



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2025 – 12:55 PM EST

PDB ID : 9EH5  
EMDB ID : EMD-48046  
Title : Structure of a mutated photosystem II complex reveals changes to the hydrogen-bonding network that affect proton egress during O-O bond formation  
Authors : Flesher, D.A.; Shin, J.; Debus, R.J.; Brudvig, G.W.  
Deposited on : 2024-11-22  
Resolution : 1.97 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.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.41.4

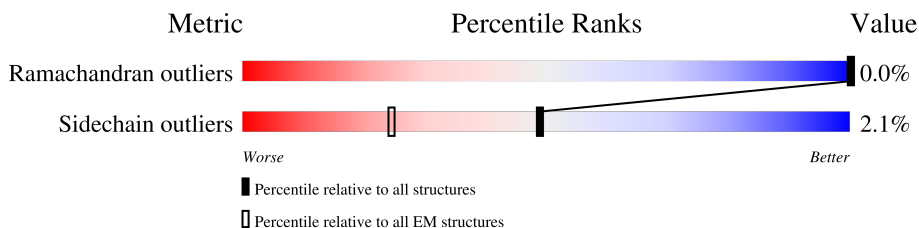
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.97 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.



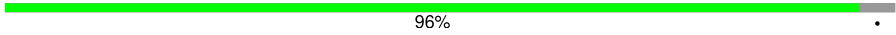


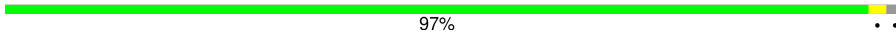
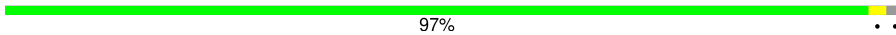
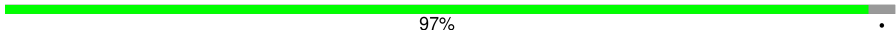
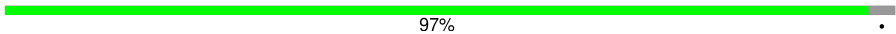


















Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	344	97% ..
1	a	344	97% ..
2	B	507	98% .
2	b	507	98% .
3	C	460	96% ..
3	c	460	96% ..
4	D	352	96% ..
4	d	352	96% ..
5	E	81	96% .

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Mol	Chain	Length	Quality of chain
5	e	81	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	45	
10	k	45	
11	L	39	
11	l	39	
12	M	35	
12	m	35	
13	O	274	
13	o	274	
14	Q	149	
14	q	149	
15	R	39	
15	r	39	
16	T	31	
16	t	31	
17	U	131	
17	u	131	

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Mol	Chain	Length	Quality of chain
18	V	160	
18	v	160	
19	X	39	
19	x	39	
20	Y	39	
20	y	39	
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
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 55154 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2625	1718	429	463	15		
1	a	334	Total	C	N	O	S	0	0
			2625	1718	429	463	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		
2	b	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3493	2293	584	603	13		
3	c	450	Total	C	N	O	S	0	0
			3493	2293	584	603	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2722	1804	442	464	12		
4	d	341	Total	C	N	O	S	0	0
			2722	1804	442	464	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	317	ALA	LYS	conflict	UNP P09192

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Chain	Residue	Modelled	Actual	Comment	Reference
d	317	ALA	LYS	conflict	UNP P09192

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	78	Total	C	N	O	S	0	0
			645	419	104	121	1		
5	e	78	Total	C	N	O	S	0	0
			645	419	104	121	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	35	Total	C	N	O	S	0	0
			279	189	46	43	1		
6	f	35	Total	C	N	O	S	0	0
			279	189	46	43	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	63	Total	C	N	O	S	0	0
			494	328	79	85	2		
7	h	63	Total	C	N	O	S	0	0
			494	328	79	85	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			297	201	46	49	1		
8	i	37	Total	C	N	O	S	0	0
			297	201	46	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			279	188	43	46	2		
9	j	39	Total	C	N	O	S	0	0
			279	188	43	46	2		

- 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	0	0
			299	210	42	47		
10	k	37	Total	C	N	O	0	0
			299	210	42	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	39	Total	C	N	O	S	0	0
			316	204	54	57	1		
11	l	39	Total	C	N	O	S	0	0
			316	204	54	57	1		

- 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	S	0	0
			245	169	36	39	1		
12	m	31	Total	C	N	O	S	0	0
			245	169	36	39	1		

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		
13	o	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	115	Total	C	N	O	S	0	0
			896	564	160	170	2		
14	q	115	Total	C	N	O	S	0	0
			896	564	160	170	2		

- Molecule 15 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	34	Total	C	N	O	0	0
			258	170	45	43		
15	r	34	Total	C	N	O	0	0
			258	170	45	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			241	163	36	40	2		
16	t	30	Total	C	N	O	S	0	0
			241	163	36	40	2		

- Molecule 17 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	95	Total	C	N	O	0	0
			740	461	123	156		
17	u	95	Total	C	N	O	0	0
			740	461	123	156		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		
18	v	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total	C	N	O	S	0	0
			288	193	46	48	1		
19	x	38	Total	C	N	O	S	0	0
			288	193	46	48	1		

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total	C	N	O	0	0
			242	165	37	40		

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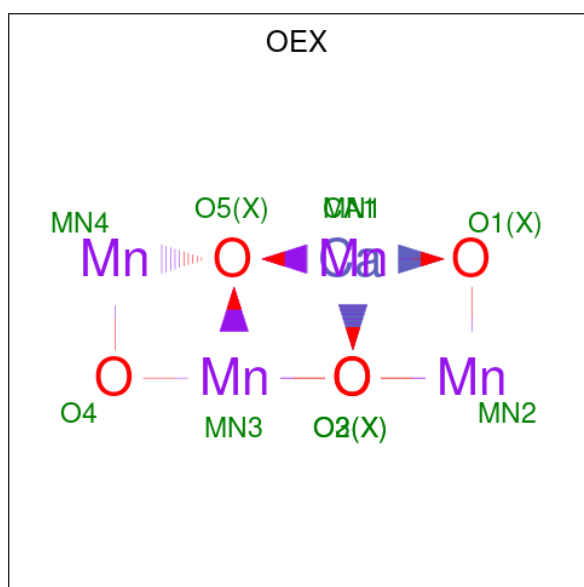
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Mol	Chain	Residues	Atoms				AltConf	Trace
20	y	32	Total	C	N	O	0	0
			242	165	37	40		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Z	60	Total	C	N	O	S	0
			460	317	70	72	1	0
21	z	60	Total	C	N	O	S	0
			460	317	70	72	1	0

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

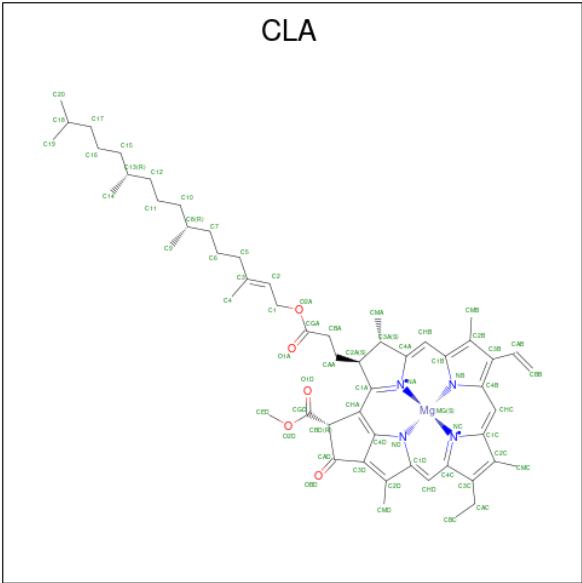
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 25 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
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
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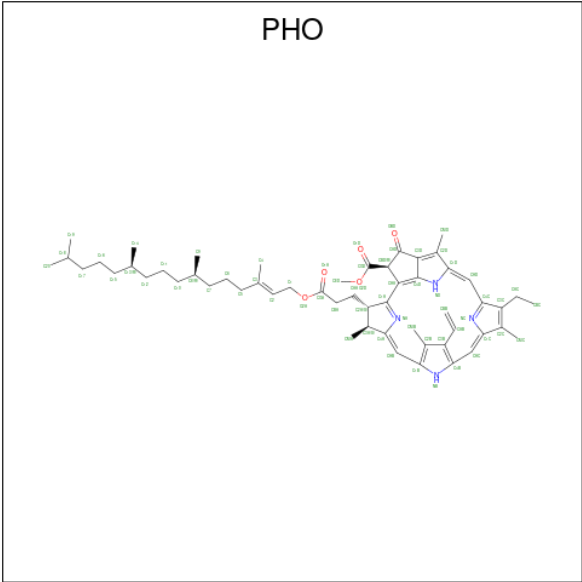
Mol	Chain	Residues	Atoms					AltConf
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25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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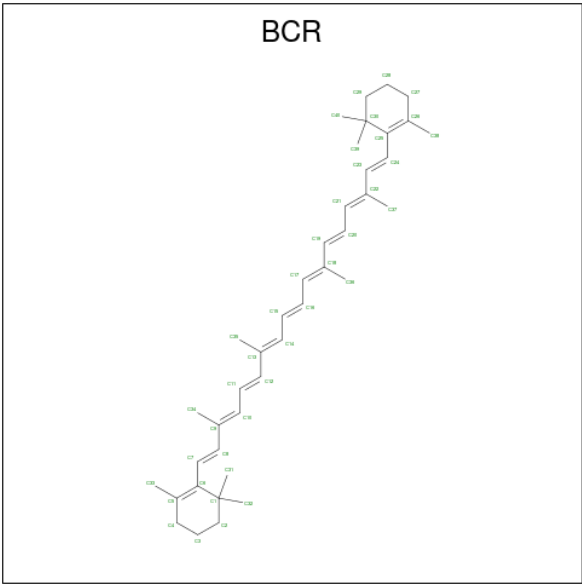
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



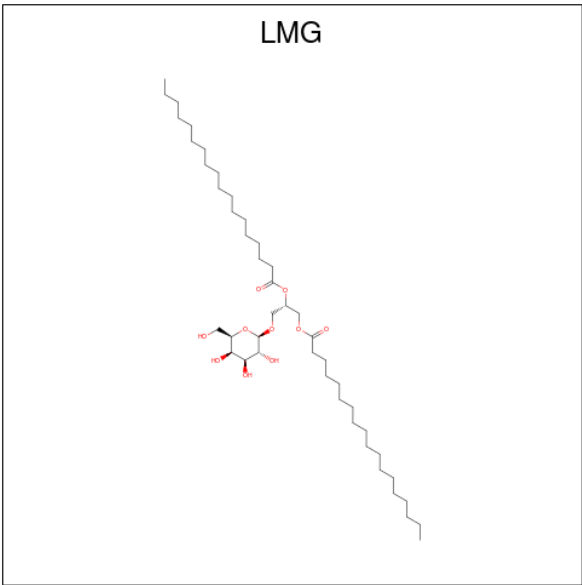
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



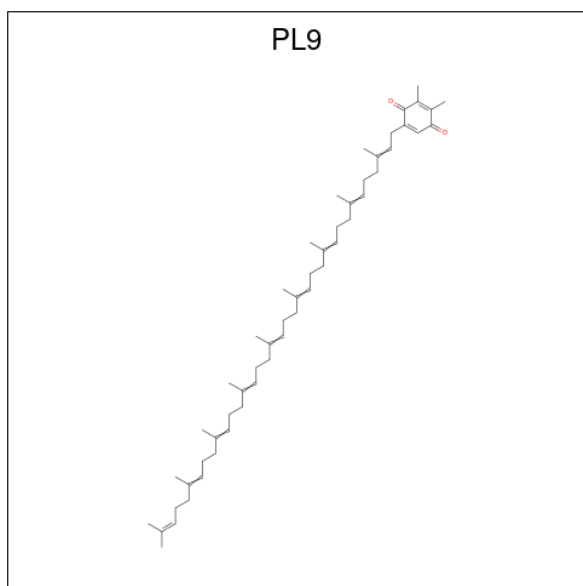
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	41	10	
28	A	1	Total	C	O	0
			36	26	10	
28	B	1	Total	C	O	0
			51	41	10	
28	B	1	Total	C	O	0
			47	37	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			49	39	10	
28	D	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			55	45	10	
28	a	1	Total	C	O	0
			51	41	10	
28	a	1	Total	C	O	0
			36	26	10	
28	b	1	Total	C	O	0
			51	41	10	
28	b	1	Total	C	O	0
			47	37	10	
28	c	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			49	39	10	

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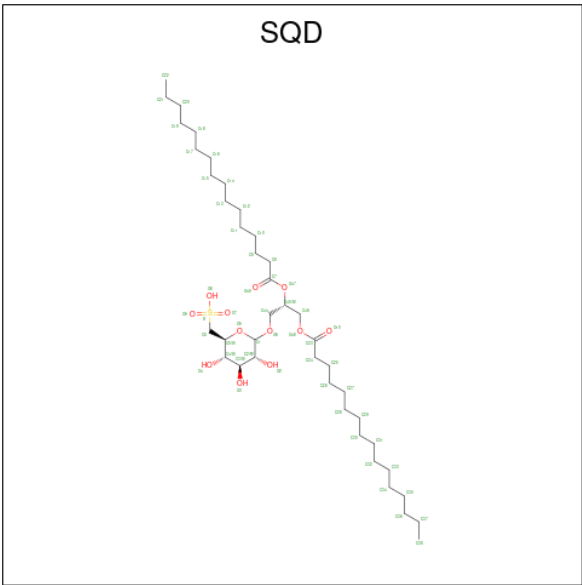
Mol	Chain	Residues	Atoms			AltConf
28	d	1	Total	C	O	0
			55	45	10	
28	j	1	Total	C	O	0
			55	45	10	

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



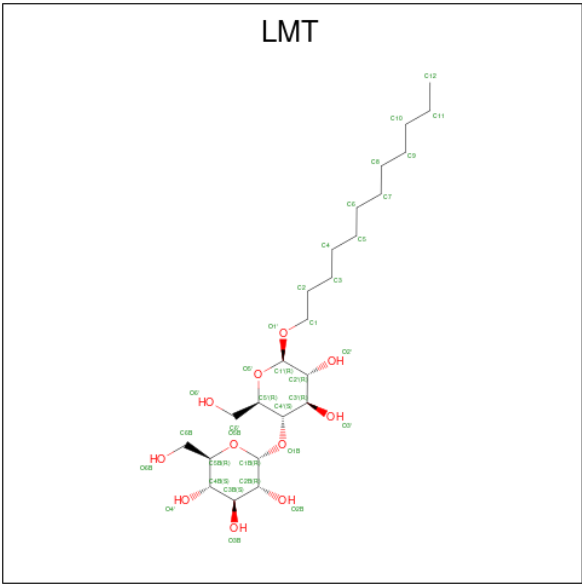
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			48	35	12	1	
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	F	1	Total	C	O	S	0
			34	21	12	1	
30	H	1	Total	C	O	S	0
			54	41	12	1	
30	K	1	Total	C	O		0
			41	32	9		
30	a	1	Total	C	O	S	0
			48	35	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	f	1	Total	C	O	S	0
			34	21	12	1	
30	h	1	Total	C	O	S	0
			54	41	12	1	
30	k	1	Total	C	O		0
			41	32	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	C	1	Total	C	O	0
			24	18	6	
31	C	1	Total	C	O	0
			35	24	11	
31	C	1	Total	C	O	0
			21	15	6	
31	C	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			24	18	6	
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			24	18	6	
31	E	1	Total	C	O	0
			22	16	6	
31	E	1	Total	C	O	0
			35	24	11	
31	F	1	Total	C	O	0
			35	24	11	
31	H	1	Total	C	O	0
			19	13	6	
31	I	1	Total	C	O	0
			24	18	6	
31	I	1	Total	C	O	0
			35	24	11	
31	I	1	Total	C	O	0
			22	16	6	
31	I	1	Total	C	O	0
			24	18	6	
31	J	1	Total	C	O	0
			35	24	11	
31	J	1	Total	C	O	0
			21	15	6	
31	M	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			24	18	6	
31	T	1	Total	C	O	0
			24	18	6	
31	X	1	Total	C	O	0
			22	17	5	
31	X	1	Total	C	O	0
			22	16	6	
31	X	1	Total	C	O	0
			35	24	11	

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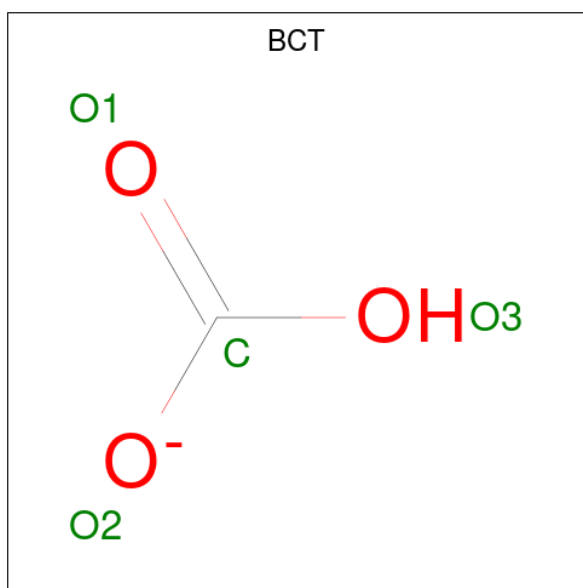
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			35	24	11	
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			21	15	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			24	18	6	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			24	18	6	
31	e	1	Total	C	O	0
			22	16	6	
31	e	1	Total	C	O	0
			35	24	11	
31	f	1	Total	C	O	0
			35	24	11	
31	h	1	Total	C	O	0
			19	13	6	

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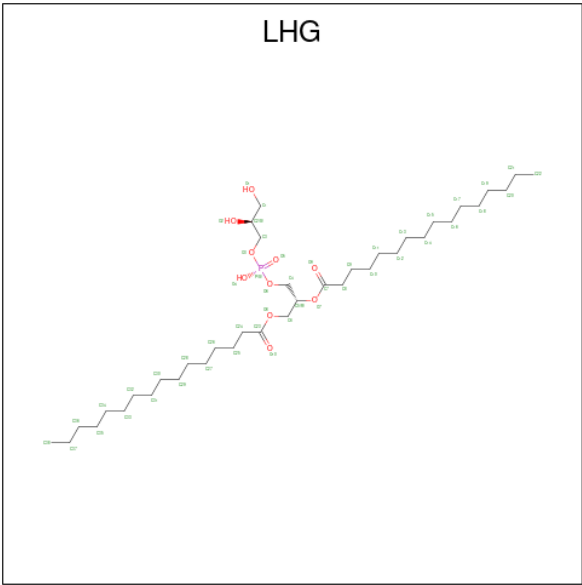
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			35	24	11	
31	i	1	Total	C	O	0
			22	16	6	
31	i	1	Total	C	O	0
			24	18	6	
31	j	1	Total	C	O	0
			35	24	11	
31	j	1	Total	C	O	0
			21	15	6	
31	m	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			22	17	5	
31	x	1	Total	C	O	0
			22	16	6	
31	x	1	Total	C	O	0
			35	24	11	

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



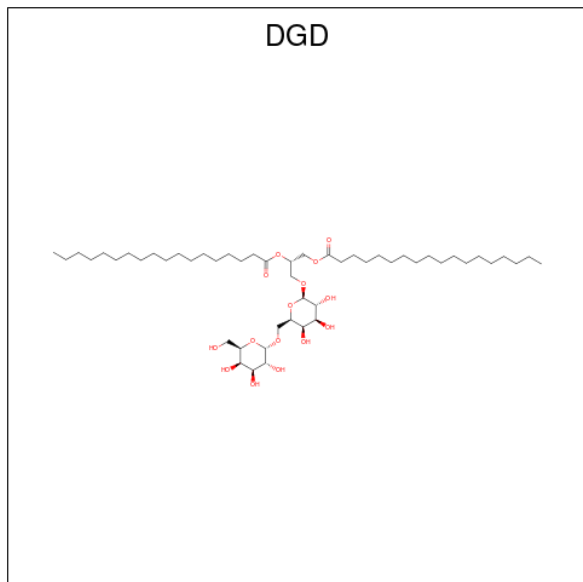
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	L	1	Total	C	O	P	0
			49	38	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	e	1	Total	C	O	P	0
			40	29	10	1	
33	l	1	Total	C	O	P	0
			49	38	10	1	
33	z	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



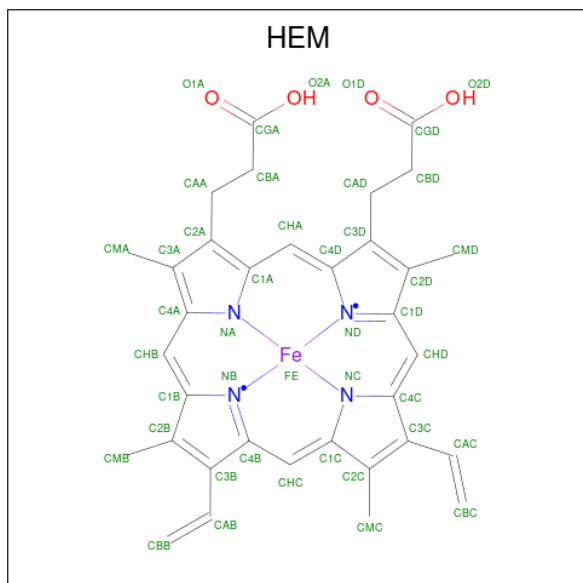
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	

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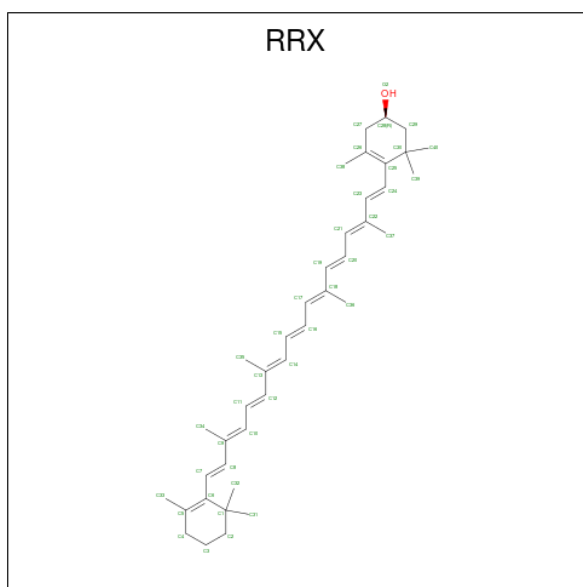
Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).



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

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
37	K	1	Total	Ca	0
			1	1	
37	U	1	Total	Ca	0
			1	1	
37	V	1	Total	Ca	0
			1	1	
37	k	1	Total	Ca	0
			1	1	
37	u	1	Total	Ca	0
			1	1	
37	v	1	Total	Ca	0
			1	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	131	Total	O	0
			131	131	

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Mol	Chain	Residues	Atoms		AltConf
38	B	147	Total 147	O 147	0
38	C	112	Total 112	O 112	0
38	D	110	Total 110	O 110	0
38	E	15	Total 15	O 15	0
38	F	5	Total 5	O 5	0
38	H	13	Total 13	O 13	0
38	I	5	Total 5	O 5	0
38	J	2	Total 2	O 2	0
38	K	2	Total 2	O 2	0
38	L	10	Total 10	O 10	0
38	M	7	Total 7	O 7	0
38	O	35	Total 35	O 35	0
38	T	11	Total 11	O 11	0
38	U	10	Total 10	O 10	0
38	V	28	Total 28	O 28	0
38	X	4	Total 4	O 4	0
38	a	132	Total 132	O 132	0
38	b	147	Total 147	O 147	0
38	c	112	Total 112	O 112	0
38	d	109	Total 109	O 109	0
38	e	15	Total 15	O 15	0

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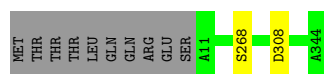
Mol	Chain	Residues	Atoms		AltConf
38	f	5	Total 5	O 5	0
38	h	13	Total 13	O 13	0
38	i	5	Total 5	O 5	0
38	j	2	Total 2	O 2	0
38	k	2	Total 2	O 2	0
38	l	10	Total 10	O 10	0
38	m	7	Total 7	O 7	0
38	o	35	Total 35	O 35	0
38	t	11	Total 11	O 11	0
38	u	10	Total 10	O 10	0
38	v	28	Total 28	O 28	0
38	x	4	Total 4	O 4	0

### 3 Residue-property plots [i](#)

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

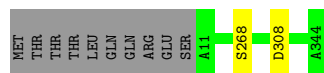
- Molecule 1: Photosystem II protein D1 2

Chain A:  97%



- Molecule 1: Photosystem II protein D1 2

Chain a:  97%



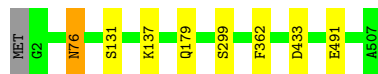
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  96%



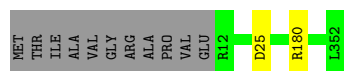
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96% ..



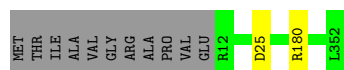
- Molecule 4: Photosystem II D2 protein

Chain D:  96% ..



- Molecule 4: Photosystem II D2 protein

Chain d:  96% ..



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  96% .




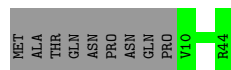
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  96% .




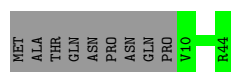
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  80% 20%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  80% 20%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  97% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  97% ..



- Molecule 8: Photosystem II reaction center protein I

Chain I:  97% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  97% .



- Molecule 9: Photosystem II reaction center protein J

Chain J:  92% 8%



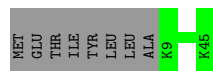
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%




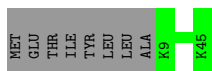
- Molecule 10: Photosystem II reaction center protein K

Chain K:  82% 18%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  82% 18%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

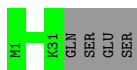
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

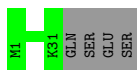
- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 11%




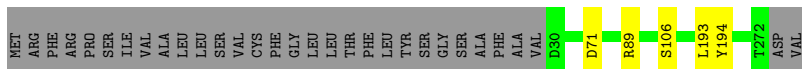
- Molecule 12: Photosystem II reaction center protein M

Chain m:  89% 11%




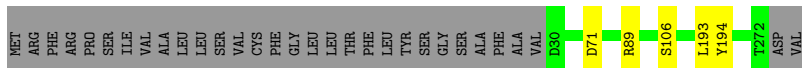
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  87% 11%



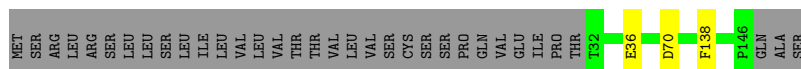
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  87% 11%

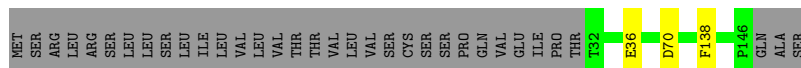


- Molecule 14: Sll1638 protein

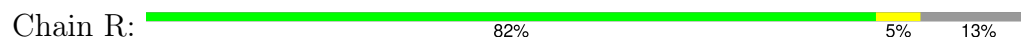
Chain Q:  75% 23%



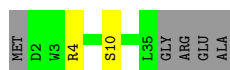
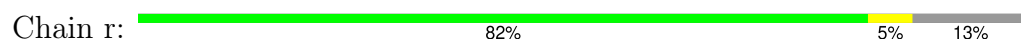
- Molecule 14: Sll1638 protein



- Molecule 15: Photosystem II protein Y



- Molecule 15: Photosystem II protein Y



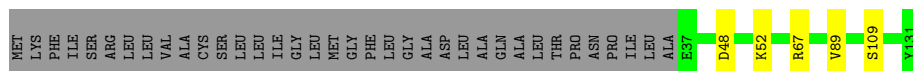
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T

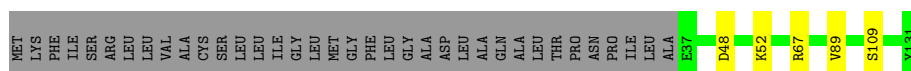


- Molecule 17: Photosystem II 12 kDa extrinsic protein

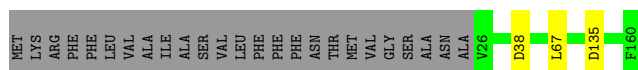
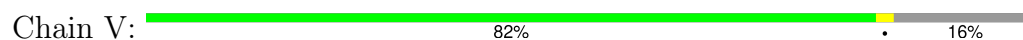


- Molecule 17: Photosystem II 12 kDa extrinsic protein

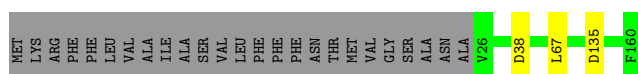




- Molecule 18: Cytochrome c-550



- Molecule 18: Cytochrome c-550



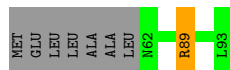
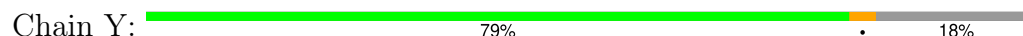
- Molecule 19: Photosystem II reaction center X protein



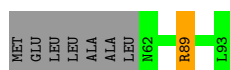
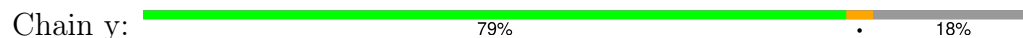
- Molecule 19: Photosystem II reaction center X protein



- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 21: Photosystem II reaction center protein Z





- Molecule 21: Photosystem II reaction center protein Z

Chain z: 94% . .





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ( $\text{\AA}$ )	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.832, 0.832, 0.832	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, LMG, BCR, SQD, CLA, FME, PHO, OEX, HEM, BCT, LMT, CL, LHG, DGD, PL9, CA, RRX

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	0.42	0/2710	0.60	0/3694
1	a	0.42	0/2710	0.60	0/3694
2	B	0.41	0/4091	0.59	0/5568
2	b	0.41	0/4091	0.59	0/5568
3	C	0.40	0/3608	0.58	0/4912
3	c	0.40	0/3608	0.58	0/4912
4	D	0.39	0/2819	0.59	0/3839
4	d	0.39	0/2819	0.59	0/3839
5	E	0.38	0/664	0.61	0/906
5	e	0.38	0/664	0.61	0/906
6	F	0.42	0/288	0.67	0/393
6	f	0.42	0/288	0.67	0/393
7	H	0.33	0/506	0.59	0/687
7	h	0.33	0/506	0.59	0/687
8	I	0.38	0/294	0.57	0/397
8	i	0.38	0/294	0.57	0/397
9	J	0.35	0/278	0.54	0/375
9	j	0.35	0/278	0.54	0/375
10	K	0.40	0/310	0.58	0/424
10	k	0.40	0/310	0.58	0/424
11	L	0.35	0/322	0.53	0/435
11	l	0.35	0/322	0.53	0/435
12	M	0.32	0/239	0.49	0/325
12	m	0.32	0/239	0.49	0/325
13	O	0.39	0/1911	0.64	0/2590
13	o	0.39	0/1911	0.64	0/2590
14	Q	0.37	0/910	0.61	0/1229
14	q	0.37	0/910	0.61	0/1229
15	R	0.30	0/262	0.60	0/361
15	r	0.30	0/262	0.60	0/361
16	T	0.32	0/236	0.49	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	t	0.32	0/236	0.50	0/321
17	U	0.33	0/751	0.61	0/1018
17	u	0.33	0/751	0.61	0/1018
18	V	0.34	0/1086	0.58	0/1476
18	v	0.34	0/1086	0.58	0/1476
19	X	0.28	0/293	0.55	0/399
19	x	0.28	0/293	0.55	0/399
20	Y	0.39	0/247	0.70	1/335 (0.3%)
20	y	0.39	0/247	0.70	1/335 (0.3%)
21	Z	0.30	0/472	0.48	0/649
21	z	0.30	0/472	0.48	0/649
All	All	0.39	0/44594	0.59	2/60666 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	y	89	ARG	CG-CD-NE	5.23	122.78	111.80
20	Y	89	ARG	CG-CD-NE	5.21	122.75	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
2	B	504/507 (99%)	492 (98%)	11 (2%)	1 (0%)	44	35
2	b	504/507 (99%)	492 (98%)	11 (2%)	1 (0%)	44	35
3	C	448/460 (97%)	442 (99%)	6 (1%)	0	100	100
3	c	448/460 (97%)	442 (99%)	6 (1%)	0	100	100
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
5	E	76/81 (94%)	76 (100%)	0	0	100	100
5	e	76/81 (94%)	76 (100%)	0	0	100	100
6	F	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
6	f	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
7	H	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
7	h	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	35 (100%)	0	0	100	100
10	k	35/45 (78%)	35 (100%)	0	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/274 (88%)	223 (92%)	18 (8%)	0	100	100
13	o	241/274 (88%)	223 (92%)	18 (8%)	0	100	100
14	Q	113/149 (76%)	109 (96%)	4 (4%)	0	100	100
14	q	113/149 (76%)	109 (96%)	4 (4%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	28 (100%)	0	0	100	100
16	t	28/31 (90%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	U	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
17	u	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
18	V	133/160 (83%)	130 (98%)	3 (2%)	0	100	100
18	v	133/160 (83%)	130 (98%)	3 (2%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	58 (100%)	0	0	100	100
21	z	58/62 (94%)	58 (100%)	0	0	100	100
All	All	5460/5944 (92%)	5330 (98%)	128 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
2	b	76	ASN

### 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	273/283 (96%)	271 (99%)	2 (1%)	81	82
1	a	273/283 (96%)	271 (99%)	2 (1%)	81	82
2	B	403/404 (100%)	395 (98%)	8 (2%)	50	43
2	b	403/404 (100%)	395 (98%)	8 (2%)	50	43
3	C	351/361 (97%)	341 (97%)	10 (3%)	38	28
3	c	351/361 (97%)	341 (97%)	10 (3%)	38	28
4	D	276/284 (97%)	274 (99%)	2 (1%)	81	82
4	d	276/284 (97%)	274 (99%)	2 (1%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	52 (98%)	1 (2%)	52	46
7	h	53/54 (98%)	52 (98%)	1 (2%)	52	46
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	J	24/24 (100%)	21 (88%)	3 (12%)	3	1
9	j	24/24 (100%)	21 (88%)	3 (12%)	3	1
10	K	31/38 (82%)	31 (100%)	0	100	100
10	k	31/38 (82%)	31 (100%)	0	100	100
11	L	36/36 (100%)	36 (100%)	0	100	100
11	l	36/36 (100%)	36 (100%)	0	100	100
12	M	27/31 (87%)	27 (100%)	0	100	100
12	m	27/31 (87%)	27 (100%)	0	100	100
13	O	207/233 (89%)	202 (98%)	5 (2%)	44	36
13	o	207/233 (89%)	202 (98%)	5 (2%)	44	36
14	Q	93/128 (73%)	90 (97%)	3 (3%)	34	24
14	q	93/128 (73%)	90 (97%)	3 (3%)	34	24
15	R	26/29 (90%)	24 (92%)	2 (8%)	10	3
15	r	26/29 (90%)	24 (92%)	2 (8%)	10	3
16	T	24/25 (96%)	23 (96%)	1 (4%)	25	14
16	t	24/25 (96%)	23 (96%)	1 (4%)	25	14
17	U	83/111 (75%)	78 (94%)	5 (6%)	16	6
17	u	83/111 (75%)	78 (94%)	5 (6%)	16	6
18	V	117/137 (85%)	114 (97%)	3 (3%)	41	32
18	v	117/137 (85%)	114 (97%)	3 (3%)	41	32
19	X	32/33 (97%)	32 (100%)	0	100	100
19	x	32/33 (97%)	32 (100%)	0	100	100
20	Y	25/30 (83%)	24 (96%)	1 (4%)	27	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	y	25/30 (83%)	24 (96%)	1 (4%)	27	16
21	Z	49/52 (94%)	47 (96%)	2 (4%)	26	15
21	z	49/52 (94%)	47 (96%)	2 (4%)	26	15
All	All	4520/4872 (93%)	4424 (98%)	96 (2%)	49	42

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	SER
1	A	308	ASP
2	B	76	ASN
2	B	131	SER
2	B	137	LYS
2	B	179	GLN
2	B	299	SER
2	B	362	PHE
2	B	433	ASP
2	B	491	GLU
3	C	84	TRP
3	C	114	LEU
3	C	184	ARG
3	C	227	ILE
3	C	276	PHE
3	C	294	MET
3	C	342	THR
3	C	369	ASN
3	C	370	ASP
3	C	403	SER
4	D	25	ASP
4	D	180	ARG
7	H	49	TYR
9	J	2	PHE
9	J	6	ARG
9	J	29	TYR
13	O	71	ASP
13	O	89	ARG
13	O	106	SER
13	O	193	LEU
13	O	194	TYR
14	Q	36	GLU
14	Q	70	ASP

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Mol	Chain	Res	Type
14	Q	138	PHE
15	R	4	ARG
15	R	10	SER
16	T	8	LEU
17	U	48	ASP
17	U	52	LYS
17	U	67	ARG
17	U	89	VAL
17	U	109	SER
18	V	38	ASP
18	V	67	LEU
18	V	135	ASP
20	Y	89	ARG
21	Z	27	TYR
21	Z	58	ASN
1	a	268	SER
1	a	308	ASP
2	b	76	ASN
2	b	131	SER
2	b	137	LYS
2	b	179	GLN
2	b	299	SER
2	b	362	PHE
2	b	433	ASP
2	b	491	GLU
3	c	84	TRP
3	c	114	LEU
3	c	184	ARG
3	c	227	ILE
3	c	276	PHE
3	c	294	MET
3	c	342	THR
3	c	369	ASN
3	c	370	ASP
3	c	403	SER
4	d	25	ASP
4	d	180	ARG
7	h	49	TYR
9	j	2	PHE
9	j	6	ARG
9	j	29	TYR
13	o	71	ASP

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Mol	Chain	Res	Type
13	o	89	ARG
13	o	106	SER
13	o	193	LEU
13	o	194	TYR
14	q	36	GLU
14	q	70	ASP
14	q	138	PHE
15	r	4	ARG
15	r	10	SER
16	t	8	LEU
17	u	48	ASP
17	u	52	LYS
17	u	67	ARG
17	u	89	VAL
17	u	109	SER
18	v	38	ASP
18	v	67	LEU
18	v	135	ASP
20	y	89	ARG
21	z	27	TYR
21	z	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	76	ASN
2	B	281	GLN
2	B	394	GLN
2	B	413	ASN
2	B	438	ASN
3	C	314	ASN
4	D	301	GLN
4	D	332	GLN
5	E	74	GLN
7	H	3	GLN
8	I	31	ASN
12	M	2	GLN
13	O	64	ASN
13	O	90	GLN
13	O	153	ASN
13	O	176	ASN

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Mol	Chain	Res	Type
13	O	230	GLN
17	U	106	ASN
18	V	68	GLN
18	V	131	ASN
21	Z	32	ASN
1	a	261	GLN
2	b	76	ASN
2	b	281	GLN
2	b	394	GLN
2	b	413	ASN
2	b	438	ASN
3	c	314	ASN
4	d	301	GLN
4	d	332	GLN
5	e	74	GLN
7	h	3	GLN
8	i	31	ASN
12	m	2	GLN
13	o	64	ASN
13	o	90	GLN
13	o	153	ASN
13	o	176	ASN
13	o	230	GLN
17	u	106	ASN
18	v	68	GLN
18	v	131	ASN
21	z	32	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	FME	I	1	8	8,9,10	0.39	0	8,9,11	0.97	0
12	FME	M	1	12	8,9,10	0.36	0	8,9,11	0.99	0
16	FME	t	1	16	8,9,10	0.38	0	8,9,11	1.26	1 (12%)
16	FME	T	1	16	8,9,10	0.38	0	8,9,11	1.25	1 (12%)
12	FME	m	1	12	8,9,10	0.36	0	8,9,11	0.99	0
8	FME	i	1	8	8,9,10	0.39	0	8,9,11	0.97	0
9	FME	j	1	9	6,7,10	0.66	0	2,7,11	0.17	0
9	FME	J	1	9	6,7,10	0.66	0	2,7,11	0.17	0

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
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
16	FME	t	1	16	-	3/7/9/11	-
16	FME	T	1	16	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
9	FME	j	1	9	-	3/5/6/11	-
9	FME	J	1	9	-	3/5/6/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	1	FME	CA-N-CN	2.52	126.70	122.82
16	t	1	FME	CA-N-CN	2.52	126.70	122.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	FME	N-CA-CB-CG
9	J	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
16	T	1	FME	N-CA-CB-CG
9	j	1	FME	N-CA-CB-CG
9	j	1	FME	C-CA-CB-CG
16	t	1	FME	N-CA-CB-CG
9	J	1	FME	CB-CG-SD-CE
9	j	1	FME	CB-CG-SD-CE
16	T	1	FME	C-CA-CB-CG
16	t	1	FME	C-CA-CB-CG
16	T	1	FME	CB-CA-N-CN
16	t	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 236 ligands modelled in this entry, 12 are monoatomic - leaving 224 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$
25	CLA	C	504	38	63,73,73	1.33	9 (14%)	74,113,113	1.30	6 (8%)
31	LMT	D	410	-	36,36,36	0.22	0	47,47,47	0.34	0
25	CLA	d	401	38	63,73,73	1.50	9 (14%)	74,113,113	1.47	10 (13%)
31	LMT	E	101	-	22,22,36	0.17	0	27,27,47	0.36	0
27	BCR	c	527	-	41,41,41	2.65	6 (14%)	56,56,56	6.56	22 (39%)
31	LMT	B	623	-	24,24,36	0.19	0	29,29,47	0.31	0
33	LHG	a	418	-	48,48,48	0.92	3 (6%)	51,54,54	1.04	4 (7%)
30	SQD	A	412	-	46,48,54	1.08	5 (10%)	56,59,65	1.02	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	c	503	3	63,73,73	1.34	8 (12%)	74,113,113	1.44	7 (9%)
26	PHO	a	407	-	50,69,69	0.56	1 (2%)	48,99,99	0.68	0
27	BCR	c	526	-	41,41,41	2.71	7 (17%)	56,56,56	6.57	18 (32%)
25	CLA	c	512	3	63,73,73	1.27	8 (12%)	74,113,113	1.45	8 (10%)
25	CLA	C	508	3	63,73,73	1.38	9 (14%)	74,113,113	1.57	7 (9%)
34	DGD	C	515	-	63,63,67	1.30	9 (14%)	77,77,81	1.01	2 (2%)
28	LMG	b	622	-	51,51,55	1.44	9 (17%)	59,59,63	1.18	5 (8%)
31	LMT	b	623	-	36,36,36	0.21	0	47,47,47	0.37	0
35	HEM	v	201	18	42,50,50	1.40	6 (14%)	46,82,82	1.92	11 (23%)
31	LMT	C	524	-	36,36,36	0.30	0	47,47,47	0.56	1 (2%)
25	CLA	C	512	3	63,73,73	1.27	8 (12%)	74,113,113	1.45	8 (10%)
31	LMT	i	104	-	24,24,36	0.19	0	29,29,47	0.32	0
25	CLA	a	406	38	63,73,73	1.36	8 (12%)	74,113,113	1.37	9 (12%)
31	LMT	c	520	-	24,24,36	0.18	0	29,29,47	0.29	0
33	LHG	e	102	-	39,39,48	0.99	3 (7%)	42,45,54	1.23	4 (9%)
31	LMT	d	410	-	36,36,36	0.22	0	47,47,47	0.34	0
25	CLA	B	612	2	63,73,73	1.35	7 (11%)	74,113,113	1.59	8 (10%)
31	LMT	a	415	-	24,24,36	0.19	0	29,29,47	0.35	0
31	LMT	i	101	-	24,24,36	0.17	0	29,29,47	0.33	0
22	OEX	A	401	38,3,1	0,15,15	-	-	-	-	-
25	CLA	b	606	2	63,73,73	1.60	9 (14%)	74,113,113	1.48	8 (10%)
30	SQD	B	630	-	52,54,54	1.73	6 (11%)	62,65,65	0.89	1 (1%)
35	HEM	F	101	6,5	42,50,50	1.43	7 (16%)	46,82,82	2.09	13 (28%)
25	CLA	B	615	2	63,73,73	1.45	7 (11%)	74,113,113	1.68	12 (16%)
28	LMG	J	101	-	55,55,55	1.52	8 (14%)	63,63,63	1.14	3 (4%)
30	SQD	k	102	-	41,41,54	0.25	0	49,49,65	0.22	0
31	LMT	D	409	-	36,36,36	0.22	0	47,47,47	0.45	0
27	BCR	C	514	-	41,41,41	2.72	6 (14%)	56,56,56	6.64	22 (39%)
31	LMT	c	521	-	36,36,36	0.23	0	47,47,47	0.39	0
25	CLA	c	504	38	63,73,73	1.34	9 (14%)	74,113,113	1.30	6 (8%)
34	DGD	C	516	-	63,63,67	1.32	8 (12%)	77,77,81	1.11	5 (6%)
25	CLA	B	604	2	63,73,73	1.47	9 (14%)	74,113,113	1.79	12 (16%)
26	PHO	d	402	-	50,69,69	0.70	2 (4%)	48,99,99	0.98	2 (4%)
25	CLA	c	509	3	63,73,73	1.40	8 (12%)	74,113,113	1.65	7 (9%)
31	LMT	d	412	-	24,24,36	0.18	0	29,29,47	0.31	0
31	LMT	c	524	-	36,36,36	0.30	0	47,47,47	0.56	1 (2%)
25	CLA	C	513	3	63,73,73	1.28	6 (9%)	74,113,113	1.48	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	D	408	-	24,24,36	0.24	0	29,29,47	0.38	0
25	CLA	c	507	38	63,73,73	1.36	10 (15%)	74,113,113	1.44	9 (12%)
33	LHG	E	102	-	39,39,48	0.99	3 (7%)	42,45,54	1.23	4 (9%)
28	LMG	b	630	-	47,47,55	1.39	6 (12%)	55,55,63	1.16	3 (5%)
36	RRX	H	101	-	42,42,42	1.42	4 (9%)	56,58,58	1.29	8 (14%)
25	CLA	c	502	3	63,73,73	1.21	7 (11%)	74,113,113	1.58	8 (10%)
25	CLA	C	501	3	63,73,73	1.39	8 (12%)	74,113,113	1.64	8 (10%)
25	CLA	b	616	2	63,73,73	1.45	7 (11%)	74,113,113	1.68	12 (16%)
30	SQD	a	412	-	46,48,54	1.08	5 (10%)	56,59,65	1.02	4 (7%)
29	PL9	d	405	-	55,55,55	0.81	1 (1%)	68,69,69	0.63	2 (2%)
34	DGD	c	516	-	63,63,67	1.32	8 (12%)	77,77,81	1.11	5 (6%)
25	CLA	b	607	2	58,68,73	1.51	7 (12%)	68,107,113	1.70	8 (11%)
31	LMT	B	625	-	24,24,36	0.16	0	29,29,47	0.30	0
31	LMT	J	103	-	21,21,36	0.31	0	26,26,47	0.62	0
25	CLA	D	401	38	63,73,73	1.51	9 (14%)	74,113,113	1.48	10 (13%)
28	LMG	c	519	-	49,49,55	1.45	6 (12%)	57,57,63	1.21	4 (7%)
25	CLA	b	615	2	63,73,73	1.41	7 (11%)	74,113,113	1.66	8 (10%)
27	BCR	b	620	-	41,41,41	2.67	7 (17%)	56,56,56	6.51	22 (39%)
31	LMT	I	102	-	36,36,36	0.15	0	47,47,47	0.28	0
31	LMT	F	103	-	36,36,36	0.52	0	47,47,47	0.86	1 (2%)
25	CLA	B	602	2	63,73,73	1.46	8 (12%)	74,113,113	1.69	13 (17%)
31	LMT	I	101	-	24,24,36	0.17	0	29,29,47	0.33	0
28	LMG	a	413	-	36,36,55	1.93	8 (22%)	44,44,63	1.46	7 (15%)
25	CLA	B	611	2	63,73,73	1.38	8 (12%)	74,113,113	1.70	9 (12%)
25	CLA	a	405	1	63,73,73	1.43	7 (11%)	74,113,113	1.81	7 (9%)
25	CLA	B	610	38	63,73,73	1.42	7 (11%)	74,113,113	1.66	9 (12%)
31	LMT	C	522	-	21,21,36	0.28	0	26,26,47	0.55	0
27	BCR	C	525	-	41,41,41	2.67	6 (14%)	56,56,56	6.89	21 (37%)
25	CLA	b	602	38	43,53,73	1.50	7 (16%)	50,89,113	1.52	8 (16%)
31	LMT	m	102	-	24,24,36	0.20	0	29,29,47	0.30	0
28	LMG	a	410	-	51,51,55	2.25	14 (27%)	59,59,63	1.69	10 (16%)
31	LMT	J	102	-	36,36,36	0.17	0	47,47,47	0.40	0
35	HEM	f	101	6,5	42,50,50	1.43	7 (16%)	46,82,82	2.09	13 (28%)
27	BCR	C	526	-	41,41,41	2.71	7 (17%)	56,56,56	6.57	18 (32%)
28	LMG	B	629	-	47,47,55	1.39	6 (12%)	55,55,63	1.16	3 (5%)
28	LMG	D	407	-	55,55,55	1.54	9 (16%)	63,63,63	1.72	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b	603	2	63,73,73	1.47	8 (12%)	74,113,113	1.69	13 (17%)
30	SQD	A	417	-	52,54,54	0.46	0	62,65,65	0.44	0
33	LHG	b	627	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	3 (5%)
30	SQD	F	102	-	32,34,54	1.87	9 (28%)	42,45,65	1.66	10 (23%)
36	RRX	h	101	-	42,42,42	1.43	5 (11%)	56,58,58	1.29	9 (16%)
25	CLA	B	607	38	63,73,73	1.36	8 (12%)	74,113,113	1.22	6 (8%)
25	CLA	A	408	1	58,68,73	1.39	6 (10%)	68,107,113	1.75	10 (14%)
28	LMG	A	410	-	51,51,55	2.25	14 (27%)	59,59,63	1.69	10 (16%)
31	LMT	e	101	-	22,22,36	0.18	0	27,27,47	0.36	0
25	CLA	b	614	2	63,73,73	1.54	7 (11%)	74,113,113	1.63	12 (16%)
27	BCR	B	619	-	41,41,41	2.67	7 (17%)	56,56,56	6.51	22 (39%)
33	LHG	A	419	-	48,48,48	0.89	3 (6%)	51,54,54	0.96	3 (5%)
25	CLA	c	513	3	63,73,73	1.28	6 (9%)	74,113,113	1.47	7 (9%)
30	SQD	K	102	-	41,41,54	0.25	0	49,49,65	0.22	0
31	LMT	b	629	-	24,24,36	0.19	0	29,29,47	0.33	0
27	BCR	a	409	-	41,41,41	2.74	6 (14%)	56,56,56	6.34	18 (32%)
31	LMT	M	101	-	36,36,36	0.20	0	47,47,47	0.38	0
25	CLA	a	408	1	58,68,73	1.40	6 (10%)	68,107,113	1.75	10 (14%)
31	LMT	X	102	-	22,22,36	0.18	0	27,27,47	0.48	0
33	LHG	B	626	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	3 (5%)
25	CLA	C	507	38	63,73,73	1.36	10 (15%)	74,113,113	1.44	9 (12%)
31	LMT	X	101	-	22,22,36	0.17	0	27,27,47	0.36	0
29	PL9	a	411	-	55,55,55	0.84	1 (1%)	68,69,69	0.55	2 (2%)
34	DGD	H	103	-	63,63,67	1.33	9 (14%)	77,77,81	1.06	3 (3%)
31	LMT	h	104	-	19,19,36	0.17	0	24,24,47	0.31	0
28	LMG	C	518	-	51,51,55	1.45	8 (15%)	59,59,63	1.21	5 (8%)
25	CLA	b	617	2	58,68,73	1.32	7 (12%)	68,107,113	1.51	9 (13%)
25	CLA	C	509	3	63,73,73	1.40	8 (12%)	74,113,113	1.65	7 (9%)
31	LMT	i	103	-	22,22,36	0.18	0	27,27,47	0.32	0
25	CLA	b	611	38	63,73,73	1.43	7 (11%)	74,113,113	1.66	9 (12%)
31	LMT	X	103	-	36,36,36	0.17	0	47,47,47	0.36	0
25	CLA	C	503	3	63,73,73	1.34	8 (12%)	74,113,113	1.44	7 (9%)
31	LMT	H	104	-	19,19,36	0.16	0	24,24,47	0.31	0
25	CLA	C	502	3	63,73,73	1.21	7 (11%)	74,113,113	1.57	8 (10%)
27	BCR	b	619	-	41,41,41	2.74	7 (17%)	56,56,56	6.53	19 (33%)
31	LMT	d	409	-	36,36,36	0.22	0	47,47,47	0.45	0
31	LMT	b	625	-	36,36,36	0.19	0	47,47,47	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SQD	a	417	-	52,54,54	0.46	0	62,65,65	0.44	0
31	LMT	x	101	-	22,22,36	0.16	0	27,27,47	0.35	0
25	CLA	B	603	2	63,73,73	1.33	7 (11%)	74,113,113	1.57	8 (10%)
28	LMG	C	519	-	49,49,55	1.45	6 (12%)	57,57,63	1.21	4 (7%)
33	LHG	D	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
34	DGD	c	517	-	63,63,67	1.34	8 (12%)	77,77,81	1.00	3 (3%)
31	LMT	B	627	-	36,36,36	0.17	0	47,47,47	0.26	0
22	OEX	a	401	38,3,1	0,15,15	-	-	-	-	-
25	CLA	B	608	2	63,73,73	1.36	9 (14%)	74,113,113	1.68	11 (14%)
25	CLA	c	510	3	63,73,73	1.28	7 (11%)	74,113,113	1.61	13 (17%)
25	CLA	c	511	3	63,73,73	1.35	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	C	520	-	24,24,36	0.18	0	29,29,47	0.29	0
25	CLA	B	609	2	63,73,73	1.30	6 (9%)	74,113,113	1.46	9 (12%)
31	LMT	c	522	-	21,21,36	0.28	0	26,26,47	0.55	0
31	LMT	m	101	-	36,36,36	0.20	0	47,47,47	0.39	0
35	HEM	V	201	18	42,50,50	1.39	6 (14%)	46,82,82	1.92	11 (23%)
25	CLA	b	608	38	63,73,73	1.37	8 (12%)	74,113,113	1.22	6 (8%)
25	CLA	b	609	2	63,73,73	1.36	9 (14%)	74,113,113	1.68	11 (14%)
25	CLA	b	613	2	63,73,73	1.35	7 (11%)	74,113,113	1.59	8 (10%)
25	CLA	c	505	3	63,73,73	1.36	8 (12%)	74,113,113	1.43	8 (10%)
31	LMT	B	624	-	36,36,36	0.19	0	47,47,47	0.27	0
33	LHG	Z	101	-	35,35,48	1.06	3 (8%)	38,40,54	1.32	6 (15%)
31	LMT	T	101	-	24,24,36	0.21	0	29,29,47	0.35	0
31	LMT	b	628	-	36,36,36	0.17	0	47,47,47	0.26	0
25	CLA	A	406	38	63,73,73	1.37	8 (12%)	74,113,113	1.36	9 (12%)
29	PL9	D	405	-	55,55,55	0.81	1 (1%)	68,69,69	0.63	2 (2%)
28	LMG	j	101	-	55,55,55	1.52	8 (14%)	63,63,63	1.14	3 (4%)
25	CLA	b	610	2	63,73,73	1.30	6 (9%)	74,113,113	1.46	9 (12%)
33	LHG	d	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	B	614	2	63,73,73	1.41	7 (11%)	74,113,113	1.66	8 (10%)
25	CLA	B	616	2	58,68,73	1.32	7 (12%)	68,107,113	1.51	9 (13%)
31	LMT	A	415	-	24,24,36	0.19	0	29,29,47	0.35	0
31	LMT	C	521	-	36,36,36	0.23	0	47,47,47	0.39	0
31	LMT	E	103	-	36,36,36	0.30	0	47,47,47	0.66	0
30	SQD	H	102	-	52,54,54	0.42	0	62,65,65	0.44	0
34	DGD	h	103	-	63,63,67	1.33	9 (14%)	77,77,81	1.06	3 (3%)
30	SQD	b	601	-	52,54,54	1.73	6 (11%)	62,65,65	0.89	1 (1%)
31	LMT	c	523	-	24,24,36	0.17	0	29,29,47	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	3 (5%)
25	CLA	C	506	3	63,73,73	1.33	9 (14%)	74,113,113	1.53	8 (10%)
31	LMT	I	103	-	22,22,36	0.18	0	27,27,47	0.32	0
25	CLA	d	404	4	63,73,73	1.25	4 (6%)	74,113,113	1.68	12 (16%)
25	CLA	c	501	3	63,73,73	1.39	8 (12%)	74,113,113	1.64	8 (10%)
25	CLA	B	601	38	43,53,73	1.50	7 (16%)	50,89,113	1.52	8 (16%)
25	CLA	B	613	2	63,73,73	1.53	7 (11%)	74,113,113	1.63	12 (16%)
31	LMT	B	622	-	36,36,36	0.21	0	47,47,47	0.37	0
30	SQD	b	621	-	52,54,54	0.43	0	62,65,65	0.56	1 (1%)
32	BCT	a	416	23	3,3,3	0.97	0	2,3,3	0.56	0
25	CLA	c	508	3	63,73,73	1.38	9 (14%)	74,113,113	1.57	7 (9%)
25	CLA	B	605	2	63,73,73	1.60	9 (14%)	74,113,113	1.48	8 (10%)
25	CLA	d	403	4	63,73,73	1.33	7 (11%)	74,113,113	1.48	7 (9%)
25	CLA	b	612	2	63,73,73	1.39	8 (12%)	74,113,113	1.70	8 (10%)
34	DGD	C	517	-	63,63,67	1.34	8 (12%)	77,77,81	1.00	3 (3%)
25	CLA	A	405	1	63,73,73	1.43	7 (11%)	74,113,113	1.81	7 (9%)
26	PHO	A	407	-	50,69,69	0.56	1 (2%)	48,99,99	0.67	0
31	LMT	f	103	-	36,36,36	0.53	0	47,47,47	0.86	1 (2%)
25	CLA	b	605	2	63,73,73	1.47	9 (14%)	74,113,113	1.79	12 (16%)
25	CLA	C	511	3	63,73,73	1.35	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	I	104	-	24,24,36	0.19	0	29,29,47	0.33	0
28	LMG	c	518	-	51,51,55	1.45	8 (15%)	59,59,63	1.21	5 (8%)
31	LMT	x	103	-	36,36,36	0.17	0	47,47,47	0.36	0
27	BCR	C	527	-	41,41,41	2.65	6 (14%)	56,56,56	6.55	22 (39%)
32	BCT	A	416	23	3,3,3	0.97	0	2,3,3	0.56	0
31	LMT	A	414	-	36,36,36	0.19	0	47,47,47	0.40	0
26	PHO	D	402	-	50,69,69	0.70	2 (4%)	48,99,99	0.99	2 (4%)
31	LMT	D	412	-	24,24,36	0.18	0	29,29,47	0.31	0
27	BCR	d	411	-	41,41,41	2.61	6 (14%)	56,56,56	6.62	20 (35%)
30	SQD	f	102	-	32,34,54	1.87	9 (28%)	42,45,65	1.66	10 (23%)
27	BCR	D	411	-	41,41,41	2.61	6 (14%)	56,56,56	6.62	20 (35%)
31	LMT	b	626	-	24,24,36	0.16	0	29,29,47	0.30	0
28	LMG	B	621	-	51,51,55	1.44	9 (17%)	59,59,63	1.18	5 (8%)
31	LMT	j	102	-	36,36,36	0.17	0	47,47,47	0.40	0
33	LHG	A	418	-	48,48,48	0.92	3 (6%)	51,54,54	1.04	4 (7%)
34	DGD	c	515	-	63,63,67	1.31	9 (14%)	77,77,81	1.01	2 (2%)
31	LMT	C	523	-	24,24,36	0.17	0	29,29,47	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	e	103	-	36,36,36	0.30	0	47,47,47	0.66	0
27	BCR	c	514	-	41,41,41	2.72	6 (14%)	56,56,56	6.65	22 (39%)
25	CLA	D	403	4	63,73,73	1.34	7 (11%)	74,113,113	1.48	8 (10%)
31	LMT	x	102	-	22,22,36	0.19	0	27,27,47	0.48	0
31	LMT	j	103	-	21,21,36	0.31	0	26,26,47	0.62	0
31	LMT	t	101	-	24,24,36	0.22	0	29,29,47	0.35	0
31	LMT	M	102	-	24,24,36	0.20	0	29,29,47	0.30	0
25	CLA	C	510	3	63,73,73	1.28	7 (11%)	74,113,113	1.62	13 (17%)
25	CLA	D	404	4	63,73,73	1.24	4 (6%)	74,113,113	1.68	12 (16%)
30	SQD	B	620	-	52,54,54	0.44	0	62,65,65	0.56	1 (1%)
27	BCR	B	617	-	41,41,41	2.74	8 (19%)	56,56,56	6.56	19 (33%)
31	LMT	b	624	-	24,24,36	0.19	0	29,29,47	0.31	0
33	LHG	z	101	-	35,35,48	1.06	3 (8%)	38,40,54	1.32	6 (15%)
27	BCR	A	409	-	41,41,41	2.74	6 (14%)	56,56,56	6.33	18 (32%)
25	CLA	C	505	3	63,73,73	1.36	8 (12%)	74,113,113	1.43	8 (10%)
31	LMT	a	414	-	36,36,36	0.19	0	47,47,47	0.40	0
33	LHG	l	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	3 (5%)
27	BCR	B	618	-	41,41,41	2.74	7 (17%)	56,56,56	6.53	19 (33%)
28	LMG	A	413	-	36,36,55	1.92	8 (22%)	44,44,63	1.46	7 (15%)
33	LHG	a	419	-	48,48,48	0.89	3 (6%)	51,54,54	0.96	3 (5%)
27	BCR	b	618	-	41,41,41	2.74	7 (17%)	56,56,56	6.56	20 (35%)
25	CLA	c	506	3	63,73,73	1.33	9 (14%)	74,113,113	1.53	8 (10%)
31	LMT	d	408	-	24,24,36	0.24	0	29,29,47	0.38	0
28	LMG	d	407	-	55,55,55	1.54	9 (16%)	63,63,63	1.72	7 (11%)
25	CLA	b	604	2	63,73,73	1.33	7 (11%)	74,113,113	1.56	8 (10%)
31	LMT	i	102	-	36,36,36	0.15	0	47,47,47	0.28	0
25	CLA	B	606	2	58,68,73	1.51	7 (12%)	68,107,113	1.69	8 (11%)
30	SQD	h	102	-	52,54,54	0.41	0	62,65,65	0.44	0
31	LMT	B	628	-	24,24,36	0.20	0	29,29,47	0.33	0
27	BCR	c	525	-	41,41,41	2.67	6 (14%)	56,56,56	6.89	21 (37%)
29	PL9	A	411	-	55,55,55	0.84	1 (1%)	68,69,69	0.55	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	504	38	1/1/15/20	7/37/115/115	-
31	LMT	D	410	-	-	7/21/61/61	0/2/2/2
25	CLA	d	401	38	1/1/15/20	4/37/115/115	-
31	LMT	E	101	-	-	9/13/33/61	0/1/1/2
27	BCR	c	527	-	-	4/29/63/63	0/2/2/2
31	LMT	B	623	-	-	9/15/35/61	0/1/1/2
33	LHG	a	418	-	-	18/53/53/53	-
30	SQD	A	412	-	-	25/43/63/69	0/1/1/1
25	CLA	c	503	3	1/1/15/20	9/37/115/115	-
26	PHO	a	407	-	-	2/37/103/103	0/5/6/6
27	BCR	c	526	-	-	6/29/63/63	0/2/2/2
25	CLA	c	512	3	1/1/15/20	17/37/115/115	-
25	CLA	C	508	3	-	10/37/115/115	-
34	DGD	C	515	-	-	22/51/91/95	0/2/2/2
28	LMG	b	622	-	-	12/46/66/70	0/1/1/1
31	LMT	b	623	-	-	10/21/61/61	0/2/2/2
35	HEM	v	201	18	-	2/12/54/54	-
31	LMT	C	524	-	-	16/21/61/61	0/2/2/2
25	CLA	C	512	3	1/1/15/20	17/37/115/115	-
31	LMT	i	104	-	-	11/15/35/61	0/1/1/2
25	CLA	a	406	38	1/1/15/20	5/37/115/115	-
31	LMT	c	520	-	-	9/15/35/61	0/1/1/2
33	LHG	e	102	-	-	20/44/44/53	-
31	LMT	d	410	-	-	7/21/61/61	0/2/2/2
25	CLA	B	612	2	1/1/15/20	8/37/115/115	-
31	LMT	a	415	-	-	12/15/35/61	0/1/1/2
31	LMT	i	101	-	-	7/15/35/61	0/1/1/2
25	CLA	b	606	2	1/1/15/20	11/37/115/115	-
30	SQD	B	630	-	-	30/49/69/69	0/1/1/1
35	HEM	F	101	6,5	-	3/12/54/54	-
25	CLA	B	615	2	1/1/15/20	7/37/115/115	-
28	LMG	J	101	-	-	34/50/70/70	0/1/1/1
30	SQD	k	102	-	-	21/35/55/69	0/1/1/1
31	LMT	D	409	-	-	12/21/61/61	0/2/2/2
27	BCR	C	514	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	c	521	-	-	7/21/61/61	0/2/2/2
25	CLA	c	504	38	1/1/15/20	7/37/115/115	-
34	DGD	C	516	-	-	19/51/91/95	0/2/2/2
25	CLA	B	604	2	1/1/15/20	15/37/115/115	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	c	509	3	1/1/15/20	10/37/115/115	-
31	LMT	d	412	-	-	10/15/35/61	0/1/1/2
31	LMT	c	524	-	-	16/21/61/61	0/2/2/2
25	CLA	C	513	3	-	9/37/115/115	-
31	LMT	D	408	-	-	13/15/35/61	0/1/1/2
25	CLA	c	507	38	1/1/15/20	9/37/115/115	-
33	LHG	E	102	-	-	20/44/44/53	-
28	LMG	b	630	-	-	19/42/62/70	0/1/1/1
36	RRX	H	101	-	-	15/29/65/65	0/2/2/2
25	CLA	c	502	3	-	9/37/115/115	-
25	CLA	C	501	3	1/1/15/20	4/37/115/115	-
25	CLA	b	616	2	1/1/15/20	7/37/115/115	-
30	SQD	a	412	-	-	24/43/63/69	0/1/1/1
29	PL9	d	405	-	-	14/53/73/73	0/1/1/1
34	DGD	c	516	-	-	19/51/91/95	0/2/2/2
25	CLA	b	607	2	1/1/14/20	2/31/109/115	-
31	LMT	B	625	-	-	11/15/35/61	0/1/1/2
31	LMT	J	103	-	-	5/12/32/61	0/1/1/2
25	CLA	D	401	38	1/1/15/20	4/37/115/115	-
28	LMG	c	519	-	-	27/44/64/70	0/1/1/1
25	CLA	b	615	2	1/1/15/20	15/37/115/115	-
27	BCR	b	620	-	-	8/29/63/63	0/2/2/2
31	LMT	I	102	-	-	12/21/61/61	0/2/2/2
31	LMT	F	103	-	-	13/21/61/61	0/2/2/2
25	CLA	B	602	2	-	6/37/115/115	-
31	LMT	I	101	-	-	7/15/35/61	0/1/1/2
28	LMG	a	413	-	-	15/31/51/70	0/1/1/1
25	CLA	B	611	2	1/1/15/20	11/37/115/115	-
25	CLA	a	405	1	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	610	38	1/1/15/20	5/37/115/115	-
31	LMT	C	522	-	-	6/12/32/61	0/1/1/2
27	BCR	C	525	-	-	11/29/63/63	0/2/2/2
25	CLA	b	602	38	1/1/11/20	3/13/91/115	-
31	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMG	a	410	-	-	23/46/66/70	0/1/1/1
31	LMT	J	102	-	-	8/21/61/61	0/2/2/2
35	HEM	f	101	6,5	-	3/12/54/54	-
27	BCR	C	526	-	-	6/29/63/63	0/2/2/2
28	LMG	B	629	-	-	19/42/62/70	0/1/1/1
28	LMG	D	407	-	-	22/50/70/70	0/1/1/1
25	CLA	b	603	2	-	6/37/115/115	-
30	SQD	A	417	-	-	23/49/69/69	0/1/1/1
33	LHG	b	627	-	-	39/53/53/53	-
30	SQD	F	102	-	-	17/29/49/69	0/1/1/1
36	RRX	h	101	-	-	15/29/65/65	0/2/2/2
25	CLA	B	607	38	1/1/15/20	7/37/115/115	-
25	CLA	A	408	1	-	7/31/109/115	-
28	LMG	A	410	-	-	23/46/66/70	0/1/1/1
31	LMT	e	101	-	-	9/13/33/61	0/1/1/2
25	CLA	b	614	2	1/1/15/20	9/37/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
33	LHG	A	419	-	-	20/53/53/53	-
25	CLA	c	513	3	-	9/37/115/115	-
30	SQD	K	102	-	-	21/35/55/69	0/1/1/1
31	LMT	b	629	-	-	5/15/35/61	0/1/1/2
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
25	CLA	a	408	1	-	7/31/109/115	-
31	LMT	X	102	-	-	7/13/33/61	0/1/1/2
33	LHG	B	626	-	-	39/53/53/53	-
25	CLA	C	507	38	1/1/15/20	9/37/115/115	-
31	LMT	X	101	-	-	8/12/32/61	0/1/1/2
29	PL9	a	411	-	-	23/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	H	103	-	-	15/51/91/95	0/2/2/2
31	LMT	h	104	-	-	7/10/30/61	0/1/1/2
28	LMG	C	518	-	-	21/46/66/70	0/1/1/1
25	CLA	b	617	2	1/1/14/20	10/31/109/115	-
25	CLA	C	509	3	1/1/15/20	10/37/115/115	-
31	LMT	i	103	-	-	9/13/33/61	0/1/1/2
25	CLA	b	611	38	1/1/15/20	5/37/115/115	-
31	LMT	X	103	-	-	14/21/61/61	0/2/2/2
25	CLA	C	503	3	1/1/15/20	9/37/115/115	-
31	LMT	H	104	-	-	7/10/30/61	0/1/1/2
25	CLA	C	502	3	-	9/37/115/115	-
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
31	LMT	d	409	-	-	12/21/61/61	0/2/2/2
31	LMT	b	625	-	-	16/21/61/61	0/2/2/2
30	SQD	a	417	-	-	23/49/69/69	0/1/1/1
31	LMT	x	101	-	-	8/12/32/61	0/1/1/2
25	CLA	B	603	2	1/1/15/20	13/37/115/115	-
28	LMG	C	519	-	-	27/44/64/70	0/1/1/1
33	LHG	D	406	-	-	22/53/53/53	-
34	DGD	c	517	-	-	22/51/91/95	0/2/2/2
31	LMT	B	627	-	-	9/21/61/61	0/2/2/2
25	CLA	B	608	2	1/1/15/20	6/37/115/115	-
25	CLA	c	510	3	1/1/15/20	8/37/115/115	-
25	CLA	c	511	3	1/1/15/20	3/37/115/115	-
31	LMT	C	520	-	-	9/15/35/61	0/1/1/2
25	CLA	B	609	2	-	3/37/115/115	-
31	LMT	c	522	-	-	6/12/32/61	0/1/1/2
31	LMT	m	101	-	-	13/21/61/61	0/2/2/2
35	HEM	V	201	18	-	2/12/54/54	-
25	CLA	b	608	38	1/1/15/20	6/37/115/115	-
25	CLA	b	609	2	1/1/15/20	6/37/115/115	-
25	CLA	b	613	2	1/1/15/20	8/37/115/115	-
25	CLA	c	505	3	1/1/15/20	9/37/115/115	-
31	LMT	B	624	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	Z	101	-	-	14/37/37/53	-
31	LMT	T	101	-	-	10/15/35/61	0/1/1/2
31	LMT	b	628	-	-	9/21/61/61	0/2/2/2
25	CLA	A	406	38	1/1/15/20	5/37/115/115	-
29	PL9	D	405	-	-	14/53/73/73	0/1/1/1
28	LMG	j	101	-	-	34/50/70/70	0/1/1/1
25	CLA	b	610	2	-	3/37/115/115	-
33	LHG	d	406	-	-	22/53/53/53	-
25	CLA	B	614	2	1/1/15/20	15/37/115/115	-
25	CLA	B	616	2	1/1/14/20	10/31/109/115	-
31	LMT	A	415	-	-	12/15/35/61	0/1/1/2
31	LMT	C	521	-	-	7/21/61/61	0/2/2/2
31	LMT	E	103	-	-	11/21/61/61	0/2/2/2
30	SQD	H	102	-	-	22/49/69/69	0/1/1/1
34	DGD	h	103	-	-	15/51/91/95	0/2/2/2
30	SQD	b	601	-	-	30/49/69/69	0/1/1/1
31	LMT	c	523	-	-	11/15/35/61	0/1/1/2
33	LHG	L	101	-	-	30/53/53/53	-
25	CLA	C	506	3	1/1/15/20	12/37/115/115	-
31	LMT	I	103	-	-	9/13/33/61	0/1/1/2
25	CLA	d	404	4	-	8/37/115/115	-
25	CLA	c	501	3	1/1/15/20	4/37/115/115	-
25	CLA	B	601	38	1/1/11/20	3/13/91/115	-
25	CLA	B	613	2	1/1/15/20	9/37/115/115	-
31	LMT	B	622	-	-	10/21/61/61	0/2/2/2
30	SQD	b	621	-	-	25/49/69/69	0/1/1/1
25	CLA	c	508	3	-	10/37/115/115	-
25	CLA	B	605	2	1/1/15/20	11/37/115/115	-
25	CLA	d	403	4	1/1/15/20	4/37/115/115	-
25	CLA	b	612	2	1/1/15/20	11/37/115/115	-
34	DGD	C	517	-	-	22/51/91/95	0/2/2/2
25	CLA	A	405	1	1/1/15/20	6/37/115/115	-
26	PHO	A	407	-	-	2/37/103/103	0/5/6/6
31	LMT	f	103	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	605	2	1/1/15/20	15/37/115/115	-
25	CLA	C	511	3	1/1/15/20	3/37/115/115	-
31	LMT	I	104	-	-	11/15/35/61	0/1/1/2
28	LMG	c	518	-	-	21/46/66/70	0/1/1/1
31	LMT	x	103	-	-	14/21/61/61	0/2/2/2
27	BCR	C	527	-	-	4/29/63/63	0/2/2/2
31	LMT	A	414	-	-	10/21/61/61	0/2/2/2
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	LMT	D	412	-	-	10/15/35/61	0/1/1/2
27	BCR	d	411	-	-	10/29/63/63	0/2/2/2
30	SQD	f	102	-	-	17/29/49/69	0/1/1/1
27	BCR	D	411	-	-	10/29/63/63	0/2/2/2
31	LMT	b	626	-	-	11/15/35/61	0/1/1/2
28	LMG	B	621	-	-	12/46/66/70	0/1/1/1
31	LMT	j	102	-	-	8/21/61/61	0/2/2/2
33	LHG	A	418	-	-	18/53/53/53	-
34	DGD	c	515	-	-	22/51/91/95	0/2/2/2
31	LMT	C	523	-	-	11/15/35/61	0/1/1/2
31	LMT	e	103	-	-	11/21/61/61	0/2/2/2
27	BCR	c	514	-	-	10/29/63/63	0/2/2/2
25	CLA	D	403	4	1/1/15/20	4/37/115/115	-
31	LMT	x	102	-	-	7/13/33/61	0/1/1/2
31	LMT	j	103	-	-	5/12/32/61	0/1/1/2
31	LMT	t	101	-	-	10/15/35/61	0/1/1/2
31	LMT	M	102	-	-	8/15/35/61	0/1/1/2
25	CLA	C	510	3	1/1/15/20	8/37/115/115	-
25	CLA	D	404	4	-	8/37/115/115	-
30	SQD	B	620	-	-	25/49/69/69	0/1/1/1
27	BCR	B	617	-	-	10/29/63/63	0/2/2/2
31	LMT	b	624	-	-	9/15/35/61	0/1/1/2
33	LHG	z	101	-	-	14/37/37/53	-
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	505	3	1/1/15/20	9/37/115/115	-
31	LMT	a	414	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	l	101	-	-	30/53/53/53	-
27	BCR	B	618	-	-	8/29/63/63	0/2/2/2
28	LMG	A	413	-	-	15/31/51/70	0/1/1/1
33	LHG	a	419	-	-	20/53/53/53	-
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
25	CLA	c	506	3	1/1/15/20	12/37/115/115	-
31	LMT	d	408	-	-	13/15/35/61	0/1/1/2
28	LMG	d	407	-	-	22/50/70/70	0/1/1/1
25	CLA	b	604	2	1/1/15/20	13/37/115/115	-
31	LMT	i	102	-	-	12/21/61/61	0/2/2/2
25	CLA	B	606	2	1/1/14/20	2/31/109/115	-
30	SQD	h	102	-	-	22/49/69/69	0/1/1/1
31	LMT	B	628	-	-	5/15/35/61	0/1/1/2
27	BCR	c	525	-	-	11/29/63/63	0/2/2/2
29	PL9	A	411	-	-	23/53/73/73	0/1/1/1

