



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 03:44 am GMT

PDB ID : 8C29  
EMDB ID : EMD-16389  
Title : Cryo-EM structure of photosystem II C2S2 supercomplex from Norway spruce (Picea abies) at 2.8 Angstrom resolution  
Authors : Kopecny, D.; Semchonok, D.A.; Kouril, R.  
Deposited on : 2022-12-21  
Resolution : 2.79 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

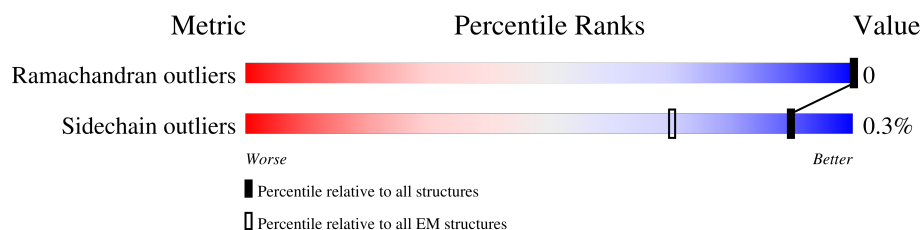
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

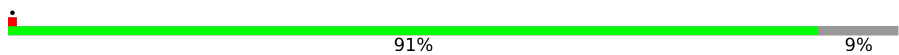
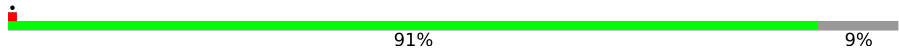
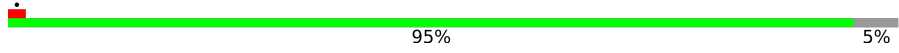
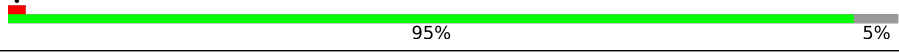
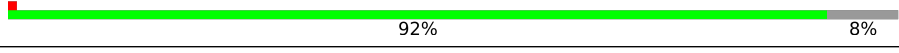
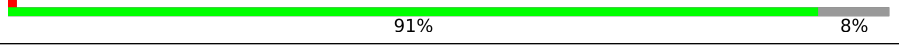
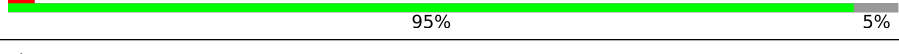
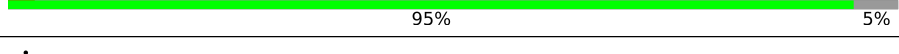

The reported resolution of this entry is 2.79 Å.

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





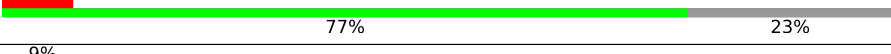

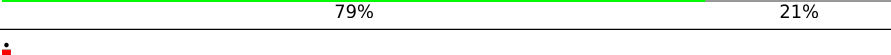
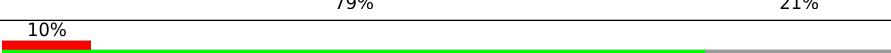
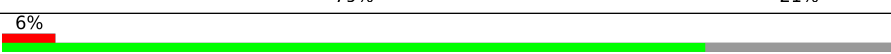
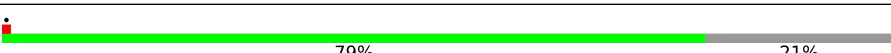


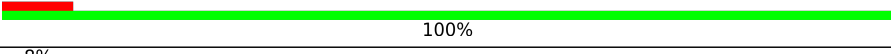
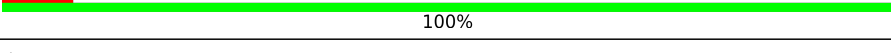


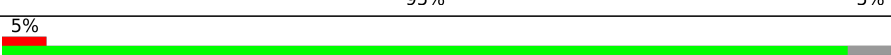
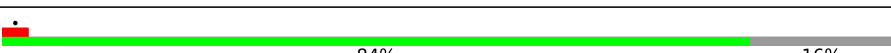


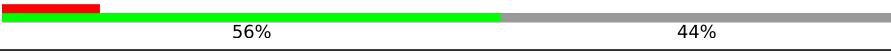


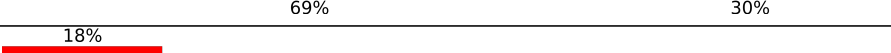



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	
5	E	83	

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Mol	Chain	Length	Quality of chain	
5	e	83	5% 	78% 22%
6	F	39	5% 	77% 23%
6	f	39	8% 	77% 23%
7	G	275	9% 	79% 21%
7	N	275	5% 	79% 21%
7	Y	275		79% 21%
7	g	275	10% 	79% 21%
7	n	275	6% 	79% 21%
7	y	275		79% 21%
8	H	75		81% 17%
8	h	75		81% 17%
9	I	36	8% 	100%
9	i	36	8% 	100%
10	K	59		63% 37%
10	k	59		63% 37%
11	L	38	5% 	95% 5%
11	l	38	5% 	95% 5%
12	M	37		84% 16%
12	m	37	5% 	84% 16%
13	O	341	10% 	56% 44%
13	o	341	11% 	56% 44%
14	R	300		73% 27%
14	r	300	5% 	73% 27%
15	S	303	18% 	69% 30%
15	s	303	18% 	69% 30%

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Mol	Chain	Length	Quality of chain
16	T	35	
16	t	35	
17	U	133	
17	u	133	
18	V	33	
18	v	33	
19	W	146	
19	w	146	
20	X	129	
20	x	129	
21	Z	62	
21	z	62	

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	402	X	-	-	-
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	406	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	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	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	G	602	X	-	-	-
23	CLA	G	603	X	-	-	-
23	CLA	G	604	X	-	-	-
23	CLA	G	610	X	-	-	-
23	CLA	G	611	X	-	-	-
23	CLA	G	612	X	-	-	-
23	CLA	G	613	X	-	-	-
23	CLA	G	614	X	-	-	-
23	CLA	N	602	X	-	-	-
23	CLA	N	603	X	-	-	-
23	CLA	N	604	X	-	-	-
23	CLA	N	610	X	-	-	-
23	CLA	N	611	X	-	-	-
23	CLA	N	612	X	-	-	-
23	CLA	N	613	X	-	-	-
23	CLA	N	614	X	-	-	-
23	CLA	R	601	X	-	-	-
23	CLA	R	602	X	-	-	-
23	CLA	R	603	X	-	-	-
23	CLA	R	604	X	-	-	-
23	CLA	R	608	X	-	-	-
23	CLA	R	609	X	-	-	-
23	CLA	R	610	X	-	-	-
23	CLA	R	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	R	612	X	-	-	-
23	CLA	S	602	X	-	-	-
23	CLA	S	603	X	-	-	-
23	CLA	S	604	X	-	-	-
23	CLA	S	608	X	-	-	-
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	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	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	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	405	X	-	-	-
23	CLA	d	406	X	-	-	-
23	CLA	g	602	X	-	-	-
23	CLA	g	603	X	-	-	-
23	CLA	g	604	X	-	-	-
23	CLA	g	610	X	-	-	-
23	CLA	g	611	X	-	-	-
23	CLA	g	612	X	-	-	-
23	CLA	g	613	X	-	-	-
23	CLA	g	614	X	-	-	-
23	CLA	n	602	X	-	-	-
23	CLA	n	603	X	-	-	-
23	CLA	n	604	X	-	-	-
23	CLA	n	610	X	-	-	-
23	CLA	n	611	X	-	-	-
23	CLA	n	612	X	-	-	-
23	CLA	n	613	X	-	-	-
23	CLA	n	614	X	-	-	-
23	CLA	r	601	X	-	-	-
23	CLA	r	602	X	-	-	-
23	CLA	r	603	X	-	-	-
23	CLA	r	604	X	-	-	-
23	CLA	r	608	X	-	-	-
23	CLA	r	609	X	-	-	-
23	CLA	r	610	X	-	-	-
23	CLA	r	611	X	-	-	-
23	CLA	r	612	X	-	-	-
23	CLA	s	602	X	-	-	-
23	CLA	s	603	X	-	-	-
23	CLA	s	604	X	-	-	-
23	CLA	s	608	X	-	-	-
23	CLA	s	609	X	-	-	-
23	CLA	s	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	s	611	X	-	-	-
23	CLA	s	612	X	-	-	-
23	CLA	s	613	X	-	-	-
23	CLA	y	304	X	-	-	-
23	CLA	y	305	X	-	-	-
23	CLA	y	306	X	-	-	-
23	CLA	y	311	X	-	-	-
23	CLA	y	312	X	-	-	-
23	CLA	y	313	X	-	-	-
23	CLA	y	314	X	-	-	-
23	CLA	y	315	X	-	-	-
39	CHL	G	601	X	-	-	-
39	CHL	G	605	X	-	-	-
39	CHL	G	606	X	-	-	-
39	CHL	G	607	X	-	-	-
39	CHL	G	608	X	-	-	-
39	CHL	G	609	X	-	-	-
39	CHL	G	620	X	-	-	-
39	CHL	N	601	X	-	-	-
39	CHL	N	605	X	-	-	-
39	CHL	N	606	X	-	-	-
39	CHL	N	607	X	-	-	-
39	CHL	N	608	X	-	-	-
39	CHL	N	609	X	-	-	-
39	CHL	R	605	X	-	-	-
39	CHL	R	606	X	-	-	-
39	CHL	R	607	X	-	-	-
39	CHL	S	601	X	-	-	-
39	CHL	S	605	X	-	-	-
39	CHL	S	606	X	-	-	-
39	CHL	S	607	X	-	-	-
39	CHL	Y	302	X	-	-	-
39	CHL	Y	306	X	-	-	-
39	CHL	Y	307	X	-	-	-
39	CHL	Y	308	X	-	-	-
39	CHL	Y	309	X	-	-	-
39	CHL	g	601	X	-	-	-
39	CHL	g	605	X	-	-	-
39	CHL	g	606	X	-	-	-
39	CHL	g	607	X	-	-	-
39	CHL	g	608	X	-	-	-
39	CHL	g	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	g	619	X	-	-	-
39	CHL	n	601	X	-	-	-
39	CHL	n	605	X	-	-	-
39	CHL	n	606	X	-	-	-
39	CHL	n	607	X	-	-	-
39	CHL	n	608	X	-	-	-
39	CHL	n	609	X	-	-	-
39	CHL	r	605	X	-	-	-
39	CHL	r	606	X	-	-	-
39	CHL	r	607	X	-	-	-
39	CHL	s	601	X	-	-	-
39	CHL	s	605	X	-	-	-
39	CHL	s	606	X	-	-	-
39	CHL	s	607	X	-	-	-
39	CHL	y	303	X	-	-	-
39	CHL	y	307	X	-	-	-
39	CHL	y	308	X	-	-	-
39	CHL	y	309	X	-	-	-
39	CHL	y	310	X	-	-	-

## 2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 71174 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	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		
1	a	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	PHE	LEU	conflict	UNP P50155
a	295	PHE	LEU	conflict	UNP P50155

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		
2	b	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	464	PHE	SER	conflict	UNP R4ZGX1
b	464	PHE	SER	conflict	UNP R4ZGX1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		
3	c	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	175	LEU	PRO	conflict	UNP R4ZGZ0
C	433	LEU	PRO	conflict	UNP R4ZGZ0
c	175	LEU	PRO	conflict	UNP R4ZGZ0
c	433	LEU	PRO	conflict	UNP R4ZGZ0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	337	Total	C	N	O	S	0	0
			2686	1781	439	455	11		
4	d	337	Total	C	N	O	S	0	0
			2685	1781	439	454	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	280	LEU	SER	conflict	UNP R4ZGX6
D	312	PHE	SER	conflict	UNP R4ZGX6
d	280	LEU	SER	conflict	UNP R4ZGX6
d	312	PHE	SER	conflict	UNP R4ZGX6

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total	C	N	O	0	0
			537	353	84	100		
5	e	65	Total	C	N	O	0	0
			537	353	84	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			240	160	41	38	1		
6	f	30	Total	C	N	O	S	0	0
			240	160	41	38	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	N	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	Y	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	g	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	n	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	y	218	Total 1659	C 1080	N 268	O 305	S 6	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	224	ILE	LEU	conflict	UNP Q40771
G	249	LEU	ILE	conflict	UNP Q40771
G	261	ASN	THR	conflict	UNP Q40771
N	224	ILE	LEU	conflict	UNP Q40771
N	249	LEU	ILE	conflict	UNP Q40771
N	261	ASN	THR	conflict	UNP Q40771
Y	224	ILE	LEU	conflict	UNP Q40771
Y	249	LEU	ILE	conflict	UNP Q40771
Y	261	ASN	THR	conflict	UNP Q40771
g	224	ILE	LEU	conflict	UNP Q40771
g	249	LEU	ILE	conflict	UNP Q40771
g	261	ASN	THR	conflict	UNP Q40771
n	224	ILE	LEU	conflict	UNP Q40771
n	249	LEU	ILE	conflict	UNP Q40771
n	261	ASN	THR	conflict	UNP Q40771
y	224	ILE	LEU	conflict	UNP Q40771
y	249	LEU	ILE	conflict	UNP Q40771
y	261	ASN	THR	conflict	UNP Q40771

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	62	Total 462	C 305	N 71	O 84	S 2	0	0
8	h	62	Total 462	C 305	N 71	O 84	S 2	0	0



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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	36	Total	C	N	O	S	0	0
			297	202	46	48	1		
9	i	36	Total	C	N	O	S	0	0
			297	202	46	48	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	N	O	S	0	0
			302	211	43	47	1		
10	k	37	Total	C	N	O	S	0	0
			302	211	43	47	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	31	PHE	SER	conflict	UNP R4ZGX8
K	45	PHE	SER	conflict	UNP R4ZGX8
k	31	PHE	SER	conflict	UNP R4ZGX8
k	45	PHE	SER	conflict	UNP R4ZGX8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	36	Total	C	N	O		0	0
			302	200	49	53			
11	l	36	Total	C	N	O		0	0
			302	200	49	53			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O		0	0
			238	165	33	40			
12	m	31	Total	C	N	O		0	0
			238	165	33	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	25	LEU	PRO	conflict	UNP A2CHR7

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Chain	Residue	Modelled	Actual	Comment	Reference
m	25	LEU	PRO	conflict	UNP A2CHR7

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		
13	o	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		
14	r	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	54	THR	PRO	conflict	UNP A9NKKX0
R	56	ALA	-	insertion	UNP A9NKKX0
R	57	VAL	-	insertion	UNP A9NKKX0
R	58	ALA	-	insertion	UNP A9NKKX0
R	59	LYS	-	insertion	UNP A9NKKX0
R	60	PRO	-	insertion	UNP A9NKKX0
R	61	LYS	-	insertion	UNP A9NKKX0
R	62	THR	-	insertion	UNP A9NKKX0
R	63	LYS	-	insertion	UNP A9NKKX0
R	64	ALA	-	insertion	UNP A9NKKX0
R	65	VAL	-	insertion	UNP A9NKKX0
R	66	ALA	-	insertion	UNP A9NKKX0
R	67	LYS	-	insertion	UNP A9NKKX0
r	54	THR	PRO	conflict	UNP A9NKKX0
r	56	ALA	-	insertion	UNP A9NKKX0
r	57	VAL	-	insertion	UNP A9NKKX0
r	58	ALA	-	insertion	UNP A9NKKX0
r	59	LYS	-	insertion	UNP A9NKKX0
r	60	PRO	-	insertion	UNP A9NKKX0
r	61	LYS	-	insertion	UNP A9NKKX0
r	62	THR	-	insertion	UNP A9NKKX0

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Chain	Residue	Modelled	Actual	Comment	Reference
r	63	LYS	-	insertion	UNP A9NKKX0
r	64	ALA	-	insertion	UNP A9NKKX0
r	65	VAL	-	insertion	UNP A9NKKX0
r	66	ALA	-	insertion	UNP A9NKKX0
r	67	LYS	-	insertion	UNP A9NKKX0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	211	Total	C	N	O	S	0	0
			1626	1067	261	294	4		
15	s	211	Total	C	N	O	S	0	0
			1626	1067	261	294	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	213	LEU	ALA	conflict	UNP A9NKM0
s	213	LEU	ALA	conflict	UNP A9NKM0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	31	Total	C	N	O	S	0	0
			254	177	36	40	1		
16	t	31	Total	C	N	O	S	0	0
			254	177	36	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	27	Total	C	N	O	S	0	0
			205	127	39	36	3		
17	u	27	Total	C	N	O	S	0	0
			205	127	39	36	3		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	31	Total	C	N	O	0	0
			228	151	37	40		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	v	31	Total	C	N	O	0	0
			228	151	37	40		

- Molecule 19 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	54	Total	C	N	O	S	0	0
			415	271	61	82	1		
19	w	54	Total	C	N	O	S	0	0
			415	271	61	82	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	98	MET	LEU	conflict	UNP A9NLC2
w	98	MET	LEU	conflict	UNP A9NLC2

- Molecule 20 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	34	Total	C	N	O	0	0
			226	146	37	43		
20	x	34	Total	C	N	O	0	0
			226	146	37	43		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	80	ALA	VAL	conflict	UNP A9NTS2
x	80	ALA	VAL	conflict	UNP A9NTS2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		
21	z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		

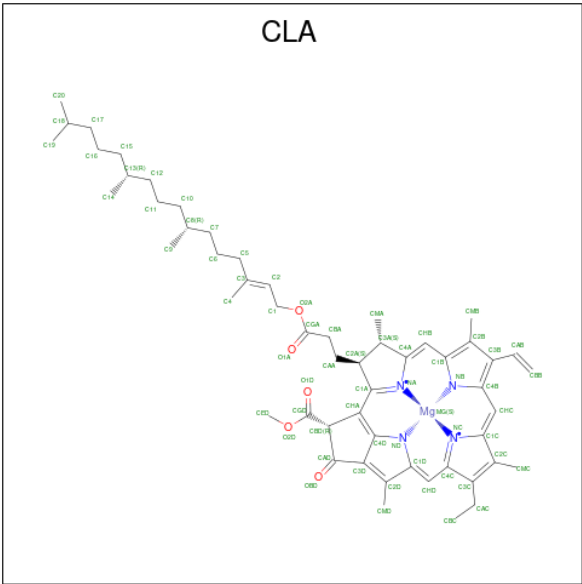
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	17	LEU	PHE	conflict	UNP R4ZGT1
z	17	LEU	PHE	conflict	UNP R4ZGT1

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C Mg N O 65 55 1 4 5	0
23	A	1	Total C Mg N O 65 55 1 4 5	0
23	A	1	Total C Mg N O 49 39 1 4 5	0
23	A	1	Total C Mg N O 60 50 1 4 5	0
23	B	1	Total C Mg N O 49 39 1 4 5	0
23	B	1	Total C Mg N O 65 55 1 4 5	0
23	B	1	Total C Mg N O 65 55 1 4 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	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 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 55	C 45	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 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	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 60	C 50	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 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 49	C 39	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	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	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 65	C 55	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 55	C 45	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 65	C 55	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	S	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	Y	1	Total 65	C 55	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 65	C 55	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 65	C 55	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 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 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 49	C 39	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 50	C 40	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

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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	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 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 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	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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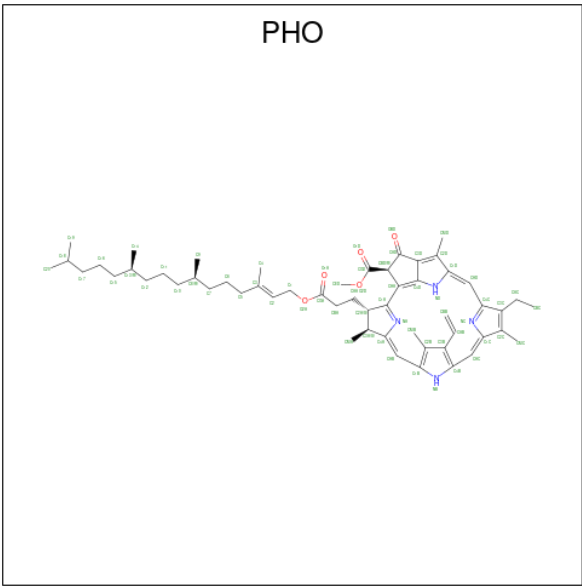
Mol	Chain	Residues	Atoms					AltConf
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	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 65	C 55	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 55	C 45	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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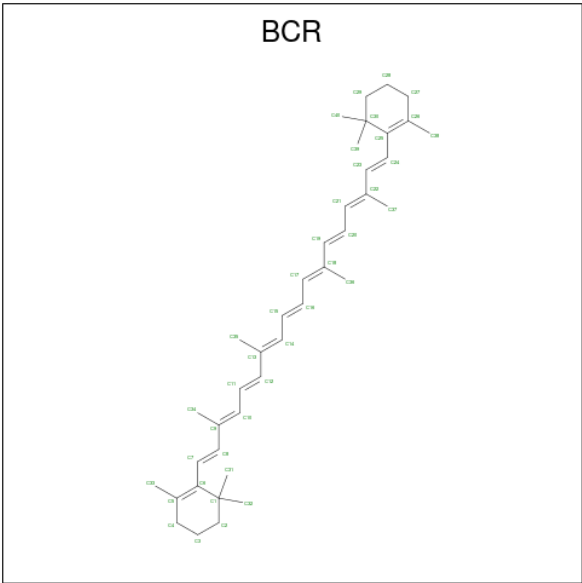
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	s	1	Total 65	C 55	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 65	C 55	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 65	C 55	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



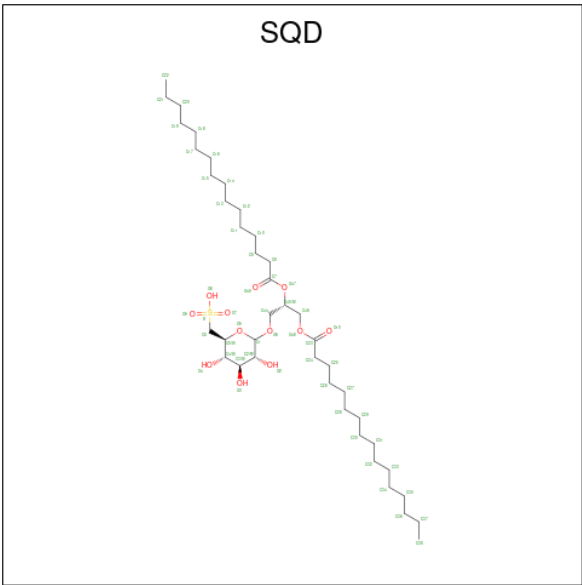
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



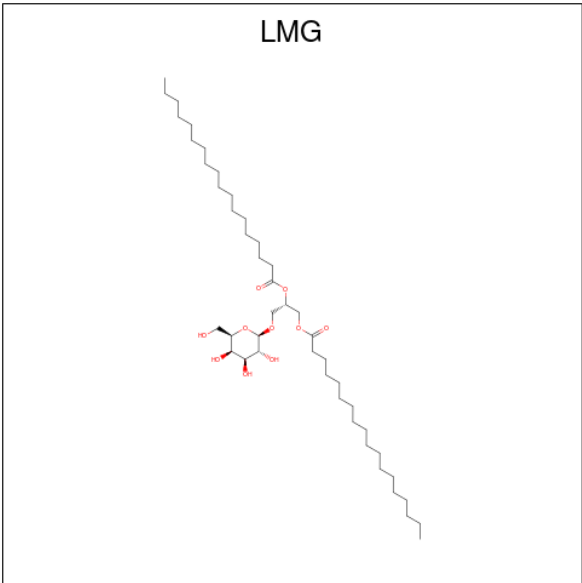
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 39 39	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	V	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 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	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	v	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



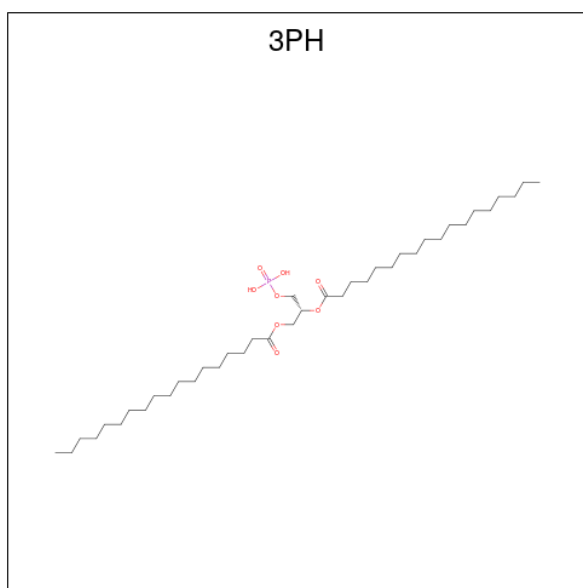
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	M	1	Total	C	O	S	0
			50	37	12	1	
26	a	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			53	43	10	
27	B	1	Total	C	O	0
			48	38	10	
27	B	1	Total	C	O	0
			49	39	10	
27	C	1	Total	C	O	0
			45	35	10	
27	D	1	Total	C	O	0
			36	26	10	
27	R	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			50	40	10	
27	c	1	Total	C	O	0
			46	36	10	
27	d	1	Total	C	O	0
			46	36	10	
27	r	1	Total	C	O	0
			51	41	10	
27	w	1	Total	C	O	0
			48	38	10	

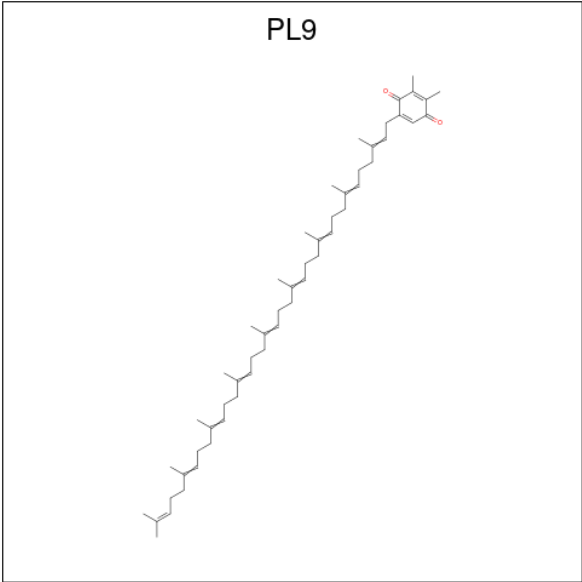
- Molecule 28 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).





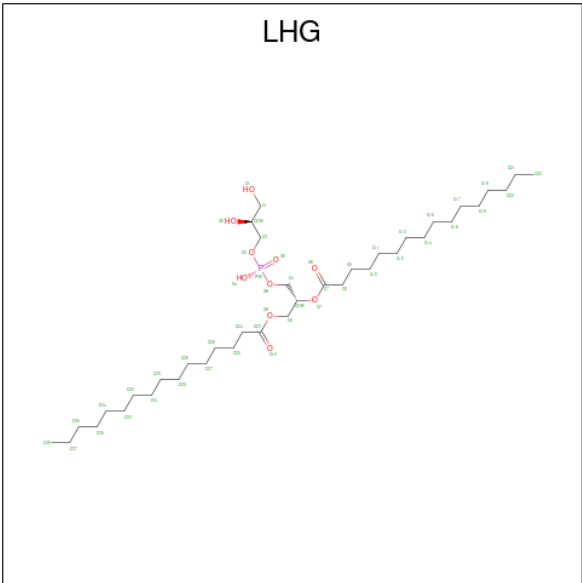
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	39	8	1	
28	C	1	Total	C	O	P	0
			48	39	8	1	
28	D	1	Total	C	O	P	0
			38	29	8	1	
28	L	1	Total	C	O	P	0
			41	32	8	1	
28	T	1	Total	C	O	P	0
			48	39	8	1	
28	W	1	Total	C	O	P	0
			46	37	8	1	
28	X	1	Total	C	O	P	0
			46	37	8	1	
28	a	1	Total	C	O	P	0
			48	39	8	1	
28	d	1	Total	C	O	P	0
			38	29	8	1	
28	s	1	Total	C	O	P	0
			38	29	8	1	
28	w	1	Total	C	O	P	0
			48	39	8	1	
28	x	1	Total	C	O	P	0
			46	37	8	1	

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



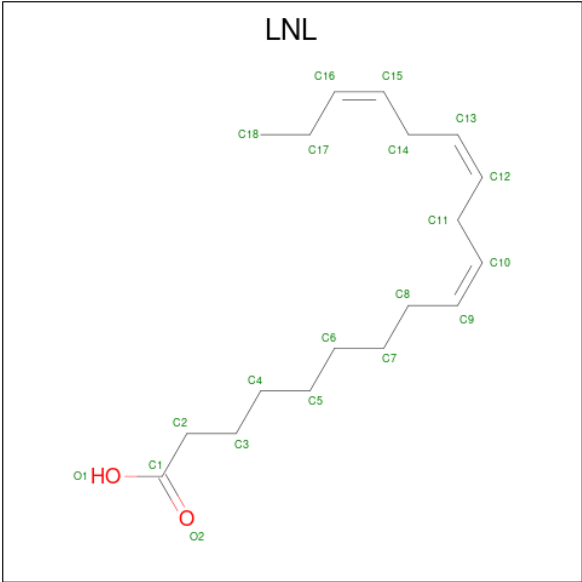
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			37	26	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	G	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
			38	27	10	1	
30	S	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
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	d	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
			49	38	10	1	
30	n	1	Total	C	O	P	0
			45	34	10	1	
30	r	1	Total	C	O	P	0
			37	26	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is ALPHA-LINOLENIC ACID (three-letter code: LNL) (formula: C<sub>18</sub>H<sub>30</sub>O<sub>2</sub>).



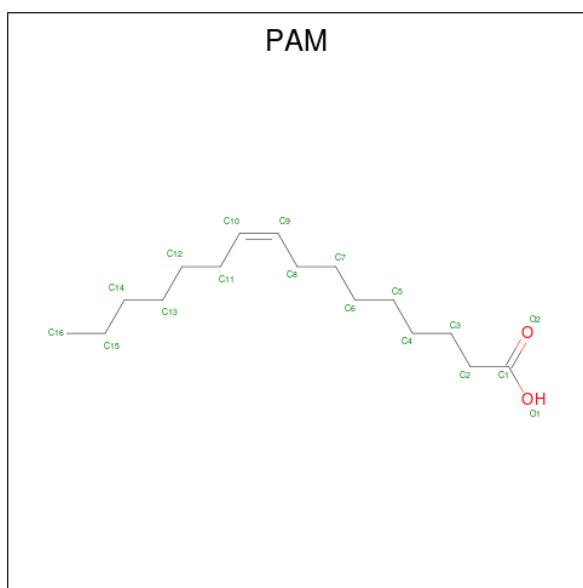
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			20	18	2	
31	A	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	I	1	Total	C	O	0
			20	18	2	
31	a	1	Total	C	O	0
			20	18	2	

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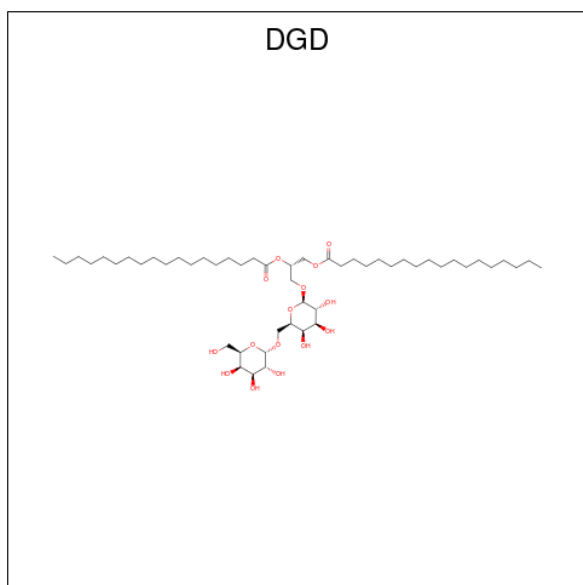
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	i	1	Total	C	O	0
			20	18	2	

- Molecule 32 is PALMITOLEIC ACID (three-letter code: PAM) (formula:  $C_{16}H_{30}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			18	16	2	
32	b	1	Total	C	O	0
			18	16	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



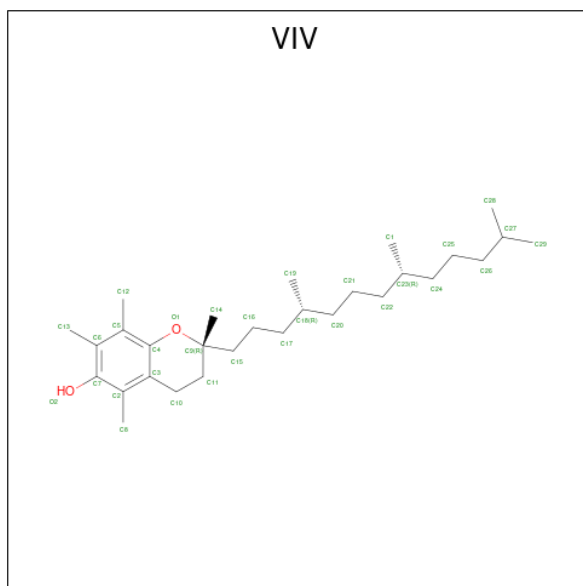
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			66	51	15	
33	H	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	d	1	Total	C	O	0
			62	47	15	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	C	1	Total	Mg	0
			1	1	
34	c	1	Total	Mg	0
			1	1	

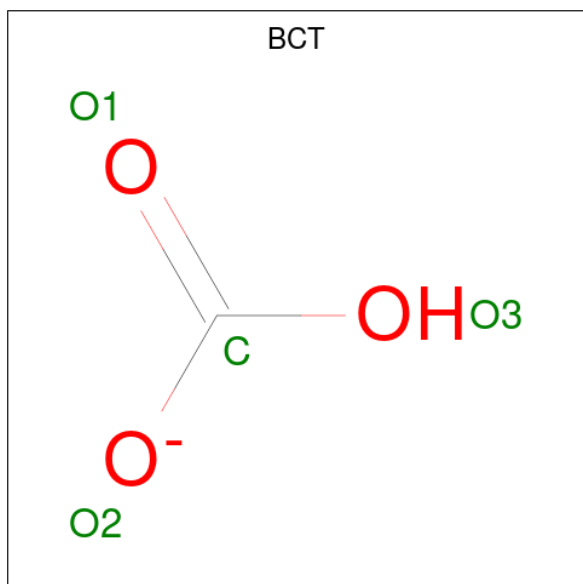
- Molecule 35 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL

]CHROMAN-6-OL (three-letter code: VIV) (formula: C<sub>29</sub>H<sub>50</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			31	29	2	
35	y	1	Total	C	O	0
			31	29	2	

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



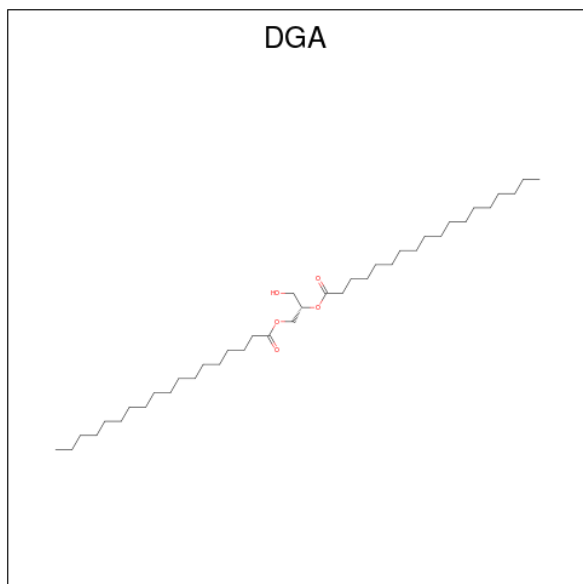
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			4	1	3	

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

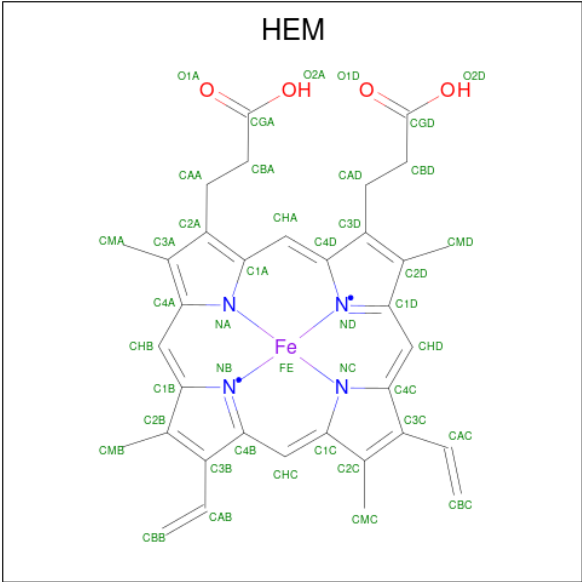
- Molecule 37 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
37	D	1	Total	C	O	0
			40	35	5	
37	b	1	Total	C	O	0
			44	39	5	

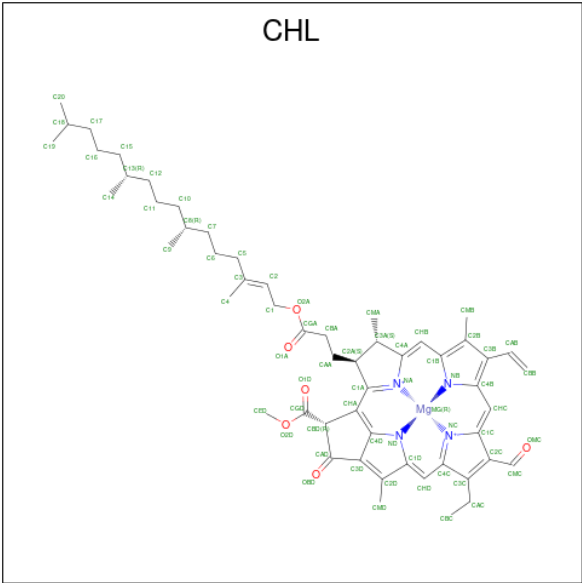
- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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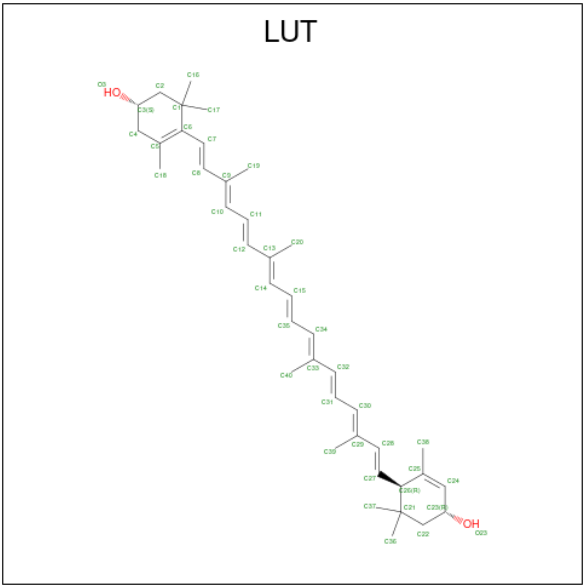
Mol	Chain	Residues	Atoms					AltConf
39	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
39	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



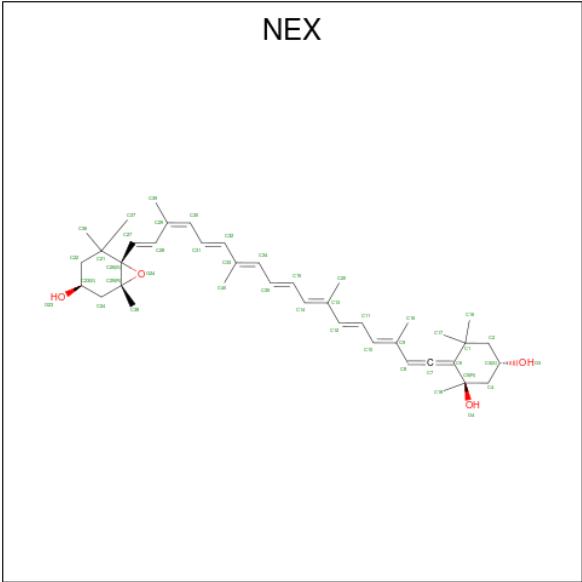
Mol	Chain	Residues	Atoms				AltConf
40	G	1	Total	C	O		0
			42	40	2		
40	G	1	Total	C	O		0
			42	40	2		
40	N	1	Total	C	O		0
			42	40	2		
40	N	1	Total	C	O		0
			42	40	2		
40	R	1	Total	C	O		0
			42	40	2		

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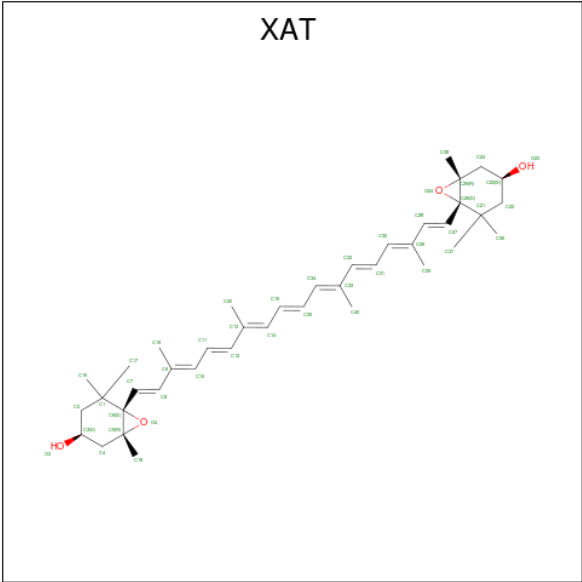
Mol	Chain	Residues	Atoms			AltConf
40	S	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	r	1	Total	C	O	0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

- Molecule 41 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
41	G	1	Total	C	O	0
			24	22	2	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	S	1	Total	C	O	0
			23	21	2	
41	Y	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	
41	s	1	Total	C	O	0
			27	25	2	

- Molecule 42 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	28	Total	O	0
			28	28	
43	B	31	Total	O	0
			31	31	
43	C	10	Total	O	0
			10	10	
43	D	18	Total	O	0
			18	18	

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Mol	Chain	Residues	Atoms		AltConf
43	E	4	Total 4	O 4	0
43	H	10	Total 10	O 10	0
43	I	1	Total 1	O 1	0
43	L	2	Total 2	O 2	0
43	N	4	Total 4	O 4	0
43	O	4	Total 4	O 4	0
43	R	8	Total 8	O 8	0
43	S	1	Total 1	O 1	0
43	T	5	Total 5	O 5	0
43	U	1	Total 1	O 1	0
43	V	1	Total 1	O 1	0
43	Y	8	Total 8	O 8	0
43	Z	1	Total 1	O 1	0
43	a	20	Total 20	O 20	0
43	b	31	Total 31	O 31	0
43	c	14	Total 14	O 14	0
43	d	25	Total 25	O 25	0
43	e	4	Total 4	O 4	0
43	f	1	Total 1	O 1	0
43	g	1	Total 1	O 1	0
43	h	11	Total 11	O 11	0

*Continued on next page...*



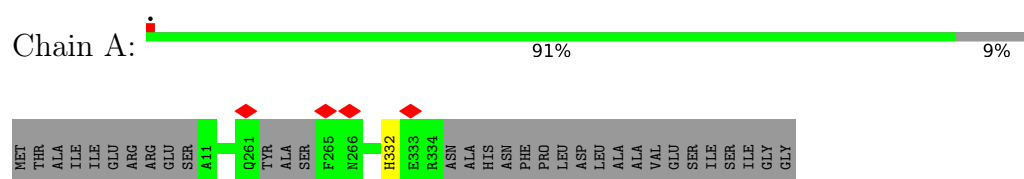
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
43	i	2	Total 2	O 2	0
43	l	4	Total 4	O 4	0
43	n	1	Total 1	O 1	0
43	o	2	Total 2	O 2	0
43	r	7	Total 7	O 7	0
43	t	4	Total 4	O 4	0
43	v	2	Total 2	O 2	0
43	x	1	Total 1	O 1	0
43	y	13	Total 13	O 13	0

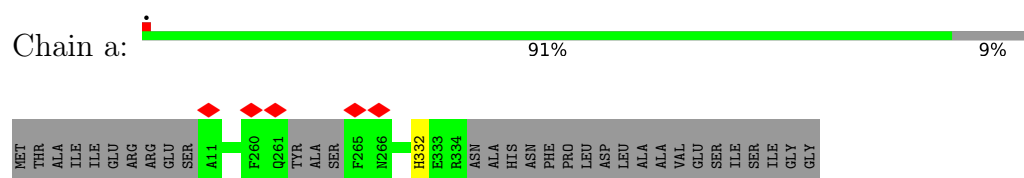
### 3 Residue-property plots

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

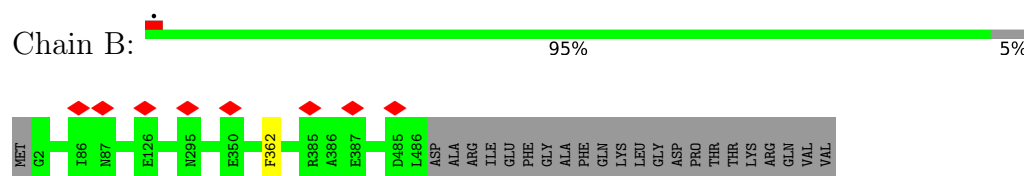
- Molecule 1: Photosystem II protein D1



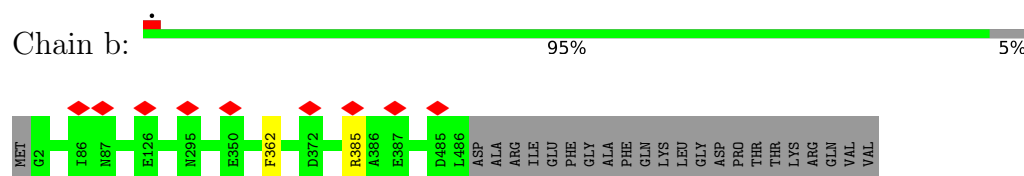
- Molecule 1: Photosystem II protein D1



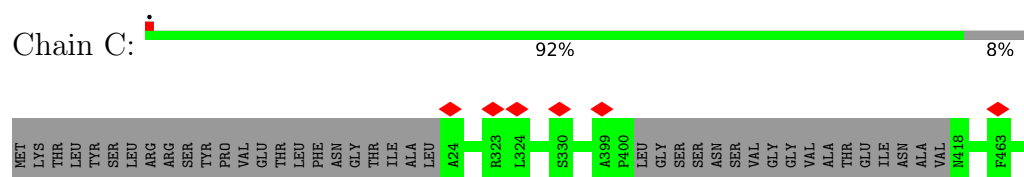
- Molecule 2: Photosystem II CP47 reaction center protein



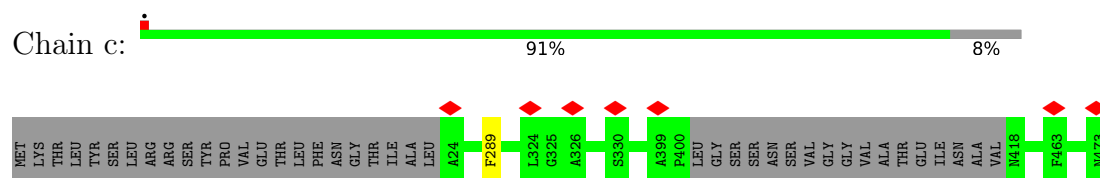
- Molecule 2: Photosystem II CP47 reaction center protein



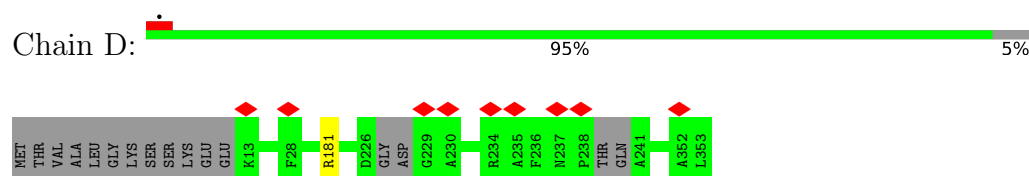
- Molecule 3: Photosystem II CP43 reaction center protein



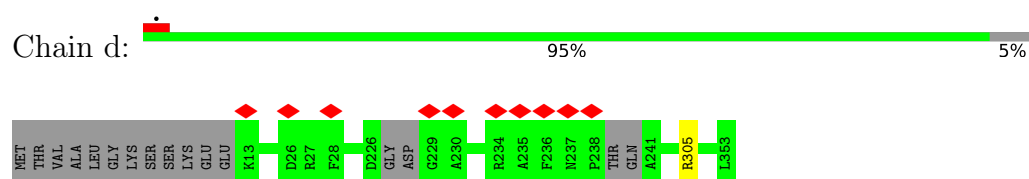
- Molecule 3: Photosystem II CP43 reaction center protein



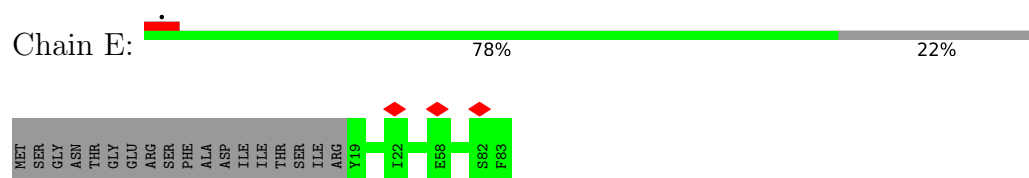
- Molecule 4: Photosystem II D2 protein



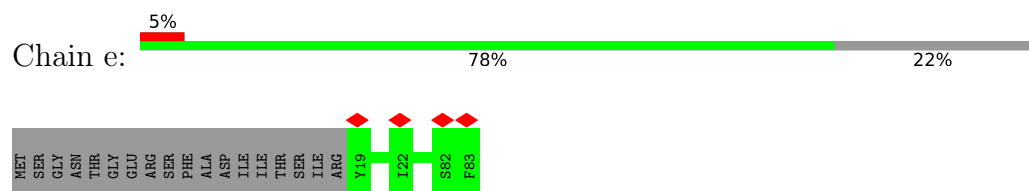
- Molecule 4: Photosystem II D2 protein



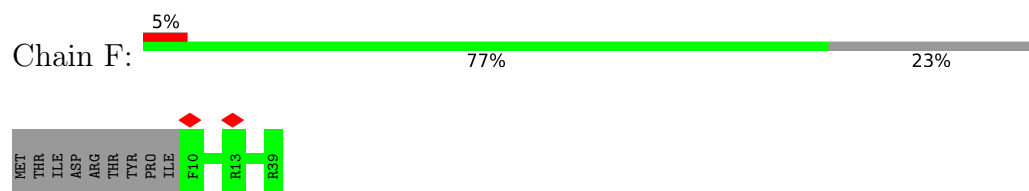
- Molecule 5: Cytochrome b559 subunit alpha



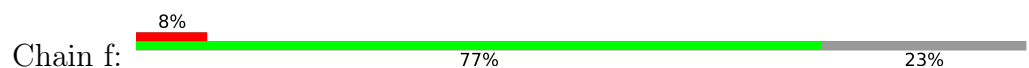
- Molecule 5: Cytochrome b559 subunit alpha

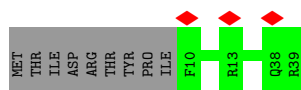


- Molecule 6: Cytochrome b559 subunit beta

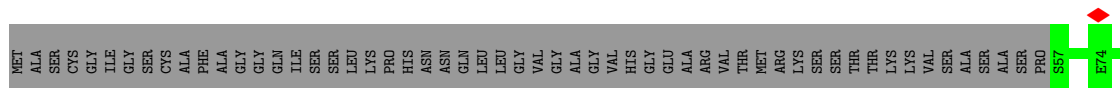
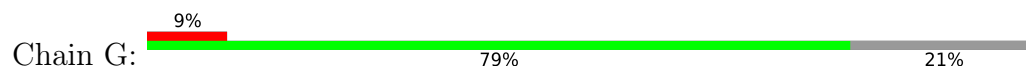


- Molecule 6: Cytochrome b559 subunit beta

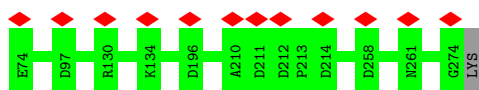
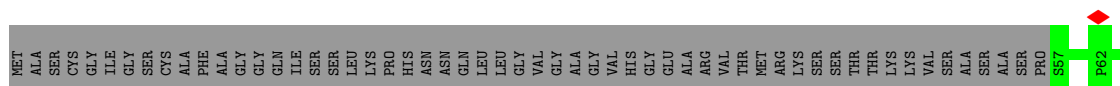
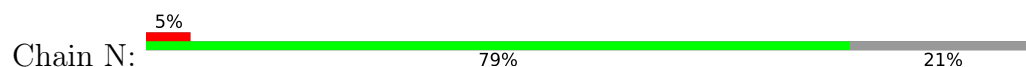




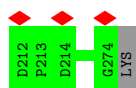
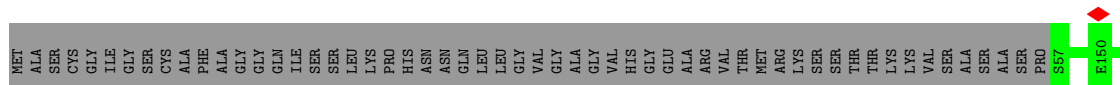
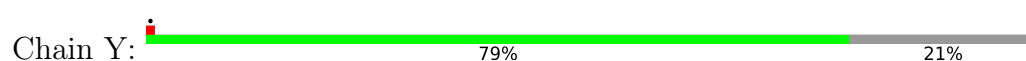
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



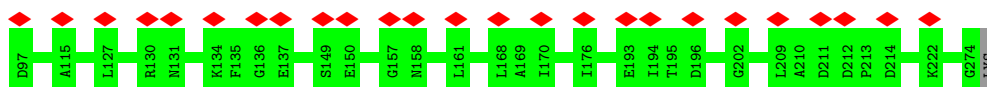
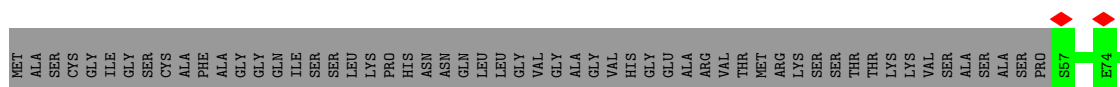
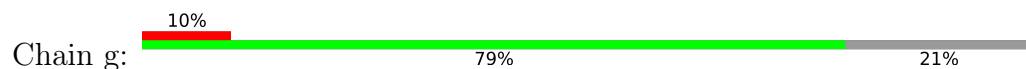
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



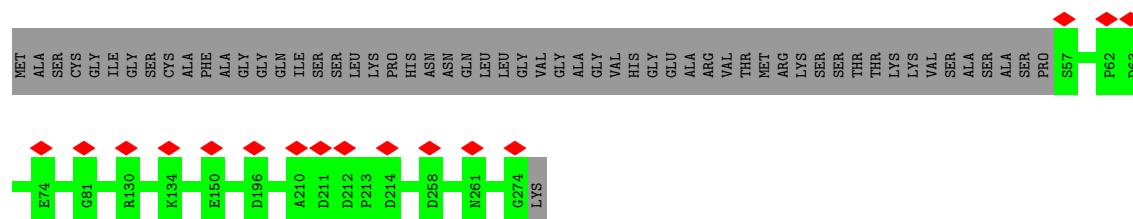
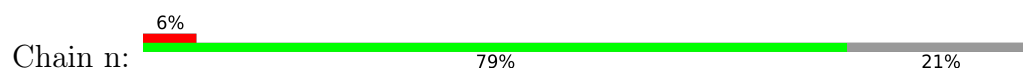
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



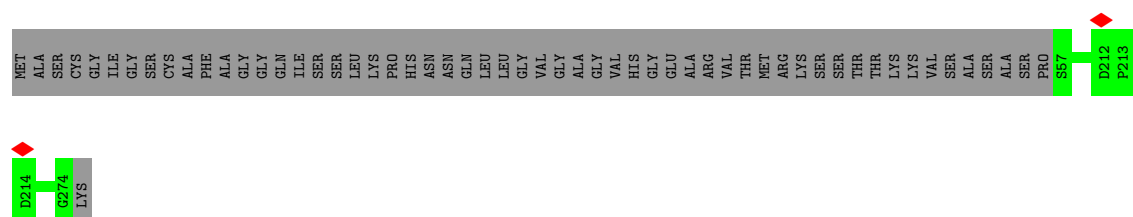
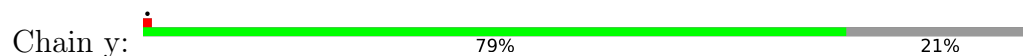
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



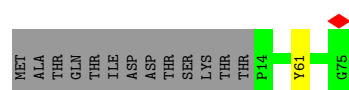
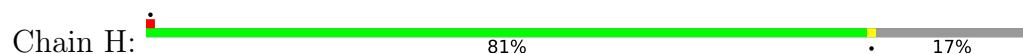
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



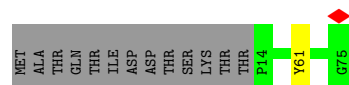
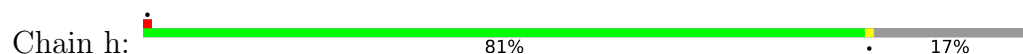
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



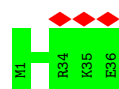
- Molecule 8: Photosystem II reaction center protein H



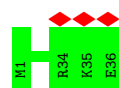
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I

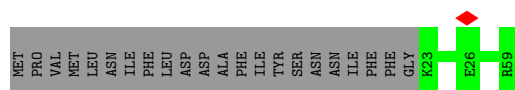


- Molecule 9: Photosystem II reaction center protein I



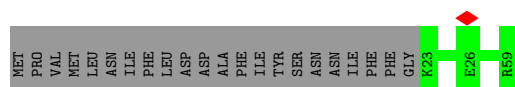
- Molecule 10: Photosystem II reaction center protein K

Chain K:  63% 37%



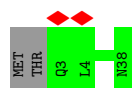
- Molecule 10: Photosystem II reaction center protein K

Chain k:  63% 37%



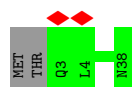
- Molecule 11: Photosystem II reaction center protein L

Chain L:  5% 95% 5%




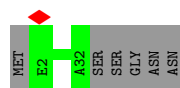
- Molecule 11: Photosystem II reaction center protein L

Chain l:  5% 95% 5%




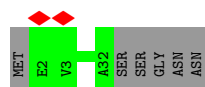
- Molecule 12: Photosystem II reaction center protein M

Chain M:  5% 84% 16%



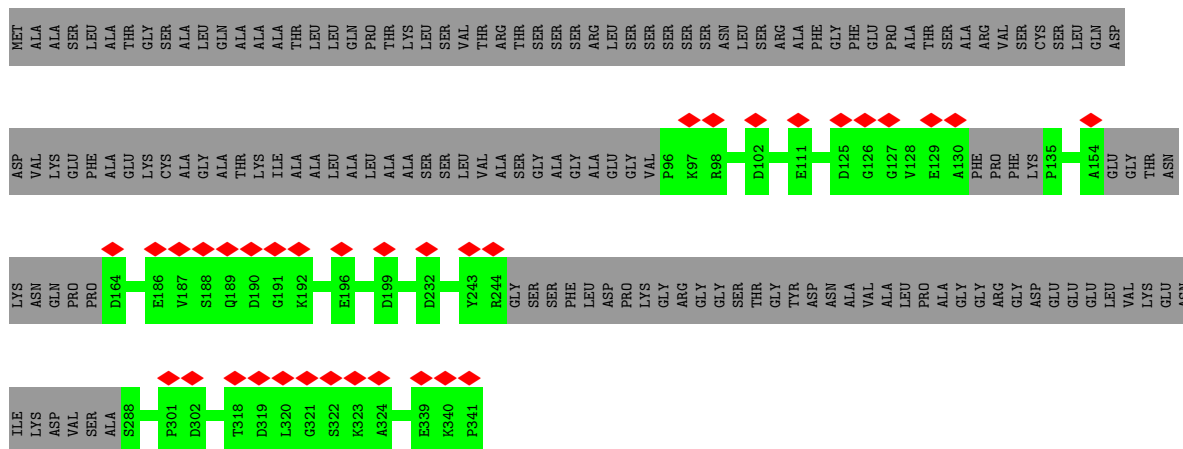
- Molecule 12: Photosystem II reaction center protein M

Chain m:  5% 84% 16%

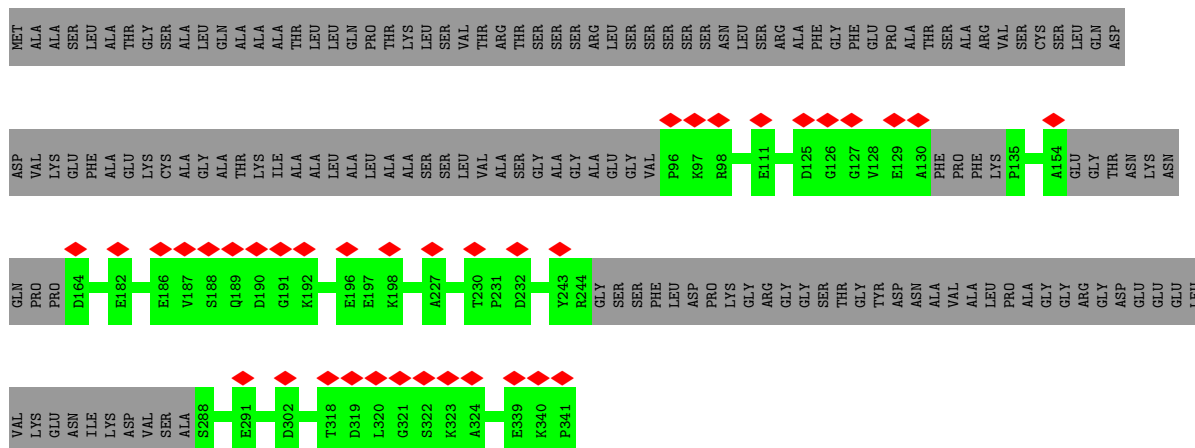


- Molecule 13: Oxygen-evolving enhancer protein 1, chloroplastic

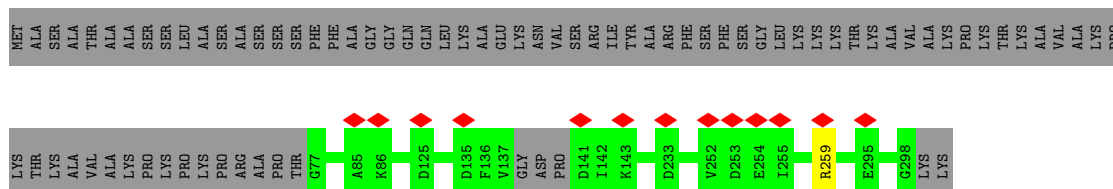
Chain O:  10% 56% 44%



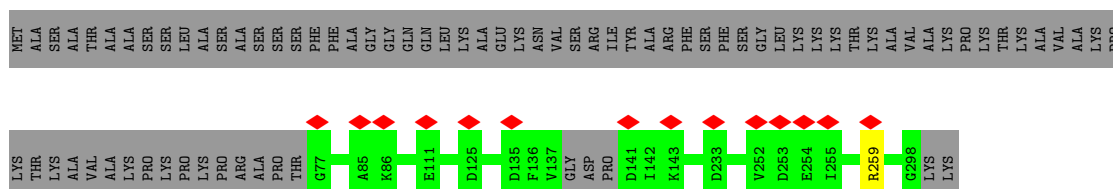
- Molecule 13: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic




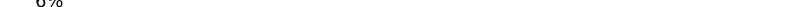

- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



- [illegible]

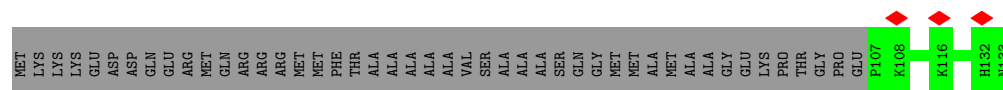
- Chain s:
- 
- 18% 69% 30%
- MET ALA SER ILE ALA LEU GLY SER THR ALA ALA LEU GLY ARG ASP GLN MET LEU GLY ASN PRO LEU ASN MET MET LEU ALA ALA SER THR ARG LEU THR PRO SER LEU GLN VAL VAL SER LEU PHE GLY PHE LYS LYS ALA ALA

- Chain T: 

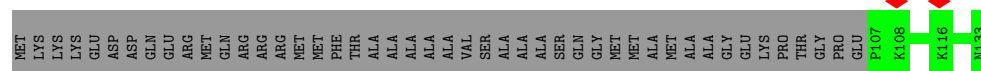
- Chain t: 
- 

- [illegible]

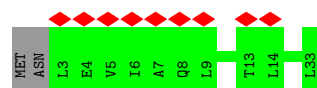




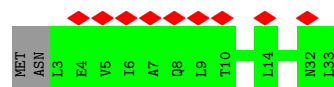
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic



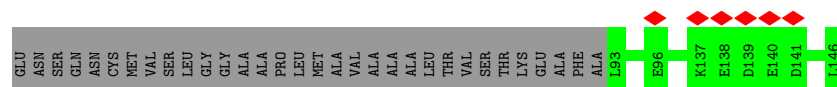
- Molecule 18: Photosystem II reaction center protein Ycf12



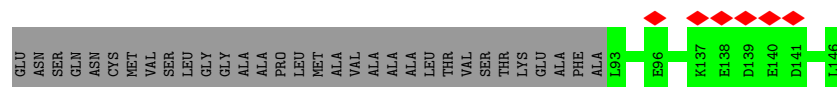
- Molecule 18: Photosystem II reaction center protein Ycf12



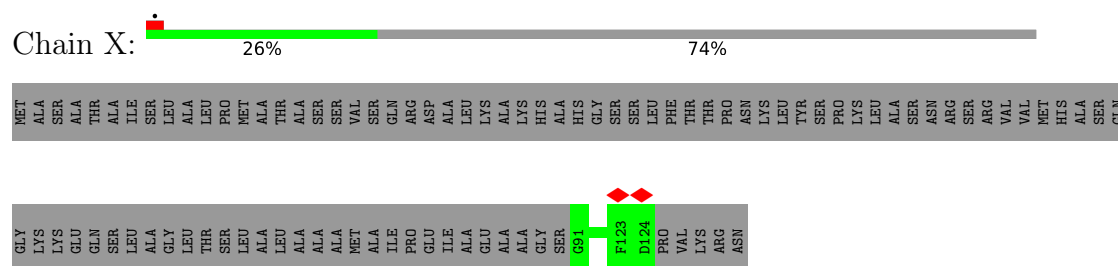
- Molecule 19: PSII 6.1 kDa protein



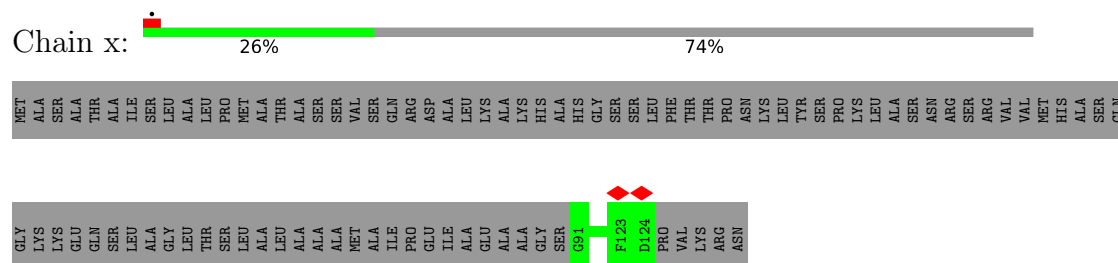
- Molecule 19: PSII 6.1 kDa protein



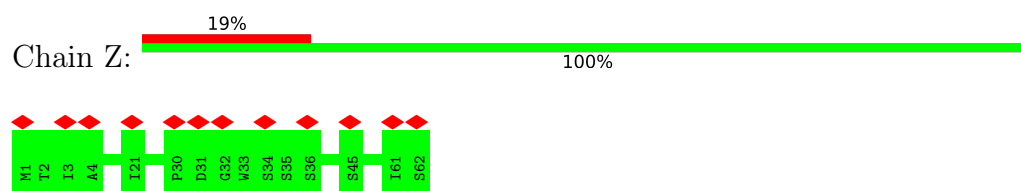
- Molecule 20: Photosystem II PsbX



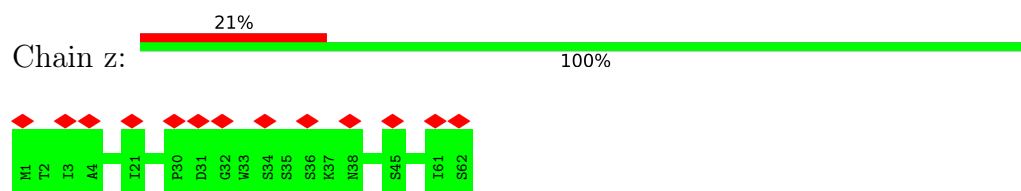
- Molecule 20: Photosystem II PsbX



- Molecule 21: Photosystem II reaction center protein Z



- Molecule 21: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	60956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	120	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.081	Depositor
Minimum map value	-3.771	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.210	Depositor
Recommended contour level	0.886	Depositor
Map size (Å)	430.64896, 430.64896, 430.64896	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96127, 0.96127, 0.96127	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, DGA, LNL, PHO, LUT, BCR, XAT, SQD, NEX, FE2, PL9, CHL, CLA, MG, VIV, LHG, LMG, PAM, HEM, 3PH, DGD

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	0.26	0/2578	0.46	0/3513
1	a	0.26	0/2578	0.47	0/3513
2	B	0.26	0/3940	0.48	0/5363
2	b	0.27	0/3940	0.49	0/5363
3	C	0.29	0/3493	0.47	0/4757
3	c	0.29	0/3493	0.48	0/4757
4	D	0.26	0/2778	0.47	0/3786
4	d	0.27	0/2777	0.47	0/3786
5	E	0.27	0/555	0.46	0/756
5	e	0.27	0/555	0.47	0/756
6	F	0.25	0/247	0.44	0/333
6	f	0.25	0/247	0.46	0/333
7	G	0.29	0/1712	0.48	0/2335
7	N	0.26	0/1712	0.43	0/2335
7	Y	0.29	0/1712	0.45	0/2335
7	g	0.27	0/1712	0.46	0/2335
7	n	0.26	0/1712	0.43	0/2335
7	y	0.26	0/1712	0.43	0/2335
8	H	0.28	0/475	0.49	0/647
8	h	0.29	0/475	0.49	0/647
9	I	0.28	0/305	0.49	0/409
9	i	0.28	0/305	0.49	0/409
10	K	0.28	0/313	0.44	0/428
10	k	0.28	0/313	0.44	0/428
11	L	0.25	0/309	0.40	0/421
11	l	0.26	0/309	0.42	0/421
12	M	0.25	0/242	0.37	0/330
12	m	0.26	0/242	0.42	0/330
13	O	0.24	0/1497	0.47	0/2017
13	o	0.25	0/1497	0.48	0/2017
14	R	0.25	0/1767	0.42	0/2397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	r	0.26	0/1767	0.44	0/2397
15	S	0.28	0/1673	0.43	0/2272
15	s	0.27	0/1673	0.45	0/2272
16	T	0.27	0/262	0.41	0/356
16	t	0.27	0/262	0.39	0/356
17	U	0.23	0/209	0.49	0/280
17	u	0.24	0/209	0.47	0/280
18	V	0.22	0/228	0.45	0/311
18	v	0.22	0/228	0.43	0/311
19	W	0.25	0/423	0.49	0/574
19	w	0.24	0/423	0.42	0/574
20	X	0.24	0/228	0.33	0/310
20	x	0.24	0/228	0.34	0/310
21	Z	0.26	0/463	0.38	0/633
21	z	0.25	0/463	0.35	0/633
All	All	0.27	0/54241	0.46	0/73796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/353 (90%)	312 (98%)	5 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
2	B	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
2	b	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
3	C	429/473 (91%)	420 (98%)	9 (2%)	0	100	100
3	c	429/473 (91%)	419 (98%)	10 (2%)	0	100	100
4	D	331/353 (94%)	319 (96%)	12 (4%)	0	100	100
4	d	331/353 (94%)	322 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	61 (97%)	2 (3%)	0	100	100
5	e	63/83 (76%)	62 (98%)	1 (2%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	216/275 (78%)	206 (95%)	10 (5%)	0	100	100
7	N	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	Y	216/275 (78%)	211 (98%)	5 (2%)	0	100	100
7	g	216/275 (78%)	207 (96%)	9 (4%)	0	100	100
7	n	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	y	216/275 (78%)	212 (98%)	4 (2%)	0	100	100
8	H	60/75 (80%)	58 (97%)	2 (3%)	0	100	100
8	h	60/75 (80%)	59 (98%)	1 (2%)	0	100	100
9	I	34/36 (94%)	34 (100%)	0	0	100	100
9	i	34/36 (94%)	34 (100%)	0	0	100	100
10	K	35/59 (59%)	33 (94%)	2 (6%)	0	100	100
10	k	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
11	L	34/38 (90%)	34 (100%)	0	0	100	100
11	l	34/38 (90%)	34 (100%)	0	0	100	100
12	M	29/37 (78%)	29 (100%)	0	0	100	100
12	m	29/37 (78%)	29 (100%)	0	0	100	100
13	O	182/341 (53%)	175 (96%)	7 (4%)	0	100	100
13	o	182/341 (53%)	173 (95%)	9 (5%)	0	100	100
14	R	215/300 (72%)	213 (99%)	2 (1%)	0	100	100
14	r	215/300 (72%)	211 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
15	s	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
16	T	29/35 (83%)	29 (100%)	0	0	100	100
16	t	29/35 (83%)	29 (100%)	0	0	100	100
17	U	25/133 (19%)	25 (100%)	0	0	100	100
17	u	25/133 (19%)	25 (100%)	0	0	100	100
18	V	29/33 (88%)	26 (90%)	3 (10%)	0	100	100
18	v	29/33 (88%)	29 (100%)	0	0	100	100
19	W	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
19	w	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
20	X	32/129 (25%)	31 (97%)	1 (3%)	0	100	100
20	x	32/129 (25%)	32 (100%)	0	0	100	100
21	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
21	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	6644/8722 (76%)	6469 (97%)	175 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	257/282 (91%)	256 (100%)	1 (0%)	89	96
1	a	257/282 (91%)	256 (100%)	1 (0%)	89	96
2	B	387/406 (95%)	386 (100%)	1 (0%)	91	97
2	b	387/406 (95%)	385 (100%)	2 (0%)	86	95
3	C	338/371 (91%)	338 (100%)	0	100	100
3	c	338/371 (91%)	337 (100%)	1 (0%)	91	97
4	D	271/284 (95%)	270 (100%)	1 (0%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	271/284 (95%)	270 (100%)	1 (0%)	89	96
5	E	59/74 (80%)	59 (100%)	0	100	100
5	e	59/74 (80%)	59 (100%)	0	100	100
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	166/208 (80%)	166 (100%)	0	100	100
7	N	166/208 (80%)	166 (100%)	0	100	100
7	Y	166/208 (80%)	166 (100%)	0	100	100
7	g	166/208 (80%)	166 (100%)	0	100	100
7	n	166/208 (80%)	166 (100%)	0	100	100
7	y	166/208 (80%)	166 (100%)	0	100	100
8	H	50/62 (81%)	49 (98%)	1 (2%)	50	78
8	h	50/62 (81%)	49 (98%)	1 (2%)	50	78
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	K	32/52 (62%)	32 (100%)	0	100	100
10	k	32/52 (62%)	32 (100%)	0	100	100
11	L	34/36 (94%)	34 (100%)	0	100	100
11	l	34/36 (94%)	34 (100%)	0	100	100
12	M	25/30 (83%)	25 (100%)	0	100	100
12	m	25/30 (83%)	25 (100%)	0	100	100
13	O	164/275 (60%)	164 (100%)	0	100	100
13	o	164/275 (60%)	164 (100%)	0	100	100
14	R	180/241 (75%)	179 (99%)	1 (1%)	84	94
14	r	180/241 (75%)	179 (99%)	1 (1%)	84	94
15	S	162/230 (70%)	161 (99%)	1 (1%)	84	94
15	s	162/230 (70%)	161 (99%)	1 (1%)	84	94
16	T	28/30 (93%)	28 (100%)	0	100	100
16	t	28/30 (93%)	28 (100%)	0	100	100
17	U	23/103 (22%)	23 (100%)	0	100	100
17	u	23/103 (22%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	V	27/29 (93%)	27 (100%)	0	100	100
18	v	27/29 (93%)	27 (100%)	0	100	100
19	W	46/116 (40%)	46 (100%)	0	100	100
19	w	46/116 (40%)	46 (100%)	0	100	100
20	X	23/94 (24%)	23 (100%)	0	100	100
20	x	23/94 (24%)	23 (100%)	0	100	100
21	Z	51/51 (100%)	51 (100%)	0	100	100
21	z	51/51 (100%)	51 (100%)	0	100	100
All	All	5426/6914 (78%)	5412 (100%)	14 (0%)	90	97

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
2	B	362	PHE
4	D	181	ARG
8	H	61	TYR
14	R	259	ARG
15	S	186	PHE
1	a	332	HIS
2	b	362	PHE
2	b	385	ARG
3	c	289	PHE
4	d	305	ARG
8	h	61	TYR
14	r	259	ARG
15	s	186	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	304	GLN
1	A	322	ASN
2	B	216	HIS
2	B	317	ASN
3	C	118	HIS
3	C	313	GLN

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Mol	Chain	Res	Type
7	G	240	GLN
7	G	251	ASN
7	N	104	ASN
14	R	156	GLN
21	Z	6	GLN
1	a	303	ASN
1	a	322	ASN
3	c	28	GLN
3	c	68	ASN
3	c	118	HIS
3	c	313	GLN
14	r	156	GLN
15	s	224	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 358 ligands modelled in this entry, 4 are monoatomic - leaving 354 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	Y	311	30	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	n	602	7	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
28	3PH	L	102	-	40,40,47	0.68	1 (2%)	44,45,52	0.64	1 (2%)
23	CLA	G	613	7	65,73,73	1.48	6 (9%)	76,113,113	1.42	7 (9%)
39	CHL	G	609	7	66,74,74	1.66	5 (7%)	73,114,114	1.72	9 (12%)
23	CLA	Y	304	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
38	HEM	f	501	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.41	7 (15%)
23	CLA	N	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.58	8 (14%)
28	3PH	w	202	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
28	3PH	x	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
27	LMG	C	525	-	45,45,55	0.20	0	53,53,63	0.14	0
39	CHL	N	608	-	50,58,74	1.81	5 (10%)	52,94,114	1.94	10 (19%)
23	CLA	G	604	-	49,57,73	1.71	5 (10%)	55,93,113	1.55	8 (14%)
24	PHO	D	402	-	51,69,69	0.98	3 (5%)	47,99,99	1.19	4 (8%)
28	3PH	a	410	-	47,47,47	0.63	1 (2%)	51,52,52	0.56	1 (1%)
23	CLA	B	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	s	611	15	49,57,73	1.70	5 (10%)	55,93,113	1.54	6 (10%)
31	LNL	i	101	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
42	XAT	N	619	-	39,47,47	3.16	23 (58%)	54,74,74	4.58	32 (59%)
28	3PH	D	403	-	37,37,47	0.70	1 (2%)	41,42,52	0.65	1 (2%)
23	CLA	R	611	-	49,57,73	1.70	6 (12%)	55,93,113	1.52	7 (12%)
23	CLA	r	611	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	7 (12%)
23	CLA	s	603	-	49,57,73	1.71	6 (12%)	55,93,113	1.54	8 (14%)
23	CLA	s	608	-	49,57,73	1.74	5 (10%)	55,93,113	1.49	7 (12%)
23	CLA	N	611	30	65,73,73	1.50	5 (7%)	76,113,113	1.34	8 (10%)
23	CLA	r	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.44	8 (11%)
23	CLA	c	513	-	60,68,73	1.52	6 (10%)	70,107,113	1.43	8 (11%)
23	CLA	c	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
25	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
23	CLA	b	602	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
41	NEX	G	617	-	21,25,46	4.26	19 (90%)	28,38,70	5.44	11 (39%)
25	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	8 (14%)
39	CHL	Y	306	7	48,56,74	1.84	5 (10%)	51,92,114	2.12	9 (17%)
23	CLA	n	613	7	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
25	BCR	k	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
31	LNL	B	622	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	Y	307	-	66,74,74	1.57	5 (7%)	73,114,114	1.63	10 (13%)
31	LNL	B	625	-	19,19,19	0.45	0	18,19,19	0.91	1 (5%)
39	CHL	y	307	7	48,56,74	1.83	5 (10%)	51,92,114	2.10	9 (17%)
31	LNL	c	518	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
28	3PH	X	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	S	608	-	49,57,73	1.72	5 (10%)	55,93,113	1.48	7 (12%)
33	DGD	H	502	-	63,63,67	0.87	1 (1%)	77,77,81	1.33	7 (9%)
23	CLA	B	616	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
26	SQD	M	101	-	49,50,54	1.59	8 (16%)	58,61,65	1.38	6 (10%)
23	CLA	n	610	7	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
27	LMG	b	620	-	51,51,55	0.19	0	59,59,63	0.22	0
31	LNL	c	519	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	N	602	7	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
32	PAM	B	621	-	17,17,17	0.61	0	17,17,17	0.78	0
39	CHL	n	606	-	66,74,74	1.58	5 (7%)	73,114,114	1.58	11 (15%)
40	LUT	Y	316	-	42,43,43	2.36	20 (47%)	51,60,60	3.15	23 (45%)
40	LUT	Y	315	-	42,43,43	1.78	10 (23%)	51,60,60	2.77	20 (39%)
25	BCR	d	410	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	6 (10%)
42	XAT	n	617	-	39,47,47	3.04	21 (53%)	54,74,74	4.50	30 (55%)
42	XAT	n	620	-	39,47,47	3.15	23 (58%)	54,74,74	4.56	31 (57%)
31	LNL	c	521	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
23	CLA	C	503	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
39	CHL	N	606	-	66,74,74	1.58	5 (7%)	73,114,114	1.59	10 (13%)
40	LUT	G	616	-	42,43,43	2.41	20 (47%)	51,60,60	3.11	21 (41%)
30	LHG	b	627	-	48,48,48	1.36	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	C	504	43	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
23	CLA	C	501	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	B	615	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
30	LHG	S	616	23	48,48,48	1.43	8 (16%)	51,54,54	0.73	2 (3%)
31	LNL	c	517	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
37	DGA	D	410	-	39,39,43	0.20	0	41,41,45	0.15	0
41	NEX	g	617	-	38,46,46	4.18	33 (86%)	50,70,70	4.94	24 (48%)
23	CLA	B	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
39	CHL	y	310	7	66,74,74	1.57	4 (6%)	73,114,114	1.58	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	r	604	43	55,63,73	1.61	5 (9%)	64,101,113	1.49	8 (12%)
31	LNL	b	624	-	19,19,19	0.43	0	18,19,19	0.88	1 (5%)
39	CHL	R	607	-	66,74,74	1.59	4 (6%)	73,114,114	1.67	12 (16%)
23	CLA	N	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.50	9 (11%)
25	BCR	D	411	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	LMG	d	409	-	46,46,55	0.19	0	54,54,63	0.15	0
30	LHG	R	616	23	37,37,48	1.56	8 (21%)	40,43,54	0.86	2 (5%)
23	CLA	R	601	14	49,57,73	1.73	6 (12%)	55,93,113	1.51	7 (12%)
39	CHL	G	608	-	50,58,74	1.85	5 (10%)	52,94,114	1.87	9 (17%)
23	CLA	g	614	-	49,57,73	1.71	5 (10%)	55,93,113	1.52	8 (14%)
31	LNL	b	625	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
23	CLA	N	610	7	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	n	603	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
40	LUT	y	317	-	42,43,43	2.38	20 (47%)	51,60,60	3.16	23 (45%)
25	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
23	CLA	c	511	3	65,73,73	1.48	6 (9%)	76,113,113	1.43	8 (10%)
23	CLA	b	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.47	8 (10%)
23	CLA	b	616	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
31	LNL	C	520	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
25	BCR	B	618	-	40,40,41	1.09	2 (5%)	52,54,56	1.25	6 (11%)
23	CLA	r	602	14	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
31	LNL	a	401	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	S	610	30	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
23	CLA	n	614	-	49,57,73	1.71	6 (12%)	55,93,113	1.54	8 (14%)
23	CLA	r	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
23	CLA	c	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
39	CHL	G	606	-	50,58,74	1.88	4 (8%)	52,94,114	1.96	9 (17%)
23	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	10 (13%)
28	3PH	A	410	-	47,47,47	0.62	1 (2%)	51,52,52	0.60	1 (1%)
30	LHG	G	618	23	48,48,48	1.39	8 (16%)	51,54,54	0.75	2 (3%)
23	CLA	C	509	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	G	614	-	49,57,73	1.73	5 (10%)	55,93,113	1.49	8 (14%)
23	CLA	Y	312	7	65,73,73	1.52	5 (7%)	76,113,113	1.35	7 (9%)
23	CLA	C	507	43	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	PL9	d	407	-	55,55,55	0.08	0	68,69,69	0.22	0
24	PHO	A	405	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	6 (12%)
39	CHL	r	605	-	50,58,74	1.78	4 (8%)	52,94,114	1.95	10 (19%)
23	CLA	c	506	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	B	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	9 (11%)
23	CLA	C	508	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	7 (9%)
42	XAT	G	619	-	39,47,47	3.01	22 (56%)	54,74,74	4.57	30 (55%)
23	CLA	S	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	Y	310	7	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
30	LHG	s	616	23	48,48,48	1.39	8 (16%)	51,54,54	0.74	2 (3%)
23	CLA	G	611	30	49,57,73	1.72	5 (10%)	55,93,113	1.52	7 (12%)
40	LUT	n	615	-	42,43,43	1.89	11 (26%)	51,60,60	2.97	19 (37%)
35	VIV	y	301	-	32,32,32	0.88	1 (3%)	41,45,45	1.13	5 (12%)
28	3PH	s	618	-	37,37,47	0.70	1 (2%)	41,42,52	0.64	1 (2%)
31	LNL	C	522	-	19,19,19	0.44	0	18,19,19	0.91	1 (5%)
28	3PH	C	524	-	47,47,47	0.63	1 (2%)	51,52,52	0.60	1 (1%)
30	LHG	N	618	23	48,48,48	1.45	8 (16%)	51,54,54	0.69	2 (3%)
30	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	0.93	3 (5%)
23	CLA	b	613	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
25	BCR	a	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
23	CLA	N	614	-	49,57,73	1.70	5 (10%)	55,93,113	1.54	8 (14%)
23	CLA	c	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
25	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
30	LHG	a	412	-	48,48,48	1.40	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	s	602	15	57,65,73	1.59	6 (10%)	66,103,113	1.45	7 (10%)
23	CLA	B	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
24	PHO	d	402	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	5 (10%)
41	NEX	s	617	-	23,27,46	4.08	19 (82%)	28,38,70	3.76	14 (50%)
23	CLA	d	406	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
41	NEX	R	618	-	38,46,46	3.93	31 (81%)	50,70,70	4.85	20 (40%)
23	CLA	c	509	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
42	XAT	r	615	-	39,47,47	3.22	20 (51%)	54,74,74	4.70	31 (57%)
23	CLA	B	606	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	8 (10%)
23	CLA	D	406	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	8 (10%)
31	LNL	C	517	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LNL	b	623	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
23	CLA	a	404	43	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
23	CLA	r	601	14	49,57,73	1.73	5 (10%)	55,93,113	1.50	6 (10%)
23	CLA	G	602	7	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
40	LUT	r	613	-	42,43,43	2.49	20 (47%)	51,60,60	3.11	24 (47%)
27	LMG	B	626	-	49,49,55	0.19	0	57,57,63	0.14	0
33	DGD	c	515	-	56,56,67	0.95	2 (3%)	70,70,81	1.45	9 (12%)
39	CHL	S	607	-	49,57,74	1.85	5 (10%)	52,93,114	1.88	10 (19%)
39	CHL	s	601	-	52,60,74	1.78	5 (9%)	56,97,114	1.86	11 (19%)
23	CLA	y	305	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
36	BCT	D	401	22	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
23	CLA	b	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	9 (11%)
40	LUT	s	614	-	42,43,43	2.74	23 (54%)	51,60,60	3.28	24 (47%)
40	LUT	N	615	-	42,43,43	2.58	21 (50%)	51,60,60	3.25	24 (47%)
40	LUT	S	615	-	42,43,43	2.65	22 (52%)	51,60,60	3.22	24 (47%)
23	CLA	S	604	-	49,57,73	1.70	5 (10%)	55,93,113	1.58	7 (12%)
25	BCR	v	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
39	CHL	n	601	7	66,74,74	1.59	5 (7%)	73,114,114	1.67	9 (12%)
23	CLA	G	612	7	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
40	LUT	G	615	-	42,43,43	1.97	12 (28%)	51,60,60	2.89	22 (43%)
39	CHL	y	303	7	66,74,74	1.58	4 (6%)	73,114,114	1.66	10 (13%)
31	LNL	b	622	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
31	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.91	1 (5%)
41	NEX	N	617	-	38,46,46	4.10	32 (84%)	50,70,70	4.96	22 (44%)
23	CLA	C	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
23	CLA	C	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
23	CLA	N	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
23	CLA	R	604	43	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
23	CLA	R	612	14	49,57,73	1.73	5 (10%)	55,93,113	1.53	7 (12%)
40	LUT	R	613	-	42,43,43	2.53	21 (50%)	51,60,60	3.16	25 (49%)
23	CLA	b	605	-	65,73,73	1.48	7 (10%)	76,113,113	1.36	7 (9%)
24	PHO	a	406	-	51,69,69	0.98	3 (5%)	47,99,99	1.14	4 (8%)
23	CLA	a	405	43	49,57,73	1.69	5 (10%)	55,93,113	1.57	8 (14%)
42	XAT	Y	301	-	39,47,47	3.30	24 (61%)	54,74,74	4.45	32 (59%)
27	LMG	B	620	-	48,48,55	0.19	0	56,56,63	0.19	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	G	601	7	66,74,74	1.57	4 (6%)	73,114,114	1.65	8 (10%)
23	CLA	y	315	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	9 (11%)
27	LMG	A	409	-	53,53,55	0.19	0	61,61,63	0.19	0
27	LMG	R	617	-	51,51,55	0.18	0	59,59,63	0.26	0
23	CLA	A	402	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
23	CLA	s	609	15	56,64,73	1.62	5 (8%)	65,102,113	1.48	7 (10%)
23	CLA	a	403	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	7 (9%)
23	CLA	g	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	g	612	7	49,57,73	1.71	6 (12%)	55,93,113	1.60	7 (12%)
40	LUT	g	615	-	42,43,43	1.88	10 (23%)	51,60,60	2.93	21 (41%)
23	CLA	D	405	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	6 (7%)
23	CLA	r	612	14	49,57,73	1.72	6 (12%)	55,93,113	1.50	7 (12%)
39	CHL	g	606	-	50,58,74	1.87	5 (10%)	52,94,114	1.98	11 (21%)
39	CHL	r	607	-	66,74,74	1.60	4 (6%)	73,114,114	1.67	12 (16%)
23	CLA	B	601	-	49,57,73	1.70	5 (10%)	55,93,113	1.58	8 (14%)
23	CLA	b	612	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	y	304	7	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
26	SQD	L	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.40	6 (9%)
23	CLA	c	502	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
25	BCR	H	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
30	LHG	r	616	23	36,36,48	1.60	8 (22%)	39,42,54	0.82	2 (5%)
39	CHL	G	605	7	48,56,74	1.87	4 (8%)	51,92,114	2.09	12 (23%)
39	CHL	S	606	-	50,58,74	1.83	4 (8%)	52,94,114	1.96	11 (21%)
23	CLA	b	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
23	CLA	y	312	30	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
39	CHL	n	609	7	66,74,74	1.56	4 (6%)	73,114,114	1.61	10 (13%)
23	CLA	C	513	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	9 (11%)
27	LMG	w	201	-	48,48,55	0.19	0	56,56,63	0.18	0
40	LUT	y	316	-	42,43,43	1.80	10 (23%)	51,60,60	2.77	19 (37%)
23	CLA	S	611	15	49,57,73	1.71	5 (10%)	55,93,113	1.53	7 (12%)
30	LHG	d	408	-	48,48,48	1.36	8 (16%)	51,54,54	0.74	2 (3%)
30	LHG	A	412	-	36,36,48	1.52	8 (22%)	39,42,54	0.89	2 (5%)
39	CHL	Y	308	-	50,58,74	1.82	5 (10%)	52,94,114	1.93	8 (15%)
31	LNL	C	521	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
23	CLA	g	604	-	49,57,73	1.71	5 (10%)	55,93,113	1.55	8 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	y	311	7	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
23	CLA	s	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.58	8 (14%)
23	CLA	R	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
40	LUT	g	616	-	42,43,43	2.40	19 (45%)	51,60,60	3.11	21 (41%)
28	3PH	T	101	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
31	LNL	C	518	-	19,19,19	0.44	0	18,19,19	0.97	1 (5%)
39	CHL	R	605	-	50,58,74	1.81	4 (8%)	52,94,114	1.91	11 (21%)
39	CHL	g	605	7	48,56,74	1.83	4 (8%)	51,92,114	2.11	11 (21%)
29	PL9	A	411	-	55,55,55	0.11	0	68,69,69	0.42	0
23	CLA	S	609	15	56,64,73	1.60	5 (8%)	65,102,113	1.43	8 (12%)
27	LMG	c	523	-	46,46,55	0.19	0	54,54,63	0.17	0
33	DGD	d	411	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
23	CLA	R	602	14	65,73,73	1.48	5 (7%)	76,113,113	1.38	6 (7%)
23	CLA	a	407	-	60,68,73	1.54	5 (8%)	70,107,113	1.46	9 (12%)
39	CHL	g	607	-	66,74,74	1.57	4 (6%)	73,114,114	1.71	9 (12%)
23	CLA	Y	313	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	614	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
28	3PH	d	403	-	37,37,47	0.71	1 (2%)	41,42,52	0.66	1 (2%)
39	CHL	G	620	-	66,74,74	1.58	5 (7%)	73,114,114	1.71	12 (16%)
30	LHG	d	404	-	48,48,48	1.36	8 (16%)	51,54,54	0.78	2 (3%)
38	HEM	F	501	-	41,50,50	1.47	3 (7%)	45,82,82	1.42	6 (13%)
39	CHL	g	619	43	66,74,74	1.58	5 (7%)	73,114,114	1.70	11 (15%)
30	LHG	n	619	23	44,44,48	1.45	8 (18%)	47,50,54	0.75	2 (4%)
40	LUT	s	615	-	42,43,43	2.55	21 (50%)	51,60,60	3.15	24 (47%)
30	LHG	g	618	-	48,48,48	1.40	8 (16%)	51,54,54	0.77	2 (3%)
30	LHG	Y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.69	2 (3%)
25	BCR	V	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
23	CLA	R	609	14	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
39	CHL	R	606	-	66,74,74	1.56	5 (7%)	73,114,114	1.67	13 (17%)
23	CLA	C	502	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
39	CHL	N	601	7	66,74,74	1.59	5 (7%)	73,114,114	1.67	10 (13%)
23	CLA	b	611	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
31	LNL	A	413	-	19,19,19	0.44	0	18,19,19	0.89	1 (5%)
39	CHL	g	609	7	66,74,74	1.60	4 (6%)	73,114,114	1.68	12 (16%)
23	CLA	A	406	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	G	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.71	10 (13%)
31	LNL	c	520	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
26	SQD	a	409	-	47,48,54	1.61	7 (14%)	56,59,65	1.45	6 (10%)
39	CHL	n	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.69	9 (12%)
23	CLA	g	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
27	LMG	r	617	-	51,51,55	0.19	0	59,59,63	0.16	0
23	CLA	s	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	c	507	43	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
40	LUT	S	614	-	42,43,43	2.60	21 (50%)	51,60,60	3.23	25 (49%)
39	CHL	y	308	43	50,58,74	1.80	5 (10%)	52,94,114	1.92	10 (19%)
23	CLA	b	610	43	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	b	615	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
23	CLA	b	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
39	CHL	g	608	-	50,58,74	1.85	5 (10%)	52,94,114	1.84	9 (17%)
36	BCT	d	401	22	2,3,3	1.15	0	2,3,3	4.51	2 (100%)
23	CLA	c	504	43	65,73,73	1.49	6 (9%)	76,113,113	1.38	6 (7%)
30	LHG	y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.71	2 (3%)
39	CHL	S	601	-	52,60,74	1.77	5 (9%)	56,97,114	1.87	11 (19%)
23	CLA	b	614	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	c	501	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
39	CHL	n	608	-	50,58,74	1.82	5 (10%)	52,94,114	1.94	10 (19%)
23	CLA	B	605	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
39	CHL	Y	309	7	66,74,74	1.60	4 (6%)	73,114,114	1.61	9 (12%)
40	LUT	n	616	-	42,43,43	2.36	19 (45%)	51,60,60	3.07	21 (41%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
30	LHG	D	404	-	42,42,48	1.43	8 (19%)	45,48,54	0.80	2 (4%)
23	CLA	B	610	43	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
31	LNL	a	413	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	s	610	30	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
29	PL9	D	407	-	55,55,55	0.08	0	68,69,69	0.21	0
23	CLA	R	608	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
41	NEX	n	618	-	38,46,46	4.08	32 (84%)	50,70,70	4.99	22 (44%)
39	CHL	n	605	7	48,56,74	1.86	5 (10%)	51,92,114	2.06	10 (19%)
39	CHL	s	605	-	50,58,74	1.81	3 (6%)	52,94,114	1.94	10 (19%)
23	CLA	Y	303	7	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LNL	B	623	-	19,19,19	0.45	0	18,19,19	0.86	1 (5%)
39	CHL	g	601	7	66,74,74	1.56	4 (6%)	73,114,114	1.64	8 (10%)
27	LMG	b	628	-	50,50,55	0.19	0	58,58,63	0.18	0
41	NEX	Y	317	-	38,46,46	4.00	31 (81%)	50,70,70	4.95	22 (44%)
39	CHL	s	606	-	50,58,74	1.81	5 (10%)	52,94,114	1.89	10 (19%)
23	CLA	s	612	15	55,63,73	1.61	6 (10%)	64,101,113	1.48	7 (10%)
31	LNL	C	519	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
39	CHL	s	607	-	49,57,74	1.85	5 (10%)	52,93,114	1.87	11 (21%)
28	3PH	W	201	-	45,45,47	0.64	1 (2%)	49,50,52	0.60	1 (2%)
35	VIV	C	523	-	32,32,32	0.93	2 (6%)	41,45,45	1.14	4 (9%)
23	CLA	N	612	7	49,57,73	1.71	6 (12%)	55,93,113	1.54	7 (12%)
42	XAT	y	302	-	39,47,47	3.39	24 (61%)	54,74,74	4.46	31 (57%)
23	CLA	S	612	15	55,63,73	1.62	6 (10%)	64,101,113	1.49	7 (10%)
23	CLA	Y	314	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	9 (11%)
23	CLA	g	602	7	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
25	BCR	h	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
27	LMG	D	409	-	36,36,55	0.20	0	44,44,63	0.14	0
30	LHG	L	103	-	48,48,48	1.36	8 (16%)	51,54,54	0.71	2 (3%)
25	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	CLA	B	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.46	8 (10%)
23	CLA	C	506	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	9 (14%)
23	CLA	B	612	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
23	CLA	c	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	A	404	43	49,57,73	1.70	6 (12%)	55,93,113	1.57	8 (14%)
39	CHL	Y	302	7	66,74,74	1.59	5 (7%)	73,114,114	1.63	10 (13%)
39	CHL	r	606	-	66,74,74	1.56	4 (6%)	73,114,114	1.65	12 (16%)
25	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
37	DGA	b	626	-	43,43,43	0.19	0	45,45,45	0.15	0
41	NEX	R	614	-	38,46,46	4.09	32 (84%)	50,70,70	4.87	22 (44%)
40	LUT	N	616	-	42,43,43	2.59	22 (52%)	51,60,60	3.21	22 (43%)
26	SQD	A	408	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
23	CLA	c	503	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
23	CLA	S	603	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	7 (12%)
23	CLA	G	610	7	65,73,73	1.46	5 (7%)	76,113,113	1.44	8 (10%)
42	XAT	R	615	-	39,47,47	3.21	20 (51%)	54,74,74	4.68	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	N	605	7	50,58,74	1.82	5 (10%)	52,94,114	2.16	9 (17%)
39	CHL	S	605	-	50,58,74	1.80	3 (6%)	52,94,114	1.99	9 (17%)
23	CLA	g	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	n	612	7	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
32	PAM	b	621	-	17,17,17	0.63	0	17,17,17	0.78	0
23	CLA	S	602	15	57,65,73	1.60	6 (10%)	66,103,113	1.45	8 (12%)
23	CLA	Y	305	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
33	DGD	C	515	-	67,67,67	0.88	2 (2%)	81,81,81	1.46	10 (12%)
23	CLA	r	609	14	65,73,73	1.47	6 (9%)	76,113,113	1.35	8 (10%)
23	CLA	y	313	7	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
41	NEX	S	617	-	19,23,46	4.24	16 (84%)	23,33,70	4.24	11 (47%)
23	CLA	b	601	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
23	CLA	R	610	30	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
23	CLA	C	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	C	511	3	65,73,73	1.48	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	g	610	7	65,73,73	1.46	5 (7%)	76,113,113	1.43	8 (10%)
31	LNL	B	624	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
23	CLA	y	306	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	G	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
23	CLA	d	405	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
23	CLA	n	611	30	49,57,73	1.73	5 (10%)	55,93,113	1.52	8 (14%)
23	CLA	b	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	r	610	30	65,73,73	1.49	5 (7%)	76,113,113	1.42	8 (10%)
23	CLA	n	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.58	8 (14%)
25	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
39	CHL	y	309	-	50,58,74	1.82	4 (8%)	52,94,114	1.89	8 (15%)
23	CLA	b	606	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	9 (11%)
23	CLA	A	403	43	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
39	CHL	N	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.68	9 (12%)
25	BCR	z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
23	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
31	LNL	A	414	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
29	PL9	a	411	-	55,55,55	0.11	0	68,69,69	0.28	0
23	CLA	y	314	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
41	NEX	r	614	-	38,46,46	3.97	31 (81%)	50,70,70	4.87	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	N	609	7	66,74,74	1.57	4 (6%)	73,114,114	1.62	10 (13%)
25	BCR	c	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
31	LNL	c	522	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)

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	Y	311	30	1/1/15/20	7/37/115/115	-
23	CLA	n	602	7	1/1/15/20	11/37/115/115	-
28	3PH	L	102	-	-	14/42/42/49	-
23	CLA	G	613	7	1/1/15/20	12/37/115/115	-
39	CHL	G	609	7	3/3/20/26	12/39/137/137	-
23	CLA	Y	304	-	1/1/15/20	12/37/115/115	-
38	HEM	f	501	6,5	-	1/12/54/54	-
23	CLA	N	604	-	1/1/11/20	7/18/96/115	-
28	3PH	w	202	-	-	17/49/49/49	-
28	3PH	x	201	-	-	13/47/47/49	-
27	LMG	C	525	-	-	10/40/60/70	0/1/1/1
39	CHL	N	608	-	3/3/16/26	6/20/118/137	-
23	CLA	G	604	-	1/1/11/20	6/18/96/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
28	3PH	a	410	-	-	21/49/49/49	-
23	CLA	B	611	-	1/1/15/20	10/37/115/115	-
23	CLA	s	611	15	1/1/11/20	8/18/96/115	-
31	LNL	i	101	-	-	9/17/17/17	-
42	XAT	N	619	-	-	13/31/93/93	0/4/4/4
28	3PH	D	403	-	-	13/39/39/49	-
23	CLA	R	611	-	1/1/11/20	6/18/96/115	-
23	CLA	r	611	-	1/1/11/20	6/18/96/115	-
23	CLA	s	603	-	1/1/11/20	12/18/96/115	-
23	CLA	s	608	-	1/1/11/20	7/18/96/115	-
23	CLA	N	611	30	1/1/15/20	9/37/115/115	-
23	CLA	r	603	-	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/14/20	8/31/109/115	-
23	CLA	c	508	-	1/1/15/20	3/37/115/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/15/20	12/37/115/115	-
41	NEX	G	617	-	-	7/16/47/83	0/2/2/3
25	BCR	b	617	-	-	11/29/63/63	0/2/2/2
39	CHL	Y	306	7	3/3/16/26	2/18/116/137	-
23	CLA	n	613	7	1/1/15/20	6/37/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
31	LNL	B	622	-	-	7/17/17/17	-
39	CHL	Y	307	-	3/3/20/26	3/39/137/137	-
31	LNL	B	625	-	-	7/17/17/17	-
39	CHL	y	307	7	3/3/16/26	2/18/116/137	-
31	LNL	c	518	-	-	12/17/17/17	-
28	3PH	X	201	-	-	13/47/47/49	-
23	CLA	S	608	-	1/1/11/20	1/18/96/115	-
33	DGD	H	502	-	-	24/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/15/20	11/37/115/115	-
26	SQD	M	101	-	-	24/45/65/69	0/1/1/1
23	CLA	n	610	7	1/1/15/20	11/37/115/115	-
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
31	LNL	c	519	-	-	11/17/17/17	-
23	CLA	N	602	7	1/1/15/20	4/37/115/115	-
23	CLA	B	607	-	1/1/15/20	21/37/115/115	-
32	PAM	B	621	-	-	5/15/15/15	-
39	CHL	n	606	-	3/3/20/26	8/39/137/137	-
40	LUT	Y	316	-	-	15/29/67/67	0/2/2/2
40	LUT	Y	315	-	-	17/29/67/67	0/2/2/2
25	BCR	d	410	-	-	9/29/63/63	0/2/2/2
42	XAT	n	617	-	-	6/31/93/93	0/4/4/4
42	XAT	n	620	-	-	9/31/93/93	0/4/4/4
31	LNL	c	521	-	-	7/17/17/17	-
23	CLA	C	503	-	1/1/15/20	8/37/115/115	-
39	CHL	N	606	-	3/3/20/26	9/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LUT	G	616	-	-	9/29/67/67	0/2/2/2
30	LHG	b	627	-	-	22/53/53/53	-
23	CLA	C	504	43	1/1/15/20	8/37/115/115	-
23	CLA	C	501	-	1/1/15/20	12/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
30	LHG	S	616	23	-	14/53/53/53	-
31	LNL	c	517	-	-	5/17/17/17	-
37	DGA	D	410	-	-	12/41/41/45	-
41	NEX	g	617	-	-	14/27/83/83	0/3/3/3
23	CLA	B	608	-	1/1/15/20	10/37/115/115	-
39	CHL	y	310	7	3/3/20/26	8/39/137/137	-
23	CLA	r	604	43	1/1/13/20	8/25/103/115	-
31	LNL	b	624	-	-	9/17/17/17	-
39	CHL	R	607	-	3/3/20/26	9/39/137/137	-
23	CLA	N	613	-	1/1/15/20	12/37/115/115	-
25	BCR	D	411	-	-	5/29/63/63	0/2/2/2
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
30	LHG	R	616	23	-	17/42/42/53	-
23	CLA	R	601	14	1/1/11/20	10/18/96/115	-
39	CHL	G	608	-	3/3/16/26	8/20/118/137	-
23	CLA	g	614	-	1/1/11/20	6/18/96/115	-
31	LNL	b	625	-	-	9/17/17/17	-
23	CLA	N	610	7	1/1/15/20	10/37/115/115	-
23	CLA	n	603	-	1/1/15/20	11/37/115/115	-
40	LUT	y	317	-	-	15/29/67/67	0/2/2/2
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
23	CLA	c	511	3	1/1/15/20	12/37/115/115	-
23	CLA	b	604	-	1/1/15/20	6/37/115/115	-
23	CLA	b	616	-	1/1/15/20	12/37/115/115	-
31	LNL	C	520	-	-	11/17/17/17	-
25	BCR	B	618	-	-	3/29/60/63	0/2/2/2
23	CLA	r	602	14	1/1/15/20	13/37/115/115	-
31	LNL	a	401	-	-	11/17/17/17	-
23	CLA	S	610	30	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	n	614	-	1/1/11/20	10/18/96/115	-
23	CLA	r	608	-	1/1/15/20	9/37/115/115	-
23	CLA	c	512	-	1/1/15/20	21/37/115/115	-
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
39	CHL	G	606	-	3/3/16/26	4/20/118/137	-
23	CLA	B	602	-	1/1/15/20	14/37/115/115	-
28	3PH	A	410	-	-	18/49/49/49	-
30	LHG	G	618	23	-	19/53/53/53	-
23	CLA	C	509	-	1/1/15/20	10/37/115/115	-
23	CLA	G	614	-	1/1/11/20	6/18/96/115	-
23	CLA	Y	312	7	1/1/15/20	9/37/115/115	-
23	CLA	C	507	43	1/1/15/20	9/37/115/115	-
29	PL9	d	407	-	-	10/53/73/73	0/1/1/1
39	CHL	r	605	-	3/3/16/26	6/20/118/137	-
24	PHO	A	405	-	-	10/37/103/103	0/5/6/6
23	CLA	c	506	-	1/1/15/20	15/37/115/115	-
23	CLA	B	609	-	1/1/15/20	8/37/115/115	-
23	CLA	C	508	-	1/1/15/20	7/37/115/115	-
42	XAT	G	619	-	-	11/31/93/93	0/4/4/4
23	CLA	S	613	-	1/1/15/20	14/37/115/115	-
23	CLA	Y	310	7	1/1/15/20	13/37/115/115	-
30	LHG	s	616	23	-	19/53/53/53	-
23	CLA	G	611	30	1/1/11/20	8/18/96/115	-
40	LUT	n	615	-	-	14/29/67/67	0/2/2/2
35	VIV	y	301	-	-	15/19/30/30	0/2/2/2
28	3PH	s	618	-	-	14/39/39/49	-
31	LNL	C	522	-	-	11/17/17/17	-
28	3PH	C	524	-	-	19/49/49/49	-
30	LHG	N	618	23	-	25/53/53/53	-
30	LHG	D	408	-	-	29/53/53/53	-
23	CLA	b	613	-	1/1/15/20	13/37/115/115	-
25	BCR	a	408	-	-	4/29/63/63	0/2/2/2
23	CLA	N	614	-	1/1/11/20	7/18/96/115	-
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	617	-	-	10/29/63/63	0/2/2/2
30	LHG	a	412	-	-	26/53/53/53	-
23	CLA	s	602	15	1/1/13/20	9/28/106/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
24	PHO	d	402	-	-	5/37/103/103	0/5/6/6
41	NEX	s	617	-	-	8/15/40/83	0/1/1/3
23	CLA	d	406	-	1/1/15/20	7/37/115/115	-
41	NEX	R	618	-	-	12/27/83/83	0/3/3/3
23	CLA	c	509	-	1/1/15/20	10/37/115/115	-
42	XAT	r	615	-	-	14/31/93/93	0/4/4/4
23	CLA	B	606	-	1/1/15/20	9/37/115/115	-
23	CLA	D	406	-	1/1/15/20	15/37/115/115	-
31	LNL	C	517	-	-	12/17/17/17	-
31	LNL	b	623	-	-	10/17/17/17	-
23	CLA	a	404	43	1/1/15/20	11/37/115/115	-
23	CLA	r	601	14	1/1/11/20	10/18/96/115	-
23	CLA	G	602	7	1/1/15/20	5/37/115/115	-
40	LUT	r	613	-	-	11/29/67/67	0/2/2/2
27	LMG	B	626	-	-	8/44/64/70	0/1/1/1
33	DGD	c	515	-	-	13/44/84/95	0/2/2/2
39	CHL	S	607	-	3/3/16/26	5/19/117/137	-
39	CHL	s	601	-	3/3/17/26	6/23/121/137	-
23	CLA	y	305	-	1/1/15/20	12/37/115/115	-
23	CLA	b	609	-	1/1/15/20	10/37/115/115	-
40	LUT	s	614	-	-	18/29/67/67	0/2/2/2
40	LUT	N	615	-	-	13/29/67/67	0/2/2/2
40	LUT	S	615	-	-	16/29/67/67	0/2/2/2
23	CLA	S	604	-	1/1/11/20	7/18/96/115	-
25	BCR	v	101	-	-	10/29/63/63	0/2/2/2
39	CHL	n	601	7	3/3/20/26	8/39/137/137	-
23	CLA	G	612	7	1/1/11/20	6/18/96/115	-
40	LUT	G	615	-	-	22/29/67/67	0/2/2/2
39	CHL	y	303	7	3/3/20/26	13/39/137/137	-
31	LNL	b	622	-	-	8/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LNL	I	101	-	-	11/17/17/17	-
41	NEX	N	617	-	-	12/27/83/83	0/3/3/3
23	CLA	C	510	-	1/1/15/20	12/37/115/115	-
23	CLA	C	512	-	1/1/15/20	17/37/115/115	-
23	CLA	N	603	-	1/1/15/20	10/37/115/115	-
23	CLA	R	604	43	1/1/13/20	9/25/103/115	-
23	CLA	R	612	14	1/1/11/20	8/18/96/115	-
40	LUT	R	613	-	-	16/29/67/67	0/2/2/2
23	CLA	b	605	-	1/1/15/20	15/37/115/115	-
24	PHO	a	406	-	-	10/37/103/103	0/5/6/6
23	CLA	a	405	43	1/1/11/20	1/18/96/115	-
42	XAT	Y	301	-	-	17/31/93/93	0/4/4/4
27	LMG	B	620	-	-	7/43/63/70	0/1/1/1
39	CHL	G	601	7	3/3/20/26	9/39/137/137	-
23	CLA	y	315	-	1/1/15/20	18/37/115/115	-
27	LMG	A	409	-	-	11/48/68/70	0/1/1/1
27	LMG	R	617	-	-	14/46/66/70	0/1/1/1
23	CLA	A	402	-	1/1/15/20	10/37/115/115	-
23	CLA	s	609	15	1/1/13/20	11/27/105/115	-
23	CLA	a	403	-	1/1/15/20	10/37/115/115	-
23	CLA	g	603	-	1/1/15/20	10/37/115/115	-
23	CLA	g	612	7	1/1/11/20	6/18/96/115	-
40	LUT	g	615	-	-	19/29/67/67	0/2/2/2
23	CLA	D	405	-	1/1/15/20	9/37/115/115	-
23	CLA	r	612	14	1/1/11/20	5/18/96/115	-
39	CHL	g	606	-	3/3/16/26	4/20/118/137	-
39	CHL	r	607	-	3/3/20/26	9/39/137/137	-
23	CLA	B	601	-	1/1/11/20	10/18/96/115	-
23	CLA	b	612	-	1/1/15/20	12/37/115/115	-
23	CLA	y	304	7	1/1/15/20	13/37/115/115	-
26	SQD	L	101	-	-	24/49/69/69	0/1/1/1
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
25	BCR	H	501	-	-	7/29/63/63	0/2/2/2
39	CHL	S	606	-	3/3/16/26	6/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	G	605	7	3/3/16/26	6/18/116/137	-
30	LHG	r	616	23	-	19/41/41/53	-
23	CLA	b	607	-	1/1/15/20	16/37/115/115	-
23	CLA	y	312	30	1/1/15/20	7/37/115/115	-
39	CHL	n	609	7	3/3/20/26	8/39/137/137	-
23	CLA	C	513	-	1/1/15/20	12/37/115/115	-
27	LMG	w	201	-	-	5/43/63/70	0/1/1/1
40	LUT	y	316	-	-	17/29/67/67	0/2/2/2
23	CLA	S	611	15	1/1/11/20	9/18/96/115	-
30	LHG	d	408	-	-	15/53/53/53	-
30	LHG	A	412	-	-	21/41/41/53	-
39	CHL	Y	308	-	3/3/16/26	6/20/118/137	-
31	LNL	C	521	-	-	11/17/17/17	-
23	CLA	g	604	-	1/1/11/20	8/18/96/115	-
23	CLA	y	311	7	1/1/15/20	10/37/115/115	-
23	CLA	s	604	-	1/1/11/20	8/18/96/115	-
23	CLA	R	603	-	1/1/14/20	5/31/109/115	-
40	LUT	g	616	-	-	10/29/67/67	0/2/2/2
28	3PH	T	101	-	-	22/49/49/49	-
31	LNL	C	518	-	-	8/17/17/17	-
39	CHL	R	605	-	3/3/16/26	2/20/118/137	-
39	CHL	g	605	7	3/3/16/26	5/18/116/137	-
29	PL9	A	411	-	-	7/53/73/73	0/1/1/1
23	CLA	S	609	15	1/1/13/20	12/27/105/115	-
27	LMG	c	523	-	-	9/41/61/70	0/1/1/1
33	DGD	d	411	-	-	18/51/91/95	0/2/2/2
23	CLA	R	602	14	1/1/15/20	6/37/115/115	-
23	CLA	a	407	-	1/1/14/20	5/31/109/115	-
39	CHL	g	607	-	3/3/20/26	13/39/137/137	-
23	CLA	Y	313	-	1/1/15/20	10/37/115/115	-
23	CLA	B	614	-	1/1/15/20	13/37/115/115	-
28	3PH	d	403	-	-	10/39/39/49	-
39	CHL	G	620	-	3/3/20/26	12/39/137/137	-
30	LHG	d	404	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEM	F	501	-	-	3/12/54/54	-
39	CHL	g	619	43	3/3/20/26	8/39/137/137	-
30	LHG	n	619	23	-	23/49/49/53	-
40	LUT	s	615	-	-	11/29/67/67	0/2/2/2
30	LHG	g	618	-	-	15/53/53/53	-
30	LHG	Y	318	23	-	21/53/53/53	-
25	BCR	V	101	-	-	11/29/63/63	0/2/2/2
23	CLA	R	609	14	1/1/15/20	6/37/115/115	-
39	CHL	R	606	-	3/3/20/26	9/39/137/137	-
23	CLA	C	502	-	1/1/15/20	12/37/115/115	-
39	CHL	N	601	7	3/3/20/26	7/39/137/137	-
23	CLA	b	611	-	1/1/15/20	6/37/115/115	-
31	LNL	A	413	-	-	10/17/17/17	-
39	CHL	g	609	7	3/3/20/26	11/39/137/137	-
23	CLA	A	406	-	1/1/14/20	1/31/109/115	-
39	CHL	G	607	-	3/3/20/26	9/39/137/137	-
31	LNL	c	520	-	-	6/17/17/17	-
26	SQD	a	409	-	-	18/43/63/69	0/1/1/1
39	CHL	n	607	-	3/3/20/26	8/39/137/137	-
23	CLA	g	611	-	1/1/15/20	11/37/115/115	-
27	LMG	r	617	-	-	11/46/66/70	0/1/1/1
23	CLA	s	613	-	1/1/15/20	16/37/115/115	-
23	CLA	c	507	43	1/1/15/20	6/37/115/115	-
40	LUT	S	614	-	-	15/29/67/67	0/2/2/2
39	CHL	y	308	43	3/3/16/26	3/20/118/137	-
23	CLA	b	610	43	1/1/15/20	10/37/115/115	-
23	CLA	b	615	-	1/1/15/20	6/37/115/115	-
23	CLA	b	603	-	1/1/15/20	11/37/115/115	-
39	CHL	g	608	-	3/3/16/26	8/20/118/137	-
23	CLA	c	504	43	1/1/15/20	8/37/115/115	-
30	LHG	y	318	23	-	22/53/53/53	-
39	CHL	S	601	-	3/3/17/26	4/23/121/137	-
23	CLA	b	614	-	1/1/15/20	12/37/115/115	-
23	CLA	c	501	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	n	608	-	3/3/16/26	4/20/118/137	-
23	CLA	B	605	-	1/1/15/20	13/37/115/115	-
39	CHL	Y	309	7	3/3/20/26	4/39/137/137	-
40	LUT	n	616	-	-	14/29/67/67	0/2/2/2
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LHG	D	404	-	-	10/47/47/53	-
23	CLA	B	610	43	1/1/15/20	8/37/115/115	-
31	LNL	a	413	-	-	9/17/17/17	-
23	CLA	s	610	30	1/1/15/20	14/37/115/115	-
29	PL9	D	407	-	-	10/53/73/73	0/1/1/1
23	CLA	R	608	-	1/1/15/20	7/37/115/115	-
41	NEX	n	618	-	-	14/27/83/83	0/3/3/3
39	CHL	n	605	7	3/3/16/26	4/18/116/137	-
39	CHL	s	605	-	3/3/16/26	5/20/118/137	-
23	CLA	Y	303	7	1/1/15/20	13/37/115/115	-
31	LNL	B	623	-	-	10/17/17/17	-
39	CHL	g	601	7	3/3/20/26	6/39/137/137	-
27	LMG	b	628	-	-	11/45/65/70	0/1/1/1
41	NEX	Y	317	-	-	14/27/83/83	0/3/3/3
39	CHL	s	606	-	3/3/16/26	4/20/118/137	-
23	CLA	s	612	15	1/1/13/20	7/25/103/115	-
31	LNL	C	519	-	-	5/17/17/17	-
39	CHL	s	607	-	3/3/16/26	6/19/117/137	-
28	3PH	W	201	-	-	23/47/47/49	-
35	VIV	C	523	-	-	12/19/30/30	0/2/2/2
23	CLA	N	612	7	1/1/11/20	9/18/96/115	-
42	XAT	y	302	-	-	18/31/93/93	0/4/4/4
23	CLA	S	612	15	1/1/13/20	9/25/103/115	-
23	CLA	Y	314	-	1/1/15/20	11/37/115/115	-
23	CLA	g	602	7	1/1/15/20	5/37/115/115	-
25	BCR	h	501	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	1/31/51/70	0/1/1/1
30	LHG	L	103	-	-	25/53/53/53	-
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	604	-	1/1/15/20	9/37/115/115	-
23	CLA	C	506	-	1/1/13/20	9/25/103/115	-
23	CLA	B	612	-	1/1/15/20	11/37/115/115	-
23	CLA	c	505	-	1/1/15/20	8/37/115/115	-
23	CLA	A	404	43	1/1/11/20	4/18/96/115	-
39	CHL	Y	302	7	3/3/20/26	11/39/137/137	-
39	CHL	r	606	-	3/3/20/26	10/39/137/137	-
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
37	DGA	b	626	-	-	14/45/45/45	-
41	NEX	R	614	-	-	13/27/83/83	0/3/3/3
40	LUT	N	616	-	-	20/29/67/67	0/2/2/2
26	SQD	A	408	-	-	29/45/65/69	0/1/1/1
23	CLA	c	503	-	1/1/15/20	7/37/115/115	-
23	CLA	S	603	-	1/1/11/20	12/18/96/115	-
23	CLA	G	610	7	1/1/15/20	10/37/115/115	-
42	XAT	R	615	-	-	14/31/93/93	0/4/4/4
39	CHL	N	605	7	3/3/16/26	5/20/118/137	-
39	CHL	S	605	-	3/3/16/26	6/20/118/137	-
23	CLA	g	613	-	1/1/15/20	10/37/115/115	-
23	CLA	n	612	7	1/1/11/20	5/18/96/115	-
32	PAM	b	621	-	-	3/15/15/15	-
23	CLA	S	602	15	1/1/13/20	10/28/106/115	-
23	CLA	Y	305	-	1/1/15/20	12/37/115/115	-
33	DGD	C	515	-	-	20/55/95/95	0/2/2/2
23	CLA	r	609	14	1/1/15/20	7/37/115/115	-
23	CLA	y	313	7	1/1/15/20	9/37/115/115	-
41	NEX	S	617	-	-	6/11/36/83	0/1/1/3
23	CLA	b	601	-	1/1/12/20	5/19/97/115	-
23	CLA	R	610	30	1/1/15/20	9/37/115/115	-
23	CLA	C	505	-	1/1/15/20	6/37/115/115	-
23	CLA	C	511	3	1/1/15/20	11/37/115/115	-
23	CLA	g	610	7	1/1/15/20	10/37/115/115	-
31	LNL	B	624	-	-	8/17/17/17	-
23	CLA	y	306	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	603	-	1/1/14/20	3/31/109/115	-
23	CLA	d	405	-	1/1/15/20	7/37/115/115	-
23	CLA	n	611	30	1/1/11/20	5/18/96/115	-
23	CLA	b	608	-	1/1/15/20	10/37/115/115	-
23	CLA	r	610	30	1/1/15/20	10/37/115/115	-
23	CLA	n	604	-	1/1/11/20	7/18/96/115	-
39	CHL	y	309	-	3/3/16/26	3/20/118/137	-
25	BCR	A	407	-	-	4/29/63/63	0/2/2/2
23	CLA	b	606	-	1/1/15/20	10/37/115/115	-
23	CLA	A	403	43	1/1/15/20	10/37/115/115	-
39	CHL	N	607	-	3/3/20/26	7/39/137/137	-
25	BCR	z	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/15/20	10/37/115/115	-
31	LNL	A	414	-	-	8/17/17/17	-
29	PL9	a	411	-	-	12/53/73/73	0/1/1/1
23	CLA	y	314	-	1/1/15/20	14/37/115/115	-
41	NEX	r	614	-	-	9/27/83/83	0/3/3/3
39	CHL	N	609	7	3/3/20/26	7/39/137/137	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
31	LNL	c	522	-	-	7/17/17/17	-

All (2109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	609	CHL	C4B-NB	11.99	1.45	1.35
39	G	606	CHL	C4B-NB	11.72	1.45	1.35
39	g	606	CHL	C4B-NB	11.72	1.45	1.35
39	g	608	CHL	C4B-NB	11.53	1.45	1.35
39	G	608	CHL	C4B-NB	11.52	1.45	1.35
39	G	605	CHL	C4B-NB	11.50	1.45	1.35
39	g	609	CHL	C4B-NB	11.44	1.45	1.35
39	Y	309	CHL	C4B-NB	11.44	1.45	1.35
39	r	607	CHL	C4B-NB	11.43	1.45	1.35
39	R	607	CHL	C4B-NB	11.40	1.45	1.35
39	s	607	CHL	C4B-NB	11.39	1.45	1.35
39	n	601	CHL	C4B-NB	11.39	1.45	1.35
39	N	601	CHL	C4B-NB	11.38	1.45	1.35
39	S	607	CHL	C4B-NB	11.38	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	302	CHL	C4B-NB	11.36	1.45	1.35
39	S	606	CHL	C4B-NB	11.36	1.45	1.35
39	Y	308	CHL	C4B-NB	11.32	1.45	1.35
39	n	606	CHL	C4B-NB	11.30	1.45	1.35
39	y	309	CHL	C4B-NB	11.29	1.45	1.35
39	N	606	CHL	C4B-NB	11.29	1.45	1.35
39	g	619	CHL	C4B-NB	11.28	1.45	1.35
39	n	608	CHL	C4B-NB	11.28	1.45	1.35
39	N	605	CHL	C4B-NB	11.28	1.45	1.35
39	s	605	CHL	C4B-NB	11.27	1.45	1.35
39	R	605	CHL	C4B-NB	11.27	1.45	1.35
39	n	607	CHL	C4B-NB	11.27	1.45	1.35
39	S	605	CHL	C4B-NB	11.26	1.45	1.35
39	n	605	CHL	C4B-NB	11.26	1.45	1.35
39	y	303	CHL	C4B-NB	11.26	1.45	1.35
39	G	607	CHL	C4B-NB	11.25	1.45	1.35
39	s	606	CHL	C4B-NB	11.23	1.45	1.35
39	N	608	CHL	C4B-NB	11.23	1.45	1.35
39	N	607	CHL	C4B-NB	11.22	1.45	1.35
39	s	601	CHL	C4B-NB	11.20	1.45	1.35
39	G	620	CHL	C4B-NB	11.18	1.45	1.35
39	N	609	CHL	C4B-NB	11.18	1.45	1.35
39	g	607	CHL	C4B-NB	11.17	1.45	1.35
39	y	310	CHL	C4B-NB	11.17	1.45	1.35
39	S	601	CHL	C4B-NB	11.17	1.45	1.35
39	Y	306	CHL	C4B-NB	11.16	1.45	1.35
39	G	601	CHL	C4B-NB	11.16	1.45	1.35
39	Y	307	CHL	C4B-NB	11.15	1.45	1.35
39	g	605	CHL	C4B-NB	11.14	1.45	1.35
39	y	308	CHL	C4B-NB	11.13	1.45	1.35
39	y	307	CHL	C4B-NB	11.11	1.45	1.35
39	g	601	CHL	C4B-NB	11.10	1.45	1.35
39	R	606	CHL	C4B-NB	11.08	1.45	1.35
39	n	609	CHL	C4B-NB	11.08	1.45	1.35
39	r	605	CHL	C4B-NB	11.06	1.45	1.35
39	r	606	CHL	C4B-NB	11.02	1.45	1.35
42	y	302	XAT	C10-C9	8.32	1.46	1.35
40	s	614	LUT	C34-C33	8.21	1.46	1.35
42	n	620	XAT	C10-C9	8.08	1.46	1.35
40	N	616	LUT	C34-C33	8.05	1.46	1.35
40	S	615	LUT	C34-C33	8.04	1.46	1.35
42	N	619	XAT	C10-C9	7.97	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	301	XAT	C10-C9	7.94	1.46	1.35
40	S	614	LUT	C34-C33	7.89	1.46	1.35
41	G	617	NEX	C34-C33	7.84	1.46	1.35
40	R	613	LUT	C34-C33	7.84	1.46	1.35
23	B	606	CLA	C4B-NB	7.83	1.42	1.35
23	Y	312	CLA	C4B-NB	7.82	1.42	1.35
23	y	313	CLA	C4B-NB	7.77	1.42	1.35
40	s	615	LUT	C34-C33	7.74	1.46	1.35
40	N	615	LUT	C34-C33	7.73	1.46	1.35
40	r	613	LUT	C34-C33	7.72	1.46	1.35
23	b	606	CLA	C4B-NB	7.71	1.42	1.35
23	G	614	CLA	C4B-NB	7.67	1.42	1.35
23	s	608	CLA	C4B-NB	7.67	1.42	1.35
23	y	315	CLA	C4B-NB	7.65	1.42	1.35
23	R	601	CLA	C4B-NB	7.64	1.42	1.35
23	B	615	CLA	C4B-NB	7.64	1.42	1.35
23	N	611	CLA	C4B-NB	7.62	1.42	1.35
23	r	601	CLA	C4B-NB	7.61	1.42	1.35
23	S	610	CLA	C4B-NB	7.61	1.42	1.35
23	g	603	CLA	C4B-NB	7.60	1.42	1.35
23	R	612	CLA	C4B-NB	7.60	1.42	1.35
23	d	405	CLA	C4B-NB	7.59	1.42	1.35
23	y	306	CLA	C4B-NB	7.59	1.42	1.35
23	n	611	CLA	C4B-NB	7.58	1.42	1.35
23	r	612	CLA	C4B-NB	7.57	1.42	1.35
23	n	612	CLA	C4B-NB	7.56	1.42	1.35
23	y	314	CLA	C4B-NB	7.56	1.42	1.35
23	D	406	CLA	C4B-NB	7.56	1.41	1.35
23	s	610	CLA	C4B-NB	7.56	1.41	1.35
23	b	603	CLA	C4B-NB	7.55	1.41	1.35
23	s	613	CLA	C4B-NB	7.54	1.41	1.35
23	G	611	CLA	C4B-NB	7.54	1.41	1.35
23	D	405	CLA	C4B-NB	7.54	1.41	1.35
23	S	608	CLA	C4B-NB	7.53	1.41	1.35
23	c	511	CLA	C4B-NB	7.53	1.41	1.35
41	g	617	NEX	C34-C33	7.53	1.45	1.35
23	s	609	CLA	C4B-NB	7.52	1.41	1.35
23	n	614	CLA	C4B-NB	7.52	1.41	1.35
23	s	603	CLA	C4B-NB	7.52	1.41	1.35
23	G	612	CLA	C4B-NB	7.52	1.41	1.35
23	S	613	CLA	C4B-NB	7.51	1.41	1.35
23	B	610	CLA	C4B-NB	7.51	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	614	CLA	C4B-NB	7.50	1.41	1.35
23	g	614	CLA	C4B-NB	7.50	1.41	1.35
23	C	506	CLA	C4B-NB	7.50	1.41	1.35
23	S	612	CLA	C4B-NB	7.50	1.41	1.35
23	b	601	CLA	C4B-NB	7.50	1.41	1.35
23	R	610	CLA	C4B-NB	7.50	1.41	1.35
23	Y	305	CLA	C4B-NB	7.49	1.41	1.35
23	G	604	CLA	C4B-NB	7.49	1.41	1.35
23	N	604	CLA	C4B-NB	7.49	1.41	1.35
23	Y	313	CLA	C4B-NB	7.49	1.41	1.35
23	b	615	CLA	C4B-NB	7.49	1.41	1.35
23	n	604	CLA	C4B-NB	7.49	1.41	1.35
23	c	506	CLA	C4B-NB	7.49	1.41	1.35
23	c	504	CLA	C4B-NB	7.48	1.41	1.35
23	C	501	CLA	C4B-NB	7.48	1.41	1.35
23	N	613	CLA	C4B-NB	7.47	1.41	1.35
23	B	602	CLA	C4B-NB	7.47	1.41	1.35
23	c	505	CLA	C4B-NB	7.47	1.41	1.35
23	s	602	CLA	C4B-NB	7.46	1.41	1.35
23	R	609	CLA	C4B-NB	7.46	1.41	1.35
23	g	612	CLA	C4B-NB	7.46	1.41	1.35
23	Y	314	CLA	C4B-NB	7.46	1.41	1.35
23	c	501	CLA	C4B-NB	7.46	1.41	1.35
23	g	611	CLA	C4B-NB	7.45	1.41	1.35
23	B	605	CLA	C4B-NB	7.45	1.41	1.35
23	b	609	CLA	C4B-NB	7.45	1.41	1.35
23	C	504	CLA	C4B-NB	7.44	1.41	1.35
23	r	608	CLA	C4B-NB	7.44	1.41	1.35
23	R	604	CLA	C4B-NB	7.44	1.41	1.35
23	n	613	CLA	C4B-NB	7.44	1.41	1.35
23	C	505	CLA	C4B-NB	7.44	1.41	1.35
23	s	611	CLA	C4B-NB	7.44	1.41	1.35
23	s	612	CLA	C4B-NB	7.43	1.41	1.35
23	g	604	CLA	C4B-NB	7.43	1.41	1.35
23	S	602	CLA	C4B-NB	7.43	1.41	1.35
23	S	611	CLA	C4B-NB	7.43	1.41	1.35
23	c	507	CLA	C4B-NB	7.43	1.41	1.35
23	S	603	CLA	C4B-NB	7.43	1.41	1.35
23	B	607	CLA	C4B-NB	7.43	1.41	1.35
23	N	612	CLA	C4B-NB	7.43	1.41	1.35
23	R	608	CLA	C4B-NB	7.43	1.41	1.35
23	a	407	CLA	C4B-NB	7.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C4B-NB	7.42	1.41	1.35
23	C	507	CLA	C4B-NB	7.42	1.41	1.35
23	B	603	CLA	C4B-NB	7.42	1.41	1.35
23	R	611	CLA	C4B-NB	7.42	1.41	1.35
23	c	503	CLA	C4B-NB	7.42	1.41	1.35
23	r	611	CLA	C4B-NB	7.42	1.41	1.35
23	b	610	CLA	C4B-NB	7.41	1.41	1.35
23	y	304	CLA	C4B-NB	7.41	1.41	1.35
23	C	510	CLA	C4B-NB	7.41	1.41	1.35
23	r	610	CLA	C4B-NB	7.41	1.41	1.35
23	C	503	CLA	C4B-NB	7.41	1.41	1.35
23	c	510	CLA	C4B-NB	7.41	1.41	1.35
23	R	602	CLA	C4B-NB	7.41	1.41	1.35
23	b	612	CLA	C4B-NB	7.40	1.41	1.35
23	b	605	CLA	C4B-NB	7.40	1.41	1.35
23	B	614	CLA	C4B-NB	7.40	1.41	1.35
23	C	511	CLA	C4B-NB	7.40	1.41	1.35
23	A	402	CLA	C4B-NB	7.39	1.41	1.35
23	g	613	CLA	C4B-NB	7.39	1.41	1.35
23	r	602	CLA	C4B-NB	7.39	1.41	1.35
23	b	613	CLA	C4B-NB	7.39	1.41	1.35
23	S	604	CLA	C4B-NB	7.39	1.41	1.35
23	B	613	CLA	C4B-NB	7.39	1.41	1.35
23	Y	311	CLA	C4B-NB	7.38	1.41	1.35
23	C	502	CLA	C4B-NB	7.38	1.41	1.35
23	S	609	CLA	C4B-NB	7.38	1.41	1.35
23	y	312	CLA	C4B-NB	7.38	1.41	1.35
23	r	604	CLA	C4B-NB	7.37	1.41	1.35
40	G	616	LUT	C34-C33	7.37	1.45	1.35
23	b	608	CLA	C4B-NB	7.37	1.41	1.35
23	B	601	CLA	C4B-NB	7.37	1.41	1.35
23	G	603	CLA	C4B-NB	7.37	1.41	1.35
23	A	404	CLA	C4B-NB	7.37	1.41	1.35
23	G	613	CLA	C4B-NB	7.37	1.41	1.35
23	B	608	CLA	C4B-NB	7.36	1.41	1.35
23	C	512	CLA	C4B-NB	7.36	1.41	1.35
23	b	607	CLA	C4B-NB	7.36	1.41	1.35
23	c	502	CLA	C4B-NB	7.36	1.41	1.35
40	y	317	LUT	C34-C33	7.36	1.45	1.35
23	C	509	CLA	C4B-NB	7.36	1.41	1.35
23	c	509	CLA	C4B-NB	7.36	1.41	1.35
23	B	616	CLA	C4B-NB	7.35	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	602	CLA	C4B-NB	7.35	1.41	1.35
23	g	602	CLA	C4B-NB	7.34	1.41	1.35
23	r	603	CLA	C4B-NB	7.34	1.41	1.35
23	s	604	CLA	C4B-NB	7.34	1.41	1.35
23	C	508	CLA	C4B-NB	7.34	1.41	1.35
40	n	616	LUT	C34-C33	7.34	1.45	1.35
23	y	305	CLA	C4B-NB	7.33	1.41	1.35
23	d	406	CLA	C4B-NB	7.33	1.41	1.35
23	A	406	CLA	C4B-NB	7.33	1.41	1.35
23	C	513	CLA	C4B-NB	7.32	1.41	1.35
23	a	405	CLA	C4B-NB	7.32	1.41	1.35
23	a	403	CLA	C4B-NB	7.32	1.41	1.35
23	c	512	CLA	C4B-NB	7.32	1.41	1.35
23	b	614	CLA	C4B-NB	7.32	1.41	1.35
23	B	604	CLA	C4B-NB	7.32	1.41	1.35
23	n	602	CLA	C4B-NB	7.31	1.41	1.35
23	n	603	CLA	C4B-NB	7.31	1.41	1.35
23	r	609	CLA	C4B-NB	7.31	1.41	1.35
23	Y	303	CLA	C4B-NB	7.31	1.41	1.35
23	b	602	CLA	C4B-NB	7.31	1.41	1.35
23	b	616	CLA	C4B-NB	7.31	1.41	1.35
23	R	603	CLA	C4B-NB	7.30	1.41	1.35
40	g	616	LUT	C34-C33	7.30	1.45	1.35
23	b	604	CLA	C4B-NB	7.30	1.41	1.35
23	N	602	CLA	C4B-NB	7.28	1.41	1.35
23	B	612	CLA	C4B-NB	7.28	1.41	1.35
40	Y	316	LUT	C34-C33	7.28	1.45	1.35
23	n	610	CLA	C4B-NB	7.27	1.41	1.35
23	N	610	CLA	C4B-NB	7.26	1.41	1.35
23	c	513	CLA	C4B-NB	7.26	1.41	1.35
23	g	610	CLA	C4B-NB	7.26	1.41	1.35
23	Y	304	CLA	C4B-NB	7.25	1.41	1.35
23	c	508	CLA	C4B-NB	7.25	1.41	1.35
23	N	603	CLA	C4B-NB	7.25	1.41	1.35
23	A	403	CLA	C4B-NB	7.24	1.41	1.35
23	G	610	CLA	C4B-NB	7.23	1.41	1.35
23	Y	310	CLA	C4B-NB	7.22	1.41	1.35
23	a	404	CLA	C4B-NB	7.22	1.41	1.35
23	B	611	CLA	C4B-NB	7.21	1.41	1.35
23	b	611	CLA	C4B-NB	7.21	1.41	1.35
23	y	311	CLA	C4B-NB	7.20	1.41	1.35
41	n	618	NEX	C34-C33	7.16	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R	614	NEX	C34-C33	7.12	1.45	1.35
41	N	617	NEX	C34-C33	7.08	1.45	1.35
41	S	617	NEX	C12-C13	7.08	1.61	1.45
41	G	617	NEX	C28-C29	7.07	1.61	1.45
41	g	617	NEX	C28-C29	7.00	1.61	1.45
41	s	617	NEX	C12-C13	6.96	1.60	1.45
42	G	619	XAT	C12-C13	-6.91	1.31	1.45
42	n	617	XAT	C10-C9	6.90	1.44	1.35
41	r	614	NEX	C34-C33	6.86	1.44	1.35
41	Y	317	NEX	C34-C33	6.83	1.44	1.35
41	N	617	NEX	C28-C29	6.80	1.60	1.45
41	n	618	NEX	C28-C29	6.80	1.60	1.45
41	g	617	NEX	C12-C13	6.77	1.60	1.45
41	R	614	NEX	C12-C13	6.75	1.60	1.45
41	R	618	NEX	C34-C33	6.74	1.44	1.35
42	r	615	XAT	C14-C13	6.70	1.44	1.35
41	S	617	NEX	C10-C9	6.68	1.44	1.35
42	n	617	XAT	C12-C13	-6.66	1.31	1.45
42	R	615	XAT	C14-C13	6.63	1.44	1.35
41	s	617	NEX	C10-C9	6.60	1.44	1.35
41	n	618	NEX	C12-C13	6.60	1.60	1.45
41	R	614	NEX	C10-C9	6.60	1.44	1.35
42	r	615	XAT	C10-C9	6.54	1.44	1.35
42	N	619	XAT	C12-C13	-6.53	1.31	1.45
41	g	617	NEX	C10-C9	6.53	1.44	1.35
41	R	614	NEX	C28-C29	6.50	1.59	1.45
41	N	617	NEX	C10-C9	6.49	1.44	1.35
41	N	617	NEX	C12-C13	6.49	1.59	1.45
42	n	620	XAT	C12-C13	-6.47	1.32	1.45
42	R	615	XAT	C12-C13	-6.45	1.32	1.45
42	R	615	XAT	C10-C9	6.44	1.44	1.35
42	r	615	XAT	C12-C13	-6.43	1.32	1.45
41	r	614	NEX	C12-C13	6.41	1.59	1.45
40	G	615	LUT	C34-C33	6.40	1.44	1.35
41	r	614	NEX	C28-C29	6.32	1.59	1.45
41	R	618	NEX	C10-C9	6.29	1.44	1.35
41	Y	317	NEX	C12-C13	6.28	1.59	1.45
41	S	617	NEX	C14-C13	6.27	1.44	1.35
42	y	302	XAT	C34-C33	6.25	1.44	1.35
41	Y	317	NEX	C28-C29	6.24	1.59	1.45
42	Y	301	XAT	C12-C13	-6.23	1.32	1.45
40	n	615	LUT	C34-C33	6.23	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R	618	NEX	C28-C29	6.22	1.59	1.45
42	y	302	XAT	C14-C13	6.20	1.44	1.35
41	Y	317	NEX	C10-C9	6.19	1.44	1.35
40	g	615	LUT	C34-C33	6.16	1.43	1.35
41	n	618	NEX	C10-C9	6.13	1.43	1.35
42	r	615	XAT	C30-C29	6.12	1.43	1.35
41	R	618	NEX	C12-C13	6.10	1.59	1.45
42	y	302	XAT	C12-C13	-6.06	1.32	1.45
42	R	615	XAT	C30-C29	6.05	1.43	1.35
41	r	614	NEX	C10-C9	5.95	1.43	1.35
41	Y	317	NEX	C1-C6	5.94	1.64	1.54
41	s	617	NEX	C14-C13	5.80	1.43	1.35
42	n	617	XAT	C32-C33	-5.78	1.33	1.45
40	y	316	LUT	C34-C33	5.70	1.43	1.35
42	r	615	XAT	C32-C33	-5.68	1.33	1.45
40	Y	315	LUT	C34-C33	5.67	1.43	1.35
41	n	618	NEX	C1-C6	5.66	1.64	1.54
42	R	615	XAT	C32-C33	-5.65	1.33	1.45
42	y	302	XAT	C32-C33	-5.64	1.33	1.45
42	G	619	XAT	C32-C33	-5.64	1.33	1.45
42	Y	301	XAT	C14-C13	5.58	1.43	1.35
41	N	617	NEX	C1-C6	5.58	1.63	1.54
42	Y	301	XAT	C32-C33	-5.58	1.34	1.45
42	n	620	XAT	C32-C33	-5.57	1.34	1.45
41	g	617	NEX	C14-C13	5.57	1.43	1.35
40	s	614	LUT	C14-C13	5.57	1.43	1.35
42	N	619	XAT	C32-C33	-5.49	1.34	1.45
41	G	617	NEX	C31-C30	5.39	1.60	1.43
40	N	616	LUT	C14-C13	5.36	1.42	1.35
42	Y	301	XAT	C34-C33	5.36	1.42	1.35
40	S	615	LUT	C14-C13	5.34	1.42	1.35
41	R	618	NEX	C1-C6	5.33	1.63	1.54
42	n	620	XAT	C14-C13	5.31	1.42	1.35
40	N	615	LUT	C14-C13	5.28	1.42	1.35
42	Y	301	XAT	C30-C29	5.27	1.42	1.35
41	n	618	NEX	C14-C13	5.26	1.42	1.35
42	N	619	XAT	C14-C13	5.26	1.42	1.35
41	R	614	NEX	C14-C13	5.25	1.42	1.35
41	g	617	NEX	C31-C30	5.24	1.59	1.43
40	R	613	LUT	C14-C13	5.24	1.42	1.35
40	S	614	LUT	C14-C13	5.22	1.42	1.35
42	R	615	XAT	C34-C33	5.21	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	S	617	NEX	C1-C6	5.21	1.63	1.54
40	s	615	LUT	C14-C13	5.20	1.42	1.35
41	n	618	NEX	C31-C30	5.18	1.59	1.43
42	r	615	XAT	C34-C33	5.18	1.42	1.35
41	R	614	NEX	C31-C30	5.17	1.59	1.43
41	N	617	NEX	C14-C13	5.16	1.42	1.35
41	s	617	NEX	C1-C6	5.14	1.63	1.54
41	N	617	NEX	C24-C23	5.14	1.59	1.52
41	N	617	NEX	C31-C30	5.14	1.59	1.43
42	y	302	XAT	C2-C3	5.13	1.59	1.52
42	G	619	XAT	C10-C9	5.13	1.42	1.35
41	R	614	NEX	C1-C6	5.12	1.63	1.54
41	n	618	NEX	C24-C23	5.11	1.59	1.52
40	r	613	LUT	C14-C13	5.09	1.42	1.35
42	Y	301	XAT	C2-C3	5.08	1.59	1.52
41	r	614	NEX	C31-C30	5.08	1.59	1.43
41	g	617	NEX	C1-C6	5.06	1.63	1.54
41	Y	317	NEX	C31-C30	5.05	1.59	1.43
42	N	619	XAT	C34-C33	5.04	1.42	1.35
41	Y	317	NEX	C14-C13	5.03	1.42	1.35
41	G	617	NEX	C24-C23	5.01	1.59	1.52
41	R	618	NEX	C31-C30	5.01	1.59	1.43
41	Y	317	NEX	C24-C23	4.98	1.59	1.52
41	r	614	NEX	C14-C13	4.97	1.42	1.35
41	R	618	NEX	C24-C23	4.96	1.59	1.52
41	r	614	NEX	C24-C23	4.95	1.59	1.52
41	r	614	NEX	C1-C6	4.95	1.62	1.54
41	g	617	NEX	C24-C23	4.93	1.59	1.52
40	g	616	LUT	C14-C13	4.93	1.42	1.35
41	R	614	NEX	C24-C23	4.92	1.59	1.52
41	g	617	NEX	C22-C23	4.92	1.59	1.52
40	G	616	LUT	C14-C13	4.89	1.42	1.35
40	n	616	LUT	C14-C13	4.87	1.42	1.35
41	G	617	NEX	C22-C23	4.85	1.59	1.52
41	R	618	NEX	C14-C13	4.83	1.42	1.35
41	G	617	NEX	C35-C34	4.83	1.58	1.43
41	s	617	NEX	C35-C34	4.83	1.58	1.43
42	G	619	XAT	C30-C29	4.82	1.42	1.35
40	N	615	LUT	C10-C9	4.81	1.42	1.35
41	R	614	NEX	C22-C23	4.77	1.59	1.52
41	n	618	NEX	C22-C23	4.76	1.59	1.52
41	r	614	NEX	C2-C3	4.76	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	s	614	LUT	C10-C9	4.73	1.42	1.35
42	n	620	XAT	C34-C33	4.73	1.42	1.35
42	G	619	XAT	C34-C33	4.73	1.42	1.35
41	S	617	NEX	C11-C10	4.73	1.58	1.43
41	G	617	NEX	C24-C25	4.72	1.58	1.52
41	R	618	NEX	C22-C23	4.72	1.59	1.52
41	N	617	NEX	C22-C23	4.71	1.59	1.52
26	M	101	SQD	O48-C23	4.70	1.47	1.33
41	Y	317	NEX	C2-C3	4.69	1.59	1.52
41	Y	317	NEX	C22-C23	4.69	1.59	1.52
41	G	617	NEX	C32-C33	4.68	1.56	1.45
41	r	614	NEX	C22-C23	4.67	1.59	1.52
40	y	317	LUT	C14-C13	4.67	1.42	1.35
41	s	617	NEX	C11-C10	4.67	1.57	1.43
40	Y	316	LUT	C14-C13	4.66	1.42	1.35
26	L	101	SQD	O48-C23	4.65	1.46	1.33
26	a	409	SQD	O48-C23	4.64	1.46	1.33
41	g	617	NEX	C35-C34	4.63	1.57	1.43
41	s	617	NEX	C2-C3	4.63	1.59	1.52
41	N	617	NEX	C24-C25	4.63	1.58	1.52
41	R	614	NEX	C2-C3	4.61	1.59	1.52
26	A	408	SQD	O48-C23	4.61	1.46	1.33
41	n	618	NEX	C24-C25	4.59	1.58	1.52
41	R	614	NEX	C11-C10	4.59	1.57	1.43
41	g	617	NEX	C24-C25	4.57	1.58	1.52
41	g	617	NEX	C11-C10	4.55	1.57	1.43
41	g	617	NEX	C18-C5	4.53	1.60	1.52
41	S	617	NEX	C7-C8	4.53	1.39	1.32
41	s	617	NEX	C34-C33	4.52	1.46	1.35
41	Y	317	NEX	C18-C5	4.51	1.60	1.52
41	R	618	NEX	C2-C3	4.51	1.58	1.52
41	R	614	NEX	C18-C5	4.51	1.60	1.52
41	g	617	NEX	C32-C33	4.51	1.55	1.45
41	r	614	NEX	C18-C5	4.49	1.60	1.52
42	n	620	XAT	C2-C3	4.48	1.58	1.52
41	S	617	NEX	C2-C3	4.48	1.58	1.52
41	N	617	NEX	C11-C10	4.48	1.57	1.43
42	N	619	XAT	C2-C3	4.48	1.58	1.52
41	s	617	NEX	C7-C8	4.48	1.39	1.32
41	Y	317	NEX	C24-C25	4.47	1.58	1.52
41	N	617	NEX	C2-C3	4.47	1.58	1.52
41	R	614	NEX	C35-C34	4.47	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	n	617	XAT	C30-C29	4.47	1.41	1.35
41	n	618	NEX	C18-C5	4.47	1.60	1.52
41	s	617	NEX	C15-C14	4.47	1.57	1.43
41	g	617	NEX	C4-C3	4.45	1.58	1.52
41	n	618	NEX	C32-C33	4.45	1.55	1.45
41	R	618	NEX	C24-C25	4.45	1.58	1.52
41	G	617	NEX	C28-C27	4.45	1.42	1.32
41	r	614	NEX	C4-C3	4.44	1.58	1.52
41	R	614	NEX	C4-C3	4.44	1.58	1.52
40	r	613	LUT	C10-C9	4.44	1.41	1.35
41	N	617	NEX	C18-C5	4.43	1.60	1.52
40	N	616	LUT	C10-C9	4.43	1.41	1.35
41	n	618	NEX	C35-C34	4.42	1.57	1.43
41	G	617	NEX	C30-C29	4.42	1.41	1.35
40	S	615	LUT	C10-C9	4.41	1.41	1.35
41	g	617	NEX	C7-C8	4.41	1.39	1.32
41	R	618	NEX	C18-C5	4.41	1.59	1.52
40	R	613	LUT	C10-C9	4.40	1.41	1.35
41	N	617	NEX	C35-C34	4.40	1.57	1.43
40	S	614	LUT	C10-C9	4.39	1.41	1.35
42	G	619	XAT	C8-C9	-4.39	1.36	1.45
41	R	618	NEX	C11-C10	4.38	1.57	1.43
40	s	615	LUT	C10-C9	4.37	1.41	1.35
41	N	617	NEX	C32-C33	4.36	1.55	1.45
41	R	614	NEX	C7-C8	4.35	1.39	1.32
41	Y	317	NEX	C11-C10	4.35	1.56	1.43
42	n	617	XAT	C14-C13	4.35	1.41	1.35
42	R	615	XAT	C2-C3	4.35	1.58	1.52
41	Y	317	NEX	C35-C34	4.35	1.56	1.43
41	s	617	NEX	C18-C5	4.34	1.59	1.52
41	n	618	NEX	C11-C10	4.33	1.56	1.43
42	y	302	XAT	C30-C29	4.32	1.41	1.35
41	N	617	NEX	C7-C8	4.32	1.39	1.32
41	Y	317	NEX	C4-C3	4.32	1.58	1.52
42	r	615	XAT	C2-C3	4.32	1.58	1.52
40	G	616	LUT	C10-C9	4.31	1.41	1.35
41	g	617	NEX	C28-C27	4.29	1.42	1.32
41	r	614	NEX	C11-C10	4.28	1.56	1.43
41	n	618	NEX	C7-C8	4.28	1.39	1.32
40	g	616	LUT	C10-C9	4.28	1.41	1.35
41	S	617	NEX	C18-C5	4.27	1.59	1.52
41	R	614	NEX	C32-C33	4.26	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	N	617	NEX	C4-C3	4.26	1.58	1.52
41	g	617	NEX	C15-C14	4.25	1.56	1.43
41	s	617	NEX	C4-C3	4.25	1.58	1.52
41	n	618	NEX	C2-C3	4.25	1.58	1.52
41	r	614	NEX	C35-C34	4.24	1.56	1.43
41	S	617	NEX	C15-C14	4.23	1.58	1.45
42	G	619	XAT	C22-C23	4.23	1.58	1.52
40	n	615	LUT	C14-C13	4.23	1.41	1.35
42	n	617	XAT	C8-C9	-4.23	1.36	1.45
41	R	618	NEX	C35-C34	4.22	1.56	1.43
41	r	614	NEX	C7-C8	4.21	1.39	1.32
41	S	617	NEX	C4-C3	4.21	1.58	1.52
41	N	617	NEX	C28-C27	4.21	1.41	1.32
41	Y	317	NEX	C7-C8	4.21	1.39	1.32
41	R	614	NEX	C24-C25	4.20	1.58	1.52
41	n	618	NEX	C28-C27	4.19	1.41	1.32
41	r	614	NEX	C24-C25	4.19	1.58	1.52
42	Y	301	XAT	C8-C9	-4.18	1.37	1.45
42	y	302	XAT	C8-C9	-4.18	1.37	1.45
41	R	614	NEX	C15-C14	4.17	1.56	1.43
41	n	618	NEX	C15-C14	4.15	1.56	1.43
40	s	614	LUT	C30-C29	4.15	1.41	1.35
40	n	616	LUT	C10-C9	4.14	1.41	1.35
41	g	617	NEX	C30-C29	4.12	1.41	1.35
41	N	617	NEX	C15-C14	4.12	1.56	1.43
40	Y	316	LUT	C10-C9	4.10	1.41	1.35
40	y	317	LUT	C10-C9	4.10	1.41	1.35
41	Y	317	NEX	C32-C33	4.10	1.54	1.45
42	r	615	XAT	C8-C9	-4.09	1.37	1.45
41	R	614	NEX	C28-C27	4.08	1.41	1.32
41	R	618	NEX	C7-C8	4.08	1.38	1.32
42	n	620	XAT	C22-C23	4.08	1.58	1.52
42	R	615	XAT	C8-C9	-4.06	1.37	1.45
42	G	619	XAT	C11-C10	-4.05	1.30	1.43
41	R	618	NEX	C32-C33	4.04	1.54	1.45
40	S	614	LUT	C30-C29	4.04	1.41	1.35
41	Y	317	NEX	C15-C14	4.04	1.56	1.43
40	s	614	LUT	C12-C13	4.03	1.54	1.45
42	y	302	XAT	C11-C12	4.03	1.45	1.34
41	r	614	NEX	C32-C33	4.01	1.54	1.45
42	y	302	XAT	C22-C23	4.00	1.58	1.52
41	r	614	NEX	C15-C14	4.00	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R	618	NEX	C4-C3	3.99	1.58	1.52
23	G	613	CLA	C1D-ND	3.99	1.42	1.37
23	n	611	CLA	C1D-ND	3.98	1.42	1.37
40	S	615	LUT	C30-C29	3.95	1.41	1.35
23	s	609	CLA	C1D-ND	3.95	1.42	1.37
23	s	612	CLA	C1D-ND	3.94	1.42	1.37
23	S	608	CLA	C1D-ND	3.94	1.42	1.37
23	s	608	CLA	C1D-ND	3.94	1.42	1.37
23	S	610	CLA	C1D-ND	3.93	1.42	1.37
41	g	617	NEX	C2-C3	3.93	1.58	1.52
23	a	405	CLA	C1D-ND	3.92	1.42	1.37
41	r	614	NEX	C28-C27	3.92	1.41	1.32
23	S	602	CLA	C1D-ND	3.92	1.42	1.37
23	n	610	CLA	C1D-ND	3.92	1.42	1.37
40	N	616	LUT	C30-C29	3.92	1.41	1.35
23	r	610	CLA	C1D-ND	3.92	1.42	1.37
41	R	618	NEX	C15-C14	3.92	1.55	1.43
23	G	612	CLA	C1D-ND	3.91	1.42	1.37
23	n	602	CLA	C1D-ND	3.91	1.42	1.37
23	r	601	CLA	C1D-ND	3.91	1.42	1.37
23	c	504	CLA	C1D-ND	3.91	1.42	1.37
23	D	406	CLA	C1D-ND	3.91	1.42	1.37
23	g	613	CLA	C1D-ND	3.91	1.42	1.37
23	Y	314	CLA	C1D-ND	3.90	1.42	1.37
23	r	602	CLA	C1D-ND	3.90	1.42	1.37
23	N	613	CLA	C1D-ND	3.90	1.42	1.37
23	R	612	CLA	C1D-ND	3.90	1.42	1.37
42	N	619	XAT	C22-C23	3.90	1.57	1.52
23	c	507	CLA	C1D-ND	3.90	1.42	1.37
23	y	311	CLA	C1D-ND	3.90	1.42	1.37
23	y	315	CLA	C1D-ND	3.90	1.42	1.37
23	B	615	CLA	C1D-ND	3.90	1.42	1.37
23	g	612	CLA	C1D-ND	3.90	1.42	1.37
23	r	612	CLA	C1D-ND	3.89	1.42	1.37
23	N	602	CLA	C1D-ND	3.89	1.42	1.37
23	R	610	CLA	C1D-ND	3.89	1.42	1.37
23	c	502	CLA	C1D-ND	3.89	1.42	1.37
42	G	619	XAT	C14-C13	3.89	1.40	1.35
23	G	614	CLA	C1D-ND	3.89	1.42	1.37
23	R	602	CLA	C1D-ND	3.89	1.42	1.37
23	r	611	CLA	C1D-ND	3.89	1.42	1.37
23	R	601	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C1D-ND	3.88	1.42	1.37
42	Y	301	XAT	C11-C12	3.88	1.44	1.34
23	G	610	CLA	C1D-ND	3.88	1.42	1.37
23	n	613	CLA	C1D-ND	3.88	1.42	1.37
23	y	305	CLA	C1D-ND	3.88	1.42	1.37
23	S	611	CLA	C1D-ND	3.88	1.42	1.37
41	Y	317	NEX	C28-C27	3.88	1.41	1.32
23	G	611	CLA	C1D-ND	3.88	1.42	1.37
23	R	609	CLA	C1D-ND	3.88	1.42	1.37
23	S	603	CLA	C1D-ND	3.88	1.42	1.37
38	F	501	HEM	C3C-CAC	3.88	1.55	1.47
23	N	612	CLA	C1D-ND	3.88	1.42	1.37
23	R	611	CLA	C1D-ND	3.87	1.42	1.37
23	d	406	CLA	C1D-ND	3.87	1.42	1.37
23	s	604	CLA	C1D-ND	3.87	1.42	1.37
40	S	615	LUT	C12-C13	3.87	1.54	1.45
23	G	604	CLA	C1D-ND	3.87	1.42	1.37
23	Y	304	CLA	C1D-ND	3.87	1.42	1.37
23	Y	303	CLA	C1D-ND	3.87	1.42	1.37
23	s	610	CLA	C1D-ND	3.87	1.42	1.37
23	S	612	CLA	C1D-ND	3.87	1.42	1.37
42	n	617	XAT	C2-C3	3.87	1.57	1.52
42	G	619	XAT	C2-C3	3.87	1.57	1.52
42	n	617	XAT	C11-C10	-3.87	1.31	1.43
23	s	611	CLA	C1D-ND	3.87	1.42	1.37
38	f	501	HEM	C3C-CAC	3.86	1.55	1.47
23	s	602	CLA	C1D-ND	3.86	1.42	1.37
23	Y	313	CLA	C1D-ND	3.86	1.42	1.37
23	C	511	CLA	C1D-ND	3.86	1.42	1.37
23	Y	310	CLA	C1D-ND	3.86	1.42	1.37
23	y	314	CLA	C1D-ND	3.86	1.42	1.37
41	n	618	NEX	C4-C3	3.86	1.57	1.52
23	g	611	CLA	C1D-ND	3.86	1.42	1.37
23	n	612	CLA	C1D-ND	3.86	1.42	1.37
23	B	616	CLA	C1D-ND	3.85	1.42	1.37
23	S	609	CLA	C1D-ND	3.85	1.42	1.37
23	a	407	CLA	C1D-ND	3.85	1.42	1.37
23	N	614	CLA	C1D-ND	3.85	1.42	1.37
23	c	508	CLA	C1D-ND	3.85	1.42	1.37
23	B	610	CLA	C1D-ND	3.84	1.42	1.37
23	C	501	CLA	C1D-ND	3.84	1.42	1.37
23	b	611	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1D-ND	3.84	1.42	1.37
23	a	404	CLA	C1D-ND	3.84	1.42	1.37
23	N	610	CLA	C1D-ND	3.84	1.42	1.37
23	C	504	CLA	C1D-ND	3.84	1.42	1.37
23	n	614	CLA	C1D-ND	3.84	1.42	1.37
23	b	610	CLA	C1D-ND	3.84	1.42	1.37
23	C	509	CLA	C1D-ND	3.84	1.42	1.37
23	r	609	CLA	C1D-ND	3.84	1.42	1.37
23	g	602	CLA	C1D-ND	3.84	1.42	1.37
23	y	306	CLA	C1D-ND	3.84	1.42	1.37
41	R	618	NEX	C28-C27	3.84	1.41	1.32
23	b	616	CLA	C1D-ND	3.83	1.42	1.37
23	Y	311	CLA	C1D-ND	3.83	1.42	1.37
23	c	509	CLA	C1D-ND	3.83	1.42	1.37
40	S	614	LUT	C12-C13	3.83	1.54	1.45
23	B	611	CLA	C1D-ND	3.83	1.42	1.37
23	B	607	CLA	C1D-ND	3.83	1.42	1.37
23	c	506	CLA	C1D-ND	3.83	1.42	1.37
23	c	505	CLA	C1D-ND	3.83	1.42	1.37
23	S	604	CLA	C1D-ND	3.83	1.42	1.37
23	s	603	CLA	C1D-ND	3.83	1.42	1.37
23	B	601	CLA	C1D-ND	3.83	1.42	1.37
23	C	508	CLA	C1D-ND	3.83	1.42	1.37
23	y	304	CLA	C1D-ND	3.83	1.42	1.37
23	r	603	CLA	C1D-ND	3.82	1.42	1.37
23	B	602	CLA	C1D-ND	3.82	1.42	1.37
23	b	606	CLA	C1D-ND	3.82	1.42	1.37
23	g	610	CLA	C1D-ND	3.82	1.42	1.37
23	C	510	CLA	C1D-ND	3.82	1.42	1.37
23	S	613	CLA	C1D-ND	3.82	1.42	1.37
23	b	601	CLA	C1D-ND	3.82	1.42	1.37
23	b	613	CLA	C1D-ND	3.82	1.42	1.37
40	R	613	LUT	C30-C29	3.82	1.40	1.35
23	G	602	CLA	C1D-ND	3.82	1.42	1.37
23	b	615	CLA	C1D-ND	3.81	1.42	1.37
38	f	501	HEM	C3C-C2C	-3.81	1.35	1.40
23	N	611	CLA	C1D-ND	3.81	1.42	1.37
23	Y	305	CLA	C1D-ND	3.81	1.42	1.37
23	c	501	CLA	C1D-ND	3.81	1.42	1.37
23	g	604	CLA	C1D-ND	3.81	1.42	1.37
23	B	613	CLA	C1D-ND	3.81	1.42	1.37
23	A	402	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	312	CLA	C1D-ND	3.81	1.42	1.37
41	n	618	NEX	C30-C29	3.81	1.40	1.35
23	B	604	CLA	C1D-ND	3.81	1.42	1.37
23	b	604	CLA	C1D-ND	3.81	1.42	1.37
42	N	619	XAT	C30-C29	3.81	1.40	1.35
23	r	608	CLA	C1D-ND	3.80	1.42	1.37
23	y	313	CLA	C1D-ND	3.80	1.42	1.37
23	b	603	CLA	C1D-ND	3.80	1.42	1.37
23	B	614	CLA	C1D-ND	3.80	1.42	1.37
23	A	403	CLA	C1D-ND	3.80	1.42	1.37
23	b	614	CLA	C1D-ND	3.80	1.42	1.37
42	R	615	XAT	C11-C10	-3.80	1.31	1.43
23	c	511	CLA	C1D-ND	3.80	1.42	1.37
23	c	503	CLA	C1D-ND	3.80	1.42	1.37
23	B	609	CLA	C1D-ND	3.79	1.42	1.37
42	n	617	XAT	C31-C30	-3.79	1.31	1.43
40	N	615	LUT	C12-C13	3.79	1.54	1.45
23	R	603	CLA	C1D-ND	3.79	1.42	1.37
42	N	619	XAT	C8-C9	-3.79	1.37	1.45
23	r	604	CLA	C1D-ND	3.79	1.42	1.37
23	G	603	CLA	C1D-ND	3.79	1.42	1.37
41	N	617	NEX	C30-C29	3.78	1.40	1.35
23	b	602	CLA	C1D-ND	3.78	1.42	1.37
23	B	605	CLA	C1D-ND	3.78	1.42	1.37
23	R	608	CLA	C1D-ND	3.78	1.42	1.37
23	C	502	CLA	C1D-ND	3.78	1.42	1.37
23	g	603	CLA	C1D-ND	3.78	1.42	1.37
38	F	501	HEM	C3C-C2C	-3.78	1.35	1.40
23	N	604	CLA	C1D-ND	3.78	1.42	1.37
23	A	406	CLA	C1D-ND	3.77	1.42	1.37
23	b	607	CLA	C1D-ND	3.77	1.42	1.37
23	y	312	CLA	C1D-ND	3.77	1.42	1.37
23	b	609	CLA	C1D-ND	3.77	1.42	1.37
40	N	616	LUT	C12-C13	3.77	1.54	1.45
23	C	505	CLA	C1D-ND	3.77	1.42	1.37
42	r	615	XAT	C11-C10	-3.77	1.31	1.43
23	c	512	CLA	C1D-ND	3.77	1.42	1.37
23	C	513	CLA	C1D-ND	3.77	1.42	1.37
23	n	603	CLA	C1D-ND	3.77	1.42	1.37
23	C	503	CLA	C1D-ND	3.77	1.42	1.37
42	n	617	XAT	C22-C23	3.77	1.57	1.52
42	n	620	XAT	C31-C30	-3.76	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1D-ND	3.76	1.42	1.37
40	s	615	LUT	C30-C29	3.76	1.40	1.35
23	C	506	CLA	C1D-ND	3.76	1.42	1.37
23	s	613	CLA	C1D-ND	3.76	1.42	1.37
40	N	615	LUT	C30-C29	3.76	1.40	1.35
23	a	403	CLA	C1D-ND	3.75	1.42	1.37
23	c	510	CLA	C1D-ND	3.75	1.42	1.37
42	y	302	XAT	C31-C30	-3.75	1.31	1.43
23	B	603	CLA	C1D-ND	3.75	1.42	1.37
23	c	513	CLA	C1D-ND	3.74	1.42	1.37
23	g	614	CLA	C1D-ND	3.74	1.42	1.37
23	n	604	CLA	C1D-ND	3.74	1.42	1.37
42	n	617	XAT	C34-C33	3.74	1.40	1.35
23	b	608	CLA	C1D-ND	3.74	1.42	1.37
23	B	608	CLA	C1D-ND	3.74	1.42	1.37
42	n	620	XAT	C8-C9	-3.73	1.37	1.45
23	B	606	CLA	C1D-ND	3.73	1.42	1.37
40	r	613	LUT	C12-C13	3.73	1.54	1.45
23	b	605	CLA	C1D-ND	3.72	1.42	1.37
40	s	614	LUT	C26-C27	3.72	1.55	1.50
23	N	603	CLA	C1D-ND	3.72	1.42	1.37
40	S	614	LUT	C26-C27	3.72	1.55	1.50
40	s	615	LUT	C12-C13	3.72	1.53	1.45
41	R	614	NEX	C30-C29	3.71	1.40	1.35
23	R	604	CLA	C1D-ND	3.70	1.42	1.37
42	G	619	XAT	C31-C30	-3.69	1.32	1.43
42	N	619	XAT	C31-C30	-3.69	1.32	1.43
41	g	617	NEX	C22-C21	3.67	1.60	1.54
23	B	612	CLA	C1D-ND	3.67	1.42	1.37
42	n	617	XAT	C15-C14	-3.66	1.32	1.43
42	Y	301	XAT	C31-C30	-3.65	1.32	1.43
41	R	614	NEX	C22-C21	3.65	1.60	1.54
42	R	615	XAT	C22-C23	3.65	1.57	1.52
41	R	618	NEX	C36-C21	3.63	1.60	1.53
41	r	614	NEX	C36-C21	3.63	1.60	1.53
41	G	617	NEX	C22-C21	3.63	1.60	1.54
42	G	619	XAT	C15-C14	-3.62	1.32	1.43
41	Y	317	NEX	C36-C21	3.62	1.60	1.53
35	y	301	VIV	C10-C3	-3.62	1.45	1.51
42	R	615	XAT	C31-C30	-3.61	1.32	1.43
41	R	614	NEX	C36-C21	3.61	1.60	1.53
41	n	618	NEX	C36-C21	3.61	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	615	XAT	C31-C30	-3.60	1.32	1.43
40	r	613	LUT	C30-C29	3.59	1.40	1.35
40	G	615	LUT	C14-C13	3.59	1.40	1.35
42	r	615	XAT	C22-C23	3.58	1.57	1.52
40	R	613	LUT	C12-C13	3.58	1.53	1.45
41	N	617	NEX	C36-C21	3.57	1.60	1.53
42	N	619	XAT	C11-C10	-3.57	1.32	1.43
40	y	316	LUT	C10-C9	3.57	1.40	1.35
42	n	617	XAT	C35-C34	-3.56	1.32	1.43
41	r	614	NEX	C17-C1	3.55	1.60	1.53
23	D	405	CLA	C1D-ND	3.55	1.42	1.37
23	b	612	CLA	C1D-ND	3.55	1.42	1.37
25	h	501	BCR	C1-C6	-3.55	1.48	1.53
41	g	617	NEX	C17-C1	3.55	1.60	1.53
25	d	410	BCR	C1-C6	-3.54	1.48	1.53
25	v	101	BCR	C1-C6	-3.54	1.48	1.53
41	g	617	NEX	C36-C21	3.54	1.60	1.53
40	n	615	LUT	C10-C9	3.53	1.40	1.35
41	n	618	NEX	C17-C1	3.53	1.60	1.53
40	Y	315	LUT	C10-C9	3.52	1.40	1.35
42	Y	301	XAT	C22-C23	3.52	1.57	1.52
40	S	615	LUT	C26-C27	3.52	1.55	1.50
41	r	614	NEX	C22-C21	3.52	1.60	1.54
25	H	501	BCR	C1-C6	-3.52	1.48	1.53
40	Y	316	LUT	C30-C29	3.51	1.40	1.35
42	n	620	XAT	C11-C10	-3.51	1.32	1.43
41	G	617	NEX	C36-C21	3.50	1.60	1.53
41	R	614	NEX	C17-C1	3.50	1.60	1.53
25	V	101	BCR	C1-C6	-3.50	1.49	1.53
42	Y	301	XAT	C15-C14	-3.50	1.32	1.43
40	y	317	LUT	C30-C29	3.49	1.40	1.35
41	R	618	NEX	C22-C21	3.49	1.60	1.54
42	N	619	XAT	C15-C14	-3.49	1.32	1.43
25	d	410	BCR	C30-C25	-3.48	1.49	1.53
23	d	405	CLA	C1D-ND	3.48	1.42	1.37
42	Y	301	XAT	C11-C10	-3.48	1.32	1.43
41	g	617	NEX	C39-C29	3.47	1.58	1.50
26	M	101	SQD	O5-C1	3.47	1.50	1.41
42	n	620	XAT	C15-C14	-3.47	1.32	1.43
25	B	618	BCR	C1-C6	-3.46	1.49	1.53
42	y	302	XAT	C11-C10	-3.46	1.32	1.43
41	Y	317	NEX	C22-C21	3.46	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	G	617	NEX	C39-C29	3.46	1.58	1.50
42	n	620	XAT	C35-C34	-3.45	1.32	1.43
26	M	101	SQD	O47-C7	3.45	1.44	1.34
25	C	514	BCR	C1-C6	-3.44	1.49	1.53
41	N	617	NEX	C17-C1	3.44	1.60	1.53
26	A	408	SQD	O47-C45	-3.44	1.38	1.46
41	s	617	NEX	C17-C1	3.44	1.60	1.53
25	c	514	BCR	C1-C6	-3.44	1.49	1.53
26	a	409	SQD	O47-C45	-3.44	1.38	1.46
42	G	619	XAT	C35-C34	-3.44	1.32	1.43
40	G	616	LUT	C30-C29	3.44	1.40	1.35
42	N	619	XAT	C35-C34	-3.44	1.32	1.43
41	r	614	NEX	C30-C29	3.43	1.40	1.35
40	s	614	LUT	C11-C10	3.43	1.54	1.43
25	K	101	BCR	C1-C6	-3.43	1.49	1.53
40	g	616	LUT	C30-C29	3.43	1.40	1.35
41	Y	317	NEX	C30-C29	3.43	1.40	1.35
41	S	617	NEX	C17-C1	3.41	1.60	1.53
25	b	618	BCR	C1-C6	-3.41	1.49	1.53
40	G	615	LUT	C30-C29	3.41	1.40	1.35
41	S	617	NEX	C35-C15	3.41	1.41	1.32
40	G	616	LUT	C12-C13	3.41	1.53	1.45
40	y	316	LUT	C14-C13	3.41	1.40	1.35
25	A	407	BCR	C1-C6	-3.40	1.49	1.53
25	b	619	BCR	C1-C6	-3.40	1.49	1.53
42	Y	301	XAT	C35-C34	-3.40	1.32	1.43
40	Y	315	LUT	C14-C13	3.40	1.40	1.35
26	L	101	SQD	O47-C7	3.39	1.43	1.34
40	n	616	LUT	C30-C29	3.39	1.40	1.35
41	G	617	NEX	C35-C15	3.38	1.40	1.32
26	L	101	SQD	O5-C1	3.38	1.50	1.41
40	g	616	LUT	C12-C13	3.38	1.53	1.45
25	a	408	BCR	C1-C6	-3.38	1.49	1.53
25	k	101	BCR	C1-C6	-3.38	1.49	1.53
40	N	615	LUT	C11-C10	3.38	1.53	1.43
41	N	617	NEX	C16-C1	3.37	1.60	1.53
42	Y	301	XAT	C31-C32	3.37	1.43	1.34
41	R	618	NEX	C30-C29	3.37	1.40	1.35
40	g	615	LUT	C30-C29	3.36	1.40	1.35
41	g	617	NEX	C20-C13	3.35	1.57	1.50
40	G	615	LUT	C10-C9	3.35	1.40	1.35
41	s	617	NEX	C20-C13	3.35	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	y	302	XAT	C15-C14	-3.34	1.33	1.43
40	s	614	LUT	C32-C33	3.34	1.53	1.45
41	g	617	NEX	C16-C1	3.33	1.60	1.53
42	r	615	XAT	O24-C25	3.33	1.51	1.46
23	s	609	CLA	CHC-C1C	3.33	1.43	1.35
42	n	620	XAT	O24-C25	3.32	1.51	1.46
28	X	201	3PH	P-O11	3.32	1.70	1.60
42	R	615	XAT	C24-C23	3.32	1.57	1.52
42	N	619	XAT	O24-C25	3.31	1.51	1.46
42	r	615	XAT	C35-C34	-3.31	1.33	1.43
42	R	615	XAT	O24-C25	3.31	1.51	1.46
30	r	616	LHG	P-O3	3.30	1.72	1.59
41	n	618	NEX	C39-C29	3.30	1.57	1.50
28	L	102	3PH	P-O11	3.30	1.70	1.60
41	g	617	NEX	C19-C9	3.30	1.57	1.50
42	R	615	XAT	C35-C34	-3.30	1.33	1.43
28	x	201	3PH	P-O11	3.29	1.70	1.60
42	n	620	XAT	C30-C29	3.29	1.40	1.35
26	a	409	SQD	O47-C7	3.28	1.43	1.34
28	d	403	3PH	P-O11	3.28	1.70	1.60
41	N	617	NEX	C39-C29	3.28	1.57	1.50
25	Z	101	BCR	C30-C25	-3.28	1.49	1.53
41	r	614	NEX	C16-C1	3.28	1.60	1.53
28	W	201	3PH	P-O11	3.28	1.70	1.60
26	a	409	SQD	O5-C1	3.27	1.50	1.41
28	T	101	3PH	P-O11	3.27	1.70	1.60
41	G	617	NEX	C40-C33	3.27	1.57	1.50
25	z	101	BCR	C30-C25	-3.27	1.49	1.53
41	r	614	NEX	C19-C9	3.27	1.57	1.50
28	C	524	3PH	P-O11	3.27	1.70	1.60
41	R	618	NEX	C17-C1	3.27	1.60	1.53
42	y	302	XAT	C35-C34	-3.26	1.33	1.43
41	Y	317	NEX	C16-C1	3.26	1.60	1.53
28	a	410	3PH	P-O11	3.26	1.70	1.60
40	S	614	LUT	C28-C27	3.26	1.40	1.32
40	S	615	LUT	C32-C33	3.26	1.52	1.45
28	w	202	3PH	P-O11	3.26	1.70	1.60
41	R	614	NEX	C16-C1	3.25	1.60	1.53
28	s	618	3PH	P-O11	3.25	1.70	1.60
41	n	618	NEX	C16-C1	3.25	1.60	1.53
41	R	614	NEX	C19-C9	3.25	1.57	1.50
41	S	617	NEX	C16-C1	3.25	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	N	617	NEX	C22-C21	3.25	1.59	1.54
28	D	403	3PH	P-O11	3.25	1.70	1.60
23	S	609	CLA	CHC-C1C	3.24	1.43	1.35
41	g	617	NEX	C40-C33	3.24	1.57	1.50
41	n	618	NEX	C19-C9	3.24	1.57	1.50
41	s	617	NEX	C19-C9	3.24	1.57	1.50
40	s	614	LUT	C28-C27	3.24	1.40	1.32
42	R	615	XAT	C15-C14	-3.24	1.33	1.43
40	y	317	LUT	C12-C13	3.24	1.52	1.45
41	r	614	NEX	C40-C33	3.24	1.57	1.50
40	s	614	LUT	C8-C9	3.24	1.52	1.45
41	Y	317	NEX	C17-C1	3.24	1.60	1.53
41	R	618	NEX	C19-C9	3.23	1.57	1.50
26	A	408	SQD	O5-C1	3.23	1.50	1.41
42	Y	301	XAT	C2-C1	3.23	1.59	1.54
42	r	615	XAT	C15-C14	-3.23	1.33	1.43
41	n	618	NEX	C22-C21	3.23	1.59	1.54
41	S	617	NEX	C20-C13	3.23	1.57	1.50
23	S	602	CLA	CHC-C1C	3.23	1.43	1.35
42	r	615	XAT	C24-C23	3.23	1.57	1.52
41	S	617	NEX	C19-C9	3.23	1.57	1.50
41	N	617	NEX	C19-C9	3.22	1.57	1.50
26	A	408	SQD	O47-C7	3.22	1.43	1.34
41	s	617	NEX	C16-C1	3.22	1.60	1.53
41	R	614	NEX	C40-C33	3.22	1.57	1.50
23	R	609	CLA	CHC-C1C	3.21	1.43	1.35
42	N	619	XAT	C11-C12	3.21	1.42	1.34
23	r	610	CLA	CHC-C1C	3.21	1.43	1.35
42	n	620	XAT	C11-C12	3.21	1.42	1.34
28	A	410	3PH	P-O11	3.21	1.70	1.60
23	s	603	CLA	CHC-C1C	3.21	1.43	1.35
23	C	510	CLA	CHC-C1C	3.21	1.43	1.35
41	R	614	NEX	C39-C29	3.20	1.57	1.50
41	Y	317	NEX	C40-C33	3.20	1.57	1.50
40	n	616	LUT	C12-C13	3.20	1.52	1.45
23	n	610	CLA	CHC-C1C	3.20	1.43	1.35
40	g	615	LUT	C14-C13	3.20	1.40	1.35
23	c	510	CLA	CHC-C1C	3.20	1.43	1.35
23	r	609	CLA	CHC-C1C	3.20	1.43	1.35
23	B	606	CLA	CHC-C1C	3.20	1.43	1.35
25	H	501	BCR	C30-C25	-3.20	1.49	1.53
23	B	601	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	610	CLA	CHC-C1C	3.19	1.43	1.35
41	R	618	NEX	C40-C33	3.19	1.57	1.50
23	R	601	CLA	CHC-C1C	3.19	1.43	1.35
42	N	619	XAT	C31-C32	3.19	1.42	1.34
30	N	618	LHG	P-O3	3.19	1.72	1.59
25	h	501	BCR	C30-C25	-3.19	1.49	1.53
41	N	617	NEX	C40-C33	3.19	1.57	1.50
23	b	616	CLA	CHC-C1C	3.19	1.43	1.35
23	B	610	CLA	CHC-C1C	3.19	1.43	1.35
23	R	608	CLA	CHC-C1C	3.19	1.43	1.35
40	N	616	LUT	C26-C27	3.19	1.55	1.50
23	c	511	CLA	CHC-C1C	3.19	1.43	1.35
23	N	610	CLA	CHC-C1C	3.19	1.43	1.35
40	S	615	LUT	C11-C10	3.19	1.53	1.43
23	g	602	CLA	CHC-C1C	3.18	1.43	1.35
23	s	602	CLA	CHC-C1C	3.18	1.43	1.35
23	N	604	CLA	CHC-C1C	3.18	1.43	1.35
41	R	618	NEX	C16-C1	3.18	1.60	1.53
23	N	614	CLA	CHC-C1C	3.18	1.43	1.35
23	C	511	CLA	CHC-C1C	3.18	1.43	1.35
30	A	412	LHG	P-O3	3.18	1.72	1.59
23	R	602	CLA	CHC-C1C	3.18	1.43	1.35
25	b	617	BCR	C1-C6	-3.18	1.49	1.53
40	S	615	LUT	C28-C27	3.18	1.39	1.32
23	b	603	CLA	CHC-C1C	3.18	1.43	1.35
30	n	619	LHG	P-O3	3.18	1.72	1.59
41	Y	317	NEX	C19-C9	3.18	1.57	1.50
42	n	617	XAT	O24-C25	3.18	1.50	1.46
41	n	618	NEX	C40-C33	3.18	1.57	1.50
23	n	602	CLA	CHC-C1C	3.18	1.43	1.35
42	G	619	XAT	C31-C32	3.18	1.42	1.34
23	G	602	CLA	CHC-C1C	3.17	1.43	1.35
23	b	614	CLA	CHC-C1C	3.17	1.43	1.35
40	Y	316	LUT	C12-C13	3.17	1.52	1.45
23	S	610	CLA	CHC-C1C	3.17	1.43	1.35
30	a	412	LHG	P-O3	3.17	1.72	1.59
23	b	612	CLA	CHC-C1C	3.17	1.43	1.35
23	s	613	CLA	CHC-C1C	3.17	1.43	1.35
23	a	403	CLA	CHC-C1C	3.17	1.43	1.35
23	b	610	CLA	CHC-C1C	3.17	1.43	1.35
23	b	608	CLA	CHC-C1C	3.17	1.43	1.35
23	N	602	CLA	CHC-C1C	3.17	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	608	CLA	CHC-C1C	3.17	1.43	1.35
42	y	302	XAT	C2-C1	3.17	1.59	1.54
23	a	407	CLA	CHC-C1C	3.17	1.43	1.35
30	d	404	LHG	O7-C7	3.17	1.43	1.34
23	n	614	CLA	CHC-C1C	3.17	1.43	1.35
42	y	302	XAT	O24-C25	3.17	1.50	1.46
23	n	604	CLA	CHC-C1C	3.16	1.43	1.35
23	S	613	CLA	CHC-C1C	3.16	1.43	1.35
23	r	608	CLA	CHC-C1C	3.16	1.43	1.35
23	c	513	CLA	CHC-C1C	3.16	1.43	1.35
23	B	614	CLA	CHC-C1C	3.16	1.43	1.35
23	b	613	CLA	CHC-C1C	3.16	1.43	1.35
23	r	601	CLA	CHC-C1C	3.16	1.43	1.35
23	b	601	CLA	CHC-C1C	3.16	1.43	1.35
23	g	614	CLA	CHC-C1C	3.16	1.43	1.35
30	r	616	LHG	P-O6	3.16	1.72	1.59
23	B	603	CLA	CHC-C1C	3.16	1.43	1.35
23	n	613	CLA	CHC-C1C	3.16	1.43	1.35
23	b	606	CLA	CHC-C1C	3.16	1.43	1.35
23	B	613	CLA	CHC-C1C	3.16	1.43	1.35
23	R	611	CLA	CHC-C1C	3.16	1.43	1.35
23	G	614	CLA	CHC-C1C	3.16	1.43	1.35
23	y	312	CLA	CHC-C1C	3.16	1.43	1.35
23	S	603	CLA	CHC-C1C	3.16	1.43	1.35
23	y	311	CLA	CHC-C1C	3.16	1.43	1.35
23	B	616	CLA	CHC-C1C	3.16	1.43	1.35
23	Y	314	CLA	CHC-C1C	3.16	1.43	1.35
23	b	607	CLA	CHC-C1C	3.15	1.43	1.35
23	y	304	CLA	CHC-C1C	3.15	1.43	1.35
23	y	314	CLA	CHC-C1C	3.15	1.43	1.35
23	C	513	CLA	CHC-C1C	3.15	1.43	1.35
23	R	604	CLA	CHC-C1C	3.15	1.43	1.35
23	Y	303	CLA	CHC-C1C	3.15	1.43	1.35
23	y	315	CLA	CHC-C1C	3.15	1.43	1.35
30	N	618	LHG	P-O6	3.15	1.72	1.59
40	s	614	LUT	C31-C30	3.15	1.53	1.43
23	B	609	CLA	CHC-C1C	3.15	1.43	1.35
23	r	611	CLA	CHC-C1C	3.15	1.43	1.35
23	s	610	CLA	CHC-C1C	3.15	1.43	1.35
23	N	612	CLA	CHC-C1C	3.15	1.43	1.35
23	A	402	CLA	CHC-C1C	3.15	1.43	1.35
40	S	614	LUT	C11-C10	3.15	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CHC-C1C	3.15	1.43	1.35
23	r	602	CLA	CHC-C1C	3.15	1.43	1.35
23	Y	310	CLA	CHC-C1C	3.15	1.43	1.35
23	c	509	CLA	CHC-C1C	3.14	1.43	1.35
41	r	614	NEX	C20-C13	3.14	1.57	1.50
23	Y	311	CLA	CHC-C1C	3.14	1.43	1.35
23	Y	313	CLA	CHC-C1C	3.14	1.43	1.35
23	B	608	CLA	CHC-C1C	3.14	1.43	1.35
26	M	101	SQD	O47-C45	-3.14	1.38	1.46
23	Y	305	CLA	CHC-C1C	3.14	1.43	1.35
23	b	602	CLA	CHC-C1C	3.14	1.43	1.35
23	g	611	CLA	CHC-C1C	3.14	1.43	1.35
23	N	611	CLA	CHC-C1C	3.14	1.43	1.35
23	R	612	CLA	CHC-C1C	3.14	1.43	1.35
25	C	514	BCR	C30-C25	-3.14	1.49	1.53
23	C	509	CLA	CHC-C1C	3.14	1.43	1.35
23	G	610	CLA	CHC-C1C	3.14	1.43	1.35
23	S	608	CLA	CHC-C1C	3.14	1.43	1.35
23	b	605	CLA	CHC-C1C	3.14	1.43	1.35
23	B	602	CLA	CHC-C1C	3.13	1.43	1.35
23	g	610	CLA	CHC-C1C	3.13	1.43	1.35
30	R	616	LHG	P-O3	3.13	1.72	1.59
42	Y	301	XAT	O24-C25	3.13	1.50	1.46
23	s	604	CLA	CHC-C1C	3.13	1.43	1.35
23	b	609	CLA	CHC-C1C	3.13	1.43	1.35
23	C	503	CLA	CHC-C1C	3.13	1.43	1.35
23	g	612	CLA	CHC-C1C	3.13	1.43	1.35
23	s	612	CLA	CHC-C1C	3.13	1.43	1.35
23	C	508	CLA	CHC-C1C	3.13	1.43	1.35
23	R	603	CLA	CHC-C1C	3.13	1.43	1.35
23	r	612	CLA	CHC-C1C	3.13	1.43	1.35
23	B	615	CLA	CHC-C1C	3.13	1.43	1.35
40	g	615	LUT	C10-C9	3.13	1.39	1.35
40	N	615	LUT	C26-C27	3.13	1.54	1.50
23	B	607	CLA	CHC-C1C	3.13	1.43	1.35
23	A	406	CLA	CHC-C1C	3.12	1.43	1.35
23	n	612	CLA	CHC-C1C	3.12	1.43	1.35
23	g	604	CLA	CHC-C1C	3.12	1.43	1.35
30	R	616	LHG	O7-C7	3.12	1.43	1.34
40	N	615	LUT	C28-C27	3.12	1.39	1.32
40	S	614	LUT	C32-C33	3.12	1.52	1.45
23	a	405	CLA	CHC-C1C	3.12	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	611	CLA	CHC-C1C	3.12	1.43	1.35
23	C	512	CLA	CHC-C1C	3.12	1.43	1.35
23	G	611	CLA	CHC-C1C	3.12	1.43	1.35
23	G	612	CLA	CHC-C1C	3.12	1.43	1.35
23	A	404	CLA	CHC-C1C	3.12	1.43	1.35
30	a	412	LHG	P-O6	3.12	1.71	1.59
42	G	619	XAT	O24-C25	3.12	1.50	1.46
23	s	611	CLA	CHC-C1C	3.12	1.43	1.35
23	r	604	CLA	CHC-C1C	3.12	1.43	1.35
26	L	101	SQD	O47-C45	-3.12	1.38	1.46
23	G	603	CLA	CHC-C1C	3.12	1.43	1.35
23	S	604	CLA	CHC-C1C	3.11	1.43	1.35
23	Y	312	CLA	CHC-C1C	3.11	1.42	1.35
23	C	502	CLA	CHC-C1C	3.11	1.42	1.35
23	N	613	CLA	CHC-C1C	3.11	1.42	1.35
25	D	411	BCR	C30-C25	-3.11	1.49	1.53
23	C	505	CLA	CHC-C1C	3.11	1.42	1.35
23	c	505	CLA	CHC-C1C	3.11	1.42	1.35
23	c	508	CLA	CHC-C1C	3.11	1.42	1.35
23	r	603	CLA	CHC-C1C	3.11	1.42	1.35
30	Y	318	LHG	P-O6	3.11	1.71	1.59
23	C	504	CLA	CHC-C1C	3.11	1.42	1.35
23	g	613	CLA	CHC-C1C	3.11	1.42	1.35
30	N	618	LHG	O7-C7	3.11	1.43	1.34
25	Z	101	BCR	C1-C6	-3.11	1.49	1.53
23	c	507	CLA	CHC-C1C	3.11	1.42	1.35
41	N	617	NEX	C20-C13	3.11	1.57	1.50
23	c	512	CLA	CHC-C1C	3.10	1.42	1.35
40	R	613	LUT	C28-C27	3.10	1.39	1.32
23	S	611	CLA	CHC-C1C	3.10	1.42	1.35
23	d	406	CLA	CHC-C1C	3.10	1.42	1.35
40	N	616	LUT	C28-C27	3.10	1.39	1.32
30	G	618	LHG	P-O3	3.10	1.71	1.59
41	R	618	NEX	C39-C29	3.10	1.57	1.50
40	s	615	LUT	C28-C27	3.10	1.39	1.32
41	r	614	NEX	C39-C29	3.10	1.57	1.50
23	C	507	CLA	CHC-C1C	3.10	1.42	1.35
23	G	604	CLA	CHC-C1C	3.10	1.42	1.35
23	c	504	CLA	CHC-C1C	3.10	1.42	1.35
23	b	611	CLA	CHC-C1C	3.10	1.42	1.35
23	D	406	CLA	CHC-C1C	3.10	1.42	1.35
42	y	302	XAT	C31-C32	3.10	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	306	CLA	CHC-C1C	3.10	1.42	1.35
40	N	616	LUT	C11-C10	3.10	1.53	1.43
25	c	514	BCR	C30-C25	-3.10	1.49	1.53
23	A	403	CLA	CHC-C1C	3.09	1.42	1.35
23	b	615	CLA	CHC-C1C	3.09	1.42	1.35
23	B	605	CLA	CHC-C1C	3.09	1.42	1.35
40	r	613	LUT	C11-C10	3.09	1.53	1.43
30	S	616	LHG	P-O6	3.09	1.71	1.59
23	G	613	CLA	CHC-C1C	3.09	1.42	1.35
23	D	405	CLA	CHC-C1C	3.09	1.42	1.35
23	S	612	CLA	CHC-C1C	3.09	1.42	1.35
23	g	603	CLA	CHC-C1C	3.09	1.42	1.35
23	a	404	CLA	CHC-C1C	3.09	1.42	1.35
23	y	313	CLA	CHC-C1C	3.09	1.42	1.35
23	c	503	CLA	CHC-C1C	3.08	1.42	1.35
23	c	501	CLA	CHC-C1C	3.08	1.42	1.35
23	B	611	CLA	CHC-C1C	3.08	1.42	1.35
30	S	616	LHG	P-O3	3.08	1.71	1.59
40	N	616	LUT	C32-C33	3.08	1.52	1.45
23	c	506	CLA	CHC-C1C	3.08	1.42	1.35
41	n	618	NEX	C20-C13	3.08	1.57	1.50
23	C	506	CLA	CHC-C1C	3.08	1.42	1.35
23	c	502	CLA	CHC-C1C	3.08	1.42	1.35
23	n	603	CLA	CHC-C1C	3.08	1.42	1.35
30	r	616	LHG	O7-C7	3.07	1.43	1.34
25	z	101	BCR	C1-C6	-3.07	1.49	1.53
40	R	613	LUT	C26-C27	3.07	1.54	1.50
23	d	405	CLA	CHC-C1C	3.07	1.42	1.35
25	a	408	BCR	C30-C25	-3.07	1.49	1.53
40	R	613	LUT	C11-C10	3.07	1.53	1.43
23	C	501	CLA	CHC-C1C	3.07	1.42	1.35
40	s	615	LUT	C11-C10	3.07	1.52	1.43
25	B	619	BCR	C1-C6	-3.06	1.49	1.53
38	F	501	HEM	CAB-C3B	3.06	1.55	1.47
26	M	101	SQD	C24-C23	3.06	1.59	1.50
25	D	411	BCR	C1-C6	-3.05	1.49	1.53
41	Y	317	NEX	C39-C29	3.05	1.57	1.50
30	s	616	LHG	P-O3	3.05	1.71	1.59
26	a	409	SQD	C24-C23	3.05	1.59	1.50
25	b	617	BCR	C30-C25	-3.05	1.49	1.53
23	N	603	CLA	CHC-C1C	3.05	1.42	1.35
40	S	615	LUT	C8-C9	3.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S	616	LHG	O7-C7	3.04	1.42	1.34
23	b	610	CLA	C4D-ND	-3.04	1.33	1.37
30	d	408	LHG	P-O3	3.04	1.71	1.59
23	y	305	CLA	CHC-C1C	3.04	1.42	1.35
25	B	617	BCR	C1-C6	-3.04	1.49	1.53
38	f	501	HEM	CAB-C3B	3.04	1.55	1.47
40	N	615	LUT	C32-C33	3.04	1.52	1.45
30	Y	318	LHG	P-O3	3.03	1.71	1.59
23	Y	304	CLA	CHC-C1C	3.03	1.42	1.35
42	R	615	XAT	C31-C32	3.03	1.42	1.34
26	L	101	SQD	C24-C23	3.03	1.59	1.50
40	Y	316	LUT	C28-C27	3.03	1.39	1.32
30	b	627	LHG	O7-C7	3.03	1.42	1.34
40	y	317	LUT	C28-C27	3.03	1.39	1.32
42	r	615	XAT	C31-C32	3.02	1.42	1.34
25	B	618	BCR	C30-C25	-3.02	1.49	1.53
40	s	615	LUT	C8-C9	3.02	1.52	1.45
23	B	611	CLA	C4D-ND	-3.02	1.33	1.37
40	r	613	LUT	C28-C27	3.02	1.39	1.32
25	A	407	BCR	C30-C25	-3.01	1.49	1.53
25	b	618	BCR	C30-C25	-3.00	1.49	1.53
26	A	408	SQD	C24-C23	3.00	1.59	1.50
41	R	614	NEX	C20-C13	3.00	1.57	1.50
40	G	615	LUT	C28-C27	3.00	1.39	1.32
30	g	618	LHG	P-O3	3.00	1.71	1.59
23	b	611	CLA	C4D-ND	-2.99	1.33	1.37
40	N	615	LUT	C8-C9	2.99	1.52	1.45
30	y	318	LHG	P-O3	2.99	1.71	1.59
30	s	616	LHG	P-O6	2.99	1.71	1.59
23	A	402	CLA	C4D-ND	-2.99	1.33	1.37
40	S	615	LUT	C31-C30	2.98	1.52	1.43
42	y	302	XAT	C28-C29	-2.98	1.39	1.45
23	d	406	CLA	C4D-ND	-2.98	1.33	1.37
25	B	617	BCR	C30-C25	-2.98	1.49	1.53
40	s	615	LUT	C32-C33	2.98	1.52	1.45
23	B	605	CLA	C4D-ND	-2.98	1.33	1.37
41	Y	317	NEX	C20-C13	2.98	1.57	1.50
30	R	616	LHG	P-O6	2.98	1.71	1.59
23	A	403	CLA	C4D-ND	-2.98	1.33	1.37
23	b	604	CLA	C4D-ND	-2.98	1.33	1.37
23	B	604	CLA	CHC-C1C	2.98	1.42	1.35
23	b	604	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	618	LHG	O7-C7	2.97	1.42	1.34
41	R	618	NEX	C20-C13	2.97	1.57	1.50
40	g	615	LUT	C28-C27	2.97	1.39	1.32
23	c	506	CLA	C4D-ND	-2.97	1.33	1.37
23	S	613	CLA	C4D-ND	-2.97	1.33	1.37
30	G	618	LHG	O7-C7	2.97	1.42	1.34
30	L	103	LHG	O7-C7	2.97	1.42	1.34
23	c	509	CLA	C4D-ND	-2.97	1.33	1.37
23	B	606	CLA	C4D-ND	-2.96	1.33	1.37
23	a	407	CLA	C4D-ND	-2.96	1.33	1.37
40	G	616	LUT	C28-C27	2.96	1.39	1.32
23	b	608	CLA	C4D-ND	-2.96	1.33	1.37
30	a	412	LHG	O7-C7	2.96	1.42	1.34
40	r	613	LUT	C8-C9	2.96	1.52	1.45
23	a	403	CLA	C4D-ND	-2.96	1.33	1.37
23	g	604	CLA	C4D-ND	-2.96	1.33	1.37
23	a	404	CLA	C4D-ND	-2.96	1.33	1.37
23	C	503	CLA	C4D-ND	-2.95	1.33	1.37
40	g	616	LUT	C28-C27	2.95	1.39	1.32
30	n	619	LHG	O7-C7	2.95	1.42	1.34
23	B	604	CLA	C4D-ND	-2.95	1.33	1.37
23	a	405	CLA	C4D-ND	-2.95	1.33	1.37
30	Y	318	LHG	O7-C7	2.95	1.42	1.34
23	B	610	CLA	C4D-ND	-2.95	1.33	1.37
40	n	616	LUT	C28-C27	2.95	1.39	1.32
40	s	615	LUT	C26-C27	2.95	1.54	1.50
23	c	513	CLA	C4D-ND	-2.95	1.33	1.37
23	Y	305	CLA	C4D-ND	-2.94	1.33	1.37
23	y	306	CLA	C4D-ND	-2.94	1.33	1.37
30	A	412	LHG	O7-C7	2.94	1.42	1.34
30	A	412	LHG	P-O6	2.94	1.71	1.59
23	r	603	CLA	C4D-ND	-2.94	1.33	1.37
23	A	406	CLA	C4D-ND	-2.94	1.33	1.37
23	C	509	CLA	C4D-ND	-2.94	1.33	1.37
40	S	614	LUT	C31-C30	2.94	1.52	1.43
23	C	501	CLA	C4D-ND	-2.94	1.33	1.37
23	c	503	CLA	C4D-ND	-2.94	1.33	1.37
23	c	502	CLA	C4D-ND	-2.94	1.33	1.37
30	n	619	LHG	P-O6	2.93	1.71	1.59
25	v	101	BCR	C30-C25	-2.93	1.49	1.53
23	y	312	CLA	C4D-ND	-2.93	1.33	1.37
23	B	614	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	614	LUT	C8-C9	2.93	1.52	1.45
42	n	620	XAT	C28-C29	-2.93	1.39	1.45
23	B	612	CLA	C4D-ND	-2.93	1.33	1.37
23	R	612	CLA	C4D-ND	-2.93	1.33	1.37
23	D	406	CLA	C4D-ND	-2.92	1.33	1.37
23	b	616	CLA	C4D-ND	-2.92	1.33	1.37
40	N	616	LUT	C1-C6	2.92	1.57	1.53
40	R	613	LUT	C8-C9	2.92	1.52	1.45
23	R	602	CLA	C4D-ND	-2.92	1.33	1.37
23	Y	312	CLA	C4D-ND	-2.92	1.33	1.37
30	L	103	LHG	P-O3	2.92	1.71	1.59
23	G	611	CLA	C4D-ND	-2.92	1.33	1.37
23	C	513	CLA	C4D-ND	-2.92	1.33	1.37
25	B	619	BCR	C30-C25	-2.91	1.49	1.53
23	r	604	CLA	C4D-ND	-2.91	1.33	1.37
30	y	318	LHG	P-O6	2.91	1.71	1.59
35	C	523	VIV	C10-C3	-2.91	1.46	1.51
23	B	608	CLA	C4D-ND	-2.91	1.33	1.37
23	B	603	CLA	C4D-ND	-2.91	1.33	1.37
23	S	602	CLA	C4D-ND	-2.91	1.33	1.37
23	y	314	CLA	C4D-ND	-2.91	1.33	1.37
23	C	506	CLA	C4D-ND	-2.91	1.33	1.37
23	c	510	CLA	C4D-ND	-2.91	1.33	1.37
23	c	501	CLA	C4D-ND	-2.91	1.33	1.37
30	N	618	LHG	C6-C5	2.91	1.59	1.50
23	S	611	CLA	C4D-ND	-2.91	1.33	1.37
30	s	616	LHG	O7-C7	2.90	1.42	1.34
42	n	620	XAT	C31-C32	2.90	1.42	1.34
23	C	508	CLA	C4D-ND	-2.90	1.33	1.37
23	C	502	CLA	C4D-ND	-2.90	1.33	1.37
23	d	405	CLA	C4D-ND	-2.90	1.33	1.37
23	N	613	CLA	C4D-ND	-2.90	1.33	1.37
30	R	616	LHG	O8-C23	2.90	1.41	1.33
23	C	512	CLA	C4D-ND	-2.90	1.33	1.37
23	b	605	CLA	C4D-ND	-2.90	1.33	1.37
25	V	101	BCR	C30-C25	-2.90	1.49	1.53
23	b	606	CLA	C4D-ND	-2.90	1.33	1.37
23	B	616	CLA	C4D-ND	-2.90	1.33	1.37
23	D	405	CLA	C4D-ND	-2.90	1.33	1.37
23	B	602	CLA	C4D-ND	-2.90	1.33	1.37
23	N	602	CLA	C4D-ND	-2.90	1.33	1.37
23	c	507	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C4D-ND	-2.89	1.33	1.37
23	s	602	CLA	C4D-ND	-2.89	1.33	1.37
23	c	511	CLA	C4D-ND	-2.89	1.33	1.37
30	n	619	LHG	O8-C23	2.89	1.41	1.33
30	D	404	LHG	O7-C7	2.89	1.42	1.34
23	Y	304	CLA	C4D-ND	-2.89	1.33	1.37
42	N	619	XAT	C24-C23	2.89	1.56	1.52
23	b	602	CLA	C4D-ND	-2.89	1.33	1.37
40	G	616	LUT	C8-C9	2.89	1.52	1.45
23	y	305	CLA	C4D-ND	-2.89	1.33	1.37
40	g	616	LUT	C8-C9	2.89	1.52	1.45
25	k	101	BCR	C30-C25	-2.89	1.49	1.53
42	r	615	XAT	C28-C29	-2.89	1.39	1.45
23	R	609	CLA	C4D-ND	-2.88	1.33	1.37
25	b	619	BCR	C30-C25	-2.88	1.49	1.53
23	R	601	CLA	C4D-ND	-2.88	1.33	1.37
23	b	612	CLA	C4D-ND	-2.88	1.33	1.37
23	g	614	CLA	C4D-ND	-2.88	1.33	1.37
23	C	507	CLA	C4D-ND	-2.88	1.33	1.37
23	R	610	CLA	C4D-ND	-2.88	1.33	1.37
23	B	613	CLA	C4D-ND	-2.88	1.33	1.37
23	r	610	CLA	C4D-ND	-2.88	1.33	1.37
23	s	611	CLA	C4D-ND	-2.88	1.33	1.37
30	b	627	LHG	P-O3	2.88	1.71	1.59
30	D	404	LHG	P-O3	2.88	1.71	1.59
23	r	611	CLA	C4D-ND	-2.88	1.33	1.37
23	N	611	CLA	C4D-ND	-2.88	1.33	1.37
23	G	614	CLA	C4D-ND	-2.88	1.33	1.37
42	n	617	XAT	C31-C32	2.88	1.42	1.34
23	r	601	CLA	C4D-ND	-2.88	1.33	1.37
23	G	602	CLA	C4D-ND	-2.88	1.33	1.37
23	Y	311	CLA	C4D-ND	-2.88	1.33	1.37
23	Y	313	CLA	C4D-ND	-2.88	1.33	1.37
40	s	614	LUT	C22-C21	2.88	1.58	1.54
23	A	404	CLA	C4D-ND	-2.87	1.33	1.37
30	y	318	LHG	O8-C23	2.87	1.41	1.33
23	B	601	CLA	C4D-ND	-2.87	1.33	1.37
23	n	613	CLA	C4D-ND	-2.87	1.33	1.37
40	G	616	LUT	C11-C10	2.87	1.52	1.43
23	c	508	CLA	C4D-ND	-2.87	1.33	1.37
23	G	604	CLA	C4D-ND	-2.87	1.33	1.37
23	R	603	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	610	CLA	C4D-ND	-2.87	1.33	1.37
23	b	614	CLA	C4D-ND	-2.87	1.33	1.37
23	b	603	CLA	C4D-ND	-2.87	1.33	1.37
23	G	613	CLA	C4D-ND	-2.87	1.33	1.37
30	G	618	LHG	P-O6	2.87	1.70	1.59
23	c	512	CLA	C4D-ND	-2.86	1.33	1.37
30	r	616	LHG	C8-C7	2.86	1.59	1.50
23	n	602	CLA	C4D-ND	-2.86	1.33	1.37
23	S	612	CLA	C4D-ND	-2.86	1.33	1.37
30	g	618	LHG	O8-C23	2.86	1.41	1.33
23	b	615	CLA	C4D-ND	-2.86	1.33	1.37
23	Y	310	CLA	C4D-ND	-2.86	1.33	1.37
23	b	613	CLA	C4D-ND	-2.86	1.33	1.37
23	n	603	CLA	C4D-ND	-2.86	1.33	1.37
42	n	617	XAT	C11-C12	2.86	1.41	1.34
23	g	612	CLA	C4D-ND	-2.86	1.33	1.37
40	g	616	LUT	C11-C10	2.86	1.52	1.43
23	r	608	CLA	C4D-ND	-2.86	1.33	1.37
40	s	615	LUT	C22-C21	2.86	1.58	1.54
23	r	612	CLA	C4D-ND	-2.86	1.33	1.37
23	s	613	CLA	C4D-ND	-2.86	1.33	1.37
23	g	613	CLA	C4D-ND	-2.86	1.33	1.37
40	n	616	LUT	C1-C6	2.85	1.57	1.53
30	y	318	LHG	O7-C7	2.85	1.42	1.34
40	R	613	LUT	C32-C33	2.85	1.52	1.45
23	y	311	CLA	C4D-ND	-2.85	1.33	1.37
25	K	101	BCR	C30-C25	-2.85	1.49	1.53
30	g	618	LHG	P-O6	2.85	1.70	1.59
23	S	610	CLA	C4D-ND	-2.85	1.33	1.37
23	s	604	CLA	C4D-ND	-2.85	1.33	1.37
23	B	615	CLA	C4D-ND	-2.85	1.33	1.37
23	R	608	CLA	C4D-ND	-2.85	1.33	1.37
23	b	609	CLA	C4D-ND	-2.85	1.33	1.37
23	B	609	CLA	C4D-ND	-2.85	1.33	1.37
23	r	602	CLA	C4D-ND	-2.85	1.33	1.37
23	y	304	CLA	C4D-ND	-2.85	1.33	1.37
23	y	313	CLA	C4D-ND	-2.85	1.33	1.37
23	N	612	CLA	C4D-ND	-2.85	1.33	1.37
23	g	611	CLA	C4D-ND	-2.85	1.33	1.37
30	Y	318	LHG	C8-C7	2.84	1.59	1.50
30	d	408	LHG	O7-C7	2.84	1.42	1.34
23	C	510	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	612	CLA	C4D-ND	-2.84	1.33	1.37
30	d	404	LHG	C8-C7	2.84	1.59	1.50
23	N	603	CLA	C4D-ND	-2.84	1.33	1.37
30	R	616	LHG	C8-C7	2.84	1.59	1.50
40	G	616	LUT	C26-C27	2.84	1.54	1.50
30	N	618	LHG	O8-C23	2.83	1.41	1.33
23	g	602	CLA	C4D-ND	-2.83	1.33	1.37
23	C	511	CLA	C4D-ND	-2.83	1.33	1.37
30	d	404	LHG	P-O3	2.83	1.70	1.59
23	N	604	CLA	C4D-ND	-2.83	1.33	1.37
40	s	614	LUT	C15-C14	2.83	1.52	1.43
23	G	603	CLA	C4D-ND	-2.83	1.33	1.37
40	S	615	LUT	C1-C6	2.83	1.57	1.53
30	S	616	LHG	O8-C23	2.83	1.41	1.33
23	R	604	CLA	C4D-ND	-2.83	1.33	1.37
23	G	610	CLA	C4D-ND	-2.83	1.33	1.37
23	C	504	CLA	C4D-ND	-2.83	1.33	1.37
30	r	616	LHG	O8-C23	2.82	1.41	1.33
42	n	620	XAT	C24-C23	2.82	1.56	1.52
23	R	611	CLA	C4D-ND	-2.82	1.33	1.37
30	s	616	LHG	O8-C23	2.82	1.41	1.33
40	N	616	LUT	C31-C30	2.82	1.52	1.43
40	Y	316	LUT	C26-C27	2.82	1.54	1.50
30	G	618	LHG	O8-C23	2.82	1.41	1.33
23	s	612	CLA	C4D-ND	-2.82	1.33	1.37
23	r	609	CLA	C4D-ND	-2.82	1.33	1.37
40	y	317	LUT	C26-C27	2.82	1.54	1.50
42	G	619	XAT	C24-C25	-2.82	1.48	1.52
30	g	618	LHG	C8-C7	2.81	1.58	1.50
23	S	604	CLA	C4D-ND	-2.81	1.33	1.37
23	g	603	CLA	C4D-ND	-2.81	1.33	1.37
30	S	616	LHG	C8-C7	2.81	1.58	1.50
23	n	611	CLA	C4D-ND	-2.80	1.33	1.37
23	G	612	CLA	C4D-ND	-2.80	1.33	1.37
23	s	603	CLA	C4D-ND	-2.80	1.33	1.37
23	s	608	CLA	C4D-ND	-2.80	1.33	1.37
30	Y	318	LHG	O8-C23	2.80	1.41	1.33
30	D	408	LHG	P-O3	2.80	1.70	1.59
40	N	615	LUT	C31-C30	2.80	1.52	1.43
23	n	610	CLA	C4D-ND	-2.80	1.33	1.37
30	a	412	LHG	O8-C23	2.80	1.41	1.33
23	Y	303	CLA	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	609	CLA	C4D-ND	-2.79	1.33	1.37
23	n	604	CLA	C4D-ND	-2.79	1.33	1.37
40	S	614	LUT	C1-C6	2.79	1.57	1.53
23	S	603	CLA	C4D-ND	-2.79	1.33	1.37
40	r	613	LUT	C15-C14	2.79	1.52	1.43
40	S	615	LUT	C5-C6	2.79	1.39	1.34
23	Y	314	CLA	C4D-ND	-2.79	1.33	1.37
30	L	103	LHG	O8-C23	2.79	1.41	1.33
30	b	627	LHG	C8-C7	2.79	1.58	1.50
30	D	404	LHG	C8-C7	2.78	1.58	1.50
23	s	610	CLA	C4D-ND	-2.78	1.33	1.37
30	b	627	LHG	O8-C23	2.78	1.41	1.33
23	B	607	CLA	C4D-ND	-2.78	1.33	1.37
23	y	315	CLA	C4D-ND	-2.78	1.33	1.37
30	G	618	LHG	C8-C7	2.77	1.58	1.50
30	N	618	LHG	C8-C7	2.77	1.58	1.50
30	L	103	LHG	P-O6	2.77	1.70	1.59
40	y	317	LUT	C8-C9	2.77	1.51	1.45
42	R	615	XAT	C28-C29	-2.77	1.40	1.45
23	b	607	CLA	C4D-ND	-2.77	1.33	1.37
42	N	619	XAT	C28-C29	-2.76	1.40	1.45
30	D	404	LHG	O8-C23	2.76	1.41	1.33
23	g	610	CLA	C4D-ND	-2.76	1.33	1.37
40	G	615	LUT	C22-C21	2.76	1.58	1.54
40	N	616	LUT	C8-C9	2.76	1.51	1.45
23	N	614	CLA	C4D-ND	-2.76	1.33	1.37
30	n	619	LHG	C8-C7	2.75	1.58	1.50
40	Y	316	LUT	C11-C10	2.75	1.52	1.43
40	y	317	LUT	C11-C10	2.75	1.52	1.43
40	r	613	LUT	C32-C33	2.75	1.51	1.45
40	R	613	LUT	C31-C30	2.75	1.52	1.43
23	c	505	CLA	C4D-ND	-2.75	1.33	1.37
30	b	627	LHG	P-O6	2.74	1.70	1.59
40	s	615	LUT	C31-C30	2.74	1.51	1.43
30	d	404	LHG	O8-C23	2.74	1.41	1.33
23	s	609	CLA	C4D-ND	-2.74	1.33	1.37
30	d	408	LHG	O8-C23	2.74	1.41	1.33
40	s	615	LUT	C1-C6	2.74	1.57	1.53
23	b	601	CLA	C4D-ND	-2.74	1.33	1.37
23	n	614	CLA	C4D-ND	-2.73	1.33	1.37
40	s	614	LUT	C11-C12	2.73	1.41	1.34
30	d	404	LHG	P-O6	2.73	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	N	615	LUT	C11-C12	2.73	1.41	1.34
40	R	613	LUT	C5-C6	2.73	1.39	1.34
30	y	318	LHG	C8-C7	2.73	1.58	1.50
23	S	608	CLA	C4D-ND	-2.73	1.33	1.37
40	n	616	LUT	C11-C10	2.72	1.51	1.43
30	d	408	LHG	P-O6	2.72	1.70	1.59
40	g	616	LUT	C5-C6	2.72	1.39	1.34
40	g	616	LUT	C26-C27	2.71	1.54	1.50
23	C	505	CLA	C4D-ND	-2.71	1.34	1.37
30	A	412	LHG	C8-C7	2.71	1.58	1.50
40	s	615	LUT	C5-C6	2.71	1.39	1.34
40	Y	316	LUT	C8-C9	2.70	1.51	1.45
40	n	616	LUT	C26-C27	2.70	1.54	1.50
30	d	408	LHG	C8-C7	2.70	1.58	1.50
30	s	616	LHG	C8-C7	2.69	1.58	1.50
40	N	616	LUT	C15-C14	2.69	1.51	1.43
30	r	616	LHG	C6-C5	2.69	1.59	1.50
40	N	615	LUT	C5-C6	2.69	1.39	1.34
40	y	317	LUT	C5-C6	2.68	1.39	1.34
40	S	615	LUT	C15-C14	2.68	1.51	1.43
40	y	316	LUT	C28-C27	2.68	1.38	1.32
30	A	412	LHG	O8-C23	2.68	1.41	1.33
30	S	616	LHG	C6-C5	2.68	1.58	1.50
40	r	613	LUT	C26-C27	2.67	1.54	1.50
30	L	103	LHG	C8-C7	2.67	1.58	1.50
40	s	614	LUT	C5-C6	2.67	1.39	1.34
40	N	615	LUT	C1-C6	2.66	1.57	1.53
40	r	613	LUT	C5-C6	2.66	1.39	1.34
40	S	614	LUT	C15-C14	2.66	1.51	1.43
24	a	406	PHO	CAC-C3C	-2.66	1.47	1.52
24	d	402	PHO	CAC-C3C	-2.65	1.47	1.52
40	Y	316	LUT	C5-C6	2.65	1.39	1.34
40	Y	315	LUT	C28-C27	2.65	1.38	1.32
30	n	619	LHG	C6-C5	2.65	1.58	1.50
40	s	614	LUT	C1-C6	2.65	1.57	1.53
30	D	404	LHG	P-O6	2.65	1.70	1.59
40	n	615	LUT	C28-C27	2.64	1.38	1.32
24	A	405	PHO	CAC-C3C	-2.64	1.47	1.52
30	R	616	LHG	C6-C5	2.64	1.58	1.50
42	G	619	XAT	C24-C23	2.64	1.56	1.52
40	S	615	LUT	C11-C12	2.64	1.41	1.34
30	g	618	LHG	C6-C5	2.64	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	N	615	LUT	C15-C14	2.64	1.51	1.43
23	Y	305	CLA	CMB-C2B	-2.63	1.46	1.51
40	S	614	LUT	C11-C12	2.63	1.41	1.34
40	S	614	LUT	C5-C6	2.63	1.39	1.34
23	y	306	CLA	CMB-C2B	-2.62	1.46	1.51
41	s	617	NEX	C40-C33	2.62	1.57	1.50
24	D	402	PHO	CAC-C3C	-2.61	1.47	1.52
42	y	302	XAT	O4-C5	-2.61	1.42	1.46
40	G	616	LUT	C5-C6	2.61	1.38	1.34
30	y	318	LHG	C6-C5	2.61	1.58	1.50
42	r	615	XAT	C11-C12	2.61	1.41	1.34
30	N	618	LHG	C4-C5	2.61	1.58	1.50
40	N	616	LUT	C11-C12	2.61	1.41	1.34
40	R	613	LUT	C11-C12	2.60	1.41	1.34
30	a	412	LHG	C8-C7	2.60	1.58	1.50
42	n	617	XAT	C24-C23	2.59	1.56	1.52
40	R	613	LUT	C15-C14	2.59	1.51	1.43
40	g	616	LUT	C1-C6	2.59	1.57	1.53
40	s	614	LUT	C28-C29	2.59	1.51	1.45
40	G	616	LUT	C32-C33	2.59	1.51	1.45
23	g	604	CLA	CMB-C2B	-2.59	1.46	1.51
40	s	615	LUT	C11-C12	2.58	1.41	1.34
40	r	613	LUT	C11-C12	2.58	1.41	1.34
40	y	317	LUT	C32-C33	2.58	1.51	1.45
40	r	613	LUT	C31-C30	2.58	1.51	1.43
41	r	614	NEX	C37-C21	2.57	1.58	1.53
23	C	506	CLA	CMB-C2B	-2.57	1.46	1.51
42	Y	301	XAT	O4-C5	-2.57	1.42	1.46
40	G	616	LUT	C1-C6	2.57	1.57	1.53
23	S	604	CLA	CMB-C2B	-2.57	1.46	1.51
40	g	616	LUT	C32-C33	2.57	1.51	1.45
40	N	616	LUT	C5-C6	2.57	1.38	1.34
23	R	604	CLA	CMB-C2B	-2.56	1.46	1.51
40	Y	316	LUT	C31-C30	2.56	1.51	1.43
40	y	316	LUT	C5-C6	2.56	1.38	1.34
30	b	627	LHG	C6-C5	2.56	1.58	1.50
42	n	617	XAT	C28-C29	-2.56	1.40	1.45
30	d	408	LHG	C6-C5	2.56	1.58	1.50
41	R	618	NEX	C37-C21	2.56	1.58	1.53
40	n	616	LUT	C5-C6	2.56	1.38	1.34
30	G	618	LHG	C6-C5	2.55	1.58	1.50
42	R	615	XAT	C11-C12	2.55	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R	614	NEX	C37-C21	2.55	1.58	1.53
23	s	604	CLA	CMB-C2B	-2.55	1.46	1.51
23	N	604	CLA	CMB-C2B	-2.55	1.46	1.51
41	N	617	NEX	C38-C25	2.55	1.55	1.51
40	s	615	LUT	C15-C14	2.55	1.51	1.43
40	n	615	LUT	C5-C6	2.55	1.38	1.34
42	y	302	XAT	C24-C25	-2.54	1.48	1.52
23	G	604	CLA	CMB-C2B	-2.54	1.46	1.51
30	L	103	LHG	C6-C5	2.54	1.58	1.50
40	Y	316	LUT	C32-C33	2.54	1.51	1.45
40	G	616	LUT	C11-C12	2.54	1.41	1.34
40	g	616	LUT	C11-C12	2.54	1.41	1.34
42	Y	301	XAT	C28-C29	-2.54	1.40	1.45
40	G	616	LUT	C31-C30	2.53	1.51	1.43
23	c	506	CLA	CMB-C2B	-2.53	1.46	1.51
40	y	317	LUT	C31-C30	2.53	1.51	1.43
35	C	523	VIV	O1-C9	-2.53	1.43	1.46
30	Y	318	LHG	C6-C5	2.53	1.58	1.50
23	n	604	CLA	CMB-C2B	-2.53	1.46	1.51
41	Y	317	NEX	C37-C21	2.53	1.58	1.53
41	G	617	NEX	C38-C25	2.52	1.55	1.51
23	s	609	CLA	CMB-C2B	-2.52	1.46	1.51
30	a	412	LHG	C6-C5	2.52	1.58	1.50
40	y	317	LUT	C1-C6	2.52	1.57	1.53
30	D	404	LHG	C6-C5	2.52	1.58	1.50
40	n	615	LUT	C12-C13	2.51	1.51	1.45
23	r	604	CLA	CMB-C2B	-2.51	1.46	1.51
42	Y	301	XAT	C24-C23	2.51	1.55	1.52
41	r	614	NEX	C38-C25	2.51	1.55	1.51
40	g	616	LUT	C31-C30	2.51	1.51	1.43
41	G	617	NEX	C37-C21	2.51	1.58	1.53
41	g	617	NEX	C37-C21	2.50	1.58	1.53
23	b	604	CLA	CMB-C2B	-2.50	1.46	1.51
41	N	617	NEX	C37-C21	2.50	1.58	1.53
30	d	404	LHG	C6-C5	2.50	1.58	1.50
41	g	617	NEX	C38-C25	2.50	1.55	1.51
41	n	618	NEX	C37-C21	2.49	1.58	1.53
23	D	406	CLA	CMB-C2B	-2.49	1.46	1.51
33	C	515	DGD	O1G-C1G	-2.49	1.39	1.45
42	y	302	XAT	C24-C23	2.49	1.55	1.52
30	D	408	LHG	O7-C7	2.49	1.41	1.34
42	n	620	XAT	C4-C3	2.48	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	CMB-C2B	-2.48	1.46	1.51
40	G	615	LUT	C26-C27	2.48	1.53	1.50
30	S	616	LHG	C4-C5	2.48	1.58	1.50
40	R	613	LUT	C1-C6	2.48	1.57	1.53
23	Y	314	CLA	CMB-C2B	-2.47	1.46	1.51
42	N	619	XAT	C4-C3	2.47	1.55	1.52
23	y	311	CLA	CMB-C2B	-2.47	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.47	1.46	1.51
41	R	614	NEX	C38-C25	2.47	1.55	1.51
42	y	302	XAT	C37-C21	2.47	1.58	1.53
23	B	604	CLA	CMB-C2B	-2.47	1.46	1.51
23	B	608	CLA	CMB-C2B	-2.47	1.46	1.51
42	r	615	XAT	C4-C3	2.47	1.55	1.52
40	n	616	LUT	C31-C30	2.46	1.51	1.43
40	n	616	LUT	C32-C33	2.46	1.51	1.45
42	n	617	XAT	O4-C5	-2.46	1.42	1.46
40	S	614	LUT	C28-C29	2.46	1.51	1.45
39	g	619	CHL	C3B-C2B	-2.46	1.37	1.40
23	G	611	CLA	CMB-C2B	-2.46	1.46	1.51
23	C	502	CLA	CMB-C2B	-2.46	1.46	1.51
23	c	501	CLA	CMB-C2B	-2.46	1.46	1.51
41	R	618	NEX	C38-C25	2.46	1.55	1.51
23	B	610	CLA	CMB-C2B	-2.46	1.46	1.51
40	s	614	LUT	C31-C32	2.46	1.40	1.34
40	S	615	LUT	C28-C29	2.45	1.51	1.45
30	R	616	LHG	C24-C23	2.45	1.57	1.50
30	y	318	LHG	C24-C23	2.45	1.57	1.50
23	B	606	CLA	CMB-C2B	-2.45	1.46	1.51
30	A	412	LHG	C6-C5	2.45	1.58	1.50
39	n	607	CHL	C3B-C2B	-2.45	1.37	1.40
23	y	315	CLA	CMB-C2B	-2.45	1.46	1.51
41	n	618	NEX	C38-C25	2.45	1.55	1.51
23	S	609	CLA	CMB-C2B	-2.45	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.45	1.46	1.51
23	a	404	CLA	CMB-C2B	-2.45	1.46	1.51
42	G	619	XAT	O4-C5	-2.45	1.42	1.46
40	g	615	LUT	C26-C27	2.44	1.53	1.50
40	n	616	LUT	C8-C9	2.44	1.51	1.45
42	R	615	XAT	C4-C3	2.44	1.55	1.52
23	S	613	CLA	CMB-C2B	-2.44	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.44	1.46	1.51
40	Y	316	LUT	C1-C6	2.44	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	403	CLA	CMB-C2B	-2.44	1.46	1.51
39	R	607	CHL	C3B-C2B	-2.44	1.37	1.40
30	r	616	LHG	C4-C5	2.43	1.58	1.50
30	s	616	LHG	C6-C5	2.43	1.58	1.50
39	R	606	CHL	C3B-C2B	-2.43	1.37	1.40
23	Y	311	CLA	CMB-C2B	-2.43	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.43	1.46	1.51
23	r	612	CLA	CMB-C2B	-2.43	1.46	1.51
40	n	616	LUT	C11-C12	2.43	1.40	1.34
40	y	317	LUT	C11-C12	2.43	1.40	1.34
23	b	601	CLA	CMB-C2B	-2.43	1.46	1.51
23	C	501	CLA	CMB-C2B	-2.43	1.46	1.51
23	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
23	s	613	CLA	CMB-C2B	-2.43	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.43	1.46	1.51
23	R	612	CLA	CMB-C2B	-2.43	1.46	1.51
23	C	508	CLA	CMB-C2B	-2.42	1.46	1.51
23	r	601	CLA	CMB-C2B	-2.42	1.46	1.51
42	y	302	XAT	C17-C1	2.42	1.58	1.53
40	S	615	LUT	C31-C32	2.42	1.40	1.34
23	y	312	CLA	CMB-C2B	-2.42	1.46	1.51
23	s	610	CLA	CMB-C2B	-2.42	1.46	1.51
23	R	603	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.42	1.46	1.51
40	s	614	LUT	C35-C15	2.42	1.42	1.36
40	Y	316	LUT	C11-C12	2.42	1.40	1.34
40	y	316	LUT	C12-C13	2.42	1.51	1.45
40	Y	315	LUT	C5-C6	2.42	1.38	1.34
23	n	611	CLA	CMB-C2B	-2.42	1.46	1.51
23	S	610	CLA	CMB-C2B	-2.41	1.46	1.51
30	D	404	LHG	C24-C23	2.41	1.57	1.50
30	g	618	LHG	C24-C23	2.41	1.57	1.50
23	R	601	CLA	CMB-C2B	-2.41	1.46	1.51
23	s	602	CLA	CMB-C2B	-2.41	1.46	1.51
23	Y	310	CLA	CMB-C2B	-2.41	1.46	1.51
23	g	614	CLA	CMB-C2B	-2.41	1.46	1.51
23	n	603	CLA	CMB-C2B	-2.41	1.46	1.51
33	C	515	DGD	O2G-C2G	-2.41	1.40	1.46
23	C	503	CLA	CMB-C2B	-2.41	1.46	1.51
42	Y	301	XAT	C24-C25	-2.41	1.48	1.52
39	r	606	CHL	C3B-C2B	-2.41	1.37	1.40
23	B	605	CLA	CMB-C2B	-2.41	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	405	CLA	CMB-C2B	-2.41	1.46	1.51
23	y	314	CLA	CMB-C2B	-2.41	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.41	1.46	1.51
23	Y	303	CLA	CMB-C2B	-2.41	1.46	1.51
23	B	601	CLA	CMB-C2B	-2.41	1.46	1.51
23	R	611	CLA	CMB-C2B	-2.41	1.46	1.51
23	Y	312	CLA	CMB-C2B	-2.41	1.46	1.51
23	G	610	CLA	CMB-C2B	-2.40	1.46	1.51
23	A	406	CLA	CMB-C2B	-2.40	1.46	1.51
42	Y	301	XAT	C17-C1	2.40	1.58	1.53
23	B	613	CLA	CMB-C2B	-2.40	1.46	1.51
23	S	612	CLA	CMB-C2B	-2.40	1.46	1.51
42	G	619	XAT	C4-C5	-2.40	1.48	1.52
23	s	603	CLA	CMB-C2B	-2.40	1.46	1.51
23	G	612	CLA	CMB-C2B	-2.40	1.46	1.51
39	G	620	CHL	C3B-C2B	-2.40	1.37	1.40
23	C	509	CLA	CMB-C2B	-2.40	1.46	1.51
23	N	611	CLA	CMB-C2B	-2.40	1.46	1.51
23	R	610	CLA	CMB-C2B	-2.40	1.46	1.51
33	c	515	DGD	O2G-C2G	-2.40	1.40	1.46
40	S	614	LUT	C31-C32	2.40	1.40	1.34
23	y	313	CLA	CMB-C2B	-2.40	1.46	1.51
23	B	611	CLA	CMB-C2B	-2.40	1.46	1.51
23	Y	304	CLA	CMB-C2B	-2.40	1.46	1.51
23	s	611	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	606	CLA	CMB-C2B	-2.39	1.46	1.51
23	s	612	CLA	CMB-C2B	-2.39	1.46	1.51
23	g	610	CLA	CMB-C2B	-2.39	1.46	1.51
23	G	602	CLA	CMB-C2B	-2.39	1.46	1.51
23	S	602	CLA	CMB-C2B	-2.39	1.46	1.51
23	s	608	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	605	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.39	1.46	1.51
39	N	608	CHL	C3B-C2B	-2.39	1.37	1.40
23	b	611	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	405	CLA	CMB-C2B	-2.39	1.46	1.51
23	N	612	CLA	CMB-C2B	-2.39	1.46	1.51
23	g	613	CLA	CMB-C2B	-2.39	1.46	1.51
39	y	303	CHL	C3B-C2B	-2.39	1.37	1.40
42	y	302	XAT	C4-C5	-2.39	1.48	1.52
23	g	612	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CMB-C2B	-2.38	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.38	1.46	1.51
40	g	615	LUT	C5-C6	2.38	1.38	1.34
30	N	618	LHG	C24-C23	2.38	1.57	1.50
23	S	611	CLA	CMB-C2B	-2.38	1.46	1.51
42	N	619	XAT	C24-C25	-2.38	1.48	1.52
23	N	613	CLA	CMB-C2B	-2.38	1.46	1.51
23	R	602	CLA	CMB-C2B	-2.38	1.46	1.51
23	g	602	CLA	CMB-C2B	-2.38	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.38	1.46	1.51
39	r	607	CHL	C3B-C2B	-2.38	1.37	1.40
42	n	617	XAT	C24-C25	-2.38	1.48	1.52
30	Y	318	LHG	C24-C23	2.38	1.57	1.50
23	r	602	CLA	CMB-C2B	-2.38	1.46	1.51
39	N	607	CHL	C3B-C2B	-2.38	1.37	1.40
23	a	407	CLA	CMB-C2B	-2.38	1.46	1.51
23	n	614	CLA	CMB-C2B	-2.38	1.46	1.51
39	G	607	CHL	C3B-C2B	-2.38	1.37	1.40
30	Y	318	LHG	C4-C5	2.38	1.58	1.50
23	b	616	CLA	CMB-C2B	-2.38	1.46	1.51
23	c	504	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	614	CLA	CMB-C2B	-2.38	1.46	1.51
23	n	613	CLA	CMB-C2B	-2.38	1.46	1.51
42	n	620	XAT	C24-C25	-2.38	1.48	1.52
30	n	619	LHG	C24-C23	2.38	1.57	1.50
23	N	602	CLA	CMB-C2B	-2.38	1.46	1.51
23	S	608	CLA	CMB-C2B	-2.37	1.46	1.51
23	Y	313	CLA	CMB-C2B	-2.37	1.46	1.51
42	n	617	XAT	C4-C5	-2.37	1.48	1.52
23	G	614	CLA	CMB-C2B	-2.37	1.46	1.51
23	y	305	CLA	CMB-C2B	-2.37	1.46	1.51
23	r	609	CLA	CMB-C2B	-2.37	1.46	1.51
30	s	616	LHG	C4-C5	2.37	1.58	1.50
39	s	606	CHL	C3B-C2B	-2.37	1.37	1.40
23	d	406	CLA	CMB-C2B	-2.37	1.46	1.51
23	D	405	CLA	CMB-C2B	-2.37	1.46	1.51
23	n	602	CLA	CMB-C2B	-2.37	1.46	1.51
40	G	616	LUT	C15-C14	2.37	1.50	1.43
23	N	610	CLA	CMB-C2B	-2.37	1.46	1.51
23	R	609	CLA	CMB-C2B	-2.37	1.46	1.51
23	C	511	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	603	CLA	CMB-C2B	-2.37	1.46	1.51
23	c	509	CLA	CMB-C2B	-2.37	1.46	1.51
30	s	616	LHG	C24-C23	2.37	1.57	1.50
23	b	602	CLA	CMB-C2B	-2.37	1.46	1.51
40	S	614	LUT	C24-C25	2.36	1.36	1.33
23	b	615	CLA	CMB-C2B	-2.36	1.46	1.51
23	y	304	CLA	CMB-C2B	-2.36	1.46	1.51
30	r	616	LHG	C24-C23	2.36	1.57	1.50
23	N	603	CLA	CMB-C2B	-2.36	1.46	1.51
40	R	613	LUT	C24-C25	2.36	1.36	1.33
23	n	610	CLA	CMB-C2B	-2.36	1.46	1.51
30	S	616	LHG	C24-C23	2.36	1.57	1.50
23	b	609	CLA	CMB-C2B	-2.36	1.46	1.51
39	g	601	CHL	C3B-C2B	-2.36	1.37	1.40
23	n	612	CLA	CMB-C2B	-2.36	1.46	1.51
23	R	608	CLA	CMB-C2B	-2.36	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.36	1.46	1.51
23	N	614	CLA	CMB-C2B	-2.36	1.46	1.51
23	c	505	CLA	CMB-C2B	-2.36	1.46	1.51
23	r	610	CLA	CMB-C2B	-2.36	1.46	1.51
39	G	601	CHL	C3B-C2B	-2.36	1.37	1.40
23	A	404	CLA	CMB-C2B	-2.36	1.46	1.51
40	Y	315	LUT	C12-C13	2.36	1.51	1.45
39	y	309	CHL	C3B-C2B	-2.36	1.37	1.40
40	N	615	LUT	C24-C25	2.36	1.36	1.33
23	b	607	CLA	CMB-C2B	-2.36	1.46	1.51
40	r	613	LUT	C24-C25	2.35	1.36	1.33
23	r	611	CLA	CMB-C2B	-2.35	1.46	1.51
39	G	608	CHL	C3B-C2B	-2.35	1.37	1.40
39	Y	308	CHL	C3B-C2B	-2.35	1.37	1.40
23	r	608	CLA	CMB-C2B	-2.35	1.46	1.51
23	G	613	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	403	CLA	CMB-C2B	-2.35	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.35	1.46	1.51
30	d	408	LHG	C24-C23	2.35	1.57	1.50
40	N	615	LUT	C31-C32	2.35	1.40	1.34
23	c	512	CLA	CMB-C2B	-2.35	1.46	1.51
39	n	608	CHL	C3B-C2B	-2.35	1.37	1.40
39	Y	302	CHL	C3B-C2B	-2.35	1.37	1.40
23	C	505	CLA	CMB-C2B	-2.35	1.46	1.51
23	C	512	CLA	CMB-C2B	-2.35	1.46	1.51
23	B	612	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	616	LUT	C15-C14	2.34	1.50	1.43
23	G	603	CLA	CMB-C2B	-2.34	1.46	1.51
40	r	613	LUT	C1-C6	2.34	1.57	1.53
40	g	616	LUT	C24-C25	2.34	1.36	1.33
23	S	603	CLA	CMB-C2B	-2.34	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.34	1.46	1.51
23	r	603	CLA	CMB-C2B	-2.34	1.46	1.51
23	g	611	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	612	CLA	CMB-C2B	-2.34	1.46	1.51
23	B	607	CLA	CMB-C2B	-2.33	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.33	1.46	1.51
30	a	412	LHG	C4-C5	2.33	1.57	1.50
41	Y	317	NEX	C38-C25	2.33	1.55	1.51
39	S	606	CHL	C3B-C2B	-2.32	1.37	1.40
39	Y	309	CHL	C3B-C2B	-2.32	1.37	1.40
23	c	510	CLA	CMB-C2B	-2.32	1.46	1.51
23	A	402	CLA	CMB-C2B	-2.32	1.46	1.51
40	N	616	LUT	C31-C32	2.32	1.40	1.34
23	C	510	CLA	CMB-C2B	-2.32	1.46	1.51
40	G	616	LUT	C24-C25	2.31	1.36	1.33
39	g	607	CHL	C3B-C2B	-2.31	1.37	1.40
40	s	614	LUT	C8-C7	2.31	1.40	1.33
30	a	412	LHG	C24-C23	2.31	1.57	1.50
33	c	515	DGD	O1G-C1G	-2.30	1.39	1.45
40	s	615	LUT	C31-C32	2.30	1.40	1.34
38	f	501	HEM	FE-ND	2.30	2.08	1.96
40	n	615	LUT	C15-C14	2.30	1.50	1.43
30	D	408	LHG	C8-C7	2.30	1.57	1.50
39	g	606	CHL	C3B-C2B	-2.30	1.37	1.40
40	N	616	LUT	C24-C25	2.30	1.36	1.33
39	n	605	CHL	CHC-C1C	2.30	1.40	1.35
39	N	609	CHL	C3B-C2B	-2.30	1.37	1.40
30	G	618	LHG	C24-C23	2.30	1.57	1.50
40	R	613	LUT	C31-C32	2.30	1.40	1.34
39	n	609	CHL	C3B-C2B	-2.30	1.37	1.40
30	A	412	LHG	C4-C5	2.29	1.57	1.50
39	S	607	CHL	C3B-C2B	-2.29	1.37	1.40
40	S	615	LUT	C8-C7	2.29	1.40	1.33
40	N	616	LUT	C35-C15	2.29	1.41	1.36
41	Y	317	NEX	O24-C25	-2.29	1.42	1.46
40	S	615	LUT	C35-C15	2.28	1.41	1.36
39	g	608	CHL	C3B-C2B	-2.28	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	614	LUT	C35-C15	2.28	1.41	1.36
40	S	614	LUT	C8-C7	2.28	1.39	1.33
30	A	412	LHG	C24-C23	2.28	1.57	1.50
40	G	615	LUT	C5-C6	2.28	1.38	1.34
41	R	618	NEX	O24-C25	-2.27	1.43	1.46
39	N	605	CHL	CHC-C1C	2.27	1.40	1.35
30	y	318	LHG	C4-C5	2.27	1.57	1.50
40	s	615	LUT	C8-C7	2.27	1.39	1.33
39	y	310	CHL	C3B-C2B	-2.27	1.37	1.40
40	N	615	LUT	C8-C7	2.27	1.39	1.33
23	d	405	CLA	CMD-C2D	-2.27	1.46	1.50
39	G	606	CHL	C3B-C2B	-2.27	1.37	1.40
40	N	615	LUT	C35-C15	2.26	1.41	1.36
39	G	607	CHL	C1D-C2D	-2.26	1.40	1.45
41	G	617	NEX	C31-C32	2.26	1.40	1.34
40	n	615	LUT	C30-C29	2.26	1.38	1.35
39	g	607	CHL	C1D-C2D	-2.26	1.40	1.45
39	G	620	CHL	C1D-C2D	-2.26	1.40	1.45
39	S	601	CHL	C3B-C2B	-2.26	1.37	1.40
39	g	609	CHL	C3B-C2B	-2.26	1.37	1.40
23	c	505	CLA	CMD-C2D	-2.25	1.46	1.50
40	S	615	LUT	C22-C21	2.25	1.57	1.54
40	g	615	LUT	C1-C6	2.25	1.56	1.53
30	R	616	LHG	C4-C5	2.25	1.57	1.50
40	n	616	LUT	C15-C14	2.25	1.50	1.43
39	y	303	CHL	C1D-C2D	-2.25	1.40	1.45
40	S	615	LUT	C24-C25	2.25	1.35	1.33
30	D	408	LHG	C24-C23	2.25	1.57	1.50
40	g	616	LUT	C8-C7	2.24	1.39	1.33
42	n	620	XAT	O4-C5	-2.24	1.43	1.46
40	s	615	LUT	C28-C29	2.24	1.50	1.45
41	S	617	NEX	C11-C12	2.24	1.40	1.34
42	G	619	XAT	C22-C21	2.24	1.58	1.54
40	G	616	LUT	C8-C7	2.24	1.39	1.33
42	N	619	XAT	O4-C5	-2.24	1.43	1.46
39	s	601	CHL	C3B-C2B	-2.24	1.37	1.40
39	y	308	CHL	C3B-C2B	-2.24	1.37	1.40
39	y	309	CHL	C1D-C2D	-2.24	1.40	1.45
41	r	614	NEX	O24-C25	-2.23	1.43	1.46
39	N	608	CHL	C1D-C2D	-2.23	1.40	1.45
40	y	317	LUT	C8-C7	2.23	1.39	1.33
41	N	617	NEX	O24-C25	-2.23	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	r	613	LUT	C8-C7	2.23	1.39	1.33
39	G	606	CHL	C1D-C2D	-2.23	1.40	1.45
39	Y	307	CHL	C1D-C2D	-2.23	1.40	1.45
39	N	607	CHL	C1D-C2D	-2.23	1.40	1.45
39	N	601	CHL	C3B-C2B	-2.23	1.37	1.40
40	Y	315	LUT	C30-C29	2.23	1.38	1.35
40	N	616	LUT	C8-C7	2.23	1.39	1.33
40	R	613	LUT	C35-C15	2.23	1.41	1.36
40	y	316	LUT	C30-C29	2.23	1.38	1.35
40	y	317	LUT	C24-C25	2.23	1.35	1.33
39	g	605	CHL	C1D-C2D	-2.22	1.40	1.45
39	N	605	CHL	C3B-C2B	-2.22	1.37	1.40
40	R	613	LUT	C8-C7	2.22	1.39	1.33
40	n	616	LUT	C24-C25	2.22	1.35	1.33
26	L	101	SQD	O9-S	2.22	1.51	1.45
39	R	605	CHL	C3B-C2B	-2.22	1.37	1.40
41	R	614	NEX	O24-C25	-2.22	1.43	1.46
40	r	613	LUT	C31-C32	2.22	1.40	1.34
40	N	615	LUT	C28-C29	2.22	1.50	1.45
23	C	505	CLA	CMD-C2D	-2.22	1.46	1.50
39	Y	307	CHL	C3B-C2B	-2.21	1.37	1.40
39	n	601	CHL	C1D-C2D	-2.21	1.41	1.45
40	G	615	LUT	C17-C1	2.21	1.58	1.53
39	R	607	CHL	C1D-C2D	-2.21	1.41	1.45
39	G	609	CHL	C3B-C2B	-2.21	1.37	1.40
39	s	607	CHL	C3B-C2B	-2.21	1.37	1.40
40	s	615	LUT	C35-C15	2.21	1.41	1.36
39	g	609	CHL	C1D-C2D	-2.21	1.41	1.45
40	N	616	LUT	C28-C29	2.21	1.50	1.45
39	y	308	CHL	C1D-C2D	-2.21	1.41	1.45
23	b	607	CLA	CMD-C2D	-2.21	1.46	1.50
39	r	607	CHL	C1D-C2D	-2.21	1.41	1.45
23	D	405	CLA	CMD-C2D	-2.21	1.46	1.50
40	y	317	LUT	C31-C32	2.21	1.40	1.34
42	Y	301	XAT	C4-C5	-2.21	1.48	1.52
40	Y	316	LUT	C8-C7	2.21	1.39	1.33
40	Y	316	LUT	C31-C32	2.21	1.40	1.34
40	Y	315	LUT	C1-C6	2.20	1.56	1.53
39	g	606	CHL	C1D-C2D	-2.20	1.41	1.45
30	L	103	LHG	C24-C23	2.20	1.57	1.50
40	Y	316	LUT	C15-C14	2.20	1.50	1.43
40	y	317	LUT	C15-C14	2.20	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	308	CHL	C1D-C2D	-2.20	1.41	1.45
30	n	619	LHG	C4-C5	2.20	1.57	1.50
39	N	601	CHL	C1D-C2D	-2.20	1.41	1.45
40	r	613	LUT	C35-C15	2.20	1.41	1.36
41	s	617	NEX	C11-C12	2.19	1.40	1.34
40	G	616	LUT	C31-C32	2.19	1.40	1.34
23	B	607	CLA	CMD-C2D	-2.19	1.46	1.50
39	n	601	CHL	C3B-C2B	-2.19	1.37	1.40
39	r	605	CHL	C1D-C2D	-2.19	1.41	1.45
39	n	607	CHL	C1D-C2D	-2.19	1.41	1.45
39	Y	302	CHL	C1D-C2D	-2.19	1.41	1.45
42	r	615	XAT	O4-C5	-2.19	1.43	1.46
39	R	605	CHL	C1D-C2D	-2.19	1.41	1.45
26	a	409	SQD	O9-S	2.19	1.51	1.45
30	g	618	LHG	C4-C5	2.19	1.57	1.50
40	n	615	LUT	C1-C6	2.19	1.56	1.53
39	G	605	CHL	C1D-C2D	-2.19	1.41	1.45
39	G	609	CHL	CHC-C1C	2.18	1.40	1.35
39	g	619	CHL	C1D-C2D	-2.18	1.41	1.45
39	s	601	CHL	C1D-C2D	-2.18	1.41	1.45
40	g	615	LUT	C17-C1	2.18	1.58	1.53
39	s	607	CHL	C1D-C2D	-2.18	1.41	1.45
39	N	606	CHL	C1D-C2D	-2.18	1.41	1.45
26	A	408	SQD	O9-S	2.18	1.51	1.45
26	M	101	SQD	O9-S	2.18	1.51	1.45
42	R	615	XAT	O4-C5	-2.18	1.43	1.46
39	N	609	CHL	C1D-C2D	-2.18	1.41	1.45
39	r	606	CHL	C1D-C2D	-2.18	1.41	1.45
39	S	606	CHL	C1D-C2D	-2.17	1.41	1.45
39	S	607	CHL	C1D-C2D	-2.17	1.41	1.45
39	G	601	CHL	C1D-C2D	-2.17	1.41	1.45
23	b	612	CLA	CMD-C2D	-2.17	1.46	1.50
40	R	613	LUT	C17-C1	2.17	1.58	1.53
39	g	601	CHL	C1D-C2D	-2.17	1.41	1.45
39	G	608	CHL	C1D-C2D	-2.17	1.41	1.45
41	s	617	NEX	C32-C33	2.17	1.56	1.50
42	G	619	XAT	C28-C29	-2.17	1.41	1.45
39	S	605	CHL	C1D-C2D	-2.17	1.41	1.45
40	n	616	LUT	C8-C7	2.17	1.39	1.33
39	n	608	CHL	C1D-C2D	-2.17	1.41	1.45
39	R	606	CHL	C1D-C2D	-2.16	1.41	1.45
40	g	616	LUT	C31-C32	2.16	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	606	CHL	C1D-C2D	-2.16	1.41	1.45
40	Y	316	LUT	C24-C25	2.16	1.35	1.33
26	a	409	SQD	O7-S	2.16	1.51	1.45
39	g	608	CHL	C1D-C2D	-2.16	1.41	1.45
39	Y	309	CHL	C1D-C2D	-2.16	1.41	1.45
40	n	615	LUT	C17-C1	2.16	1.58	1.53
39	Y	306	CHL	C1D-C2D	-2.16	1.41	1.45
23	A	402	CLA	CMD-C2D	-2.16	1.46	1.50
30	b	627	LHG	C24-C23	2.16	1.57	1.50
39	S	601	CHL	C1D-C2D	-2.15	1.41	1.45
40	G	615	LUT	C1-C6	2.15	1.56	1.53
39	S	607	CHL	C3D-C4D	-2.15	1.39	1.44
39	s	605	CHL	C1D-C2D	-2.15	1.41	1.45
40	y	316	LUT	C1-C6	2.15	1.56	1.53
40	r	613	LUT	C17-C1	2.15	1.58	1.53
41	n	618	NEX	O24-C25	-2.14	1.43	1.46
39	s	606	CHL	C1D-C2D	-2.14	1.41	1.45
23	a	403	CLA	CMC-C2C	-2.14	1.46	1.50
40	n	615	LUT	C11-C12	2.14	1.40	1.34
39	n	609	CHL	C1D-C2D	-2.14	1.41	1.45
39	S	605	CHL	C3B-C2B	-2.14	1.37	1.40
26	M	101	SQD	O7-S	2.13	1.51	1.45
39	y	309	CHL	C3D-C4D	-2.13	1.39	1.44
40	n	616	LUT	C31-C32	2.13	1.40	1.34
39	y	310	CHL	C1D-C2D	-2.13	1.41	1.45
39	y	307	CHL	C1D-C2D	-2.13	1.41	1.45
30	d	404	LHG	C24-C23	2.13	1.56	1.50
23	C	510	CLA	CMD-C2D	-2.13	1.46	1.50
33	H	502	DGD	O1G-C1G	-2.12	1.40	1.45
40	g	615	LUT	C22-C21	2.12	1.57	1.54
39	g	608	CHL	CHC-C1C	2.12	1.40	1.35
30	G	618	LHG	C4-C5	2.12	1.57	1.50
39	G	609	CHL	C1D-C2D	-2.12	1.41	1.45
23	A	402	CLA	CMC-C2C	-2.12	1.46	1.50
23	B	612	CLA	CMD-C2D	-2.12	1.46	1.50
23	a	403	CLA	CMD-C2D	-2.12	1.46	1.50
39	g	605	CHL	CHC-C1C	2.12	1.40	1.35
26	L	101	SQD	O7-S	2.12	1.51	1.45
39	S	601	CHL	C3D-C4D	-2.11	1.39	1.44
40	G	615	LUT	C31-C30	2.11	1.50	1.43
40	n	616	LUT	C17-C1	2.11	1.57	1.53
40	Y	316	LUT	C17-C1	2.11	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	y	317	LUT	C17-C1	2.11	1.57	1.53
41	g	617	NEX	C11-C12	2.11	1.40	1.34
39	N	605	CHL	C1D-C2D	-2.11	1.41	1.45
39	s	601	CHL	CHC-C1C	2.11	1.40	1.35
39	G	605	CHL	C3B-C2B	-2.11	1.37	1.40
26	A	408	SQD	O7-S	2.10	1.51	1.45
33	d	411	DGD	O1G-C1G	-2.10	1.40	1.45
30	d	408	LHG	C4-C5	2.10	1.57	1.50
39	n	608	CHL	CHC-C1C	2.10	1.40	1.35
39	y	308	CHL	C3D-C4D	-2.10	1.39	1.44
40	N	616	LUT	C17-C1	2.10	1.57	1.53
39	s	601	CHL	C3D-C4D	-2.10	1.39	1.44
42	G	619	XAT	C11-C12	2.10	1.40	1.34
39	y	303	CHL	C3D-C4D	-2.10	1.39	1.44
39	Y	308	CHL	C3D-C4D	-2.10	1.39	1.44
39	S	601	CHL	CHC-C1C	2.10	1.40	1.35
39	N	606	CHL	CHC-C1C	2.10	1.40	1.35
39	y	307	CHL	CHC-C1C	2.09	1.40	1.35
30	b	627	LHG	C4-C5	2.09	1.57	1.50
42	n	620	XAT	C2-C1	2.09	1.57	1.54
39	N	606	CHL	C3B-C2B	-2.09	1.37	1.40
23	g	603	CLA	CMD-C2D	-2.09	1.46	1.50
39	Y	306	CHL	CHC-C1C	2.09	1.40	1.35
39	G	605	CHL	CHC-C1C	2.09	1.40	1.35
30	d	404	LHG	C4-C5	2.09	1.57	1.50
24	A	405	PHO	CMC-C2C	-2.09	1.46	1.51
39	n	605	CHL	C1D-C2D	-2.09	1.41	1.45
23	B	604	CLA	CMD-C2D	-2.09	1.46	1.50
39	Y	302	CHL	C3D-C4D	-2.09	1.39	1.44
39	y	307	CHL	C3B-C2B	-2.09	1.37	1.40
23	b	605	CLA	CMC-C2C	-2.08	1.46	1.50
39	s	607	CHL	C3D-C4D	-2.08	1.39	1.44
39	g	608	CHL	C3D-C4D	-2.08	1.39	1.44
23	g	612	CLA	CMD-C2D	-2.08	1.46	1.50
41	g	617	NEX	C31-C32	2.08	1.39	1.34
41	R	614	NEX	C11-C12	2.08	1.39	1.34
42	N	619	XAT	C37-C21	2.08	1.57	1.53
39	G	620	CHL	CHC-C1C	2.08	1.40	1.35
23	c	510	CLA	CMD-C2D	-2.08	1.46	1.50
39	N	606	CHL	C3D-C4D	-2.08	1.39	1.44
41	g	617	NEX	O24-C25	-2.08	1.43	1.46
39	y	310	CHL	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	606	CHL	CHC-C1C	2.08	1.40	1.35
23	b	616	CLA	CMC-C2C	-2.07	1.46	1.50
40	R	613	LUT	C28-C29	2.07	1.50	1.45
23	B	616	CLA	CMC-C2C	-2.07	1.46	1.50
24	d	402	PHO	CMC-C2C	-2.07	1.46	1.51
40	y	316	LUT	C11-C10	2.07	1.49	1.43
39	n	605	CHL	C3B-C2B	-2.07	1.37	1.40
23	n	603	CLA	CMD-C2D	-2.07	1.46	1.50
23	y	315	CLA	CMD-C2D	-2.07	1.46	1.50
39	r	605	CHL	C3D-C4D	-2.07	1.39	1.44
39	n	608	CHL	C3D-C4D	-2.07	1.39	1.44
24	D	402	PHO	CMC-C2C	-2.07	1.46	1.51
39	r	605	CHL	C3B-C2B	-2.06	1.37	1.40
40	N	615	LUT	C17-C1	2.06	1.57	1.53
40	s	615	LUT	C17-C1	2.06	1.57	1.53
23	b	606	CLA	CMC-C2C	-2.06	1.46	1.50
23	B	606	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	501	CLA	CMD-C2D	-2.06	1.46	1.50
40	S	615	LUT	C17-C1	2.06	1.57	1.53
40	Y	316	LUT	C22-C21	2.06	1.57	1.54
23	c	509	CLA	CMD-C2D	-2.06	1.46	1.50
41	G	617	NEX	O24-C25	-2.06	1.43	1.46
39	Y	306	CHL	C3B-C2B	-2.06	1.37	1.40
23	B	603	CLA	CMD-C2D	-2.06	1.46	1.50
23	n	604	CLA	CMD-C2D	-2.06	1.46	1.50
39	R	607	CHL	C3D-C4D	-2.06	1.39	1.44
23	b	604	CLA	CMD-C2D	-2.06	1.46	1.50
40	s	614	LUT	C17-C1	2.06	1.57	1.53
23	b	608	CLA	CMD-C2D	-2.06	1.46	1.50
39	G	601	CHL	C3D-C4D	-2.06	1.39	1.44
39	G	620	CHL	C3D-C4D	-2.06	1.39	1.44
24	a	406	PHO	CMD-C2D	-2.06	1.46	1.51
42	Y	301	XAT	C37-C21	2.06	1.57	1.53
23	c	513	CLA	CMD-C2D	-2.06	1.46	1.50
39	G	608	CHL	C3D-C4D	-2.06	1.39	1.44
40	y	316	LUT	C11-C12	2.06	1.39	1.34
23	B	615	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.06	1.46	1.50
39	s	606	CHL	CHC-C1C	2.06	1.40	1.35
40	G	615	LUT	C2-C3	2.06	1.55	1.52
39	r	607	CHL	C3D-C4D	-2.05	1.39	1.44
23	c	501	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CMD-C2D	-2.05	1.46	1.50
39	n	607	CHL	C3D-C4D	-2.05	1.39	1.44
23	R	603	CLA	CMD-C2D	-2.05	1.46	1.50
39	Y	309	CHL	C3D-C4D	-2.05	1.39	1.44
24	a	406	PHO	CMC-C2C	-2.05	1.46	1.51
39	n	609	CHL	C3D-C4D	-2.05	1.39	1.44
23	b	603	CLA	CMD-C2D	-2.05	1.46	1.50
24	A	405	PHO	CMD-C2D	-2.05	1.46	1.51
39	G	607	CHL	C3D-C4D	-2.04	1.39	1.44
42	n	620	XAT	C37-C21	2.04	1.57	1.53
24	D	402	PHO	CMD-C2D	-2.04	1.46	1.51
23	r	603	CLA	CMD-C2D	-2.04	1.46	1.50
39	N	601	CHL	CHC-C1C	2.04	1.40	1.35
40	S	614	LUT	C17-C1	2.04	1.57	1.53
39	N	608	CHL	C3D-C4D	-2.04	1.39	1.44
23	R	604	CLA	CMD-C2D	-2.04	1.46	1.50
39	G	609	CHL	C3D-C4D	-2.04	1.39	1.44
39	r	606	CHL	C3D-C4D	-2.04	1.39	1.44
39	n	601	CHL	CHC-C1C	2.04	1.40	1.35
40	G	616	LUT	C35-C15	2.04	1.41	1.36
39	G	608	CHL	CHC-C1C	2.04	1.40	1.35
23	B	606	CLA	CMC-C2C	-2.04	1.46	1.50
39	N	608	CHL	CHC-C1C	2.04	1.40	1.35
39	n	601	CHL	C3D-C4D	-2.04	1.39	1.44
39	g	601	CHL	C3D-C4D	-2.04	1.39	1.44
39	s	605	CHL	C3B-C2B	-2.04	1.37	1.40
40	g	616	LUT	C35-C15	2.04	1.41	1.36
39	Y	307	CHL	CHC-C1C	2.04	1.40	1.35
39	n	606	CHL	C3D-C4D	-2.04	1.39	1.44
40	Y	315	LUT	C11-C12	2.04	1.39	1.34
23	C	513	CLA	CMD-C2D	-2.03	1.46	1.50
39	R	605	CHL	C3D-C4D	-2.03	1.39	1.44
39	G	606	CHL	CHC-C1C	2.03	1.40	1.35
39	g	619	CHL	CHC-C1C	2.03	1.40	1.35
23	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	614	CLA	CMD-C2D	-2.03	1.46	1.50
23	C	506	CLA	CMD-C2D	-2.03	1.46	1.50
39	N	609	CHL	C3D-C4D	-2.03	1.39	1.44
23	r	608	CLA	CMD-C2D	-2.03	1.46	1.50
23	A	403	CLA	CMD-C2D	-2.03	1.46	1.50
40	Y	315	LUT	C11-C10	2.03	1.49	1.43
23	C	504	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	607	CHL	C3D-C4D	-2.03	1.39	1.44
39	N	601	CHL	C3D-C4D	-2.03	1.39	1.44
39	N	605	CHL	C3D-C4D	-2.03	1.39	1.44
41	N	617	NEX	C11-C12	2.03	1.39	1.34
23	c	506	CLA	CMD-C2D	-2.03	1.46	1.50
23	n	610	CLA	CMD-C2D	-2.03	1.46	1.50
40	s	614	LUT	C24-C25	2.03	1.35	1.33
39	y	308	CHL	CHC-C1C	2.03	1.40	1.35
23	N	604	CLA	CMD-C2D	-2.03	1.46	1.50
26	M	101	SQD	C8-C7	2.03	1.56	1.50
39	Y	307	CHL	C3D-C4D	-2.03	1.39	1.44
39	g	619	CHL	C3D-C4D	-2.03	1.39	1.44
24	d	402	PHO	CMB-C2B	-2.02	1.46	1.51
23	Y	304	CLA	CMD-C2D	-2.02	1.46	1.50
23	n	602	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	605	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	602	CLA	CMD-C2D	-2.02	1.46	1.50
23	N	610	CLA	CMD-C2D	-2.02	1.46	1.50
40	N	616	LUT	C22-C21	2.02	1.57	1.54
23	G	603	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
23	n	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	612	CLA	CMD-C2D	-2.02	1.46	1.50
39	Y	306	CHL	C3D-C4D	-2.02	1.39	1.44
39	n	605	CHL	C3D-C4D	-2.02	1.39	1.44
23	G	613	CLA	CMD-C2D	-2.02	1.46	1.50
23	R	611	CLA	CMD-C2D	-2.02	1.46	1.50
40	s	614	LUT	C35-C34	2.02	1.49	1.43
39	Y	302	CHL	CHC-C1C	2.02	1.40	1.35
39	Y	308	CHL	CHC-C1C	2.02	1.40	1.35
30	L	103	LHG	C4-C5	2.02	1.56	1.50
23	G	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	504	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.02	1.46	1.50
23	n	614	CLA	CMD-C2D	-2.02	1.46	1.50
26	L	101	SQD	C8-C7	2.02	1.56	1.50
23	A	404	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.02	1.46	1.50
39	y	307	CHL	C3D-C4D	-2.02	1.39	1.44
39	s	607	CHL	CHC-C1C	2.02	1.40	1.35
23	Y	314	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	508	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	602	CLA	CMD-C2D	-2.02	1.46	1.50
40	G	616	LUT	C17-C1	2.02	1.57	1.53
39	S	607	CHL	CHC-C1C	2.02	1.40	1.35
23	b	601	CLA	CMD-C2D	-2.02	1.46	1.50
38	f	501	HEM	CMB-C2B	2.02	1.55	1.50
39	g	605	CHL	C3B-C2B	-2.02	1.37	1.40
39	S	606	CHL	C3D-C4D	-2.02	1.39	1.44
39	g	606	CHL	C3D-C4D	-2.02	1.39	1.44
23	S	612	CLA	CMD-C2D	-2.02	1.46	1.50
39	R	606	CHL	C3D-C4D	-2.02	1.39	1.44
23	R	601	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	613	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	404	CLA	CMD-C2D	-2.01	1.46	1.50
24	d	402	PHO	CMD-C2D	-2.01	1.46	1.51
39	g	606	CHL	CHC-C1C	2.01	1.40	1.35
23	r	612	CLA	CMD-C2D	-2.01	1.46	1.50
40	y	317	LUT	C2-C3	2.01	1.55	1.52
23	s	603	CLA	CMD-C2D	-2.01	1.46	1.50
23	y	314	CLA	CMD-C2D	-2.01	1.46	1.50
39	n	606	CHL	C3B-C2B	-2.01	1.37	1.40
39	s	606	CHL	C3D-C4D	-2.01	1.39	1.44
23	S	602	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	614	CLA	CMD-C2D	-2.01	1.46	1.50
41	n	618	NEX	C31-C32	2.01	1.39	1.34
23	N	603	CLA	CMD-C2D	-2.01	1.46	1.50
39	g	609	CHL	CHC-C1C	2.01	1.40	1.35
42	N	619	XAT	C2-C1	2.01	1.57	1.54
23	N	612	CLA	CMD-C2D	-2.01	1.46	1.50
23	s	604	CLA	CMD-C2D	-2.00	1.46	1.50
30	D	404	LHG	C4-C5	2.00	1.56	1.50
23	b	611	CLA	CMC-C2C	-2.00	1.46	1.50
23	C	509	CLA	CMD-C2D	-2.00	1.46	1.50
23	c	511	CLA	CMD-C2D	-2.00	1.46	1.50
39	g	607	CHL	C3D-C4D	-2.00	1.39	1.44
39	R	606	CHL	CHC-C1C	2.00	1.40	1.35
23	c	507	CLA	CMD-C2D	-2.00	1.46	1.50
23	r	609	CLA	CMD-C2D	-2.00	1.46	1.50

