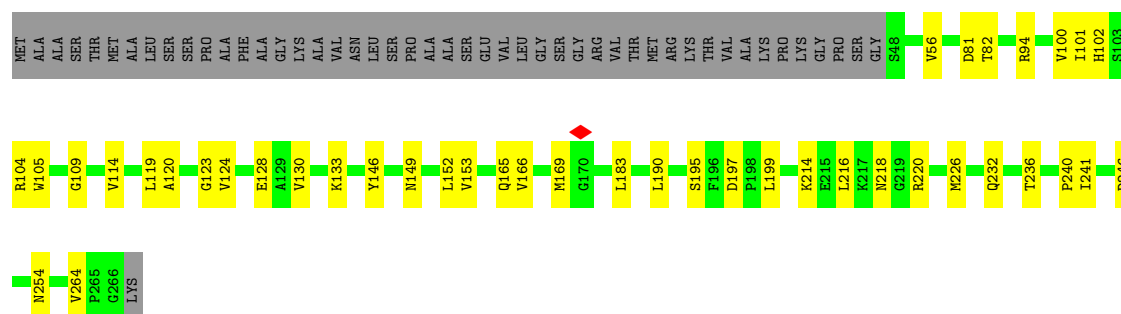
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain N: 71% 11% 18%



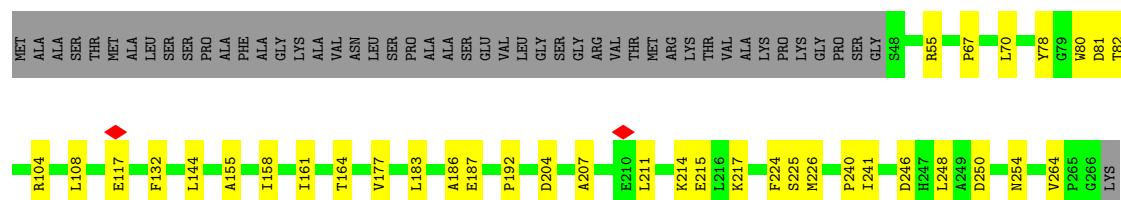
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain g: 66% 16% 18%



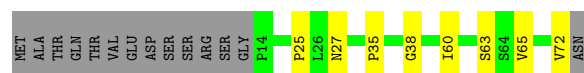
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain n: 68% 14% 18%



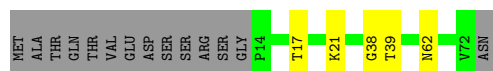
- Molecule 8: Photosystem II reaction center protein H

Chain H: 70% 11% 19%




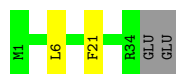
- Molecule 8: Photosystem II reaction center protein H

Chain h:  74% 7% 19%




• Molecule 9: Photosystem II reaction center protein I

Chain I:  89% 6% 6%




• Molecule 9: Photosystem II reaction center protein I

Chain i:  86% 8% 6%



• Molecule 10: Photosystem II reaction center protein J

Chain J:  40% 68% 5% 28%



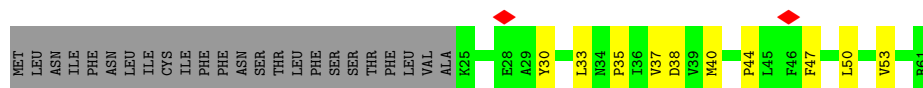
• Molecule 10: Photosystem II reaction center protein J

Chain j:  35% 65% 8% 28%



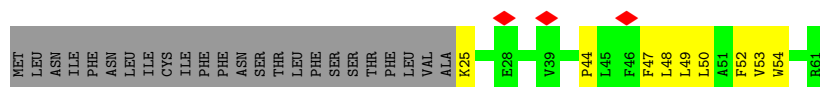
• Molecule 11: Photosystem II reaction center protein K

Chain K:  44% 16% 39%



• Molecule 11: Photosystem II reaction center protein K

Chain k:  5% 46% 15% 39%




- Molecule 12: Photosystem II reaction center protein L

Chain L:  95%




- Molecule 12: Photosystem II reaction center protein L

Chain l:  84% 13%




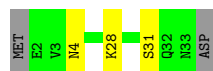
- Molecule 13: Photosystem II reaction center protein M

Chain M:  82% 12% 6%



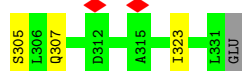
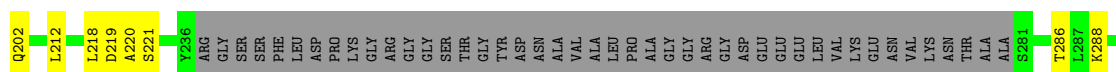
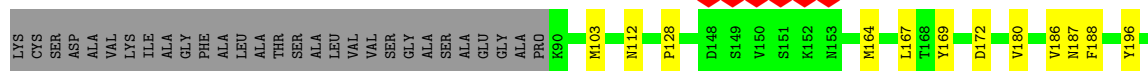
- Molecule 13: Photosystem II reaction center protein M

Chain m:  85% 9% 6%



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

Chain O:  53% 7% 40%

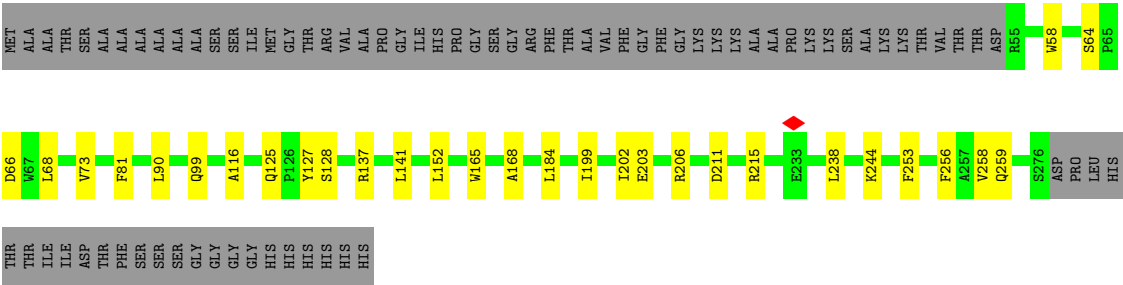


- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

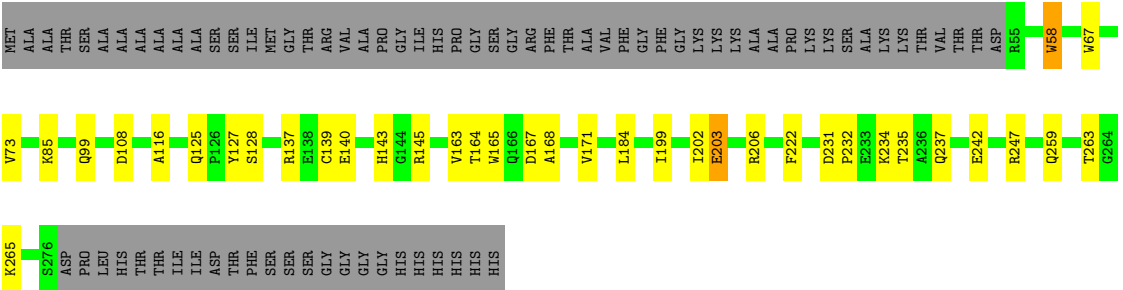
Chain o:  53% 7% 40%



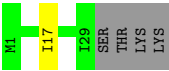
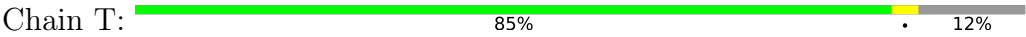
● Molecule 15: Chlorophyll a-b binding protein CP29.1, chloroplastic



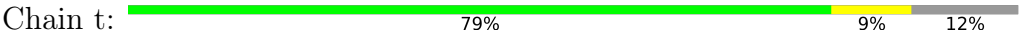
● Molecule 15: Chlorophyll a-b binding protein CP29.1, chloroplastic

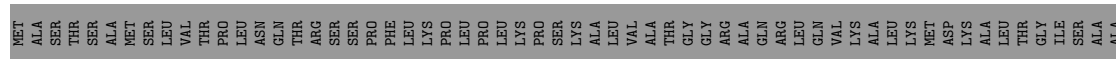


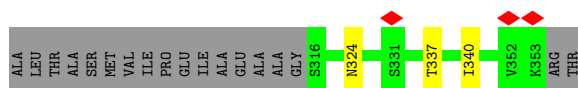
● Molecule 16: Photosystem II reaction center protein T



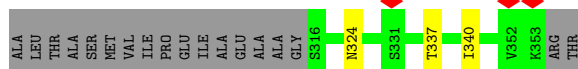
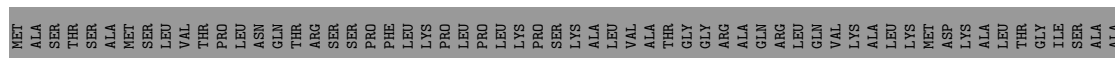
● Molecule 16: Photosystem II reaction center protein T



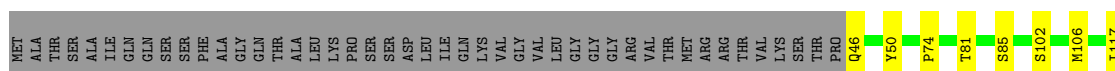




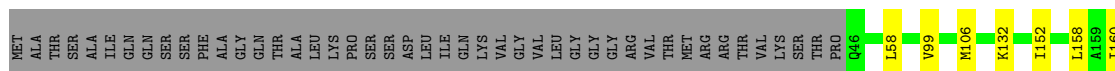
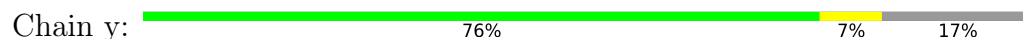
- Molecule 19: (thale cress) hypothetical protein



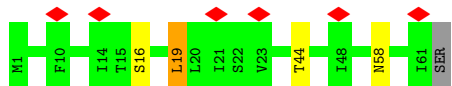
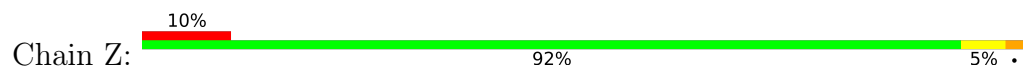
- Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic



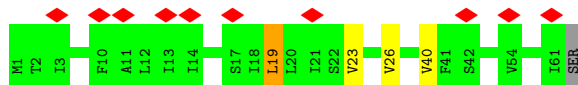
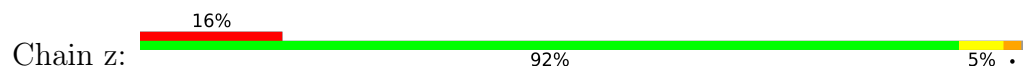
- Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic



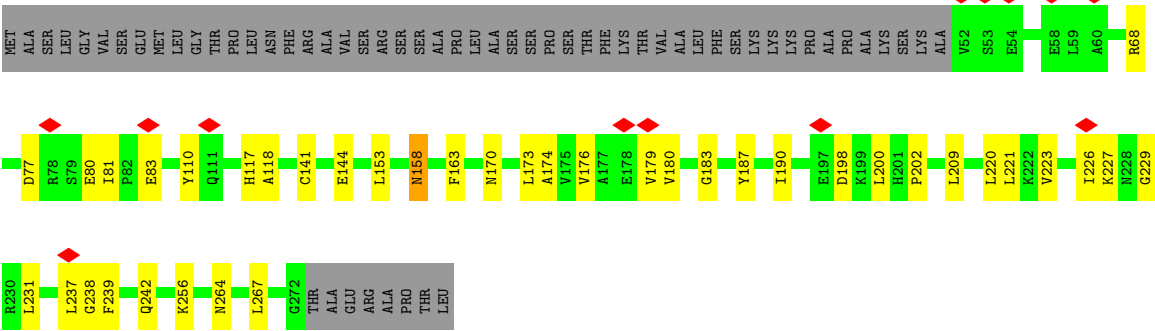
- Molecule 21: Photosystem II reaction center protein Z



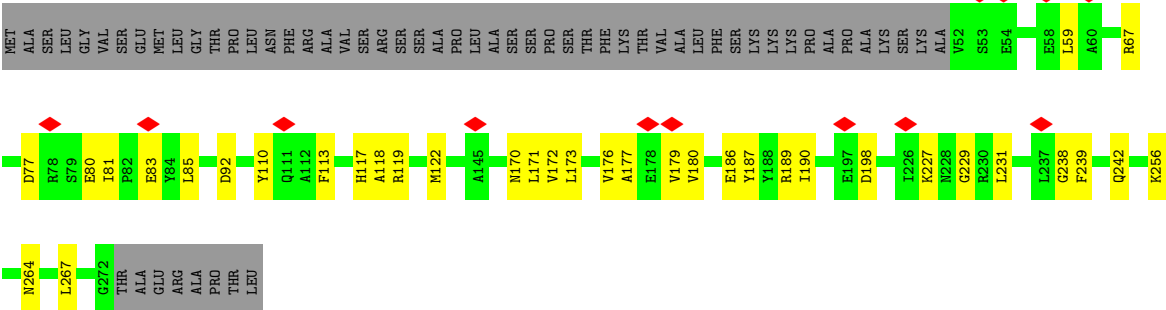
- Molecule 21: Photosystem II reaction center protein Z



- Molecule 22: Chlorophyll a-b binding protein CP26, chloroplastic



● Molecule 22: Chlorophyll a-b binding protein CP26, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67864	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	37.376	Depositor
Minimum map value	-22.323	Depositor
Average map value	0.013	Depositor
Map value standard deviation	1.095	Depositor
Recommended contour level	3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/2680	0.65	0/3654
1	a	0.38	0/2680	0.69	1/3654 (0.0%)
2	B	0.35	0/3959	0.58	2/5394 (0.0%)
2	b	0.33	0/3959	0.57	0/5394
3	C	0.35	0/3595	0.73	2/4899 (0.0%)
3	c	0.34	0/3595	0.71	1/4899 (0.0%)
4	D	0.35	0/2789	0.61	0/3803
4	d	0.35	0/2789	0.64	0/3803
5	E	0.37	1/557 (0.2%)	0.71	0/758
5	e	0.38	1/557 (0.2%)	0.75	0/758
6	F	0.31	0/230	0.68	0/313
6	f	0.29	0/230	0.66	0/313
7	G	0.32	0/1716	0.64	0/2336
7	N	0.33	0/1716	0.70	1/2336 (0.0%)
7	g	0.33	0/1716	0.67	0/2336
7	n	0.33	0/1716	0.67	0/2336
8	H	0.34	0/447	0.67	0/608
8	h	0.33	0/447	0.60	0/608
9	I	0.38	0/285	0.74	0/385
9	i	0.38	0/285	0.80	0/385
10	J	0.26	0/225	0.48	0/306
10	j	0.32	0/225	0.58	0/306
11	K	0.40	0/312	0.87	0/428
11	k	0.37	0/312	0.84	0/428
12	L	0.31	0/317	0.55	0/431
12	l	0.28	0/317	0.53	0/431
13	M	0.30	0/254	0.61	0/348
13	m	0.30	0/254	0.65	0/348
14	O	0.26	0/1556	0.63	2/2104 (0.1%)
14	o	0.27	0/1556	0.63	0/2104
15	R	0.29	0/1772	0.60	0/2414
15	r	0.27	0/1772	0.65	1/2414 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	T	0.28	0/246	0.59	0/333
16	t	0.28	0/246	0.58	0/333
17	U	0.22	0/181	0.57	0/242
17	u	0.18	0/181	0.45	0/242
18	W	0.28	0/438	0.57	0/594
18	w	0.28	0/438	0.55	0/594
19	X	0.28	0/270	0.63	0/367
19	x	0.28	0/270	0.59	0/367
20	Y	0.31	0/1753	0.64	2/2385 (0.1%)
20	y	0.29	0/1753	0.59	0/2385
21	Z	0.28	0/468	0.67	2/641 (0.3%)
21	z	0.31	0/468	0.70	2/641 (0.3%)
22	S	0.35	0/1750	0.77	2/2376 (0.1%)
22	s	0.32	0/1750	0.73	3/2376 (0.1%)
All	All	0.33	2/55032 (0.0%)	0.66	21/74910 (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
3	c	0	1
15	R	0	1
15	r	0	1
22	S	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	27	ILE	C-N	6.30	1.40	1.34
5	E	27	ILE	C-N	5.79	1.39	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	r	203	GLU	CA-CB-CG	6.87	127.83	114.10
7	N	232	GLN	CA-CB-CG	6.59	127.28	114.10
3	c	224	ILE	N-CA-C	-6.57	106.72	113.10
1	a	179	THR	CA-CB-OG1	6.47	119.31	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	38	GLY	CA-C-N	-6.32	111.69	122.56
3	C	38	GLY	C-N-CA	-6.32	111.69	122.56
22	s	198	ASP	CA-C-N	6.18	133.35	121.54
22	s	198	ASP	C-N-CA	6.18	133.35	121.54
20	Y	197	LEU	CA-C-N	5.97	132.95	121.54
20	Y	197	LEU	C-N-CA	5.97	132.95	121.54
14	O	218	LEU	CA-C-N	5.63	132.29	121.54
14	O	218	LEU	C-N-CA	5.63	132.29	121.54
21	z	19	LEU	CA-C-N	5.62	132.28	121.54
21	z	19	LEU	C-N-CA	5.62	132.28	121.54
22	S	198	ASP	CA-C-N	5.35	131.75	121.54
22	S	198	ASP	C-N-CA	5.35	131.75	121.54
21	Z	19	LEU	CA-C-N	5.29	131.64	121.54
21	Z	19	LEU	C-N-CA	5.29	131.64	121.54
22	s	59	LEU	CA-CB-CG	5.16	134.36	116.30
2	B	294	GLU	CA-C-N	5.12	129.39	122.07
2	B	294	GLU	C-N-CA	5.12	129.39	122.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	39	ASN	Peptide
15	R	58	TRP	Peptide
22	S	200	LEU	Peptide
3	c	80	PRO	Peptide
15	r	58	TRP	Peptide

5.2 Too-close contacts [i](#)

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	2599	0	2501	30	0
1	a	2599	0	2501	30	0
2	B	3829	0	3707	45	0
2	b	3829	0	3707	41	0
3	C	3480	0	3409	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3480	0	3409	65	0
4	D	2696	0	2585	42	0
4	d	2696	0	2585	44	0
5	E	540	0	521	7	0
5	e	540	0	521	10	0
6	F	224	0	229	5	0
6	f	224	0	229	5	0
7	G	1666	0	1593	31	0
7	N	1666	0	1593	26	0
7	g	1666	0	1593	35	0
7	n	1666	0	1593	27	0
8	H	438	0	465	7	0
8	h	438	0	465	4	0
9	I	277	0	289	2	0
9	i	277	0	289	3	0
10	J	219	0	231	1	0
10	j	219	0	231	2	0
11	K	301	0	313	6	0
11	k	301	0	313	6	0
12	L	309	0	298	1	0
12	l	309	0	298	4	0
13	M	250	0	273	4	0
13	m	250	0	273	3	0
14	O	1523	0	1504	16	0
14	o	1523	0	1504	15	0
15	R	1724	0	1684	25	0
15	r	1724	0	1684	30	0
16	T	239	0	255	1	0
16	t	239	0	255	3	0
17	U	179	0	190	4	0
17	u	179	0	190	2	0
18	W	427	0	405	8	0
18	w	427	0	405	7	0
19	X	267	0	292	2	0
19	x	267	0	292	2	0
20	Y	1699	0	1630	21	0
20	y	1699	0	1630	14	0
21	Z	458	0	490	3	0
21	z	458	0	490	2	0
22	S	1705	0	1681	28	0
22	s	1705	0	1681	24	0
23	A	175	0	169	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1040	0	1152	27	0
23	C	810	0	854	24	0
23	D	195	0	216	9	0
23	G	448	0	429	11	0
23	N	435	0	396	7	0
23	R	530	0	466	10	0
23	S	414	0	313	9	0
23	Y	466	0	454	6	0
23	a	240	0	242	8	0
23	b	1040	0	1152	29	0
23	c	810	0	854	29	0
23	d	130	0	144	9	0
23	g	448	0	429	12	0
23	n	435	0	396	6	0
23	r	530	0	466	14	0
23	s	414	0	313	11	0
23	y	466	0	454	6	0
24	A	64	0	74	2	0
24	D	64	0	74	7	0
24	a	64	0	74	1	0
24	d	64	0	74	4	0
25	A	40	0	56	4	0
25	B	120	0	168	6	0
25	C	80	0	112	9	0
25	F	40	0	56	2	0
25	H	40	0	56	4	0
25	K	40	0	56	2	0
25	Z	40	0	56	3	0
25	a	40	0	56	2	0
25	b	120	0	168	8	0
25	c	120	0	168	15	0
25	d	40	0	56	2	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
26	A	104	0	145	1	0
26	L	54	0	78	4	0
26	M	54	0	78	3	0
26	a	54	0	78	1	0
26	d	50	0	67	2	0
27	A	40	0	50	0	0
27	B	91	0	122	5	0
27	C	48	0	66	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D	46	0	62	2	0
27	a	48	0	66	2	0
27	b	51	0	72	4	0
27	d	46	0	62	0	0
28	A	59	0	76	4	0
28	C	55	0	68	4	0
28	H	62	0	82	4	0
28	a	59	0	76	3	0
28	c	55	0	68	2	0
28	d	62	0	82	4	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	A	95	0	139	4	0
30	B	98	0	148	2	0
30	C	49	0	74	3	0
30	G	46	0	65	3	0
30	L	98	0	148	5	0
30	N	49	0	74	2	0
30	R	42	0	57	2	0
30	S	49	0	74	3	0
30	T	49	0	74	2	0
30	W	49	0	74	1	0
30	Y	49	0	74	1	0
30	a	95	0	139	4	0
30	b	98	0	148	2	0
30	c	49	0	74	2	0
30	d	49	0	74	6	0
30	g	46	0	65	3	0
30	n	49	0	74	1	0
30	r	42	0	57	2	0
30	s	49	0	74	2	0
30	w	49	0	74	1	0
30	y	49	0	74	1	0
31	D	4	0	0	2	0
31	d	4	0	0	3	0
32	D	55	0	80	2	0
32	d	55	0	80	3	0
33	E	43	0	30	1	0
33	e	43	0	30	0	0
34	G	391	0	356	12	0
34	N	338	0	305	8	0
34	R	195	0	146	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	S	184	0	125	5	0
34	Y	299	0	284	10	0
34	g	391	0	356	19	0
34	n	338	0	305	7	0
34	r	195	0	146	4	0
34	s	184	0	125	2	0
34	y	299	0	284	8	0
35	G	84	0	112	8	0
35	N	84	0	112	7	0
35	R	42	0	56	2	0
35	S	84	0	112	8	0
35	Y	84	0	112	6	0
35	g	84	0	112	13	0
35	n	84	0	112	4	0
35	r	42	0	56	3	0
35	s	84	0	112	4	0
35	y	84	0	112	5	0
36	G	44	0	56	3	0
36	N	44	0	56	2	0
36	R	44	0	56	2	0
36	S	44	0	56	0	0
36	Y	44	0	56	0	0
36	g	44	0	56	3	0
36	n	44	0	56	3	0
36	r	44	0	56	2	0
36	s	44	0	56	2	0
36	y	44	0	56	0	0
37	G	44	0	56	6	0
37	N	44	0	56	0	0
37	R	44	0	56	1	0
37	Y	44	0	56	5	0
37	g	44	0	56	3	0
37	n	44	0	56	2	0
37	r	44	0	56	0	0
37	y	44	0	56	4	0
All	All	70366	0	70511	980	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 7.

All (980) 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)
3:C:37:ALA:O	3:C:40:ALA:HB3	1.77	0.84
22:s:242:GLN:OE1	23:s:612:CLA:NA	2.15	0.79
34:g:606:CHL:HBB2	35:g:616:LUT:H7	1.68	0.74
7:N:226:MET:HG2	35:N:317:LUT:H12	1.69	0.74
5:e:43:ALA:O	5:e:47:PHE:HB2	1.88	0.74
20:Y:224:MET:HG2	35:Y:316:LUT:H12	1.70	0.72
23:A:402:CLA:HBB1	23:D:404:CLA:H51	1.71	0.71
3:C:38:GLY:O	3:C:41:ARG:HB2	1.91	0.71
7:n:226:MET:HG2	35:n:317:LUT:H12	1.71	0.71
20:y:224:MET:HG2	35:y:316:LUT:H12	1.72	0.71
23:a:403:CLA:HBB1	23:d:404:CLA:H51	1.73	0.69
7:n:211:LEU:HA	7:n:214:LYS:HG2	1.75	0.69
7:g:216:LEU:O	7:g:220:ARG:HB2	1.93	0.68
7:g:264:VAL:HG21	34:g:619:CHL:HED3	1.76	0.68
7:N:211:LEU:HB3	23:N:311:CLA:H3A	1.74	0.68
7:n:108:LEU:HB3	23:n:305:CLA:HBB2	1.76	0.67
20:Y:74:PRO:HG2	20:Y:210:LYS:HD2	1.76	0.67
7:G:264:VAL:HG21	34:G:619:CHL:HED3	1.76	0.67
7:n:183:LEU:HD13	34:n:309:CHL:HAB	1.77	0.66
1:a:272:HIS:CE1	31:d:403:BCT:O2	2.48	0.66
14:o:186:VAL:O	14:o:221:SER:HA	1.95	0.66
20:Y:226:GLY:O	20:Y:230:GLN:HB3	1.95	0.66
3:c:311:GLN:HG3	3:c:361:LEU:HD13	1.78	0.65
1:A:217:SER:O	1:A:221:SER:HB3	1.97	0.65
7:G:138:ILE:HG21	7:G:158:ILE:HD12	1.79	0.65
7:N:108:LEU:HB3	23:N:305:CLA:HBB2	1.79	0.65
7:n:117:GLU:HB3	7:n:241:ILE:HD12	1.78	0.65
3:c:246:PHE:HB2	30:c:517:LHG:H211	1.80	0.64
3:C:311:GLN:HG3	3:C:361:LEU:HD13	1.78	0.64
34:g:607:CHL:HBB1	34:n:302:CHL:H192	1.80	0.64
14:O:188:PHE:O	14:O:219:ASP:HA	1.97	0.64
4:d:91:LEU:HD13	4:d:110:GLY:HA2	1.79	0.64
1:A:272:HIS:CE1	31:D:403:BCT:O2	2.50	0.63
4:D:94:TRP:HB2	19:X:324:ASN:HB3	1.81	0.63
3:C:46:SER:H	3:C:139:THR:HG22	1.63	0.63
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.80	0.62
3:c:46:SER:H	3:c:139:THR:HG22	1.64	0.62
34:n:308:CHL:HBB2	34:n:310:CHL:HBC1	1.82	0.62
22:S:242:GLN:OE1	23:S:612:CLA:NA	2.32	0.62
1:A:272:HIS:CD2	4:D:215:HIS:NE2	2.68	0.62
2:B:251:VAL:HG12	28:H:102:DGD:HB52	1.82	0.62
14:O:187:ASN:HA	14:O:220:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:226:MET:HE1	35:g:616:LUT:H35	1.83	0.61
15:r:242:GLU:OE1	23:r:609:CLA:NA	2.32	0.61
7:G:211:LEU:HD23	7:G:214:LYS:HD3	1.83	0.61
7:g:104:ARG:NH2	7:g:190:LEU:O	2.34	0.60
23:G:604:CLA:HBB1	36:G:617:NEX:H27	1.83	0.60
1:A:103:ASP:HB3	14:O:164:MET:HE1	1.83	0.60
22:s:170:ASN:HB2	22:s:173:LEU:HD23	1.83	0.60
15:r:58:TRP:O	23:r:601:CLA:NB	2.35	0.60
2:B:110:ALA:HB2	25:B:619:BCR:H17C	1.84	0.60
3:C:393:ALA:O	3:C:396:MET:HB3	2.02	0.59
4:D:336:PRO:HB2	5:E:65:LEU:HD11	1.83	0.59
34:G:619:CHL:HED2	20:Y:132:LYS:HA	1.84	0.59
3:c:410:VAL:HG12	3:c:412:THR:H	1.67	0.59
2:b:110:ALA:HB2	25:b:619:BCR:H17C	1.84	0.59
2:b:251:VAL:HG12	28:d:410:DGD:HB52	1.85	0.59
3:c:55:ALA:HA	3:c:126:GLY:HA2	1.84	0.59
7:g:220:ARG:HG2	30:g:618:LHG:H252	1.84	0.59
2:b:385:ARG:H	4:d:352:ALA:HB1	1.67	0.59
22:S:202:PRO:HG3	34:S:607:CHL:HBC2	1.82	0.59
5:E:34:GLY:HA2	5:E:38:VAL:HB	1.85	0.59
28:A:408:DGD:HD5	2:b:75:TRP:HB3	1.85	0.59
4:D:124:ILE:HD11	28:H:102:DGD:HAH2	1.83	0.59
34:N:308:CHL:HBB2	34:N:310:CHL:HBC1	1.83	0.59
23:b:607:CLA:H12	27:b:620:LMG:H121	1.85	0.59
5:E:55:TYR:O	5:E:60:ARG:NH1	2.36	0.58
37:Y:301:XAT:H32	34:Y:302:CHL:H111	1.84	0.58
3:C:225:VAL:O	3:C:293:ASN:ND2	2.36	0.58
3:C:87:ILE:HG21	23:C:505:CLA:HMB3	1.86	0.58
20:Y:197:LEU:HD12	35:Y:315:LUT:H222	1.85	0.58
4:D:91:LEU:HD13	4:D:110:GLY:HA2	1.85	0.58
3:c:37:ALA:O	3:c:40:ALA:HB3	2.03	0.58
3:c:164:HIS:HA	3:c:167:LEU:HD12	1.85	0.58
7:G:216:LEU:O	7:G:220:ARG:HB2	2.04	0.58
34:g:601:CHL:HMC	37:g:620:XAT:H222	1.84	0.58
1:A:29:TYR:O	1:A:129:ARG:NH1	2.37	0.58
23:B:607:CLA:H12	27:B:620:LMG:H121	1.86	0.58
2:B:235:GLU:HB3	2:B:473:THR:HB	1.86	0.58
5:e:44:TYR:OH	5:e:51:ARG:NH1	2.36	0.58
7:G:223:MET:SD	7:G:223:MET:N	2.76	0.58
34:N:310:CHL:HMC	34:Y:302:CHL:H72	1.85	0.58
15:r:73:VAL:O	15:r:137:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:LEU:HD22	24:D:402:PHO:HBC3	1.86	0.57
3:c:305:THR:HG22	3:c:307:PRO:HD2	1.87	0.57
15:R:203:GLU:OE1	15:R:206:ARG:NH2	2.37	0.57
3:C:39:ASN:N	3:C:39:ASN:HD22	2.00	0.57
3:c:79:LYS:HD2	3:c:80:PRO:HD2	1.85	0.57
4:d:130:GLN:NE2	24:d:401:PHO:OBD	2.37	0.57
3:C:39:ASN:HD22	3:C:39:ASN:H	1.51	0.57
37:y:301:XAT:H32	34:y:302:CHL:H111	1.86	0.57
22:s:227:LYS:HE3	30:s:617:LHG:HC62	1.87	0.57
23:B:603:CLA:H161	25:H:101:BCR:H313	1.87	0.57
23:b:603:CLA:H161	25:h:101:BCR:H313	1.86	0.57
4:d:94:TRP:HB2	19:x:324:ASN:HB3	1.87	0.57
2:b:370:LEU:HD12	2:b:379:ALA:HB3	1.86	0.57
34:Y:306:CHL:HBA1	15:r:184:LEU:HD13	1.87	0.57
3:C:362:ARG:NH2	14:O:103:MET:SD	2.78	0.56
1:a:272:HIS:CD2	4:d:215:HIS:NE2	2.73	0.56
1:A:272:HIS:CD2	4:D:215:HIS:HE2	2.21	0.56
15:R:244:LYS:NZ	30:R:618:LHG:O4	2.39	0.56
20:Y:127:GLU:HG2	20:Y:132:LYS:HB2	1.87	0.56
23:a:402:CLA:H2A	23:a:402:CLA:HED3	1.87	0.56
17:U:90:GLN:HA	17:U:93:VAL:HG12	1.87	0.56
22:s:122:MET:HE3	23:s:609:CLA:HAB	1.86	0.56
7:g:214:LYS:O	7:g:218:ASN:HB2	2.05	0.56
2:B:357:ARG:NH1	17:U:94:THR:O	2.39	0.56
3:C:246:PHE:HB2	30:C:518:LHG:H211	1.87	0.56
1:A:174:LEU:HD22	24:A:403:PHO:H151	1.88	0.56
2:B:75:TRP:HB3	28:a:408:DGD:HD5	1.86	0.56
23:a:401:CLA:H203	30:d:408:LHG:H172	1.87	0.56
2:B:256:MET:HG3	2:B:448:ARG:HG3	1.87	0.55
15:R:184:LEU:HD13	34:y:306:CHL:HBA1	1.89	0.55
7:g:246:ASP:O	7:g:254:ASN:ND2	2.40	0.55
14:o:174:ILE:HD11	14:o:195:ASP:HB3	1.88	0.55
23:b:610:CLA:H141	23:b:612:CLA:HBD	1.88	0.55
2:B:357:ARG:NH2	4:D:338:GLU:OE1	2.39	0.55
2:b:347:ARG:O	2:b:397:VAL:HA	2.06	0.55
22:s:110:TYR:HB3	23:s:602:CLA:HHB	1.88	0.55
14:O:305:SER:HB3	14:O:323:ILE:HB	1.88	0.55
20:Y:85:SER:HB2	23:Y:303:CLA:HBA1	1.89	0.55
30:a:412:LHG:H161	30:a:412:LHG:H342	1.89	0.55
22:s:77:ASP:HB2	22:s:80:GLU:HB2	1.88	0.55
1:A:217:SER:HB2	4:D:143:ASN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	4:D:257:ILE:O	2.40	0.55
3:C:55:ALA:HB2	3:C:129:GLY:HA3	1.89	0.55
2:B:385:ARG:H	4:D:352:ALA:HB1	1.72	0.54
8:H:63:SER:HB3	8:H:72:VAL:HG13	1.90	0.54
23:g:610:CLA:HBB2	35:g:615:LUT:H34	1.89	0.54
3:C:60:ILE:HD13	23:C:504:CLA:H201	1.88	0.54
7:G:109:GLY:HA2	35:G:616:LUT:H182	1.89	0.54
15:R:259:GLN:OE1	23:R:612:CLA:NA	2.41	0.54
2:b:269:GLY:O	2:b:448:ARG:NH1	2.40	0.54
7:N:246:ASP:O	7:N:254:ASN:ND2	2.40	0.54
34:R:605:CHL:HBC2	34:R:606:CHL:HHD	1.89	0.54
15:r:125:GLN:HE21	23:r:614:CLA:HED1	1.71	0.54
3:C:178:LYS:HB2	23:C:503:CLA:H193	1.90	0.54
34:S:605:CHL:HBC2	34:S:606:CHL:HBC3	1.90	0.54
3:C:55:ALA:HA	3:C:126:GLY:HA2	1.90	0.54
20:Y:172:GLU:OE1	20:Y:175:ARG:NH2	2.41	0.54
3:c:233:ILE:HG12	25:c:515:BCR:H282	1.89	0.54
3:C:61:VAL:HG13	3:C:118:HIS:HD1	1.72	0.54
15:R:73:VAL:O	15:R:137:ARG:NH2	2.41	0.54
4:D:187:GLN:HB2	23:D:404:CLA:HBC1	1.90	0.54
22:s:67:ARG:HH12	22:s:85:LEU:HB3	1.72	0.54
2:B:341:LEU:HD12	2:B:429:ILE:HG22	1.90	0.54
15:r:263:THR:HB	15:r:265:LYS:HE3	1.89	0.54
2:B:370:LEU:HD12	2:B:379:ALA:HB3	1.90	0.54
3:C:121:SER:HB2	25:C:515:BCR:H14C	1.90	0.54
20:Y:117:ILE:HD11	20:Y:239:ILE:HD13	1.90	0.54
3:C:132:HIS:HE1	23:C:514:CLA:HMA3	1.73	0.53
7:N:250:ASP:OD1	7:N:254:ASN:ND2	2.42	0.53
4:D:107:GLN:NE2	5:E:48:GLY:O	2.41	0.53
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.91	0.53
1:a:272:HIS:HE1	31:d:403:BCT:O2	1.88	0.53
1:a:29:TYR:O	1:a:129:ARG:NH1	2.38	0.53
1:a:140:ARG:NH2	30:a:412:LHG:O5	2.38	0.53
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.90	0.53
34:G:606:CHL:HBB2	35:G:616:LUT:H7	1.91	0.53
23:A:401:CLA:H203	30:L:101:LHG:H172	1.89	0.53
30:A:412:LHG:H161	30:A:412:LHG:H342	1.90	0.53
2:b:222:PRO:HB3	8:h:38:GLY:H	1.73	0.53
7:g:214:LYS:O	7:g:218:ASN:CB	2.57	0.53
7:n:78:TYR:OH	7:n:217:LYS:NZ	2.41	0.53
3:C:114:SER:HA	3:C:117:LEU:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:259:GLN:HE22	35:R:615:LUT:H42	1.73	0.53
3:c:58:GLY:O	3:c:122:SER:OG	2.27	0.53
34:g:619:CHL:HED2	20:y:132:LYS:HA	1.90	0.53
3:c:114:SER:HA	3:c:117:LEU:HB2	1.91	0.53
20:y:218:ARG:HB3	23:y:303:CLA:HBC3	1.89	0.53
2:b:45:PHE:HD1	2:b:60:MET:HE3	1.74	0.53
8:h:17:THR:O	8:h:21:LYS:NZ	2.42	0.53
3:C:264:LEU:HD21	25:C:516:BCR:H322	1.91	0.52
27:b:620:LMG:O10	13:m:4:ASN:ND2	2.41	0.52
3:c:246:PHE:HA	3:c:249:ILE:HG12	1.90	0.52
7:n:144:LEU:HB3	7:n:155:ALA:HB3	1.91	0.52
3:c:225:VAL:HG21	28:c:516:DGD:HG32	1.91	0.52
3:c:225:VAL:O	3:c:293:ASN:ND2	2.42	0.52
1:A:269:ARG:NH1	4:D:232:THR:O	2.40	0.52
2:b:45:PHE:O	2:b:58:GLN:NE2	2.41	0.52
3:c:39:ASN:ND2	23:c:510:CLA:O1A	2.38	0.52
27:B:620:LMG:O10	13:M:4:ASN:ND2	2.40	0.52
19:X:337:THR:HA	19:X:340:ILE:HG22	1.92	0.52
23:b:613:CLA:H2A	23:b:613:CLA:H12	1.91	0.52
7:g:100:VAL:HB	7:g:190:LEU:HD11	1.91	0.52
23:y:313:CLA:H93	30:y:318:LHG:H132	1.90	0.52
4:D:20:ASP:OD1	4:D:33:TRP:NE1	2.41	0.52
3:C:164:HIS:HA	3:C:167:LEU:HD12	1.92	0.52
3:c:47:GLY:H	3:c:139:THR:HA	1.74	0.52
2:B:71:ILE:HD11	23:B:606:CLA:H2A	1.91	0.51
3:C:261:ARG:HA	3:C:266:TRP:HE1	1.75	0.51
10:J:19:ILE:HA	10:J:22:ILE:HB	1.91	0.51
15:R:168:ALA:HB1	23:R:604:CLA:HED1	1.92	0.51
2:b:227:LYS:O	2:b:230:ARG:NH1	2.43	0.51
3:c:294:ASN:ND2	3:c:308:GLU:OE2	2.40	0.51
7:n:250:ASP:OD1	7:n:254:ASN:ND2	2.43	0.51
34:n:307:CHL:HBB2	34:n:308:CHL:HBB1	1.92	0.51
15:r:140:GLU:OE2	15:r:247:ARG:NE	2.39	0.51
22:S:110:TYR:HB3	23:S:602:CLA:HHB	1.91	0.51
22:s:177:ALA:HB1	34:s:605:CHL:HMA3	1.91	0.51
2:B:45:PHE:O	2:B:58:GLN:NE2	2.39	0.51
23:Y:313:CLA:H93	30:Y:318:LHG:H132	1.91	0.51
4:d:160:ILE:HG21	4:d:288:VAL:HG22	1.92	0.51
15:r:164:THR:HG23	15:r:167:ASP:H	1.75	0.51
22:S:117:HIS:HD2	35:S:615:LUT:H34	1.75	0.51
1:A:14:TRP:HB3	18:W:119:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:613:CLA:H12	23:B:613:CLA:H2A	1.91	0.51
15:R:64:SER:HB2	15:R:68:LEU:HD21	1.93	0.51
4:d:81:THR:OG1	4:d:168:TRP:O	2.26	0.51
7:g:128:GLU:HG2	7:g:133:LYS:HB2	1.92	0.51
34:g:619:CHL:H121	34:y:309:CHL:H102	1.92	0.51
7:n:225:SER:HA	23:n:314:CLA:HAB	1.92	0.51
1:A:93:PHE:HZ	23:A:404:CLA:HAA1	1.76	0.51
20:Y:209:LEU:HD23	20:Y:212:LYS:HD2	1.92	0.51
2:b:391:SER:OG	2:b:394:GLN:OE1	2.28	0.51
3:c:166:ILE:HG13	3:c:248:GLY:HA3	1.92	0.51
34:G:601:CHL:HMC	37:G:620:XAT:H222	1.93	0.51
14:O:112:ASN:HD22	14:O:167:LEU:HD12	1.75	0.51
23:c:508:CLA:H12	23:c:511:CLA:HAC1	1.93	0.51
3:C:59:LEU:HD13	23:C:511:CLA:HMD2	1.93	0.51
3:C:151:TRP:HA	3:C:157:MET:HE1	1.92	0.51
26:L:103:SQD:H121	30:T:101:LHG:H101	1.93	0.51
3:c:61:VAL:HG13	3:c:118:HIS:HD1	1.75	0.51
7:g:197:ASP:N	7:g:197:ASP:OD1	2.43	0.51
19:x:337:THR:HA	19:x:340:ILE:HG22	1.92	0.51
7:G:149:ASN:HD22	7:G:152:LEU:HD22	1.76	0.51
22:s:67:ARG:HD2	22:s:92:ASP:HB3	1.93	0.51
4:D:68:TYR:HB2	6:F:34:MET:HG3	1.93	0.51
30:n:319:LHG:H282	30:n:319:LHG:H112	1.94	0.51
22:s:118:ALA:HB1	22:s:229:GLY:HA3	1.93	0.51
4:D:102:PHE:O	4:D:106:CYS:CB	2.60	0.50
23:b:603:CLA:H143	23:b:608:CLA:HAC1	1.91	0.50
22:S:183:GLY:O	22:S:187:TYR:HB2	2.11	0.50
3:C:156:LYS:O	3:C:159:THR:OG1	2.29	0.50
1:a:93:PHE:HZ	23:a:405:CLA:HAA1	1.76	0.50
23:c:506:CLA:H42	25:c:515:BCR:H10C	1.92	0.50
25:c:514:BCR:H321	22:s:267:LEU:HD22	1.93	0.50
2:b:181:VAL:HG11	2:b:195:PRO:HB2	1.93	0.50
26:L:103:SQD:H61	26:L:103:SQD:H92	1.93	0.50
23:a:401:CLA:H152	23:a:402:CLA:H152	1.93	0.50
2:b:477:ASP:OD1	2:b:477:ASP:N	2.45	0.50
1:a:91:LEU:O	3:c:219:GLY:N	2.40	0.50
1:a:127:MET:HE2	3:c:442:LEU:HD11	1.92	0.50
23:c:513:CLA:H93	25:c:514:BCR:H23C	1.93	0.50
4:d:124:ILE:HD11	28:d:410:DGD:HAH2	1.92	0.50
14:o:128:PRO:HA	14:o:180:VAL:HG13	1.94	0.50
3:C:90:PRO:HB3	3:C:302:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:186:VAL:O	14:O:221:SER:HA	2.11	0.50
1:a:269:ARG:NH2	4:d:232:THR:OG1	2.44	0.50
7:G:82:THR:HG21	34:Y:309:CHL:HAA2	1.93	0.50
7:N:211:LEU:HA	7:N:214:LYS:HG2	1.94	0.50
7:n:246:ASP:O	7:n:254:ASN:ND2	2.44	0.50
7:N:98:LEU:HD11	20:Y:81:THR:HG22	1.94	0.50
34:r:605:CHL:HBC2	34:r:606:CHL:HHD	1.93	0.50
23:A:401:CLA:H152	23:D:401:CLA:H152	1.93	0.50
1:a:272:HIS:CD2	4:d:215:HIS:HE2	2.26	0.50
3:c:261:ARG:NH1	18:w:129:SER:OG	2.45	0.50
25:d:406:BCR:H14C	6:f:27:PHE:HD2	1.77	0.50
7:N:183:LEU:HG	34:N:309:CHL:HAB	1.94	0.49
1:a:297:LEU:HA	3:c:402:GLY:HA3	1.93	0.49
22:S:158:ASN:C	22:S:158:ASN:HD22	2.20	0.49
7:G:246:ASP:O	7:G:254:ASN:ND2	2.40	0.49
34:Y:306:CHL:HED2	15:r:184:LEU:HD11	1.94	0.49
3:c:121:SER:HB2	25:c:514:BCR:H14C	1.94	0.49
34:g:601:CHL:HED3	30:g:618:LHG:H131	1.94	0.49
15:r:206:ARG:NH2	23:r:608:CLA:O1D	2.43	0.49
2:B:10:THR:O	15:R:99:GLN:NE2	2.45	0.49
30:B:623:LHG:H101	26:M:101:SQD:H121	1.94	0.49
23:C:503:CLA:H3A	23:C:504:CLA:OBD	2.12	0.49
4:D:130:GLN:NE2	24:D:402:PHO:OBD	2.45	0.49
4:D:165:GLN:HE22	4:D:293:ASN:HD21	1.60	0.49
23:N:311:CLA:H52	35:N:316:LUT:H30	1.94	0.49
3:c:264:LEU:HD21	25:c:515:BCR:H322	1.93	0.49
3:C:166:ILE:HG13	3:C:248:GLY:HA3	1.95	0.49
9:I:6:LEU:HA	18:W:101:LEU:HD11	1.93	0.49
22:S:68:ARG:HH12	30:S:617:LHG:HC31	1.77	0.49
30:B:623:LHG:H282	26:M:101:SQD:H171	1.95	0.49
3:C:246:PHE:HA	3:C:249:ILE:HG12	1.93	0.49
7:G:94:ARG:NH1	7:N:81:ASP:O	2.46	0.49
7:N:55:ARG:NH2	7:N:70:LEU:O	2.44	0.49
7:N:195:SER:HA	22:S:209:LEU:HD21	1.93	0.49
4:d:108:LEU:HD13	5:e:66:ILE:HD13	1.95	0.49
4:d:251:ASN:ND2	4:d:262:PHE:O	2.43	0.49
7:n:211:LEU:HB3	23:n:311:CLA:H3A	1.95	0.49
3:C:54:VAL:HG22	23:C:513:CLA:HED2	1.94	0.49
3:C:97:TRP:HB3	3:C:110:PRO:HB2	1.94	0.49
23:b:603:CLA:HBB2	23:b:605:CLA:H18	1.95	0.49
3:c:261:ARG:HA	3:c:266:TRP:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:81:ILE:HG22	22:S:83:GLU:H	1.78	0.49
28:A:408:DGD:HAW1	25:b:618:BCR:H391	1.95	0.49
3:C:39:ASN:H	3:C:39:ASN:ND2	2.11	0.49
7:G:81:ASP:OD1	35:G:616:LUT:O23	2.30	0.49
7:G:117:GLU:HB3	7:G:241:ILE:HD13	1.94	0.49
22:S:144:GLU:HB3	22:S:153:LEU:HD11	1.95	0.49
22:s:171:LEU:HG	22:s:172:VAL:HG13	1.94	0.49
1:A:326:LEU:HA	3:C:412:THR:HG22	1.95	0.49
2:B:158:VAL:HG22	2:B:166:ILE:HD11	1.95	0.49
7:N:250:ASP:OD1	7:N:250:ASP:N	2.46	0.49
15:R:152:LEU:HG	23:R:604:CLA:HAC1	1.94	0.49
3:c:453:ALA:HB1	9:i:31:ASN:HD22	1.77	0.49
7:n:132:PHE:HE2	20:y:263:PRO:HG3	1.78	0.49
7:n:240:PRO:O	35:n:316:LUT:O3	2.31	0.49
6:F:21:ALA:O	6:F:25:VAL:N	2.46	0.48
7:g:214:LYS:NZ	23:g:612:CLA:O1A	2.44	0.48
2:B:227:LYS:O	2:B:230:ARG:NH1	2.46	0.48
34:G:601:CHL:HED3	30:G:618:LHG:H131	1.94	0.48
7:n:55:ARG:NH2	7:n:70:LEU:O	2.45	0.48
2:b:257:TRP:HB2	2:b:452:THR:HG21	1.95	0.48
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.45	0.48
1:a:103:ASP:HB3	14:o:164:MET:HE1	1.95	0.48
3:C:418:ASN:C	3:C:418:ASN:HD22	2.22	0.48
4:D:183:ILE:HG23	23:D:404:CLA:HAC1	1.95	0.48
7:G:128:GLU:HG2	7:G:133:LYS:HB2	1.96	0.48
7:G:232:GLN:O	7:G:236:THR:OG1	2.32	0.48
3:c:346:THR:OG1	3:c:348:GLU:OE1	2.28	0.48
3:C:261:ARG:NH1	18:W:129:SER:OG	2.45	0.48
3:C:402:GLY:HA2	3:C:420:VAL:HA	1.96	0.48
34:N:309:CHL:HAA2	34:N:309:CHL:H152	1.95	0.48
2:b:55:MET:HE3	2:b:64:PRO:HG3	1.94	0.48
34:g:606:CHL:HBB2	35:g:616:LUT:H192	1.95	0.48
23:s:612:CLA:HMA3	23:s:613:CLA:HBC3	1.96	0.48
1:A:293:MET:HE2	1:A:293:MET:HB3	1.78	0.48
30:A:412:LHG:O3	30:A:412:LHG:O1	2.32	0.48
2:B:58:GLN:HG3	2:B:60:MET:HE2	1.96	0.48
2:B:399:VAL:HB	2:B:417:VAL:HG23	1.96	0.48
4:D:60:TYR:HD2	5:E:66:ILE:HD11	1.79	0.48
4:D:81:THR:OG1	4:D:168:TRP:O	2.27	0.48
14:O:128:PRO:HA	14:O:180:VAL:HG13	1.95	0.48
23:n:311:CLA:H52	35:n:316:LUT:H30	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:612:CLA:H72	23:s:613:CLA:HMD3	1.95	0.48
3:C:225:VAL:HG11	28:C:517:DGD:HG32	1.95	0.48
2:b:10:THR:O	15:r:99:GLN:NE2	2.47	0.48
23:b:601:CLA:H143	25:h:101:BCR:H21C	1.95	0.48
3:c:215:LYS:HE2	3:c:221:GLU:HB2	1.95	0.48
7:G:102:HIS:HD1	23:G:602:CLA:HAB	1.78	0.48
26:L:103:SQD:H171	30:T:101:LHG:H282	1.95	0.48
23:c:502:CLA:H3A	23:c:503:CLA:OBD	2.13	0.48
22:s:119:ARG:NH1	34:s:607:CHL:OBD	2.43	0.48
2:B:133:LEU:HD23	8:H:27:ASN:HD21	1.79	0.47
23:B:615:CLA:HED1	23:B:616:CLA:HHC	1.96	0.47
25:B:618:BCR:H391	28:a:408:DGD:HAW1	1.95	0.47
3:C:50:LEU:HD13	23:C:513:CLA:HMD2	1.96	0.47
15:R:81:PHE:HD2	37:R:616:XAT:H221	1.79	0.47
1:a:14:TRP:HB3	18:w:119:TYR:HB2	1.95	0.47
23:b:603:CLA:HAB	23:b:605:CLA:H162	1.96	0.47
4:d:222:THR:HG21	4:d:250:ALA:HB2	1.96	0.47
7:n:186:ALA:HB2	34:n:309:CHL:HBC1	1.95	0.47
15:r:203:GLU:OE2	15:r:206:ARG:NH2	2.46	0.47
2:B:347:ARG:O	2:B:397:VAL:HA	2.14	0.47
15:R:258:VAL:HG11	23:R:612:CLA:HAC2	1.96	0.47
15:r:163:VAL:HG21	15:r:171:VAL:HG21	1.96	0.47
22:S:77:ASP:HB2	22:S:80:GLU:HB2	1.96	0.47
22:s:231:LEU:HD13	23:s:610:CLA:HBC1	1.95	0.47
2:B:315:ILE:HG12	2:B:321:LYS:HG3	1.95	0.47
23:B:610:CLA:H111	23:B:610:CLA:H72	1.75	0.47
7:G:95:ASN:ND2	23:G:602:CLA:O1A	2.46	0.47
20:Y:195:ASP:OD1	35:Y:315:LUT:O23	2.32	0.47
3:c:262:ARG:NH1	18:w:125:GLU:OE2	2.47	0.47
7:g:109:GLY:HA2	35:g:616:LUT:H182	1.95	0.47
11:k:49:LEU:HA	11:k:52:PHE:HB2	1.95	0.47
14:o:212:LEU:O	14:o:307:GLN:NE2	2.42	0.47
7:g:183:LEU:HD22	7:g:195:SER:HB3	1.97	0.47
21:z:19:LEU:HD22	21:z:23:VAL:HG23	1.96	0.47
23:S:612:CLA:H72	23:S:613:CLA:HMD3	1.95	0.47
2:B:460:LEU:HB3	4:D:281:TRP:HZ3	1.80	0.47
24:D:402:PHO:HBA2	24:D:402:PHO:H3A	1.66	0.47
7:N:244:LEU:HA	23:N:314:CLA:HMA2	1.96	0.47
2:b:460:LEU:HB3	4:d:281:TRP:HZ3	1.80	0.47
15:r:231:ASP:OD1	15:r:234:LYS:NZ	2.38	0.47
23:r:609:CLA:H52	35:r:615:LUT:H30	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:608:CLA:H18	23:d:405:CLA:HAA2	1.96	0.47
4:d:193:THR:HG23	23:d:404:CLA:HBC2	1.95	0.47
7:g:94:ARG:NH1	7:n:81:ASP:O	2.48	0.47
20:y:99:VAL:HB	20:y:188:LEU:HD11	1.96	0.47
23:B:610:CLA:H141	23:B:612:CLA:HBD	1.95	0.47
2:b:341:LEU:HD12	2:b:429:ILE:HG22	1.96	0.47
4:d:46:LEU:HD11	23:d:404:CLA:H161	1.96	0.47
5:e:36:LEU:O	5:e:40:THR:OG1	2.33	0.47
23:s:602:CLA:H3A	23:s:602:CLA:HBA2	1.71	0.47
1:A:296:ASN:HB3	3:C:401:LEU:HA	1.95	0.47
2:B:294:GLU:OE2	2:B:296:GLN:NE2	2.47	0.47
4:d:127:MET:HE3	4:d:151:ILE:HD12	1.96	0.47
3:c:451:ALA:HA	3:c:456:GLU:HB2	1.97	0.47
23:g:602:CLA:H43	35:g:616:LUT:H26	1.97	0.47
15:r:145:ARG:NH1	34:r:607:CHL:OBD	2.39	0.47
2:B:45:PHE:HD1	2:B:60:MET:HE3	1.80	0.47
2:B:155:ALA:O	2:B:159:THR:OG1	2.33	0.47
3:C:29:GLU:OE2	4:D:234:ARG:NH2	2.43	0.47
7:G:226:MET:SD	35:G:616:LUT:H12	2.54	0.47
28:H:102:DGD:O5D	28:H:102:DGD:O4D	2.32	0.47
7:N:131:TRP:HE1	7:N:240:PRO:HG2	1.80	0.47
7:g:94:ARG:HH22	7:n:67:PRO:HG3	1.80	0.47
7:g:165:GLN:O	7:g:169:MET:HB3	2.14	0.47
34:g:601:CHL:H111	37:g:620:XAT:H12	1.97	0.47
7:n:104:ARG:NH2	7:n:215:GLU:OE2	2.48	0.47
17:u:85:LYS:NZ	17:u:101:CYS:O	2.43	0.47
22:s:179:VAL:HG13	22:s:180:VAL:HG23	1.96	0.47
1:A:140:ARG:NH2	30:A:412:LHG:O5	2.42	0.46
23:C:510:CLA:H112	23:C:510:CLA:HAA1	1.97	0.46
23:C:511:CLA:HBA1	23:C:511:CLA:H3A	1.67	0.46
4:D:127:MET:HB3	4:D:147:PHE:HD2	1.80	0.46
14:O:286:THR:O	14:O:286:THR:OG1	2.33	0.46
20:Y:46:GLN:NE2	20:Y:204:GLU:OE2	2.43	0.46
37:Y:301:XAT:H34	34:Y:302:CHL:H8	1.97	0.46
22:S:174:ALA:HB1	34:S:605:CHL:HBC3	1.98	0.46
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.81	0.46
8:H:25:PRO:HB2	15:R:125:GLN:HB3	1.97	0.46
15:R:152:LEU:HB3	23:R:604:CLA:HMC2	1.97	0.46
20:Y:50:TYR:OH	20:Y:207:SER:O	2.31	0.46
3:c:156:LYS:O	3:c:159:THR:OG1	2.30	0.46
3:c:305:THR:HB	3:c:308:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:118:ALA:HB1	22:S:229:GLY:HA3	1.97	0.46
3:C:331:ALA:O	14:O:196:TYR:OH	2.33	0.46
23:R:602:CLA:H141	30:R:618:LHG:H221	1.97	0.46
3:c:174:LEU:HG	23:c:502:CLA:H171	1.95	0.46
4:d:187:GLN:HB2	23:d:404:CLA:HBC1	1.98	0.46
4:d:234:ARG:HE	26:d:402:SQD:H62	1.81	0.46
23:r:614:CLA:HED2	23:r:614:CLA:H2A	1.97	0.46
2:B:74:SER:HA	2:B:92:SER:HB2	1.97	0.46
23:B:603:CLA:HBA2	23:B:603:CLA:H3A	1.64	0.46
3:C:86:LEU:HD23	3:C:89:LEU:HB2	1.97	0.46
3:C:225:VAL:HG23	3:C:289:PHE:HA	1.97	0.46
2:b:71:ILE:HD11	23:b:606:CLA:H2A	1.96	0.46
1:A:272:HIS:HE1	31:D:403:BCT:O2	1.91	0.46
23:G:610:CLA:HBA2	23:G:610:CLA:H3A	1.72	0.46
36:R:617:NEX:H11	36:R:617:NEX:H191	1.83	0.46
2:b:155:ALA:O	2:b:159:THR:OG1	2.34	0.46
7:g:232:GLN:O	7:g:236:THR:OG1	2.32	0.46
14:o:230:LYS:HD3	14:o:284:GLU:HG3	1.97	0.46
3:C:39:ASN:N	3:C:39:ASN:ND2	2.63	0.46
3:C:451:ALA:HA	3:C:456:GLU:HB2	1.98	0.46
1:a:326:LEU:HD13	3:c:412:THR:HB	1.97	0.46
23:b:608:CLA:H62	23:b:608:CLA:H41	1.74	0.46
3:c:316:THR:HA	3:c:319:VAL:HG22	1.97	0.46
10:j:19:ILE:HA	10:j:22:ILE:HB	1.97	0.46
4:D:61:THR:OG1	4:D:62:HIS:N	2.48	0.46
18:W:117:PHE:HA	18:W:120:THR:HG22	1.98	0.46
1:A:221:SER:HA	4:D:140:ARG:HB2	1.98	0.46
34:G:608:CHL:H51	34:G:608:CHL:H11	1.76	0.46
7:N:132:PHE:HE2	20:Y:263:PRO:HG3	1.80	0.46
14:o:164:MET:HE2	14:o:202:GLN:HB2	1.97	0.46
22:S:223:VAL:HA	22:S:226:ILE:HG22	1.98	0.46
1:A:262:TYR:OH	4:D:27:ARG:O	2.34	0.46
23:C:512:CLA:H13	25:Z:101:BCR:H21C	1.97	0.46
18:W:126:ASP:OD1	18:W:127:GLU:N	2.48	0.46
1:a:129:ARG:NH2	4:d:257:ILE:O	2.49	0.46
3:c:178:LYS:HD3	23:c:502:CLA:H202	1.98	0.46
4:d:183:ILE:HG23	23:d:404:CLA:HAC1	1.97	0.46
20:y:197:LEU:HD12	35:y:315:LUT:H222	1.97	0.46
23:B:601:CLA:C3B	23:B:602:CLA:HAB	2.46	0.46
4:D:237:ASN:HB3	4:D:240:GLN:HB2	1.97	0.46
1:a:156:ALA:HA	1:a:160:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:235:GLU:HB3	2:b:473:THR:HB	1.97	0.46
4:d:126:PHE:CE2	24:d:401:PHO:HBD	2.51	0.46
22:S:179:VAL:HG13	22:S:180:VAL:HG23	1.98	0.46
22:s:81:ILE:HG22	22:s:83:GLU:H	1.81	0.46
1:A:155:THR:HG21	28:C:517:DGD:HBN1	1.98	0.45
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.97	0.45
4:D:102:PHE:O	4:D:106:CYS:HB2	2.16	0.45
23:D:401:CLA:H142	32:D:406:PL9:H453	1.98	0.45
5:e:78:GLU:HA	5:e:81:ARG:HG2	1.97	0.45
34:g:601:CHL:H12	30:g:618:LHG:H142	1.99	0.45
2:B:222:PRO:HB3	8:H:38:GLY:H	1.82	0.45
14:O:180:VAL:HA	14:O:186:VAL:HG12	1.98	0.45
14:O:212:LEU:O	14:O:307:GLN:NE2	2.45	0.45
1:a:262:TYR:OH	4:d:27:ARG:O	2.35	0.45
2:b:74:SER:HA	2:b:92:SER:HB2	1.98	0.45
23:c:505:CLA:H61	23:c:505:CLA:H41	1.67	0.45
22:s:256:LYS:HE2	22:s:264:ASN:HB3	1.97	0.45
4:D:126:PHE:CE2	24:D:402:PHO:HBD	2.52	0.45
1:a:77:ILE:HB	12:l:34:ASN:HD21	1.81	0.45
1:a:82:ILE:HB	1:a:174:LEU:HD12	1.98	0.45
7:n:161:ILE:HA	7:n:164:THR:HG22	1.98	0.45
23:S:612:CLA:HMA1	23:S:613:CLA:HBC3	1.99	0.45
7:G:51:TYR:OH	7:G:209:ALA:O	2.34	0.45
23:b:608:CLA:H93	4:d:37:LEU:HD22	1.97	0.45
3:c:27:ASP:O	3:c:31:THR:OG1	2.33	0.45
7:g:199:LEU:HD23	35:g:615:LUT:H222	1.98	0.45
23:B:612:CLA:H3A	23:B:612:CLA:HBA2	1.40	0.45
3:C:343:ARG:HH21	14:O:172:ASP:HB2	1.81	0.45
23:C:503:CLA:H112	23:C:503:CLA:H171	1.98	0.45
24:D:402:PHO:HHB	23:D:404:CLA:H142	1.97	0.45
7:N:163:ALA:HA	7:N:166:VAL:HG12	1.99	0.45
23:b:603:CLA:H41	23:b:603:CLA:H61	1.64	0.45
4:d:269:HIS:CD2	31:d:403:BCT:O3	2.46	0.45
20:y:195:ASP:OD1	35:y:315:LUT:O23	2.30	0.45
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.98	0.45
4:D:86:LEU:HD11	4:D:108:LEU:HD23	1.99	0.45
30:L:101:LHG:H292	16:T:17:ILE:HG23	1.98	0.45
15:R:116:ALA:O	15:R:128:SER:OG	2.34	0.45
15:R:199:ILE:HA	15:R:202:ILE:HG22	1.98	0.45
23:g:611:CLA:HBA2	23:g:611:CLA:H3A	1.39	0.45
34:n:307:CHL:HBA2	34:n:307:CHL:HBD	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:y:316:LUT:H15	35:y:316:LUT:H201	1.83	0.45
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.98	0.45
7:N:182:PRO:HG2	34:N:309:CHL:HBB2	1.96	0.45
23:N:312:CLA:HBB2	30:N:319:LHG:H302	1.98	0.45
7:g:216:LEU:O	7:g:220:ARG:CB	2.62	0.45
15:r:116:ALA:O	15:r:128:SER:OG	2.34	0.45
23:S:613:CLA:HBC1	35:S:614:LUT:H162	1.97	0.45
37:G:620:XAT:H15	37:G:620:XAT:H201	1.83	0.45
7:N:246:ASP:N	7:N:246:ASP:OD1	2.48	0.45
20:Y:215:LYS:NZ	23:Y:311:CLA:O1D	2.44	0.45
25:b:617:BCR:H15C	25:b:617:BCR:H351	1.81	0.45
23:B:603:CLA:HAB	23:B:605:CLA:H162	1.99	0.45
23:C:507:CLA:H42	25:C:516:BCR:H10C	1.98	0.45
4:D:146:ALA:HB2	4:D:273:LEU:HD11	1.98	0.45
4:D:222:THR:HG21	4:D:250:ALA:HB2	1.98	0.45
15:R:211:ASP:N	15:R:211:ASP:OD1	2.44	0.45
23:r:609:CLA:H51	23:r:611:CLA:H3A	1.99	0.45
22:S:256:LYS:HZ3	22:S:264:ASN:HB3	1.82	0.45
12:L:27:VAL:HG11	30:L:102:LHG:H201	1.99	0.45
4:d:20:ASP:OD1	4:d:33:TRP:NE1	2.47	0.45
23:d:404:CLA:H141	23:d:404:CLA:H162	1.84	0.45
7:g:146:TYR:HE2	23:g:604:CLA:HBA2	1.81	0.45
25:k:101:BCR:H20C	25:k:101:BCR:H361	1.86	0.45
15:r:165:TRP:HA	15:r:168:ALA:HB2	1.99	0.45
15:r:199:ILE:HA	15:r:202:ILE:HG22	1.99	0.45
20:y:234:THR:HG23	20:y:236:LYS:H	1.82	0.45
23:B:603:CLA:H143	23:B:608:CLA:HAC1	1.98	0.44
3:C:426:LEU:HD23	3:C:426:LEU:HA	1.85	0.44
7:G:120:ALA:HB2	7:G:126:PHE:HD2	1.82	0.44
23:d:405:CLA:H121	23:d:405:CLA:H193	1.98	0.44
11:k:44:PRO:HA	11:k:47:PHE:HD2	1.82	0.44
11:k:50:LEU:O	11:k:53:VAL:HB	2.17	0.44
23:S:602:CLA:H3A	23:S:602:CLA:HBA2	1.70	0.44
25:A:405:BCR:H15C	25:A:405:BCR:H351	1.86	0.44
23:D:404:CLA:H192	27:D:407:LMG:H222	1.99	0.44
23:c:510:CLA:HBA1	23:c:510:CLA:H3A	1.58	0.44
14:o:144:THR:HB	14:o:158:PHE:HB3	1.98	0.44
15:r:125:GLN:NE2	15:r:127:TYR:O	2.50	0.44
6:F:27:PHE:CE2	25:F:101:BCR:H12C	2.52	0.44
25:H:101:BCR:H371	25:H:101:BCR:H24C	1.77	0.44
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:154:ARG:HE	3:c:266:TRP:CD1	2.35	0.44
23:c:511:CLA:H62	23:c:511:CLA:H101	1.81	0.44
7:g:102:HIS:HE1	23:g:603:CLA:NA	2.15	0.44
23:r:602:CLA:H3A	23:r:602:CLA:HBA2	1.70	0.44
23:s:613:CLA:HBC1	35:s:614:LUT:H162	1.99	0.44
23:A:404:CLA:H2	27:C:501:LMG:H112	2.00	0.44
23:C:504:CLA:H142	23:C:504:CLA:H112	1.84	0.44
37:Y:301:XAT:H22	34:Y:302:CHL:HMC	1.98	0.44
23:a:403:CLA:HMB2	24:d:401:PHO:H152	1.98	0.44
3:c:307:PRO:HB2	3:c:361:LEU:HD12	2.00	0.44
3:c:406:SER:O	3:c:418:ASN:ND2	2.44	0.44
36:g:617:NEX:H15	36:g:617:NEX:H201	1.75	0.44
3:c:424:SER:O	3:c:428:THR:OG1	2.26	0.44
30:d:408:LHG:H311	16:t:21:ILE:HD11	1.99	0.44
36:r:617:NEX:H191	36:r:617:NEX:H11	1.75	0.44
30:a:412:LHG:O4	4:d:232:THR:OG1	2.36	0.44
2:b:348:ASN:OD1	2:b:352:ARG:N	2.50	0.44
4:d:69:LEU:HD13	6:f:34:MET:HG2	1.99	0.44
36:g:617:NEX:H35	36:g:617:NEX:H401	1.79	0.44
25:h:101:BCR:H371	25:h:101:BCR:H24C	1.79	0.44
7:G:194:GLY:N	7:G:197:ASP:OD1	2.50	0.44
25:a:406:BCR:H24C	25:a:406:BCR:H371	1.84	0.44
3:c:178:LYS:HD2	3:c:182:PHE:HB2	1.99	0.44
3:c:402:GLY:HA2	3:c:420:VAL:HG13	1.99	0.44
7:g:114:VAL:HG22	7:g:241:ILE:HD11	1.99	0.44
12:l:5:ASN:HB3	12:l:8:GLU:HG3	1.99	0.44
7:n:158:ILE:HA	7:n:161:ILE:HG22	2.00	0.44
15:r:108:ASP:OD1	15:r:108:ASP:N	2.50	0.44
37:y:301:XAT:H34	34:y:302:CHL:H8	2.00	0.44
22:s:176:VAL:HA	22:s:179:VAL:HG12	1.98	0.44
25:A:405:BCR:H11C	25:A:405:BCR:H341	1.87	0.44
23:C:502:CLA:HBC2	23:C:503:CLA:H51	2.00	0.44
11:K:30:TYR:OH	21:Z:58:ASN:OD1	2.35	0.44
25:Z:101:BCR:H24C	25:Z:101:BCR:H371	1.74	0.44
1:a:269:ARG:HH21	4:d:223:LEU:HD13	1.83	0.44
2:b:66:MET:HB3	2:b:71:ILE:HB	2.00	0.44
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.99	0.44
4:d:190:HIS:HE1	4:d:293:ASN:HD22	1.65	0.44
7:g:149:ASN:HD22	7:g:152:LEU:HD22	1.82	0.44
23:s:612:CLA:H3A	23:s:612:CLA:HBA2	1.70	0.44
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LEU:HD22	23:R:614:CLA:H3A	2.00	0.44
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.85	0.44
3:c:252:ILE:HG22	3:c:253:LEU:HD23	1.99	0.44
28:c:516:DGD:HB82	28:c:516:DGD:HBE1	1.86	0.44
35:r:615:LUT:H15	35:r:615:LUT:H201	1.86	0.44
2:B:348:ASN:OD1	2:B:352:ARG:N	2.51	0.43
8:H:35:PRO:HB3	15:R:90:LEU:HD23	2.00	0.43
30:b:622:LHG:HC82	4:d:270:PHE:HE2	1.82	0.43
1:A:38:ILE:O	1:A:42:LEU:HB2	2.18	0.43
2:B:257:TRP:HB2	2:B:452:THR:HG21	2.00	0.43
23:G:610:CLA:CBB	35:G:615:LUT:H32	2.48	0.43
7:N:240:PRO:O	35:N:316:LUT:O3	2.36	0.43
34:Y:309:CHL:H3A	34:Y:309:CHL:HBA2	1.86	0.43
1:a:85:THR:HA	1:a:109:GLY:HA3	1.99	0.43
25:b:619:BCR:H24C	25:b:619:BCR:H371	1.79	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.88	0.43
4:d:90:LEU:HG	8:h:62:ASN:HD22	1.83	0.43
4:d:210:LEU:HD22	32:d:407:PL9:H162	1.99	0.43
7:g:166:VAL:HG23	34:g:609:CHL:HBB2	1.99	0.43
34:g:607:CHL:HED1	7:n:264:VAL:HG13	2.00	0.43
35:g:615:LUT:H35	35:g:615:LUT:H401	1.83	0.43
23:r:601:CLA:H3A	23:r:601:CLA:HBA1	1.73	0.43
23:r:611:CLA:H2A	23:r:611:CLA:HED2	2.00	0.43
23:y:303:CLA:H3A	23:y:303:CLA:HBA2	1.46	0.43
22:S:237:LEU:HD13	23:S:603:CLA:HBB2	1.99	0.43
25:A:405:BCR:H24C	25:A:405:BCR:H371	1.85	0.43
2:B:263:THR:O	2:B:263:THR:OG1	2.30	0.43
3:C:64:ALA:O	3:C:68:ASN:HB2	2.18	0.43
25:C:515:BCR:H321	22:S:267:LEU:HD22	1.99	0.43
7:N:214:LYS:O	7:N:218:ASN:HB2	2.19	0.43
35:N:317:LUT:H15	35:N:317:LUT:H201	1.83	0.43
2:b:321:LYS:NZ	2:b:363:PHE:O	2.51	0.43
4:d:22:TRP:HE3	4:d:23:LEU:HD22	1.82	0.43
15:r:67:TRP:HE1	15:r:85:LYS:HG3	1.84	0.43
15:r:259:GLN:HE22	35:r:615:LUT:H42	1.82	0.43
36:r:617:NEX:H15	36:r:617:NEX:H201	1.77	0.43
35:s:614:LUT:H193	30:s:617:LHG:H381	2.00	0.43
23:B:608:CLA:H62	23:B:608:CLA:H41	1.70	0.43
30:G:618:LHG:HC92	37:G:620:XAT:H361	2.00	0.43
15:R:66:ASP:OD1	15:R:66:ASP:N	2.47	0.43
23:b:601:CLA:H141	23:b:601:CLA:H162	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:601:CLA:H93	25:h:101:BCR:H402	2.00	0.43
15:r:168:ALA:HB1	23:r:604:CLA:HED1	1.99	0.43
34:y:309:CHL:H3A	34:y:309:CHL:HBA2	1.76	0.43
22:S:176:VAL:HA	22:S:179:VAL:HG12	2.00	0.43
2:B:240:SER:OG	23:B:608:CLA:OBD	2.36	0.43
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.82	0.43
3:C:154:ARG:HE	3:C:266:TRP:CD1	2.36	0.43
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.31	0.43
4:D:295:ARG:HG3	4:D:297:TYR:HB2	2.00	0.43
4:D:337:HIS:CD2	4:D:338:GLU:HG2	2.54	0.43
35:Y:315:LUT:H35	35:Y:315:LUT:H401	1.82	0.43
23:c:510:CLA:H101	23:c:510:CLA:H13	1.80	0.43
23:c:511:CLA:H13	25:c:518:BCR:H19C	1.99	0.43
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.88	0.43
4:d:55:PHE:O	5:e:49:SER:OG	2.36	0.43
4:d:125:GLY:HA2	4:d:128:LEU:HD12	2.00	0.43
5:e:23:HIS:HA	5:e:26:THR:HG22	2.00	0.43
23:D:404:CLA:H141	23:D:404:CLA:H162	1.79	0.43
7:G:114:VAL:HG13	7:G:241:ILE:HD11	2.00	0.43
8:H:60:ILE:HD13	8:H:65:VAL:HG23	2.01	0.43
23:Y:311:CLA:H92	23:Y:311:CLA:H61	1.90	0.43
27:a:407:LMG:H332	27:a:407:LMG:H302	1.79	0.43
23:c:510:CLA:H101	23:c:510:CLA:H62	1.87	0.43
34:g:606:CHL:HMC	35:g:616:LUT:H22	2.00	0.43
22:S:221:LEU:HB3	23:S:609:CLA:HHB	2.01	0.43
28:A:408:DGD:HAE2	28:A:408:DGD:HA81	1.89	0.43
2:B:23:HIS:ND1	23:B:615:CLA:OBD	2.43	0.43
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.50	0.43
3:C:265:VAL:HG22	18:W:131:LEU:HB2	1.99	0.43
3:C:401:LEU:HD21	3:C:410:VAL:HG22	1.99	0.43
23:C:504:CLA:H143	23:C:504:CLA:H61	2.00	0.43
7:G:102:HIS:HE1	23:G:603:CLA:NA	2.16	0.43
23:G:603:CLA:HBB1	34:G:609:CHL:H13	2.00	0.43
25:c:515:BCR:H351	25:c:515:BCR:H15C	1.77	0.43
23:g:610:CLA:H3A	23:g:610:CLA:HBA2	1.69	0.43
7:n:177:VAL:HG11	20:y:58:LEU:HD13	2.01	0.43
21:z:26:VAL:HG21	21:z:40:VAL:HB	2.01	0.43
7:N:59:LEU:HB3	7:N:62:PHE:HB2	2.01	0.43
35:N:317:LUT:H35	35:N:317:LUT:H401	1.91	0.43
2:b:315:ILE:HG12	2:b:321:LYS:HG3	2.01	0.43
15:r:139:CYS:O	15:r:143:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:r:607:CHL:H2	34:r:607:CHL:H62	1.68	0.43
37:y:301:XAT:H35	37:y:301:XAT:H401	1.88	0.43
23:y:311:CLA:H92	23:y:311:CLA:H61	1.85	0.43
35:S:615:LUT:H35	35:S:615:LUT:H401	1.90	0.43
37:G:620:XAT:H35	37:G:620:XAT:H401	1.87	0.43
26:M:101:SQD:H61	26:M:101:SQD:H92	1.99	0.43
37:Y:301:XAT:H201	37:Y:301:XAT:H15	1.79	0.43
23:a:401:CLA:H61	23:a:401:CLA:H41	1.75	0.43
25:c:518:BCR:H371	25:c:518:BCR:H24C	1.79	0.43
37:n:301:XAT:H15	37:n:301:XAT:H201	1.88	0.43
1:A:217:SER:O	1:A:221:SER:CB	2.67	0.43
7:N:172:VAL:HG21	36:N:318:NEX:H34	2.01	0.43
15:R:141:LEU:HD23	15:R:141:LEU:HA	1.79	0.43
3:c:262:ARG:NH2	18:w:120:THR:OG1	2.52	0.43
30:d:408:LHG:H261	30:d:408:LHG:H121	2.00	0.43
23:g:604:CLA:HMB2	36:g:617:NEX:H383	2.01	0.43
15:r:222:PHE:HB3	34:r:607:CHL:H8	2.01	0.43
23:A:402:CLA:HMB2	24:D:402:PHO:H152	2.00	0.42
24:A:403:PHO:H8	24:A:403:PHO:H122	1.78	0.42
30:C:518:LHG:H171	30:C:518:LHG:H202	1.88	0.42
35:R:615:LUT:H35	35:R:615:LUT:H401	1.88	0.42
20:Y:102:SER:HB3	20:Y:217:GLY:HA3	2.01	0.42
22:s:187:TYR:HA	22:s:190:ILE:HG22	2.01	0.42
2:B:391:SER:OG	2:B:392:VAL:N	2.51	0.42
23:B:613:CLA:H111	23:B:613:CLA:H72	1.88	0.42
27:C:501:LMG:HC2	18:W:95:GLY:HA3	2.01	0.42
4:D:160:ILE:HG21	4:D:288:VAL:HG22	2.01	0.42
23:D:401:CLA:H162	30:L:101:LHG:H212	2.00	0.42
7:G:54:ASP:OD1	7:G:54:ASP:N	2.51	0.42
7:G:240:PRO:O	35:G:615:LUT:O3	2.38	0.42
1:a:221:SER:HA	4:d:140:ARG:HB2	2.00	0.42
2:b:489:GLN:HG2	2:b:490:VAL:HG13	2.01	0.42
23:b:614:CLA:H52	23:b:614:CLA:H8	1.72	0.42
3:c:89:LEU:HD23	3:c:89:LEU:HA	1.83	0.42
3:c:318:LEU:HG	3:c:328:VAL:HG11	2.01	0.42
23:c:503:CLA:H143	23:c:503:CLA:H61	2.00	0.42
24:d:401:PHO:H3A	23:d:404:CLA:H142	2.00	0.42
7:n:224:PHE:HZ	23:n:314:CLA:H92	1.84	0.42
23:r:610:CLA:HBC2	30:r:618:LHG:HC92	2.00	0.42
3:C:66:ALA:HA	11:K:40:MET:HE2	2.01	0.42
34:G:607:CHL:HED1	7:N:264:VAL:HG13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:101:BCR:HC22	21:Z:16:SER:HB2	2.01	0.42
15:R:127:TYR:OH	15:R:215:ARG:NE	2.52	0.42
15:R:202:ILE:HD11	34:R:607:CHL:C4B	2.49	0.42
23:R:614:CLA:H3A	23:R:614:CLA:HBA2	1.71	0.42
20:Y:175:ARG:HH21	34:Y:309:CHL:HMA3	1.83	0.42
25:Z:101:BCR:H15C	25:Z:101:BCR:H351	1.83	0.42
30:a:412:LHG:H131	30:a:412:LHG:H102	1.84	0.42
23:b:603:CLA:HBA2	23:b:603:CLA:H3A	1.63	0.42
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.87	0.42
23:c:502:CLA:H151	23:c:502:CLA:H112	1.80	0.42
36:n:318:NEX:H191	36:n:318:NEX:H11	1.79	0.42
14:o:185:SER:HA	14:o:222:GLY:O	2.19	0.42
22:s:238:GLY:O	22:s:242:GLN:HG3	2.18	0.42
14:O:164:MET:HE2	14:O:202:GLN:HB2	2.02	0.42
3:c:72:VAL:O	11:k:25:LYS:N	2.53	0.42
3:c:206:PRO:O	3:c:210:PHE:HB2	2.19	0.42
30:r:618:LHG:H111	30:r:618:LHG:H272	2.01	0.42
23:A:401:CLA:H41	23:A:401:CLA:H61	1.75	0.42
23:B:602:CLA:H42	28:H:102:DGD:HB22	2.01	0.42
3:C:223:TRP:HE3	28:C:517:DGD:HB21	1.85	0.42
6:F:27:PHE:HD2	25:F:101:BCR:H14C	1.84	0.42
7:G:94:ARG:HA	7:G:94:ARG:HD3	1.94	0.42
26:L:103:SQD:H441	26:L:103:SQD:H102	2.02	0.42
30:d:408:LHG:H292	16:t:17:ILE:HG23	2.02	0.42
5:e:72:SER:O	5:e:76:LEU:HB2	2.19	0.42
34:n:309:CHL:H143	34:n:309:CHL:H111	1.90	0.42
20:y:160:ILE:HD13	34:y:306:CHL:HAC1	2.01	0.42
22:S:238:GLY:O	22:S:242:GLN:HG3	2.20	0.42
34:S:606:CHL:HHB	35:S:615:LUT:H172	2.01	0.42
22:s:113:PHE:O	22:s:117:HIS:ND1	2.34	0.42
36:s:616:NEX:H35	36:s:616:NEX:H401	1.94	0.42
2:B:311:PHE:O	2:B:317:ASN:ND2	2.52	0.42
35:G:615:LUT:H35	35:G:615:LUT:H401	1.82	0.42
7:N:51:TYR:HE1	7:N:75:PRO:HA	1.84	0.42
34:N:307:CHL:HBA2	34:N:307:CHL:HBD	2.02	0.42
20:Y:238:PRO:O	35:Y:315:LUT:O3	2.34	0.42
23:Y:303:CLA:H3A	23:Y:303:CLA:HBA2	1.45	0.42
23:b:605:CLA:H141	23:b:610:CLA:HMA2	2.01	0.42
3:c:36:TRP:CE2	26:d:402:SQD:H461	2.54	0.42
7:g:240:PRO:O	35:g:615:LUT:O3	2.37	0.42
15:r:234:LYS:HB2	15:r:237:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:408:DGD:HA41	28:A:408:DGD:HB81	2.02	0.42
7:G:59:LEU:HB3	7:G:62:PHE:HB2	2.01	0.42
36:R:617:NEX:H15	36:R:617:NEX:H201	1.78	0.42
7:g:101:ILE:HA	7:g:104:ARG:HD2	2.02	0.42
10:j:16:VAL:HA	10:j:19:ILE:HG22	2.01	0.42
12:l:22:LEU:HB3	16:t:16:ILE:HD13	2.02	0.42
36:n:318:NEX:H15	36:n:318:NEX:H201	1.82	0.42
15:r:231:ASP:OD1	15:r:231:ASP:N	2.50	0.42
22:S:239:PHE:CZ	35:S:614:LUT:H8	2.54	0.42
34:S:601:CHL:H3A	34:S:601:CHL:HBA1	1.75	0.42
22:s:173:LEU:HA	22:s:176:VAL:HG12	2.02	0.42
26:A:409:SQD:H282	26:A:409:SQD:H312	1.93	0.42
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.01	0.42
23:B:610:CLA:H8	23:B:610:CLA:H51	1.80	0.42
23:B:615:CLA:H112	23:B:616:CLA:H152	2.01	0.42
11:K:44:PRO:HA	11:K:47:PHE:HD2	1.85	0.42
25:K:101:BCR:H11C	25:K:101:BCR:H341	1.93	0.42
34:N:309:CHL:H143	34:N:309:CHL:H111	1.89	0.42
23:a:402:CLA:H142	32:d:407:PL9:H453	2.02	0.42
2:b:216:HIS:HD2	23:b:609:CLA:HED2	1.84	0.42
25:c:514:BCR:H11C	25:c:514:BCR:H341	1.80	0.42
4:d:91:LEU:HD23	4:d:91:LEU:HA	1.93	0.42
25:d:406:BCR:H12C	6:f:27:PHE:CE2	2.55	0.42
37:n:301:XAT:H31	37:n:301:XAT:H391	1.91	0.42
35:n:317:LUT:H15	35:n:317:LUT:H201	1.86	0.42
14:o:140:PRO:HA	14:o:325:GLY:HA3	2.00	0.42
1:A:293:MET:HA	1:A:297:LEU:H	1.84	0.42
26:a:409:SQD:H312	26:a:409:SQD:H162	2.02	0.42
2:b:140:GLY:HA3	2:b:217:LEU:HB2	2.01	0.42
5:e:24:SER:HA	5:e:27:ILE:HG22	2.01	0.42
5:e:28:PRO:HA	5:e:31:PHE:HB3	2.01	0.42
20:y:209:LEU:HD23	20:y:212:LYS:HD2	2.01	0.42
1:A:48:PHE:O	1:A:52:PHE:HB2	2.20	0.42
3:C:33:PHE:HB2	3:C:41:ARG:HG3	2.01	0.42
25:C:516:BCR:H351	25:C:516:BCR:H15C	1.77	0.42
7:G:214:LYS:HE2	23:G:612:CLA:HAA2	2.02	0.42
7:N:231:VAL:HG11	23:N:314:CLA:HAC2	2.01	0.42
36:N:318:NEX:H35	36:N:318:NEX:H401	1.82	0.42
21:Z:19:LEU:HD21	21:Z:44:THR:HG22	2.02	0.42
27:a:407:LMG:HC2	18:w:95:GLY:HA3	2.02	0.42
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:n:318:NEX:H35	36:n:318:NEX:H401	1.77	0.42
15:r:242:GLU:OE1	23:r:609:CLA:C4A	2.68	0.42
1:A:316:THR:N	1:A:319:ASP:OD2	2.52	0.41
3:C:388:GLN:O	3:C:392:SER:OG	2.35	0.41
11:K:33:LEU:HG	11:K:37:VAL:HG23	2.02	0.41
23:b:603:CLA:HAC2	23:b:606:CLA:HBB2	2.02	0.41
23:g:603:CLA:HBA1	23:g:603:CLA:H3A	1.89	0.41
7:n:248:LEU:HB2	23:n:315:CLA:HBB1	2.02	0.41
35:y:315:LUT:H35	35:y:315:LUT:H401	1.85	0.41
22:S:170:ASN:HB2	22:S:173:LEU:HG	2.00	0.41
27:B:620:LMG:H341	27:B:620:LMG:H372	1.83	0.41
27:D:407:LMG:HC62	6:F:35:GLN:HG2	2.01	0.41
34:G:601:CHL:HBC1	30:G:618:LHG:HC11	2.02	0.41
34:G:619:CHL:H112	34:Y:309:CHL:H152	2.02	0.41
30:W:201:LHG:H122	30:W:201:LHG:H152	1.83	0.41
2:b:25:MET:HE1	2:b:108:PHE:HD1	1.85	0.41
2:b:42:LEU:HD13	2:b:94:GLU:HG3	2.01	0.41
2:b:231:MET:HB2	23:b:610:CLA:HAC2	2.02	0.41
2:b:474:LEU:O	4:d:135:ARG:NH1	2.53	0.41
23:c:501:CLA:H192	23:c:501:CLA:H161	1.90	0.41
30:c:517:LHG:H321	30:c:517:LHG:H352	1.87	0.41
35:S:614:LUT:H193	30:S:617:LHG:H381	2.01	0.41
23:C:509:CLA:H43	23:C:512:CLA:HAC1	2.02	0.41
23:C:514:CLA:H101	25:C:515:BCR:H21C	2.02	0.41
7:G:239:GLY:HA2	7:G:240:PRO:HD3	1.88	0.41
37:G:620:XAT:H31	37:G:620:XAT:H391	1.86	0.41
34:R:607:CHL:H62	34:R:607:CHL:H2	1.70	0.41
3:c:464:GLU:HA	3:c:465:PRO:HD3	1.79	0.41
7:g:153:VAL:HA	34:g:605:CHL:C4D	2.51	0.41
25:h:101:BCR:H20C	25:h:101:BCR:H361	1.84	0.41
1:A:9:GLU:HB3	1:A:10:SER:H	1.72	0.41
3:C:60:ILE:HG23	23:C:511:CLA:HMC2	2.03	0.41
3:C:132:HIS:CE1	23:C:514:CLA:NA	2.87	0.41
4:D:127:MET:HB2	4:D:144:ALA:HB1	2.01	0.41
23:G:602:CLA:H171	35:G:616:LUT:H393	2.01	0.41
25:H:101:BCR:H20C	25:H:101:BCR:H361	1.82	0.41
23:R:609:CLA:H202	23:R:609:CLA:H162	1.94	0.41
23:b:608:CLA:H43	23:b:609:CLA:H101	2.03	0.41
27:b:620:LMG:H341	27:b:620:LMG:H372	1.82	0.41
3:c:331:ALA:O	14:o:196:TYR:OH	2.34	0.41
23:g:611:CLA:H91	23:g:611:CLA:H112	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:220:LEU:HA	22:S:223:VAL:HG12	2.02	0.41
22:S:227:LYS:HE3	30:S:617:LHG:HC62	2.02	0.41
23:B:603:CLA:HAC2	23:B:606:CLA:HBB2	2.03	0.41
17:U:97:THR:HA	17:U:102:ARG:HH21	1.84	0.41
1:a:95:PRO:HD2	1:a:98:GLU:HB2	2.01	0.41
28:a:408:DGD:O3D	14:o:162:LYS:NZ	2.54	0.41
2:b:54:PRO:HD2	2:b:57:ARG:HB2	2.01	0.41
2:b:458:PHE:HB3	23:b:604:CLA:HBC2	2.02	0.41
14:o:145:VAL:HG22	14:o:321:VAL:HG23	2.02	0.41
22:S:141:CYS:HA	22:S:163:PHE:HA	2.02	0.41
22:S:231:LEU:HD13	23:S:610:CLA:HBC1	2.03	0.41
35:S:614:LUT:H15	35:S:614:LUT:H201	1.94	0.41
25:A:405:BCR:H20C	25:A:405:BCR:H361	1.86	0.41
2:B:276:ASP:HA	17:U:95:MET:HE1	2.02	0.41
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.79	0.41
3:C:89:LEU:HD23	3:C:89:LEU:HA	1.81	0.41
7:G:98:LEU:HD21	34:G:609:CHL:HED3	2.01	0.41
37:Y:301:XAT:H31	37:Y:301:XAT:H391	1.78	0.41
1:a:288:LEU:HD12	3:c:432:VAL:HG22	2.02	0.41
23:b:605:CLA:H142	23:b:605:CLA:H112	1.94	0.41
25:b:617:BCR:H11C	25:b:617:BCR:H341	1.80	0.41
3:c:117:LEU:HD23	3:c:117:LEU:HA	1.91	0.41
23:g:614:CLA:HMA2	20:y:158:LEU:HD11	2.02	0.41
37:g:620:XAT:H31	37:g:620:XAT:H391	1.87	0.41
15:r:232:PRO:HA	15:r:235:THR:HB	2.01	0.41
23:C:510:CLA:HBD	23:C:510:CLA:H121	2.03	0.41
23:C:513:CLA:H3A	23:C:513:CLA:HBA1	1.67	0.41
33:E:101:HEM:HHC	33:E:101:HEM:HBB2	2.03	0.41
14:O:112:ASN:HD21	14:O:169:TYR:H	1.69	0.41
15:R:238:LEU:HG	23:R:609:CLA:H3A	2.03	0.41
20:Y:106:MET:SD	23:Y:310:CLA:HAB	2.61	0.41
1:a:172:MET:HA	1:a:173:PRO:HD3	1.94	0.41
23:c:508:CLA:H43	23:c:511:CLA:HAC1	2.02	0.41
23:c:512:CLA:H3A	23:c:512:CLA:HBA1	1.77	0.41
7:g:130:VAL:HG13	7:g:240:PRO:HD3	2.01	0.41
34:g:608:CHL:HMB1	34:g:608:CHL:H122	2.03	0.41
14:o:180:VAL:HA	14:o:186:VAL:HG12	2.02	0.41
20:y:167:LEU:HD23	20:y:167:LEU:HA	1.94	0.41
36:s:616:NEX:H15	36:s:616:NEX:H201	1.77	0.41
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.86	0.41
4:D:22:TRP:HD1	4:D:23:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:HA	4:D:30:PHE:HE1	1.85	0.41
7:G:77:ASP:HA	23:G:602:CLA:HED3	2.03	0.41
36:G:617:NEX:H35	36:G:617:NEX:H401	1.78	0.41
11:K:50:LEU:O	11:K:53:VAL:HB	2.20	0.41
7:N:226:MET:HB3	35:N:317:LUT:H14	2.01	0.41
23:N:314:CLA:H93	30:N:319:LHG:H172	2.03	0.41
15:R:253:PHE:HA	15:R:256:PHE:HB2	2.02	0.41
25:a:406:BCR:H15C	25:a:406:BCR:H351	1.85	0.41
3:c:118:HIS:HE1	23:c:503:CLA:NC	2.18	0.41
23:c:503:CLA:H202	23:c:503:CLA:H162	1.91	0.41
7:g:119:LEU:O	7:g:123:GLY:N	2.54	0.41
15:r:184:LEU:HA	15:r:184:LEU:HD12	1.87	0.41
22:S:187:TYR:HA	22:S:190:ILE:HG22	2.02	0.41
35:S:614:LUT:H35	35:S:614:LUT:H401	1.91	0.41
30:A:412:LHG:H242	30:A:412:LHG:H271	1.84	0.41
2:B:321:LYS:NZ	2:B:363:PHE:O	2.53	0.41
2:B:366:PHE:O	2:B:425:GLN:NE2	2.46	0.41
2:B:372:ASP:OD1	2:B:376:ILE:N	2.54	0.41
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	2.02	0.41
23:B:612:CLA:H93	23:B:612:CLA:H62	1.93	0.41
27:B:620:LMG:H162	27:B:620:LMG:H192	1.88	0.41
3:C:294:ASN:H	28:C:517:DGD:HE61	1.86	0.41
32:D:406:PL9:H121	30:L:101:LHG:H101	2.03	0.41
13:M:28:LYS:HG3	13:m:31:SER:HB2	2.02	0.41
35:N:316:LUT:H31	35:N:316:LUT:H391	1.89	0.41
1:a:174:LEU:HD22	24:a:404:PHO:H151	2.03	0.41
1:a:195:HIS:CD2	1:a:197:PHE:HB2	2.56	0.41
2:b:240:SER:OG	23:b:608:CLA:OBD	2.38	0.41
23:b:602:CLA:H42	28:d:410:DGD:HB22	2.03	0.41
23:b:609:CLA:OBD	8:h:39:THR:OG1	2.32	0.41
23:b:610:CLA:HHC	23:b:610:CLA:HAB	1.91	0.41
3:c:229:ASP:HB3	3:c:231:GLU:H	1.85	0.41
23:c:511:CLA:HBA1	25:c:518:BCR:H271	2.03	0.41
4:d:54:THR:HG23	6:f:34:MET:HE1	2.03	0.41
4:d:186:PHE:CD1	4:d:190:HIS:HD2	2.39	0.41
4:d:330:MET:O	4:d:334:ASP:HB2	2.19	0.41
32:d:407:PL9:H121	30:d:408:LHG:H101	2.03	0.41
30:d:408:LHG:H132	30:d:408:LHG:H281	2.03	0.41
7:g:81:ASP:OD1	35:g:616:LUT:O23	2.39	0.41
34:g:601:CHL:HBA1	34:g:601:CHL:H3A	1.91	0.41
34:g:608:CHL:H11	34:g:608:CHL:H51	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:187:GLU:H	7:n:192:PRO:HA	1.86	0.41
23:y:312:CLA:H112	23:y:312:CLA:H91	1.89	0.41
23:B:605:CLA:H141	23:B:610:CLA:HMA2	2.04	0.41
23:B:614:CLA:H52	23:B:614:CLA:H8	1.71	0.41
25:C:515:BCR:H11C	25:C:515:BCR:H341	1.84	0.41
30:C:518:LHG:H352	30:C:518:LHG:H321	1.90	0.41
5:E:69:ARG:NH2	8:H:63:SER:O	2.55	0.41
7:G:211:LEU:HA	7:G:214:LYS:HG2	2.03	0.41
34:N:310:CHL:H93	34:N:310:CHL:H111	1.90	0.41
14:O:288:LYS:HB2	14:O:288:LYS:HE2	1.82	0.41
2:b:55:MET:HE2	2:b:55:MET:HB3	1.87	0.41
7:g:105:TRP:HB2	35:g:616:LUT:H202	2.03	0.41
7:g:120:ALA:HA	7:g:124:VAL:H	1.85	0.41
20:y:106:MET:SD	23:y:310:CLA:HAB	2.61	0.41
23:B:601:CLA:H143	25:H:101:BCR:H21C	2.02	0.40
27:B:620:LMG:H392	13:M:14:PHE:HD1	1.86	0.40
34:R:607:CHL:H92	34:R:607:CHL:H61	1.91	0.40
3:c:53:HIS:CD2	23:c:509:CLA:NA	2.90	0.40
23:c:509:CLA:H13	23:c:512:CLA:C3D	2.50	0.40
23:c:510:CLA:H43	23:c:510:CLA:HED1	2.02	0.40
7:g:56:VAL:HB	34:g:601:CHL:HBC1	2.03	0.40
34:g:619:CHL:H143	34:g:619:CHL:H161	1.92	0.40
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.96	0.40
23:C:506:CLA:H41	23:C:506:CLA:H61	1.67	0.40
23:G:603:CLA:HBA1	23:G:603:CLA:H3A	1.93	0.40
37:G:620:XAT:H11	37:G:620:XAT:H191	1.89	0.40
9:I:21:PHE:HD2	18:W:112:ILE:HG22	1.86	0.40
13:M:27:VAL:HG12	13:m:28:LYS:HB2	2.03	0.40
25:b:618:BCR:H11C	25:b:618:BCR:H341	1.92	0.40
27:b:620:LMG:H192	27:b:620:LMG:H162	1.87	0.40
3:c:190:ALA:HB3	3:c:194:GLY:HA2	2.02	0.40
23:c:503:CLA:H142	23:c:503:CLA:H112	1.88	0.40
23:c:508:CLA:H122	11:k:48:LEU:HD22	2.03	0.40
23:c:513:CLA:H121	25:c:514:BCR:H19C	2.03	0.40
23:g:602:CLA:H171	35:g:616:LUT:H393	2.02	0.40
7:n:80:TRP:HE1	7:n:82:THR:HB	1.86	0.40
23:r:608:CLA:HBA2	23:r:608:CLA:H3A	1.63	0.40
37:y:301:XAT:H22	34:y:302:CHL:HMC	2.02	0.40
35:s:614:LUT:H31	35:s:614:LUT:H391	1.98	0.40
23:B:615:CLA:H193	23:B:615:CLA:H161	1.94	0.40
23:C:510:CLA:H13	23:C:513:CLA:C3D	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:516:BCR:H20C	25:C:516:BCR:H361	1.95	0.40
34:G:601:CHL:HBA1	34:G:601:CHL:H3A	1.86	0.40
36:G:617:NEX:H201	36:G:617:NEX:H15	1.74	0.40
20:Y:117:ILE:HD13	20:Y:117:ILE:HA	1.91	0.40
35:Y:316:LUT:H35	35:Y:316:LUT:H401	1.95	0.40
3:c:174:LEU:HD11	23:s:613:CLA:HMB1	2.04	0.40
3:c:262:ARG:HD2	9:i:26:ASN:HB2	2.03	0.40
23:c:511:CLA:H2	11:k:54:TRP:HH2	1.85	0.40
4:d:69:LEU:HD12	6:f:37:ILE:HG21	2.03	0.40
9:i:5:LYS:HD2	18:w:85:MET:HE1	2.03	0.40
17:u:90:GLN:HA	17:u:93:VAL:HG22	2.02	0.40
18:w:117:PHE:HA	18:w:120:THR:HG22	2.02	0.40
30:w:201:LHG:H122	30:w:201:LHG:H152	1.84	0.40
22:s:239:PHE:CZ	35:s:614:LUT:H8	2.56	0.40
1:A:84:PRO:HA	1:A:112:TYR:CG	2.57	0.40
2:B:124:CYS:SG	2:B:125:ASP:N	2.94	0.40
4:D:123:LEU:HD22	24:D:402:PHO:H41	2.04	0.40
5:E:63:ILE:HA	5:E:64:PRO:HD3	1.93	0.40
11:K:35:PRO:O	11:K:38:ASP:HB2	2.22	0.40
1:a:289:GLY:O	1:a:293:MET:HG3	2.21	0.40
2:b:5:TRP:HZ3	23:b:611:CLA:H51	1.87	0.40
30:b:622:LHG:H201	12:l:27:VAL:HG11	2.03	0.40
3:c:116:VAL:HG21	25:c:514:BCR:HC32	2.04	0.40
3:c:130:ILE:HD11	23:c:511:CLA:H161	2.03	0.40
28:d:410:DGD:HBN1	28:d:410:DGD:HBW1	1.83	0.40
7:g:82:THR:HG21	34:y:309:CHL:HAA2	2.02	0.40
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.97	0.40
7:n:204:ASP:OD1	7:n:207:ALA:N	2.45	0.40
23:B:605:CLA:H92	23:B:605:CLA:H62	1.93	0.40
3:C:116:VAL:HG11	25:C:515:BCR:HC32	2.02	0.40
15:R:165:TRP:HA	15:R:168:ALA:HB2	2.03	0.40
1:a:38:ILE:O	1:a:42:LEU:HB2	2.21	0.40
4:d:146:ALA:HB2	4:d:273:LEU:HD11	2.04	0.40
14:o:313:LEU:HD23	14:o:313:LEU:HA	1.93	0.40
22:s:186:GLU:HA	22:s:189:ARG:HD3	2.04	0.40
23:s:612:CLA:H51	23:s:612:CLA:H8	1.89	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	330/353 (94%)	314 (95%)	16 (5%)	0	100	100
1	a	330/353 (94%)	313 (95%)	17 (5%)	0	100	100
2	B	487/508 (96%)	465 (96%)	22 (4%)	0	100	100
2	b	487/508 (96%)	468 (96%)	19 (4%)	0	100	100
3	C	447/473 (94%)	415 (93%)	32 (7%)	0	100	100
3	c	447/473 (94%)	416 (93%)	31 (7%)	0	100	100
4	D	337/353 (96%)	321 (95%)	16 (5%)	0	100	100
4	d	337/353 (96%)	320 (95%)	17 (5%)	0	100	100
5	E	64/83 (77%)	64 (100%)	0	0	100	100
5	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
6	F	27/39 (69%)	26 (96%)	1 (4%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	G	217/267 (81%)	209 (96%)	7 (3%)	1 (0%)	25	58
7	N	217/267 (81%)	198 (91%)	19 (9%)	0	100	100
7	g	217/267 (81%)	204 (94%)	13 (6%)	0	100	100
7	n	217/267 (81%)	201 (93%)	16 (7%)	0	100	100
8	H	57/73 (78%)	54 (95%)	3 (5%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
9	i	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
10	J	27/40 (68%)	26 (96%)	1 (4%)	0	100	100
10	j	27/40 (68%)	27 (100%)	0	0	100	100
11	K	35/61 (57%)	34 (97%)	1 (3%)	0	100	100
11	k	35/61 (57%)	33 (94%)	2 (6%)	0	100	100
12	L	35/38 (92%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	35/38 (92%)	35 (100%)	0	0	100	100
13	M	30/34 (88%)	28 (93%)	2 (7%)	0	100	100
13	m	30/34 (88%)	28 (93%)	2 (7%)	0	100	100
14	O	194/332 (58%)	182 (94%)	12 (6%)	0	100	100
14	o	194/332 (58%)	183 (94%)	11 (6%)	0	100	100
15	R	220/300 (73%)	211 (96%)	9 (4%)	0	100	100
15	r	220/300 (73%)	209 (95%)	11 (5%)	0	100	100
16	T	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
16	t	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
17	U	21/103 (20%)	20 (95%)	1 (5%)	0	100	100
17	u	21/103 (20%)	20 (95%)	1 (5%)	0	100	100
18	W	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
18	w	52/133 (39%)	50 (96%)	2 (4%)	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%)	203 (93%)	14 (6%)	1 (0%)	25	58
20	y	218/265 (82%)	208 (95%)	9 (4%)	1 (0%)	25	58
21	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
21	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
22	S	219/280 (78%)	202 (92%)	17 (8%)	0	100	100
22	s	219/280 (78%)	206 (94%)	13 (6%)	0	100	100
All	All	6776/8498 (80%)	6419 (95%)	354 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	Y	152	ILE
20	y	152	ILE
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	269/285 (94%)	269 (100%)	0	100	100
1	a	269/285 (94%)	269 (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%)	350 (99%)	2 (1%)	84	91
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	59/73 (81%)	59 (100%)	0	100	100
5	e	59/73 (81%)	59 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (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%)	35 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	o	170/268 (63%)	170 (100%)	0	100	100
15	R	176/231 (76%)	176 (100%)	0	100	100
15	r	176/231 (76%)	176 (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
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	S	172/219 (78%)	171 (99%)	1 (1%)	84	91
22	s	172/219 (78%)	172 (100%)	0	100	100
All	All	5522/6768 (82%)	5519 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	39	ASN
3	C	418	ASN
22	S	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	165	GLN
1	A	301	ASN
1	A	335	ASN
2	B	100	HIS
2	B	157	HIS

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Mol	Chain	Res	Type
2	B	281	GLN
2	B	317	ASN
3	C	327	ASN
3	C	418	ASN
4	D	84	ASN
4	D	99	GLN
4	D	165	GLN
4	D	187	GLN
4	D	256	GLN
5	E	61	GLN
7	G	102	HIS
9	I	26	ASN
12	L	7	ASN
7	N	95	ASN
14	O	217	GLN
14	O	330	GLN
15	R	205	GLN
20	Y	155	GLN
20	Y	164	GLN
20	Y	230	GLN
20	Y	241	ASN
20	Y	252	ASN
1	a	108	ASN
1	a	303	ASN
2	b	100	HIS
3	c	237	HIS
3	c	311	GLN
3	c	327	ASN
4	d	99	GLN
4	d	293	ASN
7	g	102	HIS
7	g	149	ASN
7	g	180	ASN
9	i	31	ASN
12	l	7	ASN
12	l	34	ASN
12	l	38	ASN
7	n	95	ASN
14	o	113	GLN
14	o	330	GLN
15	r	125	GLN
20	y	164	GLN

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Mol	Chain	Res	Type
20	y	230	GLN
20	y	252	ASN
22	S	158	ASN
22	s	161	ASN
22	s	166	ASN
22	s	264	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 322 ligands modelled in this entry, 2 are monoatomic - leaving 320 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	$\# Z > 2$
23	CLA	B	609	2	65,73,73	1.54	11 (16%)	76,113,113	1.31	8 (10%)
27	LMG	B	622	-	40,40,55	1.09	2 (5%)	48,48,63	1.10	2 (4%)
23	CLA	Y	314	20	45,53,73	1.69	6 (13%)	52,89,113	1.82	9 (17%)
28	DGD	A	408	-	60,60,67	0.90	2 (3%)	74,74,81	1.02	2 (2%)
30	LHG	B	623	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
23	CLA	r	604	-	48,56,73	1.66	7 (14%)	55,92,113	1.83	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	a	412	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	3 (5%)
34	CHL	g	608	-	66,74,74	1.48	7 (10%)	73,114,114	1.29	10 (13%)
23	CLA	c	512	3	56,64,73	1.63	9 (16%)	65,102,113	1.67	17 (26%)
30	LHG	r	618	-	41,41,48	1.03	2 (4%)	44,47,54	1.22	4 (9%)
34	CHL	n	308	-	46,54,74	1.70	9 (19%)	49,90,114	1.76	11 (22%)
23	CLA	N	304	7	59,67,73	1.56	9 (15%)	68,105,113	1.59	11 (16%)
26	SQD	a	409	-	53,54,54	1.19	4 (7%)	62,65,65	3.64	8 (12%)
34	CHL	R	605	-	46,54,74	1.76	7 (15%)	49,90,114	1.61	8 (16%)
30	LHG	s	617	23	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
25	BCR	h	101	-	41,41,41	0.73	0	56,56,56	1.59	10 (17%)
34	CHL	g	607	-	43,51,74	1.80	7 (16%)	45,86,114	1.98	12 (26%)
25	BCR	B	618	-	41,41,41	0.78	0	56,56,56	1.89	17 (30%)
35	LUT	g	615	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	14 (27%)
35	LUT	S	614	-	42,43,43	0.78	0	51,60,60	1.70	16 (31%)
23	CLA	R	604	-	48,56,73	1.66	7 (14%)	55,92,113	1.79	9 (16%)
28	DGD	a	408	-	60,60,67	0.91	2 (3%)	74,74,81	1.03	2 (2%)
34	CHL	S	605	-	46,54,74	1.80	11 (23%)	49,90,114	1.81	16 (32%)
23	CLA	N	315	7	41,49,73	1.81	5 (12%)	47,84,113	1.67	10 (21%)
23	CLA	c	504	-	60,68,73	1.59	7 (11%)	70,107,113	1.32	6 (8%)
23	CLA	B	606	2	65,73,73	1.52	8 (12%)	76,113,113	1.30	7 (9%)
23	CLA	c	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.47	12 (15%)
23	CLA	S	612	22	55,63,73	1.69	7 (12%)	64,101,113	1.69	8 (12%)
30	LHG	R	618	23	41,41,48	1.04	2 (4%)	44,47,54	1.10	2 (4%)
23	CLA	n	312	30	60,68,73	1.55	9 (15%)	70,107,113	1.47	8 (11%)
34	CHL	r	613	15	42,50,74	1.82	6 (14%)	44,85,114	1.68	9 (20%)
25	BCR	A	405	-	41,41,41	0.73	0	56,56,56	1.71	13 (23%)
35	LUT	S	615	-	42,43,43	0.74	0	51,60,60	1.64	10 (19%)
23	CLA	Y	303	20	61,69,73	1.50	8 (13%)	71,108,113	1.41	9 (12%)
34	CHL	N	302	7	66,74,74	1.40	7 (10%)	73,114,114	1.41	10 (13%)
30	LHG	A	411	-	45,45,48	0.95	2 (4%)	48,51,54	1.02	2 (4%)
34	CHL	g	619	-	66,74,74	1.40	7 (10%)	73,114,114	1.51	10 (13%)
25	BCR	Z	101	-	41,41,41	0.69	0	56,56,56	1.78	15 (26%)
23	CLA	A	401	1	65,73,73	1.43	8 (12%)	76,113,113	1.78	16 (21%)
23	CLA	S	609	22	45,53,73	1.83	9 (20%)	52,89,113	1.52	10 (19%)
23	CLA	D	404	4	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.84	13 (23%)
25	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
23	CLA	C	503	3	65,73,73	1.50	10 (15%)	76,113,113	1.60	11 (14%)
34	CHL	G	608	-	66,74,74	1.45	7 (10%)	73,114,114	1.36	10 (13%)
23	CLA	b	609	2	65,73,73	1.50	9 (13%)	76,113,113	1.36	8 (10%)
35	LUT	y	316	-	42,43,43	0.80	1 (2%)	51,60,60	1.51	10 (19%)
23	CLA	R	608	23,15	58,66,73	1.60	7 (12%)	67,104,113	1.36	6 (8%)
23	CLA	y	311	30	60,68,73	1.58	10 (16%)	70,107,113	1.48	9 (12%)
30	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	3 (5%)
23	CLA	C	511	3	65,73,73	1.48	8 (12%)	76,113,113	1.50	11 (14%)
23	CLA	C	507	3	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
25	BCR	a	406	-	41,41,41	0.73	0	56,56,56	1.73	15 (26%)
34	CHL	R	613	15	42,50,74	1.82	6 (14%)	44,85,114	1.64	9 (20%)
23	CLA	c	501	3	65,73,73	1.49	9 (13%)	76,113,113	1.35	7 (9%)
23	CLA	n	305	-	50,58,73	1.60	8 (16%)	58,95,113	1.69	9 (15%)
23	CLA	C	504	3	65,73,73	1.48	8 (12%)	76,113,113	1.42	8 (10%)
23	CLA	r	608	15	58,66,73	1.64	9 (15%)	67,104,113	1.34	8 (11%)
23	CLA	b	616	2	65,73,73	1.50	8 (12%)	76,113,113	1.33	9 (11%)
23	CLA	B	612	2	65,73,73	1.41	8 (12%)	76,113,113	1.58	6 (7%)
35	LUT	G	616	-	42,43,43	0.79	0	51,60,60	1.47	7 (13%)
23	CLA	G	613	7	58,66,73	1.57	9 (15%)	67,104,113	1.55	9 (13%)
23	CLA	g	614	7	42,50,73	1.82	6 (14%)	48,85,113	1.54	7 (14%)
34	CHL	n	306	7	48,56,74	1.66	7 (14%)	51,92,114	1.49	8 (15%)
30	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	2 (3%)
27	LMG	A	407	-	40,40,55	1.07	2 (5%)	48,48,63	1.13	3 (6%)
32	PL9	d	407	-	55,55,55	4.23	20 (36%)	68,69,69	3.80	33 (48%)
23	CLA	g	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.40	8 (11%)
23	CLA	d	404	4	65,73,73	1.46	8 (12%)	76,113,113	1.44	8 (10%)
23	CLA	R	609	15	65,73,73	1.47	8 (12%)	76,113,113	1.31	8 (10%)
34	CHL	r	607	-	61,69,74	1.47	5 (8%)	67,108,114	1.35	7 (10%)
34	CHL	G	619	-	66,74,74	1.41	7 (10%)	73,114,114	1.52	10 (13%)
23	CLA	c	506	3	51,59,73	1.67	8 (15%)	59,96,113	1.59	7 (11%)
24	PHO	d	401	-	51,69,69	0.75	1 (1%)	47,99,99	1.10	3 (6%)
25	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.78	13 (23%)
23	CLA	C	505	-	60,68,73	1.58	6 (10%)	70,107,113	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	n	313	7	45,53,73	1.75	6 (13%)	52,89,113	1.69	9 (17%)
27	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	3 (5%)
36	NEX	S	616	-	38,46,46	0.96	2 (5%)	50,70,70	2.52	14 (28%)
23	CLA	y	303	20	61,69,73	1.55	8 (13%)	71,108,113	1.46	9 (12%)
25	BCR	b	618	-	41,41,41	0.78	0	56,56,56	1.87	18 (32%)
23	CLA	B	605	2	65,73,73	1.47	10 (15%)	76,113,113	1.53	14 (18%)
37	XAT	y	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.54	20 (37%)
23	CLA	C	506	3	58,66,73	1.53	8 (13%)	67,104,113	1.64	12 (17%)
35	LUT	Y	315	-	42,43,43	0.75	0	51,60,60	1.44	8 (15%)
23	CLA	s	612	22	55,63,73	1.70	7 (12%)	64,101,113	1.68	9 (14%)
34	CHL	g	605	7	46,54,74	1.76	6 (13%)	49,90,114	1.61	10 (20%)
23	CLA	B	601	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
30	LHG	W	201	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
27	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	3 (5%)
34	CHL	N	308	-	46,54,74	1.69	8 (17%)	49,90,114	1.78	12 (24%)
30	LHG	B	621	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
34	CHL	n	309	-	66,74,74	1.42	9 (13%)	73,114,114	1.45	8 (10%)
23	CLA	b	614	2	65,73,73	1.46	8 (12%)	76,113,113	1.40	10 (13%)
23	CLA	c	513	3	65,73,73	1.50	9 (13%)	76,113,113	1.32	11 (14%)
23	CLA	G	614	7	42,50,73	1.83	7 (16%)	48,85,113	1.55	7 (14%)
25	BCR	B	617	-	41,41,41	0.75	0	56,56,56	1.75	11 (19%)
23	CLA	R	612	15	47,55,73	1.74	6 (12%)	54,91,113	1.63	7 (12%)
23	CLA	N	305	-	50,58,73	1.64	10 (20%)	58,95,113	1.62	8 (13%)
23	CLA	d	405	4	65,73,73	1.50	8 (12%)	76,113,113	1.45	7 (9%)
28	DGD	c	516	-	56,56,67	0.88	2 (3%)	70,70,81	1.14	7 (10%)
34	CHL	N	310	7	66,74,74	1.47	9 (13%)	73,114,114	1.92	12 (16%)
23	CLA	s	611	22	45,53,73	1.79	9 (20%)	52,89,113	1.58	9 (17%)
23	CLA	r	612	15	47,55,73	1.70	6 (12%)	54,91,113	1.64	9 (16%)
36	NEX	y	317	-	38,46,46	1.40	4 (10%)	50,70,70	4.19	20 (40%)
34	CHL	g	609	7	61,69,74	1.55	9 (14%)	67,108,114	1.87	14 (20%)
23	CLA	B	610	-	65,73,73	1.39	9 (13%)	76,113,113	1.56	8 (10%)
23	CLA	c	510	3	65,73,73	1.47	8 (12%)	76,113,113	1.52	9 (11%)
23	CLA	B	613	2	65,73,73	1.47	9 (13%)	76,113,113	1.50	8 (10%)
31	BCT	D	403	29	2,3,3	0.88	0	2,3,3	3.02	2 (100%)
34	CHL	G	605	7	46,54,74	1.79	6 (13%)	49,90,114	1.60	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	Y	318	23	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
23	CLA	B	607	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	7 (9%)
23	CLA	g	612	7	45,53,73	1.81	9 (20%)	52,89,113	1.60	10 (19%)
37	XAT	N	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.55	19 (35%)
35	LUT	N	316	-	42,43,43	0.73	0	51,60,60	1.60	9 (17%)
25	BCR	B	619	-	41,41,41	0.72	0	56,56,56	1.91	14 (25%)
34	CHL	y	306	20	51,59,74	1.62	8 (15%)	55,96,114	1.76	12 (21%)
36	NEX	G	617	-	38,46,46	1.00	2 (5%)	50,70,70	2.81	16 (32%)
34	CHL	N	307	-	46,54,74	1.74	9 (19%)	49,90,114	1.84	11 (22%)
23	CLA	y	314	20	45,53,73	1.69	6 (13%)	52,89,113	1.81	8 (15%)
23	CLA	G	602	7	65,73,73	1.53	8 (12%)	76,113,113	1.34	8 (10%)
23	CLA	N	303	7	61,69,73	1.53	9 (14%)	71,108,113	1.44	10 (14%)
23	CLA	C	509	3	65,73,73	1.41	8 (12%)	76,113,113	1.49	7 (9%)
23	CLA	R	603	15	60,68,73	1.53	8 (13%)	70,107,113	1.42	9 (12%)
23	CLA	B	604	2	65,73,73	1.50	8 (12%)	76,113,113	1.49	8 (10%)
23	CLA	y	310	20	60,68,73	1.52	7 (11%)	70,107,113	1.40	8 (11%)
23	CLA	b	602	2	65,73,73	1.41	7 (10%)	76,113,113	1.32	7 (9%)
23	CLA	r	610	-	49,57,73	1.73	6 (12%)	55,93,113	1.49	7 (12%)
34	CHL	N	306	7	48,56,74	1.64	6 (12%)	51,92,114	1.48	7 (13%)
23	CLA	r	614	15	45,53,73	1.77	6 (13%)	52,89,113	1.67	7 (13%)
23	CLA	A	404	1	60,68,73	1.46	8 (13%)	70,107,113	1.56	7 (10%)
35	LUT	g	616	-	42,43,43	0.81	0	51,60,60	1.56	13 (25%)
23	CLA	s	610	30	42,50,73	1.80	6 (14%)	48,85,113	1.54	8 (16%)
23	CLA	r	611	15	49,57,73	1.69	6 (12%)	55,93,113	1.47	9 (16%)
23	CLA	S	613	22	41,49,73	1.92	7 (17%)	47,84,113	1.51	8 (17%)
23	CLA	g	610	7	64,72,73	1.49	6 (9%)	74,111,113	1.43	8 (10%)
23	CLA	Y	312	20	60,68,73	1.50	7 (11%)	70,107,113	1.62	12 (17%)
34	CHL	N	309	-	66,74,74	1.41	7 (10%)	73,114,114	1.41	11 (15%)
23	CLA	g	603	7	65,73,73	1.51	11 (16%)	76,113,113	1.40	10 (13%)
25	BCR	c	518	-	41,41,41	0.68	0	56,56,56	1.82	14 (25%)
25	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.89	14 (25%)
23	CLA	R	614	23,15	45,53,73	1.78	9 (20%)	52,89,113	1.59	7 (13%)
35	LUT	n	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.34	7 (13%)
35	LUT	n	316	-	42,43,43	0.71	0	51,60,60	1.67	11 (21%)
24	PHO	a	404	-	51,69,69	0.74	0	47,99,99	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	CHL	r	605	-	46,54,74	1.74	7 (15%)	49,90,114	1.52	8 (16%)
23	CLA	R	611	15	49,57,73	1.71	7 (14%)	55,93,113	1.44	9 (16%)
23	CLA	D	405	4	65,73,73	1.49	9 (13%)	76,113,113	1.50	8 (10%)
34	CHL	n	307	-	46,54,74	1.75	9 (19%)	49,90,114	1.90	11 (22%)
23	CLA	n	303	7	61,69,73	1.52	9 (14%)	71,108,113	1.40	9 (12%)
23	CLA	S	610	30	42,50,73	1.78	6 (14%)	48,85,113	1.57	9 (18%)
34	CHL	S	601	22	46,54,74	1.71	6 (13%)	49,90,114	1.72	9 (18%)
25	BCR	H	101	-	41,41,41	0.75	0	56,56,56	1.67	10 (17%)
23	CLA	b	613	2	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
34	CHL	G	601	7	66,74,74	1.45	9 (13%)	73,114,114	1.62	15 (20%)
34	CHL	S	606	-	43,51,74	1.81	6 (13%)	45,86,114	2.00	11 (24%)
23	CLA	y	305	-	50,58,73	1.67	9 (18%)	58,95,113	1.57	8 (13%)
36	NEX	n	318	-	38,46,46	0.96	2 (5%)	50,70,70	2.27	16 (32%)
37	XAT	R	616	-	39,47,47	0.96	2 (5%)	54,74,74	2.62	19 (35%)
23	CLA	a	401	1	65,73,73	1.41	8 (12%)	76,113,113	1.80	19 (25%)
23	CLA	b	610	-	65,73,73	1.40	8 (12%)	76,113,113	1.54	8 (10%)
27	LMG	C	501	-	48,48,55	0.96	2 (4%)	56,56,63	1.23	6 (10%)
23	CLA	n	311	7	59,67,73	1.53	7 (11%)	68,105,113	1.48	8 (11%)
34	CHL	r	606	-	46,54,74	1.77	6 (13%)	49,90,114	1.55	8 (16%)
34	CHL	S	607	-	49,57,74	1.72	6 (12%)	52,93,114	1.64	14 (26%)
23	CLA	b	605	2	65,73,73	1.46	10 (15%)	76,113,113	1.58	14 (18%)
28	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.11	3 (3%)
36	NEX	r	617	-	38,46,46	0.93	2 (5%)	50,70,70	2.52	16 (32%)
37	XAT	Y	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.51	20 (37%)
36	NEX	N	318	-	38,46,46	0.92	2 (5%)	50,70,70	2.38	20 (40%)
23	CLA	S	604	-	50,58,73	1.74	7 (14%)	58,95,113	1.62	8 (13%)
23	CLA	B	608	2	65,73,73	1.47	9 (13%)	76,113,113	1.56	9 (11%)
34	CHL	Y	309	20	66,74,74	1.53	9 (13%)	73,114,114	1.46	9 (12%)
23	CLA	b	604	2	65,73,73	1.51	8 (12%)	76,113,113	1.50	9 (11%)
24	PHO	D	402	-	51,69,69	0.76	2 (3%)	47,99,99	1.15	2 (4%)
26	SQD	A	409	-	53,54,54	1.18	4 (7%)	62,65,65	3.65	9 (14%)
30	LHG	g	618	23	45,45,48	0.95	2 (4%)	48,51,54	1.13	3 (6%)
23	CLA	s	613	22	41,49,73	1.94	7 (17%)	47,84,113	1.58	8 (17%)
23	CLA	G	603	7	65,73,73	1.50	11 (16%)	76,113,113	1.41	10 (13%)
31	BCT	d	403	29	2,3,3	0.88	0	2,3,3	3.06	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	402	-	50,58,73	1.71	7 (14%)	58,95,113	1.54	9 (15%)
23	CLA	b	606	2	65,73,73	1.52	8 (12%)	76,113,113	1.28	7 (9%)
23	CLA	B	614	2	65,73,73	1.46	8 (12%)	76,113,113	1.40	10 (13%)
25	BCR	c	515	-	41,41,41	0.76	0	56,56,56	1.82	15 (26%)
23	CLA	y	304	20	65,73,73	1.50	11 (16%)	76,113,113	1.50	11 (14%)
34	CHL	Y	302	20	66,74,74	1.38	7 (10%)	73,114,114	1.47	9 (12%)
23	CLA	C	514	3	65,73,73	1.49	6 (9%)	76,113,113	1.29	9 (11%)
23	CLA	B	603	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
30	LHG	S	617	23	48,48,48	0.92	2 (4%)	51,54,54	1.04	2 (3%)
27	LMG	a	407	-	48,48,55	0.95	2 (4%)	56,56,63	1.30	6 (10%)
23	CLA	B	602	2	65,73,73	1.44	7 (10%)	76,113,113	1.33	7 (9%)
23	CLA	C	513	3	56,64,73	1.63	10 (17%)	65,102,113	1.56	15 (23%)
37	XAT	n	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.56	16 (29%)
34	CHL	s	601	22	46,54,74	1.70	6 (13%)	49,90,114	1.76	8 (16%)
23	CLA	c	502	3	65,73,73	1.50	11 (16%)	76,113,113	1.71	10 (13%)
23	CLA	s	608	22	45,53,73	1.79	6 (13%)	52,89,113	1.63	10 (19%)
37	XAT	g	620	-	39,47,47	0.93	1 (2%)	54,74,74	2.53	17 (31%)
34	CHL	R	607	-	61,69,74	1.51	7 (11%)	67,108,114	1.38	8 (11%)
23	CLA	s	602	22	46,54,73	1.72	10 (21%)	53,90,113	1.55	8 (15%)
35	LUT	s	614	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
35	LUT	N	317	-	42,43,43	0.93	1 (2%)	51,60,60	1.42	7 (13%)
36	NEX	g	617	23	38,46,46	0.97	2 (5%)	50,70,70	2.62	10 (20%)
23	CLA	b	611	2	65,73,73	1.46	8 (12%)	76,113,113	1.39	6 (7%)
33	HEM	E	101	5,6	41,50,50	1.47	3 (7%)	45,82,82	1.64	9 (20%)
23	CLA	r	609	15	65,73,73	1.47	9 (13%)	76,113,113	1.23	9 (11%)
26	SQD	M	101	-	53,54,54	1.15	4 (7%)	62,65,65	1.16	4 (6%)
23	CLA	c	509	3	65,73,73	1.59	8 (12%)	76,113,113	1.36	10 (13%)
34	CHL	y	302	20	66,74,74	1.38	7 (10%)	73,114,114	1.52	8 (10%)
23	CLA	n	314	7	60,68,73	1.56	11 (18%)	70,107,113	1.62	11 (15%)
28	DGD	C	517	-	56,56,67	0.88	2 (3%)	70,70,81	1.15	7 (10%)
37	XAT	G	620	-	39,47,47	0.94	1 (2%)	54,74,74	2.55	17 (31%)
23	CLA	b	615	2	65,73,73	1.49	8 (12%)	76,113,113	1.39	9 (11%)
27	LMG	d	409	-	46,46,55	1.00	2 (4%)	54,54,63	1.01	2 (3%)
23	CLA	N	312	30	60,68,73	1.54	8 (13%)	70,107,113	1.44	8 (11%)
23	CLA	D	401	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	CHL	y	309	20	66,74,74	1.48	8 (12%)	73,114,114	1.38	7 (9%)
23	CLA	Y	304	20	65,73,73	1.49	10 (15%)	76,113,113	1.52	11 (14%)
23	CLA	S	608	22	45,53,73	1.77	6 (13%)	52,89,113	1.64	10 (19%)
23	CLA	r	603	15	60,68,73	1.54	10 (16%)	70,107,113	1.44	8 (11%)
23	CLA	S	602	22	46,54,73	1.74	9 (19%)	53,90,113	1.55	9 (16%)
37	XAT	r	616	-	39,47,47	0.96	1 (2%)	54,74,74	2.62	18 (33%)
23	CLA	C	502	3	65,73,73	1.49	8 (12%)	76,113,113	1.34	9 (11%)
23	CLA	R	602	15	60,68,73	1.53	8 (13%)	70,107,113	1.45	7 (10%)
34	CHL	s	607	-	49,57,74	1.66	6 (12%)	52,93,114	1.64	10 (19%)
23	CLA	Y	311	30	60,68,73	1.56	10 (16%)	70,107,113	1.49	9 (12%)
34	CHL	G	606	-	43,51,74	1.74	9 (20%)	45,86,114	1.51	8 (17%)
30	LHG	y	318	23	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
23	CLA	R	610	30	49,57,73	1.73	6 (12%)	55,93,113	1.55	8 (14%)
30	LHG	A	412	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
30	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	2 (3%)
30	LHG	b	622	-	48,48,48	0.88	2 (4%)	51,54,54	1.10	4 (7%)
36	NEX	s	616	-	38,46,46	0.87	2 (5%)	50,70,70	2.52	13 (26%)
23	CLA	n	315	7	41,49,73	1.84	5 (12%)	47,84,113	1.61	9 (19%)
30	LHG	w	201	-	48,48,48	0.94	2 (4%)	51,54,54	1.17	3 (5%)
34	CHL	G	609	7	61,69,74	1.54	9 (14%)	67,108,114	1.98	17 (25%)
23	CLA	s	604	-	50,58,73	1.72	8 (16%)	58,95,113	1.59	10 (17%)
23	CLA	g	613	7	58,66,73	1.56	10 (17%)	67,104,113	1.55	9 (13%)
34	CHL	y	308	-	66,74,74	1.42	7 (10%)	73,114,114	1.29	7 (9%)
23	CLA	Y	313	20	65,73,73	1.51	10 (15%)	76,113,113	1.45	9 (11%)
23	CLA	N	311	7	59,67,73	1.52	8 (13%)	68,105,113	1.40	7 (10%)
23	CLA	s	609	22	45,53,73	1.81	8 (17%)	52,89,113	1.54	8 (15%)
26	SQD	L	103	-	53,54,54	1.16	4 (7%)	62,65,65	1.16	5 (8%)
30	LHG	C	518	-	48,48,48	0.92	2 (4%)	51,54,54	0.90	2 (3%)
23	CLA	a	403	-	50,58,73	1.73	8 (16%)	58,95,113	1.52	9 (15%)
23	CLA	C	508	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	11 (14%)
23	CLA	G	612	7	45,53,73	1.80	9 (20%)	52,89,113	1.76	11 (21%)
28	DGD	d	410	-	63,63,67	0.88	2 (3%)	77,77,81	1.09	2 (2%)
23	CLA	B	615	2	65,73,73	1.48	8 (12%)	76,113,113	1.39	11 (14%)
34	CHL	G	607	-	43,51,74	1.79	6 (13%)	45,86,114	1.86	11 (24%)
25	BCR	K	101	-	41,41,41	0.68	0	56,56,56	1.72	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	b	621	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
25	BCR	F	101	-	41,41,41	0.69	0	56,56,56	1.65	15 (26%)
23	CLA	s	603	22	45,53,73	1.82	10 (22%)	52,89,113	1.74	9 (17%)
34	CHL	g	601	7	66,74,74	1.44	10 (15%)	73,114,114	1.62	16 (21%)
35	LUT	R	615	-	42,43,43	0.73	0	51,60,60	1.72	12 (23%)
23	CLA	y	312	20	60,68,73	1.50	7 (11%)	70,107,113	1.58	11 (15%)
34	CHL	n	310	7	66,74,74	1.45	9 (13%)	73,114,114	1.82	10 (13%)
23	CLA	a	402	1	65,73,73	1.53	11 (16%)	76,113,113	1.47	12 (15%)
23	CLA	C	512	3	65,73,73	1.53	9 (13%)	76,113,113	1.36	9 (11%)
25	BCR	b	619	-	41,41,41	0.71	0	56,56,56	1.87	14 (25%)
23	CLA	Y	310	20	60,68,73	1.54	7 (11%)	70,107,113	1.38	7 (10%)
23	CLA	B	611	2	65,73,73	1.46	9 (13%)	76,113,113	1.40	7 (9%)
25	BCR	b	617	-	41,41,41	0.75	0	56,56,56	1.76	12 (21%)
23	CLA	N	313	7	45,53,73	1.82	8 (17%)	52,89,113	1.61	8 (15%)
23	CLA	g	604	36	49,57,73	1.67	10 (20%)	55,93,113	1.56	6 (10%)
26	SQD	d	402	-	49,50,54	1.23	4 (8%)	58,61,65	1.13	4 (6%)
35	LUT	r	615	-	42,43,43	0.74	0	51,60,60	1.72	10 (19%)
35	LUT	G	615	-	42,43,43	0.87	2 (4%)	51,60,60	1.74	14 (27%)
30	LHG	T	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
34	CHL	R	606	-	46,54,74	1.75	6 (13%)	49,90,114	1.57	8 (16%)
23	CLA	B	616	2	65,73,73	1.49	8 (12%)	76,113,113	1.34	10 (13%)
23	CLA	b	608	2	65,73,73	1.51	10 (15%)	76,113,113	1.61	11 (14%)
23	CLA	n	304	7	59,67,73	1.57	8 (13%)	68,105,113	1.53	9 (13%)
30	LHG	c	517	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
23	CLA	r	602	15	60,68,73	1.53	9 (15%)	70,107,113	1.30	7 (10%)
23	CLA	N	314	7	60,68,73	1.56	8 (13%)	70,107,113	1.75	14 (20%)
30	LHG	N	319	23	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
23	CLA	c	511	3	65,73,73	1.50	8 (12%)	76,113,113	1.42	9 (11%)
23	CLA	b	603	2	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
24	PHO	A	403	-	51,69,69	0.74	1 (1%)	47,99,99	0.95	2 (4%)
23	CLA	r	601	15	49,57,73	1.76	7 (14%)	55,93,113	1.66	12 (21%)
27	LMG	D	407	-	46,46,55	1.01	2 (4%)	54,54,63	1.00	2 (3%)
35	LUT	s	615	-	42,43,43	0.73	0	51,60,60	1.59	11 (21%)
23	CLA	G	610	7	64,72,73	1.49	6 (9%)	74,111,113	1.42	7 (9%)
36	NEX	R	617	-	38,46,46	0.94	2 (5%)	50,70,70	2.50	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	CHL	Y	308	-	66,74,74	1.42	7 (10%)	73,114,114	1.30	8 (10%)
23	CLA	c	503	3	65,73,73	1.48	8 (12%)	76,113,113	1.33	4 (5%)
33	HEM	e	101	5,6	41,50,50	1.51	4 (9%)	45,82,82	1.62	11 (24%)
34	CHL	s	605	-	46,54,74	1.78	6 (13%)	49,90,114	1.50	8 (16%)
34	CHL	s	606	-	43,51,74	1.81	6 (13%)	45,86,114	1.83	9 (20%)
23	CLA	G	604	-	49,57,73	1.66	10 (20%)	55,93,113	1.56	7 (12%)
23	CLA	a	405	1	60,68,73	1.47	8 (13%)	70,107,113	1.53	7 (10%)
32	PL9	D	406	-	55,55,55	4.24	20 (36%)	68,69,69	3.79	34 (50%)
23	CLA	y	313	20	65,73,73	1.52	10 (15%)	76,113,113	1.59	11 (14%)
23	CLA	b	601	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	8 (10%)
23	CLA	b	607	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	6 (7%)
23	CLA	g	602	7	65,73,73	1.52	8 (12%)	76,113,113	1.36	8 (10%)
25	BCR	d	406	-	41,41,41	0.69	0	56,56,56	1.72	15 (26%)
34	CHL	Y	307	-	50,58,74	1.56	7 (14%)	52,94,114	1.52	6 (11%)
30	LHG	G	618	23	45,45,48	0.96	2 (4%)	48,51,54	1.15	3 (6%)
23	CLA	S	611	22	45,53,73	1.80	9 (20%)	52,89,113	1.57	10 (19%)
23	CLA	R	601	15	49,57,73	1.78	8 (16%)	55,93,113	1.56	10 (18%)
34	CHL	n	302	7	66,74,74	1.40	7 (10%)	73,114,114	1.55	10 (13%)
35	LUT	y	315	-	42,43,43	0.76	0	51,60,60	1.46	7 (13%)
36	NEX	Y	317	-	38,46,46	1.16	3 (7%)	50,70,70	4.24	20 (40%)
23	CLA	C	510	3	65,73,73	1.45	7 (10%)	76,113,113	1.68	13 (17%)
23	CLA	S	603	22	45,53,73	1.78	8 (17%)	52,89,113	1.76	10 (19%)
26	SQD	A	406	-	49,50,54	1.23	4 (8%)	58,61,65	1.18	4 (6%)
35	LUT	Y	316	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	9 (17%)
23	CLA	G	611	30	60,68,73	1.60	9 (15%)	70,107,113	1.35	6 (8%)
34	CHL	g	606	-	43,51,74	1.74	7 (16%)	45,86,114	1.73	12 (26%)
30	LHG	n	319	23	48,48,48	0.94	2 (4%)	51,54,54	1.04	2 (3%)
23	CLA	Y	305	-	50,58,73	1.63	8 (16%)	58,95,113	1.58	7 (12%)
30	LHG	a	411	-	45,45,48	0.94	2 (4%)	48,51,54	1.03	2 (4%)
34	CHL	y	307	-	50,58,74	1.55	6 (12%)	52,94,114	1.59	9 (17%)
23	CLA	b	612	2	65,73,73	1.41	8 (12%)	76,113,113	1.60	8 (10%)
23	CLA	c	508	3	65,73,73	1.39	8 (12%)	76,113,113	1.56	10 (13%)
23	CLA	c	505	3	58,66,73	1.52	8 (13%)	67,104,113	1.55	11 (16%)
34	CHL	Y	306	20	51,59,74	1.63	8 (15%)	55,96,114	1.86	12 (21%)

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
23	CLA	B	609	2	1/1/15/20	13/37/115/115	-
27	LMG	B	622	-	-	5/35/55/70	0/1/1/1
23	CLA	Y	314	20	1/1/11/20	4/13/91/115	-
28	DGD	A	408	-	-	10/48/88/95	0/2/2/2
30	LHG	B	623	-	-	10/53/53/53	-
23	CLA	r	604	-	1/1/11/20	9/17/95/115	-
30	LHG	a	412	-	-	11/53/53/53	-
34	CHL	g	608	-	3/3/20/26	19/39/137/137	-
23	CLA	c	512	3	1/1/13/20	9/27/105/115	-
30	LHG	r	618	-	-	11/46/46/53	-
34	CHL	n	308	-	3/3/16/26	11/15/113/137	-
23	CLA	N	304	7	1/1/13/20	10/30/108/115	-
26	SQD	a	409	-	-	16/49/69/69	0/1/1/1
34	CHL	R	605	-	3/3/16/26	1/15/113/137	-
30	LHG	s	617	23	-	10/53/53/53	-
25	BCR	h	101	-	-	7/29/63/63	0/2/2/2
34	CHL	g	607	-	3/3/15/26	8/12/110/137	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
35	LUT	g	615	-	-	2/29/67/67	0/2/2/2
35	LUT	S	614	-	-	2/29/67/67	0/2/2/2
23	CLA	R	604	-	1/1/11/20	7/17/95/115	-
28	DGD	a	408	-	-	10/48/88/95	0/2/2/2
34	CHL	S	605	-	3/3/16/26	11/15/113/137	-
23	CLA	N	315	7	1/1/10/20	2/8/86/115	-
23	CLA	c	504	-	1/1/14/20	13/31/109/115	-
23	CLA	B	606	2	1/1/15/20	7/37/115/115	-
23	CLA	c	507	-	1/1/15/20	10/37/115/115	-
23	CLA	S	612	22	1/1/13/20	12/25/103/115	-
30	LHG	R	618	23	-	11/46/46/53	-
23	CLA	n	312	30	1/1/14/20	9/31/109/115	-
34	CHL	r	613	15	3/3/15/26	7/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	A	405	-	-	2/29/63/63	0/2/2/2
35	LUT	S	615	-	-	6/29/67/67	0/2/2/2
23	CLA	Y	303	20	1/1/14/20	17/33/111/115	-
34	CHL	N	302	7	3/3/20/26	14/39/137/137	-
30	LHG	A	411	-	-	10/50/50/53	-
34	CHL	g	619	-	3/3/20/26	25/39/137/137	-
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
23	CLA	A	401	1	1/1/15/20	15/37/115/115	-
23	CLA	S	609	22	1/1/11/20	8/13/91/115	-
23	CLA	D	404	4	1/1/15/20	10/37/115/115	-
25	BCR	C	516	-	-	4/29/63/63	0/2/2/2
25	BCR	C	515	-	-	5/29/63/63	0/2/2/2
23	CLA	C	503	3	1/1/15/20	22/37/115/115	-
34	CHL	G	608	-	3/3/20/26	19/39/137/137	-
23	CLA	b	609	2	1/1/15/20	13/37/115/115	-
35	LUT	y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	R	608	23,15	1/1/13/20	6/29/107/115	-
23	CLA	y	311	30	1/1/14/20	12/31/109/115	-
30	LHG	L	102	-	-	10/53/53/53	-
23	CLA	C	511	3	1/1/15/20	16/37/115/115	-
23	CLA	C	507	3	1/1/12/20	9/21/99/115	-
25	BCR	a	406	-	-	2/29/63/63	0/2/2/2
34	CHL	R	613	15	3/3/15/26	7/10/108/137	-
23	CLA	c	501	3	1/1/15/20	9/37/115/115	-
23	CLA	n	305	-	1/1/12/20	9/19/97/115	-
23	CLA	C	504	3	1/1/15/20	17/37/115/115	-
23	CLA	r	608	15	1/1/13/20	9/29/107/115	-
23	CLA	b	616	2	1/1/15/20	12/37/115/115	-
23	CLA	B	612	2	1/1/15/20	15/37/115/115	-
35	LUT	G	616	-	-	2/29/67/67	0/2/2/2
23	CLA	G	613	7	1/1/13/20	7/29/107/115	-
23	CLA	g	614	7	1/1/10/20	2/10/88/115	-
34	CHL	n	306	7	3/3/16/26	9/18/116/137	-
30	LHG	L	101	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	A	407	-	-	6/35/55/70	0/1/1/1
32	PL9	d	407	-	-	25/53/73/73	0/1/1/1
23	CLA	g	611	30	1/1/14/20	10/31/109/115	-
23	CLA	d	404	4	1/1/15/20	9/37/115/115	-
23	CLA	R	609	15	1/1/15/20	11/37/115/115	-
34	CHL	r	607	-	3/3/19/26	12/33/131/137	-
34	CHL	G	619	-	3/3/20/26	23/39/137/137	-
23	CLA	c	506	3	1/1/12/20	9/21/99/115	-
24	PHO	d	401	-	-	12/37/103/103	0/5/6/6
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/14/20	11/31/109/115	-
23	CLA	n	313	7	1/1/11/20	8/13/91/115	-
27	LMG	B	620	-	-	9/46/66/70	0/1/1/1
36	NEX	S	616	-	-	3/27/83/83	0/3/3/3
23	CLA	y	303	20	1/1/14/20	17/33/111/115	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	B	605	2	1/1/15/20	11/37/115/115	-
37	XAT	y	301	-	-	2/31/93/93	0/4/4/4
23	CLA	C	506	3	1/1/13/20	13/29/107/115	-
35	LUT	Y	315	-	-	5/29/67/67	0/2/2/2
23	CLA	s	612	22	1/1/13/20	10/25/103/115	-
34	CHL	g	605	7	3/3/16/26	8/15/113/137	-
23	CLA	B	601	-	1/1/15/20	14/37/115/115	-
30	LHG	W	201	-	-	18/53/53/53	-
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
34	CHL	N	308	-	3/3/16/26	11/15/113/137	-
30	LHG	B	621	-	-	12/53/53/53	-
34	CHL	n	309	-	3/3/20/26	14/39/137/137	-
23	CLA	b	614	2	1/1/15/20	21/37/115/115	-
23	CLA	c	513	3	1/1/15/20	13/37/115/115	-
23	CLA	G	614	7	1/1/10/20	0/10/88/115	-
25	BCR	B	617	-	-	6/29/63/63	0/2/2/2
23	CLA	R	612	15	1/1/11/20	8/16/94/115	-
23	CLA	N	305	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	405	4	1/1/15/20	13/37/115/115	-
28	DGD	c	516	-	-	10/44/84/95	0/2/2/2
34	CHL	N	310	7	3/3/20/26	16/39/137/137	-
23	CLA	s	611	22	1/1/11/20	6/13/91/115	-
23	CLA	r	612	15	1/1/11/20	7/16/94/115	-
36	NEX	y	317	-	-	4/27/83/83	0/3/3/3
34	CHL	g	609	7	3/3/19/26	8/33/131/137	-
23	CLA	B	610	-	1/1/15/20	14/37/115/115	-
23	CLA	c	510	3	1/1/15/20	18/37/115/115	-
23	CLA	B	613	2	1/1/15/20	11/37/115/115	-
34	CHL	G	605	7	3/3/16/26	11/15/113/137	-
30	LHG	Y	318	23	-	12/53/53/53	-
23	CLA	B	607	-	1/1/15/20	14/37/115/115	-
23	CLA	g	612	7	1/1/11/20	6/13/91/115	-
37	XAT	N	301	-	-	1/31/93/93	0/4/4/4
35	LUT	N	316	-	-	3/29/67/67	0/2/2/2
25	BCR	B	619	-	-	6/29/63/63	0/2/2/2
34	CHL	y	306	20	3/3/17/26	9/21/119/137	-
36	NEX	G	617	-	-	2/27/83/83	0/3/3/3
34	CHL	N	307	-	3/3/16/26	10/15/113/137	-
23	CLA	y	314	20	1/1/11/20	4/13/91/115	-
23	CLA	G	602	7	1/1/15/20	13/37/115/115	-
23	CLA	N	303	7	1/1/14/20	11/33/111/115	-
23	CLA	C	509	3	1/1/15/20	10/37/115/115	-
23	CLA	R	603	15	1/1/14/20	5/31/109/115	-
23	CLA	B	604	2	1/1/15/20	14/37/115/115	-
23	CLA	y	310	20	1/1/14/20	8/31/109/115	-
23	CLA	b	602	2	1/1/15/20	8/37/115/115	-
23	CLA	r	610	-	1/1/11/20	7/18/96/115	-
34	CHL	N	306	7	3/3/16/26	9/18/116/137	-
23	CLA	r	614	15	1/1/11/20	8/13/91/115	-
23	CLA	A	404	1	1/1/14/20	11/31/109/115	-
35	LUT	g	616	-	-	5/29/67/67	0/2/2/2
23	CLA	s	610	30	1/1/10/20	6/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	r	611	15	1/1/11/20	6/18/96/115	-
23	CLA	S	613	22	1/1/10/20	5/8/86/115	-
23	CLA	g	610	7	1/1/14/20	11/36/114/115	-
23	CLA	Y	312	20	1/1/14/20	9/31/109/115	-
34	CHL	N	309	-	3/3/20/26	14/39/137/137	-
23	CLA	g	603	7	1/1/15/20	8/37/115/115	-
25	BCR	c	518	-	-	6/29/63/63	0/2/2/2
25	BCR	c	514	-	-	5/29/63/63	0/2/2/2
23	CLA	R	614	23,15	1/1/11/20	7/13/91/115	-
35	LUT	n	317	-	-	5/29/67/67	0/2/2/2
35	LUT	n	316	-	-	2/29/67/67	0/2/2/2
24	PHO	a	404	-	-	13/37/103/103	0/5/6/6
34	CHL	r	605	-	3/3/16/26	2/15/113/137	-
23	CLA	R	611	15	1/1/11/20	3/18/96/115	-
23	CLA	D	405	4	1/1/15/20	12/37/115/115	-
34	CHL	n	307	-	3/3/16/26	8/15/113/137	-
23	CLA	n	303	7	1/1/14/20	9/33/111/115	-
23	CLA	S	610	30	1/1/10/20	4/10/88/115	-
34	CHL	S	601	22	3/3/16/26	7/15/113/137	-
25	BCR	H	101	-	-	5/29/63/63	0/2/2/2
23	CLA	b	613	2	1/1/15/20	11/37/115/115	-
34	CHL	G	601	7	3/3/20/26	11/39/137/137	-
34	CHL	S	606	-	3/3/15/26	9/12/110/137	-
23	CLA	y	305	-	1/1/12/20	7/19/97/115	-
36	NEX	n	318	-	-	4/27/83/83	0/3/3/3
37	XAT	R	616	-	-	2/31/93/93	0/4/4/4
23	CLA	a	401	1	1/1/15/20	15/37/115/115	-
23	CLA	b	610	-	1/1/15/20	11/37/115/115	-
27	LMG	C	501	-	-	7/43/63/70	0/1/1/1
23	CLA	n	311	7	1/1/13/20	10/30/108/115	-
34	CHL	r	606	-	3/3/16/26	8/15/113/137	-
34	CHL	S	607	-	3/3/16/26	13/19/117/137	-
23	CLA	b	605	2	1/1/15/20	10/37/115/115	-
28	DGD	H	102	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	r	617	-	-	3/27/83/83	0/3/3/3
37	XAT	Y	301	-	-	2/31/93/93	0/4/4/4
36	NEX	N	318	-	-	3/27/83/83	0/3/3/3
23	CLA	S	604	-	1/1/12/20	4/19/97/115	-
23	CLA	B	608	2	1/1/15/20	16/37/115/115	-
34	CHL	Y	309	20	3/3/20/26	23/39/137/137	-
23	CLA	b	604	2	1/1/15/20	13/37/115/115	-
24	PHO	D	402	-	-	13/37/103/103	0/5/6/6
26	SQD	A	409	-	-	14/49/69/69	0/1/1/1
30	LHG	g	618	23	-	11/50/50/53	-
23	CLA	s	613	22	1/1/10/20	5/8/86/115	-
23	CLA	G	603	7	1/1/15/20	7/37/115/115	-
23	CLA	A	402	-	1/1/12/20	9/19/97/115	-
23	CLA	b	606	2	1/1/15/20	6/37/115/115	-
23	CLA	B	614	2	1/1/15/20	20/37/115/115	-
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2
23	CLA	y	304	20	1/1/15/20	13/37/115/115	-
34	CHL	Y	302	20	3/3/20/26	14/39/137/137	-
23	CLA	C	514	3	1/1/15/20	10/37/115/115	-
23	CLA	B	603	2	1/1/15/20	15/37/115/115	-
30	LHG	S	617	23	-	10/53/53/53	-
27	LMG	a	407	-	-	7/43/63/70	0/1/1/1
23	CLA	B	602	2	1/1/15/20	7/37/115/115	-
23	CLA	C	513	3	1/1/13/20	8/27/105/115	-
37	XAT	n	301	-	-	2/31/93/93	0/4/4/4
34	CHL	s	601	22	3/3/16/26	9/15/113/137	-
23	CLA	c	502	3	1/1/15/20	20/37/115/115	-
23	CLA	s	608	22	1/1/11/20	7/13/91/115	-
37	XAT	g	620	-	-	1/31/93/93	0/4/4/4
34	CHL	R	607	-	3/3/19/26	10/33/131/137	-
23	CLA	s	602	22	1/1/11/20	7/15/93/115	-
35	LUT	s	614	-	-	2/29/67/67	0/2/2/2
35	LUT	N	317	-	-	3/29/67/67	0/2/2/2
36	NEX	g	617	23	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	611	2	1/1/15/20	8/37/115/115	-
33	HEM	E	101	5,6	-	5/12/54/54	-
23	CLA	r	609	15	1/1/15/20	10/37/115/115	-
26	SQD	M	101	-	-	16/49/69/69	0/1/1/1
23	CLA	c	509	3	1/1/15/20	14/37/115/115	-
34	CHL	y	302	20	3/3/20/26	18/39/137/137	-
23	CLA	n	314	7	1/1/14/20	13/31/109/115	-
28	DGD	C	517	-	-	6/44/84/95	0/2/2/2
37	XAT	G	620	-	-	0/31/93/93	0/4/4/4
23	CLA	b	615	2	1/1/15/20	11/37/115/115	-
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
23	CLA	N	312	30	1/1/14/20	7/31/109/115	-
23	CLA	D	401	-	1/1/15/20	17/37/115/115	-
34	CHL	y	309	20	3/3/20/26	25/39/137/137	-
23	CLA	Y	304	20	1/1/15/20	13/37/115/115	-
23	CLA	S	608	22	1/1/11/20	4/13/91/115	-
23	CLA	r	603	15	1/1/14/20	7/31/109/115	-
23	CLA	S	602	22	1/1/11/20	8/15/93/115	-
37	XAT	r	616	-	-	2/31/93/93	0/4/4/4
23	CLA	C	502	3	1/1/15/20	13/37/115/115	-
23	CLA	R	602	15	1/1/14/20	8/31/109/115	-
34	CHL	s	607	-	3/3/16/26	14/19/117/137	-
23	CLA	Y	311	30	1/1/14/20	11/31/109/115	-
34	CHL	G	606	-	3/3/15/26	8/12/110/137	-
30	LHG	y	318	23	-	10/53/53/53	-
23	CLA	R	610	30	1/1/11/20	7/18/96/115	-
30	LHG	A	412	-	-	15/53/53/53	-
30	LHG	d	408	-	-	8/53/53/53	-
30	LHG	b	622	-	-	8/53/53/53	-
36	NEX	s	616	-	-	2/27/83/83	0/3/3/3
23	CLA	n	315	7	1/1/10/20	2/8/86/115	-
34	CHL	G	609	7	3/3/19/26	13/33/131/137	-
30	LHG	w	201	-	-	19/53/53/53	-
23	CLA	s	604	-	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	613	7	1/1/13/20	5/29/107/115	-
34	CHL	y	308	-	3/3/20/26	17/39/137/137	-
23	CLA	Y	313	20	1/1/15/20	15/37/115/115	-
23	CLA	N	311	7	1/1/13/20	10/30/108/115	-
23	CLA	s	609	22	1/1/11/20	8/13/91/115	-
26	SQD	L	103	-	-	17/49/69/69	0/1/1/1
30	LHG	C	518	-	-	11/53/53/53	-
23	CLA	a	403	-	1/1/12/20	9/19/97/115	-
23	CLA	C	508	-	1/1/15/20	11/37/115/115	-
23	CLA	G	612	7	1/1/11/20	6/13/91/115	-
28	DGD	d	410	-	-	10/51/91/95	0/2/2/2
23	CLA	B	615	2	1/1/15/20	12/37/115/115	-
34	CHL	G	607	-	3/3/15/26	7/12/110/137	-
25	BCR	K	101	-	-	6/29/63/63	0/2/2/2
30	LHG	b	621	-	-	11/53/53/53	-
25	BCR	F	101	-	-	5/29/63/63	0/2/2/2
23	CLA	s	603	22	1/1/11/20	7/13/91/115	-
34	CHL	g	601	7	3/3/20/26	10/39/137/137	-
35	LUT	R	615	-	-	3/29/67/67	0/2/2/2
23	CLA	y	312	20	1/1/14/20	10/31/109/115	-
34	CHL	n	310	7	3/3/20/26	18/39/137/137	-
23	CLA	a	402	1	1/1/15/20	16/37/115/115	-
23	CLA	C	512	3	1/1/15/20	17/37/115/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	Y	310	20	1/1/14/20	8/31/109/115	-
23	CLA	B	611	2	1/1/15/20	7/37/115/115	-
25	BCR	b	617	-	-	6/29/63/63	0/2/2/2
23	CLA	N	313	7	1/1/11/20	5/13/91/115	-
23	CLA	g	604	36	1/1/11/20	5/18/96/115	-
26	SQD	d	402	-	-	11/45/65/69	0/1/1/1
35	LUT	r	615	-	-	3/29/67/67	0/2/2/2
35	LUT	G	615	-	-	2/29/67/67	0/2/2/2
30	LHG	T	101	-	-	10/53/53/53	-
34	CHL	R	606	-	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	616	2	1/1/15/20	11/37/115/115	-
23	CLA	b	608	2	1/1/15/20	14/37/115/115	-
23	CLA	n	304	7	1/1/13/20	9/30/108/115	-
30	LHG	c	517	-	-	11/53/53/53	-
23	CLA	r	602	15	1/1/14/20	9/31/109/115	-
23	CLA	N	314	7	1/1/14/20	12/31/109/115	-
30	LHG	N	319	23	-	11/53/53/53	-
23	CLA	c	511	3	1/1/15/20	14/37/115/115	-
23	CLA	b	603	2	1/1/15/20	16/37/115/115	-
24	PHO	A	403	-	-	12/37/103/103	0/5/6/6
23	CLA	r	601	15	1/1/11/20	8/18/96/115	-
27	LMG	D	407	-	-	5/41/61/70	0/1/1/1
35	LUT	s	615	-	-	6/29/67/67	0/2/2/2
23	CLA	G	610	7	1/1/14/20	12/36/114/115	-
36	NEX	R	617	-	-	3/27/83/83	0/3/3/3
34	CHL	Y	308	-	3/3/20/26	14/39/137/137	-
23	CLA	c	503	3	1/1/15/20	18/37/115/115	-
33	HEM	e	101	5,6	-	4/12/54/54	-
34	CHL	s	605	-	3/3/16/26	9/15/113/137	-
34	CHL	s	606	-	3/3/15/26	6/12/110/137	-
23	CLA	G	604	-	1/1/11/20	9/18/96/115	-
23	CLA	a	405	1	1/1/14/20	14/31/109/115	-
32	PL9	D	406	-	-	24/53/73/73	0/1/1/1
23	CLA	y	313	20	1/1/15/20	15/37/115/115	-
23	CLA	b	601	-	1/1/15/20	14/37/115/115	-
23	CLA	b	607	-	1/1/15/20	14/37/115/115	-
23	CLA	g	602	7	1/1/15/20	19/37/115/115	-
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
34	CHL	Y	307	-	3/3/16/26	10/20/118/137	-
30	LHG	G	618	23	-	15/50/50/53	-
23	CLA	S	611	22	1/1/11/20	8/13/91/115	-
23	CLA	R	601	15	1/1/11/20	5/18/96/115	-
34	CHL	n	302	7	3/3/20/26	13/39/137/137	-
35	LUT	y	315	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	Y	317	-	-	3/27/83/83	0/3/3/3
23	CLA	C	510	3	1/1/15/20	16/37/115/115	-
23	CLA	S	603	22	1/1/11/20	7/13/91/115	-
26	SQD	A	406	-	-	11/45/65/69	0/1/1/1
35	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	G	611	30	1/1/14/20	9/31/109/115	-
34	CHL	g	606	-	3/3/15/26	9/12/110/137	-
30	LHG	n	319	23	-	15/53/53/53	-
23	CLA	Y	305	-	1/1/12/20	8/19/97/115	-
30	LHG	a	411	-	-	13/50/50/53	-
34	CHL	y	307	-	3/3/16/26	11/20/118/137	-
23	CLA	b	612	2	1/1/15/20	15/37/115/115	-
23	CLA	c	508	3	1/1/15/20	11/37/115/115	-
23	CLA	c	505	3	1/1/13/20	14/29/107/115	-
34	CHL	Y	306	20	3/3/17/26	11/21/119/137	-