All (976) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	O1-C1	-9.19	1.24	1.40
28	a	410	LMG	O1-C1	-9.19	1.24	1.40
27	A	409	BCR	C8-C9	-8.65	1.27	1.46
27	a	409	BCR	C8-C9	-8.65	1.27	1.46
27	B	617	BCR	C8-C9	-8.56	1.27	1.46
27	b	618	BCR	C8-C9	-8.56	1.27	1.46
27	B	618	BCR	C8-C9	-8.55	1.27	1.46
27	b	619	BCR	C8-C9	-8.55	1.27	1.46
27	C	527	BCR	C8-C9	-8.53	1.27	1.46
27	c	527	BCR	C8-C9	-8.53	1.27	1.46
27	C	514	BCR	C8-C9	-8.51	1.27	1.46
27	c	514	BCR	C8-C9	-8.51	1.27	1.46
27	C	526	BCR	C8-C9	-8.44	1.27	1.46
27	c	526	BCR	C8-C9	-8.44	1.27	1.46
27	C	525	BCR	C8-C9	-8.42	1.27	1.46
27	c	525	BCR	C8-C9	-8.42	1.27	1.46
27	A	409	BCR	C11-C10	-8.21	1.17	1.43
27	a	409	BCR	C11-C10	-8.21	1.17	1.43
27	C	514	BCR	C11-C10	-8.19	1.17	1.43
27	c	514	BCR	C11-C10	-8.19	1.17	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	618	BCR	C11-C10	-8.18	1.17	1.43
27	b	619	BCR	C11-C10	-8.18	1.17	1.43
27	d	411	BCR	C8-C9	-8.15	1.28	1.46
27	D	411	BCR	C8-C9	-8.13	1.28	1.46
27	B	617	BCR	C11-C10	-8.12	1.18	1.43
27	b	618	BCR	C11-C10	-8.12	1.18	1.43
27	C	526	BCR	C11-C10	-8.10	1.18	1.43
27	c	526	BCR	C11-C10	-8.10	1.18	1.43
27	B	619	BCR	C8-C9	-8.08	1.28	1.46
27	b	620	BCR	C8-C9	-8.08	1.28	1.46
27	d	411	BCR	C11-C10	-8.01	1.18	1.43
27	c	525	BCR	C11-C10	-8.00	1.18	1.43
27	C	525	BCR	C11-C10	-8.00	1.18	1.43
27	D	411	BCR	C11-C10	-7.98	1.18	1.43
27	B	619	BCR	C11-C10	-7.92	1.18	1.43
27	b	620	BCR	C11-C10	-7.92	1.18	1.43
27	C	527	BCR	C11-C10	-7.87	1.18	1.43
27	c	527	BCR	C11-C10	-7.87	1.18	1.43
27	B	617	BCR	C20-C21	-7.70	1.19	1.43
27	b	618	BCR	C20-C21	-7.70	1.19	1.43
27	C	526	BCR	C20-C21	-7.60	1.19	1.43
27	c	526	BCR	C20-C21	-7.60	1.19	1.43
27	B	619	BCR	C16-C17	-7.54	1.19	1.43
27	b	620	BCR	C16-C17	-7.54	1.19	1.43
27	B	618	BCR	C20-C21	-7.52	1.19	1.43
27	b	619	BCR	C20-C21	-7.52	1.19	1.43
27	A	409	BCR	C20-C21	-7.48	1.20	1.43
27	a	409	BCR	C20-C21	-7.48	1.20	1.43
27	C	514	BCR	C20-C21	-7.45	1.20	1.43
27	c	514	BCR	C20-C21	-7.45	1.20	1.43
27	A	409	BCR	C16-C17	-7.42	1.20	1.43
27	a	409	BCR	C16-C17	-7.42	1.20	1.43
27	B	617	BCR	C16-C17	-7.41	1.20	1.43
27	b	618	BCR	C16-C17	-7.41	1.20	1.43
27	B	618	BCR	C16-C17	-7.41	1.20	1.43
27	b	619	BCR	C16-C17	-7.41	1.20	1.43
27	B	619	BCR	C20-C21	-7.40	1.20	1.43
27	b	620	BCR	C20-C21	-7.40	1.20	1.43
27	C	526	BCR	C16-C17	-7.39	1.20	1.43
27	c	526	BCR	C16-C17	-7.39	1.20	1.43
27	C	525	BCR	C20-C21	-7.36	1.20	1.43
27	c	525	BCR	C20-C21	-7.36	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	411	BCR	C20-C21	-7.31	1.20	1.43
27	d	411	BCR	C20-C21	-7.29	1.20	1.43
27	c	525	BCR	C16-C17	-7.29	1.20	1.43
27	C	525	BCR	C16-C17	-7.29	1.20	1.43
27	C	527	BCR	C20-C21	-7.28	1.20	1.43
27	c	527	BCR	C20-C21	-7.28	1.20	1.43
27	c	514	BCR	C16-C17	-7.26	1.20	1.43
27	C	514	BCR	C16-C17	-7.26	1.20	1.43
27	d	411	BCR	C16-C17	-7.24	1.20	1.43
27	D	411	BCR	C16-C17	-7.24	1.20	1.43
27	C	527	BCR	C16-C17	-7.18	1.20	1.43
27	c	527	BCR	C16-C17	-7.17	1.20	1.43
30	B	630	SQD	O3-C3	6.65	1.59	1.43
30	b	601	SQD	O3-C3	6.65	1.59	1.43
28	A	413	LMG	O1-C1	-6.29	1.29	1.40
28	a	413	LMG	O1-C1	-6.29	1.29	1.40
25	b	606	CLA	CHB-C4A	6.26	1.38	1.33
25	B	612	CLA	CHB-C4A	6.25	1.38	1.33
25	b	613	CLA	CHB-C4A	6.25	1.38	1.33
30	B	630	SQD	O2-C2	-6.24	1.27	1.43
30	b	601	SQD	O2-C2	-6.24	1.27	1.43
25	B	605	CLA	CHB-C4A	6.24	1.38	1.33
25	b	614	CLA	CHB-C4A	6.23	1.38	1.33
25	b	603	CLA	CHB-C4A	6.16	1.38	1.33
25	B	614	CLA	CHB-C4A	6.16	1.38	1.33
25	b	615	CLA	CHB-C4A	6.16	1.38	1.33
25	B	613	CLA	CHB-C4A	6.14	1.38	1.33
25	B	602	CLA	CHB-C4A	6.10	1.38	1.33
30	B	630	SQD	O4-C4	-5.93	1.28	1.43
30	b	601	SQD	O4-C4	-5.93	1.28	1.43
25	A	405	CLA	CHB-C4A	5.83	1.38	1.33
25	a	405	CLA	CHB-C4A	5.83	1.38	1.33
25	B	604	CLA	CHB-C4A	5.82	1.38	1.33
25	b	605	CLA	CHB-C4A	5.82	1.38	1.33
25	B	615	CLA	CHB-C4A	5.79	1.38	1.33
25	b	616	CLA	CHB-C4A	5.79	1.38	1.33
25	b	612	CLA	CHB-C4A	5.79	1.38	1.33
25	b	614	CLA	MG-NC	5.76	2.20	2.06
25	B	603	CLA	CHB-C4A	5.76	1.38	1.33
25	b	604	CLA	CHB-C4A	5.76	1.38	1.33
25	B	611	CLA	CHB-C4A	5.75	1.38	1.33
25	B	613	CLA	MG-NC	5.75	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	CLA	CHB-C4A	5.63	1.38	1.33
25	d	401	CLA	CHB-C4A	5.63	1.38	1.33
25	B	606	CLA	CHB-C4A	5.63	1.38	1.33
25	b	607	CLA	CHB-C4A	5.63	1.38	1.33
25	B	610	CLA	CHB-C4A	5.60	1.38	1.33
25	b	611	CLA	CHB-C4A	5.60	1.38	1.33
25	A	408	CLA	CHB-C4A	5.57	1.38	1.33
25	a	408	CLA	CHB-C4A	5.57	1.38	1.33
25	B	609	CLA	CHB-C4A	5.53	1.38	1.33
25	b	610	CLA	CHB-C4A	5.53	1.38	1.33
25	D	403	CLA	CHB-C4A	5.52	1.38	1.33
28	A	410	LMG	O4-C4	-5.48	1.29	1.43
28	a	410	LMG	O4-C4	-5.48	1.29	1.43
25	B	605	CLA	MG-NC	5.46	2.19	2.06
25	b	606	CLA	MG-NC	5.46	2.19	2.06
25	B	616	CLA	CHB-C4A	5.45	1.38	1.33
25	C	501	CLA	CHB-C4A	5.45	1.38	1.33
25	b	617	CLA	CHB-C4A	5.45	1.38	1.33
25	c	501	CLA	CHB-C4A	5.45	1.38	1.33
25	d	403	CLA	CHB-C4A	5.44	1.38	1.33
25	C	509	CLA	CHB-C4A	5.43	1.38	1.33
25	c	509	CLA	CHB-C4A	5.43	1.38	1.33
29	A	411	PL9	C3-C4	-5.41	1.41	1.49
29	a	411	PL9	C3-C4	-5.41	1.41	1.49
25	B	607	CLA	CHB-C4A	5.40	1.38	1.33
25	b	608	CLA	CHB-C4A	5.40	1.38	1.33
25	B	615	CLA	MG-NC	5.39	2.19	2.06
25	b	616	CLA	MG-NC	5.39	2.19	2.06
25	C	505	CLA	CHB-C4A	5.29	1.38	1.33
25	c	505	CLA	CHB-C4A	5.29	1.38	1.33
25	C	506	CLA	CHB-C4A	5.26	1.37	1.33
25	c	506	CLA	CHB-C4A	5.26	1.37	1.33
25	b	607	CLA	MG-NC	5.23	2.18	2.06
25	B	606	CLA	MG-NC	5.20	2.18	2.06
29	D	405	PL9	C3-C4	-5.18	1.41	1.49
29	d	405	PL9	C3-C4	-5.18	1.41	1.49
25	C	512	CLA	CHB-C4A	5.17	1.37	1.33
25	c	512	CLA	CHB-C4A	5.17	1.37	1.33
25	A	406	CLA	CHB-C4A	5.14	1.37	1.33
25	C	510	CLA	CHB-C4A	5.12	1.37	1.33
25	c	510	CLA	CHB-C4A	5.12	1.37	1.33
25	c	503	CLA	CHB-C4A	5.10	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	503	CLA	CHB-C4A	5.10	1.37	1.33
25	B	601	CLA	CHB-C4A	5.07	1.37	1.33
25	b	602	CLA	CHB-C4A	5.07	1.37	1.33
25	C	513	CLA	CHB-C4A	5.07	1.37	1.33
25	c	513	CLA	CHB-C4A	5.07	1.37	1.33
25	a	406	CLA	CHB-C4A	5.05	1.37	1.33
25	c	504	CLA	CHB-C4A	5.05	1.37	1.33
25	C	511	CLA	CHB-C4A	4.99	1.37	1.33
25	c	511	CLA	CHB-C4A	4.97	1.37	1.33
25	D	401	CLA	MG-ND	-4.96	1.96	2.05
25	d	401	CLA	MG-ND	-4.96	1.96	2.05
25	B	608	CLA	CHB-C4A	4.96	1.37	1.33
25	b	609	CLA	CHB-C4A	4.96	1.37	1.33
25	C	504	CLA	CHB-C4A	4.95	1.37	1.33
25	C	508	CLA	CHB-C4A	4.93	1.37	1.33
25	c	508	CLA	CHB-C4A	4.93	1.37	1.33
30	B	630	SQD	O5-C1	4.93	1.54	1.41
30	b	601	SQD	O5-C1	4.93	1.54	1.41
25	D	404	CLA	CHB-C4A	4.89	1.37	1.33
25	d	404	CLA	CHB-C4A	4.89	1.37	1.33
25	C	507	CLA	CHB-C4A	4.80	1.37	1.33
25	c	507	CLA	CHB-C4A	4.80	1.37	1.33
25	B	610	CLA	MG-NA	4.71	2.17	2.06
25	b	611	CLA	MG-NA	4.71	2.17	2.06
25	C	502	CLA	CHB-C4A	4.70	1.37	1.33
25	c	502	CLA	CHB-C4A	4.70	1.37	1.33
27	C	514	BCR	C10-C9	-4.68	1.25	1.35
27	c	514	BCR	C10-C9	-4.68	1.25	1.35
27	B	618	BCR	C10-C9	-4.64	1.25	1.35
30	F	102	SQD	O48-C23	4.62	1.46	1.33
30	f	102	SQD	O48-C23	4.62	1.46	1.33
27	A	409	BCR	C10-C9	-4.61	1.25	1.35
27	a	409	BCR	C10-C9	-4.61	1.25	1.35
27	b	619	BCR	C10-C9	-4.61	1.25	1.35
27	C	526	BCR	C10-C9	-4.46	1.25	1.35
27	c	526	BCR	C10-C9	-4.46	1.25	1.35
28	B	629	LMG	O8-C28	4.41	1.46	1.33
28	b	630	LMG	O8-C28	4.41	1.46	1.33
28	A	413	LMG	O1-C7	4.40	1.51	1.43
28	a	413	LMG	O1-C7	4.40	1.51	1.43
27	B	617	BCR	C10-C9	-4.39	1.25	1.35
27	b	618	BCR	C10-C9	-4.39	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	411	BCR	C10-C9	-4.35	1.25	1.35
27	d	411	BCR	C10-C9	-4.31	1.25	1.35
27	C	525	BCR	C10-C9	-4.28	1.25	1.35
27	c	525	BCR	C10-C9	-4.28	1.25	1.35
27	C	527	BCR	C10-C9	-4.27	1.25	1.35
27	c	527	BCR	C10-C9	-4.27	1.25	1.35
27	B	619	BCR	C10-C9	-4.27	1.25	1.35
27	b	620	BCR	C10-C9	-4.27	1.25	1.35
25	C	509	CLA	MG-NA	4.27	2.16	2.06
25	c	509	CLA	MG-NA	4.27	2.16	2.06
35	F	101	HEM	C4D-ND	-4.27	1.32	1.40
35	f	101	HEM	C4D-ND	-4.27	1.32	1.40
28	A	410	LMG	O8-C28	4.26	1.45	1.33
28	a	410	LMG	O8-C28	4.26	1.45	1.33
28	A	413	LMG	O2-C2	-4.26	1.32	1.43
28	a	413	LMG	O2-C2	-4.26	1.32	1.43
34	C	517	DGD	O1G-C1A	4.25	1.45	1.33
34	c	517	DGD	O1G-C1A	4.25	1.45	1.33
28	C	519	LMG	O8-C28	4.22	1.45	1.33
28	c	519	LMG	O8-C28	4.22	1.45	1.33
33	B	626	LHG	O7-C7	4.21	1.46	1.34
33	b	627	LHG	O7-C7	4.21	1.46	1.34
25	C	508	CLA	MG-ND	-4.19	1.97	2.05
25	c	508	CLA	MG-ND	-4.19	1.97	2.05
33	B	626	LHG	O8-C23	4.18	1.45	1.33
33	b	627	LHG	O8-C23	4.18	1.45	1.33
28	a	413	LMG	O8-C28	4.17	1.45	1.33
25	B	602	CLA	MG-ND	4.17	2.14	2.05
25	b	603	CLA	MG-ND	4.17	2.14	2.05
25	B	608	CLA	MG-NA	4.16	2.16	2.06
25	b	609	CLA	MG-NA	4.16	2.16	2.06
25	a	405	CLA	MG-NC	4.15	2.16	2.06
34	C	517	DGD	O2G-C1B	4.15	1.46	1.34
34	c	517	DGD	O2G-C1B	4.15	1.46	1.34
25	A	405	CLA	MG-NC	4.15	2.16	2.06
28	A	413	LMG	O8-C28	4.14	1.45	1.33
28	C	519	LMG	O7-C10	4.14	1.46	1.34
28	c	519	LMG	O7-C10	4.14	1.46	1.34
33	E	102	LHG	O8-C23	4.12	1.45	1.33
33	e	102	LHG	O8-C23	4.12	1.45	1.33
33	A	418	LHG	O8-C23	4.12	1.45	1.33
25	c	504	CLA	MG-ND	-4.11	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	MG-ND	-4.11	1.97	2.05
28	J	101	LMG	O8-C28	4.10	1.45	1.33
28	j	101	LMG	O8-C28	4.10	1.45	1.33
33	a	418	LHG	O8-C23	4.10	1.45	1.33
28	B	629	LMG	O7-C10	4.05	1.45	1.34
28	b	630	LMG	O7-C10	4.05	1.45	1.34
25	C	501	CLA	MG-NC	4.04	2.15	2.06
25	c	501	CLA	MG-NC	4.04	2.15	2.06
34	H	103	DGD	O1G-C1A	4.04	1.45	1.33
34	h	103	DGD	O1G-C1A	4.04	1.45	1.33
30	a	412	SQD	O2-C2	4.01	1.52	1.43
28	J	101	LMG	O7-C10	4.01	1.45	1.34
28	j	101	LMG	O7-C10	4.01	1.45	1.34
28	C	518	LMG	O8-C28	4.00	1.45	1.33
28	c	518	LMG	O8-C28	4.00	1.45	1.33
30	A	412	SQD	O2-C2	3.98	1.52	1.43
34	C	516	DGD	O1G-C1A	3.97	1.44	1.33
34	c	516	DGD	O1G-C1A	3.97	1.44	1.33
28	B	621	LMG	O8-C28	3.97	1.44	1.33
28	C	519	LMG	C37-C36	-3.96	1.32	1.51
28	c	519	LMG	C37-C36	-3.96	1.32	1.51
25	B	614	CLA	MG-NA	3.96	2.15	2.06
25	b	615	CLA	MG-NA	3.96	2.15	2.06
28	b	622	LMG	O8-C28	3.96	1.44	1.33
28	A	413	LMG	O7-C10	3.93	1.45	1.34
28	a	413	LMG	O7-C10	3.93	1.45	1.34
30	A	412	SQD	O3-C3	-3.93	1.33	1.43
30	a	412	SQD	O3-C3	-3.93	1.33	1.43
35	v	201	HEM	C1B-NB	-3.92	1.33	1.40
28	D	407	LMG	O8-C28	3.91	1.44	1.33
28	d	407	LMG	O8-C28	3.91	1.44	1.33
35	V	201	HEM	C1B-NB	-3.90	1.33	1.40
33	Z	101	LHG	O8-C23	3.87	1.44	1.33
33	z	101	LHG	O8-C23	3.87	1.44	1.33
28	C	519	LMG	C40-C39	-3.86	1.32	1.51
28	c	519	LMG	C40-C39	-3.86	1.32	1.51
25	C	507	CLA	MG-ND	-3.85	1.98	2.05
25	c	507	CLA	MG-ND	-3.85	1.98	2.05
33	L	101	LHG	O8-C23	3.84	1.44	1.33
33	l	101	LHG	O8-C23	3.84	1.44	1.33
28	C	518	LMG	O7-C10	3.84	1.45	1.34
28	a	410	LMG	C19-C18	-3.83	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	C19-C18	-3.83	1.32	1.51
28	D	407	LMG	C37-C36	-3.82	1.32	1.51
28	d	407	LMG	C37-C36	-3.82	1.32	1.51
25	B	604	CLA	MG-NA	3.82	2.15	2.06
33	a	419	LHG	O8-C23	3.82	1.44	1.33
28	c	518	LMG	O7-C10	3.82	1.45	1.34
34	H	103	DGD	CAB-C9B	-3.81	1.32	1.51
34	h	103	DGD	CAB-C9B	-3.81	1.32	1.51
25	b	605	CLA	MG-NA	3.81	2.15	2.06
33	A	419	LHG	O8-C23	3.81	1.44	1.33
28	C	518	LMG	C40-C39	-3.81	1.32	1.51
25	D	401	CLA	MG-NA	3.80	2.15	2.06
33	D	406	LHG	O7-C7	3.80	1.45	1.34
33	d	406	LHG	O7-C7	3.80	1.45	1.34
28	c	518	LMG	C40-C39	-3.79	1.32	1.51
25	d	401	CLA	MG-NA	3.78	2.15	2.06
28	A	410	LMG	C37-C36	-3.78	1.33	1.51
28	a	410	LMG	C37-C36	-3.78	1.33	1.51
28	a	410	LMG	C22-C21	-3.78	1.33	1.51
34	H	103	DGD	CDB-CCB	-3.78	1.33	1.51
34	h	103	DGD	CDB-CCB	-3.78	1.33	1.51
28	A	410	LMG	C22-C21	-3.78	1.33	1.51
28	B	621	LMG	C19-C18	-3.78	1.33	1.51
28	J	101	LMG	C22-C21	-3.78	1.33	1.51
28	j	101	LMG	C22-C21	-3.78	1.33	1.51
28	J	101	LMG	C43-C42	-3.77	1.33	1.51
33	D	406	LHG	O8-C23	3.77	1.44	1.33
33	d	406	LHG	O8-C23	3.77	1.44	1.33
34	C	515	DGD	CDB-CCB	-3.77	1.33	1.51
34	c	515	DGD	CDB-CCB	-3.77	1.33	1.51
28	B	621	LMG	C37-C36	-3.77	1.33	1.51
28	b	622	LMG	C37-C36	-3.77	1.33	1.51
28	c	518	LMG	C37-C36	-3.76	1.33	1.51
28	D	407	LMG	C43-C42	-3.76	1.33	1.51
28	b	622	LMG	C19-C18	-3.76	1.33	1.51
34	C	515	DGD	CAB-C9B	-3.76	1.33	1.51
34	c	515	DGD	CAB-C9B	-3.76	1.33	1.51
28	j	101	LMG	C43-C42	-3.76	1.33	1.51
28	J	101	LMG	C40-C39	-3.76	1.33	1.51
28	j	101	LMG	C40-C39	-3.76	1.33	1.51
28	C	518	LMG	C19-C18	-3.76	1.33	1.51
28	c	518	LMG	C19-C18	-3.76	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	102	SQD	O5-C1	3.76	1.51	1.41
28	d	407	LMG	C43-C42	-3.76	1.33	1.51
28	J	101	LMG	C19-C18	-3.76	1.33	1.51
28	j	101	LMG	C19-C18	-3.76	1.33	1.51
28	C	518	LMG	C37-C36	-3.75	1.33	1.51
28	B	629	LMG	C37-C36	-3.74	1.33	1.51
28	b	630	LMG	C37-C36	-3.74	1.33	1.51
34	c	516	DGD	CDA-CCA	-3.74	1.33	1.51
28	J	101	LMG	C37-C36	-3.74	1.33	1.51
28	j	101	LMG	C37-C36	-3.74	1.33	1.51
30	f	102	SQD	O5-C1	3.74	1.51	1.41
28	D	407	LMG	C22-C21	-3.73	1.33	1.51
28	d	407	LMG	C22-C21	-3.73	1.33	1.51
28	D	407	LMG	C40-C39	-3.73	1.33	1.51
28	d	407	LMG	C40-C39	-3.73	1.33	1.51
34	C	517	DGD	CDA-CCA	-3.73	1.33	1.51
28	b	622	LMG	C22-C21	-3.73	1.33	1.51
28	B	621	LMG	C22-C21	-3.73	1.33	1.51
34	C	516	DGD	CDA-CCA	-3.73	1.33	1.51
34	c	517	DGD	CDA-CCA	-3.73	1.33	1.51
28	D	407	LMG	C19-C18	-3.73	1.33	1.51
28	d	407	LMG	C19-C18	-3.73	1.33	1.51
28	C	519	LMG	C22-C21	-3.73	1.33	1.51
28	c	519	LMG	C22-C21	-3.73	1.33	1.51
34	C	516	DGD	CDB-CCB	-3.72	1.33	1.51
34	c	516	DGD	CDB-CCB	-3.72	1.33	1.51
28	B	621	LMG	C40-C39	-3.72	1.33	1.51
34	C	516	DGD	CAB-C9B	-3.72	1.33	1.51
33	L	101	LHG	O7-C7	3.72	1.44	1.34
33	l	101	LHG	O7-C7	3.72	1.44	1.34
28	J	101	LMG	C25-C24	-3.72	1.33	1.51
35	F	101	HEM	C1B-NB	-3.72	1.33	1.40
35	f	101	HEM	C1B-NB	-3.72	1.33	1.40
28	j	101	LMG	C25-C24	-3.71	1.33	1.51
28	B	629	LMG	C40-C39	-3.71	1.33	1.51
28	b	630	LMG	C40-C39	-3.71	1.33	1.51
35	V	201	HEM	C4D-ND	-3.71	1.33	1.40
35	v	201	HEM	C4D-ND	-3.71	1.33	1.40
34	c	516	DGD	CAB-C9B	-3.71	1.33	1.51
28	b	622	LMG	C40-C39	-3.71	1.33	1.51
34	C	517	DGD	CDB-CCB	-3.70	1.33	1.51
34	c	517	DGD	CDB-CCB	-3.70	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	418	LHG	O7-C7	3.70	1.44	1.34
33	a	418	LHG	O7-C7	3.70	1.44	1.34
34	H	103	DGD	CAA-C9A	-3.70	1.33	1.51
34	h	103	DGD	CAA-C9A	-3.70	1.33	1.51
34	C	517	DGD	CAA-C9A	-3.70	1.33	1.51
34	H	103	DGD	CDA-CCA	-3.70	1.33	1.51
34	h	103	DGD	CDA-CCA	-3.70	1.33	1.51
34	c	517	DGD	CAA-C9A	-3.69	1.33	1.51
28	D	407	LMG	C25-C24	-3.69	1.33	1.51
28	d	407	LMG	C25-C24	-3.69	1.33	1.51
34	C	516	DGD	CAA-C9A	-3.69	1.33	1.51
34	c	516	DGD	CAA-C9A	-3.69	1.33	1.51
33	Z	101	LHG	O7-C7	3.69	1.44	1.34
33	z	101	LHG	O7-C7	3.69	1.44	1.34
25	B	607	CLA	MG-NC	3.68	2.15	2.06
25	b	608	CLA	MG-NC	3.68	2.15	2.06
28	D	407	LMG	O7-C10	3.68	1.44	1.34
28	d	407	LMG	O7-C10	3.68	1.44	1.34
28	A	410	LMG	C40-C39	-3.68	1.33	1.51
28	a	410	LMG	C40-C39	-3.68	1.33	1.51
34	C	515	DGD	CAA-C9A	-3.67	1.33	1.51
34	c	515	DGD	CAA-C9A	-3.67	1.33	1.51
34	C	517	DGD	CAB-C9B	-3.67	1.33	1.51
34	c	517	DGD	CAB-C9B	-3.67	1.33	1.51
36	H	101	RRX	C8-C9	-3.67	1.38	1.46
36	h	101	RRX	C8-C9	-3.67	1.38	1.46
28	C	519	LMG	C19-C18	-3.67	1.33	1.51
28	c	519	LMG	C19-C18	-3.67	1.33	1.51
34	C	515	DGD	CDA-CCA	-3.66	1.33	1.51
34	C	516	DGD	O2G-C1B	3.66	1.44	1.34
34	c	516	DGD	O2G-C1B	3.66	1.44	1.34
28	C	518	LMG	C22-C21	-3.66	1.33	1.51
28	c	518	LMG	C22-C21	-3.66	1.33	1.51
34	c	515	DGD	CDA-CCA	-3.65	1.33	1.51
27	a	409	BCR	C11-C12	-3.65	1.25	1.34
27	A	409	BCR	C11-C12	-3.64	1.25	1.34
25	A	408	CLA	CHC-C1C	3.64	1.43	1.34
25	a	408	CLA	CHC-C1C	3.64	1.43	1.34
27	B	618	BCR	C11-C12	-3.61	1.25	1.34
27	b	619	BCR	C11-C12	-3.61	1.25	1.34
28	B	621	LMG	O7-C10	3.60	1.44	1.34
28	b	622	LMG	O7-C10	3.60	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	101	RRX	C23-C22	-3.58	1.38	1.46
36	h	101	RRX	C23-C22	-3.58	1.38	1.46
28	a	410	LMG	O7-C10	3.58	1.44	1.34
28	A	410	LMG	O7-C10	3.57	1.44	1.34
34	C	515	DGD	O1G-C1A	3.57	1.43	1.33
34	c	515	DGD	O1G-C1A	3.57	1.43	1.33
30	F	102	SQD	O47-C45	-3.55	1.38	1.46
30	f	102	SQD	O47-C45	-3.55	1.38	1.46
34	H	103	DGD	O2G-C1B	3.55	1.44	1.34
34	h	103	DGD	O2G-C1B	3.55	1.44	1.34
33	A	419	LHG	O7-C7	3.55	1.44	1.34
33	a	419	LHG	O7-C7	3.55	1.44	1.34
25	c	511	CLA	MG-NA	3.53	2.14	2.06
25	B	608	CLA	CHC-C1C	3.51	1.43	1.34
25	b	609	CLA	CHC-C1C	3.51	1.43	1.34
27	C	526	BCR	C11-C12	-3.51	1.25	1.34
27	c	526	BCR	C11-C12	-3.51	1.25	1.34
25	B	605	CLA	CHC-C1C	3.50	1.43	1.34
25	b	606	CLA	CHC-C1C	3.50	1.43	1.34
25	C	503	CLA	MG-ND	-3.50	1.98	2.05
25	c	503	CLA	MG-ND	-3.50	1.98	2.05
25	C	511	CLA	MG-NA	3.49	2.14	2.06
27	C	514	BCR	C11-C12	-3.49	1.25	1.34
27	c	514	BCR	C11-C12	-3.49	1.25	1.34
25	B	607	CLA	CHC-C1C	3.48	1.43	1.34
25	b	608	CLA	CHC-C1C	3.48	1.43	1.34
25	D	403	CLA	CHC-C1C	3.48	1.43	1.34
25	d	403	CLA	CHC-C1C	3.48	1.43	1.34
33	E	102	LHG	O7-C7	3.47	1.44	1.34
33	e	102	LHG	O7-C7	3.47	1.44	1.34
27	B	617	BCR	C11-C12	-3.47	1.25	1.34
25	B	606	CLA	C1D-ND	3.44	1.42	1.37
25	b	607	CLA	C1D-ND	3.44	1.42	1.37
25	B	612	CLA	CHC-C1C	3.44	1.43	1.34
25	b	613	CLA	CHC-C1C	3.44	1.43	1.34
27	b	618	BCR	C11-C12	-3.44	1.25	1.34
28	A	410	LMG	O5-C6	-3.44	1.28	1.42
28	a	410	LMG	O5-C6	-3.44	1.28	1.42
28	A	410	LMG	O3-C3	-3.42	1.34	1.43
28	a	410	LMG	O3-C3	-3.41	1.34	1.43
25	A	406	CLA	MG-ND	-3.41	1.99	2.05
25	a	406	CLA	MG-ND	-3.41	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	612	CLA	CHC-C1C	3.41	1.43	1.34
25	B	611	CLA	CHC-C1C	3.41	1.43	1.34
25	b	605	CLA	C1D-ND	3.40	1.42	1.37
27	C	525	BCR	C11-C12	-3.40	1.25	1.34
27	c	525	BCR	C11-C12	-3.40	1.25	1.34
34	c	515	DGD	O2G-C1B	3.38	1.43	1.34
25	B	602	CLA	CHC-C1C	3.38	1.42	1.34
25	b	603	CLA	CHC-C1C	3.38	1.42	1.34
34	C	515	DGD	O2G-C1B	3.36	1.43	1.34
25	B	604	CLA	C1D-ND	3.35	1.42	1.37
25	A	408	CLA	MG-NA	3.35	2.14	2.06
25	a	408	CLA	MG-NA	3.35	2.14	2.06
25	B	606	CLA	CHC-C1C	3.34	1.42	1.34
25	b	607	CLA	CHC-C1C	3.34	1.42	1.34
25	C	505	CLA	MG-ND	-3.32	1.99	2.05
25	c	505	CLA	MG-ND	-3.32	1.99	2.05
30	F	102	SQD	O47-C7	3.32	1.43	1.34
30	f	102	SQD	O47-C7	3.32	1.43	1.34
25	B	609	CLA	MG-NA	3.31	2.14	2.06
27	D	411	BCR	C11-C12	-3.31	1.26	1.34
27	d	411	BCR	C11-C12	-3.31	1.26	1.34
25	C	510	CLA	CHC-C1C	3.30	1.42	1.34
25	c	510	CLA	CHC-C1C	3.30	1.42	1.34
25	C	509	CLA	CHC-C1C	3.29	1.42	1.34
25	c	509	CLA	CHC-C1C	3.29	1.42	1.34
25	b	610	CLA	MG-NA	3.28	2.14	2.06
27	C	527	BCR	C11-C12	-3.28	1.26	1.34
27	c	527	BCR	C11-C12	-3.28	1.26	1.34
25	B	602	CLA	MG-NC	3.27	2.14	2.06
25	B	611	CLA	C1D-ND	3.27	1.42	1.37
25	b	612	CLA	C1D-ND	3.27	1.42	1.37
27	b	620	BCR	C11-C12	-3.27	1.26	1.34
25	b	603	CLA	MG-NC	3.26	2.14	2.06
27	B	619	BCR	C11-C12	-3.26	1.26	1.34
25	B	601	CLA	CHC-C1C	3.25	1.42	1.34
25	B	614	CLA	CHC-C1C	3.24	1.42	1.34
25	b	615	CLA	CHC-C1C	3.24	1.42	1.34
25	B	615	CLA	CHC-C1C	3.24	1.42	1.34
25	b	616	CLA	CHC-C1C	3.24	1.42	1.34
25	B	605	CLA	MG-NA	3.23	2.13	2.06
25	b	606	CLA	MG-NA	3.23	2.13	2.06
25	b	602	CLA	CHC-C1C	3.22	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	CHC-C1C	3.21	1.42	1.34
25	d	404	CLA	CHC-C1C	3.21	1.42	1.34
25	C	505	CLA	CHC-C1C	3.21	1.42	1.34
25	c	505	CLA	CHC-C1C	3.21	1.42	1.34
25	C	501	CLA	CHC-C1C	3.20	1.42	1.34
25	c	501	CLA	CHC-C1C	3.20	1.42	1.34
25	C	513	CLA	CHC-C1C	3.17	1.42	1.34
25	c	513	CLA	CHC-C1C	3.17	1.42	1.34
25	A	406	CLA	MG-NC	3.15	2.13	2.06
25	a	406	CLA	MG-NC	3.15	2.13	2.06
25	B	610	CLA	CHC-C1C	3.14	1.42	1.34
25	b	611	CLA	CHC-C1C	3.14	1.42	1.34
25	B	604	CLA	CHC-C1C	3.12	1.42	1.34
25	b	605	CLA	CHC-C1C	3.12	1.42	1.34
25	B	603	CLA	CHC-C1C	3.11	1.42	1.34
25	b	604	CLA	CHC-C1C	3.11	1.42	1.34
25	C	512	CLA	CHC-C1C	3.11	1.42	1.34
25	B	613	CLA	CHC-C1C	3.11	1.42	1.34
25	b	614	CLA	CHC-C1C	3.11	1.42	1.34
25	a	406	CLA	C1D-ND	3.11	1.41	1.37
25	C	506	CLA	CHC-C1C	3.10	1.42	1.34
25	c	506	CLA	CHC-C1C	3.10	1.42	1.34
25	c	512	CLA	CHC-C1C	3.07	1.42	1.34
25	A	406	CLA	C1D-ND	3.06	1.41	1.37
25	C	508	CLA	CHC-C1C	3.06	1.42	1.34
25	c	508	CLA	CHC-C1C	3.06	1.42	1.34
25	C	503	CLA	CHC-C1C	3.06	1.42	1.34
25	c	503	CLA	CHC-C1C	3.06	1.42	1.34
25	C	511	CLA	CHC-C1C	3.05	1.42	1.34
25	B	604	CLA	MG-NC	3.05	2.13	2.06
25	b	605	CLA	MG-NC	3.05	2.13	2.06
25	C	501	CLA	C1D-ND	3.04	1.41	1.37
25	c	501	CLA	C1D-ND	3.04	1.41	1.37
30	F	102	SQD	C24-C23	3.04	1.59	1.50
30	f	102	SQD	C24-C23	3.04	1.59	1.50
25	B	601	CLA	C1D-ND	3.04	1.41	1.37
25	b	602	CLA	C1D-ND	3.04	1.41	1.37
25	C	507	CLA	C1D-ND	3.03	1.41	1.37
25	c	507	CLA	C1D-ND	3.03	1.41	1.37
25	c	511	CLA	CHC-C1C	3.02	1.42	1.34
25	B	605	CLA	MG-ND	3.02	2.11	2.05
25	b	606	CLA	MG-ND	3.02	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	C1D-ND	3.01	1.41	1.37
25	b	611	CLA	C1D-ND	3.01	1.41	1.37
28	A	410	LMG	O2-C2	-3.01	1.35	1.43
28	a	410	LMG	O2-C2	-3.01	1.35	1.43
25	C	505	CLA	CMD-C2D	-3.01	1.44	1.50
25	c	505	CLA	CMD-C2D	-3.01	1.44	1.50
28	B	629	LMG	C19-C18	-3.00	1.33	1.51
25	b	609	CLA	C1D-ND	3.00	1.41	1.37
25	B	608	CLA	C1D-ND	2.99	1.41	1.37
25	B	614	CLA	C1D-ND	2.99	1.41	1.37
25	b	615	CLA	C1D-ND	2.99	1.41	1.37
28	b	630	LMG	C19-C18	-2.99	1.33	1.51
25	B	616	CLA	CHC-C1C	2.99	1.41	1.34
25	b	617	CLA	CHC-C1C	2.99	1.41	1.34
25	B	613	CLA	CMB-C2B	-2.99	1.45	1.51
25	b	614	CLA	CMB-C2B	-2.99	1.45	1.51
25	b	610	CLA	CHC-C1C	2.99	1.41	1.34
25	B	609	CLA	CHC-C1C	2.98	1.41	1.34
28	a	413	LMG	O5-C6	2.98	1.54	1.42
25	c	502	CLA	CHC-C1C	2.97	1.41	1.34
28	A	413	LMG	O5-C6	2.97	1.54	1.42
25	A	405	CLA	CMB-C2B	-2.97	1.45	1.51
25	a	405	CLA	CMB-C2B	-2.97	1.45	1.51
25	D	401	CLA	CHC-C1C	2.96	1.41	1.34
30	A	412	SQD	O5-C1	-2.96	1.34	1.41
30	a	412	SQD	O5-C1	-2.96	1.34	1.41
25	c	501	CLA	CMB-C2B	-2.94	1.45	1.51
25	A	405	CLA	CHC-C1C	2.94	1.41	1.34
25	a	405	CLA	CHC-C1C	2.94	1.41	1.34
25	d	401	CLA	CHC-C1C	2.94	1.41	1.34
28	B	629	LMG	C43-C42	-2.94	1.33	1.51
28	b	630	LMG	C43-C42	-2.94	1.33	1.51
25	C	502	CLA	CHC-C1C	2.93	1.41	1.34
25	c	513	CLA	C1D-ND	2.92	1.41	1.37
25	C	513	CLA	C1D-ND	2.92	1.41	1.37
25	C	504	CLA	CHC-C1C	2.92	1.41	1.34
25	c	504	CLA	CHC-C1C	2.92	1.41	1.34
25	B	612	CLA	C1D-ND	2.92	1.41	1.37
25	b	613	CLA	C1D-ND	2.92	1.41	1.37
25	B	613	CLA	C1D-ND	2.91	1.41	1.37
25	b	614	CLA	C1D-ND	2.91	1.41	1.37
25	C	501	CLA	CMB-C2B	-2.91	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CMB-C2B	-2.91	1.45	1.51
25	c	511	CLA	CMB-C2B	-2.91	1.45	1.51
25	C	504	CLA	C1D-ND	2.90	1.41	1.37
25	c	504	CLA	C1D-ND	2.90	1.41	1.37
25	B	602	CLA	CMB-C2B	-2.90	1.45	1.51
25	b	603	CLA	CMB-C2B	-2.90	1.45	1.51
25	C	506	CLA	C1D-ND	2.89	1.41	1.37
25	c	506	CLA	C1D-ND	2.89	1.41	1.37
25	B	603	CLA	CMB-C2B	-2.89	1.45	1.51
25	B	605	CLA	C1D-ND	2.89	1.41	1.37
25	b	606	CLA	C1D-ND	2.89	1.41	1.37
25	C	510	CLA	CMB-C2B	-2.88	1.45	1.51
25	c	510	CLA	CMB-C2B	-2.88	1.45	1.51
25	C	506	CLA	CMB-C2B	-2.87	1.45	1.51
25	c	506	CLA	CMB-C2B	-2.87	1.45	1.51
25	D	403	CLA	CMB-C2B	-2.87	1.45	1.51
25	d	403	CLA	CMB-C2B	-2.87	1.45	1.51
25	C	511	CLA	C1D-ND	2.86	1.41	1.37
25	c	511	CLA	C1D-ND	2.86	1.41	1.37
36	H	101	RRX	C19-C18	-2.86	1.39	1.46
36	h	101	RRX	C19-C18	-2.86	1.39	1.46
25	b	604	CLA	CMB-C2B	-2.85	1.45	1.51
25	B	603	CLA	C1D-ND	2.84	1.41	1.37
25	b	604	CLA	C1D-ND	2.84	1.41	1.37
25	C	509	CLA	CMB-C2B	-2.83	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.83	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.83	1.46	1.51
35	v	201	HEM	C4B-NB	-2.83	1.33	1.38
25	C	502	CLA	CMB-C2B	-2.83	1.46	1.51
25	C	503	CLA	C1D-ND	2.82	1.41	1.37
25	c	503	CLA	C1D-ND	2.82	1.41	1.37
35	V	201	HEM	C4B-NB	-2.82	1.33	1.38
25	C	507	CLA	CMB-C2B	-2.82	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.82	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.82	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.82	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.81	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.81	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.81	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.80	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.80	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.80	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	508	CLA	CMB-C2B	-2.80	1.46	1.51
25	b	608	CLA	C1D-ND	2.79	1.41	1.37
25	C	509	CLA	C1D-ND	2.79	1.41	1.37
25	c	509	CLA	C1D-ND	2.79	1.41	1.37
25	b	606	CLA	CMB-C2B	-2.79	1.46	1.51
25	b	617	CLA	CMB-C2B	-2.79	1.46	1.51
25	C	508	CLA	MG-NA	2.79	2.12	2.06
25	c	508	CLA	MG-NA	2.79	2.12	2.06
26	D	402	PHO	C3A-C2A	-2.78	1.52	1.54
26	d	402	PHO	C3A-C2A	-2.78	1.52	1.54
25	B	607	CLA	C1D-ND	2.78	1.41	1.37
25	B	605	CLA	CMB-C2B	-2.77	1.46	1.51
25	D	404	CLA	C1D-ND	2.77	1.41	1.37
25	d	404	CLA	C1D-ND	2.77	1.41	1.37
25	C	504	CLA	CMB-C2B	-2.76	1.46	1.51
25	A	406	CLA	CHC-C1C	2.76	1.41	1.34
25	a	406	CLA	CHC-C1C	2.76	1.41	1.34
25	c	504	CLA	CMB-C2B	-2.75	1.46	1.51
36	H	101	RRX	C12-C13	-2.75	1.40	1.46
36	h	101	RRX	C12-C13	-2.75	1.40	1.46
25	D	401	CLA	C1D-ND	2.75	1.41	1.37
25	d	401	CLA	C1D-ND	2.75	1.41	1.37
25	D	401	CLA	CMB-C2B	-2.74	1.46	1.51
25	d	401	CLA	CMB-C2B	-2.74	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.73	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.73	1.46	1.51
25	B	616	CLA	C1D-ND	2.72	1.41	1.37
25	b	617	CLA	C1D-ND	2.72	1.41	1.37
25	B	601	CLA	CMB-C2B	-2.72	1.46	1.51
25	C	505	CLA	C1D-ND	2.72	1.41	1.37
25	C	507	CLA	CHC-C1C	2.72	1.41	1.34
25	c	507	CLA	CHC-C1C	2.72	1.41	1.34
25	c	505	CLA	C1D-ND	2.71	1.41	1.37
25	B	615	CLA	CMB-C2B	-2.71	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.71	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.70	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.70	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.70	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.70	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.70	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.70	1.46	1.51
25	C	510	CLA	CMD-C2D	-2.69	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	CMD-C2D	-2.69	1.45	1.50
25	b	602	CLA	CMB-C2B	-2.68	1.46	1.51
25	C	505	CLA	MG-NC	2.66	2.12	2.06
25	c	505	CLA	MG-NC	2.66	2.12	2.06
25	B	602	CLA	C1D-ND	2.65	1.41	1.37
25	b	603	CLA	C1D-ND	2.65	1.41	1.37
25	B	615	CLA	C1D-ND	2.63	1.41	1.37
25	b	616	CLA	C1D-ND	2.63	1.41	1.37
26	D	402	PHO	CBD-CGD	-2.62	1.49	1.52
26	d	402	PHO	CBD-CGD	-2.62	1.49	1.52
25	B	611	CLA	MG-NA	2.62	2.12	2.06
25	b	612	CLA	MG-NA	2.62	2.12	2.06
35	F	101	HEM	C1D-ND	-2.62	1.33	1.38
35	f	101	HEM	C1D-ND	-2.62	1.33	1.38
25	C	503	CLA	CMB-C2B	-2.62	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.62	1.46	1.51
35	v	201	HEM	C1D-ND	-2.62	1.33	1.38
25	c	502	CLA	CMD-C2D	-2.62	1.45	1.50
35	V	201	HEM	C1D-ND	-2.61	1.33	1.38
25	C	502	CLA	CMD-C2D	-2.61	1.45	1.50
25	B	607	CLA	CMD-C2D	-2.59	1.45	1.50
25	b	608	CLA	CMD-C2D	-2.59	1.45	1.50
25	A	408	CLA	CMB-C2B	-2.58	1.46	1.51
25	a	408	CLA	CMB-C2B	-2.58	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.58	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.57	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.57	1.46	1.51
25	a	406	CLA	CMD-C2D	-2.57	1.45	1.50
25	B	603	CLA	MG-NC	2.56	2.12	2.06
25	b	604	CLA	MG-NC	2.56	2.12	2.06
25	A	406	CLA	CMD-C2D	-2.56	1.45	1.50
25	C	508	CLA	C1D-ND	2.55	1.41	1.37
25	c	508	CLA	C1D-ND	2.55	1.41	1.37
25	B	608	CLA	CMB-C2B	-2.55	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.55	1.46	1.51
25	D	404	CLA	CMB-C2B	-2.54	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.52	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.52	1.46	1.51
25	A	405	CLA	C1D-ND	2.52	1.41	1.37
25	a	405	CLA	C1D-ND	2.52	1.41	1.37
25	C	510	CLA	MG-NA	2.52	2.12	2.06
25	c	510	CLA	MG-NA	2.52	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	CMB-C2B	-2.52	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.52	1.46	1.51
26	a	407	PHO	C3A-C2A	-2.51	1.52	1.54
26	A	407	PHO	C3A-C2A	-2.51	1.52	1.54
25	A	406	CLA	CMB-C2B	-2.50	1.46	1.51
25	a	406	CLA	CMB-C2B	-2.50	1.46	1.51
25	C	509	CLA	MG-ND	-2.50	2.00	2.05
25	c	509	CLA	MG-ND	-2.50	2.00	2.05
25	C	507	CLA	C3B-C2B	-2.50	1.37	1.40
25	c	507	CLA	C3B-C2B	-2.50	1.37	1.40
35	F	101	HEM	C4B-NB	-2.49	1.34	1.38
35	f	101	HEM	C4B-NB	-2.49	1.34	1.38
25	B	612	CLA	CMD-C2D	-2.49	1.45	1.50
25	b	613	CLA	CMD-C2D	-2.49	1.45	1.50
25	C	501	CLA	CMD-C2D	-2.47	1.45	1.50
25	c	501	CLA	CMD-C2D	-2.47	1.45	1.50
25	B	612	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.45	1.46	1.51
27	B	619	BCR	C30-C25	-2.45	1.50	1.53
27	b	620	BCR	C30-C25	-2.45	1.50	1.53
25	B	603	CLA	CMD-C2D	-2.44	1.45	1.50
25	b	604	CLA	CMD-C2D	-2.44	1.45	1.50
34	H	103	DGD	CGA-CFA	-2.43	1.33	1.50
34	h	103	DGD	CGA-CFA	-2.43	1.33	1.50
25	b	617	CLA	CMC-C2C	-2.43	1.45	1.50
28	B	621	LMG	C25-C24	-2.43	1.33	1.50
28	b	622	LMG	C25-C24	-2.43	1.33	1.50
25	C	506	CLA	MG-NC	2.43	2.12	2.06
25	c	506	CLA	MG-NC	2.43	2.12	2.06
25	a	408	CLA	C1D-ND	2.43	1.41	1.37
34	h	103	DGD	CGB-CFB	-2.43	1.33	1.50
25	c	506	CLA	C3B-C2B	-2.42	1.37	1.40
25	C	501	CLA	MG-NA	2.42	2.12	2.06
25	c	501	CLA	MG-NA	2.42	2.12	2.06
34	H	103	DGD	CGB-CFB	-2.42	1.33	1.50
25	C	506	CLA	C3B-C2B	-2.42	1.37	1.40
25	B	609	CLA	C1D-ND	2.41	1.41	1.37
25	b	610	CLA	C1D-ND	2.41	1.41	1.37
28	A	410	LMG	C25-C24	-2.41	1.33	1.50
28	a	410	LMG	C25-C24	-2.41	1.33	1.50
25	a	408	CLA	CMD-C2D	-2.41	1.45	1.50
25	D	403	CLA	CMC-C2C	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	CMC-C2C	-2.41	1.45	1.50
34	c	516	DGD	CGB-CFB	-2.40	1.33	1.50
25	B	616	CLA	CMC-C2C	-2.40	1.45	1.50
25	D	403	CLA	MG-NA	2.40	2.12	2.06
25	d	403	CLA	MG-NA	2.40	2.12	2.06
25	C	513	CLA	CMD-C2D	-2.40	1.45	1.50
25	c	513	CLA	CMD-C2D	-2.40	1.45	1.50
25	C	504	CLA	CMD-C2D	-2.40	1.45	1.50
25	c	504	CLA	CMD-C2D	-2.40	1.45	1.50
25	B	601	CLA	CMD-C2D	-2.40	1.45	1.50
25	b	602	CLA	CMD-C2D	-2.40	1.45	1.50
34	C	516	DGD	CGB-CFB	-2.40	1.33	1.50
25	B	614	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	615	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	612	CLA	CMD-C2D	-2.38	1.45	1.50
25	A	405	CLA	CMD-C2D	-2.38	1.45	1.50
25	a	405	CLA	CMD-C2D	-2.38	1.45	1.50
25	B	611	CLA	CMD-C2D	-2.38	1.45	1.50
25	A	408	CLA	C1D-ND	2.38	1.41	1.37
25	c	508	CLA	CMD-C2D	-2.38	1.45	1.50
28	C	518	LMG	C25-C24	-2.38	1.33	1.50
28	c	518	LMG	C25-C24	-2.38	1.33	1.50
34	C	517	DGD	CGB-CFB	-2.38	1.33	1.50
34	c	517	DGD	CGB-CFB	-2.38	1.33	1.50
25	A	408	CLA	CMD-C2D	-2.37	1.45	1.50
25	B	605	CLA	CMD-C2D	-2.37	1.45	1.50
25	b	606	CLA	CMD-C2D	-2.37	1.45	1.50
34	C	516	DGD	CGA-CFA	-2.37	1.33	1.50
34	c	516	DGD	CGA-CFA	-2.37	1.33	1.50
35	F	101	HEM	FE-NB	2.37	2.11	1.98
35	f	101	HEM	FE-NB	2.37	2.11	1.98
25	B	611	CLA	CMC-C2C	-2.37	1.45	1.50
25	b	612	CLA	CMC-C2C	-2.37	1.45	1.50
25	C	508	CLA	CMD-C2D	-2.37	1.45	1.50
25	C	502	CLA	C1D-ND	2.36	1.41	1.37
25	c	502	CLA	C1D-ND	2.36	1.41	1.37
28	B	621	LMG	C43-C42	-2.36	1.33	1.50
34	C	517	DGD	CGA-CFA	-2.36	1.33	1.50
34	c	517	DGD	CGA-CFA	-2.36	1.33	1.50
28	C	518	LMG	C43-C42	-2.36	1.33	1.50
28	c	518	LMG	C43-C42	-2.36	1.33	1.50
25	C	503	CLA	CMD-C2D	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	CMD-C2D	-2.36	1.45	1.50
34	C	515	DGD	CGB-CFB	-2.35	1.33	1.50
34	c	515	DGD	CGB-CFB	-2.35	1.33	1.50
28	a	410	LMG	C43-C42	-2.35	1.33	1.50
28	A	410	LMG	C43-C42	-2.35	1.33	1.50
28	b	622	LMG	C43-C42	-2.35	1.33	1.50
30	f	102	SQD	O5-C5	2.34	1.50	1.44
25	C	511	CLA	CMD-C2D	-2.34	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.34	1.46	1.50
25	c	509	CLA	CMD-C2D	-2.34	1.46	1.50
34	C	515	DGD	CGA-CFA	-2.34	1.33	1.50
34	c	515	DGD	CGA-CFA	-2.34	1.33	1.50
25	C	506	CLA	CMD-C2D	-2.33	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.33	1.46	1.50
25	C	502	CLA	CMC-C2C	-2.33	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.33	1.46	1.50
25	C	507	CLA	CMC-C2C	-2.33	1.46	1.50
25	B	604	CLA	C3B-C2B	-2.33	1.37	1.40
25	b	605	CLA	C3B-C2B	-2.33	1.37	1.40
25	B	608	CLA	CMD-C2D	-2.33	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.33	1.46	1.50
25	C	503	CLA	CMC-C2C	-2.32	1.46	1.50
25	c	503	CLA	CMC-C2C	-2.32	1.46	1.50
25	d	401	CLA	CMD-C2D	-2.32	1.46	1.50
25	C	509	CLA	CMD-C2D	-2.32	1.46	1.50
25	c	507	CLA	CMC-C2C	-2.32	1.46	1.50
25	C	507	CLA	CMD-C2D	-2.31	1.46	1.50
25	c	507	CLA	CMD-C2D	-2.31	1.46	1.50
30	F	102	SQD	O5-C5	2.31	1.50	1.44
25	D	401	CLA	CMD-C2D	-2.31	1.46	1.50
28	A	413	LMG	O3-C3	2.30	1.48	1.43
28	a	413	LMG	O3-C3	2.30	1.48	1.43
25	B	609	CLA	CMD-C2D	-2.30	1.46	1.50
25	b	610	CLA	CMD-C2D	-2.30	1.46	1.50
25	C	512	CLA	C1D-ND	2.30	1.40	1.37
25	c	512	CLA	C1D-ND	2.30	1.40	1.37
25	C	510	CLA	C1D-ND	2.29	1.40	1.37
25	c	510	CLA	C1D-ND	2.29	1.40	1.37
25	B	614	CLA	CMC-C2C	-2.29	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.29	1.46	1.50
25	C	507	CLA	C4B-CHC	-2.28	1.34	1.41
25	c	507	CLA	C4B-CHC	-2.28	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	CMD-C2D	-2.28	1.46	1.50
25	b	617	CLA	CMD-C2D	-2.28	1.46	1.50
25	C	506	CLA	MG-ND	-2.27	2.01	2.05
25	c	506	CLA	MG-ND	-2.27	2.01	2.05
25	D	403	CLA	CMD-C2D	-2.26	1.46	1.50
25	d	403	CLA	CMD-C2D	-2.26	1.46	1.50
25	B	613	CLA	CMD-C2D	-2.26	1.46	1.50
25	b	614	CLA	CMD-C2D	-2.26	1.46	1.50
25	C	503	CLA	MG-NA	2.25	2.11	2.06
25	c	503	CLA	MG-NA	2.25	2.11	2.06
25	b	607	CLA	CMC-C2C	-2.24	1.46	1.50
25	C	512	CLA	CMD-C2D	-2.24	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.24	1.46	1.50
25	C	511	CLA	C3B-C2B	-2.23	1.37	1.40
25	c	511	CLA	C3B-C2B	-2.23	1.37	1.40
25	b	611	CLA	CMC-C2C	-2.23	1.46	1.50
25	B	606	CLA	CMC-C2C	-2.23	1.46	1.50
25	B	601	CLA	C3B-C2B	-2.22	1.37	1.40
25	b	602	CLA	C3B-C2B	-2.22	1.37	1.40
25	C	501	CLA	CMC-C2C	-2.21	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.21	1.46	1.50
27	B	618	BCR	C30-C25	-2.21	1.51	1.53
25	C	504	CLA	CMC-C2C	-2.21	1.46	1.50
25	c	504	CLA	CMC-C2C	-2.21	1.46	1.50
25	C	506	CLA	CMC-C2C	-2.20	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	610	CLA	CMC-C2C	-2.20	1.46	1.50
25	C	511	CLA	CMC-C2C	-2.20	1.46	1.50
25	c	511	CLA	CMC-C2C	-2.20	1.46	1.50
30	A	412	SQD	O5-C5	2.20	1.49	1.44
30	a	412	SQD	O5-C5	2.20	1.49	1.44
27	b	619	BCR	C30-C25	-2.19	1.51	1.53
25	b	616	CLA	CMD-C2D	-2.19	1.46	1.50
25	C	504	CLA	C3B-C2B	-2.18	1.37	1.40
25	c	504	CLA	C3B-C2B	-2.18	1.37	1.40
25	C	508	CLA	CMC-C2C	-2.17	1.46	1.50
25	c	508	CLA	CMC-C2C	-2.17	1.46	1.50
30	A	412	SQD	O8-S	2.17	1.55	1.47
30	a	412	SQD	O8-S	2.17	1.55	1.47
33	A	418	LHG	O7-C5	-2.17	1.41	1.46
33	a	418	LHG	O7-C5	-2.17	1.41	1.46
28	D	407	LMG	O7-C8	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	CMD-C2D	-2.15	1.46	1.50
25	C	509	CLA	CMC-C2C	-2.14	1.46	1.50
25	c	509	CLA	CMC-C2C	-2.14	1.46	1.50
25	B	602	CLA	CMC-C2C	-2.14	1.46	1.50
28	d	407	LMG	O7-C8	-2.14	1.41	1.46
35	V	201	HEM	FE-NB	2.13	2.09	1.98
35	v	201	HEM	FE-NB	2.13	2.09	1.98
25	B	605	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	606	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	603	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	604	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	604	CLA	CMC-C2C	-2.12	1.46	1.50
25	C	508	CLA	C3B-C2B	-2.12	1.37	1.40
25	c	508	CLA	C3B-C2B	-2.12	1.37	1.40
27	B	617	BCR	C30-C25	-2.12	1.51	1.53
27	b	618	BCR	C30-C25	-2.12	1.51	1.53
28	A	410	LMG	O1-C7	-2.12	1.40	1.43
28	a	410	LMG	O1-C7	-2.12	1.40	1.43
30	B	630	SQD	O5-C5	2.12	1.49	1.44
30	b	601	SQD	O5-C5	2.12	1.49	1.44
25	c	505	CLA	CMC-C2C	-2.12	1.46	1.50
25	b	614	CLA	MG-ND	-2.12	2.01	2.05
25	b	603	CLA	CMC-C2C	-2.11	1.46	1.50
25	A	405	CLA	CMC-C2C	-2.11	1.46	1.50
25	a	405	CLA	CMC-C2C	-2.11	1.46	1.50
25	C	505	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	612	CLA	MG-NA	2.11	2.11	2.06
25	b	613	CLA	MG-NA	2.11	2.11	2.06
25	B	613	CLA	MG-ND	-2.11	2.01	2.05
28	B	621	LMG	O7-C8	-2.10	1.41	1.46
28	b	622	LMG	O7-C8	-2.10	1.41	1.46
25	c	512	CLA	CMC-C2C	-2.10	1.46	1.50
28	A	413	LMG	O7-C8	-2.10	1.41	1.46
28	a	413	LMG	O7-C8	-2.10	1.41	1.46
25	B	612	CLA	CMC-C2C	-2.10	1.46	1.50
25	C	510	CLA	CMC-C2C	-2.10	1.46	1.50
25	b	613	CLA	CMC-C2C	-2.10	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.10	1.46	1.50
25	C	513	CLA	CMC-C2C	-2.10	1.46	1.50
25	c	513	CLA	CMC-C2C	-2.10	1.46	1.50
25	b	605	CLA	CMC-C2C	-2.10	1.46	1.50
30	F	102	SQD	C8-C7	2.10	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	102	SQD	C8-C7	2.10	1.56	1.50
25	B	615	CLA	CMC-C2C	-2.09	1.46	1.50
30	F	102	SQD	O9-S	2.09	1.51	1.45
30	f	102	SQD	O9-S	2.09	1.51	1.45
35	f	101	HEM	FE-ND	-2.08	1.86	1.98
35	F	101	HEM	FE-ND	-2.08	1.86	1.98
27	C	526	BCR	C30-C25	-2.08	1.51	1.53
25	C	512	CLA	MG-ND	-2.08	2.01	2.05
25	B	616	CLA	C4B-CHC	-2.08	1.35	1.41
25	b	617	CLA	C4B-CHC	-2.08	1.35	1.41
25	D	401	CLA	C4B-CHC	-2.08	1.35	1.41
25	d	401	CLA	C4B-CHC	-2.08	1.35	1.41
25	B	604	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.07	1.46	1.50
25	C	512	CLA	CMC-C2C	-2.07	1.46	1.50
25	C	504	CLA	C4B-CHC	-2.07	1.35	1.41
25	c	504	CLA	C4B-CHC	-2.07	1.35	1.41
25	c	511	CLA	MG-ND	-2.07	2.01	2.05
25	B	611	CLA	C4B-CHC	-2.07	1.35	1.41
25	b	612	CLA	C4B-CHC	-2.07	1.35	1.41
25	b	616	CLA	CMC-C2C	-2.07	1.46	1.50
27	c	526	BCR	C30-C25	-2.06	1.51	1.53
33	E	102	LHG	O7-C5	-2.06	1.41	1.46
33	e	102	LHG	O7-C5	-2.06	1.41	1.46
25	B	601	CLA	CMC-C2C	-2.06	1.46	1.50
25	b	602	CLA	CMC-C2C	-2.06	1.46	1.50
35	V	201	HEM	CHB-C1B	2.06	1.39	1.34
35	v	201	HEM	CHB-C1B	2.06	1.39	1.34
25	c	512	CLA	MG-ND	-2.06	2.01	2.05
34	C	515	DGD	O2G-C2G	-2.05	1.41	1.46
34	c	515	DGD	O2G-C2G	-2.05	1.41	1.46
25	B	610	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	611	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	502	CLA	C3B-C2B	-2.05	1.37	1.40
25	B	608	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	609	CLA	CMC-C2C	-2.05	1.46	1.50
25	C	507	CLA	MG-NA	2.05	2.11	2.06
25	c	507	CLA	MG-NA	2.05	2.11	2.06
30	B	630	SQD	O8-S	2.05	1.54	1.47
30	b	601	SQD	O8-S	2.05	1.54	1.47
25	C	512	CLA	C3B-C2B	-2.05	1.37	1.40
25	c	512	CLA	C3B-C2B	-2.05	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	MG-ND	-2.04	2.01	2.05
33	A	419	LHG	O7-C5	-2.04	1.41	1.46
33	a	419	LHG	O7-C5	-2.04	1.41	1.46
25	a	406	CLA	C4B-CHC	-2.04	1.35	1.41
25	D	401	CLA	CMC-C2C	-2.04	1.46	1.50
25	d	401	CLA	CMC-C2C	-2.04	1.46	1.50
25	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	b	603	CLA	CMD-C2D	-2.04	1.46	1.50
34	H	103	DGD	O2G-C2G	-2.04	1.41	1.46
34	h	103	DGD	O2G-C2G	-2.04	1.41	1.46
25	B	607	CLA	MG-NA	2.03	2.11	2.06
25	b	608	CLA	MG-NA	2.03	2.11	2.06
25	B	608	CLA	C3B-C2B	-2.03	1.37	1.40
30	F	102	SQD	O7-S	2.03	1.50	1.45
30	f	102	SQD	O7-S	2.03	1.50	1.45
25	B	607	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.03	1.46	1.50
35	F	101	HEM	CHB-C1B	2.03	1.39	1.34
35	f	101	HEM	CHB-C1B	2.03	1.39	1.34
25	C	502	CLA	C3B-C2B	-2.02	1.37	1.40
25	b	609	CLA	C3B-C2B	-2.02	1.37	1.40
25	B	606	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	607	CLA	CMD-C2D	-2.02	1.46	1.50
25	D	403	CLA	C1D-ND	2.02	1.40	1.37
25	d	403	CLA	C1D-ND	2.02	1.40	1.37
25	B	608	CLA	MG-ND	-2.02	2.01	2.05
25	b	609	CLA	MG-ND	-2.02	2.01	2.05
25	A	406	CLA	C4B-CHC	-2.02	1.35	1.41
36	h	101	RRX	C21-C22	2.01	1.40	1.35
27	B	617	BCR	C1-C6	-2.01	1.51	1.53
33	Z	101	LHG	O7-C5	-2.00	1.41	1.46
33	z	101	LHG	O7-C5	-2.00	1.41	1.46