All (2825) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	617	NEX	O24-C25-C24	23.84	131.29	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	n	618	NEX	O24-C25-C24	23.64	131.14	113.38
41	g	617	NEX	O24-C25-C24	23.37	130.94	113.38
41	R	618	NEX	O24-C25-C24	23.16	130.78	113.38
41	r	614	NEX	O24-C25-C24	23.13	130.76	113.38
41	R	614	NEX	O24-C25-C24	22.81	130.52	113.38
41	Y	317	NEX	O24-C25-C24	22.81	130.51	113.38
41	G	617	NEX	O24-C25-C24	22.71	130.44	113.38
42	n	620	XAT	C19-C9-C10	-13.64	103.81	122.92
42	N	619	XAT	C19-C9-C10	-13.42	104.12	122.92
42	n	617	XAT	C19-C9-C10	-12.09	105.99	122.92
42	r	615	XAT	C39-C29-C30	-12.08	106.00	122.92
42	R	615	XAT	C39-C29-C30	-12.07	106.02	122.92
42	G	619	XAT	C19-C9-C10	-11.96	106.16	122.92
42	y	302	XAT	C27-C28-C29	11.96	144.09	125.53
42	r	615	XAT	C19-C9-C10	-11.95	106.19	122.92
42	Y	301	XAT	C27-C28-C29	11.84	143.91	125.53
42	R	615	XAT	C19-C9-C10	-11.84	106.34	122.92
42	y	302	XAT	C20-C13-C14	-11.46	106.87	122.92
42	n	617	XAT	C27-C28-C29	11.42	143.25	125.53
39	N	605	CHL	C4A-NA-C1A	11.38	111.82	106.71
42	Y	301	XAT	C19-C9-C10	-11.25	107.17	122.92
39	Y	306	CHL	C4A-NA-C1A	11.19	111.74	106.71
42	y	302	XAT	C19-C9-C10	-11.19	107.25	122.92
42	Y	301	XAT	C20-C13-C14	-11.09	107.39	122.92
42	N	619	XAT	C20-C13-C14	-11.06	107.44	122.92
42	n	620	XAT	C20-C13-C14	-11.05	107.45	122.92
42	G	619	XAT	C27-C28-C29	10.99	142.58	125.53
42	N	619	XAT	C27-C28-C29	10.93	142.49	125.53
39	y	307	CHL	C4A-NA-C1A	10.93	111.62	106.71
42	n	620	XAT	C27-C28-C29	10.90	142.44	125.53
39	g	605	CHL	C4A-NA-C1A	10.79	111.56	106.71
39	G	605	CHL	C4A-NA-C1A	10.66	111.50	106.71
42	r	615	XAT	C20-C13-C14	-10.64	108.01	122.92
42	G	619	XAT	C39-C29-C30	-10.58	108.10	122.92
42	n	617	XAT	C20-C13-C14	-10.49	108.23	122.92
42	R	615	XAT	C20-C13-C14	-10.44	108.29	122.92
42	N	619	XAT	C39-C29-C30	-10.41	108.34	122.92
39	G	609	CHL	C4A-NA-C1A	10.33	111.35	106.71
42	r	615	XAT	C7-C8-C9	10.28	141.48	125.53
39	g	607	CHL	C4A-NA-C1A	10.24	111.31	106.71
39	n	605	CHL	C4A-NA-C1A	10.22	111.30	106.71
42	R	615	XAT	C7-C8-C9	10.18	141.33	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	607	CHL	C4A-NA-C1A	10.13	111.26	106.71
39	n	607	CHL	C4A-NA-C1A	10.05	111.22	106.71
39	G	620	CHL	C4A-NA-C1A	10.02	111.21	106.71
39	N	607	CHL	C4A-NA-C1A	9.96	111.19	106.71
39	N	601	CHL	C4A-NA-C1A	9.96	111.18	106.71
39	g	619	CHL	C4A-NA-C1A	9.93	111.17	106.71
39	g	609	CHL	C4A-NA-C1A	9.86	111.14	106.71
40	Y	315	LUT	C40-C33-C34	-9.85	109.13	122.92
42	G	619	XAT	C20-C13-C14	-9.84	109.13	122.92
39	S	605	CHL	C4A-NA-C1A	9.84	111.13	106.71
40	n	615	LUT	C40-C33-C34	-9.83	109.16	122.92
39	y	303	CHL	C4A-NA-C1A	9.82	111.12	106.71
39	R	607	CHL	C4A-NA-C1A	9.82	111.12	106.71
39	n	601	CHL	C4A-NA-C1A	9.79	111.11	106.71
40	y	316	LUT	C40-C33-C34	-9.79	109.22	122.92
39	g	606	CHL	C4A-NA-C1A	9.78	111.10	106.71
39	r	607	CHL	C4A-NA-C1A	9.72	111.07	106.71
39	G	601	CHL	C4A-NA-C1A	9.70	111.06	106.71
39	S	606	CHL	C4A-NA-C1A	9.67	111.06	106.71
42	n	620	XAT	C39-C29-C30	-9.67	109.38	122.92
42	n	617	XAT	C39-C29-C30	-9.65	109.40	122.92
39	G	606	CHL	C4A-NA-C1A	9.64	111.04	106.71
39	Y	302	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	r	606	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	R	606	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	N	608	CHL	C4A-NA-C1A	9.58	111.01	106.71
39	Y	307	CHL	C4A-NA-C1A	9.56	111.01	106.71
39	n	608	CHL	C4A-NA-C1A	9.54	111.00	106.71
39	y	308	CHL	C4A-NA-C1A	9.54	111.00	106.71
39	Y	308	CHL	C4A-NA-C1A	9.52	110.98	106.71
39	s	605	CHL	C4A-NA-C1A	9.50	110.98	106.71
39	r	605	CHL	C4A-NA-C1A	9.50	110.97	106.71
42	Y	301	XAT	C39-C29-C30	-9.49	109.63	122.92
40	s	614	LUT	C40-C33-C34	-9.48	109.65	122.92
39	g	601	CHL	C4A-NA-C1A	9.47	110.96	106.71
39	N	609	CHL	C4A-NA-C1A	9.33	110.90	106.71
39	R	605	CHL	C4A-NA-C1A	9.31	110.89	106.71
39	y	309	CHL	C4A-NA-C1A	9.29	110.88	106.71
42	n	620	XAT	C28-C29-C30	9.29	133.19	118.94
39	n	609	CHL	C4A-NA-C1A	9.26	110.87	106.71
39	S	601	CHL	C4A-NA-C1A	9.23	110.86	106.71
40	Y	316	LUT	C40-C33-C34	-9.23	110.00	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	y	302	XAT	C39-C29-C30	-9.21	110.03	122.92
39	s	601	CHL	C4A-NA-C1A	9.19	110.84	106.71
40	y	317	LUT	C40-C33-C34	-9.19	110.05	122.92
39	s	606	CHL	C4A-NA-C1A	9.14	110.81	106.71
39	N	606	CHL	C4A-NA-C1A	9.09	110.79	106.71
40	S	615	LUT	C40-C33-C34	-9.08	110.20	122.92
39	Y	309	CHL	C4A-NA-C1A	9.08	110.79	106.71
40	S	614	LUT	C40-C33-C34	-9.06	110.23	122.92
40	n	616	LUT	C40-C33-C34	-9.05	110.25	122.92
39	S	607	CHL	C4A-NA-C1A	9.02	110.76	106.71
39	G	608	CHL	C4A-NA-C1A	9.01	110.76	106.71
40	N	615	LUT	C40-C33-C34	-9.01	110.30	122.92
40	g	616	LUT	C40-C33-C34	-9.00	110.32	122.92
40	G	616	LUT	C40-C33-C34	-8.99	110.33	122.92
40	r	613	LUT	C40-C33-C34	-8.98	110.34	122.92
40	s	615	LUT	C40-C33-C34	-8.97	110.36	122.92
39	y	310	CHL	C4A-NA-C1A	8.95	110.73	106.71
39	n	606	CHL	C4A-NA-C1A	8.94	110.72	106.71
39	s	607	CHL	C4A-NA-C1A	8.93	110.72	106.71
41	s	617	NEX	C12-C13-C14	8.92	132.63	118.94
40	g	615	LUT	C20-C13-C14	-8.86	110.52	122.92
42	R	615	XAT	C40-C33-C34	-8.75	110.67	122.92
40	n	615	LUT	C20-C13-C14	-8.72	110.71	122.92
42	r	615	XAT	C40-C33-C34	-8.69	110.75	122.92
39	g	608	CHL	C4A-NA-C1A	8.68	110.61	106.71
40	N	616	LUT	C40-C33-C34	-8.58	110.91	122.92
41	G	617	NEX	C28-C29-C30	8.43	131.88	118.94
42	y	302	XAT	C40-C33-C34	-8.42	111.13	122.92
41	N	617	NEX	C12-C13-C14	8.42	131.85	118.94
41	Y	317	NEX	C12-C13-C14	8.41	131.84	118.94
42	R	615	XAT	C27-C28-C29	8.40	138.56	125.53
41	r	614	NEX	C12-C13-C14	8.39	131.81	118.94
42	n	617	XAT	C40-C33-C34	-8.37	111.19	122.92
40	R	613	LUT	C40-C33-C34	-8.35	111.22	122.92
42	n	617	XAT	C28-C29-C30	8.34	131.74	118.94
42	N	619	XAT	C28-C29-C30	8.34	131.74	118.94
41	R	618	NEX	C12-C13-C14	8.34	131.73	118.94
41	g	617	NEX	C12-C13-C14	8.28	131.64	118.94
41	R	614	NEX	C12-C13-C14	8.26	131.61	118.94
42	G	619	XAT	C40-C33-C34	-8.25	111.37	122.92
41	Y	317	NEX	C40-C33-C34	-8.23	111.39	122.92
42	r	615	XAT	C27-C28-C29	8.21	138.27	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	617	NEX	C40-C33-C34	-8.19	111.46	122.92
41	R	618	NEX	C40-C33-C34	-8.17	111.48	122.92
42	N	619	XAT	C40-C33-C34	-8.16	111.49	122.92
41	n	618	NEX	C40-C33-C34	-8.15	111.50	122.92
41	g	617	NEX	C40-C33-C34	-8.14	111.53	122.92
41	S	617	NEX	C12-C13-C14	8.09	131.36	118.94
40	g	615	LUT	C40-C33-C34	-8.07	111.62	122.92
42	Y	301	XAT	C40-C33-C34	-8.05	111.64	122.92
41	R	614	NEX	C40-C33-C34	-8.04	111.66	122.92
41	n	618	NEX	C12-C13-C14	8.00	131.21	118.94
42	n	620	XAT	C40-C33-C34	-7.94	111.80	122.92
41	R	614	NEX	C20-C13-C14	-7.94	111.81	122.92
42	y	302	XAT	C28-C29-C30	7.93	131.10	118.94
41	r	614	NEX	C40-C33-C34	-7.90	111.85	122.92
40	R	613	LUT	C20-C13-C14	-7.89	111.87	122.92
40	G	615	LUT	C40-C33-C34	-7.80	111.99	122.92
42	Y	301	XAT	C28-C29-C30	7.80	130.91	118.94
40	N	616	LUT	C20-C13-C14	-7.79	112.01	122.92
41	Y	317	NEX	C20-C13-C14	-7.78	112.02	122.92
40	G	616	LUT	C20-C13-C14	-7.78	112.02	122.92
40	g	616	LUT	C20-C13-C14	-7.68	112.16	122.92
41	g	617	NEX	C28-C29-C30	7.63	130.65	118.94
41	G	617	NEX	C40-C33-C34	-7.63	112.24	122.92
40	n	616	LUT	C20-C13-C14	-7.59	112.30	122.92
40	Y	316	LUT	C20-C13-C14	-7.57	112.32	122.92
41	N	617	NEX	C17-C1-C6	-7.56	103.71	110.47
40	r	613	LUT	C20-C13-C14	-7.54	112.36	122.92
41	n	618	NEX	C17-C1-C6	-7.54	103.73	110.47
40	s	615	LUT	C20-C13-C14	-7.53	112.37	122.92
40	S	614	LUT	C20-C13-C14	-7.53	112.37	122.92
41	g	617	NEX	C20-C13-C14	-7.53	112.37	122.92
40	N	615	LUT	C19-C9-C8	-7.52	106.22	118.08
42	r	615	XAT	C32-C33-C34	7.51	130.46	118.94
41	Y	317	NEX	C17-C1-C6	-7.51	103.75	110.47
41	g	617	NEX	C17-C1-C6	-7.50	103.76	110.47
41	Y	317	NEX	C19-C9-C10	-7.49	112.43	122.92
42	y	302	XAT	C32-C33-C34	7.49	130.43	118.94
40	S	615	LUT	C20-C13-C14	-7.48	112.44	122.92
40	y	317	LUT	C20-C13-C14	-7.48	112.44	122.92
42	R	615	XAT	C32-C33-C34	7.46	130.40	118.94
40	N	615	LUT	C20-C13-C14	-7.45	112.49	122.92
42	G	619	XAT	C28-C29-C30	7.43	130.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	n	618	NEX	C20-C13-C14	-7.43	112.51	122.92
41	R	614	NEX	C17-C1-C6	-7.43	103.82	110.47
41	n	618	NEX	C19-C9-C10	-7.43	112.52	122.92
41	r	614	NEX	C20-C13-C14	-7.42	112.53	122.92
40	Y	315	LUT	C19-C9-C8	-7.42	106.39	118.08
41	r	614	NEX	C19-C9-C10	-7.41	112.54	122.92
41	S	617	NEX	C17-C1-C6	-7.41	103.84	110.47
41	s	617	NEX	C17-C1-C6	-7.40	103.85	110.47
42	Y	301	XAT	C32-C33-C34	7.40	130.29	118.94
41	Y	317	NEX	C2-C1-C6	7.37	116.38	109.21
41	r	614	NEX	C17-C1-C6	-7.37	103.88	110.47
41	N	617	NEX	C20-C13-C14	-7.33	112.65	122.92
40	y	316	LUT	C19-C9-C8	-7.31	106.56	118.08
42	G	619	XAT	O4-C5-C4	7.31	118.87	113.38
41	S	617	NEX	C35-C15-C14	7.30	132.90	123.25
41	R	618	NEX	C20-C13-C14	-7.26	112.76	122.92
23	b	604	CLA	C4A-NA-C1A	7.23	109.96	106.71
41	s	617	NEX	C20-C13-C14	-7.23	112.80	122.92
40	g	615	LUT	C7-C8-C9	7.21	137.13	126.23
23	B	604	CLA	C4A-NA-C1A	7.20	109.94	106.71
41	R	618	NEX	C17-C1-C6	-7.18	104.04	110.47
41	r	614	NEX	C39-C29-C28	-7.18	106.77	118.08
41	R	614	NEX	C39-C29-C28	-7.17	106.78	118.08
41	s	617	NEX	C19-C9-C10	-7.15	112.91	122.92
40	s	614	LUT	C20-C13-C14	-7.12	112.95	122.92
42	y	302	XAT	O4-C5-C4	7.12	118.73	113.38
42	y	302	XAT	C8-C9-C10	7.11	129.85	118.94
41	g	617	NEX	C19-C9-C10	-7.11	112.97	122.92
23	B	612	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	a	403	CLA	C4A-NA-C1A	7.07	109.88	106.71
40	G	615	LUT	C7-C8-C9	7.06	136.91	126.23
23	A	402	CLA	C4A-NA-C1A	7.04	109.87	106.71
40	y	317	LUT	C19-C9-C8	-7.02	107.01	118.08
23	C	504	CLA	C4A-NA-C1A	7.02	109.86	106.71
42	G	619	XAT	C32-C33-C34	7.02	129.71	118.94
40	Y	316	LUT	C19-C9-C8	-7.02	107.02	118.08
41	n	618	NEX	C28-C29-C30	7.01	129.70	118.94
40	S	614	LUT	C19-C9-C8	-7.00	107.05	118.08
42	n	617	XAT	C32-C33-C34	6.97	129.64	118.94
23	d	406	CLA	C4A-NA-C1A	6.95	109.83	106.71
23	b	607	CLA	C4A-NA-C1A	6.94	109.83	106.71
23	c	507	CLA	C4A-NA-C1A	6.94	109.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	R	608	CLA	C4A-NA-C1A	6.93	109.82	106.71
42	n	617	XAT	O4-C5-C4	6.92	118.58	113.38
23	c	504	CLA	C4A-NA-C1A	6.91	109.81	106.71
41	S	617	NEX	C19-C9-C10	-6.91	113.25	122.92
23	C	507	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	c	503	CLA	C4A-NA-C1A	6.89	109.80	106.71
23	d	405	CLA	C4A-NA-C1A	6.88	109.80	106.71
41	R	614	NEX	C28-C29-C30	6.88	129.50	118.94
42	Y	301	XAT	O4-C5-C4	6.87	118.54	113.38
42	G	619	XAT	C7-C8-C9	6.87	136.19	125.53
23	b	615	CLA	C4A-NA-C1A	6.87	109.79	106.71
23	C	502	CLA	C4A-NA-C1A	6.85	109.78	106.71
23	r	608	CLA	C4A-NA-C1A	6.85	109.78	106.71
40	R	613	LUT	C19-C9-C8	-6.84	107.29	118.08
23	c	511	CLA	C4A-NA-C1A	6.84	109.78	106.71
41	N	617	NEX	C39-C29-C28	-6.84	107.30	118.08
40	G	615	LUT	C20-C13-C14	-6.84	113.34	122.92
23	g	612	CLA	C4A-NA-C1A	6.84	109.78	106.71
41	n	618	NEX	C39-C29-C28	-6.83	107.31	118.08
23	B	607	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	C	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	C	503	CLA	C4A-NA-C1A	6.81	109.77	106.71
41	S	617	NEX	C20-C13-C14	-6.81	113.38	122.92
23	c	502	CLA	C4A-NA-C1A	6.81	109.77	106.71
40	N	615	LUT	C12-C13-C14	6.79	129.36	118.94
23	G	613	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	S	612	CLA	C4A-NA-C1A	6.78	109.76	106.71
23	b	601	CLA	C4A-NA-C1A	6.78	109.76	106.71
23	g	613	CLA	C4A-NA-C1A	6.78	109.75	106.71
23	D	406	CLA	C4A-NA-C1A	6.78	109.75	106.71
41	g	617	NEX	C39-C29-C28	-6.77	107.41	118.08
23	r	611	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	D	405	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	b	605	CLA	C4A-NA-C1A	6.74	109.73	106.71
40	r	613	LUT	C7-C8-C9	6.73	136.40	126.23
41	R	618	NEX	C28-C29-C30	6.72	129.26	118.94
23	S	610	CLA	C4A-NA-C1A	6.72	109.73	106.71
41	Y	317	NEX	C39-C29-C28	-6.72	107.49	118.08
41	N	617	NEX	C28-C29-C30	6.72	129.25	118.94
23	s	612	CLA	C4A-NA-C1A	6.71	109.72	106.71
42	Y	301	XAT	C8-C9-C10	6.71	129.24	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C4A-NA-C1A	6.70	109.72	106.71
42	n	617	XAT	C7-C8-C9	6.70	135.93	125.53
23	B	605	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	y	314	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	B	613	CLA	C4A-NA-C1A	6.70	109.72	106.71
41	R	618	NEX	C39-C29-C28	-6.68	107.55	118.08
23	r	602	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	a	404	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	N	603	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	Y	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	G	611	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	c	506	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	y	305	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	b	613	CLA	C4A-NA-C1A	6.67	109.70	106.71
40	r	613	LUT	C19-C9-C8	-6.67	107.57	118.08
40	R	613	LUT	C7-C8-C9	6.67	136.31	126.23
23	C	506	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	R	612	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	n	613	CLA	C4A-NA-C1A	6.65	109.70	106.71
23	b	614	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	s	610	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	C	508	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	g	611	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	B	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	R	602	CLA	C4A-NA-C1A	6.64	109.69	106.71
41	G	617	NEX	C39-C29-C28	-6.63	107.63	118.08
40	S	615	LUT	C19-C9-C8	-6.63	107.64	118.08
23	c	505	CLA	C4A-NA-C1A	6.62	109.68	106.71
41	G	617	NEX	C38-C25-C26	-6.62	111.17	122.26
23	B	615	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	A	403	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	S	611	CLA	C4A-NA-C1A	6.61	109.68	106.71
40	N	616	LUT	C7-C8-C9	6.60	136.22	126.23
23	B	614	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	A	404	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	s	611	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	R	603	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	B	616	CLA	C4A-NA-C1A	6.59	109.67	106.71
42	G	619	XAT	C20-C13-C12	6.59	128.46	118.08
23	R	611	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	n	603	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	G	610	CLA	C4A-NA-C1A	6.58	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	c	510	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	s	603	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	S	604	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	b	616	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	r	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	C	513	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	c	501	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	S	603	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	G	602	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	c	509	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	C	505	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	N	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
41	Y	317	NEX	C28-C29-C30	6.55	129.00	118.94
23	r	603	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	G	603	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	Y	313	CLA	C4A-NA-C1A	6.55	109.65	106.71
41	r	614	NEX	C28-C29-C30	6.54	128.98	118.94
23	N	612	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	C	509	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	b	602	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	C	512	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	a	407	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	b	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	Y	303	CLA	C4A-NA-C1A	6.52	109.64	106.71
40	N	616	LUT	C19-C9-C8	-6.52	107.81	118.08
23	C	501	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	N	613	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	n	611	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	Y	305	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	s	604	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	Y	311	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	y	315	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	n	604	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	G	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	g	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	R	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	g	610	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	g	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	r	612	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	N	604	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	n	602	CLA	C4A-NA-C1A	6.48	109.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	y	304	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	B	601	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	g	602	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	S	602	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	b	611	CLA	C4A-NA-C1A	6.46	109.61	106.71
40	n	616	LUT	C7-C8-C9	6.46	135.99	126.23
23	B	609	CLA	C4A-NA-C1A	6.45	109.61	106.71
40	S	615	LUT	C7-C8-C9	6.45	135.98	126.23
41	n	618	NEX	C2-C1-C6	6.45	115.48	109.21
23	c	512	CLA	C4A-NA-C1A	6.45	109.60	106.71
23	c	508	CLA	C4A-NA-C1A	6.44	109.60	106.71
40	n	615	LUT	C19-C9-C8	-6.44	107.93	118.08
23	n	614	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	B	602	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	y	306	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	A	406	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	N	602	CLA	C4A-NA-C1A	6.43	109.59	106.71
23	a	405	CLA	C4A-NA-C1A	6.42	109.59	106.71
41	g	617	NEX	C38-C25-C26	-6.41	111.52	122.26
23	N	614	CLA	C4A-NA-C1A	6.41	109.59	106.71
41	S	617	NEX	C20-C13-C12	-6.39	108.00	118.08
23	C	510	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	B	606	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	s	602	CLA	C4A-NA-C1A	6.37	109.57	106.71
42	N	619	XAT	O4-C5-C4	6.36	118.16	113.38
23	G	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
23	b	610	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	r	601	CLA	C4A-NA-C1A	6.35	109.56	106.71
40	y	316	LUT	C20-C13-C14	-6.35	114.03	122.92
23	n	612	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	b	606	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	g	614	CLA	C4A-NA-C1A	6.33	109.55	106.71
40	Y	315	LUT	C20-C13-C14	-6.33	114.06	122.92
23	Y	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
42	r	615	XAT	C28-C29-C30	6.32	128.64	118.94
40	g	616	LUT	C19-C9-C8	-6.31	108.14	118.08
23	R	610	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	y	312	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	R	609	CLA	C4A-NA-C1A	6.29	109.53	106.71
40	G	616	LUT	C19-C9-C8	-6.29	108.17	118.08
23	r	609	CLA	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	Y	312	CLA	C4A-NA-C1A	6.27	109.52	106.71
40	Y	316	LUT	C7-C8-C9	6.27	135.71	126.23
23	b	608	CLA	C4A-NA-C1A	6.26	109.52	106.71
41	N	617	NEX	C19-C9-C10	-6.26	114.15	122.92
23	R	601	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	y	311	CLA	C4A-NA-C1A	6.25	109.52	106.71
41	R	614	NEX	C11-C10-C9	6.25	136.22	127.31
41	N	617	NEX	C38-C25-C26	-6.24	111.80	122.26
23	y	313	CLA	C4A-NA-C1A	6.24	109.51	106.71
42	n	620	XAT	O4-C5-C4	6.24	118.07	113.38
41	n	618	NEX	C38-C25-C26	-6.23	111.82	122.26
23	Y	310	CLA	C4A-NA-C1A	6.23	109.50	106.71
41	S	617	NEX	C11-C10-C9	6.22	136.19	127.31
41	R	618	NEX	C38-C25-C26	-6.22	111.84	122.26
40	s	614	LUT	C7-C8-C9	6.21	135.62	126.23
40	y	317	LUT	C7-C8-C9	6.20	135.61	126.23
40	G	616	LUT	C7-C8-C9	6.20	135.60	126.23
42	G	619	XAT	C26-C27-C28	6.20	139.10	125.99
42	R	615	XAT	C28-C29-C30	6.19	128.44	118.94
42	N	619	XAT	C32-C33-C34	6.19	128.44	118.94
23	B	608	CLA	C4A-NA-C1A	6.18	109.49	106.71
23	G	614	CLA	C4A-NA-C1A	6.18	109.48	106.71
40	g	616	LUT	C7-C8-C9	6.17	135.56	126.23
23	S	613	CLA	C4A-NA-C1A	6.17	109.48	106.71
40	s	615	LUT	C19-C9-C8	-6.15	108.39	118.08
23	n	610	CLA	C4A-NA-C1A	6.14	109.47	106.71
41	Y	317	NEX	C38-C25-C26	-6.14	111.97	122.26
40	n	616	LUT	C19-C9-C8	-6.13	108.42	118.08
40	N	616	LUT	C32-C33-C34	6.13	128.34	118.94
41	R	614	NEX	C38-C25-C26	-6.12	112.00	122.26
23	N	610	CLA	C4A-NA-C1A	6.11	109.45	106.71
41	Y	317	NEX	C20-C13-C12	-6.11	108.45	118.08
41	N	617	NEX	C11-C10-C9	6.11	136.03	127.31
23	S	608	CLA	C4A-NA-C1A	6.09	109.44	106.71
23	s	608	CLA	C4A-NA-C1A	6.09	109.44	106.71
42	N	619	XAT	C7-C8-C9	6.09	134.98	125.53
40	s	614	LUT	C19-C9-C8	-6.07	108.51	118.08
41	r	614	NEX	C38-C25-C26	-6.05	112.12	122.26
41	R	618	NEX	C2-C1-C6	6.05	115.09	109.21
42	r	615	XAT	C38-C25-C24	6.05	121.08	114.28
41	R	614	NEX	C19-C9-C10	-6.04	114.46	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	610	CLA	C4A-NA-C1A	6.03	109.42	106.71
40	g	615	LUT	C19-C9-C8	-5.99	108.65	118.08
23	s	613	CLA	C4A-NA-C1A	5.98	109.39	106.71
41	n	618	NEX	C11-C10-C9	5.97	135.83	127.31
42	R	615	XAT	C38-C25-C24	5.97	120.99	114.28
40	y	316	LUT	C7-C8-C9	5.95	135.22	126.23
42	n	620	XAT	C32-C33-C34	5.94	128.06	118.94
41	R	618	NEX	C11-C10-C9	5.91	135.74	127.31
41	R	618	NEX	C19-C9-C10	-5.87	114.70	122.92
23	S	609	CLA	C4A-NA-C1A	5.87	109.34	106.71
41	g	617	NEX	C20-C13-C12	-5.86	108.84	118.08
40	N	615	LUT	C7-C8-C9	5.86	135.08	126.23
40	s	614	LUT	C12-C13-C14	5.85	127.92	118.94
42	n	617	XAT	C20-C13-C12	5.83	127.27	118.08
40	Y	315	LUT	C7-C8-C9	5.81	135.01	126.23
40	S	614	LUT	C7-C8-C9	5.81	135.01	126.23
23	s	609	CLA	C4A-NA-C1A	5.80	109.31	106.71
42	n	620	XAT	C7-C8-C9	5.78	134.50	125.53
42	r	615	XAT	C39-C29-C28	-5.78	108.97	118.08
41	R	614	NEX	C20-C13-C12	-5.68	109.12	118.08
40	n	615	LUT	C7-C8-C9	5.68	134.82	126.23
42	R	615	XAT	O4-C5-C4	5.65	117.63	113.38
41	S	617	NEX	C2-C1-C6	5.65	114.70	109.21
40	s	615	LUT	C12-C13-C14	5.64	127.59	118.94
41	s	617	NEX	C20-C13-C12	-5.64	109.20	118.08
40	N	615	LUT	C35-C15-C14	5.63	135.01	123.47
42	R	615	XAT	C39-C29-C28	-5.61	109.25	118.08
42	G	619	XAT	C18-C5-C6	-5.59	112.89	122.26
40	Y	316	LUT	C21-C26-C27	5.58	119.75	112.70
36	D	401	BCT	O2-C-O1	5.58	134.02	119.55
42	r	615	XAT	O4-C5-C4	5.58	117.57	113.38
42	R	615	XAT	C19-C9-C8	5.57	126.85	118.08
41	r	614	NEX	C20-C13-C12	-5.57	109.30	118.08
36	d	401	BCT	O2-C-O1	5.57	133.98	119.55
42	r	615	XAT	C19-C9-C8	5.55	126.82	118.08
42	N	619	XAT	C26-C27-C28	5.54	137.70	125.99
41	n	618	NEX	C20-C13-C12	-5.53	109.36	118.08
41	s	617	NEX	C2-C1-C6	5.53	114.58	109.21
42	n	617	XAT	C18-C5-C6	-5.52	113.00	122.26
40	y	317	LUT	C21-C26-C27	5.52	119.68	112.70
40	G	615	LUT	C19-C9-C8	-5.51	109.39	118.08
40	S	614	LUT	C12-C13-C14	5.49	127.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	617	NEX	C11-C10-C9	5.48	135.13	127.31
42	r	615	XAT	C18-C5-C6	-5.48	113.08	122.26
40	g	616	LUT	C12-C13-C14	5.47	127.33	118.94
42	n	620	XAT	C38-C25-C26	-5.46	113.11	122.26
40	S	615	LUT	C21-C26-C27	5.44	119.57	112.70
42	N	619	XAT	C38-C25-C26	-5.43	113.15	122.26
42	R	615	XAT	C18-C5-C6	-5.42	113.17	122.26
42	y	302	XAT	C38-C25-C24	5.41	120.37	114.28
42	R	615	XAT	C20-C13-C12	5.40	126.58	118.08
41	N	617	NEX	C20-C13-C12	-5.39	109.58	118.08
40	s	614	LUT	C8-C9-C10	5.39	127.21	118.94
42	n	620	XAT	C26-C27-C28	5.37	137.35	125.99
40	N	615	LUT	C35-C34-C33	5.37	134.97	127.31
41	s	617	NEX	C11-C10-C9	5.36	134.96	127.31
40	G	616	LUT	C12-C13-C14	5.36	127.16	118.94
42	R	615	XAT	C38-C25-C26	-5.34	113.31	122.26
42	N	619	XAT	C38-C25-C24	5.34	120.28	114.28
41	R	618	NEX	C20-C13-C12	-5.34	109.67	118.08
42	r	615	XAT	C20-C13-C12	5.33	126.48	118.08
41	Y	317	NEX	C11-C10-C9	5.33	134.92	127.31
40	G	615	LUT	C21-C26-C27	5.29	119.39	112.70
42	r	615	XAT	C38-C25-C26	-5.29	113.39	122.26
40	S	615	LUT	C32-C33-C34	5.28	127.04	118.94
41	N	617	NEX	C2-C1-C6	5.26	114.32	109.21
42	Y	301	XAT	C7-C8-C9	5.26	133.68	125.53
42	Y	301	XAT	C20-C13-C12	5.25	126.34	118.08
40	s	614	LUT	C21-C26-C27	5.22	119.30	112.70
42	N	619	XAT	C18-C5-C6	-5.21	113.52	122.26
42	n	620	XAT	C38-C25-C24	5.21	120.14	114.28
40	g	615	LUT	C21-C26-C27	5.21	119.28	112.70
42	n	620	XAT	C18-C5-C6	-5.18	113.58	122.26
41	R	614	NEX	C2-C1-C6	5.16	114.22	109.21
41	r	614	NEX	C11-C10-C9	5.15	134.66	127.31
40	S	615	LUT	C12-C13-C14	5.15	126.84	118.94
42	Y	301	XAT	C38-C25-C24	5.14	120.06	114.28
42	N	619	XAT	C20-C13-C12	5.11	126.13	118.08
40	r	613	LUT	C35-C15-C14	5.10	133.92	123.47
42	n	617	XAT	C26-C27-C28	5.09	136.75	125.99
40	N	616	LUT	C15-C35-C34	5.08	133.89	123.47
41	N	617	NEX	C39-C29-C30	-5.07	115.83	122.92
42	n	620	XAT	C20-C13-C12	5.05	126.04	118.08
40	N	616	LUT	C15-C14-C13	5.03	134.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	y	317	LUT	C12-C13-C14	5.02	126.65	118.94
40	s	615	LUT	C21-C26-C27	5.02	119.05	112.70
42	Y	301	XAT	C18-C5-C6	-5.01	113.86	122.26
40	s	615	LUT	C8-C9-C10	5.00	126.62	118.94
40	S	614	LUT	C32-C33-C34	5.00	126.61	118.94
40	g	616	LUT	C21-C26-C27	4.99	119.01	112.70
40	G	616	LUT	C21-C26-C27	4.99	119.01	112.70
41	n	618	NEX	C39-C29-C30	-4.98	115.94	122.92
42	G	619	XAT	C38-C25-C24	4.98	119.88	114.28
41	R	614	NEX	C39-C29-C30	-4.98	115.95	122.92
40	S	614	LUT	C21-C26-C27	4.96	118.97	112.70
40	n	615	LUT	C8-C9-C10	4.95	126.54	118.94
40	N	616	LUT	C21-C26-C27	4.93	118.94	112.70
40	S	615	LUT	C15-C35-C34	4.93	133.58	123.47
41	r	614	NEX	C2-C1-C6	4.93	114.00	109.21
41	r	614	NEX	C39-C29-C30	-4.92	116.04	122.92
40	S	615	LUT	C15-C14-C13	4.91	134.32	127.31
40	N	615	LUT	C21-C26-C27	4.91	118.91	112.70
42	N	619	XAT	O24-C25-C24	4.91	117.07	113.38
40	R	613	LUT	C32-C33-C34	4.90	126.46	118.94
40	n	616	LUT	C21-C26-C27	4.88	118.87	112.70
40	r	613	LUT	C32-C33-C34	4.88	126.43	118.94
41	G	617	NEX	C32-C33-C34	4.87	126.42	118.94
40	N	615	LUT	C8-C9-C10	4.87	126.41	118.94
42	r	615	XAT	C8-C9-C10	4.87	126.41	118.94
40	s	615	LUT	C7-C8-C9	4.87	133.59	126.23
40	S	614	LUT	C15-C35-C34	4.84	133.40	123.47
40	n	616	LUT	C12-C13-C14	4.82	126.34	118.94
40	Y	316	LUT	C12-C13-C14	4.82	126.34	118.94
42	R	615	XAT	C8-C9-C10	4.81	126.32	118.94
40	R	613	LUT	C15-C14-C13	4.80	134.16	127.31
42	R	615	XAT	O24-C25-C26	-4.78	55.01	58.96
40	R	613	LUT	C21-C26-C27	4.77	118.73	112.70
42	r	615	XAT	O24-C25-C26	-4.77	55.01	58.96
42	r	615	XAT	C26-C27-C28	4.76	136.06	125.99
41	Y	317	NEX	C32-C33-C34	4.76	126.25	118.94
42	Y	301	XAT	O24-C25-C26	-4.76	55.02	58.96
41	g	617	NEX	C39-C29-C30	-4.76	116.26	122.92
40	r	613	LUT	C21-C26-C27	4.75	118.71	112.70
42	y	302	XAT	C18-C5-C6	-4.75	114.30	122.26
40	N	616	LUT	C12-C13-C14	4.75	126.23	118.94
41	g	617	NEX	C2-C1-C6	4.74	113.81	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	G	619	XAT	C38-C25-C26	-4.73	114.34	122.26
42	y	302	XAT	C20-C13-C12	4.72	125.52	118.08
42	n	617	XAT	O24-C25-C26	-4.71	55.06	58.96
40	S	614	LUT	C8-C9-C10	4.70	126.16	118.94
33	C	515	DGD	O3G-C3G-C2G	-4.69	99.59	110.90
40	s	614	LUT	C15-C35-C34	4.68	133.06	123.47
40	s	615	LUT	C8-C7-C6	4.68	140.35	127.20
41	G	617	NEX	C39-C29-C30	-4.68	116.37	122.92
42	n	617	XAT	C38-C25-C24	4.67	119.53	114.28
40	g	616	LUT	C8-C9-C10	4.66	126.09	118.94
42	n	617	XAT	C38-C25-C26	-4.66	114.45	122.26
40	G	616	LUT	C8-C9-C10	4.65	126.08	118.94
40	G	615	LUT	C32-C33-C34	4.65	126.08	118.94
40	R	613	LUT	C12-C13-C14	4.65	126.07	118.94
40	R	613	LUT	C15-C35-C34	4.64	132.97	123.47
42	n	617	XAT	C8-C9-C10	4.63	126.05	118.94
42	n	620	XAT	O24-C25-C24	4.63	116.86	113.38
42	n	620	XAT	O24-C25-C26	-4.63	55.13	58.96
40	g	615	LUT	C32-C33-C34	4.62	126.03	118.94
42	y	302	XAT	O24-C25-C26	-4.62	55.14	58.96
40	S	614	LUT	C15-C14-C13	4.61	133.89	127.31
42	n	620	XAT	C35-C34-C33	4.60	133.88	127.31
41	R	618	NEX	C32-C33-C34	4.59	125.98	118.94
40	s	614	LUT	C15-C14-C13	4.57	133.83	127.31
40	G	615	LUT	C12-C13-C14	4.56	125.94	118.94
40	Y	316	LUT	C32-C33-C34	4.56	125.94	118.94
42	N	619	XAT	O24-C25-C26	-4.55	55.19	58.96
33	c	515	DGD	O3G-C3G-C2G	-4.55	99.92	110.90
40	Y	316	LUT	C15-C35-C34	4.55	132.79	123.47
40	y	317	LUT	C32-C33-C34	4.54	125.92	118.94
39	N	605	CHL	CHD-C1D-ND	-4.54	120.28	124.45
42	R	615	XAT	C26-C27-C28	4.54	135.59	125.99
40	y	317	LUT	C15-C35-C34	4.53	132.76	123.47
40	s	615	LUT	C32-C33-C34	4.53	125.89	118.94
42	y	302	XAT	C38-C25-C26	-4.53	114.67	122.26
23	G	610	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
42	G	619	XAT	O24-C25-C24	4.51	116.77	113.38
42	G	619	XAT	O24-C25-C26	-4.51	55.22	58.96
40	s	614	LUT	C35-C34-C33	4.51	133.74	127.31
42	N	619	XAT	C35-C34-C33	4.51	133.74	127.31
42	G	619	XAT	C19-C9-C8	4.50	125.17	118.08
39	n	605	CHL	CHD-C1D-ND	-4.50	120.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s	614	LUT	C35-C15-C14	4.50	132.69	123.47
40	S	614	LUT	C8-C7-C6	4.49	139.81	127.20
23	s	609	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
23	g	610	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
42	G	619	XAT	C8-C9-C10	4.42	125.72	118.94
40	G	616	LUT	C35-C15-C14	4.41	132.50	123.47
40	G	615	LUT	C1-C6-C5	-4.40	116.41	122.61
39	s	601	CHL	CHD-C1D-ND	-4.39	120.42	124.45
40	s	615	LUT	C15-C35-C34	4.37	132.44	123.47
39	G	609	CHL	CHD-C1D-ND	-4.37	120.43	124.45
40	n	616	LUT	C8-C9-C10	4.37	125.65	118.94
40	r	613	LUT	C15-C35-C34	4.37	132.42	123.47
39	S	601	CHL	CHD-C1D-ND	-4.36	120.45	124.45
39	Y	306	CHL	CHD-C1D-ND	-4.35	120.46	124.45
39	n	601	CHL	CHD-C1D-ND	-4.35	120.46	124.45
39	y	307	CHL	CHD-C1D-ND	-4.35	120.46	124.45
40	y	317	LUT	C8-C7-C6	4.34	139.40	127.20
40	Y	316	LUT	C8-C7-C6	4.34	139.39	127.20
40	g	616	LUT	C35-C15-C14	4.33	132.35	123.47
41	n	618	NEX	C32-C33-C34	4.33	125.59	118.94
40	g	615	LUT	C15-C35-C34	4.33	132.35	123.47
40	y	317	LUT	C15-C14-C13	4.32	133.48	127.31
39	Y	309	CHL	CHD-C1D-ND	-4.31	120.49	124.45
40	g	616	LUT	C32-C33-C34	4.31	125.56	118.94
40	S	615	LUT	C8-C9-C10	4.31	125.55	118.94
41	N	617	NEX	C32-C33-C34	4.31	125.55	118.94
40	G	616	LUT	C32-C33-C34	4.31	125.55	118.94
39	g	601	CHL	CHD-C1D-ND	-4.31	120.50	124.45
23	N	604	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
40	N	615	LUT	C8-C7-C6	4.30	139.29	127.20
41	Y	317	NEX	C39-C29-C30	-4.30	116.90	122.92
41	g	617	NEX	C32-C33-C34	4.30	125.53	118.94
23	n	604	CLA	CMB-C2B-C1B	-4.29	121.86	128.46
39	s	607	CHL	CHD-C1D-ND	-4.29	120.51	124.45
39	g	608	CHL	CHD-C1D-ND	-4.29	120.51	124.45
40	s	615	LUT	C35-C15-C14	4.28	132.24	123.47
40	n	615	LUT	C35-C15-C14	4.27	132.23	123.47
42	Y	301	XAT	C26-C27-C28	4.27	135.03	125.99
23	C	508	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
40	n	615	LUT	C32-C33-C34	4.27	125.49	118.94
40	n	616	LUT	C15-C14-C13	4.26	133.39	127.31
40	Y	316	LUT	C15-C14-C13	4.26	133.39	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	605	CHL	CHD-C1D-ND	-4.26	120.54	124.45
23	y	306	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
41	R	618	NEX	C39-C29-C30	-4.26	116.96	122.92
39	G	601	CHL	CHD-C1D-ND	-4.25	120.55	124.45
39	Y	302	CHL	CHD-C1D-ND	-4.24	120.56	124.45
42	y	302	XAT	C7-C8-C9	4.24	132.11	125.53
39	n	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
39	n	609	CHL	CHD-C1D-ND	-4.24	120.56	124.45
40	s	614	LUT	C8-C7-C6	4.24	139.10	127.20
42	Y	301	XAT	C38-C25-C26	-4.24	115.16	122.26
39	S	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
23	c	508	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
41	R	614	NEX	C32-C33-C34	4.23	125.44	118.94
39	G	608	CHL	CHD-C1D-ND	-4.23	120.57	124.45
39	r	605	CHL	CHD-C1D-ND	-4.23	120.57	124.45
39	y	310	CHL	CHD-C1D-ND	-4.23	120.57	124.45
40	N	616	LUT	C8-C9-C10	4.23	125.42	118.94
39	y	303	CHL	CHD-C1D-ND	-4.23	120.57	124.45
23	Y	305	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
39	N	609	CHL	CHD-C1D-ND	-4.22	120.58	124.45
39	r	606	CHL	CHD-C1D-ND	-4.21	120.58	124.45
40	s	615	LUT	C15-C14-C13	4.20	133.30	127.31
39	N	601	CHL	CHD-C1D-ND	-4.19	120.60	124.45
40	n	616	LUT	C15-C35-C34	4.19	132.06	123.47
39	R	605	CHL	CHD-C1D-ND	-4.19	120.60	124.45
40	s	614	LUT	C32-C33-C34	4.19	125.37	118.94
39	R	606	CHL	CHD-C1D-ND	-4.19	120.61	124.45
39	g	605	CHL	CHD-C1D-ND	-4.19	120.61	124.45
42	R	615	XAT	O24-C25-C24	4.18	116.52	113.38
39	Y	307	CHL	CHD-C1D-ND	-4.18	120.61	124.45
39	G	620	CHL	CHD-C1D-ND	-4.18	120.61	124.45
41	r	614	NEX	C32-C33-C34	4.18	125.36	118.94
42	Y	301	XAT	C11-C12-C13	4.18	138.15	126.42
39	S	607	CHL	CHD-C1D-ND	-4.17	120.62	124.45
39	Y	308	CHL	CHD-C1D-ND	-4.17	120.62	124.45
23	a	403	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
40	g	616	LUT	C15-C35-C34	4.17	132.01	123.47
23	S	609	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
39	N	608	CHL	CHD-C1D-ND	-4.16	120.63	124.45
39	g	619	CHL	CHD-C1D-ND	-4.16	120.63	124.45
23	B	602	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
23	A	402	CLA	CMB-C2B-C1B	-4.16	122.07	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	308	CHL	CHD-C1D-ND	-4.16	120.63	124.45
42	R	615	XAT	C11-C12-C13	4.16	138.10	126.42
39	y	309	CHL	CHD-C1D-ND	-4.16	120.64	124.45
39	s	605	CHL	CHD-C1D-ND	-4.15	120.64	124.45
39	n	608	CHL	CHD-C1D-ND	-4.15	120.64	124.45
23	R	604	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
39	N	606	CHL	CHD-C1D-ND	-4.15	120.64	124.45
40	G	616	LUT	C15-C35-C34	4.15	131.97	123.47
40	g	616	LUT	C8-C7-C6	4.14	138.82	127.20
42	r	615	XAT	C11-C12-C13	4.14	138.04	126.42
23	r	608	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
40	S	615	LUT	C8-C7-C6	4.13	138.81	127.20
40	y	317	LUT	C8-C9-C10	4.13	125.28	118.94
39	s	606	CHL	CHD-C1D-ND	-4.13	120.66	124.45
23	G	613	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
23	C	511	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
23	b	607	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
40	s	614	LUT	C31-C30-C29	4.13	133.20	127.31
39	G	607	CHL	CHD-C1D-ND	-4.13	120.66	124.45
39	S	605	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	N	607	CHL	CHD-C1D-ND	-4.12	120.67	124.45
23	c	511	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
39	R	607	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	g	606	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	G	606	CHL	CHD-C1D-ND	-4.12	120.67	124.45
26	L	101	SQD	O7-S-C6	4.12	111.83	106.94
23	R	603	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
40	G	616	LUT	C8-C7-C6	4.11	138.75	127.20
39	r	607	CHL	CHD-C1D-ND	-4.11	120.68	124.45
40	n	615	LUT	C15-C35-C34	4.10	131.88	123.47
40	Y	315	LUT	C35-C15-C14	4.10	131.87	123.47
23	B	607	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
40	y	316	LUT	C35-C15-C14	4.10	131.87	123.47
40	S	614	LUT	C35-C15-C14	4.10	131.86	123.47
23	r	603	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
40	n	616	LUT	C35-C15-C14	4.09	131.86	123.47
39	n	607	CHL	CHD-C1D-ND	-4.09	120.70	124.45
23	b	616	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
42	r	615	XAT	O24-C25-C24	4.07	116.44	113.38
23	b	602	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
42	y	302	XAT	C11-C12-C13	4.07	137.85	126.42
23	R	608	CLA	CMB-C2B-C1B	-4.06	122.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
26	M	101	SQD	O7-S-C6	4.06	111.77	106.94
23	B	616	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	B	611	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
42	y	302	XAT	C26-C27-C28	4.06	134.58	125.99
40	Y	316	LUT	C8-C9-C10	4.05	125.16	118.94
23	C	513	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
40	n	616	LUT	C32-C33-C34	4.04	125.15	118.94
23	b	611	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
39	g	609	CHL	CHD-C1D-ND	-4.04	120.74	124.45
23	r	604	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
39	g	607	CHL	CHD-C1D-ND	-4.03	120.75	124.45
23	A	403	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
23	c	512	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	A	408	SQD	O47-C7-C8	3.99	120.10	111.50
23	B	612	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
23	c	513	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
23	g	611	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
41	s	617	NEX	C35-C15-C14	3.98	131.62	123.47
40	G	615	LUT	C15-C35-C34	3.98	131.62	123.47
26	M	101	SQD	O47-C7-C8	3.98	120.07	111.50
40	N	616	LUT	C8-C7-C6	3.98	138.37	127.20
40	S	615	LUT	C35-C15-C14	3.97	131.62	123.47
40	R	613	LUT	C35-C15-C14	3.97	131.60	123.47
26	a	409	SQD	O47-C7-C8	3.97	120.05	111.50
23	C	512	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
23	C	510	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
41	R	614	NEX	C35-C15-C14	3.94	131.55	123.47
23	b	608	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
23	r	610	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
40	R	613	LUT	C8-C7-C6	3.93	138.24	127.20
23	n	613	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
40	s	615	LUT	C35-C34-C33	3.93	132.92	127.31
23	B	608	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
23	N	613	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
40	r	613	LUT	C8-C7-C6	3.93	138.23	127.20
23	C	506	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
42	r	615	XAT	C10-C11-C12	3.92	135.46	123.22
40	r	613	LUT	C12-C13-C14	3.92	124.96	118.94
23	b	612	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	s	604	CLA	CMB-C2B-C1B	-3.91	122.46	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	408	SQD	O9-S-C6	3.91	111.58	106.94
41	N	617	NEX	C35-C15-C14	3.90	131.47	123.47
23	Y	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	N	602	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	y	311	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	C	509	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	b	609	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	Y	313	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
23	y	304	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
40	r	613	LUT	C8-C9-C10	3.89	124.92	118.94
40	G	616	LUT	C35-C34-C33	3.89	132.87	127.31
23	S	604	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
26	L	101	SQD	O47-C7-C8	3.89	119.88	111.50
42	n	617	XAT	C10-C11-C12	3.89	135.34	123.22
41	g	617	NEX	C35-C15-C14	3.88	131.43	123.47
23	c	509	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
40	n	616	LUT	C35-C34-C33	3.88	132.85	127.31
23	S	613	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
40	N	616	LUT	C35-C15-C14	3.87	131.41	123.47
23	B	609	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
23	G	603	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
23	s	612	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
23	G	604	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
23	c	506	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
26	a	409	SQD	O7-S-C6	3.86	111.52	106.94
23	N	613	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
40	g	616	LUT	C35-C34-C33	3.85	132.81	127.31
23	b	613	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
40	y	317	LUT	C35-C15-C14	3.85	131.36	123.47
23	s	613	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	Y	310	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	g	613	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	g	603	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
23	n	602	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
42	R	615	XAT	C10-C11-C12	3.84	135.20	123.22
23	y	305	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
42	y	302	XAT	C15-C14-C13	3.83	132.78	127.31
40	g	615	LUT	C1-C6-C5	-3.83	117.22	122.61
41	N	617	NEX	C5-C6-C1	-3.83	115.89	119.70
40	Y	316	LUT	C35-C15-C14	3.83	131.31	123.47
42	N	619	XAT	C11-C12-C13	3.83	137.17	126.42
41	S	617	NEX	C10-C11-C12	3.82	135.15	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	N	610	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	A	406	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
23	g	604	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
41	n	618	NEX	C35-C15-C14	3.81	131.27	123.47
23	y	314	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
23	g	602	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
39	n	605	CHL	C2A-C1A-CHA	3.80	130.51	123.86
23	a	407	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
23	B	613	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
26	a	409	SQD	O9-S-O7	-3.79	100.82	113.95
23	r	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
23	C	502	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
42	n	620	XAT	C11-C12-C13	3.79	137.06	126.42
23	G	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
41	r	614	NEX	C35-C15-C14	3.79	131.23	123.47
41	r	614	NEX	C5-C6-C1	-3.78	115.94	119.70
41	R	614	NEX	C10-C11-C12	3.78	135.02	123.22
40	G	616	LUT	C15-C14-C13	3.78	132.71	127.31
23	s	602	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
23	S	603	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
40	s	614	LUT	C10-C11-C12	3.78	135.00	123.22
23	c	502	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
23	R	602	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
40	s	615	LUT	C18-C5-C6	-3.77	120.30	124.53
23	S	612	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
23	b	614	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
40	G	616	LUT	C1-C6-C5	-3.76	117.31	122.61
40	n	616	LUT	C8-C7-C6	3.76	137.76	127.20
23	n	610	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
40	g	616	LUT	C15-C14-C13	3.75	132.67	127.31
23	B	614	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
26	A	408	SQD	O9-S-O7	-3.75	100.96	113.95
23	C	505	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
40	N	615	LUT	C31-C30-C29	3.75	132.66	127.31
23	n	612	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
26	L	101	SQD	O9-S-O7	-3.75	100.98	113.95
40	Y	315	LUT	C32-C33-C34	3.75	124.69	118.94
40	S	614	LUT	C35-C34-C33	3.74	132.65	127.31
23	S	602	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
23	Y	304	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
23	g	612	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
40	R	613	LUT	C8-C9-C10	3.74	124.67	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	G	619	XAT	C11-C12-C13	3.73	136.91	126.42
39	n	609	CHL	CHC-C1C-NC	3.73	129.87	124.20
26	M	101	SQD	O9-S-C6	3.73	111.37	106.94
23	c	505	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
41	n	618	NEX	C10-C11-C12	3.72	134.84	123.22
39	N	609	CHL	CHC-C1C-NC	3.72	129.85	124.20
23	N	614	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
23	s	611	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
23	n	614	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
42	Y	301	XAT	C15-C14-C13	3.71	132.60	127.31
23	G	610	CLA	CMB-C2B-C3B	3.70	131.60	124.68
40	Y	315	LUT	C21-C26-C27	3.70	117.37	112.70
42	G	619	XAT	C35-C34-C33	3.70	132.58	127.31
23	r	611	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
39	Y	309	CHL	CHC-C1C-NC	3.69	129.80	124.20
41	R	614	NEX	C5-C6-C1	-3.69	116.03	119.70
39	r	605	CHL	CMB-C2B-C1B	-3.69	122.79	128.46
41	N	617	NEX	C10-C11-C12	3.69	134.72	123.22
40	y	316	LUT	C32-C33-C34	3.68	124.59	118.94
39	R	607	CHL	CHC-C1C-NC	3.68	129.79	124.20
23	b	603	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
42	G	619	XAT	C10-C11-C12	3.68	134.70	123.22
39	G	601	CHL	CHC-C1C-NC	3.68	129.79	124.20
23	s	603	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
39	y	310	CHL	CHC-C1C-NC	3.67	129.77	124.20
25	b	617	BCR	C2-C1-C6	3.67	116.13	110.48
41	Y	317	NEX	C35-C15-C14	3.67	130.98	123.47
40	R	613	LUT	C35-C34-C33	3.66	132.54	127.31
40	g	616	LUT	C1-C6-C5	-3.66	117.46	122.61
41	n	618	NEX	C5-C6-C1	-3.66	116.06	119.70
23	d	406	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
23	N	603	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
39	g	601	CHL	CHC-C1C-NC	3.65	129.75	124.20
23	r	609	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
39	G	608	CHL	CHC-C1C-NC	3.65	129.74	124.20
23	g	610	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	s	609	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	B	603	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
40	y	316	LUT	C21-C26-C27	3.65	117.31	112.70
41	R	618	NEX	C35-C15-C14	3.65	130.94	123.47
39	s	607	CHL	CHC-C1C-NC	3.65	129.74	124.20
23	N	612	CLA	CMB-C2B-C1B	-3.64	122.87	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	609	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
39	g	608	CHL	CHC-C1C-NC	3.63	129.72	124.20
40	n	616	LUT	C1-C6-C5	-3.63	117.50	122.61
39	s	605	CHL	CMB-C2B-C1B	-3.63	122.89	128.46
39	r	605	CHL	CHC-C1C-NC	3.63	129.71	124.20
23	D	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
40	Y	315	LUT	C1-C6-C5	-3.63	117.51	122.61
23	Y	314	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
40	G	615	LUT	C15-C14-C13	3.62	132.48	127.31
39	N	606	CHL	CMB-C2B-C1B	-3.62	122.90	128.46
39	S	605	CHL	CHC-C1C-NC	3.62	129.70	124.20
39	g	619	CHL	CHC-C1C-NC	3.62	129.69	124.20
42	n	617	XAT	C19-C9-C8	3.62	123.78	118.08
39	r	607	CHL	CHC-C1C-NC	3.62	129.69	124.20
42	n	617	XAT	C35-C34-C33	3.61	132.47	127.31
39	S	606	CHL	CHC-C1C-NC	3.61	129.68	124.20
39	S	605	CHL	CMB-C2B-C1B	-3.61	122.91	128.46
23	d	405	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
40	r	613	LUT	C35-C34-C33	3.61	132.46	127.31
23	b	606	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	B	606	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	c	503	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	S	611	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
26	A	408	SQD	O7-S-C6	3.60	111.22	106.94
23	b	604	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	y	312	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	C	503	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	a	405	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
39	n	606	CHL	CMB-C2B-C1B	-3.59	122.94	128.46
39	R	605	CHL	CHC-C1C-NC	3.59	129.65	124.20
23	B	604	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	B	605	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
40	n	615	LUT	C21-C26-C27	3.59	117.23	112.70
26	M	101	SQD	O9-S-O7	-3.59	101.54	113.95
23	n	603	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
39	N	601	CHL	CHC-C1C-NC	3.58	129.64	124.20
39	G	607	CHL	CHC-C1C-NC	3.58	129.64	124.20
41	R	618	NEX	C10-C11-C12	3.58	134.39	123.22
39	s	605	CHL	CHC-C1C-NC	3.58	129.63	124.20
39	S	607	CHL	CHC-C1C-NC	3.58	129.63	124.20
23	c	504	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
39	g	606	CHL	CHC-C1C-NC	3.57	129.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	609	CHL	CHC-C1C-NC	3.57	129.62	124.20
39	n	607	CHL	CHC-C1C-NC	3.57	129.62	124.20
40	N	615	LUT	C32-C33-C34	3.57	124.42	118.94
39	g	607	CHL	CHC-C1C-NC	3.56	129.61	124.20
39	S	601	CHL	CHC-C1C-NC	3.56	129.61	124.20
39	n	608	CHL	CHC-C1C-NC	3.56	129.60	124.20
40	y	316	LUT	C1-C6-C5	-3.55	117.61	122.61
42	R	615	XAT	C17-C1-C6	3.55	119.64	110.05
42	r	615	XAT	C17-C1-C6	3.55	119.63	110.05
39	y	309	CHL	CHC-C1C-NC	3.55	129.59	124.20
23	A	404	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
39	G	609	CHL	CMB-C2B-C1B	-3.55	123.01	128.46
23	C	504	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
39	g	605	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	s	601	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	Y	302	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	y	303	CHL	CHC-C1C-NC	3.54	129.58	124.20
23	C	508	CLA	CMB-C2B-C3B	3.54	131.30	124.68
39	n	606	CHL	CHC-C1C-NC	3.54	129.57	124.20
39	Y	308	CHL	CHC-C1C-NC	3.54	129.57	124.20
39	N	608	CHL	CHC-C1C-NC	3.54	129.57	124.20
39	g	605	CHL	CMB-C2B-C1B	-3.54	123.03	128.46
23	c	508	CLA	CMB-C2B-C3B	3.54	131.29	124.68
39	s	606	CHL	CHC-C1C-NC	3.53	129.57	124.20
42	n	620	XAT	C10-C11-C12	3.53	134.25	123.22
23	Y	312	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
39	Y	307	CHL	CHC-C1C-NC	3.53	129.56	124.20
39	n	601	CHL	CHC-C1C-NC	3.53	129.55	124.20
39	N	606	CHL	CHC-C1C-NC	3.52	129.54	124.20
23	g	614	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
39	S	601	CHL	CMB-C2B-C1B	-3.52	123.06	128.46
39	G	605	CHL	CHC-C1C-NC	3.52	129.54	124.20
25	B	618	BCR	C8-C7-C6	-3.51	121.09	127.09
39	G	606	CHL	CHC-C1C-NC	3.51	129.53	124.20
30	A	412	LHG	O7-C7-C8	3.51	119.06	111.50
39	y	308	CHL	CHC-C1C-NC	3.51	129.52	124.20
23	b	605	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
23	b	610	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
42	N	619	XAT	C8-C9-C10	3.50	124.32	118.94
26	L	101	SQD	O9-S-C6	3.50	111.10	106.94
41	g	617	NEX	C10-C11-C12	3.50	134.13	123.22
39	y	307	CHL	CHC-C1C-NC	3.50	129.51	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	601	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
40	N	616	LUT	C1-C6-C5	-3.49	117.70	122.61
23	G	612	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
39	G	620	CHL	CHC-C1C-NC	3.49	129.49	124.20
23	y	313	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	B	610	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
42	n	617	XAT	C11-C12-C13	3.48	136.19	126.42
23	B	602	CLA	CMB-C2B-C3B	3.47	131.18	124.68
42	Y	301	XAT	C19-C9-C8	3.47	123.55	118.08
39	N	605	CHL	CHC-C1C-NC	3.47	129.47	124.20
40	G	615	LUT	C8-C9-C10	3.47	124.26	118.94
39	s	601	CHL	CMB-C2B-C1B	-3.47	123.14	128.46
23	r	608	CLA	CMB-C2B-C3B	3.47	131.16	124.68
23	S	609	CLA	CMB-C2B-C3B	3.46	131.16	124.68
23	A	402	CLA	CMB-C2B-C3B	3.46	131.16	124.68
39	G	606	CHL	CMB-C2B-C1B	-3.46	123.14	128.46
23	R	601	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
40	S	615	LUT	C1-C6-C5	-3.46	117.74	122.61
40	y	316	LUT	C8-C9-C10	3.46	124.25	118.94
23	b	602	CLA	CMB-C2B-C3B	3.46	131.15	124.68
23	b	615	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
42	y	302	XAT	C37-C21-C26	3.46	119.37	110.05
23	C	511	CLA	CMB-C2B-C3B	3.45	131.14	124.68
39	r	606	CHL	CHC-C1C-NC	3.45	129.44	124.20
23	a	403	CLA	CMB-C2B-C3B	3.45	131.14	124.68
23	C	513	CLA	CMB-C2B-C3B	3.45	131.13	124.68
39	R	606	CHL	CHC-C1C-NC	3.45	129.44	124.20
42	N	619	XAT	C10-C11-C12	3.45	133.98	123.22
23	C	501	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	b	616	CLA	CMB-C2B-C3B	3.45	131.12	124.68
23	r	610	CLA	O2D-CGD-CBD	3.44	117.39	111.27
24	a	406	PHO	CMB-C2B-C3B	3.44	131.11	124.68
23	c	511	CLA	CMB-C2B-C3B	3.44	131.11	124.68
39	Y	306	CHL	CHC-C1C-NC	3.44	129.41	124.20
23	N	604	CLA	CMB-C2B-C3B	3.44	131.10	124.68
23	G	613	CLA	CMB-C2B-C3B	3.43	131.10	124.68
39	N	609	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
23	c	512	CLA	CMB-C2B-C3B	3.43	131.10	124.68
23	C	512	CLA	CMB-C2B-C3B	3.43	131.10	124.68
39	g	606	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
40	S	615	LUT	C35-C34-C33	3.43	132.21	127.31
23	b	607	CLA	CMB-C2B-C3B	3.43	131.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	605	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
40	r	613	LUT	C1-C6-C5	-3.43	117.78	122.61
25	B	617	BCR	C2-C1-C6	3.43	115.76	110.48
40	s	615	LUT	C1-C6-C5	-3.43	117.79	122.61
39	N	607	CHL	CHC-C1C-NC	3.42	129.40	124.20
23	c	501	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
33	C	515	DGD	O6D-C1D-O3G	-3.42	101.87	109.97
23	Y	311	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
42	n	620	XAT	C8-C9-C10	3.42	124.19	118.94
23	C	513	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
23	B	616	CLA	CMB-C2B-C3B	3.42	131.07	124.68
39	G	605	CHL	CMB-C2B-C1B	-3.42	123.21	128.46
41	s	617	NEX	C10-C11-C12	3.42	133.88	123.22
23	S	608	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
39	n	605	CHL	CHC-C1C-NC	3.41	129.38	124.20
40	y	316	LUT	C8-C7-C6	3.41	136.78	127.20
23	G	611	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
39	n	609	CHL	CMB-C2B-C1B	-3.41	123.22	128.46
23	B	607	CLA	CMB-C2B-C3B	3.41	131.06	124.68
23	n	604	CLA	CMB-C2B-C3B	3.41	131.05	124.68
26	a	409	SQD	O9-S-C6	3.41	110.99	106.94
23	r	612	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
39	R	606	CHL	CMB-C2B-C1B	-3.41	123.23	128.46
23	b	601	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
23	G	614	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
23	R	603	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	R	616	LHG	O7-C7-C8	3.40	118.83	111.50
39	N	605	CHL	CMB-C2B-C1B	-3.40	123.24	128.46
40	g	615	LUT	C15-C14-C13	3.40	132.16	127.31
40	Y	315	LUT	C8-C9-C10	3.39	124.15	118.94
23	s	610	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	R	608	CLA	CMB-C2B-C3B	3.39	131.03	124.68
40	Y	316	LUT	C1-C6-C5	-3.39	117.84	122.61
40	R	613	LUT	C1-C6-C5	-3.39	117.84	122.61
42	y	302	XAT	C10-C11-C12	3.39	133.79	123.22
39	G	620	CHL	CMB-C2B-C1B	-3.39	123.26	128.46
23	c	513	CLA	CMB-C2B-C3B	3.38	131.01	124.68
23	R	612	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	r	610	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	y	315	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	B	611	CLA	CMB-C2B-C3B	3.38	131.00	124.68
30	D	404	LHG	O7-C7-C8	3.38	118.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	S	610	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	b	611	CLA	CMB-C2B-C3B	3.38	131.00	124.68
42	G	619	XAT	C17-C1-C6	3.38	119.16	110.05
24	A	405	PHO	CMB-C2B-C3B	3.38	131.00	124.68
39	s	606	CHL	CMB-C2B-C1B	-3.38	123.27	128.46
39	Y	309	CHL	CMB-C2B-C1B	-3.38	123.28	128.46
23	B	601	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
40	n	615	LUT	C12-C13-C14	3.37	124.12	118.94
39	y	310	CHL	CMB-C2B-C1B	-3.37	123.28	128.46
39	G	607	CHL	CMB-C2B-C1B	-3.37	123.29	128.46
23	N	611	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
23	a	404	CLA	CMB-C2B-C3B	3.37	130.98	124.68
30	G	618	LHG	O7-C7-C8	3.36	118.75	111.50
23	r	603	CLA	CMB-C2B-C3B	3.36	130.97	124.68
40	s	615	LUT	C10-C11-C12	3.36	133.71	123.22
41	r	614	NEX	C10-C11-C12	3.36	133.70	123.22
39	g	607	CHL	CMB-C2B-C1B	-3.36	123.30	128.46
39	g	608	CHL	CMB-C2B-C1B	-3.36	123.30	128.46
40	N	615	LUT	C31-C32-C33	3.36	135.85	126.42
30	g	618	LHG	O7-C7-C8	3.36	118.73	111.50
23	R	610	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
39	n	605	CHL	CMB-C2B-C1B	-3.36	123.31	128.46
40	Y	315	LUT	C8-C7-C6	3.36	136.62	127.20
40	r	613	LUT	C18-C5-C6	-3.35	120.76	124.53
23	n	611	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
39	g	607	CHL	CHB-C4A-NA	3.35	129.15	124.51
23	s	608	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
23	Y	305	CLA	CMB-C2B-C3B	3.35	130.94	124.68
39	S	606	CHL	CMB-C2B-C1B	-3.35	123.32	128.46
40	G	615	LUT	C35-C15-C14	3.34	130.32	123.47
39	y	308	CHL	CMB-C2B-C1B	-3.34	123.33	128.46
30	s	616	LHG	O7-C7-C8	3.34	118.71	111.50
33	c	515	DGD	O6D-C1D-O3G	-3.34	102.06	109.97
26	a	409	SQD	O8-S-C6	3.34	111.07	105.74
23	y	306	CLA	CMB-C2B-C3B	3.34	130.93	124.68
23	c	510	CLA	CMB-C2B-C3B	3.34	130.93	124.68
30	d	404	LHG	O7-C7-C8	3.34	118.70	111.50
23	B	612	CLA	CMB-C2B-C3B	3.34	130.93	124.68
23	R	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
39	G	607	CHL	CHB-C4A-NA	3.34	129.13	124.51
39	g	609	CHL	CMB-C2B-C1B	-3.34	123.34	128.46
39	n	608	CHL	CMB-C2B-C1B	-3.33	123.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	403	CLA	CMB-C2B-C3B	3.33	130.92	124.68
39	N	607	CHL	CHB-C4A-NA	3.33	129.12	124.51
40	y	317	LUT	C1-C6-C5	-3.33	117.92	122.61
39	r	606	CHL	CMB-C2B-C1B	-3.33	123.35	128.46
40	S	614	LUT	C1-C6-C5	-3.33	117.93	122.61
39	G	620	CHL	CHB-C4A-NA	3.32	129.11	124.51
39	Y	307	CHL	CMB-C2B-C1B	-3.32	123.36	128.46
42	n	620	XAT	C37-C21-C26	3.32	119.00	110.05
39	g	609	CHL	CHC-C1C-NC	3.32	129.24	124.20
41	Y	317	NEX	C10-C11-C12	3.32	133.56	123.22
42	Y	301	XAT	C37-C21-C26	3.31	118.99	110.05
39	s	607	CHL	CMB-C2B-C1B	-3.31	123.38	128.46
39	n	607	CHL	CMB-C2B-C1B	-3.31	123.38	128.46
39	y	307	CHL	CMB-C2B-C1B	-3.31	123.38	128.46
24	d	402	PHO	CMB-C2B-C3B	3.31	130.86	124.68
40	S	615	LUT	C31-C30-C29	3.30	132.03	127.31
42	N	619	XAT	C11-C10-C9	3.30	132.02	127.31
39	Y	308	CHL	CMB-C2B-C1B	-3.30	123.39	128.46
39	r	607	CHL	CMB-C2B-C1B	-3.30	123.39	128.46
24	D	402	PHO	CMB-C2B-C3B	3.30	130.85	124.68
42	n	617	XAT	C17-C1-C6	3.30	118.95	110.05
40	n	615	LUT	C1-C6-C5	-3.30	117.97	122.61
39	G	608	CHL	CMB-C2B-C1B	-3.30	123.40	128.46
23	C	510	CLA	CMB-C2B-C3B	3.29	130.84	124.68
39	N	608	CHL	CMB-C2B-C1B	-3.29	123.40	128.46
23	a	405	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
40	S	614	LUT	C10-C11-C12	3.29	133.48	123.22
33	d	411	DGD	O3G-C3G-C2G	-3.29	102.97	110.90
23	g	611	CLA	CMB-C2B-C3B	3.29	130.83	124.68
39	S	607	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
39	n	607	CHL	CHB-C4A-NA	3.28	129.05	124.51
23	C	509	CLA	CMB-C2B-C3B	3.28	130.82	124.68
41	s	617	NEX	C15-C35-C34	3.28	130.19	123.47
39	y	309	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
23	R	604	CLA	CMB-C2B-C3B	3.28	130.81	124.68
39	g	619	CHL	CMB-C2B-C1B	-3.28	123.42	128.46
23	B	615	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
23	D	406	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
39	g	619	CHL	CHB-C4A-NA	3.28	129.04	124.51
23	Y	303	CLA	CMB-C2B-C3B	3.28	130.81	124.68
42	n	620	XAT	C11-C10-C9	3.27	131.98	127.31
39	R	606	CHL	CHB-C4A-NA	3.27	129.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
42	Y	301	XAT	C10-C11-C12	3.27	133.42	123.22
23	b	612	CLA	CMB-C2B-C3B	3.27	130.79	124.68
42	N	619	XAT	C37-C21-C26	3.27	118.86	110.05
23	s	613	CLA	CMB-C2B-C3B	3.26	130.78	124.68
30	b	627	LHG	O7-C7-C8	3.26	118.53	111.50
23	y	304	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	B	609	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	b	609	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	S	613	CLA	CMB-C2B-C3B	3.26	130.78	124.68
42	G	619	XAT	C36-C21-C26	-3.26	101.25	110.05
23	b	608	CLA	CMB-C2B-C3B	3.25	130.77	124.68
40	N	616	LUT	C35-C34-C33	3.25	131.96	127.31
23	n	613	CLA	CMB-C2B-C3B	3.25	130.77	124.68
40	N	615	LUT	C15-C35-C34	3.25	130.14	123.47
42	n	617	XAT	O24-C25-C24	3.25	115.83	113.38
23	N	602	CLA	CMB-C2B-C3B	3.25	130.76	124.68
23	A	406	CLA	CMB-C2B-C3B	3.25	130.76	124.68
23	a	407	CLA	CMB-C2B-C3B	3.25	130.76	124.68
39	r	607	CHL	CHB-C4A-NA	3.25	129.00	124.51
30	a	412	LHG	O7-C7-C8	3.24	118.49	111.50
23	y	305	CLA	CMB-C2B-C3B	3.24	130.75	124.68
23	c	509	CLA	CMB-C2B-C3B	3.24	130.74	124.68
23	Y	313	CLA	CMB-C2B-C3B	3.24	130.74	124.68
39	N	607	CHL	CMB-C2B-C1B	-3.24	123.49	128.46
23	B	608	CLA	CMB-C2B-C3B	3.23	130.73	124.68
39	y	303	CHL	CMB-C2B-C1B	-3.23	123.50	128.46
33	H	502	DGD	O3G-C3G-C2G	-3.23	103.10	110.90
39	n	601	CHL	CMB-C2B-C1B	-3.23	123.50	128.46
23	y	311	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	r	604	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	N	610	CLA	CMB-C2B-C3B	3.23	130.71	124.68
39	R	607	CHL	CMB-C2B-C1B	-3.22	123.51	128.46
39	N	601	CHL	CMB-C2B-C1B	-3.22	123.51	128.46
23	C	507	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
39	r	606	CHL	CHB-C4A-NA	3.22	128.96	124.51
42	R	615	XAT	C15-C14-C13	3.22	131.90	127.31
40	y	317	LUT	C35-C34-C33	3.22	131.90	127.31
23	N	613	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	g	603	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	n	610	CLA	CMB-C2B-C3B	3.21	130.69	124.68
39	Y	309	CHL	CHB-C4A-NA	3.21	128.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	408	LHG	O7-C7-C8	3.21	118.42	111.50
40	s	614	LUT	C30-C31-C32	3.21	133.24	123.22
23	s	612	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	G	603	CLA	CMB-C2B-C3B	3.21	130.68	124.68
30	S	616	LHG	O7-C7-C8	3.20	118.40	111.50
31	C	518	LNL	C15-C14-C13	-3.20	96.29	112.02
23	g	612	CLA	CMB-C2B-C3B	3.20	130.66	124.68
30	r	616	LHG	O7-C7-C8	3.19	118.39	111.50
39	Y	302	CHL	CMB-C2B-C1B	-3.19	123.56	128.46
39	g	605	CHL	C4D-CHA-C1A	3.19	125.13	121.25
30	n	619	LHG	O7-C7-C8	3.19	118.38	111.50
23	n	602	CLA	CMB-C2B-C3B	3.19	130.64	124.68
23	y	314	CLA	CMB-C2B-C3B	3.19	130.64	124.68
39	G	609	CHL	C2A-C1A-CHA	3.18	129.42	123.86
39	n	609	CHL	CHB-C4A-NA	3.18	128.91	124.51
39	R	607	CHL	CHB-C4A-NA	3.18	128.91	124.51
39	g	601	CHL	CMB-C2B-C1B	-3.18	123.58	128.46
23	c	507	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	C	506	CLA	CMB-C2B-C3B	3.18	130.62	124.68
39	Y	306	CHL	CMB-C2B-C1B	-3.18	123.58	128.46
23	C	505	CLA	CMB-C2B-C3B	3.17	130.62	124.68
30	L	103	LHG	O7-C7-C8	3.17	118.34	111.50
23	g	602	CLA	CMB-C2B-C3B	3.17	130.62	124.68
39	N	609	CHL	CHB-C4A-NA	3.17	128.90	124.51
23	g	613	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	s	604	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	n	612	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	b	613	CLA	CMB-C2B-C3B	3.17	130.60	124.68
42	G	619	XAT	C31-C30-C29	3.16	131.82	127.31
39	y	303	CHL	CHB-C4A-NA	3.16	128.88	124.51
23	G	602	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	c	505	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	Y	304	CLA	CMB-C2B-C3B	3.16	130.58	124.68
23	Y	310	CLA	CMB-C2B-C3B	3.15	130.58	124.68
40	G	616	LUT	C31-C30-C29	3.15	131.81	127.31
42	r	615	XAT	C15-C14-C13	3.15	131.81	127.31
39	g	609	CHL	CHB-C4A-NA	3.15	128.87	124.51
39	G	601	CHL	CMB-C2B-C1B	-3.15	123.63	128.46
23	B	614	CLA	CMB-C2B-C3B	3.15	130.57	124.68
23	S	604	CLA	CMB-C2B-C3B	3.15	130.56	124.68
40	s	614	LUT	C1-C6-C5	-3.14	118.19	122.61
23	b	614	CLA	CMB-C2B-C3B	3.14	130.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Y	316	LUT	C35-C34-C33	3.14	131.79	127.31
23	B	613	CLA	CMB-C2B-C3B	3.14	130.56	124.68
23	R	602	CLA	CMB-C2B-C3B	3.14	130.56	124.68
36	D	401	BCT	O3-C-O1	-3.14	111.41	119.55
23	s	602	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	y	312	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
31	C	519	LNL	C15-C14-C13	-3.14	96.58	112.02
23	n	614	CLA	CMB-C2B-C3B	3.13	130.54	124.68
40	N	615	LUT	C10-C11-C12	3.13	133.00	123.22
23	N	614	CLA	CMB-C2B-C3B	3.13	130.54	124.68
23	r	602	CLA	CMB-C2B-C3B	3.13	130.53	124.68
39	y	310	CHL	CHB-C4A-NA	3.13	128.83	124.51
40	g	616	LUT	C31-C30-C29	3.13	131.77	127.31
42	n	620	XAT	C31-C32-C33	3.12	135.19	126.42
23	N	603	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	S	603	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	C	502	CLA	CMB-C2B-C3B	3.12	130.52	124.68
40	N	616	LUT	C31-C32-C33	3.12	135.18	126.42
23	S	604	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	c	506	CLA	CMB-C2B-C3B	3.12	130.51	124.68
23	b	603	CLA	CMB-C2B-C3B	3.12	130.51	124.68
30	y	318	LHG	O7-C7-C8	3.12	118.22	111.50
39	s	606	CHL	CHB-C4A-NA	3.12	128.82	124.51
40	G	616	LUT	C10-C11-C12	3.11	132.94	123.22
23	c	502	CLA	CMB-C2B-C3B	3.11	130.50	124.68
40	y	317	LUT	C10-C11-C12	3.11	132.93	123.22
42	n	617	XAT	C37-C21-C26	3.11	118.44	110.05
39	Y	302	CHL	CHB-C4A-NA	3.11	128.81	124.51
23	S	612	CLA	CMB-C2B-C3B	3.11	130.49	124.68
36	d	401	BCT	O3-C-O1	-3.11	111.48	119.55
31	c	521	LNL	C15-C14-C13	-3.11	96.73	112.02
23	B	610	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
40	g	616	LUT	C10-C11-C12	3.10	132.90	123.22
40	n	615	LUT	C10-C11-C12	3.10	132.90	123.22
40	n	615	LUT	C8-C7-C6	3.10	135.91	127.20
40	Y	316	LUT	C10-C11-C12	3.10	132.90	123.22
39	G	620	CHL	C4D-CHA-C1A	3.10	125.02	121.25
23	r	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	S	605	CHL	CHB-C4A-NA	3.10	128.80	124.51
23	B	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	g	619	CHL	C4D-CHA-C1A	3.10	125.02	121.25
35	y	301	VIV	C10-C3-C4	-3.10	117.02	120.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
23	S	602	CLA	CMB-C2B-C3B	3.09	130.47	124.68
23	s	611	CLA	CMB-C2B-C3B	3.09	130.46	124.68
23	B	601	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	C	505	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	606	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
31	i	101	LNL	C15-C14-C13	-3.09	96.81	112.02
40	R	613	LUT	C18-C5-C6	-3.09	121.06	124.53
41	Y	317	NEX	C35-C34-C33	-3.09	122.90	127.31
40	r	613	LUT	C31-C30-C29	3.08	131.71	127.31
23	c	505	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
23	r	611	CLA	CMB-C2B-C3B	3.08	130.44	124.68
39	G	605	CHL	C4D-CHA-C1A	3.08	124.99	121.25
23	D	405	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	B	603	CLA	CMB-C2B-C3B	3.07	130.43	124.68
39	S	606	CHL	CHB-C4A-NA	3.07	128.75	124.51
41	R	618	NEX	C35-C34-C33	-3.07	122.93	127.31
23	B	614	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
39	g	606	CHL	CHB-C4A-NA	3.06	128.75	124.51
39	Y	307	CHL	CHB-C4A-NA	3.06	128.75	124.51
31	c	519	LNL	C15-C14-C13	-3.06	96.95	112.02
23	a	407	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	d	405	CLA	CMB-C2B-C3B	3.05	130.39	124.68
40	G	615	LUT	C31-C32-C33	3.05	134.99	126.42
39	N	605	CHL	C4D-CHA-C1A	3.05	124.96	121.25
23	s	609	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	G	604	CLA	CMB-C2B-C3B	3.05	130.38	124.68
23	d	406	CLA	CMB-C2B-C3B	3.05	130.38	124.68
23	g	604	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	b	617	BCR	C15-C16-C17	-3.05	117.24	123.47
23	r	609	CLA	CMB-C2B-C3B	3.04	130.38	124.68
23	b	604	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	Y	311	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	610	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	614	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	N	612	CLA	CMB-C2B-C3B	3.04	130.36	124.68
40	N	615	LUT	C1-C6-C5	-3.04	118.33	122.61
40	N	616	LUT	C31-C30-C29	3.04	131.65	127.31
23	s	603	CLA	CMB-C2B-C3B	3.04	130.36	124.68
40	S	615	LUT	C30-C31-C32	3.04	132.70	123.22
31	c	517	LNL	C15-C14-C13	-3.04	97.07	112.02
23	C	508	CLA	O2D-CGD-O1D	-3.04	117.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	R	601	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	y	312	CLA	CMB-C2B-C3B	3.03	130.35	124.68
31	a	401	LNL	C15-C14-C13	-3.03	97.10	112.02
23	s	604	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	R	609	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	N	612	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	b	602	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
39	s	605	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	A	406	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
39	S	606	CHL	C4D-CHA-C1A	3.02	124.92	121.25
23	B	604	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
31	c	522	LNL	C15-C14-C13	-3.02	97.16	112.02
39	n	608	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	b	601	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	c	520	LNL	C15-C14-C13	-3.02	97.17	112.02
31	A	414	LNL	C15-C14-C13	-3.01	97.18	112.02
23	a	405	CLA	CMB-C2B-C3B	3.01	130.32	124.68
39	g	605	CHL	C2A-C1A-CHA	3.01	129.13	123.86
23	b	615	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	b	625	LNL	C15-C14-C13	-3.01	97.19	112.02
23	B	615	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	B	622	LNL	C15-C14-C13	-3.01	97.20	112.02
39	G	606	CHL	CHB-C4A-NA	3.01	128.68	124.51
23	A	403	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	b	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	C	521	LNL	C15-C14-C13	-3.01	97.21	112.02
23	a	404	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
39	N	608	CHL	CHB-C4A-NA	3.01	128.67	124.51
38	F	501	HEM	C4D-ND-C1D	3.00	108.18	105.07
41	g	617	NEX	C5-C4-C3	3.00	115.30	111.75
39	S	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
23	S	611	CLA	CMB-C2B-C3B	3.00	130.30	124.68
23	c	503	CLA	CMB-C2B-C3B	3.00	130.30	124.68
31	a	413	LNL	C15-C14-C13	-3.00	97.24	112.02
23	b	616	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
41	g	617	NEX	C15-C35-C34	3.00	129.62	123.47
23	n	603	CLA	CMB-C2B-C3B	3.00	130.29	124.68
31	c	518	LNL	C15-C14-C13	-3.00	97.27	112.02
23	d	405	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	B	605	CLA	CMB-C2B-C3B	3.00	130.28	124.68
40	N	616	LUT	C18-C5-C6	-2.99	121.17	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	N	619	XAT	C17-C1-C6	2.99	118.13	110.05
39	y	308	CHL	CHB-C4A-NA	2.99	128.65	124.51
39	g	606	CHL	C4D-CHA-C1A	2.99	124.89	121.25
39	R	606	CHL	C4D-CHA-C1A	2.99	124.89	121.25
25	b	617	BCR	C15-C14-C13	-2.99	123.04	127.31
42	G	619	XAT	C15-C14-C13	2.99	131.57	127.31
23	B	612	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
39	n	601	CHL	CHB-C4A-NA	2.98	128.64	124.51
39	G	606	CHL	C4D-CHA-C1A	2.98	124.88	121.25
23	D	405	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	b	622	LNL	C15-C14-C13	-2.98	97.35	112.02
40	n	616	LUT	C31-C30-C29	2.98	131.56	127.31
23	g	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	s	613	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
23	Y	314	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	N	614	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
40	n	615	LUT	C16-C1-C6	-2.98	105.47	110.30
41	G	617	NEX	C34-C35-C15	2.97	130.22	123.42
23	c	504	CLA	CMB-C2B-C3B	2.97	130.24	124.68
40	S	614	LUT	C30-C31-C32	2.97	132.50	123.22
39	Y	306	CHL	C4D-CHA-C1A	2.97	124.87	121.25
23	B	616	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	Y	314	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	y	315	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
42	y	302	XAT	C19-C9-C8	2.97	122.76	118.08
39	N	607	CHL	C4D-CHA-C1A	2.97	124.87	121.25
39	Y	308	CHL	CHB-C4A-NA	2.97	128.62	124.51
39	g	601	CHL	CHB-C4A-NA	2.97	128.62	124.51
23	g	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	R	604	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
40	Y	315	LUT	C15-C35-C34	2.96	129.54	123.47
39	S	605	CHL	C4D-CHA-C1A	2.96	124.86	121.25
23	S	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	g	614	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	A	404	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	y	304	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
42	n	620	XAT	C17-C1-C6	2.96	118.03	110.05
23	r	604	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
40	y	316	LUT	C15-C35-C34	2.95	129.52	123.47
23	b	607	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
39	n	607	CHL	C4D-CHA-C1A	2.95	124.84	121.25
25	b	617	BCR	C11-C10-C9	-2.95	123.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	601	CHL	CHB-C4A-NA	2.95	128.59	124.51
40	S	614	LUT	C18-C5-C6	-2.95	121.21	124.53
39	S	601	CHL	C2A-C1A-CHA	2.95	129.02	123.86
23	C	504	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	C	503	CLA	CMB-C2B-C3B	2.95	130.19	124.68
39	y	307	CHL	C4D-CHA-C1A	2.95	124.84	121.25
23	b	605	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	n	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
40	R	613	LUT	C31-C30-C29	2.95	131.51	127.31
23	s	613	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
31	B	625	LNL	C15-C14-C13	-2.94	97.52	112.02
40	g	615	LUT	C35-C15-C14	2.94	129.51	123.47
39	s	605	CHL	C4D-CHA-C1A	2.94	124.83	121.25
23	B	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	C	507	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	R	602	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	G	608	CHL	CHB-C4A-NA	2.94	128.58	124.51
23	n	614	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
40	g	615	LUT	C31-C32-C33	2.94	134.68	126.42
39	y	309	CHL	CHB-C4A-NA	2.94	128.57	124.51
23	S	613	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	s	610	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	N	613	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	B	617	BCR	C11-C10-C9	-2.93	123.12	127.31
39	n	606	CHL	CHB-C4A-NA	2.93	128.57	124.51
39	Y	306	CHL	C2A-C1A-CHA	2.93	128.99	123.86
39	r	606	CHL	C4D-CHA-C1A	2.93	124.82	121.25
31	I	101	LNL	C15-C14-C13	-2.93	97.59	112.02
23	Y	303	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
31	C	517	LNL	C15-C14-C13	-2.93	97.61	112.02
39	N	606	CHL	CHB-C4A-NA	2.93	128.56	124.51
39	r	605	CHL	CHB-C4A-NA	2.92	128.55	124.51
23	C	501	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
30	N	618	LHG	O7-C7-C8	2.92	117.80	111.50
40	g	615	LUT	C16-C1-C6	-2.92	105.56	110.30
23	C	509	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	s	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	b	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	b	615	CLA	CMB-C2B-C3B	2.92	130.14	124.68
41	Y	317	NEX	C15-C35-C34	2.92	129.45	123.47
23	n	613	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	n	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	c	501	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	B	604	CLA	CMB-C2B-C3B	2.91	130.12	124.68
39	r	607	CHL	C4D-CHA-C1A	2.91	124.79	121.25
23	S	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
40	S	615	LUT	C10-C11-C12	2.91	132.29	123.22
40	n	616	LUT	C10-C11-C12	2.91	132.29	123.22
23	G	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	c	507	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	R	610	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	S	601	CHL	C4D-CHA-C1A	2.90	124.78	121.25
30	Y	318	LHG	O7-C7-C8	2.90	117.76	111.50
23	R	611	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
42	y	302	XAT	C36-C21-C26	-2.90	102.21	110.05
31	C	522	LNL	C15-C14-C13	-2.90	97.74	112.02
31	b	623	LNL	C15-C14-C13	-2.90	97.74	112.02
39	r	605	CHL	C4D-CHA-C1A	2.90	124.78	121.25
42	r	615	XAT	C16-C1-C6	-2.90	102.22	110.05
23	N	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	G	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	A	413	LNL	C15-C14-C13	-2.89	97.77	112.02
23	c	511	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	N	605	CHL	C2A-C1A-CHA	2.89	128.92	123.86
39	g	608	CHL	CHB-C4A-NA	2.89	128.51	124.51
23	b	603	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	s	601	CHL	CHB-C4A-NA	2.89	128.51	124.51
40	s	615	LUT	C31-C30-C29	2.89	131.44	127.31
23	B	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	N	601	CHL	C4D-CHA-C1A	2.89	124.77	121.25
23	B	609	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	C	503	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
39	R	607	CHL	C4D-CHA-C1A	2.89	124.77	121.25
23	S	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
40	g	615	LUT	C8-C7-C6	2.89	135.32	127.20
23	C	511	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
39	y	307	CHL	C2A-C1A-CHA	2.89	128.91	123.86
23	R	612	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
40	s	614	LUT	C16-C1-C6	-2.88	105.62	110.30
23	s	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	s	606	CHL	C4D-CHA-C1A	2.88	124.76	121.25
39	g	608	CHL	C2A-C1A-CHA	2.88	128.90	123.86
23	B	603	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	605	CHL	CHB-C4A-NA	2.88	128.50	124.51
39	G	620	CHL	C2A-C1A-CHA	2.88	128.90	123.86
23	G	612	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	D	406	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
39	G	607	CHL	C4D-CHA-C1A	2.88	124.75	121.25
23	G	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	r	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
42	R	615	XAT	C16-C1-C6	-2.88	102.28	110.05
23	c	502	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	b	605	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
23	g	603	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
23	r	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	B	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
41	n	618	NEX	C15-C35-C34	2.87	129.36	123.47
39	N	601	CHL	CHB-C4A-NA	2.87	128.49	124.51
23	C	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	C	510	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
40	N	616	LUT	C10-C11-C12	2.87	132.18	123.22
23	Y	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	D	402	PHO	O1D-CGD-CBD	2.87	129.52	124.74
39	n	601	CHL	C2A-C1A-CHA	2.87	128.88	123.86
23	c	503	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	g	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	d	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	c	504	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	s	601	CHL	C2A-C1A-CHA	2.87	128.87	123.86
39	Y	306	CHL	CHB-C4A-NA	2.87	128.48	124.51
39	g	607	CHL	C4D-CHA-C1A	2.87	124.74	121.25
31	C	520	LNL	C15-C14-C13	-2.87	97.91	112.02
23	c	512	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	Y	311	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	r	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	b	609	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	b	610	CLA	CMB-C2B-C3B	2.86	130.04	124.68
42	G	619	XAT	C37-C21-C26	2.86	117.78	110.05
25	B	618	BCR	C15-C16-C17	-2.86	117.61	123.47
23	r	601	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
39	G	605	CHL	C2A-C1A-CHA	2.86	128.86	123.86
23	R	603	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
40	y	317	LUT	C31-C30-C29	2.86	131.39	127.31
39	S	601	CHL	CHB-C4A-NA	2.86	128.47	124.51
23	b	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	b	608	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	c	510	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	y	313	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	C	504	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	B	624	LNL	C15-C14-C13	-2.86	97.96	112.02
23	y	305	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	R	605	CHL	C4D-CHA-C1A	2.86	124.72	121.25
23	n	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
40	G	615	LUT	C16-C1-C6	-2.85	105.67	110.30
39	R	605	CHL	CHB-C4A-NA	2.85	128.46	124.51
23	N	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	Y	304	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	S	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	G	605	CHL	CHB-C4A-NA	2.85	128.45	124.51
23	s	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	s	607	CHL	C4D-CHA-C1A	2.85	124.72	121.25
23	B	601	CLA	CMB-C2B-C3B	2.85	130.01	124.68
39	s	607	CHL	CHB-C4A-NA	2.85	128.45	124.51
40	G	615	LUT	C8-C7-C6	2.85	135.19	127.20
40	s	614	LUT	C18-C5-C6	-2.85	121.33	124.53
40	n	616	LUT	C31-C32-C33	2.84	134.40	126.42
23	S	609	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
40	G	616	LUT	C31-C32-C33	2.84	134.40	126.42
23	r	610	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	s	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
42	N	619	XAT	C31-C32-C33	2.84	134.39	126.42
40	R	613	LUT	C16-C1-C6	-2.84	105.70	110.30
23	y	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
42	n	617	XAT	C31-C30-C29	2.83	131.35	127.31
40	R	613	LUT	C30-C31-C32	2.83	132.05	123.22
23	Y	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	y	306	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
40	R	613	LUT	C10-C11-C12	2.83	132.05	123.22
23	R	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	A	405	PHO	O1D-CGD-CBD	2.83	129.45	124.74
39	N	605	CHL	CHB-C4A-NA	2.83	128.43	124.51
40	g	616	LUT	C31-C32-C33	2.83	134.36	126.42
23	b	611	CLA	C1-C2-C3	-2.83	121.15	126.04
23	S	608	CLA	CMB-C2B-C3B	2.83	129.97	124.68
23	G	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	L	101	SQD	O8-S-C6	2.83	110.24	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	608	CHL	C4D-CHA-C1A	2.83	124.69	121.25
41	R	614	NEX	C15-C35-C34	2.82	129.26	123.47
23	S	608	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	n	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
41	s	617	NEX	C5-C6-C1	-2.82	116.89	119.70
39	G	609	CHL	CHB-C4A-NA	2.82	128.42	124.51
39	y	307	CHL	CHB-C4A-NA	2.82	128.42	124.51
41	R	618	NEX	C15-C35-C34	2.82	129.26	123.47
38	F	501	HEM	C4B-CHC-C1C	2.82	126.28	122.56
23	N	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	y	308	CHL	C4D-CHA-C1A	2.82	124.68	121.25
25	B	617	BCR	C15-C16-C17	-2.82	117.70	123.47
39	g	619	CHL	C2A-C1A-CHA	2.82	128.79	123.86
41	N	617	NEX	C15-C35-C34	2.82	129.24	123.47
23	r	601	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	g	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
40	Y	316	LUT	C31-C30-C29	2.82	131.33	127.31
39	N	608	CHL	C4D-CHA-C1A	2.82	124.68	121.25
39	S	607	CHL	C4D-CHA-C1A	2.81	124.67	121.25
23	c	513	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	d	402	PHO	O1D-CGD-CBD	2.81	129.42	124.74
23	N	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	Y	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	R	601	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	Y	312	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	C	513	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	d	410	BCR	C24-C23-C22	-2.81	121.99	126.23
23	n	611	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
23	r	609	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
24	D	402	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
40	s	615	LUT	C31-C32-C33	2.80	134.29	126.42
40	n	616	LUT	C18-C5-C6	-2.80	121.38	124.53
25	d	410	BCR	C33-C5-C6	-2.80	121.38	124.53
23	r	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	G	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	C	501	CLA	CMB-C2B-C3B	2.80	129.91	124.68
24	d	402	PHO	O2D-CGD-O1D	-2.80	118.37	123.84
39	Y	307	CHL	C4D-CHA-C1A	2.80	124.65	121.25
25	B	617	BCR	C15-C14-C13	-2.80	123.32	127.31
23	g	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	g	613	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	y	315	CLA	CMB-C2B-C3B	2.79	129.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	601	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	N	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
40	S	615	LUT	C18-C5-C6	-2.79	121.40	124.53
23	B	610	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	c	501	CLA	CMB-C2B-C3B	2.79	129.90	124.68
39	s	601	CHL	C4D-CHA-C1A	2.79	124.64	121.25
40	y	317	LUT	C16-C1-C6	-2.79	105.78	110.30
23	R	610	CLA	CMB-C2B-C3B	2.78	129.89	124.68
40	Y	316	LUT	C16-C1-C6	-2.78	105.78	110.30
23	y	313	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	n	611	CLA	CMB-C2B-C3B	2.78	129.88	124.68
40	r	613	LUT	C16-C1-C6	-2.78	105.79	110.30
23	G	614	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	c	507	CLA	CMB-C2B-C3B	2.78	129.87	124.68
38	f	501	HEM	C4D-ND-C1D	2.78	107.94	105.07
40	N	615	LUT	C18-C5-C6	-2.77	121.41	124.53
40	S	614	LUT	C16-C1-C6	-2.77	105.80	110.30
23	N	611	CLA	CMB-C2B-C3B	2.77	129.87	124.68
23	G	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	n	603	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	G	613	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	C	507	CLA	CMB-C2B-C3B	2.77	129.85	124.68
31	b	624	LNL	C15-C14-C13	-2.77	98.41	112.02
35	C	523	VIV	C12-C5-C4	-2.76	117.04	121.30
40	Y	316	LUT	C30-C31-C32	2.76	131.84	123.22
23	R	611	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	s	608	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	g	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	a	406	PHO	O1D-CGD-CBD	2.76	129.33	124.74
26	A	408	SQD	O8-S-C6	2.76	110.14	105.74
23	G	610	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	R	608	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	r	612	CLA	CMB-C2B-C3B	2.76	129.83	124.68
24	A	405	PHO	O2D-CGD-O1D	-2.75	118.45	123.84
23	b	606	CLA	CMB-C2B-C3B	2.75	129.83	124.68
42	Y	301	XAT	C16-C1-C6	-2.75	102.61	110.05
40	N	615	LUT	C16-C1-C6	-2.75	105.83	110.30
23	c	507	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	b	618	BCR	C15-C16-C17	-2.75	117.83	123.47
42	n	620	XAT	C37-C21-C36	-2.75	103.31	107.37
23	s	612	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	S	610	CLA	CMB-C2B-C3B	2.75	129.83	124.68
39	N	601	CHL	C2A-C1A-CHA	2.75	128.67	123.86
39	G	601	CHL	C4D-CHA-C1A	2.75	124.60	121.25
42	N	619	XAT	C15-C14-C13	2.75	131.24	127.31
23	S	612	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	G	611	CLA	CMB-C2B-C3B	2.75	129.82	124.68
41	S	617	NEX	C5-C6-C1	-2.75	116.97	119.70
41	r	614	NEX	C15-C35-C34	2.75	129.10	123.47
23	s	610	CLA	CMB-C2B-C3B	2.74	129.81	124.68
40	N	616	LUT	C16-C1-C6	-2.74	105.85	110.30
24	a	406	PHO	O2D-CGD-O1D	-2.74	118.48	123.84
40	S	614	LUT	C31-C30-C29	2.74	131.22	127.31
23	S	613	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
40	r	613	LUT	C30-C31-C32	2.74	131.77	123.22
39	G	606	CHL	C2A-C1A-CHA	2.74	128.65	123.86
39	R	605	CHL	C2A-C1A-CHA	2.74	128.65	123.86
23	g	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
41	R	618	NEX	O24-C25-C38	-2.74	111.77	115.06
39	r	605	CHL	C2A-C1A-CHA	2.74	128.65	123.86
25	B	618	BCR	C15-C14-C13	-2.74	123.40	127.31
39	G	609	CHL	C4D-CHA-C1A	2.74	124.58	121.25
41	Y	317	NEX	C5-C6-C1	-2.74	116.98	119.70
39	g	609	CHL	C2A-C1A-CHA	2.74	128.64	123.86
40	y	317	LUT	C30-C31-C32	2.74	131.76	123.22
39	g	606	CHL	C2A-C1A-CHA	2.73	128.64	123.86
23	R	612	CLA	CMB-C2B-C3B	2.73	129.79	124.68
40	n	615	LUT	C18-C5-C6	-2.73	121.46	124.53
23	y	314	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
33	d	411	DGD	O6D-C1D-O3G	-2.73	103.50	109.97
39	N	608	CHL	C2A-C1A-CHA	2.73	128.64	123.86
40	s	615	LUT	C30-C31-C32	2.73	131.75	123.22
39	g	601	CHL	C2A-C1A-CHA	2.73	128.64	123.86
25	h	501	BCR	C24-C23-C22	-2.73	122.11	126.23
42	R	615	XAT	C37-C21-C26	2.73	117.42	110.05
40	y	317	LUT	C18-C5-C6	-2.73	121.46	124.53
40	G	615	LUT	C35-C34-C33	2.73	131.20	127.31
40	G	615	LUT	C10-C11-C12	2.73	131.73	123.22
39	G	601	CHL	C2A-C1A-CHA	2.73	128.63	123.86
39	R	606	CHL	C2A-C1A-CHA	2.73	128.63	123.86
40	Y	316	LUT	C18-C5-C6	-2.72	121.47	124.53
42	Y	301	XAT	C36-C21-C26	-2.72	102.69	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	615	LUT	C15-C14-C13	2.72	131.20	127.31
33	c	515	DGD	CDB-CCB-CBB	-2.72	100.60	114.42
40	G	615	LUT	C39-C29-C28	-2.72	113.79	118.08
41	g	617	NEX	C1-C2-C3	-2.72	107.50	113.64
40	S	615	LUT	C16-C1-C6	-2.72	105.89	110.30
39	G	607	CHL	C2A-C1A-CHA	2.72	128.61	123.86
39	Y	308	CHL	C4D-CHA-C1A	2.72	124.56	121.25
39	y	303	CHL	C4D-CHA-C1A	2.72	124.55	121.25
39	g	607	CHL	C2A-C1A-CHA	2.71	128.60	123.86
39	n	605	CHL	CHB-C4A-NA	2.71	128.26	124.51
25	d	410	BCR	C27-C26-C25	2.71	126.67	122.73
40	n	616	LUT	C16-C1-C6	-2.71	105.90	110.30
26	L	101	SQD	O48-C23-C24	2.71	120.41	111.91
42	y	302	XAT	C16-C1-C6	-2.71	102.73	110.05
31	B	623	LNL	C15-C14-C13	-2.71	98.68	112.02
39	N	607	CHL	C2A-C1A-CHA	2.71	128.59	123.86
40	N	616	LUT	C30-C31-C32	2.71	131.66	123.22
33	d	411	DGD	CDB-CCB-CBB	-2.70	100.69	114.42
40	r	613	LUT	C10-C11-C12	2.70	131.65	123.22
33	H	502	DGD	CDB-CCB-CBB	-2.70	100.70	114.42
23	B	615	CLA	CMB-C2B-C3B	2.70	129.73	124.68
39	y	309	CHL	C2A-C1A-CHA	2.70	128.58	123.86
33	H	502	DGD	O6D-C1D-O3G	-2.70	103.58	109.97
39	n	606	CHL	C2A-C1A-CHA	2.70	128.58	123.86
25	H	501	BCR	C27-C26-C25	2.70	126.65	122.73
23	a	403	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	b	615	CLA	CHB-C4A-NA	2.70	128.24	124.51
33	C	515	DGD	CDB-CCB-CBB	-2.69	100.75	114.42
23	b	613	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
39	n	608	CHL	C2A-C1A-CHA	2.69	128.57	123.86
25	k	101	BCR	C24-C23-C22	-2.69	122.17	126.23
23	N	613	CLA	CHB-C4A-NA	2.69	128.24	124.51
39	Y	308	CHL	C2A-C1A-CHA	2.69	128.56	123.86
23	D	406	CLA	CMB-C2B-C3B	2.69	129.70	124.68
25	b	618	BCR	C15-C14-C13	-2.69	123.48	127.31
41	Y	317	NEX	C30-C31-C32	2.68	131.59	123.22
25	H	501	BCR	C24-C23-C22	-2.68	122.18	126.23
25	k	101	BCR	C15-C16-C17	-2.68	117.98	123.47
39	n	607	CHL	C2A-C1A-CHA	2.68	128.55	123.86
23	A	402	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	K	101	BCR	C24-C23-C22	-2.68	122.19	126.23
39	r	607	CHL	C2A-C1A-CHA	2.67	128.53	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Y	315	LUT	C16-C1-C6	-2.67	105.96	110.30
41	r	614	NEX	O24-C25-C38	-2.67	111.85	115.06
25	h	501	BCR	C27-C26-C25	2.67	126.61	122.73
40	s	615	LUT	C16-C1-C6	-2.67	105.97	110.30
39	n	605	CHL	C4D-CHA-C1A	2.67	124.50	121.25
33	C	515	DGD	O5D-C6D-C5D	-2.67	104.11	109.05
39	y	309	CHL	C4D-CHA-C1A	2.67	124.50	121.25
39	Y	307	CHL	C2A-C1A-CHA	2.67	128.52	123.86
23	C	507	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	C	513	CLA	CHB-C4A-NA	2.66	128.20	124.51
26	a	409	SQD	O48-C23-C24	2.66	120.26	111.91
42	Y	301	XAT	C17-C1-C6	2.66	117.23	110.05
26	M	101	SQD	O8-S-C6	2.66	109.98	105.74
23	B	615	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	s	609	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
30	D	408	LHG	O7-C7-C8	2.66	117.23	111.50
42	r	615	XAT	C37-C21-C26	2.66	117.22	110.05
26	A	408	SQD	O48-C23-C24	2.66	120.24	111.91
39	y	310	CHL	C2A-C1A-CHA	2.65	128.50	123.86
23	d	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	N	613	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
39	s	605	CHL	C2A-C1A-CHA	2.65	128.49	123.86
23	S	609	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
39	G	608	CHL	C2A-C1A-CHA	2.64	128.48	123.86
23	B	605	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
40	g	616	LUT	C18-C5-C6	-2.64	121.56	124.53
40	s	614	LUT	C31-C32-C33	2.64	133.83	126.42
23	G	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	n	605	CHL	C3B-C4B-NB	-2.64	105.80	109.21
39	n	601	CHL	C4D-CHA-C1A	2.64	124.46	121.25
26	M	101	SQD	O48-C23-C24	2.64	120.18	111.91
23	B	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
39	G	608	CHL	C4D-CHA-C1A	2.63	124.45	121.25
42	n	620	XAT	C15-C14-C13	2.63	131.06	127.31
38	f	501	HEM	C4B-CHC-C1C	2.63	126.03	122.56
39	g	609	CHL	C1-C2-C3	-2.63	121.50	126.04
39	s	607	CHL	C2A-C1A-CHA	2.62	128.44	123.86
25	v	101	BCR	C33-C5-C6	-2.62	121.58	124.53
41	N	617	NEX	O24-C25-C38	-2.62	111.91	115.06
39	n	609	CHL	C2A-C1A-CHA	2.62	128.44	123.86
40	g	615	LUT	C39-C29-C28	-2.62	113.95	118.08
39	g	601	CHL	C4D-CHA-C1A	2.62	124.44	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	BCR	C15-C16-C17	-2.62	118.11	123.47
40	r	613	LUT	C31-C32-C33	2.62	133.77	126.42
40	y	316	LUT	C16-C1-C6	-2.62	106.06	110.30
42	n	617	XAT	C15-C14-C13	2.61	131.04	127.31
23	D	406	CLA	CHB-C4A-NA	2.61	128.13	124.51
42	R	615	XAT	O4-C5-C6	-2.61	56.79	58.96
42	R	615	XAT	C31-C32-C33	2.61	133.76	126.42
39	N	606	CHL	C4D-CHA-C1A	2.61	124.43	121.25
42	Y	301	XAT	C35-C34-C33	2.61	131.04	127.31
40	R	613	LUT	C38-C25-C24	-2.61	117.97	123.56
42	N	619	XAT	C37-C21-C36	-2.61	103.52	107.37
39	N	609	CHL	C4D-CHA-C1A	2.61	124.43	121.25
42	r	615	XAT	O4-C5-C6	-2.61	56.80	58.96
23	B	601	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	f	501	HEM	C1B-NB-C4B	2.61	107.77	105.07
23	g	610	CLA	C1-C2-C3	-2.61	121.53	126.04
41	n	618	NEX	O24-C25-C38	-2.61	111.93	115.06
38	f	501	HEM	C4C-CHD-C1D	2.60	125.99	122.56
40	y	317	LUT	C31-C32-C33	2.60	133.73	126.42
23	c	506	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
33	C	515	DGD	C3G-C2G-C1G	-2.60	105.63	111.79
23	C	501	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	y	305	CLA	CHB-C4A-NA	2.60	128.11	124.51
41	Y	317	NEX	O24-C25-C38	-2.60	111.94	115.06
33	c	515	DGD	O5D-C6D-C5D	-2.60	104.24	109.05
38	F	501	HEM	C1B-NB-C4B	2.60	107.76	105.07
39	r	606	CHL	C2A-C1A-CHA	2.60	128.40	123.86
39	N	605	CHL	C3B-C4B-NB	-2.60	105.85	109.21
39	S	606	CHL	C2A-C1A-CHA	2.60	128.40	123.86
25	H	501	BCR	C33-C5-C6	-2.59	121.61	124.53
42	n	620	XAT	C35-C15-C14	2.59	128.78	123.47
23	r	608	CLA	CHB-C4A-NA	2.59	128.09	124.51
40	G	616	LUT	C16-C1-C6	-2.59	106.10	110.30
23	C	506	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
42	r	615	XAT	C31-C32-C33	2.59	133.69	126.42
23	c	501	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	N	606	CHL	C2A-C1A-CHA	2.58	128.38	123.86
35	C	523	VIV	C11-C10-C3	2.58	115.80	111.75
41	N	617	NEX	C35-C34-C33	-2.58	123.62	127.31
39	Y	309	CHL	C4D-CHA-C1A	2.58	124.39	121.25
40	S	615	LUT	C31-C32-C33	2.58	133.67	126.42
23	C	506	CLA	O2D-CGD-O1D	-2.58	118.79	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	608	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	b	601	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	B	601	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
23	B	612	CLA	CHB-C4A-NA	2.58	128.08	124.51
40	g	615	LUT	C12-C13-C14	2.58	122.90	118.94
41	R	618	NEX	C30-C31-C32	2.58	131.26	123.22
40	y	316	LUT	C10-C11-C12	2.58	131.26	123.22
42	N	619	XAT	C35-C15-C14	2.57	128.75	123.47
40	y	317	LUT	C39-C29-C28	-2.57	114.02	118.08
40	Y	315	LUT	C10-C11-C12	2.57	131.25	123.22
25	z	101	BCR	C15-C16-C17	-2.57	118.20	123.47
42	y	302	XAT	C17-C1-C6	2.57	116.99	110.05
23	C	502	CLA	CHB-C4A-NA	2.57	128.07	124.51
39	y	308	CHL	C2A-C1A-CHA	2.57	128.35	123.86
25	h	501	BCR	C33-C5-C6	-2.57	121.64	124.53
23	S	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
40	S	614	LUT	C31-C32-C33	2.57	133.62	126.42
23	s	613	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
25	V	101	BCR	C33-C5-C6	-2.56	121.65	124.53
23	a	407	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	A	402	CLA	O2D-CGD-CBD	2.56	115.82	111.27
40	Y	315	LUT	C30-C31-C32	2.56	131.21	123.22
42	Y	301	XAT	C30-C31-C32	2.56	131.21	123.22
40	Y	316	LUT	C39-C29-C28	-2.56	114.05	118.08
23	c	506	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
40	R	613	LUT	C31-C32-C33	2.56	133.60	126.42
39	R	607	CHL	C2A-C1A-CHA	2.56	128.33	123.86
42	n	620	XAT	O4-C5-C6	-2.56	56.84	58.96
25	D	411	BCR	C15-C16-C17	-2.56	118.24	123.47
23	G	603	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	a	403	CLA	O2D-CGD-CBD	2.55	115.80	111.27
40	Y	316	LUT	C31-C32-C33	2.55	133.58	126.42
40	y	316	LUT	C30-C31-C32	2.55	131.17	123.22
23	b	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	B	603	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	g	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
40	g	616	LUT	C30-C31-C32	2.55	131.17	123.22
23	S	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	r	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	Z	101	BCR	C27-C26-C25	2.54	126.42	122.73
25	b	618	BCR	C27-C26-C25	2.54	126.42	122.73
25	b	619	BCR	C24-C23-C22	-2.54	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	N	619	XAT	O4-C5-C6	-2.54	56.85	58.96
23	G	602	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	b	607	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	B	616	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	s	611	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	c	502	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	Y	309	CHL	C2A-C1A-CHA	2.54	128.30	123.86
25	Z	101	BCR	C15-C16-C17	-2.54	118.28	123.47
38	F	501	HEM	C4C-CHD-C1D	2.54	125.91	122.56
40	n	615	LUT	C17-C1-C6	2.54	114.41	110.30
23	Y	304	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	n	603	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	G	609	CHL	C3B-C4B-NB	-2.53	105.93	109.21
23	a	404	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	b	613	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	b	616	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	N	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
39	S	605	CHL	C2A-C1A-CHA	2.53	128.29	123.86
25	z	101	BCR	C24-C23-C22	-2.53	122.41	126.23
40	S	614	LUT	C22-C23-C24	-2.53	108.86	111.74
23	B	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
41	n	618	NEX	C35-C34-C33	-2.53	123.70	127.31
39	n	606	CHL	C4D-CHA-C1A	2.53	124.33	121.25
39	y	303	CHL	C2A-C1A-CHA	2.53	128.28	123.86
23	C	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	b	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
40	G	616	LUT	C18-C5-C6	-2.53	121.69	124.53
23	S	613	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
40	G	616	LUT	C30-C31-C32	2.52	131.09	123.22
39	n	609	CHL	C4D-CHA-C1A	2.52	124.32	121.25
23	A	403	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	C	511	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	N	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	y	310	CHL	C4D-CHA-C1A	2.52	124.31	121.25
23	n	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
40	g	616	LUT	C16-C1-C6	-2.52	106.21	110.30
25	v	101	BCR	C24-C23-C22	-2.52	122.43	126.23
25	B	618	BCR	C27-C26-C25	2.52	126.39	122.73
23	b	603	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	S	610	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	R	611	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	S	604	CLA	CHB-C4A-NA	2.51	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	s	604	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	C	508	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	s	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	Y	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	B	619	BCR	C24-C23-C22	-2.51	122.44	126.23
42	R	615	XAT	C35-C15-C14	2.51	128.62	123.47
23	c	504	CLA	CHB-C4A-NA	2.51	127.98	124.51
42	r	615	XAT	C35-C15-C14	2.51	128.61	123.47
23	R	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	s	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	z	101	BCR	C27-C26-C25	2.51	126.37	122.73
23	A	406	CLA	CHB-C4A-NA	2.51	127.98	124.51
39	N	609	CHL	C2A-C1A-CHA	2.51	128.24	123.86
40	Y	315	LUT	C35-C34-C33	2.50	130.88	127.31
33	c	515	DGD	C3G-C2G-C1G	-2.50	105.86	111.79
23	B	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	r	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	V	101	BCR	C24-C23-C22	-2.50	122.45	126.23
23	r	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	A	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	g	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	K	101	BCR	C33-C5-C6	-2.50	121.72	124.53
25	C	514	BCR	C15-C16-C17	-2.50	118.35	123.47
23	Y	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	Z	101	BCR	C24-C23-C22	-2.50	122.46	126.23
23	c	511	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	B	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	a	403	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	G	610	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	n	612	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
23	g	604	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
23	B	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	r	609	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
23	y	313	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	R	609	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
40	y	316	LUT	C38-C25-C24	-2.49	118.24	123.56
23	c	503	CLA	CHB-C4A-NA	2.49	127.95	124.51
42	G	619	XAT	C31-C32-C33	2.49	133.40	126.42
25	c	514	BCR	C15-C16-C17	-2.49	118.38	123.47
23	y	304	CLA	CHB-C4A-NA	2.48	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	y	316	LUT	C18-C5-C6	-2.48	121.74	124.53
23	N	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	n	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
39	g	609	CHL	C4D-CHA-C1A	2.48	124.27	121.25
23	S	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
40	G	615	LUT	C17-C1-C6	2.48	114.32	110.30
23	r	603	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	a	405	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	b	602	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	R	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	C	503	CLA	CHB-C4A-NA	2.48	127.94	124.51
40	g	615	LUT	C17-C1-C6	2.48	114.32	110.30
23	C	501	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	y	315	CLA	CHB-C4A-NA	2.48	127.94	124.51
40	Y	315	LUT	C38-C25-C24	-2.48	118.26	123.56
23	s	608	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	k	101	BCR	C33-C5-C6	-2.47	121.75	124.53
23	N	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	s	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	R	604	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	B	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	Y	310	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	N	610	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	A	402	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	n	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	Y	305	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
39	s	606	CHL	C2A-C1A-CHA	2.47	128.18	123.86
23	b	606	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
23	c	501	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
23	Y	311	CLA	CHB-C4A-NA	2.47	127.92	124.51
39	Y	302	CHL	C2A-C1A-CHA	2.47	128.17	123.86
23	S	602	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	c	509	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	c	510	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	S	608	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	y	312	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
40	n	616	LUT	C30-C31-C32	2.46	130.90	123.22
23	n	611	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	g	610	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	c	514	BCR	C11-C10-C9	-2.46	123.80	127.31
23	n	610	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	y	306	CLA	C1B-CHB-C4A	-2.46	125.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	r	614	NEX	C35-C34-C33	-2.46	123.80	127.31
23	S	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	b	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	n	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
40	y	316	LUT	C35-C34-C33	2.45	130.81	127.31
23	R	612	CLA	CHB-C4A-NA	2.45	127.91	124.51
23	Y	314	CLA	CHB-C4A-NA	2.45	127.91	124.51
40	r	613	LUT	C3-C4-C5	2.45	116.74	111.85
23	D	405	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	s	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	s	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
39	Y	302	CHL	C4D-CHA-C1A	2.45	124.23	121.25
23	R	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	c	507	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
41	R	614	NEX	O24-C25-C38	-2.45	112.12	115.06
30	D	408	LHG	O8-C23-O10	-2.45	117.42	123.59
23	R	601	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	c	508	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	G	604	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	Y	314	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	C	508	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
25	A	407	BCR	C15-C14-C13	-2.44	123.82	127.31
25	a	408	BCR	C15-C14-C13	-2.44	123.82	127.31
23	b	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
41	g	617	NEX	C5-C6-C1	-2.44	117.27	119.70
23	a	407	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	b	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	y	311	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	B	608	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	B	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	G	613	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	b	605	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	b	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	B	602	CLA	C1-C2-C3	-2.44	121.83	126.04
23	B	601	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	Y	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
40	g	616	LUT	C38-C25-C24	-2.43	118.35	123.56
23	c	508	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
42	n	620	XAT	C16-C1-C6	-2.43	103.48	110.05
42	n	620	XAT	C31-C30-C29	2.43	130.78	127.31
41	Y	317	NEX	C19-C9-C8	-2.43	113.29	118.93
23	c	513	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	514	BCR	C33-C5-C6	-2.43	121.80	124.53
25	b	617	BCR	C3-C4-C5	-2.43	109.74	114.08
23	C	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	g	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	R	609	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	r	601	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	C	513	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	C	507	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	d	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	C	505	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	g	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	B	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	G	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	c	505	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	N	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	r	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	C	509	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
40	R	613	LUT	C3-C4-C5	2.42	116.67	111.85
23	G	614	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
42	n	617	XAT	C35-C15-C14	2.42	128.43	123.47
42	N	619	XAT	C16-C1-C6	-2.42	103.52	110.05
30	D	408	LHG	O8-C23-C24	2.42	119.49	111.91
23	B	605	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
33	d	411	DGD	C1D-C2D-C3D	-2.42	104.96	110.00
23	G	604	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	G	611	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	g	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	B	606	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	r	610	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	b	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	b	605	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	y	313	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	y	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	n	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	a	405	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	B	605	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	B	608	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
40	n	615	LUT	C38-C25-C24	-2.41	118.41	123.56
25	c	514	BCR	C33-C5-C6	-2.41	121.83	124.53
23	B	602	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
39	g	608	CHL	C4D-CHA-C1A	2.40	124.17	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	314	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	N	604	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	b	619	BCR	C27-C26-C25	2.40	126.22	122.73
25	A	407	BCR	C15-C16-C17	-2.40	118.56	123.47
23	b	611	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	g	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	S	607	CHL	C2A-C1A-CHA	2.40	128.05	123.86
23	A	406	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	B	611	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	N	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	c	514	BCR	C7-C8-C9	-2.40	122.61	126.23
23	b	606	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	Y	312	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	g	610	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
42	Y	301	XAT	C18-C5-C4	2.39	116.97	114.28
23	D	406	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	r	610	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	B	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	N	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	n	604	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	D	411	BCR	C27-C26-C25	2.39	126.20	122.73
23	r	612	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	G	610	CLA	C1-C2-C3	-2.39	121.91	126.04
23	D	405	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	C	506	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	y	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	c	506	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	a	405	CLA	O2D-CGD-CBD	2.38	115.50	111.27
42	y	302	XAT	C18-C5-C4	2.38	116.96	114.28
23	s	604	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	n	610	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	y	315	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	Y	313	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	C	514	BCR	C7-C8-C9	-2.38	122.64	126.23
25	A	407	BCR	C11-C10-C9	-2.38	123.91	127.31
23	g	614	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	C	514	BCR	C27-C26-C25	2.38	126.19	122.73
40	G	616	LUT	C38-C25-C24	-2.38	118.47	123.56
23	c	509	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	b	614	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	d	406	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	d	405	CLA	CHB-C4A-NA	2.38	127.80	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C27-C26-C25	2.38	126.18	122.73
23	N	613	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	Y	311	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
23	Y	305	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	A	407	BCR	C33-C5-C6	-2.37	121.86	124.53
23	B	606	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	C	513	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
23	r	608	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	a	408	BCR	C15-C16-C17	-2.37	118.61	123.47
35	y	301	VIV	C12-C5-C4	-2.37	117.64	121.30
42	n	617	XAT	C36-C21-C26	-2.37	103.64	110.05
23	S	604	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	b	609	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	R	608	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	r	604	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	A	404	CLA	O2D-CGD-CBD	2.37	115.47	111.27
23	B	606	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
25	b	618	BCR	C33-C5-C6	-2.36	121.87	124.53
23	A	403	CLA	CHD-C1D-ND	-2.36	122.28	124.45
23	A	404	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	R	604	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
40	g	615	LUT	C8-C9-C10	2.36	122.56	118.94
40	G	615	LUT	C18-C5-C6	-2.36	121.88	124.53
23	R	612	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	G	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	y	306	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	B	619	BCR	C27-C26-C25	2.36	126.16	122.73
40	n	615	LUT	C30-C31-C32	2.36	130.58	123.22
25	B	617	BCR	C27-C26-C25	2.36	126.16	122.73
23	r	612	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	S	611	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	C	509	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
40	S	614	LUT	C3-C4-C5	2.35	116.54	111.85
25	a	408	BCR	C33-C5-C6	-2.35	121.89	124.53
23	b	601	CLA	C1-C2-C3	-2.35	122.95	126.75
41	r	614	NEX	C30-C31-C32	2.35	130.56	123.22
40	N	615	LUT	C30-C31-C32	2.35	130.55	123.22
40	g	615	LUT	C18-C5-C6	-2.35	121.89	124.53
42	Y	301	XAT	C31-C30-C29	2.35	130.66	127.31
33	H	502	DGD	C1D-C2D-C3D	-2.35	105.11	110.00
23	c	512	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	s	602	CLA	C1B-CHB-C4A	-2.35	125.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	R	614	NEX	C30-C31-C32	2.34	130.53	123.22
23	B	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	s	608	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	a	408	BCR	C27-C26-C25	2.34	126.13	122.73
23	s	611	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
41	N	617	NEX	C30-C31-C32	2.34	130.52	123.22
39	Y	306	CHL	C3B-C4B-NB	-2.34	106.19	109.21
23	s	609	CLA	CHB-C4A-NA	2.34	127.74	124.51
23	C	504	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
35	C	523	VIV	O1-C4-C3	2.34	124.79	122.36
41	s	617	NEX	C35-C34-C33	-2.33	123.95	127.30
23	C	512	CLA	CHB-C4A-NA	2.33	127.74	124.51
42	N	619	XAT	C36-C21-C26	-2.33	103.74	110.05
39	y	307	CHL	C3B-C4B-NB	-2.33	106.19	109.21
42	R	615	XAT	C31-C30-C29	2.33	130.64	127.31
23	g	610	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	B	614	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	A	408	SQD	O5-C5-C4	2.33	113.92	109.69
23	N	614	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	N	612	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
42	r	615	XAT	C31-C30-C29	2.33	130.63	127.31
39	s	601	CHL	C3B-C4B-NB	-2.33	106.20	109.21
23	a	404	CLA	CHD-C1D-ND	-2.33	122.32	124.45
23	c	513	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
25	a	408	BCR	C11-C10-C9	-2.32	124.00	127.31
41	G	617	NEX	C14-C15-C35	2.32	131.38	125.55
23	A	403	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
39	g	605	CHL	C3B-C4B-NB	-2.32	106.21	109.21
23	b	610	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	n	611	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	B	610	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	b	609	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	c	504	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	g	613	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	C	502	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	a	404	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
40	S	614	LUT	C38-C25-C24	-2.31	118.61	123.56
42	y	302	XAT	C30-C31-C32	2.31	130.43	123.22
40	r	613	LUT	C4-C5-C6	2.31	126.00	120.85
23	s	610	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
39	r	605	CHL	CMB-C2B-C3B	2.31	129.00	124.68
23	B	604	CLA	C1-C2-C3	-2.31	122.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	B	609	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
40	s	615	LUT	C3-C4-C5	2.31	116.45	111.85
41	n	618	NEX	C30-C31-C32	2.31	130.42	123.22
23	R	610	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
40	s	614	LUT	C3-C4-C5	2.30	116.44	111.85
23	y	315	CLA	C1-C2-C3	-2.30	122.06	126.04
23	N	611	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	n	602	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
41	R	614	NEX	C35-C34-C33	-2.30	124.03	127.31
23	S	602	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
39	G	606	CHL	C3B-C4B-NB	-2.30	106.24	109.21
40	S	614	LUT	C17-C1-C6	2.30	114.02	110.30
23	b	601	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	Y	310	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
41	g	617	NEX	O24-C25-C38	-2.29	112.31	115.06
39	g	606	CHL	C3B-C4B-NB	-2.29	106.25	109.21
25	k	101	BCR	C15-C14-C13	-2.29	124.04	127.31
23	c	502	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	S	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	b	606	CLA	CHB-C4A-NA	2.29	127.68	124.51
28	T	101	3PH	O13-P-O11	-2.29	100.63	106.73
25	b	617	BCR	C27-C26-C25	2.29	126.06	122.73
38	F	501	HEM	CMC-C2C-C3C	2.29	128.96	124.68
40	N	615	LUT	C38-C25-C24	-2.29	118.66	123.56
39	S	601	CHL	C3B-C4B-NB	-2.29	106.25	109.21
39	s	605	CHL	CMB-C2B-C3B	2.29	128.96	124.68
25	A	407	BCR	C27-C26-C25	2.29	126.05	122.73
40	R	613	LUT	C39-C29-C28	-2.29	114.47	118.08
25	Z	101	BCR	C33-C5-C6	-2.29	121.96	124.53
23	g	613	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
33	C	515	DGD	C1D-C2D-C3D	-2.28	105.24	110.00
23	y	305	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
40	S	615	LUT	C38-C25-C24	-2.28	118.67	123.56
23	s	602	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	G	602	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	G	612	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
40	r	613	LUT	C38-C25-C24	-2.28	118.68	123.56
39	S	605	CHL	CMB-C2B-C3B	2.28	128.94	124.68
42	n	617	XAT	C31-C32-C33	2.28	132.82	126.42
23	n	613	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
39	G	605	CHL	C3B-C4B-NB	-2.28	106.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	603	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	S	610	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
33	c	515	DGD	C1D-C2D-C3D	-2.28	105.25	110.00
23	N	602	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
42	G	619	XAT	C35-C15-C14	2.27	128.13	123.47
23	b	611	CLA	CHD-C1D-ND	-2.27	122.36	124.45
25	z	101	BCR	C33-C5-C6	-2.27	121.98	124.53
23	g	603	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
40	r	613	LUT	C17-C1-C6	2.27	113.98	110.30
42	R	615	XAT	C18-C5-C4	2.27	116.83	114.28
23	G	611	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
42	r	615	XAT	C18-C5-C4	2.27	116.83	114.28
25	V	101	BCR	C27-C26-C25	2.27	126.02	122.73
23	b	604	CLA	C1-C2-C3	-2.27	122.12	126.04
23	a	403	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
23	N	603	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
23	b	607	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
23	G	613	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	B	611	CLA	CHD-C1D-ND	-2.26	122.37	124.45
23	g	611	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	Y	304	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
28	L	102	3PH	O13-P-O11	-2.26	100.72	106.73
24	A	405	PHO	C1-C2-C3	-2.26	122.14	126.04
23	A	402	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	S	612	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	y	304	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
40	Y	315	LUT	C18-C5-C6	-2.26	121.99	124.53
40	g	615	LUT	C38-C25-C24	-2.26	118.73	123.56
23	n	614	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
23	b	616	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
28	W	201	3PH	O13-P-O11	-2.25	100.74	106.73
23	Y	313	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
39	N	606	CHL	CMB-C2B-C3B	2.25	128.89	124.68
23	y	314	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	g	602	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
40	S	615	LUT	C39-C29-C28	-2.25	114.53	118.08
25	b	619	BCR	C11-C10-C9	-2.25	124.10	127.31
23	N	613	CLA	C1-C2-C3	-2.25	122.16	126.04
23	C	510	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	R	603	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	c	510	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	Y	303	CLA	C1B-CHB-C4A	-2.24	125.67	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	616	LUT	C38-C25-C24	-2.24	118.76	123.56
25	c	514	BCR	C15-C14-C13	-2.24	124.11	127.31
25	K	101	BCR	C15-C14-C13	-2.24	124.11	127.31
23	y	311	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
23	R	601	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
30	S	616	LHG	O8-C23-C24	2.24	118.94	111.91
23	N	610	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
38	F	501	HEM	C3D-C4D-ND	-2.24	107.67	110.17
25	v	101	BCR	C27-C26-C25	2.24	125.98	122.73
30	d	404	LHG	O8-C23-C24	2.24	118.92	111.91
23	B	607	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
28	A	410	3PH	O13-P-O11	-2.24	100.78	106.73
25	d	410	BCR	C11-C10-C9	-2.24	124.12	127.31
33	C	515	DGD	CFB-CEB-CDB	-2.23	103.08	114.42
23	R	611	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
28	C	524	3PH	O13-P-O11	-2.23	100.79	106.73
41	g	617	NEX	C30-C31-C32	2.23	130.19	123.22
25	d	410	BCR	C15-C16-C17	-2.23	118.90	123.47
23	r	611	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
38	f	501	HEM	CMC-C2C-C3C	2.23	128.85	124.68
39	n	606	CHL	CMB-C2B-C3B	2.23	128.85	124.68
23	n	610	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	C	510	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	B	616	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
40	N	615	LUT	C17-C1-C6	2.23	113.92	110.30
33	H	502	DGD	CBB-CAB-C9B	-2.23	103.11	114.42
42	N	619	XAT	C31-C30-C29	2.23	130.49	127.31
39	r	607	CHL	CAA-C2A-C1A	2.23	119.27	111.97
30	R	616	LHG	O8-C23-C24	2.23	118.90	111.91
39	g	605	CHL	CMB-C2B-C3B	2.23	128.84	124.68
23	R	602	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
33	d	411	DGD	C3G-C2G-C1G	-2.22	106.53	111.79
23	C	503	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
42	y	302	XAT	C31-C32-C33	2.22	132.66	126.42
41	G	617	NEX	C30-C31-C32	2.22	130.15	123.22
23	B	604	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	s	603	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	B	615	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	b	611	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	b	615	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	r	601	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
40	G	615	LUT	C38-C25-C24	-2.22	118.82	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
23	a	407	CLA	C1-C2-C3	-2.22	122.21	126.04
23	b	606	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	G	614	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	S	603	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	N	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	R	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	y	306	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	c	505	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	R	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
30	g	618	LHG	O8-C23-C24	2.21	118.84	111.91
23	b	615	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	c	501	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
30	A	412	LHG	O8-C23-C24	2.21	118.83	111.91
23	a	407	CLA	CHD-C1D-ND	-2.21	122.43	124.45
25	z	101	BCR	C15-C14-C13	-2.21	124.16	127.31
23	S	613	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
23	r	602	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	B	608	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	S	608	CLA	CHB-C4A-NA	2.20	127.56	124.51
23	C	501	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
28	w	202	3PH	O13-P-O11	-2.20	100.87	106.73
23	y	312	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	g	603	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	Y	318	LHG	O8-C23-C24	2.20	118.81	111.91
40	s	614	LUT	C17-C1-C6	2.20	113.86	110.30
30	d	408	LHG	O8-C23-C24	2.20	118.81	111.91
23	r	603	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
33	H	502	DGD	C3G-C2G-C1G	-2.20	106.59	111.79
39	G	620	CHL	CHA-C1A-NA	-2.20	121.37	126.40
23	B	603	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
23	r	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	n	603	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	r	602	CLA	O2D-CGD-CBD	2.19	115.17	111.27
23	n	602	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	s	612	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
39	g	608	CHL	C3B-C4B-NB	-2.19	106.38	109.21
25	D	411	BCR	C33-C5-C6	-2.19	122.07	124.53
25	b	619	BCR	C33-C5-C6	-2.19	122.07	124.53
23	b	604	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	b	613	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
42	y	302	XAT	C31-C30-C29	2.19	130.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	604	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	C	505	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	N	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	s	613	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
41	s	617	NEX	C40-C33-C34	-2.18	111.09	122.73
23	c	512	CLA	CHD-C1D-ND	-2.18	122.45	124.45
40	y	316	LUT	C12-C13-C14	2.18	122.29	118.94
23	Y	311	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	A	405	PHO	CMC-C2C-C3C	2.18	129.06	124.94
25	C	514	BCR	C15-C14-C13	-2.18	124.20	127.31
40	R	613	LUT	C17-C1-C6	2.18	113.83	110.30
40	y	317	LUT	C38-C25-C24	-2.18	118.89	123.56
23	b	616	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	c	514	BCR	C24-C23-C22	-2.18	122.94	126.23
40	Y	316	LUT	C38-C25-C24	-2.18	118.90	123.56
23	B	612	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
28	X	201	3PH	O13-P-O11	-2.18	100.94	106.73
39	g	605	CHL	CHA-C1A-NA	-2.18	121.41	126.40
33	c	515	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
23	y	312	CLA	O2D-CGD-CBD	2.18	115.13	111.27
23	S	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	B	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
40	s	615	LUT	C38-C25-C24	-2.17	118.91	123.56
23	b	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	y	312	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	D	406	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	S	612	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
39	g	619	CHL	CHA-C1A-NA	-2.17	121.43	126.40
33	C	515	DGD	CBB-CAB-C9B	-2.17	103.42	114.42
40	Y	315	LUT	C17-C1-C6	2.17	113.82	110.30
23	a	404	CLA	C1-C2-C3	-2.17	122.29	126.04
23	B	606	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	B	610	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	Y	305	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	c	510	CLA	CHD-C1D-ND	-2.16	122.47	124.45
40	s	614	LUT	C38-C25-C24	-2.16	118.93	123.56
30	a	412	LHG	O8-C23-C24	2.16	118.69	111.91
23	B	615	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	506	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
40	y	316	LUT	C17-C1-C6	2.16	113.80	110.30
23	c	511	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
41	S	617	NEX	C19-C9-C8	-2.16	113.93	118.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	y	301	VIV	C11-C10-C3	-2.16	108.38	111.75
24	a	406	PHO	CMC-C2C-C3C	2.16	129.01	124.94
23	n	613	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
30	r	616	LHG	O8-C23-C24	2.16	118.67	111.91
41	s	617	NEX	C19-C9-C8	-2.16	113.93	118.93
23	s	610	CLA	C1-C2-C3	-2.15	122.32	126.04
23	s	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
40	S	615	LUT	C3-C4-C5	2.15	116.14	111.85
23	G	613	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	S	609	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	y	313	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	y	305	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	A	406	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	S	610	CLA	C1-C2-C3	-2.15	122.32	126.04
25	D	411	BCR	C24-C23-C22	-2.15	122.98	126.23
25	b	617	BCR	C24-C23-C22	-2.15	122.98	126.23
23	G	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	b	612	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
39	G	607	CHL	CHA-C1A-NA	-2.15	121.47	126.40
39	n	601	CHL	C3B-C4B-NB	-2.15	106.43	109.21
23	B	613	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
41	G	617	NEX	C38-C25-C24	-2.15	111.86	114.28
23	Y	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	C	514	BCR	C24-C23-C22	-2.15	122.99	126.23
23	C	511	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	Y	305	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	b	608	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	b	617	BCR	C8-C7-C6	-2.15	121.18	127.20
39	r	607	CHL	CHA-C1A-NA	-2.14	121.49	126.40
25	Z	101	BCR	C15-C14-C13	-2.14	124.25	127.31
42	Y	301	XAT	C11-C10-C9	2.14	130.37	127.31
23	b	608	CLA	CHD-C1D-ND	-2.14	122.48	124.45
23	n	604	CLA	CHD-C1D-ND	-2.14	122.48	124.45
23	A	403	CLA	C1-C2-C3	-2.14	122.34	126.04
23	C	512	CLA	C1-C2-C3	-2.14	122.34	126.04
25	b	618	BCR	C24-C23-C22	-2.14	123.00	126.23
41	R	614	NEX	C25-C24-C23	-2.14	108.51	112.75
25	k	101	BCR	C27-C26-C25	2.14	125.84	122.73
39	S	601	CHL	CMB-C2B-C3B	2.14	128.68	124.68
39	n	605	CHL	CHD-C1D-C2D	2.14	129.97	125.48
42	n	620	XAT	C36-C21-C26	-2.14	104.27	110.05
39	n	608	CHL	C3B-C4B-NB	-2.14	106.45	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	s	616	LHG	O8-C23-C24	2.14	118.62	111.91
23	g	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	B	612	CLA	C1-C2-C3	-2.14	122.35	126.04
33	c	515	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
39	N	607	CHL	CHA-C1A-NA	-2.14	121.51	126.40
23	r	610	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	G	603	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
42	y	302	XAT	O4-C5-C6	-2.13	57.19	58.96
23	b	613	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
30	N	618	LHG	O8-C23-C24	2.13	118.60	111.91
23	y	304	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	S	613	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	a	407	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	r	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	G	610	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	y	314	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	616	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	G	602	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	g	612	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	g	607	CHL	CHA-C1A-NA	-2.13	121.52	126.40
23	b	606	CLA	C1-C2-C3	-2.13	122.36	126.04
23	s	613	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	c	512	CLA	C1-C2-C3	-2.13	122.36	126.04
33	C	515	DGD	C5B-C4B-C3B	-2.13	103.62	114.42
23	b	609	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	G	608	CHL	C3B-C4B-NB	-2.13	106.46	109.21
25	B	619	BCR	C33-C5-C6	-2.13	122.14	124.53
39	R	606	CHL	CMB-C2B-C3B	2.12	128.65	124.68
23	R	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
39	n	605	CHL	CHA-C1A-NA	-2.12	121.53	126.40
23	y	306	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	b	612	CLA	C1-C2-C3	-2.12	122.37	126.04
41	N	617	NEX	C38-C25-C24	-2.12	111.89	114.28
23	B	608	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	d	406	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	R	601	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	R	612	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	y	311	CLA	C1-C2-C3	-2.12	122.38	126.04
39	Y	308	CHL	C3B-C4B-NB	-2.12	106.47	109.21
40	R	613	LUT	C4-C5-C6	2.12	125.57	120.85
39	R	606	CHL	CHA-C1A-NA	-2.12	121.55	126.40
42	y	302	XAT	C11-C10-C9	2.12	130.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	609	CHL	CMB-C2B-C3B	2.12	128.64	124.68
39	R	607	CHL	CAA-C2A-C1A	2.12	118.92	111.97
23	N	610	CLA	C1-C2-C3	-2.12	122.38	126.04
23	Y	303	CLA	C1-C2-C3	-2.12	122.38	126.04
30	D	404	LHG	O8-C23-C24	2.12	118.55	111.91
25	K	101	BCR	C27-C26-C25	2.12	125.81	122.73
23	G	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	s	609	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	Y	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	G	609	CHL	CHD-C1D-C2D	2.12	129.92	125.48
23	B	616	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	N	609	CHL	CMB-C2B-C3B	2.11	128.63	124.68
35	y	301	VIV	O2-C7-C6	2.11	123.67	118.10
28	x	201	3PH	O13-P-O11	-2.11	101.11	106.73
39	G	620	CHL	C3B-C4B-NB	-2.11	106.48	109.21
39	R	606	CHL	C3B-C4B-NB	-2.11	106.48	109.21
40	y	317	LUT	C17-C1-C6	2.11	113.72	110.30
38	f	501	HEM	C3D-C4D-ND	-2.11	107.82	110.17
39	n	607	CHL	CHA-C1A-NA	-2.11	121.56	126.40
23	s	610	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	h	501	BCR	C38-C26-C25	-2.11	122.16	124.53
23	C	507	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
39	N	601	CHL	C3B-C4B-NB	-2.11	106.48	109.21
23	s	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	b	610	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	A	406	CLA	C1-C2-C3	-2.11	122.40	126.04
23	N	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	Y	310	CLA	C1-C2-C3	-2.11	122.40	126.04
23	c	502	CLA	CHD-C1D-ND	-2.11	122.52	124.45
28	s	618	3PH	O13-P-O11	-2.11	101.13	106.73
23	b	603	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	B	618	BCR	C11-C10-C9	-2.11	124.31	127.31
23	B	609	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
25	b	618	BCR	C11-C10-C9	-2.10	124.31	127.31
41	g	617	NEX	C19-C9-C8	-2.10	114.05	118.93
23	B	603	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	c	508	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
39	N	605	CHL	CHD-C1D-C2D	2.10	129.89	125.48
39	N	608	CHL	C3B-C4B-NB	-2.10	106.49	109.21
30	y	318	LHG	O8-C23-C24	2.10	118.51	111.91
33	C	515	DGD	CAB-C9B-C8B	-2.10	103.75	114.42
25	B	618	BCR	C24-C23-C22	-2.10	123.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	d	402	PHO	CMC-C2C-C3C	2.10	128.91	124.94
23	n	610	CLA	C1-C2-C3	-2.10	122.41	126.04
23	n	614	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
40	Y	315	LUT	C12-C13-C14	2.10	122.17	118.94
23	D	406	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	D	402	PHO	CMC-C2C-C3C	2.10	128.90	124.94
30	n	619	LHG	O8-C23-C24	2.10	118.50	111.91
23	b	603	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
41	r	614	NEX	C25-C24-C23	-2.10	108.59	112.75
42	n	617	XAT	C12-C13-C14	2.10	122.16	118.94
23	g	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
33	d	411	DGD	CBB-CAB-C9B	-2.10	103.78	114.42
25	H	501	BCR	C38-C26-C25	-2.10	122.17	124.53
39	r	607	CHL	C3A-C2A-C1A	2.10	104.48	101.34
23	A	406	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
42	R	615	XAT	C30-C31-C32	2.10	129.75	123.22
23	c	506	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	G	607	CHL	C3B-C4B-NB	-2.09	106.50	109.21
39	y	308	CHL	C3B-C4B-NB	-2.09	106.50	109.21
23	B	607	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	601	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	C	506	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	r	607	CHL	C3B-C4B-NB	-2.09	106.50	109.21
39	g	609	CHL	CAA-C2A-C1A	2.09	118.83	111.97
23	C	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
39	S	607	CHL	CHA-C1A-NA	-2.09	121.61	126.40
23	Y	313	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	N	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	607	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
39	s	601	CHL	CMB-C2B-C3B	2.09	128.59	124.68
41	g	617	NEX	C35-C34-C33	-2.09	124.33	127.31
42	r	615	XAT	C30-C31-C32	2.09	129.74	123.22
23	d	406	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	Y	303	CLA	CHD-C1D-ND	-2.09	122.53	124.45
42	Y	301	XAT	O4-C5-C6	-2.09	57.23	58.96
39	s	606	CHL	C3B-C4B-NB	-2.09	106.51	109.21
23	R	610	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	s	608	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	Y	302	CHL	C1-C2-C3	-2.09	122.43	126.04
25	B	617	BCR	C24-C23-C22	-2.09	123.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	S	603	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
28	D	403	3PH	O13-P-O11	-2.09	101.18	106.73
30	b	627	LHG	O8-C23-C24	2.09	118.45	111.91
23	n	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
39	S	606	CHL	CHA-C1A-NA	-2.08	121.62	126.40
39	s	607	CHL	C3B-C4B-NB	-2.08	106.52	109.21
39	N	601	CHL	CHA-C1A-NA	-2.08	121.63	126.40
39	G	620	CHL	CMB-C2B-C3B	2.08	128.58	124.68
39	g	609	CHL	C3B-C4B-NB	-2.08	106.52	109.21
23	C	506	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	Y	311	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	n	602	CLA	CHD-C1D-ND	-2.08	122.54	124.45
35	C	523	VIV	O2-C7-C6	2.08	123.58	118.10
23	y	315	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	S	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	g	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	R	607	CHL	CHA-C1A-NA	-2.08	121.63	126.40
23	y	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	g	611	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	C	505	CLA	C1-C2-C3	-2.08	122.45	126.04
23	a	405	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	s	605	CHL	CHA-C1A-NA	-2.08	121.64	126.40
39	S	607	CHL	C3B-C4B-NB	-2.08	106.52	109.21
39	G	605	CHL	CHA-C1A-NA	-2.08	121.64	126.40
39	y	303	CHL	C3B-C4B-NB	-2.08	106.52	109.21
23	Y	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	c	511	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	B	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	y	315	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
39	s	601	CHL	CHD-C1D-C2D	2.08	129.84	125.48
39	s	606	CHL	CMB-C2B-C3B	2.08	128.56	124.68
23	N	614	CLA	CHD-C1D-ND	-2.08	122.55	124.45
23	R	608	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	S	601	CHL	CHD-C1D-C2D	2.08	129.83	125.48
23	C	509	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	N	614	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
39	g	619	CHL	C3B-C4B-NB	-2.08	106.53	109.21
30	G	618	LHG	O8-C23-C24	2.07	118.42	111.91
23	g	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	L	103	LHG	O8-C23-C24	2.07	118.42	111.91
39	r	606	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	B	605	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	611	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	c	505	CLA	O2D-CGD-CBD	2.07	114.95	111.27
42	y	302	XAT	C37-C21-C36	-2.07	104.31	107.37
39	R	606	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	b	601	CLA	CHD-C1D-ND	-2.07	122.55	124.45
33	c	515	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
28	d	403	3PH	O13-P-O11	-2.07	101.23	106.73
40	S	614	LUT	C4-C5-C6	2.07	125.46	120.85
23	g	613	CLA	C1-C2-C3	-2.07	122.47	126.04
39	S	601	CHL	CHA-C1A-NA	-2.07	121.67	126.40
39	G	605	CHL	CAA-C2A-C1A	2.07	118.75	111.97
39	N	609	CHL	CHC-C1C-C2C	-2.07	118.62	126.11
40	r	613	LUT	C15-C14-C13	2.07	130.26	127.31
23	c	513	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
39	Y	306	CHL	CHD-C1D-C2D	2.07	129.81	125.48
40	Y	316	LUT	C17-C1-C6	2.06	113.65	110.30
40	g	615	LUT	C10-C11-C12	2.06	129.66	123.22
39	g	606	CHL	C3A-C2A-C1A	2.06	104.43	101.34
23	C	512	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	N	608	CHL	CAA-C2A-C1A	2.06	118.74	111.97
40	G	615	LUT	C40-C33-C32	2.06	121.33	118.08
23	Y	314	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	c	505	CLA	C1-C2-C3	-2.06	122.47	126.04
23	S	602	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
39	s	606	CHL	CHA-C1A-NA	-2.06	121.67	126.40
23	r	611	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	r	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
42	G	619	XAT	C16-C1-C6	-2.06	104.48	110.05
23	S	604	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
39	R	605	CHL	CMB-C2B-C3B	2.06	128.53	124.68
23	n	612	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
40	n	615	LUT	C20-C13-C12	-2.06	114.83	118.08
25	a	408	BCR	C24-C23-C22	-2.06	123.12	126.23
23	b	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	r	606	CHL	CHA-C1A-NA	-2.06	121.68	126.40
39	Y	302	CHL	C3B-C4B-NB	-2.06	106.55	109.21
39	y	307	CHL	CHD-C1D-C2D	2.06	129.79	125.48
23	b	616	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	S	611	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
40	s	615	LUT	C4-C5-C6	2.06	125.43	120.85
23	C	511	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	B	619	BCR	C2-C1-C6	2.06	113.65	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	306	CLA	C1-C2-C3	-2.05	122.49	126.04
23	C	503	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	n	601	CHL	CHD-C1D-C2D	2.05	129.79	125.48
39	y	309	CHL	C3B-C4B-NB	-2.05	106.55	109.21
40	s	614	LUT	C4-C5-C6	2.05	125.43	120.85
39	Y	309	CHL	CHD-C1D-C2D	2.05	129.79	125.48
39	G	607	CHL	CMB-C2B-C3B	2.05	128.52	124.68
23	Y	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	s	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	B	617	BCR	C3-C4-C5	-2.05	110.41	114.08
39	s	607	CHL	CHA-C1A-NA	-2.05	121.70	126.40
39	r	606	CHL	CMB-C2B-C3B	2.05	128.52	124.68
23	B	609	CLA	C1-C2-C3	-2.05	122.50	126.04
39	S	606	CHL	CMB-C2B-C3B	2.05	128.51	124.68
39	g	607	CHL	CMB-C2B-C3B	2.05	128.51	124.68
25	d	410	BCR	C15-C14-C13	-2.05	124.38	127.31
23	C	502	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	c	513	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	n	614	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	C	505	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	y	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	G	605	CHL	CMB-C2B-C3B	2.05	128.51	124.68
39	Y	309	CHL	C3B-C4B-NB	-2.05	106.56	109.21
23	n	602	CLA	C1-C2-C3	-2.05	122.50	126.04
23	N	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	R	605	CHL	CHA-C1A-NA	-2.05	121.71	126.40
39	R	607	CHL	C3B-C4B-NB	-2.05	106.56	109.21
23	r	603	CLA	CHD-C1D-ND	-2.05	122.57	124.45
40	N	615	LUT	C3-C4-C5	2.05	115.93	111.85
39	g	601	CHL	CHD-C1D-C2D	2.05	129.77	125.48
39	s	607	CHL	CHD-C1D-C2D	2.05	129.77	125.48
23	B	613	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
39	r	606	CHL	C3B-C4B-NB	-2.05	106.56	109.21
39	G	606	CHL	CHA-C1A-NA	-2.04	121.72	126.40
39	s	601	CHL	CHA-C1A-NA	-2.04	121.72	126.40
39	y	310	CHL	CHD-C1D-C2D	2.04	129.77	125.48
39	Y	307	CHL	CHA-C1A-NA	-2.04	121.72	126.40
23	B	602	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	K	101	BCR	C11-C10-C9	-2.04	124.39	127.31
23	B	610	CLA	O2D-CGD-CBD	2.04	114.90	111.27
28	a	410	3PH	O13-P-O11	-2.04	101.30	106.73
39	y	308	CHL	CMB-C2B-C3B	2.04	128.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	607	CHL	CHC-C1C-C2C	-2.04	118.70	126.11
23	C	506	CLA	C1-C2-C3	-2.04	122.51	126.04
24	A	405	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
39	n	606	CHL	C3B-C4B-NB	-2.04	106.57	109.21
23	R	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	b	612	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	S	606	CHL	C3B-C4B-NB	-2.04	106.57	109.21
39	g	608	CHL	CHD-C1D-C2D	2.04	129.76	125.48
23	b	605	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	B	612	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	b	619	BCR	C15-C14-C13	-2.04	124.40	127.31
39	n	609	CHL	CHC-C1C-C2C	-2.04	118.72	126.11
39	y	310	CHL	CMB-C2B-C3B	2.04	128.49	124.68
39	r	605	CHL	CHA-C1A-NA	-2.04	121.73	126.40
23	N	603	CLA	C1-C2-C3	-2.04	122.52	126.04
23	B	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	r	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
42	n	617	XAT	C16-C1-C6	-2.04	104.54	110.05
42	Y	301	XAT	C25-C24-C23	-2.04	108.72	112.75
23	S	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
40	N	615	LUT	C4-C5-C6	2.04	125.39	120.85
23	G	611	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	G	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
39	G	601	CHL	CHD-C1D-C2D	2.04	129.75	125.48
39	n	606	CHL	CHD-C1D-C2D	2.04	129.75	125.48
40	n	616	LUT	C38-C25-C24	-2.04	119.20	123.56
23	c	509	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
39	G	605	CHL	CHD-C1D-C2D	2.04	129.75	125.48
39	S	606	CHL	CHD-C1D-C2D	2.04	129.75	125.48
25	B	619	BCR	C15-C16-C17	-2.04	119.31	123.47
39	R	605	CHL	C3B-C4B-NB	-2.04	106.58	109.21
39	Y	302	CHL	CHD-C1D-C2D	2.03	129.75	125.48
42	N	619	XAT	C39-C29-C28	-2.03	114.87	118.08
38	f	501	HEM	C3B-C2B-C1B	2.03	108.00	106.49
39	g	606	CHL	CHA-C1A-NA	-2.03	121.74	126.40
25	D	411	BCR	C15-C14-C13	-2.03	124.41	127.31
25	B	617	BCR	C8-C7-C6	-2.03	121.49	127.20
39	n	609	CHL	CHD-C1D-C2D	2.03	129.74	125.48
39	g	606	CHL	CAA-C2A-C1A	2.03	118.63	111.97
23	g	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	c	502	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	v	101	BCR	C16-C15-C14	-2.03	119.31	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	S	615	LUT	C4-C5-C6	2.03	125.37	120.85
39	Y	307	CHL	C3B-C4B-NB	-2.03	106.59	109.21
39	y	308	CHL	CHA-C1A-NA	-2.03	121.75	126.40
23	G	602	CLA	C1-C2-C3	-2.03	122.53	126.04
23	Y	304	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	n	603	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	R	607	CHL	C3A-C2A-C1A	2.03	104.38	101.34
39	N	606	CHL	C3B-C4B-NB	-2.03	106.59	109.21
23	N	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	Y	307	CHL	CMB-C2B-C3B	2.03	128.47	124.68
39	R	606	CHL	CHD-C1D-C2D	2.03	129.73	125.48
39	n	607	CHL	C3B-C4B-NB	-2.03	106.59	109.21
23	g	603	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
39	S	605	CHL	CHA-C1A-NA	-2.03	121.76	126.40
25	D	411	BCR	C2-C1-C6	2.03	113.60	110.48
23	C	513	CLA	C1-C2-C3	-2.03	122.54	126.04
23	R	608	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
39	N	609	CHL	CHD-C1D-C2D	2.03	129.73	125.48
23	g	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	r	605	CHL	CHD-C1D-C2D	2.02	129.73	125.48
39	R	606	CHL	CAA-C2A-C1A	2.02	118.61	111.97
23	n	611	CLA	CHD-C1D-ND	-2.02	122.59	124.45
42	G	619	XAT	C12-C13-C14	2.02	122.05	118.94
39	R	605	CHL	CHD-C1D-C2D	2.02	129.72	125.48
23	N	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
23	y	305	CLA	CHD-C1D-ND	-2.02	122.59	124.45
23	S	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
39	r	606	CHL	CHD-C1D-C2D	2.02	129.72	125.48
39	N	607	CHL	C3B-C4B-NB	-2.02	106.60	109.21
23	r	602	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
39	n	608	CHL	CHA-C1A-NA	-2.02	121.77	126.40
39	r	607	CHL	CMB-C2B-C3B	2.02	128.46	124.68
23	N	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	y	301	VIV	C15-C16-C17	-2.02	108.62	112.74
39	N	608	CHL	CHA-C1A-NA	-2.02	121.78	126.40
23	B	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	N	611	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	C	502	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	R	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	G	620	CHL	CHD-C1D-C2D	2.02	129.71	125.48
39	G	620	CHL	CAA-C2A-C1A	2.02	118.59	111.97
39	N	601	CHL	CHD-C1D-C2D	2.02	129.71	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C11-C10-C9	-2.02	124.43	127.31
23	n	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
40	Y	315	LUT	C3-C4-C5	2.02	115.87	111.85
39	n	608	CHL	CMB-C2B-C3B	2.02	128.45	124.68
40	N	616	LUT	C17-C1-C6	2.02	113.57	110.30
39	y	303	CHL	CHA-C1A-NA	-2.02	121.78	126.40
39	g	609	CHL	C3A-C2A-C1A	2.02	104.36	101.34
23	b	610	CLA	O2D-CGD-CBD	2.02	114.85	111.27
23	c	507	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
39	n	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
23	c	512	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
40	g	615	LUT	C40-C33-C32	2.01	121.25	118.08
23	b	614	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
39	G	608	CHL	CHD-C1D-C2D	2.01	129.71	125.48
23	A	404	CLA	CHD-C1D-ND	-2.01	122.60	124.45
23	C	509	CLA	CHD-C1D-ND	-2.01	122.60	124.45
23	r	603	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
39	y	303	CHL	CHD-C1D-C2D	2.01	129.70	125.48
39	s	607	CHL	CMB-C2B-C3B	2.01	128.44	124.68
40	s	615	LUT	C17-C1-C6	2.01	113.56	110.30
39	g	609	CHL	CMB-C2B-C3B	2.01	128.44	124.68
23	B	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	c	511	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	V	101	BCR	C16-C15-C14	-2.01	119.36	123.47
23	g	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	c	508	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	r	612	CLA	CHD-C1D-ND	-2.01	122.61	124.45
42	Y	301	XAT	C31-C32-C33	2.01	132.06	126.42
39	S	607	CHL	CHC-C1C-C2C	-2.01	118.83	126.11
23	Y	314	CLA	C1-C2-C3	-2.01	122.57	126.04
41	n	618	NEX	C38-C25-C24	-2.01	112.02	114.28
23	y	304	CLA	C1-C2-C3	-2.01	122.57	126.04
23	b	604	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
39	g	619	CHL	C3A-C2A-C1A	2.01	104.34	101.34
33	d	411	DGD	C1E-O6E-C5E	2.01	117.63	113.69
23	b	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	s	604	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	G	614	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	B	605	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	s	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	y	311	CLA	CHD-C1D-ND	-2.01	122.61	124.45
39	s	605	CHL	CHD-C1D-C2D	2.01	129.69	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
39	y	310	CHL	CHC-C1C-C2C	-2.00	118.84	126.11
39	g	605	CHL	CHD-C1D-C2D	2.00	129.68	125.48
23	c	503	CLA	CHD-C1D-ND	-2.00	122.61	124.45
33	H	502	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
24	d	402	PHO	O2A-CGA-O1A	-2.00	118.54	123.59
23	b	609	CLA	C1-C2-C3	-2.00	122.58	126.04
39	g	619	CHL	CMB-C2B-C3B	2.00	128.42	124.68
23	r	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	N	606	CHL	CHA-C1A-NA	-2.00	121.82	126.40