All (1846) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	407	PL9	C23-C24	10.19	1.57	1.33
32	D	406	PL9	C23-C24	10.15	1.57	1.33
32	D	406	PL9	C38-C39	9.99	1.56	1.33
32	d	407	PL9	C38-C39	9.88	1.56	1.33
32	d	407	PL9	C18-C19	9.44	1.55	1.33
32	D	406	PL9	C18-C19	9.42	1.55	1.33
32	D	406	PL9	C28-C29	9.39	1.55	1.33
32	d	407	PL9	C28-C29	9.34	1.55	1.33
32	d	407	PL9	C8-C9	8.90	1.54	1.33
32	D	406	PL9	C8-C9	8.86	1.54	1.33
32	D	406	PL9	C43-C44	8.79	1.54	1.33
32	d	407	PL9	C43-C44	8.77	1.54	1.33
32	D	406	PL9	C33-C34	8.74	1.53	1.33
32	d	407	PL9	C33-C34	8.73	1.53	1.33
23	s	612	CLA	C4B-NB	8.50	1.42	1.35
23	S	612	CLA	C4B-NB	8.45	1.42	1.35
23	c	509	CLA	C4B-NB	8.17	1.42	1.35
23	R	601	CLA	C4B-NB	7.96	1.42	1.35
23	G	611	CLA	C4B-NB	7.89	1.42	1.35
23	g	611	CLA	C4B-NB	7.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	G	605	CHL	C4B-NB	7.83	1.42	1.35
32	D	406	PL9	C13-C14	7.82	1.51	1.33
23	r	610	CLA	C4B-NB	7.81	1.42	1.35
32	d	407	PL9	C13-C14	7.78	1.51	1.33
23	N	313	CLA	C4B-NB	7.75	1.42	1.35
34	s	605	CHL	C4B-NB	7.73	1.42	1.35
23	R	610	CLA	C4B-NB	7.73	1.42	1.35
23	S	604	CLA	C4B-NB	7.72	1.42	1.35
34	g	605	CHL	C4B-NB	7.71	1.42	1.35
23	C	505	CLA	C4B-NB	7.71	1.42	1.35
23	S	613	CLA	C4B-NB	7.70	1.42	1.35
23	g	610	CLA	C4B-NB	7.66	1.42	1.35
23	s	613	CLA	C4B-NB	7.66	1.42	1.35
23	S	609	CLA	C4B-NB	7.65	1.42	1.35
23	y	311	CLA	C4B-NB	7.63	1.42	1.35
23	C	513	CLA	C4B-NB	7.63	1.42	1.35
23	B	606	CLA	C4B-NB	7.62	1.42	1.35
23	C	511	CLA	C4B-NB	7.62	1.42	1.35
34	G	608	CHL	C4B-NB	7.62	1.42	1.35
23	g	602	CLA	C4B-NB	7.61	1.42	1.35
23	b	606	CLA	C4B-NB	7.61	1.42	1.35
34	r	613	CHL	C4B-NB	7.60	1.42	1.35
23	r	601	CLA	C4B-NB	7.60	1.42	1.35
34	r	606	CHL	C4B-NB	7.59	1.42	1.35
23	G	614	CLA	C4B-NB	7.58	1.42	1.35
23	c	504	CLA	C4B-NB	7.58	1.42	1.35
23	G	602	CLA	C4B-NB	7.57	1.42	1.35
23	c	510	CLA	C4B-NB	7.57	1.42	1.35
34	g	608	CHL	C4B-NB	7.56	1.42	1.35
34	R	613	CHL	C4B-NB	7.56	1.41	1.35
34	S	605	CHL	C4B-NB	7.55	1.41	1.35
34	s	606	CHL	C4B-NB	7.54	1.41	1.35
23	c	511	CLA	C4B-NB	7.53	1.41	1.35
23	C	514	CLA	C4B-NB	7.52	1.41	1.35
23	c	512	CLA	C4B-NB	7.52	1.41	1.35
23	n	315	CLA	C4B-NB	7.52	1.41	1.35
23	g	612	CLA	C4B-NB	7.51	1.41	1.35
23	g	614	CLA	C4B-NB	7.50	1.41	1.35
23	y	313	CLA	C4B-NB	7.50	1.41	1.35
34	n	306	CHL	C4B-NB	7.47	1.41	1.35
23	s	610	CLA	C4B-NB	7.46	1.41	1.35
34	R	605	CHL	C4B-NB	7.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	407	PL9	C48-C49	7.45	1.53	1.32
23	Y	311	CLA	C4B-NB	7.44	1.41	1.35
32	D	406	PL9	C48-C49	7.44	1.53	1.32
34	S	606	CHL	C4B-NB	7.43	1.41	1.35
23	C	512	CLA	C4B-NB	7.42	1.41	1.35
23	G	612	CLA	C4B-NB	7.42	1.41	1.35
34	R	606	CHL	C4B-NB	7.42	1.41	1.35
23	n	304	CLA	C4B-NB	7.42	1.41	1.35
23	R	612	CLA	C4B-NB	7.41	1.41	1.35
23	G	610	CLA	C4B-NB	7.41	1.41	1.35
23	R	611	CLA	C4B-NB	7.41	1.41	1.35
23	s	609	CLA	C4B-NB	7.41	1.41	1.35
23	s	604	CLA	C4B-NB	7.40	1.41	1.35
23	r	608	CLA	C4B-NB	7.40	1.41	1.35
32	d	407	PL9	O1-C4	7.40	1.39	1.23
23	r	614	CLA	C4B-NB	7.37	1.41	1.35
23	Y	313	CLA	C4B-NB	7.37	1.41	1.35
23	c	513	CLA	C4B-NB	7.35	1.41	1.35
32	D	406	PL9	O1-C4	7.35	1.39	1.23
23	r	611	CLA	C4B-NB	7.35	1.41	1.35
34	G	607	CHL	C4B-NB	7.34	1.41	1.35
23	s	603	CLA	C4B-NB	7.32	1.41	1.35
23	R	608	CLA	C4B-NB	7.32	1.41	1.35
23	R	609	CLA	C4B-NB	7.32	1.41	1.35
23	B	616	CLA	C4B-NB	7.32	1.41	1.35
23	N	312	CLA	C4B-NB	7.31	1.41	1.35
34	s	607	CHL	C4B-NB	7.29	1.41	1.35
34	S	607	CHL	C4B-NB	7.29	1.41	1.35
23	n	312	CLA	C4B-NB	7.29	1.41	1.35
34	Y	308	CHL	C4B-NB	7.29	1.41	1.35
34	g	607	CHL	C4B-NB	7.28	1.41	1.35
23	b	608	CLA	C4B-NB	7.28	1.41	1.35
23	R	602	CLA	C4B-NB	7.27	1.41	1.35
23	a	402	CLA	C4B-NB	7.27	1.41	1.35
23	b	615	CLA	C4B-NB	7.24	1.41	1.35
23	b	616	CLA	C4B-NB	7.24	1.41	1.35
23	Y	304	CLA	C4B-NB	7.23	1.41	1.35
34	R	607	CHL	C4B-NB	7.23	1.41	1.35
23	b	609	CLA	C4B-NB	7.23	1.41	1.35
34	y	308	CHL	C4B-NB	7.23	1.41	1.35
23	n	314	CLA	C4B-NB	7.22	1.41	1.35
23	N	315	CLA	C4B-NB	7.22	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	403	CLA	C4B-NB	7.21	1.41	1.35
34	s	601	CHL	C4B-NB	7.21	1.41	1.35
34	N	306	CHL	C4B-NB	7.21	1.41	1.35
34	Y	306	CHL	C4B-NB	7.20	1.41	1.35
23	s	611	CLA	C4B-NB	7.19	1.41	1.35
23	c	506	CLA	C4B-NB	7.18	1.41	1.35
23	A	402	CLA	C4B-NB	7.18	1.41	1.35
23	B	615	CLA	C4B-NB	7.18	1.41	1.35
23	R	614	CLA	C4B-NB	7.18	1.41	1.35
23	G	603	CLA	C4B-NB	7.17	1.41	1.35
23	y	304	CLA	C4B-NB	7.16	1.41	1.35
23	b	603	CLA	C4B-NB	7.16	1.41	1.35
23	g	603	CLA	C4B-NB	7.16	1.41	1.35
23	d	405	CLA	C4B-NB	7.15	1.41	1.35
23	y	303	CLA	C4B-NB	7.14	1.41	1.35
34	Y	309	CHL	C4B-NB	7.14	1.41	1.35
23	Y	310	CLA	C4B-NB	7.14	1.41	1.35
23	r	602	CLA	C4B-NB	7.14	1.41	1.35
34	S	601	CHL	C4B-NB	7.13	1.41	1.35
23	s	608	CLA	C4B-NB	7.13	1.41	1.35
23	n	311	CLA	C4B-NB	7.12	1.41	1.35
23	B	609	CLA	C4B-NB	7.11	1.41	1.35
34	r	605	CHL	C4B-NB	7.11	1.41	1.35
23	r	612	CLA	C4B-NB	7.10	1.41	1.35
23	b	601	CLA	C4B-NB	7.09	1.41	1.35
23	S	603	CLA	C4B-NB	7.09	1.41	1.35
23	b	604	CLA	C4B-NB	7.09	1.41	1.35
23	S	608	CLA	C4B-NB	7.09	1.41	1.35
34	n	307	CHL	C4B-NB	7.08	1.41	1.35
23	r	603	CLA	C4B-NB	7.07	1.41	1.35
23	G	613	CLA	C4B-NB	7.07	1.41	1.35
23	n	313	CLA	C4B-NB	7.07	1.41	1.35
23	D	405	CLA	C4B-NB	7.06	1.41	1.35
23	S	611	CLA	C4B-NB	7.06	1.41	1.35
23	B	607	CLA	C4B-NB	7.06	1.41	1.35
34	y	306	CHL	C4B-NB	7.06	1.41	1.35
23	N	314	CLA	C4B-NB	7.06	1.41	1.35
23	C	506	CLA	C4B-NB	7.05	1.41	1.35
23	b	607	CLA	C4B-NB	7.05	1.41	1.35
23	R	603	CLA	C4B-NB	7.04	1.41	1.35
34	G	619	CHL	C4B-NB	7.03	1.41	1.35
23	S	610	CLA	C4B-NB	7.03	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4B-NB	7.02	1.41	1.35
23	C	504	CLA	C4B-NB	7.02	1.41	1.35
23	y	312	CLA	C4B-NB	7.01	1.41	1.35
23	N	304	CLA	C4B-NB	7.01	1.41	1.35
34	y	309	CHL	C4B-NB	6.98	1.41	1.35
23	c	505	CLA	C4B-NB	6.98	1.41	1.35
23	C	507	CLA	C4B-NB	6.98	1.41	1.35
23	Y	312	CLA	C4B-NB	6.96	1.41	1.35
23	C	508	CLA	C4B-NB	6.96	1.41	1.35
23	b	611	CLA	C4B-NB	6.95	1.41	1.35
23	c	503	CLA	C4B-NB	6.94	1.41	1.35
23	B	613	CLA	C4B-NB	6.94	1.41	1.35
23	B	611	CLA	C4B-NB	6.93	1.41	1.35
34	r	607	CHL	C4B-NB	6.93	1.41	1.35
23	y	305	CLA	C4B-NB	6.93	1.41	1.35
23	C	502	CLA	C4B-NB	6.93	1.41	1.35
34	y	302	CHL	C4B-NB	6.93	1.41	1.35
23	r	609	CLA	C4B-NB	6.92	1.41	1.35
34	g	609	CHL	C4B-NB	6.92	1.41	1.35
23	B	608	CLA	C4B-NB	6.92	1.41	1.35
23	B	604	CLA	C4B-NB	6.92	1.41	1.35
23	g	613	CLA	C4B-NB	6.92	1.41	1.35
34	N	309	CHL	C4B-NB	6.91	1.41	1.35
23	c	507	CLA	C4B-NB	6.91	1.41	1.35
23	Y	303	CLA	C4B-NB	6.90	1.41	1.35
23	D	404	CLA	C4B-NB	6.90	1.41	1.35
34	Y	302	CHL	C4B-NB	6.90	1.41	1.35
23	y	314	CLA	C4B-NB	6.88	1.41	1.35
23	N	303	CLA	C4B-NB	6.88	1.41	1.35
23	c	501	CLA	C4B-NB	6.87	1.41	1.35
23	B	603	CLA	C4B-NB	6.87	1.41	1.35
23	D	401	CLA	C4B-NB	6.87	1.41	1.35
23	S	602	CLA	C4B-NB	6.86	1.41	1.35
23	B	614	CLA	C4B-NB	6.85	1.41	1.35
34	N	308	CHL	C4B-NB	6.85	1.41	1.35
34	g	619	CHL	C4B-NB	6.84	1.41	1.35
34	N	307	CHL	C4B-NB	6.83	1.41	1.35
23	d	404	CLA	C4B-NB	6.82	1.41	1.35
34	g	601	CHL	C4B-NB	6.80	1.41	1.35
23	Y	305	CLA	C4B-NB	6.79	1.41	1.35
34	n	308	CHL	C4B-NB	6.79	1.41	1.35
23	R	604	CLA	C4B-NB	6.78	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	n	309	CHL	C4B-NB	6.78	1.41	1.35
23	N	311	CLA	C4B-NB	6.77	1.41	1.35
23	b	614	CLA	C4B-NB	6.76	1.41	1.35
23	s	602	CLA	C4B-NB	6.75	1.41	1.35
23	g	604	CLA	C4B-NB	6.75	1.41	1.35
23	Y	314	CLA	C4B-NB	6.74	1.41	1.35
23	r	604	CLA	C4B-NB	6.74	1.41	1.35
32	d	407	PL9	C3-C4	-6.73	1.38	1.49
23	n	303	CLA	C4B-NB	6.72	1.41	1.35
23	y	310	CLA	C4B-NB	6.71	1.41	1.35
23	C	503	CLA	C4B-NB	6.71	1.41	1.35
32	D	406	PL9	C3-C4	-6.68	1.38	1.49
23	N	305	CLA	C4B-NB	6.66	1.41	1.35
23	C	510	CLA	C4B-NB	6.65	1.41	1.35
23	B	601	CLA	C4B-NB	6.65	1.41	1.35
23	G	604	CLA	C4B-NB	6.64	1.41	1.35
34	n	302	CHL	C4B-NB	6.62	1.41	1.35
34	g	606	CHL	C4B-NB	6.61	1.41	1.35
34	G	601	CHL	C4B-NB	6.59	1.41	1.35
23	C	509	CLA	C4B-NB	6.59	1.41	1.35
34	Y	307	CHL	C4B-NB	6.57	1.41	1.35
23	c	502	CLA	C4B-NB	6.56	1.41	1.35
34	N	310	CHL	C4B-NB	6.55	1.41	1.35
23	b	612	CLA	C4B-NB	6.54	1.41	1.35
34	G	606	CHL	C4B-NB	6.53	1.41	1.35
23	B	612	CLA	C4B-NB	6.53	1.41	1.35
23	a	405	CLA	C4B-NB	6.53	1.41	1.35
23	n	305	CLA	C4B-NB	6.53	1.41	1.35
34	N	302	CHL	C4B-NB	6.52	1.41	1.35
23	B	605	CLA	C4B-NB	6.50	1.41	1.35
23	b	610	CLA	C4B-NB	6.47	1.41	1.35
23	A	404	CLA	C4B-NB	6.46	1.41	1.35
23	c	508	CLA	C4B-NB	6.46	1.41	1.35
23	b	605	CLA	C4B-NB	6.44	1.41	1.35
23	B	602	CLA	C4B-NB	6.44	1.41	1.35
34	G	609	CHL	C4B-NB	6.41	1.40	1.35
23	b	602	CLA	C4B-NB	6.39	1.40	1.35
34	y	307	CHL	C4B-NB	6.34	1.40	1.35
34	n	310	CHL	C4B-NB	6.32	1.40	1.35
32	d	407	PL9	C6-C1	-6.21	1.37	1.48
23	B	610	CLA	C4B-NB	6.19	1.40	1.35
23	A	401	CLA	C4B-NB	6.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406	PL9	C6-C1	-6.18	1.37	1.48
23	a	401	CLA	C4B-NB	5.98	1.40	1.35
32	D	406	PL9	O2-C1	5.43	1.39	1.24
32	d	407	PL9	O2-C1	5.42	1.39	1.24
26	A	409	SQD	O8-S	5.00	1.65	1.47
26	a	409	SQD	O8-S	4.98	1.65	1.47
36	y	317	NEX	C7-C8	-4.72	1.24	1.32
26	d	402	SQD	O8-S	4.63	1.64	1.47
26	A	406	SQD	O8-S	4.60	1.63	1.47
26	L	103	SQD	O8-S	4.54	1.63	1.47
26	M	101	SQD	O8-S	4.54	1.63	1.47
30	r	618	LHG	O7-C7	4.45	1.46	1.34
27	B	622	LMG	O8-C28	4.37	1.46	1.33
27	D	407	LMG	O8-C28	4.37	1.46	1.33
27	d	409	LMG	O8-C28	4.36	1.46	1.33
27	A	407	LMG	O8-C28	4.34	1.46	1.33
28	a	408	DGD	O2G-C1B	4.33	1.46	1.34
28	H	102	DGD	O1G-C1A	4.33	1.46	1.33
28	A	408	DGD	O2G-C1B	4.32	1.46	1.34
27	B	622	LMG	O7-C10	4.31	1.46	1.34
30	R	618	LHG	O7-C7	4.30	1.46	1.34
23	N	314	CLA	C4D-ND	-4.29	1.31	1.37
30	w	201	LHG	O8-C23	4.28	1.45	1.33
28	d	410	DGD	O1G-C1A	4.27	1.45	1.33
30	R	618	LHG	O8-C23	4.27	1.45	1.33
28	H	102	DGD	O2G-C1B	4.27	1.46	1.34
27	A	407	LMG	O7-C10	4.27	1.46	1.34
36	y	317	NEX	C1-C6	-4.24	1.47	1.54
30	S	617	LHG	O7-C7	4.23	1.46	1.34
30	s	617	LHG	O7-C7	4.22	1.46	1.34
30	N	319	LHG	O8-C23	4.22	1.45	1.33
23	s	608	CLA	C1D-ND	4.22	1.43	1.37
26	d	402	SQD	O48-C23	4.21	1.45	1.33
30	n	319	LHG	O8-C23	4.20	1.45	1.33
27	D	407	LMG	O7-C10	4.20	1.46	1.34
30	b	621	LHG	O7-C7	4.19	1.46	1.34
30	c	517	LHG	O7-C7	4.19	1.46	1.34
26	A	406	SQD	O48-C23	4.18	1.45	1.33
33	e	101	HEM	C3C-CAC	4.18	1.56	1.47
26	A	406	SQD	O47-C7	4.18	1.46	1.34
26	a	409	SQD	O48-C23	4.17	1.45	1.33
27	b	620	LMG	O8-C28	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	SQD	O48-C23	4.17	1.45	1.33
30	B	621	LHG	O7-C7	4.17	1.46	1.34
30	W	201	LHG	O8-C23	4.17	1.45	1.33
27	d	409	LMG	O7-C10	4.16	1.46	1.34
28	A	408	DGD	O1G-C1A	4.15	1.45	1.33
30	r	618	LHG	O8-C23	4.15	1.45	1.33
27	B	620	LMG	O8-C28	4.15	1.45	1.33
32	D	406	PL9	C7-C3	4.14	1.55	1.51
30	n	319	LHG	O7-C7	4.14	1.46	1.34
30	G	618	LHG	O7-C7	4.14	1.46	1.34
28	a	408	DGD	O1G-C1A	4.14	1.45	1.33
23	c	509	CLA	C1D-ND	4.14	1.42	1.37
33	E	101	HEM	C3C-CAC	4.13	1.56	1.47
28	C	517	DGD	O2G-C1B	4.13	1.45	1.34
27	C	501	LMG	O8-C28	4.13	1.45	1.33
30	C	518	LHG	O7-C7	4.11	1.45	1.34
30	G	618	LHG	O8-C23	4.11	1.45	1.33
28	c	516	DGD	O2G-C1B	4.11	1.45	1.34
27	C	501	LMG	O7-C10	4.11	1.45	1.34
23	S	608	CLA	C1D-ND	4.10	1.42	1.37
27	a	407	LMG	O7-C10	4.09	1.45	1.34
26	d	402	SQD	O47-C7	4.09	1.45	1.34
23	N	313	CLA	C1D-ND	4.09	1.42	1.37
23	R	608	CLA	C1D-ND	4.09	1.42	1.37
30	L	101	LHG	O8-C23	4.08	1.45	1.33
28	d	410	DGD	O2G-C1B	4.08	1.45	1.34
30	g	618	LHG	O7-C7	4.08	1.45	1.34
30	a	412	LHG	O8-C23	4.08	1.45	1.33
30	y	318	LHG	O8-C23	4.08	1.45	1.33
26	a	409	SQD	O47-C7	4.08	1.45	1.34
30	g	618	LHG	O8-C23	4.08	1.45	1.33
30	Y	318	LHG	O8-C23	4.06	1.45	1.33
30	A	412	LHG	O8-C23	4.06	1.45	1.33
30	A	411	LHG	O7-C7	4.06	1.45	1.34
26	L	103	SQD	O48-C23	4.06	1.45	1.33
30	T	101	LHG	O8-C23	4.06	1.45	1.33
32	d	407	PL9	C7-C3	4.05	1.55	1.51
27	a	407	LMG	O8-C28	4.05	1.45	1.33
36	Y	317	NEX	C7-C8	-4.04	1.25	1.32
30	w	201	LHG	O7-C7	4.04	1.45	1.34
30	a	411	LHG	O7-C7	4.04	1.45	1.34
30	W	201	LHG	O7-C7	4.04	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M	101	SQD	O48-C23	4.03	1.45	1.33
26	L	103	SQD	O47-C7	4.03	1.45	1.34
30	Y	318	LHG	O7-C7	4.03	1.45	1.34
30	B	623	LHG	O8-C23	4.02	1.45	1.33
30	T	101	LHG	O7-C7	4.02	1.45	1.34
34	S	606	CHL	C1D-ND	4.02	1.42	1.37
26	A	409	SQD	O47-C7	4.02	1.45	1.34
23	n	313	CLA	C1D-ND	4.01	1.42	1.37
23	s	613	CLA	C1D-ND	4.01	1.42	1.37
30	B	623	LHG	O7-C7	4.01	1.45	1.34
23	S	613	CLA	C1D-ND	4.00	1.42	1.37
30	d	408	LHG	O8-C23	4.00	1.45	1.33
23	r	608	CLA	C1D-ND	3.99	1.42	1.37
30	A	411	LHG	O8-C23	3.99	1.45	1.33
30	C	518	LHG	O8-C23	3.98	1.45	1.33
27	b	620	LMG	O7-C10	3.98	1.45	1.34
30	y	318	LHG	O7-C7	3.97	1.45	1.34
26	M	101	SQD	O47-C7	3.96	1.45	1.34
23	c	504	CLA	C1D-ND	3.95	1.42	1.37
27	B	620	LMG	O7-C10	3.95	1.45	1.34
30	N	319	LHG	O7-C7	3.95	1.45	1.34
23	a	403	CLA	C4D-ND	-3.94	1.32	1.37
30	a	411	LHG	O8-C23	3.93	1.44	1.33
23	R	612	CLA	C1D-ND	3.93	1.42	1.37
23	a	402	CLA	C4D-ND	-3.92	1.32	1.37
30	c	517	LHG	O8-C23	3.92	1.44	1.33
30	L	102	LHG	O7-C7	3.92	1.45	1.34
30	a	412	LHG	O7-C7	3.91	1.45	1.34
30	s	617	LHG	O8-C23	3.90	1.44	1.33
30	b	622	LHG	O7-C7	3.89	1.45	1.34
34	N	310	CHL	C4D-ND	-3.89	1.32	1.37
30	S	617	LHG	O8-C23	3.87	1.44	1.33
28	C	517	DGD	O1G-C1A	3.87	1.44	1.33
28	c	516	DGD	O1G-C1A	3.87	1.44	1.33
34	S	607	CHL	C1D-ND	3.87	1.42	1.37
23	A	402	CLA	C4D-ND	-3.87	1.32	1.37
30	A	412	LHG	O7-C7	3.86	1.45	1.34
34	G	607	CHL	C1D-ND	3.86	1.42	1.37
23	s	604	CLA	C1D-ND	3.85	1.42	1.37
30	B	621	LHG	O8-C23	3.85	1.44	1.33
23	y	313	CLA	C4D-ND	-3.84	1.32	1.37
23	R	614	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	621	LHG	O8-C23	3.83	1.44	1.33
23	Y	313	CLA	C4D-ND	-3.83	1.32	1.37
23	C	510	CLA	C1D-ND	3.82	1.42	1.37
30	b	622	LHG	O8-C23	3.81	1.44	1.33
23	b	608	CLA	CMB-C2B	-3.81	1.43	1.51
34	s	606	CHL	C1D-ND	3.80	1.42	1.37
34	R	613	CHL	C1D-ND	3.80	1.42	1.37
23	S	603	CLA	C1D-ND	3.80	1.42	1.37
30	L	102	LHG	O8-C23	3.80	1.44	1.33
23	D	401	CLA	C4D-ND	-3.79	1.32	1.37
23	c	501	CLA	C4D-ND	-3.79	1.32	1.37
34	N	310	CHL	CMB-C2B	-3.79	1.43	1.51
23	r	612	CLA	C1D-ND	3.78	1.42	1.37
30	d	408	LHG	O7-C7	3.78	1.45	1.34
23	S	604	CLA	C1D-ND	3.78	1.42	1.37
23	R	610	CLA	C1D-ND	3.78	1.42	1.37
23	d	405	CLA	C1D-ND	3.77	1.42	1.37
34	n	310	CHL	C4D-ND	-3.77	1.32	1.37
30	L	101	LHG	O7-C7	3.76	1.44	1.34
23	g	612	CLA	C1D-ND	3.76	1.42	1.37
34	Y	309	CHL	CMB-C2B	-3.76	1.43	1.51
23	n	303	CLA	C4D-ND	-3.75	1.32	1.37
23	N	303	CLA	C4D-ND	-3.74	1.32	1.37
34	g	609	CHL	C1D-ND	3.74	1.42	1.37
23	C	503	CLA	C4D-ND	-3.73	1.32	1.37
23	c	503	CLA	C1D-ND	3.72	1.42	1.37
34	r	613	CHL	C1D-ND	3.72	1.42	1.37
23	S	611	CLA	C1D-ND	3.71	1.42	1.37
34	g	605	CHL	C1D-ND	3.71	1.42	1.37
23	n	314	CLA	C4D-ND	-3.69	1.32	1.37
34	G	609	CHL	C4D-ND	-3.69	1.32	1.37
23	C	505	CLA	C1D-ND	3.69	1.42	1.37
23	Y	310	CLA	C1D-ND	3.67	1.42	1.37
23	R	603	CLA	C1D-ND	3.67	1.42	1.37
34	g	607	CHL	C1D-ND	3.67	1.42	1.37
23	D	405	CLA	C1D-ND	3.67	1.42	1.37
23	C	512	CLA	C1D-ND	3.66	1.42	1.37
23	G	614	CLA	C1D-ND	3.65	1.42	1.37
23	Y	312	CLA	C1D-ND	3.65	1.42	1.37
23	R	602	CLA	C1D-ND	3.65	1.42	1.37
23	N	312	CLA	C4D-ND	-3.65	1.32	1.37
23	y	310	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	610	CLA	C1D-ND	3.64	1.42	1.37
23	c	512	CLA	C1D-ND	3.64	1.42	1.37
34	G	606	CHL	C1D-ND	3.64	1.42	1.37
34	n	310	CHL	CMB-C2B	-3.62	1.44	1.51
23	C	504	CLA	C1D-ND	3.62	1.42	1.37
23	B	607	CLA	C1D-ND	3.62	1.42	1.37
23	N	315	CLA	C1D-ND	3.62	1.42	1.37
23	s	610	CLA	C1D-ND	3.62	1.42	1.37
23	A	401	CLA	C1D-ND	3.62	1.42	1.37
23	r	610	CLA	C1D-ND	3.61	1.42	1.37
23	B	609	CLA	C4D-ND	-3.61	1.32	1.37
23	b	607	CLA	C1D-ND	3.61	1.42	1.37
23	r	614	CLA	C1D-ND	3.61	1.42	1.37
23	y	312	CLA	C1D-ND	3.60	1.42	1.37
23	s	603	CLA	C1D-ND	3.60	1.42	1.37
23	B	605	CLA	C4D-ND	-3.60	1.32	1.37
23	r	602	CLA	C1D-ND	3.60	1.42	1.37
23	a	401	CLA	C1D-ND	3.59	1.42	1.37
34	N	306	CHL	C1D-ND	3.59	1.42	1.37
34	G	609	CHL	C1D-ND	3.59	1.42	1.37
23	n	315	CLA	C1D-ND	3.58	1.42	1.37
34	s	601	CHL	C1D-ND	3.58	1.42	1.37
23	s	609	CLA	C1D-ND	3.58	1.42	1.37
23	g	614	CLA	C1D-ND	3.58	1.42	1.37
23	B	608	CLA	C4D-ND	-3.57	1.32	1.37
34	G	605	CHL	C1D-ND	3.57	1.42	1.37
23	B	601	CLA	C1D-ND	3.57	1.42	1.37
23	s	612	CLA	C1D-ND	3.57	1.42	1.37
23	g	602	CLA	C1D-ND	3.56	1.42	1.37
23	G	610	CLA	C1D-ND	3.56	1.42	1.37
34	g	609	CHL	C4D-ND	-3.56	1.32	1.37
34	r	605	CHL	C1D-ND	3.55	1.42	1.37
23	B	601	CLA	C4D-ND	-3.55	1.32	1.37
23	C	509	CLA	C4D-ND	-3.55	1.32	1.37
23	b	609	CLA	C4D-ND	-3.54	1.32	1.37
34	s	605	CHL	C1D-ND	3.54	1.42	1.37
23	c	508	CLA	C4D-ND	-3.54	1.32	1.37
23	s	611	CLA	C1D-ND	3.54	1.42	1.37
23	r	601	CLA	C1D-ND	3.53	1.42	1.37
23	c	513	CLA	C4D-ND	-3.53	1.32	1.37
23	c	506	CLA	C4D-ND	-3.53	1.32	1.37
34	R	607	CHL	C4D-ND	-3.53	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C1D-ND	3.53	1.42	1.37
23	r	604	CLA	C1D-ND	3.53	1.42	1.37
23	a	403	CLA	C1D-ND	3.52	1.42	1.37
23	b	604	CLA	C1D-ND	3.52	1.42	1.37
34	r	606	CHL	C1D-ND	3.52	1.42	1.37
34	g	606	CHL	C1D-ND	3.51	1.42	1.37
23	S	612	CLA	C1D-ND	3.51	1.42	1.37
34	S	601	CHL	C1D-ND	3.50	1.42	1.37
23	c	502	CLA	C4D-ND	-3.50	1.32	1.37
34	g	608	CHL	C4D-ND	-3.50	1.32	1.37
23	B	611	CLA	C4D-ND	-3.50	1.32	1.37
23	G	604	CLA	C4D-ND	-3.50	1.32	1.37
23	R	601	CLA	C1D-ND	3.49	1.42	1.37
23	r	603	CLA	C1D-ND	3.49	1.42	1.37
23	S	609	CLA	C1D-ND	3.49	1.42	1.37
23	b	605	CLA	C1D-ND	3.49	1.42	1.37
23	A	402	CLA	C1D-ND	3.49	1.42	1.37
23	N	305	CLA	C4D-ND	-3.49	1.32	1.37
23	n	311	CLA	C4D-ND	-3.49	1.32	1.37
23	d	404	CLA	C4D-ND	-3.49	1.32	1.37
23	b	601	CLA	C1D-ND	3.48	1.42	1.37
23	b	615	CLA	C1D-ND	3.48	1.42	1.37
23	C	509	CLA	C1D-ND	3.48	1.42	1.37
23	R	609	CLA	C1D-ND	3.48	1.42	1.37
23	b	608	CLA	C4D-ND	-3.48	1.32	1.37
23	B	602	CLA	C1D-ND	3.48	1.42	1.37
23	b	602	CLA	C1D-ND	3.48	1.42	1.37
23	A	404	CLA	C4D-ND	-3.48	1.32	1.37
23	C	513	CLA	C1D-ND	3.47	1.42	1.37
23	b	611	CLA	C4D-ND	-3.47	1.32	1.37
23	B	615	CLA	C1D-ND	3.47	1.42	1.37
23	N	311	CLA	C1D-ND	3.47	1.42	1.37
23	c	508	CLA	C1D-ND	3.47	1.42	1.37
23	B	602	CLA	C4D-ND	-3.47	1.32	1.37
23	n	312	CLA	C4D-ND	-3.47	1.32	1.37
34	Y	309	CHL	C1D-ND	3.47	1.42	1.37
23	y	303	CLA	C1D-ND	3.47	1.42	1.37
23	C	507	CLA	C4D-ND	-3.46	1.32	1.37
34	Y	309	CHL	C4D-ND	-3.46	1.32	1.37
34	n	308	CHL	C1D-ND	3.46	1.42	1.37
23	c	506	CLA	C1D-ND	3.45	1.42	1.37
23	C	502	CLA	C4D-ND	-3.45	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4D-ND	-3.45	1.32	1.37
23	S	602	CLA	C4D-ND	-3.45	1.33	1.37
23	C	502	CLA	CMD-C2D	-3.45	1.43	1.50
23	N	304	CLA	C1D-ND	3.45	1.42	1.37
23	C	514	CLA	C4D-ND	-3.45	1.33	1.37
23	n	305	CLA	C4D-ND	-3.45	1.33	1.37
34	n	310	CHL	C1D-ND	3.44	1.42	1.37
23	y	314	CLA	C1D-ND	3.44	1.42	1.37
23	n	312	CLA	C1D-ND	3.44	1.42	1.37
34	s	607	CHL	C1D-ND	3.44	1.42	1.37
34	n	309	CHL	C4D-ND	-3.44	1.33	1.37
34	N	307	CHL	C1D-ND	3.44	1.42	1.37
23	G	612	CLA	C1D-ND	3.43	1.42	1.37
34	r	607	CHL	C1D-ND	3.43	1.42	1.37
23	r	609	CLA	C1D-ND	3.43	1.42	1.37
23	B	606	CLA	C4D-ND	-3.43	1.33	1.37
23	G	602	CLA	C1D-ND	3.42	1.42	1.37
23	b	606	CLA	C1D-ND	3.42	1.42	1.37
23	g	613	CLA	C4D-ND	-3.42	1.33	1.37
23	b	606	CLA	C4D-ND	-3.42	1.33	1.37
23	S	602	CLA	C1D-ND	3.41	1.42	1.37
23	y	311	CLA	C1D-ND	3.41	1.42	1.37
23	G	611	CLA	C4D-ND	-3.41	1.33	1.37
23	Y	314	CLA	C4D-ND	-3.41	1.33	1.37
23	b	613	CLA	C1D-ND	3.41	1.42	1.37
23	R	604	CLA	C1D-ND	3.41	1.42	1.37
34	S	605	CHL	C1D-ND	3.40	1.42	1.37
34	y	306	CHL	C1D-ND	3.40	1.42	1.37
34	Y	306	CHL	C1D-ND	3.40	1.42	1.37
23	g	610	CLA	C1D-ND	3.39	1.42	1.37
23	s	602	CLA	C4D-ND	-3.39	1.33	1.37
23	G	610	CLA	C4D-ND	-3.39	1.33	1.37
23	a	405	CLA	C4D-ND	-3.39	1.33	1.37
34	R	607	CHL	C1D-ND	3.39	1.42	1.37
23	B	609	CLA	C3B-C2B	-3.39	1.35	1.40
34	R	606	CHL	C1D-ND	3.39	1.42	1.37
34	N	308	CHL	C1D-ND	3.39	1.41	1.37
23	b	601	CLA	C4D-ND	-3.38	1.33	1.37
23	b	610	CLA	C4D-ND	-3.38	1.33	1.37
23	D	405	CLA	C4D-ND	-3.37	1.33	1.37
23	y	304	CLA	C4D-ND	-3.37	1.33	1.37
23	D	404	CLA	C4D-ND	-3.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	310	CLA	C4D-ND	-3.37	1.33	1.37
23	y	311	CLA	C4D-ND	-3.37	1.33	1.37
34	y	309	CHL	CMB-C2B	-3.37	1.44	1.51
23	d	405	CLA	C4D-ND	-3.36	1.33	1.37
23	b	605	CLA	C4D-ND	-3.36	1.33	1.37
23	Y	311	CLA	C1D-ND	3.36	1.41	1.37
23	n	314	CLA	C1D-ND	3.36	1.41	1.37
23	b	614	CLA	C4D-ND	-3.35	1.33	1.37
23	y	305	CLA	CMB-C2B	-3.35	1.44	1.51
23	n	304	CLA	C1D-ND	3.35	1.41	1.37
23	b	616	CLA	C1D-ND	3.35	1.41	1.37
23	g	611	CLA	C1D-ND	3.35	1.41	1.37
23	B	616	CLA	C1D-ND	3.35	1.41	1.37
23	s	609	CLA	C4D-ND	-3.35	1.33	1.37
23	c	505	CLA	C4D-ND	-3.35	1.33	1.37
23	B	614	CLA	C4D-ND	-3.35	1.33	1.37
23	g	604	CLA	C4D-ND	-3.34	1.33	1.37
23	Y	303	CLA	C1D-ND	3.34	1.41	1.37
23	B	610	CLA	C4D-ND	-3.34	1.33	1.37
34	N	307	CHL	C4D-ND	-3.34	1.33	1.37
23	C	506	CLA	C4D-ND	-3.34	1.33	1.37
23	Y	312	CLA	C4D-ND	-3.34	1.33	1.37
23	B	606	CLA	C1D-ND	3.34	1.41	1.37
23	B	613	CLA	C1D-ND	3.34	1.41	1.37
23	Y	311	CLA	C4D-ND	-3.33	1.33	1.37
34	N	310	CHL	C1D-ND	3.33	1.41	1.37
34	R	606	CHL	C4D-ND	-3.33	1.33	1.37
34	R	605	CHL	C1D-ND	3.33	1.41	1.37
23	R	602	CLA	C4D-ND	-3.33	1.33	1.37
34	g	608	CHL	C1D-ND	3.32	1.41	1.37
23	Y	314	CLA	C1D-ND	3.32	1.41	1.37
23	r	602	CLA	C4D-ND	-3.32	1.33	1.37
34	g	607	CHL	C4D-ND	-3.32	1.33	1.37
23	b	602	CLA	C4D-ND	-3.31	1.33	1.37
23	G	613	CLA	C4D-ND	-3.31	1.33	1.37
23	N	315	CLA	C4D-ND	-3.31	1.33	1.37
34	n	309	CHL	C1D-ND	3.31	1.41	1.37
23	C	510	CLA	C4D-ND	-3.31	1.33	1.37
34	y	309	CHL	C1D-ND	3.30	1.41	1.37
23	A	404	CLA	C1D-ND	3.30	1.41	1.37
23	B	609	CLA	CMB-C2B	-3.30	1.44	1.51
34	n	307	CHL	C4D-ND	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1D-ND	3.30	1.41	1.37
23	B	614	CLA	C1D-ND	3.30	1.41	1.37
23	B	605	CLA	C1D-ND	3.29	1.41	1.37
23	b	614	CLA	C1D-ND	3.29	1.41	1.37
23	S	609	CLA	C4D-ND	-3.29	1.33	1.37
23	S	611	CLA	C4D-ND	-3.29	1.33	1.37
23	b	613	CLA	C4D-ND	-3.29	1.33	1.37
23	b	612	CLA	C4D-ND	-3.28	1.33	1.37
23	C	507	CLA	C1D-ND	3.28	1.41	1.37
23	B	608	CLA	CMB-C2B	-3.28	1.44	1.51
34	r	606	CHL	C4D-ND	-3.28	1.33	1.37
33	e	101	HEM	C3C-C2C	-3.27	1.35	1.40
34	R	605	CHL	C4D-ND	-3.27	1.33	1.37
23	c	511	CLA	C4D-ND	-3.27	1.33	1.37
34	S	607	CHL	CHC-C1C	3.27	1.43	1.35
23	Y	310	CLA	CHC-C1C	3.27	1.43	1.35
23	y	310	CLA	CHC-C1C	3.26	1.43	1.35
23	Y	304	CLA	C4D-ND	-3.26	1.33	1.37
23	N	311	CLA	C4D-ND	-3.26	1.33	1.37
23	b	604	CLA	C4D-ND	-3.26	1.33	1.37
23	Y	313	CLA	C1D-ND	3.26	1.41	1.37
23	B	613	CLA	C4D-ND	-3.26	1.33	1.37
23	c	504	CLA	C4D-ND	-3.25	1.33	1.37
34	r	605	CHL	C4D-ND	-3.25	1.33	1.37
34	G	608	CHL	C4D-ND	-3.25	1.33	1.37
23	G	603	CLA	C1D-ND	3.25	1.41	1.37
34	g	607	CHL	CHC-C1C	3.25	1.43	1.35
23	y	313	CLA	C1D-ND	3.24	1.41	1.37
23	C	503	CLA	CMB-C2B	-3.24	1.44	1.51
23	c	507	CLA	C4D-ND	-3.24	1.33	1.37
23	Y	310	CLA	C4D-ND	-3.24	1.33	1.37
23	n	315	CLA	C4D-ND	-3.24	1.33	1.37
23	B	603	CLA	C4D-ND	-3.23	1.33	1.37
23	g	610	CLA	C4D-ND	-3.23	1.33	1.37
23	r	603	CLA	C4D-ND	-3.23	1.33	1.37
23	n	305	CLA	C1D-ND	3.23	1.41	1.37
23	G	610	CLA	CHC-C1C	3.23	1.43	1.35
23	B	604	CLA	C4D-ND	-3.23	1.33	1.37
34	G	619	CHL	C1D-ND	3.22	1.41	1.37
23	g	603	CLA	C1D-ND	3.22	1.41	1.37
23	n	311	CLA	C1D-ND	3.22	1.41	1.37
23	s	603	CLA	C4D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	611	CLA	C1D-ND	3.22	1.41	1.37
23	N	312	CLA	C1D-ND	3.21	1.41	1.37
23	b	609	CLA	C1D-ND	3.21	1.41	1.37
23	b	611	CLA	C1D-ND	3.21	1.41	1.37
23	y	312	CLA	C4D-ND	-3.20	1.33	1.37
34	n	307	CHL	C1D-ND	3.20	1.41	1.37
23	y	314	CLA	C4D-ND	-3.20	1.33	1.37
34	N	309	CHL	C4D-ND	-3.20	1.33	1.37
23	b	607	CLA	C4D-ND	-3.20	1.33	1.37
23	S	602	CLA	CHC-C1C	3.20	1.43	1.35
23	B	611	CLA	C1D-ND	3.19	1.41	1.37
34	g	619	CHL	C1D-ND	3.19	1.41	1.37
23	S	610	CLA	C4D-ND	-3.19	1.33	1.37
34	y	307	CHL	C1D-ND	3.19	1.41	1.37
23	g	611	CLA	C4D-ND	-3.18	1.33	1.37
23	r	609	CLA	C4D-ND	-3.18	1.33	1.37
23	B	607	CLA	C4D-ND	-3.18	1.33	1.37
23	G	613	CLA	C1D-ND	3.18	1.41	1.37
34	y	306	CHL	C4D-ND	-3.18	1.33	1.37
23	b	603	CLA	C4D-ND	-3.17	1.33	1.37
34	G	607	CHL	C4D-ND	-3.17	1.33	1.37
23	a	405	CLA	C1D-ND	3.17	1.41	1.37
34	n	306	CHL	C1D-ND	3.17	1.41	1.37
34	n	306	CHL	C4D-ND	-3.17	1.33	1.37
23	y	305	CLA	C4D-ND	-3.17	1.33	1.37
23	G	611	CLA	CHC-C1C	3.17	1.43	1.35
23	G	612	CLA	C4D-ND	-3.17	1.33	1.37
23	s	602	CLA	C1D-ND	3.16	1.41	1.37
23	c	502	CLA	C1D-ND	3.16	1.41	1.37
23	c	512	CLA	C4D-ND	-3.16	1.33	1.37
23	D	401	CLA	C1D-ND	3.16	1.41	1.37
23	G	613	CLA	CHC-C1C	3.16	1.43	1.35
36	n	318	NEX	C7-C8	-3.16	1.26	1.32
23	c	510	CLA	C1D-ND	3.16	1.41	1.37
34	N	302	CHL	C4D-ND	-3.15	1.33	1.37
34	r	607	CHL	C4D-ND	-3.15	1.33	1.37
23	S	604	CLA	C4D-ND	-3.15	1.33	1.37
34	G	607	CHL	CHC-C1C	3.15	1.43	1.35
23	b	604	CLA	CMB-C2B	-3.15	1.45	1.51
23	Y	305	CLA	C4D-ND	-3.15	1.33	1.37
23	S	604	CLA	CHC-C1C	3.14	1.43	1.35
33	e	101	HEM	CAB-C3B	3.14	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	N	302	CHL	CHC-C1C	3.14	1.43	1.35
23	s	602	CLA	CHC-C1C	3.14	1.43	1.35
34	G	608	CHL	CHC-C1C	3.14	1.43	1.35
23	c	511	CLA	C1D-ND	3.14	1.41	1.37
23	s	611	CLA	C4D-ND	-3.14	1.33	1.37
23	b	616	CLA	CHC-C1C	3.14	1.43	1.35
23	R	611	CLA	C1D-ND	3.14	1.41	1.37
23	G	614	CLA	C4D-ND	-3.14	1.33	1.37
36	S	616	NEX	C7-C8	-3.13	1.26	1.32
23	C	505	CLA	C4D-ND	-3.13	1.33	1.37
23	s	604	CLA	C4D-ND	-3.13	1.33	1.37
23	A	401	CLA	C4D-ND	-3.13	1.33	1.37
23	G	602	CLA	C4D-ND	-3.13	1.33	1.37
23	N	303	CLA	CHC-C1C	3.13	1.43	1.35
34	y	308	CHL	CHC-C1C	3.13	1.43	1.35
23	B	604	CLA	CMB-C2B	-3.13	1.45	1.51
34	G	609	CHL	CMB-C2B	-3.13	1.45	1.51
36	Y	317	NEX	C1-C6	-3.13	1.49	1.54
23	g	613	CLA	C1D-ND	3.13	1.41	1.37
23	B	612	CLA	CMD-C2D	-3.12	1.44	1.50
23	R	603	CLA	C4D-ND	-3.12	1.33	1.37
34	n	308	CHL	C4D-ND	-3.12	1.33	1.37
34	S	601	CHL	C4D-ND	-3.12	1.33	1.37
23	c	507	CLA	C1D-ND	3.12	1.41	1.37
34	n	309	CHL	CHC-C1C	3.12	1.43	1.35
23	B	612	CLA	C4D-ND	-3.12	1.33	1.37
23	R	608	CLA	C4D-ND	-3.12	1.33	1.37
23	n	303	CLA	CHC-C1C	3.11	1.43	1.35
23	B	616	CLA	CHC-C1C	3.11	1.42	1.35
23	g	612	CLA	C4D-ND	-3.11	1.33	1.37
23	S	603	CLA	C4D-ND	-3.11	1.33	1.37
23	b	603	CLA	C1D-ND	3.11	1.41	1.37
33	E	101	HEM	C3C-C2C	-3.10	1.36	1.40
34	Y	306	CHL	C4D-ND	-3.10	1.33	1.37
34	Y	308	CHL	CHC-C1C	3.10	1.42	1.35
23	N	303	CLA	C1D-ND	3.10	1.41	1.37
23	g	610	CLA	CHC-C1C	3.10	1.42	1.35
23	n	303	CLA	C1D-ND	3.09	1.41	1.37
34	y	302	CHL	C4D-ND	-3.09	1.33	1.37
34	n	302	CHL	C4D-ND	-3.09	1.33	1.37
23	g	614	CLA	C4D-ND	-3.09	1.33	1.37
23	s	610	CLA	C4D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	y	308	CHL	C4D-ND	-3.09	1.33	1.37
23	r	608	CLA	C4D-ND	-3.09	1.33	1.37
34	s	601	CHL	CHC-C1C	3.09	1.42	1.35
34	y	309	CHL	C4D-ND	-3.09	1.33	1.37
23	N	305	CLA	C1D-ND	3.09	1.41	1.37
34	Y	307	CHL	C1D-ND	3.09	1.41	1.37
23	B	609	CLA	C1D-ND	3.08	1.41	1.37
34	G	601	CHL	C1D-ND	3.08	1.41	1.37
23	g	613	CLA	CHC-C1C	3.08	1.42	1.35
34	g	608	CHL	CHC-C1C	3.08	1.42	1.35
34	g	609	CHL	CMB-C2B	-3.08	1.45	1.51
23	c	510	CLA	CHC-C1C	3.08	1.42	1.35
23	g	602	CLA	C4D-ND	-3.08	1.33	1.37
34	s	601	CHL	C4D-ND	-3.08	1.33	1.37
23	y	303	CLA	C4D-ND	-3.08	1.33	1.37
23	c	509	CLA	C4D-ND	-3.07	1.33	1.37
23	C	511	CLA	CHC-C1C	3.07	1.42	1.35
23	Y	303	CLA	C4D-ND	-3.07	1.33	1.37
34	S	601	CHL	CHC-C1C	3.07	1.42	1.35
34	r	607	CHL	CHC-C1C	3.07	1.42	1.35
34	y	307	CHL	C4D-ND	-3.06	1.33	1.37
34	Y	302	CHL	C4D-ND	-3.06	1.33	1.37
34	Y	307	CHL	C4D-ND	-3.06	1.33	1.37
34	g	601	CHL	C4D-ND	-3.06	1.33	1.37
23	g	604	CLA	C1D-ND	3.06	1.41	1.37
23	c	513	CLA	C1D-ND	3.06	1.41	1.37
23	g	603	CLA	C4D-ND	-3.06	1.33	1.37
23	C	508	CLA	C4D-ND	-3.06	1.33	1.37
34	N	309	CHL	C1D-ND	3.06	1.41	1.37
23	r	602	CLA	CHC-C1C	3.05	1.42	1.35
23	R	609	CLA	CHC-C1C	3.05	1.42	1.35
23	C	508	CLA	C1D-ND	3.05	1.41	1.37
34	N	302	CHL	C1D-ND	3.05	1.41	1.37
23	B	603	CLA	C1D-ND	3.05	1.41	1.37
33	E	101	HEM	CAB-C3B	3.05	1.55	1.47
34	s	607	CHL	CHC-C1C	3.05	1.42	1.35
23	c	510	CLA	C4D-ND	-3.05	1.33	1.37
23	R	612	CLA	C4D-ND	-3.04	1.33	1.37
23	n	312	CLA	CHC-C1C	3.04	1.42	1.35
34	s	606	CHL	CHC-C1C	3.04	1.42	1.35
34	r	606	CHL	CHC-C1C	3.04	1.42	1.35
23	B	615	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	608	CLA	CHC-C1C	3.04	1.42	1.35
23	S	608	CLA	C4D-ND	-3.04	1.33	1.37
23	R	609	CLA	C4D-ND	-3.04	1.33	1.37
23	g	611	CLA	CHC-C1C	3.03	1.42	1.35
34	S	606	CHL	CHC-C1C	3.03	1.42	1.35
23	c	501	CLA	C1D-ND	3.03	1.41	1.37
23	s	609	CLA	CHC-C1C	3.03	1.42	1.35
23	C	503	CLA	C1D-ND	3.02	1.41	1.37
23	G	603	CLA	C4D-ND	-3.02	1.33	1.37
34	N	306	CHL	CHC-C1C	3.01	1.42	1.35
23	B	602	CLA	CHC-C1C	3.01	1.42	1.35
23	C	504	CLA	C4D-ND	-3.01	1.33	1.37
23	s	613	CLA	C4D-ND	-3.01	1.33	1.37
23	g	602	CLA	CHC-C1C	3.01	1.42	1.35
23	C	505	CLA	CHC-C1C	3.01	1.42	1.35
23	a	401	CLA	C4D-ND	-3.01	1.33	1.37
23	Y	303	CLA	CHC-C1C	3.01	1.42	1.35
23	s	604	CLA	CHC-C1C	3.01	1.42	1.35
34	N	309	CHL	CHC-C1C	3.01	1.42	1.35
23	N	304	CLA	C4D-ND	-3.01	1.33	1.37
34	N	308	CHL	C4D-ND	-3.00	1.33	1.37
23	R	602	CLA	CHC-C1C	3.00	1.42	1.35
23	R	608	CLA	CHC-C1C	3.00	1.42	1.35
23	Y	305	CLA	CMB-C2B	-3.00	1.45	1.51
23	B	603	CLA	CHC-C1C	3.00	1.42	1.35
23	g	603	CLA	CMB-C2B	-3.00	1.45	1.51
34	n	302	CHL	CHC-C1C	3.00	1.42	1.35
34	Y	309	CHL	C3B-C2B	-3.00	1.36	1.40
34	R	606	CHL	CHC-C1C	2.99	1.42	1.35
23	g	612	CLA	CHC-C1C	2.99	1.42	1.35
34	s	605	CHL	CHC-C1C	2.99	1.42	1.35
23	r	614	CLA	C4D-ND	-2.99	1.33	1.37
34	y	302	CHL	CHC-C1C	2.99	1.42	1.35
23	C	513	CLA	C4D-ND	-2.99	1.33	1.37
23	b	603	CLA	CHC-C1C	2.99	1.42	1.35
34	g	619	CHL	C4D-ND	-2.98	1.33	1.37
23	S	613	CLA	C4D-ND	-2.98	1.33	1.37
23	G	602	CLA	CHC-C1C	2.98	1.42	1.35
23	c	502	CLA	CMB-C2B	-2.98	1.45	1.51
23	C	511	CLA	C4D-ND	-2.98	1.33	1.37
23	N	314	CLA	C1D-ND	2.98	1.41	1.37
34	Y	308	CHL	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHC-C1C	2.97	1.42	1.35
23	R	614	CLA	CMB-C2B	-2.97	1.45	1.51
23	Y	314	CLA	CHC-C1C	2.97	1.42	1.35
23	b	609	CLA	CMB-C2B	-2.97	1.45	1.51
23	C	508	CLA	CHC-C1C	2.97	1.42	1.35
23	B	616	CLA	C4D-ND	-2.96	1.33	1.37
26	A	406	SQD	C6-S	-2.96	1.66	1.77
23	s	608	CLA	C4D-ND	-2.96	1.33	1.37
34	G	605	CHL	CHC-C1C	2.96	1.42	1.35
23	c	506	CLA	CHC-C1C	2.96	1.42	1.35
34	g	606	CHL	C4D-ND	-2.96	1.33	1.37
23	S	610	CLA	CHC-C1C	2.96	1.42	1.35
23	r	611	CLA	C4D-ND	-2.96	1.33	1.37
23	D	404	CLA	CHC-C1C	2.96	1.42	1.35
23	N	305	CLA	CMB-C2B	-2.96	1.45	1.51
34	Y	302	CHL	CHC-C1C	2.96	1.42	1.35
23	G	611	CLA	C1D-ND	2.96	1.41	1.37
23	y	303	CLA	CHC-C1C	2.96	1.42	1.35
23	a	402	CLA	C3B-C2B	-2.96	1.36	1.40
23	b	612	CLA	C1D-ND	2.96	1.41	1.37
26	d	402	SQD	C6-S	-2.95	1.66	1.77
23	R	610	CLA	C4D-ND	-2.95	1.33	1.37
34	N	306	CHL	C4D-ND	-2.95	1.33	1.37
23	B	614	CLA	CHC-C1C	2.95	1.42	1.35
23	b	614	CLA	CHC-C1C	2.95	1.42	1.35
23	C	507	CLA	CHC-C1C	2.94	1.42	1.35
23	S	609	CLA	CMB-C2B	-2.94	1.45	1.51
23	S	612	CLA	C4D-ND	-2.94	1.33	1.37
23	s	608	CLA	CHC-C1C	2.94	1.42	1.35
23	b	602	CLA	CHC-C1C	2.94	1.42	1.35
34	G	606	CHL	C4D-ND	-2.94	1.33	1.37
34	s	607	CHL	C4D-ND	-2.94	1.33	1.37
34	R	607	CHL	CHC-C1C	2.93	1.42	1.35
23	Y	305	CLA	C1D-ND	2.93	1.41	1.37
23	d	404	CLA	CHC-C1C	2.93	1.42	1.35
23	R	604	CLA	C4D-ND	-2.93	1.33	1.37
34	n	306	CHL	CHC-C1C	2.93	1.42	1.35
23	r	612	CLA	C4D-ND	-2.93	1.33	1.37
23	R	610	CLA	CHC-C1C	2.93	1.42	1.35
23	y	314	CLA	CHC-C1C	2.93	1.42	1.35
23	c	509	CLA	CMB-C2B	-2.93	1.45	1.51
34	g	619	CHL	CHC-C1C	2.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	G	619	CHL	CHC-C1C	2.93	1.42	1.35
23	c	513	CLA	CHC-C1C	2.93	1.42	1.35
23	n	304	CLA	CHC-C1C	2.93	1.42	1.35
23	b	615	CLA	C4D-ND	-2.92	1.33	1.37
34	R	613	CHL	CHC-C1C	2.92	1.42	1.35
23	G	604	CLA	CHC-C1C	2.92	1.42	1.35
23	S	608	CLA	CHC-C1C	2.92	1.42	1.35
23	n	305	CLA	CMB-C2B	-2.92	1.45	1.51
34	R	605	CHL	CHC-C1C	2.92	1.42	1.35
23	b	610	CLA	C1D-ND	2.92	1.41	1.37
23	c	507	CLA	CHC-C1C	2.92	1.42	1.35
23	Y	304	CLA	C1D-ND	2.92	1.41	1.37
34	G	619	CHL	C4D-ND	-2.92	1.33	1.37
23	r	610	CLA	C4D-ND	-2.92	1.33	1.37
23	C	512	CLA	CHC-C1C	2.92	1.42	1.35
34	G	605	CHL	C4D-ND	-2.91	1.33	1.37
23	c	504	CLA	CMB-C2B	-2.91	1.45	1.51
23	r	614	CLA	CMB-C2B	-2.91	1.45	1.51
23	a	403	CLA	C3B-C2B	-2.91	1.36	1.40
23	c	501	CLA	CMB-C2B	-2.91	1.45	1.51
23	C	510	CLA	CHC-C1C	2.91	1.42	1.35
23	R	614	CLA	C4D-ND	-2.91	1.33	1.37
23	B	610	CLA	C1D-ND	2.91	1.41	1.37
23	B	613	CLA	CHC-C1C	2.91	1.42	1.35
23	y	304	CLA	C1D-ND	2.90	1.41	1.37
34	G	606	CHL	CMB-C2B	-2.90	1.45	1.51
23	c	503	CLA	C4D-ND	-2.90	1.33	1.37
23	C	506	CLA	C1D-ND	2.90	1.41	1.37
23	C	502	CLA	C1D-ND	2.90	1.41	1.37
23	g	604	CLA	CHC-C1C	2.90	1.42	1.35
23	b	613	CLA	CHC-C1C	2.90	1.42	1.35
23	C	514	CLA	C1D-ND	2.90	1.41	1.37
23	G	604	CLA	C1D-ND	2.89	1.41	1.37
34	n	307	CHL	CHC-C1C	2.89	1.42	1.35
34	g	606	CHL	C3B-C2B	-2.89	1.36	1.40
23	A	402	CLA	CHC-C1C	2.89	1.42	1.35
23	r	610	CLA	CHC-C1C	2.89	1.42	1.35
34	r	613	CHL	CHC-C1C	2.89	1.42	1.35
34	G	606	CHL	CHC-C1C	2.89	1.42	1.35
34	g	601	CHL	C1D-ND	2.89	1.41	1.37
23	B	607	CLA	CHC-C1C	2.89	1.42	1.35
23	n	315	CLA	CHC-C1C	2.89	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	612	CLA	CHC-C1C	2.88	1.42	1.35
23	B	612	CLA	CHC-C1C	2.88	1.42	1.35
23	c	506	CLA	CMB-C2B	-2.88	1.45	1.51
23	y	312	CLA	CHC-C1C	2.88	1.42	1.35
23	R	604	CLA	CHC-C1C	2.88	1.42	1.35
34	G	601	CHL	C4D-ND	-2.88	1.33	1.37
23	b	616	CLA	C4D-ND	-2.88	1.33	1.37
34	g	606	CHL	CHC-C1C	2.88	1.42	1.35
23	b	612	CLA	CHC-C1C	2.88	1.42	1.35
23	a	403	CLA	CHC-C1C	2.88	1.42	1.35
23	b	609	CLA	CHC-C1C	2.87	1.42	1.35
23	G	603	CLA	CMB-C2B	-2.87	1.45	1.51
34	r	605	CHL	CHC-C1C	2.87	1.42	1.35
23	Y	311	CLA	CHC-C1C	2.87	1.42	1.35
23	N	304	CLA	CMB-C2B	-2.87	1.45	1.51
23	r	604	CLA	CMB-C2B	-2.87	1.45	1.51
23	N	313	CLA	C4D-ND	-2.87	1.33	1.37
23	R	611	CLA	C4D-ND	-2.86	1.33	1.37
23	b	607	CLA	CHC-C1C	2.86	1.42	1.35
23	D	401	CLA	CMB-C2B	-2.86	1.45	1.51
23	y	311	CLA	CHC-C1C	2.86	1.42	1.35
23	N	304	CLA	CHC-C1C	2.86	1.42	1.35
23	b	601	CLA	CHC-C1C	2.86	1.42	1.35
34	n	307	CHL	CMB-C2B	-2.86	1.45	1.51
23	r	609	CLA	CHC-C1C	2.85	1.42	1.35
34	y	308	CHL	C1D-ND	2.85	1.41	1.37
23	g	604	CLA	CMB-C2B	-2.85	1.45	1.51
23	N	311	CLA	CHC-C1C	2.85	1.42	1.35
23	R	604	CLA	CMB-C2B	-2.85	1.45	1.51
34	g	605	CHL	CHC-C1C	2.85	1.42	1.35
23	n	304	CLA	CMB-C2B	-2.85	1.45	1.51
23	B	606	CLA	CMB-C2B	-2.85	1.45	1.51
23	a	402	CLA	C1D-ND	2.84	1.41	1.37
23	n	303	CLA	CMC-C2C	-2.84	1.44	1.50
23	B	611	CLA	CMB-C2B	-2.84	1.45	1.51
23	y	305	CLA	C1D-ND	2.84	1.41	1.37
23	D	401	CLA	CHC-C1C	2.84	1.42	1.35
23	R	611	CLA	CHC-C1C	2.84	1.42	1.35
26	L	103	SQD	C6-S	-2.84	1.66	1.77
23	Y	312	CLA	CHC-C1C	2.84	1.42	1.35
26	M	101	SQD	C6-S	-2.84	1.66	1.77
23	s	613	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	303	CLA	CMB-C2B	-2.84	1.45	1.51
34	S	605	CHL	C4D-ND	-2.84	1.33	1.37
23	r	611	CLA	CHC-C1C	2.84	1.42	1.35
23	D	405	CLA	CMB-C2B	-2.84	1.45	1.51
34	n	302	CHL	C1D-ND	2.84	1.41	1.37
34	S	607	CHL	CMD-C2D	-2.84	1.44	1.50
23	a	405	CLA	CHC-C1C	2.83	1.42	1.35
23	c	501	CLA	CMD-C2D	-2.83	1.44	1.50
23	R	603	CLA	CHC-C1C	2.83	1.42	1.35
23	r	601	CLA	CHC-C1C	2.83	1.42	1.35
34	N	307	CHL	CHC-C1C	2.83	1.42	1.35
23	A	404	CLA	CHC-C1C	2.83	1.42	1.35
23	c	505	CLA	C1D-ND	2.83	1.41	1.37
23	N	315	CLA	CHC-C1C	2.83	1.42	1.35
23	A	402	CLA	C3B-C2B	-2.83	1.36	1.40
23	s	612	CLA	C4D-ND	-2.83	1.33	1.37
23	s	613	CLA	CMB-C2B	-2.83	1.45	1.51
23	r	604	CLA	C4D-ND	-2.83	1.33	1.37
34	G	608	CHL	C1D-ND	2.82	1.41	1.37
23	Y	305	CLA	CHC-C1C	2.82	1.42	1.35
23	B	613	CLA	CMB-C2B	-2.82	1.45	1.51
23	c	510	CLA	CMD-C2D	-2.81	1.44	1.50
23	c	502	CLA	C3B-C2B	-2.81	1.36	1.40
23	C	503	CLA	C3B-C2B	-2.81	1.36	1.40
34	y	307	CHL	CHC-C1C	2.81	1.42	1.35
23	g	603	CLA	C3B-C2B	-2.81	1.36	1.40
34	r	613	CHL	C4D-ND	-2.80	1.33	1.37
34	Y	308	CHL	C1D-ND	2.80	1.41	1.37
23	Y	304	CLA	CMB-C2B	-2.80	1.45	1.51
34	g	619	CHL	CMD-C2D	-2.80	1.44	1.50
23	n	311	CLA	CHC-C1C	2.80	1.42	1.35
23	b	613	CLA	CMB-C2B	-2.80	1.45	1.51
23	N	314	CLA	MG-ND	-2.80	2.00	2.05
34	g	606	CHL	CMB-C2B	-2.80	1.45	1.51
23	n	304	CLA	C4D-ND	-2.80	1.33	1.37
23	S	613	CLA	CHC-C1C	2.80	1.42	1.35
34	y	309	CHL	C3B-C2B	-2.80	1.36	1.40
23	c	511	CLA	CHC-C1C	2.79	1.42	1.35
34	y	306	CHL	CHC-C1C	2.79	1.42	1.35
34	Y	307	CHL	CHC-C1C	2.79	1.42	1.35
23	B	615	CLA	CHC-C1C	2.79	1.42	1.35
23	B	608	CLA	MG-ND	-2.79	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	G	601	CHL	CMD-C2D	-2.79	1.44	1.50
23	s	612	CLA	CHC-C1C	2.79	1.42	1.35
23	b	611	CLA	CMB-C2B	-2.79	1.45	1.51
23	d	405	CLA	CMB-C2B	-2.79	1.45	1.51
23	G	604	CLA	CMB-C2B	-2.78	1.45	1.51
23	r	604	CLA	CHC-C1C	2.78	1.42	1.35
23	N	312	CLA	CHC-C1C	2.78	1.42	1.35
23	b	616	CLA	CMD-C2D	-2.78	1.44	1.50
23	D	404	CLA	CMB-C2B	-2.78	1.45	1.51
23	c	503	CLA	CMB-C2B	-2.78	1.45	1.51
23	d	404	CLA	CMB-C2B	-2.78	1.45	1.51
34	Y	306	CHL	CHC-C1C	2.78	1.42	1.35
23	b	615	CLA	CHC-C1C	2.77	1.42	1.35
23	b	605	CLA	C3B-C2B	-2.77	1.36	1.40
34	R	613	CHL	C4D-ND	-2.77	1.33	1.37
23	b	610	CLA	CHC-C1C	2.77	1.42	1.35
23	B	616	CLA	CMB-C2B	-2.77	1.45	1.51
23	r	612	CLA	CHC-C1C	2.76	1.42	1.35
23	S	612	CLA	CHC-C1C	2.76	1.42	1.35
23	D	404	CLA	CMC-C2C	-2.76	1.45	1.50
23	r	603	CLA	CHC-C1C	2.75	1.42	1.35
23	B	601	CLA	CHC-C1C	2.75	1.42	1.35
23	n	313	CLA	C4D-ND	-2.75	1.33	1.37
34	S	607	CHL	C4D-ND	-2.75	1.33	1.37
23	c	507	CLA	CMB-C2B	-2.75	1.45	1.51
23	d	405	CLA	CHC-C1C	2.75	1.42	1.35
23	b	616	CLA	CMB-C2B	-2.75	1.45	1.51
36	R	617	NEX	C7-C8	-2.74	1.27	1.32
23	B	608	CLA	CHC-C1C	2.74	1.42	1.35
23	R	601	CLA	C4D-ND	-2.74	1.33	1.37
23	c	509	CLA	CHC-C1C	2.74	1.42	1.35
34	s	606	CHL	C4D-ND	-2.73	1.33	1.37
23	B	605	CLA	C3B-C2B	-2.73	1.36	1.40
23	s	610	CLA	CHC-C1C	2.72	1.41	1.35
23	a	401	CLA	CHC-C1C	2.72	1.41	1.35
23	C	504	CLA	CHC-C1C	2.72	1.41	1.35
23	R	612	CLA	CHC-C1C	2.71	1.41	1.35
23	b	606	CLA	CMB-C2B	-2.71	1.46	1.51
34	n	308	CHL	CMB-C2B	-2.71	1.46	1.51
23	y	304	CLA	CMB-C2B	-2.71	1.46	1.51
23	A	401	CLA	CHC-C1C	2.71	1.41	1.35
34	s	605	CHL	C4D-ND	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	602	CLA	CMC-C2C	-2.71	1.45	1.50
23	y	303	CLA	C3B-C2B	-2.71	1.36	1.40
23	R	601	CLA	CHC-C1C	2.71	1.41	1.35
23	C	508	CLA	CMB-C2B	-2.71	1.46	1.51
23	S	603	CLA	CHC-C1C	2.70	1.41	1.35
23	y	305	CLA	CHC-C1C	2.70	1.41	1.35
23	a	403	CLA	CMB-C2B	-2.70	1.46	1.51
23	s	603	CLA	CHC-C1C	2.70	1.41	1.35
23	s	611	CLA	CHC-C1C	2.70	1.41	1.35
34	N	307	CHL	CMB-C2B	-2.70	1.46	1.51
34	G	619	CHL	CMD-C2D	-2.70	1.45	1.50
23	B	612	CLA	C1D-ND	2.69	1.41	1.37
34	r	605	CHL	CMB-C2B	-2.69	1.46	1.51
23	C	506	CLA	CHC-C1C	2.69	1.41	1.35
23	D	405	CLA	CHC-C1C	2.69	1.41	1.35
23	N	313	CLA	CHC-C1C	2.69	1.41	1.35
23	C	507	CLA	CMB-C2B	-2.69	1.46	1.51
34	g	601	CHL	CMB-C2B	-2.69	1.46	1.51
23	b	612	CLA	CMD-C2D	-2.69	1.45	1.50
23	c	505	CLA	CMB-C2B	-2.68	1.46	1.51
23	r	614	CLA	CHC-C1C	2.68	1.41	1.35
34	g	609	CHL	CHC-C1C	2.68	1.41	1.35
34	G	606	CHL	C3B-C2B	-2.68	1.36	1.40
36	G	617	NEX	C7-C8	-2.68	1.27	1.32
23	B	614	CLA	CMB-C2B	-2.68	1.46	1.51
23	b	614	CLA	CMB-C2B	-2.68	1.46	1.51
23	S	609	CLA	CHC-C1C	2.68	1.41	1.35
23	r	601	CLA	C4D-ND	-2.68	1.34	1.37
34	S	606	CHL	C4D-ND	-2.68	1.34	1.37
23	d	404	CLA	C1D-ND	2.67	1.41	1.37
34	N	309	CHL	CMB-C2B	-2.67	1.46	1.51
23	g	614	CLA	CHC-C1C	2.67	1.41	1.35
23	Y	304	CLA	CHC-C1C	2.67	1.41	1.35
23	C	511	CLA	CMD-C2D	-2.67	1.45	1.50
34	g	605	CHL	C4D-ND	-2.67	1.34	1.37
23	C	502	CLA	CMB-C2B	-2.67	1.46	1.51
23	a	401	CLA	CMD-C2D	-2.67	1.45	1.50
23	n	313	CLA	CHC-C1C	2.67	1.41	1.35
23	c	511	CLA	CMD-C2D	-2.66	1.45	1.50
23	n	314	CLA	CMB-C2B	-2.66	1.46	1.51
23	c	505	CLA	CHC-C1C	2.66	1.41	1.35
23	G	603	CLA	CHC-C1C	2.66	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	S	605	CHL	CMB-C2B	-2.66	1.46	1.51
23	d	404	CLA	CMC-C2C	-2.66	1.45	1.50
34	S	601	CHL	CMB-C2B	-2.66	1.46	1.51
23	S	611	CLA	CHC-C1C	2.66	1.41	1.35
23	c	503	CLA	CHC-C1C	2.66	1.41	1.35
23	R	611	CLA	CMB-C2B	-2.65	1.46	1.51
23	Y	303	CLA	CMB-C2B	-2.65	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.65	1.46	1.51
23	Y	311	CLA	CMB-C2B	-2.65	1.46	1.51
23	g	614	CLA	CMB-C2B	-2.65	1.46	1.51
23	N	312	CLA	CMB-C2B	-2.65	1.46	1.51
23	D	404	CLA	CMD-C2D	-2.65	1.45	1.50
34	y	306	CHL	CMB-C2B	-2.65	1.46	1.51
34	G	601	CHL	CMB-C2B	-2.65	1.46	1.51
23	N	303	CLA	CMB-C2B	-2.65	1.46	1.51
23	y	304	CLA	CHC-C1C	2.65	1.41	1.35
23	R	614	CLA	CHC-C1C	2.64	1.41	1.35
23	y	305	CLA	C3B-C2B	-2.64	1.36	1.40
23	G	603	CLA	C3B-C2B	-2.64	1.36	1.40
34	Y	306	CHL	CMB-C2B	-2.64	1.46	1.51
23	R	601	CLA	C3B-C2B	-2.64	1.36	1.40
23	a	402	CLA	CMB-C2B	-2.64	1.46	1.51
23	G	614	CLA	CHC-C1C	2.64	1.41	1.35
23	d	404	CLA	CMD-C2D	-2.64	1.45	1.50
36	r	617	NEX	C7-C8	-2.64	1.27	1.32
34	Y	307	CHL	CMB-C2B	-2.64	1.46	1.51
23	b	611	CLA	CHC-C1C	2.64	1.41	1.35
23	Y	313	CLA	CMB-C2B	-2.64	1.46	1.51
23	C	504	CLA	CMD-C2D	-2.64	1.45	1.50
34	g	601	CHL	CHC-C1C	2.63	1.41	1.35
23	A	402	CLA	CMB-C2B	-2.63	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.63	1.46	1.51
23	b	608	CLA	CHC-C1C	2.63	1.41	1.35
34	G	609	CHL	CMD-C2D	-2.63	1.45	1.50
34	n	309	CHL	CMB-C2B	-2.63	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.63	1.46	1.51
34	S	605	CHL	CHC-C1C	2.63	1.41	1.35
23	C	509	CLA	CHC-C1C	2.62	1.41	1.35
23	B	608	CLA	CMD-C2D	-2.62	1.45	1.50
23	B	615	CLA	CMB-C2B	-2.62	1.46	1.51
23	y	313	CLA	CMB-C2B	-2.62	1.46	1.51
23	b	608	CLA	MG-ND	-2.62	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	CMB-C2B	-2.62	1.46	1.51
23	G	602	CLA	CMB-C2B	-2.62	1.46	1.51
23	Y	310	CLA	CMB-C2B	-2.62	1.46	1.51
23	y	304	CLA	C3B-C2B	-2.62	1.36	1.40
34	s	607	CHL	CMD-C2D	-2.61	1.45	1.50
34	N	308	CHL	CMB-C2B	-2.61	1.46	1.51
34	y	307	CHL	CMB-C2B	-2.61	1.46	1.51
34	Y	302	CHL	CMB-C2B	-2.61	1.46	1.51
36	g	617	NEX	C7-C8	-2.61	1.27	1.32
23	g	602	CLA	CMB-C2B	-2.61	1.46	1.51
23	n	303	CLA	CMB-C2B	-2.61	1.46	1.51
23	y	311	CLA	CMB-C2B	-2.60	1.46	1.51
23	b	608	CLA	CMD-C2D	-2.60	1.45	1.50
32	D	406	PL9	C36-C34	2.60	1.56	1.51
23	c	502	CLA	CHC-C1C	2.60	1.41	1.35
34	n	306	CHL	CMB-C2B	-2.60	1.46	1.51
23	B	610	CLA	CHC-C1C	2.60	1.41	1.35
23	D	404	CLA	C1D-ND	2.59	1.41	1.37
32	d	407	PL9	C36-C34	2.59	1.56	1.51
23	B	609	CLA	CHC-C1C	2.59	1.41	1.35
23	G	614	CLA	CMB-C2B	-2.59	1.46	1.51
23	S	612	CLA	CMB-C2B	-2.59	1.46	1.51
23	B	603	CLA	CMD-C2D	-2.59	1.45	1.50
23	C	505	CLA	CMB-C2B	-2.59	1.46	1.51
23	b	605	CLA	CMB-C2B	-2.58	1.46	1.51
23	g	613	CLA	CMB-C2B	-2.58	1.46	1.51
23	s	612	CLA	CMB-C2B	-2.58	1.46	1.51
23	r	601	CLA	C3B-C2B	-2.58	1.36	1.40
23	B	607	CLA	CMB-C2B	-2.58	1.46	1.51
23	N	303	CLA	CMC-C2C	-2.58	1.45	1.50
32	D	406	PL9	C21-C19	2.58	1.56	1.51
34	Y	309	CHL	CMD-C2D	-2.58	1.45	1.50
23	B	616	CLA	C3B-C2B	-2.58	1.36	1.40
23	c	507	CLA	CMD-C2D	-2.57	1.45	1.50
32	d	407	PL9	C21-C19	2.57	1.56	1.51
23	Y	314	CLA	CMB-C2B	-2.57	1.46	1.51
23	S	603	CLA	CMB-C2B	-2.57	1.46	1.51
23	B	611	CLA	CHC-C1C	2.57	1.41	1.35
23	b	615	CLA	CMB-C2B	-2.57	1.46	1.51
23	b	606	CLA	CHC-C1C	2.57	1.41	1.35
23	n	314	CLA	CHC-C1C	2.57	1.41	1.35
23	r	603	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CMB-C2B	-2.56	1.46	1.51
23	y	310	CLA	CMB-C2B	-2.56	1.46	1.51
34	y	302	CHL	CMB-C2B	-2.56	1.46	1.51
23	c	503	CLA	C3B-C2B	-2.56	1.36	1.40
23	B	601	CLA	CMB-C2B	-2.56	1.46	1.51
23	b	616	CLA	C3B-C2B	-2.56	1.36	1.40
34	g	601	CHL	CMD-C2D	-2.56	1.45	1.50
23	A	404	CLA	CMB-C2B	-2.56	1.46	1.51
23	A	401	CLA	CMC-C2C	-2.56	1.45	1.50
23	B	604	CLA	CHC-C1C	2.55	1.41	1.35
23	C	503	CLA	CHC-C1C	2.55	1.41	1.35
34	G	619	CHL	CMB-C2B	-2.55	1.46	1.51
23	c	508	CLA	CHC-C1C	2.55	1.41	1.35
23	A	401	CLA	CMD-C2D	-2.55	1.45	1.50
23	c	513	CLA	CMD-C2D	-2.55	1.45	1.50
34	S	607	CHL	CMB-C2B	-2.55	1.46	1.51
23	a	405	CLA	CMB-C2B	-2.55	1.46	1.51
26	a	409	SQD	C6-S	-2.55	1.68	1.77
23	c	511	CLA	CMB-C2B	-2.54	1.46	1.51
23	r	609	CLA	C3B-C2B	-2.54	1.36	1.40
34	N	309	CHL	CMD-C2D	-2.54	1.45	1.50
23	G	613	CLA	CMB-C2B	-2.54	1.46	1.51
23	s	609	CLA	CMB-C2B	-2.54	1.46	1.51
23	c	504	CLA	CHC-C1C	2.54	1.41	1.35
34	G	609	CHL	CHC-C1C	2.54	1.41	1.35
23	y	314	CLA	CMB-C2B	-2.54	1.46	1.51
26	A	409	SQD	C6-S	-2.54	1.68	1.77
23	s	603	CLA	CMB-C2B	-2.54	1.46	1.51
23	Y	304	CLA	C3B-C2B	-2.54	1.36	1.40
23	n	312	CLA	CMB-C2B	-2.54	1.46	1.51
34	y	309	CHL	CMD-C2D	-2.54	1.45	1.50
23	C	513	CLA	CHC-C1C	2.54	1.41	1.35
23	B	606	CLA	CHC-C1C	2.54	1.41	1.35
23	n	311	CLA	CMB-C2B	-2.54	1.46	1.51
23	b	603	CLA	CMD-C2D	-2.53	1.45	1.50
23	c	512	CLA	CMB-C2B	-2.53	1.46	1.51
34	R	606	CHL	CMB-C2B	-2.53	1.46	1.51
34	r	606	CHL	CMB-C2B	-2.53	1.46	1.51
34	G	601	CHL	CHC-C1C	2.53	1.41	1.35
36	N	318	NEX	C7-C8	-2.53	1.27	1.32
34	N	306	CHL	CMB-C2B	-2.53	1.46	1.51
23	b	604	CLA	CHC-C1C	2.53	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	CMB-C2B	-2.53	1.46	1.51
23	S	604	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.53	1.46	1.51
23	R	603	CLA	CMB-C2B	-2.53	1.46	1.51
34	N	302	CHL	CMB-C2B	-2.52	1.46	1.51
23	c	512	CLA	CHC-C1C	2.52	1.41	1.35
23	B	604	CLA	C3B-C2B	-2.52	1.36	1.40
23	N	311	CLA	CMD-C2D	-2.52	1.45	1.50
23	a	401	CLA	CMC-C2C	-2.52	1.45	1.50
34	Y	302	CHL	C1D-ND	2.51	1.40	1.37
23	D	405	CLA	C3B-C2B	-2.50	1.36	1.40
23	n	304	CLA	C3B-C2B	-2.50	1.36	1.40
23	g	603	CLA	CHC-C1C	2.50	1.41	1.35
23	r	611	CLA	CMB-C2B	-2.50	1.46	1.51
34	G	601	CHL	MG-ND	-2.50	2.00	2.05
23	r	609	CLA	CMB-C2B	-2.50	1.46	1.51
23	C	502	CLA	MG-ND	-2.50	2.00	2.05
23	B	610	CLA	CMB-C2B	-2.50	1.46	1.51
23	s	609	CLA	CMC-C2C	-2.50	1.45	1.50
23	N	314	CLA	CHC-C1C	2.50	1.41	1.35
34	y	302	CHL	C1D-ND	2.50	1.40	1.37
23	c	501	CLA	MG-ND	-2.49	2.00	2.05
23	R	608	CLA	CMB-C2B	-2.49	1.46	1.51
34	g	619	CHL	CMB-C2B	-2.49	1.46	1.51
23	Y	313	CLA	CHC-C1C	2.49	1.41	1.35
34	s	607	CHL	CMB-C2B	-2.49	1.46	1.51
23	N	314	CLA	CMB-C2B	-2.49	1.46	1.51
23	G	612	CLA	CMB-C2B	-2.49	1.46	1.51
34	n	309	CHL	CMD-C2D	-2.49	1.45	1.50
23	B	602	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	604	CLA	C3B-C2B	-2.49	1.36	1.40
23	c	509	CLA	C3B-C2B	-2.49	1.36	1.40
34	N	307	CHL	C3B-C2B	-2.48	1.36	1.40
23	s	604	CLA	CMB-C2B	-2.48	1.46	1.51
23	C	508	CLA	C3B-C2B	-2.48	1.36	1.40
23	y	313	CLA	CHC-C1C	2.48	1.41	1.35
34	g	608	CHL	CMB-C2B	-2.48	1.46	1.51
34	y	308	CHL	CMB-C2B	-2.48	1.46	1.51
23	b	604	CLA	CMD-C2D	-2.48	1.45	1.50
23	C	513	CLA	MG-ND	-2.48	2.00	2.05
34	g	605	CHL	CMB-C2B	-2.48	1.46	1.51
23	r	609	CLA	C3B-CAB	-2.48	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	402	CLA	CHC-C1C	2.48	1.41	1.35
32	D	406	PL9	C5-C4	-2.48	1.38	1.47
34	s	605	CHL	CMB-C2B	-2.48	1.46	1.51
32	d	407	PL9	C5-C4	-2.47	1.38	1.47
23	C	508	CLA	CMD-C2D	-2.47	1.45	1.50
23	G	612	CLA	CMD-C2D	-2.47	1.45	1.50
23	g	612	CLA	CMB-C2B	-2.47	1.46	1.51
34	Y	308	CHL	CMB-C2B	-2.47	1.46	1.51
23	R	601	CLA	CMB-C2B	-2.47	1.46	1.51
23	S	602	CLA	CMB-C2B	-2.47	1.46	1.51
23	G	602	CLA	C3B-C2B	-2.47	1.36	1.40
23	G	611	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.46	1.46	1.51
23	r	611	CLA	CMD-C2D	-2.46	1.45	1.50
23	c	512	CLA	MG-ND	-2.46	2.00	2.05
23	r	608	CLA	CMB-C2B	-2.46	1.46	1.51
34	R	607	CHL	CMB-C2B	-2.46	1.46	1.51
23	g	610	CLA	CMC-C2C	-2.46	1.45	1.50
23	b	610	CLA	CMB-C2B	-2.46	1.46	1.51
23	N	304	CLA	C3B-C2B	-2.46	1.37	1.40
34	r	605	CHL	C3B-C2B	-2.46	1.37	1.40
34	N	309	CHL	C3B-C2B	-2.46	1.37	1.40
34	s	601	CHL	CMB-C2B	-2.46	1.46	1.51
23	N	313	CLA	CMB-C2B	-2.45	1.46	1.51
23	B	610	CLA	CMD-C2D	-2.45	1.45	1.50
23	N	305	CLA	CHC-C1C	2.45	1.41	1.35
34	r	607	CHL	CMB-C2B	-2.45	1.46	1.51
23	r	601	CLA	CMB-C2B	-2.45	1.46	1.51
34	G	605	CHL	CMB-C2B	-2.45	1.46	1.51
23	Y	303	CLA	CMC-C2C	-2.45	1.45	1.50
23	r	610	CLA	CMD-C2D	-2.44	1.45	1.50
23	d	405	CLA	C3B-C2B	-2.44	1.37	1.40
23	n	311	CLA	CMD-C2D	-2.44	1.45	1.50
23	C	510	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	605	CLA	C4B-CHC	-2.44	1.34	1.41
34	G	608	CHL	CMD-C2D	-2.44	1.45	1.50
34	R	613	CHL	CMB-C2B	-2.44	1.46	1.51
23	c	507	CLA	C3B-C2B	-2.44	1.37	1.40
23	b	610	CLA	CMD-C2D	-2.44	1.45	1.50
23	R	610	CLA	CMB-C2B	-2.44	1.46	1.51
34	r	613	CHL	CMB-C2B	-2.44	1.46	1.51
23	B	606	CLA	CMC-C2C	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	315	CLA	CMB-C2B	-2.43	1.46	1.51
23	G	611	CLA	CMD-C2D	-2.43	1.45	1.50
23	n	313	CLA	CMB-C2B	-2.43	1.46	1.51
23	B	612	CLA	CMC-C2C	-2.43	1.45	1.50
34	N	310	CHL	CHC-C1C	2.43	1.41	1.35
23	b	602	CLA	CMB-C2B	-2.43	1.46	1.51
23	r	610	CLA	CMB-C2B	-2.43	1.46	1.51
34	N	302	CHL	CMD-C2D	-2.43	1.45	1.50
23	R	611	CLA	CMD-C2D	-2.43	1.45	1.50
23	g	602	CLA	CMC-C2C	-2.43	1.45	1.50
23	b	608	CLA	C1D-ND	2.43	1.40	1.37
23	N	315	CLA	CMB-C2B	-2.43	1.46	1.51
34	G	601	CHL	C3B-C2B	-2.42	1.37	1.40
23	g	611	CLA	CMB-C2B	-2.42	1.46	1.51
34	R	605	CHL	CMB-C2B	-2.42	1.46	1.51
36	s	616	NEX	C7-C8	-2.42	1.27	1.32
23	Y	312	CLA	CMB-C2B	-2.42	1.46	1.51
23	y	303	CLA	C3B-CAB	-2.42	1.43	1.47
34	G	607	CHL	CMB-C2B	-2.41	1.46	1.51
23	y	313	CLA	C3B-C2B	-2.41	1.37	1.40
34	n	310	CHL	C4B-CHC	-2.41	1.34	1.41
34	n	302	CHL	CMB-C2B	-2.41	1.46	1.51
23	c	502	CLA	CAA-C2A	-2.41	1.49	1.54
23	B	605	CLA	CAC-C3C	-2.41	1.44	1.51
23	B	615	CLA	C3B-C2B	-2.41	1.37	1.40
23	s	610	CLA	CMB-C2B	-2.41	1.46	1.51
23	s	611	CLA	CMB-C2B	-2.40	1.46	1.51
23	N	311	CLA	CMB-C2B	-2.40	1.46	1.51
23	S	604	CLA	CMC-C2C	-2.40	1.45	1.50
23	C	512	CLA	CMD-C2D	-2.40	1.45	1.50
23	b	612	CLA	CMB-C2B	-2.40	1.46	1.51
23	y	312	CLA	CMB-C2B	-2.40	1.46	1.51
23	r	602	CLA	CMB-C2B	-2.40	1.46	1.51
34	g	609	CHL	CMD-C2D	-2.40	1.45	1.50
23	B	612	CLA	CMB-C2B	-2.40	1.46	1.51
23	C	514	CLA	CMD-C2D	-2.40	1.45	1.50
23	B	604	CLA	CMD-C2D	-2.39	1.45	1.50
23	s	602	CLA	CMB-C2B	-2.39	1.46	1.51
23	y	304	CLA	MG-ND	-2.39	2.01	2.05
34	g	607	CHL	CMB-C2B	-2.39	1.46	1.51
23	c	501	CLA	C3B-C2B	-2.39	1.37	1.40
23	r	602	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C3B-C2B	-2.39	1.37	1.40
23	n	305	CLA	CHC-C1C	2.39	1.41	1.35
34	g	606	CHL	C3B-CAB	-2.39	1.43	1.47
23	R	612	CLA	CMB-C2B	-2.39	1.46	1.51
23	C	504	CLA	C3B-C2B	-2.38	1.37	1.40
23	A	401	CLA	CMB-C2B	-2.38	1.46	1.51
34	N	310	CHL	C4B-CHC	-2.38	1.34	1.41
34	Y	309	CHL	C4B-CHC	-2.38	1.34	1.41
23	b	612	CLA	CMC-C2C	-2.38	1.45	1.50
23	C	514	CLA	CMB-C2B	-2.38	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.38	1.46	1.51
23	s	608	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	606	CLA	C3B-C2B	-2.38	1.37	1.40
34	g	601	CHL	C3B-C2B	-2.38	1.37	1.40
23	S	611	CLA	CMB-C2B	-2.38	1.46	1.51
23	Y	305	CLA	C3B-C2B	-2.37	1.37	1.40
23	S	609	CLA	C3B-C2B	-2.37	1.37	1.40
23	c	503	CLA	CMD-C2D	-2.37	1.45	1.50
23	S	613	CLA	CMB-C2B	-2.37	1.46	1.51
34	y	309	CHL	CHC-C1C	2.37	1.41	1.35
34	N	307	CHL	C3B-CAB	-2.37	1.43	1.47
23	B	603	CLA	CMC-C2C	-2.37	1.45	1.50
23	b	605	CLA	CMD-C2D	-2.37	1.45	1.50
23	R	602	CLA	CMB-C2B	-2.36	1.46	1.51
23	B	605	CLA	C4B-CHC	-2.36	1.34	1.41
34	G	608	CHL	CMB-C2B	-2.36	1.46	1.51
34	N	307	CHL	CMD-C2D	-2.36	1.45	1.50
23	C	502	CLA	CHC-C1C	2.36	1.41	1.35
34	G	609	CHL	C4B-CHC	-2.36	1.34	1.41
23	a	401	CLA	CMB-C2B	-2.36	1.46	1.51
34	R	605	CHL	CMD-C2D	-2.36	1.45	1.50
34	y	302	CHL	CMD-C2D	-2.36	1.45	1.50
34	n	307	CHL	C3B-C2B	-2.35	1.37	1.40
23	Y	313	CLA	C3B-C2B	-2.35	1.37	1.40
23	S	608	CLA	CMB-C2B	-2.35	1.46	1.51
23	R	609	CLA	CMB-C2B	-2.35	1.46	1.51
23	B	609	CLA	CMC-C2C	-2.35	1.45	1.50
23	G	602	CLA	C3B-CAB	-2.35	1.43	1.47
23	g	603	CLA	CMC-C2C	-2.35	1.45	1.50
34	G	609	CHL	MG-ND	-2.34	2.01	2.05
34	n	307	CHL	CMD-C2D	-2.34	1.45	1.50
23	B	605	CLA	CHC-C1C	2.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CMB-C2B	-2.34	1.46	1.51
23	N	304	CLA	C3B-CAB	-2.34	1.43	1.47
23	r	612	CLA	CMB-C2B	-2.34	1.46	1.51
23	c	504	CLA	C3B-C2B	-2.34	1.37	1.40
23	c	507	CLA	C3B-CAB	-2.34	1.43	1.47
23	S	610	CLA	CMB-C2B	-2.34	1.46	1.51
23	B	605	CLA	CMD-C2D	-2.34	1.45	1.50
34	n	309	CHL	C3B-C2B	-2.34	1.37	1.40
23	y	303	CLA	CMC-C2C	-2.34	1.45	1.50
33	e	101	HEM	FE-NB	2.33	2.08	1.96
23	Y	304	CLA	MG-ND	-2.33	2.01	2.05
23	B	607	CLA	CMD-C2D	-2.33	1.45	1.50
23	a	402	CLA	C4B-CHC	-2.33	1.34	1.41
23	b	615	CLA	C3B-C2B	-2.33	1.37	1.40
34	N	310	CHL	CMD-C2D	-2.33	1.45	1.50
23	n	312	CLA	CMD-C2D	-2.33	1.45	1.50
23	y	312	CLA	CMD-C2D	-2.33	1.45	1.50
34	S	606	CHL	CMB-C2B	-2.33	1.46	1.51
23	Y	303	CLA	C3B-C2B	-2.33	1.37	1.40
23	S	611	CLA	C3B-C2B	-2.33	1.37	1.40
23	G	603	CLA	CMC-C2C	-2.33	1.45	1.50
23	b	607	CLA	CMD-C2D	-2.33	1.45	1.50
23	G	612	CLA	C3B-C2B	-2.32	1.37	1.40
34	y	309	CHL	C4B-CHC	-2.32	1.34	1.41
23	c	506	CLA	CMC-C2C	-2.32	1.45	1.50
23	c	508	CLA	CMC-C2C	-2.32	1.45	1.50
23	G	603	CLA	MG-ND	-2.32	2.01	2.05
23	S	613	CLA	CMD-C2D	-2.32	1.45	1.50
23	C	508	CLA	C3B-CAB	-2.32	1.43	1.47
23	s	602	CLA	C3B-CAB	-2.32	1.43	1.47
23	n	305	CLA	C4B-CHC	-2.32	1.34	1.41
23	B	602	CLA	CMD-C2D	-2.32	1.45	1.50
23	b	614	CLA	CMD-C2D	-2.32	1.45	1.50
23	b	606	CLA	CMC-C2C	-2.31	1.45	1.50
23	g	602	CLA	C3B-CAB	-2.31	1.43	1.47
23	C	507	CLA	CMD-C2D	-2.31	1.45	1.50
23	g	603	CLA	CMD-C2D	-2.31	1.45	1.50
23	r	603	CLA	CMC-C2C	-2.31	1.45	1.50
34	G	605	CHL	CMD-C2D	-2.31	1.45	1.50
23	C	507	CLA	CMC-C2C	-2.31	1.45	1.50
23	B	608	CLA	C1D-ND	2.31	1.40	1.37
23	B	609	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	606	CHL	CMB-C2B	-2.30	1.46	1.51
23	y	313	CLA	MG-ND	-2.30	2.01	2.05
23	C	509	CLA	CMC-C2C	-2.30	1.45	1.50
23	c	505	CLA	CMD-C2D	-2.30	1.45	1.50
34	y	307	CHL	CMD-C2D	-2.30	1.45	1.50
23	s	613	CLA	CMD-C2D	-2.30	1.45	1.50
34	Y	307	CHL	CMD-C2D	-2.30	1.45	1.50
35	n	317	LUT	C26-C27	2.30	1.53	1.50
23	N	305	CLA	C3B-C2B	-2.30	1.37	1.40
34	n	310	CHL	CMD-C2D	-2.30	1.45	1.50
23	a	403	CLA	CMD-C2D	-2.30	1.45	1.50
23	C	503	CLA	CMD-C2D	-2.30	1.45	1.50
34	n	308	CHL	CHC-C1C	2.30	1.40	1.35
34	n	310	CHL	CHC-C1C	2.30	1.40	1.35
23	b	606	CLA	CMD-C2D	-2.29	1.45	1.50
34	g	601	CHL	CAC-C3C	-2.29	1.45	1.51
23	s	613	CLA	C3B-C2B	-2.29	1.37	1.40
23	g	603	CLA	C4B-CHC	-2.29	1.34	1.41
23	B	601	CLA	C3B-C2B	-2.29	1.37	1.40
23	C	506	CLA	CMD-C2D	-2.29	1.45	1.50
23	G	604	CLA	C3B-CAB	-2.29	1.43	1.47
23	B	614	CLA	CMD-C2D	-2.29	1.45	1.50
34	g	601	CHL	MG-ND	-2.29	2.01	2.05
23	r	608	CLA	C1B-NB	2.29	1.37	1.35
34	N	308	CHL	CHC-C1C	2.29	1.40	1.35
34	n	308	CHL	C3B-C2B	-2.29	1.37	1.40
23	N	305	CLA	CMD-C2D	-2.29	1.46	1.50
23	G	611	CLA	MG-ND	-2.29	2.01	2.05
34	n	307	CHL	C3B-CAB	-2.29	1.43	1.47
23	b	611	CLA	CMD-C2D	-2.28	1.46	1.50
23	b	605	CLA	CHC-C1C	2.28	1.40	1.35
23	d	404	CLA	MG-ND	-2.28	2.01	2.05
23	B	606	CLA	CMD-C2D	-2.28	1.46	1.50
34	G	601	CHL	C4B-CHC	-2.28	1.34	1.41
23	C	512	CLA	MG-NA	2.28	2.11	2.06
23	n	314	CLA	CMC-C2C	-2.28	1.46	1.50
34	S	605	CHL	C3B-C2B	-2.28	1.37	1.40
35	G	615	LUT	C22-C21	-2.28	1.51	1.54
23	s	602	CLA	CMC-C2C	-2.28	1.46	1.50
23	Y	312	CLA	CMD-C2D	-2.28	1.46	1.50
23	A	402	CLA	CMD-C2D	-2.28	1.46	1.50
23	y	313	CLA	C4B-CHC	-2.28	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	CMD-C2D	-2.27	1.46	1.50
23	r	609	CLA	CMC-C2C	-2.27	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.27	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.27	1.46	1.50
34	Y	302	CHL	CMD-C2D	-2.27	1.46	1.50
23	a	401	CLA	C4B-CHC	-2.27	1.34	1.41
23	B	610	CLA	CMC-C2C	-2.27	1.46	1.50
23	N	305	CLA	C4B-CHC	-2.27	1.34	1.41
23	r	614	CLA	CMD-C2D	-2.27	1.46	1.50
34	G	606	CHL	CMD-C2D	-2.27	1.46	1.50
23	s	611	CLA	C3B-C2B	-2.27	1.37	1.40
23	s	603	CLA	C3B-C2B	-2.26	1.37	1.40
23	G	603	CLA	CMD-C2D	-2.26	1.46	1.50
23	r	603	CLA	CMD-C2D	-2.26	1.46	1.50
23	Y	312	CLA	CMC-C2C	-2.26	1.46	1.50
23	D	404	CLA	MG-ND	-2.26	2.01	2.05
23	B	601	CLA	C3B-CAB	-2.26	1.43	1.47
23	b	616	CLA	CMC-C2C	-2.26	1.46	1.50
23	B	616	CLA	CMC-C2C	-2.26	1.46	1.50
23	C	509	CLA	CMD-C2D	-2.26	1.46	1.50
23	n	303	CLA	C3B-C2B	-2.26	1.37	1.40
34	n	302	CHL	CMD-C2D	-2.25	1.46	1.50
34	S	605	CHL	CMD-C2D	-2.25	1.46	1.50
23	a	402	CLA	CMD-C2D	-2.25	1.46	1.50
34	y	308	CHL	CMD-C2D	-2.25	1.46	1.50
23	b	605	CLA	CAC-C3C	-2.25	1.45	1.51
23	b	613	CLA	CMC-C2C	-2.25	1.46	1.50
32	D	406	PL9	C41-C39	2.25	1.56	1.51
23	s	610	CLA	CMD-C2D	-2.25	1.46	1.50
23	G	603	CLA	C3B-CAB	-2.25	1.43	1.47
23	C	511	CLA	CMC-C2C	-2.25	1.46	1.50
37	r	616	XAT	O4-C5	-2.25	1.43	1.46
23	a	405	CLA	CMD-C2D	-2.25	1.46	1.50
23	D	401	CLA	CMC-C2C	-2.25	1.46	1.50
23	g	603	CLA	C3B-CAB	-2.25	1.43	1.47
23	Y	303	CLA	C3B-CAB	-2.24	1.43	1.47
23	g	612	CLA	C3B-CAB	-2.24	1.43	1.47
34	G	609	CHL	C3B-C2B	-2.24	1.37	1.40
37	g	620	XAT	O4-C5	-2.24	1.43	1.46
23	G	604	CLA	MG-ND	-2.24	2.01	2.05
23	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
23	y	304	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	303	CLA	C3B-CAB	-2.24	1.43	1.47
23	Y	310	CLA	CMC-C2C	-2.24	1.46	1.50
23	D	401	CLA	C3B-C2B	-2.24	1.37	1.40
23	b	601	CLA	C3B-C2B	-2.23	1.37	1.40
23	b	613	CLA	CMD-C2D	-2.23	1.46	1.50
34	Y	308	CHL	CMD-C2D	-2.23	1.46	1.50
23	g	604	CLA	C3B-C2B	-2.23	1.37	1.40
23	S	603	CLA	C3B-C2B	-2.23	1.37	1.40
23	R	603	CLA	CMC-C2C	-2.23	1.46	1.50
23	g	612	CLA	CMC-C2C	-2.23	1.46	1.50
23	c	501	CLA	CHC-C1C	2.23	1.40	1.35
23	b	611	CLA	CMC-C2C	-2.23	1.46	1.50
23	B	611	CLA	CMD-C2D	-2.23	1.46	1.50
23	r	609	CLA	CMD-C2D	-2.23	1.46	1.50
23	g	604	CLA	C3B-CAB	-2.23	1.43	1.47
23	G	612	CLA	C3B-CAB	-2.23	1.43	1.47
23	c	508	CLA	CMD-C2D	-2.23	1.46	1.50
23	s	602	CLA	CMD-C2D	-2.23	1.46	1.50
23	s	603	CLA	MG-ND	-2.23	2.01	2.05
23	C	513	CLA	CMD-C2D	-2.23	1.46	1.50
23	D	401	CLA	CMD-C2D	-2.23	1.46	1.50
23	b	609	CLA	CMD-C2D	-2.22	1.46	1.50
23	r	603	CLA	C3B-C2B	-2.22	1.37	1.40
23	R	603	CLA	CMD-C2D	-2.22	1.46	1.50
34	Y	308	CHL	C3B-C2B	-2.22	1.37	1.40
23	R	609	CLA	CMC-C2C	-2.22	1.46	1.50
23	G	604	CLA	CMD-C2D	-2.22	1.46	1.50
23	R	609	CLA	CMD-C2D	-2.22	1.46	1.50
23	c	506	CLA	CMD-C2D	-2.22	1.46	1.50
23	r	608	CLA	CMD-C2D	-2.22	1.46	1.50
23	s	609	CLA	C3B-C2B	-2.22	1.37	1.40
23	C	510	CLA	MG-ND	-2.21	2.01	2.05
23	b	609	CLA	CMC-C2C	-2.21	1.46	1.50
23	g	610	CLA	CMB-C2B	-2.21	1.47	1.51
32	d	407	PL9	C41-C39	2.21	1.55	1.51
23	B	616	CLA	CMD-C2D	-2.21	1.46	1.50
23	b	609	CLA	C3B-C2B	-2.21	1.37	1.40
23	R	614	CLA	CMD-C2D	-2.21	1.46	1.50
23	c	511	CLA	MG-ND	-2.21	2.01	2.05
23	d	405	CLA	CMC-C2C	-2.21	1.46	1.50
23	Y	313	CLA	CMC-C2C	-2.21	1.46	1.50
23	g	602	CLA	C3B-C2B	-2.21	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	305	CLA	MG-ND	-2.21	2.01	2.05
23	B	613	CLA	CMC-C2C	-2.21	1.46	1.50
23	g	612	CLA	C3B-C2B	-2.20	1.37	1.40
23	g	613	CLA	C3B-CAB	-2.20	1.43	1.47
23	B	612	CLA	CMA-C3A	-2.20	1.48	1.53
23	B	613	CLA	CMD-C2D	-2.20	1.46	1.50
23	B	611	CLA	CMC-C2C	-2.20	1.46	1.50
23	S	602	CLA	CMC-C2C	-2.20	1.46	1.50
23	S	602	CLA	C3B-CAB	-2.20	1.43	1.47
34	g	609	CHL	C3B-C2B	-2.20	1.37	1.40
23	N	303	CLA	C3B-CAB	-2.20	1.43	1.47
34	n	310	CHL	C3B-C2B	-2.20	1.37	1.40
23	A	404	CLA	CMD-C2D	-2.20	1.46	1.50
23	g	611	CLA	MG-ND	-2.20	2.01	2.05
34	g	608	CHL	CMD-C2D	-2.20	1.46	1.50
35	y	316	LUT	C22-C21	-2.20	1.52	1.54
34	N	306	CHL	CMD-C2D	-2.20	1.46	1.50
23	N	311	CLA	CMC-C2C	-2.20	1.46	1.50
34	R	606	CHL	CMD-C2D	-2.19	1.46	1.50
23	y	313	CLA	CMC-C2C	-2.19	1.46	1.50
23	G	613	CLA	C3B-CAB	-2.19	1.43	1.47
23	G	610	CLA	CMB-C2B	-2.19	1.47	1.51
23	y	311	CLA	MG-ND	-2.19	2.01	2.05
23	B	608	CLA	CMC-C2C	-2.19	1.46	1.50
23	G	612	CLA	CMC-C2C	-2.19	1.46	1.50
34	s	605	CHL	CMD-C2D	-2.19	1.46	1.50
23	N	305	CLA	MG-ND	-2.19	2.01	2.05
23	Y	313	CLA	C4B-CHC	-2.19	1.34	1.41
23	B	603	CLA	C3B-C2B	-2.19	1.37	1.40
23	b	608	CLA	C3B-C2B	-2.19	1.37	1.40
23	b	607	CLA	CMC-C2C	-2.19	1.46	1.50
37	R	616	XAT	O4-C5	-2.18	1.43	1.46
23	A	401	CLA	C4B-CHC	-2.18	1.34	1.41
23	B	607	CLA	CMC-C2C	-2.18	1.46	1.50
23	r	602	CLA	CMC-C2C	-2.18	1.46	1.50
34	y	306	CHL	C3B-C2B	-2.18	1.37	1.40
34	R	607	CHL	CMD-C2D	-2.18	1.46	1.50
23	D	405	CLA	CMC-C2C	-2.18	1.46	1.50
23	G	604	CLA	C3B-C2B	-2.18	1.37	1.40
23	n	305	CLA	CMD-C2D	-2.18	1.46	1.50
34	G	607	CHL	CMD-C2D	-2.18	1.46	1.50
24	D	402	PHO	C3A-C2A	-2.17	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406	PL9	C7-C8	2.17	1.53	1.50
23	C	503	CLA	CMC-C2C	-2.17	1.46	1.50
23	c	513	CLA	MG-ND	-2.17	2.01	2.05
34	n	306	CHL	CMD-C2D	-2.17	1.46	1.50
36	S	616	NEX	O24-C25	-2.17	1.43	1.46
23	y	304	CLA	C3B-CAB	-2.17	1.43	1.47
24	d	401	PHO	C1C-NC	-2.17	1.31	1.38
23	b	603	CLA	CMC-C2C	-2.17	1.46	1.50
23	b	608	CLA	CMC-C2C	-2.17	1.46	1.50
23	C	503	CLA	C4B-CHC	-2.17	1.35	1.41
34	N	310	CHL	MG-ND	-2.17	2.01	2.05
23	c	510	CLA	CMC-C2C	-2.17	1.46	1.50
34	R	605	CHL	MG-ND	-2.17	2.01	2.05
23	g	603	CLA	MG-ND	-2.17	2.01	2.05
34	n	310	CHL	MG-ND	-2.16	2.01	2.05
23	B	610	CLA	MG-ND	-2.16	2.01	2.05
23	c	509	CLA	CMD-C2D	-2.16	1.46	1.50
23	N	303	CLA	MG-ND	-2.16	2.01	2.05
23	Y	311	CLA	MG-ND	-2.16	2.01	2.05
23	s	612	CLA	CMD-C2D	-2.16	1.46	1.50
23	Y	305	CLA	CMD-C2D	-2.16	1.46	1.50
37	G	620	XAT	O4-C5	-2.16	1.43	1.46
23	y	312	CLA	CMC-C2C	-2.16	1.46	1.50
36	y	317	NEX	O24-C25	-2.16	1.43	1.46
23	g	604	CLA	CMD-C2D	-2.16	1.46	1.50
34	y	308	CHL	C3B-C2B	-2.16	1.37	1.40
23	D	401	CLA	C3B-CAB	-2.15	1.43	1.47
23	s	611	CLA	MG-ND	-2.15	2.01	2.05
23	C	511	CLA	CMB-C2B	-2.15	1.47	1.51
23	s	608	CLA	CMD-C2D	-2.15	1.46	1.50
23	y	305	CLA	CMD-C2D	-2.15	1.46	1.50
23	b	610	CLA	MG-ND	-2.15	2.01	2.05
34	y	306	CHL	CMD-C2D	-2.15	1.46	1.50
34	N	308	CHL	MG-ND	-2.15	2.01	2.05
34	Y	309	CHL	CHC-C1C	2.15	1.40	1.35
36	Y	317	NEX	O24-C25	-2.15	1.43	1.46
23	n	314	CLA	C3B-C2B	-2.15	1.37	1.40
34	g	608	CHL	C3B-C2B	-2.15	1.37	1.40
23	b	601	CLA	C3B-CAB	-2.15	1.43	1.47
23	C	511	CLA	CAC-C3C	-2.15	1.45	1.51
23	C	513	CLA	C4B-CHC	-2.15	1.35	1.41
23	g	612	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	304	CLA	CMD-C2D	-2.15	1.46	1.50
23	B	609	CLA	C3B-CAB	-2.15	1.43	1.47
23	b	604	CLA	C4B-CHC	-2.14	1.35	1.41
34	R	607	CHL	MG-ND	-2.14	2.01	2.05
23	C	503	CLA	MG-ND	-2.14	2.01	2.05
23	S	613	CLA	C3B-C2B	-2.14	1.37	1.40
23	S	611	CLA	C4B-CHC	-2.14	1.35	1.41
23	G	613	CLA	CMD-C2D	-2.14	1.46	1.50
23	S	609	CLA	CMD-C2D	-2.14	1.46	1.50
34	N	308	CHL	CMD-C2D	-2.14	1.46	1.50
34	Y	306	CHL	CMD-C2D	-2.14	1.46	1.50
32	d	407	PL9	C7-C8	2.14	1.53	1.50
23	N	304	CLA	CMD-C2D	-2.14	1.46	1.50
23	S	611	CLA	CMD-C2D	-2.14	1.46	1.50
23	C	506	CLA	CMC-C2C	-2.14	1.46	1.50
23	n	314	CLA	CMD-C2D	-2.14	1.46	1.50
23	Y	313	CLA	MG-ND	-2.14	2.01	2.05
23	y	313	CLA	CMD-C2D	-2.14	1.46	1.50
23	Y	313	CLA	CMD-C2D	-2.14	1.46	1.50
23	B	614	CLA	C3B-C2B	-2.14	1.37	1.40
23	s	609	CLA	CMD-C2D	-2.14	1.46	1.50
23	g	613	CLA	CMD-C2D	-2.14	1.46	1.50
23	N	314	CLA	CMC-C2C	-2.14	1.46	1.50
23	Y	311	CLA	CMD-C2D	-2.14	1.46	1.50
23	S	604	CLA	CMD-C2D	-2.13	1.46	1.50
34	R	613	CHL	CMD-C2D	-2.13	1.46	1.50
36	G	617	NEX	O24-C25	-2.13	1.43	1.46
36	N	318	NEX	O24-C25	-2.13	1.43	1.46
23	g	613	CLA	C3B-C2B	-2.13	1.37	1.40
23	c	502	CLA	C4B-CHC	-2.13	1.35	1.41
23	C	502	CLA	C3B-C2B	-2.13	1.37	1.40
23	Y	304	CLA	C3B-CAB	-2.13	1.43	1.47
23	R	614	CLA	C3B-C2B	-2.13	1.37	1.40
23	b	614	CLA	C3B-C2B	-2.13	1.37	1.40
34	r	606	CHL	CMD-C2D	-2.13	1.46	1.50
23	c	505	CLA	CMC-C2C	-2.13	1.46	1.50
34	Y	306	CHL	C3B-C2B	-2.13	1.37	1.40
23	N	312	CLA	CMD-C2D	-2.13	1.46	1.50
23	r	604	CLA	CMC-C2C	-2.13	1.46	1.50
23	R	608	CLA	CMD-C2D	-2.13	1.46	1.50
23	s	604	CLA	CMC-C2C	-2.13	1.46	1.50
23	N	314	CLA	C4B-CHC	-2.13	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	611	CLA	MG-ND	-2.12	2.01	2.05
23	R	602	CLA	CMC-C2C	-2.12	1.46	1.50
23	n	311	CLA	CMC-C2C	-2.12	1.46	1.50
23	n	314	CLA	C3B-CAB	-2.12	1.43	1.47
34	n	307	CHL	MG-ND	-2.12	2.01	2.05
23	a	405	CLA	C3B-CAB	-2.12	1.43	1.47
35	N	317	LUT	C26-C27	2.12	1.53	1.50
23	c	507	CLA	CMC-C2C	-2.12	1.46	1.50
23	s	603	CLA	C4B-CHC	-2.12	1.35	1.41
23	r	603	CLA	MG-ND	-2.12	2.01	2.05
23	S	612	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	509	CLA	CMB-C2B	-2.12	1.47	1.51
23	C	513	CLA	CAC-C3C	-2.12	1.45	1.51
23	s	611	CLA	C4B-CHC	-2.12	1.35	1.41
23	S	603	CLA	C4B-CHC	-2.12	1.35	1.41
34	S	605	CHL	CAC-C3C	-2.12	1.45	1.51
23	y	310	CLA	CMC-C2C	-2.12	1.46	1.50
23	C	513	CLA	C3B-C2B	-2.12	1.37	1.40
34	Y	302	CHL	MG-ND	-2.12	2.01	2.05
23	R	601	CLA	C4B-CHC	-2.12	1.35	1.41
23	B	611	CLA	C3B-C2B	-2.11	1.37	1.40
23	r	608	CLA	C3B-C2B	-2.11	1.37	1.40
23	y	304	CLA	C4B-CHC	-2.11	1.35	1.41
34	S	605	CHL	C3B-CAB	-2.11	1.43	1.47
23	y	311	CLA	CMD-C2D	-2.11	1.46	1.50
23	b	612	CLA	CMA-C3A	-2.11	1.48	1.53
23	a	402	CLA	CAC-C3C	-2.11	1.45	1.51
23	B	604	CLA	C4B-CHC	-2.11	1.35	1.41
23	R	608	CLA	C3B-C2B	-2.11	1.37	1.40
23	B	609	CLA	MG-ND	-2.11	2.01	2.05
23	B	608	CLA	C3B-CAB	-2.11	1.43	1.47
23	N	312	CLA	MG-ND	-2.11	2.01	2.05
23	n	303	CLA	MG-ND	-2.11	2.01	2.05
34	n	302	CHL	MG-ND	-2.11	2.01	2.05
32	D	406	PL9	C26-C24	2.11	1.55	1.51
23	R	604	CLA	CMC-C2C	-2.11	1.46	1.50
23	R	610	CLA	CMD-C2D	-2.10	1.46	1.50
23	c	508	CLA	CMB-C2B	-2.10	1.47	1.51
23	b	610	CLA	CMC-C2C	-2.10	1.46	1.50
23	b	615	CLA	CMC-C2C	-2.10	1.46	1.50
23	n	304	CLA	CMC-C2C	-2.10	1.46	1.50
23	B	603	CLA	C3B-CAB	-2.10	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	g	601	CHL	C4B-CHC	-2.10	1.35	1.41
34	n	308	CHL	CMD-C2D	-2.10	1.46	1.50
23	n	313	CLA	C3B-C2B	-2.10	1.37	1.40
23	c	502	CLA	CMD-C2D	-2.10	1.46	1.50
23	Y	311	CLA	CMC-C2C	-2.10	1.46	1.50
23	r	604	CLA	CMD-C2D	-2.10	1.46	1.50
23	s	611	CLA	CMD-C2D	-2.10	1.46	1.50
34	g	607	CHL	CMD-C2D	-2.10	1.46	1.50
23	R	609	CLA	C3B-CAB	-2.10	1.43	1.47
36	g	617	NEX	O24-C25	-2.09	1.43	1.46
23	N	304	CLA	CMC-C2C	-2.09	1.46	1.50
34	g	605	CHL	CMD-C2D	-2.09	1.46	1.50
24	D	402	PHO	C1C-NC	-2.09	1.32	1.38
34	G	606	CHL	C3B-CAB	-2.09	1.43	1.47
23	s	603	CLA	CMC-C2C	-2.09	1.46	1.50
23	g	614	CLA	C3B-C2B	-2.09	1.37	1.40
23	c	508	CLA	C4B-CHC	-2.09	1.35	1.41
23	R	611	CLA	C3B-C2B	-2.09	1.37	1.40
23	Y	311	CLA	C3B-CAB	-2.09	1.43	1.47
34	g	609	CHL	MG-ND	-2.09	2.01	2.05
23	c	512	CLA	C4B-CHC	-2.09	1.35	1.41
23	b	601	CLA	CMD-C2D	-2.09	1.46	1.50
23	G	603	CLA	C4B-CHC	-2.09	1.35	1.41
23	a	405	CLA	CMC-C2C	-2.08	1.46	1.50
23	R	603	CLA	C3B-C2B	-2.08	1.37	1.40
23	Y	305	CLA	MG-ND	-2.08	2.01	2.05
23	g	613	CLA	MG-ND	-2.08	2.01	2.05
23	B	610	CLA	C4B-CHC	-2.08	1.35	1.41
34	g	619	CHL	MG-ND	-2.08	2.01	2.05
36	s	616	NEX	O24-C25	-2.08	1.43	1.46
23	y	305	CLA	C4B-CHC	-2.08	1.35	1.41
34	g	609	CHL	C4B-CHC	-2.08	1.35	1.41
23	D	405	CLA	CMD-C2D	-2.08	1.46	1.50
23	a	402	CLA	CMC-C2C	-2.08	1.46	1.50
23	y	311	CLA	CMC-C2C	-2.08	1.46	1.50
23	R	614	CLA	C4B-CHC	-2.08	1.35	1.41
23	y	304	CLA	CMC-C2C	-2.08	1.46	1.50
23	B	613	CLA	C3B-C2B	-2.08	1.37	1.40
23	Y	310	CLA	CMD-C2D	-2.08	1.46	1.50
34	s	601	CHL	CMD-C2D	-2.08	1.46	1.50
34	r	605	CHL	CMD-C2D	-2.08	1.46	1.50
34	y	302	CHL	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	602	CLA	C3B-C2B	-2.07	1.37	1.40
23	n	305	CLA	MG-ND	-2.07	2.01	2.05
23	S	608	CLA	CMD-C2D	-2.07	1.46	1.50
23	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
23	b	613	CLA	C3B-C2B	-2.07	1.37	1.40
23	B	609	CLA	C4B-CHC	-2.07	1.35	1.41
36	R	617	NEX	C1-C6	-2.07	1.51	1.54
23	n	304	CLA	CMD-C2D	-2.07	1.46	1.50
23	r	602	CLA	C3B-C2B	-2.07	1.37	1.40
34	S	601	CHL	CMD-C2D	-2.07	1.46	1.50
36	n	318	NEX	O24-C25	-2.07	1.43	1.46
23	C	505	CLA	CMD-C2D	-2.07	1.46	1.50
23	y	310	CLA	CMD-C2D	-2.07	1.46	1.50
34	g	607	CHL	C3B-CAB	-2.07	1.43	1.47
23	b	611	CLA	C3B-C2B	-2.07	1.37	1.40
23	s	604	CLA	C3B-C2B	-2.07	1.37	1.40
23	N	311	CLA	C3B-CAB	-2.07	1.43	1.47
34	n	308	CHL	C4B-CHC	-2.07	1.35	1.41
23	C	508	CLA	MG-ND	-2.06	2.01	2.05
23	C	509	CLA	C4B-CHC	-2.06	1.35	1.41
23	B	602	CLA	CMC-C2C	-2.06	1.46	1.50
23	R	602	CLA	CMD-C2D	-2.06	1.46	1.50
23	S	610	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	508	CLA	CMC-C2C	-2.06	1.46	1.50
23	B	601	CLA	CMD-C2D	-2.06	1.46	1.50
23	c	513	CLA	CMC-C2C	-2.06	1.46	1.50
23	a	402	CLA	C3B-CAB	-2.06	1.43	1.47
23	c	511	CLA	CMC-C2C	-2.06	1.46	1.50
23	s	604	CLA	C3B-CAB	-2.06	1.43	1.47
23	C	512	CLA	C3B-CAB	-2.06	1.43	1.47
23	G	604	CLA	CMC-C2C	-2.06	1.46	1.50
23	g	611	CLA	CMD-C2D	-2.06	1.46	1.50
23	Y	314	CLA	CMD-C2D	-2.06	1.46	1.50
23	n	312	CLA	MG-ND	-2.06	2.01	2.05
23	c	502	CLA	C3B-CAB	-2.06	1.43	1.47
23	N	303	CLA	C3B-C2B	-2.06	1.37	1.40
23	y	311	CLA	C3B-C2B	-2.06	1.37	1.40
34	S	606	CHL	C3D-C4D	2.06	1.48	1.44
23	s	603	CLA	CMD-C2D	-2.06	1.46	1.50
32	d	407	PL9	C26-C24	2.05	1.55	1.51
23	G	613	CLA	C3B-C2B	-2.05	1.37	1.40
23	S	612	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-CAB	-2.05	1.43	1.47
23	g	611	CLA	C3B-C2B	-2.05	1.37	1.40
34	N	310	CHL	C3B-C2B	-2.05	1.37	1.40
35	Y	316	LUT	C22-C21	-2.05	1.52	1.54
23	Y	304	CLA	C4B-CHC	-2.05	1.35	1.41
23	g	604	CLA	MG-ND	-2.05	2.01	2.05
23	g	613	CLA	CMC-C2C	-2.05	1.46	1.50
23	b	602	CLA	CMC-C2C	-2.05	1.46	1.50
23	A	404	CLA	CMC-C2C	-2.05	1.46	1.50
23	c	510	CLA	CMB-C2B	-2.04	1.47	1.51
23	c	513	CLA	C3B-C2B	-2.04	1.37	1.40
23	B	611	CLA	C4B-CHC	-2.04	1.35	1.41
34	r	613	CHL	CMD-C2D	-2.04	1.46	1.50
23	c	510	CLA	CAC-C3C	-2.04	1.45	1.51
23	B	614	CLA	CMC-C2C	-2.04	1.46	1.50
23	r	602	CLA	C3B-CAB	-2.04	1.43	1.47
34	N	308	CHL	C3B-C2B	-2.04	1.37	1.40
23	B	613	CLA	MG-ND	-2.04	2.01	2.05
23	n	312	CLA	CMC-C2C	-2.04	1.46	1.50
23	S	603	CLA	CMD-C2D	-2.04	1.46	1.50
34	Y	306	CHL	MG-ND	-2.04	2.01	2.05
34	Y	307	CHL	MG-ND	-2.04	2.01	2.05
23	N	313	CLA	CMD-C2D	-2.04	1.46	1.50
23	S	609	CLA	CMC-C2C	-2.04	1.46	1.50
23	c	503	CLA	C4B-CHC	-2.04	1.35	1.41
34	N	302	CHL	C3B-CAB	-2.03	1.43	1.47
23	y	314	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	613	CLA	MG-ND	-2.03	2.01	2.05
23	r	603	CLA	C3B-CAB	-2.03	1.43	1.47
23	G	614	CLA	C3B-C2B	-2.03	1.37	1.40
23	S	602	CLA	C3B-C2B	-2.03	1.37	1.40
23	r	601	CLA	C4B-CHC	-2.03	1.35	1.41
23	b	608	CLA	C4B-CHC	-2.03	1.35	1.41
34	s	606	CHL	C3D-C4D	2.03	1.48	1.44
23	Y	311	CLA	C3B-C2B	-2.03	1.37	1.40
23	y	311	CLA	C3B-CAB	-2.03	1.43	1.47
23	d	405	CLA	CMD-C2D	-2.03	1.46	1.50
23	n	314	CLA	C4B-CHC	-2.03	1.35	1.41
23	N	313	CLA	C3B-C2B	-2.03	1.37	1.40
34	y	306	CHL	MG-ND	-2.03	2.01	2.05
37	N	301	XAT	O4-C5	-2.03	1.43	1.46
23	N	313	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CMC-C2C	-2.03	1.46	1.50
34	n	309	CHL	MG-ND	-2.03	2.01	2.05
23	C	504	CLA	C4B-CHC	-2.03	1.35	1.41
34	G	619	CHL	MG-ND	-2.02	2.01	2.05
34	n	308	CHL	MG-ND	-2.02	2.01	2.05
35	G	615	LUT	C10-C9	-2.02	1.33	1.35
34	Y	309	CHL	MG-ND	-2.02	2.01	2.05
37	R	616	XAT	O24-C25	-2.02	1.43	1.46
23	B	601	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	614	CLA	CMD-C2D	-2.02	1.46	1.50
23	R	614	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	611	CLA	C3D-C4D	2.02	1.48	1.44
35	g	615	LUT	C10-C9	-2.02	1.33	1.35
23	S	602	CLA	CMD-C2D	-2.02	1.46	1.50
37	y	301	XAT	O4-C5	-2.02	1.43	1.46
34	S	605	CHL	MG-ND	-2.02	2.01	2.05
23	g	604	CLA	CMC-C2C	-2.02	1.46	1.50
23	N	305	CLA	C3B-CAB	-2.02	1.43	1.47
23	D	405	CLA	C4B-CHC	-2.02	1.35	1.41
23	s	602	CLA	MG-ND	-2.02	2.01	2.05
23	c	505	CLA	C4B-CHC	-2.02	1.35	1.41
34	n	309	CHL	C3B-CAB	-2.02	1.43	1.47
23	G	613	CLA	CMC-C2C	-2.02	1.46	1.50
23	B	601	CLA	C4B-CHC	-2.02	1.35	1.41
23	C	506	CLA	C4B-CHC	-2.02	1.35	1.41
34	N	307	CHL	C4B-CHC	-2.02	1.35	1.41
34	S	605	CHL	C4B-CHC	-2.02	1.35	1.41
23	G	610	CLA	CMD-C2D	-2.02	1.46	1.50
23	n	312	CLA	C3B-C2B	-2.02	1.37	1.40
23	a	403	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	611	CLA	C3B-CAB	-2.02	1.43	1.47
23	c	501	CLA	CMC-C2C	-2.01	1.46	1.50
36	y	317	NEX	C11-C10	2.01	1.49	1.43
37	Y	301	XAT	O4-C5	-2.01	1.43	1.46
23	b	609	CLA	MG-ND	-2.01	2.01	2.05
23	c	502	CLA	CMC-C2C	-2.01	1.46	1.50
23	r	612	CLA	CMC-C2C	-2.01	1.46	1.50
23	c	507	CLA	MG-ND	-2.01	2.01	2.05
23	R	601	CLA	CMD-C2D	-2.01	1.46	1.50
23	g	611	CLA	C3B-CAB	-2.01	1.43	1.47
34	n	306	CHL	MG-ND	-2.01	2.01	2.05
23	b	605	CLA	C3B-CAB	-2.01	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CAC-C3C	-2.01	1.46	1.51
23	C	512	CLA	C4B-CHC	-2.01	1.35	1.41
23	c	504	CLA	CMD-C2D	-2.01	1.46	1.50
23	S	609	CLA	C4B-CHC	-2.01	1.35	1.41
23	R	604	CLA	CMD-C2D	-2.01	1.46	1.50
23	c	509	CLA	CMC-C2C	-2.01	1.46	1.50
37	n	301	XAT	O4-C5	-2.01	1.43	1.46
34	G	606	CHL	MG-ND	-2.01	2.01	2.05
23	s	612	CLA	CMC-C2C	-2.00	1.46	1.50
23	A	404	CLA	C3B-CAB	-2.00	1.43	1.47
23	R	612	CLA	CMC-C2C	-2.00	1.46	1.50
23	s	602	CLA	C3B-C2B	-2.00	1.37	1.40
24	A	403	PHO	C1C-NC	-2.00	1.32	1.38
36	r	617	NEX	O24-C25	-2.00	1.43	1.46
23	r	608	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	512	CLA	C3B-C2B	-2.00	1.37	1.40
23	n	314	CLA	MG-ND	-2.00	2.01	2.05
23	N	312	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	506	CLA	C3B-C2B	-2.00	1.37	1.40
34	G	608	CHL	C3B-C2B	-2.00	1.37	1.40