All (1264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	525	BCR	C20-C21-C22	24.79	162.05	127.28
27	c	525	BCR	C20-C21-C22	24.79	162.05	127.28
27	C	514	BCR	C20-C21-C22	22.93	159.43	127.28
27	c	514	BCR	C20-C21-C22	22.93	159.43	127.28
27	D	411	BCR	C20-C21-C22	21.21	157.02	127.28
27	d	411	BCR	C20-C21-C22	21.20	157.01	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	525	BCR	C16-C17-C18	20.86	156.54	127.28
27	C	527	BCR	C20-C21-C22	20.84	156.50	127.28
27	c	527	BCR	C20-C21-C22	20.84	156.50	127.28
27	C	525	BCR	C16-C17-C18	20.84	156.50	127.28
27	C	526	BCR	C20-C21-C22	20.77	156.41	127.28
27	c	526	BCR	C20-C21-C22	20.77	156.41	127.28
27	B	618	BCR	C20-C21-C22	20.56	156.11	127.28
27	b	619	BCR	C20-C21-C22	20.56	156.11	127.28
27	d	411	BCR	C15-C16-C17	20.50	165.46	123.52
27	B	617	BCR	C16-C17-C18	20.48	156.00	127.28
27	b	618	BCR	C16-C17-C18	20.48	156.00	127.28
27	D	411	BCR	C15-C16-C17	20.47	165.41	123.52
27	c	514	BCR	C15-C16-C17	20.47	165.41	123.52
27	C	514	BCR	C15-C16-C17	20.45	165.37	123.52
27	B	618	BCR	C16-C17-C18	20.45	155.96	127.28
27	b	619	BCR	C16-C17-C18	20.45	155.96	127.28
27	B	617	BCR	C20-C21-C22	20.31	155.76	127.28
27	b	618	BCR	C20-C21-C22	20.31	155.76	127.28
27	c	527	BCR	C15-C16-C17	20.26	164.97	123.52
27	c	526	BCR	C15-C16-C17	20.24	164.94	123.52
27	C	526	BCR	C15-C16-C17	20.24	164.92	123.52
27	C	527	BCR	C15-C16-C17	20.23	164.92	123.52
27	B	619	BCR	C20-C21-C22	20.22	155.64	127.28
27	b	620	BCR	C20-C21-C22	20.22	155.64	127.28
27	A	409	BCR	C15-C16-C17	20.17	164.78	123.52
27	a	409	BCR	C15-C16-C17	20.17	164.78	123.52
27	B	618	BCR	C15-C16-C17	19.96	164.35	123.52
27	b	619	BCR	C15-C16-C17	19.96	164.35	123.52
27	B	619	BCR	C15-C16-C17	19.89	164.21	123.52
27	b	620	BCR	C15-C16-C17	19.89	164.21	123.52
27	B	619	BCR	C16-C17-C18	19.68	154.88	127.28
27	b	620	BCR	C16-C17-C18	19.68	154.88	127.28
27	B	617	BCR	C15-C16-C17	19.61	163.65	123.52
27	b	618	BCR	C15-C16-C17	19.61	163.65	123.52
27	c	514	BCR	C16-C17-C18	19.51	154.65	127.28
27	C	526	BCR	C16-C17-C18	19.51	154.64	127.28
27	c	525	BCR	C15-C16-C17	19.50	163.43	123.52
27	c	526	BCR	C16-C17-C18	19.49	154.61	127.28
27	C	514	BCR	C16-C17-C18	19.49	154.61	127.28
27	C	525	BCR	C15-C16-C17	19.48	163.38	123.52
27	C	527	BCR	C10-C11-C12	19.48	179.63	123.20
27	c	527	BCR	C10-C11-C12	19.48	179.63	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	411	BCR	C16-C17-C18	19.36	154.43	127.28
27	D	411	BCR	C16-C17-C18	19.32	154.38	127.28
27	c	527	BCR	C16-C17-C18	19.31	154.35	127.28
27	C	527	BCR	C16-C17-C18	19.27	154.31	127.28
27	B	617	BCR	C10-C11-C12	19.27	179.03	123.20
27	b	618	BCR	C10-C11-C12	19.26	179.01	123.20
27	A	409	BCR	C16-C17-C18	19.15	154.14	127.28
27	a	409	BCR	C16-C17-C18	19.15	154.14	127.28
27	c	525	BCR	C10-C11-C12	19.09	178.50	123.20
27	C	525	BCR	C10-C11-C12	19.07	178.46	123.20
27	C	514	BCR	C10-C11-C12	18.90	177.96	123.20
27	c	514	BCR	C10-C11-C12	18.90	177.96	123.20
27	C	526	BCR	C10-C11-C12	18.87	177.88	123.20
27	c	526	BCR	C10-C11-C12	18.87	177.88	123.20
27	B	618	BCR	C10-C11-C12	18.70	177.39	123.20
27	b	619	BCR	C10-C11-C12	18.70	177.39	123.20
27	A	409	BCR	C10-C11-C12	18.55	176.96	123.20
27	a	409	BCR	C10-C11-C12	18.55	176.94	123.20
27	D	411	BCR	C10-C11-C12	18.04	175.47	123.20
27	d	411	BCR	C10-C11-C12	18.03	175.45	123.20
27	A	409	BCR	C20-C21-C22	18.03	152.56	127.28
27	a	409	BCR	C20-C21-C22	18.02	152.54	127.28
27	B	619	BCR	C10-C11-C12	17.85	174.93	123.20
27	b	620	BCR	C10-C11-C12	17.84	174.89	123.20
27	d	411	BCR	C11-C10-C9	14.64	147.81	127.28
27	D	411	BCR	C11-C10-C9	14.62	147.78	127.28
27	d	411	BCR	C21-C20-C19	14.45	165.06	123.20
27	D	411	BCR	C21-C20-C19	14.44	165.05	123.20
27	C	527	BCR	C21-C20-C19	14.23	164.43	123.20
27	c	527	BCR	C21-C20-C19	14.23	164.43	123.20
27	B	617	BCR	C21-C20-C19	14.21	164.36	123.20
27	b	618	BCR	C21-C20-C19	14.21	164.36	123.20
27	B	619	BCR	C21-C20-C19	14.20	164.33	123.20
27	b	620	BCR	C21-C20-C19	14.20	164.33	123.20
27	C	526	BCR	C21-C20-C19	14.13	164.15	123.20
27	c	526	BCR	C21-C20-C19	14.13	164.15	123.20
27	B	618	BCR	C21-C20-C19	14.05	163.90	123.20
27	b	619	BCR	C21-C20-C19	14.05	163.90	123.20
27	C	514	BCR	C21-C20-C19	13.90	163.48	123.20
27	c	514	BCR	C21-C20-C19	13.90	163.48	123.20
27	C	525	BCR	C16-C15-C14	13.70	151.55	123.52
27	c	525	BCR	C16-C15-C14	13.70	151.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	409	BCR	C11-C10-C9	13.60	146.36	127.28
27	a	409	BCR	C11-C10-C9	13.60	146.36	127.28
27	C	527	BCR	C16-C15-C14	13.18	150.49	123.52
27	c	527	BCR	C16-C15-C14	13.18	150.49	123.52
27	B	619	BCR	C11-C10-C9	13.01	145.52	127.28
27	b	620	BCR	C11-C10-C9	13.01	145.52	127.28
27	c	525	BCR	C11-C10-C9	12.73	145.13	127.28
27	C	525	BCR	C11-C10-C9	12.70	145.09	127.28
27	B	617	BCR	C16-C15-C14	12.67	149.44	123.52
27	b	618	BCR	C16-C15-C14	12.67	149.44	123.52
27	d	411	BCR	C16-C15-C14	12.66	149.42	123.52
27	D	411	BCR	C16-C15-C14	12.66	149.42	123.52
27	C	525	BCR	C21-C20-C19	12.61	159.74	123.20
27	c	525	BCR	C21-C20-C19	12.61	159.74	123.20
27	B	618	BCR	C16-C15-C14	12.51	149.11	123.52
27	b	619	BCR	C16-C15-C14	12.51	149.11	123.52
27	a	409	BCR	C21-C20-C19	12.41	159.15	123.20
27	A	409	BCR	C21-C20-C19	12.39	159.11	123.20
27	C	514	BCR	C16-C15-C14	12.31	148.71	123.52
27	c	514	BCR	C16-C15-C14	12.31	148.71	123.52
27	C	526	BCR	C11-C10-C9	12.21	144.40	127.28
27	c	526	BCR	C11-C10-C9	12.21	144.40	127.28
27	B	619	BCR	C11-C12-C13	12.21	159.84	126.36
27	b	620	BCR	C11-C12-C13	12.19	159.80	126.36
27	B	619	BCR	C16-C15-C14	12.17	148.42	123.52
27	b	620	BCR	C16-C15-C14	12.17	148.42	123.52
27	c	526	BCR	C16-C15-C14	12.11	148.31	123.52
27	C	526	BCR	C16-C15-C14	12.11	148.29	123.52
27	b	619	BCR	C11-C10-C9	11.86	143.91	127.28
27	A	409	BCR	C16-C15-C14	11.86	147.78	123.52
27	a	409	BCR	C16-C15-C14	11.86	147.78	123.52
27	B	618	BCR	C11-C10-C9	11.84	143.88	127.28
27	C	514	BCR	C11-C10-C9	11.53	143.44	127.28
27	c	514	BCR	C11-C10-C9	11.53	143.44	127.28
27	B	617	BCR	C11-C10-C9	11.41	143.28	127.28
27	b	618	BCR	C11-C10-C9	11.41	143.28	127.28
25	A	405	CLA	C4A-NA-C1A	11.15	111.77	106.68
25	a	405	CLA	C4A-NA-C1A	11.15	111.77	106.68
27	a	409	BCR	C11-C12-C13	11.11	156.83	126.36
27	A	409	BCR	C11-C12-C13	11.10	156.80	126.36
27	B	618	BCR	C11-C12-C13	11.07	156.72	126.36
27	b	619	BCR	C11-C12-C13	11.07	156.72	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	514	BCR	C11-C12-C13	11.05	156.66	126.36
27	c	514	BCR	C11-C12-C13	11.05	156.66	126.36
27	D	411	BCR	C11-C12-C13	11.04	156.63	126.36
27	d	411	BCR	C11-C12-C13	11.04	156.63	126.36
27	C	526	BCR	C11-C12-C13	11.03	156.59	126.36
27	c	526	BCR	C11-C12-C13	11.03	156.59	126.36
27	C	525	BCR	C11-C12-C13	10.92	156.30	126.36
27	c	525	BCR	C11-C12-C13	10.92	156.30	126.36
27	b	618	BCR	C11-C12-C13	10.79	155.96	126.36
27	B	617	BCR	C11-C12-C13	10.79	155.95	126.36
27	C	527	BCR	C11-C12-C13	10.71	155.73	126.36
27	c	527	BCR	C11-C12-C13	10.71	155.73	126.36
27	C	527	BCR	C11-C10-C9	10.42	141.89	127.28
27	c	527	BCR	C11-C10-C9	10.42	141.89	127.28
25	B	604	CLA	C4A-NA-C1A	9.57	111.04	106.68
25	b	605	CLA	C4A-NA-C1A	9.57	111.04	106.68
25	B	611	CLA	C4A-NA-C1A	9.49	111.01	106.68
25	b	612	CLA	C4A-NA-C1A	9.49	111.01	106.68
25	b	615	CLA	C4A-NA-C1A	9.09	110.83	106.68
25	B	614	CLA	C4A-NA-C1A	9.08	110.82	106.68
25	c	501	CLA	C4A-NA-C1A	8.90	110.74	106.68
25	B	610	CLA	C4A-NA-C1A	8.89	110.73	106.68
25	b	611	CLA	C4A-NA-C1A	8.89	110.73	106.68
25	C	501	CLA	C4A-NA-C1A	8.88	110.73	106.68
25	C	509	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	c	509	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	B	612	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	b	613	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	b	607	CLA	C4A-NA-C1A	8.47	110.54	106.68
25	B	606	CLA	C4A-NA-C1A	8.34	110.49	106.68
25	D	404	CLA	C4A-NA-C1A	8.34	110.48	106.68
25	d	404	CLA	C4A-NA-C1A	8.34	110.48	106.68
25	B	602	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	b	603	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	B	603	CLA	C4A-NA-C1A	8.09	110.37	106.68
25	C	506	CLA	C4A-NA-C1A	8.08	110.36	106.68
25	c	506	CLA	C4A-NA-C1A	8.08	110.36	106.68
25	b	604	CLA	C4A-NA-C1A	8.06	110.35	106.68
27	C	525	BCR	C20-C19-C18	8.03	148.39	126.36
27	c	525	BCR	C20-C19-C18	8.03	148.39	126.36
25	B	608	CLA	C4A-NA-C1A	7.99	110.32	106.68
25	b	609	CLA	C4A-NA-C1A	7.99	110.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	CLA	C4A-NA-C1A	7.98	110.32	106.68
25	a	408	CLA	C4A-NA-C1A	7.98	110.32	106.68
25	B	615	CLA	C4A-NA-C1A	7.91	110.29	106.68
25	b	616	CLA	C4A-NA-C1A	7.90	110.28	106.68
25	c	508	CLA	C4A-NA-C1A	7.90	110.28	106.68
25	C	508	CLA	C4A-NA-C1A	7.88	110.27	106.68
25	d	403	CLA	C4A-NA-C1A	7.53	110.12	106.68
25	D	403	CLA	C4A-NA-C1A	7.48	110.09	106.68
25	B	605	CLA	C4A-NA-C1A	7.40	110.06	106.68
25	b	606	CLA	C4A-NA-C1A	7.40	110.06	106.68
25	b	614	CLA	C4A-NA-C1A	7.33	110.02	106.68
25	B	613	CLA	C4A-NA-C1A	7.29	110.01	106.68
28	D	407	LMG	O1-C1-C2	7.11	119.07	108.27
28	d	407	LMG	O1-C1-C2	7.11	119.07	108.27
27	A	409	BCR	C24-C23-C22	-6.95	115.95	126.23
27	a	409	BCR	C24-C23-C22	-6.95	115.95	126.23
27	A	409	BCR	C20-C19-C18	6.93	145.37	126.36
27	a	409	BCR	C20-C19-C18	6.93	145.37	126.36
25	D	401	CLA	C4A-NA-C1A	6.87	109.81	106.68
27	C	526	BCR	C24-C23-C22	-6.76	116.23	126.23
27	c	526	BCR	C24-C23-C22	-6.76	116.23	126.23
28	A	410	LMG	C7-O1-C1	6.75	128.28	113.80
28	a	410	LMG	C7-O1-C1	6.75	128.28	113.80
27	C	527	BCR	C20-C19-C18	6.73	144.80	126.36
27	c	527	BCR	C20-C19-C18	6.73	144.80	126.36
25	d	401	CLA	C4A-NA-C1A	6.72	109.75	106.68
27	b	620	BCR	C20-C19-C18	6.71	144.75	126.36
27	B	619	BCR	C20-C19-C18	6.69	144.70	126.36
27	C	526	BCR	C20-C19-C18	6.63	144.54	126.36
27	c	526	BCR	C20-C19-C18	6.63	144.54	126.36
27	C	514	BCR	C20-C19-C18	6.60	144.45	126.36
27	c	514	BCR	C20-C19-C18	6.60	144.45	126.36
27	B	617	BCR	C20-C19-C18	6.57	144.39	126.36
27	b	618	BCR	C20-C19-C18	6.57	144.39	126.36
27	B	618	BCR	C20-C19-C18	6.57	144.38	126.36
27	b	619	BCR	C20-C19-C18	6.56	144.36	126.36
25	C	513	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	C	503	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	c	503	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	c	513	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	B	616	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	b	617	CLA	C4A-NA-C1A	6.33	109.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	502	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	c	502	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	C	510	CLA	C4A-NA-C1A	6.30	109.56	106.68
25	c	510	CLA	C4A-NA-C1A	6.26	109.54	106.68
27	D	411	BCR	C20-C19-C18	6.21	143.39	126.36
27	d	411	BCR	C20-C19-C18	6.21	143.39	126.36
25	C	507	CLA	C4A-NA-C1A	6.15	109.49	106.68
25	c	507	CLA	C4A-NA-C1A	6.15	109.49	106.68
35	v	201	HEM	CHC-C4B-NB	6.15	131.05	124.44
35	V	201	HEM	CHC-C4B-NB	6.11	131.01	124.44
25	B	609	CLA	C4A-NA-C1A	5.98	109.41	106.68
35	F	101	HEM	CBD-CAD-C3D	-5.97	96.03	112.53
35	f	101	HEM	CBD-CAD-C3D	-5.97	96.03	112.53
25	b	610	CLA	C4A-NA-C1A	5.94	109.39	106.68
25	C	505	CLA	C4A-NA-C1A	5.88	109.36	106.68
25	c	505	CLA	C4A-NA-C1A	5.88	109.36	106.68
25	C	511	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	c	511	CLA	C4A-NA-C1A	5.87	109.36	106.68
35	F	101	HEM	CHC-C4B-NB	5.87	130.75	124.44
35	f	101	HEM	CHC-C4B-NB	5.87	130.75	124.44
27	C	527	BCR	C24-C23-C22	-5.64	117.90	126.23
27	c	527	BCR	C24-C23-C22	-5.64	117.90	126.23
27	B	617	BCR	C24-C23-C22	-5.58	117.99	126.23
27	b	618	BCR	C24-C23-C22	-5.58	117.99	126.23
25	C	512	CLA	C4A-NA-C1A	5.48	109.18	106.68
25	c	512	CLA	C4A-NA-C1A	5.48	109.18	106.68
25	B	604	CLA	C1-C2-C3	-5.46	117.25	126.20
25	b	605	CLA	C1-C2-C3	-5.44	117.28	126.20
27	B	618	BCR	C24-C23-C22	-5.42	118.21	126.23
27	b	619	BCR	C24-C23-C22	-5.42	118.21	126.23
27	c	525	BCR	C24-C23-C22	-5.26	118.45	126.23
27	C	525	BCR	C24-C23-C22	-5.24	118.48	126.23
25	a	406	CLA	C4A-NA-C1A	5.23	109.07	106.68
28	D	407	LMG	O7-C10-C11	5.20	122.72	111.48
28	d	407	LMG	O7-C10-C11	5.20	122.72	111.48
25	a	408	CLA	CMB-C2B-C1B	-5.19	120.85	128.46
25	A	408	CLA	CMB-C2B-C1B	-5.17	120.88	128.46
25	A	406	CLA	C4A-NA-C1A	5.17	109.04	106.68
27	D	411	BCR	C24-C23-C22	-5.13	118.64	126.23
27	d	411	BCR	C24-C23-C22	-5.13	118.64	126.23
35	F	101	HEM	CHD-C1D-ND	5.08	129.90	124.44
35	f	101	HEM	CHD-C1D-ND	5.08	129.90	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	618	BCR	C7-C8-C9	-5.05	118.76	126.23
27	B	617	BCR	C7-C8-C9	-5.03	118.80	126.23
27	C	514	BCR	C7-C8-C9	-4.98	118.86	126.23
27	c	514	BCR	C7-C8-C9	-4.98	118.86	126.23
34	C	516	DGD	O2G-C1B-C2B	4.85	121.98	111.48
34	c	516	DGD	O2G-C1B-C2B	4.85	121.98	111.48
25	C	510	CLA	CMB-C2B-C1B	-4.85	121.35	128.46
25	c	510	CLA	CMB-C2B-C1B	-4.85	121.35	128.46
25	c	513	CLA	CMB-C2B-C1B	-4.77	121.47	128.46
25	C	513	CLA	CMB-C2B-C1B	-4.77	121.47	128.46
25	c	502	CLA	CMB-C2B-C1B	-4.69	121.59	128.46
25	C	502	CLA	CMB-C2B-C1B	-4.67	121.61	128.46
25	A	405	CLA	CMB-C2B-C1B	-4.64	121.66	128.46
25	a	405	CLA	CMB-C2B-C1B	-4.64	121.66	128.46
25	B	601	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	b	602	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	B	615	CLA	CMB-C2B-C1B	-4.62	121.69	128.46
25	b	616	CLA	CMB-C2B-C1B	-4.62	121.69	128.46
25	c	504	CLA	CMB-C2B-C1B	-4.60	121.71	128.46
25	C	504	CLA	CMB-C2B-C1B	-4.60	121.72	128.46
30	B	630	SQD	C1-O5-C5	-4.59	104.76	113.72
30	b	601	SQD	C1-O5-C5	-4.59	104.76	113.72
25	C	503	CLA	CMB-C2B-C1B	-4.56	121.77	128.46
25	c	503	CLA	CMB-C2B-C1B	-4.56	121.77	128.46
25	C	508	CLA	CMB-C2B-C1B	-4.53	121.83	128.46
25	c	508	CLA	CMB-C2B-C1B	-4.53	121.83	128.46
25	B	608	CLA	CMB-C2B-C1B	-4.42	121.97	128.46
25	b	609	CLA	CMB-C2B-C1B	-4.42	121.98	128.46
26	D	402	PHO	C1-C2-C3	-4.37	119.04	126.20
28	B	621	LMG	O7-C10-C11	4.36	120.92	111.48
28	b	622	LMG	O7-C10-C11	4.36	120.92	111.48
27	C	525	BCR	C33-C5-C6	-4.36	119.73	124.48
27	c	525	BCR	C33-C5-C6	-4.36	119.73	124.48
26	d	402	PHO	C1-C2-C3	-4.36	119.06	126.20
25	B	607	CLA	C4A-NA-C1A	4.33	108.66	106.68
25	b	608	CLA	C4A-NA-C1A	4.33	108.66	106.68
25	b	614	CLA	C1-C2-C3	-4.32	119.11	126.20
25	c	501	CLA	CMB-C2B-C1B	-4.32	122.13	128.46
25	C	509	CLA	CMB-C2B-C1B	-4.31	122.15	128.46
28	J	101	LMG	O7-C10-C11	4.30	120.79	111.48
28	j	101	LMG	O7-C10-C11	4.30	120.79	111.48
25	B	606	CLA	CMB-C2B-C1B	-4.30	122.15	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	CMB-C2B-C1B	-4.30	122.15	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.30	122.15	128.46
25	c	509	CLA	CMB-C2B-C1B	-4.30	122.16	128.46
25	B	613	CLA	C1-C2-C3	-4.30	119.16	126.20
28	A	413	LMG	O7-C10-C11	4.27	120.72	111.48
28	a	413	LMG	O7-C10-C11	4.27	120.72	111.48
34	C	515	DGD	O2G-C1B-C2B	4.26	120.70	111.48
34	c	515	DGD	O2G-C1B-C2B	4.25	120.68	111.48
25	c	512	CLA	CMB-C2B-C1B	-4.25	122.23	128.46
25	C	512	CLA	CMB-C2B-C1B	-4.24	122.24	128.46
25	B	609	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
25	C	511	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
25	b	610	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
25	c	511	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
28	B	629	LMG	O7-C10-C11	4.21	120.58	111.48
28	b	630	LMG	O7-C10-C11	4.21	120.58	111.48
35	V	201	HEM	CHD-C1D-ND	4.18	128.93	124.44
25	B	613	CLA	CMB-C2B-C1B	-4.17	122.35	128.46
25	b	614	CLA	CMB-C2B-C1B	-4.17	122.35	128.46
35	v	201	HEM	CHD-C1D-ND	4.17	128.92	124.44
27	B	618	BCR	C33-C5-C6	-4.16	119.94	124.48
27	b	619	BCR	C33-C5-C6	-4.15	119.96	124.48
25	c	504	CLA	C4A-NA-C1A	4.14	108.57	106.68
25	b	604	CLA	CMB-C2B-C1B	-4.12	122.42	128.46
25	B	603	CLA	CMB-C2B-C1B	-4.12	122.42	128.46
25	C	504	CLA	C4A-NA-C1A	4.12	108.56	106.68
25	B	610	CLA	CMB-C2B-C1B	-4.11	122.44	128.46
25	b	611	CLA	CMB-C2B-C1B	-4.11	122.44	128.46
25	C	510	CLA	C1-C2-C3	-4.10	119.47	126.20
25	c	510	CLA	C1-C2-C3	-4.10	119.47	126.20
27	D	411	BCR	C38-C26-C25	-4.08	120.03	124.48
27	d	411	BCR	C38-C26-C25	-4.08	120.03	124.48
25	B	611	CLA	CMB-C2B-C1B	-4.08	122.48	128.46
25	b	612	CLA	CMB-C2B-C1B	-4.08	122.48	128.46
25	B	614	CLA	C1-C2-C3	-4.06	119.54	126.20
25	b	615	CLA	C1-C2-C3	-4.06	119.54	126.20
27	C	526	BCR	C7-C8-C9	-4.06	120.23	126.23
27	c	526	BCR	C7-C8-C9	-4.06	120.23	126.23
27	B	619	BCR	C24-C23-C22	-4.05	120.24	126.23
27	b	620	BCR	C24-C23-C22	-4.05	120.24	126.23
28	C	519	LMG	O7-C10-C11	4.01	120.15	111.48
28	c	519	LMG	O7-C10-C11	4.01	120.15	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	CMB-C2B-C1B	-4.01	122.59	128.46
25	d	404	CLA	CMB-C2B-C1B	-4.00	122.60	128.46
25	A	408	CLA	CMB-C2B-C3B	3.97	132.62	124.68
25	b	617	CLA	CMB-C2B-C1B	-3.97	122.65	128.46
25	a	408	CLA	CMB-C2B-C3B	3.96	132.61	124.68
25	B	605	CLA	CMB-C2B-C1B	-3.96	122.65	128.46
25	B	602	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
25	b	603	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
25	B	616	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
33	L	101	LHG	O7-C7-C8	3.95	120.02	111.48
33	l	101	LHG	O7-C7-C8	3.95	120.02	111.48
25	B	607	CLA	CMB-C2B-C1B	-3.94	122.68	128.46
25	b	606	CLA	CMB-C2B-C1B	-3.94	122.69	128.46
25	b	608	CLA	CMB-C2B-C1B	-3.93	122.69	128.46
33	Z	101	LHG	O7-C7-C8	3.91	119.94	111.48
33	z	101	LHG	O7-C7-C8	3.91	119.94	111.48
33	b	627	LHG	O7-C7-C8	3.91	119.94	111.48
33	B	626	LHG	O7-C7-C8	3.91	119.93	111.48
30	F	102	SQD	O47-C7-C8	3.90	119.91	111.48
30	f	102	SQD	O47-C7-C8	3.90	119.91	111.48
25	b	602	CLA	CMB-C2B-C1B	-3.89	122.75	128.46
25	D	404	CLA	CHB-C4A-NA	3.89	130.02	124.40
25	d	404	CLA	CHB-C4A-NA	3.89	130.02	124.40
25	c	502	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
25	c	513	CLA	CMB-C2B-C3B	3.89	132.45	124.68
25	C	502	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
25	C	513	CLA	CMB-C2B-C3B	3.88	132.44	124.68
25	D	403	CLA	CMB-C2B-C1B	-3.88	122.78	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.88	122.78	128.46
25	B	601	CLA	CMB-C2B-C1B	-3.87	122.78	128.46
28	A	410	LMG	O7-C10-C11	3.87	119.85	111.48
28	a	410	LMG	O7-C10-C11	3.86	119.83	111.48
25	B	614	CLA	CMB-C2B-C1B	-3.84	122.82	128.46
25	b	615	CLA	CMB-C2B-C1B	-3.84	122.83	128.46
27	c	526	BCR	C3-C4-C5	-3.84	107.21	114.06
27	C	526	BCR	C3-C4-C5	-3.82	107.24	114.06
33	E	102	LHG	O7-C7-C8	3.82	119.75	111.48
28	d	407	LMG	O6-C1-O1	-3.81	101.03	110.04
34	C	517	DGD	O2G-C1B-C2B	3.81	119.72	111.48
34	c	517	DGD	O2G-C1B-C2B	3.81	119.72	111.48
28	D	407	LMG	O6-C1-O1	-3.81	101.05	110.04
33	e	102	LHG	O7-C7-C8	3.81	119.72	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	525	BCR	C38-C26-C25	-3.80	120.34	124.48
27	c	525	BCR	C38-C26-C25	-3.80	120.34	124.48
25	b	613	CLA	CMB-C2B-C1B	-3.80	122.89	128.46
27	C	526	BCR	C38-C26-C25	-3.79	120.35	124.48
27	c	526	BCR	C38-C26-C25	-3.79	120.35	124.48
25	B	612	CLA	CMB-C2B-C1B	-3.79	122.91	128.46
27	B	617	BCR	C33-C5-C6	-3.78	120.36	124.48
25	C	501	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
25	c	501	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
25	c	505	CLA	CMB-C2B-C1B	-3.78	122.92	128.46
25	C	505	CLA	CMB-C2B-C1B	-3.77	122.93	128.46
27	b	618	BCR	C33-C5-C6	-3.77	120.37	124.48
30	F	102	SQD	O9-S-O7	-3.74	101.64	113.82
30	f	102	SQD	O9-S-O7	-3.74	101.64	113.82
28	C	518	LMG	O7-C10-C11	3.74	119.58	111.48
25	C	502	CLA	C1-C2-C3	-3.74	120.07	126.20
25	c	502	CLA	C1-C2-C3	-3.74	120.07	126.20
28	c	518	LMG	O7-C10-C11	3.73	119.56	111.48
25	c	506	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
25	C	506	CLA	CMB-C2B-C1B	-3.71	123.02	128.46
30	F	102	SQD	O5-C5-C4	3.70	116.37	109.70
30	f	102	SQD	O5-C5-C4	3.69	116.34	109.70
35	v	201	HEM	C1B-NB-C4B	3.68	109.56	105.21
27	a	409	BCR	C38-C26-C25	-3.67	120.48	124.48
35	V	201	HEM	C1B-NB-C4B	3.67	109.55	105.21
25	D	401	CLA	CMB-C2B-C1B	-3.65	123.10	128.46
25	d	401	CLA	CMB-C2B-C1B	-3.65	123.10	128.46
25	C	510	CLA	CMB-C2B-C3B	3.64	131.96	124.68
25	c	510	CLA	CMB-C2B-C3B	3.64	131.96	124.68
27	A	409	BCR	C38-C26-C25	-3.64	120.51	124.48
25	B	612	CLA	CHB-C4A-NA	3.64	129.65	124.40
25	b	613	CLA	CHB-C4A-NA	3.64	129.65	124.40
27	B	619	BCR	C7-C8-C9	-3.63	120.86	126.23
27	b	620	BCR	C7-C8-C9	-3.63	120.86	126.23
25	B	606	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
25	b	607	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
25	D	401	CLA	CHB-C4A-NA	3.62	129.63	124.40
34	H	103	DGD	O2G-C1B-C2B	3.61	119.29	111.48
34	h	103	DGD	O2G-C1B-C2B	3.61	119.29	111.48
27	C	527	BCR	C33-C5-C6	-3.61	120.55	124.48
25	C	503	CLA	CMB-C2B-C3B	3.60	131.88	124.68
25	c	503	CLA	CMB-C2B-C3B	3.60	131.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	418	LHG	O7-C7-C8	3.60	119.27	111.48
25	d	401	CLA	CHB-C4A-NA	3.59	129.59	124.40
33	a	418	LHG	O7-C7-C8	3.59	119.24	111.48
25	c	507	CLA	CMB-C2B-C1B	-3.58	123.20	128.46
27	B	619	BCR	C33-C5-C6	-3.58	120.58	124.48
27	A	409	BCR	C37-C22-C21	-3.57	117.03	122.82
27	a	409	BCR	C37-C22-C21	-3.57	117.03	122.82
27	c	527	BCR	C33-C5-C6	-3.56	120.60	124.48
25	C	507	CLA	CMB-C2B-C1B	-3.56	123.24	128.46
27	C	514	BCR	C24-C23-C22	-3.56	120.97	126.23
27	c	514	BCR	C24-C23-C22	-3.56	120.97	126.23
33	E	102	LHG	C5-O7-C7	-3.55	109.30	117.80
33	e	102	LHG	C5-O7-C7	-3.55	109.30	117.80
25	B	615	CLA	C1D-ND-C4D	3.55	108.80	106.31
25	b	616	CLA	C1D-ND-C4D	3.55	108.80	106.31
29	D	405	PL9	C7-C3-C4	3.55	119.83	116.91
29	d	405	PL9	C7-C3-C4	3.55	119.83	116.91
27	b	620	BCR	C33-C5-C6	-3.54	120.62	124.48
25	b	609	CLA	CHB-C4A-NA	3.54	129.51	124.40
25	B	608	CLA	CHB-C4A-NA	3.53	129.50	124.40
25	B	614	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
25	C	505	CLA	C1-C2-C3	-3.51	120.44	126.20
25	c	505	CLA	C1-C2-C3	-3.51	120.44	126.20
25	B	602	CLA	O2D-CGD-CBD	3.51	117.36	111.23
25	b	603	CLA	O2D-CGD-CBD	3.51	117.36	111.23
25	b	615	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
25	B	610	CLA	C1-C2-C3	-3.50	120.46	126.20
25	b	611	CLA	C1-C2-C3	-3.50	120.46	126.20
25	a	406	CLA	O2D-CGD-CBD	3.50	117.34	111.23
35	v	201	HEM	CBA-CAA-C2A	-3.50	106.66	112.54
35	V	201	HEM	CBA-CAA-C2A	-3.49	106.66	112.54
27	c	526	BCR	C33-C5-C6	-3.49	120.68	124.48
25	C	512	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
25	c	512	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
27	C	526	BCR	C33-C5-C6	-3.48	120.69	124.48
25	A	406	CLA	O2D-CGD-CBD	3.48	117.31	111.23
25	C	502	CLA	CMB-C2B-C3B	3.48	131.63	124.68
25	c	502	CLA	CMB-C2B-C3B	3.47	131.62	124.68
28	A	410	LMG	O1-C1-C2	3.46	113.53	108.27
28	a	410	LMG	O1-C1-C2	3.46	113.53	108.27
25	C	508	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
25	c	508	CLA	O2D-CGD-O1D	-3.45	117.13	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	618	BCR	C38-C26-C25	-3.44	120.72	124.48
27	C	527	BCR	C19-C18-C17	3.44	124.41	119.01
27	c	527	BCR	C19-C18-C17	3.44	124.41	119.01
27	b	619	BCR	C38-C26-C25	-3.43	120.74	124.48
25	b	605	CLA	CMB-C2B-C1B	-3.43	123.43	128.46
27	C	525	BCR	C3-C4-C5	-3.43	107.94	114.06
27	C	514	BCR	C3-C4-C5	-3.43	107.95	114.06
27	c	514	BCR	C3-C4-C5	-3.43	107.95	114.06
35	V	201	HEM	CHA-C4D-ND	3.42	128.62	124.37
35	v	201	HEM	CHA-C4D-ND	3.42	128.62	124.37
25	B	608	CLA	CMB-C2B-C3B	3.42	131.52	124.68
25	b	609	CLA	CMB-C2B-C3B	3.42	131.52	124.68
27	c	525	BCR	C3-C4-C5	-3.42	107.96	114.06
25	B	601	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
25	B	604	CLA	CMB-C2B-C1B	-3.41	123.46	128.46
35	F	101	HEM	CHA-C4D-ND	3.40	128.59	124.37
35	f	101	HEM	CHA-C4D-ND	3.40	128.59	124.37
27	C	525	BCR	C31-C1-C6	-3.39	104.92	110.24
25	C	509	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
27	c	527	BCR	C38-C26-C25	-3.39	120.79	124.48
25	B	609	CLA	CMB-C2B-C3B	3.39	131.45	124.68
25	b	610	CLA	CMB-C2B-C3B	3.39	131.45	124.68
30	F	102	SQD	C1-O5-C5	3.39	120.33	113.72
25	c	509	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
25	B	613	CLA	C1D-ND-C4D	3.38	108.69	106.31
25	b	614	CLA	C1D-ND-C4D	3.38	108.69	106.31
27	c	525	BCR	C31-C1-C6	-3.38	104.94	110.24
30	f	102	SQD	C1-O5-C5	3.38	120.32	113.72
27	B	617	BCR	C3-C4-C5	-3.38	108.03	114.06
27	b	618	BCR	C3-C4-C5	-3.38	108.03	114.06
25	D	404	CLA	CMB-C2B-C3B	3.38	131.43	124.68
27	B	619	BCR	C3-C4-C5	-3.38	108.03	114.06
27	b	620	BCR	C3-C4-C5	-3.38	108.03	114.06
25	d	404	CLA	CMB-C2B-C3B	3.37	131.43	124.68
25	A	408	CLA	O2D-CGD-CBD	3.37	117.12	111.23
25	a	408	CLA	O2D-CGD-CBD	3.37	117.12	111.23
25	C	509	CLA	CMB-C2B-C3B	3.36	131.40	124.68
25	c	509	CLA	CMB-C2B-C3B	3.36	131.40	124.68
25	c	504	CLA	CMB-C2B-C3B	3.36	131.40	124.68
25	C	504	CLA	CMB-C2B-C3B	3.36	131.39	124.68
36	H	101	RRX	C37-C22-C21	-3.35	117.39	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	527	BCR	C38-C26-C25	-3.34	120.84	124.48
27	D	411	BCR	C19-C18-C17	3.34	124.27	119.01
27	d	411	BCR	C19-C18-C17	3.34	124.27	119.01
36	h	101	RRX	C37-C22-C21	-3.33	117.42	122.82
25	B	615	CLA	CMB-C2B-C3B	3.33	131.34	124.68
25	b	616	CLA	CMB-C2B-C3B	3.33	131.34	124.68
27	C	514	BCR	C33-C5-C6	-3.31	120.87	124.48
27	c	514	BCR	C33-C5-C6	-3.31	120.87	124.48
25	A	405	CLA	CMB-C2B-C3B	3.31	131.30	124.68
25	a	405	CLA	CMB-C2B-C3B	3.31	131.30	124.68
25	B	615	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
25	b	616	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
27	A	409	BCR	C33-C5-C6	-3.29	120.89	124.48
27	a	409	BCR	C33-C5-C6	-3.29	120.89	124.48
25	D	401	CLA	CMB-C2B-C3B	3.29	131.25	124.68
25	d	401	CLA	CMB-C2B-C3B	3.29	131.25	124.68
27	C	525	BCR	C15-C14-C13	-3.28	122.67	127.28
27	c	525	BCR	C15-C14-C13	-3.28	122.67	127.28
25	A	406	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	a	406	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	C	508	CLA	CMB-C2B-C3B	3.28	131.24	124.68
25	c	508	CLA	CMB-C2B-C3B	3.28	131.24	124.68
25	c	501	CLA	CMB-C2B-C3B	3.27	131.22	124.68
25	B	602	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
25	b	603	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
25	C	501	CLA	CMB-C2B-C3B	3.26	131.20	124.68
25	b	617	CLA	CMB-C2B-C3B	3.24	131.16	124.68
25	c	504	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
25	c	511	CLA	CMB-C2B-C3B	3.23	131.14	124.68
34	H	103	DGD	O1G-C1A-C2A	3.23	121.69	111.83
34	h	103	DGD	O1G-C1A-C2A	3.23	121.69	111.83
25	C	511	CLA	CMB-C2B-C3B	3.23	131.14	124.68
25	B	616	CLA	CMB-C2B-C3B	3.23	131.13	124.68
25	C	512	CLA	CMB-C2B-C3B	3.23	131.13	124.68
25	c	512	CLA	CMB-C2B-C3B	3.23	131.13	124.68
36	h	101	RRX	C34-C9-C10	-3.22	117.60	122.82
25	B	604	CLA	O2D-CGD-CBD	3.21	116.84	111.23
25	b	605	CLA	O2D-CGD-CBD	3.21	116.84	111.23
36	H	101	RRX	C34-C9-C10	-3.20	117.62	122.82
33	D	406	LHG	O7-C7-C8	3.20	118.41	111.48
33	d	406	LHG	O7-C7-C8	3.20	118.41	111.48
28	B	629	LMG	O8-C28-C29	3.20	121.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	630	LMG	O8-C28-C29	3.20	121.60	111.83
25	C	504	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
28	C	518	LMG	O8-C28-C29	3.20	121.59	111.83
28	c	518	LMG	O8-C28-C29	3.20	121.59	111.83
27	C	514	BCR	C19-C18-C17	3.20	124.04	119.01
27	c	514	BCR	C19-C18-C17	3.20	124.04	119.01
27	c	527	BCR	C28-C27-C26	-3.20	108.36	114.06
27	B	617	BCR	C38-C26-C25	-3.19	121.00	124.48
27	b	618	BCR	C38-C26-C25	-3.19	121.00	124.48
27	C	527	BCR	C28-C27-C26	-3.19	108.37	114.06
36	H	101	RRX	C15-C16-C17	3.18	130.03	123.52
36	h	101	RRX	C15-C16-C17	3.18	130.03	123.52
25	B	606	CLA	CMB-C2B-C3B	3.18	131.04	124.68
25	b	607	CLA	CMB-C2B-C3B	3.18	131.04	124.68
25	B	608	CLA	C1-C2-C3	-3.17	121.00	126.20
25	b	609	CLA	C1-C2-C3	-3.17	121.00	126.20
25	B	606	CLA	O2D-CGD-CBD	3.16	116.76	111.23
25	b	607	CLA	O2D-CGD-CBD	3.16	116.76	111.23
25	B	612	CLA	CMB-C2B-C3B	3.16	131.00	124.68
25	A	408	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
25	a	408	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
25	B	611	CLA	CMB-C2B-C3B	3.16	130.99	124.68
25	b	612	CLA	CMB-C2B-C3B	3.16	130.99	124.68
27	C	514	BCR	C38-C26-C25	-3.15	121.04	124.48
27	c	514	BCR	C38-C26-C25	-3.15	121.04	124.48
25	b	613	CLA	CMB-C2B-C3B	3.15	130.98	124.68
25	C	505	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
27	c	514	BCR	C31-C1-C6	-3.14	105.31	110.24
25	c	505	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
27	d	411	BCR	C15-C14-C13	-3.13	122.89	127.28
27	C	514	BCR	C31-C1-C6	-3.12	105.34	110.24
27	D	411	BCR	C15-C14-C13	-3.12	122.90	127.28
30	F	102	SQD	O7-S-C6	3.12	111.41	106.76
25	C	508	CLA	O2D-CGD-CBD	3.11	116.67	111.23
25	c	508	CLA	O2D-CGD-CBD	3.11	116.67	111.23
25	A	406	CLA	CMB-C2B-C1B	-3.10	123.91	128.46
30	f	102	SQD	O7-S-C6	3.10	111.39	106.76
25	d	404	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
33	D	406	LHG	O8-C23-C24	3.09	121.27	111.83
33	d	406	LHG	O8-C23-C24	3.09	121.27	111.83
30	A	412	SQD	O3-C3-C4	3.09	117.66	110.38
30	a	412	SQD	O3-C3-C4	3.09	117.66	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	CMB-C2B-C1B	-3.09	123.93	128.46
27	C	527	BCR	C15-C14-C13	-3.09	122.95	127.28
27	c	527	BCR	C15-C14-C13	-3.09	122.95	127.28
33	L	101	LHG	O8-C23-C24	3.09	121.24	111.83
33	l	101	LHG	O8-C23-C24	3.09	121.24	111.83
28	C	519	LMG	O8-C28-C29	3.08	121.24	111.83
28	c	519	LMG	O8-C28-C29	3.08	121.24	111.83
25	D	404	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
28	a	410	LMG	O3-C3-C2	3.07	117.62	110.38
25	C	512	CLA	CHB-C4A-NA	3.07	128.84	124.40
25	c	512	CLA	CHB-C4A-NA	3.07	128.84	124.40
28	A	410	LMG	O3-C3-C2	3.07	117.62	110.38
27	C	525	BCR	C28-C27-C26	-3.06	108.59	114.06
27	c	525	BCR	C28-C27-C26	-3.06	108.59	114.06
28	a	410	LMG	O8-C28-C29	3.06	121.17	111.83
25	b	609	CLA	O2D-CGD-CBD	3.06	116.58	111.23
28	A	410	LMG	O8-C28-C29	3.05	121.15	111.83
25	B	608	CLA	O2D-CGD-CBD	3.05	116.57	111.23
28	A	410	LMG	O2-C2-C3	-3.04	103.20	110.38
28	a	410	LMG	O2-C2-C3	-3.04	103.20	110.38
27	C	527	BCR	C36-C18-C17	-3.03	117.91	122.82
27	c	527	BCR	C36-C18-C17	-3.03	117.91	122.82
25	D	401	CLA	C1B-CHB-C4A	-3.03	124.26	130.04
25	C	505	CLA	O2D-CGD-CBD	3.03	116.53	111.23
25	c	511	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	C	507	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	C	511	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	c	505	CLA	O2D-CGD-CBD	3.02	116.51	111.23
27	B	619	BCR	C38-C26-C25	-3.02	121.19	124.48
25	d	401	CLA	C1B-CHB-C4A	-3.01	124.29	130.04
25	c	507	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
27	b	620	BCR	C38-C26-C25	-3.00	121.21	124.48
33	B	626	LHG	O8-C23-C24	2.98	120.92	111.83
33	b	627	LHG	O8-C23-C24	2.98	120.92	111.83
25	c	507	CLA	CMB-C2B-C3B	2.97	130.63	124.68
25	b	609	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	c	503	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	C	503	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	B	608	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
28	D	407	LMG	O8-C28-C29	2.97	120.89	111.83
28	d	407	LMG	O8-C28-C29	2.97	120.89	111.83
25	C	507	CLA	CHB-C4A-NA	2.96	128.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	CHB-C4A-NA	2.96	128.68	124.40
25	B	602	CLA	CMB-C2B-C3B	2.96	130.60	124.68
25	b	603	CLA	CMB-C2B-C3B	2.96	130.60	124.68
25	C	507	CLA	CMB-C2B-C3B	2.96	130.59	124.68
25	b	604	CLA	CMB-C2B-C3B	2.96	130.59	124.68
25	B	603	CLA	CMB-C2B-C3B	2.96	130.59	124.68
27	c	527	BCR	C3-C4-C5	-2.95	108.79	114.06
25	b	608	CLA	CMB-C2B-C3B	2.94	130.57	124.68
25	B	607	CLA	CMB-C2B-C3B	2.94	130.56	124.68
25	C	505	CLA	CMB-C2B-C3B	2.94	130.55	124.68
25	c	505	CLA	CMB-C2B-C3B	2.94	130.55	124.68
25	b	602	CLA	CMB-C2B-C3B	2.94	130.55	124.68
27	C	527	BCR	C3-C4-C5	-2.93	108.82	114.06
25	C	513	CLA	C1-C2-C3	-2.93	121.39	126.20
25	c	513	CLA	C1-C2-C3	-2.93	121.39	126.20
25	C	502	CLA	C1B-CHB-C4A	-2.93	124.45	130.04
25	c	502	CLA	C1B-CHB-C4A	-2.93	124.45	130.04
25	C	509	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	c	509	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	B	601	CLA	CMB-C2B-C3B	2.92	130.52	124.68
25	B	607	CLA	CHB-C4A-NA	2.91	128.60	124.40
25	b	608	CLA	CHB-C4A-NA	2.91	128.60	124.40
27	B	619	BCR	C37-C22-C21	-2.90	118.11	122.82
27	b	620	BCR	C37-C22-C21	-2.90	118.11	122.82
36	H	101	RRX	C36-C18-C17	-2.90	118.12	122.82
36	h	101	RRX	C36-C18-C17	-2.90	118.12	122.82
27	B	618	BCR	C19-C18-C17	2.90	123.56	119.01
35	F	101	HEM	CBA-CAA-C2A	-2.89	107.67	112.54
35	f	101	HEM	CBA-CAA-C2A	-2.89	107.67	112.54
27	B	617	BCR	C28-C27-C26	-2.89	108.90	114.06
27	B	618	BCR	C7-C8-C9	-2.89	121.96	126.23
27	b	619	BCR	C7-C8-C9	-2.89	121.97	126.23
27	b	618	BCR	C28-C27-C26	-2.88	108.91	114.06
28	B	621	LMG	O8-C28-C29	2.88	120.63	111.83
27	A	409	BCR	C23-C22-C21	2.88	123.54	119.01
27	a	409	BCR	C23-C22-C21	2.88	123.54	119.01
27	b	619	BCR	C19-C18-C17	2.88	123.54	119.01
28	b	622	LMG	O8-C28-C29	2.88	120.61	111.83
25	B	616	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
36	H	101	RRX	C35-C13-C14	-2.87	118.17	122.82
25	B	605	CLA	CMB-C2B-C3B	2.86	130.41	124.68
25	C	506	CLA	CHB-C4A-NA	2.86	128.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	CHB-C4A-NA	2.86	128.53	124.40
28	D	407	LMG	C8-O7-C10	-2.86	110.95	117.80
25	B	609	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	b	610	CLA	CHB-C4A-NA	2.86	128.53	124.40
28	d	407	LMG	C8-O7-C10	-2.86	110.95	117.80
25	C	513	CLA	C1B-CHB-C4A	-2.86	124.59	130.04
25	c	513	CLA	C1B-CHB-C4A	-2.86	124.59	130.04
33	Z	101	LHG	O8-C23-C24	2.86	120.55	111.83
36	h	101	RRX	C35-C13-C14	-2.85	118.19	122.82
25	B	602	CLA	C1D-ND-C4D	2.85	108.31	106.31
25	b	603	CLA	C1D-ND-C4D	2.85	108.31	106.31
25	B	602	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	b	617	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
33	z	101	LHG	O8-C23-C24	2.85	120.52	111.83
25	b	606	CLA	CMB-C2B-C3B	2.85	130.37	124.68
25	b	603	CLA	CHB-C4A-NA	2.85	128.51	124.40
35	F	101	HEM	CHC-C4B-C3B	-2.83	120.23	124.57
35	f	101	HEM	CHC-C4B-C3B	-2.83	120.23	124.57
35	F	101	HEM	CHD-C1D-C2D	-2.83	120.56	125.03
35	f	101	HEM	CHD-C1D-C2D	-2.83	120.56	125.03
27	A	409	BCR	C19-C18-C17	2.83	123.46	119.01
27	a	409	BCR	C19-C18-C17	2.83	123.46	119.01
28	A	413	LMG	O8-C28-C29	2.83	120.46	111.83
25	A	406	CLA	CMB-C2B-C3B	2.82	130.32	124.68
25	a	406	CLA	CMB-C2B-C3B	2.82	130.32	124.68
28	a	413	LMG	O8-C28-C29	2.82	120.44	111.83
25	b	611	CLA	CMB-C2B-C3B	2.82	130.32	124.68
28	D	407	LMG	O2-C2-C3	-2.82	103.74	110.38
28	d	407	LMG	O2-C2-C3	-2.82	103.74	110.38
35	V	201	HEM	CHB-C1B-NB	2.82	127.86	124.37
35	F	101	HEM	C1B-NB-C4B	2.81	108.53	105.21
35	f	101	HEM	C1B-NB-C4B	2.81	108.53	105.21
25	d	403	CLA	CED-O2D-CGD	2.81	122.28	115.92
25	B	610	CLA	CMB-C2B-C3B	2.80	130.29	124.68
25	C	513	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
25	c	513	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
27	B	619	BCR	C36-C18-C17	-2.79	118.29	122.82
27	b	620	BCR	C36-C18-C17	-2.79	118.29	122.82
25	D	403	CLA	CED-O2D-CGD	2.79	122.25	115.92
35	v	201	HEM	CHB-C1B-NB	2.79	127.83	124.37
34	C	517	DGD	O1G-C1A-C2A	2.78	120.31	111.83
34	c	517	DGD	O1G-C1A-C2A	2.78	120.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	B	611	CLA	O2D-CGD-CBD	2.78	116.09	111.23
25	b	612	CLA	O2D-CGD-CBD	2.78	116.09	111.23
25	B	612	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	b	613	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
25	C	507	CLA	C1B-CHB-C4A	-2.78	124.74	130.04
25	c	507	CLA	C1B-CHB-C4A	-2.78	124.74	130.04
30	f	102	SQD	O9-S-C6	2.78	110.90	106.76
28	J	101	LMG	O8-C28-C29	2.77	120.29	111.83
28	j	101	LMG	O8-C28-C29	2.77	120.29	111.83
25	C	506	CLA	C1-C2-C3	-2.77	121.65	126.20
30	F	102	SQD	O9-S-C6	2.77	110.89	106.76
27	B	619	BCR	C23-C22-C21	2.77	123.37	119.01
27	b	620	BCR	C23-C22-C21	2.77	123.37	119.01
25	B	613	CLA	CMB-C2B-C3B	2.77	130.21	124.68
25	b	614	CLA	CMB-C2B-C3B	2.77	130.21	124.68
25	c	506	CLA	C1-C2-C3	-2.77	121.66	126.20
25	A	406	CLA	CHB-C4A-NA	2.76	128.39	124.40
33	A	419	LHG	O7-C7-C8	2.76	117.44	111.48
33	a	419	LHG	O7-C7-C8	2.76	117.44	111.48
25	B	611	CLA	C1-C2-C3	-2.75	121.69	126.20
25	b	612	CLA	C1-C2-C3	-2.75	121.69	126.20
25	B	604	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	b	605	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
36	H	101	RRX	C19-C18-C17	2.74	123.32	119.01
36	h	101	RRX	C19-C18-C17	2.74	123.32	119.01
30	A	412	SQD	O5-C5-C4	2.74	114.64	109.70
35	F	101	HEM	C4D-ND-C1D	2.74	108.45	105.21
35	f	101	HEM	C4D-ND-C1D	2.74	108.45	105.21
25	B	614	CLA	CMB-C2B-C3B	2.74	130.15	124.68
25	b	615	CLA	CMB-C2B-C3B	2.74	130.15	124.68
27	c	525	BCR	C37-C22-C21	-2.73	118.39	122.82
25	A	408	CLA	C1-C2-C3	-2.73	121.73	126.20
27	C	525	BCR	C37-C22-C21	-2.73	118.40	122.82
25	A	405	CLA	C7-C6-C5	-2.72	106.00	113.26
30	a	412	SQD	O5-C5-C4	2.72	114.60	109.70
25	a	408	CLA	C1-C2-C3	-2.72	121.74	126.20
25	a	405	CLA	C7-C6-C5	-2.72	106.03	113.26
35	F	101	HEM	CHB-C1B-NB	2.71	127.73	124.37
35	f	101	HEM	CHB-C1B-NB	2.71	127.73	124.37
27	d	411	BCR	C7-C8-C9	-2.71	122.23	126.23
25	B	601	CLA	C1B-CHB-C4A	-2.71	124.88	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	C1B-CHB-C4A	-2.71	124.88	130.04
25	a	406	CLA	C1B-CHB-C4A	-2.70	124.90	130.04
27	C	514	BCR	C36-C18-C17	-2.69	118.45	122.82
27	c	514	BCR	C36-C18-C17	-2.69	118.45	122.82
25	A	406	CLA	C1B-CHB-C4A	-2.69	124.90	130.04
28	j	101	LMG	C8-O7-C10	-2.69	111.36	117.80
28	J	101	LMG	C8-O7-C10	-2.69	111.36	117.80
27	C	525	BCR	C7-C8-C9	-2.69	122.26	126.23
27	c	525	BCR	C7-C8-C9	-2.69	122.26	126.23
25	C	506	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
25	c	506	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
27	D	411	BCR	C7-C8-C9	-2.69	122.26	126.23
25	b	611	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
34	C	516	DGD	O1G-C1A-C2A	2.68	120.01	111.83
34	c	516	DGD	O1G-C1A-C2A	2.68	120.01	111.83
25	B	610	CLA	CAA-CBA-CGA	-2.68	105.60	113.21
25	c	506	CLA	CMB-C2B-C3B	2.67	130.02	124.68
33	a	418	LHG	O8-C23-C24	2.67	119.98	111.83
28	A	410	LMG	O4-C4-C3	2.67	116.66	110.38
28	a	410	LMG	O4-C4-C3	2.67	116.66	110.38
30	A	412	SQD	O5-C1-C2	2.67	115.85	110.37
30	a	412	SQD	O5-C1-C2	2.67	115.85	110.37
25	C	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
33	A	418	LHG	O8-C23-C24	2.66	119.95	111.83
25	B	605	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
25	b	606	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
27	a	409	BCR	C31-C1-C6	-2.66	106.08	110.24
27	B	617	BCR	C37-C22-C21	-2.66	118.51	122.82
27	b	618	BCR	C37-C22-C21	-2.66	118.51	122.82
25	C	511	CLA	CHB-C4A-NA	2.65	128.23	124.40
27	C	526	BCR	C19-C18-C17	2.65	123.18	119.01
25	C	506	CLA	CMB-C2B-C3B	2.65	129.98	124.68
33	Z	101	LHG	C5-O7-C7	-2.65	111.45	117.80
33	z	101	LHG	C5-O7-C7	-2.65	111.45	117.80
25	c	510	CLA	CHB-C4A-NA	2.65	128.23	124.40
28	c	518	LMG	C8-O7-C10	-2.65	111.45	117.80
27	D	411	BCR	C36-C18-C17	-2.65	118.53	122.82
27	d	411	BCR	C36-C18-C17	-2.65	118.53	122.82
33	E	102	LHG	O8-C23-C24	2.64	119.89	111.83
28	A	410	LMG	O3-C3-C4	-2.64	104.16	110.38
28	C	518	LMG	C8-O7-C10	-2.64	111.48	117.80
25	B	616	CLA	C1B-CHB-C4A	-2.63	125.02	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	409	BCR	C31-C1-C6	-2.63	106.11	110.24
27	c	526	BCR	C19-C18-C17	2.63	123.15	119.01
25	b	617	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
25	C	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	c	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	C	512	CLA	C1B-CHB-C4A	-2.63	125.03	130.04
33	e	102	LHG	O8-C23-C24	2.63	119.85	111.83
25	c	511	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	C	527	BCR	C7-C8-C9	-2.63	122.35	126.23
27	c	527	BCR	C7-C8-C9	-2.63	122.35	126.23
28	a	410	LMG	O3-C3-C4	-2.63	104.19	110.38
25	B	609	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
25	b	610	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
25	c	512	CLA	C1B-CHB-C4A	-2.62	125.04	130.04
28	B	621	LMG	C8-O7-C10	-2.61	111.54	117.80
28	b	622	LMG	C8-O7-C10	-2.61	111.54	117.80
30	F	102	SQD	O48-C23-C24	2.61	119.78	111.83
30	f	102	SQD	O48-C23-C24	2.61	119.78	111.83
25	c	504	CLA	C1B-CHB-C4A	-2.60	125.07	130.04
25	B	611	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
25	b	612	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
33	A	419	LHG	O8-C23-C24	2.60	119.77	111.83
25	D	403	CLA	CMB-C2B-C3B	2.60	129.88	124.68
25	d	403	CLA	CMB-C2B-C3B	2.60	129.88	124.68
25	B	616	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	b	617	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	C	504	CLA	C1B-CHB-C4A	-2.59	125.09	130.04
33	a	419	LHG	O8-C23-C24	2.59	119.74	111.83
36	H	101	RRX	C12-C13-C14	2.59	123.08	119.01
27	C	526	BCR	C36-C18-C17	-2.59	118.63	122.82
35	V	201	HEM	CHD-C1D-C2D	-2.58	120.95	125.03
35	v	201	HEM	CHD-C1D-C2D	-2.58	120.95	125.03
25	C	501	CLA	C1-C2-C3	-2.58	121.96	126.20
25	c	501	CLA	C1-C2-C3	-2.58	121.96	126.20
36	h	101	RRX	C12-C13-C14	2.58	123.07	119.01
25	D	404	CLA	C1B-CHB-C4A	-2.58	125.12	130.04
29	A	411	PL9	C3-C4-C5	2.57	121.78	118.57
29	a	411	PL9	C3-C4-C5	2.57	121.78	118.57
25	b	615	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	b	620	BCR	C19-C18-C17	2.57	123.05	119.01
27	B	617	BCR	C19-C18-C17	2.57	123.05	119.01
27	b	618	BCR	C19-C18-C17	2.57	123.05	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	CHB-C4A-NA	2.57	128.10	124.40
25	B	610	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	b	611	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
27	c	526	BCR	C36-C18-C17	-2.57	118.66	122.82
25	d	404	CLA	C1B-CHB-C4A	-2.57	125.15	130.04
25	B	607	CLA	C1B-CHB-C4A	-2.56	125.15	130.04
25	b	608	CLA	C1B-CHB-C4A	-2.56	125.15	130.04
28	A	413	LMG	C8-O7-C10	-2.56	111.66	117.80
28	a	413	LMG	C8-O7-C10	-2.56	111.66	117.80
25	B	615	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	b	616	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	B	609	CLA	C1B-CHB-C4A	-2.56	125.17	130.04
25	b	610	CLA	C1B-CHB-C4A	-2.56	125.17	130.04
25	B	610	CLA	C1B-CHB-C4A	-2.55	125.17	130.04
25	C	509	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
25	c	509	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
27	B	619	BCR	C19-C18-C17	2.54	123.01	119.01
27	c	514	BCR	C28-C27-C26	-2.54	109.53	114.06
25	b	611	CLA	C1B-CHB-C4A	-2.54	125.20	130.04
25	C	510	CLA	C1D-ND-C4D	2.54	108.09	106.31
25	c	510	CLA	C1D-ND-C4D	2.54	108.09	106.31
25	B	603	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
25	b	604	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
25	C	510	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	c	510	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
34	C	516	DGD	O2G-C1B-O1B	-2.53	117.80	123.70
34	c	516	DGD	O2G-C1B-O1B	-2.53	117.80	123.70
27	C	514	BCR	C28-C27-C26	-2.53	109.55	114.06
25	B	613	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
25	b	614	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
27	B	617	BCR	C36-C18-C17	-2.51	118.75	122.82
27	b	618	BCR	C36-C18-C17	-2.51	118.75	122.82
25	c	502	CLA	O2D-CGD-CBD	2.51	115.62	111.23
25	C	507	CLA	C2A-C1A-CHA	2.51	128.22	123.87
25	c	507	CLA	C2A-C1A-CHA	2.51	128.22	123.87
25	C	502	CLA	O2D-CGD-CBD	2.51	115.61	111.23
25	B	615	CLA	C2D-C1D-ND	-2.50	107.65	110.13
25	b	616	CLA	C2D-C1D-ND	-2.50	107.65	110.13
25	A	406	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
25	B	604	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	b	605	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	B	613	CLA	C7-C6-C5	-2.50	106.61	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	C7-C6-C5	-2.50	106.61	113.26
25	a	406	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
25	C	508	CLA	C1B-CHB-C4A	-2.48	125.30	130.04
25	c	508	CLA	C1B-CHB-C4A	-2.48	125.30	130.04
25	B	611	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	C	519	LMG	C8-O7-C10	-2.47	111.88	117.80
28	c	519	LMG	C8-O7-C10	-2.47	111.88	117.80
27	C	526	BCR	C37-C22-C21	-2.47	118.81	122.82
27	c	526	BCR	C37-C22-C21	-2.47	118.81	122.82
25	C	506	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
25	c	506	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
25	b	612	CLA	CHB-C4A-NA	2.47	127.96	124.40
27	B	618	BCR	C37-C22-C21	-2.46	118.83	122.82
25	C	510	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
35	F	101	HEM	CAD-CBD-CGD	2.44	120.14	113.67
35	f	101	HEM	CAD-CBD-CGD	2.44	120.14	113.67
25	B	610	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	b	611	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	b	605	CLA	CMB-C2B-C3B	2.44	129.56	124.68
25	b	609	CLA	CAC-C3C-C4C	2.44	127.96	124.79
25	C	511	CLA	C1-C2-C3	-2.44	122.20	126.20
25	c	511	CLA	C1-C2-C3	-2.44	122.20	126.20
28	B	621	LMG	O7-C10-O9	-2.44	118.01	123.70
28	b	622	LMG	O7-C10-O9	-2.44	118.01	123.70
25	c	510	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
27	b	619	BCR	C37-C22-C21	-2.44	118.87	122.82
25	B	608	CLA	CAC-C3C-C4C	2.44	127.96	124.79
25	B	603	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
25	b	604	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
25	c	503	CLA	C1B-CHB-C4A	-2.43	125.40	130.04
25	C	503	CLA	C1B-CHB-C4A	-2.43	125.40	130.04
25	C	512	CLA	O2D-CGD-CBD	2.43	115.47	111.23
25	c	512	CLA	O2D-CGD-CBD	2.43	115.47	111.23
25	B	604	CLA	CMB-C2B-C3B	2.43	129.53	124.68
25	c	503	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	C	503	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	A	405	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	a	405	CLA	CHB-C4A-NA	2.42	127.89	124.40
34	C	515	DGD	O2G-C1B-O1B	-2.41	118.07	123.70
25	B	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	B	602	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
25	b	603	CLA	O2A-CGA-O1A	-2.40	117.62	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	407	LMG	O7-C10-O9	-2.40	118.09	123.70
28	d	407	LMG	O7-C10-O9	-2.40	118.09	123.70
25	b	604	CLA	CHB-C4A-NA	2.40	127.86	124.40
34	c	515	DGD	O2G-C1B-O1B	-2.40	118.09	123.70
25	C	510	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
25	c	510	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
25	B	615	CLA	O2D-CGD-CBD	2.40	115.42	111.23
25	b	616	CLA	O2D-CGD-CBD	2.40	115.42	111.23
25	b	613	CLA	CHD-C1D-ND	-2.39	121.44	124.80
27	A	409	BCR	C7-C8-C9	-2.39	122.70	126.23
27	a	409	BCR	C7-C8-C9	-2.39	122.70	126.23
25	b	608	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
25	C	510	CLA	CHD-C1D-C2D	2.37	130.43	125.49
25	c	510	CLA	CHD-C1D-C2D	2.37	130.43	125.49
33	z	101	LHG	O4-P-O5	2.37	120.08	110.83
25	B	606	CLA	C1B-CHB-C4A	-2.37	125.51	130.04
25	b	607	CLA	C1B-CHB-C4A	-2.37	125.51	130.04
34	C	516	DGD	C2G-O2G-C1B	-2.37	112.12	117.80
34	c	516	DGD	C2G-O2G-C1B	-2.37	112.12	117.80
25	B	607	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
33	Z	101	LHG	O4-P-O5	2.37	120.06	110.83
25	B	612	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	B	605	CLA	C1-C2-C3	-2.36	122.33	126.20
25	b	606	CLA	C1-C2-C3	-2.36	122.33	126.20
35	V	201	HEM	C3B-C4B-NB	-2.35	107.78	109.47
29	D	405	PL9	C7-C3-C2	-2.35	120.61	123.39
31	F	103	LMT	C1'-O5'-C5'	2.35	118.31	113.72
27	B	619	BCR	C32-C1-C6	-2.35	106.56	110.24
25	C	505	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
25	c	505	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
27	b	620	BCR	C32-C1-C6	-2.34	106.57	110.24
25	B	615	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
25	b	616	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
33	D	406	LHG	C5-O7-C7	-2.34	112.19	117.80
33	d	406	LHG	C5-O7-C7	-2.34	112.19	117.80
31	f	103	LMT	C1'-O5'-C5'	2.34	118.29	113.72
27	C	526	BCR	C35-C13-C12	2.34	121.66	118.09
27	c	526	BCR	C35-C13-C12	2.34	121.66	118.09
25	B	613	CLA	CED-O2D-CGD	2.34	121.22	115.92
25	b	614	CLA	CED-O2D-CGD	2.34	121.22	115.92
35	v	201	HEM	C3B-C4B-NB	-2.34	107.79	109.47
28	A	413	LMG	O3-C3-C4	-2.33	104.88	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413	LMG	O3-C3-C4	-2.33	104.88	110.38
30	f	102	SQD	O8-S-C6	2.33	110.47	105.97
28	C	518	LMG	O1-C7-C8	-2.33	105.16	110.82
28	c	518	LMG	O1-C7-C8	-2.33	105.16	110.82
25	A	408	CLA	C3C-C4C-NC	-2.33	107.45	110.43
27	C	527	BCR	C37-C22-C21	-2.32	119.05	122.82
27	c	527	BCR	C37-C22-C21	-2.32	119.05	122.82
25	C	507	CLA	CHA-C1A-NA	-2.32	121.13	126.39
25	c	507	CLA	CHA-C1A-NA	-2.32	121.13	126.39
25	B	601	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	b	602	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	d	405	PL9	C7-C3-C2	-2.32	120.65	123.39
25	C	502	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	c	502	CLA	CHB-C4A-NA	2.32	127.75	124.40
33	z	101	LHG	O3-P-O6	-2.32	100.62	106.67
30	F	102	SQD	O8-S-C6	2.32	110.45	105.97
25	B	604	CLA	C6-C7-C8	-2.32	108.26	115.97
25	b	605	CLA	C6-C7-C8	-2.32	108.26	115.97
25	a	405	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
25	a	408	CLA	C3C-C4C-NC	-2.32	107.46	110.43
33	Z	101	LHG	O3-P-O6	-2.32	100.63	106.67
25	A	405	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
25	c	508	CLA	CHB-C4A-NA	2.31	127.74	124.40
31	C	524	LMT	C1'-O5'-C5'	2.31	118.24	113.72
25	B	611	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
28	A	413	LMG	O1-C1-C2	-2.31	104.76	108.27
28	a	413	LMG	O1-C1-C2	-2.31	104.76	108.27
25	D	404	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	B	609	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	C	508	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	b	612	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
27	c	527	BCR	C31-C1-C6	-2.30	106.64	110.24
25	d	404	CLA	CHD-C1D-ND	-2.30	121.57	124.80
34	H	103	DGD	O1G-C1A-O1A	-2.30	117.88	123.63
34	h	103	DGD	O1G-C1A-O1A	-2.30	117.88	123.63
27	C	527	BCR	C31-C1-C6	-2.30	106.64	110.24
31	c	524	LMT	C1'-O5'-C5'	2.29	118.20	113.72
25	B	606	CLA	CHB-C4A-NA	2.29	127.71	124.40
25	b	607	CLA	CHB-C4A-NA	2.29	127.71	124.40
28	B	629	LMG	C8-O7-C10	-2.29	112.32	117.80
28	b	630	LMG	C8-O7-C10	-2.29	112.32	117.80
25	C	506	CLA	O1D-CGD-CBD	2.29	129.03	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	O1D-CGD-CBD	2.29	129.03	124.52
25	b	606	CLA	C1B-CHB-C4A	-2.28	125.69	130.04
25	b	610	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	C	510	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	c	510	CLA	CHD-C1D-ND	-2.28	121.59	124.80
35	V	201	HEM	CAD-CBD-CGD	-2.28	107.62	113.67
35	v	201	HEM	CAD-CBD-CGD	-2.28	107.62	113.67
25	c	503	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
25	B	605	CLA	C1B-CHB-C4A	-2.27	125.70	130.04
28	a	410	LMG	C8-O7-C10	-2.27	112.36	117.80
25	C	512	CLA	CHD-C1D-ND	-2.27	121.61	124.80
25	c	512	CLA	CHD-C1D-ND	-2.27	121.61	124.80
34	C	517	DGD	C2G-O2G-C1B	-2.27	112.36	117.80
27	C	527	BCR	C34-C9-C10	-2.27	119.14	122.82
27	c	527	BCR	C34-C9-C10	-2.27	119.14	122.82
35	F	101	HEM	C4B-C3B-C2B	-2.27	105.20	107.28
35	f	101	HEM	C4B-C3B-C2B	-2.27	105.20	107.28
27	d	411	BCR	C34-C9-C10	-2.27	119.15	122.82
25	C	503	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
27	d	411	BCR	C37-C22-C21	-2.26	119.16	122.82
25	b	610	CLA	C1-C2-C3	-2.26	122.50	126.20
27	D	411	BCR	C37-C22-C21	-2.26	119.16	122.82
34	c	517	DGD	C2G-O2G-C1B	-2.25	112.40	117.80
28	A	410	LMG	C8-O7-C10	-2.25	112.41	117.80
25	B	609	CLA	C1-C2-C3	-2.25	122.51	126.20
27	D	411	BCR	C34-C9-C10	-2.25	119.17	122.82
25	D	404	CLA	O2D-CGD-CBD	2.25	115.17	111.23
25	d	404	CLA	O2D-CGD-CBD	2.25	115.17	111.23
36	H	101	RRX	C16-C15-C14	2.25	128.11	123.52
36	h	101	RRX	C16-C15-C14	2.25	128.11	123.52
35	F	101	HEM	O2A-CGA-CBA	2.24	121.09	114.00
35	f	101	HEM	O2A-CGA-CBA	2.24	121.09	114.00
25	B	605	CLA	C3C-C4C-NC	-2.24	107.56	110.43
25	b	606	CLA	C3C-C4C-NC	-2.24	107.56	110.43
25	B	616	CLA	C1-C2-C3	-2.24	122.53	126.20
25	b	617	CLA	C1-C2-C3	-2.24	122.53	126.20
27	C	525	BCR	C23-C22-C21	2.23	122.52	119.01
27	c	525	BCR	C23-C22-C21	2.23	122.52	119.01
27	B	618	BCR	C36-C18-C17	-2.23	119.20	122.82
27	b	619	BCR	C36-C18-C17	-2.23	119.20	122.82
25	D	404	CLA	C1-C2-C3	-2.23	122.54	126.20
25	d	404	CLA	C1-C2-C3	-2.23	122.54	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEM	CHC-C4B-C3B	-2.23	121.16	124.57
25	b	609	CLA	C1D-ND-C4D	2.23	107.88	106.31
25	d	401	CLA	C1-C2-C3	-2.23	122.55	126.20
25	B	604	CLA	C16-C15-C13	-2.23	108.56	115.97
25	B	608	CLA	C1D-ND-C4D	2.23	107.87	106.31
27	B	619	BCR	C35-C13-C12	2.22	121.48	118.09
27	b	620	BCR	C35-C13-C12	2.22	121.48	118.09
27	D	411	BCR	C38-C26-C27	2.22	118.33	113.60
27	d	411	BCR	C38-C26-C27	2.22	118.33	113.60
33	E	102	LHG	O7-C7-O9	-2.22	118.52	123.70
33	e	102	LHG	O7-C7-O9	-2.22	118.52	123.70
25	A	408	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	a	408	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	D	401	CLA	C1-C2-C3	-2.22	122.57	126.20
25	b	605	CLA	C16-C15-C13	-2.22	108.60	115.97
33	A	418	LHG	C5-O7-C7	-2.22	112.49	117.80
33	a	418	LHG	C5-O7-C7	-2.22	112.49	117.80
33	a	418	LHG	C9-C8-C7	-2.21	105.59	113.69
25	B	606	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	b	607	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
33	D	406	LHG	O8-C23-O10	-2.21	118.10	123.63
33	d	406	LHG	O8-C23-O10	-2.21	118.10	123.63
33	A	418	LHG	C9-C8-C7	-2.21	105.61	113.69
35	V	201	HEM	CHC-C4B-C3B	-2.19	121.21	124.57
25	b	609	CLA	C1B-CHB-C4A	-2.19	125.86	130.04
25	B	613	CLA	C2D-C1D-ND	-2.19	107.96	110.13
25	b	614	CLA	C2D-C1D-ND	-2.19	107.96	110.13
27	B	618	BCR	C15-C14-C13	-2.19	124.21	127.28
27	C	514	BCR	C34-C9-C10	-2.19	119.28	122.82
27	c	514	BCR	C34-C9-C10	-2.19	119.28	122.82
25	B	608	CLA	C1B-CHB-C4A	-2.18	125.87	130.04
25	B	613	CLA	O1D-CGD-CBD	2.18	128.83	124.52
25	b	614	CLA	O1D-CGD-CBD	2.18	128.83	124.52
25	c	507	CLA	O2D-CGD-CBD	2.18	115.05	111.23
25	B	601	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	b	602	CLA	CHD-C1D-ND	-2.18	121.73	124.80
29	A	411	PL9	C7-C3-C4	2.18	118.71	116.91
29	a	411	PL9	C7-C3-C4	2.18	118.71	116.91
25	A	408	CLA	C1B-CHB-C4A	-2.18	125.88	130.04
25	a	408	CLA	C1B-CHB-C4A	-2.18	125.88	130.04
25	B	614	CLA	C1B-CHB-C4A	-2.18	125.88	130.04
25	b	615	CLA	C1B-CHB-C4A	-2.18	125.88	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	619	BCR	C15-C14-C13	-2.18	124.22	127.28
25	C	507	CLA	O2D-CGD-CBD	2.18	115.04	111.23
25	B	602	CLA	CHD-C1D-C2D	2.18	130.01	125.49
25	b	603	CLA	CHD-C1D-C2D	2.18	130.01	125.49
25	b	605	CLA	C6-C5-C3	-2.17	108.17	113.47
25	B	604	CLA	C6-C5-C3	-2.17	108.17	113.47
33	B	626	LHG	C5-O7-C7	-2.17	112.61	117.80
33	b	627	LHG	C5-O7-C7	-2.17	112.61	117.80
25	C	510	CLA	C2D-C1D-ND	-2.17	107.98	110.13
25	c	510	CLA	C2D-C1D-ND	-2.17	107.98	110.13
25	b	606	CLA	C3B-C4B-NB	-2.16	106.42	109.21
25	B	603	CLA	C1B-CHB-C4A	-2.16	125.92	130.04
25	b	604	CLA	C1B-CHB-C4A	-2.16	125.92	130.04
25	D	403	CLA	CHD-C1D-ND	-2.16	121.77	124.80
25	d	403	CLA	CHD-C1D-ND	-2.16	121.77	124.80
25	B	605	CLA	C3B-C4B-NB	-2.16	106.42	109.21
27	A	409	BCR	C8-C7-C6	-2.16	121.24	127.00
27	a	409	BCR	C8-C7-C6	-2.16	121.24	127.00
33	Z	101	LHG	O8-C23-O10	-2.15	118.25	123.63
33	z	101	LHG	O8-C23-O10	-2.15	118.25	123.63
25	b	613	CLA	CHD-C4C-NC	2.15	127.56	124.23
26	D	402	PHO	CMA-C3A-C4A	-2.14	110.00	114.61
26	d	402	PHO	CMA-C3A-C4A	-2.14	110.00	114.61
25	B	612	CLA	CHD-C4C-NC	2.14	127.55	124.23
25	b	609	CLA	C2D-C1D-ND	-2.14	108.01	110.13
25	B	615	CLA	C4D-CHA-C1A	2.14	123.79	121.24
25	b	616	CLA	C4D-CHA-C1A	2.14	123.79	121.24
25	C	501	CLA	O2D-CGD-CBD	2.14	114.96	111.23
25	c	501	CLA	O2D-CGD-CBD	2.14	114.96	111.23
25	B	608	CLA	C2D-C1D-ND	-2.13	108.01	110.13
25	A	405	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
25	C	511	CLA	O2D-CGD-CBD	2.13	114.96	111.23
27	C	514	BCR	C23-C24-C25	-2.13	121.31	127.00
27	c	514	BCR	C23-C24-C25	-2.13	121.31	127.00
25	a	405	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
35	V	201	HEM	C4D-ND-C1D	2.12	107.72	105.21
25	B	616	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	b	617	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	B	612	CLA	C1-C2-C3	-2.12	122.72	126.20
25	b	613	CLA	C1-C2-C3	-2.12	122.72	126.20
25	B	604	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
25	b	605	CLA	CAA-CBA-CGA	-2.12	107.19	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	O2D-CGD-CBD	2.12	114.94	111.23
25	b	603	CLA	C1B-CHB-C4A	-2.12	126.00	130.04
25	C	505	CLA	CHB-C4A-NA	2.11	127.45	124.40
25	c	505	CLA	CHB-C4A-NA	2.11	127.45	124.40
25	A	406	CLA	CHA-C1A-NA	-2.11	121.60	126.39
35	v	201	HEM	C4D-ND-C1D	2.11	107.71	105.21
30	F	102	SQD	O6-C1-C2	2.11	111.48	108.27
30	f	102	SQD	O6-C1-C2	2.11	111.48	108.27
30	f	102	SQD	O5-C1-C2	2.11	114.70	110.37
33	L	101	LHG	O8-C23-O10	-2.10	118.36	123.63
33	l	101	LHG	O8-C23-O10	-2.10	118.36	123.63
25	B	604	CLA	C1D-ND-C4D	2.10	107.79	106.31
27	c	525	BCR	C36-C18-C17	-2.10	119.41	122.82
25	a	406	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	B	602	CLA	C1B-CHB-C4A	-2.09	126.05	130.04
25	C	509	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	c	509	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
30	F	102	SQD	O5-C1-C2	2.09	114.67	110.37
25	D	404	CLA	C1D-ND-C4D	2.09	107.78	106.31
25	B	602	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	b	603	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	b	604	CLA	C7-C6-C5	-2.09	107.69	113.26
25	B	602	CLA	C11-C12-C13	-2.09	109.03	115.97
25	b	603	CLA	C11-C12-C13	-2.09	109.03	115.97
25	B	615	CLA	CHA-C1A-NA	-2.08	121.67	126.39
25	b	616	CLA	CHA-C1A-NA	-2.08	121.67	126.39
25	B	603	CLA	C7-C6-C5	-2.08	107.71	113.26
27	C	525	BCR	C38-C26-C27	2.08	118.04	113.60
27	c	525	BCR	C38-C26-C27	2.08	118.04	113.60
27	d	411	BCR	C34-C9-C8	2.08	121.27	118.09
27	C	525	BCR	C36-C18-C17	-2.08	119.44	122.82
25	C	511	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
28	A	413	LMG	C9-C8-C7	-2.08	106.94	111.78
28	a	413	LMG	C9-C8-C7	-2.08	106.94	111.78
25	B	610	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	b	611	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	B	609	CLA	O1D-CGD-CBD	2.07	128.61	124.52
25	b	610	CLA	O1D-CGD-CBD	2.07	128.61	124.52
27	B	617	BCR	C33-C5-C4	2.07	118.01	113.60
27	b	618	BCR	C33-C5-C4	2.07	118.01	113.60
27	b	620	BCR	C29-C30-C25	2.07	113.44	110.44
27	B	619	BCR	C29-C30-C25	2.07	113.44	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	CHA-C4D-ND	2.07	136.81	132.55
28	A	413	LMG	C4-C3-C2	-2.07	107.20	110.83
28	a	413	LMG	C4-C3-C2	-2.07	107.20	110.83
25	D	403	CLA	C3B-C4B-NB	-2.07	106.54	109.21
25	d	403	CLA	C3B-C4B-NB	-2.07	106.54	109.21
25	c	504	CLA	CHB-C4A-NA	2.07	127.38	124.40
25	C	504	CLA	CHB-C4A-NA	2.06	127.38	124.40
25	B	602	CLA	C2D-C1D-ND	-2.06	108.08	110.13
25	b	603	CLA	C2D-C1D-ND	-2.06	108.08	110.13
25	D	401	CLA	O2D-CGD-CBD	2.06	114.84	111.23
25	D	403	CLA	C4-C3-C5	2.06	118.81	115.23
25	d	403	CLA	C4-C3-C5	2.06	118.81	115.23
30	a	412	SQD	O4-C4-C5	-2.06	104.24	109.32
25	d	404	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	C	518	LMG	O8-C28-O10	-2.06	118.47	123.63
28	c	518	LMG	O8-C28-O10	-2.06	118.47	123.63
25	c	511	CLA	C1B-CHB-C4A	-2.06	126.11	130.04
25	d	401	CLA	O2D-CGD-CBD	2.06	114.83	111.23
27	C	527	BCR	C8-C9-C10	2.06	122.25	119.01
27	c	527	BCR	C8-C9-C10	2.06	122.25	119.01
27	D	411	BCR	C34-C9-C8	2.06	121.23	118.09
27	d	411	BCR	C40-C30-C25	-2.05	107.02	110.24
27	b	619	BCR	C34-C9-C10	-2.05	119.49	122.82
25	D	404	CLA	CHD-C1D-C2D	2.05	129.76	125.49
33	a	419	LHG	O8-C23-O10	-2.05	118.49	123.63
27	D	411	BCR	C40-C30-C25	-2.05	107.03	110.24
25	d	404	CLA	C1D-ND-C4D	2.05	107.75	106.31
30	A	412	SQD	O4-C4-C5	-2.05	104.27	109.32
27	C	514	BCR	C37-C22-C21	-2.05	119.50	122.82
27	c	514	BCR	C37-C22-C21	-2.05	119.50	122.82
25	B	613	CLA	CHA-C4D-ND	2.05	136.78	132.55
25	D	401	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
25	d	401	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
25	D	404	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	D	401	CLA	CED-O2D-CGD	2.05	120.56	115.92
33	A	419	LHG	O8-C23-O10	-2.05	118.51	123.63
25	d	404	CLA	CHD-C1D-C2D	2.04	129.74	125.49
25	d	401	CLA	CED-O2D-CGD	2.04	120.55	115.92
34	c	516	DGD	O1G-C1A-O1A	-2.04	118.51	123.63
30	b	621	SQD	O8-S-C6	-2.04	102.03	105.97
27	B	618	BCR	C34-C9-C10	-2.04	119.51	122.82
25	b	605	CLA	C1D-ND-C4D	2.04	107.74	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	O1D-CGD-CBD	2.04	128.54	124.52
25	c	501	CLA	O1D-CGD-CBD	2.04	128.54	124.52
27	C	514	BCR	C33-C5-C4	2.04	117.94	113.60
27	c	514	BCR	C33-C5-C4	2.04	117.94	113.60
34	C	516	DGD	O1G-C1A-O1A	-2.04	118.53	123.63
25	B	615	CLA	C3C-C4C-NC	-2.04	107.82	110.43
25	b	616	CLA	C3C-C4C-NC	-2.04	107.82	110.43
28	C	519	LMG	O7-C10-O9	-2.03	118.95	123.70
28	c	519	LMG	O7-C10-O9	-2.03	118.95	123.70
30	B	620	SQD	O8-S-C6	-2.03	102.04	105.97
25	C	501	CLA	C1B-CHB-C4A	-2.03	126.17	130.04
25	C	511	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	c	511	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	B	601	CLA	O2D-CGD-CBD	2.02	114.77	111.23
25	b	602	CLA	O2D-CGD-CBD	2.02	114.77	111.23
25	D	401	CLA	CHD-C1D-ND	-2.02	121.95	124.80
25	d	401	CLA	CHD-C1D-ND	-2.02	121.95	124.80
25	b	614	CLA	C1B-CHB-C4A	-2.02	126.18	130.04
25	B	614	CLA	O1D-CGD-CBD	2.02	128.51	124.52
25	b	615	CLA	O1D-CGD-CBD	2.02	128.51	124.52
27	B	619	BCR	C33-C5-C4	2.02	117.90	113.60
27	b	620	BCR	C33-C5-C4	2.02	117.90	113.60
25	A	408	CLA	C11-C10-C8	-2.02	109.25	115.97
25	a	408	CLA	C11-C10-C8	-2.02	109.25	115.97
27	b	618	BCR	C32-C1-C6	-2.02	107.08	110.24
28	B	621	LMG	O8-C28-O10	-2.02	118.58	123.63
28	A	410	LMG	O8-C28-O10	-2.02	118.58	123.63
28	a	410	LMG	O8-C28-O10	-2.02	118.58	123.63
25	c	501	CLA	C1B-CHB-C4A	-2.01	126.20	130.04
25	B	613	CLA	C1B-CHB-C4A	-2.01	126.20	130.04
27	B	618	BCR	C28-C27-C26	-2.01	110.47	114.06
28	b	622	LMG	O8-C28-O10	-2.01	118.60	123.63
25	B	616	CLA	CHD-C1D-ND	-2.01	121.98	124.80
25	b	617	CLA	CHD-C1D-ND	-2.01	121.98	124.80
27	b	619	BCR	C28-C27-C26	-2.01	110.48	114.06
25	C	510	CLA	O1D-CGD-CBD	2.00	128.47	124.52
25	D	403	CLA	CHD-C4C-NC	2.00	127.34	124.23
36	h	101	RRX	C34-C9-C8	2.00	121.15	118.09
25	B	611	CLA	CGD-CBD-CAD	-2.00	104.36	110.85
25	c	510	CLA	O1D-CGD-CBD	2.00	128.47	124.52

All (56) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	B	601	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	D	401	CLA	ND
25	D	403	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	b	602	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	617	CLA	ND
25	c	501	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND

All (2642) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C9
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	513	CLA	C6-C7-C8-C9
25	b	602	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O1D
25	b	615	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	C11-C12-C13-C15
25	c	506	CLA	C6-C7-C8-C9
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	c	513	CLA	C6-C7-C8-C9
27	A	409	BCR	C10-C11-C12-C13
27	A	409	BCR	C11-C12-C13-C14
27	A	409	BCR	C11-C12-C13-C35
27	B	617	BCR	C7-C8-C9-C10
27	B	617	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	B	617	BCR	C11-C10-C9-C34
27	B	617	BCR	C10-C11-C12-C13
27	B	618	BCR	C7-C8-C9-C10
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C10-C9-C8
27	B	618	BCR	C11-C10-C9-C34
27	B	619	BCR	C7-C8-C9-C10
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C10-C9-C8
27	B	619	BCR	C11-C10-C9-C34
27	B	619	BCR	C10-C11-C12-C13
27	B	619	BCR	C11-C12-C13-C14
27	C	514	BCR	C7-C8-C9-C10
27	C	514	BCR	C11-C10-C9-C8
27	C	514	BCR	C11-C10-C9-C34
27	C	514	BCR	C10-C11-C12-C13
27	C	525	BCR	C5-C6-C7-C8
27	C	525	BCR	C7-C8-C9-C10
27	C	525	BCR	C10-C11-C12-C13
27	C	525	BCR	C11-C12-C13-C14
27	C	525	BCR	C11-C12-C13-C35
27	C	526	BCR	C11-C10-C9-C8
27	C	526	BCR	C11-C10-C9-C34
27	D	411	BCR	C11-C10-C9-C8
27	D	411	BCR	C11-C10-C9-C34
27	D	411	BCR	C10-C11-C12-C13
27	a	409	BCR	C10-C11-C12-C13
27	a	409	BCR	C11-C12-C13-C14
27	a	409	BCR	C11-C12-C13-C35
27	b	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C7-C8-C9-C10
27	b	619	BCR	C7-C8-C9-C34
27	b	619	BCR	C11-C10-C9-C8
27	b	619	BCR	C11-C10-C9-C34
27	b	620	BCR	C7-C8-C9-C10
27	b	620	BCR	C7-C8-C9-C34
27	b	620	BCR	C11-C10-C9-C8
27	b	620	BCR	C11-C10-C9-C34
27	b	620	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	b	620	BCR	C11-C12-C13-C14
27	c	514	BCR	C7-C8-C9-C10
27	c	514	BCR	C11-C10-C9-C8
27	c	514	BCR	C11-C10-C9-C34
27	c	514	BCR	C10-C11-C12-C13
27	c	525	BCR	C5-C6-C7-C8
27	c	525	BCR	C7-C8-C9-C10
27	c	525	BCR	C10-C11-C12-C13
27	c	525	BCR	C11-C12-C13-C14
27	c	525	BCR	C11-C12-C13-C35
27	c	526	BCR	C11-C10-C9-C8
27	c	526	BCR	C11-C10-C9-C34
27	d	411	BCR	C11-C10-C9-C8
27	d	411	BCR	C11-C10-C9-C34
27	d	411	BCR	C10-C11-C12-C13
28	A	410	LMG	O6-C1-O1-C7
28	C	519	LMG	O6-C1-O1-C7
28	C	519	LMG	O9-C10-O7-C8
28	C	519	LMG	C11-C10-O7-C8
28	D	407	LMG	C2-C1-O1-C7
28	D	407	LMG	O6-C1-O1-C7
28	D	407	LMG	O1-C7-C8-O7
28	D	407	LMG	O9-C10-O7-C8
28	D	407	LMG	C11-C10-O7-C8
28	J	101	LMG	C2-C1-O1-C7
28	J	101	LMG	O6-C1-O1-C7
28	J	101	LMG	C29-C28-O8-C9
28	a	410	LMG	O6-C1-O1-C7
28	c	519	LMG	O6-C1-O1-C7
28	c	519	LMG	O9-C10-O7-C8
28	c	519	LMG	C11-C10-O7-C8
28	d	407	LMG	C2-C1-O1-C7
28	d	407	LMG	O6-C1-O1-C7
28	d	407	LMG	O1-C7-C8-O7
28	d	407	LMG	O9-C10-O7-C8
28	d	407	LMG	C11-C10-O7-C8
28	j	101	LMG	C2-C1-O1-C7
28	j	101	LMG	O6-C1-O1-C7
28	j	101	LMG	C29-C28-O8-C9
29	A	411	PL9	C12-C13-C14-C16
29	A	411	PL9	C37-C38-C39-C40
29	A	411	PL9	C37-C38-C39-C41