All (304) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	402	CLA	ND
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	406	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
23	C	507	CLA	ND
23	C	508	CLA	ND

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Mol	Chain	Res	Type	Atom
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	405	CLA	ND
23	D	406	CLA	ND
23	G	602	CLA	ND
23	G	603	CLA	ND
23	G	604	CLA	ND
23	G	610	CLA	ND
23	G	611	CLA	ND
23	G	612	CLA	ND
23	G	613	CLA	ND
23	G	614	CLA	ND
23	N	602	CLA	ND
23	N	603	CLA	ND
23	N	604	CLA	ND
23	N	610	CLA	ND
23	N	611	CLA	ND
23	N	612	CLA	ND
23	N	613	CLA	ND
23	N	614	CLA	ND
23	R	601	CLA	ND
23	R	602	CLA	ND
23	R	603	CLA	ND
23	R	604	CLA	ND
23	R	608	CLA	ND
23	R	609	CLA	ND
23	R	610	CLA	ND
23	R	611	CLA	ND
23	R	612	CLA	ND
23	S	602	CLA	ND
23	S	603	CLA	ND
23	S	604	CLA	ND
23	S	608	CLA	ND
23	S	609	CLA	ND
23	S	610	CLA	ND
23	S	611	CLA	ND
23	S	612	CLA	ND
23	S	613	CLA	ND
23	Y	303	CLA	ND

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Mol	Chain	Res	Type	Atom
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	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	407	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
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	405	CLA	ND
23	d	406	CLA	ND

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Mol	Chain	Res	Type	Atom
23	g	602	CLA	ND
23	g	603	CLA	ND
23	g	604	CLA	ND
23	g	610	CLA	ND
23	g	611	CLA	ND
23	g	612	CLA	ND
23	g	613	CLA	ND
23	g	614	CLA	ND
23	n	602	CLA	ND
23	n	603	CLA	ND
23	n	604	CLA	ND
23	n	610	CLA	ND
23	n	611	CLA	ND
23	n	612	CLA	ND
23	n	613	CLA	ND
23	n	614	CLA	ND
23	r	601	CLA	ND
23	r	602	CLA	ND
23	r	603	CLA	ND
23	r	604	CLA	ND
23	r	608	CLA	ND
23	r	609	CLA	ND
23	r	610	CLA	ND
23	r	611	CLA	ND
23	r	612	CLA	ND
23	s	602	CLA	ND
23	s	603	CLA	ND
23	s	604	CLA	ND
23	s	608	CLA	ND
23	s	609	CLA	ND
23	s	610	CLA	ND
23	s	611	CLA	ND
23	s	612	CLA	ND
23	s	613	CLA	ND
23	y	304	CLA	ND
23	y	305	CLA	ND
23	y	306	CLA	ND
23	y	311	CLA	ND
23	y	312	CLA	ND
23	y	313	CLA	ND
23	y	314	CLA	ND
23	y	315	CLA	ND

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Mol	Chain	Res	Type	Atom
39	G	601	CHL	NA
39	G	601	CHL	NC
39	G	601	CHL	ND
39	G	605	CHL	NA
39	G	605	CHL	NC
39	G	605	CHL	ND
39	G	606	CHL	NA
39	G	606	CHL	NC
39	G	606	CHL	ND
39	G	607	CHL	NA
39	G	607	CHL	NC
39	G	607	CHL	ND
39	G	608	CHL	NA
39	G	608	CHL	NC
39	G	608	CHL	ND
39	G	609	CHL	NA
39	G	609	CHL	NC
39	G	609	CHL	ND
39	G	620	CHL	NA
39	G	620	CHL	NC
39	G	620	CHL	ND
39	N	601	CHL	NA
39	N	601	CHL	NC
39	N	601	CHL	ND
39	N	605	CHL	NA
39	N	605	CHL	NC
39	N	605	CHL	ND
39	N	606	CHL	NA
39	N	606	CHL	NC
39	N	606	CHL	ND
39	N	607	CHL	NA
39	N	607	CHL	NC
39	N	607	CHL	ND
39	N	608	CHL	NA
39	N	608	CHL	NC
39	N	608	CHL	ND
39	N	609	CHL	NA
39	N	609	CHL	NC
39	N	609	CHL	ND
39	R	605	CHL	NA
39	R	605	CHL	NC
39	R	605	CHL	ND

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Mol	Chain	Res	Type	Atom
39	R	606	CHL	NA
39	R	606	CHL	NC
39	R	606	CHL	ND
39	R	607	CHL	NA
39	R	607	CHL	NC
39	R	607	CHL	ND
39	S	601	CHL	NA
39	S	601	CHL	NC
39	S	601	CHL	ND
39	S	605	CHL	NA
39	S	605	CHL	NC
39	S	605	CHL	ND
39	S	606	CHL	NA
39	S	606	CHL	NC
39	S	606	CHL	ND
39	S	607	CHL	NA
39	S	607	CHL	NC
39	S	607	CHL	ND
39	Y	302	CHL	NA
39	Y	302	CHL	NC
39	Y	302	CHL	ND
39	Y	306	CHL	NA
39	Y	306	CHL	NC
39	Y	306	CHL	ND
39	Y	307	CHL	NA
39	Y	307	CHL	NC
39	Y	307	CHL	ND
39	Y	308	CHL	NA
39	Y	308	CHL	NC
39	Y	308	CHL	ND
39	Y	309	CHL	NA
39	Y	309	CHL	NC
39	Y	309	CHL	ND
39	g	601	CHL	NA
39	g	601	CHL	NC
39	g	601	CHL	ND
39	g	605	CHL	NA
39	g	605	CHL	NC
39	g	605	CHL	ND
39	g	606	CHL	NA
39	g	606	CHL	NC
39	g	606	CHL	ND

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Mol	Chain	Res	Type	Atom
39	g	607	CHL	NA
39	g	607	CHL	NC
39	g	607	CHL	ND
39	g	608	CHL	NA
39	g	608	CHL	NC
39	g	608	CHL	ND
39	g	609	CHL	NA
39	g	609	CHL	NC
39	g	609	CHL	ND
39	g	619	CHL	NA
39	g	619	CHL	NC
39	g	619	CHL	ND
39	n	601	CHL	NA
39	n	601	CHL	NC
39	n	601	CHL	ND
39	n	605	CHL	NA
39	n	605	CHL	NC
39	n	605	CHL	ND
39	n	606	CHL	NA
39	n	606	CHL	NC
39	n	606	CHL	ND
39	n	607	CHL	NA
39	n	607	CHL	NC
39	n	607	CHL	ND
39	n	608	CHL	NA
39	n	608	CHL	NC
39	n	608	CHL	ND
39	n	609	CHL	NA
39	n	609	CHL	NC
39	n	609	CHL	ND
39	r	605	CHL	NA
39	r	605	CHL	NC
39	r	605	CHL	ND
39	r	606	CHL	NA
39	r	606	CHL	NC
39	r	606	CHL	ND
39	r	607	CHL	NA
39	r	607	CHL	NC
39	r	607	CHL	ND
39	s	601	CHL	NA
39	s	601	CHL	NC
39	s	601	CHL	ND

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Mol	Chain	Res	Type	Atom
39	s	605	CHL	NA
39	s	605	CHL	NC
39	s	605	CHL	ND
39	s	606	CHL	NA
39	s	606	CHL	NC
39	s	606	CHL	ND
39	s	607	CHL	NA
39	s	607	CHL	NC
39	s	607	CHL	ND
39	y	303	CHL	NA
39	y	303	CHL	NC
39	y	303	CHL	ND
39	y	307	CHL	NA
39	y	307	CHL	NC
39	y	307	CHL	ND
39	y	308	CHL	NA
39	y	308	CHL	NC
39	y	308	CHL	ND
39	y	309	CHL	NA
39	y	309	CHL	NC
39	y	309	CHL	ND
39	y	310	CHL	NA
39	y	310	CHL	NC
39	y	310	CHL	ND

All (3614) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	403	CLA	C2A-CAA-CBA-CGA
23	A	403	CLA	CHA-CBD-CGD-O1D
23	A	403	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	C4-C3-C5-C6
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C4-C3-C5-C6
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	C12-C13-C15-C16
23	B	612	CLA	C1A-C2A-CAA-CBA
23	B	612	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	501	CLA	CHA-CBD-CGD-O1D
23	C	501	CLA	CHA-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	C1A-C2A-CAA-CBA
23	G	604	CLA	CHA-CBD-CGD-O1D
23	G	604	CLA	CHA-CBD-CGD-O2D
23	G	610	CLA	CBD-CGD-O2D-CED
23	R	601	CLA	CHA-CBD-CGD-O1D
23	R	601	CLA	CHA-CBD-CGD-O2D
23	R	610	CLA	C1A-C2A-CAA-CBA
23	R	610	CLA	C3A-C2A-CAA-CBA
23	R	611	CLA	CBD-CGD-O2D-CED
23	R	612	CLA	CHA-CBD-CGD-O1D
23	R	612	CLA	CHA-CBD-CGD-O2D
23	S	603	CLA	C1A-C2A-CAA-CBA
23	S	603	CLA	C3A-C2A-CAA-CBA
23	S	604	CLA	CHA-CBD-CGD-O1D
23	S	604	CLA	CHA-CBD-CGD-O2D
23	S	609	CLA	C1A-C2A-CAA-CBA
23	S	609	CLA	C3A-C2A-CAA-CBA
23	S	611	CLA	CBD-CGD-O2D-CED
23	S	613	CLA	C1A-C2A-CAA-CBA
23	Y	310	CLA	CBD-CGD-O2D-CED
23	a	403	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CHA-CBD-CGD-O1D
23	a	404	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	C1A-C2A-CAA-CBA
23	b	601	CLA	C3A-C2A-CAA-CBA
23	b	602	CLA	C2-C3-C5-C6
23	b	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	C1A-C2A-CAA-CBA
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	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	b	613	CLA	C11-C12-C13-C14
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CHA-CBD-CGD-O1D
23	c	501	CLA	CHA-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O1D
23	c	501	CLA	C14-C13-C15-C16
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	C6-C7-C8-C9
23	g	604	CLA	CHA-CBD-CGD-O1D
23	g	604	CLA	CHA-CBD-CGD-O2D
23	g	610	CLA	CBD-CGD-O2D-CED
23	n	614	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	C1A-C2A-CAA-CBA
23	r	610	CLA	C3A-C2A-CAA-CBA
23	r	611	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	C1A-C2A-CAA-CBA
23	r	612	CLA	C3A-C2A-CAA-CBA
23	r	612	CLA	CHA-CBD-CGD-O1D
23	r	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	C1A-C2A-CAA-CBA
23	s	602	CLA	C3A-C2A-CAA-CBA
23	s	602	CLA	C2-C3-C5-C6
23	s	602	CLA	C4-C3-C5-C6
23	s	604	CLA	CHA-CBD-CGD-O1D
23	s	604	CLA	CHA-CBD-CGD-O2D
23	s	609	CLA	C1A-C2A-CAA-CBA
23	s	609	CLA	C3A-C2A-CAA-CBA
23	s	609	CLA	CBD-CGD-O2D-CED
23	s	611	CLA	CBD-CGD-O2D-CED
23	s	613	CLA	C1A-C2A-CAA-CBA
25	B	617	BCR	C11-C12-C13-C14
25	B	617	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
25	B	617	BCR	C20-C21-C22-C37
25	B	617	BCR	C21-C22-C23-C24
25	B	618	BCR	C5-C6-C7-C8
25	C	514	BCR	C1-C6-C7-C8
25	C	514	BCR	C20-C21-C22-C37
25	H	501	BCR	C1-C6-C7-C8
25	H	501	BCR	C7-C8-C9-C34
25	K	101	BCR	C1-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	618	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	c	514	BCR	C20-C21-C22-C37
25	d	410	BCR	C6-C7-C8-C9
25	h	501	BCR	C7-C8-C9-C34
25	k	101	BCR	C1-C6-C7-C8
25	v	101	BCR	C21-C22-C23-C24
26	A	408	SQD	C5-C6-S-O7
26	A	408	SQD	C5-C6-S-O8
26	A	408	SQD	C5-C6-S-O9
26	L	101	SQD	O5-C1-O6-C44
26	L	101	SQD	C8-C7-O47-C45
26	M	101	SQD	C2-C1-O6-C44
26	M	101	SQD	O5-C1-O6-C44
26	M	101	SQD	O5-C5-C6-S
27	A	409	LMG	C2-C1-O1-C7
27	A	409	LMG	O6-C1-O1-C7
27	C	525	LMG	C2-C1-O1-C7
27	C	525	LMG	O6-C1-O1-C7
27	c	523	LMG	C2-C1-O1-C7
27	c	523	LMG	O6-C1-O1-C7
28	D	403	3PH	C1-O11-P-O13
28	L	102	3PH	C1-O11-P-O13
28	L	102	3PH	C1-O11-P-O14
28	L	102	3PH	C1-O11-P-O12
28	L	102	3PH	O22-C21-O21-C2
28	T	101	3PH	C1-O11-P-O13
28	T	101	3PH	C1-O11-P-O14
28	T	101	3PH	O11-C1-C2-O21
28	T	101	3PH	O22-C21-O21-C2
28	X	201	3PH	C22-C21-O21-C2
28	s	618	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
28	s	618	3PH	C1-O11-P-O14
28	s	618	3PH	C1-O11-P-O12
28	w	202	3PH	C1-O11-P-O13
28	w	202	3PH	C1-O11-P-O14
28	w	202	3PH	C1-O11-P-O12
28	x	201	3PH	O11-C1-C2-O21
28	x	201	3PH	C22-C21-O21-C2
29	A	411	PL9	C34-C36-C37-C38
29	A	411	PL9	C43-C44-C46-C47
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C29-C31-C32-C33
30	A	412	LHG	O1-C1-C2-C3
30	A	412	LHG	C3-O3-P-O5
30	A	412	LHG	C4-O6-P-O4
30	D	404	LHG	O1-C1-C2-C3
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C4-O6-P-O4
30	G	618	LHG	C3-O3-P-O4
30	G	618	LHG	C3-O3-P-O5
30	L	103	LHG	O1-C1-C2-C3
30	L	103	LHG	C3-O3-P-O4
30	L	103	LHG	C3-O3-P-O5
30	L	103	LHG	C3-O3-P-O6
30	L	103	LHG	C4-O6-P-O3
30	L	103	LHG	C4-O6-P-O4
30	L	103	LHG	C4-O6-P-O5
30	N	618	LHG	O1-C1-C2-C3
30	N	618	LHG	C4-C5-O7-C7
30	N	618	LHG	O9-C7-O7-C5
30	N	618	LHG	C8-C7-O7-C5
30	R	616	LHG	O1-C1-C2-O2
30	R	616	LHG	O1-C1-C2-C3
30	R	616	LHG	C8-C7-O7-C5
30	S	616	LHG	O1-C1-C2-C3
30	S	616	LHG	O2-C2-C3-O3
30	S	616	LHG	C4-O6-P-O4
30	S	616	LHG	C4-O6-P-O5
30	Y	318	LHG	O1-C1-C2-O2
30	Y	318	LHG	O1-C1-C2-C3
30	Y	318	LHG	C1-C2-C3-O3
30	a	412	LHG	O1-C1-C2-C3
30	a	412	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
30	a	412	LHG	C3-O3-P-O5
30	a	412	LHG	C3-O3-P-O6
30	b	627	LHG	O1-C1-C2-C3
30	b	627	LHG	C3-O3-P-O4
30	b	627	LHG	C4-O6-P-O3
30	b	627	LHG	C4-O6-P-O4
30	b	627	LHG	C4-O6-P-O5
30	d	404	LHG	O1-C1-C2-C3
30	d	404	LHG	C4-O6-P-O4
30	d	404	LHG	C4-O6-P-O5
30	d	408	LHG	O1-C1-C2-C3
30	d	408	LHG	C4-O6-P-O4
30	g	618	LHG	O2-C2-C3-O3
30	g	618	LHG	C3-O3-P-O5
30	g	618	LHG	O10-C23-O8-C6
30	g	618	LHG	C24-C23-O8-C6
30	n	619	LHG	O1-C1-C2-O2
30	n	619	LHG	O1-C1-C2-C3
30	r	616	LHG	O1-C1-C2-C3
30	s	616	LHG	O1-C1-C2-C3
30	s	616	LHG	O2-C2-C3-O3
30	s	616	LHG	C4-O6-P-O5
30	s	616	LHG	O7-C5-C6-O8
30	y	318	LHG	O1-C1-C2-O2
30	y	318	LHG	O1-C1-C2-C3
30	y	318	LHG	C1-C2-C3-O3
31	A	413	LNL	C9-C10-C11-C12
31	A	414	LNL	C15-C16-C17-C18
31	C	517	LNL	C13-C14-C15-C16
31	C	518	LNL	C15-C16-C17-C18
31	C	519	LNL	C15-C16-C17-C18
31	C	520	LNL	C9-C10-C11-C12
31	C	520	LNL	C13-C14-C15-C16
31	C	521	LNL	C15-C16-C17-C18
31	C	522	LNL	C13-C14-C15-C16
31	b	622	LNL	C15-C16-C17-C18
31	b	624	LNL	C10-C11-C12-C13
31	b	624	LNL	C15-C16-C17-C18
31	c	518	LNL	C9-C10-C11-C12
31	c	518	LNL	C15-C16-C17-C18
31	c	521	LNL	C9-C10-C11-C12
33	d	411	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
33	d	411	DGD	O6E-C1E-O5D-C6D
35	y	301	VIV	C16-C15-C9-O1
35	y	301	VIV	C16-C15-C9-C11
35	y	301	VIV	C16-C15-C9-C14
37	D	410	DGA	CB2-CB1-OG2-CG2
37	D	410	DGA	OG2-CG2-CG3-OXT
37	b	626	DGA	CB2-CB1-OG2-CG2
39	G	601	CHL	C1C-C2C-CMC-OMC
39	G	601	CHL	C3C-C2C-CMC-OMC
39	G	601	CHL	CHA-CBD-CGD-O1D
39	G	601	CHL	CHA-CBD-CGD-O2D
39	G	605	CHL	C1C-C2C-CMC-OMC
39	G	605	CHL	C3C-C2C-CMC-OMC
39	G	606	CHL	C1C-C2C-CMC-OMC
39	G	606	CHL	C3C-C2C-CMC-OMC
39	G	607	CHL	C1C-C2C-CMC-OMC
39	G	607	CHL	C3C-C2C-CMC-OMC
39	G	608	CHL	C1C-C2C-CMC-OMC
39	G	608	CHL	C3C-C2C-CMC-OMC
39	G	609	CHL	C1C-C2C-CMC-OMC
39	G	609	CHL	C3C-C2C-CMC-OMC
39	G	609	CHL	C2-C3-C5-C6
39	G	609	CHL	C4-C3-C5-C6
39	G	609	CHL	C6-C7-C8-C9
39	G	620	CHL	C3C-C2C-CMC-OMC
39	N	601	CHL	C1A-C2A-CAA-CBA
39	N	601	CHL	C3A-C2A-CAA-CBA
39	N	601	CHL	C1C-C2C-CMC-OMC
39	N	601	CHL	C3C-C2C-CMC-OMC
39	N	601	CHL	CHA-CBD-CGD-O1D
39	N	601	CHL	CHA-CBD-CGD-O2D
39	N	605	CHL	C1C-C2C-CMC-OMC
39	N	605	CHL	C3C-C2C-CMC-OMC
39	N	606	CHL	C1C-C2C-CMC-OMC
39	N	608	CHL	C3C-C2C-CMC-OMC
39	N	609	CHL	C1C-C2C-CMC-OMC
39	N	609	CHL	C3C-C2C-CMC-OMC
39	R	605	CHL	C1C-C2C-CMC-OMC
39	R	605	CHL	C3C-C2C-CMC-OMC
39	R	606	CHL	C3C-C2C-CMC-OMC
39	R	606	CHL	C14-C13-C15-C16
39	R	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	R	607	CHL	C1C-C2C-CMC-OMC
39	S	601	CHL	C1C-C2C-CMC-OMC
39	S	601	CHL	C3C-C2C-CMC-OMC
39	S	605	CHL	C1C-C2C-CMC-OMC
39	S	605	CHL	C3C-C2C-CMC-OMC
39	S	606	CHL	C3A-C2A-CAA-CBA
39	S	606	CHL	C1C-C2C-CMC-OMC
39	S	606	CHL	C3C-C2C-CMC-OMC
39	S	607	CHL	C1A-C2A-CAA-CBA
39	S	607	CHL	C3A-C2A-CAA-CBA
39	S	607	CHL	C1C-C2C-CMC-OMC
39	S	607	CHL	C3C-C2C-CMC-OMC
39	Y	302	CHL	C1C-C2C-CMC-OMC
39	Y	302	CHL	C3C-C2C-CMC-OMC
39	Y	302	CHL	C4-C3-C5-C6
39	Y	306	CHL	C1C-C2C-CMC-OMC
39	Y	306	CHL	C3C-C2C-CMC-OMC
39	Y	308	CHL	C1C-C2C-CMC-OMC
39	Y	308	CHL	C3C-C2C-CMC-OMC
39	Y	309	CHL	C1C-C2C-CMC-OMC
39	Y	309	CHL	C3C-C2C-CMC-OMC
39	g	601	CHL	C1C-C2C-CMC-OMC
39	g	601	CHL	C3C-C2C-CMC-OMC
39	g	601	CHL	CHA-CBD-CGD-O1D
39	g	601	CHL	CHA-CBD-CGD-O2D
39	g	605	CHL	C1C-C2C-CMC-OMC
39	g	605	CHL	C3C-C2C-CMC-OMC
39	g	606	CHL	C1C-C2C-CMC-OMC
39	g	606	CHL	C3C-C2C-CMC-OMC
39	g	607	CHL	C1C-C2C-CMC-OMC
39	g	607	CHL	C3C-C2C-CMC-OMC
39	g	607	CHL	C6-C7-C8-C9
39	g	608	CHL	C1A-C2A-CAA-CBA
39	g	608	CHL	C1C-C2C-CMC-OMC
39	g	608	CHL	C3C-C2C-CMC-OMC
39	g	608	CHL	CHA-CBD-CGD-O1D
39	g	608	CHL	CHA-CBD-CGD-O2D
39	g	609	CHL	C1A-C2A-CAA-CBA
39	g	609	CHL	CHA-CBD-CGD-O1D
39	g	609	CHL	CHA-CBD-CGD-O2D
39	g	619	CHL	C1C-C2C-CMC-OMC
39	g	619	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
39	n	601	CHL	C3C-C2C-CMC-OMC
39	n	601	CHL	CHA-CBD-CGD-O1D
39	n	601	CHL	CHA-CBD-CGD-O2D
39	n	605	CHL	C1C-C2C-CMC-OMC
39	n	605	CHL	C3C-C2C-CMC-OMC
39	n	606	CHL	C1C-C2C-CMC-OMC
39	n	607	CHL	C3C-C2C-CMC-OMC
39	n	608	CHL	C3C-C2C-CMC-OMC
39	n	609	CHL	C1C-C2C-CMC-OMC
39	n	609	CHL	C3C-C2C-CMC-OMC
39	r	605	CHL	C1C-C2C-CMC-OMC
39	r	605	CHL	C3C-C2C-CMC-OMC
39	r	606	CHL	C3C-C2C-CMC-OMC
39	r	607	CHL	C1A-C2A-CAA-CBA
39	r	607	CHL	C1C-C2C-CMC-OMC
39	s	601	CHL	C1C-C2C-CMC-OMC
39	s	601	CHL	C3C-C2C-CMC-OMC
39	s	601	CHL	C2-C3-C5-C6
39	s	605	CHL	C1A-C2A-CAA-CBA
39	s	605	CHL	C3A-C2A-CAA-CBA
39	s	605	CHL	C1C-C2C-CMC-OMC
39	s	605	CHL	C3C-C2C-CMC-OMC
39	s	606	CHL	C1C-C2C-CMC-OMC
39	s	606	CHL	C3C-C2C-CMC-OMC
39	s	607	CHL	C1C-C2C-CMC-OMC
39	s	607	CHL	C3C-C2C-CMC-OMC
39	y	303	CHL	C1C-C2C-CMC-OMC
39	y	303	CHL	C3C-C2C-CMC-OMC
39	y	303	CHL	C2-C3-C5-C6
39	y	303	CHL	C4-C3-C5-C6
39	y	307	CHL	C1C-C2C-CMC-OMC
39	y	307	CHL	C3C-C2C-CMC-OMC
39	y	308	CHL	C1C-C2C-CMC-OMC
39	y	309	CHL	C1C-C2C-CMC-OMC
39	y	309	CHL	C3C-C2C-CMC-OMC
39	y	310	CHL	C1C-C2C-CMC-OMC
39	y	310	CHL	C3C-C2C-CMC-OMC
40	G	615	LUT	C1-C6-C7-C8
40	G	615	LUT	C7-C8-C9-C10
40	G	615	LUT	C10-C11-C12-C13
40	G	615	LUT	C11-C12-C13-C14
40	G	615	LUT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
40	G	615	LUT	C26-C27-C28-C29
40	G	615	LUT	C27-C28-C29-C30
40	G	615	LUT	C28-C29-C30-C31
40	G	615	LUT	C39-C29-C30-C31
40	G	615	LUT	C30-C31-C32-C33
40	G	615	LUT	C31-C32-C33-C34
40	G	615	LUT	C31-C32-C33-C40
40	G	616	LUT	C11-C10-C9-C8
40	G	616	LUT	C11-C10-C9-C19
40	G	616	LUT	C11-C12-C13-C20
40	G	616	LUT	C31-C32-C33-C40
40	N	615	LUT	C1-C6-C7-C8
40	N	615	LUT	C6-C7-C8-C9
40	N	615	LUT	C7-C8-C9-C10
40	N	615	LUT	C7-C8-C9-C19
40	N	615	LUT	C11-C10-C9-C19
40	N	615	LUT	C9-C10-C11-C12
40	N	615	LUT	C11-C12-C13-C20
40	N	615	LUT	C27-C28-C29-C39
40	N	615	LUT	C31-C32-C33-C40
40	N	616	LUT	C7-C8-C9-C10
40	N	616	LUT	C11-C10-C9-C19
40	N	616	LUT	C10-C11-C12-C13
40	N	616	LUT	C11-C12-C13-C14
40	N	616	LUT	C20-C13-C14-C15
40	N	616	LUT	C26-C27-C28-C29
40	N	616	LUT	C27-C28-C29-C39
40	N	616	LUT	C39-C29-C30-C31
40	R	613	LUT	C11-C10-C9-C19
40	R	613	LUT	C10-C11-C12-C13
40	R	613	LUT	C11-C12-C13-C14
40	R	613	LUT	C26-C27-C28-C29
40	R	613	LUT	C39-C29-C30-C31
40	R	613	LUT	C31-C32-C33-C34
40	S	614	LUT	C6-C7-C8-C9
40	S	614	LUT	C7-C8-C9-C10
40	S	614	LUT	C7-C8-C9-C19
40	S	614	LUT	C11-C10-C9-C19
40	S	614	LUT	C10-C11-C12-C13
40	S	614	LUT	C11-C12-C13-C20
40	S	614	LUT	C21-C26-C27-C28
40	S	614	LUT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
40	S	614	LUT	C26-C27-C28-C29
40	S	614	LUT	C27-C28-C29-C30
40	S	614	LUT	C30-C31-C32-C33
40	S	615	LUT	C1-C6-C7-C8
40	S	615	LUT	C6-C7-C8-C9
40	S	615	LUT	C7-C8-C9-C19
40	S	615	LUT	C11-C10-C9-C19
40	S	615	LUT	C10-C11-C12-C13
40	S	615	LUT	C11-C12-C13-C20
40	S	615	LUT	C27-C28-C29-C30
40	S	615	LUT	C28-C29-C30-C31
40	S	615	LUT	C39-C29-C30-C31
40	S	615	LUT	C31-C32-C33-C34
40	Y	315	LUT	C6-C7-C8-C9
40	Y	315	LUT	C7-C8-C9-C19
40	Y	315	LUT	C11-C10-C9-C8
40	Y	315	LUT	C10-C11-C12-C13
40	Y	315	LUT	C27-C28-C29-C30
40	Y	315	LUT	C39-C29-C30-C31
40	Y	316	LUT	C6-C7-C8-C9
40	Y	316	LUT	C7-C8-C9-C19
40	Y	316	LUT	C11-C12-C13-C20
40	Y	316	LUT	C21-C26-C27-C28
40	Y	316	LUT	C25-C26-C27-C28
40	Y	316	LUT	C26-C27-C28-C29
40	Y	316	LUT	C27-C28-C29-C30
40	Y	316	LUT	C28-C29-C30-C31
40	Y	316	LUT	C39-C29-C30-C31
40	g	615	LUT	C7-C8-C9-C10
40	g	615	LUT	C11-C10-C9-C19
40	g	615	LUT	C11-C12-C13-C20
40	g	615	LUT	C20-C13-C14-C15
40	g	615	LUT	C26-C27-C28-C29
40	g	615	LUT	C27-C28-C29-C30
40	g	615	LUT	C28-C29-C30-C31
40	g	615	LUT	C39-C29-C30-C31
40	g	615	LUT	C29-C30-C31-C32
40	g	615	LUT	C30-C31-C32-C33
40	g	615	LUT	C31-C32-C33-C34
40	g	615	LUT	C31-C32-C33-C40
40	g	615	LUT	C40-C33-C34-C35
40	g	616	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	g	616	LUT	C11-C10-C9-C8
40	g	616	LUT	C11-C10-C9-C19
40	g	616	LUT	C11-C12-C13-C20
40	g	616	LUT	C39-C29-C30-C31
40	g	616	LUT	C31-C32-C33-C40
40	n	615	LUT	C20-C13-C14-C15
40	n	615	LUT	C14-C15-C35-C34
40	n	615	LUT	C26-C27-C28-C29
40	n	615	LUT	C27-C28-C29-C39
40	n	615	LUT	C28-C29-C30-C31
40	n	615	LUT	C30-C31-C32-C33
40	n	615	LUT	C31-C32-C33-C40
40	n	616	LUT	C7-C8-C9-C10
40	n	616	LUT	C11-C10-C9-C19
40	n	616	LUT	C10-C11-C12-C13
40	n	616	LUT	C11-C12-C13-C20
40	n	616	LUT	C20-C13-C14-C15
40	n	616	LUT	C26-C27-C28-C29
40	n	616	LUT	C27-C28-C29-C39
40	n	616	LUT	C31-C32-C33-C40
40	r	613	LUT	C11-C10-C9-C19
40	r	613	LUT	C11-C12-C13-C20
40	r	613	LUT	C26-C27-C28-C29
40	r	613	LUT	C27-C28-C29-C39
40	s	614	LUT	C1-C6-C7-C8
40	s	614	LUT	C5-C6-C7-C8
40	s	614	LUT	C6-C7-C8-C9
40	s	614	LUT	C9-C10-C11-C12
40	s	614	LUT	C11-C12-C13-C14
40	s	614	LUT	C26-C27-C28-C29
40	s	614	LUT	C27-C28-C29-C30
40	s	614	LUT	C39-C29-C30-C31
40	s	615	LUT	C5-C6-C7-C8
40	s	615	LUT	C6-C7-C8-C9
40	s	615	LUT	C7-C8-C9-C19
40	s	615	LUT	C11-C12-C13-C20
40	s	615	LUT	C31-C32-C33-C40
40	y	316	LUT	C6-C7-C8-C9
40	y	316	LUT	C7-C8-C9-C19
40	y	316	LUT	C11-C10-C9-C8
40	y	316	LUT	C10-C11-C12-C13
40	y	316	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
40	y	316	LUT	C39-C29-C30-C31
40	y	317	LUT	C6-C7-C8-C9
40	y	317	LUT	C7-C8-C9-C19
40	y	317	LUT	C11-C12-C13-C20
40	y	317	LUT	C21-C26-C27-C28
40	y	317	LUT	C25-C26-C27-C28
40	y	317	LUT	C26-C27-C28-C29
40	y	317	LUT	C27-C28-C29-C30
40	y	317	LUT	C28-C29-C30-C31
40	y	317	LUT	C39-C29-C30-C31
40	y	317	LUT	C31-C32-C33-C40
41	G	617	NEX	O24-C26-C27-C28
41	N	617	NEX	C20-C13-C14-C15
41	N	617	NEX	O24-C26-C27-C28
41	N	617	NEX	C27-C28-C29-C39
41	N	617	NEX	C39-C29-C30-C31
41	N	617	NEX	C40-C33-C34-C35
41	R	614	NEX	C7-C8-C9-C19
41	R	614	NEX	C9-C10-C11-C12
41	R	614	NEX	C11-C12-C13-C14
41	R	614	NEX	C12-C13-C14-C15
41	R	614	NEX	C14-C15-C35-C34
41	R	614	NEX	O24-C26-C27-C28
41	R	614	NEX	C27-C28-C29-C39
41	R	614	NEX	C31-C32-C33-C40
41	R	618	NEX	O24-C26-C27-C28
41	R	618	NEX	C27-C28-C29-C39
41	R	618	NEX	C29-C30-C31-C32
41	R	618	NEX	C40-C33-C34-C35
41	S	617	NEX	C20-C13-C14-C15
41	S	617	NEX	C13-C14-C15-C35
41	Y	317	NEX	C7-C8-C9-C19
41	Y	317	NEX	C11-C10-C9-C19
41	Y	317	NEX	C10-C11-C12-C13
41	Y	317	NEX	C11-C12-C13-C14
41	Y	317	NEX	C20-C13-C14-C15
41	Y	317	NEX	C14-C15-C35-C34
41	Y	317	NEX	O24-C26-C27-C28
41	Y	317	NEX	C40-C33-C34-C35
41	g	617	NEX	C11-C10-C9-C19
41	g	617	NEX	C11-C12-C13-C14
41	g	617	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
41	g	617	NEX	C29-C30-C31-C32
41	g	617	NEX	C31-C32-C33-C34
41	n	618	NEX	C7-C8-C9-C19
41	n	618	NEX	C11-C10-C9-C19
41	n	618	NEX	C11-C12-C13-C14
41	n	618	NEX	O24-C26-C27-C28
41	n	618	NEX	C27-C28-C29-C39
41	n	618	NEX	C39-C29-C30-C31
41	n	618	NEX	C40-C33-C34-C35
41	r	614	NEX	C11-C12-C13-C20
41	r	614	NEX	O24-C26-C27-C28
41	r	614	NEX	C27-C28-C29-C39
41	r	614	NEX	C31-C32-C33-C40
41	s	617	NEX	C40-C33-C34-C35
42	G	619	XAT	O4-C6-C7-C8
42	G	619	XAT	C7-C8-C9-C10
42	G	619	XAT	C31-C32-C33-C40
42	N	619	XAT	C7-C8-C9-C10
42	N	619	XAT	C11-C12-C13-C14
42	N	619	XAT	C31-C32-C33-C34
42	R	615	XAT	C11-C10-C9-C19
42	R	615	XAT	O24-C26-C27-C28
42	R	615	XAT	C26-C27-C28-C29
42	R	615	XAT	C27-C28-C29-C30
42	R	615	XAT	C27-C28-C29-C39
42	R	615	XAT	C39-C29-C30-C31
42	Y	301	XAT	O4-C6-C7-C8
42	Y	301	XAT	C31-C32-C33-C34
42	Y	301	XAT	C31-C32-C33-C40
42	n	617	XAT	O4-C6-C7-C8
42	n	617	XAT	C7-C8-C9-C19
42	n	617	XAT	C11-C10-C9-C19
42	n	617	XAT	C11-C12-C13-C14
42	n	620	XAT	O4-C6-C7-C8
42	n	620	XAT	C7-C8-C9-C10
42	n	620	XAT	C11-C12-C13-C14
42	r	615	XAT	C11-C10-C9-C19
42	r	615	XAT	O24-C26-C27-C28
42	r	615	XAT	C26-C27-C28-C29
42	r	615	XAT	C27-C28-C29-C30
42	r	615	XAT	C27-C28-C29-C39
42	r	615	XAT	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
42	y	302	XAT	O4-C6-C7-C8
42	y	302	XAT	C31-C32-C33-C34
42	y	302	XAT	C40-C33-C34-C35
23	R	611	CLA	O1D-CGD-O2D-CED
23	S	603	CLA	O1D-CGD-O2D-CED
23	s	603	CLA	O1D-CGD-O2D-CED
23	S	609	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1D-CGD-O2D-CED
23	A	402	CLA	CBD-CGD-O2D-CED
23	N	611	CLA	CBD-CGD-O2D-CED
23	R	601	CLA	CBD-CGD-O2D-CED
23	S	603	CLA	CBD-CGD-O2D-CED
23	S	604	CLA	CBD-CGD-O2D-CED
23	S	609	CLA	CBD-CGD-O2D-CED
23	n	611	CLA	CBD-CGD-O2D-CED
23	s	602	CLA	CBD-CGD-O2D-CED
23	s	603	CLA	CBD-CGD-O2D-CED
23	s	604	CLA	CBD-CGD-O2D-CED
23	y	311	CLA	CBD-CGD-O2D-CED
24	d	402	PHO	CBD-CGD-O2D-CED
23	S	612	CLA	O1A-CGA-O2A-C1
23	S	613	CLA	O1A-CGA-O2A-C1
23	s	612	CLA	O1A-CGA-O2A-C1
23	s	613	CLA	O1A-CGA-O2A-C1
24	A	405	PHO	O1A-CGA-O2A-C1
30	G	618	LHG	O10-C23-O8-C6
30	n	619	LHG	O10-C23-O8-C6
23	R	601	CLA	O1D-CGD-O2D-CED
23	S	604	CLA	O1D-CGD-O2D-CED
33	d	411	DGD	C4D-C5D-C6D-O5D
23	B	605	CLA	O1D-CGD-O2D-CED
23	Y	310	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	g	610	CLA	O1D-CGD-O2D-CED
23	s	609	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	O1D-CGD-O2D-CED
23	S	613	CLA	CBA-CGA-O2A-C1
23	s	612	CLA	CBA-CGA-O2A-C1
24	A	405	PHO	CBA-CGA-O2A-C1
30	G	618	LHG	C24-C23-O8-C6
30	n	619	LHG	C24-C23-O8-C6
23	C	502	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	G	614	CLA	CBD-CGD-O2D-CED
23	N	613	CLA	CBD-CGD-O2D-CED
23	N	614	CLA	CBD-CGD-O2D-CED
23	S	602	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
23	g	614	CLA	CBD-CGD-O2D-CED
24	D	402	PHO	CBD-CGD-O2D-CED
23	B	616	CLA	O1A-CGA-O2A-C1
23	G	611	CLA	O1A-CGA-O2A-C1
23	R	612	CLA	O1A-CGA-O2A-C1
23	S	603	CLA	O1A-CGA-O2A-C1
23	S	610	CLA	O1A-CGA-O2A-C1
23	Y	311	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1A-CGA-O2A-C1
23	n	614	CLA	O1A-CGA-O2A-C1
23	s	603	CLA	O1A-CGA-O2A-C1
23	s	610	CLA	O1A-CGA-O2A-C1
23	y	312	CLA	O1A-CGA-O2A-C1
28	s	618	3PH	O32-C31-O31-C3
30	D	408	LHG	O10-C23-O8-C6
30	N	618	LHG	O10-C23-O8-C6
30	d	408	LHG	O10-C23-O8-C6
23	G	610	CLA	O1D-CGD-O2D-CED
23	S	611	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	O1D-CGD-O2D-CED
23	s	611	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	n	614	CLA	O1D-CGD-O2D-CED
23	B	607	CLA	CBD-CGD-O2D-CED
23	N	611	CLA	O1D-CGD-O2D-CED
26	M	101	SQD	O49-C7-O47-C45
28	X	201	3PH	O22-C21-O21-C2
28	x	201	3PH	O22-C21-O21-C2
30	R	616	LHG	O9-C7-O7-C5
37	D	410	DGA	OB1-CB1-OG2-CG2
37	b	626	DGA	OB1-CB1-OG2-CG2
23	B	602	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	C	511	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	G	613	CLA	C3-C5-C6-C7
23	S	610	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7
23	s	602	CLA	C3-C5-C6-C7
23	s	609	CLA	C3-C5-C6-C7
23	s	610	CLA	C3-C5-C6-C7
23	y	306	CLA	C3-C5-C6-C7
23	y	315	CLA	C3-C5-C6-C7
24	A	405	PHO	C3-C5-C6-C7
24	a	406	PHO	C3-C5-C6-C7
39	n	609	CHL	C3-C5-C6-C7
23	G	611	CLA	CBA-CGA-O2A-C1
23	R	612	CLA	CBA-CGA-O2A-C1
23	S	603	CLA	CBA-CGA-O2A-C1
23	S	612	CLA	CBA-CGA-O2A-C1
23	n	614	CLA	CBA-CGA-O2A-C1
23	s	603	CLA	CBA-CGA-O2A-C1
23	s	613	CLA	CBA-CGA-O2A-C1
28	s	618	3PH	C32-C31-O31-C3
30	N	618	LHG	C24-C23-O8-C6
26	M	101	SQD	C8-C7-O47-C45
28	L	102	3PH	C22-C21-O21-C2
28	T	101	3PH	C22-C21-O21-C2
23	A	402	CLA	O1D-CGD-O2D-CED
23	a	403	CLA	O1D-CGD-O2D-CED
23	n	613	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C4-C3-C5-C6
23	R	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	r	604	CLA	C4-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
39	Y	302	CHL	C2-C3-C5-C6
23	b	607	CLA	CBD-CGD-O2D-CED
23	n	610	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	S	604	CLA	C2A-CAA-CBA-CGA
23	a	404	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	s	604	CLA	C2A-CAA-CBA-CGA
39	Y	308	CHL	C2A-CAA-CBA-CGA
23	R	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C3-C5-C6-C7
23	Y	305	CLA	C3-C5-C6-C7
23	Y	313	CLA	C3-C5-C6-C7
23	c	511	CLA	C3-C5-C6-C7
23	B	616	CLA	CBA-CGA-O2A-C1
23	N	614	CLA	CBA-CGA-O2A-C1
23	R	601	CLA	CBA-CGA-O2A-C1
23	S	610	CLA	CBA-CGA-O2A-C1
23	Y	311	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	g	603	CLA	CBA-CGA-O2A-C1
23	g	613	CLA	CBA-CGA-O2A-C1
23	s	610	CLA	CBA-CGA-O2A-C1
23	y	312	CLA	CBA-CGA-O2A-C1
26	M	101	SQD	C24-C23-O48-C46
28	T	101	3PH	C32-C31-O31-C3
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
33	C	515	DGD	C4E-C5E-C6E-O5E
23	s	602	CLA	O1D-CGD-O2D-CED
23	N	602	CLA	CBD-CGD-O2D-CED
23	g	604	CLA	CBD-CGD-O2D-CED
26	L	101	SQD	O49-C7-O47-C45
33	H	502	DGD	C4E-C5E-C6E-O5E
33	c	515	DGD	C4E-C5E-C6E-O5E
23	A	402	CLA	O1A-CGA-O2A-C1
23	G	604	CLA	O1A-CGA-O2A-C1
23	a	403	CLA	O1A-CGA-O2A-C1
23	g	603	CLA	O1A-CGA-O2A-C1
23	g	604	CLA	O1A-CGA-O2A-C1
28	T	101	3PH	O32-C31-O31-C3
40	G	616	LUT	C9-C10-C11-C12
40	N	616	LUT	C29-C30-C31-C32
40	R	613	LUT	C29-C30-C31-C32
40	g	616	LUT	C9-C10-C11-C12
40	n	616	LUT	C9-C10-C11-C12
40	s	614	LUT	C29-C30-C31-C32
41	N	617	NEX	C9-C10-C11-C12
41	R	614	NEX	C13-C14-C15-C35
41	R	618	NEX	C9-C10-C11-C12
41	S	617	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
41	g	617	NEX	C9-C10-C11-C12
41	n	618	NEX	C9-C10-C11-C12
41	s	617	NEX	C9-C10-C11-C12
42	G	619	XAT	C9-C10-C11-C12
42	y	302	XAT	C33-C34-C35-C15
23	C	510	CLA	CBD-CGD-O2D-CED
23	D	406	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	CBD-CGD-O2D-CED
23	N	610	CLA	CBD-CGD-O2D-CED
23	Y	305	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	CBD-CGD-O2D-CED
23	s	604	CLA	O1D-CGD-O2D-CED
30	L	103	LHG	O2-C2-C3-O3
30	Y	318	LHG	O2-C2-C3-O3
30	a	412	LHG	O2-C2-C3-O3
30	y	318	LHG	O2-C2-C3-O3
23	c	504	CLA	C3-C5-C6-C7
23	y	314	CLA	C3-C5-C6-C7
23	d	406	CLA	CBA-CGA-O2A-C1
26	L	101	SQD	C24-C23-O48-C46
28	A	410	3PH	C32-C31-O31-C3
28	a	410	3PH	C32-C31-O31-C3
26	M	101	SQD	O10-C23-O48-C46
28	A	410	3PH	O32-C31-O31-C3
33	d	411	DGD	O6E-C5E-C6E-O5E
23	B	606	CLA	CBD-CGD-O2D-CED
23	G	612	CLA	CBD-CGD-O2D-CED
23	d	406	CLA	CBD-CGD-O2D-CED
31	b	622	LNL	C2-C3-C4-C5
28	a	410	3PH	O32-C31-O31-C3
30	D	408	LHG	C24-C25-C26-C27
30	b	627	LHG	C31-C32-C33-C34
31	C	521	LNL	C3-C4-C5-C6
31	C	521	LNL	C5-C6-C7-C8
23	n	611	CLA	O1D-CGD-O2D-CED
24	d	402	PHO	O1D-CGD-O2D-CED
30	d	404	LHG	C31-C32-C33-C34
31	C	522	LNL	C2-C3-C4-C5
23	C	504	CLA	C3-C5-C6-C7
23	A	402	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	G	604	CLA	CBA-CGA-O2A-C1
23	a	403	CLA	CBA-CGA-O2A-C1
23	g	604	CLA	CBA-CGA-O2A-C1
33	C	515	DGD	O6E-C5E-C6E-O5E
33	d	411	DGD	C4E-C5E-C6E-O5E
30	N	618	LHG	C5-C4-O6-P
23	b	610	CLA	O1A-CGA-O2A-C1
33	H	502	DGD	O6E-C5E-C6E-O5E
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	D	407	PL9	C12-C11-C9-C10
29	a	411	PL9	C40-C39-C41-C42
29	d	407	PL9	C12-C11-C9-C10
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	D	407	PL9	C12-C11-C9-C8
29	a	411	PL9	C38-C39-C41-C42
29	d	407	PL9	C12-C11-C9-C8
39	g	607	CHL	C2A-CAA-CBA-CGA
39	n	608	CHL	C2A-CAA-CBA-CGA
33	c	515	DGD	O6E-C5E-C6E-O5E
23	N	614	CLA	O1A-CGA-O2A-C1
27	r	617	LMG	O6-C1-O1-C7
29	A	411	PL9	C44-C46-C47-C48
29	a	411	PL9	C19-C21-C22-C23
29	a	411	PL9	C44-C46-C47-C48
23	N	612	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
31	B	622	LNL	C2-C3-C4-C5
23	d	406	CLA	O1A-CGA-O2A-C1
26	L	101	SQD	O10-C23-O48-C46
30	A	412	LHG	C1-C2-C3-O3
30	a	412	LHG	C1-C2-C3-O3
30	g	618	LHG	C1-C2-C3-O3
23	S	602	CLA	O1D-CGD-O2D-CED
24	D	402	PHO	O1D-CGD-O2D-CED
23	D	406	CLA	CBA-CGA-O2A-C1
23	N	603	CLA	CBA-CGA-O2A-C1
23	S	611	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
23	g	611	CLA	CBA-CGA-O2A-C1
23	g	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	n	603	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBD-CGD-O2D-CED
40	S	615	LUT	C9-C10-C11-C12
42	n	617	XAT	C9-C10-C11-C12
23	s	610	CLA	C15-C16-C17-C18
31	A	413	LNL	C5-C6-C7-C8
23	C	502	CLA	O1D-CGD-O2D-CED
30	d	404	LHG	C33-C34-C35-C36
23	C	504	CLA	C5-C6-C7-C8
23	S	613	CLA	C10-C11-C12-C13
23	b	612	CLA	C15-C16-C17-C18
39	G	620	CHL	C10-C11-C12-C13
39	n	606	CHL	C10-C11-C12-C13
39	n	607	CHL	C5-C6-C7-C8
30	A	412	LHG	O2-C2-C3-O3
30	N	618	LHG	O2-C2-C3-O3
28	x	201	3PH	C26-C27-C28-C29
23	N	603	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
23	g	611	CLA	O1A-CGA-O2A-C1
23	g	612	CLA	O1A-CGA-O2A-C1
23	D	406	CLA	C4-C3-C5-C6
23	R	604	CLA	C2-C3-C5-C6
23	r	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C6-C7-C8-C9
23	B	607	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	C	504	CLA	C11-C12-C13-C14
23	C	507	CLA	C14-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C9
23	G	603	CLA	C11-C10-C8-C9
23	N	603	CLA	C11-C12-C13-C14
23	N	611	CLA	C11-C10-C8-C9
23	S	609	CLA	C6-C7-C8-C9
23	S	610	CLA	C6-C7-C8-C9
23	S	613	CLA	C11-C10-C8-C9
23	S	613	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
23	c	504	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	g	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	n	603	CLA	C11-C12-C13-C14
23	r	608	CLA	C11-C10-C8-C9
23	s	610	CLA	C6-C7-C8-C9
23	y	305	CLA	C11-C10-C8-C9
23	y	315	CLA	C11-C10-C8-C9
35	C	523	VIV	C21-C22-C23-C1
35	y	301	VIV	C21-C22-C23-C1
39	G	607	CHL	C6-C7-C8-C9
39	N	607	CHL	C6-C7-C8-C9
39	R	606	CHL	C6-C7-C8-C9
39	r	606	CHL	C11-C10-C8-C9
39	y	303	CHL	C6-C7-C8-C9
23	N	613	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
23	S	612	CLA	CBD-CGD-O2D-CED
23	g	612	CLA	CBD-CGD-O2D-CED
23	S	610	CLA	C15-C16-C17-C18
23	B	607	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	s	613	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C7-C8-C9-C34
25	V	101	BCR	C37-C22-C23-C24
25	v	101	BCR	C37-C22-C23-C24
40	G	615	LUT	C7-C8-C9-C19
40	G	615	LUT	C11-C12-C13-C20
40	R	613	LUT	C11-C12-C13-C20
40	R	613	LUT	C27-C28-C29-C39
40	R	613	LUT	C31-C32-C33-C40
40	Y	315	LUT	C27-C28-C29-C39
40	Y	316	LUT	C31-C32-C33-C40
40	g	615	LUT	C27-C28-C29-C39
40	s	614	LUT	C7-C8-C9-C19
40	s	614	LUT	C11-C12-C13-C20
40	y	316	LUT	C27-C28-C29-C39
41	G	617	NEX	C27-C28-C29-C39
41	N	617	NEX	C11-C12-C13-C20
41	R	618	NEX	C11-C12-C13-C20
41	g	617	NEX	C31-C32-C33-C40
42	N	619	XAT	C7-C8-C9-C19
42	Y	301	XAT	C7-C8-C9-C19
42	Y	301	XAT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
42	n	620	XAT	C7-C8-C9-C19
42	y	302	XAT	C31-C32-C33-C40
25	B	617	BCR	C7-C8-C9-C10
25	V	101	BCR	C21-C22-C23-C24
40	N	615	LUT	C11-C12-C13-C14
40	R	613	LUT	C27-C28-C29-C30
40	Y	316	LUT	C31-C32-C33-C34
40	s	614	LUT	C7-C8-C9-C10
40	s	614	LUT	C31-C32-C33-C34
40	s	615	LUT	C7-C8-C9-C10
40	y	317	LUT	C31-C32-C33-C34
41	N	617	NEX	C11-C12-C13-C14
41	R	618	NEX	C11-C12-C13-C14
41	s	617	NEX	C11-C12-C13-C14
42	Y	301	XAT	C7-C8-C9-C10
42	Y	301	XAT	C11-C12-C13-C14
42	y	302	XAT	C11-C12-C13-C14
30	A	412	LHG	C29-C30-C31-C32
30	D	404	LHG	C23-C24-C25-C26
31	C	521	LNL	C1-C2-C3-C4
23	n	603	CLA	O1A-CGA-O2A-C1
23	y	306	CLA	C13-C15-C16-C17
35	C	523	VIV	C23-C24-C25-C26
39	N	601	CHL	C5-C6-C7-C8
23	G	614	CLA	O1D-CGD-O2D-CED
30	N	618	LHG	C26-C27-C28-C29
23	n	604	CLA	CBD-CGD-O2D-CED
23	r	608	CLA	CBD-CGD-O2D-CED
23	g	614	CLA	O1D-CGD-O2D-CED
28	d	403	3PH	C32-C31-O31-C3
23	B	606	CLA	C13-C15-C16-C17
23	B	612	CLA	C15-C16-C17-C18
23	C	512	CLA	C5-C6-C7-C8
23	S	609	CLA	C5-C6-C7-C8
23	Y	310	CLA	C13-C15-C16-C17
23	c	504	CLA	C5-C6-C7-C8
23	c	510	CLA	C10-C11-C12-C13
23	y	313	CLA	C8-C10-C11-C12
35	C	523	VIV	C20-C21-C22-C23
39	n	609	CHL	C5-C6-C7-C8
27	B	620	LMG	C28-C29-C30-C31
31	B	625	LNL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	b	622	LNL	C1-C2-C3-C4
31	c	522	LNL	C1-C2-C3-C4
33	d	411	DGD	C1B-C2B-C3B-C4B
23	B	604	CLA	C5-C6-C7-C8
23	C	510	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	510	CLA	C15-C16-C17-C18
23	D	405	CLA	C10-C11-C12-C13
23	N	611	CLA	C8-C10-C11-C12
23	b	604	CLA	C10-C11-C12-C13
23	b	615	CLA	C10-C11-C12-C13
23	c	510	CLA	C15-C16-C17-C18
23	s	609	CLA	C5-C6-C7-C8
23	s	613	CLA	C5-C6-C7-C8
23	y	311	CLA	C5-C6-C7-C8
35	C	523	VIV	C15-C16-C17-C18
39	G	601	CHL	C5-C6-C7-C8
39	g	609	CHL	C5-C6-C7-C8
30	A	412	LHG	O1-C1-C2-O2
30	a	412	LHG	O1-C1-C2-O2
30	s	616	LHG	O1-C1-C2-O2
30	D	408	LHG	C23-C24-C25-C26
30	G	618	LHG	C7-C8-C9-C10
30	r	616	LHG	C23-C24-C25-C26
30	s	616	LHG	C23-C24-C25-C26
31	B	622	LNL	C1-C2-C3-C4
31	b	625	LNL	C1-C2-C3-C4
31	c	521	LNL	C1-C2-C3-C4
32	B	621	PAM	C1-C2-C3-C4
33	H	502	DGD	C1B-C2B-C3B-C4B
23	N	612	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
23	Y	312	CLA	C8-C10-C11-C12
23	b	613	CLA	C8-C10-C11-C12
39	Y	302	CHL	C5-C6-C7-C8
39	Y	307	CHL	C5-C6-C7-C8
39	y	303	CHL	C5-C6-C7-C8
26	a	409	SQD	C14-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18
23	c	513	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	A	405	PHO	C13-C15-C16-C17
24	a	406	PHO	C13-C15-C16-C17
26	M	101	SQD	C23-C24-C25-C26
28	A	410	3PH	C21-C22-C23-C24
31	I	101	LNL	C1-C2-C3-C4
31	a	401	LNL	C1-C2-C3-C4
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	C5-C6-C7-C8
23	C	505	CLA	C15-C16-C17-C18
23	R	604	CLA	C5-C6-C7-C8
23	c	505	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
23	r	604	CLA	C5-C6-C7-C8
23	C	509	CLA	C6-C7-C8-C10
23	N	603	CLA	C11-C12-C13-C15
23	N	613	CLA	C12-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C7
23	b	602	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C10-C8-C7
23	c	501	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C15
23	s	613	CLA	C11-C10-C8-C7
39	R	606	CHL	C12-C13-C15-C16
23	y	313	CLA	C3-C5-C6-C7
42	R	615	XAT	C13-C14-C15-C35
42	Y	301	XAT	C9-C10-C11-C12
42	r	615	XAT	C13-C14-C15-C35
42	y	302	XAT	C9-C10-C11-C12
23	B	610	CLA	C2A-CAA-CBA-CGA
23	R	604	CLA	C2A-CAA-CBA-CGA
23	S	612	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
23	r	604	CLA	C2A-CAA-CBA-CGA
23	s	612	CLA	C2A-CAA-CBA-CGA
23	N	614	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	n	602	CLA	C5-C6-C7-C8
23	r	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	C	523	VIV	C18-C20-C21-C22
39	R	606	CHL	C5-C6-C7-C8
39	g	601	CHL	C5-C6-C7-C8
30	a	412	LHG	C33-C34-C35-C36
25	b	619	BCR	C6-C7-C8-C9
23	D	406	CLA	O1A-CGA-O2A-C1
23	N	612	CLA	O1A-CGA-O2A-C1
23	S	611	CLA	O1A-CGA-O2A-C1
23	d	405	CLA	C10-C11-C12-C13
39	G	601	CHL	C8-C10-C11-C12
29	A	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C9-C11-C12-C13
25	B	617	BCR	C10-C11-C12-C13
25	V	101	BCR	C18-C19-C20-C21
25	v	101	BCR	C18-C19-C20-C21
40	Y	315	LUT	C30-C31-C32-C33
40	Y	316	LUT	C30-C31-C32-C33
40	n	616	LUT	C30-C31-C32-C33
40	r	613	LUT	C10-C11-C12-C13
40	s	614	LUT	C10-C11-C12-C13
40	s	614	LUT	C30-C31-C32-C33
40	y	316	LUT	C30-C31-C32-C33
40	y	317	LUT	C30-C31-C32-C33
42	N	619	XAT	C10-C11-C12-C13
42	n	620	XAT	C10-C11-C12-C13
30	g	618	LHG	C27-C28-C29-C30
30	d	404	LHG	O2-C2-C3-O3
30	n	619	LHG	O2-C2-C3-O3
23	B	603	CLA	C5-C6-C7-C8
23	B	612	CLA	C13-C15-C16-C17
23	Y	310	CLA	C5-C6-C7-C8
23	r	602	CLA	C5-C6-C7-C8
39	G	609	CHL	C5-C6-C7-C8
23	B	601	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
28	W	201	3PH	C3B-C3C-C3D-C3E
28	d	403	3PH	O32-C31-O31-C3
30	D	408	LHG	C7-C8-C9-C10
23	C	508	CLA	C5-C6-C7-C8
23	S	613	CLA	C13-C15-C16-C17
23	b	613	CLA	C10-C11-C12-C13
23	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	C5-C6-C7-C8
23	g	610	CLA	C5-C6-C7-C8
23	y	315	CLA	C5-C6-C7-C8
39	y	310	CHL	C8-C10-C11-C12
23	g	602	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	C8-C10-C11-C12
39	g	609	CHL	C8-C10-C11-C12
30	A	412	LHG	C3-O3-P-O6
30	A	412	LHG	C4-O6-P-O3
30	G	618	LHG	C3-O3-P-O6
30	R	616	LHG	C3-O3-P-O6
30	S	616	LHG	C4-O6-P-O3
30	b	627	LHG	C3-O3-P-O6
30	d	404	LHG	C4-O6-P-O3
30	g	618	LHG	C3-O3-P-O6
30	s	616	LHG	C4-O6-P-O3
26	L	101	SQD	C7-C8-C9-C10
23	r	602	CLA	C3-C5-C6-C7
39	G	607	CHL	C3-C5-C6-C7
23	C	513	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
30	d	404	LHG	C24-C23-O8-C6
23	B	607	CLA	O1D-CGD-O2D-CED
27	b	628	LMG	C21-C22-C23-C24
23	n	613	CLA	O1D-CGD-O2D-CED
30	N	618	LHG	C1-C2-C3-O3
30	S	616	LHG	C1-C2-C3-O3
30	d	404	LHG	C1-C2-C3-O3
30	n	619	LHG	C1-C2-C3-O3
30	s	616	LHG	C1-C2-C3-O3
29	d	407	PL9	C15-C14-C16-C17
23	B	616	CLA	C2-C3-C5-C6
23	R	602	CLA	C13-C15-C16-C17
23	y	314	CLA	C5-C6-C7-C8
23	C	501	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	n	614	CLA	C2A-CAA-CBA-CGA
39	G	607	CHL	C2A-CAA-CBA-CGA
39	N	608	CHL	C2A-CAA-CBA-CGA
23	c	506	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	C	523	VIV	C25-C26-C27-C28
30	s	616	LHG	C24-C23-O8-C6
33	d	411	DGD	O6D-C5D-C6D-O5D
37	D	410	DGA	CB4-CB5-CB6-CB7
40	Y	316	LUT	C29-C30-C31-C32
41	N	617	NEX	C29-C30-C31-C32
42	R	615	XAT	C33-C34-C35-C15
42	Y	301	XAT	C33-C34-C35-C15
42	r	615	XAT	C9-C10-C11-C12
42	r	615	XAT	C33-C34-C35-C15
31	C	522	LNL	C1-C2-C3-C4
28	w	202	3PH	C34-C35-C36-C37
30	G	618	LHG	C34-C35-C36-C37
30	N	618	LHG	C12-C13-C14-C15
31	C	522	LNL	C3-C4-C5-C6
23	Y	314	CLA	CBD-CGD-O2D-CED
23	b	611	CLA	C15-C16-C17-C18
25	b	617	BCR	C20-C21-C22-C37
40	G	615	LUT	C11-C10-C9-C19
40	G	615	LUT	C40-C33-C34-C35
40	G	616	LUT	C20-C13-C14-C15
40	G	616	LUT	C39-C29-C30-C31
40	G	616	LUT	C40-C33-C34-C35
40	N	615	LUT	C40-C33-C34-C35
40	N	616	LUT	C40-C33-C34-C35
40	R	613	LUT	C20-C13-C14-C15
40	S	614	LUT	C20-C13-C14-C15
40	Y	315	LUT	C20-C13-C14-C15
40	g	616	LUT	C20-C13-C14-C15
40	g	616	LUT	C40-C33-C34-C35
40	n	615	LUT	C39-C29-C30-C31
40	n	616	LUT	C40-C33-C34-C35
40	r	613	LUT	C20-C13-C14-C15
40	r	613	LUT	C40-C33-C34-C35
40	s	614	LUT	C20-C13-C14-C15
40	s	614	LUT	C40-C33-C34-C35
40	s	615	LUT	C39-C29-C30-C31
40	y	316	LUT	C20-C13-C14-C15
41	G	617	NEX	C39-C29-C30-C31
41	G	617	NEX	C40-C33-C34-C35
41	R	614	NEX	C39-C29-C30-C31
41	R	618	NEX	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
41	S	617	NEX	C11-C10-C9-C19
41	Y	317	NEX	C39-C29-C30-C31
41	g	617	NEX	C20-C13-C14-C15
41	g	617	NEX	C40-C33-C34-C35
41	n	618	NEX	C20-C13-C14-C15
41	r	614	NEX	C20-C13-C14-C15
41	r	614	NEX	C39-C29-C30-C31
41	s	617	NEX	C11-C10-C9-C19
41	s	617	NEX	C20-C13-C14-C15
42	G	619	XAT	C11-C10-C9-C19
42	G	619	XAT	C39-C29-C30-C31
42	N	619	XAT	C39-C29-C30-C31
42	R	615	XAT	C20-C13-C14-C15
42	Y	301	XAT	C11-C10-C9-C19
42	Y	301	XAT	C20-C13-C14-C15
42	Y	301	XAT	C40-C33-C34-C35
42	r	615	XAT	C20-C13-C14-C15
42	y	302	XAT	C11-C10-C9-C19
42	y	302	XAT	C20-C13-C14-C15
26	A	408	SQD	C30-C31-C32-C33
27	d	409	LMG	C18-C19-C20-C21
28	A	410	3PH	C3A-C3B-C3C-C3D
28	X	201	3PH	C25-C26-C27-C28
30	d	404	LHG	C26-C27-C28-C29
31	A	414	LNL	C2-C3-C4-C5
31	C	517	LNL	C2-C3-C4-C5
31	C	520	LNL	C2-C3-C4-C5
31	b	623	LNL	C3-C4-C5-C6
31	c	520	LNL	C5-C6-C7-C8
31	c	521	LNL	C2-C3-C4-C5
31	i	101	LNL	C4-C5-C6-C7
33	C	515	DGD	CAA-CBA-CCA-CDA
33	C	515	DGD	CCA-CDA-CEA-CFA
33	C	515	DGD	CBB-CCB-CDB-CEB
37	b	626	DGA	CBB-CCB-CDB-CEB
23	b	607	CLA	O1D-CGD-O2D-CED
23	g	604	CLA	O1D-CGD-O2D-CED
26	A	408	SQD	C24-C23-O48-C46
26	A	408	SQD	C9-C10-C11-C12
27	A	409	LMG	C41-C42-C43-C44
27	R	617	LMG	C16-C17-C18-C19
28	C	524	3PH	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
28	C	524	3PH	C38-C39-C3A-C3B
28	D	403	3PH	C38-C39-C3A-C3B
28	L	102	3PH	C2A-C2B-C2C-C2D
30	R	616	LHG	C33-C34-C35-C36
30	Y	318	LHG	C34-C35-C36-C37
30	a	412	LHG	C12-C13-C14-C15
31	A	414	LNL	C3-C4-C5-C6
31	a	413	LNL	C5-C6-C7-C8
31	c	518	LNL	C5-C6-C7-C8
26	L	101	SQD	C46-C45-O47-C7
23	n	610	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	C15-C16-C17-C18
23	C	512	CLA	C10-C11-C12-C13
23	C	512	CLA	C13-C15-C16-C17
23	C	513	CLA	C5-C6-C7-C8
23	a	404	CLA	C15-C16-C17-C18
23	y	315	CLA	CBD-CGD-O2D-CED
26	a	409	SQD	C11-C10-C9-C8
28	T	101	3PH	C38-C39-C3A-C3B
30	D	408	LHG	C11-C12-C13-C14
30	d	408	LHG	C12-C13-C14-C15
30	s	616	LHG	C9-C10-C11-C12
31	A	413	LNL	C3-C4-C5-C6
31	C	521	LNL	C2-C3-C4-C5
31	C	521	LNL	C4-C5-C6-C7
31	b	623	LNL	C5-C6-C7-C8
37	b	626	DGA	CAA-CBA-CCA-CDA
37	b	626	DGA	CDB-CEB-CFB-CGB
23	N	602	CLA	O1D-CGD-O2D-CED
27	b	620	LMG	C31-C32-C33-C34
27	r	617	LMG	C16-C17-C18-C19
28	A	410	3PH	C34-C35-C36-C37
37	D	410	DGA	CB7-CB8-CB9-CAB
30	D	404	LHG	O2-C2-C3-O3
27	A	409	LMG	C40-C41-C42-C43
28	W	201	3PH	C33-C34-C35-C36
30	y	318	LHG	C11-C12-C13-C14
23	b	616	CLA	C3-C5-C6-C7
30	d	404	LHG	C7-C8-C9-C10
23	C	510	CLA	O1D-CGD-O2D-CED
25	C	514	BCR	C20-C21-C22-C23
25	b	617	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	c	514	BCR	C20-C21-C22-C23
27	R	617	LMG	C2-C1-O1-C7
40	N	616	LUT	C11-C10-C9-C8
40	N	616	LUT	C12-C13-C14-C15
40	N	616	LUT	C28-C29-C30-C31
40	R	613	LUT	C28-C29-C30-C31
40	Y	315	LUT	C28-C29-C30-C31
40	Y	315	LUT	C32-C33-C34-C35
40	y	316	LUT	C28-C29-C30-C31
40	y	316	LUT	C32-C33-C34-C35
41	N	617	NEX	C32-C33-C34-C35
41	R	614	NEX	C11-C10-C9-C8
41	R	618	NEX	C11-C10-C9-C8
41	R	618	NEX	C28-C29-C30-C31
41	Y	317	NEX	C28-C29-C30-C31
41	g	617	NEX	C28-C29-C30-C31
41	r	614	NEX	C32-C33-C34-C35
42	R	615	XAT	C11-C10-C9-C8
42	Y	301	XAT	C11-C10-C9-C8
42	Y	301	XAT	C28-C29-C30-C31
42	Y	301	XAT	C32-C33-C34-C35
42	r	615	XAT	C11-C10-C9-C8
42	y	302	XAT	C11-C10-C9-C8
42	y	302	XAT	C32-C33-C34-C35
27	r	617	LMG	C31-C32-C33-C34
30	D	404	LHG	C30-C31-C32-C33
30	a	412	LHG	C24-C25-C26-C27
31	c	519	LNL	C5-C6-C7-C8
33	H	502	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C15-C16-C17-C18
23	B	613	CLA	C16-C17-C18-C20
23	Y	304	CLA	C16-C17-C18-C20
23	y	305	CLA	C16-C17-C18-C20
23	N	610	CLA	O1D-CGD-O2D-CED
23	n	602	CLA	O1D-CGD-O2D-CED
23	S	613	CLA	C4-C3-C5-C6
29	D	407	PL9	C15-C14-C16-C17
29	D	407	PL9	C45-C44-C46-C47
39	G	620	CHL	C4-C3-C5-C6
39	g	607	CHL	C4-C3-C5-C6
28	A	410	3PH	C38-C39-C3A-C3B
28	C	524	3PH	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
28	d	403	3PH	C24-C25-C26-C27
28	w	202	3PH	C35-C36-C37-C38
30	D	404	LHG	C33-C34-C35-C36
30	d	408	LHG	C11-C12-C13-C14
29	a	411	PL9	C13-C14-C16-C17
29	d	407	PL9	C13-C14-C16-C17
23	B	611	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	N	603	CLA	C11-C10-C8-C9
23	R	608	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C12-C13-C14
23	g	611	CLA	C14-C13-C15-C16
24	A	405	PHO	C14-C13-C15-C16
35	y	301	VIV	C19-C18-C20-C21
39	n	607	CHL	C11-C10-C8-C9
31	B	623	LNL	C1-C2-C3-C4
26	A	408	SQD	C12-C13-C14-C15
28	W	201	3PH	C24-C25-C26-C27
30	r	616	LHG	C29-C30-C31-C32
30	y	318	LHG	C10-C11-C12-C13
30	y	318	LHG	C29-C30-C31-C32
31	C	519	LNL	C2-C3-C4-C5
31	a	401	LNL	C2-C3-C4-C5
33	H	502	DGD	C5B-C6B-C7B-C8B
33	H	502	DGD	C7B-C8B-C9B-CAB
33	d	411	DGD	C4A-C5A-C6A-C7A
23	b	605	CLA	C5-C6-C7-C8
23	N	613	CLA	C2A-CAA-CBA-CGA
23	S	613	CLA	C2A-CAA-CBA-CGA
39	G	606	CHL	C2A-CAA-CBA-CGA
23	b	616	CLA	O1A-CGA-O2A-C1
40	G	615	LUT	C27-C28-C29-C39
40	S	614	LUT	C27-C28-C29-C39
40	n	615	LUT	C11-C12-C13-C20
41	g	617	NEX	C11-C12-C13-C20
41	n	618	NEX	C11-C12-C13-C20
42	y	302	XAT	C7-C8-C9-C19
31	I	101	LNL	C3-C4-C5-C6
31	I	101	LNL	C5-C6-C7-C8
31	a	413	LNL	C2-C3-C4-C5
31	b	625	LNL	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	c	522	LNL	C5-C6-C7-C8
40	N	616	LUT	C27-C28-C29-C30
40	Y	316	LUT	C7-C8-C9-C10
40	y	317	LUT	C7-C8-C9-C10
42	R	615	XAT	C7-C8-C9-C10
42	n	617	XAT	C7-C8-C9-C10
42	r	615	XAT	C7-C8-C9-C10
42	y	302	XAT	C7-C8-C9-C10
23	b	609	CLA	C3-C5-C6-C7
39	g	607	CHL	C3-C5-C6-C7
30	Y	318	LHG	O9-C7-O7-C5
23	g	611	CLA	C15-C16-C17-C18
23	r	608	CLA	C13-C15-C16-C17
28	s	618	3PH	C22-C21-O21-C2
30	Y	318	LHG	C8-C7-O7-C5
30	y	318	LHG	C8-C7-O7-C5
27	R	617	LMG	C39-C40-C41-C42
28	a	410	3PH	C36-C37-C38-C39
31	I	101	LNL	C2-C3-C4-C5
31	a	401	LNL	C6-C7-C8-C9
26	M	101	SQD	C10-C11-C12-C13
27	B	620	LMG	C13-C14-C15-C16
27	R	617	LMG	C32-C33-C34-C35
28	W	201	3PH	C35-C36-C37-C38
28	s	618	3PH	C3A-C3B-C3C-C3D
30	D	408	LHG	C32-C33-C34-C35
30	N	618	LHG	C11-C12-C13-C14
31	B	623	LNL	C3-C4-C5-C6
31	c	518	LNL	C4-C5-C6-C7
31	i	101	LNL	C2-C3-C4-C5
33	d	411	DGD	C9B-CAB-CBB-CCB
37	b	626	DGA	CAB-CBB-CCB-CDB
27	R	617	LMG	O6-C1-O1-C7
23	r	608	CLA	C15-C16-C17-C18
35	y	301	VIV	C15-C16-C17-C18
39	r	606	CHL	C8-C10-C11-C12
26	L	101	SQD	C30-C31-C32-C33
26	M	101	SQD	C14-C15-C16-C17
30	N	618	LHG	C32-C33-C34-C35
23	c	508	CLA	CBD-CGD-O2D-CED
23	y	306	CLA	CBD-CGD-O2D-CED
27	C	525	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	R	617	LMG	C30-C31-C32-C33
27	r	617	LMG	C23-C24-C25-C26
28	x	201	3PH	C34-C35-C36-C37
31	b	625	LNL	C4-C5-C6-C7
33	d	411	DGD	C4B-C5B-C6B-C7B
27	B	626	LMG	C28-C29-C30-C31
27	R	617	LMG	C28-C29-C30-C31
27	b	620	LMG	C28-C29-C30-C31
30	Y	318	LHG	C23-C24-C25-C26
23	b	608	CLA	C15-C16-C17-C18
39	G	601	CHL	C13-C15-C16-C17
23	C	513	CLA	O1A-CGA-O2A-C1
30	s	616	LHG	O10-C23-O8-C6
27	R	617	LMG	C36-C37-C38-C39
27	b	628	LMG	C16-C17-C18-C19
28	T	101	3PH	C2E-C2F-C2G-C2H
31	C	518	LNL	C5-C6-C7-C8
31	b	623	LNL	C2-C3-C4-C5
23	n	602	CLA	C3-C5-C6-C7
26	M	101	SQD	C15-C16-C17-C18
27	d	409	LMG	C19-C20-C21-C22
30	n	619	LHG	C29-C30-C31-C32
31	c	517	LNL	C2-C3-C4-C5
23	D	406	CLA	O1D-CGD-O2D-CED
23	G	602	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	A	402	CLA	C3A-C2A-CAA-CBA
23	N	603	CLA	C3A-C2A-CAA-CBA
23	Y	304	CLA	C3A-C2A-CAA-CBA
23	a	403	CLA	C3A-C2A-CAA-CBA
23	g	603	CLA	C3A-C2A-CAA-CBA
23	n	603	CLA	C3A-C2A-CAA-CBA
23	r	601	CLA	C3A-C2A-CAA-CBA
23	s	608	CLA	C3A-C2A-CAA-CBA
24	D	402	PHO	C3A-C2A-CAA-CBA
40	G	615	LUT	C29-C30-C31-C32
41	Y	317	NEX	C9-C10-C11-C12
26	M	101	SQD	C25-C26-C27-C28
27	b	620	LMG	C38-C39-C40-C41
31	C	518	LNL	C4-C5-C6-C7
31	A	413	LNL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	O1A-CGA-O2A-C1
30	d	404	LHG	O10-C23-O8-C6
23	Y	304	CLA	C16-C17-C18-C19
30	D	408	LHG	C28-C29-C30-C31
30	L	103	LHG	C16-C17-C18-C19
33	C	515	DGD	C8A-C9A-CAA-CBA
23	Y	305	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
30	D	408	LHG	C12-C13-C14-C15
31	B	625	LNL	C4-C5-C6-C7
33	C	515	DGD	C7A-C8A-C9A-CAA
40	G	615	LUT	C14-C15-C35-C34
40	R	613	LUT	C14-C15-C35-C34
23	g	603	CLA	C3-C5-C6-C7
28	C	524	3PH	C21-C22-C23-C24
30	n	619	LHG	C25-C26-C27-C28
31	b	623	LNL	C4-C5-C6-C7
29	d	407	PL9	C45-C44-C46-C47
39	N	606	CHL	C4-C3-C5-C6
23	C	511	CLA	CBA-CGA-O2A-C1
23	r	610	CLA	CBA-CGA-O2A-C1
23	S	613	CLA	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
39	N	606	CHL	C2-C3-C5-C6
39	g	607	CHL	C2-C3-C5-C6
39	g	619	CHL	C2-C3-C5-C6
30	a	412	LHG	C8-C7-O7-C5
28	s	618	3PH	C23-C24-C25-C26
33	C	515	DGD	C4B-C5B-C6B-C7B
30	D	408	LHG	O1-C1-C2-O2
30	L	103	LHG	O1-C1-C2-O2
30	N	618	LHG	O1-C1-C2-O2
30	S	616	LHG	O1-C1-C2-O2
30	b	627	LHG	O1-C1-C2-O2
30	d	404	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
30	r	616	LHG	O1-C1-C2-O2
26	A	408	SQD	C25-C26-C27-C28
27	w	201	LMG	C39-C40-C41-C42
30	D	408	LHG	C18-C19-C20-C21
30	n	619	LHG	C11-C10-C9-C8
31	a	413	LNL	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	d	411	DGD	C6A-C7A-C8A-C9A
33	d	411	DGD	C5B-C6B-C7B-C8B
23	N	613	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	C16-C17-C18-C19
30	b	627	LHG	O2-C2-C3-O3
23	y	311	CLA	C8-C10-C11-C12
26	a	409	SQD	C11-C12-C13-C14
23	C	512	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	CBA-CGA-O2A-C1
31	c	522	LNL	C3-C4-C5-C6
23	B	611	CLA	C8-C10-C11-C12
23	c	512	CLA	C10-C11-C12-C13
30	L	103	LHG	C1-C2-C3-O3
30	G	618	LHG	C24-C25-C26-C27
28	s	618	3PH	O22-C21-O21-C2
30	y	318	LHG	O9-C7-O7-C5
23	S	613	CLA	C2-C1-O2A-CGA
23	s	613	CLA	C2-C1-O2A-CGA
27	B	620	LMG	C31-C32-C33-C34
28	a	410	3PH	C38-C39-C3A-C3B
30	D	408	LHG	C29-C30-C31-C32
30	d	404	LHG	C13-C14-C15-C16
30	n	619	LHG	C10-C11-C12-C13
23	S	610	CLA	C5-C6-C7-C8
23	b	610	CLA	C15-C16-C17-C18
23	b	612	CLA	C13-C15-C16-C17
23	s	610	CLA	C5-C6-C7-C8
35	y	301	VIV	C18-C20-C21-C22
39	y	310	CHL	C5-C6-C7-C8
26	A	408	SQD	O10-C23-O48-C46
30	A	412	LHG	C26-C27-C28-C29
30	R	616	LHG	C31-C32-C33-C34
31	c	518	LNL	C1-C2-C3-C4
25	C	514	BCR	C5-C6-C7-C8
25	H	501	BCR	C5-C6-C7-C8
25	H	501	BCR	C23-C24-C25-C26
25	H	501	BCR	C23-C24-C25-C30
25	K	101	BCR	C5-C6-C7-C8
25	V	101	BCR	C1-C6-C7-C8
25	V	101	BCR	C5-C6-C7-C8
25	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	d	410	BCR	C1-C6-C7-C8
25	d	410	BCR	C5-C6-C7-C8
25	h	501	BCR	C1-C6-C7-C8
25	h	501	BCR	C5-C6-C7-C8
25	h	501	BCR	C23-C24-C25-C26
25	h	501	BCR	C23-C24-C25-C30
25	k	101	BCR	C5-C6-C7-C8
25	v	101	BCR	C1-C6-C7-C8
25	v	101	BCR	C5-C6-C7-C8
39	N	607	CHL	C3-C5-C6-C7
40	G	615	LUT	C5-C6-C7-C8
40	N	615	LUT	C5-C6-C7-C8
40	N	616	LUT	C1-C6-C7-C8
40	R	613	LUT	C1-C6-C7-C8
40	S	614	LUT	C1-C6-C7-C8
40	Y	315	LUT	C1-C6-C7-C8
40	g	615	LUT	C1-C6-C7-C8
40	n	615	LUT	C1-C6-C7-C8
40	n	616	LUT	C1-C6-C7-C8
40	r	613	LUT	C1-C6-C7-C8
40	s	615	LUT	C1-C6-C7-C8
40	y	316	LUT	C1-C6-C7-C8
28	C	524	3PH	C2B-C2C-C2D-C2E
30	y	318	LHG	C26-C27-C28-C29
23	R	610	CLA	CBA-CGA-O2A-C1
23	g	614	CLA	CBA-CGA-O2A-C1
39	R	606	CHL	C13-C15-C16-C17
39	g	619	CHL	C5-C6-C7-C8
28	a	410	3PH	C22-C21-O21-C2
26	L	101	SQD	C28-C29-C30-C31
28	L	102	3PH	C2D-C2E-C2F-C2G
30	G	618	LHG	C15-C16-C17-C18
31	A	414	LNL	C5-C6-C7-C8
33	C	515	DGD	C5A-C6A-C7A-C8A
33	H	502	DGD	CBA-CCA-CDA-CEA
33	c	515	DGD	C4B-C5B-C6B-C7B
26	M	101	SQD	C30-C31-C32-C33
28	d	403	3PH	C39-C3A-C3B-C3C
31	a	401	LNL	C15-C16-C17-C18
23	y	306	CLA	C15-C16-C17-C18
23	C	508	CLA	C4-C3-C5-C6
29	a	411	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
39	N	609	CHL	C4-C3-C5-C6
39	n	601	CHL	C4-C3-C5-C6
23	d	406	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C11-C12-C13-C15
23	C	506	CLA	C2-C3-C5-C6
23	C	513	CLA	C12-C13-C15-C16
23	D	406	CLA	C12-C13-C15-C16
23	G	610	CLA	C12-C13-C15-C16
23	N	603	CLA	C11-C10-C8-C7
23	R	608	CLA	C11-C12-C13-C15
23	Y	311	CLA	C11-C10-C8-C7
23	Y	313	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	501	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	y	305	CLA	C6-C7-C8-C10
23	y	306	CLA	C6-C7-C8-C10
23	y	312	CLA	C11-C10-C8-C7
23	y	314	CLA	C2-C3-C5-C6
29	d	407	PL9	C43-C44-C46-C47
35	y	301	VIV	C22-C23-C24-C25
39	G	620	CHL	C2-C3-C5-C6
23	s	613	CLA	C3-C5-C6-C7
23	C	512	CLA	O1A-CGA-O2A-C1
23	r	610	CLA	O1A-CGA-O2A-C1
40	n	615	LUT	C9-C10-C11-C12
42	R	615	XAT	C9-C10-C11-C12
35	C	523	VIV	C25-C26-C27-C29
31	C	519	LNL	C6-C7-C8-C9
31	b	622	LNL	C6-C7-C8-C9
30	a	412	LHG	O9-C7-O7-C5
23	B	607	CLA	CBA-CGA-O2A-C1
23	G	614	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	n	611	CLA	CBA-CGA-O2A-C1
30	R	616	LHG	C24-C23-O8-C6
30	D	404	LHG	C27-C28-C29-C30
30	L	103	LHG	C32-C33-C34-C35
31	C	522	LNL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	R	612	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
23	g	613	CLA	C2A-CAA-CBA-CGA
23	s	608	CLA	C2A-CAA-CBA-CGA
39	G	620	CHL	C2A-CAA-CBA-CGA
39	N	607	CHL	C2A-CAA-CBA-CGA
39	R	607	CHL	C2A-CAA-CBA-CGA
39	g	619	CHL	C2A-CAA-CBA-CGA
33	H	502	DGD	C4D-C5D-C6D-O5D
23	B	605	CLA	C5-C6-C7-C8
23	B	611	CLA	C15-C16-C17-C18
23	B	616	CLA	C5-C6-C7-C8
23	Y	313	CLA	C5-C6-C7-C8
27	d	409	LMG	C17-C18-C19-C20
28	A	410	3PH	C3D-C3E-C3F-C3G
30	S	616	LHG	C10-C11-C12-C13
31	C	520	LNL	C5-C6-C7-C8
23	B	606	CLA	O1D-CGD-O2D-CED
30	a	412	LHG	C25-C26-C27-C28
30	b	627	LHG	C28-C29-C30-C31
30	A	412	LHG	C23-C24-C25-C26
23	y	314	CLA	C8-C10-C11-C12
27	r	617	LMG	C32-C33-C34-C35
28	x	201	3PH	C38-C39-C3A-C3B
31	a	413	LNL	C3-C4-C5-C6
33	H	502	DGD	CBB-CCB-CDB-CEB
25	b	617	BCR	C6-C7-C8-C9
23	C	511	CLA	O1A-CGA-O2A-C1
23	N	611	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	CBD-CGD-O2D-CED
23	Y	310	CLA	C8-C10-C11-C12
23	c	503	CLA	C5-C6-C7-C8
23	n	602	CLA	C10-C11-C12-C13
23	y	311	CLA	C13-C15-C16-C17
27	c	523	LMG	C32-C33-C34-C35
31	A	413	LNL	C2-C3-C4-C5
30	d	408	LHG	C7-C8-C9-C10
31	c	517	LNL	C1-C2-C3-C4
30	S	616	LHG	C8-C7-O7-C5
40	Y	315	LUT	C14-C15-C35-C34
40	y	316	LUT	C14-C15-C35-C34
41	n	618	NEX	C14-C15-C35-C34

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	CBD-CGD-O2D-CED
28	a	410	3PH	O22-C21-O21-C2
23	B	607	CLA	C3-C5-C6-C7
26	A	408	SQD	C15-C16-C17-C18
31	A	414	LNL	C4-C5-C6-C7
33	C	515	DGD	CEA-CFA-CGA-CHA
26	a	409	SQD	C2-C1-O6-C44
23	B	608	CLA	C15-C16-C17-C18
26	A	408	SQD	O6-C44-C45-O47
30	R	616	LHG	O7-C5-C6-O8
30	Y	318	LHG	O7-C5-C6-O8
30	d	404	LHG	O7-C5-C6-O8
26	A	408	SQD	C29-C30-C31-C32
28	T	101	3PH	C22-C23-C24-C25
23	c	506	CLA	C16-C17-C18-C20
26	A	408	SQD	C14-C15-C16-C17
27	r	617	LMG	C18-C19-C20-C21
28	W	201	3PH	C3A-C3B-C3C-C3D
33	C	515	DGD	C9A-CAA-CBA-CCA
23	C	512	CLA	C15-C16-C17-C18
31	a	413	LNL	C6-C7-C8-C9
31	b	625	LNL	C6-C7-C8-C9
23	C	506	CLA	C4-C3-C5-C6
23	Y	313	CLA	C4-C3-C5-C6
23	y	314	CLA	C4-C3-C5-C6
30	r	616	LHG	C7-C8-C9-C10
23	D	406	CLA	C2-C3-C5-C6
29	D	407	PL9	C43-C44-C46-C47
39	N	609	CHL	C2-C3-C5-C6
29	D	407	PL9	C4-C3-C7-C8
29	d	407	PL9	C4-C3-C7-C8
28	s	618	3PH	C35-C36-C37-C38
23	A	403	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C14
23	C	512	CLA	C11-C12-C13-C14
23	C	513	CLA	C14-C13-C15-C16
23	D	406	CLA	C14-C13-C15-C16
23	G	610	CLA	C14-C13-C15-C16
23	N	613	CLA	C14-C13-C15-C16
23	S	610	CLA	C14-C13-C15-C16
23	a	404	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C11-C12-C13-C14
23	b	605	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C10-C8-C9
23	d	405	CLA	C11-C12-C13-C14
23	s	610	CLA	C14-C13-C15-C16
23	s	613	CLA	C14-C13-C15-C16
23	y	305	CLA	C6-C7-C8-C9
23	y	313	CLA	C14-C13-C15-C16
28	C	524	3PH	C3D-C3E-C3F-C3G
30	S	616	LHG	C18-C19-C20-C21
23	Y	312	CLA	C3-C5-C6-C7
39	y	303	CHL	C3-C5-C6-C7
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
27	w	201	LMG	C37-C38-C39-C40
28	D	403	3PH	C24-C25-C26-C27
30	G	618	LHG	C11-C10-C9-C8
30	a	412	LHG	C29-C30-C31-C32
37	b	626	DGA	CA2-CA1-OG1-CG1
25	b	617	BCR	C7-C8-C9-C34
42	N	619	XAT	C31-C32-C33-C40
23	G	612	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	C5-C6-C7-C8
26	L	101	SQD	C11-C12-C13-C14
27	b	620	LMG	C13-C14-C15-C16
25	b	617	BCR	C21-C22-C23-C24
25	c	514	BCR	C7-C8-C9-C10
23	R	610	CLA	O1A-CGA-O2A-C1
23	g	614	CLA	O1A-CGA-O2A-C1
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	403	CLA	C1A-C2A-CAA-CBA
23	A	406	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	N	603	CLA	C1A-C2A-CAA-CBA
23	N	610	CLA	C1A-C2A-CAA-CBA
23	Y	304	CLA	C1A-C2A-CAA-CBA
23	a	403	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	g	603	CLA	C1A-C2A-CAA-CBA
23	n	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	r	601	CLA	C1A-C2A-CAA-CBA
23	s	608	CLA	C1A-C2A-CAA-CBA
23	y	315	CLA	C1A-C2A-CAA-CBA
39	G	608	CHL	C1A-C2A-CAA-CBA
39	G	609	CHL	C1A-C2A-CAA-CBA
39	s	607	CHL	C1A-C2A-CAA-CBA
23	B	613	CLA	C16-C17-C18-C19
30	S	616	LHG	O9-C7-O7-C5
31	C	521	LNL	C7-C8-C9-C10
40	y	317	LUT	C29-C30-C31-C32
42	R	615	XAT	C29-C30-C31-C32
23	C	503	CLA	C5-C6-C7-C8
23	C	507	CLA	C8-C10-C11-C12
23	a	404	CLA	C13-C15-C16-C17
30	D	408	LHG	C4-O6-P-O3
28	d	403	3PH	C31-C32-C33-C34
23	Y	304	CLA	C3-C5-C6-C7
23	A	403	CLA	C13-C15-C16-C17
23	B	610	CLA	C15-C16-C17-C18
23	b	609	CLA	C15-C16-C17-C18
39	r	606	CHL	C5-C6-C7-C8
27	R	617	LMG	C29-C28-O8-C9
28	T	101	3PH	O11-C1-C2-C3
28	w	202	3PH	O11-C1-C2-C3
28	x	201	3PH	O11-C1-C2-C3
28	A	410	3PH	C3C-C3D-C3E-C3F
31	c	522	LNL	C2-C3-C4-C5
27	B	626	LMG	O6-C5-C6-O5
31	c	519	LNL	C6-C7-C8-C9
32	b	621	PAM	C6-C7-C8-C9
30	L	103	LHG	C14-C15-C16-C17
27	c	523	LMG	O6-C5-C6-O5
30	G	618	LHG	C1-C2-C3-O3
23	g	610	CLA	C4-C3-C5-C6
39	g	619	CHL	C4-C3-C5-C6
30	Y	318	LHG	C33-C34-C35-C36
31	c	521	LNL	C5-C6-C7-C8
27	b	628	LMG	O6-C5-C6-O5
31	B	625	LNL	C2-C3-C4-C5
31	C	518	LNL	C2-C3-C4-C5
31	b	624	LNL	C2-C3-C4-C5
31	C	519	LNL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	O1A-CGA-O2A-C1
30	n	619	LHG	C15-C16-C17-C18
23	c	513	CLA	C11-C12-C13-C14
23	S	612	CLA	O1D-CGD-O2D-CED
26	L	101	SQD	C27-C28-C29-C30
26	L	101	SQD	C32-C33-C34-C35
26	M	101	SQD	O6-C44-C45-C46
26	M	101	SQD	C44-C45-C46-O48
30	A	412	LHG	C4-C5-C6-O8
30	D	408	LHG	C4-C5-C6-O8
30	d	408	LHG	C4-C5-C6-O8
30	s	616	LHG	C4-C5-C6-O8
37	D	410	DGA	OG1-CG1-CG2-CG3
23	Y	305	CLA	C5-C6-C7-C8
30	d	408	LHG	C31-C32-C33-C34
33	C	515	DGD	C7B-C8B-C9B-CAB
23	n	611	CLA	O1A-CGA-O2A-C1
30	R	616	LHG	O10-C23-O8-C6
26	A	408	SQD	C19-C20-C21-C22
26	M	101	SQD	C31-C32-C33-C34
23	r	608	CLA	O1D-CGD-O2D-CED
23	G	614	CLA	O1A-CGA-O2A-C1
27	b	628	LMG	O6-C1-O1-C7
29	a	411	PL9	C14-C16-C17-C18
31	c	517	LNL	C4-C5-C6-C7
23	g	613	CLA	CBD-CGD-O2D-CED
30	D	404	LHG	O1-C1-C2-O2
39	S	607	CHL	O2A-C1-C2-C3
28	T	101	3PH	C32-C33-C34-C35
33	H	502	DGD	C2B-C3B-C4B-C5B
37	b	626	DGA	CA9-CAA-CBA-CCA
23	B	602	CLA	C10-C11-C12-C13
31	C	517	LNL	C1-C2-C3-C4
31	a	413	LNL	C1-C2-C3-C4
28	W	201	3PH	C26-C27-C28-C29
26	A	408	SQD	C8-C7-O47-C45
35	y	301	VIV	C20-C21-C22-C23
25	h	501	BCR	C16-C17-C18-C36
40	S	615	LUT	C20-C13-C14-C15
41	R	618	NEX	C39-C29-C30-C31
41	r	614	NEX	C11-C10-C9-C19
42	N	619	XAT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
42	n	620	XAT	C11-C10-C9-C19
39	G	607	CHL	C4-C3-C5-C6
39	y	310	CHL	C4-C3-C5-C6
23	c	512	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CBA-CGA-O2A-C1
23	b	612	CLA	CBA-CGA-O2A-C1
27	C	525	LMG	O6-C5-C6-O5
28	W	201	3PH	C25-C26-C27-C28
33	H	502	DGD	C6B-C7B-C8B-C9B
23	C	509	CLA	CBD-CGD-O2D-CED
23	Y	303	CLA	C15-C16-C17-C18
23	n	610	CLA	C13-C15-C16-C17
37	b	626	DGA	CB6-CB7-CB8-CB9
23	B	602	CLA	C2A-CAA-CBA-CGA
23	Y	313	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C15-C16-C17-C18
23	y	304	CLA	C15-C16-C17-C18
26	A	408	SQD	C10-C11-C12-C13
31	C	520	LNL	C4-C5-C6-C7
23	N	612	CLA	O1D-CGD-O2D-CED
23	n	604	CLA	O1D-CGD-O2D-CED
28	T	101	3PH	C1-O11-P-O12
28	a	410	3PH	C1-O11-P-O12
40	N	615	LUT	C26-C27-C28-C29
23	s	609	CLA	C2C-C3C-CAC-CBC
26	L	101	SQD	C9-C10-C11-C12
30	L	103	LHG	C15-C16-C17-C18
30	a	412	LHG	C31-C32-C33-C34
23	b	607	CLA	CBA-CGA-O2A-C1
26	a	409	SQD	C24-C23-O48-C46
23	B	607	CLA	O1A-CGA-O2A-C1
28	A	410	3PH	O11-C1-C2-O21
30	d	404	LHG	O6-C4-C5-O7
27	b	628	LMG	O8-C28-C29-C30
30	n	619	LHG	C9-C10-C11-C12
23	g	612	CLA	O1D-CGD-O2D-CED
37	b	626	DGA	OA1-CA1-OG1-CG1
32	b	621	PAM	C3-C4-C5-C6
23	c	506	CLA	C13-C15-C16-C17
40	S	615	LUT	C11-C10-C9-C8
42	y	302	XAT	C28-C29-C30-C31
28	a	410	3PH	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	CAA-CBA-CGA-O2A
28	W	201	3PH	O21-C2-C3-O31
30	y	318	LHG	O7-C5-C6-O8
26	a	409	SQD	C15-C16-C17-C18
23	c	507	CLA	C13-C15-C16-C17
23	C	508	CLA	O1D-CGD-O2D-CED
31	c	519	LNL	C1-C2-C3-C4
23	d	406	CLA	C5-C6-C7-C8
23	B	604	CLA	C6-C7-C8-C10
23	B	604	CLA	C11-C10-C8-C7
23	B	611	CLA	C6-C7-C8-C10
23	B	614	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	B	616	CLA	C6-C7-C8-C10
23	C	501	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C12-C13-C15
23	D	406	CLA	C11-C10-C8-C7
23	D	406	CLA	C11-C12-C13-C15
23	G	613	CLA	C11-C12-C13-C15
23	R	608	CLA	C12-C13-C15-C16
23	S	602	CLA	C11-C10-C8-C7
23	S	610	CLA	C6-C7-C8-C10
23	S	610	CLA	C11-C10-C8-C7
23	S	610	CLA	C12-C13-C15-C16
23	Y	303	CLA	C6-C7-C8-C10
23	Y	305	CLA	C11-C12-C13-C15
23	Y	312	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C10-C8-C7
23	b	603	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	b	614	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C10-C8-C7
23	d	405	CLA	C11-C12-C13-C15
23	n	603	CLA	C11-C12-C13-C15
23	s	610	CLA	C6-C7-C8-C10
23	s	610	CLA	C11-C10-C8-C7
23	s	610	CLA	C12-C13-C15-C16
23	y	304	CLA	C6-C7-C8-C10
23	y	305	CLA	C11-C10-C8-C7
23	y	311	CLA	C11-C12-C13-C15
23	y	313	CLA	C12-C13-C15-C16
23	y	314	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	y	315	CLA	C11-C12-C13-C15
35	y	301	VIV	C16-C17-C18-C20
35	y	301	VIV	C21-C22-C23-C24
39	G	620	CHL	C12-C13-C15-C16
39	N	606	CHL	C6-C7-C8-C10
39	R	606	CHL	C6-C7-C8-C10
39	g	607	CHL	C6-C7-C8-C10
39	n	601	CHL	C6-C7-C8-C10
39	r	606	CHL	C11-C10-C8-C7
33	H	502	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
23	B	603	CLA	C11-C10-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	B	605	CLA	C14-C13-C15-C16
23	B	608	CLA	C11-C12-C13-C14
23	B	616	CLA	C6-C7-C8-C9
23	C	501	CLA	C11-C10-C8-C9
23	C	502	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C12-C13-C14
23	D	405	CLA	C11-C12-C13-C14
23	D	406	CLA	C11-C10-C8-C9
23	D	406	CLA	C11-C12-C13-C14
23	G	613	CLA	C11-C12-C13-C14
23	R	608	CLA	C14-C13-C15-C16
23	R	609	CLA	C11-C12-C13-C14
23	S	602	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C10-C8-C9
23	c	502	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	g	611	CLA	C11-C12-C13-C14
23	r	609	CLA	C11-C12-C13-C14
23	y	304	CLA	C6-C7-C8-C9
23	y	306	CLA	C11-C10-C8-C9
23	y	314	CLA	C11-C12-C13-C14
23	y	314	CLA	C14-C13-C15-C16
23	y	315	CLA	C11-C12-C13-C14
24	a	406	PHO	C14-C13-C15-C16
35	y	301	VIV	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	N	606	CHL	C6-C7-C8-C9
39	n	601	CHL	C6-C7-C8-C9
27	c	523	LMG	C31-C32-C33-C34
32	B	621	PAM	C4-C5-C6-C7
23	a	404	CLA	CBA-CGA-O2A-C1
23	b	602	CLA	C13-C15-C16-C17
23	y	314	CLA	C2A-CAA-CBA-CGA
39	r	607	CHL	C2A-CAA-CBA-CGA
30	b	627	LHG	C35-C36-C37-C38
33	H	502	DGD	CCB-CDB-CEB-CFB
23	g	602	CLA	O1D-CGD-O2D-CED
25	d	410	BCR	C7-C8-C9-C34
40	N	616	LUT	C31-C32-C33-C40
23	b	613	CLA	C16-C17-C18-C20
28	A	410	3PH	C22-C23-C24-C25
28	T	101	3PH	C37-C38-C39-C3A
25	d	410	BCR	C7-C8-C9-C10
40	N	616	LUT	C31-C32-C33-C34
42	G	619	XAT	C27-C28-C29-C30
42	G	619	XAT	C31-C32-C33-C34
28	W	201	3PH	C28-C29-C2A-C2B
39	Y	302	CHL	C3-C5-C6-C7
30	D	404	LHG	C1-C2-C3-O3
23	n	603	CLA	C8-C10-C11-C12
39	G	620	CHL	C5-C6-C7-C8
23	B	612	CLA	O1A-CGA-O2A-C1
28	L	102	3PH	C35-C36-C37-C38
30	g	618	LHG	C10-C11-C12-C13
33	H	502	DGD	C4B-C5B-C6B-C7B
25	Z	101	BCR	C22-C23-C24-C25
24	A	405	PHO	CBD-CGD-O2D-CED
30	S	616	LHG	C30-C31-C32-C33
33	H	502	DGD	C5A-C6A-C7A-C8A
23	c	513	CLA	C11-C12-C13-C15
30	N	618	LHG	O6-C4-C5-C6
30	n	619	LHG	O6-C4-C5-C6
30	Y	318	LHG	C7-C8-C9-C10
23	C	512	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBA-CGA-O2A-C1
23	n	604	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	s	613	CLA	C13-C15-C16-C17
30	a	412	LHG	C27-C28-C29-C30
23	G	610	CLA	C4-C3-C5-C6
39	G	607	CHL	C2-C3-C5-C6
39	y	310	CHL	C2-C3-C5-C6
33	c	515	DGD	C5A-C6A-C7A-C8A
23	n	610	CLA	C5-C6-C7-C8
23	b	612	CLA	O1A-CGA-O2A-C1
23	G	610	CLA	C5-C6-C7-C8
28	W	201	3PH	C32-C31-O31-C3
33	H	502	DGD	CDB-CEB-CFB-CGB
23	y	306	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C3A-C2A-CAA-CBA
23	y	315	CLA	C3A-C2A-CAA-CBA
39	G	601	CHL	C3A-C2A-CAA-CBA
39	R	607	CHL	C3A-C2A-CAA-CBA
39	g	608	CHL	C3A-C2A-CAA-CBA
39	g	609	CHL	C3A-C2A-CAA-CBA
39	r	607	CHL	C3A-C2A-CAA-CBA
39	s	606	CHL	C3A-C2A-CAA-CBA
39	y	303	CHL	C3A-C2A-CAA-CBA
23	N	610	CLA	C5-C6-C7-C8
31	c	519	LNL	C2-C3-C4-C5
31	i	101	LNL	C5-C6-C7-C8
41	Y	317	NEX	C13-C14-C15-C35
42	N	619	XAT	C9-C10-C11-C12
42	r	615	XAT	C29-C30-C31-C32
23	Y	314	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	CBA-CGA-O2A-C1
23	B	611	CLA	C5-C6-C7-C8
26	A	408	SQD	O6-C44-C45-C46
27	c	523	LMG	O1-C7-C8-C9
30	a	412	LHG	C4-C5-C6-O8
30	d	404	LHG	C4-C5-C6-O8
30	g	618	LHG	C14-C15-C16-C17
23	c	512	CLA	C3-C5-C6-C7
27	b	628	LMG	C33-C34-C35-C36
23	y	315	CLA	C4-C3-C5-C6
39	r	606	CHL	C4-C3-C5-C6
23	c	508	CLA	O1D-CGD-O2D-CED
33	C	515	DGD	C2B-C3B-C4B-C5B
23	G	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	412	LHG	C9-C10-C11-C12
30	n	619	LHG	C31-C32-C33-C34
23	y	315	CLA	O1D-CGD-O2D-CED
30	y	318	LHG	C4-O6-P-O3
31	A	413	LNL	C10-C11-C12-C13
31	A	413	LNL	C13-C14-C15-C16
31	A	414	LNL	C9-C10-C11-C12
31	B	622	LNL	C13-C14-C15-C16
31	B	624	LNL	C13-C14-C15-C16
31	C	517	LNL	C12-C13-C14-C15
31	C	518	LNL	C9-C10-C11-C12
31	C	521	LNL	C10-C11-C12-C13
31	C	522	LNL	C9-C10-C11-C12
31	a	401	LNL	C12-C13-C14-C15
31	a	413	LNL	C9-C10-C11-C12
31	b	622	LNL	C12-C13-C14-C15
31	b	623	LNL	C10-C11-C12-C13
31	b	623	LNL	C13-C14-C15-C16
31	b	624	LNL	C13-C14-C15-C16
31	b	625	LNL	C12-C13-C14-C15
31	c	518	LNL	C10-C11-C12-C13
31	c	518	LNL	C12-C13-C14-C15
31	c	520	LNL	C10-C11-C12-C13
31	c	522	LNL	C9-C10-C11-C12
31	i	101	LNL	C9-C10-C11-C12
39	N	606	CHL	C3C-C2C-CMC-OMC
39	R	607	CHL	C3C-C2C-CMC-OMC
39	n	606	CHL	C3C-C2C-CMC-OMC
39	r	607	CHL	C3C-C2C-CMC-OMC
39	y	308	CHL	C3C-C2C-CMC-OMC
26	a	409	SQD	C10-C11-C12-C13
23	y	306	CLA	C2A-CAA-CBA-CGA
31	b	622	LNL	C3-C4-C5-C6
30	R	616	LHG	O6-C4-C5-O7
30	n	619	LHG	O6-C4-C5-O7
26	A	408	SQD	O49-C7-O47-C45
23	C	504	CLA	CBA-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1
26	a	409	SQD	O10-C23-O48-C46
23	B	616	CLA	C13-C15-C16-C17
23	R	609	CLA	C5-C6-C7-C8
33	d	411	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
28	D	403	3PH	C36-C37-C38-C39
33	C	515	DGD	C2A-C3A-C4A-C5A
33	d	411	DGD	C3A-C4A-C5A-C6A
37	D	410	DGA	CCA-CDA-CEA-CFA
23	b	611	CLA	C8-C10-C11-C12
23	a	404	CLA	O1A-CGA-O2A-C1
23	S	609	CLA	C3-C5-C6-C7
30	b	627	LHG	C11-C12-C13-C14
30	b	627	LHG	C16-C17-C18-C19
27	A	409	LMG	O1-C7-C8-O7
27	C	525	LMG	O1-C7-C8-O7
27	c	523	LMG	O1-C7-C8-O7
28	C	524	3PH	O21-C2-C3-O31
28	D	403	3PH	O21-C2-C3-O31
30	D	408	LHG	O7-C5-C6-O8
37	D	410	DGA	OG1-CG1-CG2-OG2
23	y	306	CLA	C10-C11-C12-C13
30	N	618	LHG	C27-C28-C29-C30
31	C	519	LNL	C5-C6-C7-C8
31	c	518	LNL	C3-C4-C5-C6
40	S	615	LUT	C29-C30-C31-C32
23	N	610	CLA	C16-C17-C18-C20
23	R	603	CLA	C11-C12-C13-C14
23	S	612	CLA	C6-C7-C8-C10
23	b	613	CLA	C16-C17-C18-C19
23	r	603	CLA	C11-C12-C13-C14
23	Y	303	CLA	C10-C11-C12-C13
37	D	410	DGA	CG1-CG2-CG3-OXT
26	M	101	SQD	C11-C10-C9-C8
30	r	616	LHG	C24-C25-C26-C27
31	a	401	LNL	C3-C4-C5-C6
33	c	515	DGD	CDB-CEB-CFB-CGB
24	a	406	PHO	C4-C3-C5-C6
23	C	502	CLA	C2-C1-O2A-CGA
23	G	611	CLA	C2-C1-O2A-CGA
23	S	612	CLA	C2-C1-O2A-CGA
23	c	502	CLA	C2-C1-O2A-CGA
23	r	603	CLA	C2-C1-O2A-CGA
23	s	603	CLA	C2-C1-O2A-CGA
23	s	612	CLA	C2-C1-O2A-CGA
39	n	606	CHL	C2-C1-O2A-CGA
39	y	303	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	c	520	LNL	C3-C4-C5-C6
23	B	603	CLA	C6-C7-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C10-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	R	608	CLA	C11-C10-C8-C9
23	Y	303	CLA	C6-C7-C8-C9
23	Y	312	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9
23	b	613	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
23	n	602	CLA	C11-C10-C8-C9
23	s	613	CLA	C11-C12-C13-C14
35	C	523	VIV	C1-C23-C24-C25
27	B	626	LMG	C32-C33-C34-C35
30	r	616	LHG	C9-C10-C11-C12
30	L	103	LHG	C10-C11-C12-C13
31	c	520	LNL	C4-C5-C6-C7
23	b	611	CLA	C13-C15-C16-C17
23	b	612	CLA	C10-C11-C12-C13
24	A	405	PHO	C5-C6-C7-C8
24	D	402	PHO	C1A-C2A-CAA-CBA
30	Y	318	LHG	C5-C4-O6-P
39	s	601	CHL	C4-C3-C5-C6
33	c	515	DGD	C4A-C5A-C6A-C7A
23	B	607	CLA	C16-C17-C18-C20
23	G	611	CLA	O2A-C1-C2-C3
25	A	407	BCR	C1-C6-C7-C8
25	A	407	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	B	618	BCR	C23-C24-C25-C30
25	B	619	BCR	C23-C24-C25-C26
25	B	619	BCR	C23-C24-C25-C30
25	C	514	BCR	C23-C24-C25-C26
25	C	514	BCR	C23-C24-C25-C30
25	D	411	BCR	C23-C24-C25-C26
25	D	411	BCR	C23-C24-C25-C30
25	K	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C23-C24-C25-C30
25	a	408	BCR	C1-C6-C7-C8
25	a	408	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	a	408	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	b	618	BCR	C1-C6-C7-C8
25	b	618	BCR	C5-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C26
25	b	618	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C26
25	c	514	BCR	C5-C6-C7-C8
25	c	514	BCR	C23-C24-C25-C26
25	c	514	BCR	C23-C24-C25-C30
25	k	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C23-C24-C25-C30
40	G	616	LUT	C1-C6-C7-C8
27	A	409	LMG	C33-C34-C35-C36
27	B	626	LMG	C18-C19-C20-C21
41	R	614	NEX	C11-C12-C13-C20
41	s	617	NEX	C11-C12-C13-C20
30	S	616	LHG	C29-C30-C31-C32
23	s	611	CLA	CBA-CGA-O2A-C1
25	C	514	BCR	C7-C8-C9-C10
41	s	617	NEX	C32-C33-C34-C35
42	r	615	XAT	C11-C12-C13-C14
31	C	518	LNL	C3-C4-C5-C6
23	c	509	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	C8-C10-C11-C12
28	a	410	3PH	C29-C2A-C2B-C2C
28	w	202	3PH	C29-C2A-C2B-C2C
31	B	624	LNL	C2-C3-C4-C5
23	B	604	CLA	C3-C5-C6-C7
23	r	604	CLA	C3-C5-C6-C7
31	A	413	LNL	C15-C16-C17-C18
31	B	622	LNL	C15-C16-C17-C18
31	B	623	LNL	C15-C16-C17-C18
31	B	624	LNL	C15-C16-C17-C18
31	B	625	LNL	C15-C16-C17-C18
31	C	520	LNL	C15-C16-C17-C18
31	I	101	LNL	C15-C16-C17-C18
31	a	413	LNL	C15-C16-C17-C18
31	b	623	LNL	C15-C16-C17-C18
31	b	625	LNL	C15-C16-C17-C18
31	c	517	LNL	C15-C16-C17-C18
31	c	519	LNL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	c	521	LNL	C15-C16-C17-C18
31	i	101	LNL	C15-C16-C17-C18
23	B	604	CLA	C10-C11-C12-C13
23	c	506	CLA	O1D-CGD-O2D-CED
27	b	628	LMG	C18-C19-C20-C21
28	T	101	3PH	C2A-C2B-C2C-C2D
23	y	304	CLA	C10-C11-C12-C13
28	X	201	3PH	O11-C1-C2-C3
28	d	403	3PH	O11-C1-C2-C3
30	a	412	LHG	O6-C4-C5-C6
39	N	607	CHL	C4-C3-C5-C6
23	B	603	CLA	C6-C7-C8-C10
23	B	603	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C12-C13-C15
23	B	605	CLA	C12-C13-C15-C16
23	B	608	CLA	C11-C12-C13-C15
23	B	612	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C15
23	C	508	CLA	C2-C3-C5-C6
23	C	508	CLA	C11-C10-C8-C7
23	C	511	CLA	C6-C7-C8-C10
23	D	405	CLA	C11-C12-C13-C15
23	N	611	CLA	C11-C10-C8-C7
23	N	613	CLA	C11-C12-C13-C15
23	R	608	CLA	C11-C10-C8-C7
23	R	609	CLA	C11-C12-C13-C15
23	S	609	CLA	C6-C7-C8-C10
23	Y	303	CLA	C11-C12-C13-C15
23	Y	312	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	612	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
23	b	615	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
23	g	603	CLA	C11-C10-C8-C7
23	g	611	CLA	C11-C12-C13-C15
23	g	611	CLA	C12-C13-C15-C16
23	n	602	CLA	C11-C10-C8-C7
23	n	603	CLA	C12-C13-C15-C16
23	r	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	y	304	CLA	C11-C12-C13-C15
23	y	306	CLA	C11-C10-C8-C7
23	y	306	CLA	C12-C13-C15-C16
23	y	314	CLA	C6-C7-C8-C10
23	y	314	CLA	C11-C12-C13-C15
35	C	523	VIV	C21-C22-C23-C24
35	C	523	VIV	C22-C23-C24-C25
39	G	609	CHL	C6-C7-C8-C10
39	g	609	CHL	C6-C7-C8-C10
39	r	606	CHL	C2-C3-C5-C6
26	A	408	SQD	C27-C28-C29-C30
24	a	406	PHO	C15-C16-C17-C18
25	V	101	BCR	C19-C20-C21-C22
42	Y	301	XAT	C29-C30-C31-C32
42	n	620	XAT	C9-C10-C11-C12
42	y	302	XAT	C13-C14-C15-C35
23	S	612	CLA	C6-C7-C8-C9
31	C	522	LNL	C6-C7-C8-C9
27	C	525	LMG	C31-C32-C33-C34
23	c	504	CLA	CBA-CGA-O2A-C1
30	L	103	LHG	C29-C30-C31-C32
31	c	519	LNL	C4-C5-C6-C7
23	B	612	CLA	C10-C11-C12-C13
23	Y	305	CLA	C2A-CAA-CBA-CGA
25	H	501	BCR	C16-C17-C18-C36
25	b	617	BCR	C11-C10-C9-C34
28	D	403	3PH	C1-O11-P-O14
40	Y	316	LUT	C11-C10-C9-C19
40	s	615	LUT	C40-C33-C34-C35
40	y	317	LUT	C11-C10-C9-C19
33	H	502	DGD	C1A-C2A-C3A-C4A
23	G	602	CLA	C3-C5-C6-C7
23	N	610	CLA	C16-C17-C18-C19
23	R	610	CLA	C16-C17-C18-C20
23	B	608	CLA	CBA-CGA-O2A-C1
23	b	608	CLA	CBA-CGA-O2A-C1
23	r	601	CLA	CBA-CGA-O2A-C1
31	a	401	LNL	C5-C6-C7-C8
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
23	G	614	CLA	CAD-CBD-CGD-O2D
23	Y	305	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	Y	310	CLA	CAD-CBD-CGD-O2D
23	Y	312	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	g	610	CLA	CAD-CBD-CGD-O2D
23	g	611	CLA	CAD-CBD-CGD-O2D
23	g	614	CLA	CAD-CBD-CGD-O2D
23	n	604	CLA	CAD-CBD-CGD-O2D
23	r	609	CLA	CAD-CBD-CGD-O2D
23	s	609	CLA	CAD-CBD-CGD-O2D
23	y	306	CLA	CAD-CBD-CGD-O2D
23	y	311	CLA	CAD-CBD-CGD-O2D
23	y	313	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
26	M	101	SQD	C46-C45-O47-C7
30	Y	318	LHG	C4-C5-O7-C7
39	S	605	CHL	CAD-CBD-CGD-O2D
39	s	605	CHL	CAD-CBD-CGD-O2D
23	b	615	CLA	C13-C15-C16-C17
39	r	607	CHL	C5-C6-C7-C8
25	z	101	BCR	C22-C23-C24-C25
40	G	615	LUT	C6-C7-C8-C9
23	S	609	CLA	C4-C3-C5-C6
23	b	607	CLA	C16-C17-C18-C20
23	y	313	CLA	C16-C17-C18-C20
28	W	201	3PH	C3D-C3E-C3F-C3G
39	y	310	CHL	C10-C11-C12-C13
39	N	607	CHL	C2-C3-C5-C6
26	L	101	SQD	C44-C45-C46-O48
27	A	409	LMG	C7-C8-C9-O8
27	C	525	LMG	O1-C7-C8-C9
28	W	201	3PH	C1-C2-C3-O31
28	a	410	3PH	C1-C2-C3-O31
30	G	618	LHG	C2-C3-O3-P
23	A	403	CLA	O1A-CGA-O2A-C1
27	r	617	LMG	C14-C15-C16-C17
28	X	201	3PH	C23-C24-C25-C26
31	B	622	LNL	C5-C6-C7-C8
28	X	201	3PH	O11-C1-C2-O21
28	d	403	3PH	O11-C1-C2-O21
30	N	618	LHG	O6-C4-C5-O7
23	B	604	CLA	C8-C10-C11-C12
23	B	614	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	N	603	CLA	C8-C10-C11-C12
23	b	606	CLA	C8-C10-C11-C12
39	Y	302	CHL	C8-C10-C11-C12
23	R	604	CLA	C3-C5-C6-C7
23	G	612	CLA	O2A-C1-C2-C3
23	R	601	CLA	O2A-C1-C2-C3
23	R	612	CLA	O2A-C1-C2-C3
23	S	611	CLA	O2A-C1-C2-C3
23	r	601	CLA	O2A-C1-C2-C3
41	R	618	NEX	C14-C15-C35-C34
26	L	101	SQD	C29-C30-C31-C32
30	L	103	LHG	C25-C26-C27-C28
33	H	502	DGD	CAB-CBB-CCB-CDB
30	G	618	LHG	O2-C2-C3-O3
23	A	404	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	N	614	CLA	CHA-CBD-CGD-O1D
23	N	614	CLA	CHA-CBD-CGD-O2D
23	S	602	CLA	CHA-CBD-CGD-O1D
23	S	602	CLA	CHA-CBD-CGD-O2D
23	S	603	CLA	CHA-CBD-CGD-O1D
23	S	603	CLA	CHA-CBD-CGD-O2D
23	Y	314	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	612	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	n	614	CLA	CHA-CBD-CGD-O1D
23	n	614	CLA	CHA-CBD-CGD-O2D
23	r	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	r	602	CLA	CHA-CBD-CGD-O2D
23	s	603	CLA	CHA-CBD-CGD-O1D
23	s	603	CLA	CHA-CBD-CGD-O2D
23	y	315	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	O1A-CGA-O2A-C1
23	n	604	CLA	O1A-CGA-O2A-C1
23	r	601	CLA	O1A-CGA-O2A-C1
28	C	524	3PH	C24-C25-C26-C27
28	D	403	3PH	C3C-C3D-C3E-C3F
30	N	618	LHG	C11-C10-C9-C8
40	N	616	LUT	C32-C33-C34-C35
40	g	615	LUT	C32-C33-C34-C35
26	M	101	SQD	C27-C28-C29-C30
28	T	101	3PH	C3C-C3D-C3E-C3F
26	L	101	SQD	O47-C45-C46-O48
28	w	202	3PH	O21-C2-C3-O31
30	A	412	LHG	O7-C5-C6-O8
30	a	412	LHG	O7-C5-C6-O8
30	n	619	LHG	O7-C5-C6-O8
26	a	409	SQD	C13-C14-C15-C16
23	B	608	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	O1A-CGA-O2A-C1
27	R	617	LMG	O10-C28-O8-C9
23	y	305	CLA	CAA-CBA-CGA-O2A
23	R	603	CLA	C11-C12-C13-C15
23	c	512	CLA	C16-C17-C18-C20
23	r	610	CLA	C16-C17-C18-C20
23	b	613	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	C9-C10-C11-C12
28	C	524	3PH	C22-C23-C24-C25
30	s	616	LHG	C24-C25-C26-C27
31	i	101	LNL	C3-C4-C5-C6
33	C	515	DGD	C6B-C7B-C8B-C9B
31	B	623	LNL	C6-C7-C8-C9
28	C	524	3PH	C23-C24-C25-C26
23	b	608	CLA	O1A-CGA-O2A-C1
23	s	611	CLA	O1A-CGA-O2A-C1
28	W	201	3PH	O32-C31-O31-C3
29	a	411	PL9	C4-C3-C7-C8
23	N	604	CLA	CBA-CGA-O2A-C1
23	B	607	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	s	613	CLA	C11-C10-C8-C9
24	d	402	PHO	C6-C7-C8-C9
35	y	301	VIV	C1-C23-C24-C25
39	G	620	CHL	C11-C12-C13-C14
23	c	504	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	C5-C6-S-O8
23	r	608	CLA	C16-C17-C18-C20
30	L	103	LHG	C28-C29-C30-C31
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C13-C15-C16-C17
33	d	411	DGD	CDB-CEB-CFB-CGB
25	V	101	BCR	C36-C18-C19-C20
40	s	614	LUT	C31-C32-C33-C40
41	Y	317	NEX	C11-C12-C13-C20
42	G	619	XAT	C7-C8-C9-C19
30	D	408	LHG	C33-C34-C35-C36
30	D	408	LHG	C35-C36-C37-C38
30	r	616	LHG	C28-C29-C30-C31
25	V	101	BCR	C17-C18-C19-C20
25	b	617	BCR	C7-C8-C9-C10
40	n	615	LUT	C11-C12-C13-C14
41	n	618	NEX	C31-C32-C33-C34
23	a	407	CLA	C1A-C2A-CAA-CBA
23	n	610	CLA	C1A-C2A-CAA-CBA
39	G	605	CHL	C1A-C2A-CAA-CBA
39	S	606	CHL	C1A-C2A-CAA-CBA
39	n	605	CHL	C1A-C2A-CAA-CBA
39	y	310	CHL	C1A-C2A-CAA-CBA
23	r	603	CLA	C11-C12-C13-C15
35	y	301	VIV	C25-C26-C27-C29
23	y	304	CLA	C13-C15-C16-C17
23	y	306	CLA	C5-C6-C7-C8
23	r	601	CLA	C2-C1-O2A-CGA
23	B	611	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
30	n	619	LHG	C14-C15-C16-C17
25	B	617	BCR	C9-C10-C11-C12
30	d	408	LHG	C4-O6-P-O3
28	X	201	3PH	C38-C39-C3A-C3B
23	y	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	410	3PH	C28-C29-C2A-C2B
31	B	624	LNL	C4-C5-C6-C7
23	n	602	CLA	C4-C3-C5-C6
30	A	412	LHG	C2-C3-O3-P
30	Y	318	LHG	C2-C3-O3-P
30	a	412	LHG	C2-C3-O3-P
30	a	412	LHG	C5-C4-O6-P
30	r	616	LHG	C2-C3-O3-P
30	s	616	LHG	C5-C4-O6-P
30	y	318	LHG	C5-C4-O6-P
23	C	509	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	C2-C3-C5-C6
30	b	627	LHG	C25-C26-C27-C28
31	A	413	LNL	C4-C5-C6-C7
30	A	412	LHG	C3-O3-P-O4
30	A	412	LHG	C4-O6-P-O5
30	D	408	LHG	C4-O6-P-O5
30	R	616	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	g	618	LHG	C3-O3-P-O4
30	s	616	LHG	C4-O6-P-O4
30	y	318	LHG	C4-O6-P-O4
23	B	607	CLA	C16-C17-C18-C19
23	R	602	CLA	C16-C17-C18-C20
23	Y	305	CLA	C16-C17-C18-C20
28	C	524	3PH	C2D-C2E-C2F-C2G
23	b	605	CLA	C15-C16-C17-C18
23	C	502	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBA-CGA-O2A-C1
28	D	403	3PH	O11-C1-C2-C3
30	R	616	LHG	O6-C4-C5-C6
26	a	409	SQD	C17-C18-C19-C20
27	A	409	LMG	C37-C38-C39-C40
30	D	408	LHG	C26-C27-C28-C29
30	n	619	LHG	C19-C20-C21-C22
28	T	101	3PH	C2D-C2E-C2F-C2G
23	G	613	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C15-C16-C17-C18
30	a	412	LHG	C32-C33-C34-C35
23	g	611	CLA	C16-C17-C18-C20
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	CAD-CBD-CGD-O1D
23	G	604	CLA	CAD-CBD-CGD-O1D
23	S	603	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	g	604	CLA	CAD-CBD-CGD-O1D
23	n	614	CLA	CAD-CBD-CGD-O1D
23	s	603	CLA	CAD-CBD-CGD-O1D
23	y	315	CLA	CAD-CBD-CGD-O1D
39	g	609	CHL	CAD-CBD-CGD-O1D
41	S	617	NEX	C7-C8-C9-C10
24	A	405	PHO	C15-C16-C17-C18
37	D	410	DGA	CB5-CB6-CB7-CB8
23	N	604	CLA	O1A-CGA-O2A-C1
26	L	101	SQD	C12-C13-C14-C15
23	S	612	CLA	C5-C6-C7-C8
23	g	611	CLA	C13-C15-C16-C17
27	w	201	LMG	C36-C37-C38-C39
28	X	201	3PH	C29-C2A-C2B-C2C
23	b	616	CLA	O1D-CGD-O2D-CED
30	D	408	LHG	C14-C15-C16-C17
23	G	613	CLA	O1D-CGD-O2D-CED
28	D	403	3PH	C35-C36-C37-C38
23	d	406	CLA	C16-C17-C18-C19
23	r	602	CLA	C16-C17-C18-C20
23	s	609	CLA	C4-C3-C5-C6
23	B	601	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	509	CLA	C11-C10-C8-C7
23	D	406	CLA	C6-C7-C8-C10
23	G	610	CLA	C11-C12-C13-C15
23	S	613	CLA	C12-C13-C15-C16
23	Y	310	CLA	C11-C12-C13-C15
23	Y	312	CLA	C11-C12-C13-C15
23	Y	313	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	c	505	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C10-C8-C7
23	g	613	CLA	C6-C7-C8-C10
23	r	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	y	305	CLA	C12-C13-C15-C16
28	D	403	3PH	O11-C1-C2-O21
28	a	410	3PH	O11-C1-C2-O21
28	w	202	3PH	O11-C1-C2-O21
35	C	523	VIV	C16-C17-C18-C20
39	G	607	CHL	C6-C7-C8-C10
39	N	607	CHL	C6-C7-C8-C10
28	X	201	3PH	C33-C34-C35-C36
33	c	515	DGD	CCB-CDB-CEB-CFB
23	c	513	CLA	O1A-CGA-O2A-C1
27	b	628	LMG	C29-C30-C31-C32
41	Y	317	NEX	C29-C30-C31-C32
26	L	101	SQD	C25-C26-C27-C28
30	D	404	LHG	C7-C8-C9-C10
30	R	616	LHG	C23-C24-C25-C26
28	a	410	3PH	C22-C23-C24-C25
30	D	408	LHG	C27-C28-C29-C30
23	C	502	CLA	O1A-CGA-O2A-C1
23	s	609	CLA	C4C-C3C-CAC-CBC
23	c	511	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	C2A-CAA-CBA-CGA
23	g	602	CLA	C2A-CAA-CBA-CGA
30	a	412	LHG	C11-C10-C9-C8
31	c	521	LNL	C3-C4-C5-C6
30	N	618	LHG	C7-C8-C9-C10
27	B	626	LMG	O8-C28-C29-C30
26	A	408	SQD	C44-C45-C46-O48
27	A	409	LMG	O1-C7-C8-C9
28	W	201	3PH	C29-C2A-C2B-C2C
30	G	618	LHG	C4-C5-C6-O8
30	R	616	LHG	C4-C5-C6-O8
30	Y	318	LHG	C4-C5-C6-O8
30	n	619	LHG	C4-C5-C6-O8
39	G	620	CHL	C1C-C2C-CMC-OMC
39	N	608	CHL	C1C-C2C-CMC-OMC
39	R	606	CHL	C1C-C2C-CMC-OMC
39	n	601	CHL	C1C-C2C-CMC-OMC
39	n	607	CHL	C1C-C2C-CMC-OMC
39	n	608	CHL	C1C-C2C-CMC-OMC
39	r	606	CHL	C1C-C2C-CMC-OMC
26	A	408	SQD	O47-C45-C46-O48
26	L	101	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
26	M	101	SQD	O47-C45-C46-O48
30	G	618	LHG	O7-C5-C6-O8
30	d	408	LHG	O7-C5-C6-O8
31	B	623	LNL	C5-C6-C7-C8
31	C	517	LNL	C6-C7-C8-C9
27	r	617	LMG	C33-C34-C35-C36
23	c	502	CLA	O1A-CGA-O2A-C1
28	w	202	3PH	C38-C39-C3A-C3B
30	b	627	LHG	C10-C11-C12-C13
27	R	617	LMG	C15-C16-C17-C18
28	w	202	3PH	C2C-C2D-C2E-C2F
27	B	626	LMG	C14-C15-C16-C17
33	c	515	DGD	C6B-C7B-C8B-C9B
24	a	406	PHO	C2-C3-C5-C6
23	s	611	CLA	O2A-C1-C2-C3
23	B	615	CLA	C5-C6-C7-C8
23	B	602	CLA	C11-C12-C13-C14
23	B	611	CLA	C6-C7-C8-C9
23	C	503	CLA	C6-C7-C8-C9
23	N	613	CLA	C11-C12-C13-C14
23	R	609	CLA	C14-C13-C15-C16
23	Y	303	CLA	C11-C12-C13-C14
23	Y	311	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	c	503	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	c	512	CLA	C11-C10-C8-C9
23	g	610	CLA	C11-C12-C13-C14
23	n	603	CLA	C14-C13-C15-C16
23	y	304	CLA	C11-C12-C13-C14
23	y	304	CLA	C14-C13-C15-C16
23	y	314	CLA	C6-C7-C8-C9
39	n	607	CHL	C6-C7-C8-C9
24	A	405	PHO	O1D-CGD-O2D-CED
23	B	611	CLA	O1A-CGA-O2A-C1
23	N	604	CLA	CBD-CGD-O2D-CED
26	A	408	SQD	C26-C27-C28-C29
26	a	409	SQD	C16-C17-C18-C19
33	H	502	DGD	O6E-C1E-O5D-C6D
25	v	101	BCR	C19-C20-C21-C22
27	w	201	LMG	C11-C12-C13-C14
33	c	515	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
23	R	610	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
31	c	520	LNL	C2-C3-C4-C5
28	x	201	3PH	C2B-C2C-C2D-C2E
30	s	616	LHG	C18-C19-C20-C21
30	d	404	LHG	C14-C15-C16-C17
23	b	607	CLA	C13-C15-C16-C17
40	G	615	LUT	C20-C13-C14-C15
28	x	201	3PH	C29-C2A-C2B-C2C
30	N	618	LHG	C31-C32-C33-C34
28	T	101	3PH	C2F-C2G-C2H-C2I
28	W	201	3PH	C36-C37-C38-C39
30	d	404	LHG	C35-C36-C37-C38
39	n	601	CHL	C2-C3-C5-C6
39	n	607	CHL	C10-C11-C12-C13
27	r	617	LMG	C11-C12-C13-C14
28	C	524	3PH	C33-C34-C35-C36
28	d	403	3PH	C34-C35-C36-C37
30	r	616	LHG	C11-C10-C9-C8
30	r	616	LHG	C31-C32-C33-C34
31	c	518	LNL	C2-C3-C4-C5
30	s	616	LHG	C13-C14-C15-C16
23	A	404	CLA	C1-C2-C3-C4
23	B	601	CLA	C1-C2-C3-C4
23	G	604	CLA	C1-C2-C3-C4
23	G	611	CLA	C1-C2-C3-C4
23	G	612	CLA	C1-C2-C3-C4
23	G	614	CLA	C1-C2-C3-C4
23	N	604	CLA	C1-C2-C3-C4
23	N	612	CLA	C1-C2-C3-C4
23	R	611	CLA	C1-C2-C3-C4
23	S	603	CLA	C1-C2-C3-C4
23	S	604	CLA	C1-C2-C3-C4
23	a	405	CLA	C1-C2-C3-C4
23	g	604	CLA	C1-C2-C3-C4
23	g	612	CLA	C1-C2-C3-C4
23	g	614	CLA	C1-C2-C3-C4
23	n	604	CLA	C1-C2-C3-C4
23	n	612	CLA	C1-C2-C3-C4
23	n	614	CLA	C1-C2-C3-C4
23	r	601	CLA	C1-C2-C3-C4
23	r	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	r	612	CLA	C1-C2-C3-C4
23	s	603	CLA	C1-C2-C3-C4
23	s	608	CLA	C1-C2-C3-C4
39	G	606	CHL	C1-C2-C3-C4
39	G	608	CHL	C1-C2-C3-C4
39	N	605	CHL	C1-C2-C3-C4
39	S	605	CHL	C1-C2-C3-C4
39	S	606	CHL	C1-C2-C3-C4
39	Y	308	CHL	C1-C2-C3-C4
39	g	606	CHL	C1-C2-C3-C4
39	g	608	CHL	C1-C2-C3-C4
39	n	608	CHL	C1-C2-C3-C4
39	r	605	CHL	C1-C2-C3-C4
39	y	308	CHL	C1-C2-C3-C4
39	y	309	CHL	C1-C2-C3-C4
28	a	410	3PH	C28-C29-C2A-C2B
31	I	101	LNL	C4-C5-C6-C7
28	A	410	3PH	O11-C1-C2-C3
30	d	404	LHG	O6-C4-C5-C6
30	r	616	LHG	O6-C4-C5-C6
23	S	602	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
23	n	602	CLA	C2A-CAA-CBA-CGA
37	b	626	DGA	CA6-CA7-CA8-CA9
30	y	318	LHG	C24-C23-O8-C6
23	B	610	CLA	C2-C1-O2A-CGA
23	C	504	CLA	C2-C1-O2A-CGA
23	R	603	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	504	CLA	C2-C1-O2A-CGA
39	Y	307	CHL	C2-C1-O2A-CGA
39	r	605	CHL	C2-C1-O2A-CGA
31	B	623	LNL	C4-C5-C6-C7
23	r	608	CLA	C16-C17-C18-C19
27	b	620	LMG	C14-C15-C16-C17
28	T	101	3PH	C35-C36-C37-C38
23	B	601	CLA	CAA-CBA-CGA-O2A
30	y	318	LHG	O10-C23-O8-C6
23	a	407	CLA	C3-C5-C6-C7
28	s	618	3PH	C2-C1-O11-P
30	S	616	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
40	S	615	LUT	C26-C27-C28-C29
40	s	615	LUT	C26-C27-C28-C29
37	b	626	DGA	CEA-CFA-CGA-CHA
40	r	613	LUT	C9-C10-C11-C12
23	s	604	CLA	O1A-CGA-O2A-C1
30	a	412	LHG	O6-C4-C5-O7
23	c	501	CLA	C16-C17-C18-C20
23	r	610	CLA	C16-C17-C18-C19
23	y	311	CLA	C16-C17-C18-C20
23	Y	303	CLA	C13-C15-C16-C17
23	S	604	CLA	O2A-C1-C2-C3
39	N	608	CHL	O2A-C1-C2-C3
23	r	602	CLA	C4-C3-C5-C6
25	A	407	BCR	C23-C24-C25-C26
25	A	407	BCR	C23-C24-C25-C30
25	D	411	BCR	C1-C6-C7-C8
25	D	411	BCR	C5-C6-C7-C8
25	Z	101	BCR	C23-C24-C25-C26
25	Z	101	BCR	C23-C24-C25-C30
25	a	408	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C30
25	d	410	BCR	C23-C24-C25-C26
25	d	410	BCR	C23-C24-C25-C30
25	z	101	BCR	C23-C24-C25-C26
25	z	101	BCR	C23-C24-C25-C30
23	g	610	CLA	C2-C3-C5-C6
28	T	101	3PH	C39-C3A-C3B-C3C
23	C	501	CLA	CBA-CGA-O2A-C1
23	s	604	CLA	CBA-CGA-O2A-C1
27	c	523	LMG	O8-C28-C29-C30
23	n	613	CLA	C15-C16-C17-C18
23	g	613	CLA	C16-C17-C18-C20
23	s	612	CLA	C6-C7-C8-C10
30	D	408	LHG	C8-C7-O7-C5
31	c	517	LNL	C7-C8-C9-C10
26	L	101	SQD	C2-C1-O6-C44
33	H	502	DGD	C2E-C1E-O5D-C6D
40	n	615	LUT	C12-C13-C14-C15
40	n	616	LUT	C28-C29-C30-C31
42	n	620	XAT	C11-C10-C9-C8
26	M	101	SQD	O6-C44-C45-O47
27	A	409	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C3-O3-P-O6
30	N	618	LHG	C4-O6-P-O3
30	Y	318	LHG	C4-O6-P-O3
30	d	408	LHG	C3-O3-P-O6
30	n	619	LHG	C4-O6-P-O3
31	C	517	LNL	C15-C16-C17-C18
31	C	522	LNL	C15-C16-C17-C18
39	n	606	CHL	C5-C6-C7-C8
30	N	618	LHG	C15-C16-C17-C18
30	g	618	LHG	C32-C33-C34-C35
24	D	402	PHO	CHA-CBD-CGD-O2D
24	d	402	PHO	CHA-CBD-CGD-O1D
24	d	402	PHO	CHA-CBD-CGD-O2D
31	B	623	LNL	C2-C3-C4-C5
23	y	305	CLA	O1D-CGD-O2D-CED
28	D	403	3PH	C1-C2-C3-O31
30	y	318	LHG	C4-C5-C6-O8
23	B	602	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	B	607	CLA	C6-C7-C8-C10
23	C	503	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	n	602	CLA	C2-C3-C5-C6
23	r	602	CLA	C6-C7-C8-C10
23	y	315	CLA	C12-C13-C15-C16
26	A	408	SQD	C11-C10-C9-C8
31	a	401	LNL	C4-C5-C6-C7
26	a	409	SQD	C23-C24-C25-C26
28	s	618	3PH	C34-C35-C36-C37
23	B	607	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	G	610	CLA	C11-C12-C13-C14
23	S	610	CLA	C11-C10-C8-C9
23	Y	311	CLA	C11-C10-C8-C9
23	Y	312	CLA	C11-C12-C13-C14
23	Y	313	CLA	C6-C7-C8-C9
23	a	407	CLA	C11-C10-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	b	606	CLA	C6-C7-C8-C9
23	n	603	CLA	C11-C10-C8-C9
23	r	602	CLA	C11-C12-C13-C14
23	s	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	y	306	CLA	C14-C13-C15-C16
23	y	311	CLA	C11-C12-C13-C14
39	G	620	CHL	C14-C13-C15-C16
39	g	609	CHL	C6-C7-C8-C9
23	b	605	CLA	C13-C15-C16-C17
25	b	617	BCR	C9-C10-C11-C12
40	Y	315	LUT	C13-C14-C15-C35
40	y	316	LUT	C13-C14-C15-C35
23	Y	305	CLA	C16-C17-C18-C19
23	g	611	CLA	C16-C17-C18-C19
28	T	101	3PH	C29-C2A-C2B-C2C
23	b	614	CLA	C8-C10-C11-C12
23	s	612	CLA	C5-C6-C7-C8
23	b	601	CLA	C2A-CAA-CBA-CGA
37	b	626	DGA	CA5-CA6-CA7-CA8
25	d	410	BCR	C11-C12-C13-C35
40	n	616	LUT	C7-C8-C9-C19
30	b	627	LHG	C5-C4-O6-P
30	y	318	LHG	C2-C3-O3-P
42	R	615	XAT	C11-C12-C13-C14
30	Y	318	LHG	C30-C31-C32-C33
23	N	614	CLA	O2A-C1-C2-C3
23	n	611	CLA	O2A-C1-C2-C3
29	A	411	PL9	C26-C27-C28-C29
29	a	411	PL9	C36-C37-C38-C39
23	C	511	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	C2-C3-C5-C6
23	R	602	CLA	C16-C17-C18-C19
23	r	602	CLA	C16-C17-C18-C19
23	Y	313	CLA	CBA-CGA-O2A-C1
23	y	314	CLA	CBA-CGA-O2A-C1
29	D	407	PL9	C2-C3-C7-C8
29	d	407	PL9	C2-C3-C7-C8
23	C	501	CLA	O1A-CGA-O2A-C1
32	B	621	PAM	O1-C1-C2-C3
28	W	201	3PH	C38-C39-C3A-C3B
39	R	607	CHL	C5-C6-C7-C8
23	Y	313	CLA	O1A-CGA-O2A-C1
23	G	613	CLA	CBA-CGA-O2A-C1
31	C	520	LNL	C7-C8-C9-C10
23	R	610	CLA	C2A-CAA-CBA-CGA
23	r	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	d	406	CLA	C16-C17-C18-C20
31	C	522	LNL	O2-C1-C2-C3
40	N	616	LUT	C9-C10-C11-C12
40	N	616	LUT	C33-C34-C35-C15
40	R	613	LUT	C33-C34-C35-C15
29	a	411	PL9	C39-C41-C42-C43
23	G	613	CLA	O1A-CGA-O2A-C1
23	y	314	CLA	O1A-CGA-O2A-C1
40	g	615	LUT	C10-C11-C12-C13
41	s	617	NEX	C10-C11-C12-C13
42	y	302	XAT	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
30	D	404	LHG	C29-C30-C31-C32
30	r	616	LHG	C30-C31-C32-C33
23	n	610	CLA	C16-C17-C18-C20
23	N	610	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	a	404	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
31	C	517	LNL	C7-C8-C9-C10
23	B	613	CLA	C13-C15-C16-C17
23	C	507	CLA	C10-C11-C12-C13
23	b	608	CLA	C13-C15-C16-C17
23	B	608	CLA	C2-C1-O2A-CGA
39	N	606	CHL	C2-C1-O2A-CGA
39	g	607	CHL	C2-C1-O2A-CGA
39	n	609	CHL	C2-C1-O2A-CGA
28	W	201	3PH	C34-C35-C36-C37
30	L	103	LHG	C11-C12-C13-C14
23	C	502	CLA	C16-C17-C18-C19
30	g	618	LHG	C29-C30-C31-C32
23	C	505	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
23	n	613	CLA	C2A-CAA-CBA-CGA
23	r	602	CLA	C2A-CAA-CBA-CGA
23	y	304	CLA	C2A-CAA-CBA-CGA
27	d	409	LMG	O1-C7-C8-O7
28	A	410	3PH	O21-C2-C3-O31
39	n	607	CHL	C2A-CAA-CBA-CGA
33	c	515	DGD	C2A-C3A-C4A-C5A
23	g	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	C	524	3PH	C2C-C2D-C2E-C2F
33	C	515	DGD	C3A-C4A-C5A-C6A
30	r	616	LHG	C5-C4-O6-P
26	L	101	SQD	C15-C16-C17-C18
23	B	607	CLA	C3A-C2A-CAA-CBA
23	D	405	CLA	C3A-C2A-CAA-CBA
23	R	604	CLA	C3A-C2A-CAA-CBA
23	S	613	CLA	C3A-C2A-CAA-CBA
23	N	604	CLA	O1D-CGD-O2D-CED
31	B	624	LNL	C7-C8-C9-C10
31	c	520	LNL	C7-C8-C9-C10
23	s	604	CLA	O2A-C1-C2-C3
25	D	411	BCR	C9-C10-C11-C12
25	d	410	BCR	C19-C20-C21-C22
41	n	618	NEX	C29-C30-C31-C32
23	B	602	CLA	C4-C3-C5-C6
23	G	613	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
28	a	410	3PH	C3B-C3C-C3D-C3E
23	G	613	CLA	C2-C3-C5-C6
30	b	627	LHG	C34-C35-C36-C37
23	B	602	CLA	C6-C7-C8-C9
23	B	605	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	G	603	CLA	C6-C7-C8-C9
23	R	603	CLA	C6-C7-C8-C9
23	Y	310	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16
23	s	613	CLA	C6-C7-C8-C9
23	y	312	CLA	C11-C12-C13-C14
23	y	315	CLA	C6-C7-C8-C9
24	a	406	PHO	C6-C7-C8-C9
39	Y	302	CHL	C14-C13-C15-C16
39	Y	307	CHL	C14-C13-C15-C16
39	g	619	CHL	C14-C13-C15-C16
28	A	410	3PH	C2C-C2D-C2E-C2F
31	b	624	LNL	C4-C5-C6-C7
26	M	101	SQD	C12-C13-C14-C15
30	A	412	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	c	511	CLA	O1D-CGD-O2D-CED
27	d	409	LMG	O1-C7-C8-C9
30	r	616	LHG	C4-C5-C6-O8
30	D	408	LHG	O9-C7-O7-C5
27	B	620	LMG	C14-C15-C16-C17
31	a	413	LNL	C7-C8-C9-C10
23	C	507	CLA	C2A-CAA-CBA-CGA
23	N	604	CLA	C2A-CAA-CBA-CGA
23	c	507	CLA	C2A-CAA-CBA-CGA
23	Y	310	CLA	C16-C17-C18-C20
23	g	613	CLA	C16-C17-C18-C19
23	s	612	CLA	C6-C7-C8-C9
39	R	607	CHL	O2A-C1-C2-C3
39	r	607	CHL	O2A-C1-C2-C3
23	B	608	CLA	C13-C15-C16-C17
23	y	306	CLA	C8-C10-C11-C12
25	V	101	BCR	C7-C8-C9-C34
25	v	101	BCR	C36-C18-C19-C20
41	S	617	NEX	C11-C12-C13-C20
27	b	620	LMG	C17-C18-C19-C20
41	G	617	NEX	C31-C32-C33-C34
30	a	412	LHG	C28-C29-C30-C31
30	y	318	LHG	C4-C5-O7-C7
23	D	405	CLA	C1A-C2A-CAA-CBA
23	S	602	CLA	C1A-C2A-CAA-CBA
23	Y	310	CLA	C1A-C2A-CAA-CBA
23	d	405	CLA	C1A-C2A-CAA-CBA
23	g	610	CLA	C1A-C2A-CAA-CBA
23	n	614	CLA	C1A-C2A-CAA-CBA
39	G	601	CHL	C1A-C2A-CAA-CBA
39	N	605	CHL	C1A-C2A-CAA-CBA
39	n	606	CHL	C1A-C2A-CAA-CBA
27	b	620	LMG	C20-C21-C22-C23
23	C	506	CLA	C6-C7-C8-C9
23	B	607	CLA	C11-C12-C13-C15
23	B	610	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	G	613	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C10-C8-C7
23	c	502	CLA	C11-C10-C8-C7
23	c	503	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C12-C13-C15
23	n	603	CLA	C11-C10-C8-C7
23	r	608	CLA	C12-C13-C15-C16
39	r	606	CHL	C6-C7-C8-C10
28	W	201	3PH	C39-C3A-C3B-C3C
30	A	412	LHG	C24-C25-C26-C27
30	g	618	LHG	C12-C13-C14-C15
31	A	414	LNL	C12-C13-C14-C15
31	B	623	LNL	C9-C10-C11-C12
31	B	624	LNL	C12-C13-C14-C15
31	C	517	LNL	C9-C10-C11-C12
31	C	521	LNL	C13-C14-C15-C16
31	I	101	LNL	C9-C10-C11-C12
31	b	622	LNL	C9-C10-C11-C12
31	b	624	LNL	C9-C10-C11-C12
31	c	519	LNL	C9-C10-C11-C12
31	i	101	LNL	C10-C11-C12-C13
28	C	524	3PH	C37-C38-C39-C3A
23	b	608	CLA	C16-C17-C18-C20
23	y	304	CLA	C16-C17-C18-C20
23	N	602	CLA	C2A-CAA-CBA-CGA
23	R	602	CLA	C2A-CAA-CBA-CGA
23	Y	303	CLA	C2A-CAA-CBA-CGA
23	n	604	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C15-C16-C17-C18
26	A	408	SQD	C31-C32-C33-C34
30	G	618	LHG	C31-C32-C33-C34
30	Y	318	LHG	C11-C10-C9-C8
23	n	612	CLA	O2A-C1-C2-C3
23	B	614	CLA	C8-C10-C11-C12
28	L	102	3PH	C2F-C2G-C2H-C2I
30	L	103	LHG	O6-C4-C5-C6
23	a	403	CLA	C5-C6-C7-C8
31	b	623	LNL	O2-C1-C2-C3
28	s	618	3PH	C36-C37-C38-C39
30	N	618	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	n	610	CLA	C4-C3-C5-C6
23	A	402	CLA	C5-C6-C7-C8
23	c	511	CLA	C8-C10-C11-C12
28	A	410	3PH	C36-C37-C38-C39
23	c	501	CLA	CBA-CGA-O2A-C1
32	B	621	PAM	O2-C1-C2-C3
39	s	607	CHL	O2A-C1-C2-C3
23	C	513	CLA	CAA-CBA-CGA-O1A
25	h	501	BCR	C16-C17-C18-C19
40	n	615	LUT	C32-C33-C34-C35
40	r	613	LUT	C12-C13-C14-C15
41	N	617	NEX	C28-C29-C30-C31
41	R	614	NEX	C28-C29-C30-C31
41	r	614	NEX	C28-C29-C30-C31
31	b	624	LNL	O1-C1-C2-C3
31	c	522	LNL	O2-C1-C2-C3
28	X	201	3PH	C39-C3A-C3B-C3C
23	C	511	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	O6-C44-C45-O47
28	L	102	3PH	O21-C2-C3-O31
30	r	616	LHG	O7-C5-C6-O8
28	d	403	3PH	C32-C33-C34-C35
42	N	619	XAT	C29-C30-C31-C32
31	C	521	LNL	O2-C1-C2-C3
40	r	613	LUT	C6-C7-C8-C9
23	B	606	CLA	C16-C17-C18-C20
26	M	101	SQD	C16-C17-C18-C19
31	C	517	LNL	C3-C4-C5-C6
39	N	606	CHL	C5-C6-C7-C8
33	d	411	DGD	C6B-C7B-C8B-C9B
23	a	404	CLA	O1D-CGD-O2D-CED
30	b	627	LHG	C1-C2-C3-O3
31	C	521	LNL	O1-C1-C2-C3
31	C	522	LNL	O1-C1-C2-C3
31	b	623	LNL	O1-C1-C2-C3
29	D	407	PL9	C40-C39-C41-C42
39	n	609	CHL	C4-C3-C5-C6
28	d	403	3PH	C23-C24-C25-C26
23	R	601	CLA	C2-C1-O2A-CGA
23	Y	305	CLA	C2-C1-O2A-CGA
39	G	609	CHL	C2-C1-O2A-CGA
39	N	608	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
39	g	601	CHL	C2-C1-O2A-CGA
40	S	615	LUT	C30-C31-C32-C33
31	c	522	LNL	O1-C1-C2-C3
30	d	408	LHG	C23-C24-C25-C26
23	Y	303	CLA	C14-C13-C15-C16
23	b	606	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
23	g	613	CLA	C6-C7-C8-C9
23	r	603	CLA	C6-C7-C8-C9
23	y	306	CLA	C11-C12-C13-C14
37	D	410	DGA	CBB-CAB-CB9-CB8
33	d	411	DGD	C9A-CAA-CBA-CCA
23	B	606	CLA	C8-C10-C11-C12
23	b	612	CLA	C8-C10-C11-C12
28	a	410	3PH	C27-C28-C29-C2A
39	g	606	CHL	C2A-CAA-CBA-CGA
23	c	511	CLA	C16-C17-C18-C20
39	n	605	CHL	C2-C1-O2A-CGA
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C30
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	V	101	BCR	C23-C24-C25-C26
25	V	101	BCR	C23-C24-C25-C30
25	Z	101	BCR	C1-C6-C7-C8
25	Z	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	v	101	BCR	C23-C24-C25-C26
25	v	101	BCR	C23-C24-C25-C30
25	z	101	BCR	C1-C6-C7-C8
25	z	101	BCR	C5-C6-C7-C8
26	a	409	SQD	C24-C25-C26-C27
30	n	619	LHG	C26-C27-C28-C29
40	Y	315	LUT	C9-C10-C11-C12
40	s	615	LUT	C29-C30-C31-C32
41	G	617	NEX	C29-C30-C31-C32
26	L	101	SQD	C13-C14-C15-C16
23	B	604	CLA	C4-C3-C5-C6
23	Y	311	CLA	C4-C3-C5-C6
23	b	614	CLA	C5-C6-C7-C8
23	c	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	Y	311	CLA	C2-C3-C5-C6
23	r	602	CLA	C2-C3-C5-C6
23	s	610	CLA	C2-C3-C5-C6
26	A	408	SQD	O47-C7-C8-C9
31	B	625	LNL	O1-C1-C2-C3
23	b	607	CLA	C8-C10-C11-C12
31	b	625	LNL	O1-C1-C2-C3
31	c	519	LNL	O1-C1-C2-C3
23	c	501	CLA	O1A-CGA-O2A-C1
28	D	403	3PH	O31-C31-C32-C33
27	R	617	LMG	C31-C32-C33-C34
28	C	524	3PH	C2A-C2B-C2C-C2D
23	c	502	CLA	C16-C17-C18-C19
32	B	621	PAM	C7-C8-C9-C10
23	B	611	CLA	C13-C15-C16-C17
23	C	509	CLA	C13-C15-C16-C17
23	c	509	CLA	C13-C15-C16-C17
30	r	616	LHG	O6-C4-C5-O7
31	B	624	LNL	O1-C1-C2-C3
31	b	625	LNL	O2-C1-C2-C3
31	c	519	LNL	O2-C1-C2-C3
23	r	601	CLA	C2A-CAA-CBA-CGA
28	X	201	3PH	C35-C36-C37-C38
31	c	519	LNL	C3-C4-C5-C6
28	a	410	3PH	O11-C1-C2-C3
30	Y	318	LHG	O6-C4-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
29	A	411	PL9	C40-C39-C41-C42
29	d	407	PL9	C40-C39-C41-C42
23	C	502	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	R	609	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	c	503	CLA	C12-C13-C15-C16
23	g	610	CLA	C11-C12-C13-C15
39	G	620	CHL	C11-C12-C13-C15
39	Y	309	CHL	C2-C3-C5-C6
39	n	609	CHL	C2-C3-C5-C6
31	C	517	LNL	O1-C1-C2-C3
23	C	510	CLA	CBA-CGA-O2A-C1
23	n	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C15-C16-C17-C18
23	C	506	CLA	C5-C6-C7-C8
41	g	617	NEX	C13-C14-C15-C35
42	G	619	XAT	C29-C30-C31-C32
27	B	626	LMG	O1-C7-C8-O7
28	a	410	3PH	O21-C2-C3-O31
30	A	412	LHG	O9-C7-O7-C5
28	w	202	3PH	C2D-C2E-C2F-C2G
30	g	618	LHG	C25-C26-C27-C28
23	b	603	CLA	C13-C15-C16-C17
31	b	624	LNL	O2-C1-C2-C3
23	N	612	CLA	O2A-C1-C2-C3
23	S	603	CLA	O2A-C1-C2-C3
39	G	608	CHL	O2A-C1-C2-C3
39	S	605	CHL	O2A-C1-C2-C3
39	Y	308	CHL	O2A-C1-C2-C3
23	c	512	CLA	CAA-CBA-CGA-O2A
24	D	402	PHO	O1A-CGA-O2A-C1
23	b	610	CLA	C2A-CAA-CBA-CGA
23	n	610	CLA	C16-C17-C18-C19
30	G	618	LHG	C16-C17-C18-C19
24	D	402	PHO	CBA-CGA-O2A-C1
23	C	510	CLA	O1A-CGA-O2A-C1
28	a	410	3PH	C1-O11-P-O14
31	B	622	LNL	C4-C5-C6-C7
41	g	617	NEX	C39-C29-C30-C31
23	N	612	CLA	CAA-CBA-CGA-O2A
23	d	405	CLA	CAA-CBA-CGA-O2A
28	W	201	3PH	O21-C21-C22-C23
31	C	518	LNL	O1-C1-C2-C3
23	S	609	CLA	C2-C3-C5-C6
28	C	524	3PH	C31-C32-C33-C34
23	b	607	CLA	C16-C17-C18-C19
23	C	512	CLA	CAA-CBA-CGA-O2A
30	L	103	LHG	O7-C7-C8-C9
30	N	618	LHG	O8-C23-C24-C25
23	B	609	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	D	406	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C6-C7-C8-C9
23	c	505	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C10-C8-C9
23	r	602	CLA	C6-C7-C8-C9
23	y	305	CLA	C14-C13-C15-C16
23	y	306	CLA	C6-C7-C8-C9
23	y	312	CLA	C11-C10-C8-C9
35	C	523	VIV	C16-C17-C18-C19
39	G	609	CHL	C14-C13-C15-C16
23	n	613	CLA	O1A-CGA-O2A-C1
31	I	101	LNL	C6-C7-C8-C9
28	W	201	3PH	C37-C38-C39-C3A
28	s	618	3PH	C37-C38-C39-C3A
27	w	201	LMG	C15-C16-C17-C18
30	L	103	LHG	C17-C18-C19-C20
30	s	616	LHG	C29-C30-C31-C32
23	Y	314	CLA	C3A-C2A-CAA-CBA
23	b	607	CLA	C3A-C2A-CAA-CBA
23	d	405	CLA	C3A-C2A-CAA-CBA
23	r	604	CLA	C3A-C2A-CAA-CBA
39	G	608	CHL	C3A-C2A-CAA-CBA
39	G	609	CHL	C3A-C2A-CAA-CBA
39	Y	302	CHL	C3A-C2A-CAA-CBA
39	s	607	CHL	C3A-C2A-CAA-CBA
28	w	202	3PH	O21-C21-C22-C23
31	A	414	LNL	C7-C8-C9-C10
31	B	625	LNL	C7-C8-C9-C10
31	C	522	LNL	C7-C8-C9-C10
31	b	623	LNL	C7-C8-C9-C10
31	b	624	LNL	C7-C8-C9-C10
31	i	101	LNL	C7-C8-C9-C10
33	C	515	DGD	C8B-C9B-CAB-CBB
23	A	404	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	G	610	CLA	CAD-CBD-CGD-O2D
23	G	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	N	604	CLA	CAD-CBD-CGD-O2D
23	N	610	CLA	CAD-CBD-CGD-O2D
23	N	613	CLA	CAD-CBD-CGD-O2D
23	R	604	CLA	CAD-CBD-CGD-O2D
23	R	609	CLA	CAD-CBD-CGD-O2D
23	S	609	CLA	CAD-CBD-CGD-O2D
23	S	610	CLA	CAD-CBD-CGD-O2D
23	S	613	CLA	CAD-CBD-CGD-O2D
23	Y	304	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	501	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	g	603	CLA	CAD-CBD-CGD-O2D
23	n	610	CLA	CAD-CBD-CGD-O2D
23	r	610	CLA	CAD-CBD-CGD-O2D
23	s	610	CLA	CAD-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O2D
23	y	305	CLA	CAD-CBD-CGD-O2D
24	A	405	PHO	CAD-CBD-CGD-O2D
30	y	318	LHG	C6-C5-O7-C7
39	G	605	CHL	CAD-CBD-CGD-O2D
39	G	607	CHL	CAD-CBD-CGD-O2D
39	N	607	CHL	CAD-CBD-CGD-O2D
39	g	605	CHL	CAD-CBD-CGD-O2D
39	g	607	CHL	CAD-CBD-CGD-O2D
39	n	607	CHL	CAD-CBD-CGD-O2D
23	B	608	CLA	C16-C17-C18-C20
23	Y	310	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C19
28	L	102	3PH	C29-C2A-C2B-C2C
40	g	615	LUT	C9-C10-C11-C12
40	y	316	LUT	C9-C10-C11-C12
27	B	620	LMG	C20-C21-C22-C23
23	N	612	CLA	C2-C1-O2A-CGA
23	S	609	CLA	C2-C1-O2A-CGA
24	a	406	PHO	C2-C1-O2A-CGA
39	N	609	CHL	C2-C1-O2A-CGA
31	B	623	LNL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	a	401	LNL	O1-C1-C2-C3
31	C	520	LNL	C1-C2-C3-C4
23	R	611	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
28	C	524	3PH	O21-C21-C22-C23
30	b	627	LHG	O7-C7-C8-C9
27	b	628	LMG	O10-C28-C29-C30
23	Y	305	CLA	CBA-CGA-O2A-C1
23	b	606	CLA	C4-C3-C5-C6
31	B	625	LNL	O2-C1-C2-C3
31	I	101	LNL	O1-C1-C2-C3
31	c	518	LNL	O1-C1-C2-C3
23	D	405	CLA	CAA-CBA-CGA-O2A
27	C	525	LMG	O8-C28-C29-C30
30	R	616	LHG	O8-C23-C24-C25
23	Y	304	CLA	O1A-CGA-O2A-C1
25	v	101	BCR	C17-C18-C19-C20
40	Y	315	LUT	C31-C32-C33-C34
40	y	316	LUT	C31-C32-C33-C34
42	N	619	XAT	C27-C28-C29-C30
31	B	622	LNL	C7-C8-C9-C10
31	c	519	LNL	C7-C8-C9-C10
30	b	627	LHG	C11-C10-C9-C8
26	L	101	SQD	O6-C44-C45-C46
42	N	619	XAT	O4-C6-C7-C8
42	N	619	XAT	O24-C26-C27-C28
42	n	620	XAT	O24-C26-C27-C28
23	s	608	CLA	O1A-CGA-O2A-C1
28	X	201	3PH	C26-C27-C28-C29
37	D	410	DGA	CB6-CB7-CB8-CB9
30	L	103	LHG	O6-C4-C5-O7
23	r	601	CLA	CAA-CBA-CGA-O2A
33	C	515	DGD	C1B-C2B-C3B-C4B
23	R	611	CLA	O2A-C1-C2-C3
23	r	611	CLA	O2A-C1-C2-C3
23	s	608	CLA	O2A-C1-C2-C3
31	C	517	LNL	O2-C1-C2-C3
23	Y	304	CLA	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
39	G	620	CHL	O2A-C1-C2-C3
39	g	607	CHL	O2A-C1-C2-C3
39	g	619	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	L	102	3PH	C37-C38-C39-C3A
23	Y	304	CLA	C2A-CAA-CBA-CGA
30	D	408	LHG	C19-C20-C21-C22
23	C	510	CLA	CAA-CBA-CGA-O2A
28	A	410	3PH	O21-C21-C22-C23
39	g	609	CHL	CAA-CBA-CGA-O2A
33	H	502	DGD	O1B-C1B-C2B-C3B
31	B	624	LNL	O2-C1-C2-C3
31	c	518	LNL	O2-C1-C2-C3
31	a	401	LNL	C7-C8-C9-C10
31	b	622	LNL	C7-C8-C9-C10
31	c	518	LNL	C7-C8-C9-C10
23	R	608	CLA	C16-C17-C18-C19
23	y	313	CLA	C16-C17-C18-C19
27	B	620	LMG	C17-C18-C19-C20
27	b	628	LMG	C28-C29-C30-C31
26	A	408	SQD	C17-C18-C19-C20
23	Y	305	CLA	O1A-CGA-O2A-C1
23	A	402	CLA	CHA-CBD-CGD-O1D
23	A	402	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CHA-CBD-CGD-O1D
23	G	603	CLA	CHA-CBD-CGD-O2D
23	G	612	CLA	CHA-CBD-CGD-O1D
23	G	612	CLA	CHA-CBD-CGD-O2D
23	N	602	CLA	CHA-CBD-CGD-O2D
23	R	602	CLA	CHA-CBD-CGD-O1D
23	R	602	CLA	CHA-CBD-CGD-O2D
23	S	611	CLA	CHA-CBD-CGD-O1D
23	S	611	CLA	CHA-CBD-CGD-O2D
23	Y	303	CLA	CHA-CBD-CGD-O1D
23	Y	303	CLA	CHA-CBD-CGD-O2D
23	Y	314	CLA	CHA-CBD-CGD-O2D
23	a	403	CLA	CHA-CBD-CGD-O1D
23	a	403	CLA	CHA-CBD-CGD-O2D
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	g	612	CLA	CHA-CBD-CGD-O2D
23	n	602	CLA	CHA-CBD-CGD-O2D
23	n	612	CLA	CHA-CBD-CGD-O1D
23	s	602	CLA	CHA-CBD-CGD-O1D
23	s	611	CLA	CHA-CBD-CGD-O1D
23	s	611	CLA	CHA-CBD-CGD-O2D
23	y	304	CLA	CHA-CBD-CGD-O1D
23	y	304	CLA	CHA-CBD-CGD-O2D
23	y	315	CLA	CHA-CBD-CGD-O2D
39	Y	302	CHL	CHA-CBD-CGD-O1D
39	Y	302	CHL	CHA-CBD-CGD-O2D
39	y	303	CHL	CHA-CBD-CGD-O1D
39	y	303	CHL	CHA-CBD-CGD-O2D
31	I	101	LNL	O2-C1-C2-C3
31	a	401	LNL	O2-C1-C2-C3
23	s	610	CLA	C4-C3-C5-C6
23	B	613	CLA	CAA-CBA-CGA-O2A
39	R	607	CHL	CAA-CBA-CGA-O2A
23	b	606	CLA	C2-C3-C5-C6
28	a	410	3PH	C2E-C2F-C2G-C2H
30	A	412	LHG	C9-C10-C11-C12
23	C	511	CLA	C8-C10-C11-C12
30	y	318	LHG	O6-C4-C5-C6
25	H	501	BCR	C16-C17-C18-C19
40	Y	315	LUT	C12-C13-C14-C15
40	y	316	LUT	C12-C13-C14-C15
41	G	617	NEX	C28-C29-C30-C31
41	n	618	NEX	C28-C29-C30-C31
27	A	409	LMG	C11-C12-C13-C14
28	x	201	3PH	C2C-C2D-C2E-C2F
23	y	304	CLA	C16-C17-C18-C19
23	C	501	CLA	CAA-CBA-CGA-O2A
23	G	611	CLA	CAA-CBA-CGA-O2A
23	R	610	CLA	CAA-CBA-CGA-O2A
23	r	610	CLA	CAA-CBA-CGA-O2A
28	a	410	3PH	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
39	S	601	CHL	CAA-CBA-CGA-O2A
39	r	607	CHL	CAA-CBA-CGA-O2A
27	D	409	LMG	O1-C7-C8-O7
23	Y	304	CLA	CBA-CGA-O2A-C1
28	x	201	3PH	C3B-C3C-C3D-C3E
31	C	518	LNL	O2-C1-C2-C3
39	r	606	CHL	C4C-C3C-CAC-CBC
23	R	612	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A
23	r	611	CLA	CAA-CBA-CGA-O2A
39	s	601	CHL	CAA-CBA-CGA-O2A
23	y	315	CLA	C2A-CAA-CBA-CGA
31	C	520	LNL	O1-C1-C2-C3
24	D	402	PHO	CHA-CBD-CGD-O1D
23	B	605	CLA	C8-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
23	g	602	CLA	C10-C11-C12-C13
23	s	608	CLA	CBA-CGA-O2A-C1
30	D	408	LHG	C25-C26-C27-C28
23	Y	304	CLA	CAA-CBA-CGA-O2A
39	g	607	CHL	CAA-CBA-CGA-O2A
23	S	610	CLA	C2-C3-C5-C6
23	Y	314	CLA	C6-C7-C8-C10
23	s	609	CLA	C2-C3-C5-C6
23	y	312	CLA	C2-C3-C5-C6
31	b	625	LNL	C7-C8-C9-C10
23	B	610	CLA	CAA-CBA-CGA-O2A
23	g	603	CLA	CAA-CBA-CGA-O2A
33	c	515	DGD	O2G-C1B-C2B-C3B
39	G	608	CHL	CAA-CBA-CGA-O2A
23	C	509	CLA	C11-C12-C13-C14
23	G	613	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C10-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	n	610	CLA	C11-C12-C13-C14
23	r	608	CLA	C14-C13-C15-C16
23	r	609	CLA	C14-C13-C15-C16
23	y	313	CLA	C11-C10-C8-C9
39	N	609	CHL	C11-C10-C8-C9
39	n	609	CHL	C6-C7-C8-C9
23	N	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
41	N	617	NEX	C33-C34-C35-C15
42	y	302	XAT	C29-C30-C31-C32
23	D	405	CLA	C15-C16-C17-C18
23	b	602	CLA	C10-C11-C12-C13
23	b	605	CLA	C10-C11-C12-C13
23	S	608	CLA	O2A-C1-C2-C3
39	N	605	CHL	O2A-C1-C2-C3
39	S	606	CHL	O2A-C1-C2-C3
39	r	605	CHL	O2A-C1-C2-C3
26	A	408	SQD	C18-C19-C20-C21
26	M	101	SQD	C28-C29-C30-C31
42	y	302	XAT	C14-C15-C35-C34
38	F	501	HEM	CAA-CBA-CGA-O2A
27	R	617	LMG	C35-C36-C37-C38
30	n	619	LHG	O7-C7-C8-C9
26	a	409	SQD	C4-C5-C6-S
23	B	606	CLA	C16-C17-C18-C19
23	r	604	CLA	C6-C7-C8-C10
31	C	520	LNL	C3-C4-C5-C6
30	A	412	LHG	C8-C7-O7-C5
23	b	608	CLA	C2A-CAA-CBA-CGA
23	D	405	CLA	CAA-CBA-CGA-O1A
30	L	103	LHG	C13-C14-C15-C16
23	b	610	CLA	CAA-CBA-CGA-O2A
31	I	101	LNL	C7-C8-C9-C10
23	R	604	CLA	C6-C7-C8-C10
23	Y	303	CLA	C16-C17-C18-C20
28	D	403	3PH	C23-C24-C25-C26
29	D	407	PL9	C38-C39-C41-C42
28	x	201	3PH	C39-C3A-C3B-C3C
30	R	616	LHG	C28-C29-C30-C31
31	B	623	LNL	O2-C1-C2-C3
23	g	603	CLA	CAA-CBA-CGA-O1A
30	L	103	LHG	O9-C7-C8-C9
33	c	515	DGD	O1B-C1B-C2B-C3B
39	G	609	CHL	C10-C11-C12-C13
28	L	102	3PH	C2C-C2D-C2E-C2F
23	A	404	CLA	C1A-C2A-CAA-CBA
23	B	607	CLA	C1A-C2A-CAA-CBA
23	G	602	CLA	C1A-C2A-CAA-CBA
23	N	611	CLA	C1A-C2A-CAA-CBA
23	R	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	Y	314	CLA	C1A-C2A-CAA-CBA
23	b	607	CLA	C1A-C2A-CAA-CBA
23	r	604	CLA	C1A-C2A-CAA-CBA
23	r	609	CLA	C1A-C2A-CAA-CBA
23	y	311	CLA	C1A-C2A-CAA-CBA
39	N	606	CHL	C1A-C2A-CAA-CBA
39	r	605	CHL	C1A-C2A-CAA-CBA
39	s	606	CHL	C1A-C2A-CAA-CBA
39	y	303	CHL	C1A-C2A-CAA-CBA
23	A	402	CLA	C16-C17-C18-C20
23	C	512	CLA	CAA-CBA-CGA-O1A
23	d	405	CLA	CAA-CBA-CGA-O1A
39	g	609	CHL	CAA-CBA-CGA-O1A
38	F	501	HEM	CAD-CBD-CGD-O2D
23	B	605	CLA	C13-C15-C16-C17
23	R	611	CLA	CAA-CBA-CGA-O1A
23	c	512	CLA	CAA-CBA-CGA-O1A
27	C	525	LMG	O10-C28-C29-C30
30	N	618	LHG	O10-C23-C24-C25
30	b	627	LHG	O9-C7-C8-C9
30	g	618	LHG	C13-C14-C15-C16
27	B	626	LMG	O1-C7-C8-C9
39	G	605	CHL	CAA-CBA-CGA-O2A
23	C	503	CLA	C8-C10-C11-C12
23	B	608	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C2A-CAA-CBA-CGA
23	s	602	CLA	C2A-CAA-CBA-CGA
33	H	502	DGD	CCA-CDA-CEA-CFA
33	H	502	DGD	C8B-C9B-CAB-CBB
23	B	608	CLA	C16-C17-C18-C19
27	b	620	LMG	C10-C11-C12-C13
23	c	510	CLA	CAA-CBA-CGA-O1A
28	W	201	3PH	O22-C21-C22-C23
28	w	202	3PH	O22-C21-C22-C23
39	r	607	CHL	CAA-CBA-CGA-O1A
27	c	523	LMG	C35-C36-C37-C38
31	C	517	LNL	C4-C5-C6-C7
27	r	617	LMG	C29-C30-C31-C32
28	C	524	3PH	C35-C36-C37-C38
23	Y	310	CLA	C4-C3-C5-C6
39	Y	309	CHL	C4-C3-C5-C6
23	S	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	W	201	3PH	O31-C31-C32-C33
28	x	201	3PH	C33-C34-C35-C36
23	R	610	CLA	CAA-CBA-CGA-O1A
23	r	611	CLA	CAA-CBA-CGA-O1A
30	n	619	LHG	O9-C7-C8-C9
31	i	101	LNL	O1-C1-C2-C3
32	b	621	PAM	C7-C8-C9-C10
23	b	609	CLA	C13-C15-C16-C17
30	D	408	LHG	C3-O3-P-O4
23	B	610	CLA	C16-C17-C18-C20
23	a	403	CLA	C16-C17-C18-C20
39	g	605	CHL	C2-C1-O2A-CGA
23	B	613	CLA	CAA-CBA-CGA-O1A
23	G	611	CLA	CAA-CBA-CGA-O1A
23	r	610	CLA	CAA-CBA-CGA-O1A
39	G	608	CHL	CAA-CBA-CGA-O1A
23	s	603	CLA	O2A-C1-C2-C3
27	r	617	LMG	O7-C10-C11-C12
23	Y	303	CLA	C8-C10-C11-C12
40	S	614	LUT	C5-C6-C7-C8
40	g	615	LUT	C5-C6-C7-C8
27	R	617	LMG	C42-C43-C44-C45
23	B	614	CLA	C13-C15-C16-C17
23	c	508	CLA	C5-C6-C7-C8
23	C	501	CLA	CAA-CBA-CGA-O1A
23	c	501	CLA	CAA-CBA-CGA-O1A
23	r	601	CLA	CAA-CBA-CGA-O1A
28	A	410	3PH	O22-C21-C22-C23
28	C	524	3PH	O22-C21-C22-C23
28	a	410	3PH	O32-C31-C32-C33
39	S	601	CHL	CAA-CBA-CGA-O1A
23	R	601	CLA	CAA-CBA-CGA-O2A
23	R	603	CLA	CAA-CBA-CGA-O2A
28	w	202	3PH	C3A-C3B-C3C-C3D
30	y	318	LHG	C27-C28-C29-C30
31	C	520	LNL	O2-C1-C2-C3
27	B	620	LMG	C12-C13-C14-C15
23	B	610	CLA	CAA-CBA-CGA-O1A
23	Y	304	CLA	CAA-CBA-CGA-O1A
33	d	411	DGD	O1B-C1B-C2B-C3B
39	R	606	CHL	C4C-C3C-CAC-CBC
23	Y	313	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	C	515	DGD	O1B-C1B-C2B-C3B
29	d	407	PL9	C38-C39-C41-C42
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	512	CLA	CAD-CBD-CGD-O1D
23	Y	314	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	612	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	512	CLA	CAD-CBD-CGD-O1D
26	A	408	SQD	O5-C5-C6-S
28	w	202	3PH	C31-C32-C33-C34
23	C	510	CLA	CAA-CBA-CGA-O1A
39	R	607	CHL	CAA-CBA-CGA-O1A
28	L	102	3PH	C25-C26-C27-C28
26	a	409	SQD	O47-C7-C8-C9
39	S	605	CHL	CAA-CBA-CGA-O2A
39	n	606	CHL	CAA-CBA-CGA-O2A
33	H	502	DGD	O6D-C5D-C6D-O5D
30	r	616	LHG	O2-C2-C3-O3
23	C	502	CLA	C11-C10-C8-C9
23	Y	314	CLA	C6-C7-C8-C9
23	Y	314	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
39	N	609	CHL	C14-C13-C15-C16
30	r	616	LHG	O9-C7-O7-C5
28	A	410	3PH	C2D-C2E-C2F-C2G
38	F	501	HEM	CAA-CBA-CGA-O1A
38	f	501	HEM	CAA-CBA-CGA-O2A
23	R	612	CLA	CAA-CBA-CGA-O1A
39	s	601	CHL	CAA-CBA-CGA-O1A
23	c	507	CLA	CBA-CGA-O2A-C1
30	Y	318	LHG	C24-C23-O8-C6
23	Y	312	CLA	CAA-CBA-CGA-O2A
23	s	603	CLA	CAA-CBA-CGA-O2A
23	S	603	CLA	C2A-CAA-CBA-CGA
23	y	306	CLA	CBA-CGA-O2A-C1
23	S	611	CLA	CAA-CBA-CGA-O2A
30	G	618	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	Y	308	CHL	CAA-CBA-CGA-O2A
23	b	611	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
33	c	515	DGD	C5B-C6B-C7B-C8B
23	A	403	CLA	CBD-CGD-O2D-CED
23	S	610	CLA	C4-C3-C5-C6
23	C	507	CLA	C12-C13-C15-C16
23	N	610	CLA	C2-C3-C5-C6
23	N	611	CLA	C6-C7-C8-C10
23	N	613	CLA	C3A-C2A-CAA-CBA
23	Y	314	CLA	C11-C12-C13-C15
23	b	604	CLA	C2-C3-C5-C6
23	b	610	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C12-C13-C15
23	c	512	CLA	C6-C7-C8-C10
23	g	610	CLA	C12-C13-C15-C16
23	n	610	CLA	C11-C12-C13-C15
23	r	609	CLA	C12-C13-C15-C16
23	s	613	CLA	C3A-C2A-CAA-CBA
23	y	306	CLA	C11-C12-C13-C15
23	y	313	CLA	C11-C10-C8-C7
35	y	301	VIV	C17-C18-C20-C21
39	y	303	CHL	C11-C12-C13-C15
39	g	607	CHL	CAA-CBA-CGA-O1A
39	n	606	CHL	CAA-CBA-CGA-O1A
26	L	101	SQD	C11-C10-C9-C8
28	w	202	3PH	C27-C28-C29-C2A
23	r	603	CLA	CAA-CBA-CGA-O2A
28	T	101	3PH	O21-C21-C22-C23
30	Y	318	LHG	O8-C23-C24-C25
37	b	626	DGA	OG2-CB1-CB2-CB3
31	c	521	LNL	C7-C8-C9-C10
41	g	617	NEX	C27-C28-C29-C30
42	G	619	XAT	C11-C12-C13-C14
23	n	612	CLA	CAA-CBA-CGA-O1A
39	G	605	CHL	CAA-CBA-CGA-O1A
31	A	413	LNL	O1-C1-C2-C3
40	g	616	LUT	C29-C30-C31-C32
42	Y	301	XAT	C13-C14-C15-C35
27	d	409	LMG	C32-C33-C34-C35
23	B	602	CLA	CAA-CBA-CGA-O2A
23	N	603	CLA	CAA-CBA-CGA-O2A

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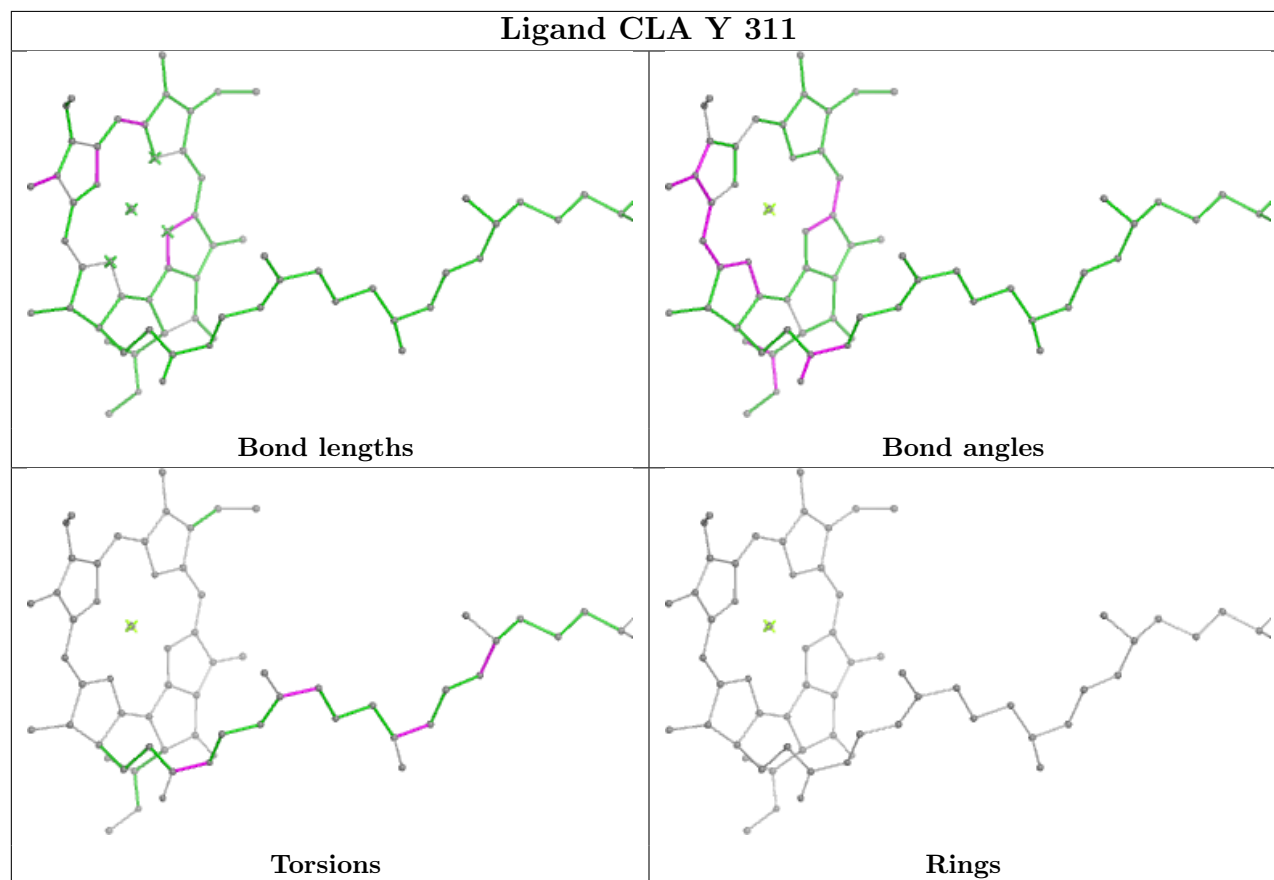
Mol	Chain	Res	Type	Atoms
23	N	613	CLA	CAA-CBA-CGA-O2A
23	s	611	CLA	CAA-CBA-CGA-O2A
39	N	608	CHL	CAA-CBA-CGA-O2A
23	g	602	CLA	C8-C10-C11-C12
23	y	306	CLA	O1A-CGA-O2A-C1
30	b	627	LHG	C17-C18-C19-C20
23	R	601	CLA	CAA-CBA-CGA-O1A
27	b	628	LMG	C15-C16-C17-C18
23	B	605	CLA	C10-C11-C12-C13
23	c	505	CLA	O1A-CGA-O2A-C1
23	n	612	CLA	CAA-CBA-CGA-O2A
30	s	616	LHG	O8-C23-C24-C25
39	g	608	CHL	CAA-CBA-CGA-O2A
23	D	406	CLA	C10-C11-C12-C13
23	S	602	CLA	CAA-CBA-CGA-O1A
23	S	611	CLA	CAA-CBA-CGA-O1A
23	b	610	CLA	CAA-CBA-CGA-O1A
23	s	603	CLA	CAA-CBA-CGA-O1A
28	W	201	3PH	O32-C31-C32-C33
23	Y	310	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C16-C17-C18-C20
27	C	525	LMG	C34-C35-C36-C37
23	s	613	CLA	C15-C16-C17-C18
30	G	618	LHG	O9-C7-C8-C9
23	y	312	CLA	C4-C3-C5-C6
26	A	408	SQD	C13-C14-C15-C16
28	X	201	3PH	O21-C21-C22-C23
33	C	515	DGD	O2G-C1B-C2B-C3B
39	g	605	CHL	CAA-CBA-CGA-O2A
39	s	607	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

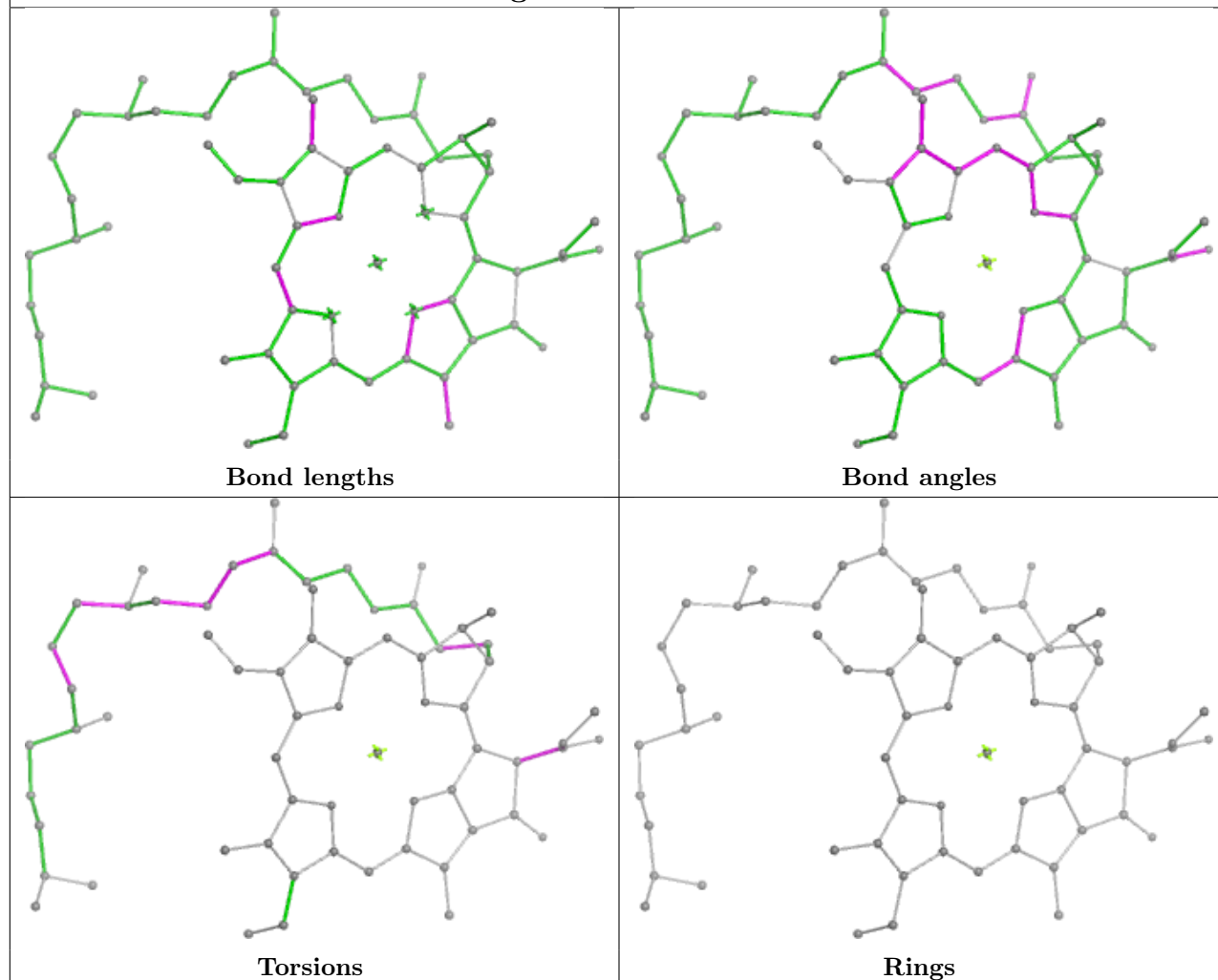
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

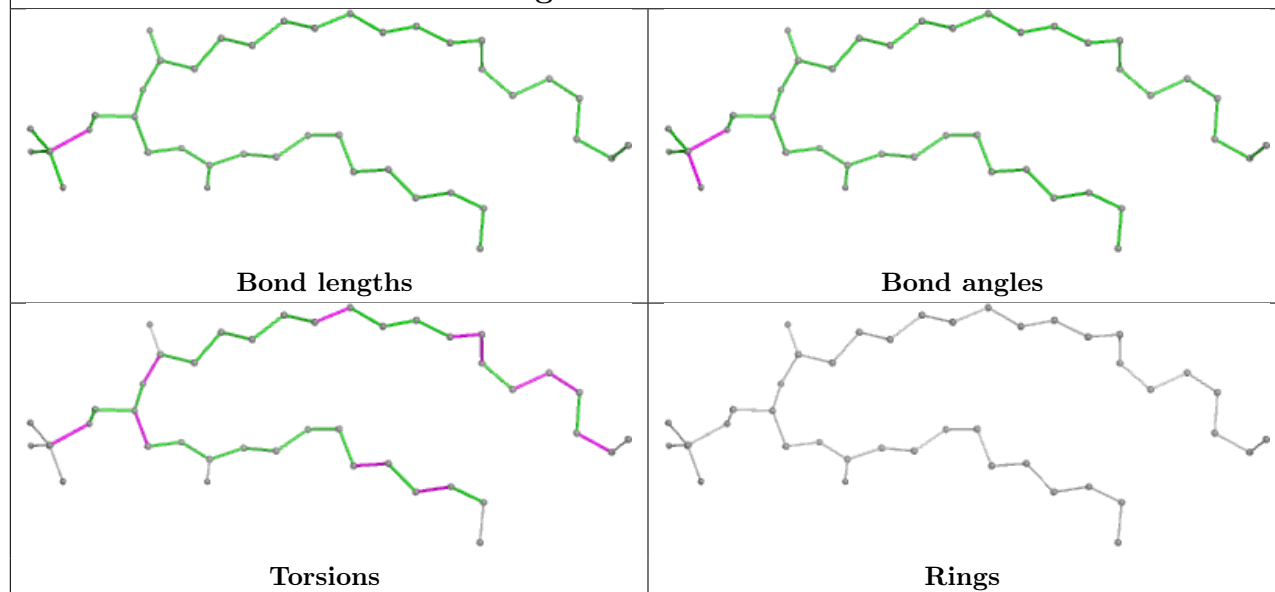
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