All (2943) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	SQD	O9-S-C6	-19.33	83.97	106.94
26	a	409	SQD	O9-S-C6	-19.29	84.01	106.94
36	Y	317	NEX	C17-C1-C6	-19.09	93.39	110.47
36	y	317	NEX	C17-C1-C6	-17.33	94.96	110.47
36	G	617	NEX	O24-C25-C24	13.28	123.36	113.38
36	g	617	NEX	O24-C25-C24	12.73	122.95	113.38
36	s	616	NEX	O24-C25-C24	11.70	122.17	113.38
26	a	409	SQD	O8-S-O9	-11.58	82.98	111.27
26	A	409	SQD	O8-S-O9	-11.56	83.04	111.27
36	S	616	NEX	O24-C25-C24	11.08	121.71	113.38
36	y	317	NEX	C16-C1-C6	10.94	120.26	110.47
36	Y	317	NEX	C16-C1-C6	10.50	119.87	110.47
37	G	620	XAT	O24-C25-C24	10.15	121.01	113.38
26	A	409	SQD	O7-S-C6	10.11	118.95	106.94
26	a	409	SQD	O7-S-C6	10.07	118.91	106.94
32	d	407	PL9	C7-C8-C9	-10.06	110.05	126.79
32	D	406	PL9	C7-C8-C9	-10.00	110.14	126.79
36	r	617	NEX	O24-C25-C24	9.89	120.81	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	617	NEX	O24-C25-C24	9.75	120.71	113.38
37	R	616	XAT	O4-C5-C4	9.44	120.47	113.38
23	c	502	CLA	C4A-NA-C1A	9.44	110.95	106.71
34	N	310	CHL	C4A-NA-C1A	9.41	110.94	106.71
34	n	310	CHL	C4A-NA-C1A	9.40	110.93	106.71
36	y	317	NEX	C17-C1-C16	-9.24	80.17	108.53
37	g	620	XAT	O24-C25-C24	9.19	120.29	113.38
26	A	409	SQD	O9-S-O7	-9.14	82.32	113.95
26	a	409	SQD	O9-S-O7	-9.12	82.40	113.95
36	Y	317	NEX	C17-C1-C16	-9.04	80.78	108.53
37	r	616	XAT	O4-C5-C4	8.82	120.01	113.38
37	n	301	XAT	O24-C25-C24	8.81	120.00	113.38
23	C	503	CLA	C4A-NA-C1A	8.78	110.65	106.71
34	G	609	CHL	C4A-NA-C1A	8.57	110.56	106.71
36	y	317	NEX	O24-C25-C24	8.48	119.75	113.38
37	y	301	XAT	O4-C5-C4	8.46	119.74	113.38
37	n	301	XAT	O4-C5-C4	8.45	119.73	113.38
34	g	609	CHL	C4A-NA-C1A	8.39	110.48	106.71
23	s	612	CLA	C4A-NA-C1A	8.36	110.47	106.71
37	N	301	XAT	O4-C5-C4	8.32	119.63	113.38
36	y	317	NEX	C2-C1-C6	8.28	117.26	109.21
23	S	612	CLA	C4A-NA-C1A	8.28	110.43	106.71
23	A	401	CLA	C4A-NA-C1A	7.97	110.29	106.71
23	R	604	CLA	C4A-NA-C1A	7.95	110.28	106.71
36	Y	317	NEX	O24-C25-C24	7.90	119.32	113.38
23	r	604	CLA	C4A-NA-C1A	7.88	110.25	106.71
37	N	301	XAT	O24-C25-C24	7.84	119.27	113.38
37	Y	301	XAT	O4-C5-C4	7.77	119.22	113.38
34	Y	309	CHL	C4A-NA-C1A	7.77	110.20	106.71
23	Y	311	CLA	C4A-NA-C1A	7.63	110.14	106.71
26	a	409	SQD	O8-S-C6	7.61	117.87	105.74
36	Y	317	NEX	C2-C1-C6	7.60	116.60	109.21
26	A	409	SQD	O8-S-C6	7.56	117.79	105.74
23	y	311	CLA	C4A-NA-C1A	7.55	110.10	106.71
23	a	401	CLA	C4A-NA-C1A	7.52	110.09	106.71
23	b	612	CLA	C4A-NA-C1A	7.29	109.98	106.71
37	r	616	XAT	O24-C25-C24	7.27	118.85	113.38
23	B	612	CLA	C4A-NA-C1A	7.27	109.97	106.71
37	R	616	XAT	O24-C25-C24	7.24	118.82	113.38
23	D	405	CLA	C4A-NA-C1A	7.23	109.96	106.71
32	d	407	PL9	C17-C18-C19	-7.13	110.50	127.66
23	d	405	CLA	C4A-NA-C1A	7.11	109.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CMB-C2B-C1B	-7.05	117.62	128.46
32	D	406	PL9	C17-C18-C19	-7.04	110.71	127.66
23	R	610	CLA	C4A-NA-C1A	7.02	109.86	106.71
34	g	607	CHL	C4A-NA-C1A	6.98	109.84	106.71
23	G	612	CLA	C4A-NA-C1A	6.96	109.83	106.71
23	g	604	CLA	C4A-NA-C1A	6.93	109.82	106.71
32	d	407	PL9	C12-C13-C14	-6.92	111.00	127.66
23	g	611	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	b	605	CLA	C4A-NA-C1A	6.85	109.78	106.71
36	n	318	NEX	O24-C25-C24	6.83	118.51	113.38
23	b	608	CLA	CMB-C2B-C1B	-6.82	117.97	128.46
23	G	611	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	B	610	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	N	314	CLA	C4A-NA-C1A	6.79	109.76	106.71
32	D	406	PL9	C12-C13-C14	-6.78	111.32	127.66
23	B	613	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	B	604	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	R	612	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	b	604	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	B	609	CLA	C4A-NA-C1A	6.71	109.72	106.71
32	D	406	PL9	C22-C23-C24	-6.71	111.51	127.66
34	y	306	CHL	C4A-NA-C1A	6.70	109.72	106.71
23	R	602	CLA	C4A-NA-C1A	6.70	109.72	106.71
32	d	407	PL9	C32-C33-C34	-6.69	111.55	127.66
23	n	305	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	n	314	CLA	C4A-NA-C1A	6.64	109.69	106.71
37	Y	301	XAT	O24-C25-C24	6.64	118.37	113.38
23	B	608	CLA	CMB-C2B-C1B	-6.63	118.27	128.46
32	D	406	PL9	C32-C33-C34	-6.61	111.73	127.66
36	N	318	NEX	O24-C25-C24	6.61	118.35	113.38
32	d	407	PL9	C22-C23-C24	-6.57	111.84	127.66
23	y	313	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	b	613	CLA	C4A-NA-C1A	6.56	109.65	106.71
23	D	401	CLA	C4A-NA-C1A	6.56	109.65	106.71
34	Y	306	CHL	C4A-NA-C1A	6.55	109.65	106.71
37	y	301	XAT	O24-C25-C24	6.55	118.30	113.38
23	B	605	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	G	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
34	N	310	CHL	CMB-C2B-C1B	-6.49	118.48	128.46
23	Y	314	CLA	CMB-C2B-C1B	-6.49	118.50	128.46
23	S	604	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	C	504	CLA	C4A-NA-C1A	6.43	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	407	PL9	C27-C28-C29	-6.40	112.26	127.66
34	y	309	CHL	C4A-NA-C1A	6.35	109.56	106.71
23	C	510	CLA	CMB-C2B-C3B	6.33	136.52	124.68
23	Y	312	CLA	C4A-NA-C1A	6.33	109.55	106.71
32	D	406	PL9	C16-C14-C13	-6.31	108.35	121.12
23	b	609	CLA	C4A-NA-C1A	6.31	109.54	106.71
23	c	508	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	c	504	CLA	C4A-NA-C1A	6.27	109.53	106.71
23	r	614	CLA	C4A-NA-C1A	6.24	109.51	106.71
34	S	606	CHL	C4A-NA-C1A	6.24	109.51	106.71
23	D	404	CLA	C4A-NA-C1A	6.23	109.51	106.71
36	G	617	NEX	C11-C10-C9	-6.23	118.42	127.31
23	N	305	CLA	C4A-NA-C1A	6.22	109.50	106.71
32	d	407	PL9	C16-C14-C13	-6.22	108.52	121.12
23	R	603	CLA	C4A-NA-C1A	6.21	109.50	106.71
32	D	406	PL9	C37-C38-C39	-6.21	112.72	127.66
34	n	308	CHL	C4A-NA-C1A	6.19	109.49	106.71
23	y	305	CLA	C4A-NA-C1A	6.18	109.48	106.71
32	d	407	PL9	C15-C14-C13	-6.18	107.83	123.68
34	G	607	CHL	C4A-NA-C1A	6.14	109.47	106.71
32	D	406	PL9	C27-C28-C29	-6.12	112.92	127.66
23	Y	305	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	S	603	CLA	C4A-NA-C1A	6.11	109.45	106.71
32	d	407	PL9	C37-C38-C39	-6.09	113.01	127.66
34	n	307	CHL	C1B-CHB-C4A	-6.07	118.09	130.12
34	N	308	CHL	C4A-NA-C1A	6.06	109.43	106.71
32	D	406	PL9	C42-C43-C44	-6.06	113.08	127.66
23	r	610	CLA	C4A-NA-C1A	6.05	109.43	106.71
32	d	407	PL9	C42-C43-C44	-6.04	113.11	127.66
23	d	404	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	A	404	CLA	C4A-NA-C1A	6.02	109.41	106.71
23	y	314	CLA	CMB-C2B-C1B	-6.02	119.21	128.46
32	D	406	PL9	C15-C14-C13	-6.01	108.26	123.68
23	r	603	CLA	C4A-NA-C1A	5.99	109.40	106.71
23	s	604	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	a	405	CLA	C4A-NA-C1A	5.97	109.39	106.71
34	N	307	CHL	C1B-CHB-C4A	-5.93	118.38	130.12
23	n	312	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	C	509	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	g	602	CLA	C4A-NA-C1A	5.90	109.36	106.71
23	r	612	CLA	C4A-NA-C1A	5.89	109.35	106.71
23	y	312	CLA	C4A-NA-C1A	5.88	109.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	313	CLA	C4A-NA-C1A	5.88	109.35	106.71
23	g	613	CLA	C4A-NA-C1A	5.86	109.34	106.71
23	G	602	CLA	C4A-NA-C1A	5.85	109.34	106.71
23	c	503	CLA	C4A-NA-C1A	5.84	109.33	106.71
23	N	315	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	C	508	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	C	507	CLA	C4A-NA-C1A	5.81	109.32	106.71
23	b	610	CLA	C4A-NA-C1A	5.80	109.31	106.71
23	s	610	CLA	C4A-NA-C1A	5.79	109.31	106.71
34	G	619	CHL	C4A-NA-C1A	5.77	109.30	106.71
34	n	309	CHL	C4A-NA-C1A	5.72	109.28	106.71
23	B	607	CLA	C4A-NA-C1A	5.72	109.28	106.71
32	d	407	PL9	C36-C34-C33	-5.71	109.56	121.12
34	y	302	CHL	C4A-NA-C1A	5.70	109.27	106.71
23	N	312	CLA	C4A-NA-C1A	5.69	109.26	106.71
23	c	506	CLA	C4A-NA-C1A	5.68	109.26	106.71
23	c	510	CLA	C4A-NA-C1A	5.67	109.26	106.71
34	S	601	CHL	C4A-NA-C1A	5.66	109.25	106.71
23	b	607	CLA	C4A-NA-C1A	5.62	109.23	106.71
32	d	407	PL9	C46-C44-C43	-5.61	109.77	121.12
34	g	619	CHL	C4A-NA-C1A	5.60	109.22	106.71
23	y	303	CLA	C4A-NA-C1A	5.59	109.22	106.71
23	G	613	CLA	C4A-NA-C1A	5.58	109.22	106.71
34	G	609	CHL	C1B-CHB-C4A	-5.58	119.07	130.12
34	s	606	CHL	C4A-NA-C1A	5.57	109.21	106.71
23	c	507	CLA	C4A-NA-C1A	5.55	109.20	106.71
34	g	609	CHL	C1B-CHB-C4A	-5.52	119.18	130.12
23	B	601	CLA	C4A-NA-C1A	5.52	109.19	106.71
32	D	406	PL9	C11-C9-C8	-5.52	109.96	121.12
37	G	620	XAT	O4-C5-C4	5.52	117.53	113.38
32	d	407	PL9	C11-C9-C8	-5.51	109.96	121.12
23	b	610	CLA	CMB-C2B-C1B	-5.51	120.00	128.46
32	D	406	PL9	C36-C34-C33	-5.47	110.04	121.12
23	Y	314	CLA	CMB-C2B-C3B	5.47	134.92	124.68
32	D	406	PL9	C45-C44-C43	-5.46	109.66	123.68
23	Y	304	CLA	C4A-NA-C1A	5.45	109.16	106.71
36	Y	317	NEX	C17-C1-C2	-5.42	84.73	109.05
37	g	620	XAT	O4-C5-C18	5.41	121.54	115.06
32	d	407	PL9	C45-C44-C43	-5.39	109.84	123.68
36	r	617	NEX	C27-C28-C29	-5.38	117.19	125.53
23	b	601	CLA	C4A-NA-C1A	5.37	109.12	106.71
23	B	611	CLA	C4A-NA-C1A	5.36	109.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	406	PL9	C35-C34-C33	-5.35	109.96	123.68
34	g	601	CHL	C4A-NA-C1A	5.33	109.10	106.71
23	n	315	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	Y	303	CLA	C4A-NA-C1A	5.32	109.10	106.71
32	d	407	PL9	C35-C34-C33	-5.32	110.03	123.68
23	C	507	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
32	d	407	PL9	C41-C39-C38	-5.30	110.39	121.12
34	r	605	CHL	C4A-NA-C1A	5.30	109.09	106.71
23	C	511	CLA	CMB-C2B-C1B	-5.29	120.34	128.46
23	C	505	CLA	C4A-NA-C1A	5.28	109.08	106.71
23	c	506	CLA	CMB-C2B-C1B	-5.27	120.37	128.46
32	D	406	PL9	C45-C44-C46	-5.27	106.41	115.27
25	k	101	BCR	C16-C17-C18	-5.27	119.79	127.31
23	G	614	CLA	C4A-NA-C1A	5.27	109.07	106.71
34	Y	307	CHL	C4A-NA-C1A	5.26	109.07	106.71
32	D	406	PL9	C46-C44-C43	-5.26	110.47	121.12
23	G	610	CLA	C4A-NA-C1A	5.26	109.07	106.71
23	C	509	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
23	n	311	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
23	N	303	CLA	C4A-NA-C1A	5.24	109.06	106.71
23	b	611	CLA	C4A-NA-C1A	5.23	109.06	106.71
23	g	614	CLA	C4A-NA-C1A	5.23	109.06	106.71
28	H	102	DGD	O2G-C1B-C2B	5.22	122.75	111.50
32	D	406	PL9	C20-C19-C18	-5.21	110.33	123.68
36	s	616	NEX	C11-C10-C9	-5.20	119.89	127.31
23	N	304	CLA	C4A-NA-C1A	5.20	109.04	106.71
34	n	302	CHL	C4A-NA-C1A	5.20	109.04	106.71
37	g	620	XAT	O4-C5-C4	5.20	117.29	113.38
23	N	313	CLA	C4A-NA-C1A	5.19	109.04	106.71
37	Y	301	XAT	O24-C25-C38	5.19	121.28	115.06
34	s	601	CHL	C4A-NA-C1A	5.19	109.04	106.71
23	A	402	CLA	C4A-NA-C1A	5.18	109.04	106.71
34	n	310	CHL	CMB-C2B-C1B	-5.18	120.50	128.46
37	g	620	XAT	C18-C5-C6	-5.16	113.60	122.26
23	c	508	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
23	Y	313	CLA	C4A-NA-C1A	5.15	109.02	106.71
23	c	510	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
37	G	620	XAT	C18-C5-C6	-5.14	113.64	122.26
32	d	407	PL9	C40-C39-C38	-5.14	110.49	123.68
32	d	407	PL9	C20-C19-C18	-5.14	110.49	123.68
36	y	317	NEX	C17-C1-C2	-5.12	86.04	109.05
36	R	617	NEX	C27-C28-C29	-5.12	117.59	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	y	307	CHL	C4A-NA-C1A	5.11	109.00	106.71
23	s	603	CLA	C4A-NA-C1A	5.11	109.00	106.71
37	y	301	XAT	O24-C25-C38	5.11	121.17	115.06
34	Y	302	CHL	C4A-NA-C1A	5.10	109.00	106.71
32	D	406	PL9	C41-C39-C38	-5.10	110.79	121.12
34	n	302	CHL	C1B-CHB-C4A	-5.10	120.02	130.12
23	c	511	CLA	CMB-C2B-C1B	-5.10	120.63	128.46
23	y	314	CLA	CMB-C2B-C3B	5.10	134.21	124.68
23	B	603	CLA	C4A-NA-C1A	5.10	109.00	106.71
32	D	406	PL9	C10-C9-C8	-5.09	110.61	123.68
23	B	606	CLA	C4A-NA-C1A	5.09	109.00	106.71
23	a	403	CLA	C4A-NA-C1A	5.08	108.99	106.71
23	A	401	CLA	O2D-CGD-O1D	-5.07	113.92	123.84
37	G	620	XAT	O4-C5-C18	5.07	121.13	115.06
23	g	603	CLA	C4A-NA-C1A	5.07	108.98	106.71
23	b	612	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
30	r	618	LHG	O7-C7-C8	5.05	122.39	111.50
32	D	406	PL9	C40-C39-C38	-5.05	110.73	123.68
23	c	501	CLA	C4A-NA-C1A	5.04	108.97	106.71
34	R	605	CHL	C4A-NA-C1A	5.03	108.97	106.71
37	y	301	XAT	C38-C25-C26	-5.02	113.85	122.26
23	b	607	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
23	B	607	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
36	n	318	NEX	C35-C34-C33	-4.99	120.19	127.31
23	B	615	CLA	C4A-NA-C1A	4.99	108.95	106.71
23	B	608	CLA	CMB-C2B-C3B	4.99	134.01	124.68
36	y	317	NEX	C19-C9-C10	-4.98	115.95	122.92
23	b	615	CLA	C4A-NA-C1A	4.98	108.94	106.71
37	R	616	XAT	C38-C25-C26	-4.97	113.92	122.26
23	b	610	CLA	CMB-C2B-C3B	4.97	133.98	124.68
23	B	612	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
36	S	616	NEX	C11-C10-C9	-4.96	120.23	127.31
32	d	407	PL9	C10-C9-C8	-4.96	110.96	123.68
25	k	101	BCR	C7-C8-C9	-4.95	118.75	126.23
36	g	617	NEX	C11-C10-C9	-4.94	120.27	127.31
37	Y	301	XAT	C38-C25-C26	-4.93	114.00	122.26
36	N	318	NEX	C38-C25-C26	-4.93	114.01	122.26
37	r	616	XAT	C38-C25-C26	-4.92	114.02	122.26
23	Y	310	CLA	CMB-C2B-C1B	-4.91	120.91	128.46
34	N	309	CHL	C4A-NA-C1A	4.91	108.91	106.71
23	g	610	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
37	R	616	XAT	C26-C27-C28	-4.91	115.62	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	617	NEX	C15-C14-C13	-4.90	120.32	127.31
23	R	614	CLA	C4A-NA-C1A	4.88	108.90	106.71
23	n	305	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
23	r	602	CLA	C4A-NA-C1A	4.87	108.90	106.71
23	y	310	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
25	K	101	BCR	C16-C17-C18	-4.86	120.37	127.31
23	b	603	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
34	y	308	CHL	C4A-NA-C1A	4.86	108.89	106.71
23	B	602	CLA	C4A-NA-C1A	4.86	108.89	106.71
23	B	603	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
23	B	610	CLA	CMB-C2B-C1B	-4.84	121.03	128.46
34	G	605	CHL	C4A-NA-C1A	4.83	108.88	106.71
23	B	616	CLA	C4A-NA-C1A	4.83	108.88	106.71
28	d	410	DGD	O2G-C1B-C2B	4.82	121.89	111.50
23	d	404	CLA	CMB-C2B-C1B	-4.81	121.06	128.46
23	G	613	CLA	CMB-C2B-C1B	-4.81	121.08	128.46
36	n	318	NEX	C38-C25-C26	-4.80	114.22	122.26
23	g	610	CLA	C4A-NA-C1A	4.79	108.86	106.71
23	S	610	CLA	C4A-NA-C1A	4.79	108.86	106.71
34	S	606	CHL	C1B-CHB-C4A	-4.78	120.65	130.12
36	r	617	NEX	C15-C14-C13	-4.78	120.49	127.31
34	g	607	CHL	C1B-CHB-C4A	-4.77	120.67	130.12
23	g	612	CLA	C4A-NA-C1A	4.77	108.85	106.71
23	b	613	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
32	D	406	PL9	C47-C48-C49	-4.76	111.48	127.75
23	y	312	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
36	S	616	NEX	C15-C14-C13	-4.75	120.53	127.31
36	N	318	NEX	C35-C34-C33	-4.75	120.54	127.31
36	Y	317	NEX	C38-C25-C26	-4.74	114.31	122.26
23	Y	312	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
23	n	303	CLA	C4A-NA-C1A	4.74	108.84	106.71
28	a	408	DGD	O2G-C1B-C2B	4.74	121.72	111.50
23	b	602	CLA	C4A-NA-C1A	4.74	108.84	106.71
23	C	512	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
23	b	614	CLA	CMB-C2B-C1B	-4.72	121.20	128.46
23	b	606	CLA	C4A-NA-C1A	4.72	108.83	106.71
37	N	301	XAT	C18-C5-C6	-4.70	114.38	122.26
23	S	608	CLA	C4A-NA-C1A	4.70	108.82	106.71
23	s	608	CLA	C4A-NA-C1A	4.70	108.82	106.71
34	G	601	CHL	C4A-NA-C1A	4.70	108.82	106.71
32	d	407	PL9	C30-C29-C28	-4.70	111.62	123.68
23	b	608	CLA	C4A-NA-C1A	4.70	108.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	4.70	108.82	106.71
25	C	516	BCR	C15-C14-C13	-4.69	120.61	127.31
25	H	101	BCR	C20-C21-C22	-4.69	120.61	127.31
23	C	509	CLA	CMB-C2B-C3B	4.69	133.44	124.68
36	s	616	NEX	C15-C14-C13	-4.68	120.63	127.31
23	C	511	CLA	CMB-C2B-C3B	4.68	133.43	124.68
28	A	408	DGD	O2G-C1B-C2B	4.67	121.58	111.50
34	g	605	CHL	C4A-NA-C1A	4.67	108.81	106.71
23	B	613	CLA	CMB-C2B-C1B	-4.67	121.28	128.46
23	B	614	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
25	c	515	BCR	C15-C14-C13	-4.66	120.66	127.31
23	G	610	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
23	n	304	CLA	C4A-NA-C1A	4.66	108.80	106.71
23	b	611	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
25	c	515	BCR	C3-C4-C5	-4.66	105.76	114.08
37	Y	301	XAT	C18-C5-C6	-4.66	114.46	122.26
23	b	603	CLA	C4A-NA-C1A	4.65	108.80	106.71
36	y	317	NEX	C38-C25-C26	-4.65	114.46	122.26
37	N	301	XAT	C38-C25-C26	-4.65	114.47	122.26
23	c	510	CLA	CMB-C2B-C3B	4.65	133.38	124.68
36	Y	317	NEX	C11-C10-C9	-4.64	120.68	127.31
34	g	606	CHL	C4A-NA-C1A	4.64	108.79	106.71
25	Z	101	BCR	C3-C4-C5	-4.64	105.80	114.08
23	y	304	CLA	C4A-NA-C1A	4.64	108.79	106.71
23	B	611	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
32	D	406	PL9	C25-C24-C23	-4.63	111.81	123.68
36	y	317	NEX	C15-C14-C13	-4.63	120.71	127.31
23	y	314	CLA	C4A-NA-C1A	4.62	108.78	106.71
37	r	616	XAT	C26-C27-C28	-4.61	116.24	125.99
23	c	508	CLA	CMB-C2B-C3B	4.61	133.30	124.68
23	D	404	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
25	H	101	BCR	C24-C23-C22	-4.60	119.28	126.23
30	G	618	LHG	O7-C7-C8	4.59	121.40	111.50
25	B	619	BCR	C33-C5-C6	-4.59	119.37	124.53
32	D	406	PL9	C30-C29-C28	-4.59	111.91	123.68
23	A	404	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
23	b	608	CLA	CMB-C2B-C3B	4.58	133.25	124.68
23	g	613	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
30	w	201	LHG	O7-C7-C8	4.56	121.32	111.50
34	R	607	CHL	CMB-C2B-C1B	-4.55	121.47	128.46
36	G	617	NEX	C15-C14-C13	-4.54	120.82	127.31
36	S	616	NEX	C27-C28-C29	-4.54	118.48	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	N	306	CHL	CMB-C2B-C1B	-4.54	121.48	128.46
23	C	506	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
34	N	310	CHL	CMB-C2B-C3B	4.52	133.13	124.68
34	s	601	CHL	CMB-C2B-C1B	-4.52	121.52	128.46
34	r	613	CHL	C4A-NA-C1A	4.52	108.74	106.71
23	C	506	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
34	r	607	CHL	CMB-C2B-C1B	-4.51	121.54	128.46
23	R	608	CLA	C4A-NA-C1A	4.51	108.73	106.71
23	b	616	CLA	C4A-NA-C1A	4.51	108.73	106.71
37	r	616	XAT	C6-C7-C8	-4.50	116.47	125.99
23	b	612	CLA	CMB-C2B-C3B	4.50	133.10	124.68
32	d	407	PL9	C26-C24-C23	-4.50	112.01	121.12
32	d	407	PL9	C47-C48-C49	-4.50	112.37	127.75
34	Y	308	CHL	C4A-NA-C1A	4.50	108.73	106.71
23	G	613	CLA	CMB-C2B-C3B	4.49	133.09	124.68
32	d	407	PL9	C21-C19-C18	-4.49	112.03	121.12
30	R	618	LHG	O7-C7-C8	4.49	121.18	111.50
23	a	401	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
34	s	601	CHL	C1B-CHB-C4A	-4.48	121.24	130.12
23	R	609	CLA	C4A-NA-C1A	4.48	108.72	106.71
32	d	407	PL9	C45-C44-C46	-4.48	107.73	115.27
23	c	505	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
36	g	617	NEX	C35-C34-C33	-4.48	120.92	127.31
37	n	301	XAT	C18-C5-C6	-4.46	114.78	122.26
32	D	406	PL9	C26-C24-C23	-4.46	112.09	121.12
34	N	302	CHL	C1B-CHB-C4A	-4.46	121.29	130.12
30	g	618	LHG	O7-C7-C8	4.45	121.10	111.50
37	g	620	XAT	C38-C25-C26	-4.45	114.80	122.26
24	d	401	PHO	CMB-C2B-C3B	4.45	133.01	124.68
34	n	306	CHL	CMB-C2B-C1B	-4.45	121.62	128.46
23	B	612	CLA	CMB-C2B-C3B	4.45	133.01	124.68
23	c	512	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
23	n	311	CLA	CMB-C2B-C3B	4.45	133.00	124.68
36	g	617	NEX	C15-C14-C13	-4.45	120.96	127.31
25	c	514	BCR	C33-C5-C6	-4.45	119.53	124.53
32	D	406	PL9	C21-C19-C18	-4.44	112.13	121.12
34	y	307	CHL	CMB-C2B-C1B	-4.43	121.65	128.46
35	G	615	LUT	C35-C15-C14	-4.43	114.40	123.47
23	B	610	CLA	CMB-C2B-C3B	4.43	132.96	124.68
32	D	406	PL9	C31-C29-C28	-4.42	112.16	121.12
24	D	402	PHO	CMB-C2B-C3B	4.42	132.95	124.68
23	r	601	CLA	CAC-C3C-C4C	4.42	130.54	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C7-C8-C9	-4.41	119.57	126.23
37	y	301	XAT	C18-C5-C6	-4.41	114.87	122.26
34	N	310	CHL	C1B-CHB-C4A	-4.41	121.39	130.12
23	C	512	CLA	CMB-C2B-C3B	4.41	132.92	124.68
25	h	101	BCR	C20-C21-C22	-4.41	121.02	127.31
23	Y	313	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
23	c	513	CLA	C4A-NA-C1A	4.40	108.68	106.71
23	y	310	CLA	C1B-CHB-C4A	-4.39	121.42	130.12
36	r	617	NEX	C11-C10-C9	-4.39	121.05	127.31
34	s	607	CHL	CMB-C2B-C1B	-4.39	121.72	128.46
23	c	505	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
23	g	610	CLA	CMB-C2B-C3B	4.38	132.88	124.68
35	g	615	LUT	C35-C15-C14	-4.38	114.50	123.47
23	y	313	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
37	n	301	XAT	C38-C25-C26	-4.38	114.92	122.26
23	a	402	CLA	C1B-CHB-C4A	-4.38	121.45	130.12
23	s	613	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
35	N	316	LUT	C35-C34-C33	-4.36	121.09	127.31
23	Y	305	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
25	b	619	BCR	C33-C5-C6	-4.36	119.64	124.53
32	d	407	PL9	C25-C24-C23	-4.35	112.51	123.68
37	y	301	XAT	C31-C30-C29	-4.35	121.10	127.31
23	c	511	CLA	C4A-NA-C1A	4.34	108.66	106.71
23	S	602	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
23	C	514	CLA	C4A-NA-C1A	4.34	108.66	106.71
25	b	617	BCR	C24-C23-C22	-4.33	119.69	126.23
25	C	516	BCR	C3-C4-C5	-4.33	106.34	114.08
23	g	613	CLA	CMB-C2B-C3B	4.32	132.77	124.68
34	s	605	CHL	C4A-NA-C1A	4.32	108.65	106.71
35	n	316	LUT	C35-C34-C33	-4.31	121.16	127.31
36	Y	317	NEX	C35-C34-C33	-4.31	121.16	127.31
25	B	617	BCR	C24-C23-C22	-4.31	119.73	126.23
25	B	618	BCR	C15-C14-C13	-4.30	121.17	127.31
37	G	620	XAT	C6-C7-C8	-4.30	116.91	125.99
37	n	301	XAT	C11-C10-C9	-4.29	121.18	127.31
30	n	319	LHG	O7-C7-C8	4.29	120.75	111.50
23	C	513	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
37	r	616	XAT	C18-C5-C6	-4.29	115.07	122.26
34	n	307	CHL	CMB-C2B-C1B	-4.29	121.88	128.46
25	b	618	BCR	C15-C14-C13	-4.29	121.19	127.31
35	S	615	LUT	C35-C34-C33	-4.29	121.19	127.31
25	b	617	BCR	C11-C10-C9	-4.28	121.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	407	PL9	C31-C29-C28	-4.28	112.46	121.12
34	r	606	CHL	CMB-C2B-C1B	-4.28	121.89	128.46
25	c	514	BCR	C24-C23-C22	-4.27	119.78	126.23
23	D	401	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
34	S	605	CHL	C1B-CHB-C4A	-4.27	121.67	130.12
34	n	310	CHL	C1B-CHB-C4A	-4.26	121.67	130.12
34	g	609	CHL	CHD-C1D-ND	-4.26	120.54	124.45
23	y	305	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
34	n	302	CHL	CMB-C2B-C1B	-4.25	121.93	128.46
25	K	101	BCR	C16-C15-C14	-4.25	114.77	123.47
34	G	606	CHL	C4A-NA-C1A	4.25	108.62	106.71
36	G	617	NEX	C35-C34-C33	-4.24	121.25	127.31
23	a	405	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
36	G	617	NEX	C31-C30-C29	-4.24	121.25	127.31
23	s	602	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
25	B	618	BCR	C3-C4-C5	-4.24	106.51	114.08
36	N	318	NEX	C15-C14-C13	-4.23	121.27	127.31
37	R	616	XAT	C18-C5-C6	-4.23	115.17	122.26
25	c	518	BCR	C16-C17-C18	-4.23	121.27	127.31
23	c	511	CLA	CMB-C2B-C3B	4.23	132.59	124.68
23	G	603	CLA	C4A-NA-C1A	4.22	108.61	106.71
25	B	617	BCR	C11-C10-C9	-4.22	121.29	127.31
23	N	314	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
34	S	605	CHL	C4A-NA-C1A	4.22	108.60	106.71
23	C	510	CLA	O2D-CGD-CBD	4.21	118.74	111.27
23	r	611	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
34	G	601	CHL	C2D-C1D-ND	-4.20	107.01	110.10
23	n	304	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
23	r	614	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
25	A	405	BCR	C7-C8-C9	-4.19	119.90	126.23
23	N	312	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
23	C	507	CLA	CMB-C2B-C3B	4.18	132.51	124.68
30	a	412	LHG	O7-C7-C8	4.18	120.52	111.50
23	c	509	CLA	C4A-NA-C1A	4.18	108.58	106.71
30	N	319	LHG	O7-C7-C8	4.18	120.51	111.50
36	N	318	NEX	C39-C29-C30	-4.18	117.07	122.92
23	R	604	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
36	R	617	NEX	C38-C25-C26	-4.17	115.27	122.26
23	y	310	CLA	CMB-C2B-C3B	4.17	132.47	124.68
37	g	620	XAT	C6-C7-C8	-4.17	117.19	125.99
23	a	401	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
23	Y	310	CLA	CMB-C2B-C3B	4.16	132.47	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
34	Y	307	CHL	CMB-C2B-C1B	-4.16	122.07	128.46
25	h	101	BCR	C24-C23-C22	-4.16	119.95	126.23
23	Y	312	CLA	CMB-C2B-C3B	4.16	132.46	124.68
23	A	401	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
23	b	609	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
37	Y	301	XAT	C31-C30-C29	-4.16	121.37	127.31
34	R	606	CHL	CMB-C2B-C1B	-4.15	122.08	128.46
25	B	619	BCR	C28-C27-C26	-4.15	106.66	114.08
23	A	404	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
23	G	610	CLA	CMB-C2B-C3B	4.15	132.44	124.68
23	b	607	CLA	CMB-C2B-C3B	4.15	132.44	124.68
34	s	606	CHL	C1B-CHB-C4A	-4.15	121.91	130.12
36	r	617	NEX	C31-C30-C29	-4.15	121.39	127.31
25	d	406	BCR	C7-C8-C9	-4.14	119.98	126.23
23	B	603	CLA	CMB-C2B-C3B	4.14	132.42	124.68
35	s	615	LUT	C35-C34-C33	-4.13	121.41	127.31
34	S	601	CHL	C1B-CHB-C4A	-4.13	121.93	130.12
25	b	617	BCR	C15-C14-C13	-4.13	121.41	127.31
28	c	516	DGD	O2G-C1B-C2B	4.13	120.40	111.50
23	B	607	CLA	CMB-C2B-C3B	4.13	132.40	124.68
23	r	612	CLA	CMB-C2B-C1B	-4.12	122.12	128.46
23	N	304	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
23	y	312	CLA	CMB-C2B-C3B	4.12	132.39	124.68
23	s	611	CLA	C4A-NA-C1A	4.12	108.56	106.71
25	d	406	BCR	C11-C10-C9	-4.12	121.43	127.31
36	N	318	NEX	C11-C10-C9	-4.11	121.45	127.31
23	s	602	CLA	C4A-NA-C1A	4.11	108.55	106.71
23	N	305	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
32	D	406	PL9	C50-C49-C48	-4.11	110.78	122.65
23	n	313	CLA	CAA-C2A-C3A	-4.10	101.54	112.78
34	R	607	CHL	C4A-NA-C1A	4.10	108.55	106.71
23	Y	310	CLA	C1B-CHB-C4A	-4.10	122.00	130.12
23	N	313	CLA	CAA-C2A-C3A	-4.10	101.56	112.78
25	c	518	BCR	C15-C14-C13	-4.10	121.46	127.31
34	G	609	CHL	CHD-C1D-ND	-4.09	120.69	124.45
23	n	314	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
23	S	604	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
36	R	617	NEX	C17-C1-C6	-4.08	106.82	110.47
23	R	611	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
34	R	605	CHL	CMB-C2B-C1B	-4.07	122.20	128.46
34	G	619	CHL	CMB-C2B-C1B	-4.07	122.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CMB-C2B-C3B	4.07	132.30	124.68
30	B	623	LHG	O7-C7-C8	4.07	120.28	111.50
23	R	601	CLA	C4A-NA-C1A	4.07	108.54	106.71
25	b	619	BCR	C28-C27-C26	-4.07	106.82	114.08
30	T	101	LHG	O7-C7-C8	4.06	120.26	111.50
34	Y	306	CHL	O2D-CGD-O1D	-4.05	115.92	123.84
30	Y	318	LHG	O7-C7-C8	4.05	120.22	111.50
23	S	602	CLA	C4A-NA-C1A	4.04	108.52	106.71
36	S	616	NEX	C38-C25-C26	-4.04	115.48	122.26
26	a	409	SQD	O47-C7-C8	4.04	120.21	111.50
32	d	407	PL9	C50-C49-C48	-4.04	110.97	122.65
25	b	618	BCR	C3-C4-C5	-4.04	106.86	114.08
30	W	201	LHG	O7-C7-C8	4.04	120.20	111.50
23	b	613	CLA	CMB-C2B-C3B	4.04	132.23	124.68
35	R	615	LUT	C15-C14-C13	-4.04	121.55	127.31
32	D	406	PL9	C51-C49-C48	-4.04	110.98	122.65
23	R	609	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
23	a	405	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
23	c	512	CLA	C4A-NA-C1A	4.03	108.52	106.71
23	s	603	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
25	B	617	BCR	C15-C14-C13	-4.03	121.56	127.31
23	s	609	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
23	A	404	CLA	CMB-C2B-C3B	4.03	132.21	124.68
23	R	614	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
30	B	621	LHG	O7-C7-C8	4.02	120.17	111.50
23	B	602	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
36	y	317	NEX	C27-C28-C29	-4.01	119.31	125.53
34	N	307	CHL	C4A-NA-C1A	4.01	108.51	106.71
32	d	407	PL9	C51-C49-C48	-4.01	111.06	122.65
34	g	619	CHL	CMB-C2B-C1B	-4.01	122.31	128.46
23	C	505	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
36	r	617	NEX	C38-C25-C26	-4.01	115.55	122.26
26	A	409	SQD	O47-C7-C8	4.01	120.13	111.50
23	r	608	CLA	C1B-CHB-C4A	-4.00	122.19	130.12
26	A	406	SQD	O47-C7-C8	4.00	120.12	111.50
25	c	514	BCR	C7-C8-C9	-4.00	120.20	126.23
37	y	301	XAT	C15-C14-C13	-4.00	121.61	127.31
37	G	620	XAT	C38-C25-C26	-3.99	115.57	122.26
23	B	601	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
30	b	621	LHG	O7-C7-C8	3.98	120.09	111.50
37	r	616	XAT	O24-C25-C38	3.98	119.83	115.06
25	a	406	BCR	C7-C8-C9	-3.98	120.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	y	318	LHG	O7-C7-C8	3.98	120.07	111.50
23	B	616	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	h	101	BCR	C16-C17-C18	-3.97	121.64	127.31
25	B	619	BCR	C1-C6-C5	-3.97	117.02	122.61
23	c	509	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
36	s	616	NEX	C27-C28-C29	-3.97	119.38	125.53
27	D	407	LMG	O7-C10-C11	3.96	120.05	111.50
25	C	515	BCR	C16-C17-C18	-3.96	121.65	127.31
23	c	506	CLA	CMB-C2B-C3B	3.96	132.09	124.68
36	Y	317	NEX	C15-C14-C13	-3.96	121.66	127.31
36	s	616	NEX	C38-C25-C26	-3.96	115.63	122.26
36	r	617	NEX	C17-C1-C6	-3.95	106.94	110.47
25	c	518	BCR	C28-C27-C26	-3.95	107.02	114.08
36	R	617	NEX	C2-C1-C6	3.95	113.05	109.21
23	b	614	CLA	CMB-C2B-C3B	3.95	132.06	124.68
37	N	301	XAT	C11-C10-C9	-3.94	121.69	127.31
30	a	411	LHG	O7-C7-C8	3.94	119.99	111.50
34	n	309	CHL	OMC-CMC-C2C	-3.94	116.79	125.69
23	s	609	CLA	C4A-NA-C1A	3.93	108.47	106.71
23	b	601	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
23	C	506	CLA	O2A-C1-C2	3.93	118.97	108.64
34	S	607	CHL	C1B-CHB-C4A	-3.93	122.33	130.12
34	S	601	CHL	CMB-C2B-C1B	-3.93	122.42	128.46
35	Y	315	LUT	C35-C34-C33	-3.93	121.70	127.31
35	r	615	LUT	C35-C34-C33	-3.93	121.71	127.31
23	B	613	CLA	CMB-C2B-C3B	3.93	132.02	124.68
23	r	604	CLA	O2D-CGD-CBD	3.93	118.24	111.27
23	b	602	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
23	Y	314	CLA	C4A-NA-C1A	3.92	108.47	106.71
27	A	407	LMG	O7-C10-C11	3.92	119.95	111.50
34	G	609	CHL	C2D-C1D-ND	-3.92	107.22	110.10
30	S	617	LHG	O7-C7-C8	3.91	119.94	111.50
23	c	501	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
37	R	616	XAT	C6-C7-C8	-3.91	117.72	125.99
23	s	613	CLA	C1B-CHB-C4A	-3.91	122.37	130.12
23	d	404	CLA	CMB-C2B-C3B	3.91	131.99	124.68
34	g	601	CHL	C1B-CHB-C4A	-3.91	122.38	130.12
23	a	402	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
34	s	606	CHL	CAA-C2A-C3A	-3.91	104.50	114.26
23	n	305	CLA	CMB-C2B-C3B	3.91	131.99	124.68
25	C	515	BCR	C33-C5-C6	-3.90	120.14	124.53
34	n	306	CHL	C4A-NA-C1A	3.90	108.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CAA-C2A-C3A	-3.90	102.09	112.78
32	d	407	PL9	C10-C9-C11	-3.90	108.71	115.27
34	s	601	CHL	CMB-C2B-C3B	3.90	131.98	124.68
23	Y	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	s	604	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	Y	314	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
37	y	301	XAT	C26-C27-C28	-3.89	117.77	125.99
23	S	603	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
23	B	614	CLA	CMB-C2B-C3B	3.89	131.95	124.68
25	Z	101	BCR	C24-C23-C22	-3.89	120.36	126.23
23	C	502	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
23	N	311	CLA	C4A-NA-C1A	3.88	108.45	106.71
36	y	317	NEX	C35-C34-C33	-3.88	121.77	127.31
23	b	614	CLA	CAA-C2A-C3A	-3.88	102.15	112.78
27	a	407	LMG	C7-O1-C1	-3.88	106.16	113.74
36	G	617	NEX	C17-C1-C6	-3.88	107.00	110.47
37	R	616	XAT	O24-C25-C38	3.87	119.70	115.06
23	R	611	CLA	C4A-NA-C1A	3.87	108.45	106.71
27	B	622	LMG	O7-C10-C11	3.87	119.84	111.50
25	b	619	BCR	C1-C6-C5	-3.87	117.17	122.61
37	Y	301	XAT	O4-C5-C18	3.86	119.69	115.06
36	g	617	NEX	C27-C28-C29	-3.86	119.53	125.53
34	G	608	CHL	C4A-NA-C1A	3.86	108.44	106.71
23	R	608	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
23	N	314	CLA	CMB-C2B-C3B	3.86	131.90	124.68
23	S	613	CLA	C1B-CHB-C4A	-3.86	122.47	130.12
35	G	616	LUT	C15-C14-C13	-3.86	121.80	127.31
23	C	506	CLA	CMB-C2B-C3B	3.86	131.90	124.68
30	A	411	LHG	O7-C7-C8	3.86	119.81	111.50
23	c	502	CLA	CAA-CBA-CGA	-3.86	101.98	113.25
37	Y	301	XAT	C26-C27-C28	-3.85	117.84	125.99
23	S	602	CLA	CMB-C2B-C3B	3.85	131.89	124.68
23	G	603	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
23	n	305	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
23	r	611	CLA	C4A-NA-C1A	3.84	108.43	106.71
34	G	607	CHL	CMB-C2B-C1B	-3.84	122.56	128.46
25	Z	101	BCR	C28-C27-C26	-3.84	107.22	114.08
31	d	403	BCT	O2-C-O1	3.83	129.48	119.55
36	n	318	NEX	O24-C25-C38	3.82	119.64	115.06
34	y	302	CHL	CMB-C2B-C1B	-3.82	122.59	128.46
23	N	305	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
34	n	302	CHL	CMB-C2B-C3B	3.81	131.81	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C16-C17-C18	-3.81	121.88	127.31
30	s	617	LHG	O7-C7-C8	3.80	119.70	111.50
23	r	609	CLA	C4A-NA-C1A	3.80	108.42	106.71
36	Y	317	NEX	O24-C25-C38	3.80	119.61	115.06
32	D	406	PL9	C10-C9-C11	-3.80	108.88	115.27
35	r	615	LUT	C31-C30-C29	-3.80	121.89	127.31
23	s	602	CLA	CMB-C2B-C3B	3.79	131.78	124.68
23	s	604	CLA	CMB-C2B-C3B	3.79	131.78	124.68
25	F	101	BCR	C11-C10-C9	-3.79	121.90	127.31
23	n	312	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
23	C	513	CLA	C4A-NA-C1A	3.79	108.41	106.71
23	b	606	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
27	d	409	LMG	O7-C10-C11	3.79	119.66	111.50
25	B	619	BCR	C11-C10-C9	-3.78	121.91	127.31
36	R	617	NEX	C31-C30-C29	-3.78	121.92	127.31
34	G	619	CHL	C1B-CHB-C4A	-3.78	122.64	130.12
34	N	302	CHL	C4A-NA-C1A	3.78	108.40	106.71
23	S	604	CLA	CMB-C2B-C3B	3.78	131.74	124.68
23	r	604	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
34	S	606	CHL	CAA-C2A-C3A	-3.77	104.83	114.26
23	B	606	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	r	604	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
23	Y	304	CLA	CAA-C2A-C3A	-3.76	102.47	112.78
23	y	313	CLA	CMB-C2B-C3B	3.76	131.72	124.68
23	S	610	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
34	S	606	CHL	CMB-C2B-C1B	-3.76	122.68	128.46
23	S	608	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
37	r	616	XAT	C15-C35-C34	-3.76	115.77	123.47
34	G	607	CHL	C1B-CHB-C4A	-3.76	122.67	130.12
35	G	615	LUT	C10-C11-C12	-3.76	111.49	123.22
23	D	404	CLA	CMB-C2B-C3B	3.76	131.71	124.68
23	a	405	CLA	CMB-C2B-C3B	3.75	131.70	124.68
25	k	101	BCR	C16-C15-C14	-3.75	115.78	123.47
23	b	611	CLA	CMB-C2B-C3B	3.75	131.69	124.68
34	R	606	CHL	C4A-NA-C1A	3.75	108.39	106.71
23	B	611	CLA	CMB-C2B-C3B	3.74	131.68	124.68
25	b	617	BCR	C7-C8-C9	-3.74	120.58	126.23
36	N	318	NEX	C2-C1-C6	3.74	112.85	109.21
34	r	607	CHL	CMB-C2B-C3B	3.74	131.68	124.68
30	A	412	LHG	O7-C7-C8	3.74	119.56	111.50
23	R	609	CLA	CMB-C2B-C3B	3.74	131.67	124.68
36	G	617	NEX	C2-C1-C6	3.74	112.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	615	LUT	C31-C30-C29	-3.74	121.97	127.31
23	n	314	CLA	CMB-C2B-C3B	3.74	131.67	124.68
23	N	303	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	y	314	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
34	g	601	CHL	OMC-CMC-C2C	-3.74	117.24	125.69
35	y	316	LUT	C15-C14-C13	-3.73	121.98	127.31
31	D	403	BCT	O2-C-O1	3.73	129.23	119.55
37	N	301	XAT	O4-C5-C18	3.73	119.53	115.06
25	A	405	BCR	C16-C17-C18	-3.73	121.99	127.31
34	S	607	CHL	CMB-C2B-C1B	-3.73	122.73	128.46
35	n	316	LUT	C31-C30-C29	-3.72	122.00	127.31
36	g	617	NEX	C38-C25-C26	-3.72	116.02	122.26
36	N	318	NEX	O24-C25-C38	3.72	119.51	115.06
34	R	607	CHL	CMB-C2B-C3B	3.72	131.63	124.68
34	Y	302	CHL	CMB-C2B-C1B	-3.72	122.75	128.46
34	Y	306	CHL	CMB-C2B-C1B	-3.72	122.75	128.46
37	Y	301	XAT	C15-C14-C13	-3.72	122.01	127.31
25	d	406	BCR	C3-C4-C5	-3.71	107.44	114.08
23	c	505	CLA	CMB-C2B-C3B	3.71	131.63	124.68
30	c	517	LHG	O7-C7-C8	3.71	119.50	111.50
25	B	617	BCR	C7-C8-C9	-3.71	120.62	126.23
23	b	605	CLA	O2D-CGD-CBD	3.71	117.86	111.27
23	Y	313	CLA	CMB-C2B-C3B	3.71	131.61	124.68
34	r	606	CHL	CMB-C2B-C3B	3.70	131.61	124.68
36	g	617	NEX	C31-C30-C29	-3.70	122.02	127.31
36	n	318	NEX	C11-C10-C9	-3.70	122.03	127.31
23	c	512	CLA	CMB-C2B-C3B	3.70	131.59	124.68
23	a	401	CLA	CMB-C2B-C3B	3.69	131.59	124.68
34	n	310	CHL	CMB-C2B-C3B	3.69	131.58	124.68
36	y	317	NEX	O24-C25-C38	3.69	119.48	115.06
25	b	618	BCR	C16-C17-C18	-3.69	122.05	127.31
35	s	615	LUT	C15-C14-C13	-3.69	122.05	127.31
23	A	401	CLA	CMB-C2B-C3B	3.68	131.57	124.68
34	s	606	CHL	CMB-C2B-C1B	-3.68	122.81	128.46
34	R	613	CHL	C1B-CHB-C4A	-3.68	122.83	130.12
36	n	318	NEX	C15-C14-C13	-3.68	122.06	127.31
23	C	502	CLA	C4A-NA-C1A	3.68	108.36	106.71
25	a	406	BCR	C16-C17-C18	-3.68	122.06	127.31
25	a	406	BCR	C15-C14-C13	-3.67	122.07	127.31
25	b	619	BCR	C11-C10-C9	-3.67	122.07	127.31
35	n	316	LUT	C11-C10-C9	-3.66	122.08	127.31
23	n	315	CLA	CMB-C2B-C1B	-3.66	122.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	n	318	NEX	C39-C29-C30	-3.66	117.80	122.92
36	S	616	NEX	C39-C29-C30	-3.65	117.80	122.92
34	g	609	CHL	CMB-C2B-C1B	-3.65	122.85	128.46
23	r	608	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
36	N	318	NEX	C24-C23-C22	-3.65	103.72	110.77
23	r	612	CLA	CMB-C2B-C3B	3.65	131.50	124.68
35	s	614	LUT	C35-C34-C33	-3.65	122.11	127.31
35	G	615	LUT	C35-C34-C33	-3.64	122.11	127.31
23	N	304	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
34	N	306	CHL	CMB-C2B-C3B	3.64	131.50	124.68
23	N	315	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
27	C	501	LMG	O7-C10-C11	3.64	119.34	111.50
23	G	604	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
36	Y	317	NEX	C27-C28-C29	-3.63	119.89	125.53
25	C	516	BCR	C16-C17-C18	-3.63	122.12	127.31
36	n	318	NEX	C24-C23-C22	-3.63	103.76	110.77
23	A	402	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
25	c	514	BCR	C16-C17-C18	-3.63	122.13	127.31
23	S	602	CLA	C1B-CHB-C4A	-3.63	122.93	130.12
30	w	201	LHG	C5-O7-C7	-3.63	108.86	117.79
23	D	401	CLA	CMB-C2B-C3B	3.63	131.47	124.68
23	r	601	CLA	C4A-NA-C1A	3.63	108.34	106.71
26	d	402	SQD	O47-C7-C8	3.63	119.31	111.50
25	b	617	BCR	C33-C5-C6	-3.62	120.46	124.53
37	N	301	XAT	O24-C25-C38	3.62	119.39	115.06
23	R	601	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
23	B	604	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
25	B	617	BCR	C33-C5-C6	-3.62	120.47	124.53
34	G	607	CHL	CMB-C2B-C3B	3.62	131.44	124.68
23	R	601	CLA	CAA-C2A-C3A	-3.61	102.89	112.78
34	r	613	CHL	C1B-CHB-C4A	-3.60	122.98	130.12
23	G	614	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
35	s	615	LUT	C35-C15-C14	-3.60	116.10	123.47
34	Y	308	CHL	CMB-C2B-C1B	-3.60	122.93	128.46
23	b	604	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	R	608	CLA	C1B-CHB-C4A	-3.60	122.99	130.12
23	g	604	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
23	s	604	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
23	r	611	CLA	CMB-C2B-C3B	3.59	131.40	124.68
23	N	314	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
34	S	606	CHL	C2A-C1A-CHA	3.59	130.14	123.86
35	y	315	LUT	C35-C34-C33	-3.59	122.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CHB-C4A-NA	3.59	129.48	124.51
37	R	616	XAT	C4-C3-C2	-3.59	103.84	110.77
25	c	518	BCR	C3-C4-C5	-3.59	107.67	114.08
34	n	306	CHL	CMB-C2B-C3B	3.58	131.38	124.68
23	B	615	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
34	g	605	CHL	CMB-C2B-C1B	-3.58	122.96	128.46
35	r	615	LUT	C15-C14-C13	-3.58	122.20	127.31
34	s	607	CHL	C1B-CHB-C4A	-3.58	123.03	130.12
34	G	601	CHL	OMC-CMC-C2C	-3.58	117.60	125.69
23	s	608	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
27	b	620	LMG	O7-C10-C11	3.57	119.20	111.50
23	C	513	CLA	CMB-C2B-C3B	3.57	131.36	124.68
27	B	620	LMG	O7-C10-C11	3.57	119.20	111.50
34	g	601	CHL	CMB-C2B-C1B	-3.57	122.97	128.46
23	c	507	CLA	CHB-C4A-NA	3.57	129.45	124.51
23	s	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
23	S	609	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
25	B	618	BCR	C16-C17-C18	-3.57	122.22	127.31
23	s	613	CLA	CMB-C2B-C3B	3.57	131.35	124.68
23	s	603	CLA	CMB-C2B-C3B	3.56	131.34	124.68
37	r	616	XAT	C4-C3-C2	-3.56	103.89	110.77
34	y	302	CHL	C1B-CHB-C4A	-3.56	123.06	130.12
23	G	613	CLA	C1B-CHB-C4A	-3.56	123.06	130.12
25	B	619	BCR	C15-C14-C13	-3.56	122.23	127.31
23	g	614	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	C	516	BCR	C11-C10-C9	-3.55	122.24	127.31
25	Z	101	BCR	C15-C14-C13	-3.55	122.24	127.31
23	g	613	CLA	C1B-CHB-C4A	-3.55	123.09	130.12
34	s	607	CHL	CMB-C2B-C3B	3.55	131.32	124.68
23	N	312	CLA	CMB-C2B-C3B	3.55	131.32	124.68
27	a	407	LMG	O7-C10-C11	3.55	119.15	111.50
25	c	514	BCR	C1-C6-C5	-3.55	117.61	122.61
25	b	619	BCR	C24-C23-C22	-3.55	120.88	126.23
34	G	608	CHL	CMB-C2B-C1B	-3.55	123.02	128.46
23	B	602	CLA	CMB-C2B-C3B	3.55	131.31	124.68
23	g	603	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	N	314	CLA	CHB-C4A-NA	3.54	129.41	124.51
23	n	303	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	S	612	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
34	g	607	CHL	CHD-C1D-ND	-3.54	121.20	124.45
34	n	309	CHL	CMB-C2B-C1B	-3.54	123.03	128.46
34	R	606	CHL	CMB-C2B-C3B	3.54	131.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C1B-CHB-C4A	-3.54	123.11	130.12
23	N	304	CLA	CMB-C2B-C3B	3.54	131.29	124.68
25	A	405	BCR	C15-C14-C13	-3.53	122.27	127.31
23	a	402	CLA	CHB-C4A-NA	3.53	129.40	124.51
36	G	617	NEX	C27-C28-C29	-3.53	120.05	125.53
23	G	610	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
36	y	317	NEX	C11-C12-C13	-3.53	116.50	126.42
23	S	609	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	r	609	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
23	S	609	CLA	C4A-NA-C1A	3.53	108.29	106.71
23	c	505	CLA	O2D-CGD-CBD	3.52	117.53	111.27
23	S	611	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
23	b	615	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
35	n	316	LUT	C10-C11-C12	-3.52	112.23	123.22
23	y	304	CLA	CAA-C2A-C3A	-3.52	103.14	112.78
23	a	403	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
25	c	518	BCR	C24-C23-C22	-3.52	120.92	126.23
25	F	101	BCR	C7-C8-C9	-3.51	120.92	126.23
23	D	401	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
23	s	611	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
34	y	307	CHL	CMB-C2B-C3B	3.51	131.24	124.68
27	a	407	LMG	O1-C1-C2	3.51	113.78	108.30
25	c	518	BCR	C11-C10-C9	-3.51	122.30	127.31
35	n	316	LUT	C7-C8-C9	-3.51	120.94	126.23
25	B	619	BCR	C24-C23-C22	-3.51	120.94	126.23
23	a	402	CLA	CMB-C2B-C3B	3.51	131.24	124.68
37	r	616	XAT	C10-C11-C12	-3.50	112.28	123.22
26	M	101	SQD	O47-C7-C8	3.50	119.05	111.50
23	c	507	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	C	515	BCR	C24-C23-C22	-3.50	120.94	126.23
23	G	603	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
36	r	617	NEX	C2-C1-C6	3.50	112.61	109.21
37	Y	301	XAT	C35-C34-C33	-3.50	122.31	127.31
23	B	608	CLA	C4A-NA-C1A	3.50	108.28	106.71
23	B	614	CLA	C4A-NA-C1A	3.50	108.28	106.71
23	r	610	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
35	N	316	LUT	C35-C15-C14	-3.50	116.30	123.47
23	n	311	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
26	L	103	SQD	O47-C7-C8	3.50	119.04	111.50
34	G	601	CHL	CMB-C2B-C1B	-3.50	123.09	128.46
34	S	601	CHL	OMC-CMC-C2C	-3.50	117.78	125.69
35	R	615	LUT	C35-C34-C33	-3.50	122.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	607	CHL	CBA-CAA-C2A	3.49	121.24	113.47
23	Y	314	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
36	n	318	NEX	C31-C30-C29	-3.49	122.33	127.31
34	N	308	CHL	CMB-C2B-C1B	-3.49	123.10	128.46
34	N	309	CHL	CMB-C2B-C1B	-3.49	123.10	128.46
23	s	602	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
30	L	101	LHG	O7-C7-C8	3.48	119.01	111.50
36	R	617	NEX	C15-C35-C34	-3.48	116.34	123.47
23	C	506	CLA	O2D-CGD-CBD	3.48	117.45	111.27
37	n	301	XAT	C6-C7-C8	-3.48	118.63	125.99
33	e	101	HEM	CMC-C2C-C3C	3.48	131.19	124.68
37	n	301	XAT	O4-C5-C18	3.48	119.22	115.06
23	y	303	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
23	b	602	CLA	CMB-C2B-C3B	3.47	131.18	124.68
34	N	309	CHL	OMC-CMC-C2C	-3.47	117.84	125.69
34	g	606	CHL	O2D-CGD-O1D	-3.47	117.05	123.84
23	y	314	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
25	b	619	BCR	C15-C14-C13	-3.47	122.36	127.31
23	S	611	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
30	L	102	LHG	O7-C7-C8	3.46	118.97	111.50
36	G	617	NEX	C38-C25-C26	-3.46	116.45	122.26
23	y	304	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	y	313	CLA	CHB-C4A-NA	3.46	129.30	124.51
23	N	313	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	S	611	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	Y	303	CLA	CMB-C2B-C3B	3.46	131.15	124.68
23	N	312	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
23	c	505	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
32	d	407	PL9	C30-C29-C31	-3.46	109.46	115.27
30	L	102	LHG	O8-C23-C24	3.45	122.75	111.91
34	R	613	CHL	CMB-C2B-C1B	-3.45	123.16	128.46
30	b	622	LHG	O7-C7-C8	3.45	118.94	111.50
23	B	605	CLA	CBC-CAC-C3C	-3.45	102.91	112.43
34	r	606	CHL	C4A-NA-C1A	3.45	108.26	106.71
34	s	607	CHL	O2D-CGD-O1D	-3.45	117.09	123.84
25	k	101	BCR	C11-C10-C9	-3.45	122.39	127.31
25	k	101	BCR	C33-C5-C6	-3.45	120.66	124.53
23	N	303	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	C	508	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
35	S	615	LUT	C15-C14-C13	-3.44	122.40	127.31
36	y	317	NEX	C39-C29-C30	-3.44	118.10	122.92
35	g	615	LUT	C10-C11-C12	-3.44	112.48	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	S	608	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
35	S	614	LUT	C35-C34-C33	-3.44	122.40	127.31
37	R	616	XAT	C35-C34-C33	-3.44	122.41	127.31
32	D	406	PL9	C30-C29-C31	-3.44	109.49	115.27
34	y	308	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
25	Z	101	BCR	C16-C17-C18	-3.43	122.41	127.31
34	y	306	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
25	K	101	BCR	C3-C4-C5	-3.43	107.95	114.08
25	c	515	BCR	C16-C17-C18	-3.43	122.42	127.31
23	s	609	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
34	Y	306	CHL	C1B-CHB-C4A	-3.43	123.33	130.12
23	n	304	CLA	CAA-C2A-C3A	-3.43	103.40	112.78
25	C	516	BCR	C7-C8-C9	-3.42	121.06	126.23
35	S	615	LUT	C35-C15-C14	-3.42	116.46	123.47
35	G	616	LUT	C15-C35-C34	-3.42	116.46	123.47
34	y	302	CHL	CMB-C2B-C3B	3.42	131.08	124.68
23	g	613	CLA	CHB-C4A-NA	3.42	129.24	124.51
23	s	611	CLA	CAA-C2A-C3A	-3.41	103.43	112.78
35	N	316	LUT	C7-C8-C9	-3.41	121.08	126.23
34	S	605	CHL	C2D-C1D-ND	-3.41	107.59	110.10
23	N	311	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
37	N	301	XAT	C26-C27-C28	-3.41	118.78	125.99
23	N	311	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
34	G	605	CHL	CMB-C2B-C1B	-3.41	123.22	128.46
35	r	615	LUT	C11-C10-C9	-3.41	122.44	127.31
23	R	604	CLA	CMB-C2B-C3B	3.41	131.06	124.68
23	s	608	CLA	C1B-CHB-C4A	-3.41	123.37	130.12
27	C	501	LMG	O1-C1-C2	3.41	113.62	108.30
23	g	612	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
23	S	608	CLA	CMB-C2B-C3B	3.41	131.05	124.68
23	G	602	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
35	g	615	LUT	C35-C34-C33	-3.40	122.45	127.31
37	R	616	XAT	C10-C11-C12	-3.40	112.60	123.22
34	g	619	CHL	C1B-CHB-C4A	-3.40	123.38	130.12
37	n	301	XAT	O24-C25-C38	3.40	119.13	115.06
28	C	517	DGD	O2G-C1B-C2B	3.40	118.83	111.50
23	n	314	CLA	CHB-C4A-NA	3.40	129.21	124.51
23	y	313	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
25	c	514	BCR	C33-C5-C4	3.39	120.14	113.62
23	g	602	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	R	612	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
34	Y	302	CHL	CMB-C2B-C3B	3.39	131.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	S	611	CLA	C4A-NA-C1A	3.39	108.23	106.71
34	g	606	CHL	C1B-CHB-C4A	-3.39	123.41	130.12
34	g	619	CHL	CMB-C2B-C3B	3.38	131.01	124.68
23	R	603	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
23	r	601	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
33	E	101	HEM	CMC-C2C-C3C	3.38	131.01	124.68
30	d	408	LHG	O7-C7-C8	3.38	118.79	111.50
37	g	620	XAT	C15-C14-C13	-3.38	122.48	127.31
23	n	304	CLA	CMB-C2B-C3B	3.38	131.00	124.68
34	n	307	CHL	CHD-C1D-ND	-3.38	121.35	124.45
35	N	317	LUT	C38-C25-C24	-3.38	116.33	123.56
34	r	613	CHL	CMB-C2B-C1B	-3.38	123.27	128.46
23	S	603	CLA	CMB-C2B-C3B	3.38	131.00	124.68
34	R	605	CHL	CMB-C2B-C3B	3.38	131.00	124.68
23	B	601	CLA	CMB-C2B-C3B	3.38	130.99	124.68
23	N	311	CLA	CMB-C2B-C3B	3.38	130.99	124.68
23	S	610	CLA	CMB-C2B-C3B	3.38	130.99	124.68
37	N	301	XAT	C15-C14-C13	-3.37	122.50	127.31
25	H	101	BCR	C10-C11-C12	-3.37	112.69	123.22
34	y	302	CHL	OMC-CMC-C2C	-3.37	118.06	125.69
23	B	608	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	S	609	CLA	O2D-CGD-CBD	3.37	117.26	111.27
23	s	609	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
23	n	303	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
23	S	612	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
23	N	314	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
34	y	306	CHL	C1B-CHB-C4A	-3.36	123.45	130.12
37	G	620	XAT	C15-C14-C13	-3.36	122.51	127.31
34	N	306	CHL	C4A-NA-C1A	3.36	108.22	106.71
23	R	611	CLA	CMB-C2B-C3B	3.36	130.97	124.68
34	g	601	CHL	C3C-C4C-NC	-3.36	106.80	110.57
25	c	514	BCR	C11-C10-C9	-3.36	122.52	127.31
23	D	405	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
34	r	606	CHL	C1B-CHB-C4A	-3.36	123.47	130.12
34	s	605	CHL	CMB-C2B-C1B	-3.36	123.30	128.46
25	c	515	BCR	C11-C10-C9	-3.36	122.52	127.31
34	G	619	CHL	CMB-C2B-C3B	3.36	130.96	124.68
34	r	605	CHL	C1B-CHB-C4A	-3.35	123.48	130.12
23	Y	313	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
34	S	601	CHL	CMB-C2B-C3B	3.35	130.95	124.68
23	c	509	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	s	610	CLA	CMB-C2B-C1B	-3.35	123.32	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	311	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
34	g	608	CHL	C1B-CHB-C4A	-3.35	123.49	130.12
34	R	606	CHL	C1B-CHB-C4A	-3.35	123.49	130.12
23	C	505	CLA	CMB-C2B-C3B	3.34	130.94	124.68
35	y	315	LUT	C10-C11-C12	-3.34	112.78	123.22
34	N	307	CHL	CHD-C1D-ND	-3.34	121.38	124.45
23	r	601	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
23	N	315	CLA	CAA-C2A-C3A	-3.34	108.30	116.10
37	y	301	XAT	C35-C34-C33	-3.34	122.54	127.31
23	y	310	CLA	C4A-NA-C1A	3.34	108.21	106.71
23	R	608	CLA	CHB-C4A-NA	3.34	129.13	124.51
23	d	405	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
37	y	301	XAT	O4-C5-C18	3.34	119.05	115.06
23	n	304	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
23	Y	304	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
23	c	502	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
23	a	405	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
25	c	518	BCR	C7-C8-C9	-3.33	121.20	126.23
23	g	611	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	K	101	BCR	C24-C23-C22	-3.33	121.20	126.23
23	A	404	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
23	r	603	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	N	305	CLA	CMB-C2B-C3B	3.33	130.90	124.68
23	D	405	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	R	608	CLA	CMB-C2B-C3B	3.33	130.90	124.68
25	b	618	BCR	C11-C10-C9	-3.33	122.56	127.31
23	b	616	CLA	CMB-C2B-C3B	3.32	130.90	124.68
25	B	619	BCR	C7-C8-C9	-3.32	121.21	126.23
35	Y	316	LUT	C15-C14-C13	-3.32	122.57	127.31
34	N	302	CHL	CMB-C2B-C1B	-3.32	123.37	128.46
34	n	307	CHL	CMB-C2B-C3B	3.32	130.88	124.68
34	S	606	CHL	CMB-C2B-C3B	3.32	130.88	124.68
34	R	613	CHL	CHD-C1D-ND	-3.32	121.41	124.45
36	r	617	NEX	C15-C35-C34	-3.32	116.68	123.47
23	N	304	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
34	S	605	CHL	C3C-C4C-NC	-3.31	106.86	110.57
23	b	614	CLA	C4A-NA-C1A	3.30	108.19	106.71
35	n	316	LUT	C35-C15-C14	-3.30	116.71	123.47
37	g	620	XAT	C35-C34-C33	-3.30	122.60	127.31
23	a	401	CLA	CHB-C4A-NA	3.30	129.07	124.51
23	R	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
33	e	101	HEM	C3B-C2B-C1B	3.30	108.93	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
23	Y	310	CLA	C4A-NA-C1A	3.29	108.19	106.71
34	g	608	CHL	CMB-C2B-C1B	-3.29	123.40	128.46
23	s	612	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
23	c	513	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
34	G	609	CHL	CMB-C2B-C1B	-3.29	123.41	128.46
23	b	605	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
30	b	622	LHG	O8-C23-C24	3.29	122.23	111.91
23	b	607	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
23	s	609	CLA	CMB-C2B-C3B	3.29	130.82	124.68
23	Y	311	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
35	r	615	LUT	C7-C8-C9	-3.28	121.27	126.23
35	n	317	LUT	C38-C25-C24	-3.28	116.53	123.56
25	B	619	BCR	C16-C17-C18	-3.28	122.63	127.31
34	Y	306	CHL	CAA-C2A-C1A	-3.28	101.22	111.97
23	Y	305	CLA	CMB-C2B-C3B	3.28	130.82	124.68
23	d	405	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	S	604	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
34	Y	302	CHL	OMC-CMC-C2C	-3.28	118.28	125.69
25	B	618	BCR	C11-C10-C9	-3.28	122.63	127.31
23	S	610	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
34	s	606	CHL	CMB-C2B-C3B	3.27	130.81	124.68
25	A	405	BCR	C11-C10-C9	-3.27	122.64	127.31
23	Y	312	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
23	c	502	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
25	B	618	BCR	C28-C27-C26	-3.27	108.24	114.08
23	A	402	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
37	Y	301	XAT	C6-C7-C8	-3.27	119.08	125.99
23	s	608	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
34	y	306	CHL	O2D-CGD-O1D	-3.26	117.46	123.84
25	B	617	BCR	C20-C21-C22	-3.26	122.66	127.31
25	b	617	BCR	C16-C17-C18	-3.26	122.66	127.31
35	g	616	LUT	C7-C8-C9	-3.26	121.31	126.23
23	G	613	CLA	CHB-C4A-NA	3.26	129.02	124.51
34	G	601	CHL	C1B-CHB-C4A	-3.26	123.66	130.12
25	b	617	BCR	C20-C21-C22	-3.26	122.66	127.31
34	G	608	CHL	C1B-CHB-C4A	-3.26	123.67	130.12
23	n	303	CLA	CMB-C2B-C3B	3.26	130.77	124.68
25	h	101	BCR	C10-C11-C12	-3.26	113.06	123.22
27	A	407	LMG	O8-C28-C29	3.26	122.12	111.91
23	c	508	CLA	O2A-C1-C2	3.25	117.19	108.64
34	g	607	CHL	CMB-C2B-C1B	-3.25	123.46	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	n	307	CHL	C4A-NA-C1A	3.25	108.17	106.71
27	C	501	LMG	C7-O1-C1	-3.25	107.39	113.74
33	E	101	HEM	C3B-C2B-C1B	3.25	108.90	106.49
23	R	610	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
34	g	605	CHL	C1B-CHB-C4A	-3.25	123.69	130.12
30	C	518	LHG	O7-C7-C8	3.25	118.50	111.50
23	g	611	CLA	CHB-C4A-NA	3.25	129.00	124.51
23	n	312	CLA	CMB-C2B-C3B	3.24	130.75	124.68
35	R	615	LUT	C7-C8-C9	-3.24	121.33	126.23
23	b	615	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
34	g	607	CHL	CMB-C2B-C3B	3.24	130.74	124.68
23	r	601	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
23	R	614	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	c	515	BCR	C7-C8-C9	-3.24	121.34	126.23
23	c	508	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
23	b	601	CLA	CMB-C2B-C3B	3.23	130.73	124.68
23	r	614	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
34	r	613	CHL	CHD-C1D-ND	-3.23	121.48	124.45
23	Y	303	CLA	CHB-C4A-NA	3.23	128.98	124.51
37	R	616	XAT	C15-C35-C34	-3.23	116.85	123.47
23	y	311	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
23	S	611	CLA	CMB-C2B-C3B	3.23	130.72	124.68
35	S	615	LUT	C18-C5-C6	-3.23	120.90	124.53
36	y	317	NEX	C26-C27-C28	-3.23	119.17	125.99
35	N	317	LUT	C32-C33-C34	3.22	123.89	118.94
26	A	406	SQD	O9-S-C6	3.22	110.77	106.94
23	a	403	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
35	Y	316	LUT	C31-C30-C29	-3.22	122.72	127.31
23	N	303	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	r	603	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	A	401	CLA	CHB-C4A-NA	3.21	128.95	124.51
35	g	616	LUT	C35-C15-C14	-3.21	116.90	123.47
25	b	619	BCR	C7-C8-C9	-3.21	121.39	126.23
25	c	514	BCR	C20-C21-C22	-3.21	122.73	127.31
34	R	613	CHL	C4A-NA-C1A	3.21	108.15	106.71
23	B	612	CLA	CHB-C4A-NA	3.20	128.94	124.51
34	Y	307	CHL	CMB-C2B-C3B	3.20	130.67	124.68
34	Y	308	CHL	CMB-C2B-C3B	3.20	130.67	124.68
34	Y	302	CHL	CHD-C1D-ND	-3.20	121.51	124.45
25	b	619	BCR	C16-C17-C18	-3.20	122.74	127.31
35	g	615	LUT	C40-C33-C32	3.20	123.12	118.08
23	c	507	CLA	CMB-C2B-C3B	3.20	130.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	614	CLA	CMB-C2B-C3B	3.20	130.66	124.68
34	N	308	CHL	C2A-C1A-CHA	3.20	129.45	123.86
35	G	615	LUT	C7-C8-C9	-3.19	121.41	126.23
23	R	601	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
23	s	611	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	b	614	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
35	N	316	LUT	C31-C30-C29	-3.19	122.76	127.31
23	s	608	CLA	CMB-C2B-C3B	3.19	130.65	124.68
32	d	407	PL9	C40-C39-C41	-3.19	109.91	115.27
34	Y	309	CHL	CMB-C2B-C1B	-3.19	123.56	128.46
23	n	312	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
33	E	101	HEM	CHC-C4B-C3B	3.19	129.45	124.57
37	G	620	XAT	C35-C34-C33	-3.19	122.76	127.31
23	b	612	CLA	CHB-C4A-NA	3.19	128.92	124.51
35	G	616	LUT	C10-C11-C12	-3.19	113.27	123.22
23	S	613	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
25	B	618	BCR	C24-C23-C22	-3.19	121.42	126.23
25	b	618	BCR	C28-C27-C26	-3.18	108.39	114.08
25	C	516	BCR	C15-C16-C17	-3.18	116.95	123.47
34	n	308	CHL	CMB-C2B-C1B	-3.18	123.57	128.46
34	G	607	CHL	CHD-C1D-ND	-3.18	121.53	124.45
25	b	618	BCR	C21-C20-C19	-3.18	113.29	123.22
32	D	406	PL9	C40-C39-C41	-3.18	109.92	115.27
23	c	511	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	G	611	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	c	506	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
25	c	515	BCR	C15-C16-C17	-3.18	116.97	123.47
24	A	403	PHO	CMB-C2B-C3B	3.18	130.62	124.68
34	Y	306	CHL	CHB-C4A-NA	3.17	128.90	124.51
23	y	313	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
34	N	306	CHL	C1B-CHB-C4A	-3.17	123.84	130.12
34	G	601	CHL	CMB-C2B-C3B	3.17	130.61	124.68
26	M	101	SQD	O7-S-C6	3.17	110.70	106.94
34	G	619	CHL	O2D-CGD-O1D	-3.17	117.64	123.84
23	g	603	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
37	r	616	XAT	C35-C34-C33	-3.17	122.79	127.31
23	c	513	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
34	y	302	CHL	CHD-C1D-ND	-3.16	121.55	124.45
35	G	615	LUT	C30-C31-C32	-3.16	113.35	123.22
25	B	617	BCR	C16-C17-C18	-3.16	122.80	127.31
23	B	603	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
23	b	610	CLA	O2D-CGD-O1D	-3.16	117.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	614	LUT	C10-C11-C12	-3.16	113.35	123.22
26	A	409	SQD	O8-S-O7	3.16	118.99	111.27
23	C	514	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
26	a	409	SQD	O8-S-O7	3.15	118.98	111.27
23	C	504	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
34	G	609	CHL	CHD-C1D-C2D	3.15	132.09	125.48
23	C	510	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	y	312	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	H	101	BCR	C3-C4-C5	-3.15	108.45	114.08
37	r	616	XAT	O4-C5-C18	3.15	118.83	115.06
34	G	607	CHL	CBA-CAA-C2A	3.15	120.47	113.47
34	G	608	CHL	CMB-C2B-C3B	3.14	130.56	124.68
36	N	318	NEX	C17-C1-C6	-3.14	107.66	110.47
23	S	603	CLA	CHB-C4A-NA	3.14	128.86	124.51
36	r	617	NEX	C35-C34-C33	-3.14	122.82	127.31
23	B	616	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	G	603	CLA	CMB-C2B-C3B	3.14	130.55	124.68
35	N	316	LUT	C10-C11-C12	-3.14	113.43	123.22
37	g	620	XAT	O24-C25-C38	3.14	118.81	115.06
23	n	315	CLA	CAA-C2A-C3A	-3.14	108.78	116.10
23	C	511	CLA	CHB-C4A-NA	3.13	128.85	124.51
23	s	603	CLA	C2A-C1A-CHA	3.13	129.34	123.86
23	r	609	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
23	b	613	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
34	G	605	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
36	n	318	NEX	C26-C27-C28	-3.13	119.38	125.99
23	n	314	CLA	CBA-CAA-C2A	3.13	123.09	113.86
23	B	613	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	r	612	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
25	a	406	BCR	C11-C10-C9	-3.13	122.85	127.31
23	G	612	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
23	a	402	CLA	O2D-CGD-CBD	3.13	116.82	111.27
36	N	318	NEX	C26-C27-C28	-3.12	119.39	125.99
23	r	608	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	B	614	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
23	n	314	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
34	G	608	CHL	CHD-C1D-ND	-3.12	121.58	124.45
23	B	610	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	B	618	BCR	C21-C20-C19	-3.12	113.48	123.22
26	L	103	SQD	O7-S-C6	3.12	110.65	106.94
34	S	607	CHL	C2D-C1D-ND	-3.12	107.81	110.10
23	C	507	CLA	C1B-CHB-C4A	-3.12	123.94	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	619	CHL	O2D-CGD-O1D	-3.12	117.74	123.84
30	r	618	LHG	O8-C23-C24	3.12	121.70	111.91
37	n	301	XAT	C26-C27-C28	-3.12	119.40	125.99
33	E	101	HEM	C1B-NB-C4B	3.12	108.29	105.07
33	e	101	HEM	CHC-C4B-C3B	3.12	129.34	124.57
23	c	510	CLA	CHB-C4A-NA	3.12	128.82	124.51
34	n	308	CHL	OMC-CMC-C2C	-3.12	118.64	125.69
25	A	405	BCR	C3-C4-C5	-3.11	108.52	114.08
34	n	309	CHL	CMB-C2B-C3B	3.11	130.50	124.68
36	s	616	NEX	C39-C29-C30	-3.11	118.57	122.92
35	Y	316	LUT	C10-C11-C12	-3.11	113.52	123.22
25	b	618	BCR	C7-C8-C9	-3.11	121.54	126.23
23	C	503	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	a	404	PHO	CMB-C2B-C3B	3.11	130.49	124.68
37	N	301	XAT	C6-C7-C8	-3.11	119.42	125.99
34	n	308	CHL	C1B-CHB-C4A	-3.11	123.97	130.12
23	r	602	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
23	N	315	CLA	CMB-C2B-C3B	3.11	130.49	124.68
25	b	618	BCR	C24-C23-C22	-3.11	121.54	126.23
23	C	508	CLA	CMB-C2B-C3B	3.10	130.49	124.68
34	N	308	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
23	b	603	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
23	s	611	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
34	r	607	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
23	S	603	CLA	C2A-C1A-CHA	3.10	129.28	123.86
23	B	608	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
34	y	306	CHL	CAA-C2A-C3A	-3.10	104.29	112.78
37	n	301	XAT	C15-C14-C13	-3.10	122.89	127.31
23	y	303	CLA	CHB-C4A-NA	3.10	128.79	124.51
34	G	609	CHL	C1D-ND-C4D	3.10	108.53	106.33
23	y	310	CLA	CHB-C4A-NA	3.09	128.79	124.51
23	N	311	CLA	CHB-C4A-NA	3.09	128.79	124.51
23	S	612	CLA	CHB-C4A-NA	3.09	128.79	124.51
23	n	303	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
34	y	306	CHL	CHB-C4A-NA	3.09	128.79	124.51
34	N	310	CHL	CHD-C1D-ND	-3.09	121.61	124.45
34	Y	309	CHL	C1B-CHB-C4A	-3.09	123.99	130.12
23	C	509	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
25	a	406	BCR	C3-C4-C5	-3.09	108.56	114.08
27	B	622	LMG	O8-C28-C29	3.09	121.60	111.91
23	s	603	CLA	CHB-C4A-NA	3.09	128.78	124.51
23	G	611	CLA	CHB-C4A-NA	3.09	128.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	313	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
35	g	616	LUT	C3-C4-C5	-3.08	105.71	111.85
35	R	615	LUT	C11-C10-C9	-3.08	122.91	127.31
23	Y	304	CLA	CHB-C4A-NA	3.08	128.77	124.51
23	C	511	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
23	s	612	CLA	CHB-C4A-NA	3.08	128.77	124.51
25	B	619	BCR	C1-C6-C7	3.08	124.49	115.78
34	g	609	CHL	C2A-C1A-CHA	3.08	129.24	123.86
34	G	606	CHL	C1B-CHB-C4A	-3.08	124.02	130.12
23	r	604	CLA	CMB-C2B-C3B	3.08	130.43	124.68
36	s	616	NEX	C31-C30-C29	-3.07	122.92	127.31
34	y	308	CHL	CMB-C2B-C3B	3.07	130.43	124.68
34	N	309	CHL	CMB-C2B-C3B	3.07	130.42	124.68
34	n	306	CHL	OMC-CMC-C2C	-3.07	118.75	125.69
25	C	515	BCR	C16-C15-C14	-3.07	117.19	123.47
23	s	612	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	y	303	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	y	304	CLA	CHB-C4A-NA	3.06	128.75	124.51
37	y	301	XAT	C6-C7-C8	-3.06	119.52	125.99
23	D	401	CLA	CHB-C4A-NA	3.06	128.75	124.51
25	b	619	BCR	C1-C6-C7	3.06	124.42	115.78
23	C	505	CLA	C1B-CHB-C4A	-3.06	124.07	130.12
23	c	510	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	B	618	BCR	C7-C8-C9	-3.05	121.62	126.23
23	c	509	CLA	O2D-CGD-CBD	3.05	116.69	111.27
23	n	313	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
23	G	612	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
23	b	609	CLA	CMB-C2B-C3B	3.05	130.39	124.68
23	S	612	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	a	406	BCR	C24-C23-C22	-3.05	121.63	126.23
37	G	620	XAT	C11-C10-C9	-3.05	122.96	127.31
34	N	307	CHL	CMB-C2B-C1B	-3.05	123.78	128.46
23	y	303	CLA	CBC-CAC-C3C	3.05	120.84	112.43
23	c	501	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
34	g	601	CHL	C2D-C1D-ND	-3.05	107.86	110.10
27	B	620	LMG	O8-C28-C29	3.05	121.47	111.91
23	G	604	CLA	CMB-C2B-C3B	3.04	130.37	124.68
35	y	316	LUT	C35-C34-C33	-3.04	122.97	127.31
23	g	610	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
23	n	315	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	r	610	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	B	615	CLA	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	610	CLA	CHB-C4A-NA	3.04	128.72	124.51
23	g	610	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	N	311	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
35	R	615	LUT	C3-C4-C5	-3.04	105.81	111.85
23	R	609	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
37	R	616	XAT	C24-C23-C22	-3.03	104.91	110.77
34	g	601	CHL	CMB-C2B-C3B	3.03	130.35	124.68
25	k	101	BCR	C24-C23-C22	-3.03	121.65	126.23
23	Y	303	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
23	g	604	CLA	CMB-C2B-C3B	3.03	130.35	124.68
23	S	602	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
34	G	608	CHL	O2D-CGD-O1D	-3.03	117.91	123.84
23	C	509	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
23	g	611	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	A	401	CLA	O1D-CGD-CBD	3.03	130.68	124.48
34	G	606	CHL	O2D-CGD-O1D	-3.02	117.92	123.84
34	G	609	CHL	C2A-C1A-CHA	3.02	129.15	123.86
23	b	605	CLA	CHB-C4A-NA	3.02	128.69	124.51
37	r	616	XAT	C24-C23-C22	-3.02	104.94	110.77
27	b	620	LMG	O8-C28-C29	3.02	121.39	111.91
30	W	201	LHG	C5-O7-C7	-3.02	110.35	117.79
34	y	302	CHL	O2D-CGD-O1D	-3.02	117.93	123.84
23	A	402	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	R	603	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	y	304	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	b	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
34	Y	306	CHL	CMB-C2B-C3B	3.01	130.32	124.68
34	r	607	CHL	C4A-NA-C1A	3.01	108.06	106.71
37	g	620	XAT	C11-C10-C9	-3.01	123.01	127.31
23	N	304	CLA	CHB-C4A-NA	3.01	128.68	124.51
23	Y	303	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
35	S	615	LUT	C38-C25-C24	-3.01	117.11	123.56
23	b	608	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	n	304	CLA	CHB-C4A-NA	3.01	128.68	124.51
35	s	614	LUT	C30-C31-C32	-3.01	113.82	123.22
23	c	507	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
23	B	602	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
23	N	303	CLA	CMB-C2B-C3B	3.01	130.31	124.68
36	S	616	NEX	C17-C1-C6	-3.01	107.78	110.47
23	b	615	CLA	CHB-C4A-NA	3.01	128.67	124.51
26	L	103	SQD	O48-C23-C24	3.00	121.34	111.91
23	c	512	CLA	O2D-CGD-CBD	3.00	116.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	N	302	CHL	O2D-CGD-O1D	-3.00	117.97	123.84
23	R	612	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
34	R	605	CHL	C1B-CHB-C4A	-3.00	124.17	130.12
23	c	508	CLA	C1-C2-C3	-3.00	120.86	126.04
34	y	306	CHL	OMC-CMC-C2C	-3.00	118.91	125.69
24	a	404	PHO	C1B-NB-C4B	3.00	113.25	107.09
37	y	301	XAT	C7-C8-C9	-3.00	120.88	125.53
37	n	301	XAT	C31-C30-C29	-3.00	123.03	127.31
23	g	612	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	b	612	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	k	101	BCR	C30-C25-C26	-2.99	118.40	122.61
34	s	606	CHL	CHD-C1D-ND	-2.99	121.70	124.45
23	G	610	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	b	615	CLA	CMB-C2B-C3B	2.99	130.27	124.68
37	N	301	XAT	C27-C28-C29	-2.99	120.89	125.53
23	G	612	CLA	CHB-C4A-NA	2.99	128.64	124.51
34	s	601	CHL	CHD-C1D-ND	-2.99	121.71	124.45
34	Y	306	CHL	OMC-CMC-C2C	-2.99	118.94	125.69
23	r	603	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
35	g	615	LUT	C30-C31-C32	-2.98	113.91	123.22
34	Y	302	CHL	C1B-CHB-C4A	-2.98	124.21	130.12
36	Y	317	NEX	C39-C29-C30	-2.98	118.75	122.92
34	N	307	CHL	OMC-CMC-C2C	-2.98	118.95	125.69
23	c	507	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	C	516	BCR	C21-C20-C19	-2.98	113.92	123.22
34	g	606	CHL	CAA-C2A-C3A	-2.98	106.82	114.26
23	B	615	CLA	CHB-C4A-NA	2.98	128.63	124.51
34	n	309	CHL	CHB-C4A-NA	2.98	128.63	124.51
23	S	611	CLA	C2A-C1A-CHA	2.98	129.06	123.86
23	c	512	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
23	c	505	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
37	R	616	XAT	C19-C9-C8	2.97	122.76	118.08
34	g	608	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
23	R	604	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
34	R	613	CHL	CMB-C2B-C3B	2.97	130.24	124.68
36	g	617	NEX	C39-C29-C30	-2.97	118.76	122.92
34	n	306	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
34	n	307	CHL	OMC-CMC-C2C	-2.97	118.97	125.69
30	B	621	LHG	O8-C23-C24	2.97	121.23	111.91
23	g	612	CLA	CMB-C2B-C3B	2.97	130.23	124.68
24	A	403	PHO	C1B-NB-C4B	2.97	113.19	107.09
34	g	608	CHL	CMB-C2B-C3B	2.97	130.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	y	315	LUT	C35-C15-C14	-2.97	117.40	123.47
23	G	610	CLA	CHB-C4A-NA	2.97	128.61	124.51
23	R	614	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	N	315	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	a	403	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	b	621	LHG	O8-C23-C24	2.96	121.20	111.91
23	r	603	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	s	612	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	g	614	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
37	N	301	XAT	C35-C34-C33	-2.96	123.09	127.31
23	y	314	CLA	CHB-C4A-NA	2.96	128.60	124.51
23	S	608	CLA	CHB-C4A-NA	2.95	128.60	124.51
34	y	308	CHL	C1B-CHB-C4A	-2.95	124.27	130.12
23	s	608	CLA	CHB-C4A-NA	2.95	128.60	124.51
34	N	308	CHL	CHB-C4A-NA	2.95	128.60	124.51
23	R	612	CLA	CMB-C2B-C3B	2.95	130.20	124.68
36	R	617	NEX	C11-C10-C9	-2.95	123.10	127.31
23	Y	313	CLA	CHB-C4A-NA	2.95	128.59	124.51
34	N	308	CHL	CMB-C2B-C3B	2.95	130.20	124.68
23	b	601	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
34	g	607	CHL	C2A-C1A-CHA	2.95	129.02	123.86
23	C	502	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	C	514	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
33	E	101	HEM	C4B-CHC-C1C	2.95	126.45	122.56
35	Y	316	LUT	C15-C35-C34	-2.95	117.44	123.47
23	r	604	CLA	CHB-C4A-NA	2.94	128.58	124.51
23	D	401	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	r	601	CLA	CMB-C2B-C3B	2.94	130.18	124.68
34	g	606	CHL	CHB-C4A-NA	2.94	128.58	124.51
37	g	620	XAT	C4-C3-C2	-2.94	105.09	110.77
36	Y	317	NEX	C24-C23-C22	-2.94	105.09	110.77
34	g	605	CHL	CMB-C2B-C3B	2.94	130.18	124.68
34	S	607	CHL	C2A-C3A-C4A	-2.94	97.12	101.87
23	b	608	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
23	S	613	CLA	CMB-C2B-C3B	2.94	130.17	124.68
35	r	615	LUT	C3-C4-C5	-2.94	106.01	111.85
23	d	405	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	b	610	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
36	N	318	NEX	C31-C30-C29	-2.93	123.13	127.31
23	G	602	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
23	c	503	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	A	402	CLA	CMB-C2B-C3B	2.93	130.16	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	614	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
36	Y	317	NEX	C16-C1-C2	2.93	122.20	109.05
23	R	604	CLA	O2D-CGD-CBD	2.93	116.47	111.27
23	S	603	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
35	Y	315	LUT	C10-C11-C12	-2.92	114.09	123.22
23	g	611	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
23	S	609	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
34	N	309	CHL	C1B-CHB-C4A	-2.92	124.33	130.12
34	S	607	CHL	CMB-C2B-C3B	2.92	130.15	124.68
23	c	507	CLA	O2D-CGD-CBD	2.92	116.46	111.27
34	r	613	CHL	CMB-C2B-C3B	2.92	130.14	124.68
34	Y	302	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
23	R	602	CLA	CMB-C2B-C3B	2.92	130.14	124.68
34	n	302	CHL	C2C-C3C-C4C	2.92	108.57	106.49
34	y	309	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
23	C	510	CLA	C4A-NA-C1A	2.92	108.02	106.71
35	G	615	LUT	C21-C26-C27	-2.92	109.01	112.70
23	D	405	CLA	CHB-C4A-NA	2.92	128.55	124.51
23	R	604	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
23	R	604	CLA	CHB-C4A-NA	2.92	128.54	124.51
35	S	615	LUT	C31-C30-C29	-2.92	123.15	127.31
34	N	309	CHL	O2D-CGD-O1D	-2.92	118.14	123.84
25	A	405	BCR	C24-C23-C22	-2.91	121.83	126.23
23	C	512	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	y	303	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
34	n	308	CHL	C2A-C1A-CHA	2.91	128.95	123.86
23	c	508	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	y	305	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
23	c	502	CLA	CHB-C4A-NA	2.91	128.54	124.51
23	N	313	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
34	G	601	CHL	C3C-C4C-NC	-2.91	107.31	110.57
23	N	304	CLA	O2D-CGD-CBD	2.91	116.44	111.27
35	Y	315	LUT	C35-C15-C14	-2.91	117.51	123.47
37	g	620	XAT	C31-C30-C29	-2.91	123.16	127.31
37	n	301	XAT	C35-C34-C33	-2.91	123.16	127.31
23	B	615	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
36	R	617	NEX	O24-C25-C38	2.91	118.54	115.06
23	g	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
34	N	310	CHL	C1D-CHD-C4C	-2.91	119.78	126.06
23	C	513	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
23	B	612	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	B	607	CLA	O2D-CGD-O1D	-2.90	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	Y	310	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	y	312	CLA	CHB-C4A-NA	2.90	128.53	124.51
35	N	316	LUT	C11-C10-C9	-2.90	123.17	127.31
35	G	616	LUT	C3-C4-C5	-2.90	106.08	111.85
23	C	513	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	G	614	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
34	S	606	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
34	S	605	CHL	C2C-C3C-C4C	2.90	108.55	106.49
37	r	616	XAT	C19-C9-C8	2.90	122.64	118.08
23	d	405	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
37	Y	301	XAT	C4-C3-C2	-2.90	105.18	110.77
34	S	605	CHL	O2D-CGD-O1D	-2.89	118.18	123.84
23	Y	312	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	B	623	LHG	O8-C23-C24	2.89	120.99	111.91
23	Y	304	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
26	M	101	SQD	O48-C23-C24	2.89	120.99	111.91
23	R	603	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
23	g	604	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	c	513	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
23	b	613	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
23	a	405	CLA	CHB-C4A-NA	2.89	128.51	124.51
28	d	410	DGD	O1G-C1A-C2A	2.89	120.98	111.91
25	H	101	BCR	C38-C26-C25	-2.89	121.28	124.53
23	n	315	CLA	CMA-C3A-C2A	-2.89	109.35	116.10
23	R	601	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	s	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
36	s	616	NEX	C15-C35-C34	-2.89	117.56	123.47
23	N	314	CLA	CBA-CAA-C2A	2.89	122.39	113.86
34	Y	308	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
34	N	306	CHL	OMC-CMC-C2C	-2.89	119.16	125.69
25	c	514	BCR	C38-C26-C25	-2.89	121.29	124.53
23	b	607	CLA	CHB-C4A-NA	2.89	128.50	124.51
23	R	603	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
35	s	614	LUT	C18-C5-C6	-2.89	121.29	124.53
23	B	610	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
23	N	305	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
34	y	309	CHL	CMB-C2B-C1B	-2.88	124.03	128.46
23	Y	305	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
37	R	616	XAT	O4-C5-C18	2.88	118.51	115.06
25	C	515	BCR	C11-C10-C9	-2.88	123.20	127.31
23	s	611	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	n	302	CHL	CHD-C1D-ND	-2.88	121.81	124.45
23	y	304	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
34	s	607	CHL	C2A-C1A-CHA	2.88	128.89	123.86
35	s	614	LUT	C10-C11-C12	-2.88	114.24	123.22
23	y	305	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	W	201	LHG	O8-C23-C24	2.88	120.93	111.91
23	B	613	CLA	CHB-C4A-NA	2.87	128.49	124.51
23	B	607	CLA	CHB-C4A-NA	2.87	128.49	124.51
34	N	302	CHL	CMB-C2B-C3B	2.87	130.05	124.68
37	g	620	XAT	C26-C27-C28	-2.87	119.92	125.99
23	r	612	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
36	R	617	NEX	C35-C34-C33	-2.87	123.21	127.31
23	N	303	CLA	O2D-CGD-CBD	2.87	116.37	111.27
30	L	102	LHG	O8-C23-O10	-2.87	116.35	123.59
23	R	612	CLA	CHB-C4A-NA	2.87	128.48	124.51
37	G	620	XAT	C31-C30-C29	-2.87	123.22	127.31
36	y	317	NEX	C24-C23-C22	-2.87	105.23	110.77
23	B	616	CLA	CHB-C4A-NA	2.87	128.48	124.51
37	G	620	XAT	C4-C3-C2	-2.87	105.23	110.77
23	r	610	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
23	G	612	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
34	s	601	CHL	OMC-CMC-C2C	-2.87	119.21	125.69
34	n	309	CHL	C1B-CHB-C4A	-2.87	124.44	130.12
23	D	401	CLA	O2D-CGD-CBD	2.87	116.36	111.27
36	Y	317	NEX	C26-C27-C28	-2.87	119.94	125.99
34	r	605	CHL	CHB-C4A-NA	2.86	128.47	124.51
34	G	601	CHL	C1D-ND-C4D	2.86	108.37	106.33
23	g	602	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	b	606	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
34	S	607	CHL	C2A-C1A-CHA	2.86	128.86	123.86
23	S	608	CLA	O2D-CGD-CBD	2.86	116.35	111.27
34	n	302	CHL	O2D-CGD-O1D	-2.86	118.25	123.84
37	y	301	XAT	C4-C3-C2	-2.86	105.25	110.77
23	C	502	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
34	r	605	CHL	CMB-C2B-C1B	-2.86	124.07	128.46
36	y	317	NEX	C31-C30-C29	-2.86	123.23	127.31
23	S	608	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	G	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	B	601	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
30	R	618	LHG	O8-C23-C24	2.86	120.87	111.91
23	A	404	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	c	512	CLA	CHB-C4A-NA	2.85	128.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	d	402	SQD	O7-S-C6	2.85	110.33	106.94
23	r	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
34	s	606	CHL	O2D-CGD-O1D	-2.85	118.26	123.84
23	n	315	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
36	G	617	NEX	C16-C1-C6	2.85	113.02	110.47
30	T	101	LHG	O8-C23-C24	2.85	120.85	111.91
34	g	608	CHL	CHD-C1D-ND	-2.85	121.83	124.45
35	y	316	LUT	C3-C4-C5	-2.85	106.18	111.85
25	F	101	BCR	C3-C4-C5	-2.85	108.99	114.08
23	g	614	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	N	303	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
23	n	312	CLA	CHD-C1D-ND	-2.85	121.84	124.45
34	G	601	CHL	CHB-C4A-NA	2.85	128.45	124.51
23	S	612	CLA	CMB-C2B-C3B	2.85	130.00	124.68
23	n	313	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
23	r	609	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
34	g	609	CHL	CHD-C1D-C2D	2.84	131.44	125.48
23	R	610	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	C	508	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
23	C	504	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
35	g	616	LUT	C38-C25-C24	-2.84	117.48	123.56
23	n	304	CLA	O2D-CGD-CBD	2.84	116.31	111.27
26	a	409	SQD	O48-C23-C24	2.84	120.82	111.91
36	s	616	NEX	C35-C34-C33	-2.84	123.26	127.31
23	b	605	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	c	513	CLA	CMB-C2B-C3B	2.84	129.99	124.68
34	s	605	CHL	C1B-CHB-C4A	-2.84	124.50	130.12
23	s	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	g	614	CLA	CAA-C2A-C3A	-2.84	107.17	114.26
23	y	305	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	S	603	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
34	R	607	CHL	C1B-CHB-C4A	-2.83	124.50	130.12
23	a	403	CLA	CMB-C2B-C3B	2.83	129.98	124.68
23	G	602	CLA	CMB-C2B-C3B	2.83	129.98	124.68
23	G	611	CLA	CMB-C2B-C3B	2.83	129.98	124.68
23	R	601	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	D	405	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	d	402	SQD	O48-C23-C24	2.83	120.79	111.91
30	G	618	LHG	O8-C23-C24	2.83	120.79	111.91
23	B	616	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	C	517	DGD	O1G-C1A-C2A	2.83	120.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
34	g	609	CHL	C2D-C1D-ND	-2.83	108.02	110.10
23	G	603	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
34	N	302	CHL	CHD-C1D-ND	-2.83	121.86	124.45
23	G	614	CLA	CAA-C2A-C3A	-2.83	107.20	114.26
35	s	614	LUT	C35-C15-C14	-2.83	117.69	123.47
23	r	612	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	Y	305	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
34	y	306	CHL	CMB-C2B-C3B	2.82	129.96	124.68
23	S	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
35	S	614	LUT	C30-C31-C32	-2.82	114.41	123.22
35	s	615	LUT	C18-C5-C6	-2.82	121.36	124.53
23	S	603	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
30	b	622	LHG	O8-C23-O10	-2.82	116.47	123.59
23	Y	304	CLA	CMB-C2B-C3B	2.82	129.95	124.68
34	r	613	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
34	N	309	CHL	CHB-C4A-NA	2.82	128.41	124.51
23	c	509	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	r	603	CLA	CHB-C4A-NA	2.82	128.41	124.51
34	g	605	CHL	O2D-CGD-O1D	-2.82	118.33	123.84
23	R	610	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
23	n	313	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	b	607	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	B	605	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	C	502	CLA	C2D-C1D-ND	-2.81	108.03	110.10
35	r	615	LUT	C35-C15-C14	-2.81	117.71	123.47
35	Y	315	LUT	C38-C25-C24	-2.81	117.54	123.56
35	y	316	LUT	C10-C11-C12	-2.81	114.44	123.22
23	r	602	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	S	602	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	G	614	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	a	402	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	r	601	CLA	CBC-CAC-C3C	2.81	120.17	112.43
23	C	503	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	w	201	LHG	O8-C23-C24	2.81	120.72	111.91
34	g	609	CHL	C1D-CHD-C4C	-2.81	120.00	126.06
23	S	604	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	h	101	BCR	C11-C10-C9	-2.80	123.31	127.31
23	b	616	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	g	603	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	606	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	B	615	CLA	C1B-CHB-C4A	-2.80	124.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	n	308	CHL	CHB-C4A-NA	2.80	128.39	124.51
23	Y	304	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	s	603	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
23	S	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
36	y	317	NEX	C16-C1-C2	2.80	121.63	109.05
23	B	601	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
34	Y	308	CHL	C1B-CHB-C4A	-2.80	124.57	130.12
34	y	308	CHL	CHB-C4A-NA	2.80	128.38	124.51
23	b	615	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
23	R	603	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	B	619	BCR	C29-C30-C25	2.80	114.79	110.48
27	a	407	LMG	C8-O7-C10	-2.80	110.91	117.79
23	s	611	CLA	CHB-C4A-NA	2.80	128.38	124.51
34	G	605	CHL	CMB-C2B-C3B	2.80	129.91	124.68
23	B	611	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
23	r	601	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	N	315	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
23	b	601	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
25	F	101	BCR	C24-C23-C22	-2.79	122.02	126.23
36	S	616	NEX	C15-C35-C34	-2.79	117.76	123.47
34	N	310	CHL	C2A-C1A-CHA	2.79	128.73	123.86
23	S	610	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
25	B	619	BCR	C33-C5-C4	2.79	118.97	113.62
33	E	101	HEM	CBA-CAA-C2A	-2.79	107.87	112.62
26	A	409	SQD	O48-C23-C24	2.78	120.65	111.91
23	s	603	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
23	b	605	CLA	CGD-CBD-CAD	-2.78	101.73	110.73
34	Y	308	CHL	CHB-C4A-NA	2.78	128.36	124.51
27	a	407	LMG	O8-C28-C29	2.78	120.63	111.91
23	Y	310	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
35	G	615	LUT	C40-C33-C32	2.78	122.45	118.08
23	a	401	CLA	O1D-CGD-CBD	2.78	130.16	124.48
34	s	605	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
23	b	603	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
23	n	312	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	Y	311	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	g	603	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
23	C	506	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
23	d	404	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
34	n	309	CHL	O2D-CGD-O1D	-2.77	118.43	123.84
23	b	616	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	c	516	DGD	O1G-C1A-C2A	2.77	120.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	620	XAT	C26-C27-C28	-2.77	120.14	125.99
34	S	607	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
25	a	406	BCR	C20-C21-C22	-2.76	123.37	127.31
23	b	611	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
23	G	612	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	n	303	CLA	CHB-C4A-NA	2.76	128.33	124.51
34	S	606	CHL	CHD-C1D-ND	-2.76	121.92	124.45
25	k	101	BCR	C20-C21-C22	-2.76	123.38	127.31
23	B	606	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
34	N	302	CHL	C2C-C3C-C4C	2.75	108.45	106.49
30	B	623	LHG	C5-O7-C7	-2.75	111.01	117.79
30	T	101	LHG	C5-O7-C7	-2.75	111.02	117.79
23	y	304	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	c	501	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	b	613	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	d	404	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	b	606	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
34	n	310	CHL	C2A-C1A-CHA	2.75	128.66	123.86
34	G	609	CHL	C1D-CHD-C4C	-2.75	120.13	126.06
23	R	609	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
23	G	602	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	B	605	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
25	C	515	BCR	C20-C21-C22	-2.75	123.39	127.31
34	G	609	CHL	O2D-CGD-O1D	-2.75	118.47	123.84
25	F	101	BCR	C16-C17-C18	-2.75	123.39	127.31
23	r	609	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	n	313	CLA	CMB-C2B-C3B	2.75	129.81	124.68
23	N	304	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
23	N	313	CLA	CMB-C2B-C3B	2.75	129.81	124.68
35	S	614	LUT	C1-C2-C3	2.74	119.84	113.64
25	b	619	BCR	C29-C30-C25	2.74	114.70	110.48
23	g	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
34	n	302	CHL	CHB-C4A-NA	2.74	128.30	124.51
34	n	310	CHL	C1D-CHD-C4C	-2.74	120.15	126.06
34	y	308	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
23	s	610	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	F	101	BCR	C30-C25-C26	-2.74	118.76	122.61
23	b	606	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	r	608	CLA	C4A-NA-C1A	2.74	107.94	106.71
34	n	307	CHL	C2D-C1D-ND	-2.74	108.09	110.10
23	C	514	CLA	CMB-C2B-C3B	2.74	129.80	124.68
36	S	616	NEX	C35-C34-C33	-2.73	123.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
35	G	616	LUT	C38-C25-C24	-2.73	117.71	123.56
30	a	412	LHG	O8-C23-C24	2.73	120.48	111.91
23	c	512	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
23	G	603	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
23	R	612	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
23	a	401	CLA	CMC-C2C-C1C	-2.73	120.88	125.04
23	a	401	CLA	C4-C3-C5	2.73	119.86	115.27
23	D	404	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
37	Y	301	XAT	C7-C8-C9	-2.73	121.30	125.53
25	B	618	BCR	C15-C16-C17	-2.73	117.89	123.47
23	B	604	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	y	311	CLA	CHB-C4A-NA	2.73	128.28	124.51
35	N	317	LUT	C15-C14-C13	-2.72	123.42	127.31
36	n	318	NEX	C35-C15-C14	-2.72	117.89	123.47
23	D	404	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	B	605	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
35	S	615	LUT	C19-C9-C8	2.72	122.37	118.08
23	b	614	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	C	512	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	g	603	CLA	CMB-C2B-C3B	2.72	129.76	124.68
33	e	101	HEM	C1B-NB-C4B	2.72	107.88	105.07
23	r	611	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	N	312	CLA	CHB-C4A-NA	2.72	128.27	124.51
34	G	607	CHL	CHB-C4A-NA	2.72	128.27	124.51
35	s	615	LUT	C19-C9-C8	2.72	122.36	118.08
23	Y	314	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	g	602	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	n	315	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	A	405	BCR	C20-C21-C22	-2.71	123.44	127.31
36	S	616	NEX	C28-C29-C30	2.71	123.10	118.94
23	n	313	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	r	604	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
23	s	603	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	n	311	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	S	610	CLA	CAA-C2A-C3A	-2.71	107.49	114.26
23	A	404	CLA	O2D-CGD-CBD	2.71	116.08	111.27
25	F	101	BCR	C1-C6-C5	-2.71	118.80	122.61
23	Y	312	CLA	CAA-C2A-C3A	-2.71	105.37	112.78
35	g	615	LUT	C19-C9-C8	2.71	122.34	118.08
23	s	609	CLA	O2D-CGD-CBD	2.70	116.07	111.27
35	y	315	LUT	C30-C31-C32	-2.70	114.78	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	605	CHL	CMB-C2B-C3B	2.70	129.74	124.68
23	r	611	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
35	s	614	LUT	C15-C14-C13	-2.70	123.45	127.31
23	n	314	CLA	CAA-C2A-C1A	2.70	120.83	111.97
23	g	610	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	R	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	N	313	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	r	609	CLA	CMB-C2B-C3B	2.70	129.73	124.68
35	g	616	LUT	C30-C31-C32	-2.70	114.80	123.22
23	C	513	CLA	CHB-C4A-NA	2.70	128.24	124.51
35	N	317	LUT	C22-C23-C24	-2.70	108.67	111.74
34	G	601	CHL	CHC-C1C-NC	2.69	128.29	124.20
23	c	508	CLA	CHB-C4A-NA	2.69	128.24	124.51
34	Y	306	CHL	O2D-CGD-CBD	2.69	116.05	111.27
35	g	616	LUT	C10-C11-C12	-2.69	114.82	123.22
36	n	318	NEX	C27-C28-C29	-2.69	121.36	125.53
23	G	611	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
23	n	304	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
25	K	101	BCR	C7-C8-C9	-2.69	122.17	126.23
23	g	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	h	101	BCR	C16-C15-C14	-2.69	117.97	123.47
23	c	504	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
37	N	301	XAT	C7-C8-C9	-2.69	121.36	125.53
35	n	316	LUT	C20-C13-C12	2.69	122.31	118.08
23	B	606	CLA	CMB-C2B-C3B	2.68	129.70	124.68
35	y	315	LUT	C38-C25-C24	-2.68	117.81	123.56
23	Y	311	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	r	614	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
25	K	101	BCR	C30-C25-C26	-2.68	118.83	122.61
28	A	408	DGD	O1G-C1A-C2A	2.68	120.33	111.91
23	C	506	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
35	s	615	LUT	C31-C30-C29	-2.68	123.48	127.31
23	s	602	CLA	CHB-C4A-NA	2.68	128.22	124.51
35	S	614	LUT	C18-C5-C6	-2.68	121.52	124.53
36	G	617	NEX	C39-C29-C30	-2.68	119.17	122.92
30	A	412	LHG	O8-C23-C24	2.68	120.31	111.91
23	r	608	CLA	CHB-C4A-NA	2.68	128.21	124.51
36	Y	317	NEX	C31-C30-C29	-2.68	123.49	127.31
23	r	610	CLA	CHB-C4A-NA	2.67	128.21	124.51
34	y	307	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
25	B	617	BCR	C15-C16-C17	-2.67	118.00	123.47
25	Z	101	BCR	C7-C8-C9	-2.67	122.20	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	r	616	XAT	C20-C13-C12	2.67	122.29	118.08
23	g	604	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	b	618	BCR	C15-C16-C17	-2.67	118.00	123.47
34	G	608	CHL	CHB-C4A-NA	2.67	128.20	124.51
23	b	602	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
35	s	615	LUT	C38-C25-C24	-2.66	117.86	123.56
34	s	607	CHL	C4A-NA-C1A	2.66	107.90	106.71
25	c	515	BCR	C21-C20-C19	-2.66	114.91	123.22
23	Y	305	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	b	610	CLA	CHB-C4A-NA	2.66	128.19	124.51
35	g	615	LUT	C21-C26-C27	-2.66	109.34	112.70
23	R	601	CLA	CHB-C4A-NA	2.66	128.19	124.51
36	S	616	NEX	C24-C23-C22	-2.66	105.64	110.77
34	R	613	CHL	O2D-CGD-O1D	-2.66	118.64	123.84
23	g	602	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
23	y	303	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
23	C	510	CLA	CHA-C1A-NA	-2.65	120.32	126.40
34	r	607	CHL	CHD-C1D-ND	-2.65	122.02	124.45
37	G	620	XAT	O24-C25-C38	2.65	118.24	115.06
23	b	605	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
37	N	301	XAT	C30-C31-C32	-2.65	114.94	123.22
34	g	605	CHL	CHD-C1D-ND	-2.65	122.02	124.45
34	n	310	CHL	CHD-C1D-ND	-2.65	122.02	124.45
25	b	619	BCR	C33-C5-C4	2.65	118.71	113.62
23	A	401	CLA	C7-C6-C5	-2.65	106.16	113.36
35	g	615	LUT	C7-C8-C9	-2.65	122.23	126.23
23	r	601	CLA	CHB-C4A-NA	2.65	128.18	124.51
35	s	614	LUT	C38-C25-C24	-2.65	117.89	123.56
23	C	505	CLA	CHB-C4A-NA	2.65	128.17	124.51
23	C	509	CLA	CHB-C4A-NA	2.65	128.17	124.51
34	G	601	CHL	CHD-C4C-C3C	2.65	128.73	124.84
23	B	614	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
34	g	601	CHL	CHD-C1D-ND	-2.65	122.02	124.45
34	g	605	CHL	CHB-C4A-NA	2.65	128.17	124.51
23	c	512	CLA	C2C-C1C-NC	2.64	112.45	109.97
37	r	616	XAT	C8-C9-C10	-2.64	114.88	118.94
23	C	508	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
34	G	605	CHL	CHB-C4A-NA	2.64	128.17	124.51
37	g	620	XAT	C24-C23-C22	-2.64	105.67	110.77
23	n	305	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
35	S	614	LUT	C38-C25-C24	-2.64	117.91	123.56
23	s	613	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CMB-C2B-C3B	2.64	129.61	124.68
35	Y	315	LUT	C30-C31-C32	-2.63	115.00	123.22
36	S	616	NEX	C2-C1-C6	2.63	111.77	109.21
23	c	504	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	c	512	CLA	CMC-C2C-C3C	2.63	133.26	126.12
23	R	611	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
35	N	316	LUT	C17-C1-C6	2.63	114.56	110.30
25	d	406	BCR	C30-C25-C26	-2.63	118.91	122.61
34	n	308	CHL	CMB-C2B-C3B	2.63	129.60	124.68
23	s	610	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	S	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	C	510	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	G	614	CLA	CHB-C4A-NA	2.63	128.14	124.51
27	C	501	LMG	C8-O7-C10	-2.63	111.33	117.79
34	Y	307	CHL	C1B-CHB-C4A	-2.63	124.92	130.12
23	g	612	CLA	O2D-CGD-CBD	2.63	115.93	111.27
27	d	409	LMG	O8-C28-C29	2.63	120.15	111.91
30	r	618	LHG	C6-C5-C4	-2.62	105.58	111.79
25	c	518	BCR	C29-C30-C25	2.62	114.52	110.48
34	g	619	CHL	CHB-C4A-NA	2.62	128.14	124.51
23	C	510	CLA	C2A-C1A-CHA	2.62	128.44	123.86
25	Z	101	BCR	C33-C5-C6	-2.62	121.59	124.53
34	g	605	CHL	OMC-CMC-C2C	-2.62	119.76	125.69
24	D	402	PHO	C1B-NB-C4B	2.62	112.47	107.09
26	A	406	SQD	O48-C23-C24	2.62	120.12	111.91
25	C	515	BCR	C33-C5-C4	2.61	118.64	113.62
23	y	311	CLA	CMB-C2B-C3B	2.61	129.57	124.68
33	E	101	HEM	C4D-ND-C1D	2.61	107.77	105.07
36	R	617	NEX	C4-C3-C2	-2.61	105.73	110.77
23	c	510	CLA	O2D-CGD-CBD	2.61	115.91	111.27
25	B	618	BCR	C10-C11-C12	-2.61	115.07	123.22
25	H	101	BCR	C15-C14-C13	-2.61	123.58	127.31
25	K	101	BCR	C11-C10-C9	-2.61	123.58	127.31
34	g	606	CHL	C2A-C1A-CHA	2.61	128.42	123.86
36	N	318	NEX	C11-C12-C13	-2.61	119.09	126.42
23	c	512	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	R	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	a	408	DGD	O1G-C1A-C2A	2.61	120.08	111.91
34	R	606	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
23	c	503	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
34	g	609	CHL	CMB-C2B-C3B	2.60	129.55	124.68
36	S	616	NEX	C11-C12-C13	-2.60	119.10	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	405	CLA	CMB-C2B-C3B	2.60	129.55	124.68
23	C	504	CLA	CMC-C2C-C1C	-2.60	121.08	125.04
35	n	317	LUT	C22-C23-C24	-2.60	108.78	111.74
23	S	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	c	505	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
30	n	319	LHG	O8-C23-C24	2.60	120.06	111.91
36	g	617	NEX	C11-C12-C13	-2.60	119.12	126.42
23	b	604	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	c	513	CLA	CHB-C4A-NA	2.60	128.10	124.51
35	S	614	LUT	C39-C29-C28	2.59	122.17	118.08
23	a	401	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	R	614	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	C	516	BCR	C37-C22-C23	2.59	122.16	118.08
23	B	604	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	c	509	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	y	303	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	s	610	CLA	CAA-C2A-C3A	-2.59	107.79	114.26
23	c	512	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
23	C	511	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
35	Y	316	LUT	C7-C8-C9	-2.59	122.33	126.23
23	G	603	CLA	CHB-C4A-NA	2.58	128.09	124.51
23	C	507	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
23	N	305	CLA	O2D-CGD-CBD	2.58	115.86	111.27
34	G	605	CHL	OMC-CMC-C2C	-2.58	119.85	125.69
34	r	605	CHL	O2D-CGD-O1D	-2.58	118.80	123.84
34	g	606	CHL	CMB-C2B-C1B	-2.58	124.50	128.46
23	B	603	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	R	602	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	d	401	PHO	C1B-NB-C4B	2.58	112.38	107.09
23	B	613	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
23	N	314	CLA	O2D-CGD-CBD	2.58	115.84	111.27
23	y	303	CLA	CHD-C1D-ND	-2.58	122.09	124.45
26	M	101	SQD	O9-S-C6	2.58	110.00	106.94
23	s	611	CLA	C2A-C1A-CHA	2.58	128.36	123.86
23	G	614	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
36	n	318	NEX	C11-C12-C13	-2.57	119.18	126.42
23	B	604	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
34	N	308	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
23	B	603	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	r	601	CLA	C2A-C1A-CHA	2.57	128.35	123.86
34	g	601	CHL	C2C-C3C-C4C	2.57	108.32	106.49
30	s	617	LHG	O8-C23-C24	2.57	119.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	301	XAT	C24-C23-C22	-2.57	105.81	110.77
23	b	604	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
25	b	617	BCR	C15-C16-C17	-2.57	118.22	123.47
23	S	609	CLA	CHB-C4A-NA	2.57	128.06	124.51
34	n	307	CHL	O2D-CGD-O1D	-2.57	118.82	123.84
34	g	606	CHL	CAA-C2A-C1A	-2.56	106.46	112.14
23	g	604	CLA	CHB-C4A-NA	2.56	128.06	124.51
35	G	616	LUT	C31-C30-C29	-2.56	123.65	127.31
23	b	604	CLA	CMB-C2B-C3B	2.56	129.47	124.68
33	e	101	HEM	C4C-CHD-C1D	2.56	125.94	122.56
23	s	609	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	C	513	CLA	C2A-C1A-CHA	2.56	128.33	123.86
25	F	101	BCR	C38-C26-C27	2.56	118.53	113.62
30	G	618	LHG	C5-O7-C7	-2.56	111.49	117.79
30	g	618	LHG	O8-C23-C24	2.56	119.93	111.91
34	S	607	CHL	CHD-C1D-ND	-2.56	122.10	124.45
23	s	610	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	G	613	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
35	n	317	LUT	C15-C14-C13	-2.56	123.66	127.31
26	L	103	SQD	O9-S-C6	2.55	109.97	106.94
34	r	606	CHL	CHD-C1D-ND	-2.55	122.11	124.45
30	N	319	LHG	O8-C23-C24	2.55	119.92	111.91
23	a	405	CLA	O2D-CGD-CBD	2.55	115.80	111.27
34	n	308	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
23	N	315	CLA	CMA-C3A-C2A	-2.55	110.15	116.10
23	c	506	CLA	CHB-C4A-NA	2.55	128.04	124.51
36	N	318	NEX	C16-C1-C6	2.55	112.75	110.47
23	G	603	CLA	O2D-CGD-CBD	2.55	115.79	111.27
23	r	614	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	a	401	CLA	C7-C6-C5	-2.54	106.45	113.36
23	r	610	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	A	401	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	g	612	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
34	S	605	CHL	CMB-C2B-C1B	-2.54	124.56	128.46
34	N	309	CHL	O2D-CGD-CBD	2.54	115.78	111.27
34	S	605	CHL	CHB-C4A-NA	2.54	128.02	124.51
23	y	304	CLA	C2D-C1D-ND	-2.54	108.23	110.10
25	b	618	BCR	C10-C11-C12	-2.54	115.30	123.22
23	c	512	CLA	C2A-C1A-CHA	2.53	128.29	123.86
25	b	618	BCR	C30-C25-C26	-2.53	119.05	122.61
23	R	608	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
36	r	617	NEX	O24-C25-C38	2.53	118.09	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	n	318	NEX	C4-C3-C2	-2.53	105.88	110.77
23	s	604	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
35	S	614	LUT	C20-C13-C12	2.53	122.06	118.08
23	C	502	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	b	604	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
34	R	613	CHL	OMC-CMC-C2C	-2.53	119.97	125.69
34	s	607	CHL	CHB-C4A-NA	2.53	128.01	124.51
23	S	609	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	g	611	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
23	g	602	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
34	S	605	CHL	C1D-ND-C4D	2.53	108.13	106.33
23	y	305	CLA	CHB-C4A-NA	2.53	128.00	124.51
34	N	310	CHL	O2A-CGA-O1A	-2.52	117.22	123.59
23	R	601	CLA	C2A-C1A-CHA	2.52	128.27	123.86
23	y	312	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
34	N	307	CHL	CMB-C2B-C3B	2.52	129.40	124.68
25	C	515	BCR	C38-C26-C25	-2.52	121.70	124.53
34	Y	307	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
34	R	606	CHL	CHD-C1D-ND	-2.52	122.14	124.45
23	C	505	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
23	y	310	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
34	s	605	CHL	CHB-C4A-NA	2.52	127.99	124.51
23	G	602	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
36	r	617	NEX	C4-C3-C2	-2.52	105.92	110.77
34	G	601	CHL	O2D-CGD-O1D	-2.51	118.92	123.84
23	G	602	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	g	613	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
37	n	301	XAT	C7-C8-C9	-2.51	121.63	125.53
34	N	308	CHL	OMC-CMC-C2C	-2.51	120.01	125.69
23	C	503	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
35	y	316	LUT	C38-C25-C24	-2.51	118.19	123.56
23	C	513	CLA	C2C-C1C-NC	2.51	112.32	109.97
23	b	616	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	B	616	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	C	507	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	N	310	CHL	OMC-CMC-C2C	-2.51	120.02	125.69
23	R	602	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
34	N	302	CHL	C3C-C4C-NC	-2.51	107.76	110.57
36	s	616	NEX	C11-C12-C13	-2.51	119.37	126.42
30	Y	318	LHG	O8-C23-C24	2.51	119.77	111.91
28	H	102	DGD	O1G-C1A-C2A	2.50	119.77	111.91
25	d	406	BCR	C24-C23-C22	-2.50	122.45	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	S	613	CLA	C4A-NA-C1A	2.50	107.83	106.71
23	c	513	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	D	405	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	R	614	CLA	O2D-CGD-CBD	2.50	115.71	111.27
25	H	101	BCR	C11-C10-C9	-2.50	123.75	127.31
25	h	101	BCR	C3-C4-C5	-2.50	109.62	114.08
23	c	511	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
34	Y	306	CHL	CAA-C2A-C3A	-2.50	105.94	112.78
23	c	510	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
35	s	614	LUT	C1-C2-C3	2.50	119.28	113.64
23	B	616	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
37	g	620	XAT	C27-C28-C29	-2.49	121.66	125.53
23	C	514	CLA	CHB-C4A-NA	2.49	127.96	124.51
27	C	501	LMG	O8-C28-C29	2.49	119.73	111.91
25	d	406	BCR	C38-C26-C27	2.49	118.40	113.62
34	S	601	CHL	CHD-C1D-ND	-2.49	122.17	124.45
25	d	406	BCR	C16-C17-C18	-2.49	123.76	127.31
34	R	605	CHL	CHD-C1D-ND	-2.49	122.17	124.45
23	A	402	CLA	O2D-CGD-CBD	2.49	115.69	111.27
23	Y	304	CLA	CAA-CBA-CGA	-2.49	105.99	113.25
25	B	618	BCR	C30-C25-C26	-2.49	119.11	122.61
23	C	513	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
23	Y	303	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
23	n	305	CLA	O2D-CGD-CBD	2.48	115.68	111.27
23	b	605	CLA	C11-C12-C13	-2.48	107.89	115.92
34	s	606	CHL	CHB-C4A-NA	2.48	127.94	124.51
23	N	303	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	s	606	CHL	C2A-C1A-CHA	2.48	128.20	123.86
23	N	313	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	d	406	BCR	C27-C26-C25	-2.48	119.13	122.73
23	G	612	CLA	O2D-CGD-CBD	2.48	115.67	111.27
23	r	602	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
34	y	307	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
34	R	607	CHL	OMC-CMC-C2C	-2.48	120.09	125.69
37	G	620	XAT	C36-C21-C22	-2.48	104.68	108.98
34	y	306	CHL	CAA-C2A-C1A	-2.48	103.86	111.97
25	Z	101	BCR	C29-C30-C25	2.48	114.29	110.48
35	S	615	LUT	C10-C11-C12	-2.47	115.50	123.22
28	C	517	DGD	O3E-C3E-C4E	-2.47	104.63	110.35
23	n	313	CLA	C2A-C1A-CHA	2.47	128.18	123.86
23	C	506	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	c	504	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	314	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
34	G	606	CHL	CMB-C2B-C1B	-2.47	124.67	128.46
23	a	401	CLA	C11-C12-C13	-2.47	107.94	115.92
30	y	318	LHG	O8-C23-C24	2.47	119.65	111.91
23	D	404	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	B	605	CLA	O2D-CGD-CBD	2.46	115.64	111.27
35	g	615	LUT	C38-C25-C24	-2.46	118.29	123.56
34	G	605	CHL	CHD-C1D-ND	-2.46	122.19	124.45
23	B	608	CLA	CAC-C3C-C4C	2.46	128.00	124.81
23	r	601	CLA	CAC-C3C-C2C	-2.46	123.32	127.53
23	c	503	CLA	CHB-C4A-NA	2.46	127.92	124.51
35	G	615	LUT	C38-C25-C24	-2.46	118.29	123.56
23	c	504	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
23	C	509	CLA	O2A-C1-C2	2.46	115.10	108.64
23	N	312	CLA	CHD-C1D-ND	-2.46	122.20	124.45
23	n	311	CLA	C4A-NA-C1A	2.46	107.81	106.71
35	r	615	LUT	C38-C25-C24	-2.46	118.31	123.56
34	g	608	CHL	OMC-CMC-C2C	-2.46	120.14	125.69
30	g	618	LHG	C5-O7-C7	-2.45	111.75	117.79
37	Y	301	XAT	C24-C23-C22	-2.45	106.03	110.77
35	s	614	LUT	C39-C29-C28	2.45	121.94	118.08
35	y	316	LUT	C7-C8-C9	-2.45	122.53	126.23
23	n	314	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
23	Y	311	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
25	c	514	BCR	C34-C9-C10	-2.45	119.50	122.92
23	R	603	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	N	314	CLA	CAA-C2A-C1A	2.44	119.98	111.97
23	c	502	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
34	G	607	CHL	C2A-C1A-CHA	2.44	128.13	123.86
23	C	511	CLA	O2D-CGD-CBD	2.44	115.61	111.27
23	Y	312	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	y	312	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	y	313	CLA	CAC-C3C-C4C	2.44	127.98	124.81
23	r	603	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
34	g	606	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
30	B	621	LHG	O8-C23-O10	-2.44	117.44	123.59
23	g	612	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
35	R	615	LUT	C38-C25-C24	-2.44	118.34	123.56
23	C	505	CLA	CHD-C1D-ND	-2.44	122.21	124.45
37	y	301	XAT	C15-C35-C34	-2.44	118.48	123.47
23	A	402	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	n	315	CLA	CHB-C4A-NA	2.44	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	Y	311	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
23	y	304	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
23	r	611	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
23	b	608	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	a	406	BCR	C29-C28-C27	-2.43	105.94	111.38
25	c	518	BCR	C33-C5-C4	2.43	118.28	113.62
23	c	506	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
27	D	407	LMG	O8-C28-C29	2.43	119.53	111.91
34	y	307	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
23	y	311	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
37	R	616	XAT	C8-C9-C10	-2.43	115.22	118.94
23	b	612	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
23	r	608	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
23	a	403	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	c	518	BCR	C33-C5-C6	-2.42	121.81	124.53
30	L	101	LHG	O8-C23-C24	2.42	119.51	111.91
23	B	611	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
23	G	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
36	R	617	NEX	C26-C27-C28	-2.42	120.88	125.99
34	n	307	CHL	CHD-C1D-C2D	2.42	130.56	125.48
23	c	502	CLA	C3A-C2A-C1A	2.42	104.96	101.34
34	N	309	CHL	CHD-C1D-ND	-2.42	122.23	124.45
23	B	606	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	b	613	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
34	N	307	CHL	C3C-C4C-NC	-2.42	107.86	110.57
34	G	601	CHL	CHD-C1D-C2D	2.42	130.55	125.48
25	F	101	BCR	C33-C5-C6	-2.42	121.82	124.53
23	g	614	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
34	n	309	CHL	O2A-CGA-O1A	-2.41	117.50	123.59
23	s	603	CLA	CHA-C1A-NA	-2.41	120.87	126.40
25	B	617	BCR	C33-C5-C4	2.41	118.25	113.62
34	s	601	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
34	n	302	CHL	C3C-C4C-NC	-2.41	107.87	110.57
23	a	403	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
23	S	611	CLA	CHA-C1A-NA	-2.41	120.88	126.40
23	r	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	s	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	b	606	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	B	602	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
34	g	601	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
25	c	514	BCR	C15-C14-C13	-2.41	123.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	Y	304	CLA	C2D-C1D-ND	-2.41	108.33	110.10
35	R	615	LUT	C35-C15-C14	-2.41	118.54	123.47
23	b	606	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
23	Y	304	CLA	O2D-CGD-CBD	2.41	115.54	111.27
27	a	407	LMG	O1-C7-C8	2.41	116.70	110.90
34	G	609	CHL	CMB-C2B-C3B	2.41	129.18	124.68
30	b	621	LHG	O8-C23-O10	-2.41	117.52	123.59
25	h	101	BCR	C15-C14-C13	-2.41	123.88	127.31
35	g	616	LUT	C20-C13-C12	2.40	121.87	118.08
26	A	406	SQD	O6-C1-C2	2.40	112.06	108.30
23	c	505	CLA	CHB-C4A-NA	2.40	127.84	124.51
37	Y	301	XAT	C11-C10-C9	-2.40	123.88	127.31
23	A	402	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
34	G	608	CHL	OMC-CMC-C2C	-2.40	120.25	125.69
23	b	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	N	309	CHL	O2A-CGA-O1A	-2.40	117.53	123.59
25	c	514	BCR	C1-C6-C7	2.40	122.57	115.78
23	C	514	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
34	N	307	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
34	N	306	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
23	R	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	r	613	CHL	OMC-CMC-C2C	-2.40	120.27	125.69
34	g	609	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
25	B	618	BCR	C20-C21-C22	-2.40	123.89	127.31
30	A	411	LHG	C5-O7-C7	-2.40	111.89	117.79
33	e	101	HEM	C4D-ND-C1D	2.40	107.55	105.07
23	y	311	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	C	512	CLA	C1D-ND-C4D	-2.39	104.63	106.33
23	s	604	CLA	CAA-C2A-C3A	-2.39	106.22	112.78
34	S	605	CHL	OMC-CMC-C2C	-2.39	120.28	125.69
23	B	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
35	G	615	LUT	C19-C9-C8	2.39	121.84	118.08
23	B	602	CLA	CHB-C4A-NA	2.39	127.82	124.51
34	N	307	CHL	C2D-C1D-ND	-2.39	108.34	110.10
23	B	609	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
33	E	101	HEM	CAB-C3B-C2B	-2.39	120.74	128.60
23	n	305	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	C	515	BCR	C38-C26-C27	2.39	118.20	113.62
23	s	613	CLA	CAA-C2A-C3A	-2.39	110.53	116.10
34	n	310	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
23	b	616	CLA	C1B-CHB-C4A	-2.38	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C4A-NA-C1A	2.38	107.78	106.71
35	s	615	LUT	C10-C11-C12	-2.38	115.78	123.22
35	S	614	LUT	C15-C14-C13	-2.38	123.91	127.31
34	S	605	CHL	CHD-C1D-ND	-2.38	122.27	124.45
34	S	601	CHL	CHB-C4A-NA	2.38	127.81	124.51
23	N	312	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
34	y	309	CHL	C1C-C2C-C3C	-2.38	105.22	107.11
23	r	602	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
37	R	616	XAT	C20-C13-C12	2.38	121.83	118.08
25	a	406	BCR	C21-C20-C19	-2.38	115.79	123.22
23	A	401	CLA	CBA-CAA-C2A	-2.38	106.84	113.86
23	b	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
36	R	617	NEX	C24-C23-C22	-2.38	106.18	110.77
23	S	610	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	Z	101	BCR	C36-C18-C17	-2.38	119.59	122.92
35	S	614	LUT	C15-C35-C34	-2.38	118.61	123.47
25	Z	101	BCR	C10-C11-C12	-2.38	115.80	123.22
23	y	311	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
25	d	406	BCR	C33-C5-C6	-2.38	121.86	124.53
34	R	606	CHL	OMC-CMC-C2C	-2.37	120.32	125.69
23	N	315	CLA	CHB-C4A-NA	2.37	127.80	124.51
25	c	515	BCR	C11-C12-C13	-2.37	119.75	126.42
34	g	619	CHL	C1-C2-C3	-2.37	121.94	126.04
23	n	303	CLA	CAC-C3C-C4C	2.37	127.89	124.81
34	g	601	CHL	CHC-C1C-NC	2.37	127.80	124.20
23	c	513	CLA	C2A-C1A-CHA	2.37	128.01	123.86
23	n	311	CLA	C1-C2-C3	-2.37	121.94	126.04
23	C	504	CLA	CMB-C2B-C3B	2.37	129.12	124.68
34	g	601	CHL	CHB-C4A-NA	2.37	127.79	124.51
35	Y	316	LUT	C38-C25-C24	-2.37	118.48	123.56
25	C	515	BCR	C30-C25-C26	-2.37	119.27	122.61
23	g	603	CLA	O2D-CGD-CBD	2.37	115.48	111.27
23	n	312	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
34	r	606	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
25	d	406	BCR	C1-C6-C5	-2.37	119.28	122.61
23	a	403	CLA	O2D-CGD-CBD	2.37	115.48	111.27
35	N	316	LUT	C20-C13-C12	2.37	121.81	118.08
25	Z	101	BCR	C21-C20-C19	-2.37	115.83	123.22
23	y	312	CLA	C11-C10-C8	-2.37	108.27	115.92
23	c	509	CLA	CHB-C4A-NA	2.37	127.78	124.51
34	g	619	CHL	C2D-C1D-ND	-2.37	108.36	110.10
23	Y	304	CLA	O2A-CGA-O1A	-2.36	117.62	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	411	LHG	C5-O7-C7	-2.36	111.97	117.79
34	S	606	CHL	CAA-C2A-C1A	2.36	117.37	112.14
25	Z	101	BCR	C33-C5-C4	2.36	118.16	113.62
23	g	603	CLA	C3A-C2A-C1A	2.36	104.88	101.34
23	B	611	CLA	CHB-C4A-NA	2.36	127.78	124.51
34	s	607	CHL	C2A-C3A-C4A	-2.36	98.05	101.87
23	b	604	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
34	G	607	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
23	b	608	CLA	C4-C3-C5	2.36	119.24	115.27
37	n	301	XAT	C4-C3-C2	-2.36	106.22	110.77
23	B	605	CLA	CMB-C2B-C3B	2.36	129.09	124.68
23	N	305	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	B	602	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
35	Y	316	LUT	C37-C21-C22	-2.36	104.97	109.44
23	r	611	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
23	y	304	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
23	c	511	CLA	CHB-C4A-NA	2.35	127.77	124.51
23	g	603	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
25	b	617	BCR	C33-C5-C4	2.35	118.13	113.62
34	G	609	CHL	O2D-CGD-CBD	2.35	115.45	111.27
34	r	607	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
34	r	613	CHL	CAA-C2A-C3A	-2.35	110.61	116.10
37	g	620	XAT	C36-C21-C22	-2.35	104.90	108.98
23	b	605	CLA	C1-C2-C3	-2.35	121.98	126.04
26	d	402	SQD	O6-C1-C2	2.35	111.97	108.30
23	C	508	CLA	CAA-C2A-C1A	2.35	119.66	111.97
23	B	614	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
34	N	308	CHL	CHA-C1A-NA	-2.34	121.03	126.40
30	S	617	LHG	O8-C23-C24	2.34	119.27	111.91
25	C	516	BCR	C11-C12-C13	-2.34	119.83	126.42
23	C	514	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
37	n	301	XAT	C27-C28-C29	-2.34	121.90	125.53
34	g	601	CHL	CHD-C4C-C3C	2.34	128.28	124.84
23	a	401	CLA	CBA-CAA-C2A	-2.34	106.95	113.86
37	G	620	XAT	C24-C23-C22	-2.34	106.25	110.77
23	y	312	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
34	S	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
23	Y	312	CLA	O2A-C1-C2	-2.34	102.49	108.64
33	e	101	HEM	CHD-C1D-ND	2.34	126.97	124.43
23	b	616	CLA	C2D-C1D-ND	-2.34	108.38	110.10
23	b	611	CLA	CHB-C4A-NA	2.34	127.74	124.51
34	G	607	CHL	O2D-CGD-O1D	-2.34	119.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	603	CLA	C3A-C2A-C1A	2.34	104.84	101.34
23	S	613	CLA	CAA-C2A-C3A	-2.34	110.65	116.10
36	s	616	NEX	C16-C1-C6	2.33	112.56	110.47
37	N	301	XAT	C4-C3-C2	-2.33	106.27	110.77
34	G	619	CHL	CHB-C4A-NA	2.33	127.74	124.51
25	F	101	BCR	C27-C26-C25	-2.33	119.34	122.73
25	F	101	BCR	C21-C20-C19	-2.33	115.94	123.22
23	b	614	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	A	401	CLA	C4-C3-C5	2.33	119.19	115.27
34	S	605	CHL	CHD-C4C-C3C	2.33	128.26	124.84
35	s	614	LUT	C20-C13-C12	2.33	121.75	118.08
33	e	101	HEM	CBA-CAA-C2A	-2.33	108.65	112.62
23	n	314	CLA	C2A-C1A-CHA	2.33	127.93	123.86
34	g	607	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
37	y	301	XAT	C10-C11-C12	-2.33	115.95	123.22
23	y	312	CLA	O2A-C1-C2	-2.33	102.52	108.64
34	g	609	CHL	C1D-ND-C4D	2.33	107.99	106.33
34	Y	302	CHL	C3C-C4C-NC	-2.32	107.96	110.57
34	R	607	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
23	C	513	CLA	O2D-CGD-CBD	2.32	115.40	111.27
34	S	606	CHL	CHA-C1A-NA	-2.32	121.08	126.40
23	D	404	CLA	CAA-CBA-CGA	-2.32	106.47	113.25
25	k	101	BCR	C27-C26-C25	-2.32	119.36	122.73
23	c	512	CLA	C1-C2-C3	-2.32	122.03	126.04
23	N	315	CLA	O2D-CGD-CBD	2.32	115.39	111.27
23	s	602	CLA	CAC-C3C-C4C	2.32	127.82	124.81
35	G	615	LUT	C11-C10-C9	-2.32	124.00	127.31
23	d	404	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	B	618	BCR	C38-C26-C25	-2.32	121.93	124.53
34	N	308	CHL	O2A-CGA-O1A	-2.32	117.53	123.30
34	S	601	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
34	y	309	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
25	A	405	BCR	C21-C20-C19	-2.31	116.00	123.22
34	g	619	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
23	b	602	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	F	101	BCR	C15-C14-C13	-2.31	124.01	127.31
23	s	613	CLA	C2D-C1D-ND	-2.31	108.40	110.10
23	Y	312	CLA	C11-C10-C8	-2.31	108.45	115.92
23	b	609	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
23	B	615	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
36	s	616	NEX	C26-C27-C28	-2.31	121.11	125.99
34	n	308	CHL	O2A-CGA-O1A	-2.31	117.54	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C39-C30-C25	-2.31	106.55	110.30
35	Y	315	LUT	C20-C13-C12	2.31	121.72	118.08
25	d	406	BCR	C21-C20-C19	-2.31	116.01	123.22
25	b	618	BCR	C38-C26-C25	-2.31	121.94	124.53
23	R	602	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	C	503	CLA	C4-C3-C5	2.31	119.15	115.27
23	c	507	CLA	CAA-C2A-C1A	2.31	119.54	111.97
23	R	611	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
23	c	507	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
23	S	609	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	c	511	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
25	c	515	BCR	C37-C22-C23	2.30	121.71	118.08
23	a	402	CLA	C4A-NA-C1A	2.30	107.74	106.71
23	S	613	CLA	C2D-C1D-ND	-2.30	108.41	110.10
34	G	605	CHL	C2D-C1D-ND	-2.30	108.41	110.10
23	G	612	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
35	N	316	LUT	C22-C23-C24	2.30	114.36	111.74
28	c	516	DGD	O3G-C3G-C2G	-2.30	105.34	110.90
25	c	515	BCR	C33-C5-C4	2.30	118.04	113.62
30	a	412	LHG	C5-O7-C7	-2.30	112.13	117.79
23	C	510	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	a	401	CLA	CHC-C1C-NC	2.30	127.69	124.20
34	G	619	CHL	OMC-CMC-C2C	-2.30	120.49	125.69
25	C	516	BCR	C23-C22-C21	-2.30	115.41	118.94
25	h	101	BCR	C38-C26-C25	-2.30	121.95	124.53
23	B	609	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
35	g	616	LUT	C35-C34-C33	-2.30	124.03	127.31
23	A	401	CLA	C11-C12-C13	-2.30	108.50	115.92
34	n	302	CHL	C1C-C2C-C3C	-2.29	105.29	107.11
34	g	608	CHL	CHB-C4A-NA	2.29	127.69	124.51
35	S	614	LUT	C11-C10-C9	-2.29	124.04	127.31
25	A	405	BCR	C29-C28-C27	-2.29	106.25	111.38
23	C	508	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
36	R	617	NEX	C16-C1-C6	2.29	112.52	110.47
23	R	610	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
34	Y	309	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
23	A	401	CLA	C3A-C2A-C1A	2.29	104.77	101.34
23	b	605	CLA	CMB-C2B-C3B	2.29	128.96	124.68
34	G	601	CHL	CHA-C4D-ND	2.29	137.28	132.50
30	d	408	LHG	O8-C23-C24	2.29	119.09	111.91
37	y	301	XAT	C24-C23-C22	-2.29	106.36	110.77
34	R	605	CHL	CHB-C4A-NA	2.29	127.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C1-C6-C5	-2.29	119.39	122.61
28	C	517	DGD	C6E-C5E-C4E	-2.29	107.65	113.00
23	Y	303	CLA	CBC-CAC-C3C	2.29	118.73	112.43
23	R	611	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
23	S	604	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
34	N	307	CHL	CHD-C1D-C2D	2.28	130.27	125.48
23	Y	305	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	N	304	CLA	C2A-C1A-CHA	2.28	127.85	123.86
34	Y	307	CHL	O2A-CGA-O1A	-2.28	117.83	123.59
23	B	605	CLA	C1-C2-C3	-2.28	122.10	126.04
36	n	318	NEX	C31-C32-C33	-2.28	120.01	126.42
23	r	608	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
34	g	605	CHL	O2D-CGD-CBD	2.28	115.32	111.27
23	B	612	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	C	503	CLA	C7-C6-C5	-2.28	107.17	113.36
25	B	617	BCR	C21-C20-C19	-2.28	116.10	123.22
34	G	606	CHL	CHB-C4A-NA	2.28	127.66	124.51
23	S	604	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
23	d	404	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
25	K	101	BCR	C20-C21-C22	-2.28	124.06	127.31
36	n	318	NEX	O24-C25-C26	-2.28	57.07	58.96
37	n	301	XAT	C24-C23-C22	-2.28	106.38	110.77
34	y	307	CHL	O2A-CGA-O1A	-2.28	117.85	123.59
25	c	515	BCR	C1-C6-C5	-2.28	119.41	122.61
23	r	604	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	c	502	CLA	C2A-C1A-CHA	2.27	127.83	123.86
35	y	316	LUT	C37-C21-C22	-2.27	105.14	109.44
25	B	619	BCR	C31-C1-C6	-2.27	106.62	110.30
34	G	606	CHL	C2A-C1A-CHA	2.27	127.83	123.86
34	y	307	CHL	C2C-C3C-C4C	2.27	108.11	106.49
34	n	307	CHL	C3C-C4C-NC	-2.27	108.03	110.57
23	b	615	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
25	a	406	BCR	C28-C27-C26	-2.27	110.03	114.08
23	R	604	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
34	Y	309	CHL	C2A-C1A-CHA	2.27	127.82	123.86
35	G	616	LUT	C11-C12-C13	2.26	132.78	126.42
23	C	510	CLA	C11-C12-C13	-2.26	108.60	115.92
36	Y	317	NEX	C11-C12-C13	-2.26	120.06	126.42
34	n	307	CHL	C2A-C1A-CHA	2.26	127.82	123.86
23	G	604	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	c	518	BCR	C21-C20-C19	-2.26	116.16	123.22
35	Y	315	LUT	C15-C14-C13	-2.26	124.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	N	314	CLA	C2D-C1D-ND	-2.26	108.44	110.10
23	r	609	CLA	O1D-CGD-CBD	2.26	129.11	124.48
34	y	302	CHL	C3C-C4C-NC	-2.26	108.04	110.57
23	D	401	CLA	CHD-C4C-NC	2.26	127.76	124.20
34	S	605	CHL	O2A-CGA-O1A	-2.26	117.67	123.30
23	B	601	CLA	CHB-C4A-NA	2.26	127.63	124.51
23	Y	303	CLA	CHD-C1D-ND	-2.26	122.38	124.45
34	y	309	CHL	CHD-C1D-ND	-2.26	122.38	124.45
23	G	604	CLA	O1D-CGD-CBD	2.25	129.10	124.48
35	N	317	LUT	C20-C13-C14	-2.25	119.77	122.92
35	g	615	LUT	C1-C2-C3	2.25	118.73	113.64
23	Y	312	CLA	O1D-CGD-CBD	2.25	129.09	124.48
23	B	605	CLA	C11-C12-C13	-2.25	108.64	115.92
23	R	601	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	S	609	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
34	Y	308	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
23	b	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	d	406	BCR	C23-C24-C25	-2.25	120.88	127.20
23	y	304	CLA	O2D-CGD-CBD	2.25	115.27	111.27
23	g	610	CLA	CHD-C1D-ND	-2.25	122.39	124.45
23	B	614	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	Y	313	CLA	CHD-C1D-ND	-2.25	122.39	124.45
23	b	610	CLA	C2A-C1A-CHA	2.25	127.79	123.86
23	b	601	CLA	CHB-C4A-NA	2.25	127.62	124.51
34	G	609	CHL	CHA-C1A-NA	-2.25	121.25	126.40
34	s	605	CHL	O2A-CGA-O1A	-2.25	117.70	123.30
23	b	608	CLA	CAA-C2A-C1A	2.24	119.33	111.97
23	Y	311	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
23	s	611	CLA	CHA-C1A-NA	-2.24	121.26	126.40
23	C	514	CLA	CMD-C2D-C1D	-2.24	120.76	124.71
25	B	618	BCR	C37-C22-C23	2.24	121.61	118.08
25	k	101	BCR	C15-C14-C13	-2.24	124.11	127.31
35	s	614	LUT	C11-C10-C9	-2.24	124.11	127.31
35	S	614	LUT	C35-C15-C14	-2.24	118.88	123.47
34	G	609	CHL	CAA-C2A-C3A	-2.24	106.64	112.78
25	c	518	BCR	C10-C11-C12	-2.24	116.22	123.22
23	c	501	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	C	512	CLA	O1D-CGD-CBD	2.24	129.07	124.48
23	N	313	CLA	C2A-C1A-CHA	2.24	127.77	123.86
23	G	613	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	g	612	CLA	CAC-C3C-C2C	2.24	131.36	127.53
25	b	617	BCR	C21-C20-C19	-2.24	116.23	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	609	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
34	N	302	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
23	a	401	CLA	C3A-C2A-C1A	2.24	104.69	101.34
34	N	302	CHL	CHB-C4A-NA	2.23	127.60	124.51
23	A	401	CLA	C2A-C1A-CHA	2.23	127.77	123.86
23	B	610	CLA	C2A-C1A-CHA	2.23	127.77	123.86
23	N	315	CLA	CHD-C1D-ND	-2.23	122.40	124.45
23	C	503	CLA	C5-C3-C2	-2.23	116.60	121.12
34	g	608	CHL	O2A-CGA-O1A	-2.23	117.96	123.59
23	r	609	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	N	305	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	c	513	CLA	CMD-C2D-C1D	-2.23	120.78	124.71
23	c	509	CLA	CHA-C1A-NA	-2.23	121.29	126.40
34	Y	309	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
23	A	401	CLA	O2D-CGD-CBD	2.23	115.23	111.27
23	n	312	CLA	CBC-CAC-C3C	2.23	118.57	112.43
36	r	617	NEX	C24-C23-C22	-2.23	106.47	110.77
23	c	512	CLA	CHA-C1A-NA	-2.23	121.30	126.40
25	b	618	BCR	C39-C30-C25	-2.23	106.69	110.30
23	C	506	CLA	C4A-NA-C1A	2.23	107.71	106.71
23	G	613	CLA	O2D-CGD-CBD	2.23	115.22	111.27
36	N	318	NEX	C38-C25-C24	2.22	116.78	114.28
25	b	618	BCR	C37-C22-C23	2.22	121.58	118.08
23	C	504	CLA	CMC-C2C-C3C	2.22	132.15	126.12
34	r	613	CHL	C1D-CHD-C4C	-2.22	121.26	126.06
25	A	405	BCR	C16-C15-C14	-2.22	118.92	123.47
36	N	318	NEX	C31-C32-C33	-2.22	120.17	126.42
23	y	313	CLA	O2D-CGD-CBD	2.22	115.22	111.27
23	G	612	CLA	CAC-C3C-C2C	2.22	131.33	127.53
35	S	614	LUT	C19-C9-C8	2.22	121.58	118.08
23	S	603	CLA	CHA-C1A-NA	-2.22	121.31	126.40
34	r	605	CHL	CMB-C2B-C3B	2.22	128.83	124.68
23	B	608	CLA	C4-C3-C5	2.22	119.00	115.27
23	C	506	CLA	CAA-C2A-C1A	-2.22	104.70	111.97
30	c	517	LHG	O8-C23-C24	2.22	118.87	111.91
36	r	617	NEX	C11-C12-C13	-2.22	120.18	126.42
34	S	605	CHL	CHD-C1D-C2D	2.22	130.13	125.48
30	B	621	LHG	C5-O7-C7	-2.22	112.33	117.79
23	b	614	CLA	C11-C12-C13	-2.22	108.75	115.92
35	n	317	LUT	C30-C31-C32	-2.21	116.31	123.22
35	Y	316	LUT	C3-C4-C5	-2.21	107.44	111.85
34	n	306	CHL	O2D-CGD-O1D	-2.21	119.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	609	CHL	C3A-C2A-C1A	2.21	104.66	101.34
23	g	603	CLA	C2A-C1A-CHA	2.21	127.73	123.86
34	N	310	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
23	C	513	CLA	C1-C2-C3	-2.21	122.22	126.04
23	s	608	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	a	406	BCR	C33-C5-C6	-2.21	122.04	124.53
34	n	310	CHL	O2A-CGA-O1A	-2.21	118.01	123.59
23	B	605	CLA	C3C-C4C-NC	-2.21	108.09	110.57
36	G	617	NEX	C11-C12-C13	-2.21	120.20	126.42
35	n	317	LUT	C35-C34-C33	-2.21	124.15	127.31
34	G	609	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
25	C	515	BCR	C29-C28-C27	2.21	116.32	111.38
34	g	601	CHL	CHD-C1D-C2D	2.21	130.12	125.48
25	d	406	BCR	C33-C5-C4	2.21	117.86	113.62
34	N	307	CHL	C2A-C1A-CHA	2.21	127.72	123.86
35	n	317	LUT	C40-C33-C34	-2.21	119.83	122.92
23	n	315	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	y	313	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	b	605	CLA	C3C-C4C-NC	-2.21	108.09	110.57
23	N	303	CLA	CMA-C3A-C2A	-2.21	104.93	113.83
23	G	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
37	Y	301	XAT	C31-C32-C33	-2.21	120.22	126.42
33	e	101	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
35	S	615	LUT	C31-C32-C33	-2.20	120.22	126.42
23	D	401	CLA	C11-C10-C8	-2.20	108.80	115.92
23	c	509	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
25	d	406	BCR	C15-C14-C13	-2.20	124.17	127.31
23	y	305	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
37	y	301	XAT	C11-C10-C9	-2.20	124.17	127.31
23	C	504	CLA	CHB-C4A-NA	2.20	127.56	124.51
23	n	313	CLA	O2D-CGD-CBD	2.20	115.18	111.27
23	a	401	CLA	C2A-C1A-CHA	2.20	127.71	123.86
30	b	621	LHG	C5-O7-C7	-2.20	112.37	117.79
23	s	612	CLA	O2D-CGD-CBD	2.20	115.18	111.27
36	R	617	NEX	C39-C29-C30	-2.20	119.84	122.92
23	N	314	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
34	N	308	CHL	CAA-C2A-C3A	-2.20	106.75	112.78
34	R	605	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
23	C	513	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
23	N	314	CLA	C2A-C1A-CHA	2.20	127.70	123.86
34	S	607	CHL	CHD-C1D-C2D	2.20	130.09	125.48
25	c	514	BCR	C30-C25-C26	-2.20	119.52	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	g	609	CHL	CHA-C1A-NA	-2.20	121.37	126.40
25	A	405	BCR	C33-C5-C6	-2.20	122.06	124.53
23	C	507	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
36	r	617	NEX	C39-C29-C30	-2.20	119.85	122.92
35	y	316	LUT	C36-C21-C26	2.20	112.87	109.55
23	b	614	CLA	CHB-C4A-NA	2.20	127.55	124.51
34	n	308	CHL	C3A-C2A-C1A	2.20	104.63	101.34
23	b	608	CLA	CBA-CAA-C2A	2.20	120.34	113.86
35	G	615	LUT	C36-C21-C26	2.19	112.87	109.55
34	n	310	CHL	O2D-CGD-O1D	-2.19	119.55	123.84
33	e	101	HEM	CAB-C3B-C2B	-2.19	121.38	128.60
23	Y	311	CLA	C2A-C1A-CHA	2.19	127.69	123.86
35	y	315	LUT	C8-C9-C10	-2.19	115.58	118.94
34	G	601	CHL	CHD-C1D-ND	-2.19	122.44	124.45
36	N	318	NEX	O24-C25-C26	-2.19	57.15	58.96
25	F	101	BCR	C38-C26-C25	-2.19	122.07	124.53
25	Z	101	BCR	C36-C18-C19	2.19	121.53	118.08
23	b	615	CLA	C3A-C2A-C1A	2.19	104.62	101.34
37	y	301	XAT	C31-C32-C33	-2.19	120.27	126.42
23	S	610	CLA	O2D-CGD-CBD	2.19	115.16	111.27
25	H	101	BCR	C20-C19-C18	-2.19	120.28	126.42
34	G	608	CHL	O2A-CGA-O1A	-2.19	118.08	123.59
23	s	610	CLA	O2D-CGD-CBD	2.19	115.15	111.27
23	b	615	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
25	d	406	BCR	C15-C16-C17	-2.18	119.00	123.47
37	N	301	XAT	C31-C30-C29	-2.18	124.19	127.31
23	r	610	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
34	G	608	CHL	O2D-CGD-CBD	2.18	115.14	111.27
25	c	515	BCR	C8-C7-C6	-2.18	121.08	127.20
35	s	615	LUT	C8-C9-C10	-2.18	115.60	118.94
28	c	516	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
25	B	618	BCR	C4-C5-C6	-2.18	119.57	122.73
23	N	304	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	c	504	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	C	514	CLA	CBA-CAA-C2A	2.17	120.28	113.86
34	S	605	CHL	C2A-C1A-CHA	2.17	127.66	123.86
23	B	614	CLA	C11-C12-C13	-2.17	108.90	115.92
23	S	602	CLA	CAC-C3C-C4C	2.17	127.63	124.81
34	S	607	CHL	C3C-C4C-NC	-2.17	108.14	110.57
34	g	607	CHL	CHA-C1A-NA	-2.17	121.42	126.40
35	r	615	LUT	C16-C1-C6	-2.17	106.78	110.30
23	R	611	CLA	CHA-C1A-NA	-2.17	121.43	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	623	LHG	O8-C23-O10	-2.17	118.11	123.59
28	c	516	DGD	O1G-C1A-O1A	-2.17	118.12	123.59
23	C	504	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
25	b	619	BCR	C3-C4-C5	-2.17	110.21	114.08
23	c	512	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
35	G	615	LUT	C12-C13-C14	-2.17	115.62	118.94
23	C	511	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
26	A	409	SQD	C45-O47-C7	-2.17	112.46	117.79
23	a	402	CLA	CHD-C4C-NC	2.17	127.62	124.20
23	Y	314	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	s	604	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
23	R	604	CLA	C2A-C1A-CHA	2.16	127.64	123.86
23	B	605	CLA	CED-O2D-CGD	2.16	120.83	115.94
23	n	303	CLA	O2D-CGD-CBD	2.16	115.11	111.27
35	n	316	LUT	C22-C23-C24	2.16	114.20	111.74
34	y	308	CHL	OMC-CMC-C2C	-2.16	120.80	125.69
34	y	306	CHL	CHD-C1D-ND	-2.16	122.47	124.45
36	g	617	NEX	O24-C25-C38	2.16	117.64	115.06
37	r	616	XAT	C12-C13-C14	-2.16	115.63	118.94
25	b	617	BCR	C1-C6-C5	-2.16	119.57	122.61
23	C	512	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
23	y	314	CLA	O2D-CGD-CBD	2.16	115.11	111.27
23	c	510	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	y	313	CLA	C2A-C1A-CHA	2.16	127.64	123.86
34	r	606	CHL	O2A-CGA-O1A	-2.16	117.92	123.30
34	G	609	CHL	C3A-C2A-C1A	2.16	104.57	101.34
23	D	405	CLA	O1D-CGD-CBD	2.16	128.90	124.48
35	r	615	LUT	C11-C12-C13	-2.16	120.36	126.42
36	N	318	NEX	C28-C29-C30	2.16	122.25	118.94
23	g	613	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
25	B	619	BCR	C3-C4-C5	-2.15	110.23	114.08
23	s	608	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
23	s	609	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
34	G	606	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
23	S	612	CLA	C3A-C2A-C1A	2.15	104.56	101.34
23	b	608	CLA	CAC-C3C-C4C	2.15	127.60	124.81
34	g	607	CHL	OMC-CMC-C2C	-2.15	120.83	125.69
23	r	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
23	a	401	CLA	C2D-C1D-ND	-2.15	108.52	110.10
36	y	317	NEX	C28-C29-C30	2.15	122.24	118.94
23	Y	314	CLA	O2D-CGD-CBD	2.15	115.09	111.27
35	N	317	LUT	C19-C9-C10	-2.15	119.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	N	304	CLA	C3A-C2A-C1A	2.15	104.56	101.34
27	A	407	LMG	O8-C28-O10	-2.15	118.17	123.59
23	C	511	CLA	C3C-C4C-NC	-2.15	108.16	110.57
25	B	619	BCR	C20-C21-C22	-2.15	124.25	127.31
25	C	515	BCR	C15-C14-C13	-2.15	124.25	127.31
28	c	516	DGD	C1E-O6E-C5E	2.14	117.90	113.69
25	b	618	BCR	C20-C21-C22	-2.14	124.25	127.31
23	b	605	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
23	c	513	CLA	CMD-C2D-C3D	2.14	132.55	127.61
34	n	306	CHL	CHB-C4A-NA	2.14	127.48	124.51
23	s	612	CLA	C3A-C2A-C1A	2.14	104.55	101.34
23	R	603	CLA	O2D-CGD-CBD	2.14	115.08	111.27
35	S	614	LUT	C2-C3-C4	2.14	113.24	110.30
23	G	612	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
23	c	512	CLA	CAA-C2A-C1A	2.14	118.99	111.97
30	T	101	LHG	O8-C23-O10	-2.14	118.19	123.59
23	y	311	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
23	B	615	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
35	Y	315	LUT	C7-C8-C9	-2.14	123.00	126.23
25	C	515	BCR	C34-C9-C10	-2.14	119.93	122.92
23	B	615	CLA	C3A-C2A-C1A	2.14	104.54	101.34
34	y	307	CHL	CHB-C4A-NA	2.14	127.47	124.51
23	s	613	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	Y	311	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
25	Z	101	BCR	C1-C6-C5	-2.14	119.60	122.61
23	g	612	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
25	c	518	BCR	C1-C6-C5	-2.14	119.61	122.61
23	y	305	CLA	C1-C2-C3	-2.14	123.30	126.75
34	s	607	CHL	CHD-C1D-ND	-2.13	122.49	124.45
23	Y	312	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
35	g	616	LUT	C1-C2-C3	2.13	118.46	113.64
23	C	512	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	G	612	CLA	C2A-C1A-CHA	2.13	127.59	123.86
23	b	603	CLA	C4-C3-C5	2.13	118.86	115.27
23	g	611	CLA	C2A-C1A-CHA	2.13	127.59	123.86
35	g	616	LUT	C18-C5-C6	-2.13	122.13	124.53
36	G	617	NEX	C20-C13-C14	-2.13	119.94	122.92
37	N	301	XAT	C40-C33-C32	2.13	121.44	118.08
23	y	314	CLA	CHD-C1D-ND	-2.13	122.50	124.45
34	N	310	CHL	CHA-C1A-NA	-2.13	121.52	126.40
34	y	306	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
23	c	507	CLA	C2A-C1A-CHA	2.13	127.58	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	301	XAT	C35-C15-C14	-2.13	119.11	123.47
25	c	515	BCR	C38-C26-C25	-2.13	122.14	124.53
36	s	616	NEX	O24-C25-C26	-2.13	57.20	58.96
23	B	604	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
28	C	517	DGD	O5D-C1E-C2E	-2.13	104.98	108.30
23	y	310	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	616	CLA	C2A-C1A-CHA	2.13	127.58	123.86
23	B	614	CLA	C2A-C1A-CHA	2.13	127.58	123.86
34	g	606	CHL	CHD-C1D-ND	-2.13	122.50	124.45
36	S	616	NEX	O24-C25-C26	-2.13	57.20	58.96
35	n	316	LUT	C12-C13-C14	-2.12	115.68	118.94
23	a	401	CLA	CMC-C2C-C3C	2.12	131.88	126.12
23	C	513	CLA	CHA-C1A-NA	-2.12	121.54	126.40
37	Y	301	XAT	C10-C11-C12	-2.12	116.59	123.22
23	R	609	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	r	604	CLA	C3A-C2A-C1A	2.12	104.52	101.34
25	c	515	BCR	C4-C5-C6	-2.12	119.65	122.73
37	Y	301	XAT	C15-C35-C34	-2.12	119.13	123.47
35	y	315	LUT	C15-C14-C13	-2.12	124.28	127.31
23	a	401	CLA	C5-C3-C2	-2.12	116.83	121.12
23	s	608	CLA	C2D-C1D-ND	-2.12	108.54	110.10
23	c	511	CLA	CAA-C2A-C1A	2.12	118.92	111.97
23	C	503	CLA	C2A-C3A-C4A	2.12	105.29	101.87
23	y	311	CLA	C2A-C1A-CHA	2.12	127.56	123.86
34	g	606	CHL	CMB-C2B-C3B	2.12	128.64	124.68
23	S	608	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	B	617	BCR	C1-C6-C5	-2.12	119.63	122.61
23	b	616	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
35	S	615	LUT	C7-C8-C9	-2.12	123.04	126.23
34	G	605	CHL	O2A-CGA-O1A	-2.12	118.03	123.30
23	b	614	CLA	C2A-C1A-CHA	2.12	127.56	123.86
34	R	613	CHL	CHB-C4A-NA	2.12	127.44	124.51
23	n	303	CLA	C6-C7-C8	-2.12	109.08	115.92
23	c	512	CLA	CAC-C3C-C4C	-2.11	122.07	124.81
34	r	605	CHL	CHD-C1D-ND	-2.11	122.51	124.45
23	n	314	CLA	CHA-C1A-NA	-2.11	121.56	126.40
23	C	503	CLA	O1D-CGD-CBD	2.11	128.81	124.48
23	b	601	CLA	CHD-C1D-ND	-2.11	122.51	124.45
23	B	601	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	g	613	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	B	608	CLA	CBA-CAA-C2A	2.11	120.10	113.86
35	R	615	LUT	C16-C1-C6	-2.11	106.87	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	614	LUT	C12-C13-C14	-2.11	115.70	118.94
23	b	605	CLA	CMC-C2C-C3C	2.11	131.85	126.12
23	A	402	CLA	CHD-C1D-ND	-2.11	122.51	124.45
23	r	611	CLA	CHA-C1A-NA	-2.11	121.56	126.40
23	N	303	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
34	Y	309	CHL	C1D-CHD-C4C	-2.11	121.50	126.06
25	F	101	BCR	C23-C24-C25	-2.11	121.28	127.20
35	s	615	LUT	C3-C4-C5	-2.11	107.65	111.85
30	C	518	LHG	O8-C23-C24	2.11	118.53	111.91
23	b	601	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	b	609	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	C	515	BCR	C40-C30-C25	-2.11	106.88	110.30
34	n	308	CHL	CHA-C1A-NA	-2.11	121.57	126.40
23	C	508	CLA	C2A-C1A-CHA	2.11	127.54	123.86
36	G	617	NEX	C31-C32-C33	-2.10	120.50	126.42
23	b	612	CLA	C2A-C1A-CHA	2.10	127.54	123.86
28	H	102	DGD	O2G-C1B-O1B	-2.10	118.62	123.70
23	s	612	CLA	C2A-C1A-CHA	2.10	127.54	123.86
25	C	516	BCR	C23-C24-C25	-2.10	121.30	127.20
23	c	502	CLA	C7-C6-C5	-2.10	107.65	113.36
23	N	311	CLA	C1-C2-C3	-2.10	122.41	126.04
34	G	619	CHL	C1-C2-C3	-2.10	122.41	126.04
23	C	502	CLA	CHB-C4A-NA	2.10	127.42	124.51
35	g	616	LUT	C40-C33-C32	2.10	121.39	118.08
23	R	610	CLA	CHD-C1D-ND	-2.10	122.53	124.45
25	a	406	BCR	C1-C6-C5	-2.10	119.66	122.61
23	b	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	s	608	CLA	O2D-CGD-CBD	2.10	115.00	111.27
23	c	502	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
23	B	603	CLA	CHD-C1D-ND	-2.10	122.53	124.45
34	r	607	CHL	O2A-CGA-O1A	-2.10	118.30	123.59
23	Y	313	CLA	O2D-CGD-CBD	2.10	114.99	111.27
23	d	405	CLA	O1D-CGD-CBD	2.10	128.77	124.48
34	Y	306	CHL	O2A-CGA-O1A	-2.10	118.30	123.59
23	r	614	CLA	O2D-CGD-CBD	2.10	114.99	111.27
23	B	613	CLA	C2A-C1A-CHA	2.09	127.52	123.86
35	g	615	LUT	C22-C23-C24	-2.09	109.36	111.74
33	E	101	HEM	C3D-C4D-ND	-2.09	107.84	110.17
37	y	301	XAT	O24-C25-C26	-2.09	57.23	58.96
23	Y	312	CLA	C2A-C1A-CHA	2.09	127.52	123.86
23	c	501	CLA	CHA-C1A-NA	-2.09	121.61	126.40
34	s	607	CHL	CAA-C2A-C3A	-2.09	107.05	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	N	309	CHL	C3C-C4C-NC	-2.09	108.22	110.57
23	R	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
35	y	316	LUT	C15-C35-C34	-2.09	119.19	123.47
37	Y	301	XAT	O24-C25-C26	-2.09	57.23	58.96
28	C	517	DGD	O1G-C1A-O1A	-2.09	118.31	123.59
34	g	608	CHL	C4A-NA-C1A	2.09	107.65	106.71
34	N	308	CHL	O1A-CGA-CBA	2.09	129.80	123.08
23	G	613	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
34	g	606	CHL	O2D-CGD-CBD	2.09	114.98	111.27
36	Y	317	NEX	O24-C25-C26	-2.09	57.23	58.96
34	g	605	CHL	O2A-CGA-O1A	-2.09	118.09	123.30
25	a	406	BCR	C16-C15-C14	-2.09	119.19	123.47
23	y	312	CLA	C2A-C1A-CHA	2.09	127.51	123.86
23	N	314	CLA	CHA-C1A-NA	-2.09	121.62	126.40
23	n	304	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	K	101	BCR	C21-C20-C19	-2.09	116.70	123.22
23	B	616	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	S	612	CLA	C2A-C1A-CHA	2.09	127.51	123.86
34	g	608	CHL	CHA-C4D-ND	2.09	136.86	132.50
35	n	316	LUT	C31-C32-C33	-2.09	120.56	126.42
23	b	613	CLA	C2A-C1A-CHA	2.09	127.51	123.86
31	D	403	BCT	O3-C-O1	-2.09	114.14	119.55
23	S	613	CLA	CHD-C1D-ND	-2.09	122.54	124.45
34	N	306	CHL	CHB-C4A-NA	2.09	127.40	124.51
37	R	616	XAT	O24-C25-C26	-2.08	57.23	58.96
34	Y	308	CHL	CHD-C1D-ND	-2.08	122.54	124.45
23	r	611	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	c	513	CLA	CHA-C1A-NA	-2.08	121.63	126.40
23	b	612	CLA	O2D-CGD-CBD	2.08	114.97	111.27
35	g	615	LUT	C18-C5-C6	-2.08	122.19	124.53
23	C	503	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
30	r	618	LHG	O8-C23-O10	-2.08	118.34	123.59
23	g	613	CLA	O2D-CGD-CBD	2.08	114.97	111.27
25	K	101	BCR	C38-C26-C27	2.08	117.61	113.62
25	a	406	BCR	C10-C11-C12	-2.08	116.73	123.22
35	s	614	LUT	C22-C23-C24	-2.08	109.37	111.74
23	N	312	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	C	515	BCR	C1-C6-C5	-2.08	119.69	122.61
23	c	507	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	C	501	LMG	O1-C7-C8	2.08	115.91	110.90
32	d	407	PL9	C53-C6-C1	2.08	119.24	114.99
25	b	619	BCR	C31-C1-C6	-2.08	106.93	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	401	CLA	CHC-C1C-NC	2.08	127.35	124.20
23	B	608	CLA	CHB-C4A-NA	2.08	127.38	124.51
34	r	605	CHL	O2A-CGA-O1A	-2.08	118.12	123.30
34	s	601	CHL	C2A-C1A-CHA	2.07	127.49	123.86
23	c	501	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
23	C	511	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
35	s	615	LUT	C31-C32-C33	-2.07	120.59	126.42
23	c	505	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
34	y	306	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	C	513	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
37	G	620	XAT	C39-C29-C30	-2.07	120.02	122.92
23	r	601	CLA	CHA-C1A-NA	-2.07	121.65	126.40
23	c	509	CLA	C2A-C1A-CHA	2.07	127.48	123.86
23	R	601	CLA	CHA-C1A-NA	-2.07	121.65	126.40
23	a	403	CLA	CHD-C1D-ND	-2.07	122.55	124.45
34	G	607	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	r	612	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
34	Y	302	CHL	CAA-C2A-C1A	-2.07	105.19	111.97
34	N	310	CHL	CHC-C1C-NC	2.07	127.34	124.20
23	S	608	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
23	A	401	CLA	CGD-CBD-CAD	2.07	117.43	110.73
37	R	616	XAT	C12-C13-C14	-2.07	115.77	118.94
28	c	516	DGD	C6D-C5D-C4D	-2.07	107.78	112.09
23	a	402	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	n	311	CLA	CMA-C3A-C2A	-2.07	105.49	113.83
34	R	607	CHL	O2A-CGA-O1A	-2.07	118.38	123.59
25	b	618	BCR	C4-C5-C6	-2.07	119.73	122.73
34	G	619	CHL	C2D-C1D-ND	-2.07	108.58	110.10
36	N	318	NEX	C4-C3-C2	-2.07	106.78	110.77
25	b	617	BCR	C32-C1-C6	-2.07	106.95	110.30
23	B	610	CLA	C1-C2-C3	-2.07	122.47	126.04
34	R	613	CHL	C1D-CHD-C4C	-2.07	121.60	126.06
27	b	620	LMG	O8-C28-O10	-2.07	118.38	123.59
24	d	401	PHO	C6-C5-C3	2.07	118.87	113.45
34	n	306	CHL	O2A-CGA-O1A	-2.07	118.38	123.59
23	r	609	CLA	CHD-C1D-ND	-2.07	122.56	124.45
23	B	609	CLA	C2A-C1A-CHA	2.06	127.47	123.86
23	B	605	CLA	CHD-C1D-ND	-2.06	122.56	124.45
36	G	617	NEX	C15-C35-C34	-2.06	119.25	123.47
23	y	310	CLA	C1-C2-C3	-2.06	122.48	126.04
23	B	615	CLA	C16-C15-C13	-2.06	109.26	115.92
23	Y	310	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	G	606	CHL	O2D-CGD-CBD	2.06	114.93	111.27
37	Y	301	XAT	O4-C5-C6	-2.06	57.25	58.96
34	S	601	CHL	C2A-C1A-CHA	2.06	127.46	123.86
25	C	516	BCR	C1-C6-C5	-2.06	119.71	122.61
35	R	615	LUT	C15-C35-C34	-2.06	119.26	123.47
34	g	601	CHL	CAC-C3C-C4C	2.06	127.48	124.81
23	B	616	CLA	CHA-C1A-NA	-2.06	121.68	126.40
34	g	607	CHL	CHB-C4A-NA	2.06	127.36	124.51
34	S	607	CHL	CHA-C4D-ND	2.06	136.80	132.50
34	R	605	CHL	O2A-CGA-O1A	-2.06	118.17	123.30
23	B	609	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
23	S	609	CLA	C1D-ND-C4D	-2.06	104.88	106.33
23	B	609	CLA	CHB-C4A-NA	2.05	127.35	124.51
35	R	615	LUT	C10-C11-C12	-2.05	116.81	123.22
23	S	611	CLA	C2C-C1C-NC	2.05	111.90	109.97
23	n	305	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
37	g	620	XAT	O24-C25-C26	-2.05	57.26	58.96
34	Y	306	CHL	C2A-C1A-CHA	2.05	127.45	123.86
23	Y	313	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
35	y	316	LUT	C30-C31-C32	-2.05	116.81	123.22
23	C	513	CLA	C7-C6-C5	-2.05	107.78	113.36
23	b	604	CLA	C6-C7-C8	-2.05	109.29	115.92
36	r	617	NEX	C26-C27-C28	-2.05	121.66	125.99
34	g	609	CHL	CAA-C2A-C3A	-2.05	107.16	112.78
23	R	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
34	R	607	CHL	CHB-C4A-NA	2.05	127.35	124.51
25	A	405	BCR	C1-C6-C5	-2.05	119.72	122.61
23	s	613	CLA	C4A-NA-C1A	2.05	107.63	106.71
23	Y	314	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	c	518	BCR	C36-C18-C17	-2.05	120.05	122.92
35	R	615	LUT	C31-C32-C33	-2.05	120.66	126.42
27	B	620	LMG	O8-C28-O10	-2.05	118.42	123.59
23	C	510	CLA	CHA-C4D-ND	2.05	136.78	132.50
30	s	617	LHG	C25-C24-C23	-2.05	106.17	113.62
23	C	510	CLA	CGD-CBD-CAD	-2.05	104.10	110.73
34	G	609	CHL	CMD-C2D-C1D	2.05	128.32	124.71
23	g	610	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
34	g	619	CHL	O2A-CGA-O1A	-2.05	118.43	123.59
23	B	609	CLA	C7-C6-C5	-2.05	107.80	113.36
35	S	614	LUT	C37-C21-C22	-2.05	105.56	109.44
23	N	314	CLA	C4D-CHA-C1A	2.05	123.74	121.25
23	r	612	CLA	CAC-C3C-C4C	2.04	127.46	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CHD-C1D-ND	-2.04	122.58	124.45
32	D	406	PL9	C35-C34-C36	-2.04	111.83	115.27
23	s	604	CLA	C3A-C2A-C1A	2.04	104.40	101.34
23	R	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
36	G	617	NEX	O24-C25-C26	-2.04	57.27	58.96
23	n	305	CLA	C1-C2-C3	-2.04	123.45	126.75
25	B	618	BCR	C38-C26-C27	2.04	117.54	113.62
23	B	605	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
23	G	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	a	402	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
35	n	317	LUT	C10-C11-C12	-2.04	116.85	123.22
30	b	622	LHG	C5-O7-C7	-2.04	112.77	117.79
23	d	404	CLA	CAC-C3C-C4C	2.04	127.45	124.81
36	Y	317	NEX	C1-C2-C3	-2.04	109.04	113.64
36	N	318	NEX	C20-C13-C14	-2.04	120.07	122.92
35	g	616	LUT	C37-C21-C22	-2.04	105.58	109.44
23	c	510	CLA	CHD-C4C-NC	2.04	127.41	124.20
34	Y	309	CHL	CHD-C1D-ND	-2.04	122.58	124.45
23	C	502	CLA	CHA-C1A-NA	-2.04	121.73	126.40
23	C	503	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
23	S	608	CLA	C2A-C1A-CHA	2.04	127.42	123.86
23	r	603	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	c	506	CLA	C2A-C1A-CHA	2.03	127.42	123.86
36	R	617	NEX	O24-C25-C26	-2.03	57.28	58.96
23	C	508	CLA	CMD-C2D-C3D	2.03	132.29	127.61
23	B	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
37	r	616	XAT	O24-C25-C26	-2.03	57.28	58.96
35	G	615	LUT	C18-C5-C6	-2.03	122.25	124.53
34	R	606	CHL	CHB-C4A-NA	2.03	127.32	124.51
34	S	605	CHL	CMB-C2B-C3B	2.03	128.48	124.68
36	R	617	NEX	C19-C9-C10	-2.03	120.08	122.92
34	r	606	CHL	CHB-C4A-NA	2.03	127.32	124.51
23	a	401	CLA	CHA-C4D-ND	2.03	136.74	132.50
23	a	402	CLA	CHC-C1C-NC	2.03	127.28	124.20
25	Z	101	BCR	C31-C1-C6	-2.03	107.01	110.30
35	s	614	LUT	C19-C9-C8	2.03	121.27	118.08
34	y	309	CHL	C2A-C1A-CHA	2.03	127.40	123.86
25	b	618	BCR	C23-C24-C25	-2.03	121.51	127.20
23	G	610	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	k	101	BCR	C21-C20-C19	-2.03	116.90	123.22
23	B	611	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
34	g	601	CHL	CHA-C4D-ND	2.02	136.73	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	S	607	CHL	CHB-C4A-NA	2.02	127.31	124.51
23	S	603	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
31	d	403	BCT	O3-C-O1	-2.02	114.30	119.55
35	g	615	LUT	C36-C21-C26	2.02	112.61	109.55
34	S	607	CHL	CAA-C2A-C3A	-2.02	107.24	112.78
23	g	611	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	h	101	BCR	C7-C8-C9	-2.02	123.18	126.23
23	b	610	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	c	508	CLA	O2D-CGD-CBD	2.02	114.86	111.27
23	S	602	CLA	CMA-C3A-C2A	-2.02	105.68	113.83
34	g	607	CHL	C1D-CHD-C4C	-2.02	121.70	126.06
32	D	406	PL9	C3-C2-C1	-2.02	118.72	122.52
32	d	407	PL9	C3-C2-C1	-2.02	118.72	122.52
25	C	516	BCR	C33-C5-C4	2.02	117.50	113.62
34	s	605	CHL	CHD-C1D-ND	-2.02	122.60	124.45
23	a	402	CLA	C11-C10-C8	-2.02	109.39	115.92
25	c	514	BCR	C38-C26-C27	2.02	117.49	113.62
23	R	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	S	602	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	B	607	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	y	313	CLA	CHC-C1C-NC	2.02	127.26	124.20
34	G	605	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
23	b	605	CLA	CHC-C1C-NC	2.02	127.26	124.20
37	R	616	XAT	C30-C31-C32	-2.02	116.92	123.22
25	k	101	BCR	C38-C26-C27	2.02	117.49	113.62
23	c	508	CLA	C2A-C1A-CHA	2.02	127.38	123.86
36	y	317	NEX	O24-C25-C26	-2.02	57.29	58.96
25	a	406	BCR	C15-C16-C17	-2.02	119.35	123.47
37	y	301	XAT	O4-C5-C6	-2.01	57.29	58.96
23	C	512	CLA	CHB-C4A-NA	2.01	127.30	124.51
35	g	615	LUT	C11-C10-C9	-2.01	124.44	127.31
23	D	405	CLA	CGD-CBD-CAD	-2.01	104.21	110.73
25	c	515	BCR	C33-C5-C6	-2.01	122.27	124.53
23	c	507	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
25	b	618	BCR	C8-C7-C6	-2.01	121.55	127.20
23	b	608	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
23	G	603	CLA	C2D-C1D-ND	-2.01	108.62	110.10
23	g	602	CLA	CHD-C1D-ND	-2.01	122.60	124.45
35	n	316	LUT	C38-C25-C24	-2.01	119.25	123.56
23	C	508	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
25	k	101	BCR	C35-C13-C12	2.01	121.25	118.08
23	s	602	CLA	CMA-C3A-C2A	-2.01	105.72	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	412	LHG	C5-O7-C7	-2.01	112.84	117.79
35	G	615	LUT	C22-C23-C24	-2.01	109.45	111.74
25	F	101	BCR	C33-C5-C4	2.01	117.48	113.62
32	D	406	PL9	C53-C6-C1	2.01	119.10	114.99
37	G	620	XAT	C27-C28-C29	-2.01	122.41	125.53
35	Y	316	LUT	C36-C21-C26	2.01	112.59	109.55
23	c	505	CLA	O2A-C1-C2	2.01	113.91	108.64
33	e	101	HEM	C3D-C4D-ND	-2.01	107.93	110.17
23	S	610	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	b	609	CLA	C2A-C1A-CHA	2.01	127.37	123.86
25	A	405	BCR	C10-C11-C12	-2.01	116.96	123.22
23	B	615	CLA	C2A-C1A-CHA	2.01	127.37	123.86
23	b	604	CLA	O2A-C1-C2	-2.01	103.36	108.64
34	G	619	CHL	CHD-C1D-ND	-2.01	122.61	124.45
34	Y	309	CHL	CHA-C4D-ND	2.01	136.69	132.50
35	g	616	LUT	C15-C14-C13	2.01	130.17	127.31
23	c	511	CLA	C2A-C1A-CHA	2.01	127.36	123.86
26	L	103	SQD	O48-C23-O10	-2.00	118.54	123.59
23	B	601	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	b	619	BCR	C20-C21-C22	-2.00	124.45	127.31
28	C	517	DGD	C3G-O3G-C1D	-2.00	109.83	113.74
35	N	317	LUT	C40-C33-C34	-2.00	120.12	122.92
23	r	612	CLA	C2D-C1D-ND	-2.00	108.63	110.10
23	s	604	CLA	C2A-C1A-CHA	2.00	127.36	123.86
34	S	607	CHL	O2A-CGA-O1A	-2.00	118.54	123.59
23	C	502	CLA	CHA-C4D-ND	2.00	136.68	132.50
23	C	511	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (312) 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
23	B	607	CLA	ND
23	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
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	404	CLA	ND
23	D	405	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	303	CLA	ND
23	N	304	CLA	ND
23	N	305	CLA	ND
23	N	311	CLA	ND
23	N	312	CLA	ND
23	N	313	CLA	ND
23	N	314	CLA	ND
23	N	315	CLA	ND
23	R	601	CLA	ND
23	R	602	CLA	ND

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Mol	Chain	Res	Type	Atom
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	R	614	CLA	ND
23	Y	303	CLA	ND
23	Y	304	CLA	ND
23	Y	305	CLA	ND
23	Y	310	CLA	ND
23	Y	311	CLA	ND
23	Y	312	CLA	ND
23	Y	313	CLA	ND
23	Y	314	CLA	ND
23	a	401	CLA	ND
23	a	402	CLA	ND
23	a	403	CLA	ND
23	a	405	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
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	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

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Mol	Chain	Res	Type	Atom
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	d	404	CLA	ND
23	d	405	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	303	CLA	ND
23	n	304	CLA	ND
23	n	305	CLA	ND
23	n	311	CLA	ND
23	n	312	CLA	ND
23	n	313	CLA	ND
23	n	314	CLA	ND
23	n	315	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	r	614	CLA	ND
23	y	303	CLA	ND
23	y	304	CLA	ND
23	y	305	CLA	ND
23	y	310	CLA	ND
23	y	311	CLA	ND
23	y	312	CLA	ND
23	y	313	CLA	ND

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Mol	Chain	Res	Type	Atom
23	y	314	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	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
34	G	601	CHL	ND
34	G	601	CHL	NA
34	G	601	CHL	NC
34	G	605	CHL	ND
34	G	605	CHL	NA
34	G	605	CHL	NC
34	G	606	CHL	ND
34	G	606	CHL	NA
34	G	606	CHL	NC
34	G	607	CHL	ND
34	G	607	CHL	NA
34	G	607	CHL	NC
34	G	608	CHL	ND
34	G	608	CHL	NA
34	G	608	CHL	NC
34	G	609	CHL	ND
34	G	609	CHL	NA
34	G	609	CHL	NC
34	G	619	CHL	ND
34	G	619	CHL	NA
34	G	619	CHL	NC
34	N	302	CHL	ND
34	N	302	CHL	NA

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Mol	Chain	Res	Type	Atom
34	N	302	CHL	NC
34	N	306	CHL	ND
34	N	306	CHL	NA
34	N	306	CHL	NC
34	N	307	CHL	ND
34	N	307	CHL	NA
34	N	307	CHL	NC
34	N	308	CHL	ND
34	N	308	CHL	NA
34	N	308	CHL	NC
34	N	309	CHL	ND
34	N	309	CHL	NA
34	N	309	CHL	NC
34	N	310	CHL	ND
34	N	310	CHL	NA
34	N	310	CHL	NC
34	R	605	CHL	ND
34	R	605	CHL	NA
34	R	605	CHL	NC
34	R	606	CHL	ND
34	R	606	CHL	NA
34	R	606	CHL	NC
34	R	607	CHL	ND
34	R	607	CHL	NA
34	R	607	CHL	NC
34	R	613	CHL	ND
34	R	613	CHL	NA
34	R	613	CHL	NC
34	Y	302	CHL	ND
34	Y	302	CHL	NA
34	Y	302	CHL	NC
34	Y	306	CHL	ND
34	Y	306	CHL	NA
34	Y	306	CHL	NC
34	Y	307	CHL	ND
34	Y	307	CHL	NA
34	Y	307	CHL	NC
34	Y	308	CHL	ND
34	Y	308	CHL	NA
34	Y	308	CHL	NC
34	Y	309	CHL	ND
34	Y	309	CHL	NA

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Mol	Chain	Res	Type	Atom
34	Y	309	CHL	NC
34	g	601	CHL	ND
34	g	601	CHL	NA
34	g	601	CHL	NC
34	g	605	CHL	ND
34	g	605	CHL	NA
34	g	605	CHL	NC
34	g	606	CHL	ND
34	g	606	CHL	NA
34	g	606	CHL	NC
34	g	607	CHL	ND
34	g	607	CHL	NA
34	g	607	CHL	NC
34	g	608	CHL	ND
34	g	608	CHL	NA
34	g	608	CHL	NC
34	g	609	CHL	ND
34	g	609	CHL	NA
34	g	609	CHL	NC
34	g	619	CHL	ND
34	g	619	CHL	NA
34	g	619	CHL	NC
34	n	302	CHL	ND
34	n	302	CHL	NA
34	n	302	CHL	NC
34	n	306	CHL	ND
34	n	306	CHL	NA
34	n	306	CHL	NC
34	n	307	CHL	ND
34	n	307	CHL	NA
34	n	307	CHL	NC
34	n	308	CHL	ND
34	n	308	CHL	NA
34	n	308	CHL	NC
34	n	309	CHL	ND
34	n	309	CHL	NA
34	n	309	CHL	NC
34	n	310	CHL	ND
34	n	310	CHL	NA
34	n	310	CHL	NC
34	r	605	CHL	ND
34	r	605	CHL	NA

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Mol	Chain	Res	Type	Atom
34	r	605	CHL	NC
34	r	606	CHL	ND
34	r	606	CHL	NA
34	r	606	CHL	NC
34	r	607	CHL	ND
34	r	607	CHL	NA
34	r	607	CHL	NC
34	r	613	CHL	ND
34	r	613	CHL	NA
34	r	613	CHL	NC
34	y	302	CHL	ND
34	y	302	CHL	NA
34	y	302	CHL	NC
34	y	306	CHL	ND
34	y	306	CHL	NA
34	y	306	CHL	NC
34	y	307	CHL	ND
34	y	307	CHL	NA
34	y	307	CHL	NC
34	y	308	CHL	ND
34	y	308	CHL	NA
34	y	308	CHL	NC
34	y	309	CHL	ND
34	y	309	CHL	NA
34	y	309	CHL	NC
34	S	601	CHL	ND
34	S	601	CHL	NA
34	S	601	CHL	NC
34	S	605	CHL	ND
34	S	605	CHL	NA
34	S	605	CHL	NC
34	S	606	CHL	ND
34	S	606	CHL	NA
34	S	606	CHL	NC
34	S	607	CHL	ND
34	S	607	CHL	NA
34	S	607	CHL	NC
34	s	601	CHL	ND
34	s	601	CHL	NA
34	s	601	CHL	NC
34	s	605	CHL	ND
34	s	605	CHL	NA

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Mol	Chain	Res	Type	Atom
34	s	605	CHL	NC
34	s	606	CHL	ND
34	s	606	CHL	NA
34	s	606	CHL	NC
34	s	607	CHL	ND
34	s	607	CHL	NA
34	s	607	CHL	NC