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Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C12-C13-C14-C15
29	D	405	PL9	C12-C13-C14-C16
29	D	405	PL9	C42-C43-C44-C45
29	D	405	PL9	C42-C43-C44-C46
29	a	411	PL9	C12-C13-C14-C16
29	a	411	PL9	C37-C38-C39-C40
29	a	411	PL9	C37-C38-C39-C41
29	d	405	PL9	C12-C13-C14-C15
29	d	405	PL9	C12-C13-C14-C16
29	d	405	PL9	C42-C43-C44-C45
29	d	405	PL9	C42-C43-C44-C46
30	A	412	SQD	C2-C1-O6-C44
30	A	412	SQD	O5-C1-O6-C44
30	A	412	SQD	C4-C5-C6-S
30	A	417	SQD	O5-C5-C6-S
30	B	620	SQD	C8-C7-O47-C45
30	B	620	SQD	O5-C5-C6-S
30	B	630	SQD	C2-C1-O6-C44
30	B	630	SQD	O5-C1-O6-C44
30	B	630	SQD	C4-C5-C6-S
30	B	630	SQD	C5-C6-S-O8
30	B	630	SQD	C5-C6-S-O9
30	F	102	SQD	C5-C6-S-O7
30	F	102	SQD	C5-C6-S-O8
30	F	102	SQD	C5-C6-S-O9
30	H	102	SQD	C8-C7-O47-C45
30	H	102	SQD	O5-C5-C6-S
30	K	102	SQD	O6-C44-C45-O47
30	K	102	SQD	O10-C23-O48-C46
30	K	102	SQD	C24-C23-O48-C46
30	a	412	SQD	C2-C1-O6-C44
30	a	412	SQD	O5-C1-O6-C44
30	a	412	SQD	C4-C5-C6-S
30	a	417	SQD	O5-C5-C6-S
30	b	601	SQD	C2-C1-O6-C44
30	b	601	SQD	O5-C1-O6-C44
30	b	601	SQD	C4-C5-C6-S
30	b	601	SQD	C5-C6-S-O8
30	b	601	SQD	C5-C6-S-O9
30	b	621	SQD	C8-C7-O47-C45
30	b	621	SQD	O5-C5-C6-S
30	f	102	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C5-C6-S-O8
30	f	102	SQD	C5-C6-S-O9
30	h	102	SQD	C8-C7-O47-C45
30	h	102	SQD	O5-C5-C6-S
30	k	102	SQD	O6-C44-C45-O47
30	k	102	SQD	O10-C23-O48-C46
30	k	102	SQD	C24-C23-O48-C46
31	A	414	LMT	C2-C1-O1'-C1'
31	A	415	LMT	C2-C1-O1'-C1'
31	B	623	LMT	O5'-C1'-O1'-C1
31	B	627	LMT	O5'-C1'-O1'-C1
31	C	520	LMT	C2-C1-O1'-C1'
31	C	522	LMT	C2-C1-O1'-C1'
31	C	523	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	C2-C1-O1'-C1'
31	D	409	LMT	O5'-C1'-O1'-C1
31	D	412	LMT	O5'-C1'-O1'-C1
31	H	104	LMT	C2'-C1'-O1'-C1
31	I	101	LMT	O5'-C1'-O1'-C1
31	I	104	LMT	O5'-C1'-O1'-C1
31	I	104	LMT	C2-C1-O1'-C1'
31	J	102	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	C2-C1-O1'-C1'
31	T	101	LMT	O5'-C1'-O1'-C1
31	a	414	LMT	C2-C1-O1'-C1'
31	a	415	LMT	C2-C1-O1'-C1'
31	b	624	LMT	O5'-C1'-O1'-C1
31	b	628	LMT	O5'-C1'-O1'-C1
31	c	520	LMT	C2-C1-O1'-C1'
31	c	522	LMT	C2-C1-O1'-C1'
31	c	523	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	C2-C1-O1'-C1'
31	d	409	LMT	O5'-C1'-O1'-C1
31	d	412	LMT	O5'-C1'-O1'-C1
31	h	104	LMT	C2'-C1'-O1'-C1
31	i	101	LMT	O5'-C1'-O1'-C1
31	i	104	LMT	O5'-C1'-O1'-C1
31	i	104	LMT	C2-C1-O1'-C1'
31	j	102	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	C2-C1-O1'-C1'
31	t	101	LMT	O5'-C1'-O1'-C1
33	A	418	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	B	626	LHG	C2-C3-O3-P
33	B	626	LHG	C8-C7-O7-C5
33	D	406	LHG	C3-O3-P-O4
33	D	406	LHG	C3-O3-P-O6
33	D	406	LHG	C4-O6-P-O3
33	D	406	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	Z	101	LHG	C4-O6-P-O3
33	Z	101	LHG	C4-O6-P-O4
33	a	418	LHG	C1-C2-C3-O3
33	b	627	LHG	C2-C3-O3-P
33	b	627	LHG	C8-C7-O7-C5
33	d	406	LHG	C3-O3-P-O4
33	d	406	LHG	C3-O3-P-O6
33	d	406	LHG	C4-O6-P-O3
33	d	406	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
33	z	101	LHG	C4-O6-P-O3
33	z	101	LHG	C4-O6-P-O4
36	H	101	RRX	C7-C8-C9-C10
36	H	101	RRX	C7-C8-C9-C34
36	h	101	RRX	C7-C8-C9-C10
36	h	101	RRX	C7-C8-C9-C34
31	J	102	LMT	C3'-C4'-O1B-C1B
31	X	103	LMT	C3'-C4'-O1B-C1B
31	j	102	LMT	C3'-C4'-O1B-C1B
31	x	103	LMT	C3'-C4'-O1B-C1B
25	C	503	CLA	O1D-CGD-O2D-CED
25	C	509	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
28	D	407	LMG	O10-C28-O8-C9
28	J	101	LMG	O10-C28-O8-C9
28	d	407	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	j	101	LMG	O10-C28-O8-C9
33	B	626	LHG	O10-C23-O8-C6
33	b	627	LHG	O10-C23-O8-C6
34	C	515	DGD	O1A-C1A-O1G-C1G
34	c	515	DGD	O1A-C1A-O1G-C1G
29	A	411	PL9	C47-C48-C49-C50
29	A	411	PL9	C47-C48-C49-C51
29	a	411	PL9	C47-C48-C49-C50
29	a	411	PL9	C47-C48-C49-C51
28	A	410	LMG	C8-C9-O8-C28
28	B	629	LMG	C8-C9-O8-C28
28	a	410	LMG	C8-C9-O8-C28
28	b	630	LMG	C8-C9-O8-C28
28	D	407	LMG	C29-C28-O8-C9
28	d	407	LMG	C29-C28-O8-C9
33	B	626	LHG	C24-C23-O8-C6
33	b	627	LHG	C24-C23-O8-C6
34	C	515	DGD	C2A-C1A-O1G-C1G
34	c	515	DGD	C2A-C1A-O1G-C1G
25	C	501	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
28	A	410	LMG	O10-C28-O8-C9
28	B	629	LMG	O10-C28-O8-C9
28	a	410	LMG	O10-C28-O8-C9
28	b	630	LMG	O10-C28-O8-C9
30	H	102	SQD	O10-C23-O48-C46
30	h	102	SQD	O10-C23-O48-C46
31	E	101	LMT	C4'-C5'-C6'-O6'
31	e	101	LMT	C4'-C5'-C6'-O6'
31	B	624	LMT	C3'-C4'-O1B-C1B
31	b	625	LMT	C3'-C4'-O1B-C1B
30	B	620	SQD	O49-C7-O47-C45
30	H	102	SQD	O49-C7-O47-C45
30	b	621	SQD	O49-C7-O47-C45
30	h	102	SQD	O49-C7-O47-C45
33	B	626	LHG	O9-C7-O7-C5
33	b	627	LHG	O9-C7-O7-C5
25	B	614	CLA	C3-C5-C6-C7
25	b	615	CLA	C3-C5-C6-C7
28	A	410	LMG	C29-C28-O8-C9
28	B	629	LMG	C29-C28-O8-C9
28	a	410	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	b	630	LMG	C29-C28-O8-C9
30	H	102	SQD	C24-C23-O48-C46
30	h	102	SQD	C24-C23-O48-C46
34	C	517	DGD	C2A-C1A-O1G-C1G
34	c	517	DGD	C2A-C1A-O1G-C1G
25	C	506	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	C4-C3-C5-C6
25	C	512	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
29	A	411	PL9	C30-C29-C31-C32
29	a	411	PL9	C30-C29-C31-C32
25	B	605	CLA	C2-C3-C5-C6
25	C	512	CLA	C2-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
29	A	411	PL9	C28-C29-C31-C32
29	a	411	PL9	C28-C29-C31-C32
31	A	414	LMT	O5B-C5B-C6B-O6B
31	B	625	LMT	O5'-C5'-C6'-O6'
31	D	412	LMT	O5'-C5'-C6'-O6'
31	a	414	LMT	O5B-C5B-C6B-O6B
31	b	626	LMT	O5'-C5'-C6'-O6'
31	d	412	LMT	O5'-C5'-C6'-O6'
25	C	512	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
30	B	620	SQD	C24-C23-O48-C46
30	b	621	SQD	C24-C23-O48-C46
33	E	102	LHG	C24-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
28	C	518	LMG	C17-C18-C19-C20
28	C	518	LMG	C20-C21-C22-C23
28	C	519	LMG	C38-C39-C40-C41
28	J	101	LMG	C17-C18-C19-C20
28	a	410	LMG	C20-C21-C22-C23
28	c	518	LMG	C17-C18-C19-C20
28	c	518	LMG	C20-C21-C22-C23
28	c	519	LMG	C38-C39-C40-C41
28	j	101	LMG	C17-C18-C19-C20
34	C	517	DGD	C8A-C9A-CAA-CBA
34	C	517	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
34	c	517	DGD	C8A-C9A-CAA-CBA
31	D	409	LMT	C4B-C5B-C6B-O6B
31	X	103	LMT	C4'-C5'-C6'-O6'
31	d	409	LMT	C4B-C5B-C6B-O6B
31	x	103	LMT	C4'-C5'-C6'-O6'
29	A	411	PL9	C12-C13-C14-C15
29	A	411	PL9	C42-C43-C44-C45
29	a	411	PL9	C12-C13-C14-C15
29	a	411	PL9	C42-C43-C44-C45
31	M	101	LMT	C3'-C4'-O1B-C1B
31	m	101	LMT	C3'-C4'-O1B-C1B
28	C	519	LMG	C17-C18-C19-C20
28	J	101	LMG	C35-C36-C37-C38
28	c	519	LMG	C17-C18-C19-C20
28	j	101	LMG	C35-C36-C37-C38
34	c	517	DGD	C8B-C9B-CAB-CBB
29	A	411	PL9	C42-C43-C44-C46
29	a	411	PL9	C42-C43-C44-C46
28	A	410	LMG	C20-C21-C22-C23
27	A	409	BCR	C19-C20-C21-C22
27	B	618	BCR	C9-C10-C11-C12
27	C	514	BCR	C9-C10-C11-C12
27	C	525	BCR	C9-C10-C11-C12
27	a	409	BCR	C19-C20-C21-C22
27	b	619	BCR	C9-C10-C11-C12
27	c	514	BCR	C9-C10-C11-C12
27	c	525	BCR	C9-C10-C11-C12
33	E	102	LHG	O10-C23-O8-C6
33	L	101	LHG	O10-C23-O8-C6
33	e	102	LHG	O10-C23-O8-C6
33	l	101	LHG	O10-C23-O8-C6
28	A	410	LMG	C17-C18-C19-C20
28	C	519	LMG	C35-C36-C37-C38
28	c	519	LMG	C35-C36-C37-C38
34	H	103	DGD	CBB-CCB-CDB-CEB
34	h	103	DGD	CBB-CCB-CDB-CEB
28	C	518	LMG	C38-C39-C40-C41
28	D	407	LMG	C17-C18-C19-C20
28	D	407	LMG	C20-C21-C22-C23
28	a	410	LMG	C17-C18-C19-C20
28	c	518	LMG	C38-C39-C40-C41
28	d	407	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	d	407	LMG	C20-C21-C22-C23
34	C	516	DGD	C8B-C9B-CAB-CBB
34	C	516	DGD	CBB-CCB-CDB-CEB
34	c	516	DGD	C8B-C9B-CAB-CBB
34	c	516	DGD	CBB-CCB-CDB-CEB
31	B	624	LMT	C4'-C5'-C6'-O6'
31	D	410	LMT	C4B-C5B-C6B-O6B
31	b	625	LMT	C4'-C5'-C6'-O6'
31	d	410	LMT	C4B-C5B-C6B-O6B
25	C	511	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
30	B	630	SQD	C24-C25-C26-C27
30	b	601	SQD	C24-C25-C26-C27
30	A	412	SQD	C24-C23-O48-C46
30	a	412	SQD	C24-C23-O48-C46
33	L	101	LHG	C24-C23-O8-C6
33	l	101	LHG	C24-C23-O8-C6
31	D	408	LMT	O5'-C5'-C6'-O6'
31	d	408	LMT	O5'-C5'-C6'-O6'
34	C	517	DGD	O1A-C1A-O1G-C1G
34	c	517	DGD	O1A-C1A-O1G-C1G
31	A	414	LMT	C4B-C5B-C6B-O6B
31	a	414	LMT	C4B-C5B-C6B-O6B
31	C	523	LMT	O5'-C5'-C6'-O6'
31	C	524	LMT	O5B-C5B-C6B-O6B
31	X	103	LMT	O5B-C5B-C6B-O6B
31	c	523	LMT	O5'-C5'-C6'-O6'
31	c	524	LMT	O5B-C5B-C6B-O6B
31	x	103	LMT	O5B-C5B-C6B-O6B
30	F	102	SQD	C8-C7-O47-C45
30	K	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
30	k	102	SQD	C8-C7-O47-C45
31	B	623	LMT	O5'-C5'-C6'-O6'
31	I	102	LMT	O5'-C5'-C6'-O6'
31	b	624	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
31	B	625	LMT	C4'-C5'-C6'-O6'
31	D	409	LMT	C4'-C5'-C6'-O6'
31	b	626	LMT	C4'-C5'-C6'-O6'
31	d	409	LMT	C4'-C5'-C6'-O6'
31	D	409	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	d	409	LMT	O5'-C5'-C6'-O6'
25	B	604	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	615	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	b	615	CLA	C2-C3-C5-C6
29	A	411	PL9	C18-C19-C21-C22
29	a	411	PL9	C18-C19-C21-C22
30	A	412	SQD	O10-C23-O48-C46
30	B	620	SQD	O10-C23-O48-C46
30	a	412	SQD	O10-C23-O48-C46
30	b	621	SQD	O10-C23-O48-C46
28	A	413	LMG	O6-C5-C6-O5
28	a	413	LMG	O6-C5-C6-O5
31	E	101	LMT	O5'-C5'-C6'-O6'
31	e	101	LMT	O5'-C5'-C6'-O6'
31	I	102	LMT	C4B-C5B-C6B-O6B
31	I	102	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4B-C5B-C6B-O6B
31	i	102	LMT	C4'-C5'-C6'-O6'
25	A	405	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
33	B	626	LHG	C5-C4-O6-P
33	b	627	LHG	C5-C4-O6-P
31	E	103	LMT	O5B-C5B-C6B-O6B
31	F	103	LMT	O5B-C5B-C6B-O6B
31	e	103	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5B-C5B-C6B-O6B
31	D	412	LMT	C4'-C5'-C6'-O6'
31	E	103	LMT	C4B-C5B-C6B-O6B
31	X	103	LMT	C4B-C5B-C6B-O6B
31	d	412	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4B-C5B-C6B-O6B
31	x	103	LMT	C4B-C5B-C6B-O6B
25	C	512	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
30	K	102	SQD	O5-C1-O6-C44
30	k	102	SQD	O5-C1-O6-C44
31	C	524	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	D	408	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	H	104	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	X	101	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	d	408	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
31	h	104	LMT	O5'-C1'-O1'-C1
31	m	102	LMT	O5'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
28	A	410	LMG	C30-C31-C32-C33
28	a	410	LMG	C30-C31-C32-C33
30	B	620	SQD	C33-C34-C35-C36
30	b	621	SQD	C33-C34-C35-C36
31	I	102	LMT	O5B-C5B-C6B-O6B
31	i	102	LMT	O5B-C5B-C6B-O6B
25	B	604	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
28	C	519	LMG	O6-C5-C6-O5
28	c	519	LMG	O6-C5-C6-O5
31	X	103	LMT	O5'-C5'-C6'-O6'
31	x	103	LMT	O5'-C5'-C6'-O6'
31	C	522	LMT	C1-C2-C3-C4
31	c	522	LMT	C1-C2-C3-C4
33	Z	101	LHG	C11-C10-C9-C8
33	z	101	LHG	C11-C10-C9-C8
31	B	624	LMT	O5'-C5'-C6'-O6'
31	D	410	LMT	O5B-C5B-C6B-O6B
31	b	625	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5B-C5B-C6B-O6B
31	B	623	LMT	C4'-C5'-C6'-O6'
31	C	524	LMT	C4'-C5'-C6'-O6'
31	b	624	LMT	C4'-C5'-C6'-O6'
31	c	524	LMT	C4'-C5'-C6'-O6'
30	A	412	SQD	C29-C30-C31-C32
30	B	620	SQD	C31-C32-C33-C34
30	B	630	SQD	C11-C10-C9-C8
30	a	412	SQD	C29-C30-C31-C32
30	b	601	SQD	C11-C10-C9-C8
30	b	621	SQD	C31-C32-C33-C34
34	C	517	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
34	c	517	DGD	CAA-CBA-CCA-CDA
31	C	524	LMT	C4B-C5B-C6B-O6B
31	c	524	LMT	C4B-C5B-C6B-O6B
27	B	617	BCR	C9-C10-C11-C12
27	b	618	BCR	C9-C10-C11-C12
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
28	A	413	LMG	C29-C28-O8-C9
28	a	413	LMG	C29-C28-O8-C9
31	D	409	LMT	O5B-C5B-C6B-O6B
31	d	409	LMT	O5B-C5B-C6B-O6B
31	C	522	LMT	C3-C4-C5-C6
31	I	102	LMT	C2-C3-C4-C5
31	J	103	LMT	C3-C4-C5-C6
31	X	103	LMT	C3-C4-C5-C6
31	c	522	LMT	C3-C4-C5-C6
31	i	102	LMT	C2-C3-C4-C5
31	j	103	LMT	C3-C4-C5-C6
31	x	103	LMT	C3-C4-C5-C6
25	C	501	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
33	B	626	LHG	C32-C33-C34-C35
31	C	523	LMT	C4'-C5'-C6'-O6'
31	c	523	LMT	C4'-C5'-C6'-O6'
33	A	419	LHG	C24-C25-C26-C27
33	a	419	LHG	C24-C25-C26-C27
33	b	627	LHG	C32-C33-C34-C35
29	A	411	PL9	C20-C19-C21-C22
29	a	411	PL9	C20-C19-C21-C22
25	A	406	CLA	C14-C13-C15-C16
25	A	408	CLA	C6-C7-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C14
25	B	611	CLA	C11-C12-C13-C14
25	B	613	CLA	C11-C12-C13-C14
25	C	509	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C12-C13-C14
25	a	406	CLA	C14-C13-C15-C16
25	a	408	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	610	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	C11-C12-C13-C14
25	b	612	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C12-C13-C14
25	c	509	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C12-C13-C14
30	H	102	SQD	C25-C26-C27-C28
28	C	519	LMG	C4-C5-C6-O5
28	c	519	LMG	C4-C5-C6-O5
31	D	408	LMT	C4'-C5'-C6'-O6'
31	F	103	LMT	C4B-C5B-C6B-O6B
31	d	408	LMT	C4'-C5'-C6'-O6'
31	f	103	LMT	C4B-C5B-C6B-O6B
30	K	102	SQD	C2-C1-O6-C44
30	k	102	SQD	C2-C1-O6-C44
31	B	623	LMT	C2'-C1'-O1'-C1
31	C	524	LMT	C2'-C1'-O1'-C1
31	D	408	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	X	101	LMT	C2'-C1'-O1'-C1
31	b	624	LMT	C2'-C1'-O1'-C1
31	c	524	LMT	C2'-C1'-O1'-C1
31	d	408	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	C2'-C1'-O1'-C1
31	m	102	LMT	C2'-C1'-O1'-C1
31	x	101	LMT	C2'-C1'-O1'-C1
28	C	518	LMG	C36-C37-C38-C39
28	C	519	LMG	C19-C20-C21-C22
28	c	518	LMG	C36-C37-C38-C39
28	c	519	LMG	C19-C20-C21-C22
30	h	102	SQD	C25-C26-C27-C28
31	B	624	LMT	C2-C3-C4-C5
31	b	625	LMT	C2-C3-C4-C5
34	C	515	DGD	C2A-C3A-C4A-C5A
33	A	418	LHG	O2-C2-C3-O3
33	a	418	LHG	O2-C2-C3-O3
31	B	627	LMT	O5'-C5'-C6'-O6'
31	b	628	LMT	O5'-C5'-C6'-O6'
34	c	515	DGD	C2A-C3A-C4A-C5A
28	a	413	LMG	O10-C28-O8-C9
31	X	101	LMT	C3-C4-C5-C6
27	B	617	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	B	617	BCR	C11-C12-C13-C35
27	B	619	BCR	C11-C12-C13-C35
27	C	514	BCR	C7-C8-C9-C34
27	C	525	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C12-C13-C35
27	b	620	BCR	C11-C12-C13-C35
27	c	514	BCR	C7-C8-C9-C34
27	c	525	BCR	C7-C8-C9-C34
27	B	617	BCR	C11-C12-C13-C14
27	b	618	BCR	C11-C12-C13-C14
31	x	101	LMT	C3-C4-C5-C6
33	Z	101	LHG	C7-C8-C9-C10
33	z	101	LHG	C7-C8-C9-C10
25	C	505	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
28	A	413	LMG	O10-C28-O8-C9
30	F	102	SQD	O49-C7-O47-C45
30	f	102	SQD	O49-C7-O47-C45
33	L	101	LHG	C8-C7-O7-C5
33	l	101	LHG	C8-C7-O7-C5
25	C	513	CLA	C8-C10-C11-C12
25	c	513	CLA	C8-C10-C11-C12
28	J	101	LMG	C13-C14-C15-C16
28	j	101	LMG	C13-C14-C15-C16
25	B	611	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
28	J	101	LMG	O6-C5-C6-O5
28	j	101	LMG	O6-C5-C6-O5
31	B	622	LMT	O5B-C5B-C6B-O6B
31	b	623	LMT	O5B-C5B-C6B-O6B
33	E	102	LHG	O1-C1-C2-O2
33	e	102	LHG	O1-C1-C2-O2
30	A	412	SQD	C23-C24-C25-C26
30	B	630	SQD	C23-C24-C25-C26
30	F	102	SQD	C23-C24-C25-C26
30	a	412	SQD	C23-C24-C25-C26
30	b	601	SQD	C23-C24-C25-C26
30	f	102	SQD	C23-C24-C25-C26
30	A	417	SQD	C31-C32-C33-C34
30	a	417	SQD	C31-C32-C33-C34
25	B	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C12-C13-C15-C16
25	D	403	CLA	C12-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C7
25	b	614	CLA	C12-C13-C15-C16
25	d	403	CLA	C12-C13-C15-C16
30	K	102	SQD	C11-C12-C13-C14
30	k	102	SQD	C11-C12-C13-C14
31	B	624	LMT	C6-C7-C8-C9
31	b	625	LMT	C6-C7-C8-C9
33	E	102	LHG	C7-C8-C9-C10
33	e	102	LHG	C7-C8-C9-C10
31	B	625	LMT	O1'-C1-C2-C3
31	b	626	LMT	O1'-C1-C2-C3
30	K	102	SQD	O49-C7-O47-C45
30	k	102	SQD	O49-C7-O47-C45
31	H	104	LMT	O1'-C1-C2-C3
31	h	104	LMT	O1'-C1-C2-C3
31	T	101	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
34	h	103	DGD	O6E-C5E-C6E-O5E
31	E	103	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4'-C5'-C6'-O6'
28	C	519	LMG	C10-C11-C12-C13
28	C	519	LMG	C28-C29-C30-C31
28	c	519	LMG	C10-C11-C12-C13
28	c	519	LMG	C28-C29-C30-C31
30	K	102	SQD	C7-C8-C9-C10
30	k	102	SQD	C7-C8-C9-C10
33	A	419	LHG	C7-C8-C9-C10
33	a	419	LHG	C7-C8-C9-C10
25	B	603	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	C13-C15-C16-C17
25	D	404	CLA	C13-C15-C16-C17
25	b	609	CLA	C13-C15-C16-C17
25	d	404	CLA	C13-C15-C16-C17
33	b	627	LHG	C17-C18-C19-C20
31	I	104	LMT	O5'-C5'-C6'-O6'
31	i	104	LMT	O5'-C5'-C6'-O6'
34	H	103	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
27	C	526	BCR	C10-C11-C12-C13
27	c	526	BCR	C10-C11-C12-C13
25	B	611	CLA	C15-C16-C17-C18
25	B	614	CLA	C13-C15-C16-C17
25	C	503	CLA	C15-C16-C17-C18
25	b	612	CLA	C15-C16-C17-C18
25	b	615	CLA	C13-C15-C16-C17
31	C	524	LMT	O5'-C5'-C6'-O6'
31	c	524	LMT	O5'-C5'-C6'-O6'
30	f	102	SQD	C7-C8-C9-C10
31	C	520	LMT	O5'-C1'-O1'-C1
31	c	520	LMT	O5'-C1'-O1'-C1
28	J	101	LMG	C22-C23-C24-C25
28	j	101	LMG	C22-C23-C24-C25
31	b	623	LMT	C3-C4-C5-C6
33	B	626	LHG	C17-C18-C19-C20
34	C	516	DGD	C6A-C7A-C8A-C9A
34	c	516	DGD	C6A-C7A-C8A-C9A
31	X	101	LMT	O1'-C1-C2-C3
31	x	101	LMT	O1'-C1-C2-C3
25	B	614	CLA	C5-C6-C7-C8
25	B	615	CLA	C5-C6-C7-C8
25	C	513	CLA	C10-C11-C12-C13
25	b	615	CLA	C5-C6-C7-C8
25	b	616	CLA	C5-C6-C7-C8
25	c	503	CLA	C15-C16-C17-C18
25	c	513	CLA	C10-C11-C12-C13
30	B	620	SQD	C11-C10-C9-C8
30	b	621	SQD	C11-C10-C9-C8
31	B	622	LMT	C3-C4-C5-C6
31	B	624	LMT	C4-C5-C6-C7
31	b	625	LMT	C4-C5-C6-C7
33	L	101	LHG	O2-C2-C3-O3
33	l	101	LHG	O2-C2-C3-O3
31	B	627	LMT	O1'-C1-C2-C3
31	b	628	LMT	O1'-C1-C2-C3
28	J	101	LMG	C4-C5-C6-O5
28	j	101	LMG	C4-C5-C6-O5
30	F	102	SQD	C7-C8-C9-C10
31	C	524	LMT	C1-C2-C3-C4
31	c	524	LMT	C1-C2-C3-C4
33	L	101	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	O9-C7-O7-C5
31	C	524	LMT	O1'-C1-C2-C3
31	I	101	LMT	O1'-C1-C2-C3
31	c	524	LMT	O1'-C1-C2-C3
31	i	101	LMT	O1'-C1-C2-C3
25	c	501	CLA	C15-C16-C17-C18
34	H	103	DGD	C4E-C5E-C6E-O5E
34	h	103	DGD	C4E-C5E-C6E-O5E
28	B	621	LMG	C10-C11-C12-C13
28	b	622	LMG	C10-C11-C12-C13
31	C	522	LMT	O1'-C1-C2-C3
31	J	102	LMT	O1'-C1-C2-C3
31	c	522	LMT	O1'-C1-C2-C3
31	j	102	LMT	O1'-C1-C2-C3
25	B	602	CLA	C8-C10-C11-C12
25	C	501	CLA	C15-C16-C17-C18
25	b	603	CLA	C8-C10-C11-C12
25	C	513	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
28	J	101	LMG	C15-C16-C17-C18
28	j	101	LMG	C15-C16-C17-C18
28	J	101	LMG	C33-C34-C35-C36
28	j	101	LMG	C33-C34-C35-C36
28	A	410	LMG	C10-C11-C12-C13
28	a	410	LMG	C10-C11-C12-C13
25	A	408	CLA	C10-C11-C12-C13
25	C	512	CLA	C13-C15-C16-C17
25	D	401	CLA	C15-C16-C17-C18
25	a	408	CLA	C10-C11-C12-C13
25	c	512	CLA	C13-C15-C16-C17
25	d	401	CLA	C15-C16-C17-C18
30	b	601	SQD	C14-C15-C16-C17
25	C	511	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	611	CLA	C8-C10-C11-C12
25	b	612	CLA	C8-C10-C11-C12
30	B	630	SQD	C14-C15-C16-C17
31	X	102	LMT	C5-C6-C7-C8
31	x	102	LMT	C5-C6-C7-C8
31	M	101	LMT	O1'-C1-C2-C3
31	m	101	LMT	O1'-C1-C2-C3
33	A	419	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	a	419	LHG	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
25	C	508	CLA	C13-C15-C16-C17
25	C	512	CLA	C15-C16-C17-C18
25	c	507	CLA	C13-C15-C16-C17
25	c	508	CLA	C13-C15-C16-C17
25	c	512	CLA	C15-C16-C17-C18
25	C	504	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
26	D	402	PHO	C4-C3-C5-C6
26	d	402	PHO	C4-C3-C5-C6
29	A	411	PL9	C40-C39-C41-C42
29	a	411	PL9	C40-C39-C41-C42
30	B	620	SQD	C13-C14-C15-C16
30	b	621	SQD	C13-C14-C15-C16
25	C	512	CLA	C8-C10-C11-C12
25	c	512	CLA	C8-C10-C11-C12
25	D	404	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
28	B	629	LMG	C11-C10-O7-C8
28	b	630	LMG	C11-C10-O7-C8
28	C	518	LMG	C40-C41-C42-C43
28	c	518	LMG	C40-C41-C42-C43
28	B	629	LMG	O9-C10-O7-C8
28	b	630	LMG	O9-C10-O7-C8
30	F	102	SQD	C2-C1-O6-C44
30	f	102	SQD	C2-C1-O6-C44
31	C	520	LMT	C2'-C1'-O1'-C1
31	D	409	LMT	C2'-C1'-O1'-C1
31	I	103	LMT	C2'-C1'-O1'-C1
31	c	520	LMT	C2'-C1'-O1'-C1
31	d	409	LMT	C2'-C1'-O1'-C1
31	i	103	LMT	C2'-C1'-O1'-C1
25	C	508	CLA	C10-C11-C12-C13
25	c	508	CLA	C10-C11-C12-C13
30	A	417	SQD	C23-C24-C25-C26
30	a	417	SQD	C23-C24-C25-C26
25	B	609	CLA	C13-C15-C16-C17
25	b	610	CLA	C13-C15-C16-C17
27	A	409	BCR	C11-C10-C9-C34
27	a	409	BCR	C11-C10-C9-C34
36	H	101	RRX	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
36	H	101	RRX	C35-C13-C14-C15
36	H	101	RRX	C11-C10-C9-C34
36	h	101	RRX	C16-C17-C18-C36
36	h	101	RRX	C35-C13-C14-C15
36	h	101	RRX	C11-C10-C9-C34
31	E	103	LMT	O5'-C5'-C6'-O6'
31	e	103	LMT	O5'-C5'-C6'-O6'
31	F	103	LMT	C11-C10-C9-C8
31	f	103	LMT	C11-C10-C9-C8
31	B	627	LMT	C4'-C5'-C6'-O6'
31	b	628	LMT	C4'-C5'-C6'-O6'
27	B	618	BCR	C11-C12-C13-C35
27	C	526	BCR	C36-C18-C19-C20
27	C	527	BCR	C7-C8-C9-C34
27	b	619	BCR	C11-C12-C13-C35
27	c	526	BCR	C36-C18-C19-C20
27	c	527	BCR	C7-C8-C9-C34
36	H	101	RRX	C37-C22-C23-C24
36	h	101	RRX	C37-C22-C23-C24
27	C	527	BCR	C7-C8-C9-C10
27	c	527	BCR	C7-C8-C9-C10
33	L	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C14-C15-C16-C17
25	C	512	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	B	616	CLA	C10-C11-C12-C13
25	b	617	CLA	C10-C11-C12-C13
28	A	410	LMG	C11-C12-C13-C14
28	a	410	LMG	C11-C12-C13-C14
33	A	418	LHG	O1-C1-C2-C3
33	B	626	LHG	O1-C1-C2-C3
33	E	102	LHG	O1-C1-C2-C3
33	a	418	LHG	O1-C1-C2-C3
33	b	627	LHG	O1-C1-C2-C3
33	e	102	LHG	O1-C1-C2-C3
30	B	620	SQD	C46-C45-O47-C7
30	b	621	SQD	C46-C45-O47-C7
29	D	405	PL9	C47-C48-C49-C51
29	d	405	PL9	C47-C48-C49-C51
25	B	616	CLA	C11-C12-C13-C14
25	B	616	CLA	C11-C12-C13-C15
25	b	617	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	617	CLA	C11-C12-C13-C15
28	B	621	LMG	C34-C35-C36-C37
28	b	622	LMG	C34-C35-C36-C37
27	A	409	BCR	C11-C10-C9-C8
27	a	409	BCR	C11-C10-C9-C8
36	H	101	RRX	C16-C17-C18-C19
36	H	101	RRX	C12-C13-C14-C15
36	H	101	RRX	C11-C10-C9-C8
36	h	101	RRX	C16-C17-C18-C19
36	h	101	RRX	C12-C13-C14-C15
36	h	101	RRX	C11-C10-C9-C8
30	F	102	SQD	O5-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	A	415	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	O5'-C1'-O1'-C1
31	a	415	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	O5'-C1'-O1'-C1
33	L	101	LHG	C5-C6-O8-C23
33	l	101	LHG	C5-C6-O8-C23
31	E	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	O1'-C1-C2-C3
31	B	622	LMT	C5-C6-C7-C8
31	b	623	LMT	C5-C6-C7-C8
25	B	616	CLA	CBA-CGA-O2A-C1
25	b	617	CLA	CBA-CGA-O2A-C1
25	B	615	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C19
26	A	407	PHO	C16-C17-C18-C20
26	a	407	PHO	C16-C17-C18-C20
28	D	407	LMG	O6-C5-C6-O5
28	d	407	LMG	O6-C5-C6-O5
30	B	630	SQD	C29-C30-C31-C32
30	b	601	SQD	C29-C30-C31-C32
31	D	409	LMT	C4-C5-C6-C7
31	d	409	LMT	C4-C5-C6-C7
34	H	103	DGD	CCA-CDA-CEA-CFA
34	h	103	DGD	CCA-CDA-CEA-CFA
36	H	101	RRX	C14-C15-C16-C17
36	h	101	RRX	C14-C15-C16-C17
30	A	412	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	B	630	SQD	C28-C29-C30-C31
30	K	102	SQD	C26-C27-C28-C29
30	b	601	SQD	C28-C29-C30-C31
30	k	102	SQD	C26-C27-C28-C29
33	Z	101	LHG	C23-C24-C25-C26
33	z	101	LHG	C23-C24-C25-C26
31	J	102	LMT	O5'-C5'-C6'-O6'
31	j	102	LMT	O5'-C5'-C6'-O6'
28	C	518	LMG	C29-C30-C31-C32
28	c	518	LMG	C29-C30-C31-C32
31	A	414	LMT	C2-C3-C4-C5
31	D	409	LMT	C11-C10-C9-C8
31	X	103	LMT	C6-C7-C8-C9
31	a	414	LMT	C2-C3-C4-C5
31	d	409	LMT	C11-C10-C9-C8
33	A	419	LHG	C29-C30-C31-C32
33	a	419	LHG	C29-C30-C31-C32
31	A	415	LMT	C1-C2-C3-C4
31	C	521	LMT	C1-C2-C3-C4
31	a	415	LMT	C1-C2-C3-C4
31	c	521	LMT	C1-C2-C3-C4
30	A	417	SQD	C9-C10-C11-C12
30	a	412	SQD	C24-C25-C26-C27
30	a	417	SQD	C9-C10-C11-C12
31	C	523	LMT	C6-C7-C8-C9
31	I	103	LMT	C3-C4-C5-C6
31	c	523	LMT	C6-C7-C8-C9
31	d	409	LMT	C3-C4-C5-C6
31	i	103	LMT	C3-C4-C5-C6
31	x	102	LMT	C2-C3-C4-C5
33	A	419	LHG	C25-C26-C27-C28
33	a	419	LHG	C25-C26-C27-C28
34	C	517	DGD	C7A-C8A-C9A-CAA
34	c	517	DGD	C7A-C8A-C9A-CAA
34	c	517	DGD	C5B-C6B-C7B-C8B
31	B	622	LMT	C2-C1-O1'-C1'
31	B	625	LMT	C2-C1-O1'-C1'
31	H	104	LMT	C2-C1-O1'-C1'
31	X	103	LMT	C2-C1-O1'-C1'
31	b	623	LMT	C2-C1-O1'-C1'
31	b	626	LMT	C2-C1-O1'-C1'
31	h	104	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	x	103	LMT	C2-C1-O1'-C1'
28	C	518	LMG	C19-C20-C21-C22
28	c	518	LMG	C19-C20-C21-C22
31	D	409	LMT	C3-C4-C5-C6
31	D	412	LMT	C5-C6-C7-C8
31	X	102	LMT	C2-C3-C4-C5
31	d	412	LMT	C5-C6-C7-C8
31	x	103	LMT	C6-C7-C8-C9
34	C	517	DGD	C5B-C6B-C7B-C8B
30	A	417	SQD	C11-C12-C13-C14
30	a	417	SQD	C11-C12-C13-C14
33	A	418	LHG	C13-C14-C15-C16
33	a	418	LHG	C13-C14-C15-C16
25	A	406	CLA	C16-C17-C18-C19
25	A	406	CLA	C16-C17-C18-C20
25	a	406	CLA	C16-C17-C18-C19
25	a	406	CLA	C16-C17-C18-C20
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
34	C	516	DGD	C3A-C4A-C5A-C6A
34	H	103	DGD	C7A-C8A-C9A-CAA
34	H	103	DGD	C7B-C8B-C9B-CAB
34	c	516	DGD	C3A-C4A-C5A-C6A
34	h	103	DGD	C7A-C8A-C9A-CAA
34	h	103	DGD	C7B-C8B-C9B-CAB
25	B	603	CLA	C15-C16-C17-C18
25	B	604	CLA	C13-C15-C16-C17
25	C	505	CLA	C13-C15-C16-C17
25	b	604	CLA	C15-C16-C17-C18
25	b	605	CLA	C13-C15-C16-C17
25	c	505	CLA	C13-C15-C16-C17
31	X	101	LMT	C1-C2-C3-C4
31	x	101	LMT	C1-C2-C3-C4
31	I	102	LMT	C7-C8-C9-C10
31	e	103	LMT	C6-C7-C8-C9
31	i	102	LMT	C7-C8-C9-C10
33	A	418	LHG	C26-C27-C28-C29
33	a	418	LHG	C26-C27-C28-C29
30	B	630	SQD	C30-C31-C32-C33
30	K	102	SQD	C11-C10-C9-C8
30	b	601	SQD	C30-C31-C32-C33
30	k	102	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	E	103	LMT	C6-C7-C8-C9
34	H	103	DGD	C6A-C7A-C8A-C9A
34	h	103	DGD	C6A-C7A-C8A-C9A
33	B	626	LHG	C23-C24-C25-C26
33	b	627	LHG	C23-C24-C25-C26
31	I	102	LMT	C1-C2-C3-C4
31	i	102	LMT	C1-C2-C3-C4
28	J	101	LMG	C18-C19-C20-C21
28	j	101	LMG	C18-C19-C20-C21
30	A	412	SQD	C14-C15-C16-C17
30	B	630	SQD	C25-C26-C27-C28
30	a	412	SQD	C14-C15-C16-C17
30	b	601	SQD	C25-C26-C27-C28
33	B	626	LHG	C14-C15-C16-C17
33	b	627	LHG	C14-C15-C16-C17
31	f	103	LMT	O1'-C1-C2-C3
25	A	405	CLA	O1D-CGD-O2D-CED
28	D	407	LMG	C15-C16-C17-C18
28	d	407	LMG	C15-C16-C17-C18
31	F	103	LMT	O1'-C1-C2-C3
31	I	101	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
31	D	412	LMT	C1-C2-C3-C4
31	d	412	LMT	C1-C2-C3-C4
25	A	405	CLA	C15-C16-C17-C18
25	B	607	CLA	C15-C16-C17-C18
25	B	613	CLA	C10-C11-C12-C13
25	a	405	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	a	405	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	C16-C17-C18-C20
25	C	504	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
25	c	504	CLA	C16-C17-C18-C20
31	C	523	LMT	C1-C2-C3-C4
31	c	523	LMT	C1-C2-C3-C4
28	C	519	LMG	C31-C32-C33-C34
28	c	519	LMG	C31-C32-C33-C34
31	B	624	LMT	C7-C8-C9-C10
31	F	103	LMT	C4-C5-C6-C7
31	b	625	LMT	C7-C8-C9-C10
31	f	103	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	Z	101	LHG	C24-C25-C26-C27
33	d	406	LHG	C28-C29-C30-C31
33	z	101	LHG	C24-C25-C26-C27
25	b	614	CLA	C10-C11-C12-C13
31	M	102	LMT	O1'-C1-C2-C3
31	m	102	LMT	O1'-C1-C2-C3
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
33	D	406	LHG	C28-C29-C30-C31
33	L	101	LHG	C10-C11-C12-C13
33	l	101	LHG	C10-C11-C12-C13
33	L	101	LHG	C1-C2-C3-O3
33	l	101	LHG	C1-C2-C3-O3
25	A	408	CLA	CBA-CGA-O2A-C1
25	a	408	CLA	CBA-CGA-O2A-C1
28	B	629	LMG	C31-C32-C33-C34
28	b	630	LMG	C31-C32-C33-C34
31	A	414	LMT	C6-C7-C8-C9
31	B	627	LMT	C6-C7-C8-C9
31	X	103	LMT	C5-C6-C7-C8
31	a	414	LMT	C6-C7-C8-C9
31	b	628	LMT	C6-C7-C8-C9
31	x	103	LMT	C5-C6-C7-C8
33	D	406	LHG	C18-C19-C20-C21
33	d	406	LHG	C18-C19-C20-C21
28	B	629	LMG	C10-C11-C12-C13
28	b	630	LMG	C10-C11-C12-C13
28	C	519	LMG	C11-C12-C13-C14
28	c	519	LMG	C11-C12-C13-C14
31	I	103	LMT	C4-C5-C6-C7
31	i	103	LMT	C4-C5-C6-C7
33	D	406	LHG	C16-C17-C18-C19
33	Z	101	LHG	C27-C28-C29-C30
33	d	406	LHG	C16-C17-C18-C19
33	z	101	LHG	C27-C28-C29-C30
34	H	103	DGD	CCB-CDB-CEB-CFB
34	h	103	DGD	CCB-CDB-CEB-CFB
30	K	102	SQD	C24-C25-C26-C27
30	f	102	SQD	C11-C10-C9-C8
30	k	102	SQD	C24-C25-C26-C27
30	F	102	SQD	C11-C10-C9-C8
31	X	103	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	x	103	LMT	C1-C2-C3-C4
31	B	628	LMT	C4'-C5'-C6'-O6'
31	b	629	LMT	C4'-C5'-C6'-O6'
28	C	518	LMG	C21-C22-C23-C24
28	c	518	LMG	C21-C22-C23-C24
30	B	620	SQD	C16-C17-C18-C19
30	b	621	SQD	C16-C17-C18-C19
31	E	103	LMT	C11-C10-C9-C8
31	e	103	LMT	C11-C10-C9-C8
33	B	626	LHG	C15-C16-C17-C18
33	E	102	LHG	C25-C26-C27-C28
33	b	627	LHG	C15-C16-C17-C18
33	e	102	LHG	C25-C26-C27-C28
28	B	621	LMG	C28-C29-C30-C31
28	b	622	LMG	C28-C29-C30-C31
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	C	525	BCR	C1-C6-C7-C8
27	D	411	BCR	C1-C6-C7-C8
27	D	411	BCR	C5-C6-C7-C8
27	D	411	BCR	C23-C24-C25-C26
27	D	411	BCR	C23-C24-C25-C30
27	b	618	BCR	C1-C6-C7-C8
27	b	618	BCR	C5-C6-C7-C8
27	c	525	BCR	C1-C6-C7-C8
27	d	411	BCR	C1-C6-C7-C8
27	d	411	BCR	C5-C6-C7-C8
27	d	411	BCR	C23-C24-C25-C26
27	d	411	BCR	C23-C24-C25-C30
36	H	101	RRX	C23-C24-C25-C30
36	H	101	RRX	C23-C24-C25-C26
36	h	101	RRX	C23-C24-C25-C30
36	h	101	RRX	C23-C24-C25-C26
31	C	520	LMT	C6-C7-C8-C9
31	c	520	LMT	C6-C7-C8-C9
33	E	102	LHG	C14-C15-C16-C17
33	Z	101	LHG	C26-C27-C28-C29
33	e	102	LHG	C14-C15-C16-C17
33	z	101	LHG	C26-C27-C28-C29
25	B	605	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
31	D	412	LMT	O1'-C1-C2-C3
31	d	412	LMT	O1'-C1-C2-C3
25	C	513	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
28	C	519	LMG	C37-C38-C39-C40
28	c	519	LMG	C37-C38-C39-C40
30	H	102	SQD	C18-C19-C20-C21
30	h	102	SQD	C18-C19-C20-C21
31	D	408	LMT	C2-C3-C4-C5
31	d	408	LMT	C2-C3-C4-C5
28	C	519	LMG	C36-C37-C38-C39
28	D	407	LMG	C13-C14-C15-C16
28	c	519	LMG	C36-C37-C38-C39
28	d	407	LMG	C13-C14-C15-C16
30	K	102	SQD	C9-C10-C11-C12
30	k	102	SQD	C9-C10-C11-C12
31	t	101	LMT	C5-C6-C7-C8
33	B	626	LHG	C26-C27-C28-C29
33	b	627	LHG	C26-C27-C28-C29
31	i	104	LMT	C1-C2-C3-C4
33	D	406	LHG	C35-C36-C37-C38
33	d	406	LHG	C35-C36-C37-C38
31	I	104	LMT	C7-C8-C9-C10
31	i	104	LMT	C7-C8-C9-C10
33	A	419	LHG	C33-C34-C35-C36
33	a	419	LHG	C33-C34-C35-C36
25	B	616	CLA	O1A-CGA-O2A-C1
25	b	617	CLA	O1A-CGA-O2A-C1
31	B	628	LMT	O1'-C1-C2-C3
31	b	629	LMT	O1'-C1-C2-C3
30	H	102	SQD	C13-C14-C15-C16
30	h	102	SQD	C13-C14-C15-C16
31	T	101	LMT	C5-C6-C7-C8
31	I	104	LMT	C1-C2-C3-C4
30	A	417	SQD	C24-C25-C26-C27
30	a	417	SQD	C24-C25-C26-C27
25	C	506	CLA	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
25	C	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C2-C3-C5-C6
29	A	411	PL9	C38-C39-C41-C42
29	a	411	PL9	C38-C39-C41-C42
28	D	407	LMG	C19-C20-C21-C22
28	J	101	LMG	C29-C30-C31-C32
28	d	407	LMG	C19-C20-C21-C22
28	j	101	LMG	C29-C30-C31-C32
30	B	620	SQD	C15-C16-C17-C18
30	B	630	SQD	C12-C13-C14-C15
30	b	601	SQD	C12-C13-C14-C15
30	b	621	SQD	C15-C16-C17-C18
33	A	418	LHG	C24-C23-O8-C6
33	a	418	LHG	C24-C23-O8-C6
25	C	509	CLA	C11-C12-C13-C14
25	c	509	CLA	C11-C12-C13-C14
28	J	101	LMG	C30-C31-C32-C33
28	j	101	LMG	C30-C31-C32-C33
31	B	627	LMT	C4-C5-C6-C7
31	X	103	LMT	C4-C5-C6-C7
31	b	628	LMT	C4-C5-C6-C7
31	x	103	LMT	C4-C5-C6-C7
28	A	410	LMG	C15-C16-C17-C18
28	C	519	LMG	C29-C30-C31-C32
28	c	519	LMG	C29-C30-C31-C32
31	C	521	LMT	C2-C3-C4-C5
31	X	102	LMT	C3-C4-C5-C6
31	c	521	LMT	C2-C3-C4-C5
31	x	102	LMT	C3-C4-C5-C6
31	I	103	LMT	O5'-C1'-O1'-C1
31	i	103	LMT	O5'-C1'-O1'-C1
34	C	516	DGD	O6E-C1E-O5D-C6D
34	c	516	DGD	O6E-C1E-O5D-C6D
28	a	410	LMG	C15-C16-C17-C18
30	H	102	SQD	C10-C11-C12-C13
30	h	102	SQD	C10-C11-C12-C13
28	A	413	LMG	C13-C14-C15-C16
28	a	413	LMG	C13-C14-C15-C16
30	B	630	SQD	C33-C34-C35-C36
30	b	601	SQD	C33-C34-C35-C36
33	A	419	LHG	C9-C10-C11-C12
33	B	626	LHG	C11-C12-C13-C14
33	a	419	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	b	627	LHG	C11-C12-C13-C14
34	C	515	DGD	C5A-C6A-C7A-C8A
34	C	515	DGD	CAA-CBA-CCA-CDA
34	c	515	DGD	C5A-C6A-C7A-C8A
34	c	515	DGD	CAA-CBA-CCA-CDA
30	B	620	SQD	C29-C30-C31-C32
30	b	621	SQD	C29-C30-C31-C32
33	a	419	LHG	C11-C10-C9-C8
34	C	516	DGD	CAB-CBB-CCB-CDB
34	c	516	DGD	CAB-CBB-CCB-CDB
28	B	621	LMG	C32-C33-C34-C35
28	b	622	LMG	C32-C33-C34-C35
30	B	630	SQD	C27-C28-C29-C30
30	b	601	SQD	C27-C28-C29-C30
31	A	415	LMT	C6-C7-C8-C9
31	H	104	LMT	C2-C3-C4-C5
31	a	415	LMT	C6-C7-C8-C9
31	h	104	LMT	C2-C3-C4-C5
33	A	419	LHG	C11-C10-C9-C8
36	H	101	RRX	C9-C10-C11-C12
36	h	101	RRX	C9-C10-C11-C12
31	D	409	LMT	C5-C6-C7-C8
31	d	409	LMT	C5-C6-C7-C8
28	A	410	LMG	C11-C10-O7-C8
28	a	410	LMG	C11-C10-O7-C8
33	E	102	LHG	C8-C7-O7-C5
33	e	102	LHG	C8-C7-O7-C5
31	J	103	LMT	O1'-C1-C2-C3
31	j	103	LMT	O1'-C1-C2-C3
28	J	101	LMG	C28-C29-C30-C31
28	j	101	LMG	C28-C29-C30-C31
28	A	410	LMG	C22-C23-C24-C25
28	a	410	LMG	C22-C23-C24-C25
31	D	410	LMT	C7-C8-C9-C10
31	d	410	LMT	C7-C8-C9-C10
25	B	602	CLA	C13-C15-C16-C17
25	B	614	CLA	C15-C16-C17-C18
25	b	603	CLA	C13-C15-C16-C17
25	b	615	CLA	C15-C16-C17-C18
28	C	518	LMG	C30-C31-C32-C33
28	c	518	LMG	C30-C31-C32-C33
30	A	417	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	a	417	SQD	C25-C26-C27-C28
30	f	102	SQD	C9-C10-C11-C12
31	C	520	LMT	C11-C10-C9-C8
31	F	103	LMT	C6-C7-C8-C9
31	c	520	LMT	C11-C10-C9-C8
31	f	103	LMT	C6-C7-C8-C9
34	c	517	DGD	CDA-CEA-CFA-CGA
30	F	102	SQD	C9-C10-C11-C12
30	H	102	SQD	C9-C10-C11-C12
30	h	102	SQD	C9-C10-C11-C12
34	C	517	DGD	CAB-CBB-CCB-CDB
34	c	517	DGD	CAB-CBB-CCB-CDB
34	C	517	DGD	CDA-CEA-CFA-CGA
27	A	409	BCR	C36-C18-C19-C20
27	a	409	BCR	C36-C18-C19-C20
31	B	623	LMT	C3-C4-C5-C6
31	b	624	LMT	C3-C4-C5-C6
25	B	604	CLA	C3-C5-C6-C7
25	b	605	CLA	C3-C5-C6-C7
36	H	101	RRX	C21-C22-C23-C24
36	h	101	RRX	C21-C22-C23-C24
30	F	102	SQD	C45-C44-O6-C1
30	f	102	SQD	C45-C44-O6-C1
30	B	630	SQD	C17-C18-C19-C20
25	C	508	CLA	C16-C17-C18-C19
25	C	508	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C20
28	A	410	LMG	C36-C37-C38-C39
28	B	629	LMG	C40-C41-C42-C43
28	D	407	LMG	C22-C23-C24-C25
28	a	410	LMG	C36-C37-C38-C39
28	b	630	LMG	C40-C41-C42-C43
30	A	412	SQD	C9-C10-C11-C12
30	a	412	SQD	C9-C10-C11-C12
30	b	601	SQD	C17-C18-C19-C20
31	E	101	LMT	C2-C3-C4-C5
31	e	101	LMT	C2-C3-C4-C5
26	D	402	PHO	C2-C3-C5-C6
26	d	402	PHO	C2-C3-C5-C6
28	D	407	LMG	C33-C34-C35-C36
28	d	407	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
28	d	407	LMG	C33-C34-C35-C36
30	A	417	SQD	C14-C15-C16-C17
30	K	102	SQD	C13-C14-C15-C16
30	a	417	SQD	C14-C15-C16-C17
30	k	102	SQD	C13-C14-C15-C16
31	B	627	LMT	C11-C10-C9-C8
31	B	628	LMT	C4-C5-C6-C7
31	b	628	LMT	C11-C10-C9-C8
31	b	629	LMT	C4-C5-C6-C7
33	B	626	LHG	C25-C26-C27-C28
33	b	627	LHG	C25-C26-C27-C28
31	J	102	LMT	C2-C3-C4-C5
31	j	102	LMT	C2-C3-C4-C5
28	C	518	LMG	C11-C12-C13-C14
28	c	518	LMG	C11-C12-C13-C14
30	B	630	SQD	C18-C19-C20-C21
30	b	601	SQD	C18-C19-C20-C21
25	A	408	CLA	O1A-CGA-O2A-C1
25	a	408	CLA	O1A-CGA-O2A-C1
30	A	417	SQD	C11-C10-C9-C8
30	a	417	SQD	C11-C10-C9-C8
28	C	518	LMG	C28-C29-C30-C31
28	c	518	LMG	C28-C29-C30-C31
28	j	101	LMG	C40-C41-C42-C43
31	T	101	LMT	C3-C4-C5-C6
31	t	101	LMT	C3-C4-C5-C6
33	A	419	LHG	C28-C29-C30-C31
33	a	419	LHG	C28-C29-C30-C31
28	J	101	LMG	C40-C41-C42-C43
26	A	407	PHO	C16-C17-C18-C19
26	a	407	PHO	C16-C17-C18-C19
30	A	417	SQD	C26-C27-C28-C29
30	a	417	SQD	C26-C27-C28-C29
33	Z	101	LHG	C10-C11-C12-C13
33	z	101	LHG	C10-C11-C12-C13
28	A	410	LMG	C39-C40-C41-C42
30	H	102	SQD	C29-C30-C31-C32
30	h	102	SQD	C29-C30-C31-C32
31	T	101	LMT	C1-C2-C3-C4
31	t	101	LMT	C1-C2-C3-C4
28	A	410	LMG	C28-C29-C30-C31
28	J	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	a	410	LMG	C28-C29-C30-C31
28	j	101	LMG	C10-C11-C12-C13
25	C	507	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
28	a	410	LMG	C39-C40-C41-C42
31	C	521	LMT	C4-C5-C6-C7
31	c	521	LMT	C4-C5-C6-C7
31	A	415	LMT	O1'-C1-C2-C3
31	a	415	LMT	O1'-C1-C2-C3
28	A	413	LMG	O7-C8-C9-O8
28	a	413	LMG	O7-C8-C9-O8
30	A	412	SQD	O47-C45-C46-O48
30	a	412	SQD	O47-C45-C46-O48
28	A	410	LMG	C14-C15-C16-C17
31	C	523	LMT	C3-C4-C5-C6
31	c	523	LMT	C3-C4-C5-C6
33	A	418	LHG	C28-C29-C30-C31
33	a	418	LHG	C28-C29-C30-C31
31	A	415	LMT	O5'-C5'-C6'-O6'
31	M	101	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5'-C5'-C6'-O6'
31	m	101	LMT	O5'-C5'-C6'-O6'
28	C	519	LMG	C33-C34-C35-C36
28	a	410	LMG	C14-C15-C16-C17
28	c	519	LMG	C33-C34-C35-C36
31	D	410	LMT	C6-C7-C8-C9
31	I	103	LMT	C5-C6-C7-C8
31	d	410	LMT	C6-C7-C8-C9
31	i	103	LMT	C5-C6-C7-C8
33	B	626	LHG	C34-C35-C36-C37
30	B	620	SQD	C34-C35-C36-C37
30	b	621	SQD	C34-C35-C36-C37
31	D	412	LMT	C4-C5-C6-C7
31	I	101	LMT	C7-C8-C9-C10
31	I	102	LMT	C6-C7-C8-C9
31	d	412	LMT	C4-C5-C6-C7
31	i	101	LMT	C7-C8-C9-C10
31	i	102	LMT	C6-C7-C8-C9
33	b	627	LHG	C34-C35-C36-C37
25	B	612	CLA	C16-C17-C18-C20
25	B	614	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C16-C17-C18-C19
31	D	408	LMT	O1'-C1-C2-C3
31	d	408	LMT	O1'-C1-C2-C3
28	C	518	LMG	C33-C34-C35-C36
28	c	518	LMG	C33-C34-C35-C36
31	B	625	LMT	C11-C10-C9-C8
31	b	626	LMT	C11-C10-C9-C8
33	B	626	LHG	C13-C14-C15-C16
33	b	627	LHG	C13-C14-C15-C16
34	C	515	DGD	O6E-C5E-C6E-O5E
34	c	515	DGD	O6E-C5E-C6E-O5E
31	I	102	LMT	C11-C10-C9-C8
31	i	102	LMT	C11-C10-C9-C8
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
30	B	630	SQD	C32-C33-C34-C35
30	b	601	SQD	C32-C33-C34-C35
31	A	414	LMT	C4-C5-C6-C7
31	I	103	LMT	C2-C3-C4-C5
31	a	414	LMT	C4-C5-C6-C7
31	i	103	LMT	C2-C3-C4-C5
28	C	518	LMG	C32-C33-C34-C35
28	c	518	LMG	C32-C33-C34-C35
30	A	417	SQD	C30-C31-C32-C33
30	B	620	SQD	C18-C19-C20-C21
30	b	621	SQD	C18-C19-C20-C21
31	B	623	LMT	C7-C8-C9-C10
31	M	101	LMT	C4-C5-C6-C7
31	b	624	LMT	C7-C8-C9-C10
31	m	101	LMT	C4-C5-C6-C7
35	F	101	HEM	C2A-CAA-CBA-CGA
35	f	101	HEM	C2A-CAA-CBA-CGA
30	B	620	SQD	C27-C28-C29-C30
30	a	417	SQD	C30-C31-C32-C33
30	b	621	SQD	C27-C28-C29-C30
31	A	414	LMT	C7-C8-C9-C10
31	a	414	LMT	C7-C8-C9-C10
25	B	608	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
29	D	405	PL9	C47-C48-C49-C50
29	d	405	PL9	C47-C48-C49-C50
28	b	630	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	A	415	LMT	C2-C3-C4-C5
31	a	415	LMT	C2-C3-C4-C5
33	A	418	LHG	O1-C1-C2-O2
33	a	418	LHG	O1-C1-C2-O2
28	B	629	LMG	C29-C30-C31-C32
31	D	408	LMT	C1-C2-C3-C4
31	d	408	LMT	C1-C2-C3-C4
25	B	611	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C15-C16-C17-C18
25	c	504	CLA	C13-C15-C16-C17
25	d	404	CLA	C15-C16-C17-C18
31	F	103	LMT	C3-C4-C5-C6
31	f	103	LMT	C3-C4-C5-C6
31	B	624	LMT	C11-C10-C9-C8
31	b	625	LMT	C11-C10-C9-C8
34	C	516	DGD	C9A-CAA-CBA-CCA
34	c	516	DGD	C9A-CAA-CBA-CCA
30	B	630	SQD	C26-C27-C28-C29
31	B	624	LMT	C3-C4-C5-C6
31	b	625	LMT	C3-C4-C5-C6
33	A	419	LHG	C13-C14-C15-C16
33	E	102	LHG	C11-C12-C13-C14
33	a	419	LHG	C13-C14-C15-C16
33	e	102	LHG	C11-C12-C13-C14
31	F	103	LMT	O5'-C5'-C6'-O6'
31	f	103	LMT	O5'-C5'-C6'-O6'
28	A	410	LMG	O9-C10-O7-C8
28	a	410	LMG	O9-C10-O7-C8
28	B	629	LMG	C16-C17-C18-C19
28	b	630	LMG	C16-C17-C18-C19
28	c	518	LMG	C34-C35-C36-C37
30	b	601	SQD	C26-C27-C28-C29
33	L	101	LHG	C12-C13-C14-C15
33	l	101	LHG	C12-C13-C14-C15
25	B	604	CLA	C11-C12-C13-C15
25	B	605	CLA	C11-C10-C8-C7
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C12-C13-C15
25	b	617	CLA	C11-C10-C8-C7
25	c	505	CLA	C12-C13-C15-C16
25	c	508	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C10-C8-C7
28	C	518	LMG	C34-C35-C36-C37
26	D	402	PHO	C5-C6-C7-C8
26	d	402	PHO	C5-C6-C7-C8
28	B	621	LMG	C37-C38-C39-C40
31	E	103	LMT	C1-C2-C3-C4
31	e	103	LMT	C1-C2-C3-C4
28	b	622	LMG	C37-C38-C39-C40
29	D	405	PL9	C40-C39-C41-C42
29	d	405	PL9	C40-C39-C41-C42
31	F	103	LMT	C7-C8-C9-C10
31	f	103	LMT	C7-C8-C9-C10
33	A	419	LHG	C11-C12-C13-C14
33	L	101	LHG	C15-C16-C17-C18
33	a	419	LHG	C11-C12-C13-C14
33	l	101	LHG	C15-C16-C17-C18
31	C	521	LMT	C7-C8-C9-C10
31	M	101	LMT	C6-C7-C8-C9
31	c	521	LMT	C7-C8-C9-C10
31	m	101	LMT	C6-C7-C8-C9
25	C	504	CLA	C13-C15-C16-C17
28	A	413	LMG	C4-C5-C6-O5
28	a	413	LMG	C4-C5-C6-O5
31	A	415	LMT	C4'-C5'-C6'-O6'
31	a	415	LMT	C4'-C5'-C6'-O6'
25	C	505	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C11-C10-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	508	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	617	CLA	C11-C10-C8-C9
25	c	505	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C6-C7-C8-C9
33	A	419	LHG	C18-C19-C20-C21
33	a	419	LHG	C18-C19-C20-C21
31	B	625	LMT	C1-C2-C3-C4
31	b	626	LMT	C1-C2-C3-C4
28	B	629	LMG	C39-C40-C41-C42
28	b	630	LMG	C39-C40-C41-C42
34	C	515	DGD	C4B-C5B-C6B-C7B
31	B	622	LMT	C4B-C5B-C6B-O6B
31	b	623	LMT	C4B-C5B-C6B-O6B
25	B	604	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
28	C	518	LMG	C29-C28-O8-C9
28	c	518	LMG	C29-C28-O8-C9
34	c	515	DGD	C4B-C5B-C6B-C7B
31	H	104	LMT	O5'-C5'-C6'-O6'
31	J	103	LMT	O5'-C5'-C6'-O6'
31	h	104	LMT	O5'-C5'-C6'-O6'
31	j	103	LMT	O5'-C5'-C6'-O6'
33	L	101	LHG	C25-C26-C27-C28
33	l	101	LHG	C25-C26-C27-C28
33	E	102	LHG	C19-C20-C21-C22
33	e	102	LHG	C19-C20-C21-C22
28	B	629	LMG	C2-C1-O1-C7
28	b	630	LMG	C2-C1-O1-C7
30	B	630	SQD	C15-C16-C17-C18
30	b	601	SQD	C15-C16-C17-C18
28	A	413	LMG	C7-C8-C9-O8
28	a	413	LMG	C7-C8-C9-O8
30	B	620	SQD	C44-C45-C46-O48
30	b	621	SQD	C44-C45-C46-O48
33	A	419	LHG	C4-C5-C6-O8
33	a	419	LHG	C4-C5-C6-O8
31	C	520	LMT	C2-C3-C4-C5
31	c	520	LMT	C2-C3-C4-C5
34	C	517	DGD	C6A-C7A-C8A-C9A
34	c	517	DGD	C6A-C7A-C8A-C9A
25	D	404	CLA	C3-C5-C6-C7
25	C	512	CLA	C10-C11-C12-C13
25	c	512	CLA	C10-C11-C12-C13
33	Z	101	LHG	C31-C32-C33-C34
33	z	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	M	102	LMT	O5'-C5'-C6'-O6'
31	m	102	LMT	O5'-C5'-C6'-O6'
31	C	522	LMT	C4-C5-C6-C7
31	c	522	LMT	C4-C5-C6-C7
33	B	626	LHG	C9-C10-C11-C12
33	b	627	LHG	C9-C10-C11-C12
28	A	413	LMG	C32-C33-C34-C35
28	B	621	LMG	C15-C16-C17-C18
28	a	413	LMG	C32-C33-C34-C35
28	b	622	LMG	C15-C16-C17-C18
31	B	625	LMT	C6-C7-C8-C9
31	D	412	LMT	C6-C7-C8-C9
31	b	626	LMT	C6-C7-C8-C9
31	d	412	LMT	C6-C7-C8-C9
25	d	404	CLA	C3-C5-C6-C7
33	A	418	LHG	O10-C23-O8-C6
33	a	418	LHG	O10-C23-O8-C6
29	D	405	PL9	C28-C29-C31-C32
29	D	405	PL9	C38-C39-C41-C42
29	d	405	PL9	C28-C29-C31-C32
29	d	405	PL9	C38-C39-C41-C42
25	C	502	CLA	C13-C15-C16-C17
25	C	510	CLA	C8-C10-C11-C12
25	c	502	CLA	C13-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
25	C	503	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
30	K	102	SQD	C10-C11-C12-C13
30	k	102	SQD	C10-C11-C12-C13
33	Z	101	LHG	C4-O6-P-O5
33	z	101	LHG	C4-O6-P-O5
33	A	418	LHG	C17-C18-C19-C20
33	a	418	LHG	C17-C18-C19-C20
34	C	515	DGD	C3B-C4B-C5B-C6B
34	c	515	DGD	C3B-C4B-C5B-C6B
31	A	415	LMT	C4-C5-C6-C7
31	B	628	LMT	C1-C2-C3-C4
31	b	629	LMT	C1-C2-C3-C4
31	A	415	LMT	C5-C6-C7-C8
31	B	622	LMT	C11-C10-C9-C8
31	I	104	LMT	C5-C6-C7-C8
31	a	415	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	a	415	LMT	C5-C6-C7-C8
31	b	623	LMT	C11-C10-C9-C8
31	i	104	LMT	C5-C6-C7-C8
34	C	515	DGD	O6D-C5D-C6D-O5D
34	c	515	DGD	O6D-C5D-C6D-O5D
27	B	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C10-C11-C12-C13
33	E	102	LHG	C24-C25-C26-C27
33	e	102	LHG	C11-C10-C9-C8
33	e	102	LHG	C24-C25-C26-C27
27	D	411	BCR	C19-C20-C21-C22
27	d	411	BCR	C19-C20-C21-C22
25	C	502	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20
31	M	101	LMT	C5'-C4'-O1B-C1B
31	m	101	LMT	C5'-C4'-O1B-C1B
28	J	101	LMG	C21-C22-C23-C24
28	j	101	LMG	C21-C22-C23-C24
31	H	104	LMT	C3-C4-C5-C6
31	h	104	LMT	C3-C4-C5-C6
33	E	102	LHG	C11-C10-C9-C8
31	C	523	LMT	C4-C5-C6-C7
31	c	523	LMT	C4-C5-C6-C7
28	A	413	LMG	C31-C32-C33-C34
28	a	413	LMG	C31-C32-C33-C34
28	A	413	LMG	C33-C34-C35-C36
28	a	413	LMG	C33-C34-C35-C36
31	I	103	LMT	C7-C8-C9-C10
31	i	103	LMT	C7-C8-C9-C10
28	C	518	LMG	C18-C19-C20-C21
28	c	518	LMG	C18-C19-C20-C21
31	C	524	LMT	C6-C7-C8-C9
31	c	524	LMT	C6-C7-C8-C9
28	A	410	LMG	C29-C30-C31-C32
28	a	410	LMG	C29-C30-C31-C32
31	B	623	LMT	C4-C5-C6-C7
31	C	524	LMT	C4-C5-C6-C7
31	b	624	LMT	C4-C5-C6-C7
31	c	524	LMT	C4-C5-C6-C7
28	B	629	LMG	C32-C33-C34-C35
28	b	630	LMG	C32-C33-C34-C35
31	E	101	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	C5-C6-C7-C8
33	A	418	LHG	C15-C16-C17-C18
33	D	406	LHG	C15-C16-C17-C18
33	a	418	LHG	C15-C16-C17-C18
33	d	406	LHG	C15-C16-C17-C18
33	l	101	LHG	C13-C14-C15-C16
34	C	516	DGD	C2A-C3A-C4A-C5A
34	C	516	DGD	C7A-C8A-C9A-CAA
34	c	516	DGD	C2A-C3A-C4A-C5A
34	c	516	DGD	C7A-C8A-C9A-CAA
30	K	102	SQD	C14-C15-C16-C17
30	k	102	SQD	C14-C15-C16-C17
31	D	408	LMT	C9-C10-C11-C12
31	d	408	LMT	C9-C10-C11-C12
34	H	103	DGD	CDA-CEA-CFA-CGA
34	h	103	DGD	CDA-CEA-CFA-CGA
33	A	419	LHG	C23-C24-C25-C26
33	a	419	LHG	C23-C24-C25-C26
25	B	610	CLA	C15-C16-C17-C18
33	A	418	LHG	C16-C17-C18-C19
33	B	626	LHG	C28-C29-C30-C31
33	L	101	LHG	C13-C14-C15-C16
33	a	418	LHG	C16-C17-C18-C19
33	b	627	LHG	C28-C29-C30-C31
33	E	102	LHG	O7-C5-C6-O8
33	e	102	LHG	O7-C5-C6-O8
30	A	412	SQD	C15-C16-C17-C18
30	a	412	SQD	C15-C16-C17-C18
33	D	406	LHG	C31-C32-C33-C34
33	d	406	LHG	C31-C32-C33-C34
25	b	611	CLA	C15-C16-C17-C18
33	A	419	LHG	C19-C20-C21-C22
33	a	419	LHG	C19-C20-C21-C22
31	B	623	LMT	C6-C7-C8-C9
25	C	506	CLA	C3-C5-C6-C7
25	c	506	CLA	C3-C5-C6-C7
31	X	103	LMT	C7-C8-C9-C10
31	b	624	LMT	C6-C7-C8-C9
31	x	103	LMT	C7-C8-C9-C10
34	C	517	DGD	C9B-CAB-CBB-CCB
34	c	517	DGD	C9B-CAB-CBB-CCB
30	F	102	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C24-C25-C26-C27
33	E	102	LHG	C26-C27-C28-C29
33	e	102	LHG	C26-C27-C28-C29
30	B	630	SQD	C16-C17-C18-C19
30	b	601	SQD	C16-C17-C18-C19
31	I	104	LMT	C9-C10-C11-C12
31	i	104	LMT	C9-C10-C11-C12
25	B	603	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
31	C	524	LMT	C11-C10-C9-C8
31	c	524	LMT	C11-C10-C9-C8
34	C	515	DGD	C2B-C3B-C4B-C5B
34	c	515	DGD	C2B-C3B-C4B-C5B
30	b	601	SQD	C35-C36-C37-C38
30	B	630	SQD	C35-C36-C37-C38
31	J	102	LMT	C3-C4-C5-C6
31	j	102	LMT	C3-C4-C5-C6
25	C	508	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
31	I	102	LMT	O1'-C1-C2-C3
31	i	102	LMT	O1'-C1-C2-C3
28	B	621	LMG	C40-C41-C42-C43
33	B	626	LHG	C19-C20-C21-C22
33	b	627	LHG	C19-C20-C21-C22
28	b	622	LMG	C40-C41-C42-C43
33	A	418	LHG	C19-C20-C21-C22
33	a	418	LHG	C19-C20-C21-C22
33	l	101	LHG	C32-C33-C34-C35
33	D	406	LHG	C30-C31-C32-C33
33	L	101	LHG	C32-C33-C34-C35
33	d	406	LHG	C30-C31-C32-C33
31	D	409	LMT	C2-C1-O1'-C1'
31	D	412	LMT	C2-C1-O1'-C1'
31	I	101	LMT	C2-C1-O1'-C1'
31	d	409	LMT	C2-C1-O1'-C1'
31	d	412	LMT	C2-C1-O1'-C1'
31	i	101	LMT	C2-C1-O1'-C1'
31	T	101	LMT	C4'-C5'-C6'-O6'
31	t	101	LMT	C4'-C5'-C6'-O6'
25	B	603	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	b	604	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C12-C13-C14
25	b	616	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C10-C8-C9
25	d	403	CLA	C14-C13-C15-C16
30	B	630	SQD	C34-C35-C36-C37
34	C	515	DGD	CCB-CDB-CEB-CFB
25	B	607	CLA	C5-C6-C7-C8
25	b	608	CLA	C5-C6-C7-C8
28	J	101	LMG	C37-C38-C39-C40
28	j	101	LMG	C37-C38-C39-C40
30	b	601	SQD	C34-C35-C36-C37
31	D	408	LMT	C3-C4-C5-C6
31	d	408	LMT	C3-C4-C5-C6
34	C	516	DGD	C2B-C3B-C4B-C5B
34	c	515	DGD	CCB-CDB-CEB-CFB
34	c	516	DGD	C2B-C3B-C4B-C5B
25	B	607	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
33	B	626	LHG	C33-C34-C35-C36
33	L	101	LHG	C27-C28-C29-C30
33	b	627	LHG	C33-C34-C35-C36
33	l	101	LHG	C27-C28-C29-C30
34	C	516	DGD	C2E-C1E-O5D-C6D
34	c	516	DGD	C2E-C1E-O5D-C6D
25	C	509	CLA	C8-C10-C11-C12
30	H	102	SQD	C17-C18-C19-C20
31	M	101	LMT	C3-C4-C5-C6
31	m	101	LMT	C3-C4-C5-C6
34	C	515	DGD	C6A-C7A-C8A-C9A
34	H	103	DGD	C9A-CAA-CBA-CCA
34	c	515	DGD	C6A-C7A-C8A-C9A
34	h	103	DGD	C9A-CAA-CBA-CCA
33	B	626	LHG	O6-C4-C5-C6
33	b	627	LHG	O6-C4-C5-C6
34	C	515	DGD	C4D-C5D-C6D-O5D
34	c	515	DGD	C4D-C5D-C6D-O5D
30	H	102	SQD	C12-C13-C14-C15
30	h	102	SQD	C12-C13-C14-C15
30	h	102	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	B	626	LHG	C10-C11-C12-C13
33	b	627	LHG	C10-C11-C12-C13
31	F	103	LMT	C9-C10-C11-C12
31	f	103	LMT	C9-C10-C11-C12
34	H	103	DGD	O2G-C1B-C2B-C3B
34	h	103	DGD	O2G-C1B-C2B-C3B
25	A	406	CLA	C12-C13-C15-C16
25	B	602	CLA	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	C	506	CLA	C6-C7-C8-C10
25	C	508	CLA	C6-C7-C8-C10
25	C	513	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C10-C8-C7
25	a	406	CLA	C12-C13-C15-C16
25	b	603	CLA	C12-C13-C15-C16
25	b	604	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
25	c	508	CLA	C6-C7-C8-C10
25	c	513	CLA	C6-C7-C8-C10
25	c	513	CLA	C11-C10-C8-C7
25	B	605	CLA	C8-C10-C11-C12
25	b	606	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
30	B	630	SQD	C19-C20-C21-C22
30	b	601	SQD	C19-C20-C21-C22
28	C	519	LMG	C30-C31-C32-C33
28	c	519	LMG	C30-C31-C32-C33
31	M	101	LMT	C2-C3-C4-C5
31	m	101	LMT	C2-C3-C4-C5
25	B	613	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
28	C	518	LMG	O10-C28-O8-C9
28	c	518	LMG	O10-C28-O8-C9
31	B	622	LMT	C6-C7-C8-C9
29	D	405	PL9	C30-C29-C31-C32
29	d	405	PL9	C30-C29-C31-C32
29	D	405	PL9	C13-C14-C16-C17
29	d	405	PL9	C13-C14-C16-C17
33	B	626	LHG	C35-C36-C37-C38
33	b	627	LHG	C35-C36-C37-C38
31	b	623	LMT	C6-C7-C8-C9
27	B	619	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	b	620	BCR	C9-C10-C11-C12
30	H	102	SQD	C32-C33-C34-C35
30	K	102	SQD	C30-C31-C32-C33
30	h	102	SQD	C32-C33-C34-C35
30	k	102	SQD	C30-C31-C32-C33
34	h	103	DGD	C5B-C6B-C7B-C8B
34	H	103	DGD	C5B-C6B-C7B-C8B
33	B	626	LHG	C1-C2-C3-O3
33	b	627	LHG	C1-C2-C3-O3
31	I	102	LMT	C9-C10-C11-C12
31	i	102	LMT	C9-C10-C11-C12
28	C	519	LMG	O1-C7-C8-C9
28	C	519	LMG	C7-C8-C9-O8
28	c	519	LMG	O1-C7-C8-C9
28	c	519	LMG	C7-C8-C9-O8
30	A	412	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48
33	L	101	LHG	C4-C5-C6-O8
33	l	101	LHG	C4-C5-C6-O8
31	C	521	LMT	C11-C10-C9-C8
31	c	521	LMT	C11-C10-C9-C8
31	M	102	LMT	C9-C10-C11-C12
31	m	102	LMT	C9-C10-C11-C12
25	C	507	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C20
25	B	612	CLA	C8-C10-C11-C12
25	b	613	CLA	C8-C10-C11-C12
30	H	102	SQD	C33-C34-C35-C36
31	C	523	LMT	O1'-C1-C2-C3
31	c	523	LMT	O1'-C1-C2-C3
30	h	102	SQD	C33-C34-C35-C36
31	I	104	LMT	C11-C10-C9-C8
31	i	104	LMT	C11-C10-C9-C8
31	X	102	LMT	C1-C2-C3-C4
31	x	102	LMT	C1-C2-C3-C4
28	C	519	LMG	C15-C16-C17-C18
28	c	519	LMG	C15-C16-C17-C18
30	B	620	SQD	C12-C13-C14-C15
30	b	621	SQD	C12-C13-C14-C15
31	J	102	LMT	C4-C5-C6-C7
31	j	102	LMT	C4-C5-C6-C7
33	E	102	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C10-C11-C12-C13
29	D	405	PL9	C15-C14-C16-C17
29	d	405	PL9	C15-C14-C16-C17
25	C	512	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
25	C	513	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
33	b	627	LHG	C31-C32-C33-C34
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	O1D-CGD-O2D-CED
33	A	419	LHG	C16-C17-C18-C19
33	a	419	LHG	C16-C17-C18-C19
33	B	626	LHG	C31-C32-C33-C34
31	X	103	LMT	O1'-C1-C2-C3
31	x	103	LMT	O1'-C1-C2-C3
27	C	514	BCR	C23-C24-C25-C30
27	c	514	BCR	C23-C24-C25-C30
33	B	626	LHG	O2-C2-C3-O3
33	b	627	LHG	O2-C2-C3-O3
31	C	521	LMT	C3-C4-C5-C6
31	c	521	LMT	C3-C4-C5-C6
33	B	626	LHG	C12-C13-C14-C15
33	b	627	LHG	C12-C13-C14-C15
25	B	607	CLA	C16-C17-C18-C20
25	D	401	CLA	C16-C17-C18-C20
25	b	608	CLA	C16-C17-C18-C20
25	d	401	CLA	C16-C17-C18-C20
28	A	413	LMG	O8-C28-C29-C30
28	a	413	LMG	O8-C28-C29-C30
25	b	606	CLA	O1D-CGD-O2D-CED
28	C	519	LMG	O1-C7-C8-O7
28	J	101	LMG	O7-C8-C9-O8
28	c	519	LMG	O1-C7-C8-O7
28	j	101	LMG	O7-C8-C9-O8
28	C	518	LMG	C22-C23-C24-C25
28	c	518	LMG	C22-C23-C24-C25
25	B	605	CLA	O1D-CGD-O2D-CED
33	l	101	LHG	C28-C29-C30-C31
33	L	101	LHG	C28-C29-C30-C31
33	A	418	LHG	C7-C8-C9-C10
33	a	418	LHG	C7-C8-C9-C10
33	D	406	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C17-C18-C19-C20
31	B	625	LMT	C9-C10-C11-C12
31	b	626	LMT	C9-C10-C11-C12
28	B	629	LMG	C34-C35-C36-C37
28	b	630	LMG	C34-C35-C36-C37
25	C	510	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
31	C	522	LMT	C5-C6-C7-C8
31	c	522	LMT	C5-C6-C7-C8
25	B	602	CLA	C14-C13-C15-C16
25	C	511	CLA	C11-C10-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C10-C8-C9
31	B	628	LMT	O5'-C5'-C6'-O6'
31	b	629	LMT	O5'-C5'-C6'-O6'
30	K	102	SQD	C25-C26-C27-C28
30	A	412	SQD	C27-C28-C29-C30
30	a	412	SQD	C27-C28-C29-C30
30	k	102	SQD	C25-C26-C27-C28
31	A	414	LMT	C1-C2-C3-C4
31	a	414	LMT	C1-C2-C3-C4
25	B	612	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C20
25	C	503	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
31	M	101	LMT	C7-C8-C9-C10
31	m	101	LMT	C7-C8-C9-C10
34	c	517	DGD	CCB-CDB-CEB-CFB
33	B	626	LHG	O1-C1-C2-O2
33	b	627	LHG	O1-C1-C2-O2
34	C	517	DGD	CCB-CDB-CEB-CFB
25	C	504	CLA	C16-C17-C18-C19
25	C	507	CLA	C16-C17-C18-C19
25	c	504	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C19
33	E	102	LHG	C17-C18-C19-C20
33	e	102	LHG	C17-C18-C19-C20
34	C	516	DGD	C6B-C7B-C8B-C9B
34	c	516	DGD	C6B-C7B-C8B-C9B
25	B	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	C13-C15-C16-C17
25	d	404	CLA	O1D-CGD-O2D-CED
31	B	625	LMT	C2-C3-C4-C5
31	C	524	LMT	C5-C6-C7-C8
31	E	103	LMT	C7-C8-C9-C10
31	b	626	LMT	C2-C3-C4-C5
31	c	524	LMT	C5-C6-C7-C8
31	e	103	LMT	C7-C8-C9-C10
33	A	418	LHG	C18-C19-C20-C21
33	B	626	LHG	C27-C28-C29-C30
33	a	418	LHG	C18-C19-C20-C21
33	b	627	LHG	C27-C28-C29-C30
28	A	413	LMG	C14-C15-C16-C17
28	a	413	LMG	C14-C15-C16-C17
25	D	404	CLA	O1D-CGD-O2D-CED
25	A	408	CLA	C11-C12-C13-C14
25	a	408	CLA	C11-C12-C13-C14
31	T	101	LMT	C6-C7-C8-C9
31	t	101	LMT	C6-C7-C8-C9
25	B	602	CLA	C11-C10-C8-C7
25	b	603	CLA	C11-C10-C8-C7
31	B	624	LMT	C1-C2-C3-C4
31	b	625	LMT	C1-C2-C3-C4
34	c	515	DGD	CCA-CDA-CEA-CFA
34	C	515	DGD	CCA-CDA-CEA-CFA
28	D	407	LMG	C24-C25-C26-C27
27	A	409	BCR	C17-C18-C19-C20
27	C	526	BCR	C17-C18-C19-C20
27	a	409	BCR	C17-C18-C19-C20
27	c	526	BCR	C17-C18-C19-C20
28	d	407	LMG	C24-C25-C26-C27
34	C	516	DGD	C2G-C3G-O3G-C1D
34	C	516	DGD	C5D-C6D-O5D-C1E
34	c	516	DGD	C2G-C3G-O3G-C1D
34	c	516	DGD	C5D-C6D-O5D-C1E
25	C	501	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
31	X	103	LMT	C2-C3-C4-C5
31	x	103	LMT	C2-C3-C4-C5
25	D	401	CLA	C16-C17-C18-C19
25	d	401	CLA	C16-C17-C18-C19
25	c	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	B	630	SQD	C9-C10-C11-C12
30	b	601	SQD	C9-C10-C11-C12
31	I	104	LMT	C4-C5-C6-C7
31	i	104	LMT	C4-C5-C6-C7
25	C	504	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1A-CGA-O2A-C1
28	B	621	LMG	C31-C32-C33-C34
28	b	622	LMG	C31-C32-C33-C34
25	B	616	CLA	C8-C10-C11-C12
25	b	617	CLA	C8-C10-C11-C12
27	D	411	BCR	C13-C14-C15-C16
27	d	411	BCR	C13-C14-C15-C16
25	b	614	CLA	C16-C17-C18-C19
25	C	510	CLA	O1A-CGA-O2A-C1
25	C	506	CLA	C15-C16-C17-C18
25	c	506	CLA	C15-C16-C17-C18
33	L	101	LHG	C11-C10-C9-C8
33	l	101	LHG	C11-C10-C9-C8
33	B	626	LHG	O6-C4-C5-O7
33	b	627	LHG	O6-C4-C5-O7
31	T	101	LMT	C4-C5-C6-C7
31	t	101	LMT	C4-C5-C6-C7
28	J	101	LMG	O1-C7-C8-C9
28	j	101	LMG	O1-C7-C8-C9
29	A	411	PL9	C14-C16-C17-C18
29	A	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C14-C16-C17-C18
29	a	411	PL9	C24-C26-C27-C28
33	Z	101	LHG	C4-C5-C6-O8
33	z	101	LHG	C4-C5-C6-O8
34	C	516	DGD	C1A-C2A-C3A-C4A
34	c	516	DGD	C1A-C2A-C3A-C4A
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
25	B	613	CLA	C16-C17-C18-C19
31	t	101	LMT	C7-C8-C9-C10
34	C	517	DGD	C7B-C8B-C9B-CAB
34	c	517	DGD	C7B-C8B-C9B-CAB
31	B	624	LMT	C5-C6-C7-C8
31	b	625	LMT	C5-C6-C7-C8
28	J	101	LMG	C14-C15-C16-C17
28	j	101	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	M	101	LMT	C11-C10-C9-C8
31	m	101	LMT	C11-C10-C9-C8
30	B	620	SQD	C26-C27-C28-C29
30	b	621	SQD	C26-C27-C28-C29
31	T	101	LMT	C7-C8-C9-C10
28	B	629	LMG	O1-C7-C8-O7
28	C	519	LMG	O7-C8-C9-O8
28	b	630	LMG	O1-C7-C8-O7
28	c	519	LMG	O7-C8-C9-O8
30	B	620	SQD	O6-C44-C45-O47
30	b	621	SQD	O6-C44-C45-O47
33	L	101	LHG	O7-C5-C6-O8
33	l	101	LHG	O7-C5-C6-O8
25	B	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	D	403	CLA	C15-C16-C17-C18
25	d	403	CLA	C15-C16-C17-C18
33	B	626	LHG	C16-C17-C18-C19
33	a	418	LHG	C14-C15-C16-C17
33	b	627	LHG	C16-C17-C18-C19
33	d	406	LHG	C29-C30-C31-C32
33	A	418	LHG	C14-C15-C16-C17
33	D	406	LHG	C29-C30-C31-C32
30	h	102	SQD	C24-C25-C26-C27
30	A	417	SQD	C8-C7-O47-C45
30	a	417	SQD	C8-C7-O47-C45
30	H	102	SQD	C24-C25-C26-C27
31	J	103	LMT	C4-C5-C6-C7
31	j	103	LMT	C4-C5-C6-C7
25	A	408	CLA	C11-C12-C13-C15
25	a	408	CLA	C11-C12-C13-C15
31	B	624	LMT	C9-C10-C11-C12
31	b	625	LMT	C9-C10-C11-C12
28	C	518	LMG	C39-C40-C41-C42
31	E	103	LMT	C5'-C4'-O1B-C1B
31	e	103	LMT	C5'-C4'-O1B-C1B
28	c	518	LMG	C39-C40-C41-C42
29	D	405	PL9	C39-C41-C42-C43
29	d	405	PL9	C39-C41-C42-C43
28	J	101	LMG	C32-C33-C34-C35
28	j	101	LMG	C32-C33-C34-C35
29	A	411	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
29	a	411	PL9	C25-C24-C26-C27
31	C	523	LMT	C9-C10-C11-C12
31	c	523	LMT	C9-C10-C11-C12
27	B	618	BCR	C11-C12-C13-C14
27	b	619	BCR	C11-C12-C13-C14
25	C	507	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
30	A	412	SQD	O49-C7-O47-C45
30	A	417	SQD	O49-C7-O47-C45
30	a	412	SQD	O49-C7-O47-C45
30	a	417	SQD	O49-C7-O47-C45
28	B	621	LMG	C16-C17-C18-C19
28	b	622	LMG	C16-C17-C18-C19
25	B	605	CLA	C12-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C15
25	B	611	CLA	C6-C7-C8-C10
25	b	606	CLA	C12-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C15
25	b	612	CLA	C6-C7-C8-C10
34	C	517	DGD	O6D-C5D-C6D-O5D
34	c	517	DGD	O6D-C5D-C6D-O5D
31	B	625	LMT	C3-C4-C5-C6
31	b	626	LMT	C3-C4-C5-C6
25	A	405	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
31	C	524	LMT	C2-C3-C4-C5
31	c	524	LMT	C2-C3-C4-C5
33	L	101	LHG	C24-C25-C26-C27
31	D	412	LMT	C3-C4-C5-C6
31	I	103	LMT	C6-C7-C8-C9
31	d	412	LMT	C3-C4-C5-C6
31	i	103	LMT	C6-C7-C8-C9
33	L	101	LHG	C34-C35-C36-C37
33	l	101	LHG	C24-C25-C26-C27
33	l	101	LHG	C34-C35-C36-C37
25	C	510	CLA	C16-C17-C18-C20
25	c	510	CLA	C16-C17-C18-C20
30	A	412	SQD	C8-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
25	D	404	CLA	C11-C10-C8-C9
25	d	404	CLA	C11-C10-C8-C9
28	A	410	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	a	410	LMG	C34-C35-C36-C37
31	X	101	LMT	C4-C5-C6-C7
31	x	101	LMT	C4-C5-C6-C7
30	h	102	SQD	C11-C12-C13-C14
30	H	102	SQD	C11-C12-C13-C14
31	E	101	LMT	C6-C7-C8-C9
28	A	410	LMG	O1-C7-C8-O7
28	J	101	LMG	O1-C7-C8-O7
28	a	410	LMG	O1-C7-C8-O7
28	j	101	LMG	O1-C7-C8-O7
30	B	620	SQD	O47-C45-C46-O48
30	b	621	SQD	O47-C45-C46-O48
33	A	419	LHG	O7-C5-C6-O8
33	a	419	LHG	O7-C5-C6-O8
31	e	101	LMT	C6-C7-C8-C9
31	i	102	LMT	C4-C5-C6-C7
34	C	517	DGD	C4A-C5A-C6A-C7A
34	c	517	DGD	C4A-C5A-C6A-C7A
25	C	510	CLA	C15-C16-C17-C18
25	c	510	CLA	C15-C16-C17-C18
31	X	102	LMT	C6-C7-C8-C9
31	x	102	LMT	C6-C7-C8-C9
28	J	101	LMG	C36-C37-C38-C39
28	j	101	LMG	C36-C37-C38-C39
28	D	407	LMG	O1-C7-C8-C9
28	d	407	LMG	O1-C7-C8-C9
30	K	102	SQD	O6-C44-C45-C46
30	k	102	SQD	O6-C44-C45-C46
25	b	604	CLA	C4-C3-C5-C6
31	I	102	LMT	C4-C5-C6-C7
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	B	612	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	C8-C10-C11-C12
25	b	605	CLA	C8-C10-C11-C12
30	H	102	SQD	C31-C32-C33-C34
31	D	410	LMT	C11-C10-C9-C8
31	d	410	LMT	C11-C10-C9-C8
30	A	412	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C11-C10-C9-C8
25	B	606	CLA	C10-C11-C12-C13
25	b	607	CLA	C10-C11-C12-C13
28	A	413	LMG	C30-C31-C32-C33
28	a	413	LMG	C30-C31-C32-C33
30	h	102	SQD	C31-C32-C33-C34
31	B	624	LMT	C5'-C4'-O1B-C1B
31	b	625	LMT	C5'-C4'-O1B-C1B
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
27	C	526	BCR	C9-C10-C11-C12
27	D	411	BCR	C9-C10-C11-C12
27	c	526	BCR	C9-C10-C11-C12
27	d	411	BCR	C9-C10-C11-C12
33	B	626	LHG	C3-O3-P-O5
33	B	626	LHG	C4-O6-P-O5
33	D	406	LHG	C4-O6-P-O5
33	b	627	LHG	C3-O3-P-O5
33	b	627	LHG	C4-O6-P-O5
33	d	406	LHG	C4-O6-P-O5
33	D	406	LHG	C34-C35-C36-C37
33	d	406	LHG	C34-C35-C36-C37
25	B	603	CLA	C4-C3-C5-C6
36	H	101	RRX	C1-C6-C7-C8
36	h	101	RRX	C1-C6-C7-C8
31	D	408	LMT	C11-C10-C9-C8
31	d	408	LMT	C11-C10-C9-C8
31	E	103	LMT	C3'-C4'-O1B-C1B
31	e	103	LMT	C3'-C4'-O1B-C1B
34	c	516	DGD	CAA-CBA-CCA-CDA
25	c	502	CLA	C15-C16-C17-C18
33	A	419	LHG	C2-C3-O3-P
33	a	419	LHG	C2-C3-O3-P
34	C	516	DGD	CAA-CBA-CCA-CDA
25	C	502	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	A	405	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
29	A	411	PL9	C4-C3-C7-C8
29	a	411	PL9	C4-C3-C7-C8
33	B	626	LHG	C7-C8-C9-C10
30	K	102	SQD	C28-C29-C30-C31
30	k	102	SQD	C28-C29-C30-C31
27	C	525	BCR	C18-C19-C20-C21
27	c	525	BCR	C18-C19-C20-C21
25	C	503	CLA	C8-C10-C11-C12
33	b	627	LHG	C7-C8-C9-C10
28	C	519	LMG	C21-C22-C23-C24
28	c	519	LMG	C21-C22-C23-C24
33	L	101	LHG	C17-C18-C19-C20
33	l	101	LHG	C17-C18-C19-C20
25	c	503	CLA	C8-C10-C11-C12
34	C	516	DGD	C1B-C2B-C3B-C4B
34	c	516	DGD	C1B-C2B-C3B-C4B
25	B	602	CLA	C11-C10-C8-C9
25	b	603	CLA	C11-C10-C8-C9
25	B	615	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	b	616	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C15
28	D	407	LMG	C34-C35-C36-C37
28	d	407	LMG	C34-C35-C36-C37
31	X	102	LMT	C7-C8-C9-C10
31	x	102	LMT	C7-C8-C9-C10
30	B	620	SQD	O48-C23-C24-C25
30	b	621	SQD	O48-C23-C24-C25
33	Z	101	LHG	O7-C5-C6-O8
33	z	101	LHG	O7-C5-C6-O8
34	C	517	DGD	C5A-C6A-C7A-C8A
34	c	517	DGD	C5A-C6A-C7A-C8A
28	J	101	LMG	C11-C10-O7-C8
28	j	101	LMG	C11-C10-O7-C8
31	X	101	LMT	C11-C10-C9-C8
31	x	101	LMT	C11-C10-C9-C8
25	B	612	CLA	CBA-CGA-O2A-C1
33	E	102	LHG	C4-C5-C6-O8
33	e	102	LHG	C4-C5-C6-O8
34	C	515	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
34	c	515	DGD	C1G-C2G-C3G-O3G
30	a	417	SQD	C29-C30-C31-C32
25	b	613	CLA	CBA-CGA-O2A-C1
34	c	515	DGD	O2G-C1B-C2B-C3B
28	J	101	LMG	C39-C40-C41-C42
28	j	101	LMG	C39-C40-C41-C42
30	A	417	SQD	C29-C30-C31-C32
31	b	623	LMT	C4'-C5'-C6'-O6'
31	B	622	LMT	C4'-C5'-C6'-O6'
28	A	410	LMG	C37-C38-C39-C40
28	a	410	LMG	C37-C38-C39-C40
34	C	515	DGD	O2G-C1B-C2B-C3B
31	D	408	LMT	C4-C5-C6-C7
31	d	408	LMT	C4-C5-C6-C7
28	b	630	LMG	C30-C31-C32-C33
31	m	102	LMT	C1-C2-C3-C4
28	B	629	LMG	C30-C31-C32-C33
31	C	524	LMT	C3'-C4'-O1B-C1B
31	c	524	LMT	C3'-C4'-O1B-C1B
31	M	102	LMT	C1-C2-C3-C4
28	B	629	LMG	C11-C12-C13-C14
28	b	630	LMG	C11-C12-C13-C14
31	b	623	LMT	C2-C3-C4-C5
31	D	408	LMT	C2-C1-O1'-C1'
31	E	101	LMT	C2-C1-O1'-C1'
31	F	103	LMT	C2-C1-O1'-C1'
31	I	103	LMT	C2-C1-O1'-C1'
31	d	408	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2-C1-O1'-C1'
31	f	103	LMT	C2-C1-O1'-C1'
31	i	103	LMT	C2-C1-O1'-C1'
25	B	605	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	b	606	CLA	C6-C7-C8-C9
31	B	622	LMT	C2-C3-C4-C5
25	B	604	CLA	C2C-C3C-CAC-CBC
30	A	417	SQD	C7-C8-C9-C10
30	a	417	SQD	C7-C8-C9-C10
25	b	605	CLA	C2C-C3C-CAC-CBC
25	B	613	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
29	A	411	PL9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
29	a	411	PL9	C23-C24-C26-C27
34	C	516	DGD	O6D-C5D-C6D-O5D
34	c	516	DGD	O6D-C5D-C6D-O5D
25	C	509	CLA	C3-C5-C6-C7
25	c	509	CLA	C3-C5-C6-C7
33	Z	101	LHG	C30-C31-C32-C33
33	z	101	LHG	C30-C31-C32-C33
25	C	509	CLA	C6-C7-C8-C10
25	c	509	CLA	C6-C7-C8-C10
28	B	621	LMG	C30-C31-C32-C33
28	b	622	LMG	C30-C31-C32-C33
33	D	406	LHG	C25-C26-C27-C28
33	d	406	LHG	C25-C26-C27-C28
34	C	517	DGD	O1G-C1G-C2G-O2G
34	c	517	DGD	O1G-C1G-C2G-O2G
29	A	411	PL9	C17-C18-C19-C20
29	a	411	PL9	C17-C18-C19-C20
33	L	101	LHG	C31-C32-C33-C34
33	l	101	LHG	C31-C32-C33-C34
27	C	525	BCR	C20-C21-C22-C37
27	c	525	BCR	C20-C21-C22-C37
28	J	101	LMG	O9-C10-O7-C8
28	j	101	LMG	O9-C10-O7-C8
33	E	102	LHG	C16-C17-C18-C19
33	A	418	LHG	C25-C26-C27-C28
33	e	102	LHG	C16-C17-C18-C19
25	C	506	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
33	a	418	LHG	C25-C26-C27-C28
31	e	101	LMT	C4-C5-C6-C7
31	E	101	LMT	C4-C5-C6-C7
33	D	406	LHG	O2-C2-C3-O3
33	d	406	LHG	O2-C2-C3-O3
28	J	101	LMG	C12-C13-C14-C15
28	j	101	LMG	C12-C13-C14-C15
31	b	628	LMT	C5-C6-C7-C8
25	B	610	CLA	C2A-CAA-CBA-CGA
31	B	627	LMT	C5-C6-C7-C8
34	H	103	DGD	O1B-C1B-C2B-C3B
34	h	103	DGD	O1B-C1B-C2B-C3B
35	F	101	HEM	CAA-CBA-CGA-O2A
35	f	101	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C11-C10-C8-C9
25	B	614	CLA	C11-C10-C8-C9
25	C	505	CLA	C11-C12-C13-C14
25	C	507	CLA	C14-C13-C15-C16
25	b	604	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C10-C8-C9
25	c	505	CLA	C11-C12-C13-C14
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
31	X	102	LMT	O1'-C1-C2-C3
31	x	102	LMT	O1'-C1-C2-C3
30	A	412	SQD	C12-C13-C14-C15
30	a	412	SQD	C12-C13-C14-C15
28	C	519	LMG	C18-C19-C20-C21
28	c	519	LMG	C18-C19-C20-C21
35	V	201	HEM	CAD-CBD-CGD-O2D
35	v	201	HEM	CAD-CBD-CGD-O2D
30	K	102	SQD	O47-C7-C8-C9
30	k	102	SQD	O47-C7-C8-C9
30	F	102	SQD	C44-C45-O47-C7
30	f	102	SQD	C44-C45-O47-C7
33	L	101	LHG	C4-C5-O7-C7
33	L	101	LHG	C6-C5-O7-C7
33	l	101	LHG	C4-C5-O7-C7
33	l	101	LHG	C6-C5-O7-C7
28	C	518	LMG	C31-C32-C33-C34
28	c	518	LMG	C31-C32-C33-C34
31	E	103	LMT	C4-C5-C6-C7
31	e	103	LMT	C4-C5-C6-C7
31	B	624	LMT	O1'-C1-C2-C3
25	b	611	CLA	C2A-CAA-CBA-CGA
31	b	625	LMT	O1'-C1-C2-C3
27	C	525	BCR	C20-C21-C22-C23
27	c	525	BCR	C20-C21-C22-C23
31	B	625	LMT	C7-C8-C9-C10
31	b	626	LMT	C7-C8-C9-C10
31	E	101	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	A	414	LMT	O1'-C1-C2-C3
31	I	104	LMT	O1'-C1-C2-C3
31	a	414	LMT	O1'-C1-C2-C3
31	i	104	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	C	514	BCR	C23-C24-C25-C26
27	C	527	BCR	C1-C6-C7-C8
27	C	527	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	c	527	BCR	C1-C6-C7-C8
27	c	527	BCR	C5-C6-C7-C8
35	f	101	HEM	CAA-CBA-CGA-O1A
28	a	410	LMG	C16-C17-C18-C19
28	A	410	LMG	C16-C17-C18-C19
35	F	101	HEM	CAA-CBA-CGA-O1A
25	B	603	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C10-C8-C7
35	V	201	HEM	CAD-CBD-CGD-O1D
35	v	201	HEM	CAD-CBD-CGD-O1D
28	J	101	LMG	C34-C35-C36-C37
28	j	101	LMG	C34-C35-C36-C37
25	B	603	CLA	C8-C10-C11-C12
25	b	604	CLA	C8-C10-C11-C12
34	C	517	DGD	C3A-C4A-C5A-C6A
34	c	517	DGD	C3A-C4A-C5A-C6A
27	C	514	BCR	C36-C18-C19-C20
27	c	514	BCR	C36-C18-C19-C20
31	B	627	LMT	C9-C10-C11-C12
31	b	628	LMT	C9-C10-C11-C12
25	B	613	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
31	M	101	LMT	C1-C2-C3-C4
31	m	101	LMT	C1-C2-C3-C4
31	J	102	LMT	C7-C8-C9-C10
30	A	412	SQD	C33-C34-C35-C36
30	a	412	SQD	C33-C34-C35-C36
30	B	630	SQD	C31-C32-C33-C34
30	b	601	SQD	C31-C32-C33-C34
31	j	102	LMT	C7-C8-C9-C10
25	C	505	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C19
25	B	614	CLA	C11-C12-C13-C14
25	C	502	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	c	502	CLA	C6-C7-C8-C9
33	D	406	LHG	C19-C20-C21-C22
33	d	406	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C5-C6-C7-C8
30	A	417	SQD	C28-C29-C30-C31
25	B	608	CLA	C8-C10-C11-C12
25	b	609	CLA	C8-C10-C11-C12
30	a	417	SQD	C28-C29-C30-C31
25	B	603	CLA	C2-C3-C5-C6
25	B	611	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
31	C	520	LMT	C7-C8-C9-C10
25	c	512	CLA	C5-C6-C7-C8
31	c	520	LMT	C7-C8-C9-C10
30	B	620	SQD	C23-C24-C25-C26
30	b	621	SQD	C23-C24-C25-C26
34	H	103	DGD	O1G-C1G-C2G-C3G
34	h	103	DGD	O1G-C1G-C2G-C3G
31	C	523	LMT	C5-C6-C7-C8
31	c	523	LMT	C5-C6-C7-C8
33	A	419	LHG	O10-C23-O8-C6
28	d	407	LMG	C39-C40-C41-C42
28	D	407	LMG	C39-C40-C41-C42
30	A	417	SQD	C15-C16-C17-C18
30	a	417	SQD	C15-C16-C17-C18
33	a	419	LHG	O10-C23-O8-C6
34	C	517	DGD	O1G-C1A-C2A-C3A
34	c	517	DGD	O1G-C1A-C2A-C3A
31	A	414	LMT	C9-C10-C11-C12
31	a	414	LMT	C9-C10-C11-C12
25	B	612	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	B	611	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
30	A	417	SQD	O6-C44-C45-O47
30	a	417	SQD	O6-C44-C45-O47
28	A	413	LMG	C28-C29-C30-C31
28	a	413	LMG	C28-C29-C30-C31
28	C	519	LMG	C34-C35-C36-C37
28	c	519	LMG	C34-C35-C36-C37
27	A	409	BCR	C15-C16-C17-C18
27	a	409	BCR	C15-C16-C17-C18
31	C	524	LMT	C5'-C4'-O1B-C1B
31	c	524	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C9
26	D	402	PHO	C6-C7-C8-C9
26	d	402	PHO	C6-C7-C8-C9
31	C	523	LMT	C11-C10-C9-C8
31	c	523	LMT	C11-C10-C9-C8
31	m	102	LMT	C5-C6-C7-C8
33	D	406	LHG	C13-C14-C15-C16
33	d	406	LHG	C13-C14-C15-C16
28	D	407	LMG	C8-C7-O1-C1
28	d	407	LMG	C8-C7-O1-C1
34	C	515	DGD	C5D-C6D-O5D-C1E
34	c	515	DGD	C5D-C6D-O5D-C1E
31	M	102	LMT	C5-C6-C7-C8
25	B	608	CLA	C2-C1-O2A-CGA
25	B	616	CLA	C2-C1-O2A-CGA
25	C	509	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
25	b	617	CLA	C2-C1-O2A-CGA
25	c	509	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
31	B	624	LMT	C4B-C5B-C6B-O6B
31	b	625	LMT	C4B-C5B-C6B-O6B
25	C	502	CLA	O1A-CGA-O2A-C1
28	A	413	LMG	O10-C28-C29-C30
28	a	413	LMG	O10-C28-C29-C30
25	c	502	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	O2A-C1-C2-C3
25	c	512	CLA	O2A-C1-C2-C3
30	A	412	SQD	C11-C12-C13-C14
30	a	412	SQD	C11-C12-C13-C14
28	D	407	LMG	C31-C32-C33-C34
28	d	407	LMG	C31-C32-C33-C34
34	c	515	DGD	C3A-C4A-C5A-C6A
34	C	515	DGD	C3A-C4A-C5A-C6A
28	J	101	LMG	C7-C8-C9-O8
28	j	101	LMG	C7-C8-C9-O8
29	A	411	PL9	C44-C46-C47-C48
29	a	411	PL9	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
30	B	620	SQD	O6-C44-C45-C46
30	b	621	SQD	O6-C44-C45-C46
31	T	101	LMT	O1'-C1-C2-C3
31	t	101	LMT	O1'-C1-C2-C3
31	A	415	LMT	C7-C8-C9-C10
31	a	415	LMT	C7-C8-C9-C10
31	J	103	LMT	C1-C2-C3-C4
31	j	103	LMT	C1-C2-C3-C4
25	B	609	CLA	C15-C16-C17-C18
25	B	612	CLA	C10-C11-C12-C13
25	b	610	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
31	I	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
33	A	419	LHG	C24-C23-O8-C6
33	a	419	LHG	C24-C23-O8-C6
31	D	410	LMT	C9-C10-C11-C12
31	d	410	LMT	C9-C10-C11-C12
34	C	515	DGD	O2G-C2G-C3G-O3G
34	H	103	DGD	O1G-C1G-C2G-O2G
34	c	515	DGD	O2G-C2G-C3G-O3G
34	h	103	DGD	O1G-C1G-C2G-O2G
25	B	611	CLA	C6-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	b	612	CLA	C6-C7-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	b	617	CLA	C6-C7-C8-C9
28	C	519	LMG	C13-C14-C15-C16
28	c	519	LMG	C13-C14-C15-C16
33	B	626	LHG	C29-C30-C31-C32
31	I	101	LMT	C5-C6-C7-C8
31	i	101	LMT	C5-C6-C7-C8
33	D	406	LHG	O8-C23-C24-C25
33	d	406	LHG	O8-C23-C24-C25
33	b	627	LHG	C29-C30-C31-C32
30	A	417	SQD	C35-C36-C37-C38
30	a	417	SQD	C35-C36-C37-C38
25	A	408	CLA	C6-C7-C8-C10
25	B	603	CLA	C12-C13-C15-C16
25	B	611	CLA	C11-C12-C13-C15
25	C	512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	a	408	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	612	CLA	C11-C12-C13-C15
25	c	512	CLA	C11-C10-C8-C7
28	B	621	LMG	C12-C13-C14-C15
28	b	622	LMG	C12-C13-C14-C15
25	C	510	CLA	C2-C1-O2A-CGA
25	c	510	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C16-C17-C18-C20
31	X	101	LMT	C7-C8-C9-C10
31	x	101	LMT	C7-C8-C9-C10
29	A	411	PL9	C29-C31-C32-C33
29	a	411	PL9	C29-C31-C32-C33
25	d	404	CLA	C16-C17-C18-C20
31	C	520	LMT	O1'-C1-C2-C3
31	c	520	LMT	O1'-C1-C2-C3
30	H	102	SQD	C28-C29-C30-C31
30	h	102	SQD	C28-C29-C30-C31
28	D	407	LMG	C4-C5-C6-O5
25	B	613	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
33	B	626	LHG	C18-C19-C20-C21
33	b	627	LHG	C18-C19-C20-C21
25	C	506	CLA	C13-C15-C16-C17
25	c	506	CLA	C13-C15-C16-C17
25	b	605	CLA	C5-C6-C7-C8
28	d	407	LMG	C4-C5-C6-O5
30	H	102	SQD	C4-C5-C6-S
30	h	102	SQD	C4-C5-C6-S
25	D	401	CLA	C2C-C3C-CAC-CBC
25	d	401	CLA	C2C-C3C-CAC-CBC
28	J	101	LMG	C24-C25-C26-C27
25	B	604	CLA	C5-C6-C7-C8
25	C	510	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
28	j	101	LMG	C24-C25-C26-C27
33	e	102	LHG	C13-C14-C15-C16
30	A	417	SQD	O47-C7-C8-C9
30	a	417	SQD	O47-C7-C8-C9
33	E	102	LHG	C13-C14-C15-C16
34	C	517	DGD	C4B-C5B-C6B-C7B
34	c	517	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
31	B	623	LMT	C2-C1-O1'-C1'
31	B	624	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
31	m	102	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C3-C4-C5-C6
31	d	410	LMT	C3-C4-C5-C6
34	C	516	DGD	CDA-CEA-CFA-CGA
34	c	516	DGD	CDA-CEA-CFA-CGA
25	B	608	CLA	C11-C12-C13-C14
25	b	609	CLA	C11-C12-C13-C14
28	J	101	LMG	C42-C43-C44-C45
28	j	101	LMG	C42-C43-C44-C45
28	B	629	LMG	O1-C7-C8-C9
28	b	630	LMG	O1-C7-C8-C9
25	B	601	CLA	C1A-C2A-CAA-CBA
25	b	602	CLA	C1A-C2A-CAA-CBA
29	D	405	PL9	C12-C11-C9-C10
29	d	405	PL9	C12-C11-C9-C10
31	C	521	LMT	O5'-C1'-O1'-C1
31	c	521	LMT	O5'-C1'-O1'-C1
34	C	515	DGD	O6E-C1E-O5D-C6D
34	c	515	DGD	O6E-C1E-O5D-C6D
33	B	626	LHG	O8-C23-C24-C25
33	b	627	LHG	O8-C23-C24-C25
27	C	514	BCR	C17-C18-C19-C20
27	c	514	BCR	C17-C18-C19-C20
25	B	611	CLA	C10-C11-C12-C13
25	b	612	CLA	C10-C11-C12-C13
25	C	502	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
33	D	406	LHG	C32-C33-C34-C35
33	d	406	LHG	C32-C33-C34-C35
30	F	102	SQD	O10-C23-O48-C46
30	B	630	SQD	C5-C6-S-O7
30	b	601	SQD	C5-C6-S-O7
25	A	406	CLA	C8-C10-C11-C12
25	a	406	CLA	C8-C10-C11-C12
25	A	405	CLA	C2-C1-O2A-CGA
25	a	405	CLA	C2-C1-O2A-CGA
25	B	608	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	C	508	CLA	C11-C12-C13-C15
25	b	609	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C12-C13-C15
33	L	101	LHG	C7-C8-C9-C10
33	l	101	LHG	C7-C8-C9-C10
34	C	517	DGD	O6E-C5E-C6E-O5E
34	c	517	DGD	O6E-C5E-C6E-O5E
25	b	605	CLA	C4C-C3C-CAC-CBC
30	f	102	SQD	O10-C23-O48-C46
33	l	101	LHG	C33-C34-C35-C36
25	B	604	CLA	C4C-C3C-CAC-CBC
30	B	630	SQD	O49-C7-O47-C45
30	b	601	SQD	O49-C7-O47-C45
33	L	101	LHG	C33-C34-C35-C36
25	C	503	CLA	C13-C15-C16-C17
25	c	503	CLA	C13-C15-C16-C17
30	F	102	SQD	O48-C23-C24-C25
30	f	102	SQD	O48-C23-C24-C25
33	D	406	LHG	O10-C23-C24-C25
33	d	406	LHG	O10-C23-C24-C25
31	A	415	LMT	C9-C10-C11-C12
31	a	415	LMT	C9-C10-C11-C12
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C45-C44-C46-C47
34	C	515	DGD	C9A-CAA-CBA-CCA
34	c	515	DGD	C9A-CAA-CBA-CCA
25	B	614	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
30	F	102	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
25	C	508	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16
28	B	621	LMG	C39-C40-C41-C42
28	b	622	LMG	C39-C40-C41-C42
30	H	102	SQD	C11-C10-C9-C8
30	h	102	SQD	C11-C10-C9-C8
31	D	409	LMT	C5'-C4'-O1B-C1B
31	d	409	LMT	C5'-C4'-O1B-C1B
34	C	517	DGD	C1B-C2B-C3B-C4B
34	c	517	DGD	C1B-C2B-C3B-C4B
25	C	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	412	SQD	O5-C5-C6-S
30	B	630	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C5-C6-S
30	b	601	SQD	O5-C5-C6-S
30	B	620	SQD	C19-C20-C21-C22
30	b	621	SQD	C19-C20-C21-C22
28	a	410	LMG	C18-C19-C20-C21
30	A	412	SQD	C45-C44-O6-C1
30	A	417	SQD	C45-C44-O6-C1
30	a	412	SQD	C45-C44-O6-C1
30	a	417	SQD	C45-C44-O6-C1
31	C	520	LMT	C3-C4-C5-C6
31	c	520	LMT	C3-C4-C5-C6
28	A	410	LMG	C18-C19-C20-C21
25	B	613	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A
33	B	626	LHG	O10-C23-C24-C25
30	H	102	SQD	C44-C45-C46-O48
30	h	102	SQD	C44-C45-C46-O48
30	A	417	SQD	O49-C7-C8-C9
30	a	417	SQD	O49-C7-C8-C9
33	b	627	LHG	O10-C23-C24-C25
30	A	417	SQD	C12-C13-C14-C15
30	a	417	SQD	C12-C13-C14-C15
28	B	629	LMG	O8-C28-C29-C30
28	b	630	LMG	O8-C28-C29-C30
31	d	408	LMT	C5-C6-C7-C8
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	612	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
31	D	408	LMT	C5-C6-C7-C8
25	B	614	CLA	C8-C10-C11-C12
31	B	622	LMT	C7-C8-C9-C10
31	I	104	LMT	C6-C7-C8-C9
31	i	104	LMT	C6-C7-C8-C9
25	C	512	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
31	b	623	LMT	C7-C8-C9-C10
33	A	418	LHG	C27-C28-C29-C30

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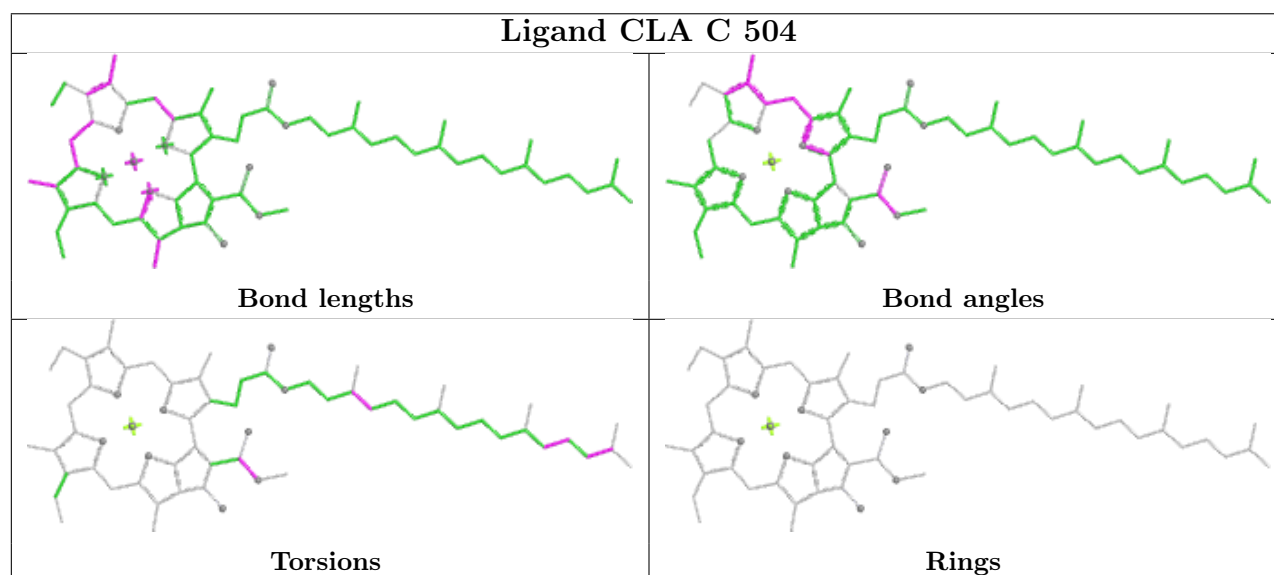
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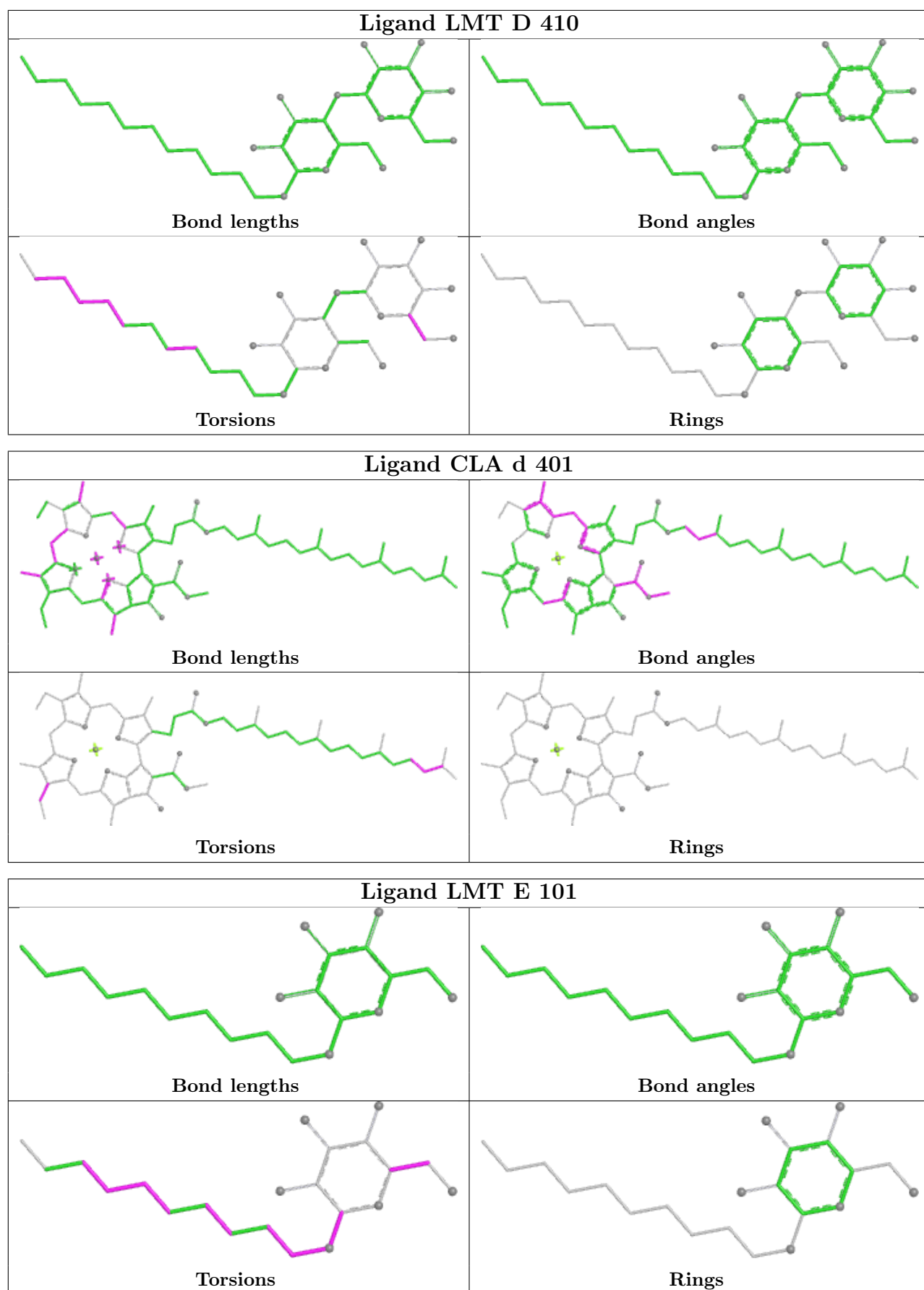
Mol	Chain	Res	Type	Atoms
33	a	418	LHG	C27-C28-C29-C30
25	C	510	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
25	b	615	CLA	C8-C10-C11-C12
28	c	518	LMG	C15-C16-C17-C18
28	C	518	LMG	C15-C16-C17-C18
34	C	515	DGD	C7B-C8B-C9B-CAB
34	c	515	DGD	C7B-C8B-C9B-CAB
30	A	412	SQD	O48-C23-C24-C25
30	a	412	SQD	O48-C23-C24-C25
25	B	605	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
30	A	412	SQD	C31-C32-C33-C34

There are no ring outliers.