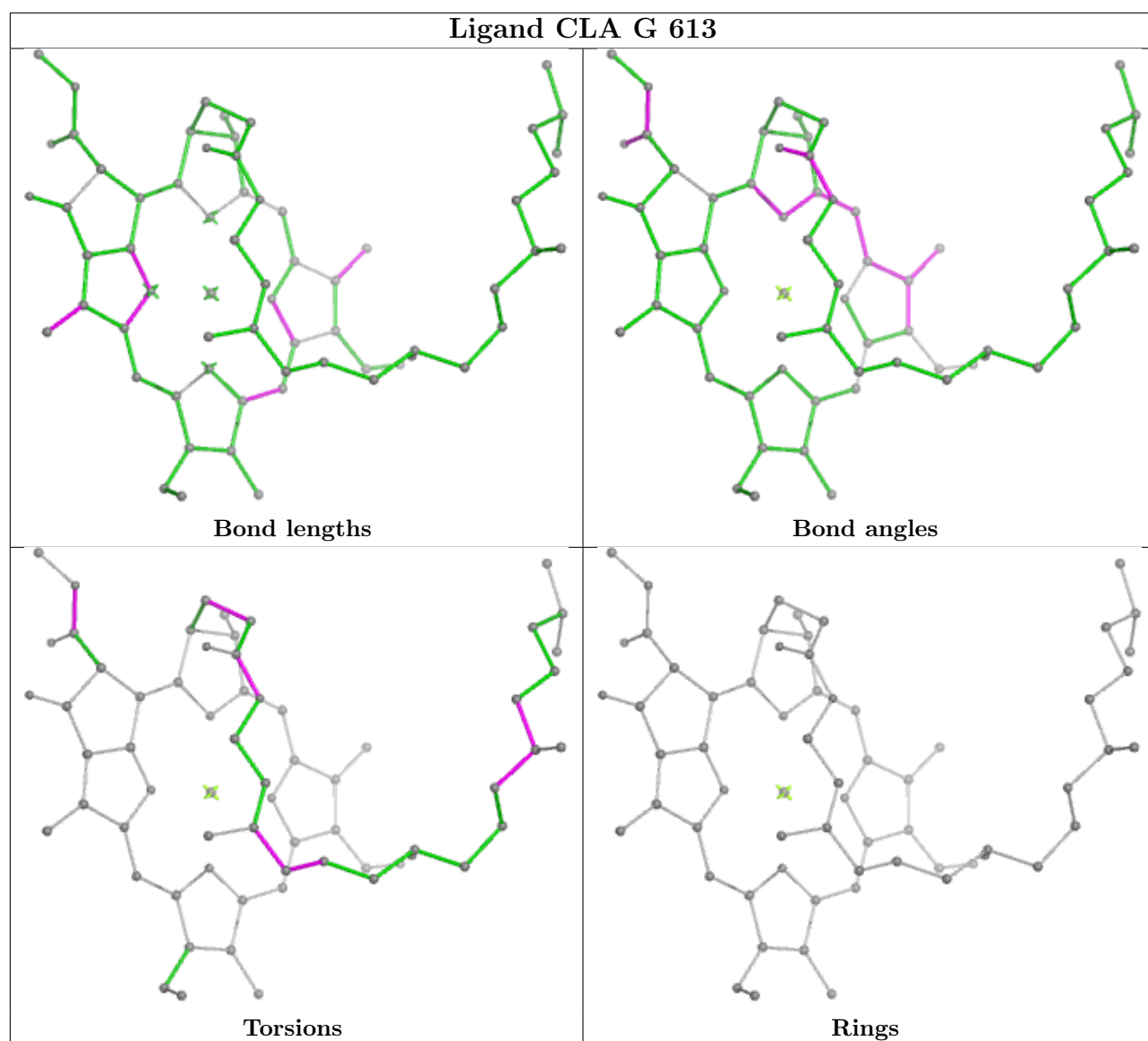


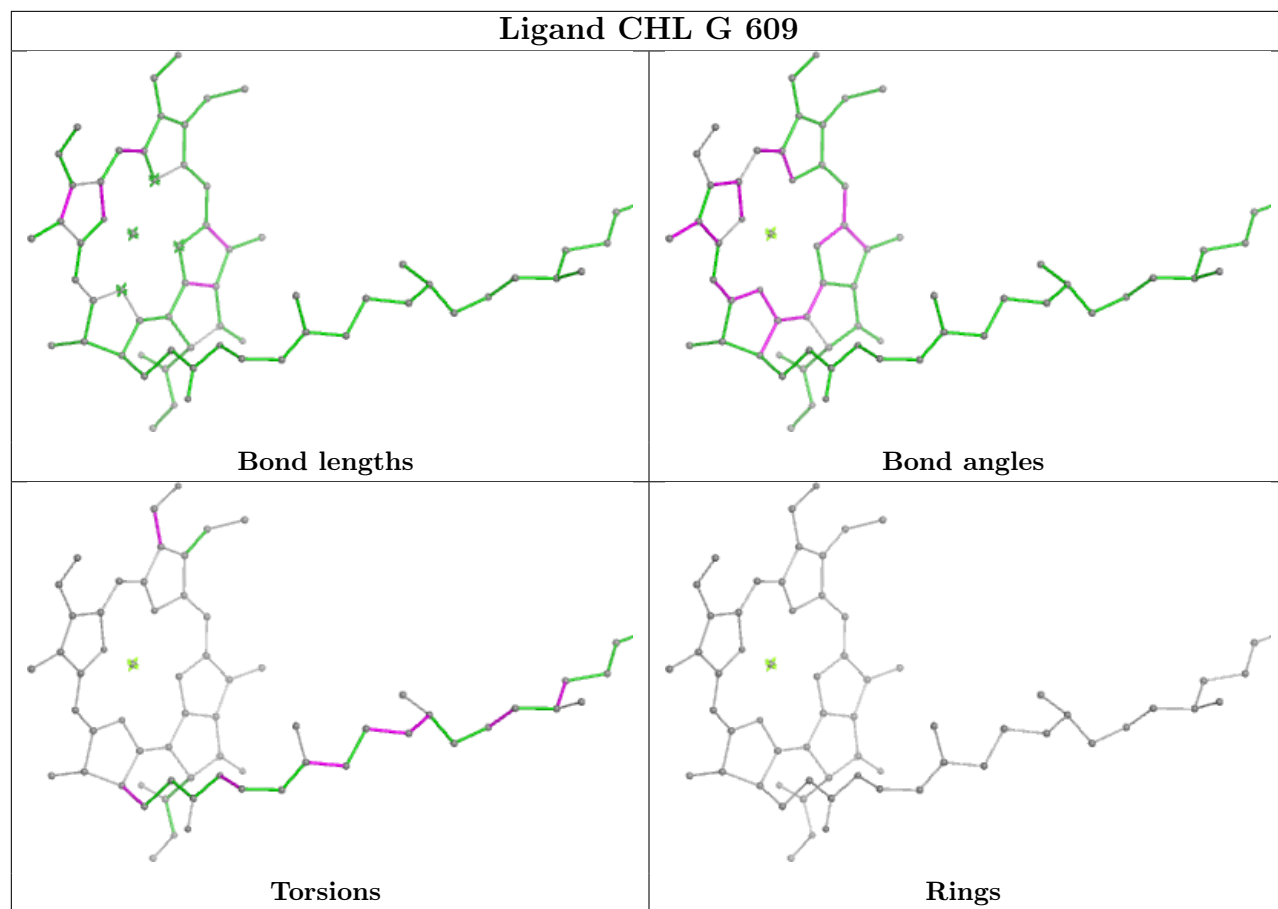
## Ligand CLA n 602

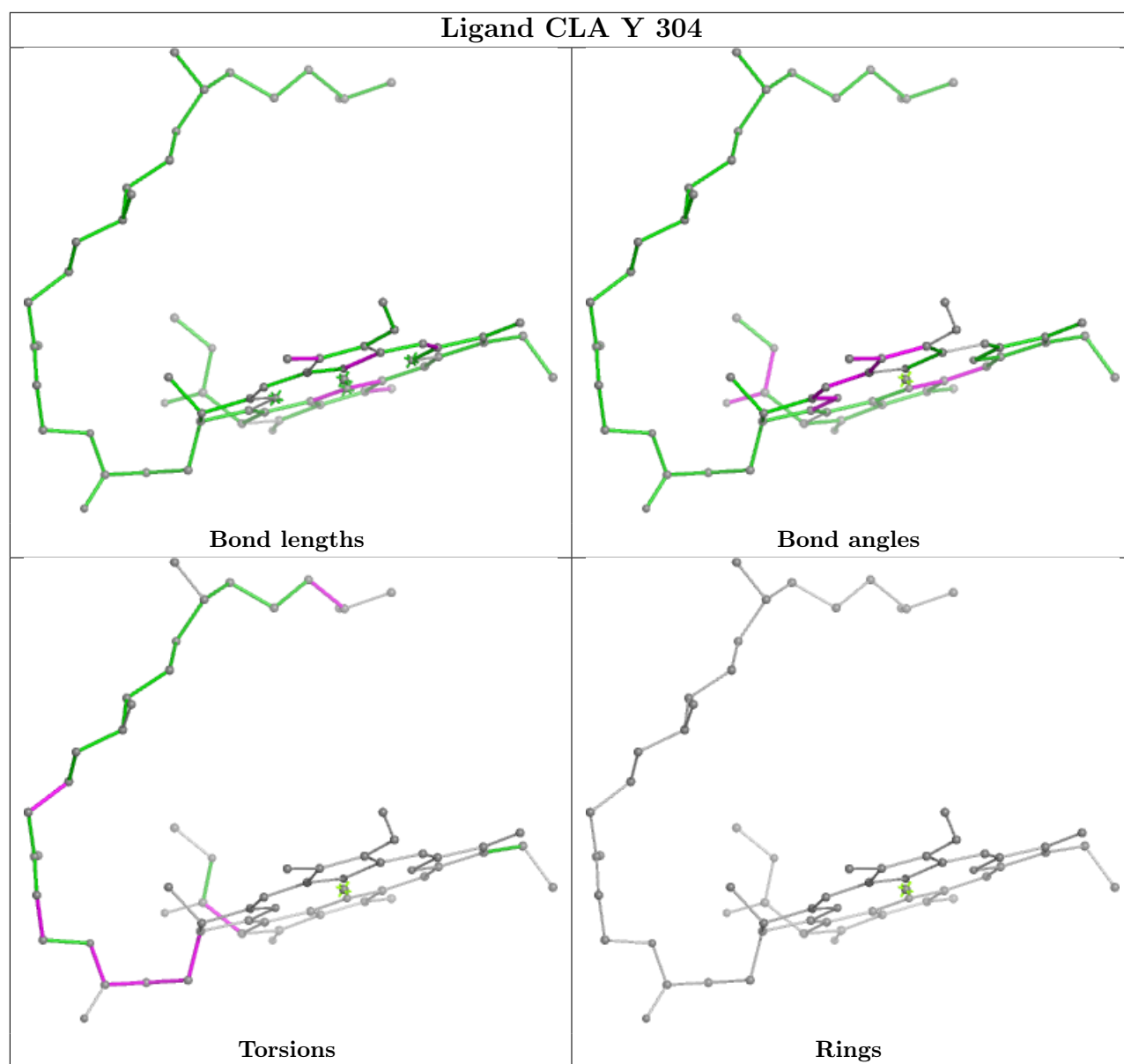


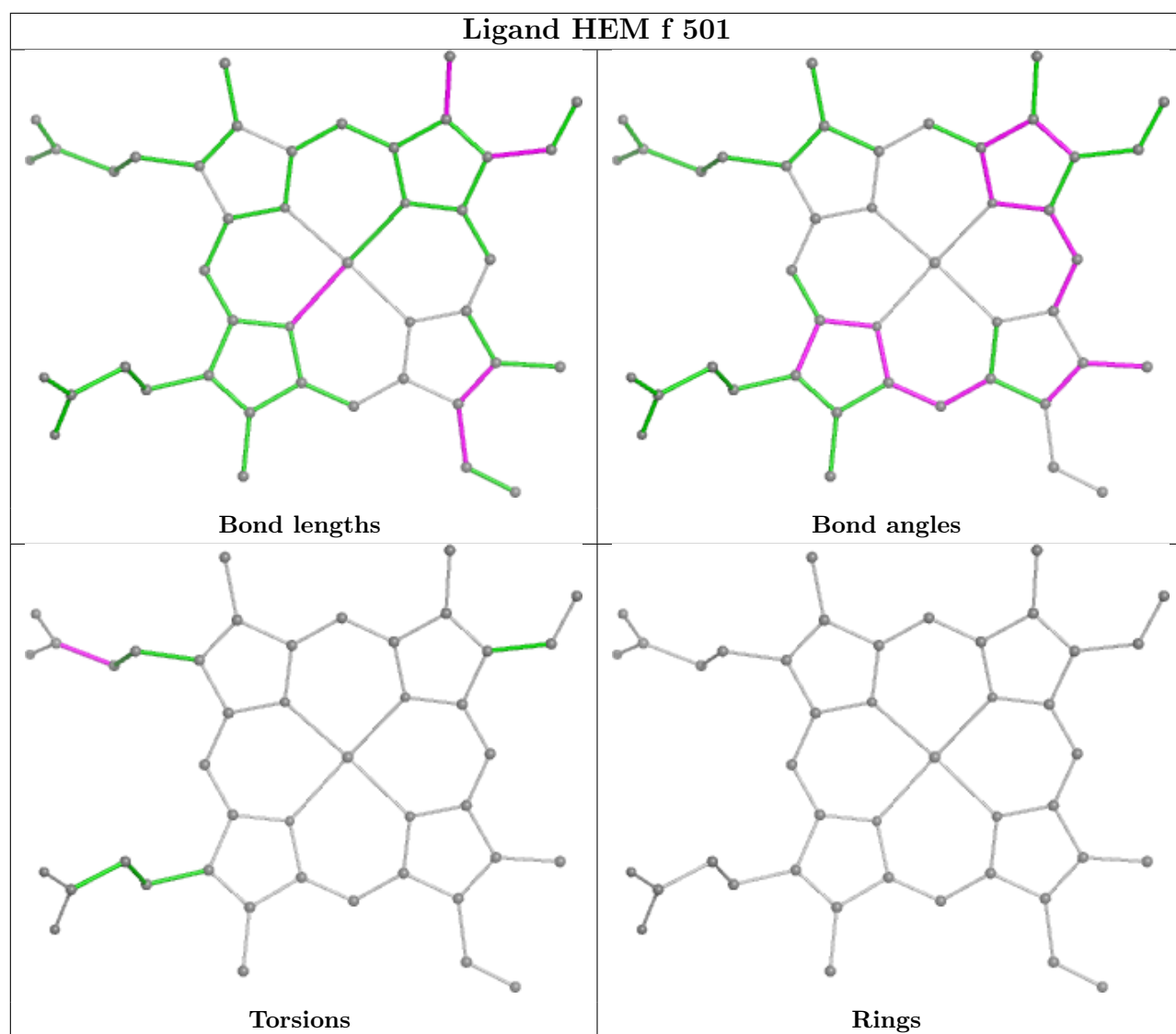
## Ligand 3PH L 102



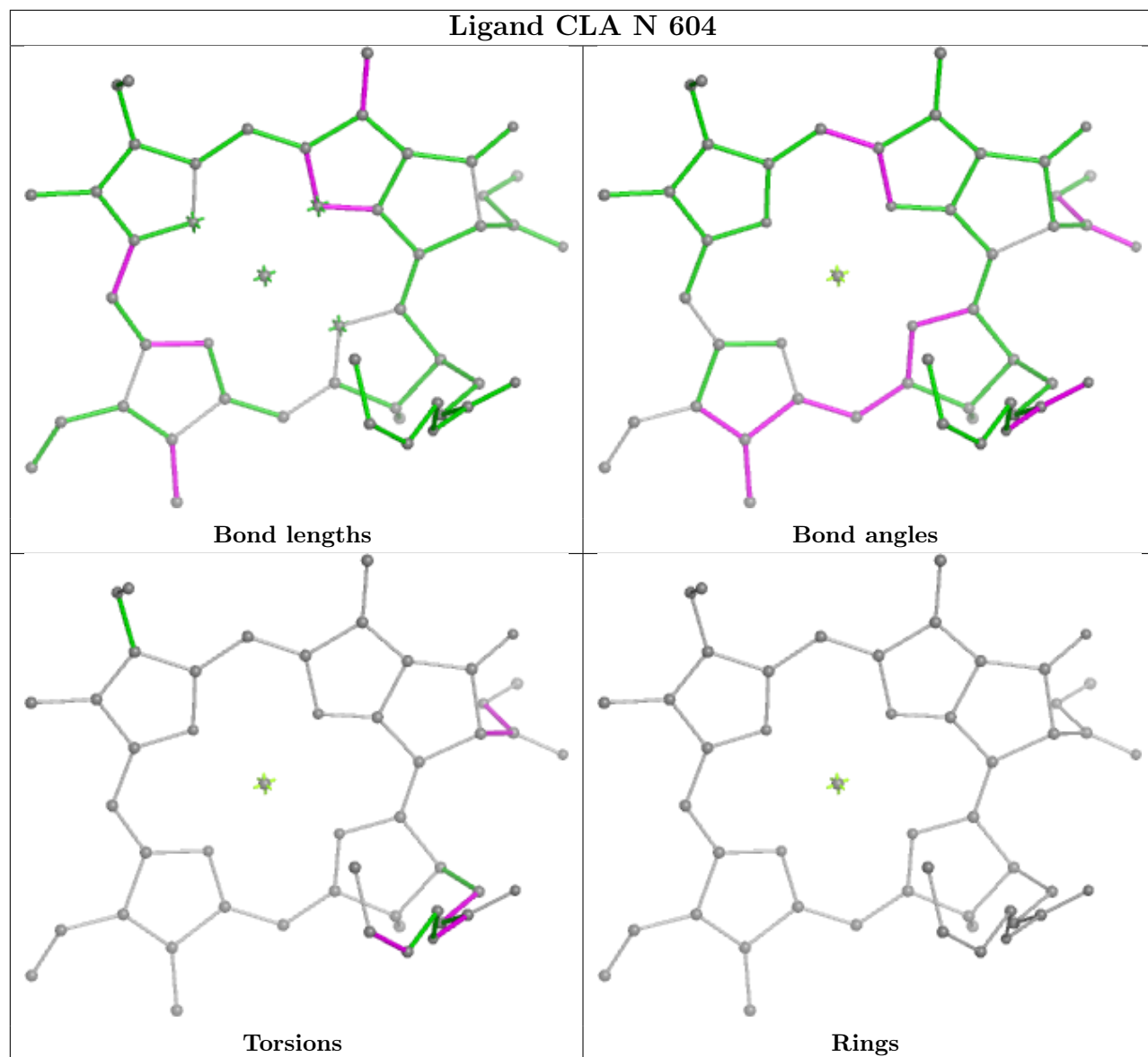


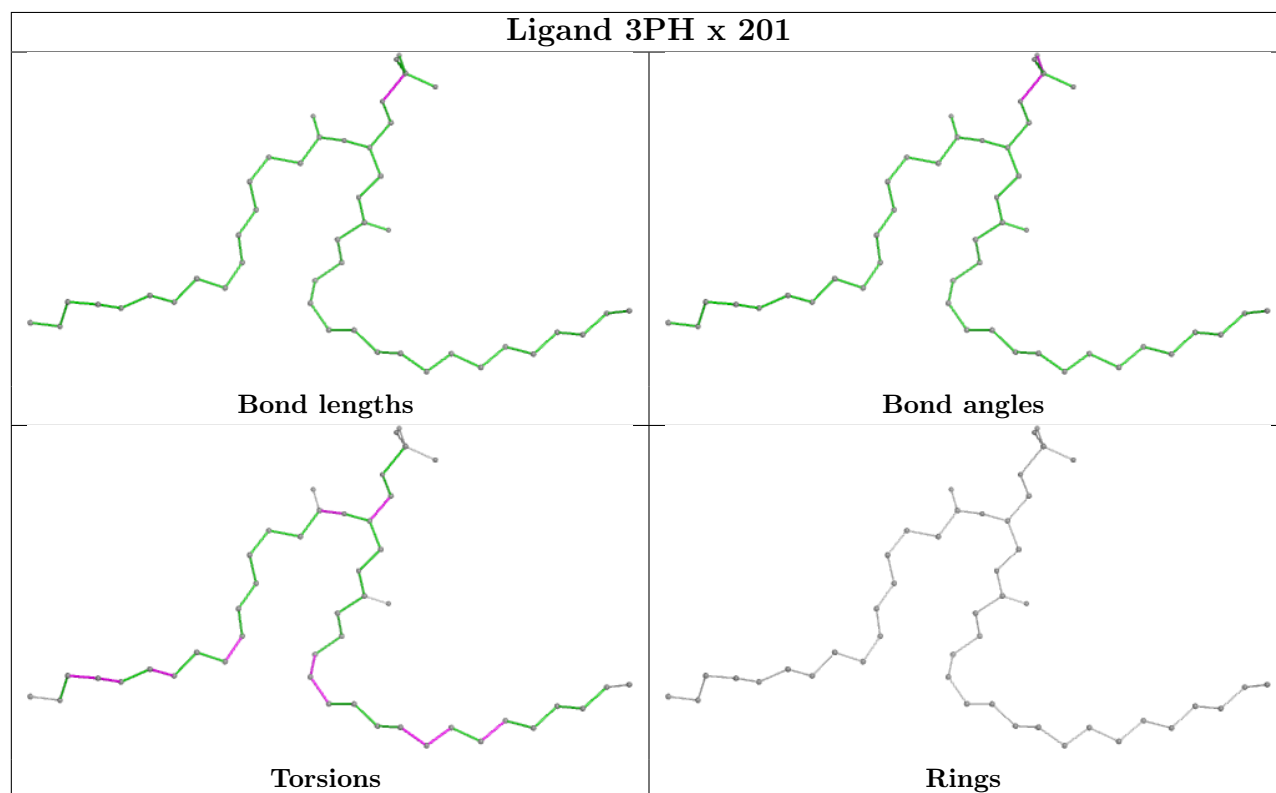
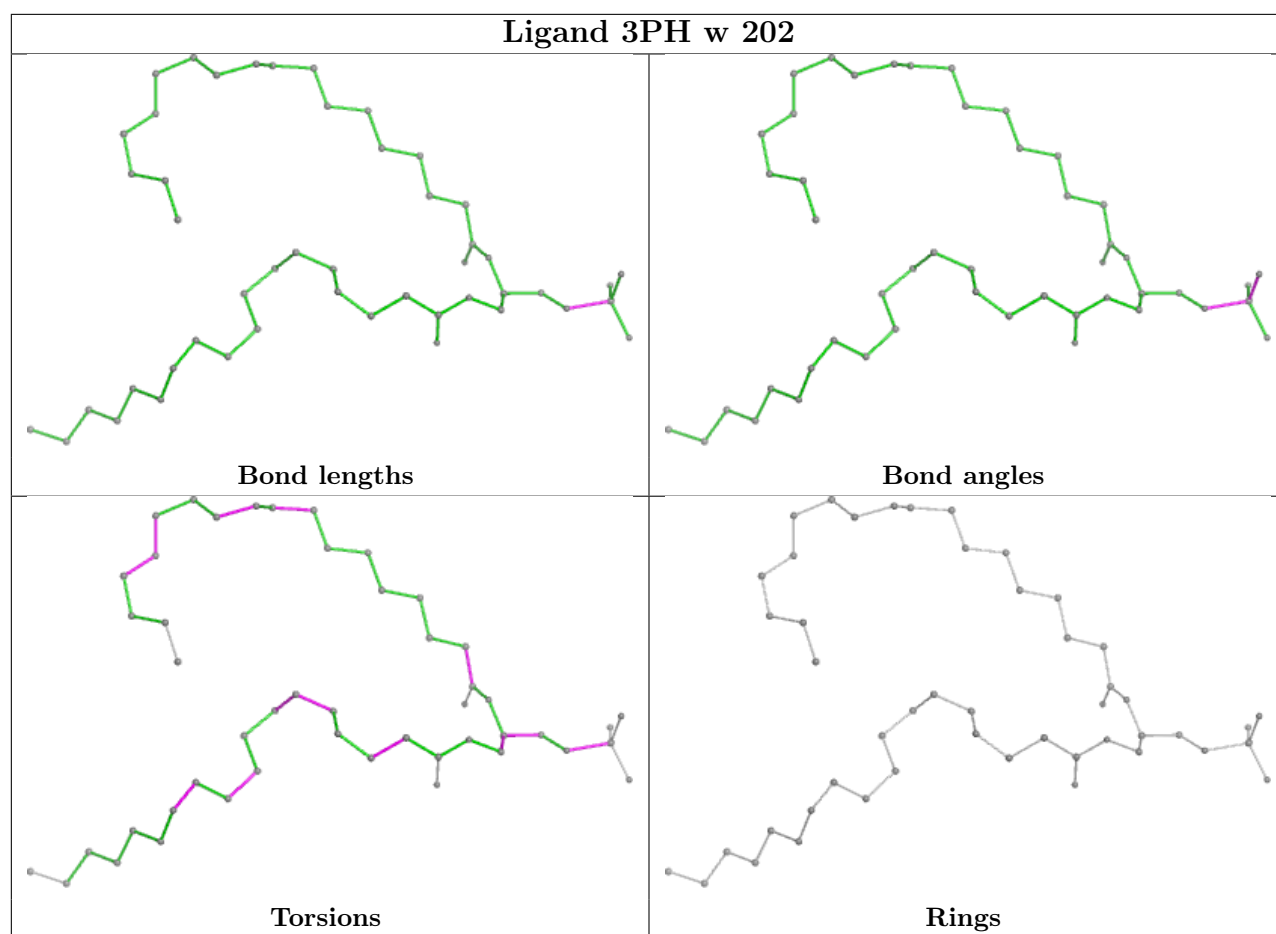


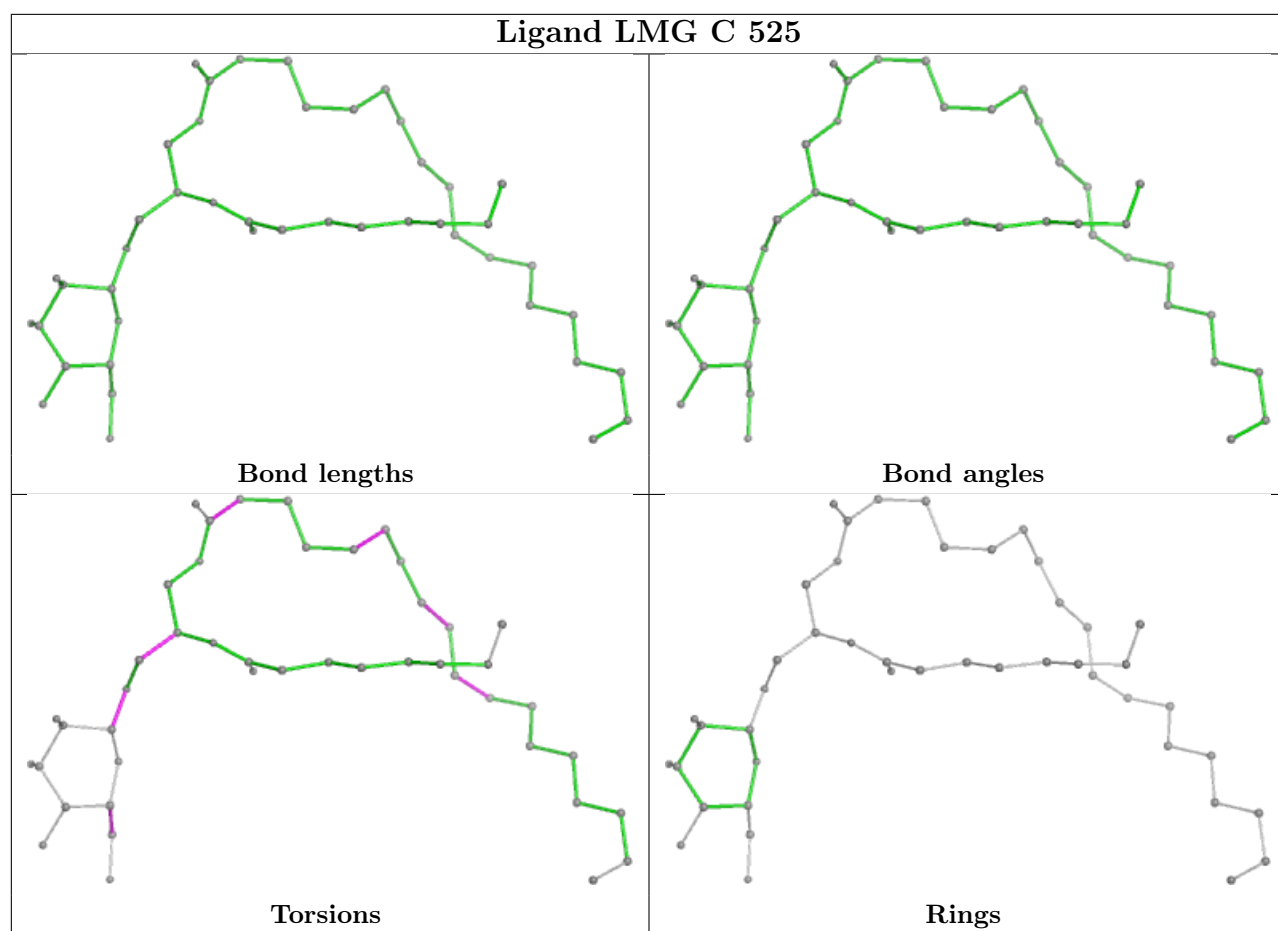


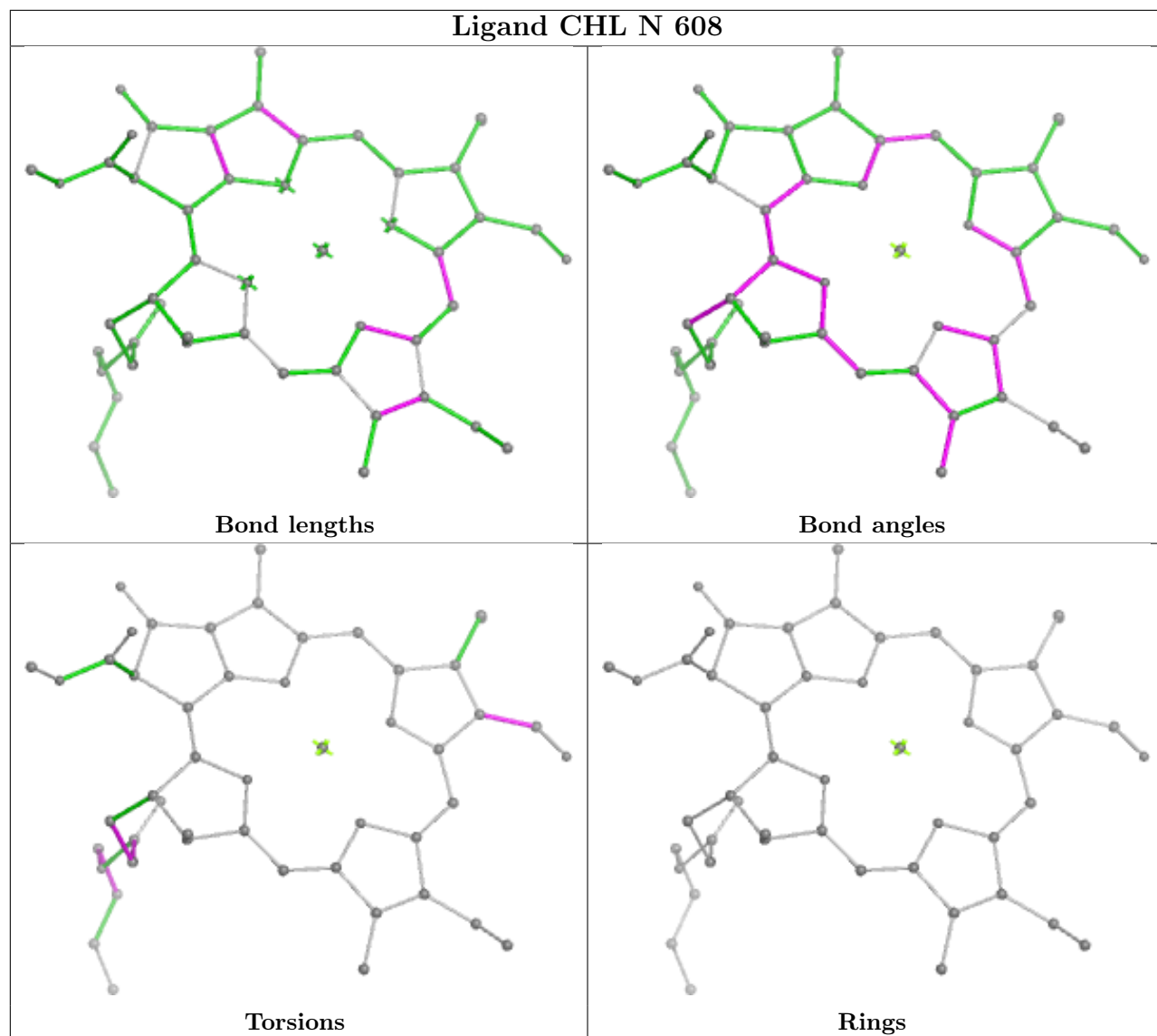




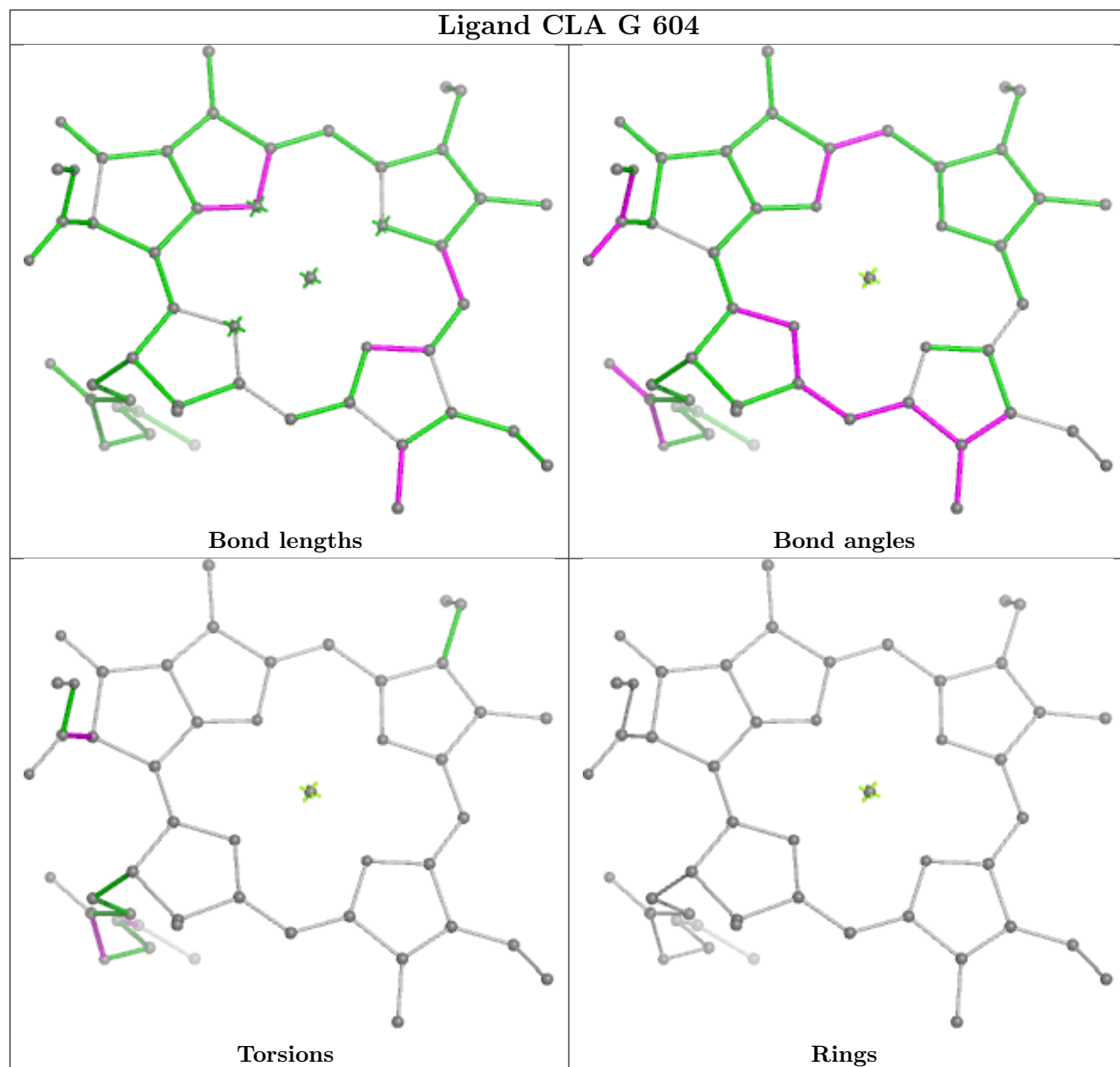


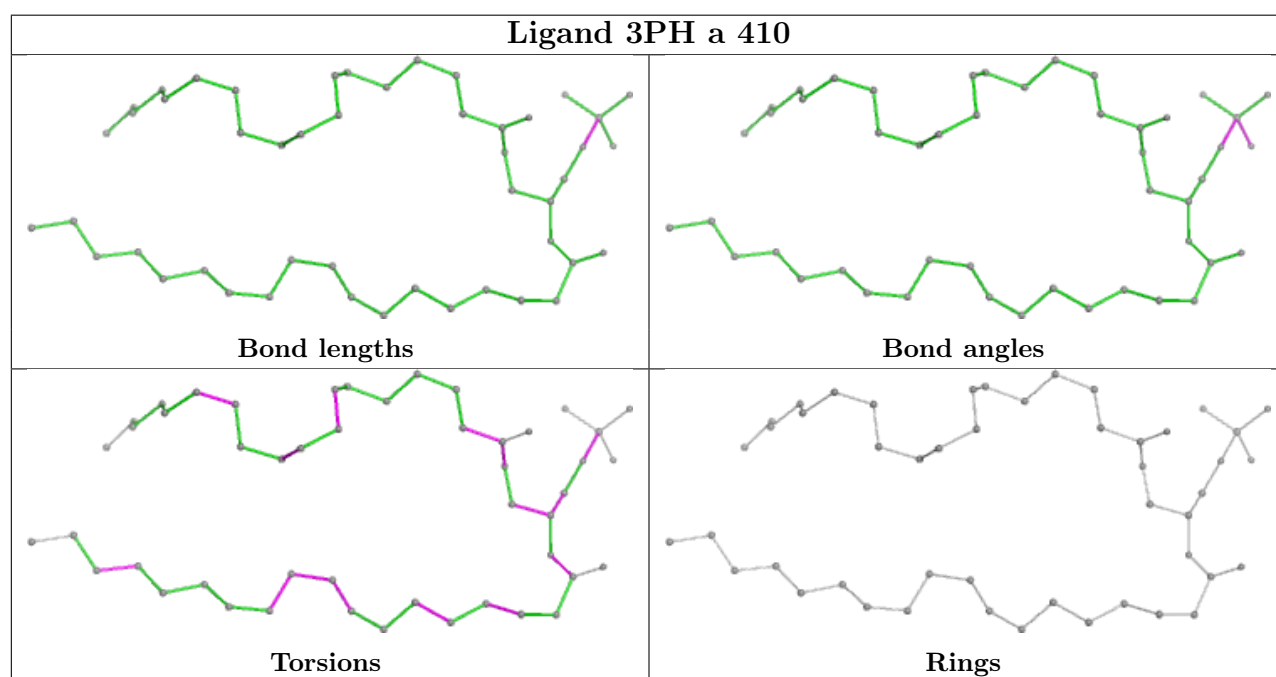
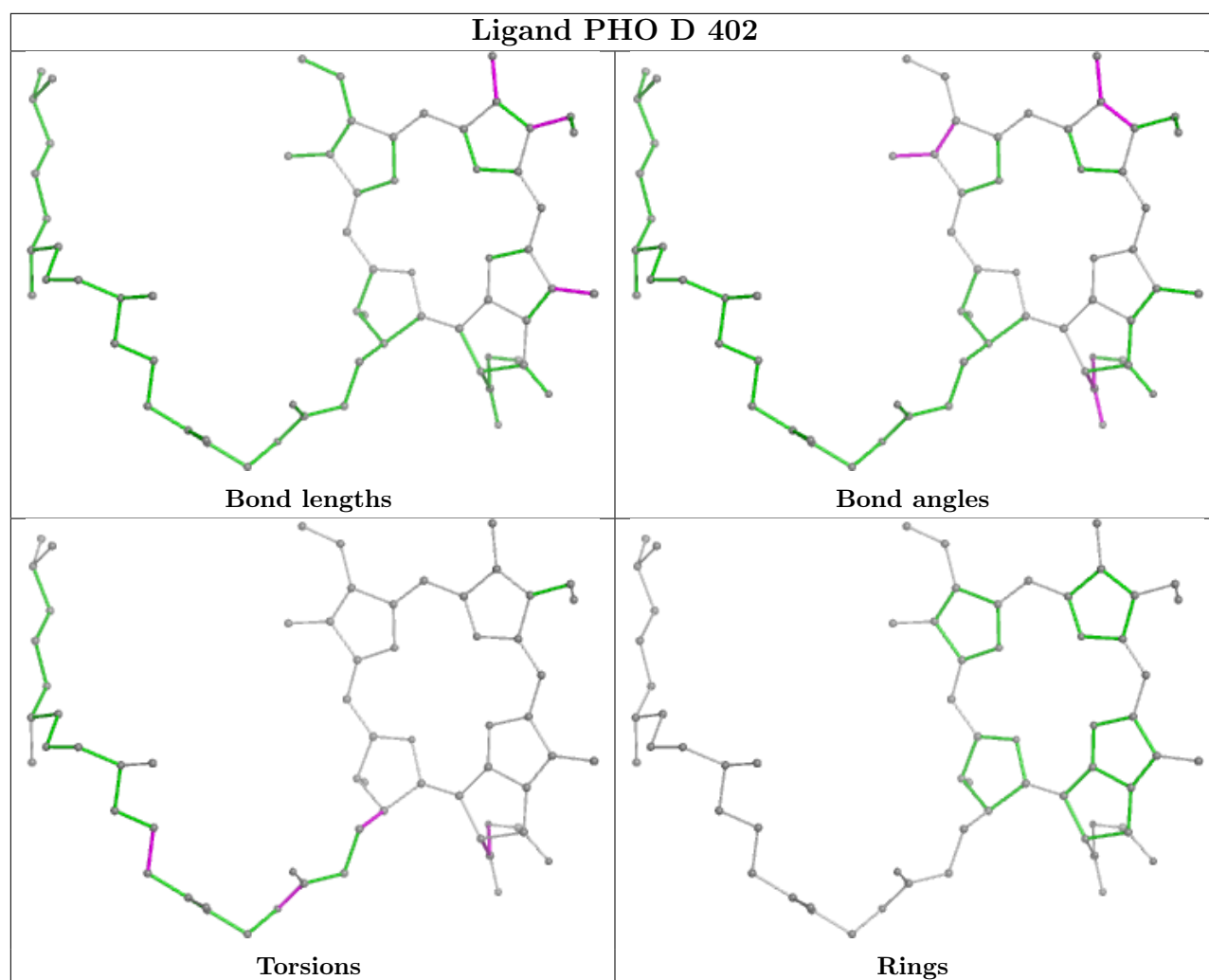


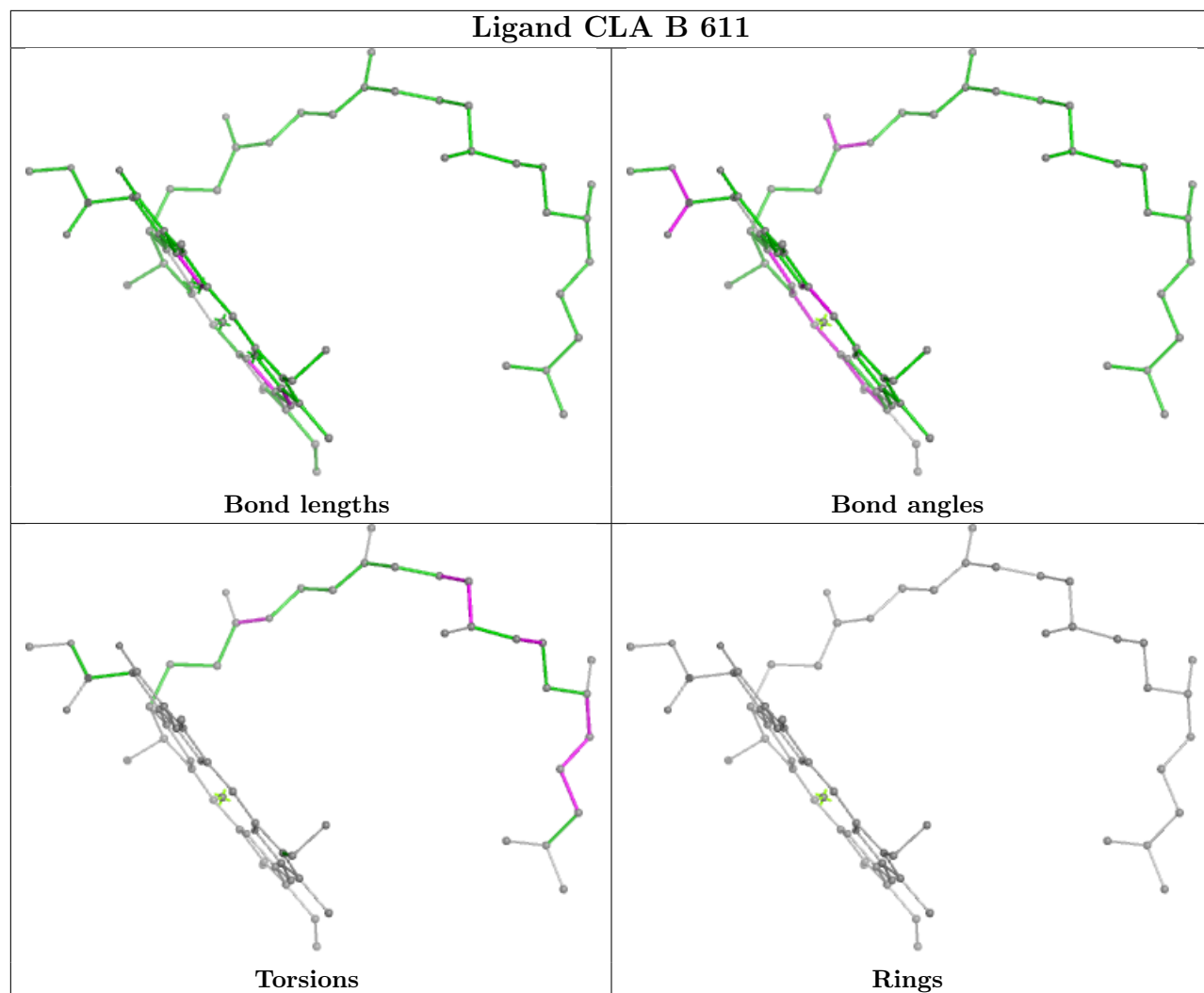




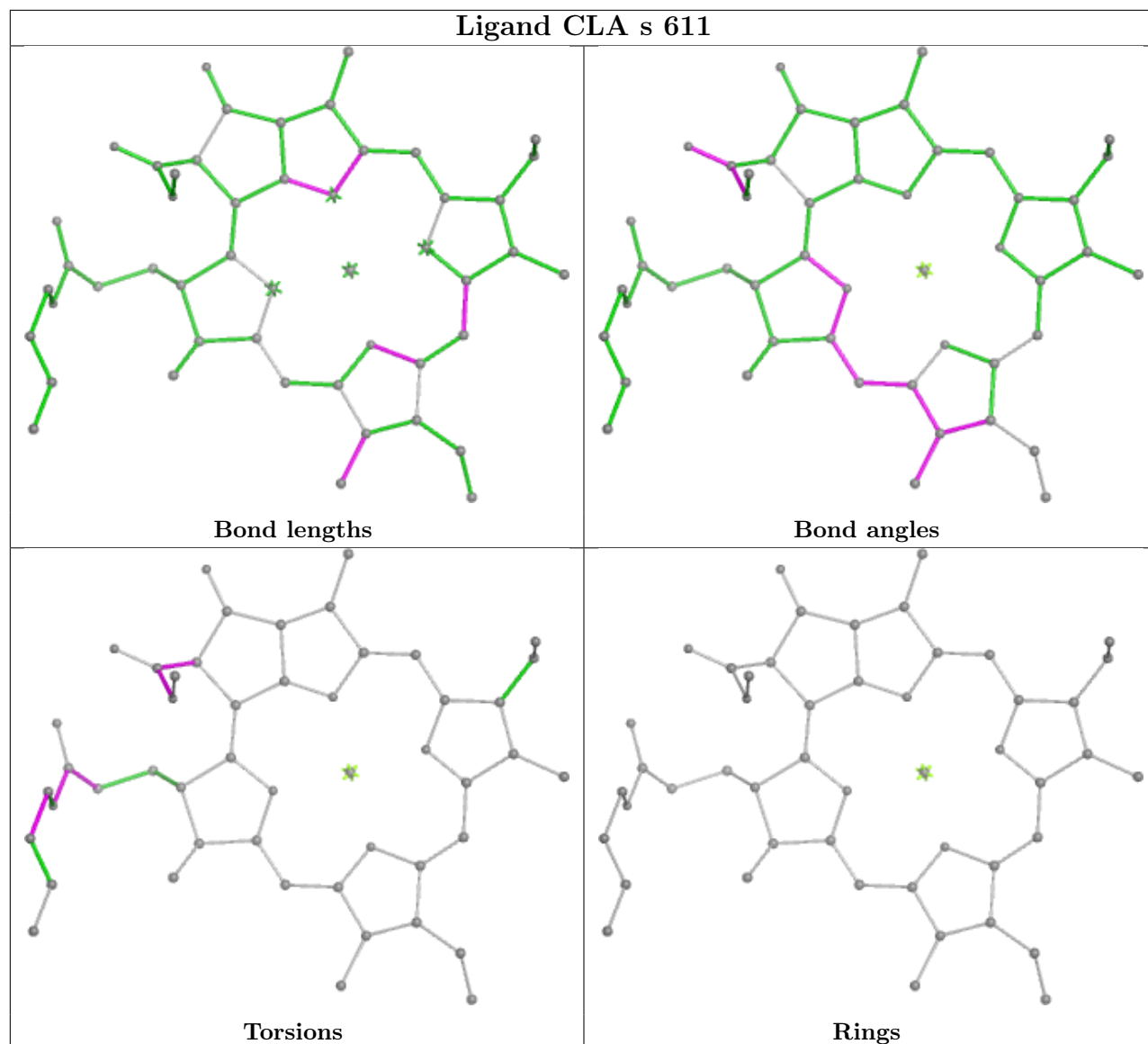
## Ligand CLA G 604



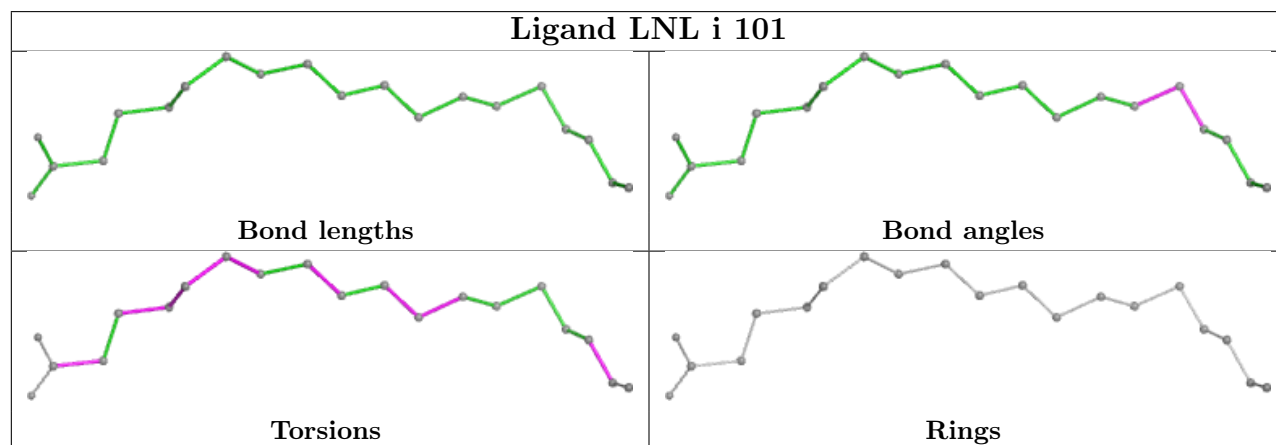




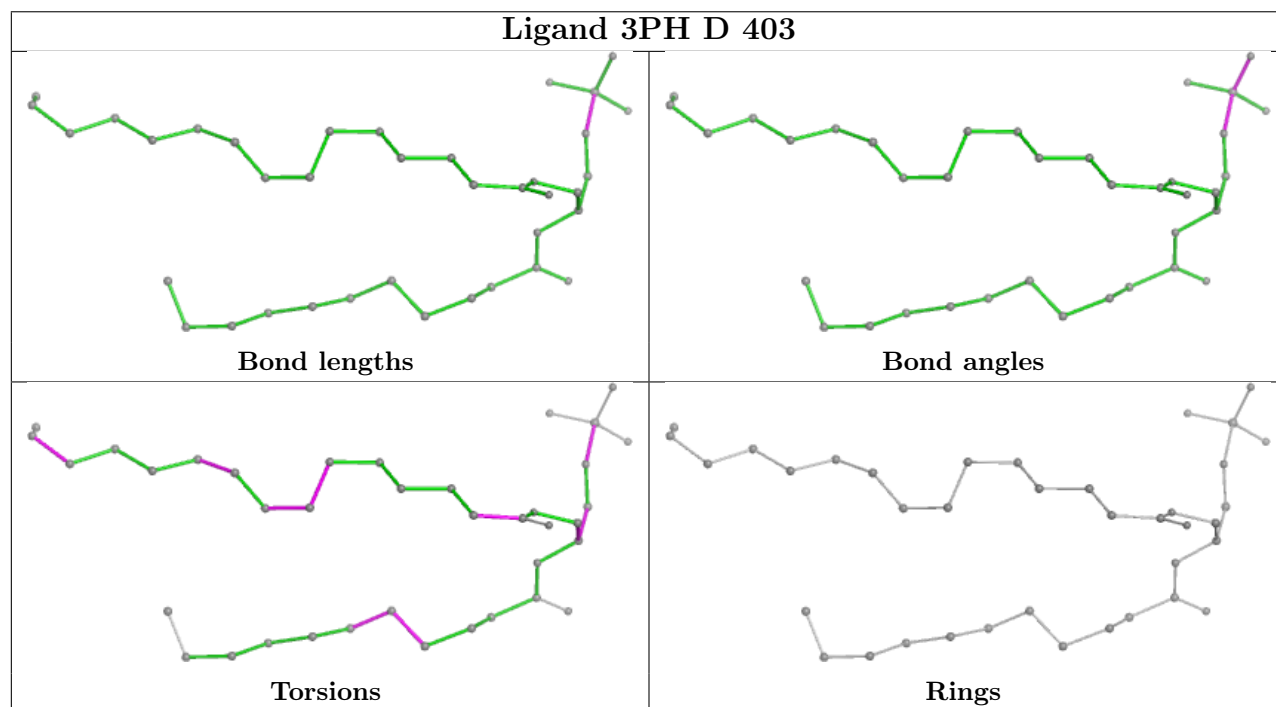
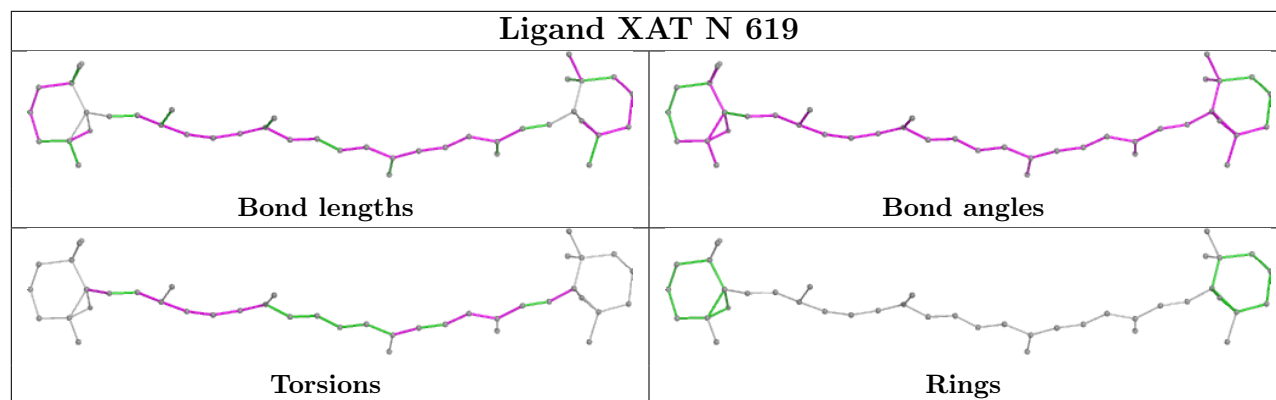
## Ligand CLA s 611

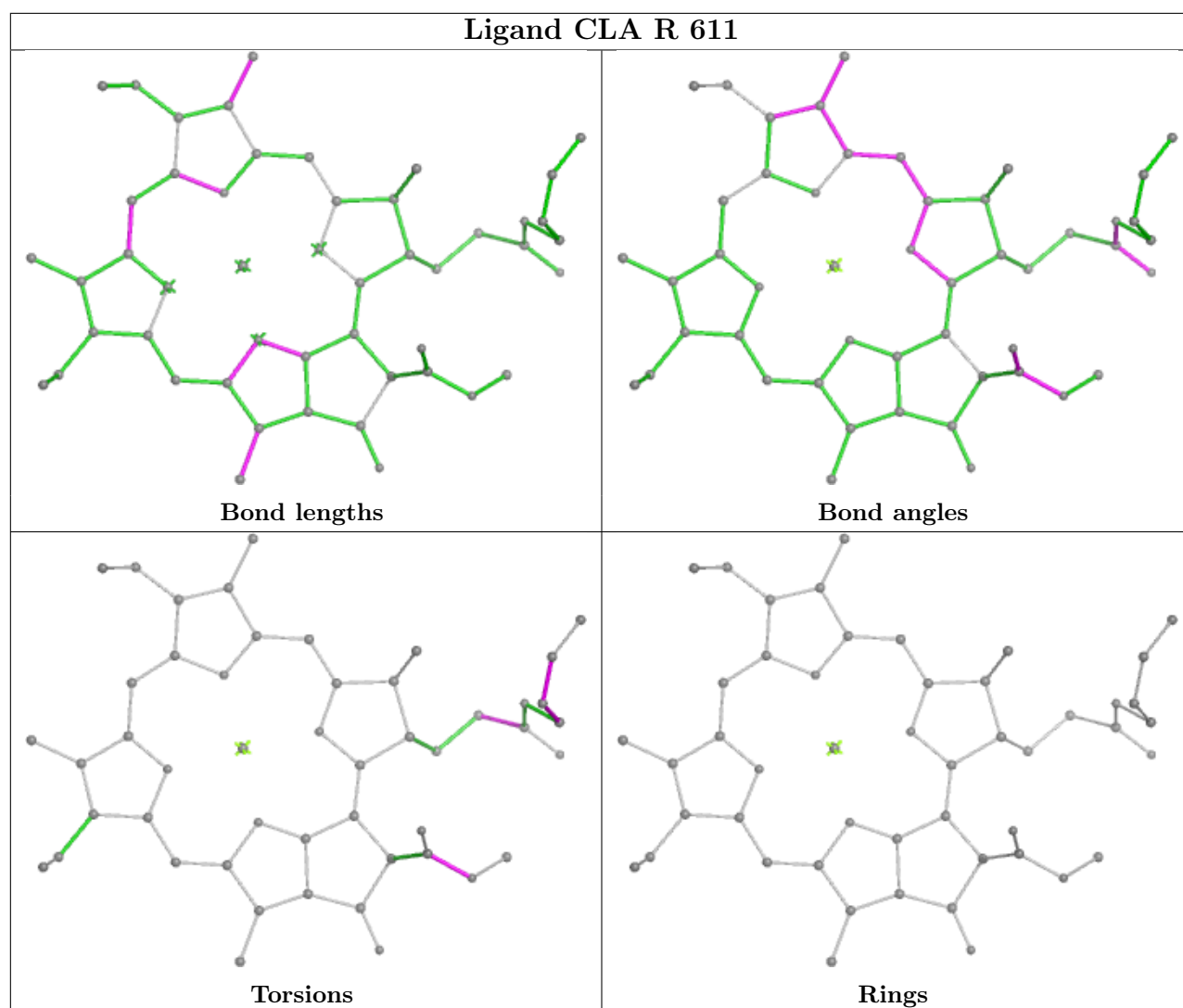


## Ligand LNL i 101

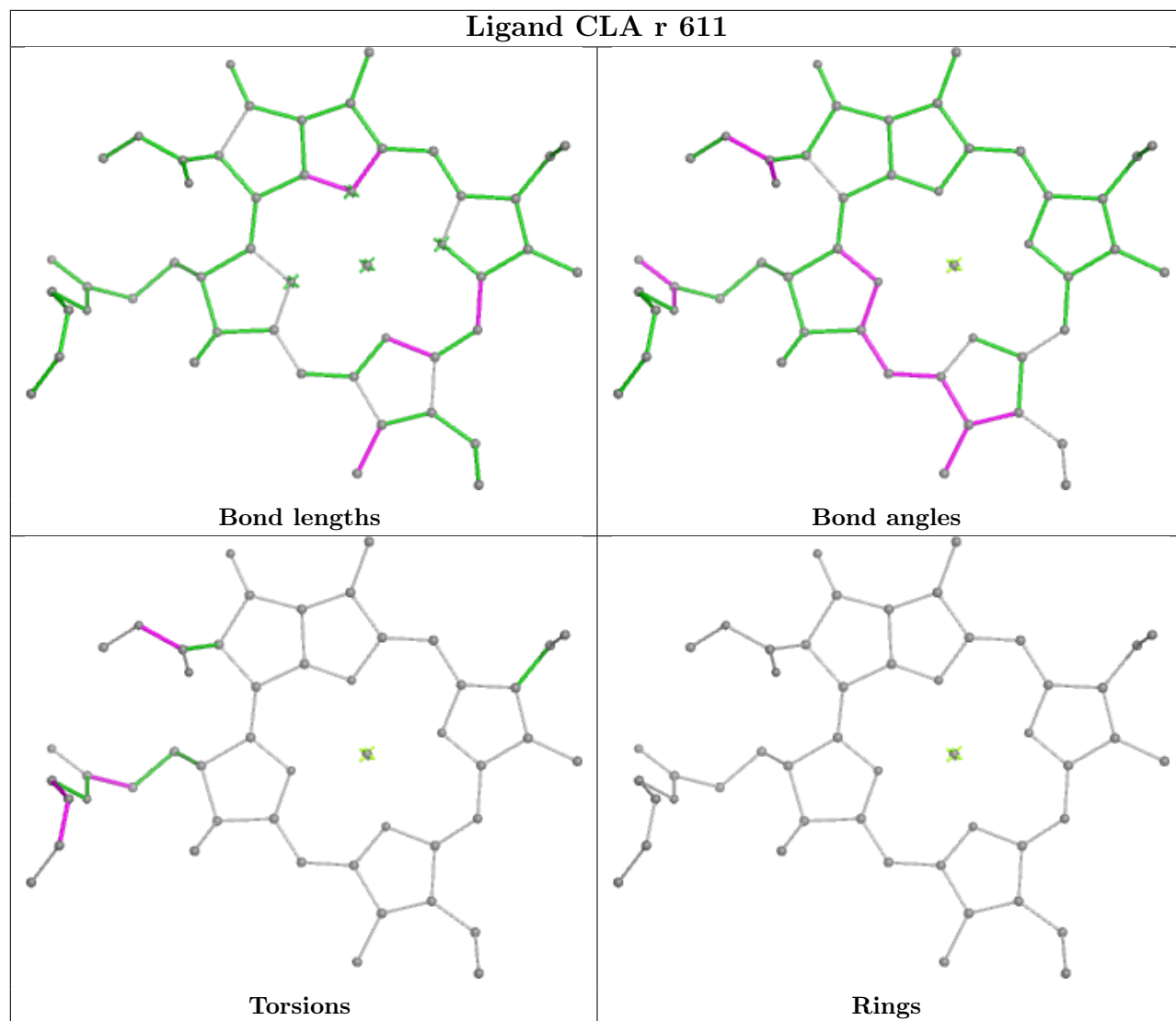


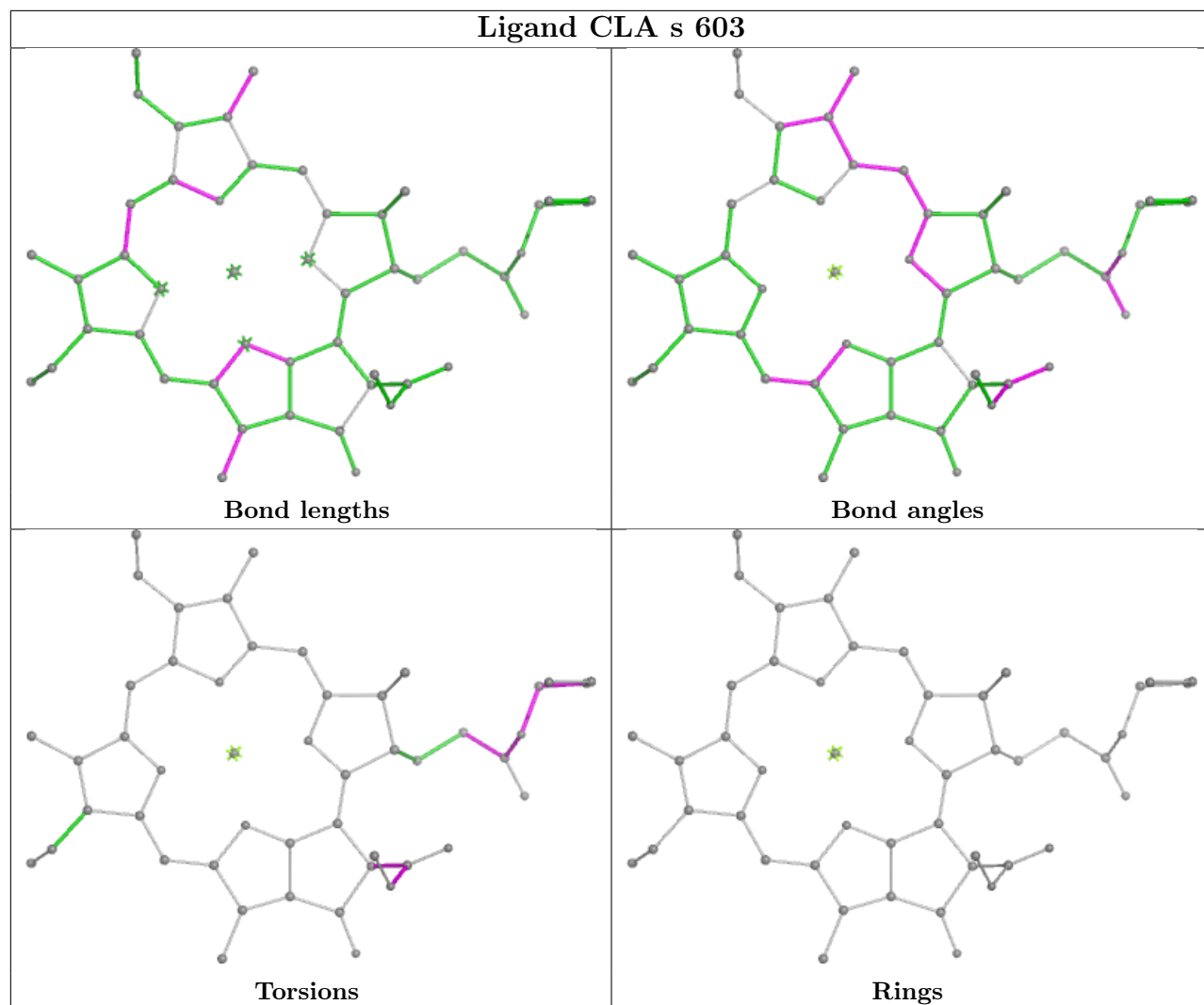


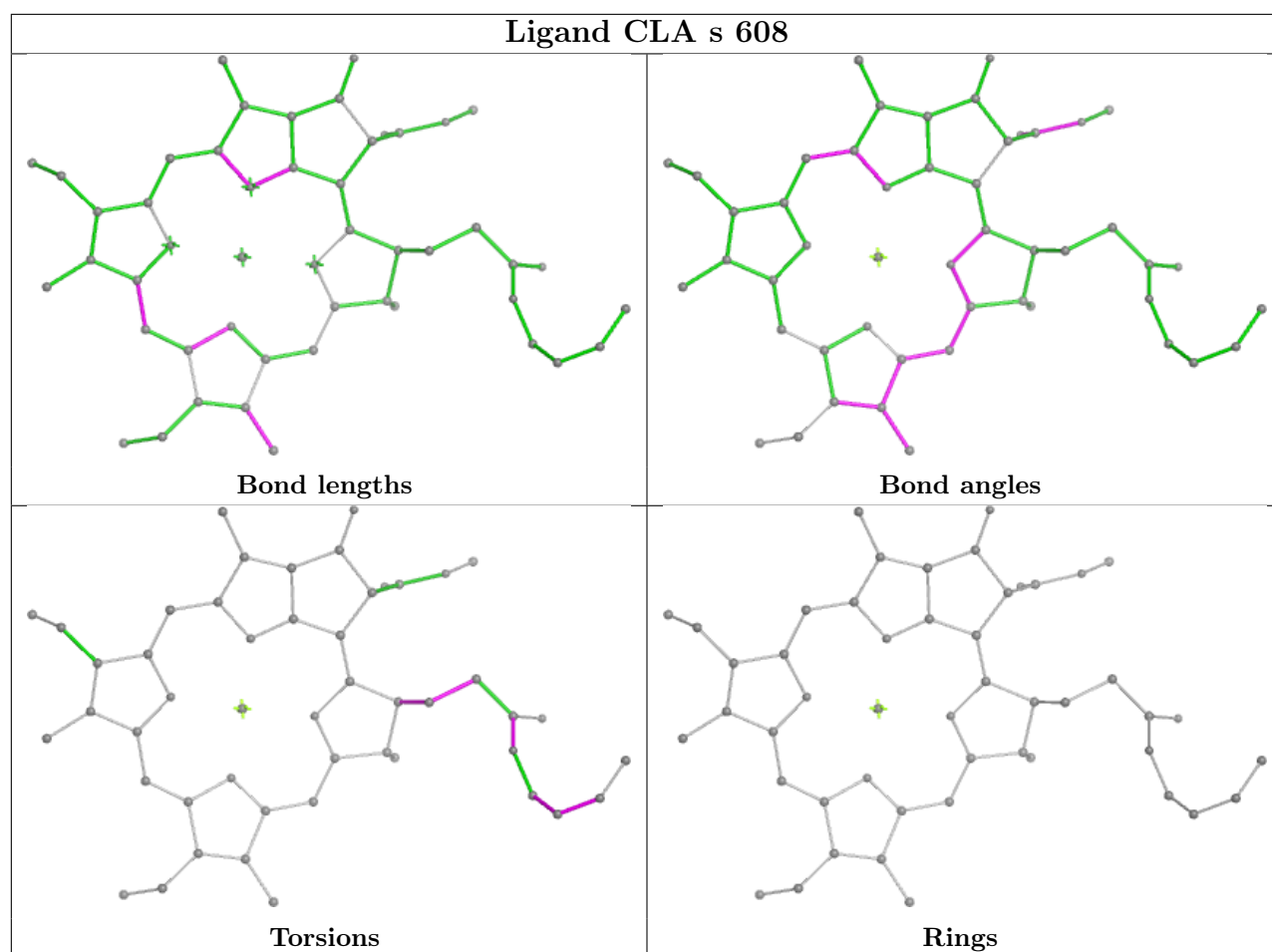


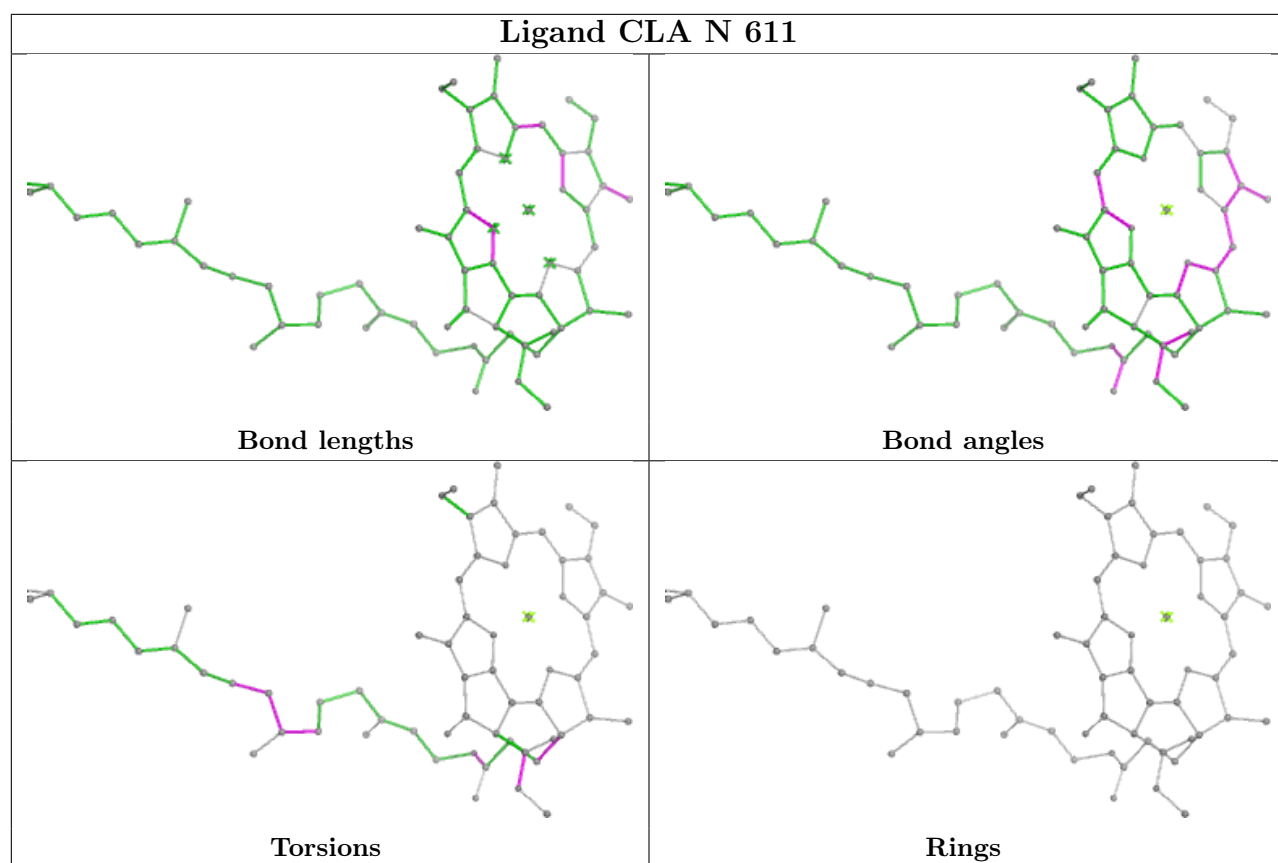


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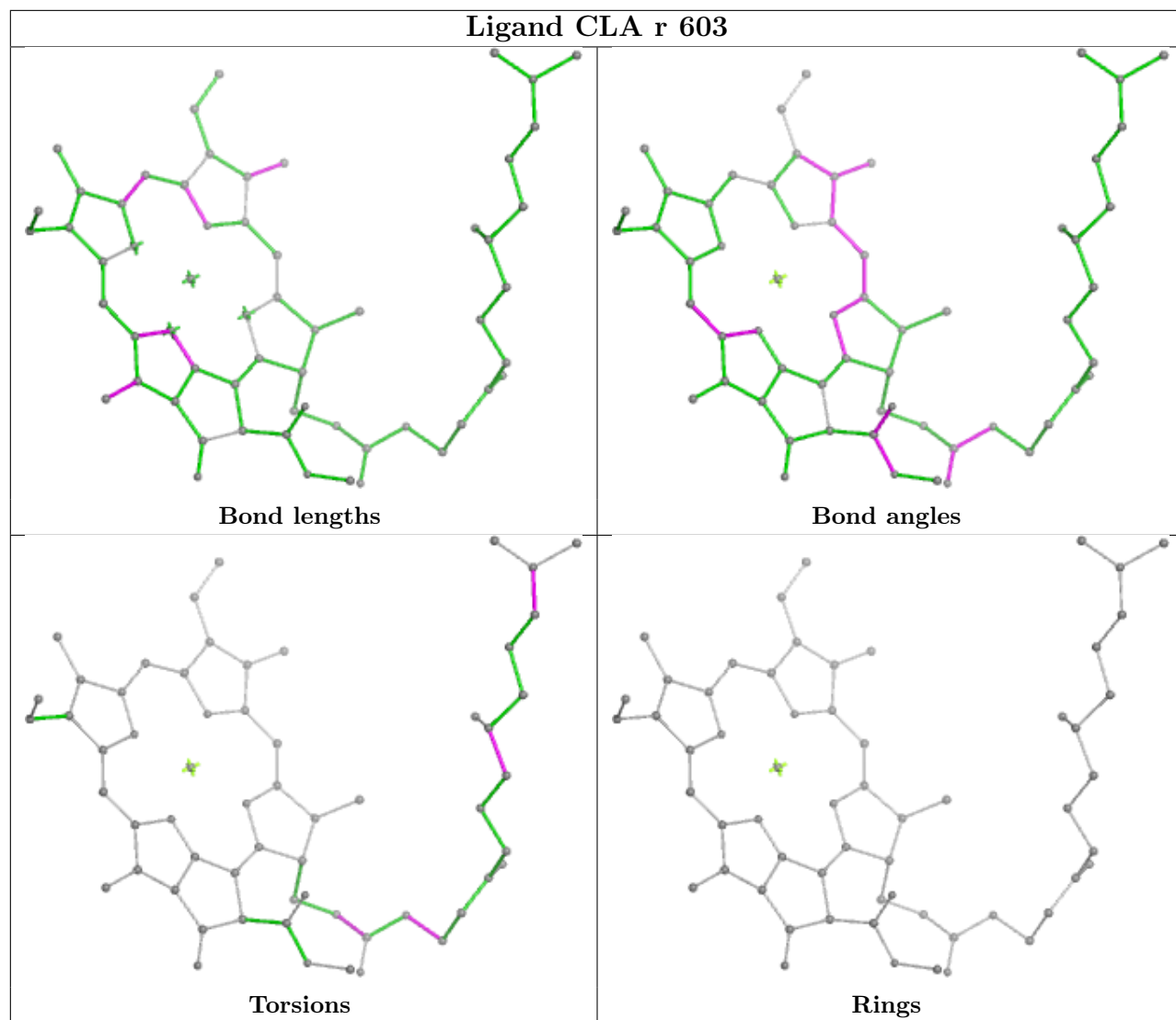




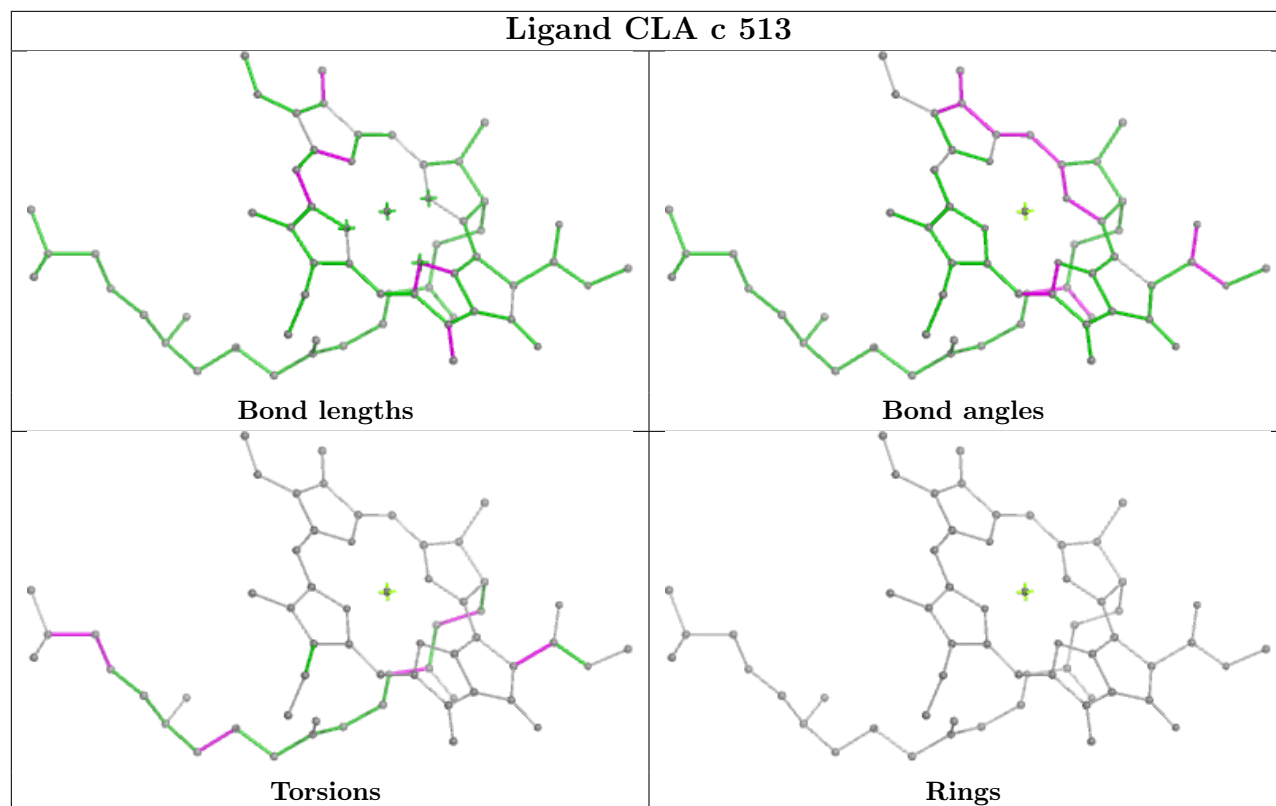




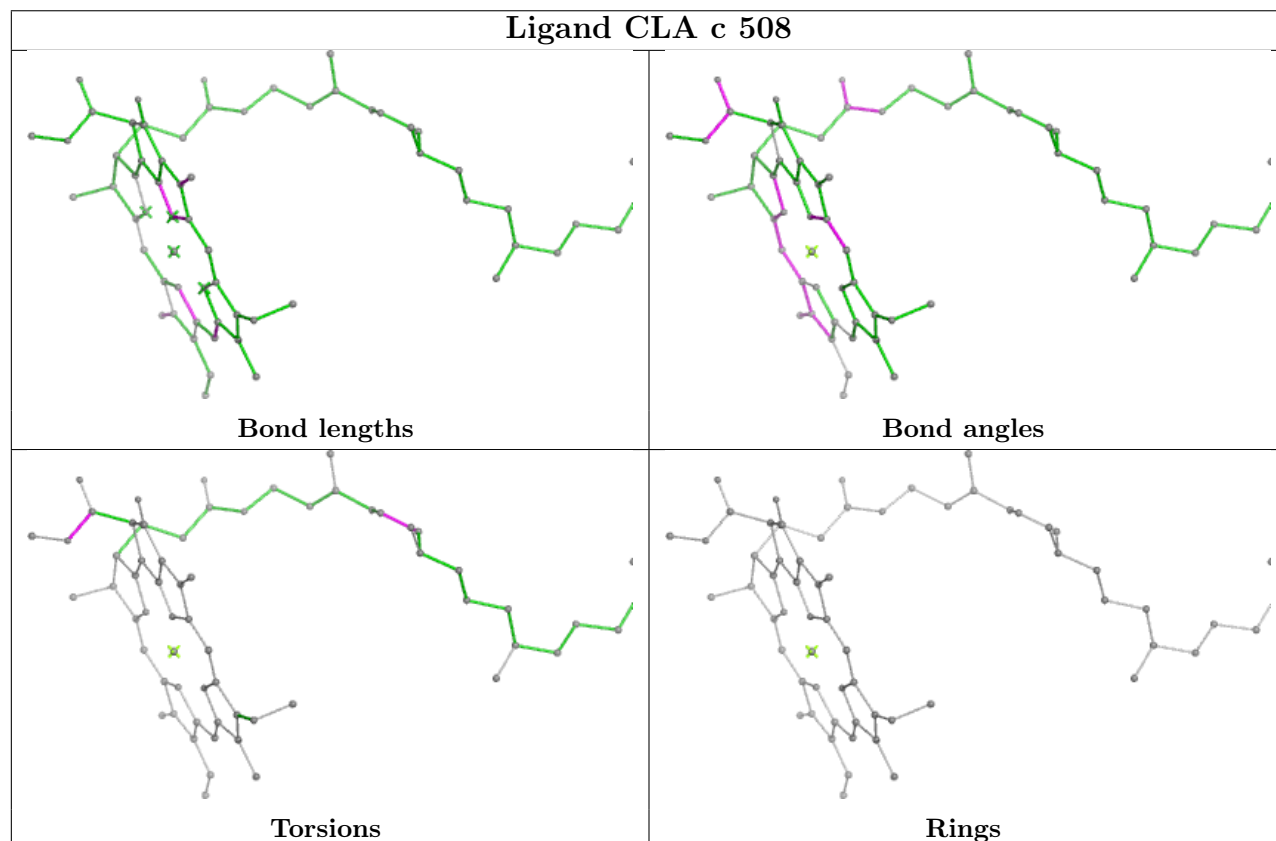
## Ligand CLA r 603



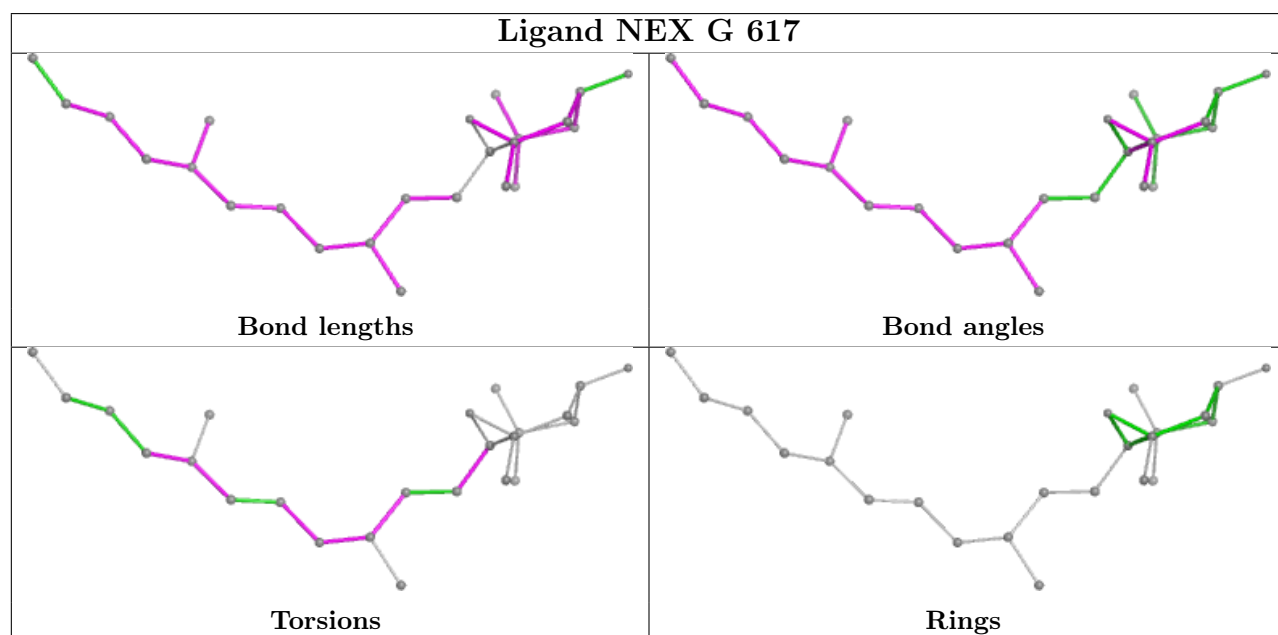
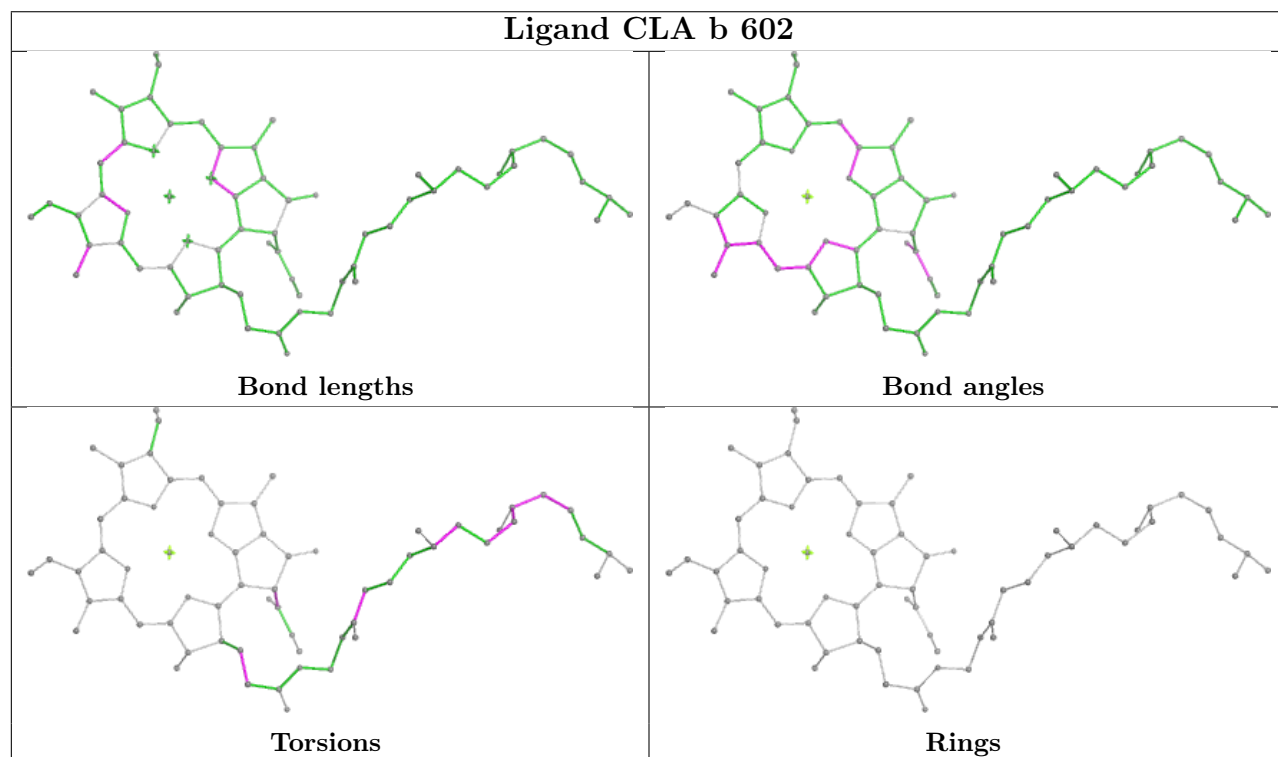
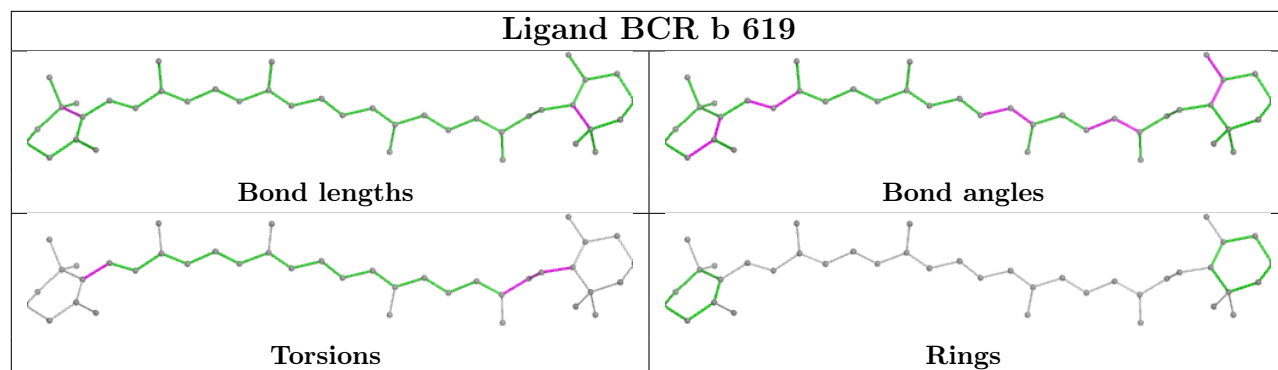
## Ligand CLA c 513



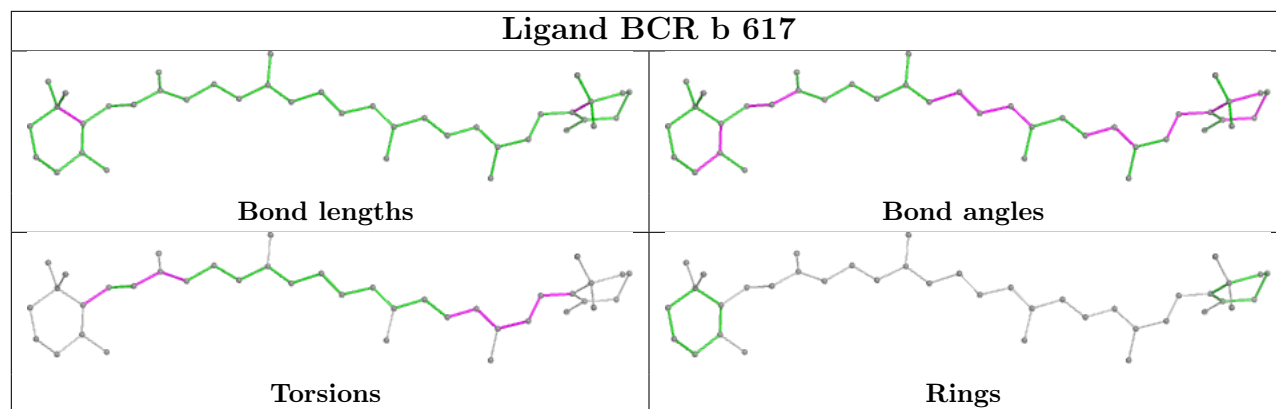
## Ligand CLA c 508



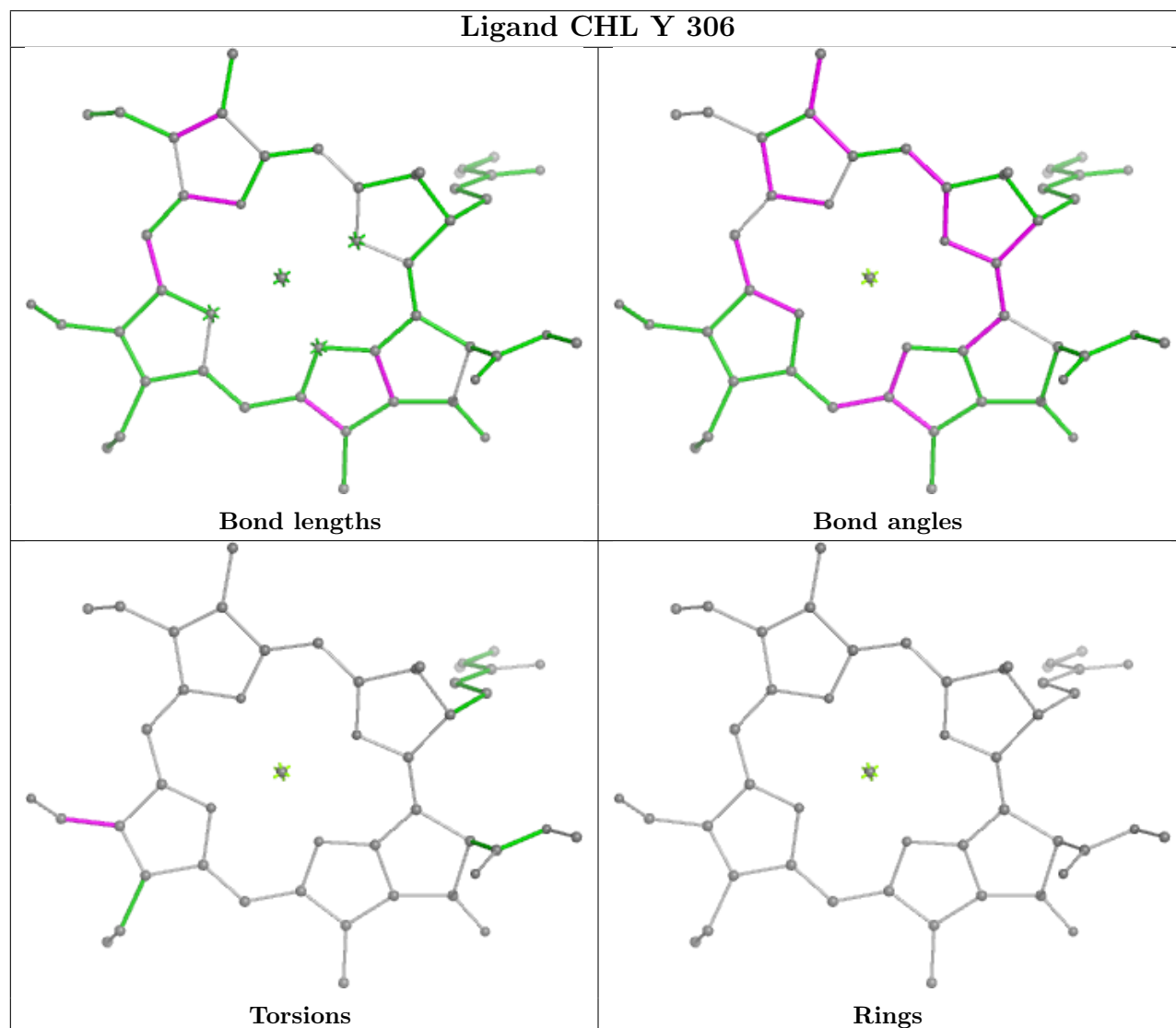




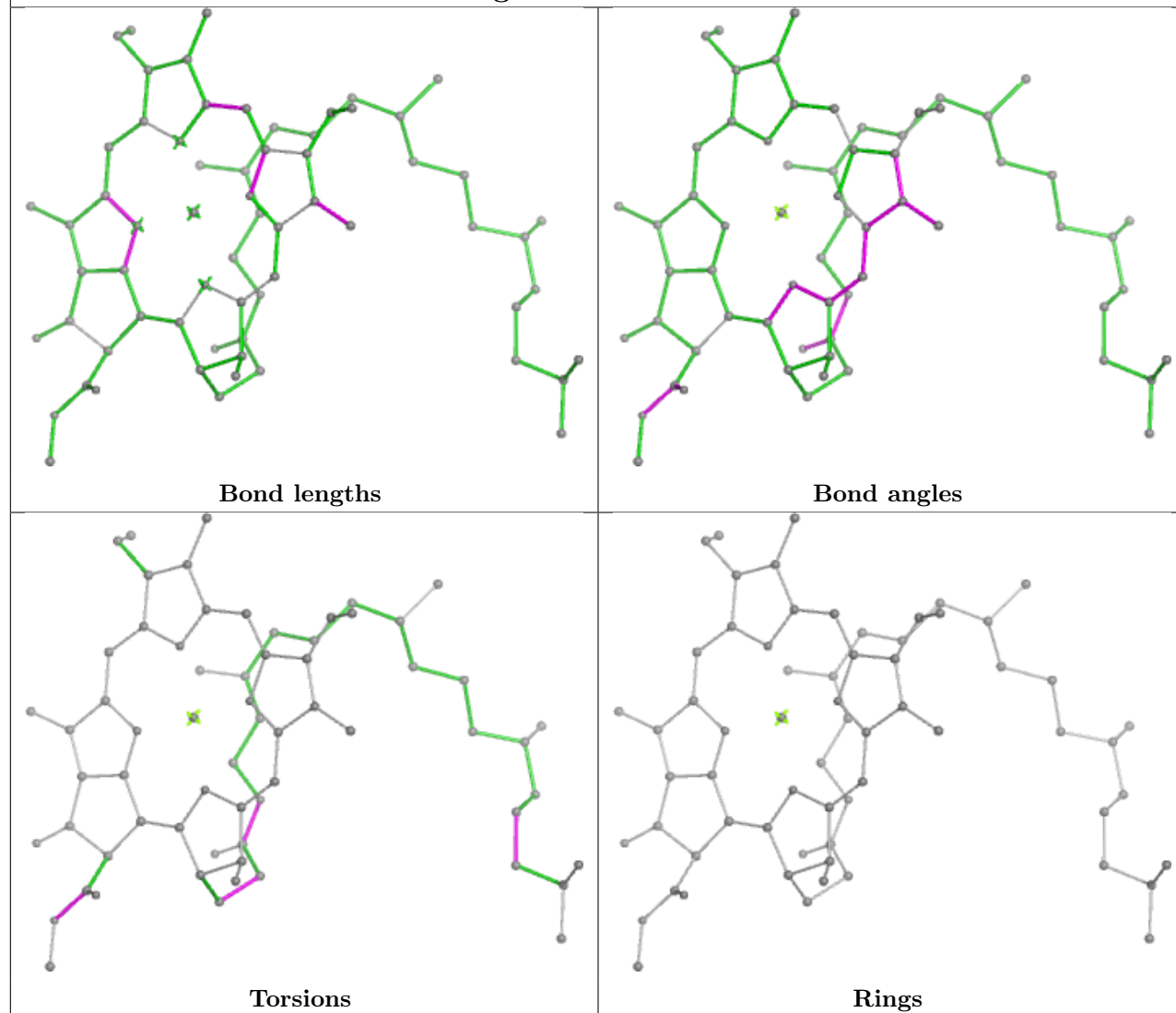
## Ligand BCR b 617



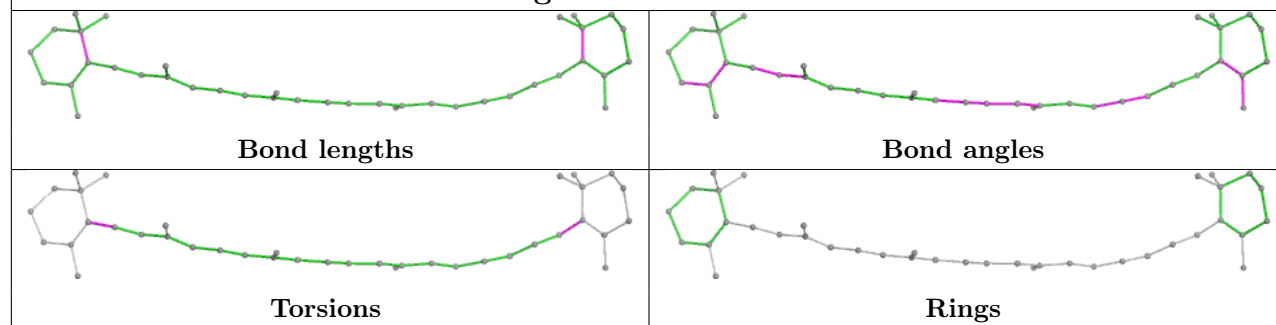
## Ligand CHL Y 306

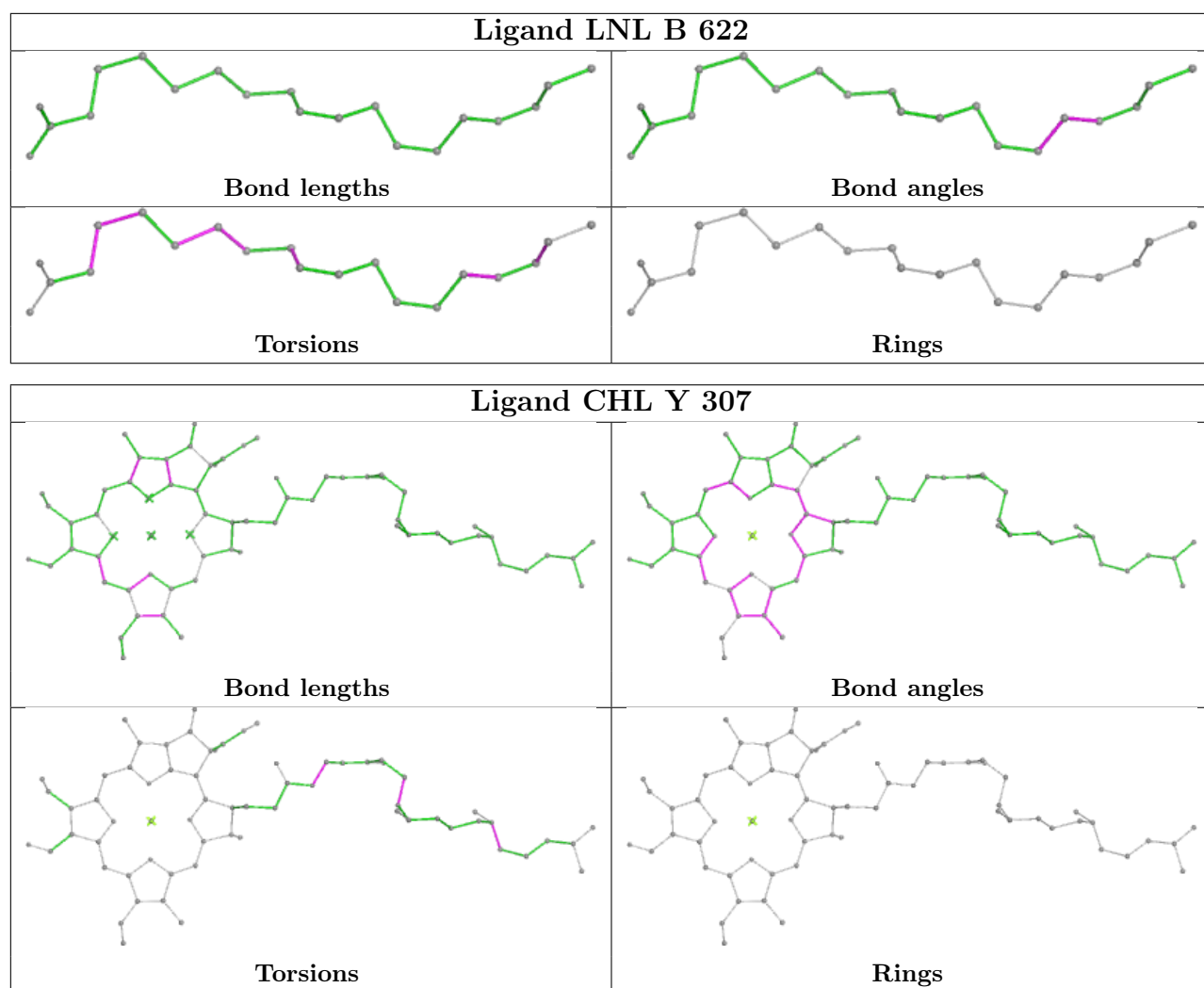


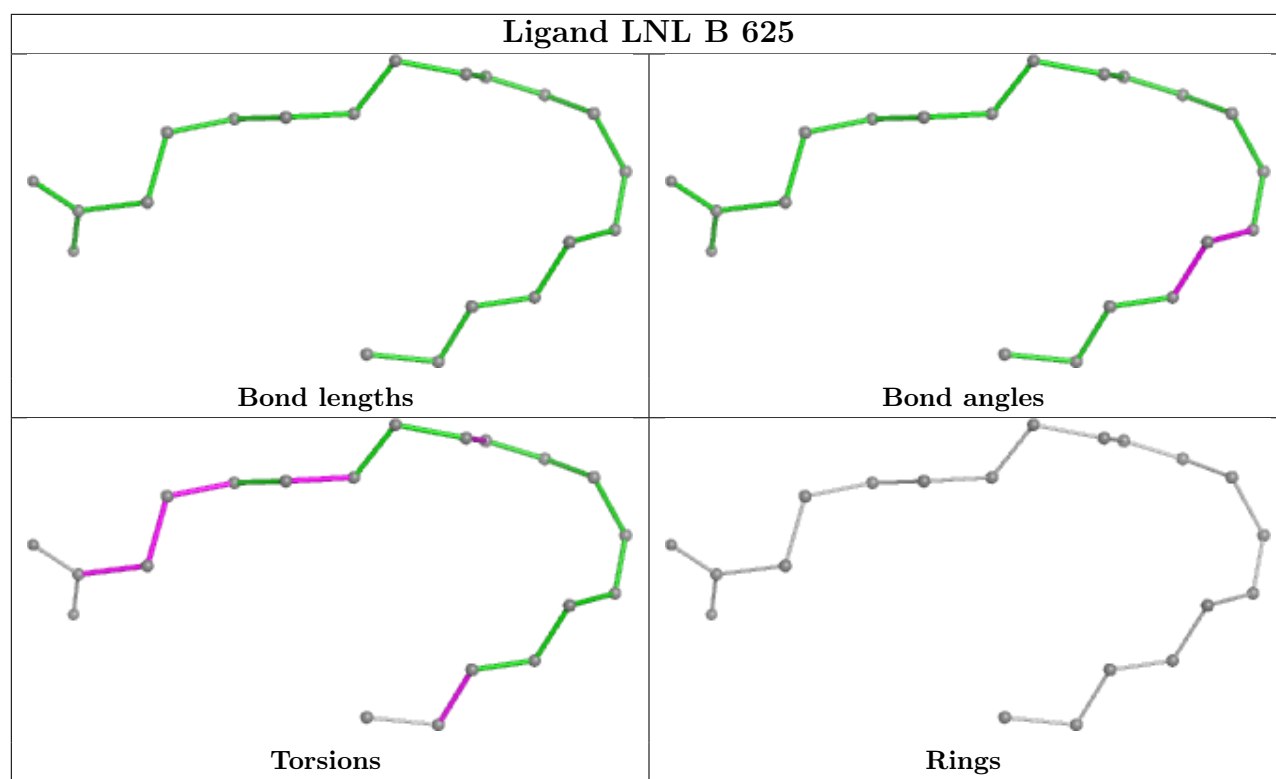
## Ligand CLA n 613

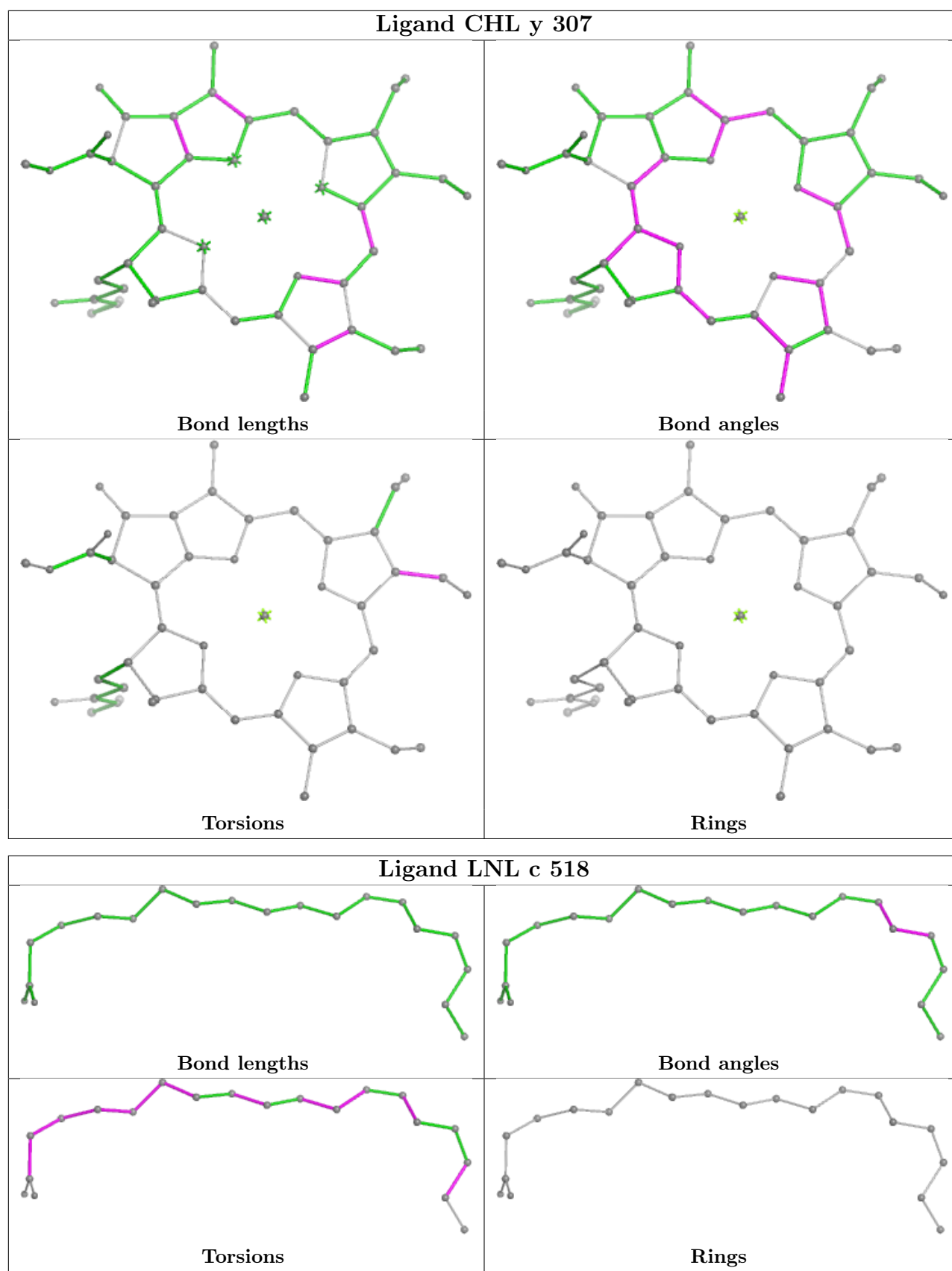


## Ligand BCR k 101

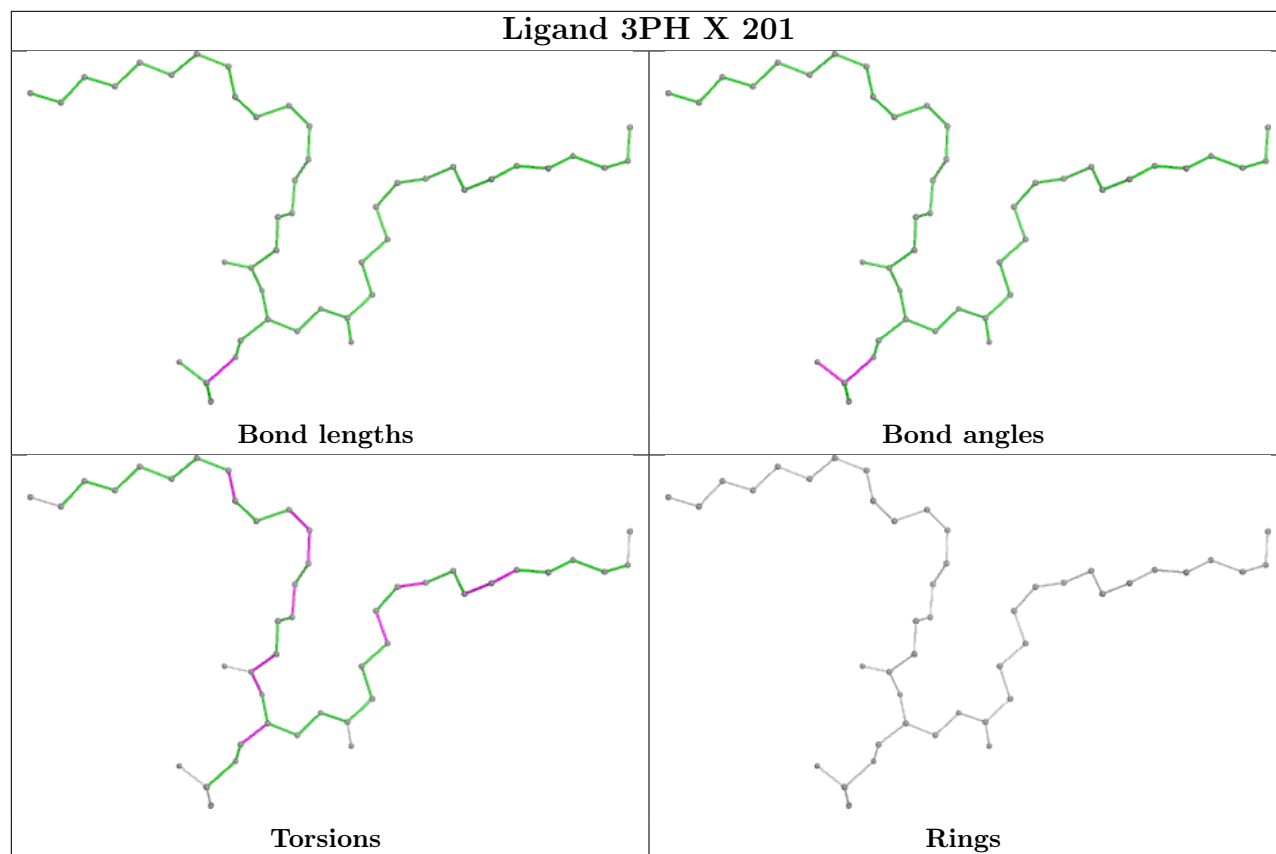




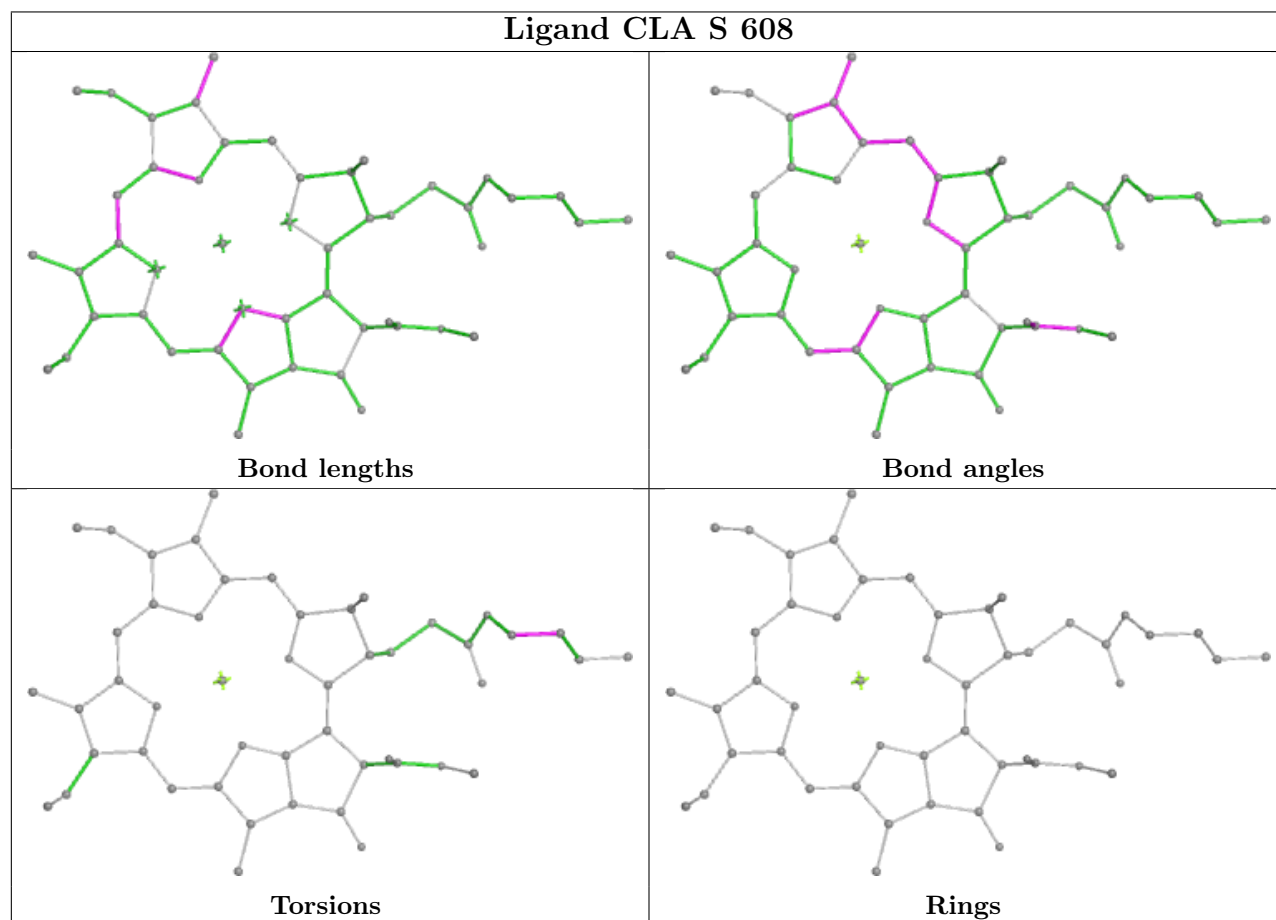


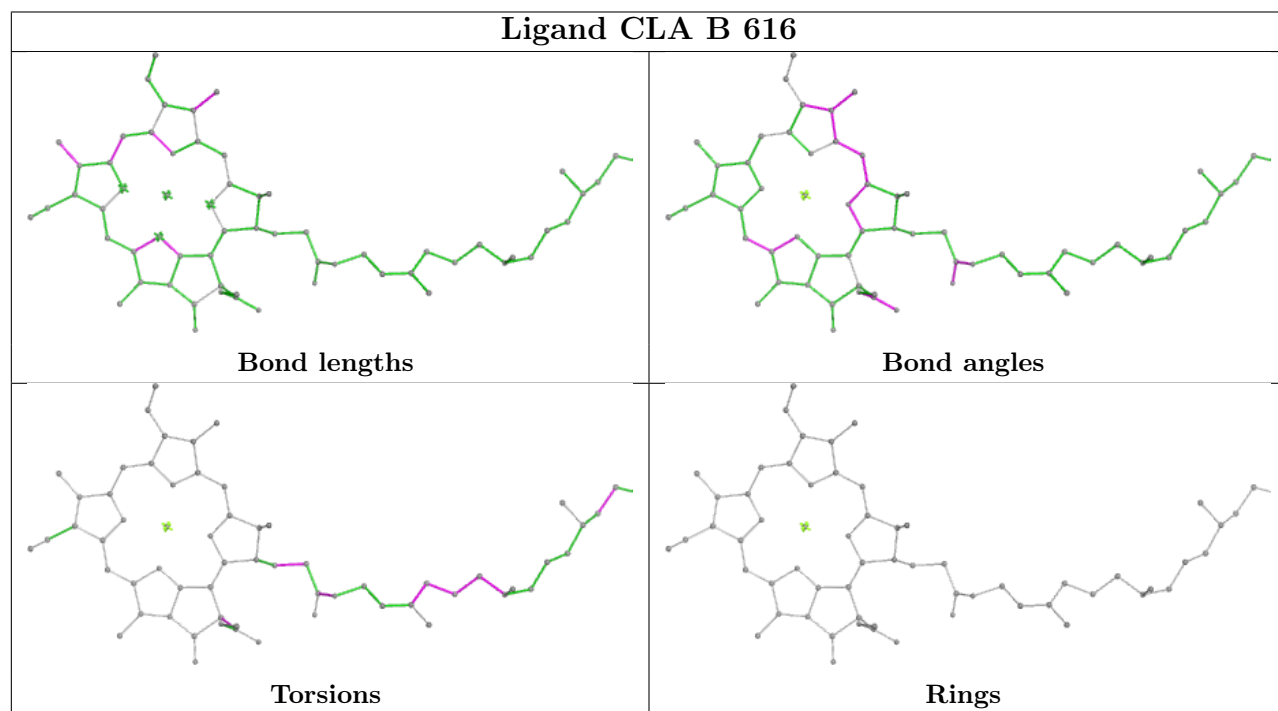
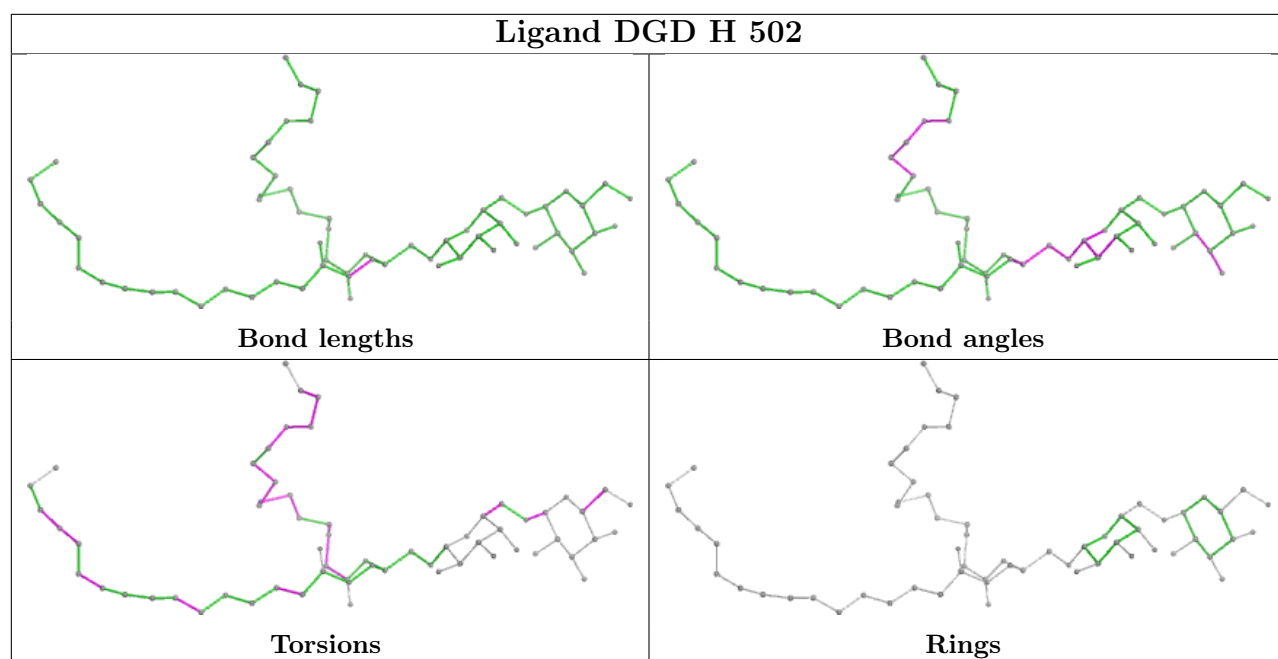


## Ligand 3PH X 201

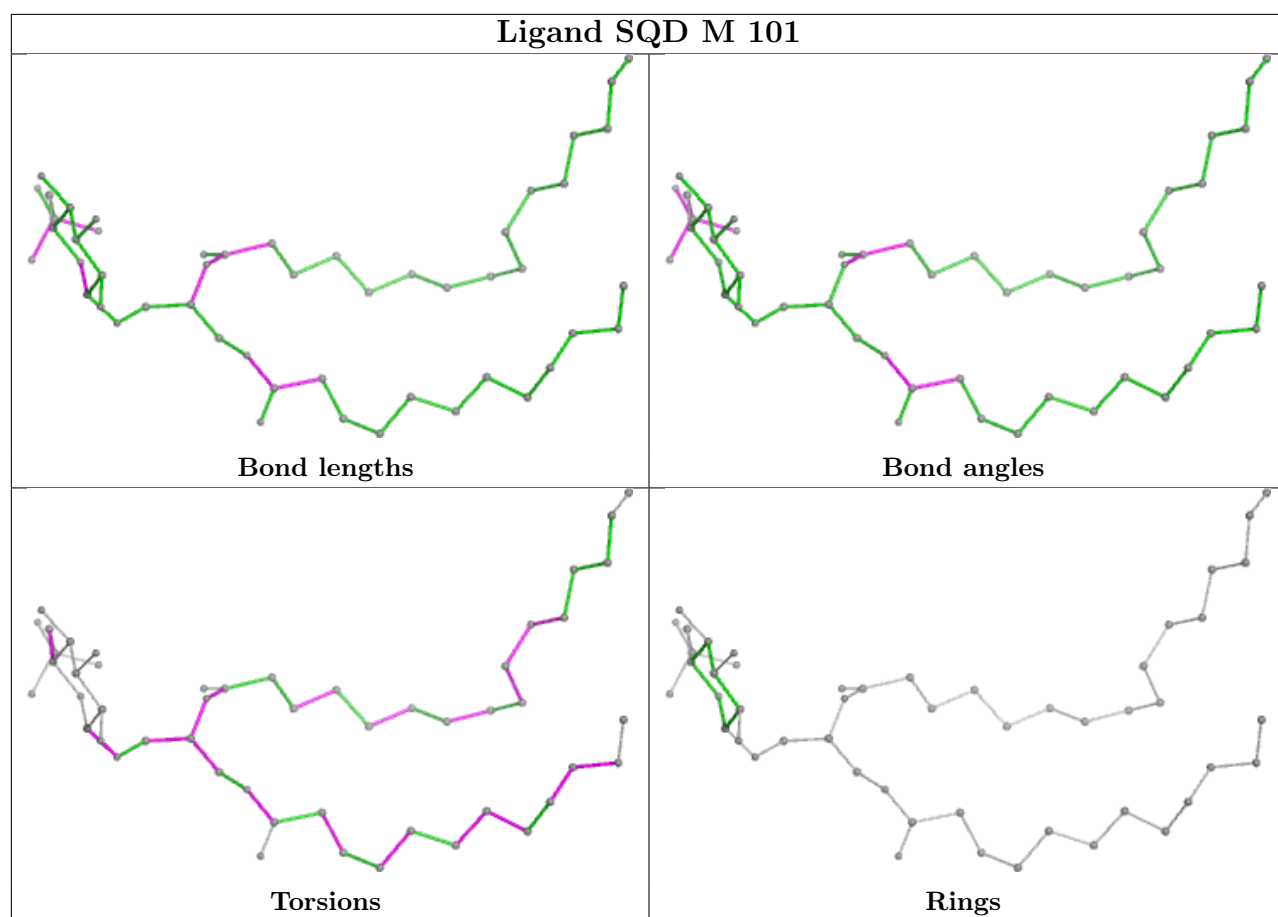


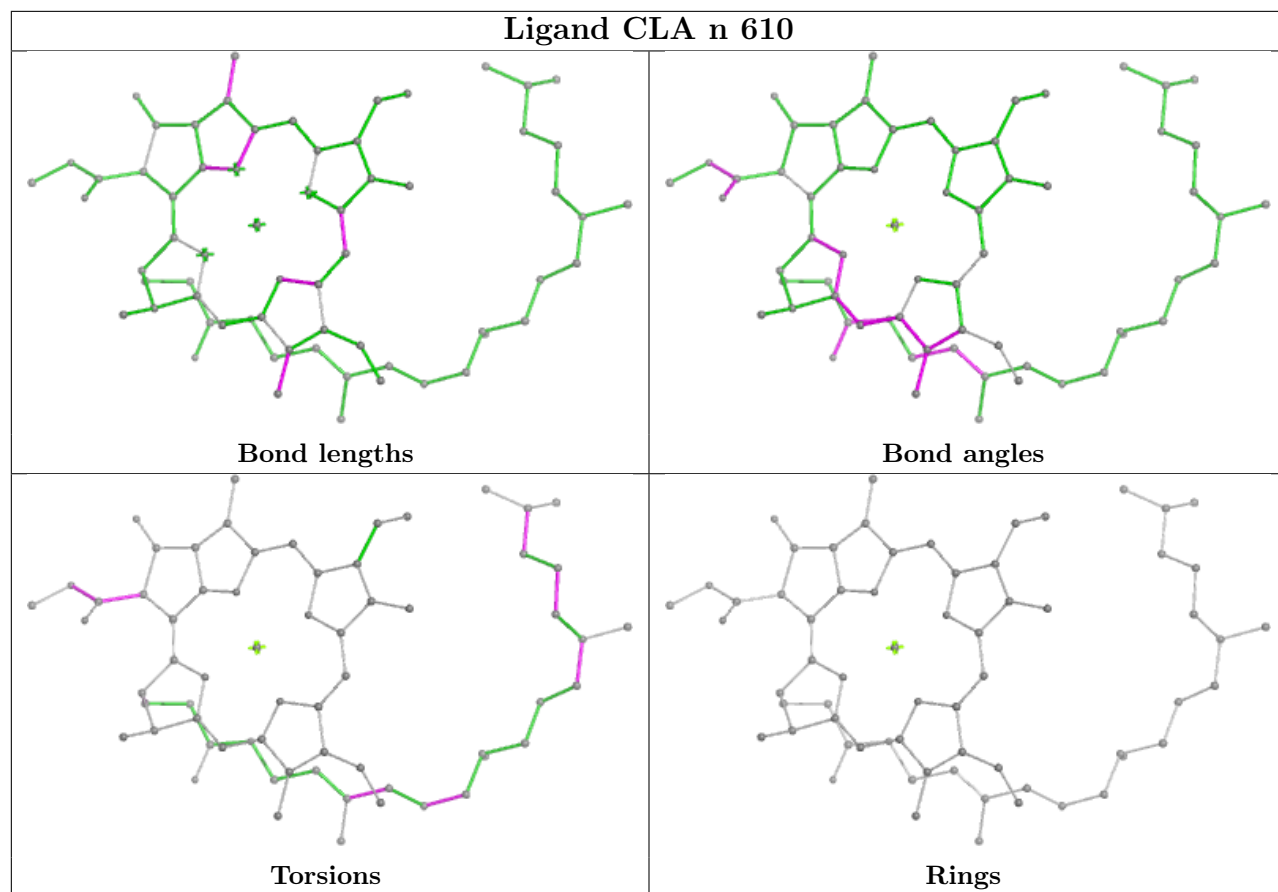
## Ligand CLA S 608

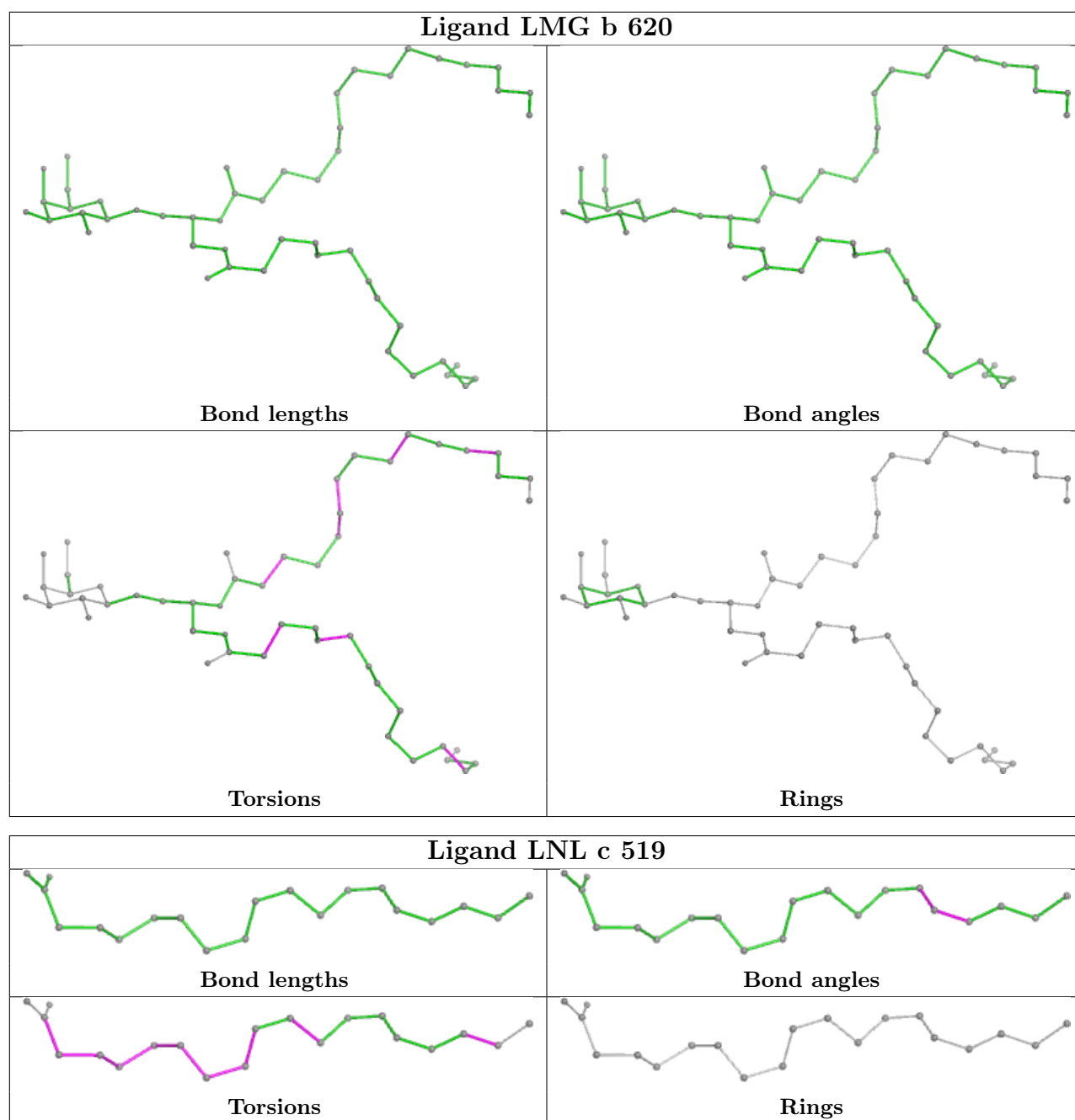


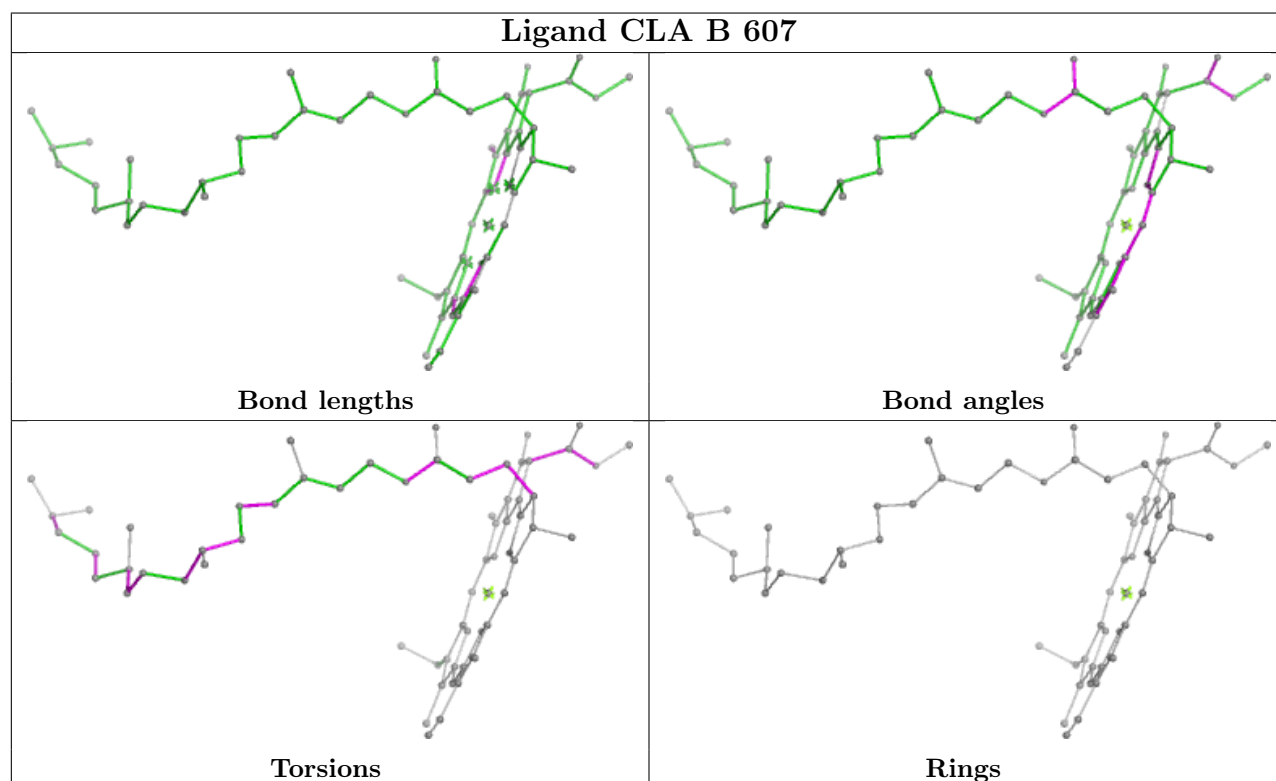
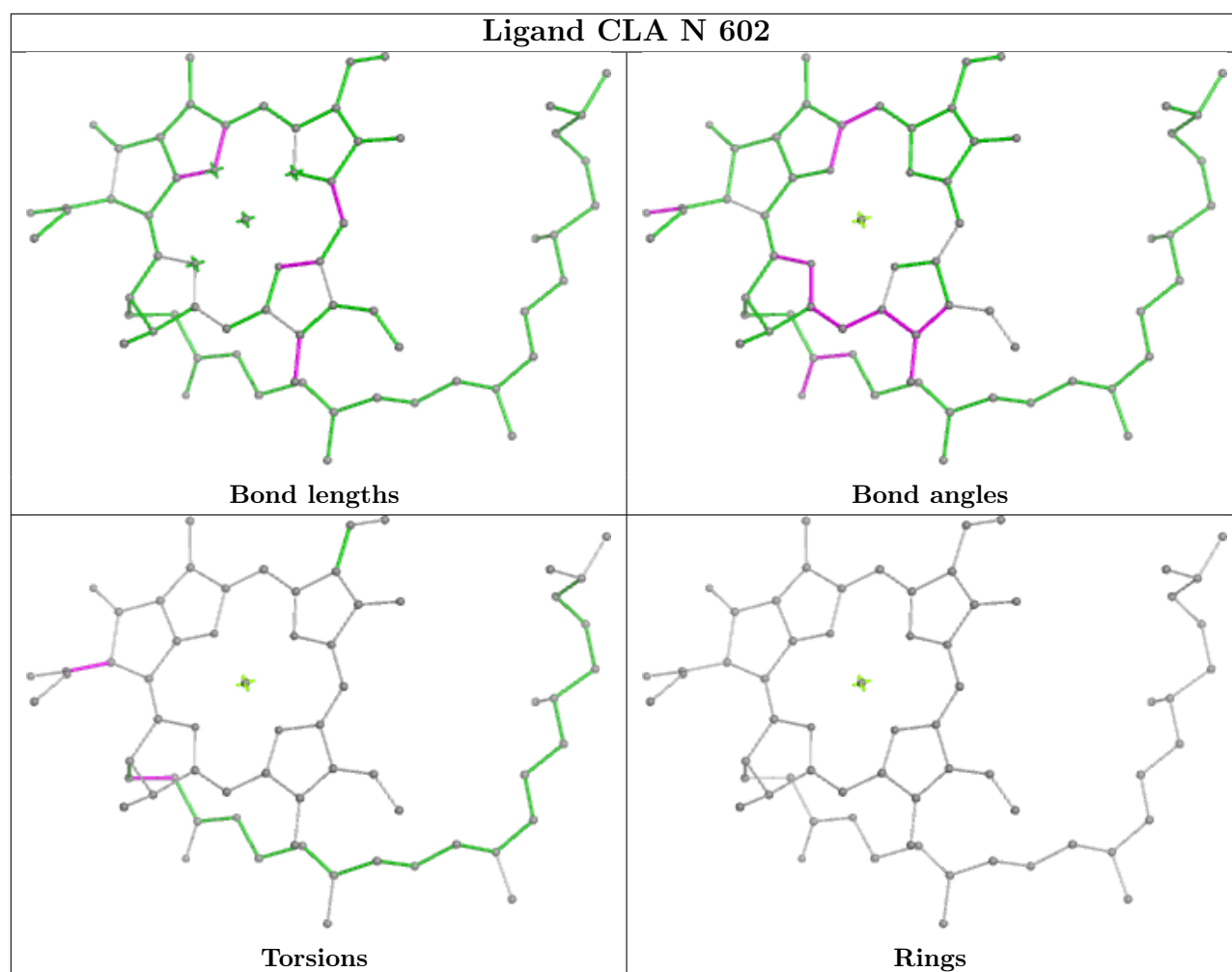


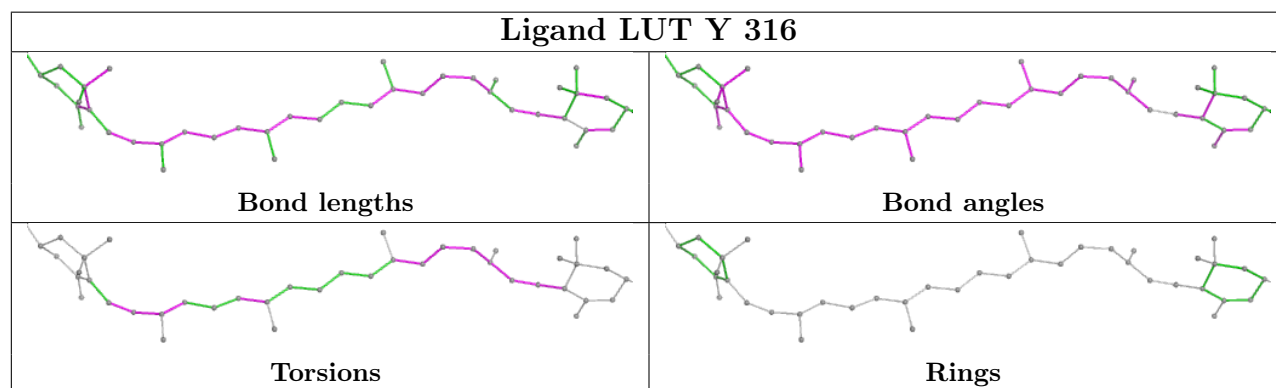
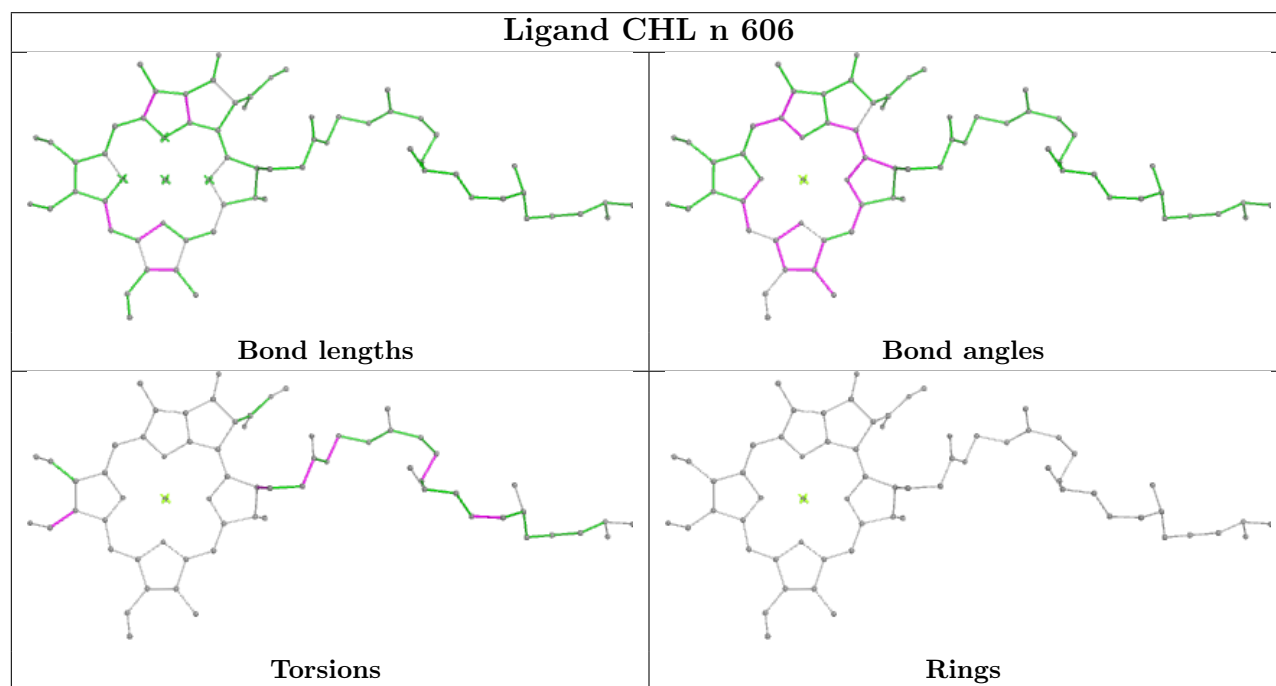
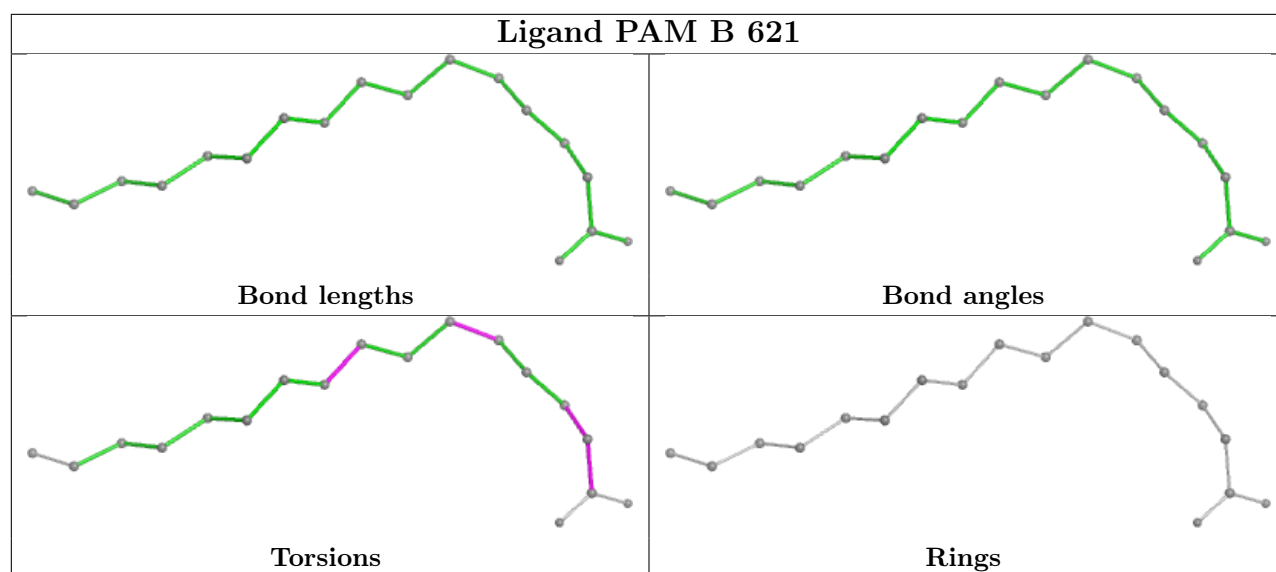


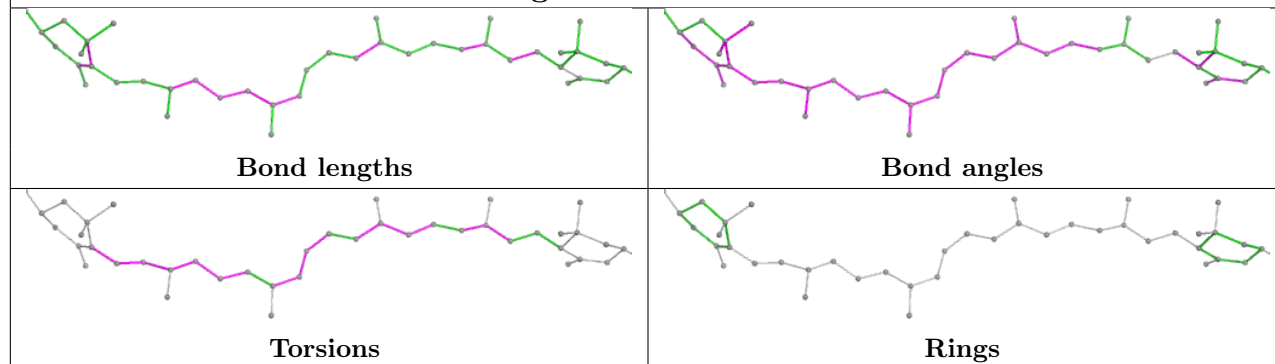
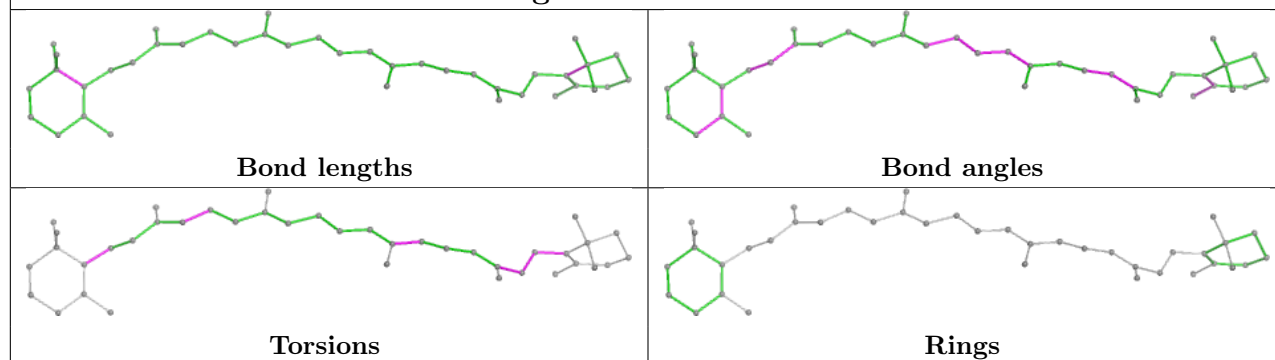
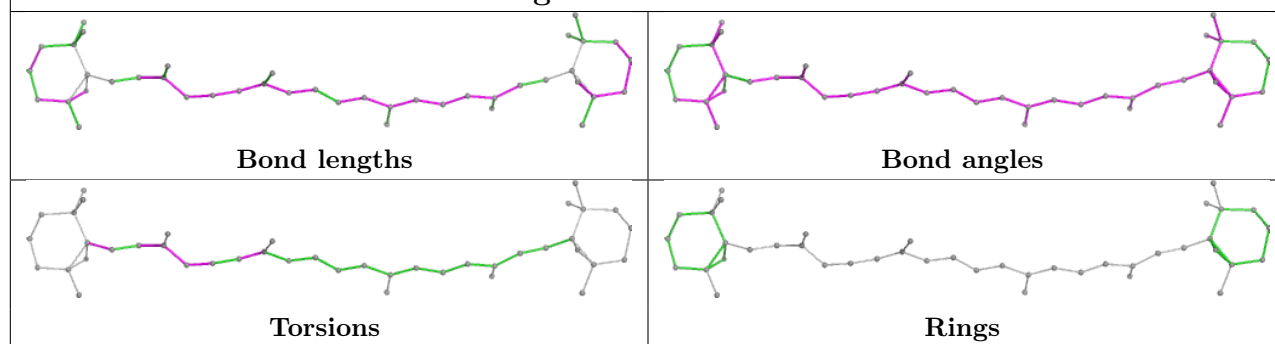
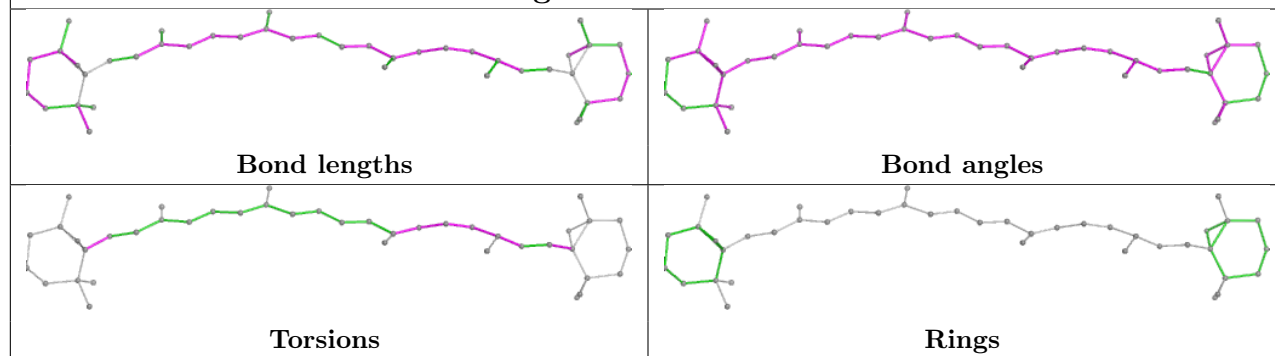


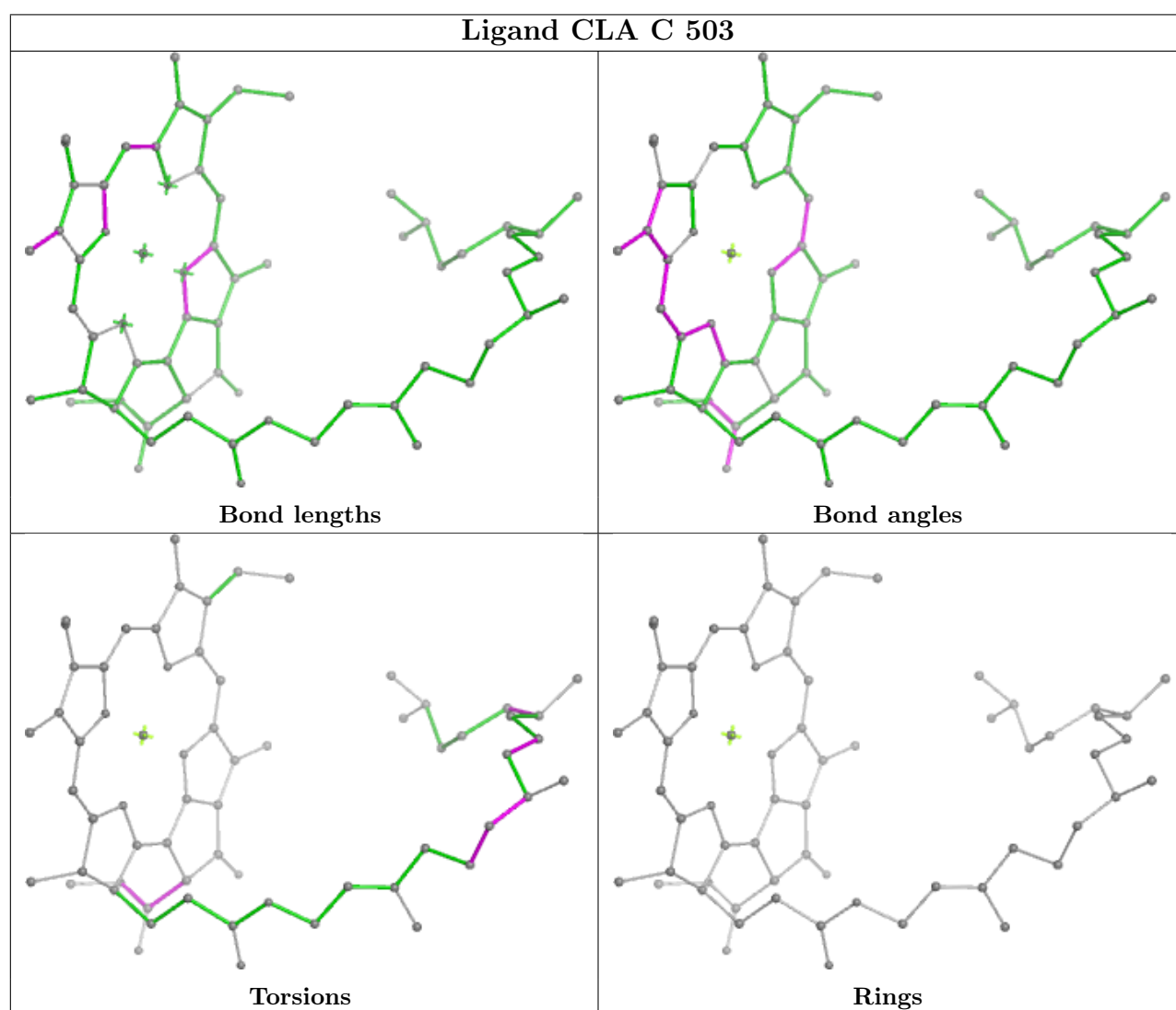
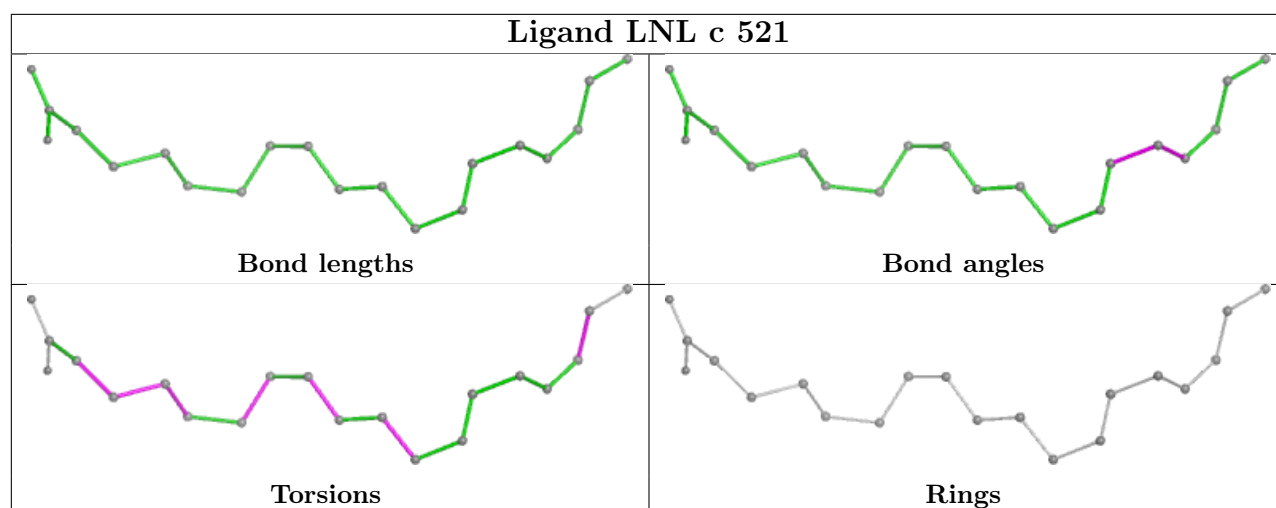


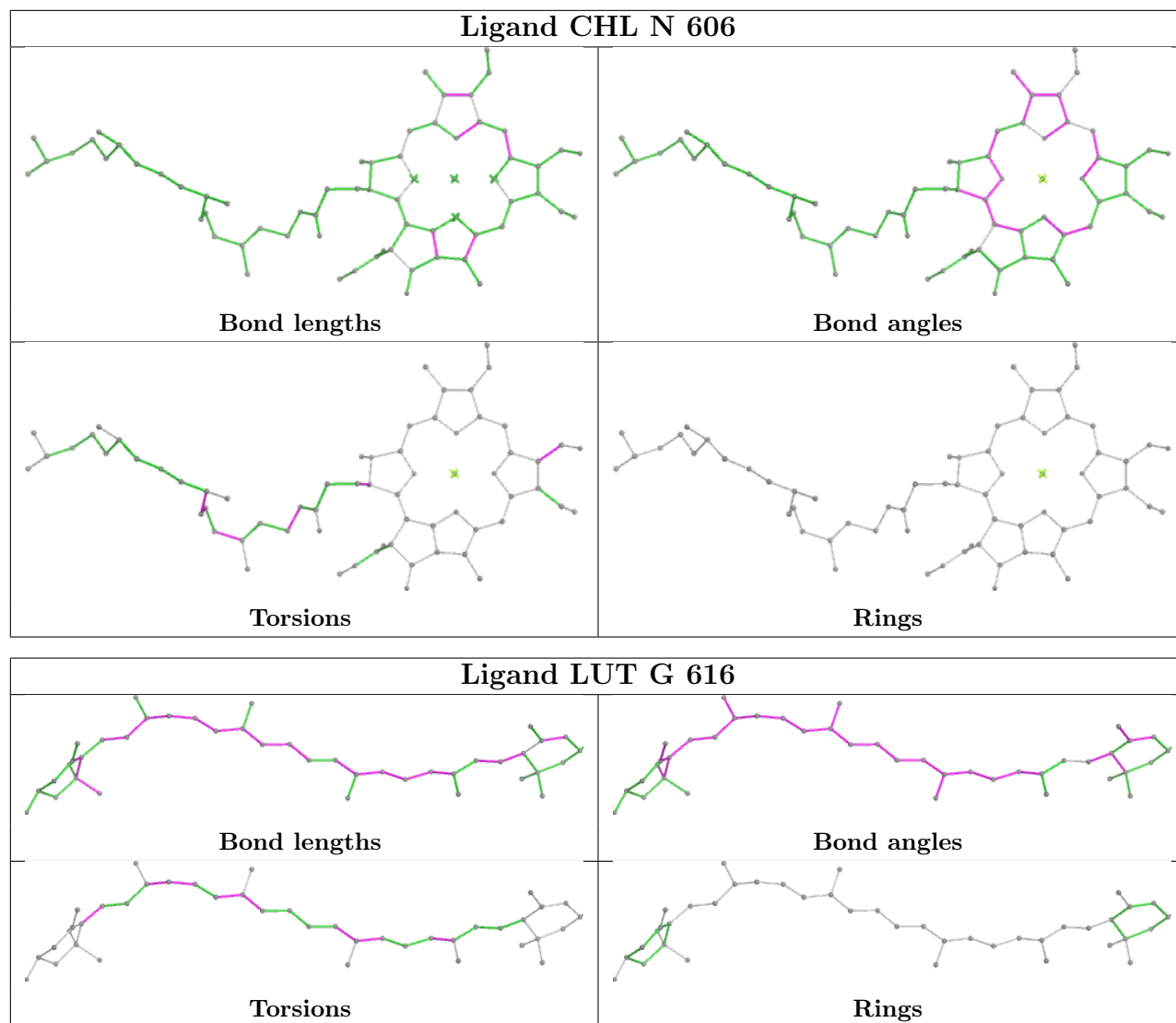




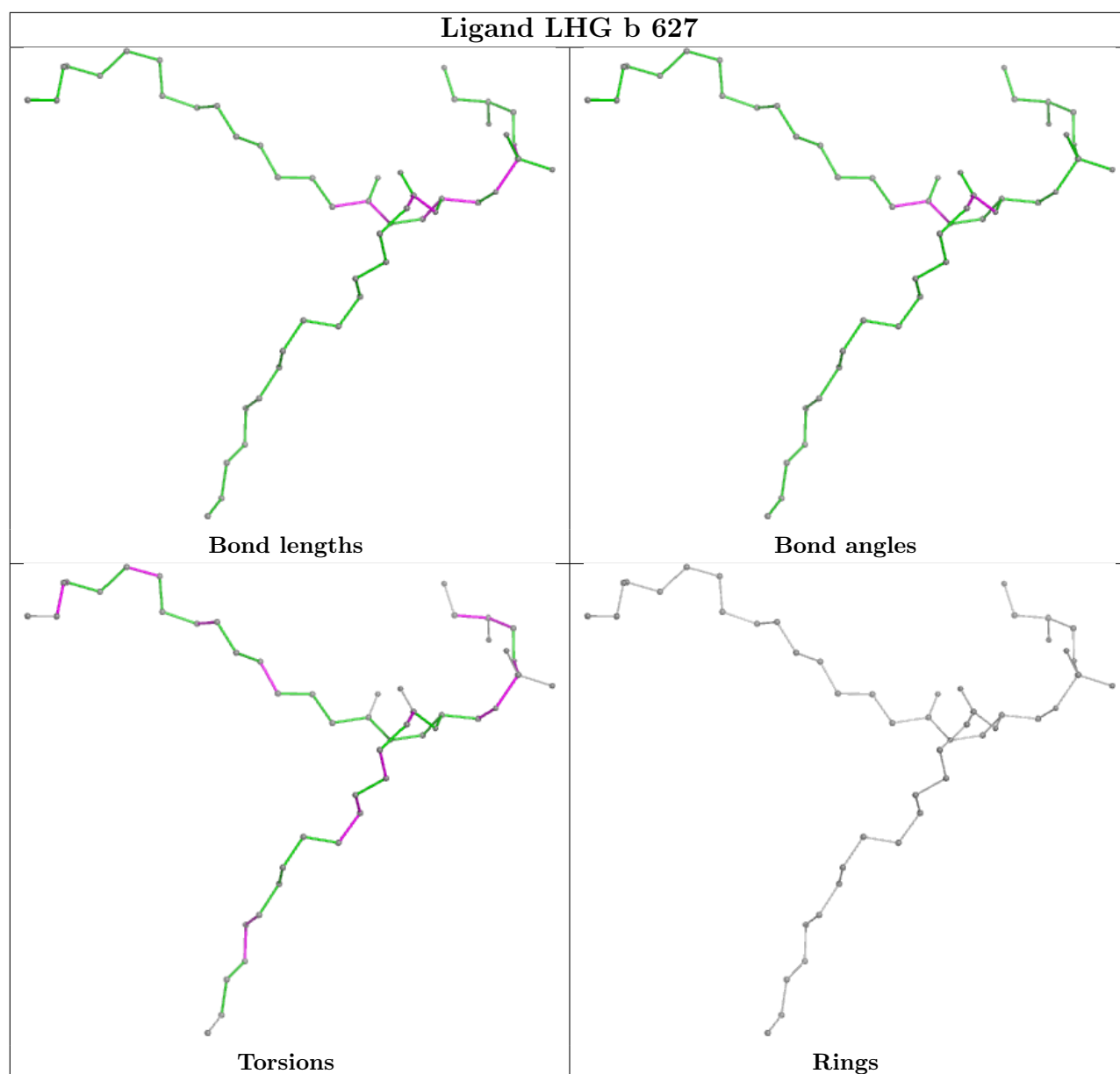


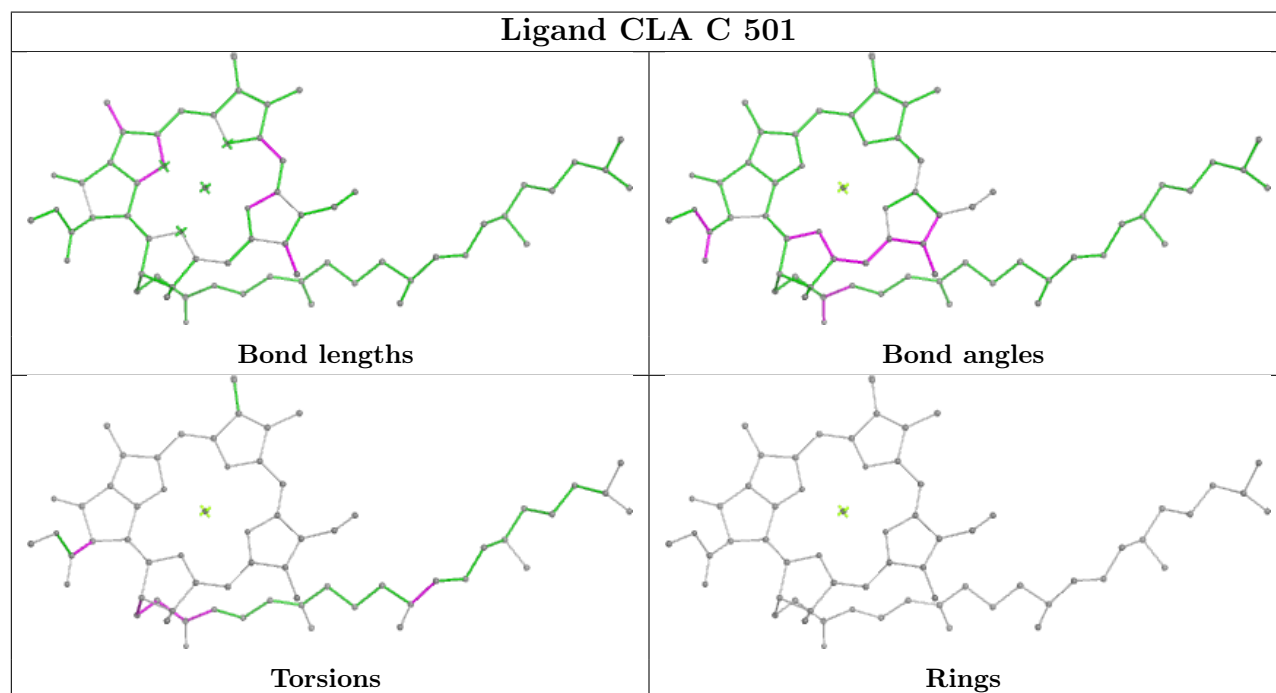
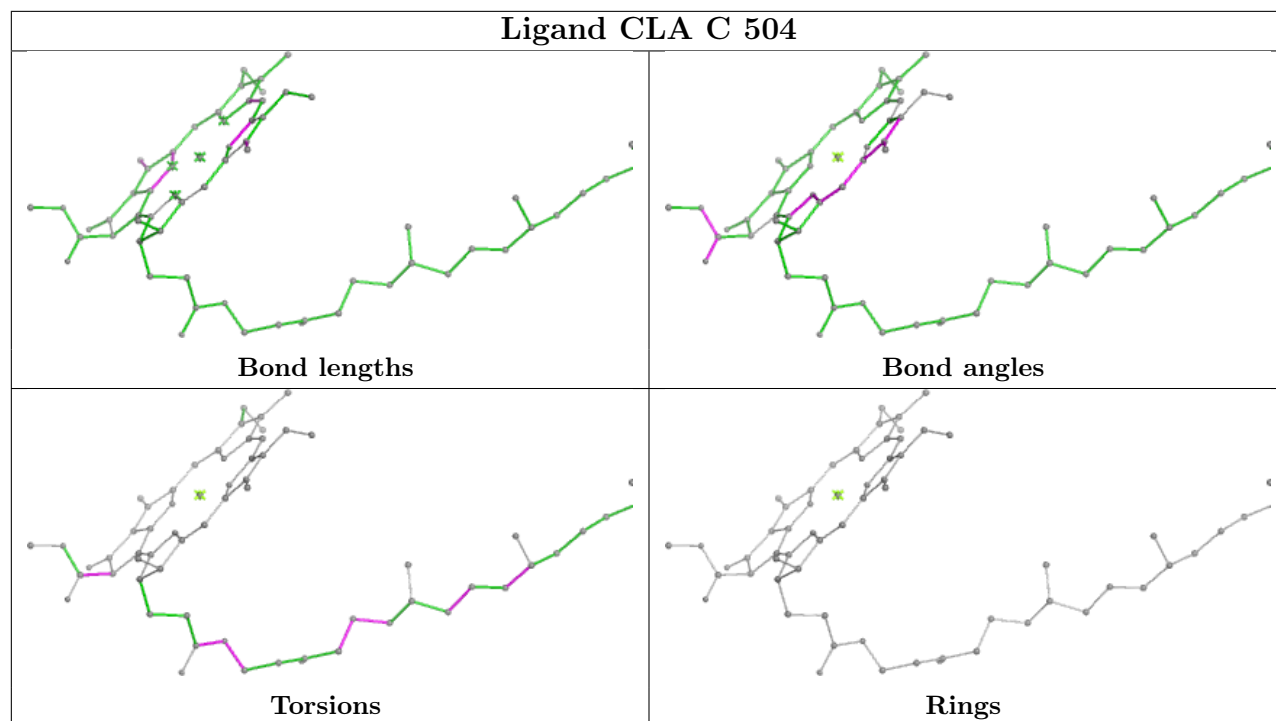
**Ligand LUT Y 315****Ligand BCR d 410****Ligand XAT n 617****Ligand XAT n 620**



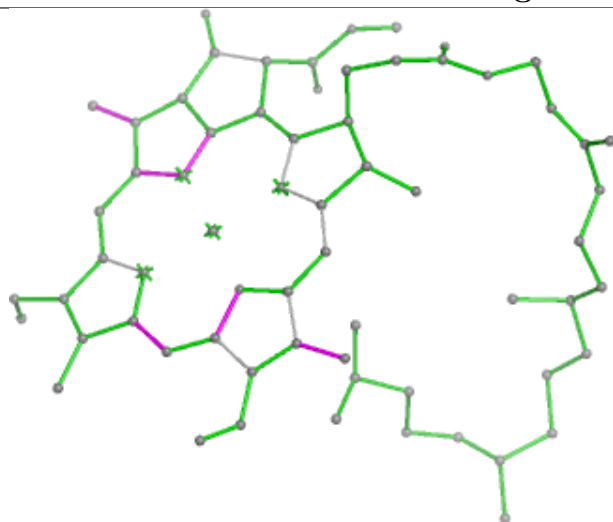




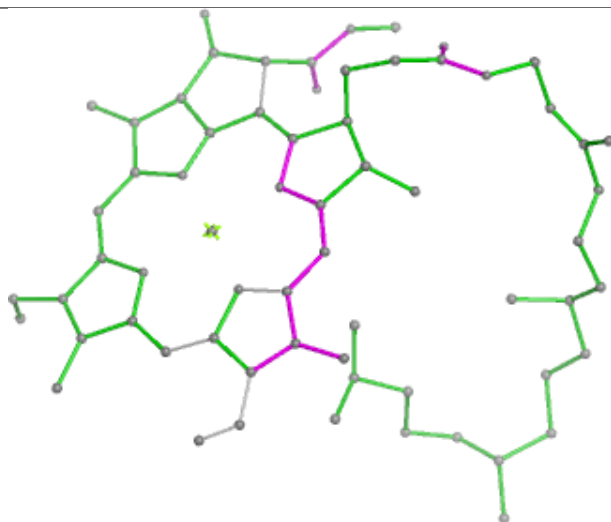




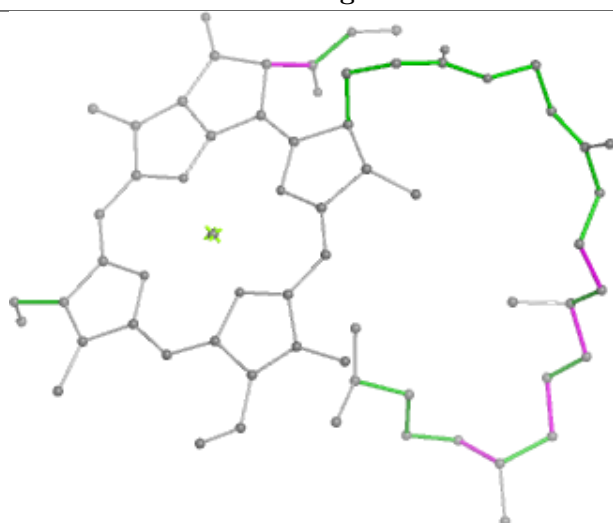
## Ligand CLA B 615



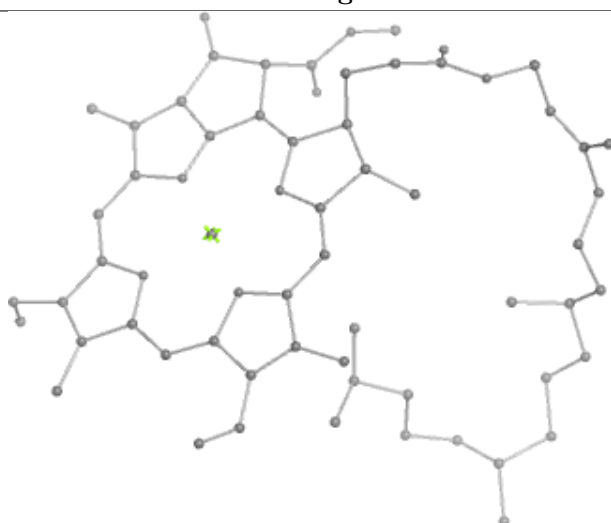
Bond lengths



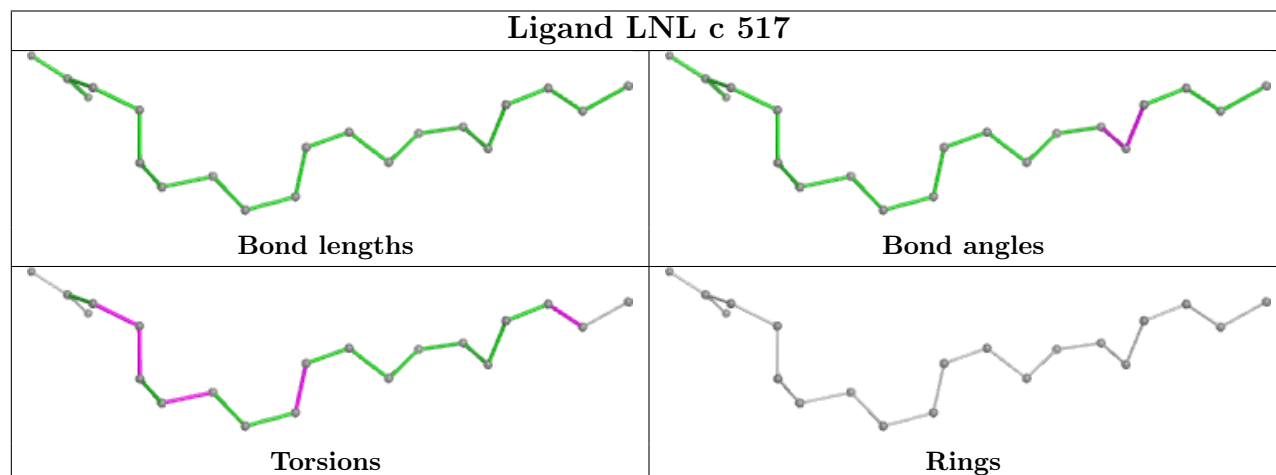
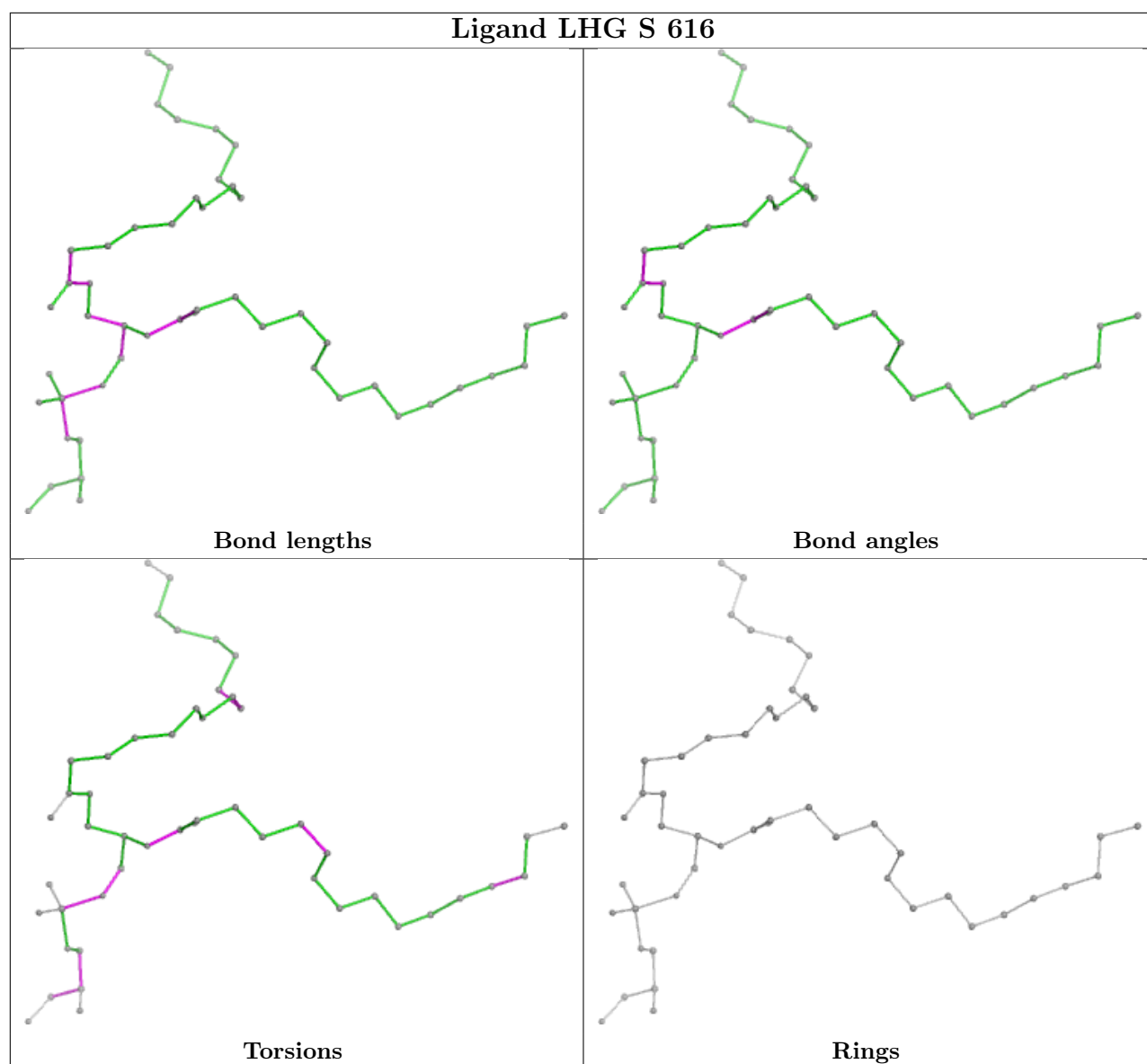
Bond angles

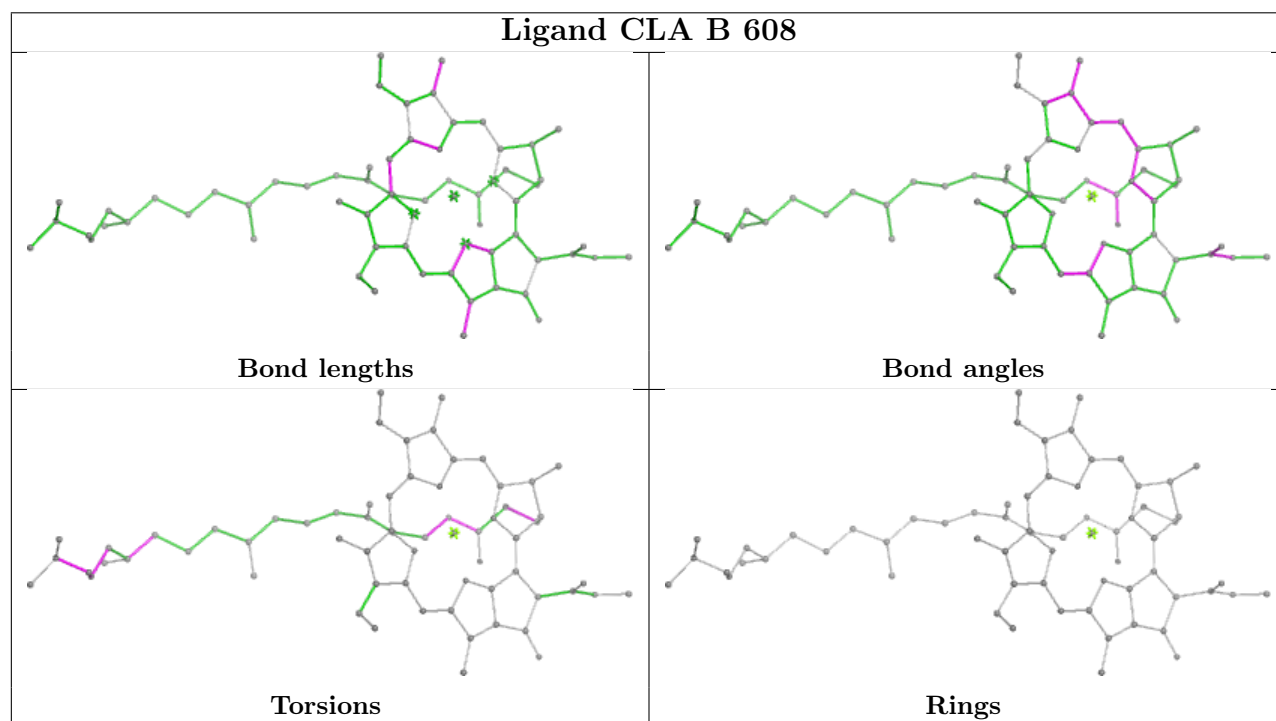
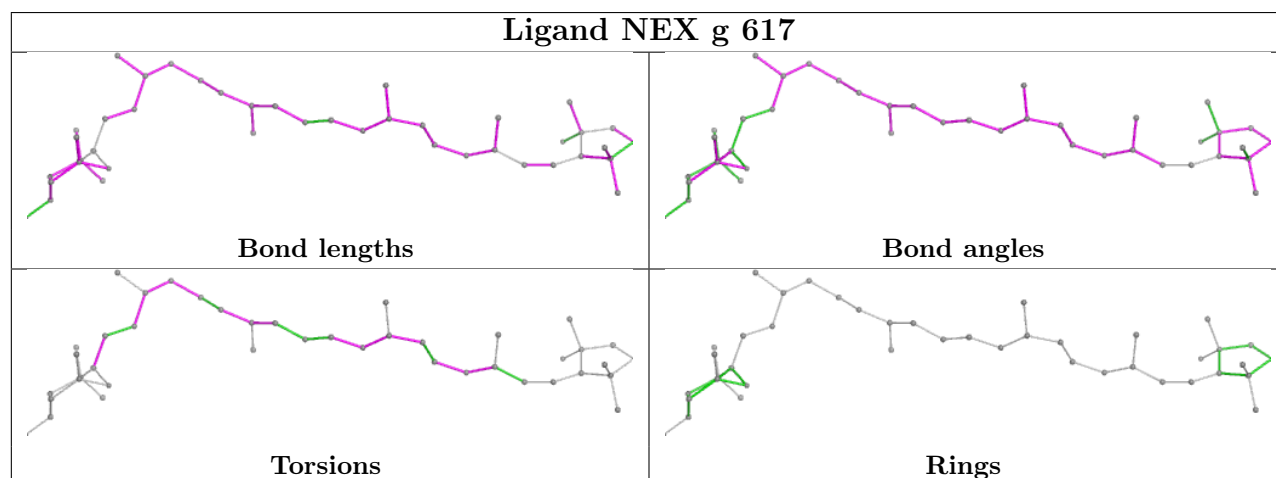
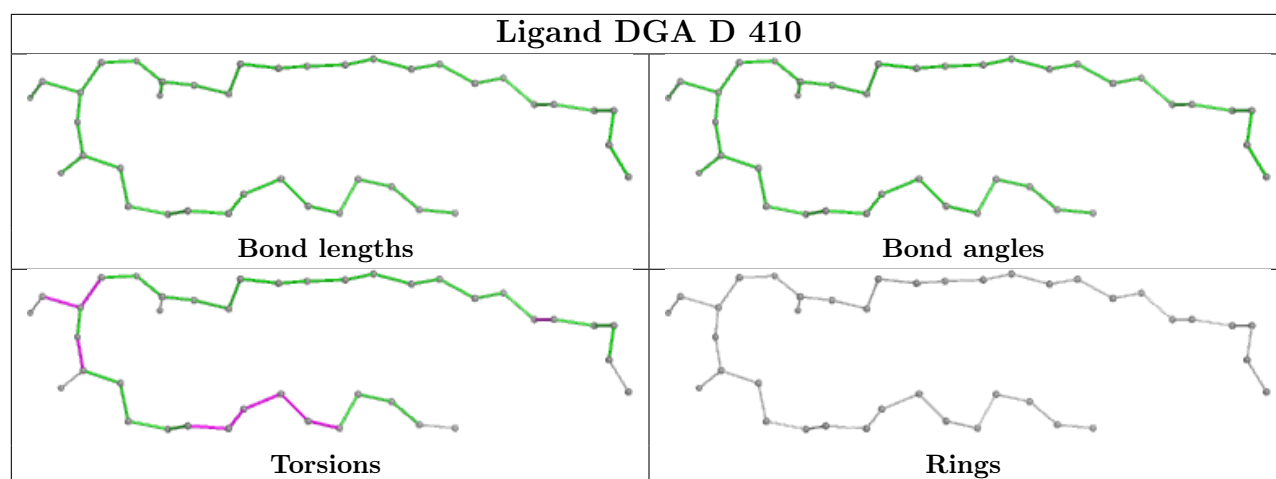


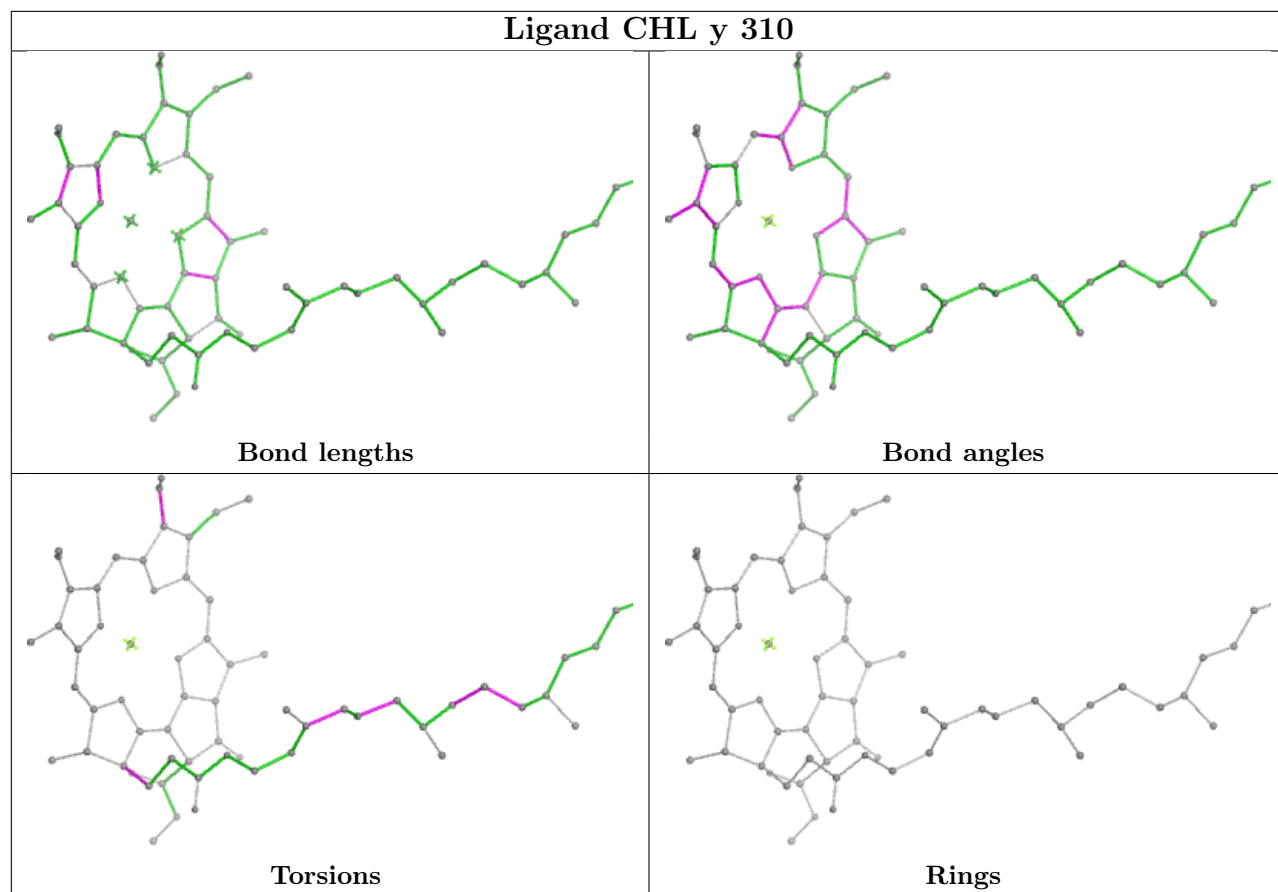
Torsions

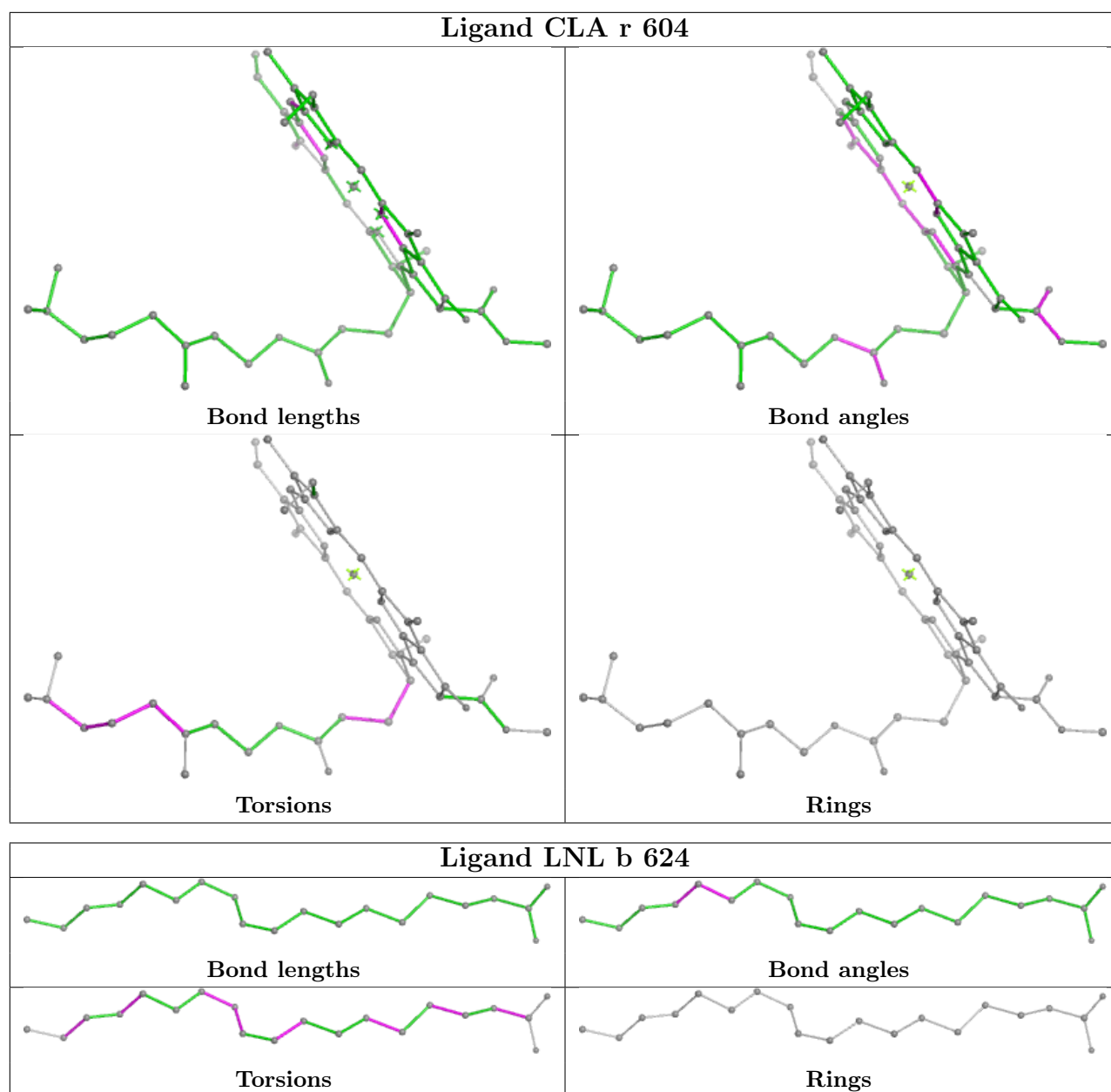


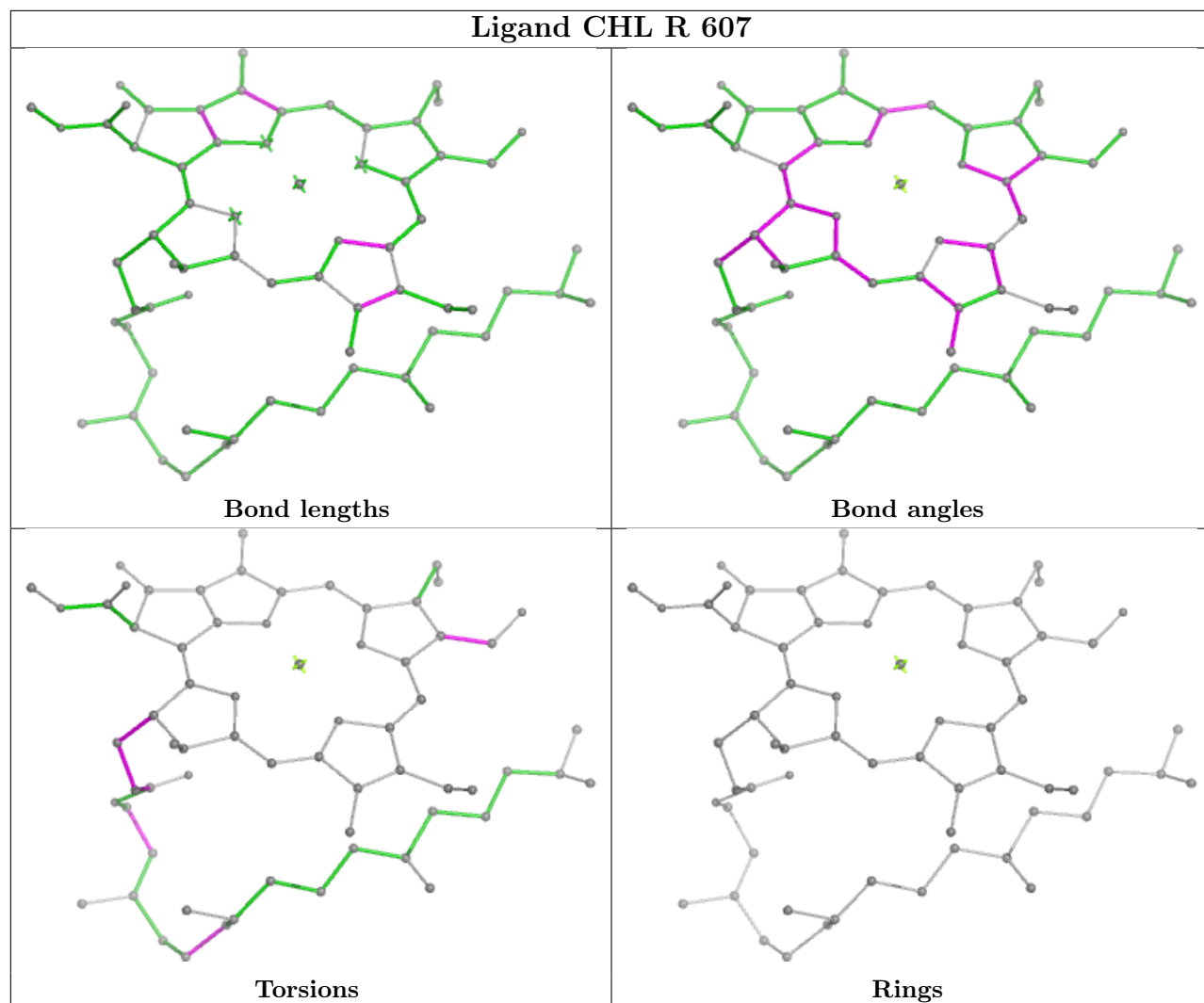
Rings



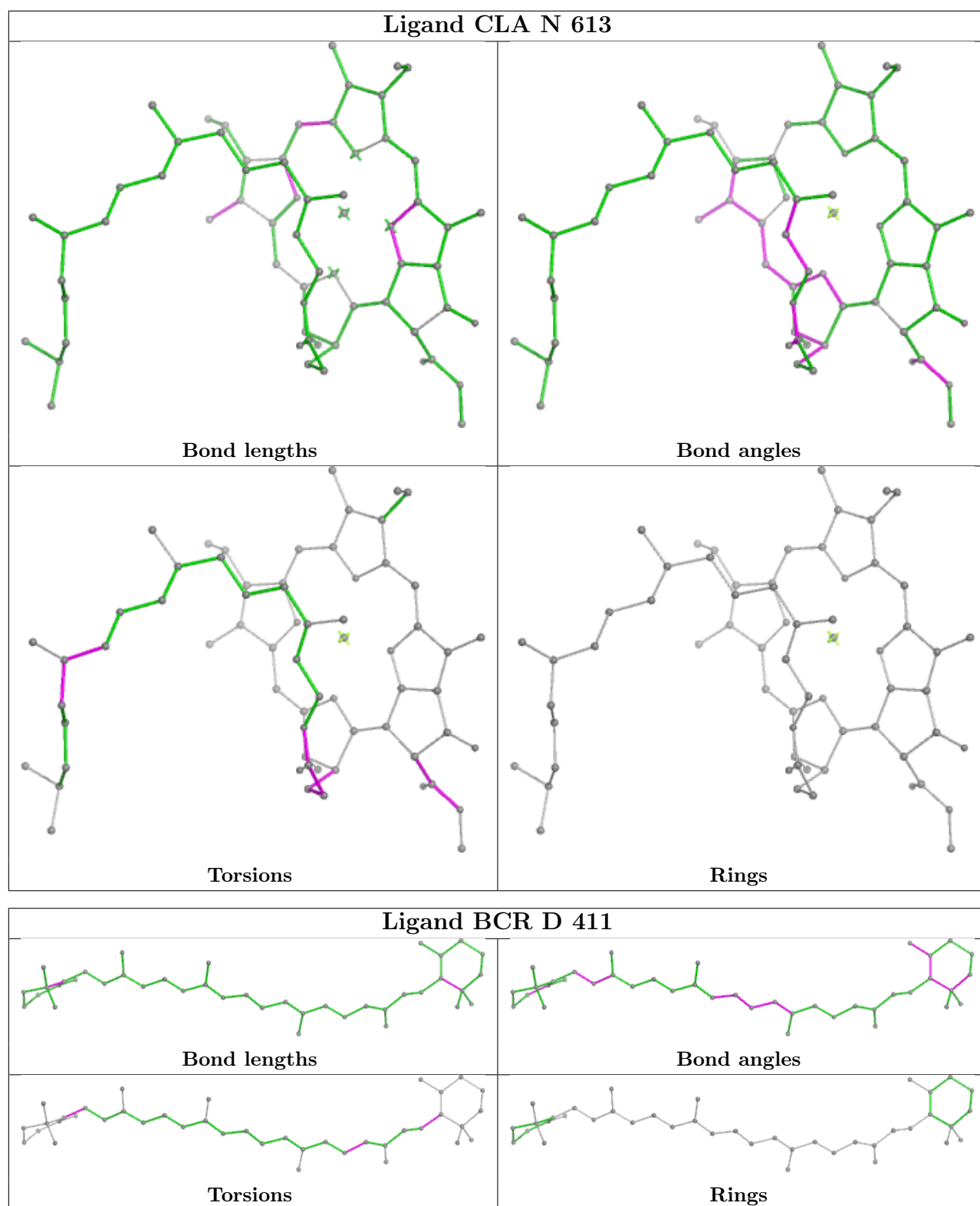


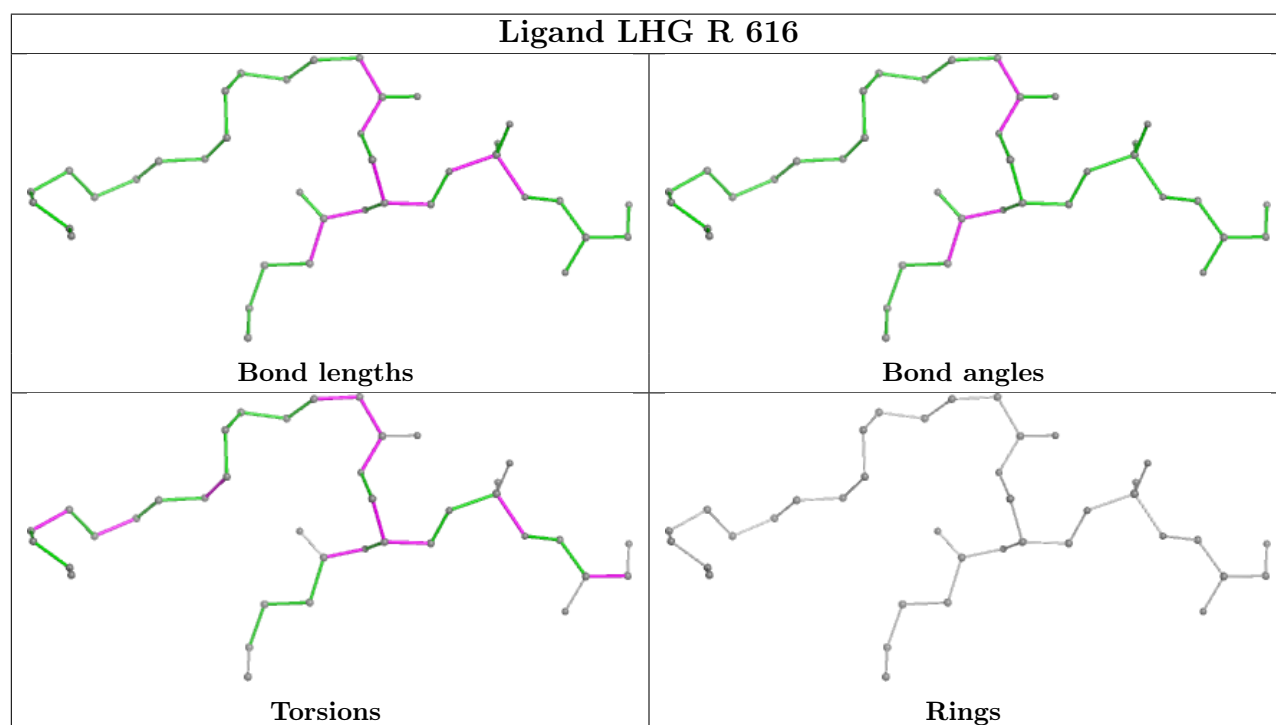
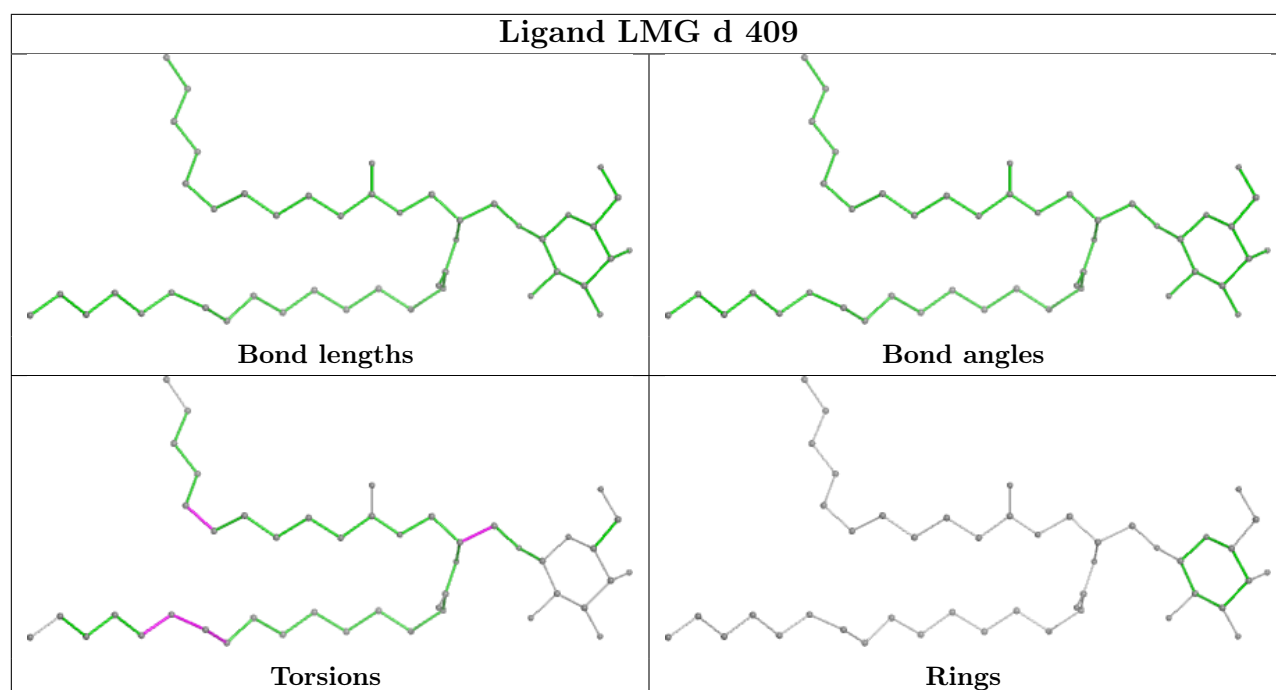




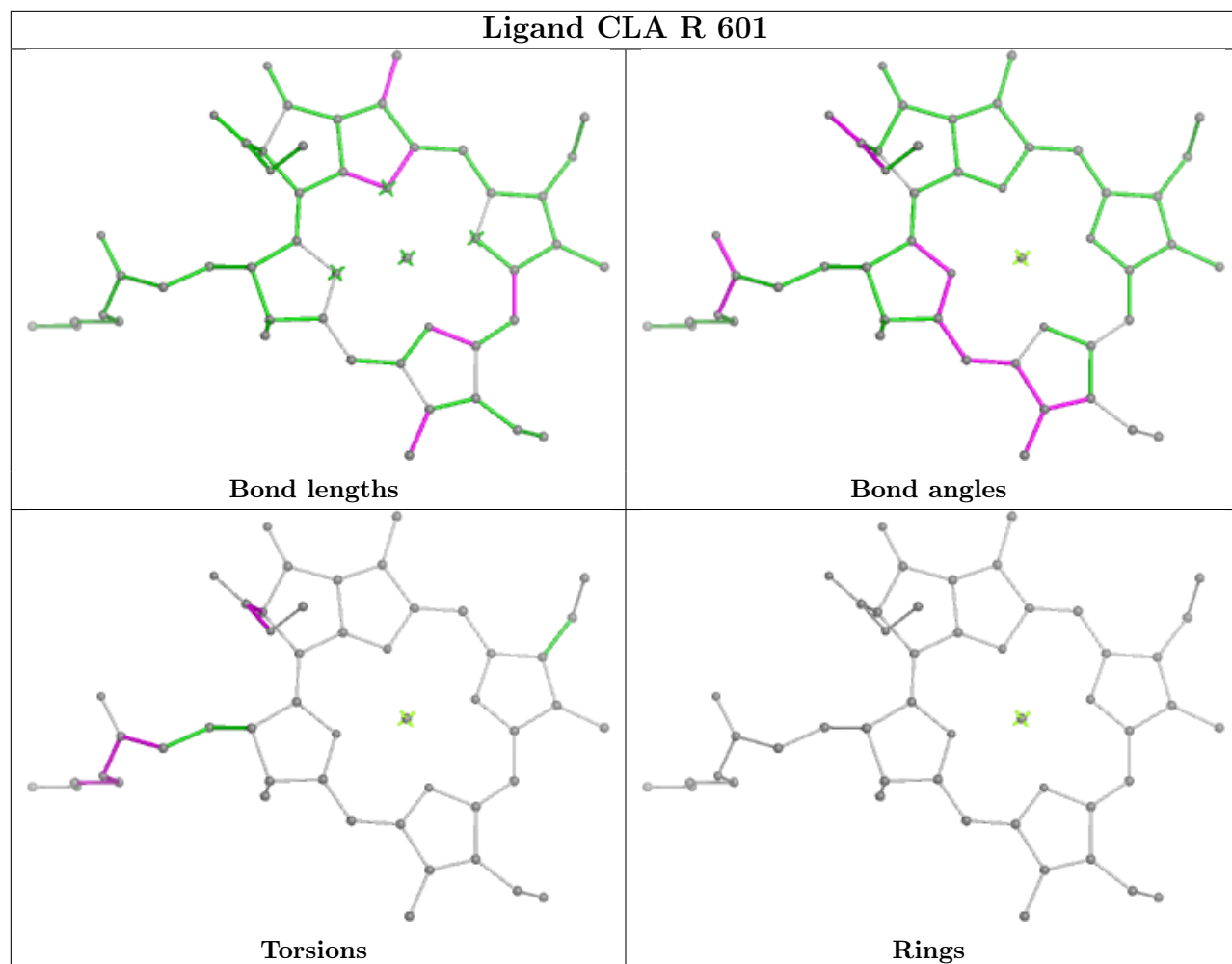


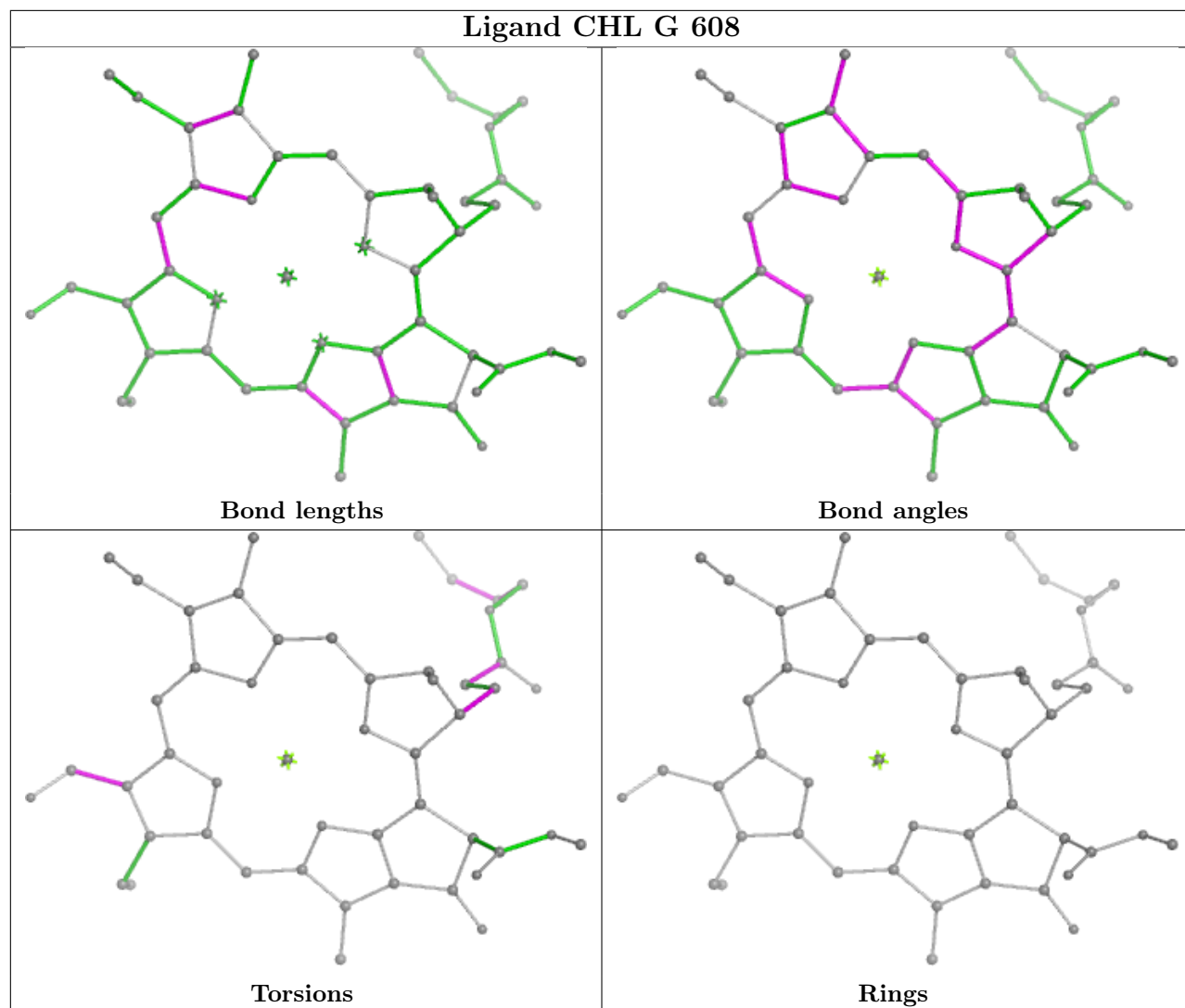


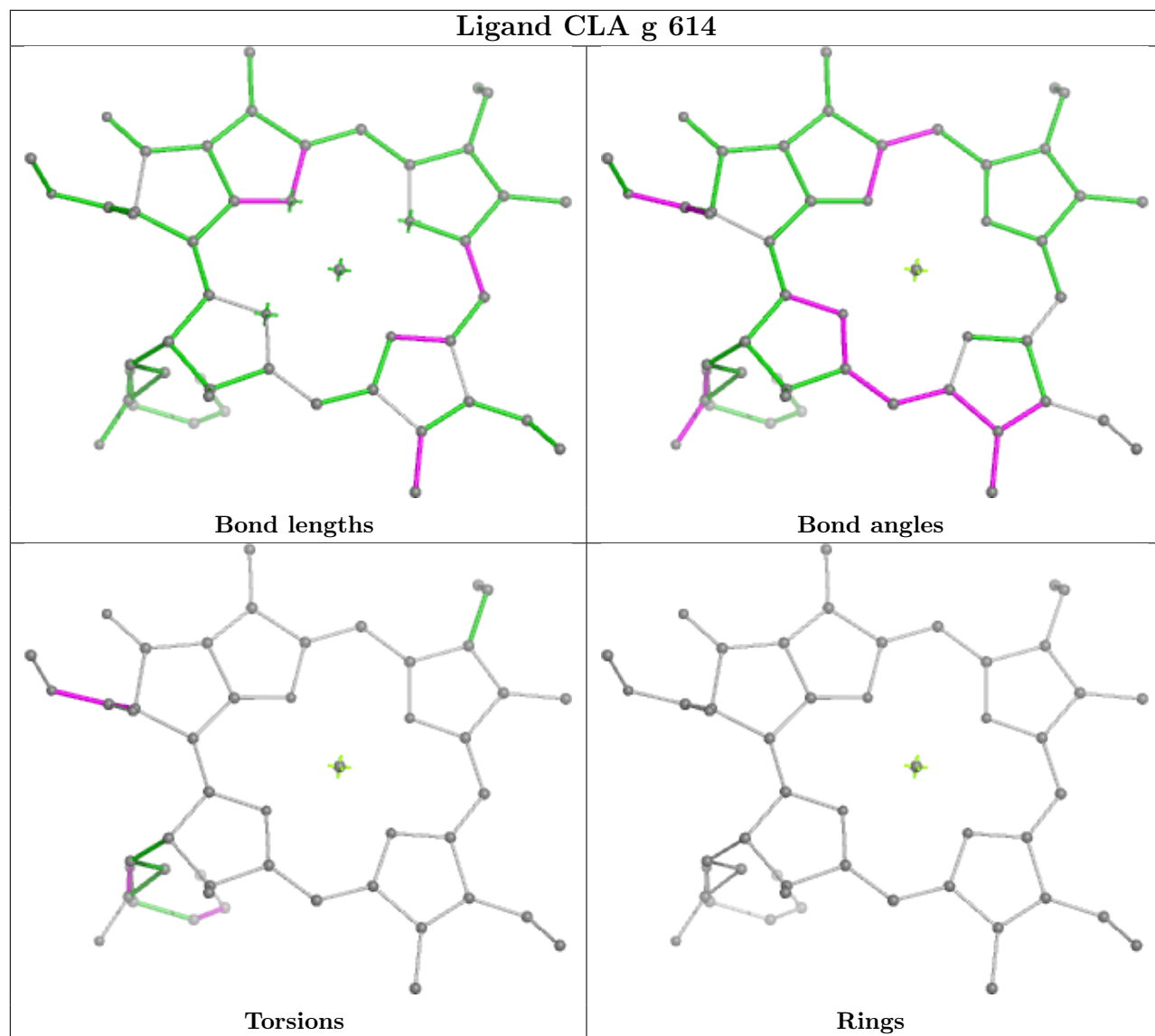


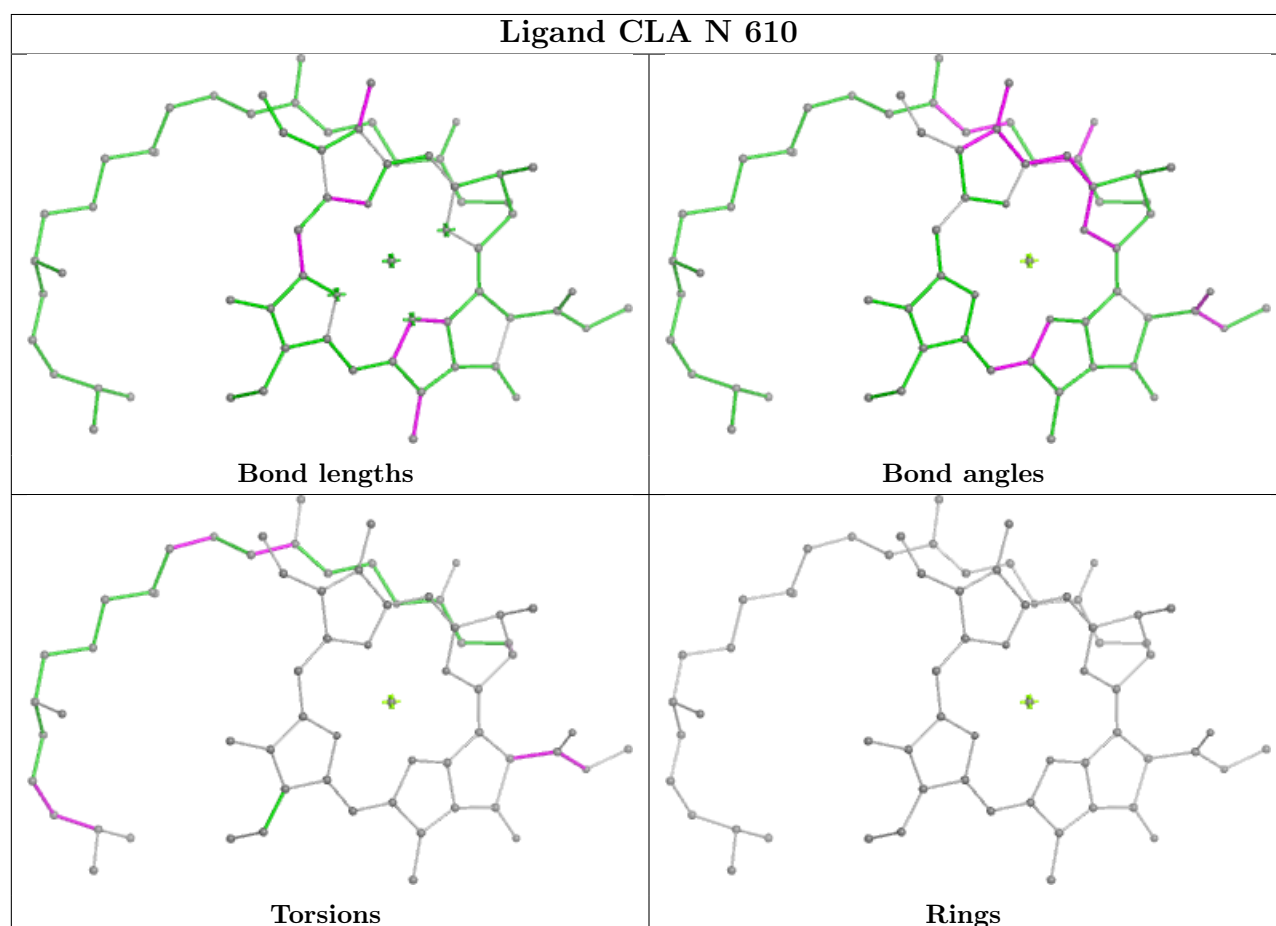
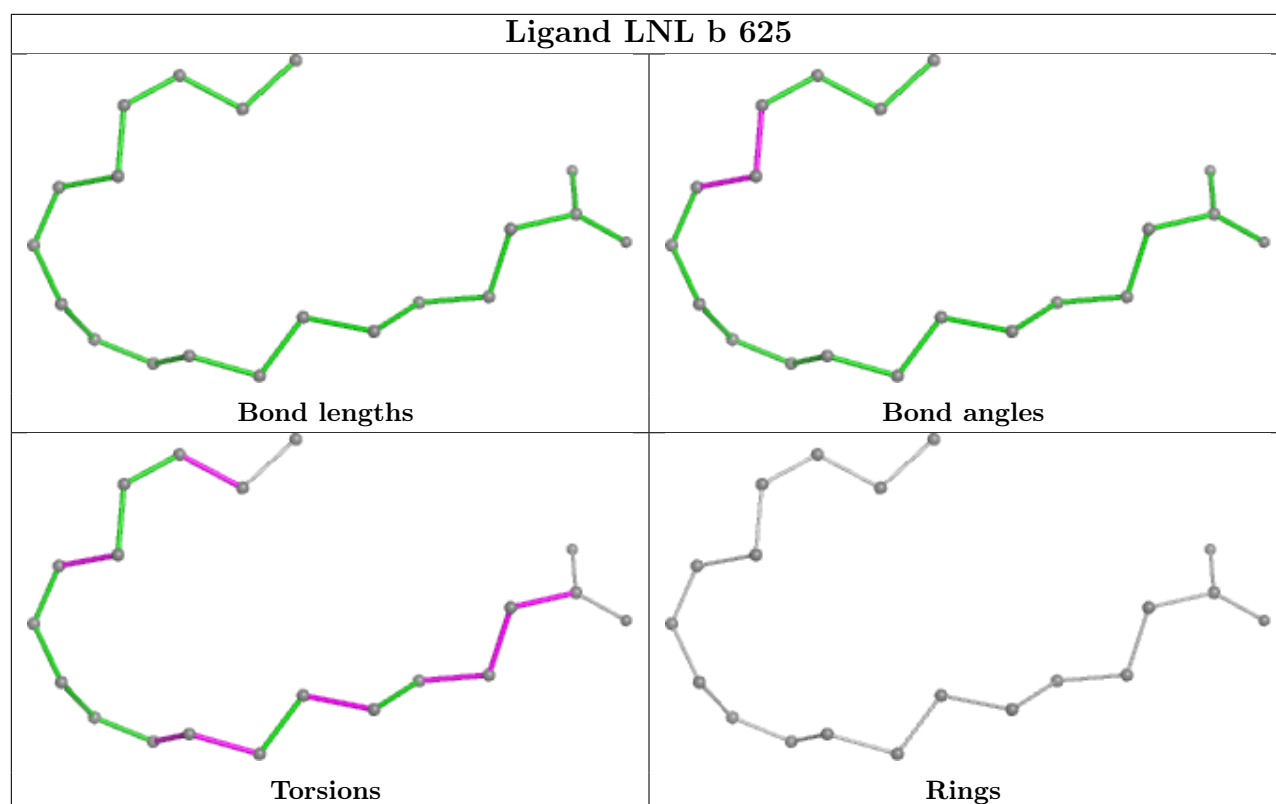