All (3010) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	401	CLA	C2-C3-C5-C6
23	A	401	CLA	C4-C3-C5-C6
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	402	CLA	C3A-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	CAD-CBD-CGD-O1D
23	A	404	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	C3A-C2A-CAA-CBA
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	608	CLA	C2-C3-C5-C6
23	B	608	CLA	C4-C3-C5-C6
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	610	CLA	C1A-C2A-CAA-CBA
23	B	612	CLA	C1A-C2A-CAA-CBA
23	B	612	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	C1A-C2A-CAA-CBA
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	C14-C13-C15-C16
23	C	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	507	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	C3A-C2A-CAA-CBA
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	C11-C10-C8-C9
23	C	512	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	CBD-CGD-O2D-CED
23	D	401	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	C1A-C2A-CAA-CBA
23	D	404	CLA	C11-C10-C8-C9
23	D	405	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	C3A-C2A-CAA-CBA
23	G	611	CLA	C3A-C2A-CAA-CBA
23	G	613	CLA	CHA-CBD-CGD-O1D
23	G	613	CLA	CHA-CBD-CGD-O2D
23	N	303	CLA	C12-C13-C15-C16
23	N	305	CLA	CHA-CBD-CGD-O1D
23	N	305	CLA	CHA-CBD-CGD-O2D
23	N	305	CLA	CAD-CBD-CGD-O1D
23	N	305	CLA	CBD-CGD-O2D-CED
23	N	311	CLA	C1A-C2A-CAA-CBA
23	N	313	CLA	C1A-C2A-CAA-CBA
23	N	313	CLA	C3A-C2A-CAA-CBA
23	N	314	CLA	C1A-C2A-CAA-CBA
23	N	314	CLA	CHA-CBD-CGD-O1D
23	N	314	CLA	CHA-CBD-CGD-O2D
23	N	314	CLA	CBD-CGD-O2D-CED
23	R	601	CLA	CBD-CGD-O2D-CED
23	R	602	CLA	CHA-CBD-CGD-O1D
23	R	602	CLA	CHA-CBD-CGD-O2D
23	R	608	CLA	C3A-C2A-CAA-CBA
23	R	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	R	609	CLA	CBD-CGD-O2D-CED
23	R	610	CLA	CBD-CGD-O2D-CED
23	R	612	CLA	CHA-CBD-CGD-O1D
23	R	612	CLA	CHA-CBD-CGD-O2D
23	R	612	CLA	CBD-CGD-O2D-CED
23	R	614	CLA	C1A-C2A-CAA-CBA
23	R	614	CLA	C3A-C2A-CAA-CBA
23	Y	303	CLA	C1A-C2A-CAA-CBA
23	Y	303	CLA	C3A-C2A-CAA-CBA
23	Y	304	CLA	O1A-CGA-O2A-C1
23	Y	304	CLA	CHA-CBD-CGD-O1D
23	Y	304	CLA	CHA-CBD-CGD-O2D
23	Y	312	CLA	CBD-CGD-O2D-CED
23	Y	312	CLA	O1D-CGD-O2D-CED
23	Y	313	CLA	CHA-CBD-CGD-O1D
23	Y	313	CLA	CHA-CBD-CGD-O2D
23	a	403	CLA	C1A-C2A-CAA-CBA
23	a	403	CLA	C3A-C2A-CAA-CBA
23	a	403	CLA	CHA-CBD-CGD-O1D
23	a	403	CLA	CHA-CBD-CGD-O2D
23	a	405	CLA	CHA-CBD-CGD-O1D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	a	405	CLA	CAD-CBD-CGD-O1D
23	a	405	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	C3A-C2A-CAA-CBA
23	b	603	CLA	C4-C3-C5-C6
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	C1A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C2-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
23	b	609	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	CHA-CBD-CGD-O1D
23	b	609	CLA	CHA-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	C2-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	c	506	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
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	513	CLA	CBD-CGD-O2D-CED
23	d	405	CLA	CBD-CGD-O2D-CED
23	g	610	CLA	C3A-C2A-CAA-CBA
23	g	611	CLA	C3A-C2A-CAA-CBA
23	g	611	CLA	CBD-CGD-O2D-CED
23	g	613	CLA	CHA-CBD-CGD-O1D
23	g	613	CLA	CBD-CGD-O2D-CED
23	g	614	CLA	C1A-C2A-CAA-CBA
23	n	303	CLA	C12-C13-C15-C16
23	n	305	CLA	CHA-CBD-CGD-O1D
23	n	305	CLA	CHA-CBD-CGD-O2D
23	n	305	CLA	CAD-CBD-CGD-O1D
23	n	311	CLA	CBD-CGD-O2D-CED
23	n	313	CLA	C1A-C2A-CAA-CBA
23	n	314	CLA	C1A-C2A-CAA-CBA
23	n	314	CLA	CHA-CBD-CGD-O1D
23	n	314	CLA	CHA-CBD-CGD-O2D
23	n	314	CLA	CBD-CGD-O2D-CED
23	r	602	CLA	CHA-CBD-CGD-O1D
23	r	602	CLA	CHA-CBD-CGD-O2D
23	r	608	CLA	CBD-CGD-O2D-CED
23	r	609	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	CHA-CBD-CGD-O1D
23	r	610	CLA	CHA-CBD-CGD-O2D
23	r	612	CLA	CHA-CBD-CGD-O1D
23	r	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	r	612	CLA	CBD-CGD-O2D-CED
23	r	614	CLA	C1A-C2A-CAA-CBA
23	y	303	CLA	C3A-C2A-CAA-CBA
23	y	304	CLA	CHA-CBD-CGD-O1D
23	y	304	CLA	CHA-CBD-CGD-O2D
23	y	311	CLA	CHA-CBD-CGD-O1D
23	y	312	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	CHA-CBD-CGD-O1D
23	y	313	CLA	CHA-CBD-CGD-O2D
23	S	602	CLA	C3A-C2A-CAA-CBA
23	S	602	CLA	CBD-CGD-O2D-CED
23	S	608	CLA	CHA-CBD-CGD-O1D
23	S	608	CLA	CHA-CBD-CGD-O2D
23	S	609	CLA	C1A-C2A-CAA-CBA
23	S	609	CLA	CHA-CBD-CGD-O1D
23	S	609	CLA	CHA-CBD-CGD-O2D
23	S	610	CLA	C1A-C2A-CAA-CBA
23	S	610	CLA	CHA-CBD-CGD-O1D
23	S	610	CLA	CHA-CBD-CGD-O2D
23	S	612	CLA	CBD-CGD-O2D-CED
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	s	602	CLA	C1A-C2A-CAA-CBA
23	s	602	CLA	C3A-C2A-CAA-CBA
23	s	602	CLA	CBD-CGD-O2D-CED
23	s	604	CLA	CHA-CBD-CGD-O1D
23	s	604	CLA	CHA-CBD-CGD-O2D
23	s	608	CLA	CHA-CBD-CGD-O1D
23	s	608	CLA	CHA-CBD-CGD-O2D
23	s	608	CLA	CAD-CBD-CGD-O1D
23	s	609	CLA	C1A-C2A-CAA-CBA
23	s	610	CLA	C1A-C2A-CAA-CBA
23	s	613	CLA	CHA-CBD-CGD-O1D
23	s	613	CLA	CHA-CBD-CGD-O2D
24	D	402	PHO	CBD-CGD-O2D-CED
25	B	617	BCR	C7-C8-C9-C10
25	B	617	BCR	C7-C8-C9-C34
25	B	617	BCR	C21-C22-C23-C24
25	B	617	BCR	C37-C22-C23-C24
25	B	618	BCR	C11-C12-C13-C14
25	B	618	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
25	B	619	BCR	C7-C8-C9-C34
25	C	516	BCR	C11-C12-C13-C35
25	F	101	BCR	C21-C22-C23-C24
25	F	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C1-C6-C7-C8
25	H	101	BCR	C7-C8-C9-C10
25	H	101	BCR	C7-C8-C9-C34
25	H	101	BCR	C9-C10-C11-C12
25	K	101	BCR	C7-C8-C9-C10
25	K	101	BCR	C7-C8-C9-C34
25	Z	101	BCR	C7-C8-C9-C10
25	Z	101	BCR	C7-C8-C9-C34
25	b	617	BCR	C7-C8-C9-C10
25	b	617	BCR	C7-C8-C9-C34
25	b	617	BCR	C21-C22-C23-C24
25	b	617	BCR	C37-C22-C23-C24
25	b	618	BCR	C11-C12-C13-C35
25	b	619	BCR	C7-C8-C9-C34
25	c	514	BCR	C37-C22-C23-C24
25	c	515	BCR	C11-C12-C13-C35
25	c	518	BCR	C15-C16-C17-C18
25	c	518	BCR	C17-C18-C19-C20
25	c	518	BCR	C36-C18-C19-C20
25	d	406	BCR	C21-C22-C23-C24
25	d	406	BCR	C37-C22-C23-C24
25	h	101	BCR	C1-C6-C7-C8
25	h	101	BCR	C7-C8-C9-C10
25	h	101	BCR	C7-C8-C9-C34
26	A	409	SQD	O47-C45-C46-O48
26	A	409	SQD	C5-C6-S-O8
26	A	409	SQD	C5-C6-S-O9
26	L	103	SQD	O5-C5-C6-S
26	M	101	SQD	O5-C5-C6-S
26	a	409	SQD	O47-C45-C46-O48
26	a	409	SQD	C5-C6-S-O8
26	a	409	SQD	C5-C6-S-O9
26	d	402	SQD	O6-C44-C45-O47
28	A	408	DGD	C2B-C1B-O2G-C2G
28	a	408	DGD	C2B-C1B-O2G-C2G
30	A	411	LHG	C3-O3-P-O5
30	A	411	LHG	C4-O6-P-O5
30	A	412	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
30	A	412	LHG	C4-O6-P-O4
30	A	412	LHG	C4-O6-P-O5
30	B	621	LHG	C3-O3-P-O4
30	B	621	LHG	C4-O6-P-O4
30	B	623	LHG	C3-O3-P-O5
30	B	623	LHG	C3-O3-P-O6
30	B	623	LHG	C8-C7-O7-C5
30	G	618	LHG	C3-O3-P-O5
30	G	618	LHG	C4-O6-P-O4
30	L	101	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O4
30	L	102	LHG	C3-O3-P-O4
30	L	102	LHG	C4-O6-P-O4
30	R	618	LHG	C4-O6-P-O3
30	R	618	LHG	C4-O6-P-O4
30	R	618	LHG	C4-O6-P-O5
30	T	101	LHG	C3-O3-P-O5
30	T	101	LHG	C3-O3-P-O6
30	T	101	LHG	C8-C7-O7-C5
30	W	201	LHG	C3-O3-P-O5
30	W	201	LHG	C4-O6-P-O4
30	W	201	LHG	C4-O6-P-O5
30	Y	318	LHG	C4-O6-P-O5
30	a	411	LHG	C4-O6-P-O5
30	a	412	LHG	C4-O6-P-O3
30	a	412	LHG	C4-O6-P-O4
30	a	412	LHG	C4-O6-P-O5
30	b	621	LHG	C3-O3-P-O4
30	b	621	LHG	C4-O6-P-O4
30	b	622	LHG	C3-O3-P-O4
30	b	622	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O6
30	d	408	LHG	C4-O6-P-O4
30	g	618	LHG	C3-O3-P-O5
30	n	319	LHG	C4-O6-P-O3
30	r	618	LHG	C4-O6-P-O4
30	r	618	LHG	C4-O6-P-O5
30	w	201	LHG	C3-O3-P-O5
30	w	201	LHG	C4-O6-P-O4
30	w	201	LHG	C4-O6-P-O5
30	y	318	LHG	C4-O6-P-O5
30	S	617	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	S	617	LHG	C4-O6-P-O4
30	S	617	LHG	C4-O6-P-O5
30	s	617	LHG	C4-O6-P-O4
30	s	617	LHG	C4-O6-P-O5
32	D	406	PL9	C12-C11-C9-C8
32	D	406	PL9	C12-C13-C14-C16
32	D	406	PL9	C13-C14-C16-C17
32	D	406	PL9	C17-C18-C19-C20
32	D	406	PL9	C17-C18-C19-C21
32	D	406	PL9	C27-C28-C29-C30
32	D	406	PL9	C47-C48-C49-C50
32	d	407	PL9	C12-C11-C9-C8
32	d	407	PL9	C12-C13-C14-C16
32	d	407	PL9	C17-C18-C19-C20
32	d	407	PL9	C17-C18-C19-C21
32	d	407	PL9	C22-C23-C24-C25
34	G	601	CHL	C1C-C2C-CMC-OMC
34	G	601	CHL	C3C-C2C-CMC-OMC
34	G	601	CHL	CHA-CBD-CGD-O1D
34	G	601	CHL	CHA-CBD-CGD-O2D
34	G	605	CHL	C1C-C2C-CMC-OMC
34	G	605	CHL	C3C-C2C-CMC-OMC
34	G	606	CHL	C1A-C2A-CAA-CBA
34	G	606	CHL	C3A-C2A-CAA-CBA
34	G	606	CHL	C1C-C2C-CMC-OMC
34	G	606	CHL	C3C-C2C-CMC-OMC
34	G	607	CHL	C1A-C2A-CAA-CBA
34	G	607	CHL	C3A-C2A-CAA-CBA
34	G	607	CHL	C1C-C2C-CMC-OMC
34	G	607	CHL	C3C-C2C-CMC-OMC
34	G	607	CHL	CHA-CBD-CGD-O1D
34	G	607	CHL	CHA-CBD-CGD-O2D
34	G	608	CHL	C1A-C2A-CAA-CBA
34	G	608	CHL	C1C-C2C-CMC-OMC
34	G	608	CHL	C3C-C2C-CMC-OMC
34	G	609	CHL	C3C-C2C-CMC-OMC
34	G	609	CHL	CHA-CBD-CGD-O1D
34	G	609	CHL	CHA-CBD-CGD-O2D
34	G	609	CHL	CBD-CGD-O2D-CED
34	G	619	CHL	C1A-C2A-CAA-CBA
34	G	619	CHL	C3A-C2A-CAA-CBA
34	G	619	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	G	619	CHL	C1C-C2C-CMC-OMC
34	G	619	CHL	C3C-C2C-CMC-OMC
34	N	302	CHL	C1C-C2C-CMC-OMC
34	N	302	CHL	C3C-C2C-CMC-OMC
34	N	302	CHL	CHA-CBD-CGD-O1D
34	N	302	CHL	CHA-CBD-CGD-O2D
34	N	306	CHL	C1C-C2C-CMC-OMC
34	N	306	CHL	C3C-C2C-CMC-OMC
34	N	307	CHL	C1C-C2C-CMC-OMC
34	N	307	CHL	C3C-C2C-CMC-OMC
34	N	307	CHL	CBD-CGD-O2D-CED
34	N	308	CHL	C1C-C2C-CMC-OMC
34	N	308	CHL	C3C-C2C-CMC-OMC
34	N	308	CHL	CHA-CBD-CGD-O1D
34	N	308	CHL	CHA-CBD-CGD-O2D
34	N	309	CHL	C1C-C2C-CMC-OMC
34	N	309	CHL	C3C-C2C-CMC-OMC
34	N	309	CHL	CHA-CBD-CGD-O1D
34	N	309	CHL	CHA-CBD-CGD-O2D
34	N	310	CHL	C1C-C2C-CMC-OMC
34	N	310	CHL	C3C-C2C-CMC-OMC
34	N	310	CHL	CHA-CBD-CGD-O1D
34	N	310	CHL	CHA-CBD-CGD-O2D
34	R	606	CHL	C1C-C2C-CMC-OMC
34	R	606	CHL	C3C-C2C-CMC-OMC
34	R	607	CHL	C1C-C2C-CMC-OMC
34	R	607	CHL	C3C-C2C-CMC-OMC
34	R	613	CHL	C1C-C2C-CMC-OMC
34	R	613	CHL	C3C-C2C-CMC-OMC
34	R	613	CHL	CHA-CBD-CGD-O1D
34	Y	302	CHL	C1C-C2C-CMC-OMC
34	Y	302	CHL	C3C-C2C-CMC-OMC
34	Y	306	CHL	C1C-C2C-CMC-OMC
34	Y	306	CHL	C3C-C2C-CMC-OMC
34	Y	306	CHL	CBD-CGD-O2D-CED
34	Y	306	CHL	O1D-CGD-O2D-CED
34	Y	307	CHL	C1C-C2C-CMC-OMC
34	Y	307	CHL	C3C-C2C-CMC-OMC
34	Y	308	CHL	C1A-C2A-CAA-CBA
34	Y	308	CHL	C3A-C2A-CAA-CBA
34	Y	308	CHL	C1C-C2C-CMC-OMC
34	Y	308	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
34	Y	308	CHL	CHA-CBD-CGD-O1D
34	Y	308	CHL	CHA-CBD-CGD-O2D
34	Y	309	CHL	C1A-C2A-CAA-CBA
34	Y	309	CHL	C1C-C2C-CMC-OMC
34	Y	309	CHL	C3C-C2C-CMC-OMC
34	Y	309	CHL	CHA-CBD-CGD-O1D
34	Y	309	CHL	CHA-CBD-CGD-O2D
34	g	601	CHL	C1C-C2C-CMC-OMC
34	g	601	CHL	C3C-C2C-CMC-OMC
34	g	601	CHL	CHA-CBD-CGD-O1D
34	g	601	CHL	CHA-CBD-CGD-O2D
34	g	605	CHL	C1C-C2C-CMC-OMC
34	g	605	CHL	C3C-C2C-CMC-OMC
34	g	605	CHL	CBD-CGD-O2D-CED
34	g	606	CHL	C1A-C2A-CAA-CBA
34	g	606	CHL	C1C-C2C-CMC-OMC
34	g	606	CHL	C3C-C2C-CMC-OMC
34	g	606	CHL	CHA-CBD-CGD-O1D
34	g	606	CHL	CHA-CBD-CGD-O2D
34	g	606	CHL	CAD-CBD-CGD-O1D
34	g	606	CHL	CBD-CGD-O2D-CED
34	g	607	CHL	C1A-C2A-CAA-CBA
34	g	607	CHL	C3A-C2A-CAA-CBA
34	g	607	CHL	C1C-C2C-CMC-OMC
34	g	607	CHL	C3C-C2C-CMC-OMC
34	g	607	CHL	CHA-CBD-CGD-O1D
34	g	607	CHL	CHA-CBD-CGD-O2D
34	g	608	CHL	C1A-C2A-CAA-CBA
34	g	608	CHL	C1C-C2C-CMC-OMC
34	g	608	CHL	C3C-C2C-CMC-OMC
34	g	609	CHL	C1C-C2C-CMC-OMC
34	g	609	CHL	C3C-C2C-CMC-OMC
34	g	609	CHL	CBD-CGD-O2D-CED
34	g	619	CHL	C3A-C2A-CAA-CBA
34	g	619	CHL	C1C-C2C-CMC-OMC
34	g	619	CHL	C3C-C2C-CMC-OMC
34	n	302	CHL	CHA-CBD-CGD-O2D
34	n	306	CHL	C1C-C2C-CMC-OMC
34	n	306	CHL	C3C-C2C-CMC-OMC
34	n	307	CHL	C1C-C2C-CMC-OMC
34	n	307	CHL	C3C-C2C-CMC-OMC
34	n	308	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
34	n	308	CHL	C3C-C2C-CMC-OMC
34	n	308	CHL	CBD-CGD-O2D-CED
34	n	309	CHL	C1C-C2C-CMC-OMC
34	n	309	CHL	C3C-C2C-CMC-OMC
34	n	309	CHL	CHA-CBD-CGD-O1D
34	n	309	CHL	CHA-CBD-CGD-O2D
34	n	310	CHL	C1C-C2C-CMC-OMC
34	n	310	CHL	C3C-C2C-CMC-OMC
34	n	310	CHL	CHA-CBD-CGD-O1D
34	n	310	CHL	CHA-CBD-CGD-O2D
34	r	605	CHL	CBD-CGD-O2D-CED
34	r	606	CHL	C1C-C2C-CMC-OMC
34	r	606	CHL	C3C-C2C-CMC-OMC
34	r	607	CHL	C1A-C2A-CAA-CBA
34	r	607	CHL	C3C-C2C-CMC-OMC
34	r	607	CHL	CBD-CGD-O2D-CED
34	r	613	CHL	C1C-C2C-CMC-OMC
34	r	613	CHL	C3C-C2C-CMC-OMC
34	r	613	CHL	CHA-CBD-CGD-O1D
34	r	613	CHL	CHA-CBD-CGD-O2D
34	y	302	CHL	C1C-C2C-CMC-OMC
34	y	302	CHL	C3C-C2C-CMC-OMC
34	y	306	CHL	C1A-C2A-CAA-CBA
34	y	306	CHL	C1C-C2C-CMC-OMC
34	y	306	CHL	C3C-C2C-CMC-OMC
34	y	308	CHL	C1A-C2A-CAA-CBA
34	y	308	CHL	C3A-C2A-CAA-CBA
34	y	308	CHL	C1C-C2C-CMC-OMC
34	y	308	CHL	C3C-C2C-CMC-OMC
34	y	308	CHL	CHA-CBD-CGD-O1D
34	y	308	CHL	CHA-CBD-CGD-O2D
34	y	309	CHL	C1A-C2A-CAA-CBA
34	y	309	CHL	C3C-C2C-CMC-OMC
34	y	309	CHL	CHA-CBD-CGD-O1D
34	y	309	CHL	CHA-CBD-CGD-O2D
34	S	601	CHL	C1C-C2C-CMC-OMC
34	S	601	CHL	C3C-C2C-CMC-OMC
34	S	601	CHL	CBD-CGD-O2D-CED
34	S	605	CHL	C1A-C2A-CAA-CBA
34	S	605	CHL	C3A-C2A-CAA-CBA
34	S	605	CHL	C1C-C2C-CMC-OMC
34	S	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
34	S	605	CHL	CHA-CBD-CGD-O1D
34	S	605	CHL	CHA-CBD-CGD-O2D
34	S	606	CHL	C1A-C2A-CAA-CBA
34	S	606	CHL	C1C-C2C-CMC-OMC
34	S	606	CHL	C3C-C2C-CMC-OMC
34	S	607	CHL	C1C-C2C-CMC-OMC
34	S	607	CHL	C3C-C2C-CMC-OMC
34	S	607	CHL	CHA-CBD-CGD-O1D
34	S	607	CHL	CHA-CBD-CGD-O2D
34	S	607	CHL	CAD-CBD-CGD-O1D
34	s	601	CHL	C1C-C2C-CMC-OMC
34	s	601	CHL	C3C-C2C-CMC-OMC
34	s	605	CHL	C1C-C2C-CMC-OMC
34	s	605	CHL	C3C-C2C-CMC-OMC
34	s	605	CHL	CBD-CGD-O2D-CED
34	s	606	CHL	C1A-C2A-CAA-CBA
34	s	606	CHL	C1C-C2C-CMC-OMC
34	s	606	CHL	C3C-C2C-CMC-OMC
34	s	607	CHL	C1C-C2C-CMC-OMC
34	s	607	CHL	C3C-C2C-CMC-OMC
34	s	607	CHL	CHA-CBD-CGD-O1D
34	s	607	CHL	CHA-CBD-CGD-O2D
34	s	607	CHL	CAD-CBD-CGD-O1D
34	s	607	CHL	CBD-CGD-O2D-CED
35	Y	316	LUT	C1-C6-C7-C8
35	g	615	LUT	C1-C6-C7-C8
35	y	315	LUT	C1-C6-C7-C8
35	S	615	LUT	C27-C28-C29-C39
35	s	615	LUT	C27-C28-C29-C30
35	s	615	LUT	C27-C28-C29-C39
36	y	317	NEX	C7-C8-C9-C19
37	Y	301	XAT	C27-C28-C29-C39
37	y	301	XAT	C27-C28-C29-C39
23	B	607	CLA	O1D-CGD-O2D-CED
23	C	507	CLA	O1D-CGD-O2D-CED
23	G	611	CLA	O1D-CGD-O2D-CED
23	N	314	CLA	O1D-CGD-O2D-CED
23	R	612	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	g	611	CLA	O1D-CGD-O2D-CED
23	n	314	CLA	O1D-CGD-O2D-CED
23	r	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	y	310	CLA	O1D-CGD-O2D-CED
23	y	312	CLA	O1D-CGD-O2D-CED
23	s	612	CLA	O1D-CGD-O2D-CED
34	G	605	CHL	O1D-CGD-O2D-CED
34	G	609	CHL	O1D-CGD-O2D-CED
34	g	609	CHL	O1D-CGD-O2D-CED
23	D	404	CLA	C15-C16-C17-C18
23	B	605	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	C	514	CLA	O1D-CGD-O2D-CED
23	G	613	CLA	O1D-CGD-O2D-CED
23	R	608	CLA	O1D-CGD-O2D-CED
23	R	610	CLA	O1D-CGD-O2D-CED
23	Y	310	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
23	r	608	CLA	O1D-CGD-O2D-CED
23	r	610	CLA	O1D-CGD-O2D-CED
23	A	401	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	CBD-CGD-O2D-CED
23	G	603	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	CBD-CGD-O2D-CED
23	G	611	CLA	CBD-CGD-O2D-CED
23	G	613	CLA	CBD-CGD-O2D-CED
23	N	303	CLA	CBD-CGD-O2D-CED
23	N	304	CLA	CBD-CGD-O2D-CED
23	N	311	CLA	CBD-CGD-O2D-CED
23	R	602	CLA	CBD-CGD-O2D-CED
23	Y	305	CLA	CBD-CGD-O2D-CED
23	Y	310	CLA	CBD-CGD-O2D-CED
23	Y	314	CLA	CBD-CGD-O2D-CED
23	a	402	CLA	CBD-CGD-O2D-CED
23	b	601	CLA	CBD-CGD-O2D-CED
23	b	605	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
23	c	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	g	610	CLA	CBD-CGD-O2D-CED
23	n	303	CLA	CBD-CGD-O2D-CED
23	n	305	CLA	CBD-CGD-O2D-CED
23	r	601	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	CBD-CGD-O2D-CED
23	r	611	CLA	CBD-CGD-O2D-CED
23	y	310	CLA	CBD-CGD-O2D-CED
23	y	311	CLA	CBD-CGD-O2D-CED
23	y	314	CLA	CBD-CGD-O2D-CED
23	S	611	CLA	CBD-CGD-O2D-CED
23	S	613	CLA	CBD-CGD-O2D-CED
23	s	612	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	CBD-CGD-O2D-CED
34	G	605	CHL	CBD-CGD-O2D-CED
34	G	606	CHL	CBD-CGD-O2D-CED
34	G	619	CHL	CBD-CGD-O2D-CED
34	N	302	CHL	CBD-CGD-O2D-CED
34	N	308	CHL	CBD-CGD-O2D-CED
34	Y	302	CHL	CBD-CGD-O2D-CED
34	n	302	CHL	CBD-CGD-O2D-CED
34	n	307	CHL	CBD-CGD-O2D-CED
34	y	302	CHL	CBD-CGD-O2D-CED
34	y	306	CHL	CBD-CGD-O2D-CED
34	S	607	CHL	CBD-CGD-O2D-CED
34	s	601	CHL	CBD-CGD-O2D-CED
23	N	312	CLA	O1A-CGA-O2A-C1
23	Y	311	CLA	O1A-CGA-O2A-C1
23	c	502	CLA	O1A-CGA-O2A-C1
23	y	304	CLA	O1A-CGA-O2A-C1
23	y	311	CLA	O1A-CGA-O2A-C1
24	A	403	PHO	O1A-CGA-O2A-C1
24	a	404	PHO	O1A-CGA-O2A-C1
34	S	607	CHL	O1A-CGA-O2A-C1
23	B	613	CLA	O1D-CGD-O2D-CED
23	N	305	CLA	O1D-CGD-O2D-CED
23	N	311	CLA	O1D-CGD-O2D-CED
23	R	601	CLA	O1D-CGD-O2D-CED
23	b	613	CLA	O1D-CGD-O2D-CED
23	g	613	CLA	O1D-CGD-O2D-CED
34	N	307	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	Y	302	CHL	O1D-CGD-O2D-CED
34	r	605	CHL	O1D-CGD-O2D-CED
34	s	601	CHL	O1D-CGD-O2D-CED
23	D	405	CLA	O1D-CGD-O2D-CED
23	N	303	CLA	O1D-CGD-O2D-CED
23	R	609	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
23	d	405	CLA	O1D-CGD-O2D-CED
23	r	601	CLA	O1D-CGD-O2D-CED
23	r	609	CLA	O1D-CGD-O2D-CED
23	S	602	CLA	O1D-CGD-O2D-CED
23	S	611	CLA	O1D-CGD-O2D-CED
23	S	612	CLA	O1D-CGD-O2D-CED
23	s	602	CLA	O1D-CGD-O2D-CED
24	D	402	PHO	O1D-CGD-O2D-CED
34	n	308	CHL	O1D-CGD-O2D-CED
34	S	601	CHL	O1D-CGD-O2D-CED
34	s	607	CHL	O1D-CGD-O2D-CED
23	c	502	CLA	CBA-CGA-O2A-C1
24	a	404	PHO	CBA-CGA-O2A-C1
32	d	407	PL9	C47-C48-C49-C50
23	A	404	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	608	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	D	401	CLA	CBD-CGD-O2D-CED
23	G	604	CLA	CBD-CGD-O2D-CED
23	R	614	CLA	CBD-CGD-O2D-CED
23	Y	303	CLA	CBD-CGD-O2D-CED
23	a	401	CLA	CBD-CGD-O2D-CED
23	a	405	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	g	603	CLA	CBD-CGD-O2D-CED
23	r	614	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	CBD-CGD-O2D-CED
23	s	608	CLA	CBD-CGD-O2D-CED
23	s	611	CLA	CBD-CGD-O2D-CED
34	R	606	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	R	607	CHL	CBD-CGD-O2D-CED
34	g	619	CHL	CBD-CGD-O2D-CED
34	r	606	CHL	CBD-CGD-O2D-CED
34	S	605	CHL	CBD-CGD-O2D-CED
23	B	607	CLA	O1A-CGA-O2A-C1
23	B	613	CLA	O1A-CGA-O2A-C1
23	N	311	CLA	O1A-CGA-O2A-C1
23	R	610	CLA	O1A-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
23	g	604	CLA	O1A-CGA-O2A-C1
23	n	311	CLA	O1A-CGA-O2A-C1
23	r	610	CLA	O1A-CGA-O2A-C1
34	Y	307	CHL	O1A-CGA-O2A-C1
34	g	619	CHL	O1A-CGA-O2A-C1
34	y	307	CHL	O1A-CGA-O2A-C1
34	s	607	CHL	O1A-CGA-O2A-C1
23	c	503	CLA	O1D-CGD-O2D-CED
23	n	311	CLA	O1D-CGD-O2D-CED
34	g	605	CHL	O1D-CGD-O2D-CED
24	a	404	PHO	C8-C10-C11-C12
34	g	606	CHL	O1D-CGD-O2D-CED
34	r	607	CHL	O1D-CGD-O2D-CED
34	s	605	CHL	O1D-CGD-O2D-CED
23	B	616	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
34	N	309	CHL	CBD-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
23	g	610	CLA	O1D-CGD-O2D-CED
28	a	408	DGD	O1B-C1B-O2G-C2G
30	B	623	LHG	O9-C7-O7-C5
30	T	101	LHG	O9-C7-O7-C5
23	G	604	CLA	O1A-CGA-O2A-C1
34	S	607	CHL	O1D-CGD-O2D-CED
23	B	603	CLA	C3-C5-C6-C7
23	B	605	CLA	C3-C5-C6-C7
23	C	512	CLA	C3-C5-C6-C7
23	G	602	CLA	C3-C5-C6-C7
23	N	304	CLA	C3-C5-C6-C7
23	b	603	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C3-C5-C6-C7
23	b	613	CLA	C3-C5-C6-C7
23	c	503	CLA	C3-C5-C6-C7
23	g	602	CLA	C3-C5-C6-C7
23	n	304	CLA	C3-C5-C6-C7
23	n	312	CLA	C3-C5-C6-C7
34	G	609	CHL	C3-C5-C6-C7
34	g	609	CHL	C3-C5-C6-C7
34	g	619	CHL	C3-C5-C6-C7
23	B	612	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	CBA-CGA-O2A-C1
23	N	311	CLA	CBA-CGA-O2A-C1
23	N	312	CLA	CBA-CGA-O2A-C1
23	R	610	CLA	CBA-CGA-O2A-C1
23	Y	311	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	g	604	CLA	CBA-CGA-O2A-C1
23	n	311	CLA	CBA-CGA-O2A-C1
23	r	610	CLA	CBA-CGA-O2A-C1
23	y	304	CLA	CBA-CGA-O2A-C1
23	y	311	CLA	CBA-CGA-O2A-C1
24	A	403	PHO	CBA-CGA-O2A-C1
34	G	619	CHL	CBA-CGA-O2A-C1
34	Y	307	CHL	CBA-CGA-O2A-C1
34	g	619	CHL	CBA-CGA-O2A-C1
34	y	307	CHL	CBA-CGA-O2A-C1
34	S	607	CHL	CBA-CGA-O2A-C1
34	s	607	CHL	CBA-CGA-O2A-C1
32	D	406	PL9	C47-C48-C49-C51
23	R	602	CLA	O1D-CGD-O2D-CED
34	Y	309	CHL	CBD-CGD-O2D-CED
23	C	511	CLA	O1A-CGA-O2A-C1
23	N	314	CLA	O1A-CGA-O2A-C1
23	n	314	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C4-C3-C5-C6
24	d	401	PHO	C4-C3-C5-C6
32	D	406	PL9	C25-C24-C26-C27
32	d	407	PL9	C25-C24-C26-C27
23	b	603	CLA	C2-C3-C5-C6
32	d	407	PL9	C13-C14-C16-C17
23	r	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	G	608	CHL	CBD-CGD-O2D-CED
23	B	610	CLA	C2A-CAA-CBA-CGA
23	N	313	CLA	C2A-CAA-CBA-CGA
23	R	602	CLA	C2A-CAA-CBA-CGA
23	Y	303	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C2A-CAA-CBA-CGA
23	g	604	CLA	C2A-CAA-CBA-CGA
23	r	602	CLA	C2A-CAA-CBA-CGA
23	r	604	CLA	C2A-CAA-CBA-CGA
23	y	303	CLA	C2A-CAA-CBA-CGA
34	Y	308	CHL	C2A-CAA-CBA-CGA
34	n	302	CHL	C2A-CAA-CBA-CGA
34	y	307	CHL	C2A-CAA-CBA-CGA
34	y	308	CHL	C2A-CAA-CBA-CGA
34	S	605	CHL	C2A-CAA-CBA-CGA
23	A	401	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C3-C5-C6-C7
23	B	613	CLA	C3-C5-C6-C7
23	C	504	CLA	C3-C5-C6-C7
34	G	619	CHL	C3-C5-C6-C7
23	B	607	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	CBA-CGA-O2A-C1
23	G	604	CLA	CBA-CGA-O2A-C1
23	N	314	CLA	CBA-CGA-O2A-C1
23	R	604	CLA	CBA-CGA-O2A-C1
23	Y	304	CLA	CBA-CGA-O2A-C1
23	b	607	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
23	n	314	CLA	CBA-CGA-O2A-C1
23	r	604	CLA	CBA-CGA-O2A-C1
34	G	608	CHL	CBA-CGA-O2A-C1
23	Y	305	CLA	O1D-CGD-O2D-CED
23	b	601	CLA	O1D-CGD-O2D-CED
32	D	406	PL9	C7-C8-C9-C10
32	D	406	PL9	C22-C23-C24-C25
32	D	406	PL9	C32-C33-C34-C35
32	D	406	PL9	C37-C38-C39-C40
32	D	406	PL9	C42-C43-C44-C45
32	d	407	PL9	C7-C8-C9-C10
32	d	407	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	d	407	PL9	C32-C33-C34-C35
32	d	407	PL9	C37-C38-C39-C40
32	d	407	PL9	C42-C43-C44-C45
23	A	402	CLA	CBD-CGD-O2D-CED
34	n	309	CHL	CBD-CGD-O2D-CED
34	y	309	CHL	CBD-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	G	610	CLA	O1D-CGD-O2D-CED
23	Y	314	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
23	y	314	CLA	O1D-CGD-O2D-CED
34	G	619	CHL	O1D-CGD-O2D-CED
34	n	302	CHL	O1D-CGD-O2D-CED
28	A	408	DGD	O1B-C1B-O2G-C2G
23	C	513	CLA	O1A-CGA-O2A-C1
23	G	610	CLA	O1A-CGA-O2A-C1
23	R	608	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	g	610	CLA	O1A-CGA-O2A-C1
23	n	312	CLA	O1A-CGA-O2A-C1
23	r	611	CLA	O1D-CGD-O2D-CED
34	G	606	CHL	O1D-CGD-O2D-CED
35	n	316	LUT	C33-C34-C35-C15
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	CBD-CGD-O2D-CED
23	N	315	CLA	CBD-CGD-O2D-CED
23	a	403	CLA	CBD-CGD-O2D-CED
23	n	313	CLA	CBD-CGD-O2D-CED
23	r	604	CLA	CBD-CGD-O2D-CED
23	S	609	CLA	CBD-CGD-O2D-CED
34	N	310	CHL	CBD-CGD-O2D-CED
34	Y	308	CHL	CBD-CGD-O2D-CED
34	r	613	CHL	CBD-CGD-O2D-CED
34	y	308	CHL	CBD-CGD-O2D-CED
34	S	606	CHL	CBD-CGD-O2D-CED
23	N	304	CLA	O1D-CGD-O2D-CED
34	y	302	CHL	O1D-CGD-O2D-CED
30	G	618	LHG	O2-C2-C3-O3
23	B	602	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C3-C5-C6-C7
23	b	612	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
34	r	607	CHL	C3-C5-C6-C7
23	C	503	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	G	610	CLA	CBA-CGA-O2A-C1
23	Y	305	CLA	CBA-CGA-O2A-C1
23	b	612	CLA	CBA-CGA-O2A-C1
23	c	503	CLA	CBA-CGA-O2A-C1
23	n	312	CLA	CBA-CGA-O2A-C1
34	g	608	CHL	CBA-CGA-O2A-C1
23	B	612	CLA	O1A-CGA-O2A-C1
23	R	604	CLA	O1A-CGA-O2A-C1
23	a	402	CLA	O1D-CGD-O2D-CED
23	n	303	CLA	O1D-CGD-O2D-CED
23	n	305	CLA	O1D-CGD-O2D-CED
34	N	302	CHL	O1D-CGD-O2D-CED
30	n	319	LHG	C8-C7-O7-C5
23	G	612	CLA	CBD-CGD-O2D-CED
23	b	602	CLA	CBD-CGD-O2D-CED
23	s	609	CLA	CBD-CGD-O2D-CED
23	s	610	CLA	CBD-CGD-O2D-CED
34	g	608	CHL	CBD-CGD-O2D-CED
24	d	401	PHO	O1D-CGD-O2D-CED
23	C	512	CLA	O1A-CGA-O2A-C1
23	G	603	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	O1D-CGD-O2D-CED
23	S	613	CLA	O1D-CGD-O2D-CED
34	n	307	CHL	O1D-CGD-O2D-CED
23	c	511	CLA	C3-C5-C6-C7
23	S	612	CLA	C3-C5-C6-C7
23	C	511	CLA	CBA-CGA-O2A-C1
23	R	608	CLA	CBA-CGA-O2A-C1
23	a	403	CLA	CBA-CGA-O2A-C1
23	g	610	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	O1D-CGD-O2D-CED
34	y	306	CHL	O1D-CGD-O2D-CED
30	n	319	LHG	O9-C7-O7-C5
23	Y	305	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	O1A-CGA-O2A-C1
23	c	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	r	604	CLA	O1A-CGA-O2A-C1
34	G	608	CHL	O1A-CGA-O2A-C1
34	g	608	CHL	O1A-CGA-O2A-C1
23	a	401	CLA	C4-C3-C5-C6
23	a	401	CLA	C2-C3-C5-C6
23	C	511	CLA	C2A-CAA-CBA-CGA
23	G	611	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C2A-CAA-CBA-CGA
34	N	307	CHL	C2A-CAA-CBA-CGA
34	Y	307	CHL	C2A-CAA-CBA-CGA
27	B	620	LMG	O6-C1-O1-C7
27	b	620	LMG	O6-C1-O1-C7
32	D	406	PL9	C9-C11-C12-C13
32	D	406	PL9	C39-C41-C42-C43
32	D	406	PL9	C44-C46-C47-C48
32	d	407	PL9	C9-C11-C12-C13
32	d	407	PL9	C39-C41-C42-C43
32	d	407	PL9	C44-C46-C47-C48
23	A	402	CLA	CBA-CGA-O2A-C1
23	C	505	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
23	y	305	CLA	CBA-CGA-O2A-C1
34	R	607	CHL	CBA-CGA-O2A-C1
23	B	608	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
23	Y	303	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
23	g	603	CLA	O1D-CGD-O2D-CED
23	s	608	CLA	O1D-CGD-O2D-CED
34	N	308	CHL	O1D-CGD-O2D-CED
34	R	607	CHL	O1D-CGD-O2D-CED
34	g	619	CHL	O1D-CGD-O2D-CED
23	a	403	CLA	O1A-CGA-O2A-C1
34	R	607	CHL	O1A-CGA-O2A-C1
23	a	401	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
23	r	614	CLA	O1D-CGD-O2D-CED
23	s	611	CLA	O1D-CGD-O2D-CED
34	r	606	CHL	O1D-CGD-O2D-CED
23	s	613	CLA	CBD-CGD-O2D-CED
34	R	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	A	402	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	O1A-CGA-O2A-C1
23	C	505	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	O1A-CGA-O2A-C1
23	s	612	CLA	C3-C5-C6-C7
23	A	404	CLA	O1D-CGD-O2D-CED
23	a	405	CLA	O1D-CGD-O2D-CED
34	S	605	CHL	O1D-CGD-O2D-CED
23	A	401	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	CBA-CGA-O2A-C1
23	a	401	CLA	CBA-CGA-O2A-C1
23	b	603	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
23	g	602	CLA	CBA-CGA-O2A-C1
23	n	304	CLA	CBA-CGA-O2A-C1
23	y	303	CLA	CBA-CGA-O2A-C1
34	N	302	CHL	CBA-CGA-O2A-C1
34	n	302	CHL	CBA-CGA-O2A-C1
34	r	607	CHL	CBA-CGA-O2A-C1
23	C	510	CLA	CBD-CGD-O2D-CED
23	b	603	CLA	CBD-CGD-O2D-CED
23	n	312	CLA	CBD-CGD-O2D-CED
34	n	310	CHL	CBD-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
34	g	608	CHL	C15-C16-C17-C18
32	d	407	PL9	C47-C48-C49-C51
23	b	604	CLA	C10-C11-C12-C13
23	c	509	CLA	C10-C11-C12-C13
34	G	608	CHL	C15-C16-C17-C18
34	n	310	CHL	C15-C16-C17-C18
30	g	618	LHG	O2-C2-C3-O3
23	b	614	CLA	C3-C5-C6-C7
28	a	408	DGD	O2G-C2G-C3G-O3G
30	Y	318	LHG	O7-C5-C6-O8
23	B	603	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	O1A-CGA-O2A-C1
23	n	304	CLA	O1A-CGA-O2A-C1
32	d	407	PL9	C20-C19-C21-C22
34	G	609	CHL	C4-C3-C5-C6
23	C	503	CLA	C2-C3-C5-C6
23	B	605	CLA	C11-C10-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	B	614	CLA	C11-C10-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	Y	311	CLA	C6-C7-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	612	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C10-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	g	602	CLA	C6-C7-C8-C9
34	Y	308	CHL	C11-C10-C8-C9
34	y	308	CHL	C11-C10-C8-C9
23	B	601	CLA	O1D-CGD-O2D-CED
23	G	604	CLA	O1D-CGD-O2D-CED
23	Y	311	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C2A-CAA-CBA-CGA
23	N	311	CLA	C2A-CAA-CBA-CGA
23	R	604	CLA	C2A-CAA-CBA-CGA
34	n	307	CHL	C2A-CAA-CBA-CGA
25	C	515	BCR	C36-C18-C19-C20
25	k	101	BCR	C7-C8-C9-C34
35	y	315	LUT	C27-C28-C29-C39
23	g	602	CLA	O1A-CGA-O2A-C1
23	y	303	CLA	O1A-CGA-O2A-C1
34	N	302	CHL	O1A-CGA-O2A-C1
34	n	302	CHL	O1A-CGA-O2A-C1
23	B	612	CLA	C10-C11-C12-C13
23	D	401	CLA	C13-C15-C16-C17
23	b	612	CLA	C10-C11-C12-C13
23	b	614	CLA	C8-C10-C11-C12
23	c	504	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	a	404	PHO	C10-C11-C12-C13
28	c	516	DGD	O6E-C5E-C6E-O5E
23	b	608	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	C3-C5-C6-C7
23	B	610	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	CBA-CGA-O2A-C1
23	S	604	CLA	CBA-CGA-O2A-C1
33	e	101	HEM	C2A-CAA-CBA-CGA
23	B	608	CLA	C5-C6-C7-C8
23	c	503	CLA	C8-C10-C11-C12
23	n	314	CLA	C10-C11-C12-C13
24	d	401	PHO	C15-C16-C17-C18
34	G	601	CHL	C13-C15-C16-C17
23	D	401	CLA	O1D-CGD-O2D-CED
23	R	614	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C10-C11-C12-C13
23	B	606	CLA	C15-C16-C17-C18
23	B	610	CLA	C15-C16-C17-C18
23	B	614	CLA	C8-C10-C11-C12
23	C	504	CLA	C5-C6-C7-C8
23	a	402	CLA	C13-C15-C16-C17
23	b	608	CLA	C5-C6-C7-C8
23	b	610	CLA	C15-C16-C17-C18
23	c	503	CLA	C5-C6-C7-C8
23	c	513	CLA	C10-C11-C12-C13
23	d	404	CLA	C10-C11-C12-C13
23	r	602	CLA	C10-C11-C12-C13
24	A	403	PHO	C10-C11-C12-C13
24	D	402	PHO	C15-C16-C17-C18
23	y	313	CLA	O1D-CGD-O2D-CED
34	r	607	CHL	O1A-CGA-O2A-C1
30	B	623	LHG	C23-C24-C25-C26
30	G	618	LHG	C23-C24-C25-C26
30	T	101	LHG	C23-C24-C25-C26
30	g	618	LHG	C23-C24-C25-C26
23	C	503	CLA	C10-C11-C12-C13
23	C	510	CLA	C10-C11-C12-C13
23	Y	311	CLA	C8-C10-C11-C12
23	b	606	CLA	C8-C10-C11-C12
23	b	613	CLA	C8-C10-C11-C12
23	c	501	CLA	C15-C16-C17-C18
23	c	511	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	Y	313	CLA	C15-C16-C17-C18
23	y	310	CLA	C5-C6-C7-C8
23	y	313	CLA	C15-C16-C17-C18
34	N	309	CHL	C15-C16-C17-C18
34	g	601	CHL	C13-C15-C16-C17
34	n	309	CHL	C8-C10-C11-C12
28	a	408	DGD	C1B-C2B-C3B-C4B
23	C	502	CLA	C15-C16-C17-C18
23	D	404	CLA	C10-C11-C12-C13
23	c	507	CLA	C13-C15-C16-C17
34	N	309	CHL	C8-C10-C11-C12
34	n	309	CHL	C15-C16-C17-C18
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C7
23	D	405	CLA	C12-C13-C15-C16
23	Y	304	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	d	405	CLA	C12-C13-C15-C16
34	n	302	CHL	C6-C7-C8-C10
23	B	612	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
23	A	401	CLA	O1A-CGA-O2A-C1
23	c	505	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
25	Z	101	BCR	C15-C16-C17-C18
25	d	406	BCR	C9-C10-C11-C12
25	h	101	BCR	C9-C10-C11-C12
34	n	306	CHL	CBA-CGA-O2A-C1
23	B	612	CLA	C2A-CAA-CBA-CGA
23	G	604	CLA	C2A-CAA-CBA-CGA
23	Y	305	CLA	C2A-CAA-CBA-CGA
23	Y	312	CLA	C2A-CAA-CBA-CGA
23	b	612	CLA	C2A-CAA-CBA-CGA
23	g	611	CLA	C2A-CAA-CBA-CGA
34	s	607	CHL	C2A-CAA-CBA-CGA
23	B	616	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	O1D-CGD-O2D-CED
34	G	608	CHL	O1D-CGD-O2D-CED
34	N	309	CHL	O1D-CGD-O2D-CED
23	B	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	R	603	CLA	C5-C6-C7-C8
23	Y	310	CLA	C5-C6-C7-C8
23	b	605	CLA	C5-C6-C7-C8
23	b	607	CLA	C5-C6-C7-C8
23	b	610	CLA	C8-C10-C11-C12
23	c	513	CLA	C5-C6-C7-C8
23	a	401	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
23	g	612	CLA	CBD-CGD-O2D-CED
34	R	613	CHL	CBD-CGD-O2D-CED
24	A	403	PHO	C15-C16-C17-C18
23	y	304	CLA	C3-C5-C6-C7
34	N	310	CHL	C3-C5-C6-C7
23	B	605	CLA	C5-C6-C7-C8
23	B	607	CLA	C5-C6-C7-C8
23	C	504	CLA	C8-C10-C11-C12
23	C	512	CLA	C8-C10-C11-C12
23	N	314	CLA	C5-C6-C7-C8
23	b	608	CLA	C8-C10-C11-C12
23	y	311	CLA	C8-C10-C11-C12
24	a	404	PHO	C15-C16-C17-C18
34	g	619	CHL	C13-C15-C16-C17
34	y	309	CHL	C10-C11-C12-C13
23	b	602	CLA	CBA-CGA-O2A-C1
30	w	201	LHG	C24-C23-O8-C6
23	C	507	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C5-C6-C7-C8
23	B	606	CLA	C8-C10-C11-C12
23	C	503	CLA	C13-C15-C16-C17
34	G	619	CHL	C15-C16-C17-C18
34	g	619	CHL	C15-C16-C17-C18
23	b	614	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	O1A-CGA-O2A-C1
23	S	604	CLA	O1A-CGA-O2A-C1
23	B	608	CLA	C8-C10-C11-C12
23	B	616	CLA	C8-C10-C11-C12
23	Y	303	CLA	C10-C11-C12-C13
23	Y	311	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
34	g	619	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	A	411	LHG	C3-O3-P-O6
30	A	411	LHG	C4-O6-P-O3
30	B	621	LHG	C3-O3-P-O6
30	B	621	LHG	C4-O6-P-O3
30	B	623	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O3
30	L	102	LHG	C3-O3-P-O6
30	L	102	LHG	C4-O6-P-O3
30	T	101	LHG	C4-O6-P-O3
30	W	201	LHG	C4-O6-P-O3
30	Y	318	LHG	C4-O6-P-O3
30	a	411	LHG	C3-O3-P-O6
30	a	411	LHG	C4-O6-P-O3
30	b	621	LHG	C3-O3-P-O6
30	b	621	LHG	C4-O6-P-O3
30	b	622	LHG	C3-O3-P-O6
30	b	622	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O3
30	r	618	LHG	C4-O6-P-O3
30	w	201	LHG	C4-O6-P-O3
30	y	318	LHG	C4-O6-P-O3
30	S	617	LHG	C4-O6-P-O3
30	s	617	LHG	C3-O3-P-O6
30	s	617	LHG	C4-O6-P-O3
23	c	507	CLA	C3-C5-C6-C7
23	B	601	CLA	CBA-CGA-O2A-C1
34	N	309	CHL	CBA-CGA-O2A-C1
23	c	503	CLA	C13-C15-C16-C17
34	Y	309	CHL	O1D-CGD-O2D-CED
23	r	603	CLA	O1D-CGD-O2D-CED
32	D	406	PL9	C20-C19-C21-C22
24	d	401	PHO	C2-C3-C5-C6
34	G	619	CHL	C13-C15-C16-C17
23	C	506	CLA	C2A-CAA-CBA-CGA
23	C	510	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
23	n	304	CLA	C2A-CAA-CBA-CGA
23	n	311	CLA	C2A-CAA-CBA-CGA
23	n	313	CLA	C2A-CAA-CBA-CGA
23	y	312	CLA	C2A-CAA-CBA-CGA
34	N	308	CHL	C2A-CAA-CBA-CGA
34	n	308	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C16-C17-C18-C19
24	a	404	PHO	C16-C17-C18-C19
23	b	602	CLA	C3-C5-C6-C7
23	n	314	CLA	C3-C5-C6-C7
34	R	607	CHL	C3-C5-C6-C7
23	D	401	CLA	CBA-CGA-O2A-C1
23	G	602	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
34	N	306	CHL	CBA-CGA-O2A-C1
34	n	309	CHL	CBA-CGA-O2A-C1
23	B	615	CLA	C8-C10-C11-C12
24	A	403	PHO	C8-C10-C11-C12
28	A	408	DGD	C1B-C2B-C3B-C4B
34	n	309	CHL	O1D-CGD-O2D-CED
23	S	603	CLA	CBD-CGD-O2D-CED
26	A	409	SQD	C8-C7-O47-C45
26	a	409	SQD	C8-C7-O47-C45
34	Y	308	CHL	O1D-CGD-O2D-CED
23	C	510	CLA	C16-C17-C18-C19
23	D	404	CLA	C16-C17-C18-C20
23	Y	311	CLA	C11-C12-C13-C15
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
23	g	602	CLA	C16-C17-C18-C20
23	N	304	CLA	CBA-CGA-O2A-C1
23	N	311	CLA	C10-C11-C12-C13
23	n	311	CLA	C10-C11-C12-C13
30	A	411	LHG	C28-C29-C30-C31
30	a	411	LHG	C28-C29-C30-C31
26	A	409	SQD	O49-C7-O47-C45
26	a	409	SQD	O49-C7-O47-C45
27	b	620	LMG	C28-C29-C30-C31
27	d	409	LMG	C10-C11-C12-C13
23	B	603	CLA	CBD-CGD-O2D-CED
23	y	311	CLA	C5-C6-C7-C8
28	d	410	DGD	C6A-C7A-C8A-C9A
30	y	318	LHG	C11-C10-C9-C8
23	C	514	CLA	C3-C5-C6-C7
23	A	402	CLA	O1D-CGD-O2D-CED
34	y	308	CHL	O1D-CGD-O2D-CED
34	y	309	CHL	O1D-CGD-O2D-CED
26	A	406	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	CBA-CGA-O2A-C1
23	G	602	CLA	O1A-CGA-O2A-C1
23	B	605	CLA	C16-C17-C18-C20
23	C	511	CLA	C16-C17-C18-C20
23	D	401	CLA	C16-C17-C18-C19
23	Y	312	CLA	C11-C12-C13-C14
23	a	402	CLA	C16-C17-C18-C19
23	y	312	CLA	C11-C12-C13-C14
23	D	401	CLA	C4-C3-C5-C6
23	B	602	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	b	615	CLA	C11-C10-C8-C9
23	y	304	CLA	C6-C7-C8-C9
23	y	304	CLA	C11-C12-C13-C14
34	N	302	CHL	C6-C7-C8-C9
23	r	604	CLA	O1D-CGD-O2D-CED
34	g	608	CHL	O1D-CGD-O2D-CED
24	a	404	PHO	C5-C6-C7-C8
23	A	402	CLA	C2A-CAA-CBA-CGA
23	C	505	CLA	C2A-CAA-CBA-CGA
23	a	403	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
23	g	602	CLA	C2A-CAA-CBA-CGA
24	d	401	PHO	C2A-CAA-CBA-CGA
34	G	619	CHL	C2A-CAA-CBA-CGA
23	b	602	CLA	O1A-CGA-O2A-C1
34	n	306	CHL	O1A-CGA-O2A-C1
30	Y	318	LHG	C11-C10-C9-C8
25	c	515	BCR	C11-C12-C13-C14
35	S	615	LUT	C27-C28-C29-C30
23	b	601	CLA	C3-C5-C6-C7
23	d	405	CLA	C3-C5-C6-C7
30	N	319	LHG	O9-C7-O7-C5
30	w	201	LHG	O9-C7-O7-C5
23	r	608	CLA	C5-C6-C7-C8
30	N	319	LHG	C8-C7-O7-C5
30	w	201	LHG	C8-C7-O7-C5
23	s	603	CLA	CBD-CGD-O2D-CED
27	B	620	LMG	C28-C29-C30-C31
27	D	407	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	403	CLA	O1D-CGD-O2D-CED
34	S	606	CHL	O1D-CGD-O2D-CED
30	N	319	LHG	C11-C12-C13-C14
30	W	201	LHG	C25-C26-C27-C28
34	N	306	CHL	O1A-CGA-O2A-C1
23	G	602	CLA	C16-C17-C18-C19
23	G	602	CLA	C16-C17-C18-C20
23	Y	310	CLA	C11-C12-C13-C14
23	Y	310	CLA	C11-C12-C13-C15
23	b	605	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
34	y	302	CHL	C16-C17-C18-C20
23	N	314	CLA	C10-C11-C12-C13
23	b	615	CLA	C8-C10-C11-C12
23	y	312	CLA	C10-C11-C12-C13
23	C	502	CLA	O1D-CGD-O2D-CED
26	A	409	SQD	C12-C13-C14-C15
30	A	412	LHG	C11-C12-C13-C14
30	B	621	LHG	C27-C28-C29-C30
30	b	621	LHG	C27-C28-C29-C30
30	w	201	LHG	C25-C26-C27-C28
27	D	407	LMG	C28-C29-C30-C31
23	C	514	CLA	C10-C11-C12-C13
23	b	616	CLA	C8-C10-C11-C12
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	CBA-CGA-O2A-C1
23	a	402	CLA	CBA-CGA-O2A-C1
23	B	614	CLA	O1D-CGD-O2D-CED
23	N	315	CLA	O1D-CGD-O2D-CED
23	n	313	CLA	O1D-CGD-O2D-CED
23	s	609	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	C3A-C2A-CAA-CBA
23	B	610	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	C3A-C2A-CAA-CBA
23	C	508	CLA	C3A-C2A-CAA-CBA
23	C	512	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
23	D	404	CLA	C3A-C2A-CAA-CBA
23	N	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	N	314	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	613	CLA	C3A-C2A-CAA-CBA
23	c	503	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	c	509	CLA	C3A-C2A-CAA-CBA
23	d	404	CLA	C3A-C2A-CAA-CBA
23	n	304	CLA	C3A-C2A-CAA-CBA
23	n	313	CLA	C3A-C2A-CAA-CBA
23	n	314	CLA	C3A-C2A-CAA-CBA
23	S	611	CLA	C3A-C2A-CAA-CBA
23	s	609	CLA	C3A-C2A-CAA-CBA
23	s	611	CLA	C3A-C2A-CAA-CBA
24	D	402	PHO	C3A-C2A-CAA-CBA
34	G	605	CHL	C3A-C2A-CAA-CBA
34	Y	306	CHL	C3A-C2A-CAA-CBA
34	Y	307	CHL	C3A-C2A-CAA-CBA
34	g	605	CHL	C3A-C2A-CAA-CBA
34	g	608	CHL	C3A-C2A-CAA-CBA
34	y	306	CHL	C3A-C2A-CAA-CBA
23	b	605	CLA	C8-C10-C11-C12
24	D	402	PHO	C10-C11-C12-C13
23	G	612	CLA	O1D-CGD-O2D-CED
23	S	609	CLA	O1D-CGD-O2D-CED
30	w	201	LHG	O10-C23-O8-C6
23	B	605	CLA	C16-C17-C18-C19
23	a	402	CLA	C16-C17-C18-C20
23	b	605	CLA	C16-C17-C18-C20
23	g	602	CLA	C16-C17-C18-C19
23	y	304	CLA	C16-C17-C18-C20
23	y	310	CLA	C11-C12-C13-C14
23	y	310	CLA	C11-C12-C13-C15
26	a	409	SQD	C12-C13-C14-C15
34	r	613	CHL	O1D-CGD-O2D-CED
23	D	401	CLA	O1A-CGA-O2A-C1
34	N	309	CHL	O1A-CGA-O2A-C1
34	n	309	CHL	O1A-CGA-O2A-C1
34	Y	302	CHL	C13-C15-C16-C17
23	N	314	CLA	C4-C3-C5-C6
34	N	310	CHL	C4-C3-C5-C6
23	y	312	CLA	CBA-CGA-O2A-C1
28	d	410	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
30	W	201	LHG	C24-C23-O8-C6
30	r	618	LHG	C24-C23-O8-C6
23	N	314	CLA	C2-C3-C5-C6
34	N	310	CHL	C2-C3-C5-C6
30	W	201	LHG	C8-C7-O7-C5
23	g	602	CLA	CBD-CGD-O2D-CED
30	n	319	LHG	C11-C12-C13-C14
26	M	101	SQD	C23-C24-C25-C26
27	d	409	LMG	C28-C29-C30-C31
23	C	510	CLA	C16-C17-C18-C20
23	Y	312	CLA	C11-C12-C13-C15
23	C	503	CLA	C5-C6-C7-C8
23	B	601	CLA	C3-C5-C6-C7
23	Y	304	CLA	C3-C5-C6-C7
34	y	308	CHL	C3-C5-C6-C7
30	G	618	LHG	C24-C23-O8-C6
30	a	412	LHG	C11-C12-C13-C14
30	W	201	LHG	O9-C7-O7-C5
23	D	401	CLA	C2-C1-O2A-CGA
23	a	402	CLA	C2-C1-O2A-CGA
23	B	605	CLA	C8-C10-C11-C12
23	b	601	CLA	C5-C6-C7-C8
24	d	401	PHO	C10-C11-C12-C13
23	N	304	CLA	O1A-CGA-O2A-C1
23	a	402	CLA	O1A-CGA-O2A-C1
23	b	614	CLA	O1A-CGA-O2A-C1
23	y	312	CLA	O1A-CGA-O2A-C1
30	L	101	LHG	C9-C10-C11-C12
23	D	401	CLA	C16-C17-C18-C20
26	a	409	SQD	C23-C24-C25-C26
23	B	608	CLA	C3-C5-C6-C7
25	A	405	BCR	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C30
25	B	617	BCR	C23-C24-C25-C26
25	C	516	BCR	C23-C24-C25-C26
25	C	516	BCR	C23-C24-C25-C30
25	F	101	BCR	C1-C6-C7-C8
25	F	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	Z	101	BCR	C23-C24-C25-C26
25	Z	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	a	406	BCR	C23-C24-C25-C26
25	a	406	BCR	C23-C24-C25-C30
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	c	515	BCR	C23-C24-C25-C26
25	c	515	BCR	C23-C24-C25-C30
25	c	518	BCR	C23-C24-C25-C26
25	c	518	BCR	C23-C24-C25-C30
25	d	406	BCR	C1-C6-C7-C8
25	d	406	BCR	C5-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
35	G	615	LUT	C1-C6-C7-C8
35	G	615	LUT	C5-C6-C7-C8
35	R	615	LUT	C1-C6-C7-C8
35	R	615	LUT	C5-C6-C7-C8
35	Y	315	LUT	C1-C6-C7-C8
35	Y	315	LUT	C5-C6-C7-C8
35	Y	316	LUT	C5-C6-C7-C8
35	g	615	LUT	C5-C6-C7-C8
35	y	315	LUT	C5-C6-C7-C8
35	S	614	LUT	C1-C6-C7-C8
35	S	614	LUT	C5-C6-C7-C8
35	s	614	LUT	C1-C6-C7-C8
35	s	614	LUT	C5-C6-C7-C8
30	L	102	LHG	C30-C31-C32-C33
23	Y	312	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	C13-C15-C16-C17
23	G	611	CLA	C10-C11-C12-C13
23	c	502	CLA	C13-C15-C16-C17
23	d	404	CLA	C13-C15-C16-C17
23	g	602	CLA	C13-C15-C16-C17
34	Y	308	CHL	C8-C10-C11-C12
34	g	608	CHL	C10-C11-C12-C13
30	c	517	LHG	C8-C7-O7-C5
23	B	602	CLA	C11-C12-C13-C15
23	B	604	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C12-C13-C15
23	B	610	CLA	C11-C12-C13-C15
23	B	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	612	CLA	C6-C7-C8-C10
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	D	401	CLA	C2-C3-C5-C6
23	b	602	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C12-C13-C15
23	b	609	CLA	C12-C13-C15-C16
23	b	612	CLA	C6-C7-C8-C10
23	b	614	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	c	502	CLA	C11-C12-C13-C15
23	c	513	CLA	C12-C13-C15-C16
23	y	304	CLA	C6-C7-C8-C10
23	y	304	CLA	C11-C12-C13-C15
24	A	403	PHO	C11-C10-C8-C7
24	D	402	PHO	C6-C7-C8-C10
24	d	401	PHO	C6-C7-C8-C10
34	N	302	CHL	C6-C7-C8-C10
34	Y	308	CHL	C11-C10-C8-C7
34	n	310	CHL	C6-C7-C8-C10
23	D	405	CLA	C3-C5-C6-C7
23	N	312	CLA	C3-C5-C6-C7
23	a	401	CLA	C3-C5-C6-C7
23	B	614	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	O1A-CGA-O2A-C1
23	Y	312	CLA	O1A-CGA-O2A-C1
28	d	410	DGD	O1A-C1A-O1G-C1G
23	a	401	CLA	C5-C6-C7-C8
34	N	302	CHL	C13-C15-C16-C17
35	n	316	LUT	C9-C10-C11-C12
23	n	315	CLA	CBD-CGD-O2D-CED
23	y	312	CLA	C11-C12-C13-C15
26	A	409	SQD	C23-C24-C25-C26
23	R	603	CLA	CBA-CGA-O2A-C1
23	Y	313	CLA	CBA-CGA-O2A-C1
30	g	618	LHG	C24-C23-O8-C6
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C2A-CAA-CBA-CGA
23	Y	313	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
23	S	608	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	O1D-CGD-O2D-CED
23	A	401	CLA	C15-C16-C17-C18
23	C	514	CLA	C5-C6-C7-C8
23	G	602	CLA	C13-C15-C16-C17
23	g	602	CLA	C5-C6-C7-C8
34	n	310	CHL	C8-C10-C11-C12
34	y	302	CHL	C13-C15-C16-C17
30	A	412	LHG	C16-C17-C18-C19
30	a	411	LHG	C11-C10-C9-C8
30	a	412	LHG	C28-C29-C30-C31
23	s	610	CLA	O1D-CGD-O2D-CED
27	b	620	LMG	C17-C18-C19-C20
30	d	408	LHG	C9-C10-C11-C12
23	B	603	CLA	C8-C10-C11-C12
23	B	604	CLA	C5-C6-C7-C8
23	B	607	CLA	C10-C11-C12-C13
30	A	412	LHG	C29-C30-C31-C32
30	b	622	LHG	C30-C31-C32-C33
27	B	620	LMG	C17-C18-C19-C20
23	C	514	CLA	CBA-CGA-O2A-C1
23	D	404	CLA	C16-C17-C18-C19
23	C	508	CLA	C15-C16-C17-C18
23	b	607	CLA	C10-C11-C12-C13
23	c	508	CLA	C5-C6-C7-C8
23	y	303	CLA	C10-C11-C12-C13
34	N	310	CHL	O1D-CGD-O2D-CED
30	A	411	LHG	C11-C10-C9-C8
33	e	101	HEM	C4B-C3B-CAB-CBB
23	B	614	CLA	C5-C6-C7-C8
23	B	616	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
23	b	604	CLA	CBD-CGD-O2D-CED
30	c	517	LHG	O9-C7-O7-C5
23	r	608	CLA	C3-C5-C6-C7
34	Y	308	CHL	C3-C5-C6-C7
30	W	201	LHG	C13-C14-C15-C16
26	L	103	SQD	O47-C45-C46-O48
26	M	101	SQD	O47-C45-C46-O48
28	A	408	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	H	102	DGD	O1G-C1G-C2G-O2G
30	y	318	LHG	O7-C5-C6-O8
23	d	404	CLA	C16-C17-C18-C20
24	a	404	PHO	C16-C17-C18-C20
30	Y	318	LHG	C28-C29-C30-C31
23	B	611	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	n	314	CLA	C2-C3-C5-C6
34	G	609	CHL	C2-C3-C5-C6
27	C	501	LMG	C29-C30-C31-C32
27	a	407	LMG	C31-C32-C33-C34
23	B	606	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	Y	304	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C12-C13-C14
23	b	609	CLA	C11-C12-C13-C14
23	b	609	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C12-C13-C14
23	c	513	CLA	C14-C13-C15-C16
24	A	403	PHO	C11-C10-C8-C9
24	D	402	PHO	C6-C7-C8-C9
24	a	404	PHO	C11-C10-C8-C9
34	G	608	CHL	C14-C13-C15-C16
34	g	608	CHL	C14-C13-C15-C16
34	n	302	CHL	C6-C7-C8-C9
23	D	405	CLA	C2A-CAA-CBA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
23	y	313	CLA	C2A-CAA-CBA-CGA
23	s	608	CLA	C2A-CAA-CBA-CGA
30	A	412	LHG	C28-C29-C30-C31
30	a	412	LHG	C29-C30-C31-C32
35	g	616	LUT	C7-C8-C9-C19
23	s	613	CLA	O1D-CGD-O2D-CED
25	b	618	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	y	301	XAT	C27-C28-C29-C30
23	b	616	CLA	O1A-CGA-O2A-C1
30	r	618	LHG	O10-C23-O8-C6
23	A	404	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	504	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C1A-C2A-CAA-CBA
23	C	510	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C1A-C2A-CAA-CBA
23	G	604	CLA	C1A-C2A-CAA-CBA
23	G	610	CLA	C1A-C2A-CAA-CBA
23	G	611	CLA	C1A-C2A-CAA-CBA
23	N	304	CLA	C1A-C2A-CAA-CBA
23	N	312	CLA	C1A-C2A-CAA-CBA
23	R	604	CLA	C1A-C2A-CAA-CBA
23	R	608	CLA	C1A-C2A-CAA-CBA
23	R	609	CLA	C1A-C2A-CAA-CBA
23	Y	310	CLA	C1A-C2A-CAA-CBA
23	Y	311	CLA	C1A-C2A-CAA-CBA
23	Y	314	CLA	C1A-C2A-CAA-CBA
23	a	402	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
23	b	601	CLA	C1A-C2A-CAA-CBA
23	b	603	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	502	CLA	C1A-C2A-CAA-CBA
23	c	504	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA
23	d	405	CLA	C1A-C2A-CAA-CBA
23	g	610	CLA	C1A-C2A-CAA-CBA
23	g	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	n	304	CLA	C1A-C2A-CAA-CBA
23	r	604	CLA	C1A-C2A-CAA-CBA
23	r	609	CLA	C1A-C2A-CAA-CBA
23	y	303	CLA	C1A-C2A-CAA-CBA
23	y	310	CLA	C1A-C2A-CAA-CBA
23	y	314	CLA	C1A-C2A-CAA-CBA
23	S	602	CLA	C1A-C2A-CAA-CBA
23	S	611	CLA	C1A-C2A-CAA-CBA
23	s	611	CLA	C1A-C2A-CAA-CBA
34	G	605	CHL	C1A-C2A-CAA-CBA
34	N	306	CHL	C1A-C2A-CAA-CBA
34	N	307	CHL	C1A-C2A-CAA-CBA
34	N	309	CHL	C1A-C2A-CAA-CBA
34	R	607	CHL	C1A-C2A-CAA-CBA
34	Y	306	CHL	C1A-C2A-CAA-CBA
34	Y	307	CHL	C1A-C2A-CAA-CBA
34	g	605	CHL	C1A-C2A-CAA-CBA
34	g	619	CHL	C1A-C2A-CAA-CBA
34	n	306	CHL	C1A-C2A-CAA-CBA
34	n	309	CHL	C1A-C2A-CAA-CBA
23	B	603	CLA	C16-C17-C18-C20
34	y	302	CHL	C16-C17-C18-C19
25	F	101	BCR	C9-C10-C11-C12
23	c	511	CLA	O1D-CGD-O2D-CED
23	g	611	CLA	C10-C11-C12-C13
34	N	310	CHL	C15-C16-C17-C18
34	y	308	CHL	C8-C10-C11-C12
30	S	617	LHG	C3-O3-P-O6
26	L	103	SQD	C10-C11-C12-C13
34	n	310	CHL	C3-C5-C6-C7
34	y	302	CHL	C3-C5-C6-C7
23	b	603	CLA	O1D-CGD-O2D-CED
23	R	603	CLA	O1A-CGA-O2A-C1
23	Y	313	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	C13-C15-C16-C17
23	C	508	CLA	C13-C15-C16-C17
23	Y	312	CLA	C10-C11-C12-C13
23	n	312	CLA	O1D-CGD-O2D-CED
23	r	601	CLA	C2C-C3C-CAC-CBC
30	S	617	LHG	C24-C25-C26-C27
28	H	102	DGD	C2A-C3A-C4A-C5A
23	Y	311	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	y	304	CLA	C16-C17-C18-C19
26	M	101	SQD	C10-C11-C12-C13
23	B	601	CLA	C13-C15-C16-C17
23	g	614	CLA	C3A-C2A-CAA-CBA
23	n	312	CLA	C2-C3-C5-C6
23	S	610	CLA	C3A-C2A-CAA-CBA
23	s	610	CLA	C3A-C2A-CAA-CBA
34	g	606	CHL	C3A-C2A-CAA-CBA
34	S	606	CHL	C3A-C2A-CAA-CBA
34	s	606	CHL	C3A-C2A-CAA-CBA
34	G	608	CHL	C5-C6-C7-C8
23	g	612	CLA	O1D-CGD-O2D-CED
30	w	201	LHG	C13-C14-C15-C16
30	G	618	LHG	O10-C23-O8-C6
30	W	201	LHG	O10-C23-O8-C6
27	b	620	LMG	C37-C38-C39-C40
28	c	516	DGD	C5B-C6B-C7B-C8B
23	B	601	CLA	C2A-CAA-CBA-CGA
23	d	405	CLA	C2A-CAA-CBA-CGA
23	n	312	CLA	C2A-CAA-CBA-CGA
34	g	619	CHL	C2A-CAA-CBA-CGA
23	B	603	CLA	C16-C17-C18-C19
26	A	406	SQD	O6-C44-C45-C46
26	A	409	SQD	C44-C45-C46-O48
26	L	103	SQD	O6-C44-C45-C46
28	a	408	DGD	C1G-C2G-C3G-O3G
30	L	101	LHG	C4-C5-C6-O8
30	N	319	LHG	C4-C5-C6-O8
30	y	318	LHG	C4-C5-C6-O8
30	S	617	LHG	C4-C5-C6-O8
34	G	601	CHL	C8-C10-C11-C12
23	b	614	CLA	CAA-CBA-CGA-O2A
26	L	103	SQD	C23-C24-C25-C26
23	C	514	CLA	O1A-CGA-O2A-C1
30	T	101	LHG	C28-C29-C30-C31
28	A	408	DGD	O6D-C1D-O3G-C3G
27	B	620	LMG	C37-C38-C39-C40
30	B	623	LHG	C28-C29-C30-C31
23	R	604	CLA	O2A-C1-C2-C3
23	r	604	CLA	O2A-C1-C2-C3
23	b	614	CLA	C5-C6-C7-C8
28	C	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
26	a	409	SQD	C16-C17-C18-C19
27	A	407	LMG	O6-C5-C6-O5
27	D	407	LMG	O6-C5-C6-O5
23	b	611	CLA	C4-C3-C5-C6
23	n	312	CLA	C4-C3-C5-C6
23	n	314	CLA	C4-C3-C5-C6
32	D	406	PL9	C28-C29-C31-C32
23	r	601	CLA	CBA-CGA-O2A-C1
23	r	602	CLA	CBA-CGA-O2A-C1
23	s	604	CLA	CBA-CGA-O2A-C1
27	B	622	LMG	O6-C5-C6-O5
23	B	606	CLA	CBD-CGD-O2D-CED
26	L	103	SQD	C15-C16-C17-C18
28	d	410	DGD	CAB-CBB-CCB-CDB
27	d	409	LMG	O6-C5-C6-O5
23	N	304	CLA	C2A-CAA-CBA-CGA
23	b	601	CLA	C2A-CAA-CBA-CGA
23	b	601	CLA	C8-C10-C11-C12
34	N	310	CHL	C2-C1-O2A-CGA
23	b	608	CLA	C3-C5-C6-C7
26	A	409	SQD	C11-C10-C9-C8
23	R	612	CLA	CBA-CGA-O2A-C1
23	r	612	CLA	CBA-CGA-O2A-C1
34	Y	302	CHL	CBA-CGA-O2A-C1
23	C	503	CLA	C16-C17-C18-C19
34	g	619	CHL	C16-C17-C18-C19
30	A	412	LHG	C25-C26-C27-C28
30	d	408	LHG	C11-C12-C13-C14
23	S	603	CLA	O1D-CGD-O2D-CED
34	R	613	CHL	O1D-CGD-O2D-CED
30	g	618	LHG	O10-C23-O8-C6
23	B	612	CLA	C5-C6-C7-C8
23	R	609	CLA	C13-C15-C16-C17
34	G	619	CHL	C8-C10-C11-C12
26	d	402	SQD	O47-C45-C46-O48
28	a	408	DGD	O1G-C1G-C2G-O2G
28	d	410	DGD	O1G-C1G-C2G-O2G
30	N	319	LHG	O7-C5-C6-O8
30	n	319	LHG	O7-C5-C6-O8
26	A	409	SQD	C16-C17-C18-C19
23	a	402	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
34	n	310	CHL	C4-C3-C5-C6
23	A	404	CLA	C11-C10-C8-C7
23	B	601	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C12-C13-C15
23	B	608	CLA	C11-C10-C8-C7
23	B	609	CLA	C12-C13-C15-C16
23	B	615	CLA	C6-C7-C8-C10
23	C	503	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C10-C8-C7
23	C	508	CLA	C6-C7-C8-C10
23	C	511	CLA	C11-C12-C13-C15
23	G	603	CLA	C12-C13-C15-C16
23	G	610	CLA	C12-C13-C15-C16
23	N	303	CLA	C6-C7-C8-C10
23	R	609	CLA	C6-C7-C8-C10
23	a	402	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	b	607	CLA	C11-C10-C8-C7
23	b	610	CLA	C12-C13-C15-C16
23	b	611	CLA	C2-C3-C5-C6
23	b	615	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16
23	g	610	CLA	C12-C13-C15-C16
23	r	609	CLA	C6-C7-C8-C10
23	y	303	CLA	C11-C12-C13-C15
23	y	312	CLA	C6-C7-C8-C10
23	y	313	CLA	C11-C10-C8-C7
23	y	313	CLA	C11-C12-C13-C15
24	A	403	PHO	C6-C7-C8-C10
24	a	404	PHO	C11-C10-C8-C7
32	d	407	PL9	C28-C29-C31-C32
34	G	601	CHL	C6-C7-C8-C10
34	G	608	CHL	C12-C13-C15-C16
34	N	310	CHL	C6-C7-C8-C10
34	Y	309	CHL	C6-C7-C8-C10
34	g	608	CHL	C12-C13-C15-C16
34	n	302	CHL	C12-C13-C15-C16
34	y	308	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
34	y	309	CHL	C6-C7-C8-C10
23	A	404	CLA	C11-C10-C8-C9
23	B	601	CLA	C11-C12-C13-C14
23	B	603	CLA	C11-C12-C13-C14
23	B	609	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C9
23	B	615	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	C	503	CLA	C6-C7-C8-C9
23	C	508	CLA	C6-C7-C8-C9
23	D	401	CLA	C14-C13-C15-C16
23	G	602	CLA	C14-C13-C15-C16
23	G	603	CLA	C14-C13-C15-C16
23	G	610	CLA	C14-C13-C15-C16
23	R	609	CLA	C6-C7-C8-C9
23	a	402	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C12-C13-C14
23	b	612	CLA	C14-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	504	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C10-C8-C9
23	g	602	CLA	C14-C13-C15-C16
23	g	610	CLA	C14-C13-C15-C16
23	y	303	CLA	C11-C12-C13-C14
23	y	313	CLA	C11-C10-C8-C9
24	d	401	PHO	C6-C7-C8-C9
34	G	601	CHL	C6-C7-C8-C9
34	G	601	CHL	C11-C12-C13-C14
34	G	609	CHL	C6-C7-C8-C9
34	N	302	CHL	C14-C13-C15-C16
34	N	310	CHL	C6-C7-C8-C9
34	N	310	CHL	C11-C12-C13-C14
34	Y	309	CHL	C6-C7-C8-C9
34	g	601	CHL	C11-C12-C13-C14
34	g	609	CHL	C6-C7-C8-C9
34	n	302	CHL	C14-C13-C15-C16
34	n	310	CHL	C6-C7-C8-C9
34	y	309	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	CBA-CGA-O2A-C1
23	R	609	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	C5-C6-C7-C8
23	c	503	CLA	C10-C11-C12-C13
23	g	602	CLA	O1D-CGD-O2D-CED
23	s	603	CLA	O1D-CGD-O2D-CED
34	n	310	CHL	O1D-CGD-O2D-CED
35	Y	315	LUT	C27-C28-C29-C39
36	n	318	NEX	C11-C12-C13-C20
23	Y	304	CLA	C16-C17-C18-C20
25	C	516	BCR	C11-C12-C13-C14
25	c	514	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C10
37	Y	301	XAT	C27-C28-C29-C30
30	G	618	LHG	C1-C2-C3-O3
23	G	602	CLA	C5-C6-C7-C8
34	G	619	CHL	C5-C6-C7-C8
34	n	302	CHL	C8-C10-C11-C12
30	C	518	LHG	C8-C7-O7-C5
30	b	621	LHG	C8-C7-O7-C5
23	n	311	CLA	C11-C12-C13-C14
26	A	409	SQD	C9-C10-C11-C12
30	C	518	LHG	C15-C16-C17-C18
23	R	602	CLA	CBA-CGA-O2A-C1
23	Y	303	CLA	CBA-CGA-O2A-C1
34	y	302	CHL	CBA-CGA-O2A-C1
23	D	405	CLA	C13-C15-C16-C17
23	d	405	CLA	C13-C15-C16-C17
26	L	103	SQD	C11-C10-C9-C8
26	M	101	SQD	C11-C10-C9-C8
30	R	618	LHG	O6-C4-C5-C6
23	c	501	CLA	C3-C5-C6-C7
26	M	101	SQD	C15-C16-C17-C18
30	W	201	LHG	C14-C15-C16-C17
23	B	616	CLA	CBA-CGA-O2A-C1
30	T	101	LHG	C24-C25-C26-C27
34	n	310	CHL	C2-C3-C5-C6
23	N	303	CLA	C14-C13-C15-C16
23	n	303	CLA	C14-C13-C15-C16
23	N	311	CLA	C11-C12-C13-C14
23	B	603	CLA	O1D-CGD-O2D-CED
30	w	201	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	s	617	LHG	C24-C25-C26-C27
30	B	621	LHG	C8-C7-O7-C5
23	y	313	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CAA-CBA-CGA-O2A
26	d	402	SQD	C7-C8-C9-C10
30	L	101	LHG	C11-C12-C13-C14
23	N	311	CLA	C3A-C2A-CAA-CBA
23	c	506	CLA	C3A-C2A-CAA-CBA
23	c	510	CLA	C3A-C2A-CAA-CBA
23	r	614	CLA	C3A-C2A-CAA-CBA
23	S	609	CLA	C3A-C2A-CAA-CBA
24	d	401	PHO	C3A-C2A-CAA-CBA
34	Y	309	CHL	C3A-C2A-CAA-CBA
34	y	309	CHL	C3A-C2A-CAA-CBA
35	Y	316	LUT	C29-C30-C31-C32
27	a	407	LMG	C29-C30-C31-C32
30	r	618	LHG	C11-C10-C9-C8
23	r	601	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	CBA-CGA-O2A-C1
23	r	608	CLA	CBA-CGA-O2A-C1
34	Y	309	CHL	CBA-CGA-O2A-C1
34	y	306	CHL	CBA-CGA-O2A-C1
34	y	309	CHL	CBA-CGA-O2A-C1
26	a	409	SQD	C9-C10-C11-C12
34	Y	309	CHL	C10-C11-C12-C13
26	M	101	SQD	O6-C44-C45-C46
26	M	101	SQD	C44-C45-C46-O48
26	d	402	SQD	O6-C44-C45-C46
28	A	408	DGD	C1G-C2G-C3G-O3G
28	C	517	DGD	C1G-C2G-C3G-O3G
28	H	102	DGD	O1G-C1G-C2G-C3G
28	c	516	DGD	C1G-C2G-C3G-O3G
28	d	410	DGD	O1G-C1G-C2G-C3G
30	Y	318	LHG	C4-C5-C6-O8
30	n	319	LHG	C4-C5-C6-O8
23	c	512	CLA	CBD-CGD-O2D-CED
30	S	617	LHG	C27-C28-C29-C30
23	b	613	CLA	C5-C6-C7-C8
23	r	601	CLA	C4C-C3C-CAC-CBC
23	C	502	CLA	C3-C5-C6-C7
34	Y	302	CHL	O1A-CGA-O2A-C1
34	g	608	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	y	309	CHL	C4-C3-C5-C6
23	r	609	CLA	CBA-CGA-O2A-C1
34	g	619	CHL	C16-C17-C18-C20
26	a	409	SQD	C11-C10-C9-C8
34	y	307	CHL	C3C-C2C-CMC-OMC
23	R	612	CLA	O1A-CGA-O2A-C1
23	s	604	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	O1D-CGD-O2D-CED
23	Y	311	CLA	O1D-CGD-O2D-CED
23	G	613	CLA	C2A-CAA-CBA-CGA
23	y	305	CLA	C2A-CAA-CBA-CGA
24	D	402	PHO	C2A-CAA-CBA-CGA
30	R	618	LHG	C11-C10-C9-C8
23	C	510	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C16-C17-C18-C20
23	C	503	CLA	C8-C10-C11-C12
23	B	613	CLA	C5-C6-C7-C8
23	r	602	CLA	O1A-CGA-O2A-C1
23	r	612	CLA	O1A-CGA-O2A-C1
34	y	302	CHL	O1A-CGA-O2A-C1
30	a	412	LHG	C25-C26-C27-C28
26	A	406	SQD	O47-C45-C46-O48
27	B	622	LMG	O7-C8-C9-O8
30	a	411	LHG	O7-C5-C6-O8
30	S	617	LHG	O7-C5-C6-O8
30	r	618	LHG	O8-C23-C24-C25
30	y	318	LHG	C28-C29-C30-C31
27	a	407	LMG	C28-C29-C30-C31
34	R	606	CHL	C2C-C3C-CAC-CBC
30	C	518	LHG	O9-C7-O7-C5
30	b	621	LHG	O9-C7-O7-C5
23	c	512	CLA	C2-C1-O2A-CGA
23	n	305	CLA	C2-C1-O2A-CGA
23	n	312	CLA	C2-C1-O2A-CGA
32	D	406	PL9	C43-C44-C46-C47
23	C	504	CLA	C10-C11-C12-C13
23	n	314	CLA	C5-C6-C7-C8
23	B	608	CLA	C11-C10-C8-C9
23	B	612	CLA	C14-C13-C15-C16
23	N	303	CLA	C6-C7-C8-C9
23	Y	304	CLA	C6-C7-C8-C9
23	Y	313	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	b	612	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	c	503	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C12-C13-C14
23	g	603	CLA	C14-C13-C15-C16
23	r	609	CLA	C6-C7-C8-C9
24	D	402	PHO	C11-C12-C13-C14
24	d	401	PHO	C11-C12-C13-C14
34	N	309	CHL	C6-C7-C8-C9
34	Y	302	CHL	C11-C12-C13-C14
34	Y	309	CHL	C11-C10-C8-C9
34	y	302	CHL	C11-C12-C13-C14
23	C	511	CLA	C15-C16-C17-C18
23	g	602	CLA	C15-C16-C17-C18
23	r	603	CLA	C5-C6-C7-C8
23	B	615	CLA	C2A-CAA-CBA-CGA
23	Y	310	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C23-C24-C25-C30
25	B	619	BCR	C5-C6-C7-C8
25	B	619	BCR	C23-C24-C25-C26
25	B	619	BCR	C23-C24-C25-C30
25	H	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C1-C6-C7-C8
35	N	316	LUT	C5-C6-C7-C8
35	n	317	LUT	C5-C6-C7-C8
35	r	615	LUT	C1-C6-C7-C8
35	r	615	LUT	C5-C6-C7-C8
35	y	316	LUT	C1-C6-C7-C8
35	y	316	LUT	C5-C6-C7-C8
35	S	615	LUT	C1-C6-C7-C8
35	S	615	LUT	C5-C6-C7-C8
35	s	615	LUT	C1-C6-C7-C8
35	s	615	LUT	C5-C6-C7-C8
30	a	412	LHG	C16-C17-C18-C19
23	R	609	CLA	O1A-CGA-O2A-C1
23	n	303	CLA	CBA-CGA-O2A-C1
25	B	619	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C7-C8-C9-C10
30	B	621	LHG	O9-C7-O7-C5
28	C	517	DGD	C4B-C5B-C6B-C7B
23	C	506	CLA	CAA-CBA-CGA-O2A
30	B	623	LHG	C24-C25-C26-C27
23	B	608	CLA	C13-C15-C16-C17
30	w	201	LHG	O6-C4-C5-C6
30	A	412	LHG	C12-C13-C14-C15
23	B	605	CLA	C11-C10-C8-C7
23	B	607	CLA	C11-C10-C8-C7
23	B	612	CLA	C11-C10-C8-C7
23	B	612	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C10-C8-C7
23	D	401	CLA	C12-C13-C15-C16
23	G	602	CLA	C12-C13-C15-C16
23	Y	303	CLA	C11-C12-C13-C15
23	Y	304	CLA	C6-C7-C8-C10
23	Y	313	CLA	C11-C10-C8-C7
23	a	402	CLA	C2-C3-C5-C6
23	a	402	CLA	C11-C12-C13-C15
23	a	405	CLA	C11-C10-C8-C7
23	b	608	CLA	C11-C10-C8-C7
23	b	612	CLA	C11-C10-C8-C7
23	b	612	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C10-C8-C7
23	c	502	CLA	C6-C7-C8-C10
23	c	503	CLA	C12-C13-C15-C16
23	c	504	CLA	C6-C7-C8-C10
23	c	507	CLA	C6-C7-C8-C10
23	c	512	CLA	C6-C7-C8-C10
23	g	602	CLA	C12-C13-C15-C16
23	g	603	CLA	C12-C13-C15-C16
23	n	303	CLA	C6-C7-C8-C10
34	G	601	CHL	C11-C12-C13-C15
34	G	609	CHL	C6-C7-C8-C10
34	G	619	CHL	C11-C10-C8-C7
34	G	619	CHL	C11-C12-C13-C15
34	N	302	CHL	C12-C13-C15-C16
34	N	310	CHL	C11-C12-C13-C15
34	Y	302	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
34	Y	309	CHL	C11-C10-C8-C7
34	g	601	CHL	C11-C12-C13-C15
34	g	609	CHL	C6-C7-C8-C10
34	g	619	CHL	C11-C10-C8-C7
34	y	302	CHL	C11-C12-C13-C15
34	Y	302	CHL	C10-C11-C12-C13
34	g	608	CHL	C5-C6-C7-C8
35	y	316	LUT	C29-C30-C31-C32
35	s	615	LUT	C13-C14-C15-C35
23	C	503	CLA	C15-C16-C17-C18
23	b	615	CLA	C2A-CAA-CBA-CGA
27	C	501	LMG	C31-C32-C33-C34
30	a	411	LHG	C29-C30-C31-C32
23	A	404	CLA	C3-C5-C6-C7
23	Y	304	CLA	C16-C17-C18-C19
23	b	609	CLA	C13-C15-C16-C17
23	b	608	CLA	CBA-CGA-O2A-C1
23	n	305	CLA	CBA-CGA-O2A-C1
28	a	408	DGD	C7A-C8A-C9A-CAA
30	G	618	LHG	C9-C10-C11-C12
23	A	401	CLA	C13-C15-C16-C17
23	B	607	CLA	C8-C10-C11-C12
23	C	509	CLA	C8-C10-C11-C12
23	b	607	CLA	C8-C10-C11-C12
23	g	602	CLA	C10-C11-C12-C13
34	g	619	CHL	C8-C10-C11-C12
23	B	604	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	CAD-CBD-CGD-O2D
23	D	405	CLA	CAD-CBD-CGD-O2D
23	G	604	CLA	CAD-CBD-CGD-O2D
23	N	305	CLA	CAD-CBD-CGD-O2D
23	N	311	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	d	405	CLA	CAD-CBD-CGD-O2D
23	n	305	CLA	CAD-CBD-CGD-O2D
23	y	305	CLA	CAD-CBD-CGD-O2D
23	y	310	CLA	CAD-CBD-CGD-O2D
34	G	619	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
34	g	619	CHL	CAD-CBD-CGD-O2D
34	y	307	CHL	CAD-CBD-CGD-O2D
34	s	607	CHL	CAD-CBD-CGD-O2D
36	g	617	NEX	C7-C8-C9-C19
28	a	408	DGD	O6D-C1D-O3G-C3G
24	A	403	PHO	C5-C6-C7-C8
30	L	101	LHG	C10-C11-C12-C13
26	L	103	SQD	C44-C45-C46-O48
26	a	409	SQD	C44-C45-C46-O48
27	B	622	LMG	C7-C8-C9-O8
30	s	617	LHG	C4-C5-C6-O8
23	B	602	CLA	O1A-CGA-O2A-C1
23	Y	303	CLA	O1A-CGA-O2A-C1
23	r	608	CLA	O1A-CGA-O2A-C1
26	A	409	SQD	C24-C25-C26-C27
30	R	618	LHG	O6-C4-C5-O7
30	b	621	LHG	O6-C4-C5-O7
23	A	401	CLA	C10-C11-C12-C13
23	B	607	CLA	C3-C5-C6-C7
34	y	307	CHL	O2A-C1-C2-C3
23	n	315	CLA	O1D-CGD-O2D-CED
33	E	101	HEM	C4B-C3B-CAB-CBB
23	G	602	CLA	C2A-CAA-CBA-CGA
34	Y	306	CHL	C2A-CAA-CBA-CGA
30	g	618	LHG	C1-C2-C3-O3
26	L	103	SQD	O49-C7-O47-C45
26	M	101	SQD	O49-C7-O47-C45
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	604	CLA	CHA-CBD-CGD-O1D
23	B	604	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	502	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	N	303	CLA	CHA-CBD-CGD-O1D
23	N	303	CLA	CHA-CBD-CGD-O2D
23	R	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	R	603	CLA	CHA-CBD-CGD-O2D
23	R	610	CLA	CHA-CBD-CGD-O1D
23	R	610	CLA	CHA-CBD-CGD-O2D
23	R	614	CLA	CHA-CBD-CGD-O1D
23	R	614	CLA	CHA-CBD-CGD-O2D
23	Y	305	CLA	CHA-CBD-CGD-O1D
23	Y	305	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	501	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	g	612	CLA	CHA-CBD-CGD-O1D
23	g	612	CLA	CHA-CBD-CGD-O2D
23	g	613	CLA	CHA-CBD-CGD-O2D
23	n	304	CLA	CHA-CBD-CGD-O1D
23	n	304	CLA	CHA-CBD-CGD-O2D
23	r	603	CLA	CHA-CBD-CGD-O1D
23	r	603	CLA	CHA-CBD-CGD-O2D
23	r	604	CLA	CHA-CBD-CGD-O1D
23	r	604	CLA	CHA-CBD-CGD-O2D
23	y	303	CLA	CHA-CBD-CGD-O1D
23	y	305	CLA	CHA-CBD-CGD-O1D
23	S	602	CLA	CHA-CBD-CGD-O1D
23	S	604	CLA	CHA-CBD-CGD-O1D
23	S	604	CLA	CHA-CBD-CGD-O2D
23	S	612	CLA	CHA-CBD-CGD-O1D
23	S	612	CLA	CHA-CBD-CGD-O2D
23	s	609	CLA	CHA-CBD-CGD-O1D
23	s	610	CLA	CHA-CBD-CGD-O1D
23	s	610	CLA	CHA-CBD-CGD-O2D
23	s	612	CLA	CHA-CBD-CGD-O1D
34	G	608	CHL	CHA-CBD-CGD-O1D
34	G	608	CHL	CHA-CBD-CGD-O2D
34	N	306	CHL	CHA-CBD-CGD-O1D
34	N	306	CHL	CHA-CBD-CGD-O2D
34	N	307	CHL	CHA-CBD-CGD-O1D
34	R	613	CHL	CHA-CBD-CGD-O2D
34	g	608	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
34	g	608	CHL	CHA-CBD-CGD-O2D
34	n	302	CHL	CHA-CBD-CGD-O1D
34	n	306	CHL	CHA-CBD-CGD-O1D
34	n	306	CHL	CHA-CBD-CGD-O2D
34	n	308	CHL	CHA-CBD-CGD-O1D
34	n	308	CHL	CHA-CBD-CGD-O2D
27	b	620	LMG	C32-C33-C34-C35
23	y	305	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	O1A-CGA-O2A-C1
23	n	303	CLA	O1A-CGA-O2A-C1
23	r	609	CLA	O1A-CGA-O2A-C1
23	y	313	CLA	O1A-CGA-O2A-C1
34	y	306	CHL	O1A-CGA-O2A-C1
26	L	103	SQD	O6-C44-C45-O47
26	M	101	SQD	O6-C44-C45-O47
27	A	407	LMG	O7-C8-C9-O8
28	C	517	DGD	O2G-C2G-C3G-O3G
28	c	516	DGD	O2G-C2G-C3G-O3G
30	A	411	LHG	O7-C5-C6-O8
30	L	101	LHG	O7-C5-C6-O8
23	B	601	CLA	C8-C10-C11-C12
23	R	602	CLA	O1A-CGA-O2A-C1
34	y	309	CHL	O1A-CGA-O2A-C1
28	C	517	DGD	O6D-C5D-C6D-O5D
26	L	103	SQD	C8-C7-O47-C45
26	a	409	SQD	C24-C25-C26-C27
34	Y	309	CHL	O1A-CGA-O2A-C1
23	b	614	CLA	C2-C3-C5-C6
23	C	502	CLA	C11-C10-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	D	405	CLA	C14-C13-C15-C16
23	a	402	CLA	C11-C12-C13-C14
23	n	303	CLA	C6-C7-C8-C9
34	G	619	CHL	C11-C10-C8-C9
34	g	619	CHL	C11-C10-C8-C9
28	C	517	DGD	C4D-C5D-C6D-O5D
30	c	517	LHG	C14-C15-C16-C17
30	d	408	LHG	C10-C11-C12-C13
34	R	606	CHL	C4C-C3C-CAC-CBC
34	s	606	CHL	CBD-CGD-O2D-CED
23	B	614	CLA	CAA-CBA-CGA-O2A
25	C	515	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	c	514	BCR	C36-C18-C19-C20
35	n	317	LUT	C31-C32-C33-C40
37	n	301	XAT	C11-C12-C13-C20
23	B	611	CLA	C5-C6-C7-C8
25	C	515	BCR	C17-C18-C19-C20
35	g	616	LUT	C7-C8-C9-C10
36	n	318	NEX	C11-C12-C13-C14
23	B	607	CLA	C1A-C2A-CAA-CBA
23	C	509	CLA	C1A-C2A-CAA-CBA
23	D	405	CLA	C1A-C2A-CAA-CBA
23	b	607	CLA	C1A-C2A-CAA-CBA
23	c	510	CLA	C1A-C2A-CAA-CBA
23	n	311	CLA	C1A-C2A-CAA-CBA
34	N	308	CHL	C1A-C2A-CAA-CBA
34	n	308	CHL	C1A-C2A-CAA-CBA
34	s	605	CHL	C1A-C2A-CAA-CBA
23	G	610	CLA	C13-C15-C16-C17
23	c	508	CLA	C13-C15-C16-C17
23	y	313	CLA	C2-C1-O2A-CGA
23	S	612	CLA	CBA-CGA-O2A-C1
35	g	616	LUT	C29-C30-C31-C32
34	G	608	CHL	C13-C15-C16-C17
30	G	618	LHG	C3-O3-P-O6
30	N	319	LHG	C4-O6-P-O3
30	g	618	LHG	C3-O3-P-O6
30	w	201	LHG	C3-O3-P-O6
23	y	305	CLA	O1D-CGD-O2D-CED
28	A	408	DGD	C7A-C8A-C9A-CAA
23	C	505	CLA	C4-C3-C5-C6
23	a	401	CLA	C15-C16-C17-C18
23	c	505	CLA	C3-C5-C6-C7
23	c	510	CLA	C3-C5-C6-C7
32	d	407	PL9	C43-C44-C46-C47
30	A	411	LHG	C4-O6-P-O4
30	B	623	LHG	C4-O6-P-O5
30	L	101	LHG	C3-O3-P-O4
30	T	101	LHG	C4-O6-P-O5
30	Y	318	LHG	C4-O6-P-O4
30	a	411	LHG	C3-O3-P-O5
30	a	411	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O4
30	n	319	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
30	y	318	LHG	C4-O6-P-O4
30	s	617	LHG	C3-O3-P-O5
34	G	619	CHL	C16-C17-C18-C19
34	Y	309	CHL	C16-C17-C18-C20
23	G	604	CLA	O2A-C1-C2-C3
23	r	611	CLA	O2A-C1-C2-C3
34	Y	307	CHL	O2A-C1-C2-C3
30	B	621	LHG	O6-C4-C5-C6
30	b	621	LHG	O6-C4-C5-C6
28	H	102	DGD	C8A-C9A-CAA-CBA
28	H	102	DGD	CAB-CBB-CCB-CDB
23	B	615	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
27	B	620	LMG	C36-C37-C38-C39
30	G	618	LHG	C27-C28-C29-C30
23	d	405	CLA	C16-C17-C18-C20
28	H	102	DGD	CAA-CBA-CCA-CDA
23	A	401	CLA	CAD-CBD-CGD-O1D
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	614	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	C	512	CLA	CAD-CBD-CGD-O1D
23	Y	305	CLA	CAD-CBD-CGD-O1D
23	a	401	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	c	501	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	S	602	CLA	CAD-CBD-CGD-O1D
23	S	608	CLA	CAD-CBD-CGD-O1D
23	s	613	CLA	CAD-CBD-CGD-O1D
26	A	406	SQD	C5-C6-S-O7
26	d	402	SQD	C5-C6-S-O7
34	N	306	CHL	CAD-CBD-CGD-O1D
34	R	613	CHL	CAD-CBD-CGD-O1D
34	n	306	CHL	CAD-CBD-CGD-O1D
34	r	613	CHL	CAD-CBD-CGD-O1D
36	g	617	NEX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	O1D-CGD-O2D-CED
30	c	517	LHG	C15-C16-C17-C18
23	b	611	CLA	C5-C6-C7-C8
23	d	405	CLA	C8-C10-C11-C12
26	A	406	SQD	C7-C8-C9-C10
23	C	509	CLA	CBA-CGA-O2A-C1
23	N	305	CLA	CBA-CGA-O2A-C1
23	b	604	CLA	O1D-CGD-O2D-CED
23	c	507	CLA	C15-C16-C17-C18
27	B	620	LMG	O9-C10-O7-C8
23	C	502	CLA	C11-C10-C8-C7
23	C	506	CLA	C11-C10-C8-C7
23	C	513	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	C6-C7-C8-C10
23	Y	303	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C7
23	c	508	CLA	C11-C10-C8-C7
23	y	303	CLA	C6-C7-C8-C10
30	B	621	LHG	O6-C4-C5-O7
30	C	518	LHG	O6-C4-C5-O7
30	c	517	LHG	O6-C4-C5-O7
30	w	201	LHG	O6-C4-C5-O7
34	N	309	CHL	C12-C13-C15-C16
34	g	619	CHL	C11-C12-C13-C15
34	n	310	CHL	C11-C12-C13-C15
28	H	102	DGD	O6E-C5E-C6E-O5E
23	C	506	CLA	C3-C5-C6-C7
35	s	615	LUT	C33-C34-C35-C15
23	b	603	CLA	C8-C10-C11-C12
26	M	101	SQD	C8-C7-O47-C45
27	B	620	LMG	C11-C10-O7-C8
28	d	410	DGD	CAA-CBA-CCA-CDA
30	w	201	LHG	C17-C18-C19-C20
34	G	608	CHL	C10-C11-C12-C13
34	G	609	CHL	C1C-C2C-CMC-OMC
34	r	607	CHL	C1C-C2C-CMC-OMC
34	y	307	CHL	C1C-C2C-CMC-OMC
34	y	309	CHL	C1C-C2C-CMC-OMC
30	s	617	LHG	O7-C5-C6-O8
30	b	621	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	C	518	LHG	C14-C15-C16-C17
23	c	512	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CAA-CBA-CGA-O2A
26	a	409	SQD	O47-C7-C8-C9
23	n	304	CLA	C5-C6-C7-C8
34	N	310	CHL	C8-C10-C11-C12
23	c	512	CLA	C3-C5-C6-C7
34	Y	306	CHL	CBA-CGA-O2A-C1
34	Y	306	CHL	CAA-CBA-CGA-O2A
23	c	510	CLA	C15-C16-C17-C18
23	g	610	CLA	C13-C15-C16-C17
23	B	607	CLA	C11-C10-C8-C9
23	B	609	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	G	602	CLA	C6-C7-C8-C9
23	Y	303	CLA	C11-C12-C13-C14
23	b	607	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
23	c	508	CLA	C11-C10-C8-C9
23	c	512	CLA	C6-C7-C8-C9
23	d	405	CLA	C14-C13-C15-C16
24	A	403	PHO	C6-C7-C8-C9
34	g	619	CHL	C11-C12-C13-C14
34	n	309	CHL	C6-C7-C8-C9
34	y	302	CHL	C6-C7-C8-C9
23	b	604	CLA	C15-C16-C17-C18
23	b	604	CLA	O1A-CGA-O2A-C1
23	b	608	CLA	O1A-CGA-O2A-C1
34	Y	306	CHL	O1A-CGA-O2A-C1
23	Y	304	CLA	C2A-CAA-CBA-CGA
34	y	302	CHL	C10-C11-C12-C13
30	N	319	LHG	C17-C18-C19-C20
30	T	101	LHG	C16-C17-C18-C19
35	y	315	LUT	C27-C28-C29-C30
34	Y	309	CHL	C13-C15-C16-C17
23	B	609	CLA	C13-C15-C16-C17
23	G	604	CLA	C1-C2-C3-C4
23	R	601	CLA	C1-C2-C3-C4
23	R	610	CLA	C1-C2-C3-C4
23	R	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	g	604	CLA	C1-C2-C3-C4
23	r	601	CLA	C1-C2-C3-C4
23	r	610	CLA	C1-C2-C3-C4
23	r	611	CLA	C1-C2-C3-C4
34	Y	307	CHL	C1-C2-C3-C4
34	y	307	CHL	C1-C2-C3-C4
23	n	305	CLA	O1A-CGA-O2A-C1
23	A	401	CLA	C3-C5-C6-C7
26	A	409	SQD	O47-C7-C8-C9
27	B	620	LMG	C32-C33-C34-C35
23	r	609	CLA	C8-C10-C11-C12
26	a	409	SQD	C46-C45-O47-C7
30	C	518	LHG	O6-C4-C5-C6
23	r	602	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C2A-CAA-CBA-CGA
23	a	401	CLA	C2A-CAA-CBA-CGA
23	g	613	CLA	C2A-CAA-CBA-CGA
23	y	304	CLA	C2A-CAA-CBA-CGA
23	y	310	CLA	C2A-CAA-CBA-CGA
23	S	612	CLA	C2A-CAA-CBA-CGA
34	Y	309	CHL	C2A-CAA-CBA-CGA
23	a	401	CLA	C13-C15-C16-C17
23	B	613	CLA	C2-C1-O2A-CGA
23	N	305	CLA	C2-C1-O2A-CGA
23	Y	303	CLA	C2-C1-O2A-CGA
23	Y	313	CLA	C2-C1-O2A-CGA
23	b	604	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	r	609	CLA	C2-C1-O2A-CGA
34	n	309	CHL	C2-C1-O2A-CGA
34	S	607	CHL	C2-C1-O2A-CGA
23	D	405	CLA	C16-C17-C18-C20
26	a	409	SQD	C29-C30-C31-C32
30	c	517	LHG	C34-C35-C36-C37
30	g	618	LHG	C11-C10-C9-C8
23	b	604	CLA	CBA-CGA-O2A-C1
37	r	616	XAT	C13-C14-C15-C35
30	A	412	LHG	O6-C4-C5-O7
34	y	306	CHL	CAA-CBA-CGA-O2A
34	N	302	CHL	C15-C16-C17-C18
34	y	309	CHL	C5-C6-C7-C8
35	g	616	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	S	612	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	CBA-CGA-O2A-C1
28	c	516	DGD	O2G-C1B-C2B-C3B
23	C	504	CLA	C4C-C3C-CAC-CBC
23	n	313	CLA	C4C-C3C-CAC-CBC
23	C	504	CLA	C16-C17-C18-C19
34	y	309	CHL	C16-C17-C18-C20
28	c	516	DGD	C2B-C1B-O2G-C2G
26	A	409	SQD	C29-C30-C31-C32
23	n	311	CLA	C8-C10-C11-C12
34	S	607	CHL	O2A-C1-C2-C3
27	a	407	LMG	C2-C1-O1-C7
30	B	623	LHG	C16-C17-C18-C19
30	A	412	LHG	C3-O3-P-O6
30	C	518	LHG	C3-O3-P-O6
30	C	518	LHG	C4-O6-P-O3
30	N	319	LHG	C3-O3-P-O6
30	R	618	LHG	C3-O3-P-O6
30	W	201	LHG	C3-O3-P-O6
30	Y	318	LHG	C3-O3-P-O6
30	a	412	LHG	C3-O3-P-O6
30	c	517	LHG	C3-O3-P-O6
30	c	517	LHG	C4-O6-P-O3
30	n	319	LHG	C3-O3-P-O6
30	r	618	LHG	C3-O3-P-O6
30	y	318	LHG	C3-O3-P-O6
30	n	319	LHG	C17-C18-C19-C20
23	C	510	CLA	C13-C15-C16-C17
30	L	102	LHG	C13-C14-C15-C16
30	s	617	LHG	C27-C28-C29-C30
34	s	606	CHL	O1D-CGD-O2D-CED
26	d	402	SQD	C44-C45-C46-O48
27	A	407	LMG	C7-C8-C9-O8
28	a	408	DGD	O1G-C1G-C2G-C3G
30	a	411	LHG	C4-C5-C6-O8
23	B	615	CLA	C11-C10-C8-C7
23	Y	312	CLA	C6-C7-C8-C10
34	y	309	CHL	C2-C3-C5-C6
27	d	409	LMG	C29-C30-C31-C32
34	n	306	CHL	CAA-CBA-CGA-O2A
23	C	508	CLA	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	Y	303	CLA	C6-C7-C8-C9
23	c	502	CLA	C6-C7-C8-C9
23	y	303	CLA	C6-C7-C8-C9
23	y	313	CLA	C11-C12-C13-C14
34	G	619	CHL	C11-C12-C13-C14
34	n	310	CHL	C11-C12-C13-C14
35	G	616	LUT	C29-C30-C31-C32
35	r	615	LUT	C29-C30-C31-C32
23	d	405	CLA	C16-C17-C18-C19
34	G	619	CHL	C16-C17-C18-C20
27	D	407	LMG	C29-C30-C31-C32
23	c	510	CLA	C10-C11-C12-C13
23	r	601	CLA	C2A-CAA-CBA-CGA
34	G	605	CHL	C2A-CAA-CBA-CGA
34	s	605	CHL	C2A-CAA-CBA-CGA
23	B	611	CLA	O1A-CGA-O2A-C1
23	b	603	CLA	C16-C17-C18-C19
34	n	310	CHL	C16-C17-C18-C20
30	L	102	LHG	C29-C30-C31-C32
23	b	611	CLA	CBA-CGA-O2A-C1
30	a	411	LHG	O2-C2-C3-O3
30	d	408	LHG	C13-C14-C15-C16
30	b	622	LHG	C10-C11-C12-C13
23	r	603	CLA	C3-C5-C6-C7
23	C	509	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	CAA-CBA-CGA-O2A
30	n	319	LHG	C12-C13-C14-C15
23	a	401	CLA	C4C-C3C-CAC-CBC
34	R	607	CHL	C5-C6-C7-C8
34	g	609	CHL	C5-C6-C7-C8
23	G	613	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	s	612	CLA	C2A-CAA-CBA-CGA
23	r	614	CLA	CAA-CBA-CGA-O1A
35	G	616	LUT	C9-C10-C11-C12
35	R	615	LUT	C29-C30-C31-C32
35	n	317	LUT	C29-C30-C31-C32
37	R	616	XAT	C13-C14-C15-C35
30	L	102	LHG	C10-C11-C12-C13
30	A	412	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	G	618	LHG	C11-C10-C9-C8
30	b	622	LHG	C13-C14-C15-C16
23	G	613	CLA	O1A-CGA-O2A-C1
34	r	606	CHL	C4C-C3C-CAC-CBC
23	G	603	CLA	C2-C3-C5-C6
23	N	305	CLA	O1A-CGA-O2A-C1
23	d	405	CLA	C15-C16-C17-C18
28	a	408	DGD	C6B-C7B-C8B-C9B
34	g	605	CHL	CAA-CBA-CGA-O1A
23	C	512	CLA	C2-C1-O2A-CGA
23	R	609	CLA	C2-C1-O2A-CGA
23	G	602	CLA	C15-C16-C17-C18
23	C	504	CLA	C16-C17-C18-C20
26	d	402	SQD	C23-C24-C25-C26
27	C	501	LMG	C2-C1-O1-C7
23	B	603	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
23	R	612	CLA	C2A-CAA-CBA-CGA
23	S	602	CLA	C2A-CAA-CBA-CGA
34	S	601	CHL	C2A-CAA-CBA-CGA
34	S	607	CHL	C2A-CAA-CBA-CGA
27	b	620	LMG	C36-C37-C38-C39
23	b	614	CLA	CAA-CBA-CGA-O1A
23	c	505	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	C3A-C2A-CAA-CBA
34	r	607	CHL	C3A-C2A-CAA-CBA
34	S	607	CHL	C3A-C2A-CAA-CBA
34	s	605	CHL	C3A-C2A-CAA-CBA
34	s	607	CHL	C3A-C2A-CAA-CBA
27	d	409	LMG	O9-C10-O7-C8
28	c	516	DGD	O1B-C1B-O2G-C2G
23	r	602	CLA	CBD-CGD-O2D-CED
28	H	102	DGD	O2G-C1B-C2B-C3B
25	C	515	BCR	C19-C20-C21-C22
34	G	605	CHL	CAA-CBA-CGA-O2A
23	G	603	CLA	C4-C3-C5-C6
32	D	406	PL9	C4-C3-C7-C8
32	d	407	PL9	C4-C3-C7-C8
23	y	311	CLA	C6-C7-C8-C9
23	y	313	CLA	C6-C7-C8-C9
34	y	309	CHL	C11-C10-C8-C9
34	Y	309	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	d	410	DGD	C9B-CAB-CBB-CCB
34	r	607	CHL	C5-C6-C7-C8
28	c	516	DGD	O1G-C1G-C2G-C3G
30	A	411	LHG	C4-C5-C6-O8
30	W	201	LHG	C1-C2-C3-O3
36	G	617	NEX	C39-C29-C30-C31
36	N	318	NEX	C39-C29-C30-C31
36	R	617	NEX	C39-C29-C30-C31
36	Y	317	NEX	C39-C29-C30-C31
36	g	617	NEX	C39-C29-C30-C31
36	n	318	NEX	C39-C29-C30-C31
36	r	617	NEX	C39-C29-C30-C31
36	y	317	NEX	C39-C29-C30-C31
36	S	616	NEX	C39-C29-C30-C31
36	s	616	NEX	C39-C29-C30-C31
34	N	307	CHL	CAA-CBA-CGA-O1A
26	A	406	SQD	C9-C10-C11-C12
23	b	603	CLA	C16-C17-C18-C20
27	C	501	LMG	O6-C1-O1-C7
27	a	407	LMG	O6-C1-O1-C7
28	H	102	DGD	C5A-C6A-C7A-C8A
34	G	605	CHL	CAA-CBA-CGA-O1A
34	g	605	CHL	CAA-CBA-CGA-O2A
34	S	605	CHL	CAA-CBA-CGA-O1A
32	D	406	PL9	C24-C26-C27-C28
34	G	609	CHL	C5-C6-C7-C8
26	a	409	SQD	C44-C45-O47-C7
32	d	407	PL9	C30-C29-C31-C32
23	C	511	CLA	C1A-C2A-CAA-CBA
23	r	602	CLA	C1A-C2A-CAA-CBA
23	S	603	CLA	C1A-C2A-CAA-CBA
23	s	603	CLA	C1A-C2A-CAA-CBA
23	s	604	CLA	C1A-C2A-CAA-CBA
34	n	307	CHL	C1A-C2A-CAA-CBA
34	n	310	CHL	C1A-C2A-CAA-CBA
34	y	307	CHL	C1A-C2A-CAA-CBA
30	A	411	LHG	C29-C30-C31-C32
23	D	405	CLA	C16-C17-C18-C19
30	R	618	LHG	O9-C7-O7-C5
23	B	607	CLA	C12-C13-C15-C16
23	B	609	CLA	C11-C12-C13-C15
23	B	614	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	Y	313	CLA	C11-C12-C13-C15
23	c	502	CLA	C11-C10-C8-C7
24	a	404	PHO	C6-C7-C8-C10
34	Y	309	CHL	C11-C12-C13-C15
34	n	309	CHL	C12-C13-C15-C16
34	y	309	CHL	C11-C12-C13-C15
34	S	606	CHL	C2C-C3C-CAC-CBC
24	d	401	PHO	C13-C15-C16-C17
23	b	611	CLA	O1A-CGA-O2A-C1
23	S	603	CLA	CAA-CBA-CGA-O1A
34	S	605	CHL	CAA-CBA-CGA-O2A
35	N	316	LUT	C33-C34-C35-C15
23	B	604	CLA	O1D-CGD-O2D-CED
23	r	614	CLA	CAA-CBA-CGA-O2A
23	s	611	CLA	CAA-CBA-CGA-O2A
23	b	604	CLA	C13-C15-C16-C17
34	g	607	CHL	CBD-CGD-O2D-CED
23	C	511	CLA	C3-C5-C6-C7
23	A	401	CLA	C2A-CAA-CBA-CGA
23	r	612	CLA	C2A-CAA-CBA-CGA
34	y	309	CHL	C2A-CAA-CBA-CGA
23	R	609	CLA	C10-C11-C12-C13
34	Y	309	CHL	C5-C6-C7-C8
30	a	412	LHG	O6-C4-C5-O7
34	N	306	CHL	CAA-CBA-CGA-O2A
34	N	307	CHL	CAA-CBA-CGA-O2A
30	b	622	LHG	C29-C30-C31-C32
23	b	615	CLA	C5-C6-C7-C8
30	n	319	LHG	C28-C29-C30-C31
30	Y	318	LHG	O6-C4-C5-C6
23	y	303	CLA	C2C-C3C-CAC-CBC
34	s	605	CHL	CAA-CBA-CGA-O1A
34	s	605	CHL	CAA-CBA-CGA-O2A
23	C	509	CLA	C13-C15-C16-C17
32	D	406	PL9	C38-C39-C41-C42
30	W	201	LHG	O2-C2-C3-O3
34	S	601	CHL	CAA-CBA-CGA-O2A
34	s	601	CHL	CAA-CBA-CGA-O1A
34	s	601	CHL	CAA-CBA-CGA-O2A
34	g	601	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	C	501	LMG	O9-C10-O7-C8
27	b	620	LMG	O9-C10-O7-C8
34	s	607	CHL	O2A-C1-C2-C3
28	c	516	DGD	C5A-C6A-C7A-C8A
34	S	606	CHL	C4C-C3C-CAC-CBC
36	G	617	NEX	C28-C29-C30-C31
36	N	318	NEX	C28-C29-C30-C31
36	R	617	NEX	C28-C29-C30-C31
36	Y	317	NEX	C28-C29-C30-C31
36	g	617	NEX	C28-C29-C30-C31
36	n	318	NEX	C28-C29-C30-C31
36	r	617	NEX	C28-C29-C30-C31
36	y	317	NEX	C28-C29-C30-C31
36	S	616	NEX	C28-C29-C30-C31
36	s	616	NEX	C28-C29-C30-C31
23	B	609	CLA	C10-C11-C12-C13
23	b	609	CLA	C10-C11-C12-C13
23	s	611	CLA	CAA-CBA-CGA-O1A
25	c	518	BCR	C9-C10-C11-C12
35	Y	315	LUT	C29-C30-C31-C32
35	y	315	LUT	C29-C30-C31-C32
35	S	615	LUT	C33-C34-C35-C15
23	s	603	CLA	CAA-CBA-CGA-O1A
23	Y	313	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	C11-C12-C13-C15
26	L	103	SQD	C32-C33-C34-C35
26	A	406	SQD	O5-C1-O6-C44
30	a	411	LHG	C1-C2-C3-O3
32	d	407	PL9	C24-C26-C27-C28
33	E	101	HEM	CAA-CBA-CGA-O2A
23	N	312	CLA	O1D-CGD-O2D-CED
23	a	405	CLA	C3-C5-C6-C7
23	B	607	CLA	C2-C1-O2A-CGA
34	r	606	CHL	C2C-C3C-CAC-CBC
23	B	611	CLA	C13-C15-C16-C17
23	g	612	CLA	CAA-CBA-CGA-O2A
33	e	101	HEM	CAD-CBD-CGD-O2D
28	d	410	DGD	O2G-C1B-C2B-C3B
23	D	401	CLA	C11-C12-C13-C14
26	L	103	SQD	C26-C27-C28-C29
23	B	616	CLA	C15-C16-C17-C18
23	S	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A	403	PHO	C13-C15-C16-C17
30	c	517	LHG	O7-C7-C8-C9
23	N	303	CLA	O1A-CGA-O2A-C1
25	B	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C1-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
35	N	316	LUT	C1-C6-C7-C8
35	N	317	LUT	C1-C6-C7-C8
35	g	616	LUT	C1-C6-C7-C8
35	n	317	LUT	C1-C6-C7-C8
34	g	601	CHL	C10-C11-C12-C13
26	M	101	SQD	C27-C28-C29-C30
23	G	612	CLA	CAA-CBA-CGA-O2A
33	E	101	HEM	CAD-CBD-CGD-O2D
25	c	514	BCR	C19-C20-C21-C22
35	S	615	LUT	C13-C14-C15-C35
35	Y	315	LUT	C27-C28-C29-C30
32	d	407	PL9	C38-C39-C41-C42
28	c	516	DGD	O1G-C1A-C2A-C3A
23	S	611	CLA	CAA-CBA-CGA-O2A
27	D	407	LMG	C8-C7-O1-C1
34	N	308	CHL	CAA-CBA-CGA-O2A
28	d	410	DGD	C2A-C3A-C4A-C5A
30	W	201	LHG	C17-C18-C19-C20
34	y	309	CHL	C16-C17-C18-C19
30	Y	318	LHG	O6-C4-C5-O7
23	G	612	CLA	CAA-CBA-CGA-O1A
23	s	603	CLA	CAA-CBA-CGA-O2A
34	S	601	CHL	CAA-CBA-CGA-O1A
23	g	612	CLA	CAA-CBA-CGA-O1A
23	c	504	CLA	C11-C12-C13-C14
30	c	517	LHG	O6-C4-C5-C6
23	c	513	CLA	C4-C3-C5-C6
23	g	602	CLA	C4-C3-C5-C6
24	D	402	PHO	C4-C3-C5-C6
34	g	619	CHL	C4-C3-C5-C6
23	C	508	CLA	C11-C12-C13-C15
23	D	401	CLA	C11-C12-C13-C15
23	D	404	CLA	C11-C10-C8-C7
23	b	614	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	g	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	D	406	PL9	C33-C34-C36-C37
32	d	407	PL9	C33-C34-C36-C37
34	r	607	CHL	C2-C3-C5-C6
33	E	101	HEM	CAA-CBA-CGA-O1A
23	G	611	CLA	CBA-CGA-O2A-C1
23	N	303	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CAA-CBA-CGA-O1A
35	N	317	LUT	C29-C30-C31-C32
23	y	303	CLA	CAA-CBA-CGA-O2A
30	W	201	LHG	O8-C23-C24-C25
30	n	319	LHG	O7-C7-C8-C9
30	B	621	LHG	C31-C32-C33-C34
23	B	604	CLA	C15-C16-C17-C18
34	N	308	CHL	CAA-CBA-CGA-O1A
34	n	308	CHL	CAA-CBA-CGA-O2A
30	w	201	LHG	O8-C23-C24-C25
23	S	612	CLA	C4-C3-C5-C6
23	A	404	CLA	C5-C6-C7-C8
23	D	405	CLA	C8-C10-C11-C12
23	C	505	CLA	C2-C3-C5-C6
23	Y	303	CLA	CAA-CBA-CGA-O2A
23	B	607	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C10-C8-C9
23	Y	313	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	508	CLA	C11-C12-C13-C14
23	g	611	CLA	C6-C7-C8-C9
24	a	404	PHO	C6-C7-C8-C9
34	Y	309	CHL	C11-C12-C13-C14
34	y	309	CHL	C11-C12-C13-C14
23	n	313	CLA	CAA-CBA-CGA-O2A
34	n	308	CHL	CAA-CBA-CGA-O1A
23	C	511	CLA	C3A-C2A-CAA-CBA
23	n	311	CLA	C3A-C2A-CAA-CBA
23	S	612	CLA	C3A-C2A-CAA-CBA
23	s	612	CLA	C3A-C2A-CAA-CBA
34	G	608	CHL	C3A-C2A-CAA-CBA
34	N	308	CHL	C3A-C2A-CAA-CBA
34	y	307	CHL	C3A-C2A-CAA-CBA
34	s	601	CHL	C3A-C2A-CAA-CBA
23	y	303	CLA	C4C-C3C-CAC-CBC
30	w	201	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C13-C15-C16-C17
23	B	615	CLA	C5-C6-C7-C8
23	C	502	CLA	C10-C11-C12-C13
23	b	611	CLA	C13-C15-C16-C17
23	G	611	CLA	O1A-CGA-O2A-C1
23	A	401	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	CAA-CBA-CGA-O2A
23	B	608	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	G	603	CLA	CAD-CBD-CGD-O2D
23	G	611	CLA	CAD-CBD-CGD-O2D
23	N	304	CLA	CAD-CBD-CGD-O2D
23	R	601	CLA	CAD-CBD-CGD-O2D
23	Y	310	CLA	CAD-CBD-CGD-O2D
23	Y	314	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	g	603	CLA	CAD-CBD-CGD-O2D
23	g	610	CLA	CAD-CBD-CGD-O2D
23	r	611	CLA	CAD-CBD-CGD-O2D
23	y	314	CLA	CAD-CBD-CGD-O2D
23	S	603	CLA	CAD-CBD-CGD-O2D
23	S	611	CLA	CAD-CBD-CGD-O2D
23	s	602	CLA	CAD-CBD-CGD-O2D
23	s	603	CLA	CAD-CBD-CGD-O2D
24	A	403	PHO	CAD-CBD-CGD-O2D
24	D	402	PHO	CAD-CBD-CGD-O2D
24	a	404	PHO	CAD-CBD-CGD-O2D
34	R	605	CHL	CAD-CBD-CGD-O2D
34	Y	302	CHL	CAD-CBD-CGD-O2D
34	Y	306	CHL	CAD-CBD-CGD-O2D
34	Y	307	CHL	CAD-CBD-CGD-O2D
34	y	302	CHL	CAD-CBD-CGD-O2D
34	S	606	CHL	CAD-CBD-CGD-O2D
34	s	601	CHL	CAD-CBD-CGD-O2D
23	c	504	CLA	C11-C12-C13-C15
23	c	512	CLA	C4C-C3C-CAC-CBC
27	a	407	LMG	O9-C10-O7-C8
30	L	101	LHG	C12-C13-C14-C15
23	Y	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	N	313	CLA	CAA-CBA-CGA-O2A
33	e	101	HEM	CAD-CBD-CGD-O1D
30	g	618	LHG	O8-C23-C24-C25
23	B	608	CLA	CBA-CGA-O2A-C1
34	n	307	CHL	CAA-CBA-CGA-O1A
23	c	511	CLA	C5-C6-C7-C8
34	G	619	CHL	CAA-CBA-CGA-O2A
34	g	619	CHL	CAA-CBA-CGA-O2A
27	C	501	LMG	C12-C13-C14-C15
25	C	515	BCR	C21-C22-C23-C24
25	c	514	BCR	C17-C18-C19-C20
26	A	406	SQD	C44-C45-C46-O48
36	N	318	NEX	O24-C26-C27-C28
36	R	617	NEX	O24-C26-C27-C28
36	Y	317	NEX	O24-C26-C27-C28
36	r	617	NEX	O24-C26-C27-C28
36	y	317	NEX	O24-C26-C27-C28
36	S	616	NEX	O24-C26-C27-C28
37	N	301	XAT	O24-C26-C27-C28
37	R	616	XAT	O4-C6-C7-C8
37	g	620	XAT	O24-C26-C27-C28
37	n	301	XAT	O24-C26-C27-C28
37	r	616	XAT	O4-C6-C7-C8
23	S	611	CLA	CAA-CBA-CGA-O1A
30	W	201	LHG	O6-C4-C5-O7
23	C	507	CLA	CAA-CBA-CGA-O2A
26	M	101	SQD	C26-C27-C28-C29
23	B	614	CLA	O2A-C1-C2-C3
23	C	506	CLA	O2A-C1-C2-C3
23	D	404	CLA	O2A-C1-C2-C3
23	b	614	CLA	O2A-C1-C2-C3
23	c	505	CLA	O2A-C1-C2-C3
23	d	404	CLA	O2A-C1-C2-C3
34	G	601	CHL	O2A-C1-C2-C3
23	g	611	CLA	CBA-CGA-O2A-C1
30	B	621	LHG	C24-C23-O8-C6
26	d	402	SQD	C9-C10-C11-C12
34	g	608	CHL	CAA-CBA-CGA-O2A
23	N	313	CLA	CAA-CBA-CGA-O1A
23	Y	313	CLA	C5-C6-C7-C8
26	L	103	SQD	C27-C28-C29-C30
23	B	605	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	N	304	CLA	CHA-CBD-CGD-O2D
23	R	604	CLA	CHA-CBD-CGD-O1D
23	R	604	CLA	CHA-CBD-CGD-O2D
23	R	611	CLA	CHA-CBD-CGD-O2D
23	Y	303	CLA	CHA-CBD-CGD-O1D
23	Y	303	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	501	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	g	602	CLA	CHA-CBD-CGD-O1D
23	g	602	CLA	CHA-CBD-CGD-O2D
23	g	603	CLA	CHA-CBD-CGD-O1D
23	r	614	CLA	CHA-CBD-CGD-O1D
23	r	614	CLA	CHA-CBD-CGD-O2D
23	y	303	CLA	CHA-CBD-CGD-O2D
23	y	311	CLA	CHA-CBD-CGD-O2D
23	S	602	CLA	CHA-CBD-CGD-O2D
23	s	609	CLA	CHA-CBD-CGD-O2D
23	s	612	CLA	CHA-CBD-CGD-O2D
34	G	605	CHL	CHA-CBD-CGD-O1D
34	G	605	CHL	CHA-CBD-CGD-O2D
34	G	606	CHL	CHA-CBD-CGD-O1D
34	N	307	CHL	CHA-CBD-CGD-O2D
23	n	313	CLA	CAA-CBA-CGA-O1A
23	C	512	CLA	CAA-CBA-CGA-O2A
23	c	506	CLA	CAA-CBA-CGA-O2A
30	w	201	LHG	C29-C30-C31-C32
23	c	513	CLA	C8-C10-C11-C12
33	E	101	HEM	CAD-CBD-CGD-O1D
23	R	602	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	r	608	CLA	CAA-CBA-CGA-O2A
26	A	406	SQD	O47-C7-C8-C9
26	d	402	SQD	O47-C7-C8-C9
34	G	608	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	B	620	LMG	O7-C8-C9-O8
28	A	408	DGD	O1G-C1G-C2G-O2G
30	G	618	LHG	O7-C5-C6-O8
23	G	602	CLA	C10-C11-C12-C13
34	n	307	CHL	CAA-CBA-CGA-O2A
30	C	518	LHG	C24-C25-C26-C27
23	b	612	CLA	C8-C10-C11-C12
23	a	401	CLA	CAA-CBA-CGA-O2A
27	A	407	LMG	C29-C30-C31-C32
34	g	601	CHL	C8-C10-C11-C12
30	g	618	LHG	C27-C28-C29-C30
27	B	622	LMG	O8-C28-C29-C30
23	C	512	CLA	C12-C13-C15-C16
34	y	302	CHL	C6-C7-C8-C10
34	y	309	CHL	C11-C10-C8-C7
34	G	608	CHL	C16-C17-C18-C20
34	n	310	CHL	C16-C17-C18-C19
23	b	602	CLA	CAA-CBA-CGA-O2A
26	L	103	SQD	O47-C7-C8-C9
26	M	101	SQD	O47-C7-C8-C9
27	A	407	LMG	O8-C28-C29-C30
23	S	609	CLA	CAA-CBA-CGA-O1A
23	D	404	CLA	C3-C5-C6-C7
23	C	505	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16
23	y	312	CLA	C6-C7-C8-C9
34	N	309	CHL	C14-C13-C15-C16
34	g	607	CHL	O1D-CGD-O2D-CED
30	Y	318	LHG	C29-C30-C31-C32
23	R	601	CLA	O2A-C1-C2-C3
23	g	604	CLA	O2A-C1-C2-C3
26	A	406	SQD	C5-C6-S-O8
26	d	402	SQD	C5-C6-S-O8
30	Y	318	LHG	C31-C32-C33-C34
27	C	501	LMG	C11-C10-O7-C8
27	b	620	LMG	C11-C10-O7-C8
27	d	409	LMG	C11-C10-O7-C8
34	G	607	CHL	CBD-CGD-O2D-CED
30	G	618	LHG	O8-C23-C24-C25
28	H	102	DGD	C9B-CAB-CBB-CCB
26	M	101	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
25	K	101	BCR	C37-C22-C23-C24
23	y	303	CLA	CAA-CBA-CGA-O1A
24	D	402	PHO	C16-C17-C18-C20
23	g	603	CLA	C4-C3-C5-C6
23	N	312	CLA	C2-C3-C5-C6
30	A	412	LHG	O7-C7-C8-C9
30	b	621	LHG	C24-C23-O8-C6
34	y	308	CHL	CBA-CGA-O2A-C1
23	n	303	CLA	C10-C11-C12-C13
28	A	408	DGD	C6B-C7B-C8B-C9B
23	c	501	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C1A-C2A-CAA-CBA
23	R	612	CLA	C1A-C2A-CAA-CBA
23	r	608	CLA	C1A-C2A-CAA-CBA
23	y	311	CLA	C1A-C2A-CAA-CBA
23	S	612	CLA	C1A-C2A-CAA-CBA
23	s	612	CLA	C1A-C2A-CAA-CBA
34	R	606	CHL	C1A-C2A-CAA-CBA
34	Y	302	CHL	C1A-C2A-CAA-CBA
34	r	606	CHL	C1A-C2A-CAA-CBA
34	s	601	CHL	C1A-C2A-CAA-CBA
34	s	607	CHL	C1A-C2A-CAA-CBA
30	A	412	LHG	C32-C33-C34-C35
34	g	619	CHL	CAA-CBA-CGA-O1A
23	g	611	CLA	O1A-CGA-O2A-C1
23	B	604	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	607	CLA	C2-C1-O2A-CGA
23	y	303	CLA	C2-C1-O2A-CGA
23	Y	303	CLA	CAA-CBA-CGA-O1A
30	n	319	LHG	O9-C7-C8-C9
28	A	408	DGD	O1G-C1G-C2G-C3G
23	A	401	CLA	C5-C6-C7-C8
23	b	612	CLA	C5-C6-C7-C8
23	g	610	CLA	C2A-CAA-CBA-CGA
23	s	602	CLA	C2A-CAA-CBA-CGA
23	C	505	CLA	C11-C12-C13-C14
30	W	201	LHG	O10-C23-C24-C25
23	B	612	CLA	C8-C10-C11-C12
34	y	308	CHL	O1A-CGA-O2A-C1
34	r	607	CHL	C4-C3-C5-C6
23	s	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	CAA-CBA-CGA-O1A
30	w	201	LHG	O10-C23-C24-C25
27	a	407	LMG	C30-C31-C32-C33
23	G	610	CLA	C5-C6-C7-C8
30	C	518	LHG	C3-O3-P-O5
30	G	618	LHG	C4-O6-P-O5
30	N	319	LHG	C3-O3-P-O5
30	c	517	LHG	C3-O3-P-O5
30	n	319	LHG	C3-O3-P-O5
30	r	618	LHG	C3-O3-P-O5
30	y	318	LHG	C3-O3-P-O5
23	c	506	CLA	CAA-CBA-CGA-O1A
26	A	406	SQD	O49-C7-C8-C9
26	d	402	SQD	O49-C7-C8-C9
30	g	618	LHG	O10-C23-C24-C25
34	G	619	CHL	CAA-CBA-CGA-O1A
23	R	611	CLA	O2A-C1-C2-C3
30	r	618	LHG	O6-C4-C5-C6
30	y	318	LHG	O6-C4-C5-C6
23	s	608	CLA	CAA-CBA-CGA-O2A
35	N	317	LUT	C5-C6-C7-C8
34	G	609	CHL	C4C-C3C-CAC-CBC
23	C	507	CLA	CAA-CBA-CGA-O1A
34	g	608	CHL	CAA-CBA-CGA-O1A
23	B	608	CLA	O1A-CGA-O2A-C1
23	r	603	CLA	O1A-CGA-O2A-C1
30	L	102	LHG	O8-C23-C24-C25
23	s	609	CLA	CAA-CBA-CGA-O2A
23	y	311	CLA	C11-C12-C13-C14
23	C	513	CLA	CAA-CBA-CGA-O1A
34	G	608	CHL	CAA-CBA-CGA-O1A
23	c	503	CLA	C15-C16-C17-C18
24	D	402	PHO	C13-C15-C16-C17
23	y	313	CLA	C5-C6-C7-C8
23	N	312	CLA	CBD-CGD-O2D-CED
23	A	401	CLA	CAA-CBA-CGA-O1A
30	G	618	LHG	O10-C23-C24-C25
30	R	618	LHG	C8-C7-O7-C5
30	a	412	LHG	C15-C16-C17-C18
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	S	611	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	s	602	CLA	CAD-CBD-CGD-O1D
34	G	606	CHL	CAD-CBD-CGD-O1D
23	a	401	CLA	CAA-CBA-CGA-O1A
30	R	618	LHG	C11-C12-C13-C14
30	C	518	LHG	O7-C7-C8-C9
34	y	302	CHL	CAA-CBA-CGA-O2A
23	a	405	CLA	C10-C11-C12-C13
23	g	611	CLA	C5-C6-C7-C8
34	n	302	CHL	C13-C15-C16-C17
23	B	608	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C10-C8-C9
23	Y	313	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
23	s	609	CLA	CAA-CBA-CGA-O1A
23	C	506	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
23	Y	304	CLA	CAA-CBA-CGA-O2A
34	Y	302	CHL	CAA-CBA-CGA-O2A
34	y	309	CHL	C13-C15-C16-C17
27	B	622	LMG	O10-C28-C29-C30
23	C	509	CLA	C5-C6-C7-C8
23	a	405	CLA	C8-C10-C11-C12
23	G	610	CLA	C2A-CAA-CBA-CGA
23	N	303	CLA	C2A-CAA-CBA-CGA
23	R	609	CLA	C2A-CAA-CBA-CGA
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
23	y	304	CLA	CAA-CBA-CGA-O2A
23	S	612	CLA	CAA-CBA-CGA-O2A
30	S	617	LHG	O8-C23-C24-C25
23	S	609	CLA	CAA-CBA-CGA-O2A
34	Y	302	CHL	C16-C17-C18-C20
23	a	405	CLA	C5-C6-C7-C8
23	C	503	CLA	C11-C12-C13-C15
23	C	510	CLA	C12-C13-C15-C16
23	G	610	CLA	C6-C7-C8-C10
23	Y	311	CLA	C6-C7-C8-C10
23	a	402	CLA	C11-C10-C8-C7
23	g	602	CLA	C6-C7-C8-C10
23	S	603	CLA	C3A-C2A-CAA-CBA
23	s	603	CLA	C3A-C2A-CAA-CBA
34	R	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
34	g	619	CHL	C2-C3-C5-C6
34	n	308	CHL	C3A-C2A-CAA-CBA
34	r	606	CHL	C3A-C2A-CAA-CBA
23	s	612	CLA	CAA-CBA-CGA-O1A
34	y	302	CHL	CAA-CBA-CGA-O1A
26	L	103	SQD	C29-C30-C31-C32
23	b	616	CLA	CAA-CBA-CGA-O2A
23	r	611	CLA	CAA-CBA-CGA-O2A
30	N	319	LHG	O7-C7-C8-C9
34	Y	308	CHL	CAA-CBA-CGA-O2A
34	Y	309	CHL	CAA-CBA-CGA-O2A
34	y	308	CHL	CAA-CBA-CGA-O2A
30	n	319	LHG	C13-C14-C15-C16
25	K	101	BCR	C21-C22-C23-C24
35	n	317	LUT	C31-C32-C33-C34
23	c	510	CLA	CAA-CBA-CGA-O1A
30	a	411	LHG	C13-C14-C15-C16
23	C	505	CLA	C11-C12-C13-C15
34	g	608	CHL	C16-C17-C18-C20
30	R	618	LHG	O7-C7-C8-C9
23	r	609	CLA	C13-C15-C16-C17
30	B	621	LHG	O10-C23-O8-C6
26	L	103	SQD	O49-C7-C8-C9
27	A	407	LMG	O10-C28-C29-C30
30	L	102	LHG	O10-C23-C24-C25
30	L	101	LHG	C24-C23-O8-C6
23	C	502	CLA	CAA-CBA-CGA-O2A
30	s	617	LHG	O8-C23-C24-C25
34	y	309	CHL	CAA-CBA-CGA-O2A
26	M	101	SQD	O49-C7-C8-C9
30	A	412	LHG	O9-C7-C8-C9
23	a	405	CLA	C2A-CAA-CBA-CGA
23	r	608	CLA	C2A-CAA-CBA-CGA
23	R	614	CLA	CAA-CBA-CGA-O1A
30	N	319	LHG	O9-C7-C8-C9
30	r	618	LHG	O10-C23-C24-C25
34	y	308	CHL	CAA-CBA-CGA-O1A
23	c	503	CLA	C4-C3-C5-C6
34	y	307	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

252 monomers are involved in 515 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	408	DGD	4	0
30	B	623	LHG	2	0
23	r	604	CLA	1	0
30	a	412	LHG	4	0
34	g	608	CHL	2	0
23	c	512	CLA	2	0
30	r	618	LHG	2	0
34	n	308	CHL	2	0
26	a	409	SQD	1	0
34	R	605	CHL	1	0
30	s	617	LHG	2	0
25	h	101	BCR	5	0
34	g	607	CHL	2	0
25	B	618	BCR	2	0
35	g	615	LUT	4	0
35	S	614	LUT	5	0
23	R	604	CLA	3	0
28	a	408	DGD	3	0
34	S	605	CHL	2	0
23	B	606	CLA	2	0
23	S	612	CLA	3	0
30	R	618	LHG	2	0
25	A	405	BCR	4	0
35	S	615	LUT	3	0
23	Y	303	CLA	2	0
34	g	619	CHL	4	0
25	Z	101	BCR	3	0
23	A	401	CLA	3	0
23	S	609	CLA	1	0
23	D	404	CLA	6	0
25	C	516	BCR	4	0
25	C	515	BCR	5	0
23	C	503	CLA	4	0
34	G	608	CHL	1	0
23	b	609	CLA	3	0
35	y	316	LUT	2	0
23	y	311	CLA	1	0
30	L	102	LHG	1	0
23	C	511	CLA	3	0
23	C	507	CLA	1	0
25	a	406	BCR	2	0
23	c	501	CLA	1	0
23	n	305	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	504	CLA	4	0
23	r	608	CLA	2	0
23	B	612	CLA	3	0
35	G	616	LUT	5	0
23	g	614	CLA	1	0
30	L	101	LHG	4	0
32	d	407	PL9	3	0
23	g	611	CLA	2	0
23	d	404	CLA	7	0
23	R	609	CLA	2	0
34	r	607	CHL	3	0
34	G	619	CHL	3	0
23	c	506	CLA	1	0
24	d	401	PHO	4	0
25	k	101	BCR	2	0
23	C	505	CLA	1	0
27	B	620	LMG	5	0
23	y	303	CLA	2	0
25	b	618	BCR	3	0
23	B	605	CLA	3	0
37	y	301	XAT	4	0
23	C	506	CLA	1	0
35	Y	315	LUT	4	0
23	s	612	CLA	5	0
34	g	605	CHL	1	0
23	B	601	CLA	2	0
30	W	201	LHG	1	0
27	b	620	LMG	4	0
34	N	308	CHL	1	0
34	n	309	CHL	3	0
23	b	614	CLA	1	0
23	c	513	CLA	2	0
25	B	617	BCR	2	0
23	R	612	CLA	2	0
23	N	305	CLA	1	0
23	d	405	CLA	2	0
28	c	516	DGD	2	0
34	N	310	CHL	3	0
34	g	609	CHL	1	0
23	B	610	CLA	4	0
23	c	510	CLA	5	0
23	B	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	403	BCT	2	0
30	Y	318	LHG	1	0
23	B	607	CLA	1	0
23	g	612	CLA	1	0
35	N	316	LUT	3	0
25	B	619	BCR	2	0
34	y	306	CHL	2	0
36	G	617	NEX	3	0
34	N	307	CHL	1	0
23	G	602	CLA	4	0
23	C	509	CLA	1	0
23	B	604	CLA	1	0
23	y	310	CLA	1	0
23	b	602	CLA	1	0
23	r	610	CLA	1	0
23	r	614	CLA	2	0
23	A	404	CLA	2	0
35	g	616	LUT	9	0
23	s	610	CLA	1	0
23	r	611	CLA	2	0
23	S	613	CLA	3	0
23	g	610	CLA	2	0
34	N	309	CHL	4	0
23	g	603	CLA	2	0
25	c	518	BCR	3	0
25	c	514	BCR	7	0
23	R	614	CLA	2	0
35	n	317	LUT	2	0
35	n	316	LUT	2	0
24	a	404	PHO	1	0
34	r	605	CHL	1	0
34	n	307	CHL	2	0
23	S	610	CLA	1	0
34	S	601	CHL	1	0
25	H	101	BCR	4	0
23	b	613	CLA	1	0
34	G	601	CHL	4	0
34	S	606	CHL	2	0
36	n	318	NEX	3	0
37	R	616	XAT	1	0
23	a	401	CLA	3	0
23	b	610	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	501	LMG	2	0
23	n	311	CLA	2	0
34	r	606	CHL	1	0
34	S	607	CHL	1	0
23	b	605	CLA	4	0
28	H	102	DGD	4	0
36	r	617	NEX	2	0
37	Y	301	XAT	5	0
36	N	318	NEX	2	0
23	B	608	CLA	3	0
34	Y	309	CHL	4	0
23	b	604	CLA	1	0
24	D	402	PHO	7	0
26	A	409	SQD	1	0
30	g	618	LHG	3	0
23	s	613	CLA	4	0
23	G	603	CLA	3	0
31	d	403	BCT	3	0
23	A	402	CLA	2	0
23	b	606	CLA	2	0
23	B	614	CLA	1	0
25	c	515	BCR	5	0
34	Y	302	CHL	4	0
23	C	514	CLA	3	0
23	B	603	CLA	5	0
30	S	617	LHG	3	0
27	a	407	LMG	2	0
23	B	602	CLA	2	0
23	C	513	CLA	4	0
37	n	301	XAT	2	0
23	c	502	CLA	4	0
37	g	620	XAT	3	0
34	R	607	CHL	3	0
23	s	602	CLA	2	0
35	s	614	LUT	4	0
35	N	317	LUT	4	0
36	g	617	NEX	3	0
23	b	611	CLA	1	0
33	E	101	HEM	1	0
23	r	609	CLA	4	0
26	M	101	SQD	3	0
23	c	509	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	y	302	CHL	3	0
23	n	314	CLA	2	0
28	C	517	DGD	4	0
37	G	620	XAT	6	0
23	N	312	CLA	1	0
23	D	401	CLA	3	0
34	y	309	CHL	3	0
23	S	602	CLA	2	0
23	C	502	CLA	1	0
23	R	602	CLA	1	0
34	s	607	CHL	1	0
23	Y	311	CLA	2	0
34	G	606	CHL	1	0
30	y	318	LHG	1	0
30	A	412	LHG	4	0
30	d	408	LHG	6	0
30	b	622	LHG	2	0
36	s	616	NEX	2	0
23	n	315	CLA	1	0
30	w	201	LHG	1	0
34	G	609	CHL	2	0
23	Y	313	CLA	1	0
23	N	311	CLA	2	0
23	s	609	CLA	1	0
26	L	103	SQD	4	0
30	C	518	LHG	3	0
23	a	403	CLA	2	0
23	G	612	CLA	1	0
28	d	410	DGD	4	0
23	B	615	CLA	4	0
34	G	607	CHL	1	0
25	K	101	BCR	2	0
25	F	101	BCR	2	0
34	g	601	CHL	6	0
35	R	615	LUT	2	0
23	y	312	CLA	1	0
34	n	310	CHL	1	0
23	a	402	CLA	3	0
23	C	512	CLA	2	0
25	b	619	BCR	3	0
23	Y	310	CLA	1	0
25	b	617	BCR	2	0

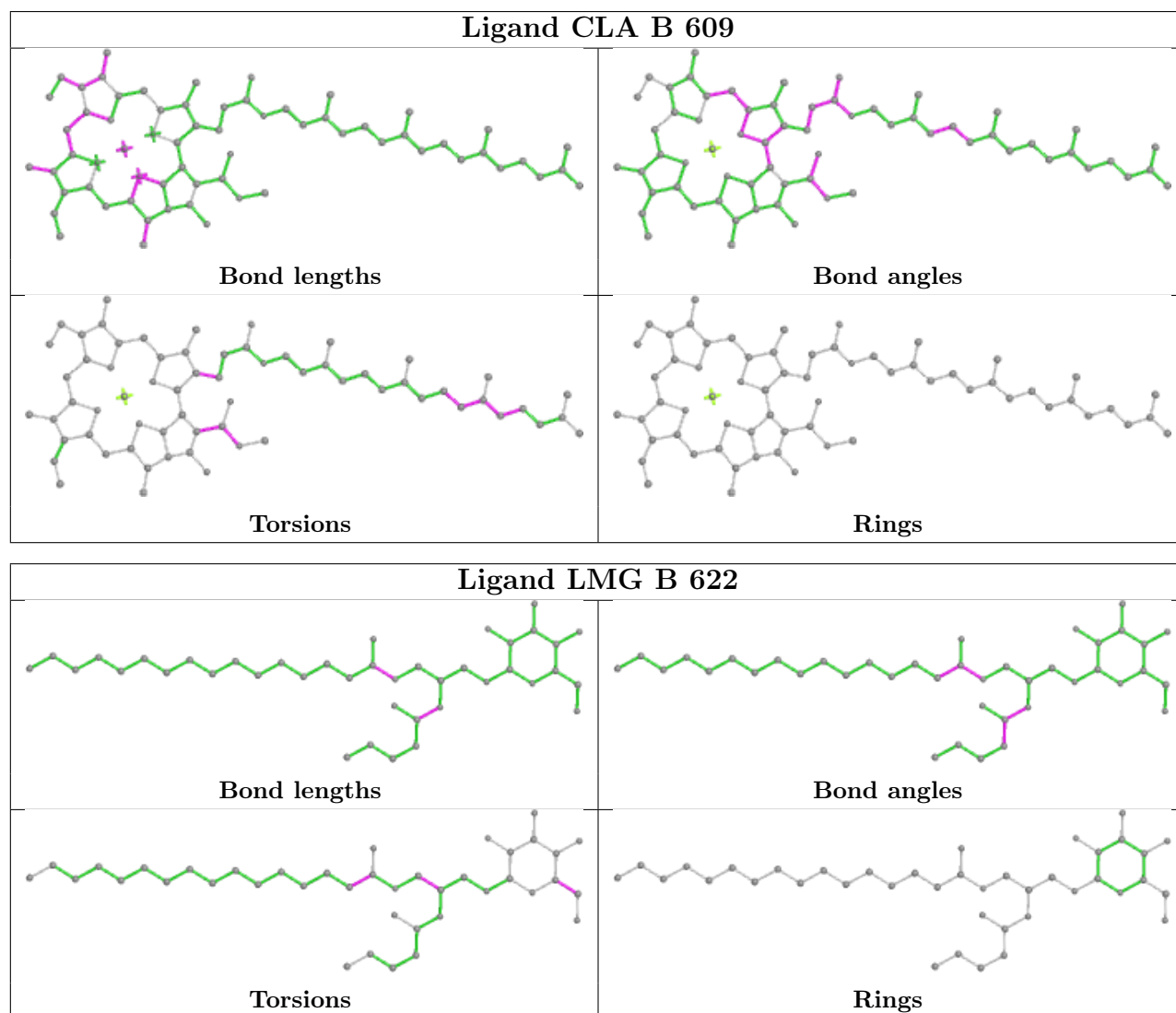
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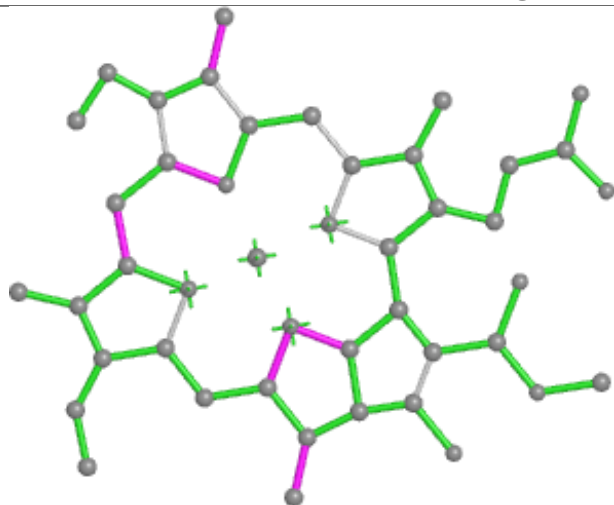
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	g	604	CLA	2	0
26	d	402	SQD	2	0
35	r	615	LUT	3	0
35	G	615	LUT	3	0
30	T	101	LHG	2	0
34	R	606	CHL	1	0
23	B	616	CLA	2	0
23	b	608	CLA	6	0
30	c	517	LHG	2	0
23	r	602	CLA	1	0
23	N	314	CLA	3	0
30	N	319	LHG	2	0
23	c	511	CLA	7	0
23	b	603	CLA	7	0
24	A	403	PHO	2	0
23	r	601	CLA	2	0
27	D	407	LMG	2	0
23	G	610	CLA	2	0
36	R	617	NEX	2	0
23	c	503	CLA	5	0
34	s	605	CHL	1	0
23	G	604	CLA	1	0
23	a	405	CLA	1	0
32	D	406	PL9	2	0
23	y	313	CLA	1	0
23	b	601	CLA	3	0
23	b	607	CLA	1	0
23	g	602	CLA	2	0
25	d	406	BCR	2	0
30	G	618	LHG	3	0
34	n	302	CHL	1	0
35	y	315	LUT	3	0
23	C	510	CLA	3	0
23	S	603	CLA	1	0
35	Y	316	LUT	2	0
34	g	606	CHL	3	0
30	n	319	LHG	1	0
23	b	612	CLA	1	0
23	c	508	CLA	3	0
23	c	505	CLA	1	0
34	Y	306	CHL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

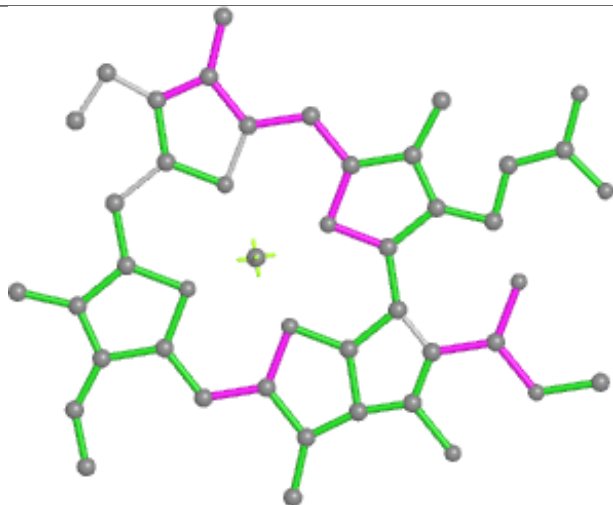
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



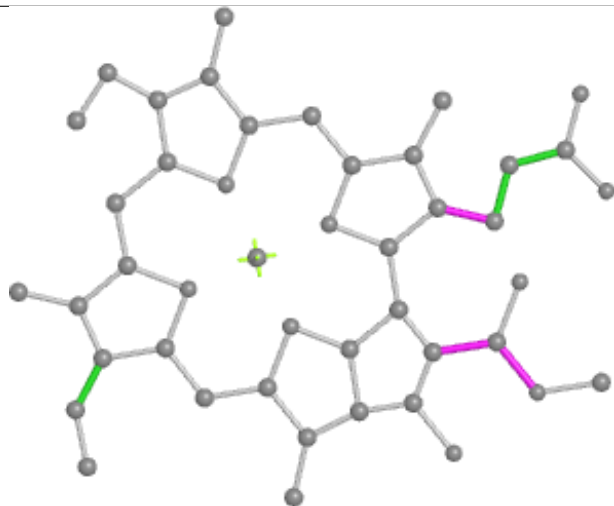
Ligand CLA Y 314



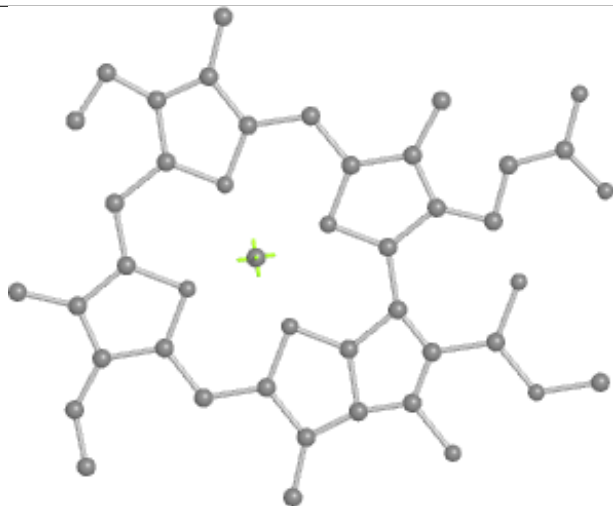
Bond lengths



Bond angles

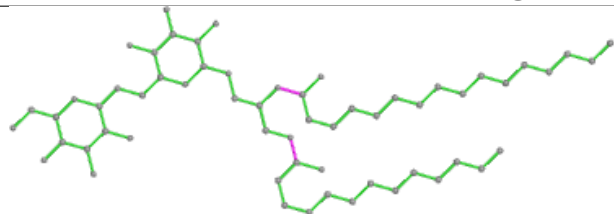


Torsions

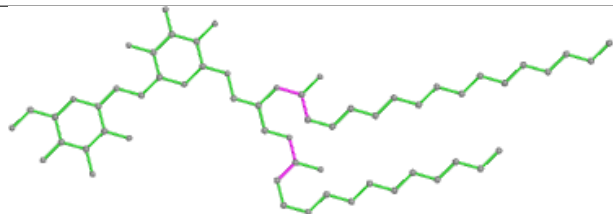


Rings

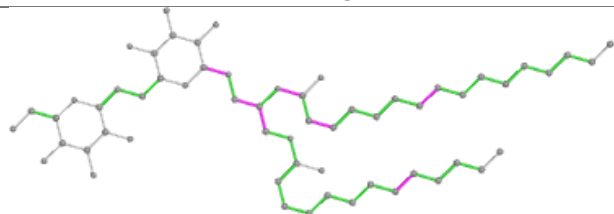
Ligand DGD A 408



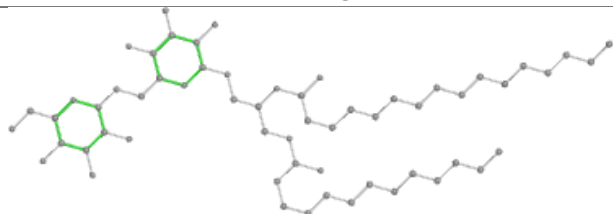
Bond lengths



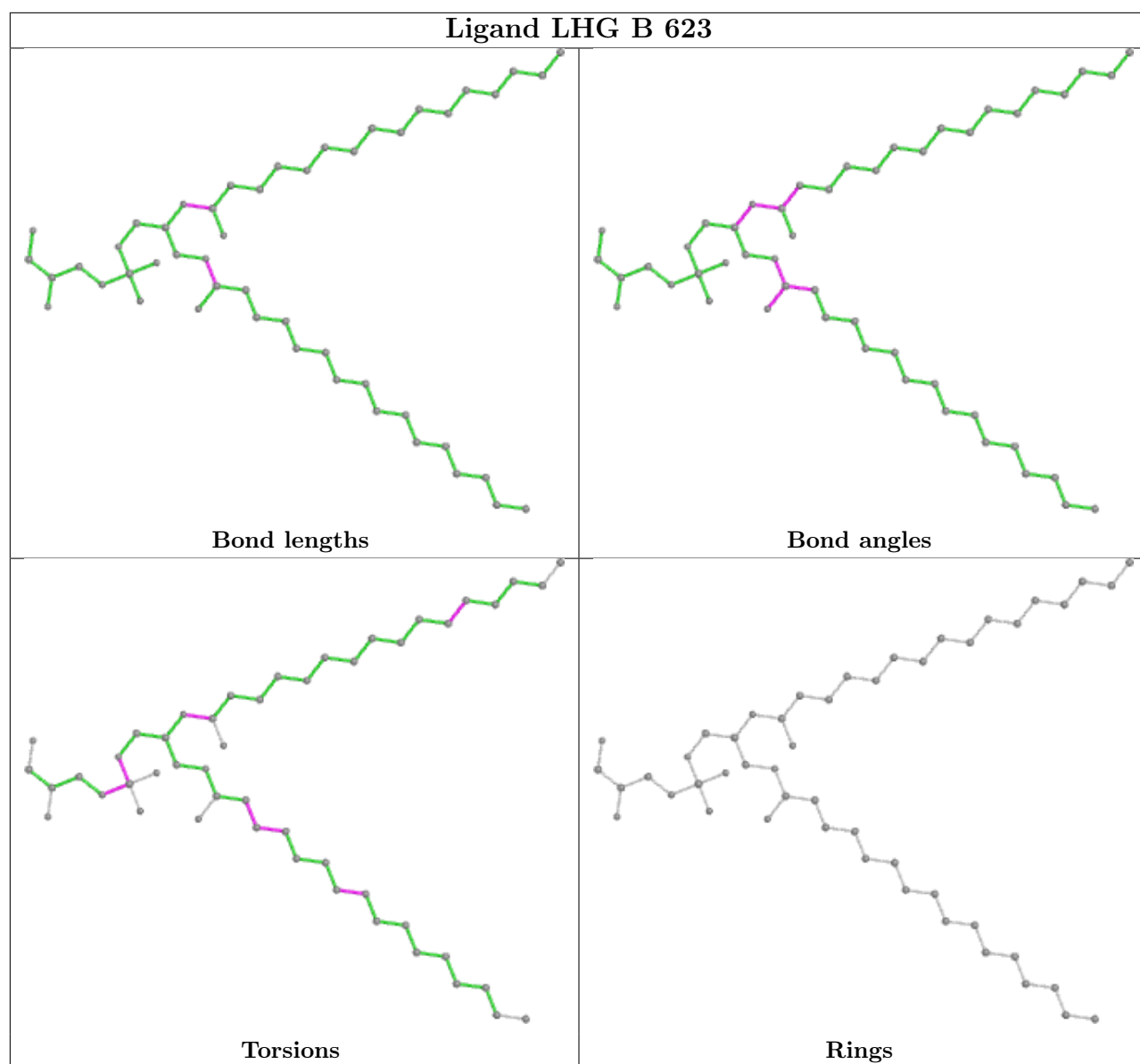
Bond angles

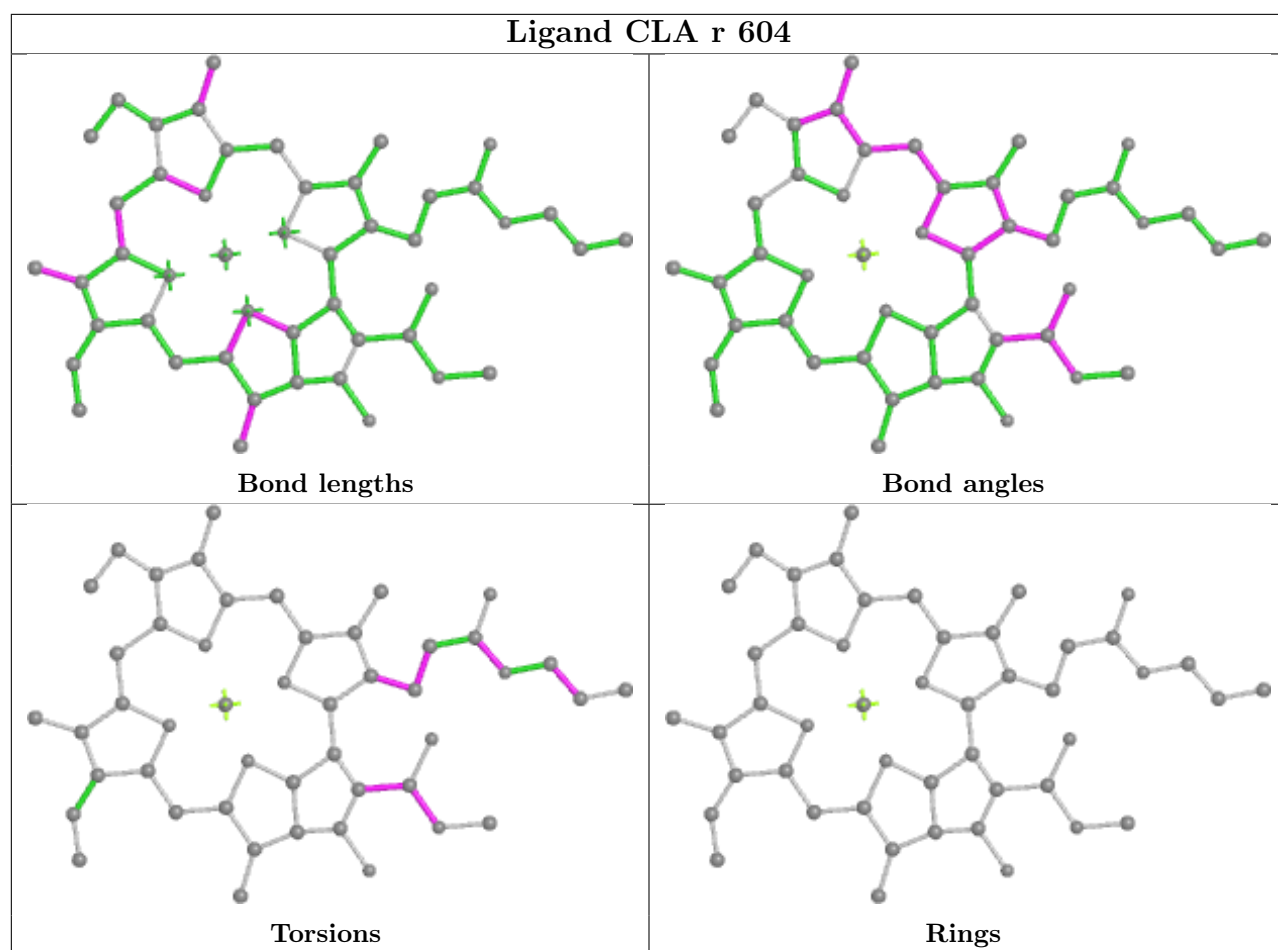


Torsions

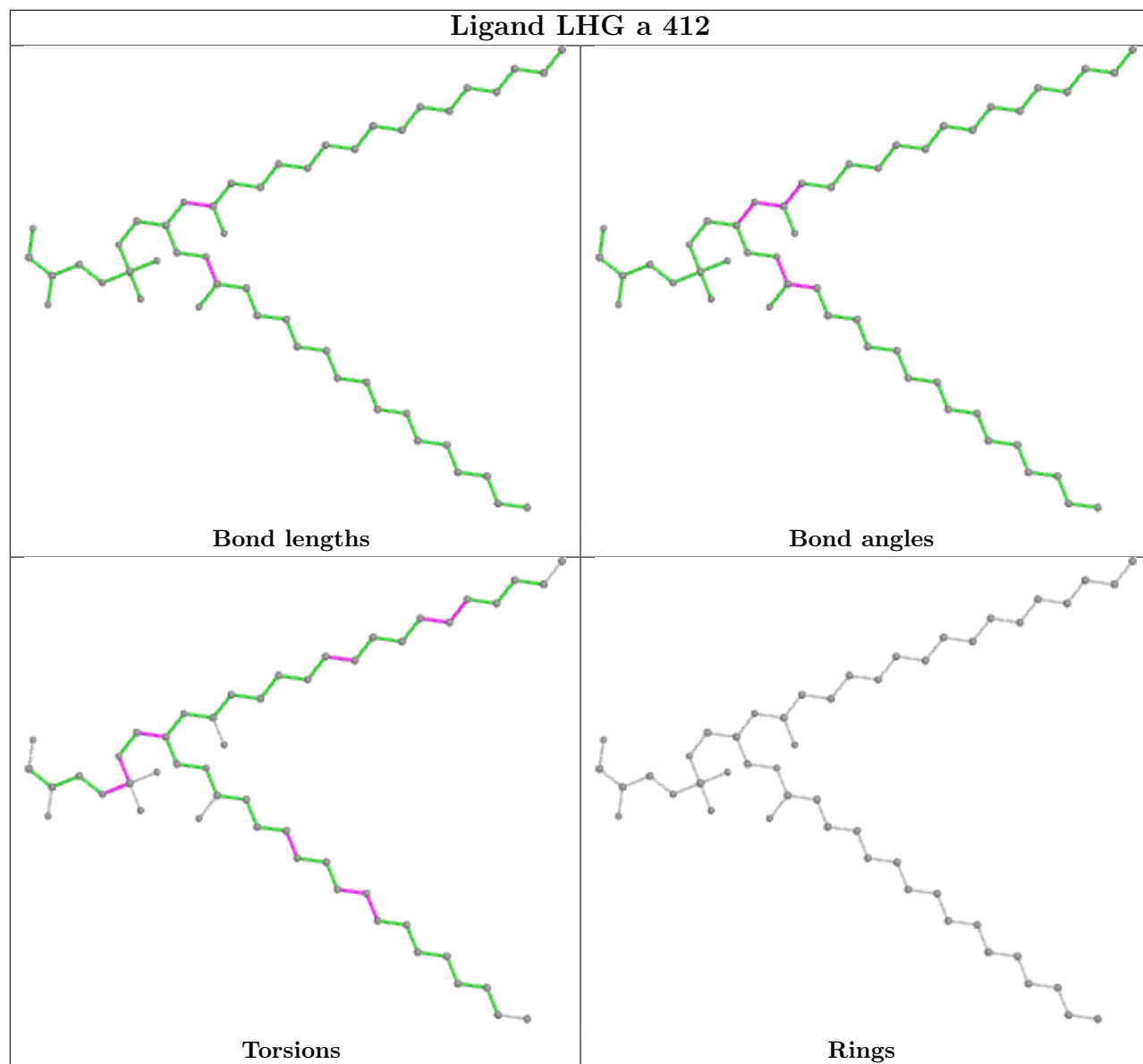


Rings

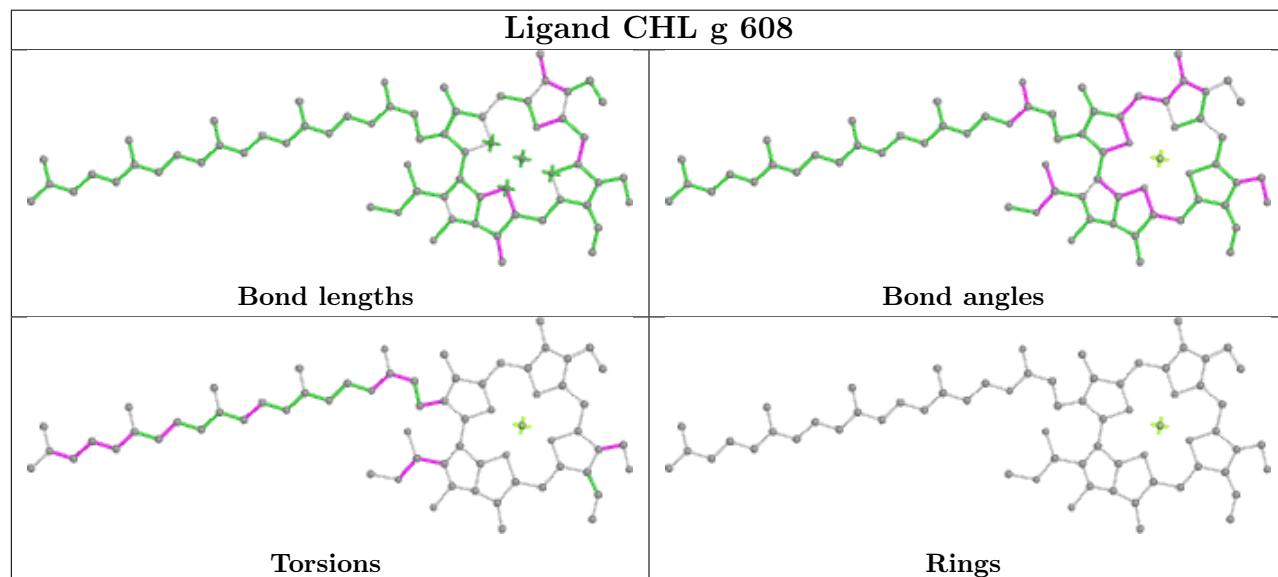




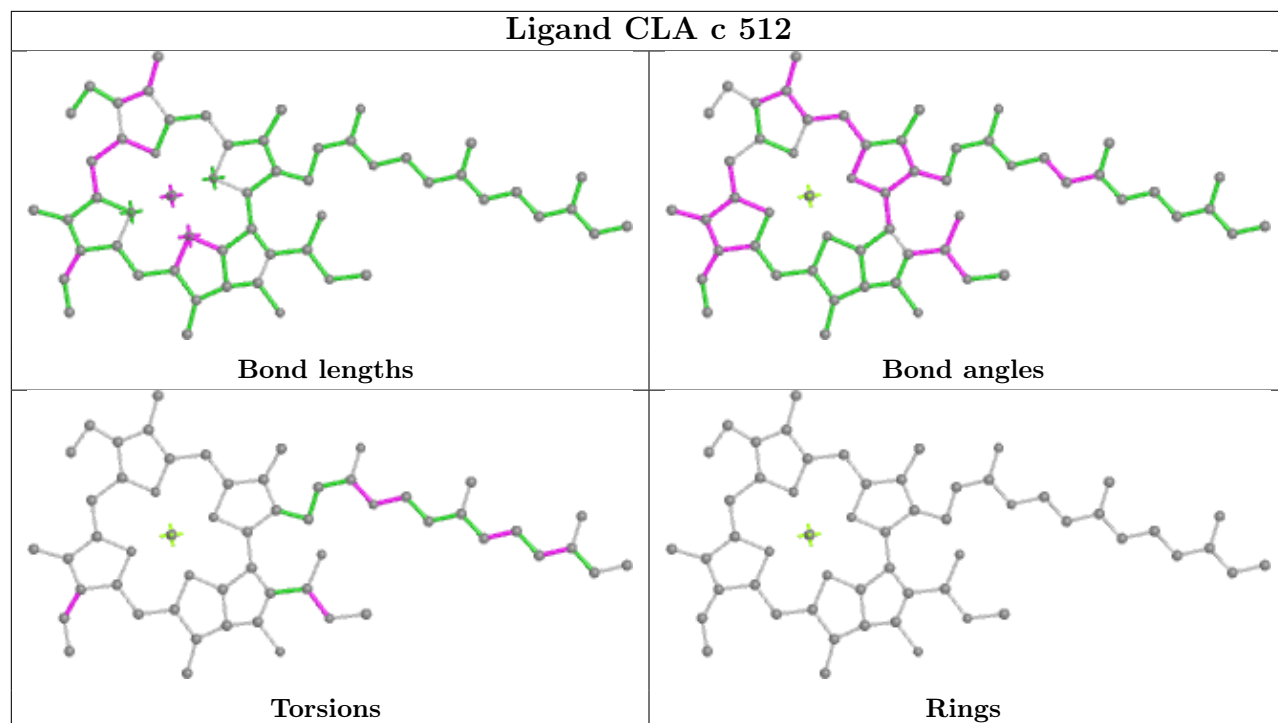
Ligand LHG a 412



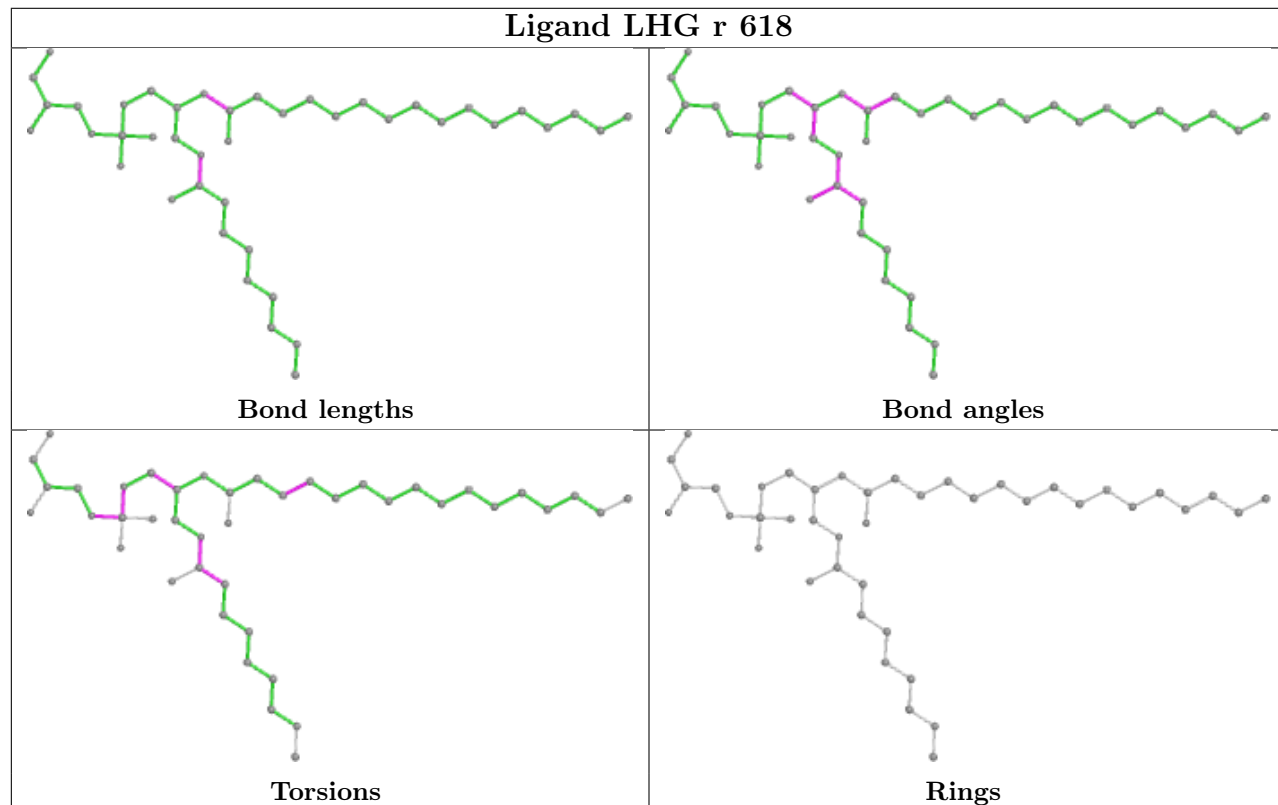
Ligand CHL g 608



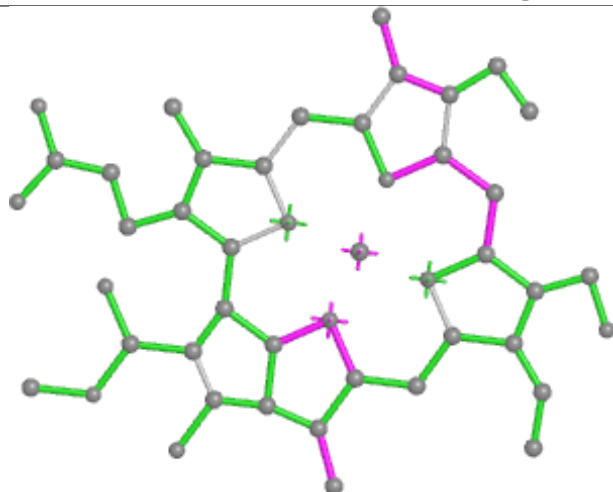
Ligand CLA c 512



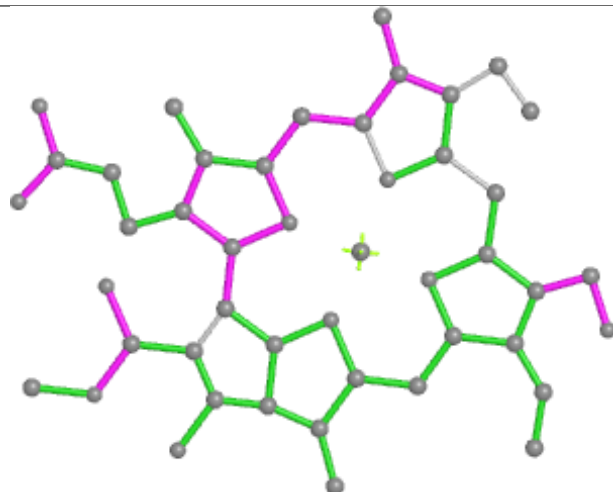
Ligand LHG r 618



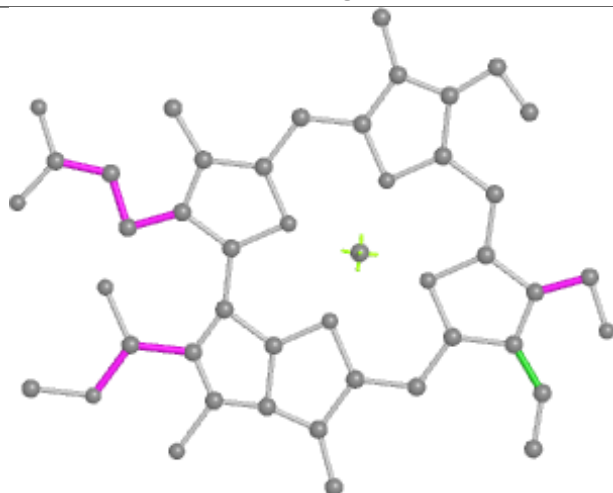
Ligand CHL n 308



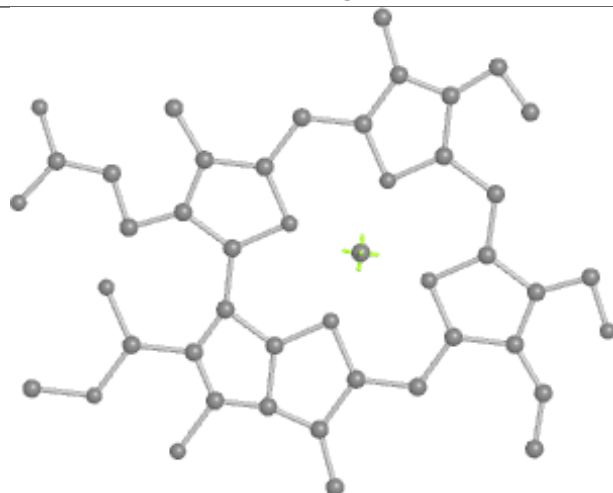
Bond lengths



Bond angles

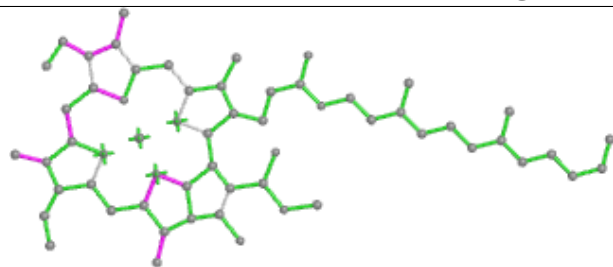


Torsions

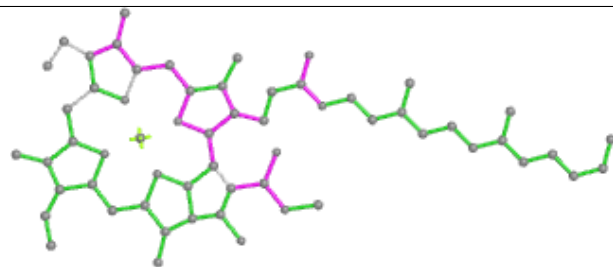


Rings

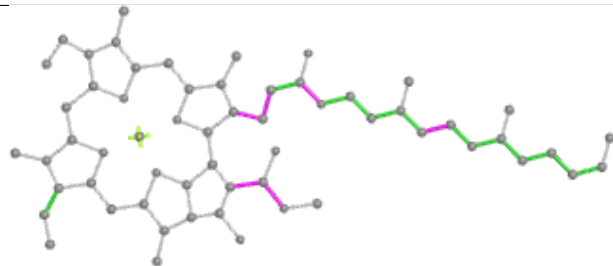
Ligand CLA N 304



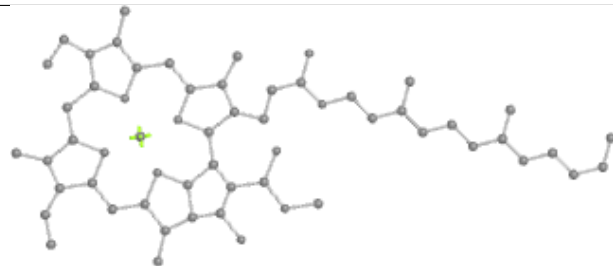
Bond lengths



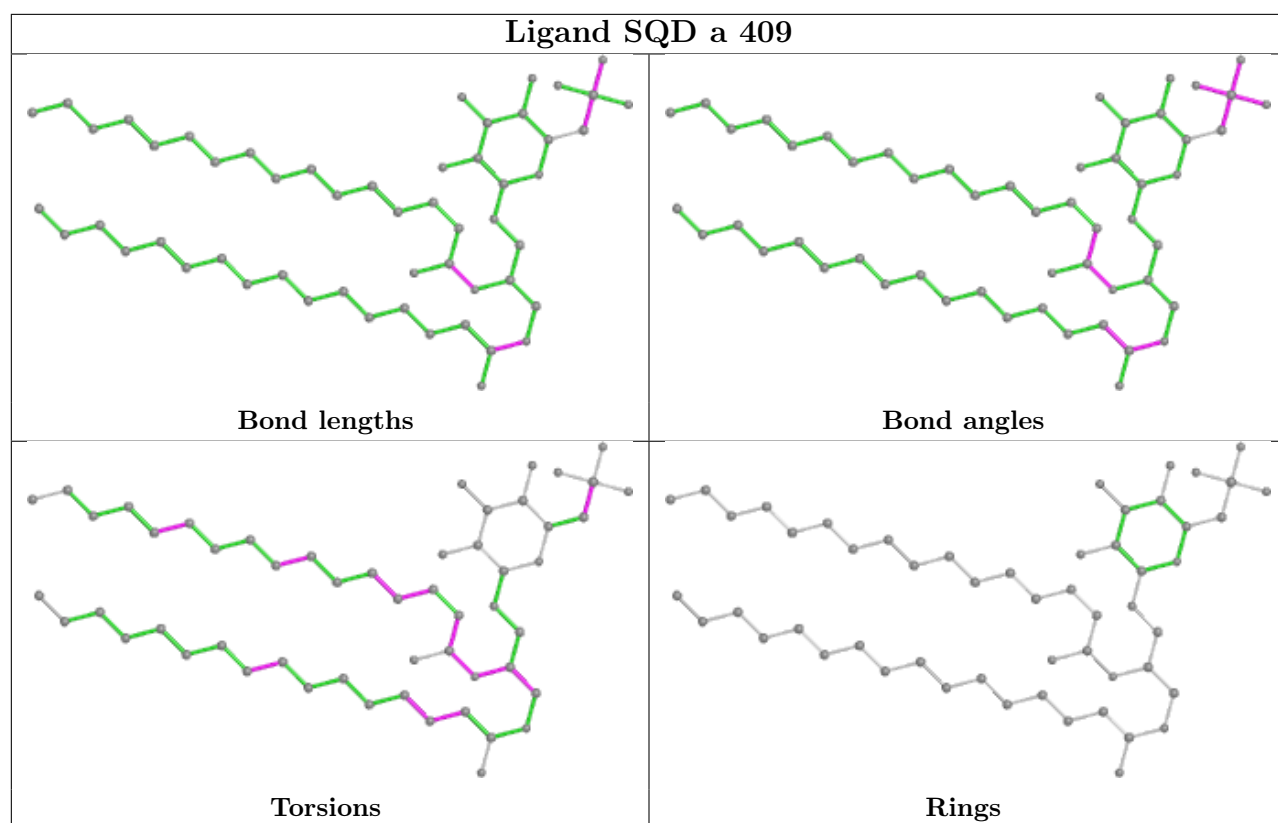
Bond angles



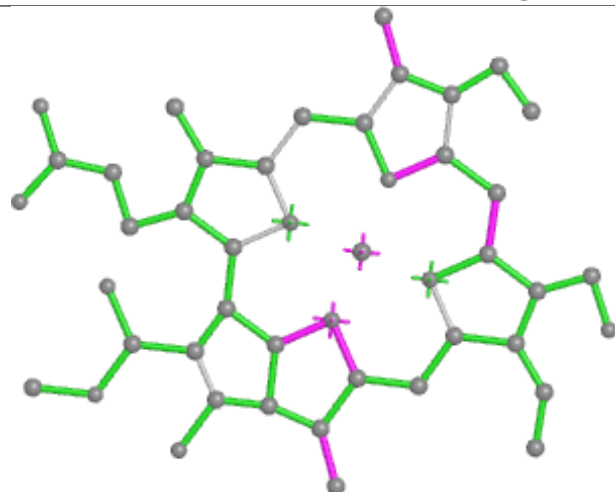
Torsions



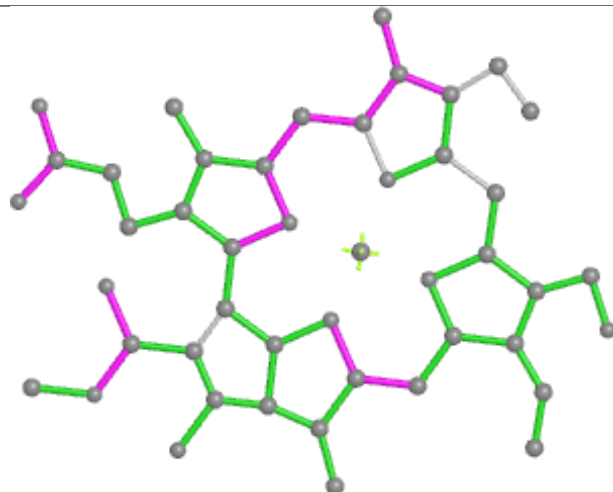
Rings



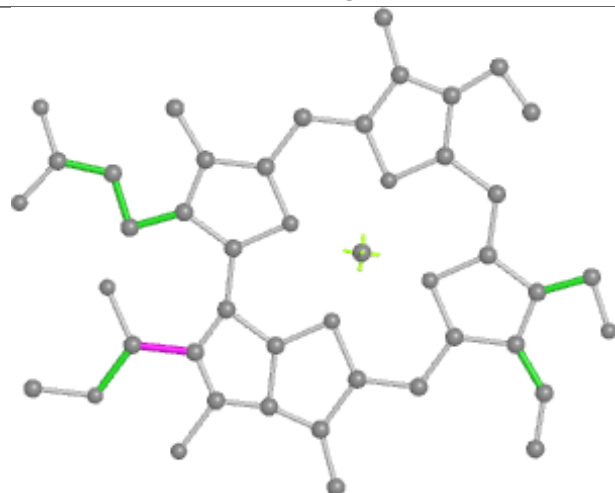
Ligand CHL R 605



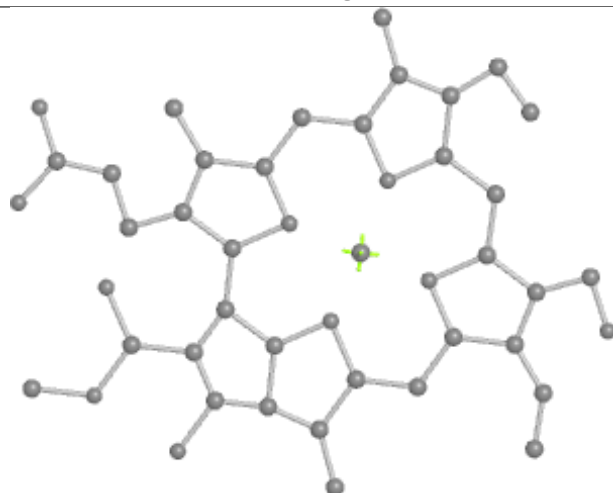
Bond lengths



Bond angles

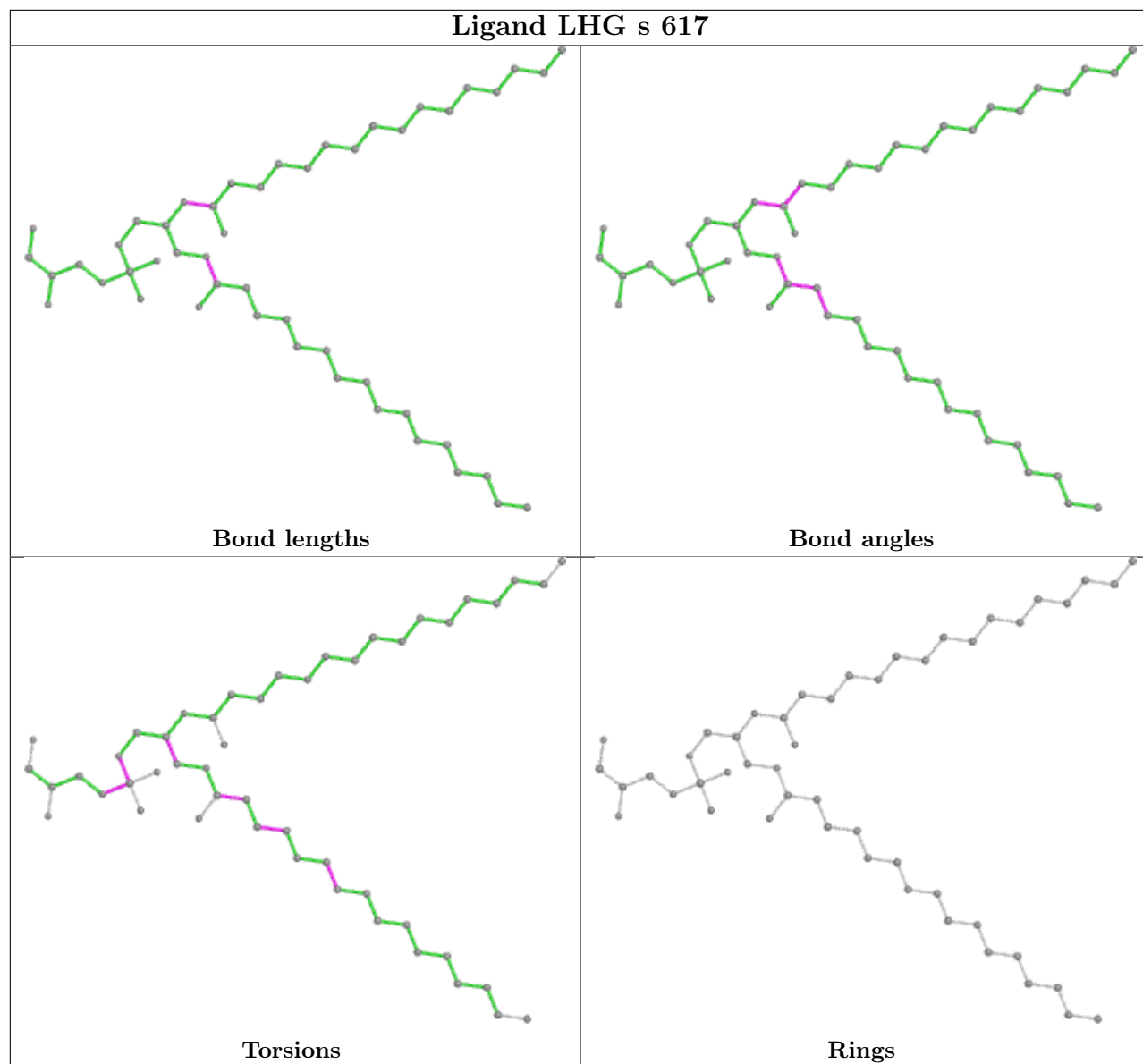


Torsions

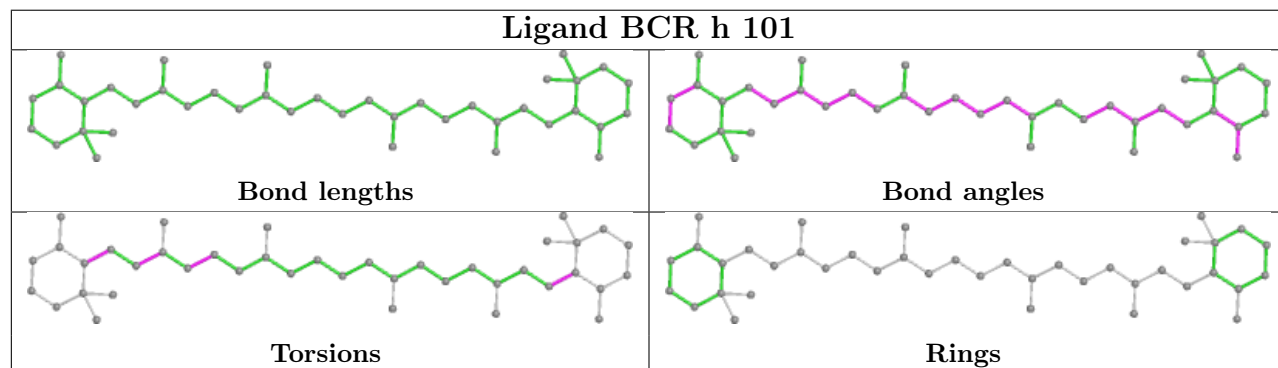


Rings

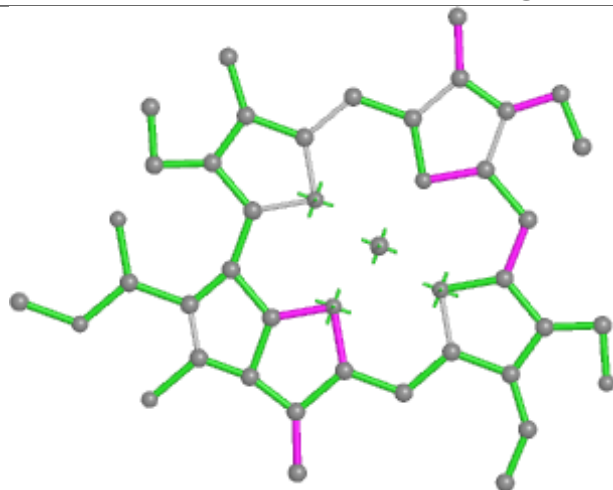
Ligand LHG s 617



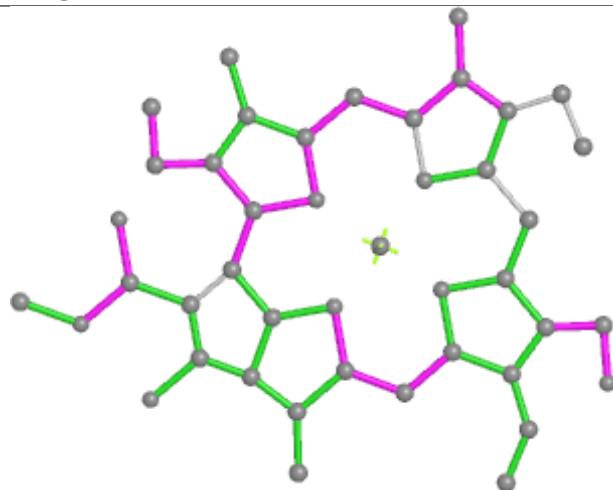
Ligand BCR h 101



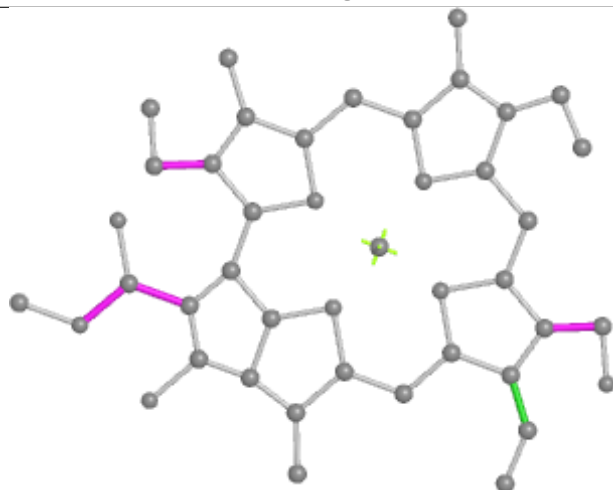
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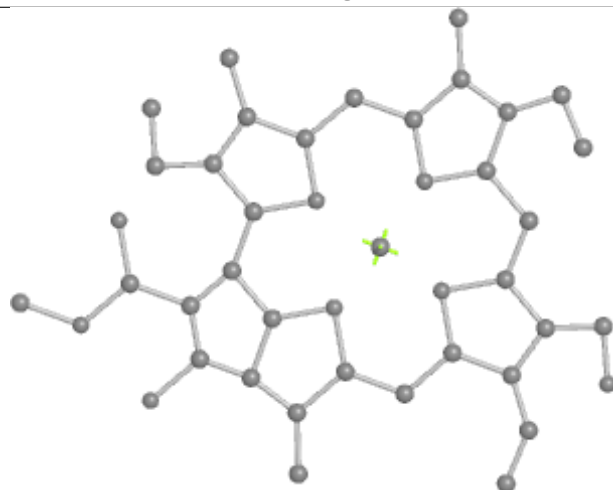
Bond lengths



Bond angles

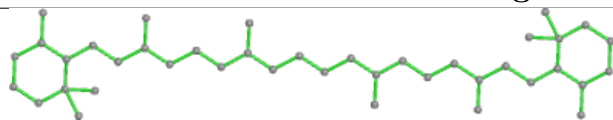


Torsions

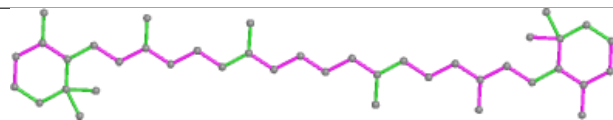


Rings

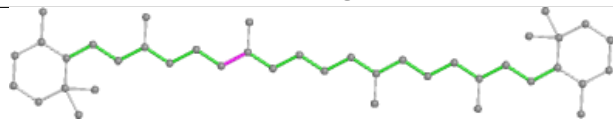
Ligand BCR B 618



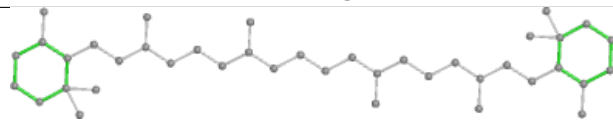
Bond lengths



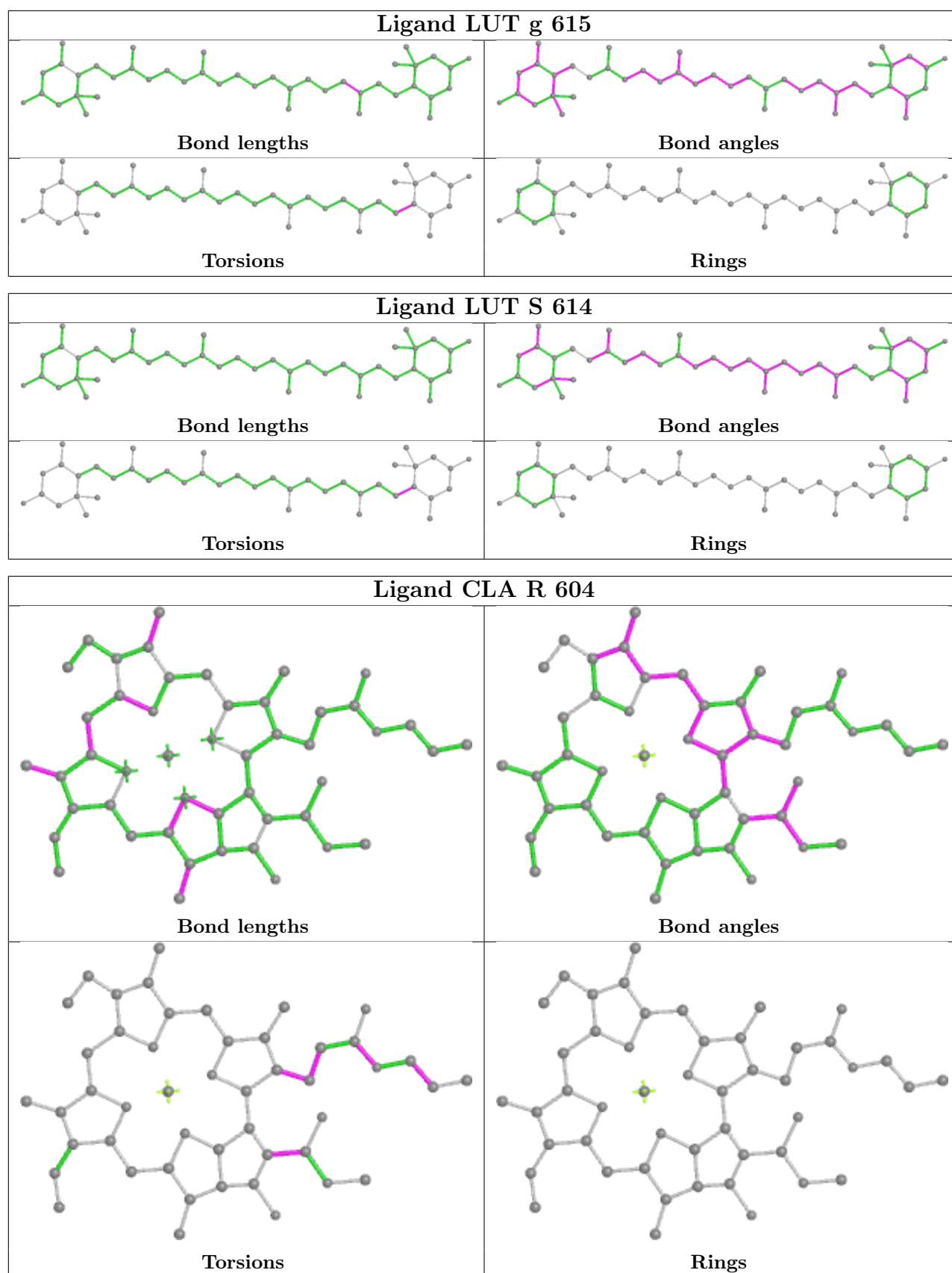
Bond angles



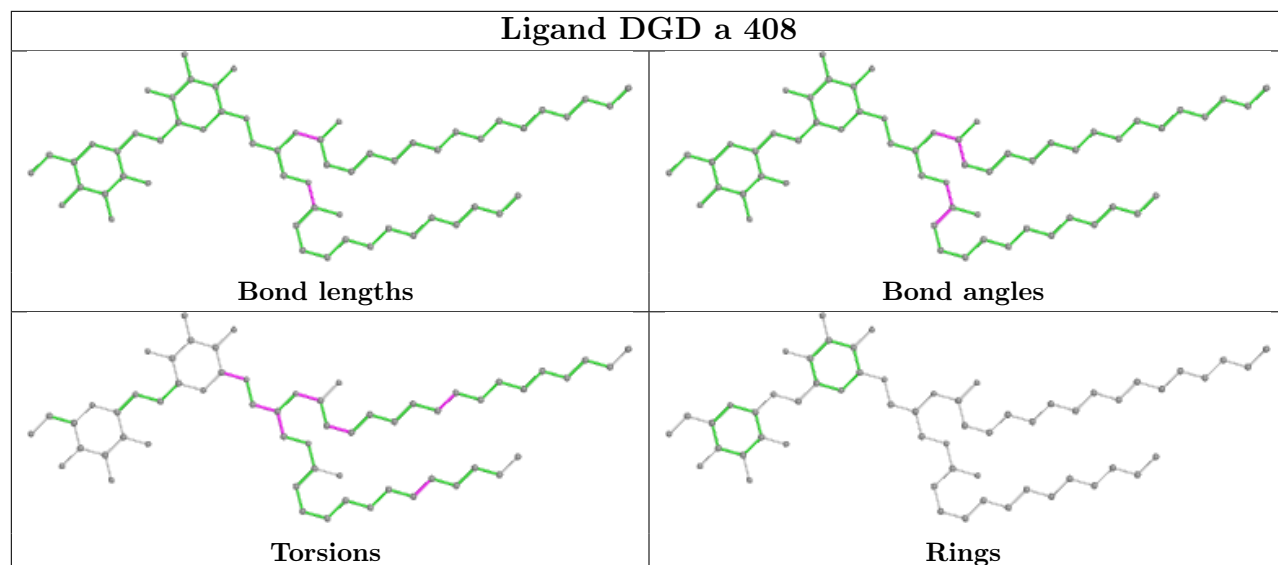
Torsions



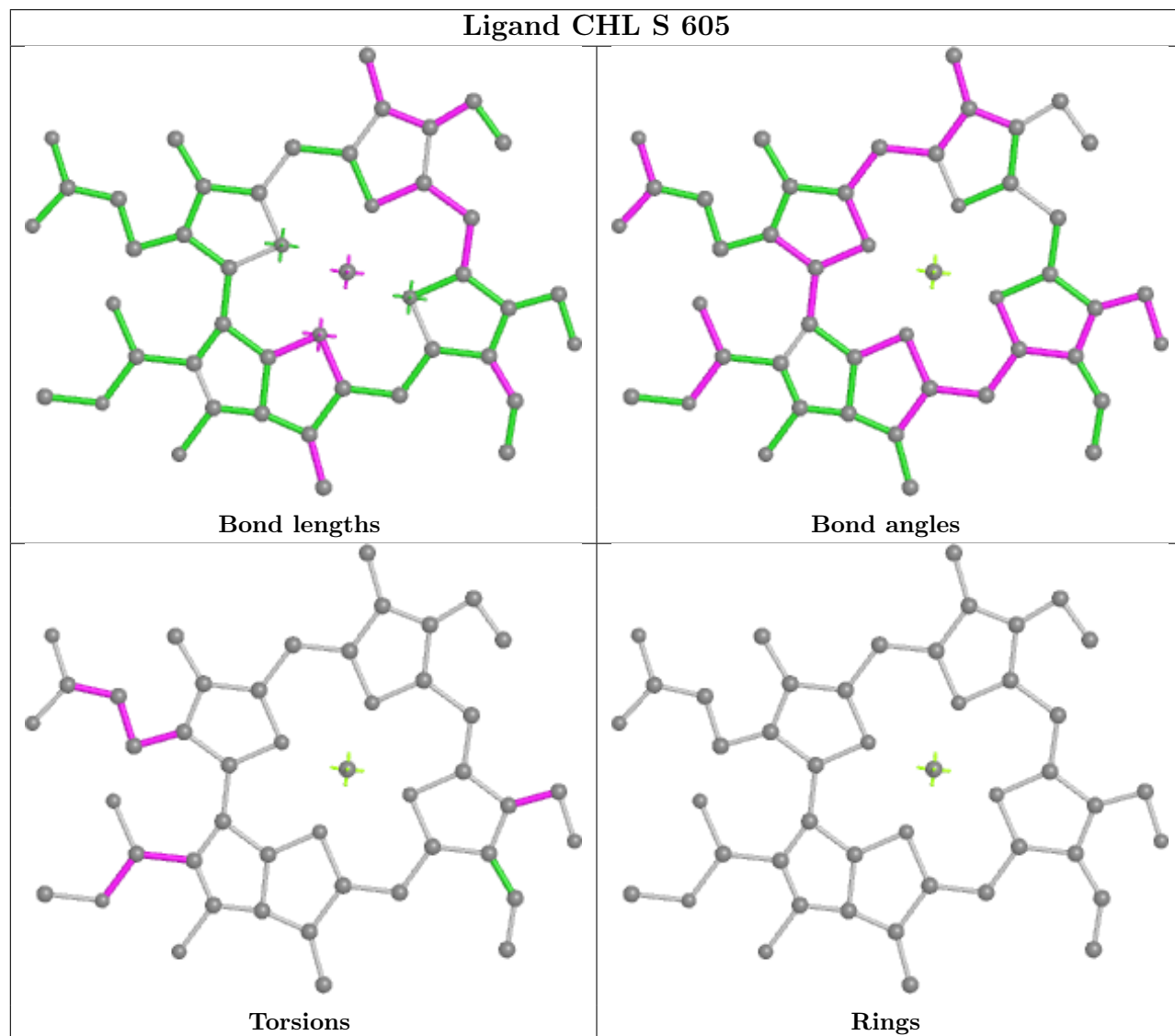
Rings



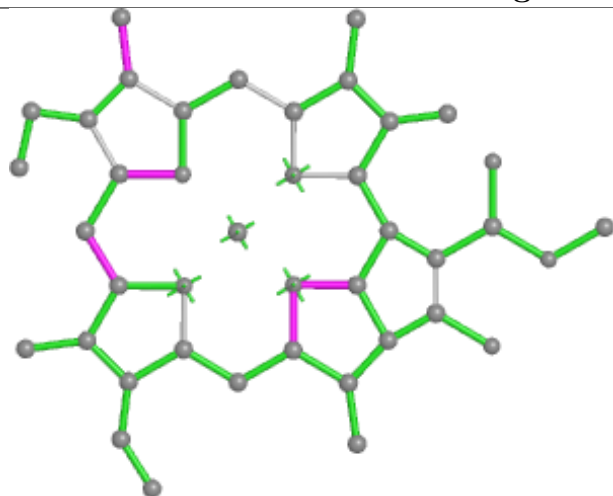
Ligand DGD a 408



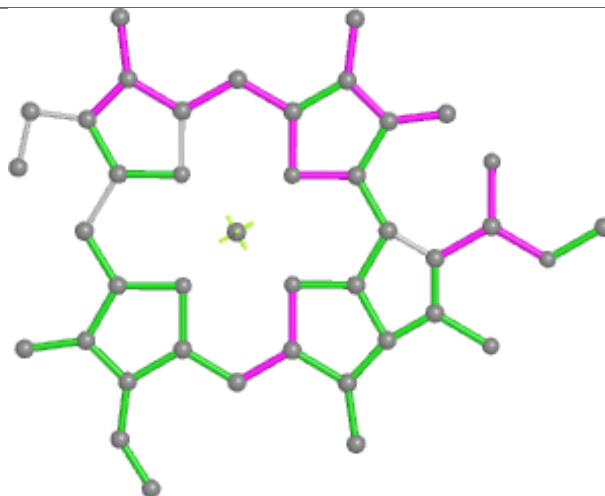
Ligand CHL S 605



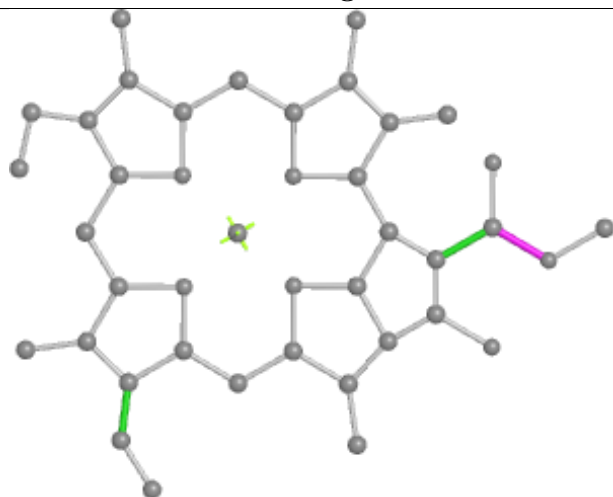
Ligand CLA N 315



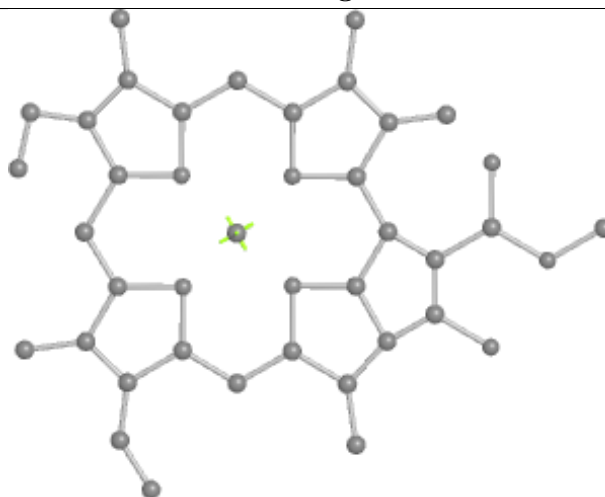
Bond lengths



Bond angles

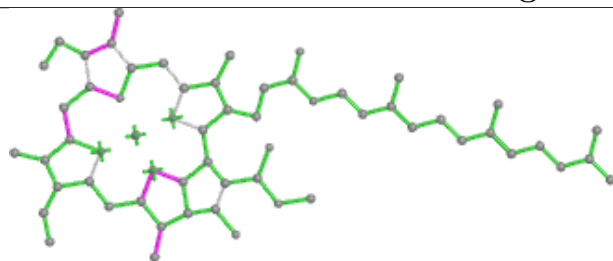


Torsions

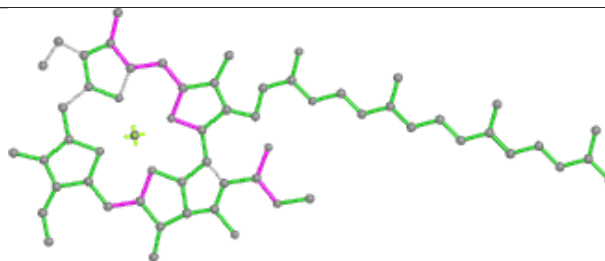


Rings

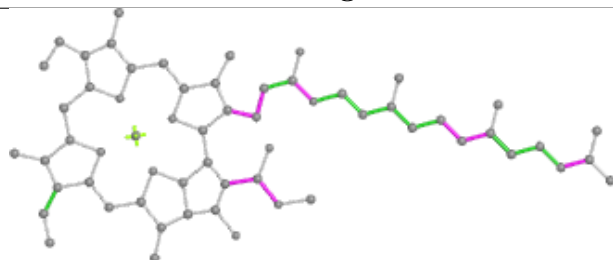
Ligand CLA c 504



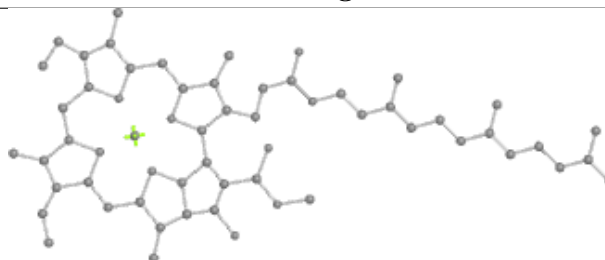
Bond lengths



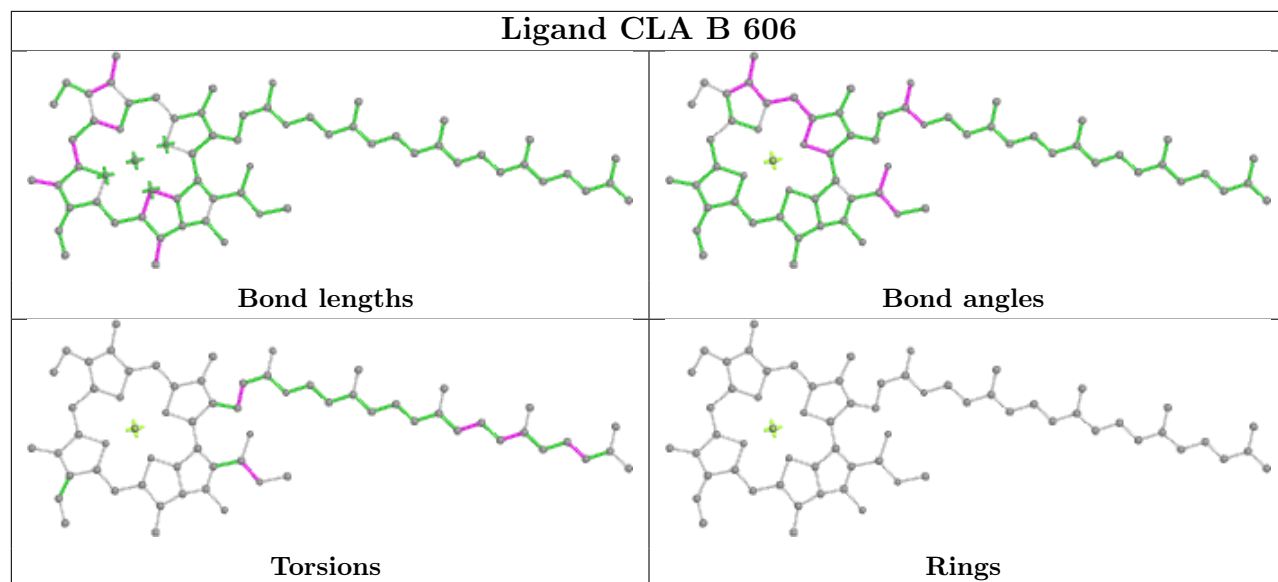
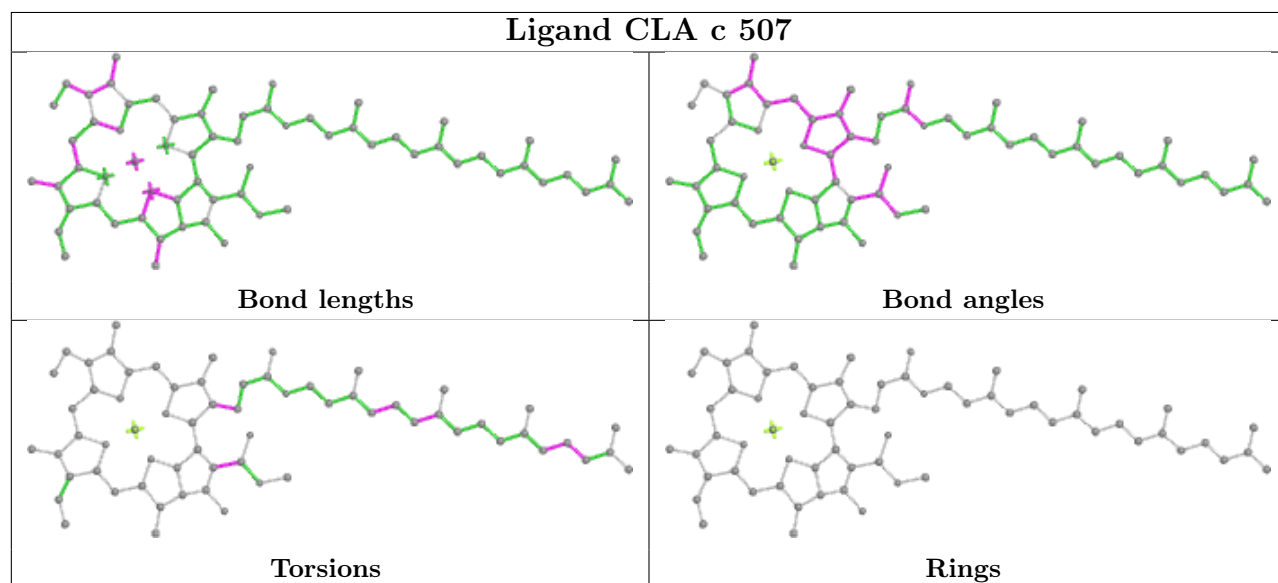
Bond angles



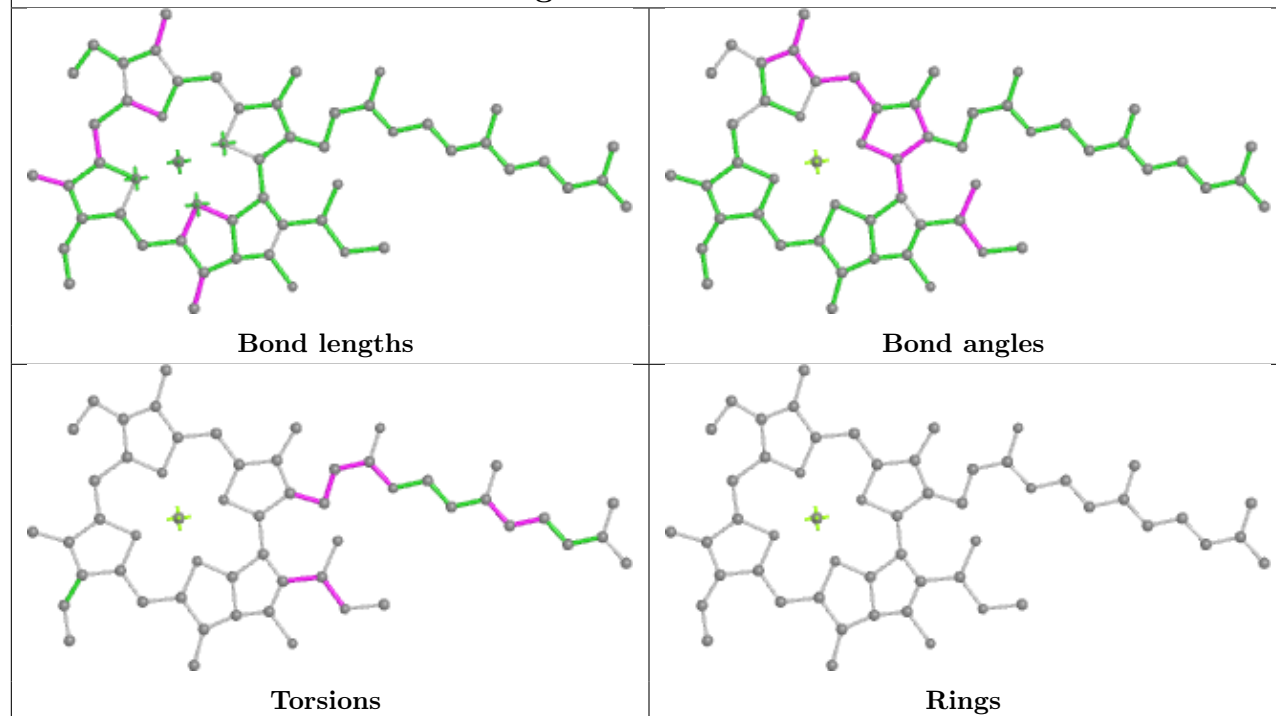
Torsions



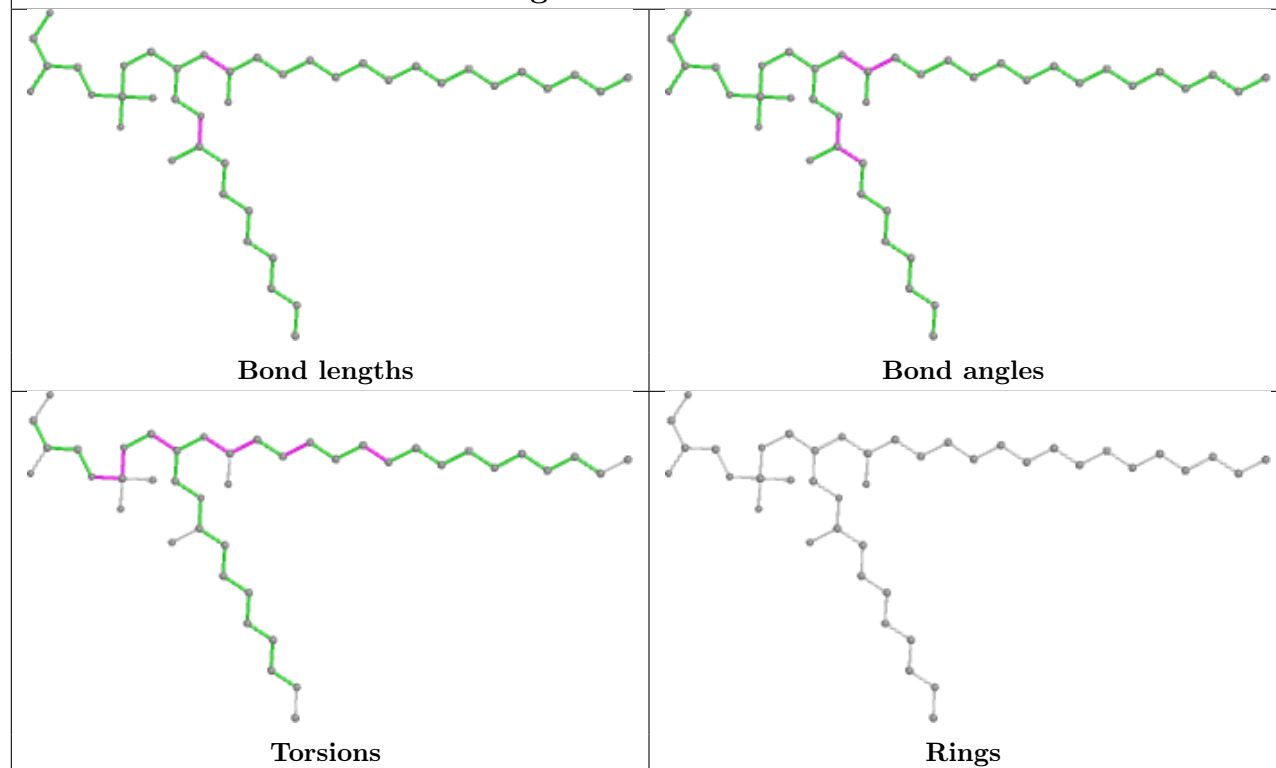
Rings

Ligand CLA B 606**Ligand CLA c 507**

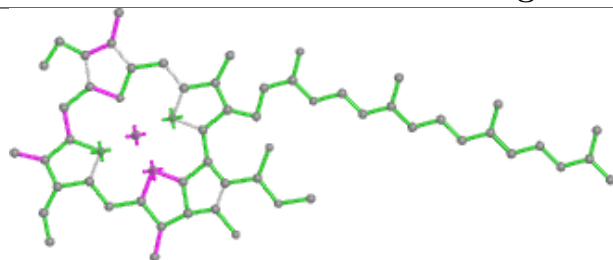
Ligand CLA S 612



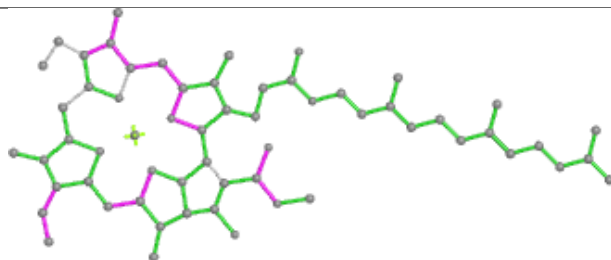
Ligand LHG R 618



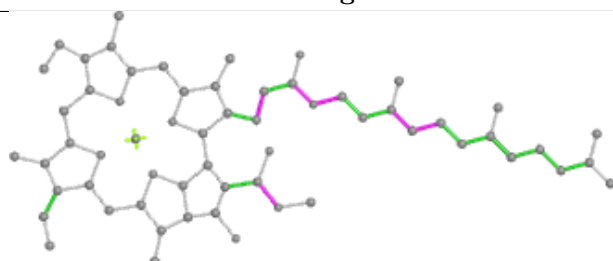
Ligand CLA n 312



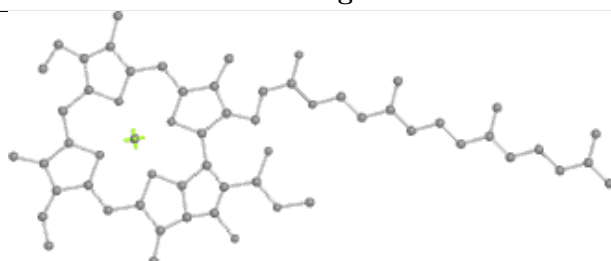
Bond lengths



Bond angles

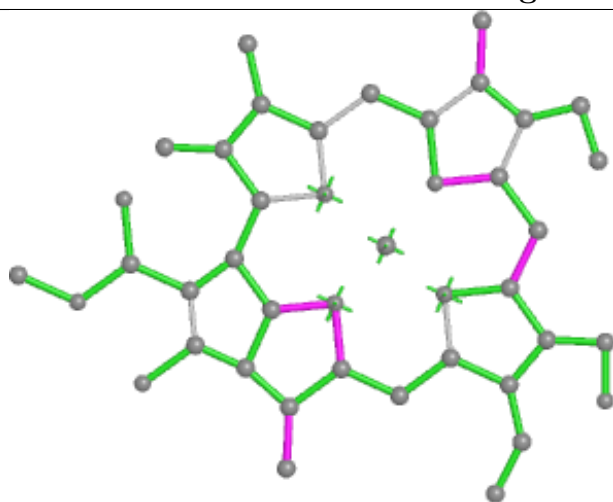


Torsions

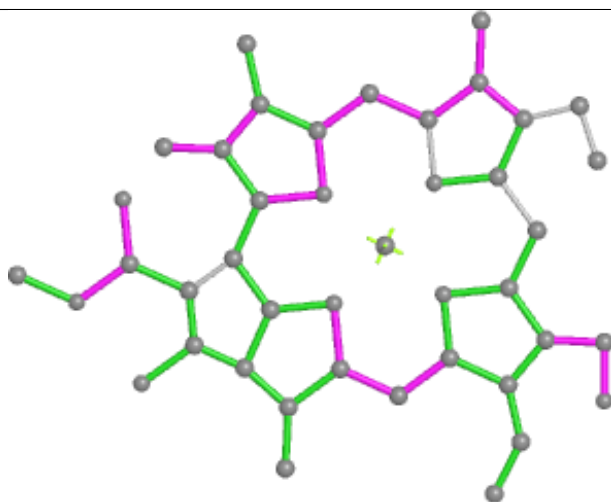


Rings

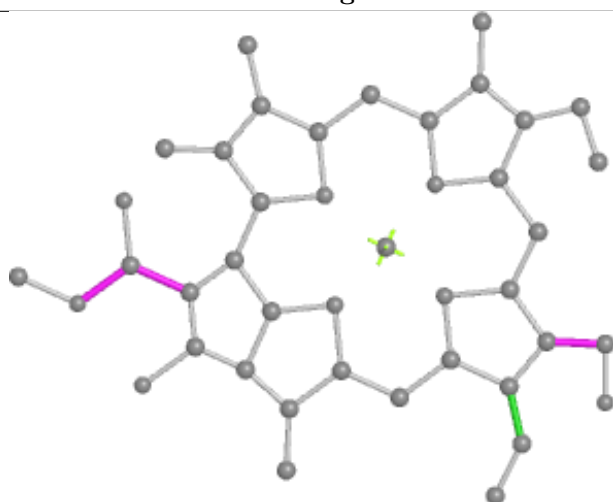
Ligand CHL r 613



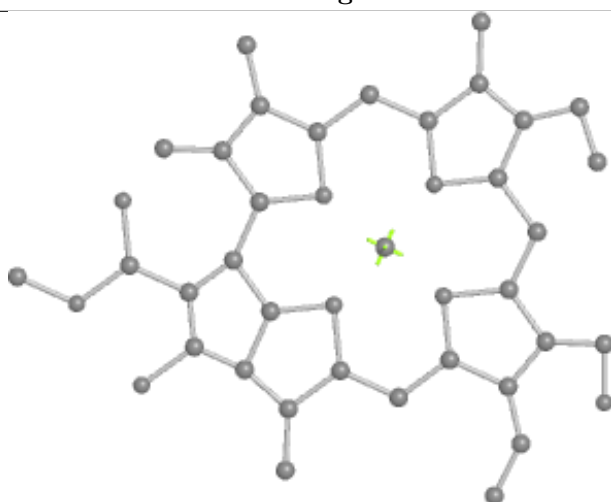
Bond lengths



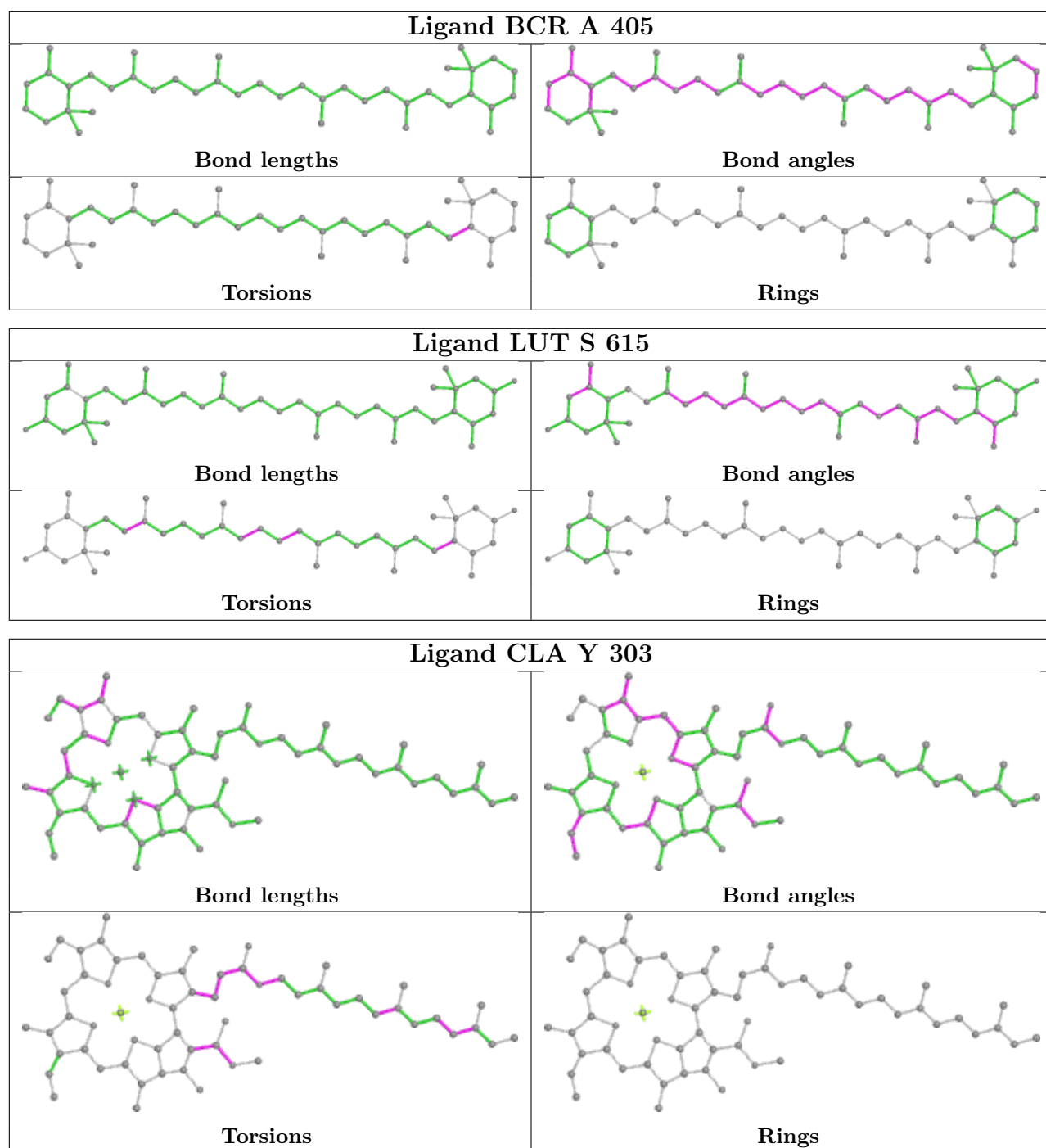
Bond angles

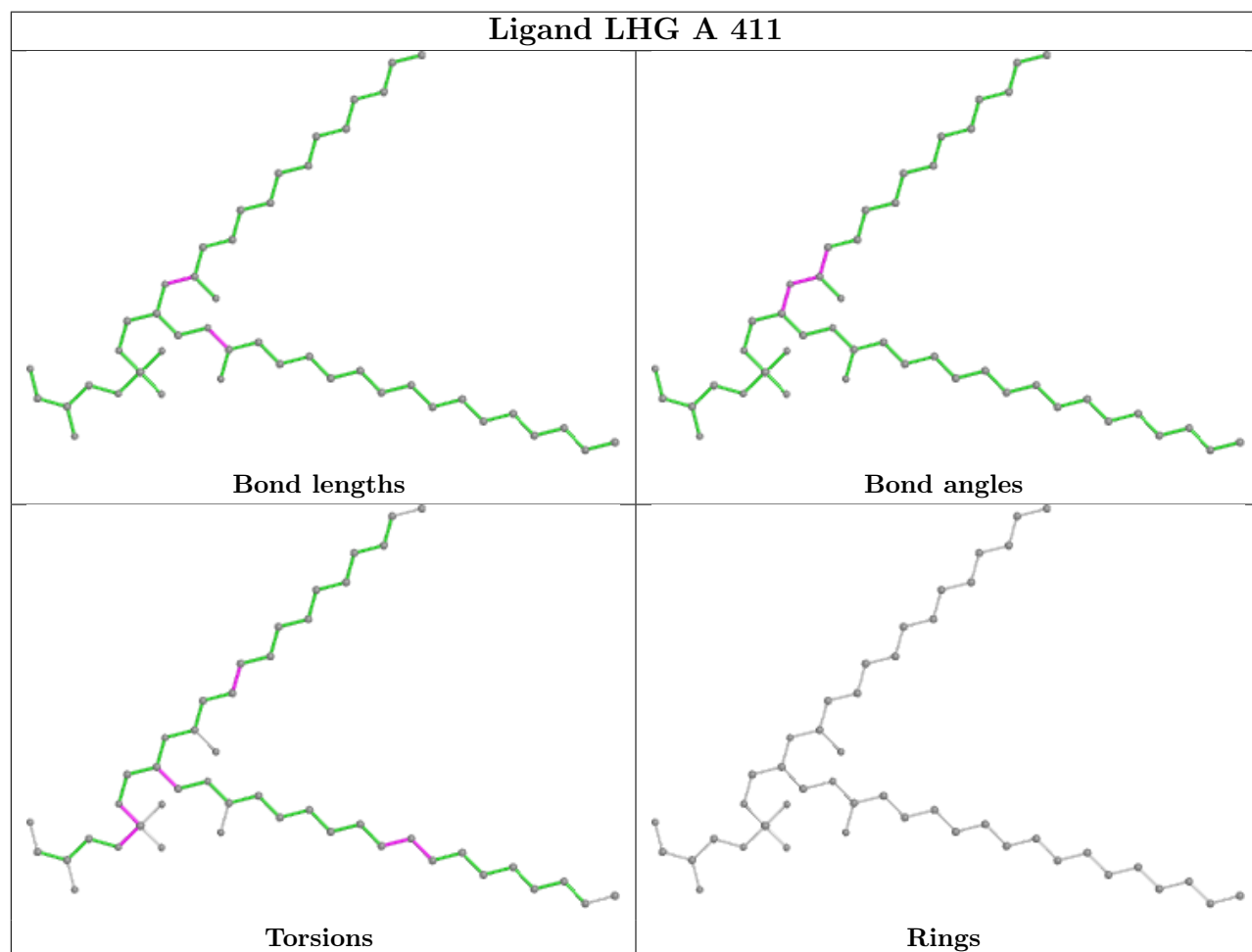
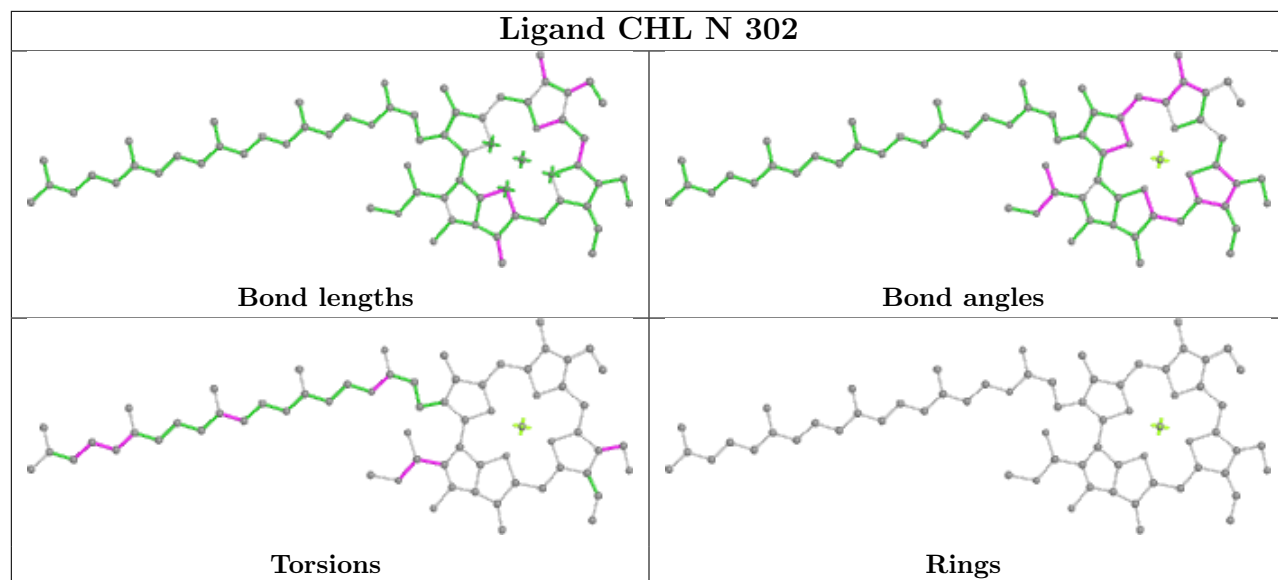