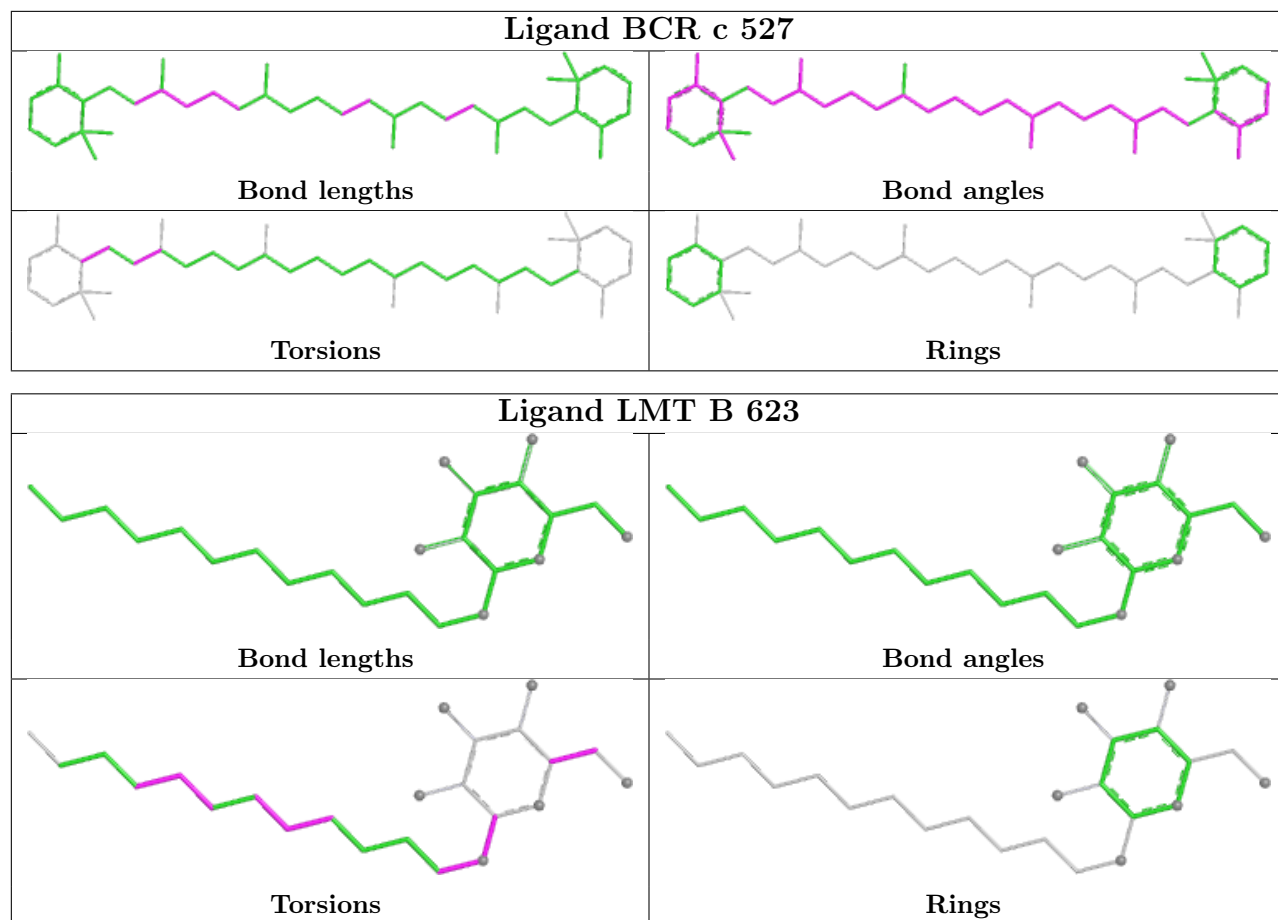
No monomer is involved in short contacts.

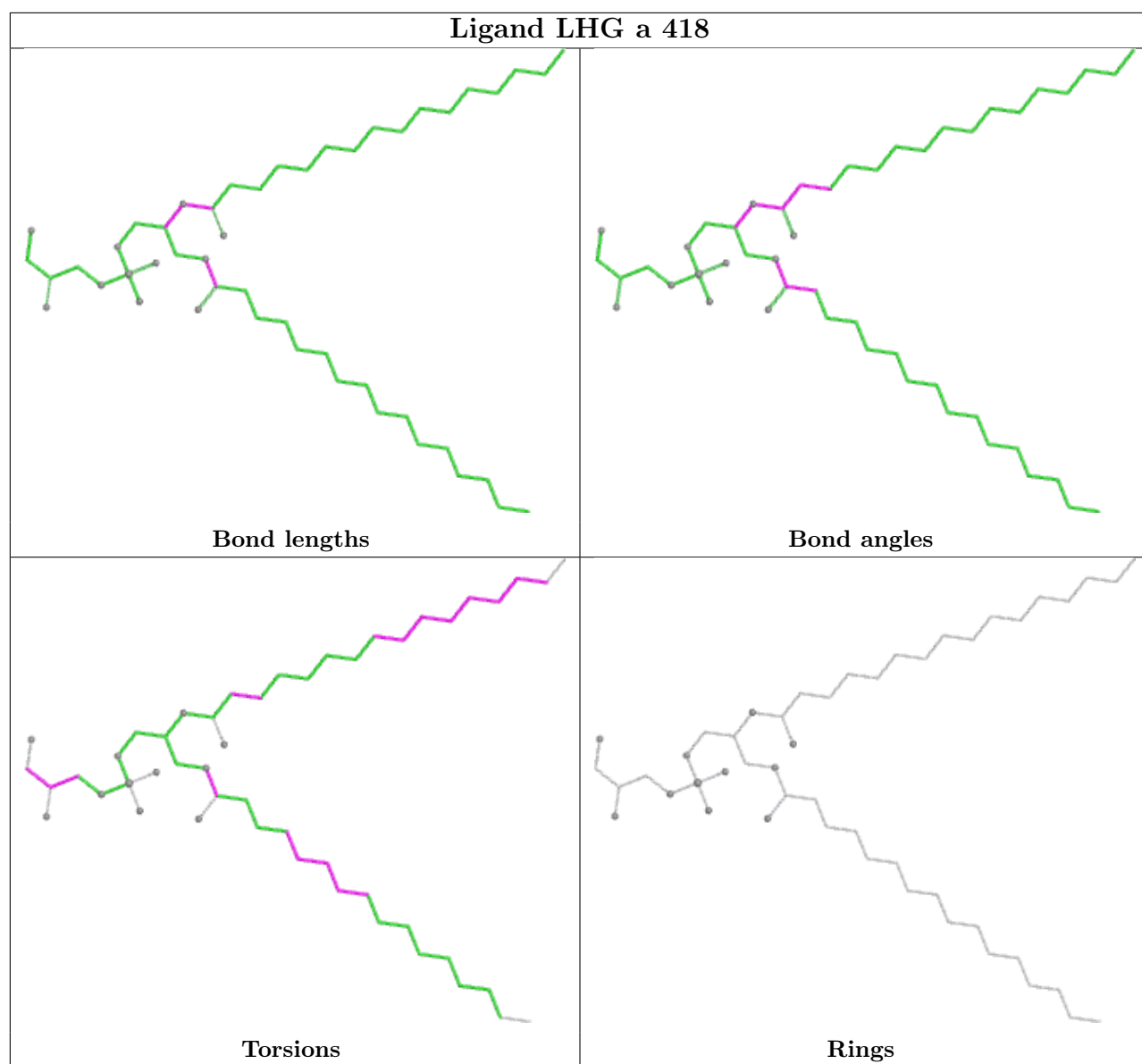
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

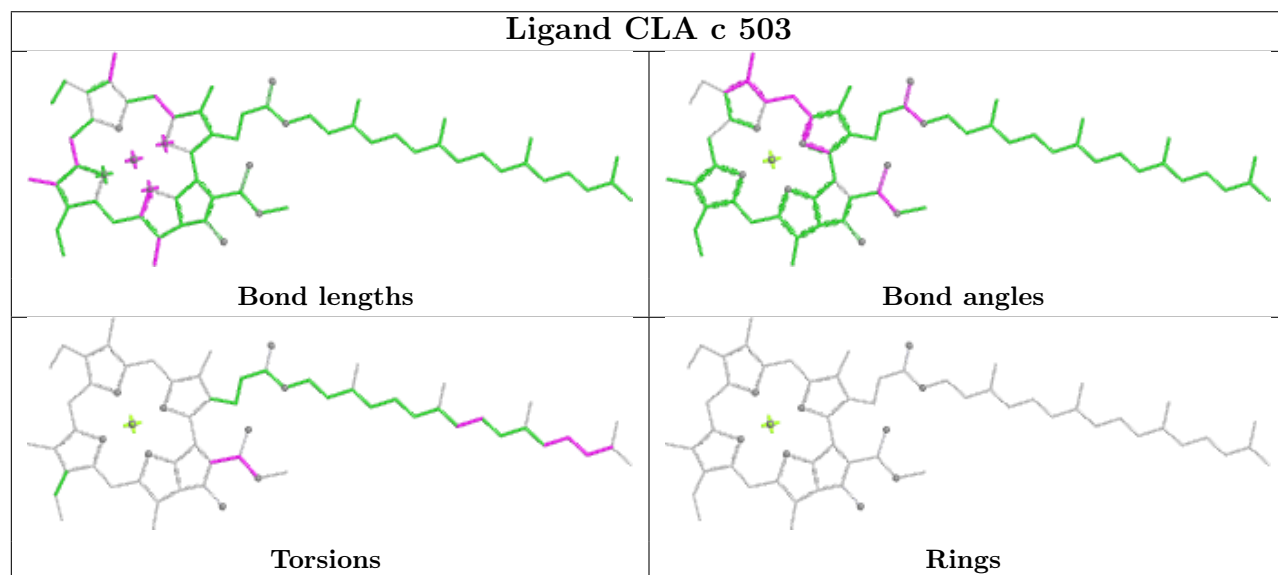
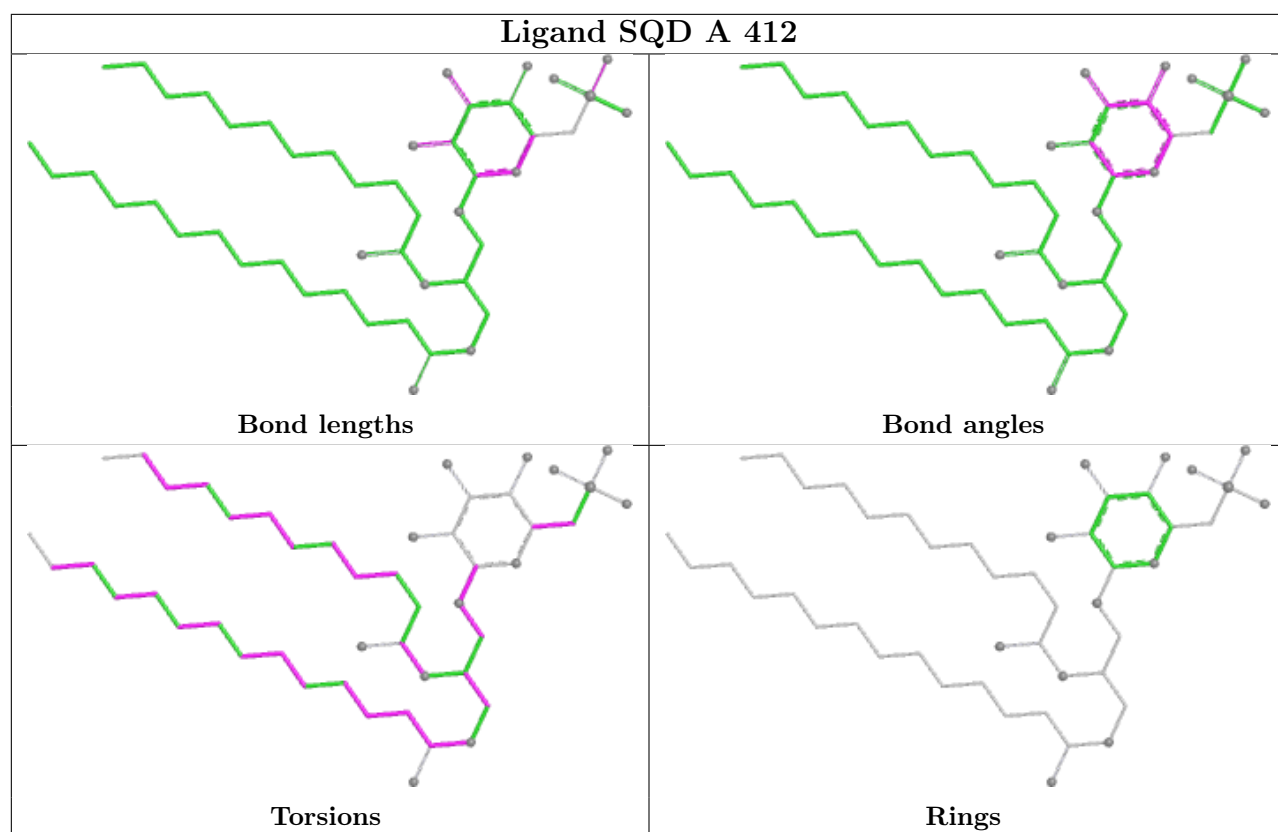


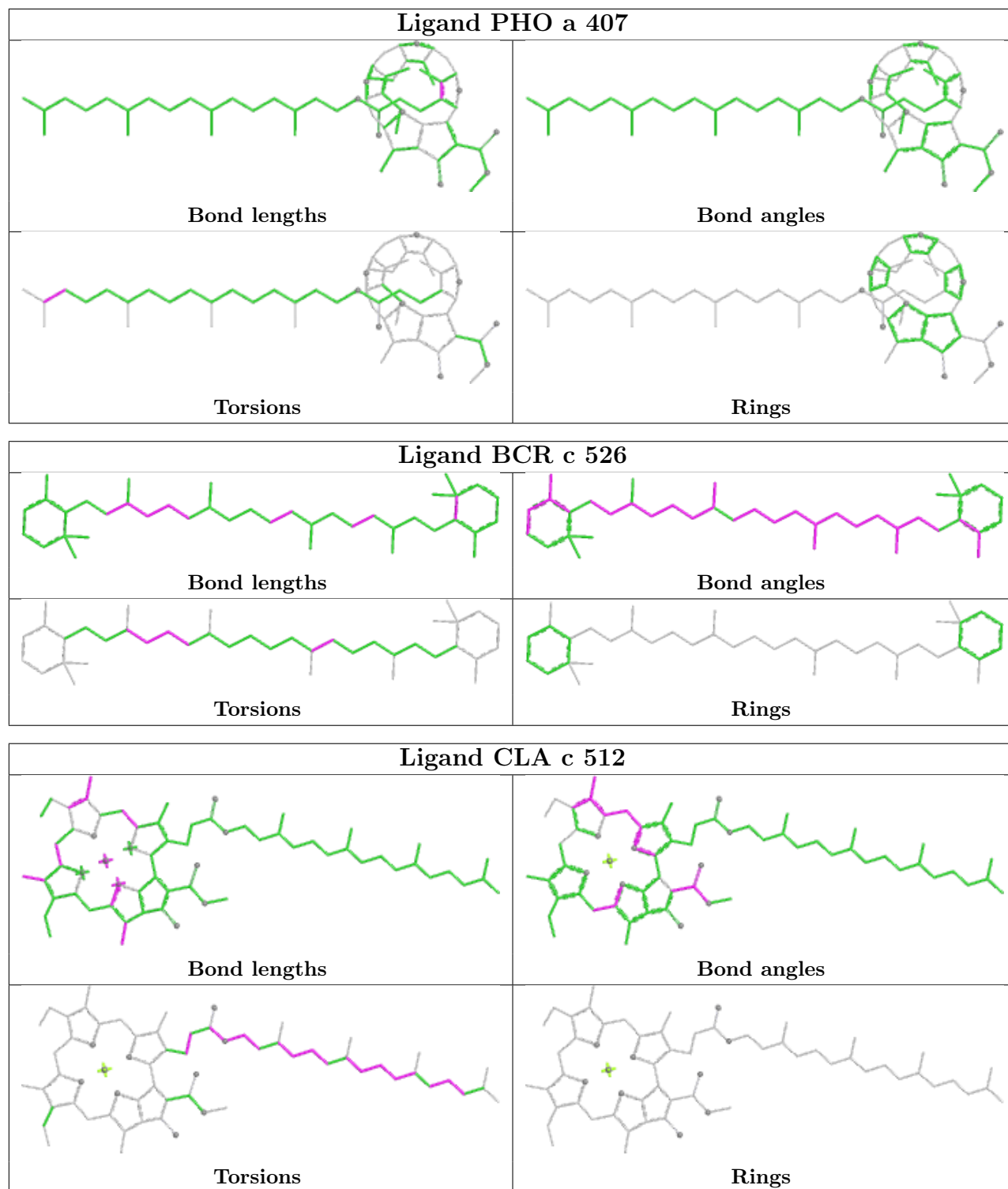


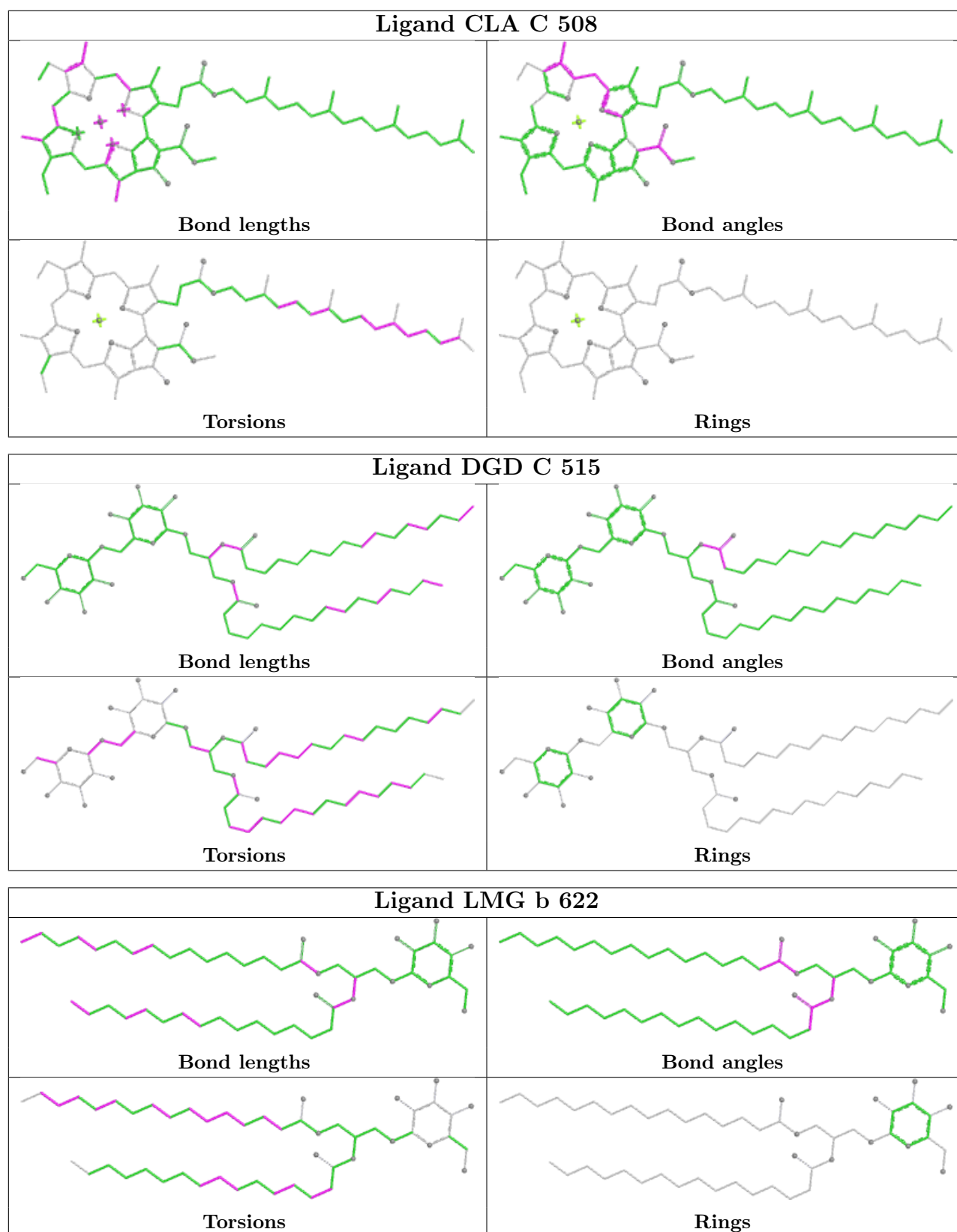


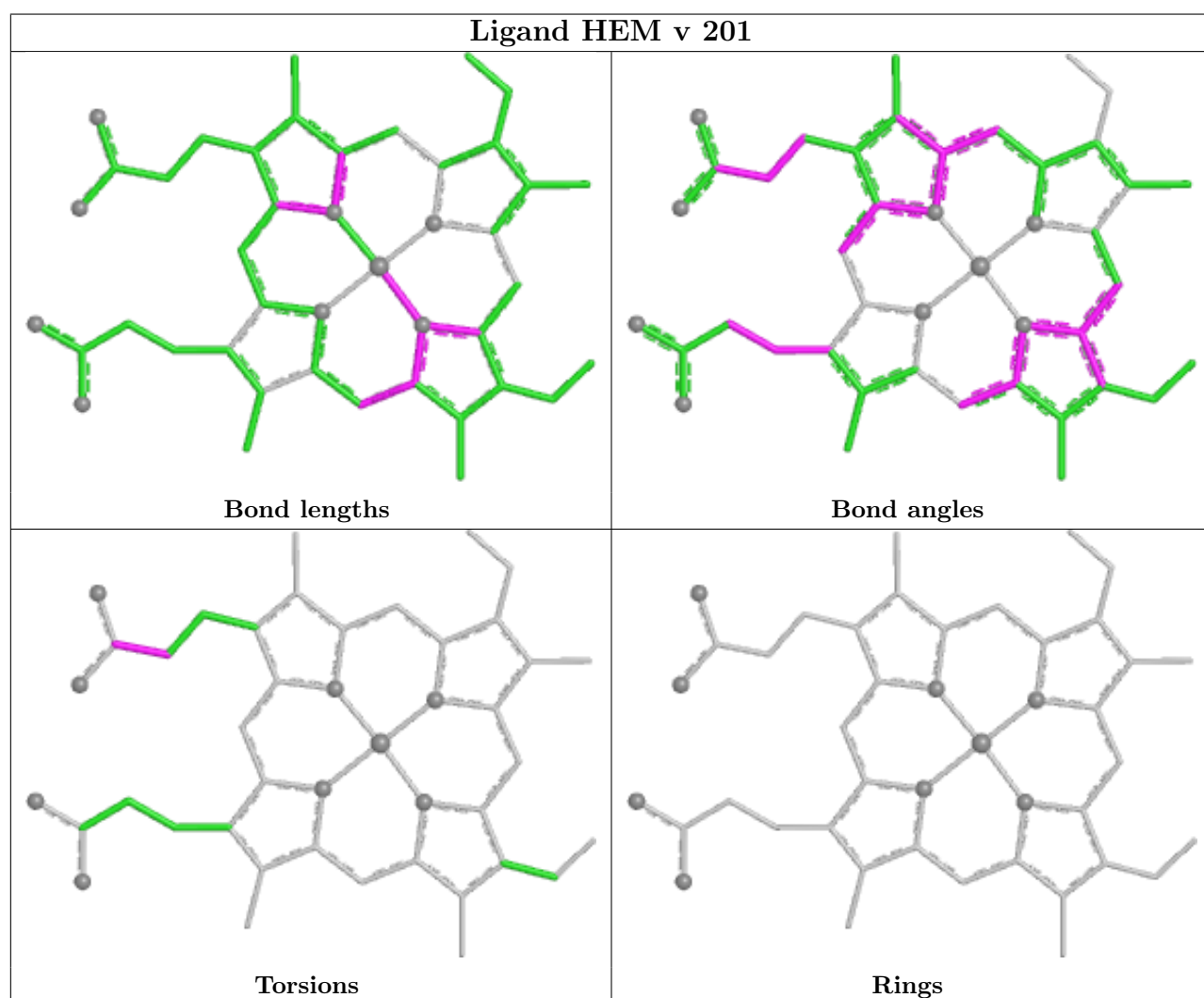
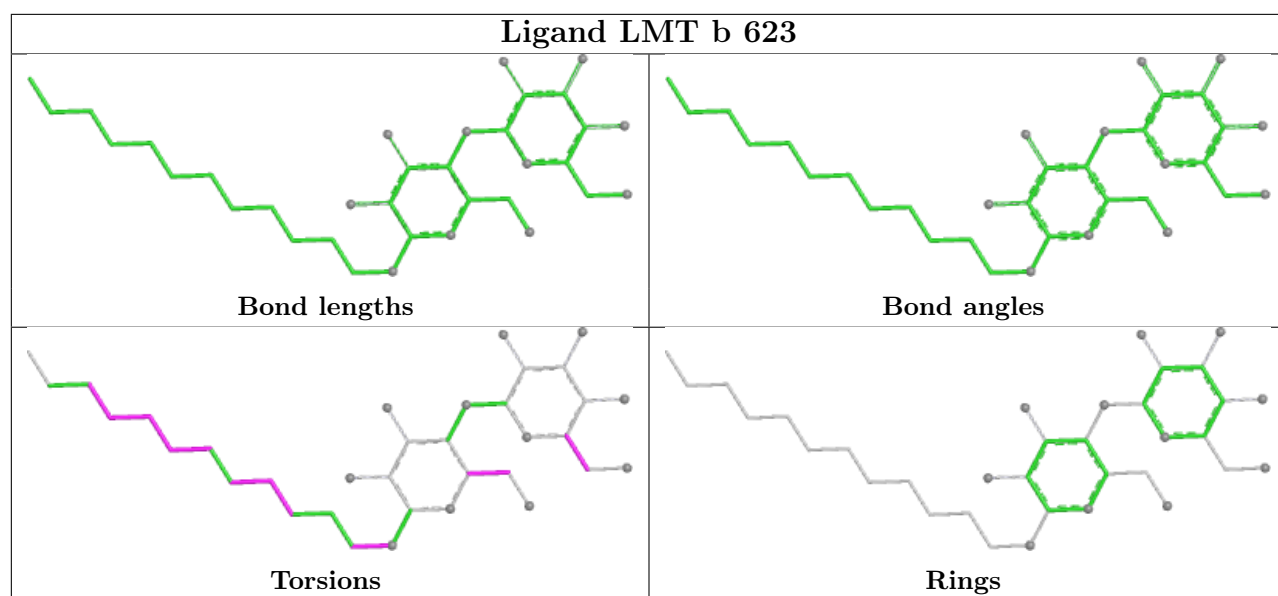


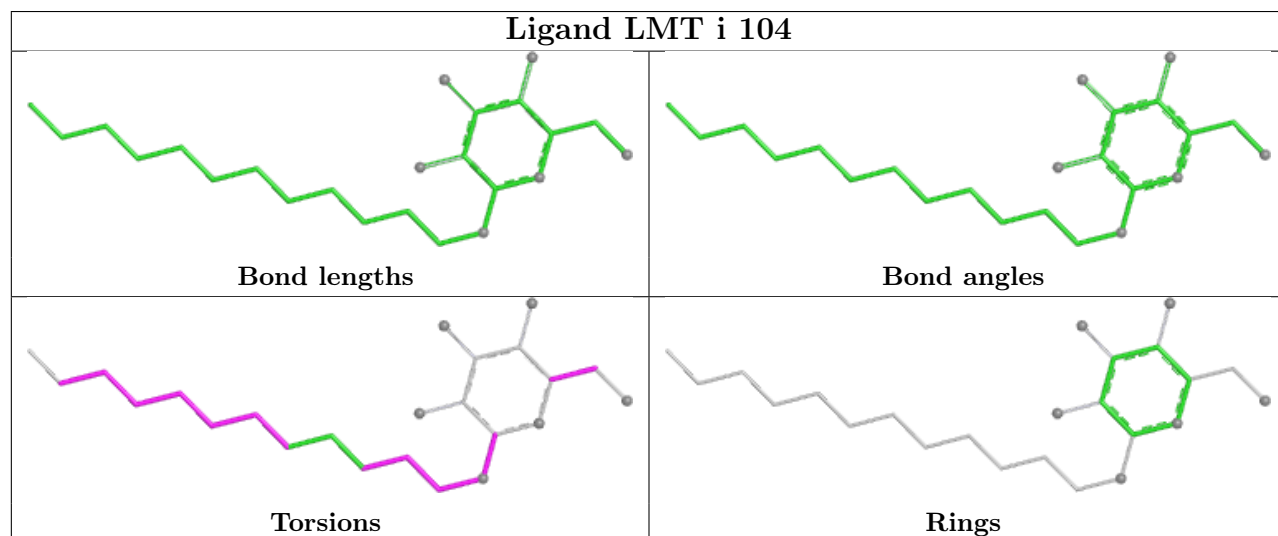
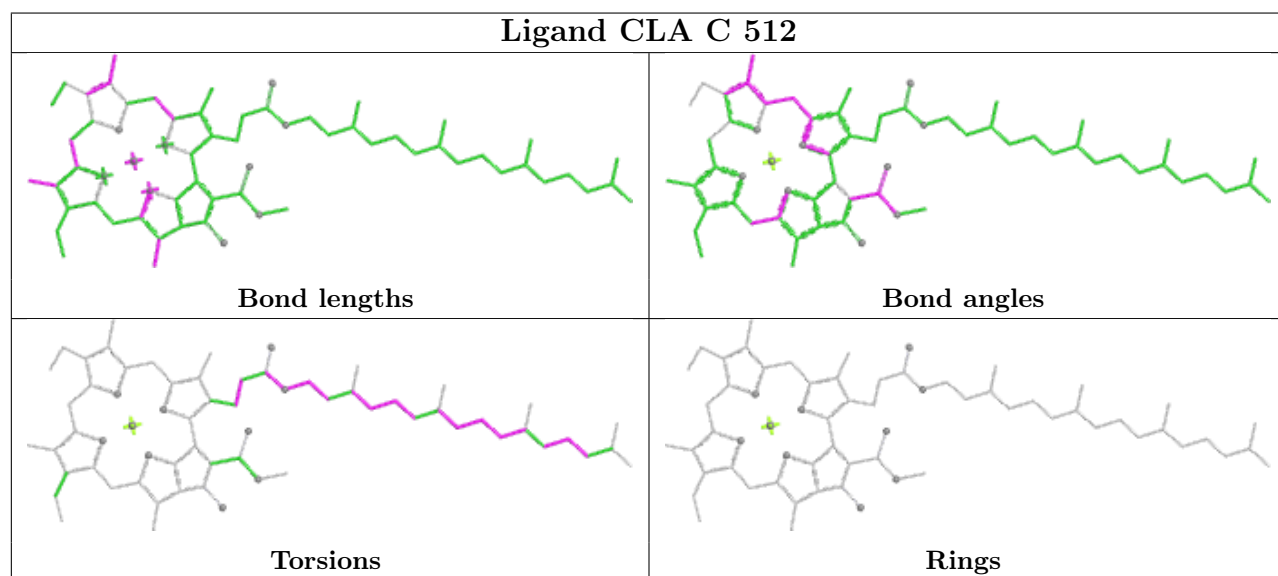
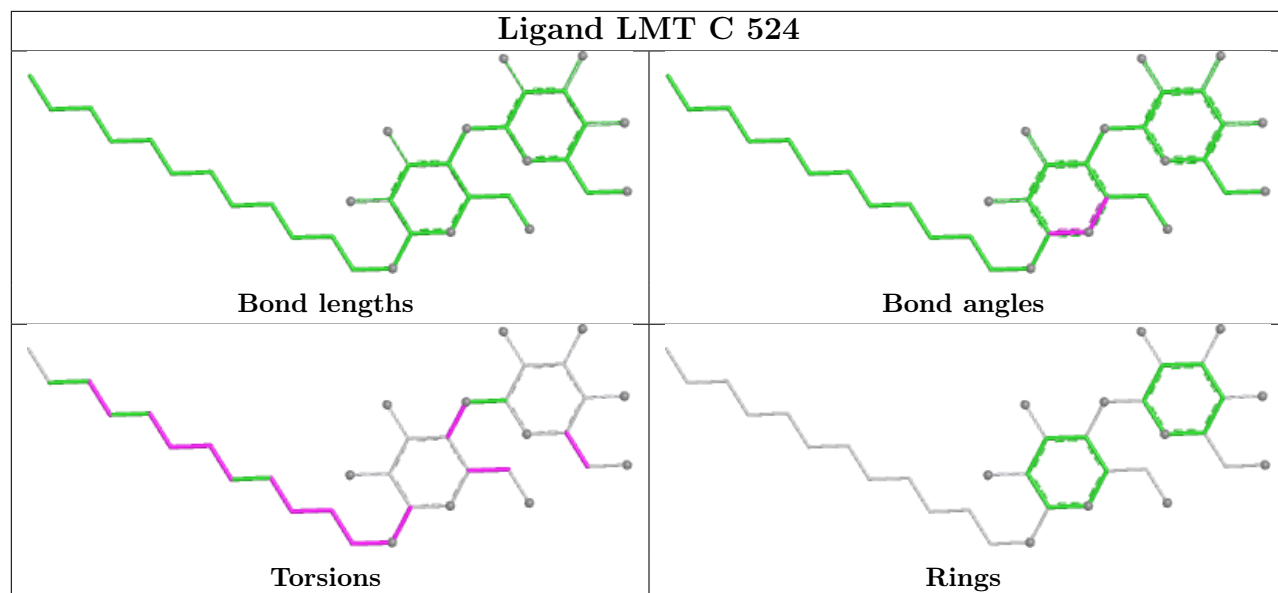


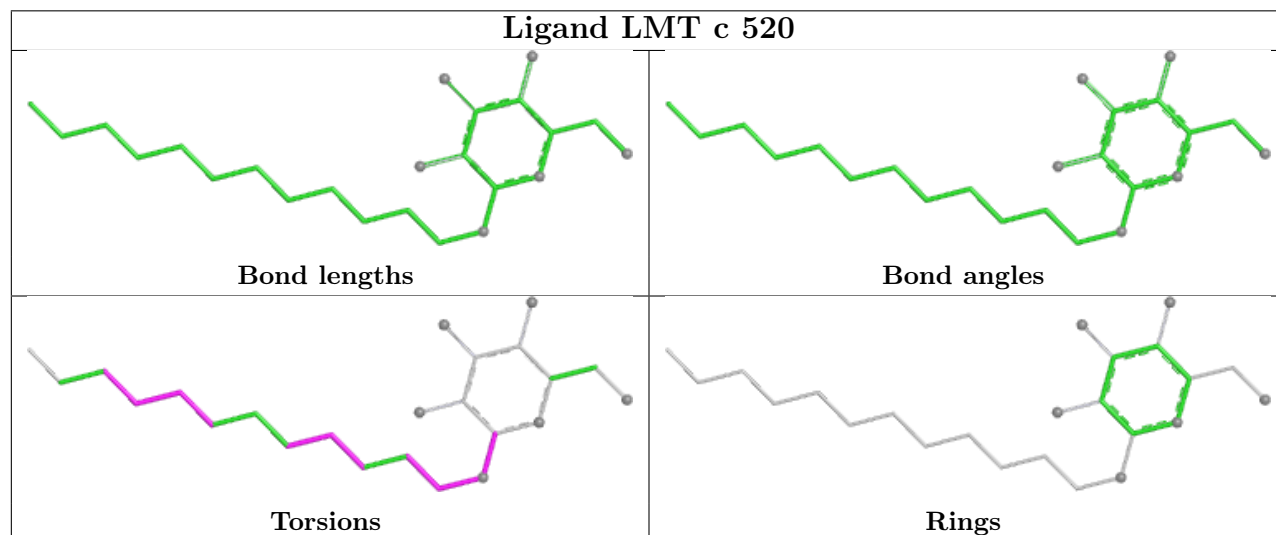
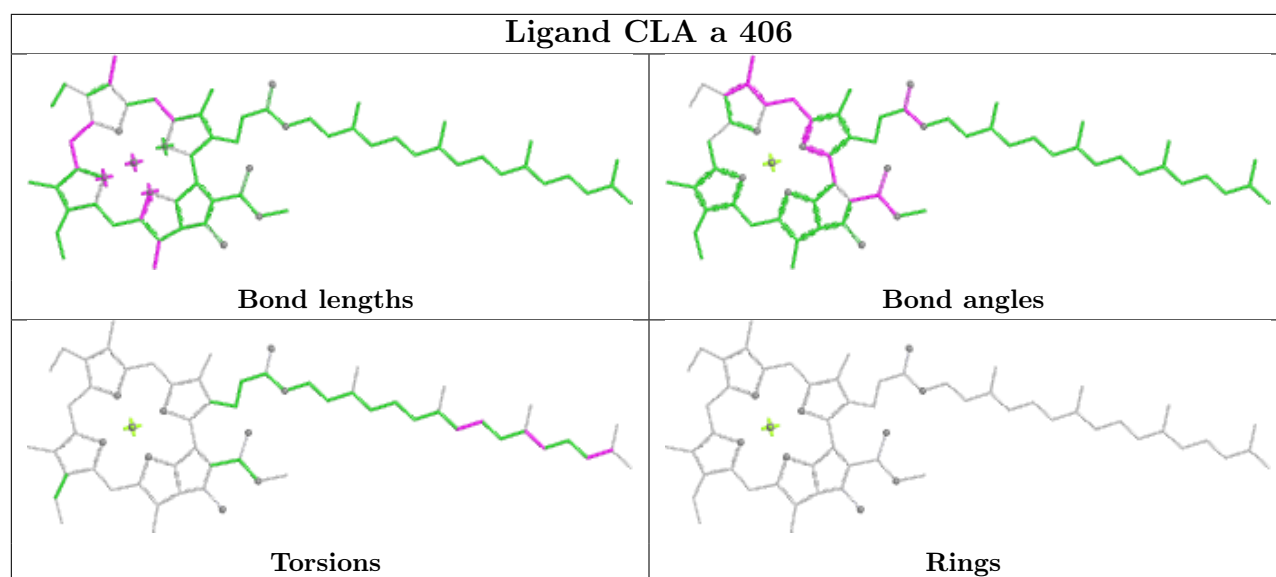




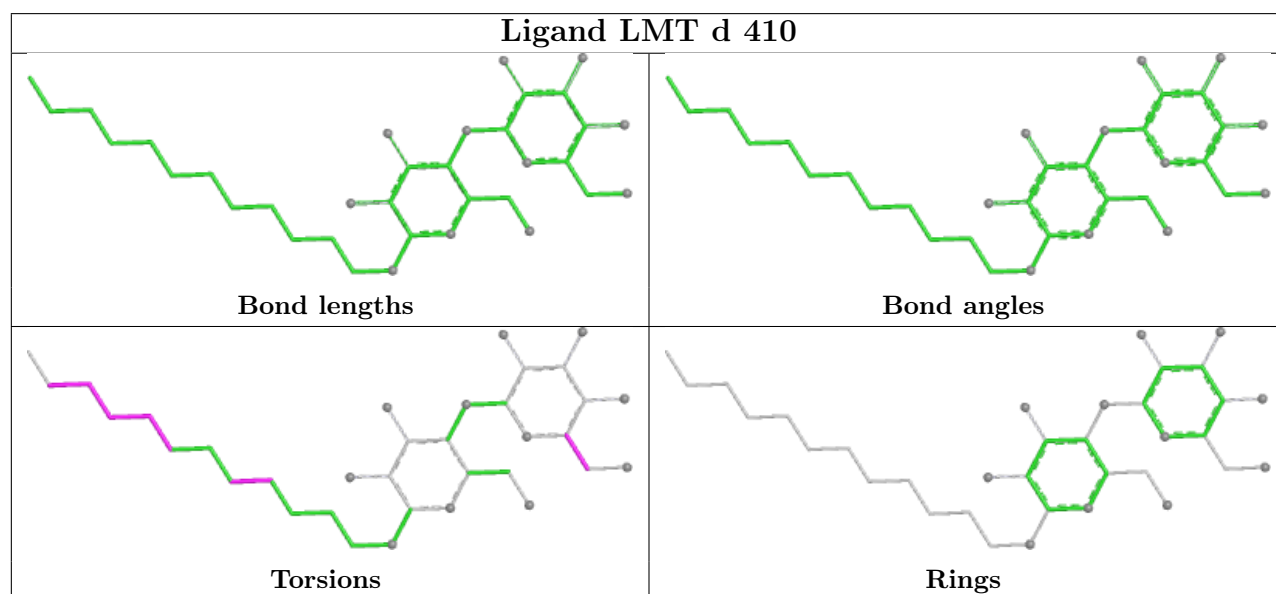
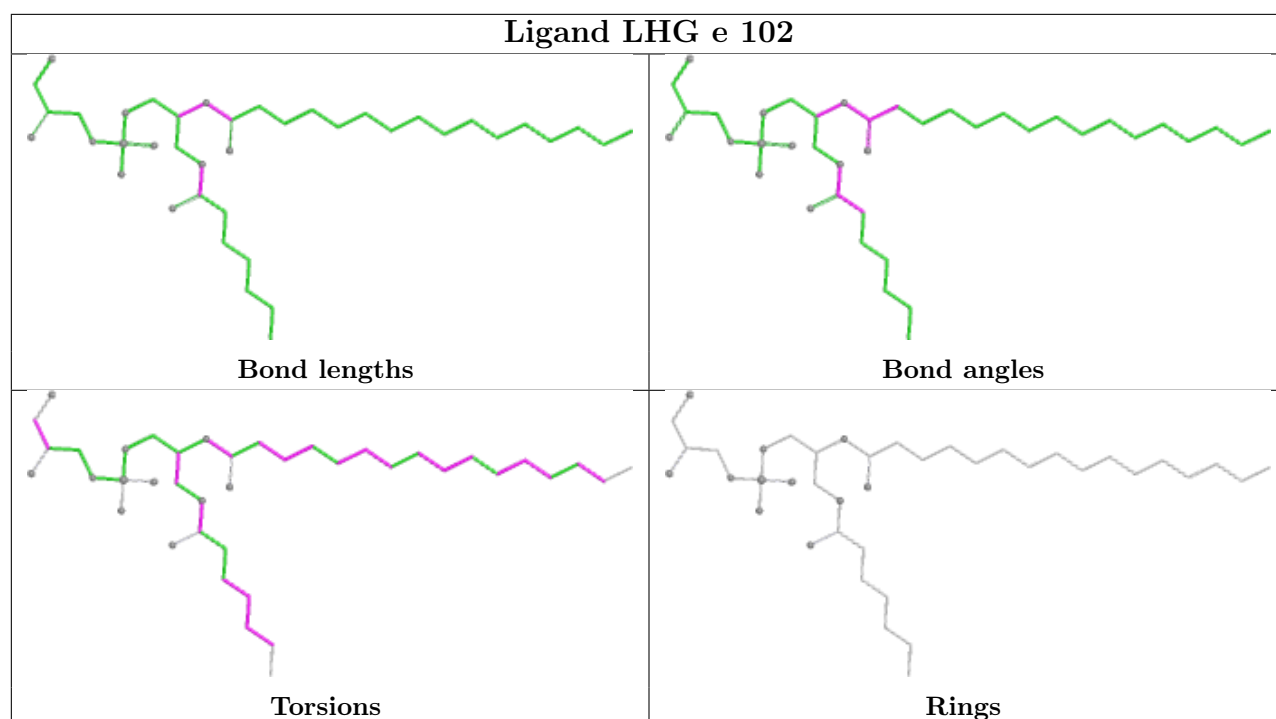


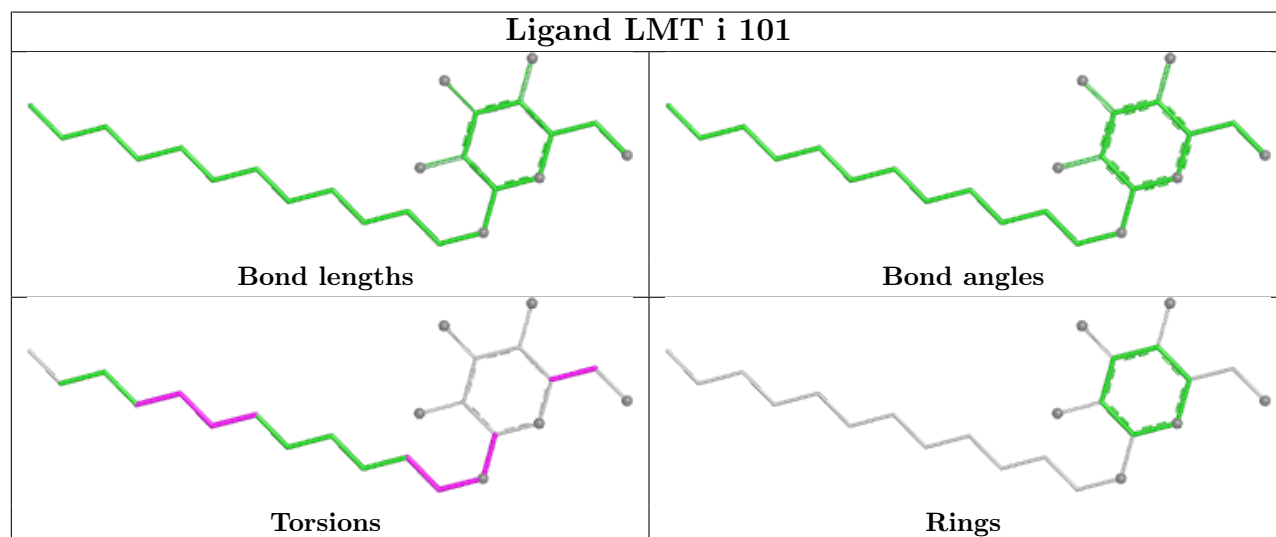
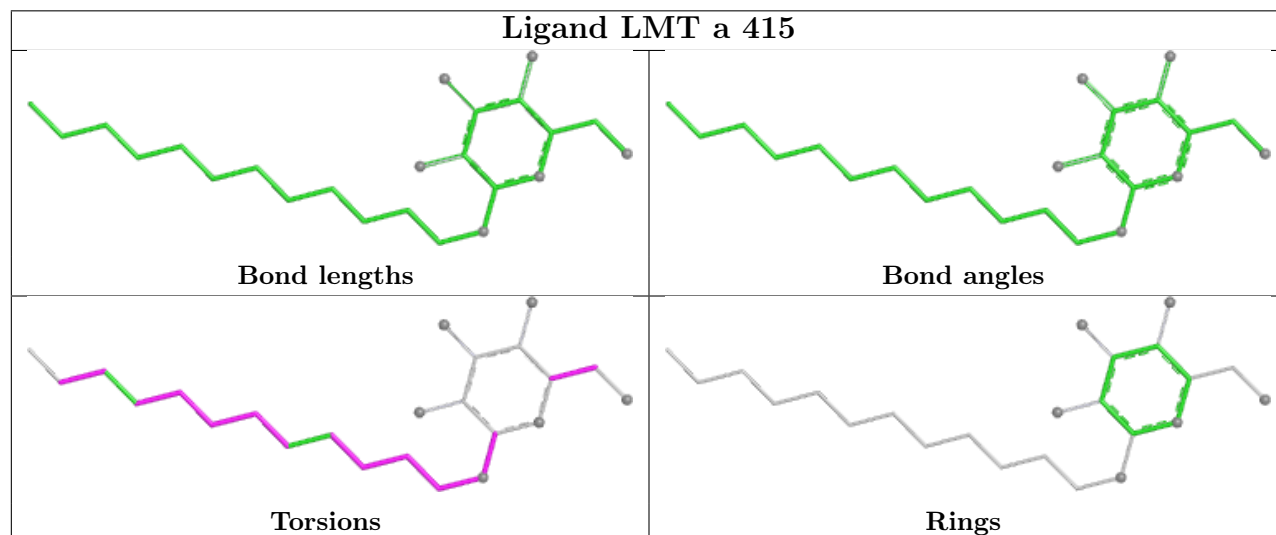
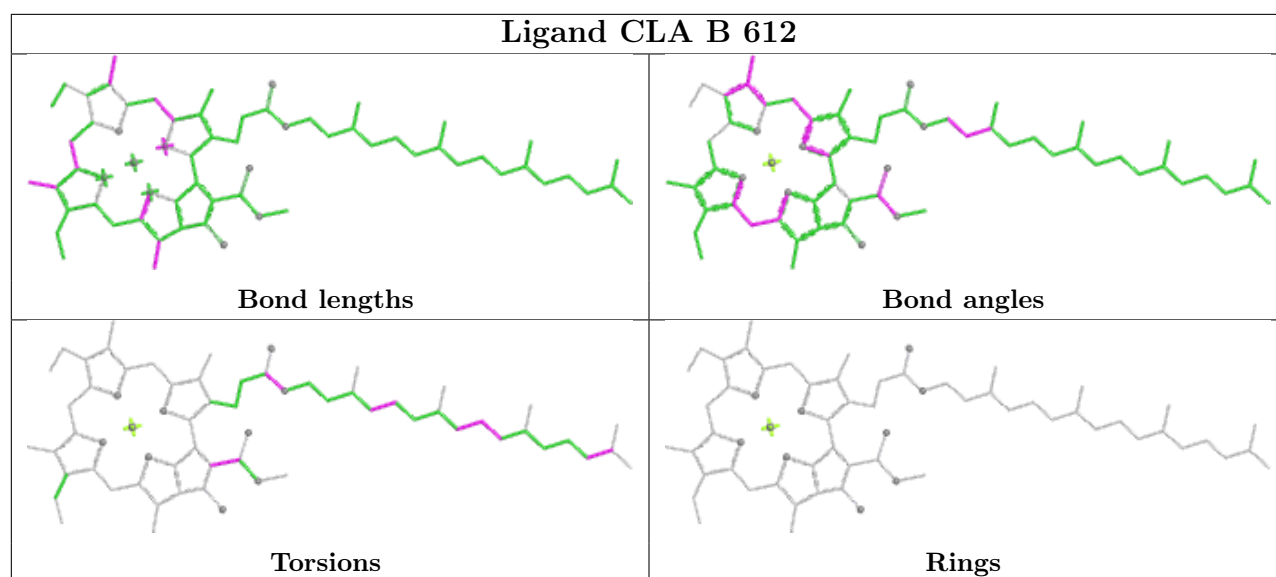


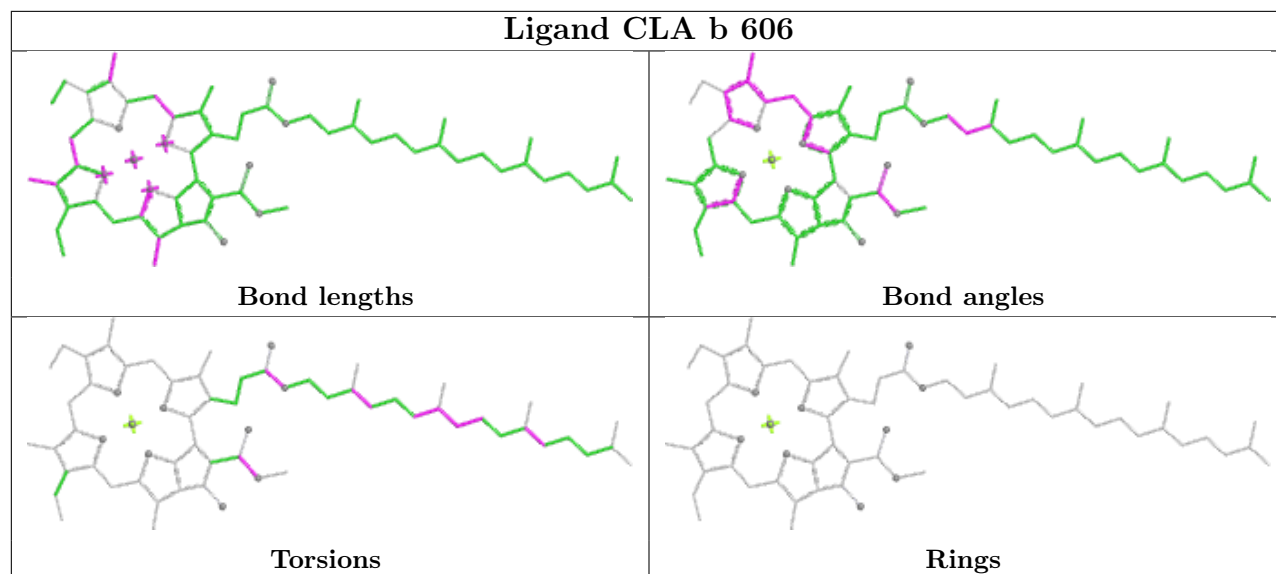
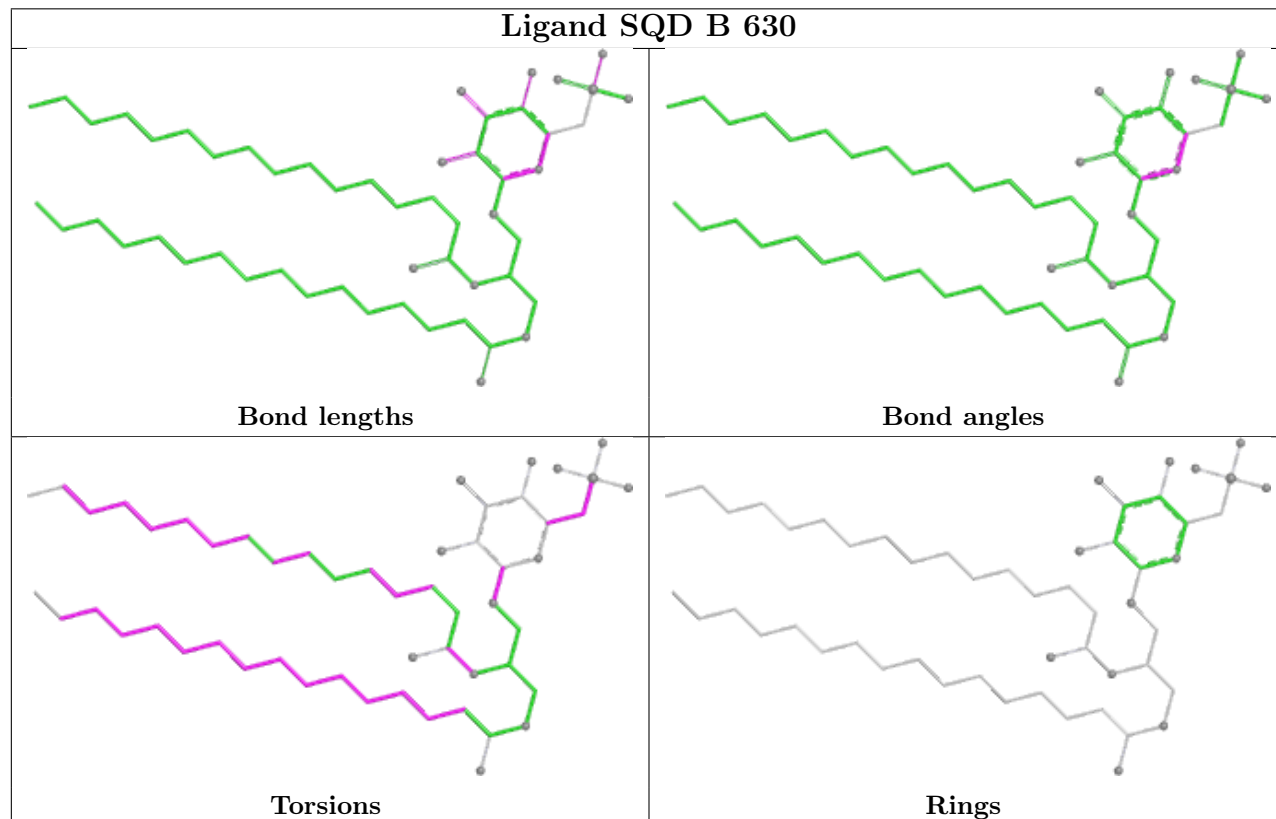


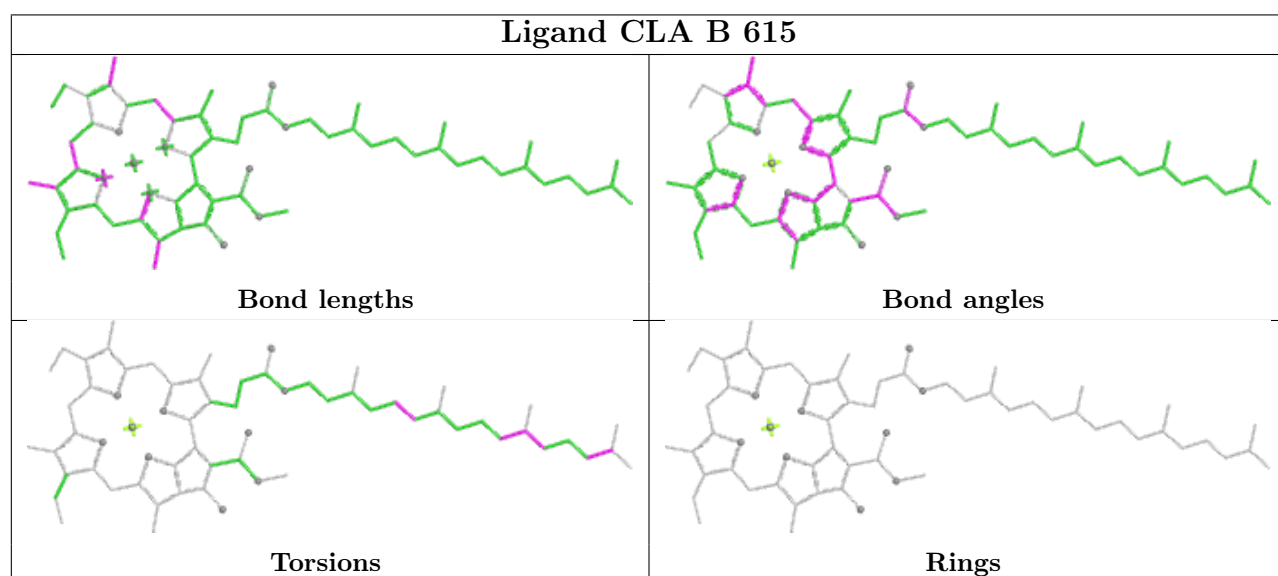
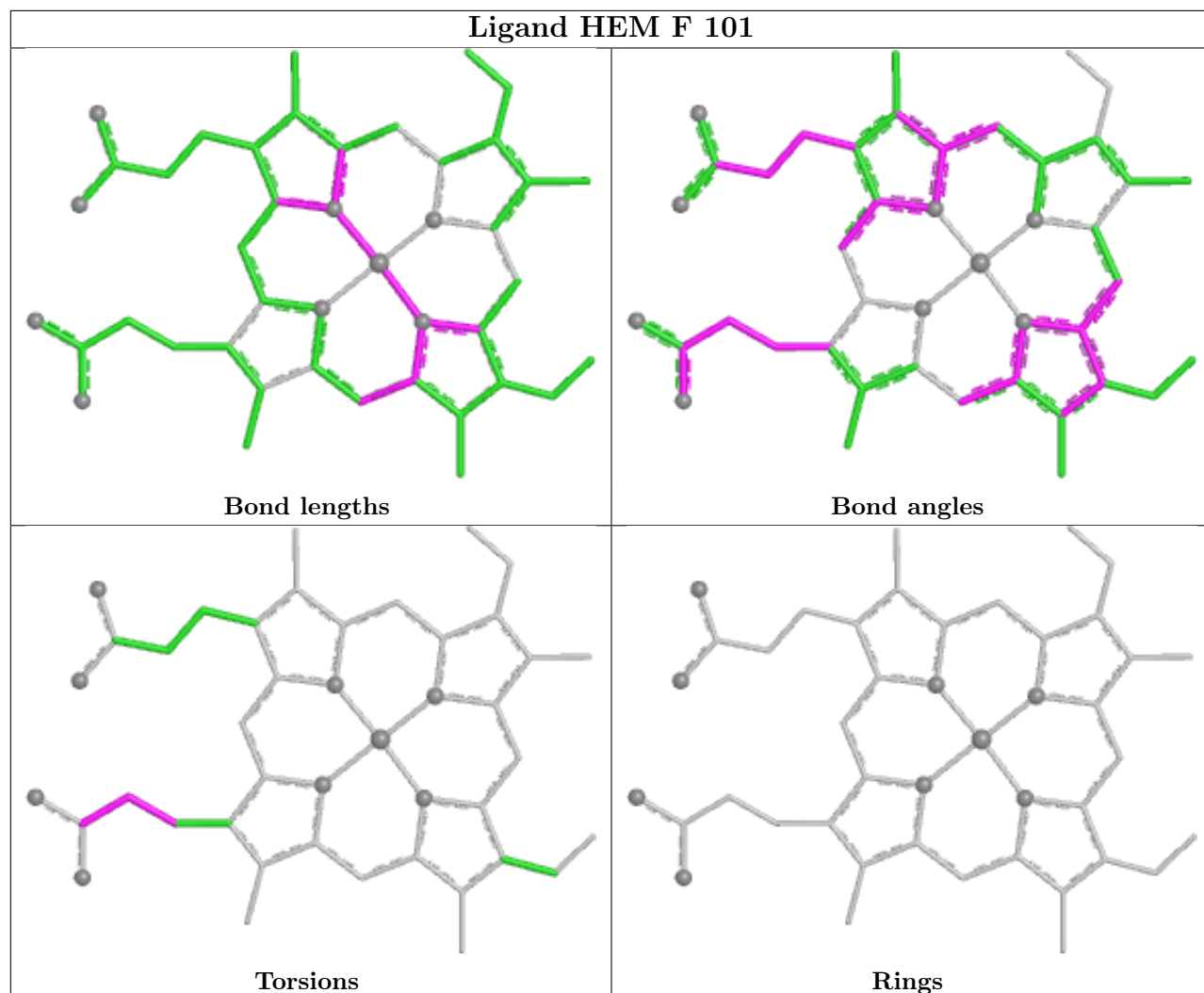


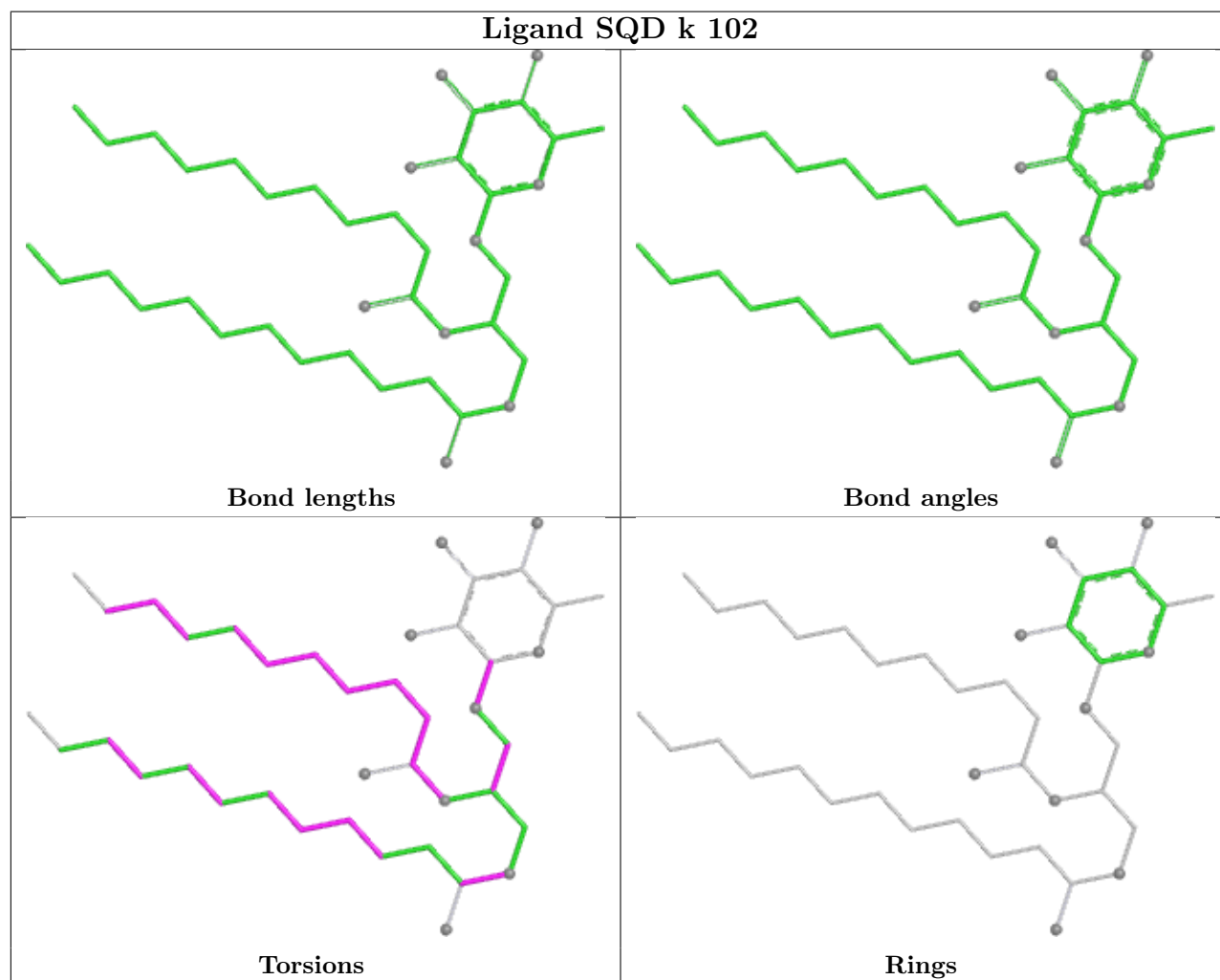
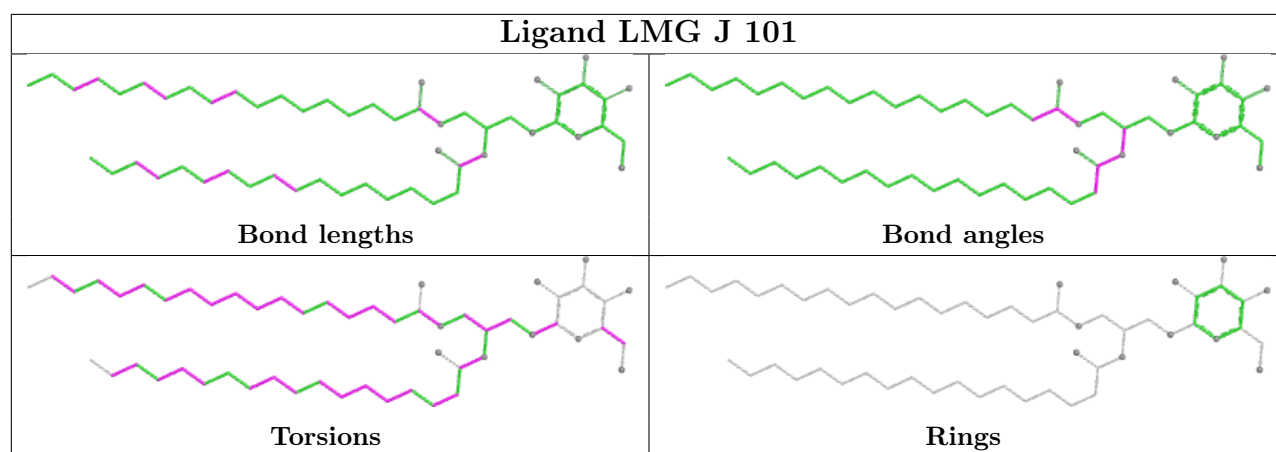


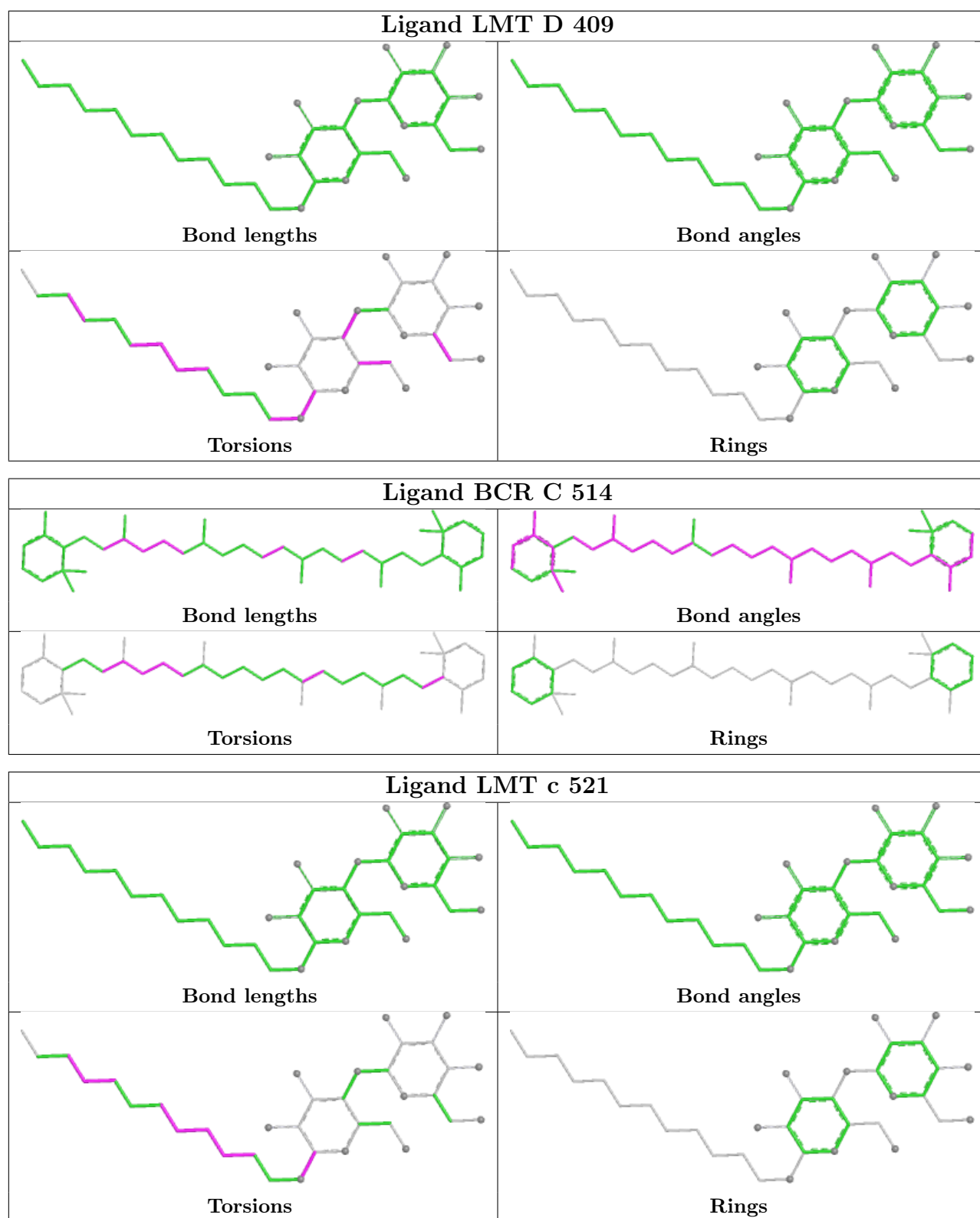




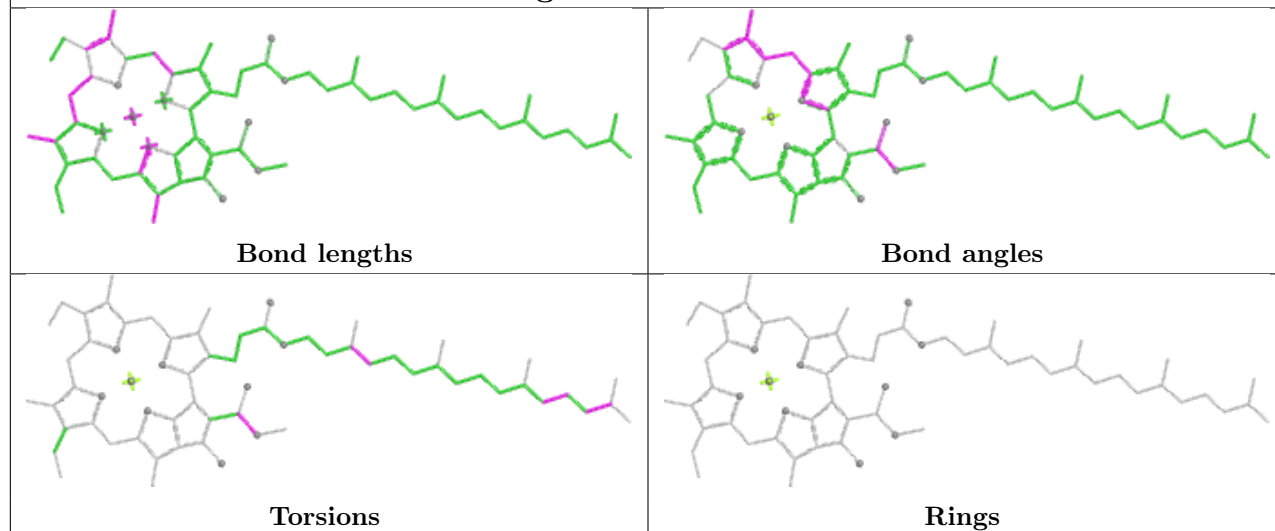
**Ligand CLA b 606****Ligand SQD B 630**