## Ligand CLA R 601

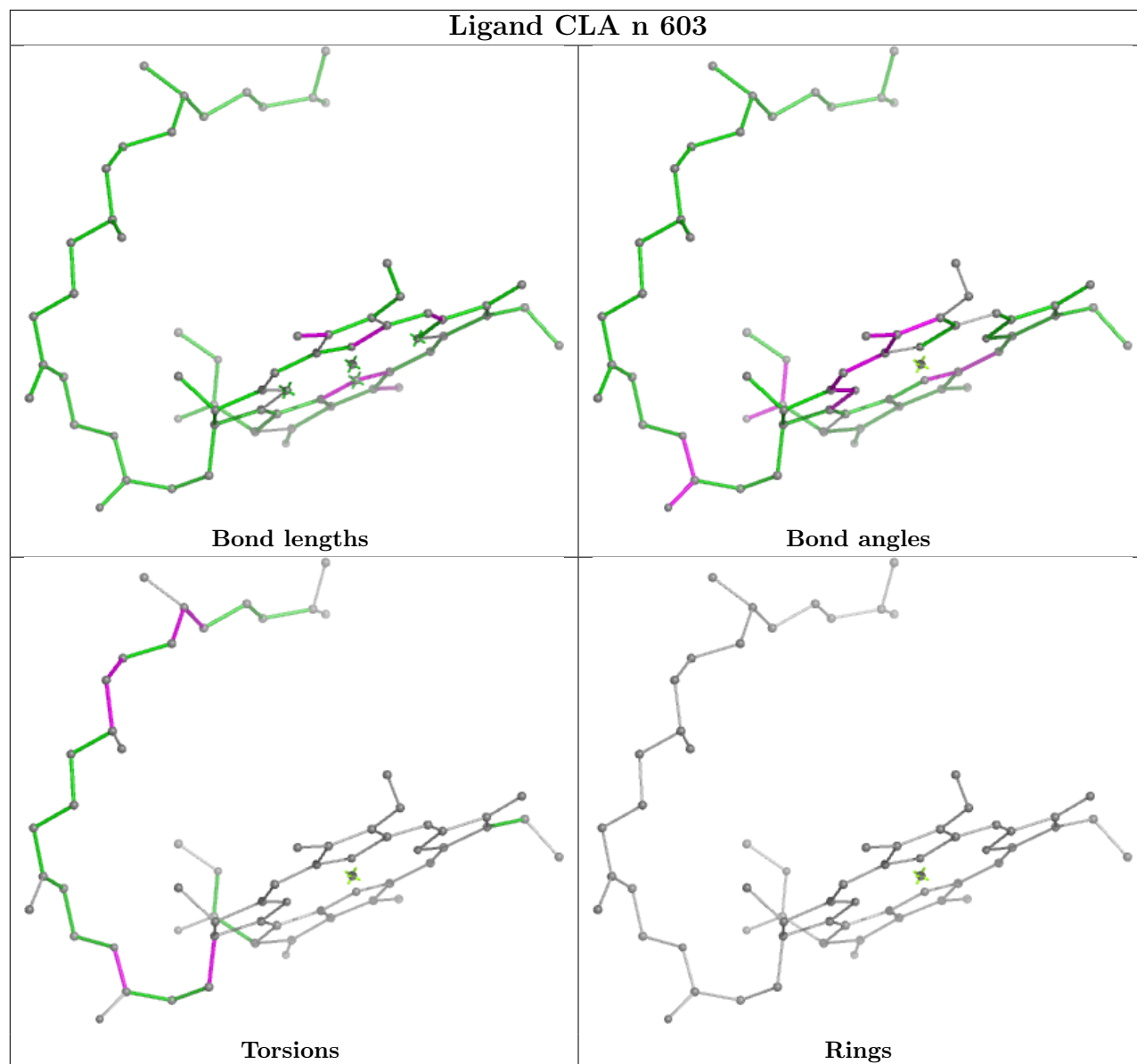




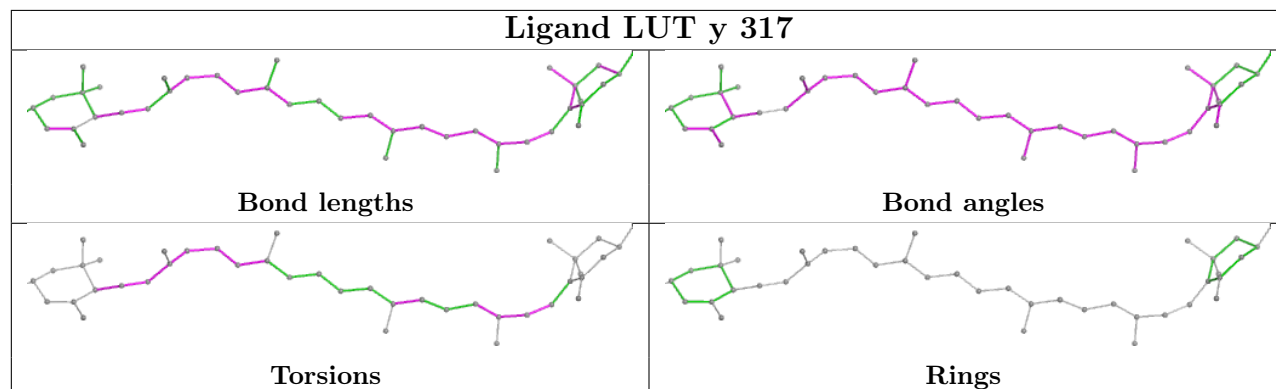


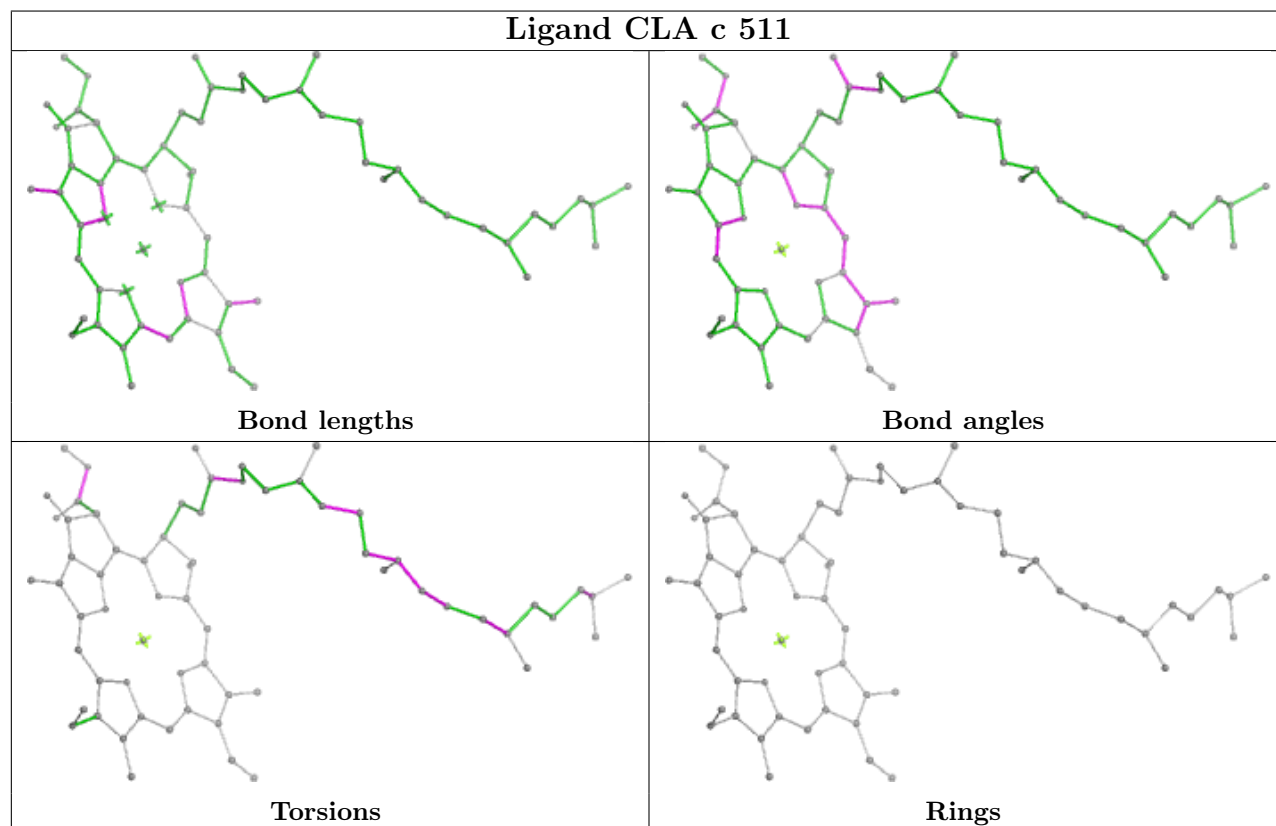
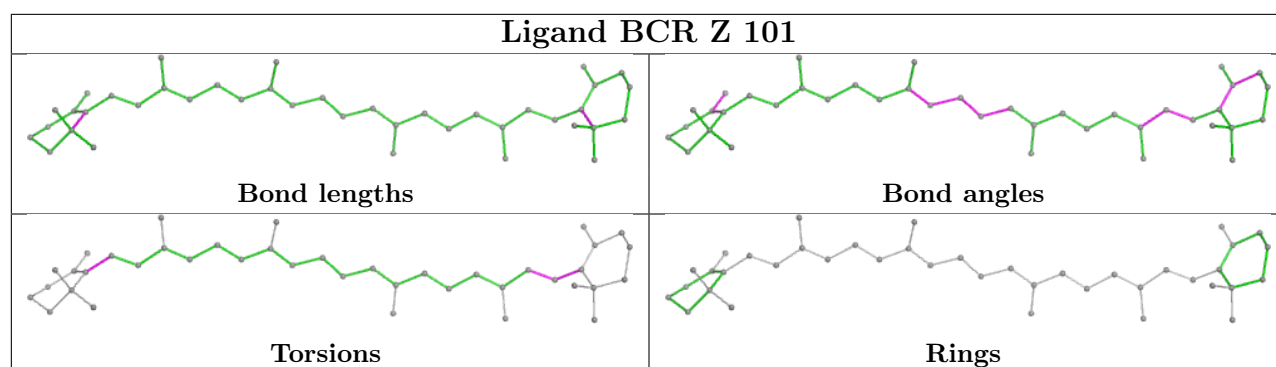


## Ligand CLA n 603

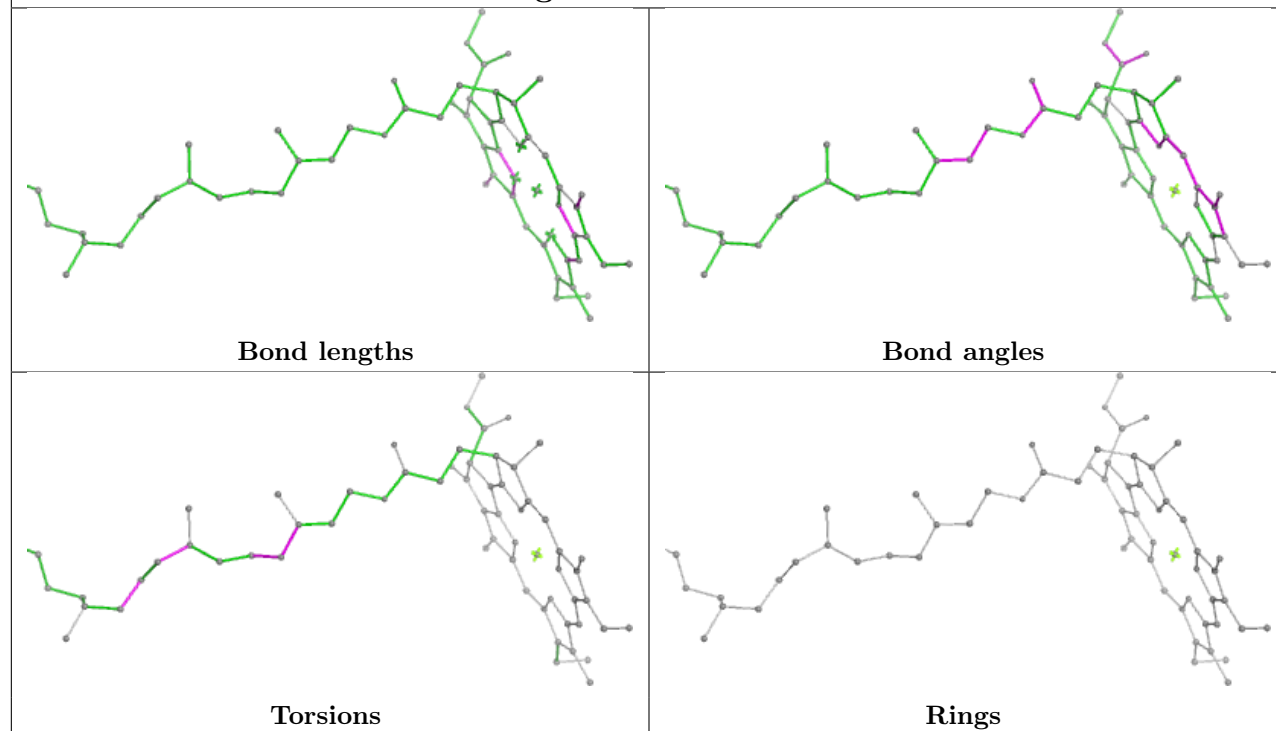
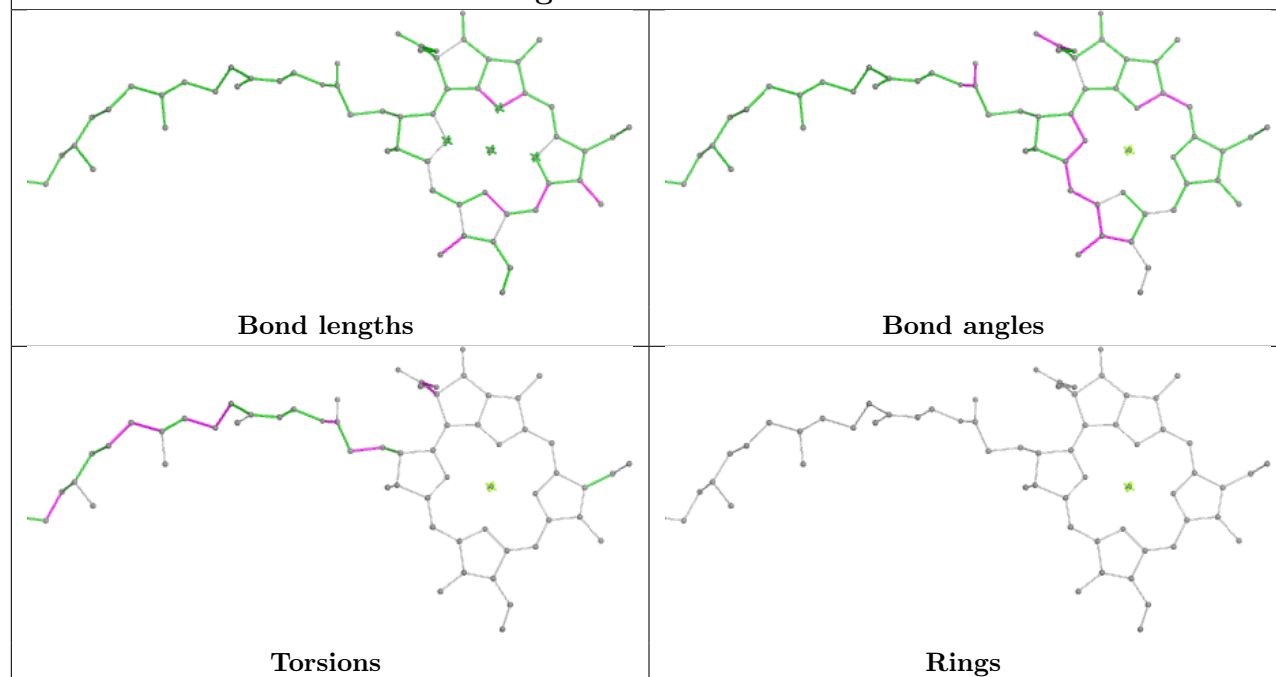


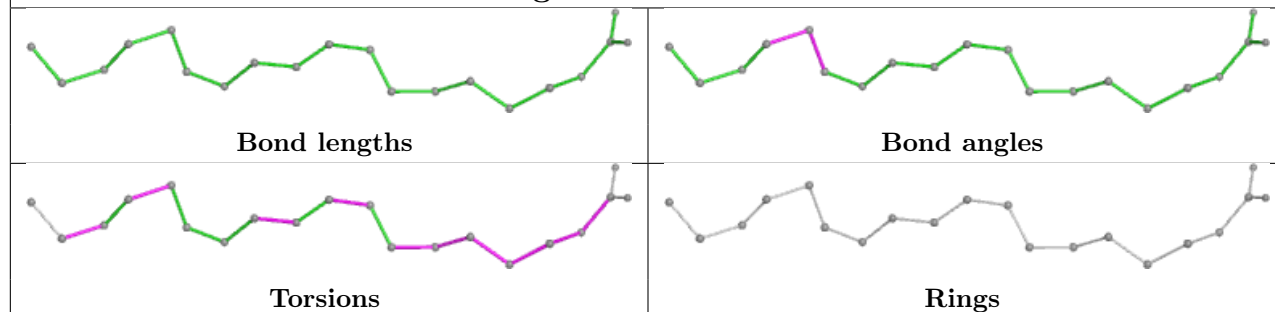
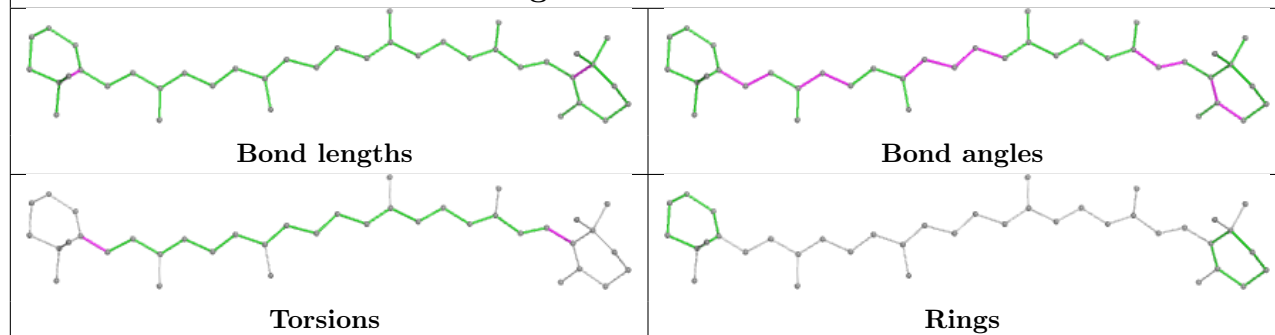
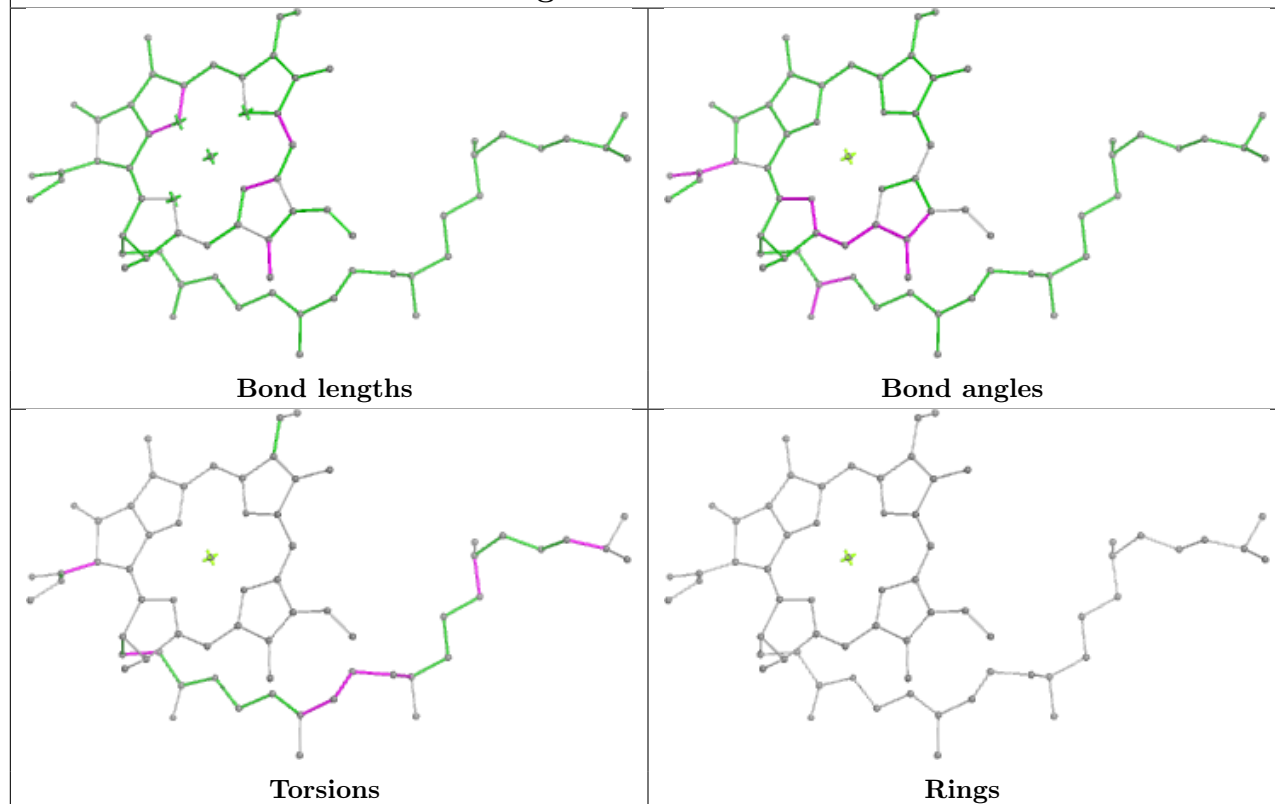
## Ligand LUT y 317

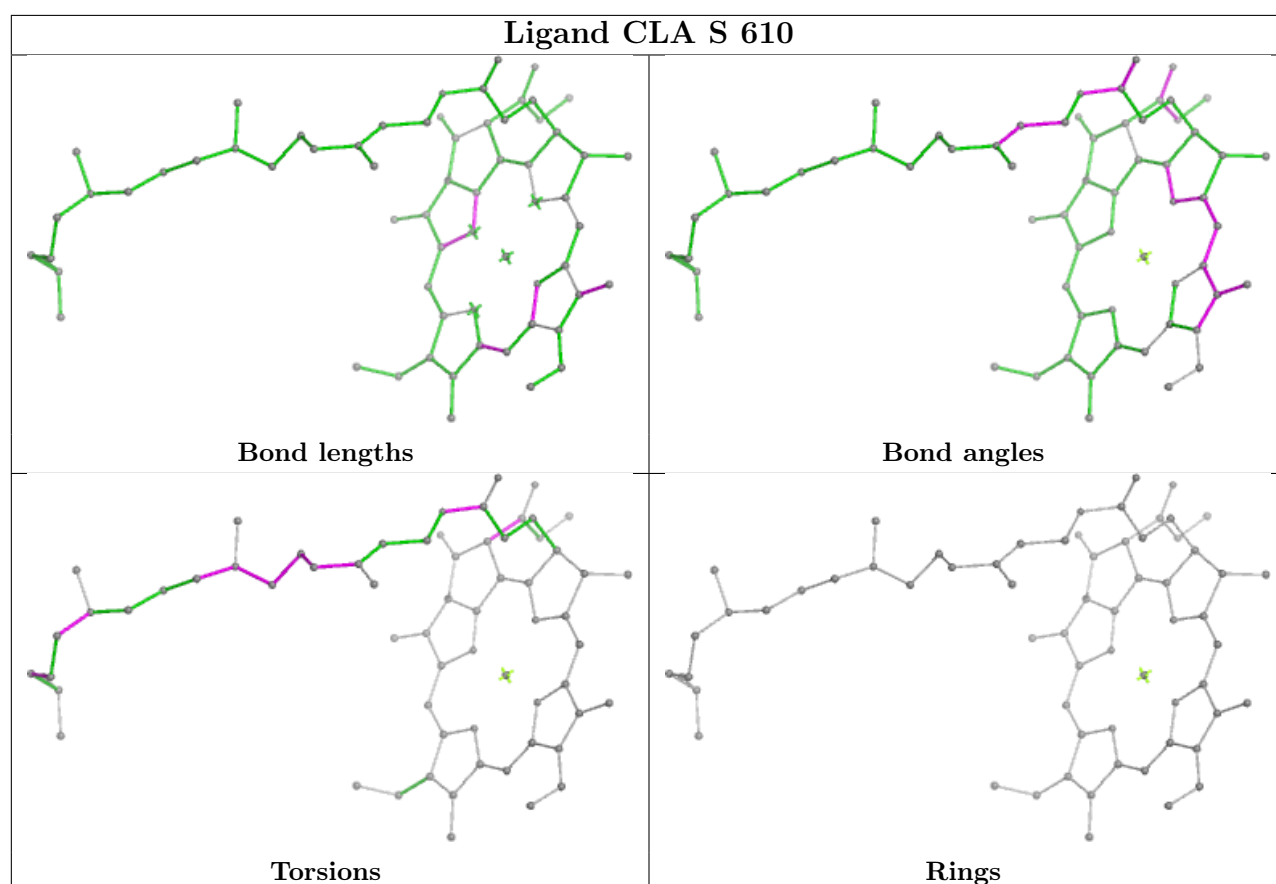
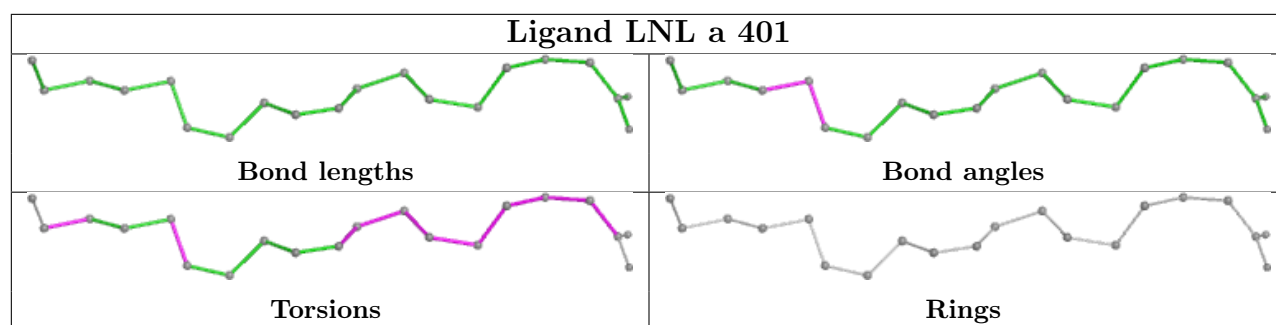




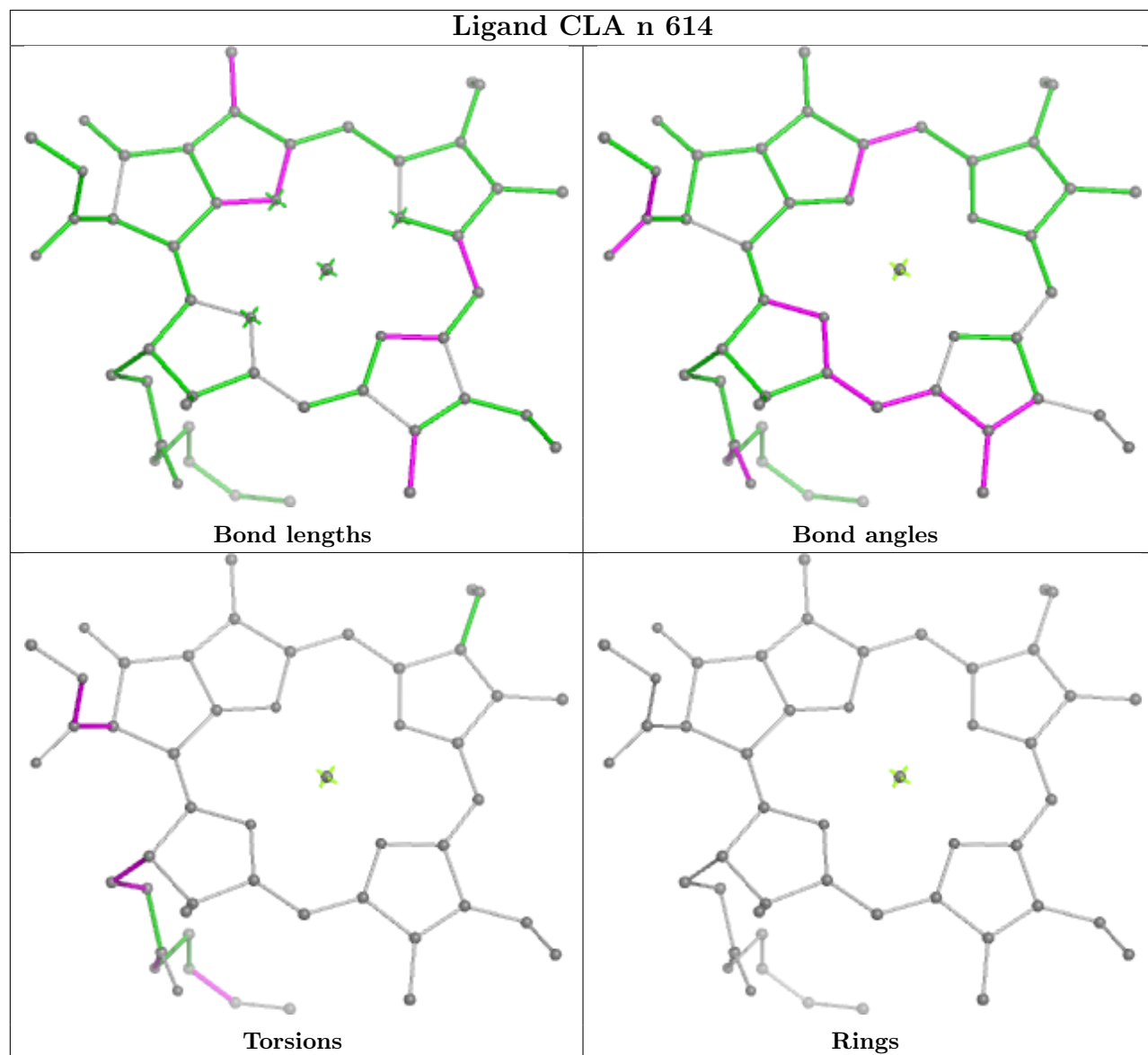


**Ligand CLA b 604****Ligand CLA b 616**

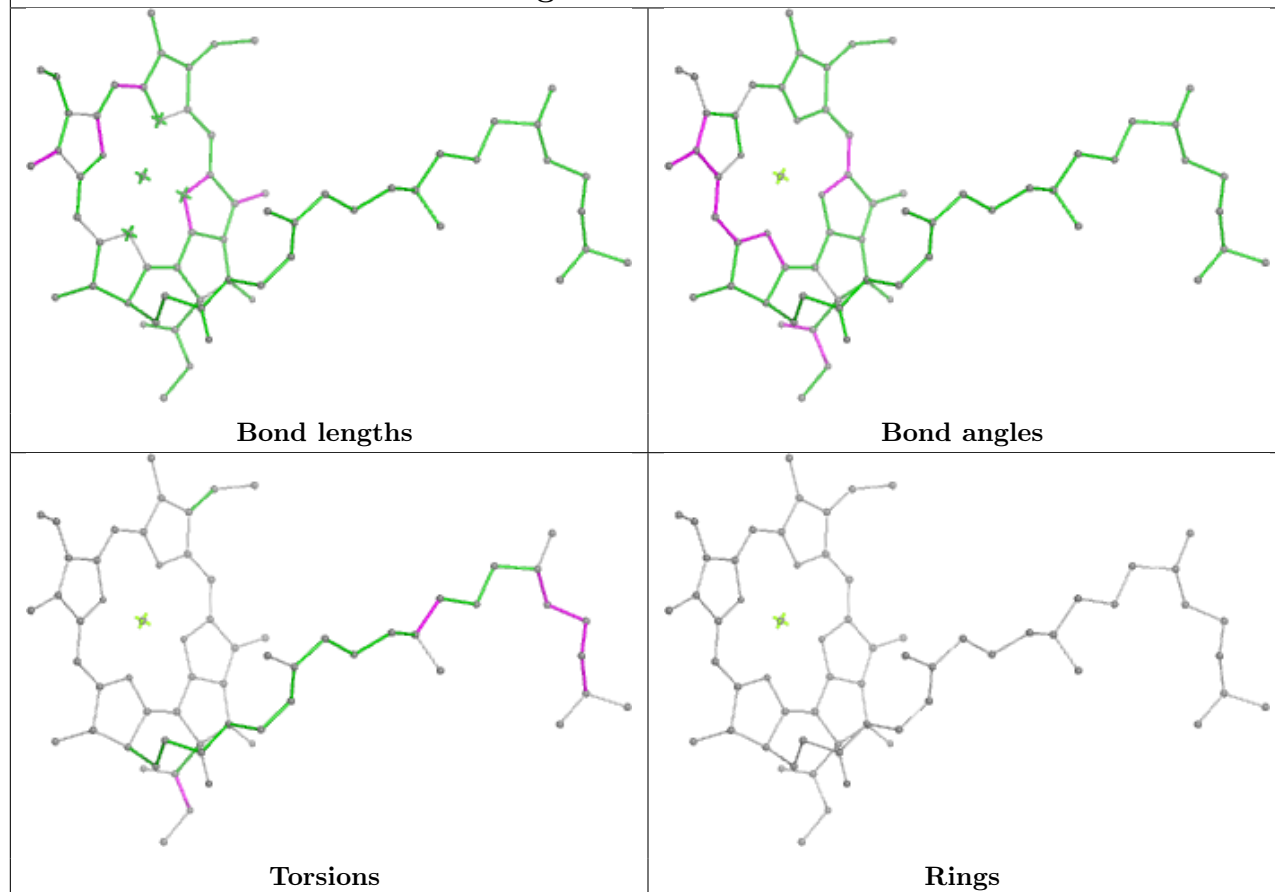
**Ligand LNL C 520****Ligand BCR B 618****Ligand CLA r 602**



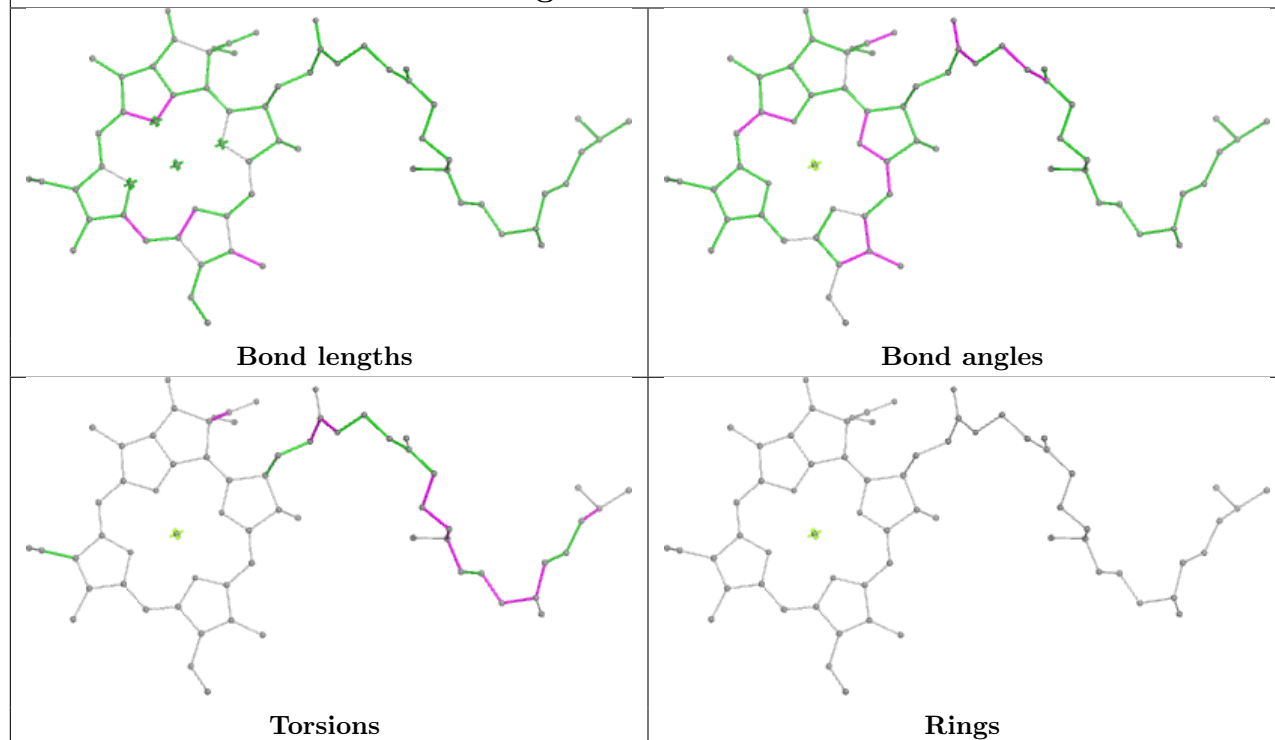
## Ligand CLA n 614

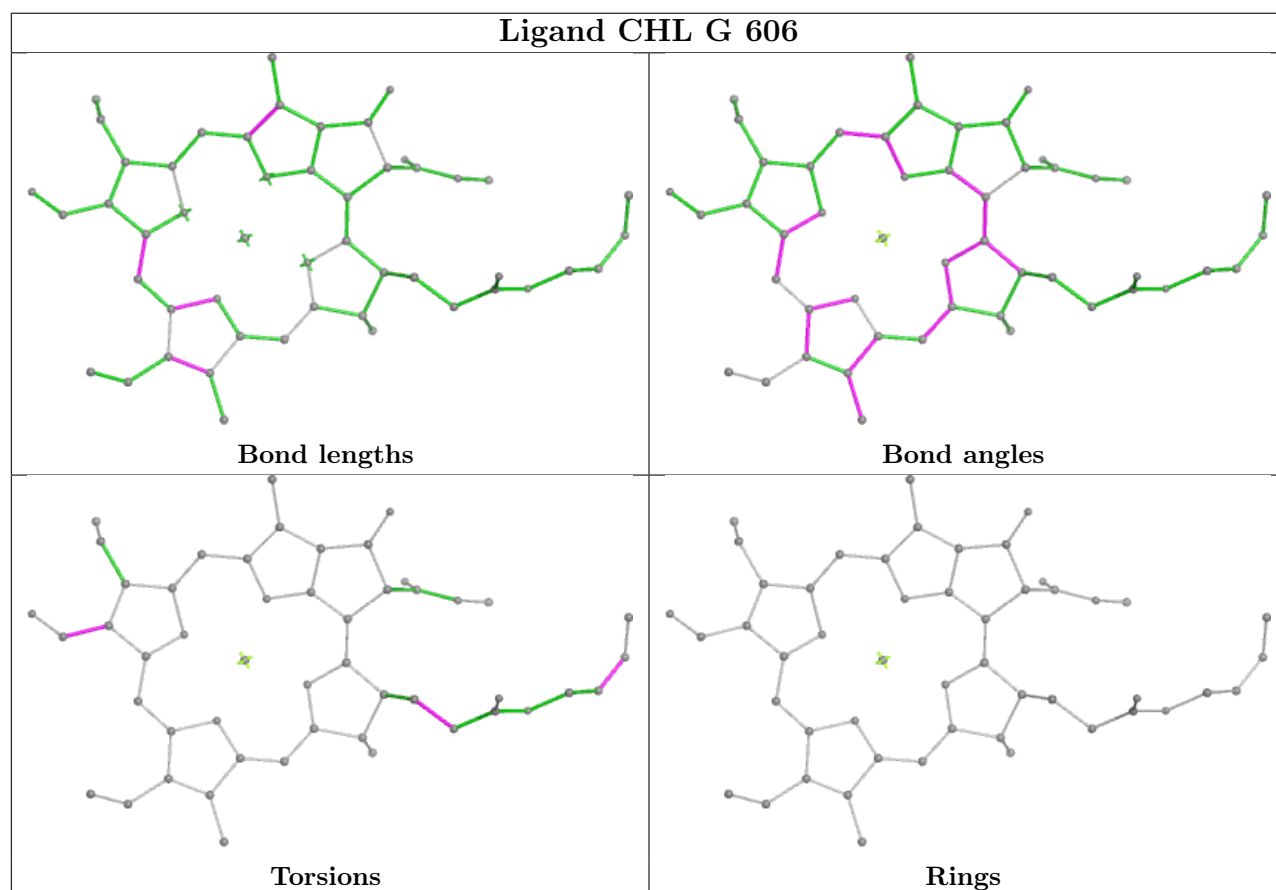
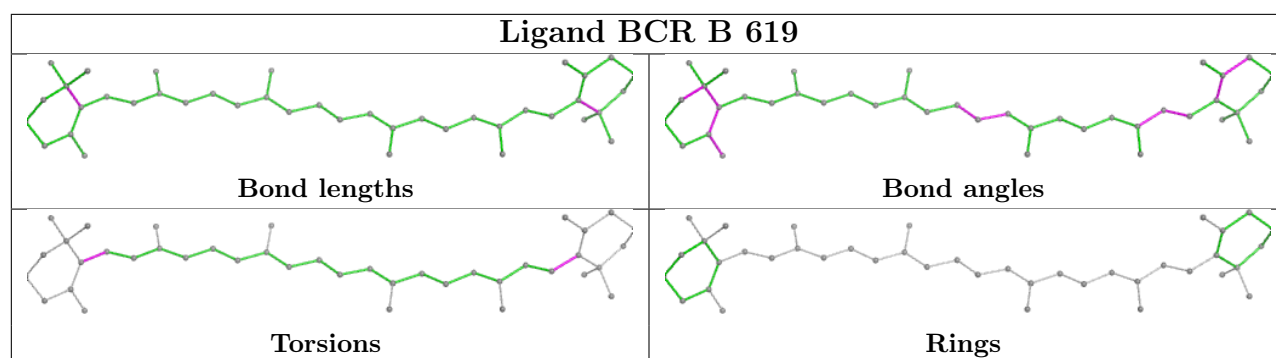


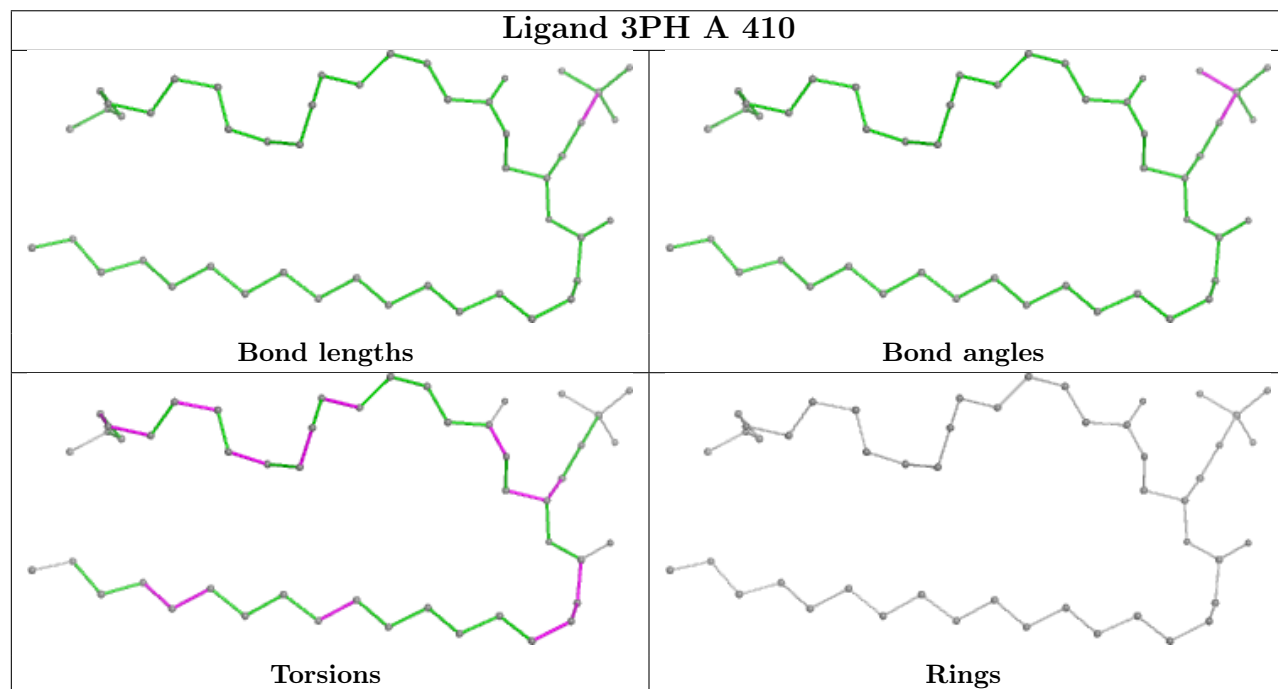
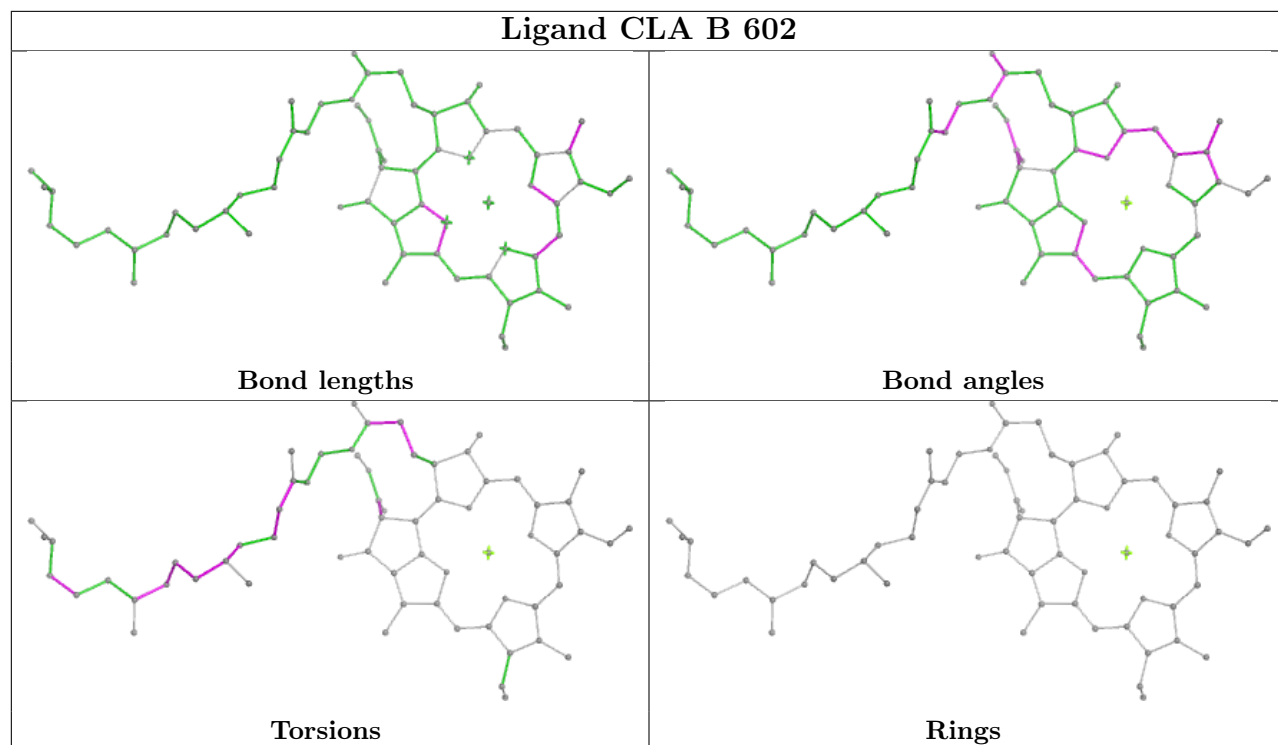
## Ligand CLA r 608

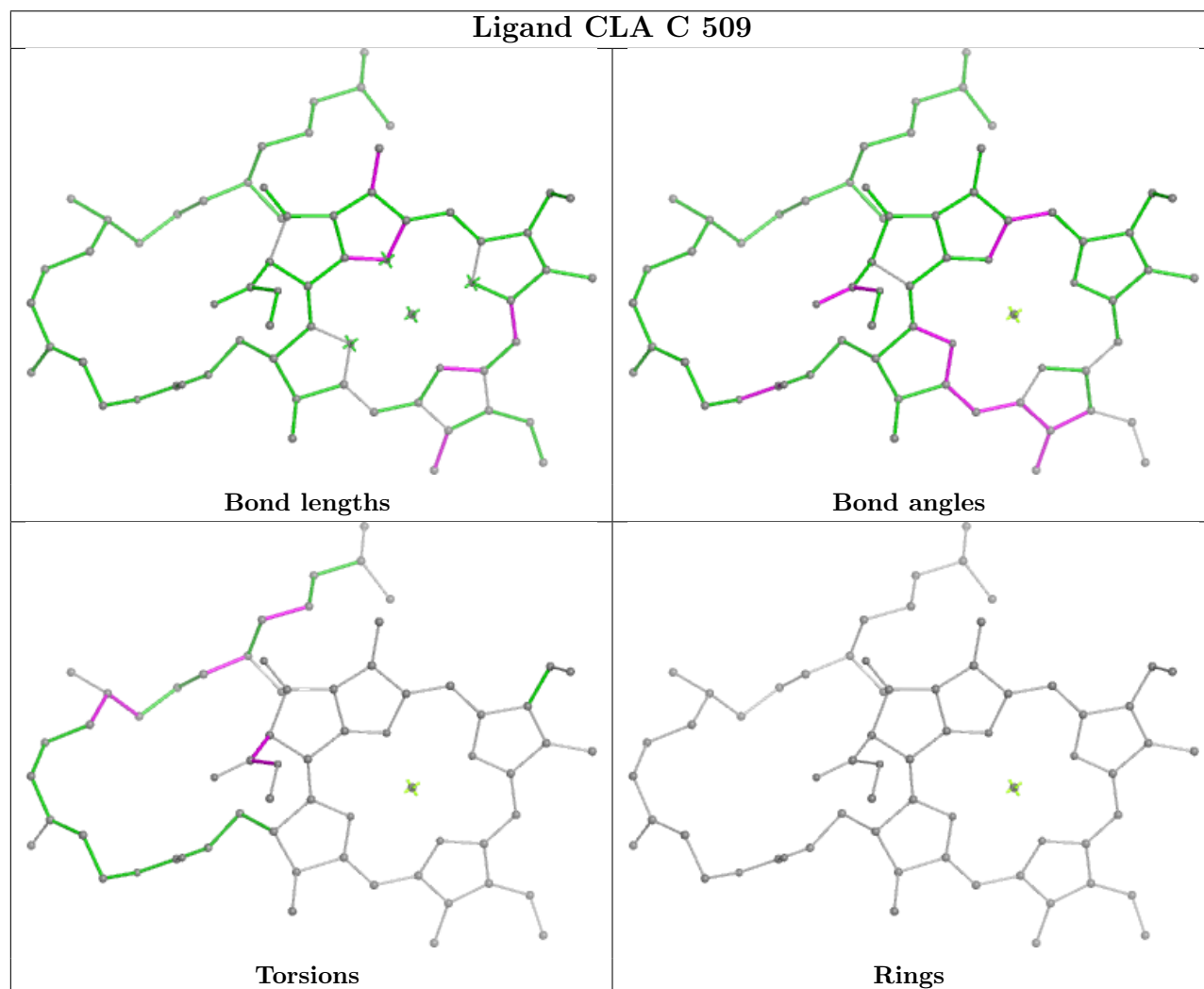
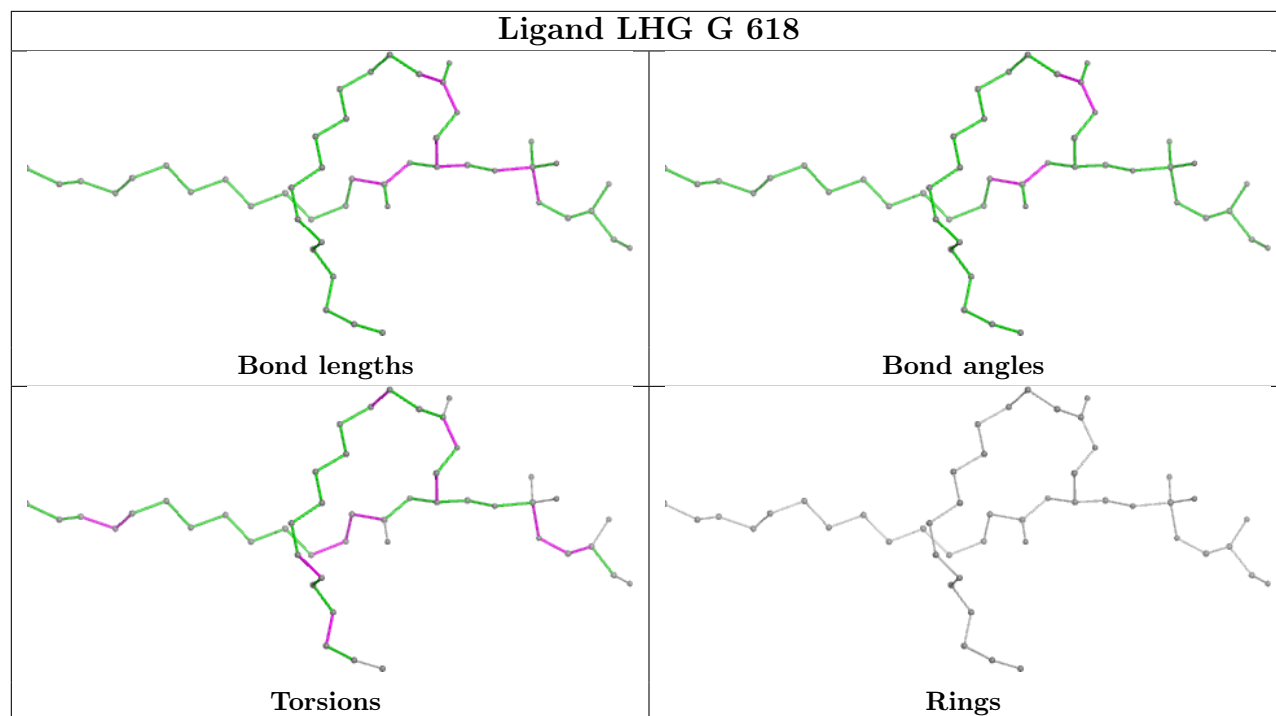


## Ligand CLA c 512

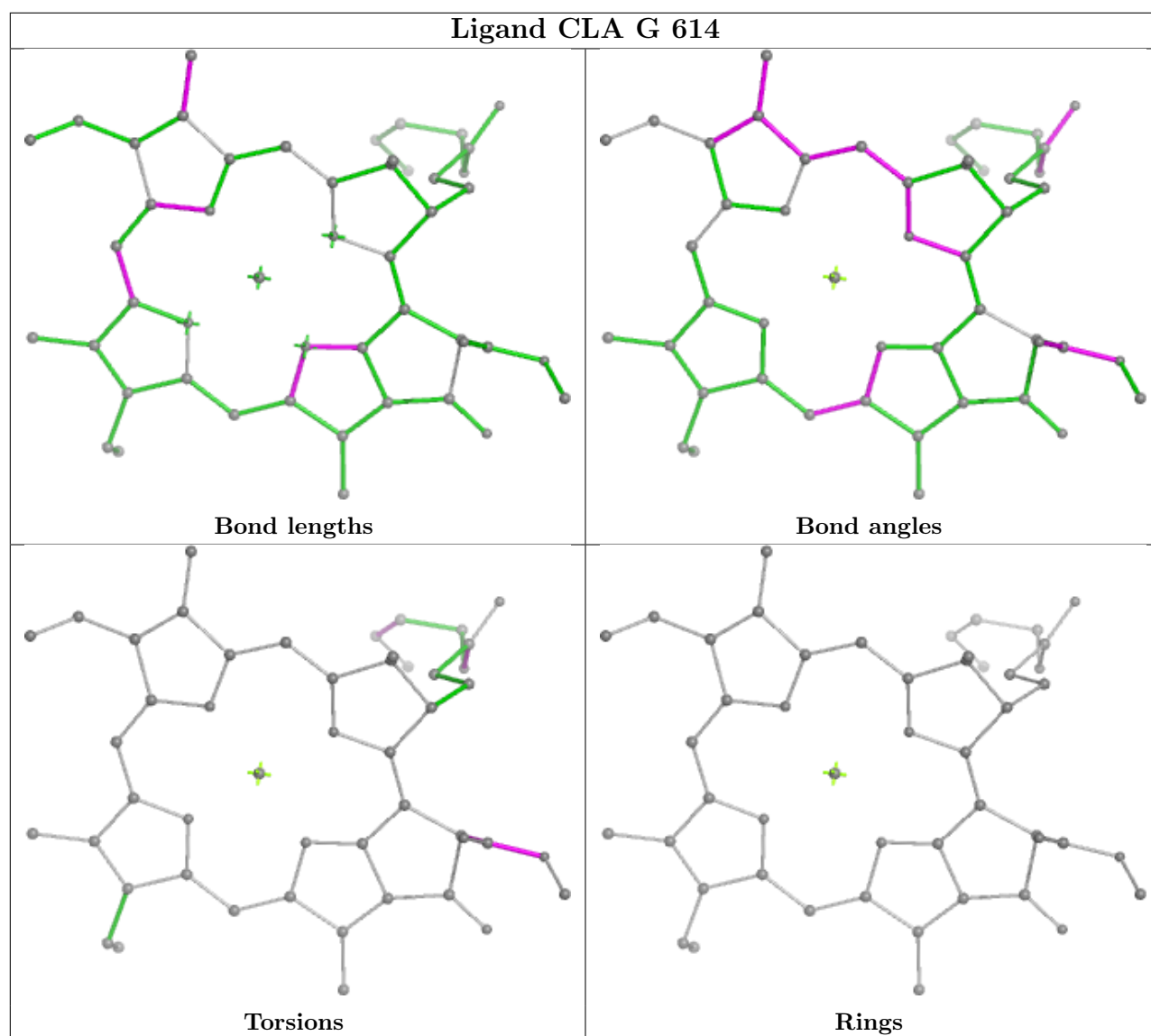




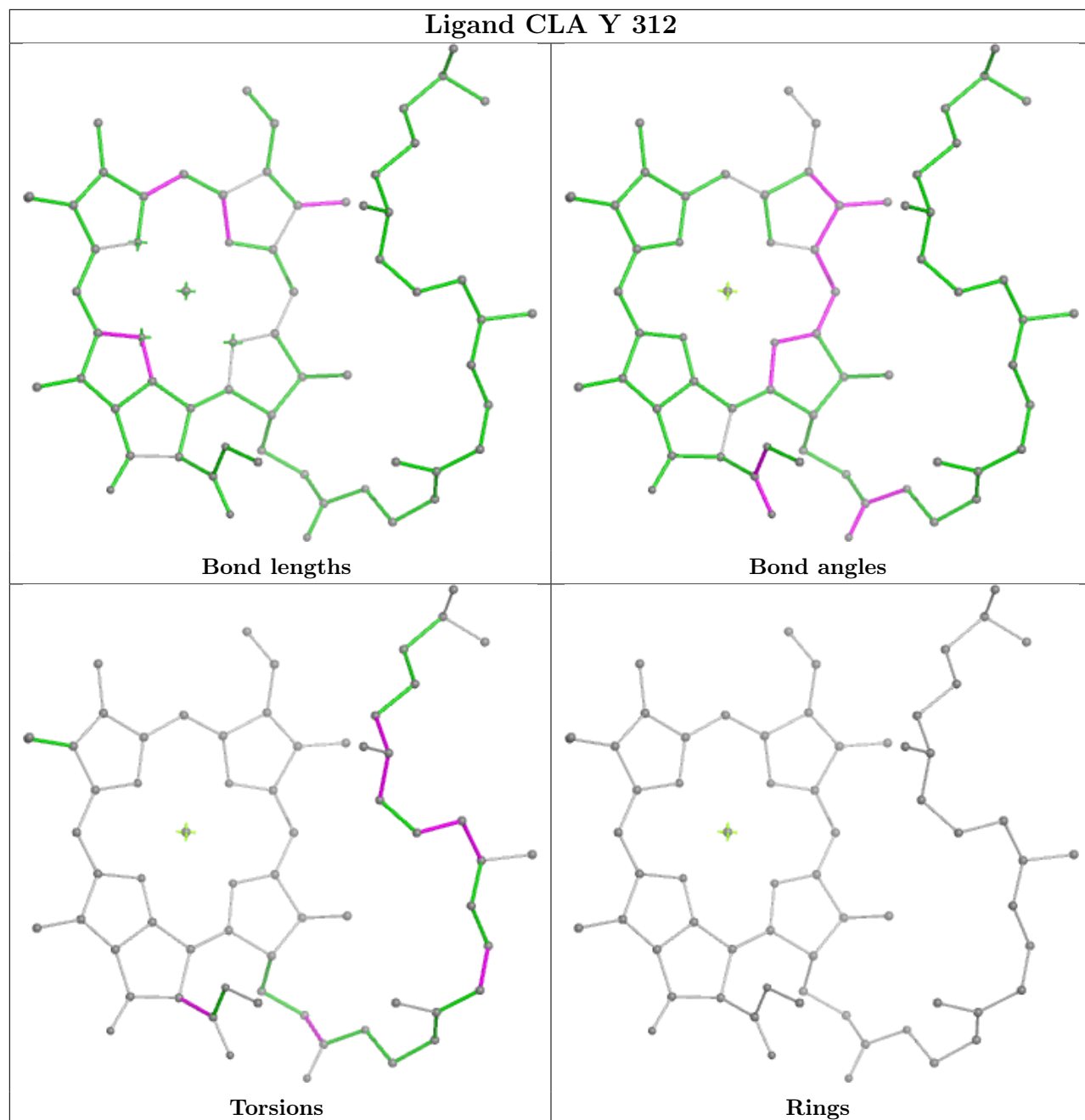


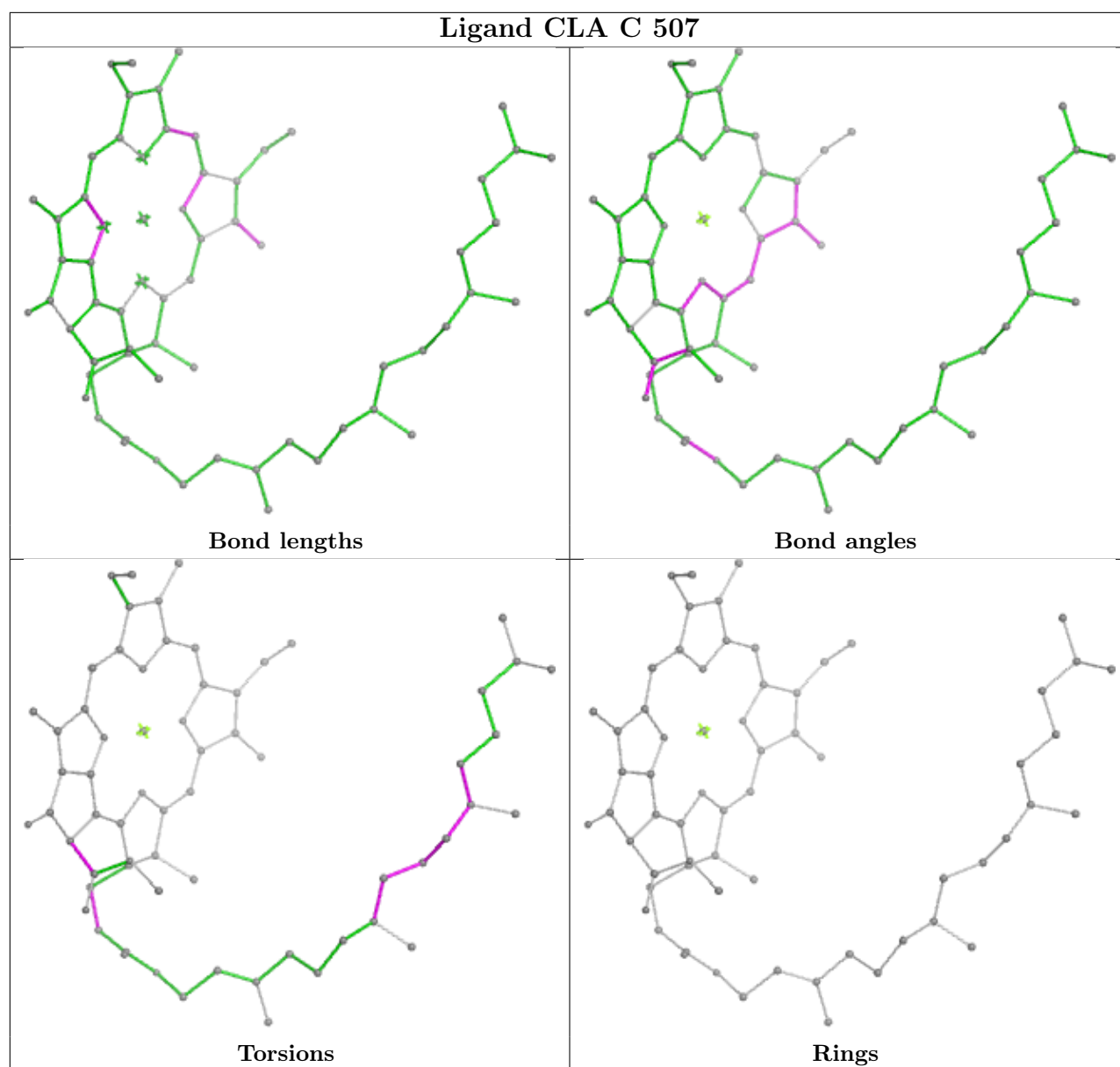


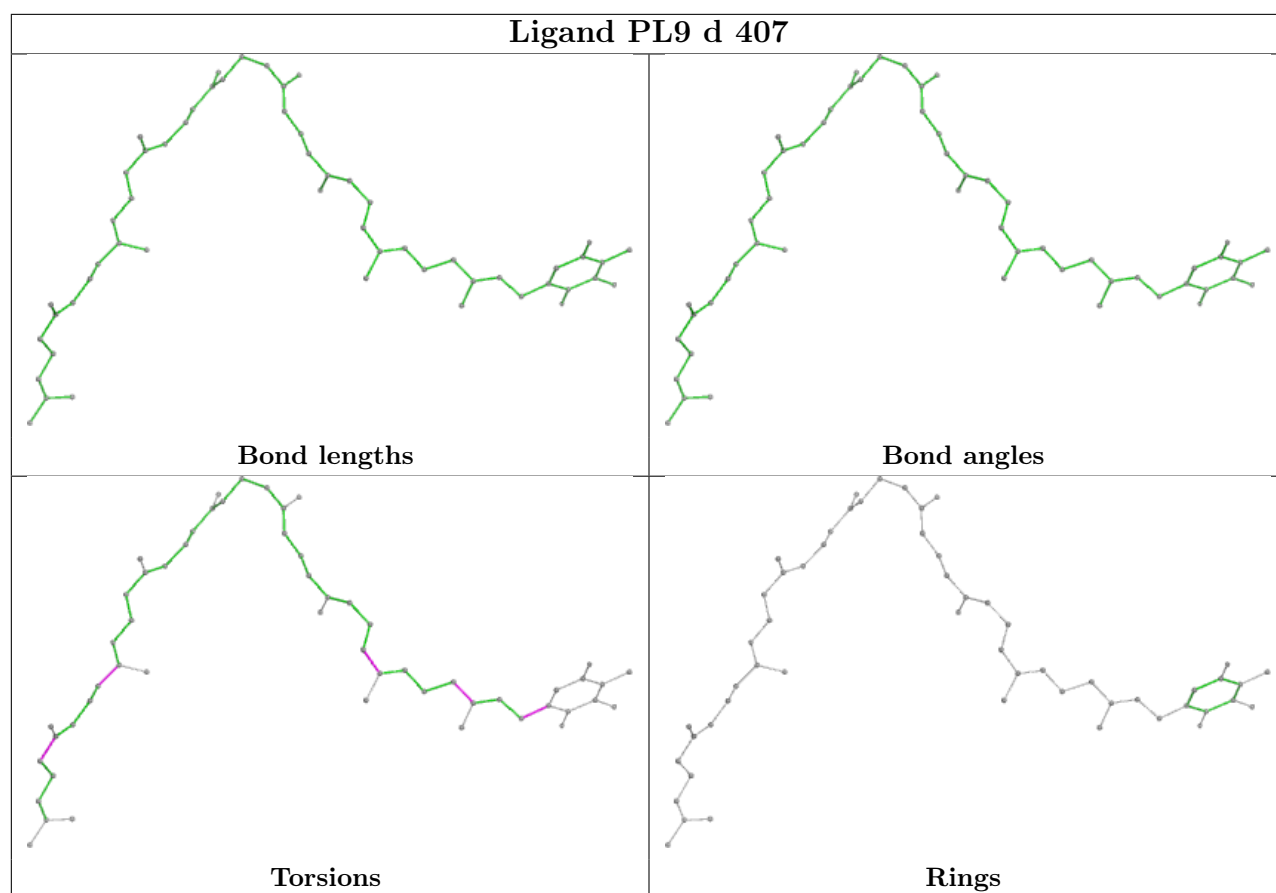


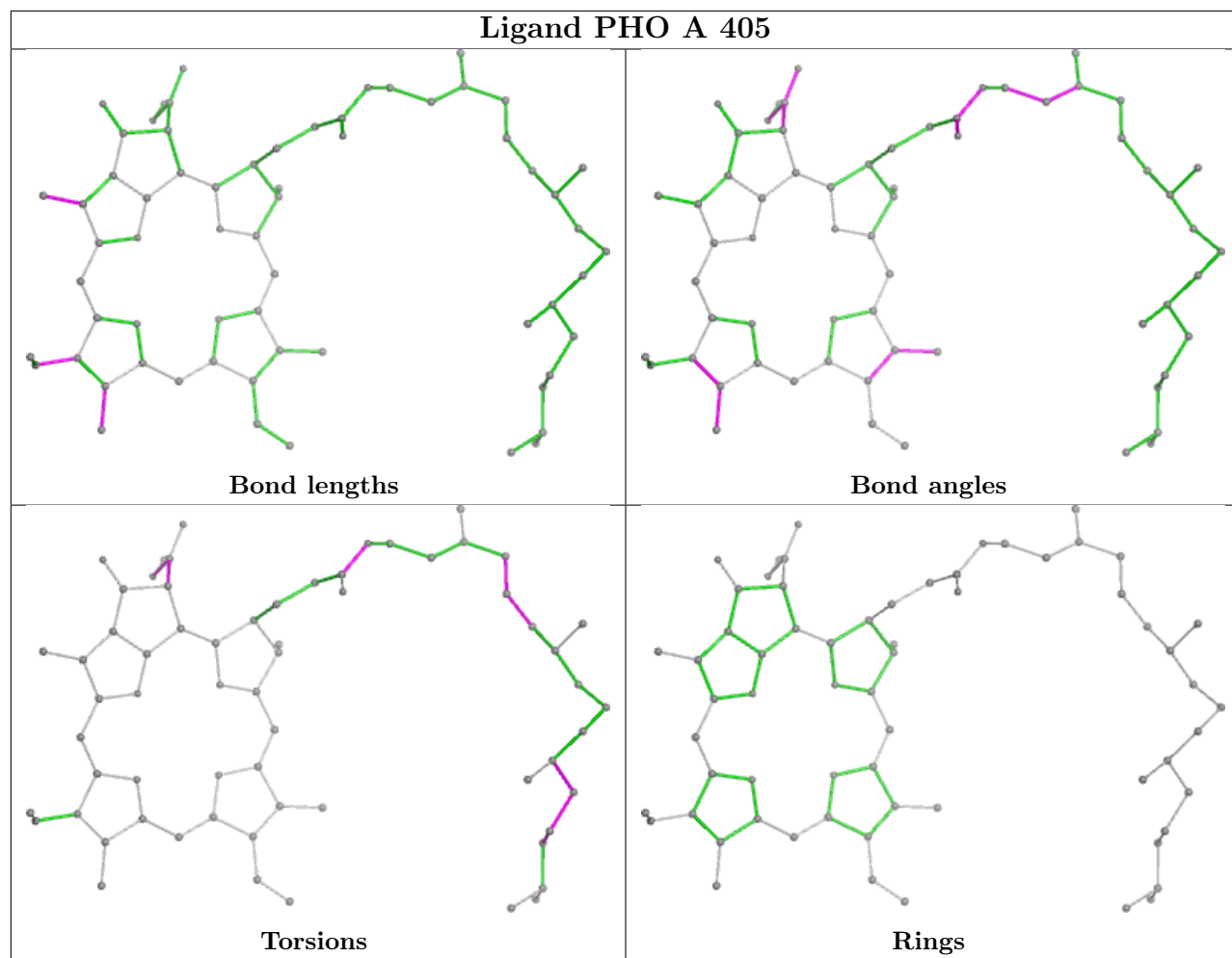


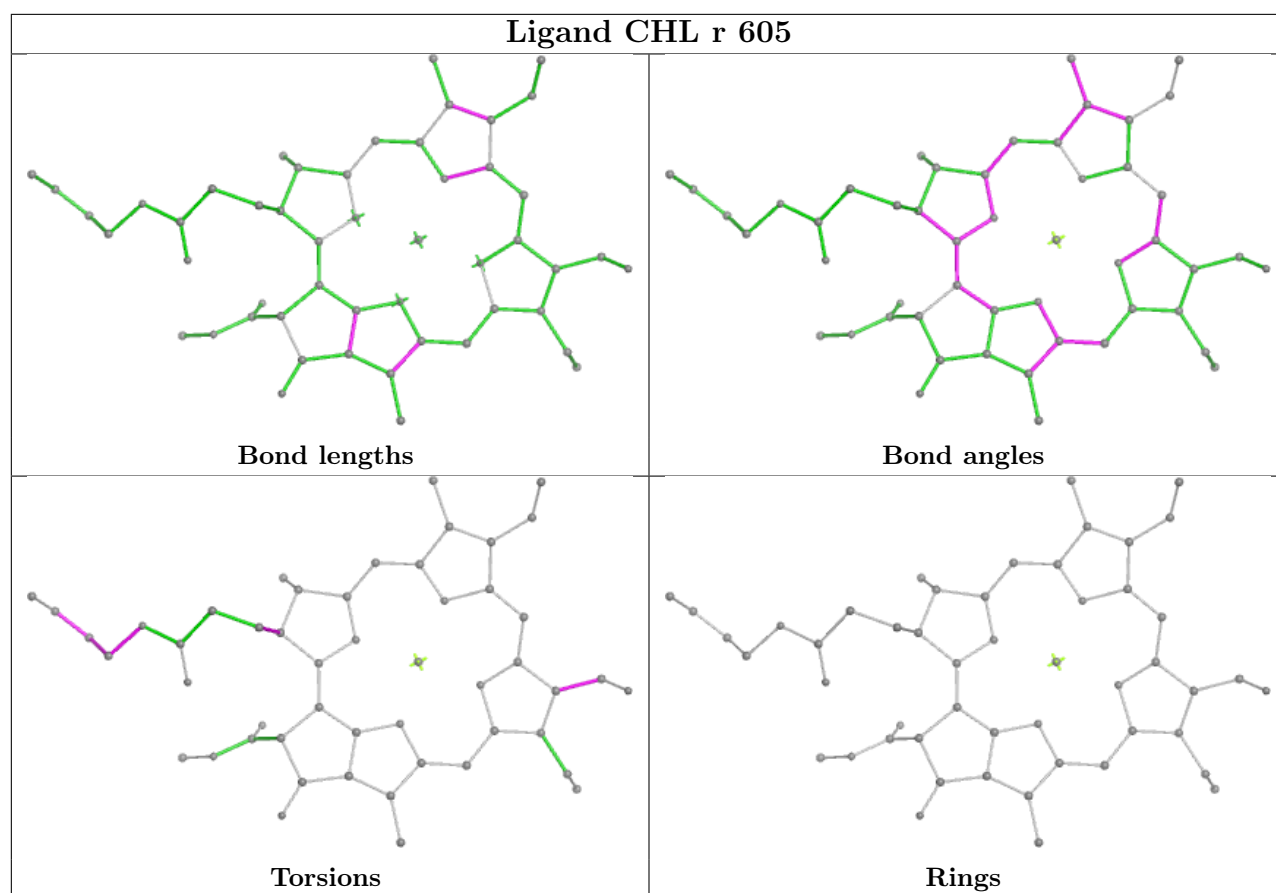
## Ligand CLA Y 312



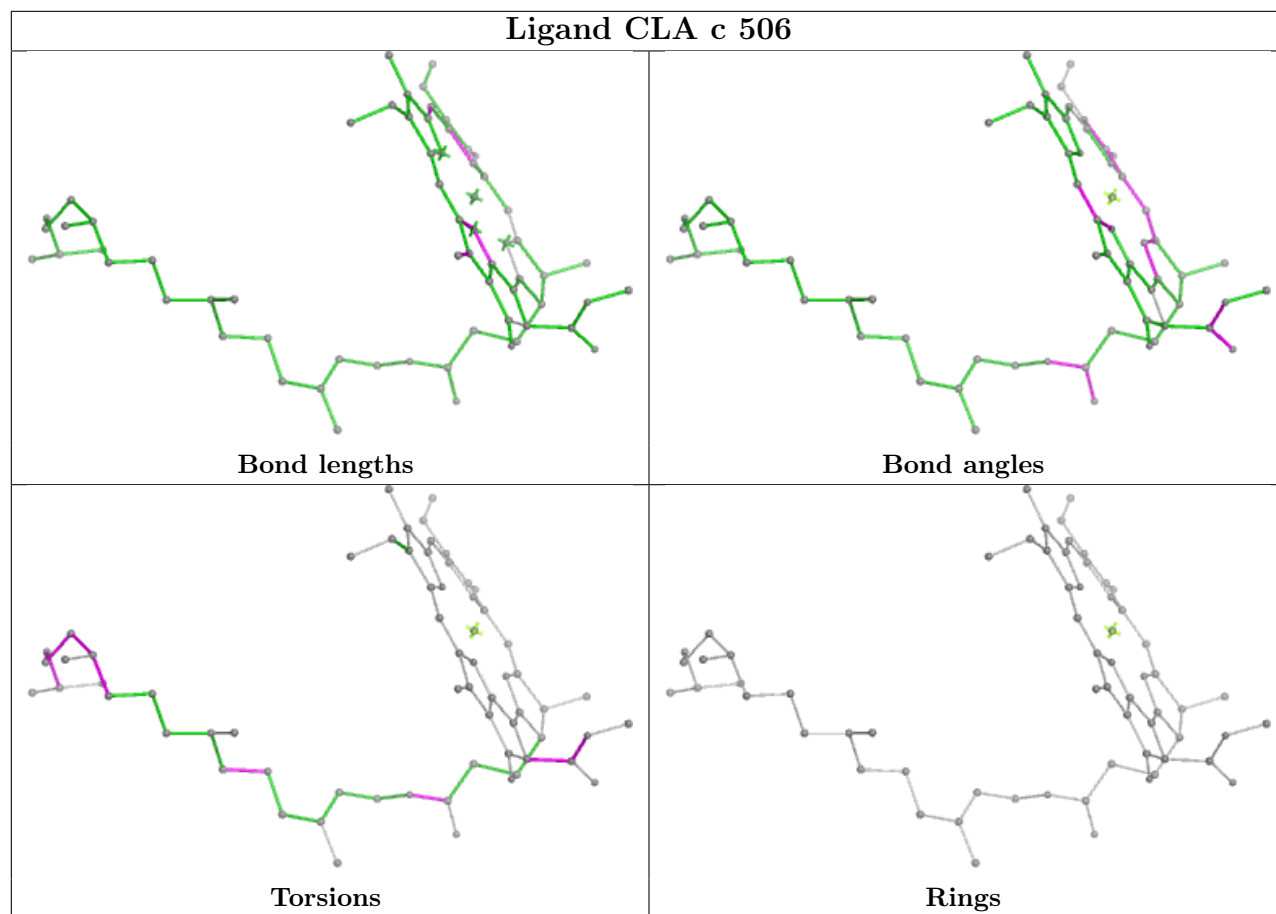




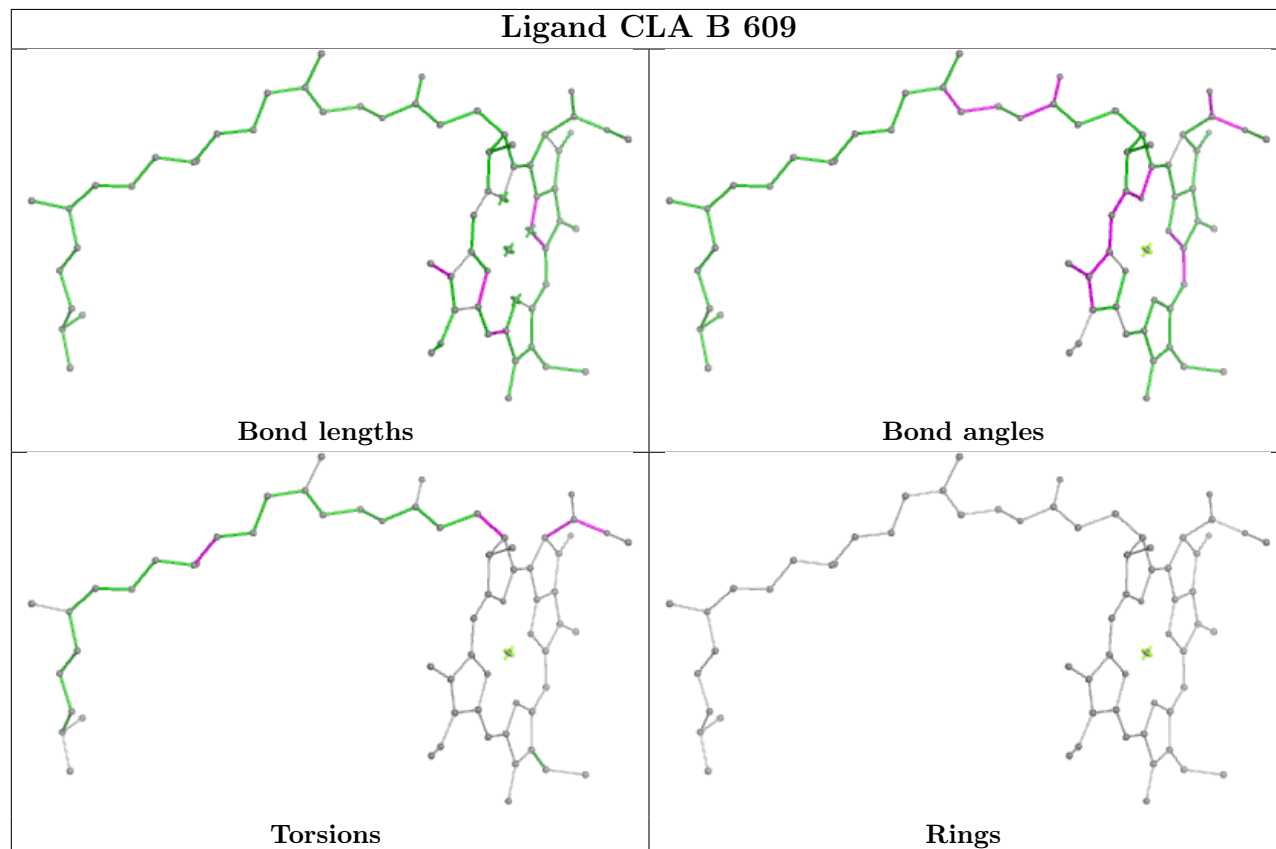


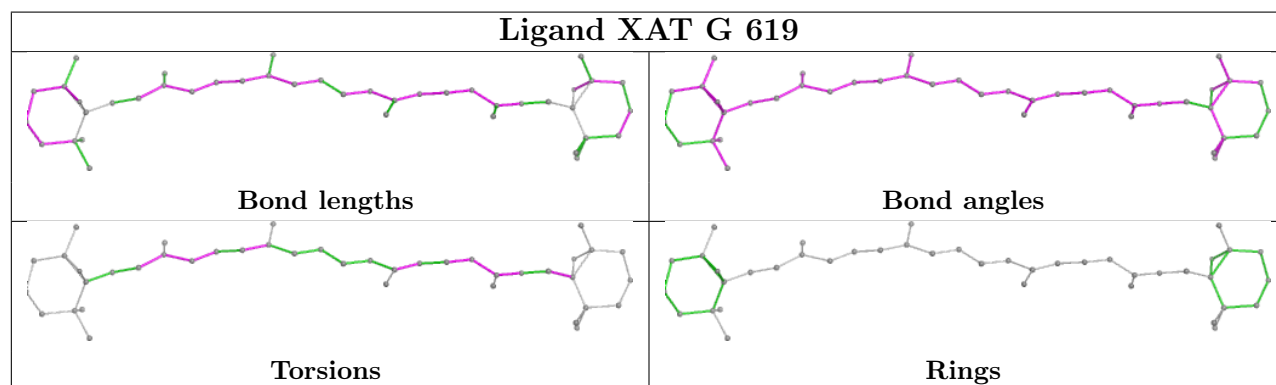
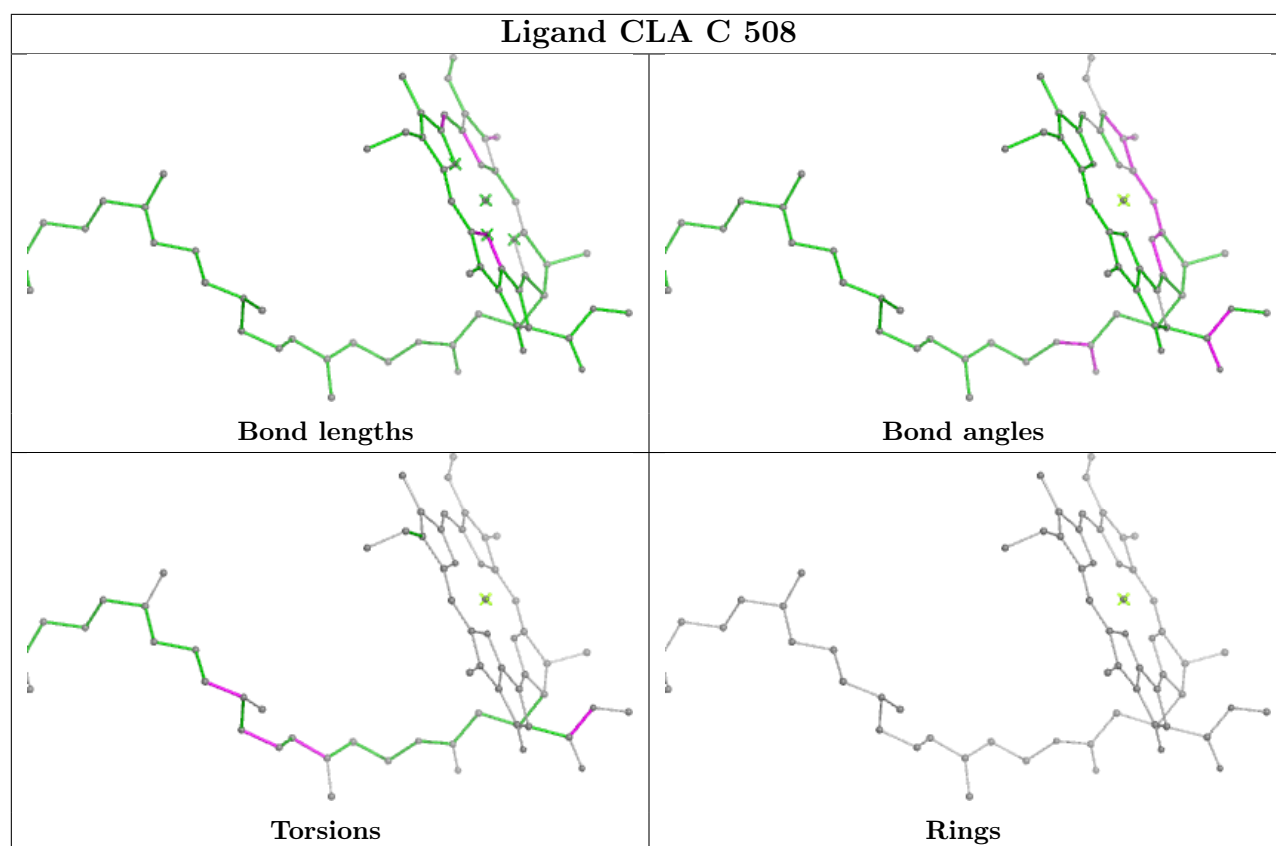


## Ligand CLA c 506



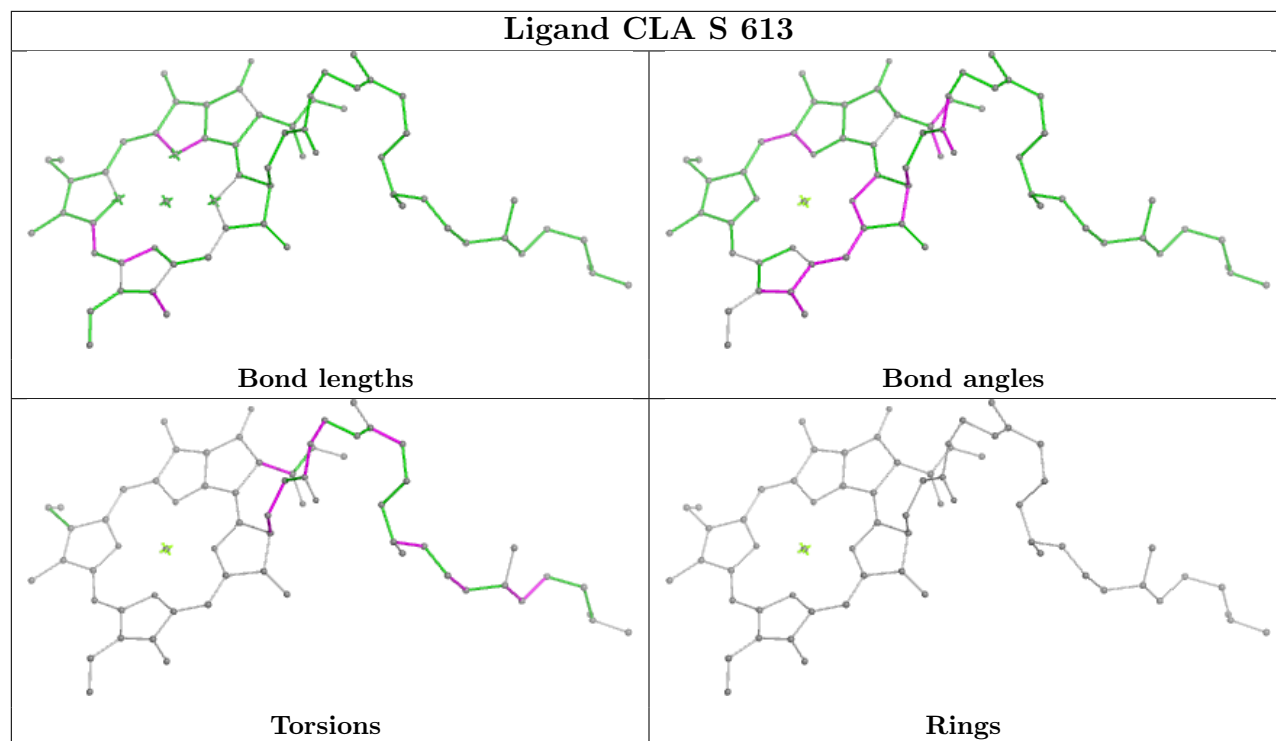
## Ligand CLA B 609



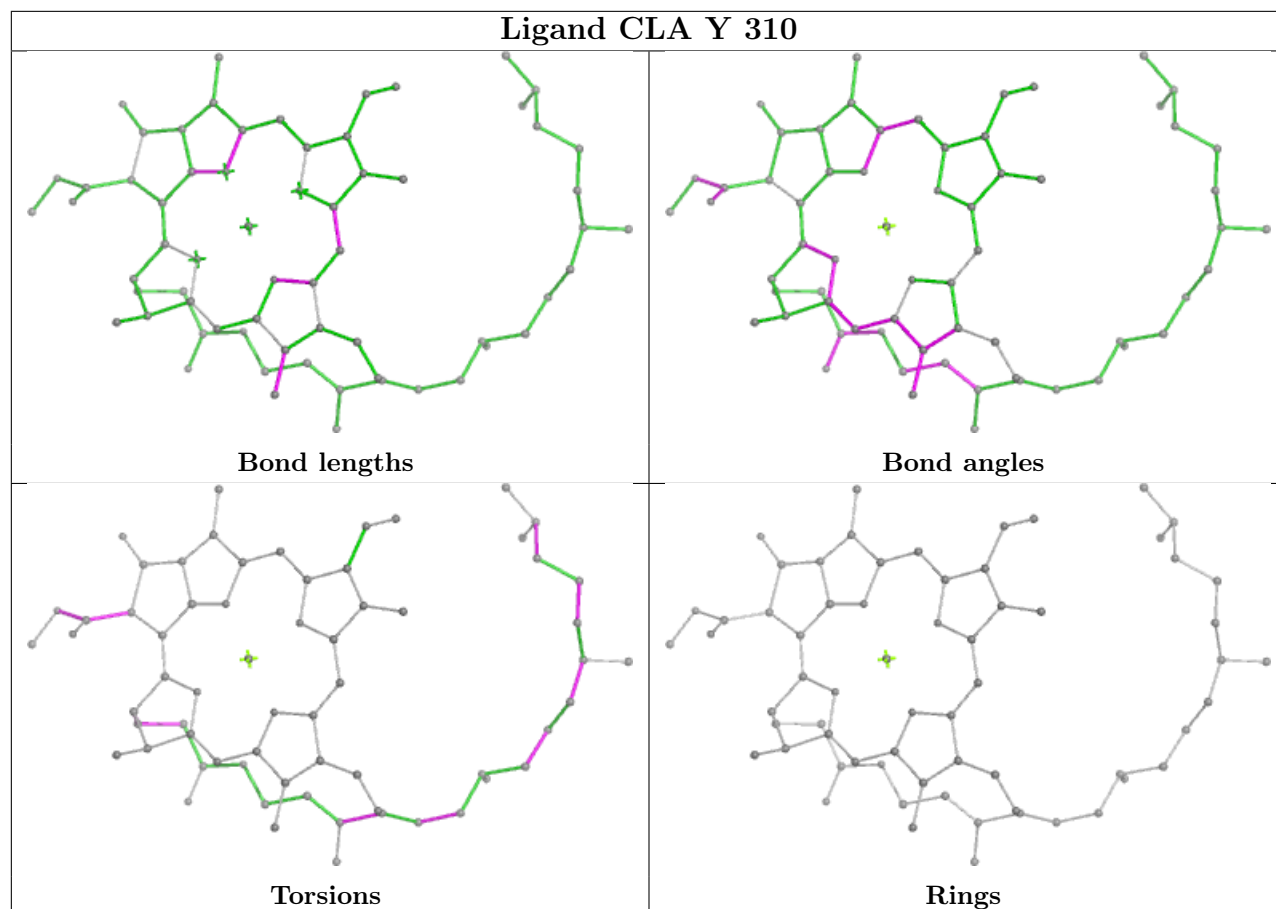




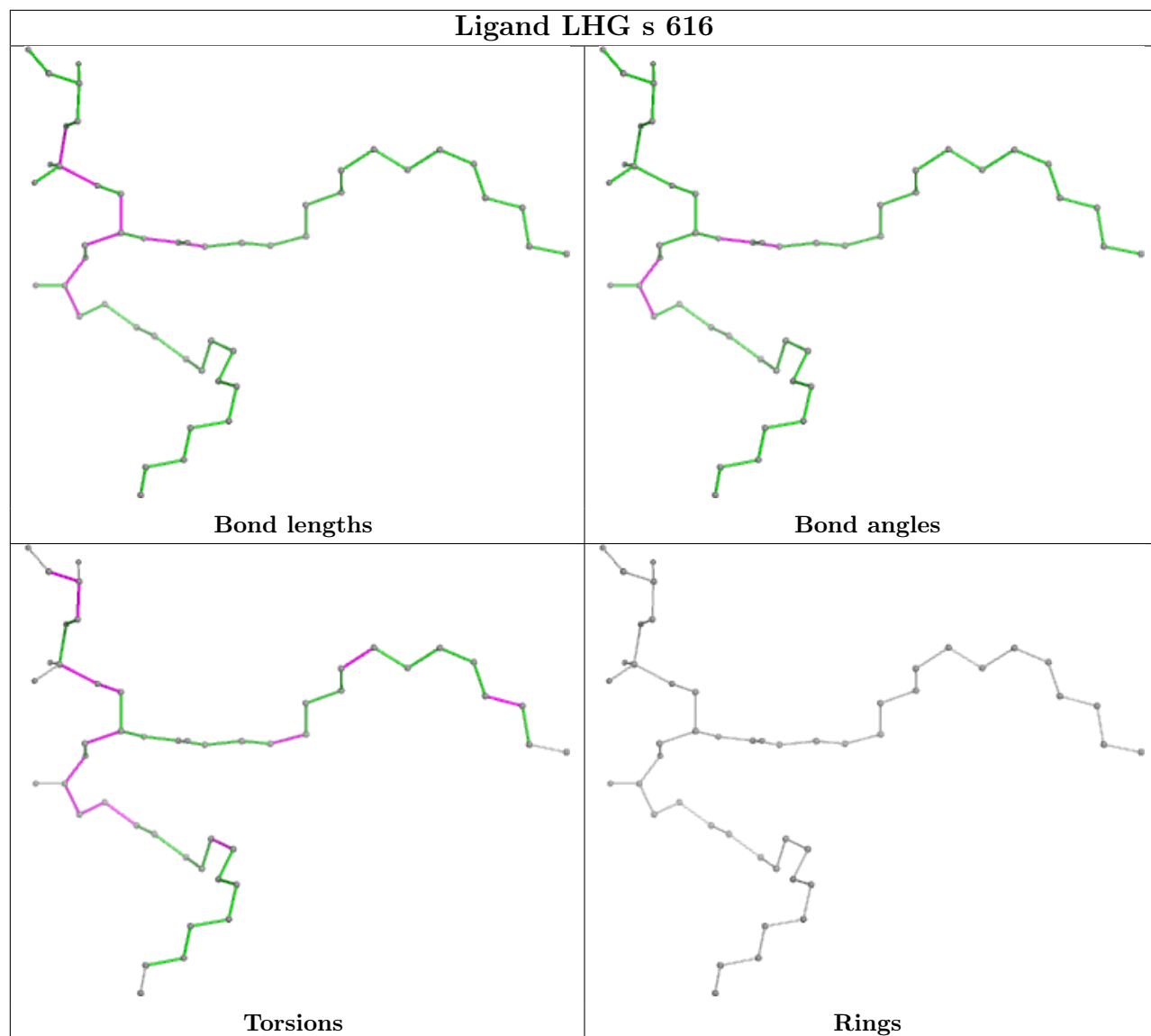
## Ligand CLA S 613

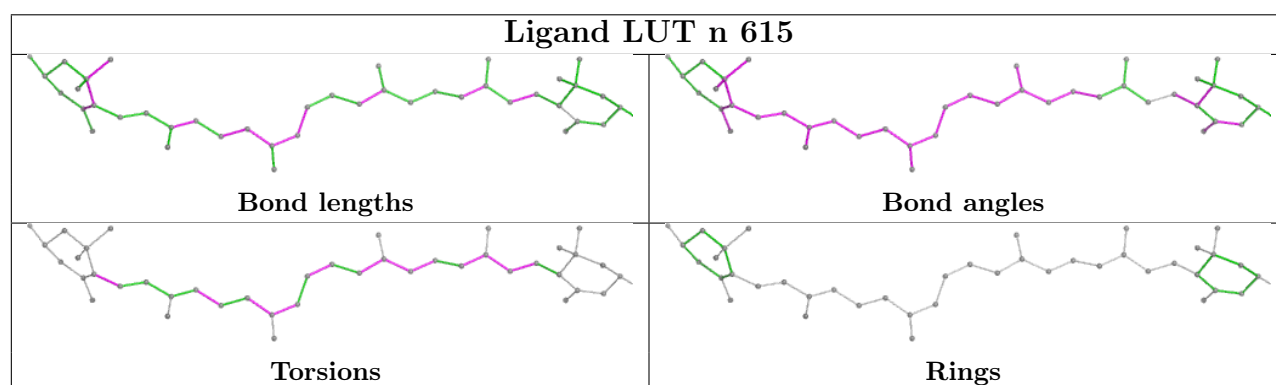
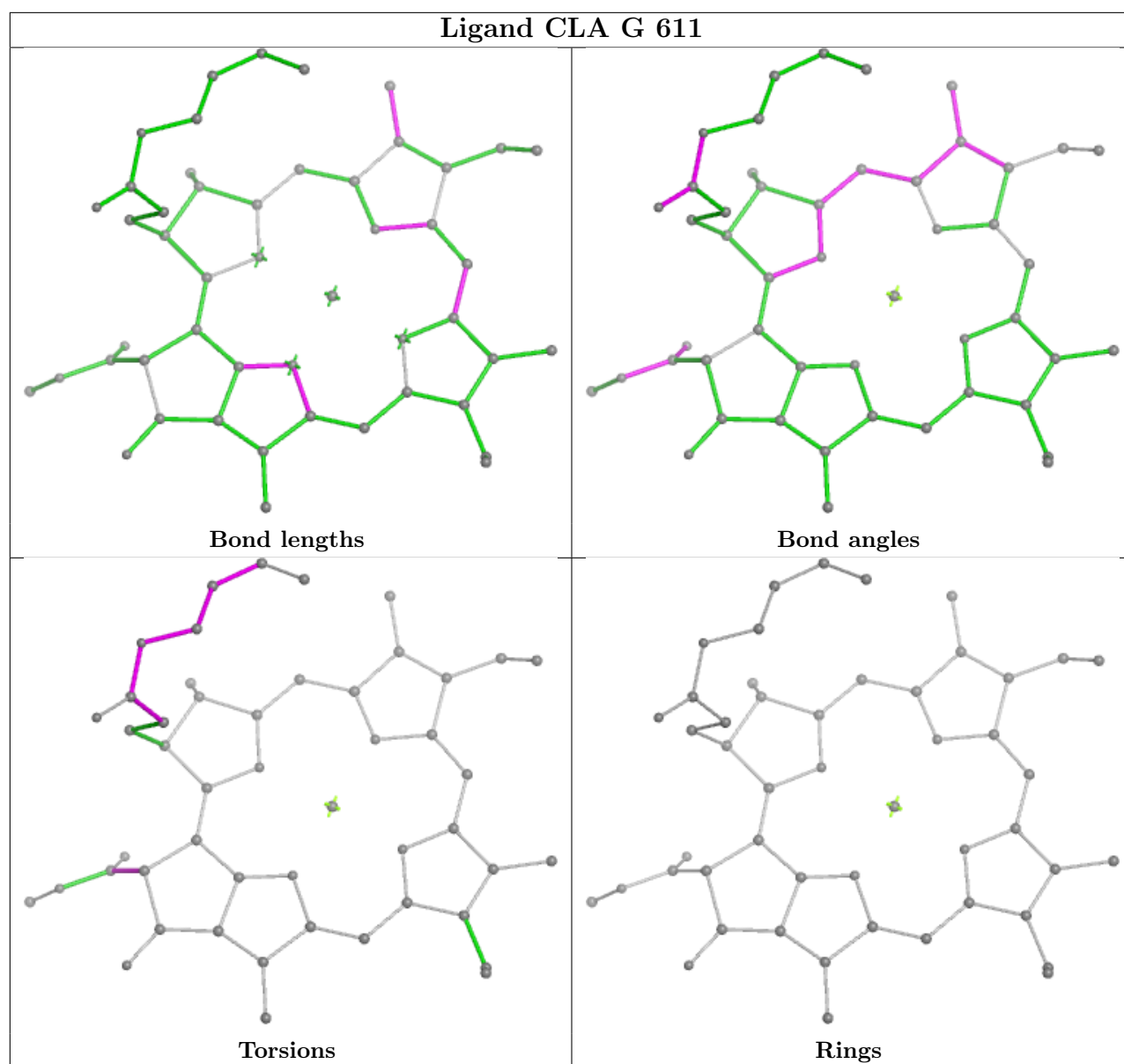


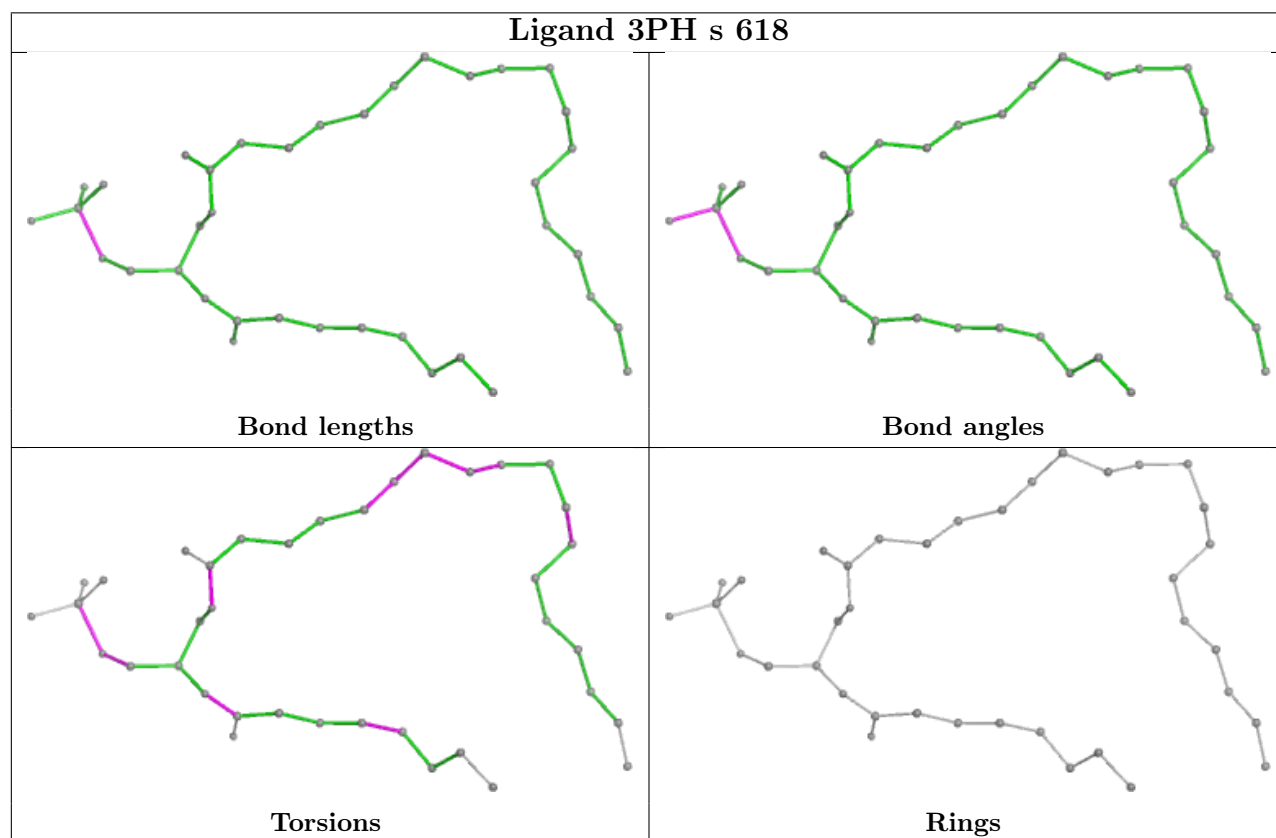
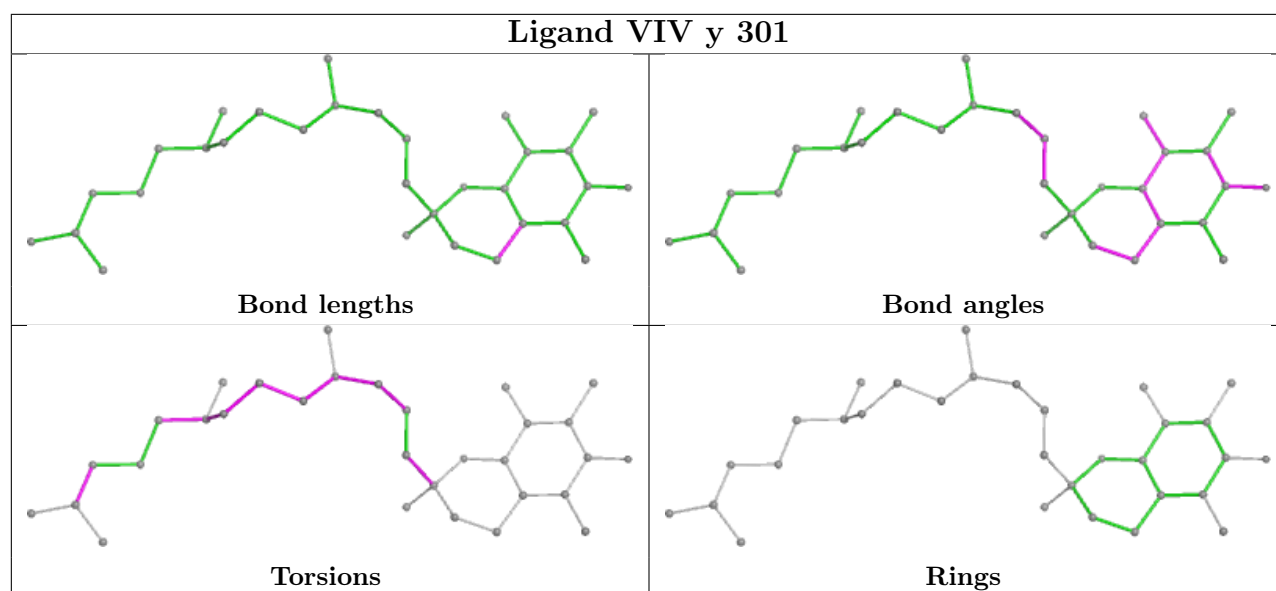
## Ligand CLA Y 310

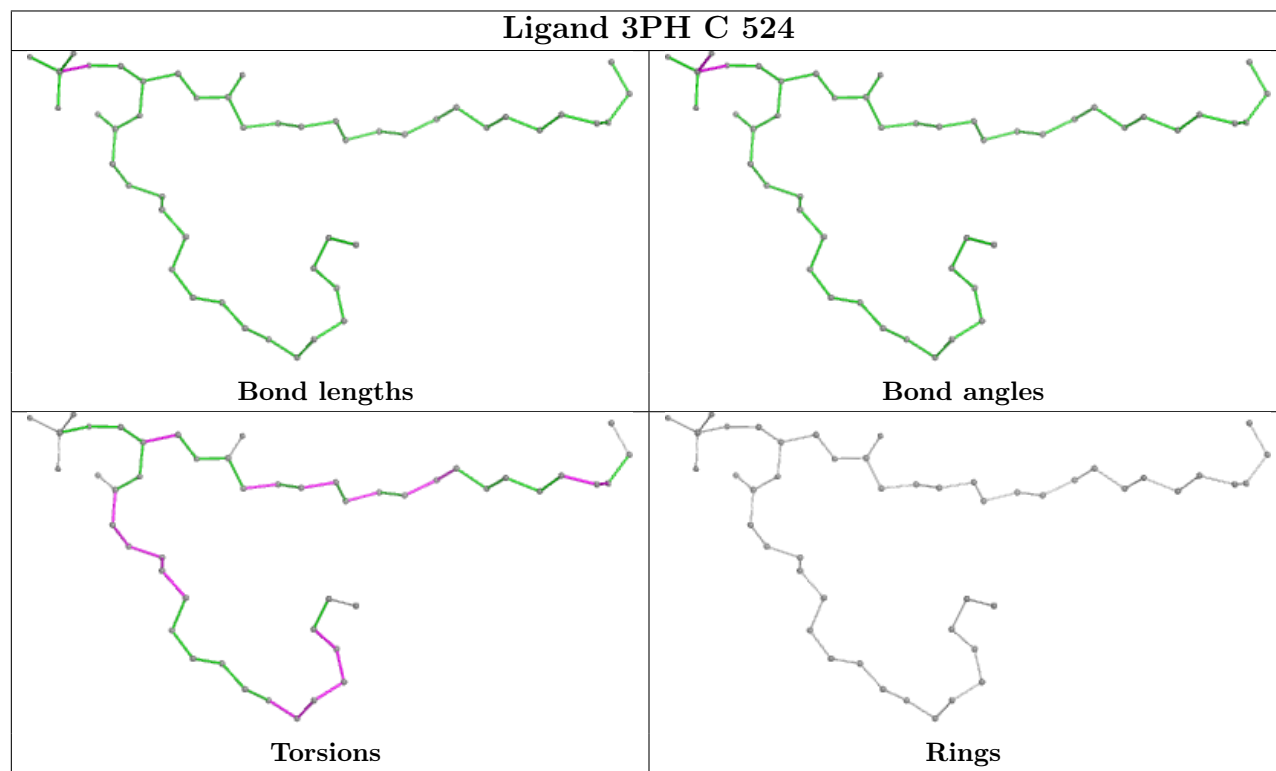
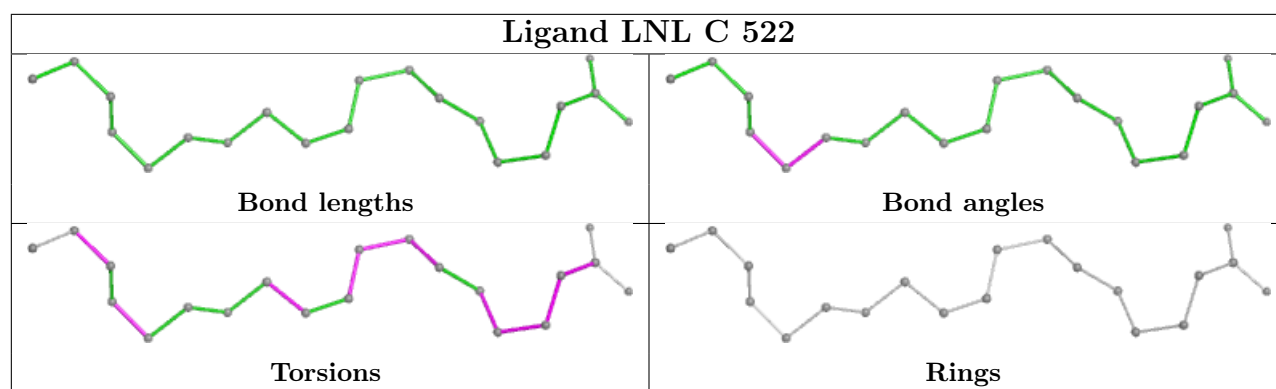


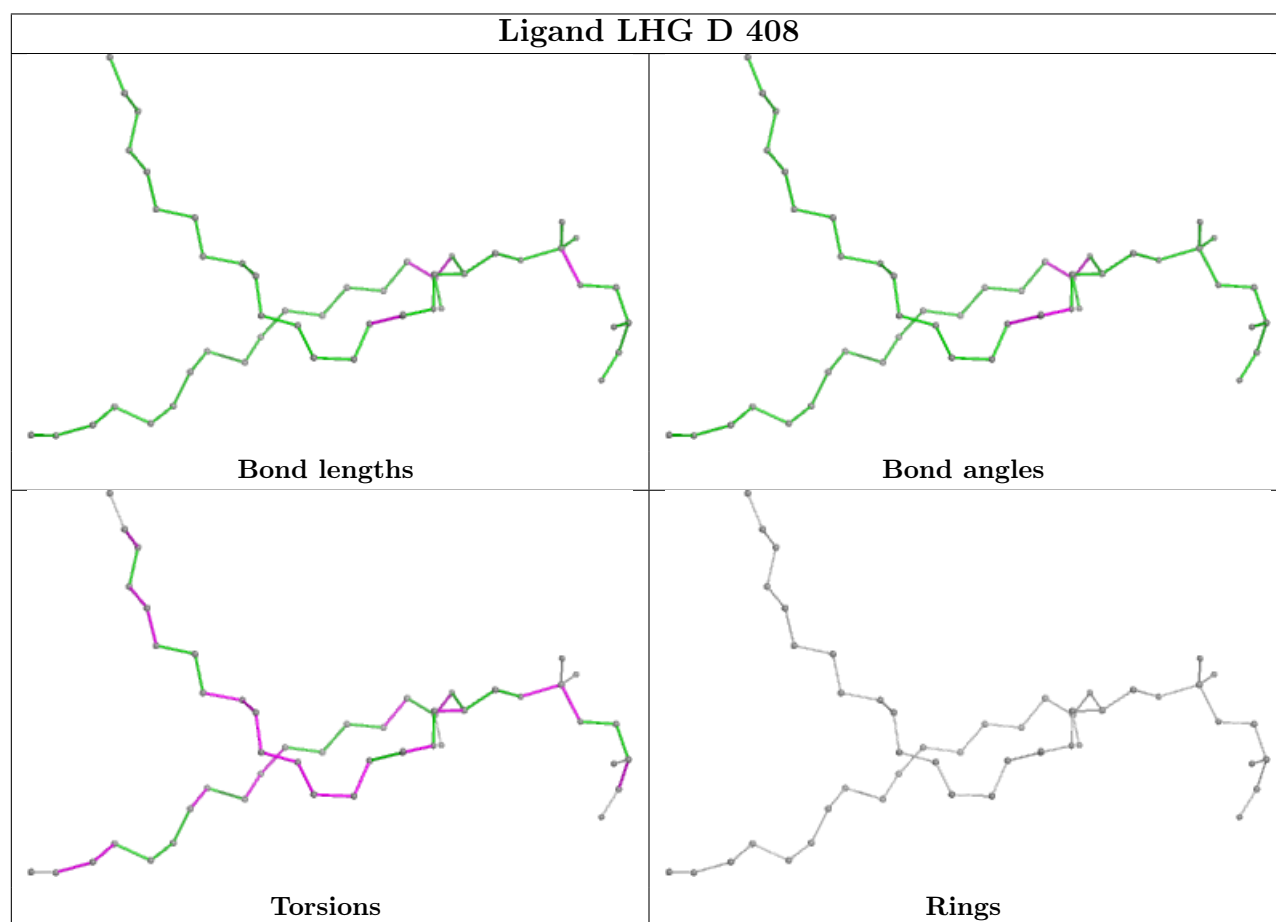
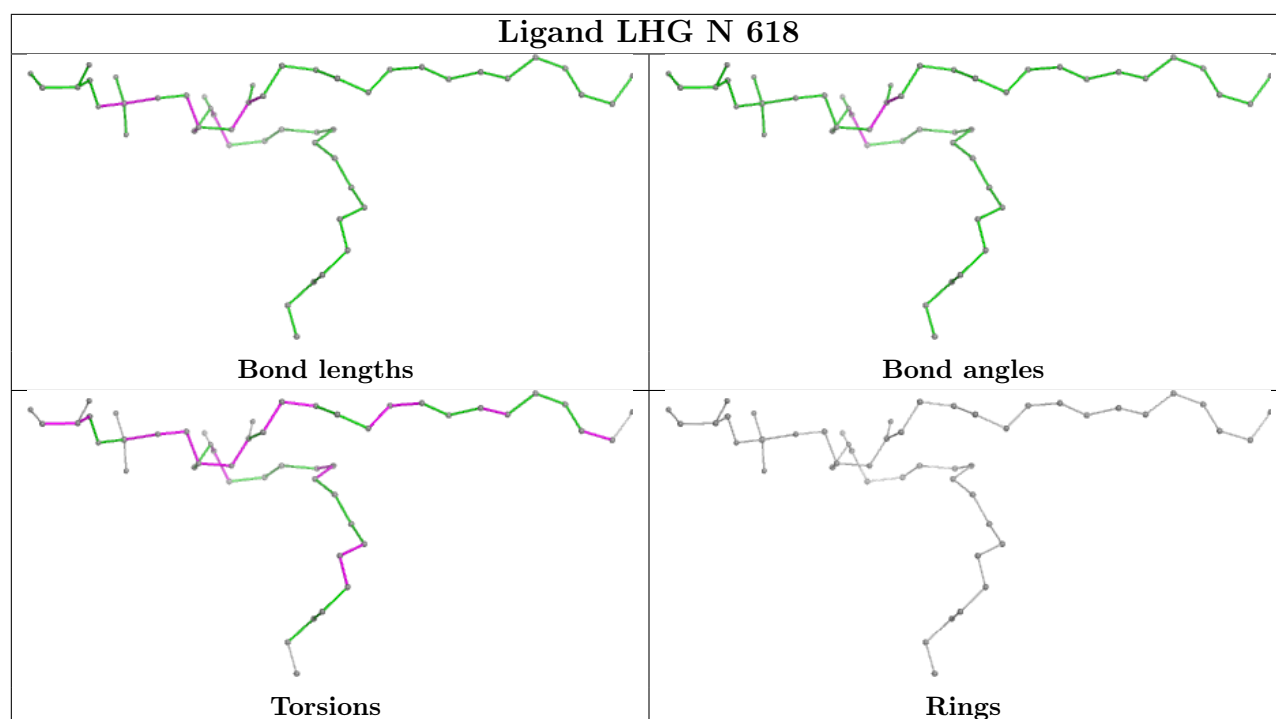
## Ligand LHG s 616

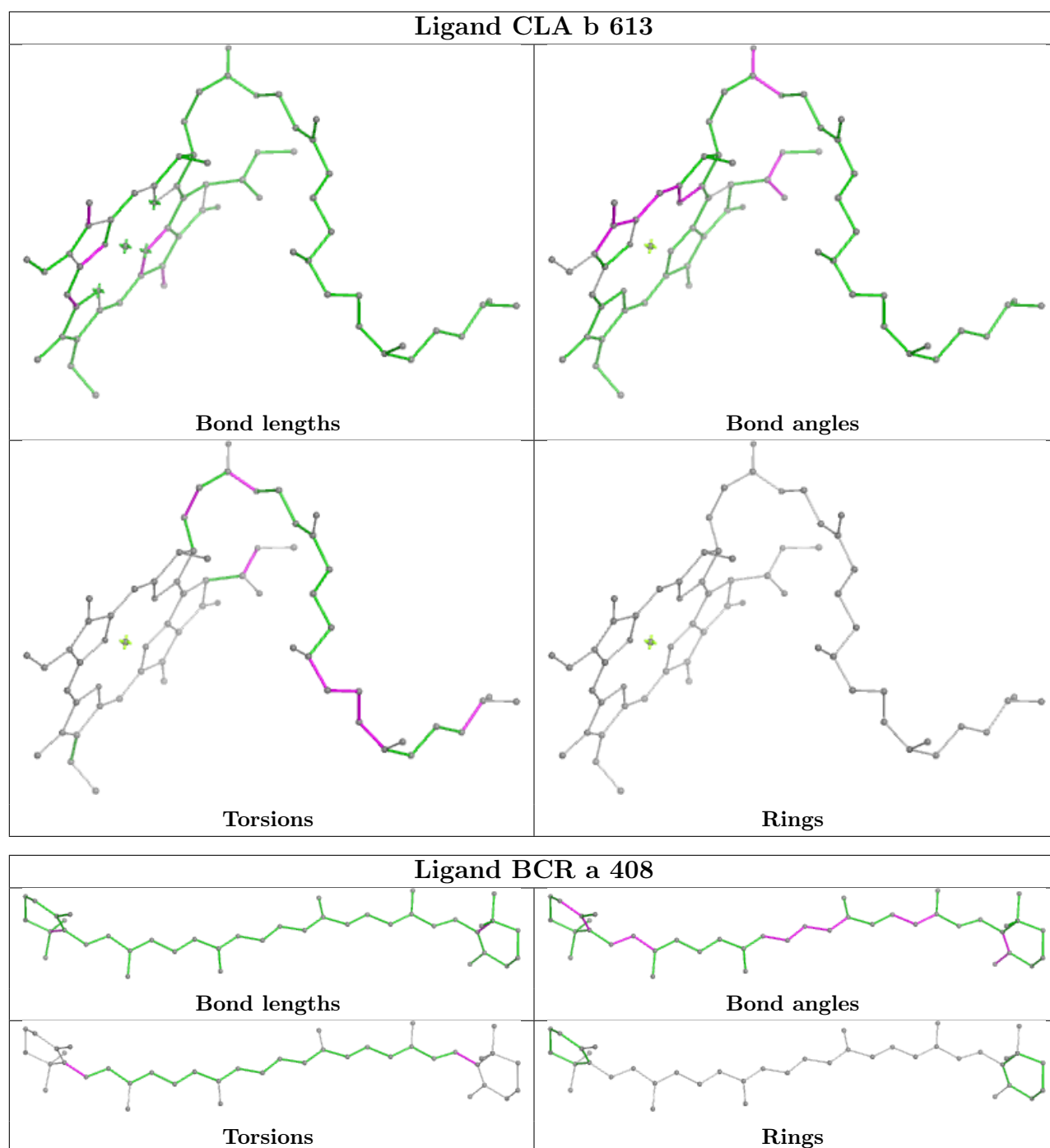




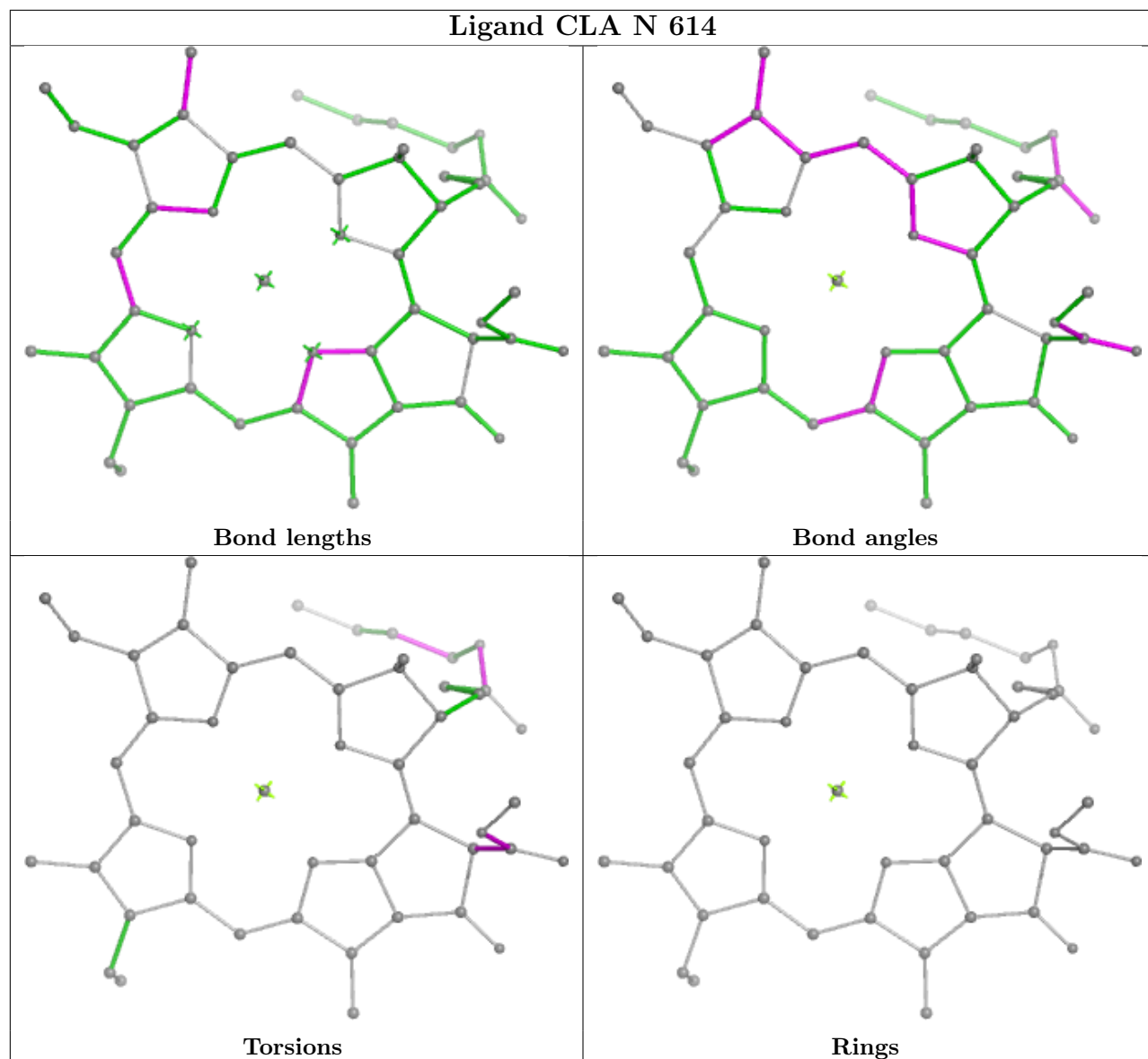






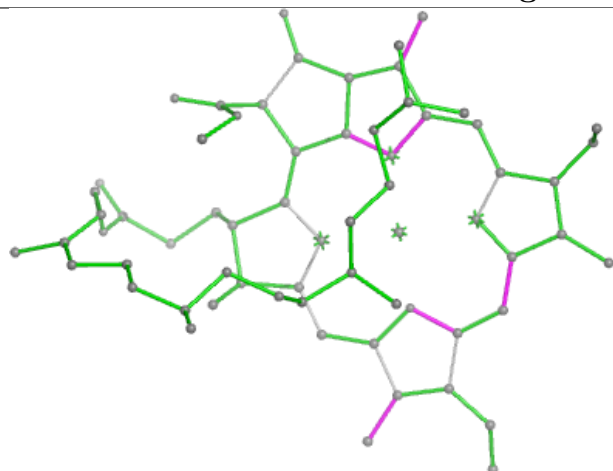


## Ligand CLA N 614

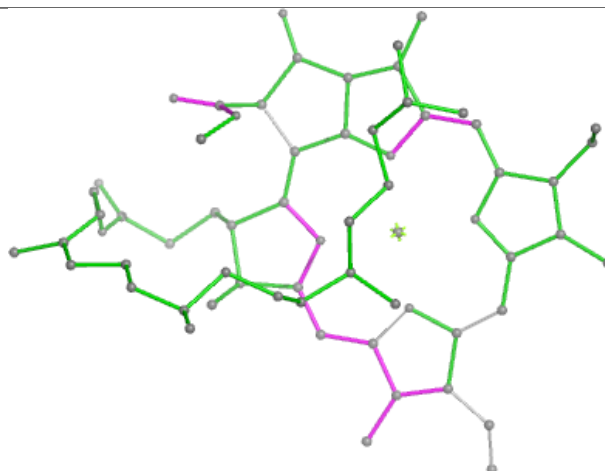




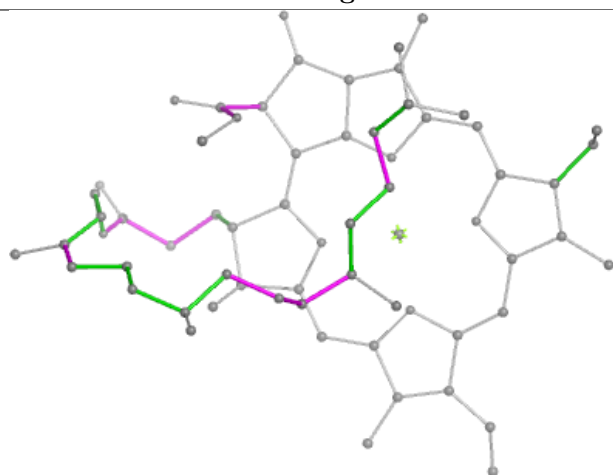
## Ligand CLA c 510



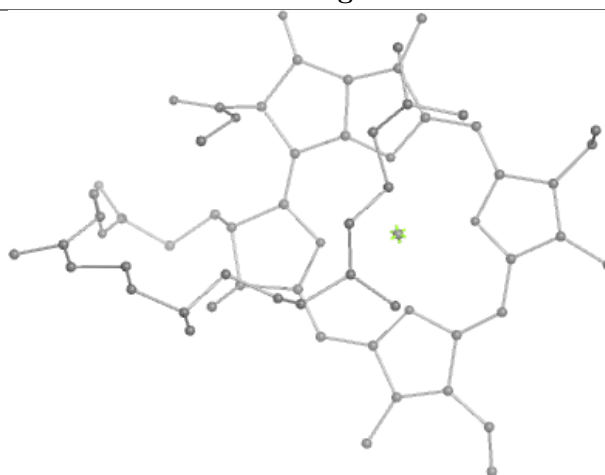
Bond lengths



Bond angles

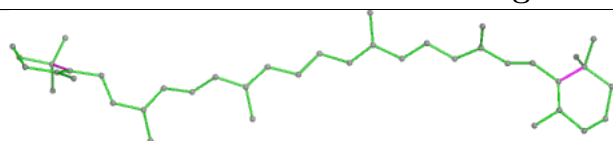


Torsions

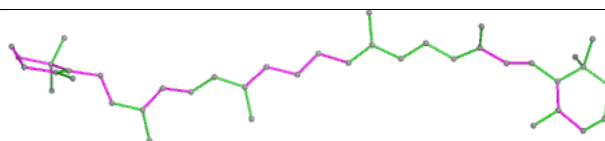


Rings

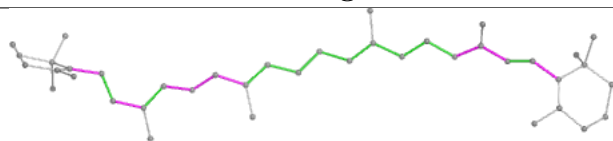
## Ligand BCR B 617



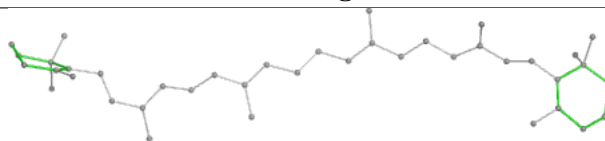
Bond lengths



Bond angles

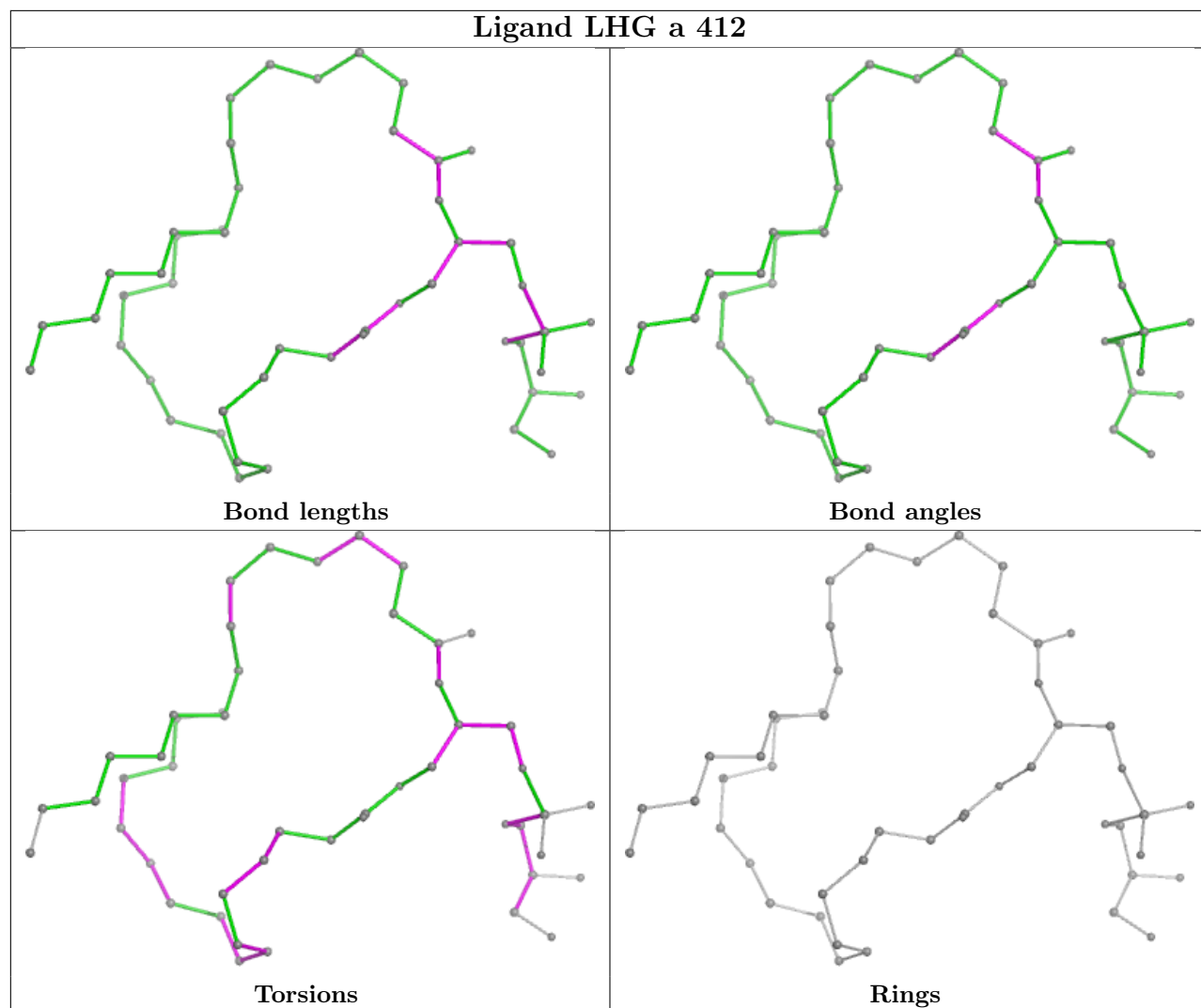


Torsions

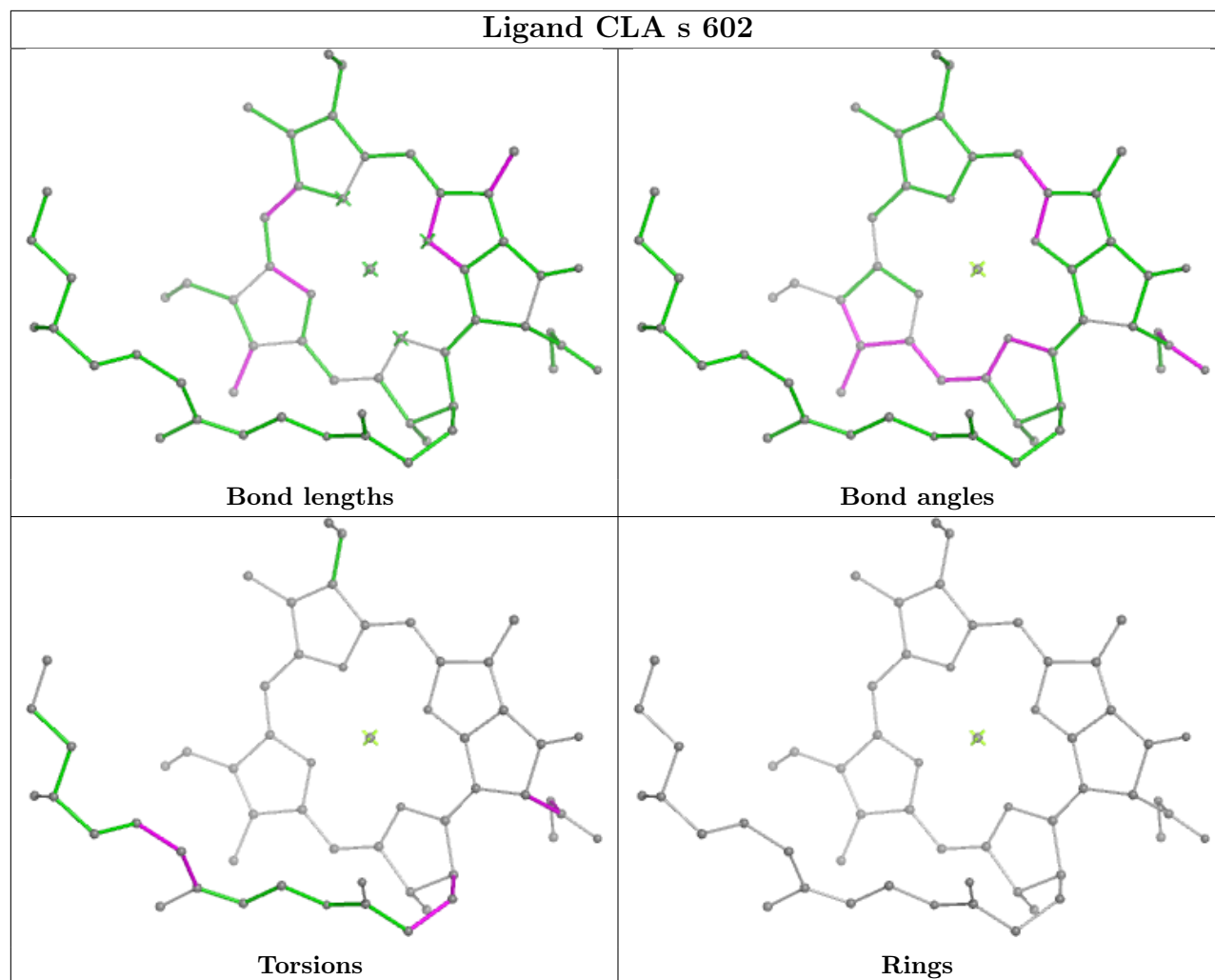


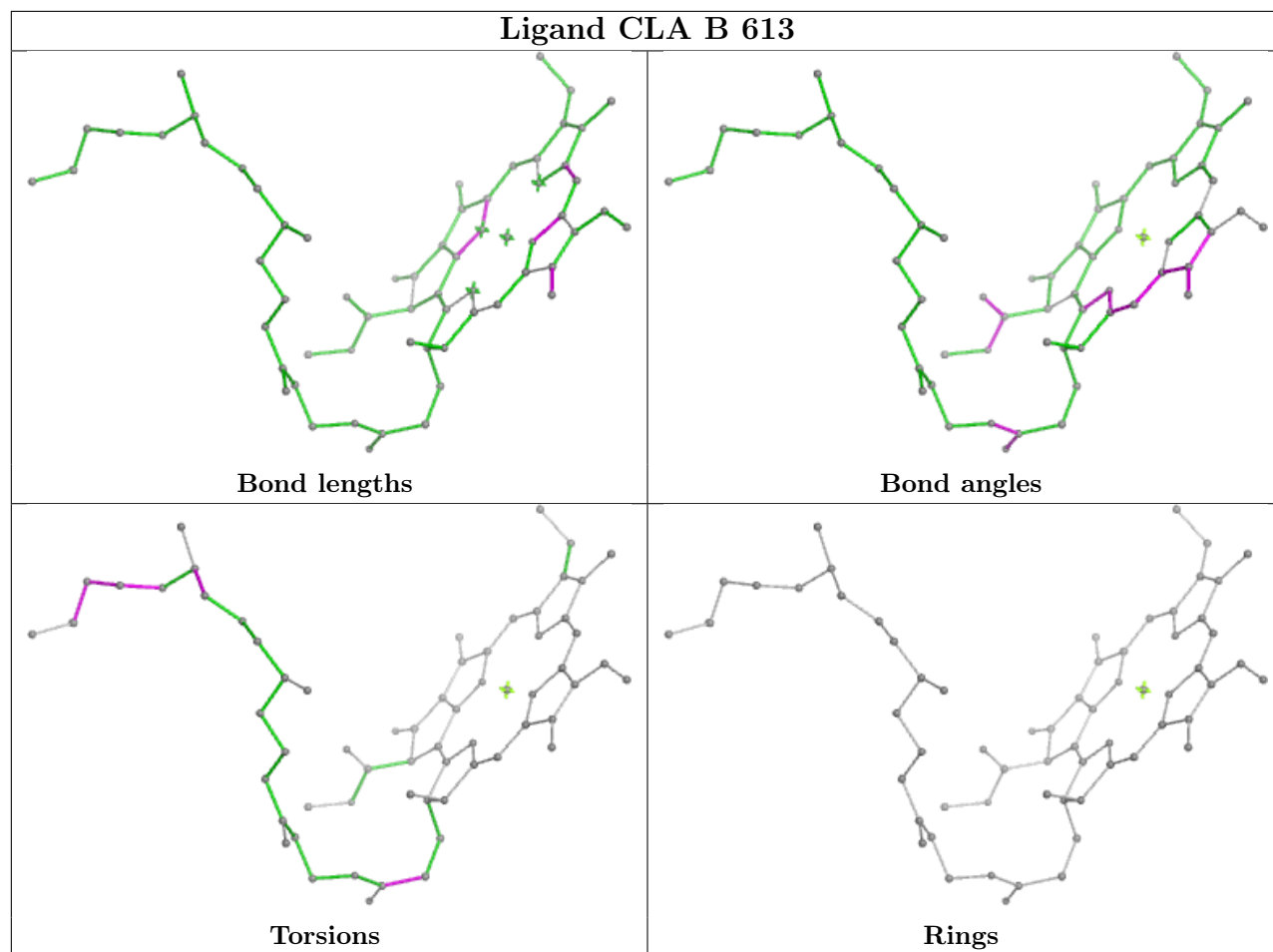
Rings

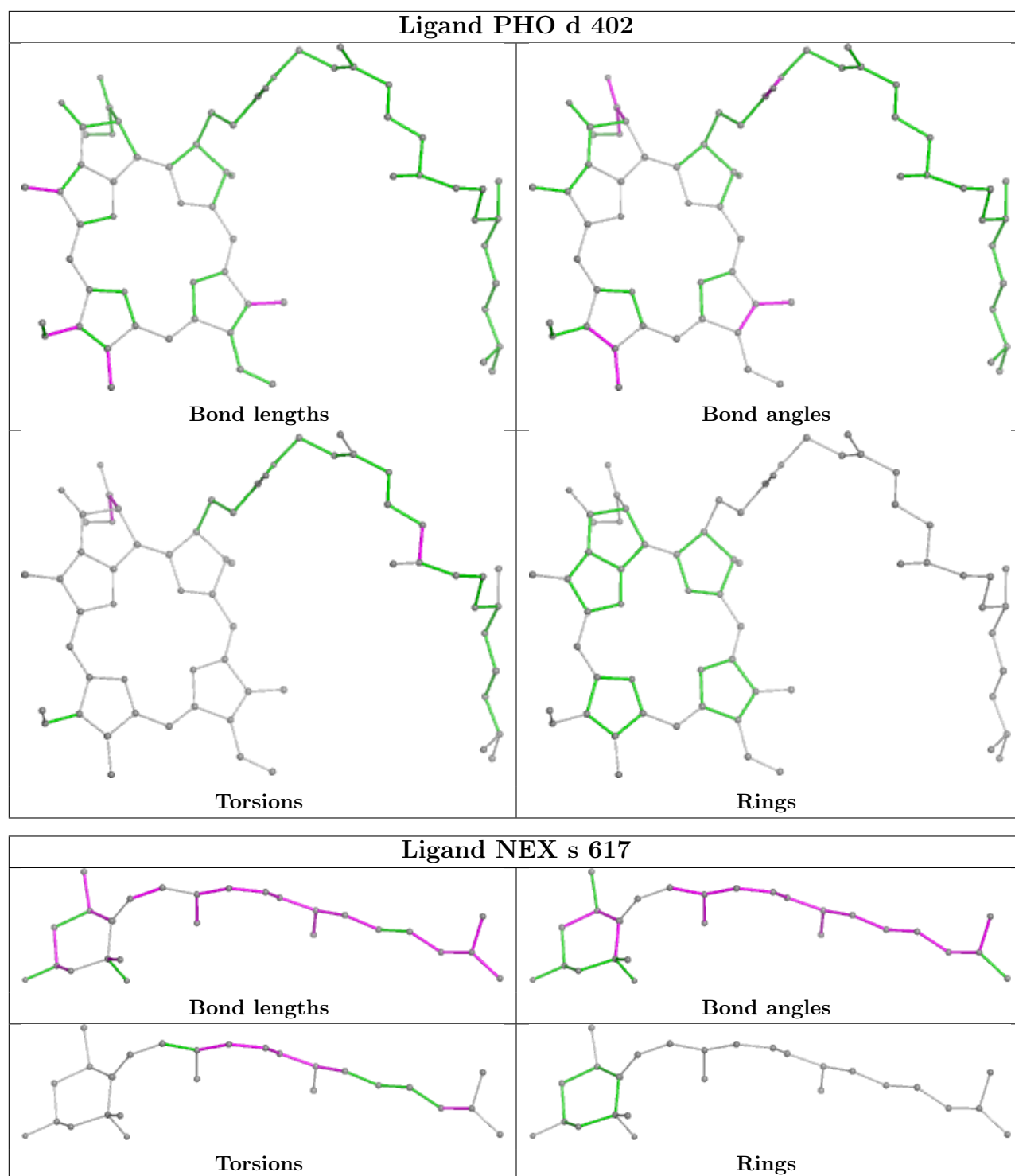
## Ligand LHG a 412

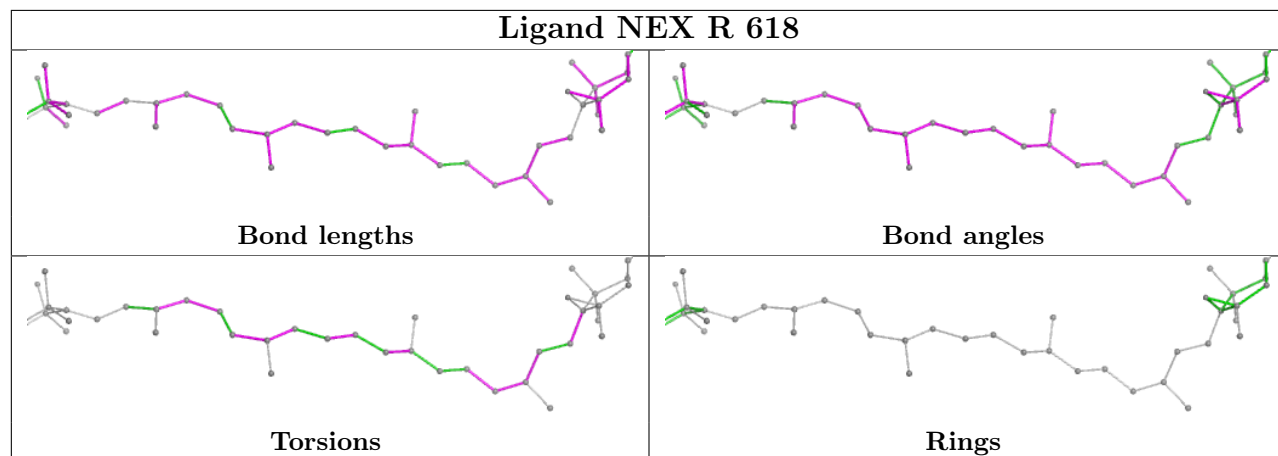
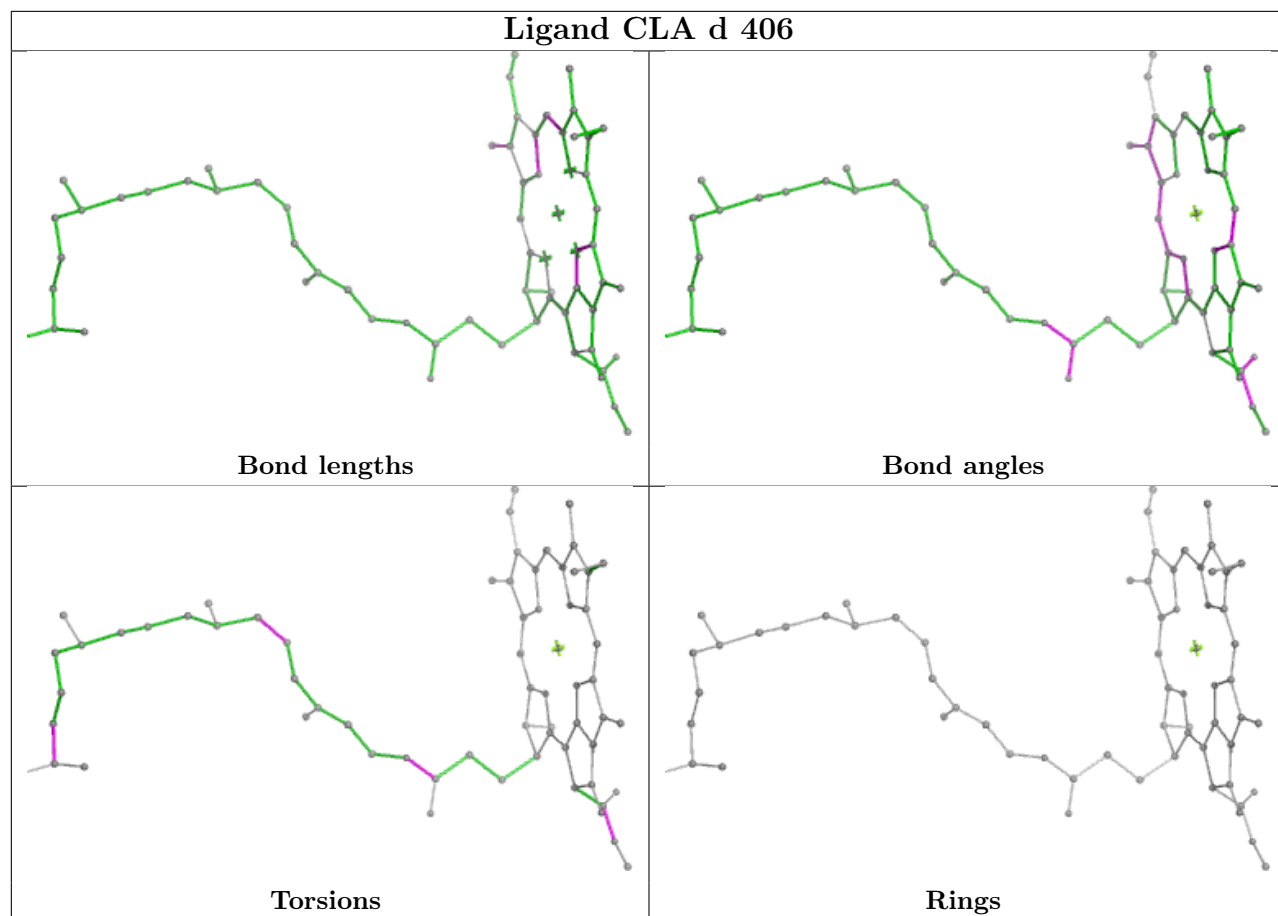


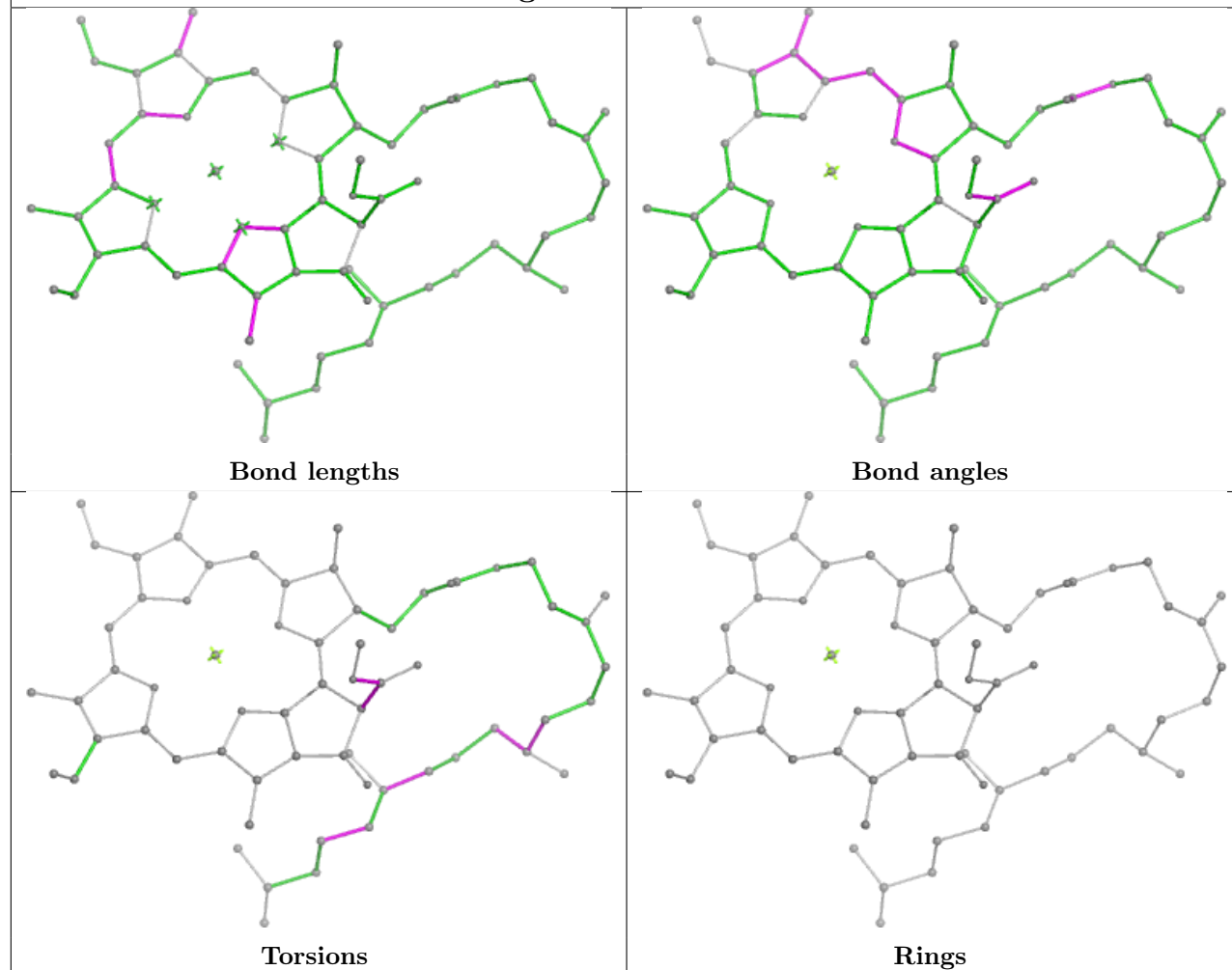
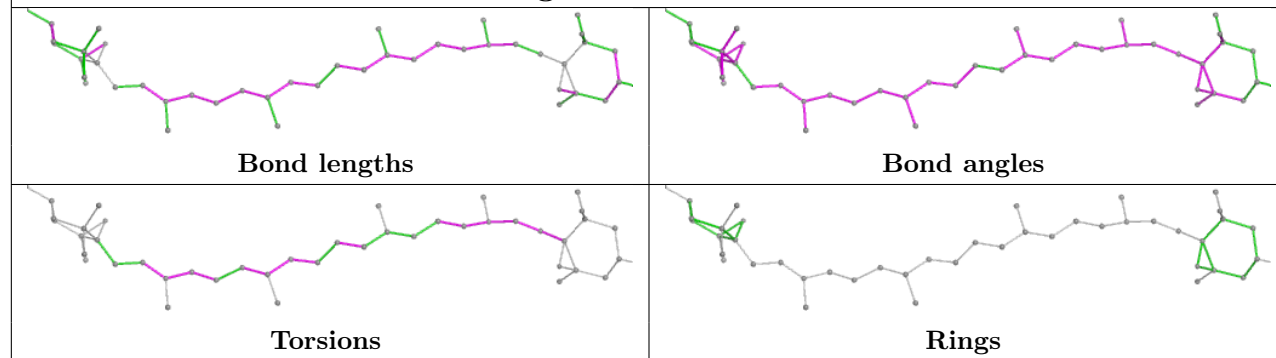
## Ligand CLA s 602

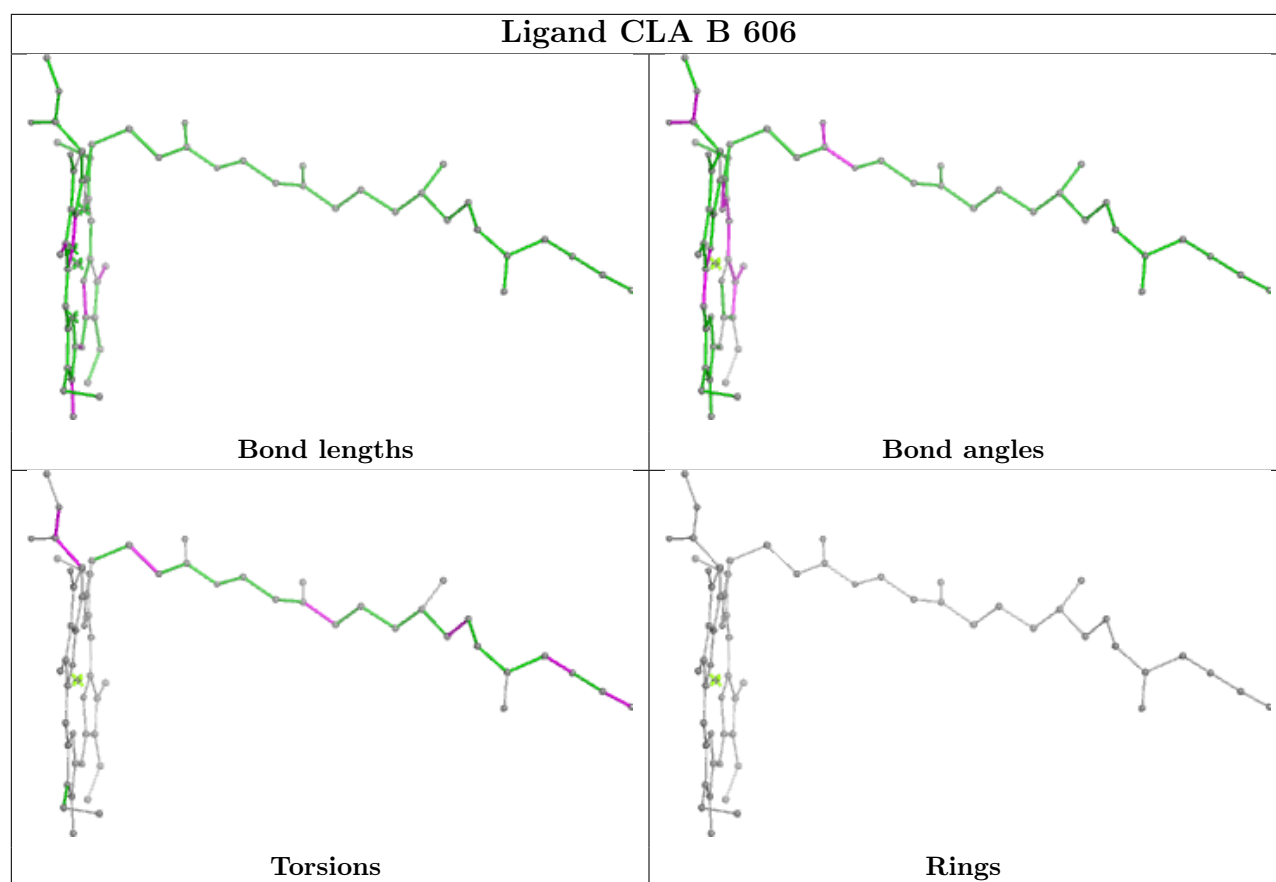






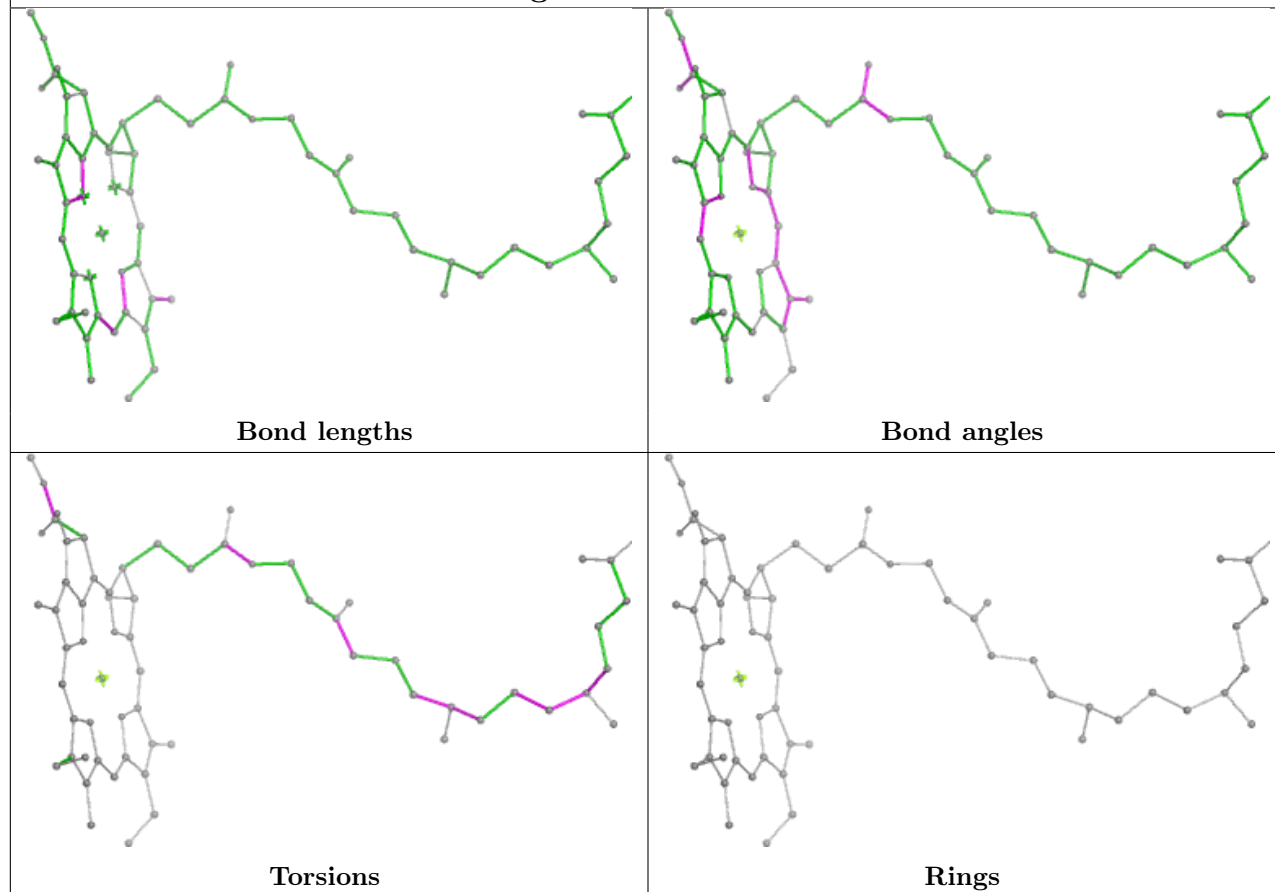


**Ligand CLA c 509****Ligand XAT r 615**

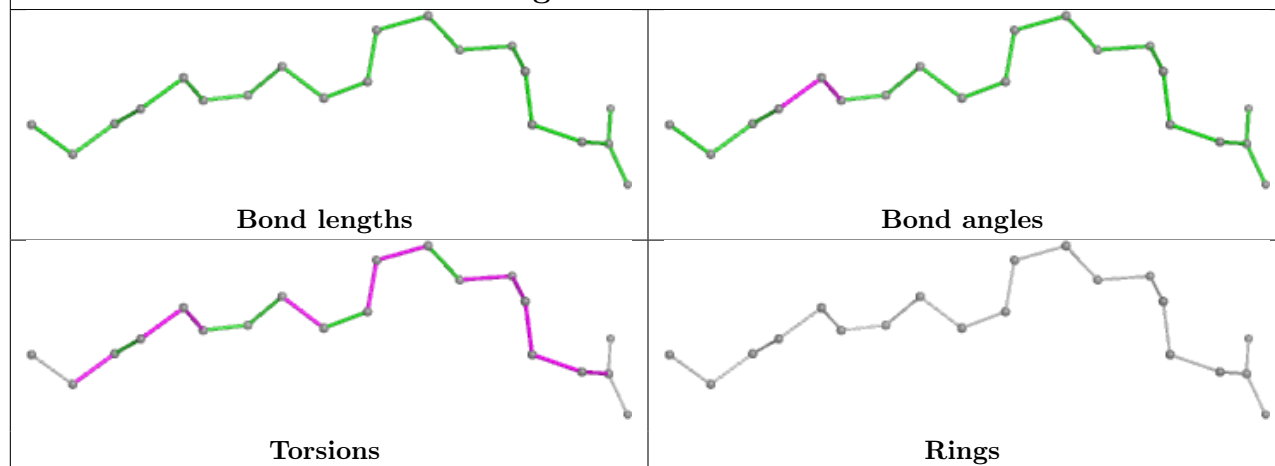


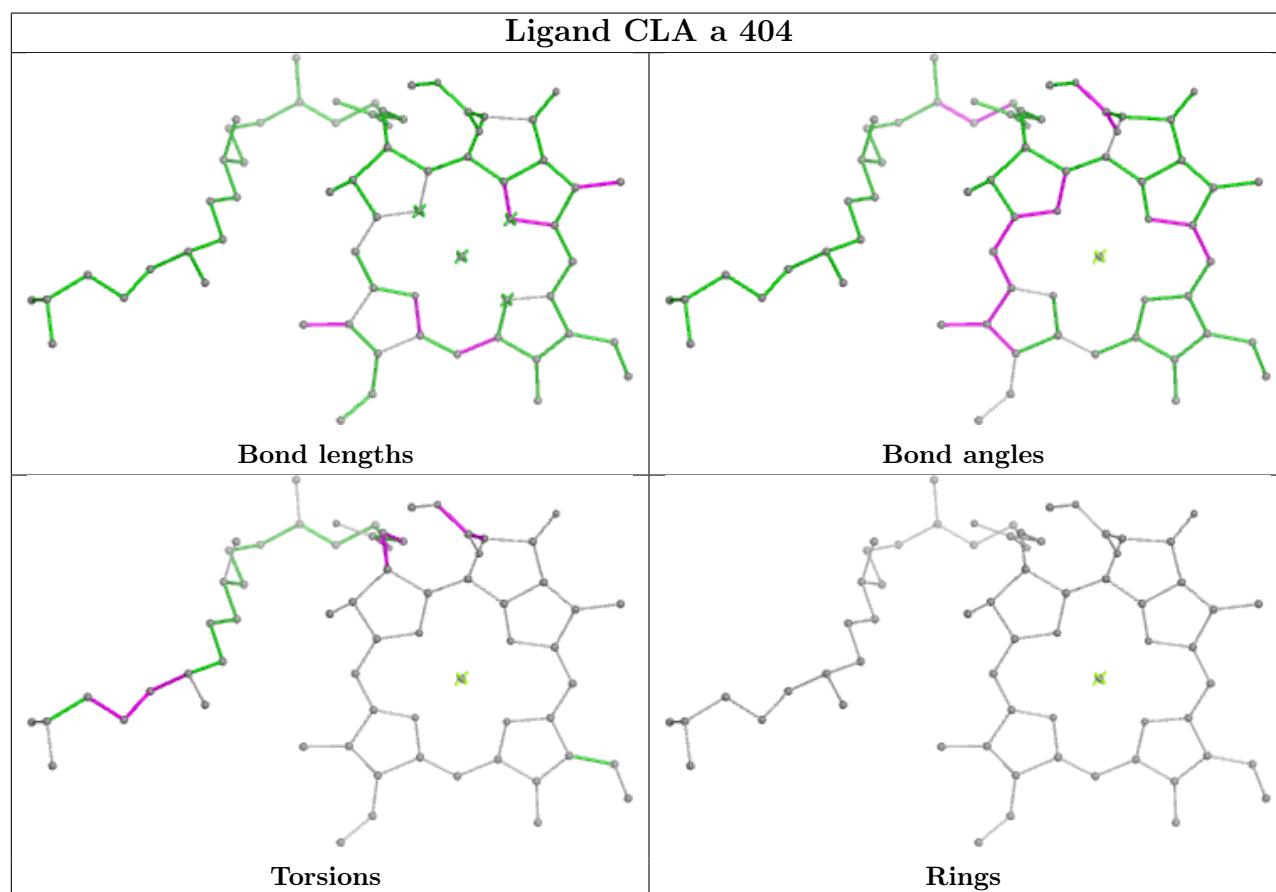
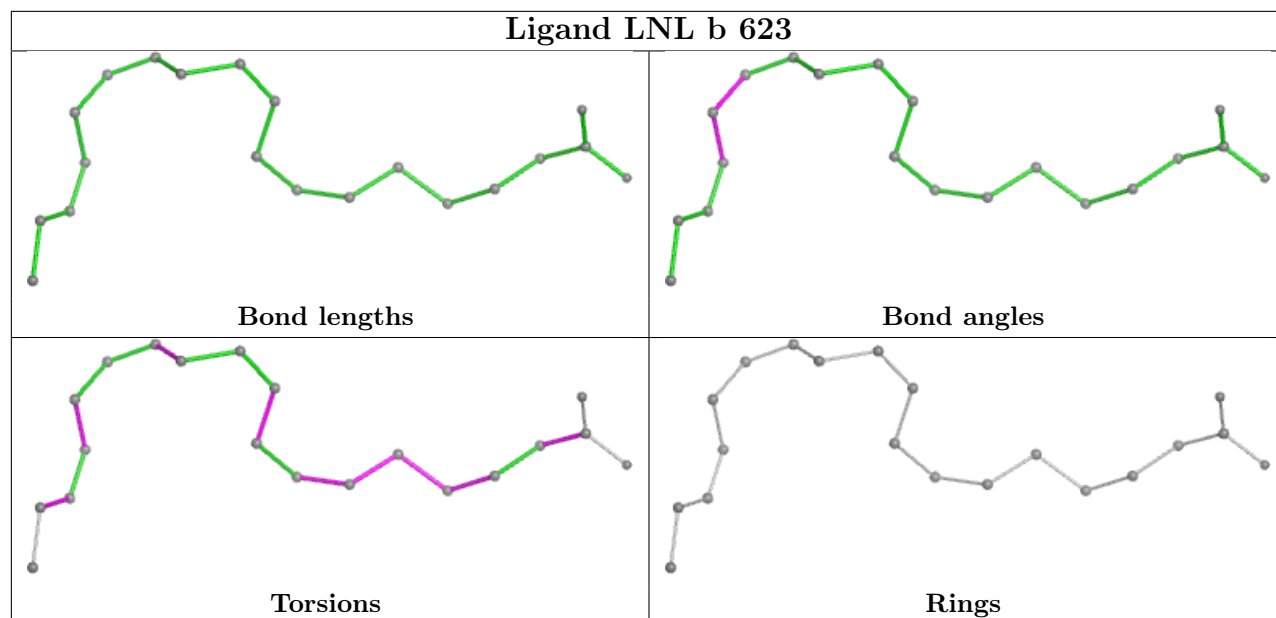


## Ligand CLA D 406

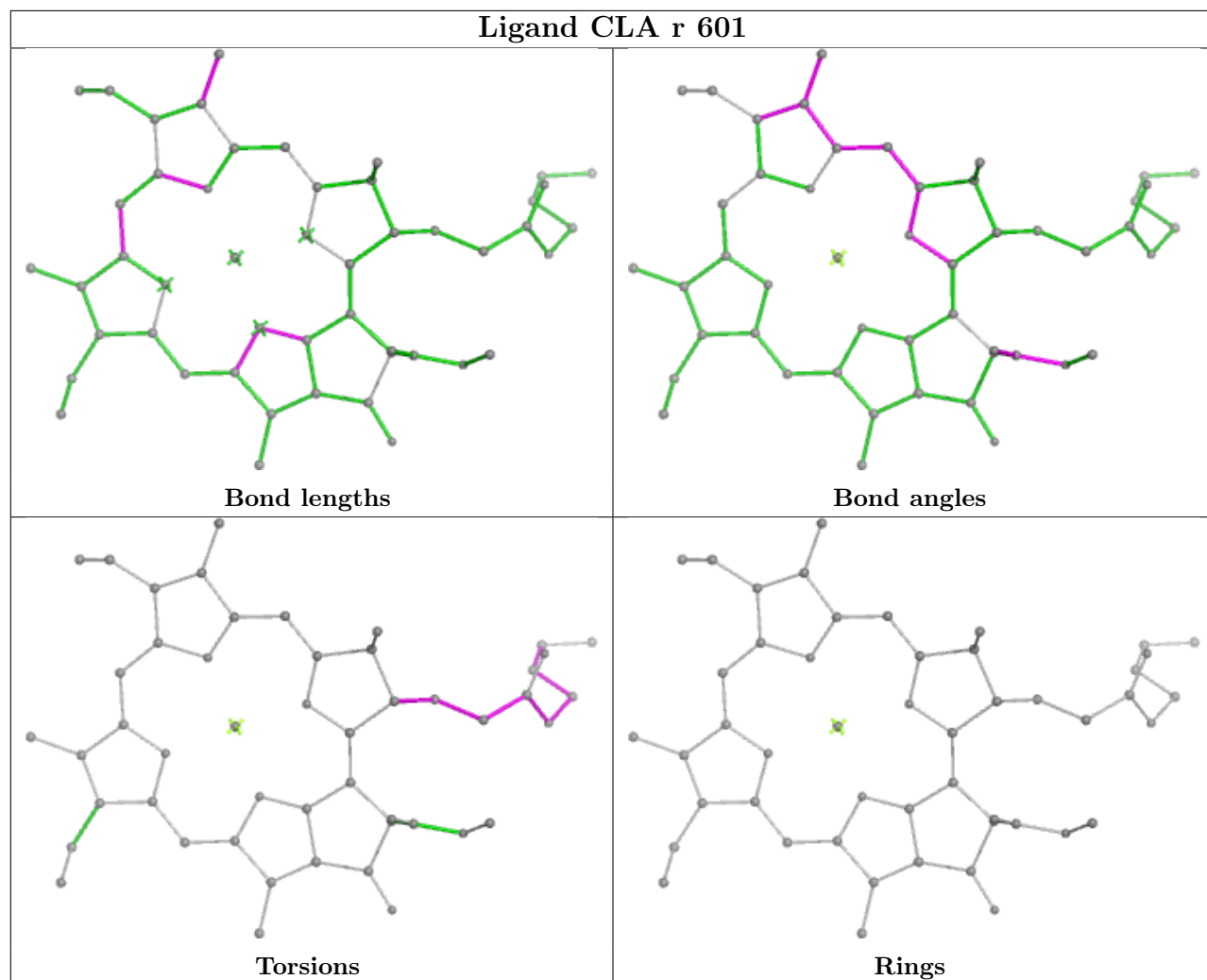


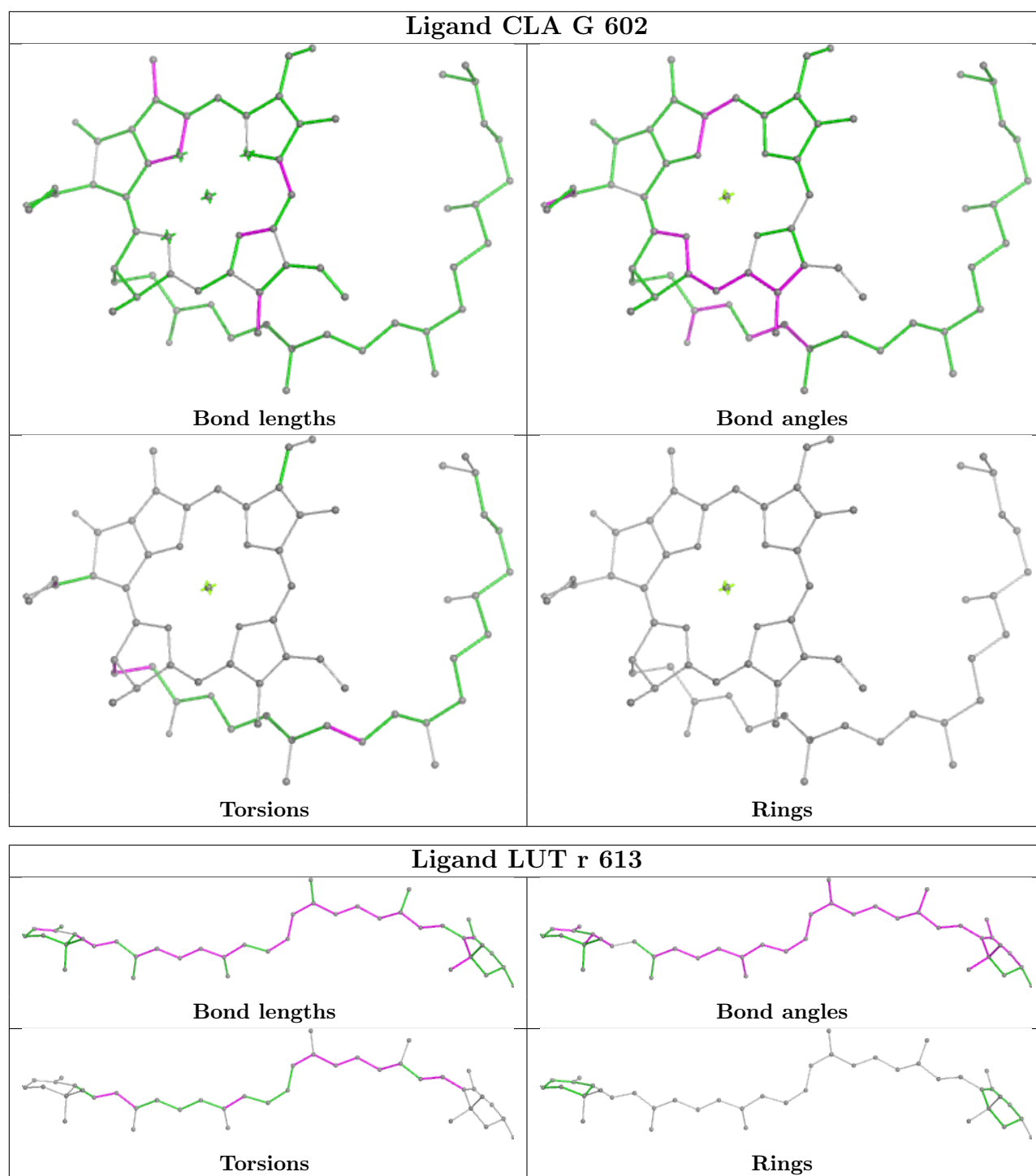
## Ligand LNL C 517

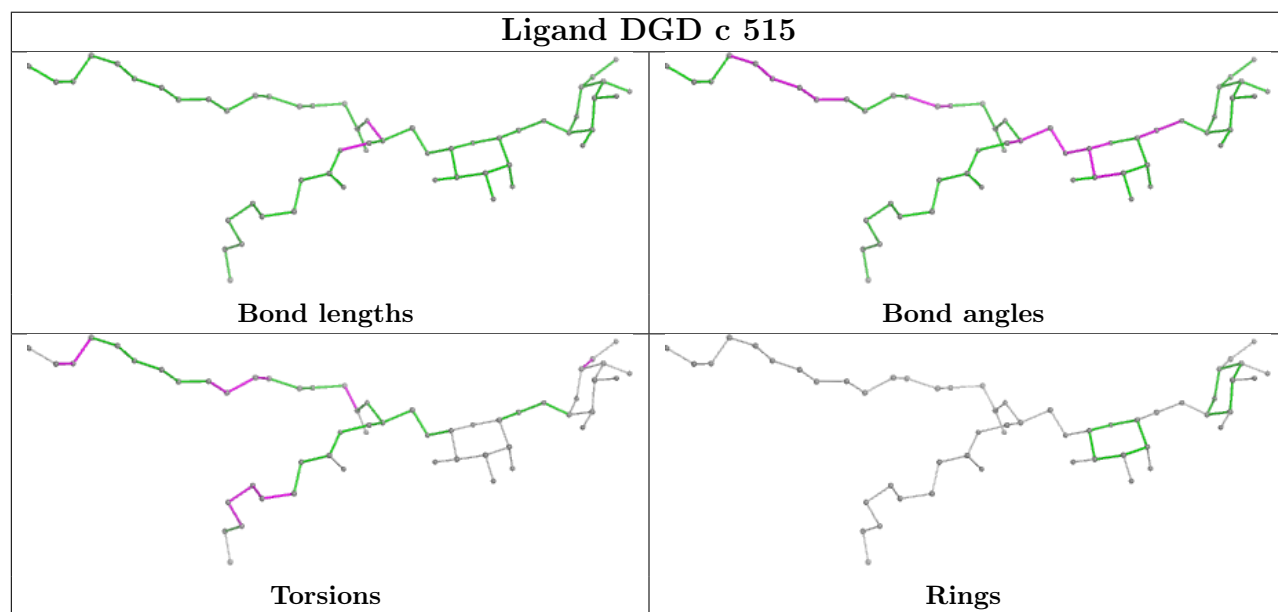
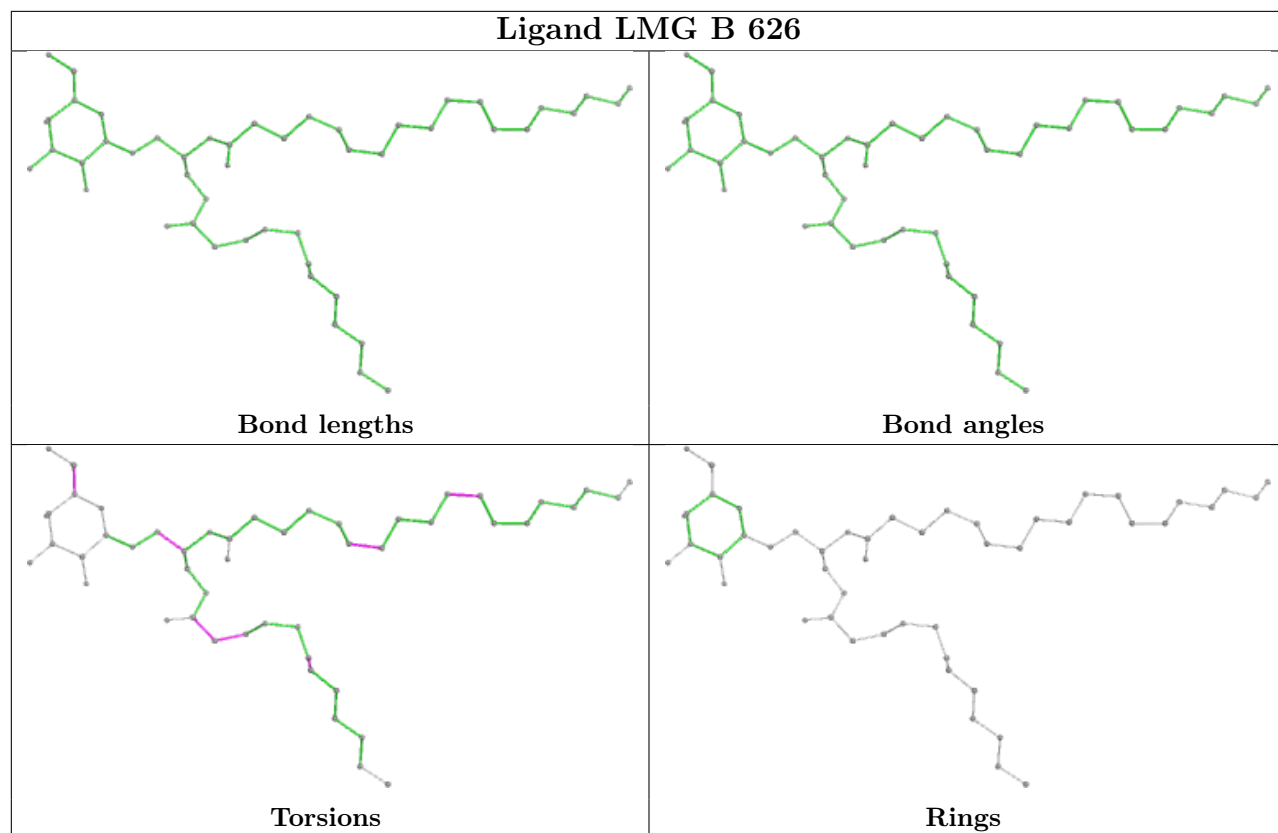