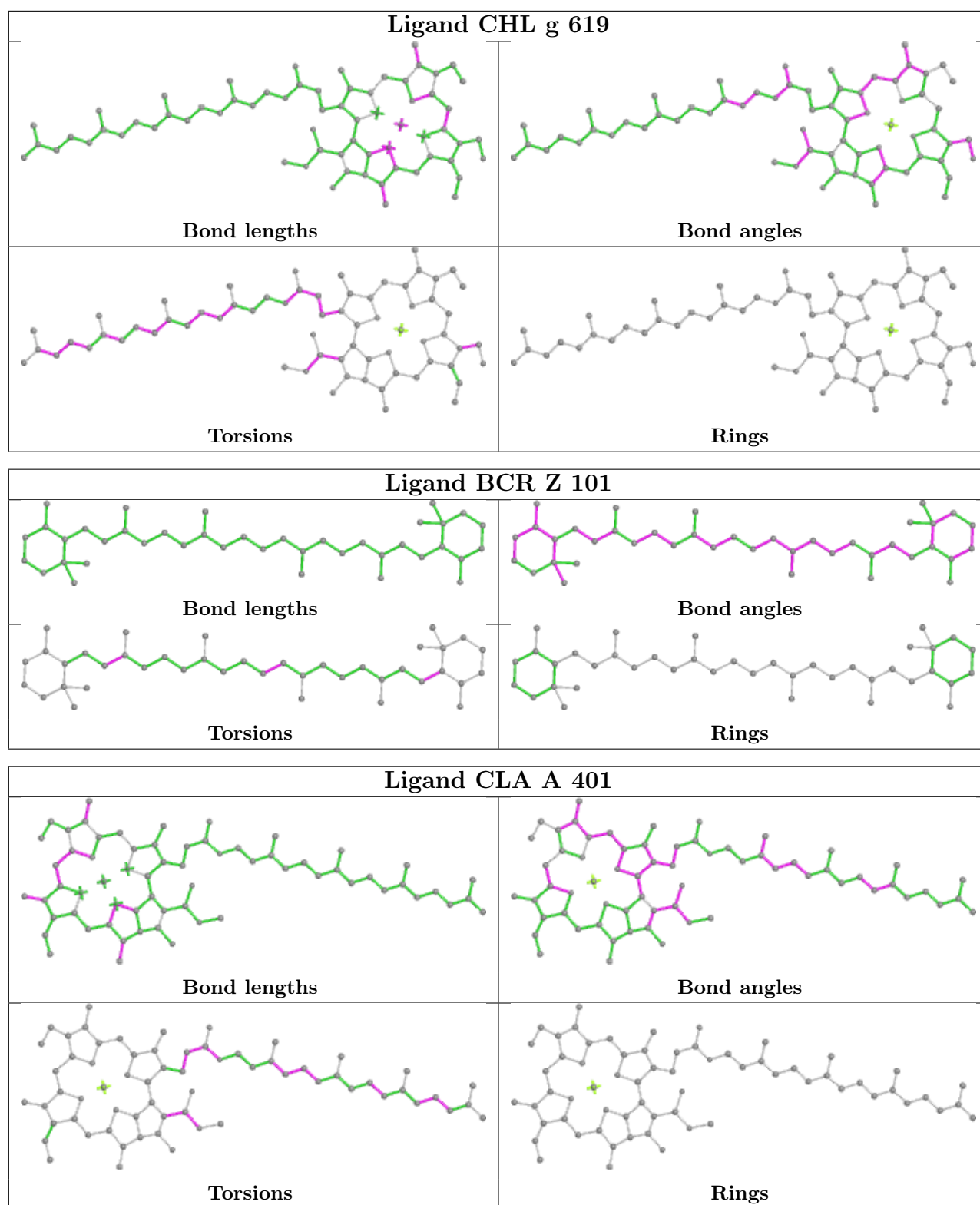
Torsions



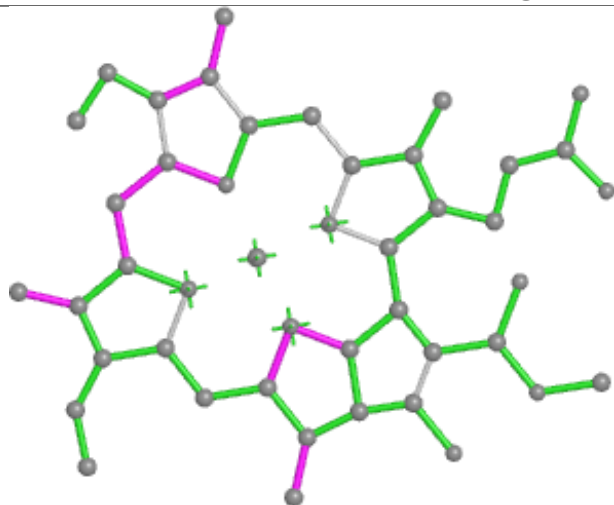
Rings



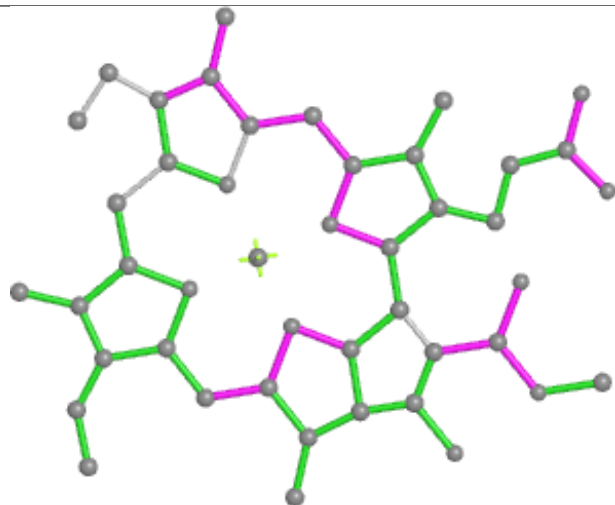




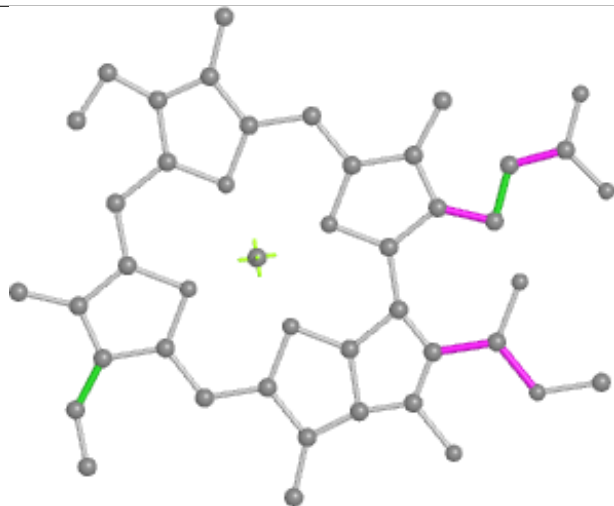
Ligand CLA S 609



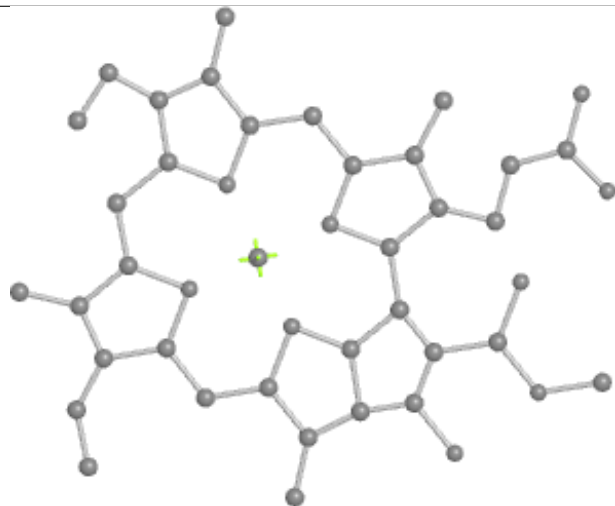
Bond lengths



Bond angles

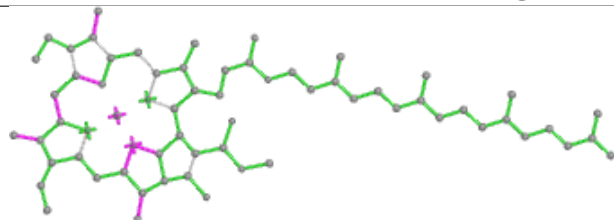


Torsions

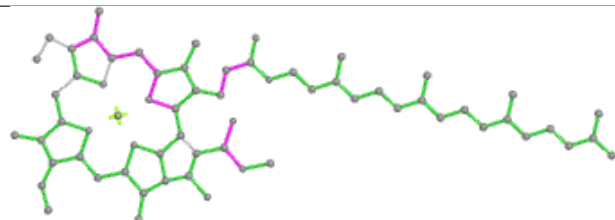


Rings

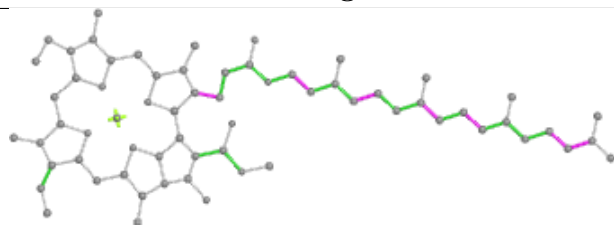
Ligand CLA D 404



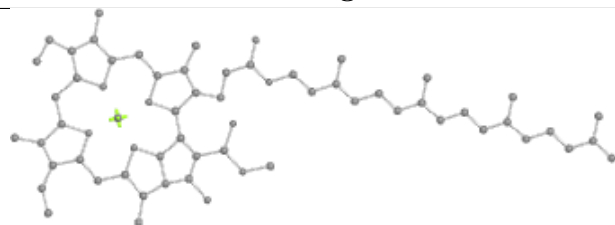
Bond lengths



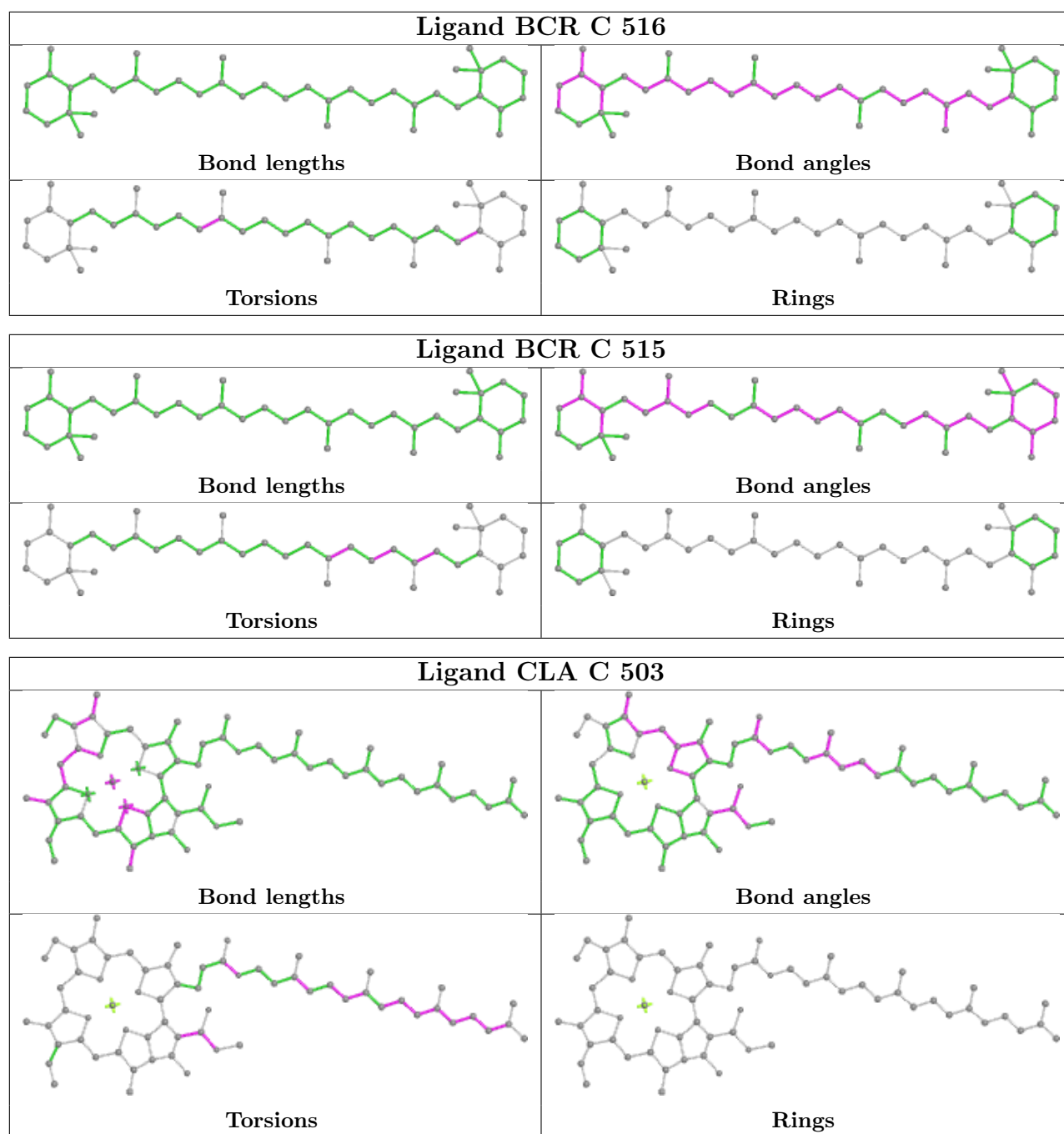
Bond angles

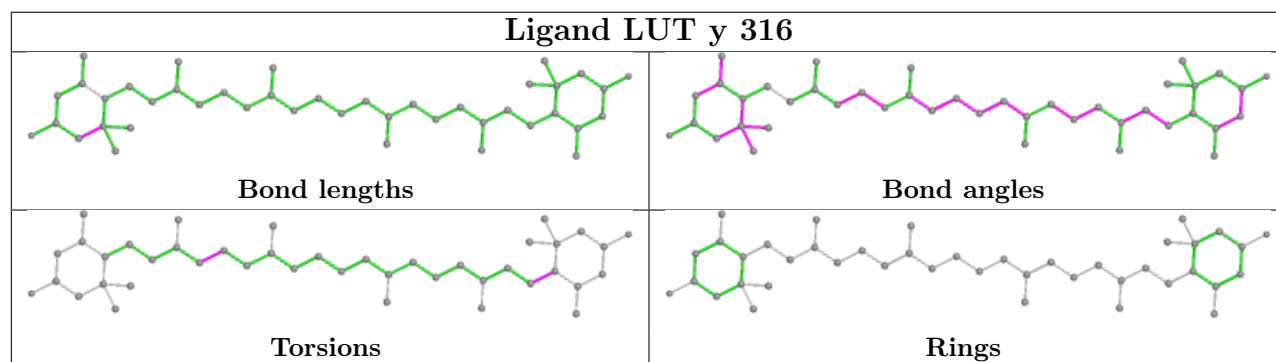
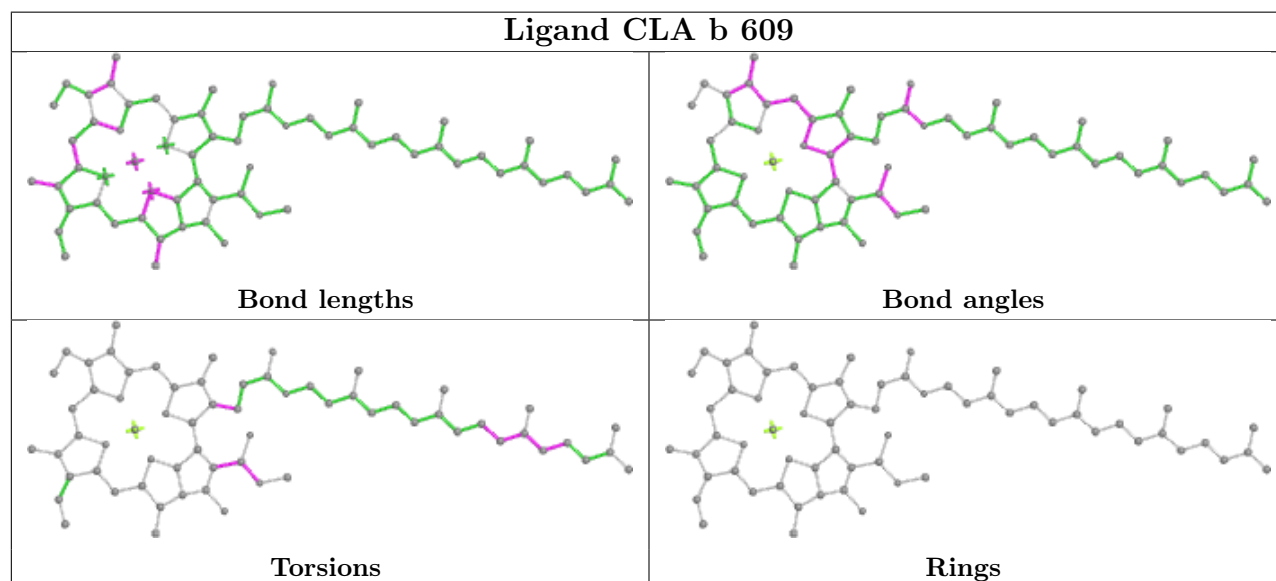
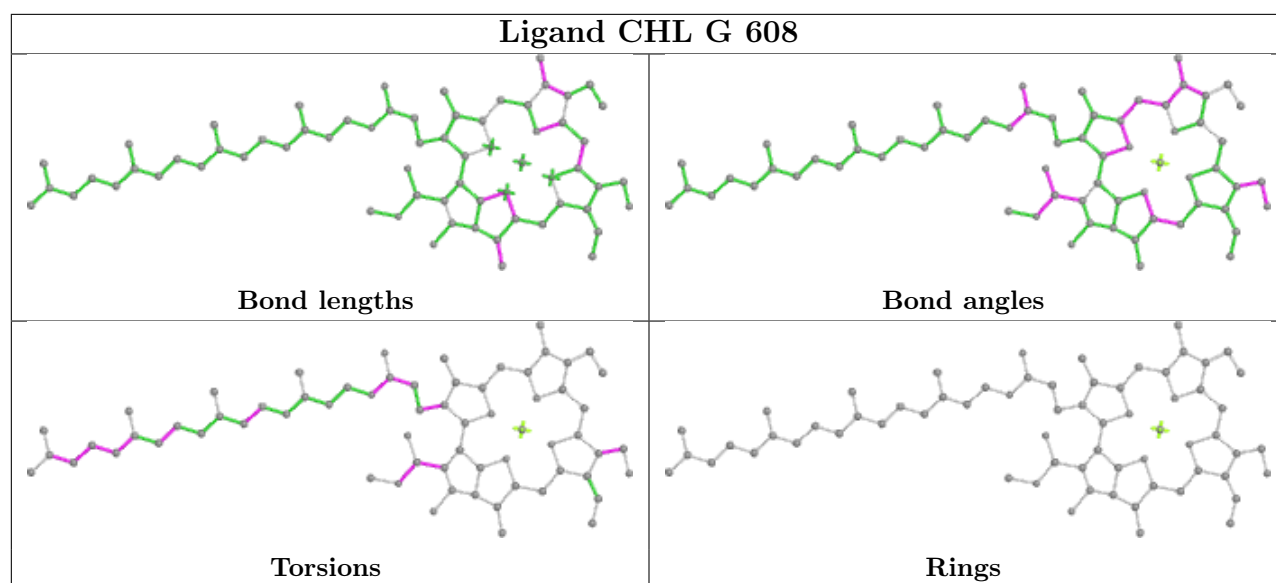


Torsions

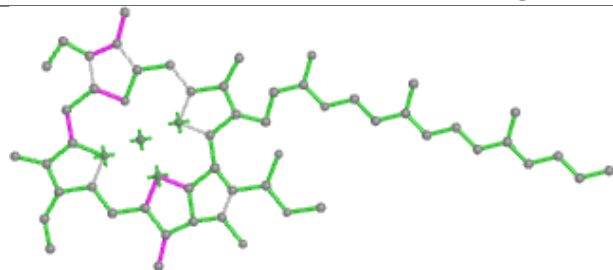


Rings

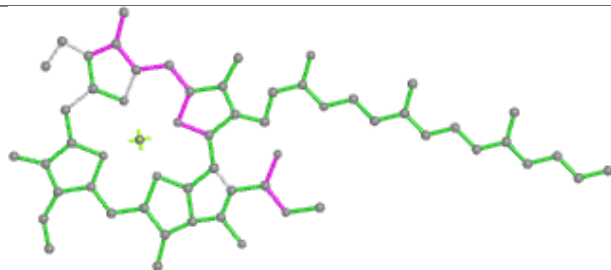




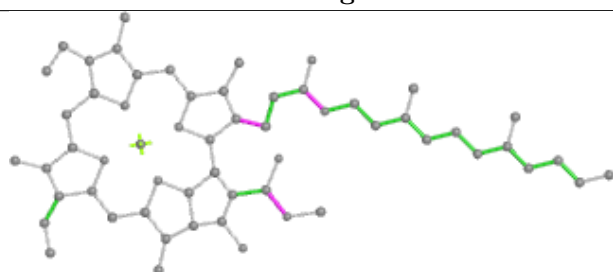
Ligand CLA R 608



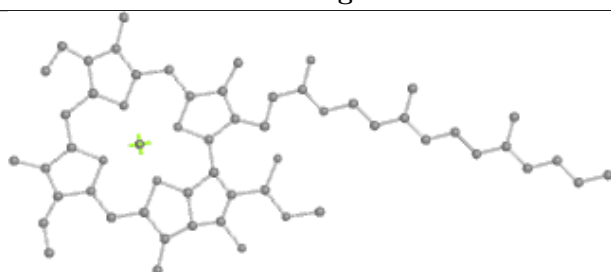
Bond lengths



Bond angles

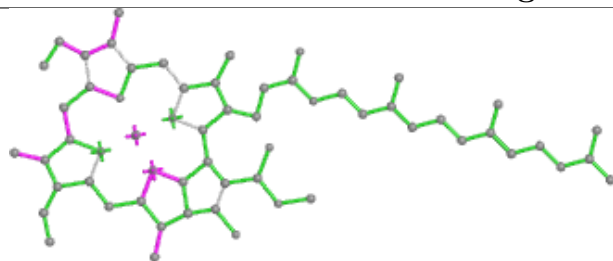


Torsions

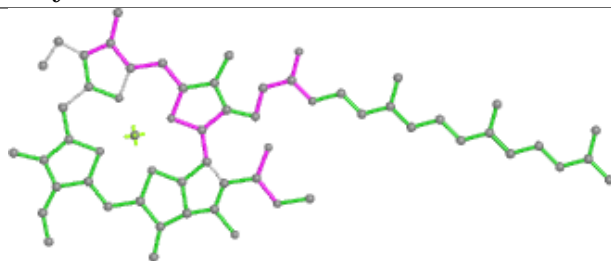


Rings

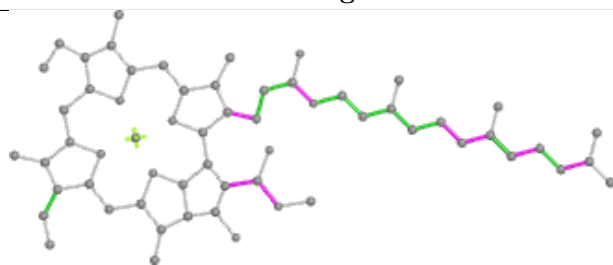
Ligand CLA y 311



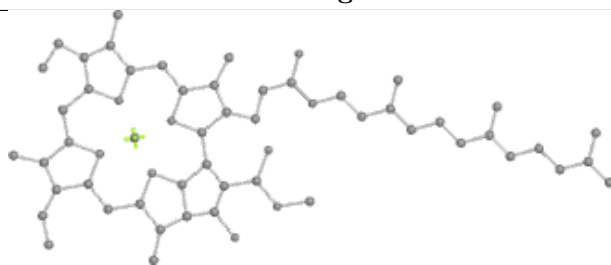
Bond lengths



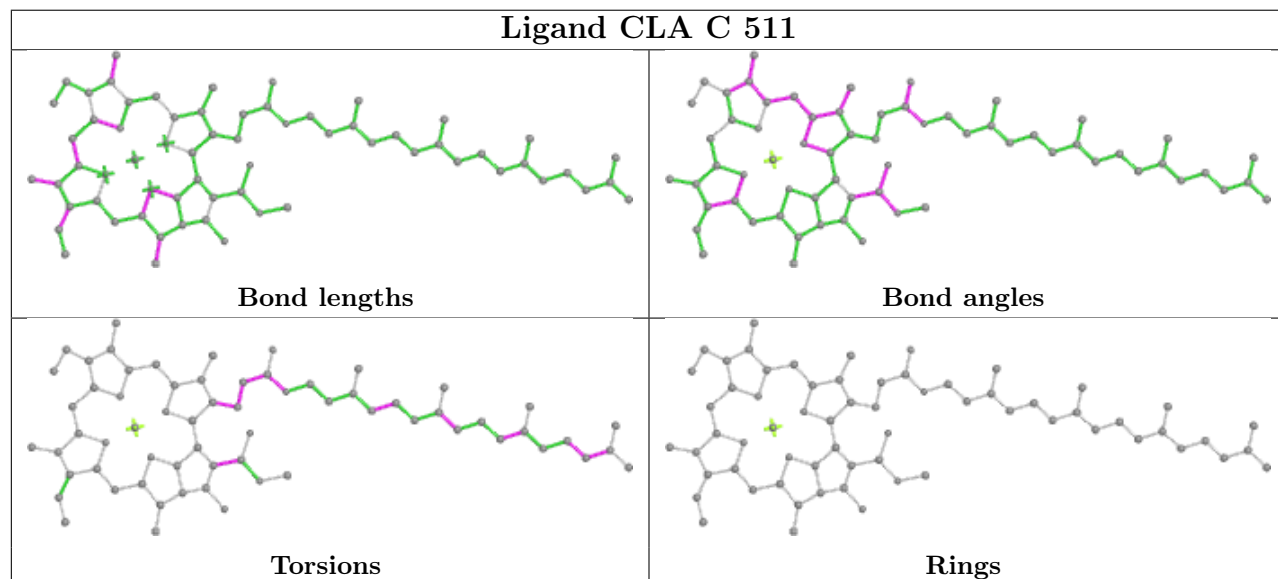
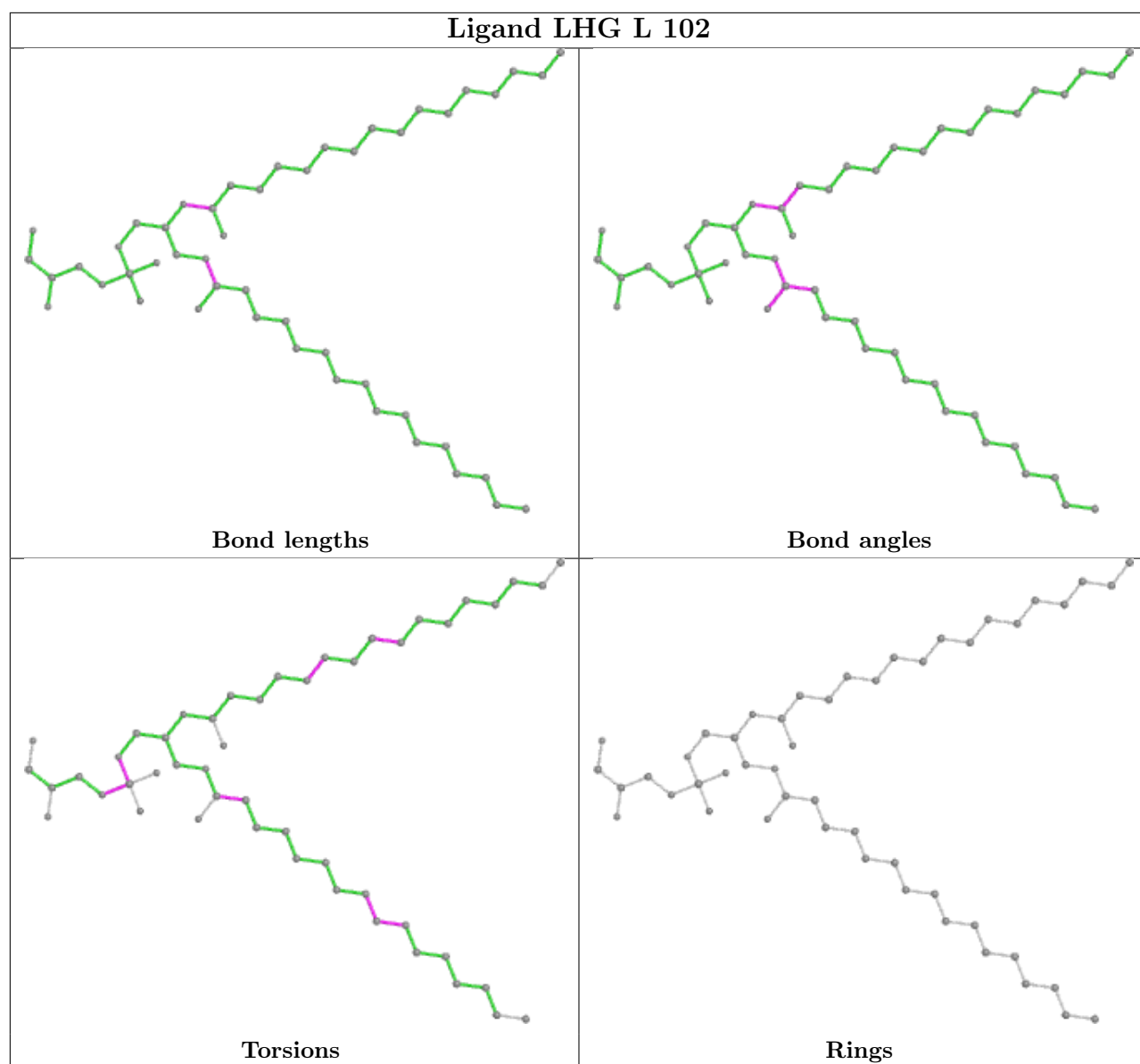
Bond angles

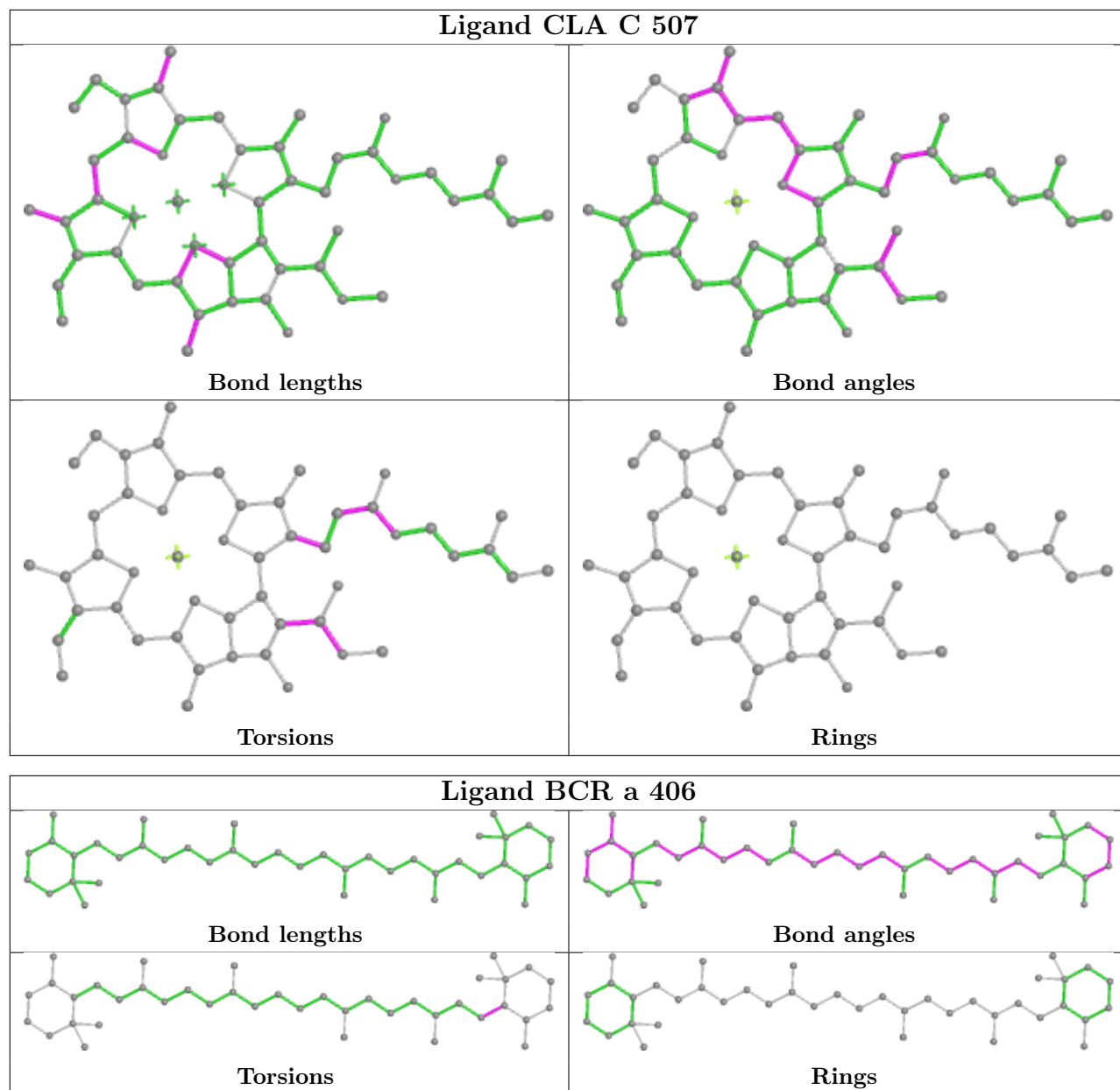


Torsions

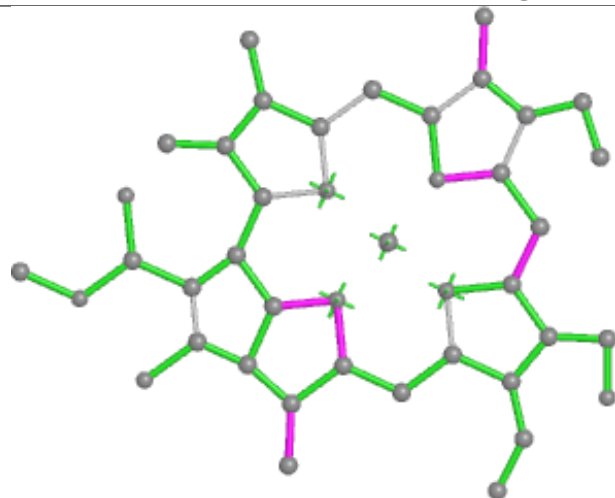


Rings

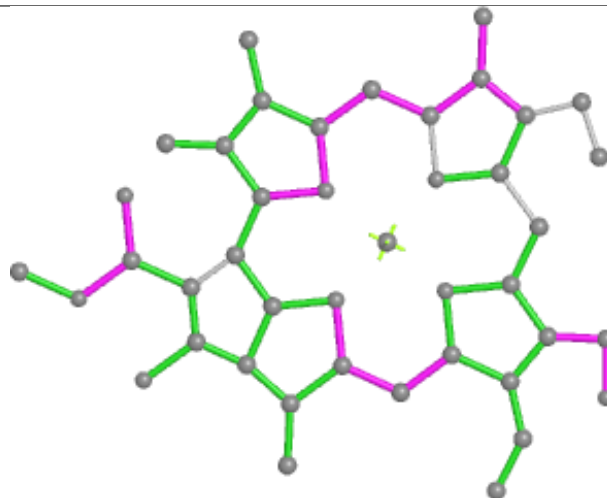




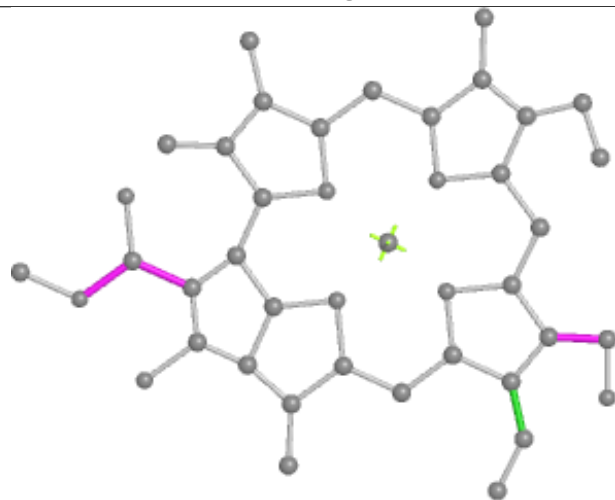
Ligand CHL R 613



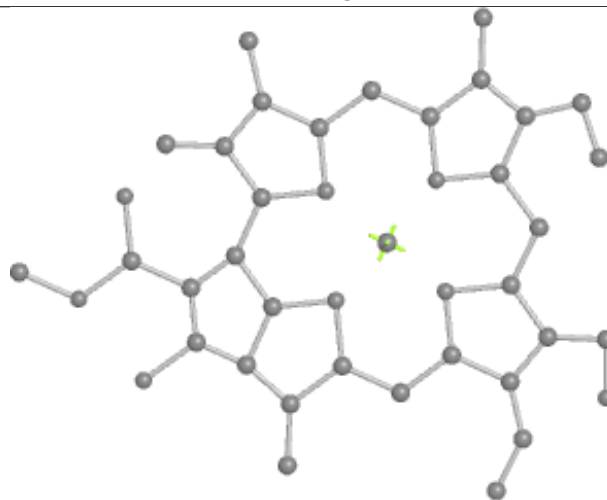
Bond lengths



Bond angles

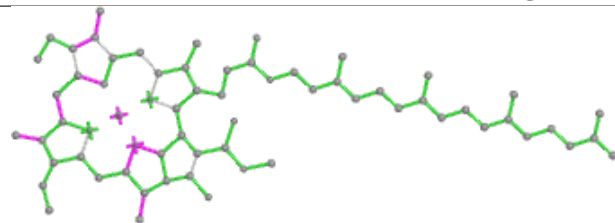


Torsions

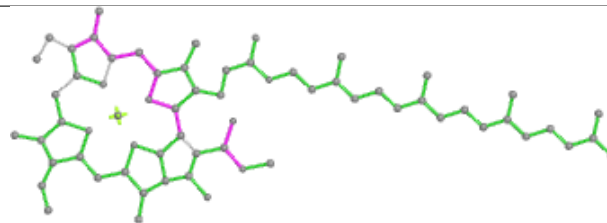


Rings

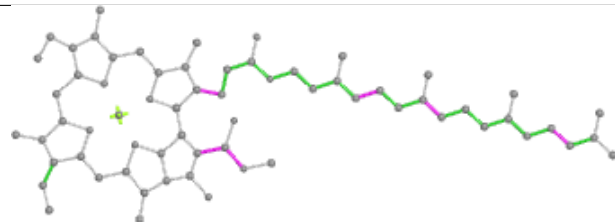
Ligand CLA c 501



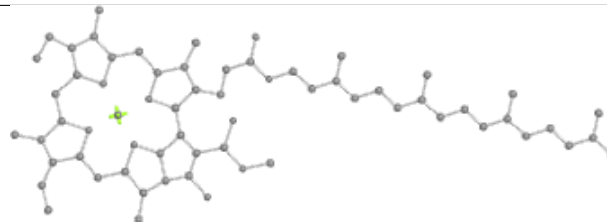
Bond lengths



Bond angles

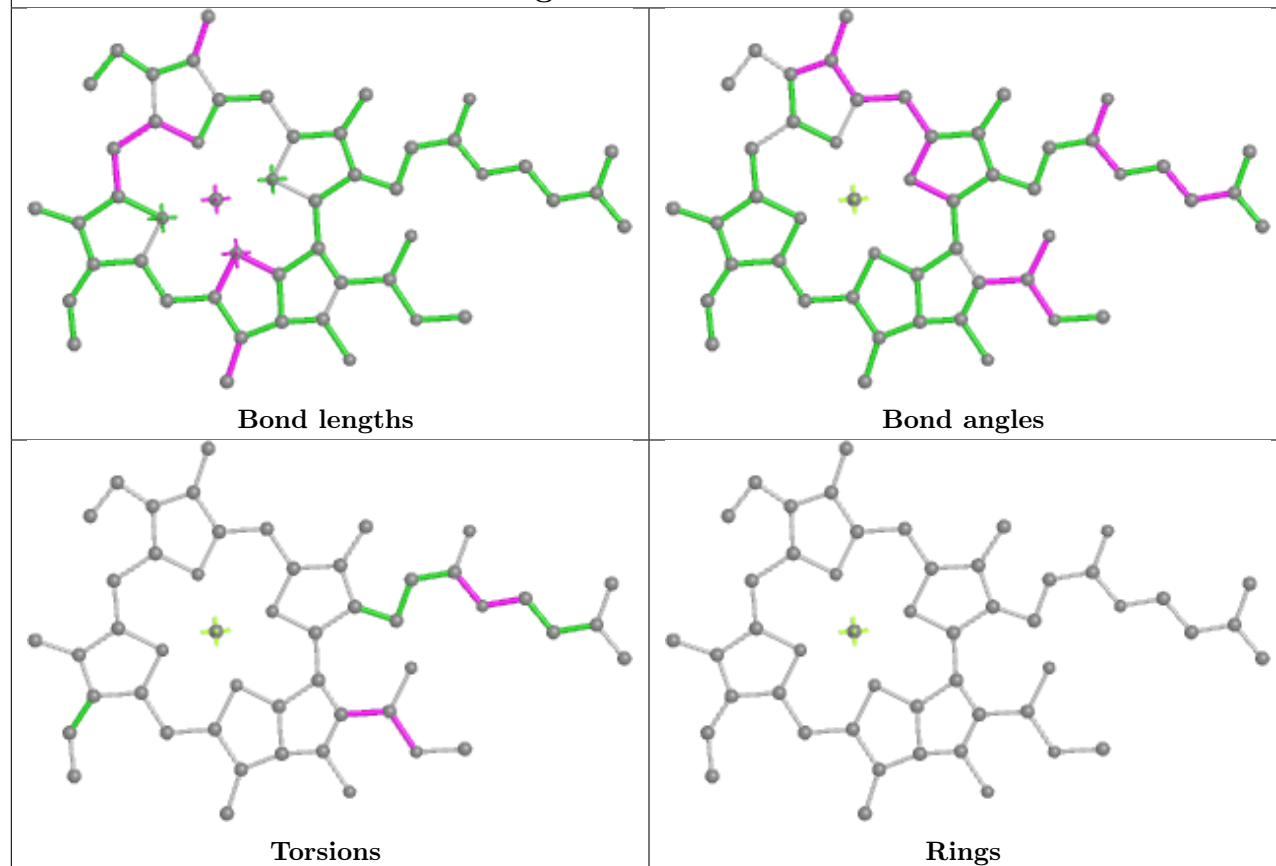


Torsions

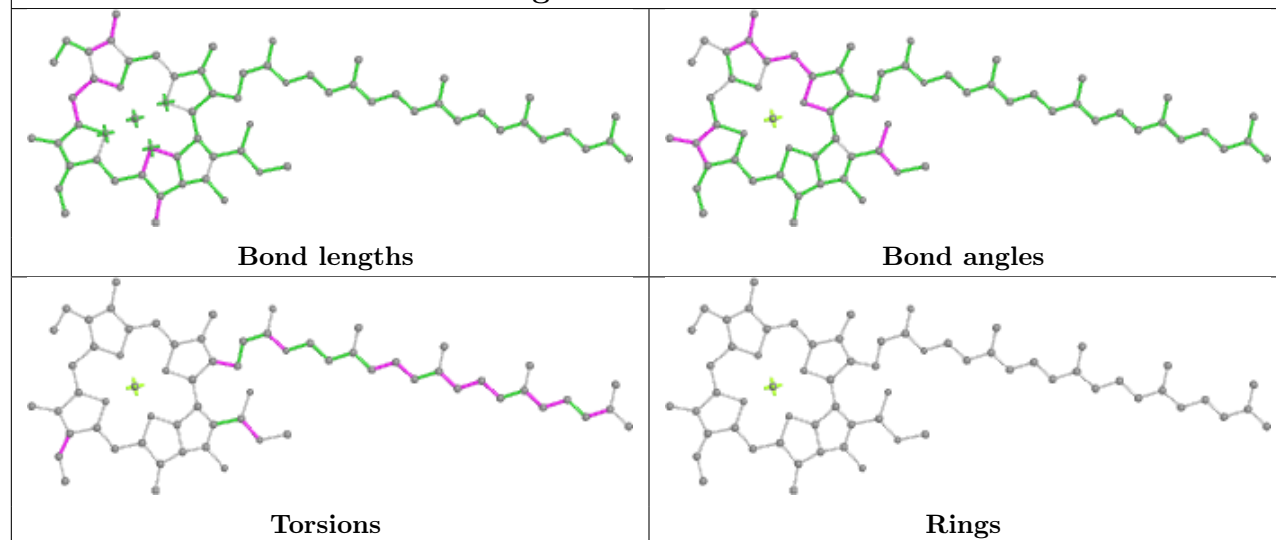


Rings

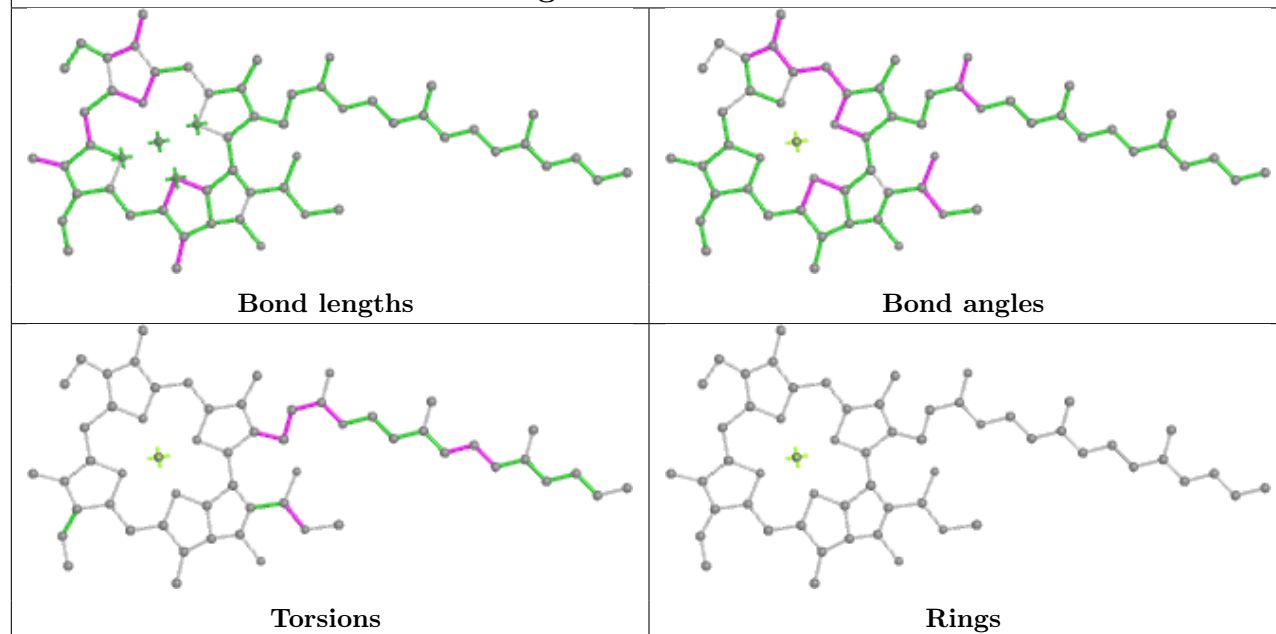
Ligand CLA n 305



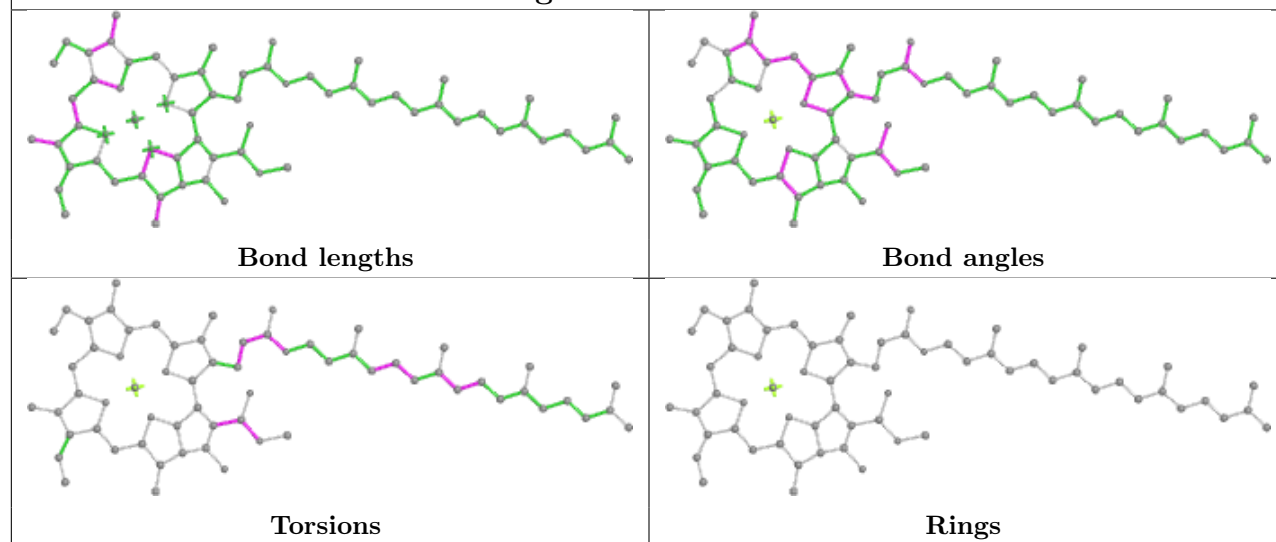
Ligand CLA C 504

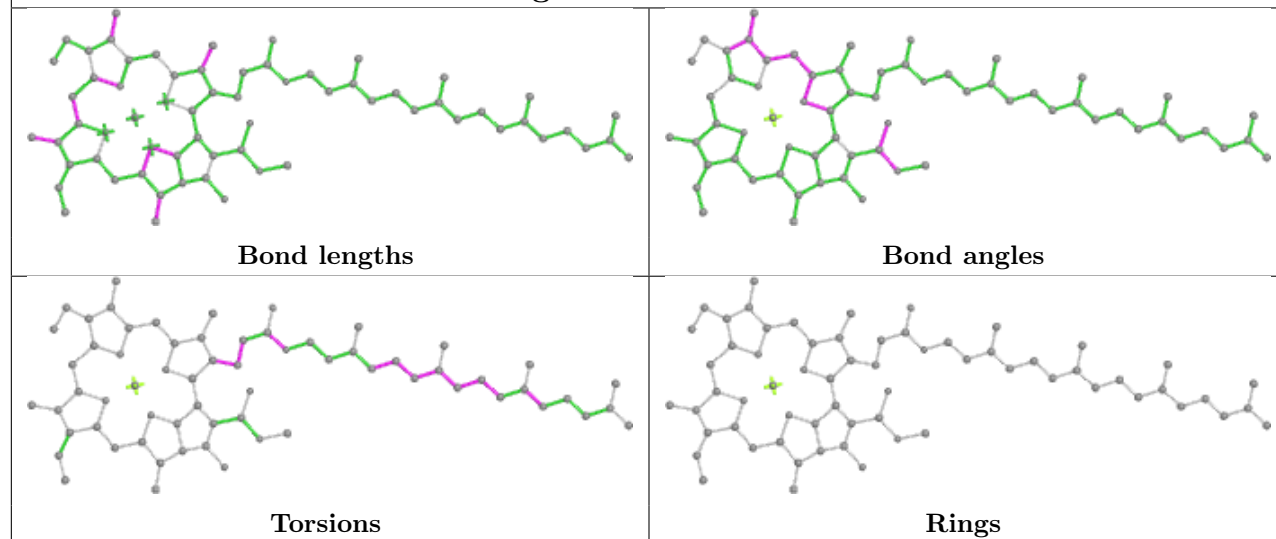
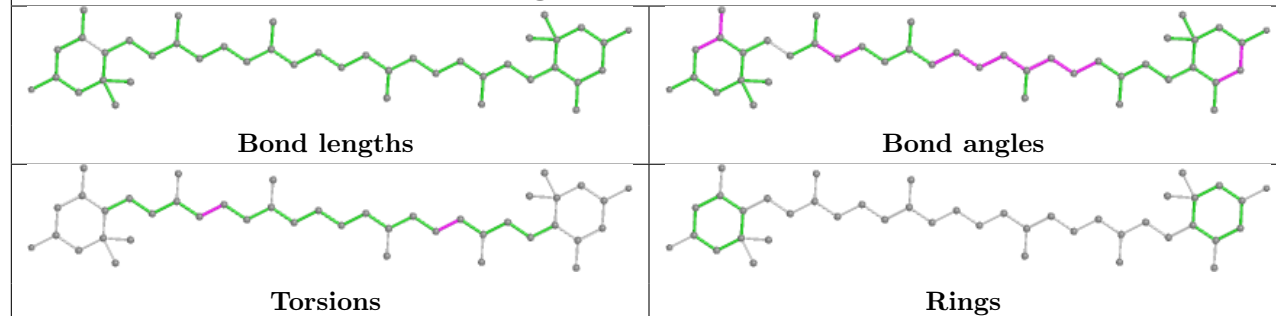
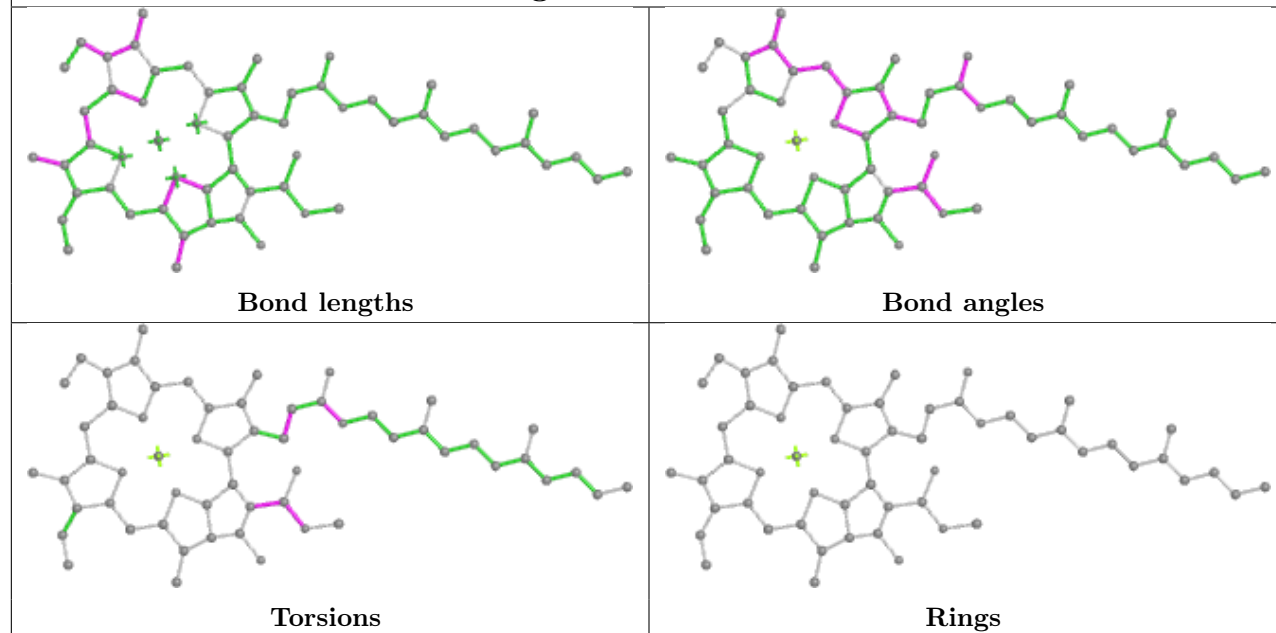


Ligand CLA r 608

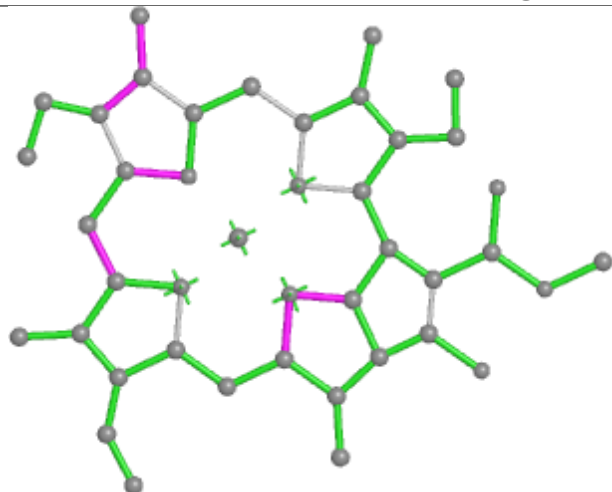


Ligand CLA b 616

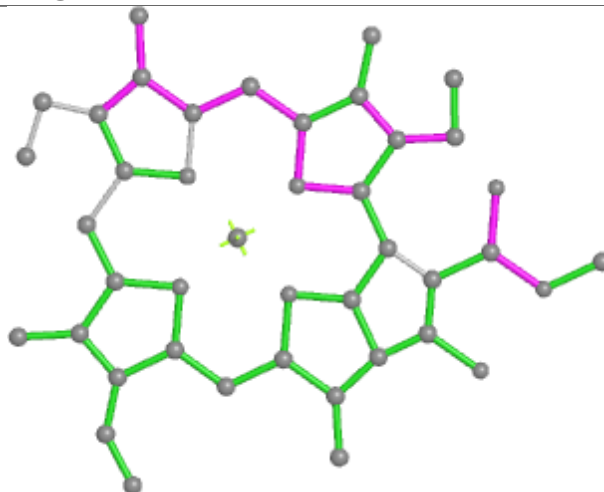


Ligand CLA B 612**Ligand LUT G 616****Ligand CLA G 613**

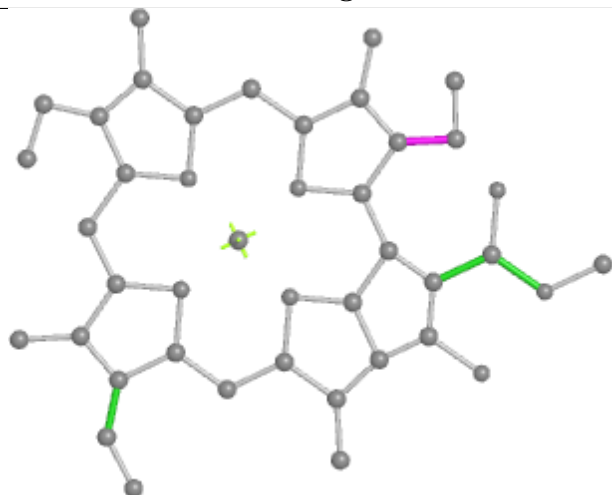
Ligand CLA g 614



Bond lengths



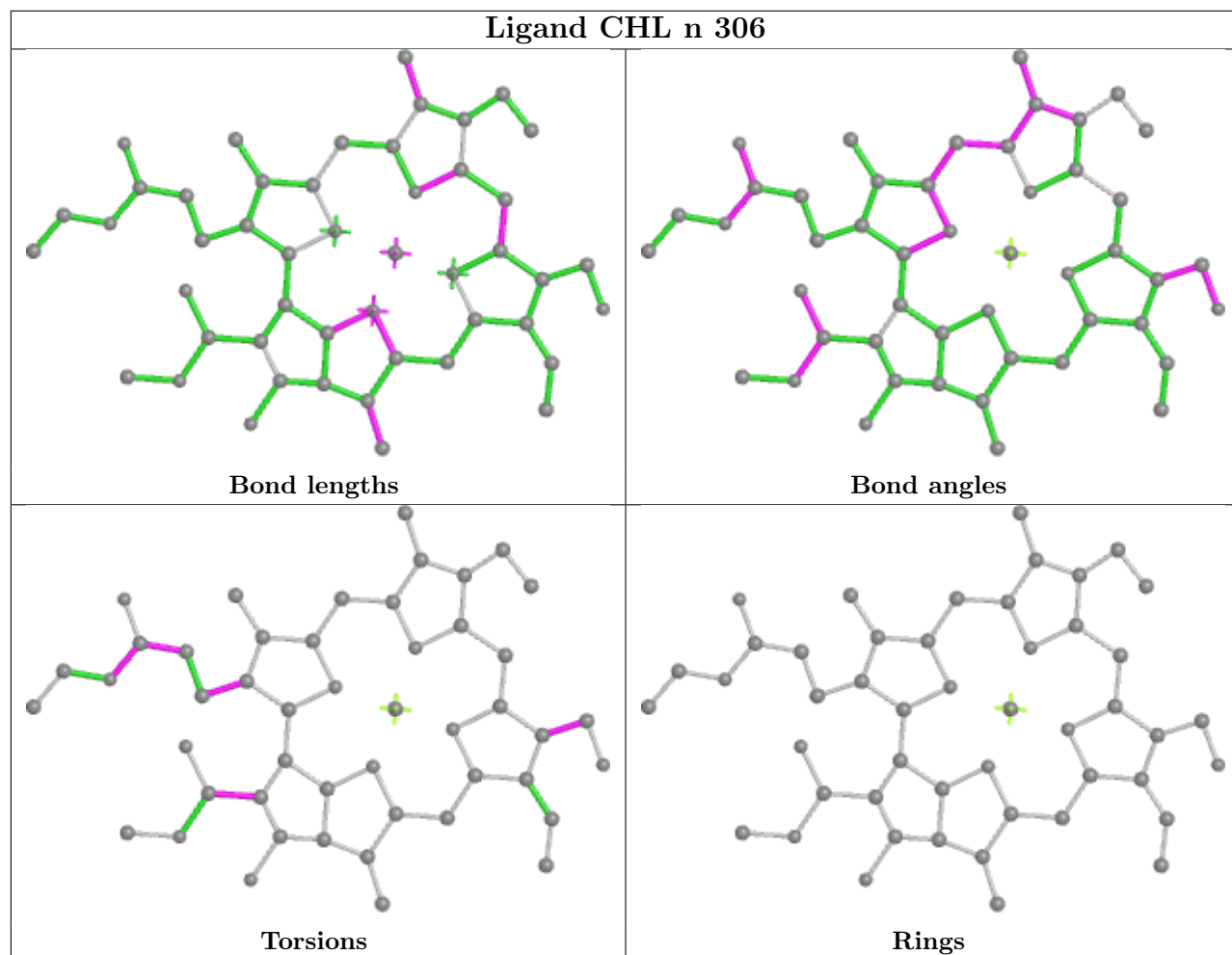
Bond angles

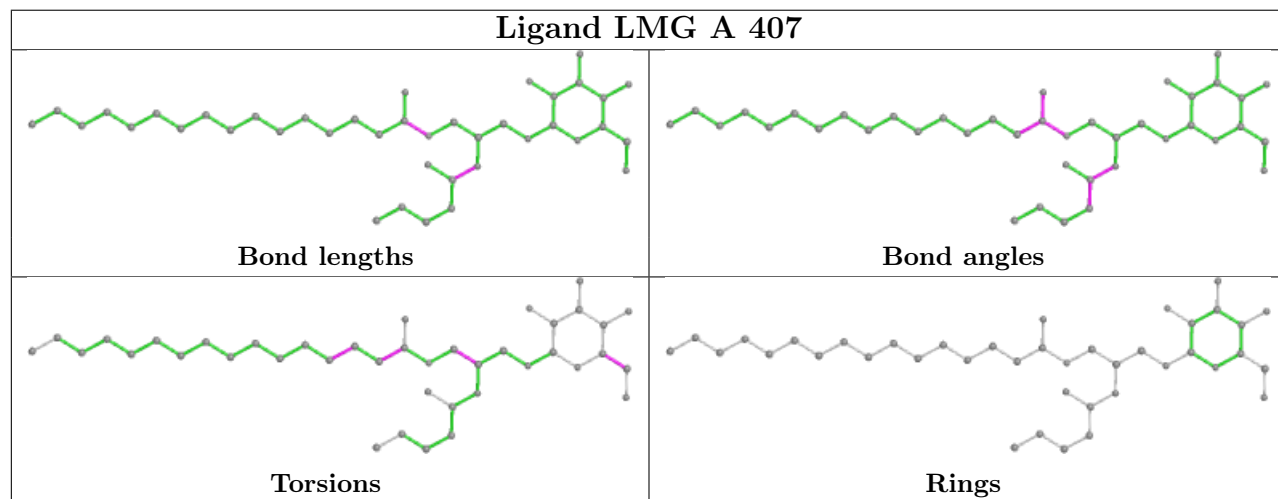
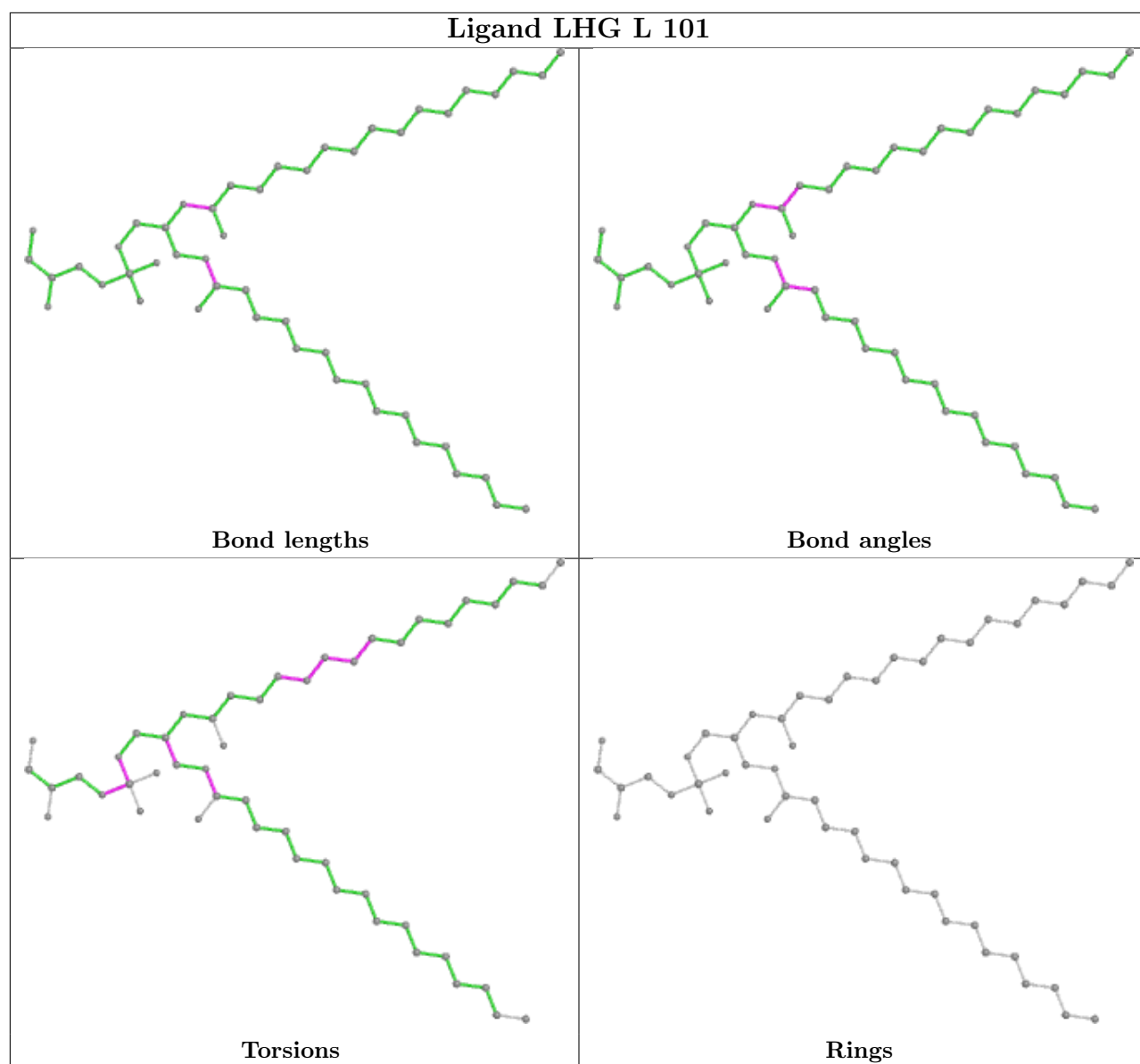


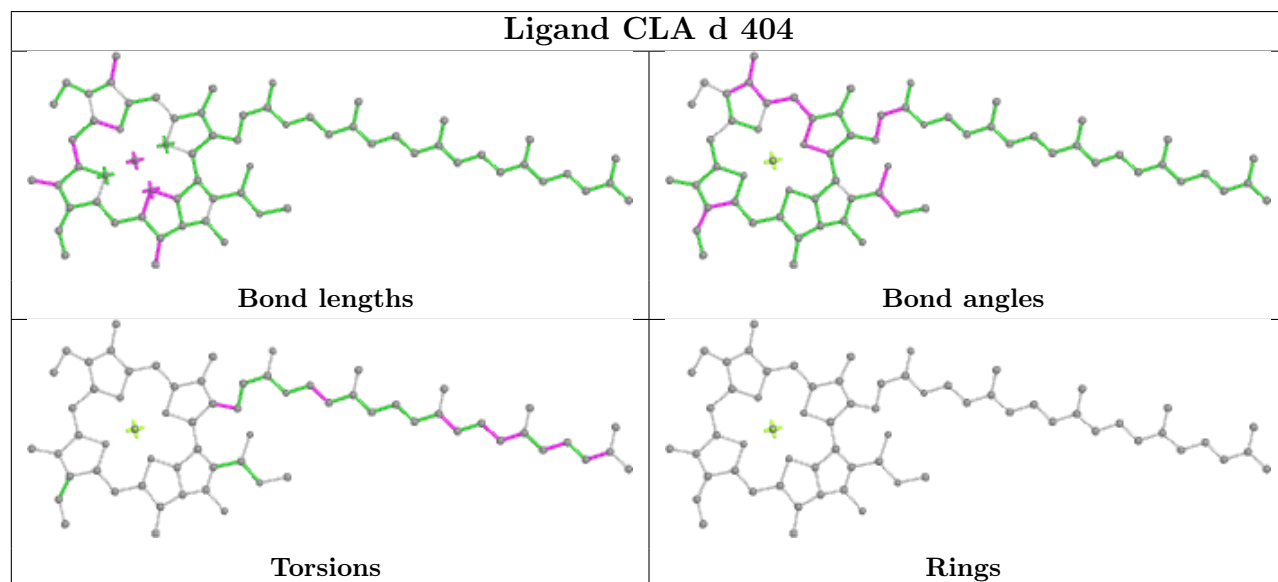
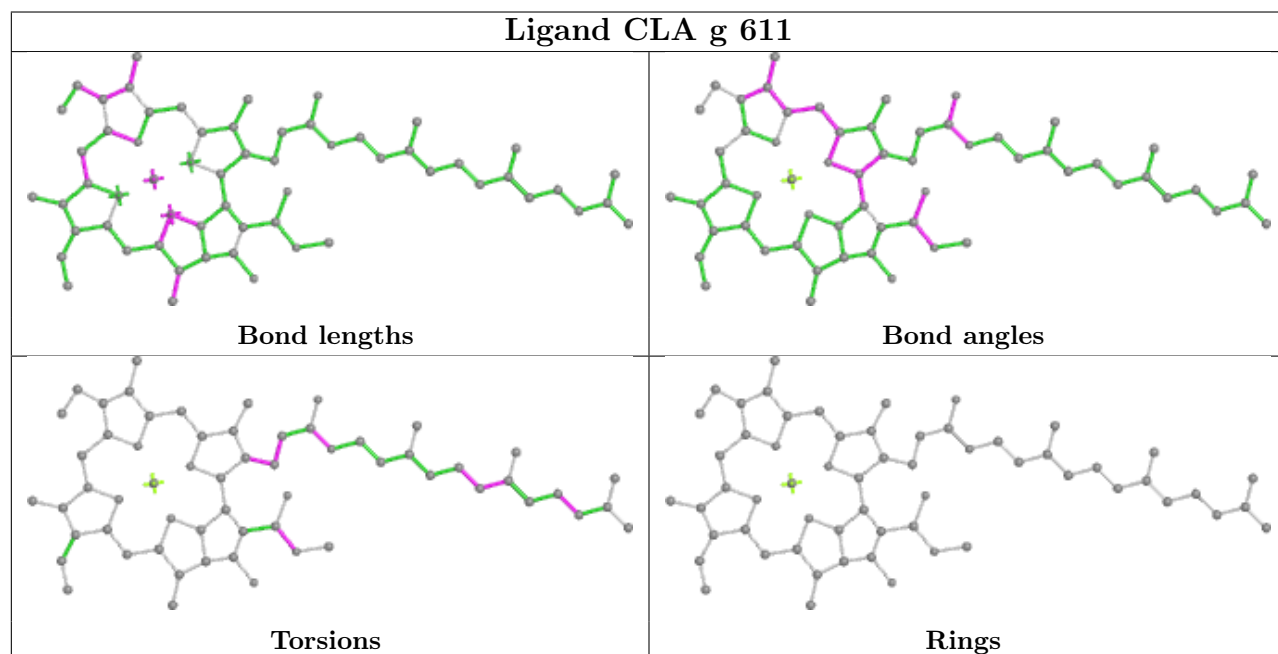
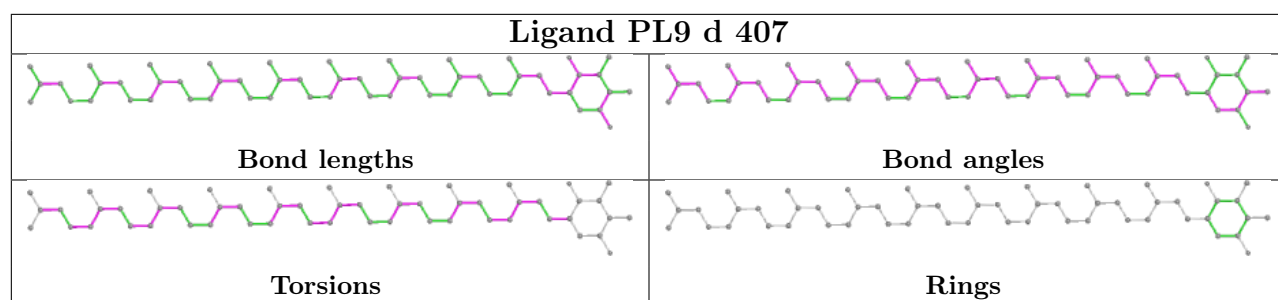
Torsions



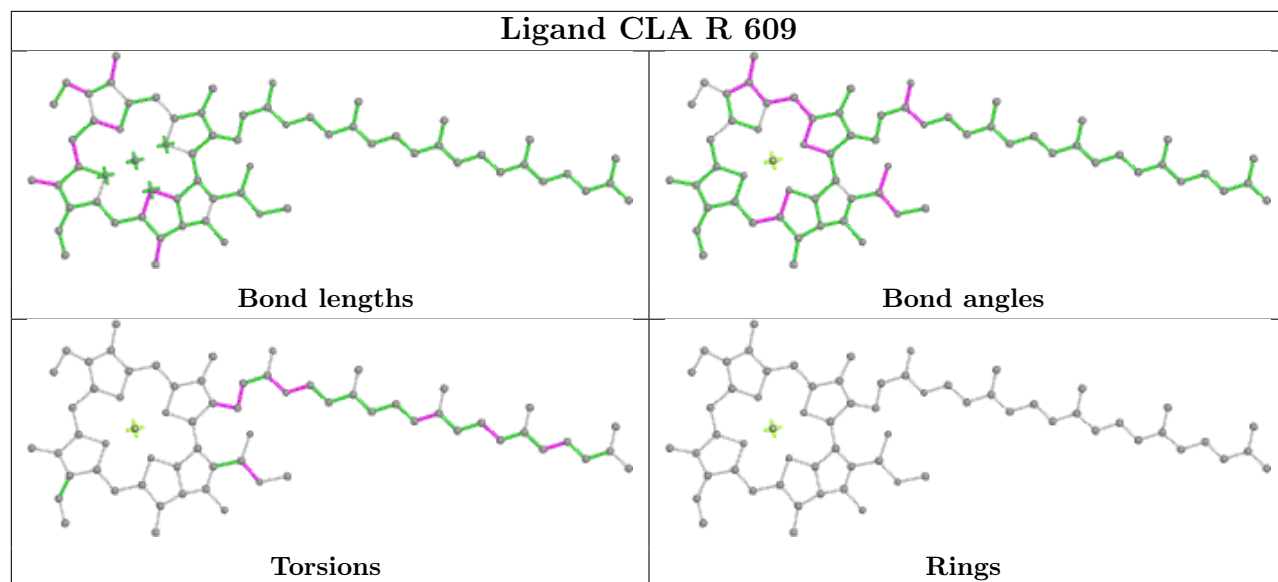
Rings



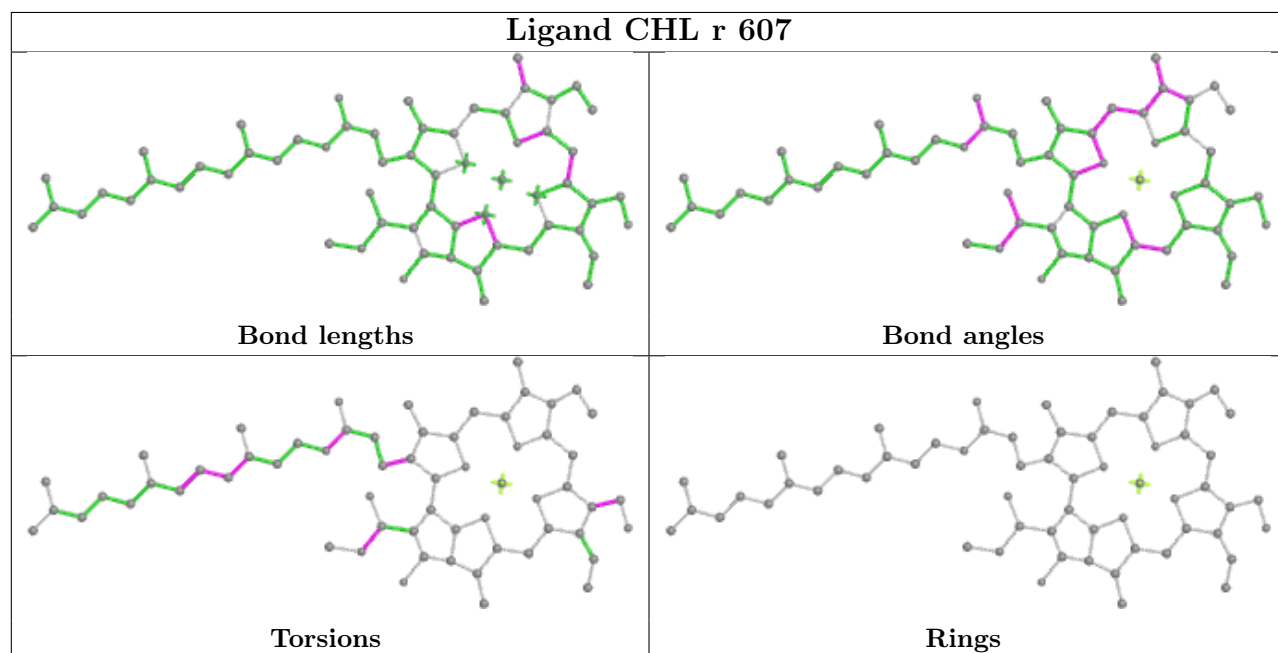


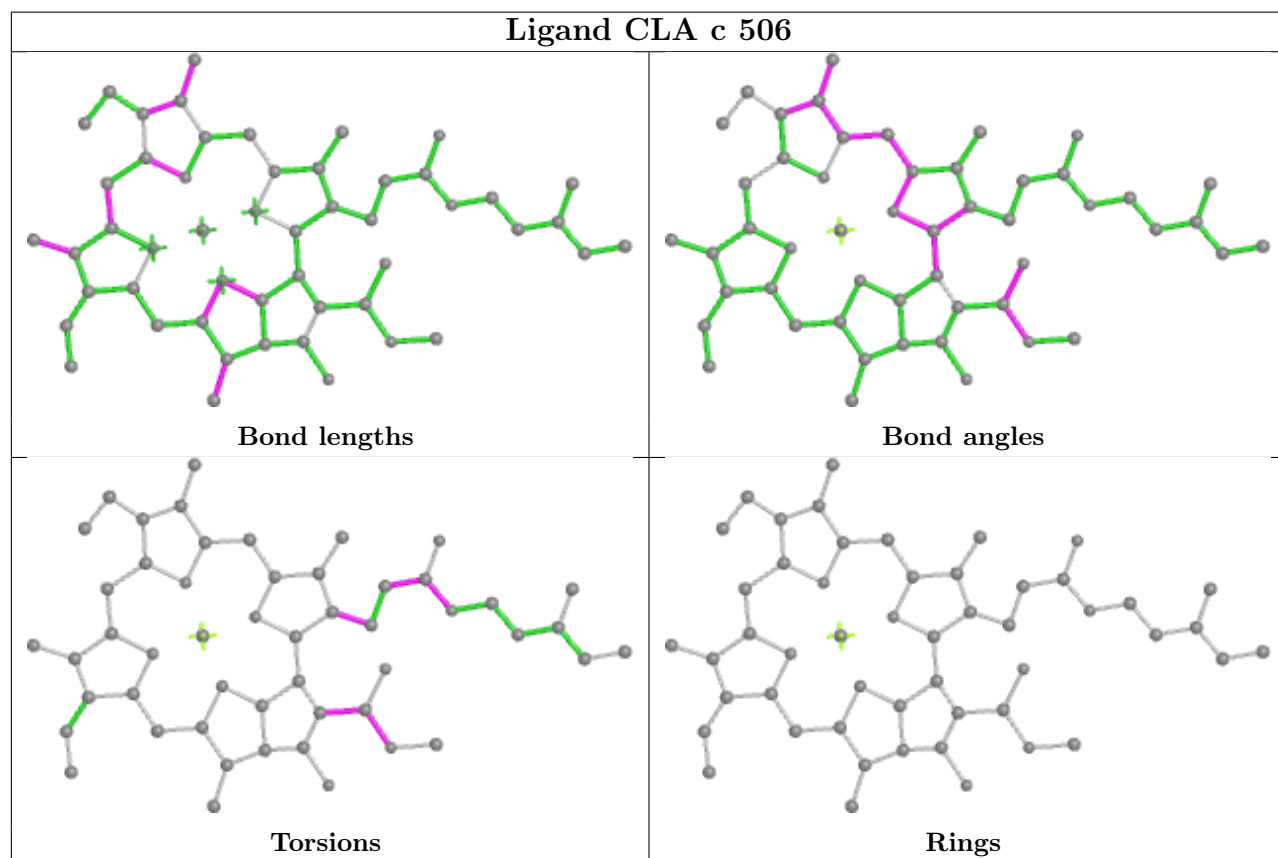
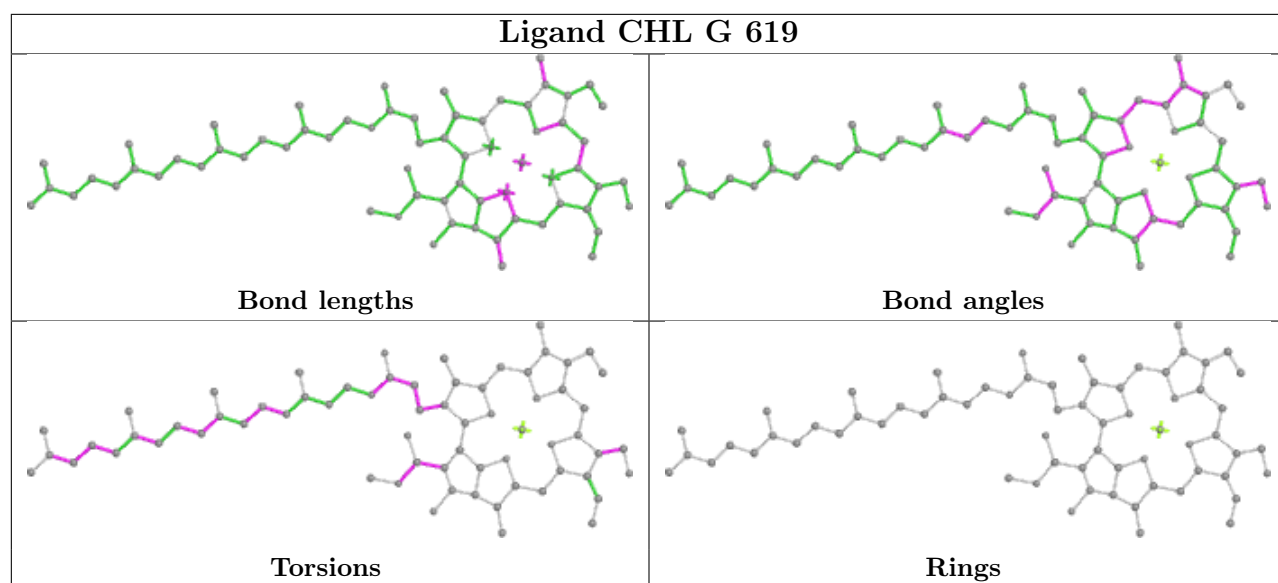


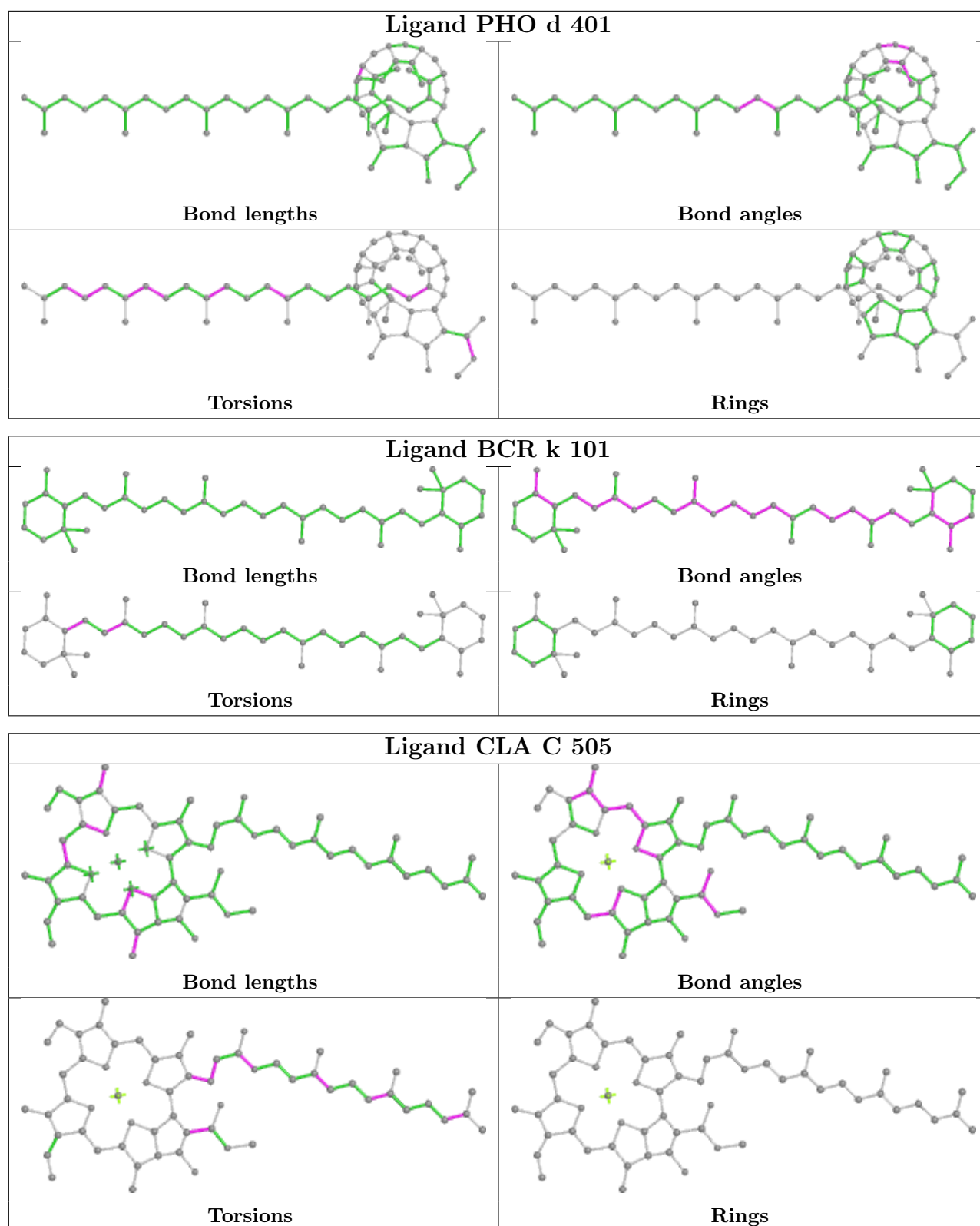
Ligand CLA R 609



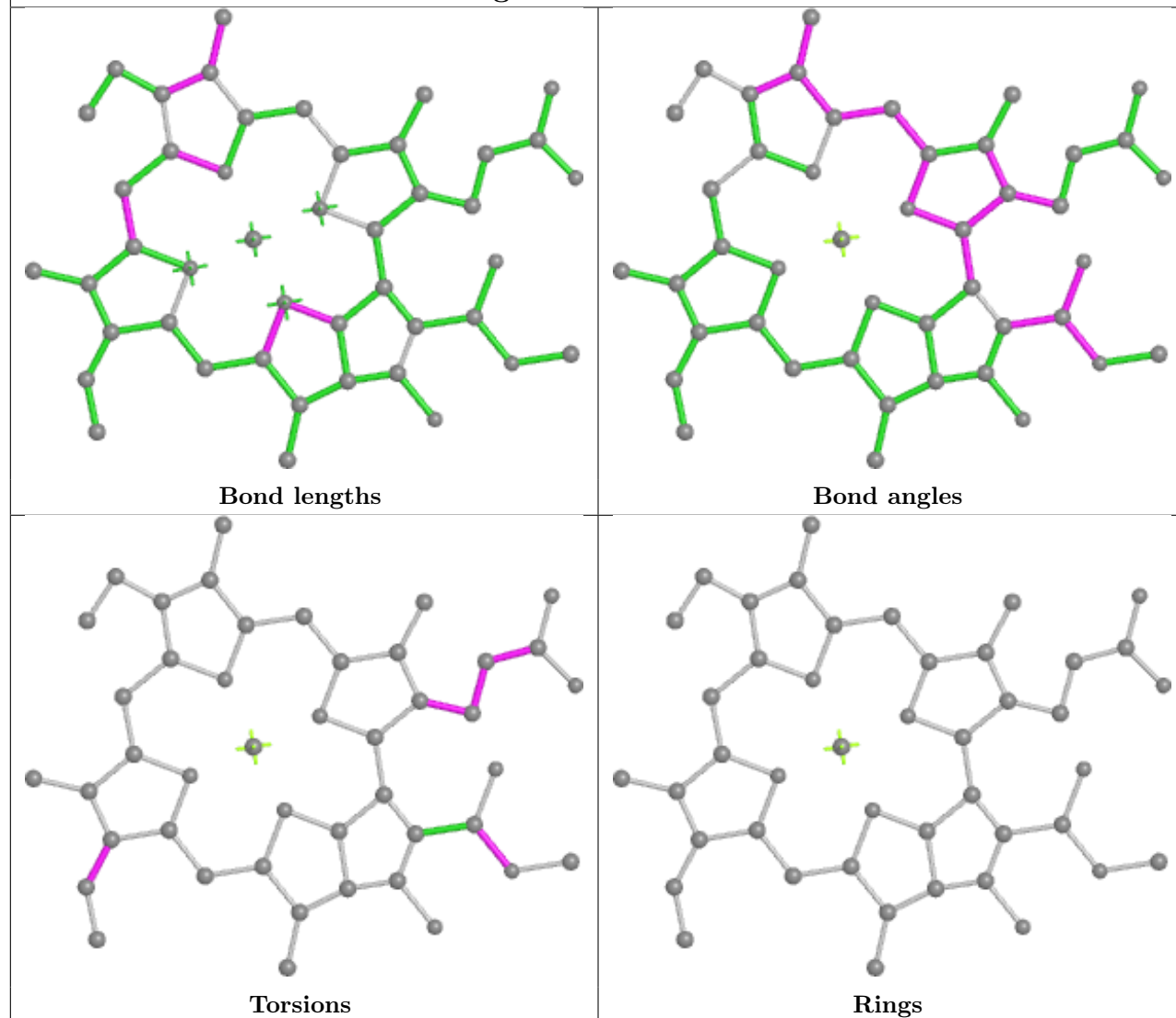
Ligand CHL r 607



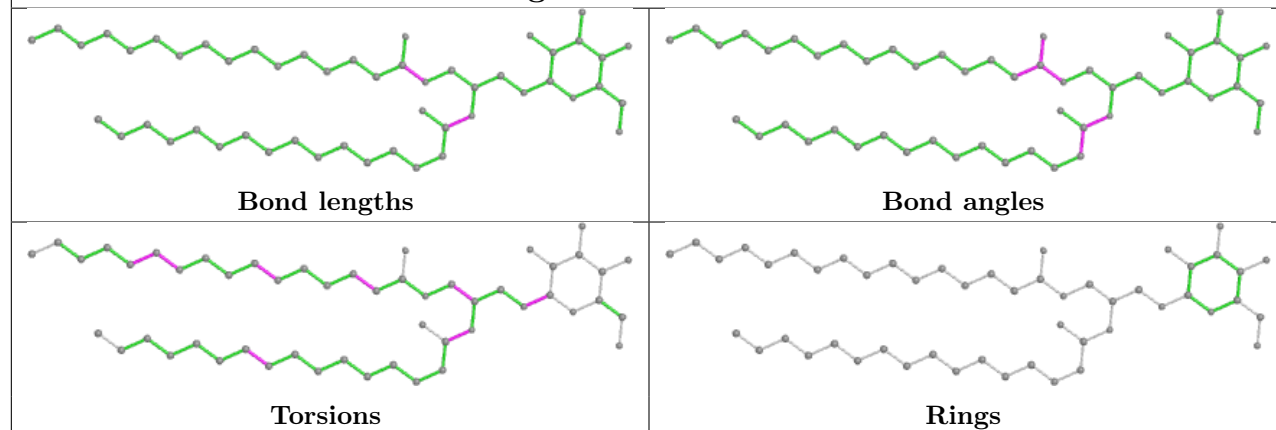


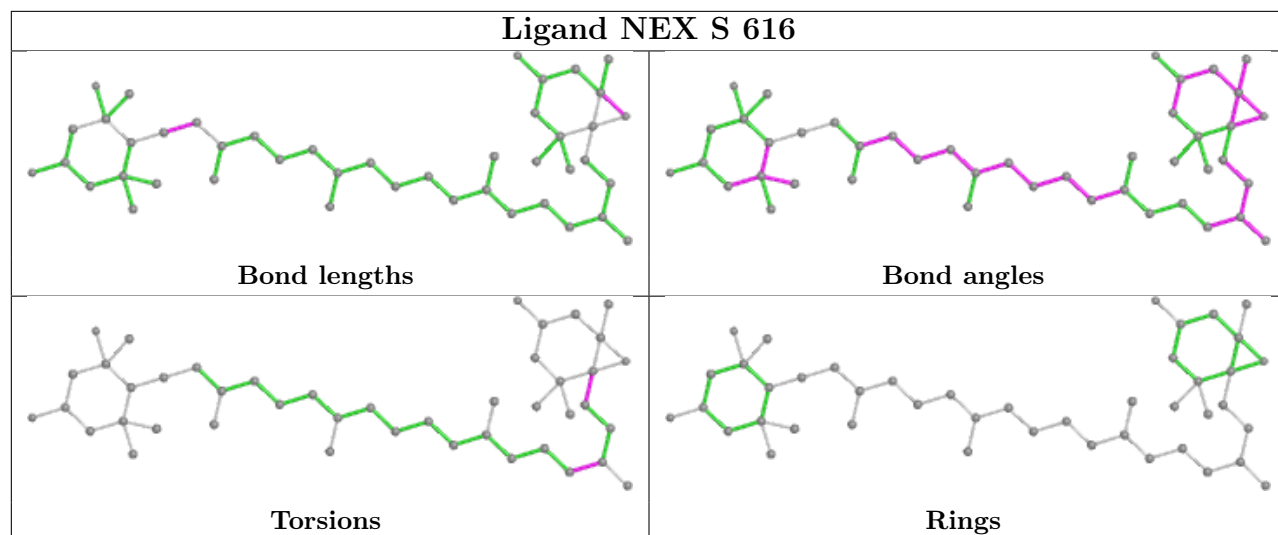
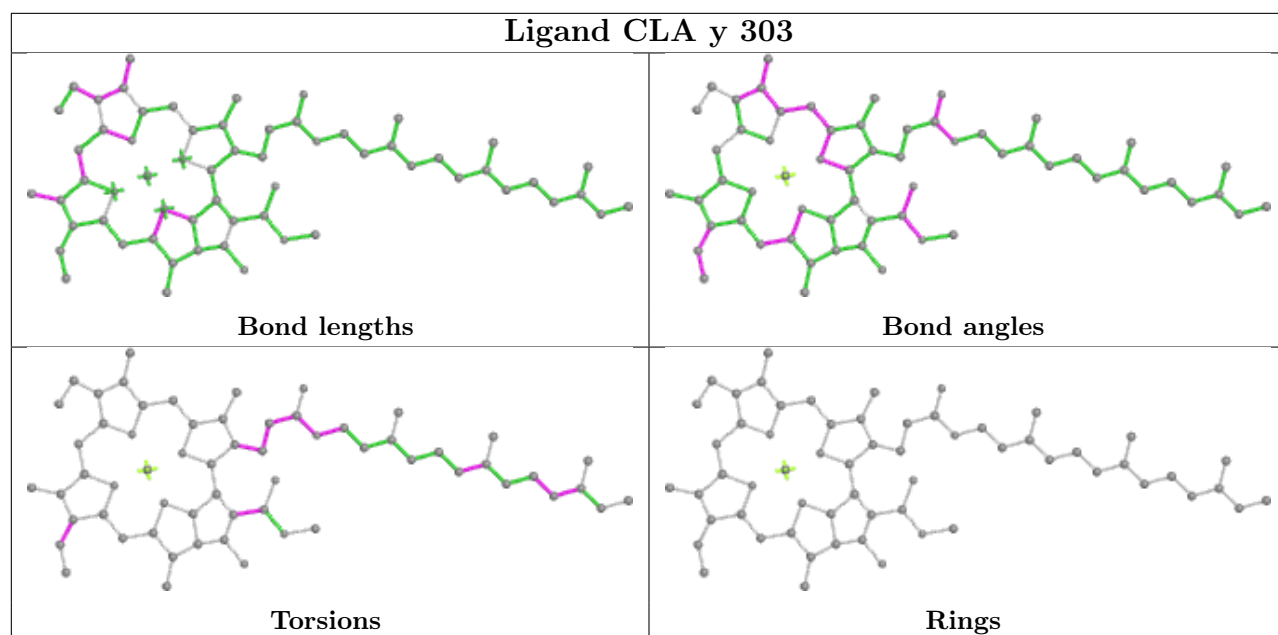
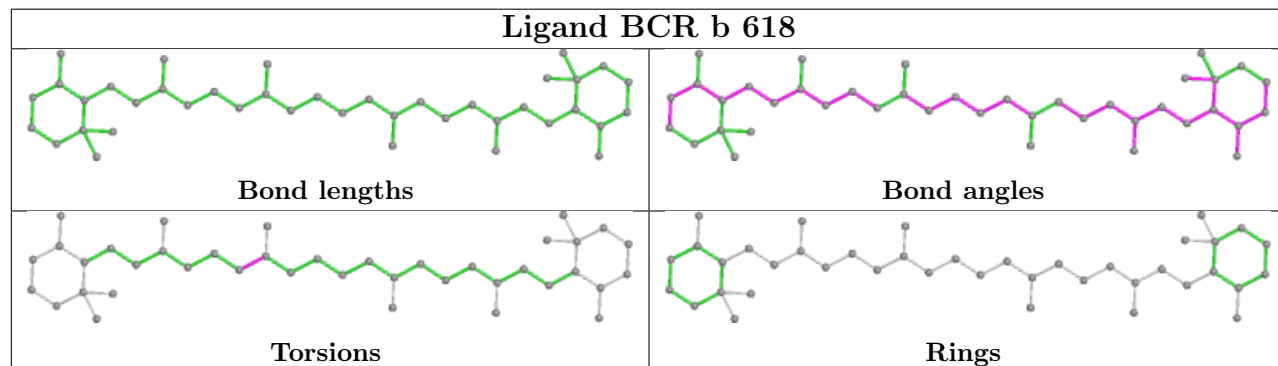


Ligand CLA n 313

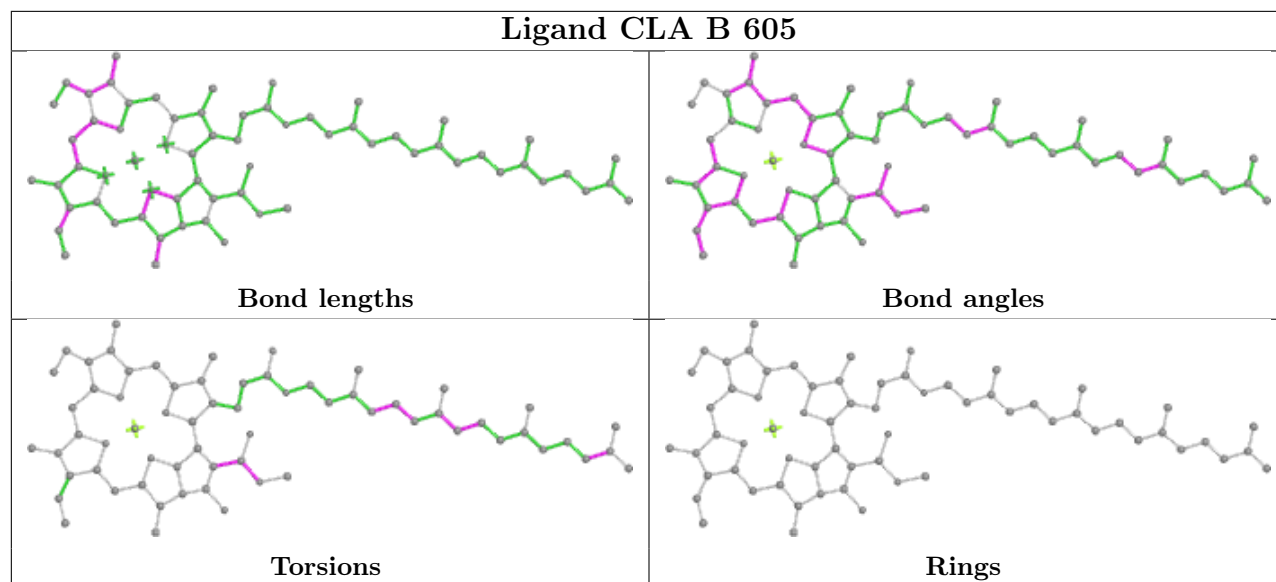


Ligand LMG B 620

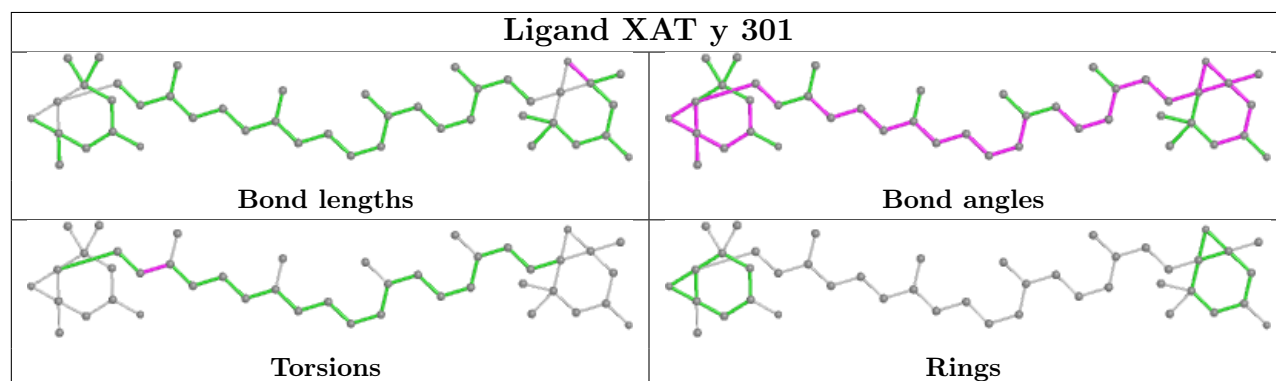


Ligand NEX S 616**Ligand CLA y 303****Ligand BCR b 618**

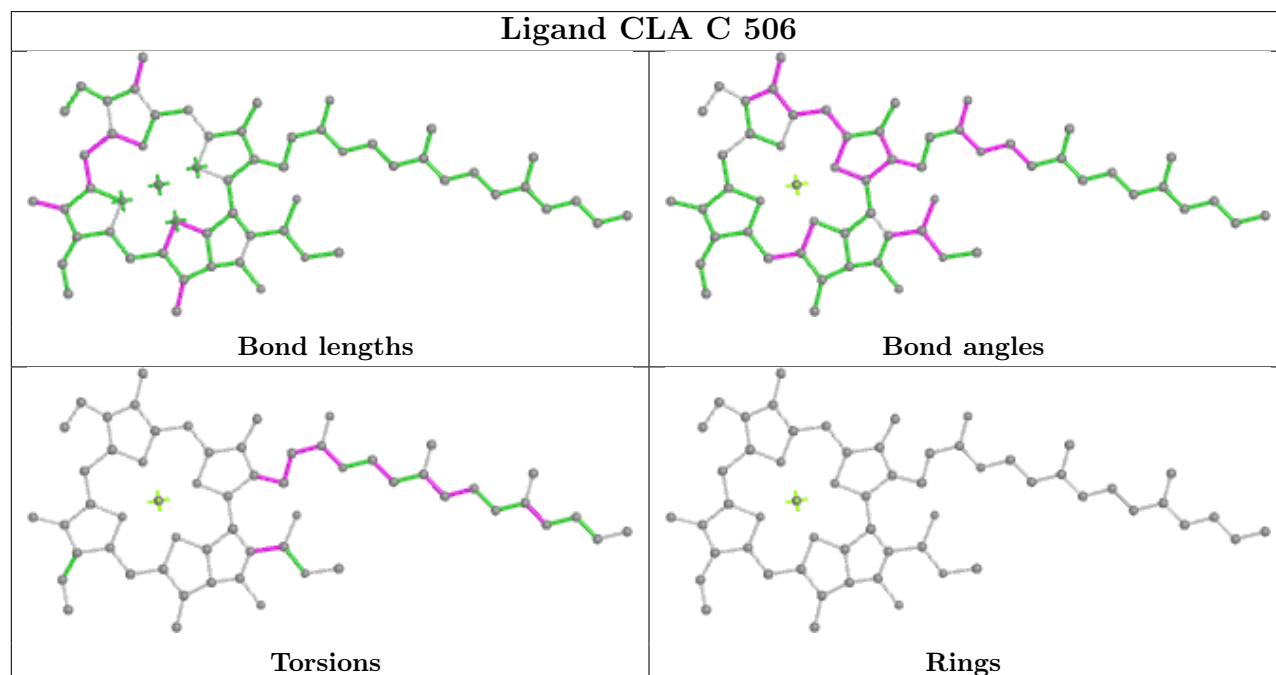
Ligand CLA B 605

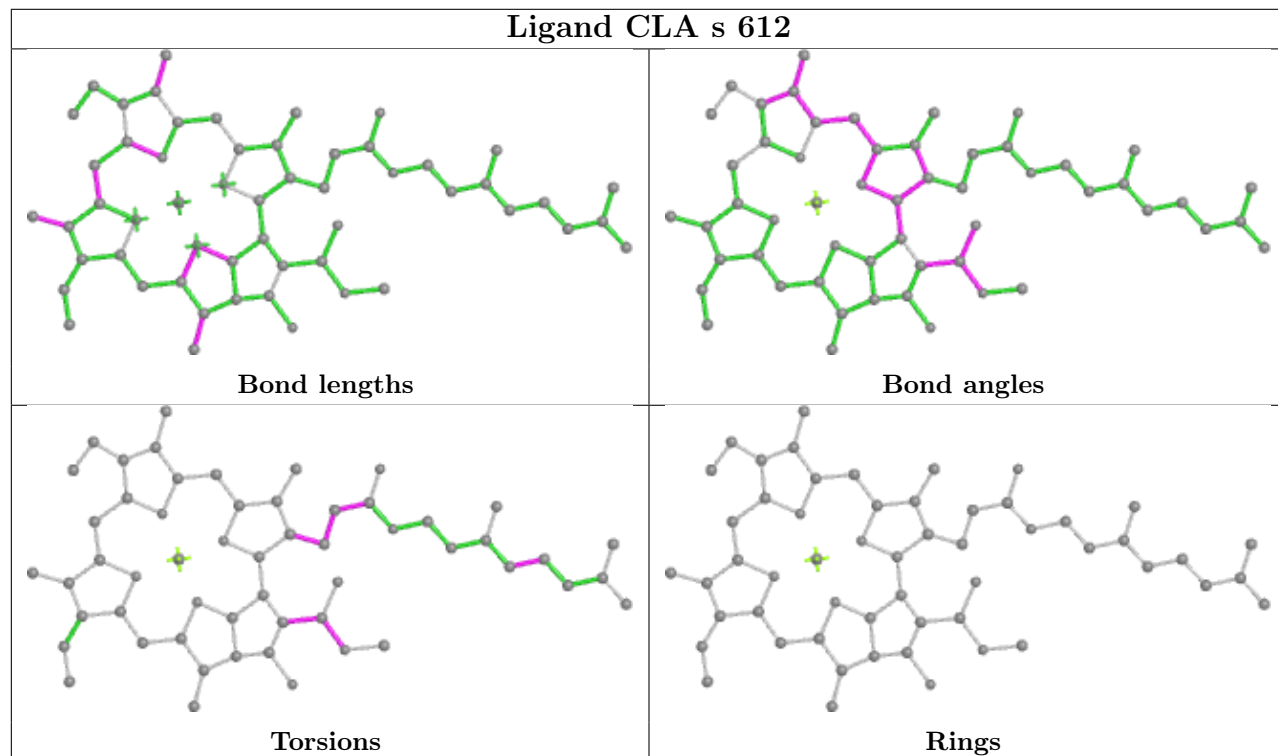
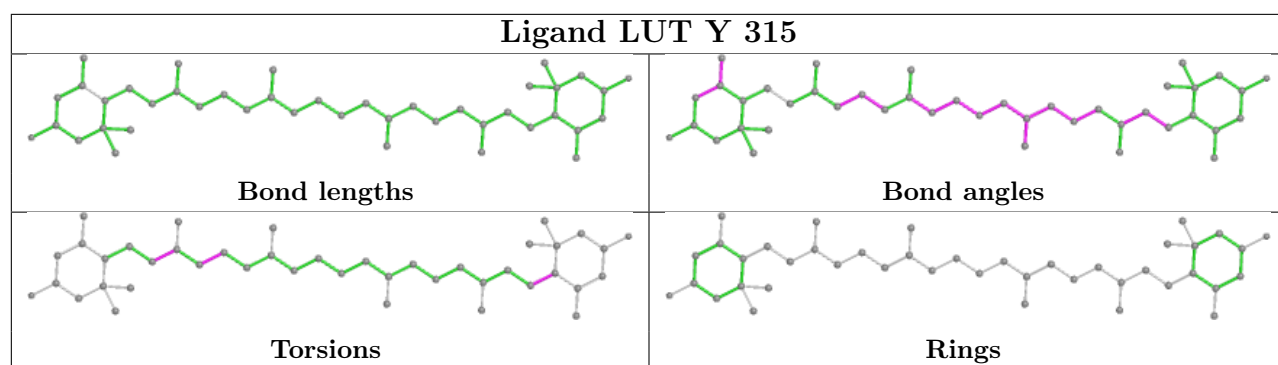


Ligand XAT y 301

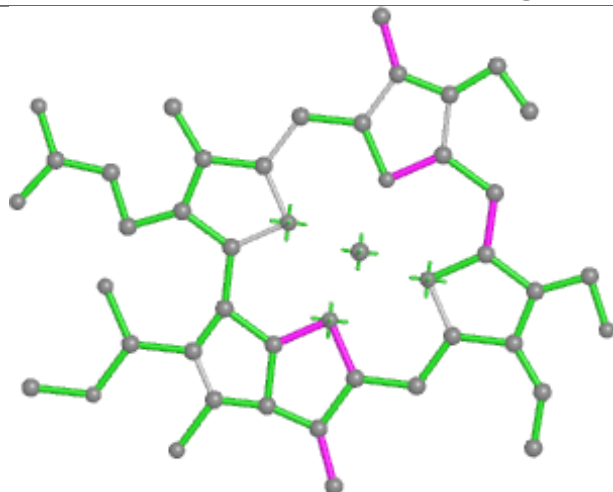


Ligand CLA C 506

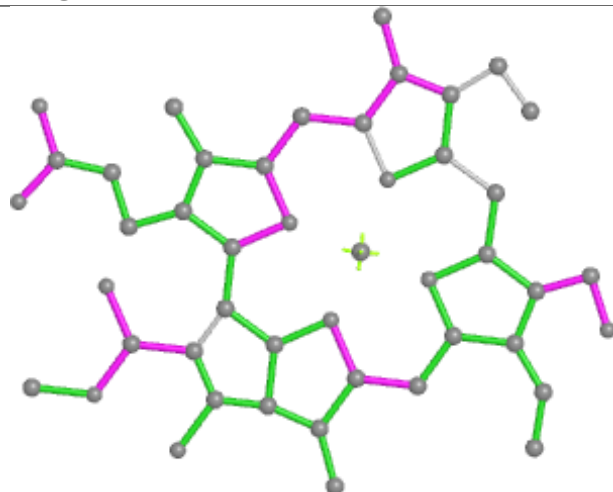




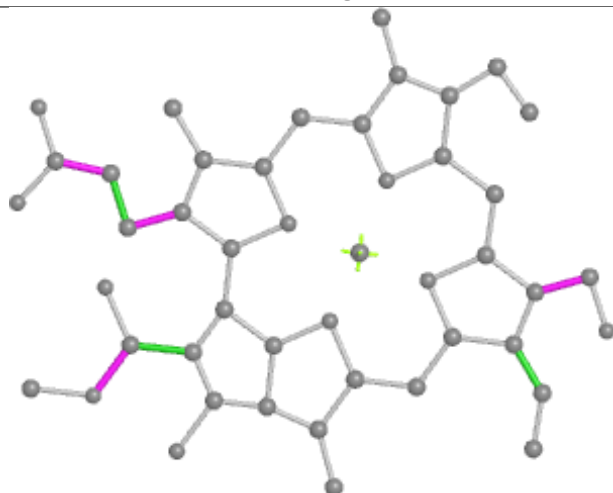
Ligand CHL g 605



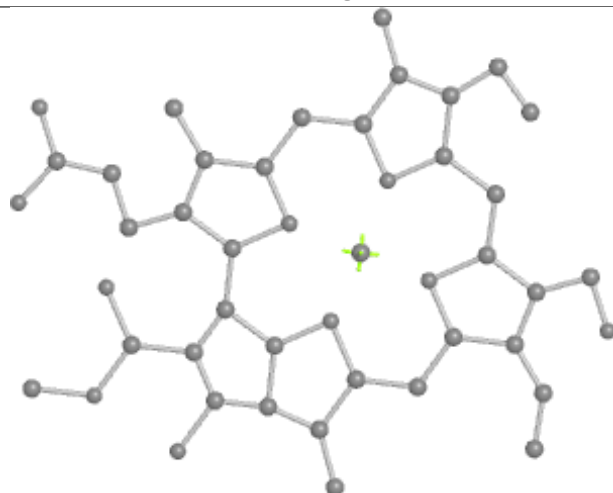
Bond lengths



Bond angles

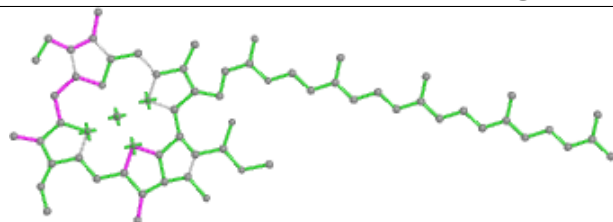


Torsions

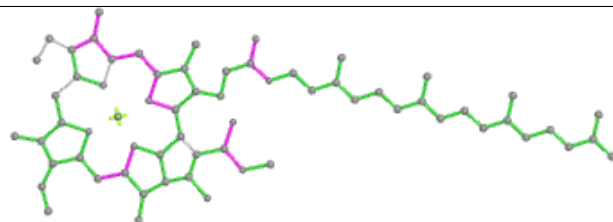


Rings

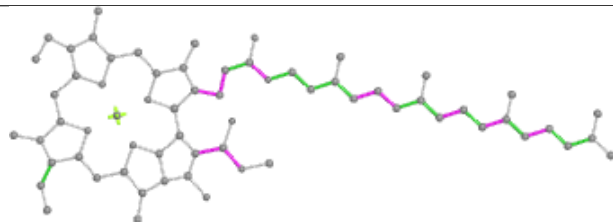
Ligand CLA B 601



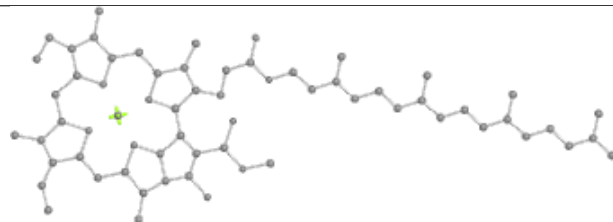
Bond lengths



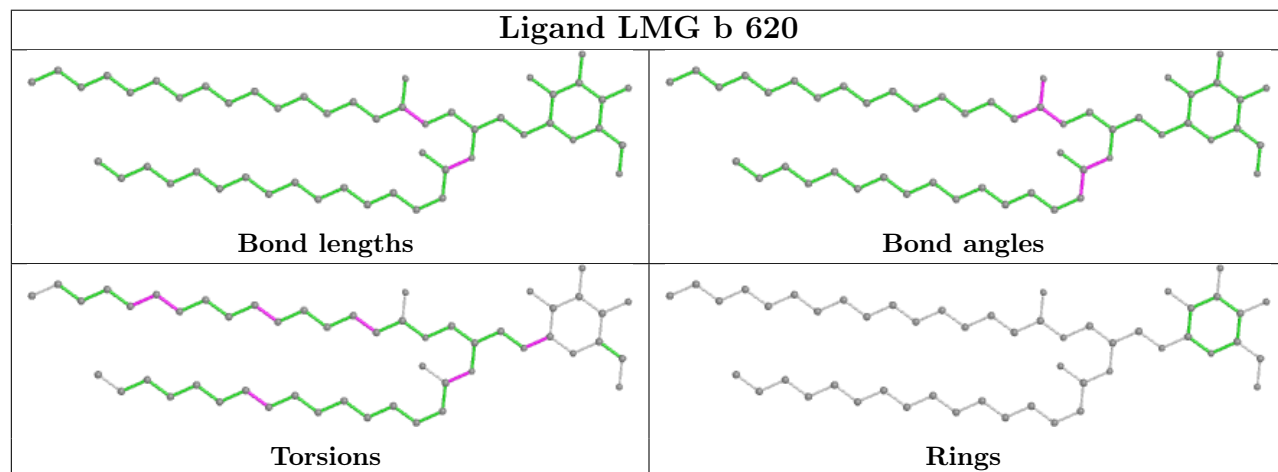
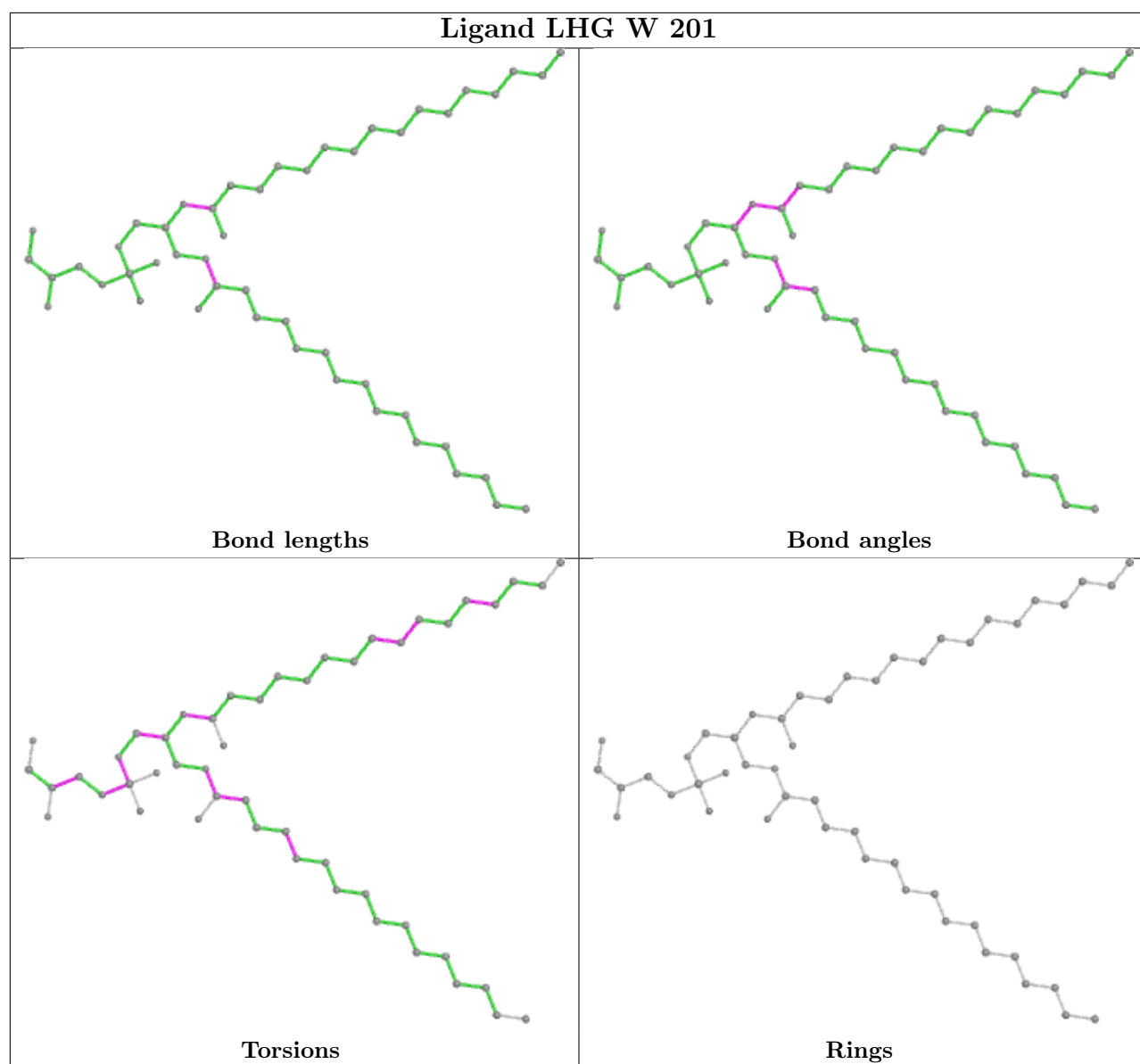
Bond angles

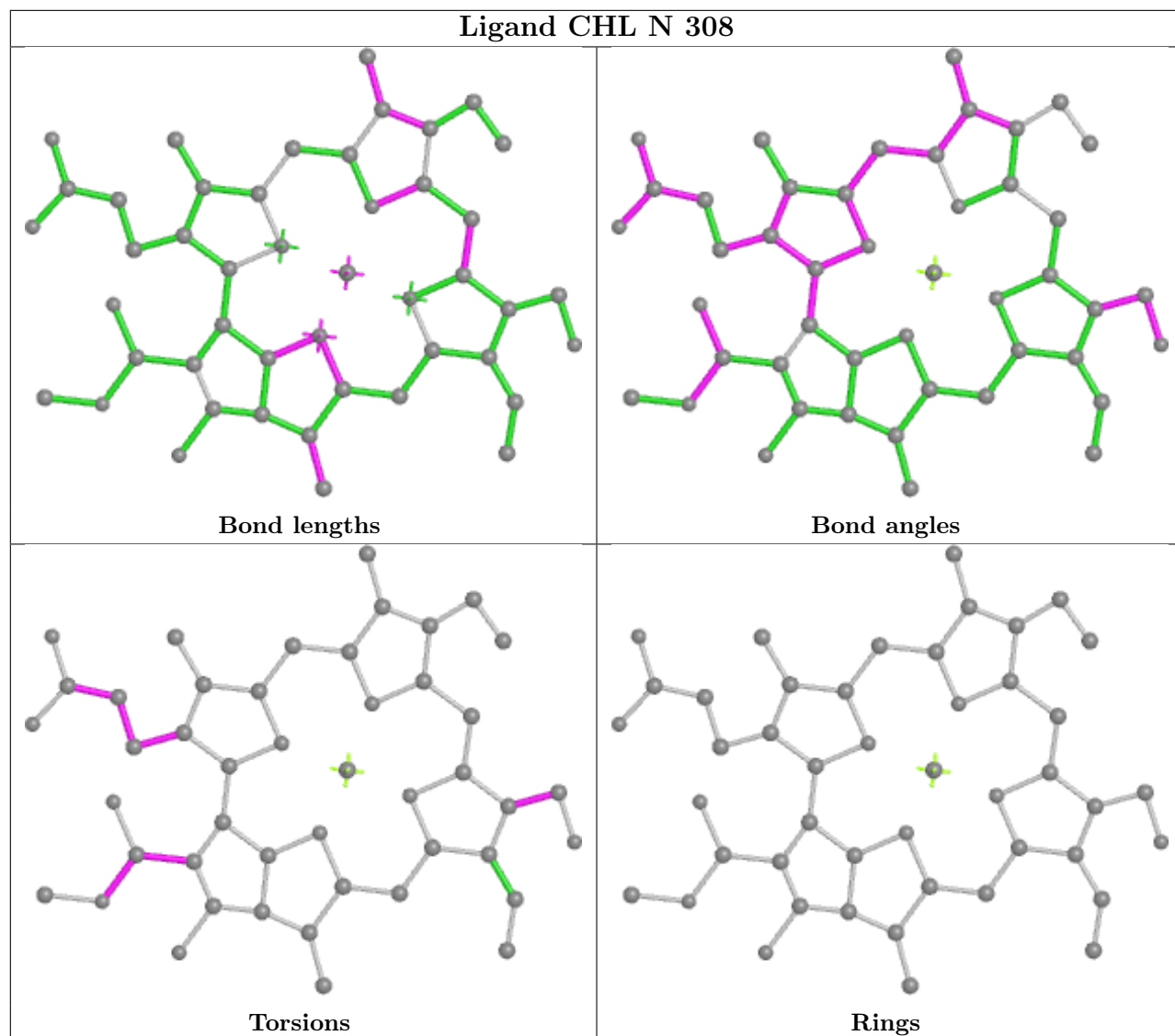


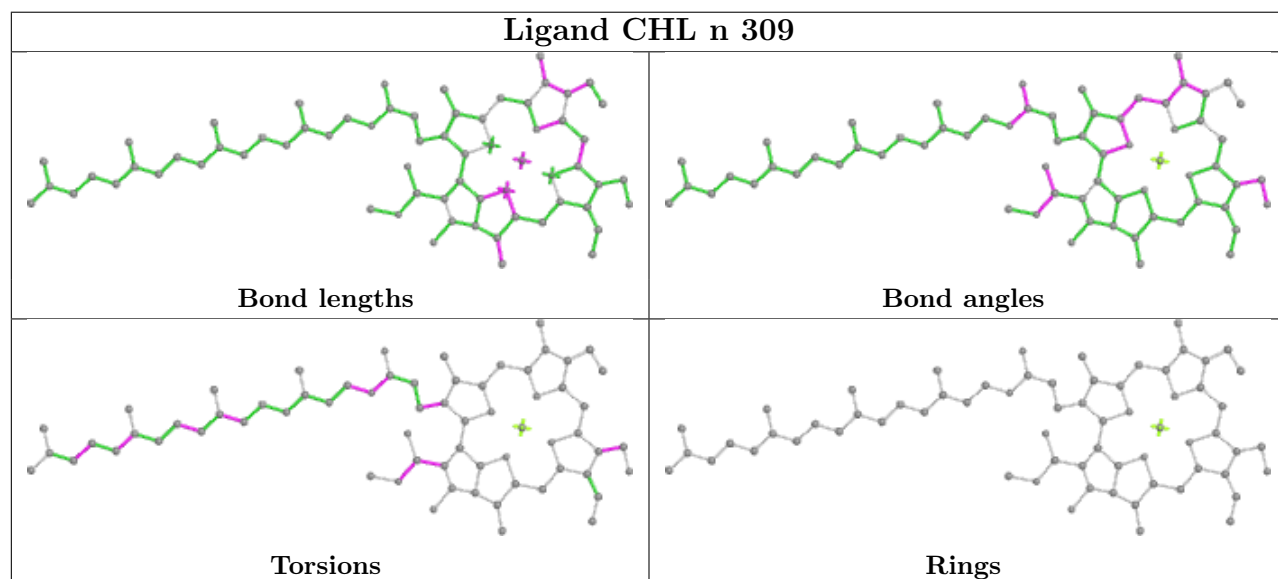
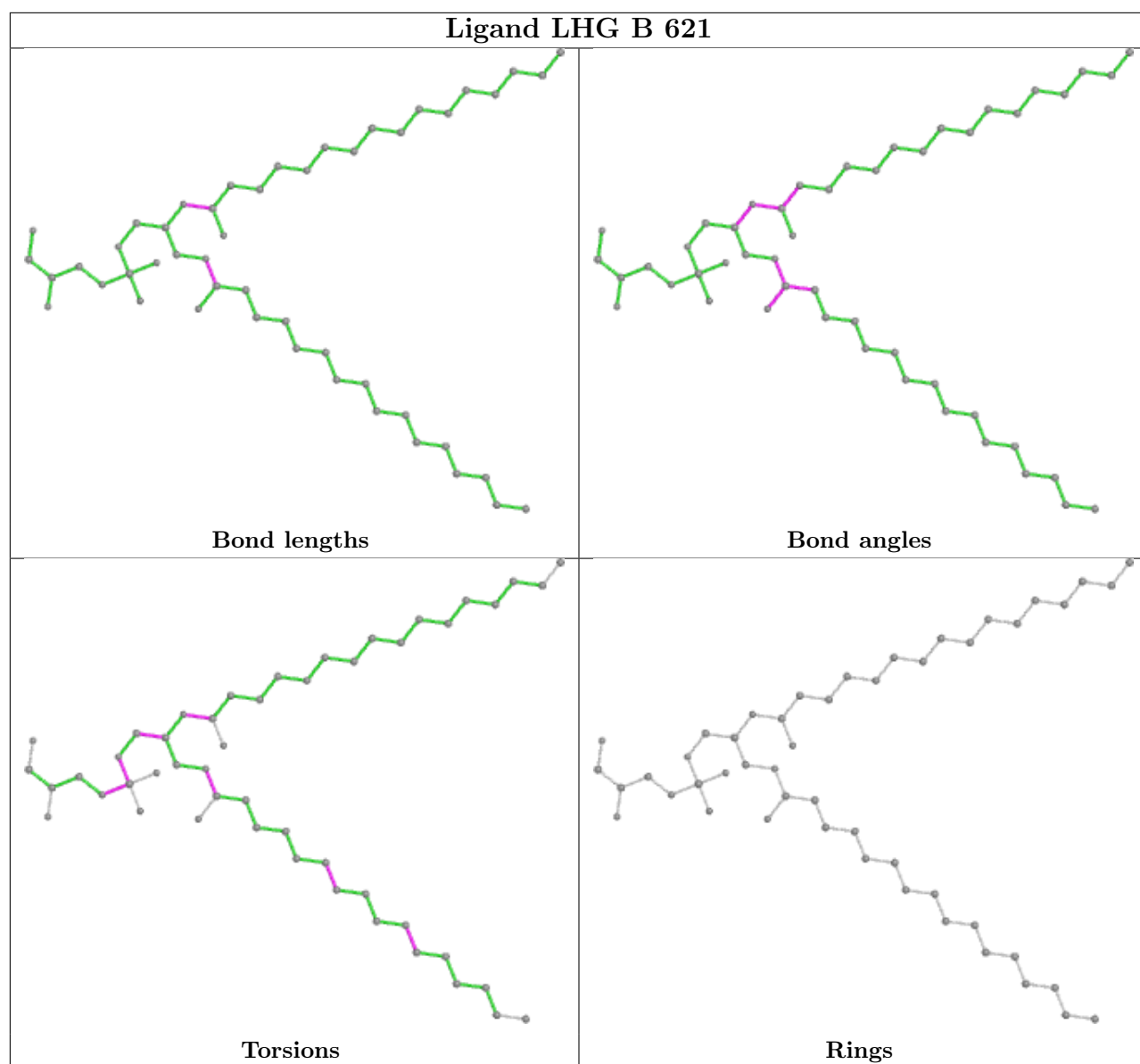
Torsions



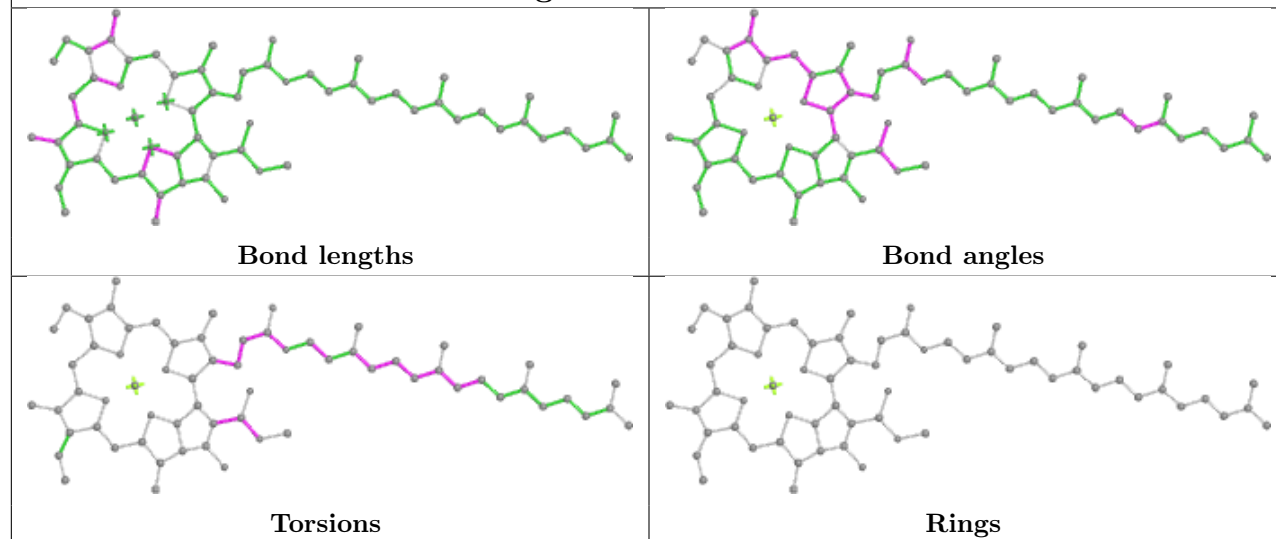
Rings



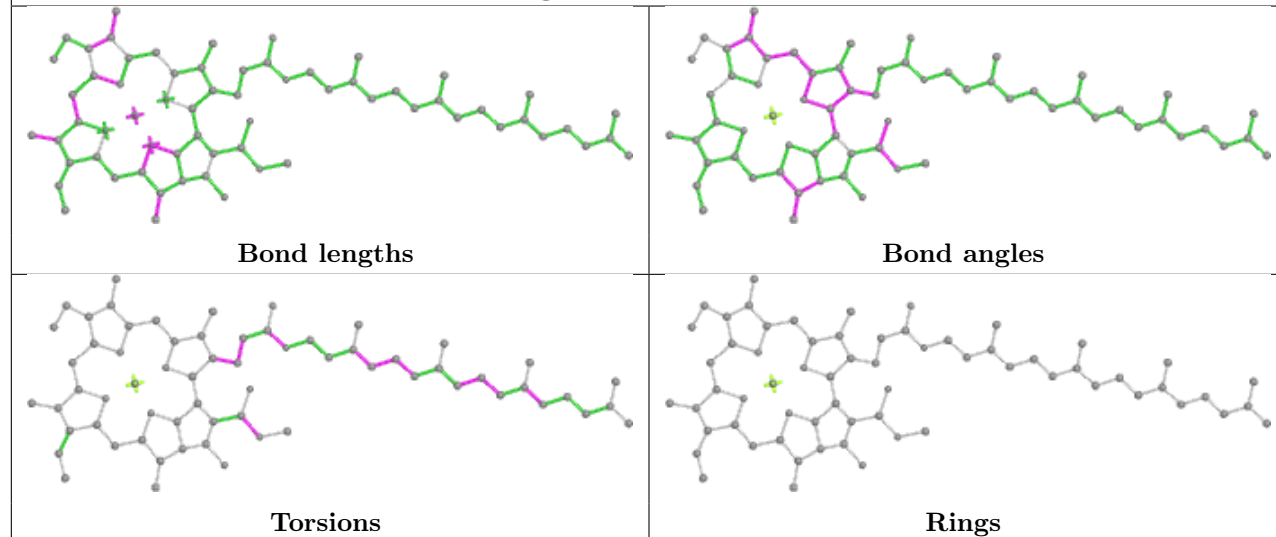




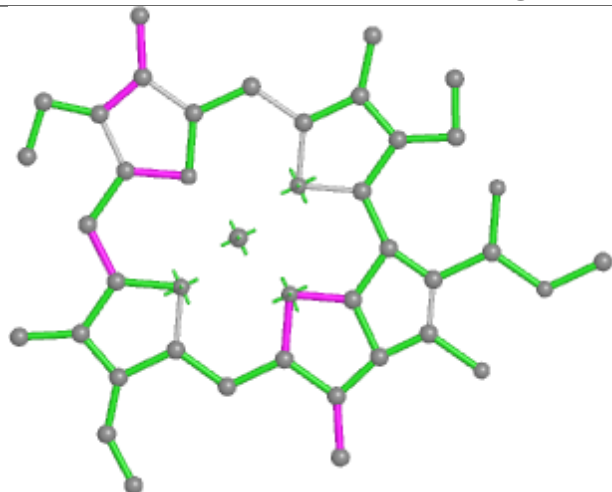
Ligand CLA b 614



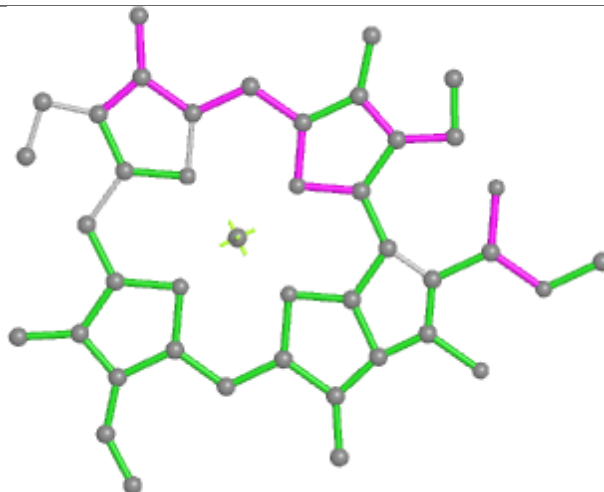
Ligand CLA c 513



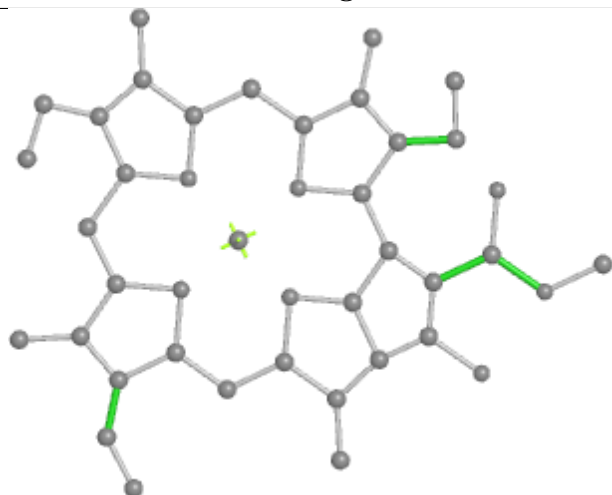
Ligand CLA G 614



Bond lengths



Bond angles

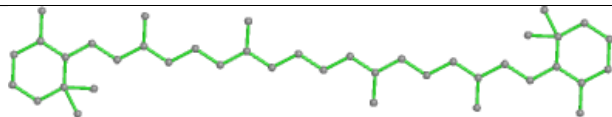


Torsions

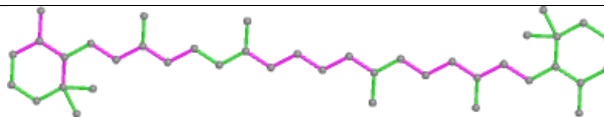


Rings

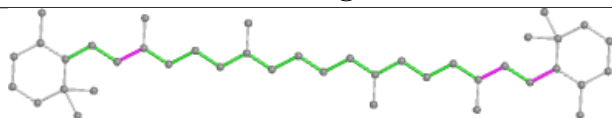
Ligand BCR B 617



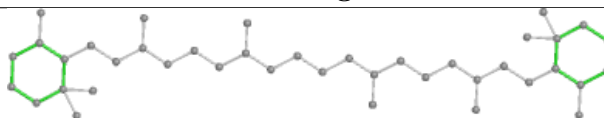
Bond lengths



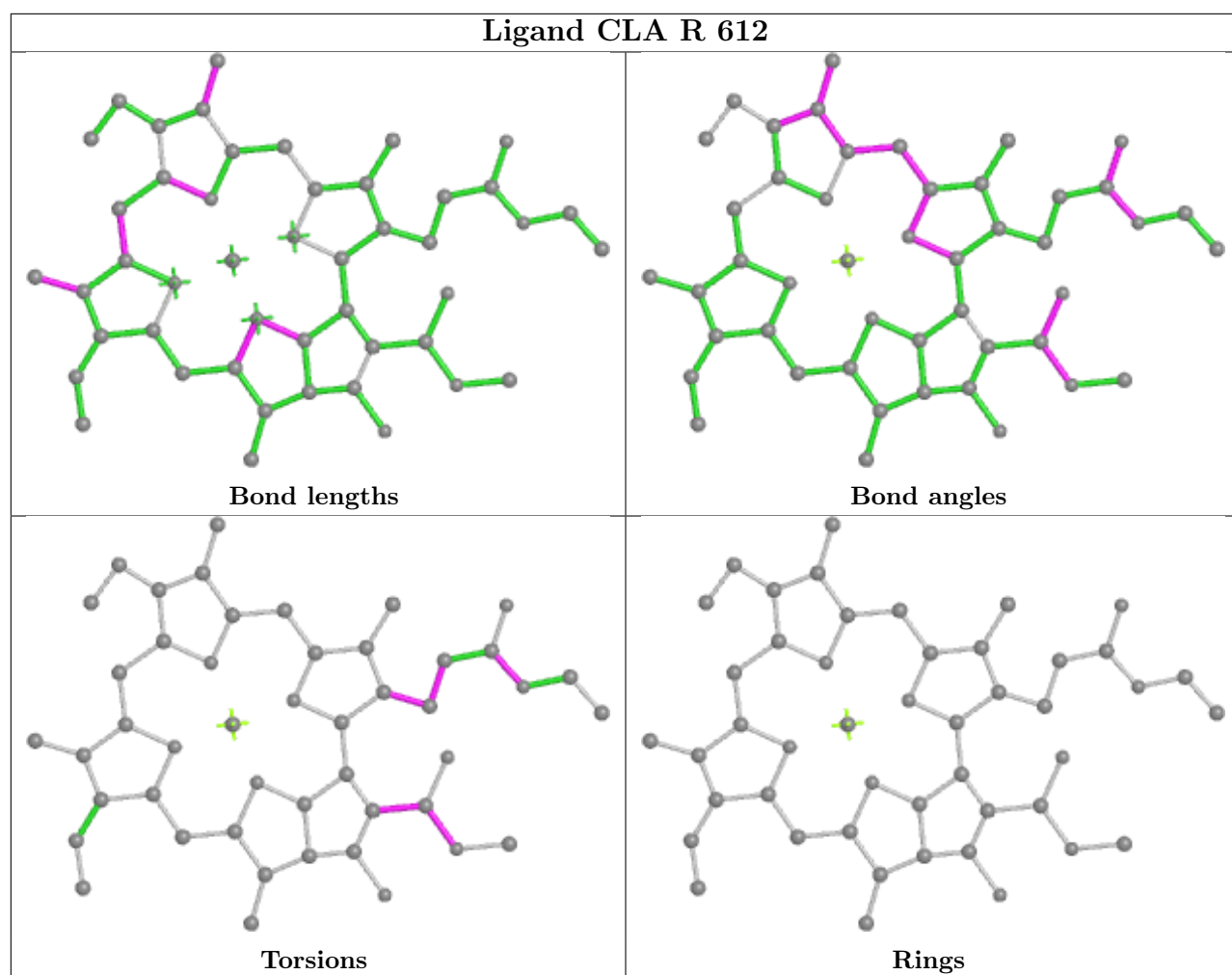
Bond angles



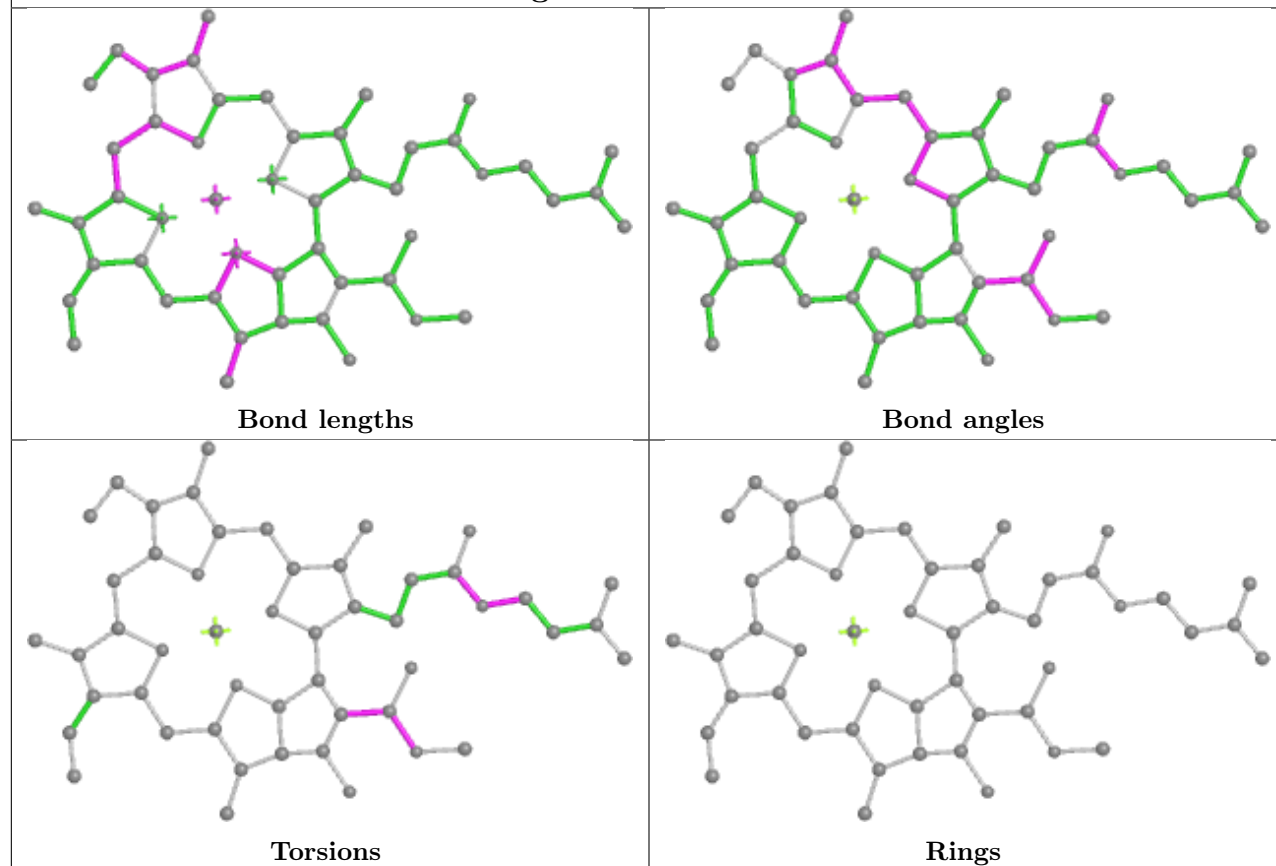
Torsions



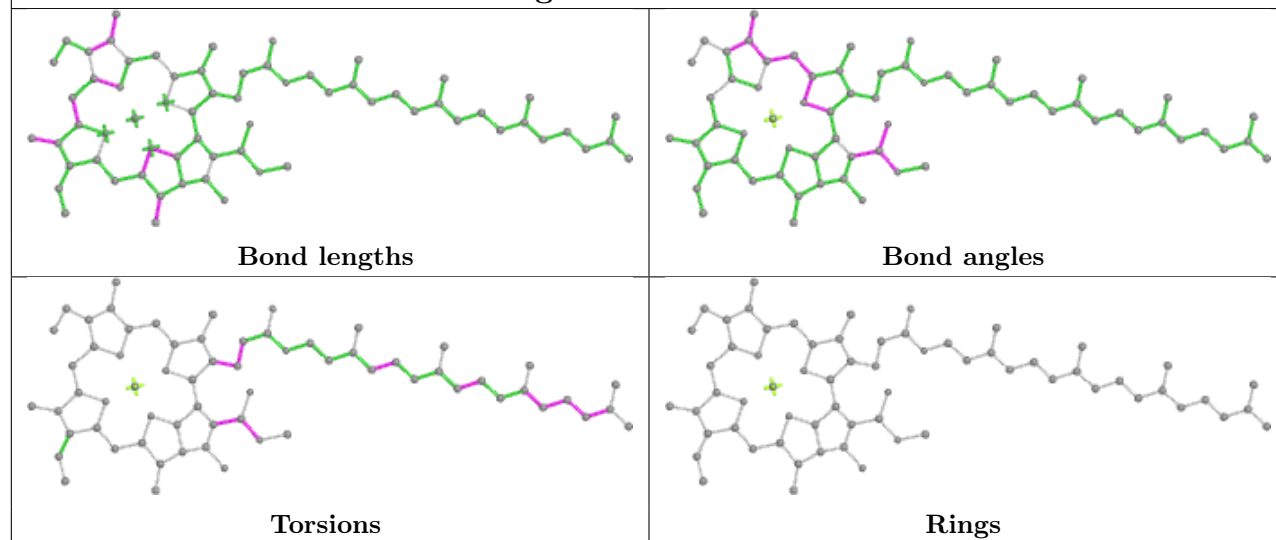
Rings

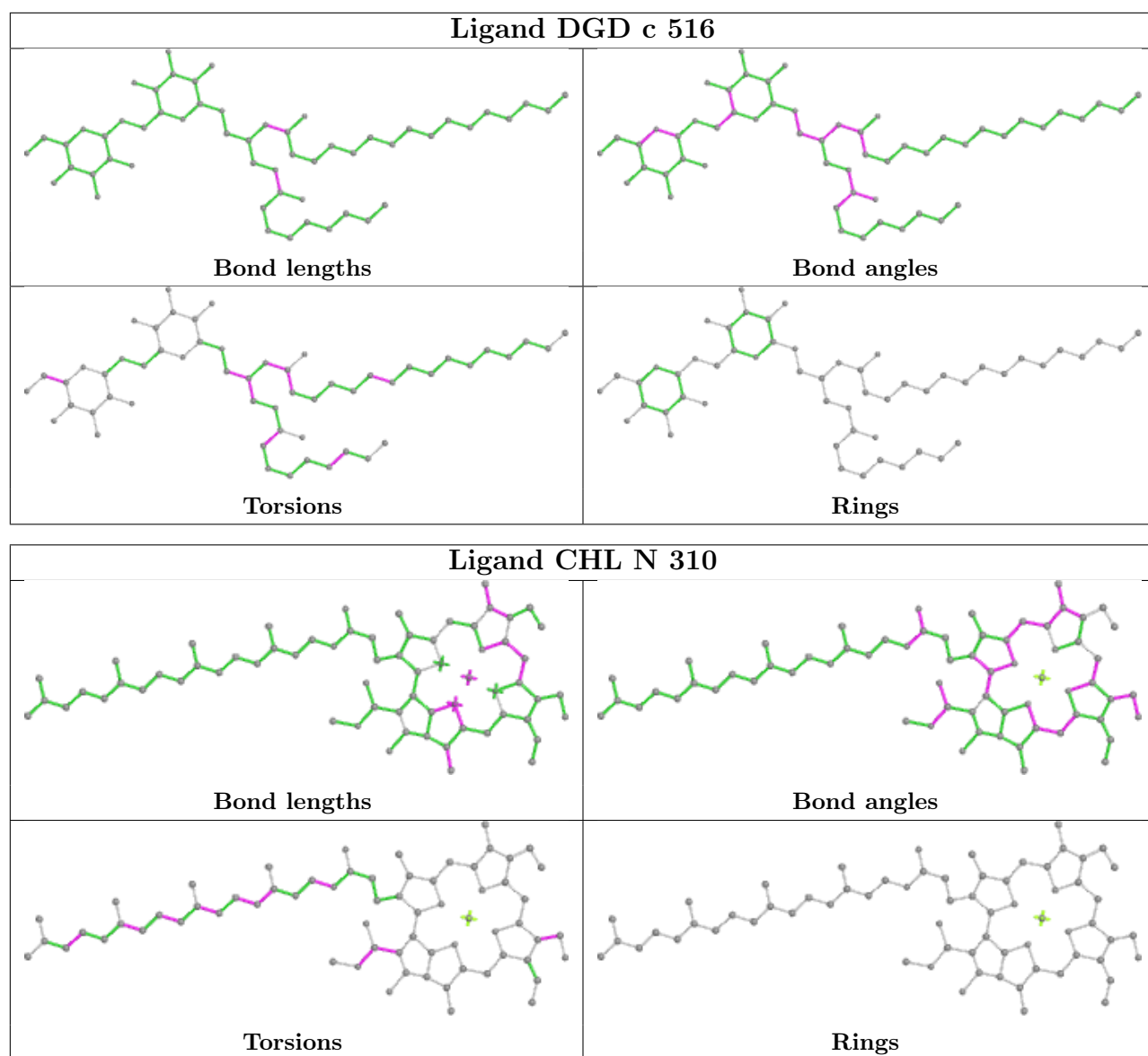


Ligand CLA N 305

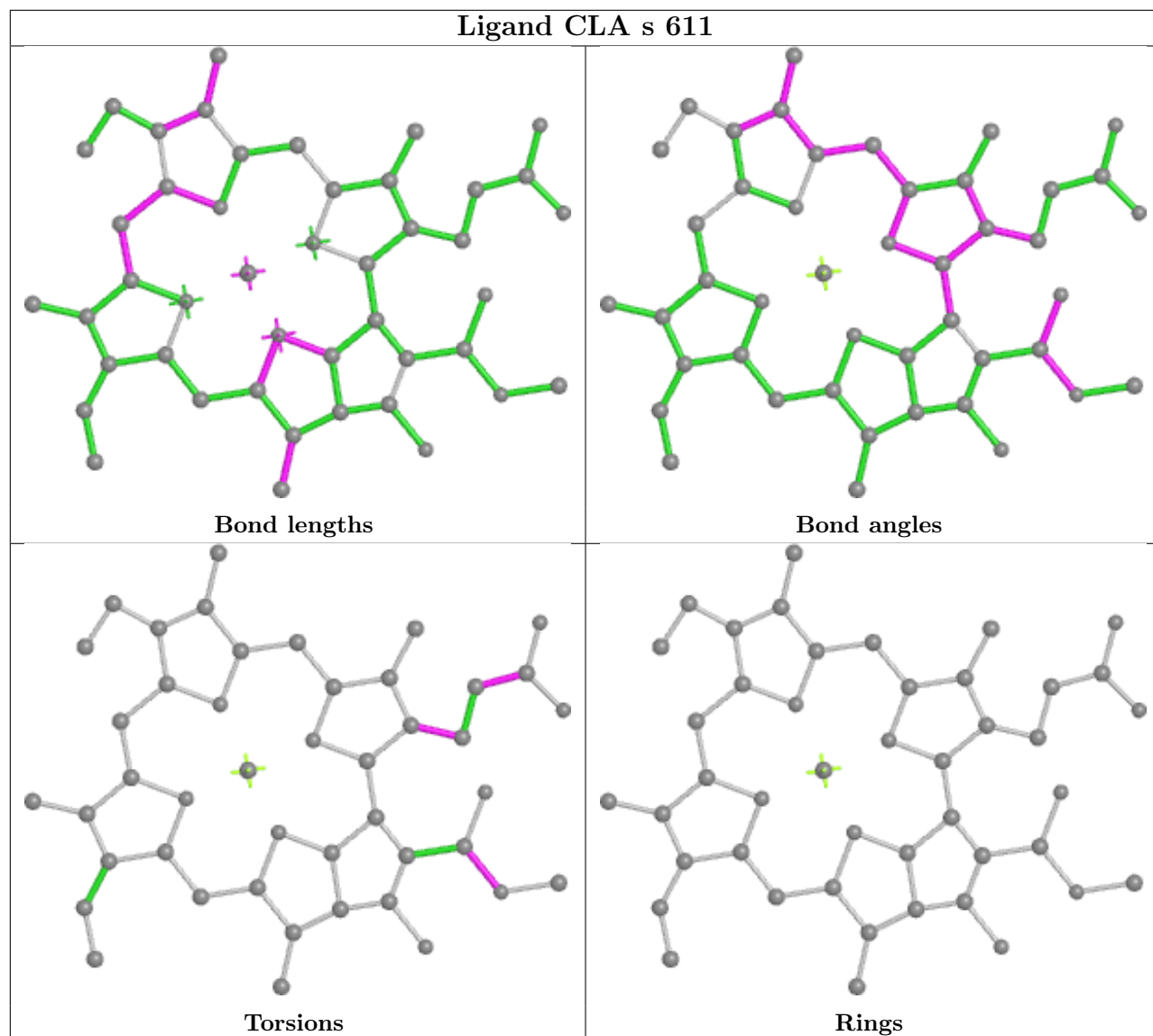


Ligand CLA d 405

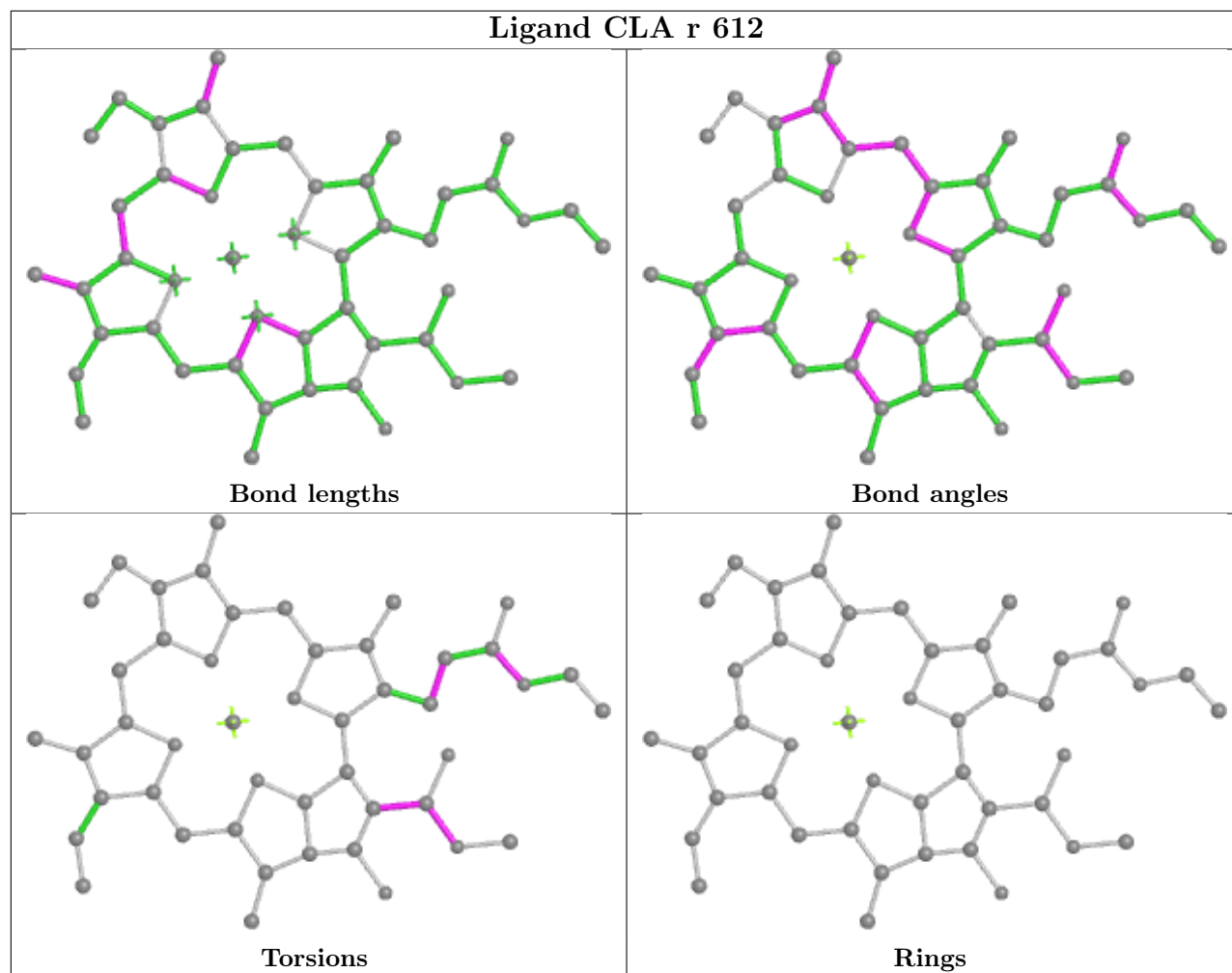




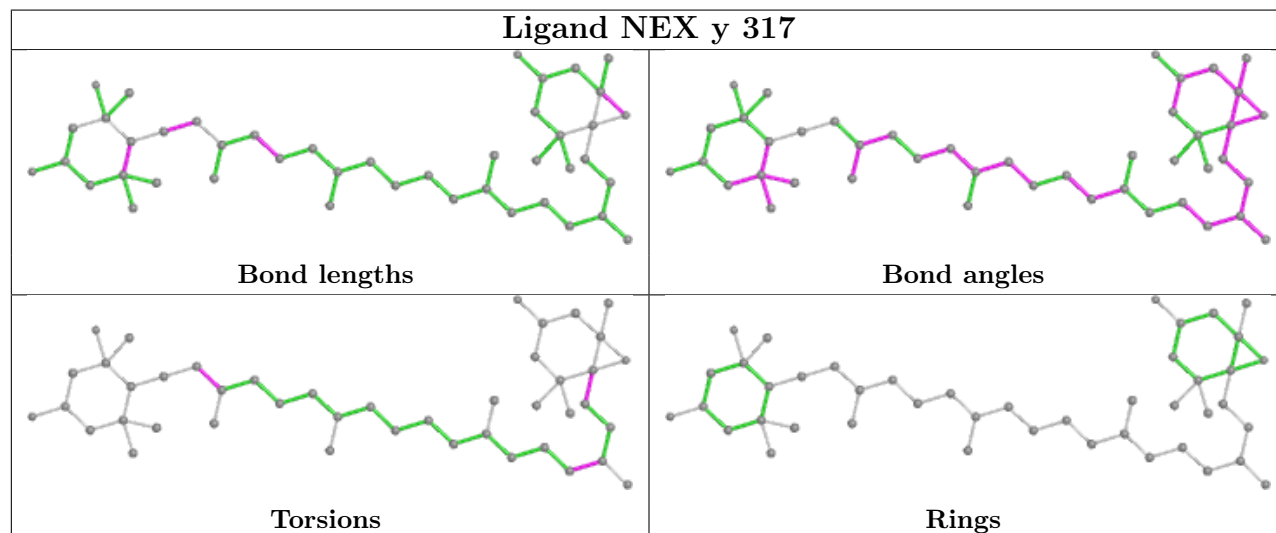
Ligand CLA s 611

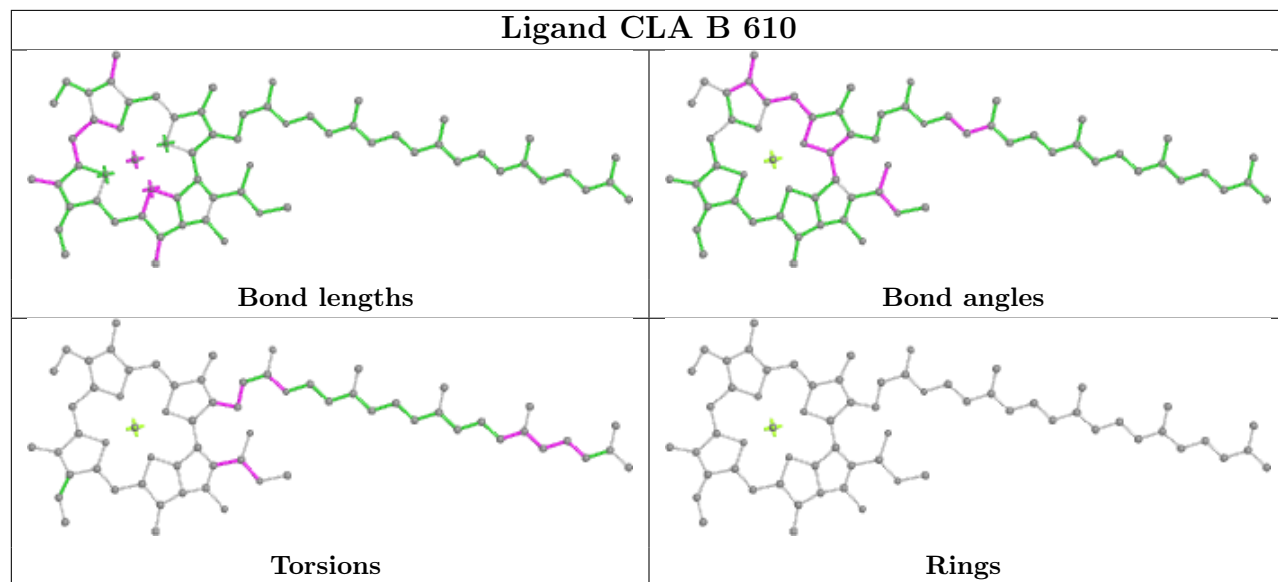
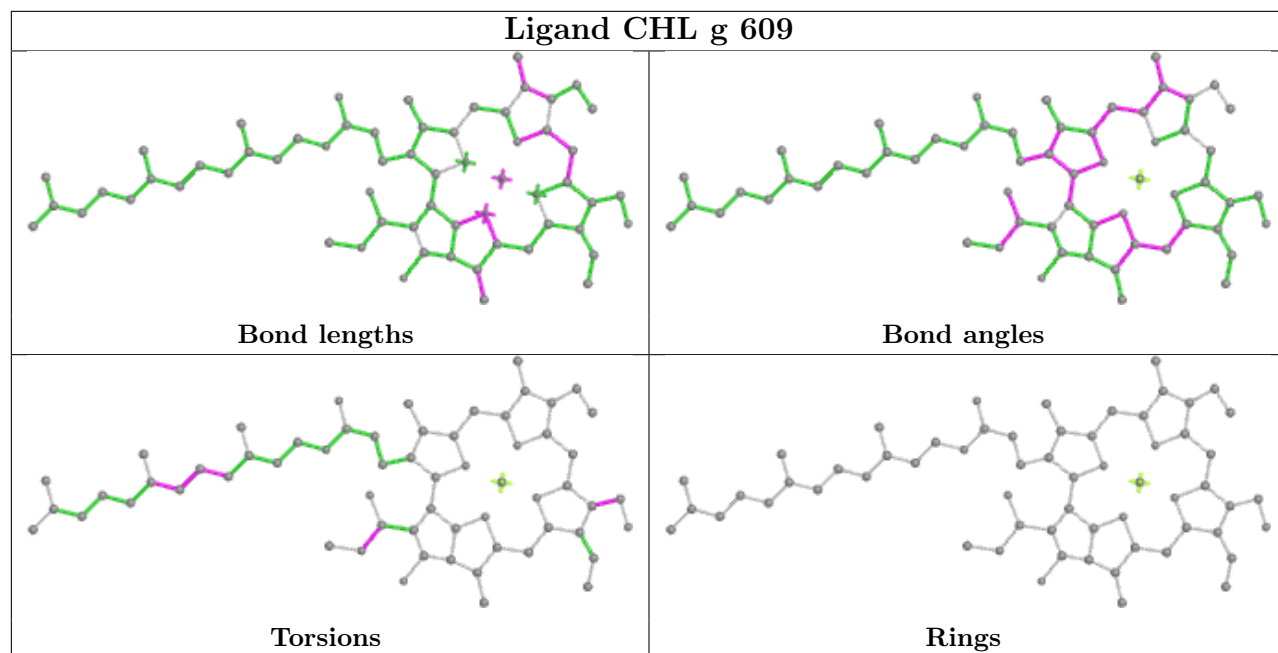


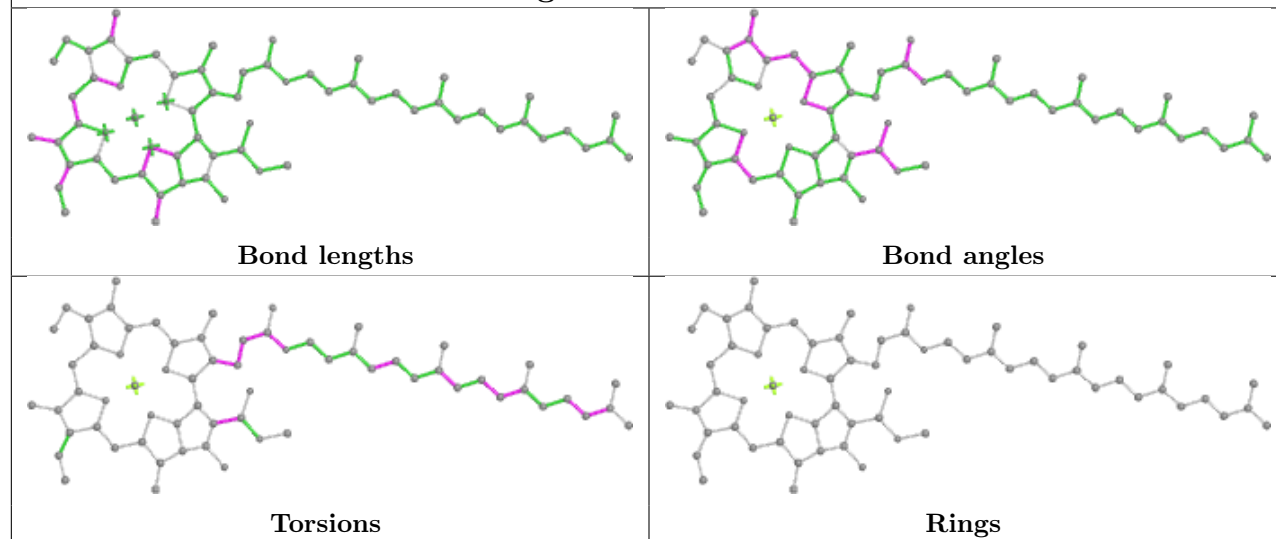
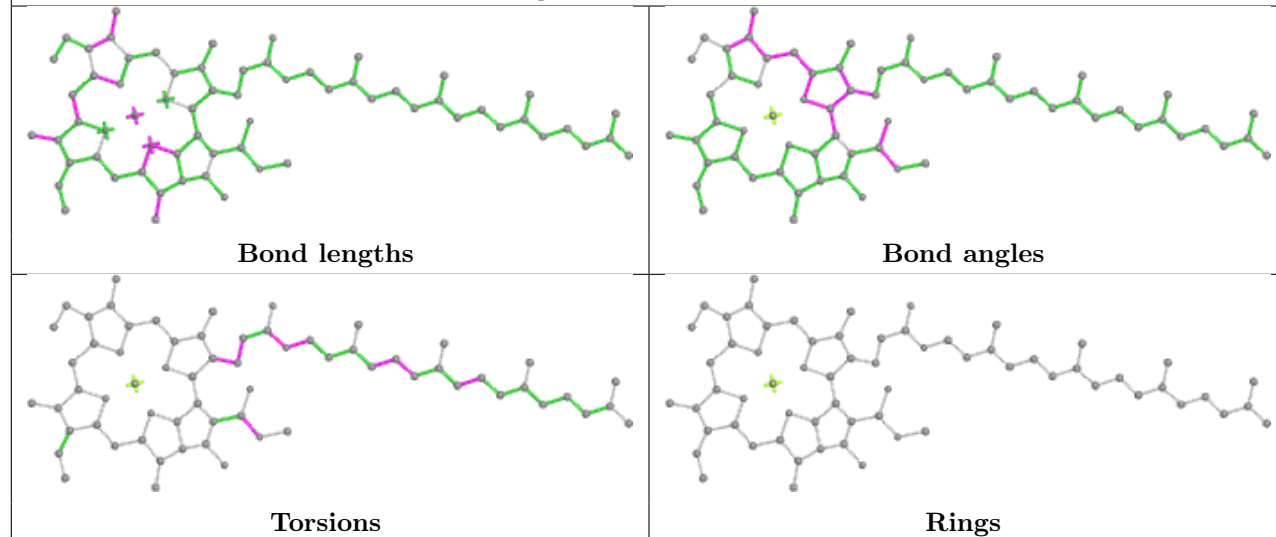
Ligand CLA r 612

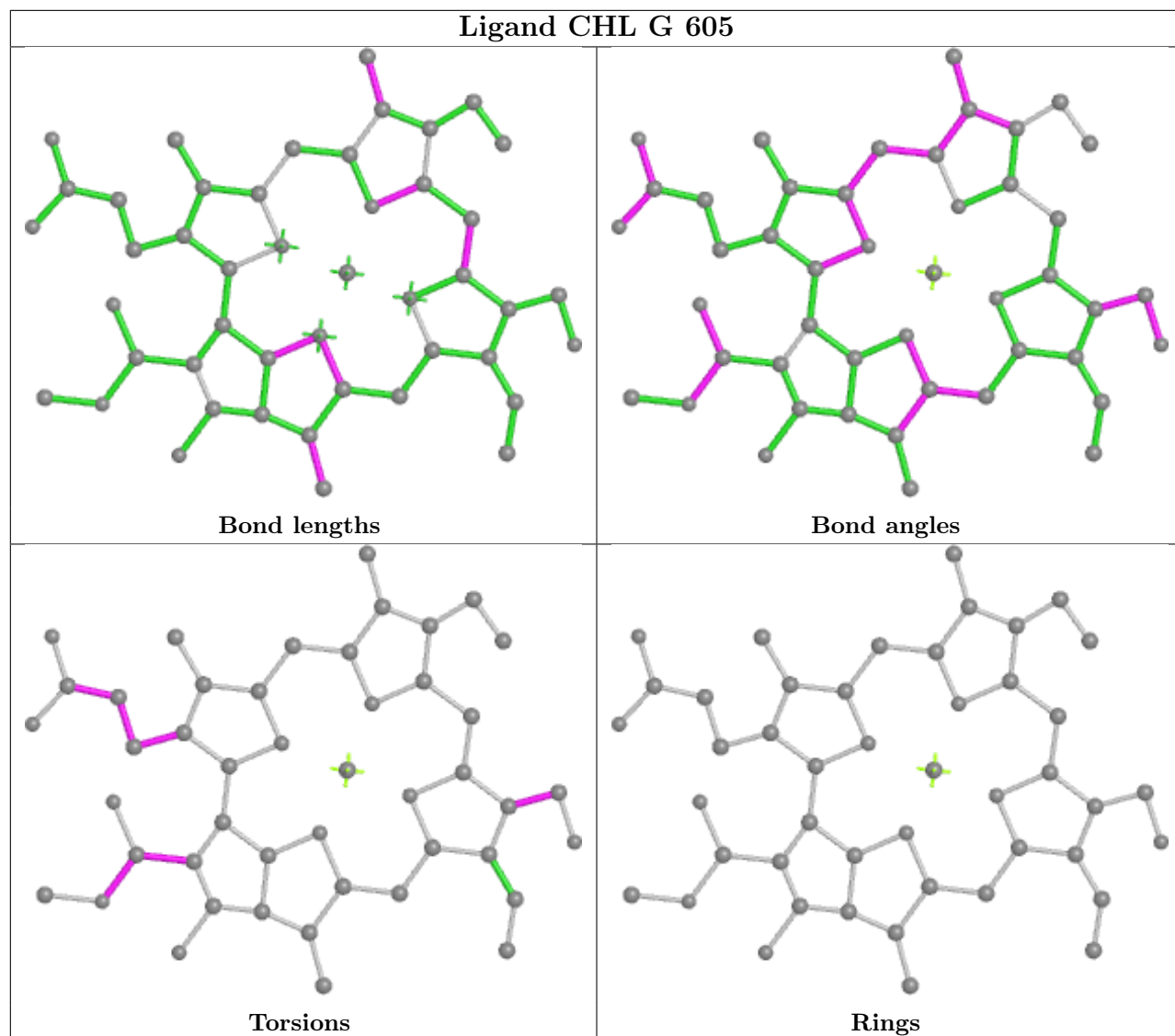


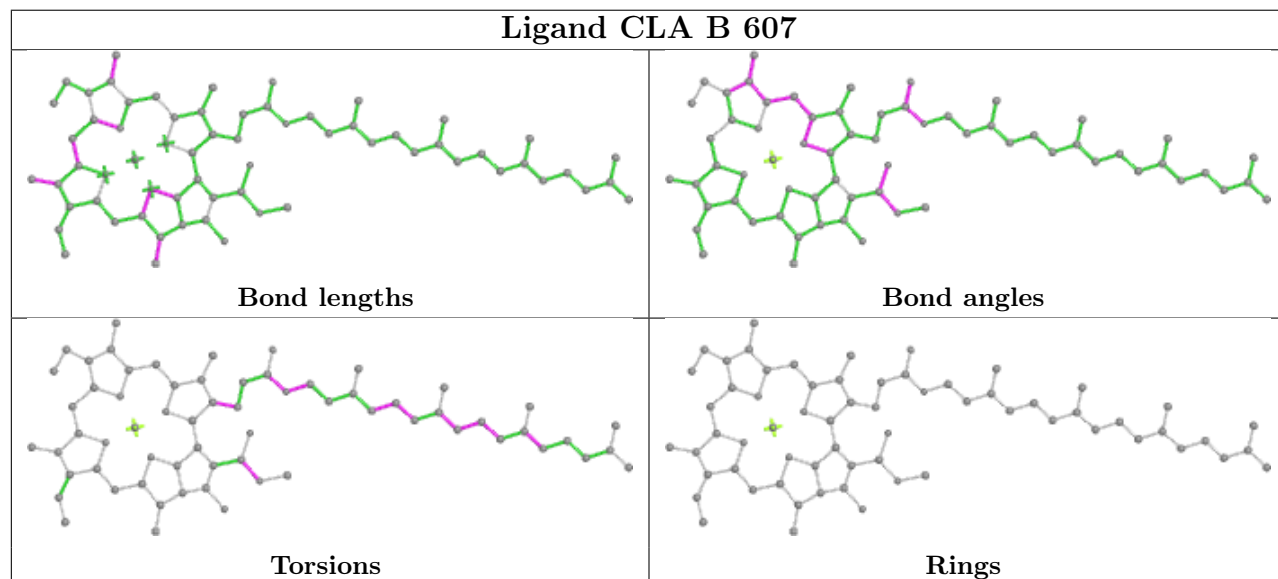
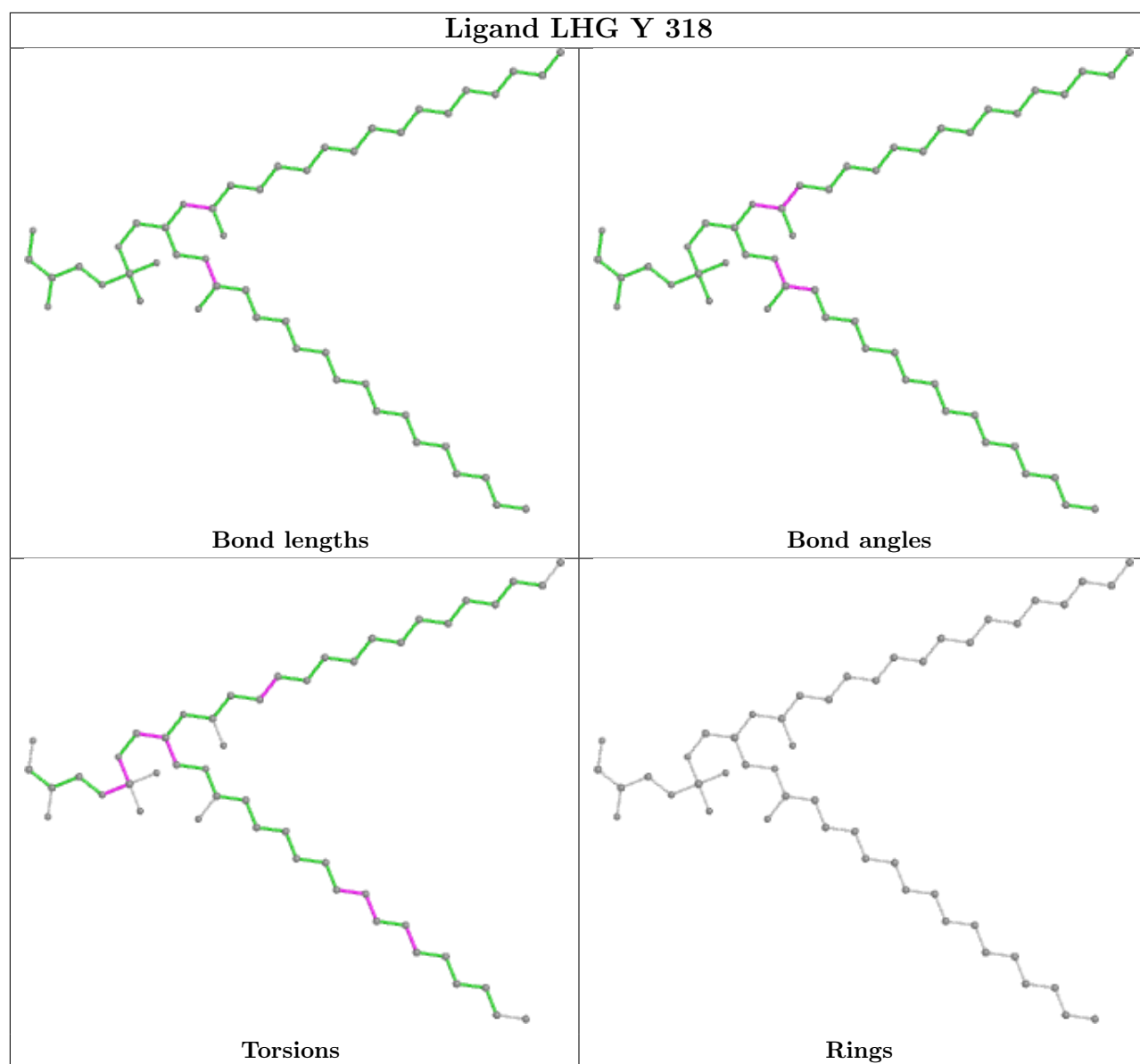
Ligand NEX y 317