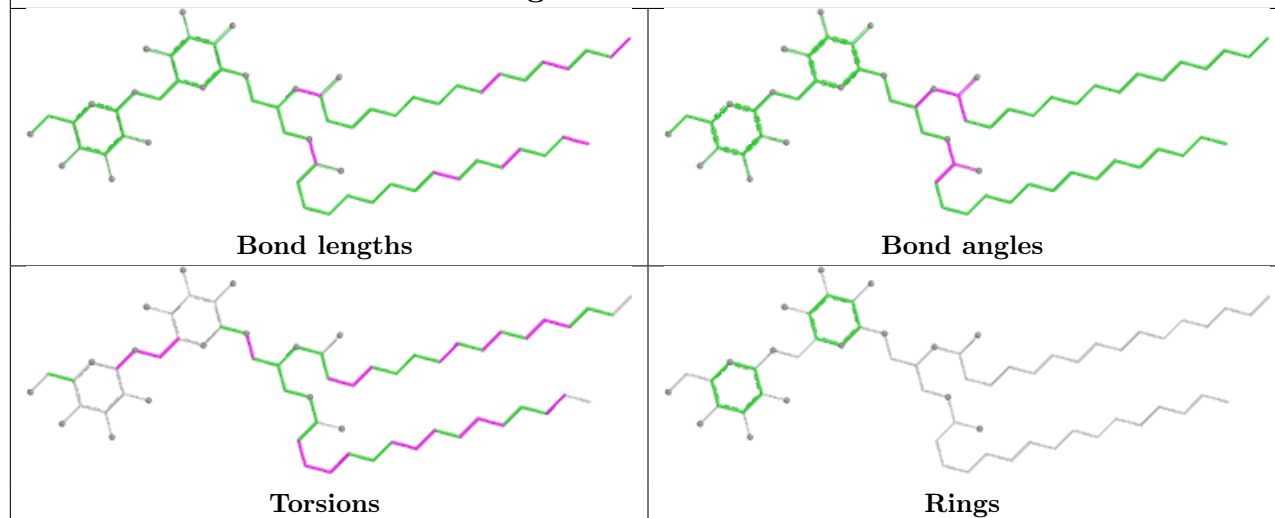




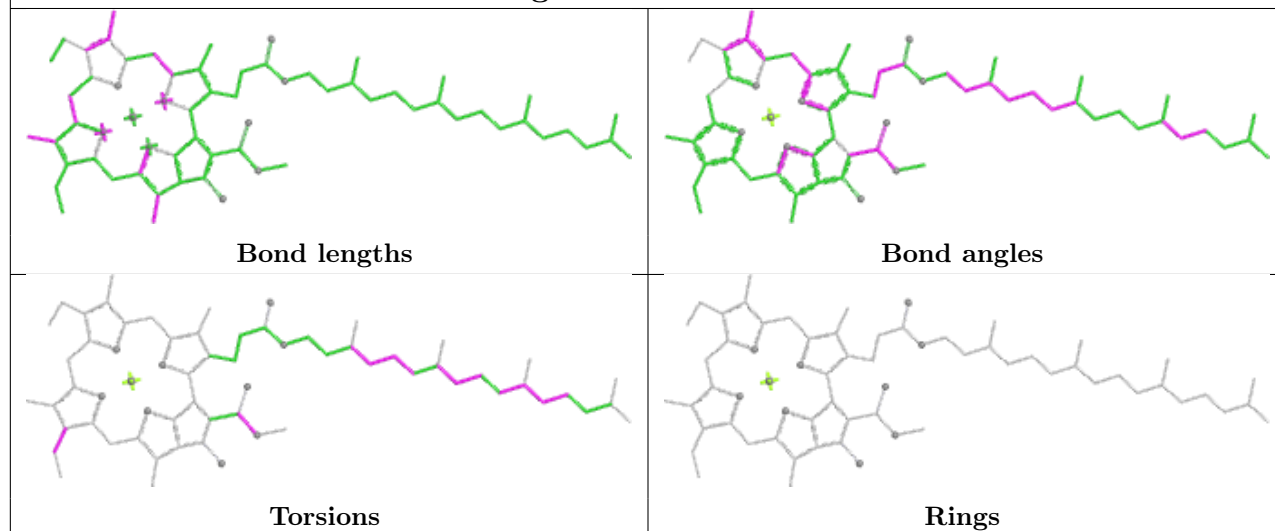
## Ligand CLA c 504

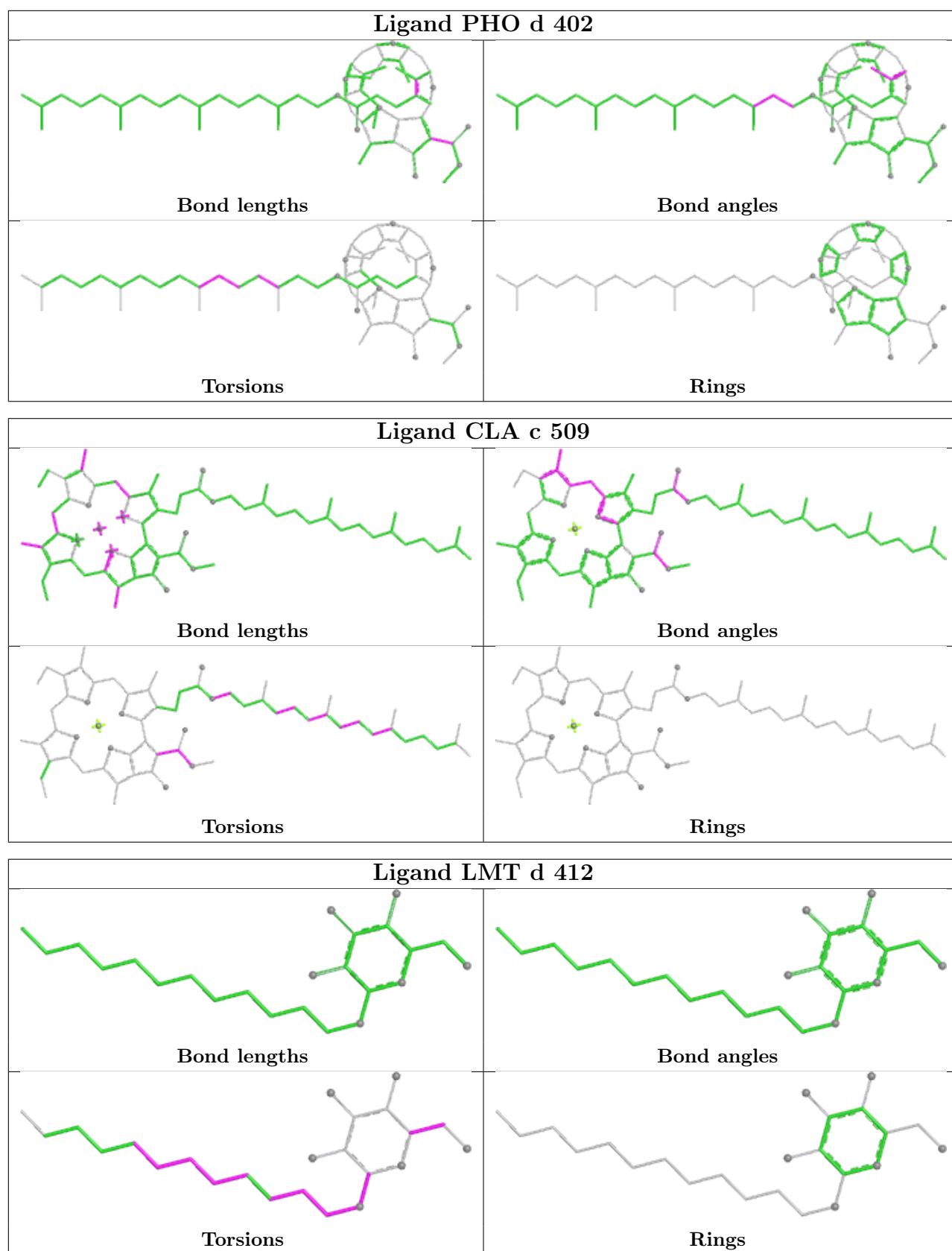


## Ligand DGD C 516

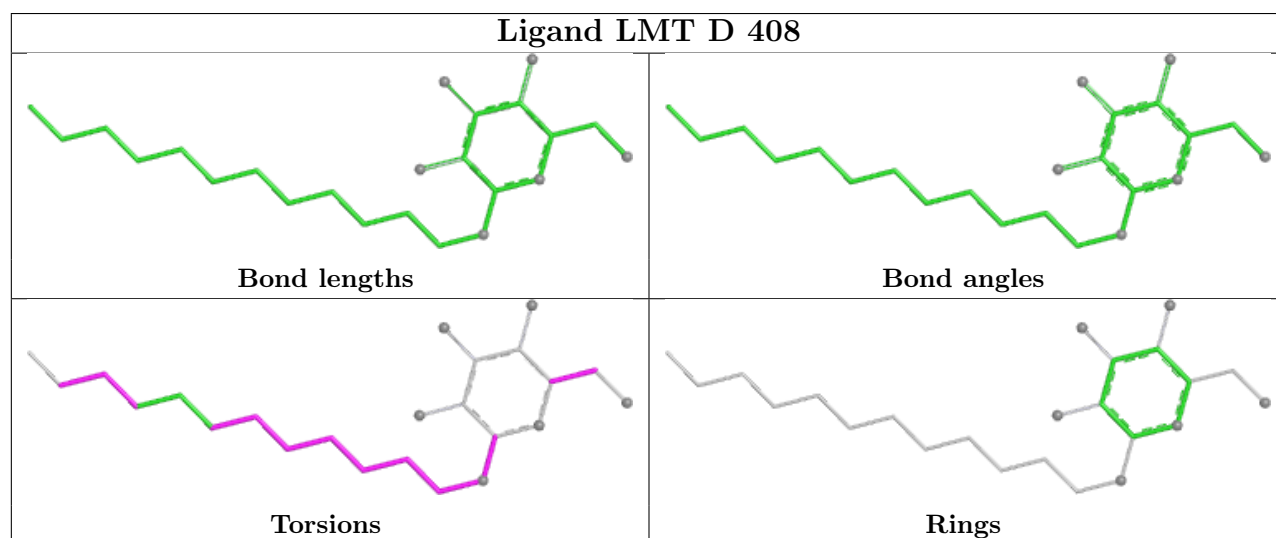
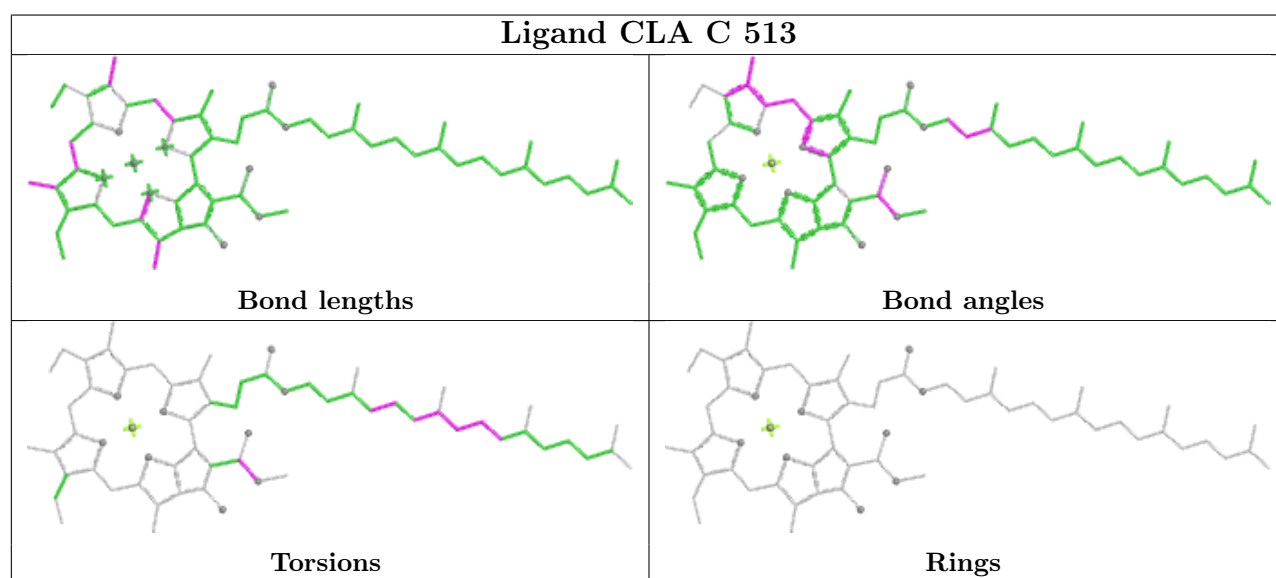
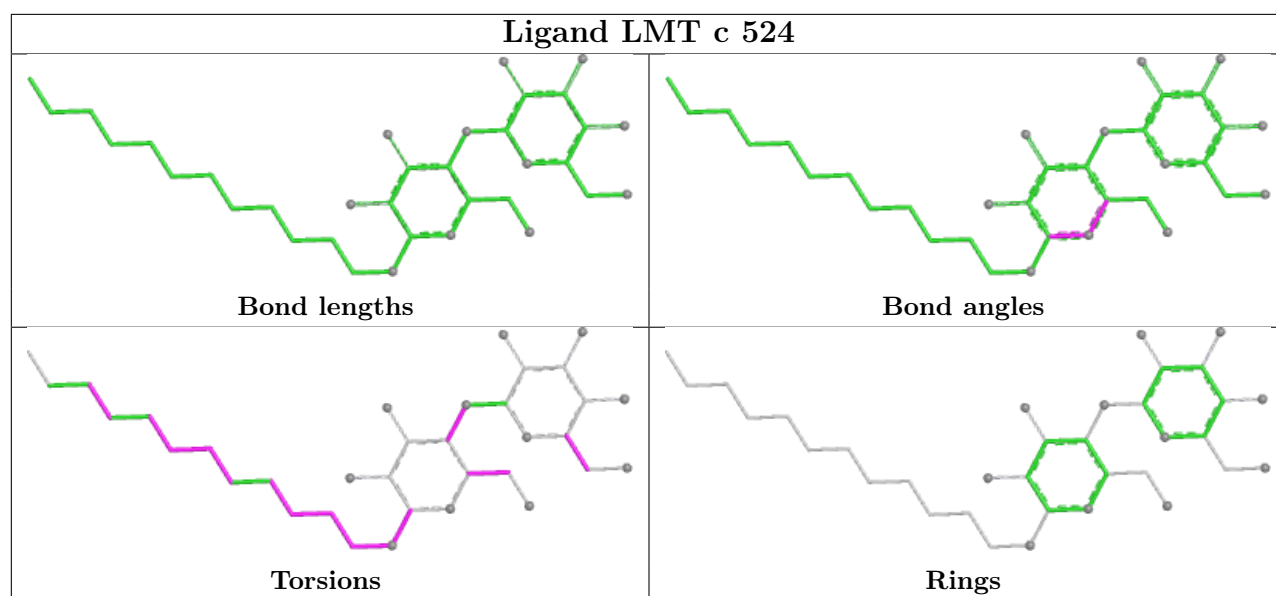


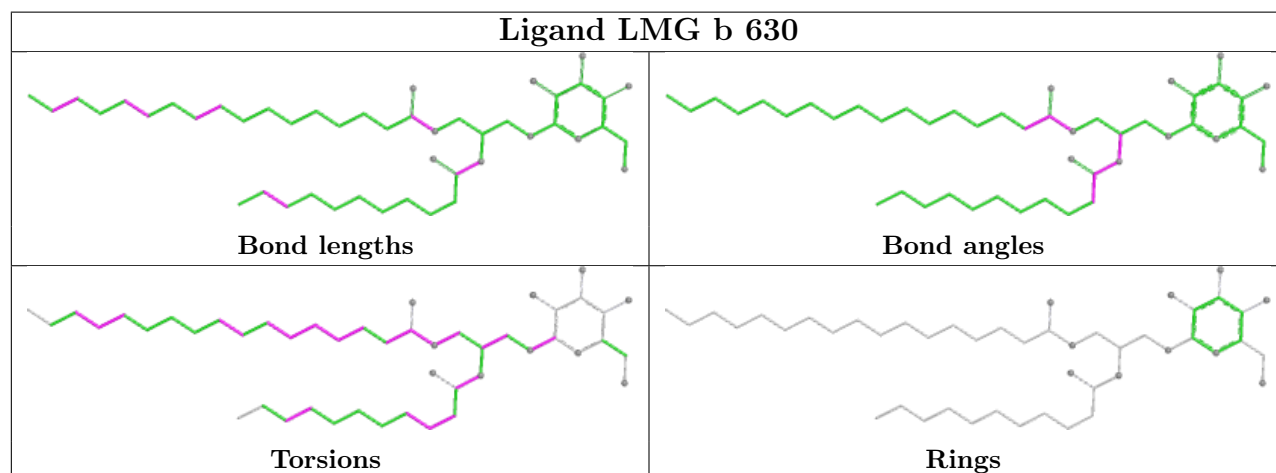
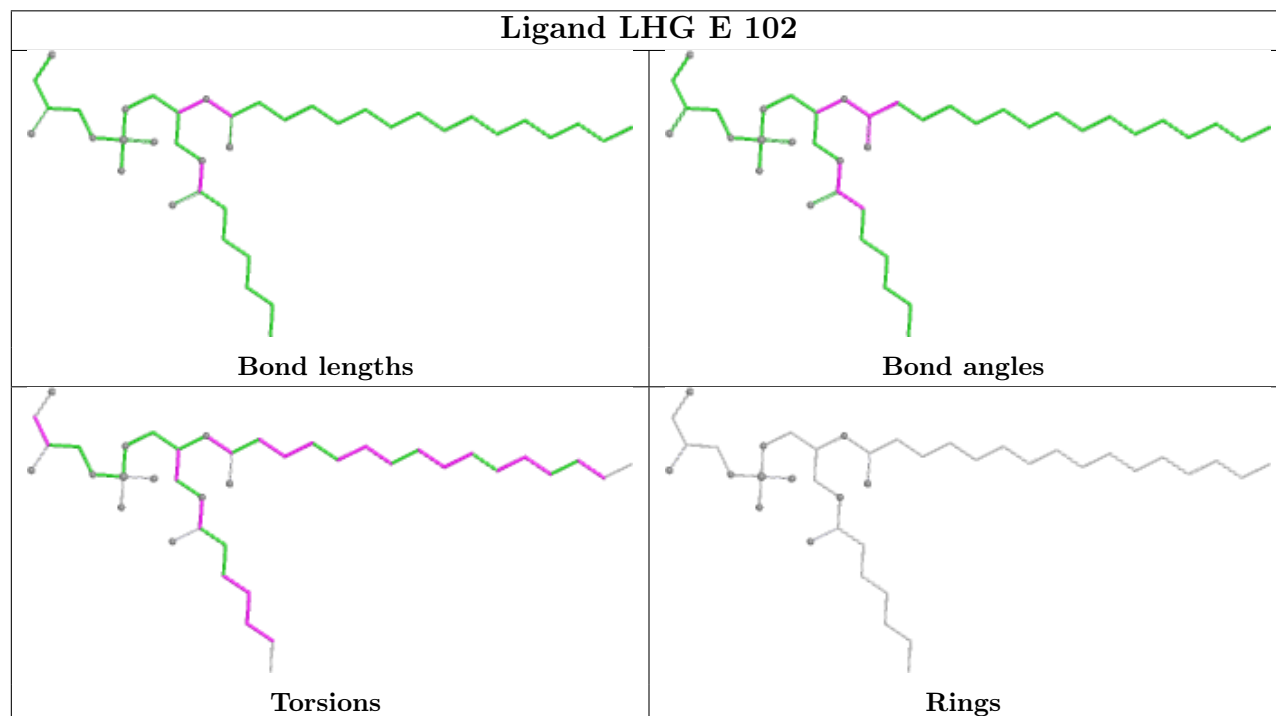
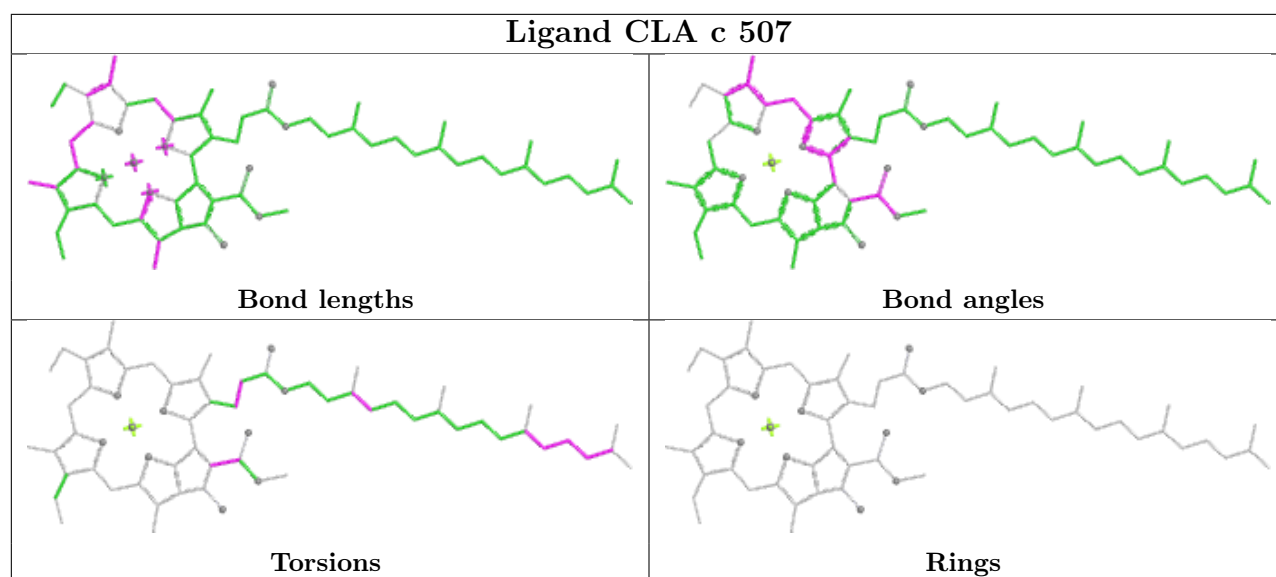
## Ligand CLA B 604

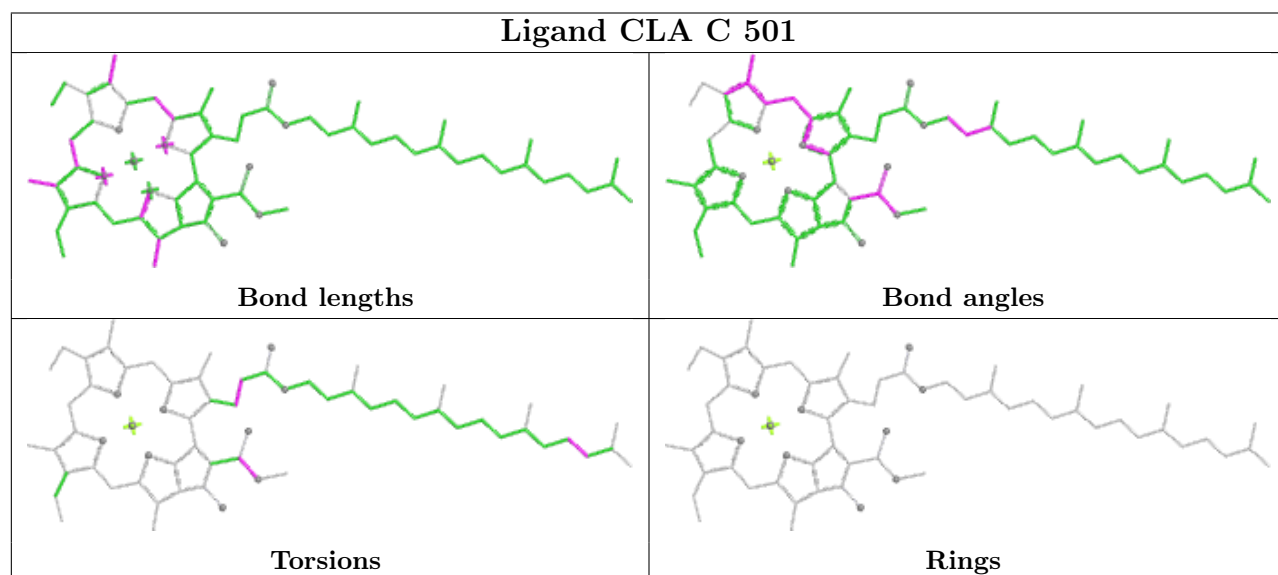
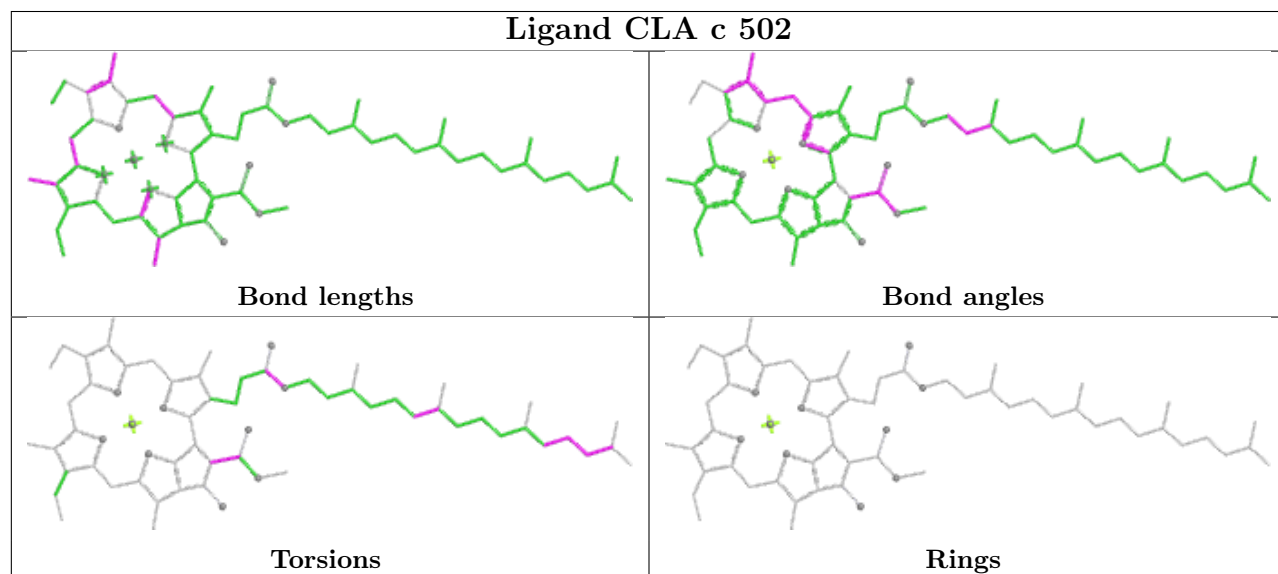
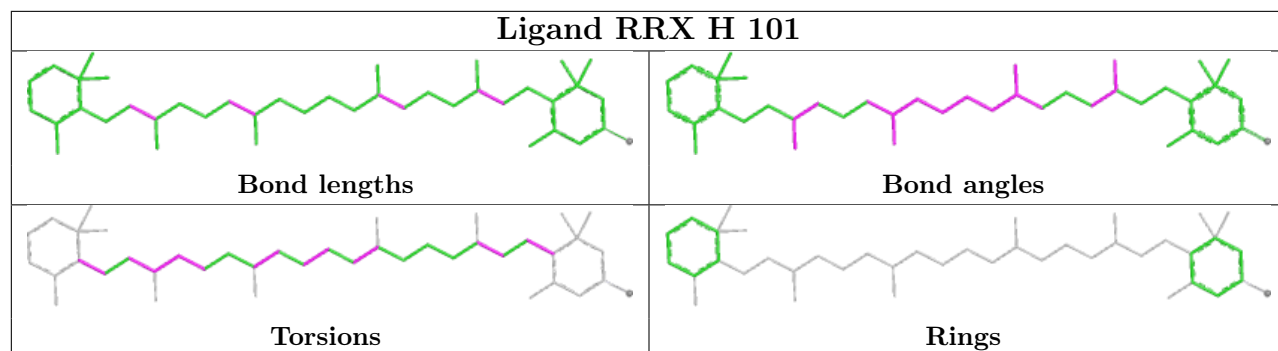


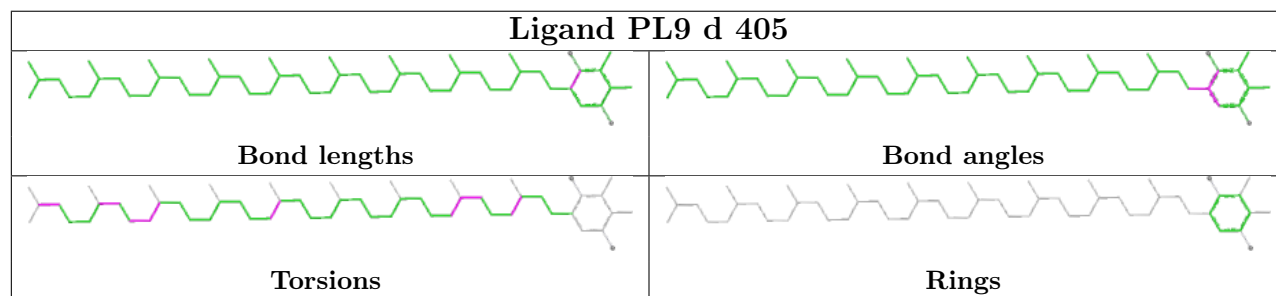
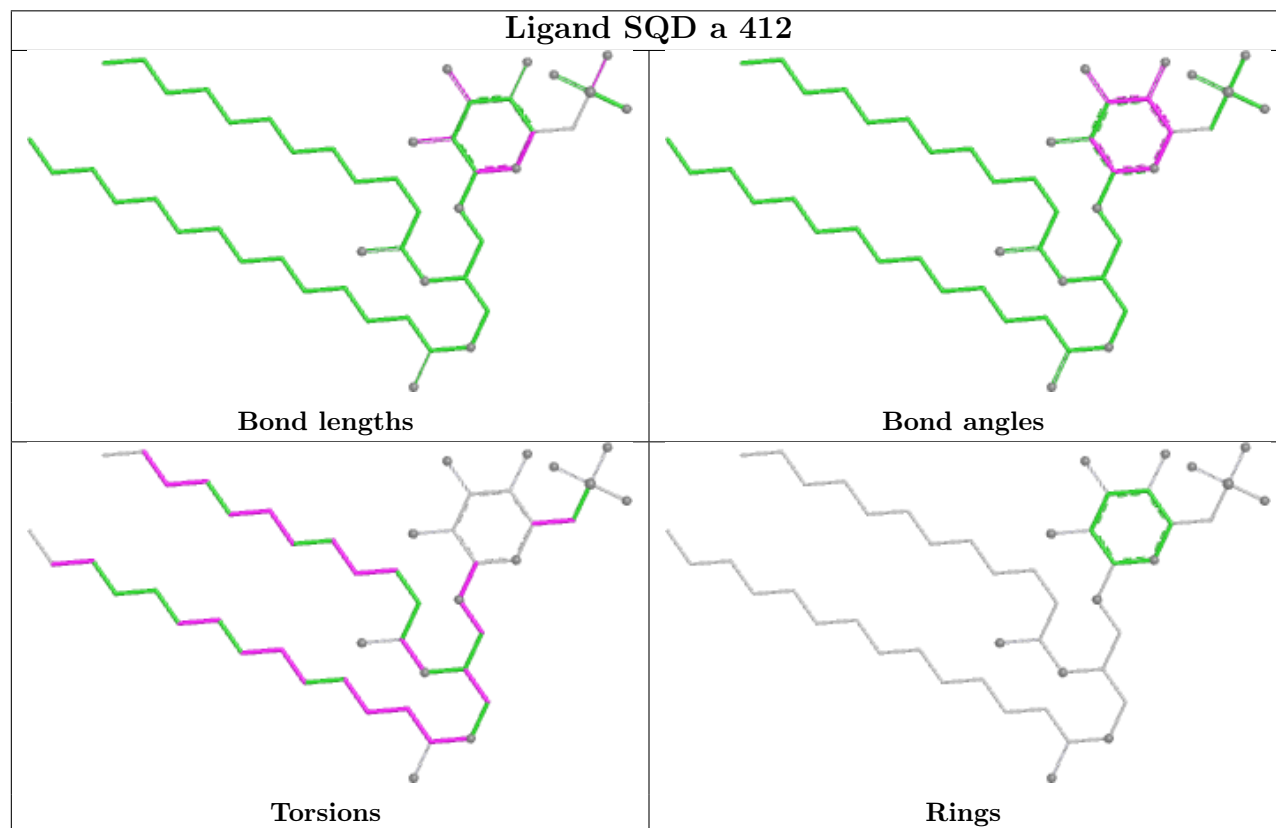
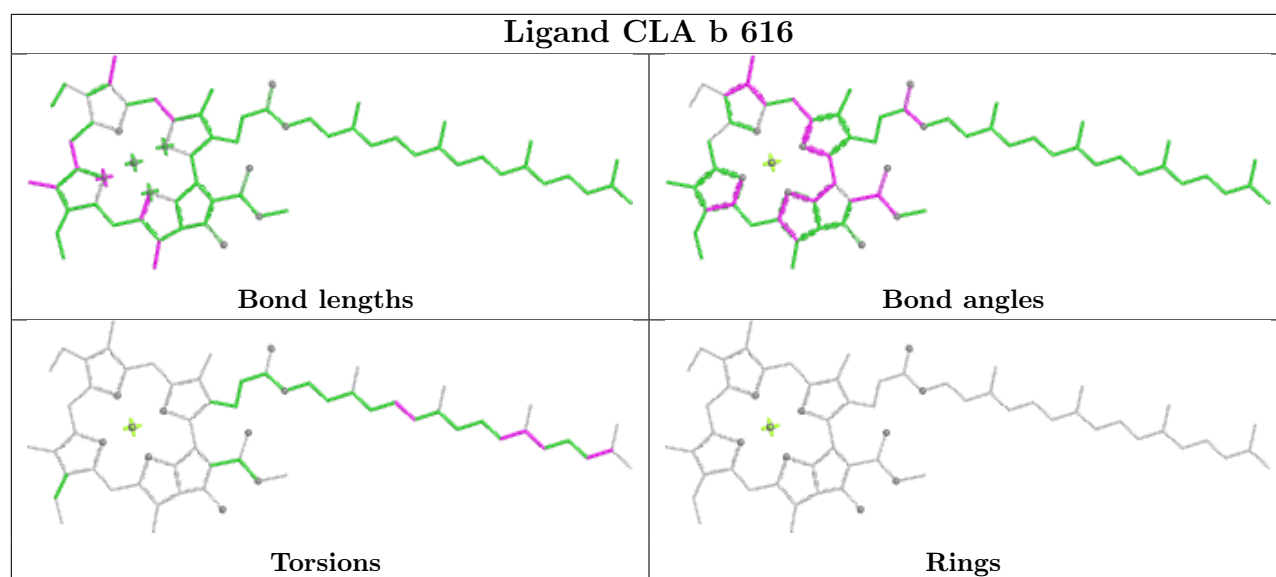


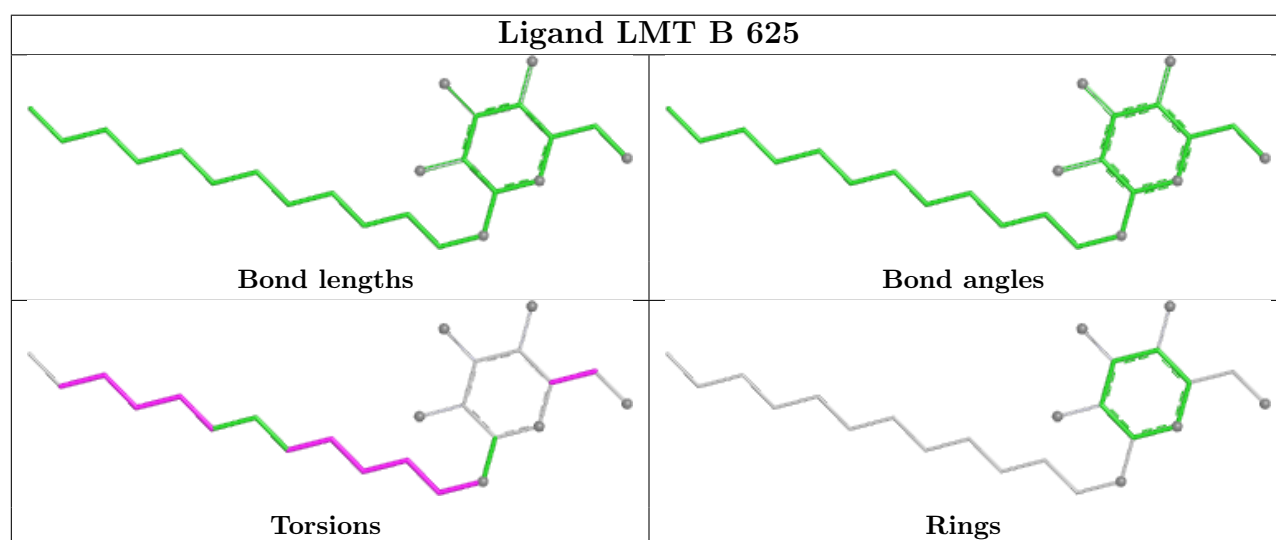
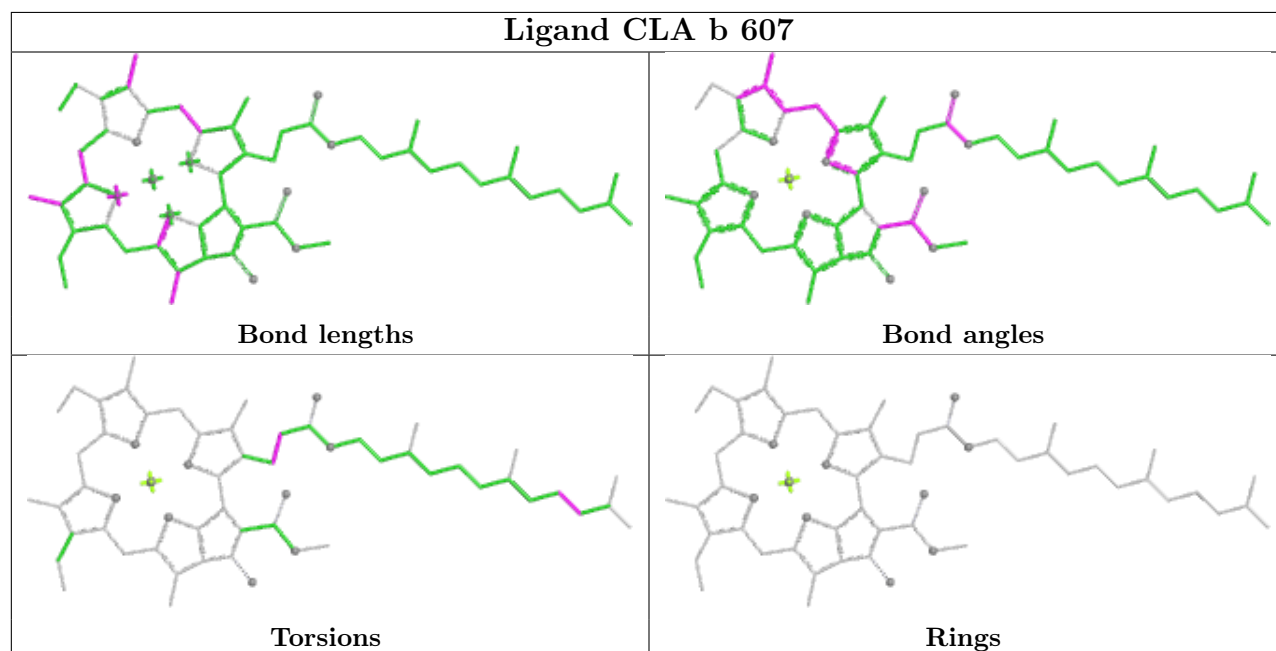
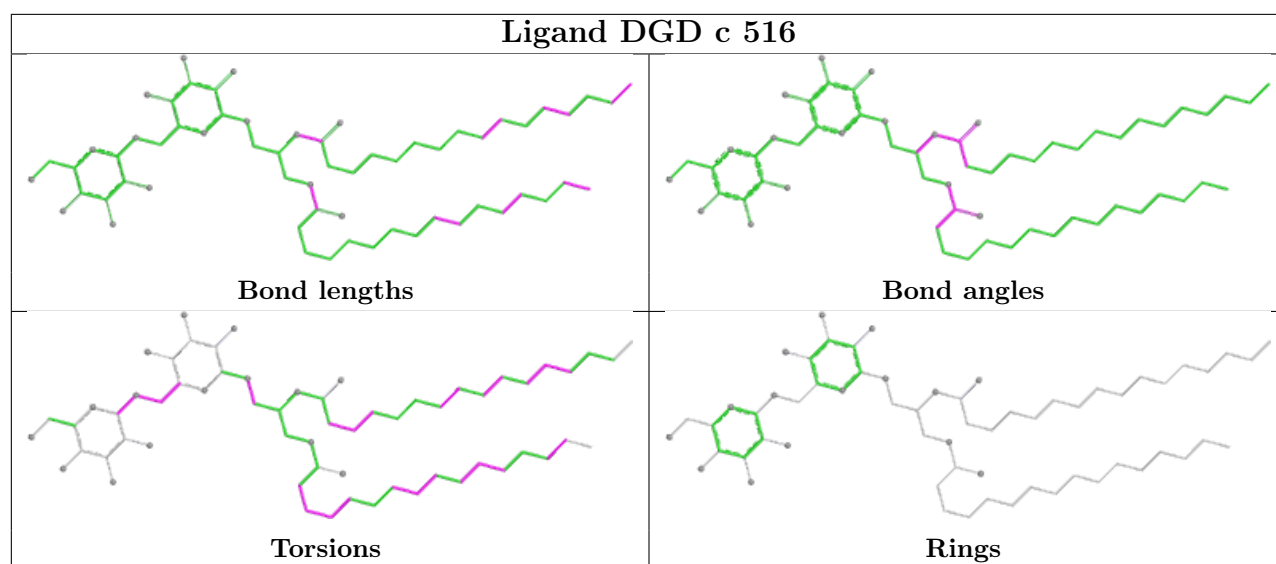


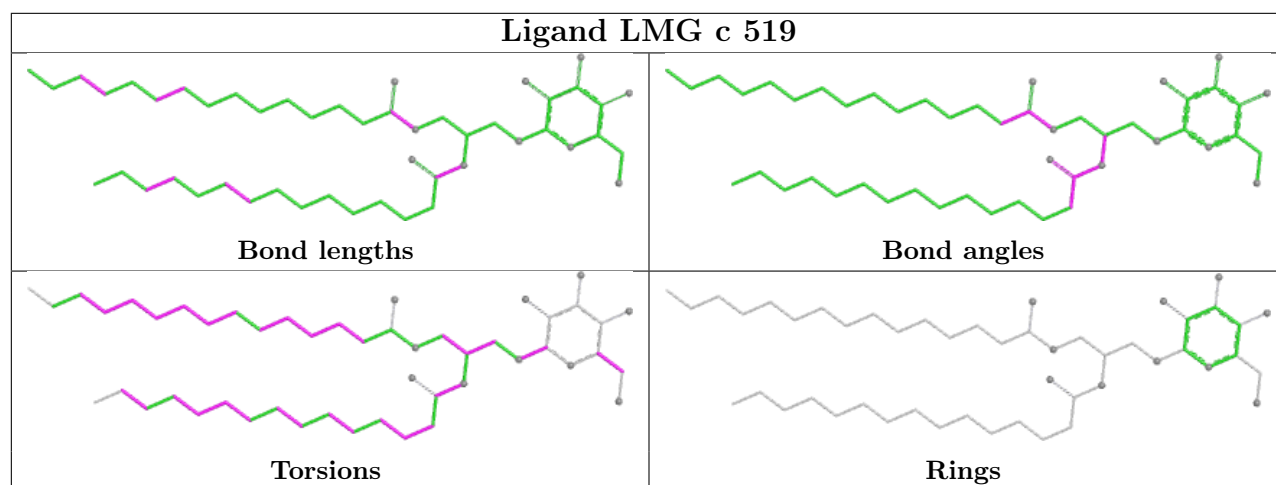
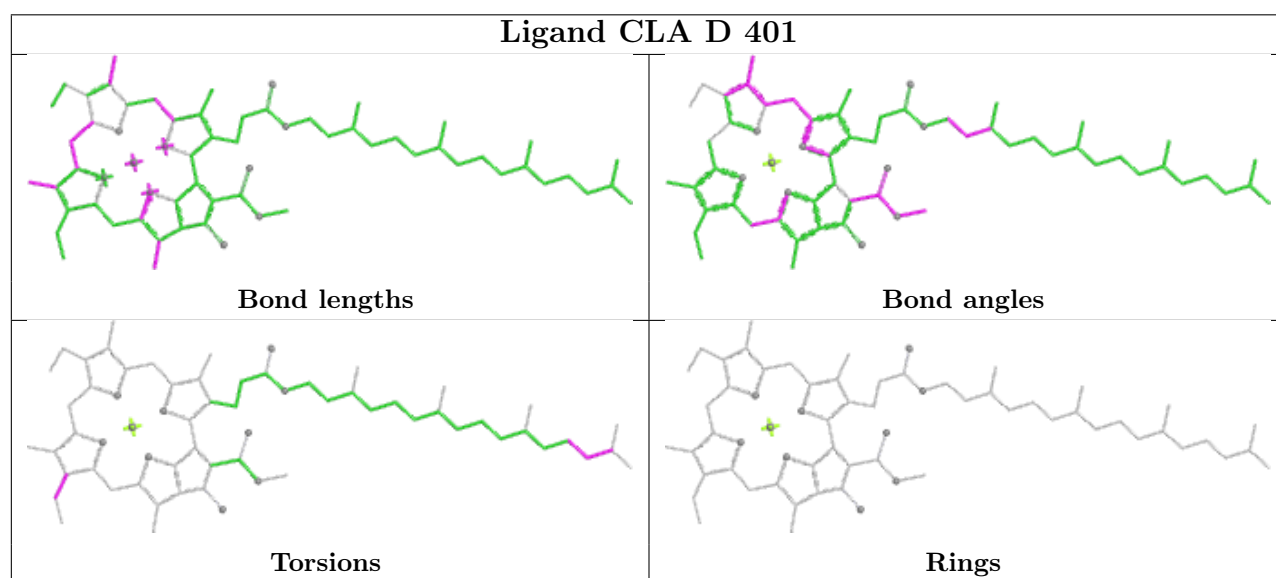
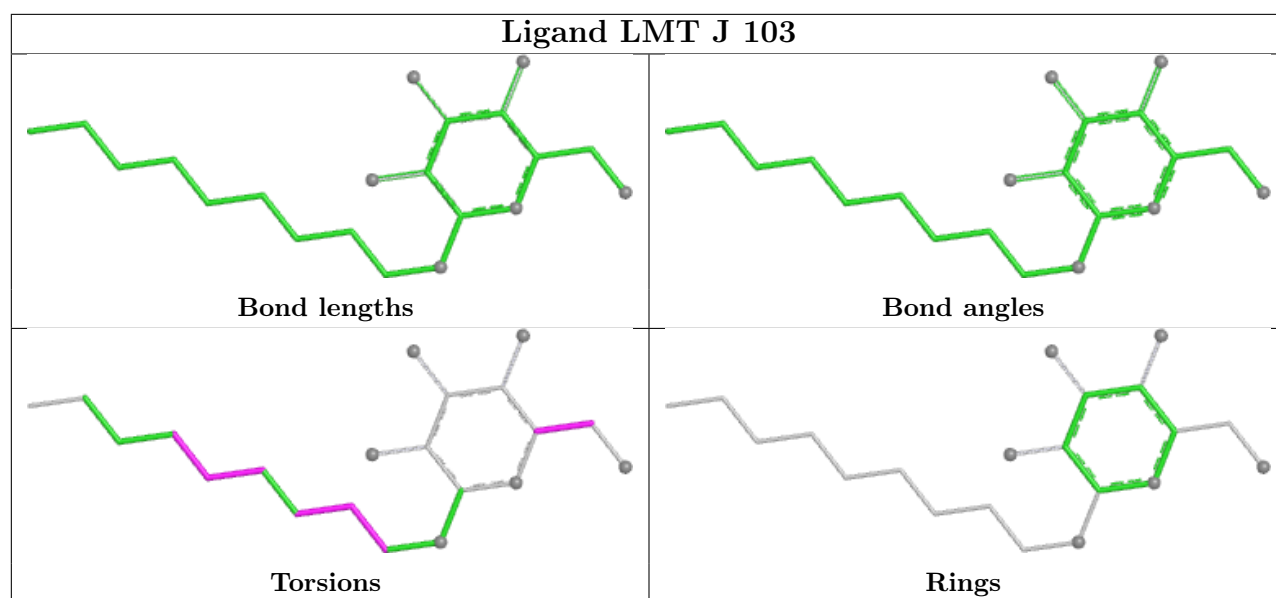


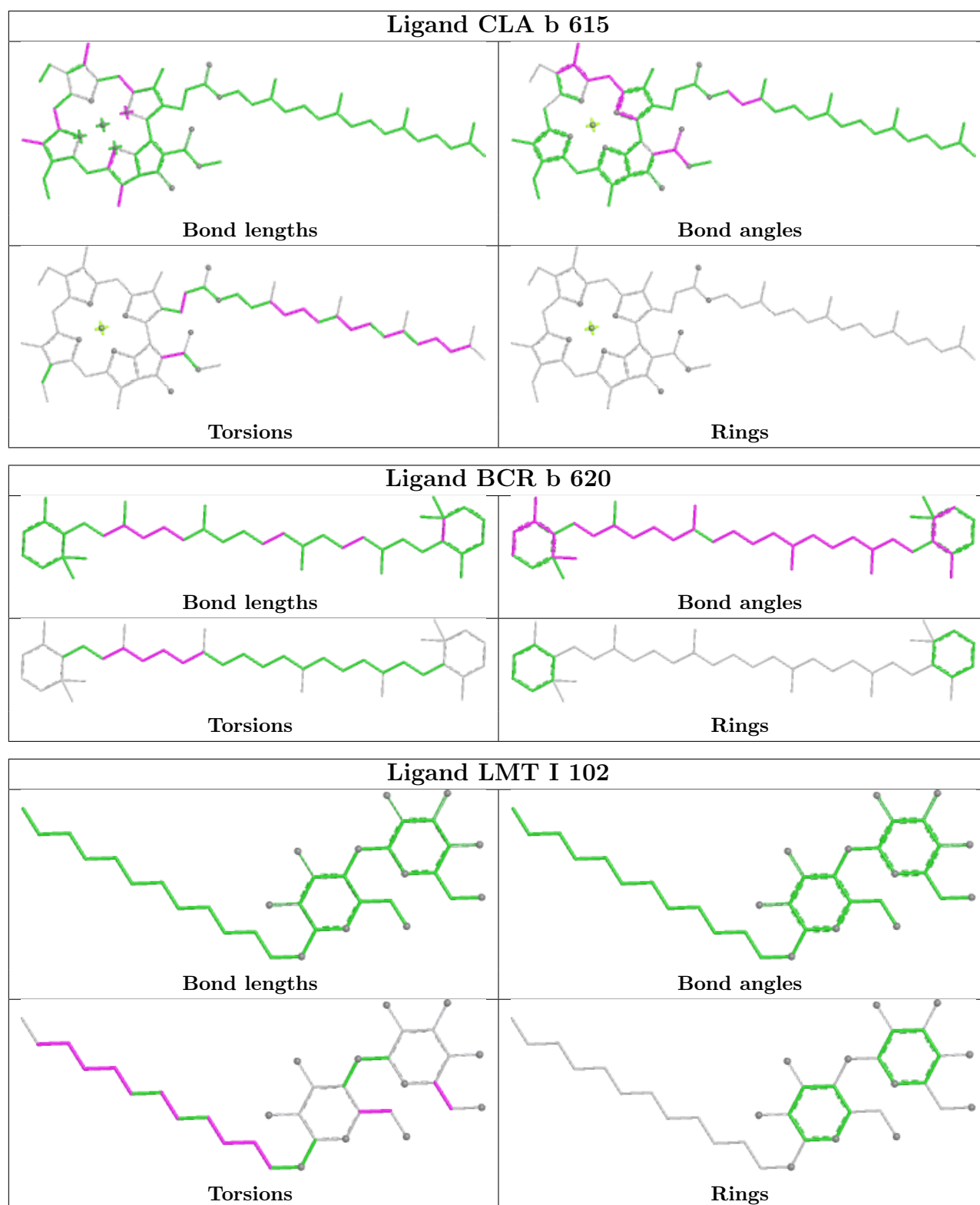


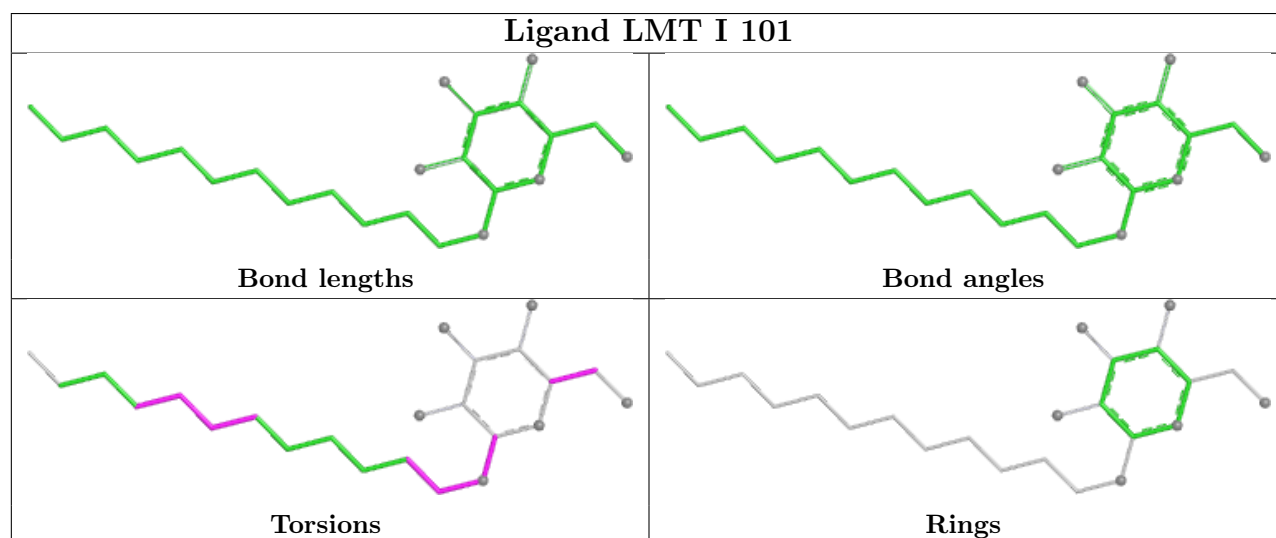
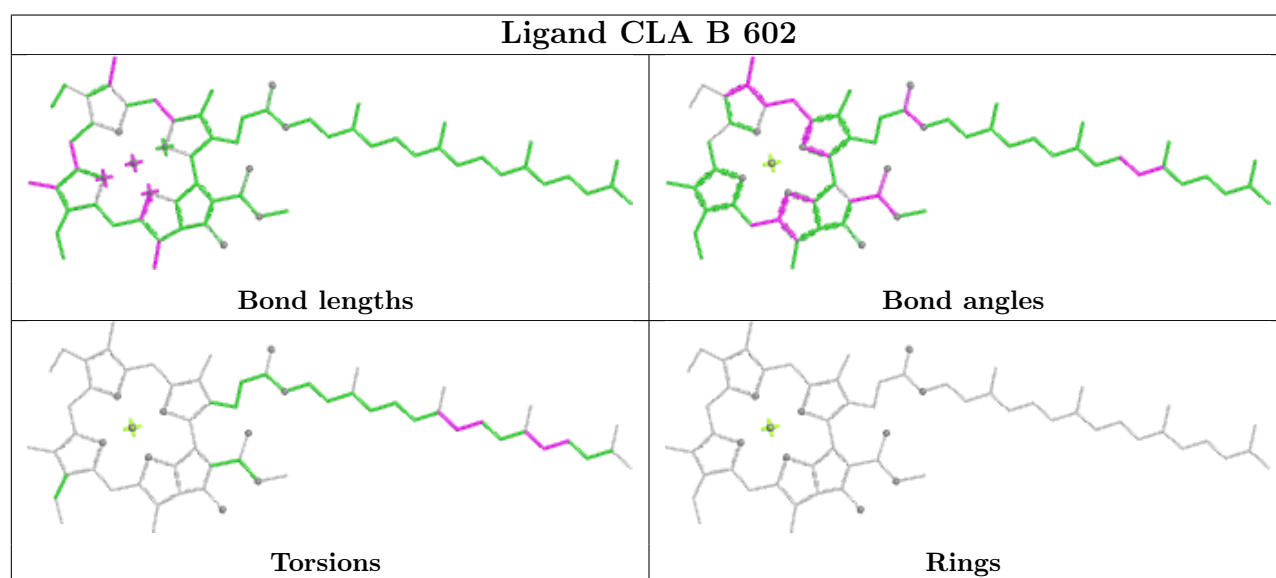
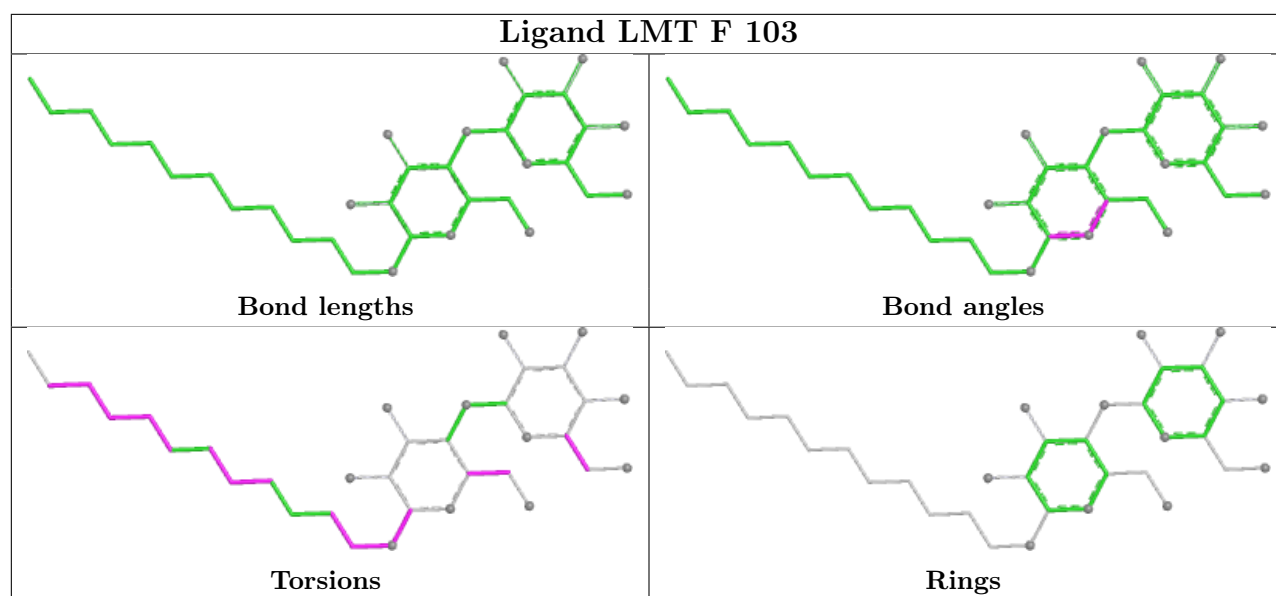




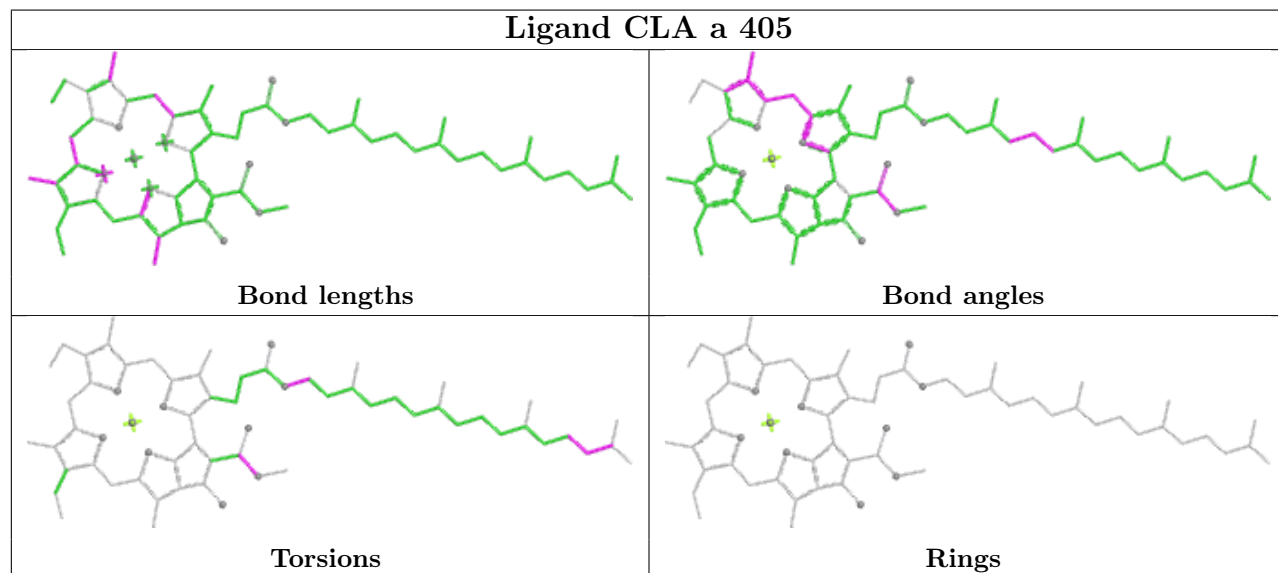
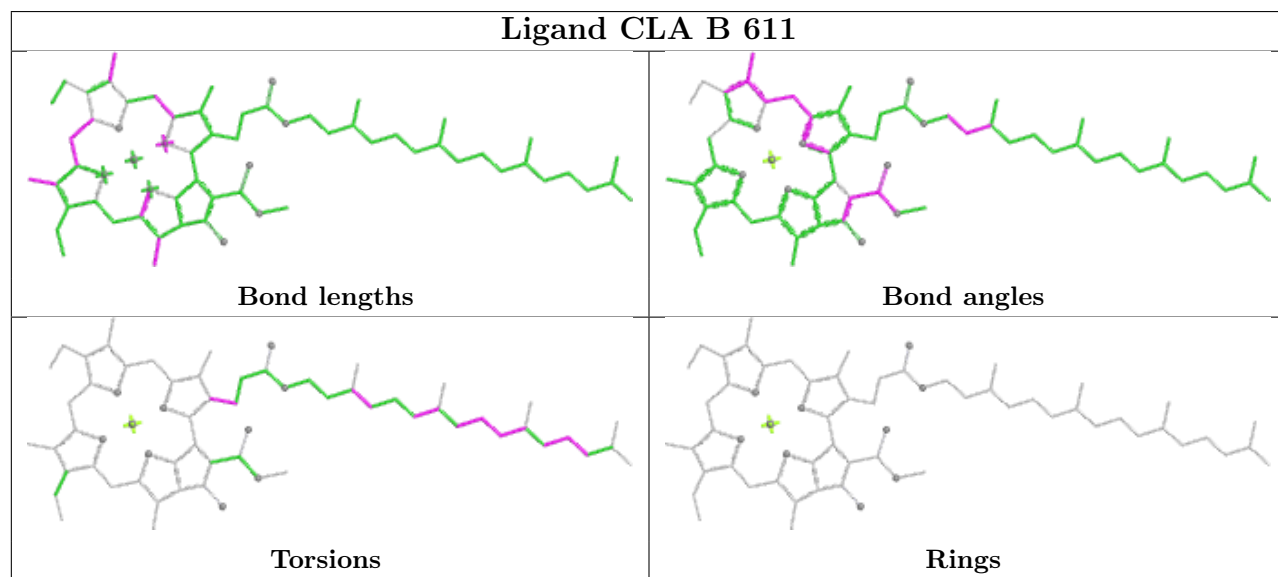
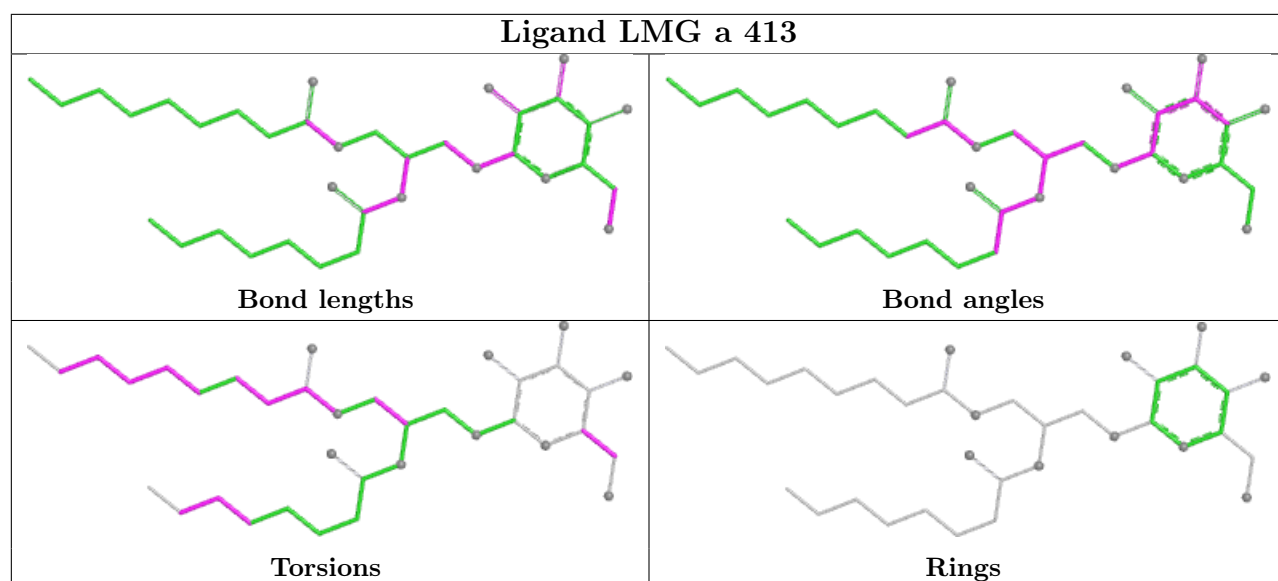


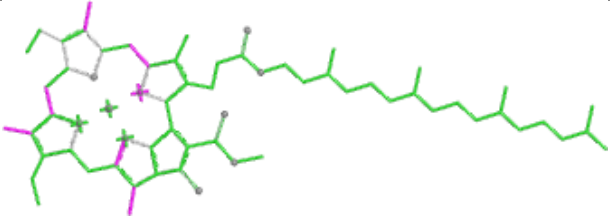
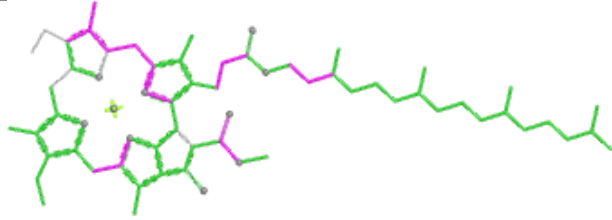
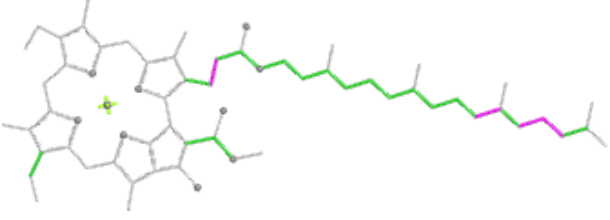
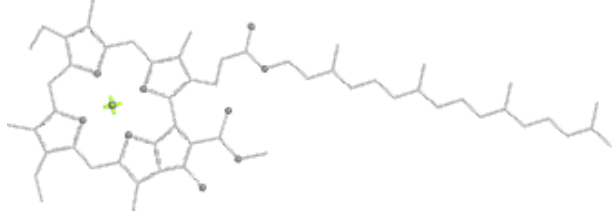
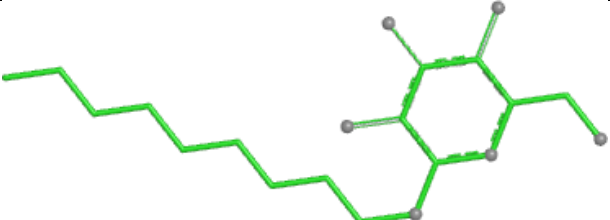
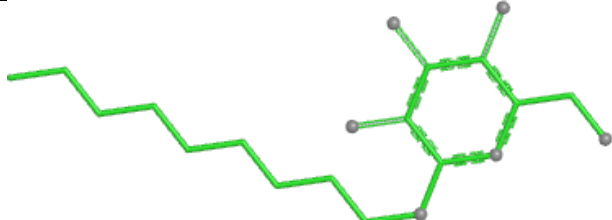
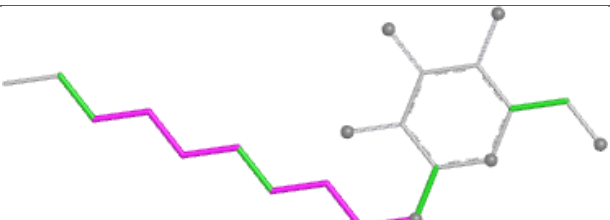
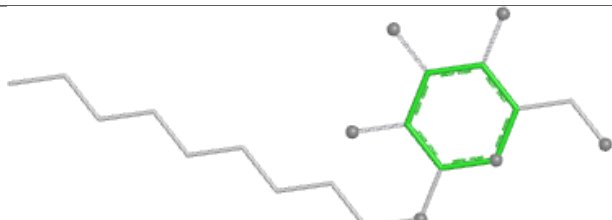
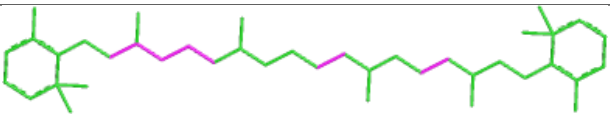
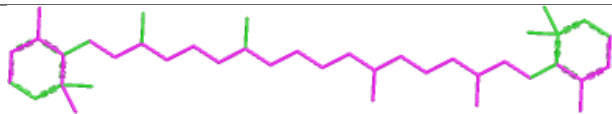
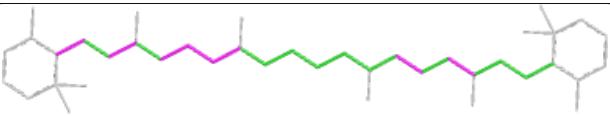
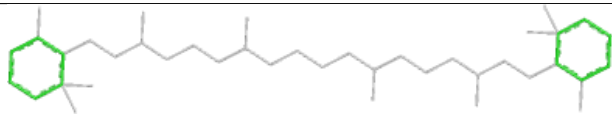




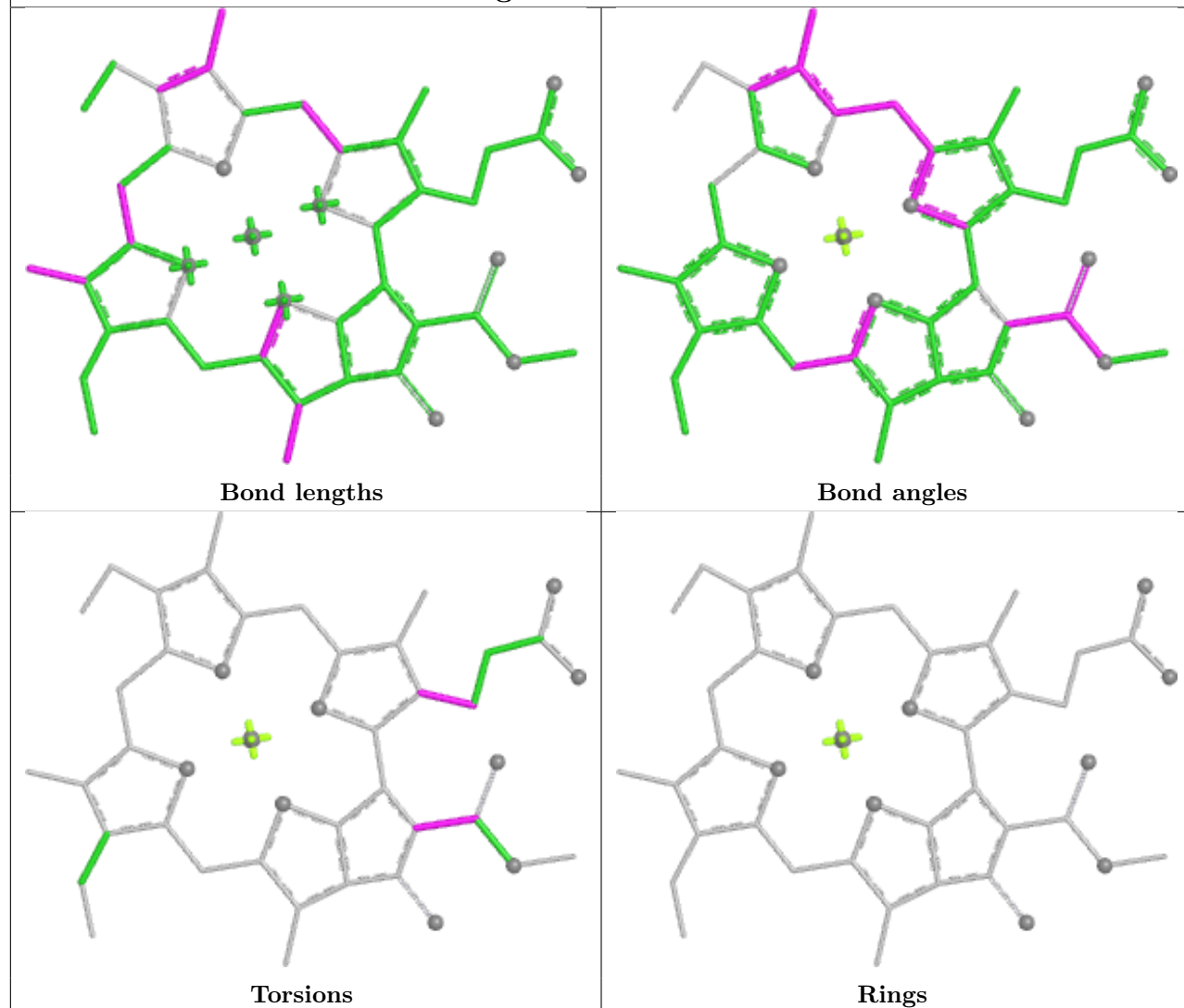




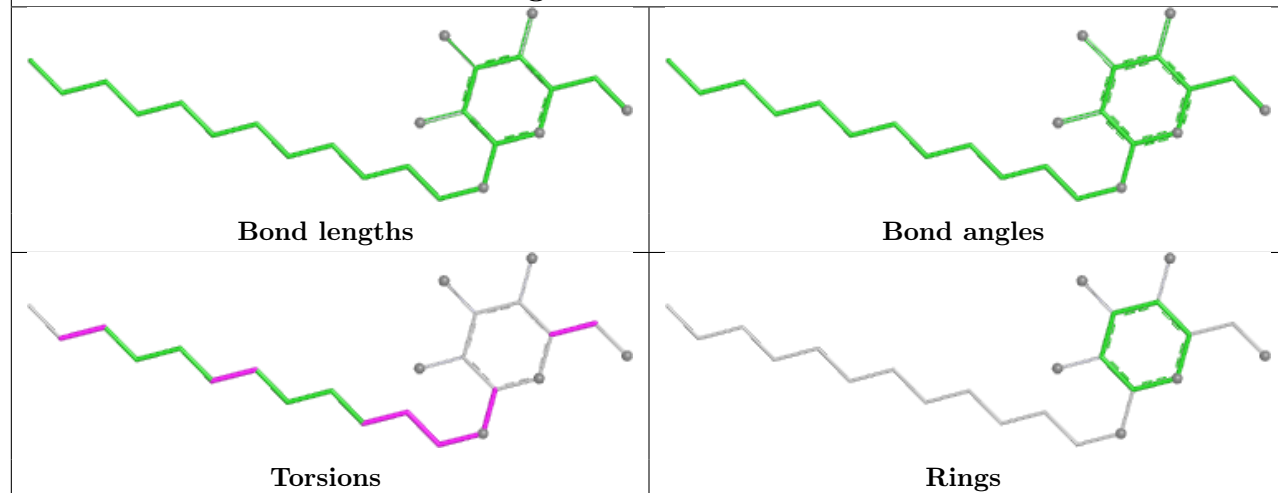


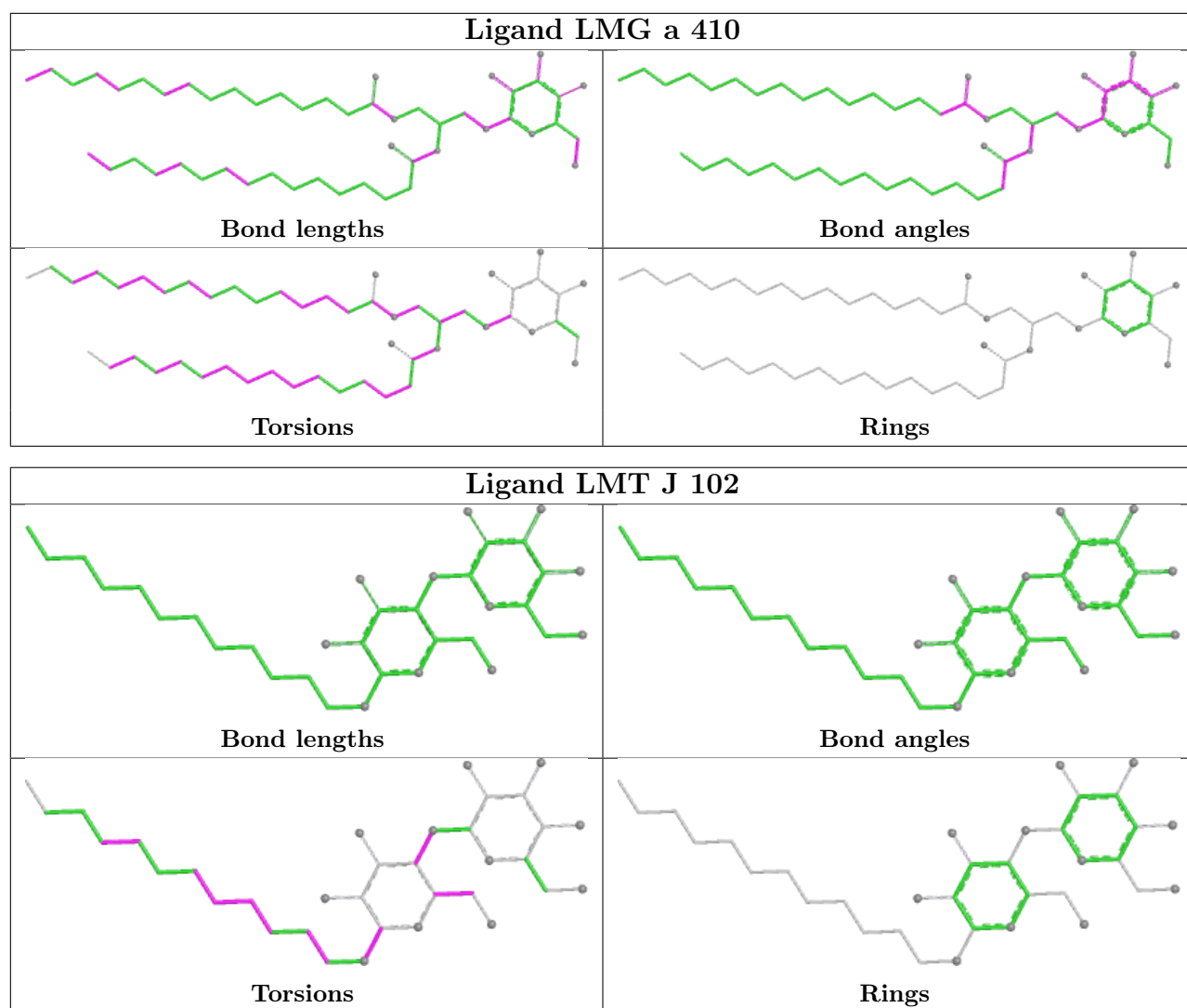
Ligand CLA B 610	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT C 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 525	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