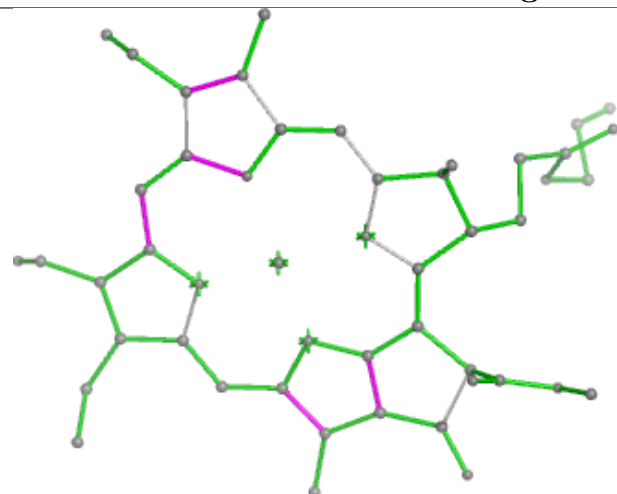
## Ligand CLA r 601



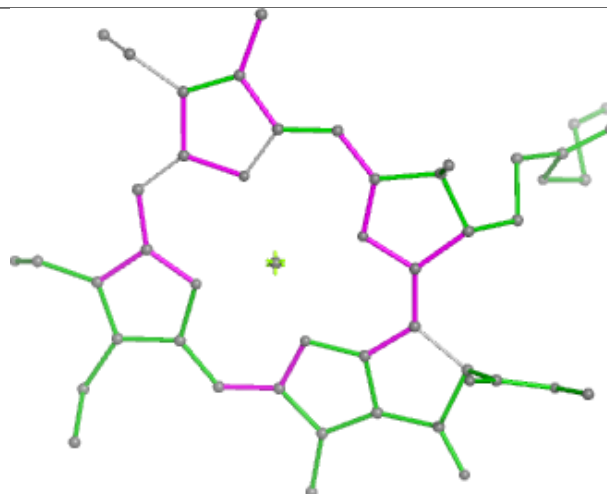




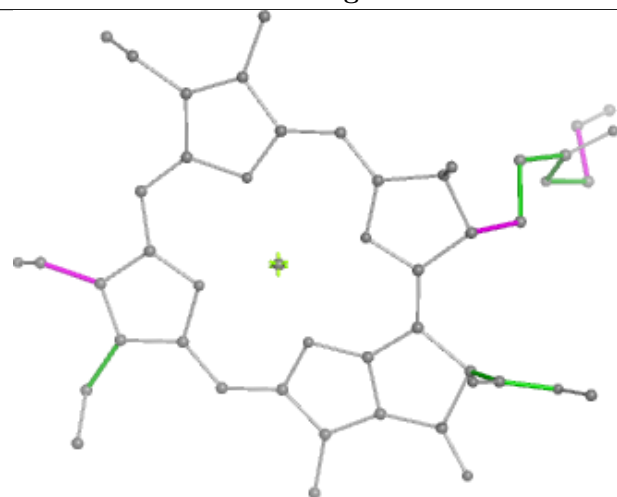
## Ligand CHL S 607



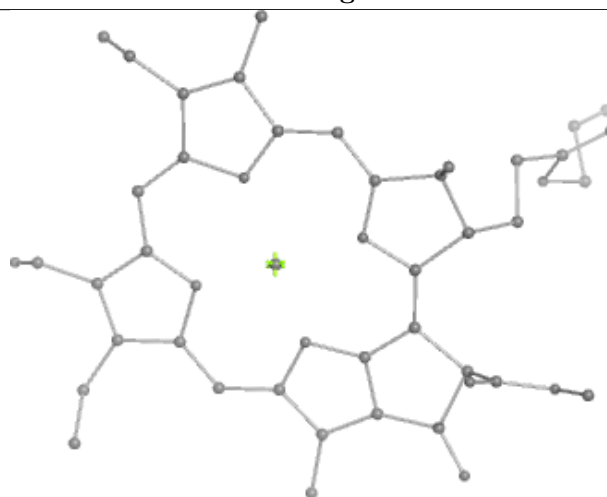
Bond lengths



Bond angles

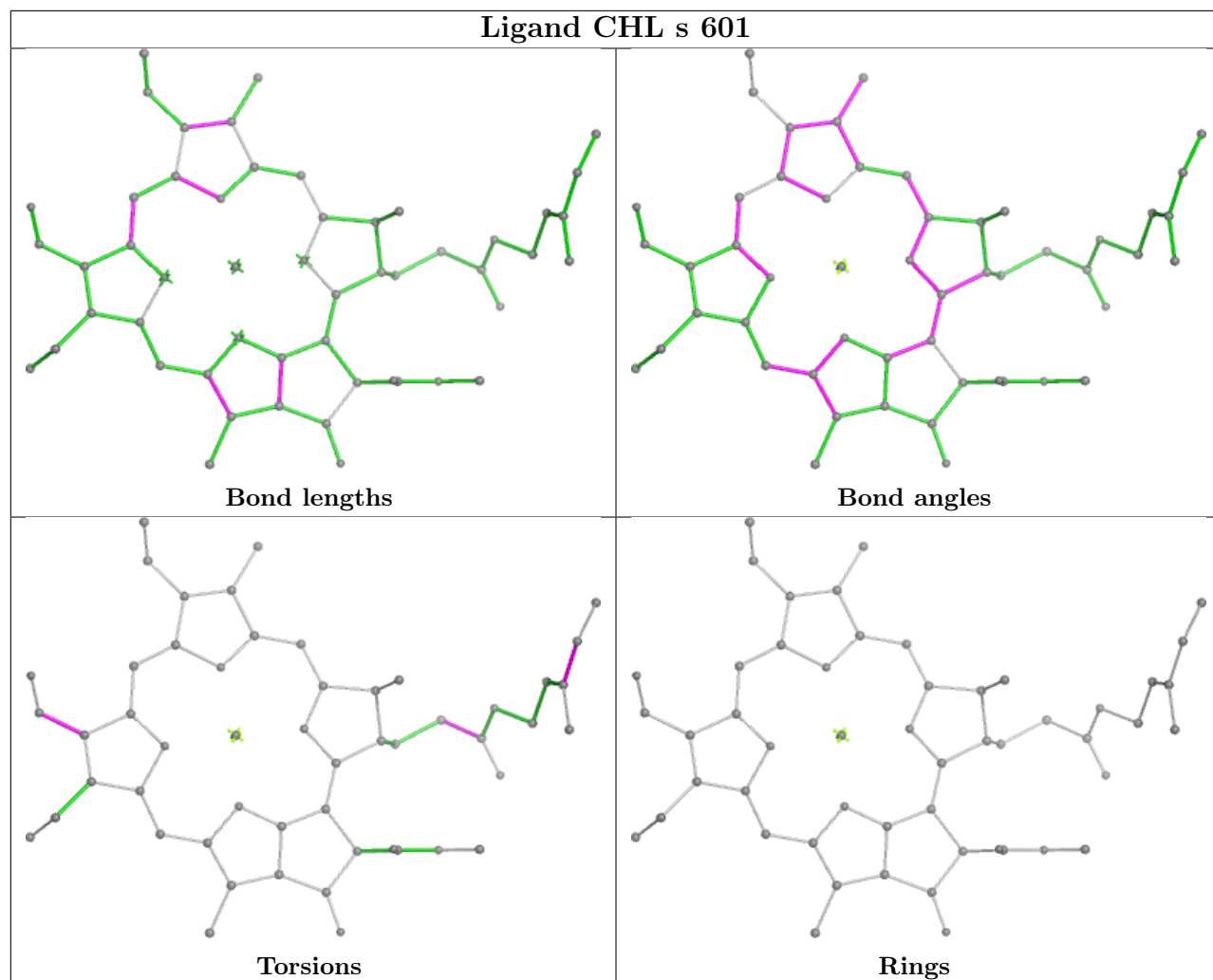


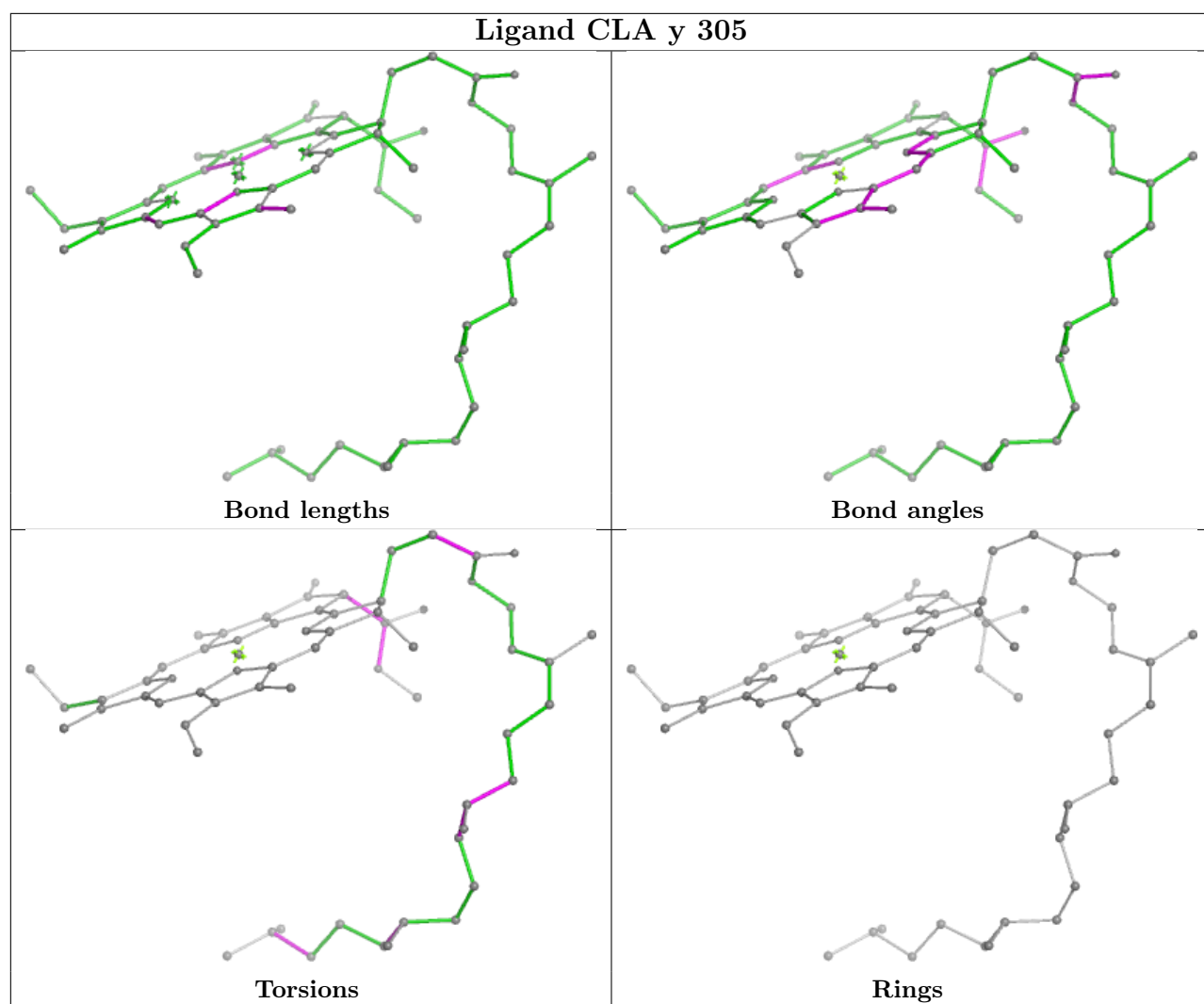
Torsions



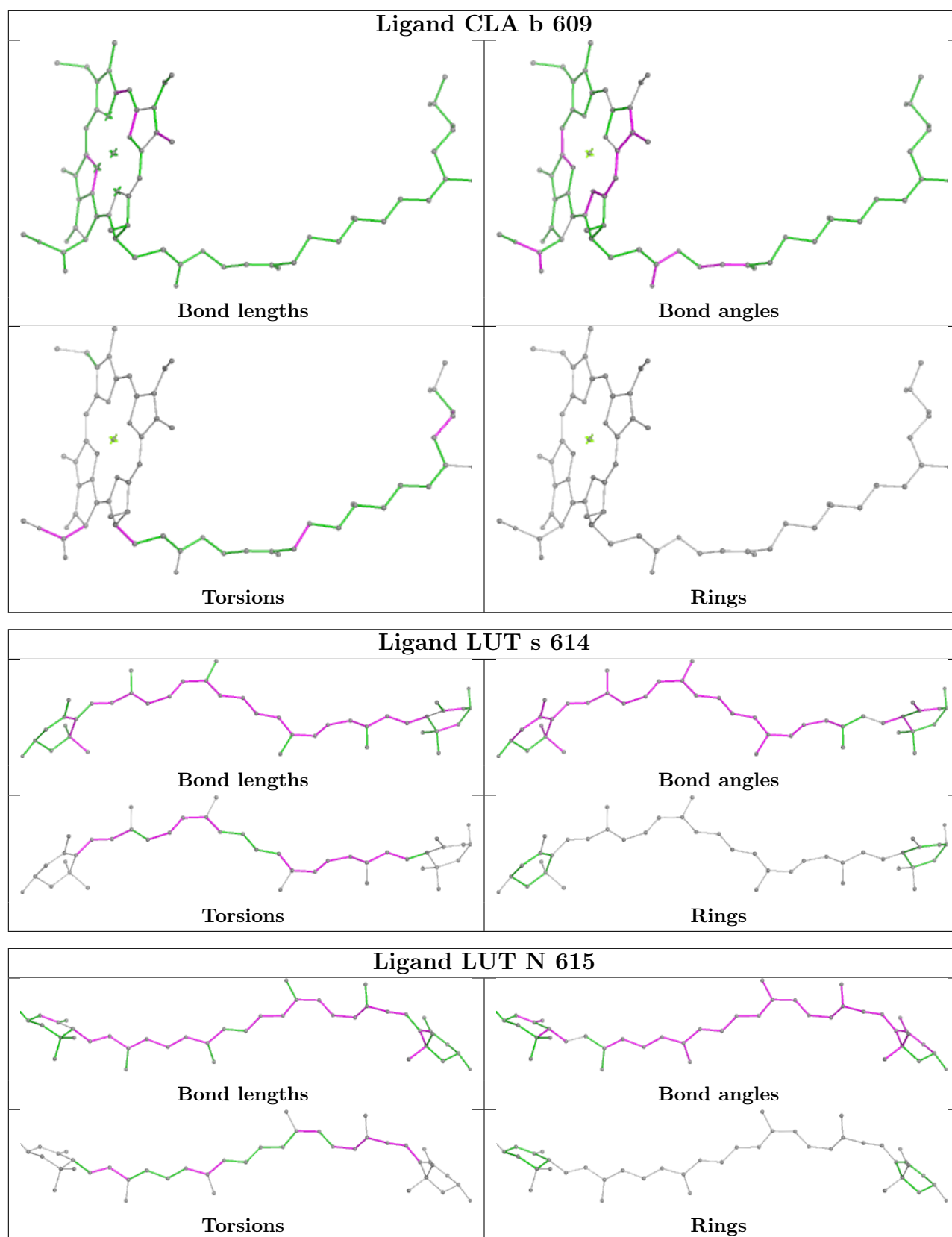
Rings

## Ligand CHL s 601

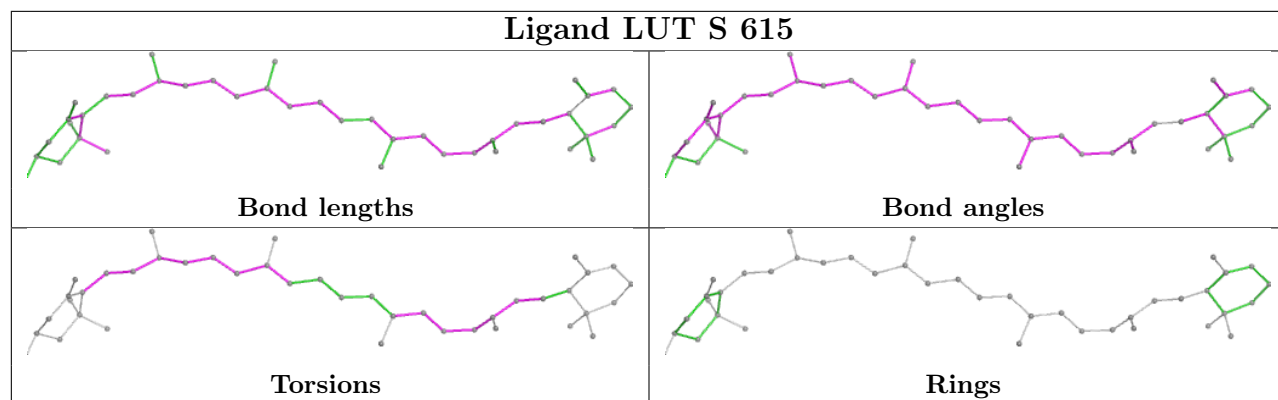




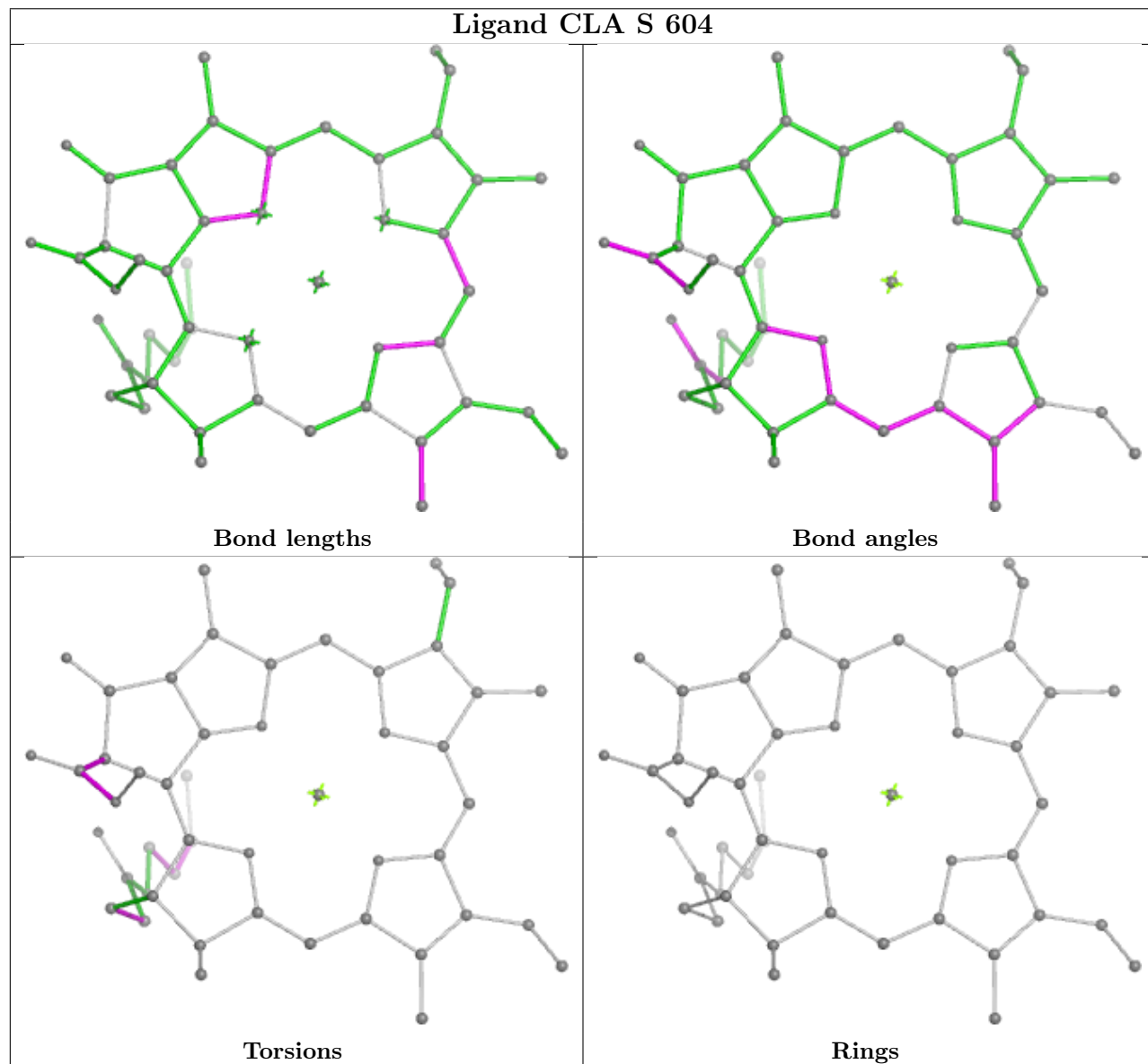




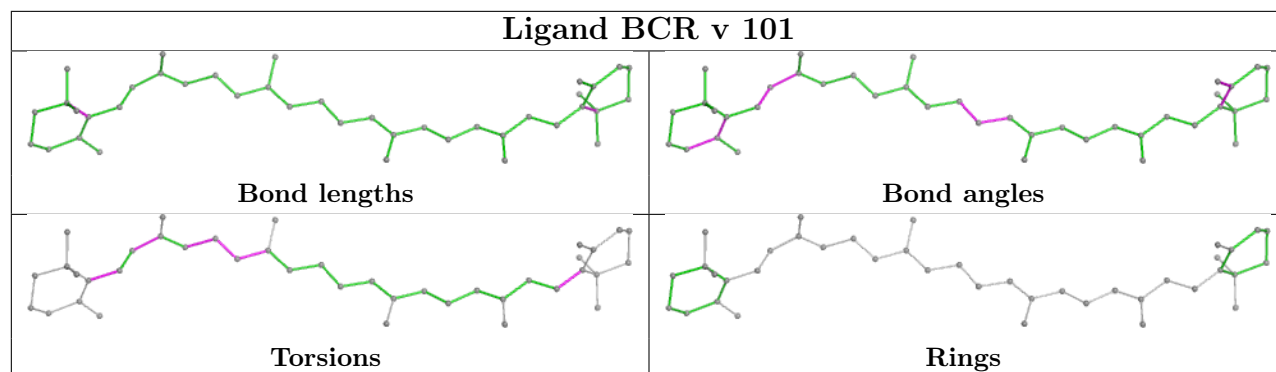
## Ligand LUT S 615



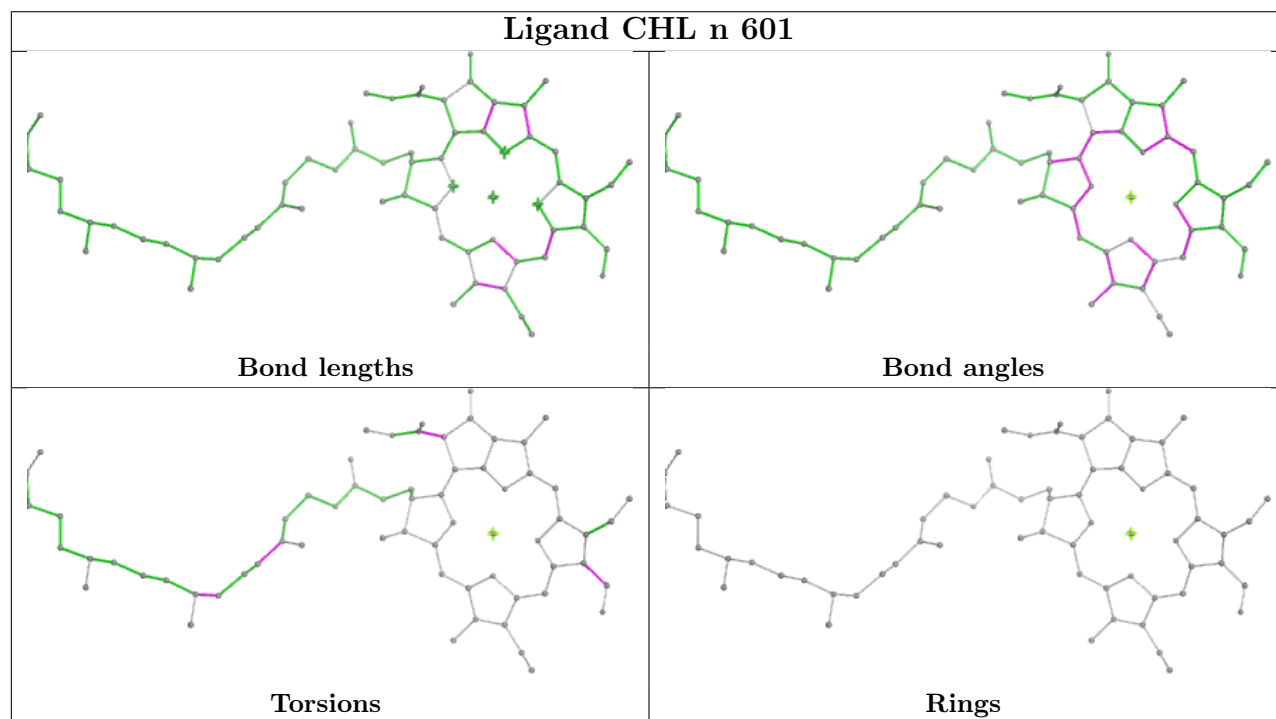
## Ligand CLA S 604

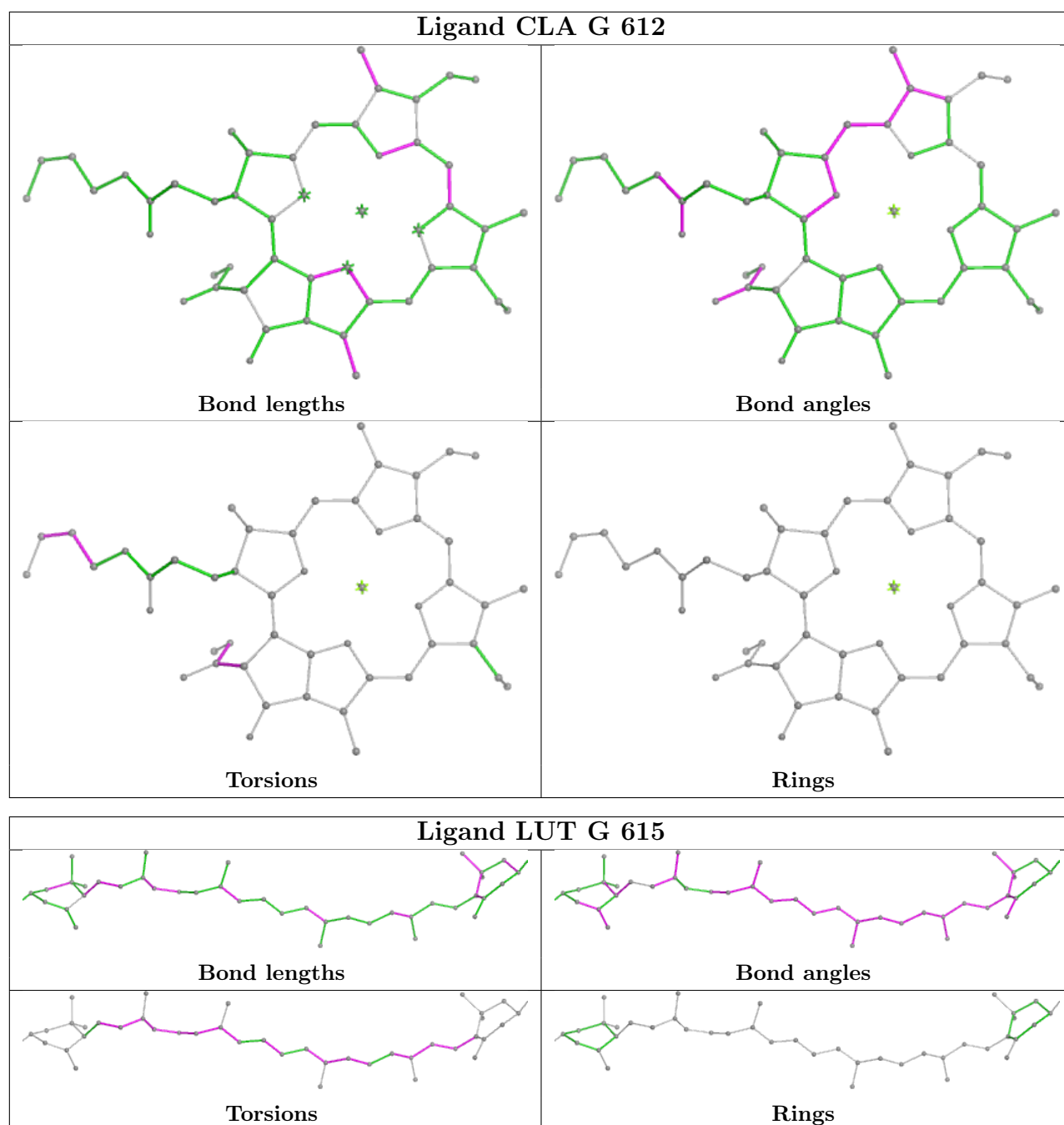


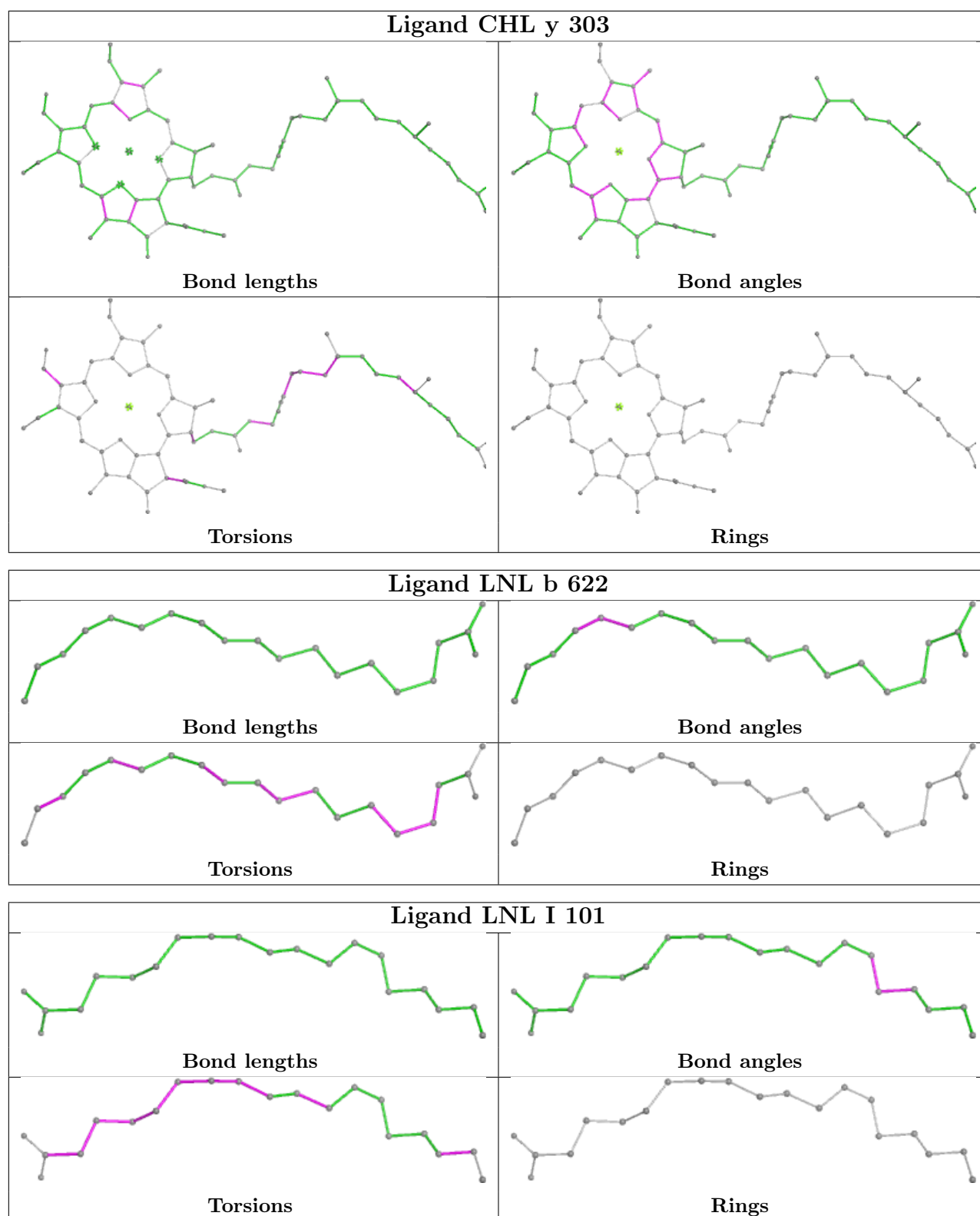
## Ligand BCR v 101

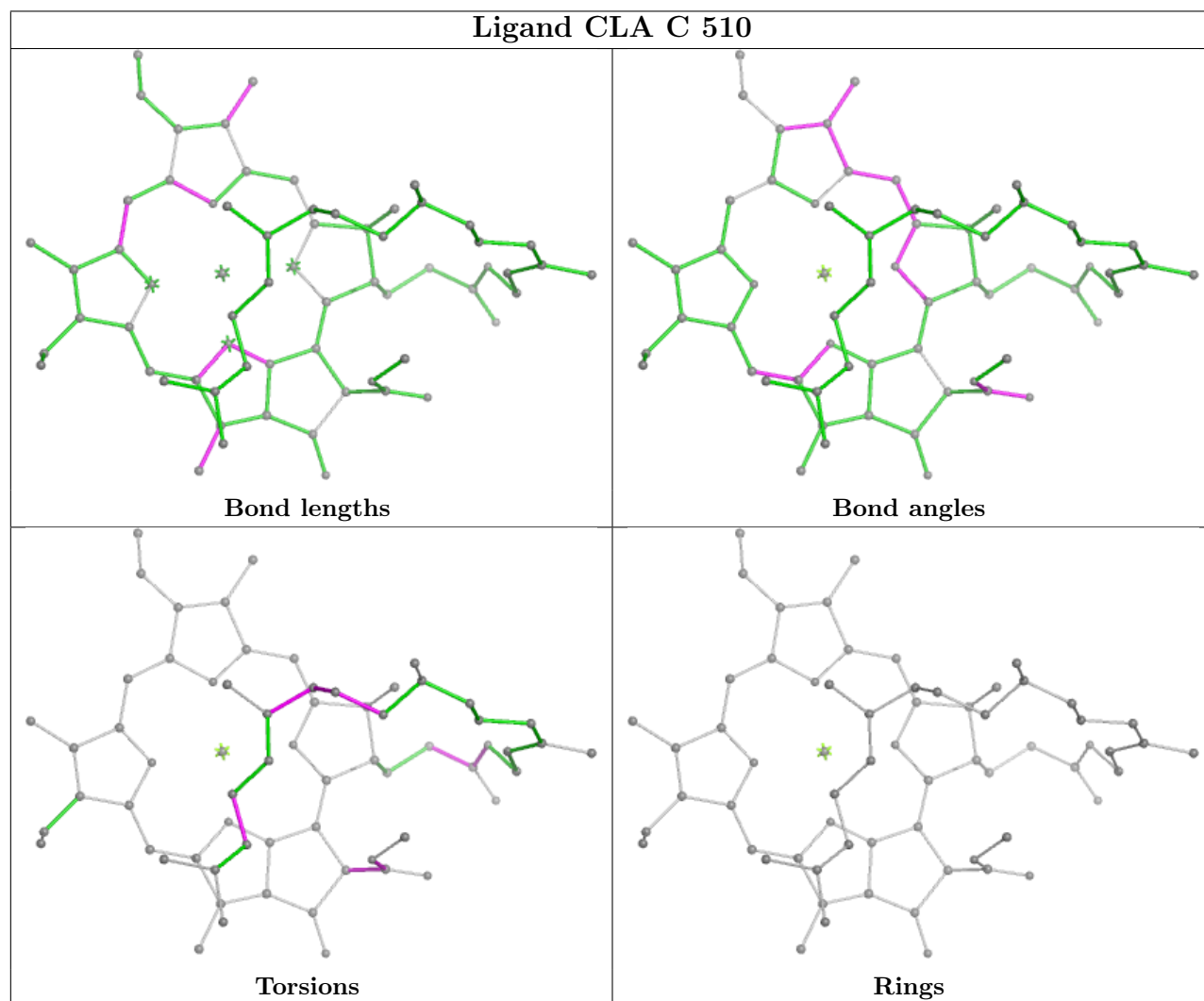
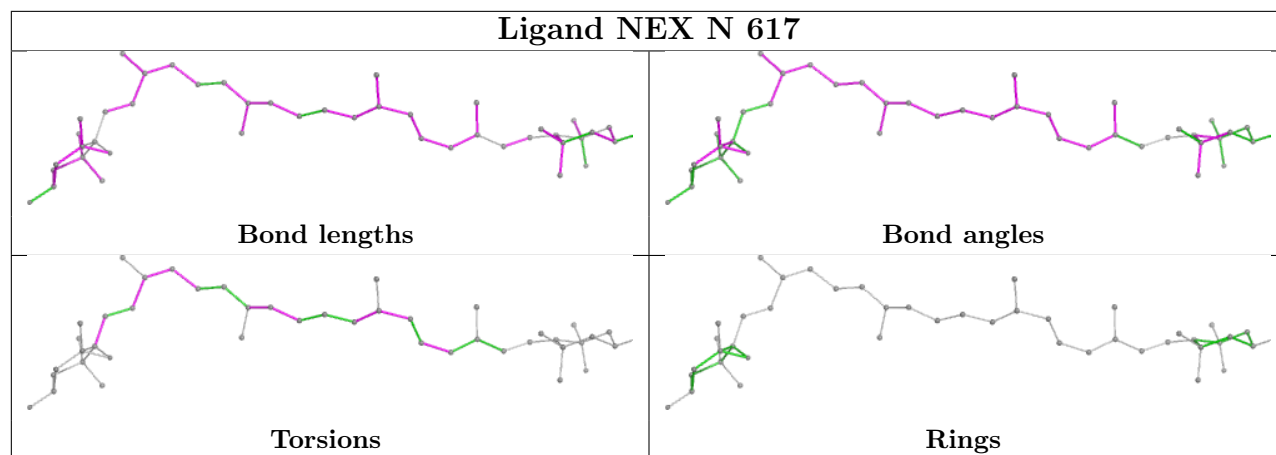


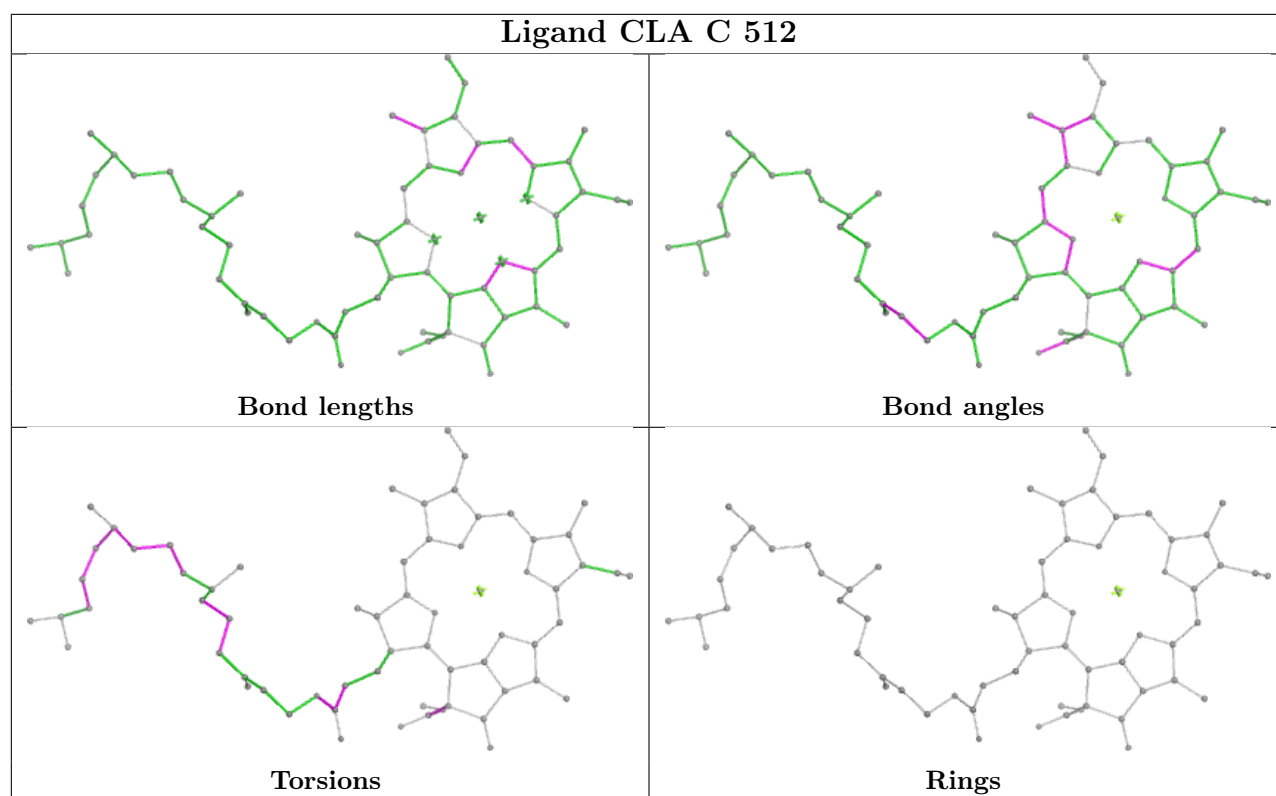
## Ligand CHL n 601

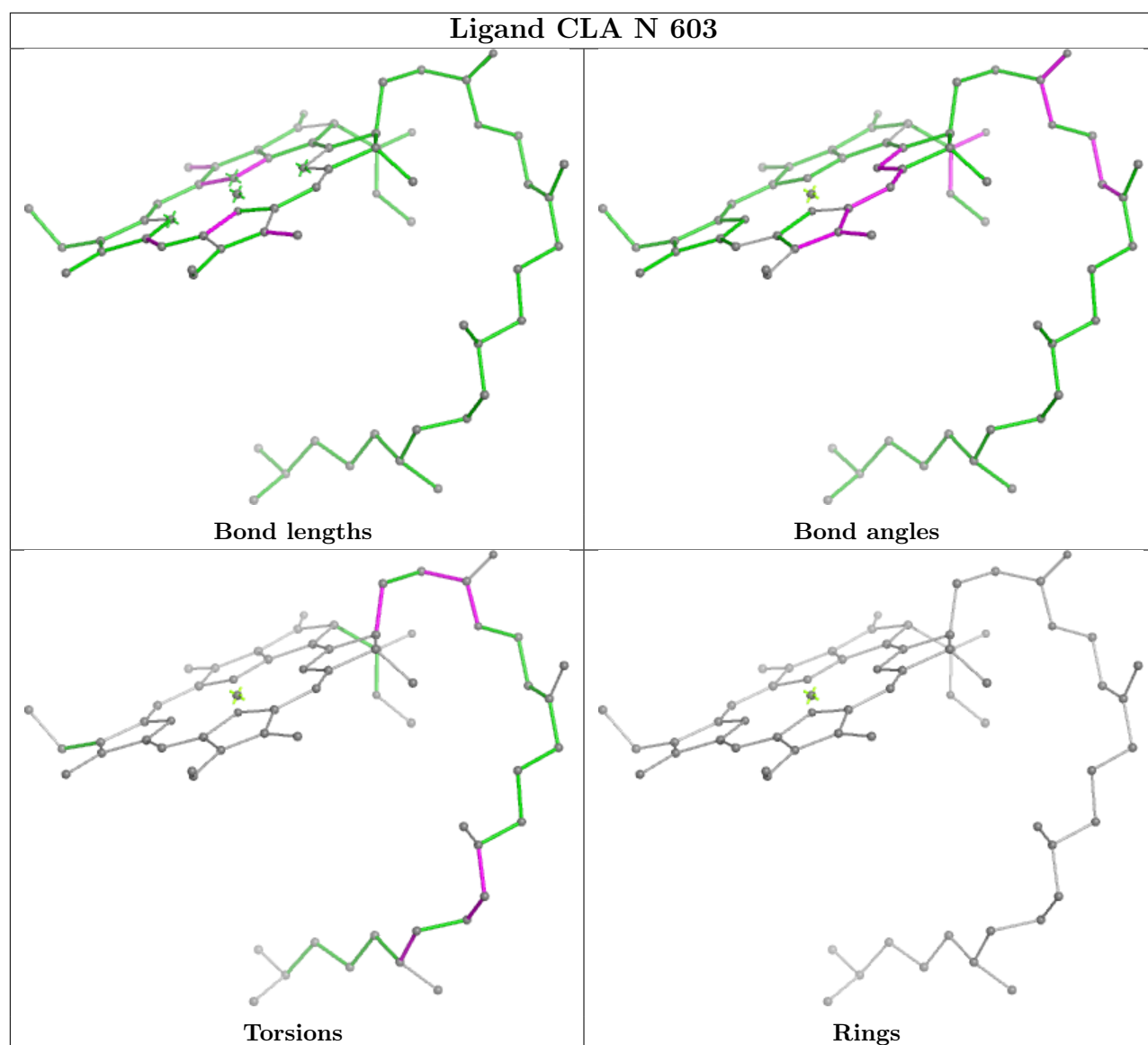




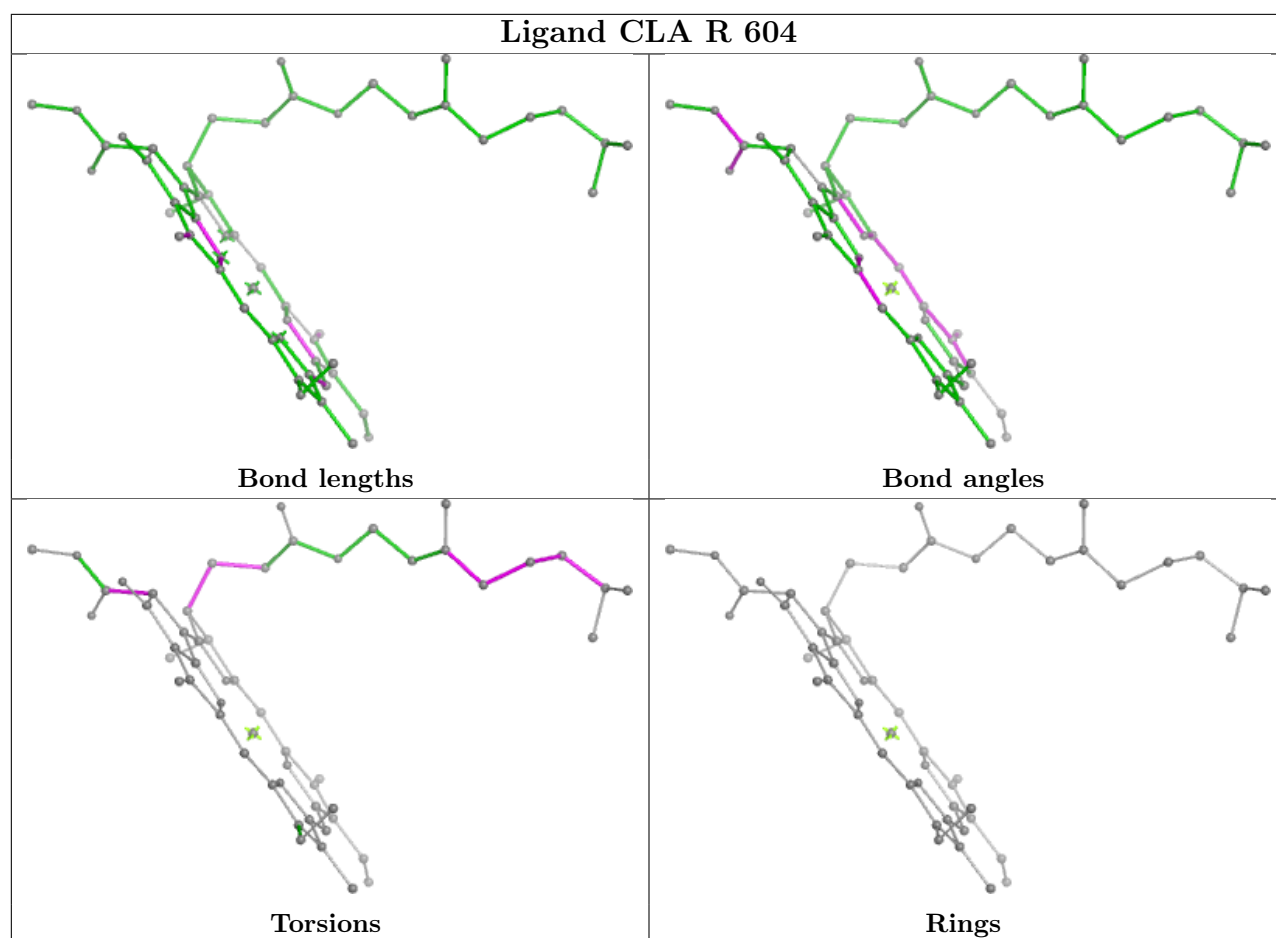




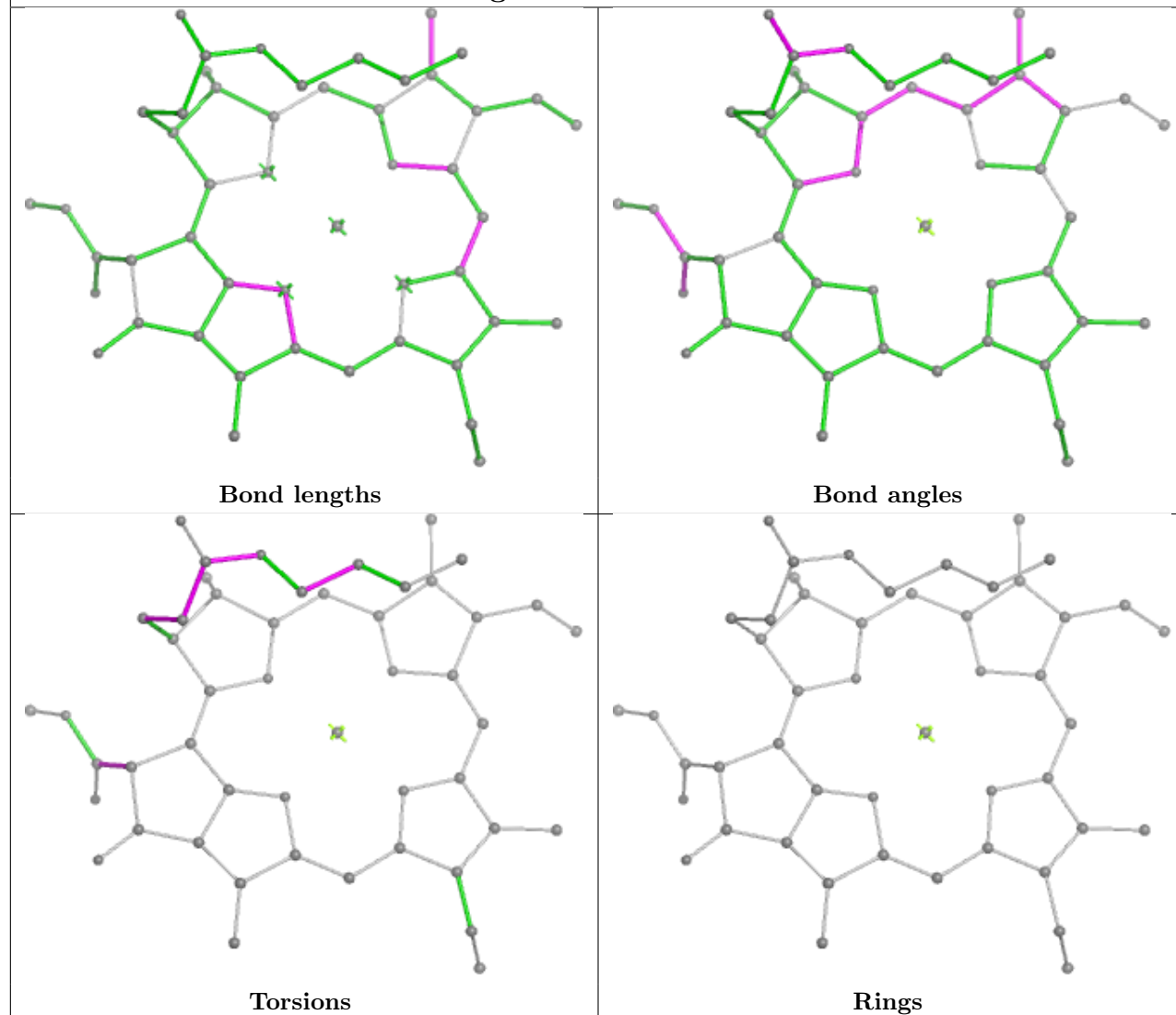




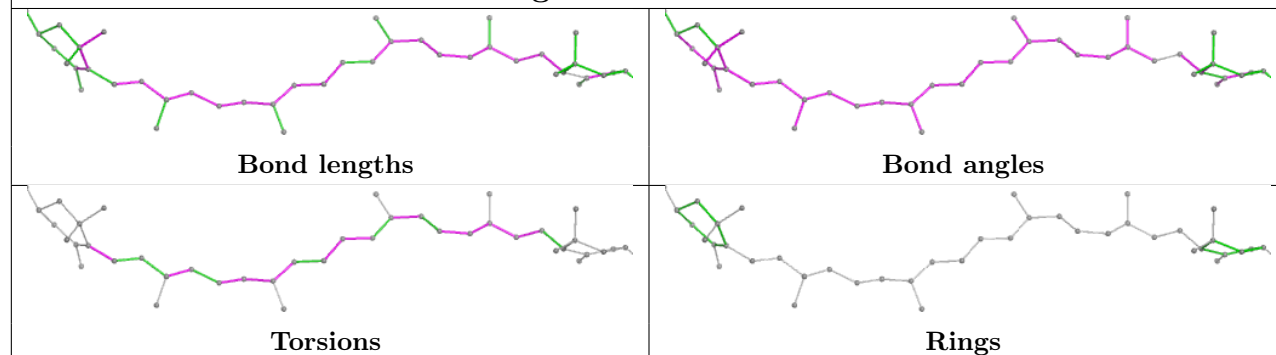




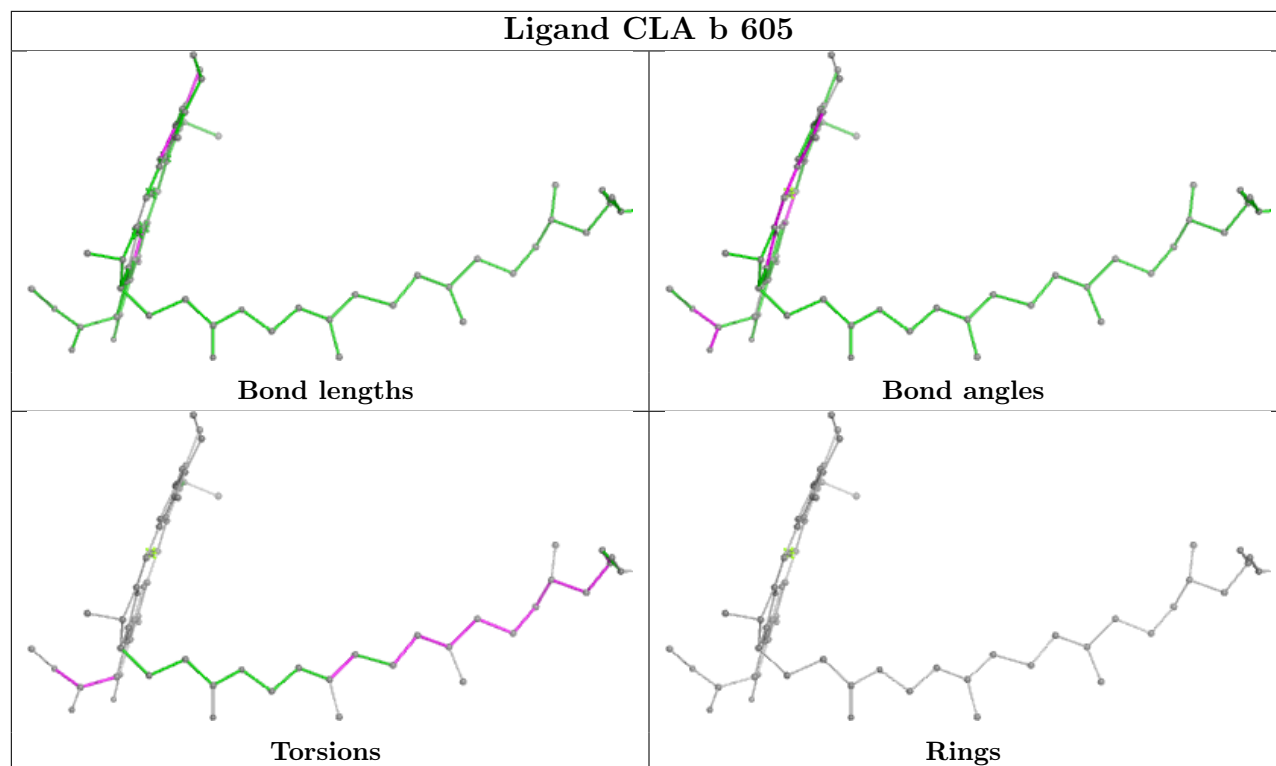
## Ligand CLA R 612



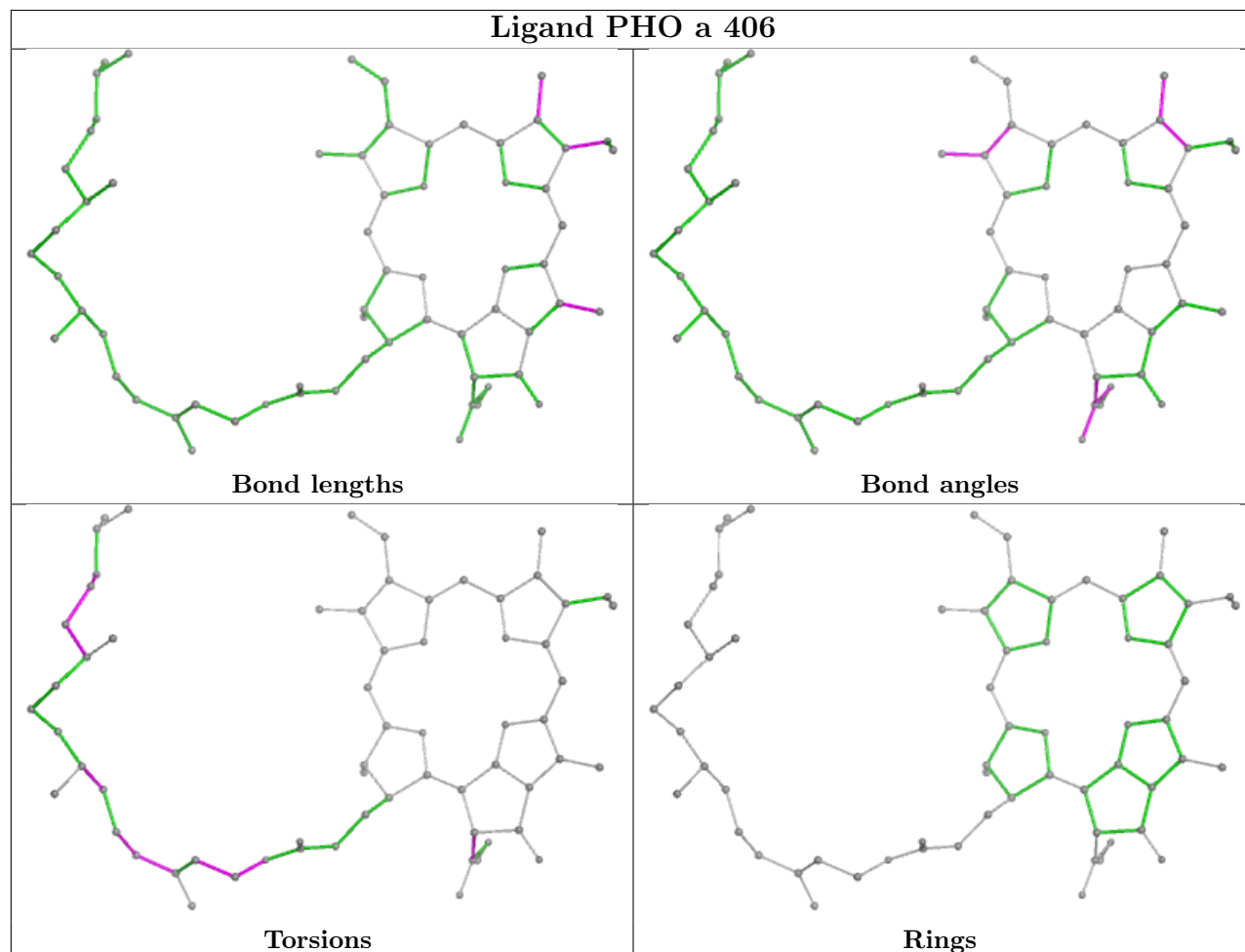
## Ligand LUT R 613



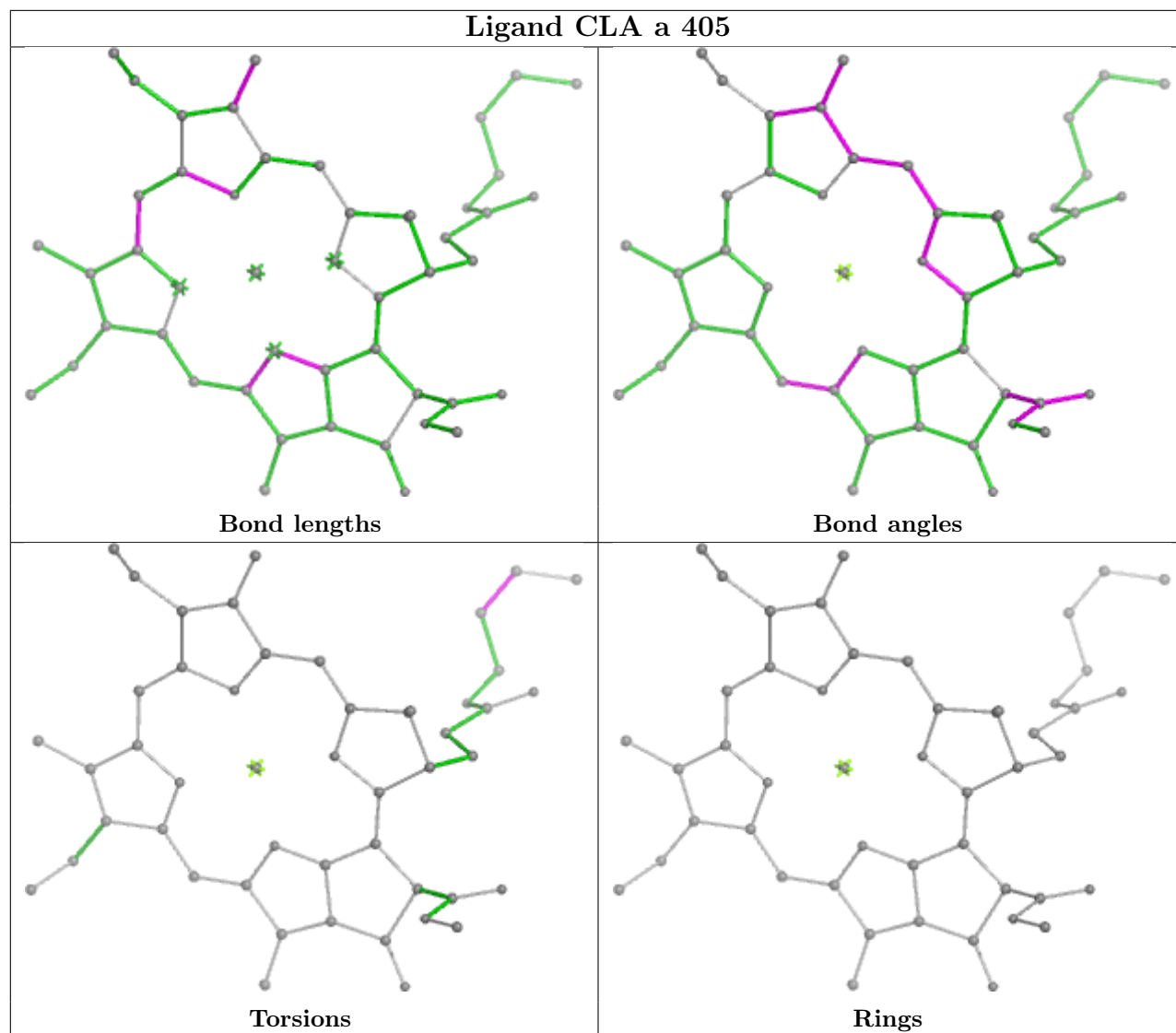
## Ligand CLA b 605



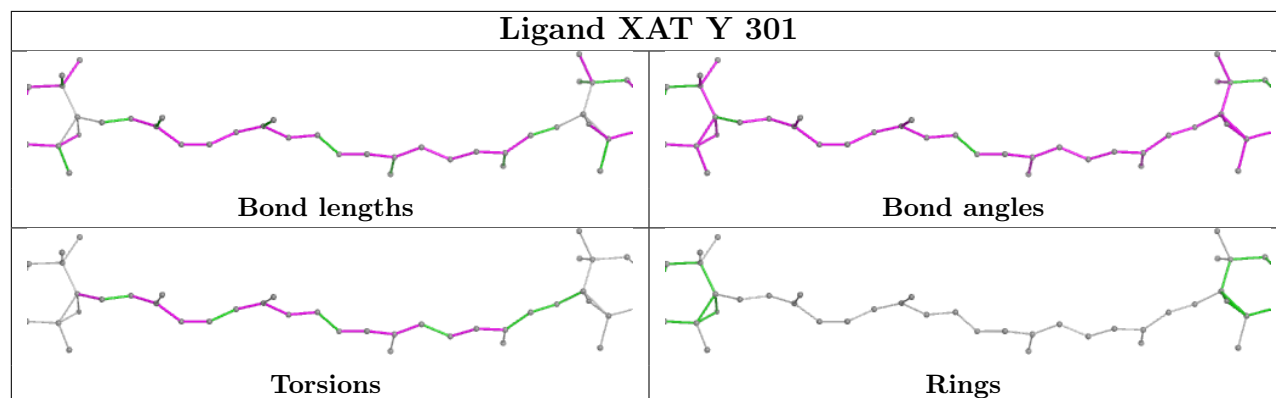
## Ligand PHO a 406

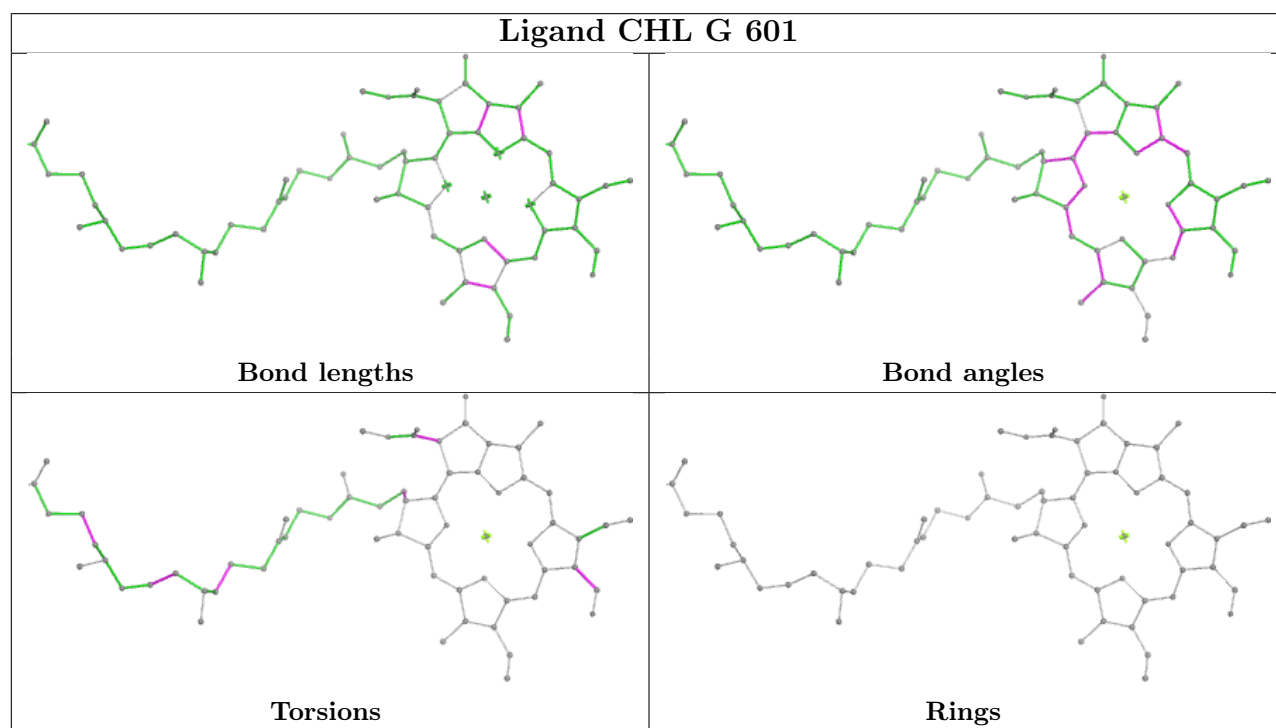
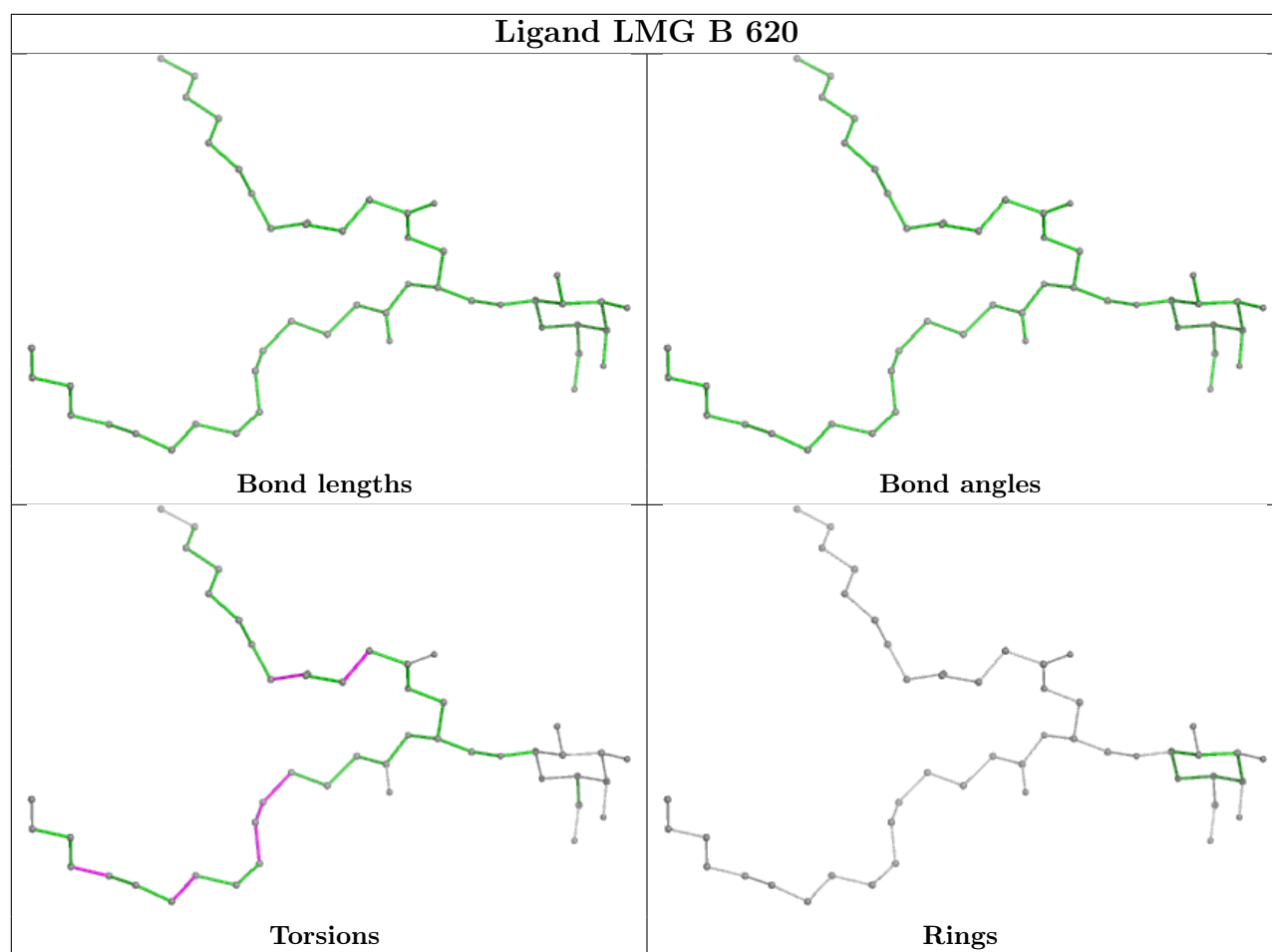


## Ligand CLA a 405

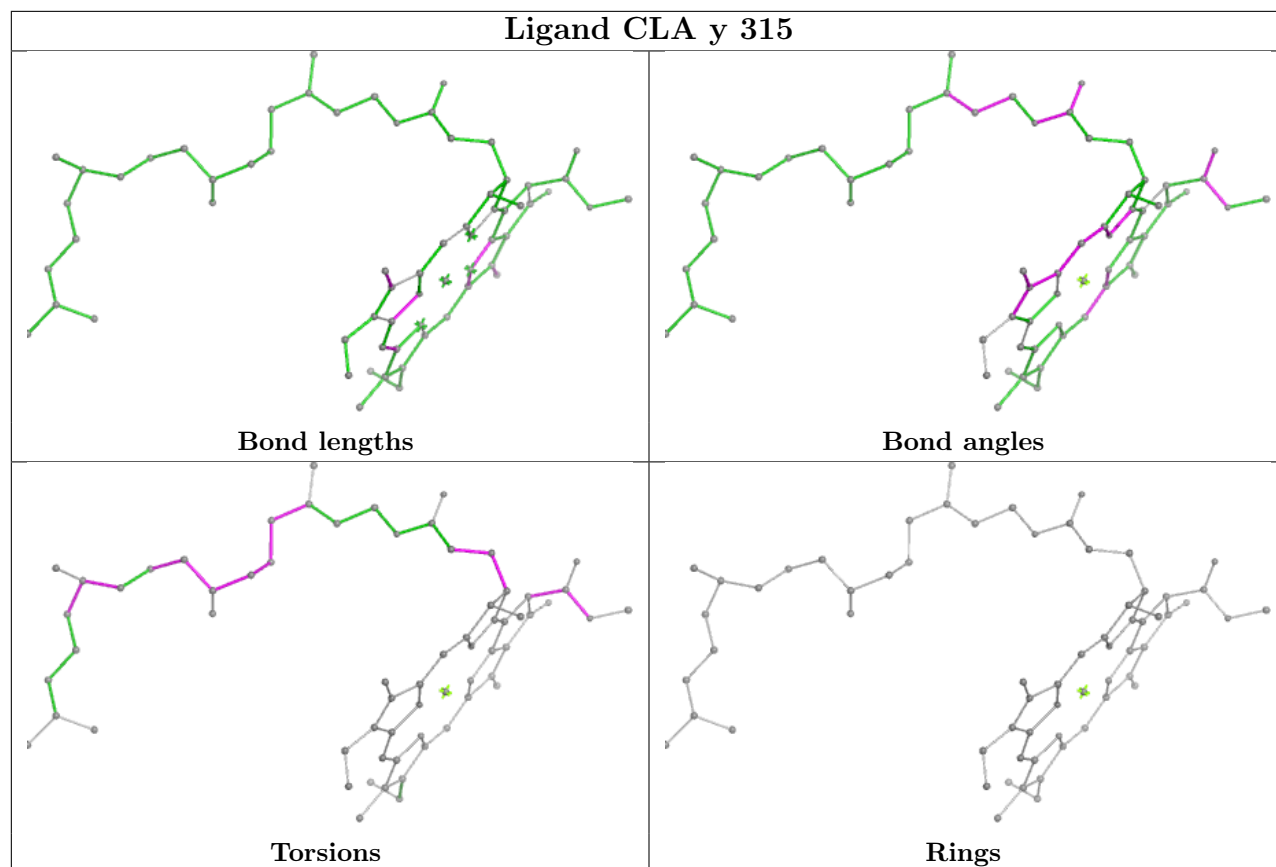


## Ligand XAT Y 301

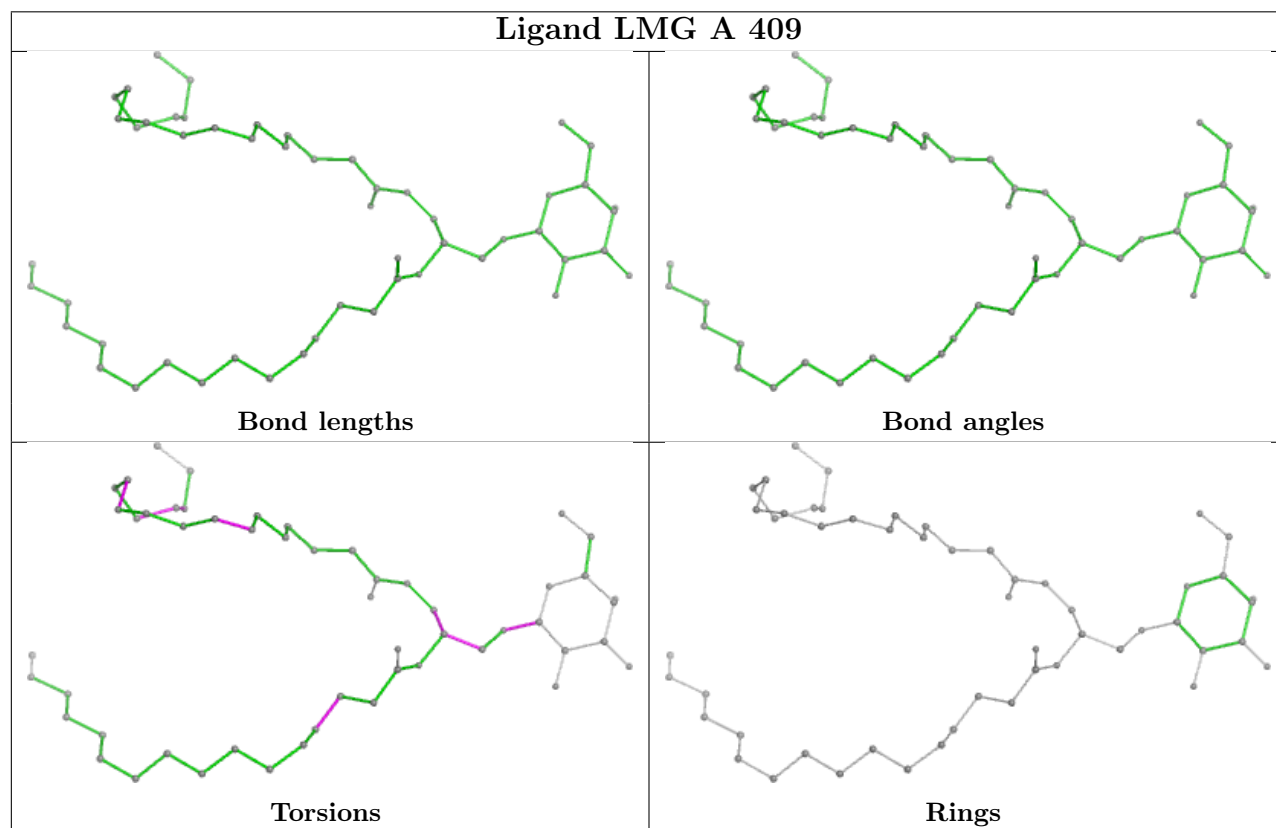


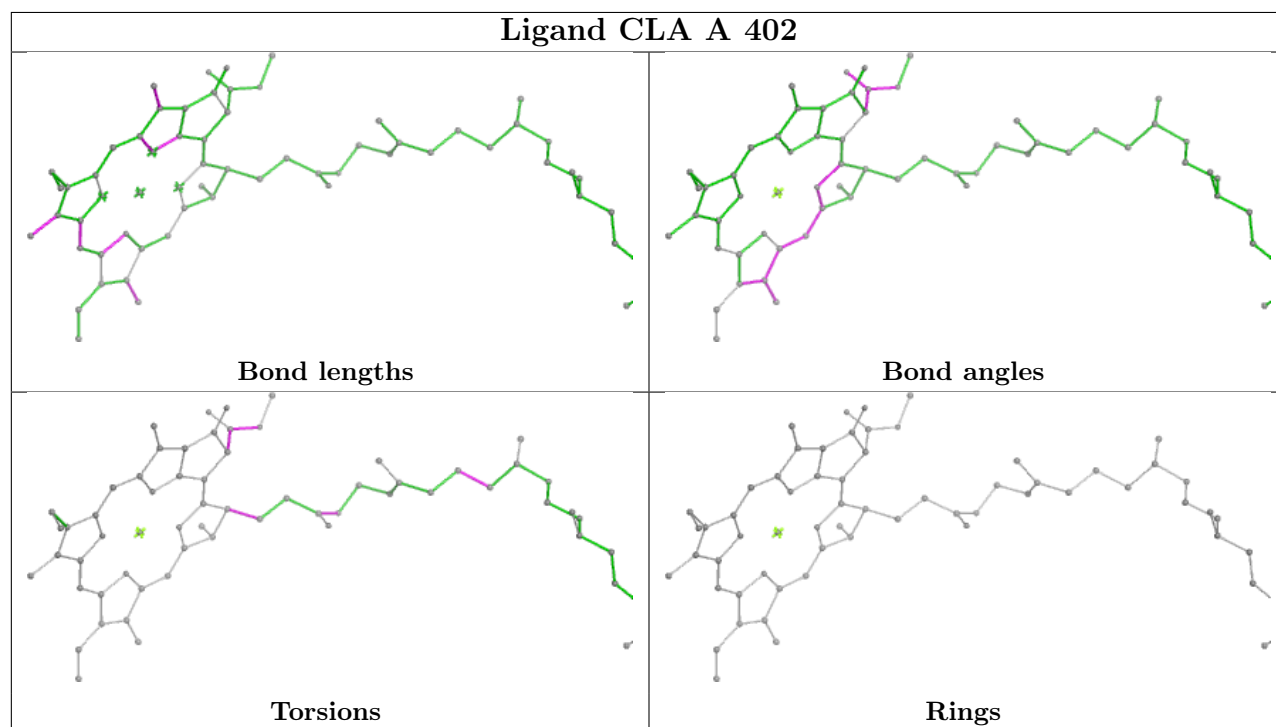
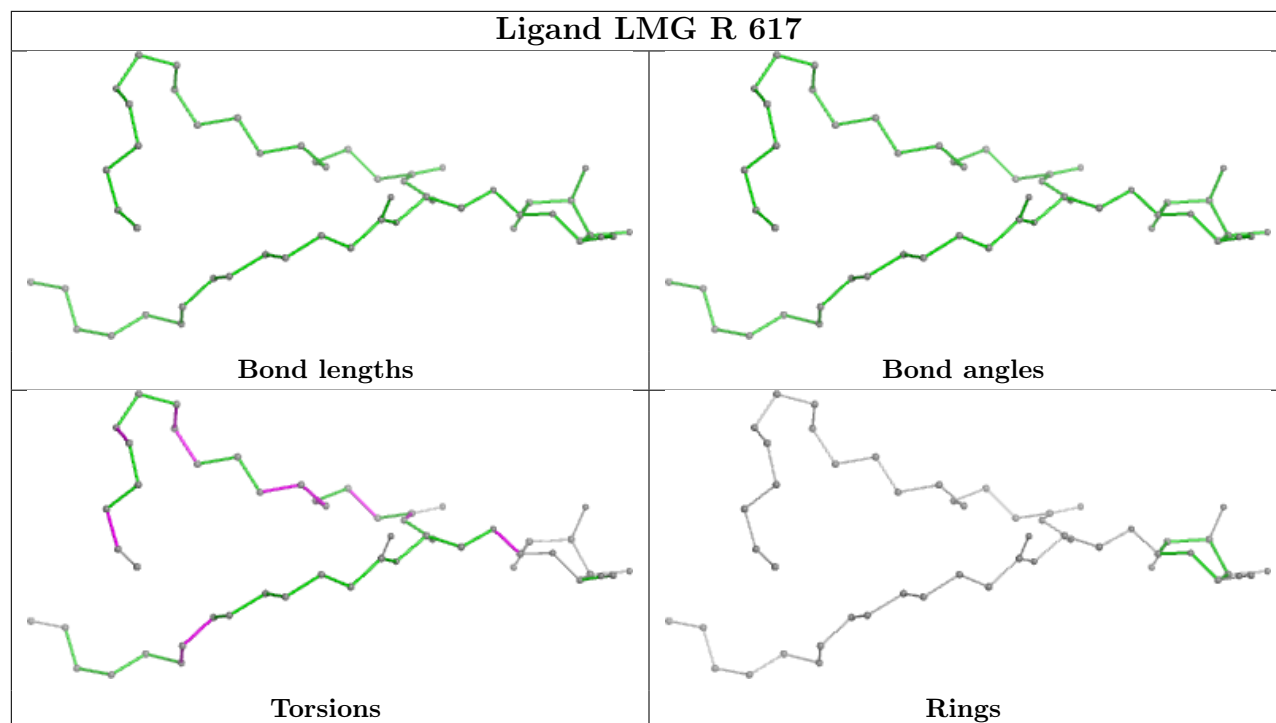


## Ligand CLA y 315

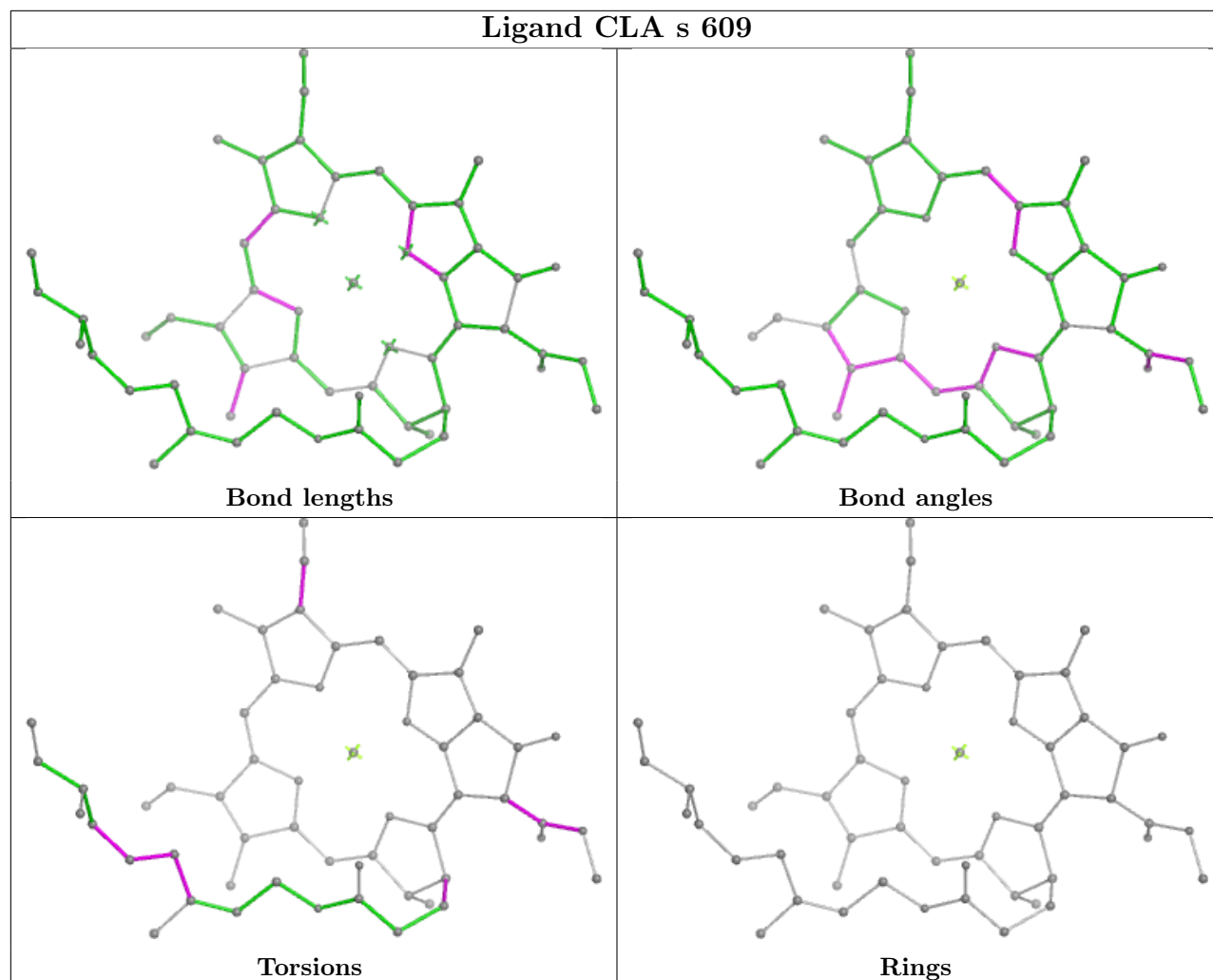


## Ligand LMG A 409

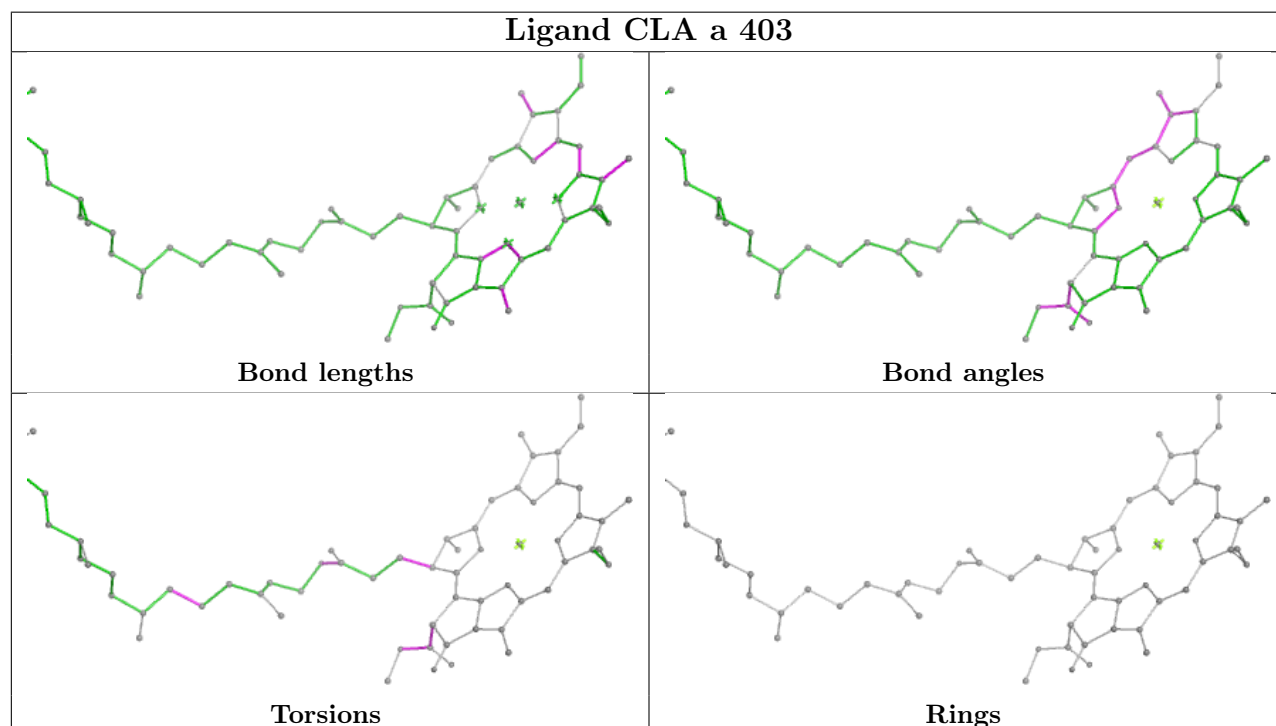




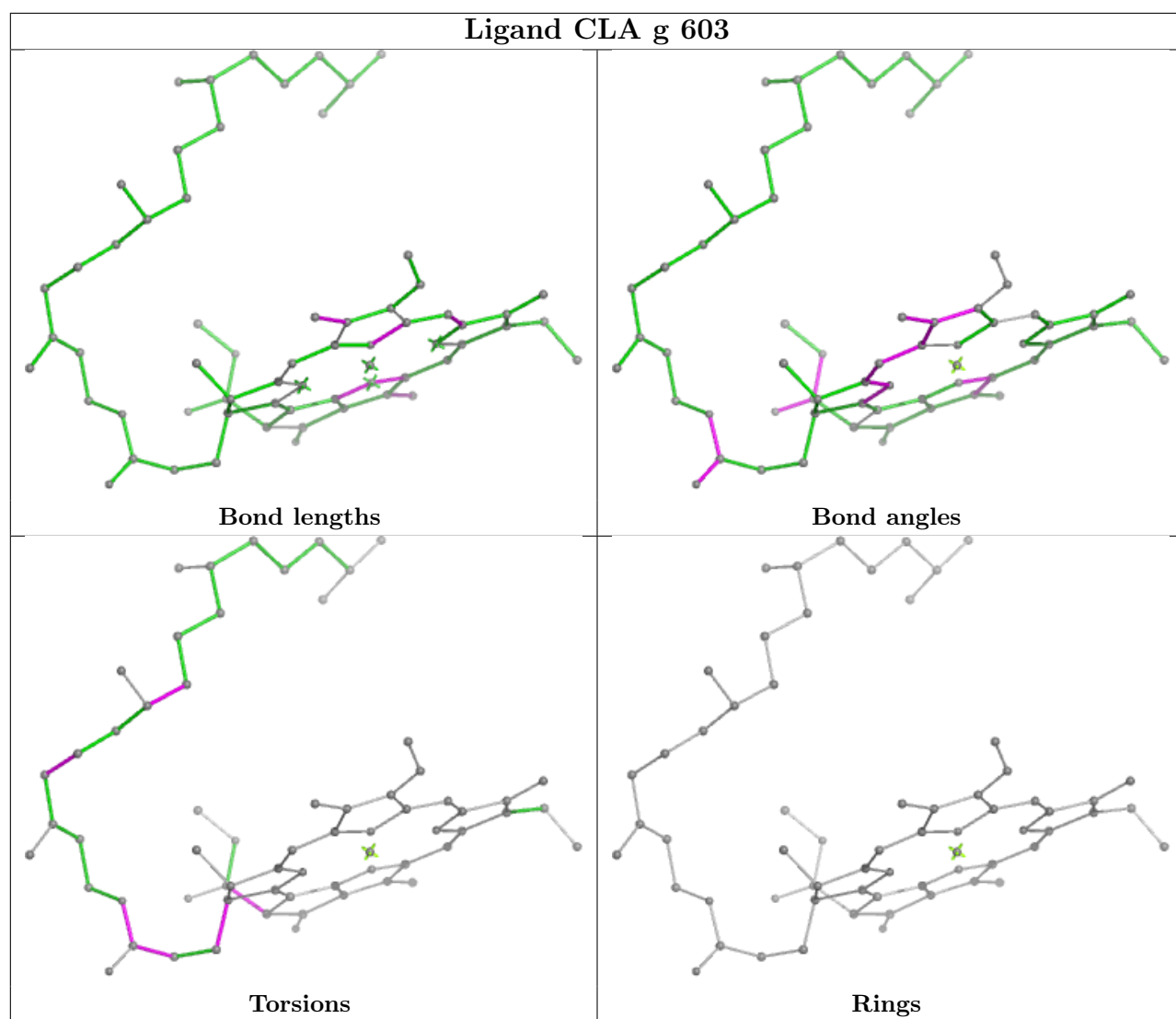
## Ligand CLA s 609



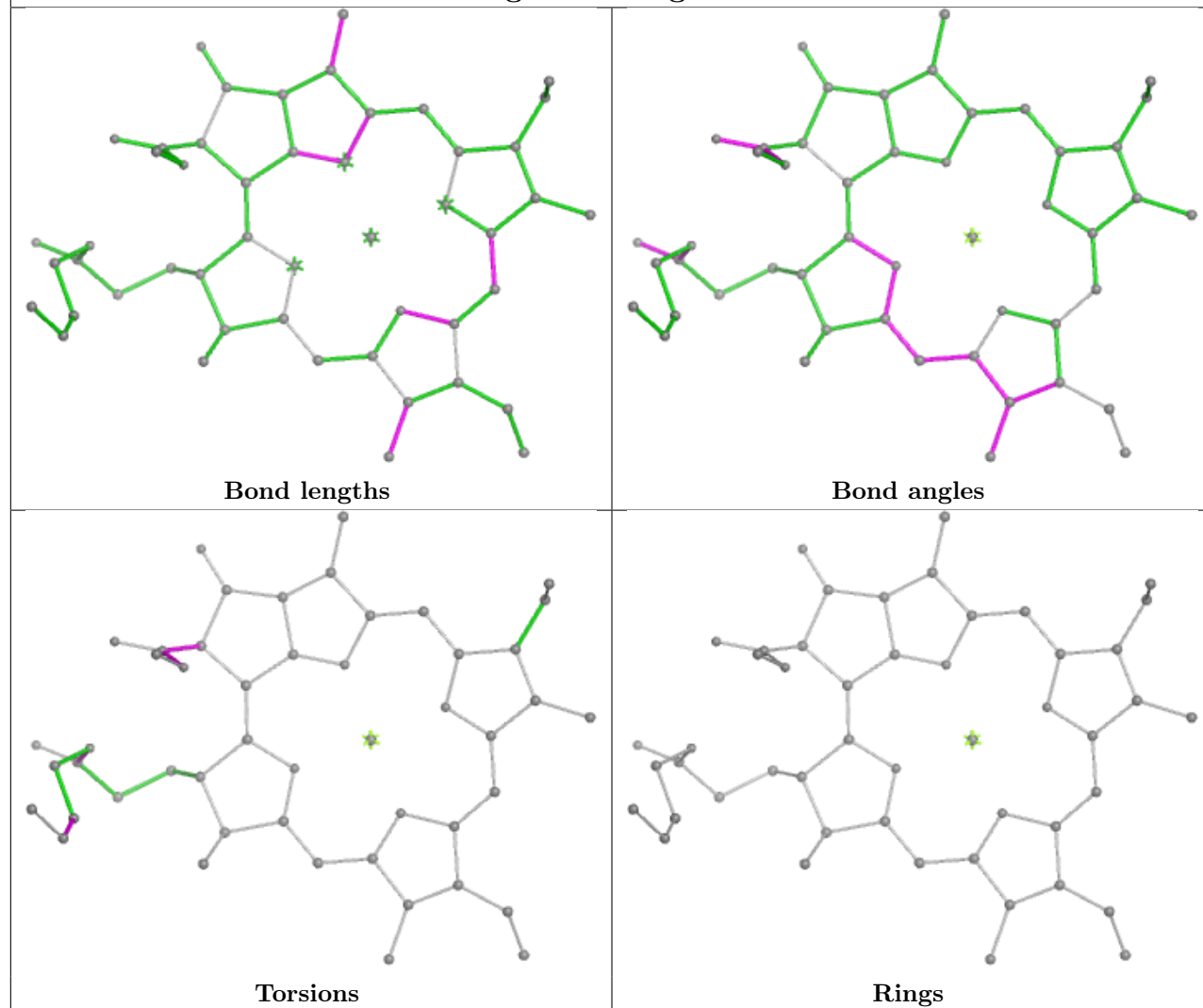
## Ligand CLA a 403



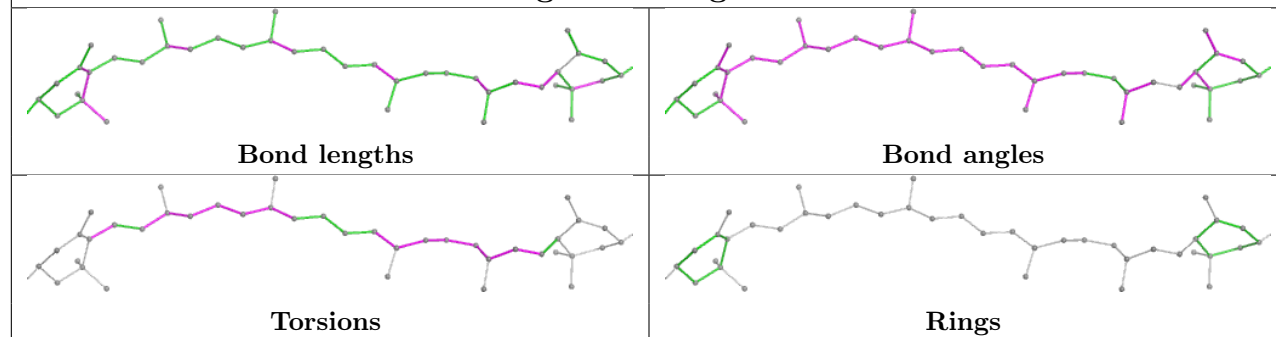


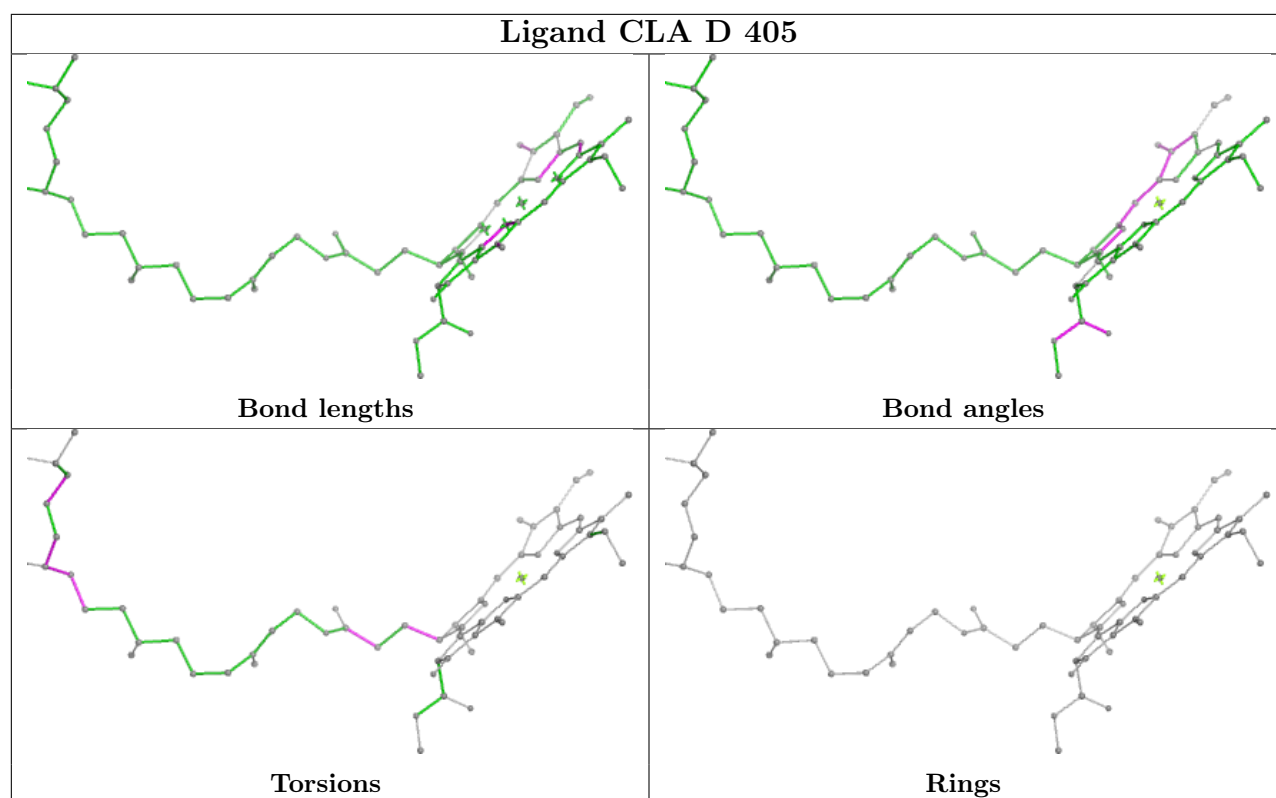


## Ligand CLA g 612

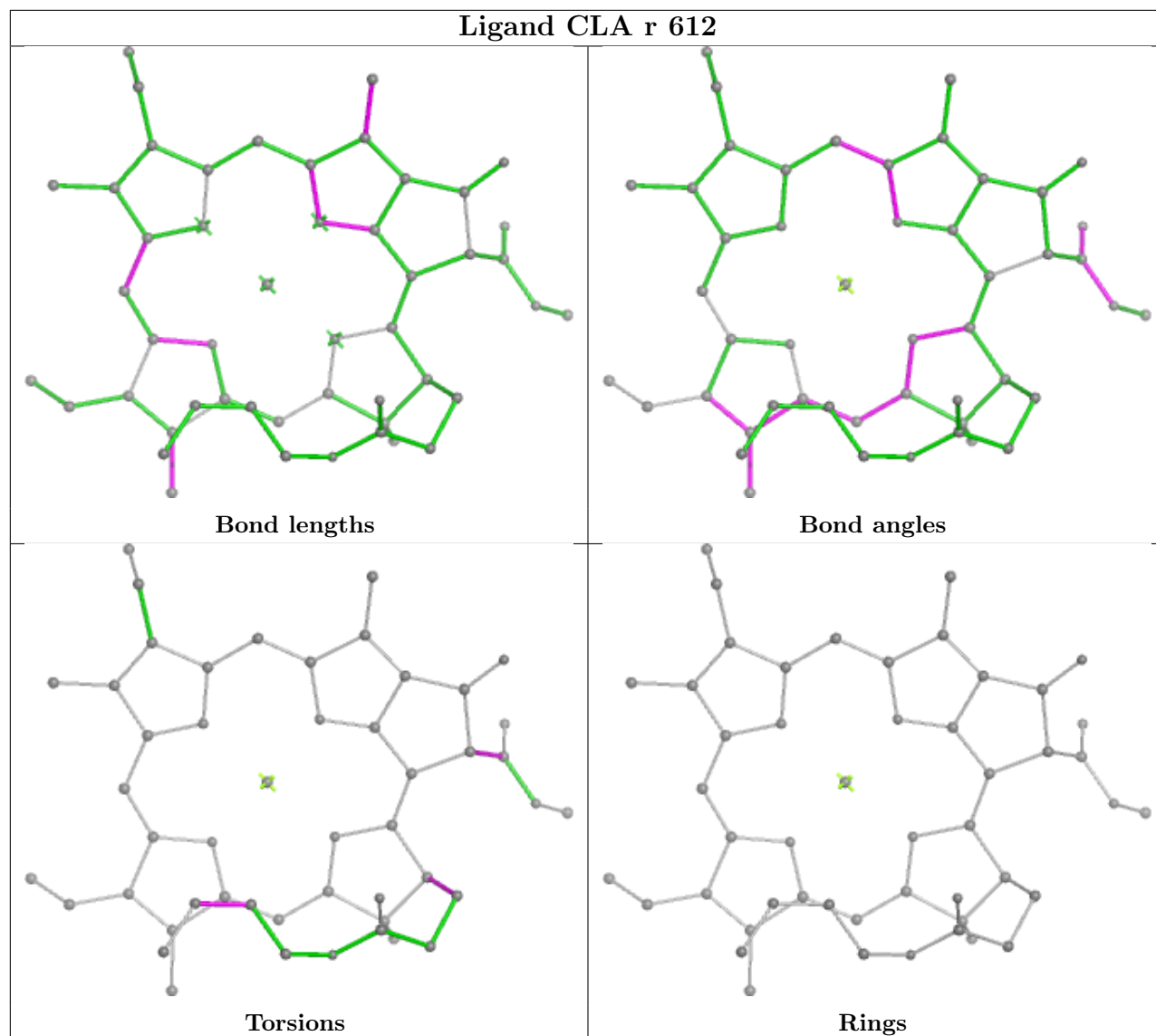


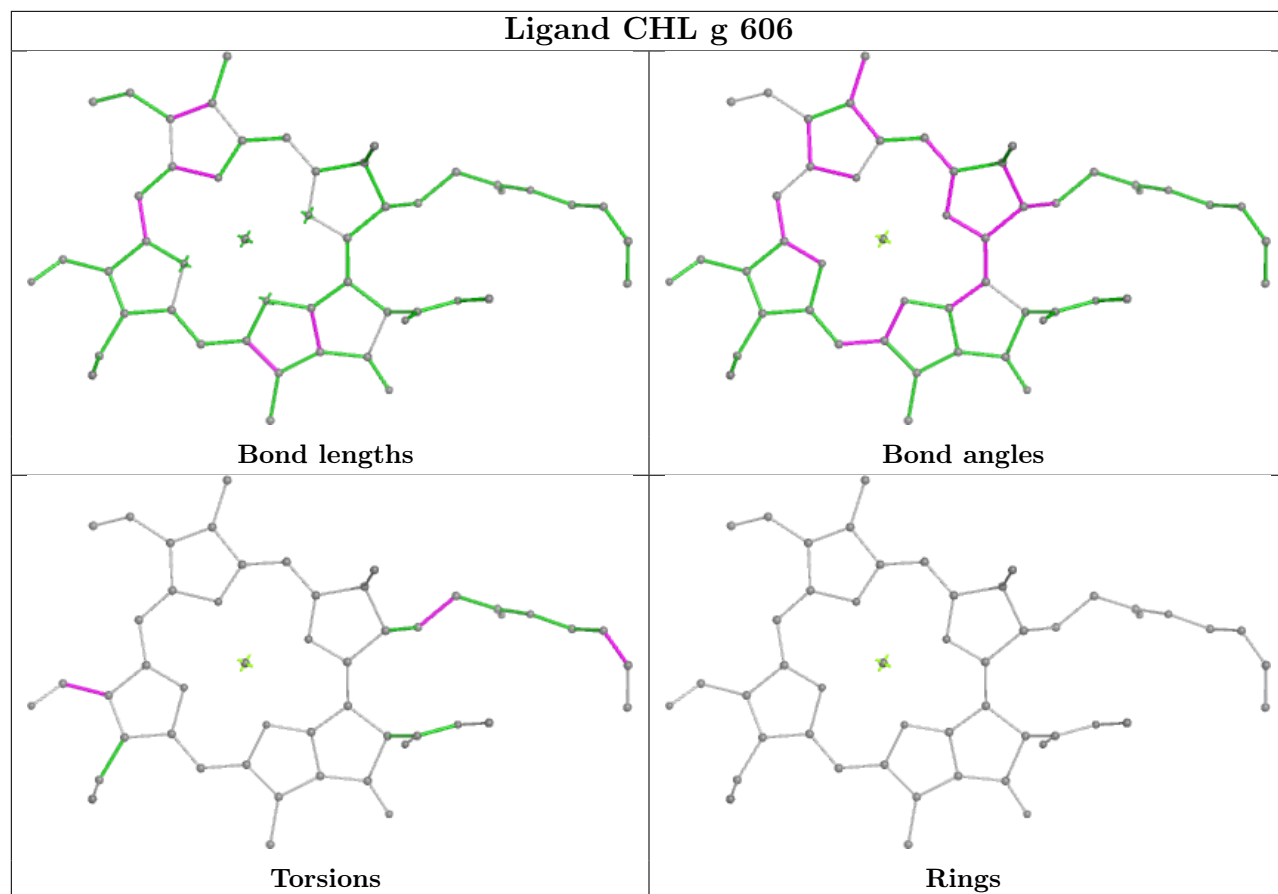
## Ligand LUT g 615



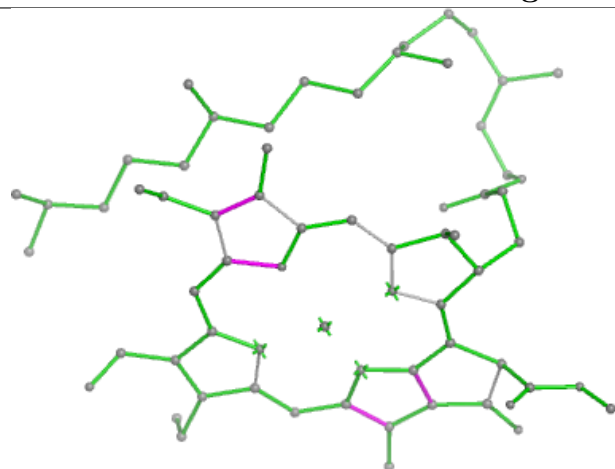


## Ligand CLA r 612

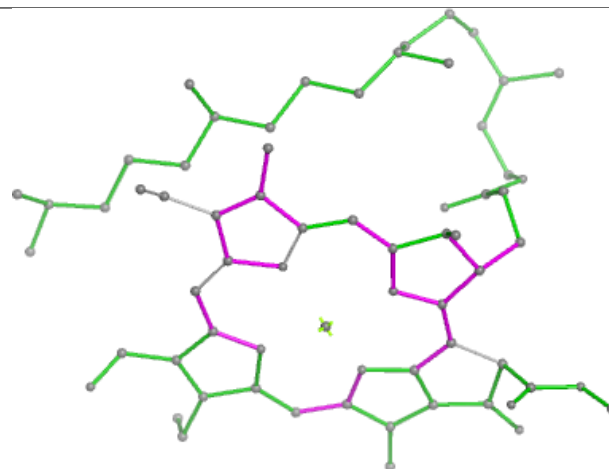




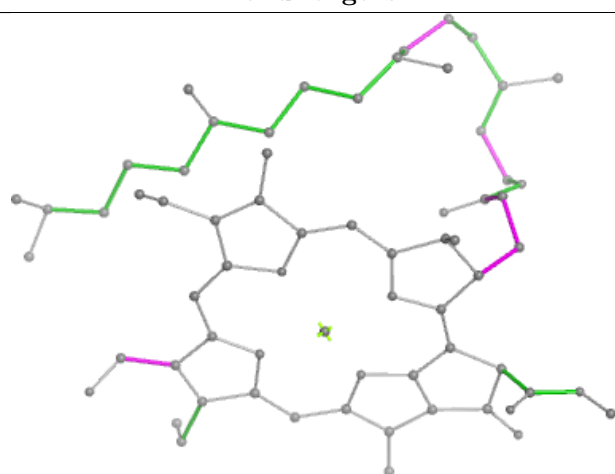
## Ligand CHL r 607



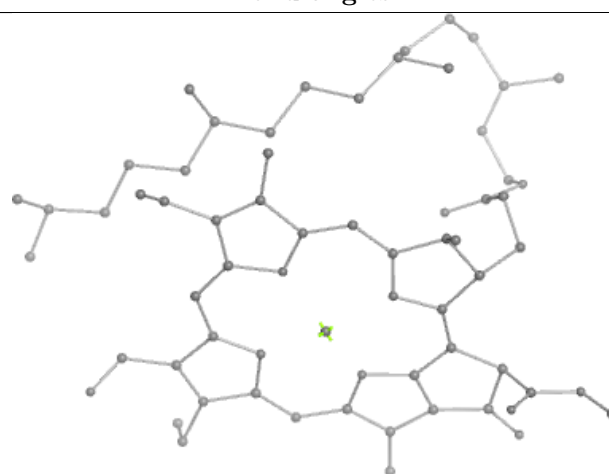
Bond lengths



Bond angles

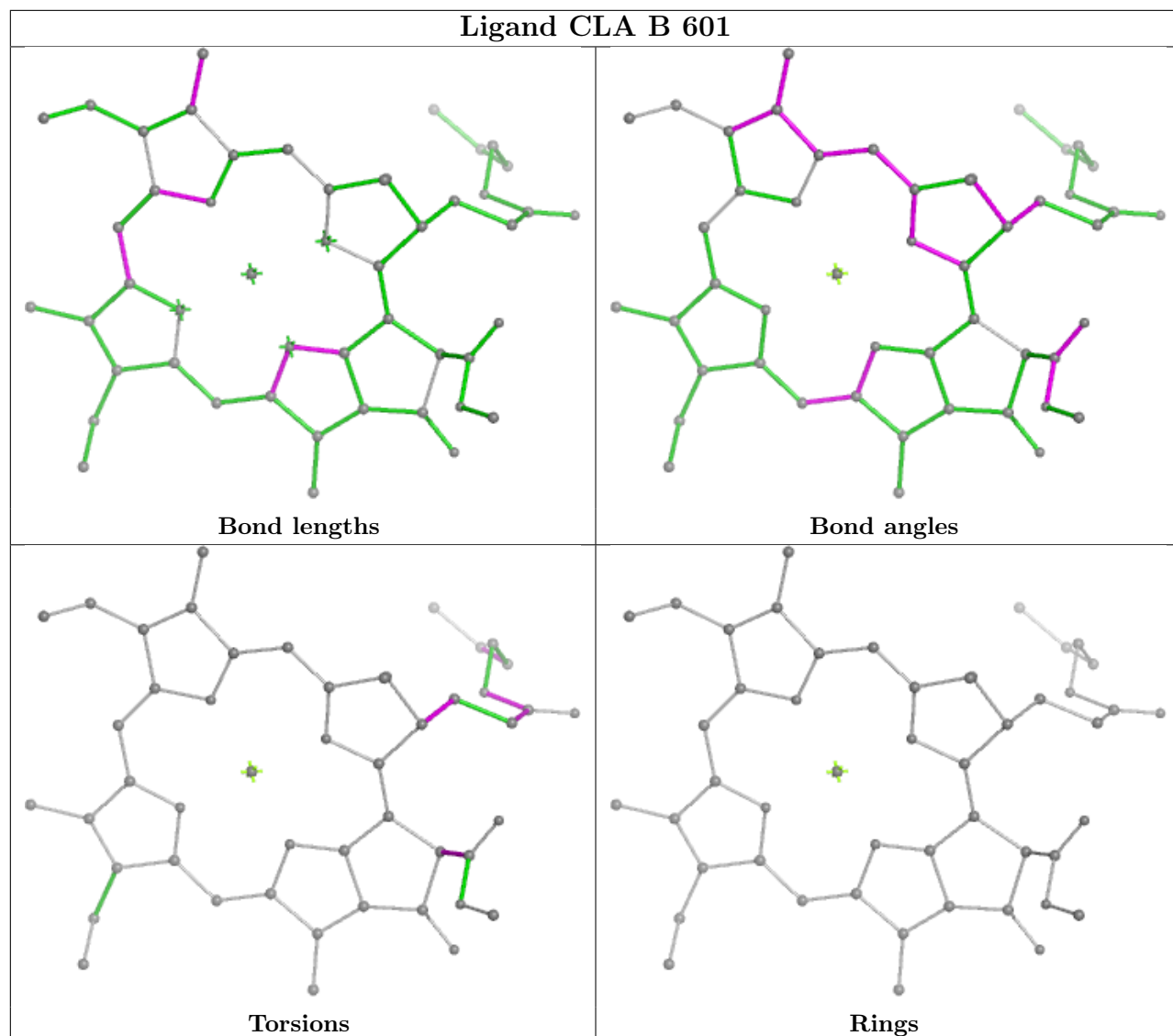


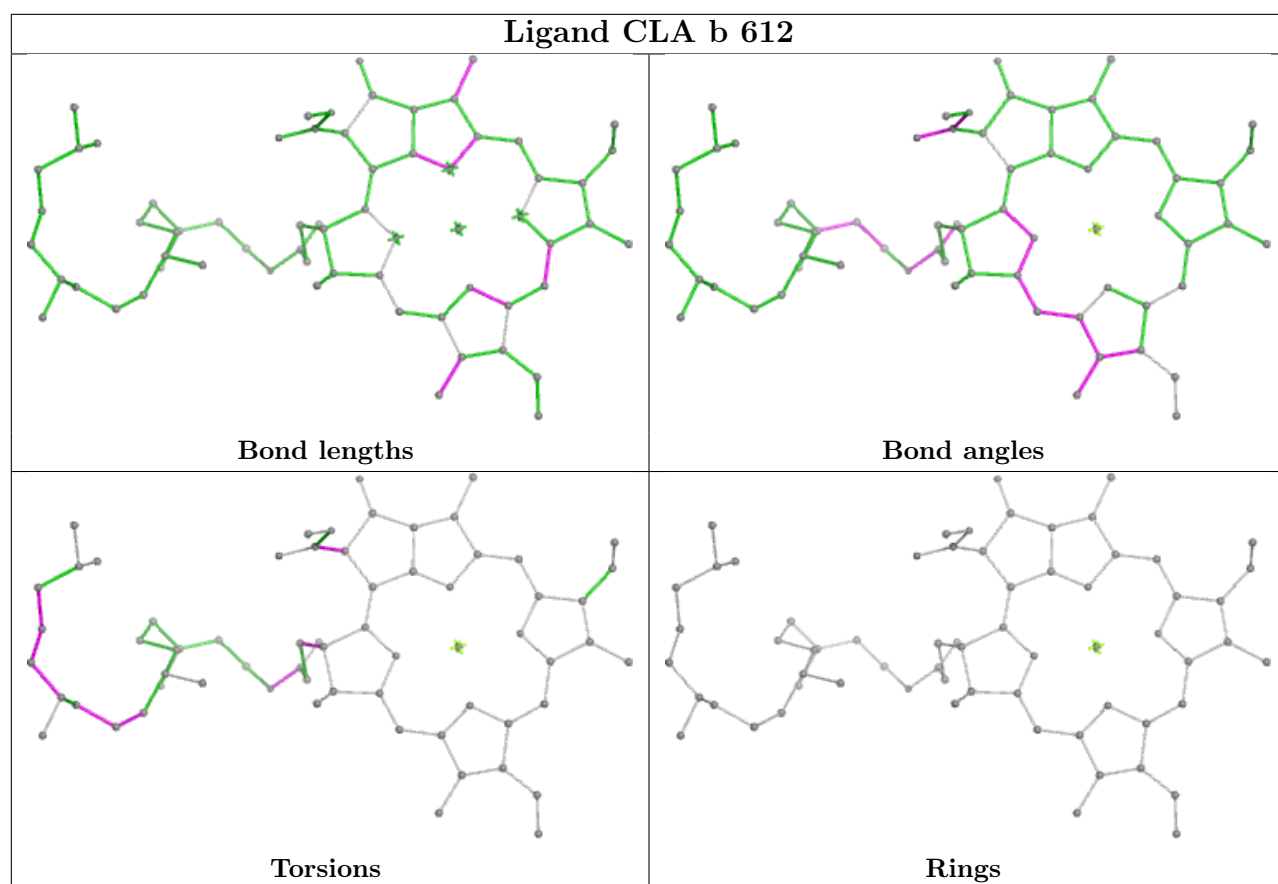
Torsions



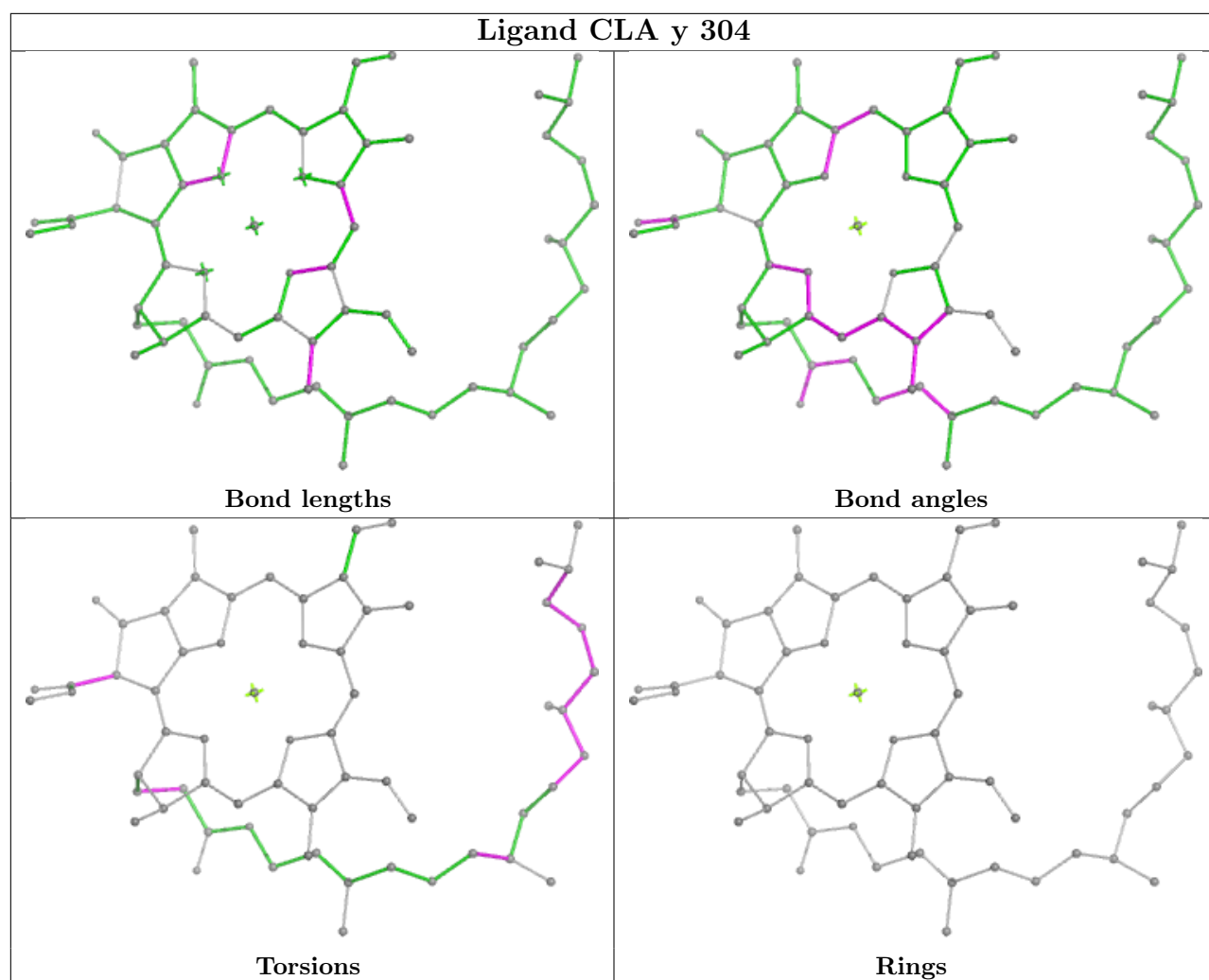
Rings

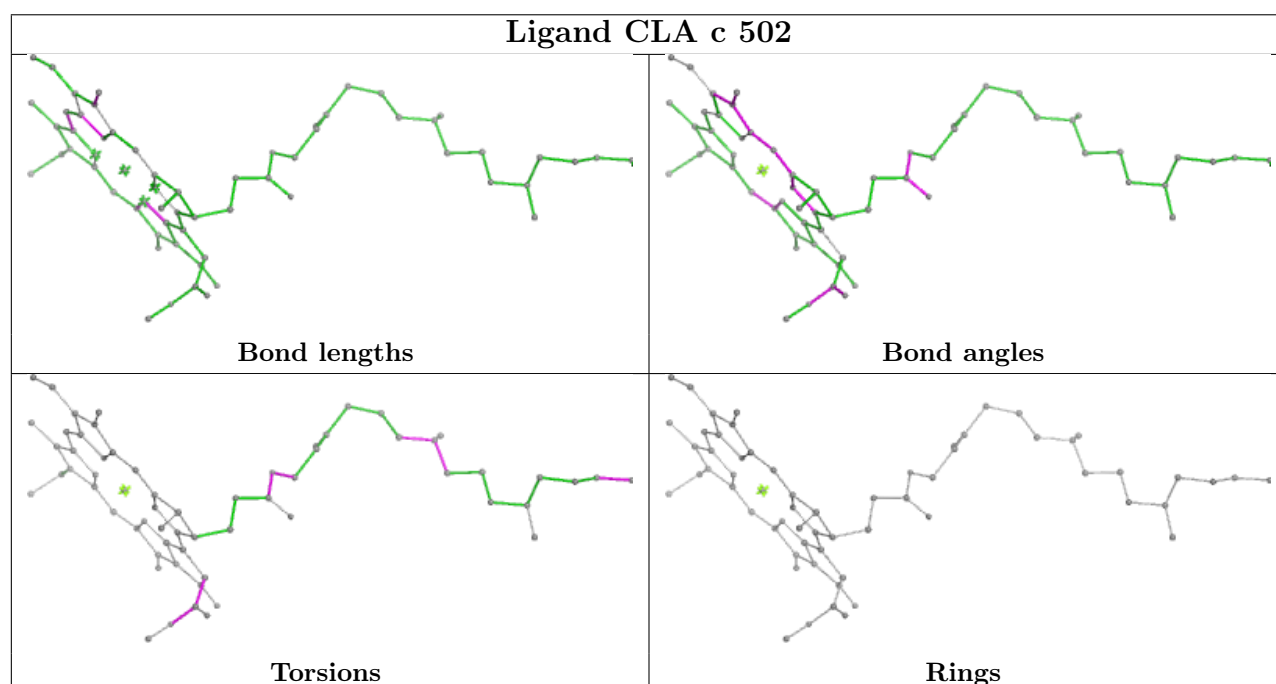
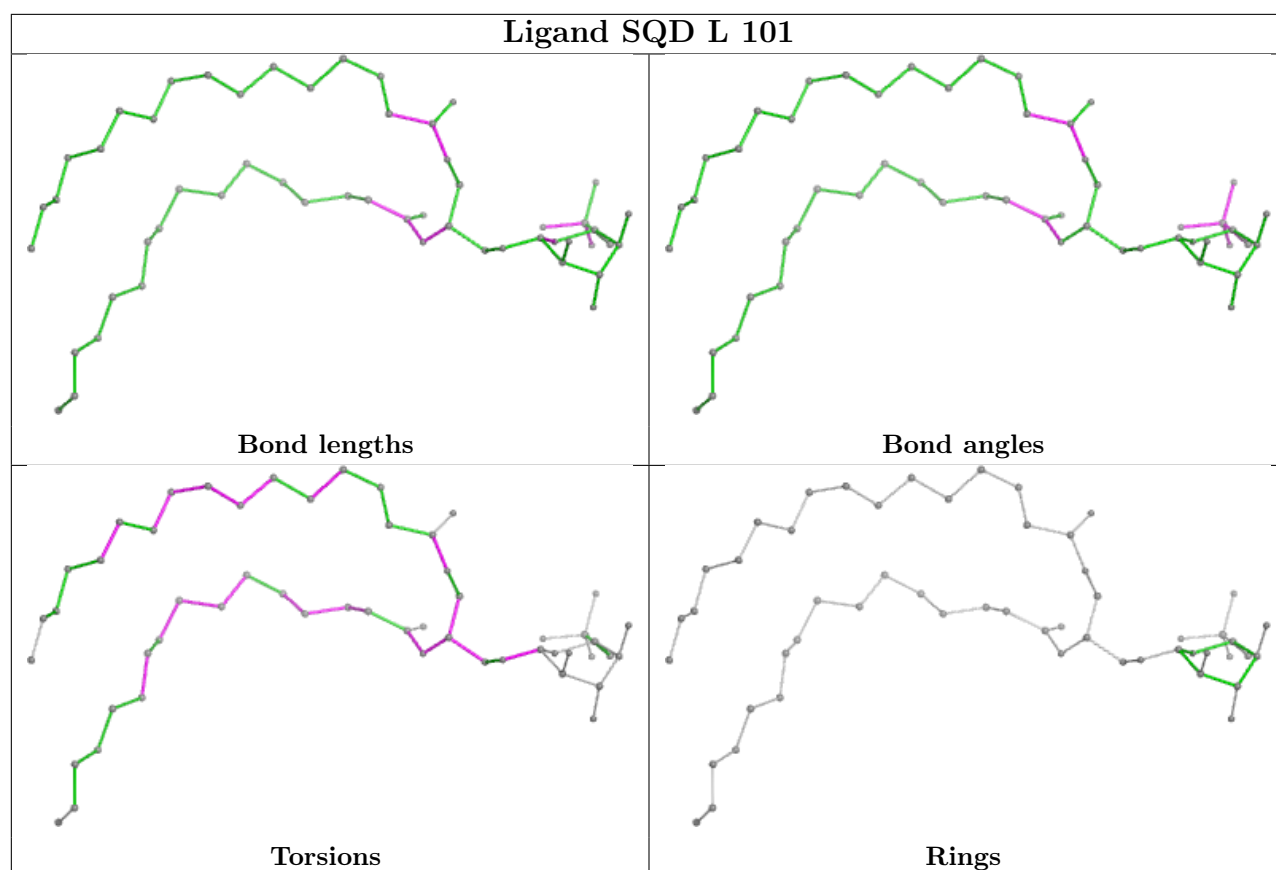
## Ligand CLA B 601

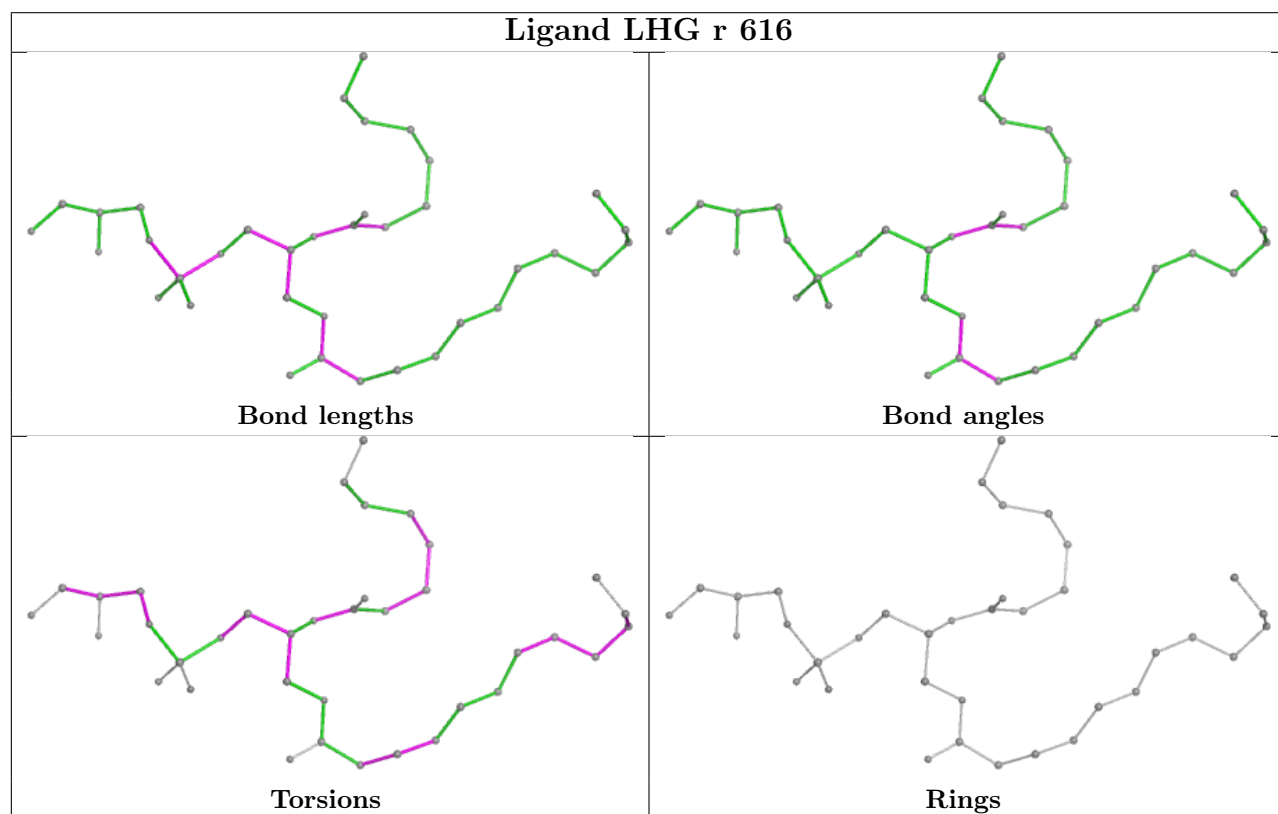
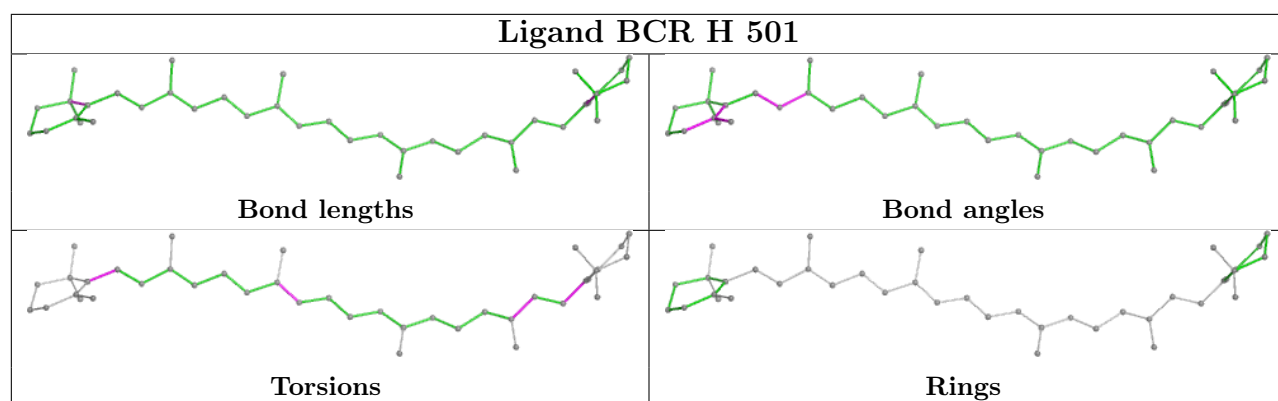


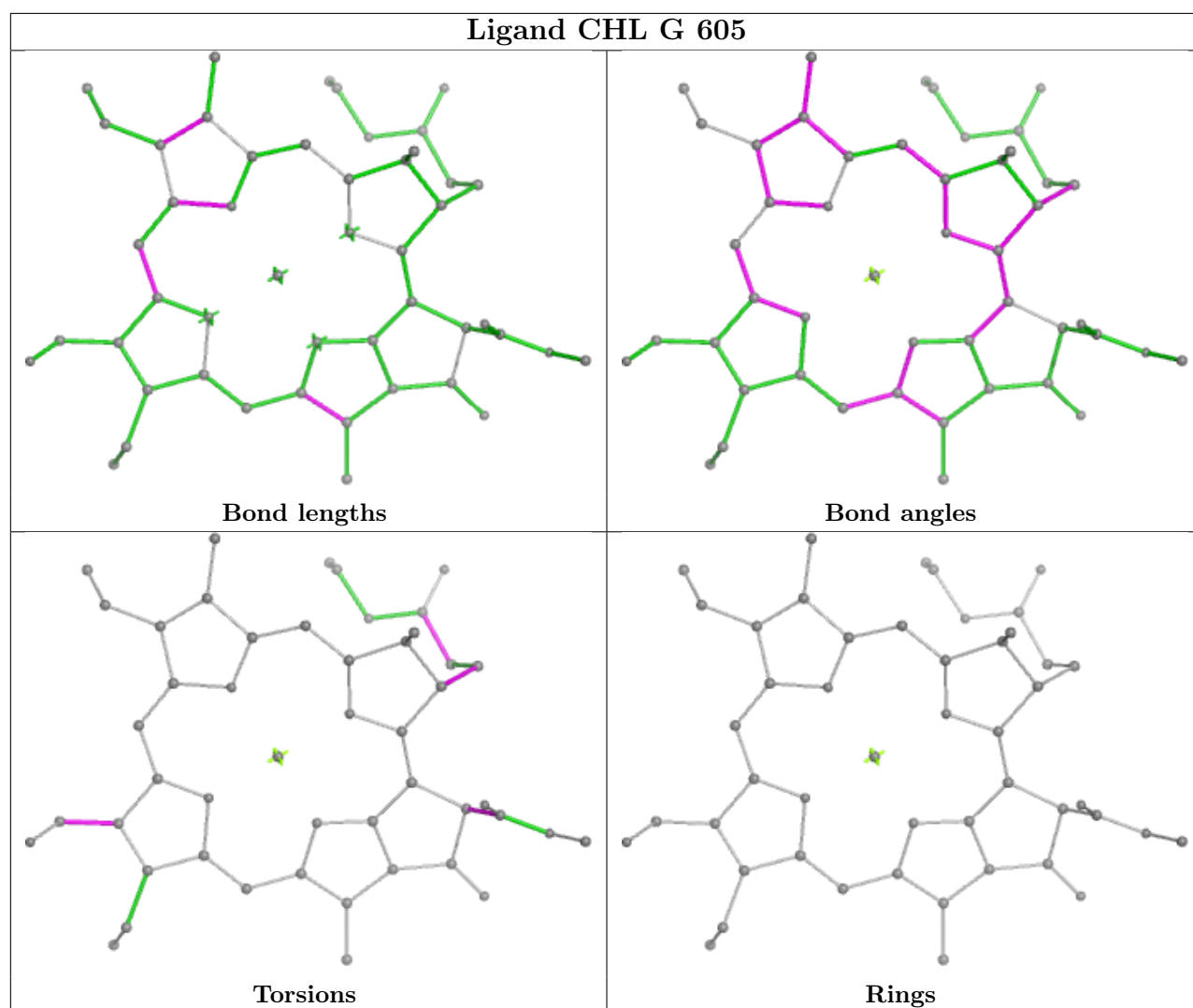




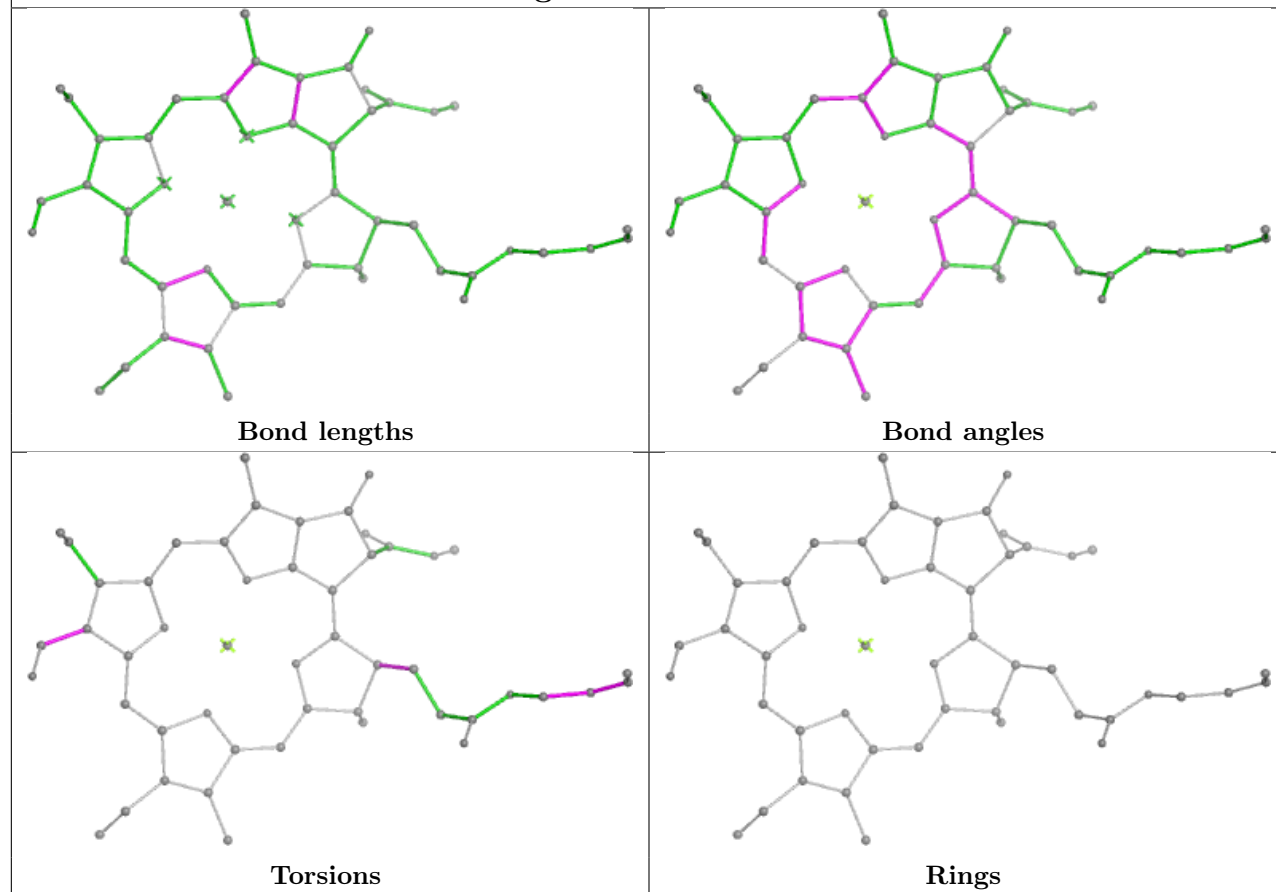




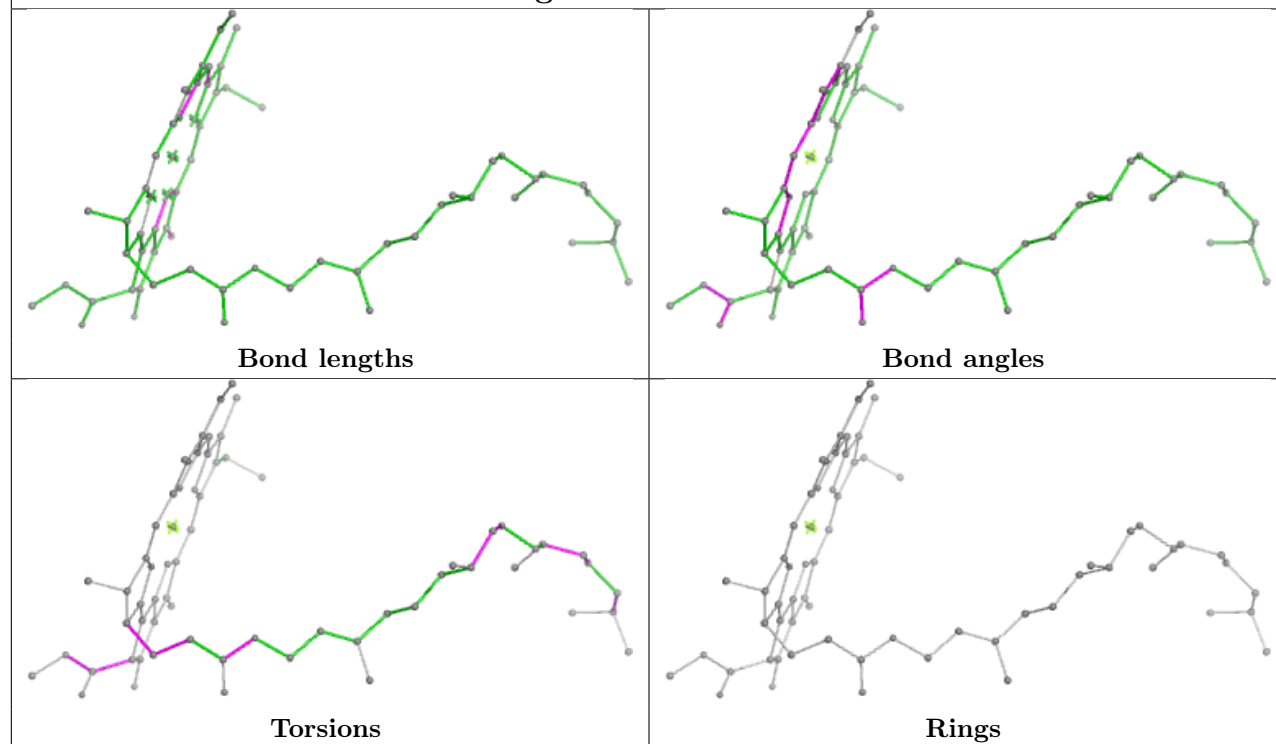




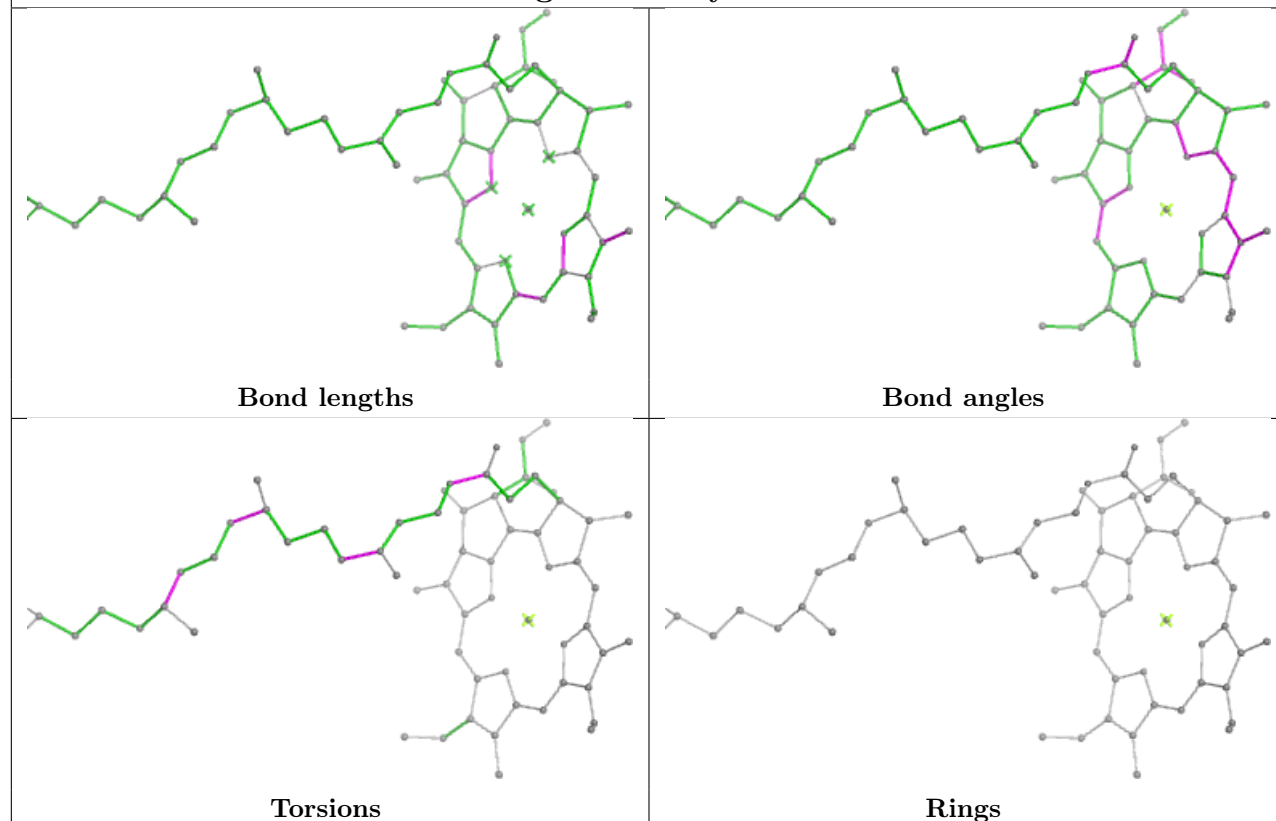
## Ligand CHL S 606



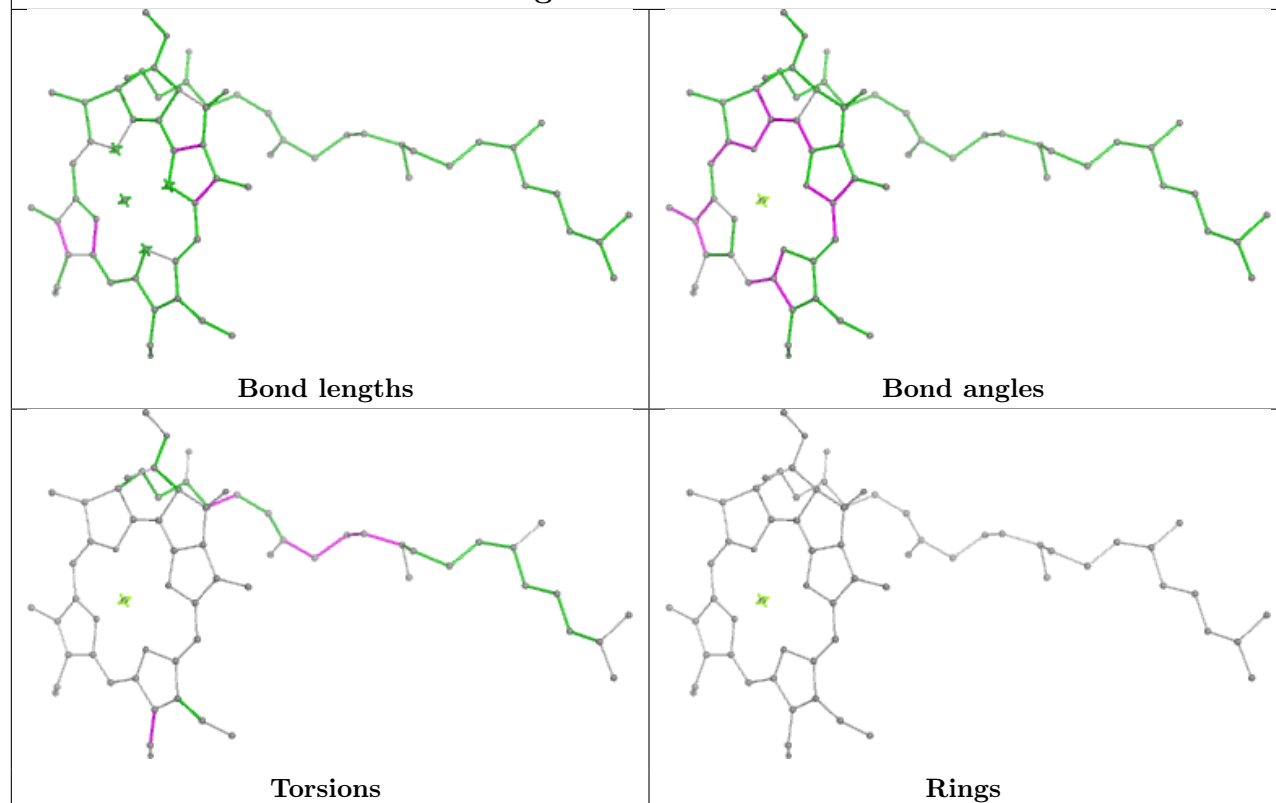
## Ligand CLA b 607

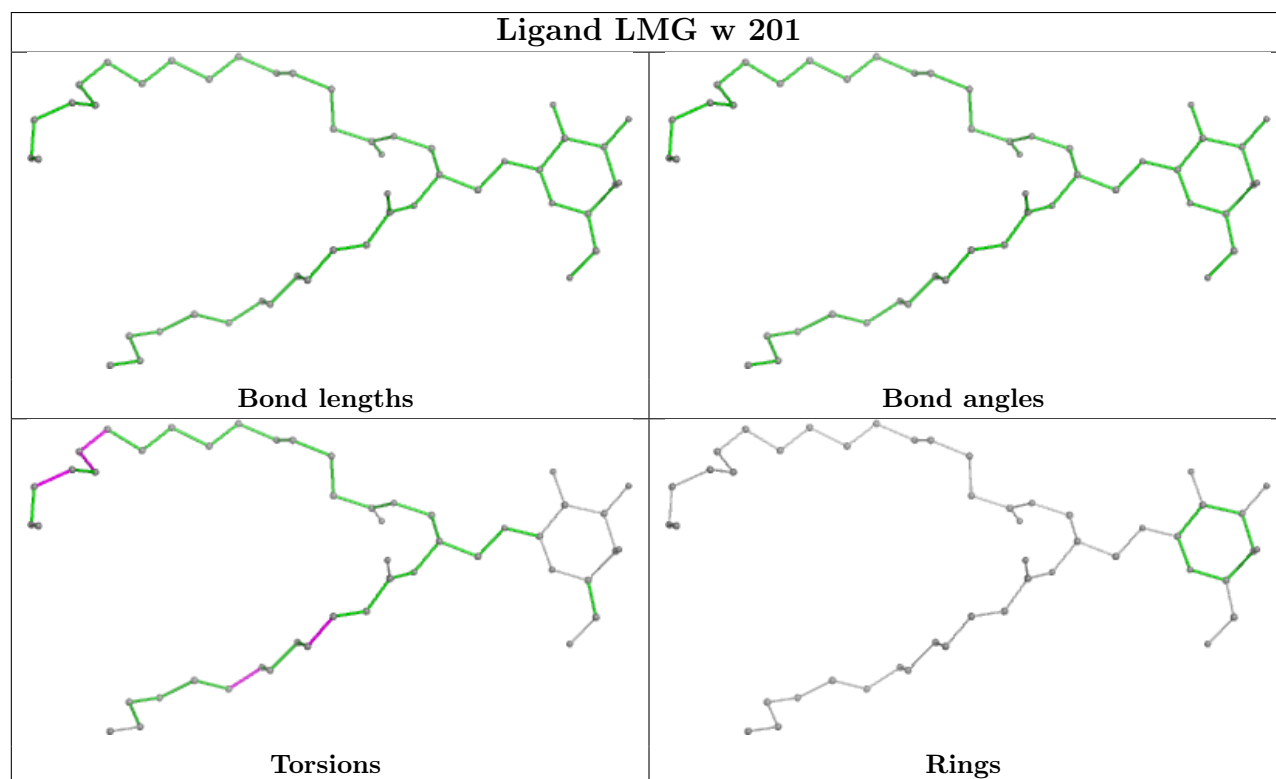
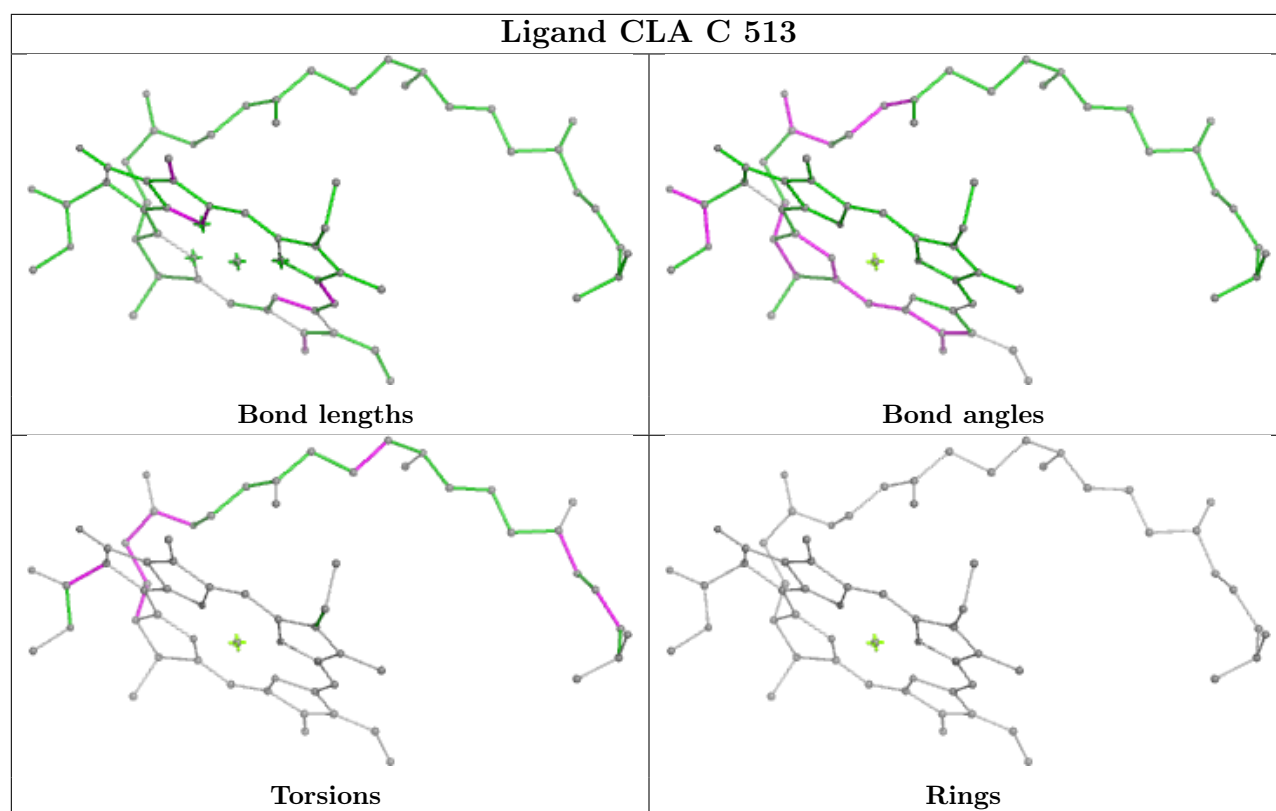


## Ligand CLA y 312

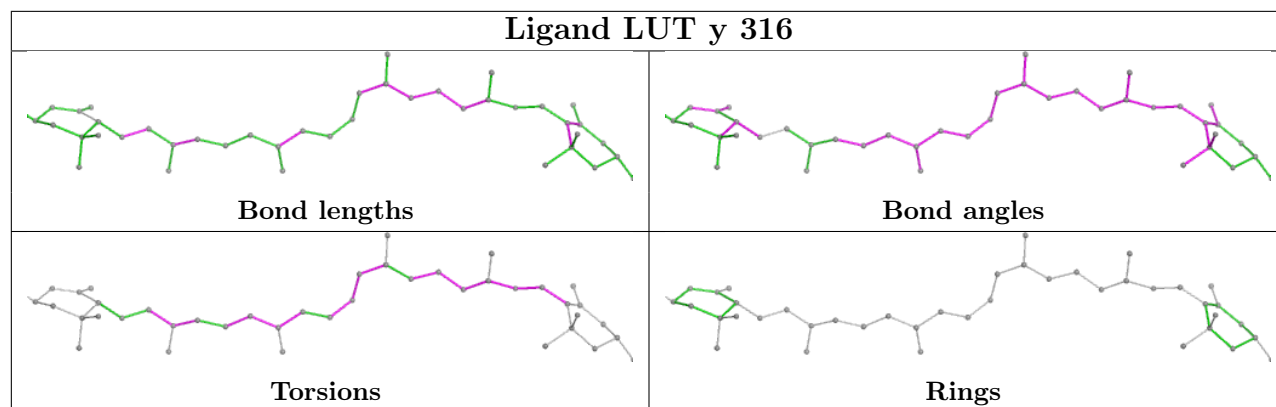


## Ligand CHL n 609

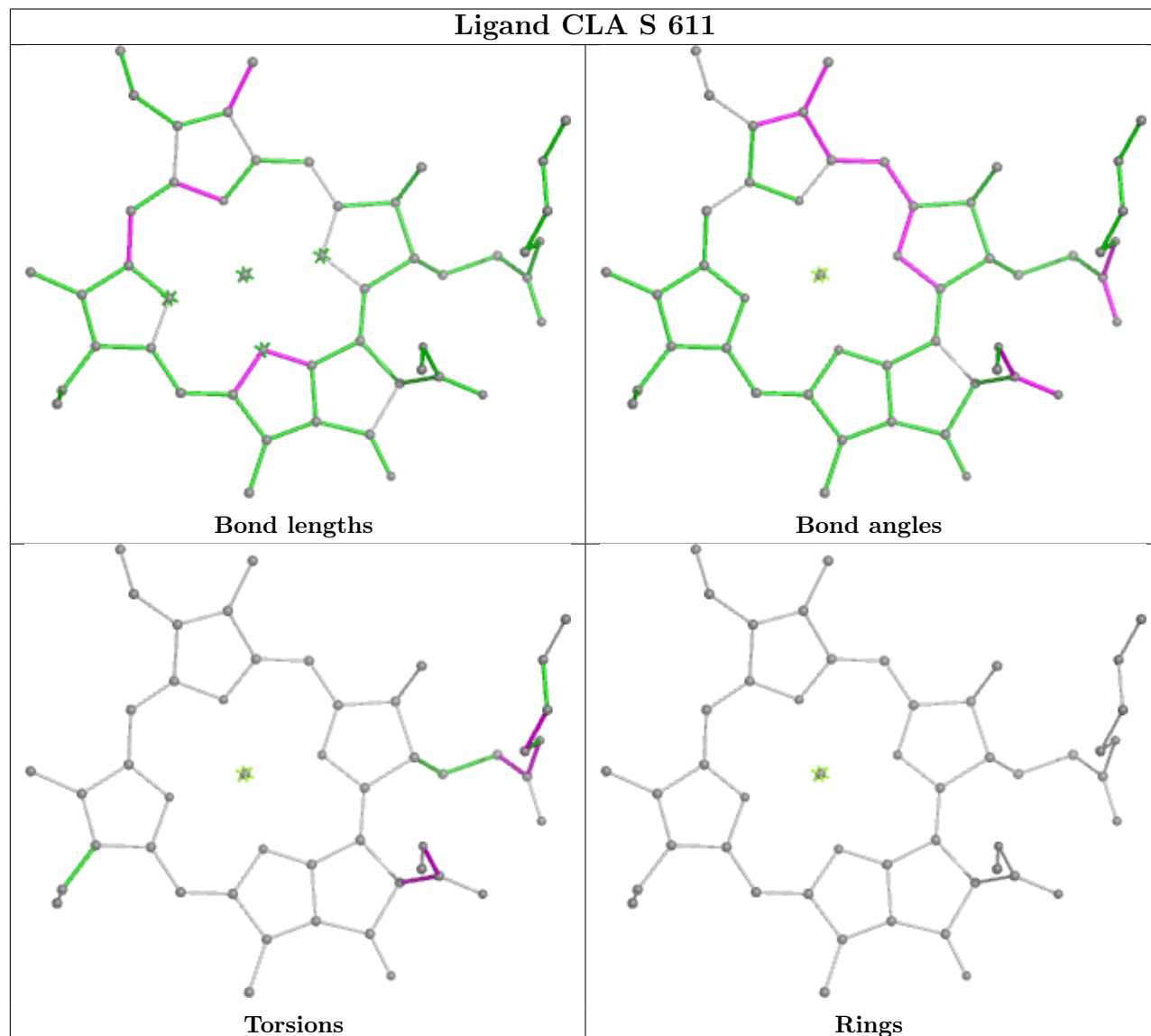




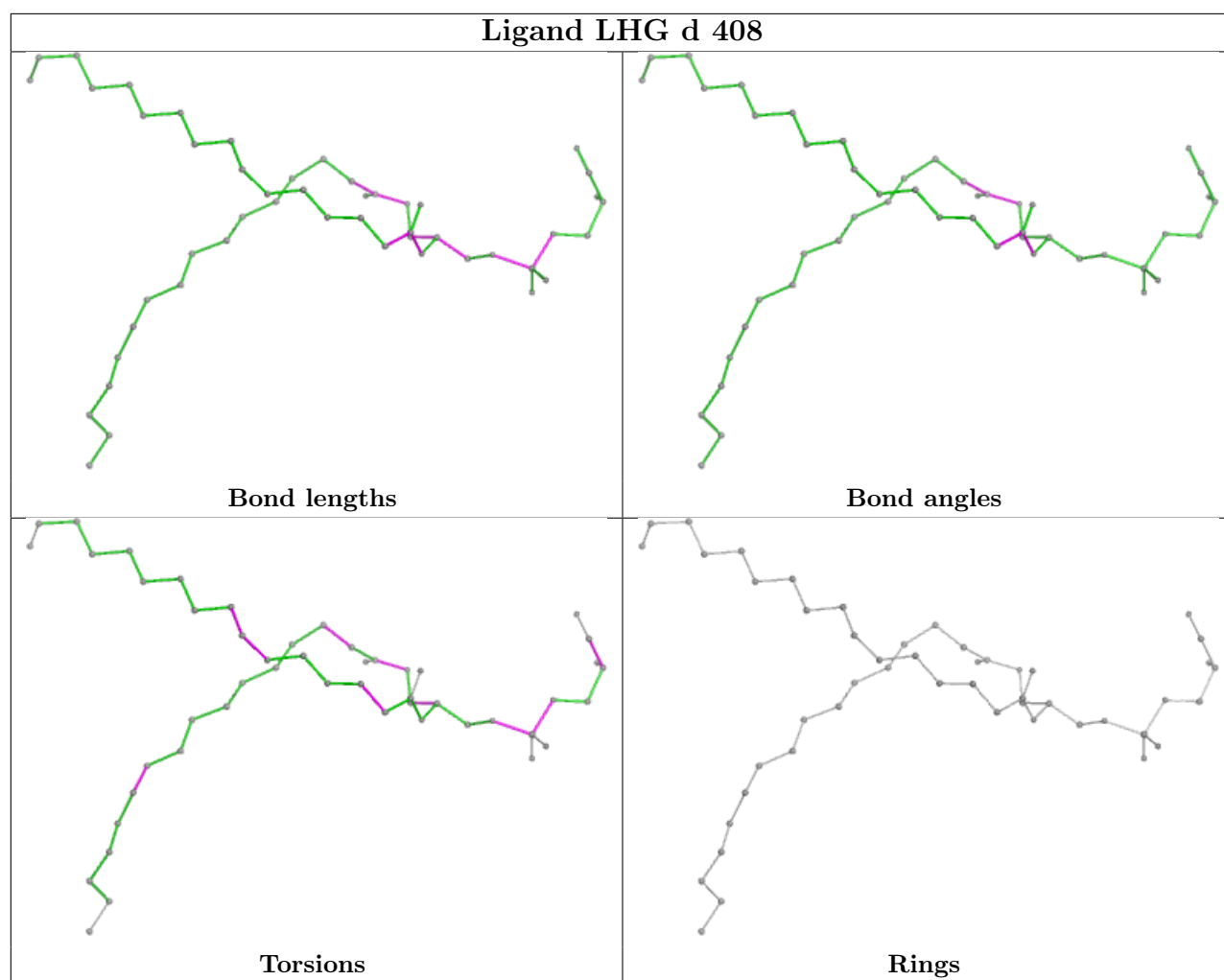
## Ligand LUT y 316

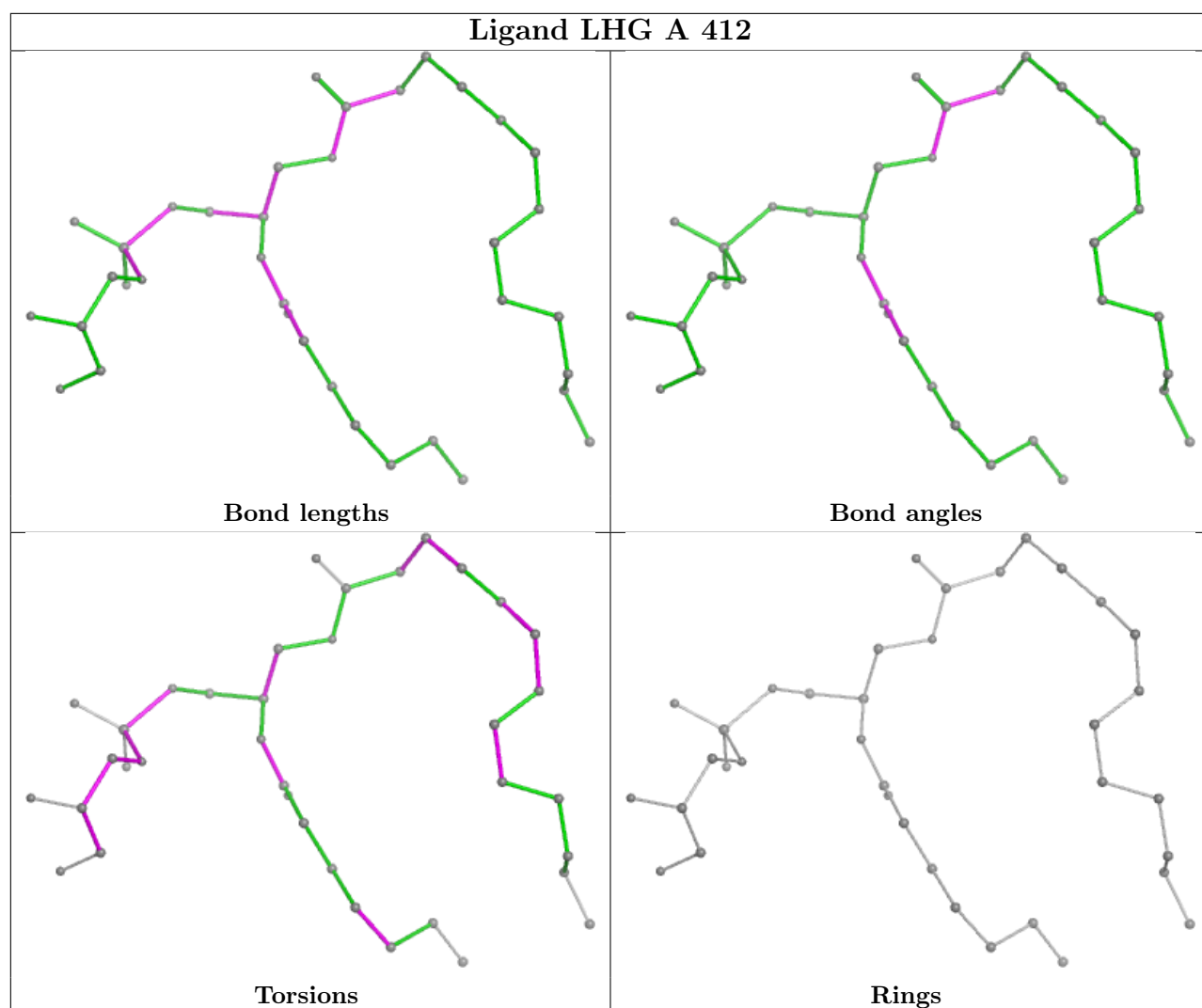


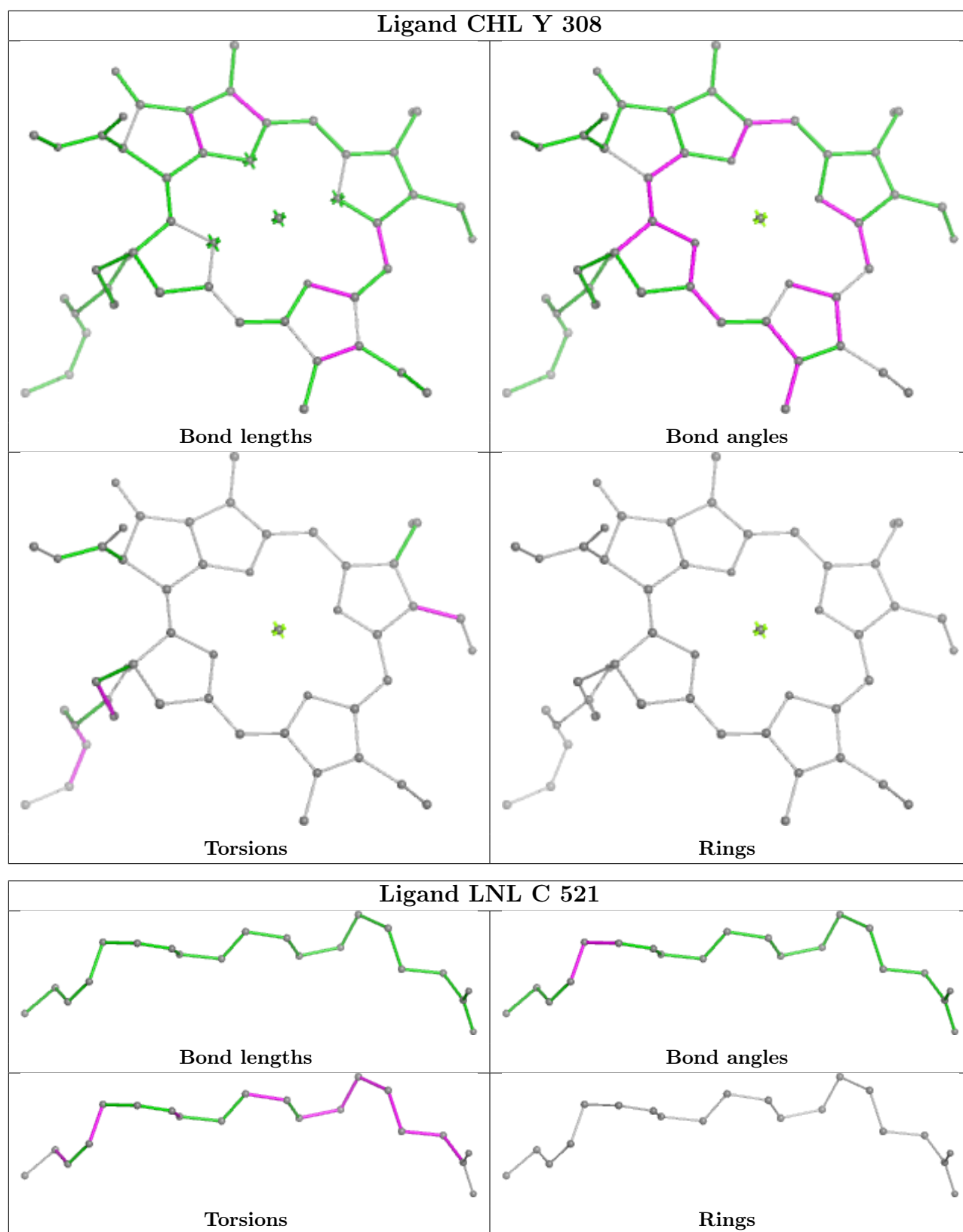
## Ligand CLA S 611

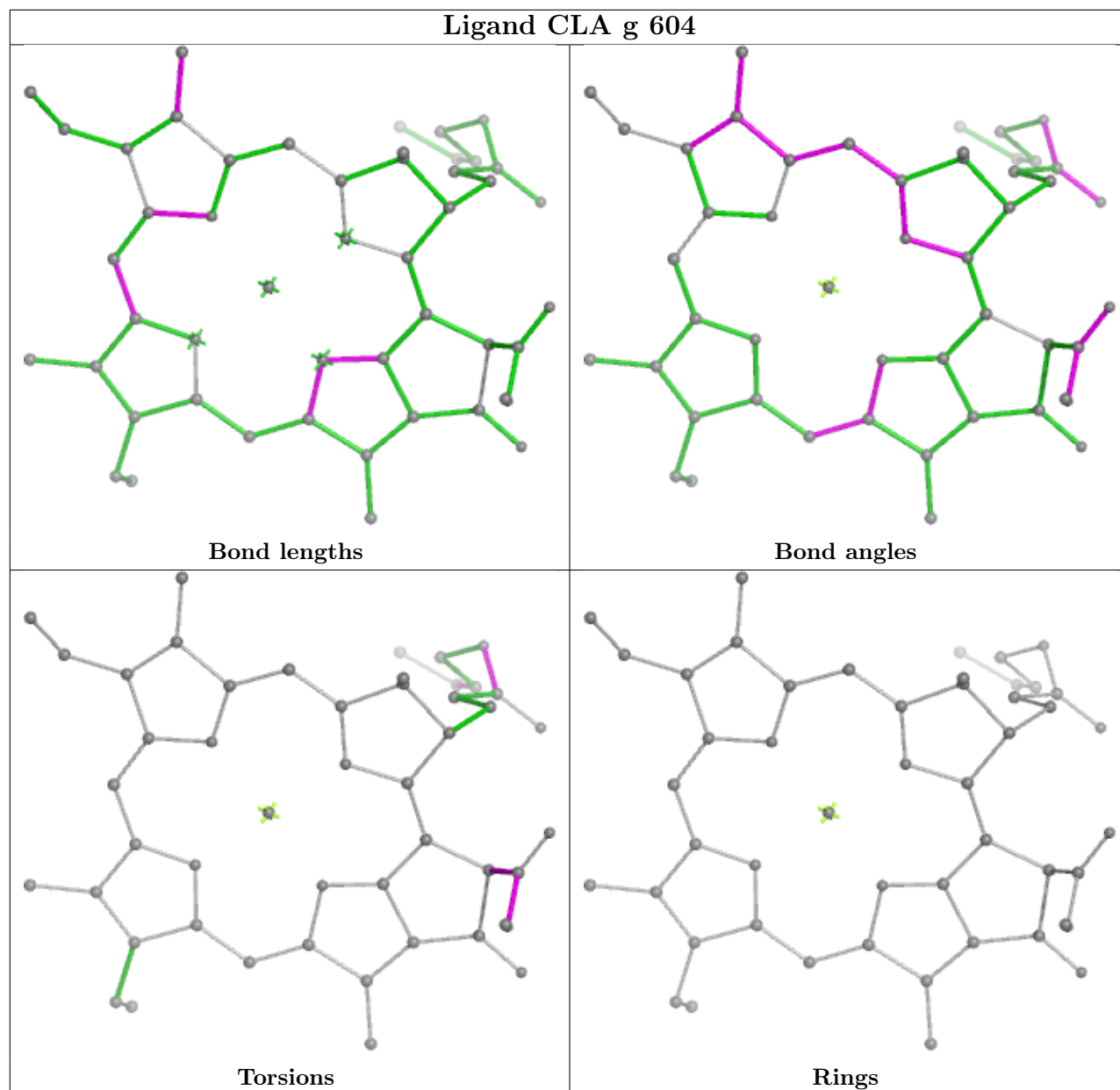


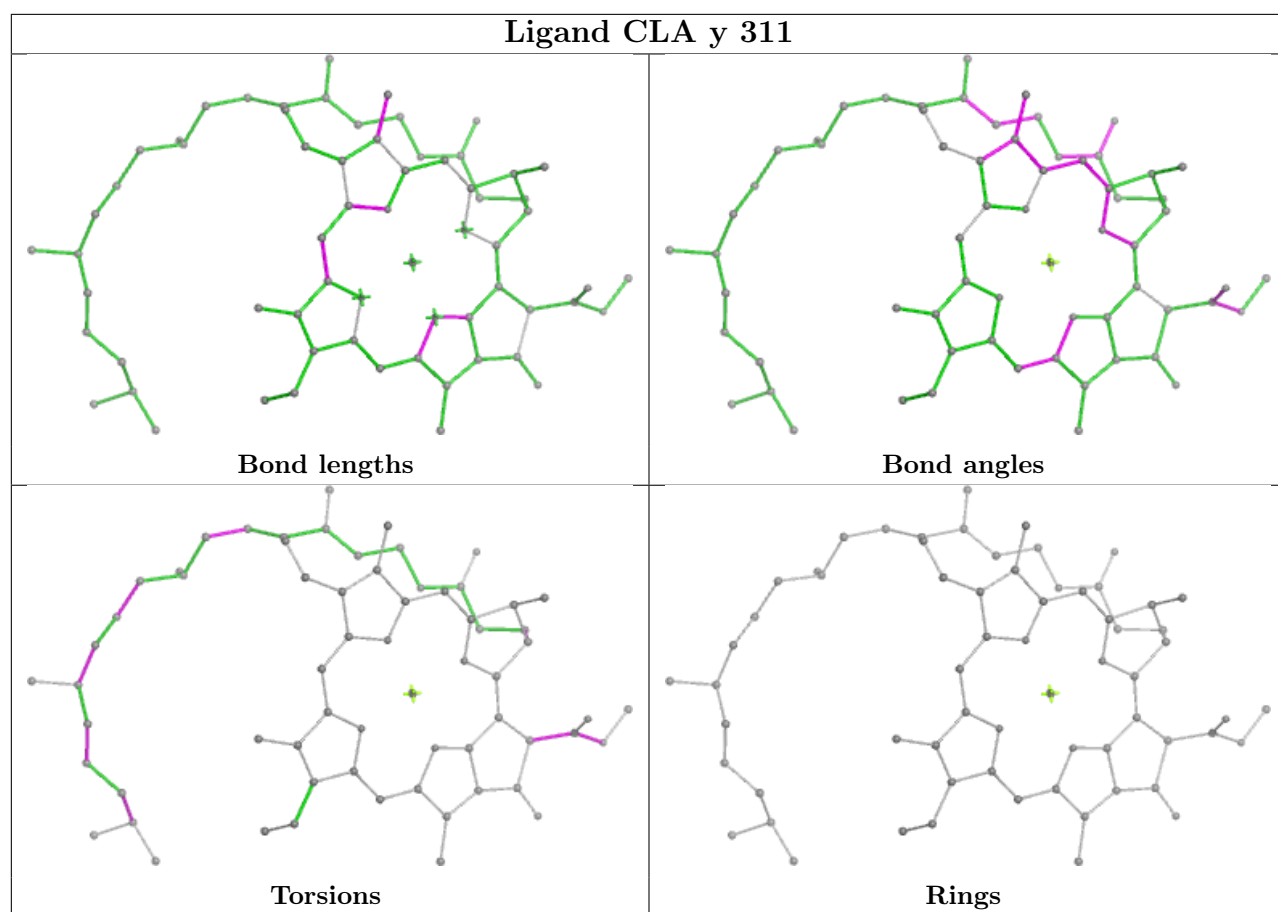




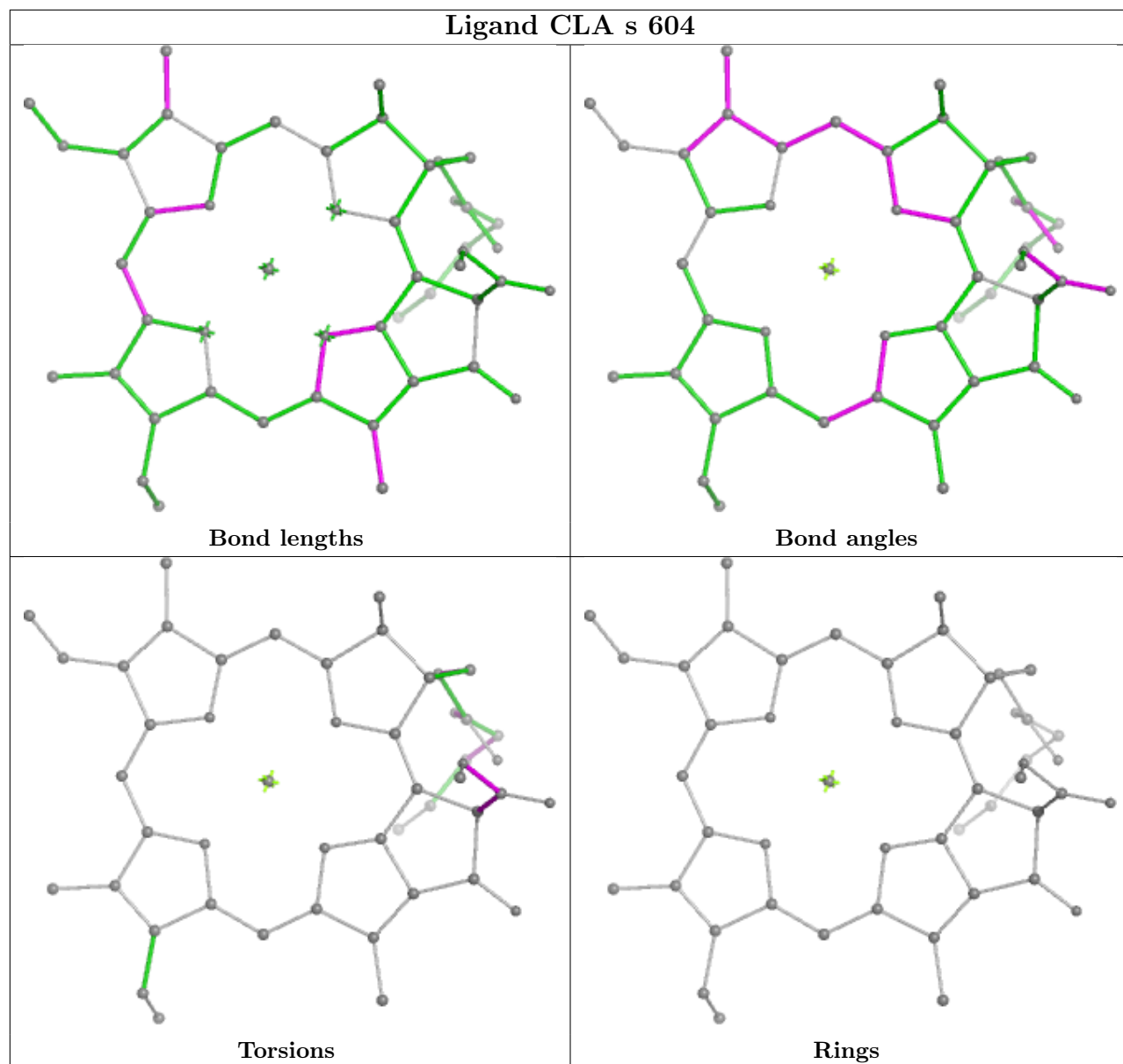




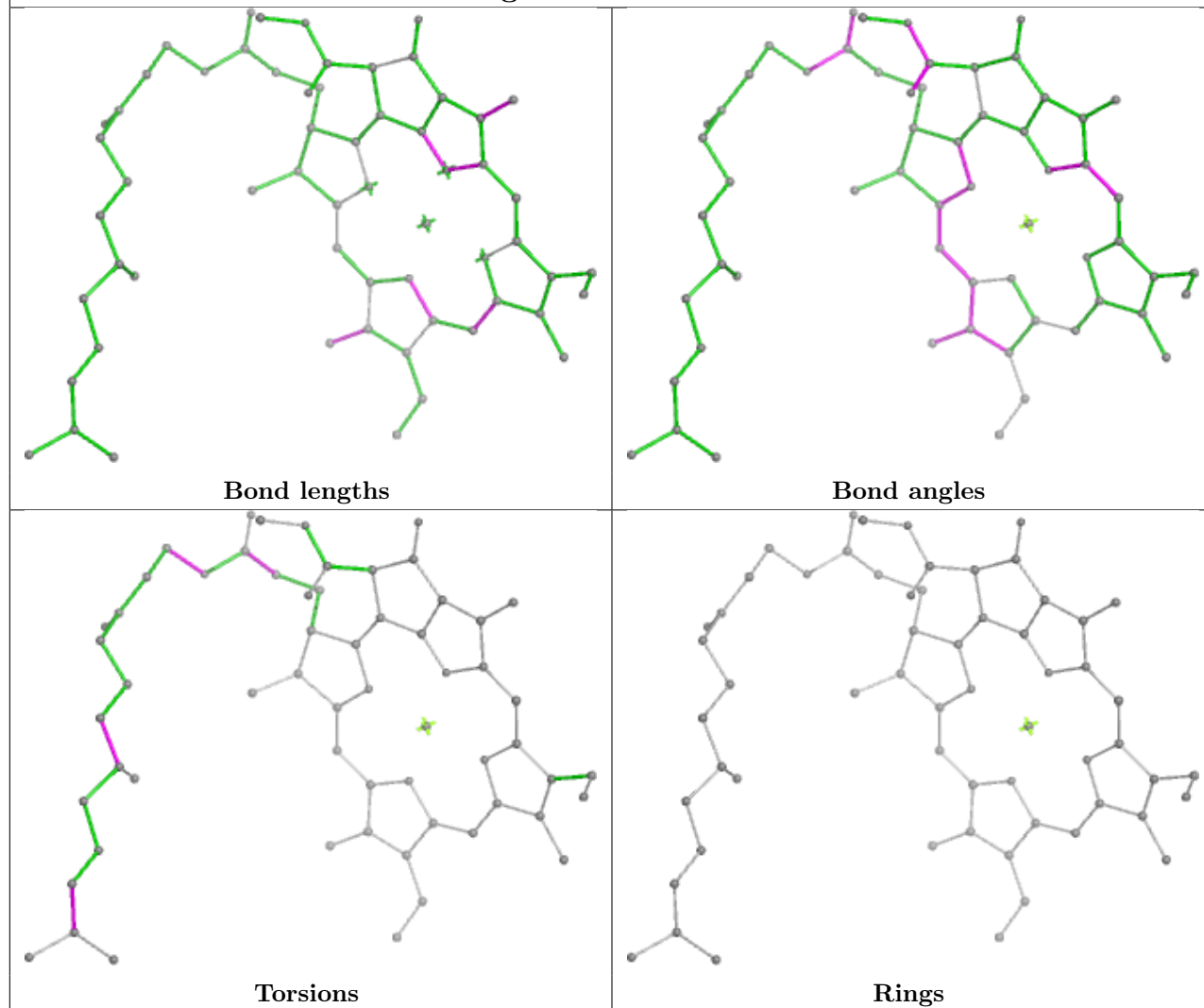




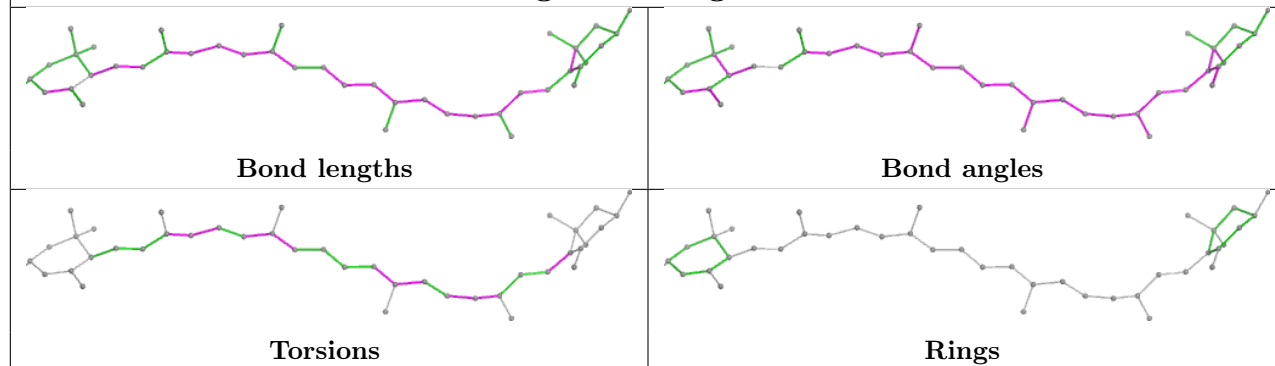
## Ligand CLA s 604

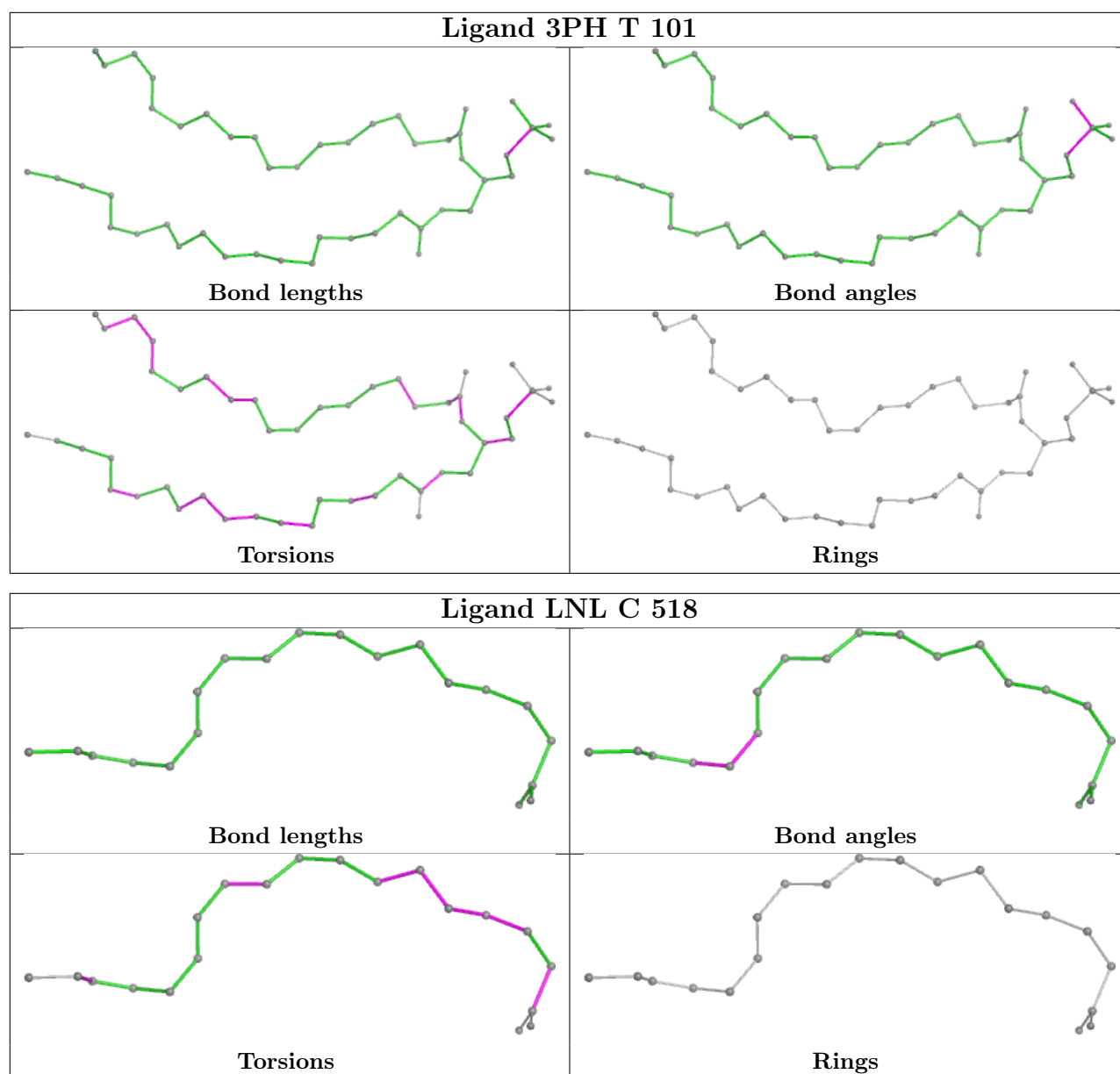


## Ligand CLA R 603

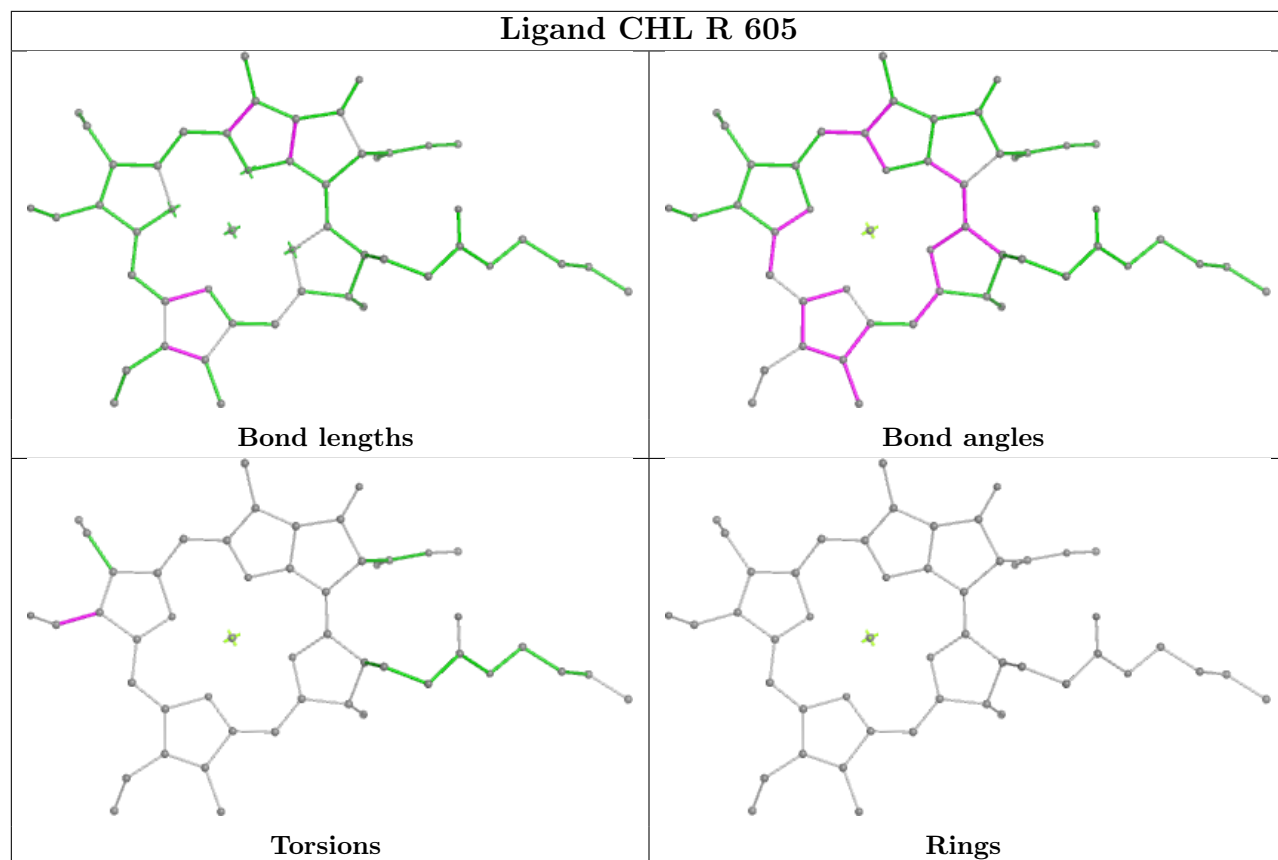


## Ligand LUT g 616

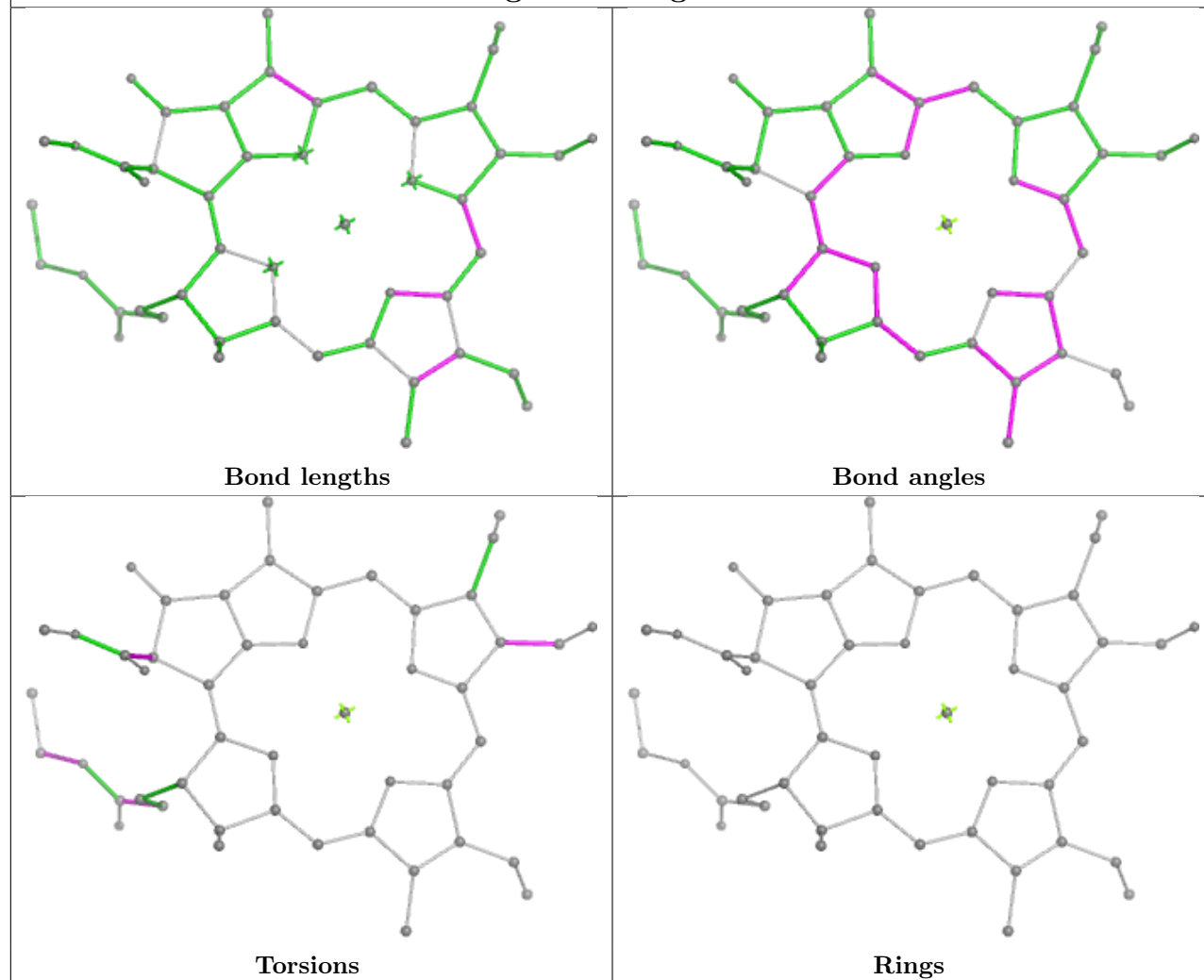




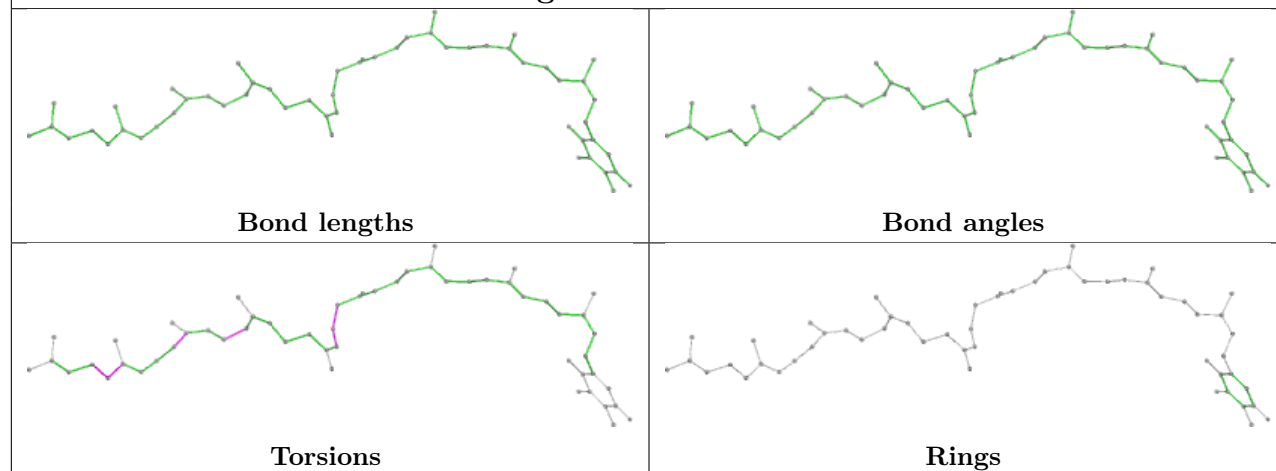


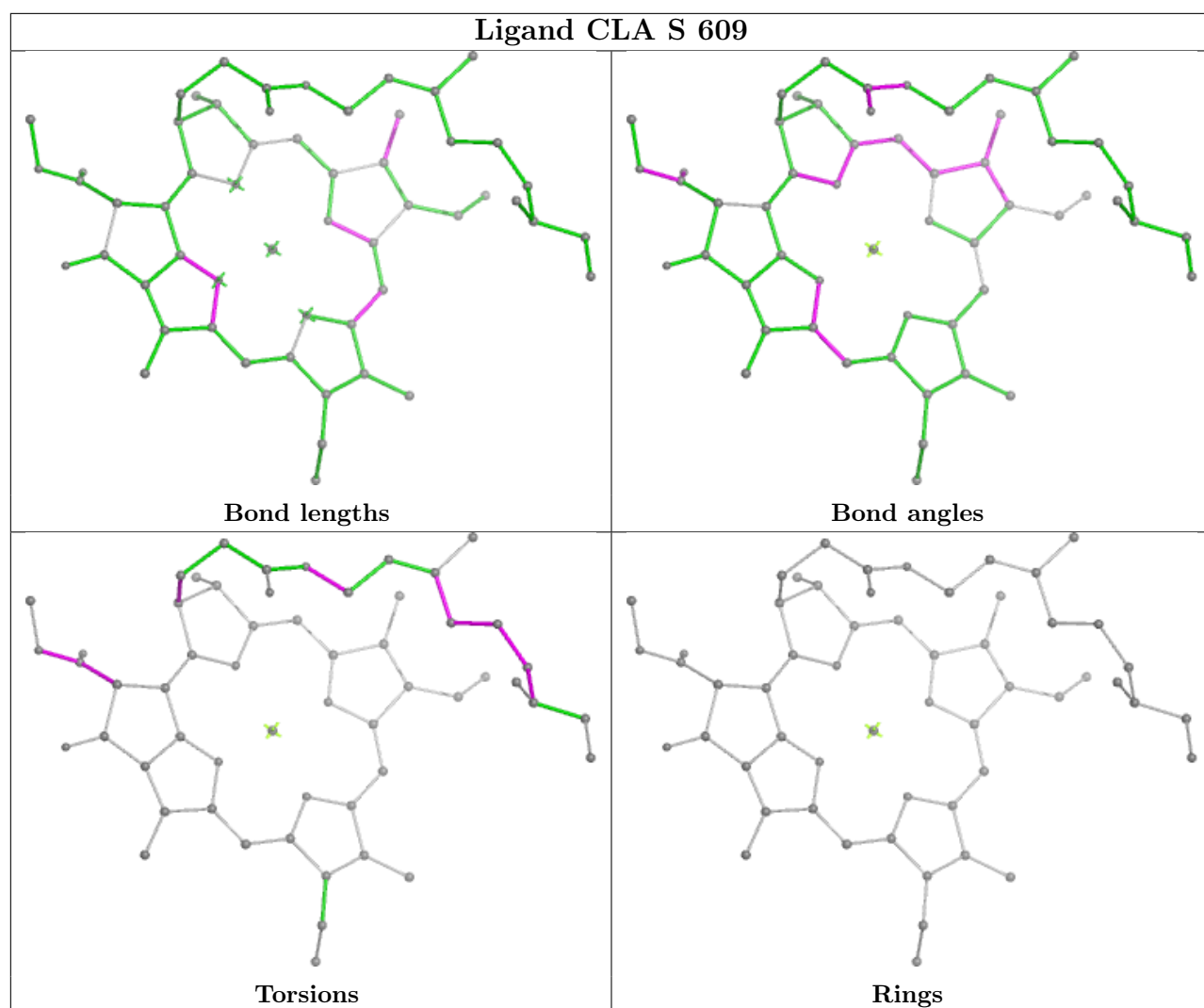


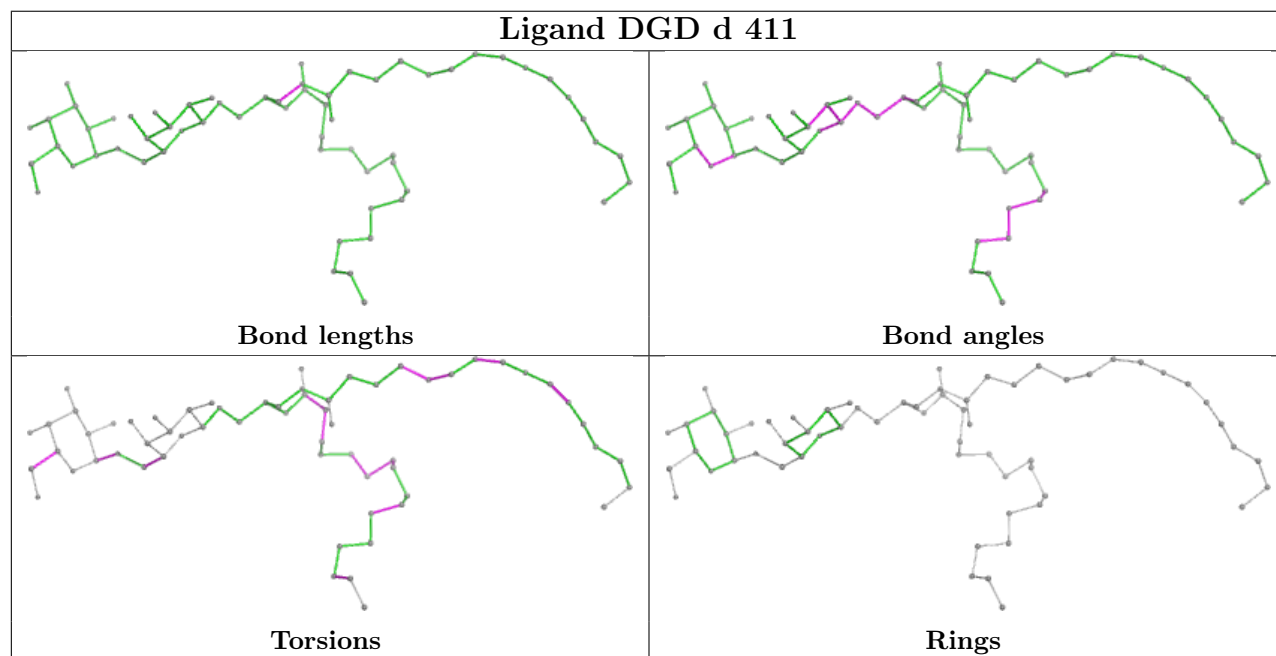
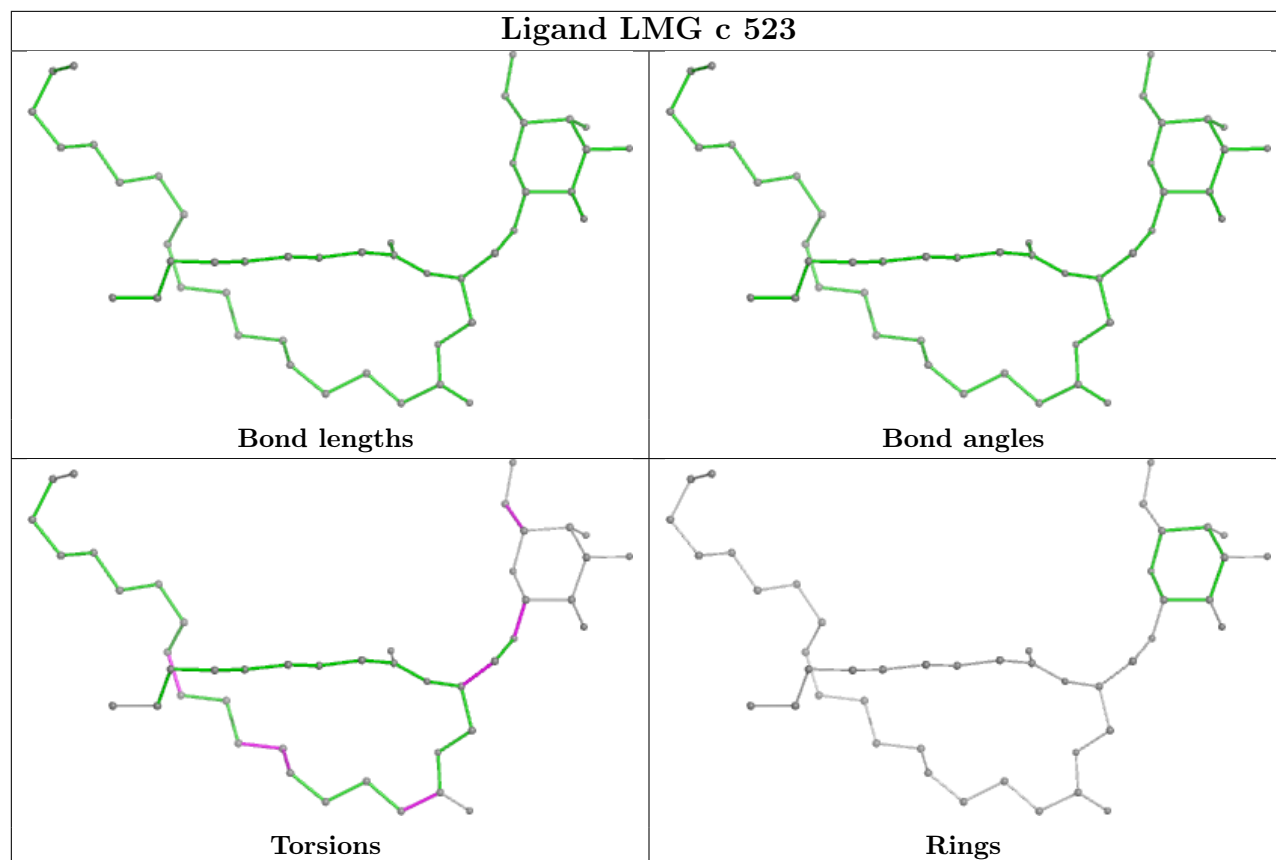
## Ligand CHL g 605