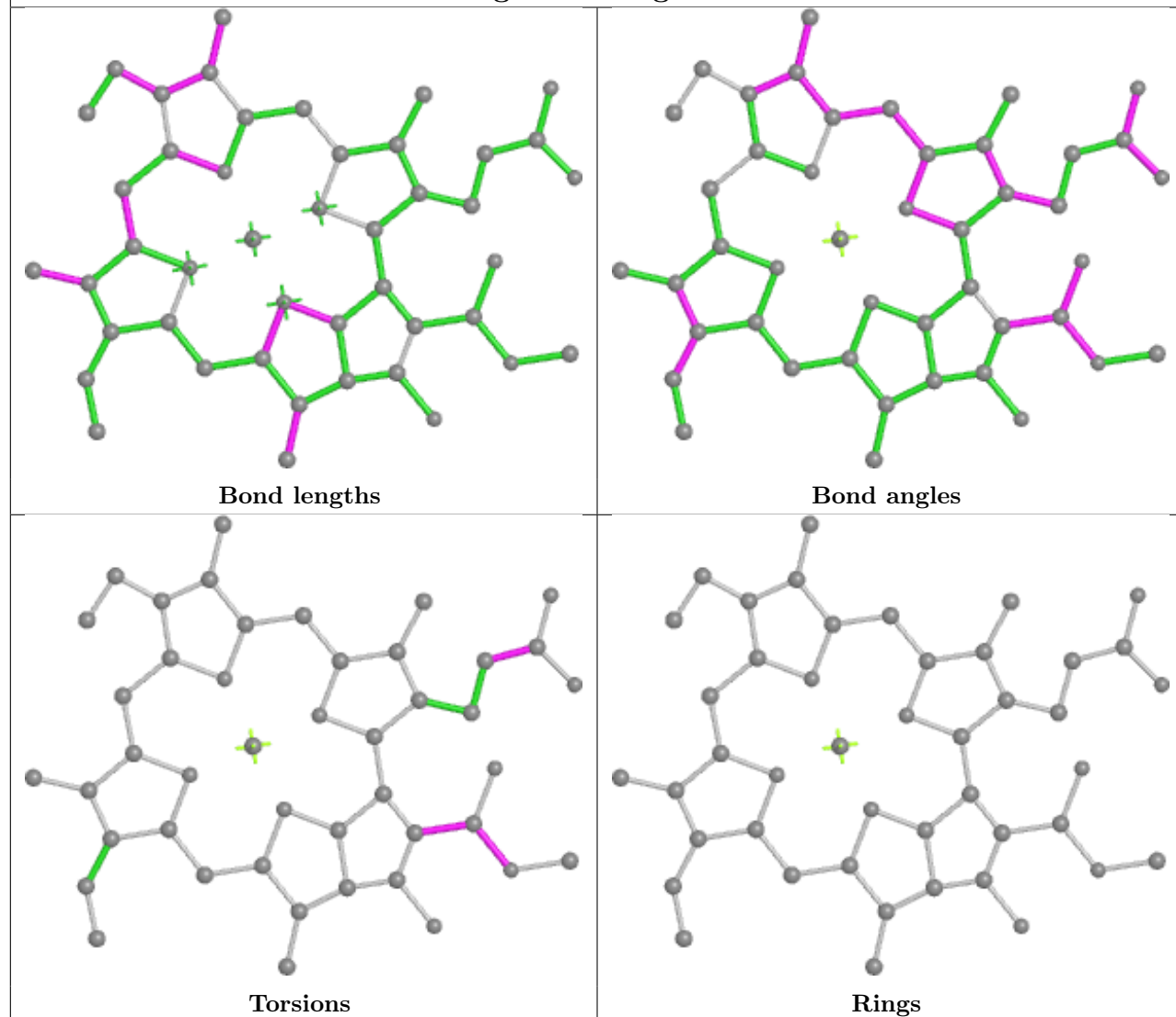


Ligand CLA c 510**Ligand CLA B 613**

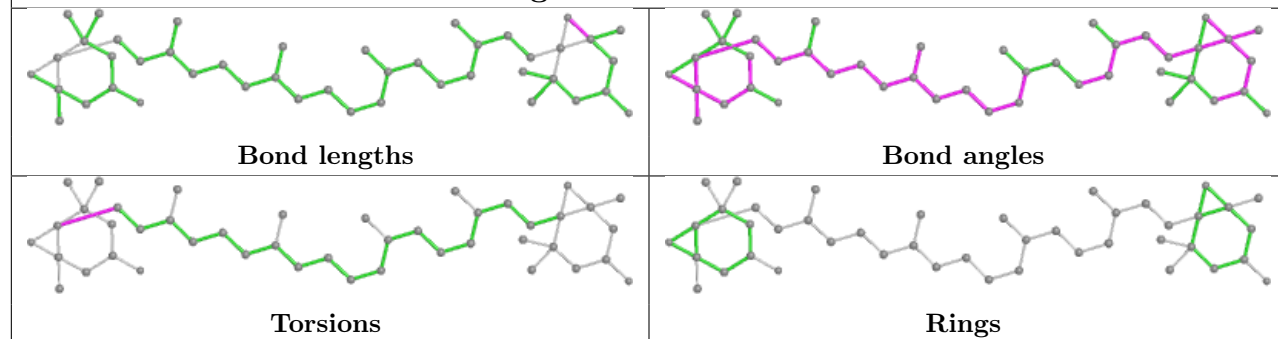


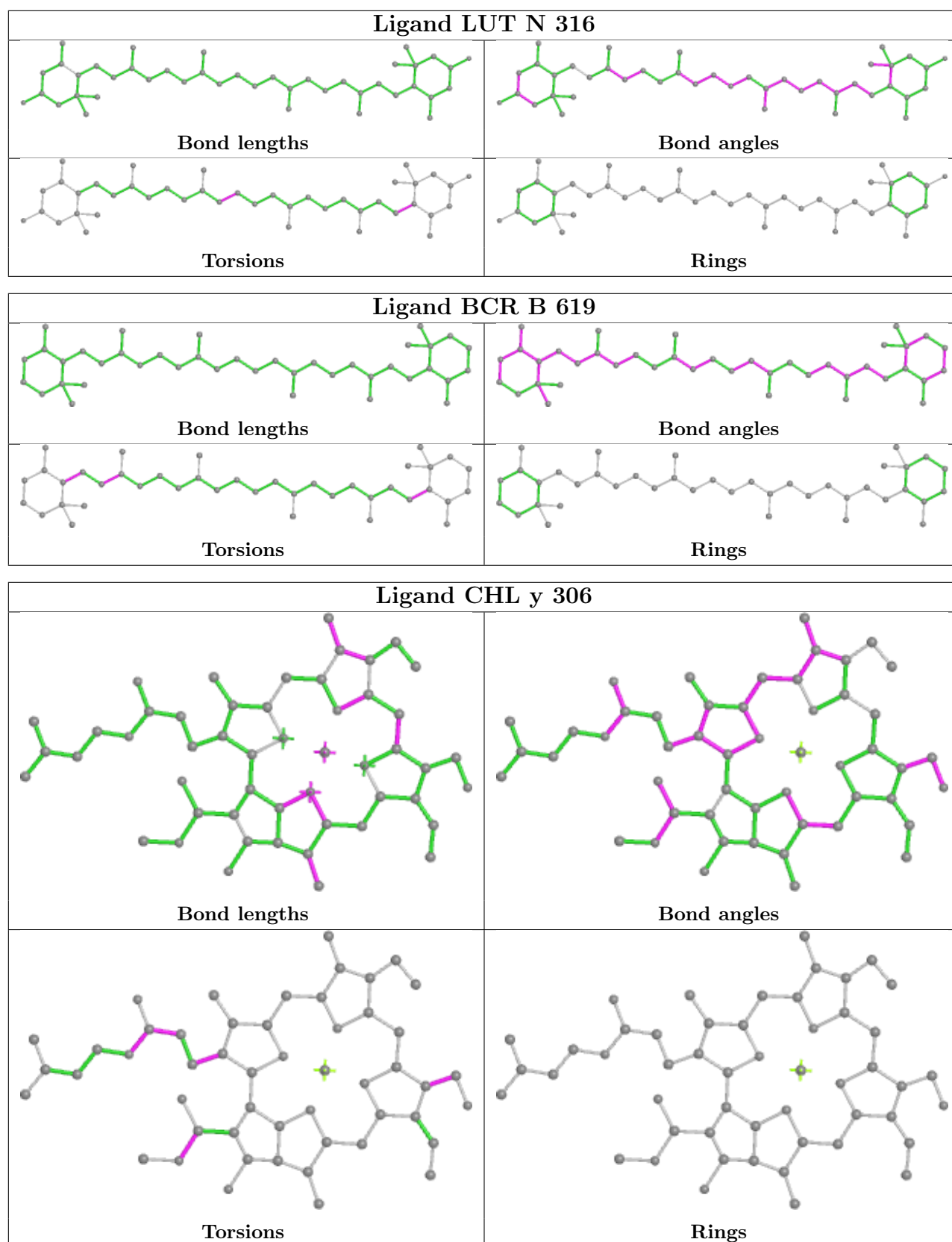


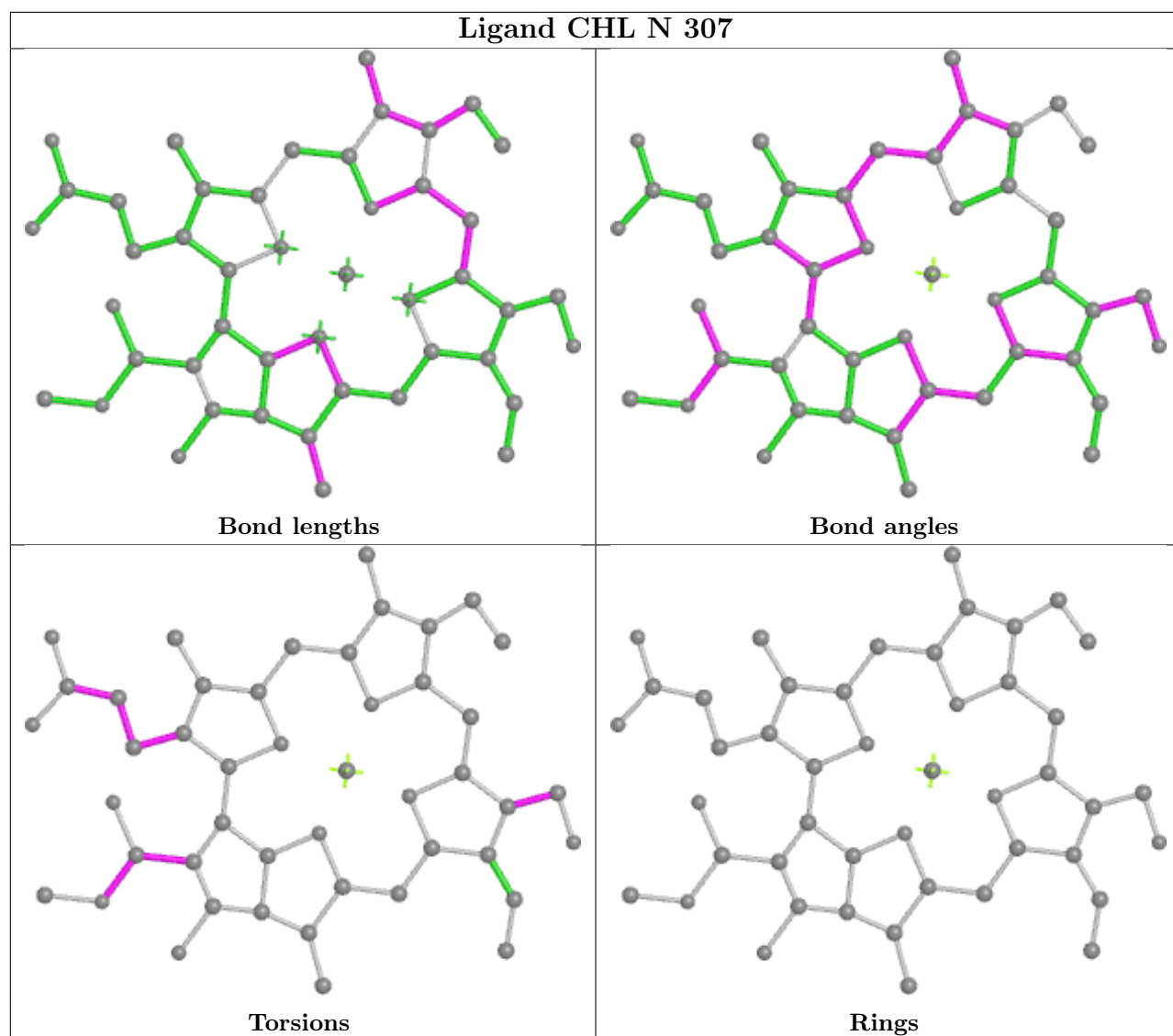
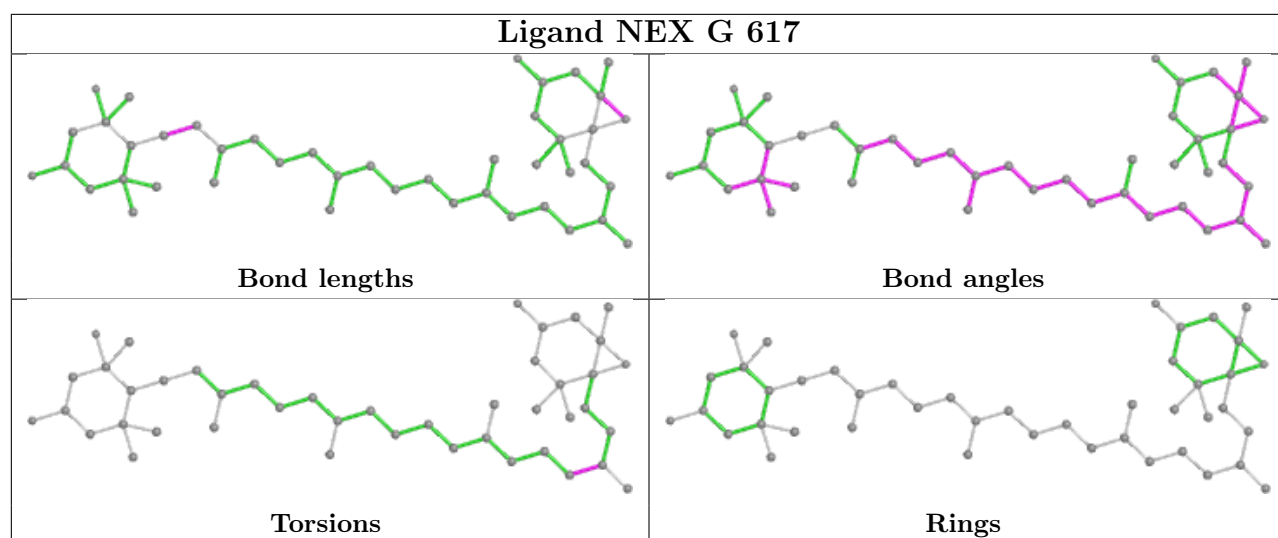
Ligand CLA g 612



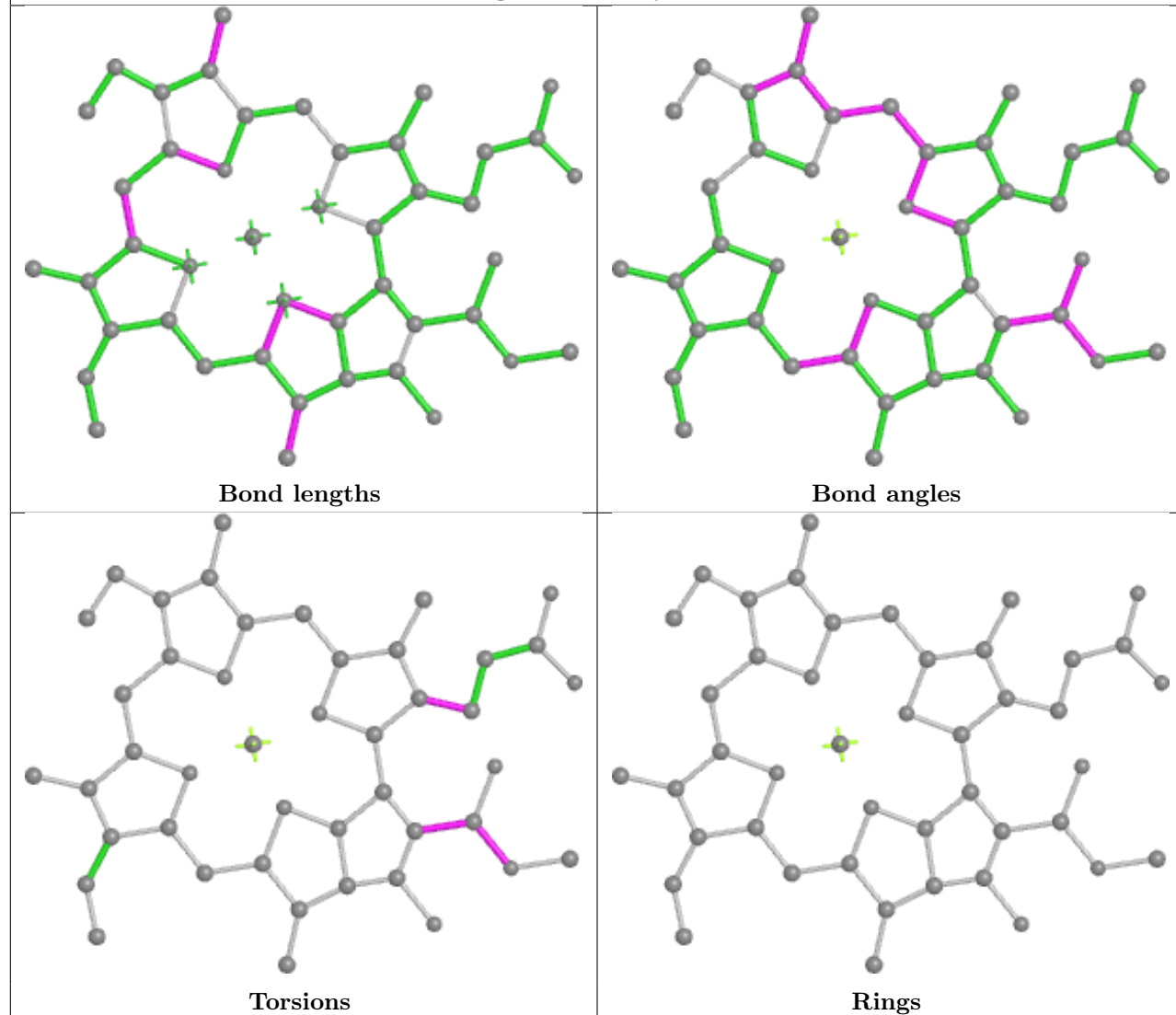
Ligand XAT N 301



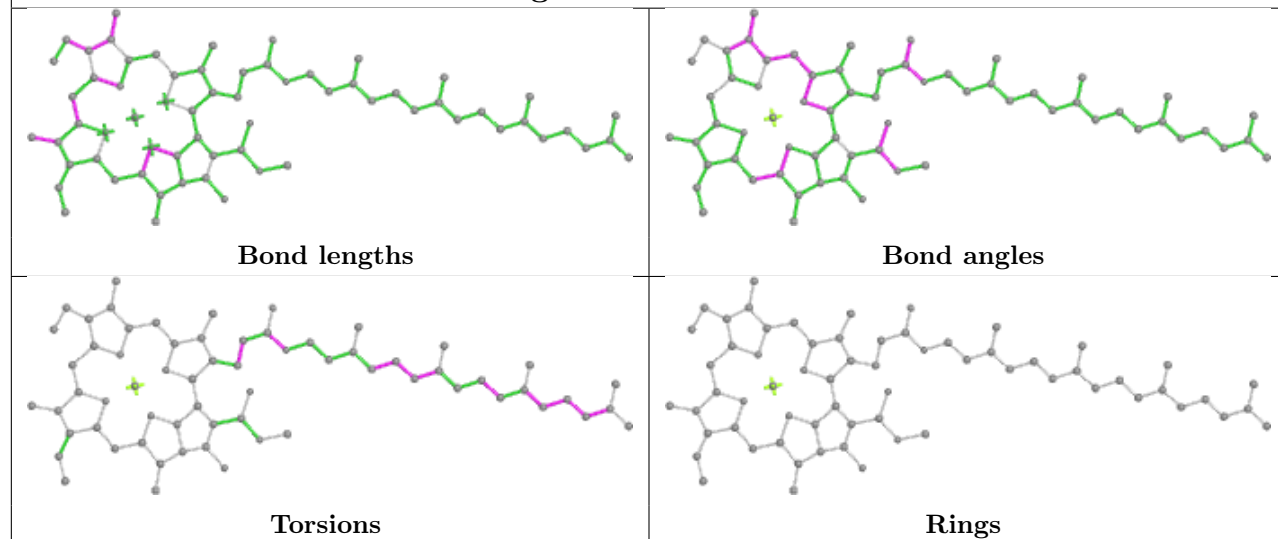


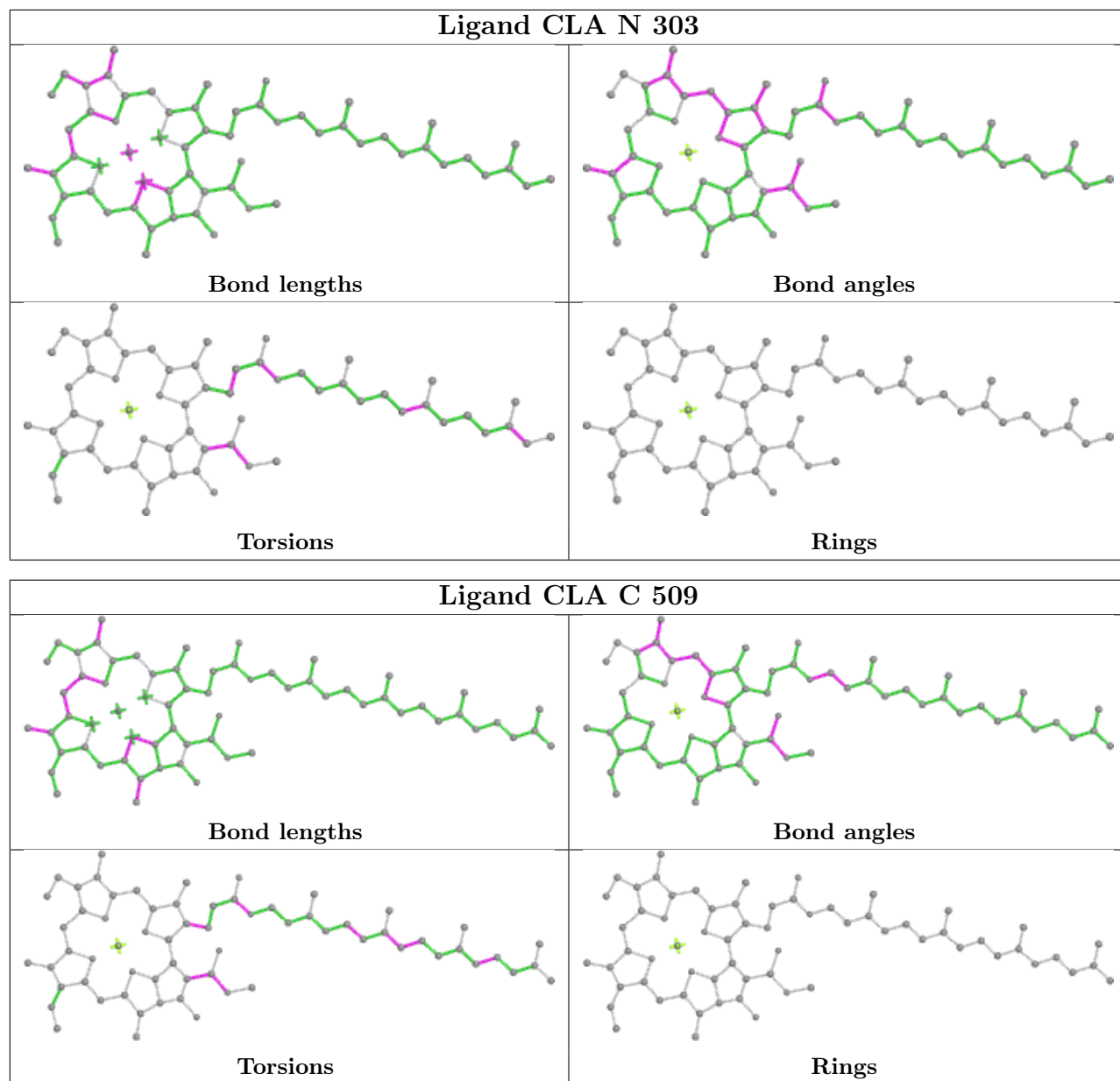


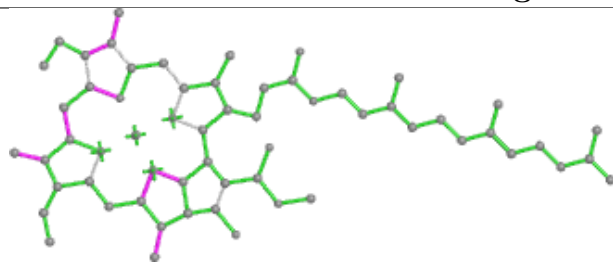
Ligand CLA y 314



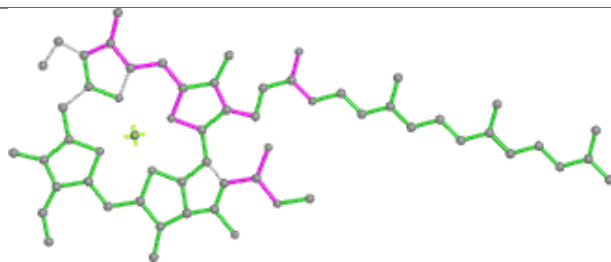
Ligand CLA G 602



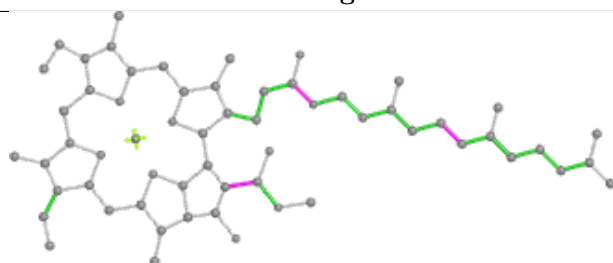


Ligand CLA R 603

Bond lengths



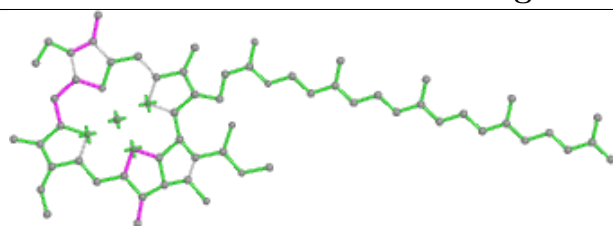
Bond angles



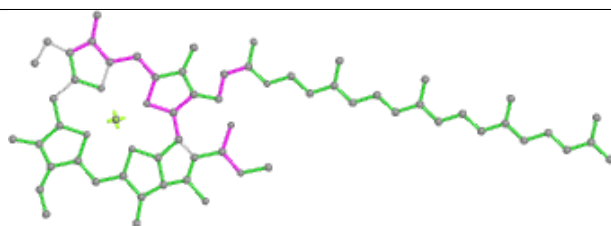
Torsions



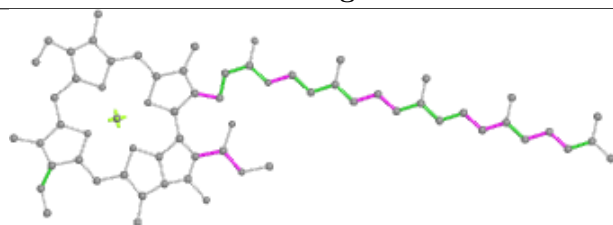
Rings

Ligand CLA B 604

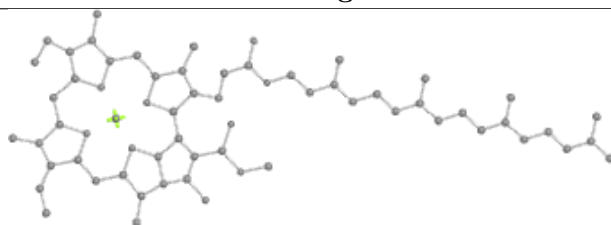
Bond lengths



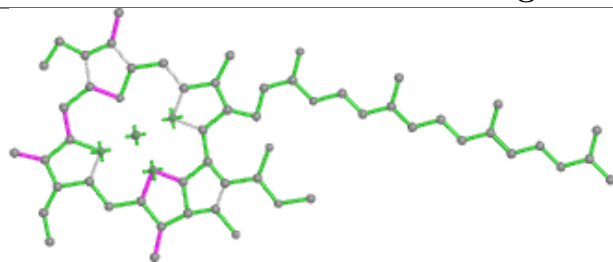
Bond angles



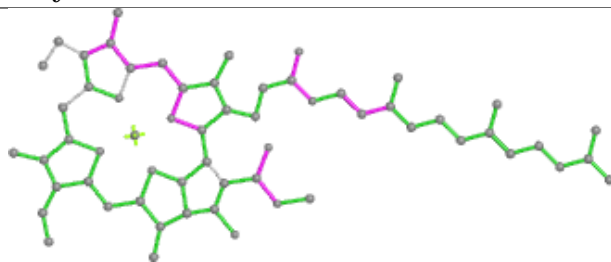
Torsions



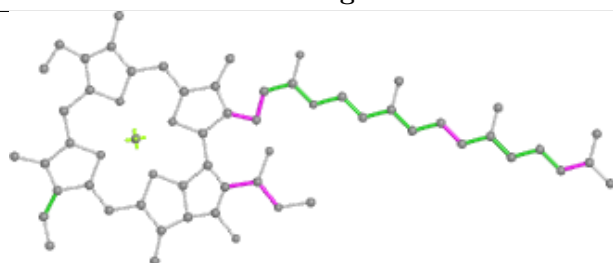
Rings

Ligand CLA y 310

Bond lengths



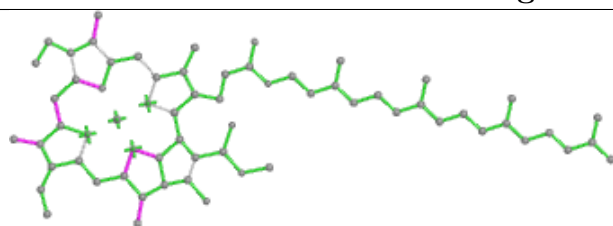
Bond angles



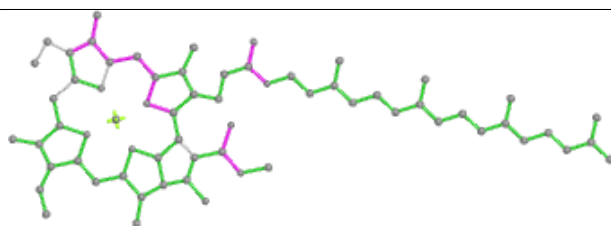
Torsions



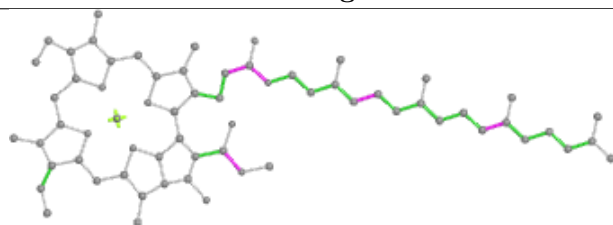
Rings

Ligand CLA b 602

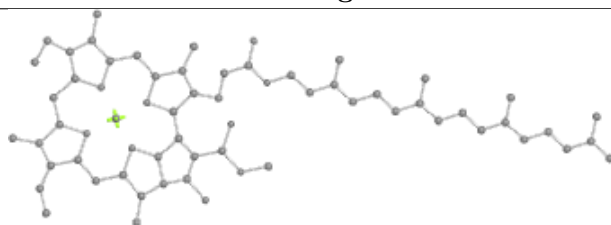
Bond lengths



Bond angles

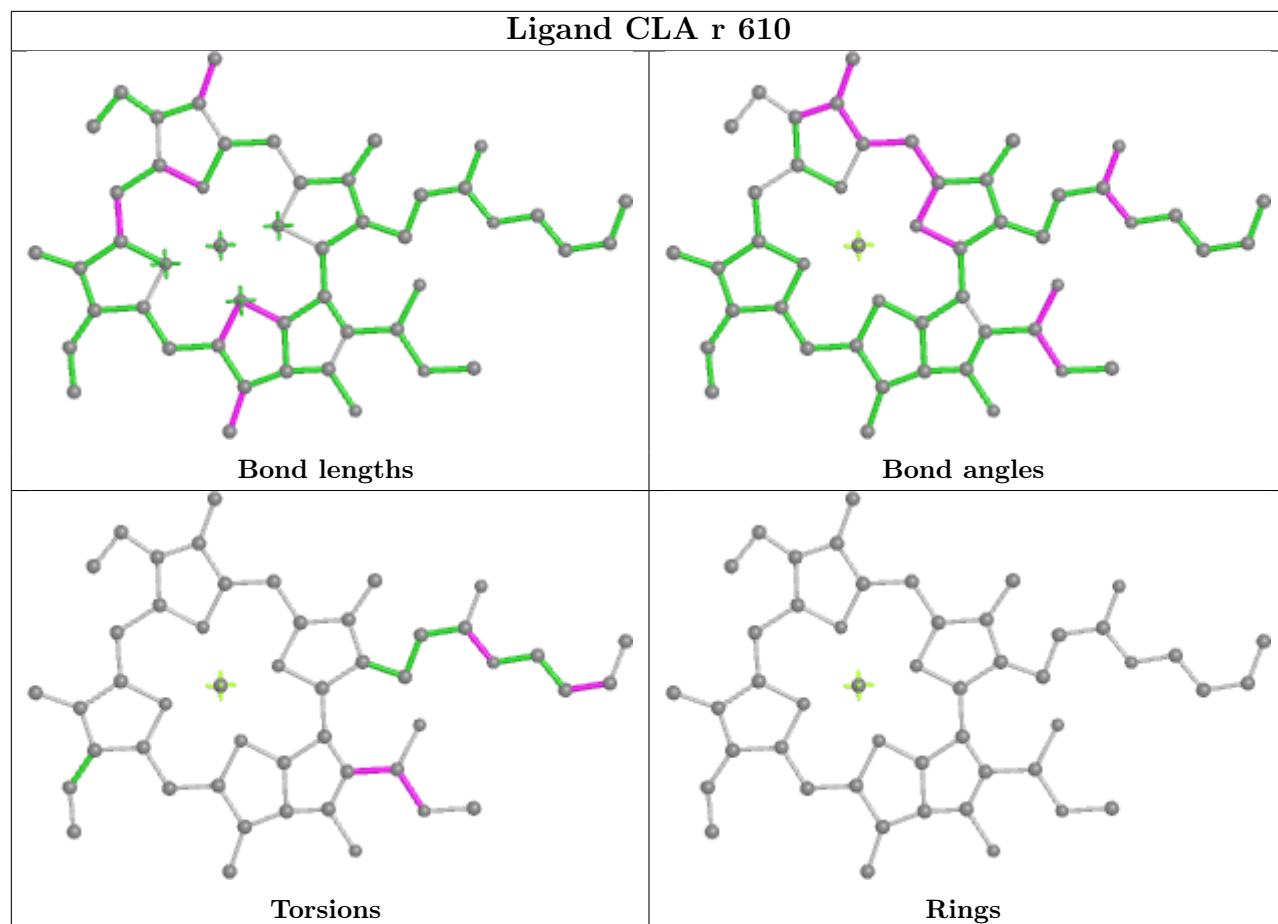


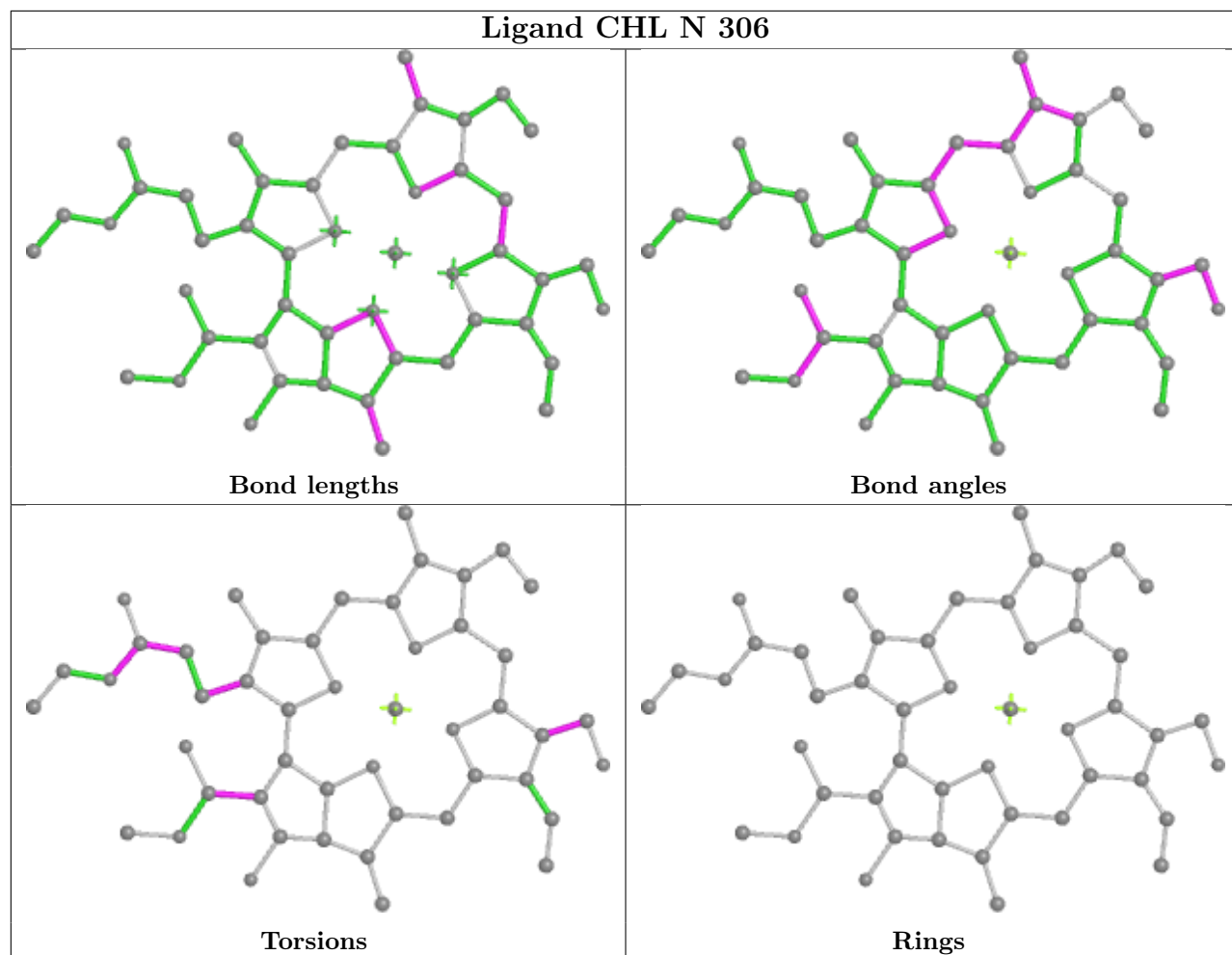
Torsions



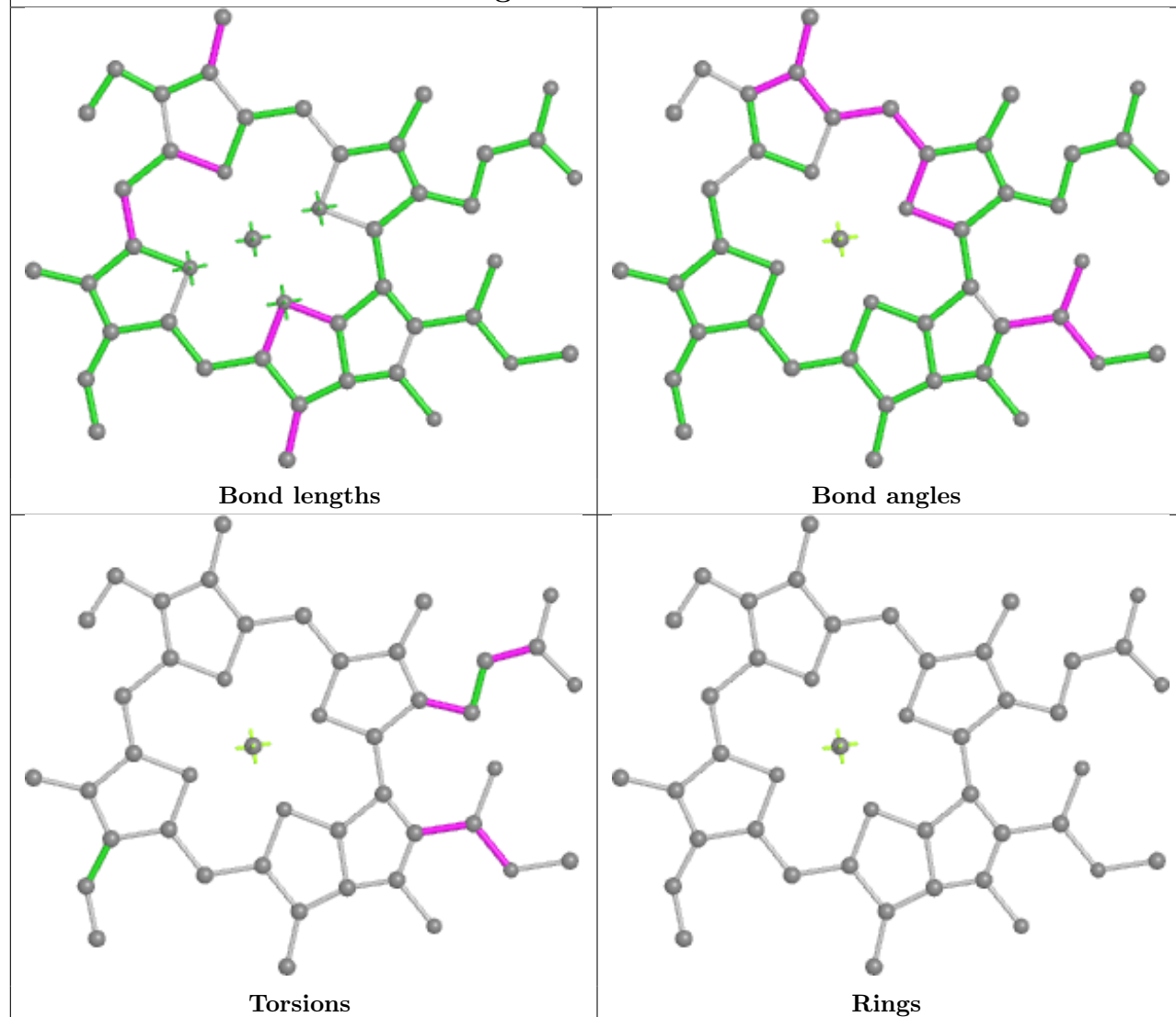
Rings

Ligand CLA r 610

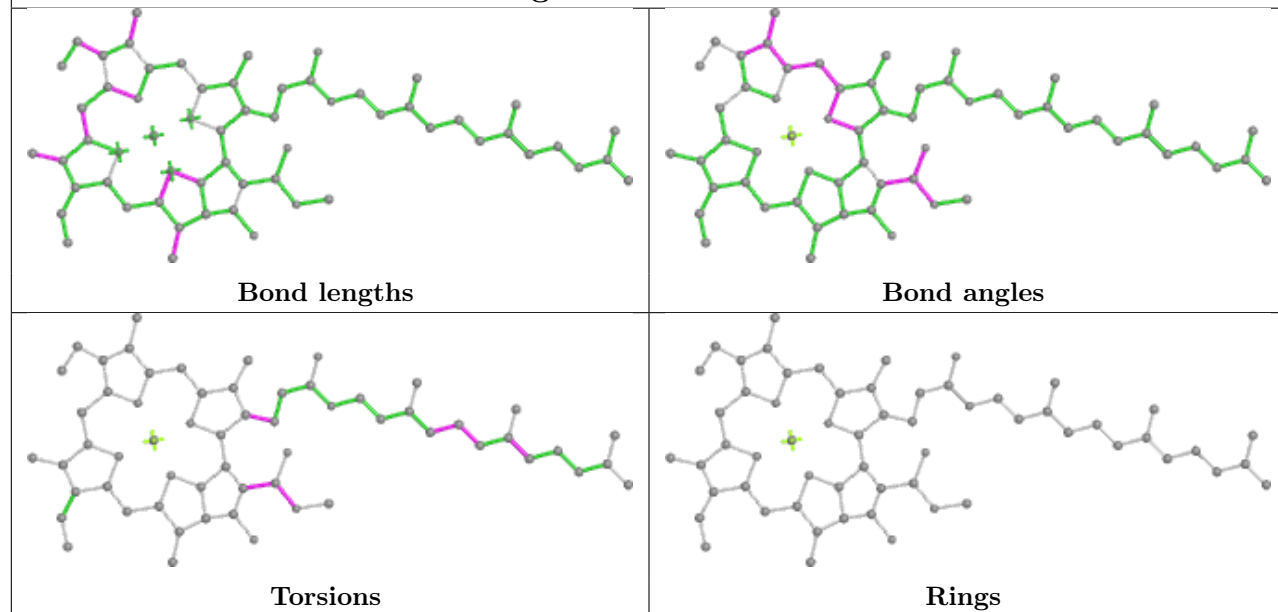


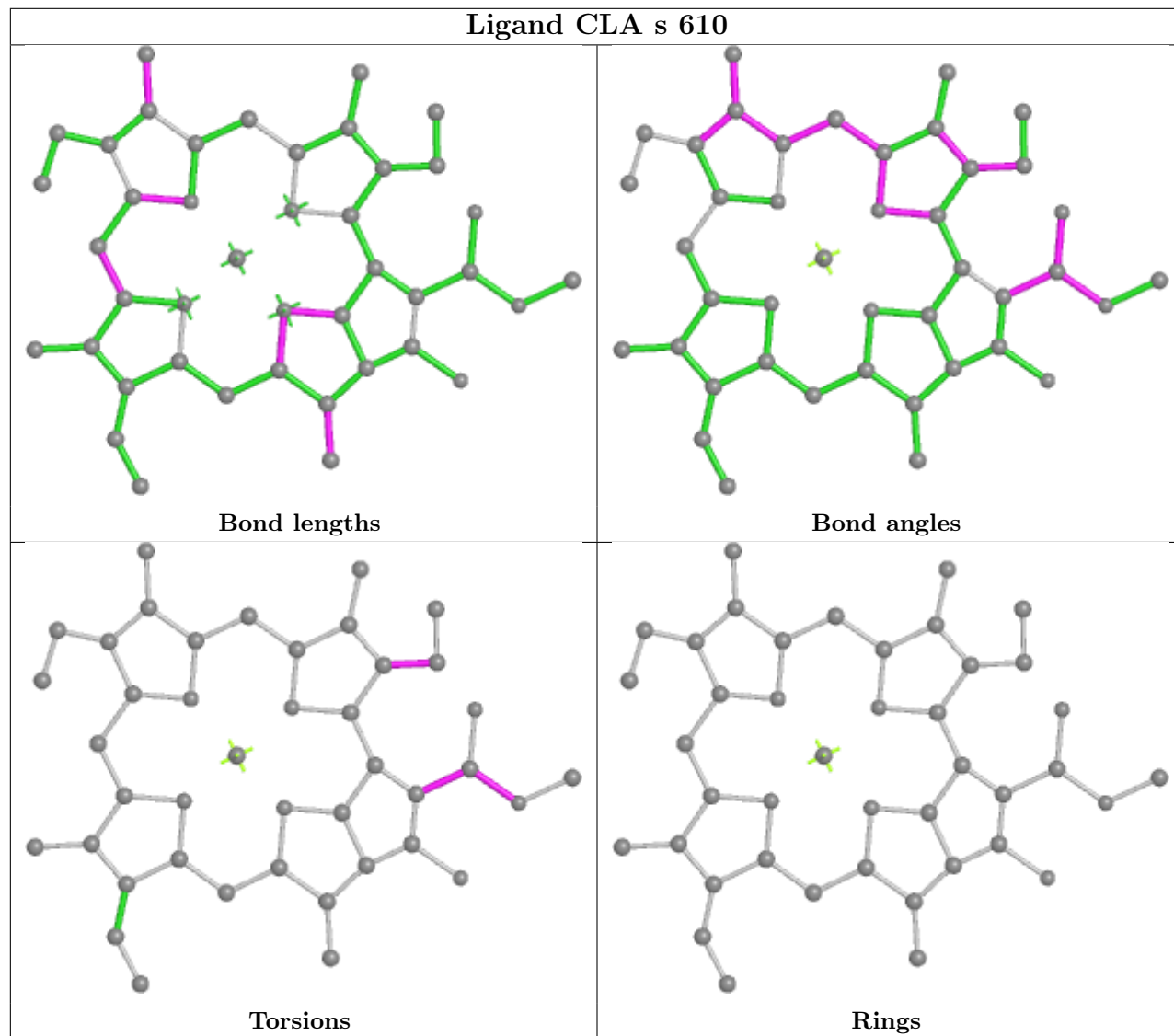
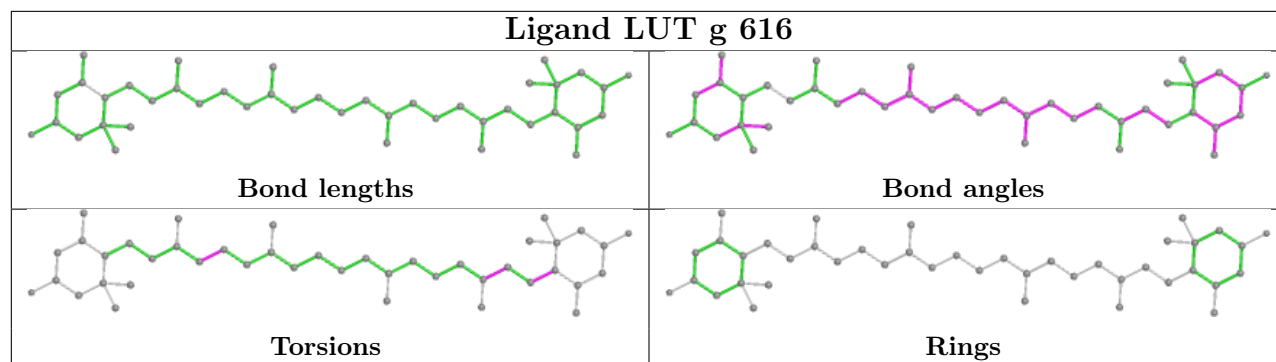


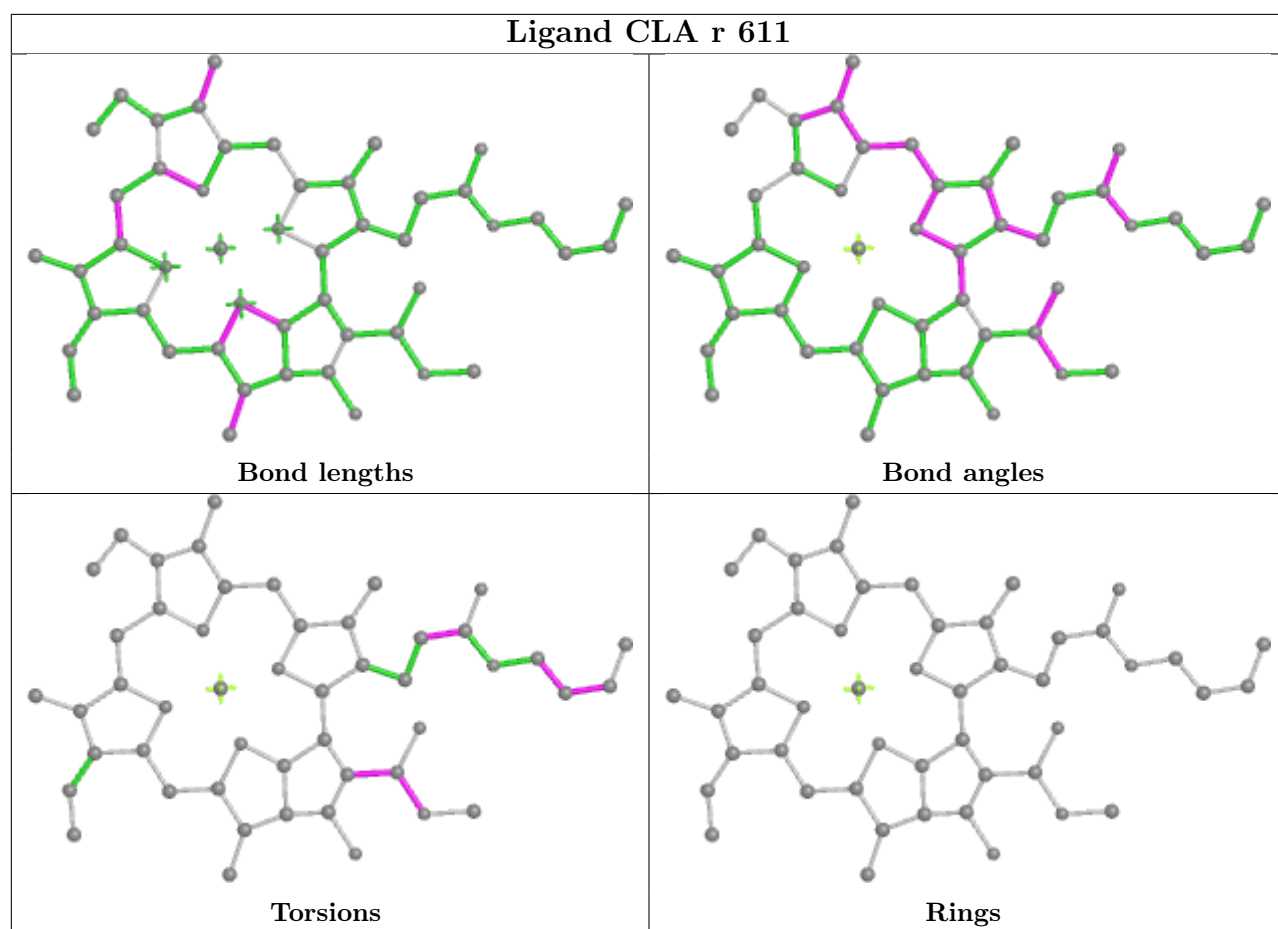
Ligand CLA r 614



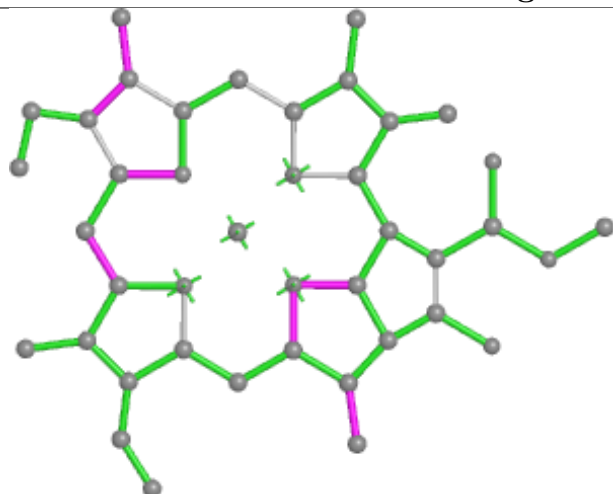
Ligand CLA A 404



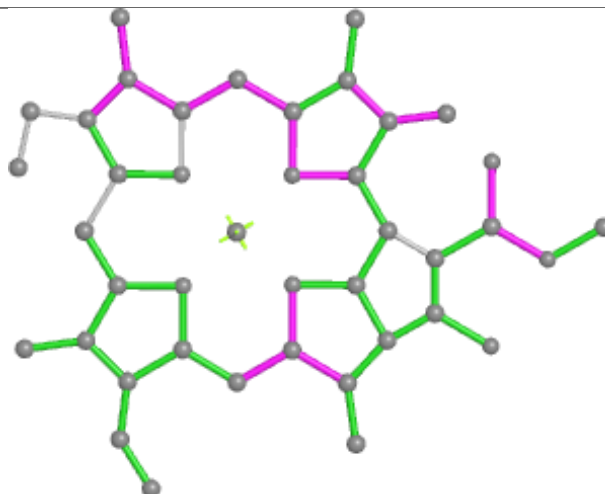




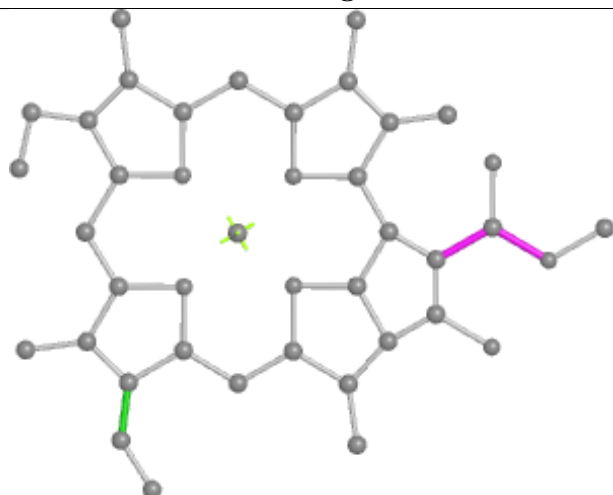
Ligand CLA S 613



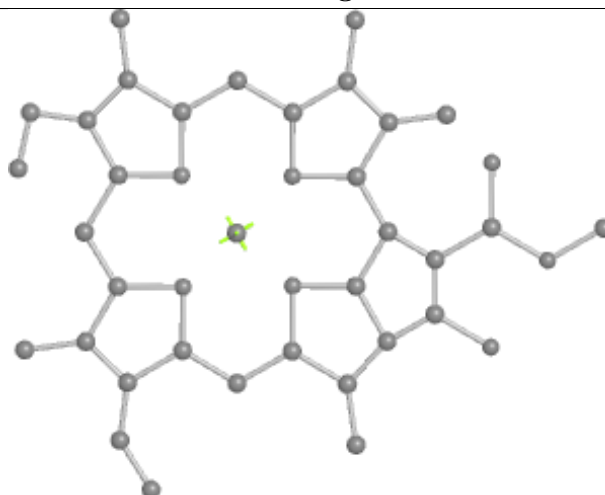
Bond lengths



Bond angles

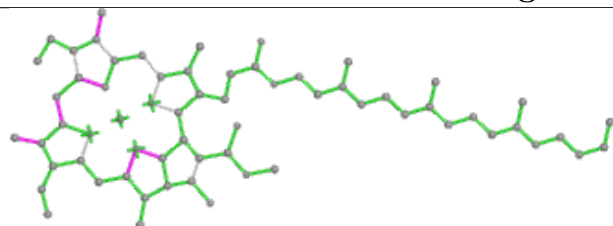


Torsions

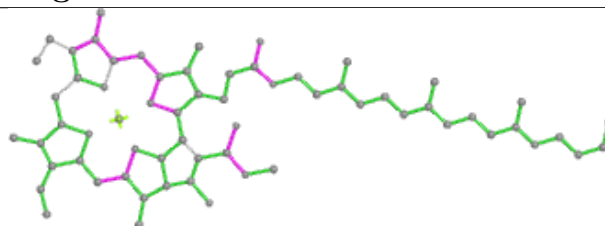


Rings

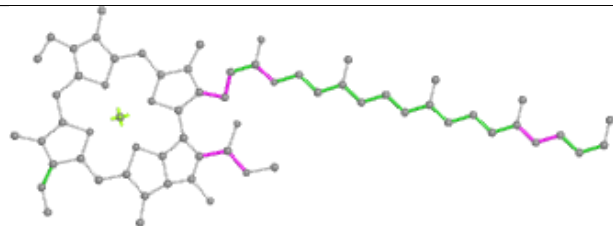
Ligand CLA g 610



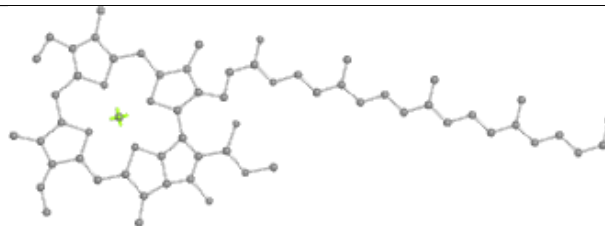
Bond lengths



Bond angles

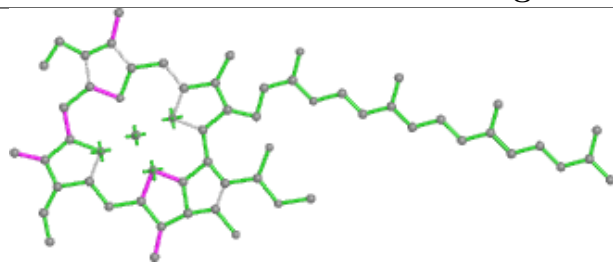


Torsions

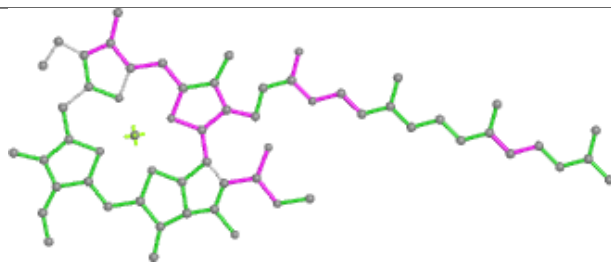


Rings

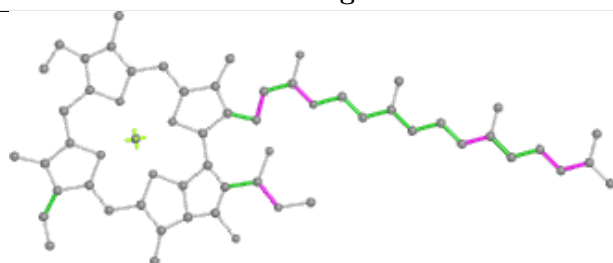
Ligand CLA Y 312



Bond lengths



Bond angles

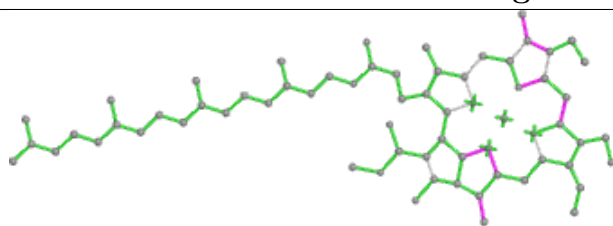


Torsions

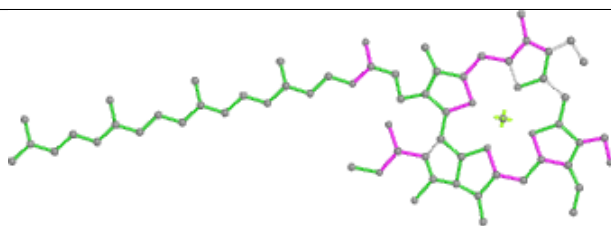


Rings

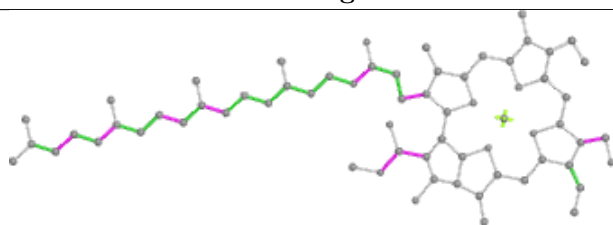
Ligand CHL N 309



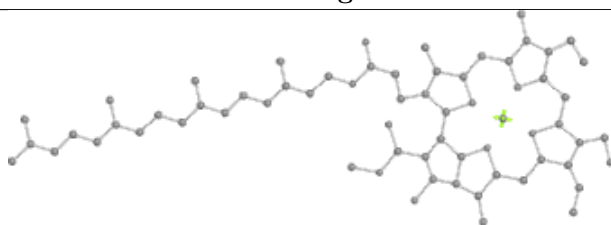
Bond lengths



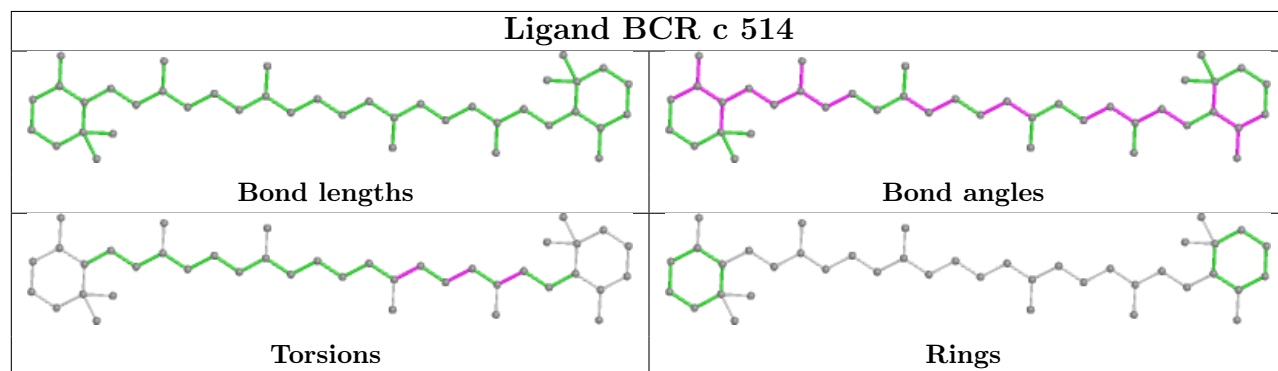
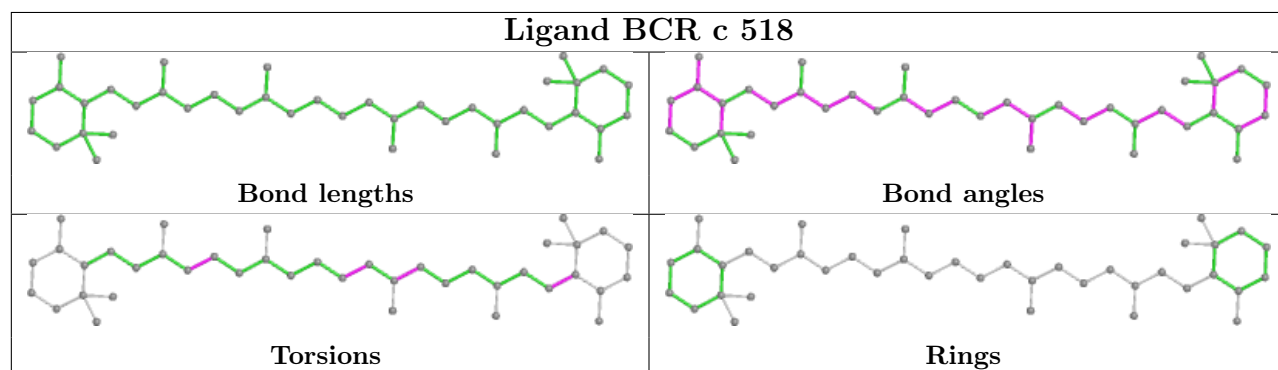
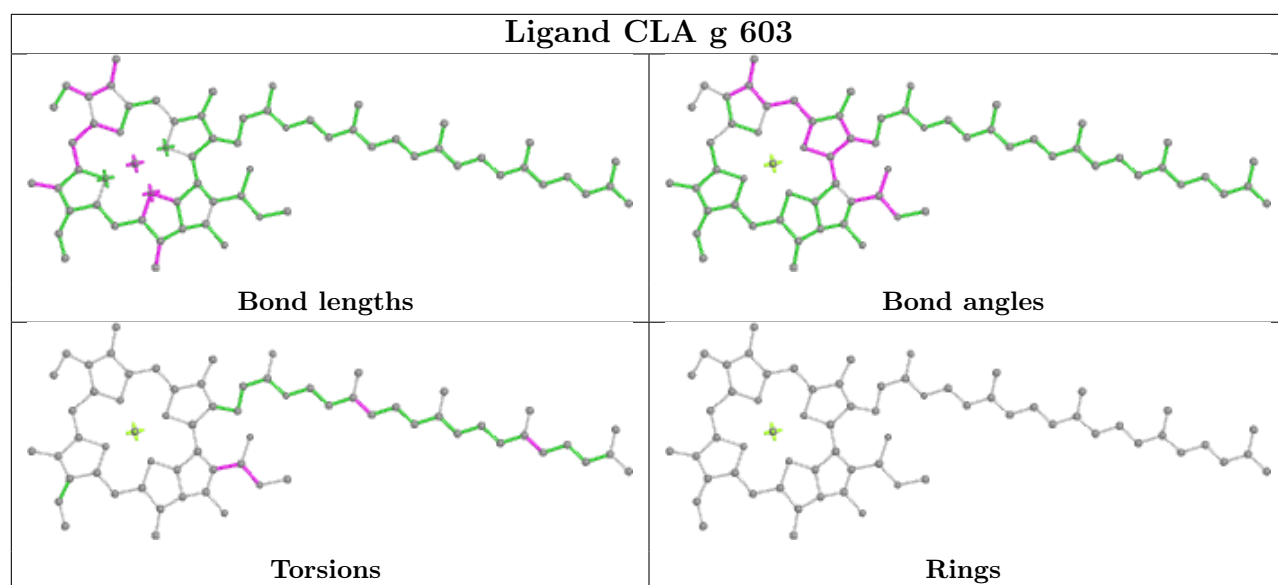
Bond angles



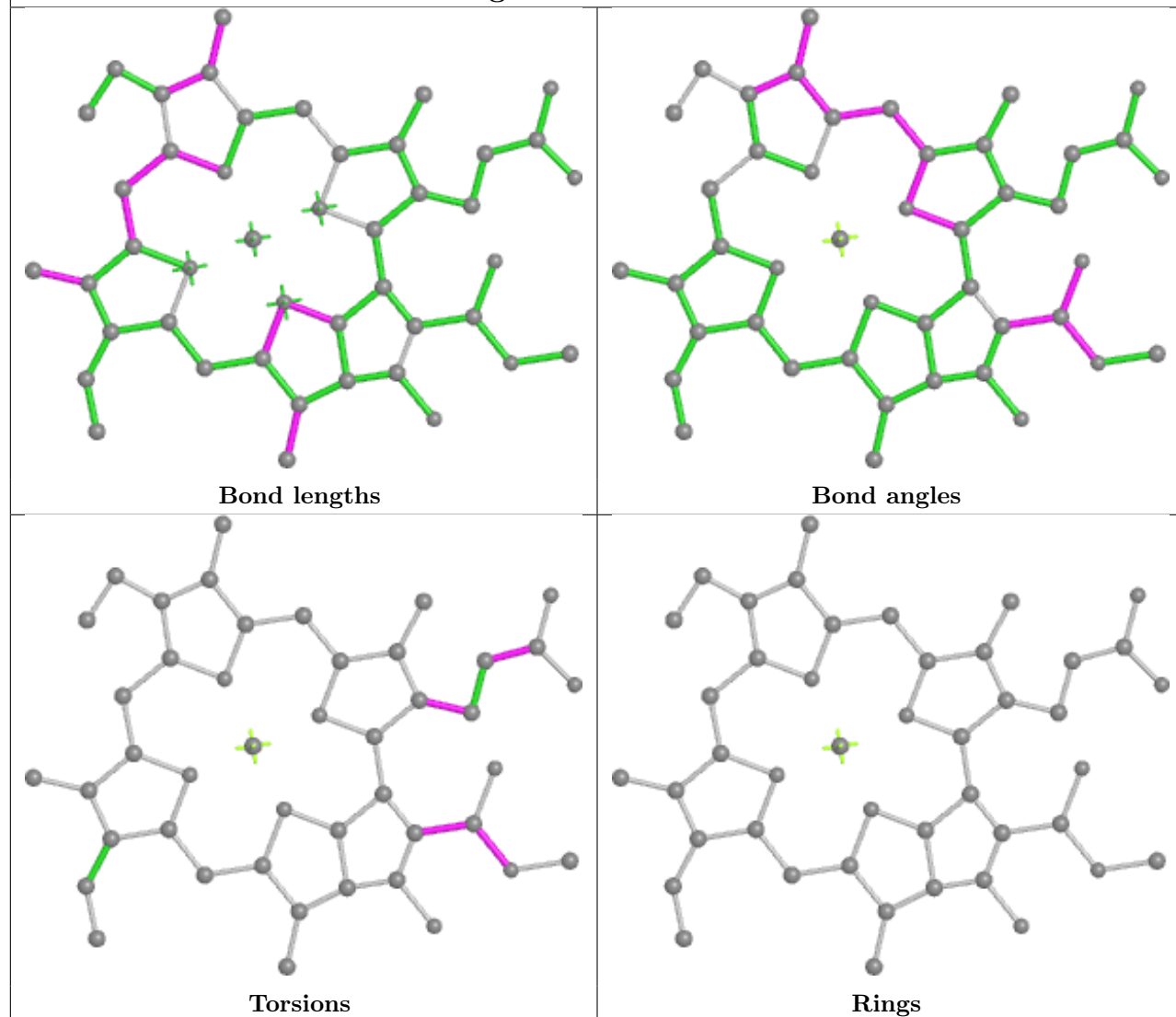
Torsions



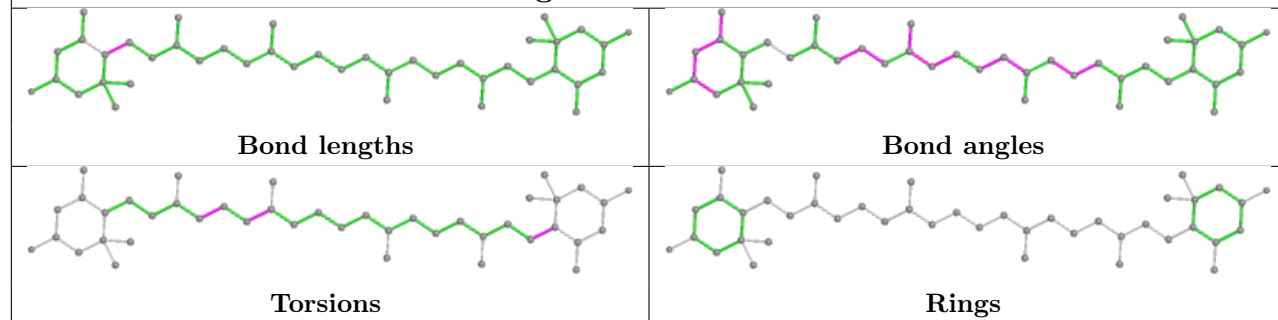
Rings

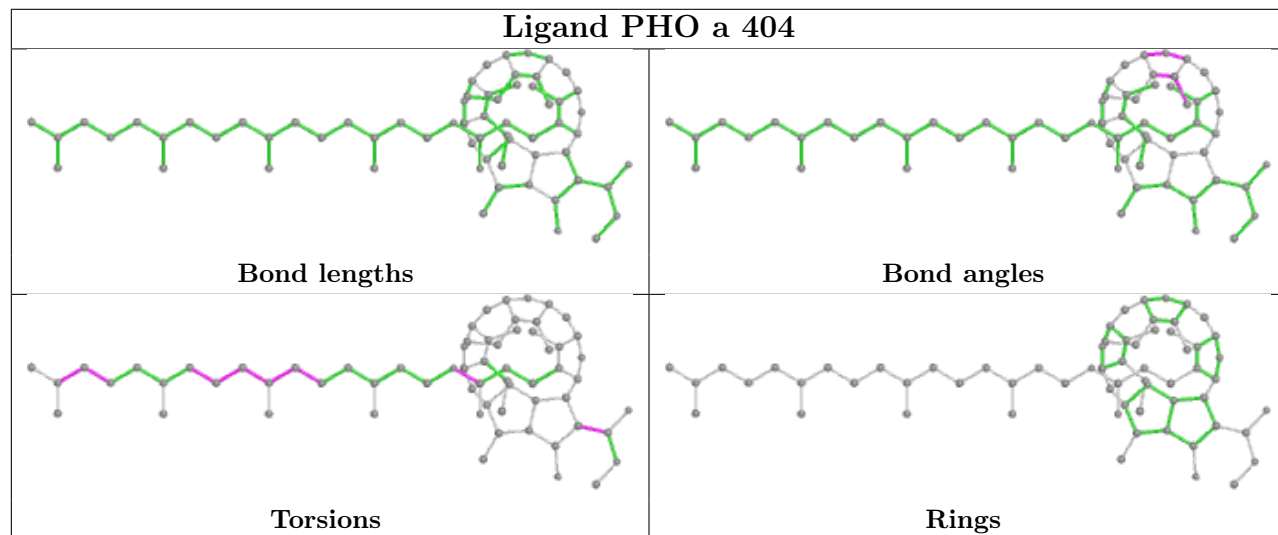
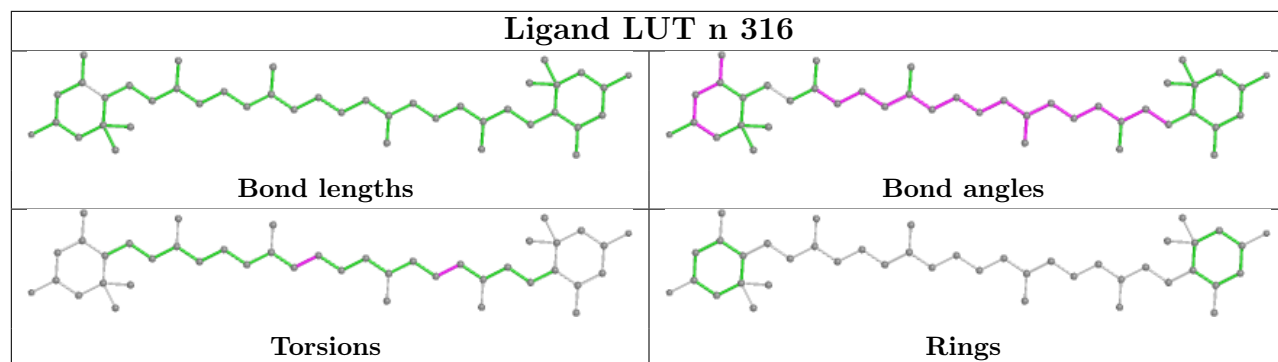


Ligand CLA R 614

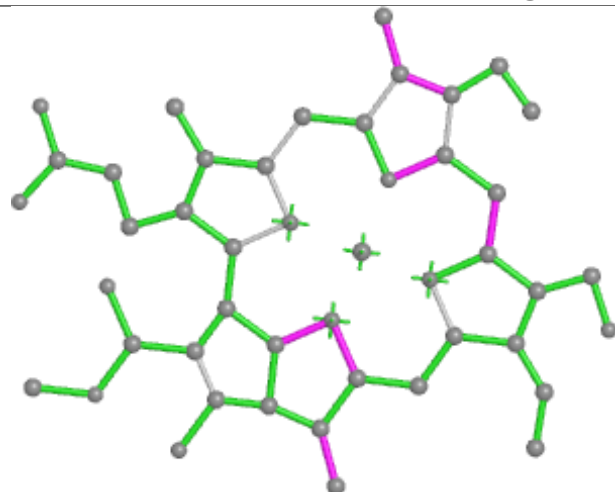


Ligand LUT n 317

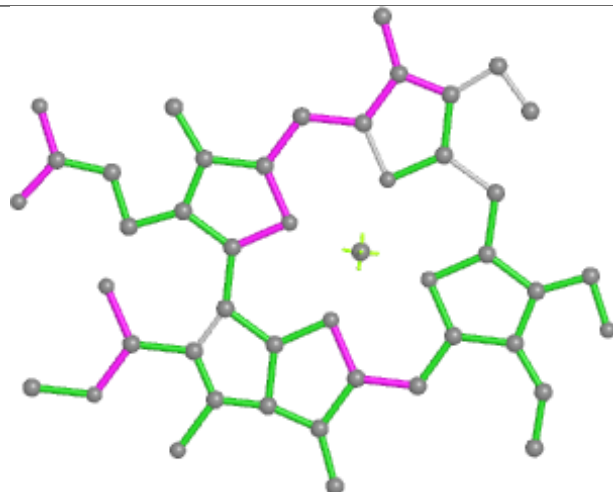




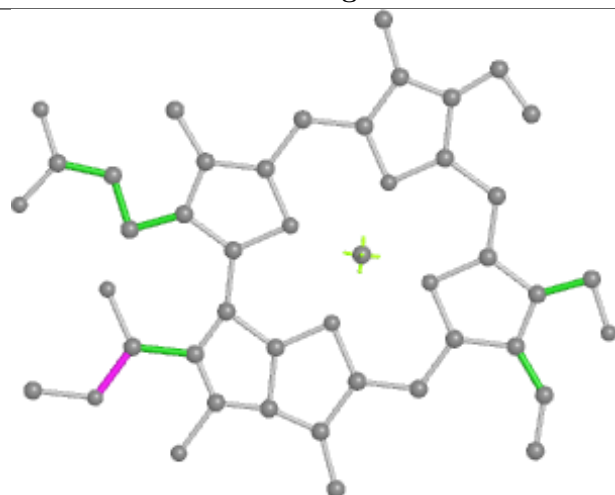
Ligand CHL r 605



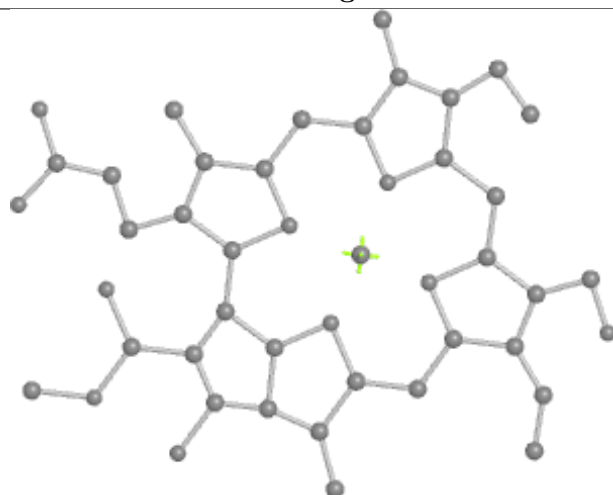
Bond lengths



Bond angles

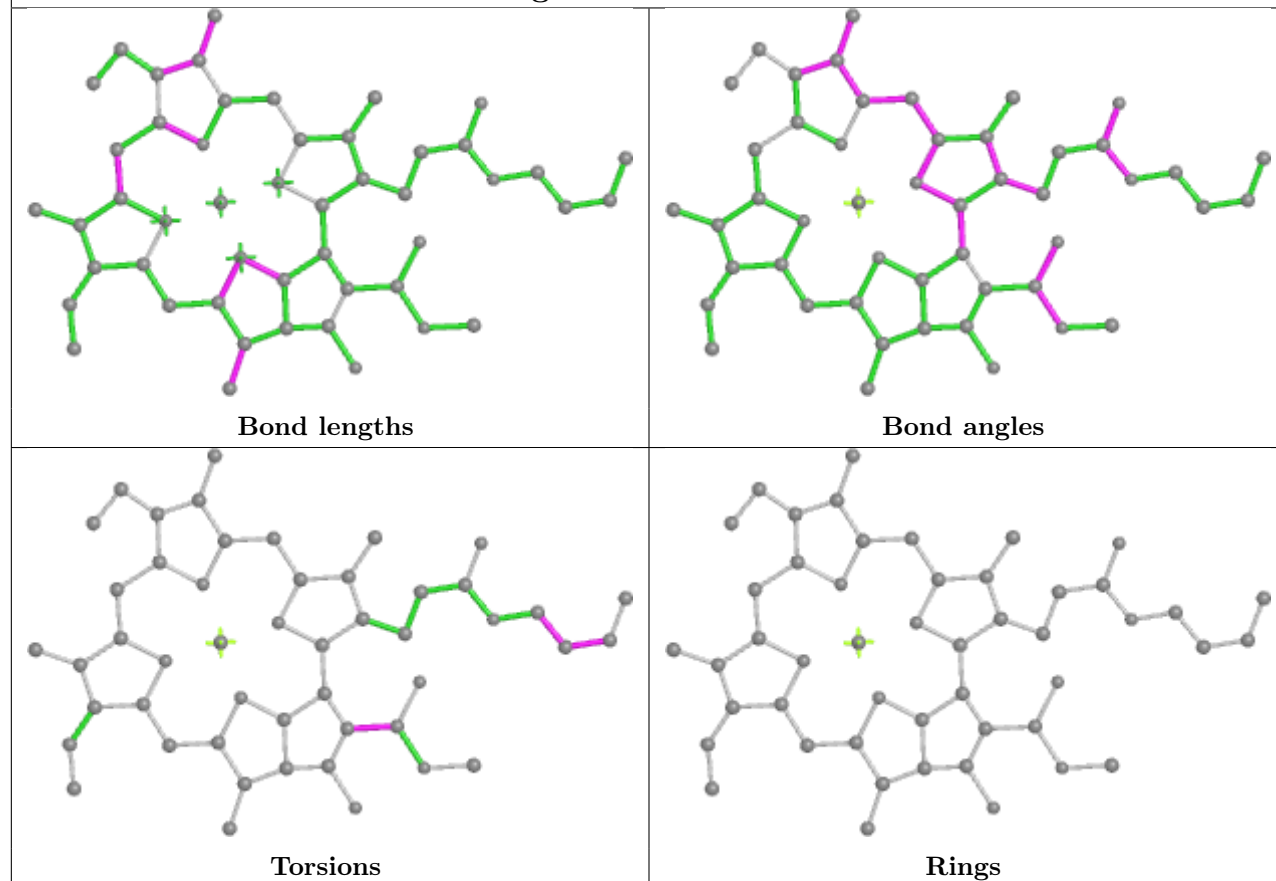


Torsions

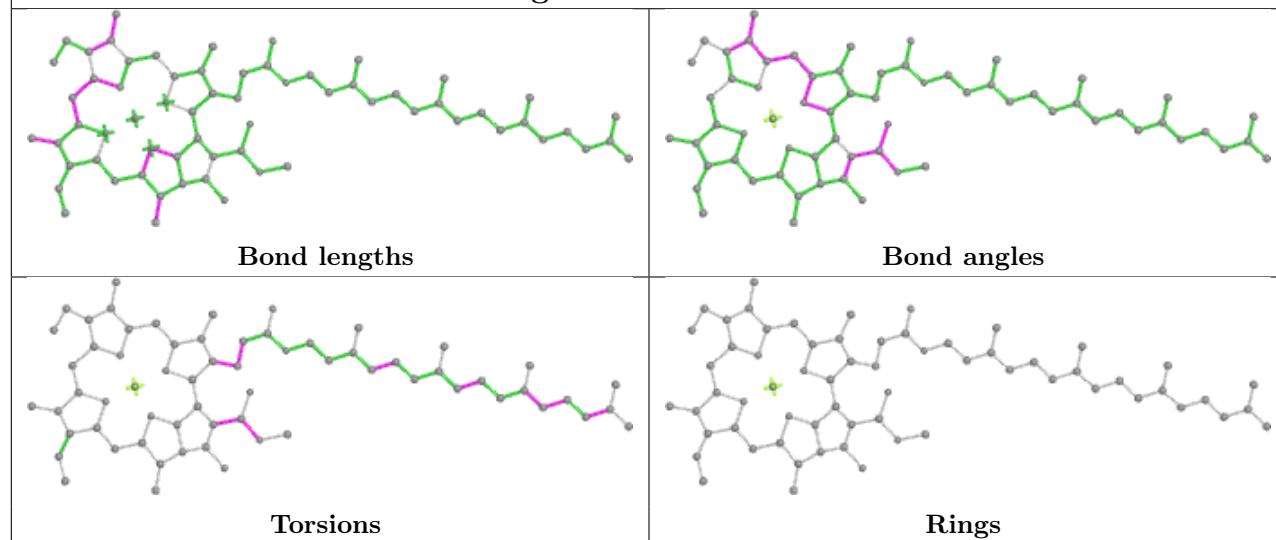


Rings

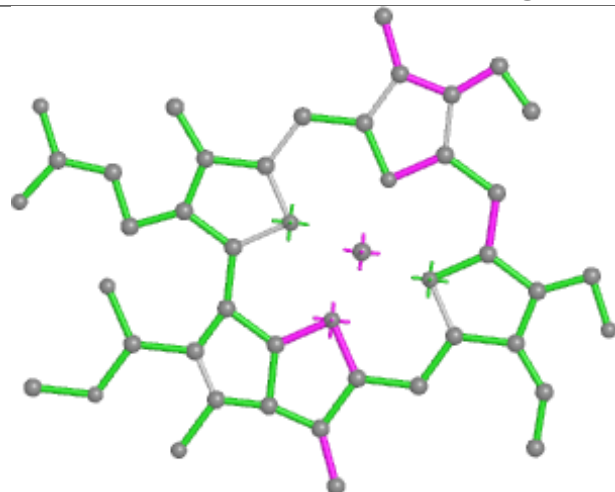
Ligand CLA R 611



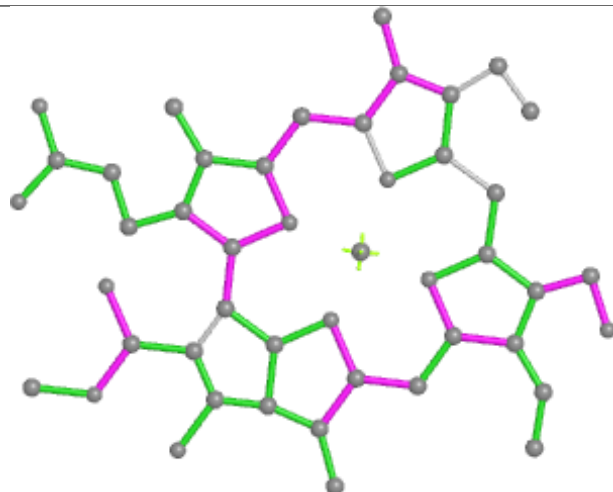
Ligand CLA D 405



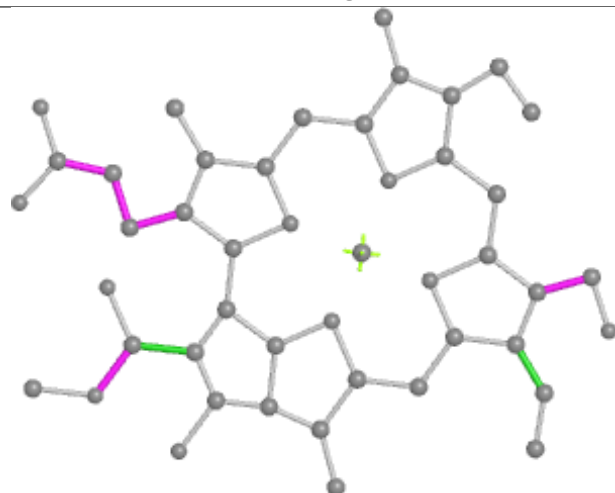
Ligand CHL n 307



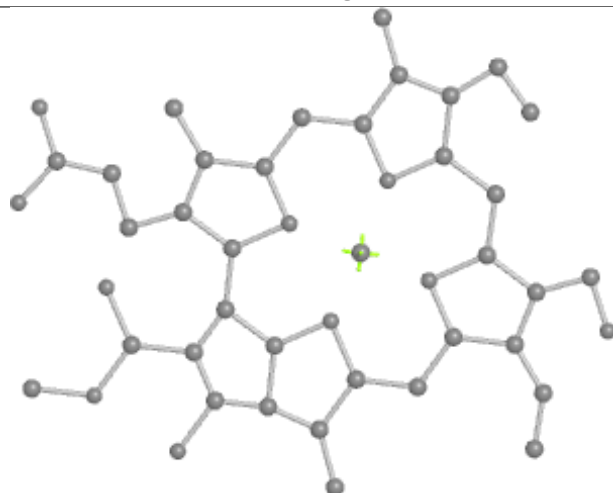
Bond lengths



Bond angles

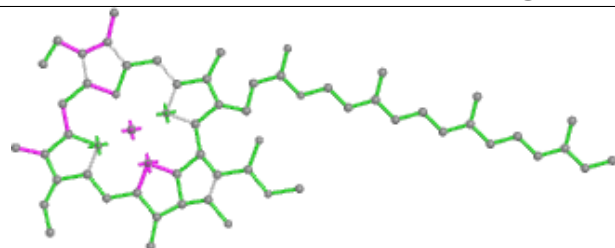


Torsions

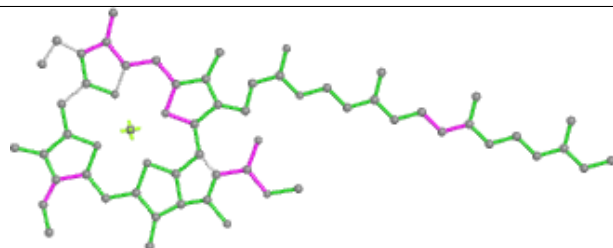


Rings

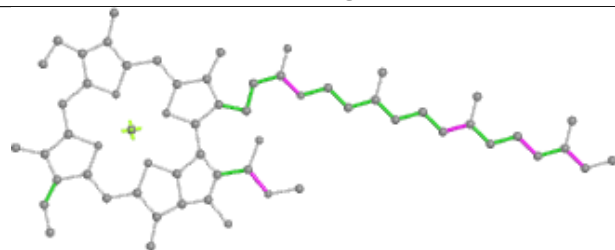
Ligand CLA n 303



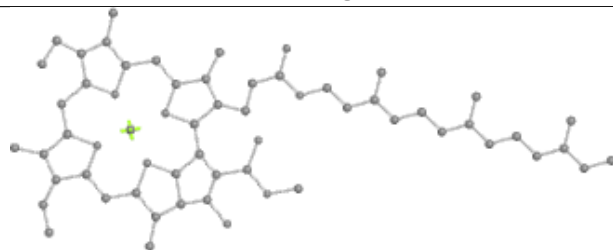
Bond lengths



Bond angles

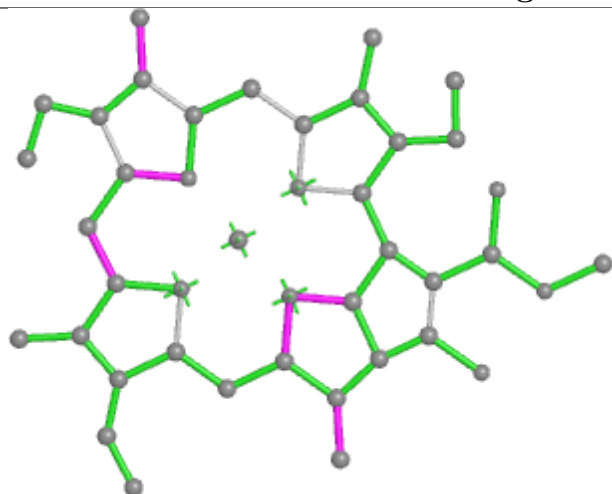


Torsions

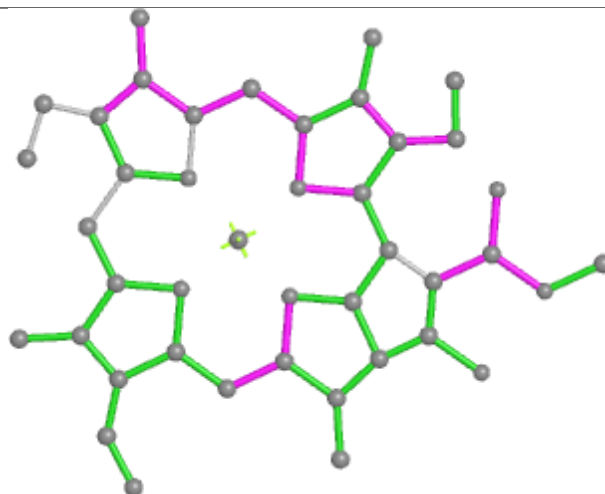


Rings

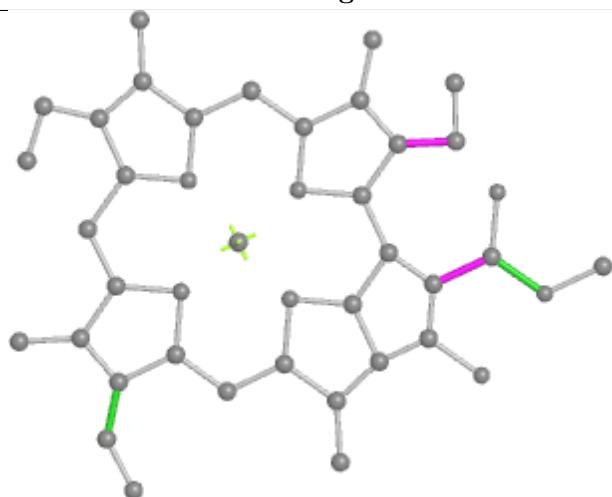
Ligand CLA S 610



Bond lengths



Bond angles

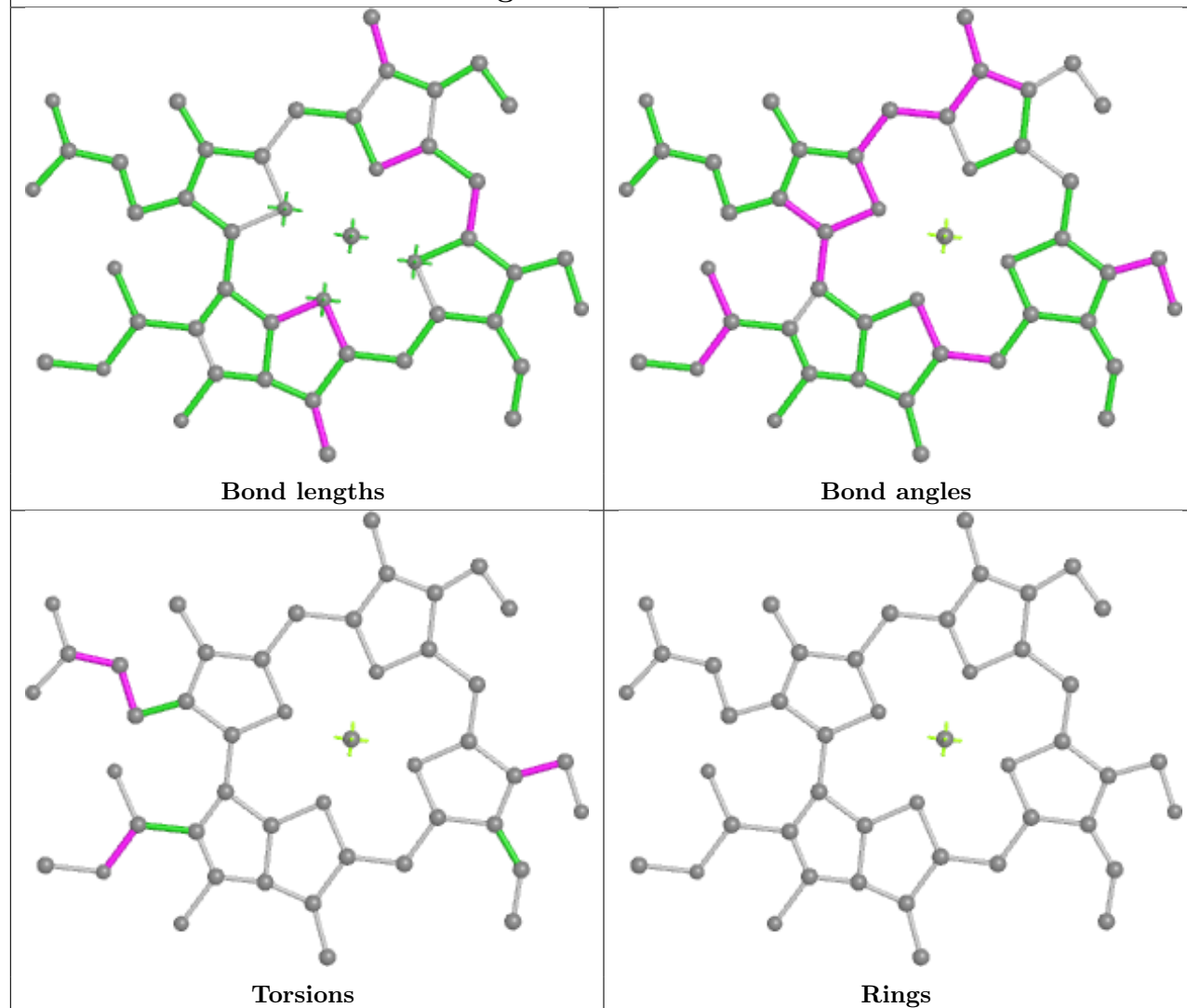


Torsions

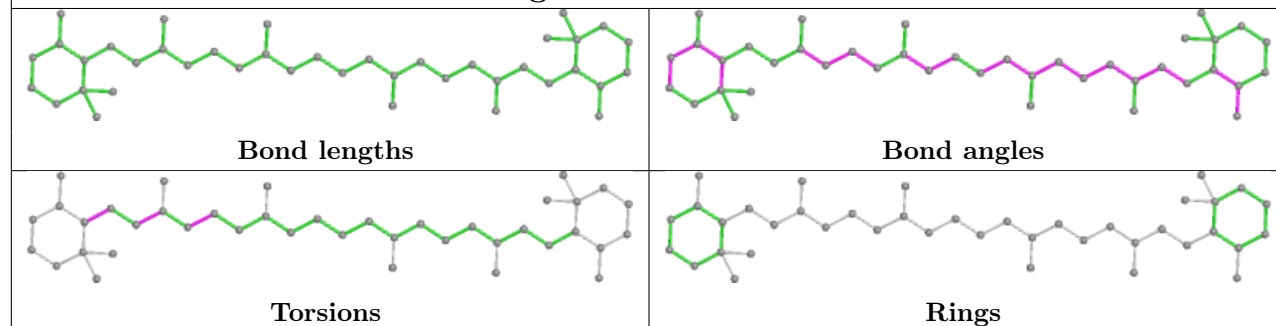


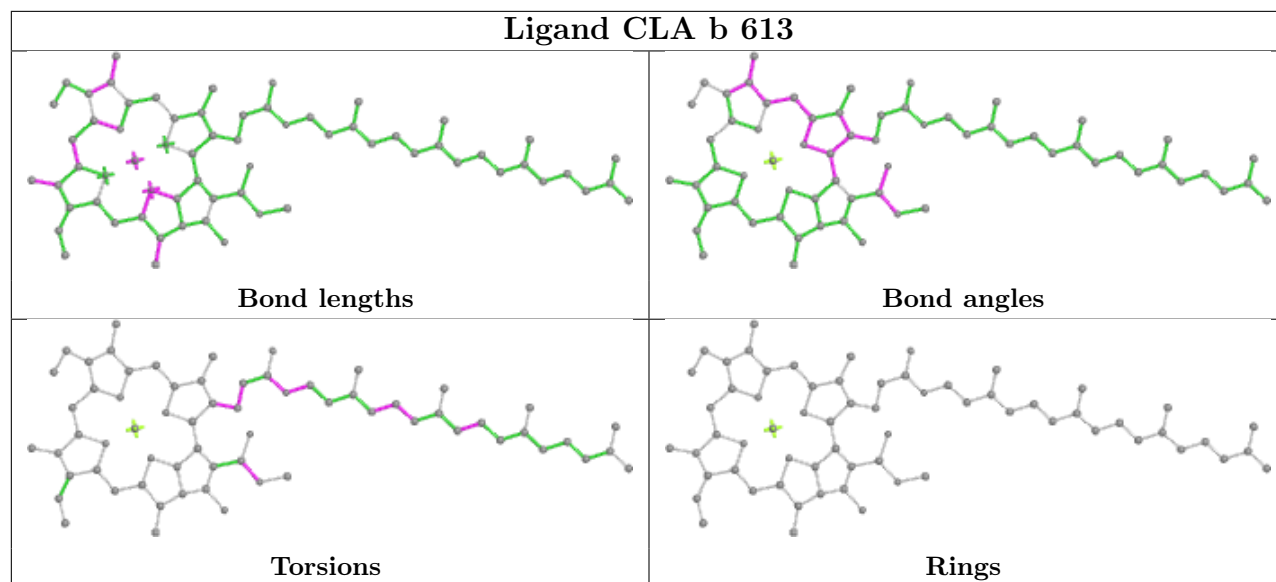
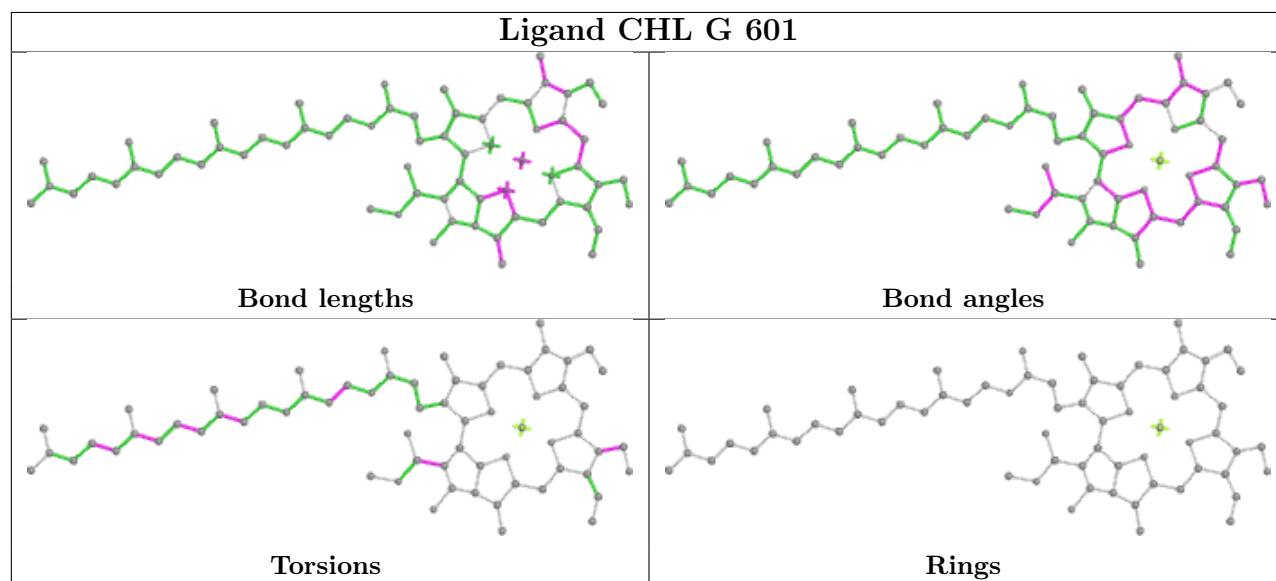
Rings

Ligand CHL S 601

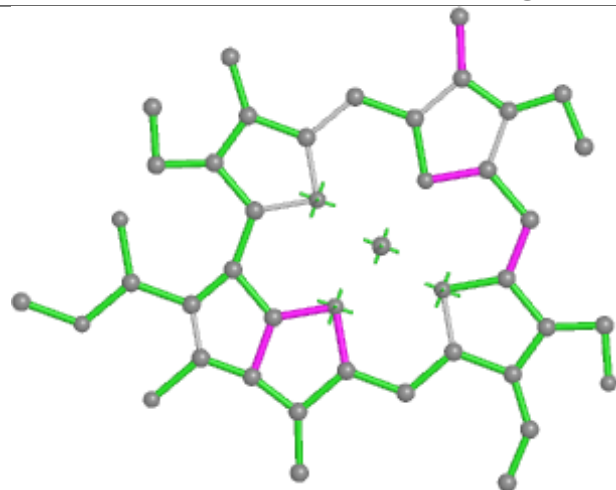


Ligand BCR H 101

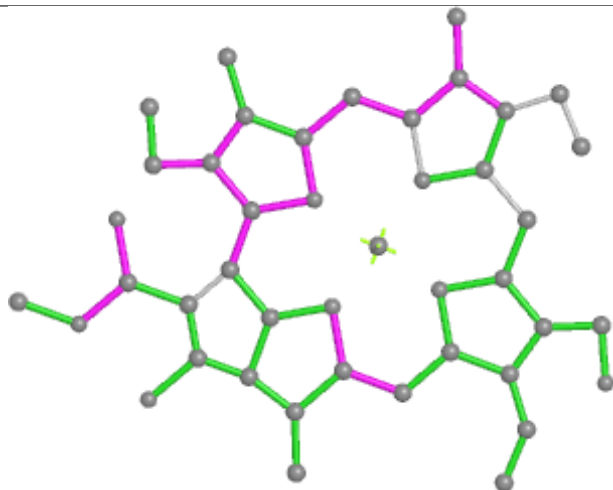


Ligand CLA b 613**Ligand CHL G 601**

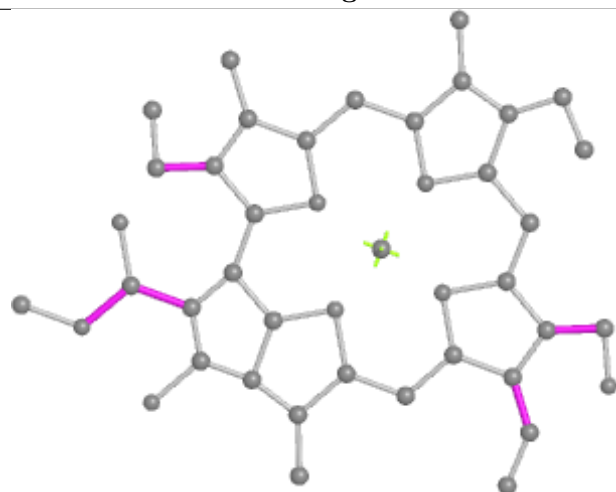
Ligand CHL S 606



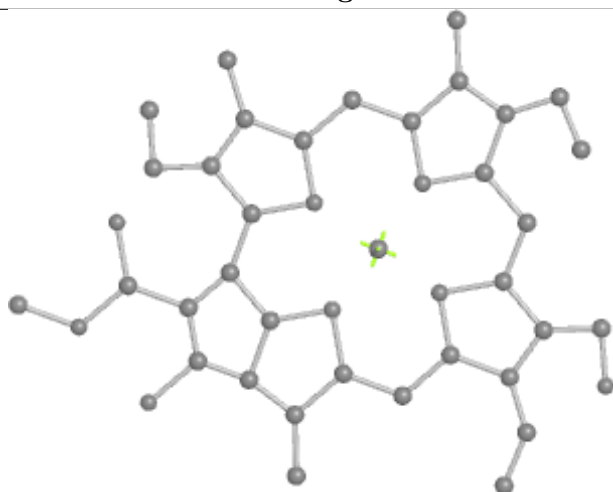
Bond lengths



Bond angles

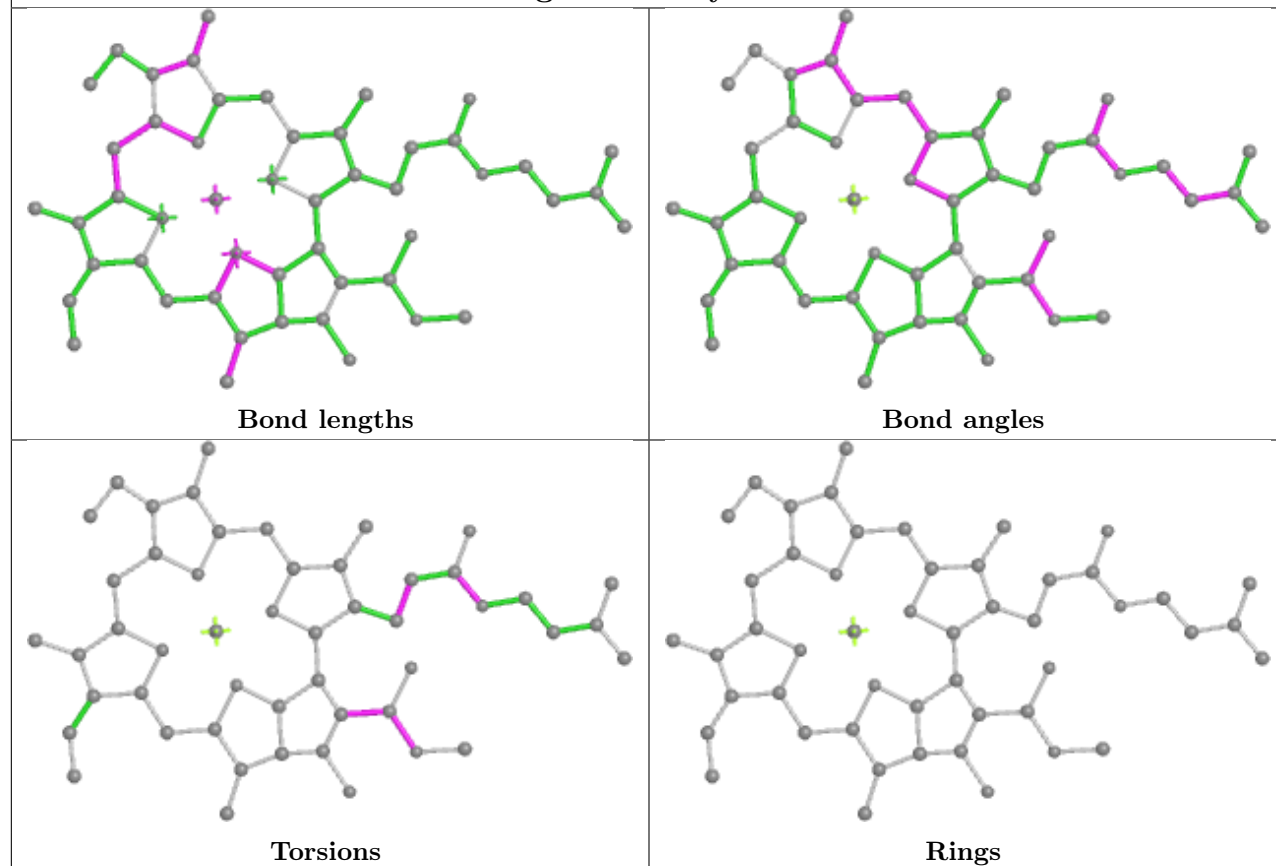


Torsions

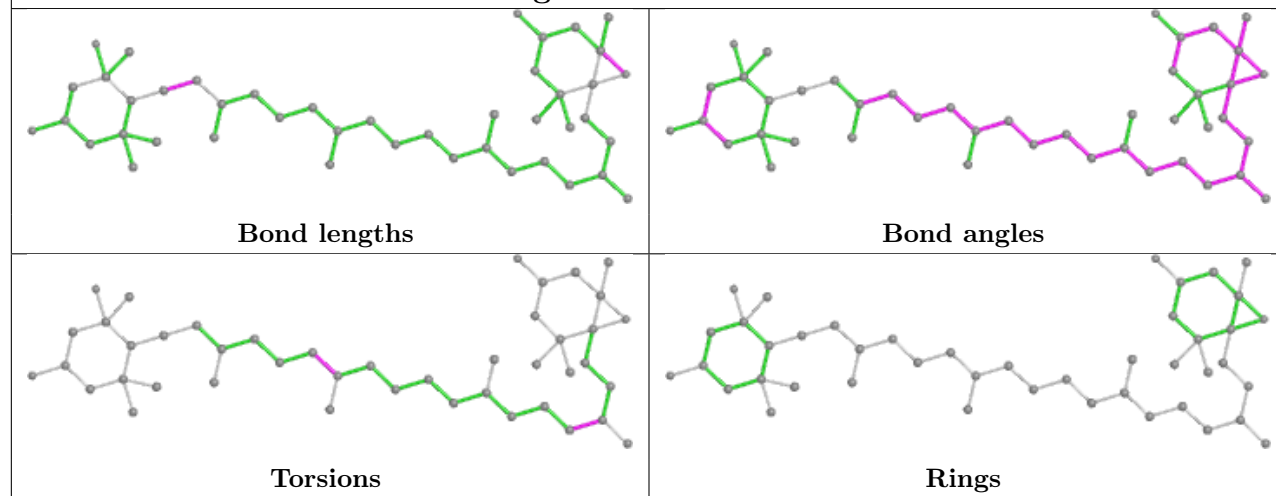


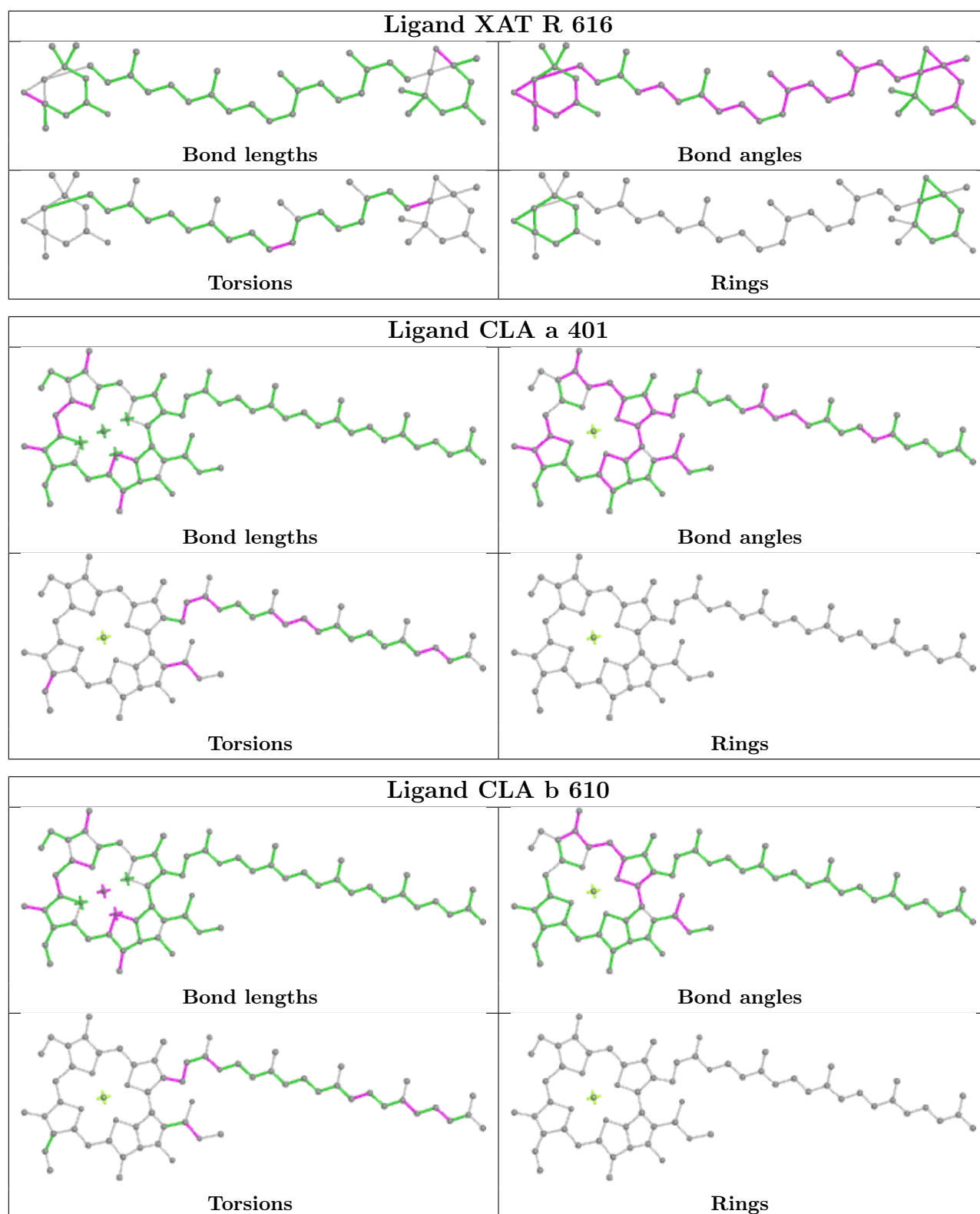
Rings

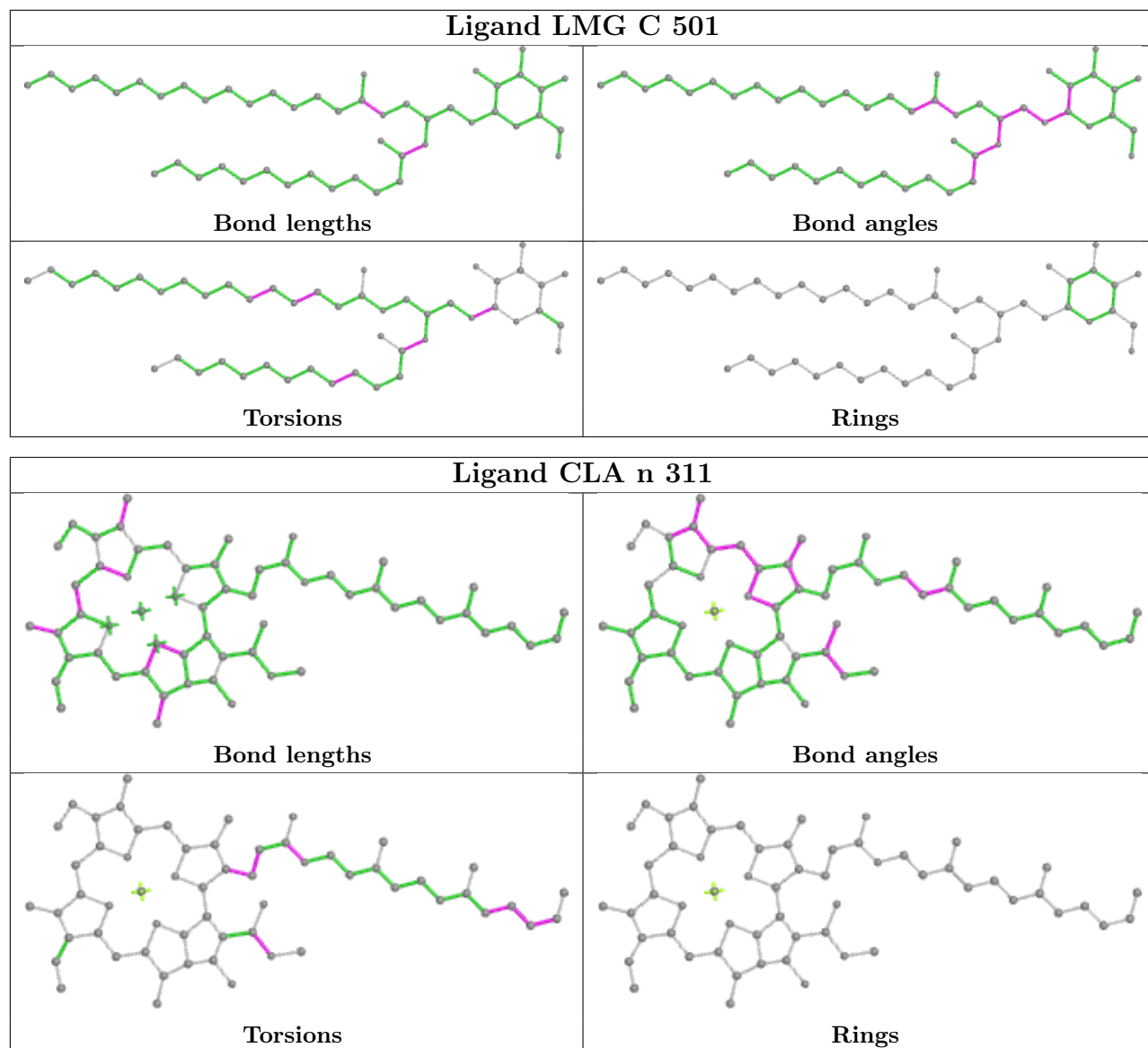
Ligand CLA y 305



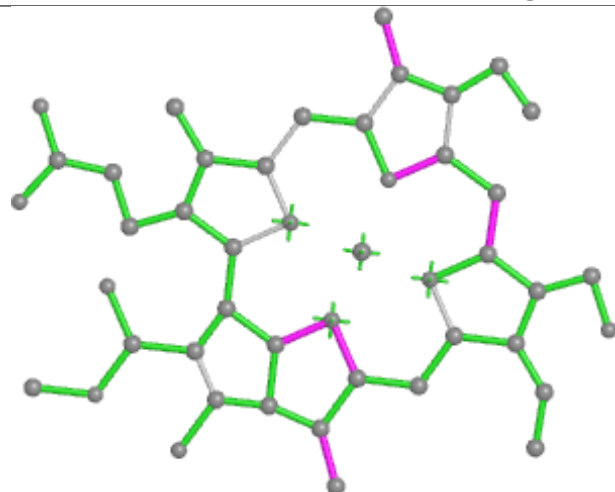
Ligand NEX n 318



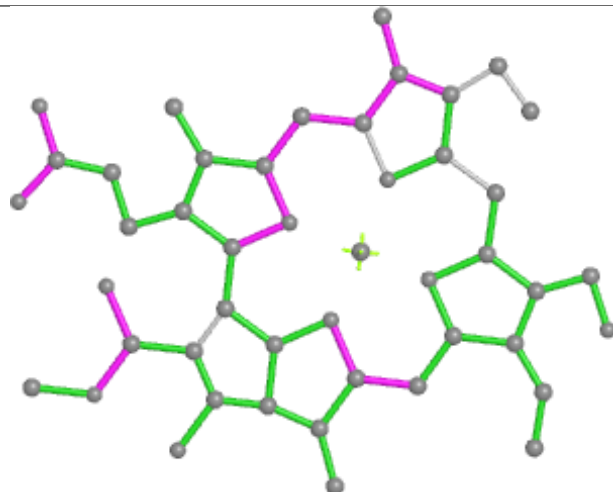




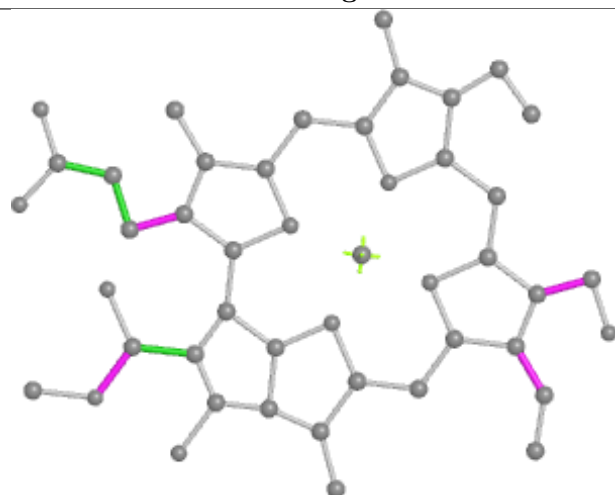
Ligand CHL r 606



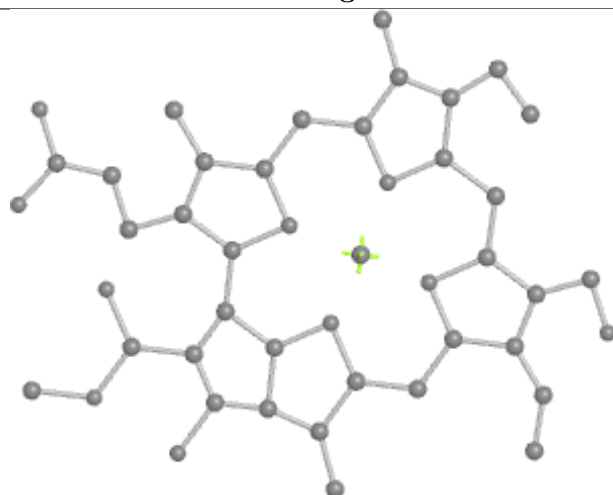
Bond lengths



Bond angles

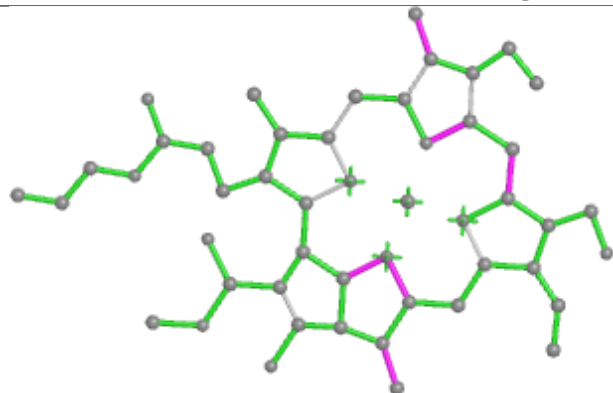


Torsions

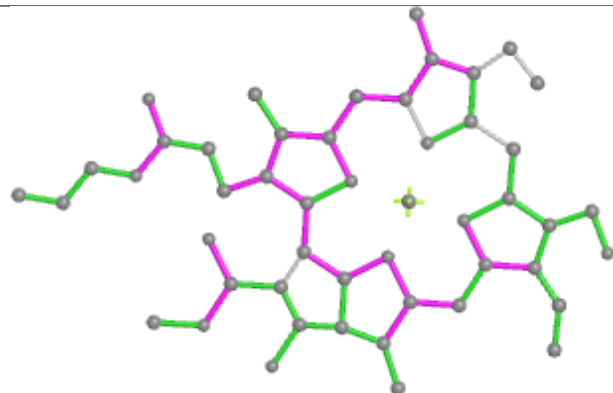


Rings

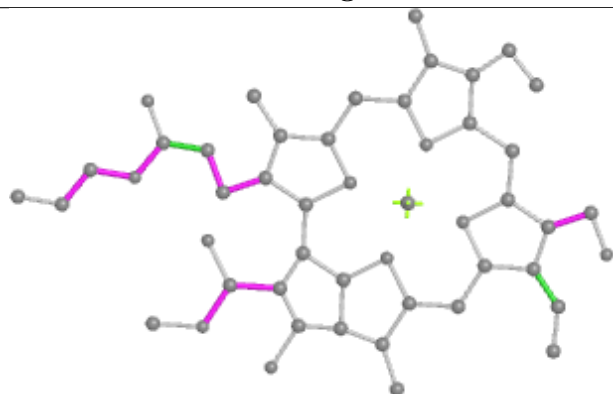
Ligand CHL S 607



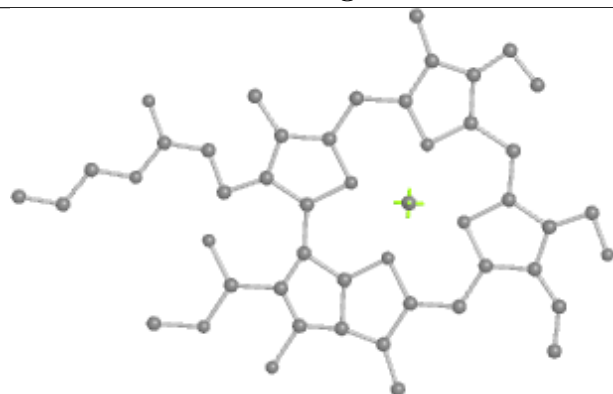
Bond lengths



Bond angles

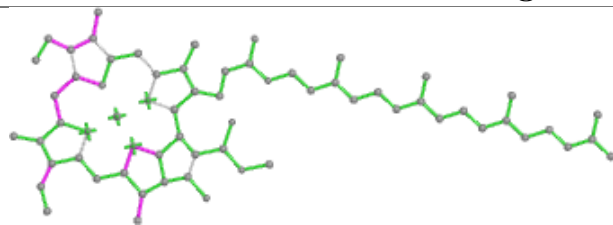


Torsions

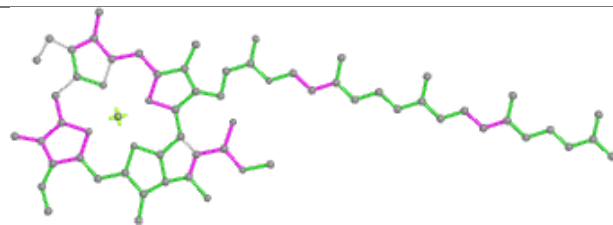


Rings

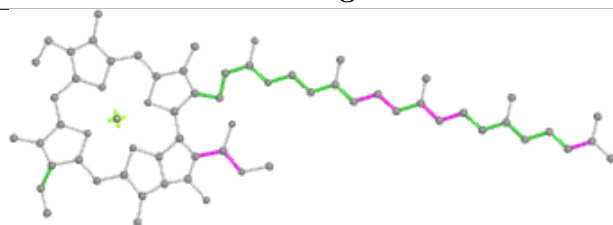
Ligand CLA b 605



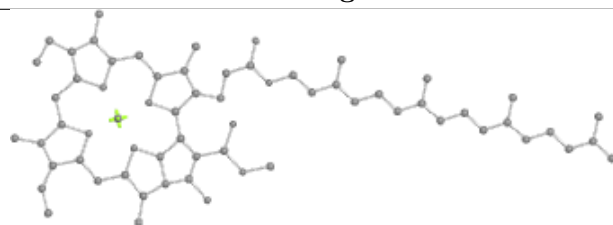
Bond lengths



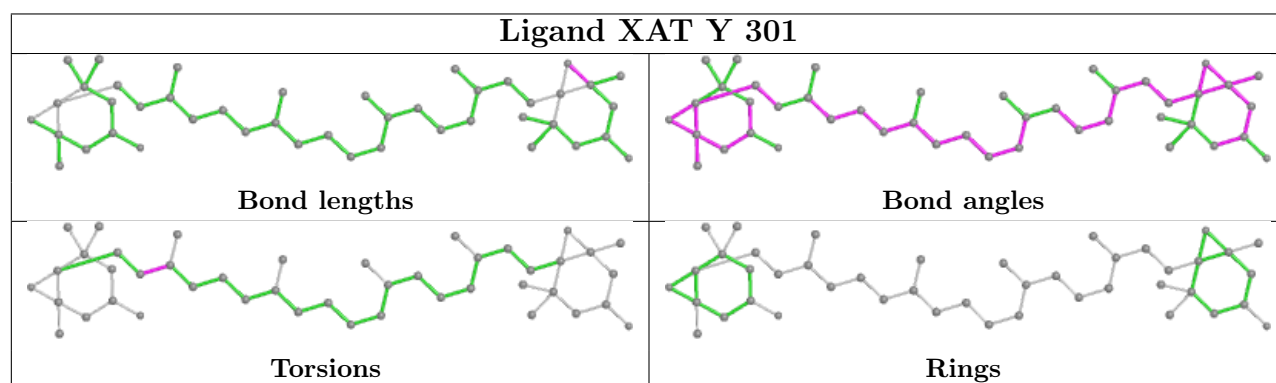
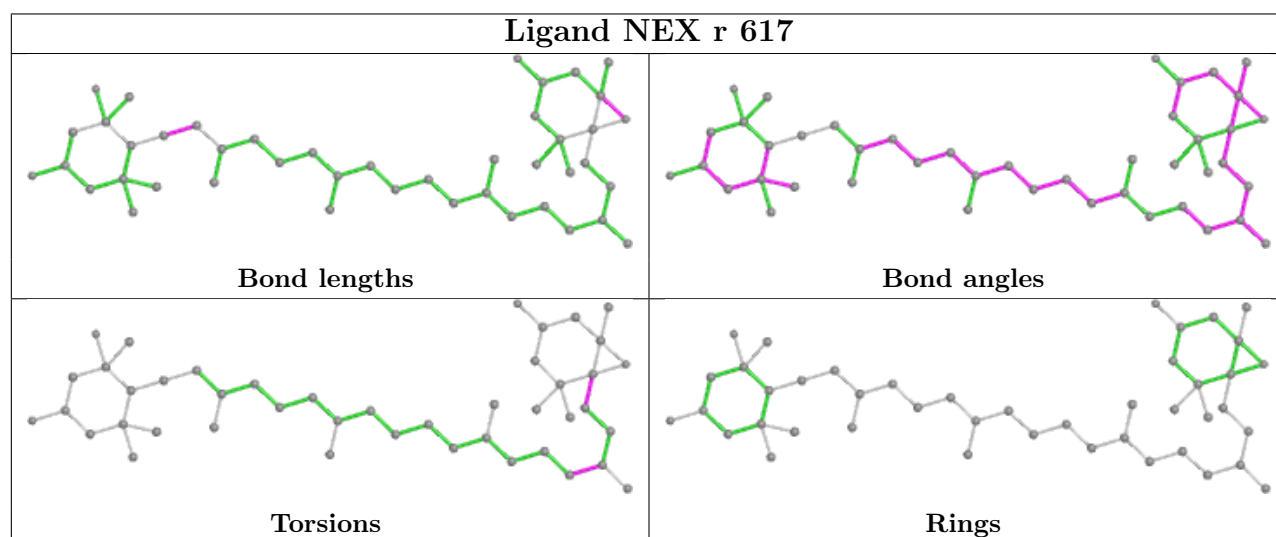
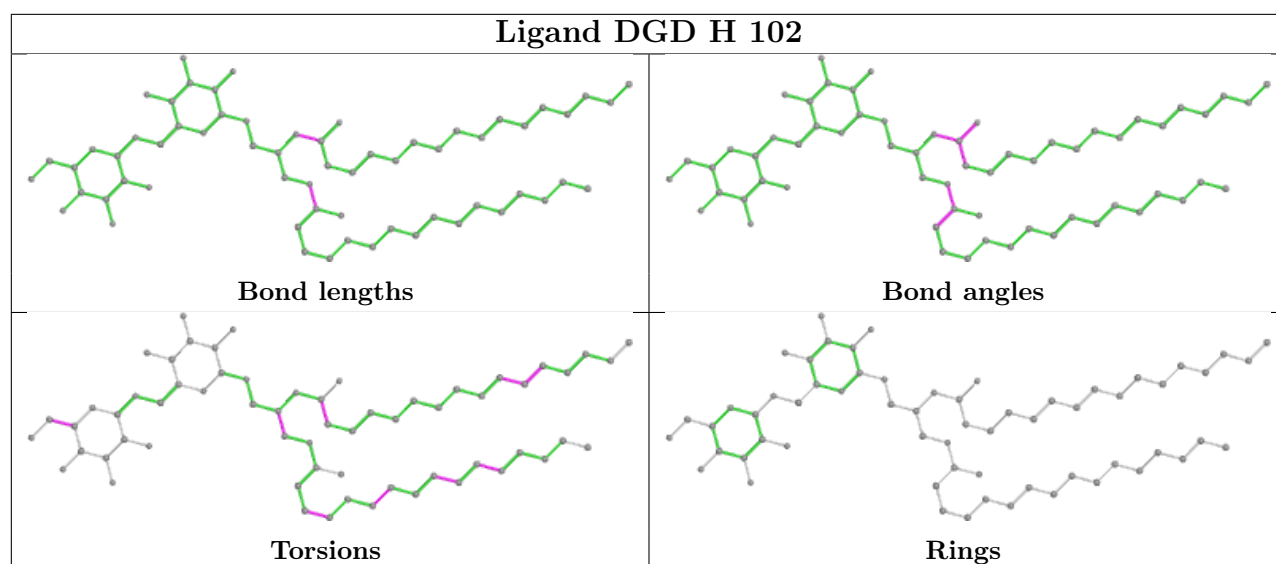
Bond angles

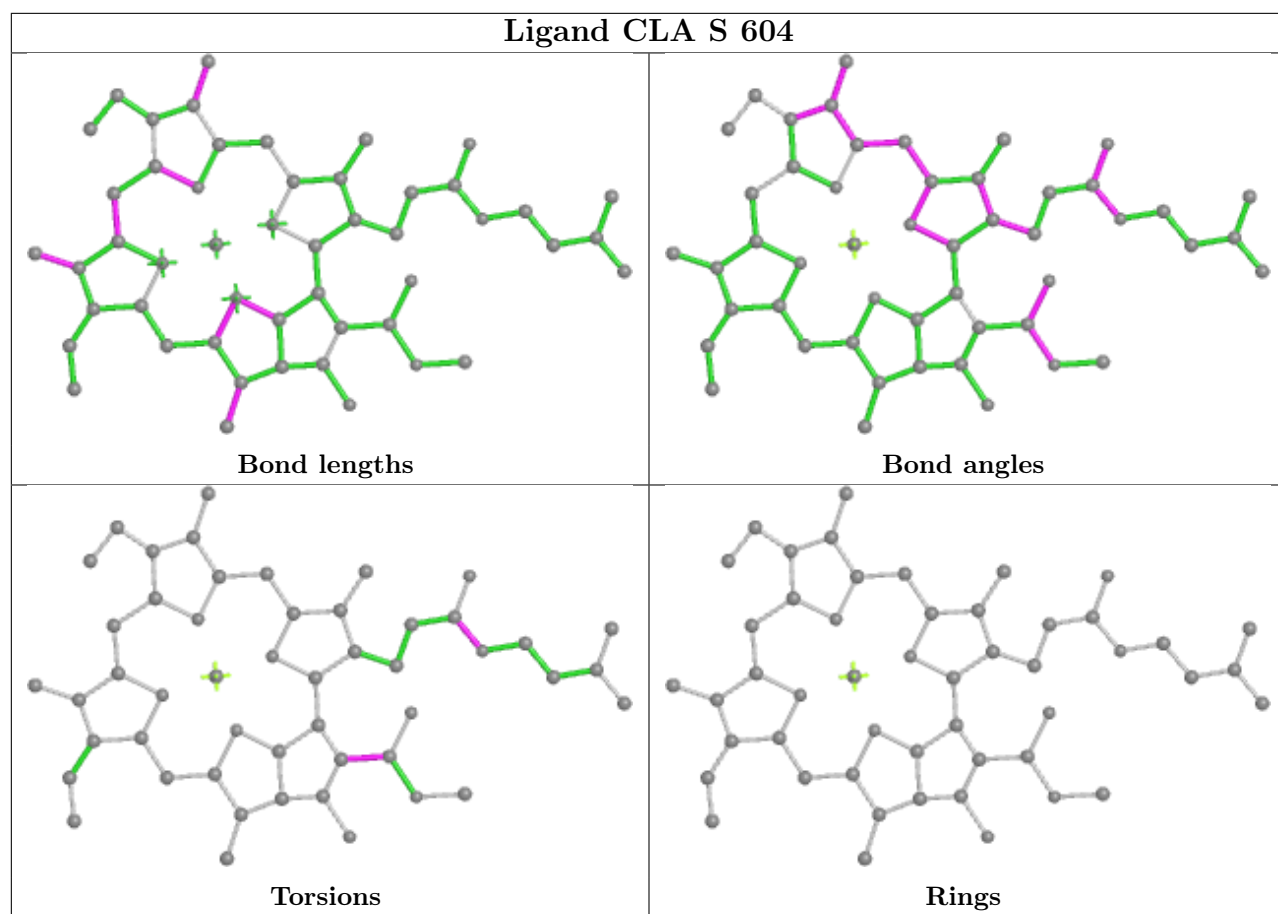
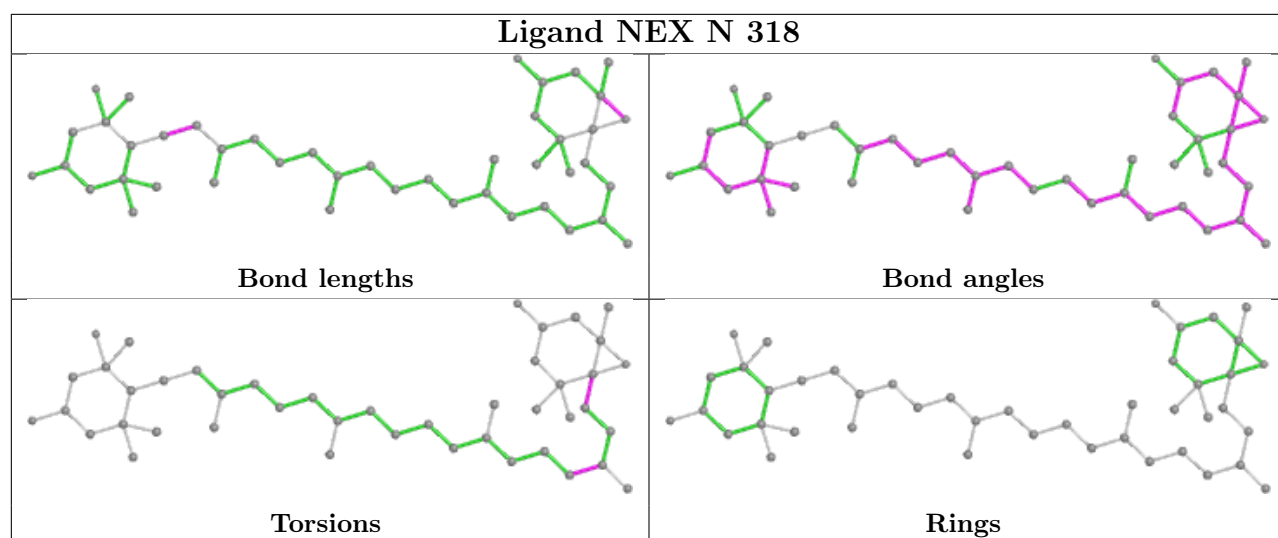


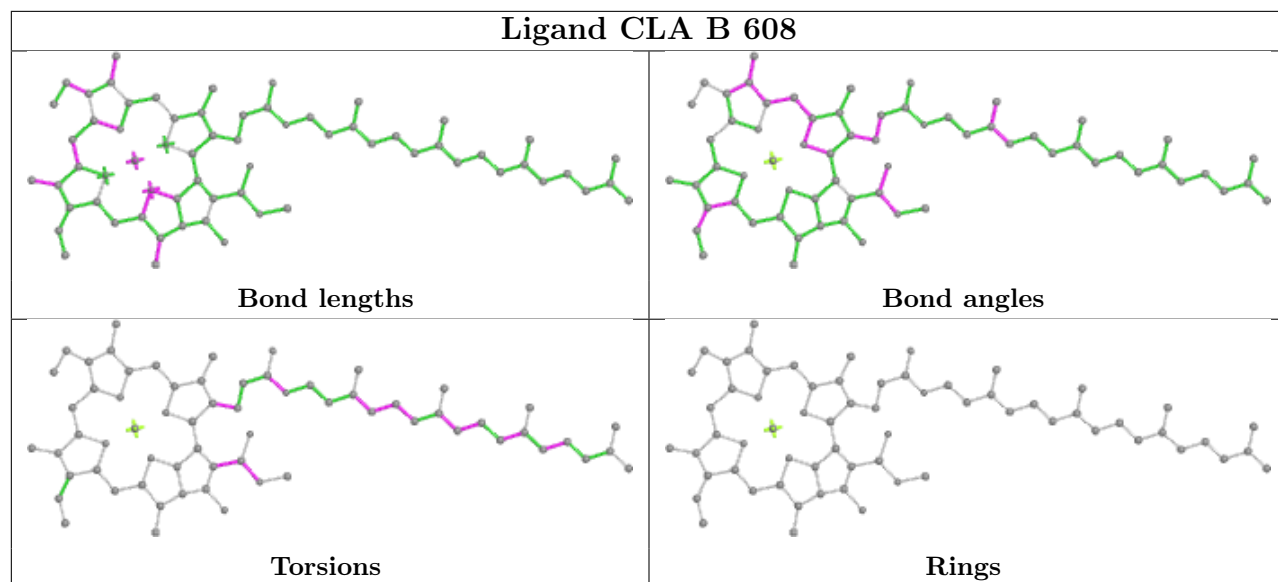
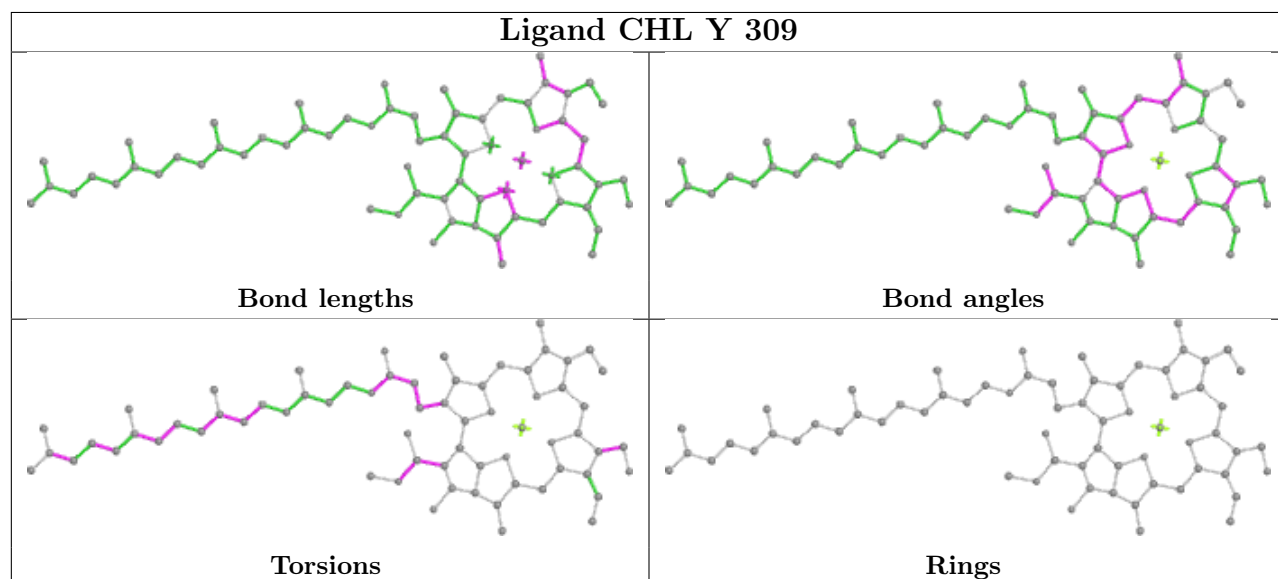
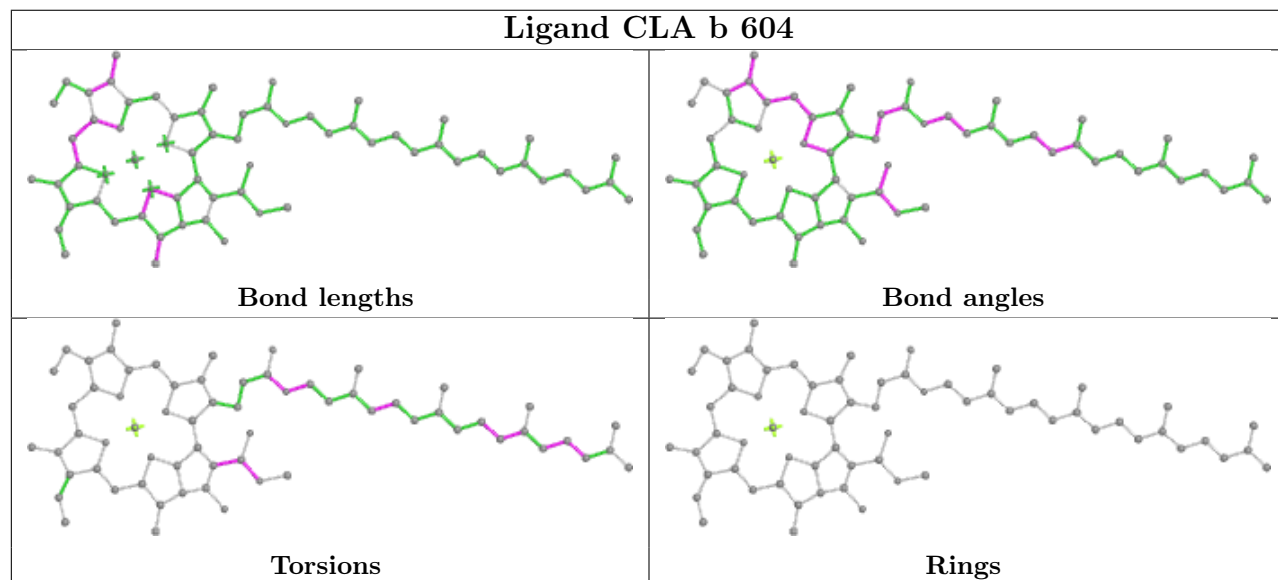
Torsions

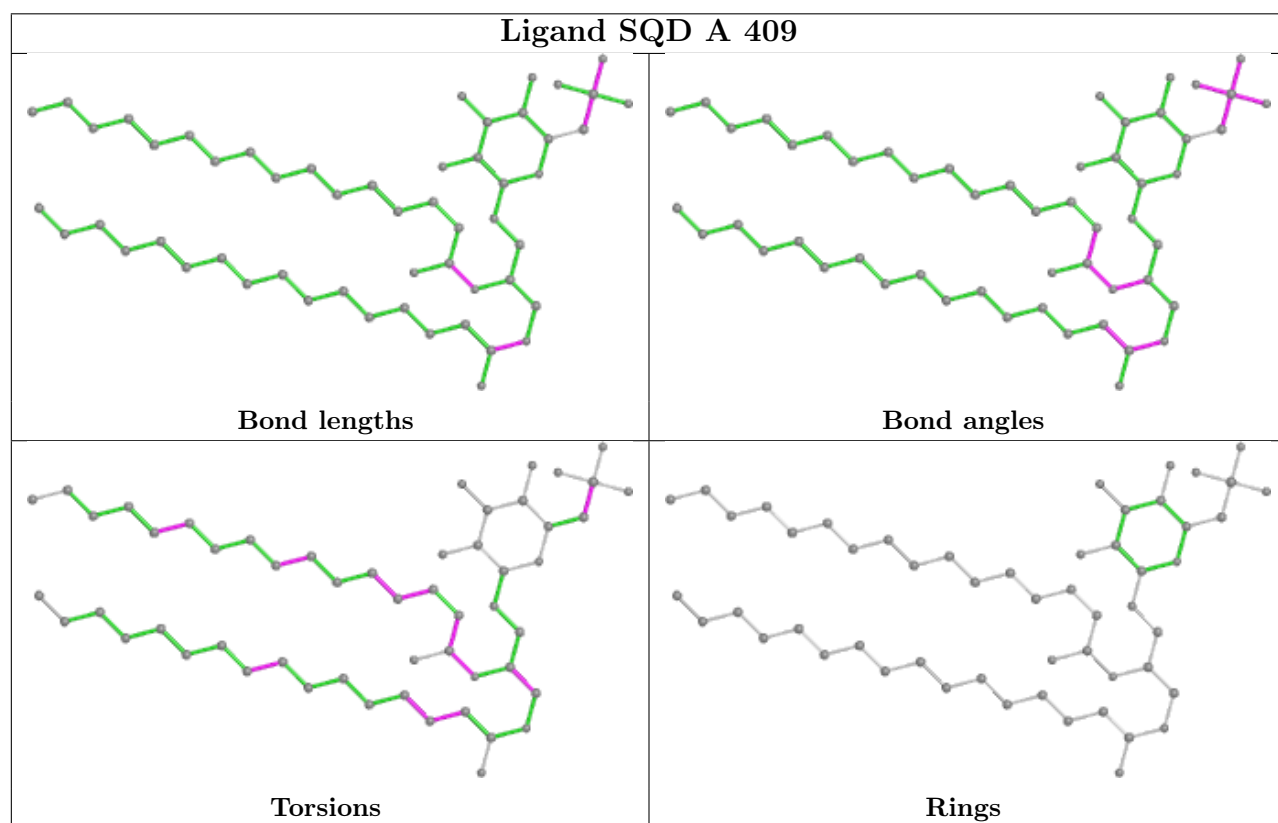
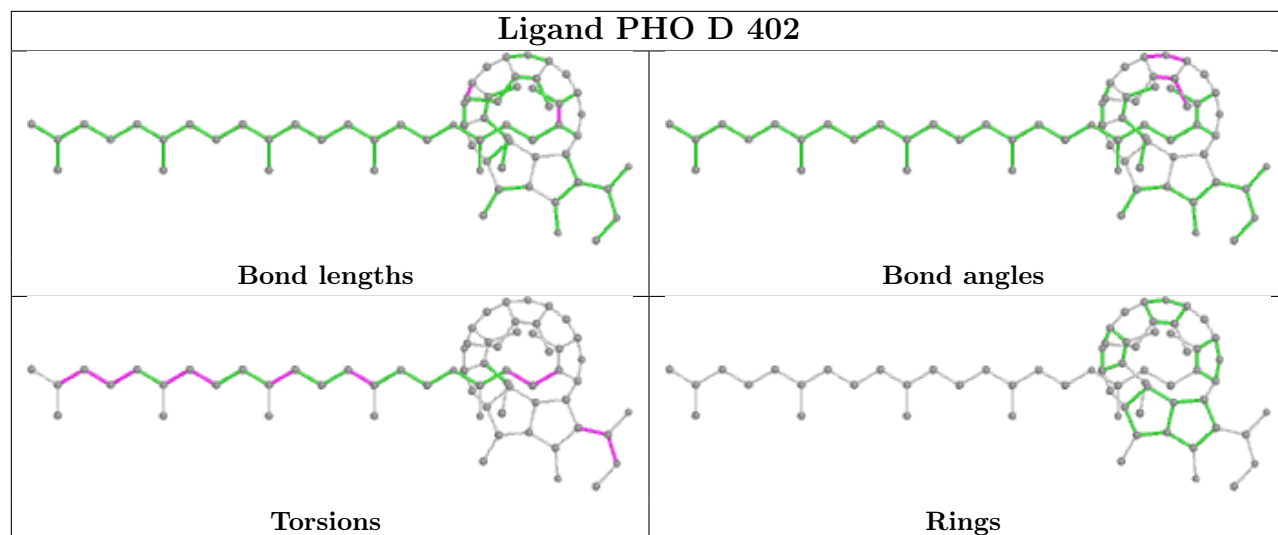


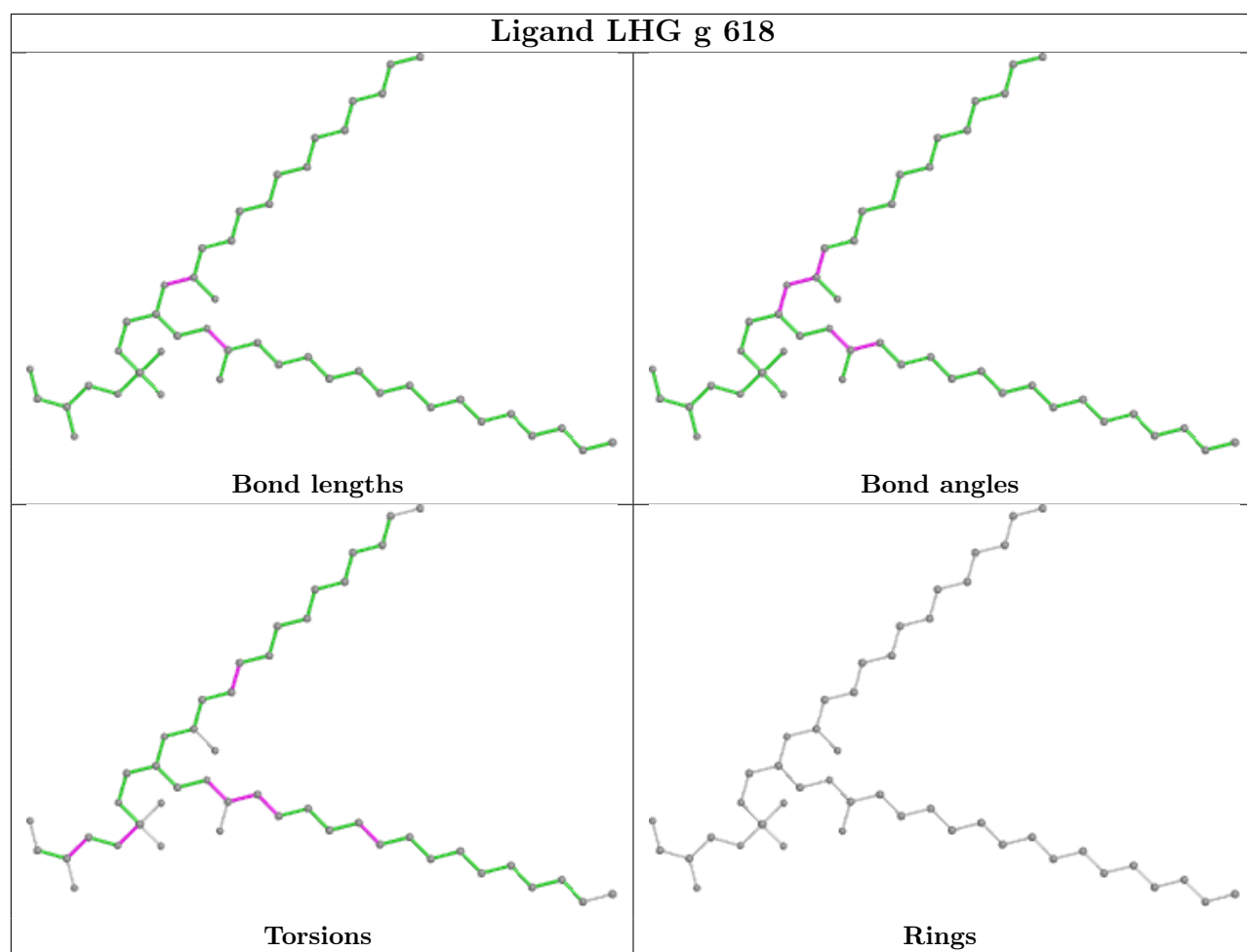
Rings



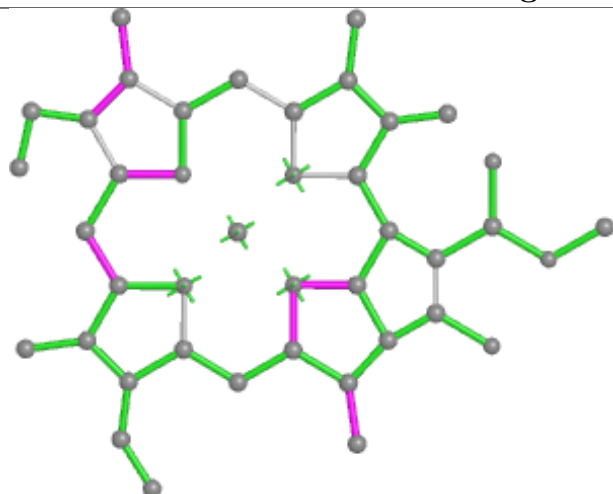


Ligand CLA B 608**Ligand CHL Y 309****Ligand CLA b 604**

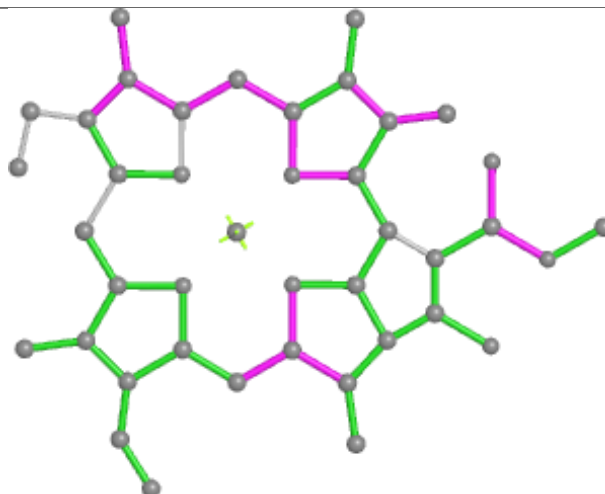




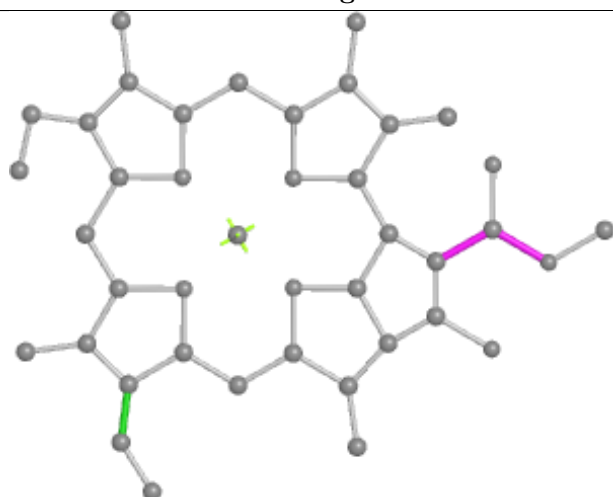
Ligand CLA s 613



Bond lengths



Bond angles

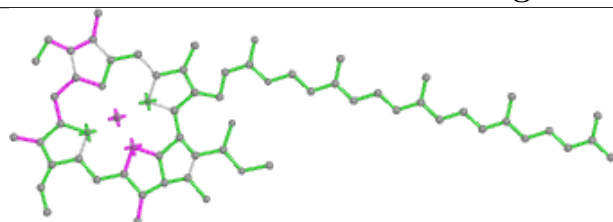


Torsions

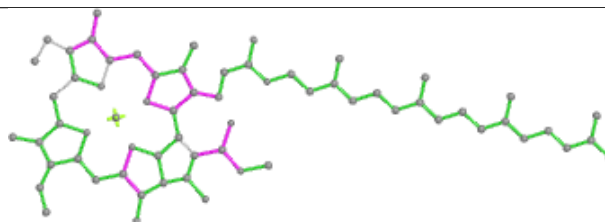


Rings

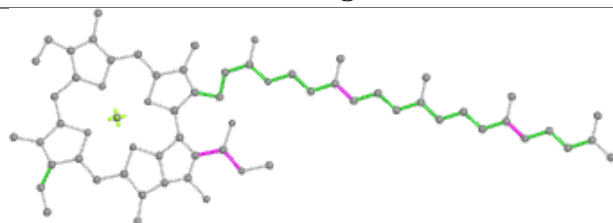
Ligand CLA G 603



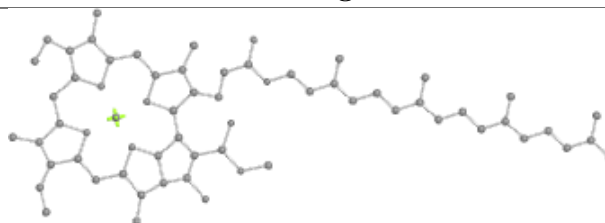
Bond lengths



Bond angles

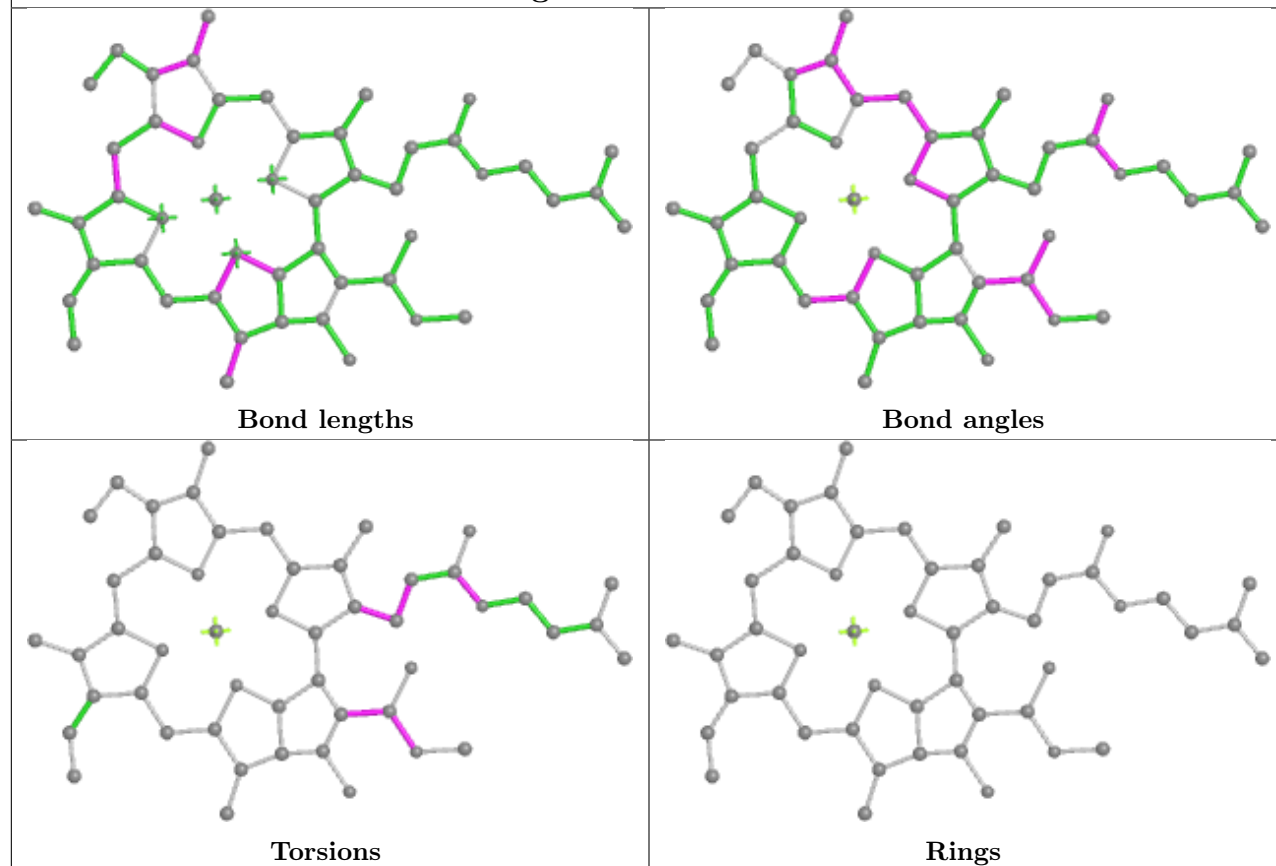


Torsions

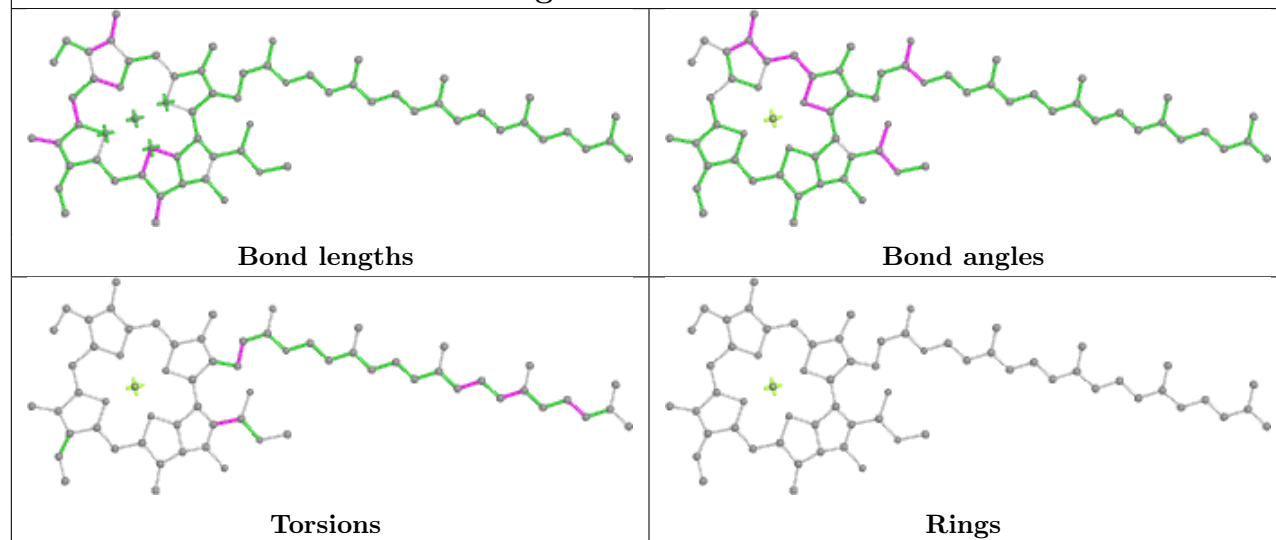


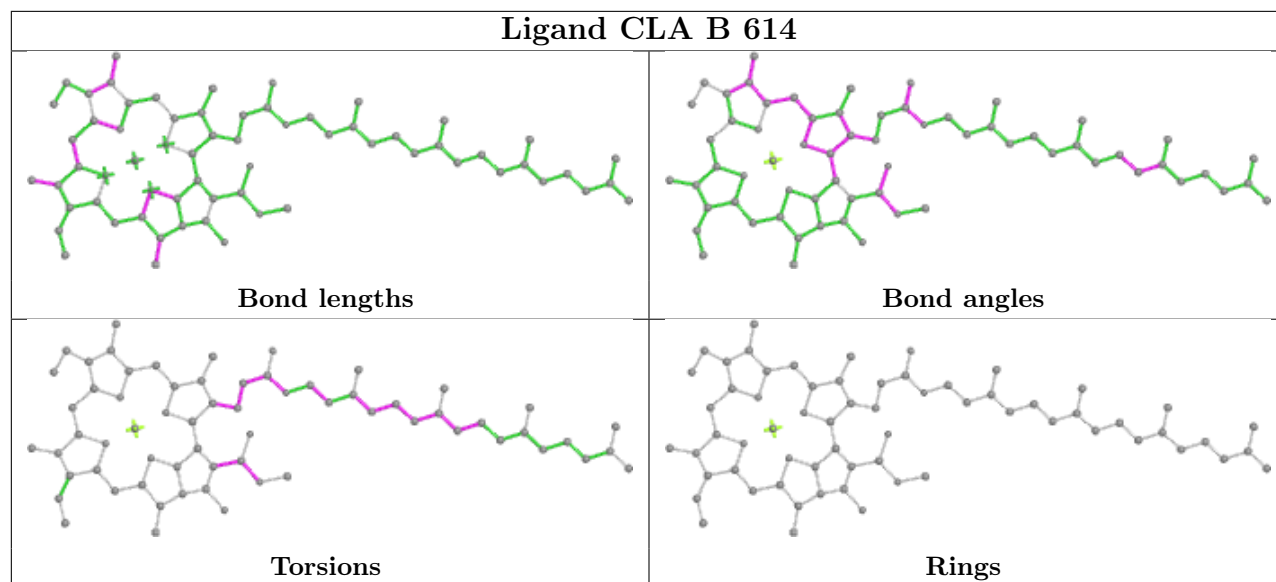
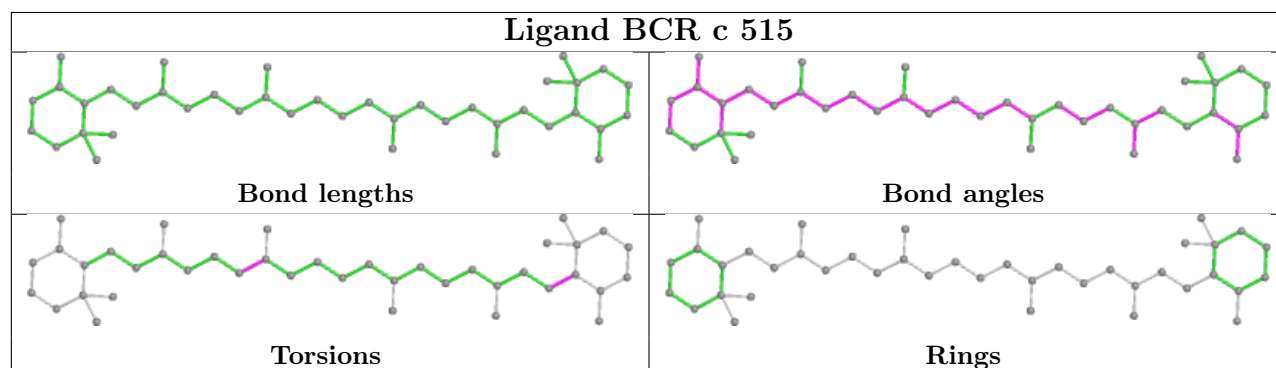
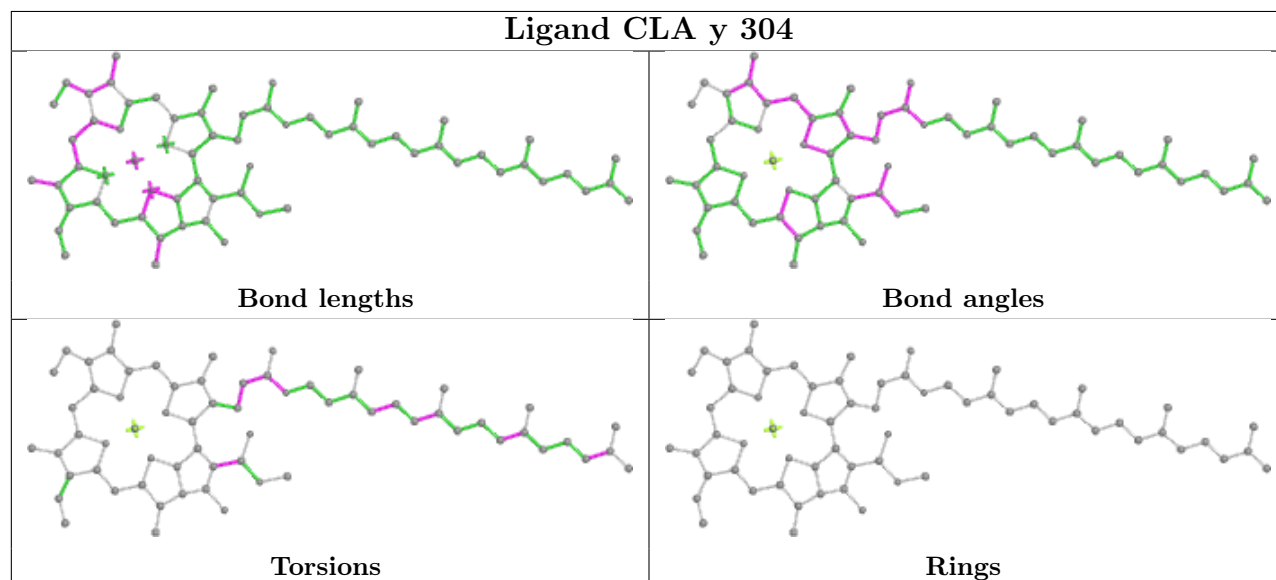
Rings