## Ligand CLA b 602

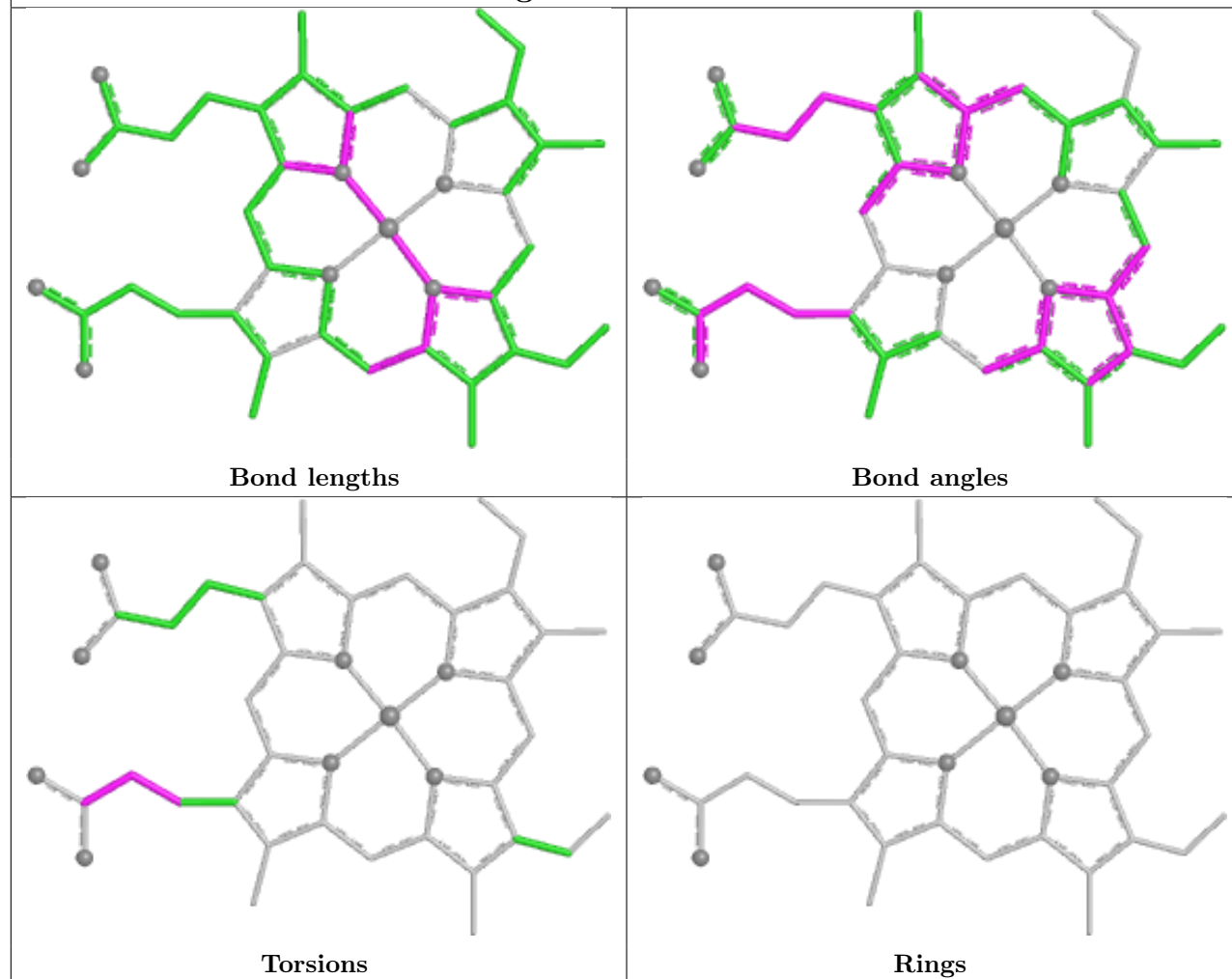


## Ligand LMT m 102

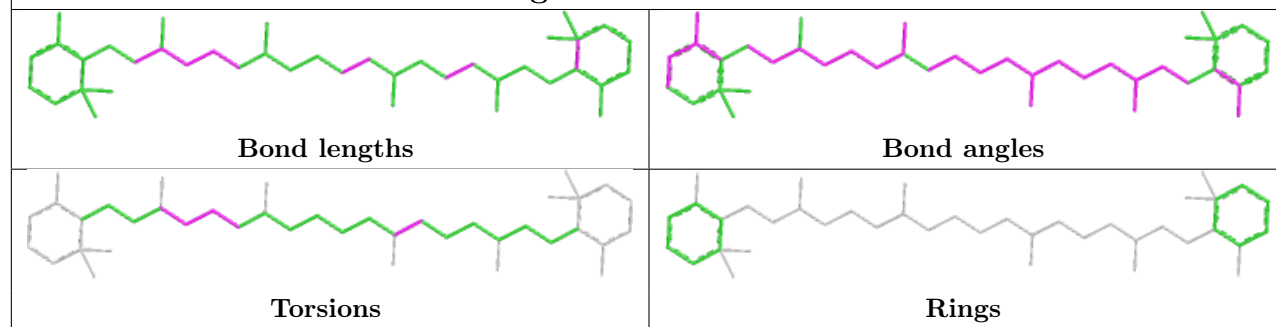


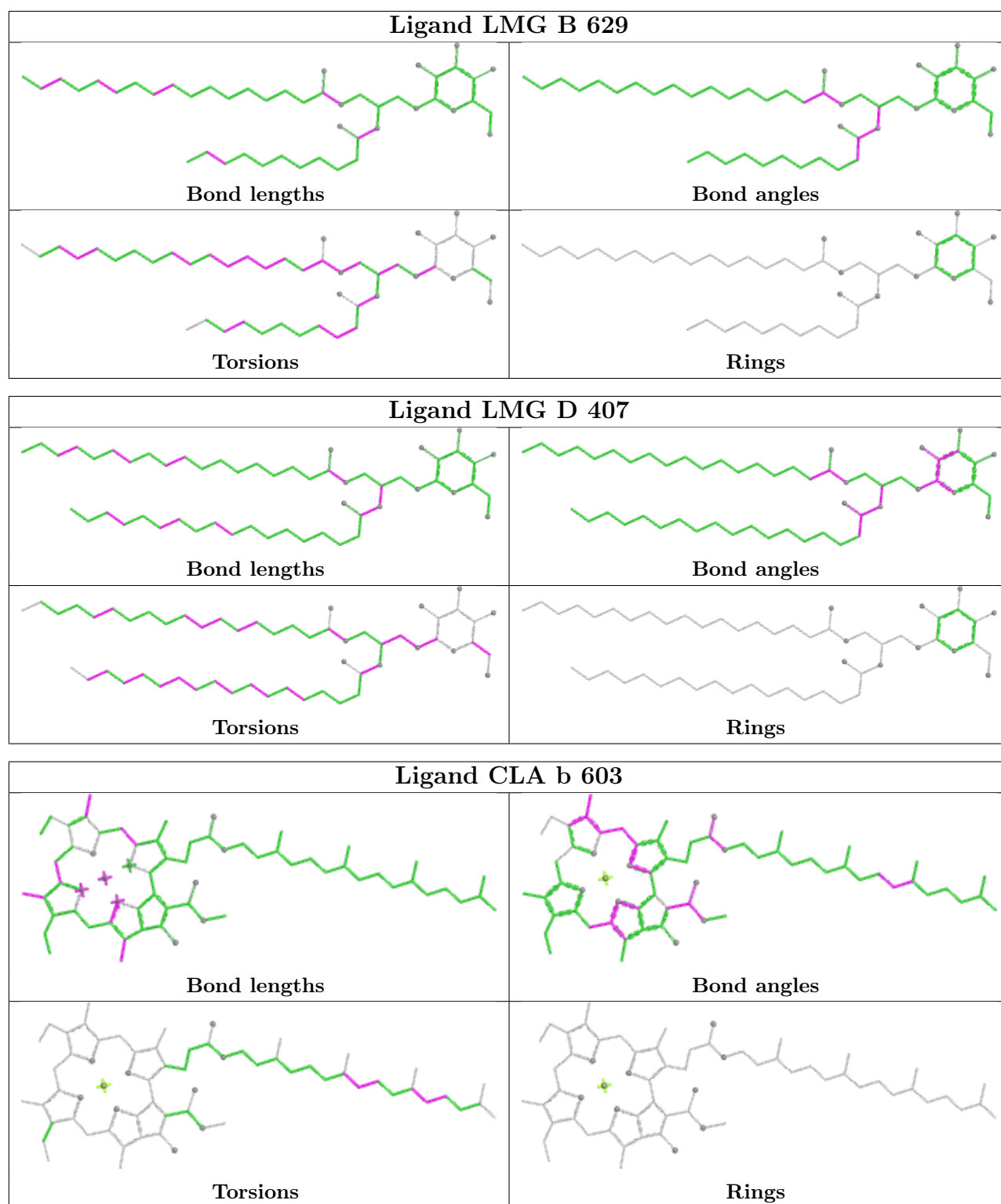


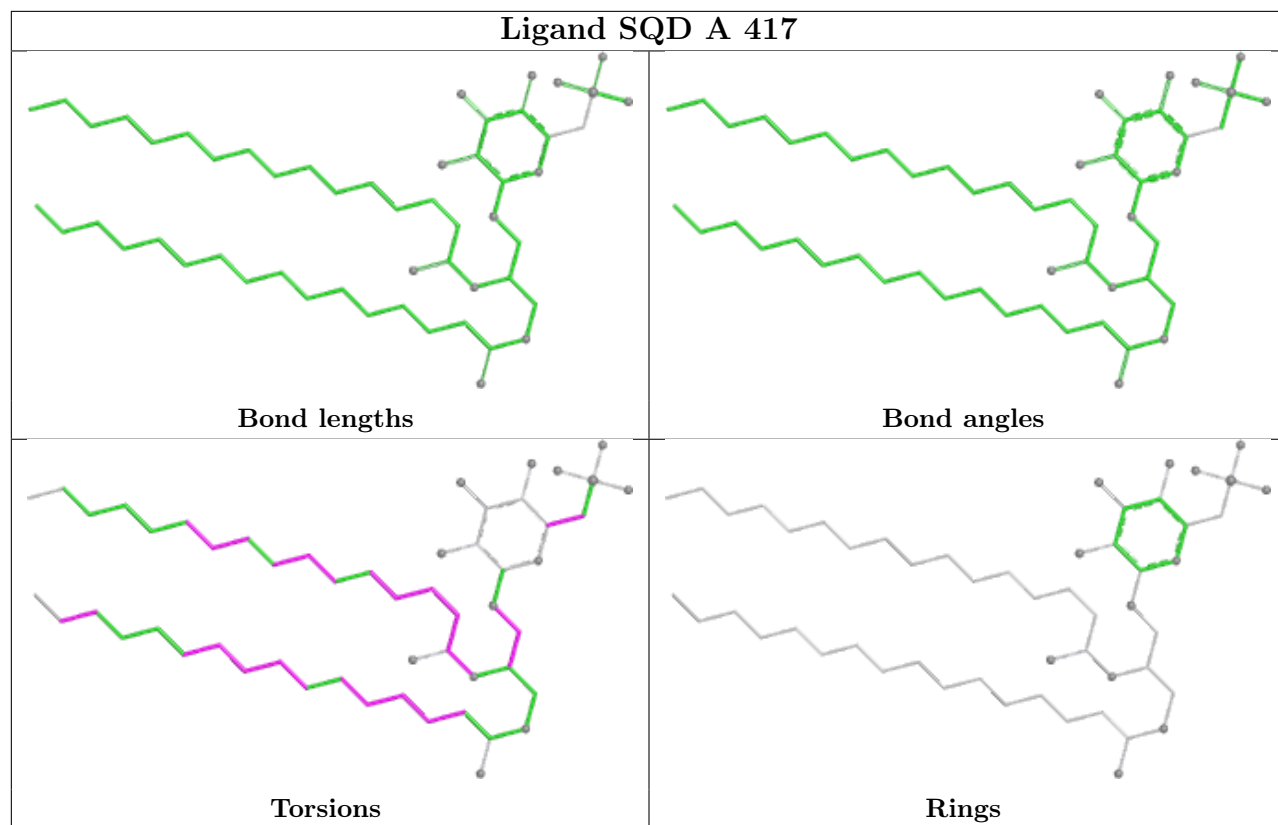
## Ligand HEM f 101

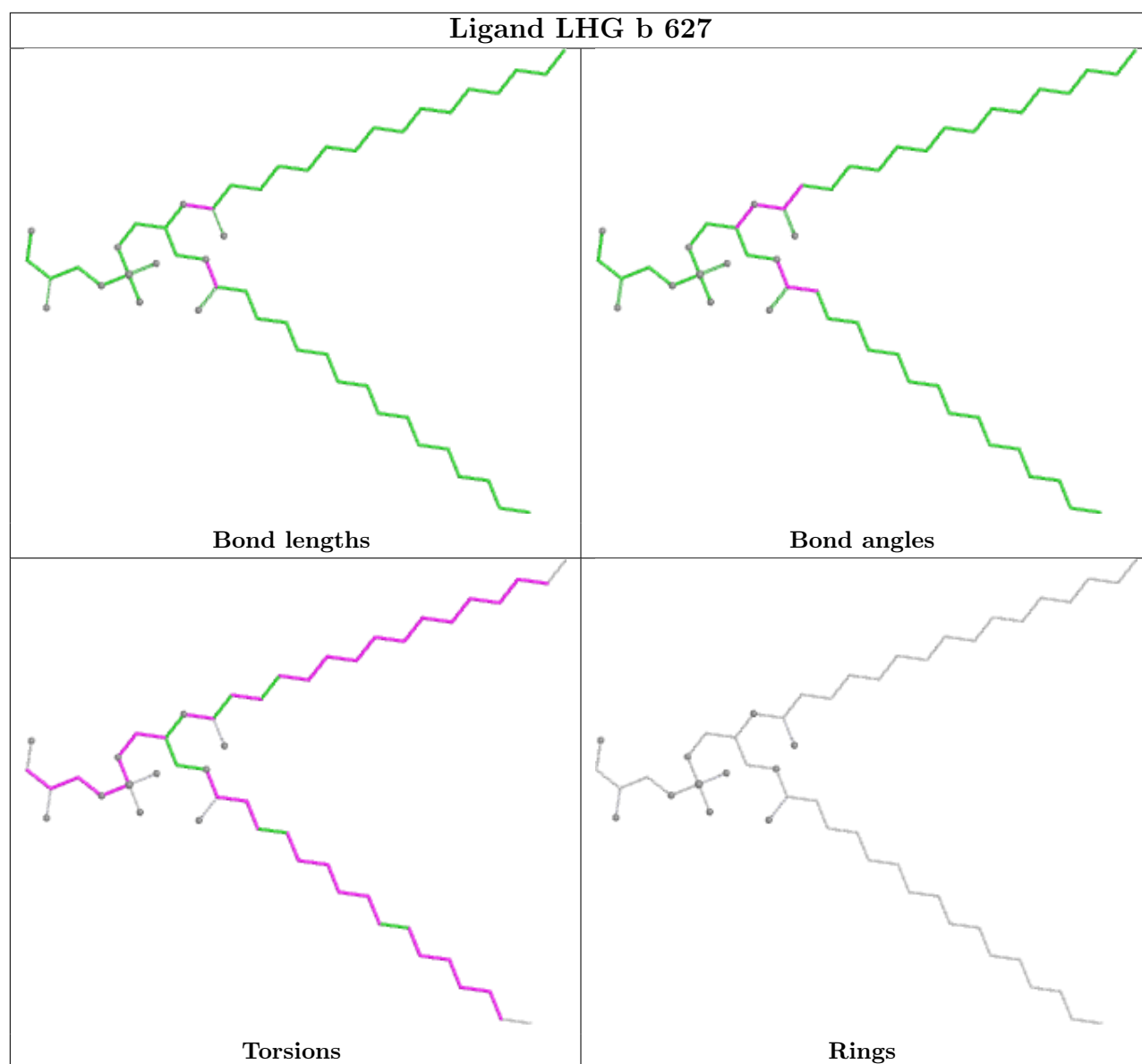


## Ligand BCR C 526



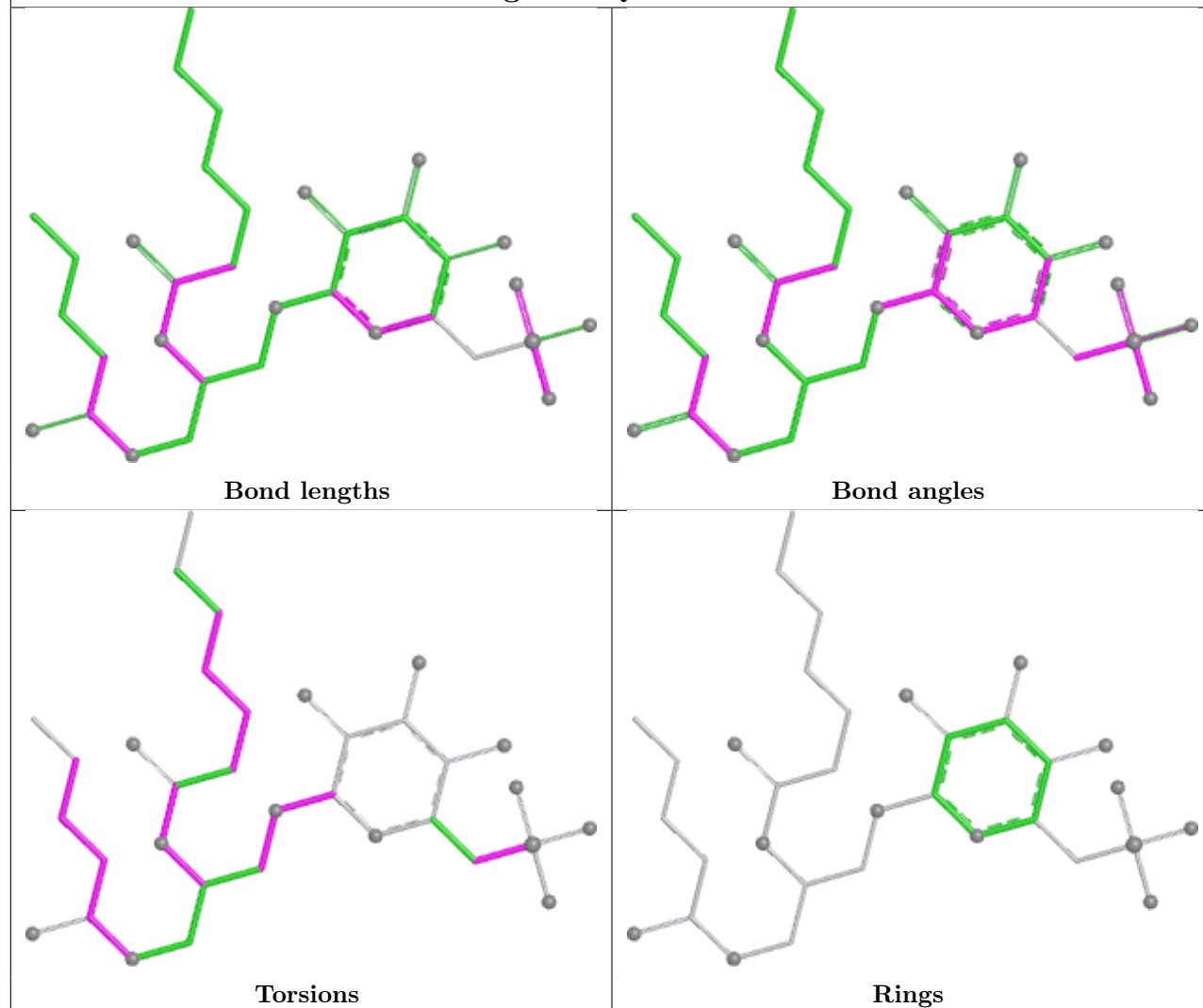




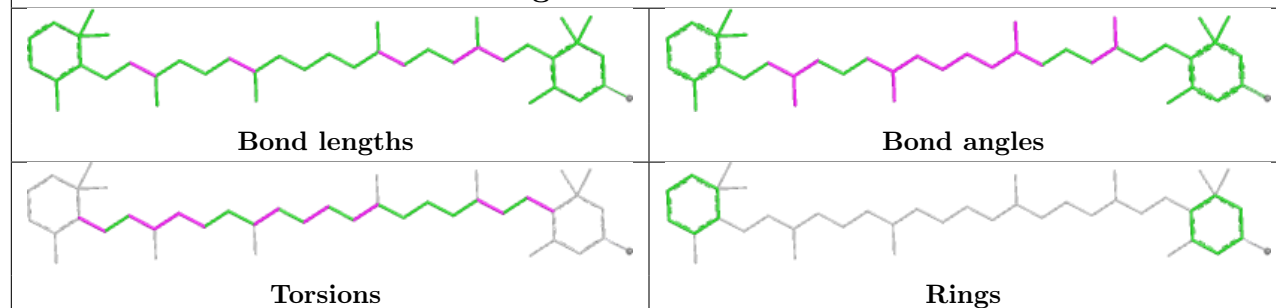


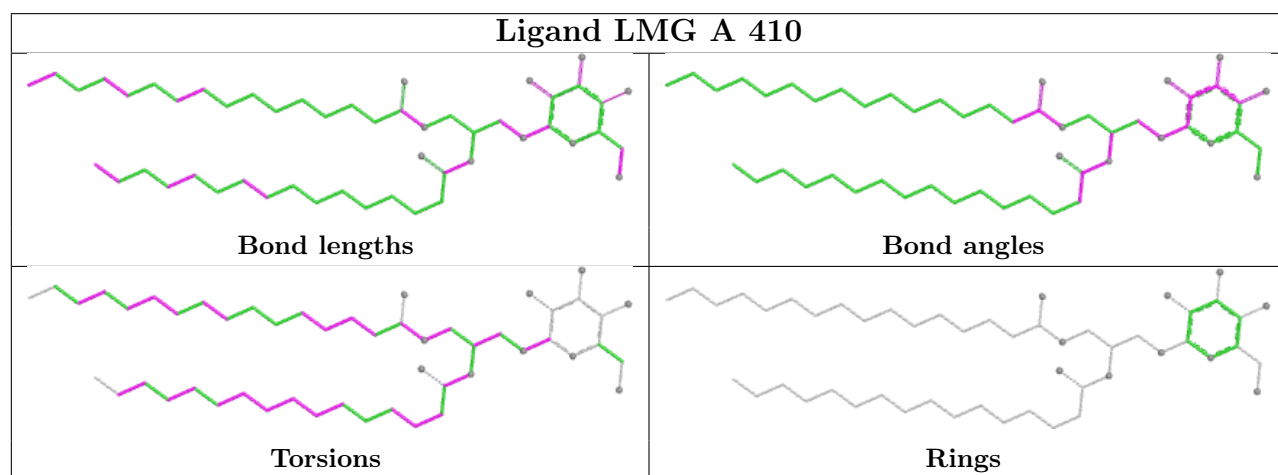
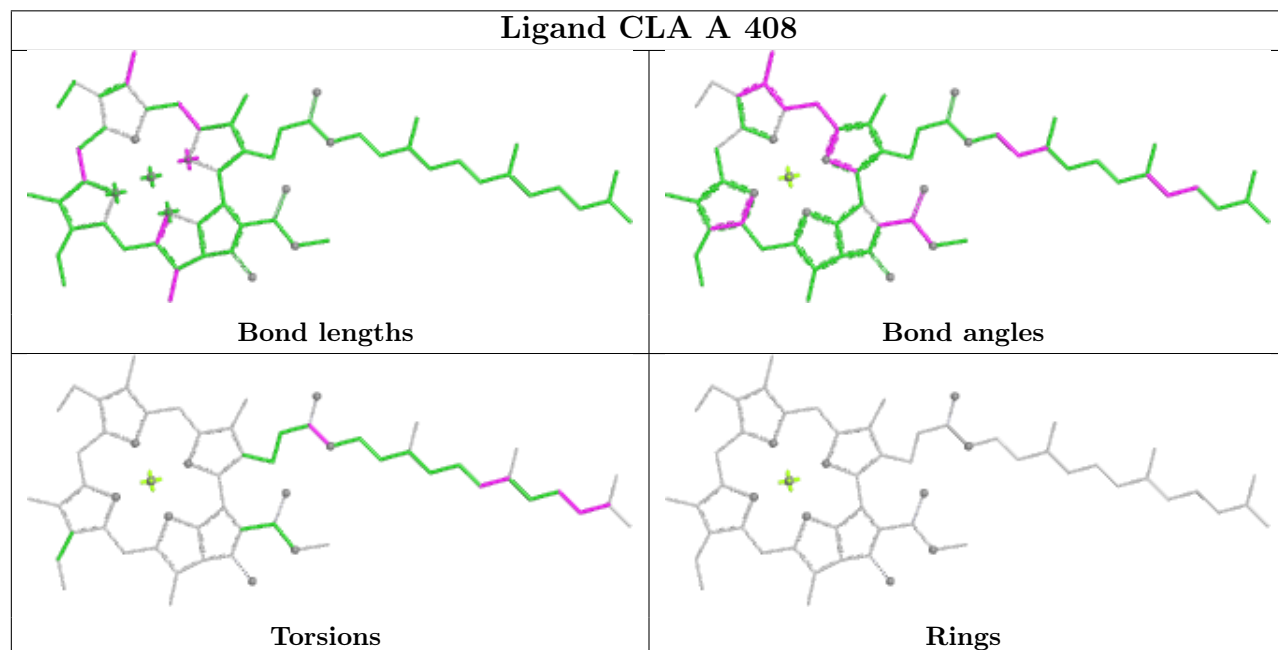
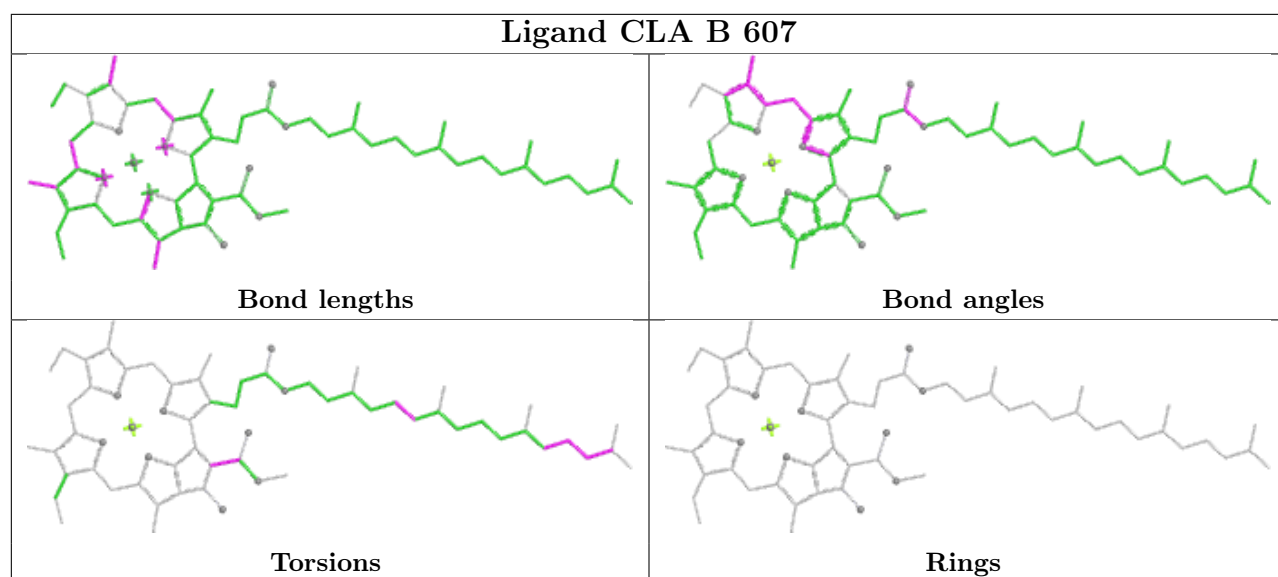


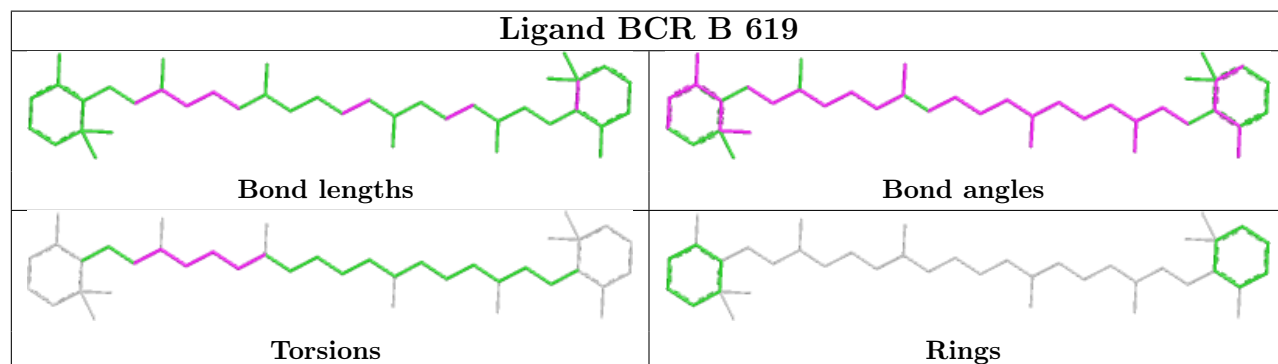
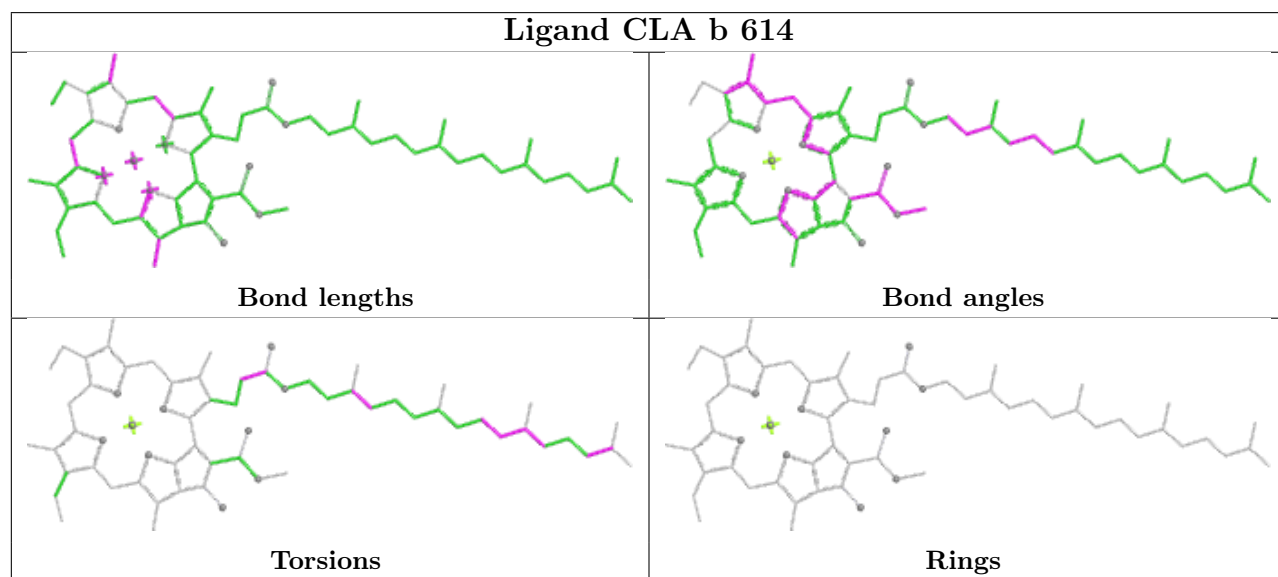
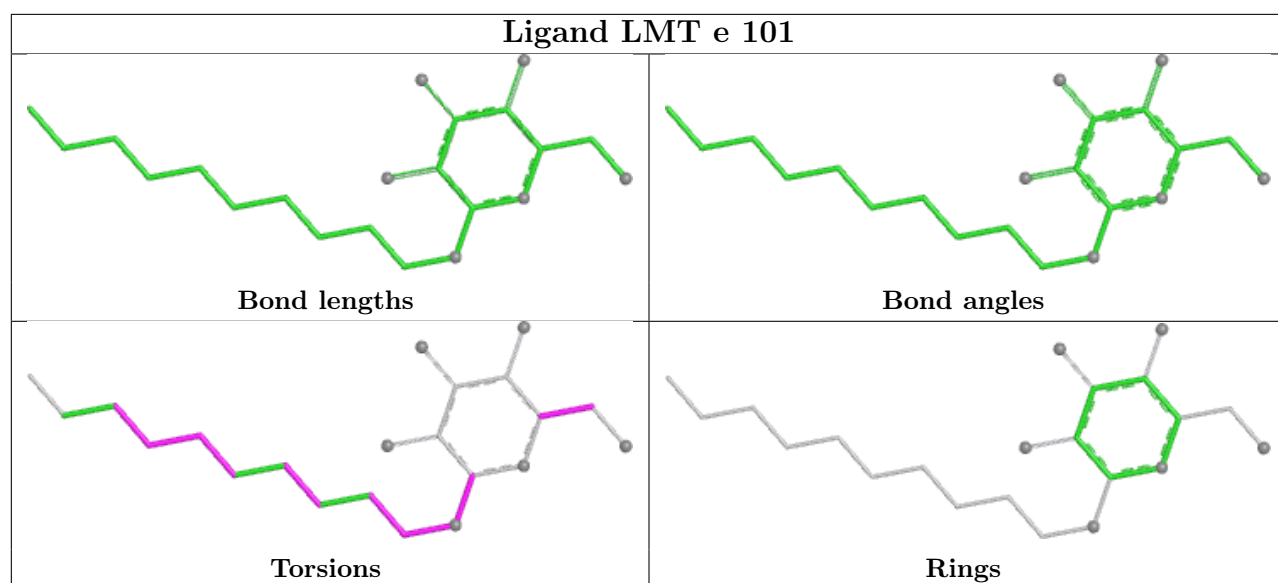
## Ligand SQD F 102

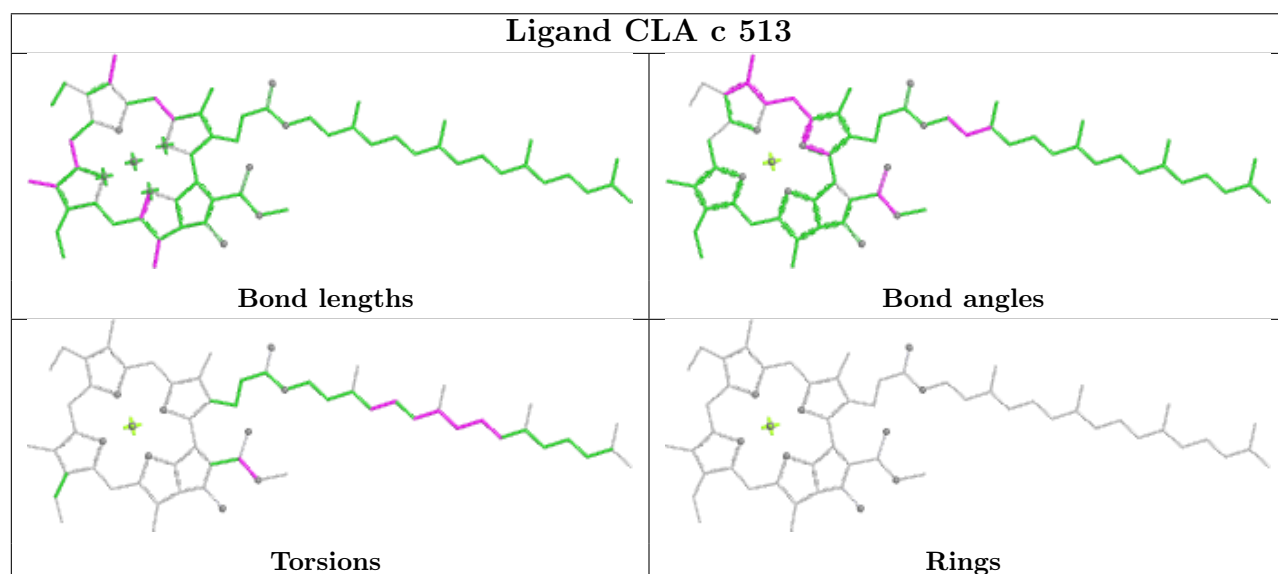
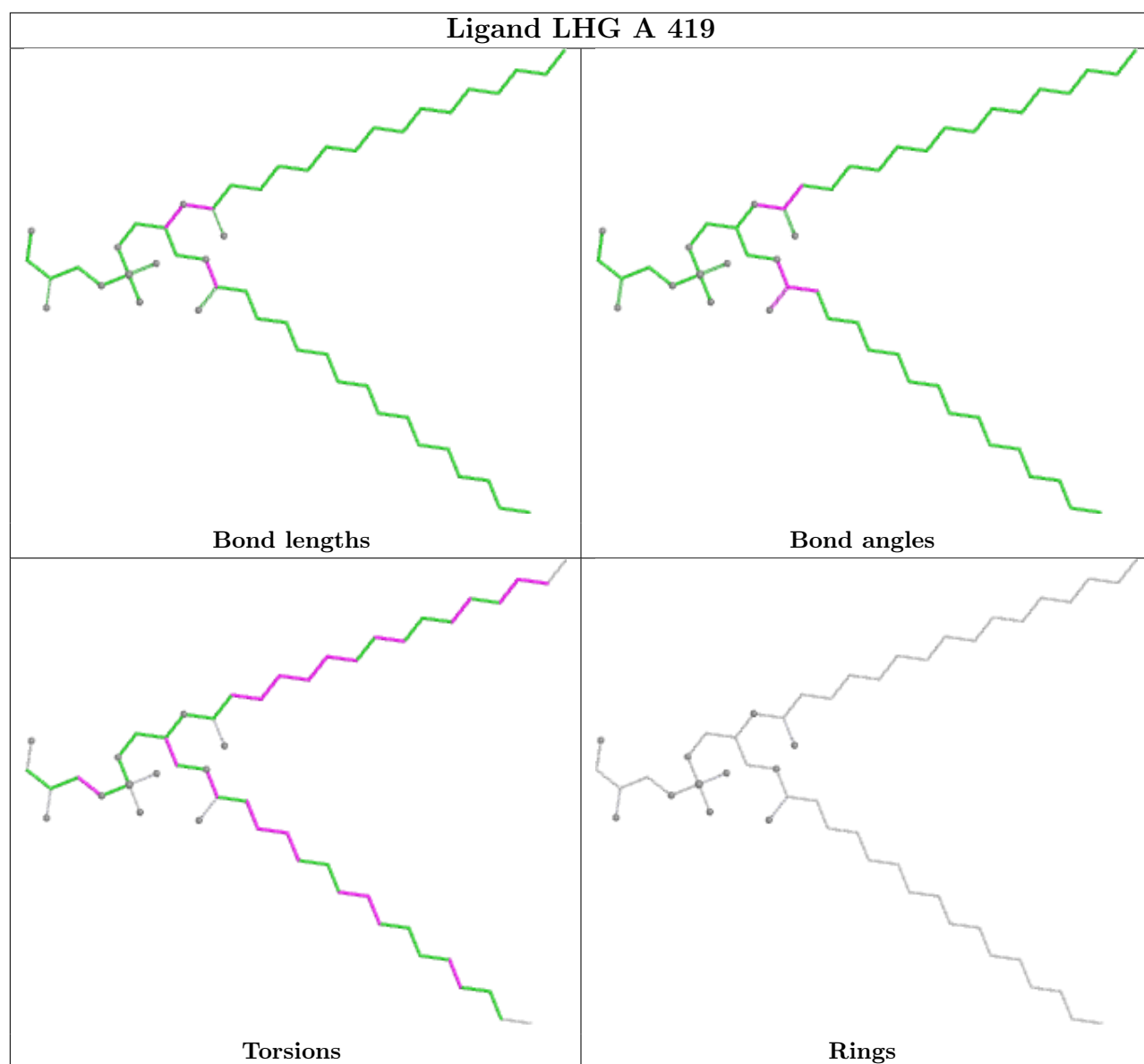


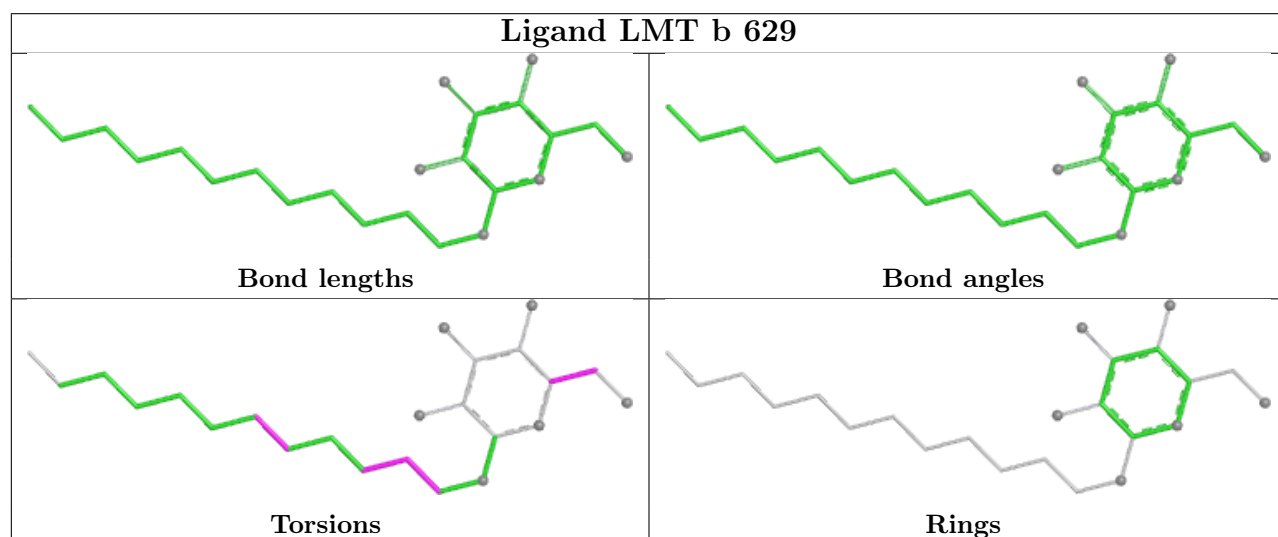
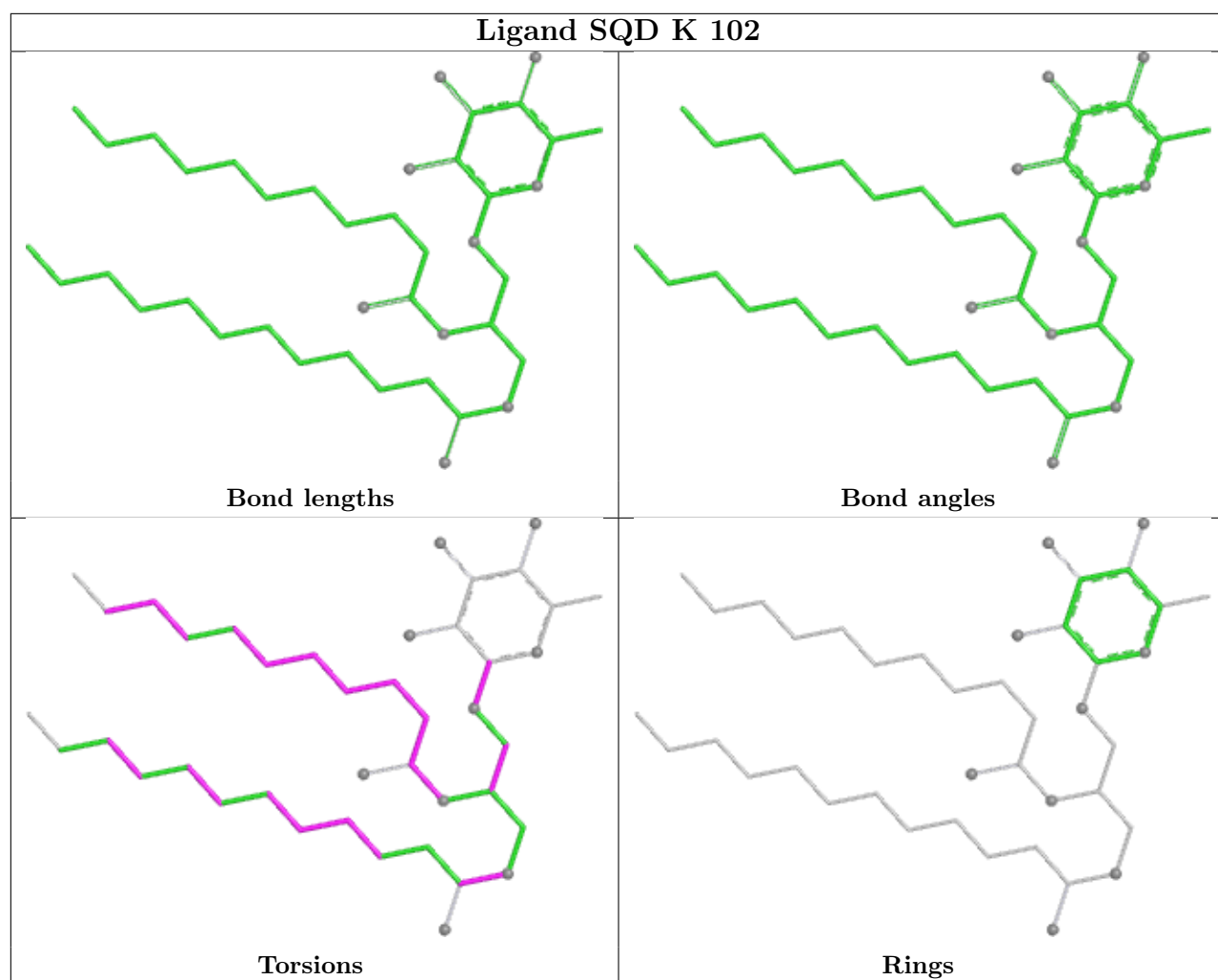
## Ligand RRX h 101

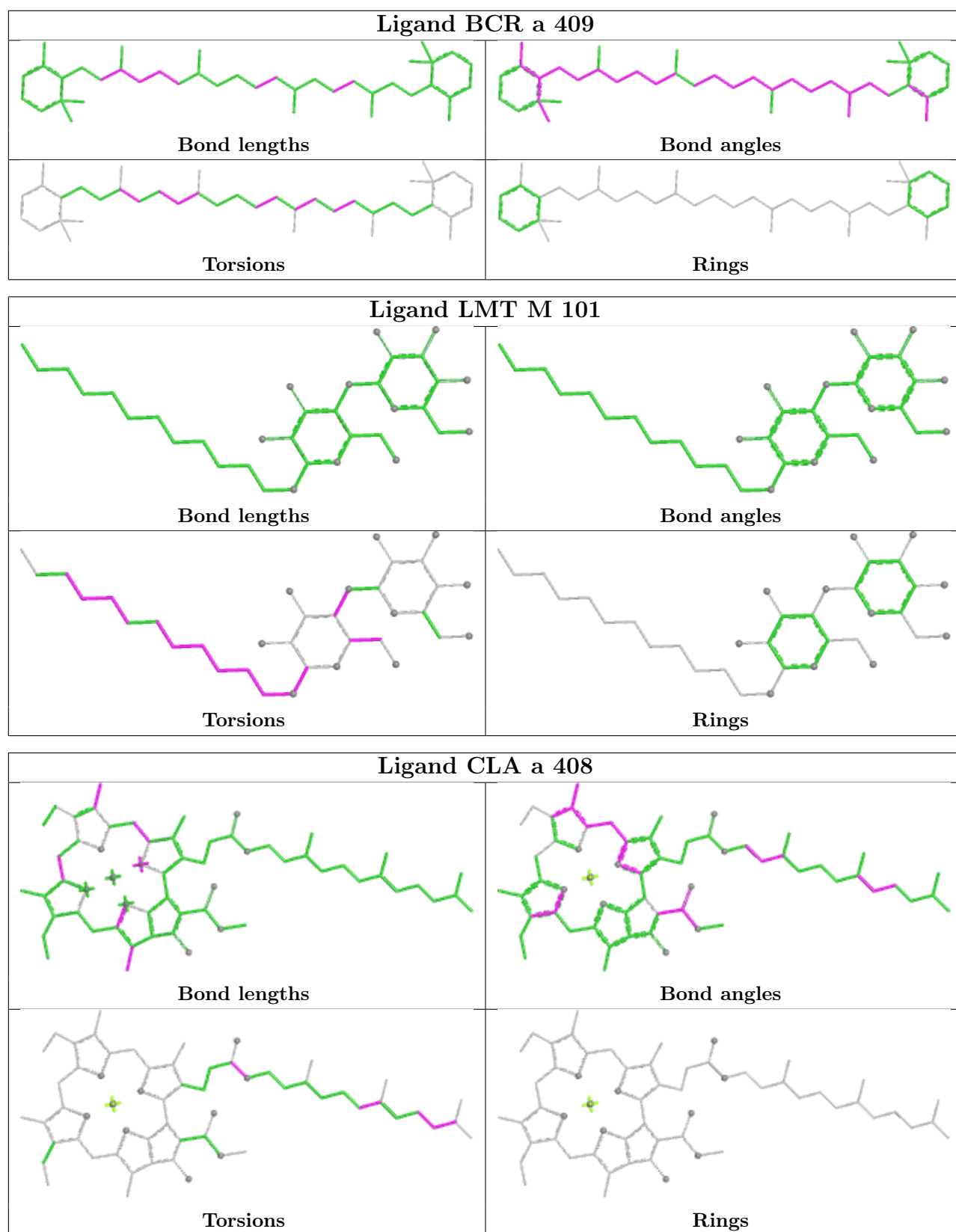


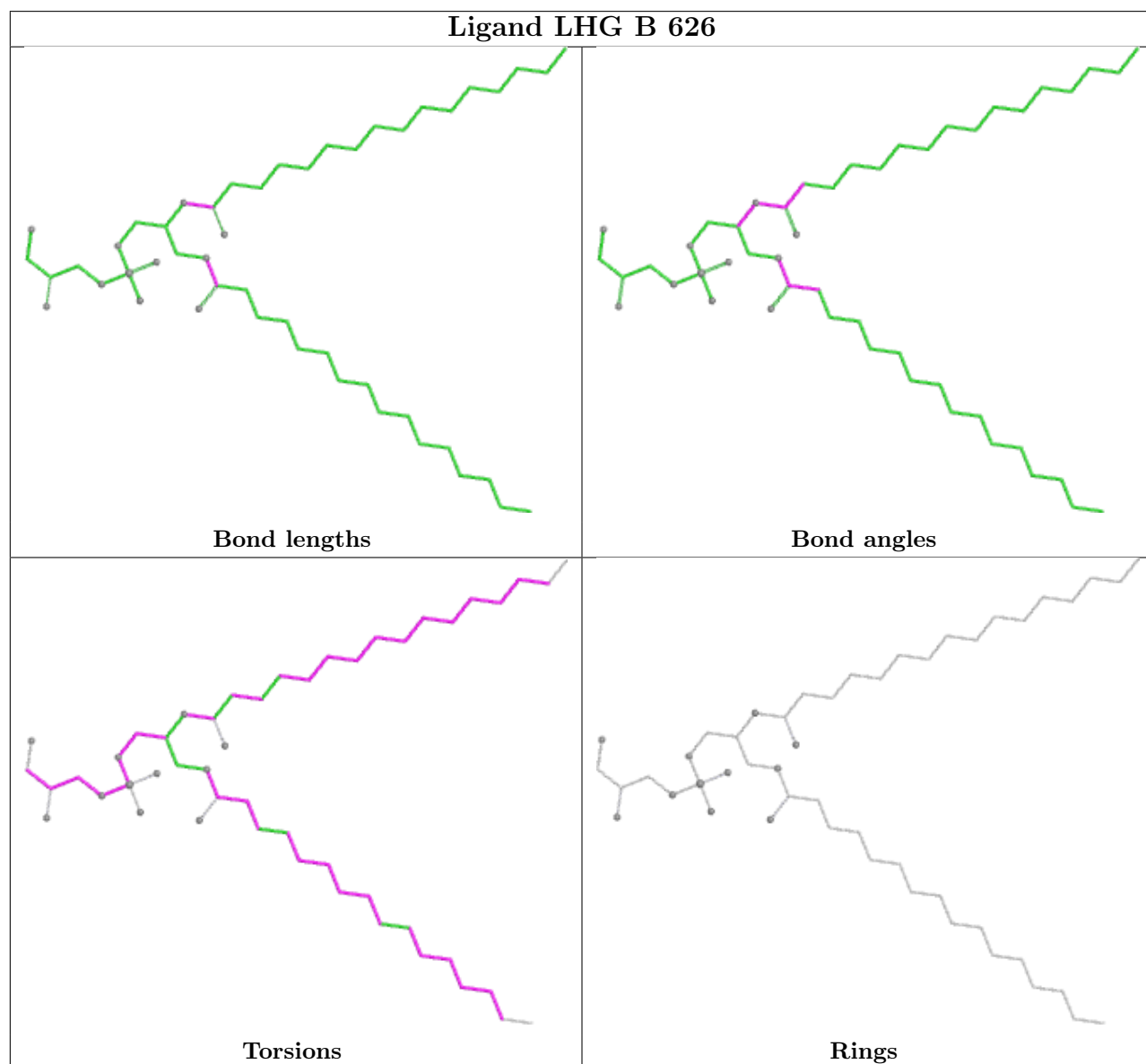
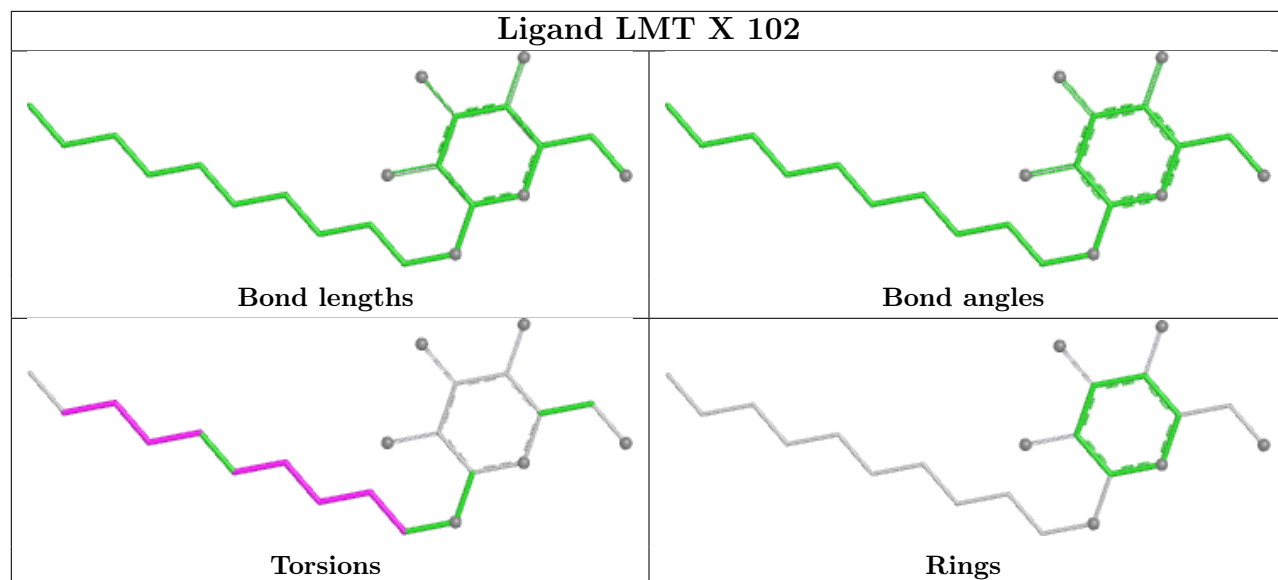


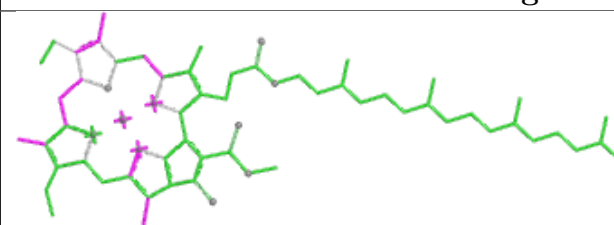
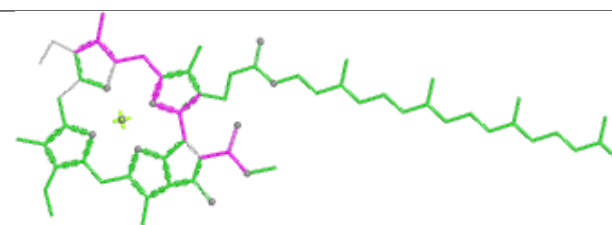
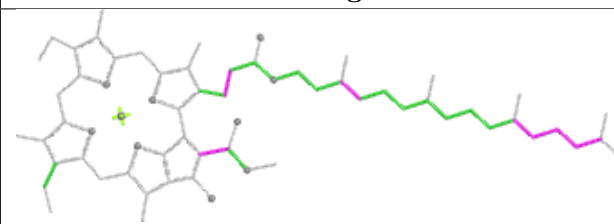
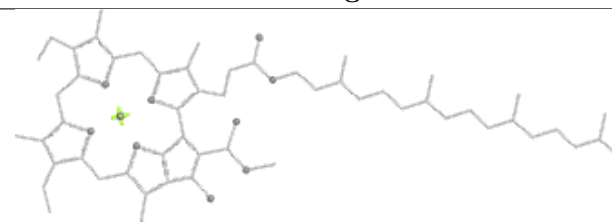




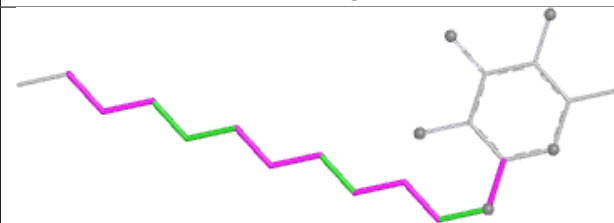
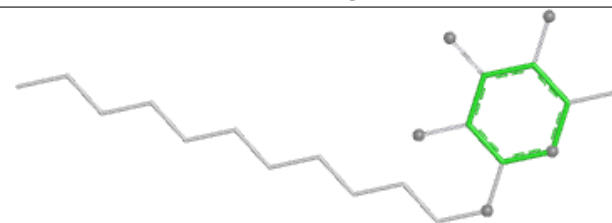


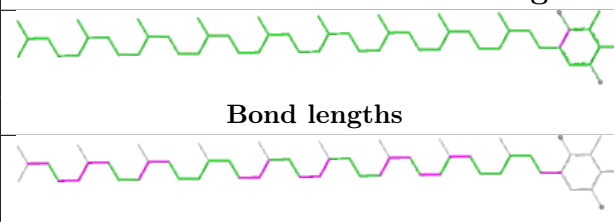
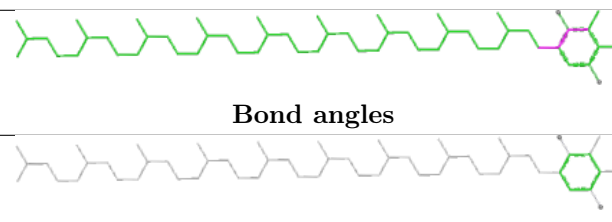
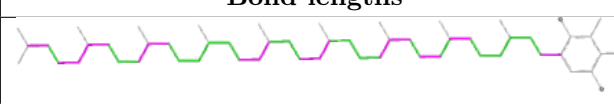
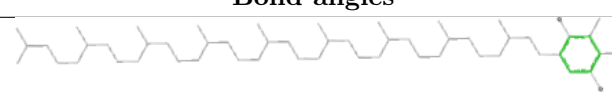




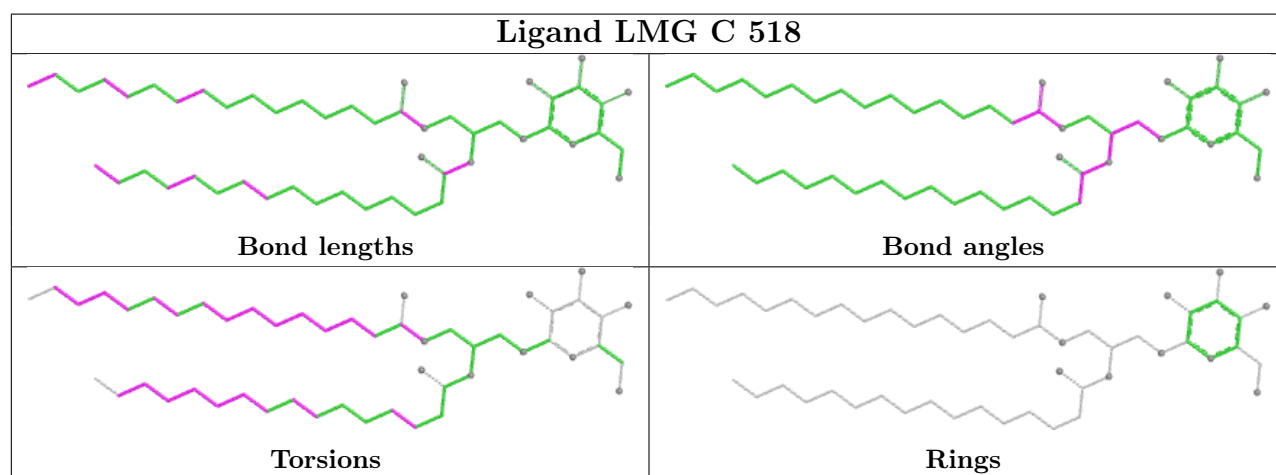
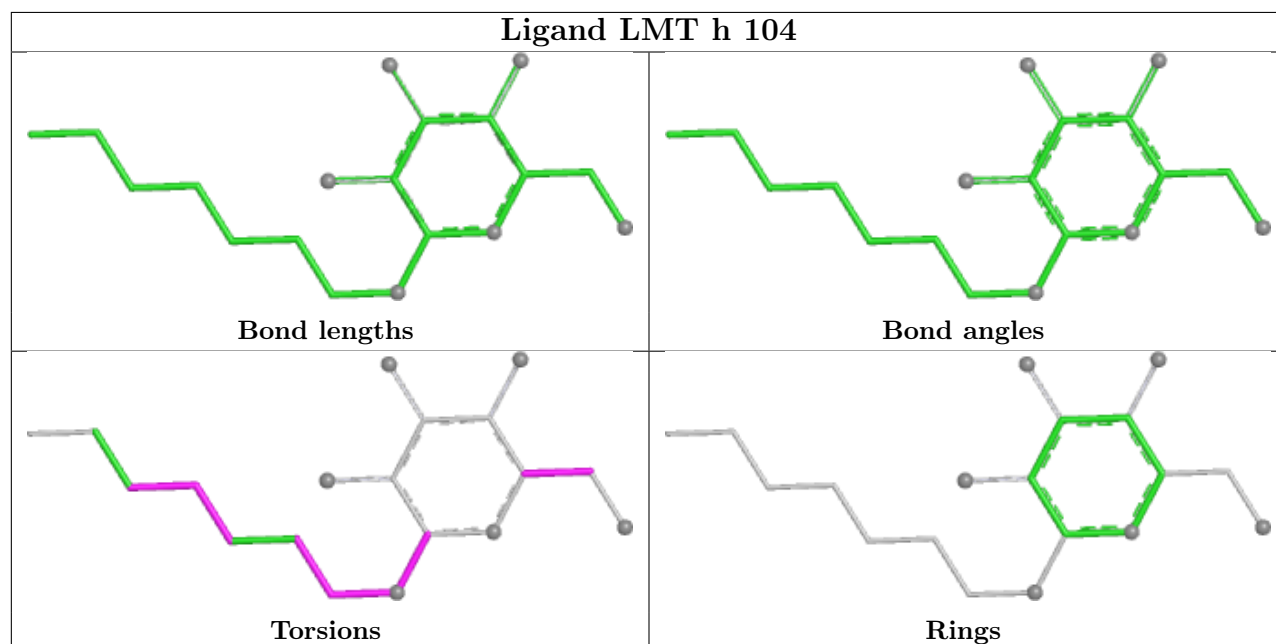
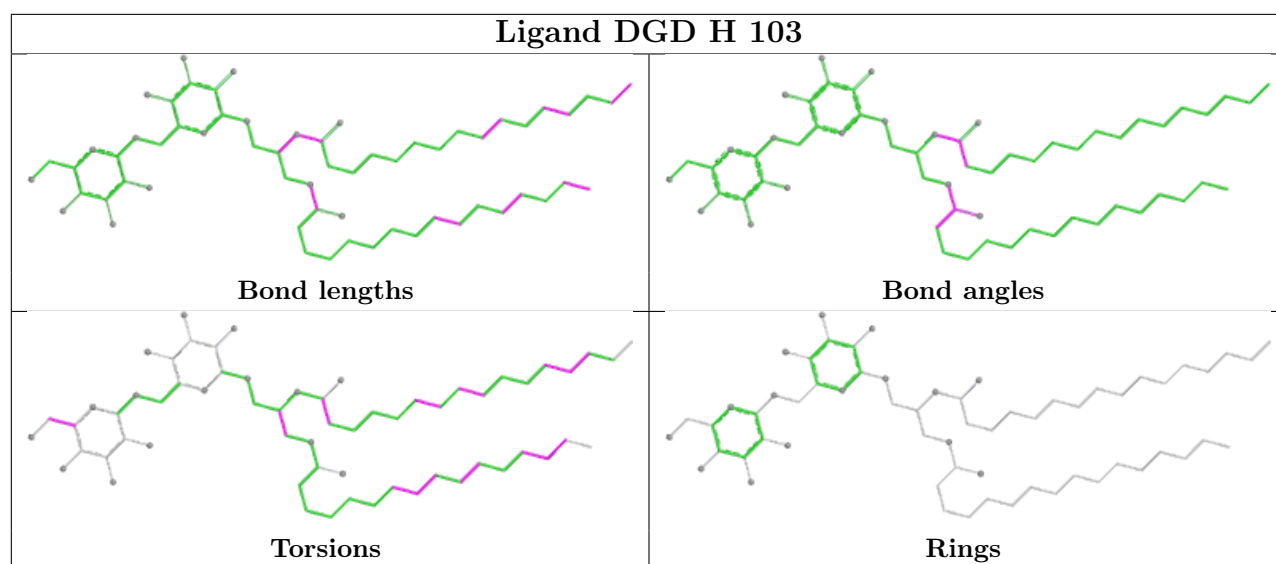


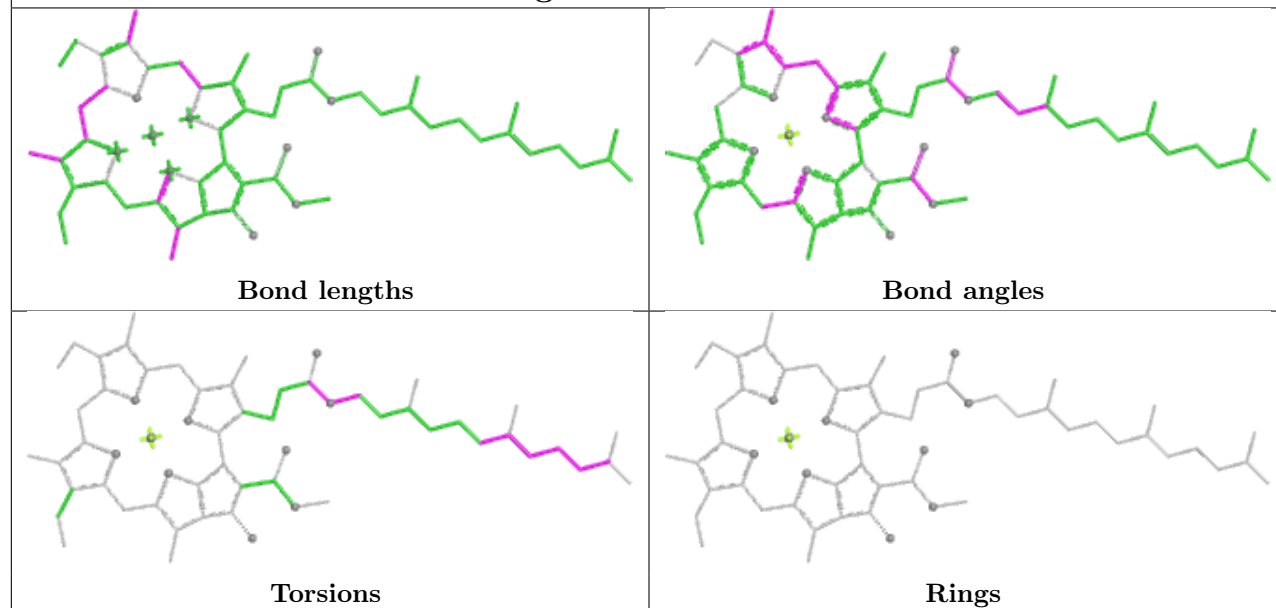
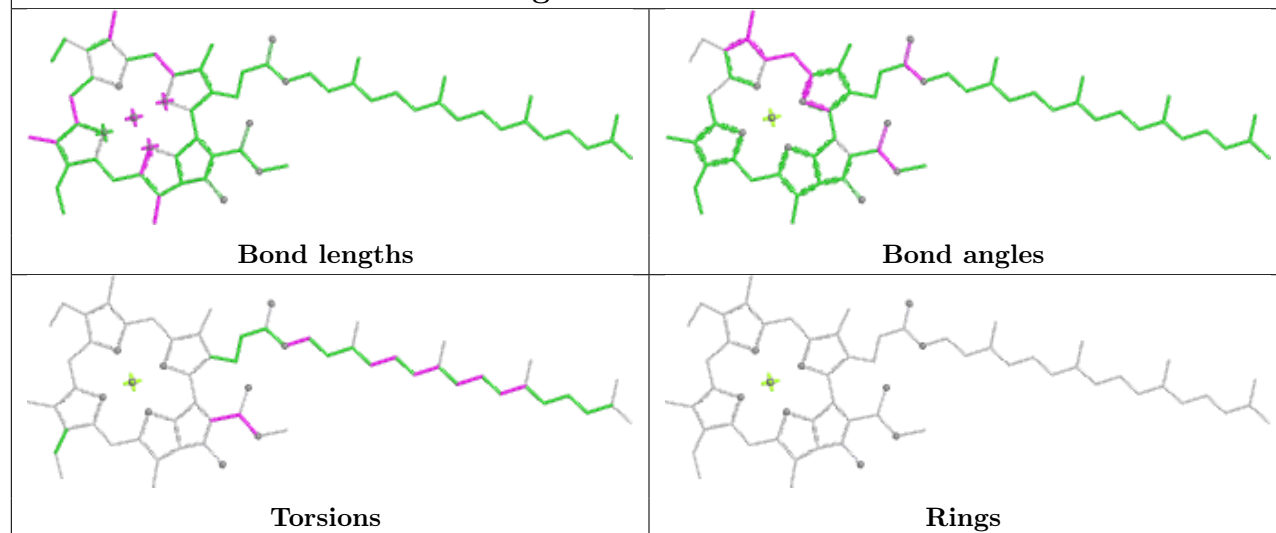
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

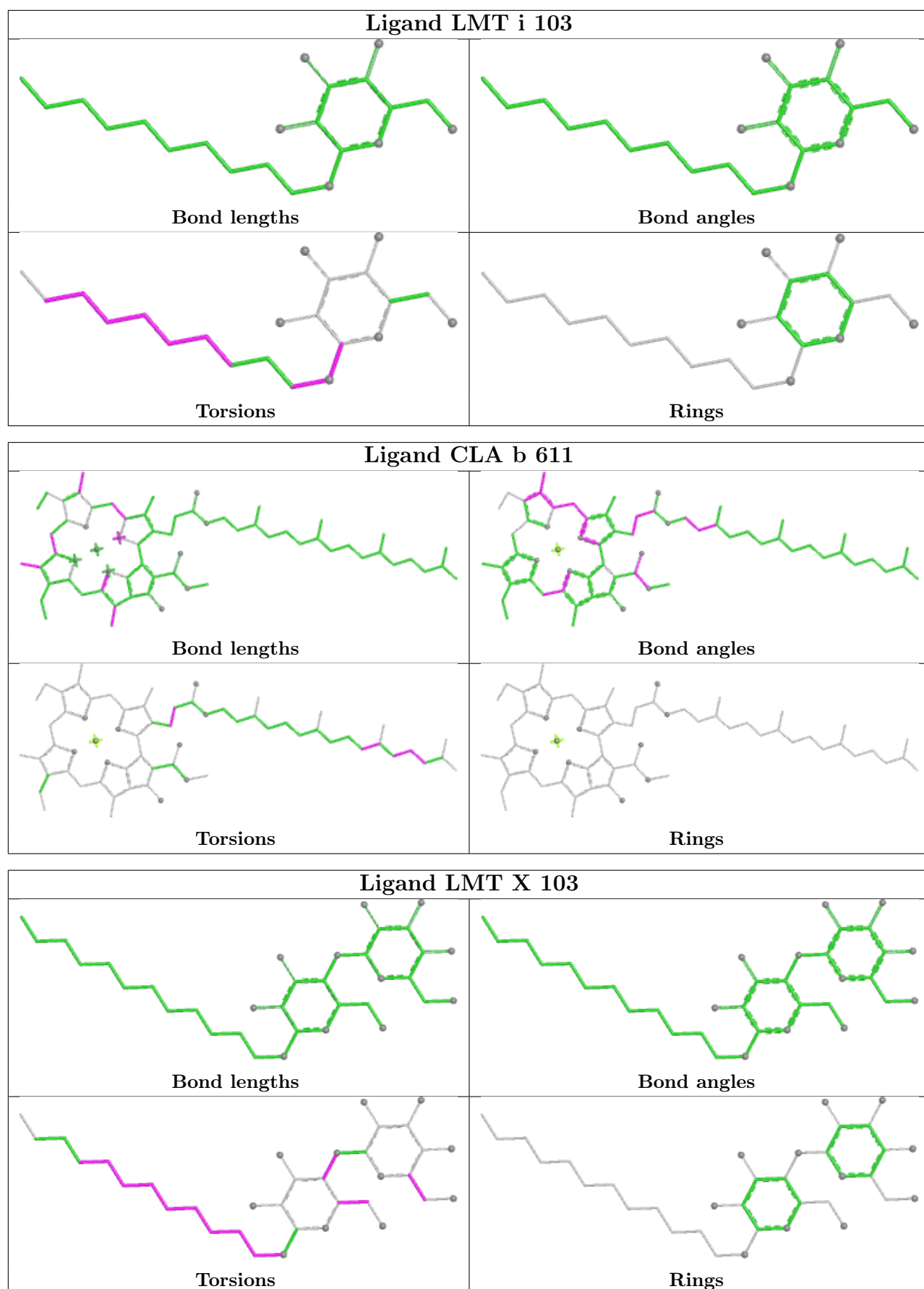
Ligand LMT X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

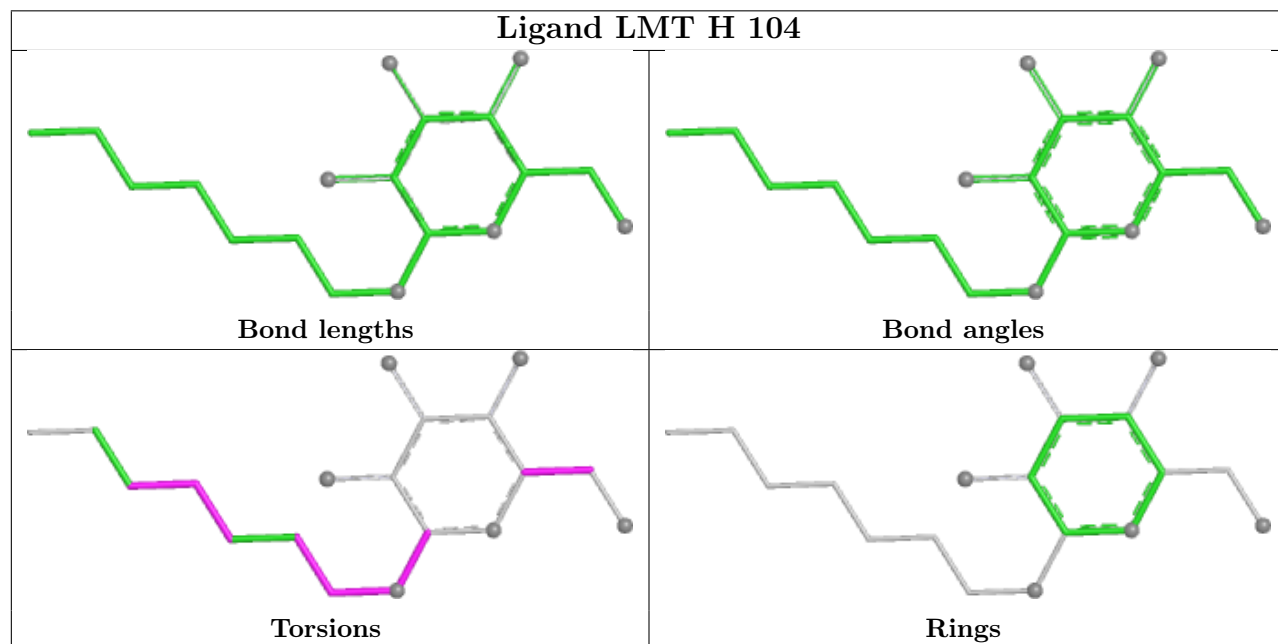
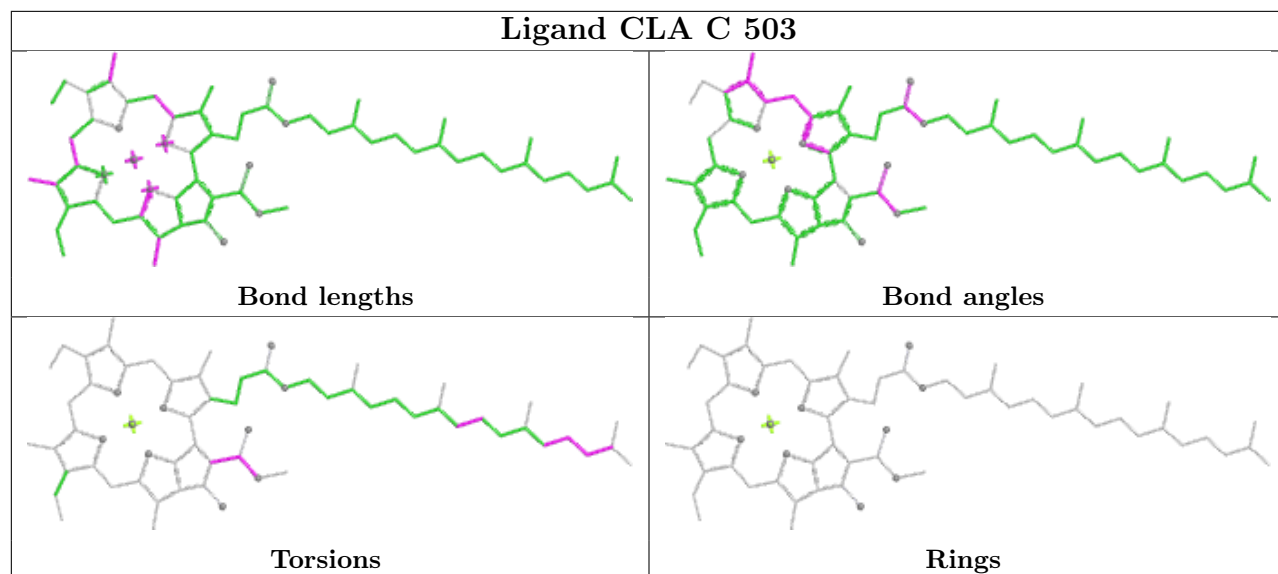
Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

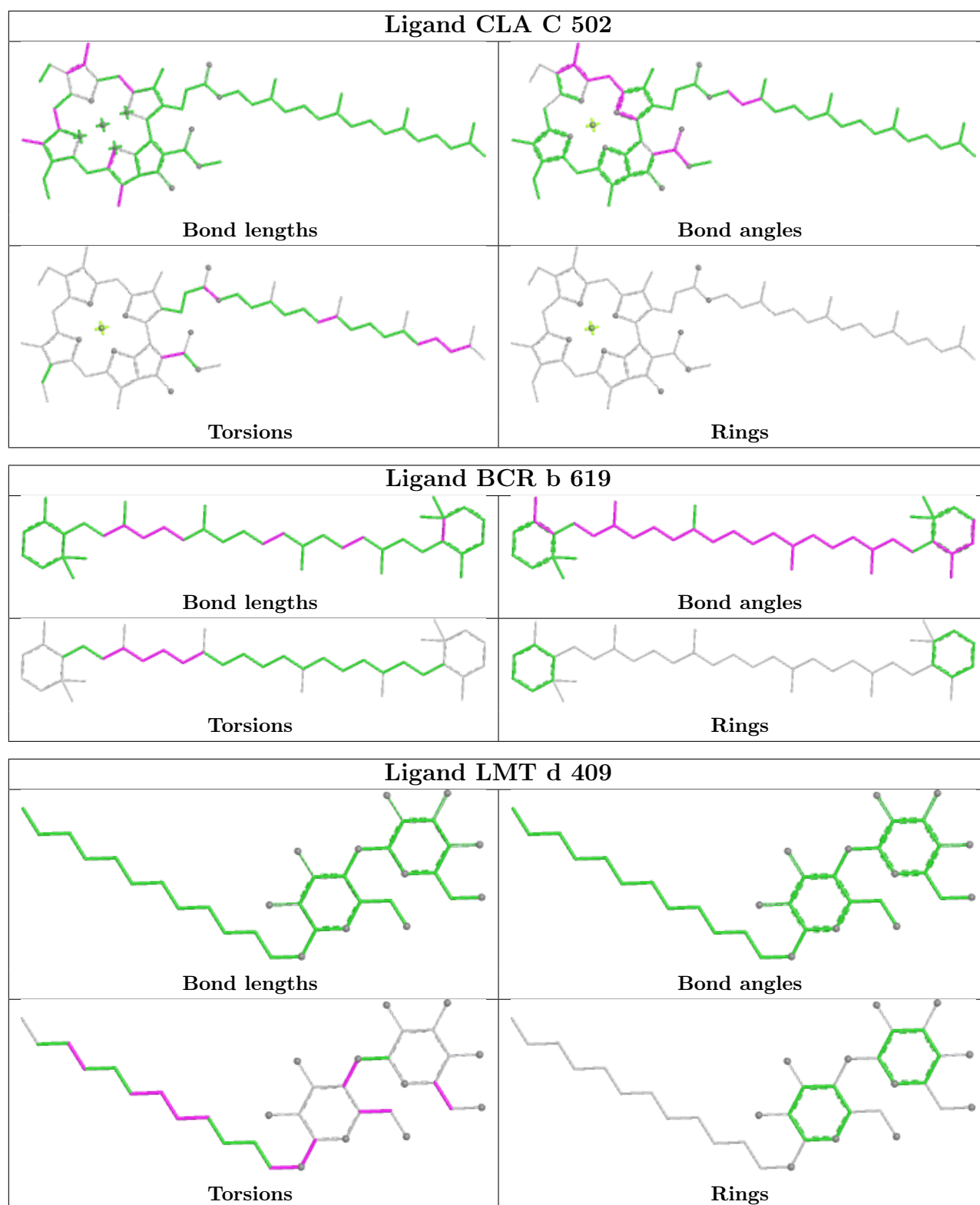


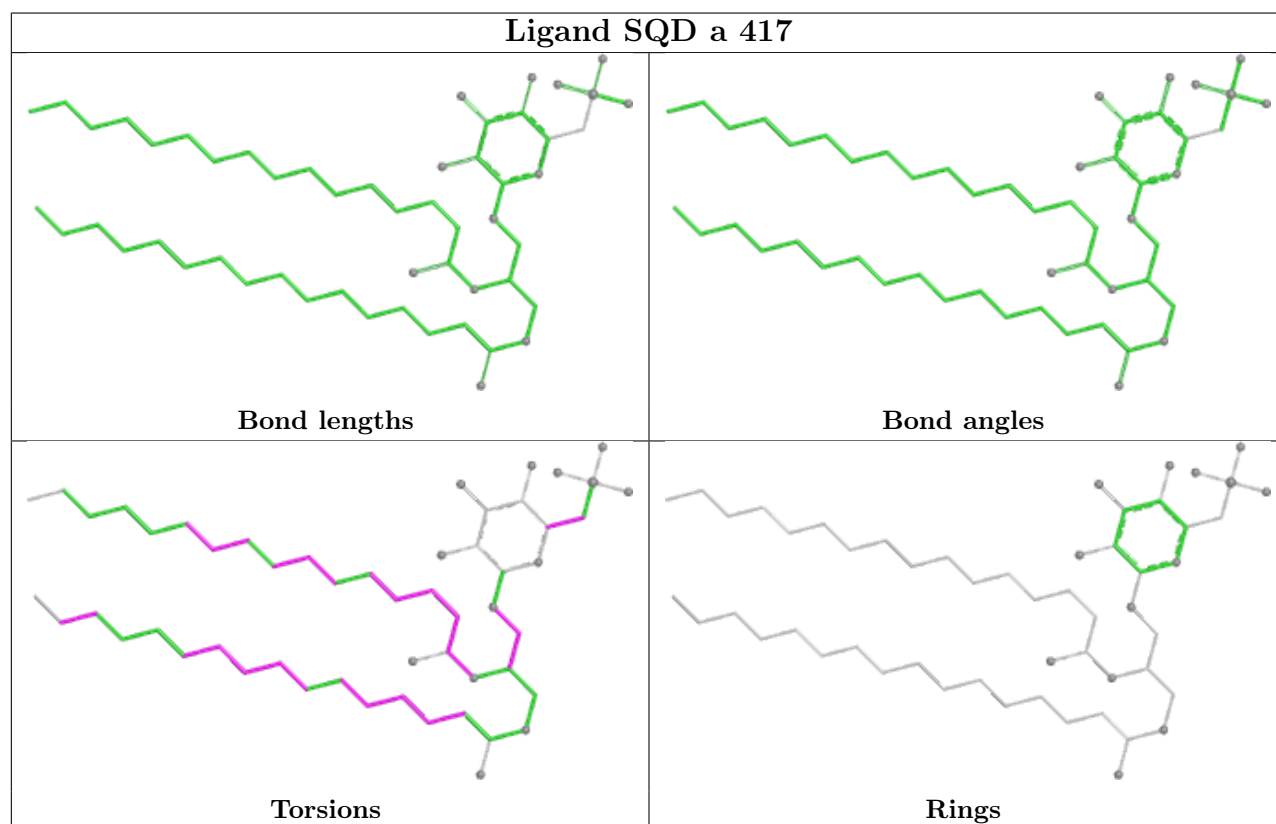
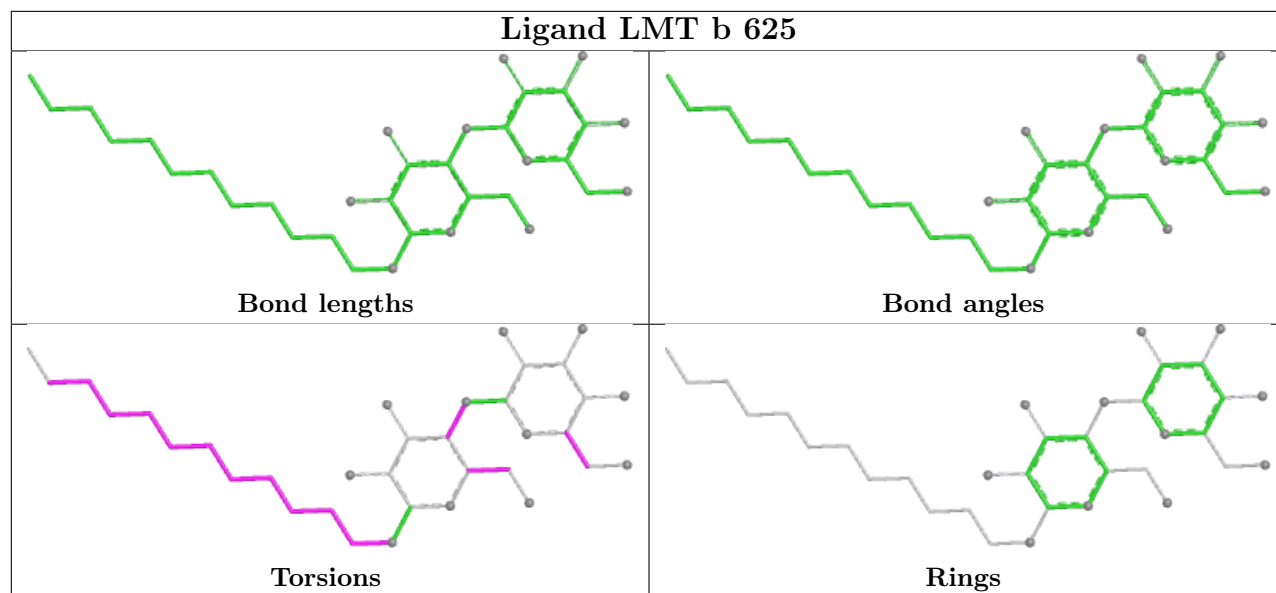


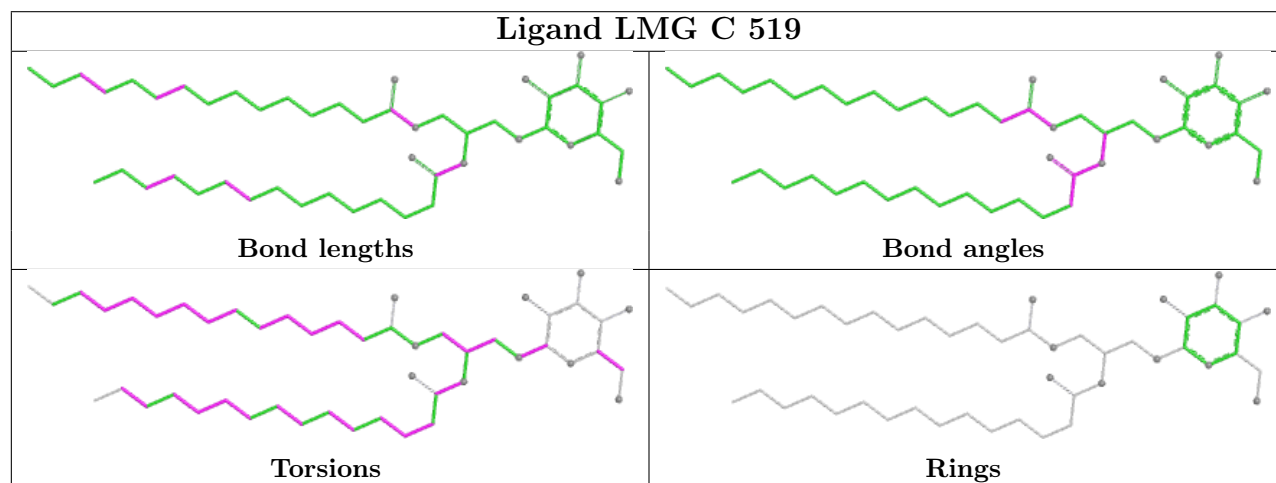
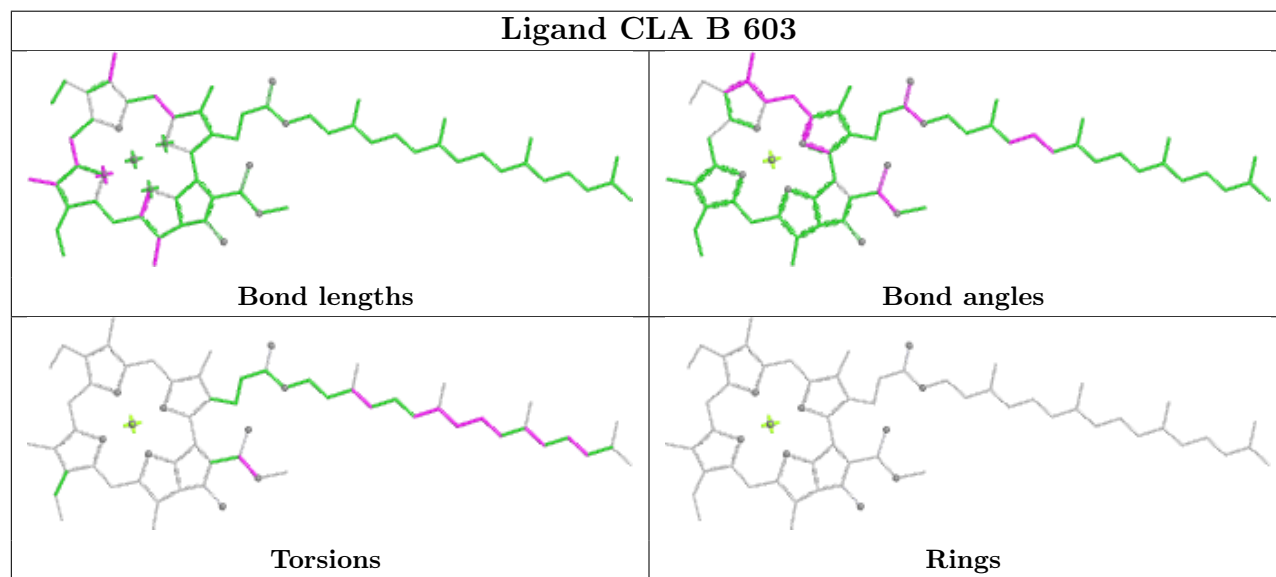
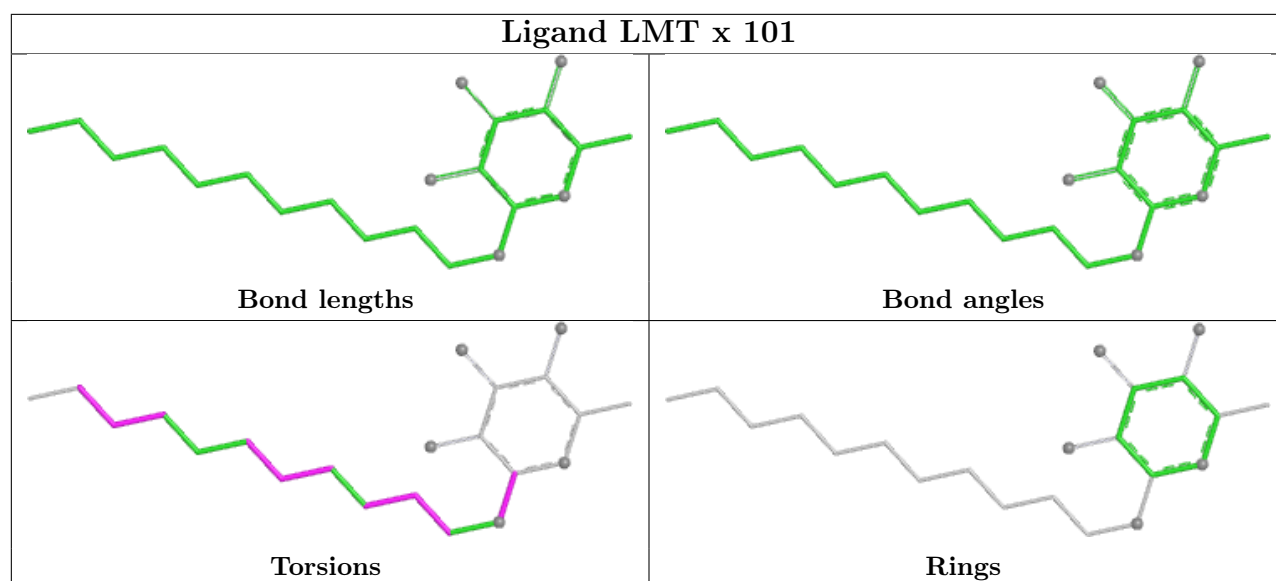
**Ligand CLA b 617****Ligand CLA C 509**