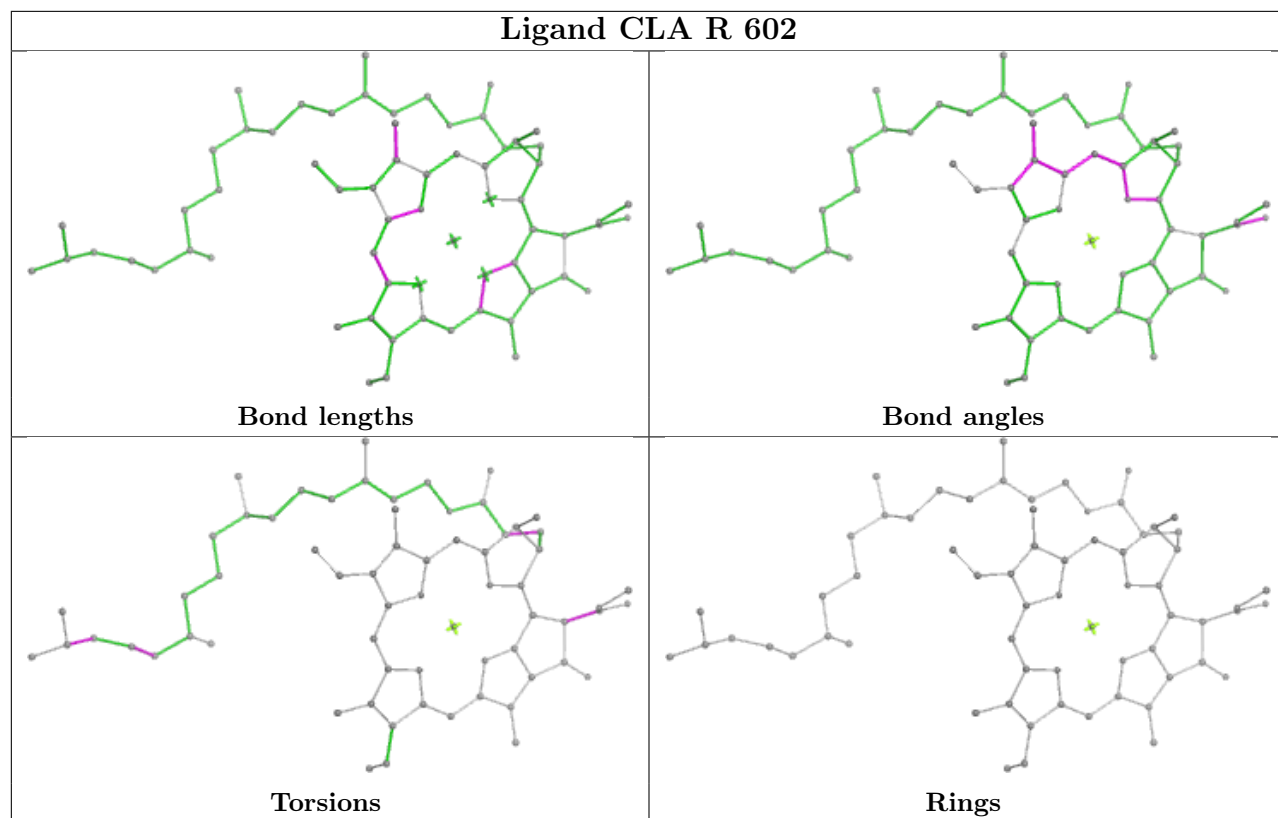


## Ligand PL9 A 411

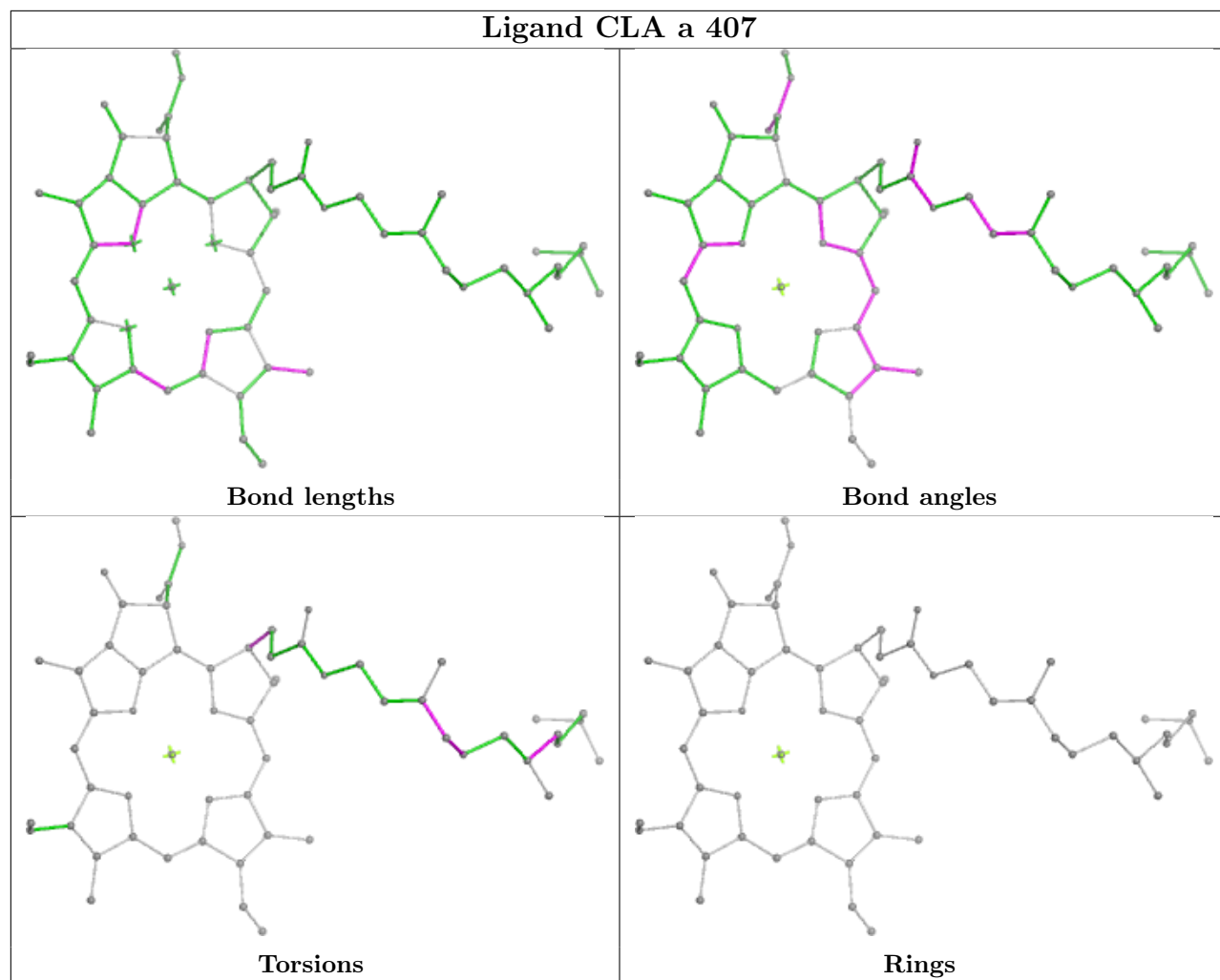




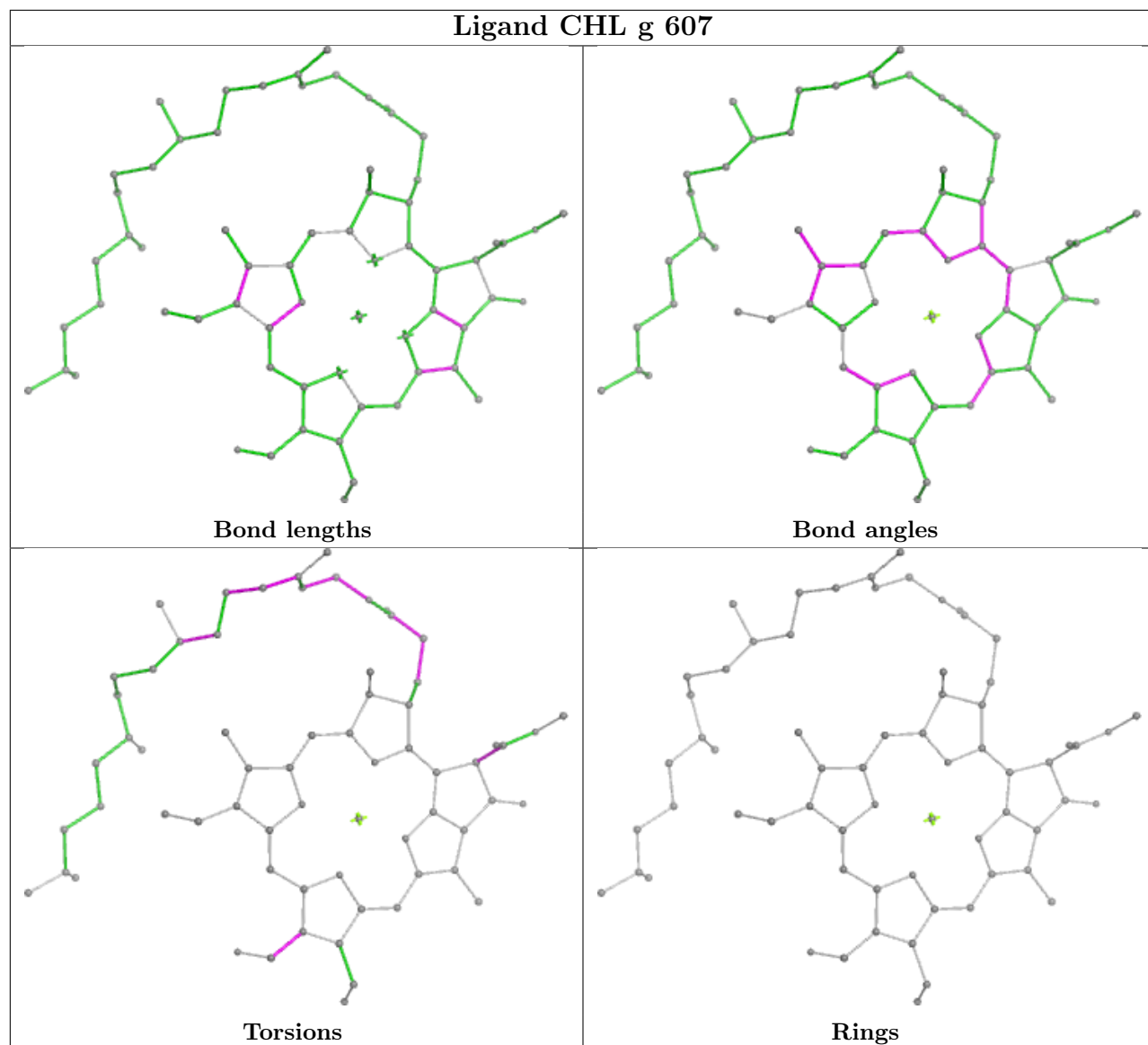




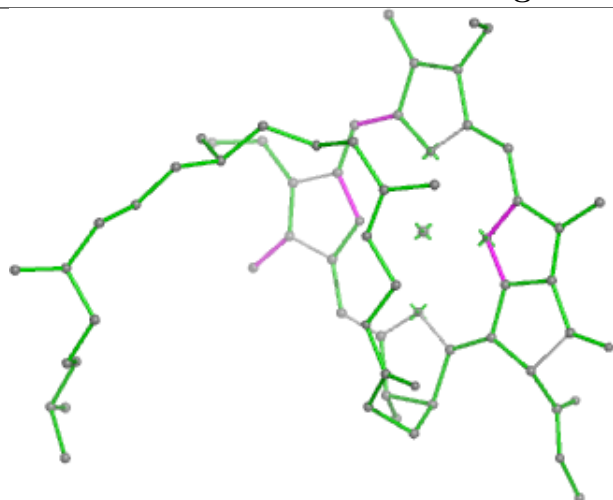
## Ligand CLA a 407



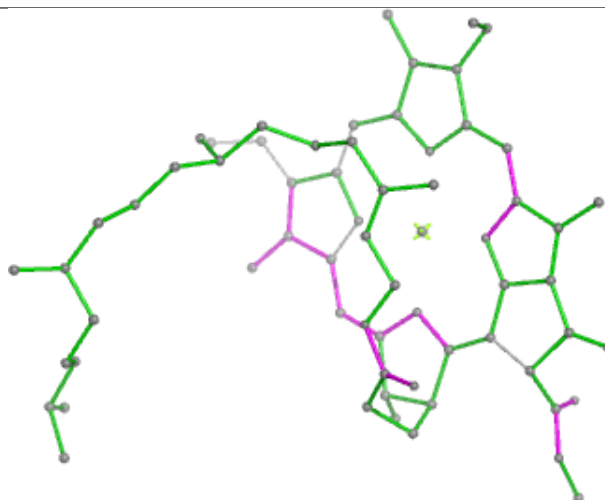
## Ligand CHL g 607



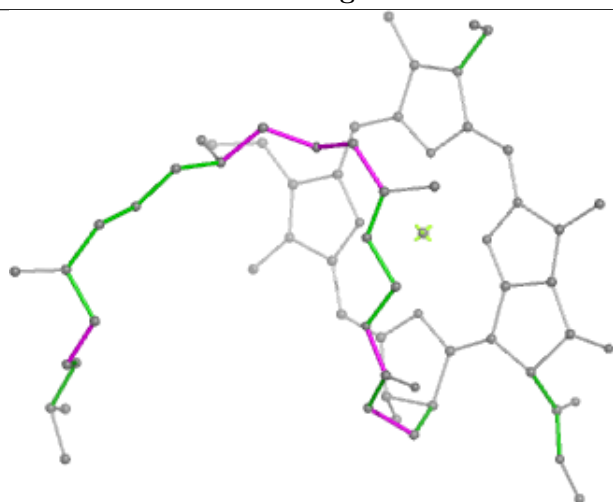
## Ligand CLA Y 313



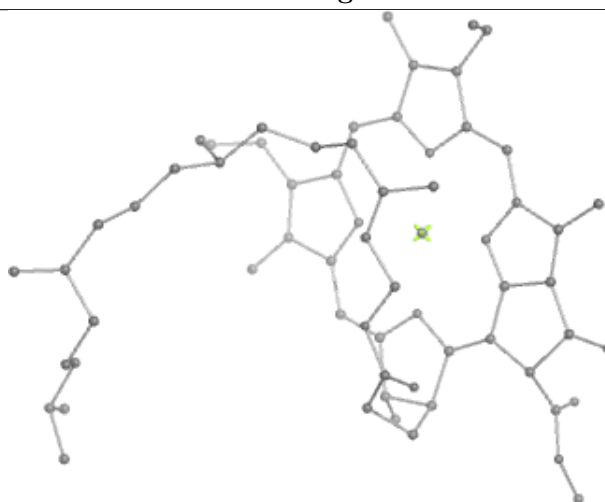
Bond lengths



Bond angles



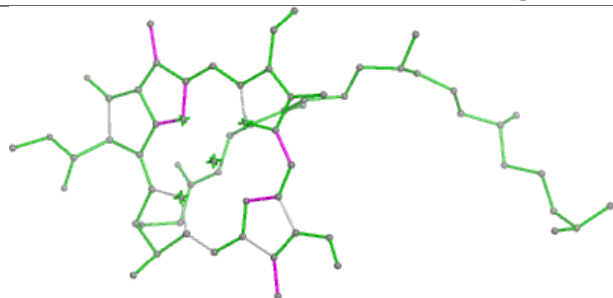
Torsions



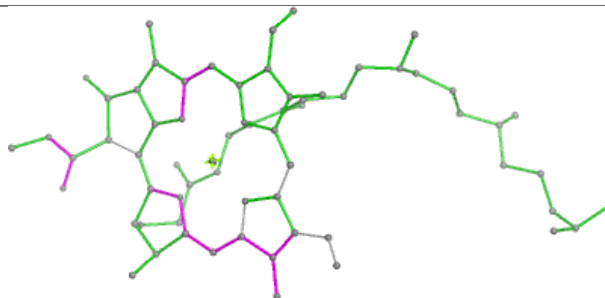
Rings



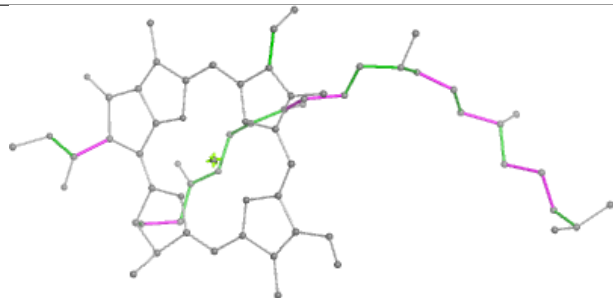
## Ligand CLA B 614



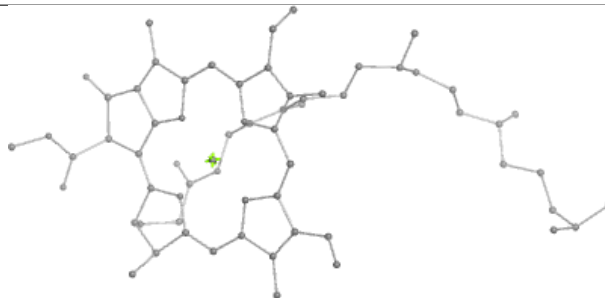
Bond lengths



Bond angles

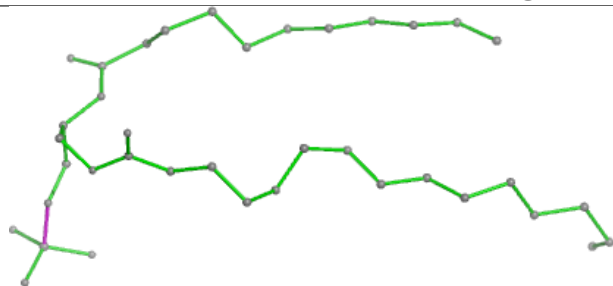


Torsions

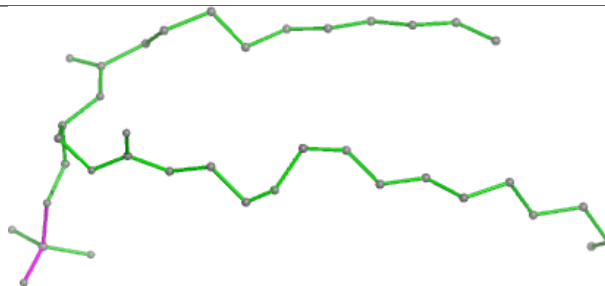


Rings

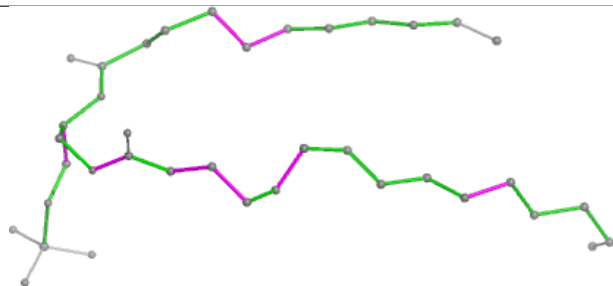
## Ligand 3PH d 403



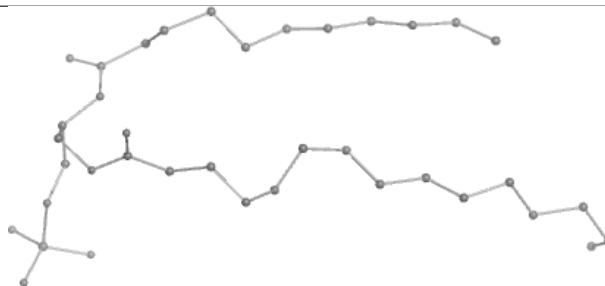
Bond lengths



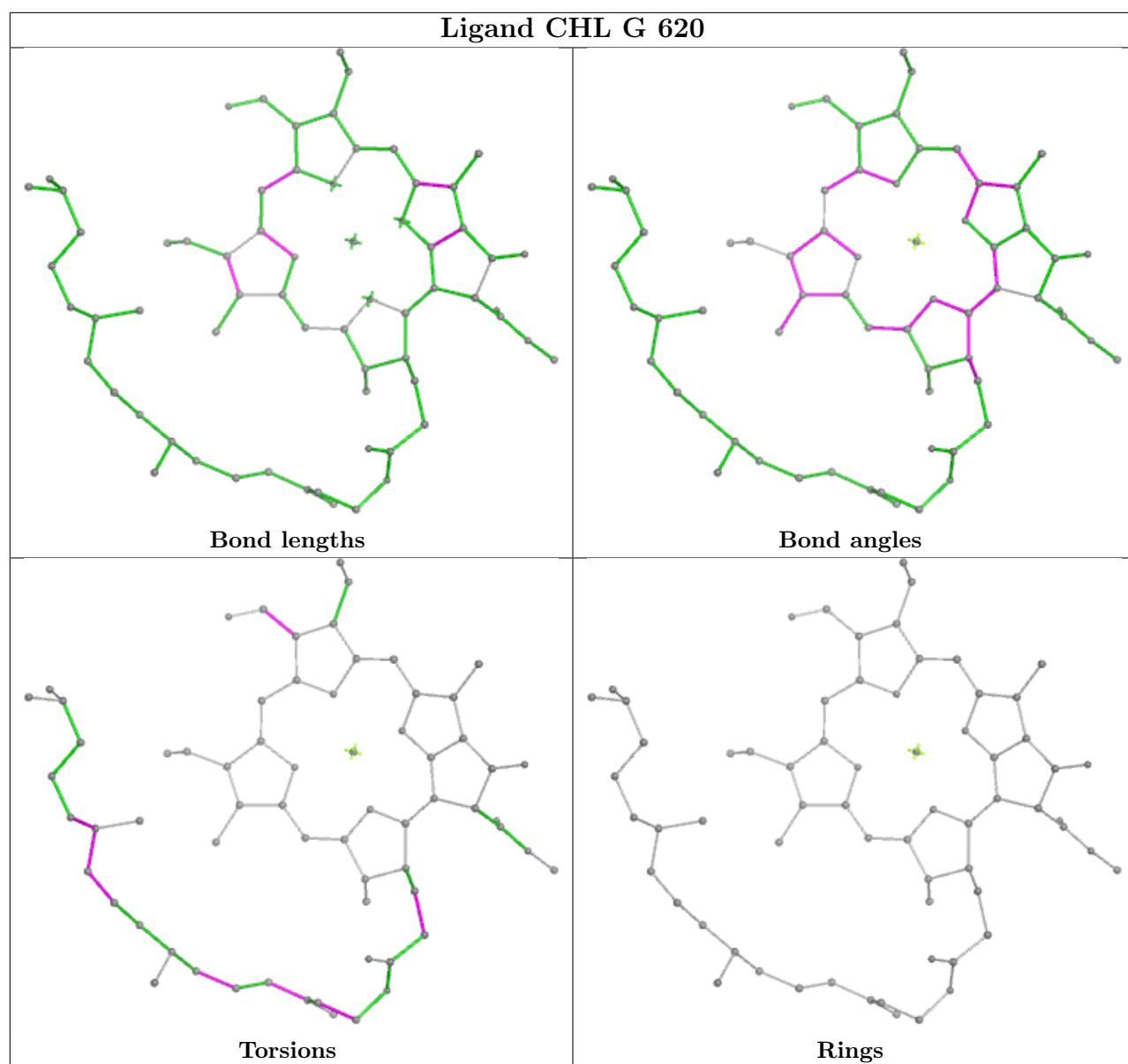
Bond angles

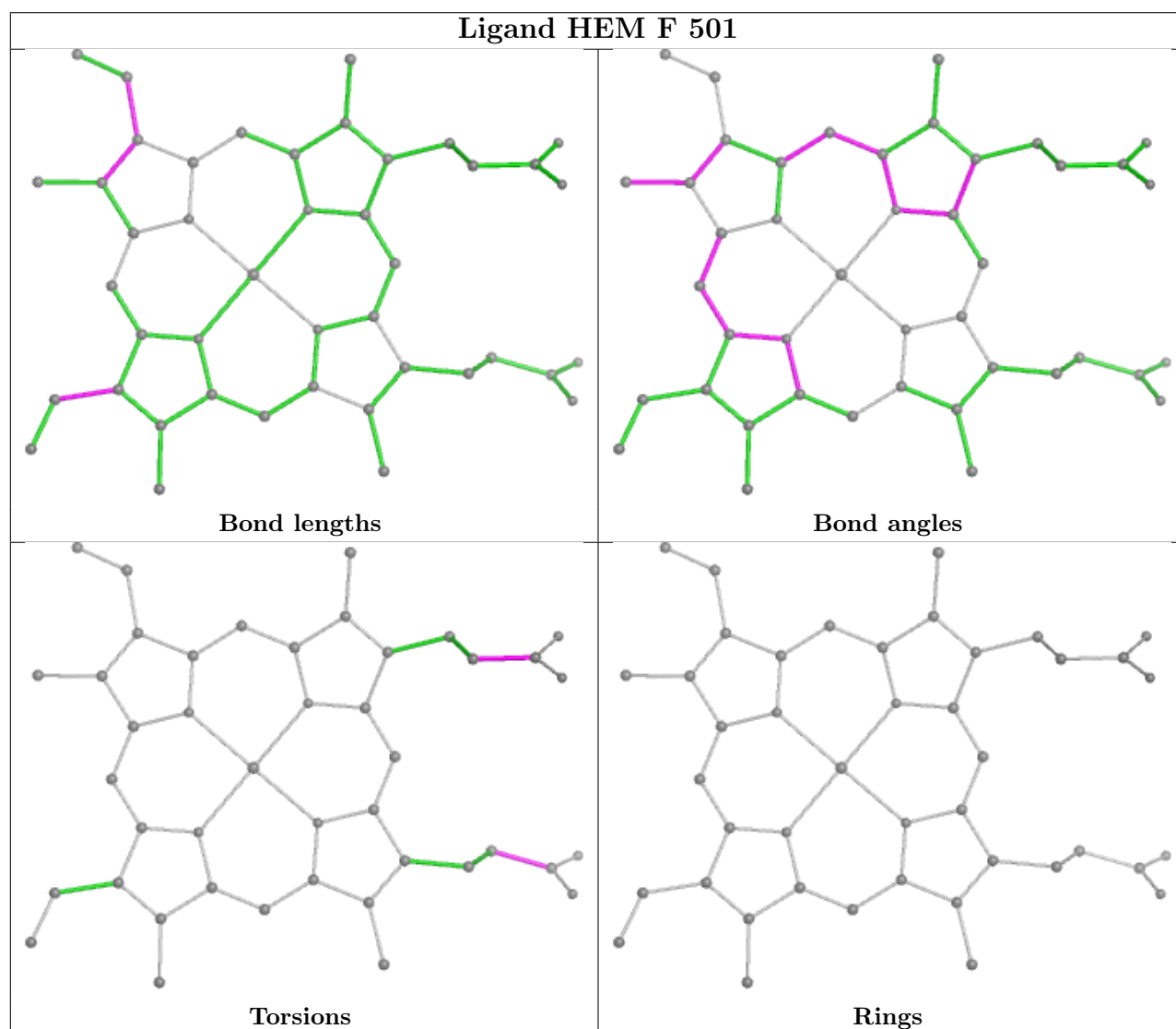
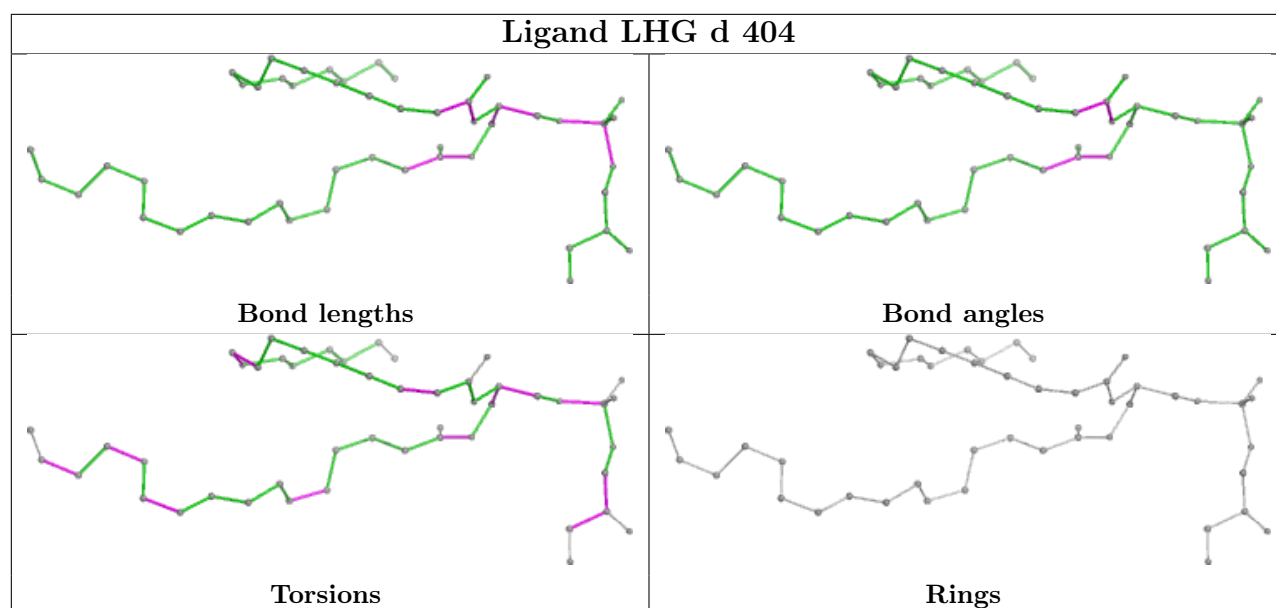


Torsions

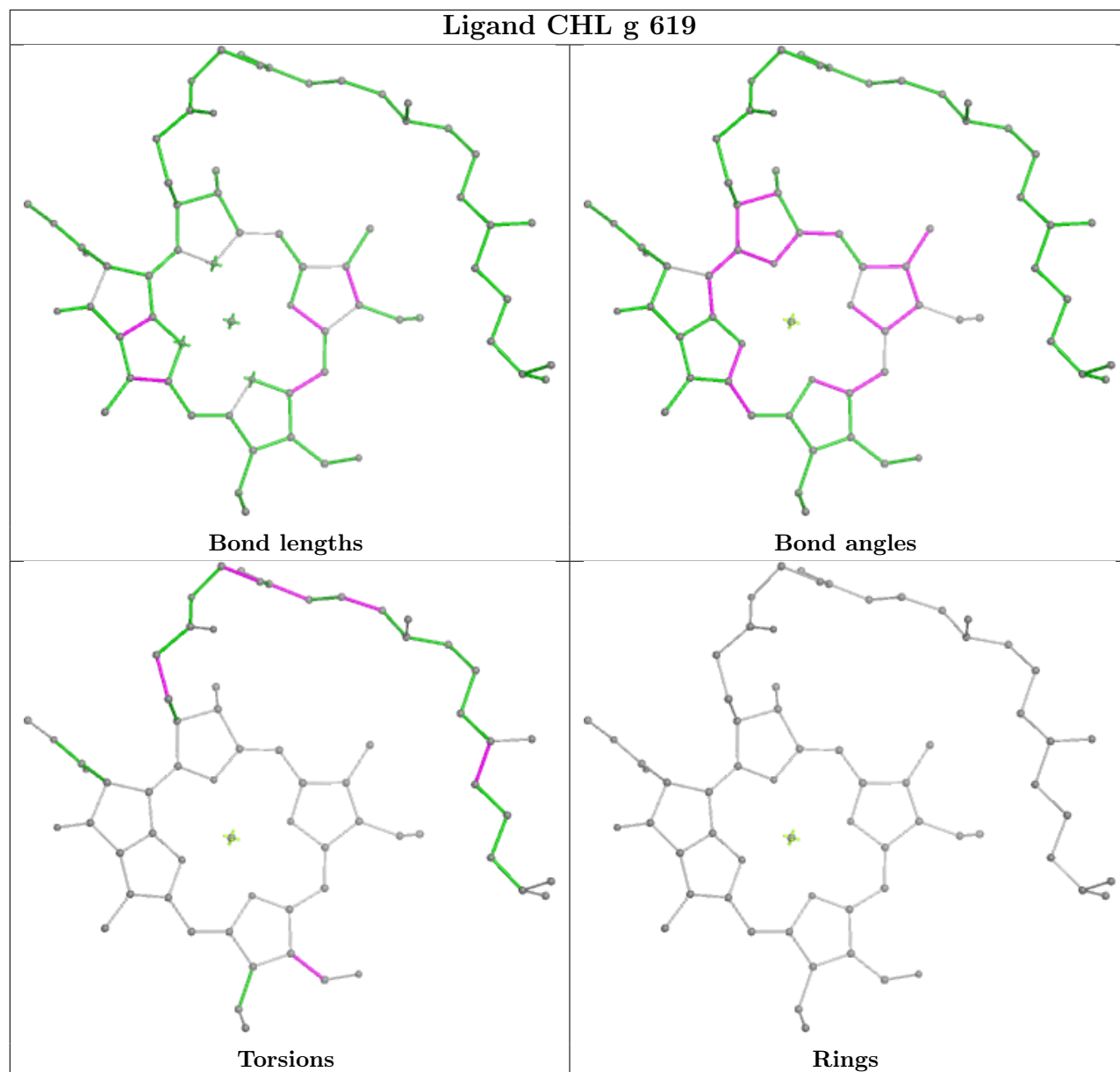


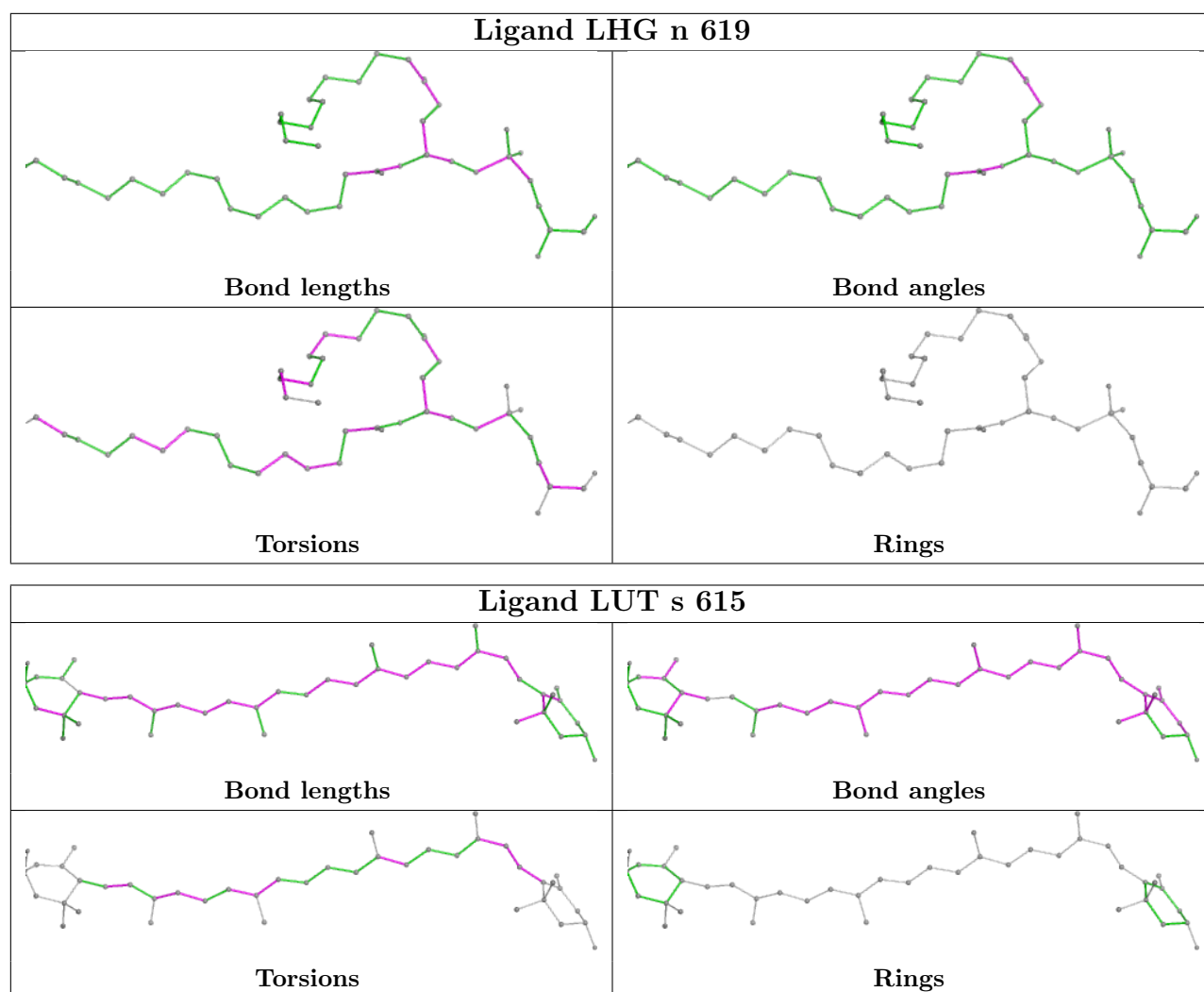
Rings

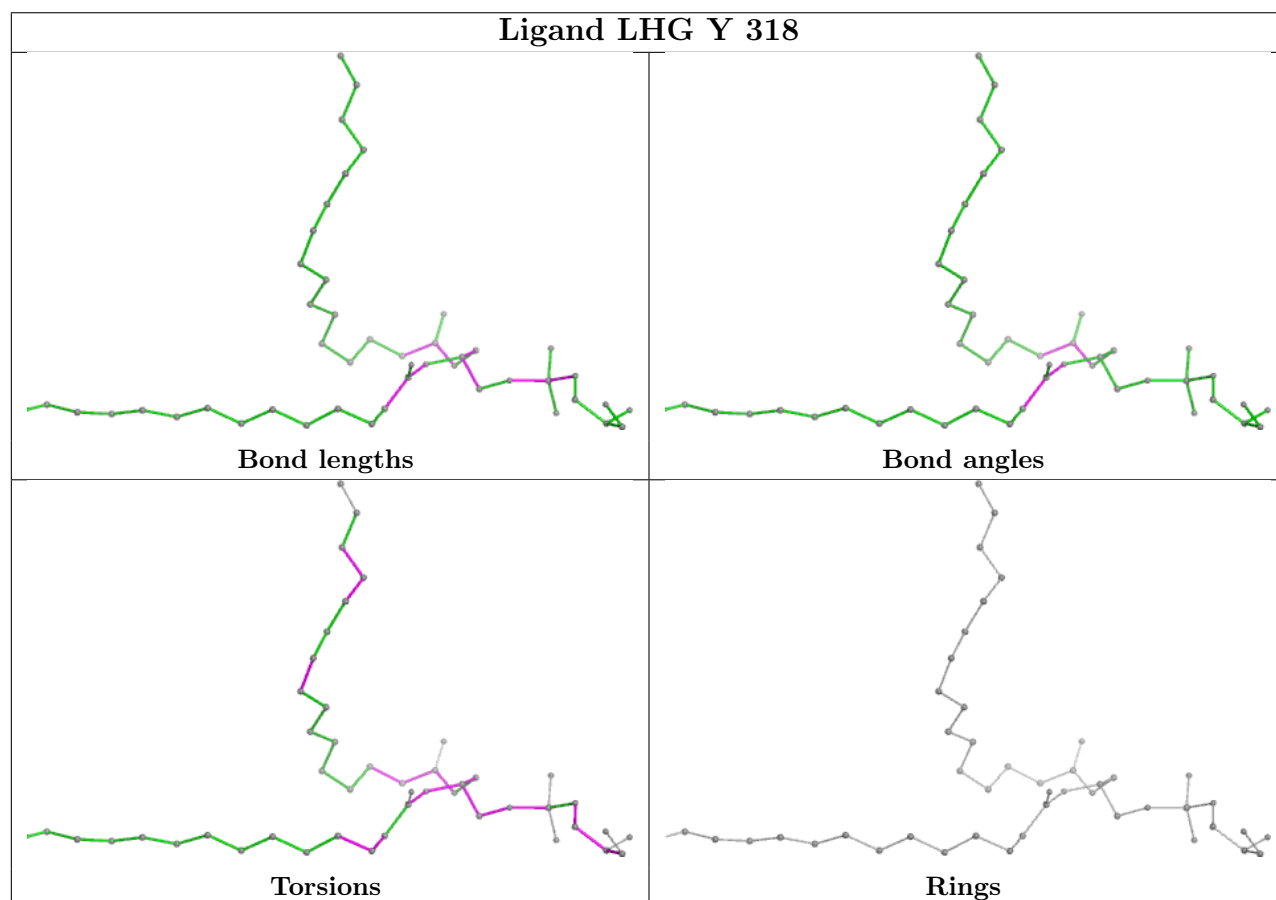
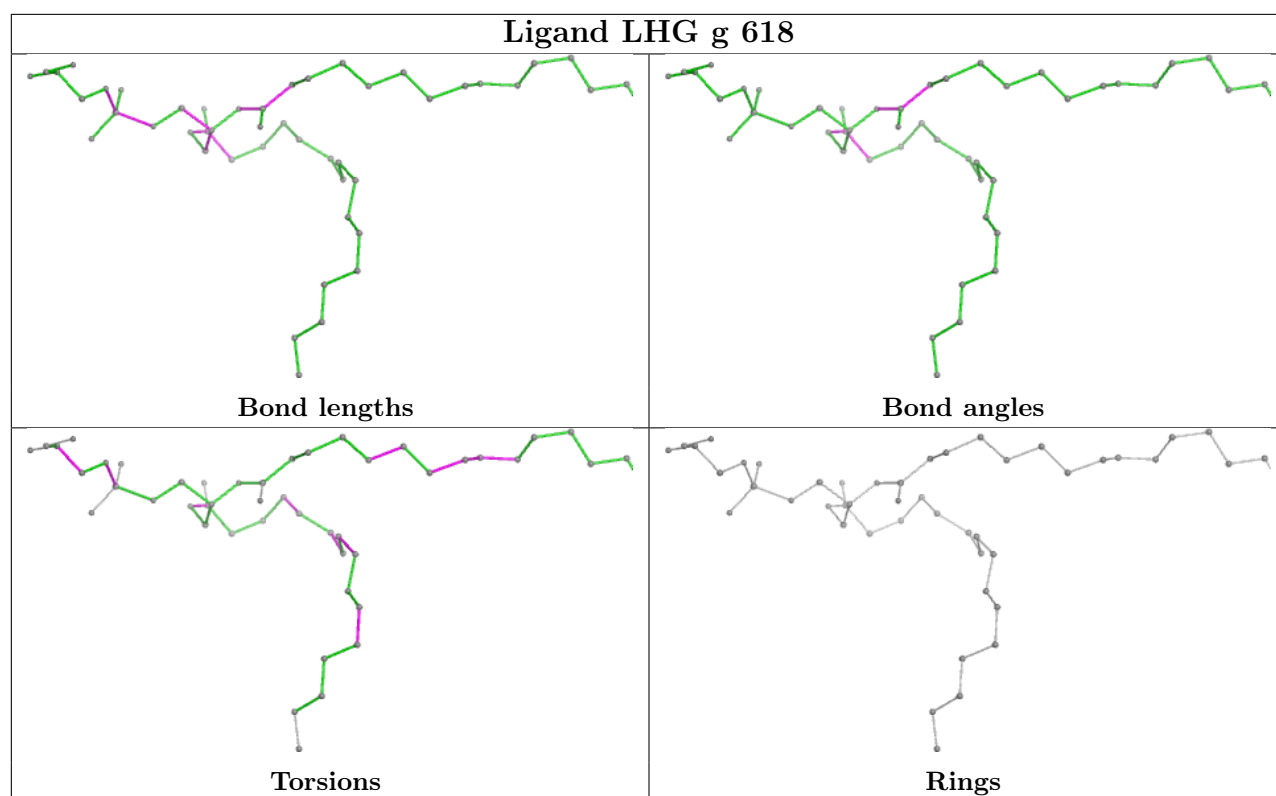


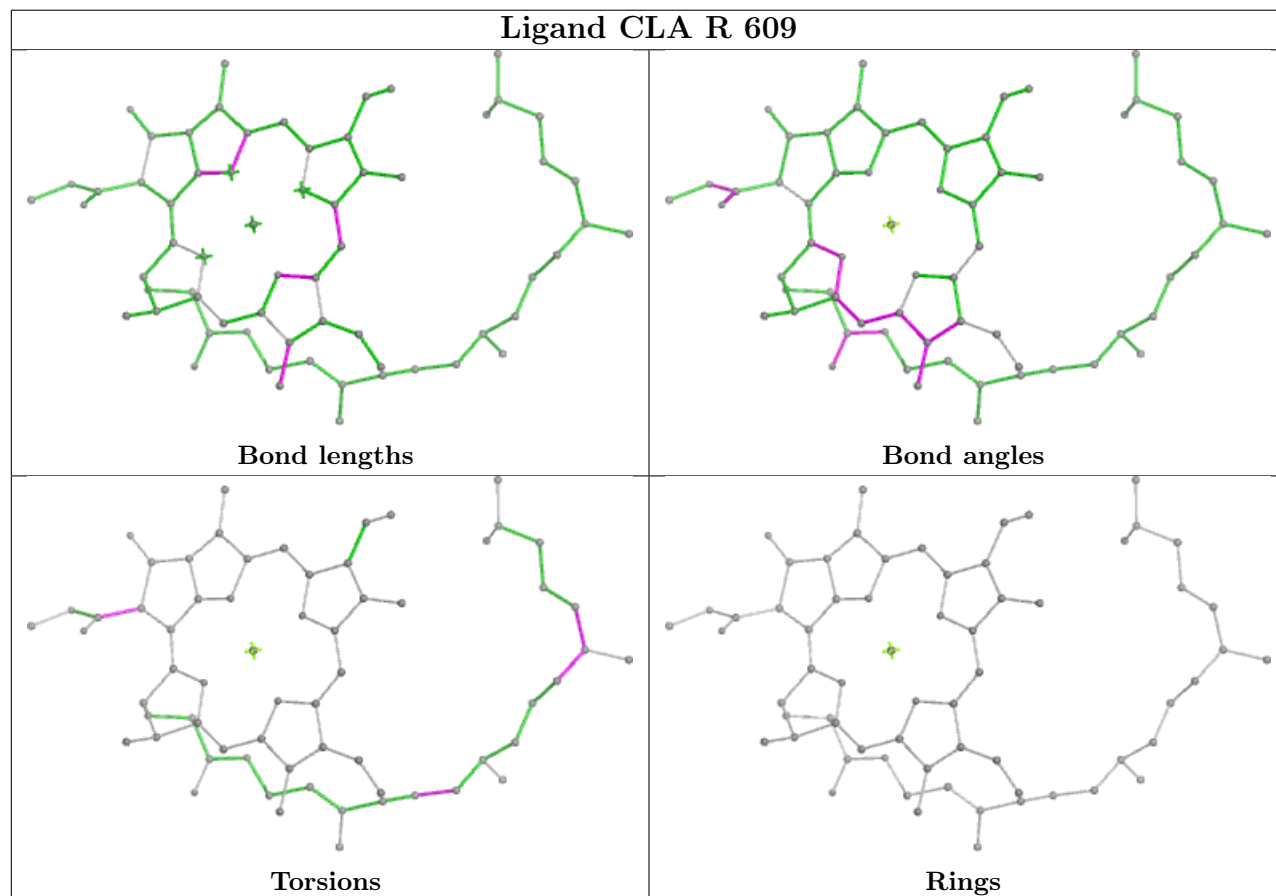
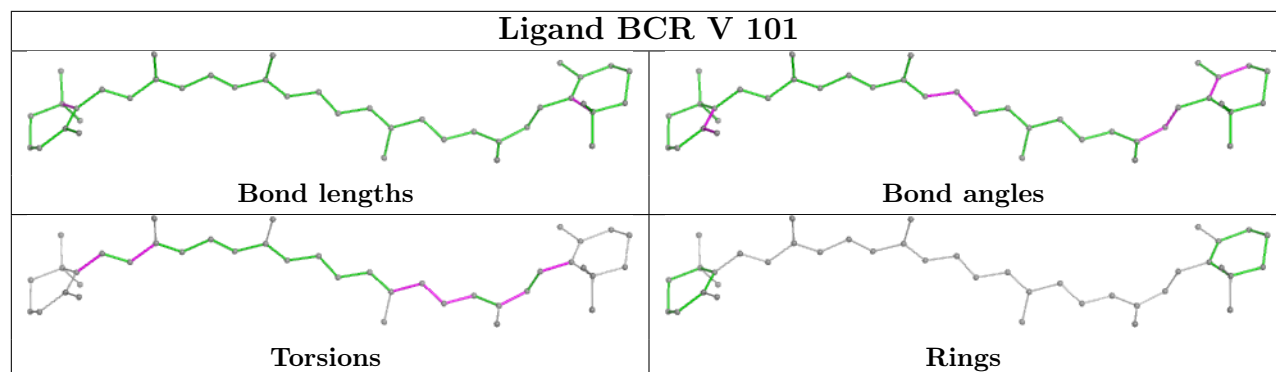


## Ligand CHL g 619

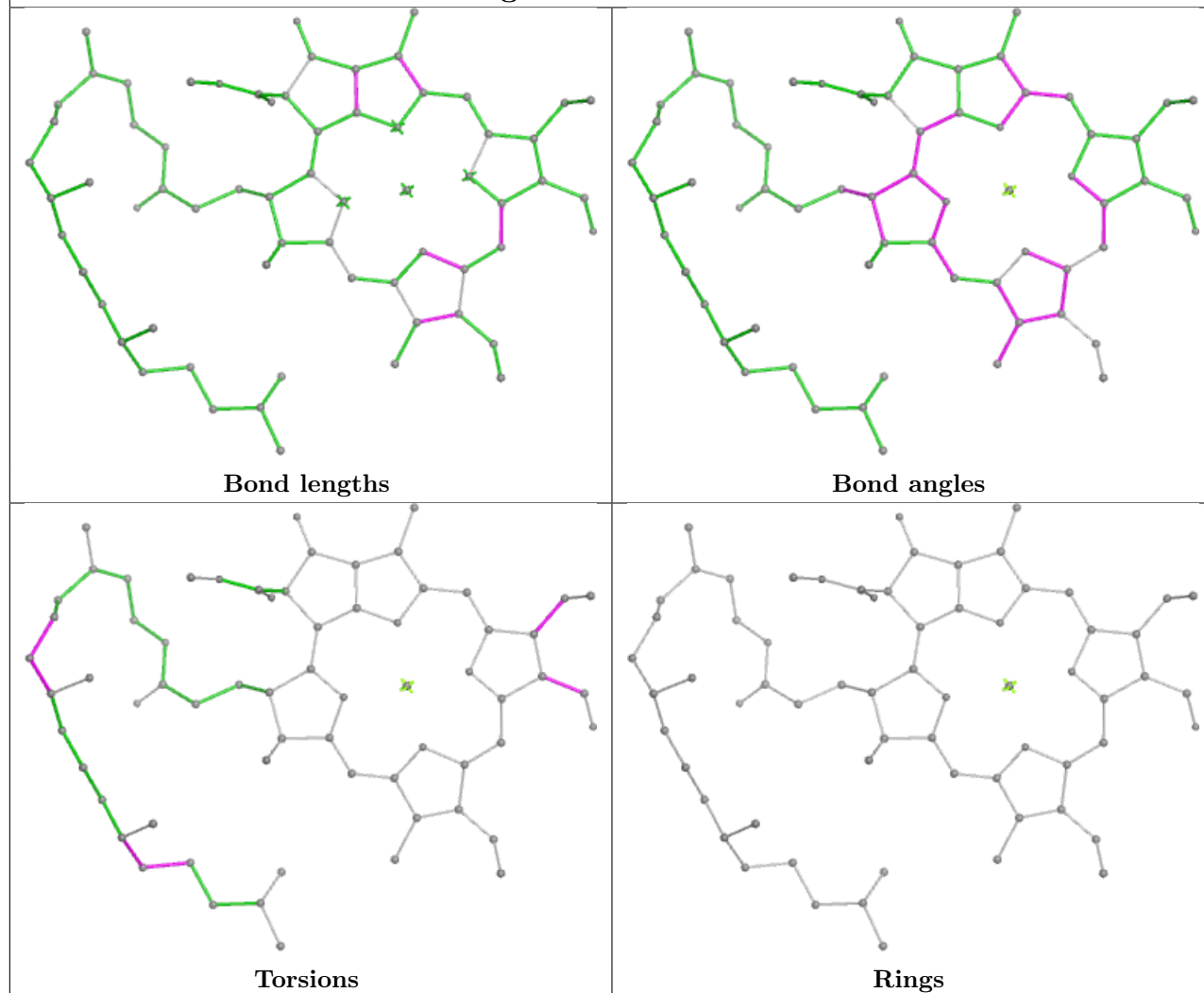




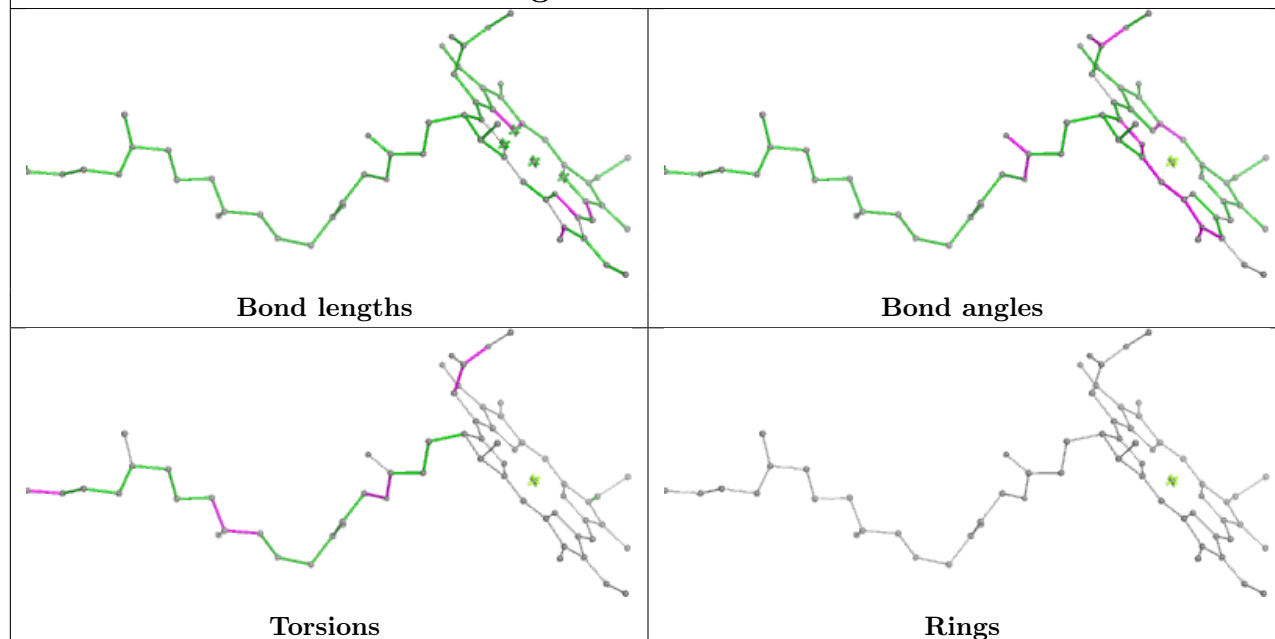




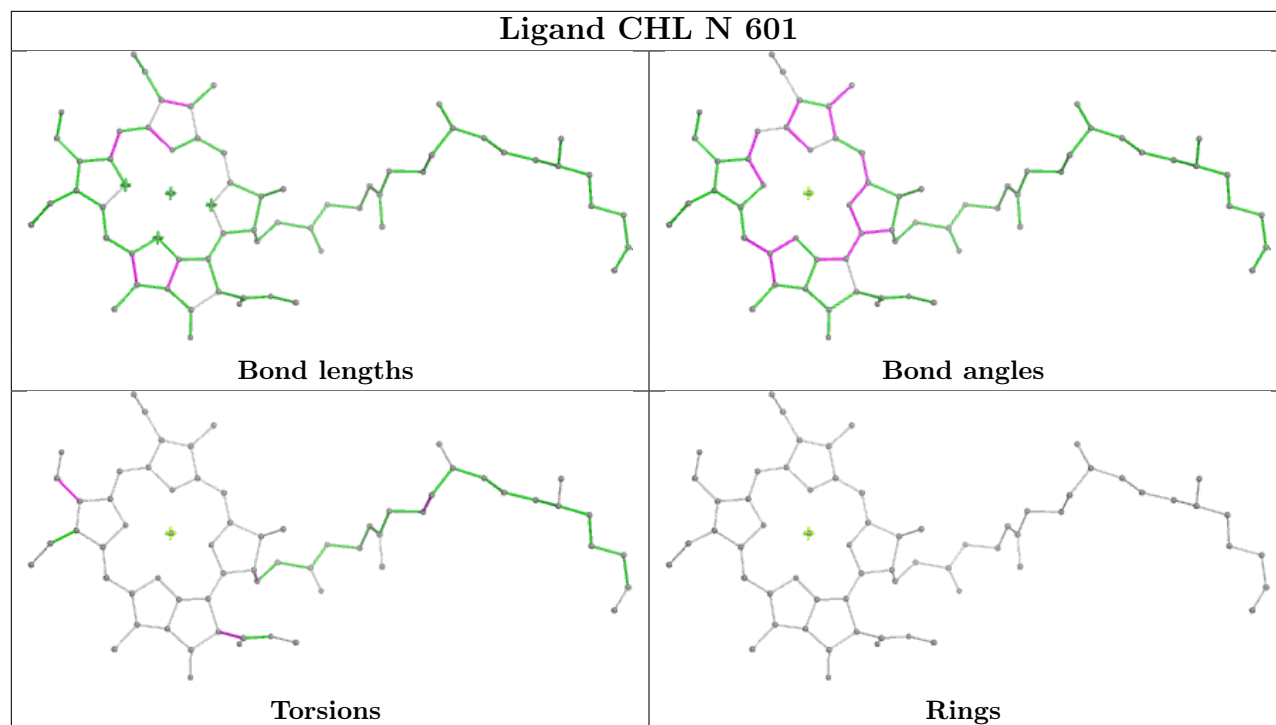
## Ligand CHL R 606



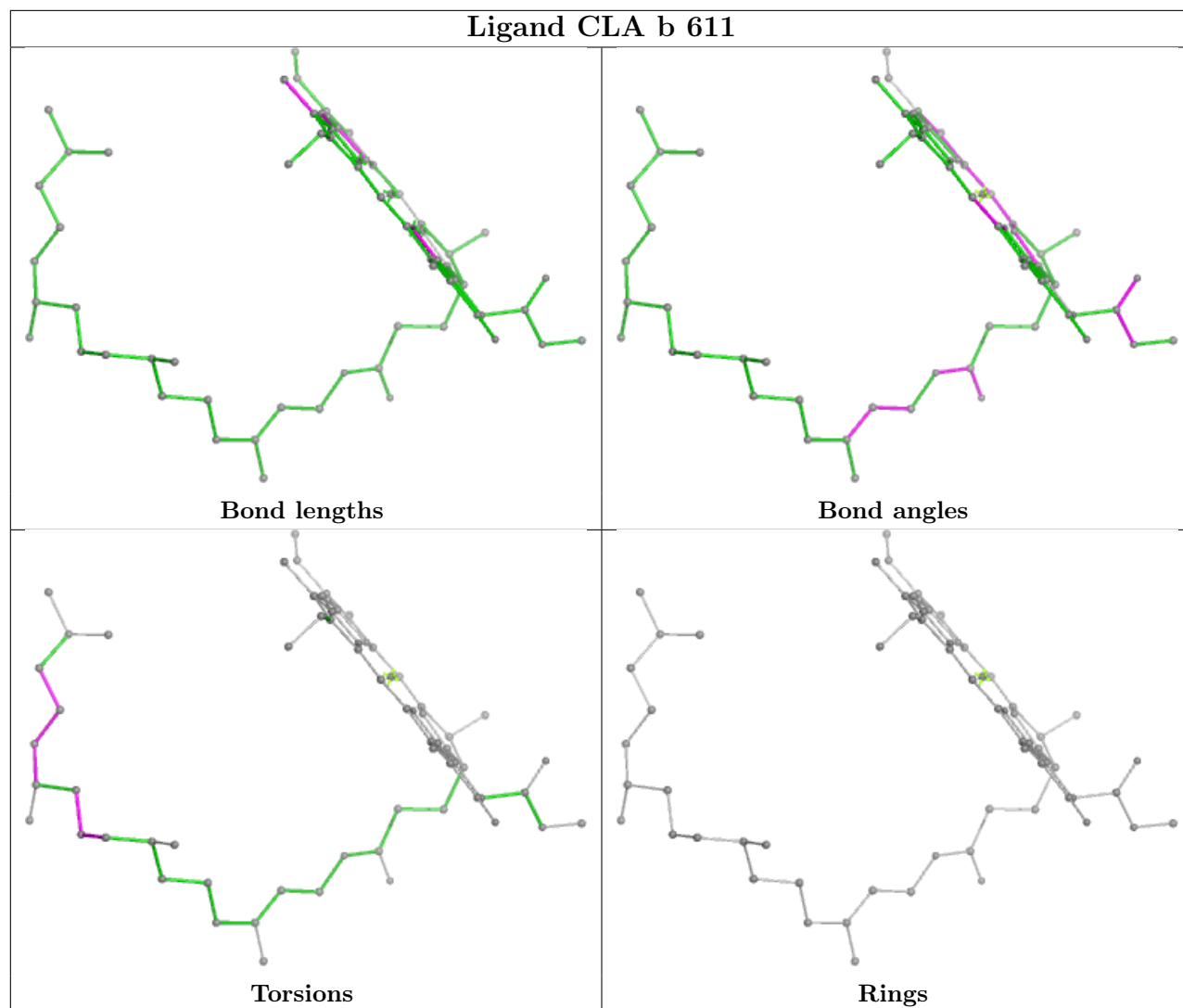
## Ligand CLA C 502



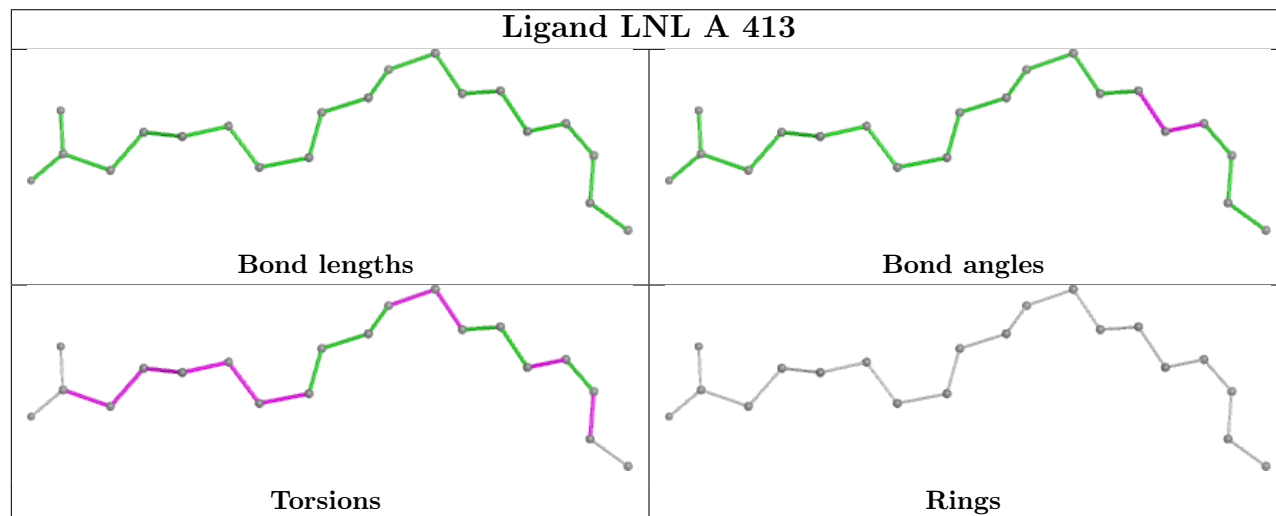


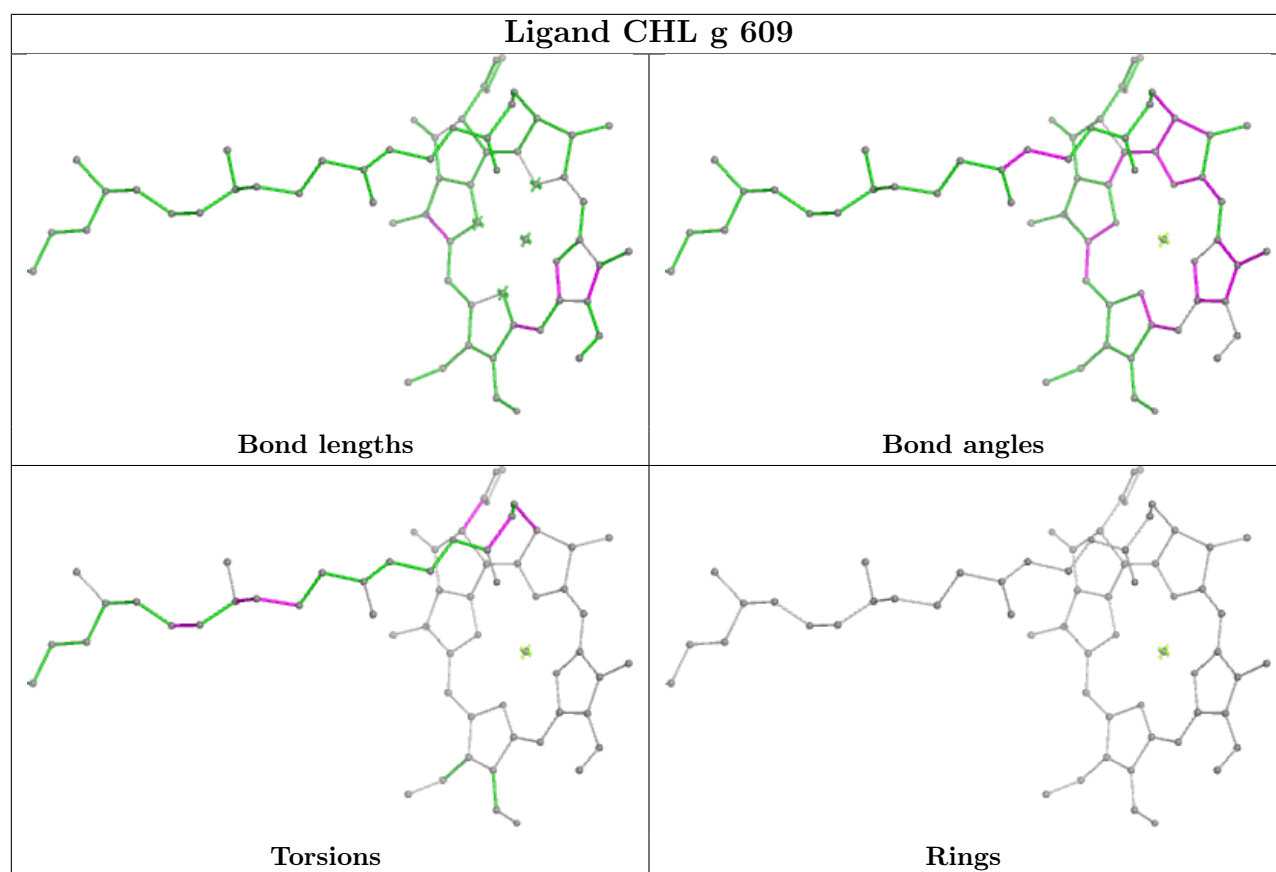


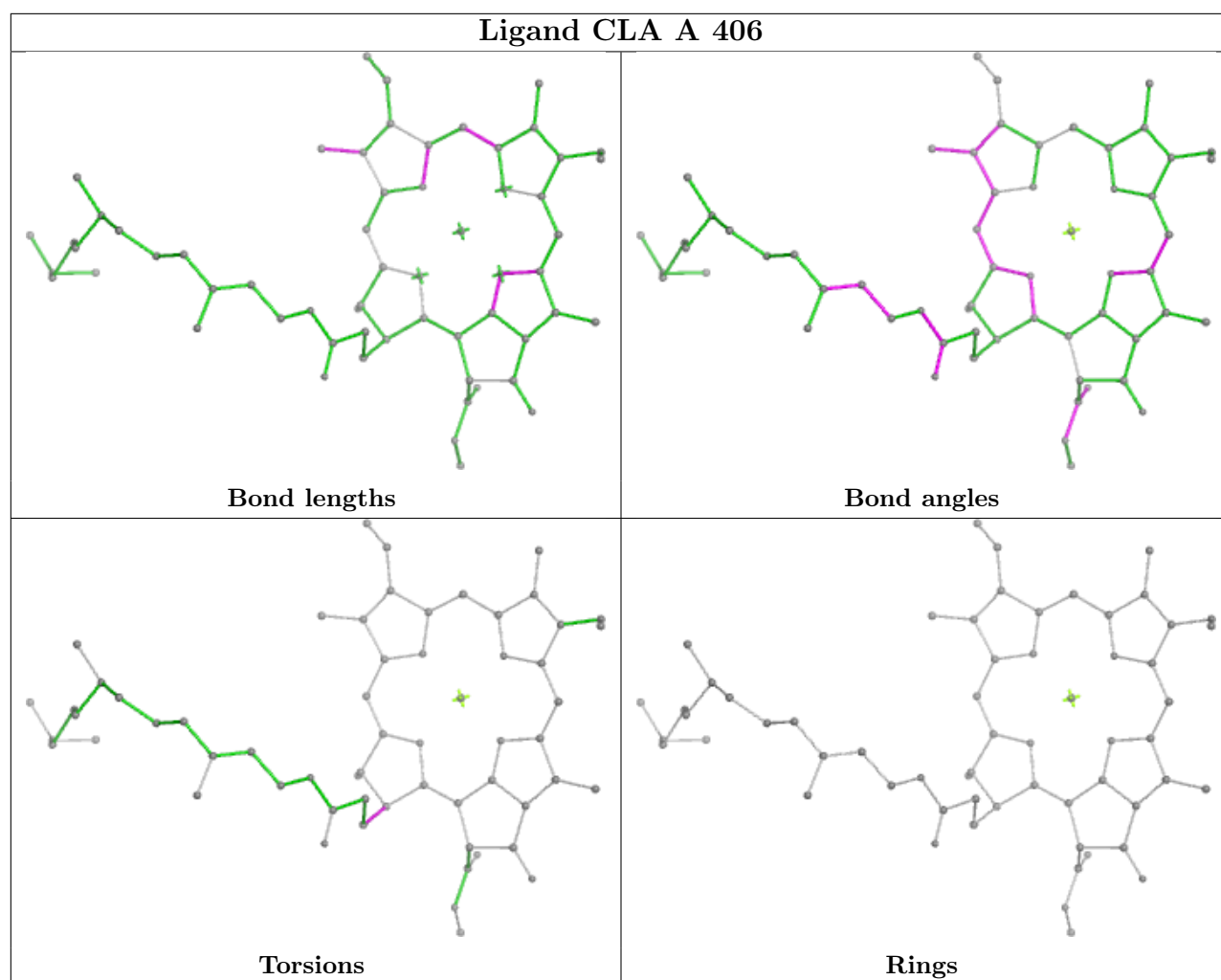
## Ligand CLA b 611

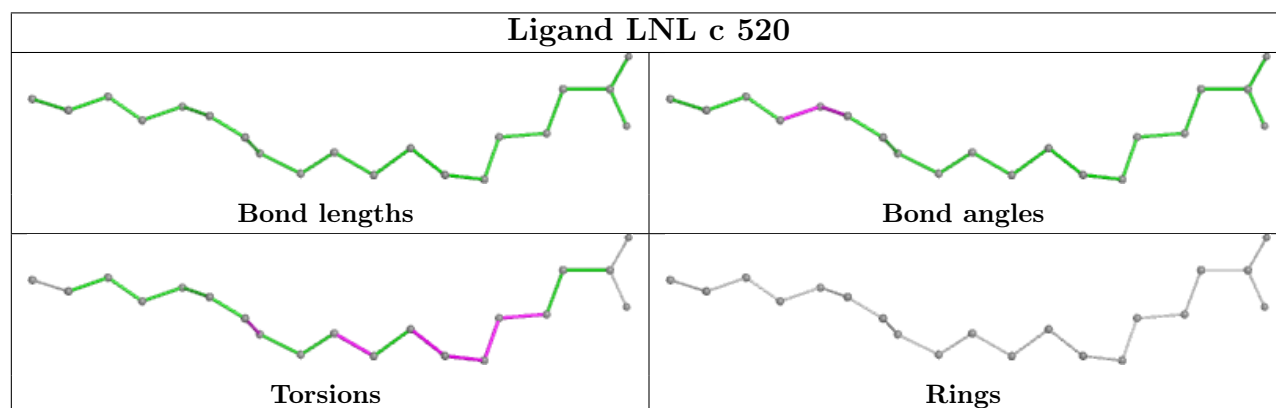
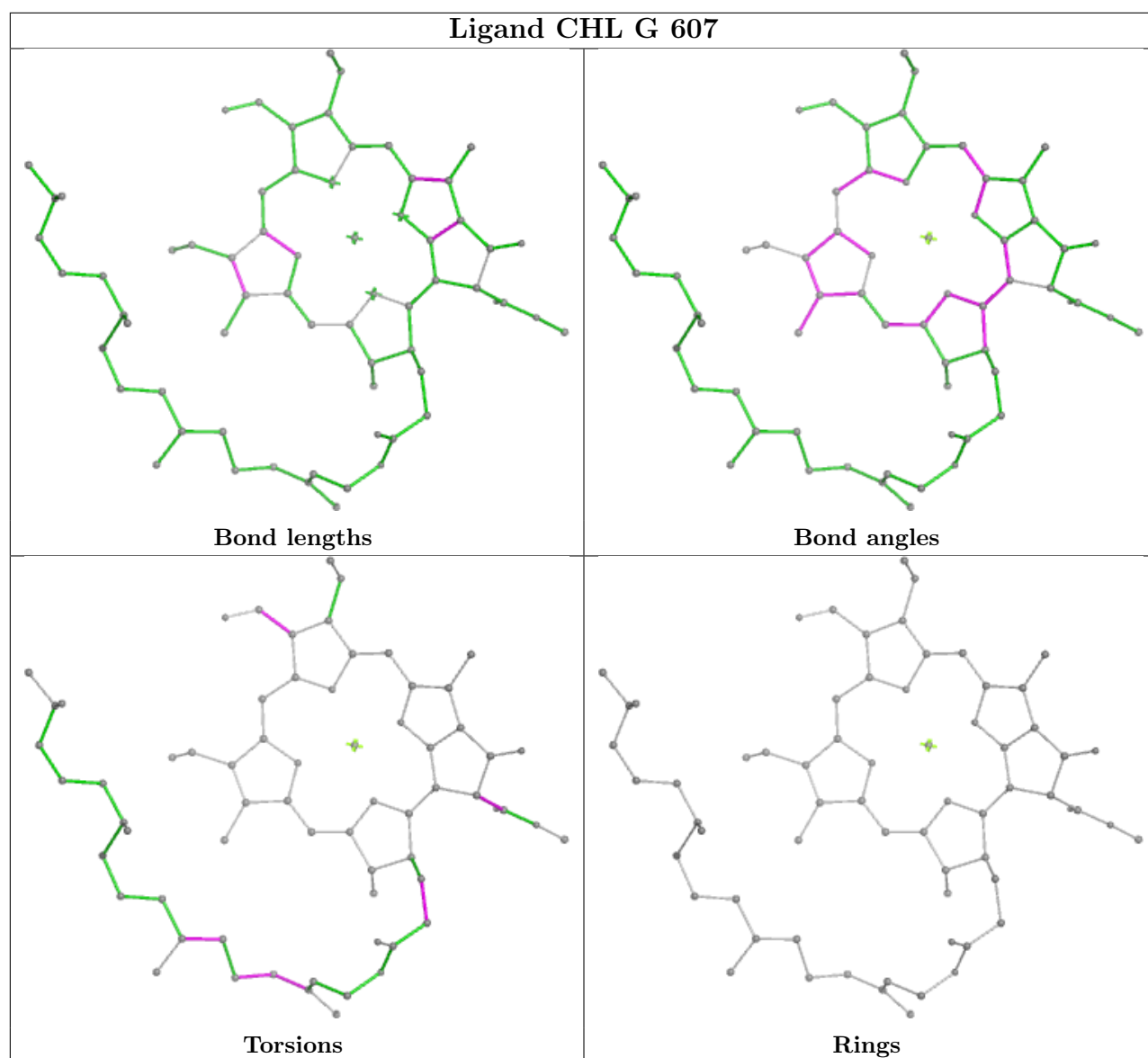


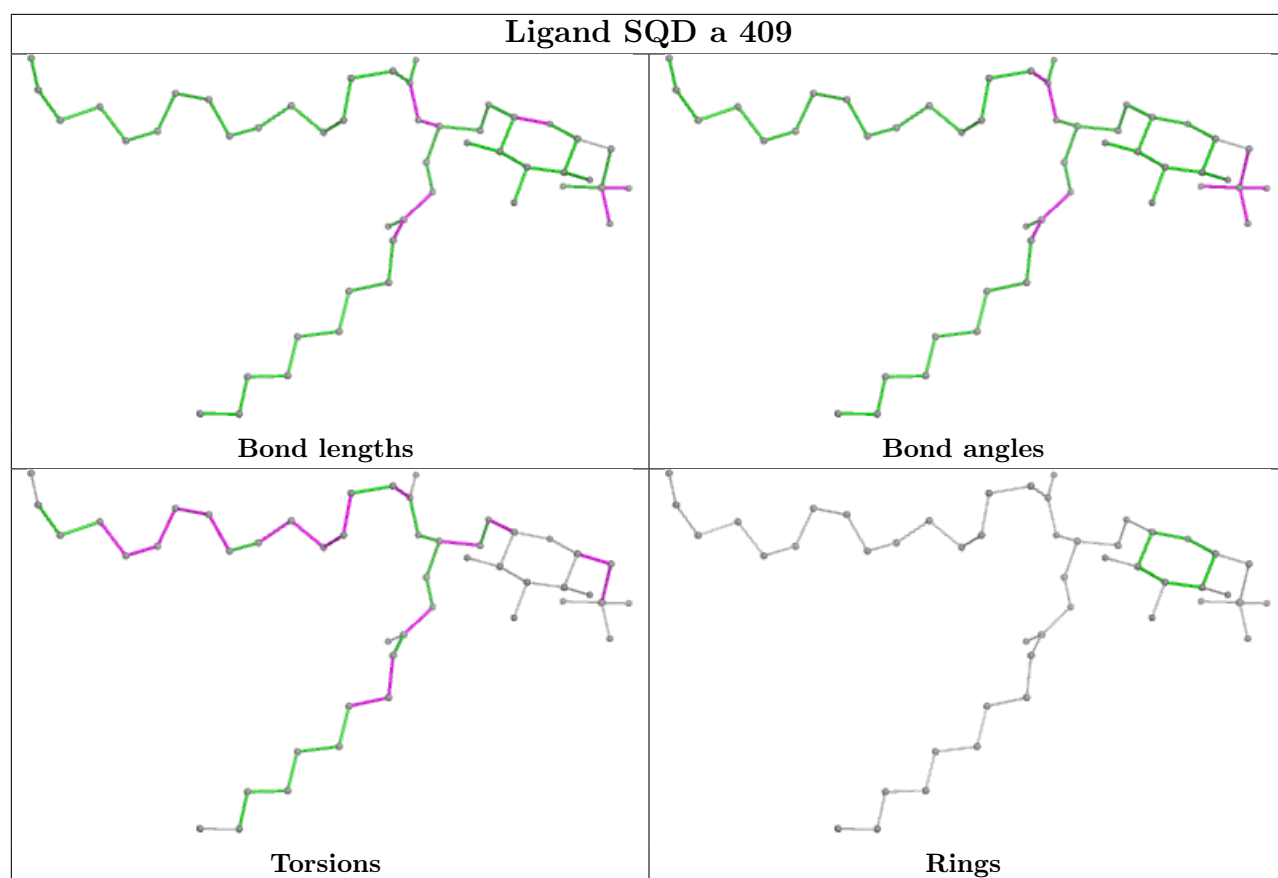
## Ligand LNL A 413



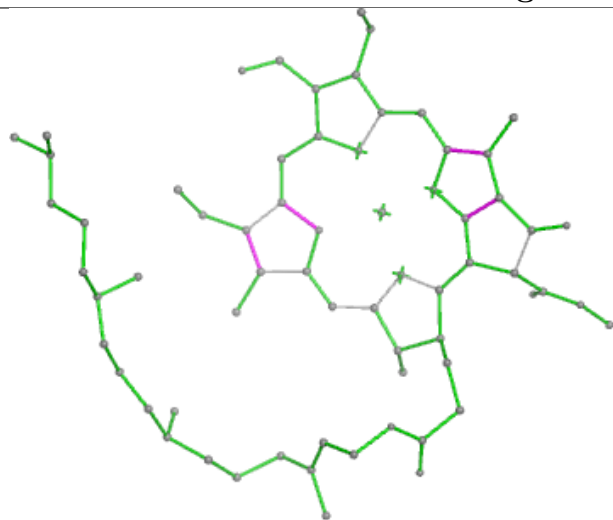




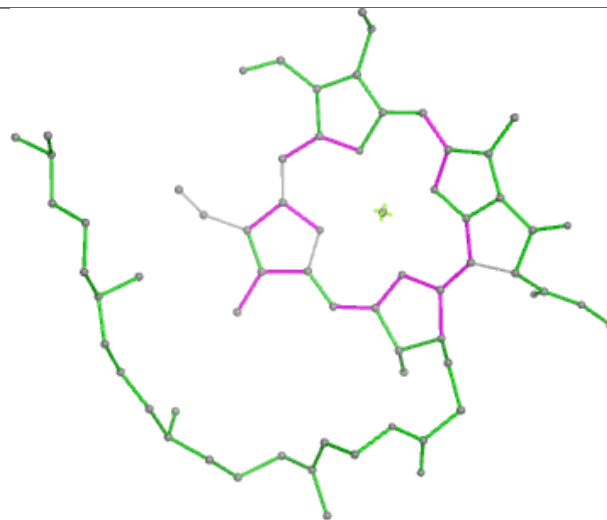




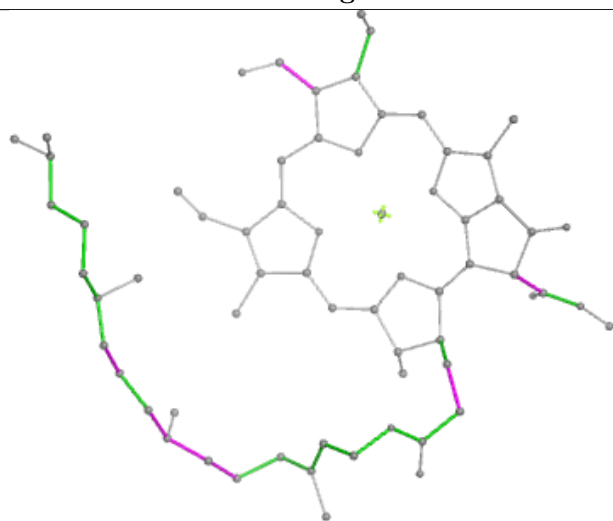
## Ligand CHL n 607



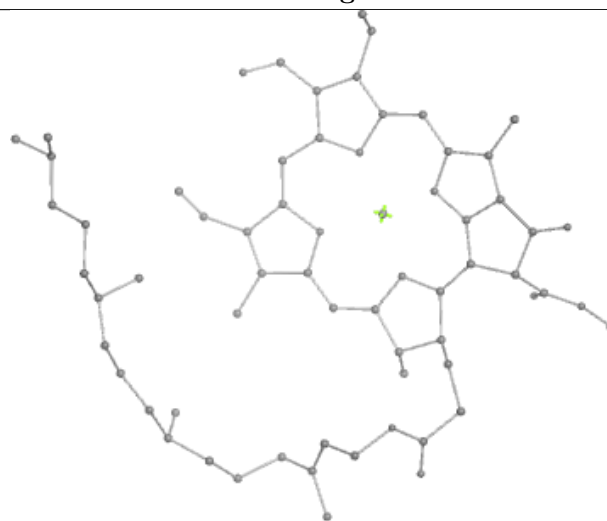
Bond lengths



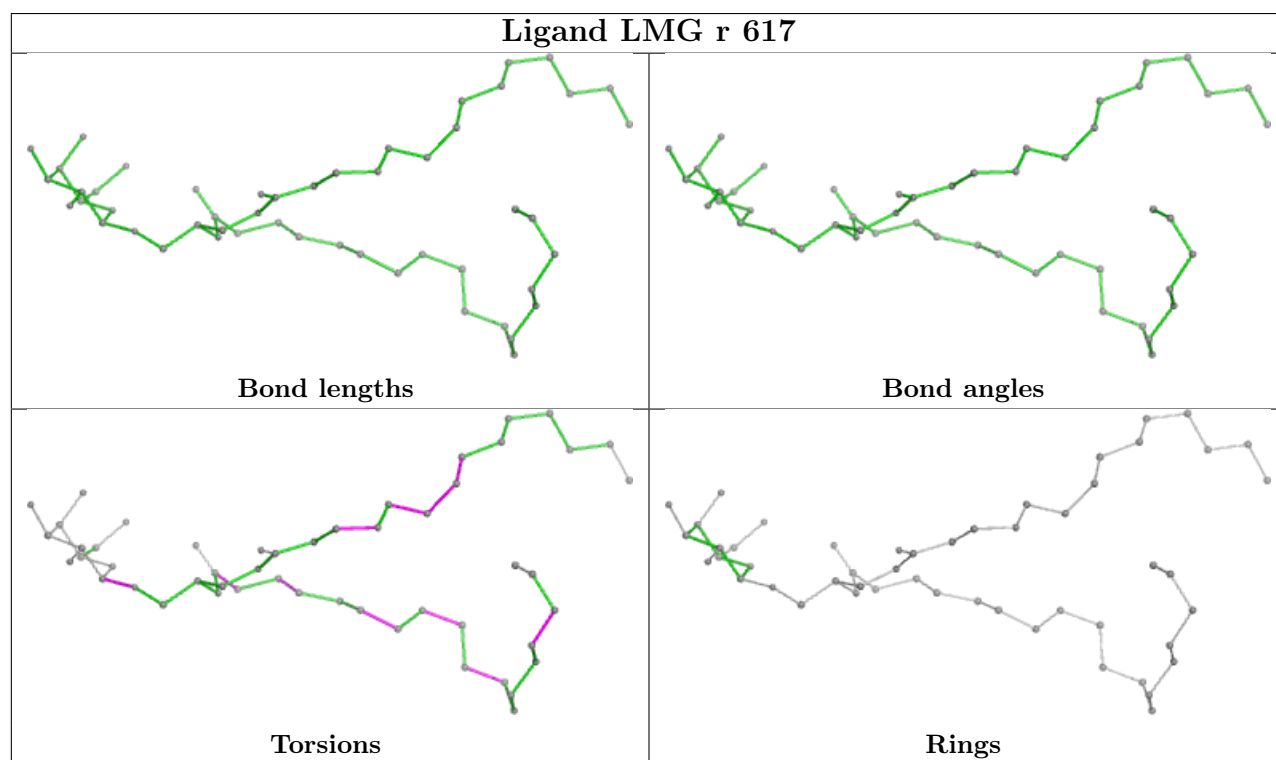
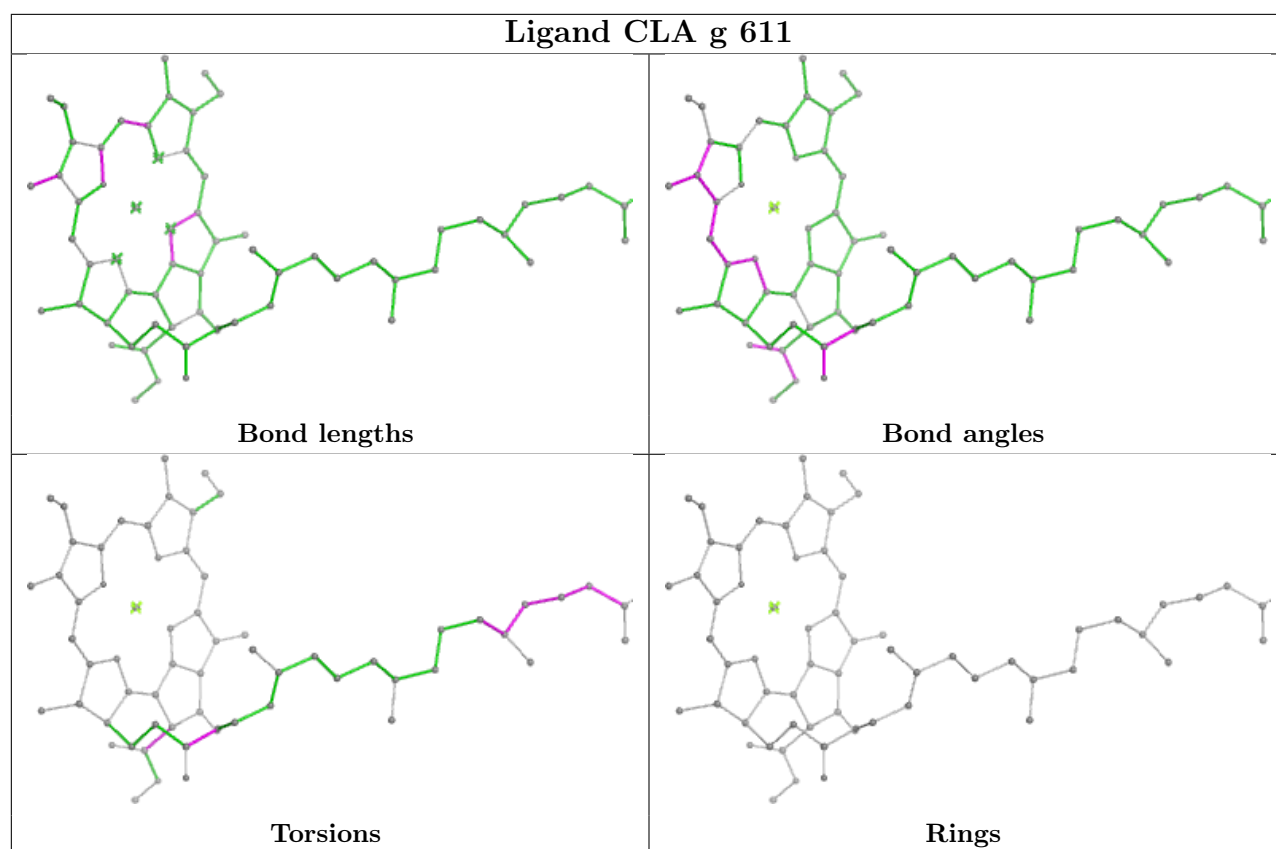
Bond angles



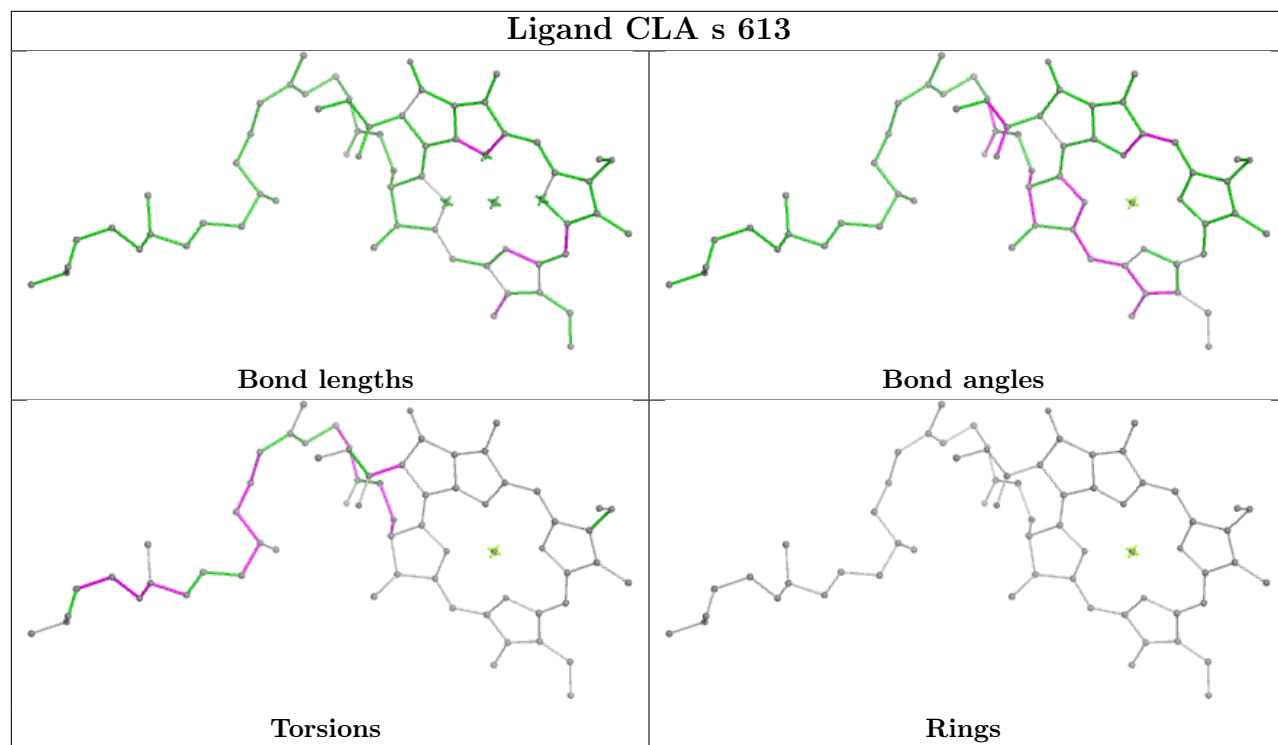
Torsions



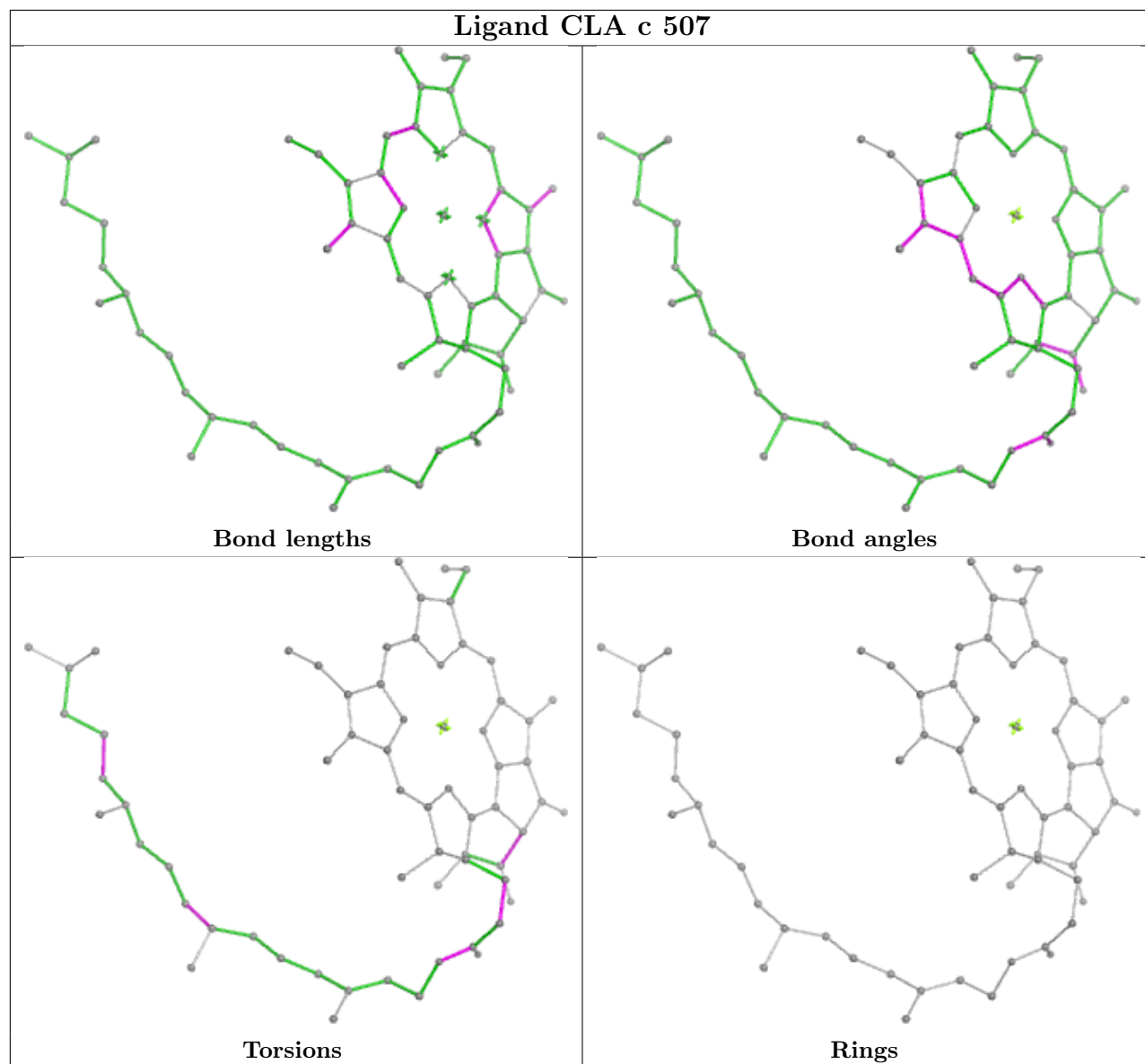
Rings



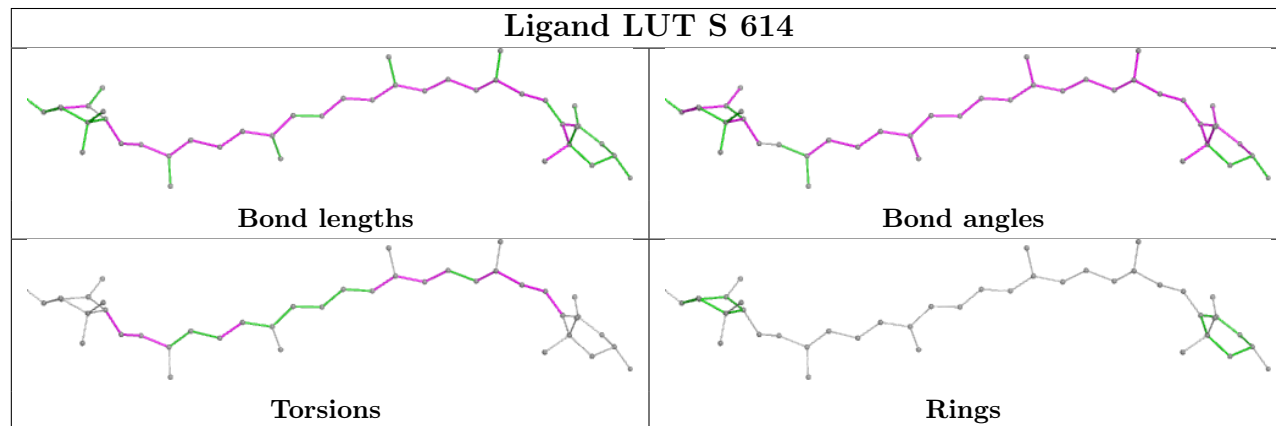


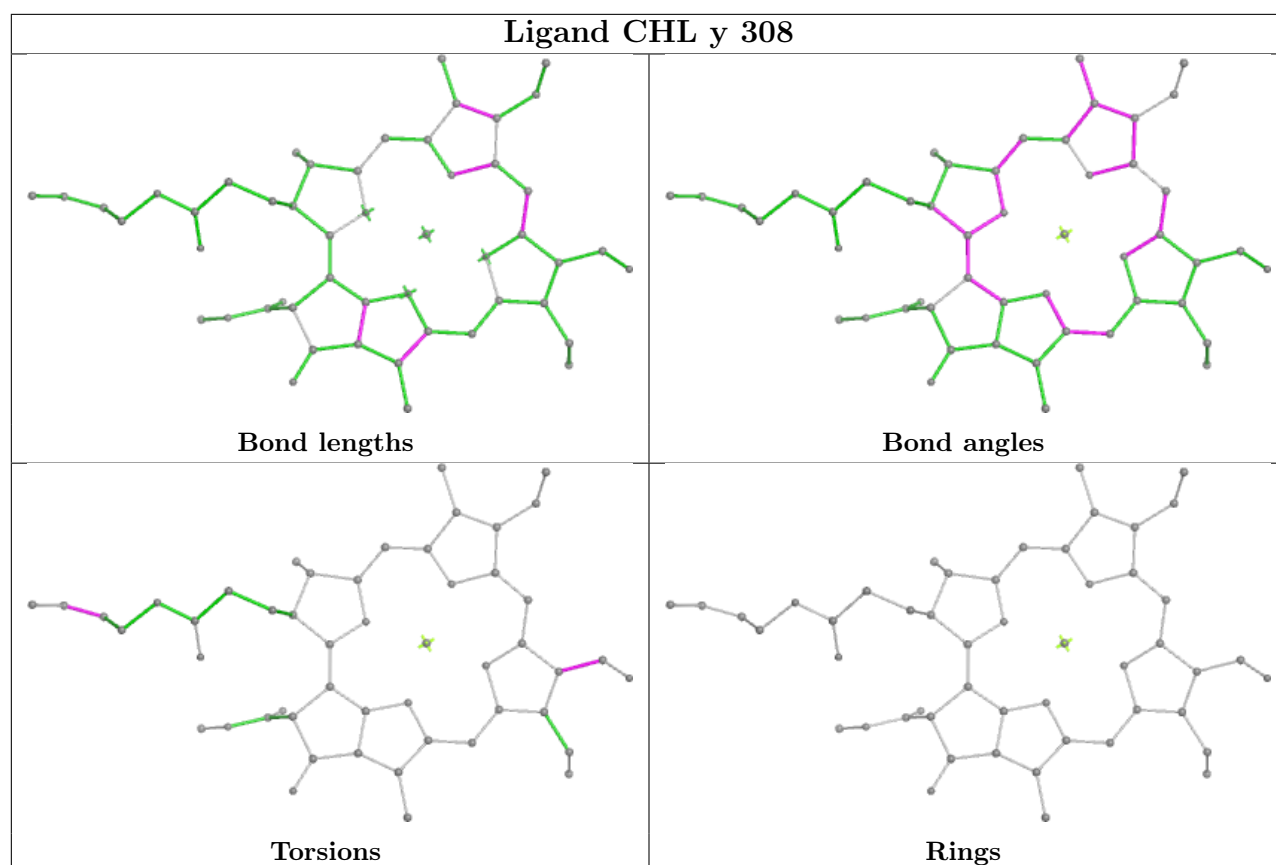


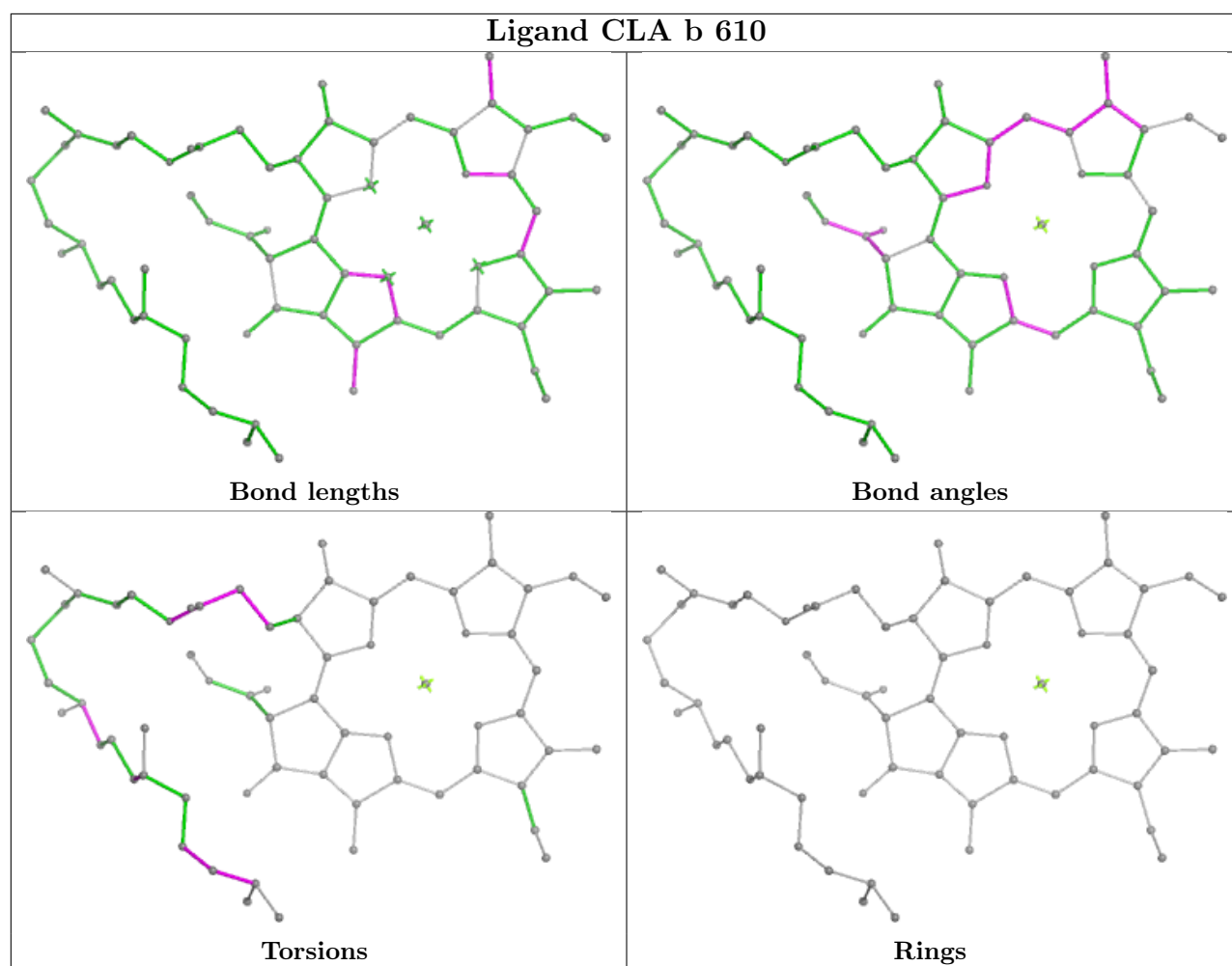
## Ligand CLA c 507



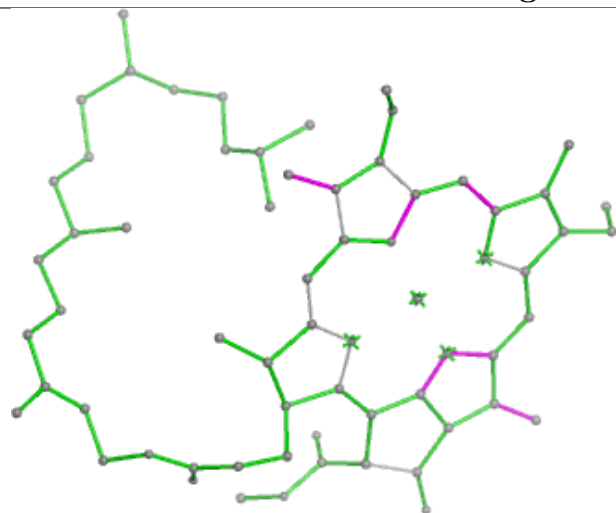
## Ligand LUT S 614



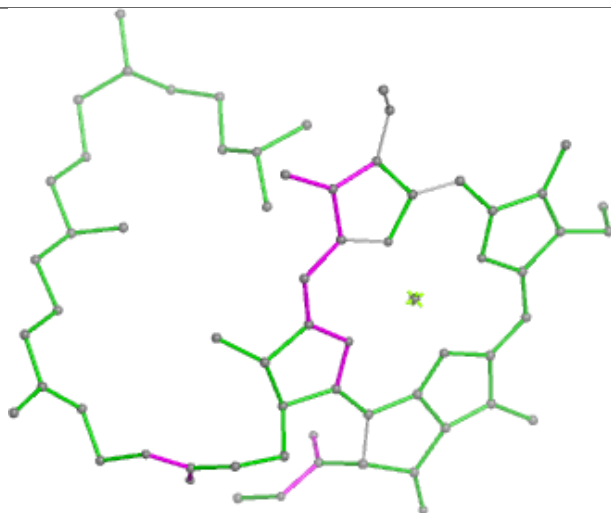




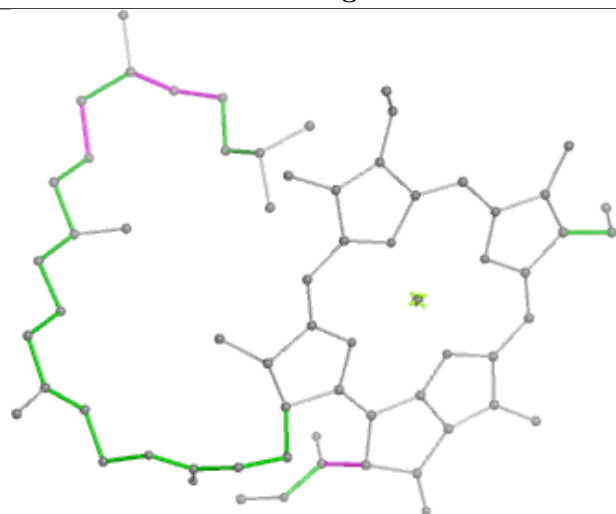
## Ligand CLA b 615



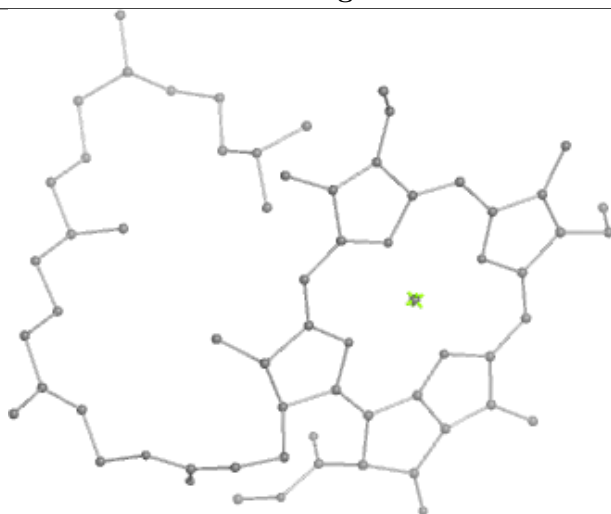
Bond lengths



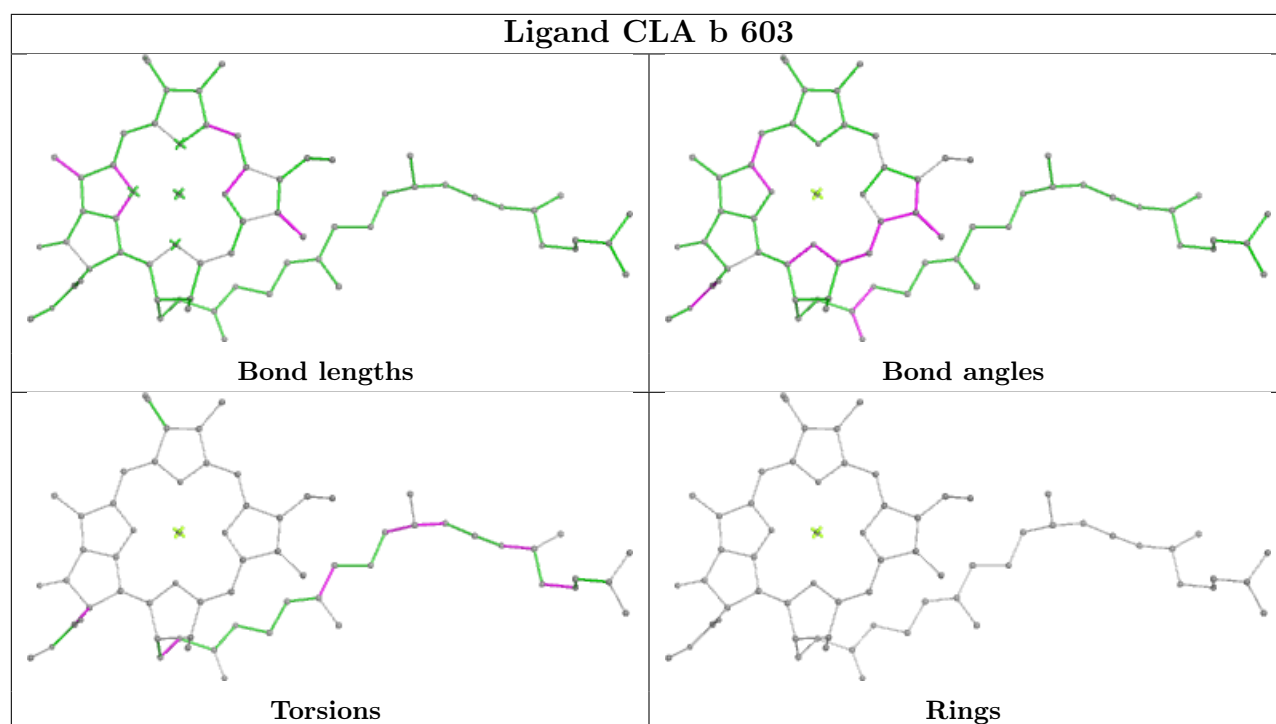
Bond angles



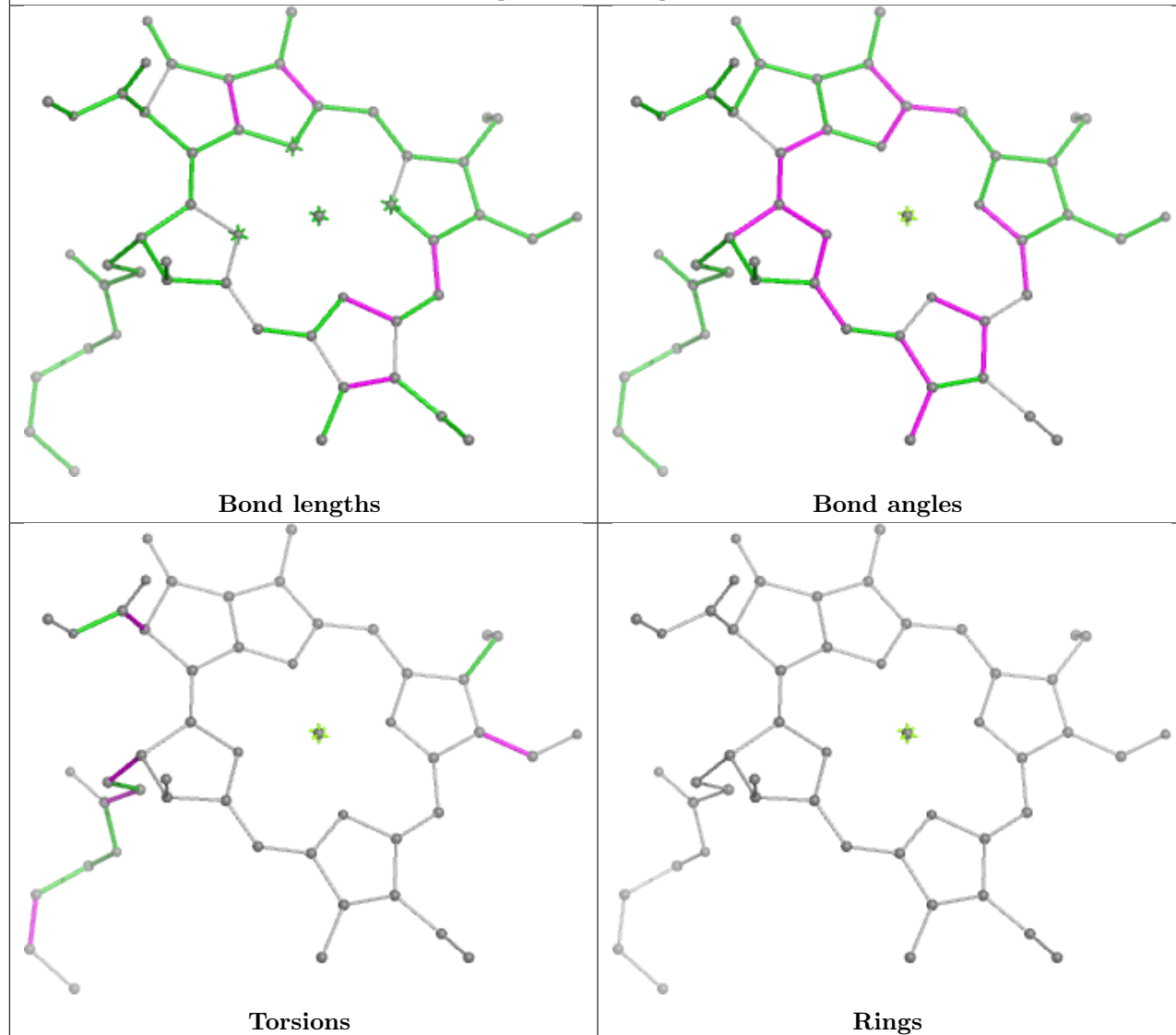
Torsions

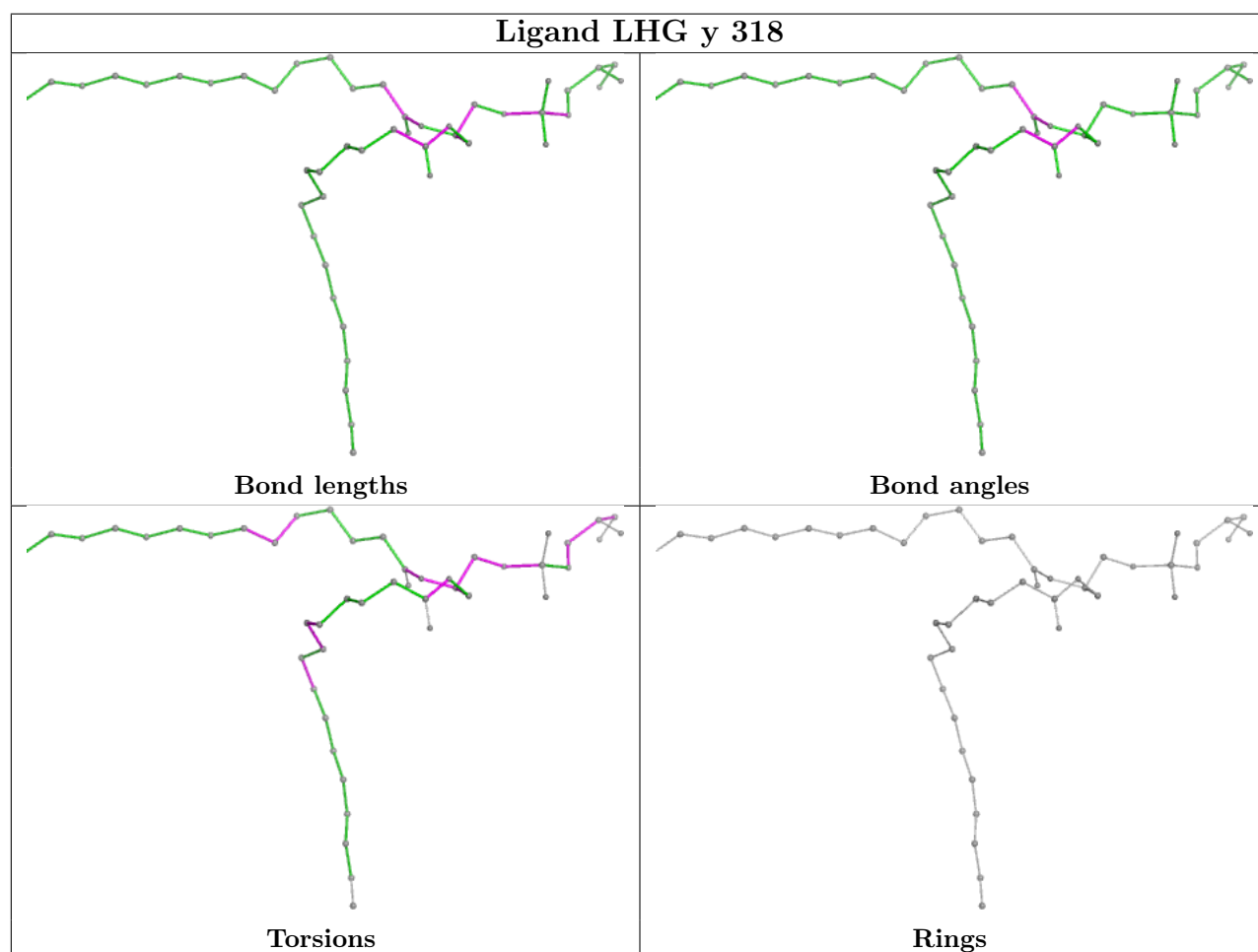
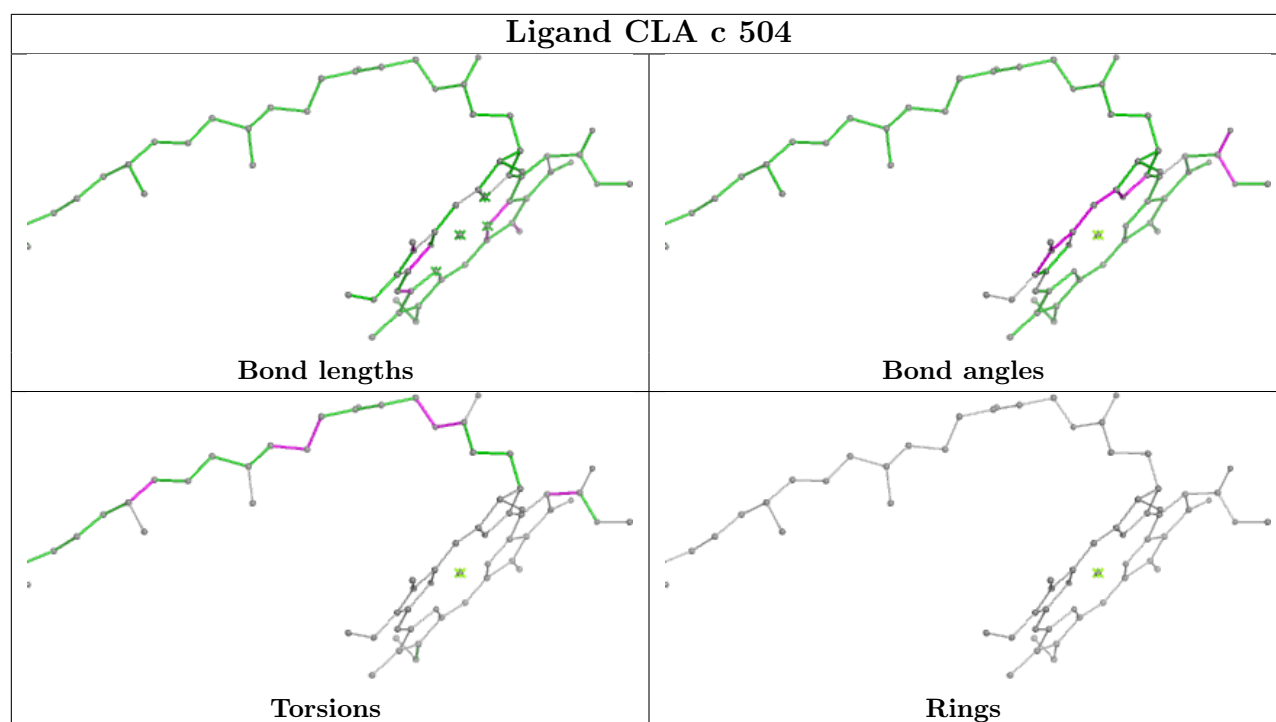


Rings



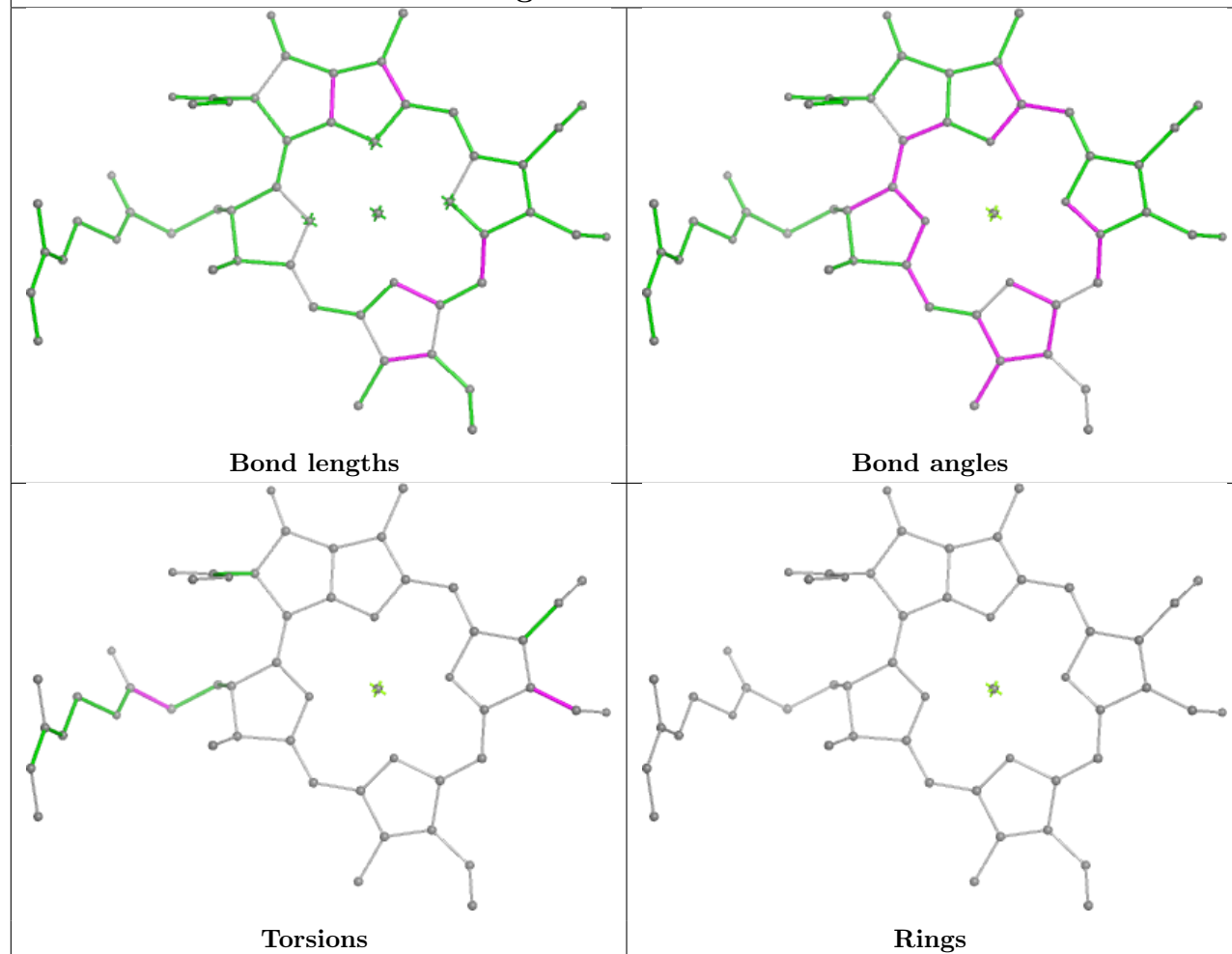
## Ligand CHL g 608



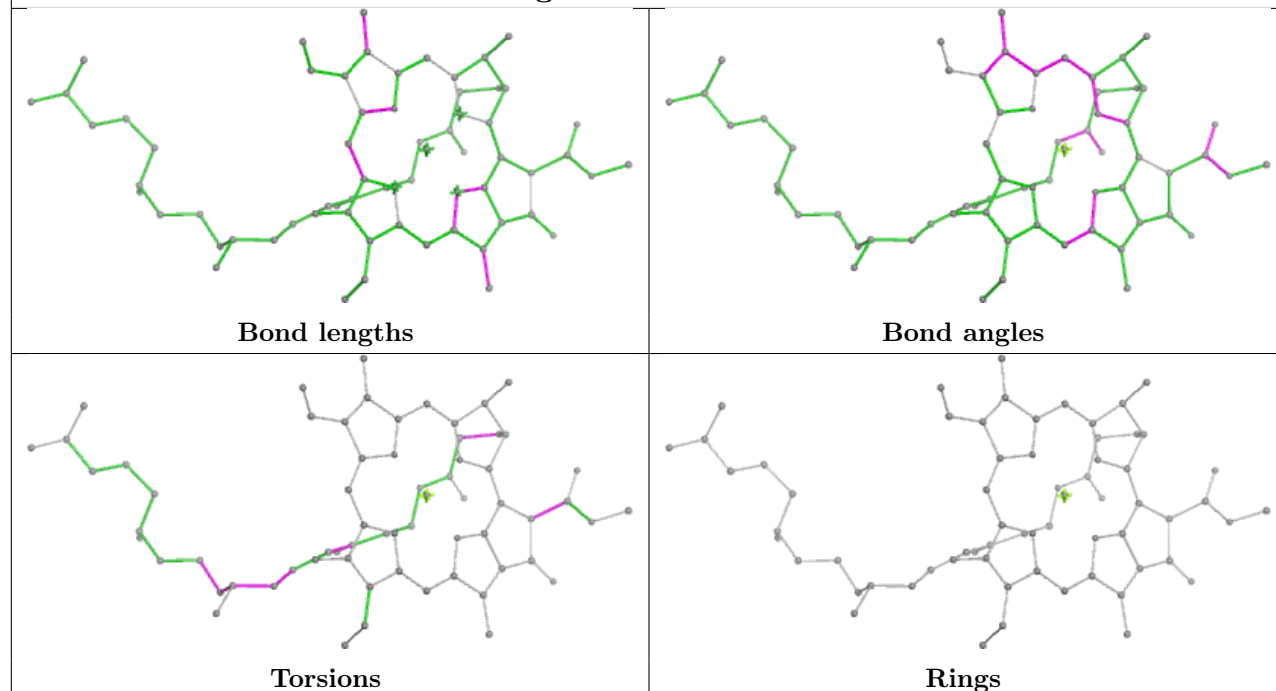




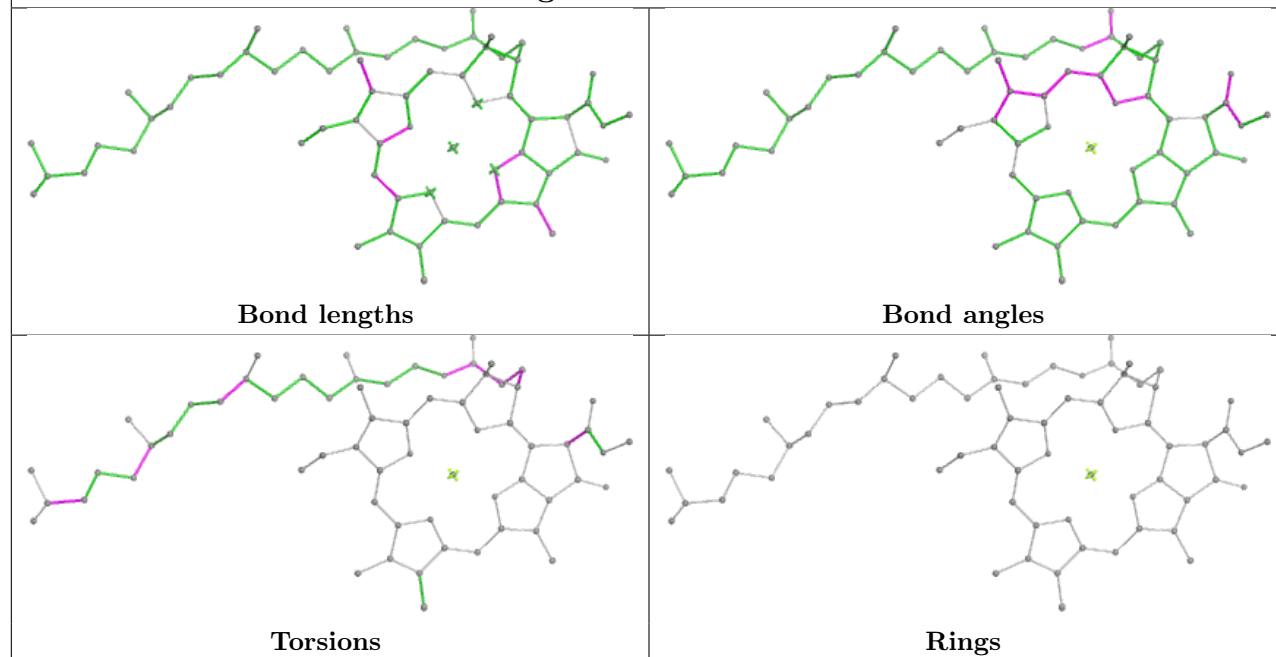
## Ligand CHL S 601



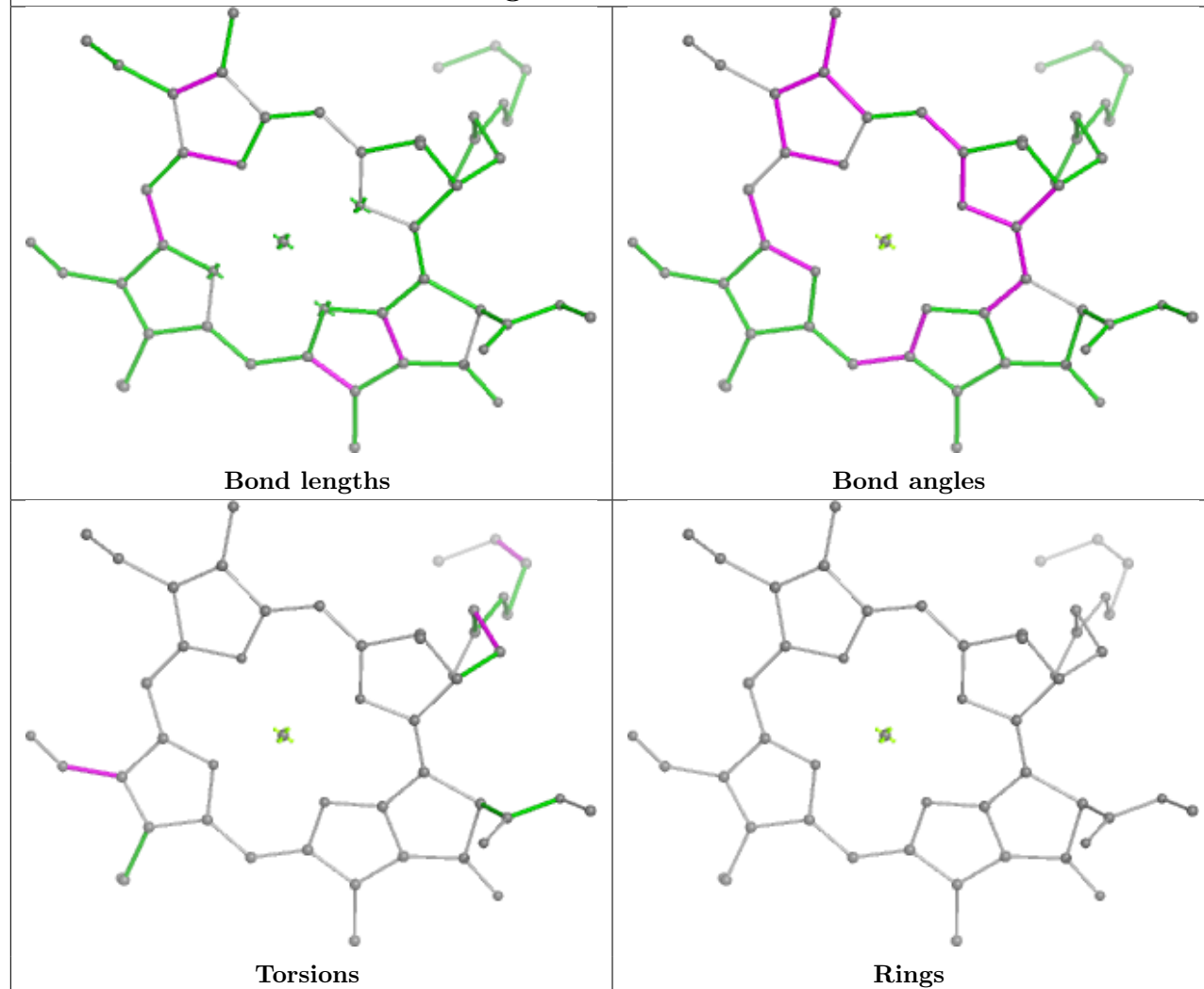
## Ligand CLA b 614

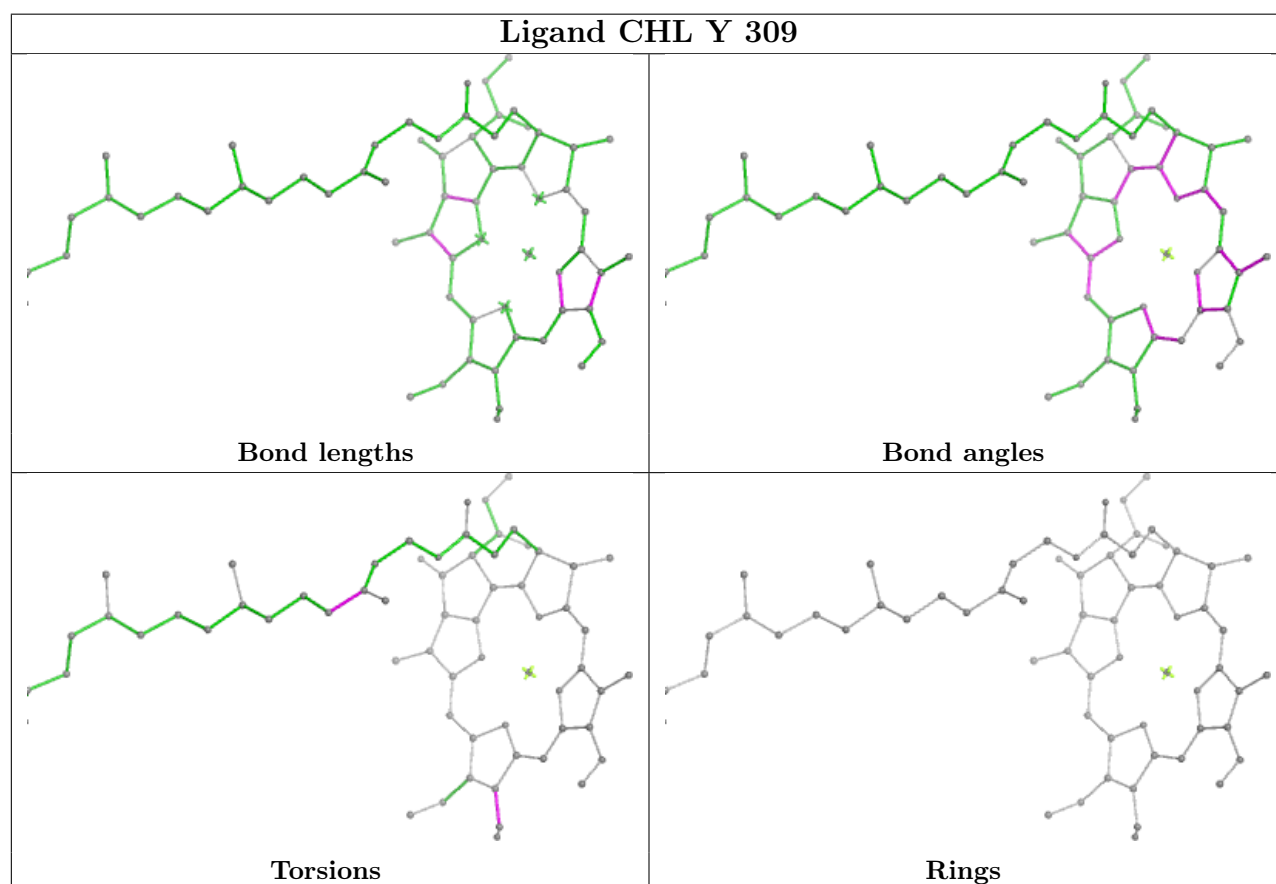
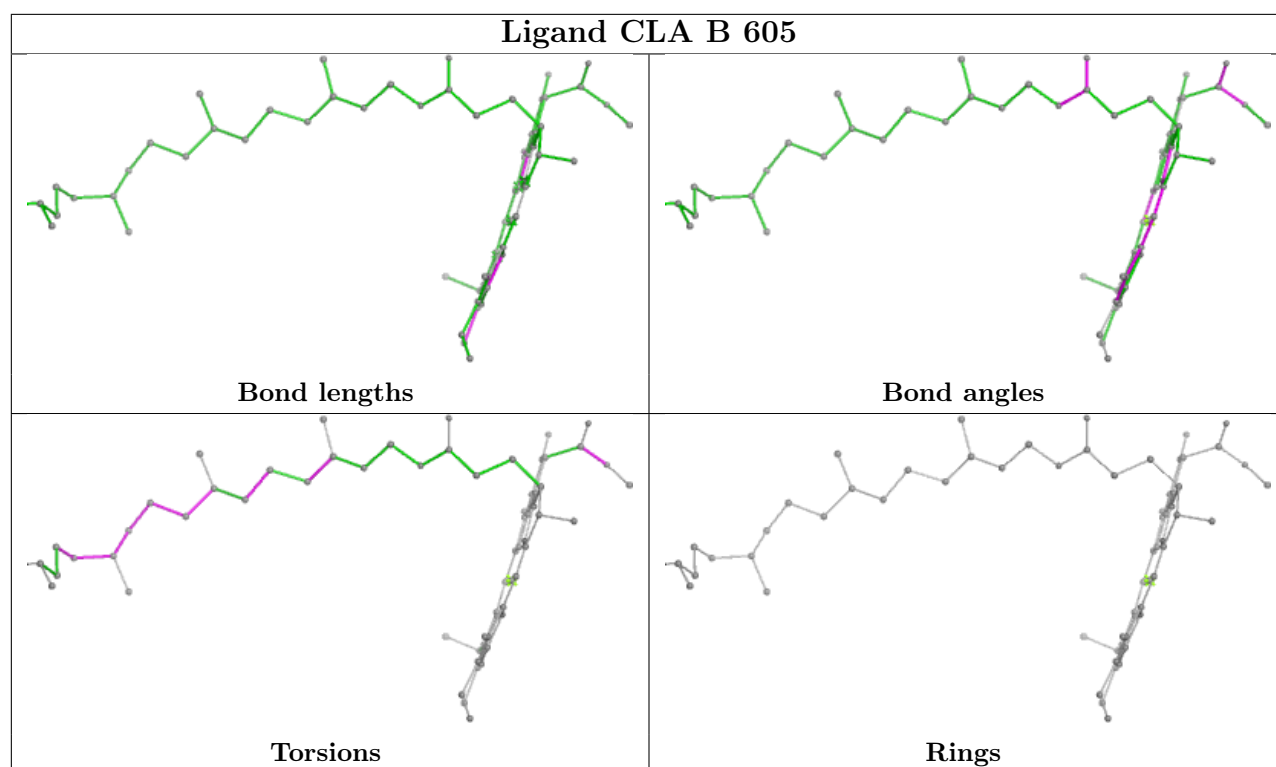


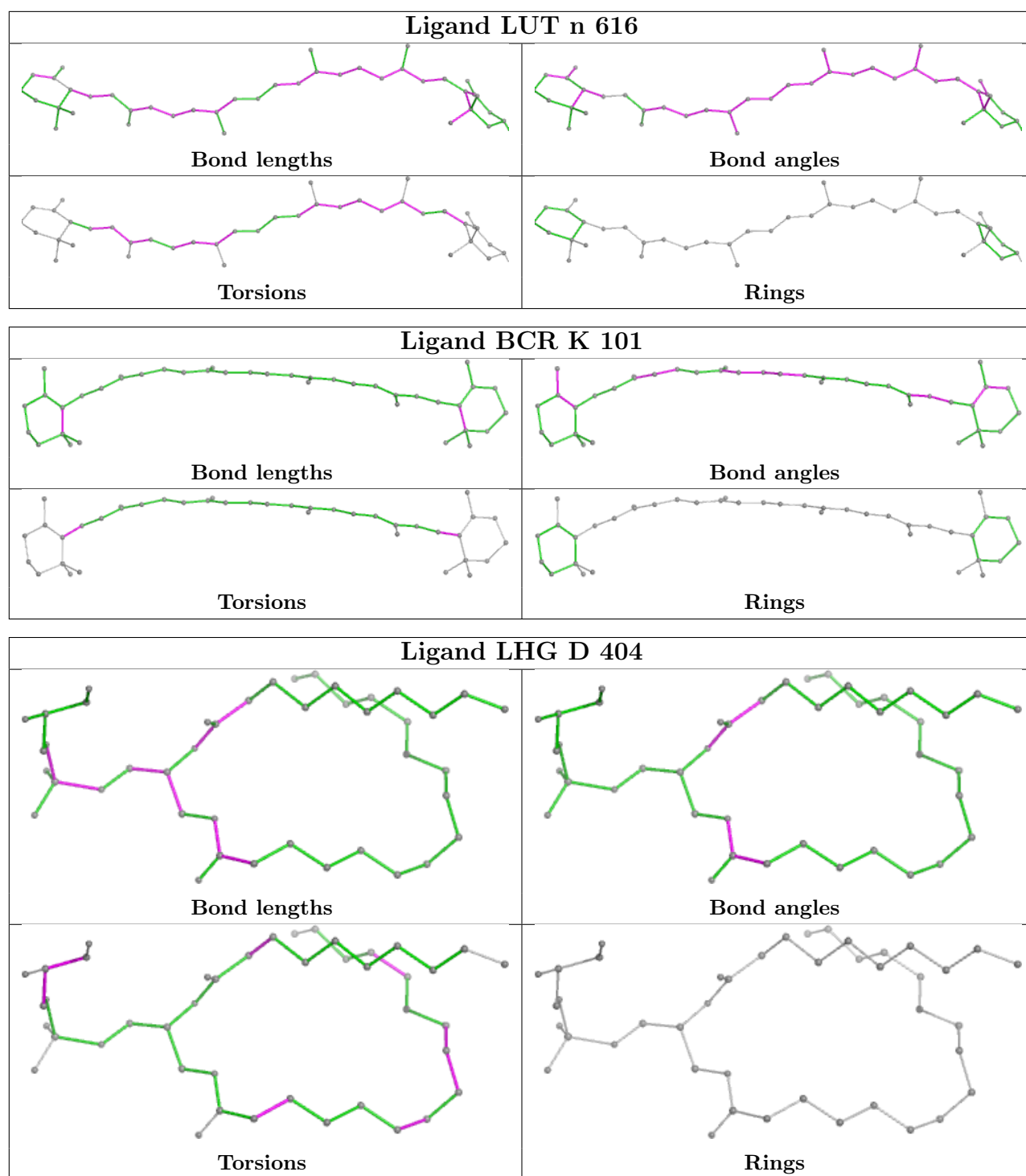
## Ligand CLA c 501



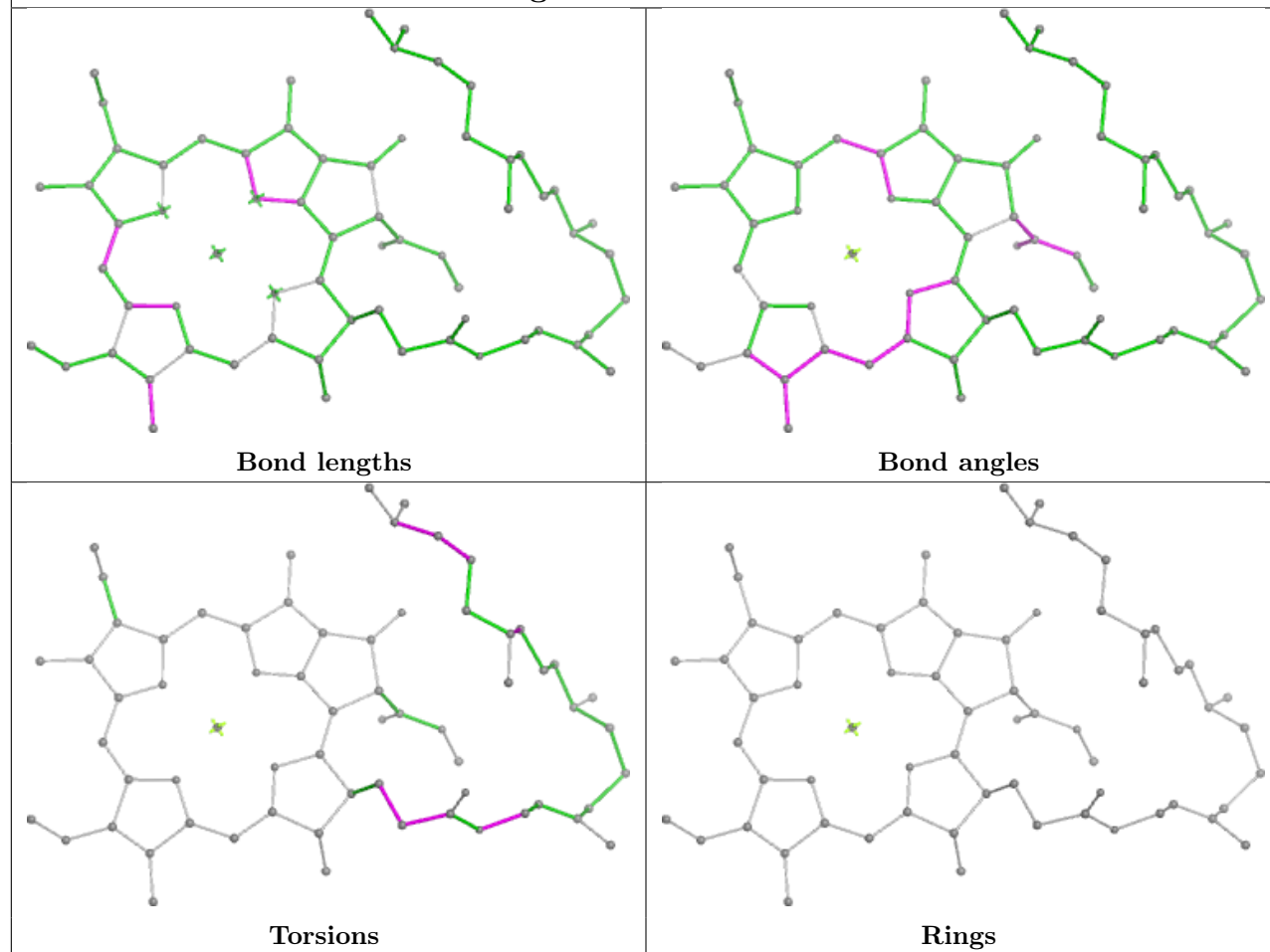
## Ligand CHL n 608



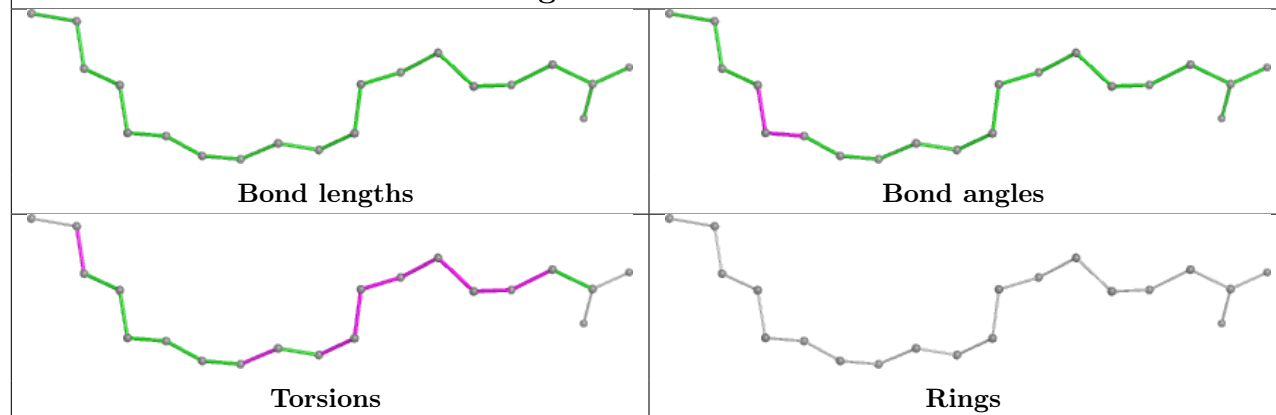




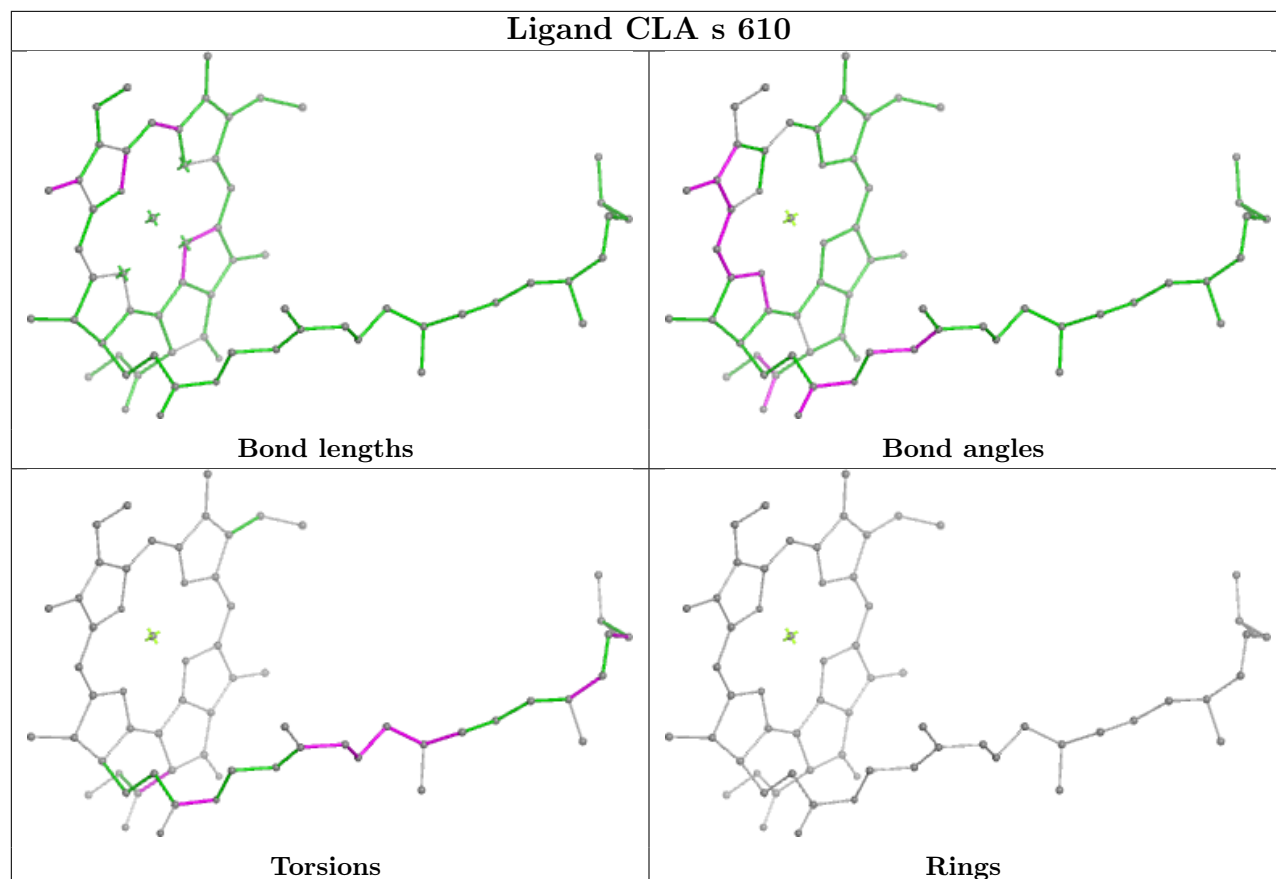
## Ligand CLA B 610



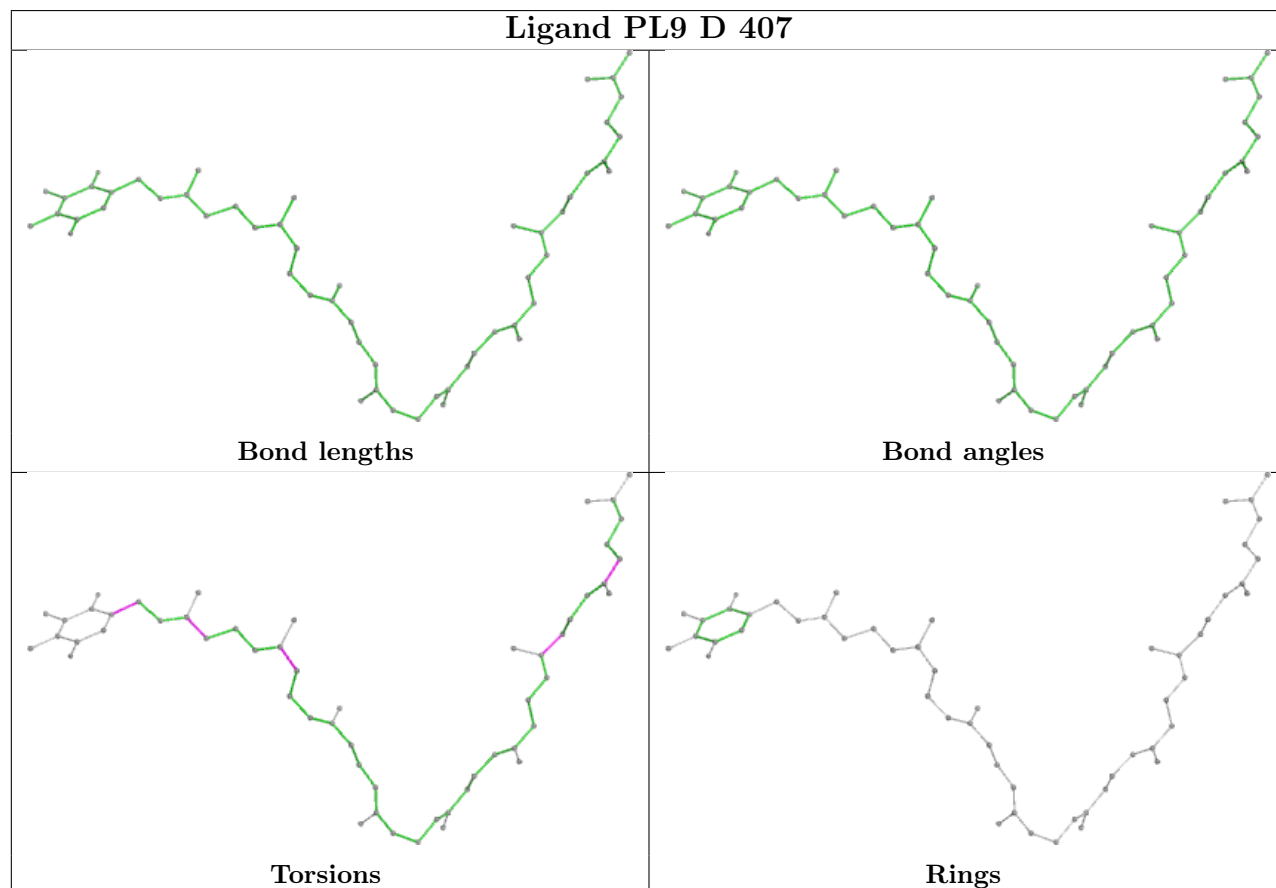
## Ligand LNL a 413

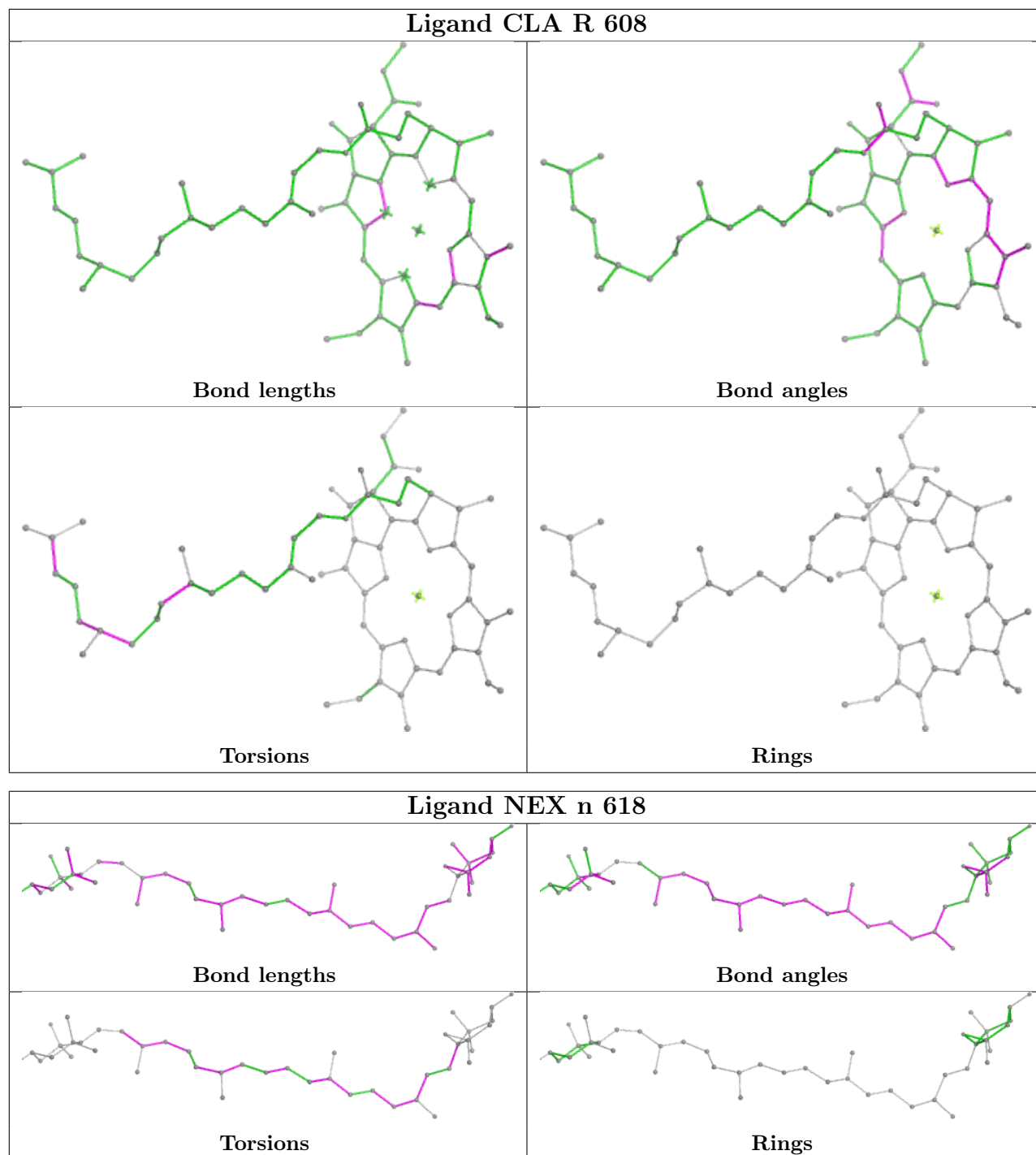


## Ligand CLA s 610

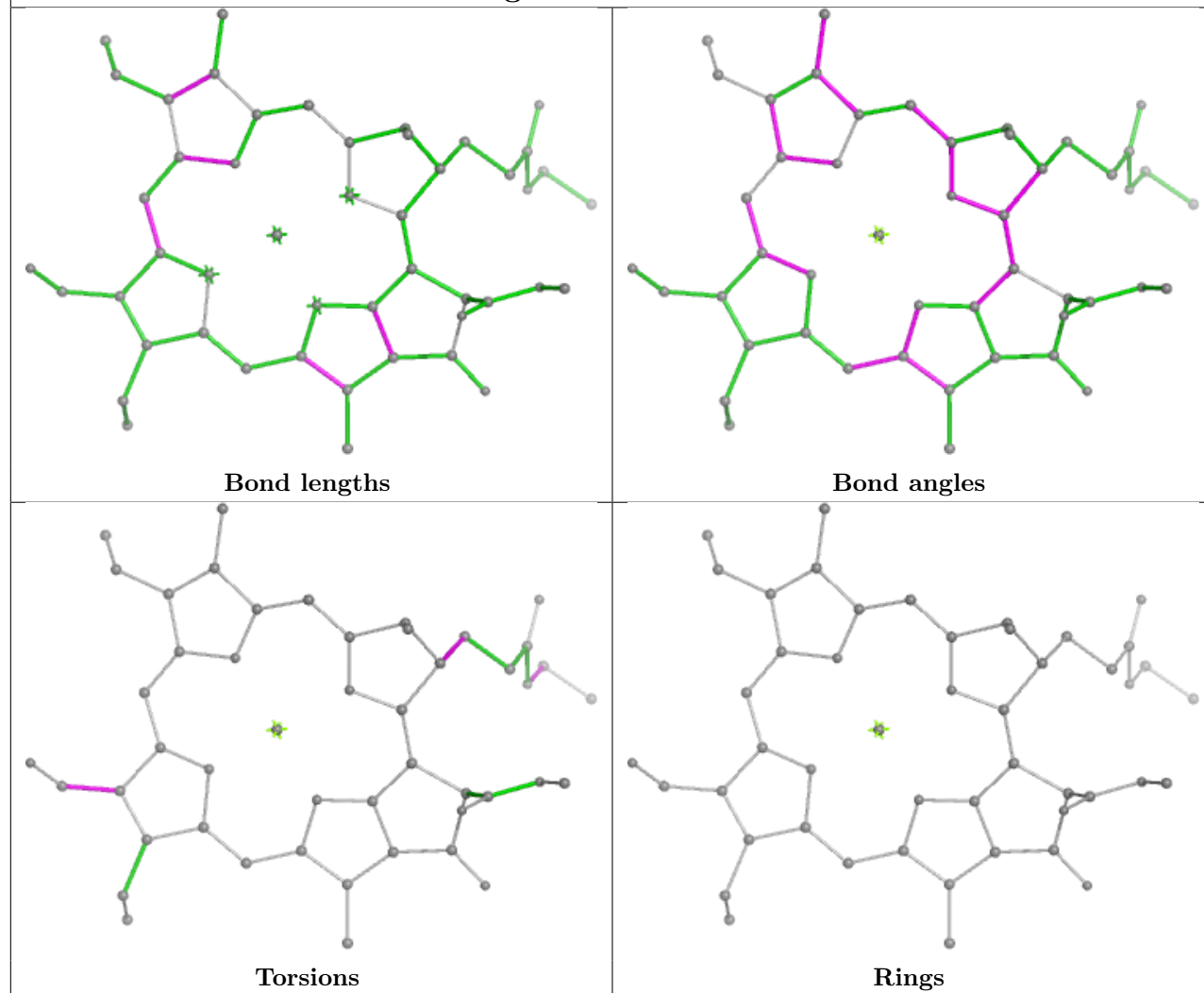


## Ligand PL9 D 407

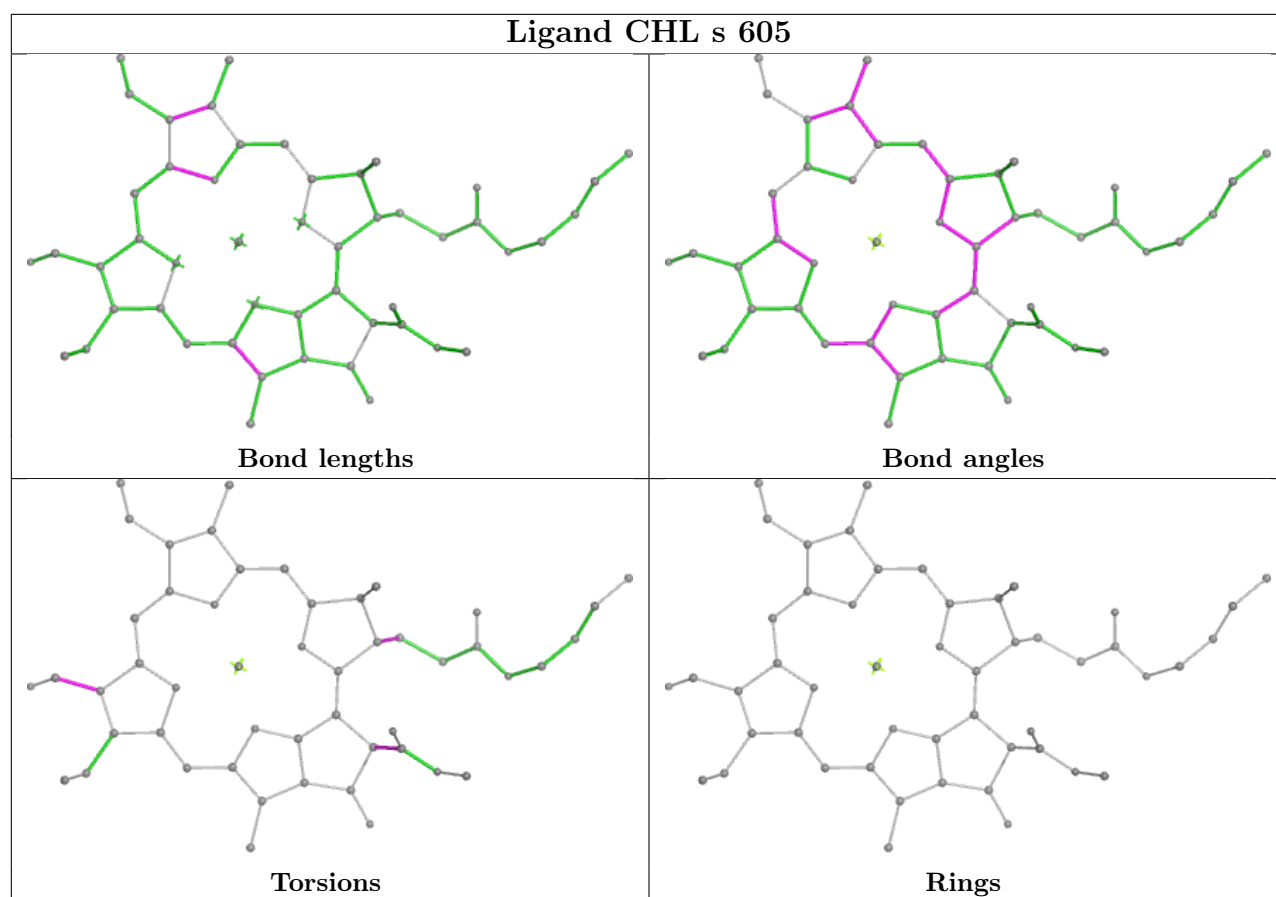




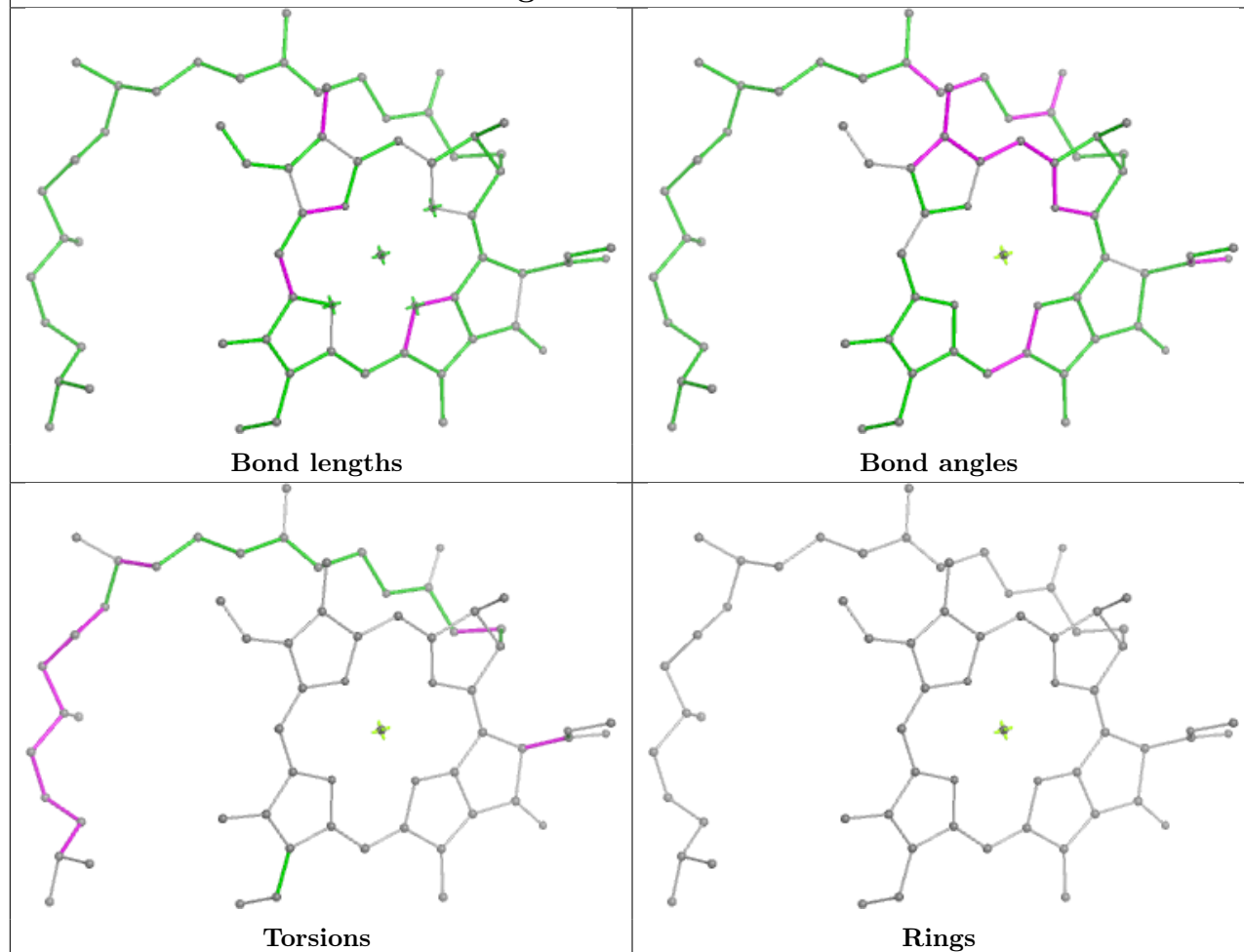
## Ligand CHL n 605



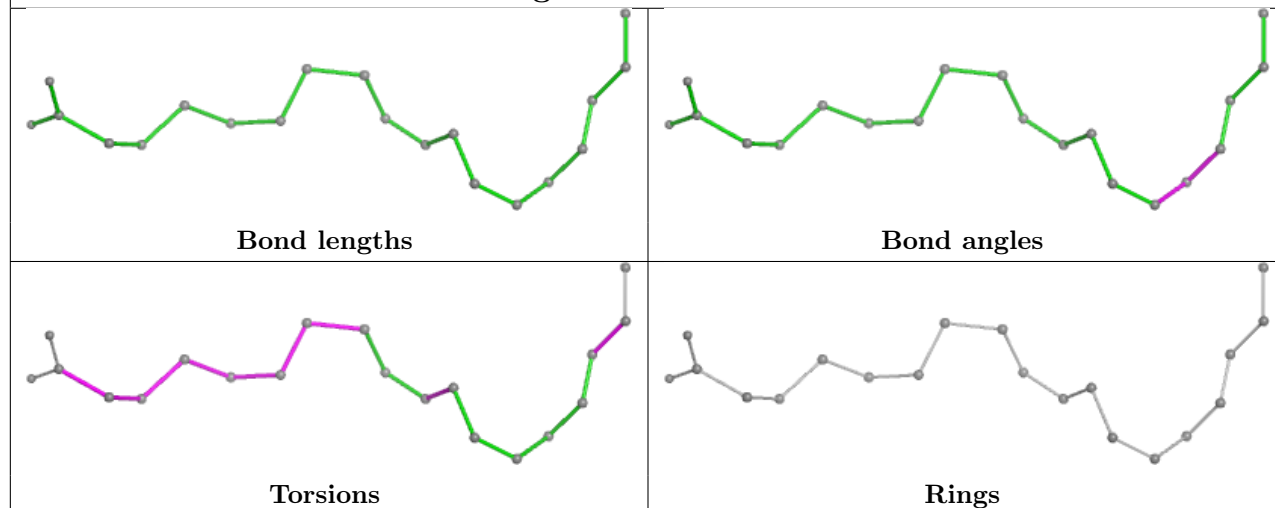


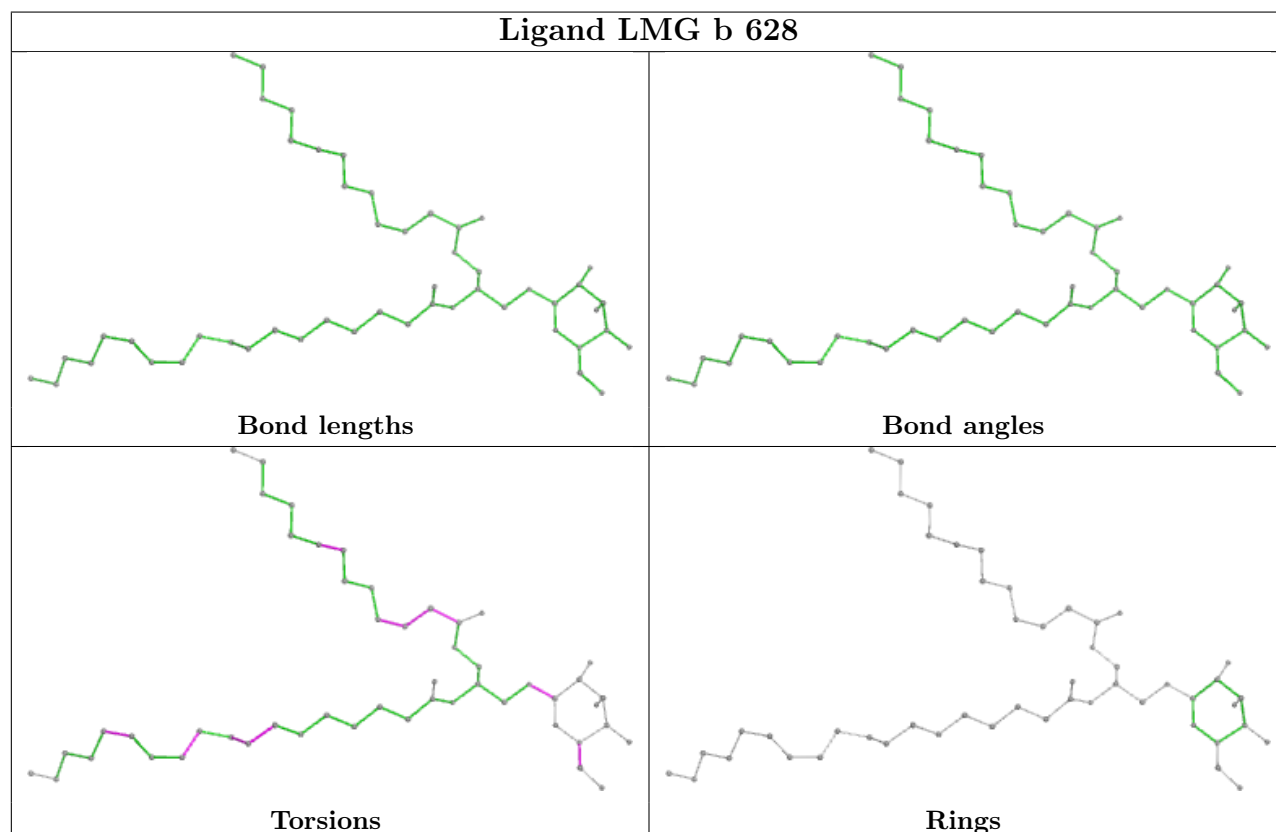
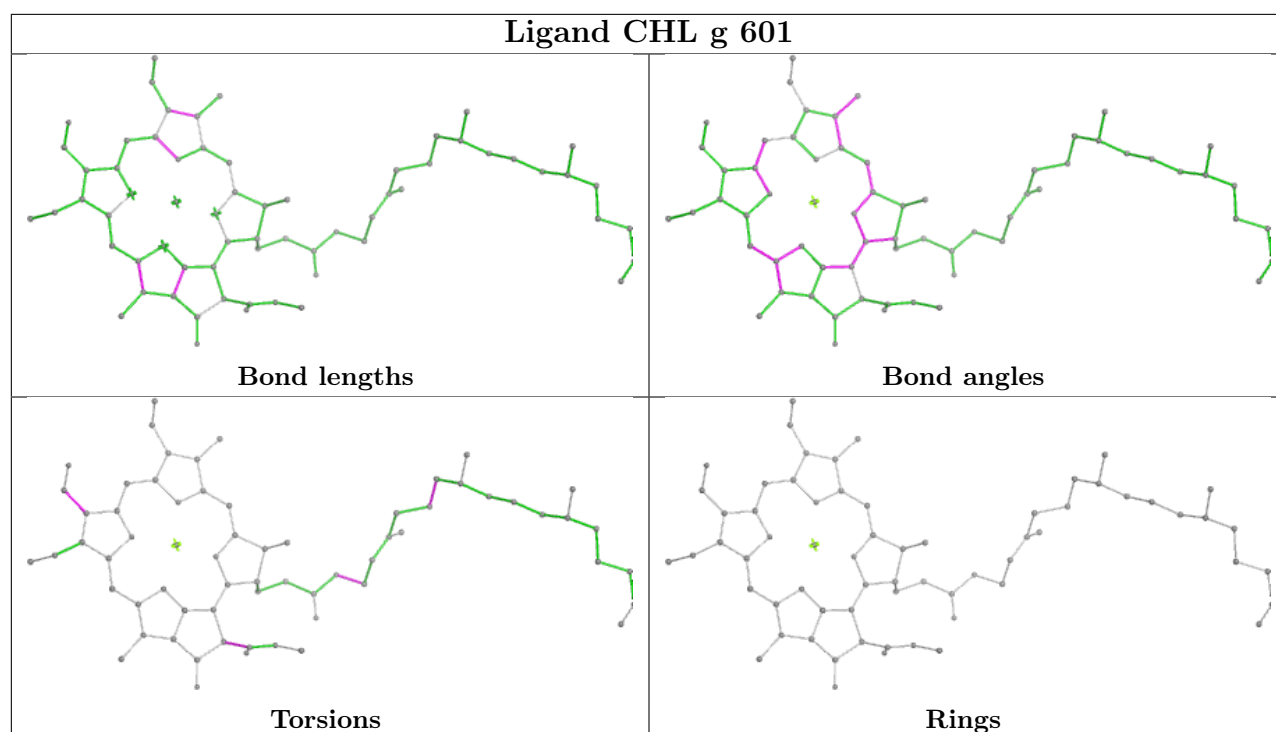


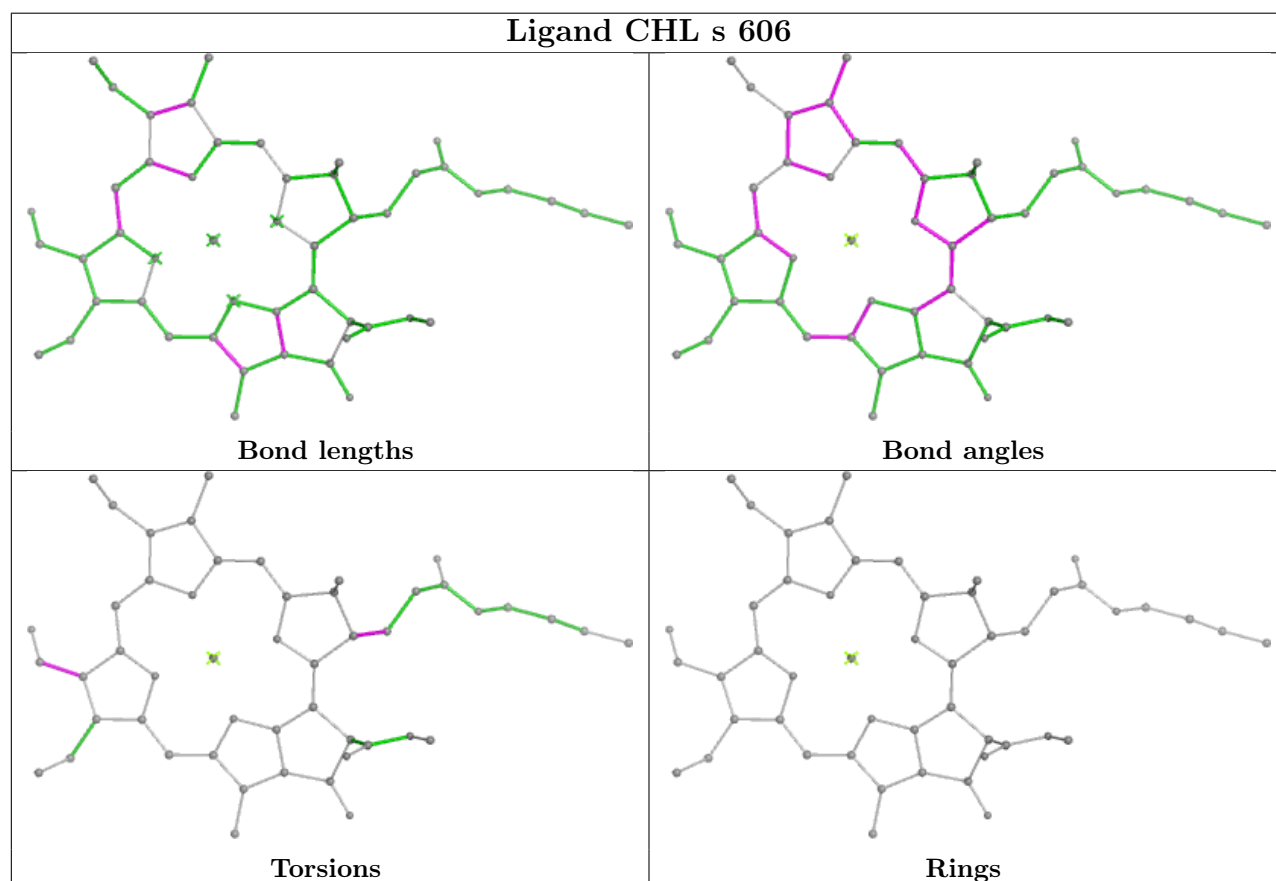
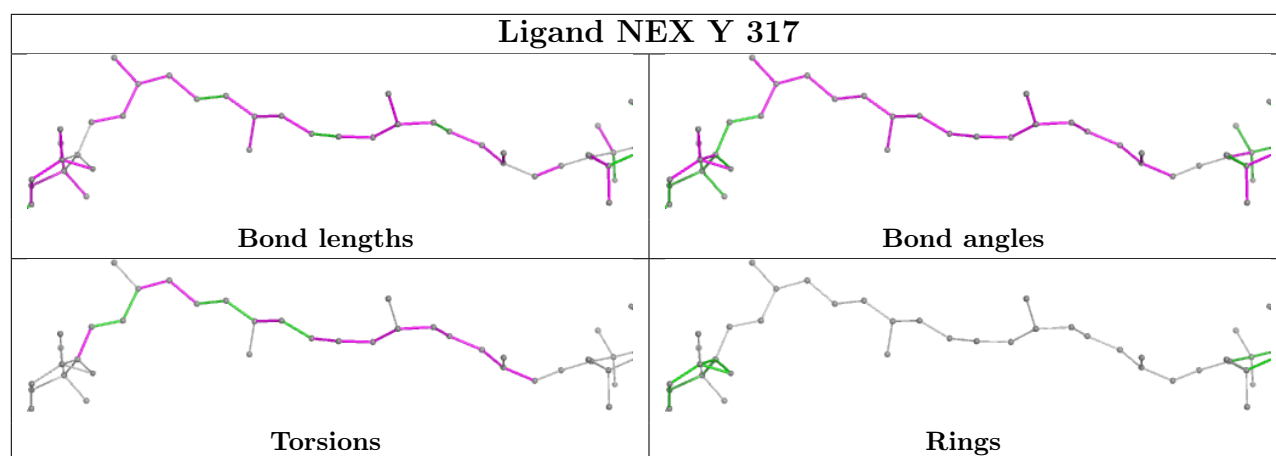
## Ligand CLA Y 303



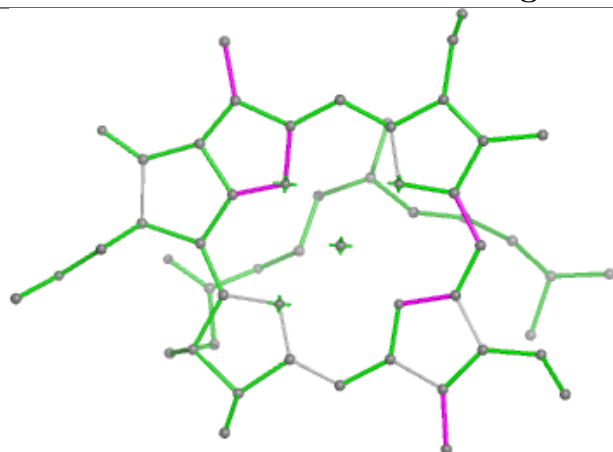
## Ligand LNL B 623



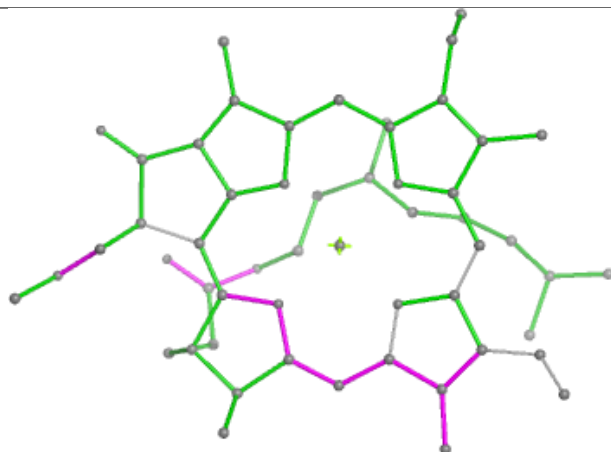




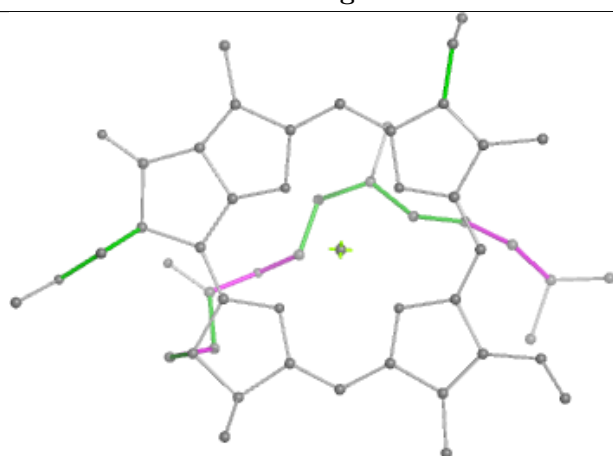
## Ligand CLA s 612



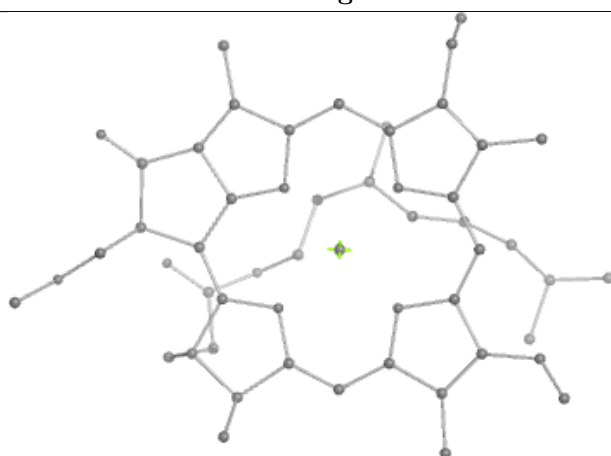
Bond lengths



Bond angles

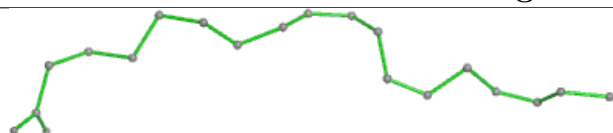


Torsions

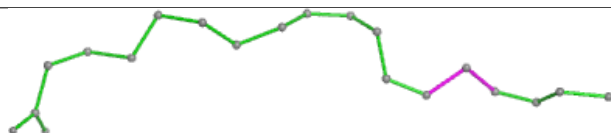


Rings

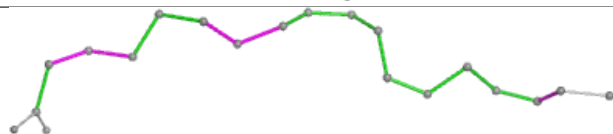
## Ligand LNL C 519



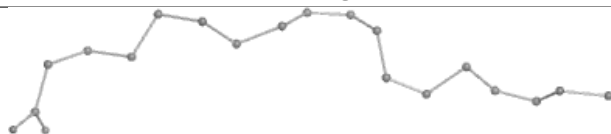
Bond lengths



Bond angles

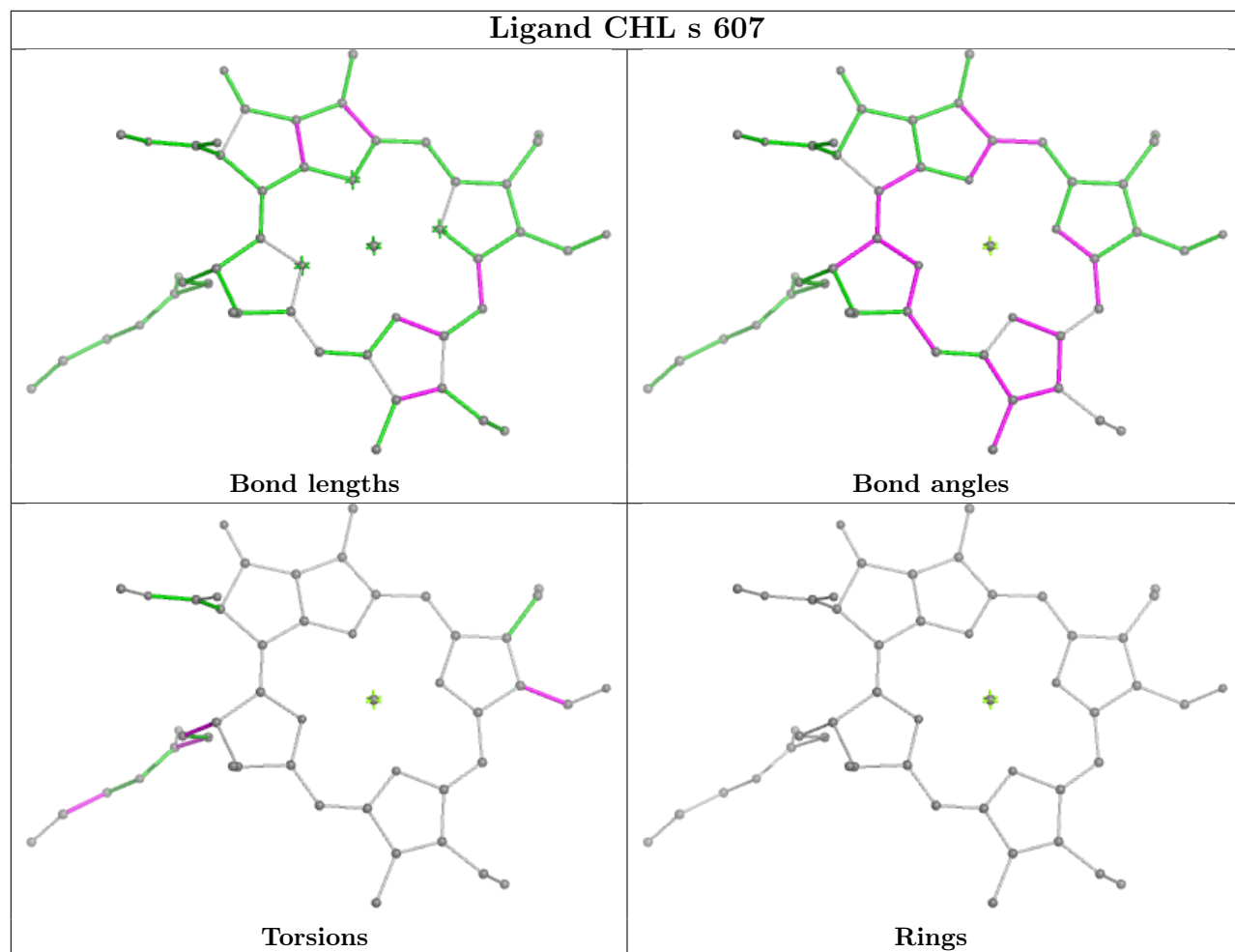


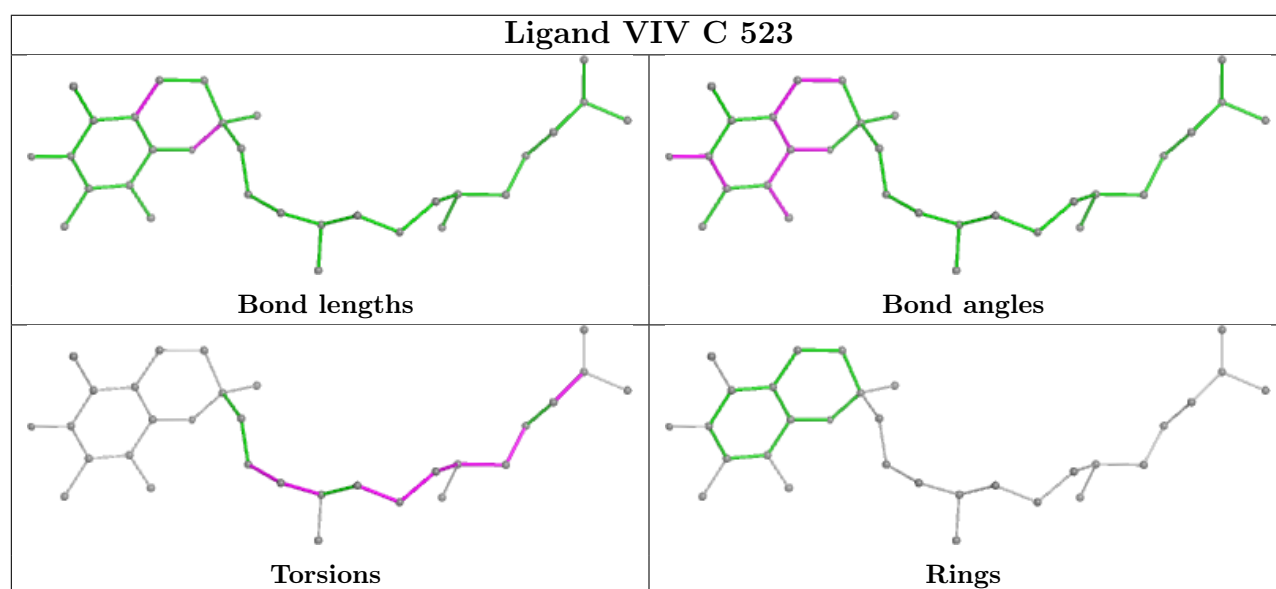
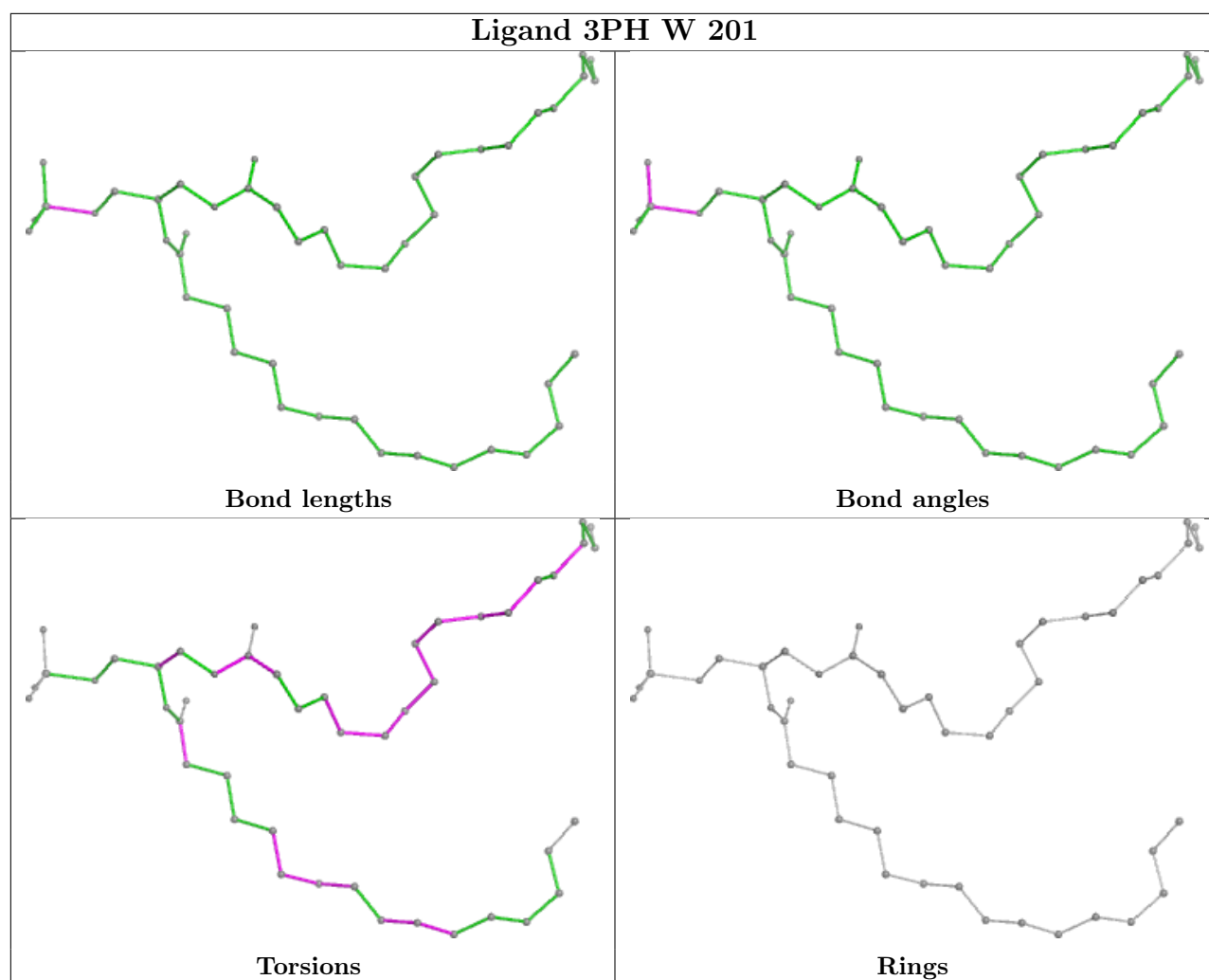
Torsions



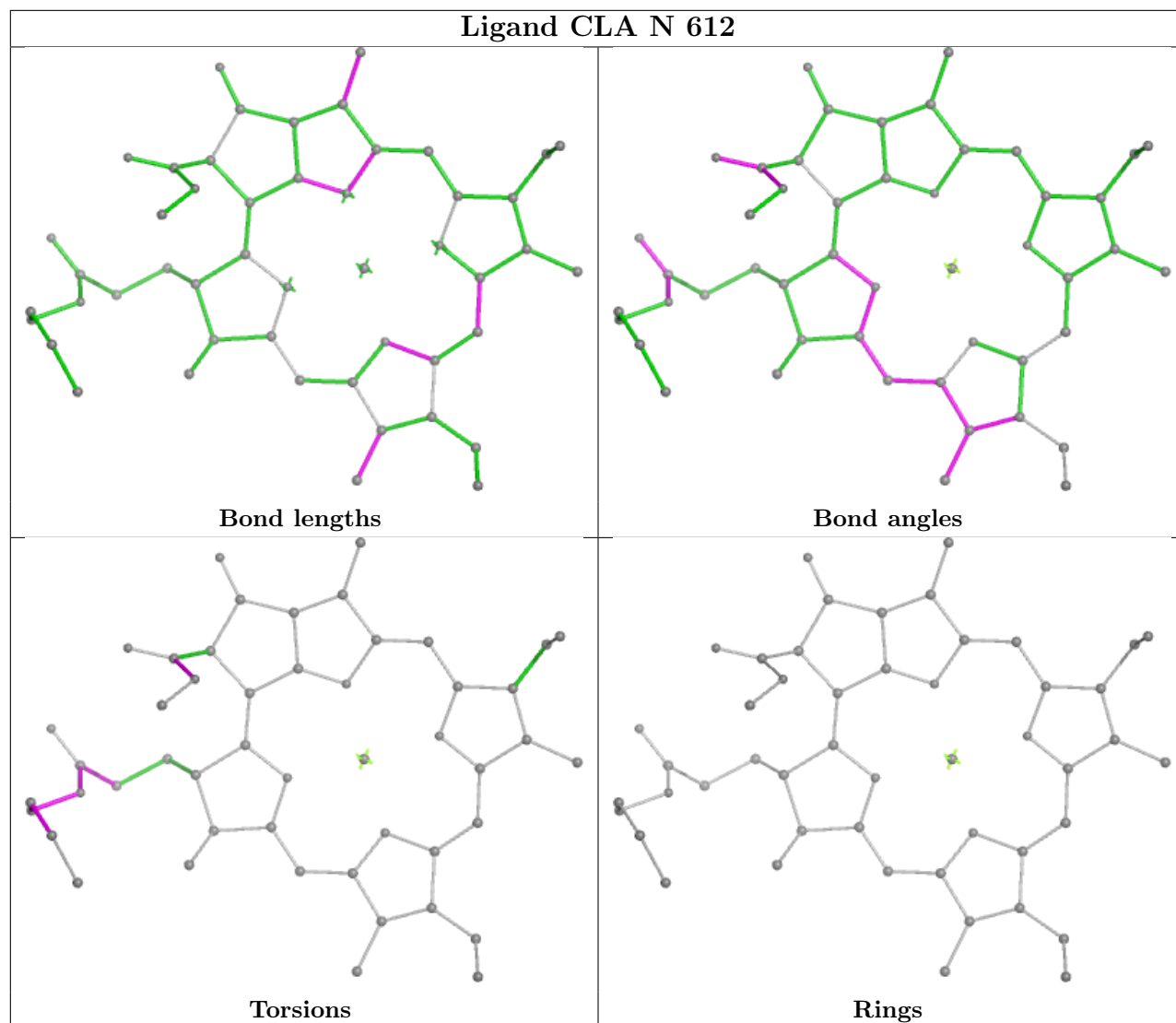
Rings

## Ligand CHL s 607

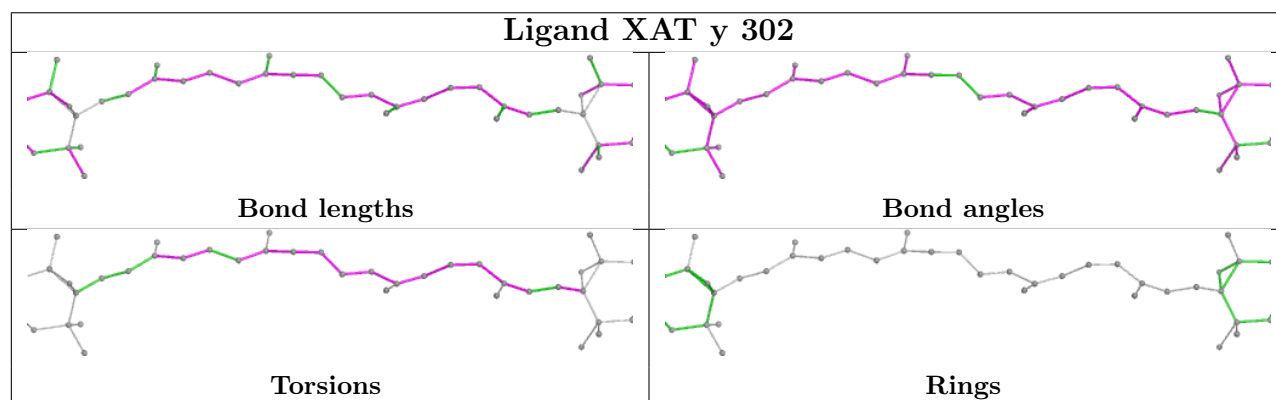




## Ligand CLA N 612

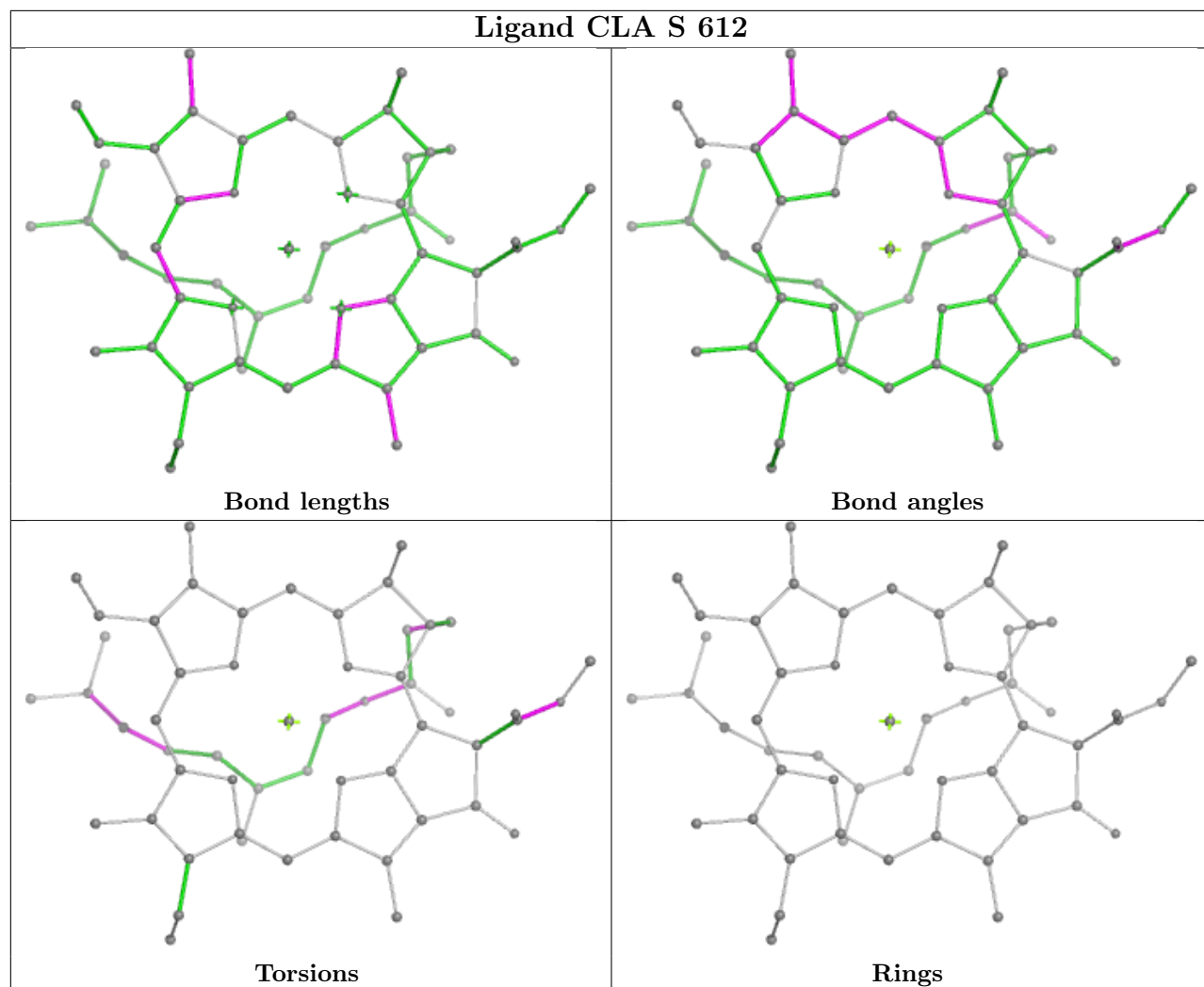


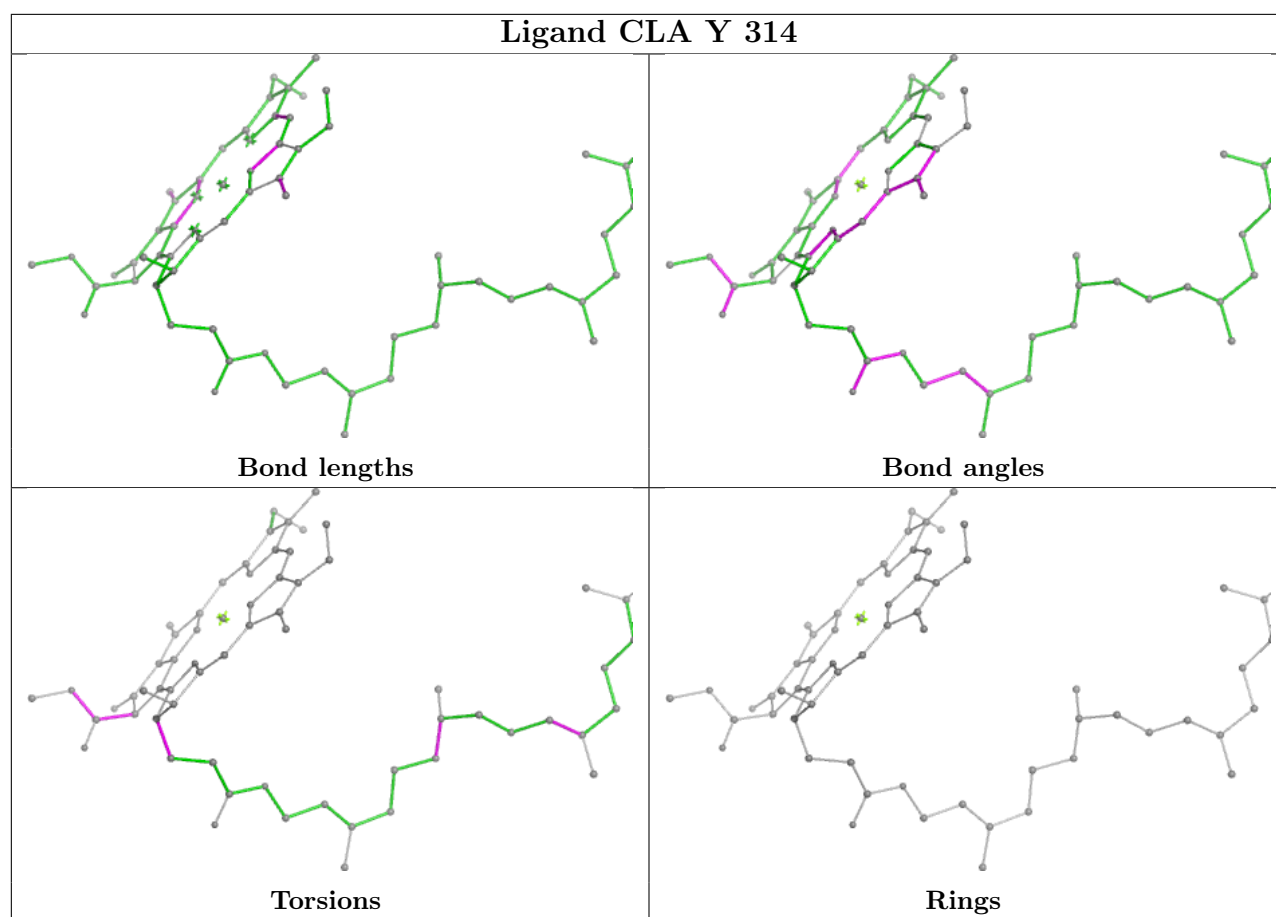
## Ligand XAT y 302



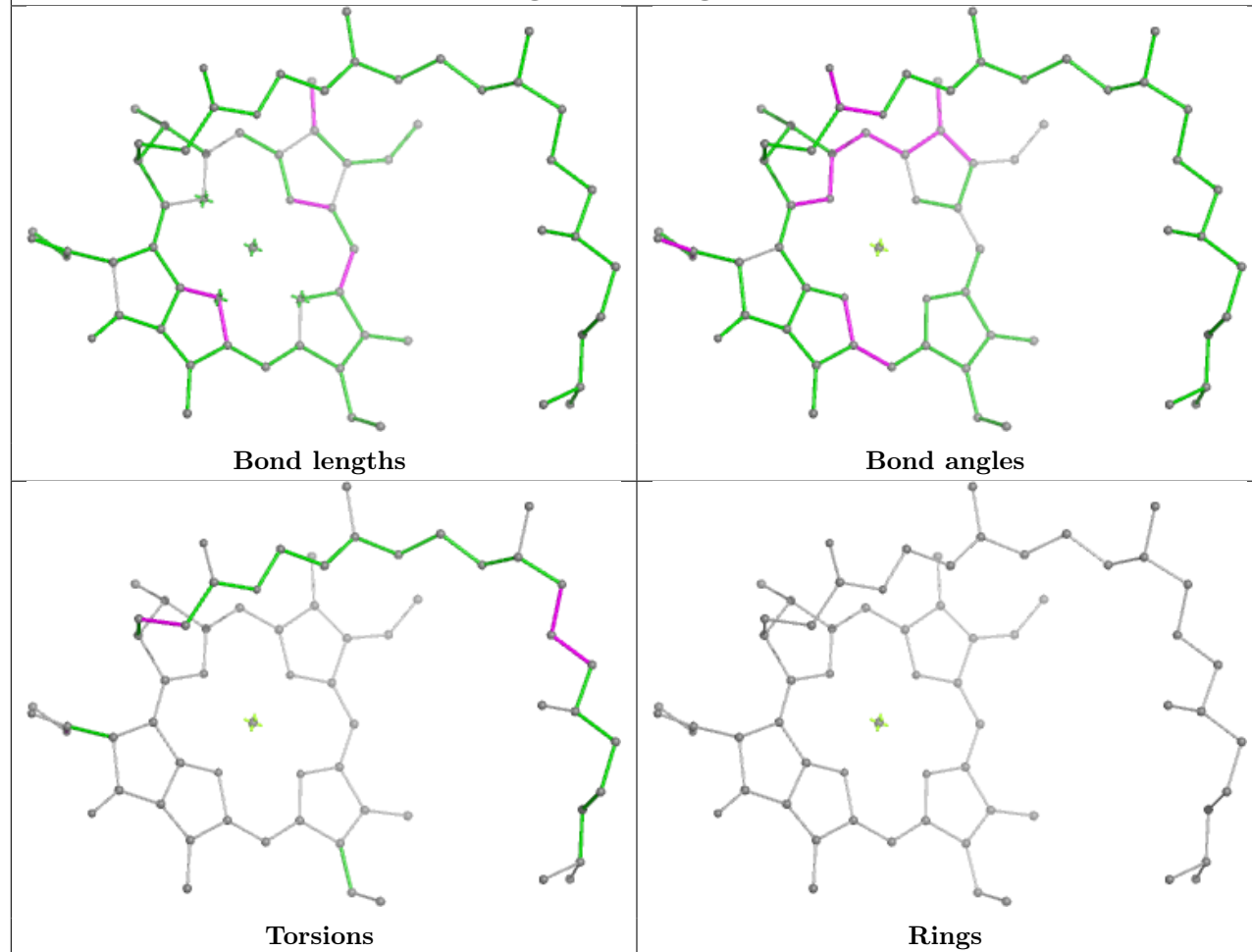


## Ligand CLA S 612

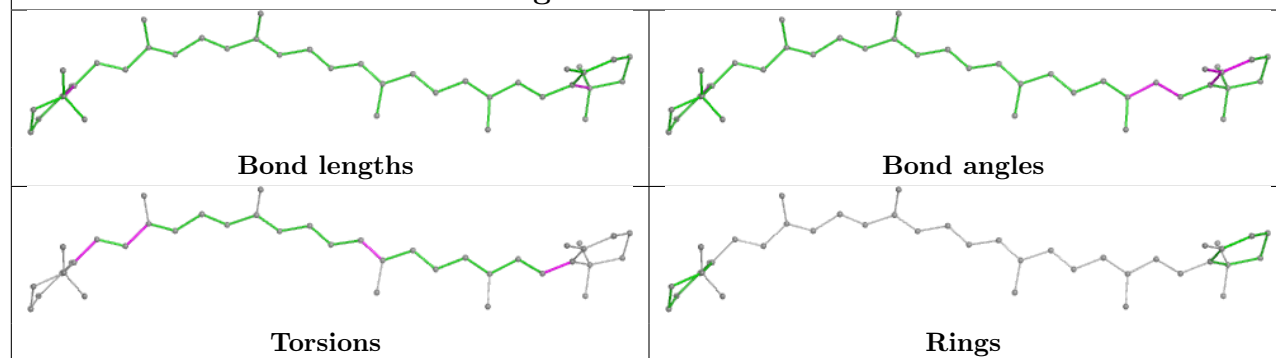


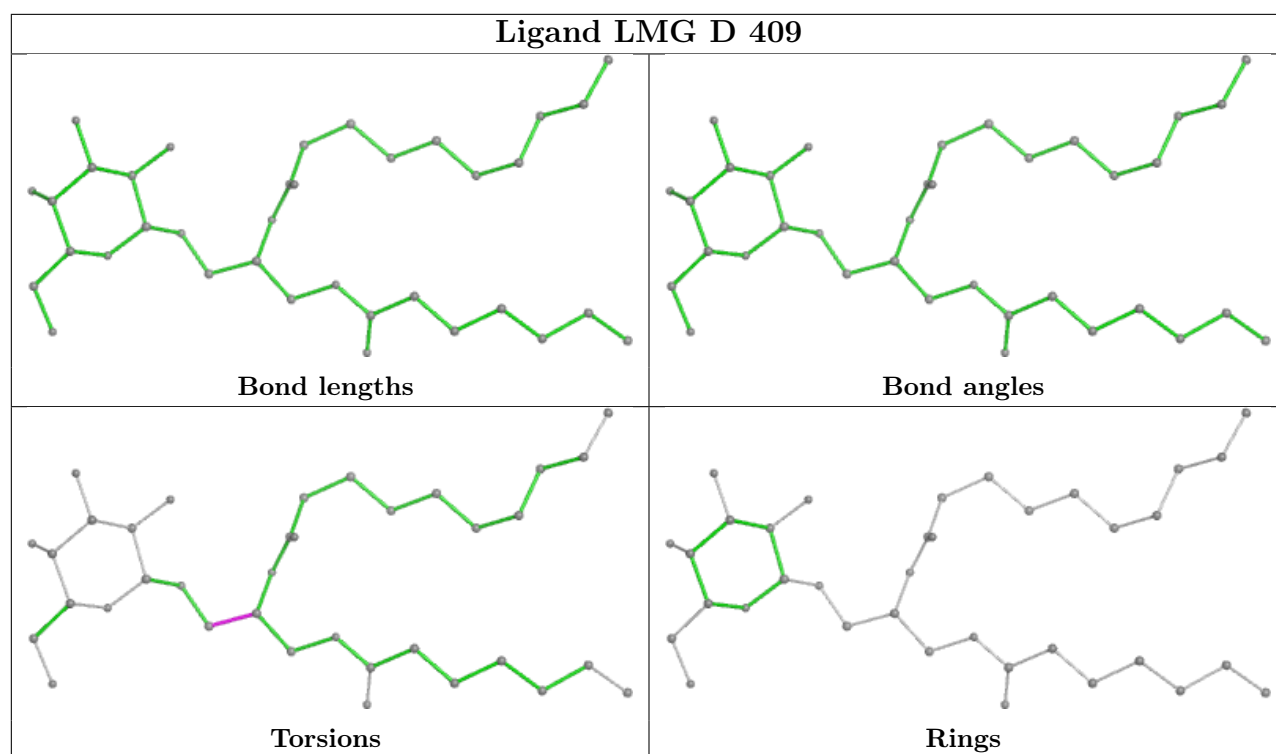


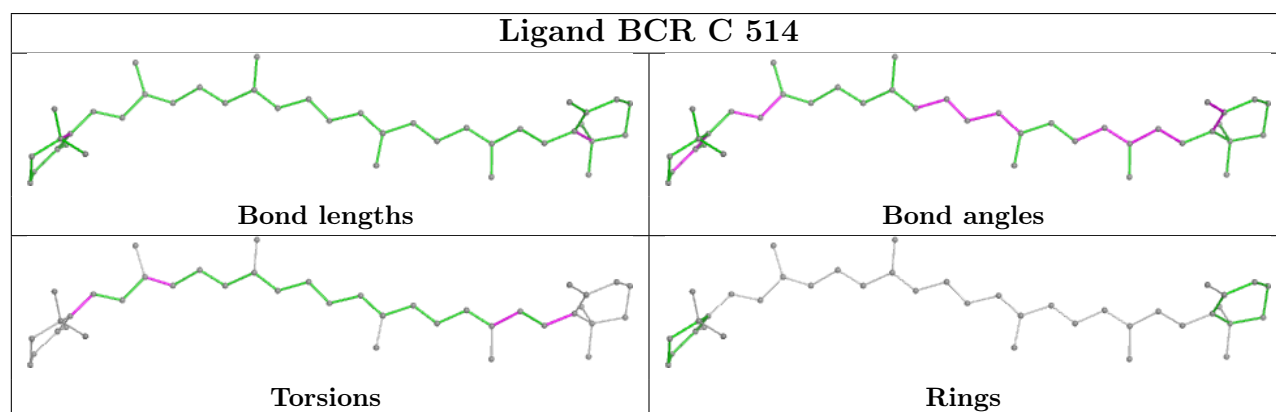
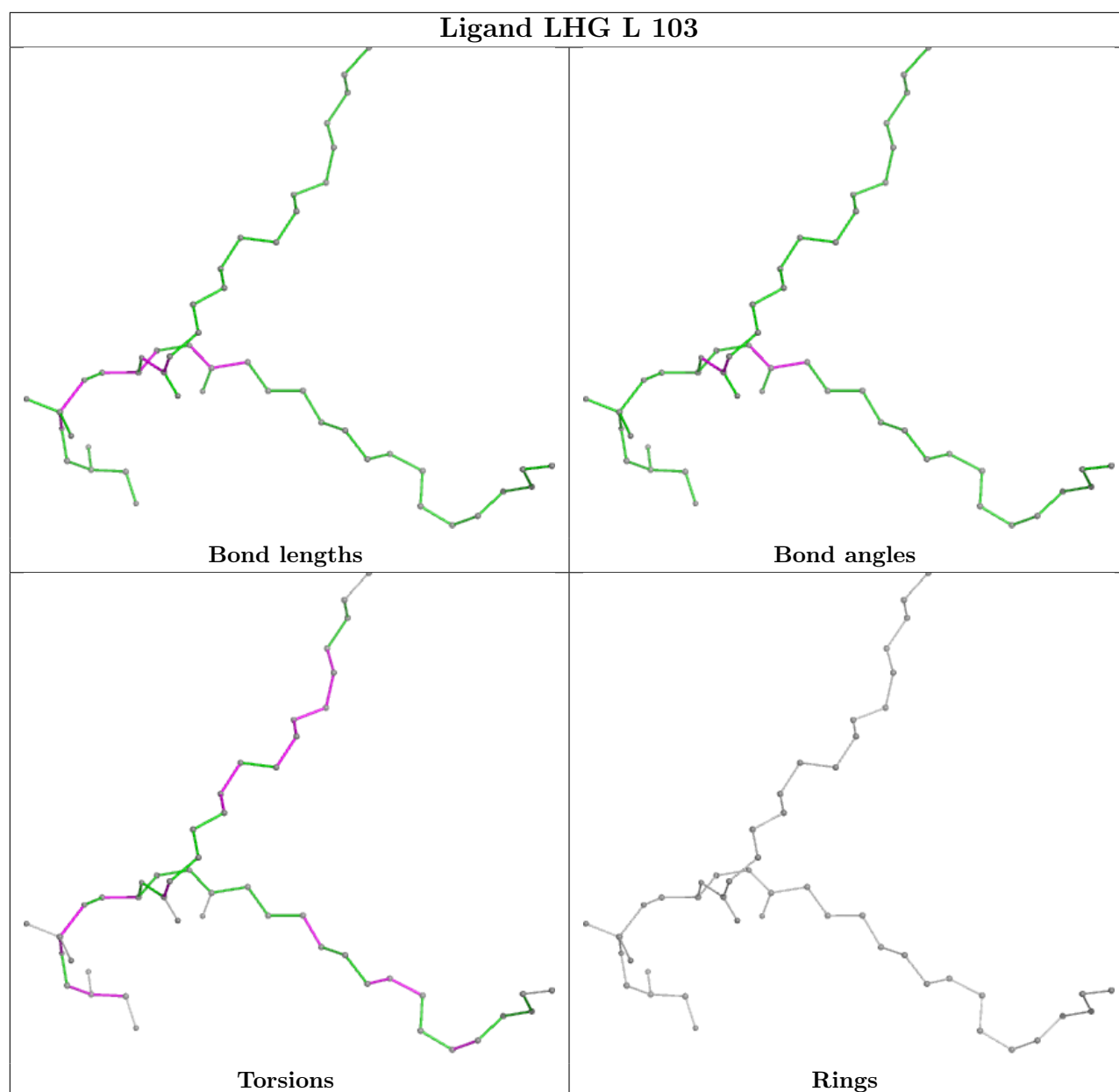
## Ligand CLA g 602