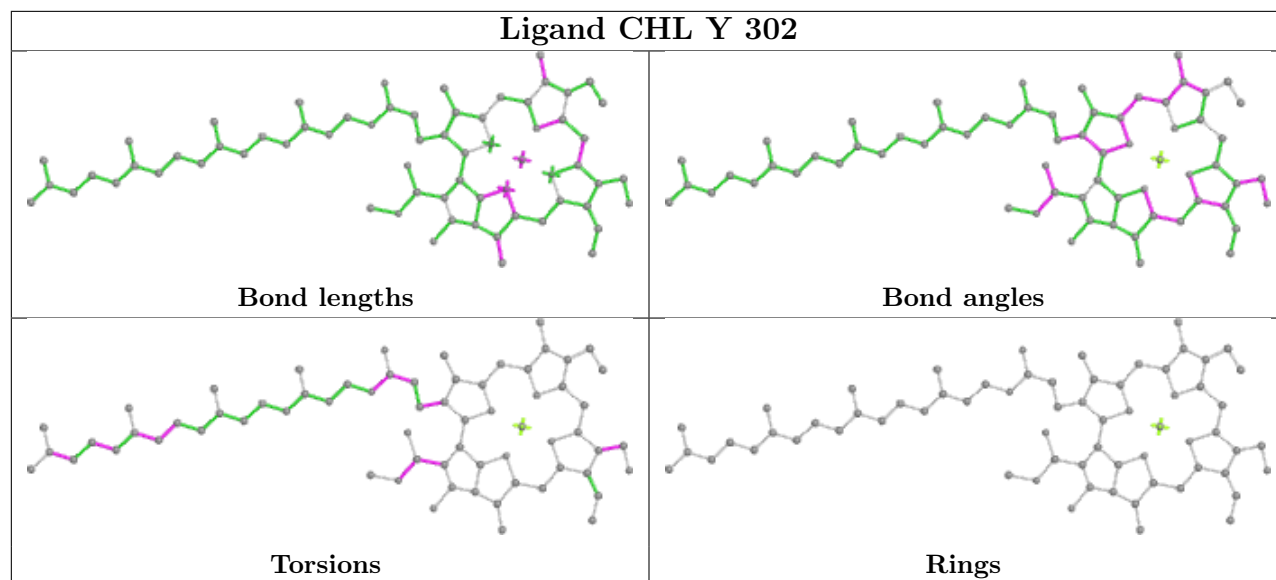
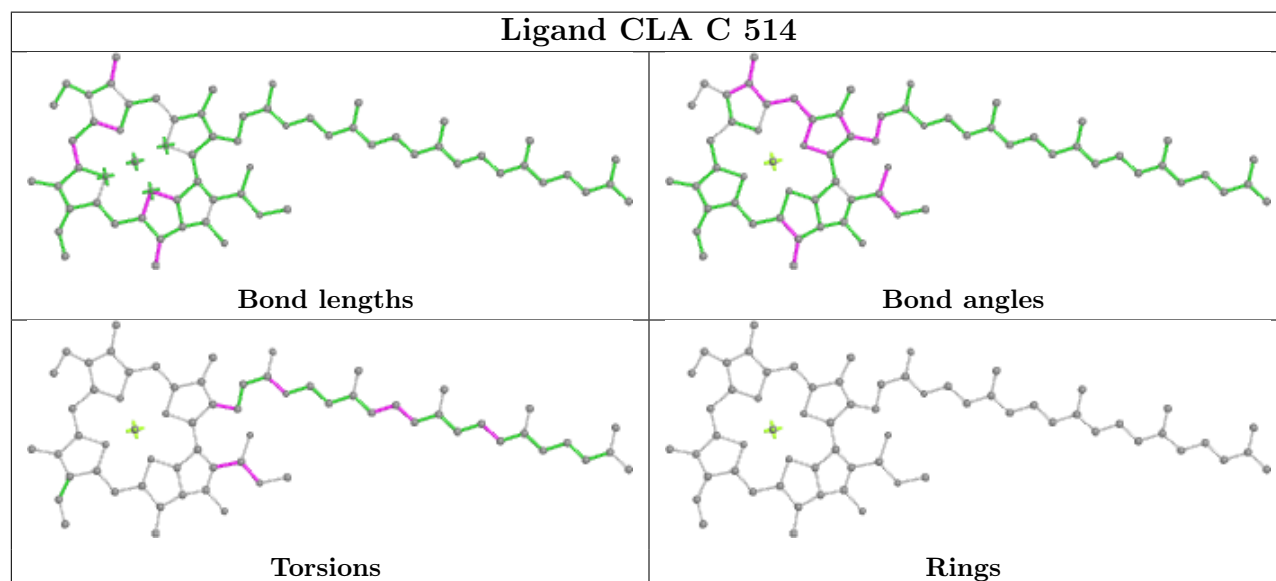
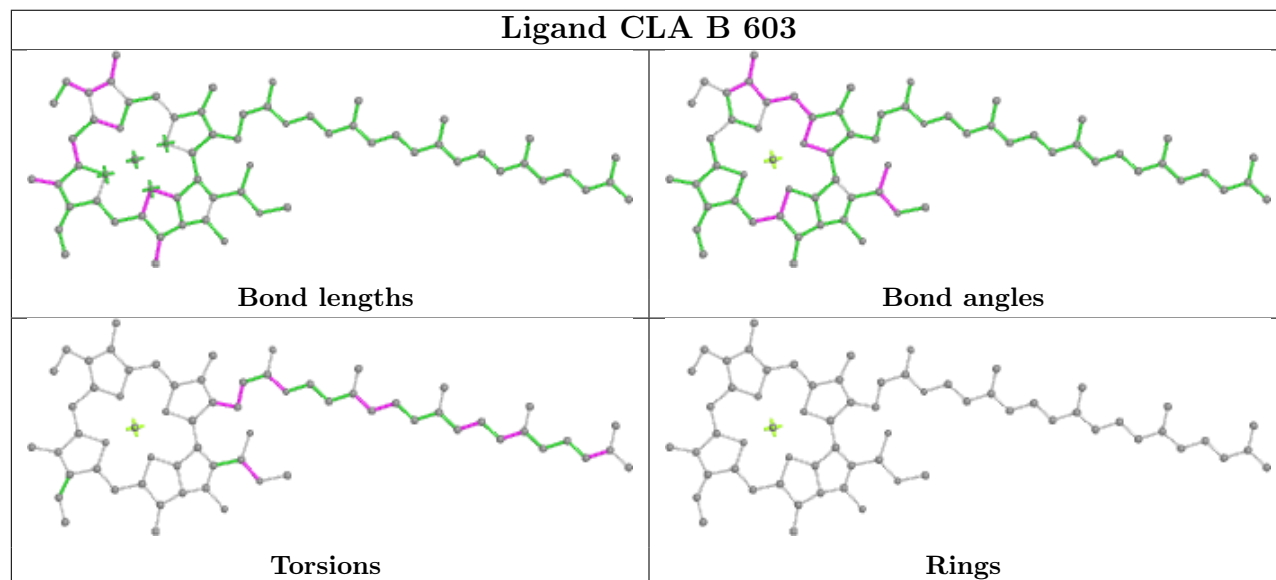
Ligand CLA A 402



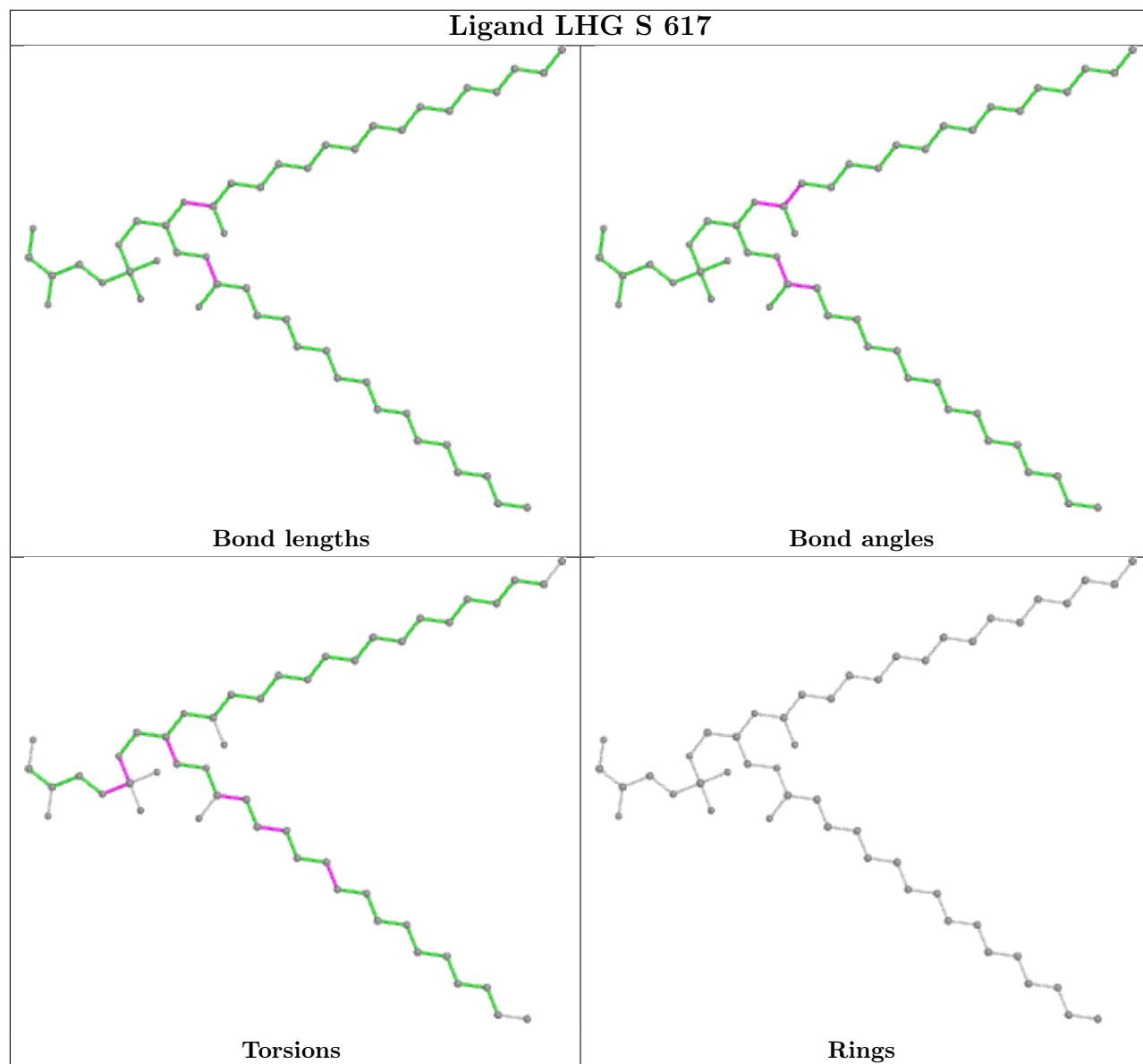
Ligand CLA b 606



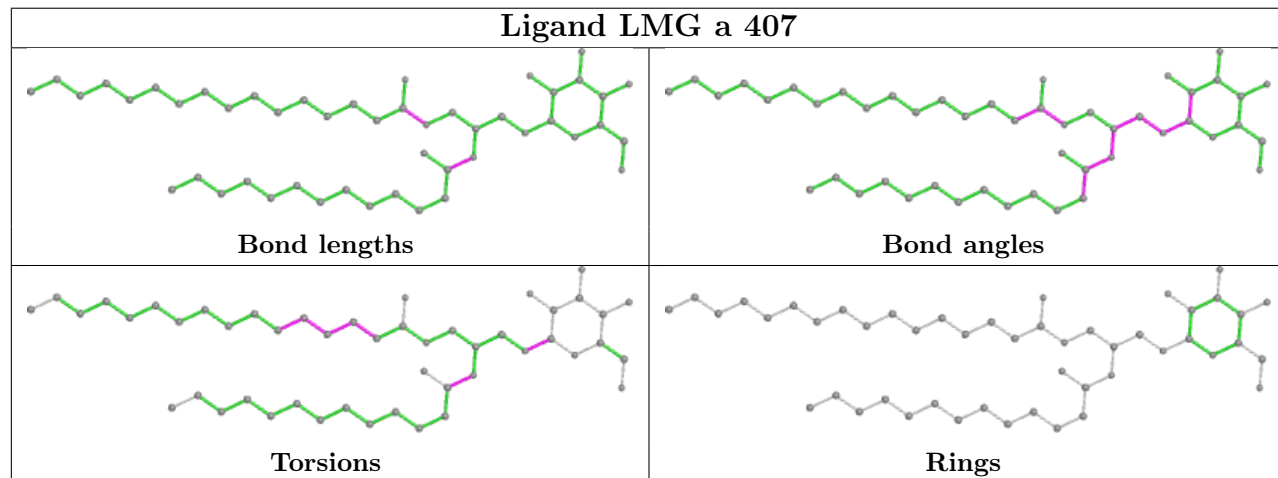
Ligand CLA B 614**Ligand BCR c 515****Ligand CLA y 304**

Ligand CHL Y 302**Ligand CLA C 514****Ligand CLA B 603**

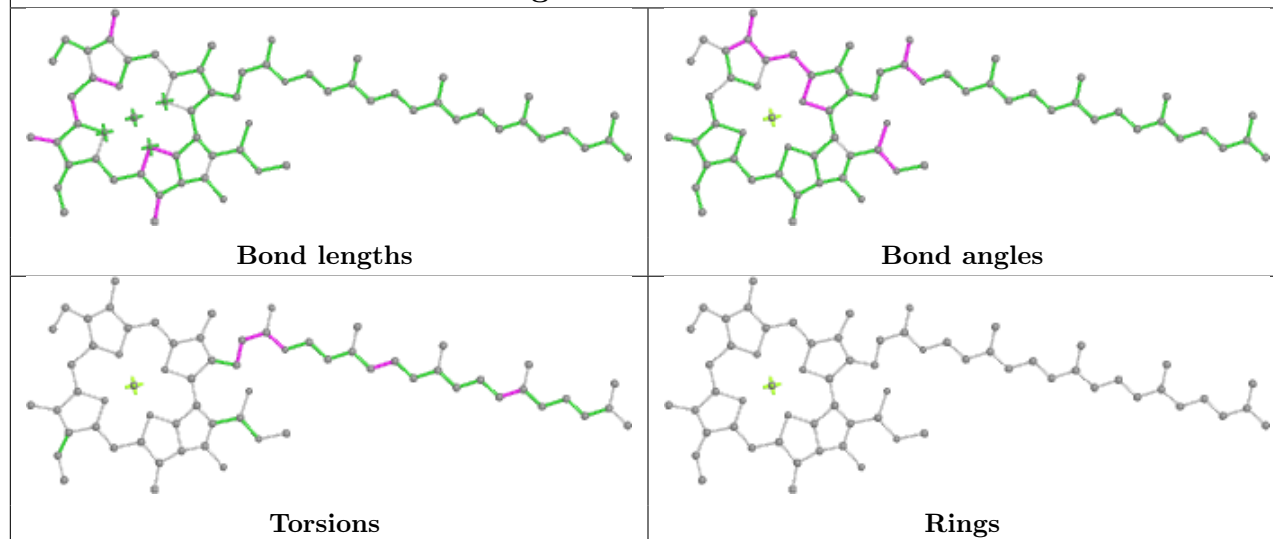
Ligand LHG S 617



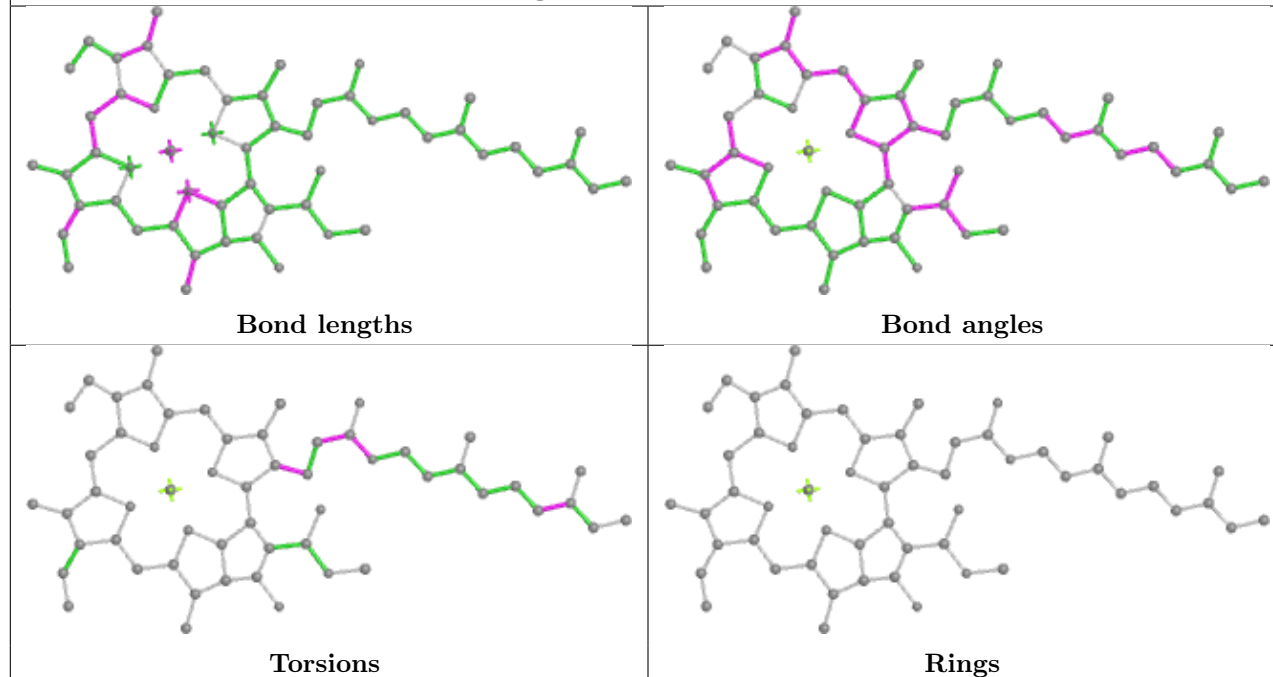
Ligand LMG a 407



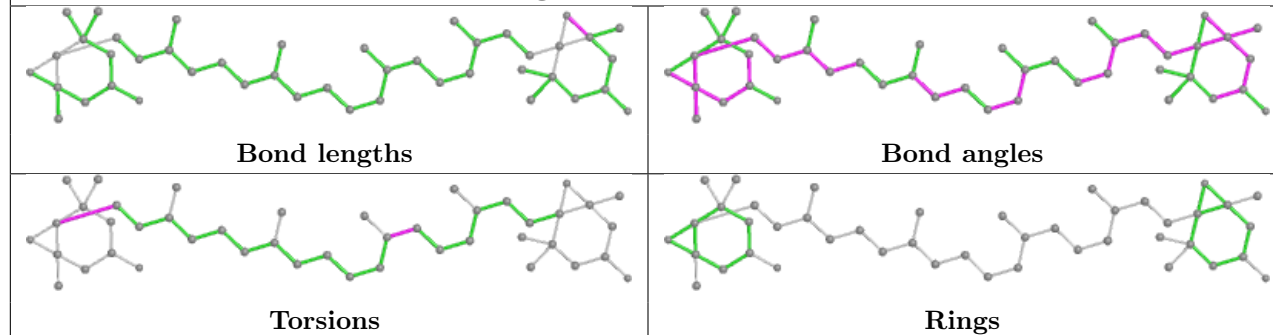
Ligand CLA B 602



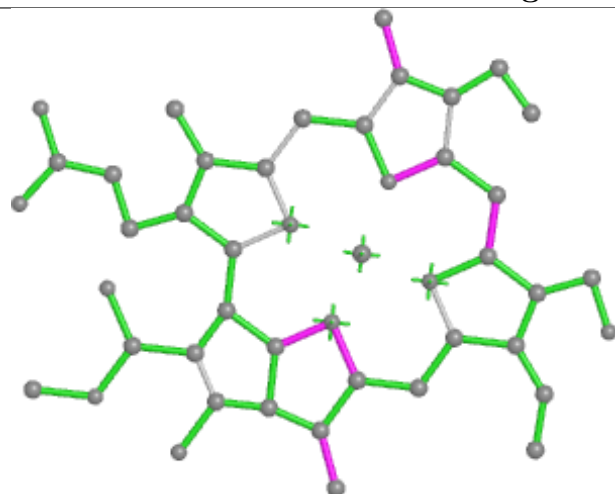
Ligand CLA C 513



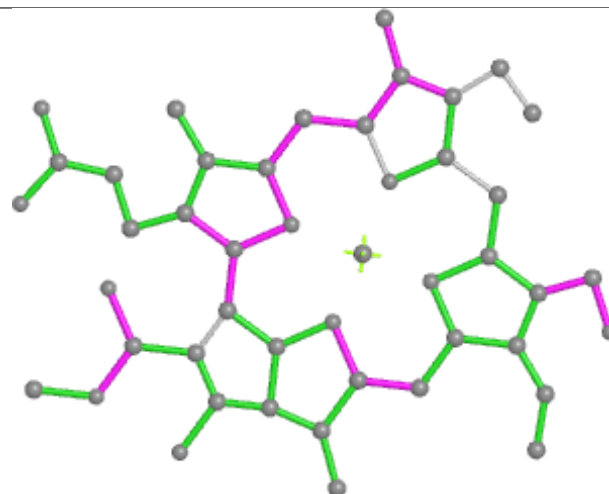
Ligand XAT n 301



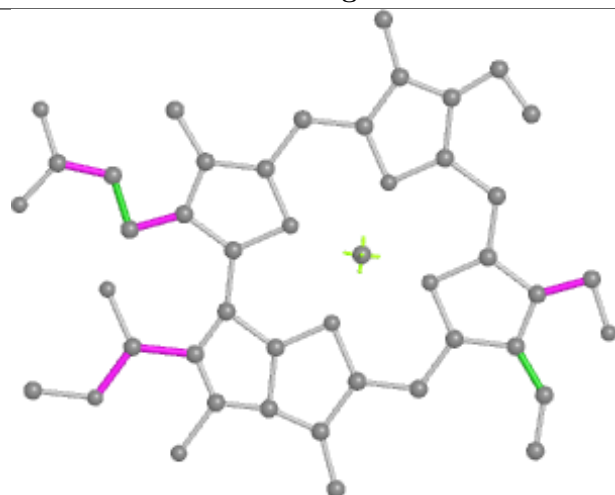
Ligand CHL s 601



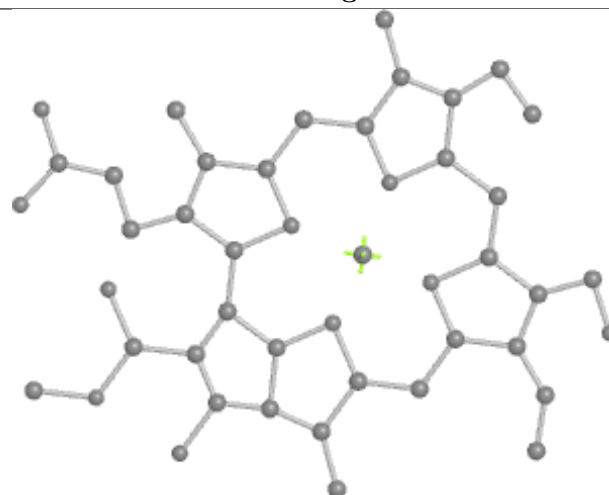
Bond lengths



Bond angles

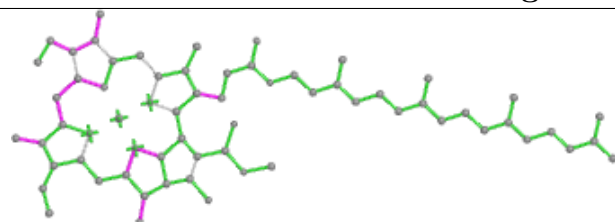


Torsions

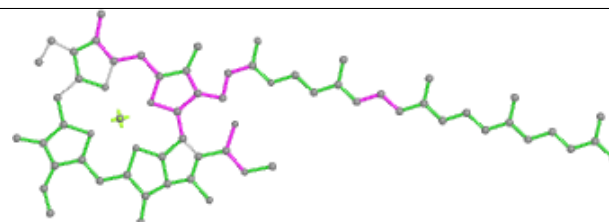


Rings

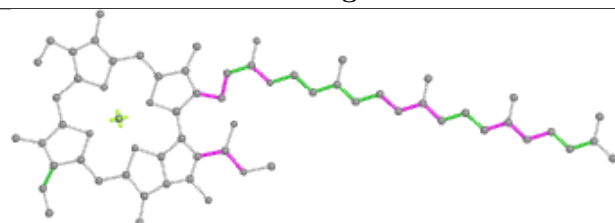
Ligand CLA c 502



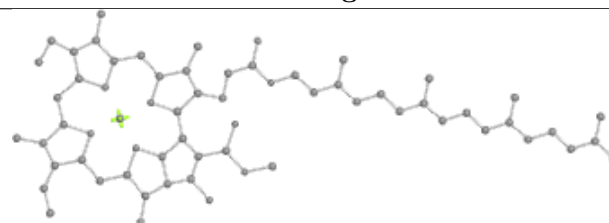
Bond lengths



Bond angles

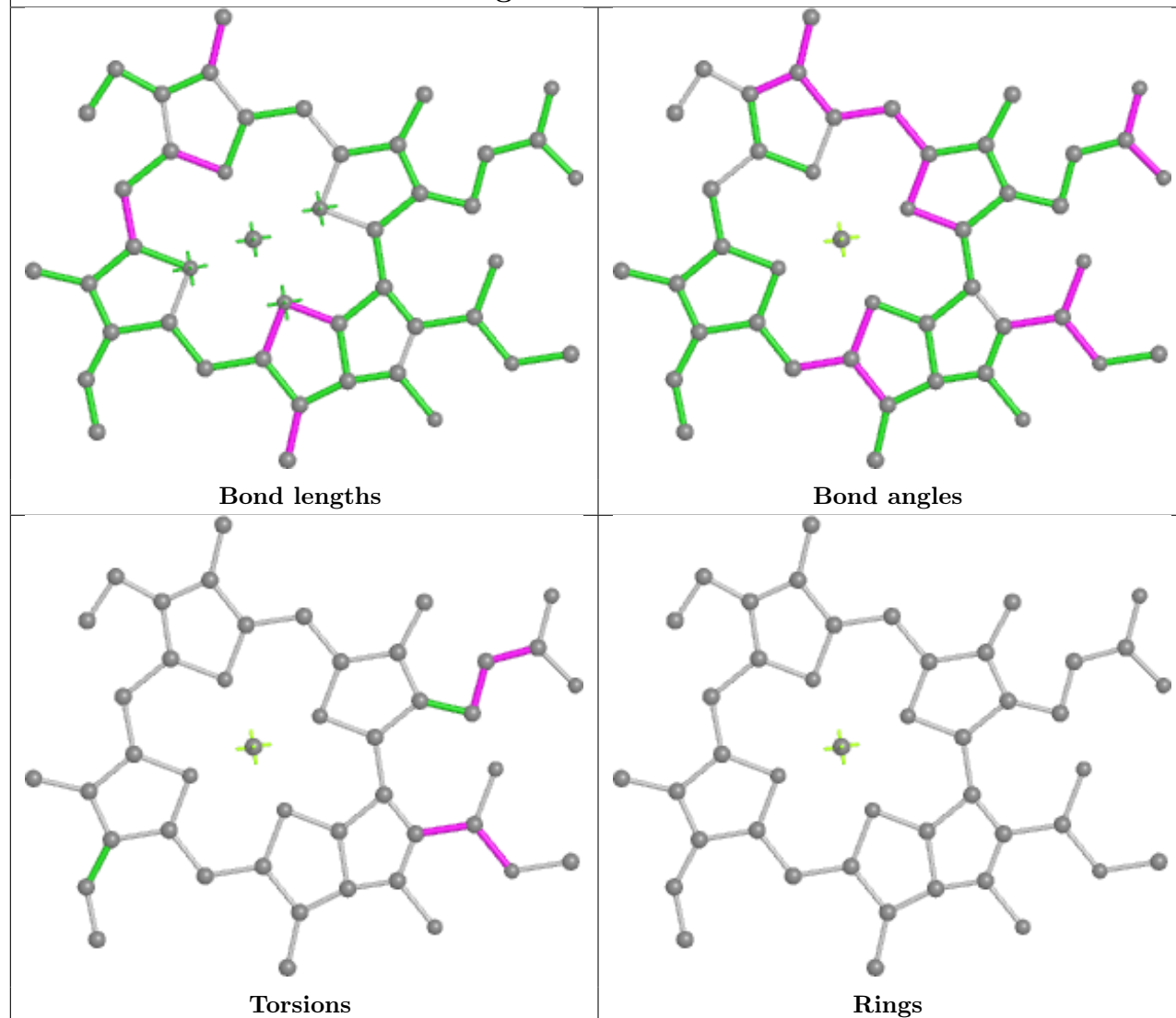


Torsions

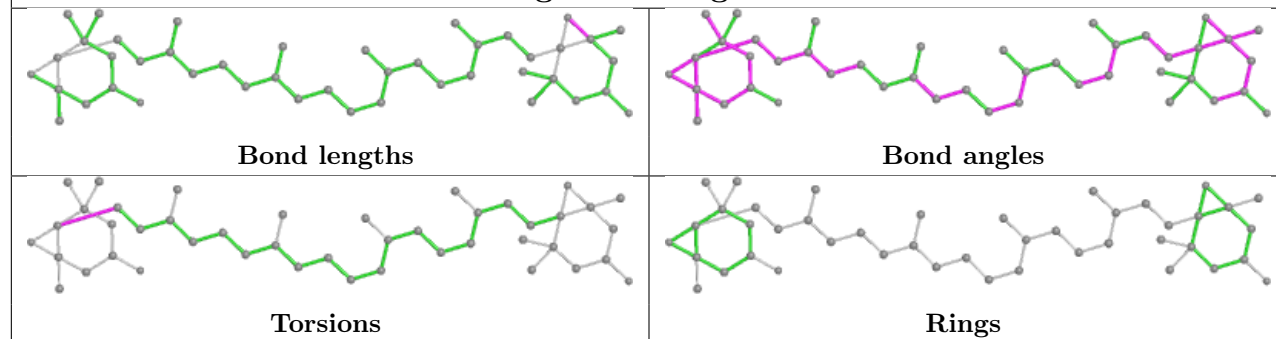


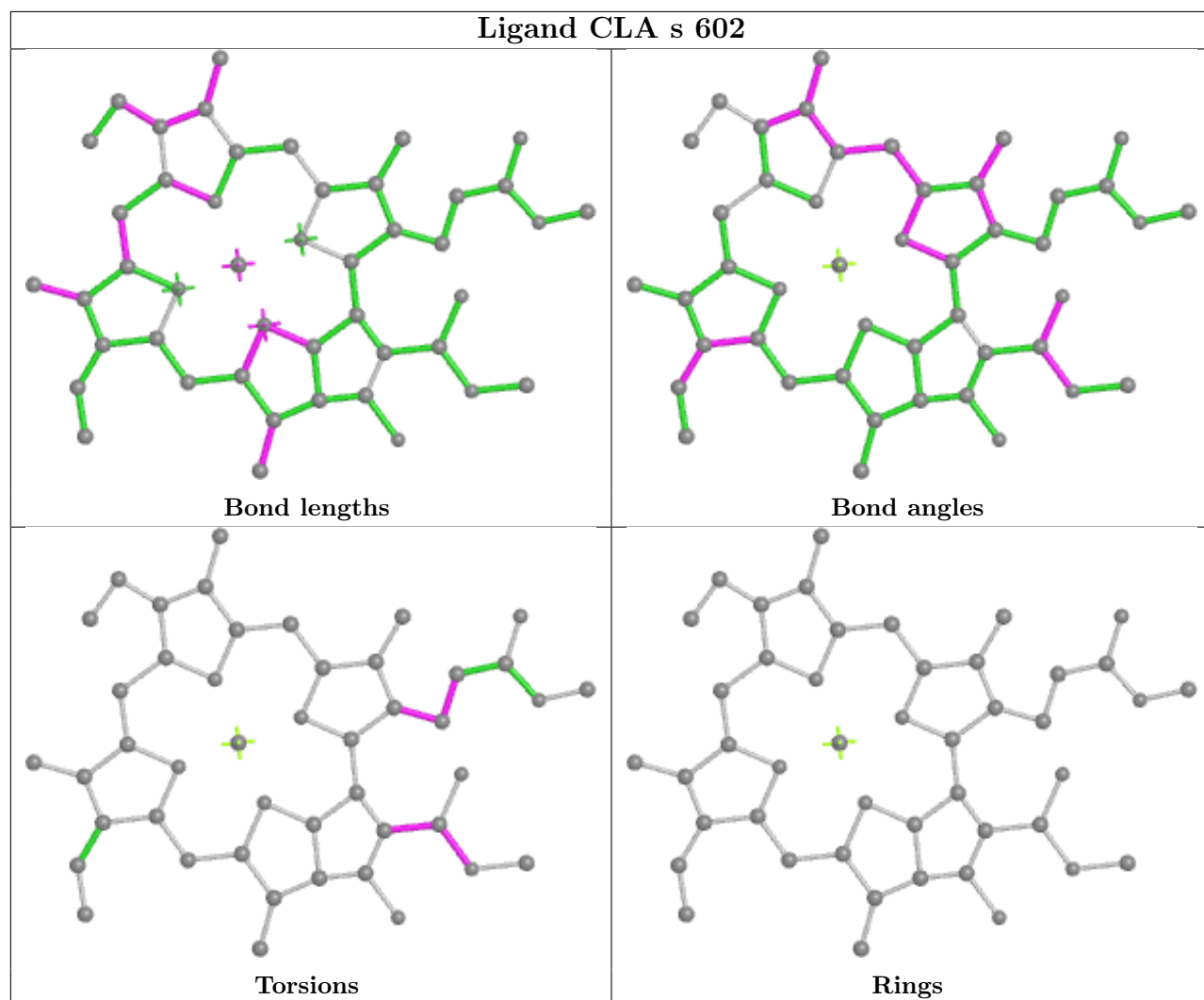
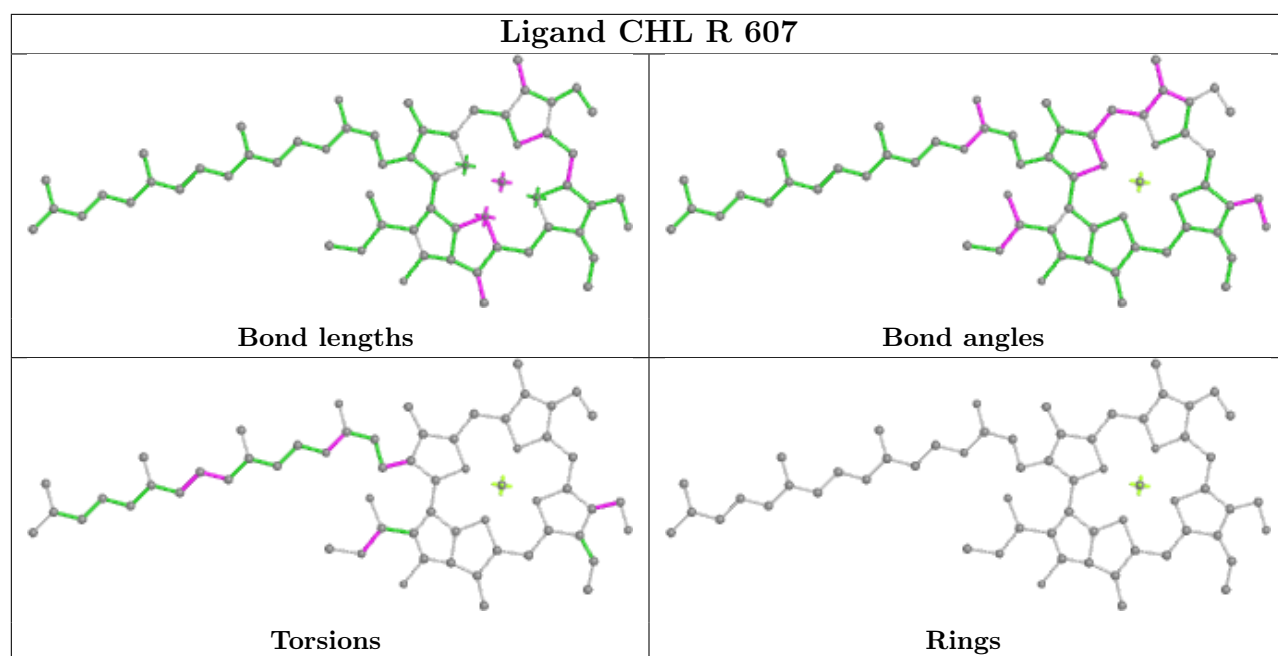
Rings

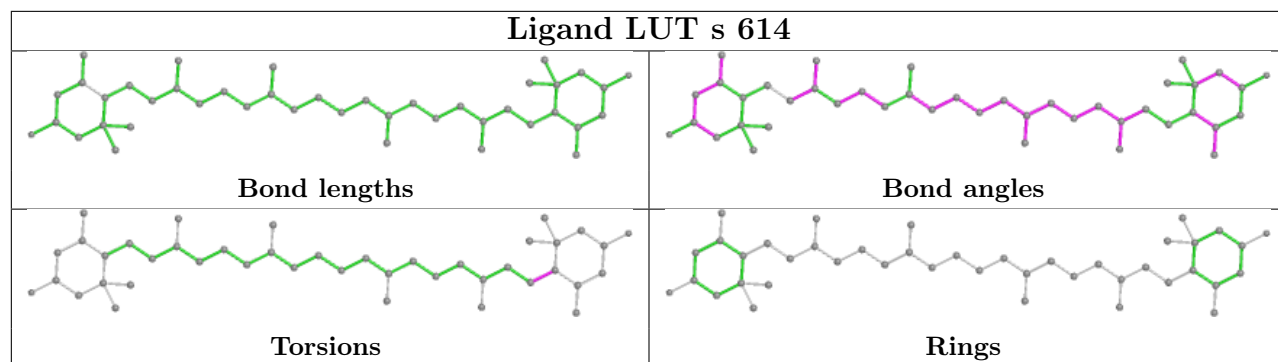
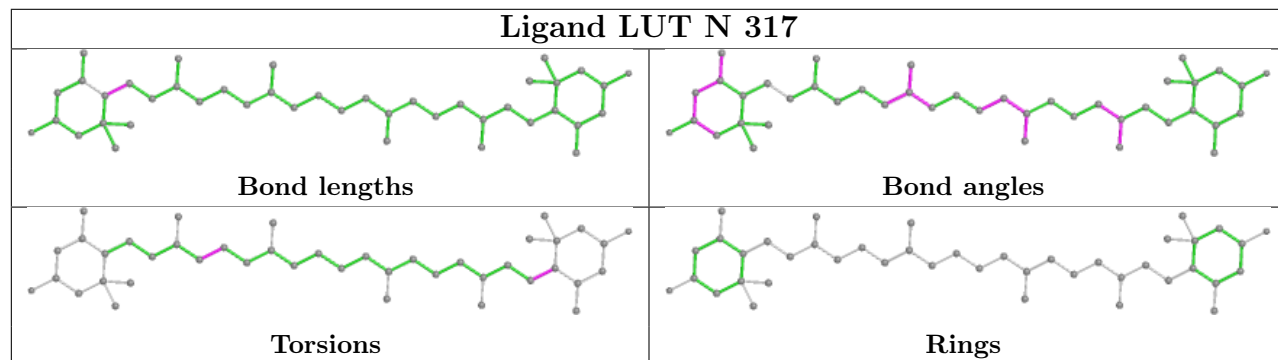
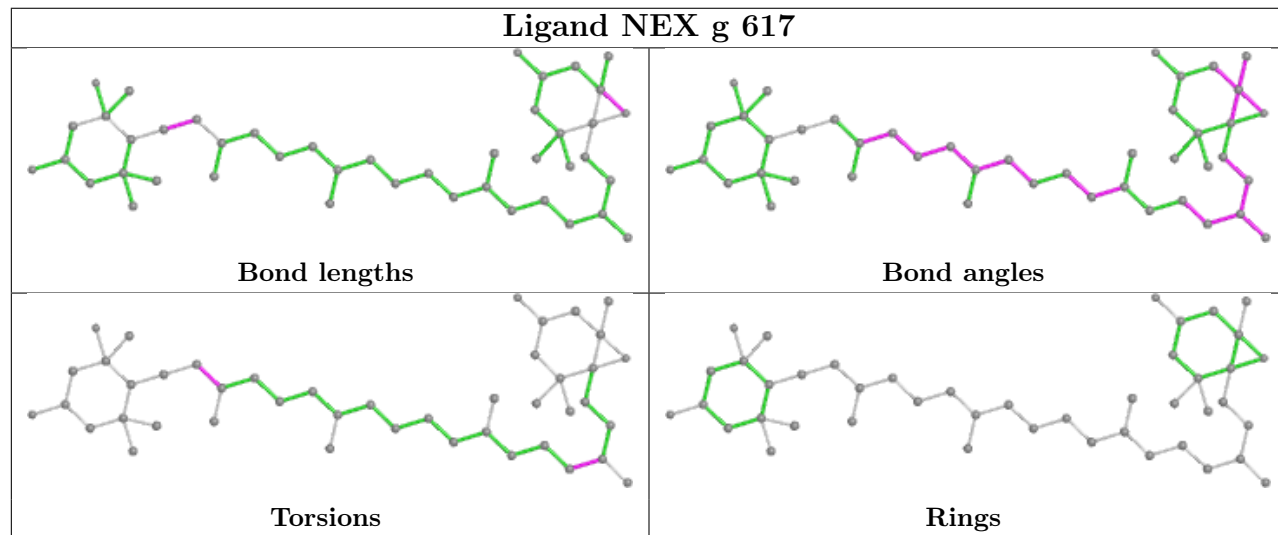
Ligand CLA s 608



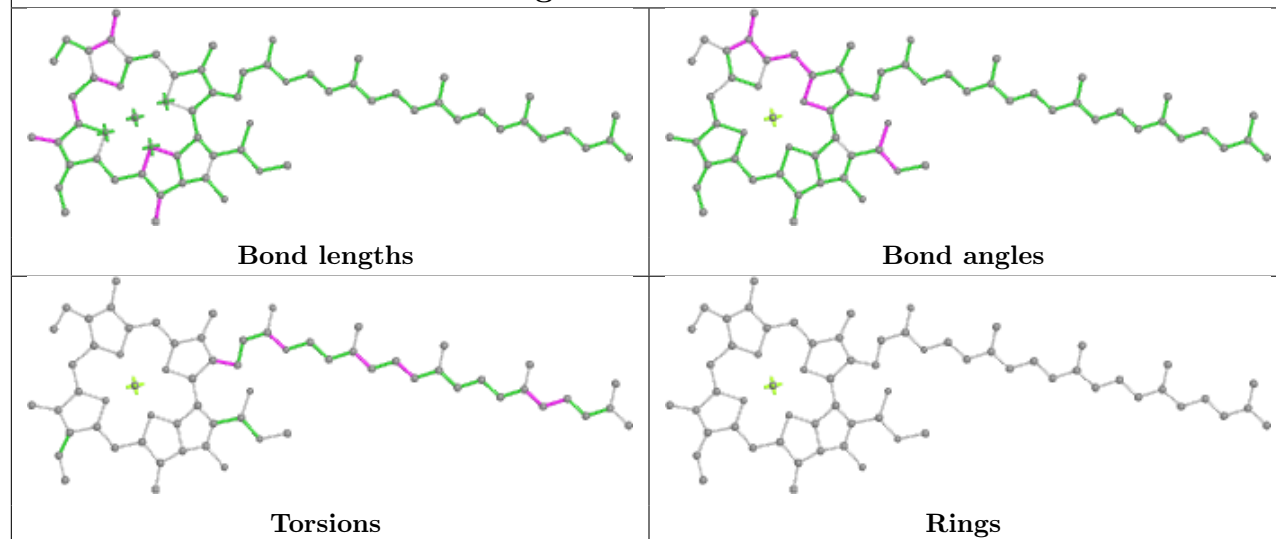
Ligand XAT g 620



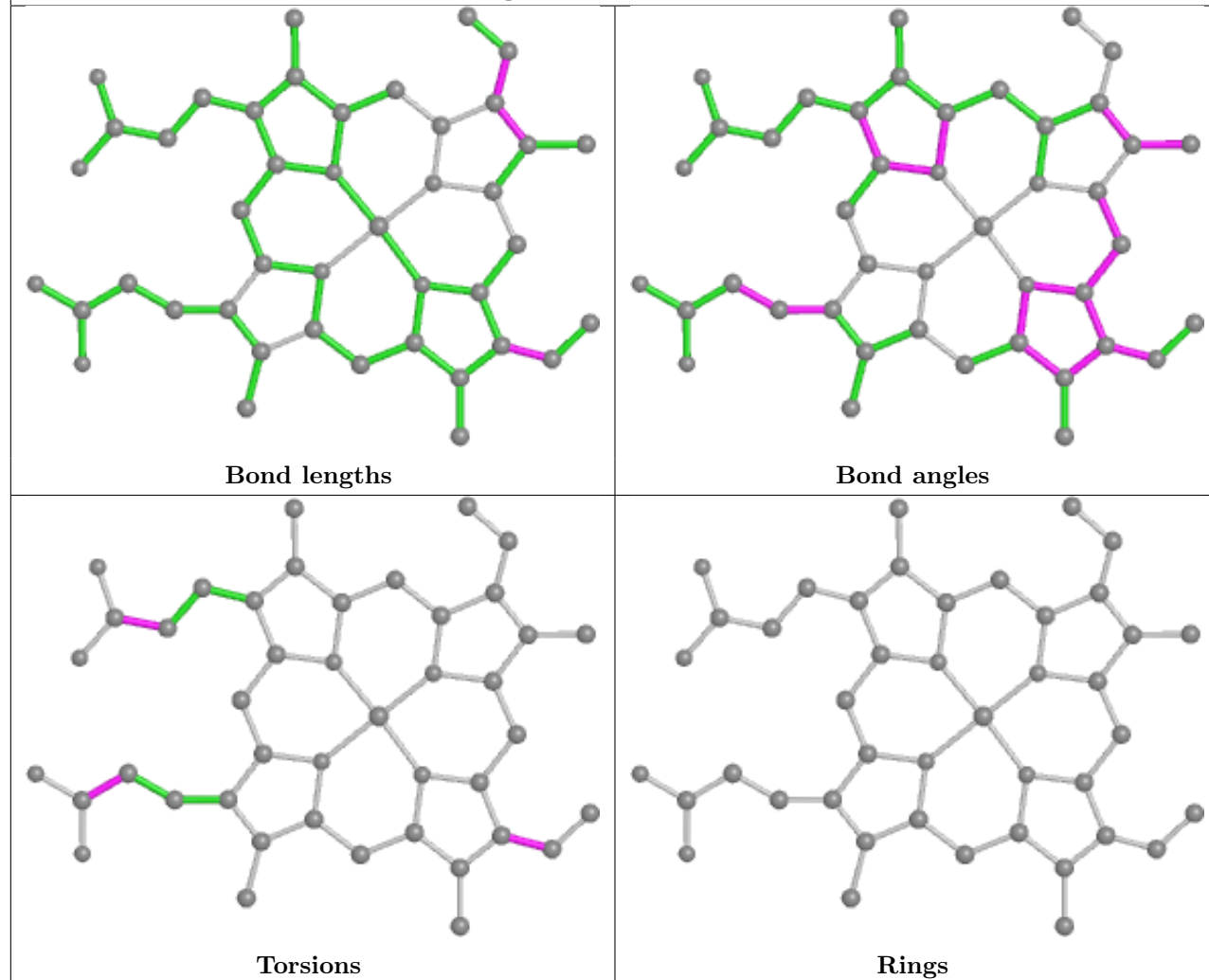


Ligand LUT s 614**Ligand LUT N 317****Ligand NEX g 617**

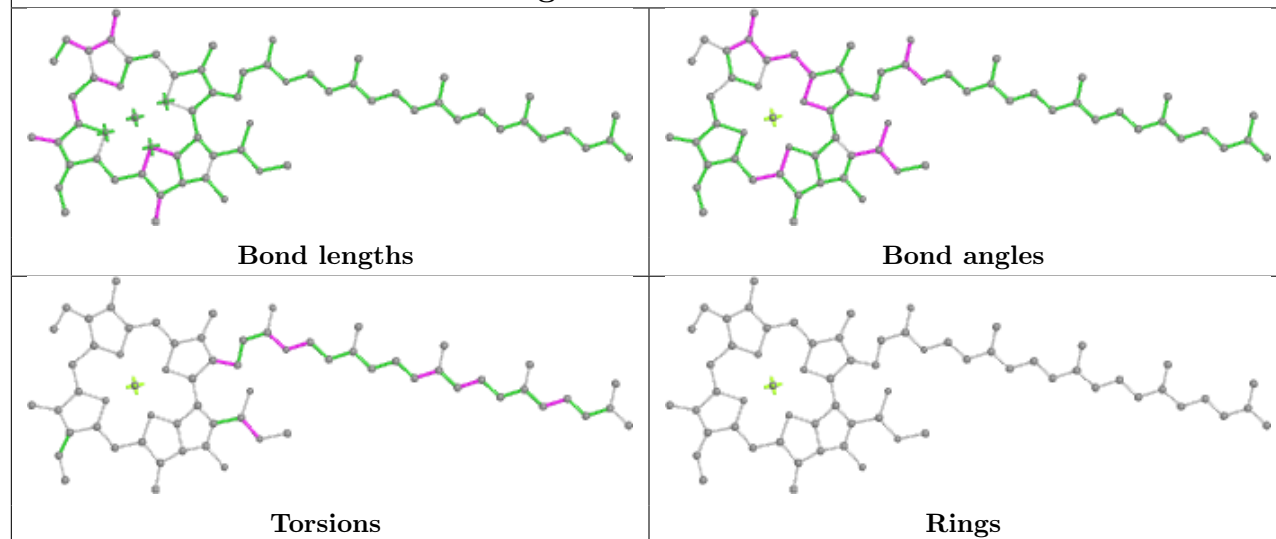
Ligand CLA b 611



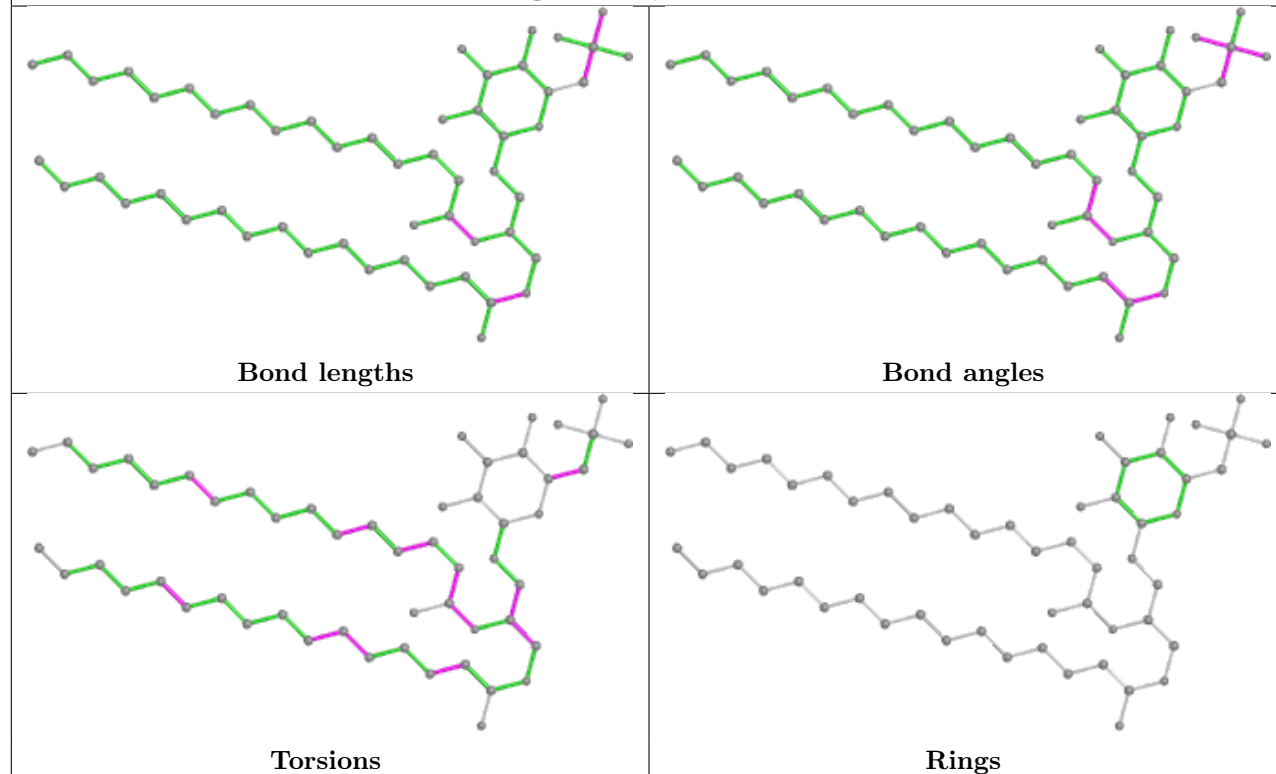
Ligand HEM E 101

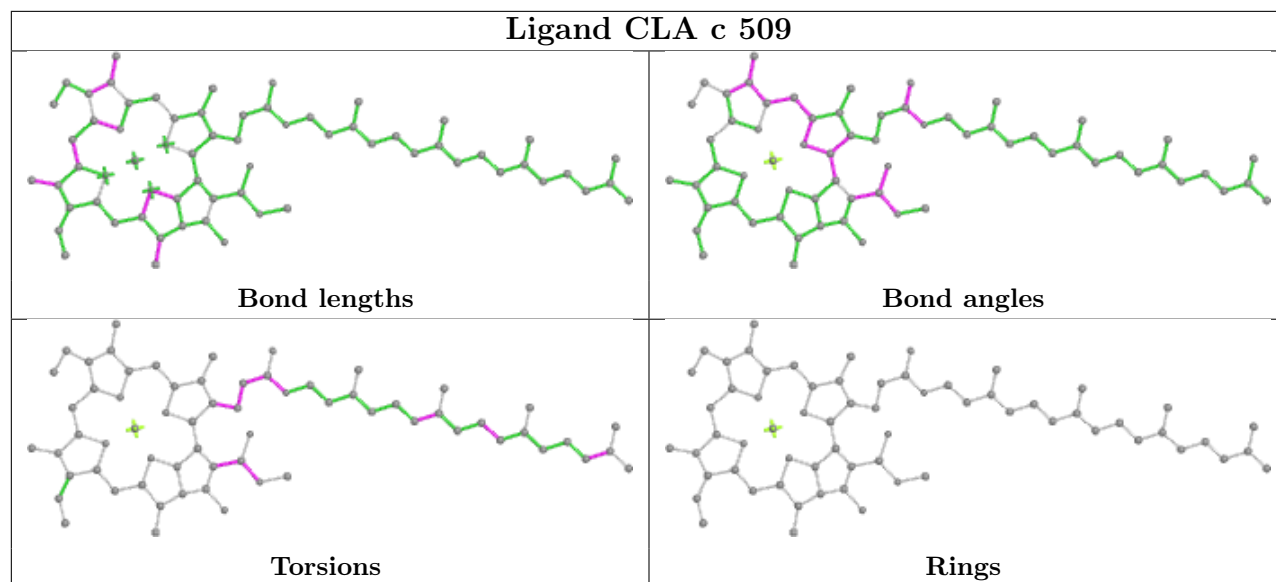
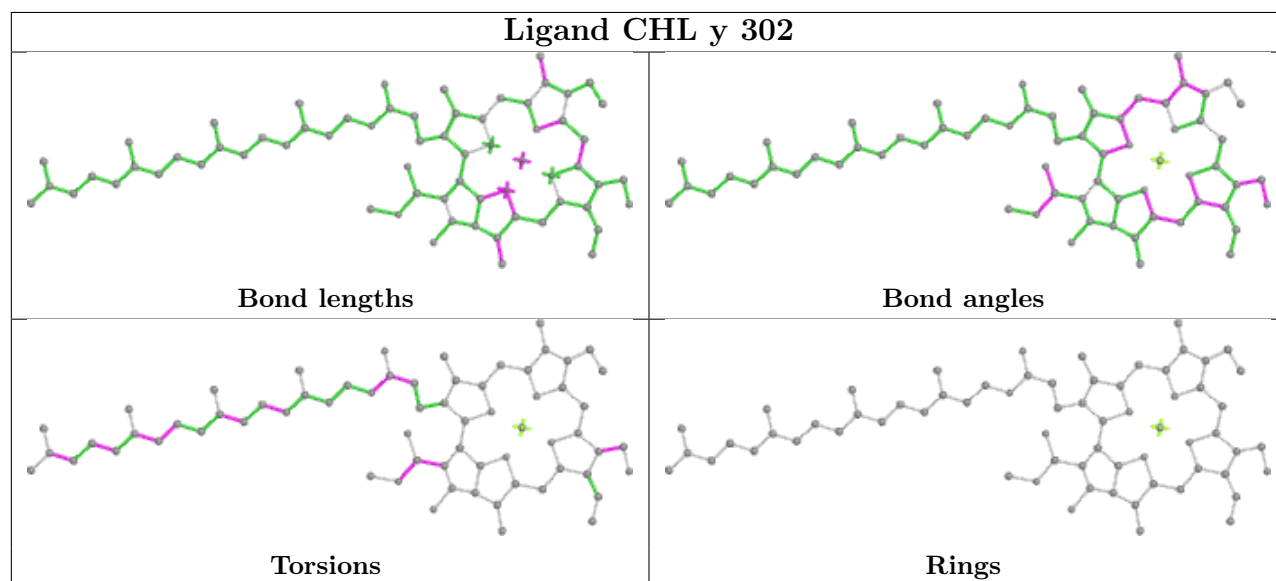


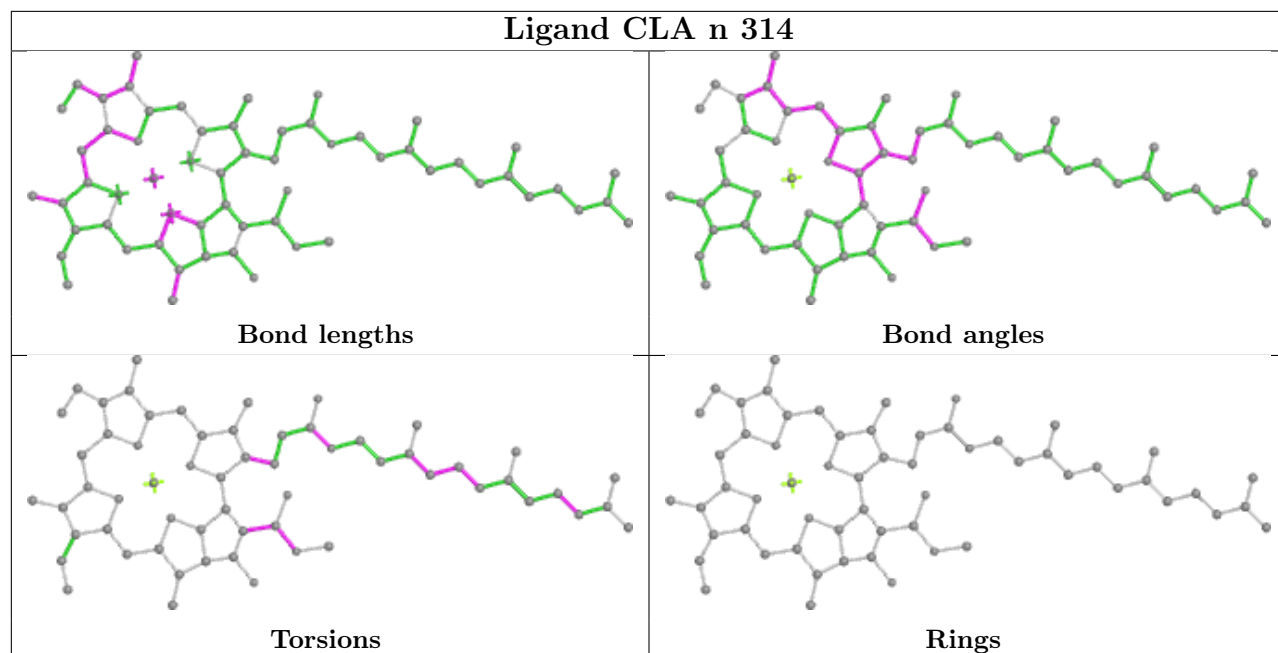
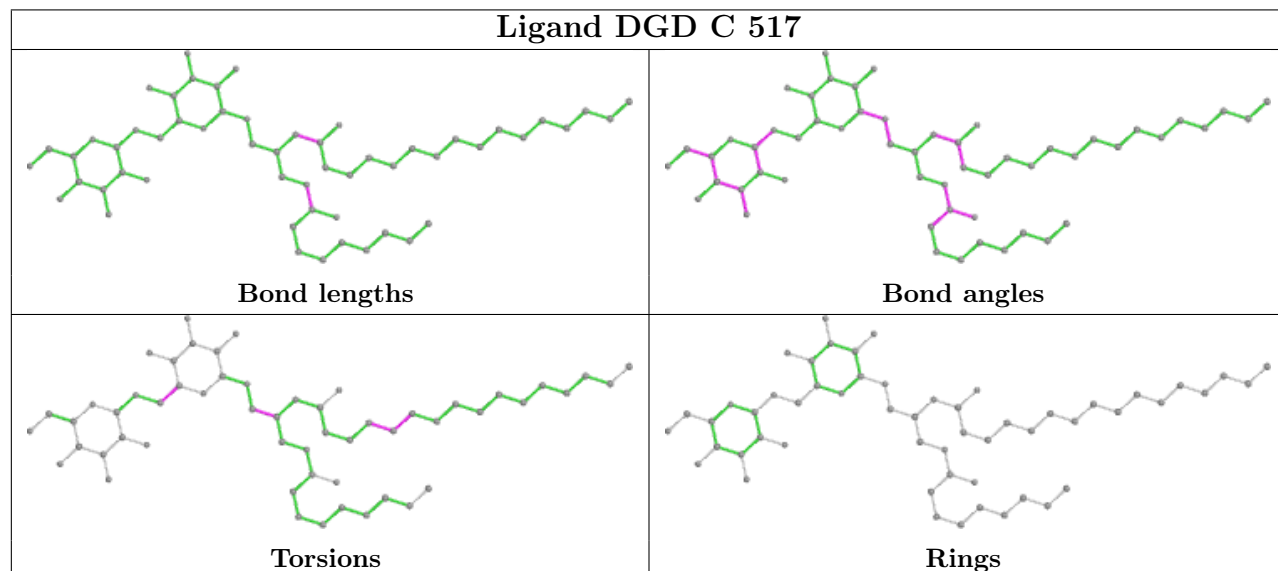
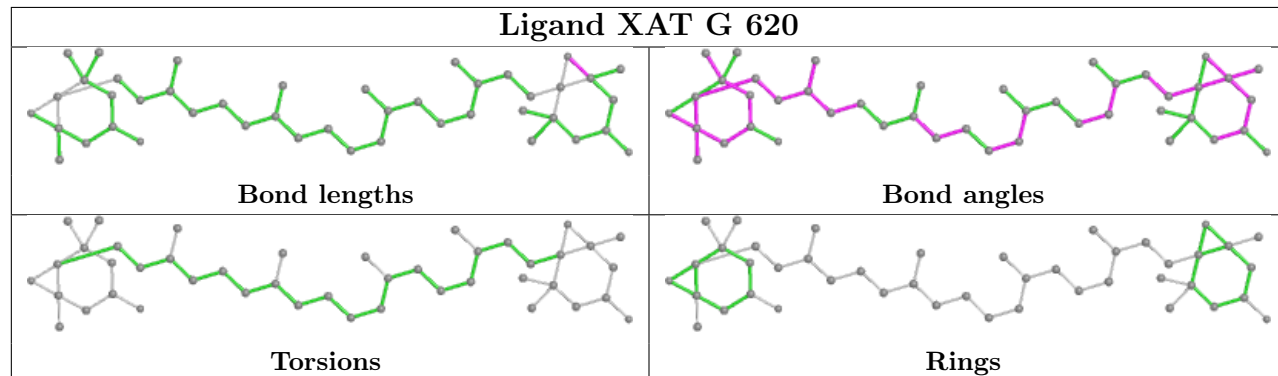
Ligand CLA r 609



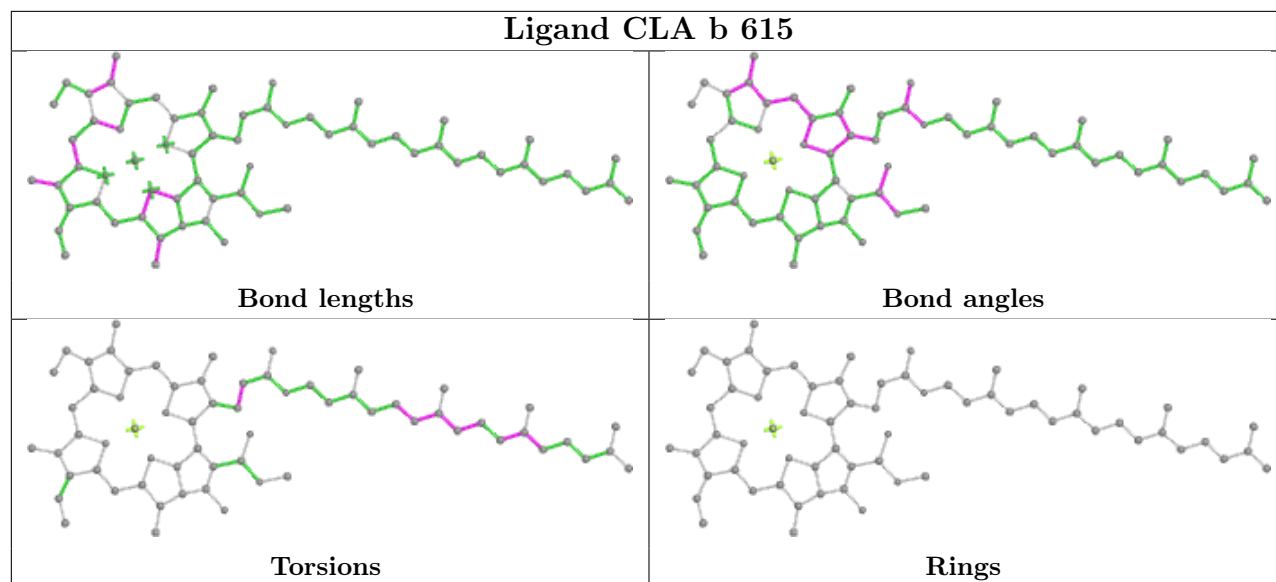
Ligand SQD M 101



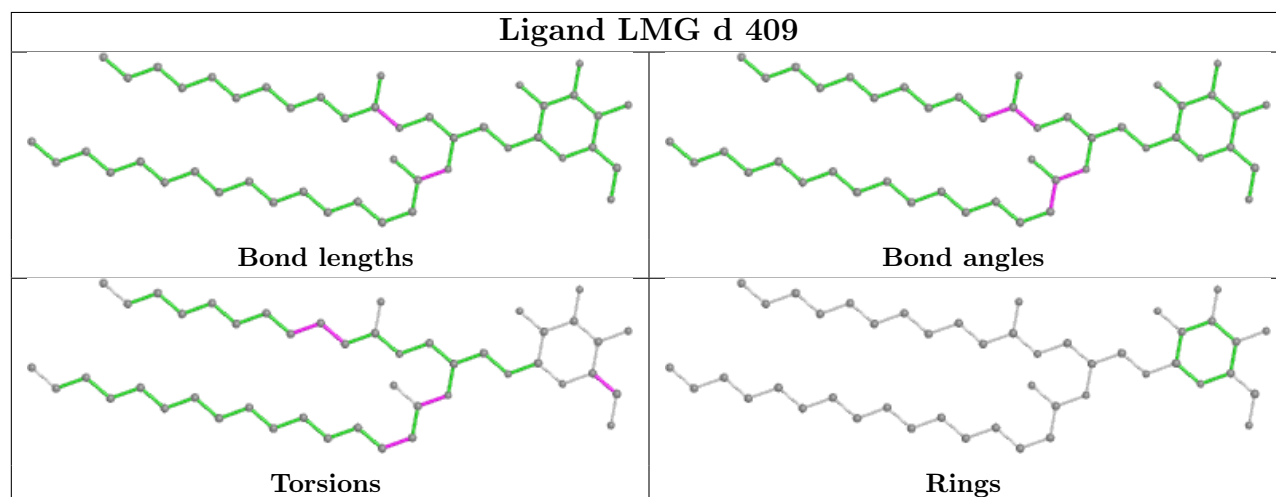
Ligand CLA c 509**Ligand CHL y 302**

Ligand CLA n 314**Ligand DGD C 517****Ligand XAT G 620**

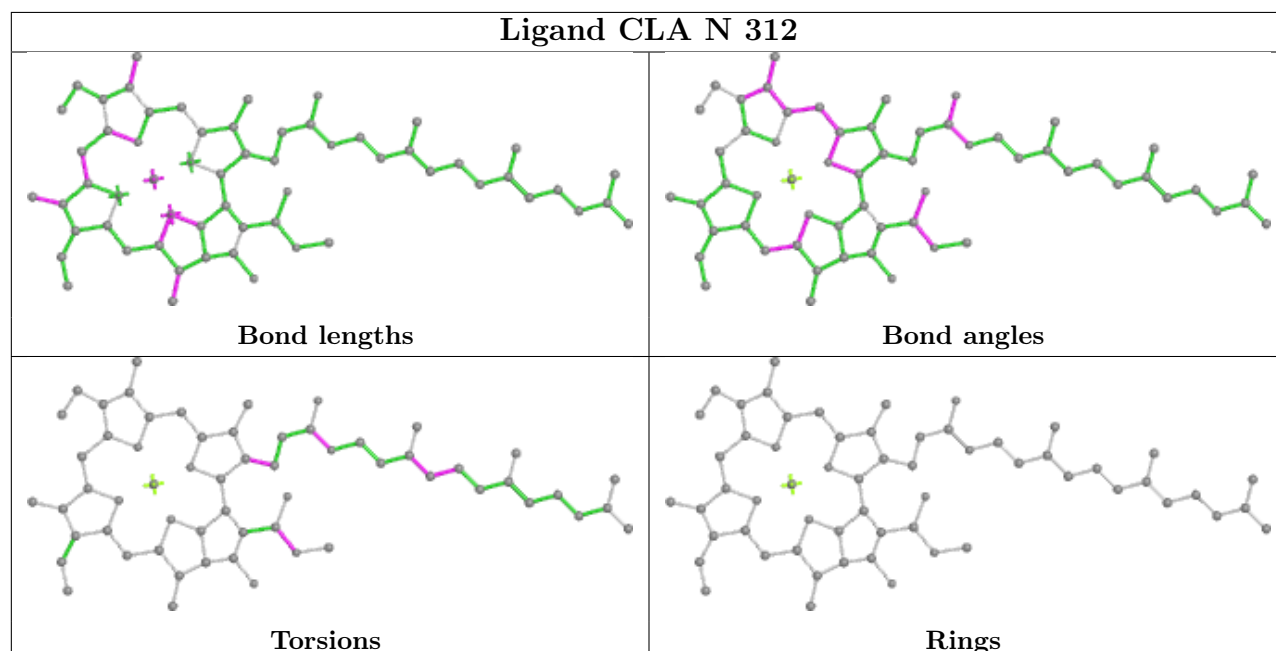
Ligand CLA b 615

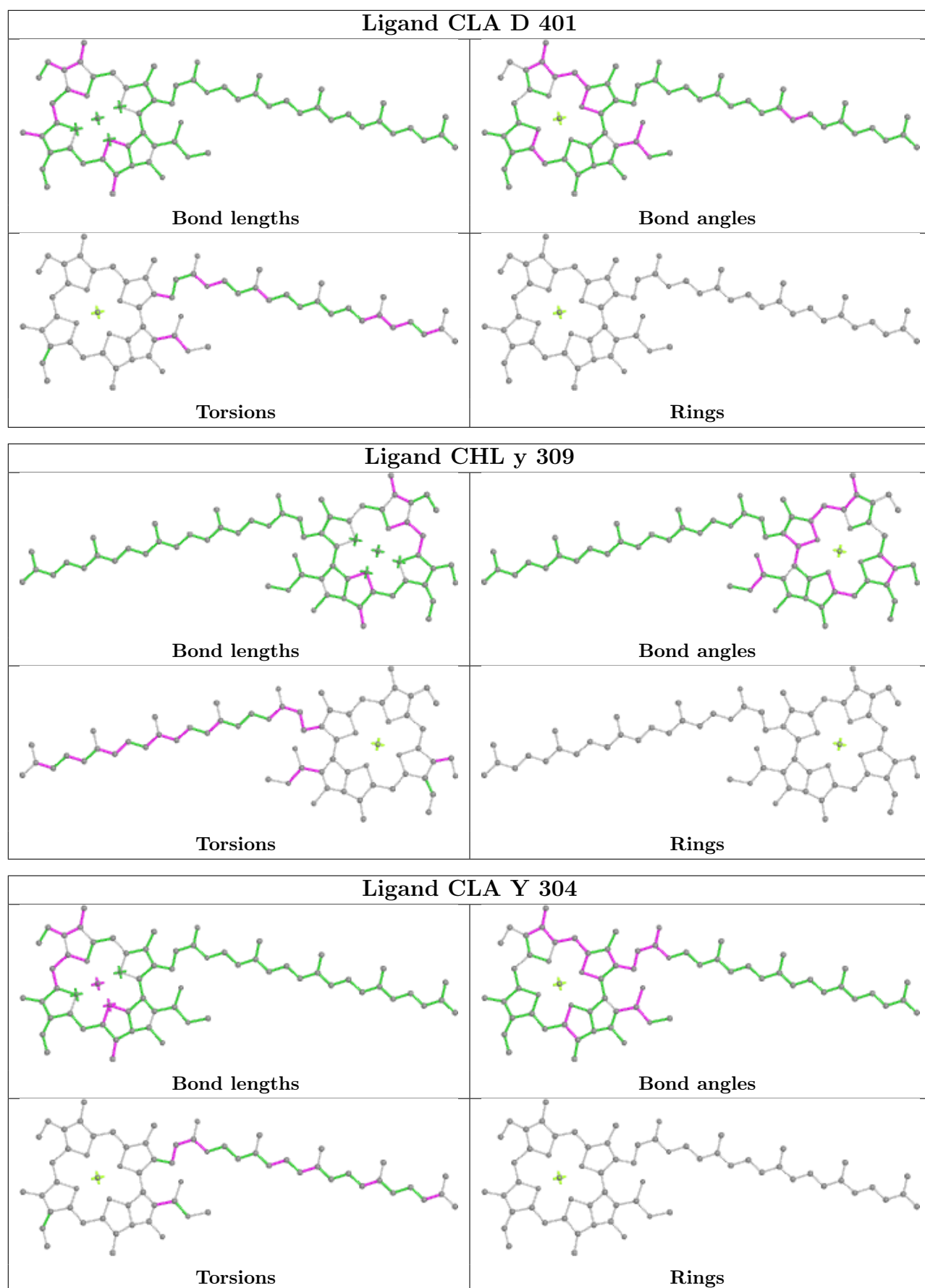


Ligand LMG d 409

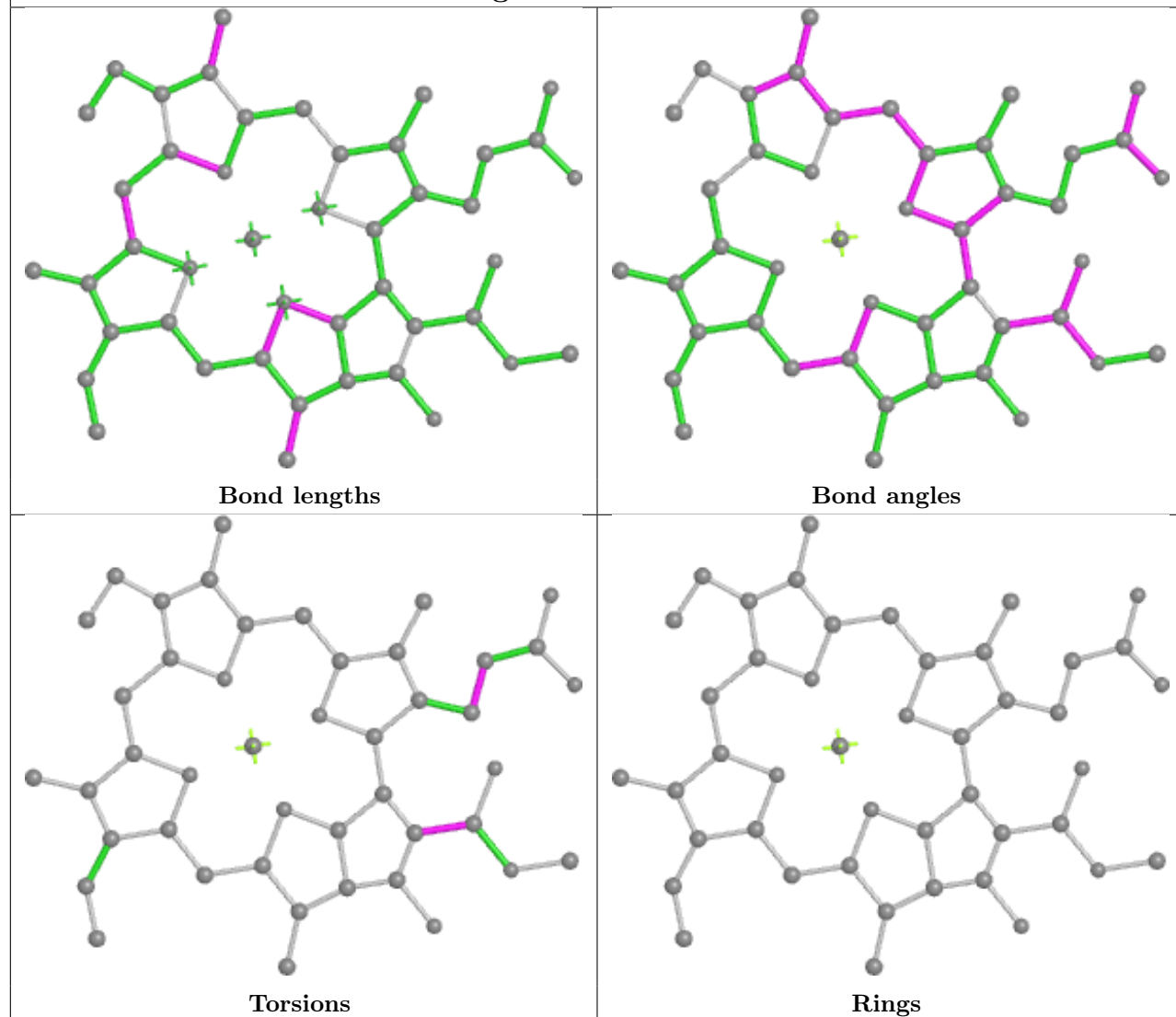


Ligand CLA N 312

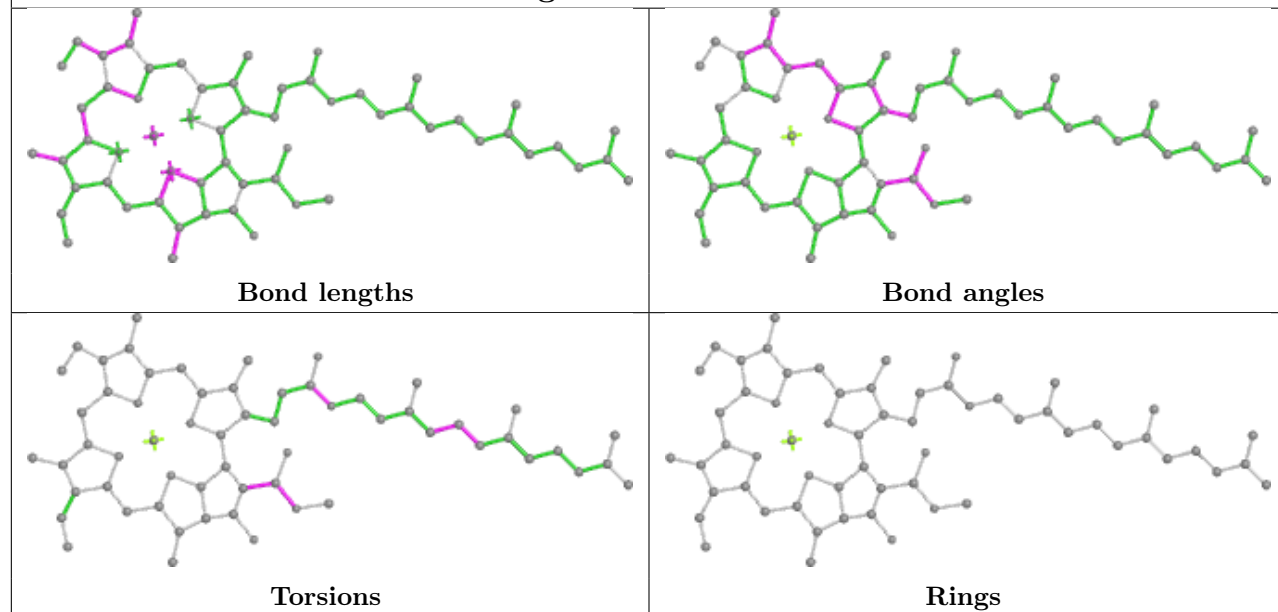




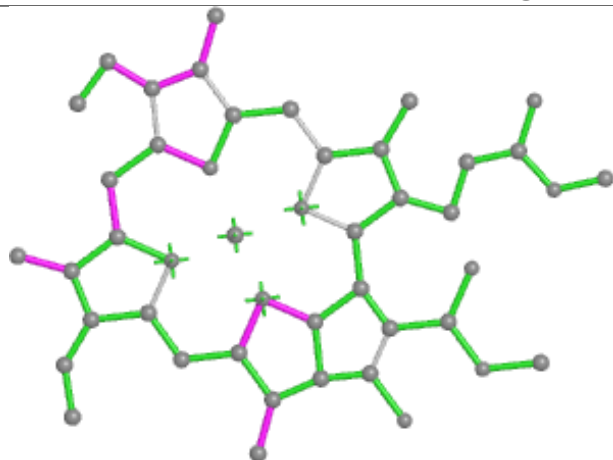
Ligand CLA S 608



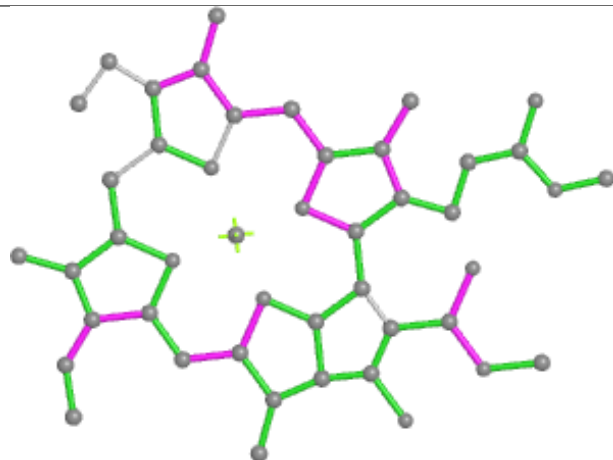
Ligand CLA r 603



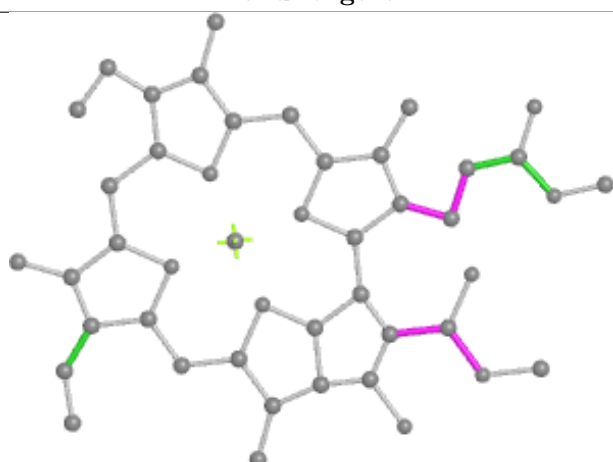
Ligand CLA S 602



Bond lengths



Bond angles

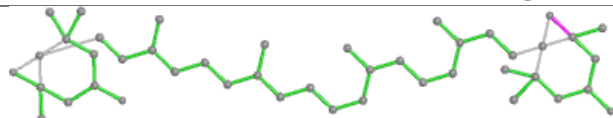


Torsions

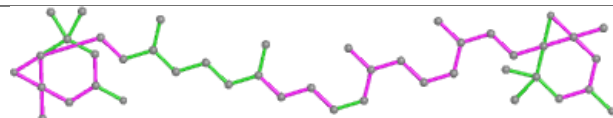


Rings

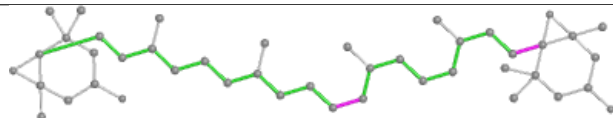
Ligand XAT r 616



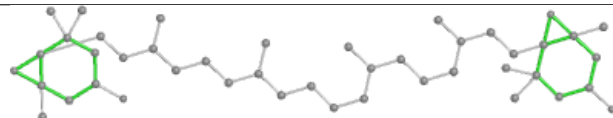
Bond lengths



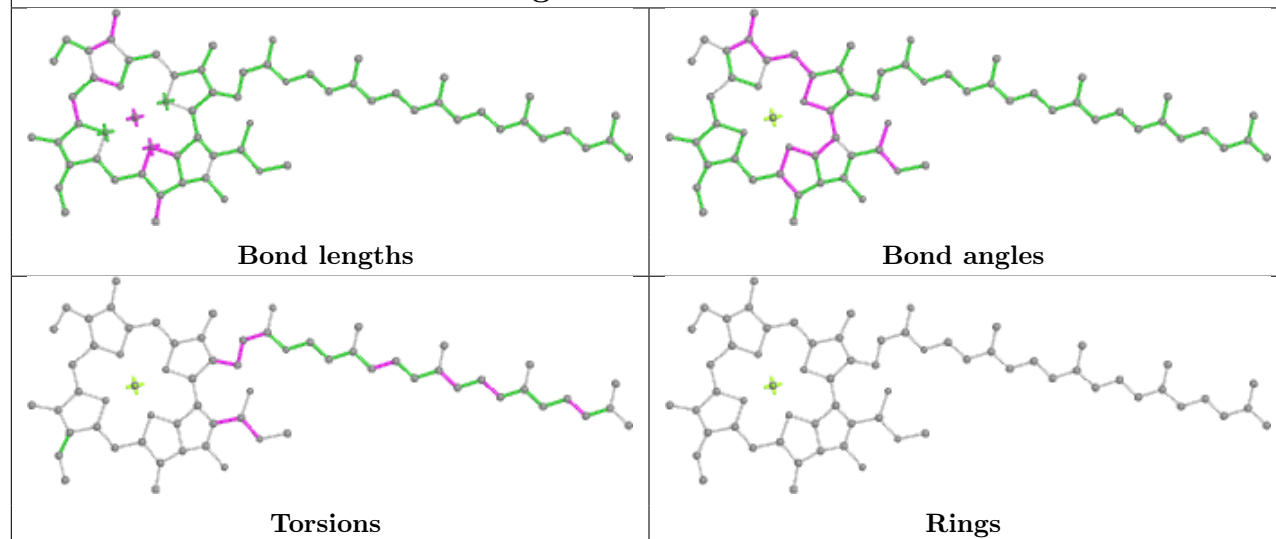
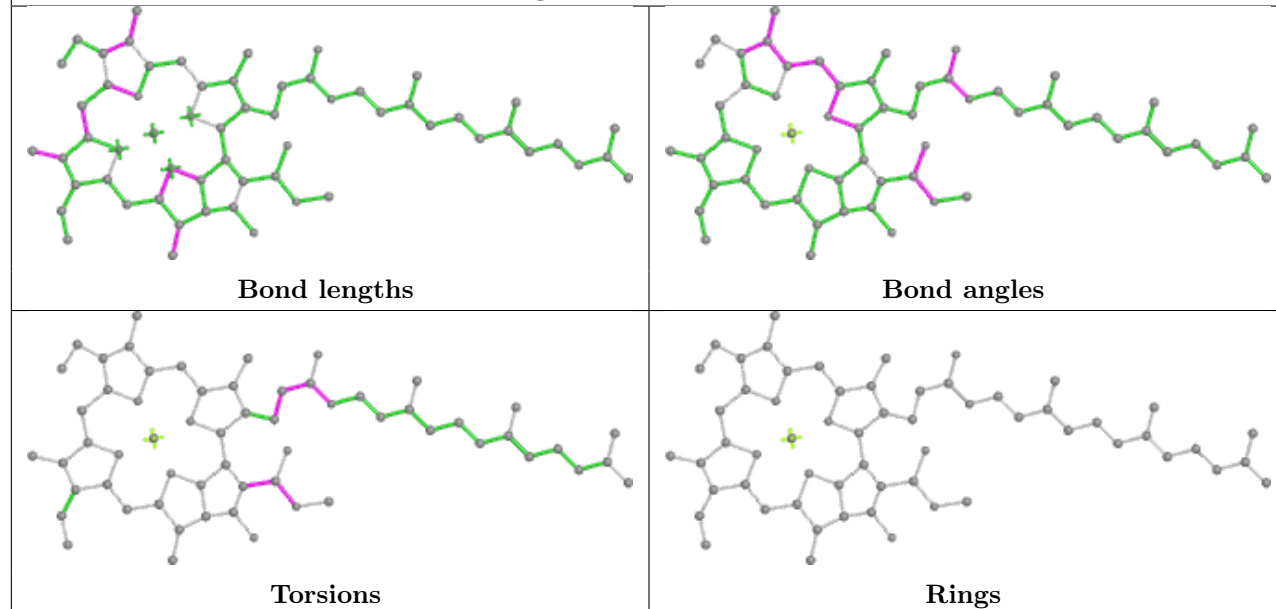
Bond angles



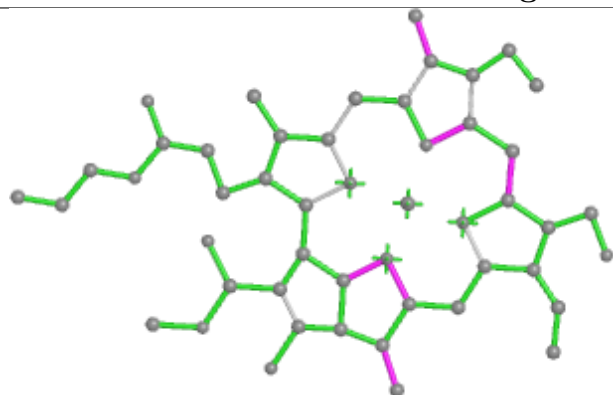
Torsions



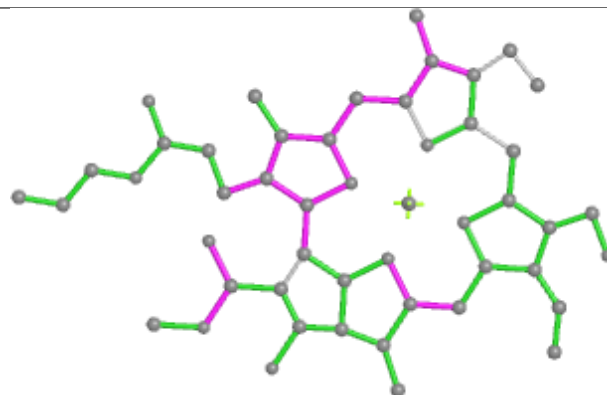
Rings

Ligand CLA C 502**Ligand CLA R 602**

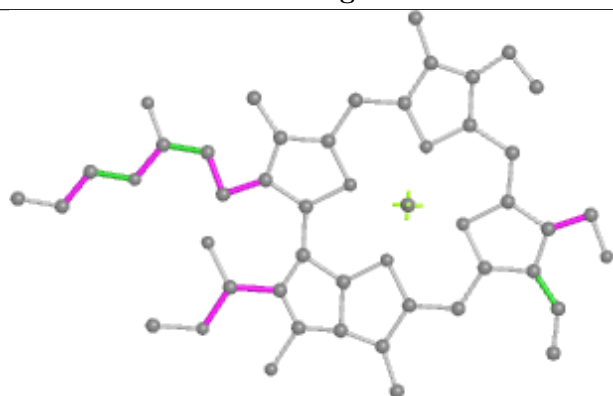
Ligand CHL s 607



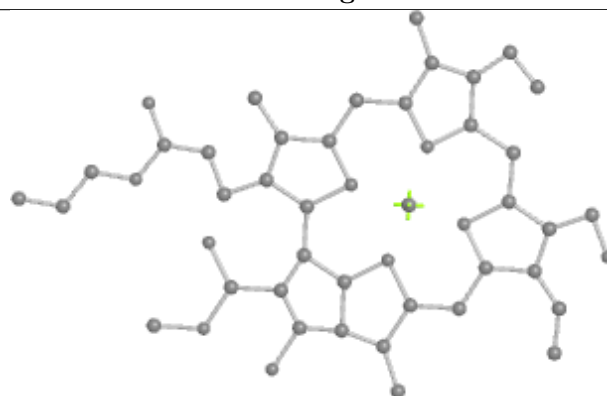
Bond lengths



Bond angles

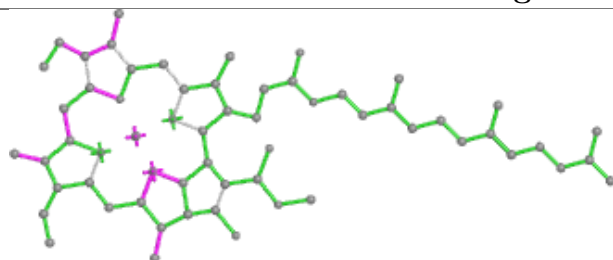


Torsions

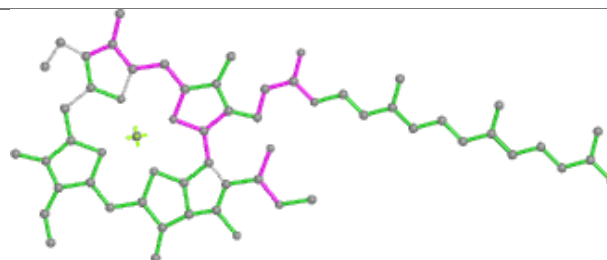


Rings

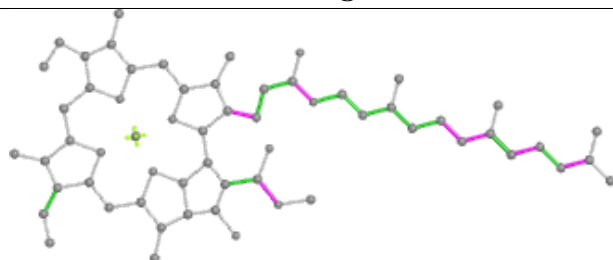
Ligand CLA Y 311



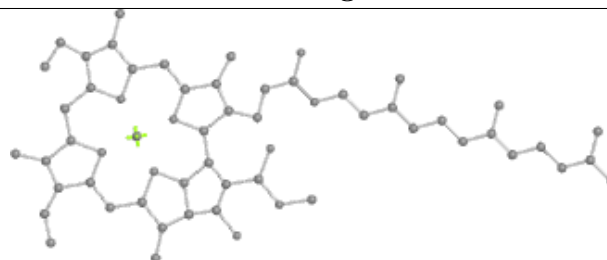
Bond lengths



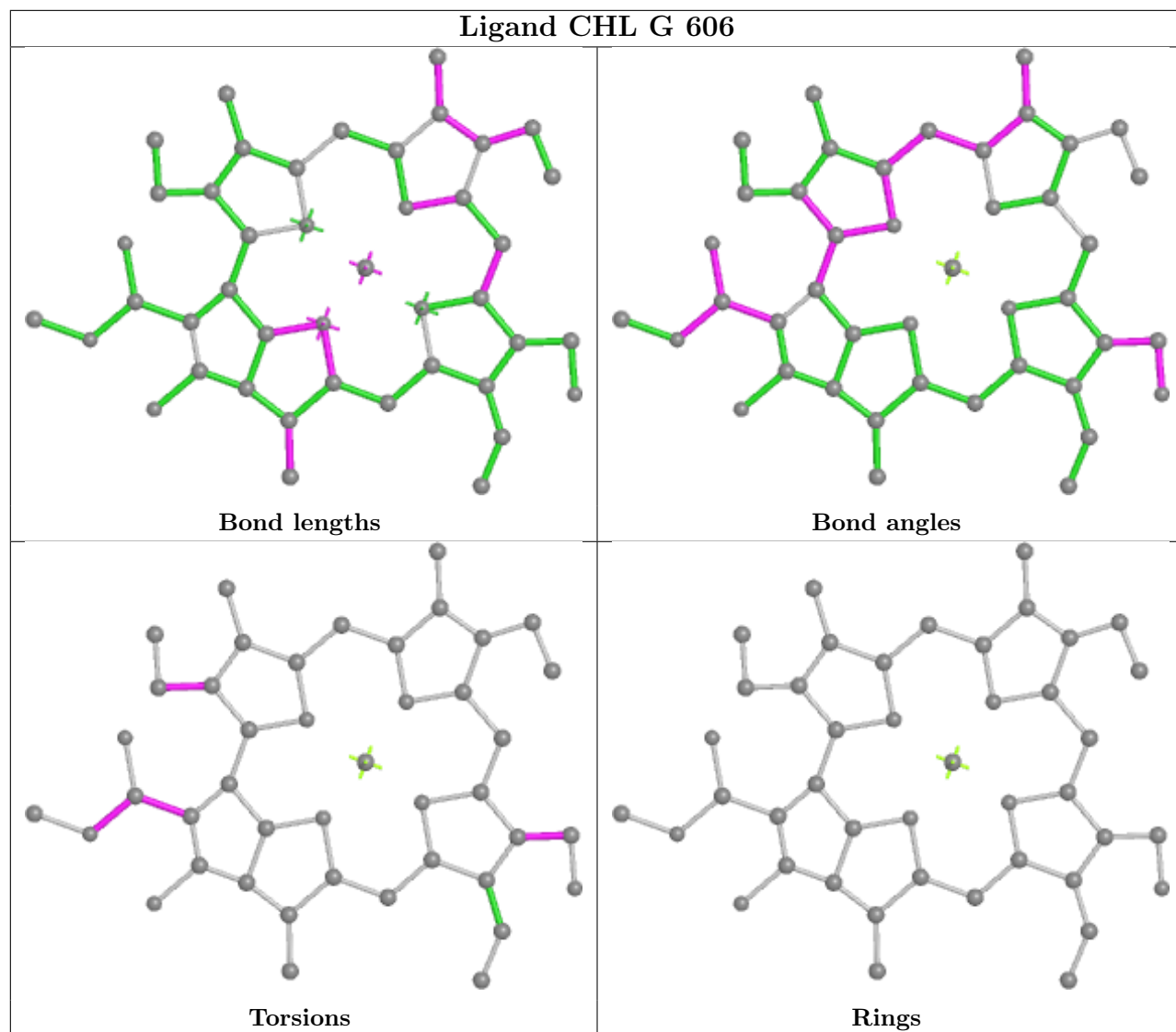
Bond angles

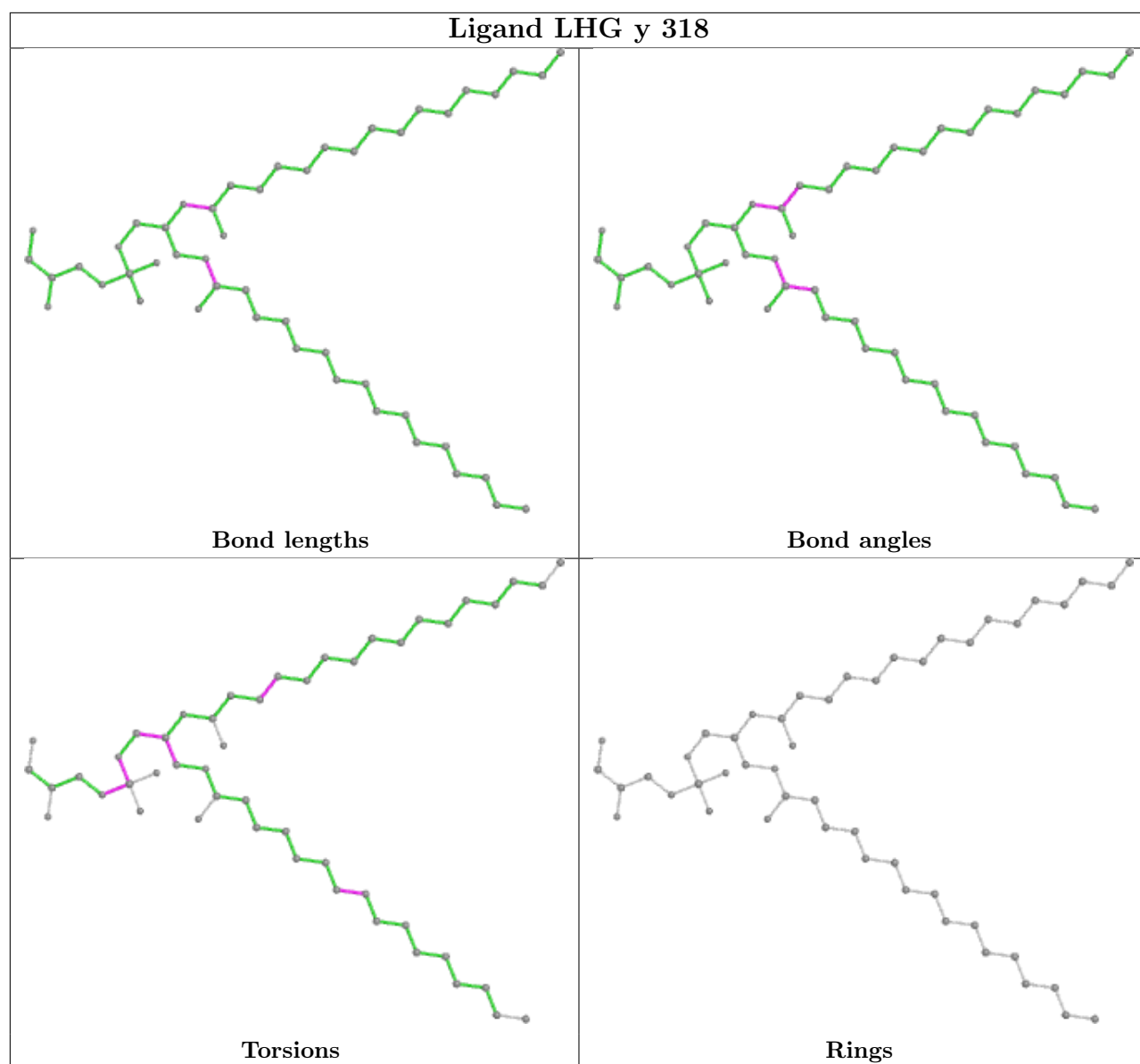


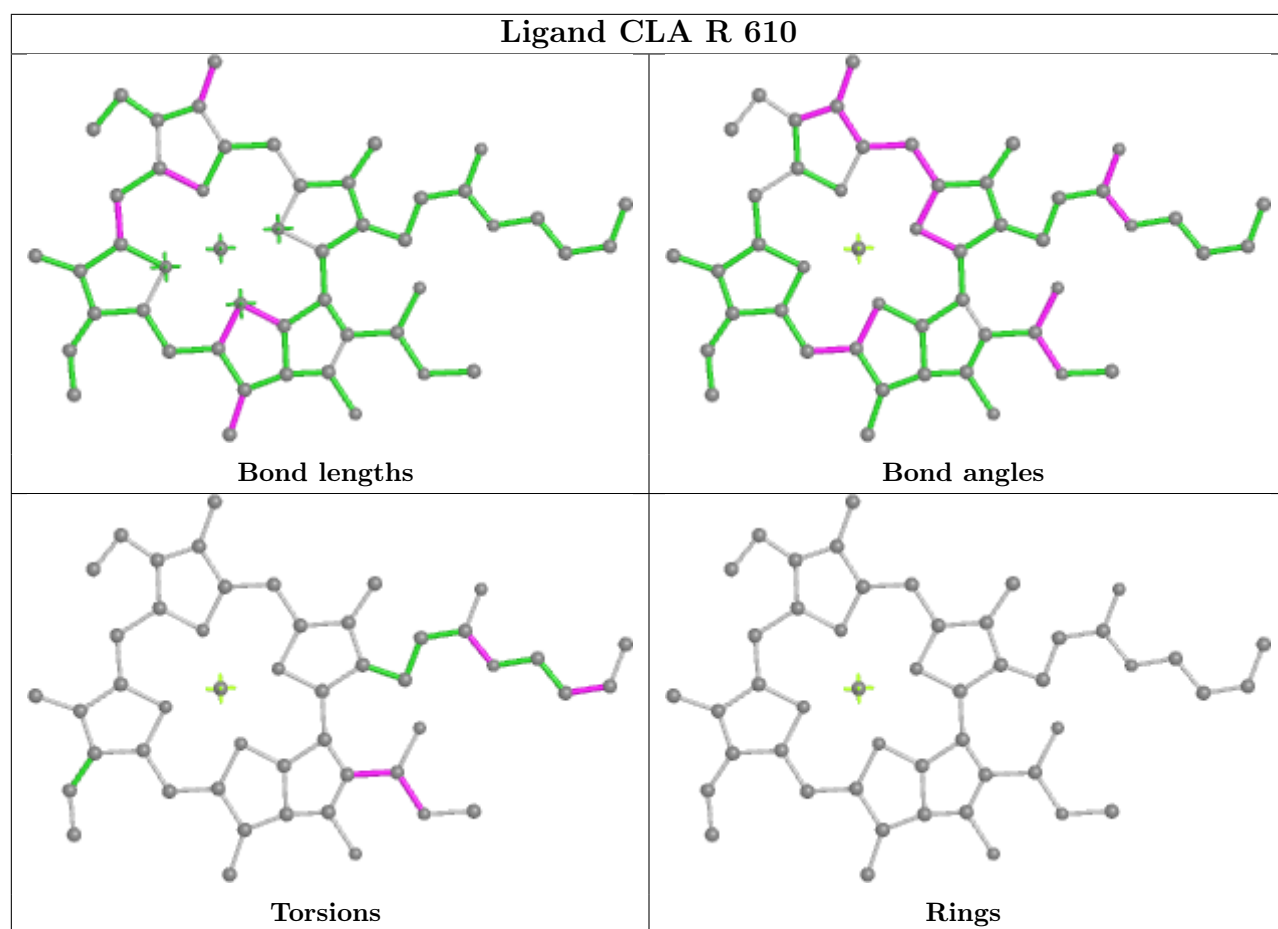
Torsions

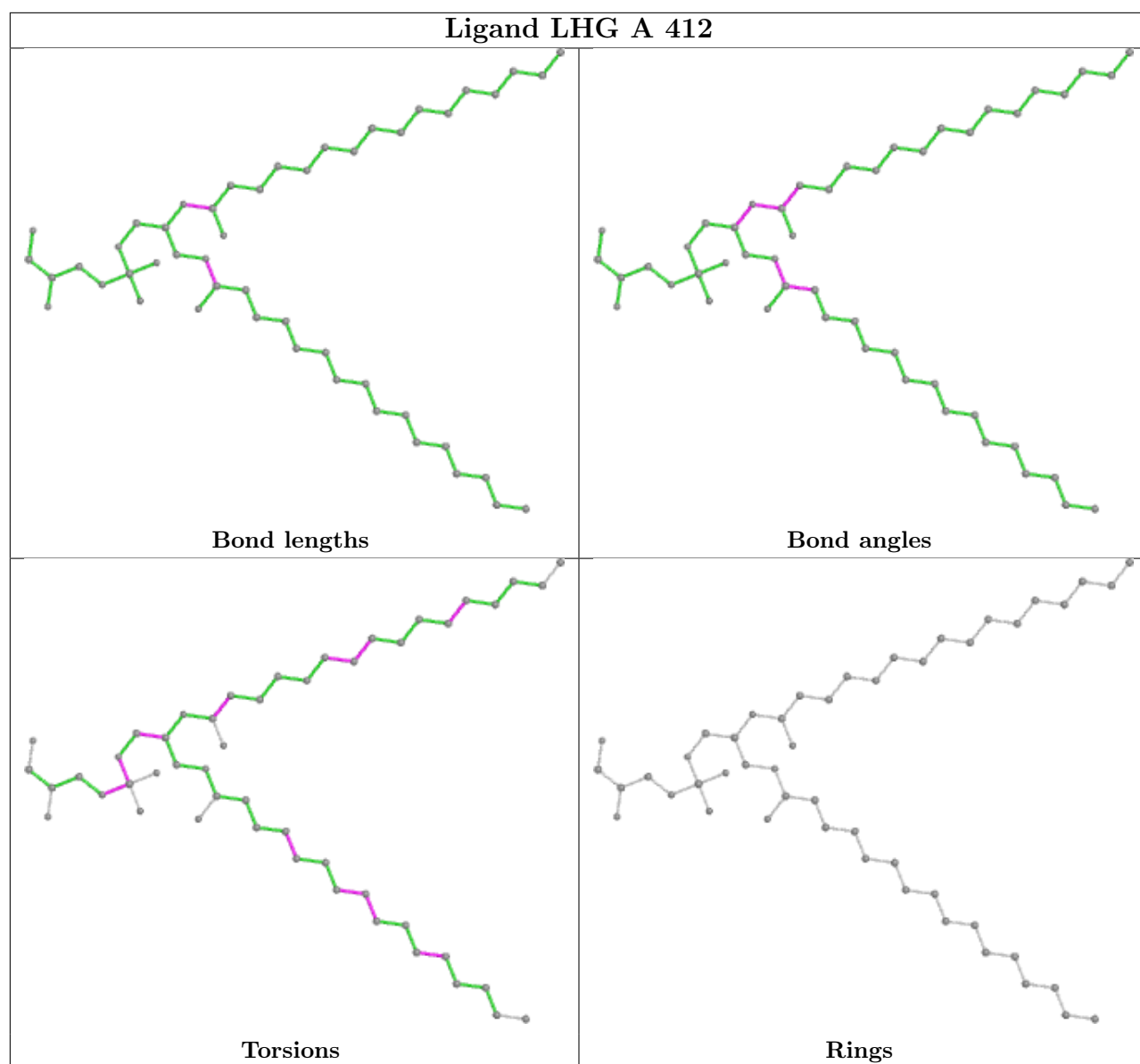


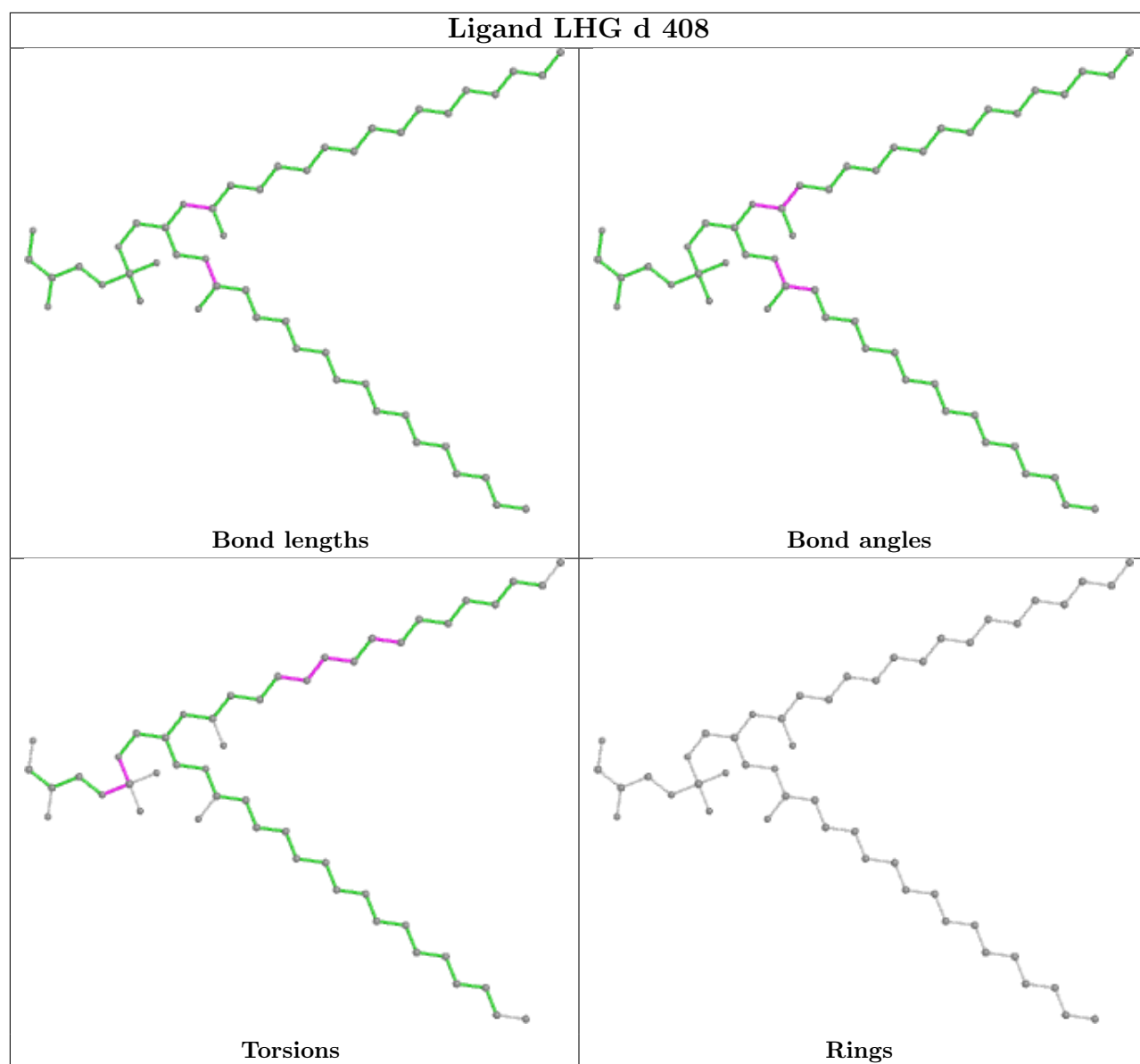
Rings

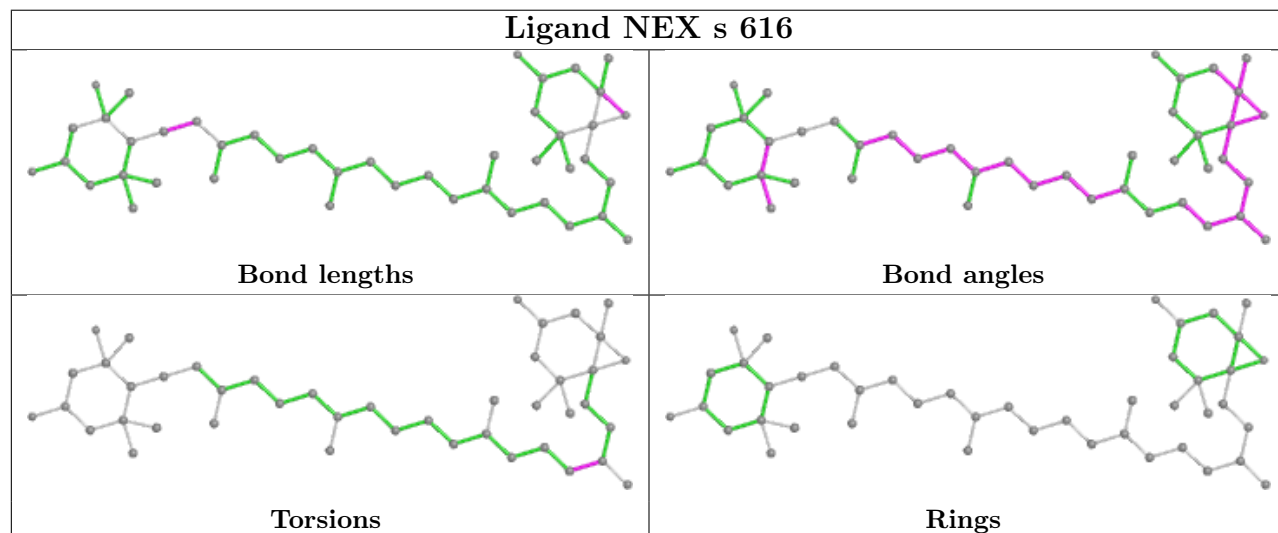
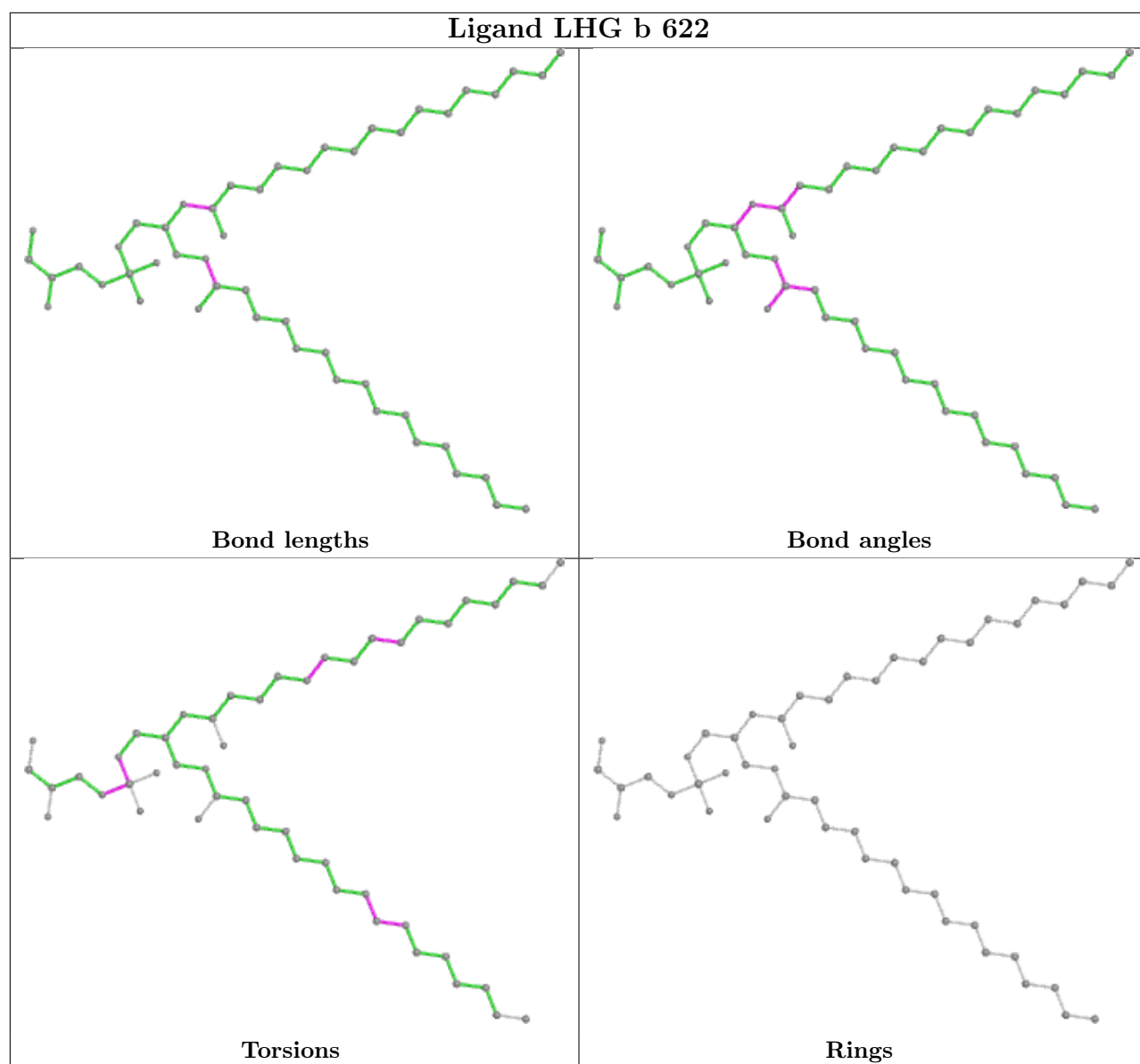




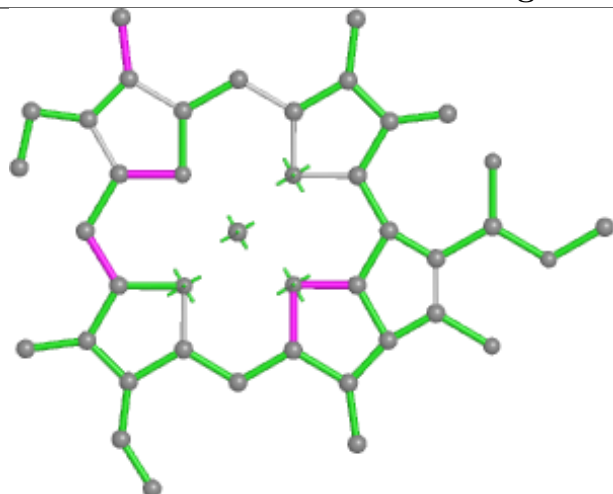




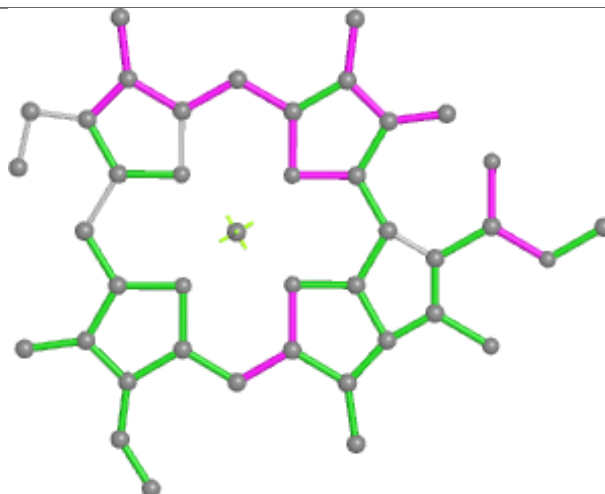




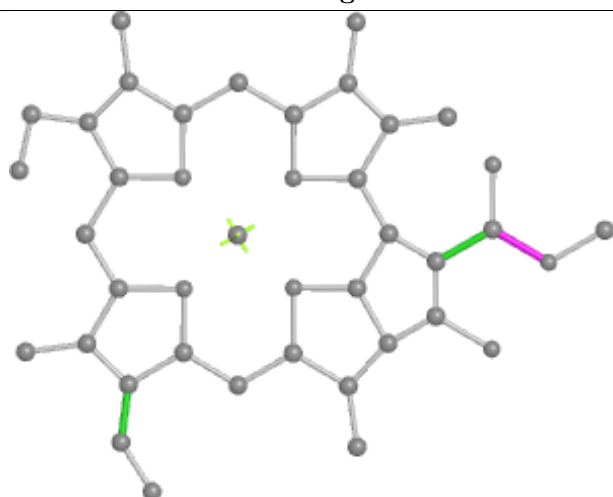
Ligand CLA n 315



Bond lengths



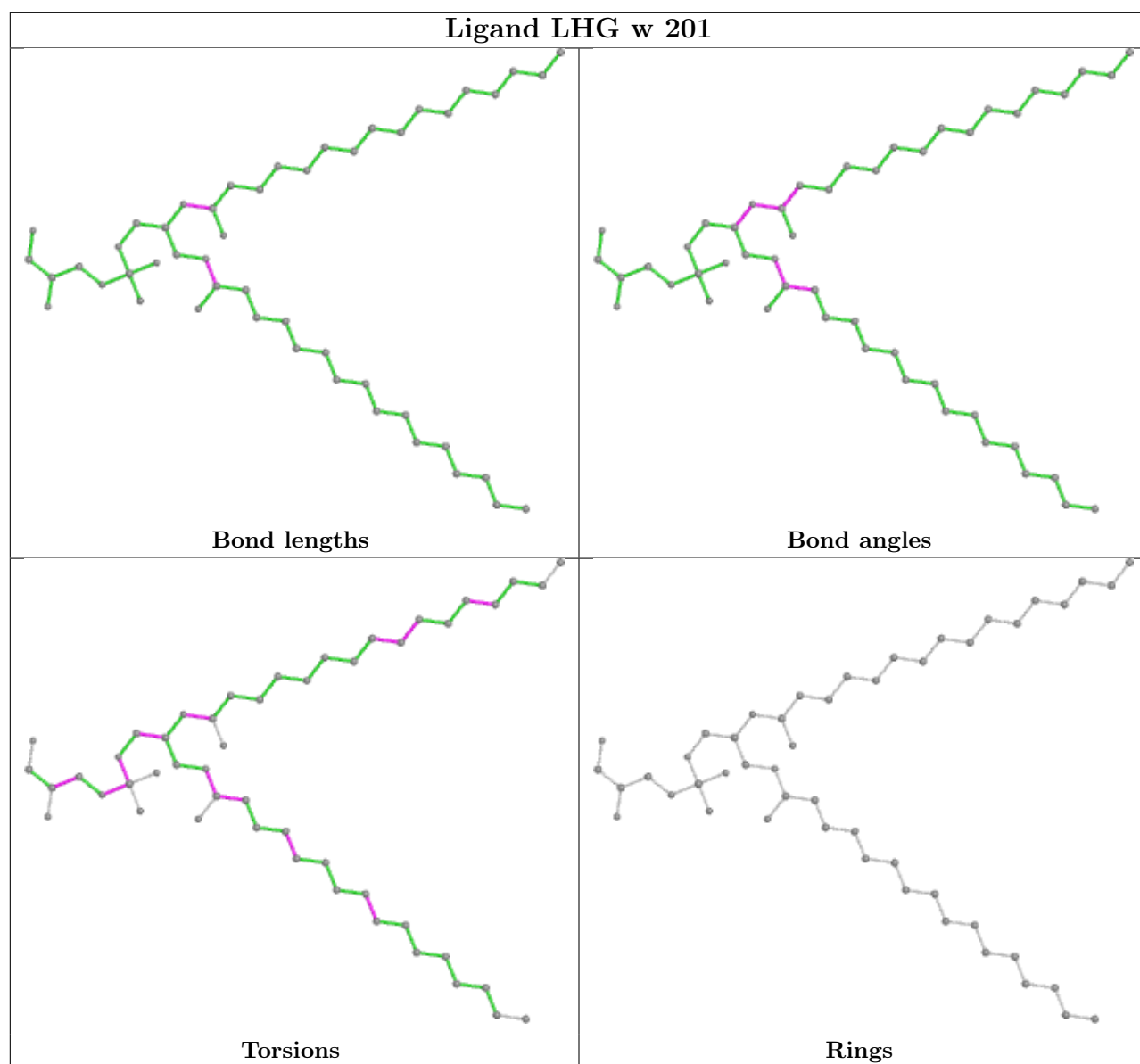
Bond angles

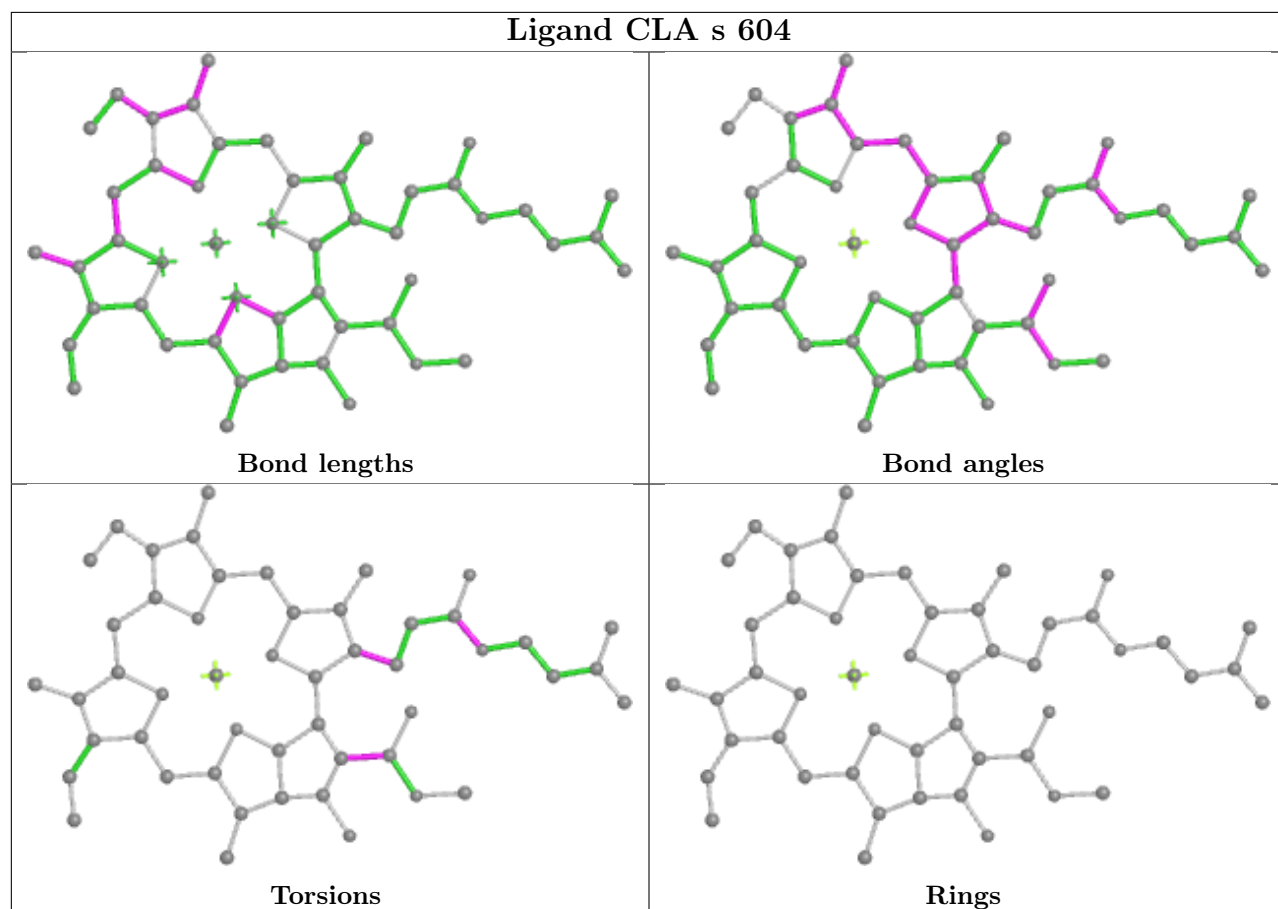
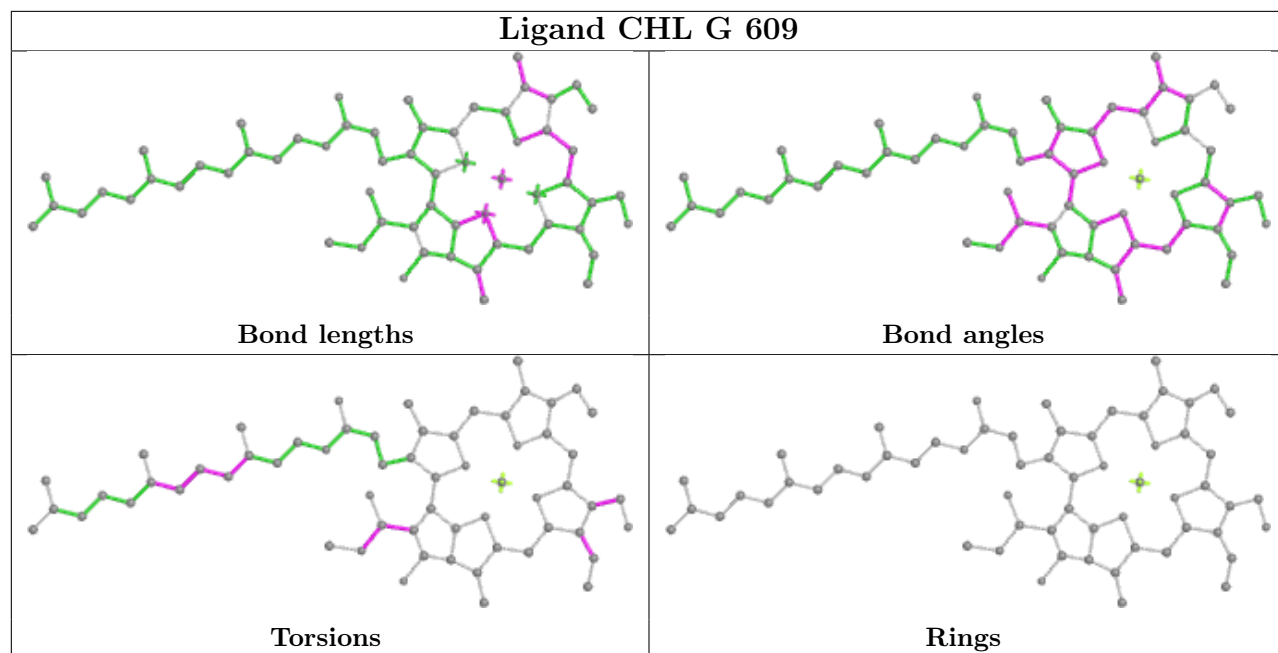


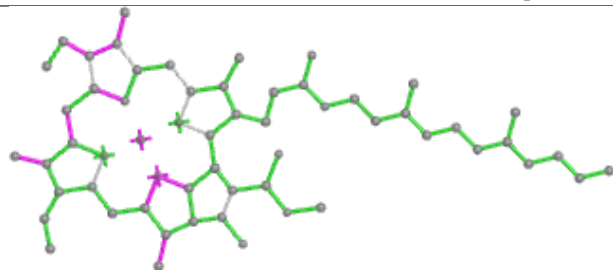
Torsions



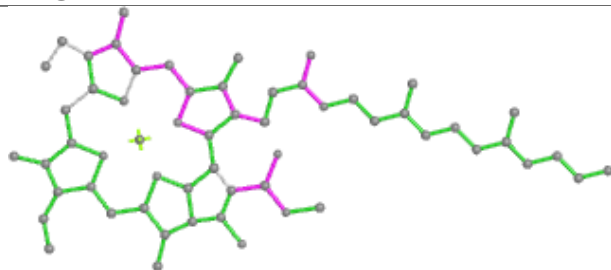
Rings



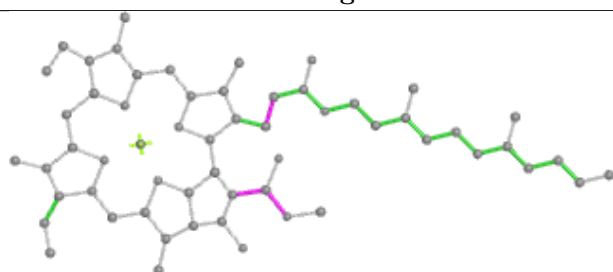


Ligand CLA g 613

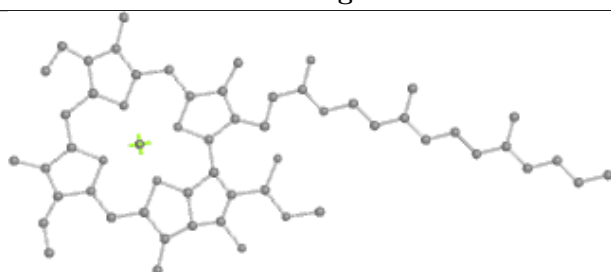
Bond lengths



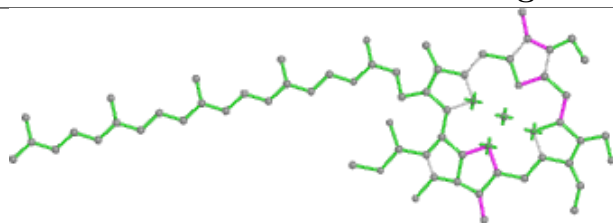
Bond angles



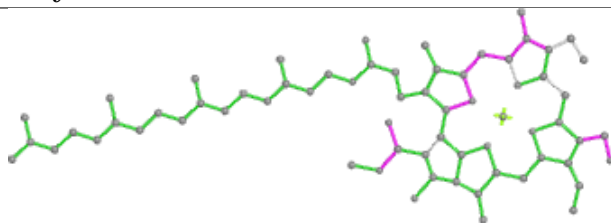
Torsions



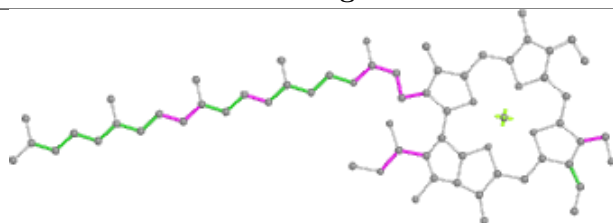
Rings

Ligand CHL y 308

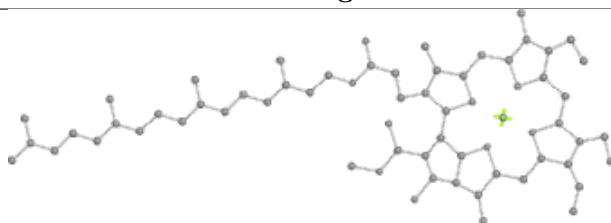
Bond lengths



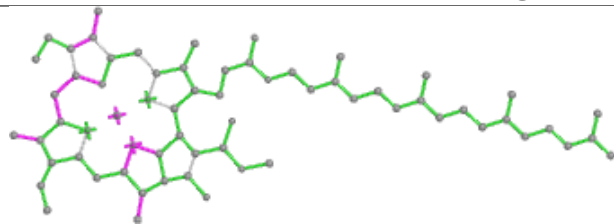
Bond angles



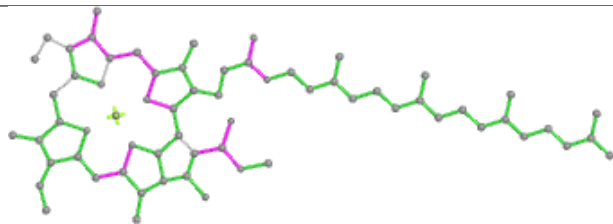
Torsions



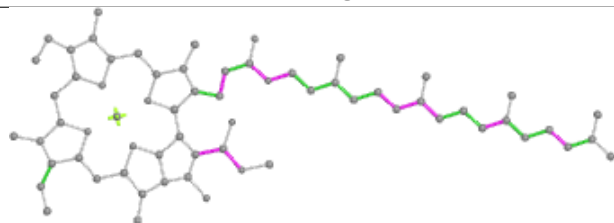
Rings

Ligand CLA Y 313

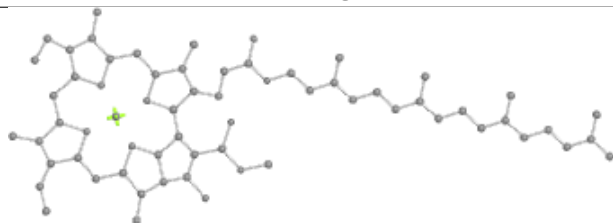
Bond lengths



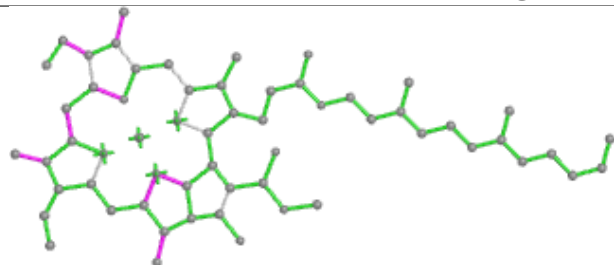
Bond angles



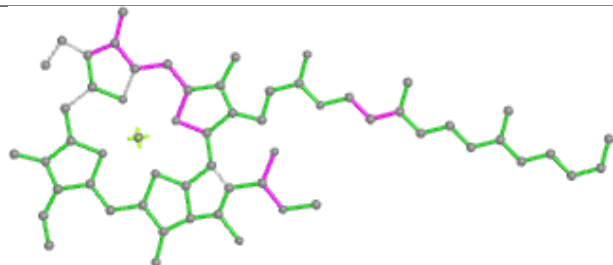
Torsions



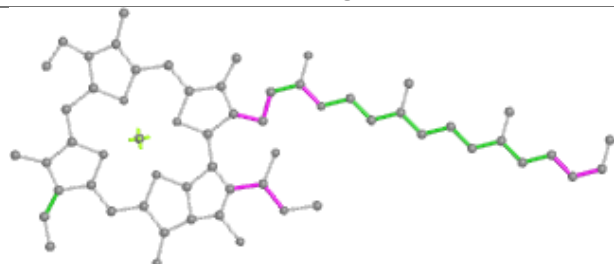
Rings

Ligand CLA N 311

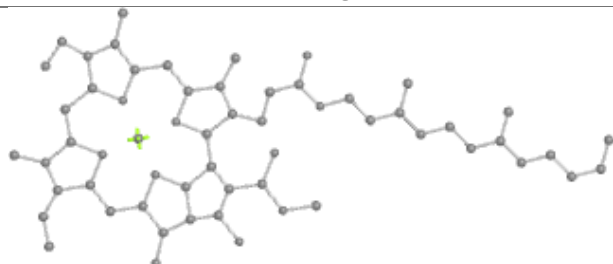
Bond lengths



Bond angles

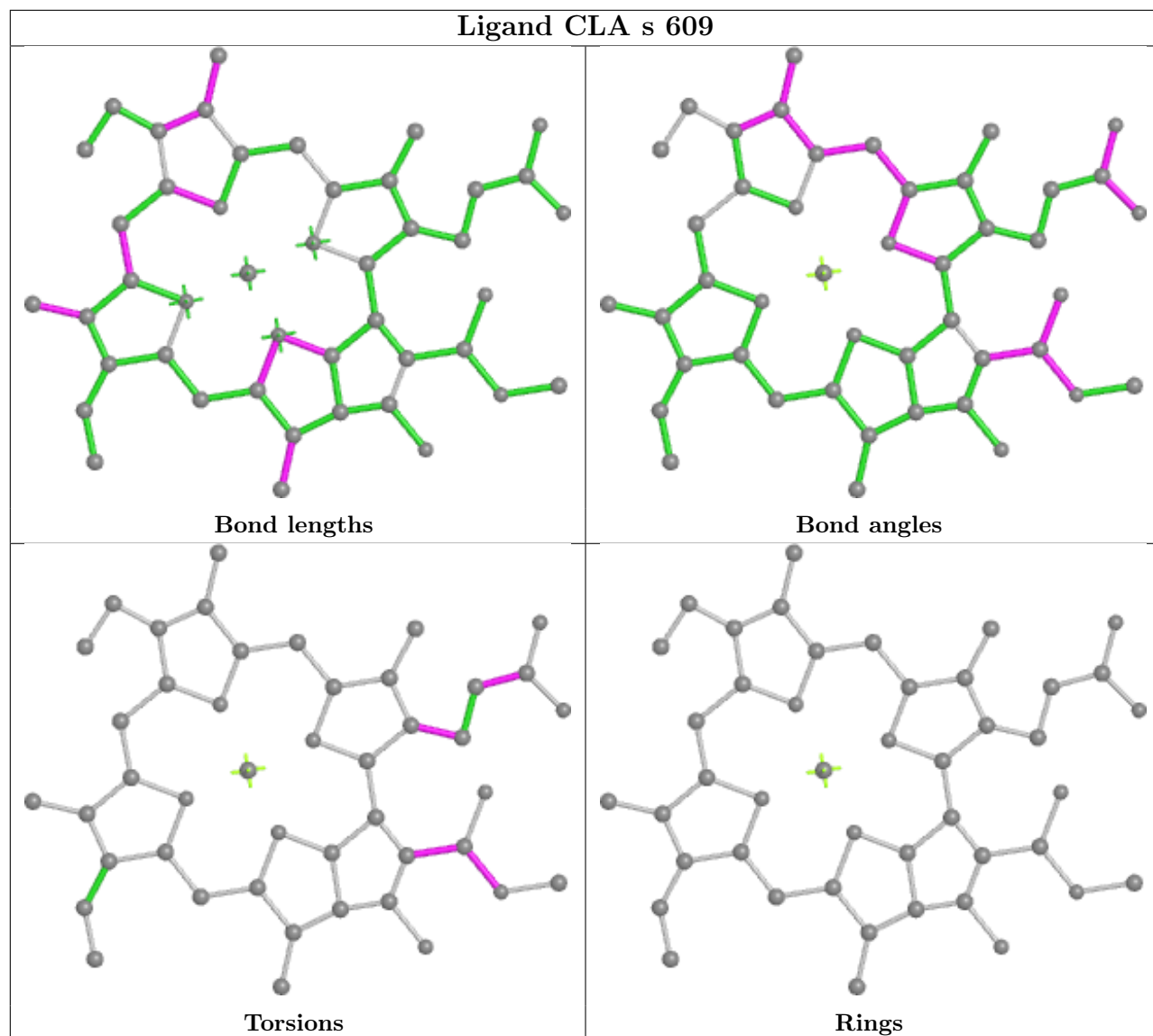


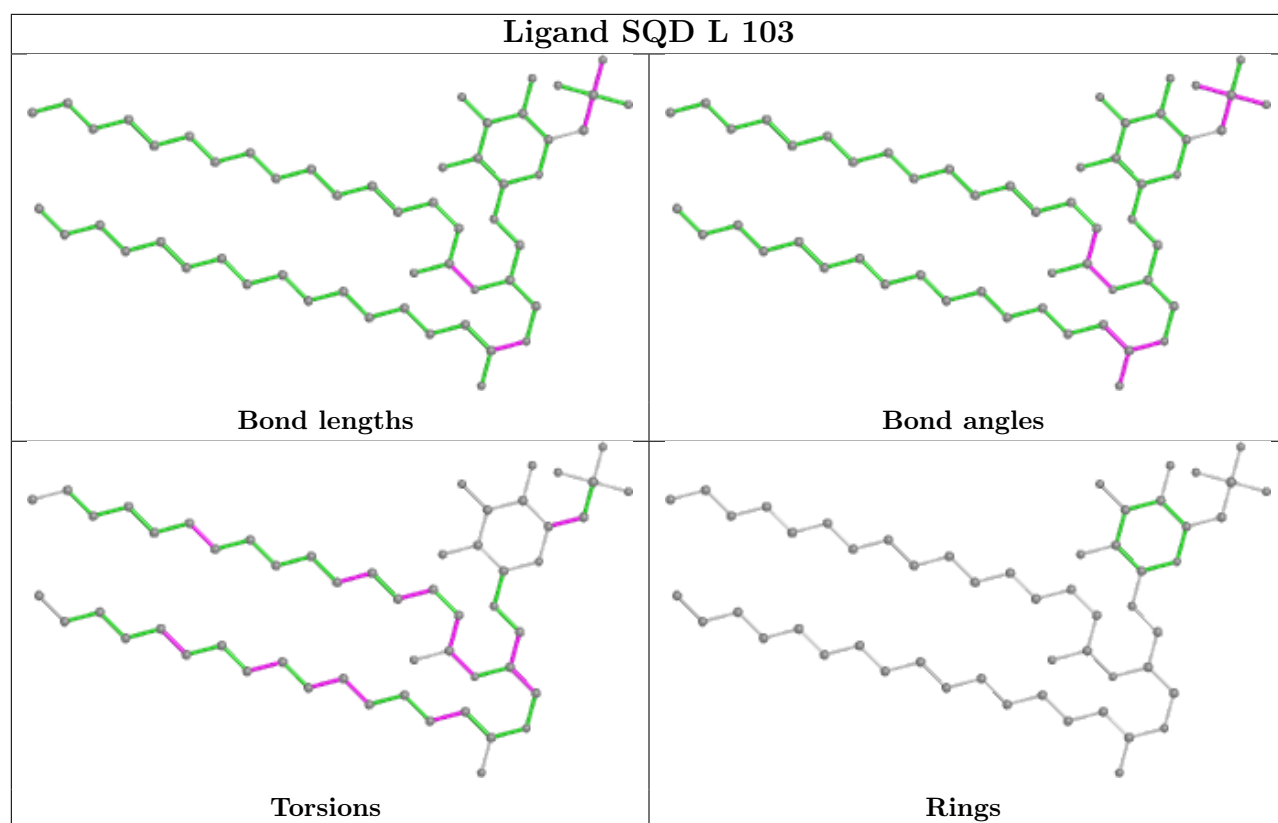
Torsions

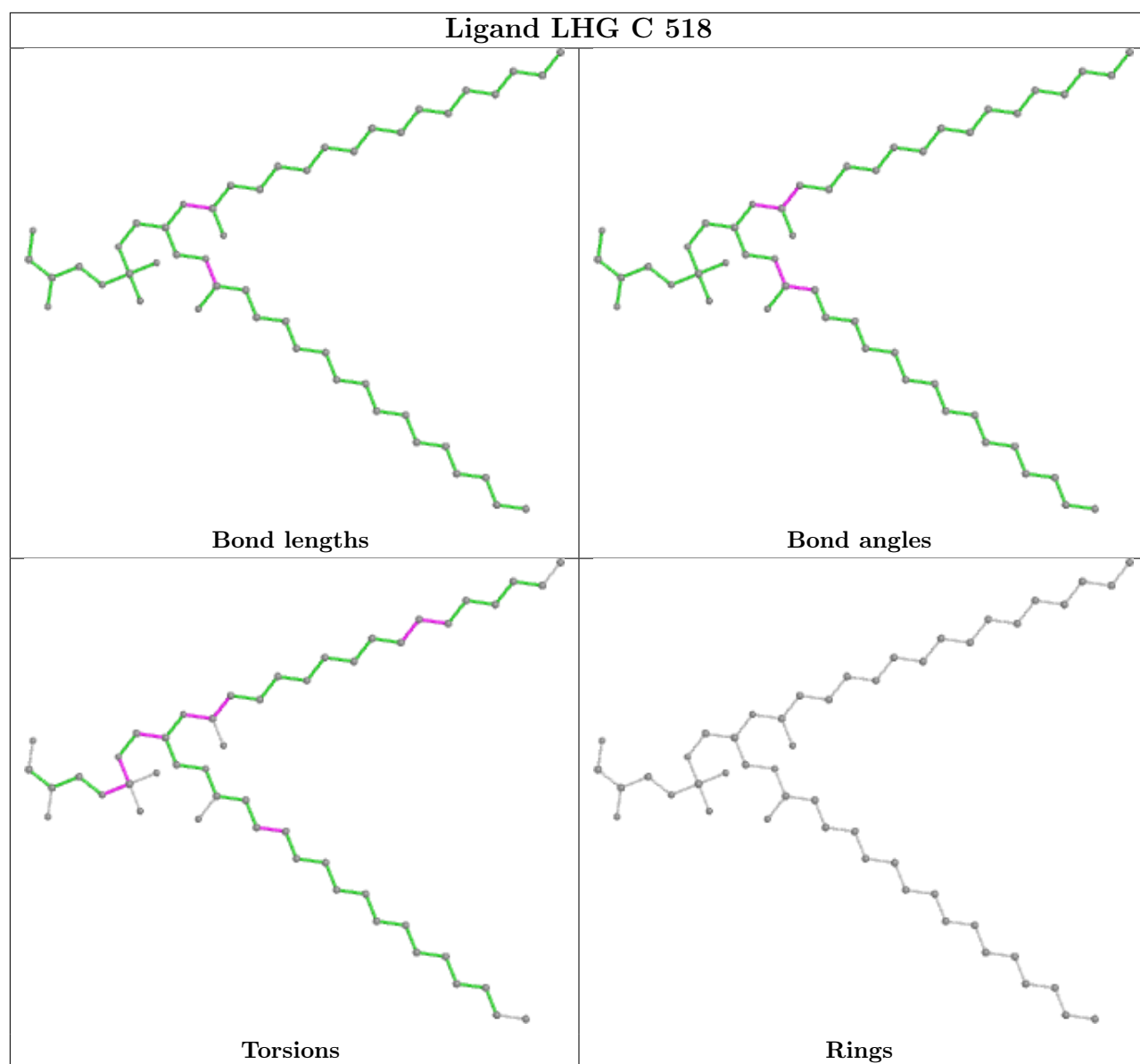


Rings

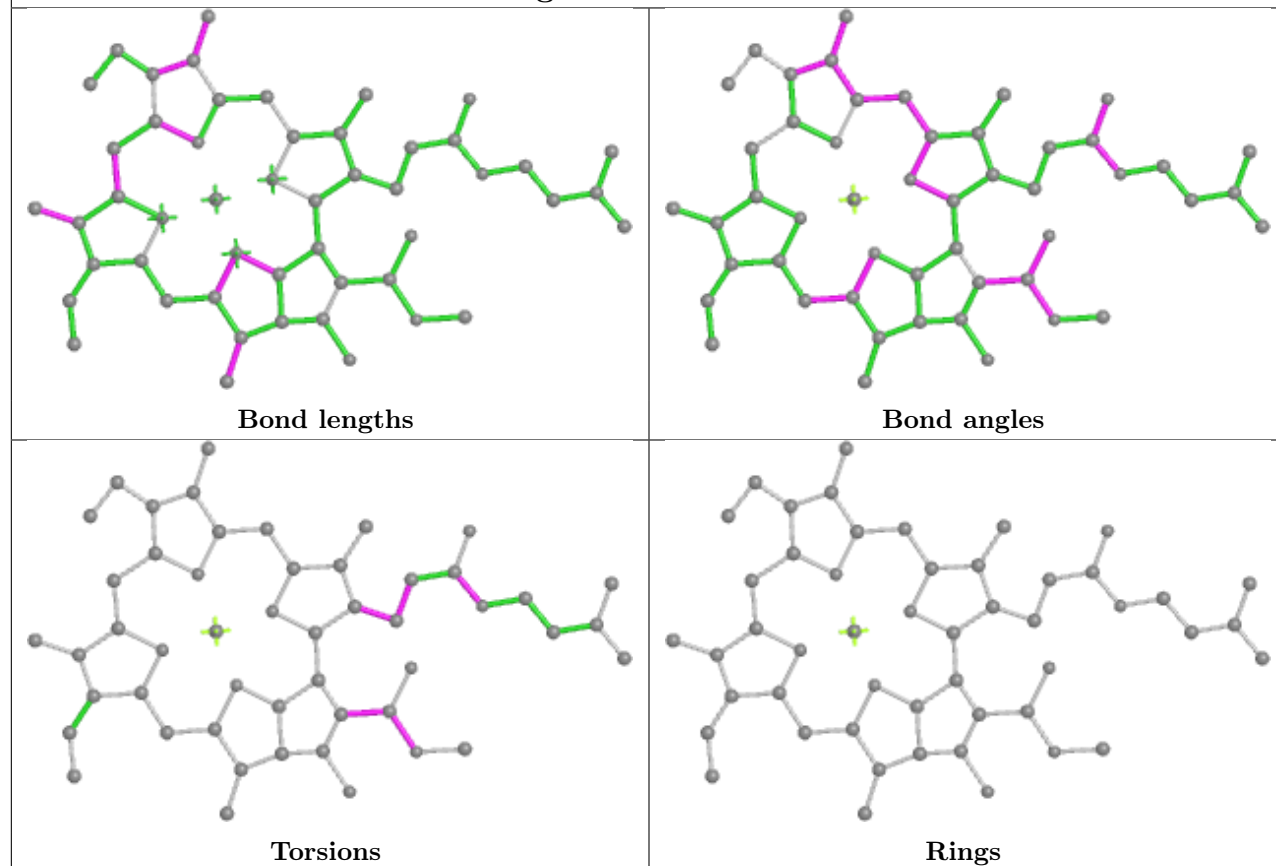
Ligand CLA s 609



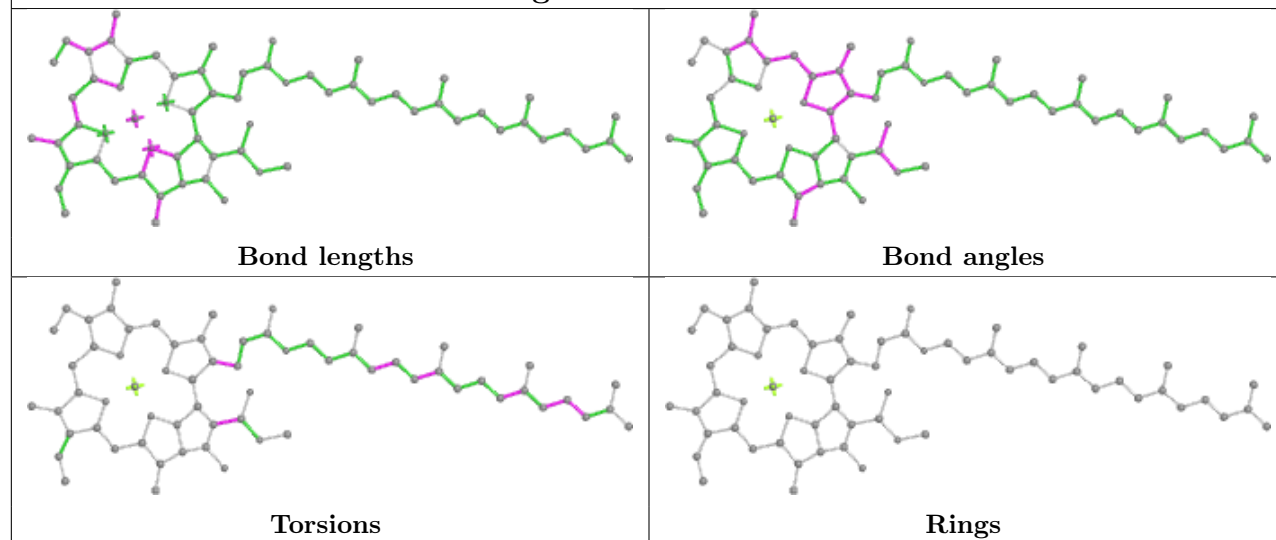




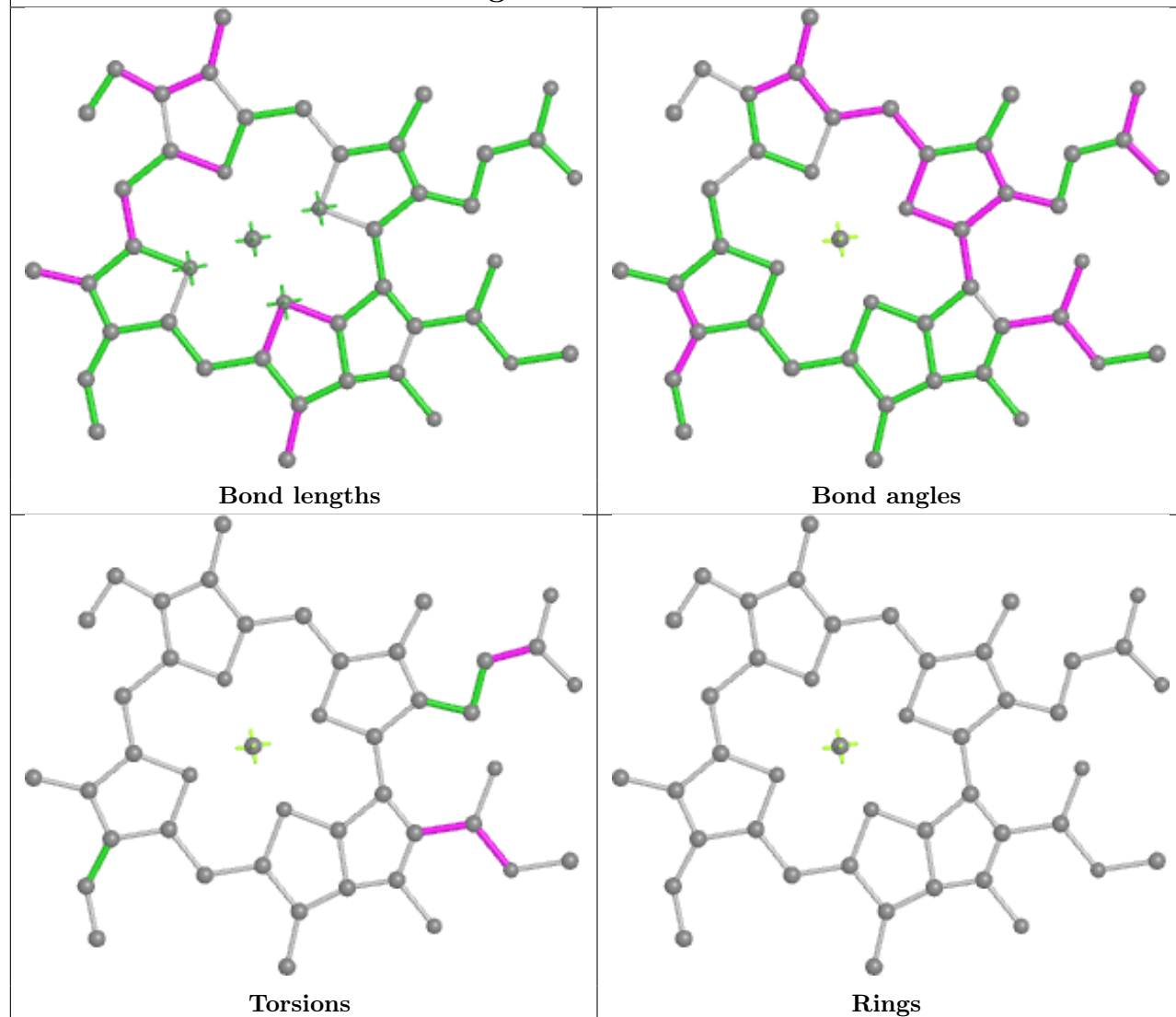
Ligand CLA a 403



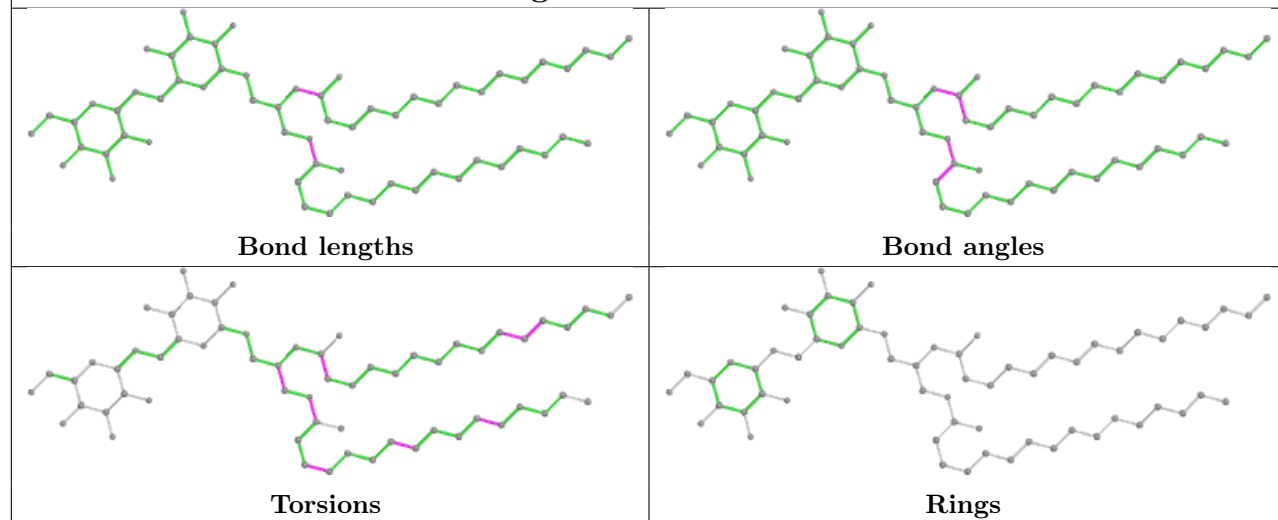
Ligand CLA C 508



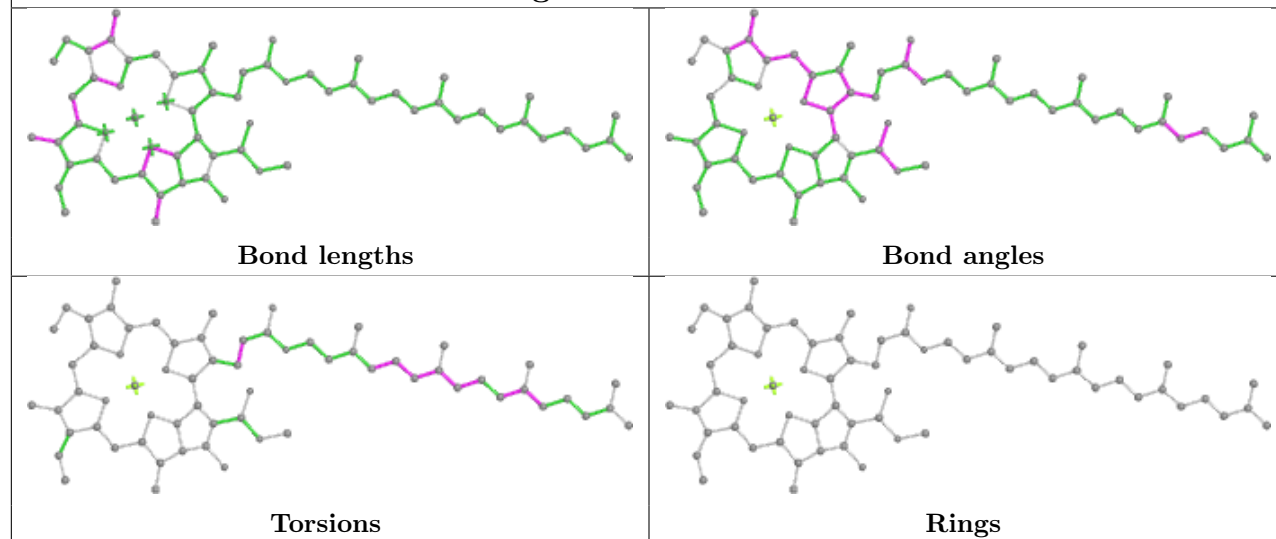
Ligand CLA G 612



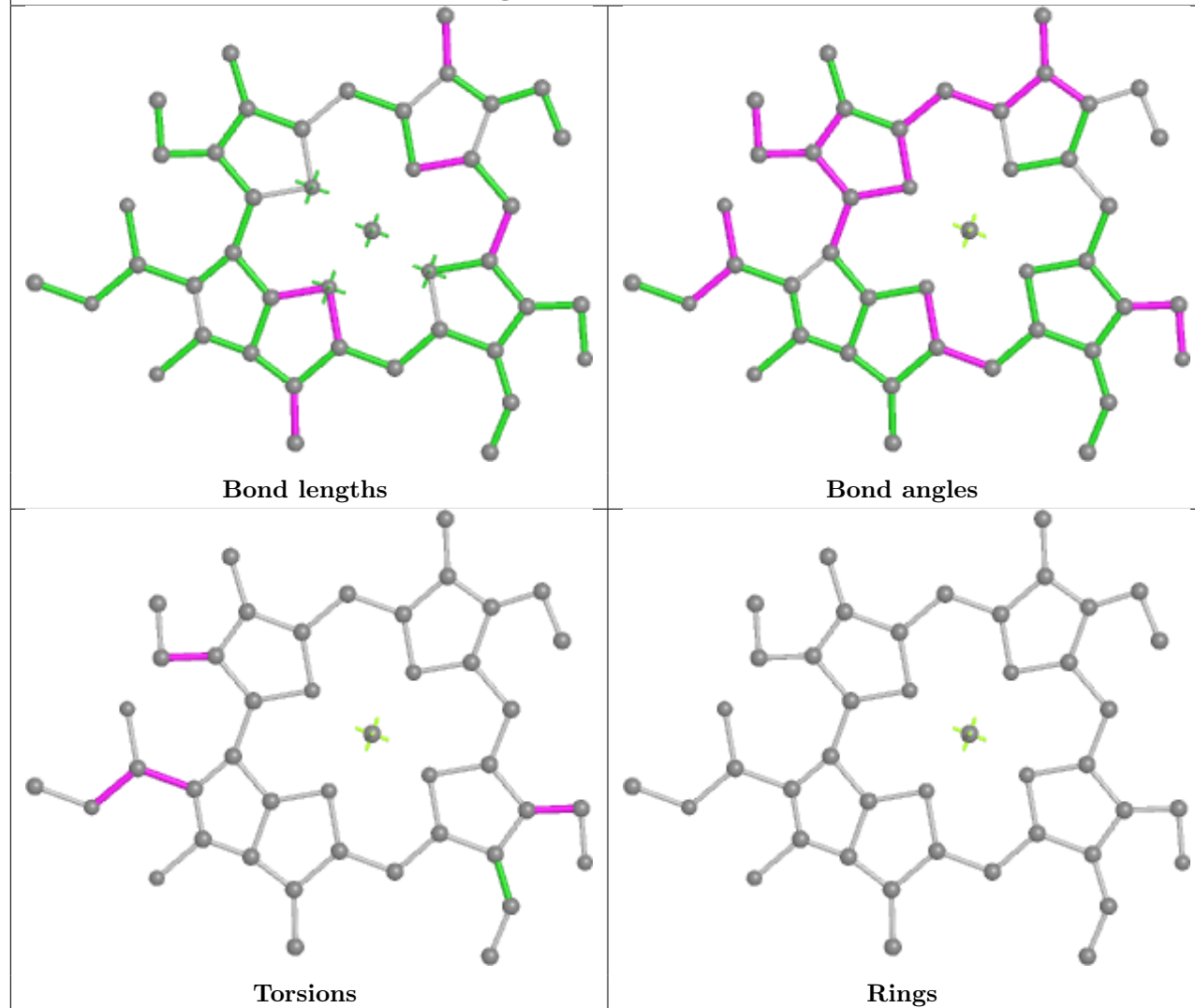
Ligand DGD d 410

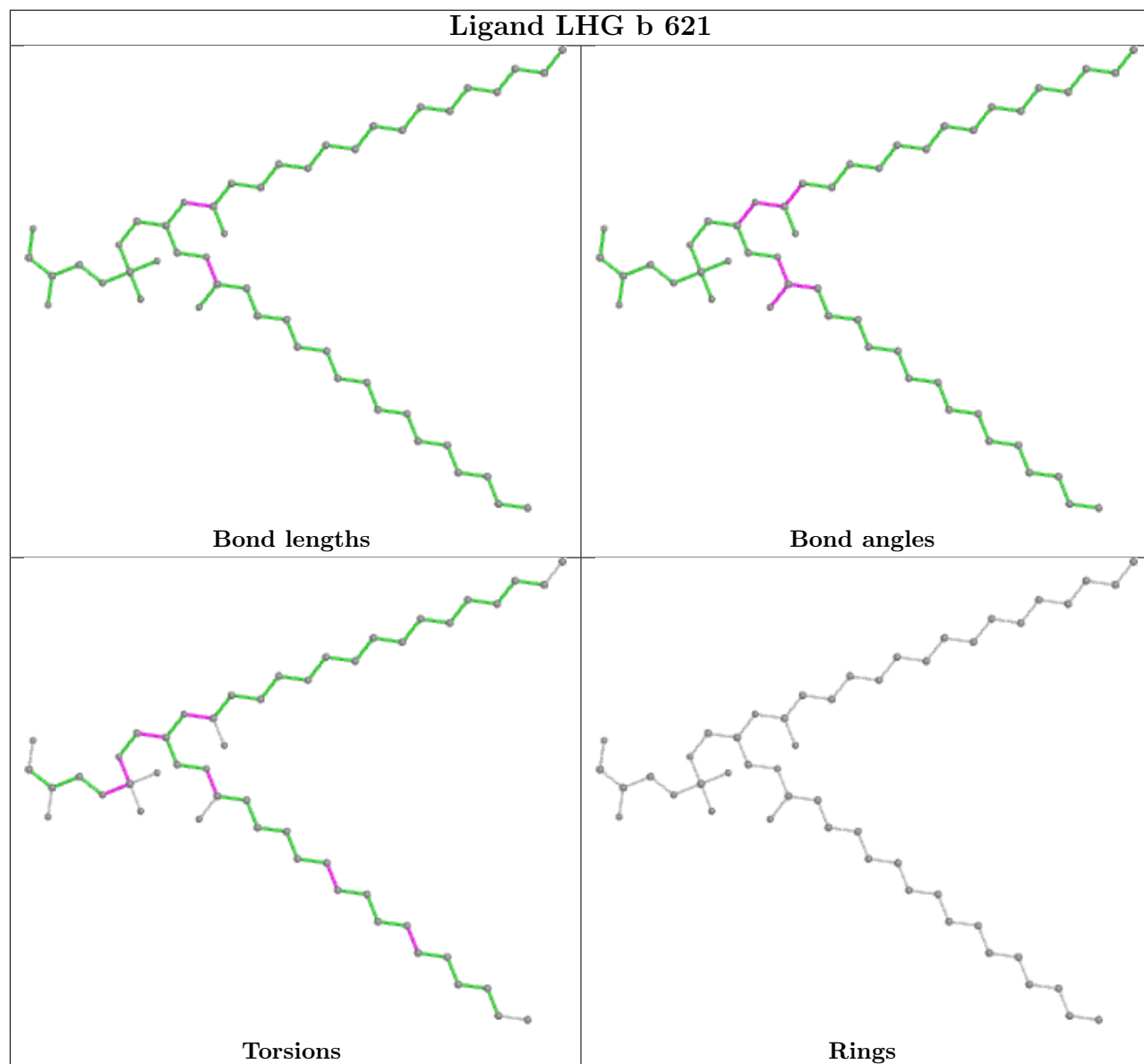
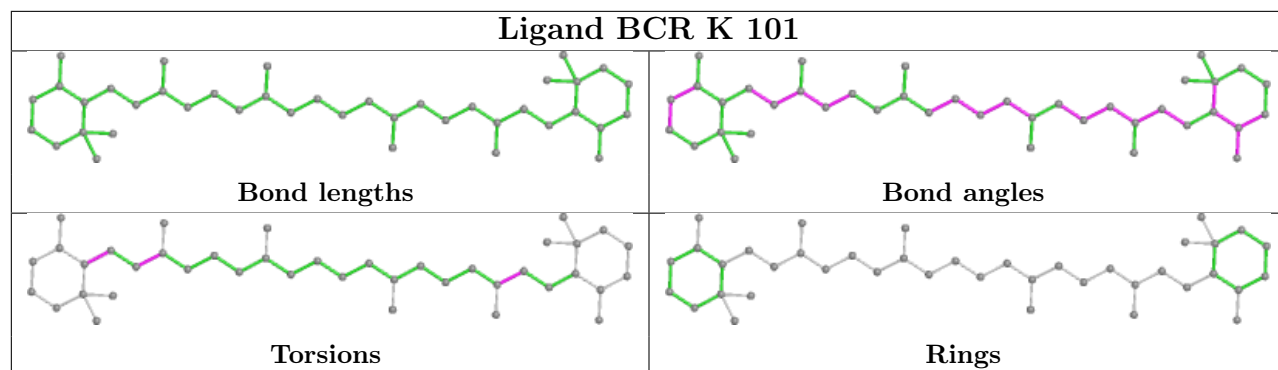


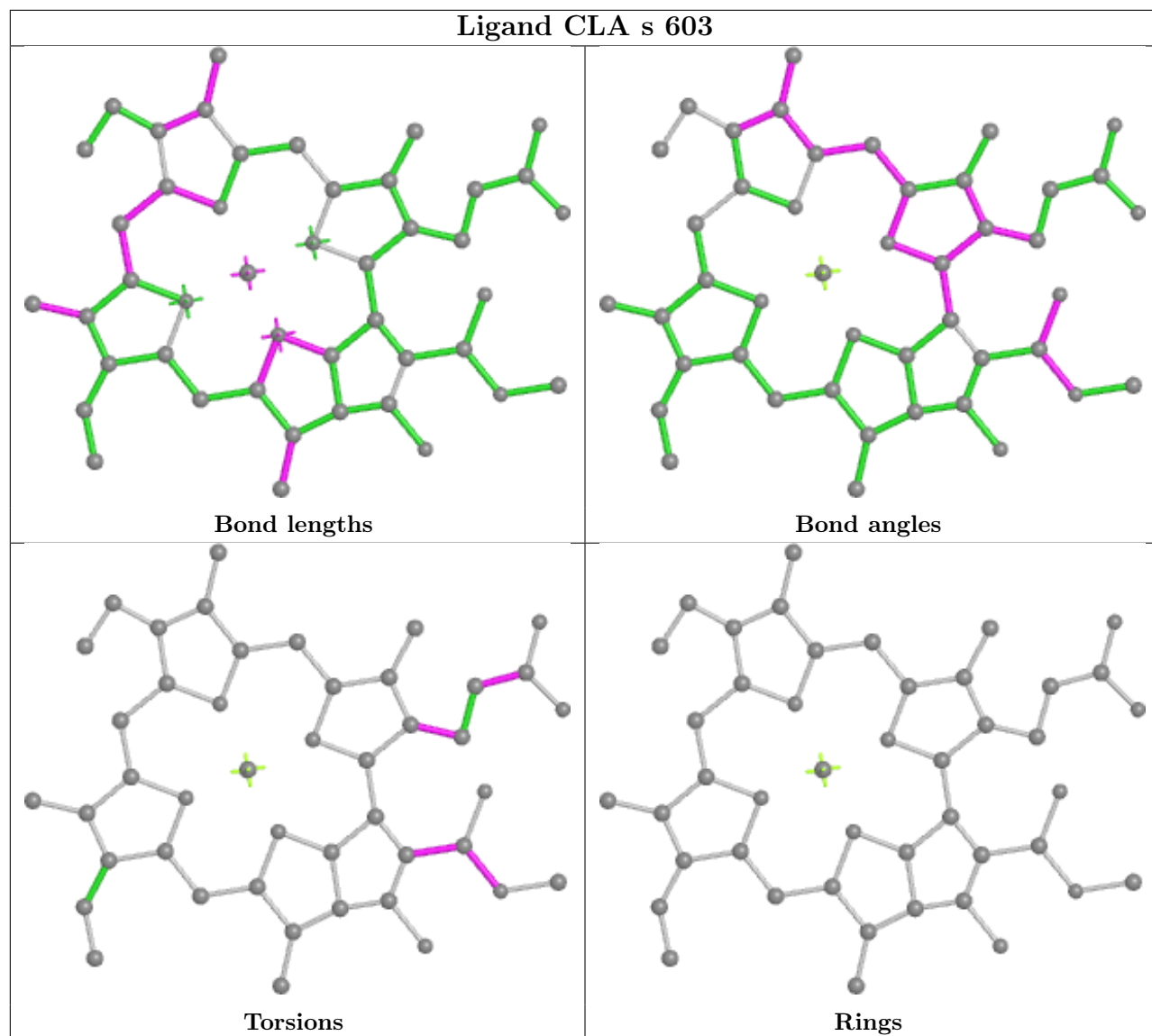
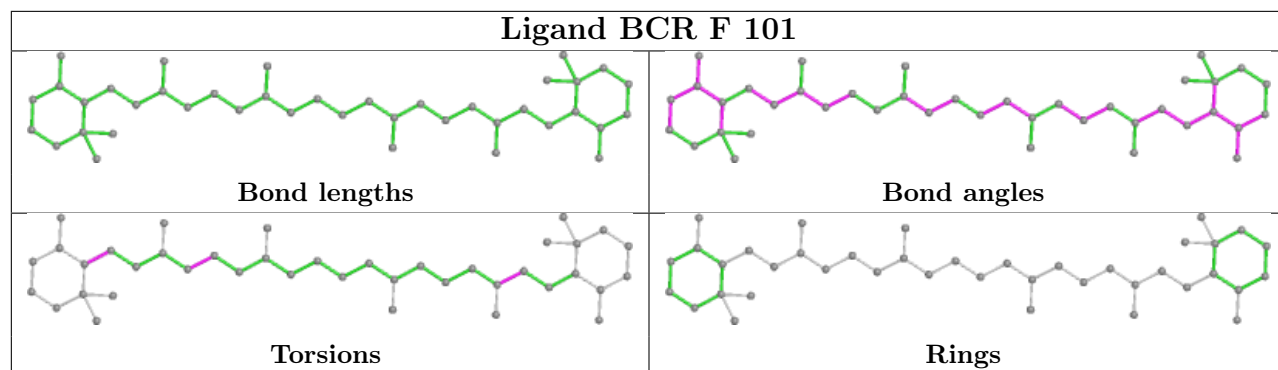
Ligand CLA B 615

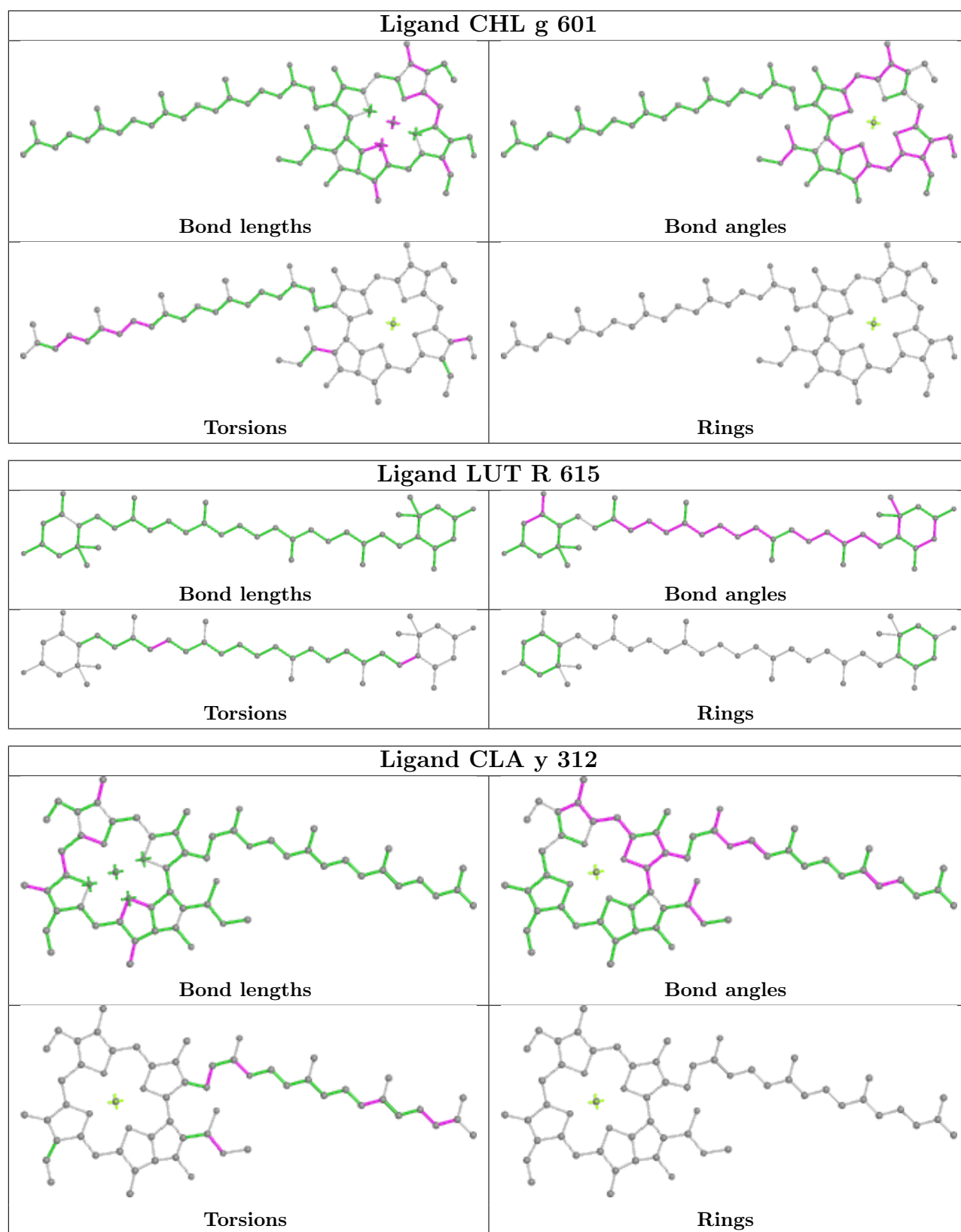


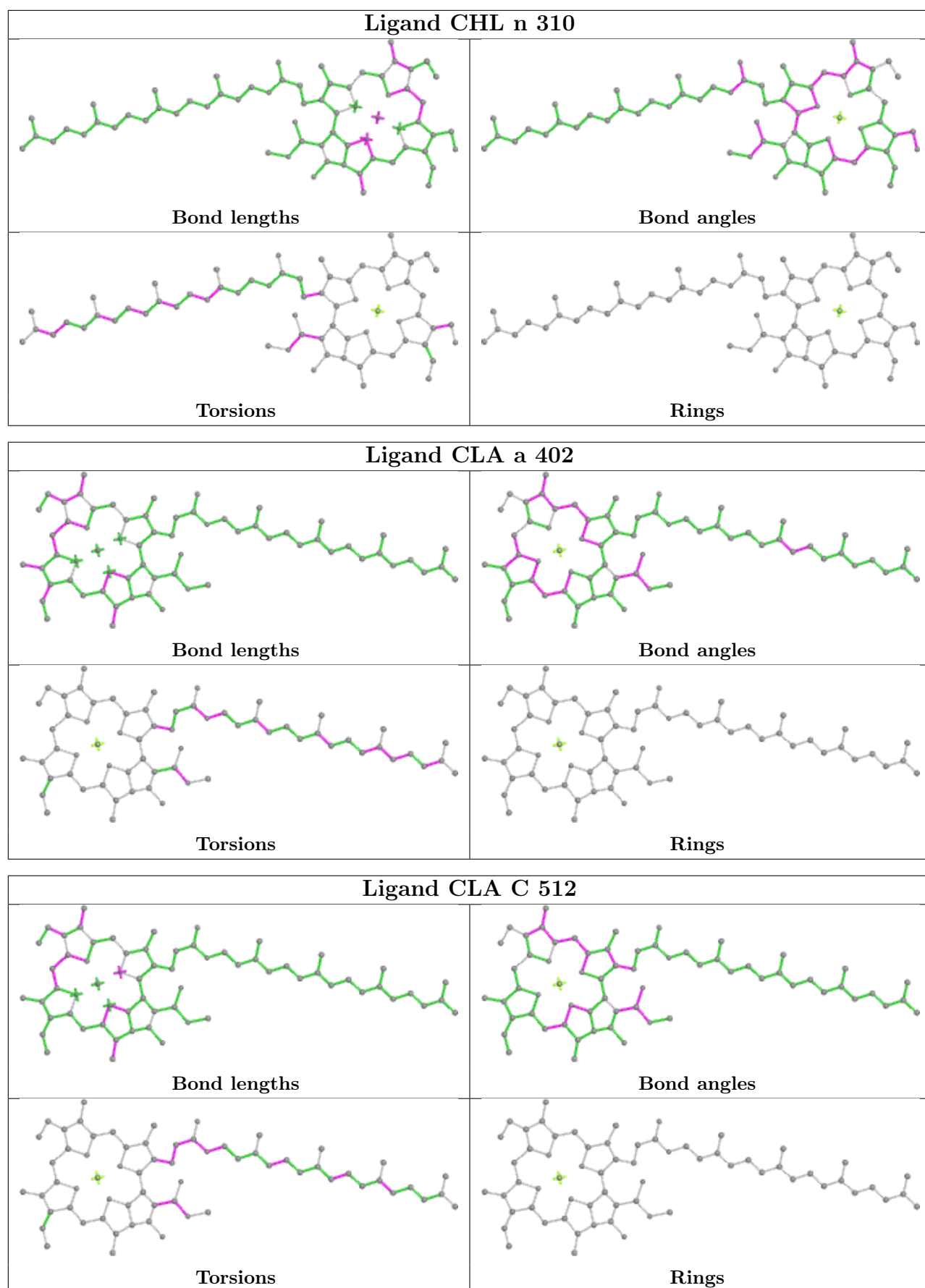
Ligand CHL G 607



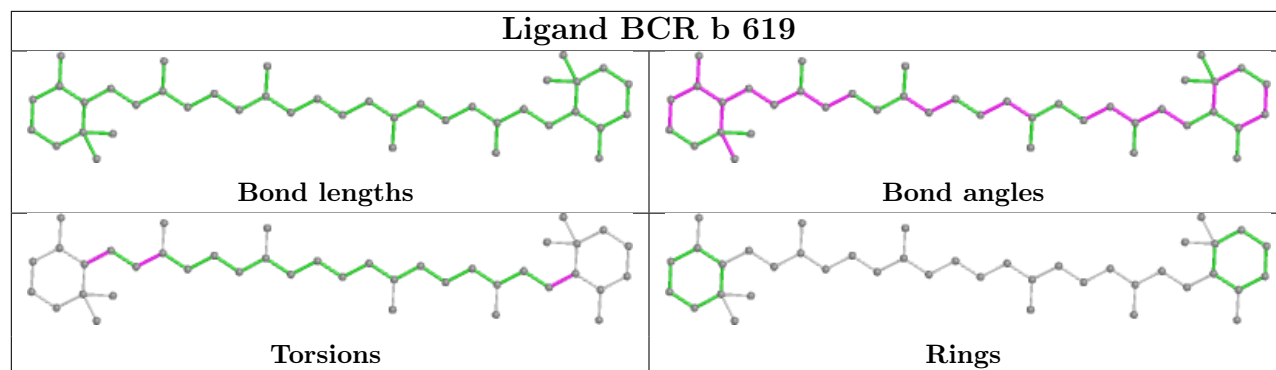




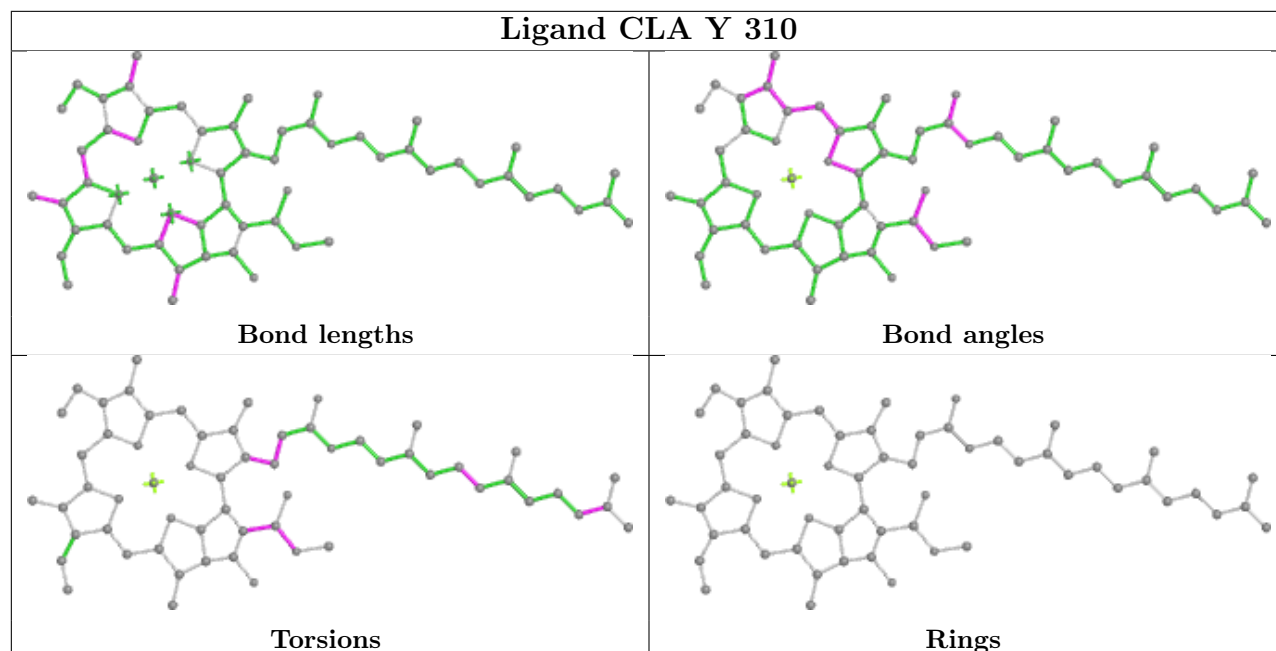




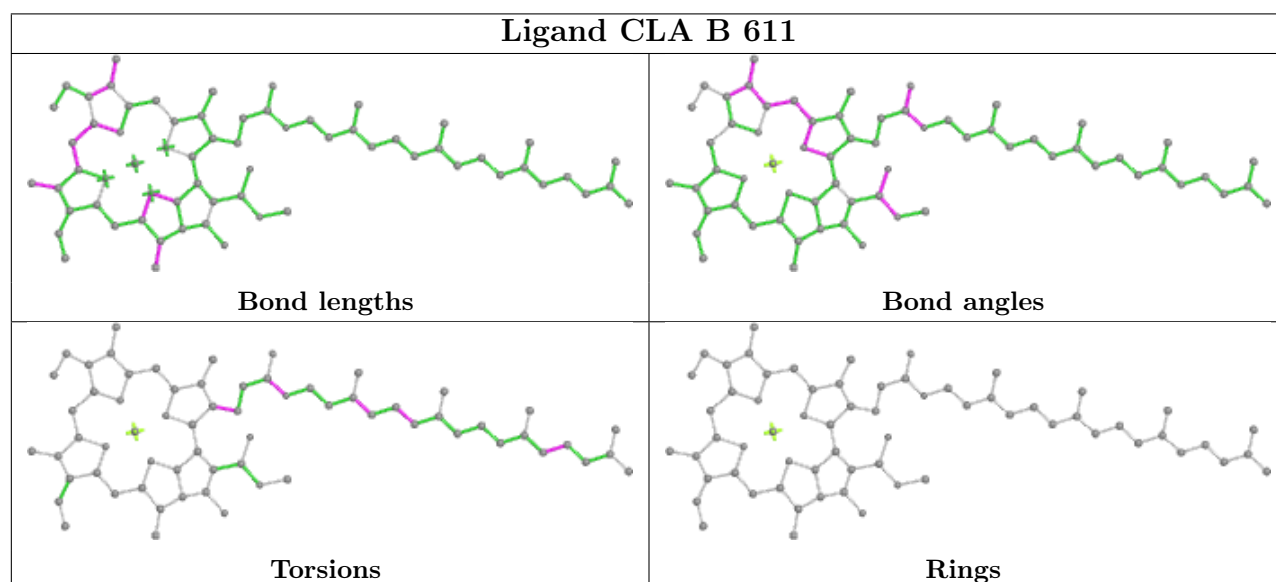
Ligand BCR b 619

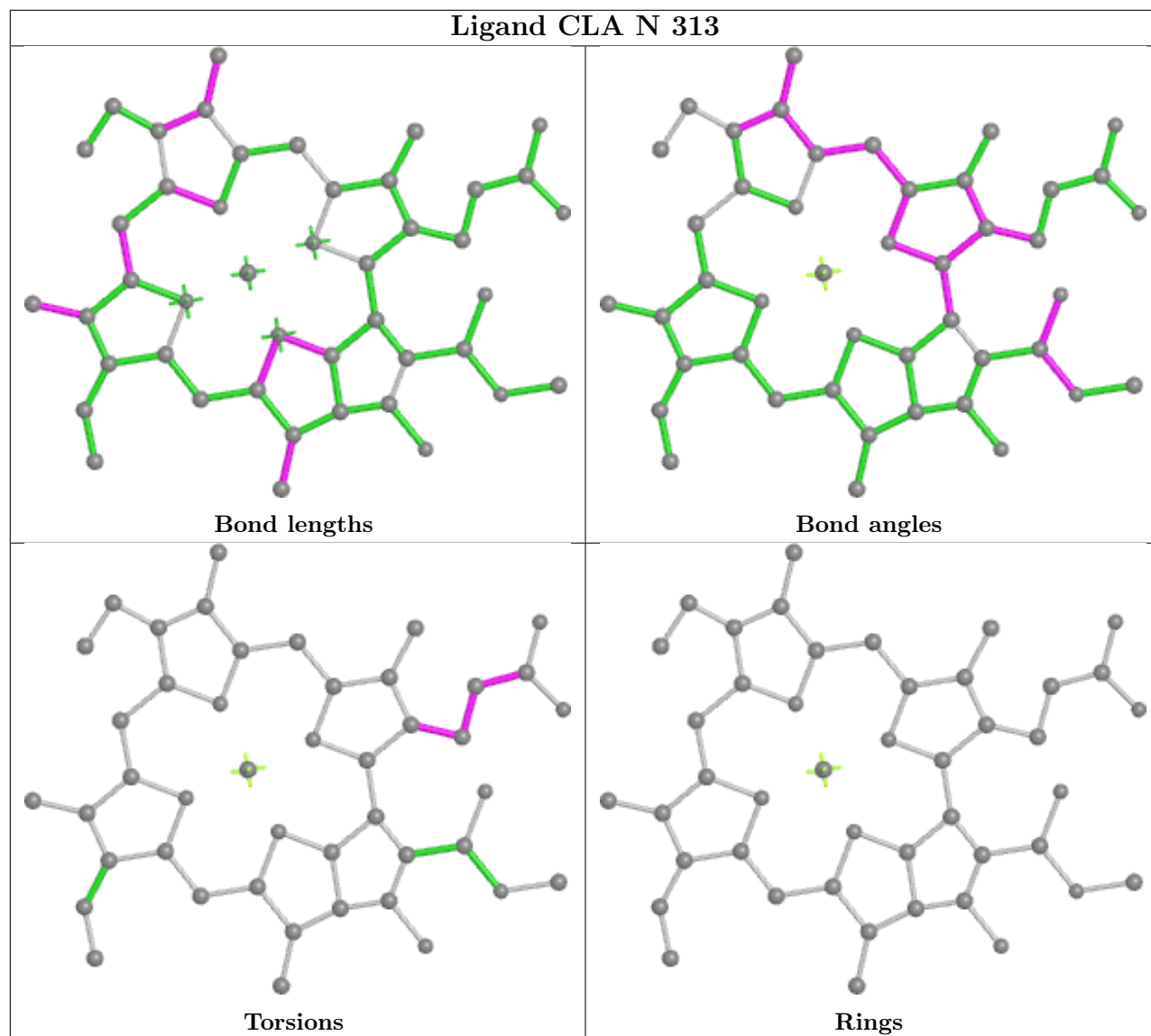
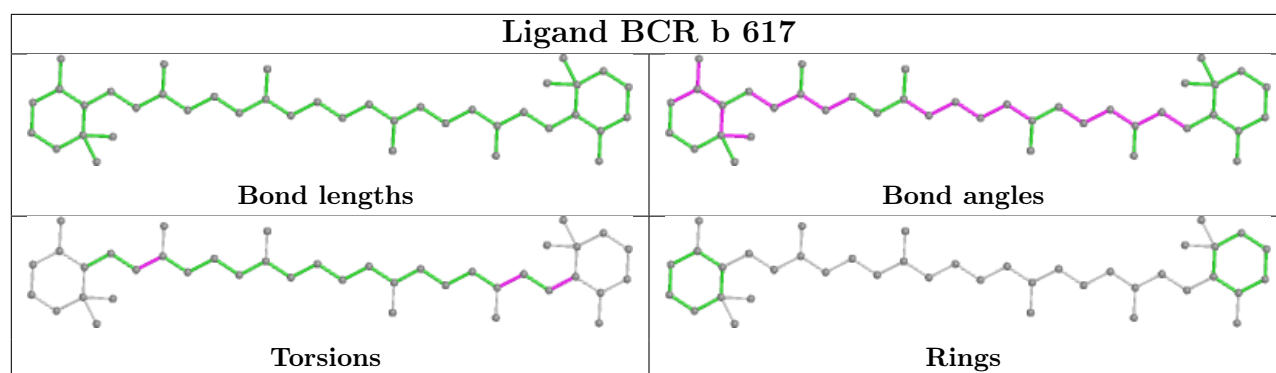


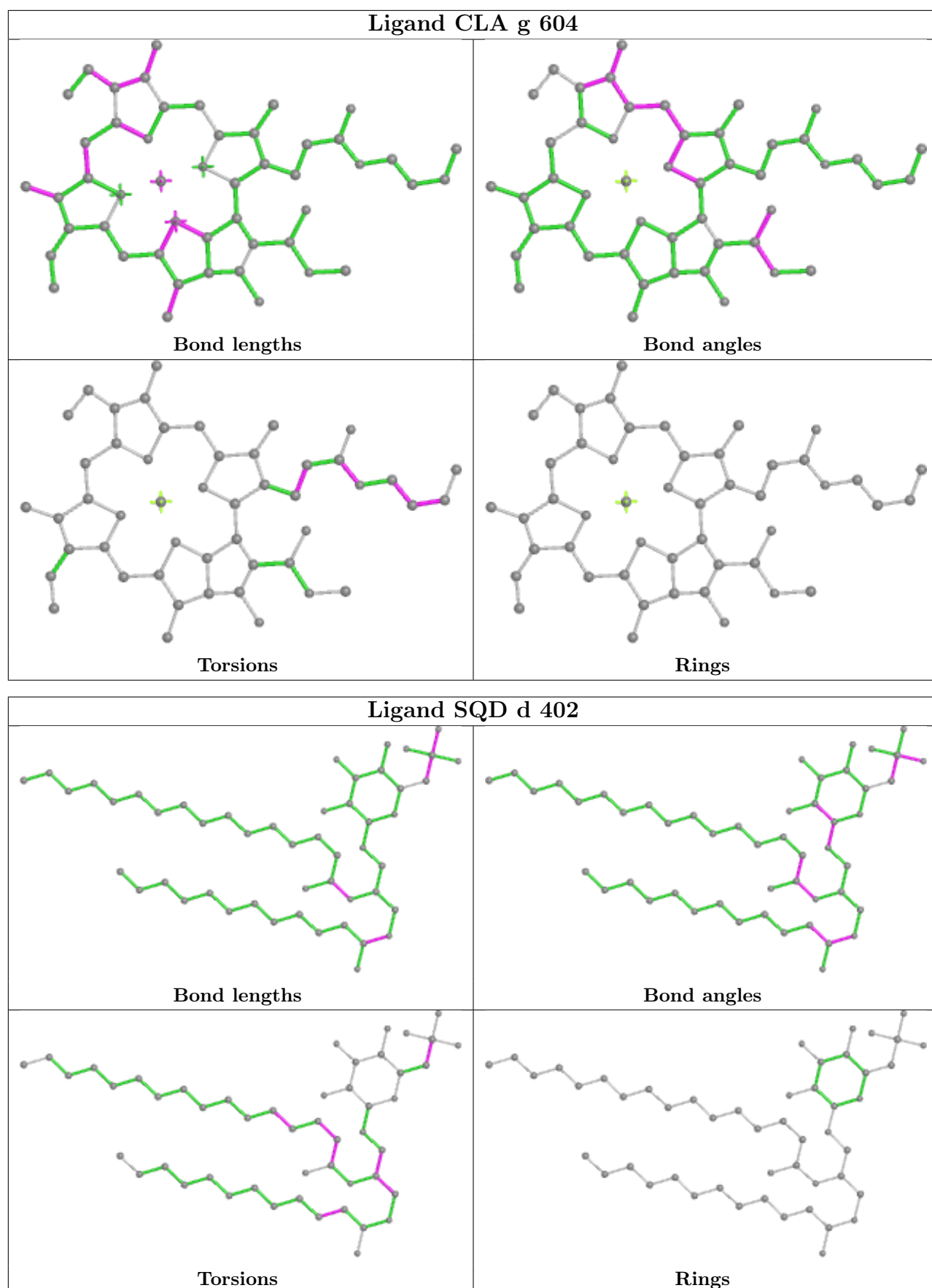
Ligand CLA Y 310

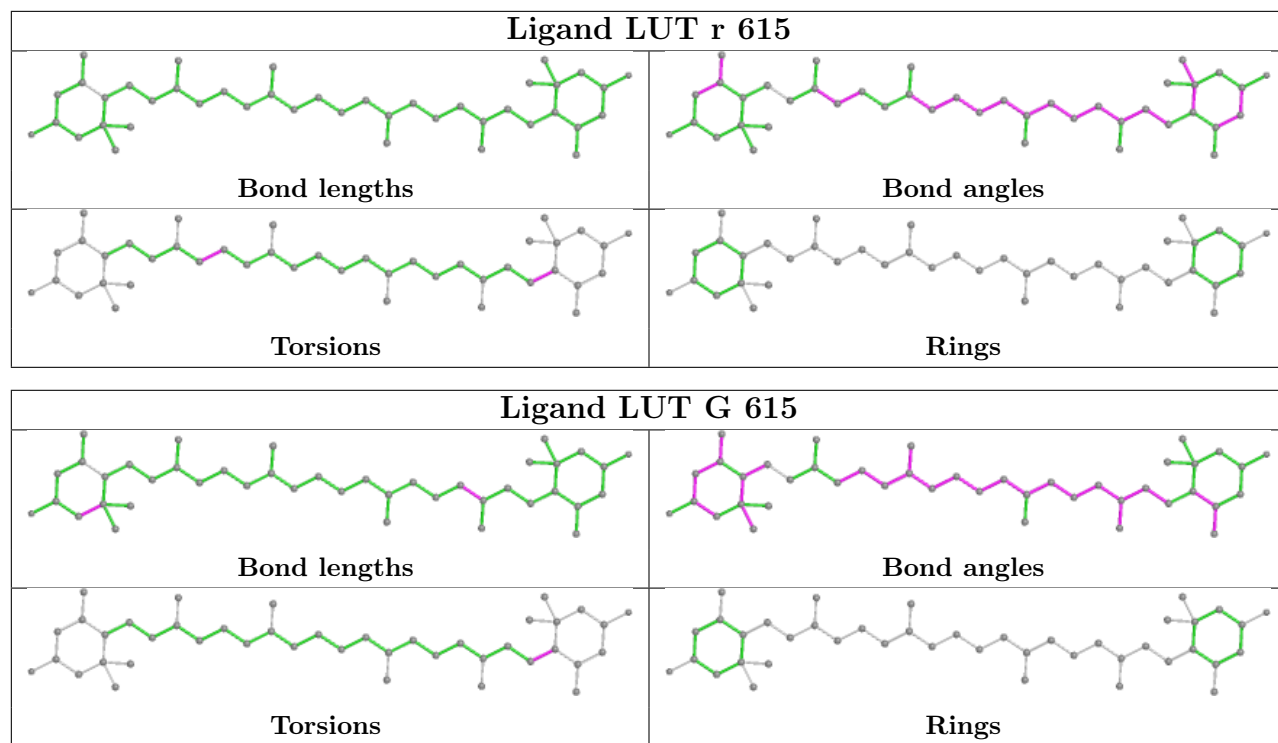


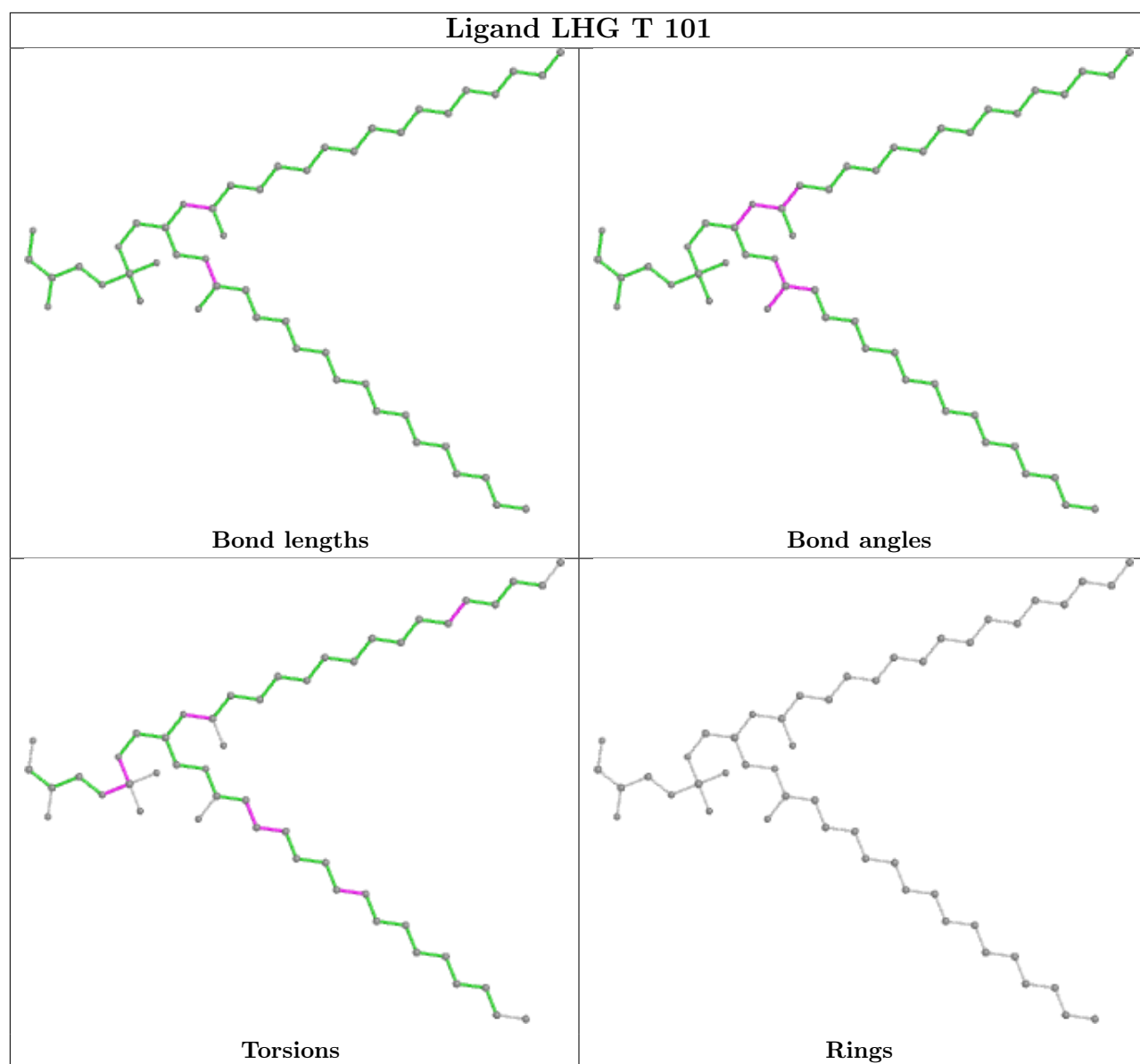
Ligand CLA B 611



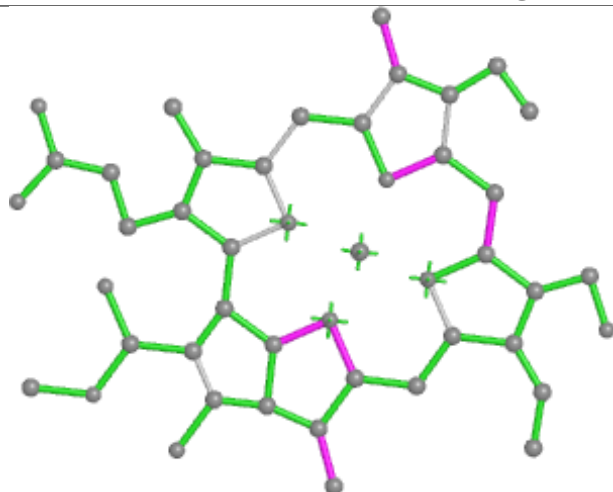




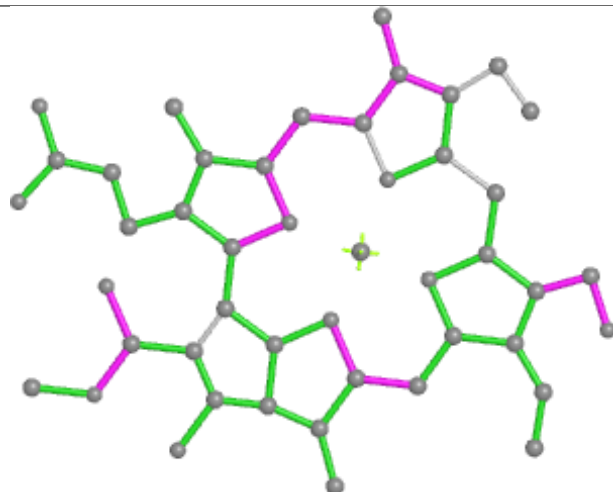




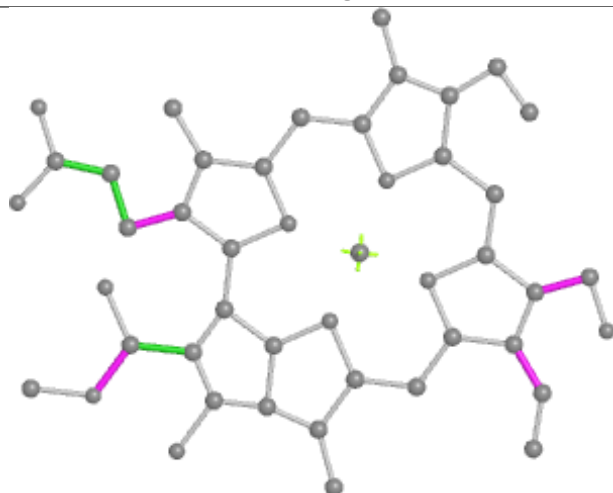
Ligand CHL R 606



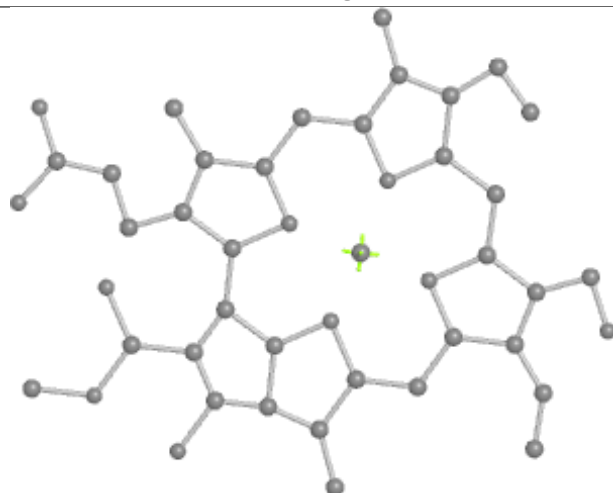
Bond lengths



Bond angles

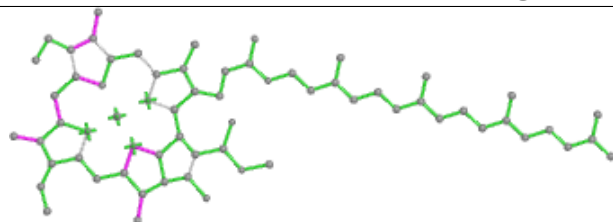


Torsions

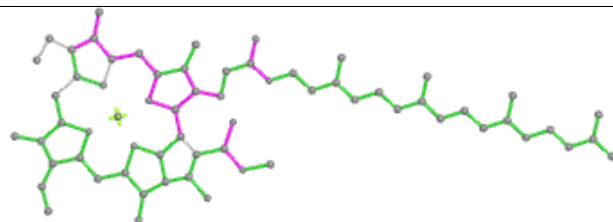


Rings

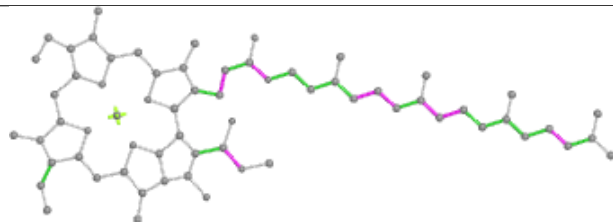
Ligand CLA B 616



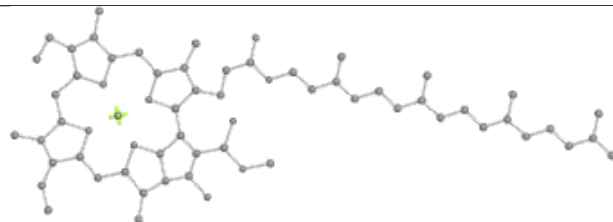
Bond lengths



Bond angles

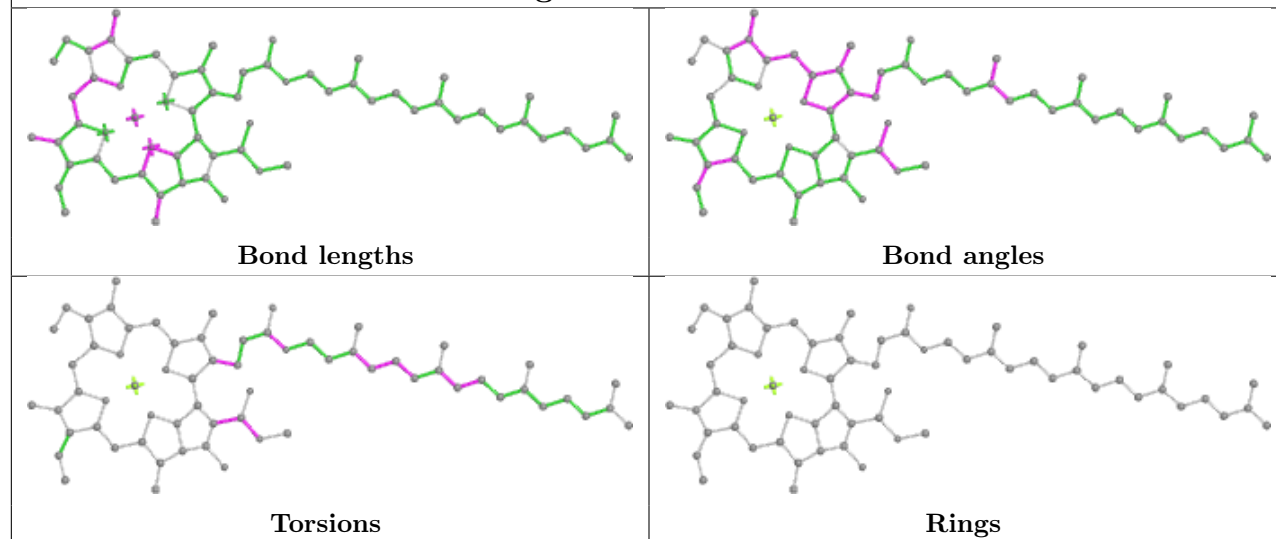


Torsions

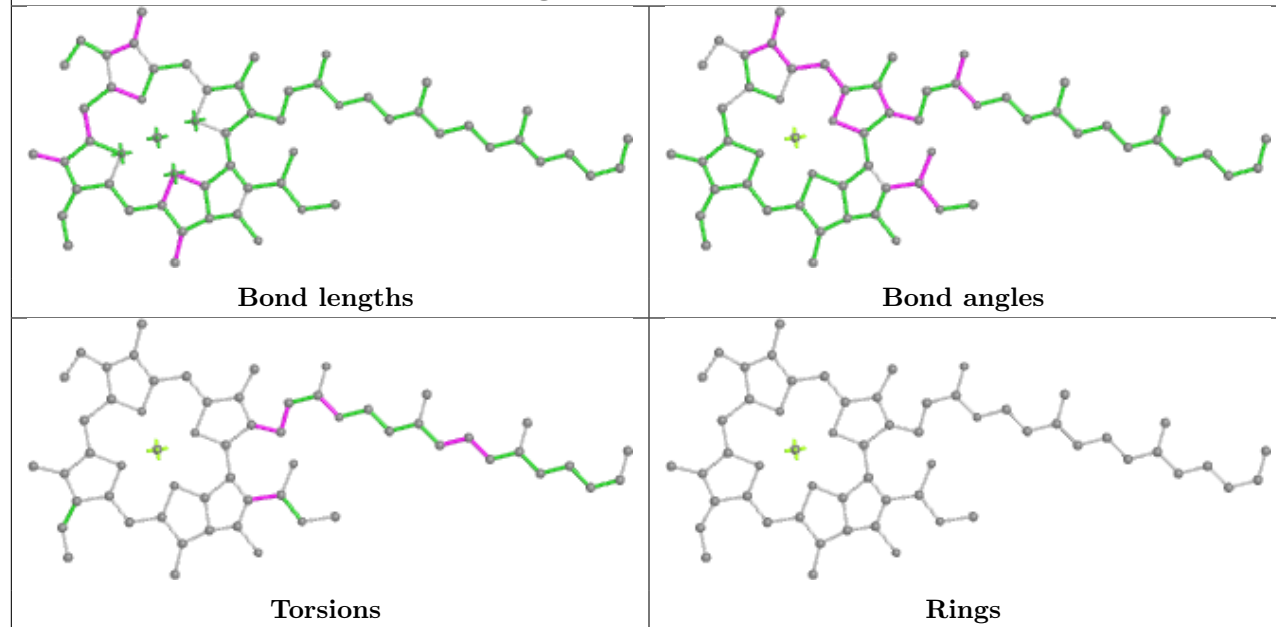


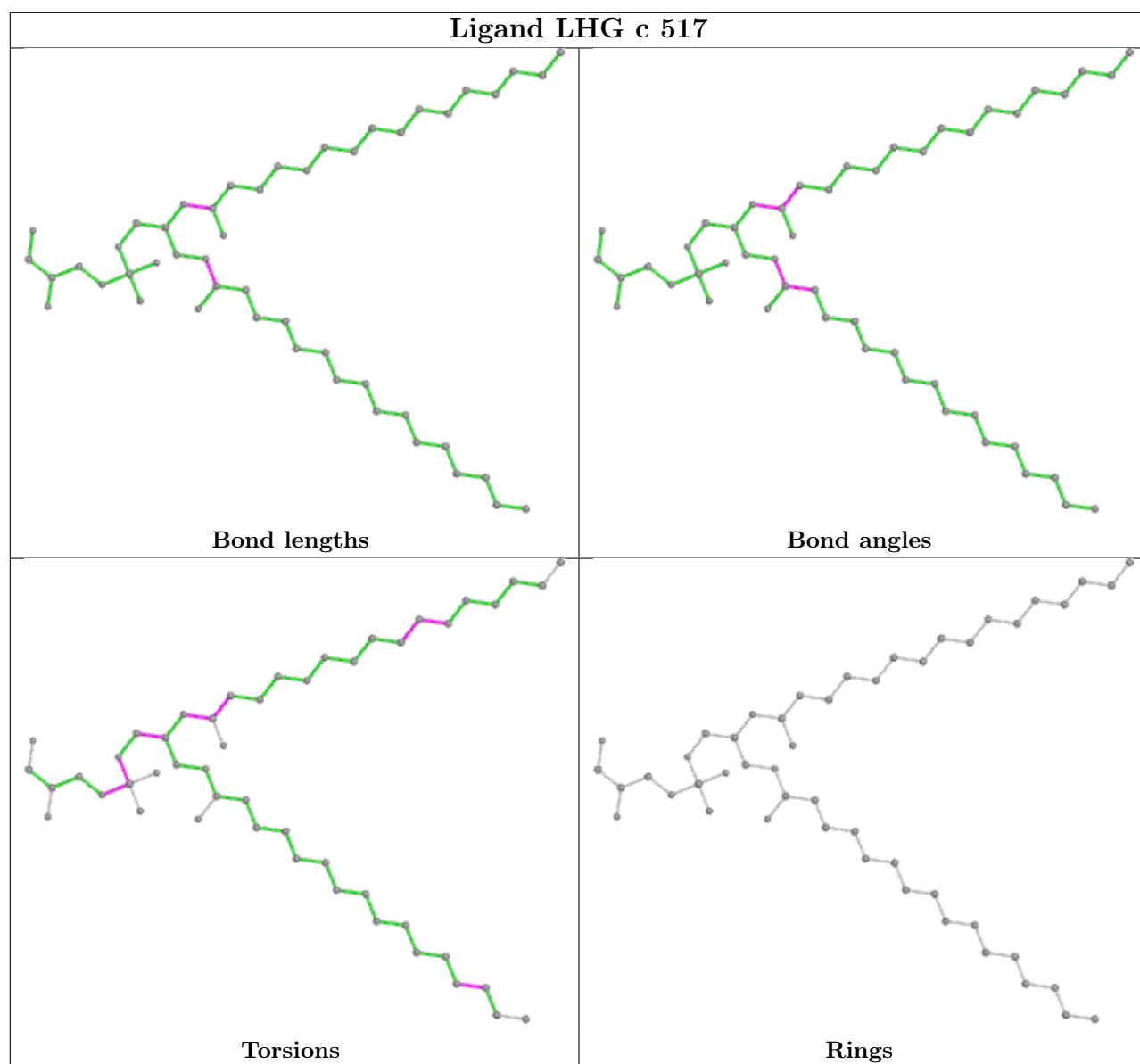
Rings

Ligand CLA b 608

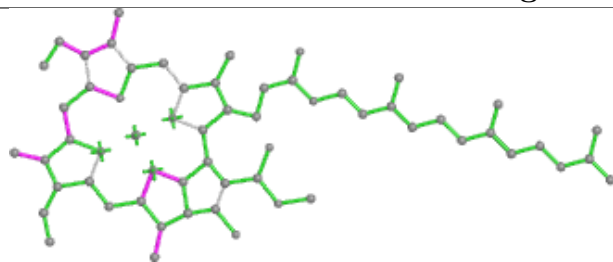


Ligand CLA n 304

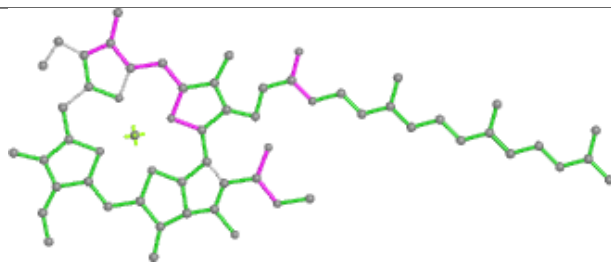




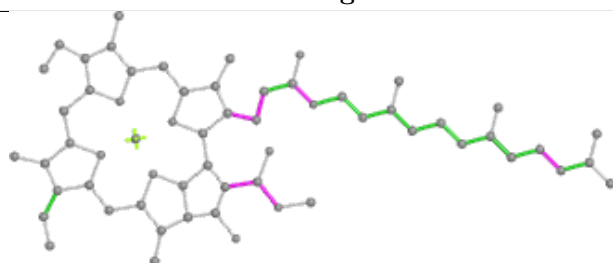
Ligand CLA r 602



Bond lengths



Bond angles

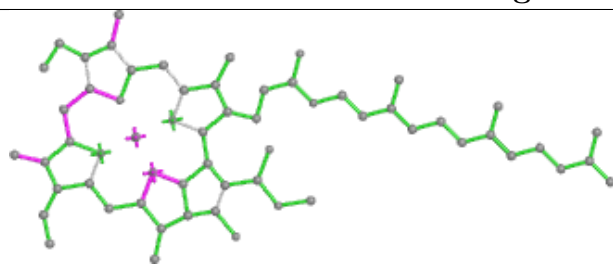


Torsions

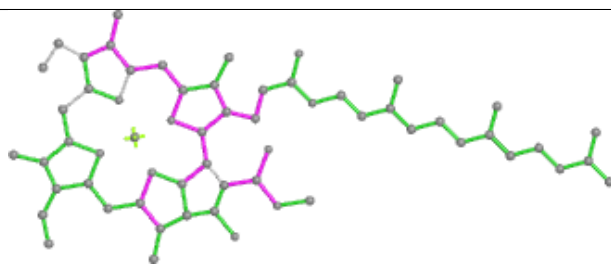


Rings

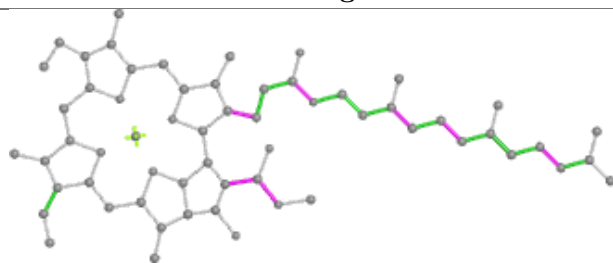
Ligand CLA N 314



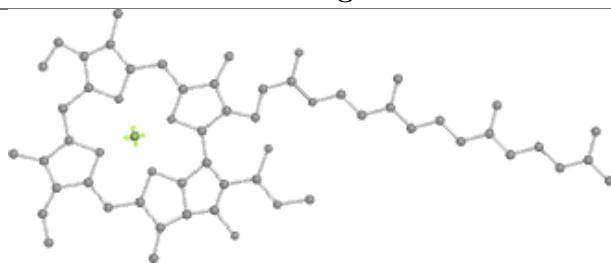
Bond lengths



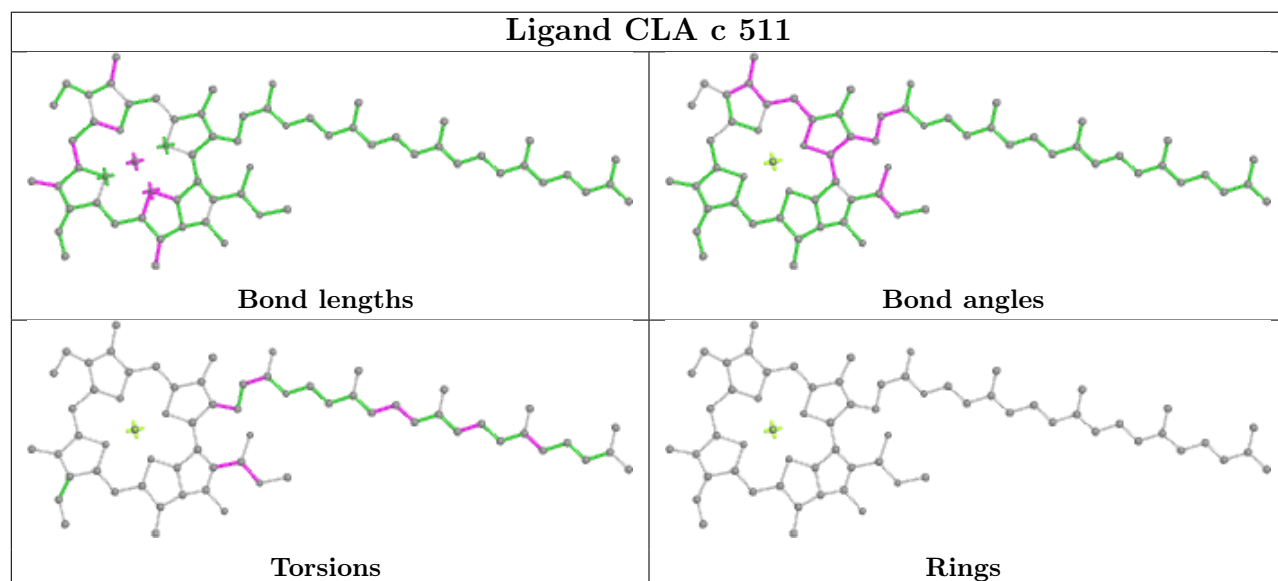
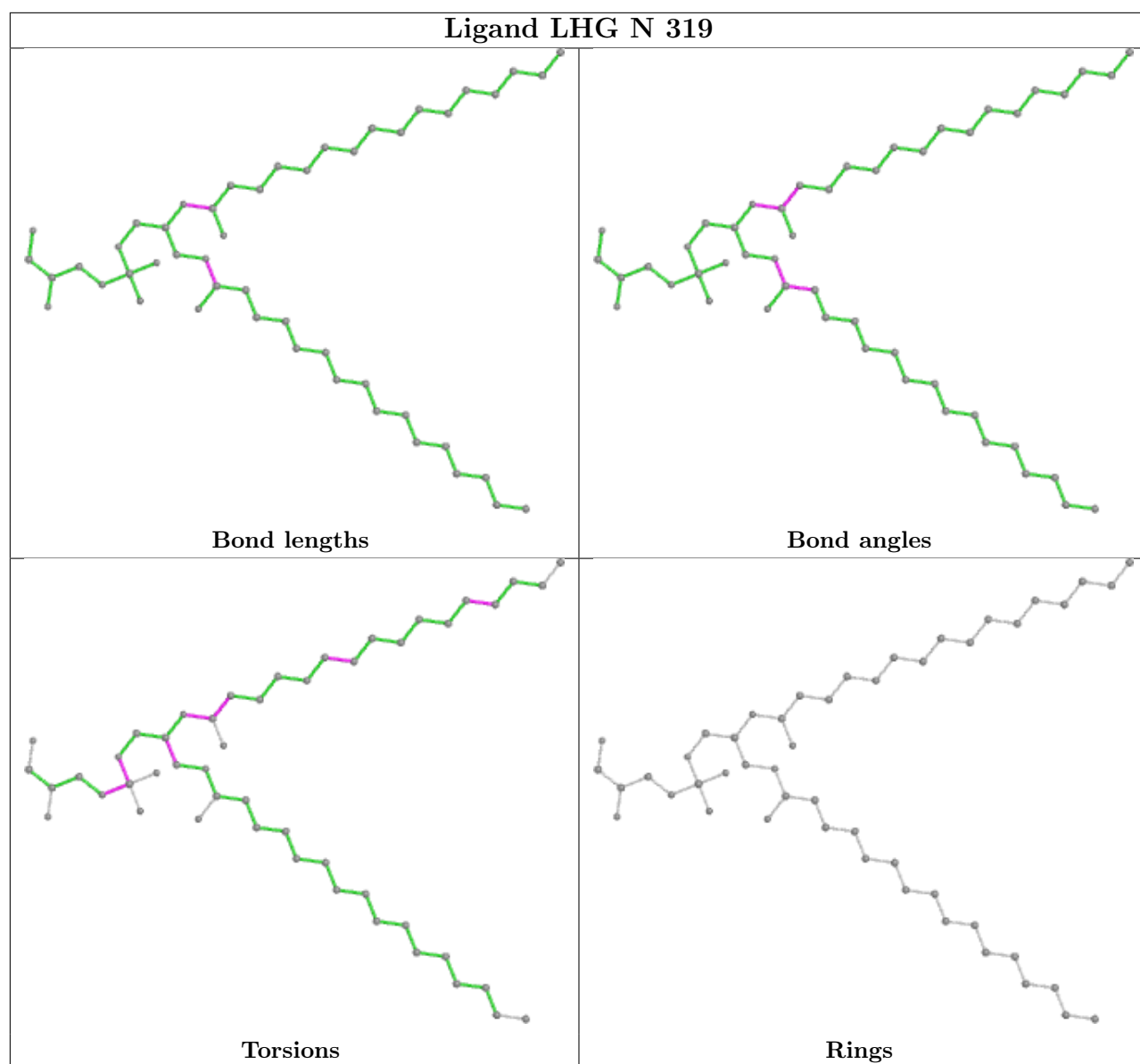
Bond angles

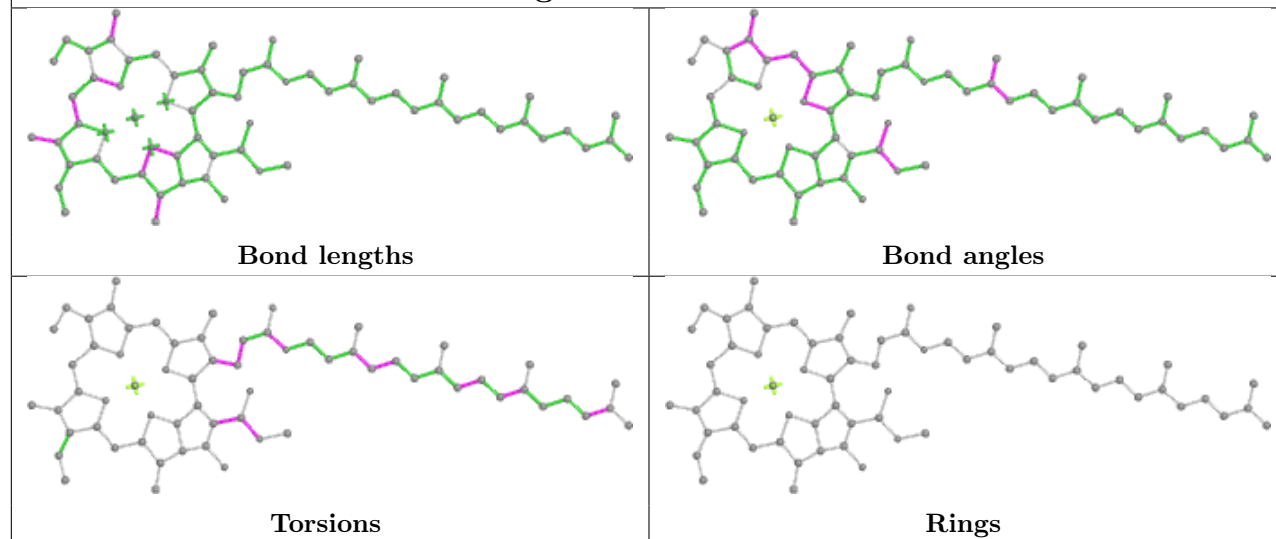
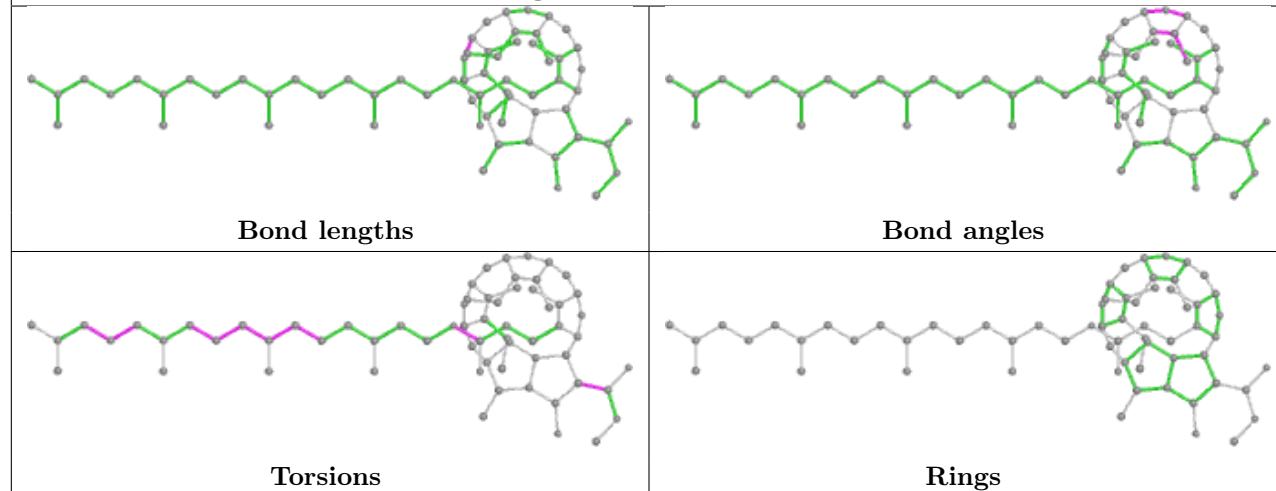


Torsions

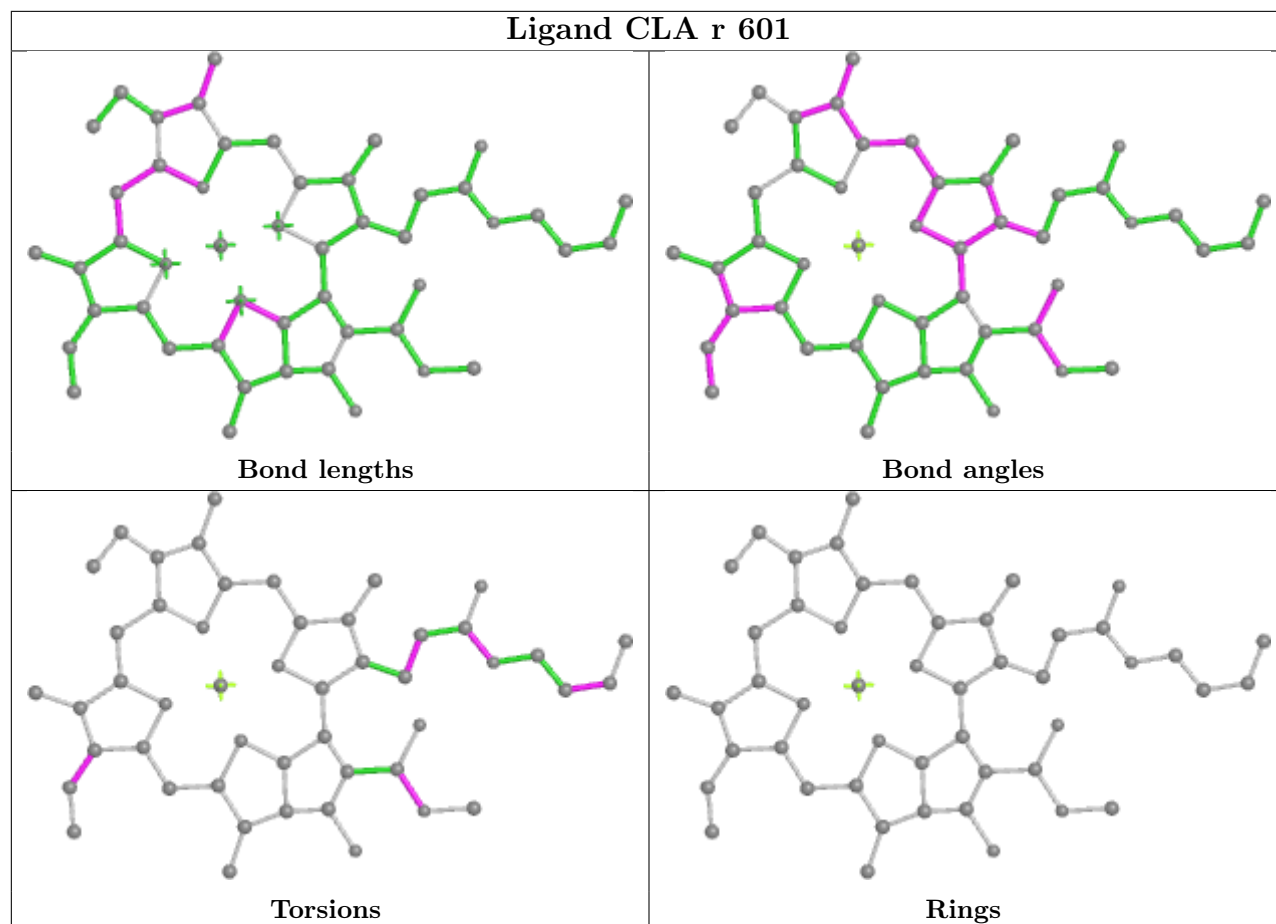


Rings

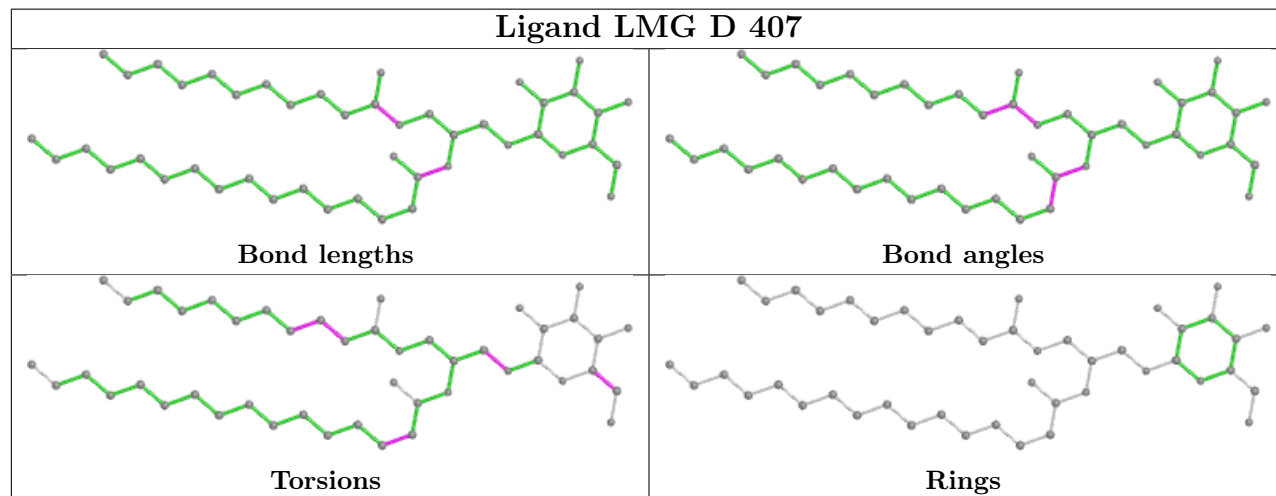


Ligand CLA b 603**Ligand PHO A 403**

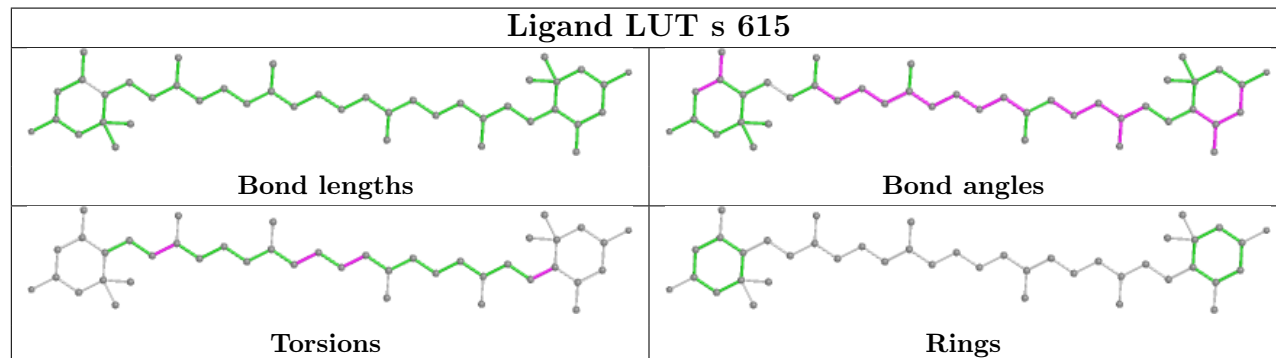
Ligand CLA r 601

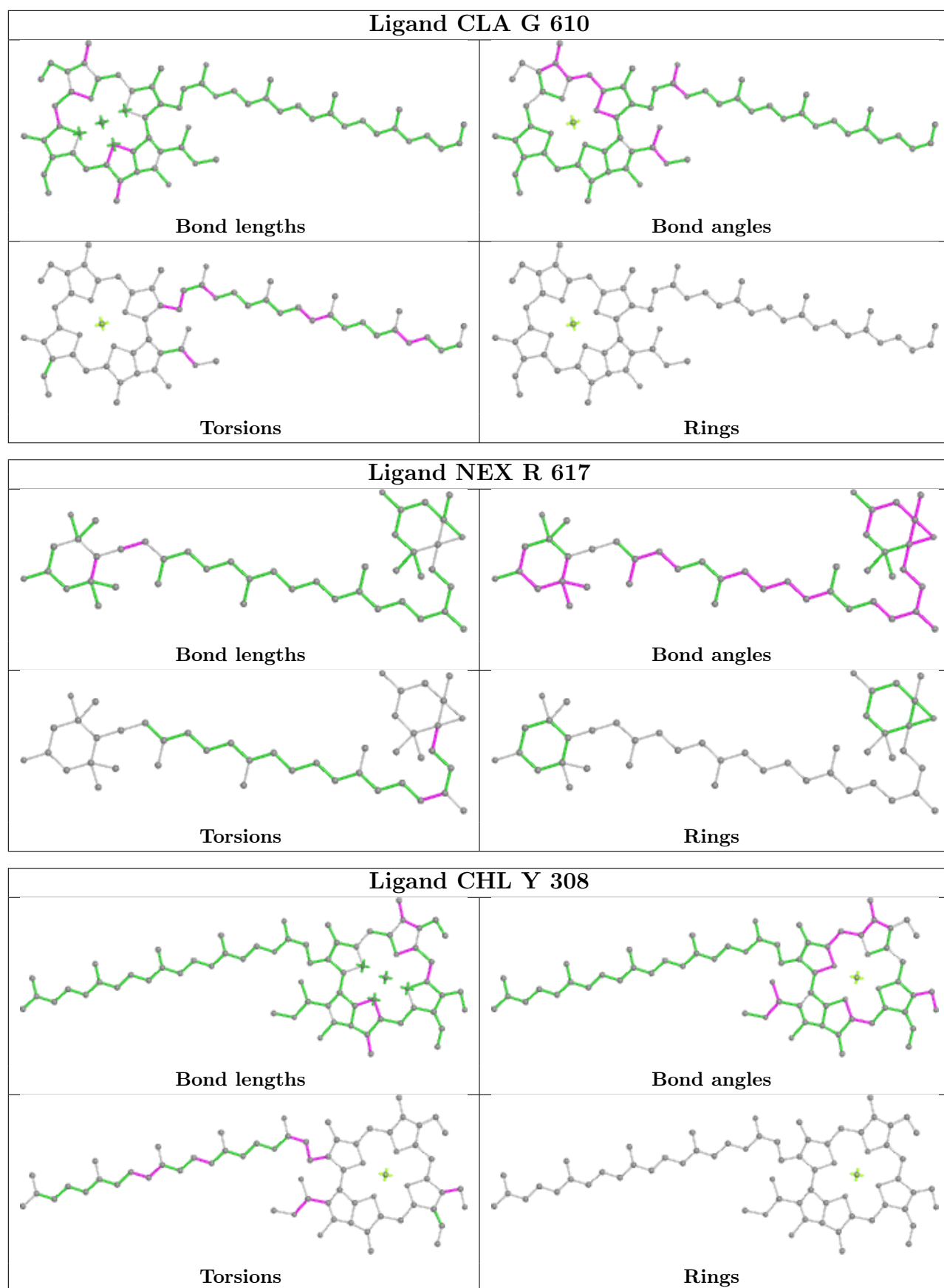


Ligand LMG D 407

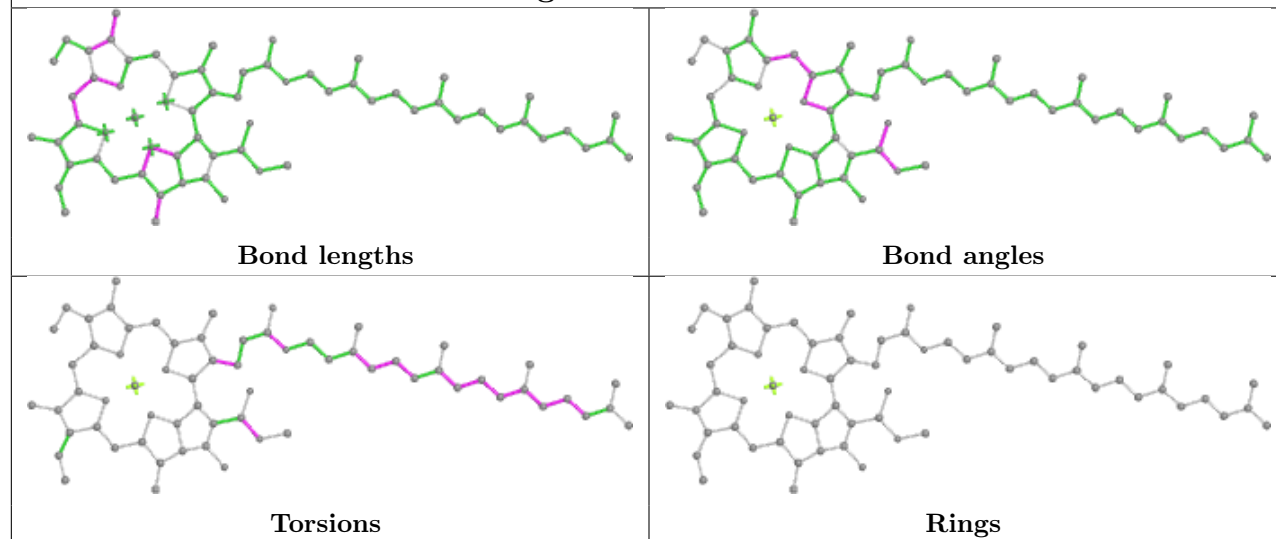


Ligand LUT s 615

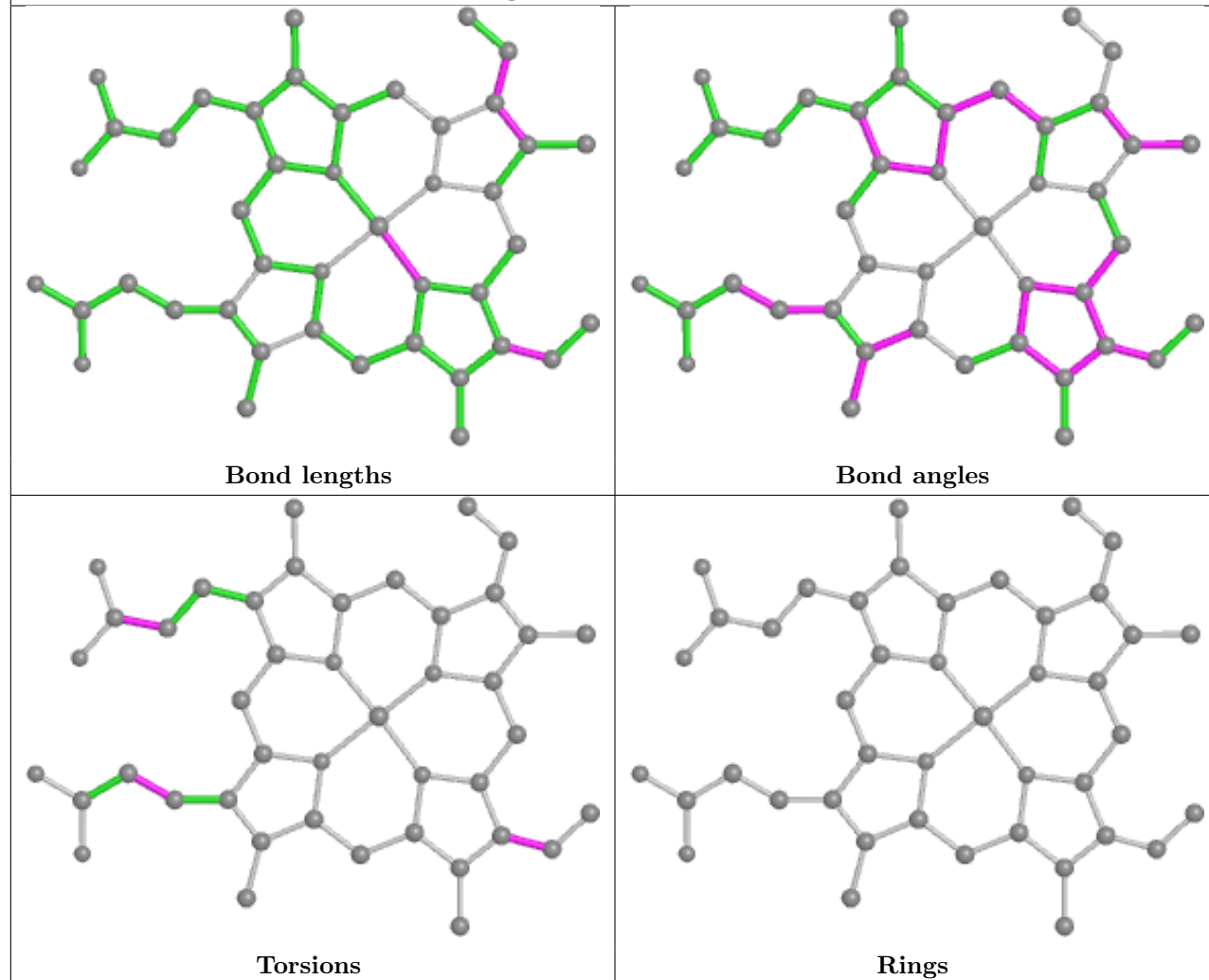




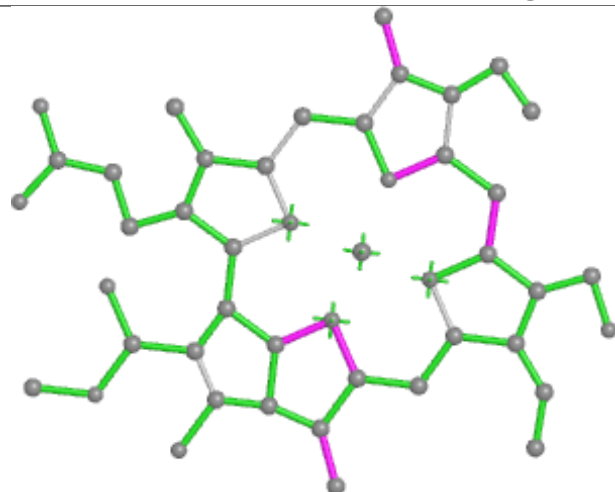
Ligand CLA c 503



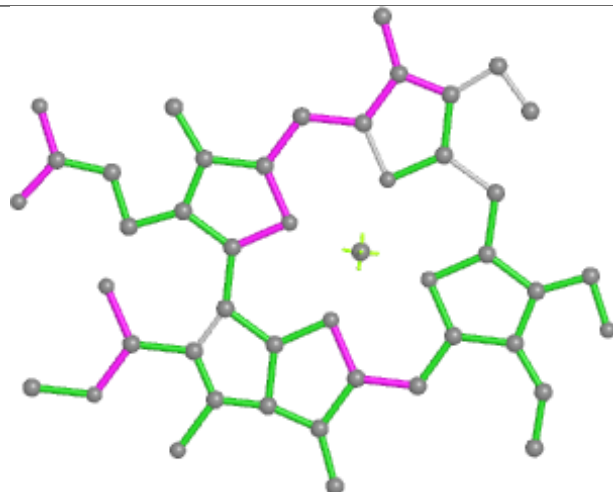
Ligand HEM e 101



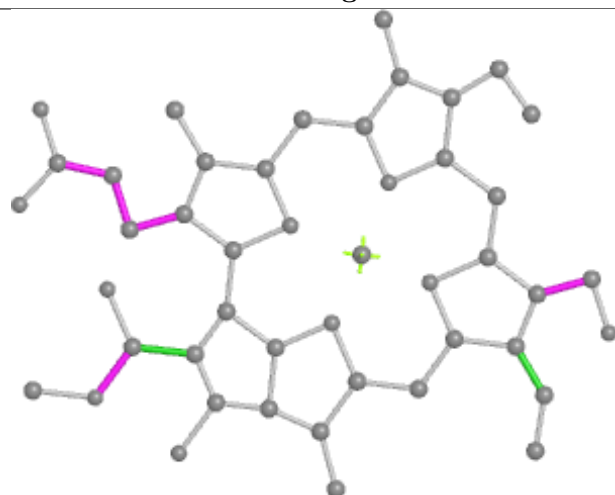
Ligand CHL s 605



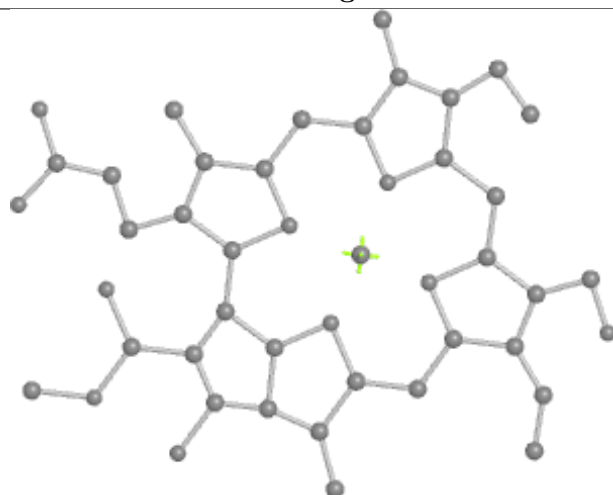
Bond lengths



Bond angles

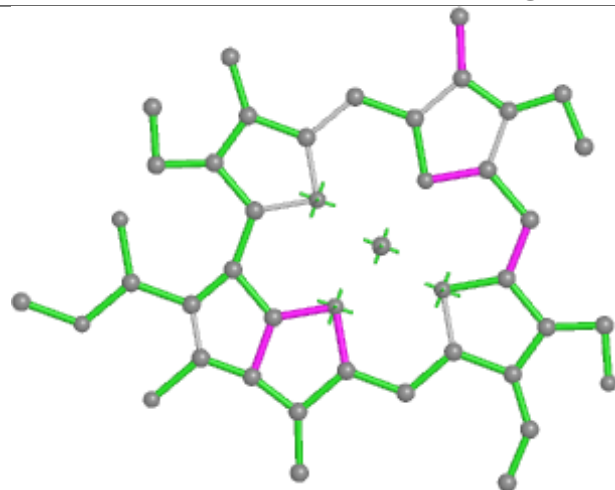


Torsions

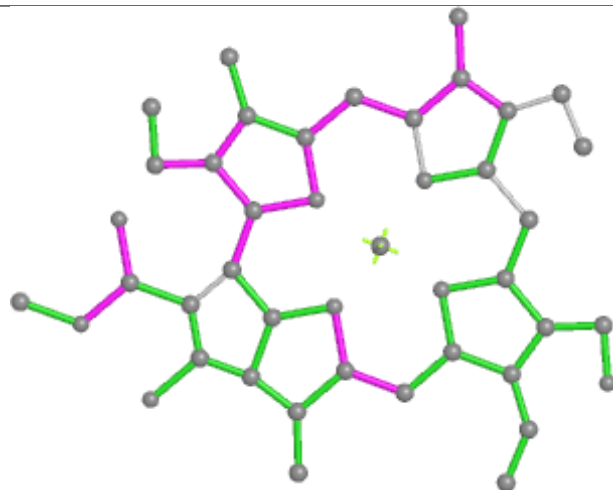


Rings

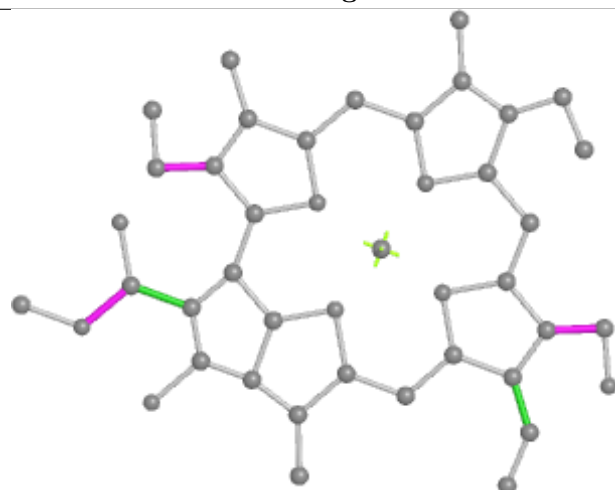
Ligand CHL s 606



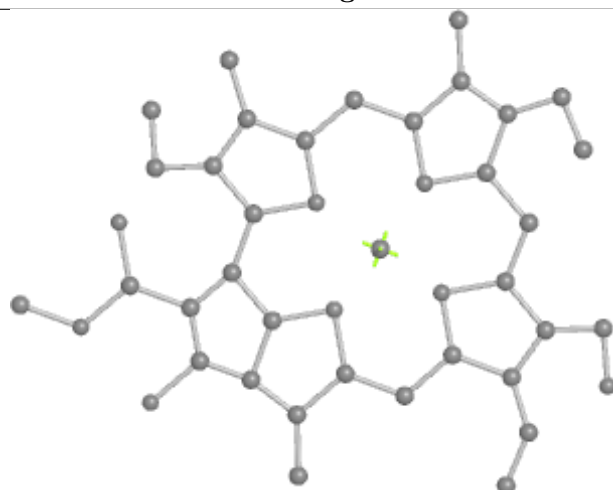
Bond lengths



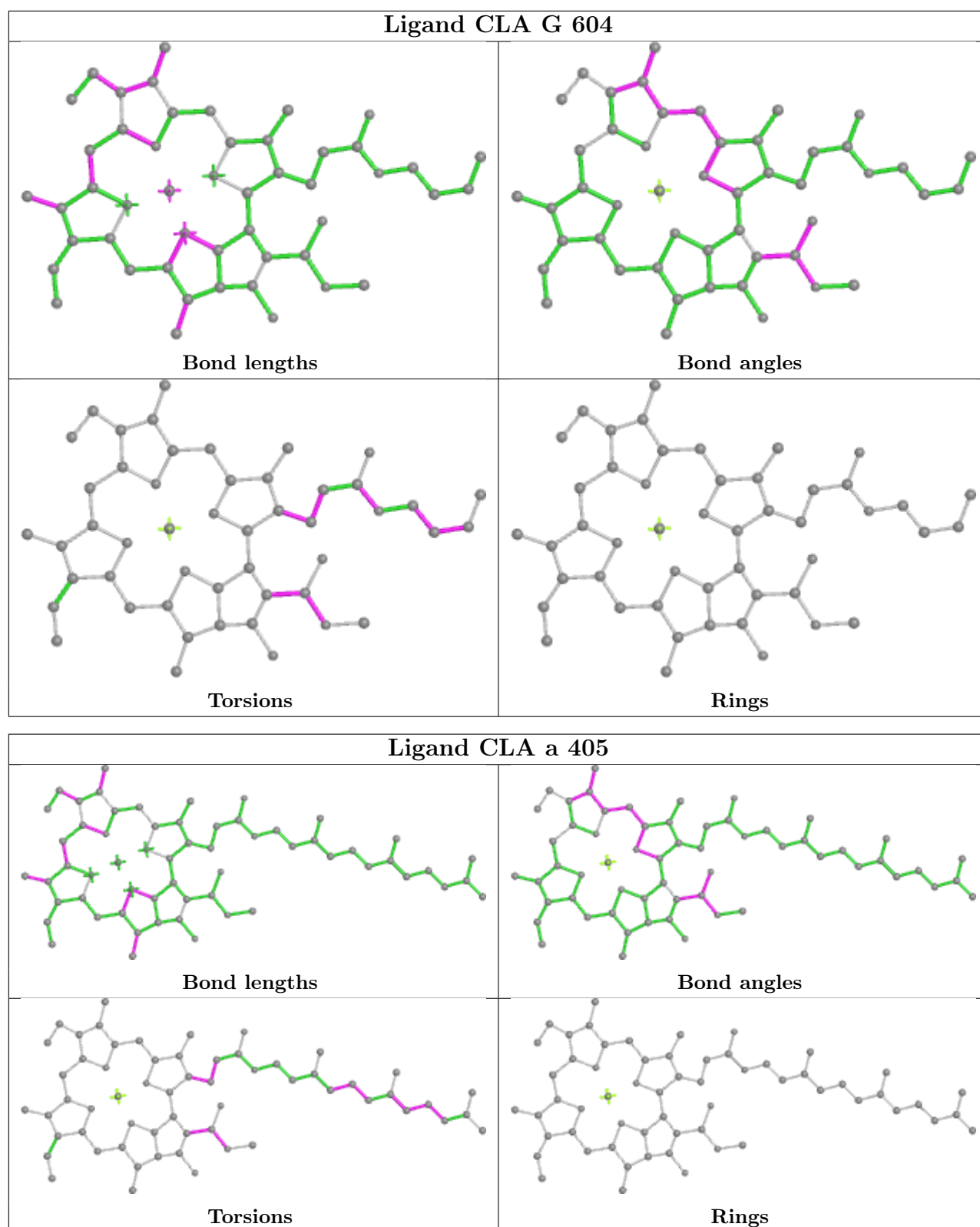
Bond angles

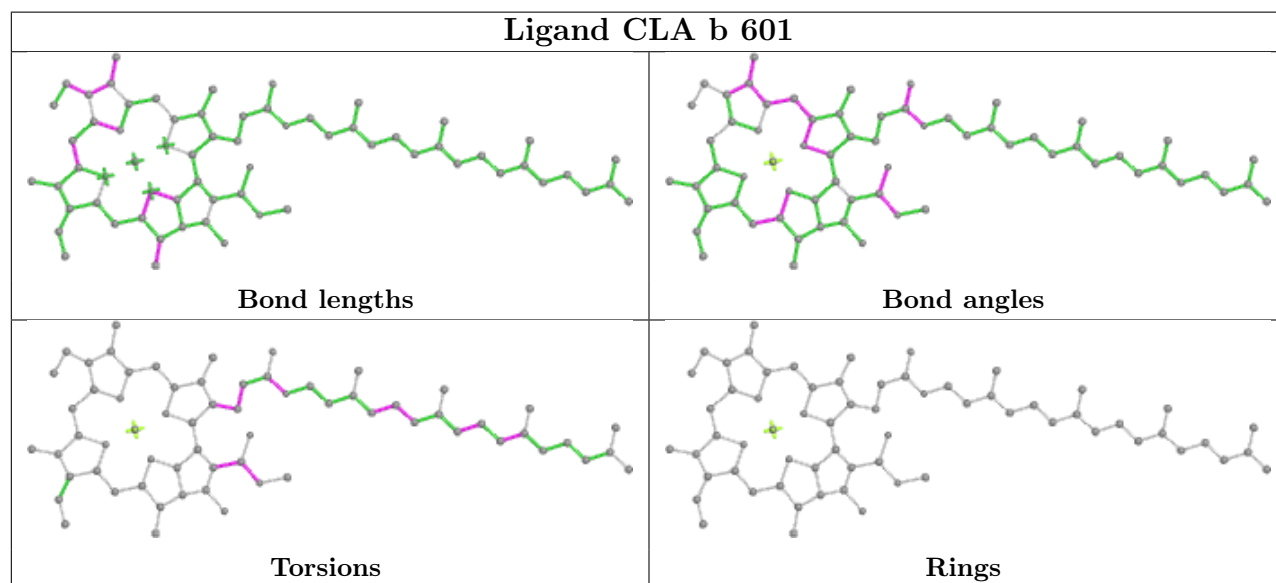
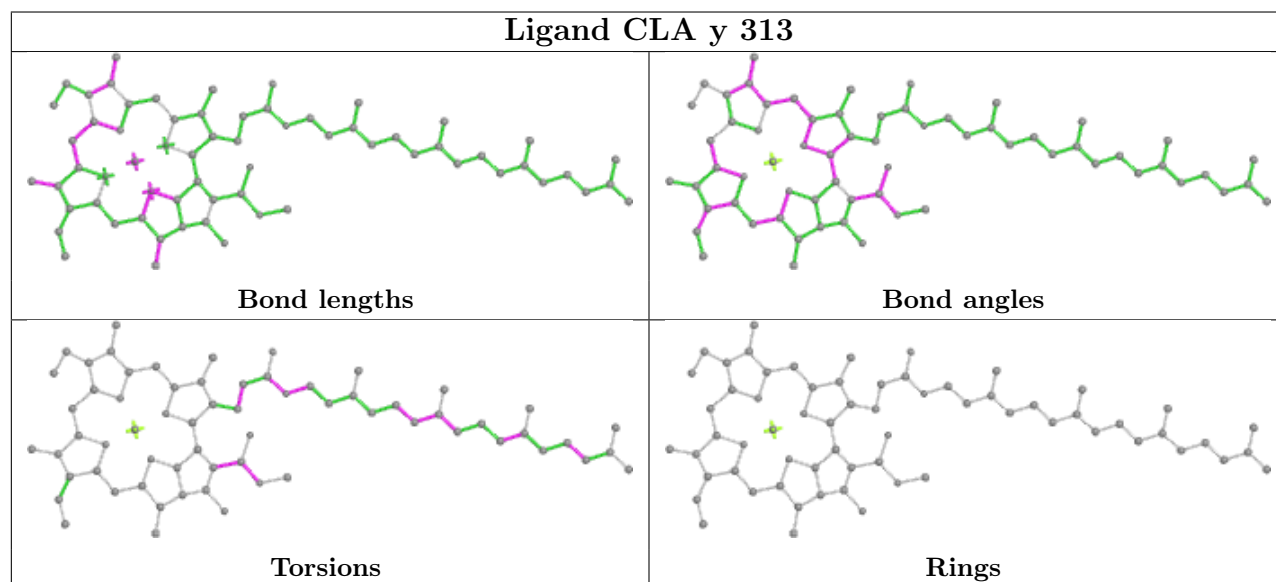
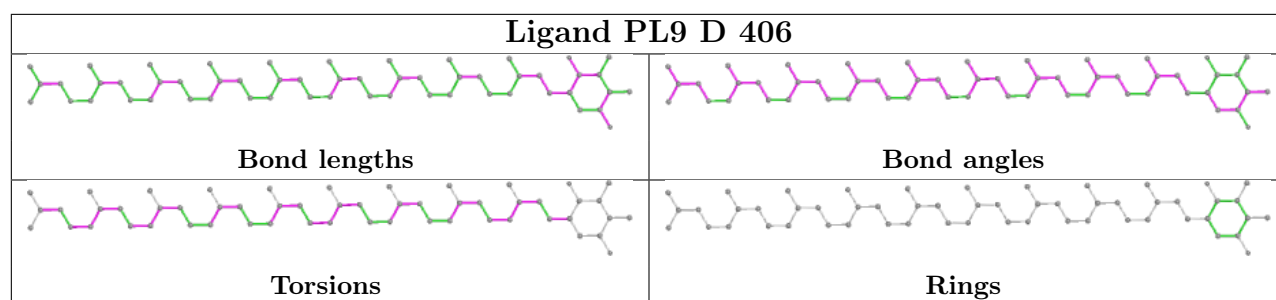


Torsions

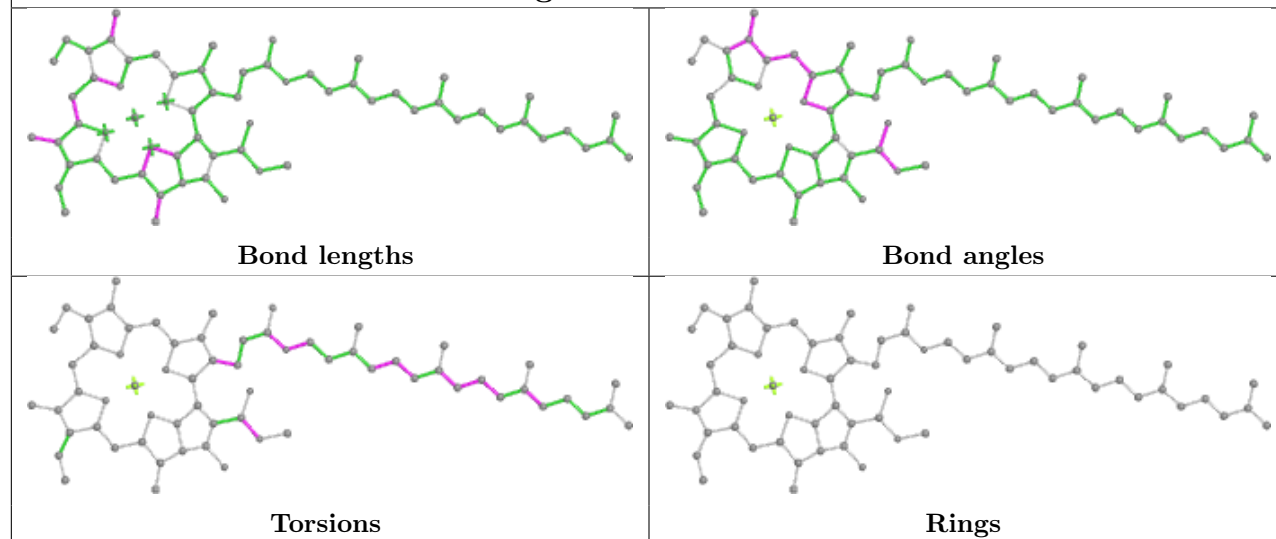


Rings

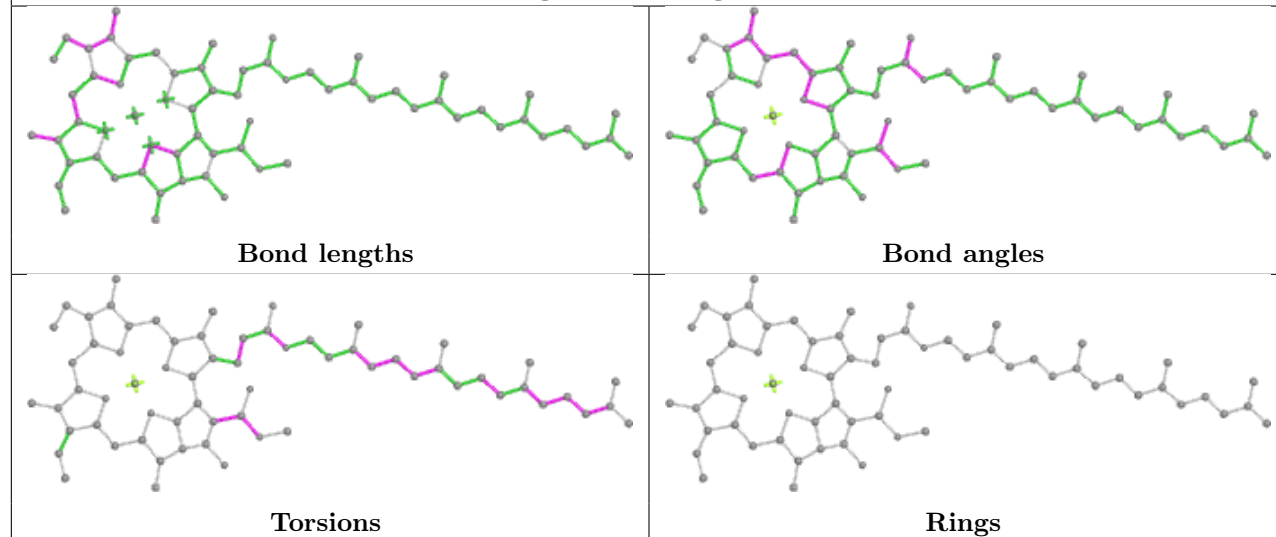




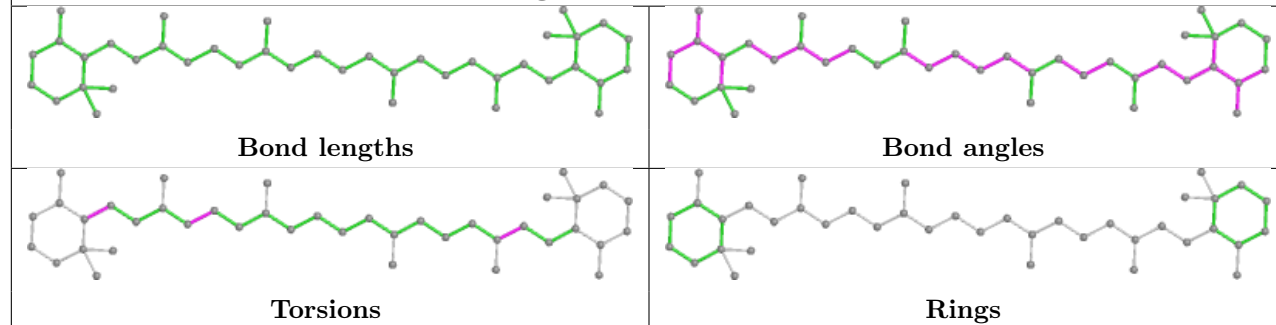
Ligand CLA b 607

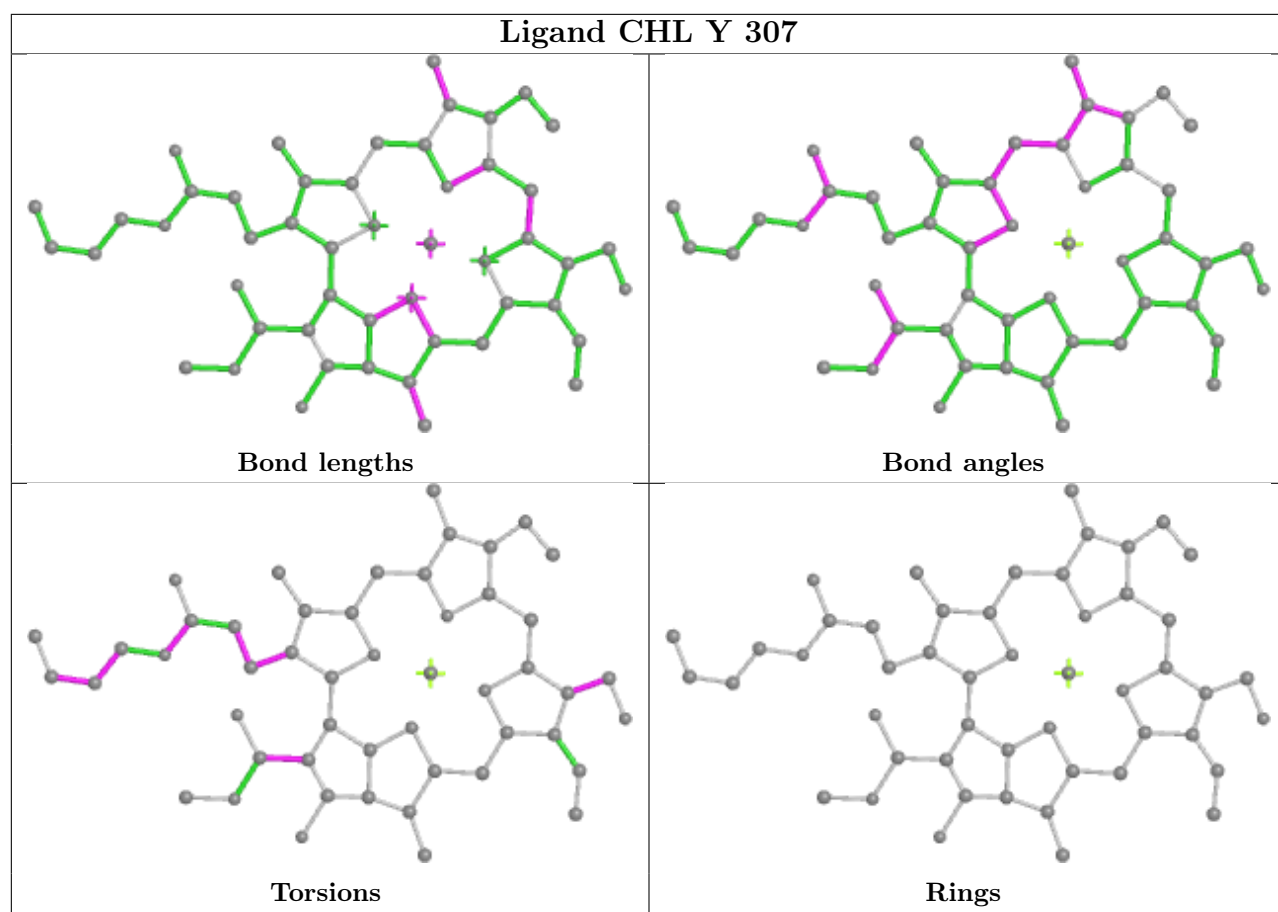


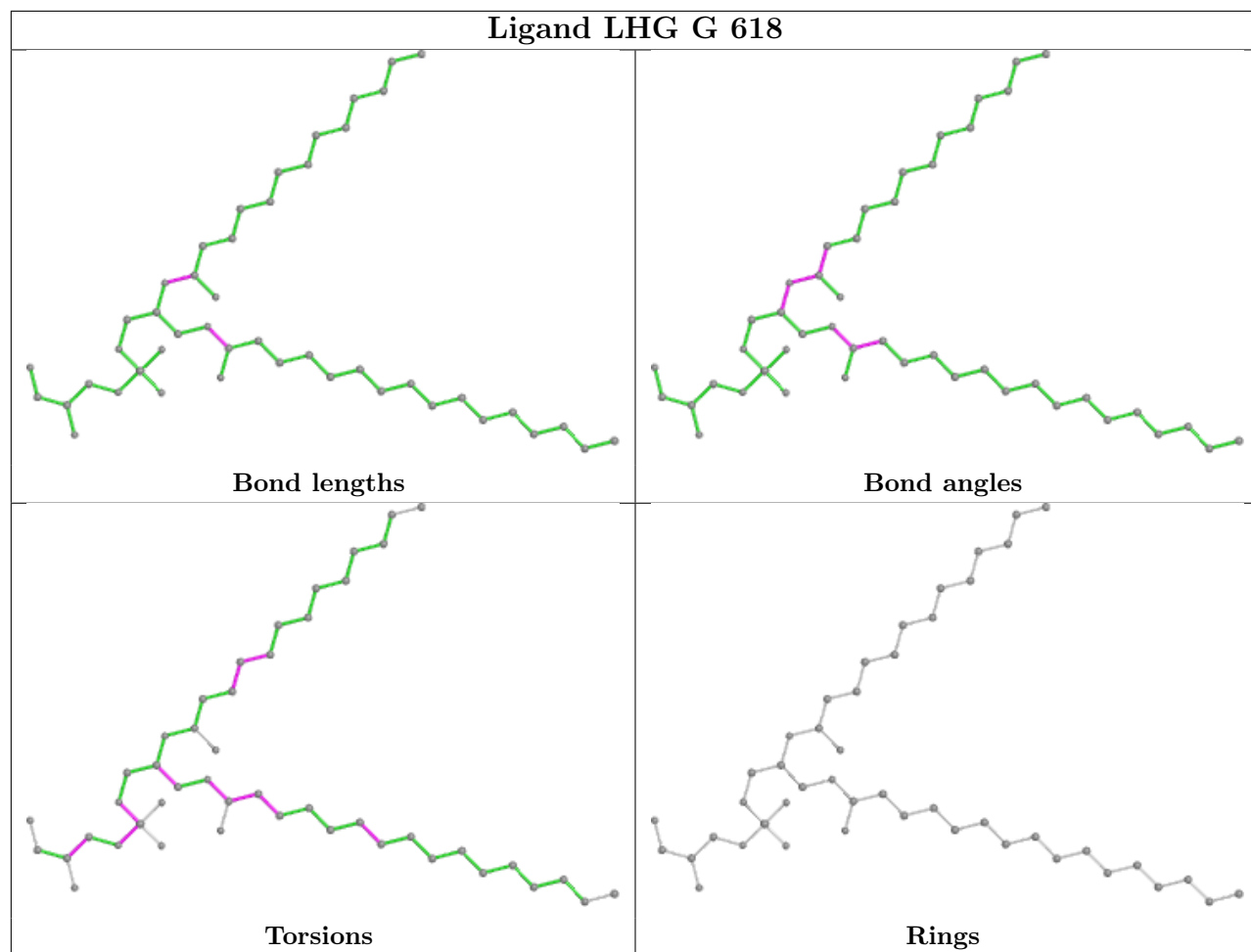
Ligand CLA g 602



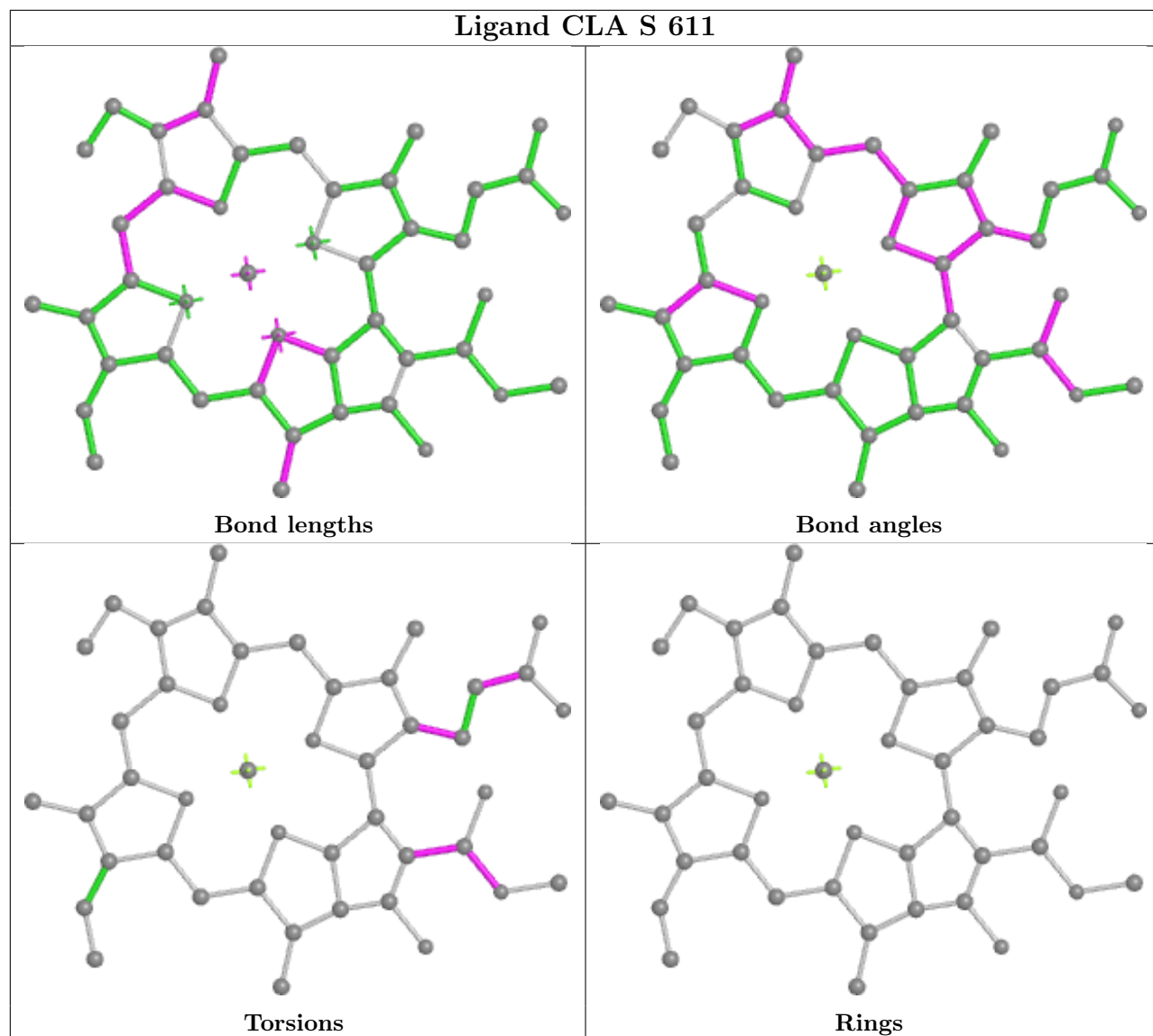
Ligand BCR d 406



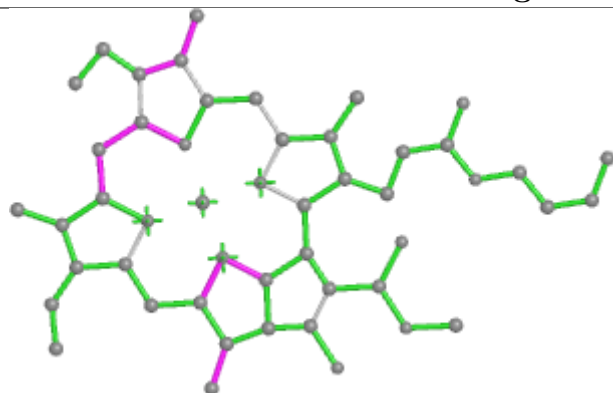




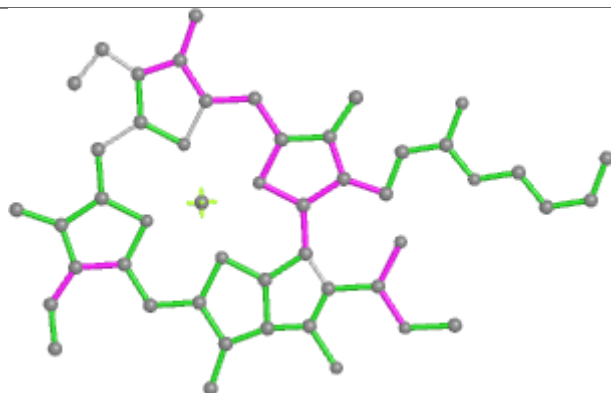
Ligand CLA S 611



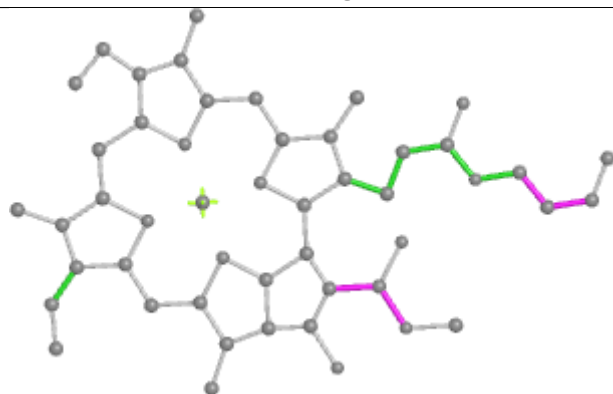
Ligand CLA R 601



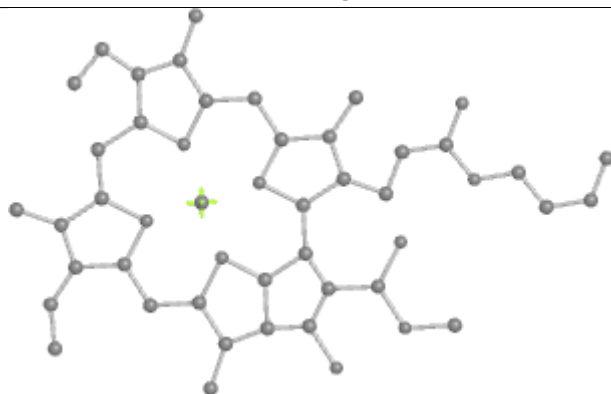
Bond lengths



Bond angles

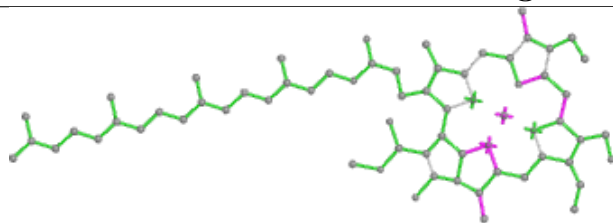


Torsions

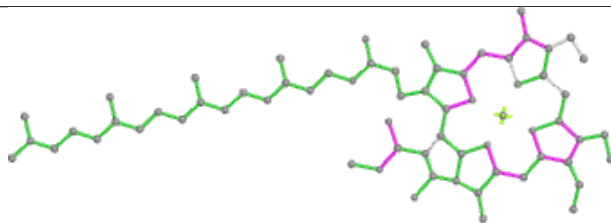


Rings

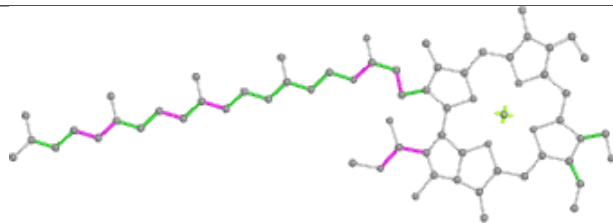
Ligand CHL n 302



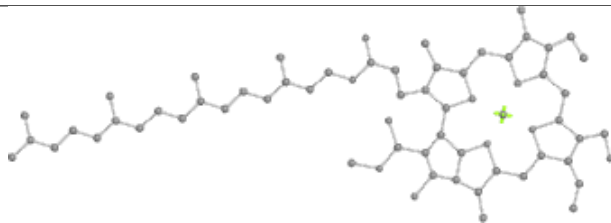
Bond lengths



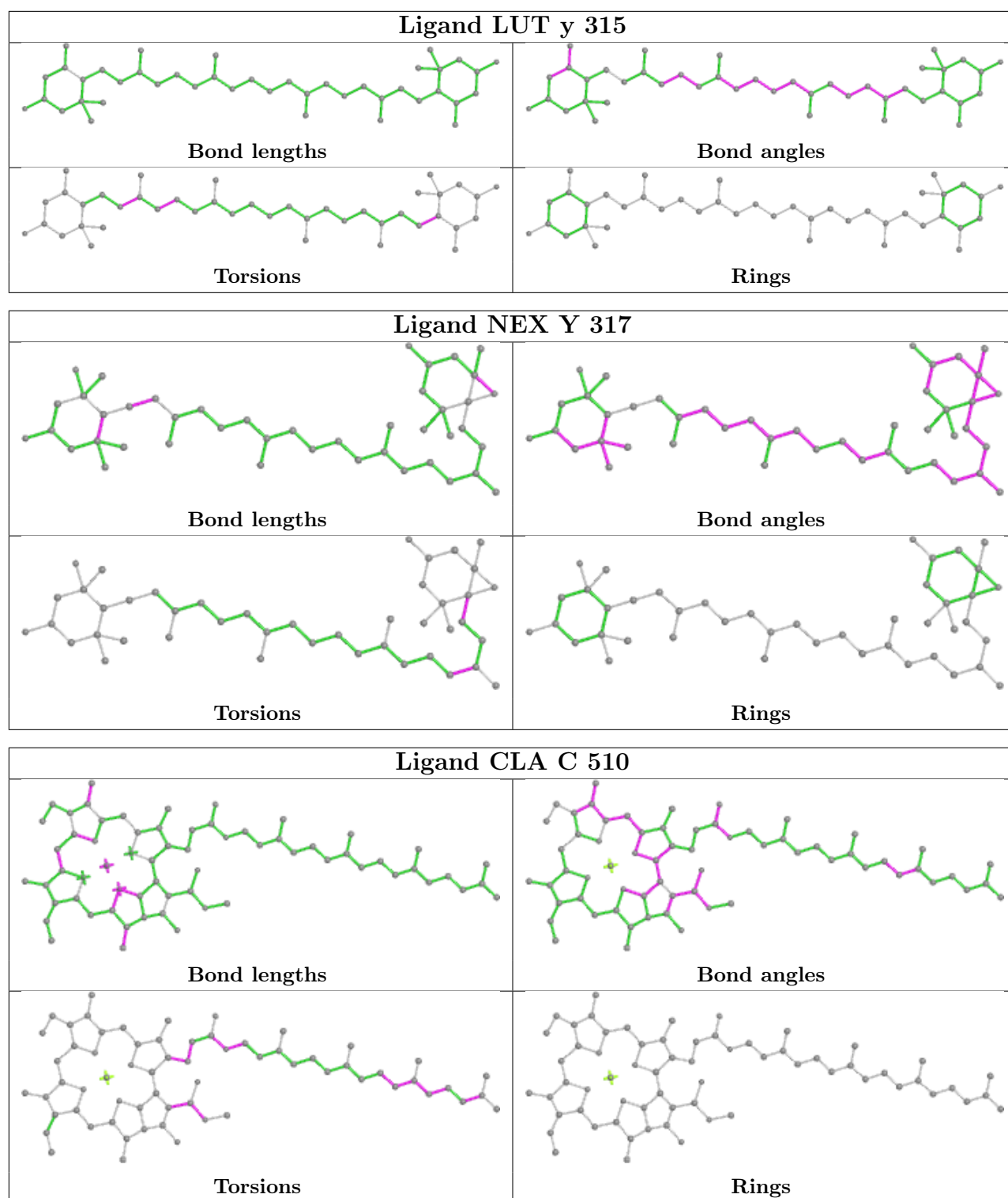
Bond angles



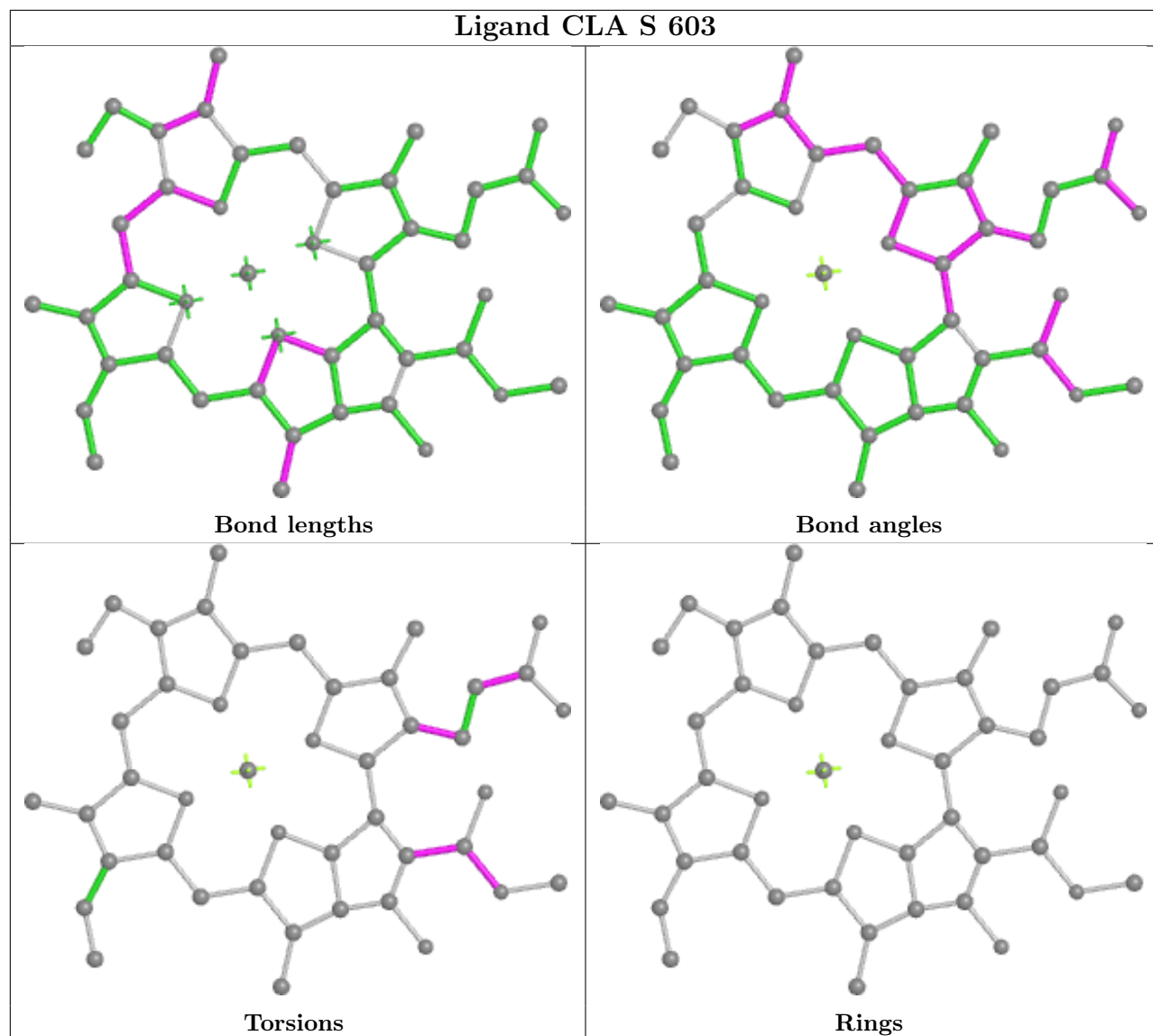
Torsions

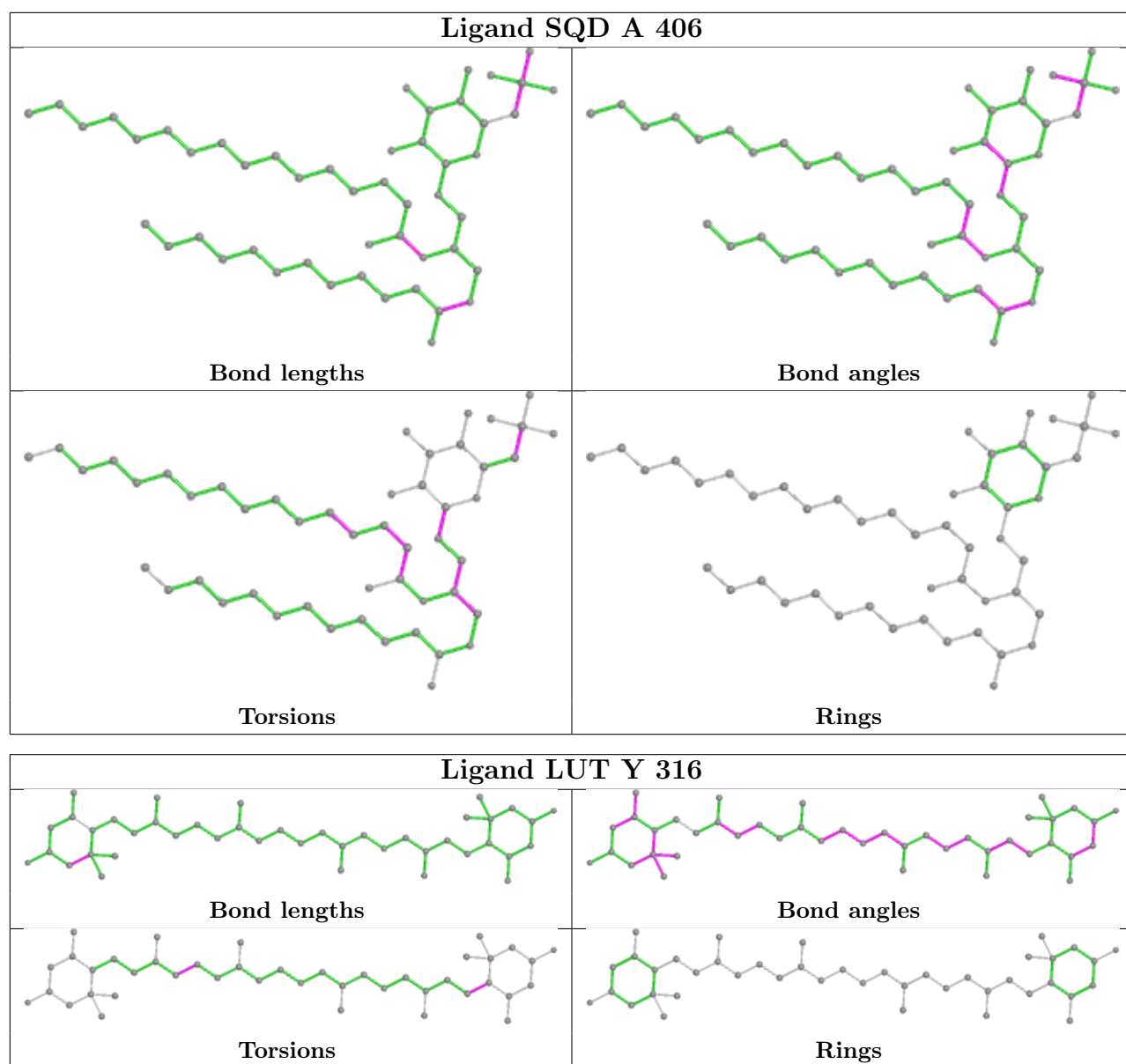


Rings

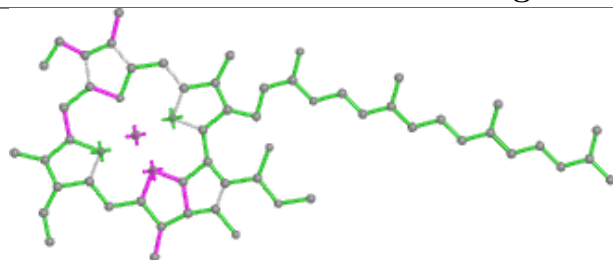


Ligand CLA S 603

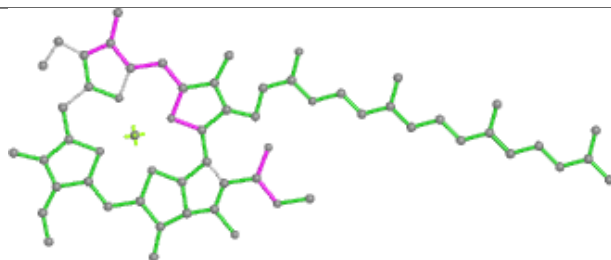




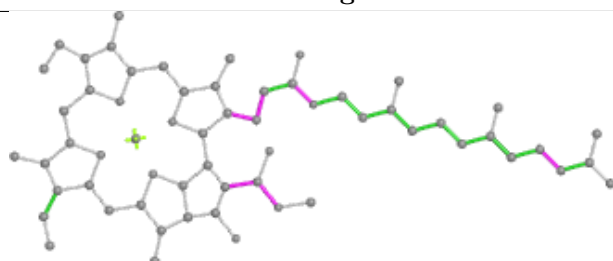
Ligand CLA G 611



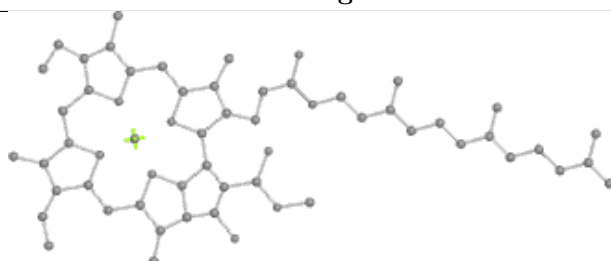
Bond lengths



Bond angles

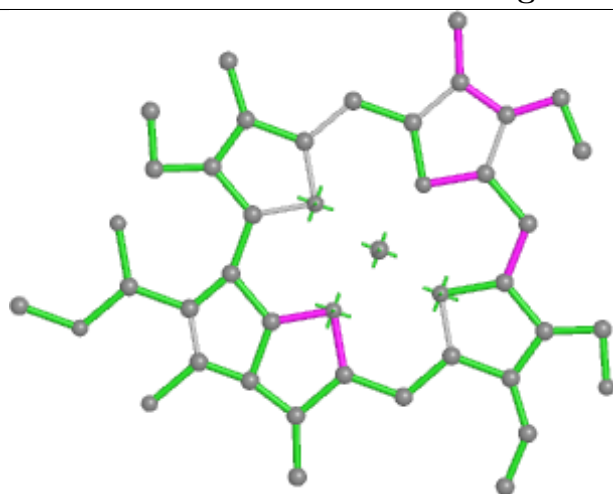


Torsions

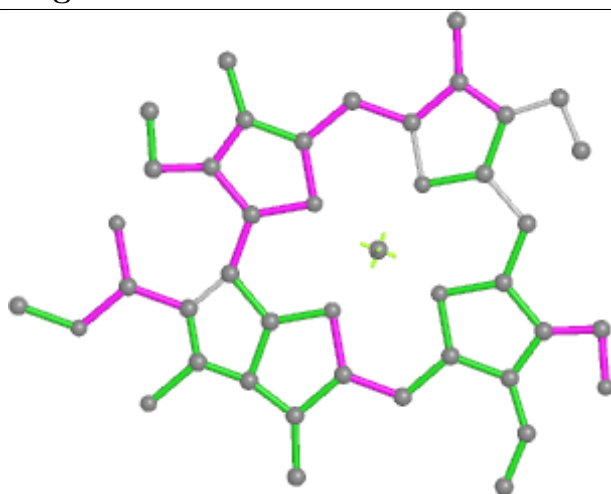


Rings

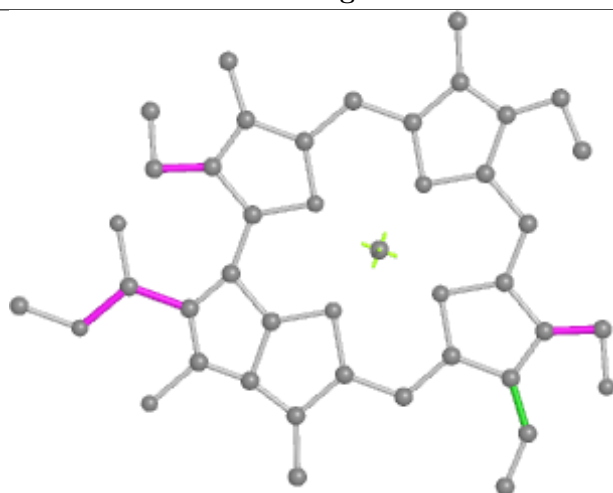
Ligand CHL g 606



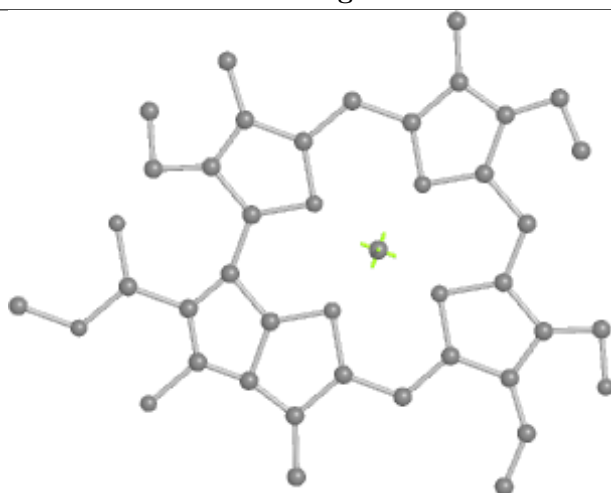
Bond lengths



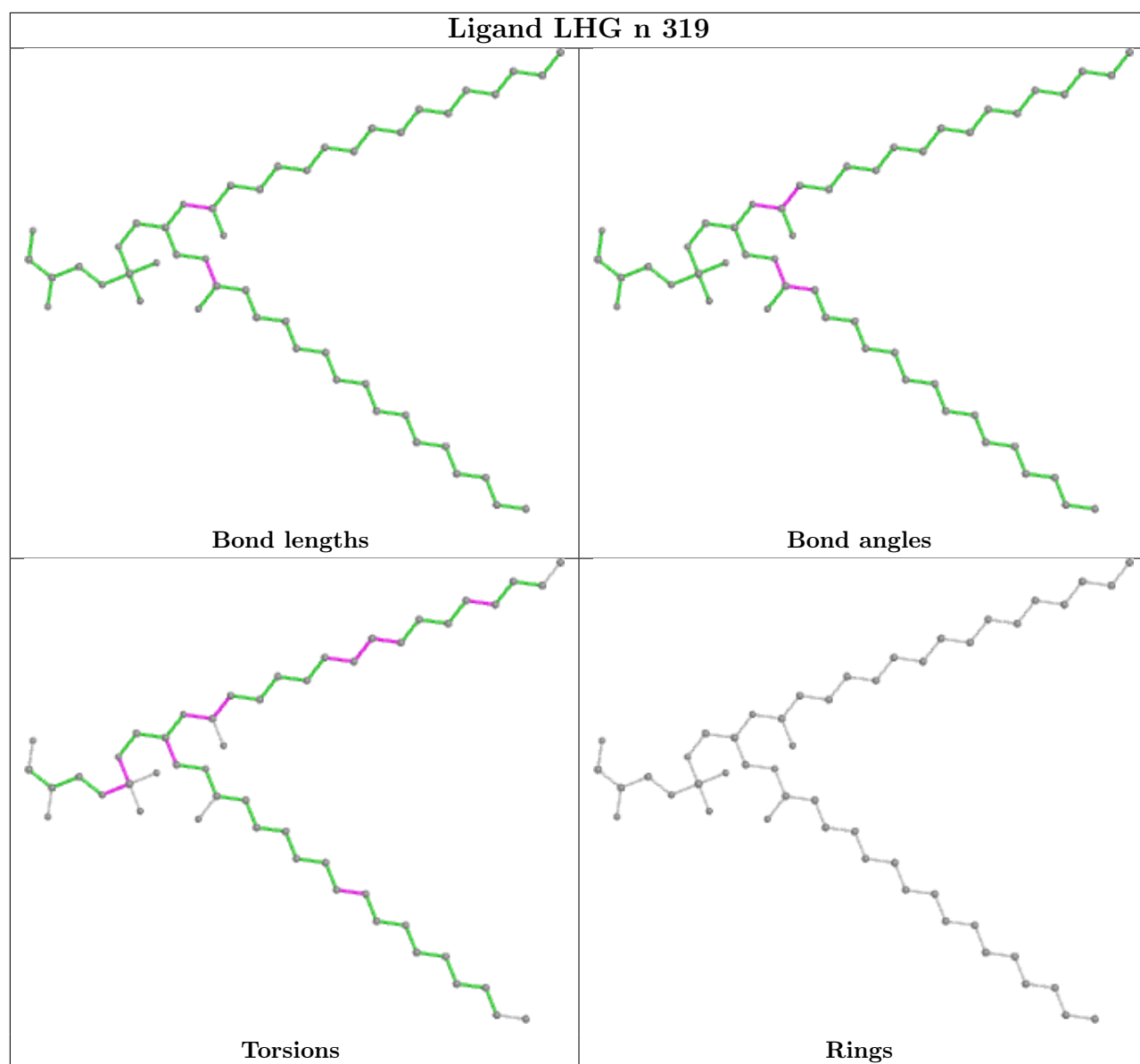
Bond angles

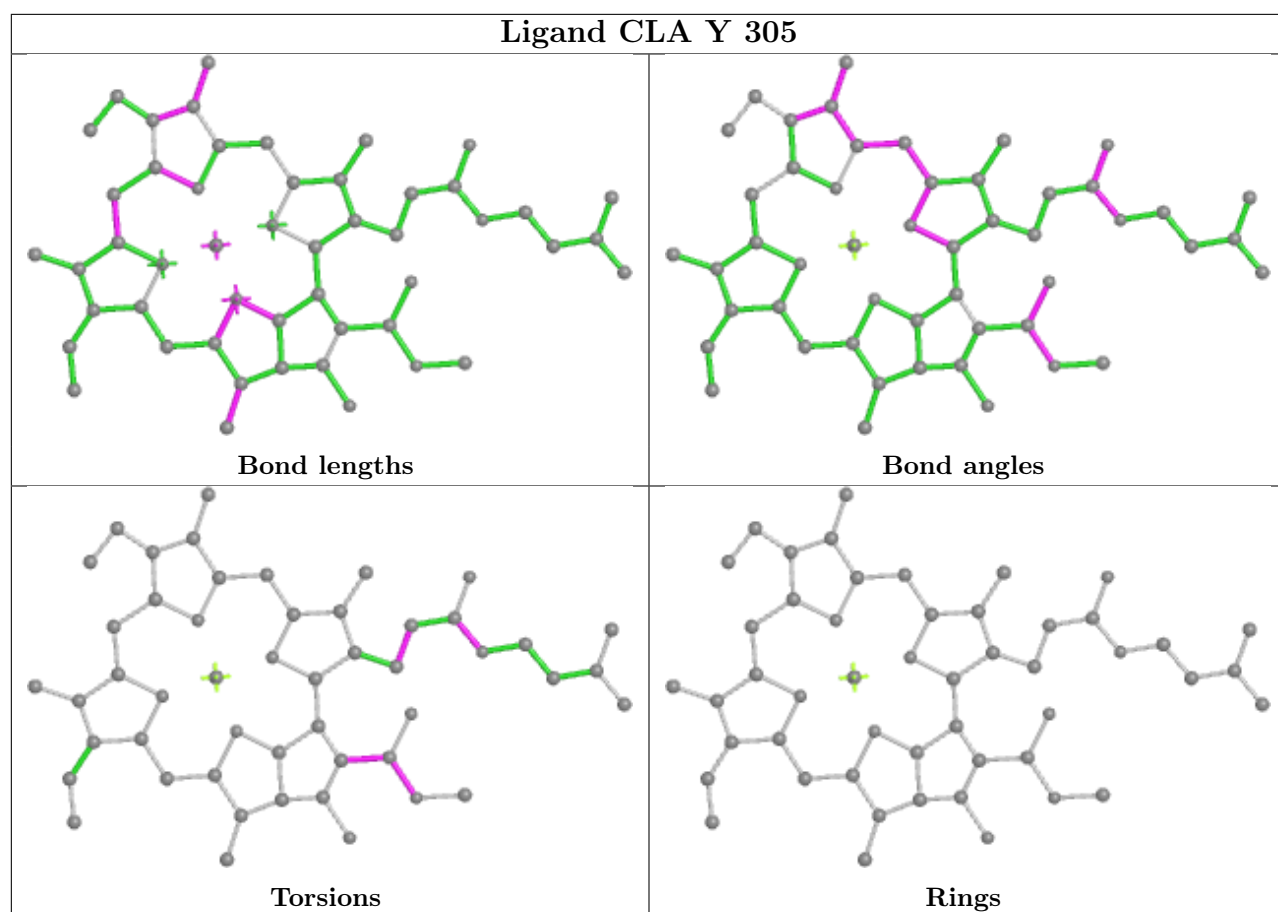


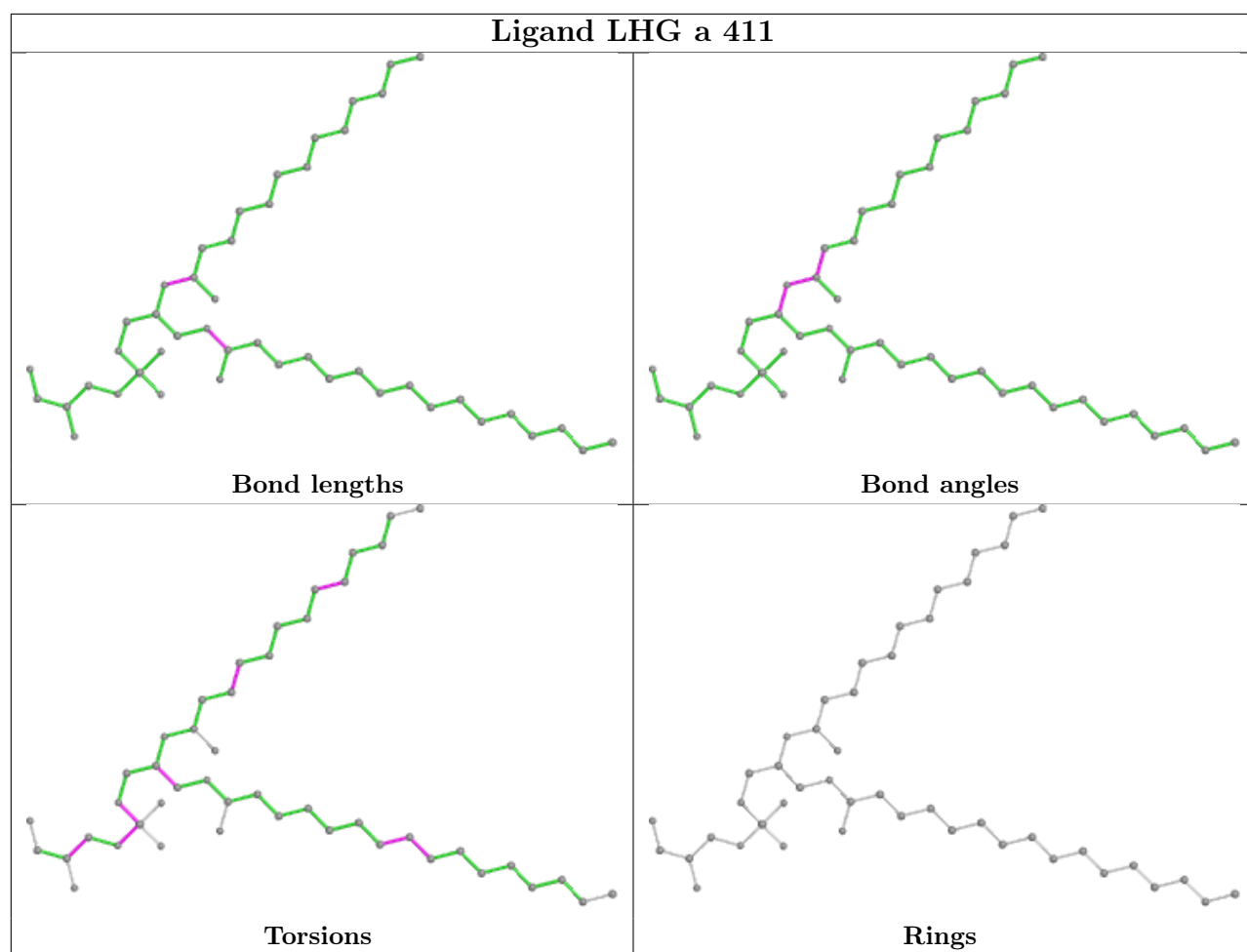
Torsions



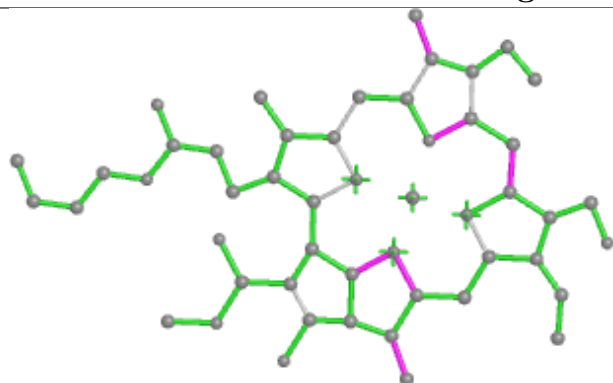
Rings



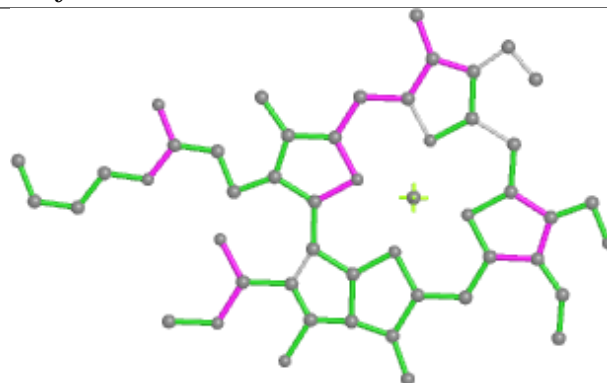




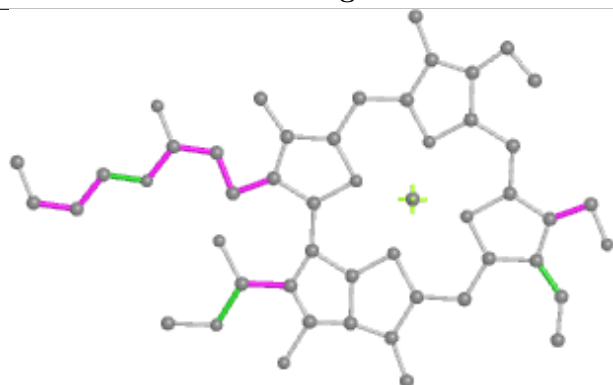
Ligand CHL y 307



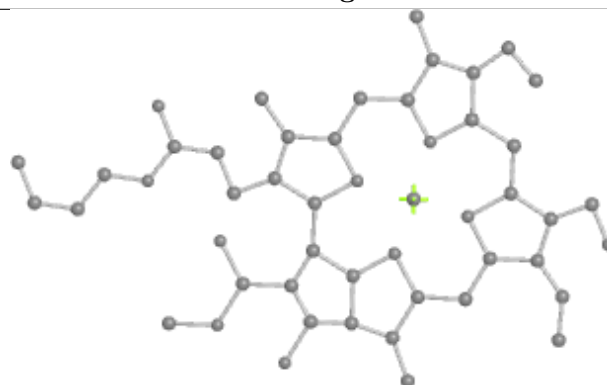
Bond lengths



Bond angles

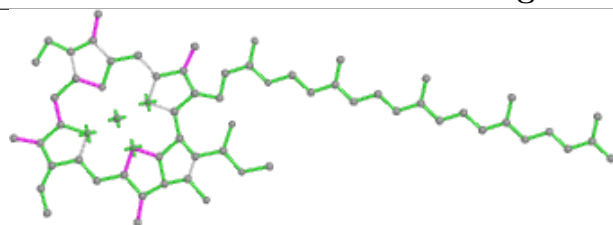


Torsions

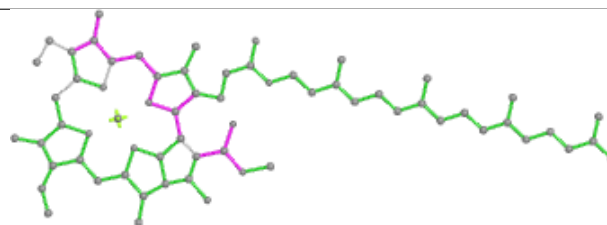


Rings

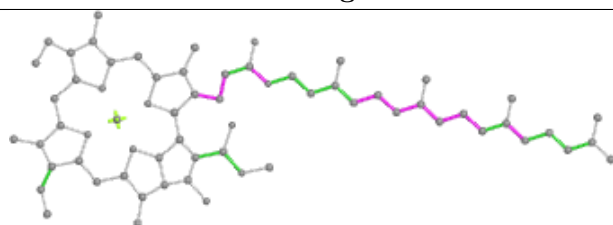
Ligand CLA b 612



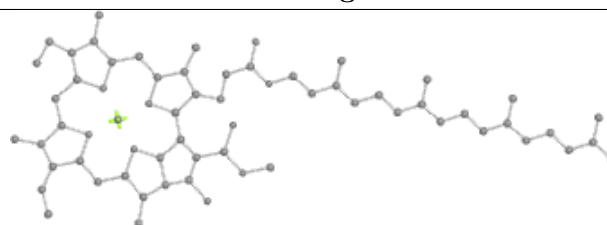
Bond lengths



Bond angles

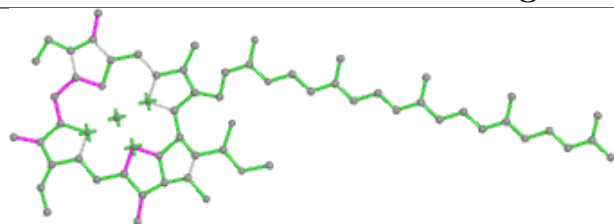


Torsions

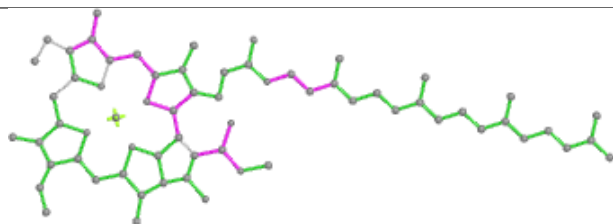


Rings

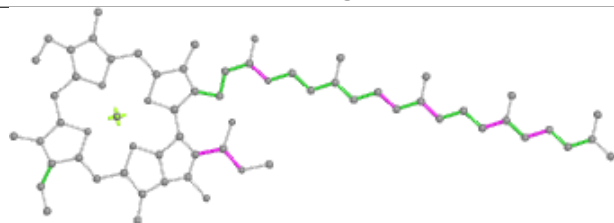
Ligand CLA c 508



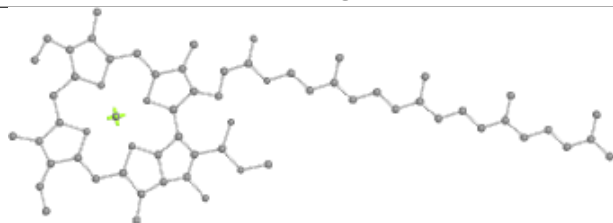
Bond lengths



Bond angles

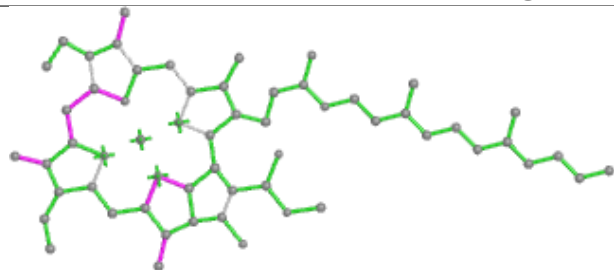


Torsions

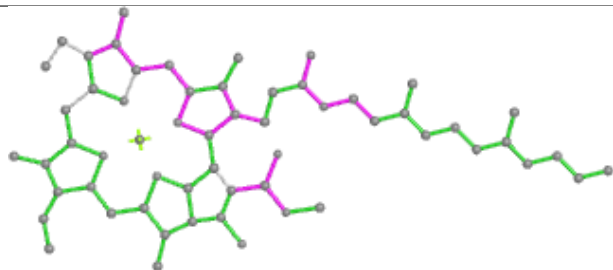


Rings

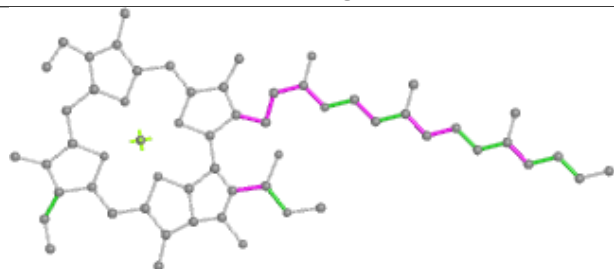
Ligand CLA c 505



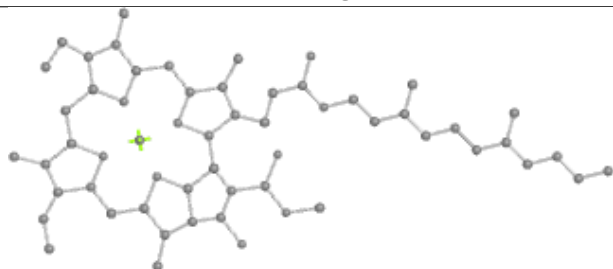
Bond lengths



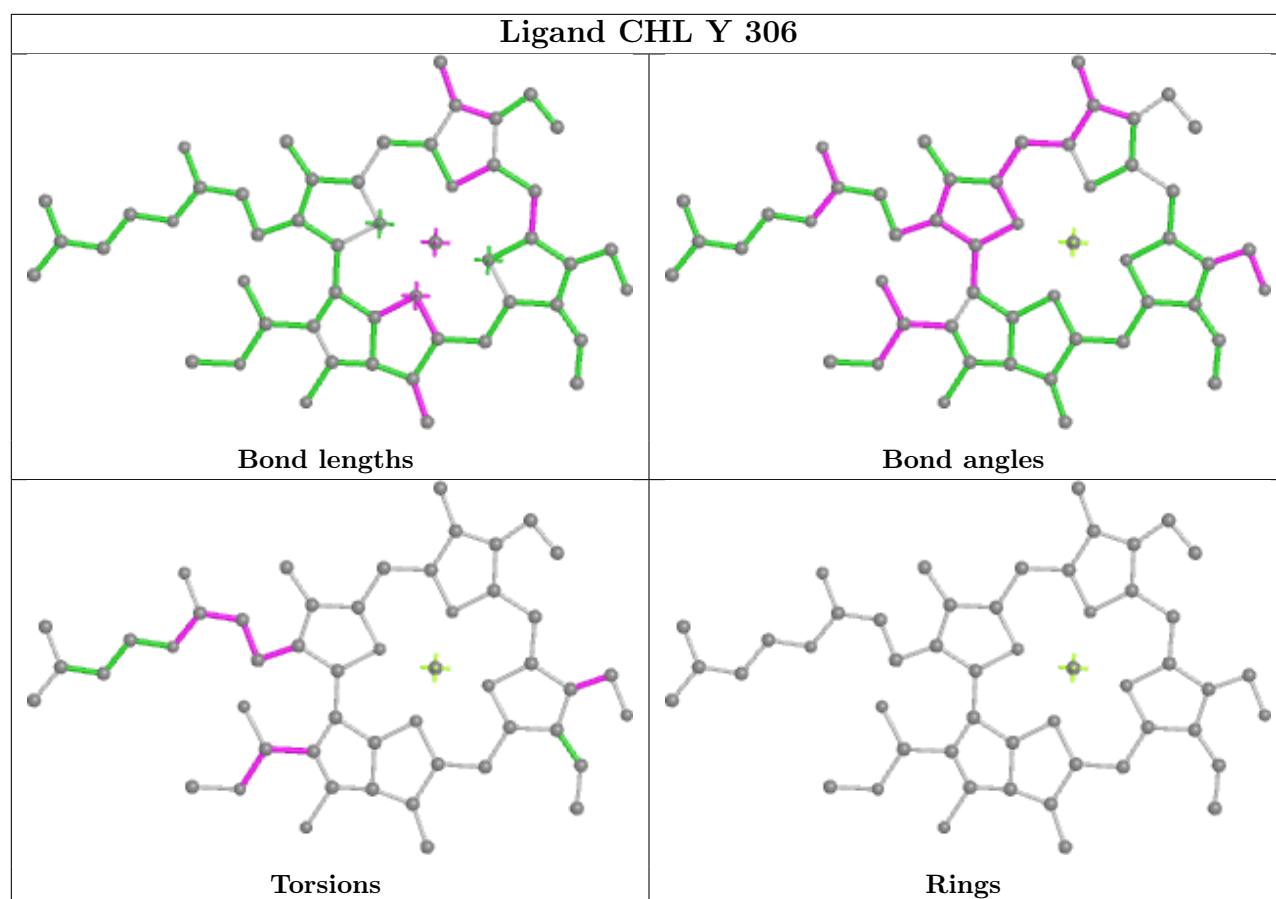
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

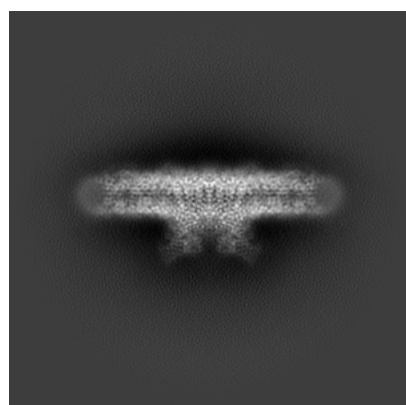
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63167. These allow visual inspection of the internal detail of the map and identification of artifacts.

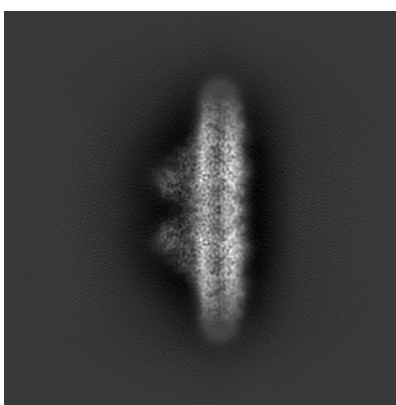
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

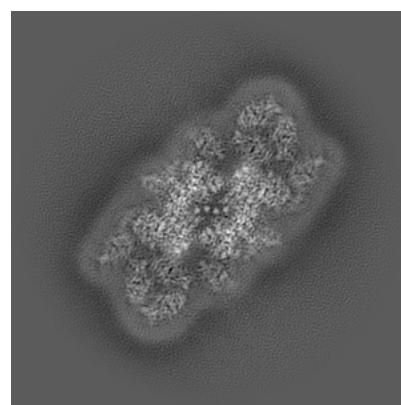
6.1.1 Primary map



X



Y

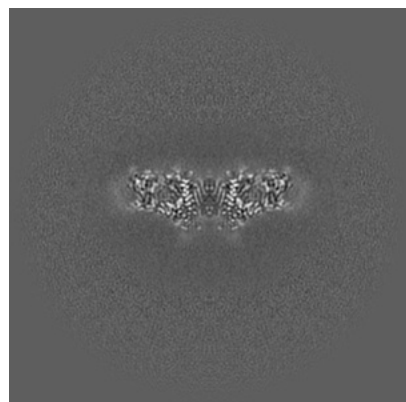


Z

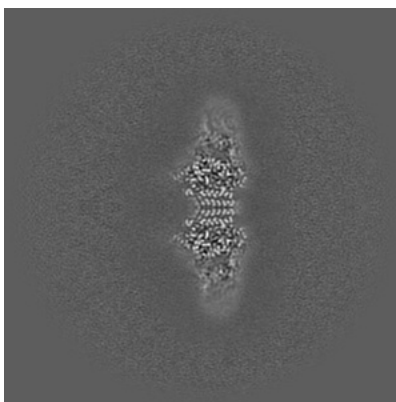
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

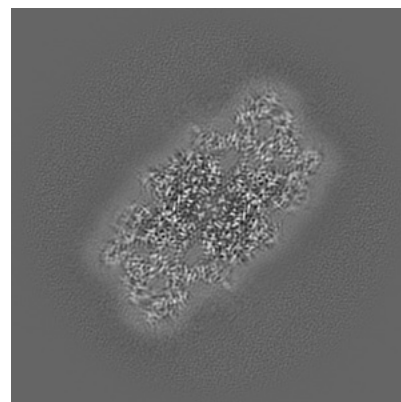
6.2.1 Primary map



X Index: 200



Y Index: 200

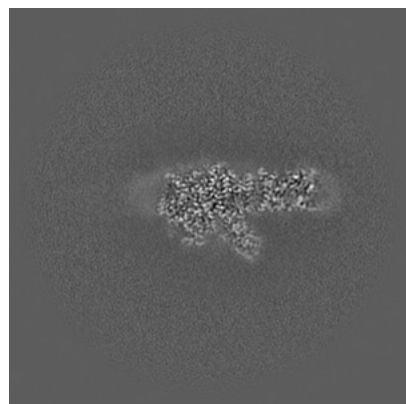


Z Index: 200

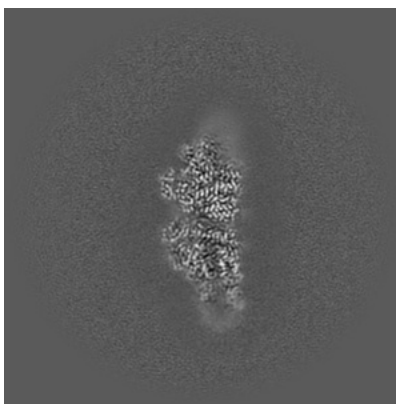
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

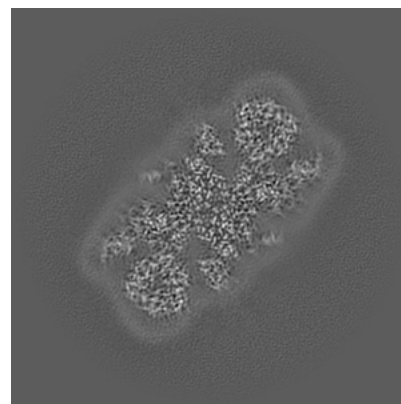
6.3.1 Primary map



X Index: 236



Y Index: 177

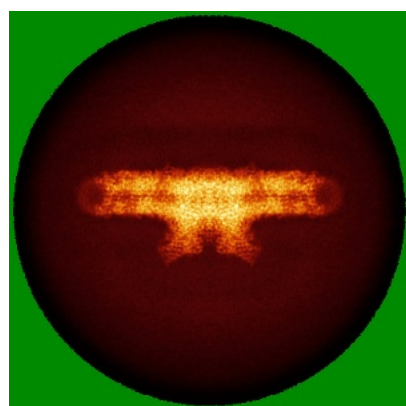


Z Index: 222

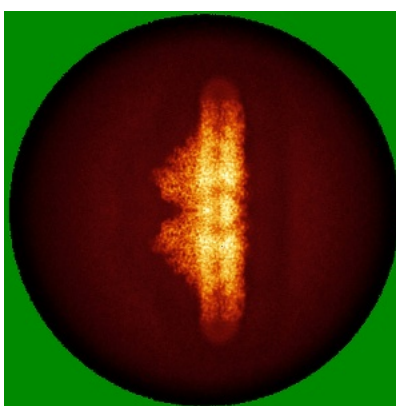
The images above show the largest variance slices of the map in three orthogonal directions.

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

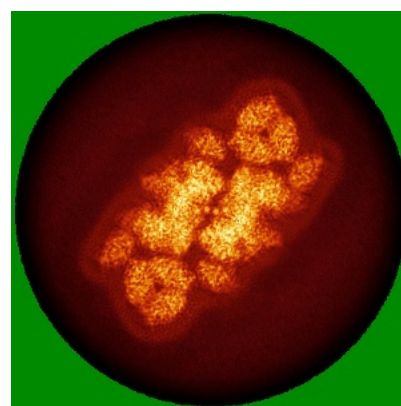
6.4.1 Primary map



X



Y

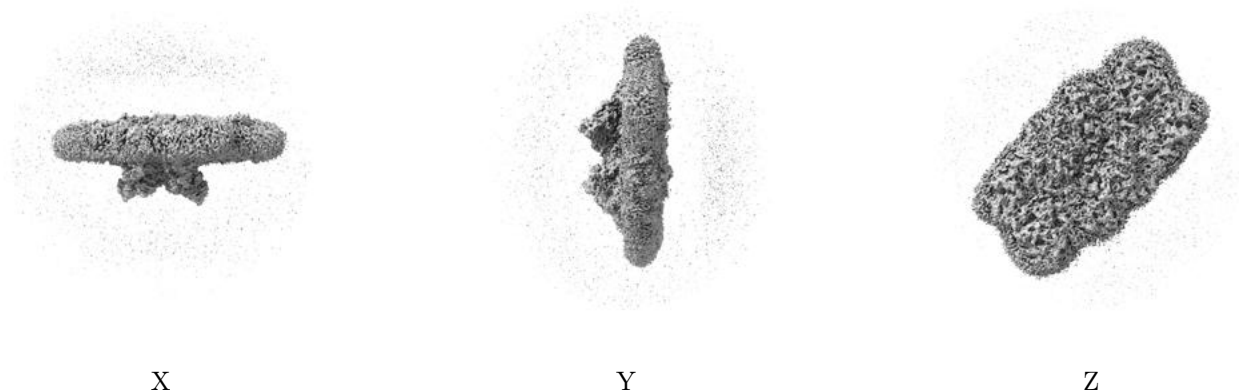


Z

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.

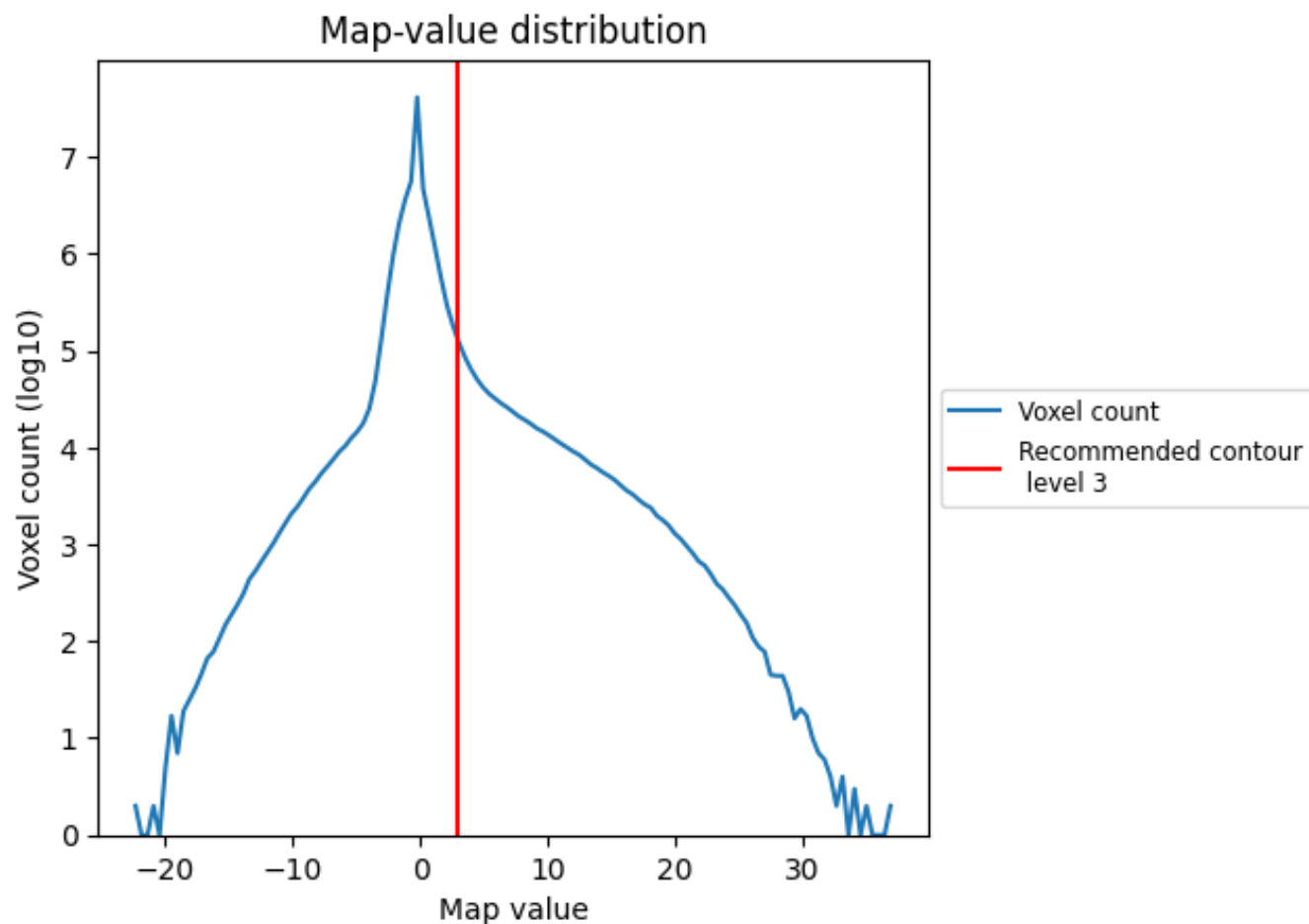
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

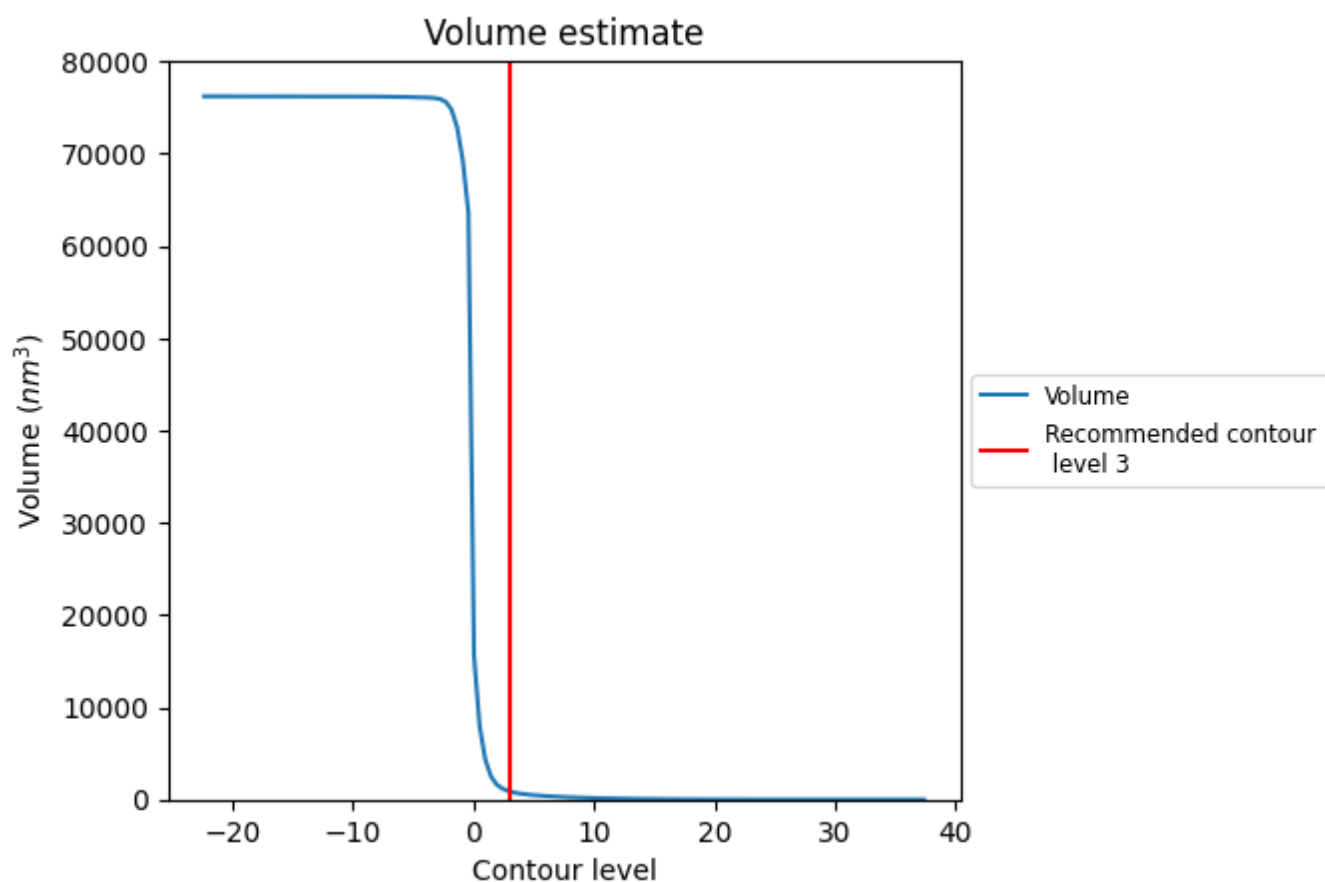
This section contains the results of statistical analysis of the map.

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.

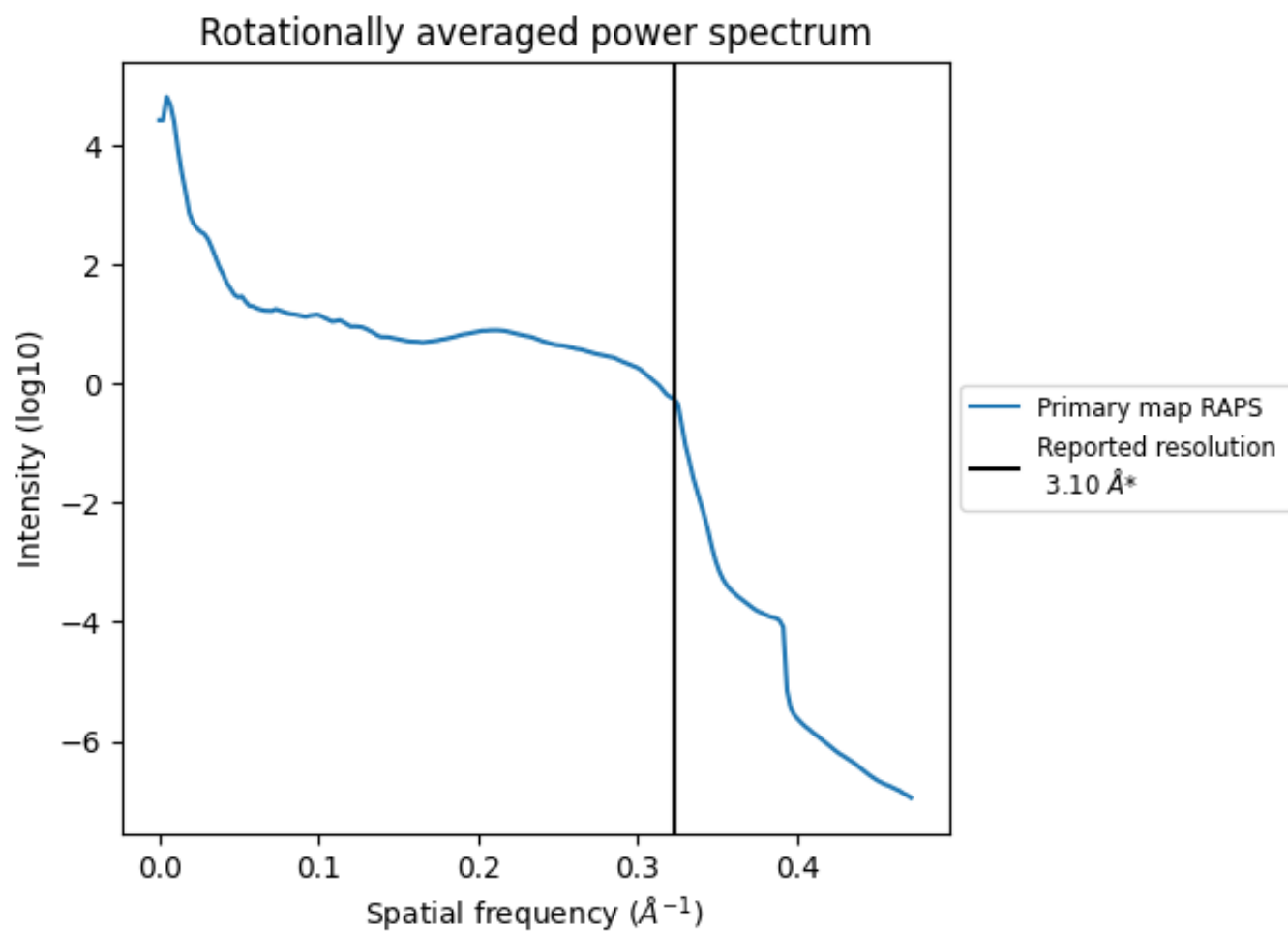
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 896 nm³; this corresponds to an approximate mass of 809 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 0.323 Å⁻¹

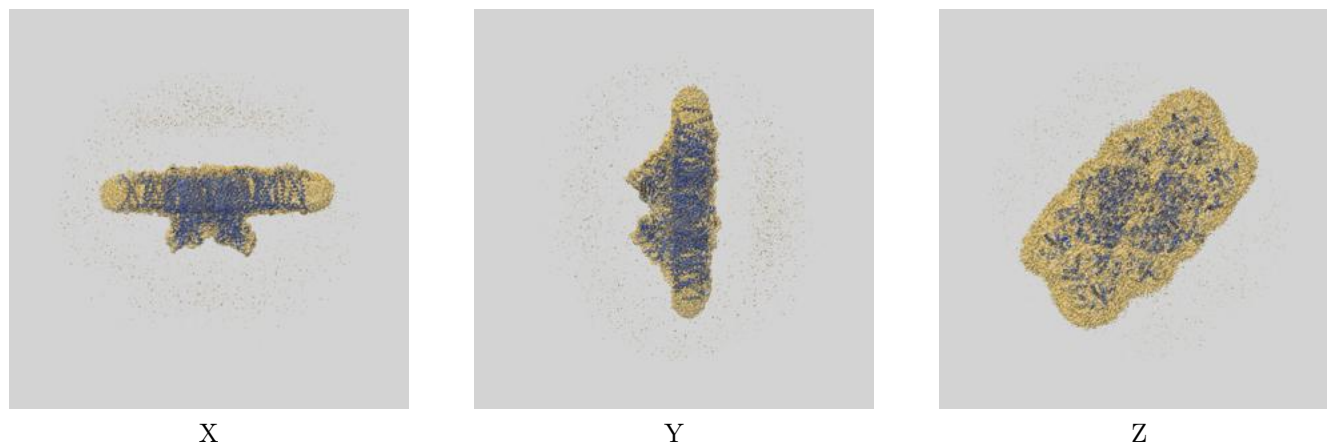
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

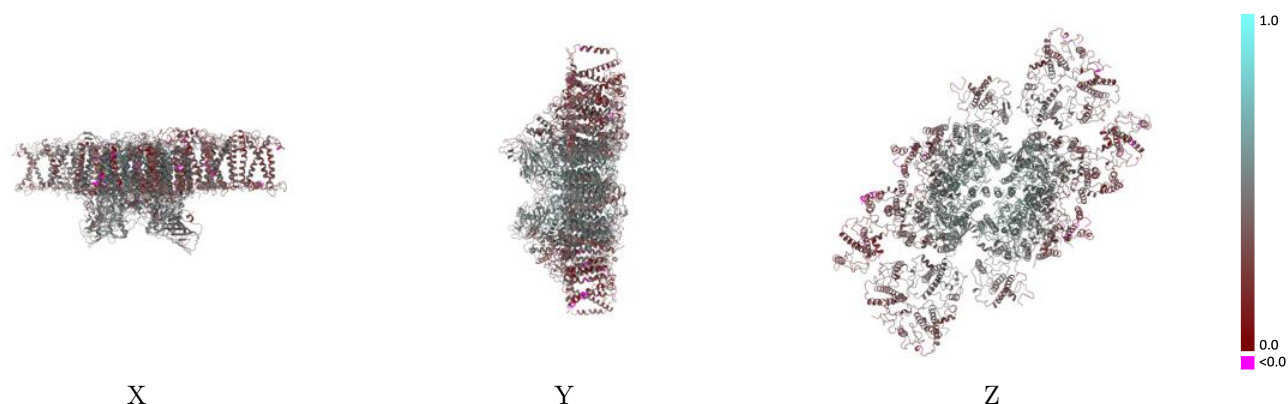
This section contains information regarding the fit between EMDB map EMD-63167 and PDB model 9LK4. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



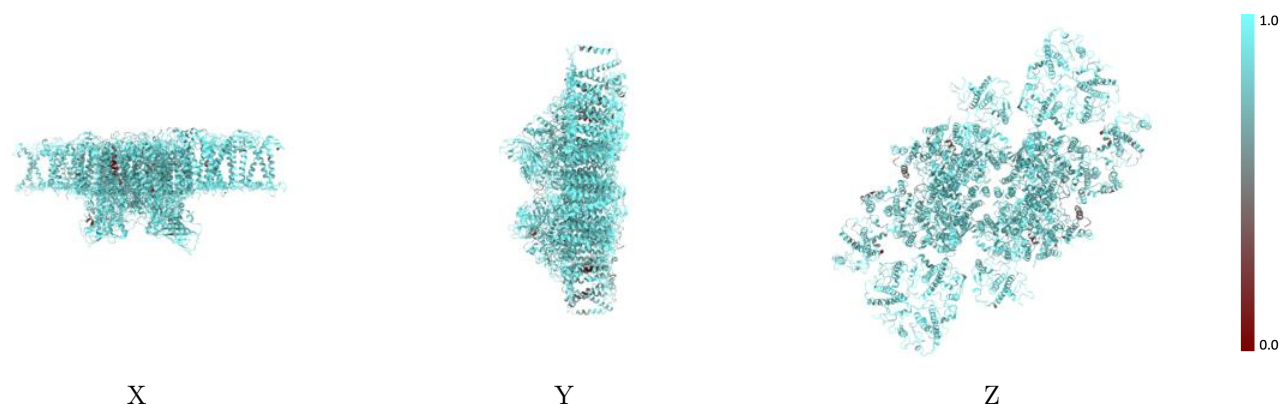
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



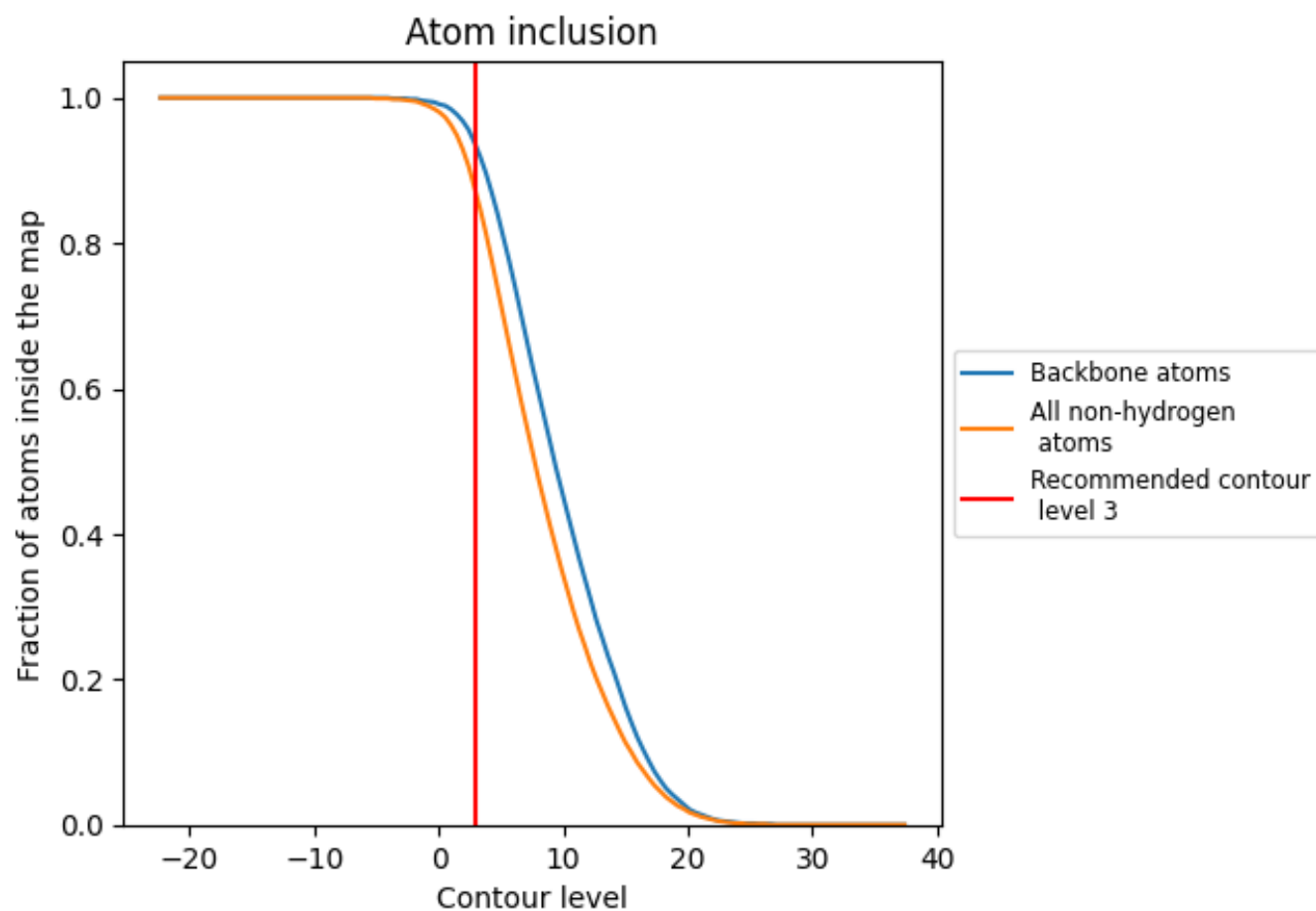
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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	 0.8680	 0.4220
A	 0.9160	 0.4940
B	 0.9350	 0.5310
C	 0.8450	 0.3820
D	 0.9130	 0.4760
E	 0.8370	 0.2940
F	 0.8050	 0.2910
G	 0.8560	 0.3620
H	 0.9180	 0.4740
I	 0.9260	 0.5020
J	 0.4020	 0.1440
K	 0.7800	 0.3440
L	 0.9250	 0.5530
M	 0.8810	 0.5120
N	 0.8230	 0.3550
O	 0.8600	 0.4430
R	 0.8590	 0.4150
S	 0.7930	 0.2840
T	 0.9260	 0.5410
U	 0.5770	 0.4010
W	 0.8340	 0.4490
X	 0.7830	 0.3340
Y	 0.8870	 0.4450
Z	 0.7420	 0.2760
a	 0.9270	 0.5010
b	 0.9380	 0.5300
c	 0.8470	 0.3790
d	 0.9030	 0.4730
e	 0.8400	 0.3080
f	 0.8640	 0.2750
g	 0.8540	 0.3540
h	 0.9260	 0.4690
i	 0.9340	 0.5030
j	 0.4530	 0.1240
k	 0.7680	 0.3350



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Chain	Atom inclusion	Q-score
l	 0.9310	 0.5420
m	 0.9120	 0.5190
n	 0.8240	 0.3470
o	 0.8660	 0.4500
r	 0.8560	 0.4050
s	 0.7940	 0.2790
t	 0.9410	 0.5460
u	 0.5600	 0.3730
w	 0.8300	 0.4500
x	 0.8090	 0.3340
y	 0.8930	 0.4490
z	 0.6970	 0.1910