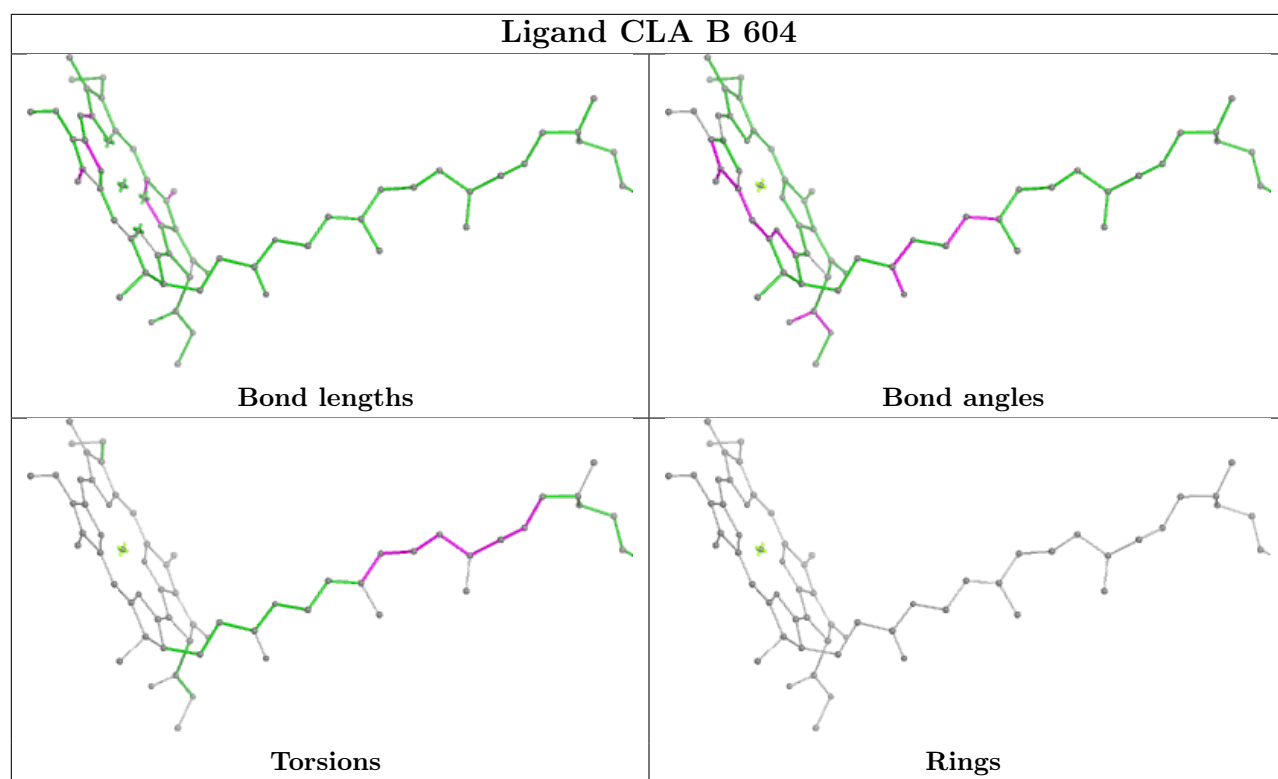


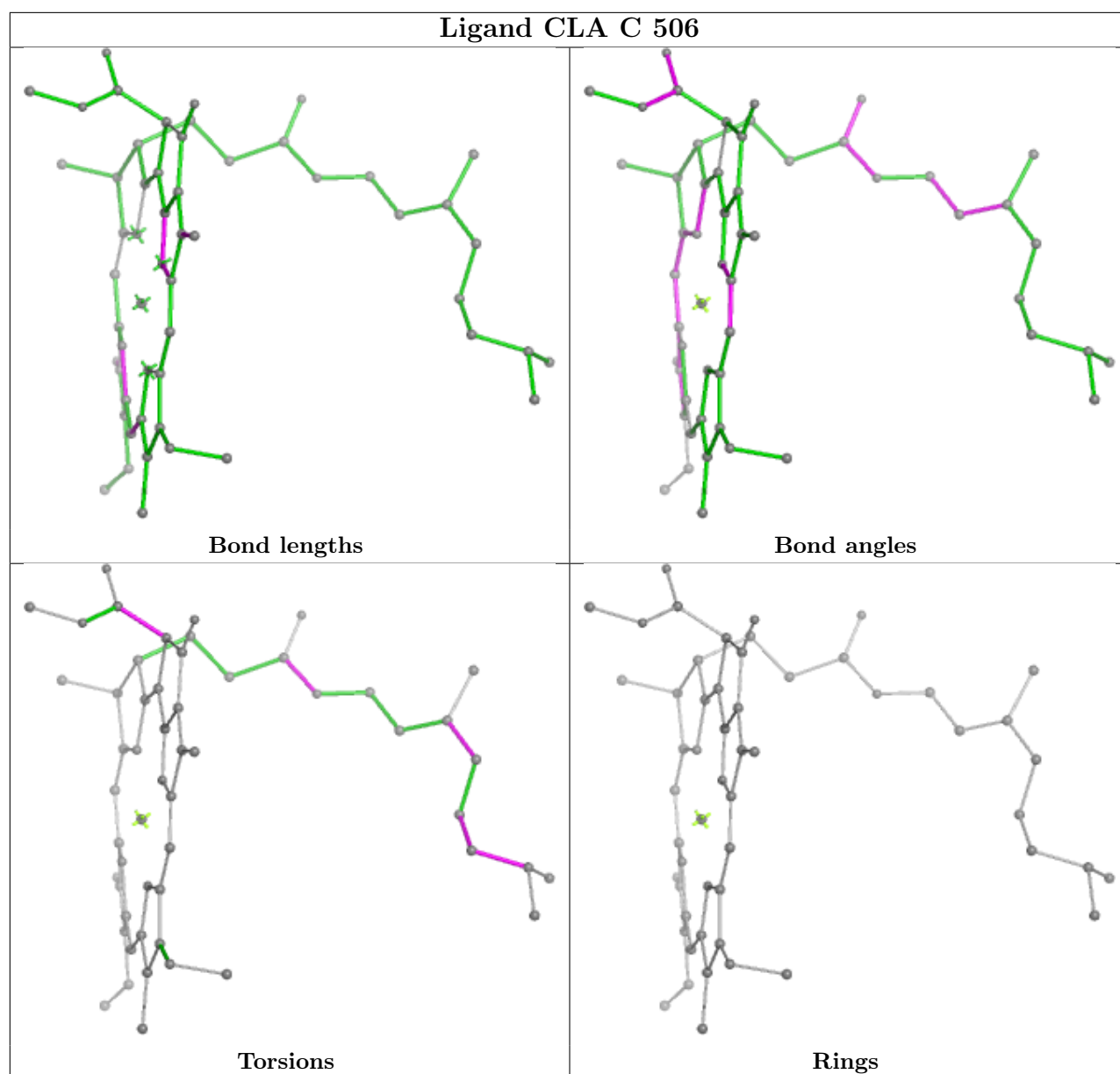
## Ligand BCR h 501



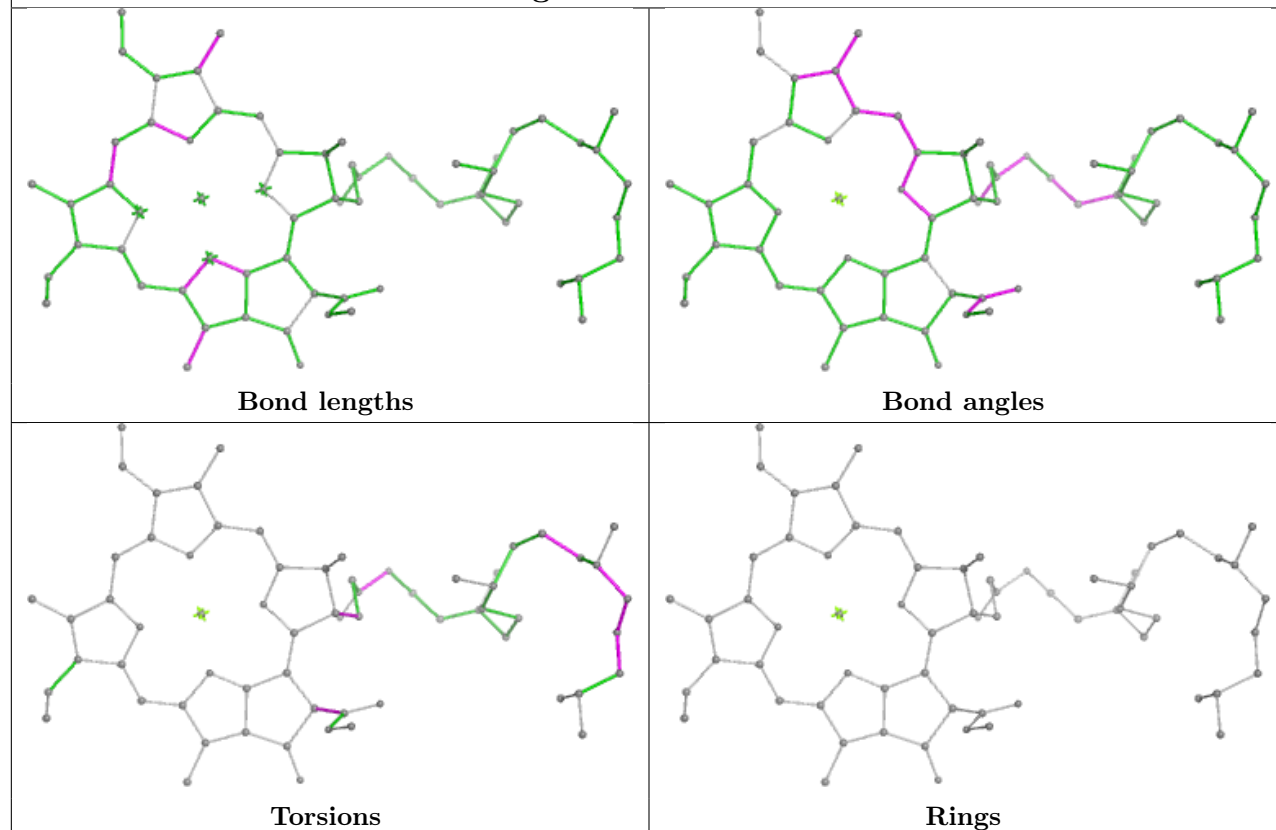




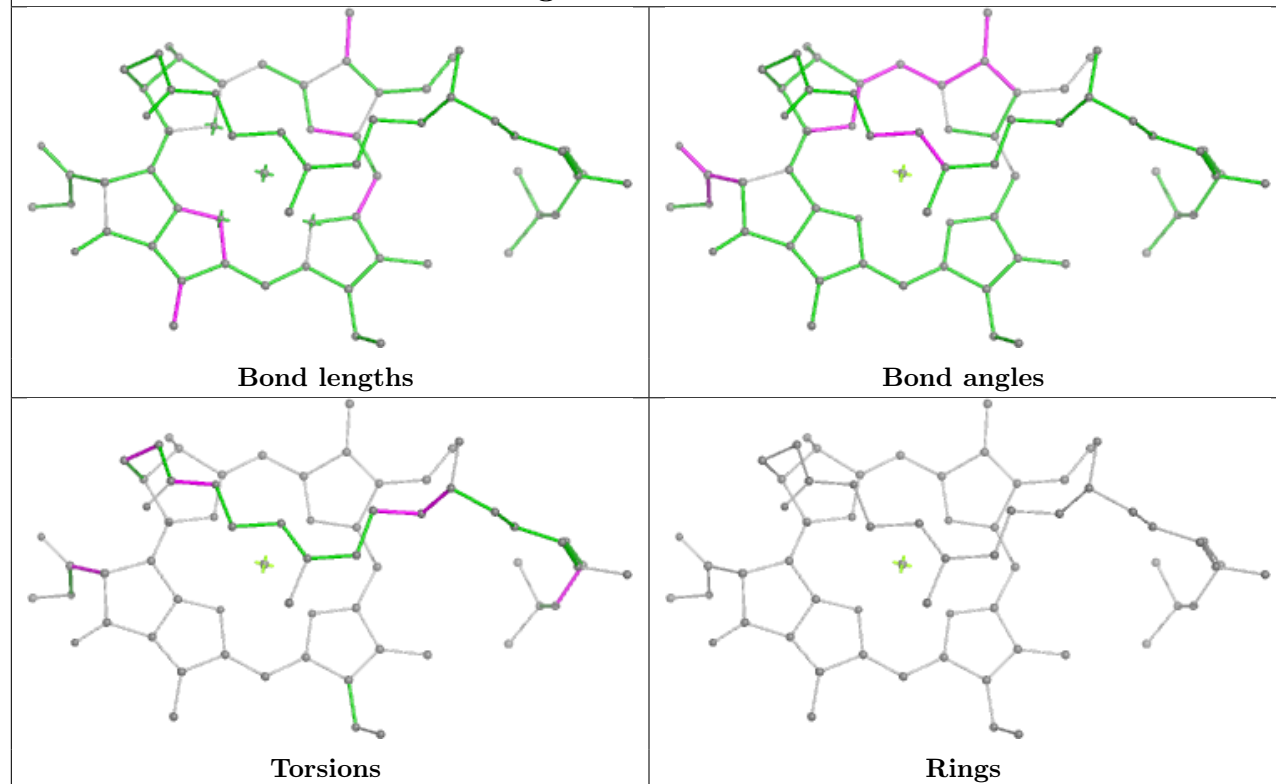




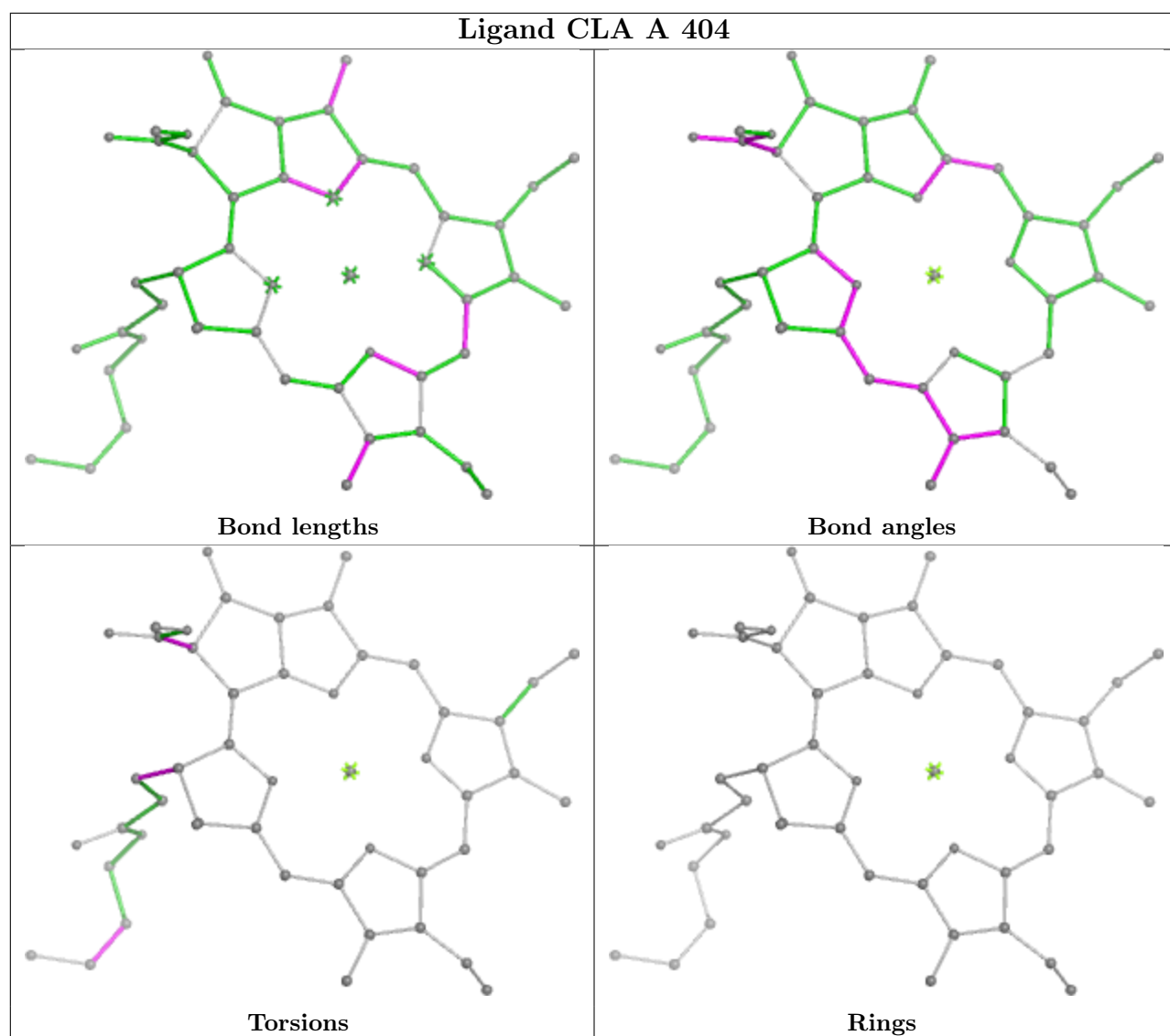
## Ligand CLA B 612

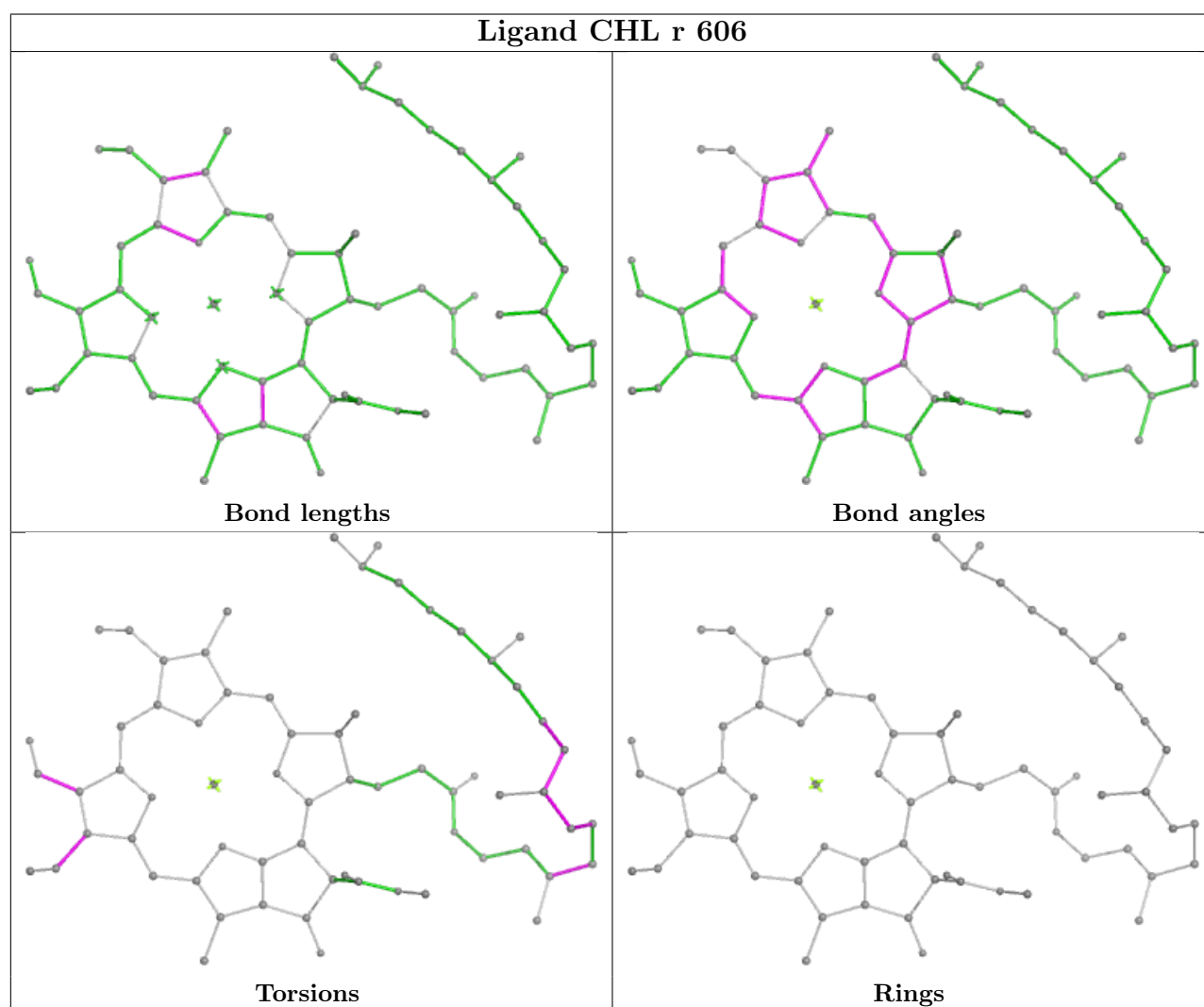
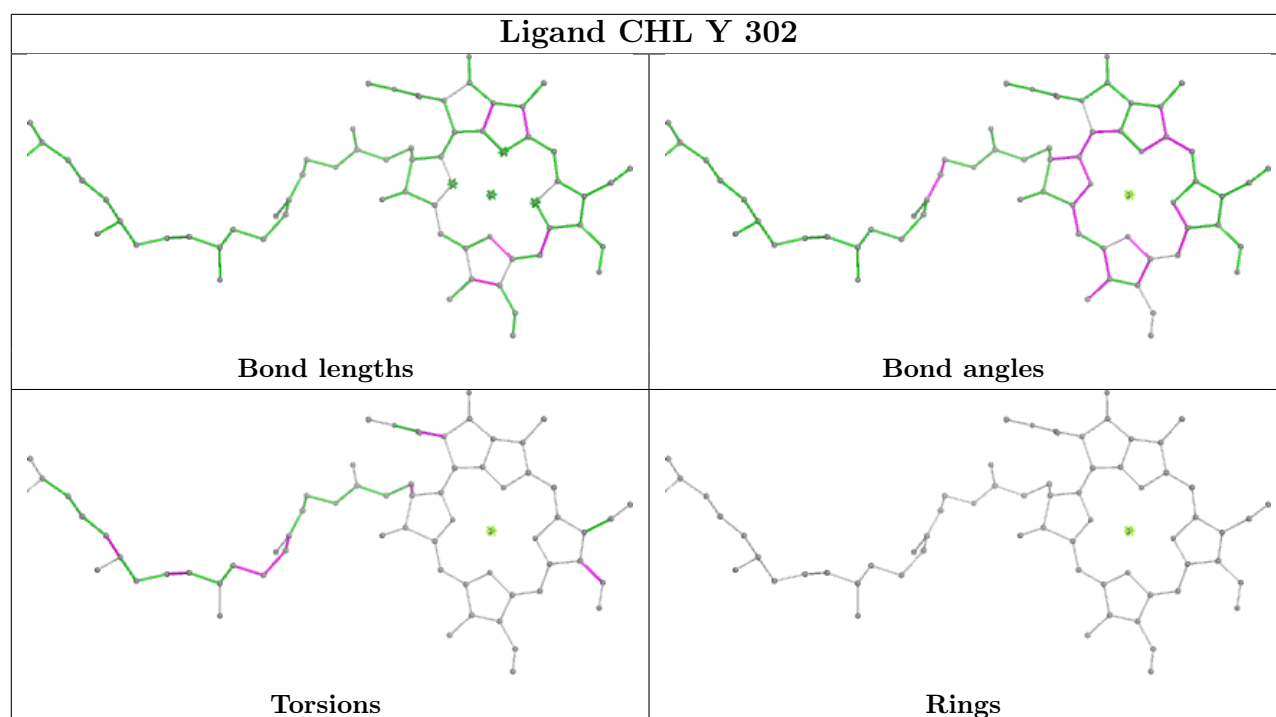


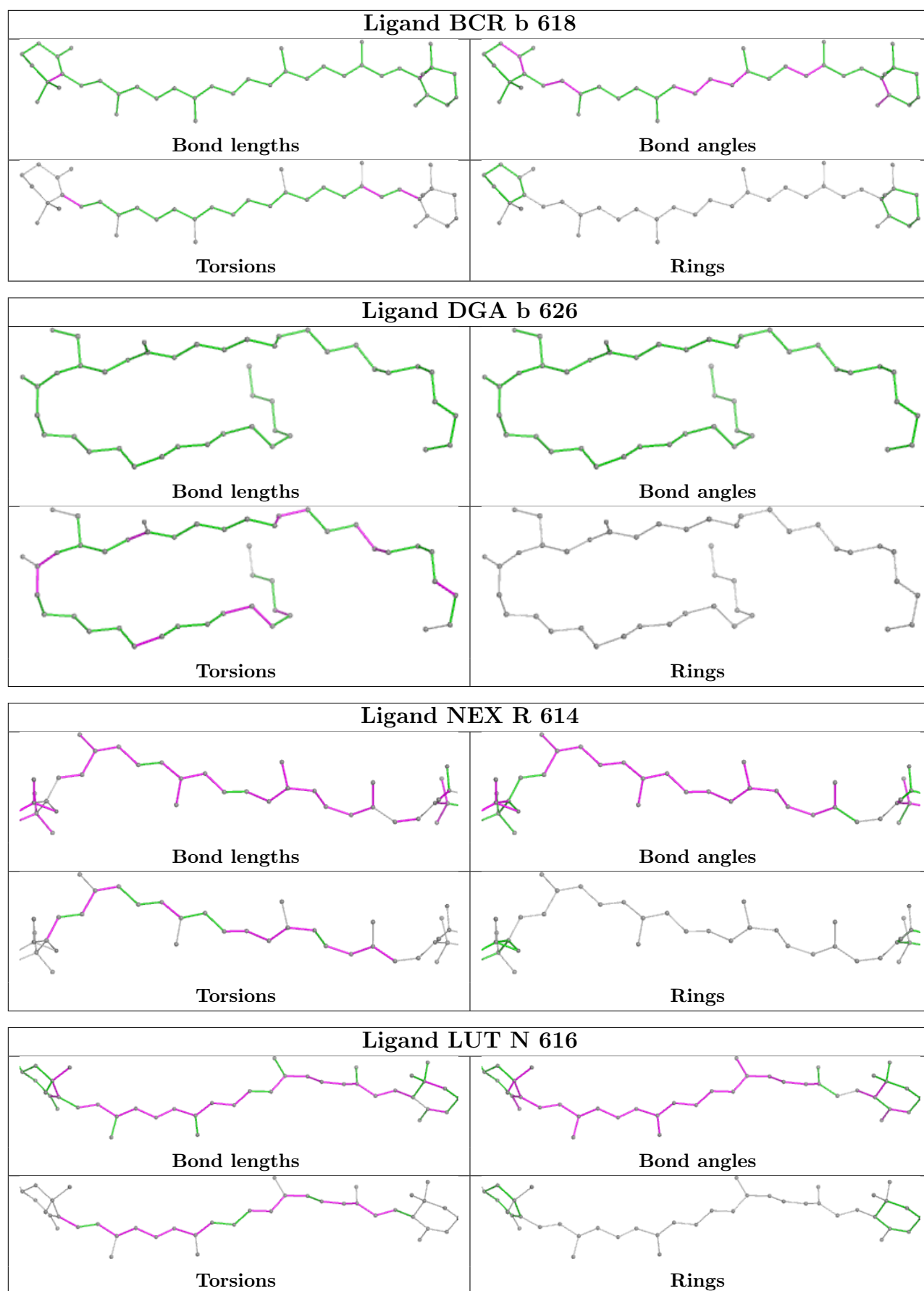
## Ligand CLA c 505

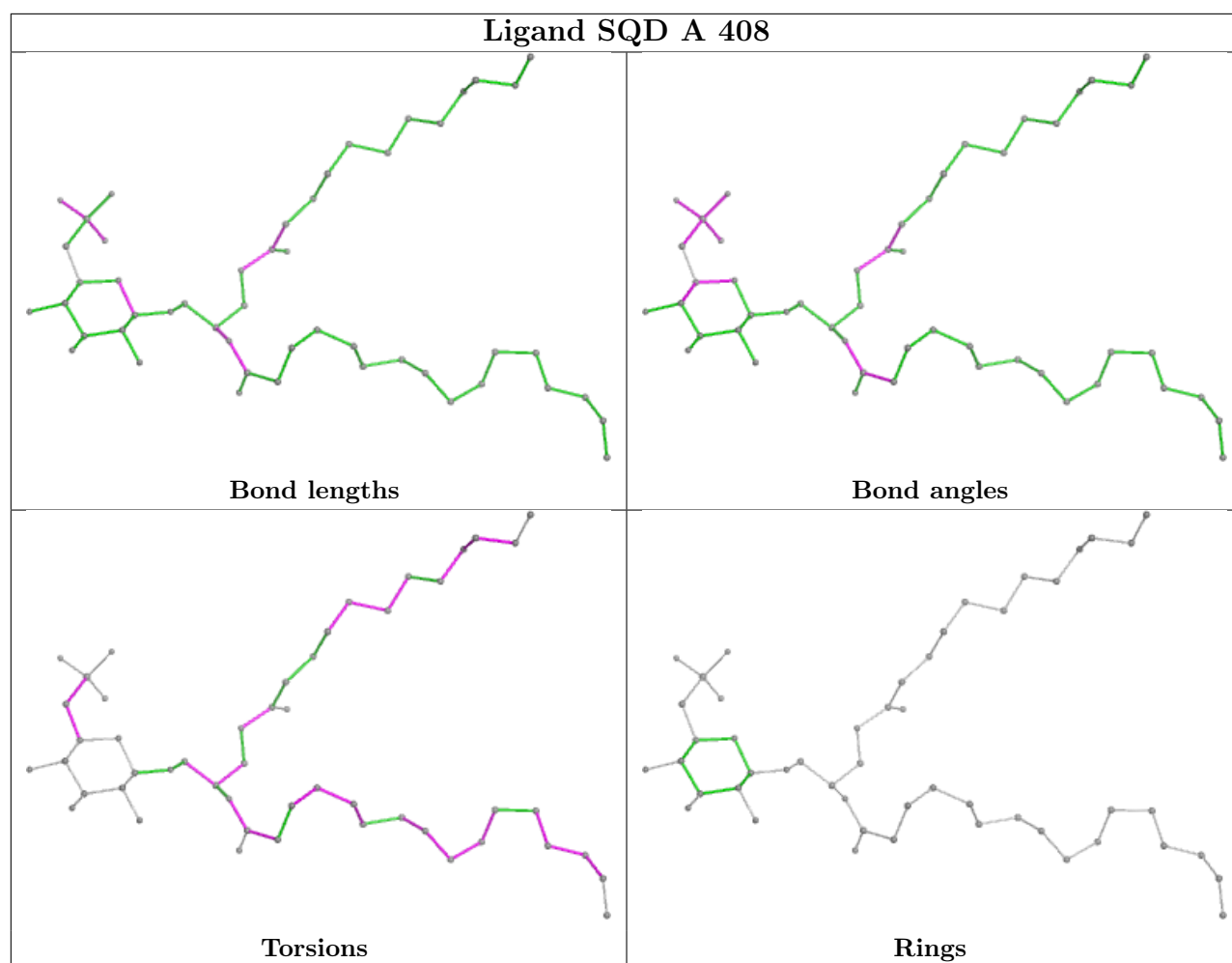




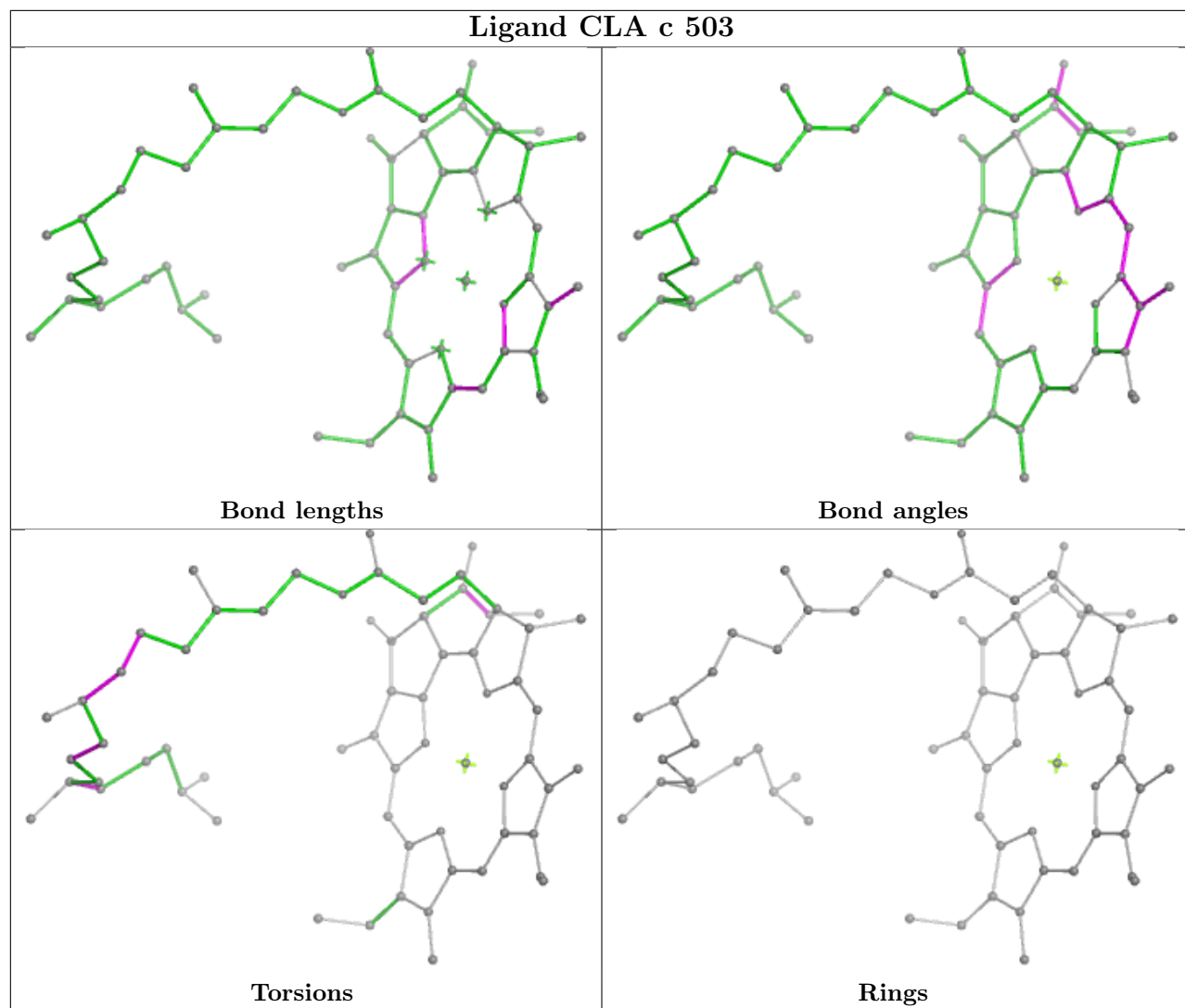




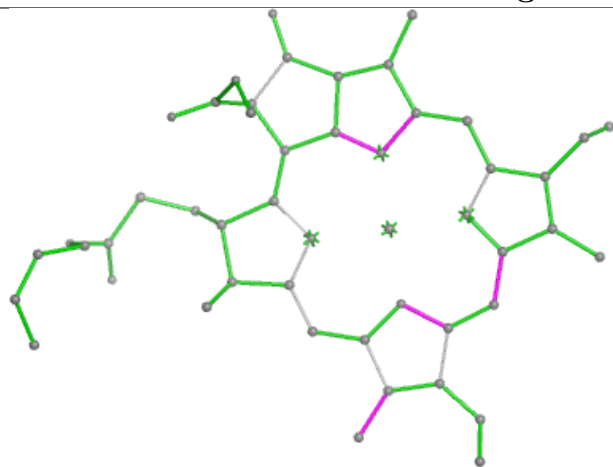




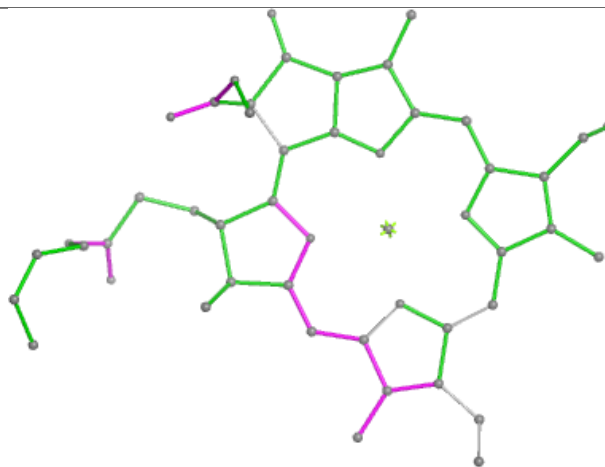
## Ligand CLA c 503



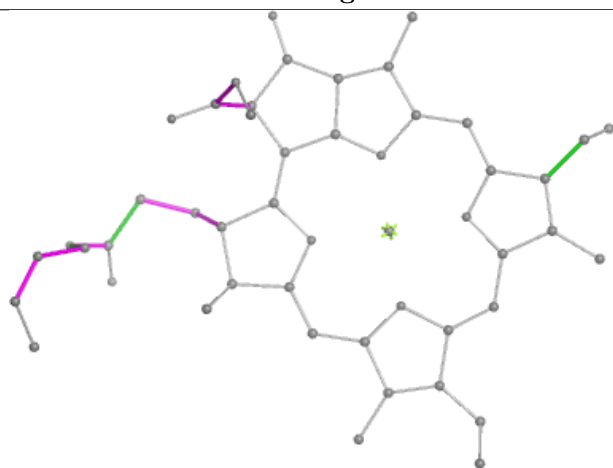
## Ligand CLA S 603



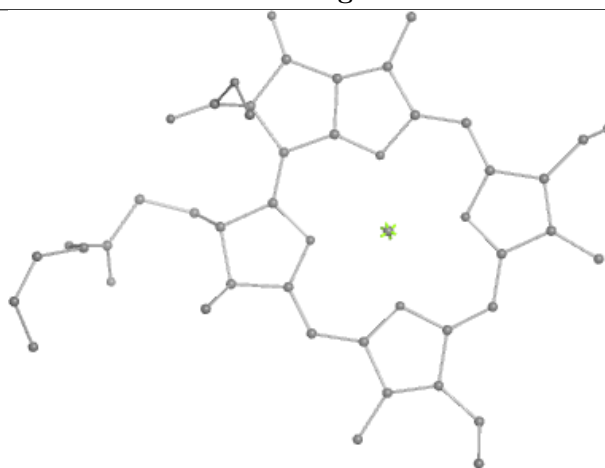
Bond lengths



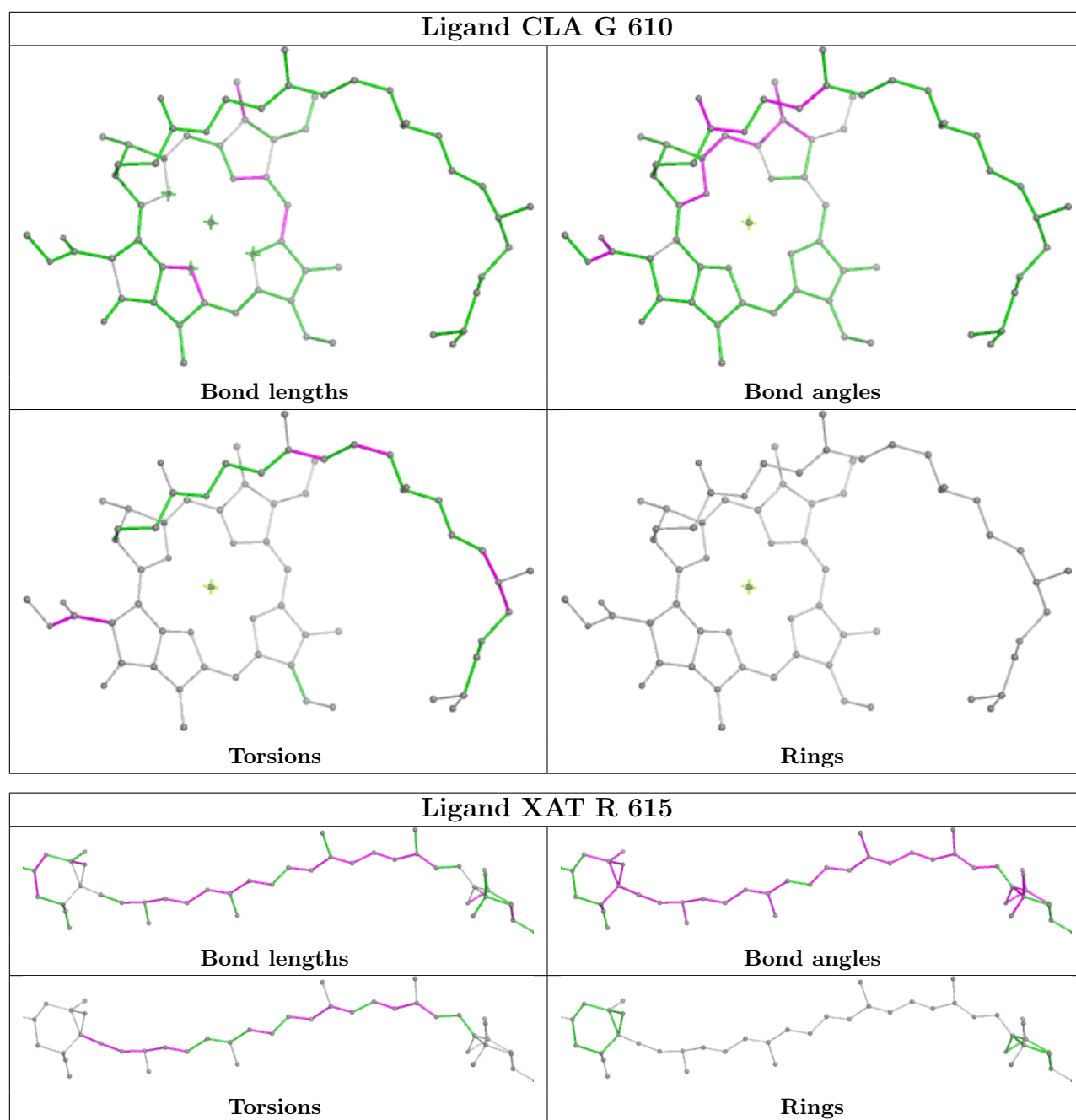
Bond angles

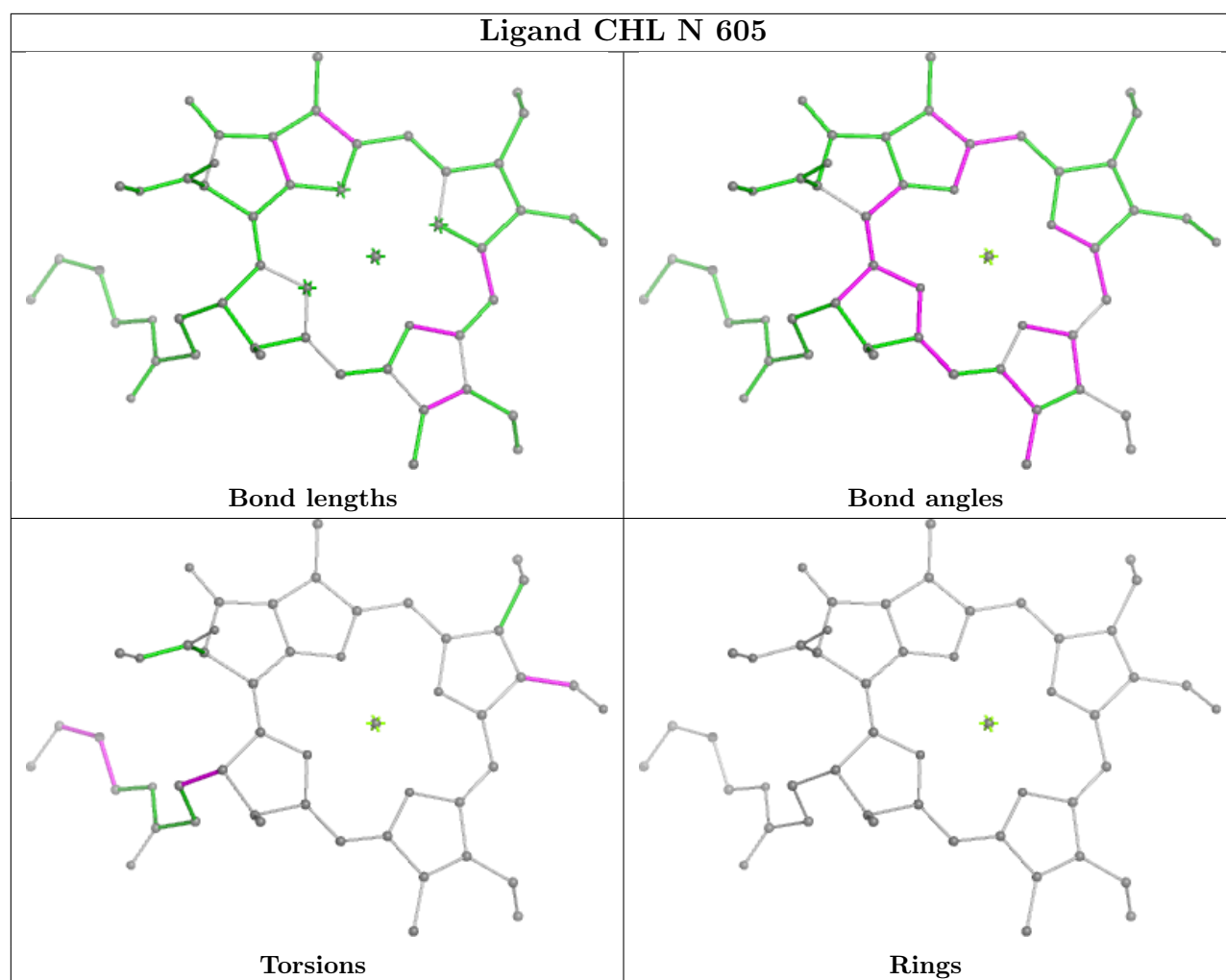


Torsions



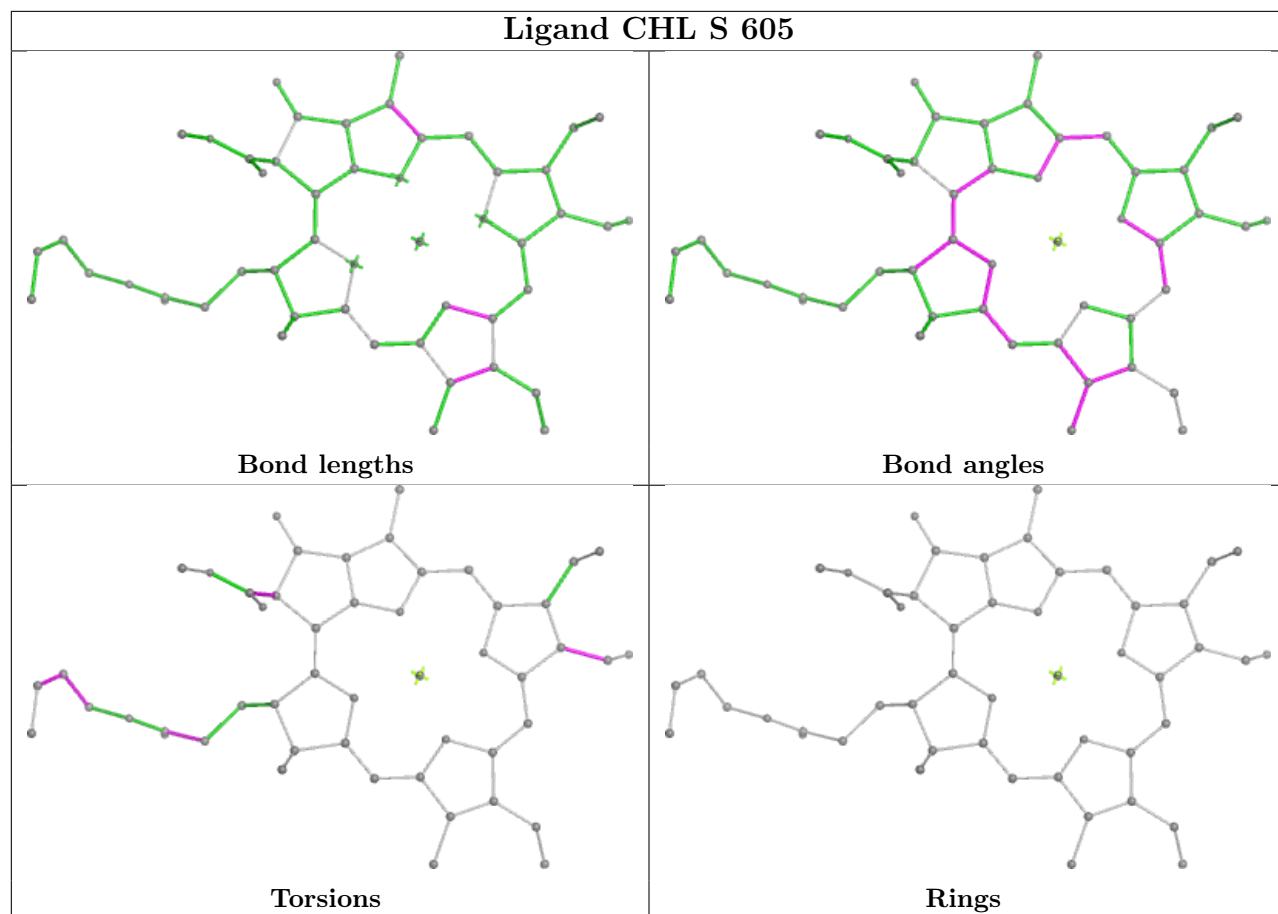
Rings



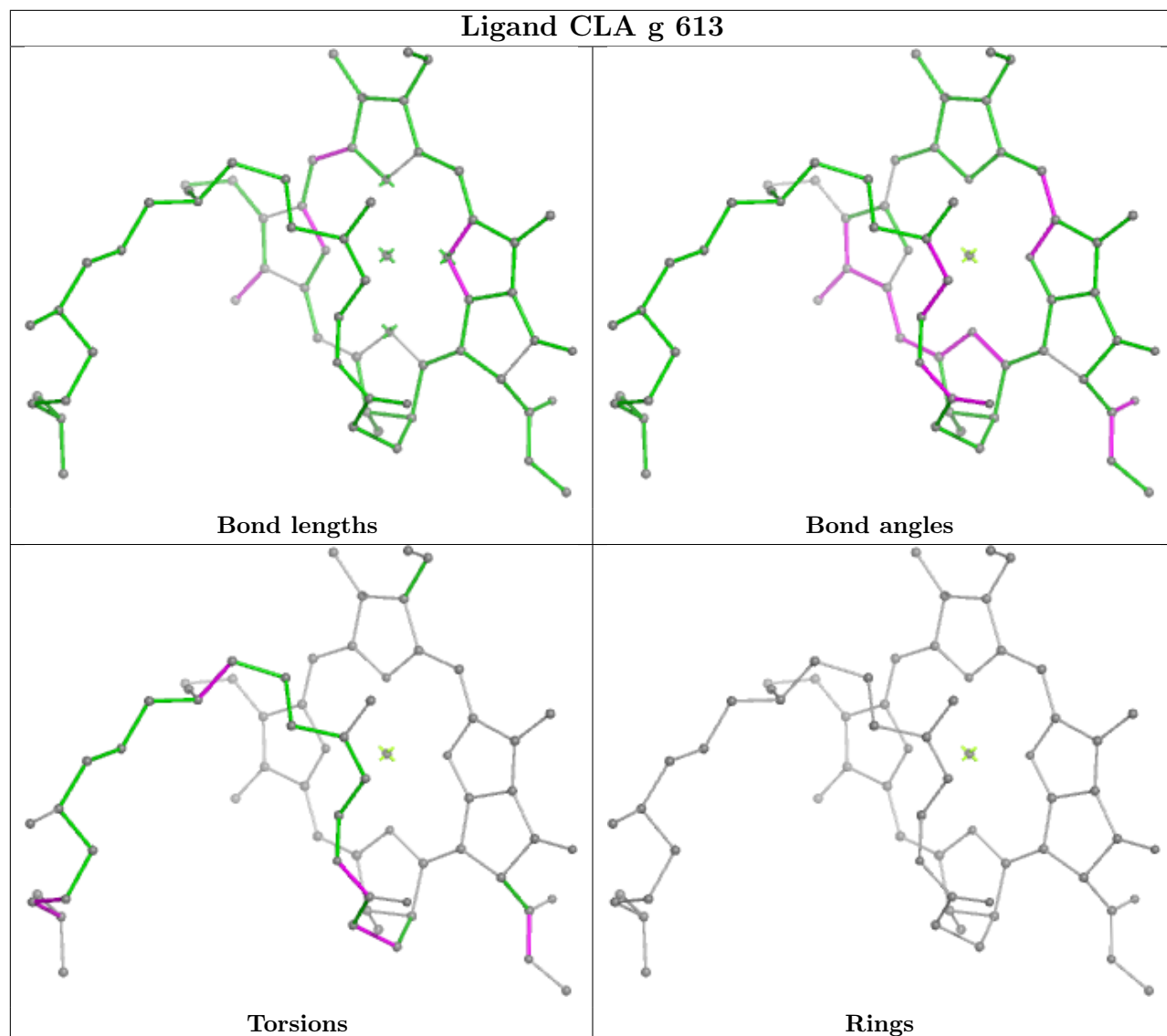




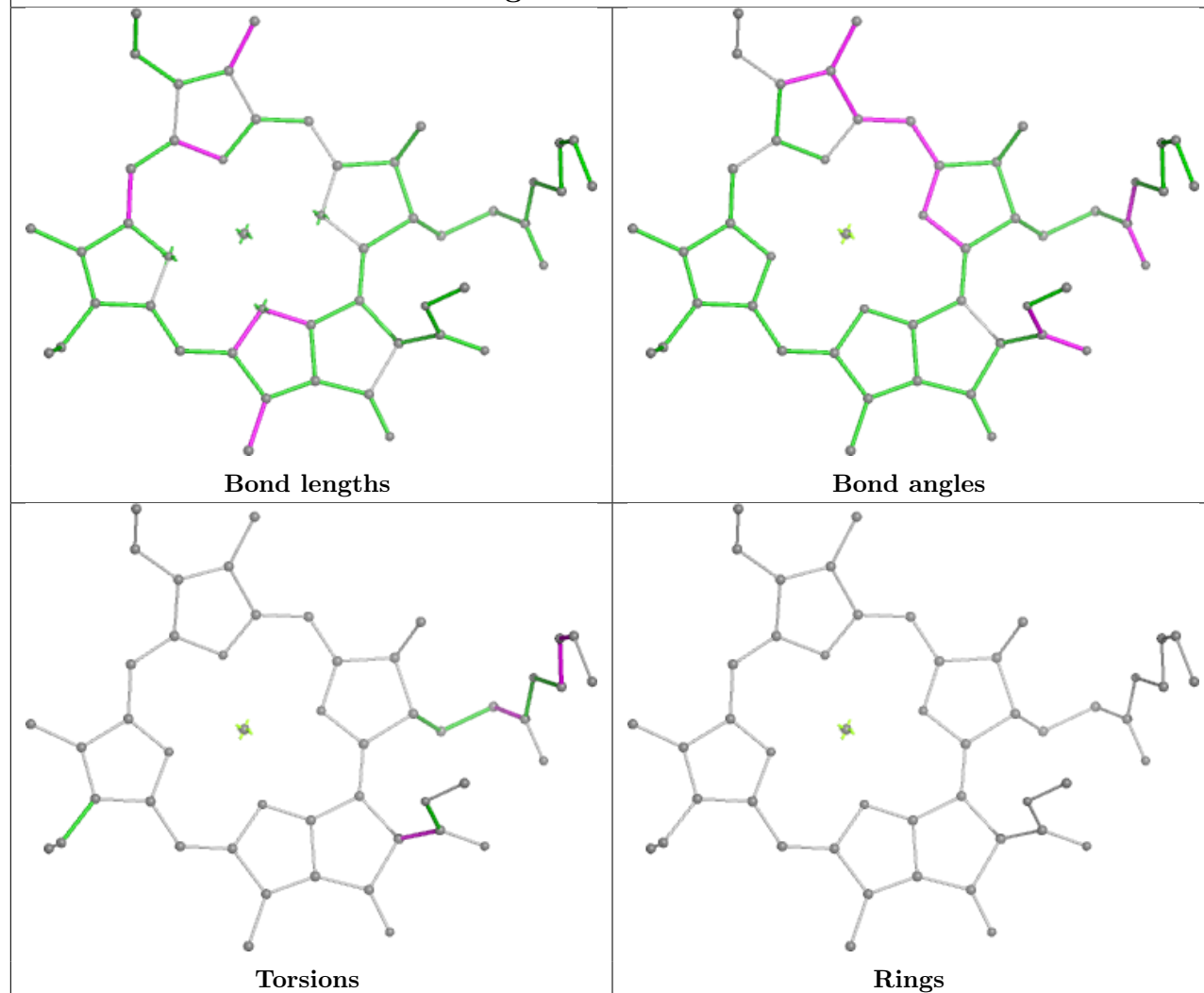
## Ligand CHL S 605



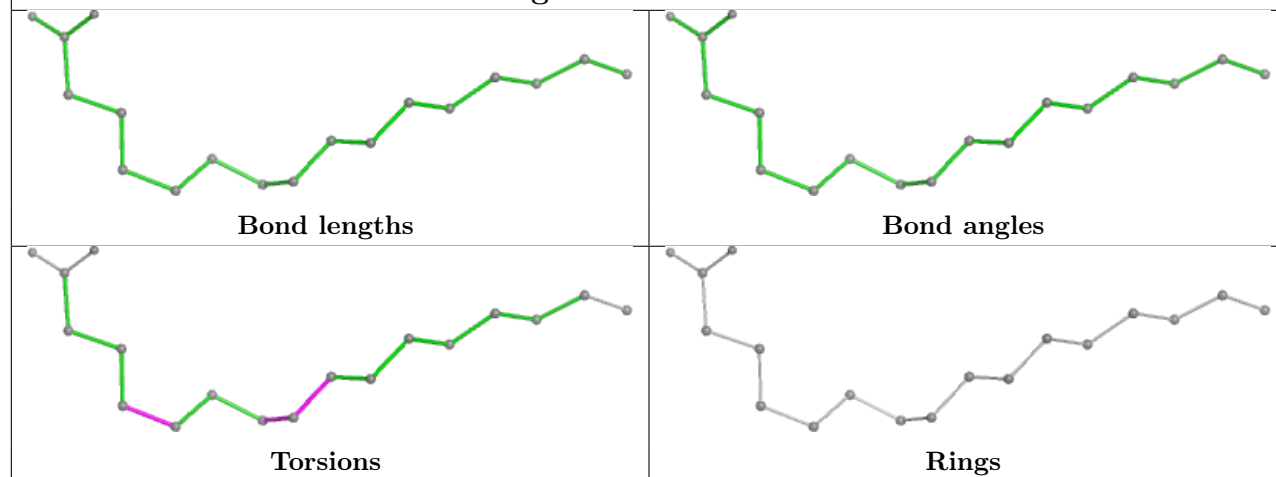
## Ligand CLA g 613



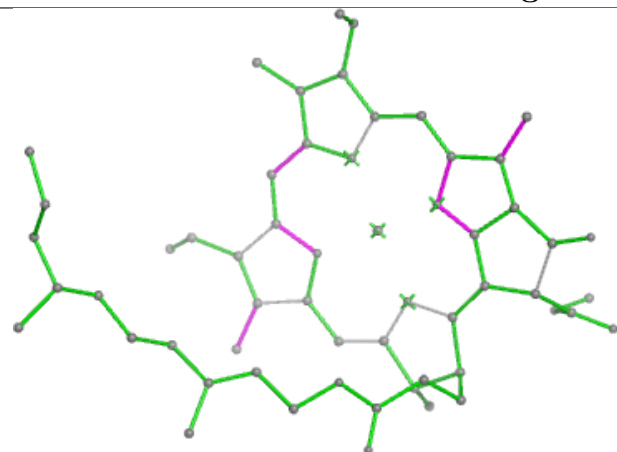
## Ligand CLA n 612



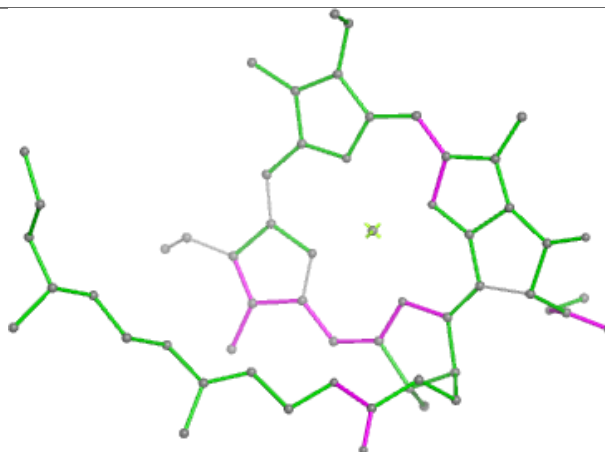
## Ligand PAM b 621



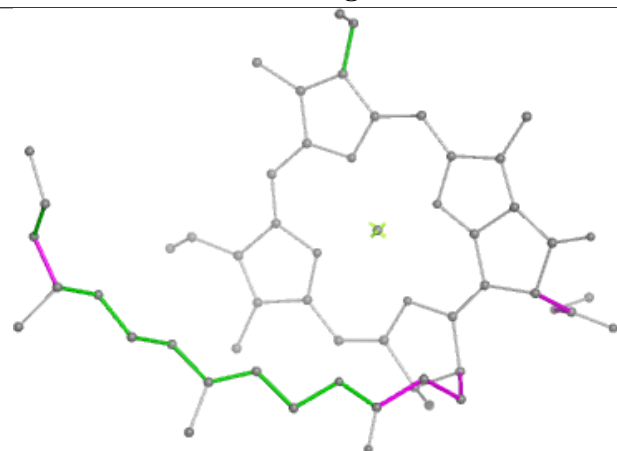
## Ligand CLA S 602



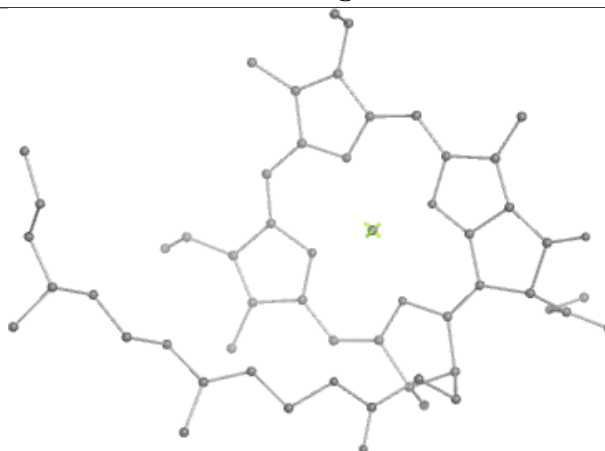
Bond lengths



Bond angles

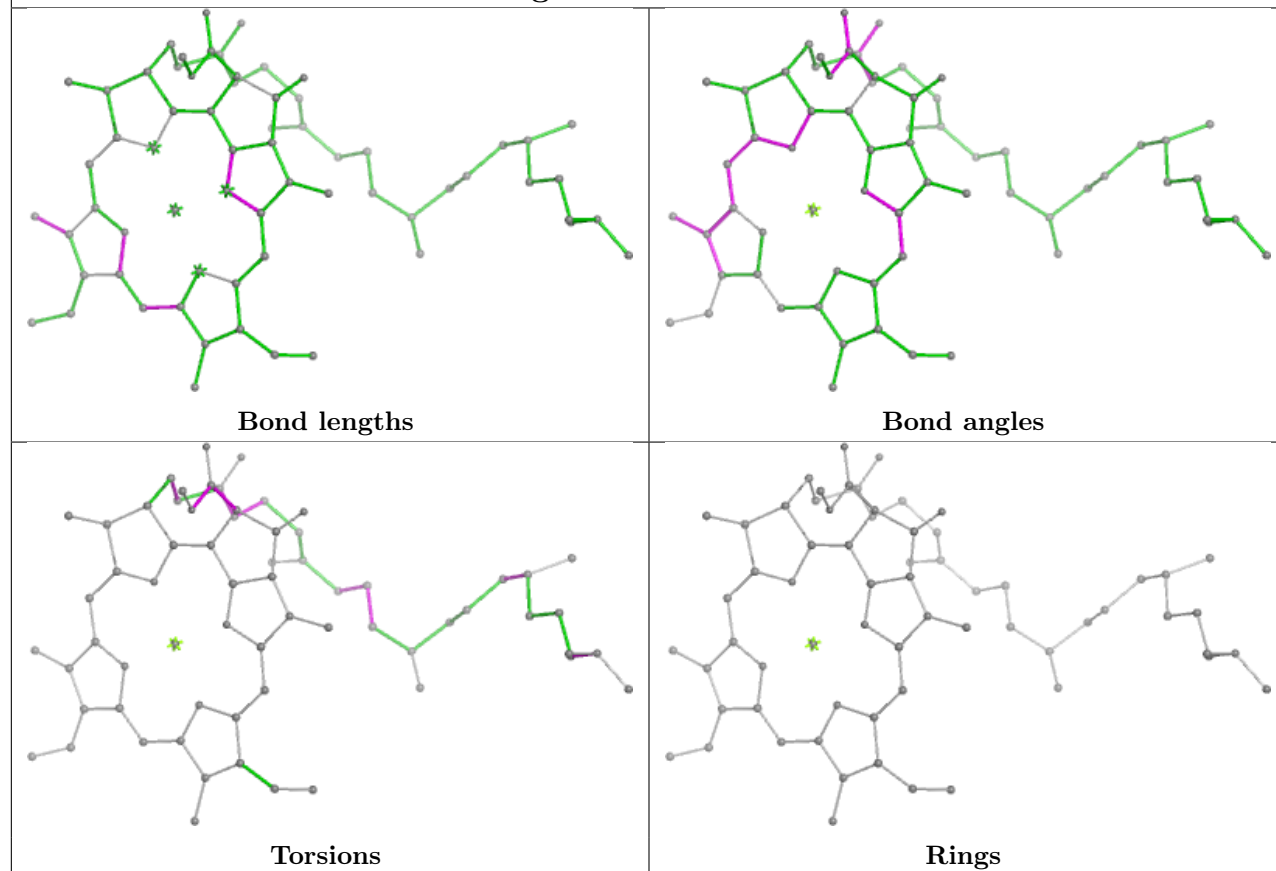


Torsions

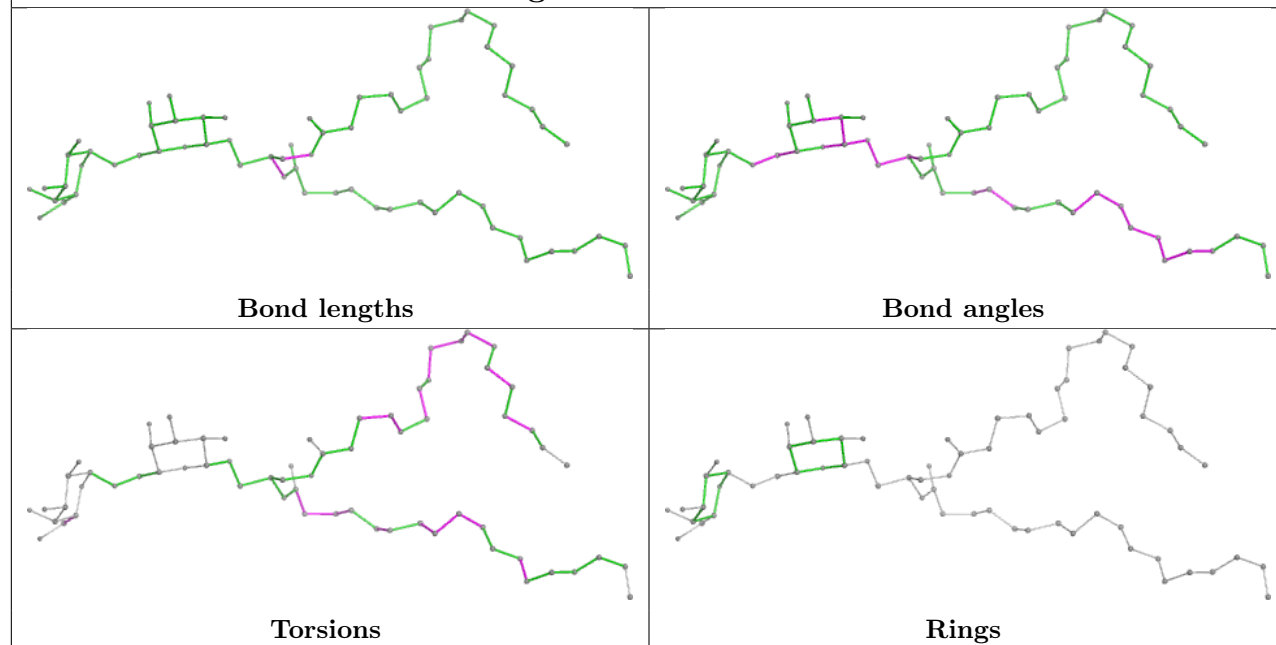


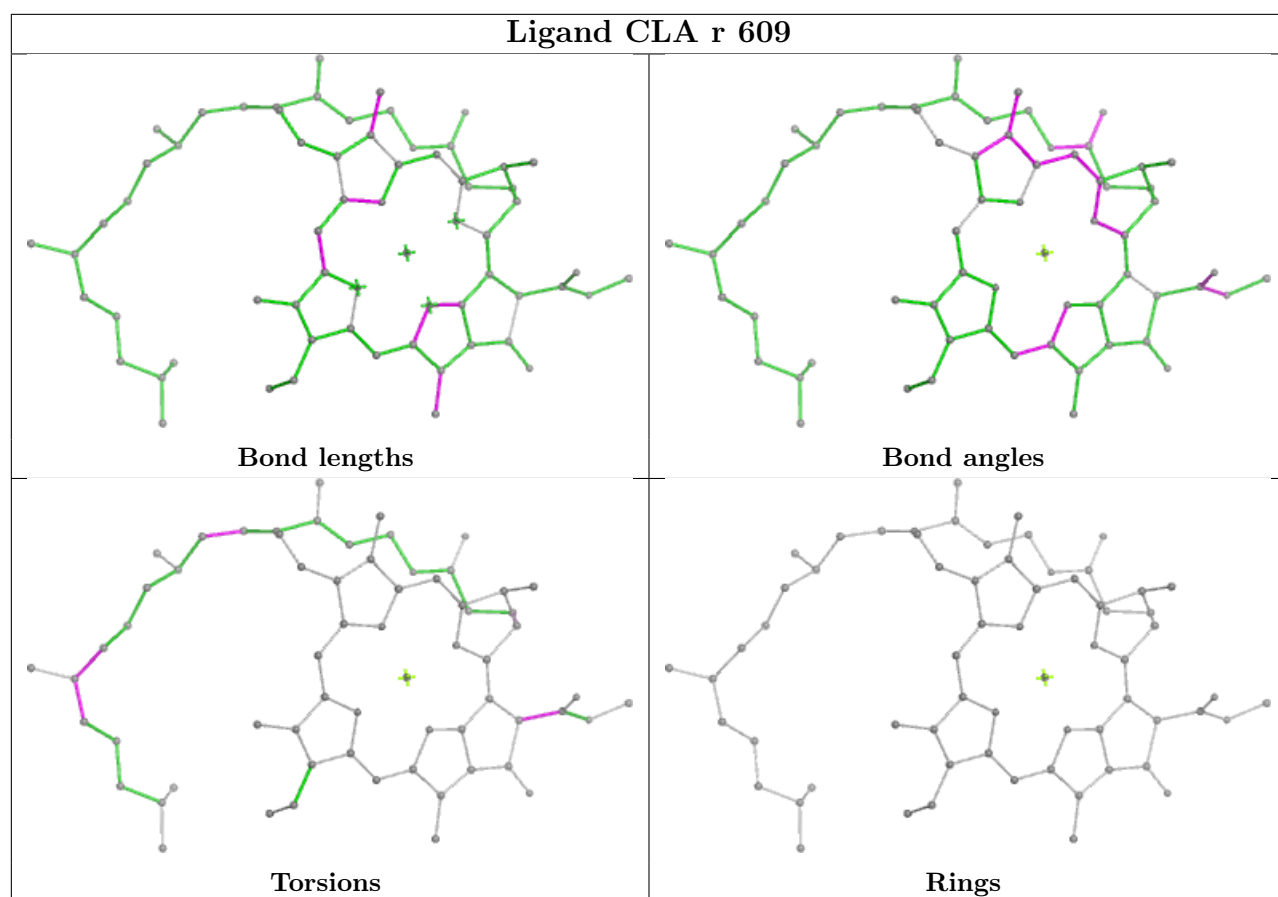
Rings

## Ligand CLA Y 305

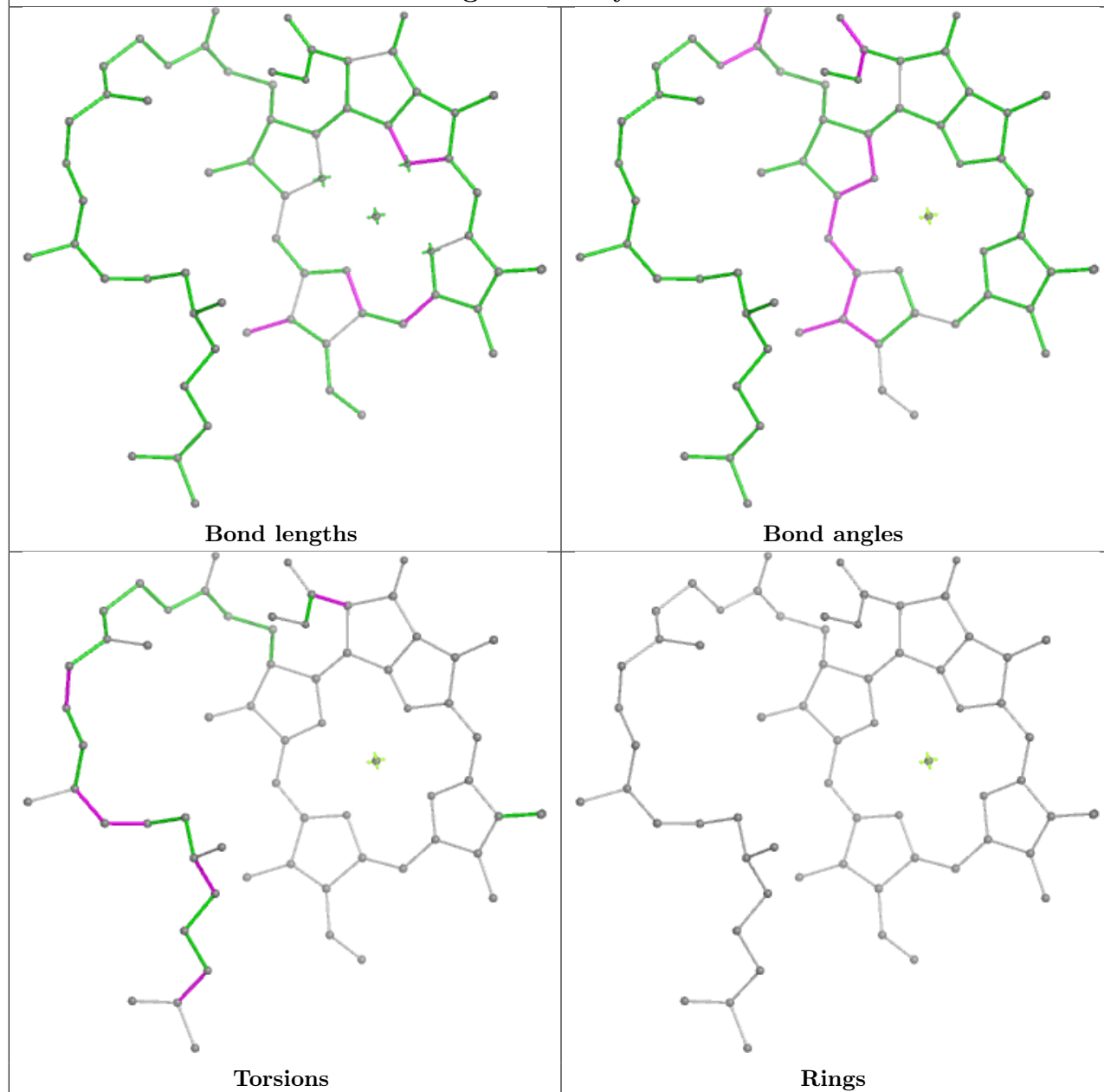


## Ligand DGD C 515

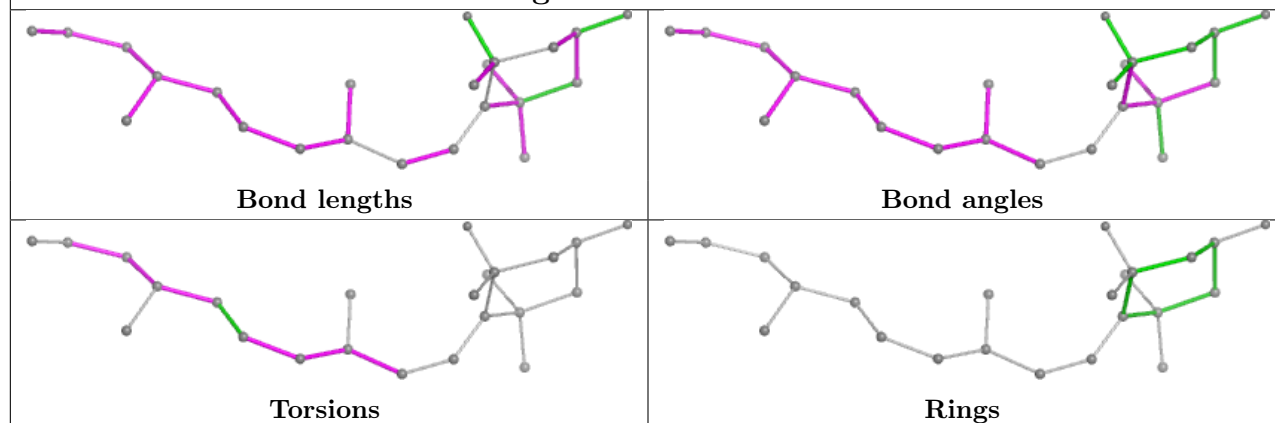




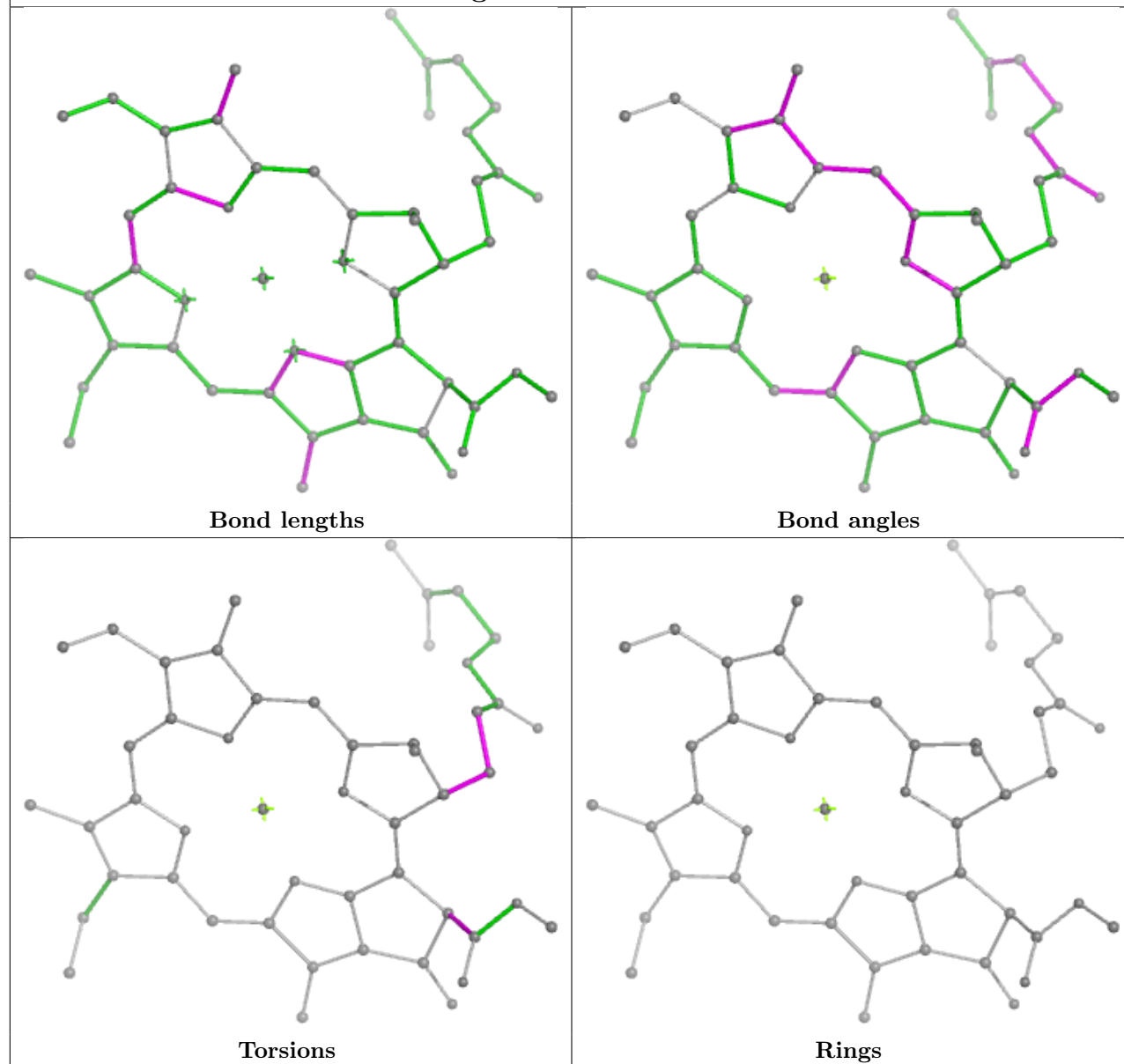
## Ligand CLA y 313



## Ligand NEX S 617

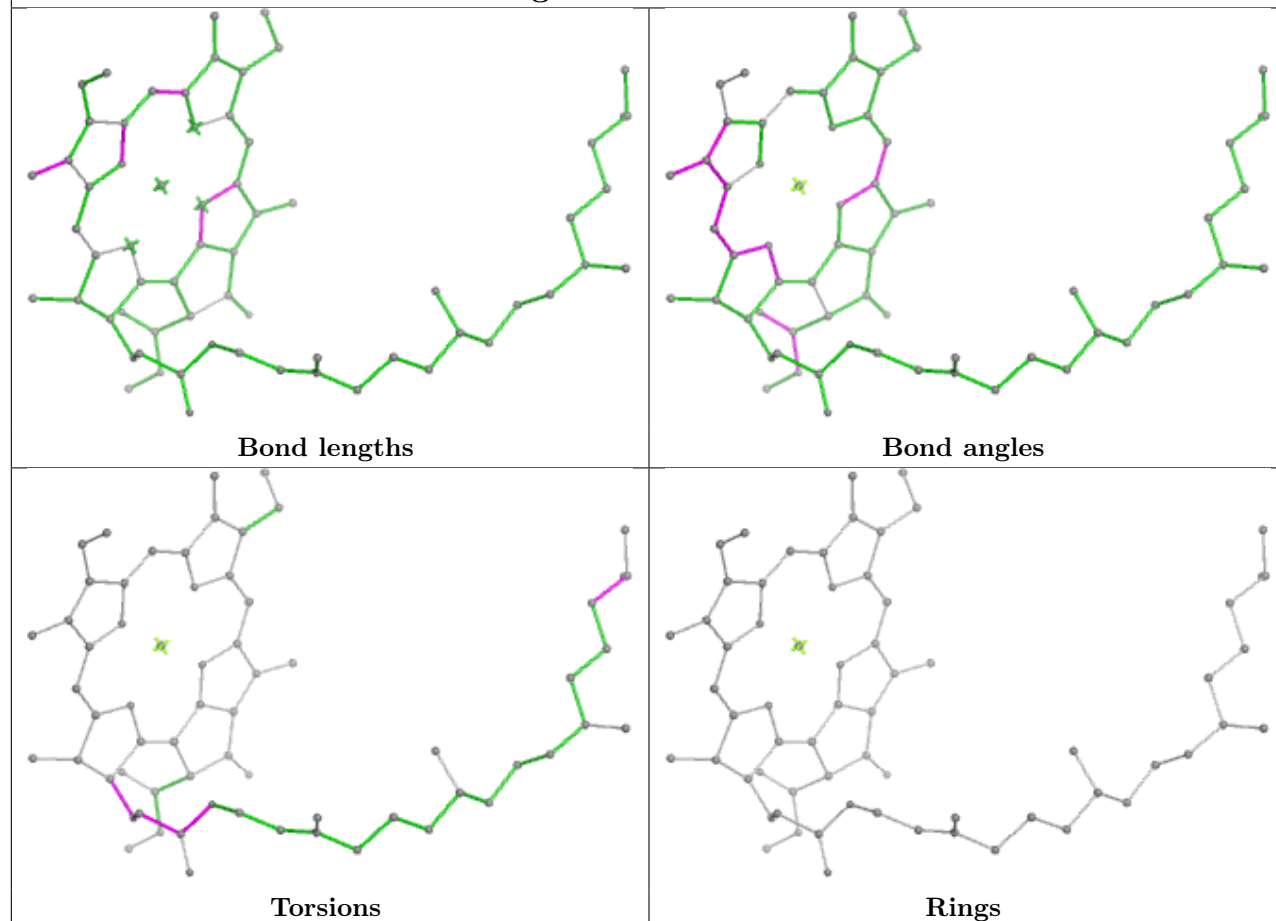


## Ligand CLA b 601

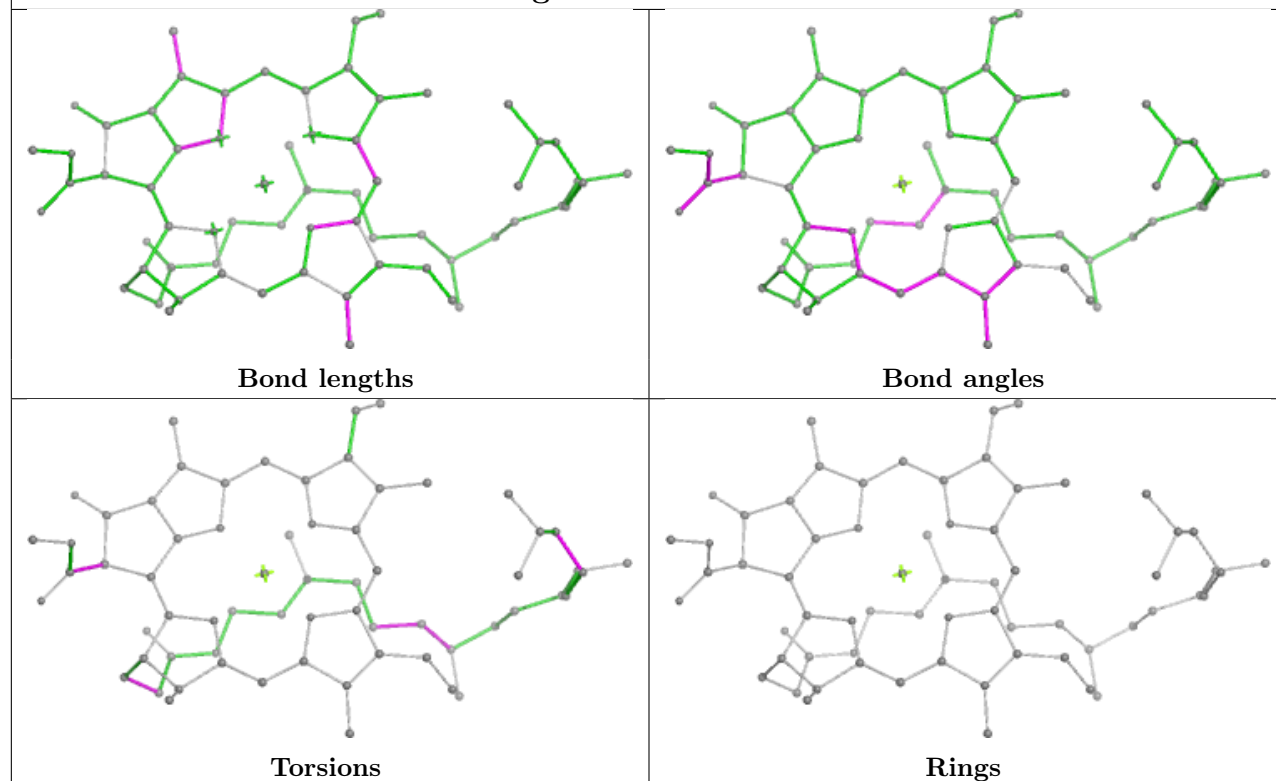


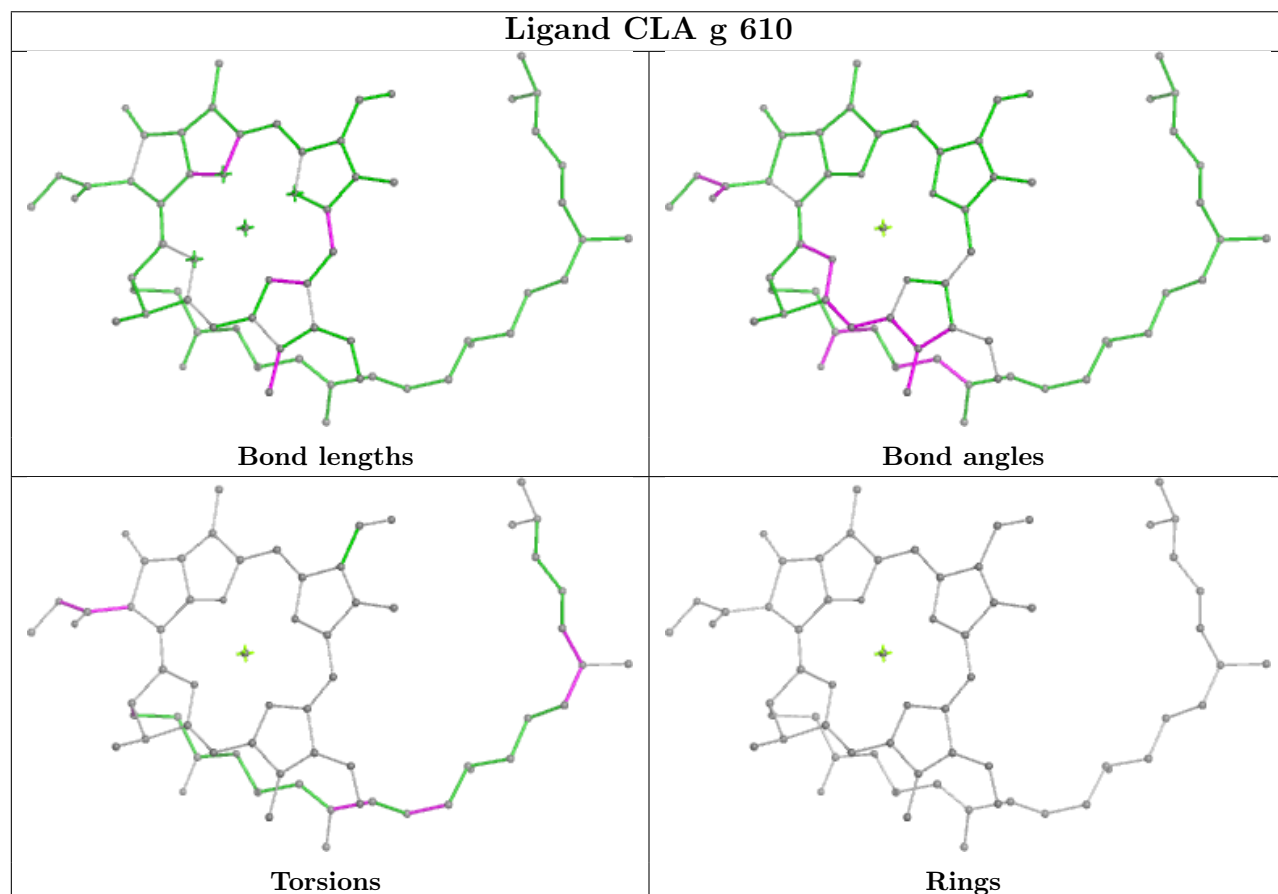
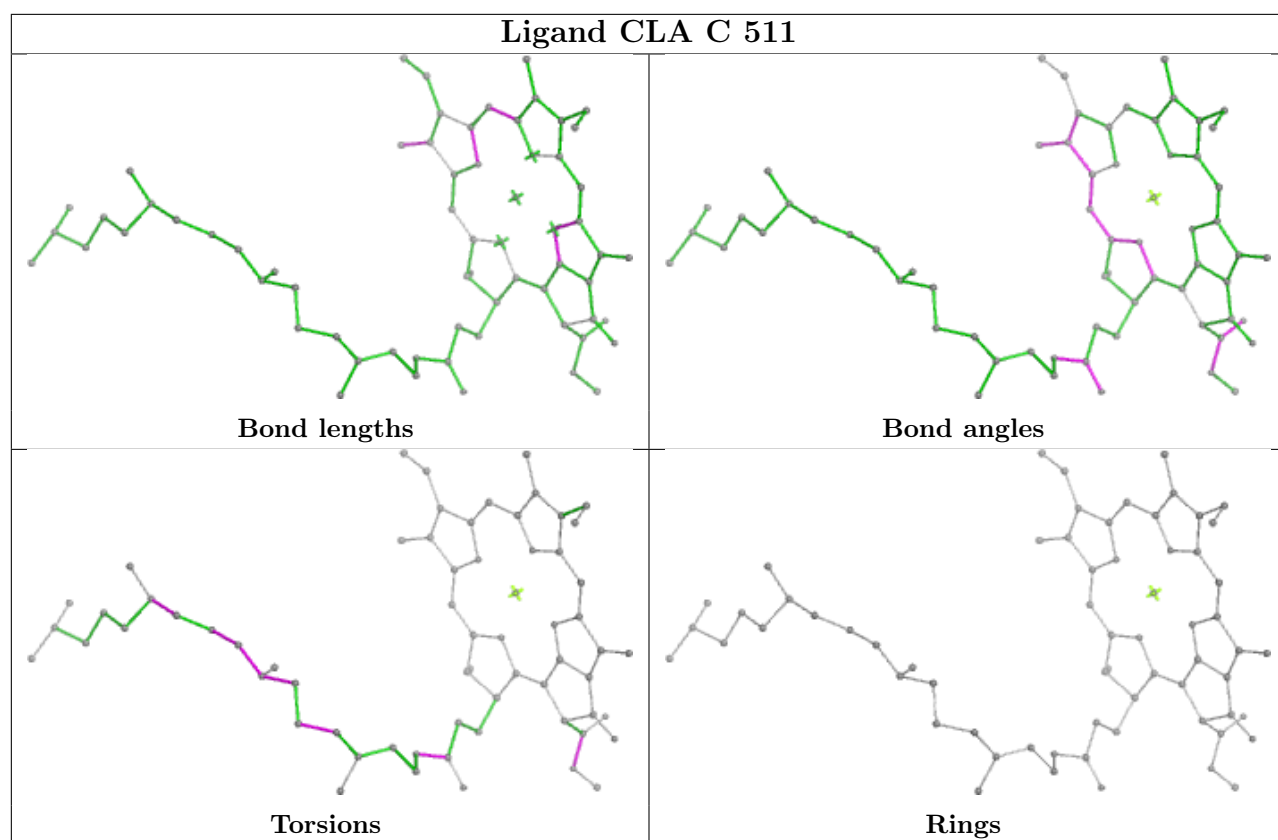


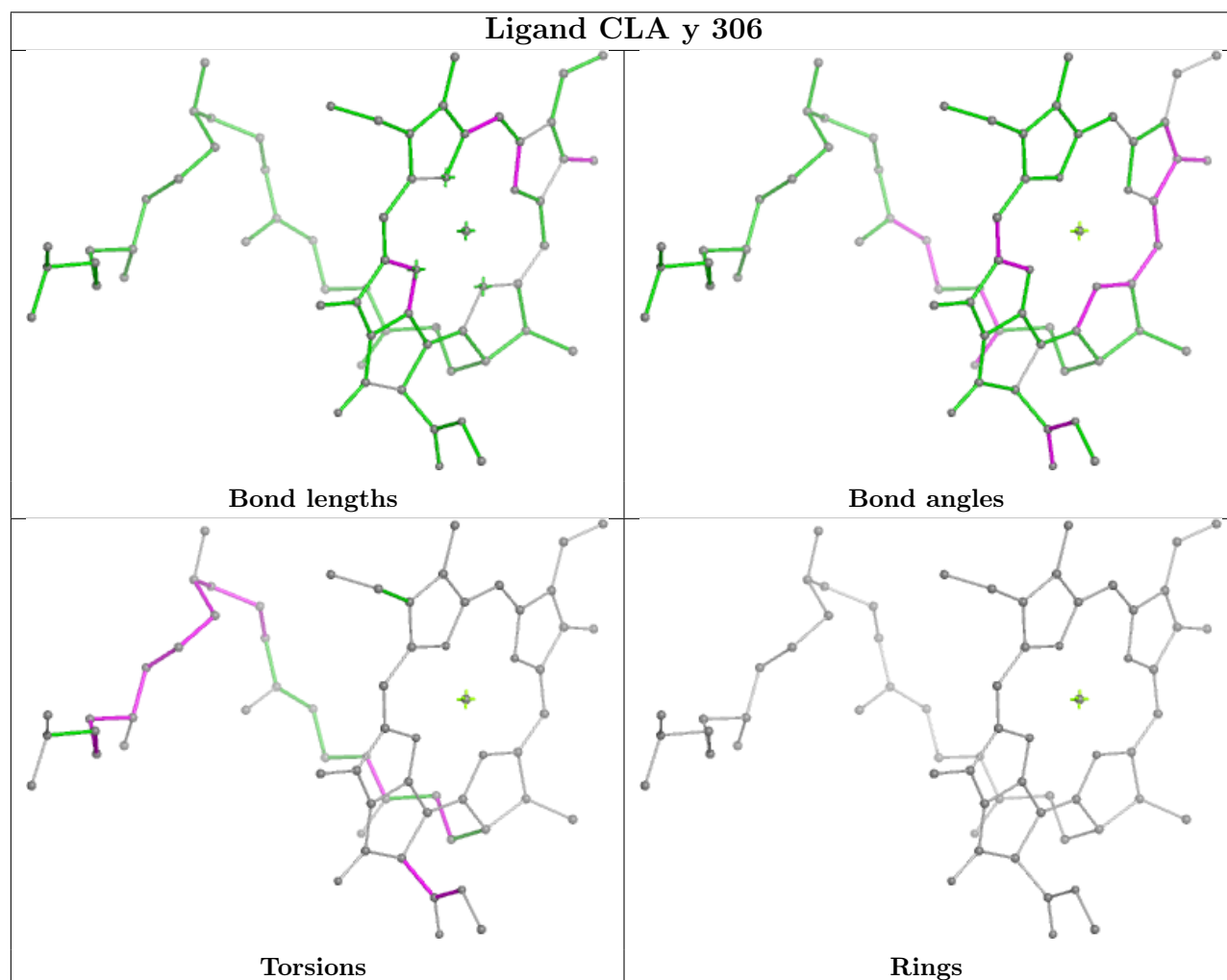
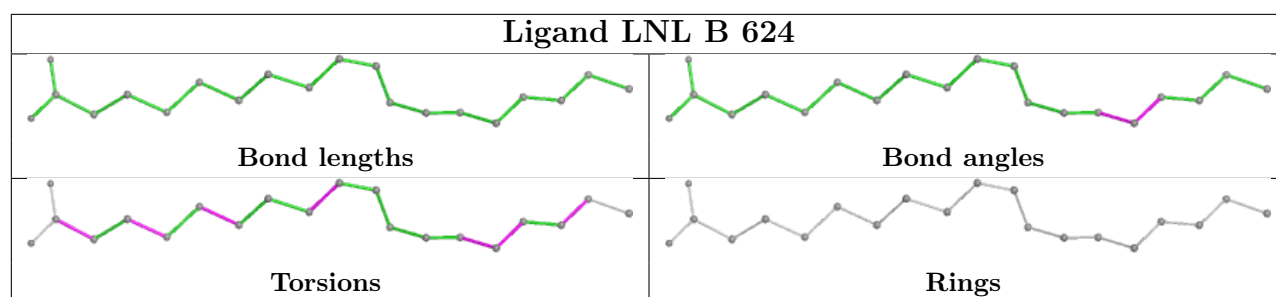
## Ligand CLA R 610

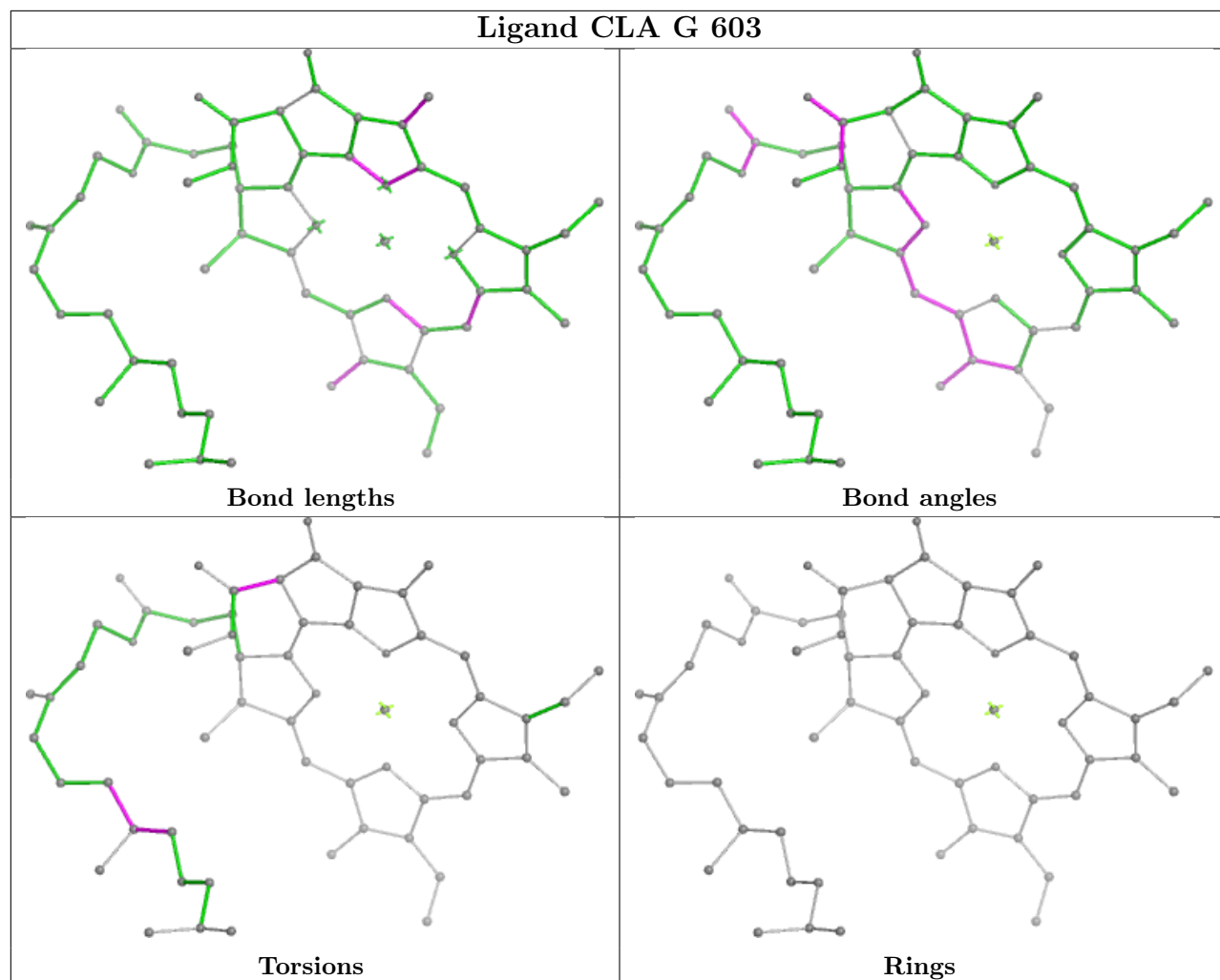


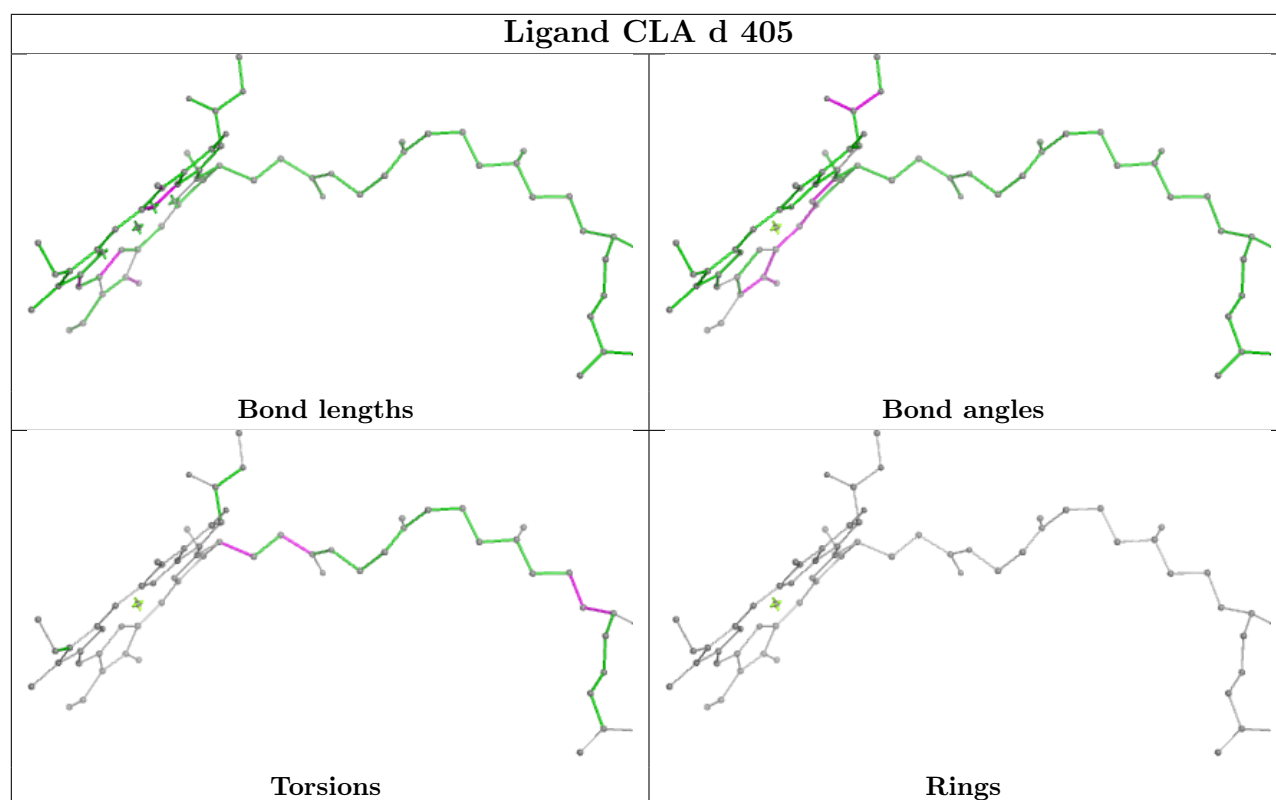
## Ligand CLA C 505



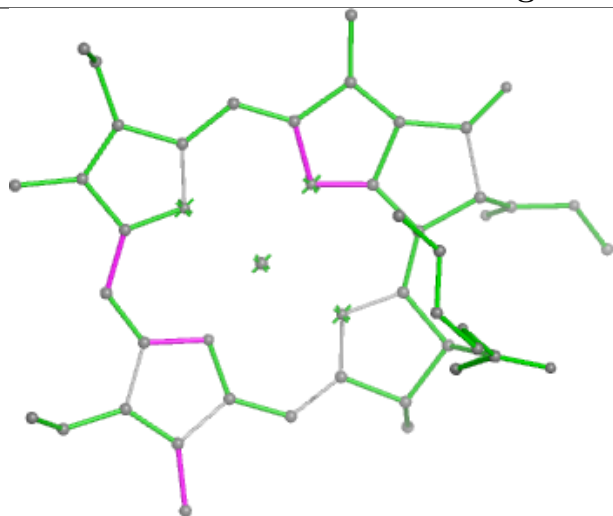




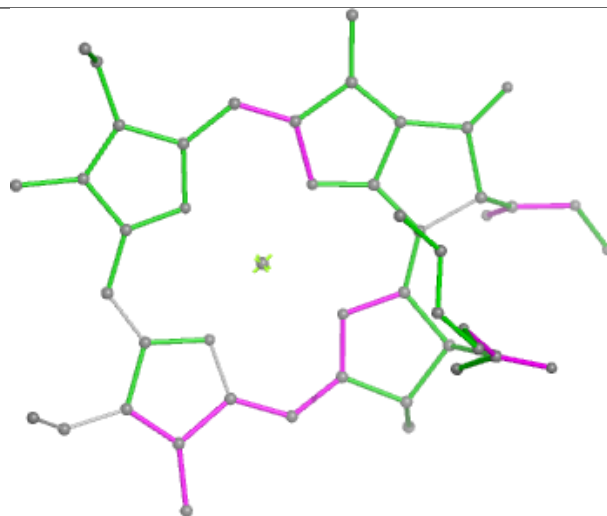




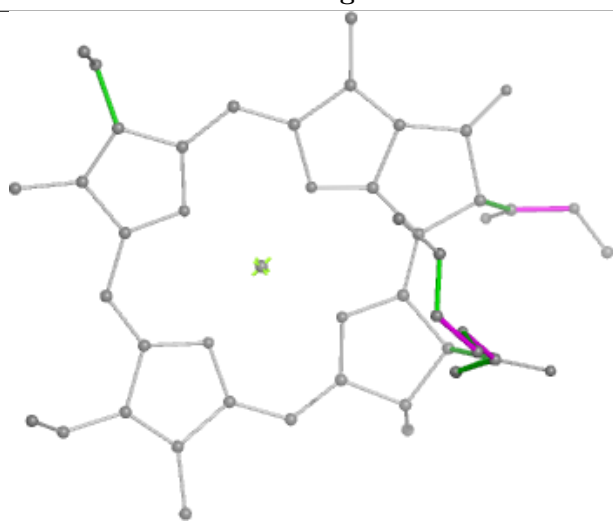
## Ligand CLA n 611



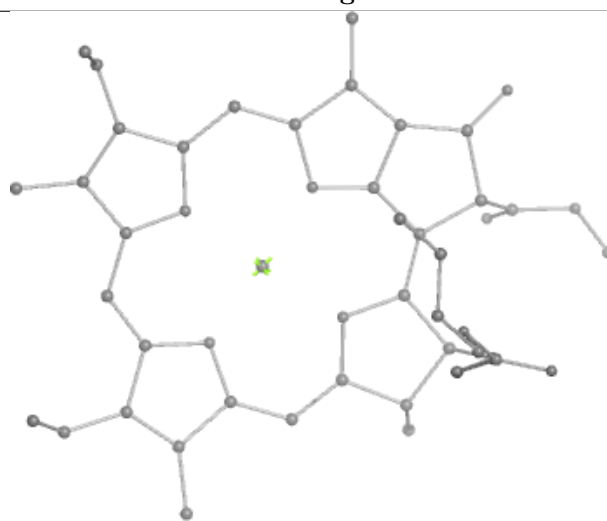
Bond lengths



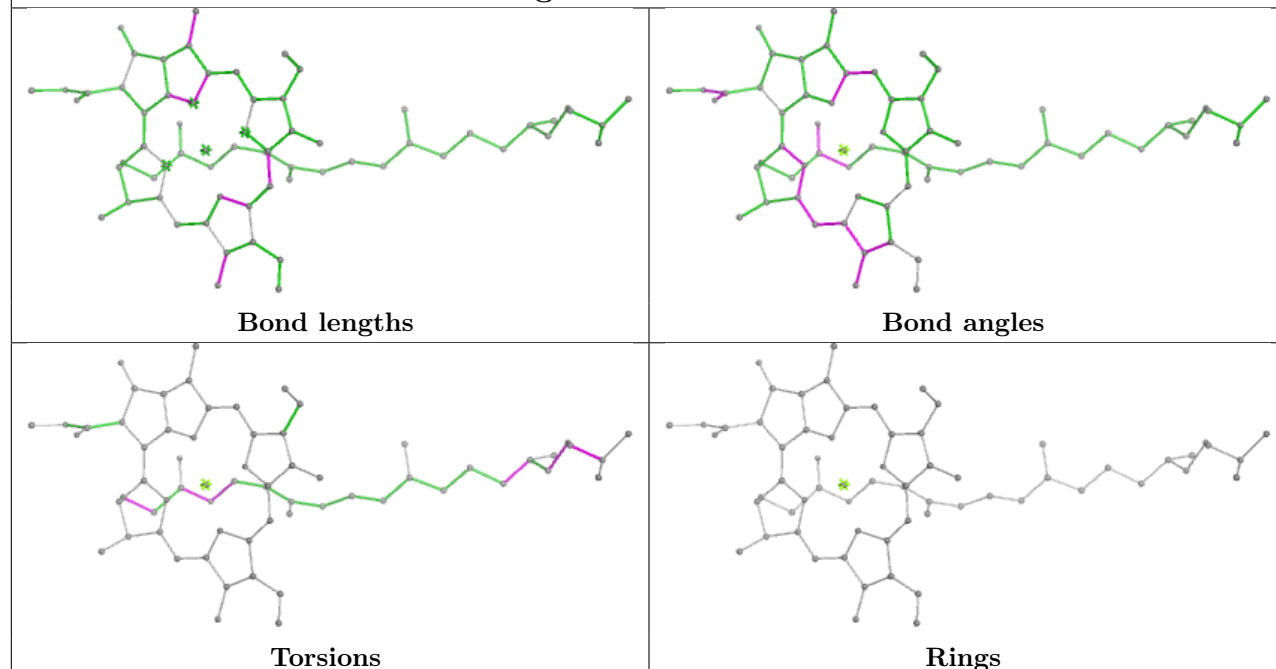
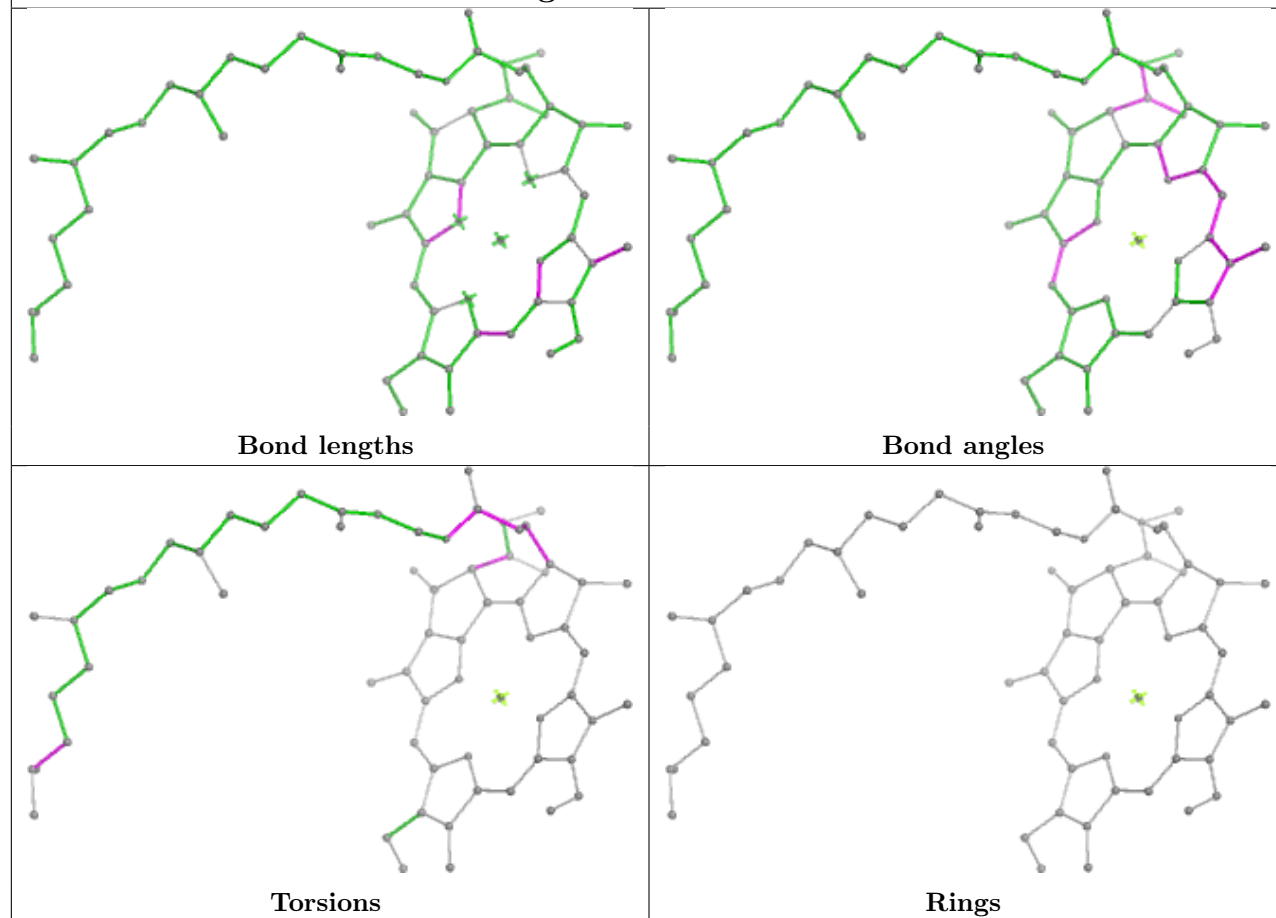
Bond angles



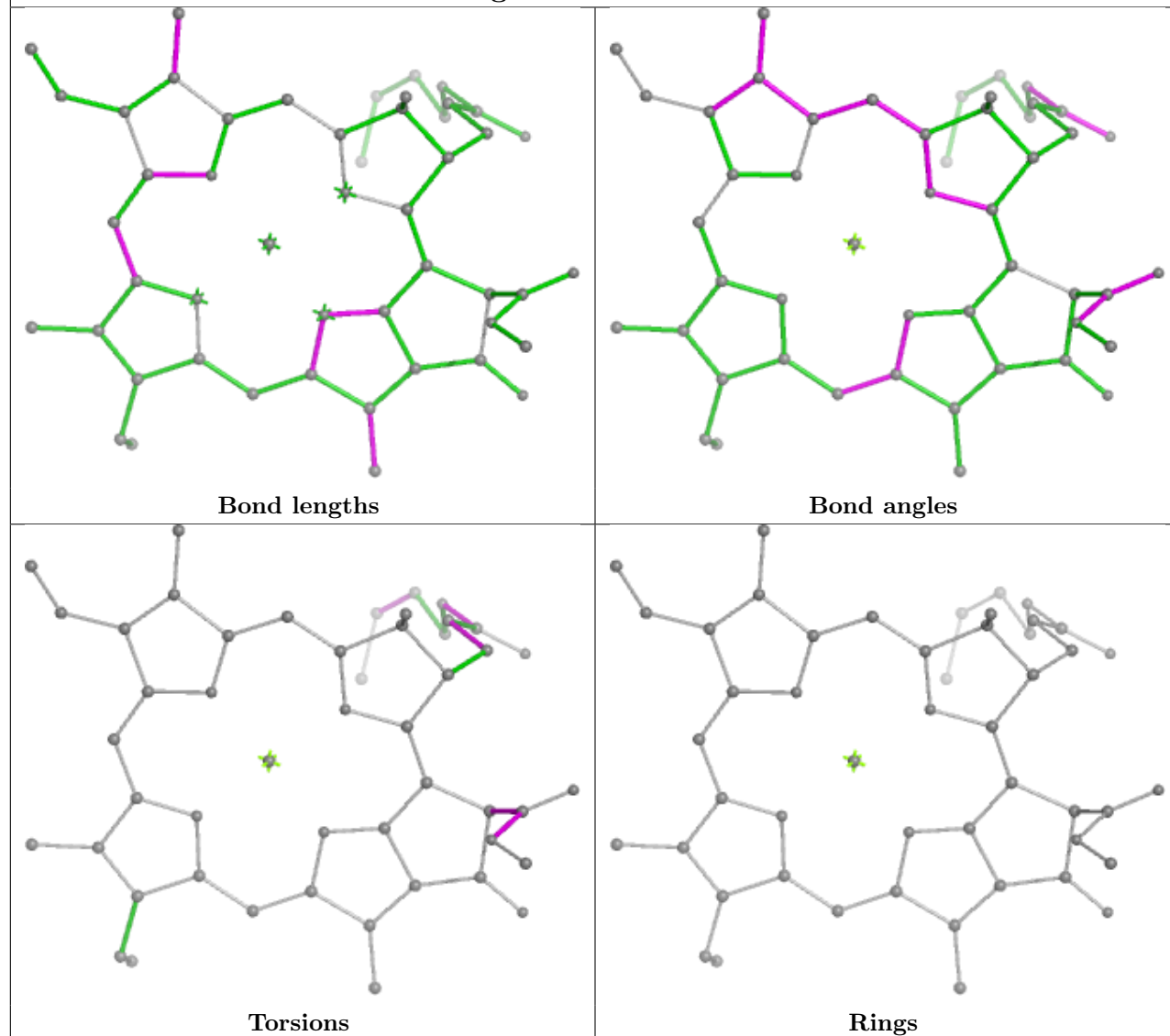
Torsions



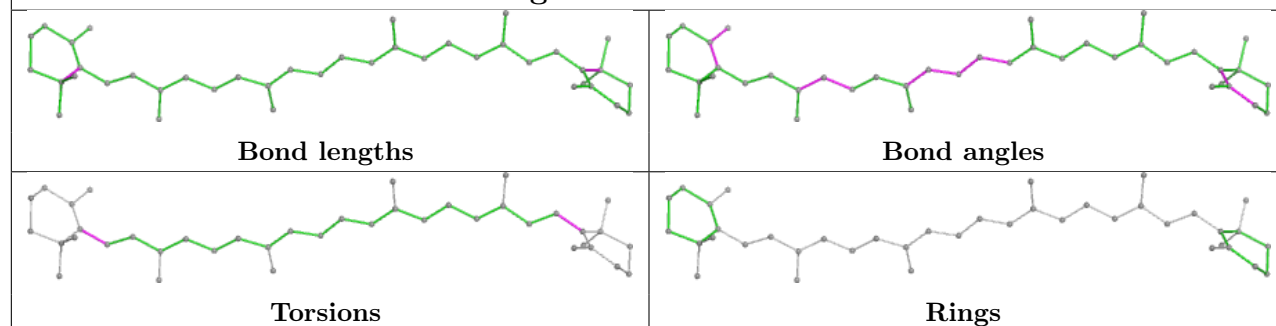
Rings

**Ligand CLA b 608****Ligand CLA r 610**

## Ligand CLA n 604

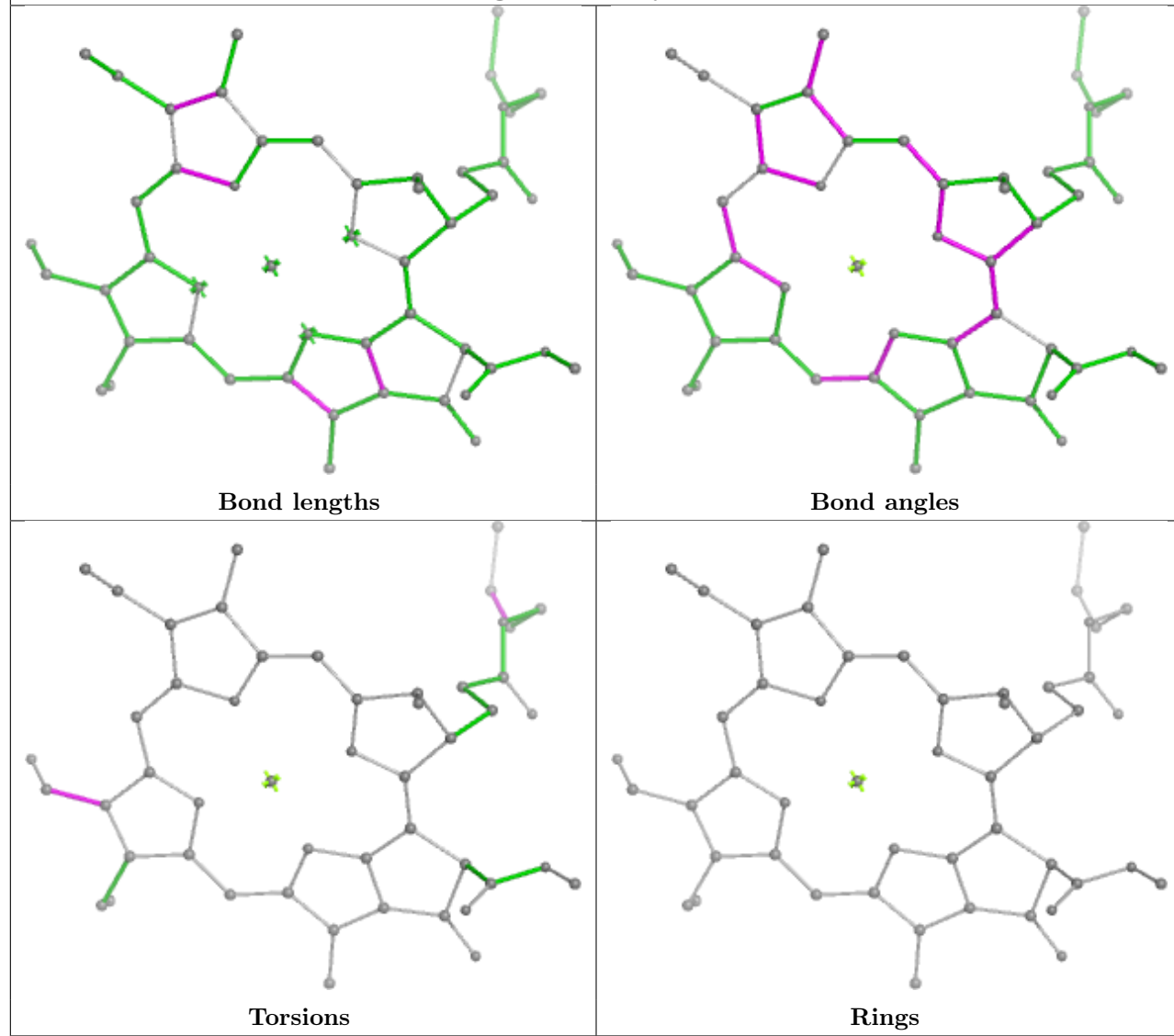


## Ligand BCR A 407

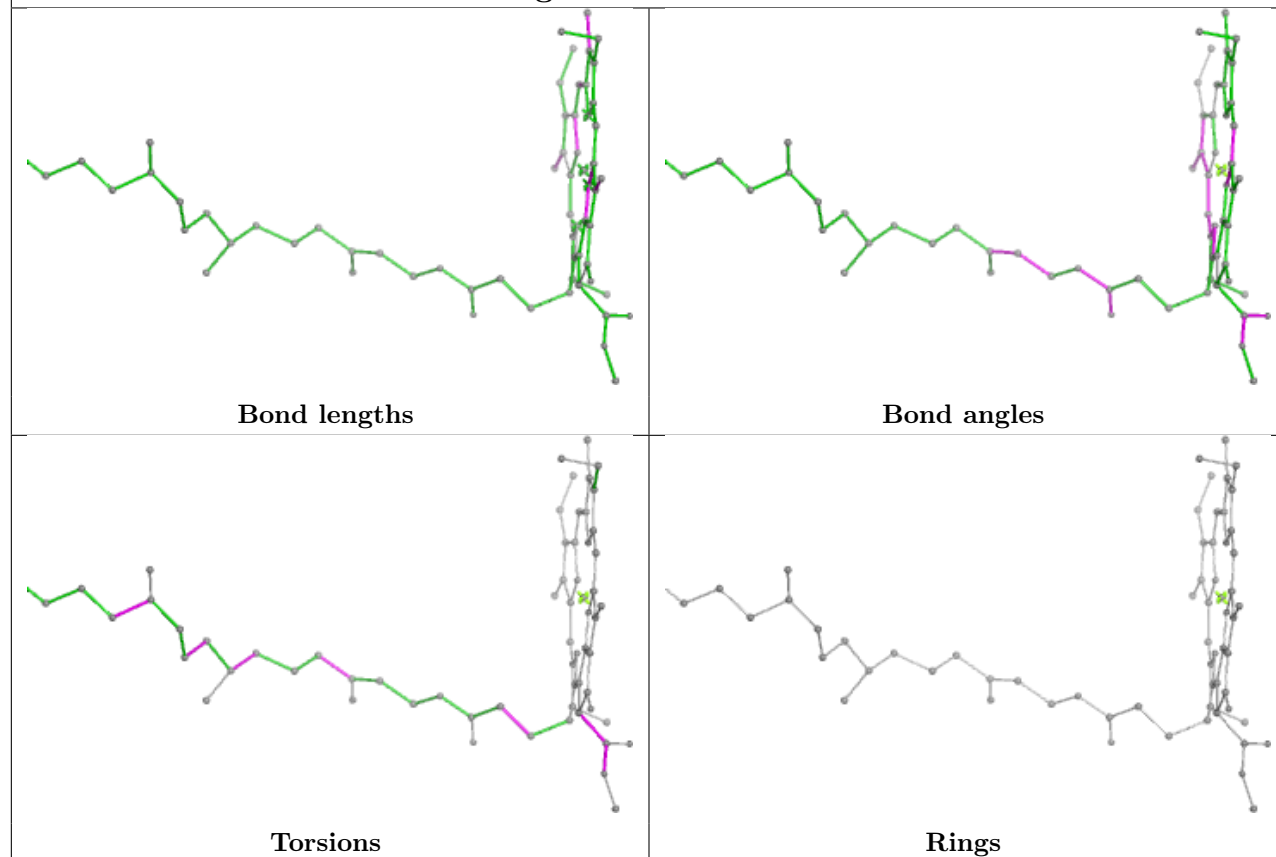




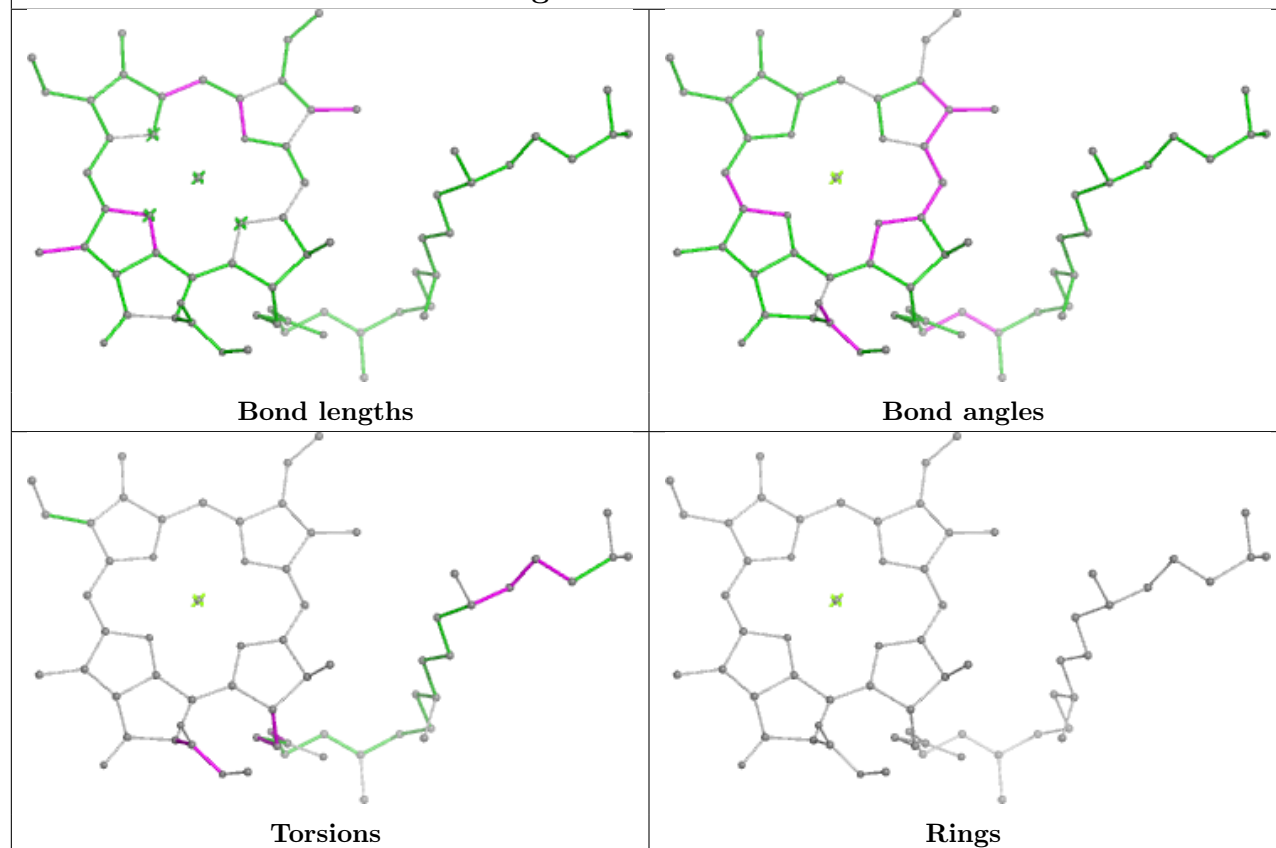
## Ligand CHL y 309

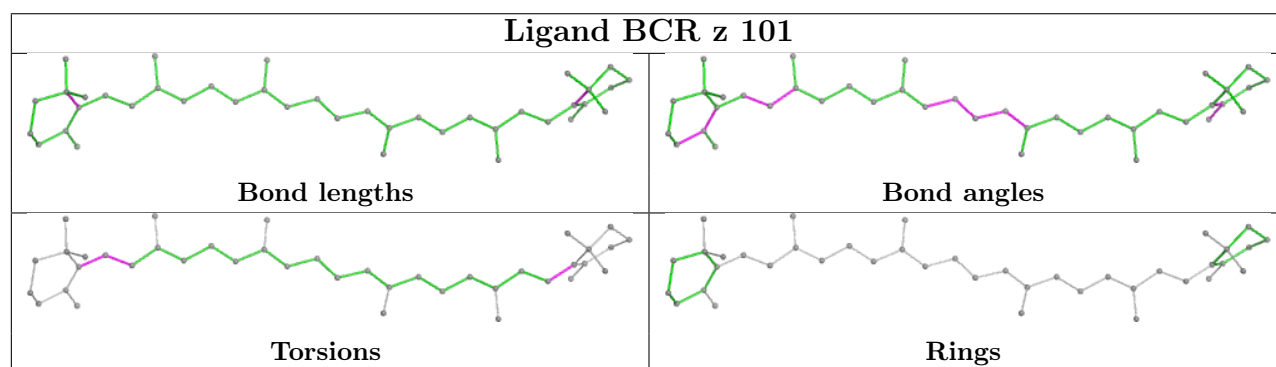
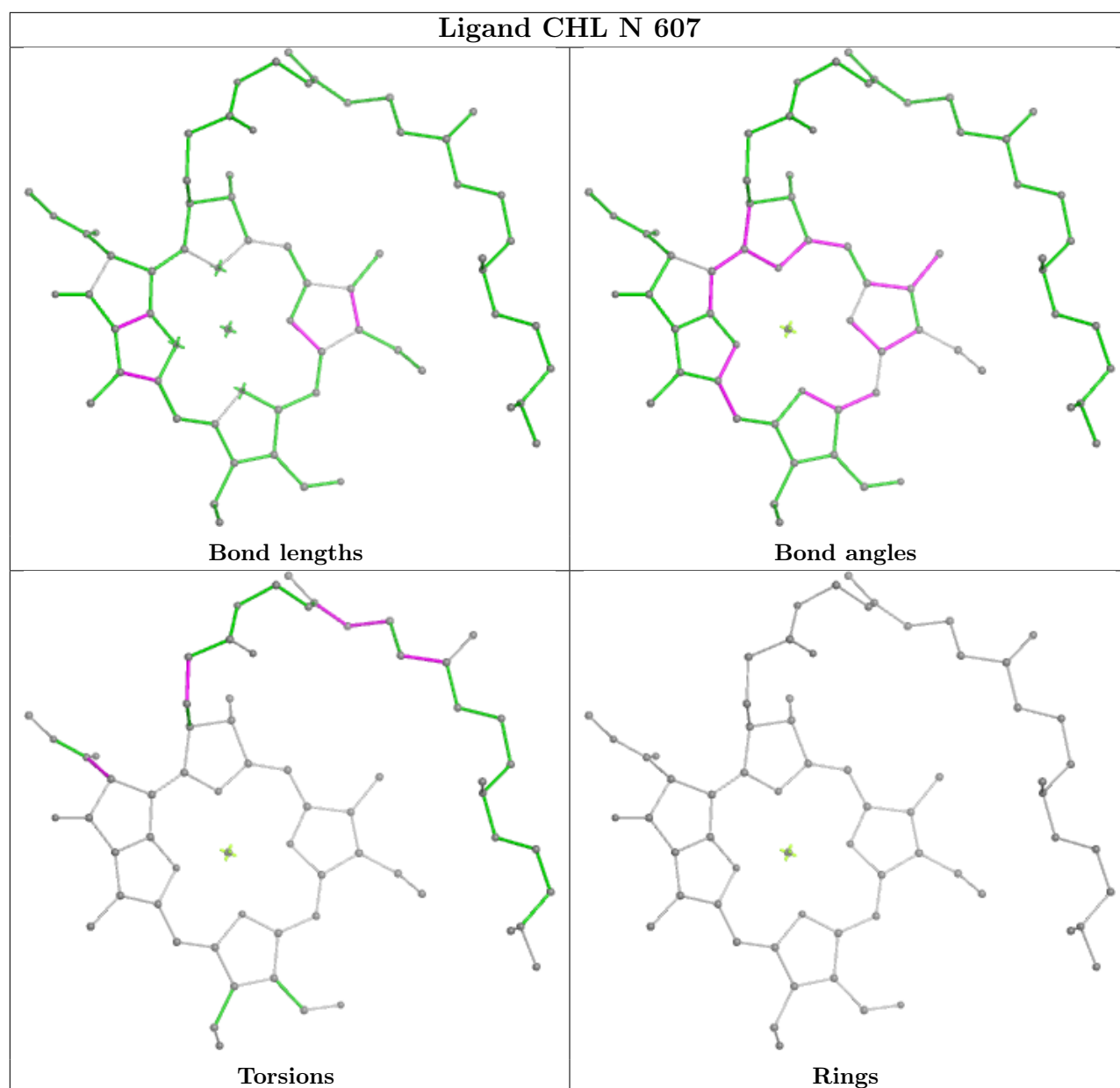


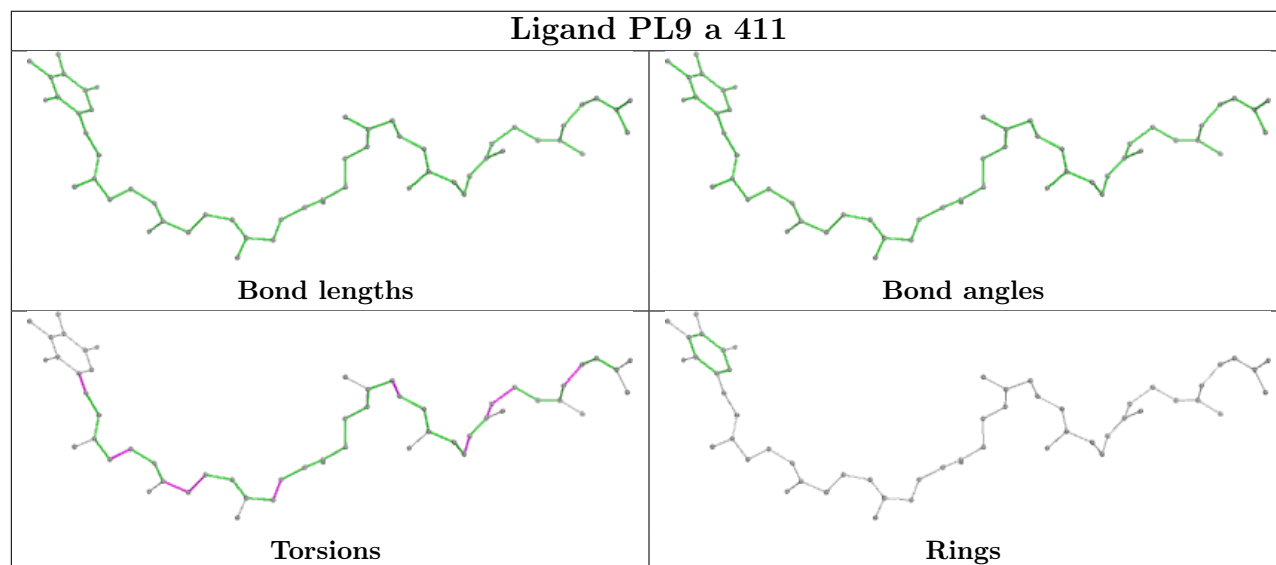
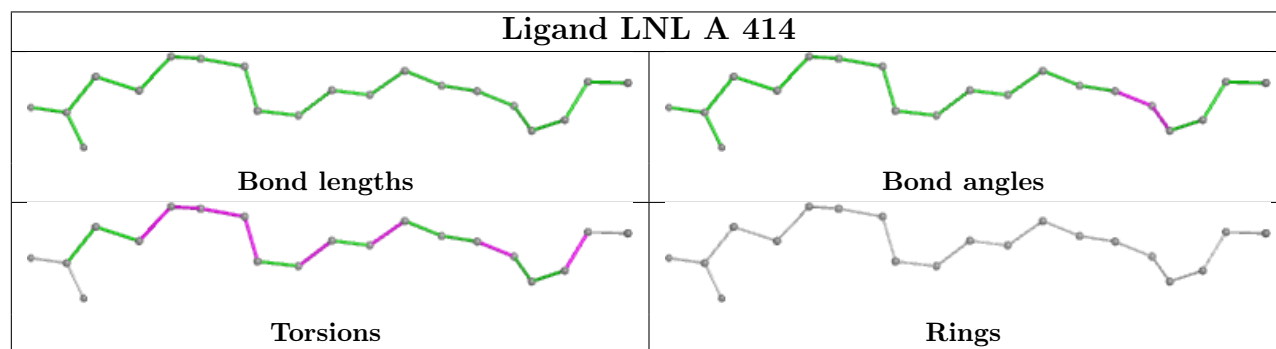
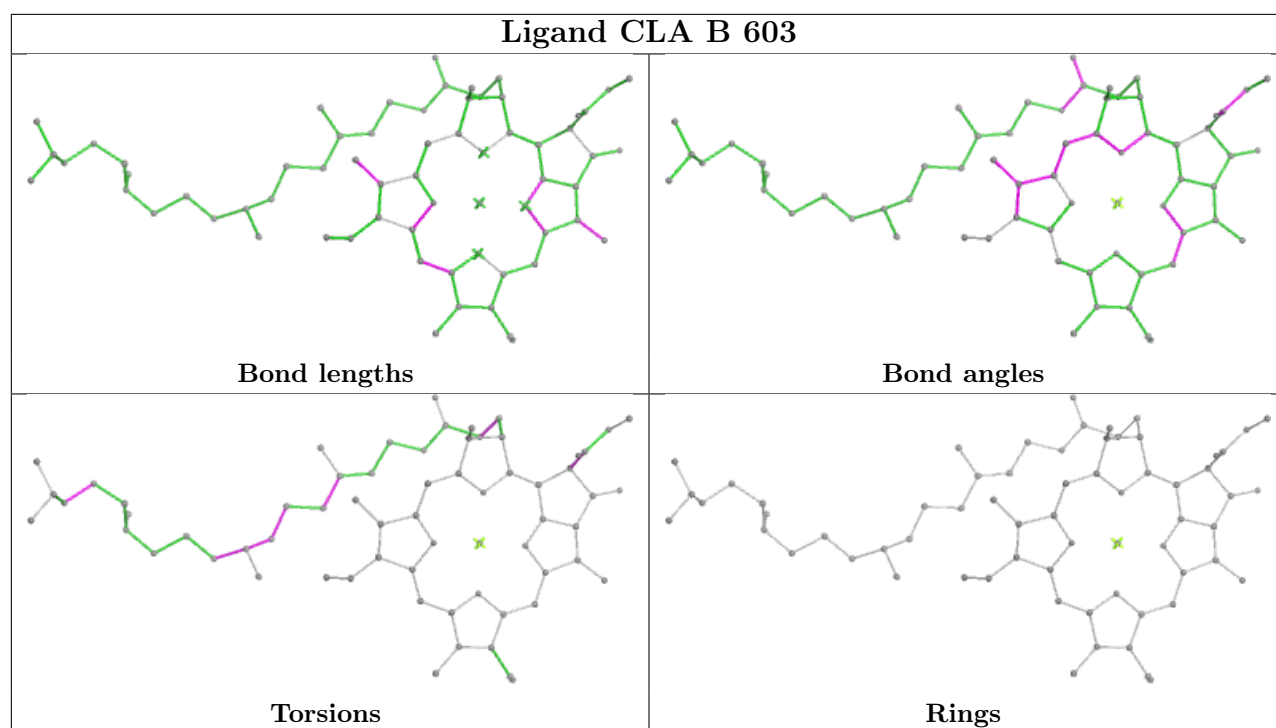
## Ligand CLA b 606

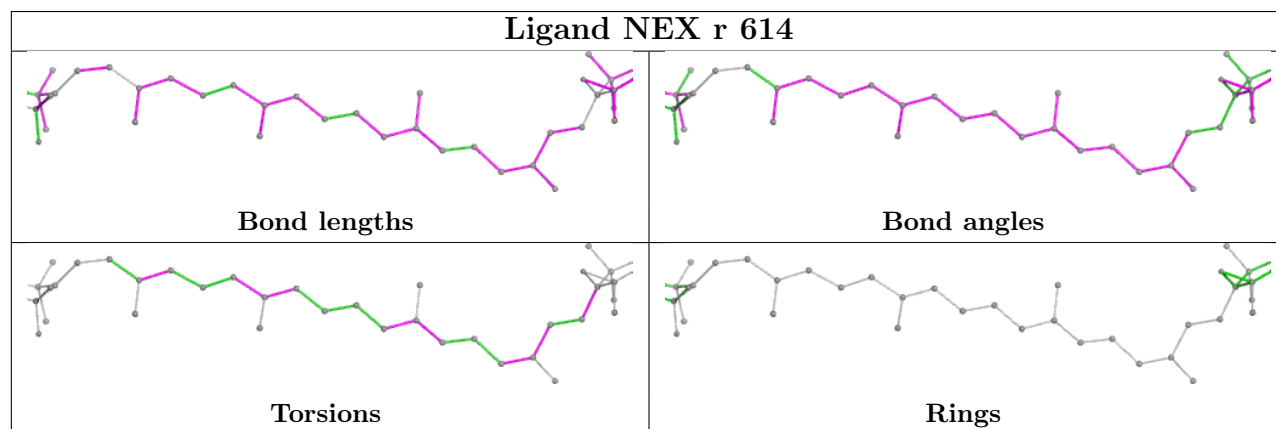
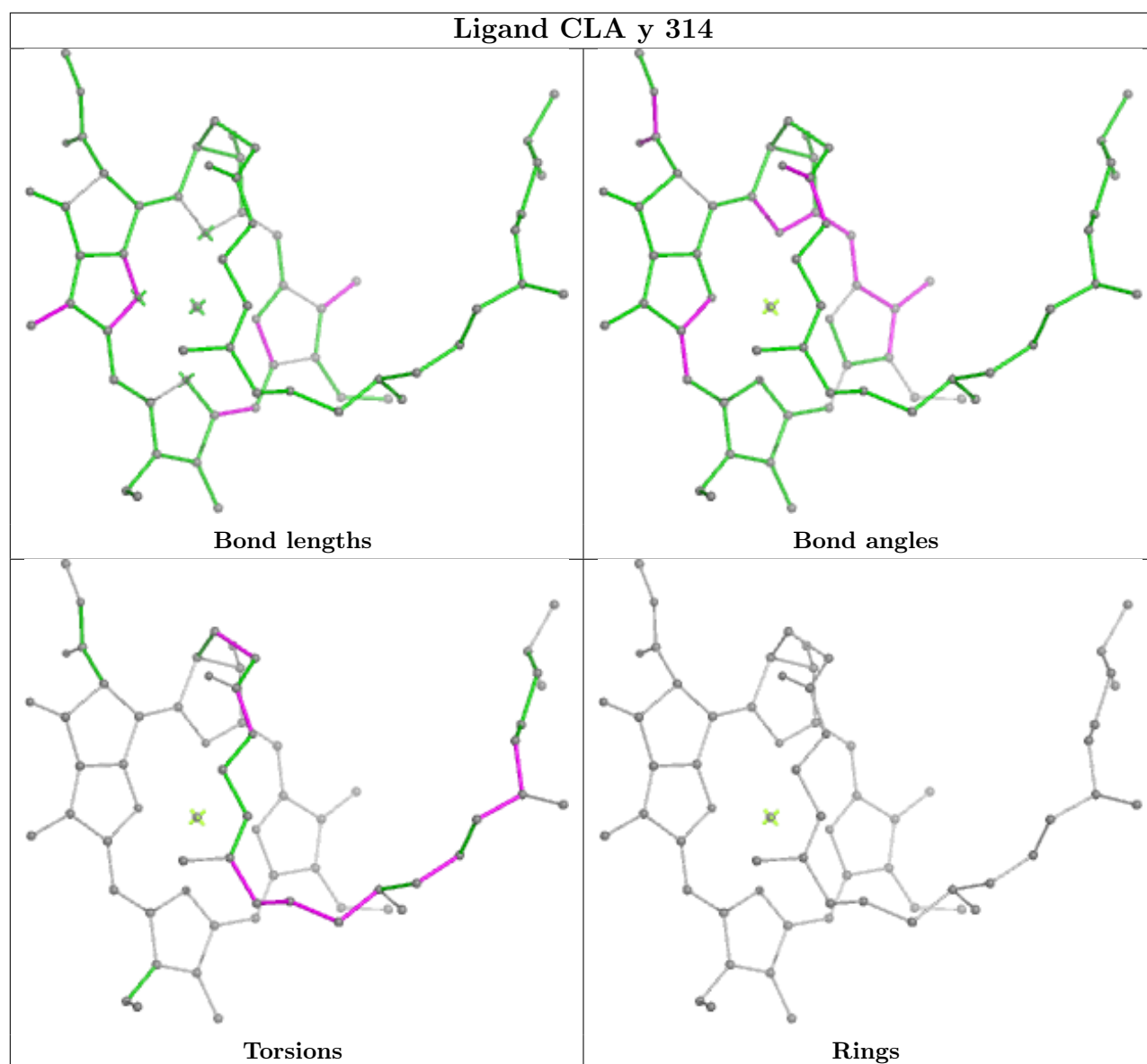


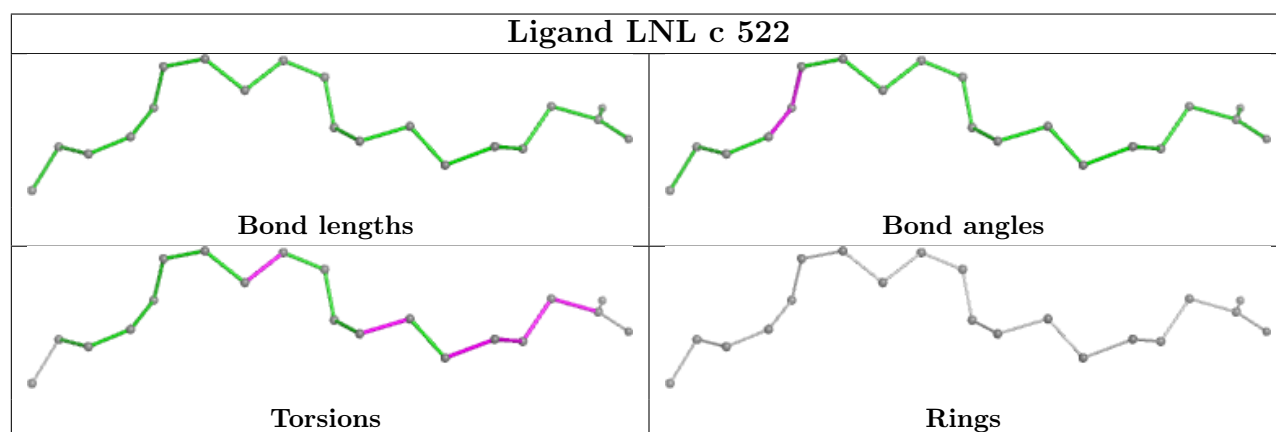
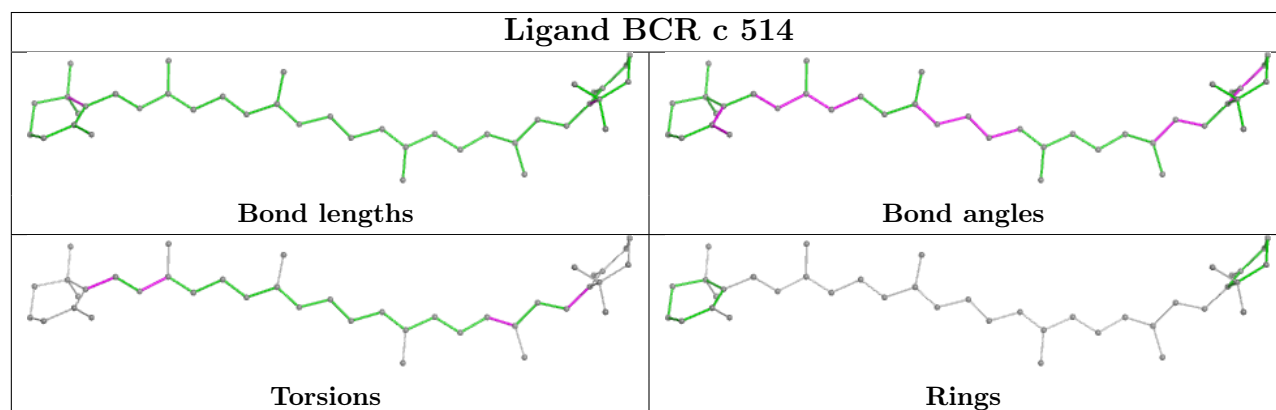
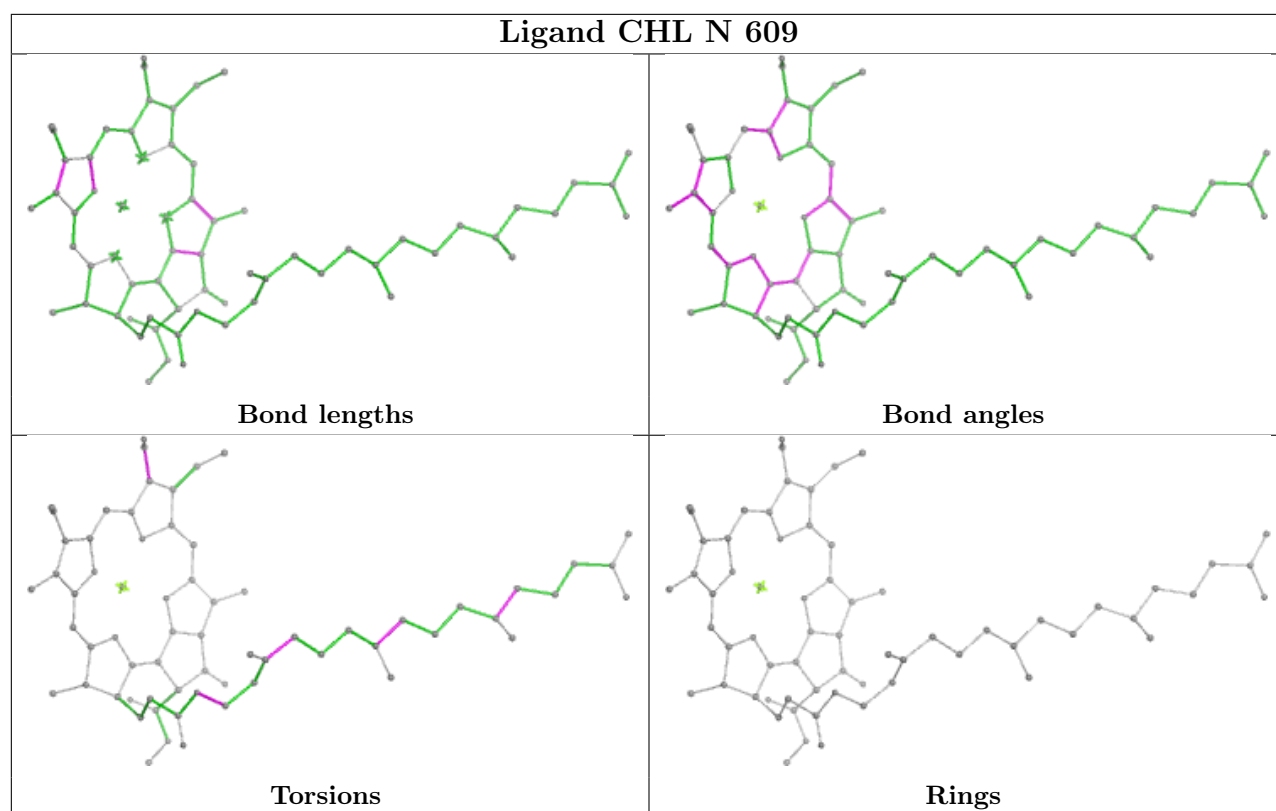
## Ligand CLA A 403











## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

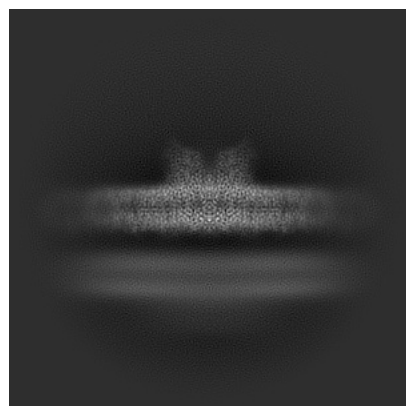
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16389. These allow visual inspection of the internal detail of the map and identification of artifacts.

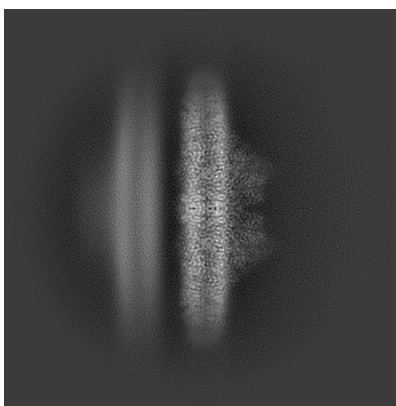
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

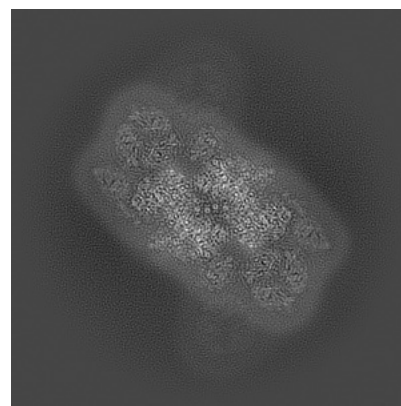
#### 6.1.1 Primary map



X

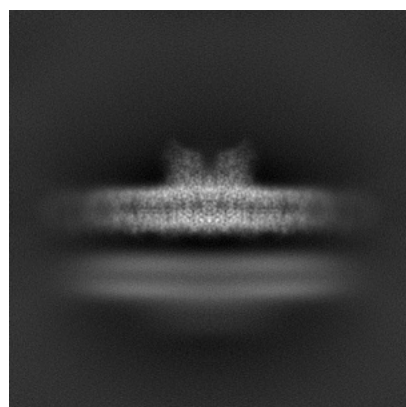


Y

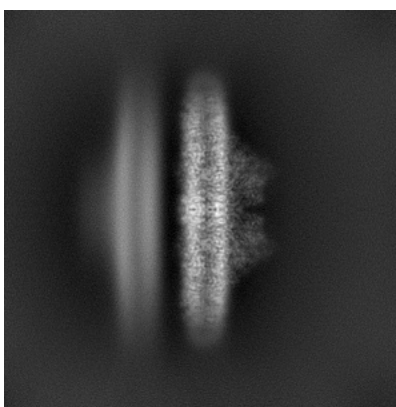


Z

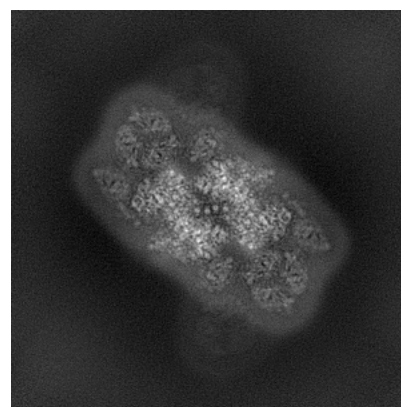
#### 6.1.2 Raw map



X



Y



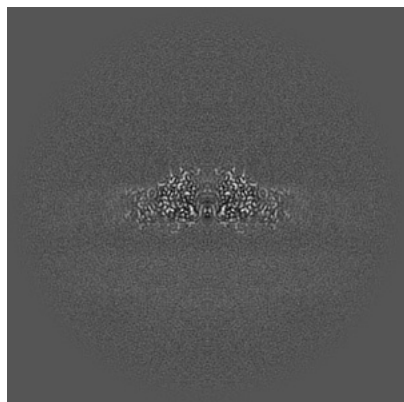
Z

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

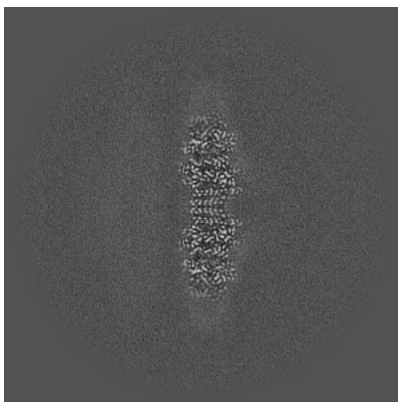


## 6.2 Central slices [i](#)

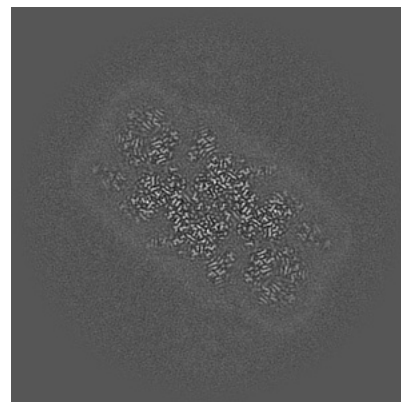
### 6.2.1 Primary map



X Index: 224

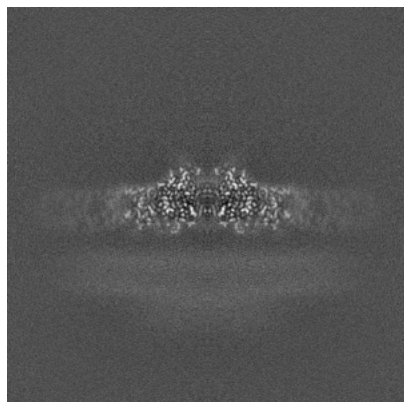


Y Index: 224

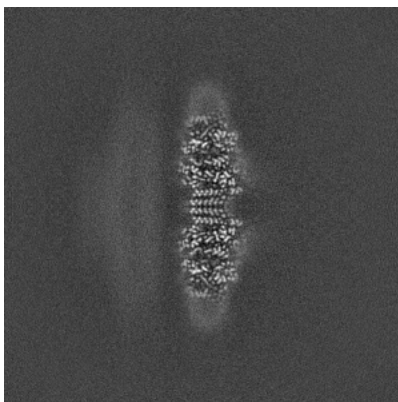


Z Index: 224

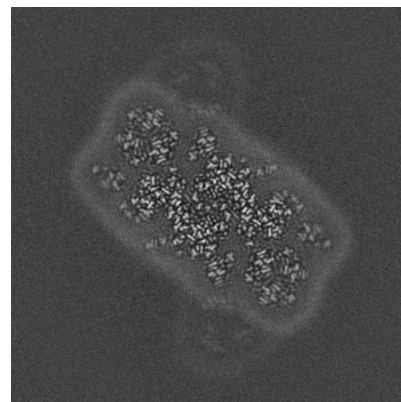
### 6.2.2 Raw map



X Index: 224



Y Index: 224

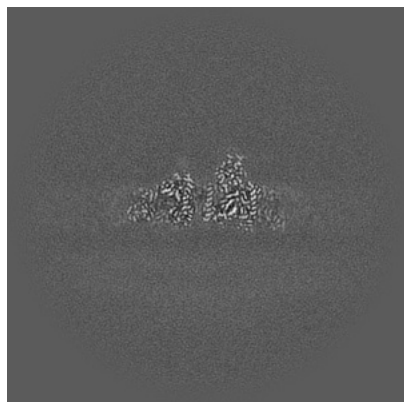


Z Index: 224

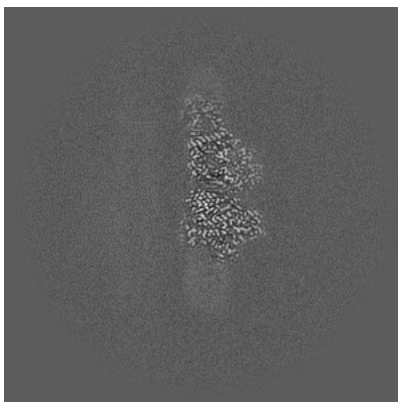
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

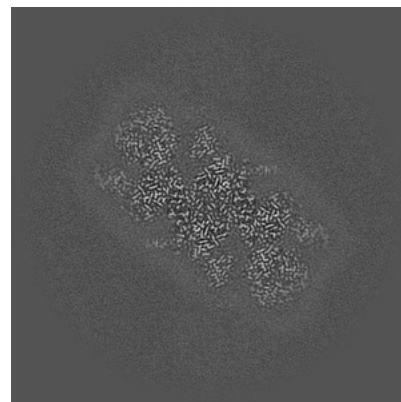
### 6.3.1 Primary map



X Index: 230

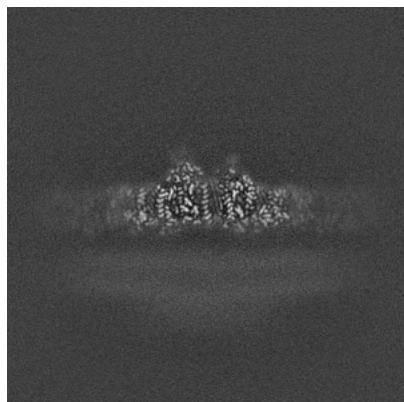


Y Index: 200

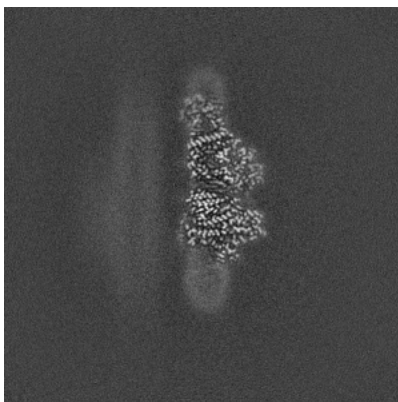


Z Index: 218

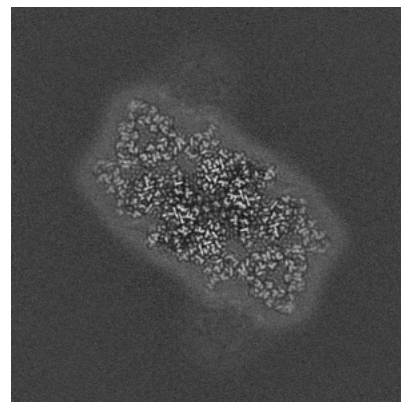
### 6.3.2 Raw map



X Index: 221



Y Index: 200

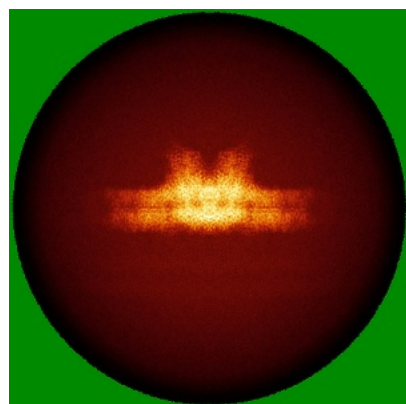


Z Index: 239

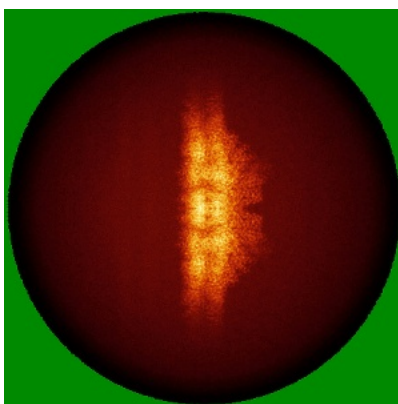
The images above show the largest variance slices of the map in three orthogonal directions.

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

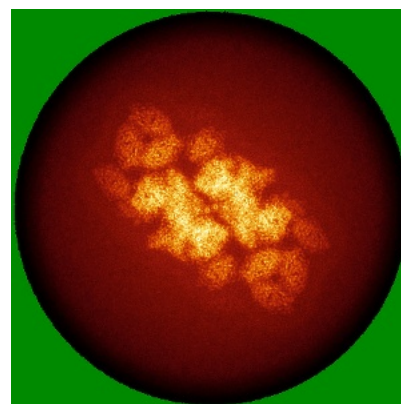
### 6.4.1 Primary map



X

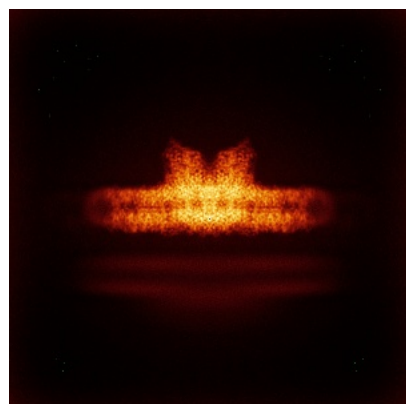


Y

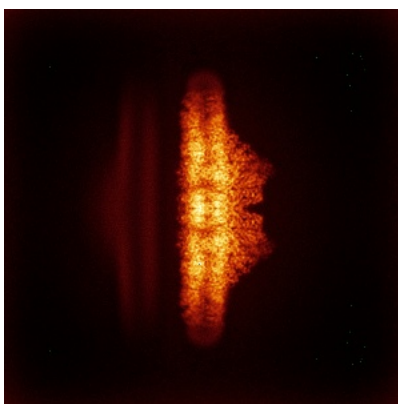


Z

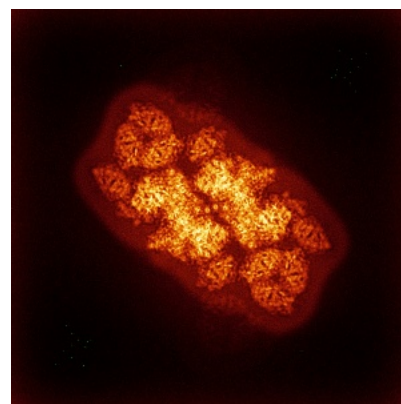
### 6.4.2 Raw map



X



Y

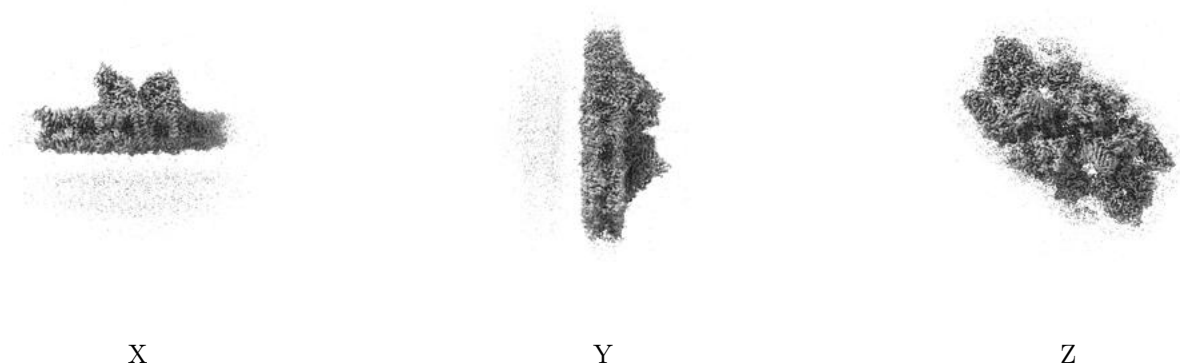


Z

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 0.886. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

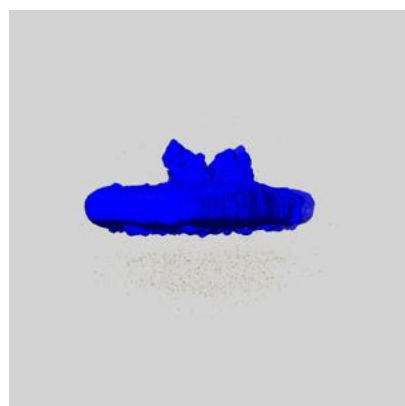
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

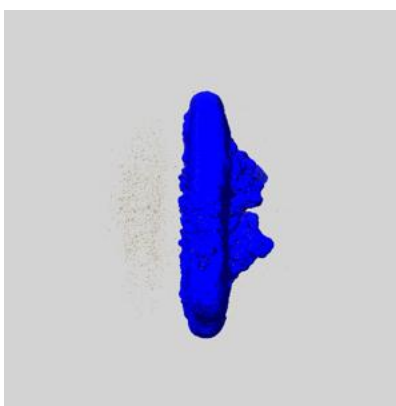
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

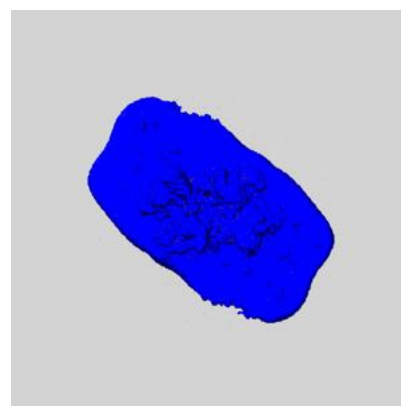
### 6.6.1 emd\_16389\_msk\_1.map [i](#)



X



Y

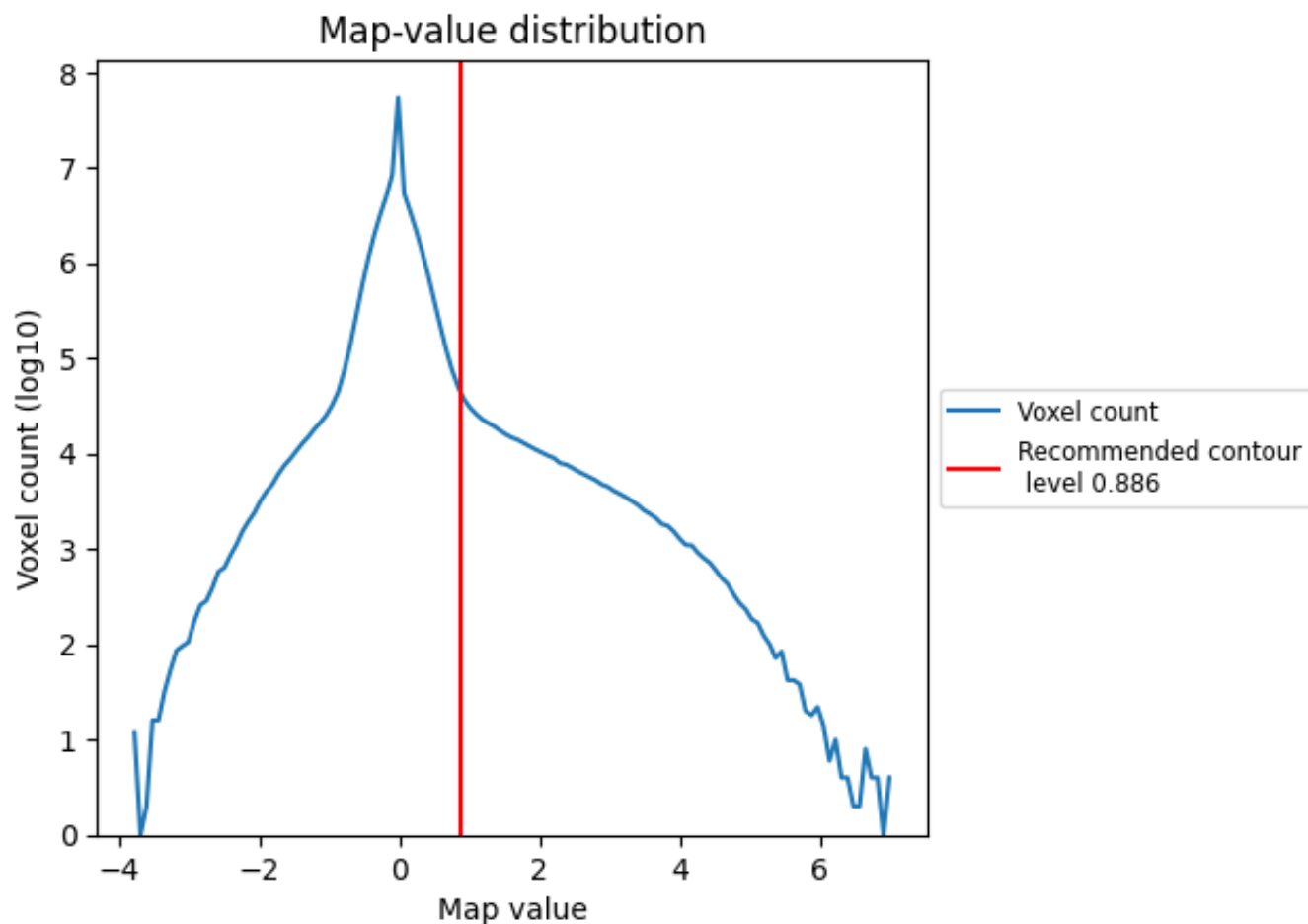


Z

## 7 Map analysis [i](#)

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

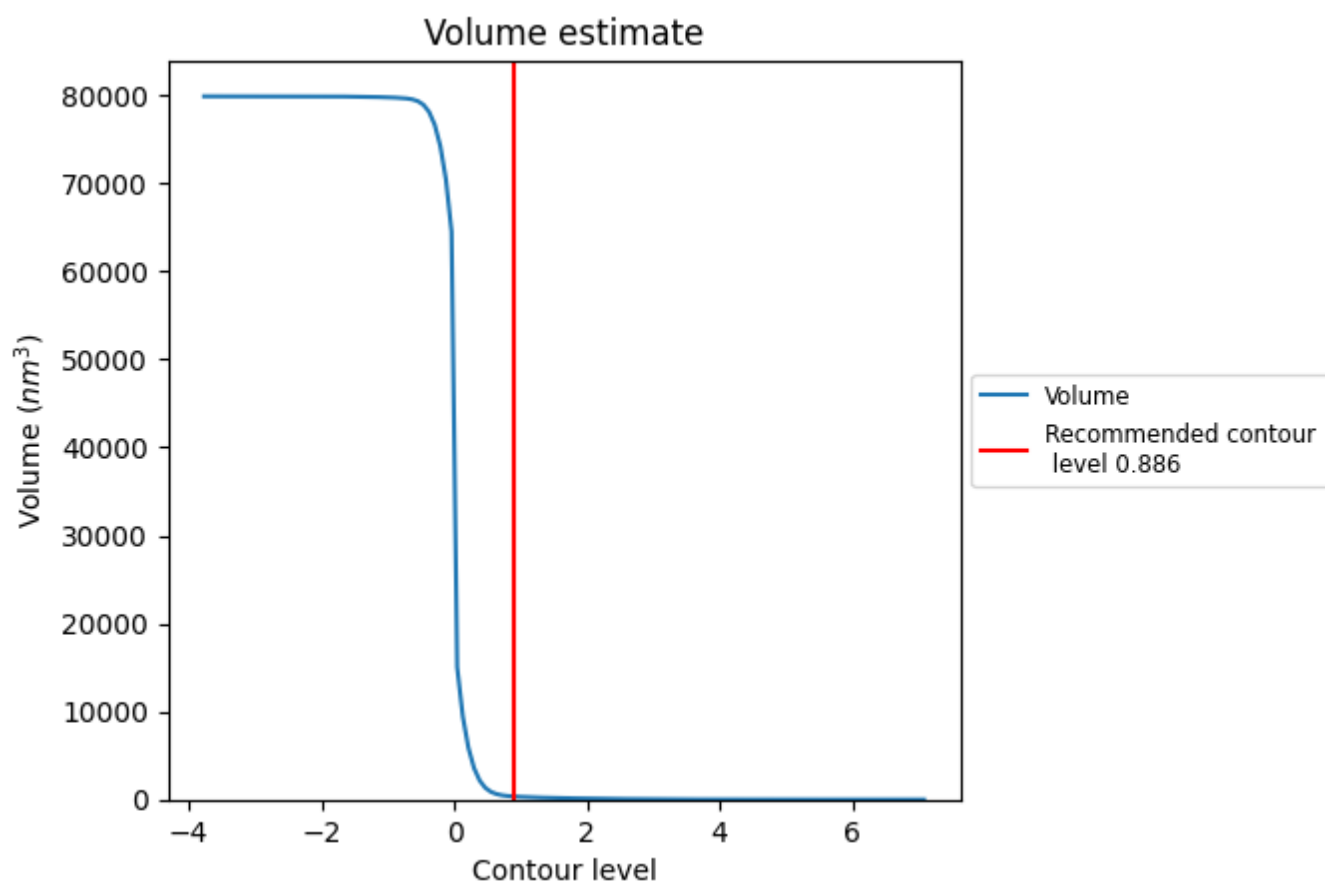
### 7.1 Map-value distribution [i](#)



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.



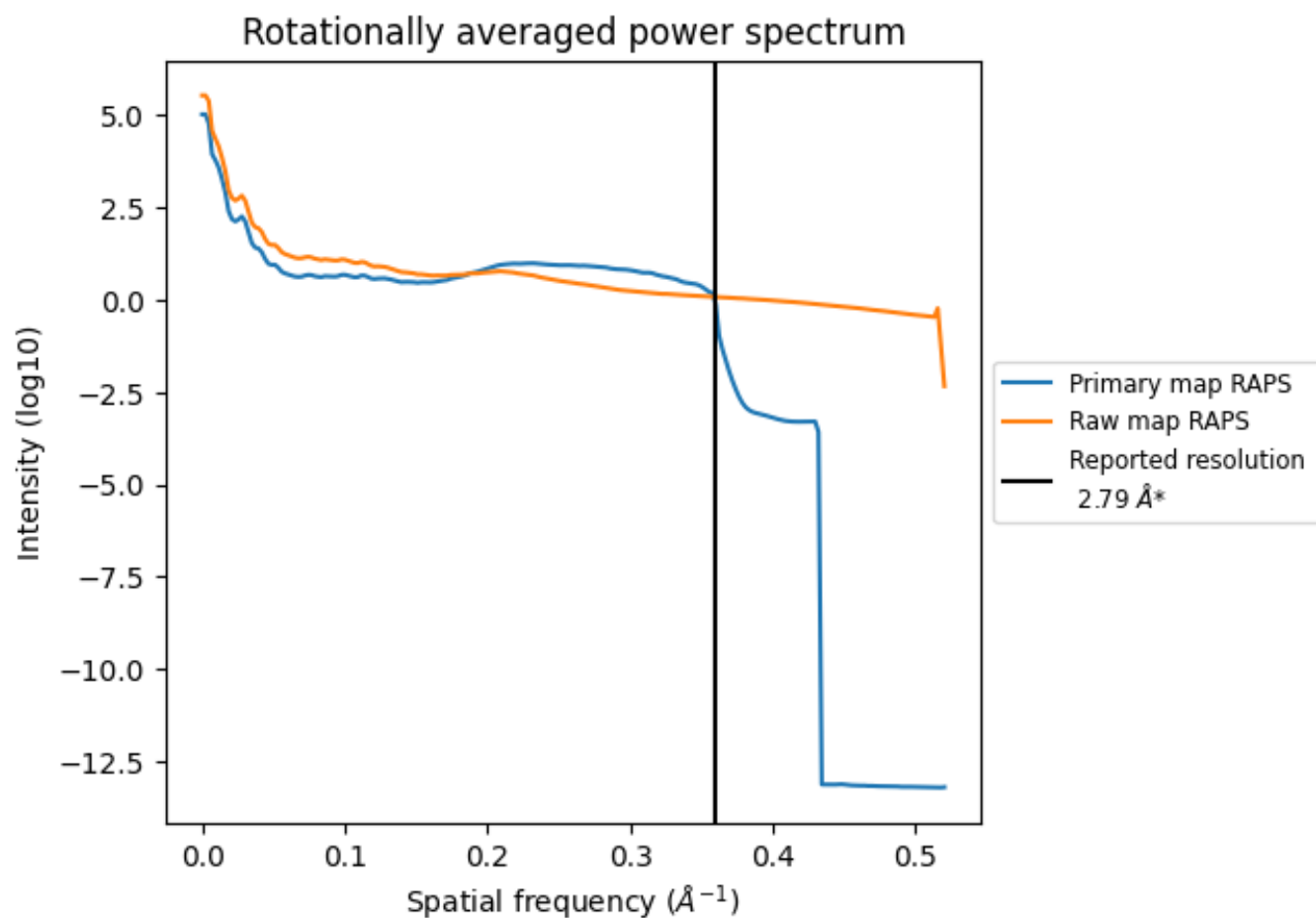
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm<sup>3</sup>; this corresponds to an approximate mass of 322 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 ⓘ



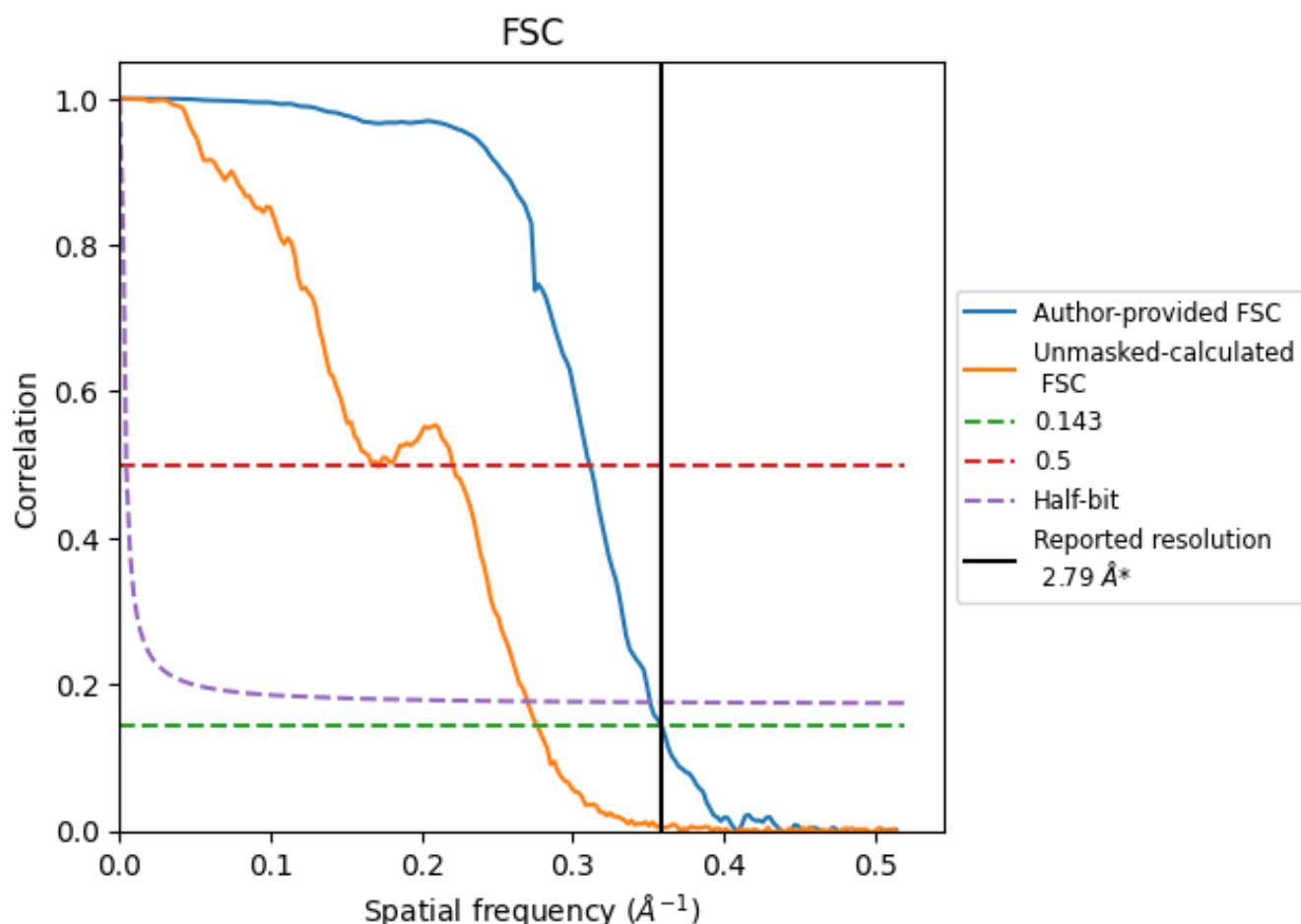
\*Reported resolution corresponds to spatial frequency of 0.359  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.359 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

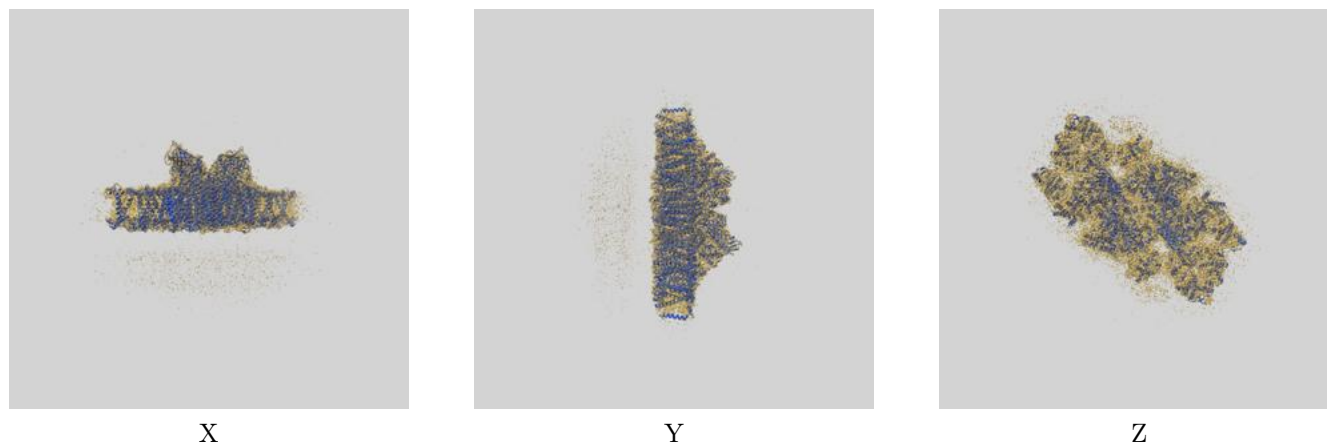
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.21	2.84
Unmasked-calculated*	3.62	5.99	3.70

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 2.785 by more than 10 %

## 9 Map-model fit [i](#)

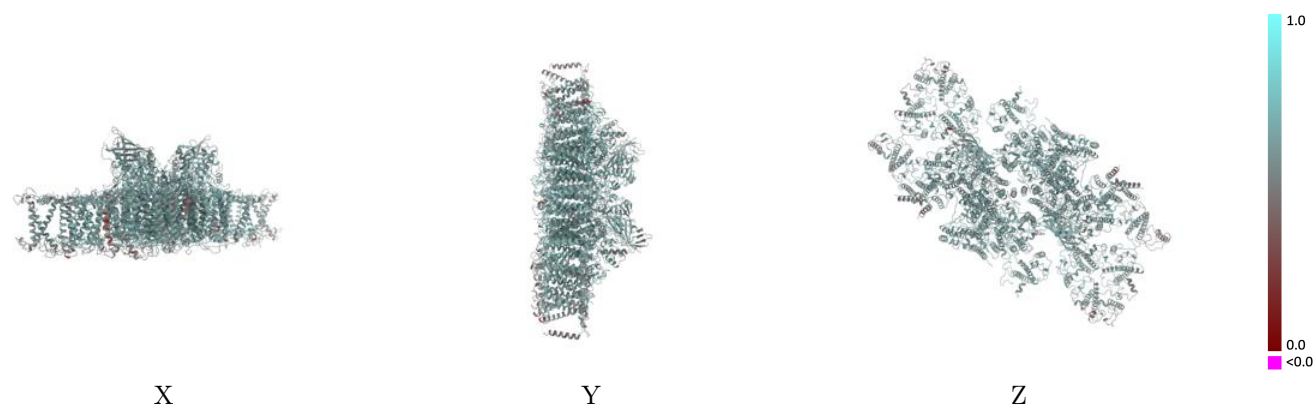
This section contains information regarding the fit between EMDB map EMD-16389 and PDB model 8C29. Per-residue inclusion information can be found in section [3](#) on page [46](#).

### 9.1 Map-model overlay [i](#)



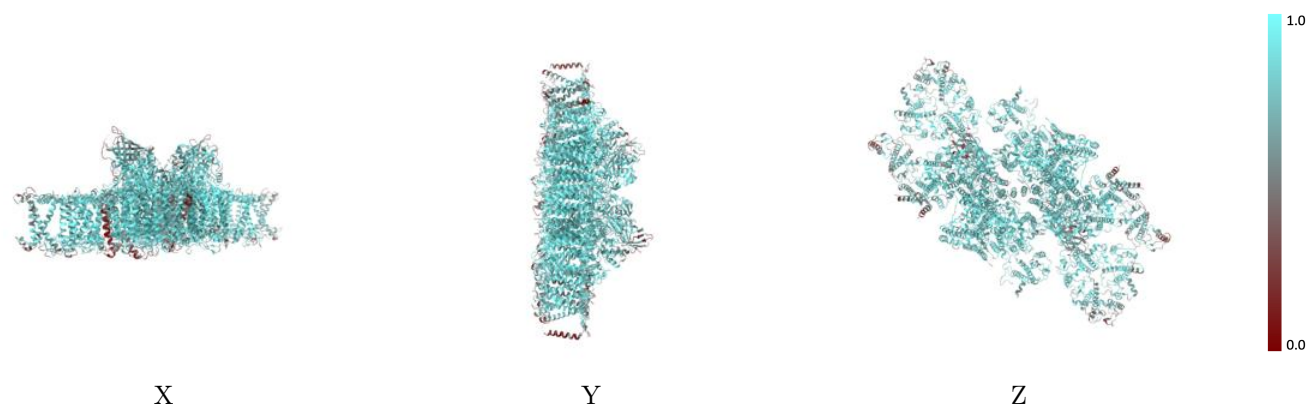
The images above show the 3D surface view of the map at the recommended contour level 0.886 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



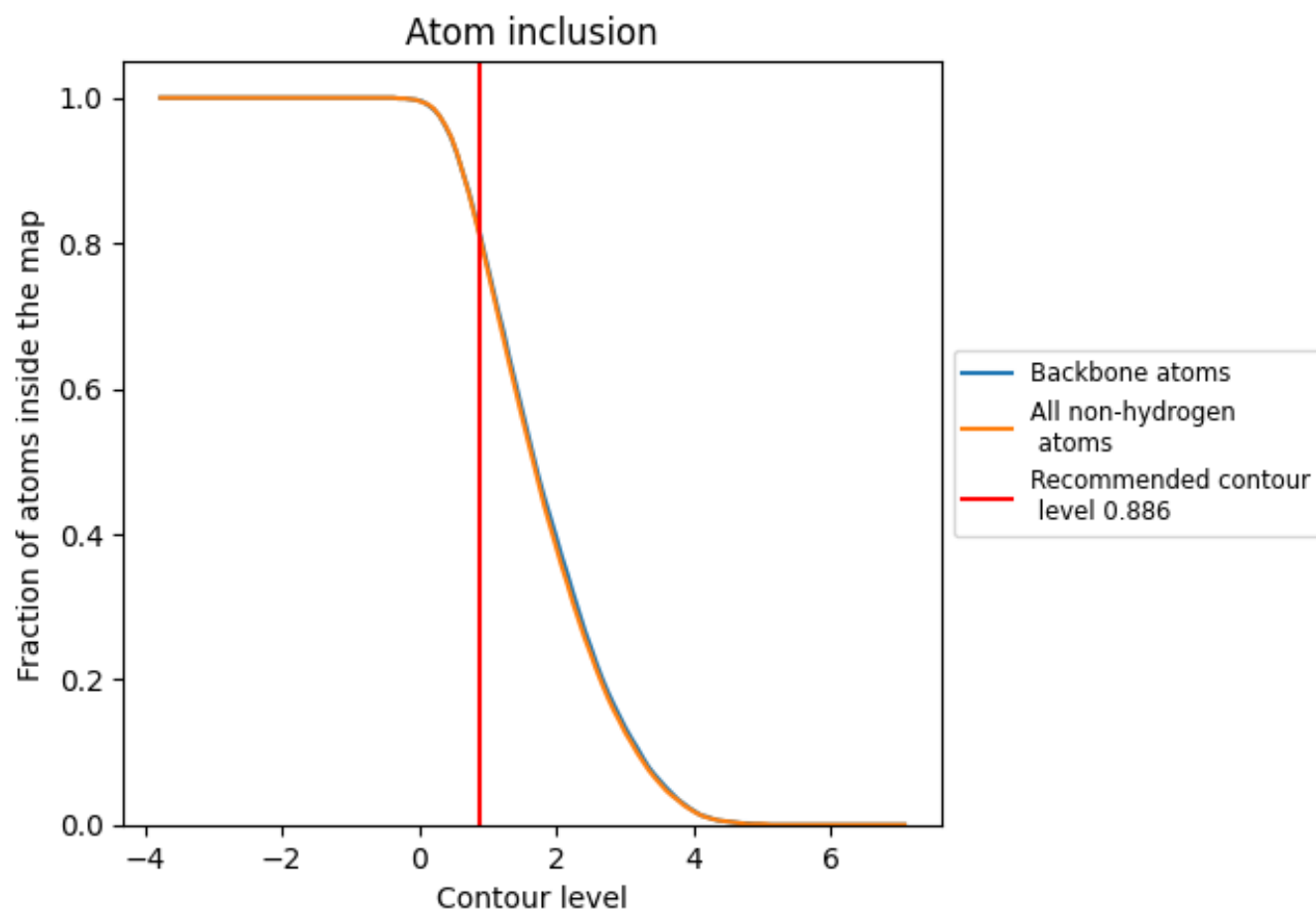
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.886).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.886) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5940
A	 0.8960	 0.6280
B	 0.9040	 0.6220
C	 0.8840	 0.6170
D	 0.8970	 0.6250
E	 0.7820	 0.5800
F	 0.7590	 0.5570
G	 0.6900	 0.5490
H	 0.8960	 0.6190
I	 0.8810	 0.6120
K	 0.8250	 0.5820
L	 0.8480	 0.6220
M	 0.8080	 0.5920
N	 0.7500	 0.5650
O	 0.6380	 0.5610
R	 0.7710	 0.5880
S	 0.6040	 0.5240
T	 0.7910	 0.6000
U	 0.6850	 0.5800
V	 0.4960	 0.5000
W	 0.7230	 0.5730
X	 0.7600	 0.5730
Y	 0.8680	 0.6120
Z	 0.6150	 0.5390
a	 0.8970	 0.6240
b	 0.9010	 0.6240
c	 0.8870	 0.6170
d	 0.8980	 0.6270
e	 0.7940	 0.5770
f	 0.7550	 0.5620
g	 0.6830	 0.5500
h	 0.8930	 0.6200
i	 0.8720	 0.6050
k	 0.8250	 0.5830
l	 0.8920	 0.6190



*Continued on next page...*

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Chain	Atom inclusion	Q-score
m	 0.8140	 0.6030
n	 0.7440	 0.5620
o	 0.6360	 0.5600
r	 0.7680	 0.5870
s	 0.6030	 0.5240
t	 0.8170	 0.6110
u	 0.7050	 0.5920
v	 0.5000	 0.5000
w	 0.7360	 0.5810
x	 0.7750	 0.5860
y	 0.8750	 0.6120
z	 0.6050	 0.5330