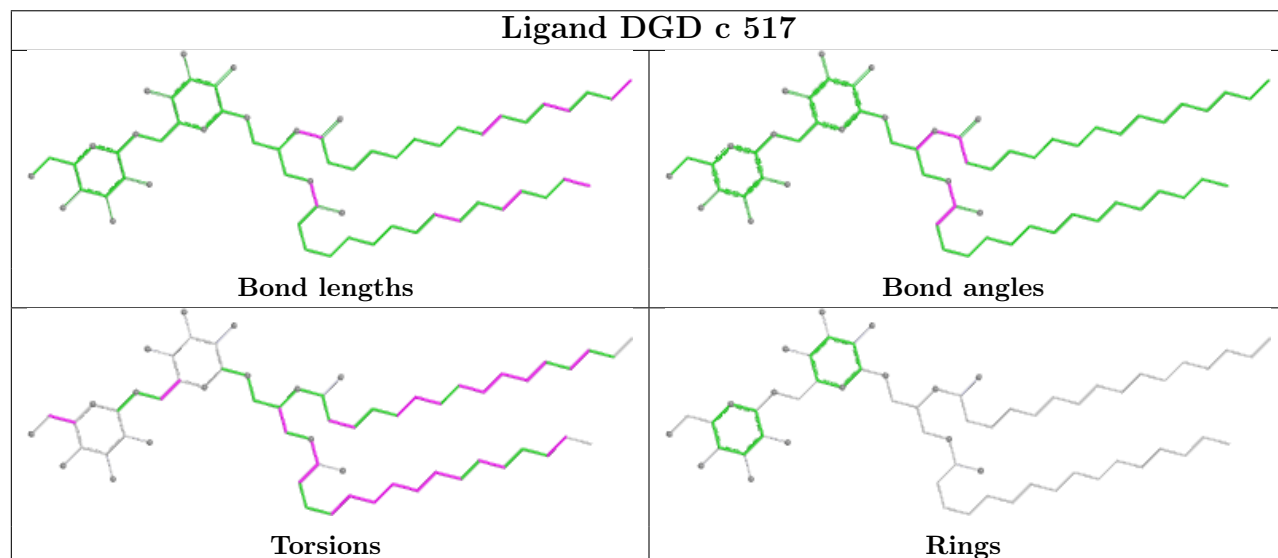
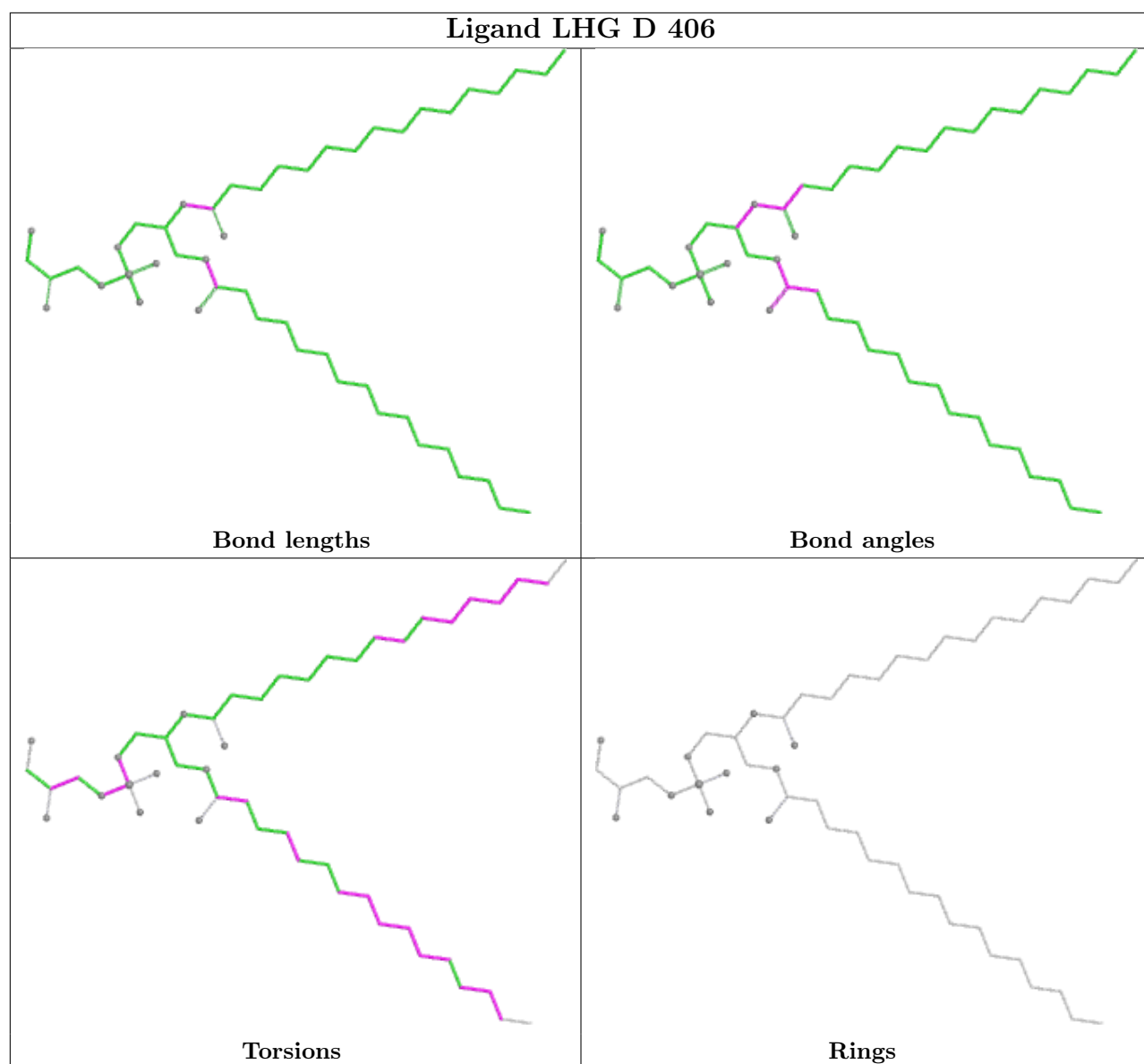




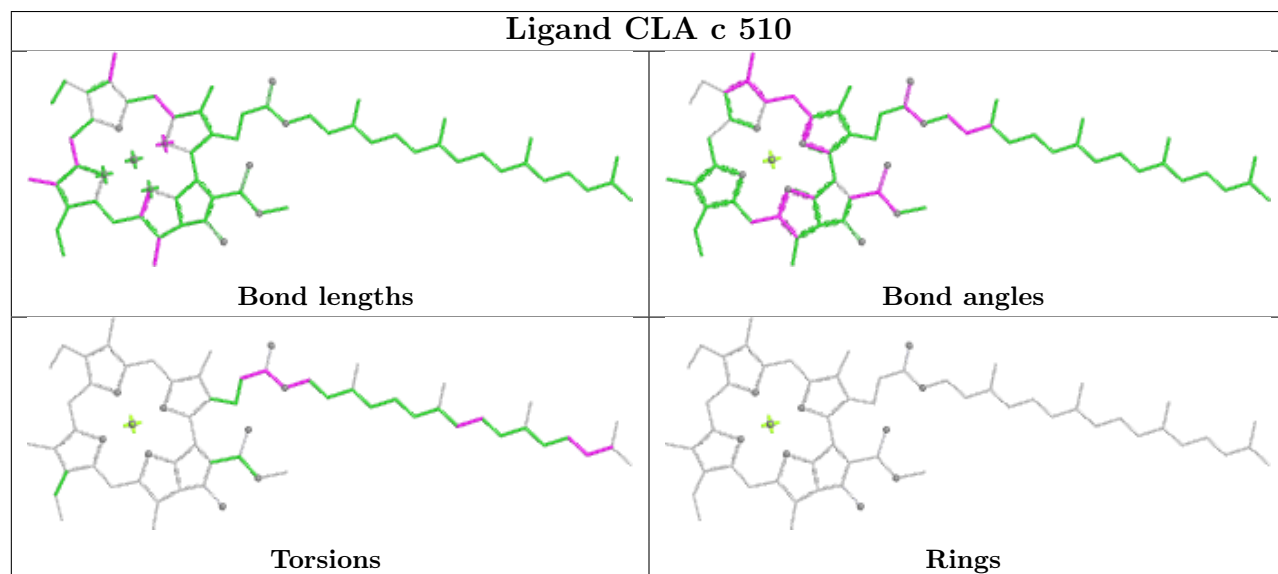
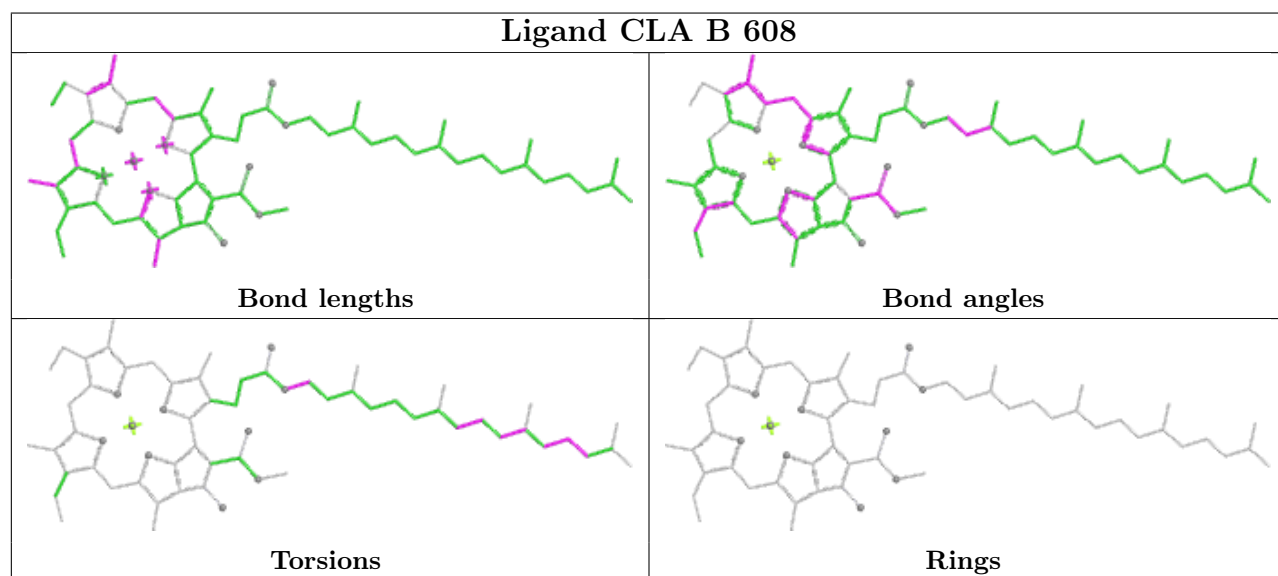
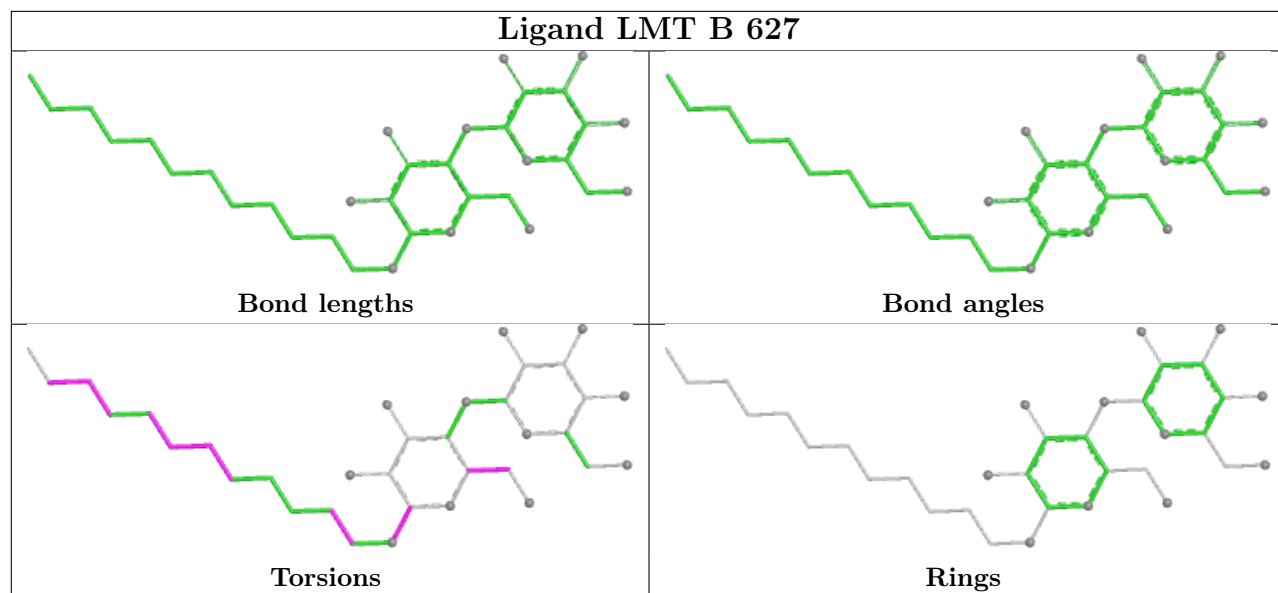


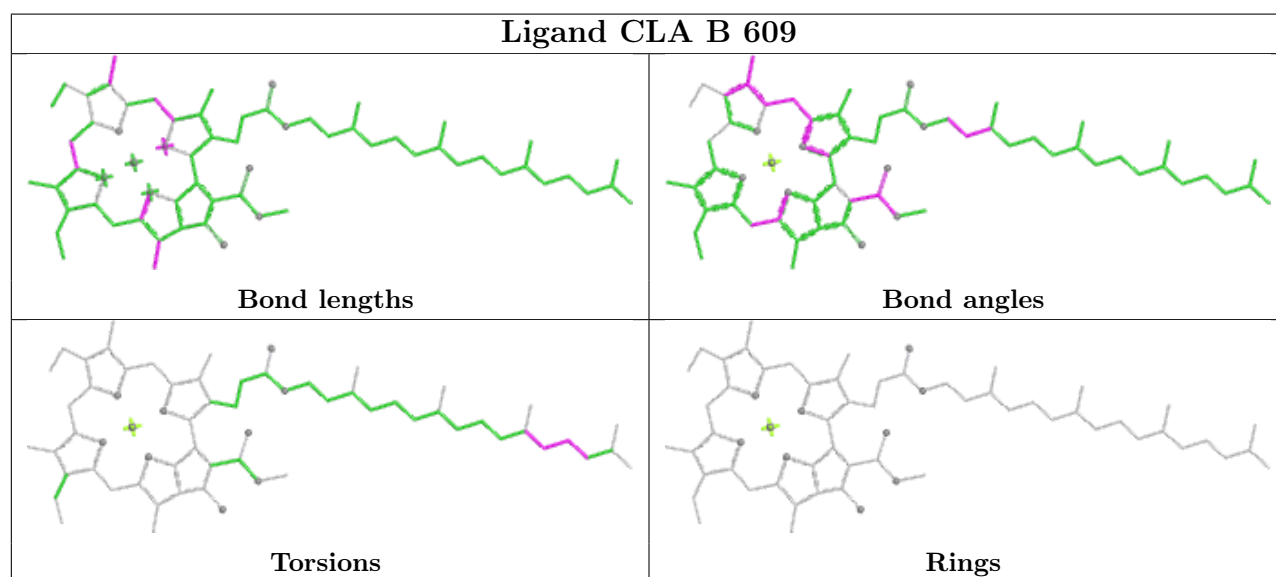
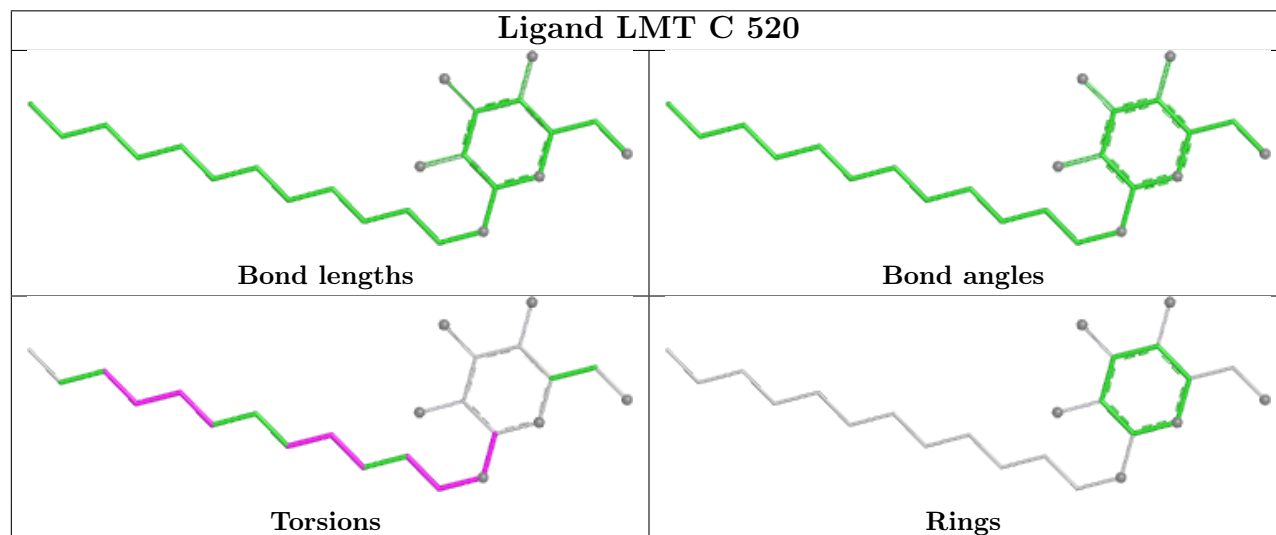
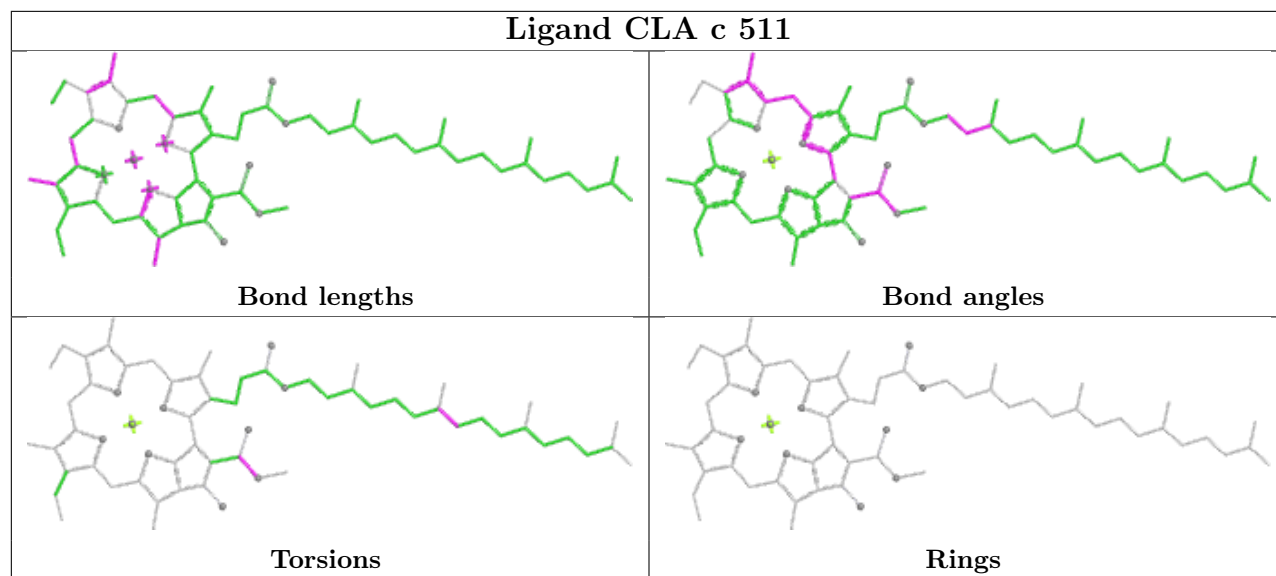


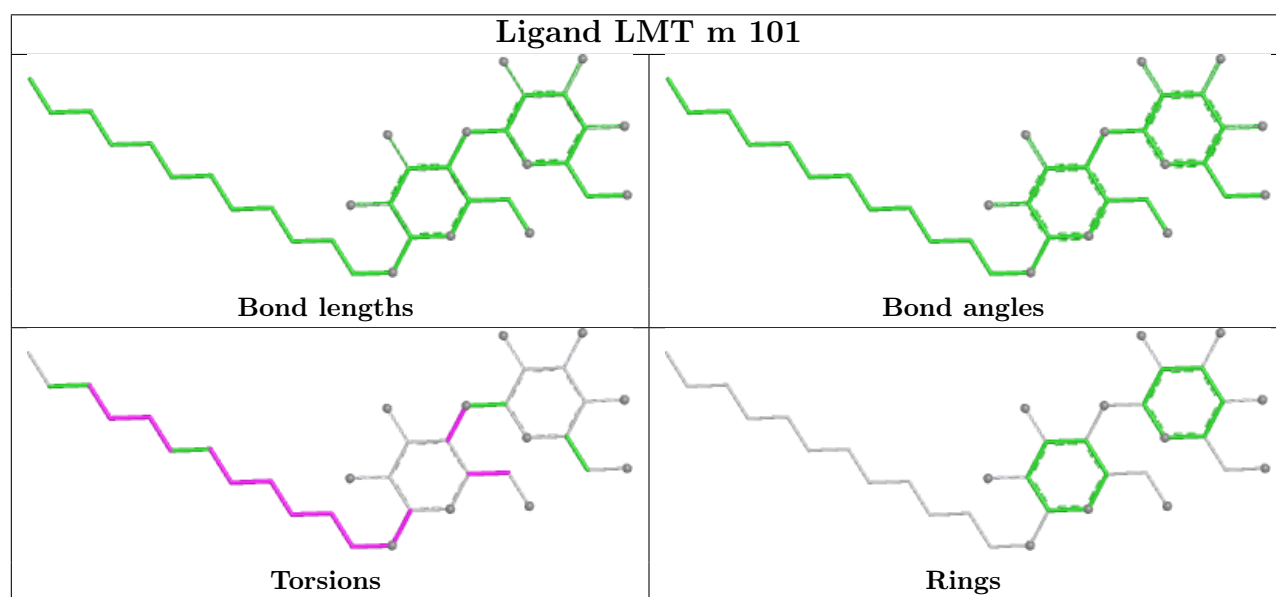
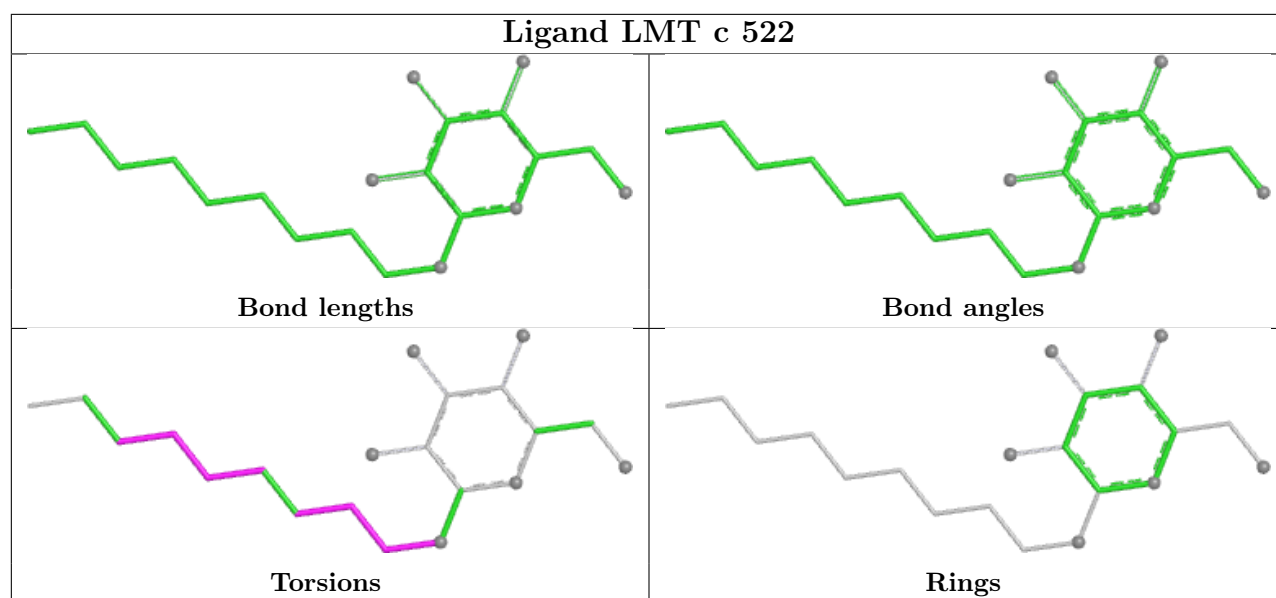


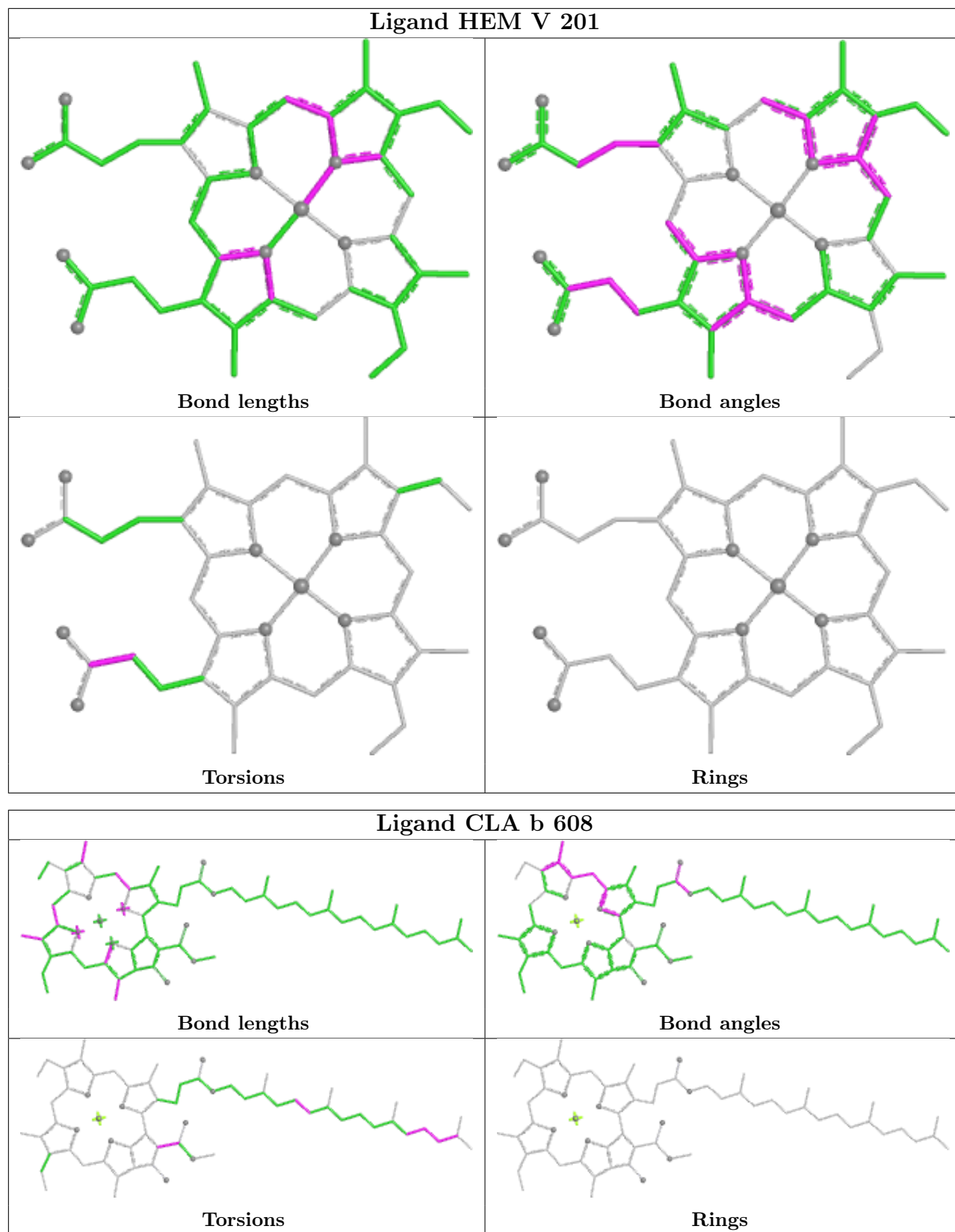


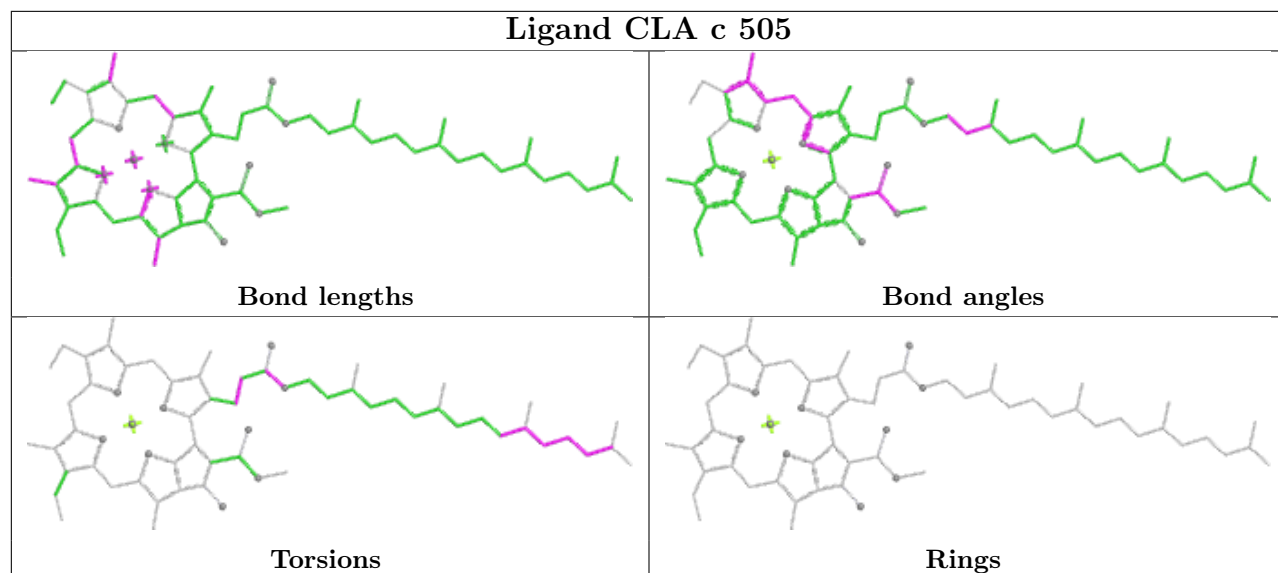
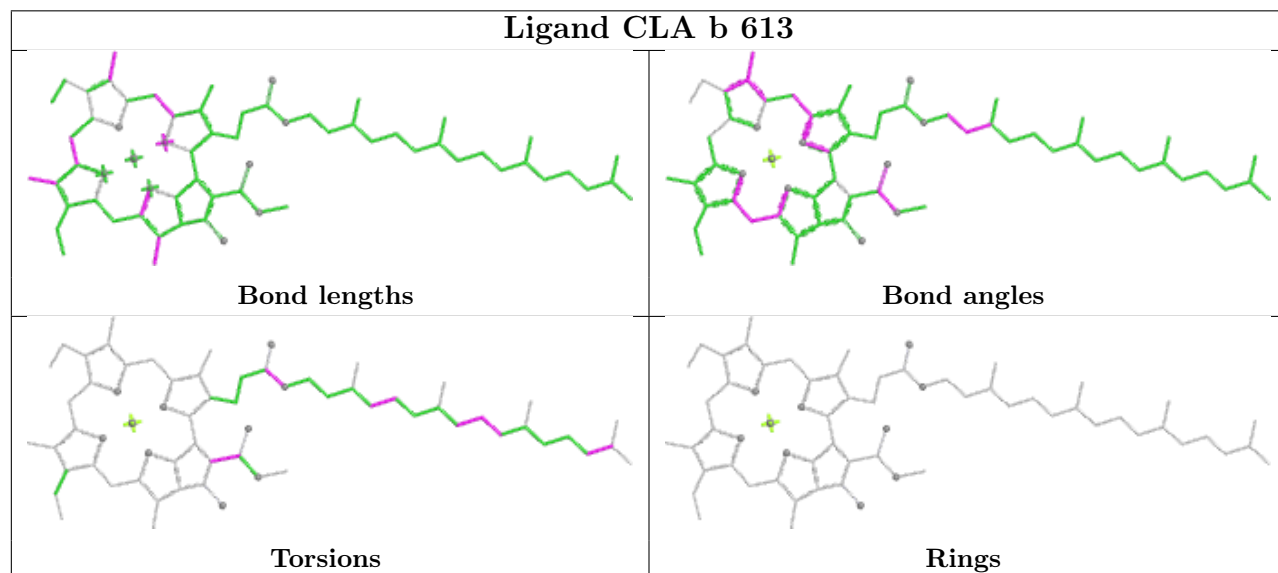
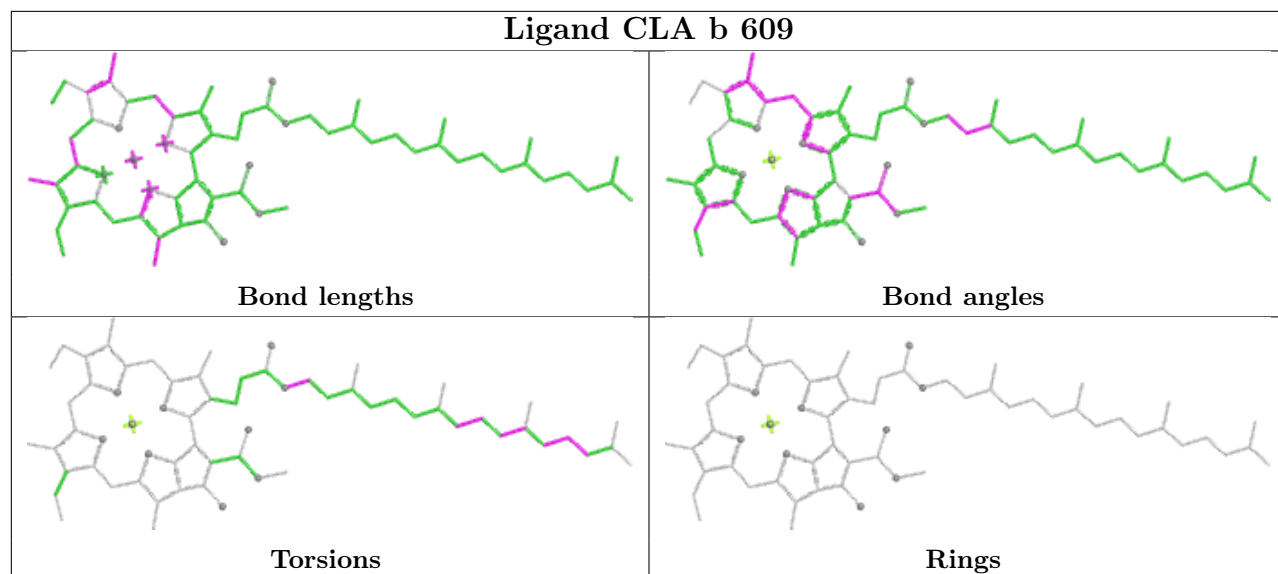


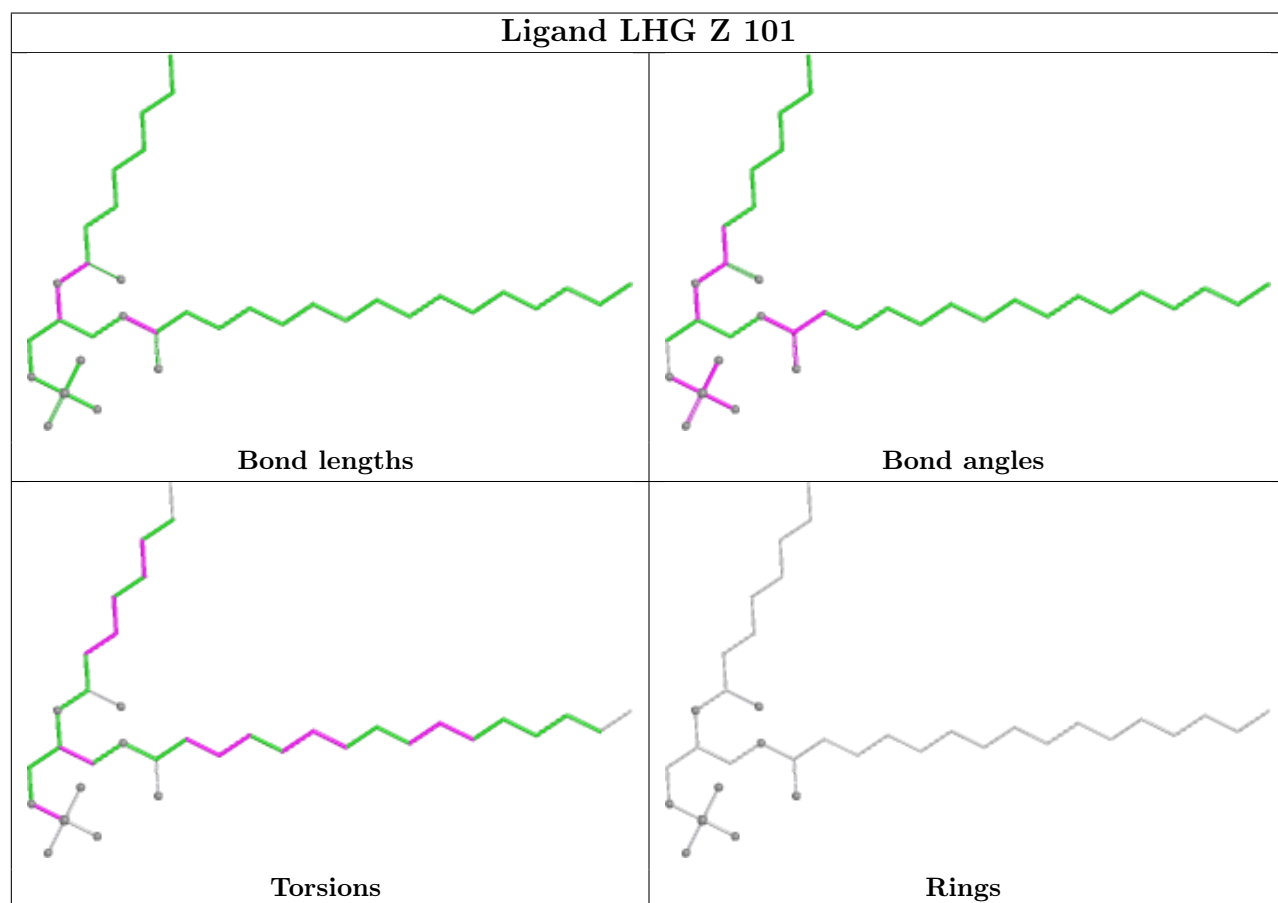
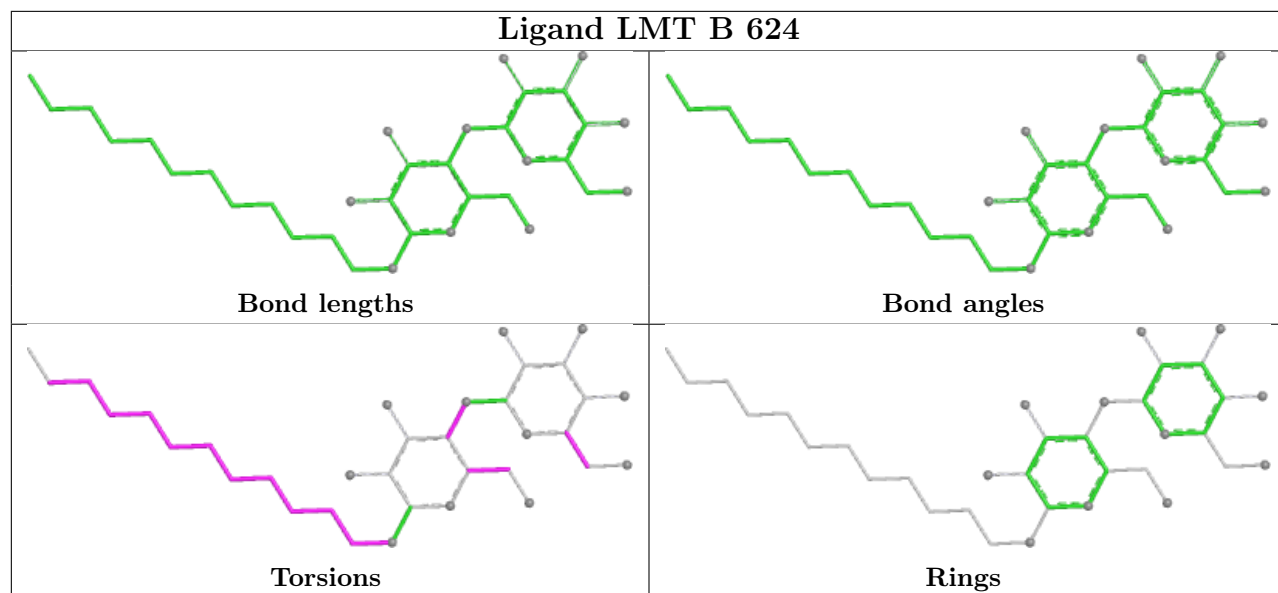


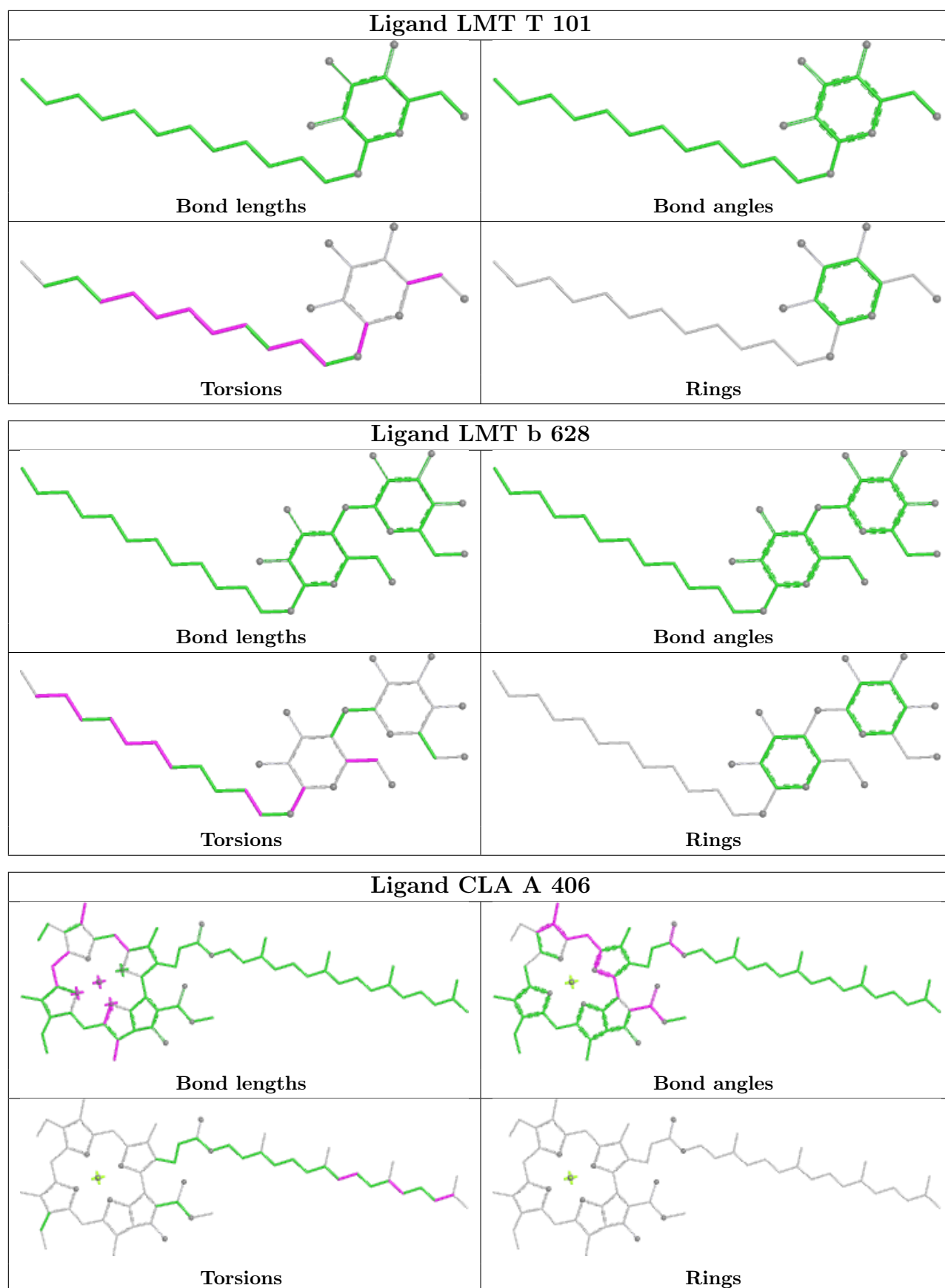


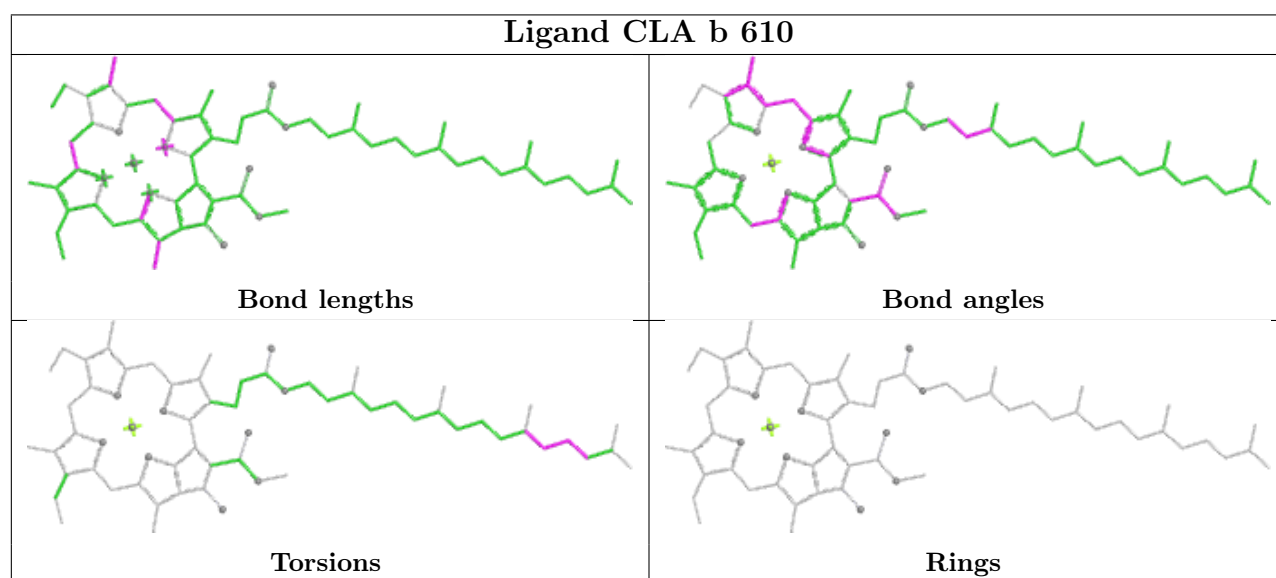
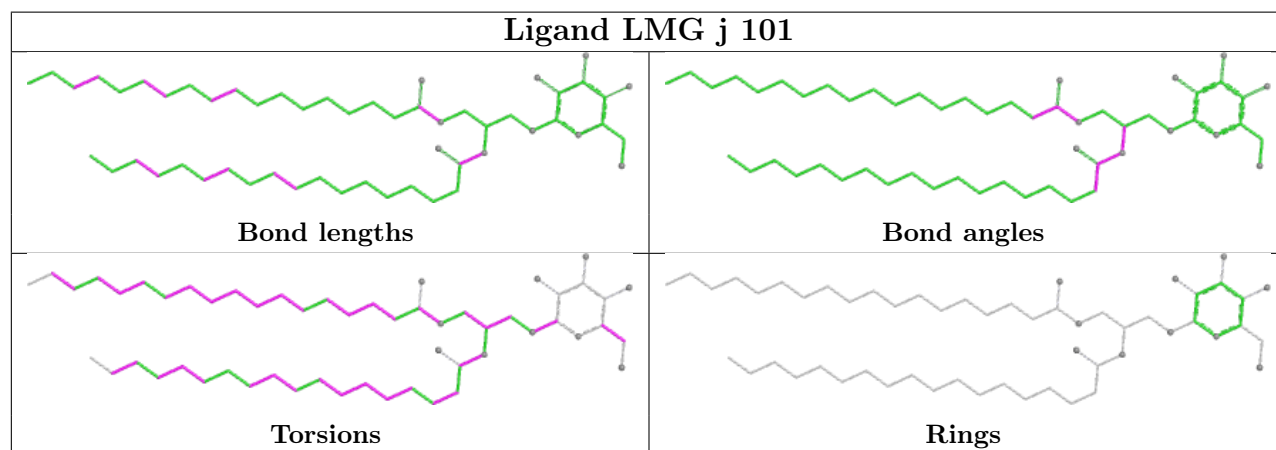
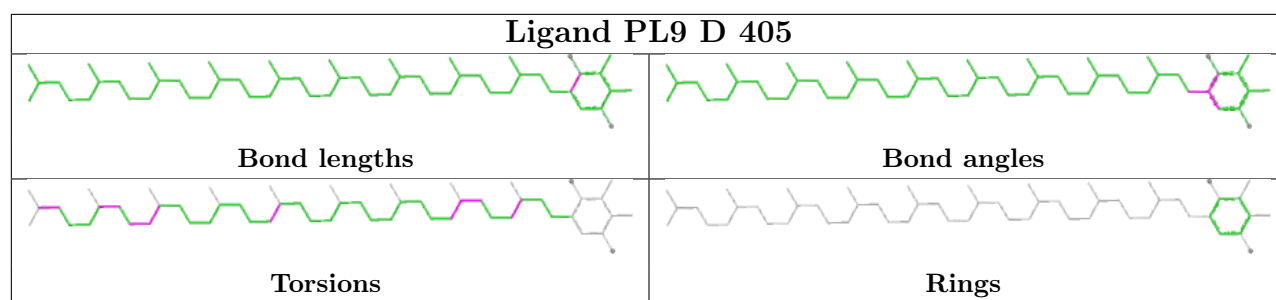




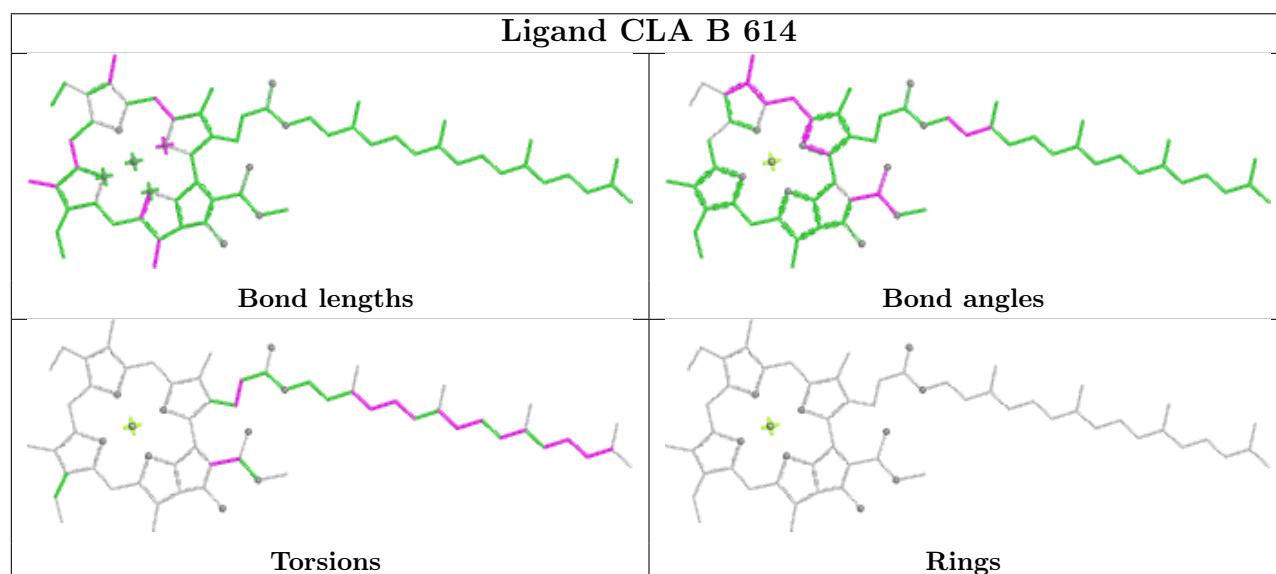
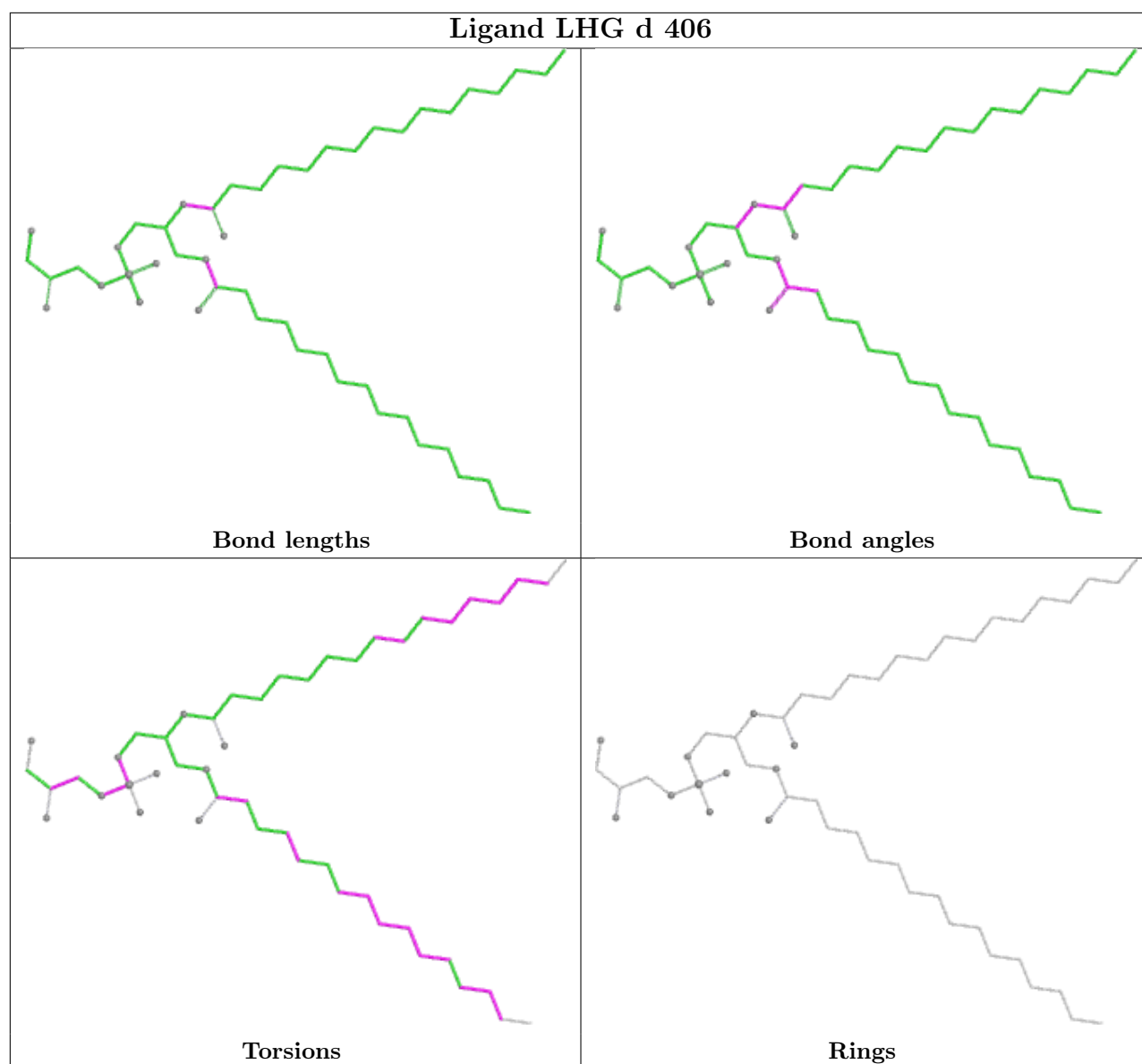


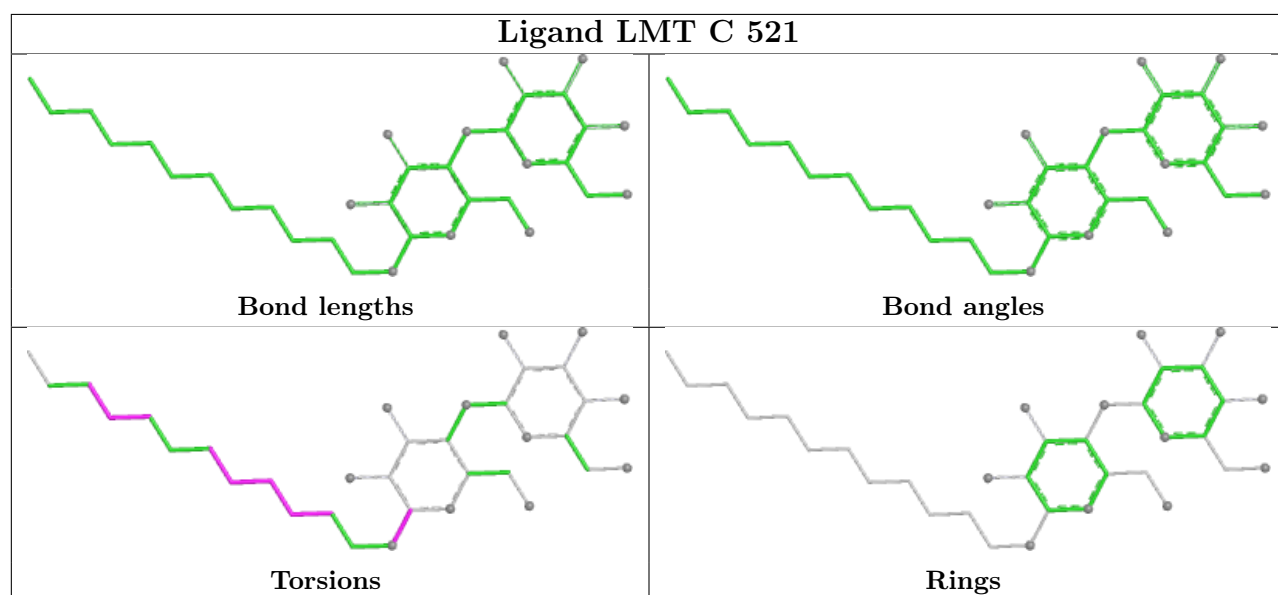
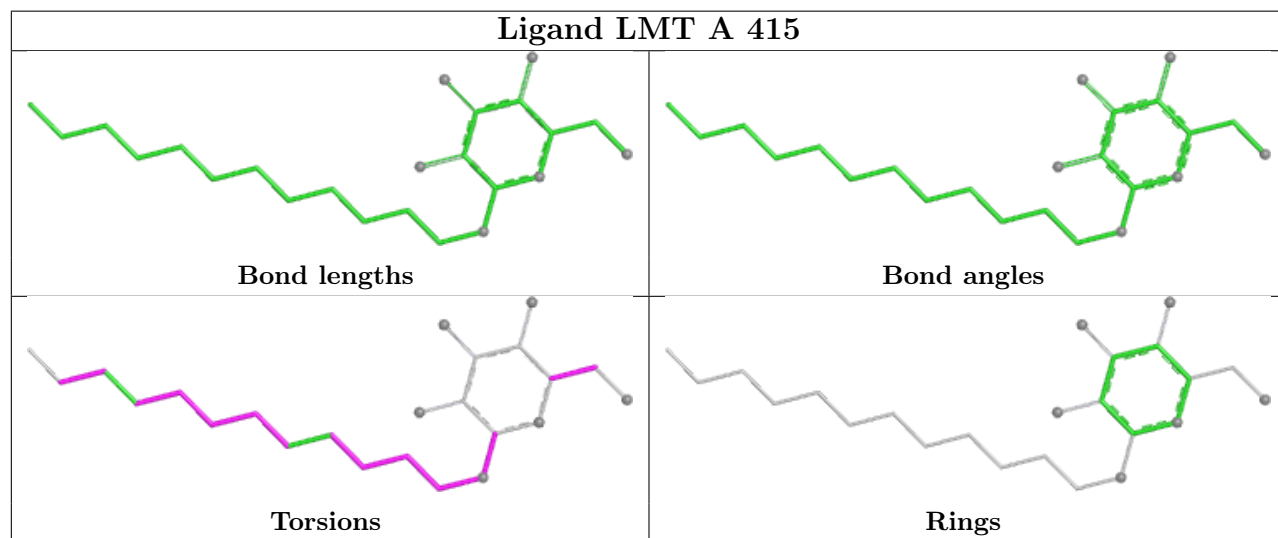
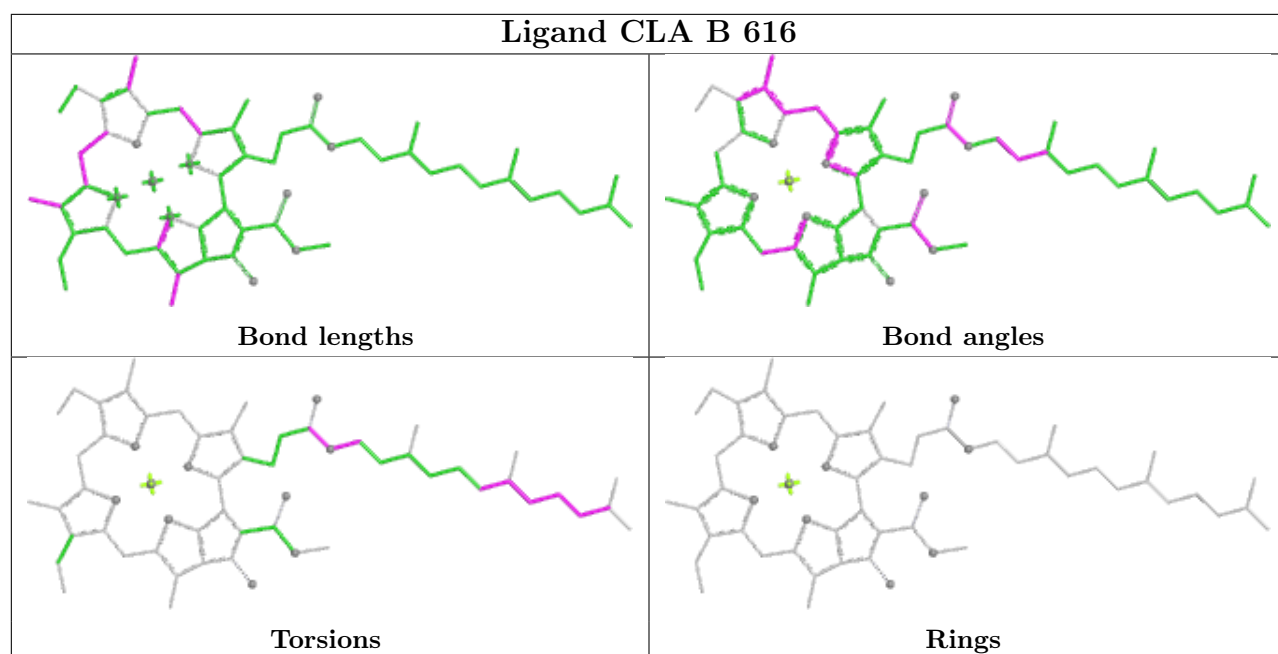


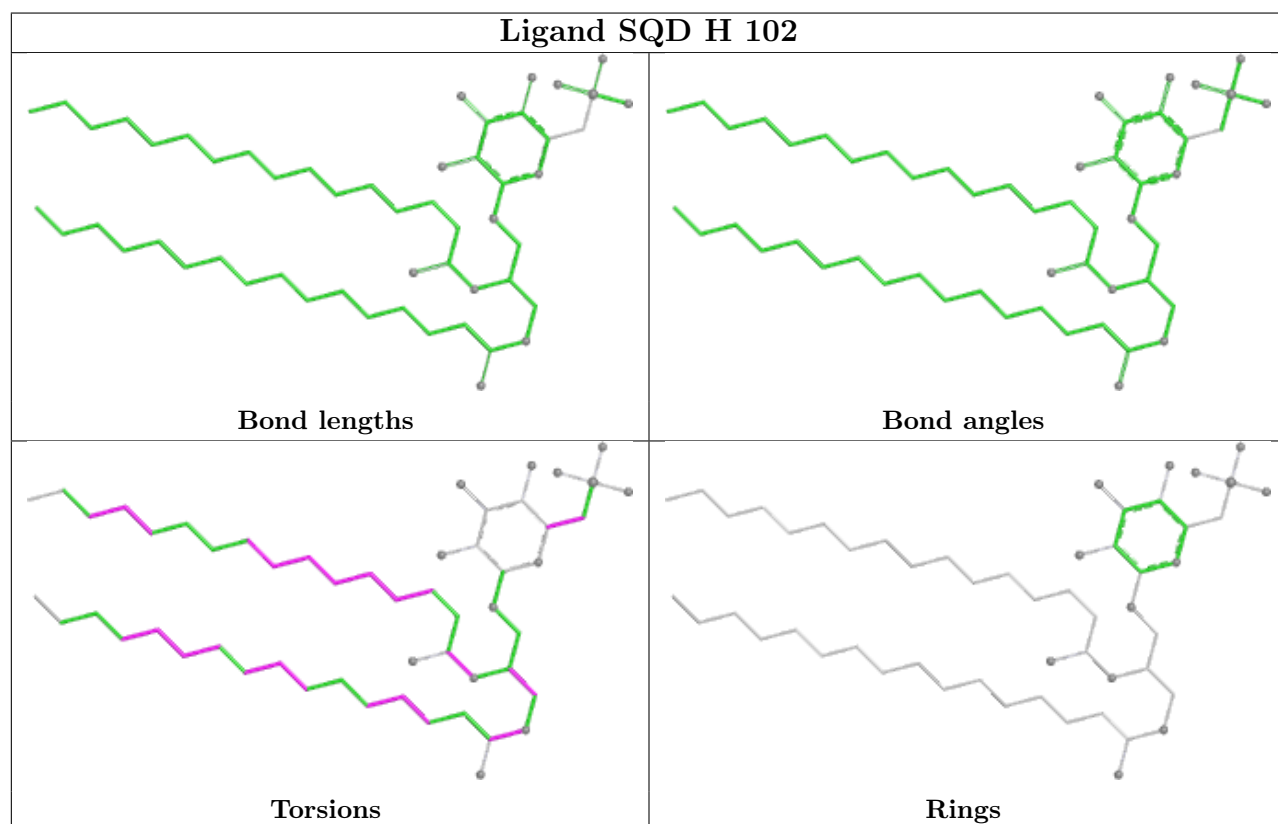
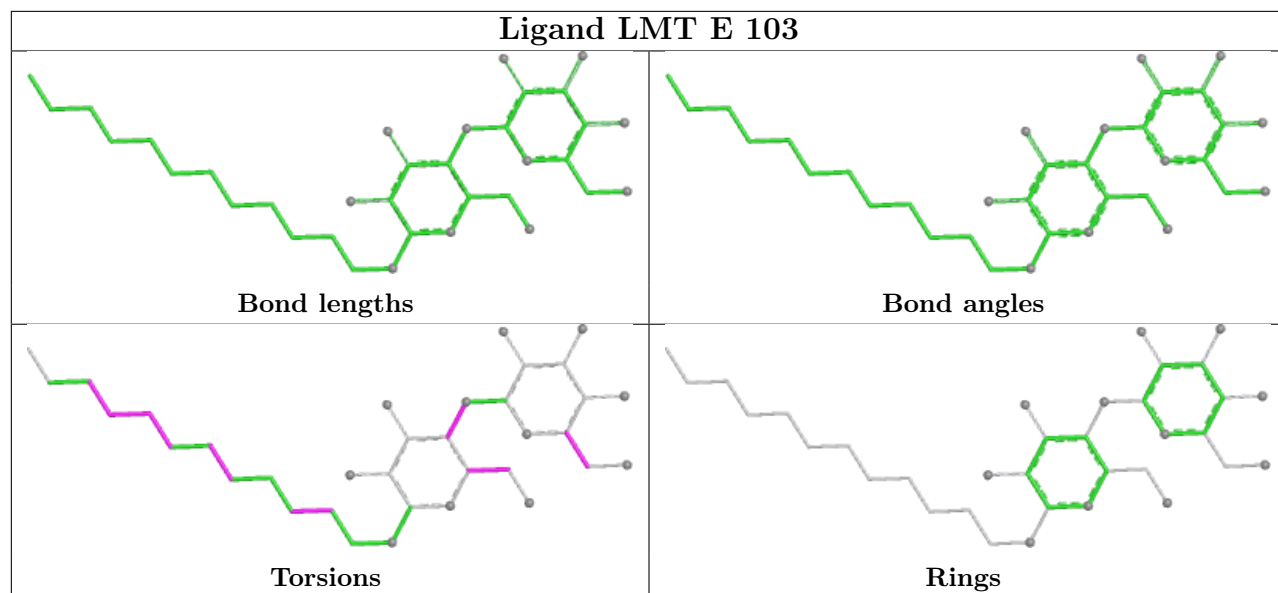


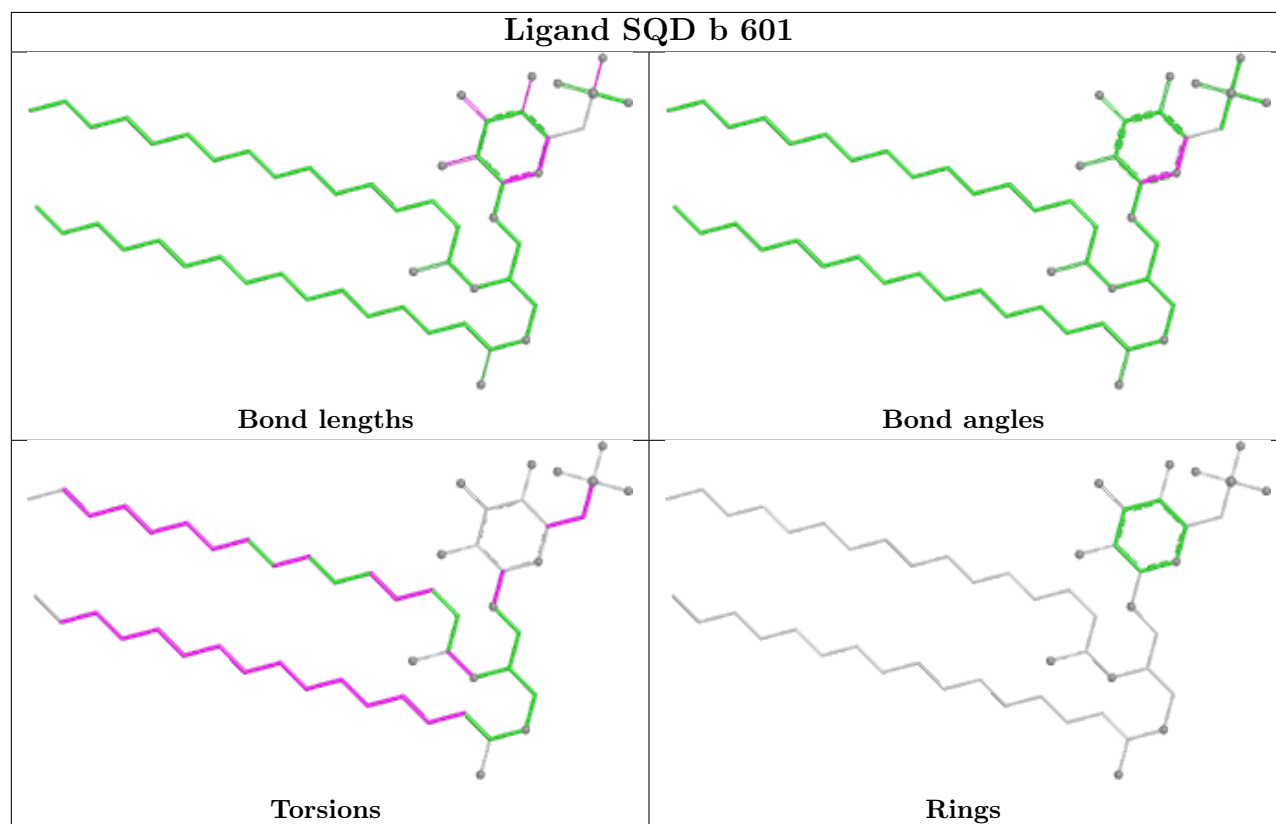
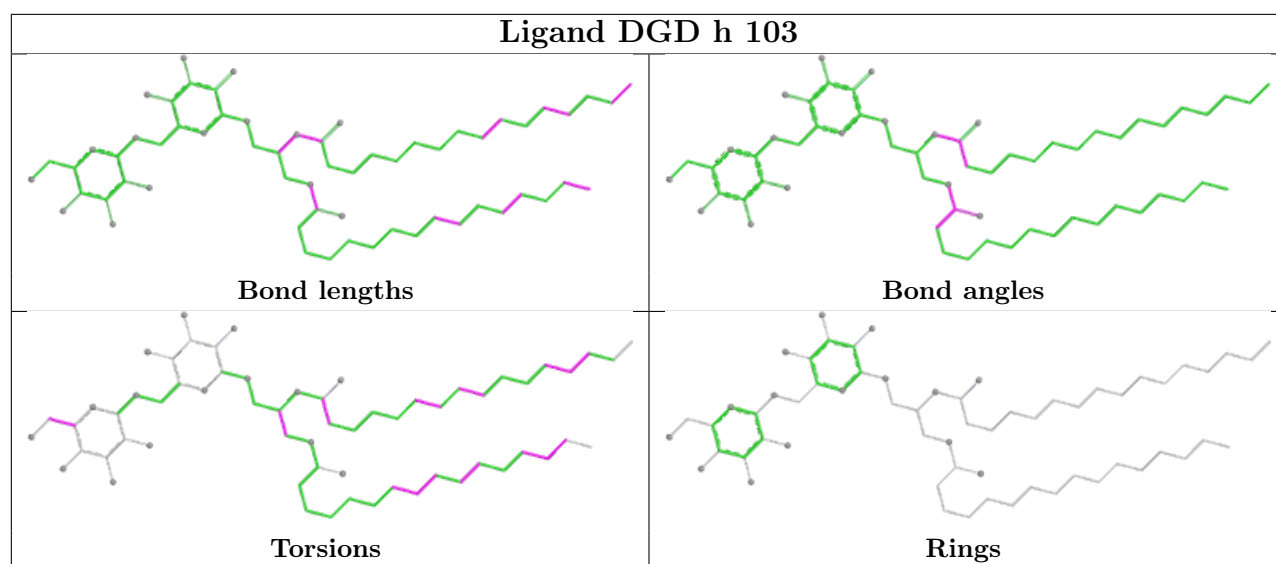


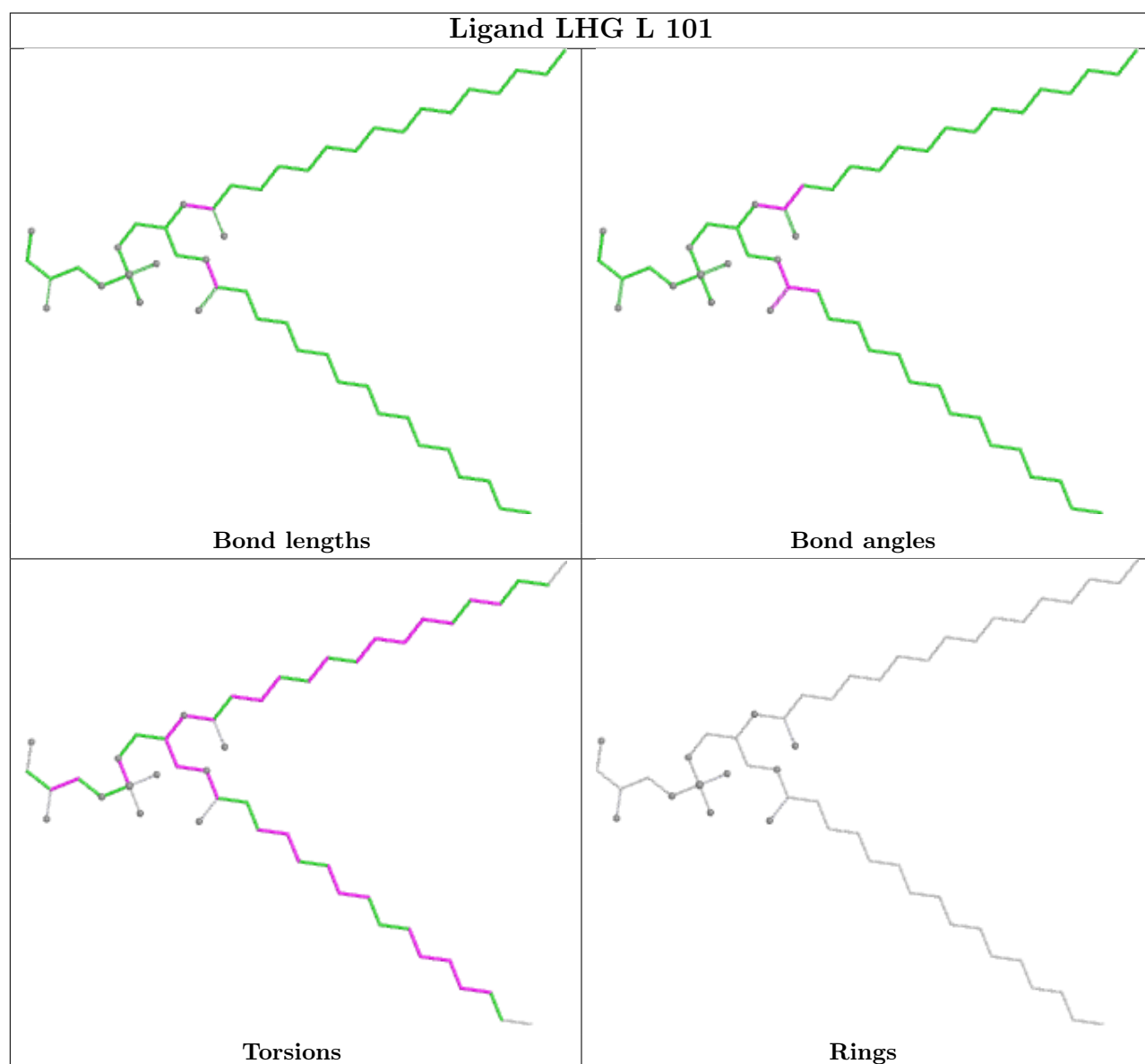
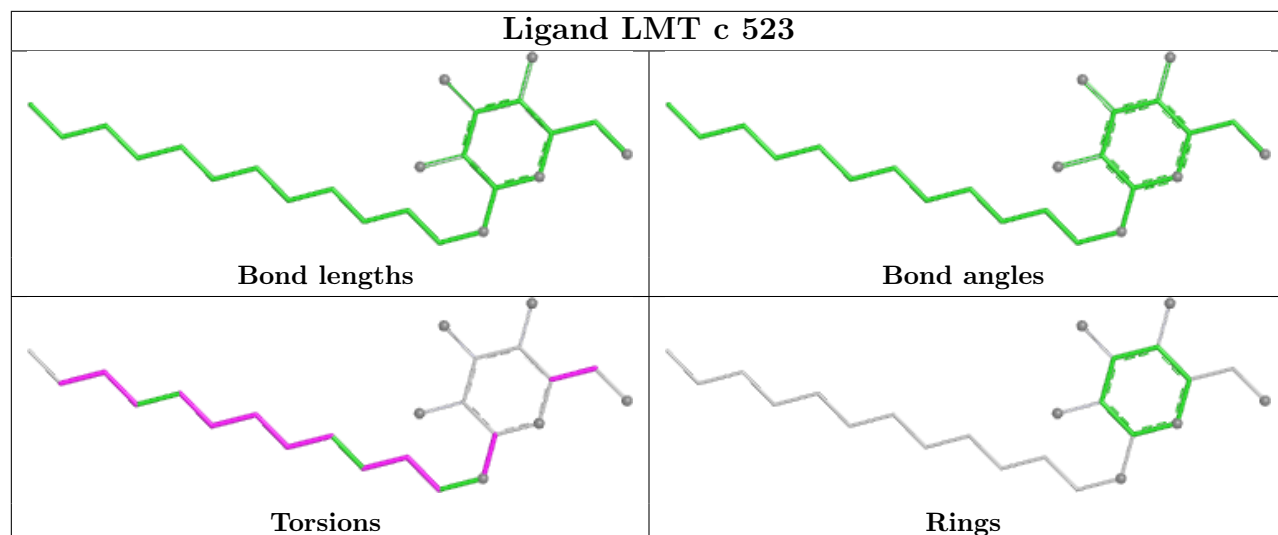




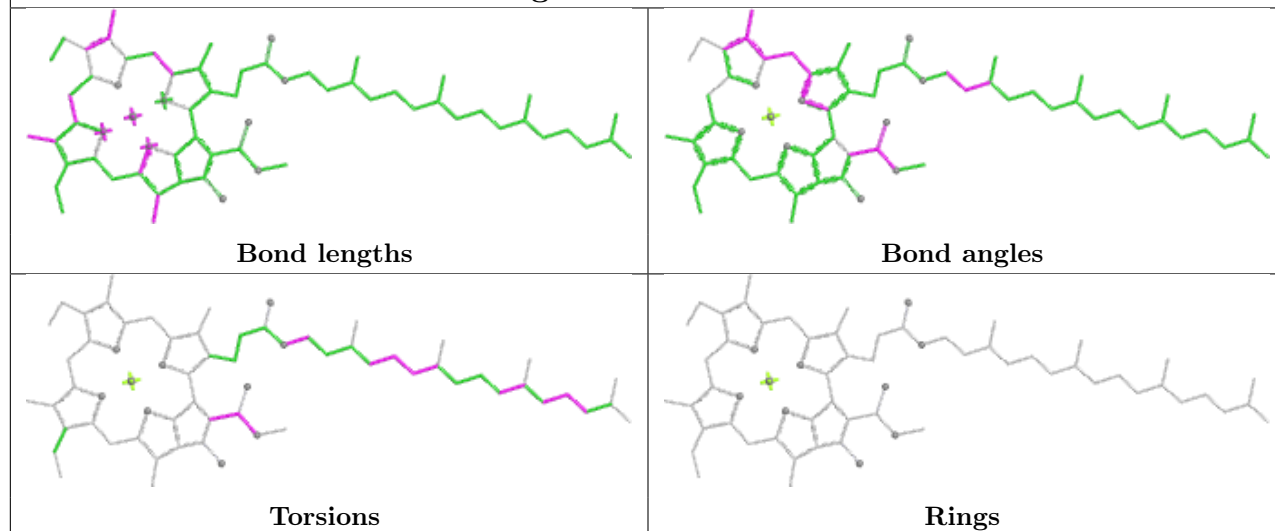




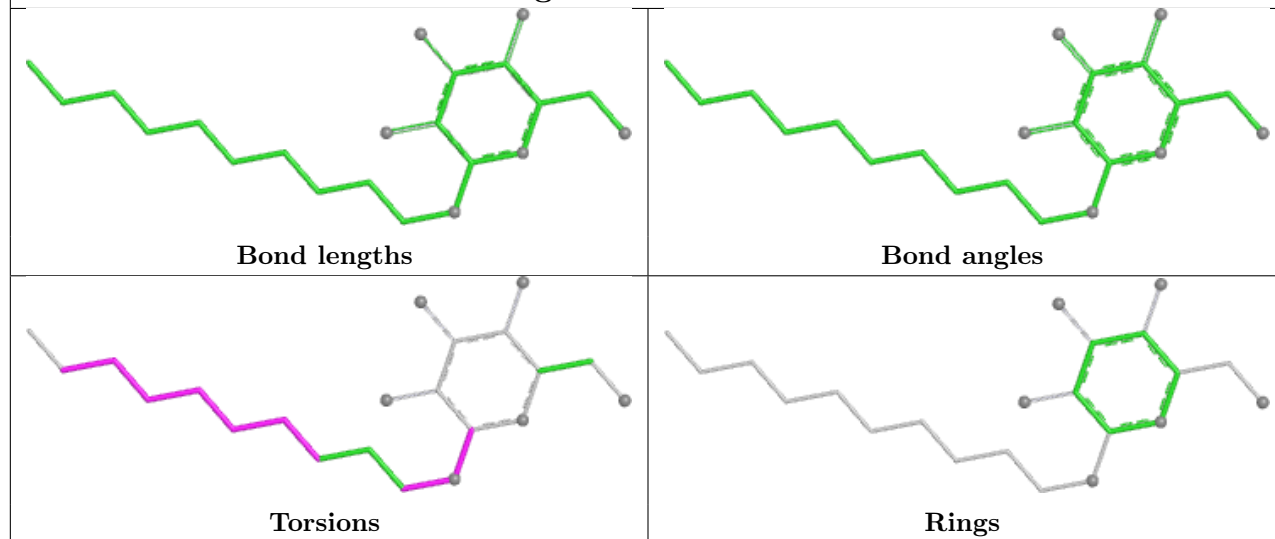




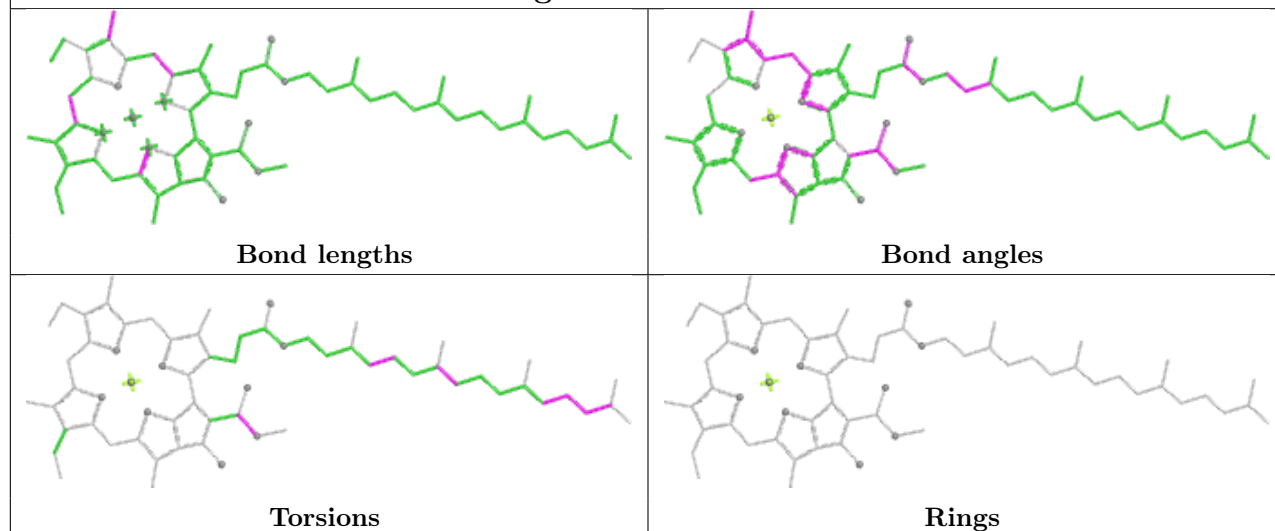
## Ligand CLA C 506



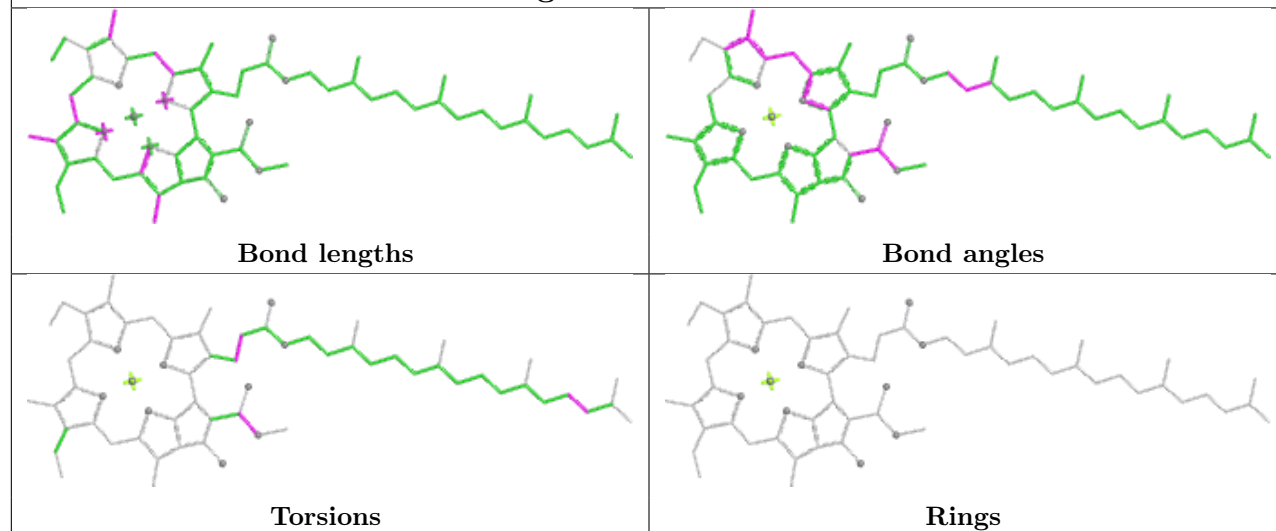
## Ligand LMT I 103



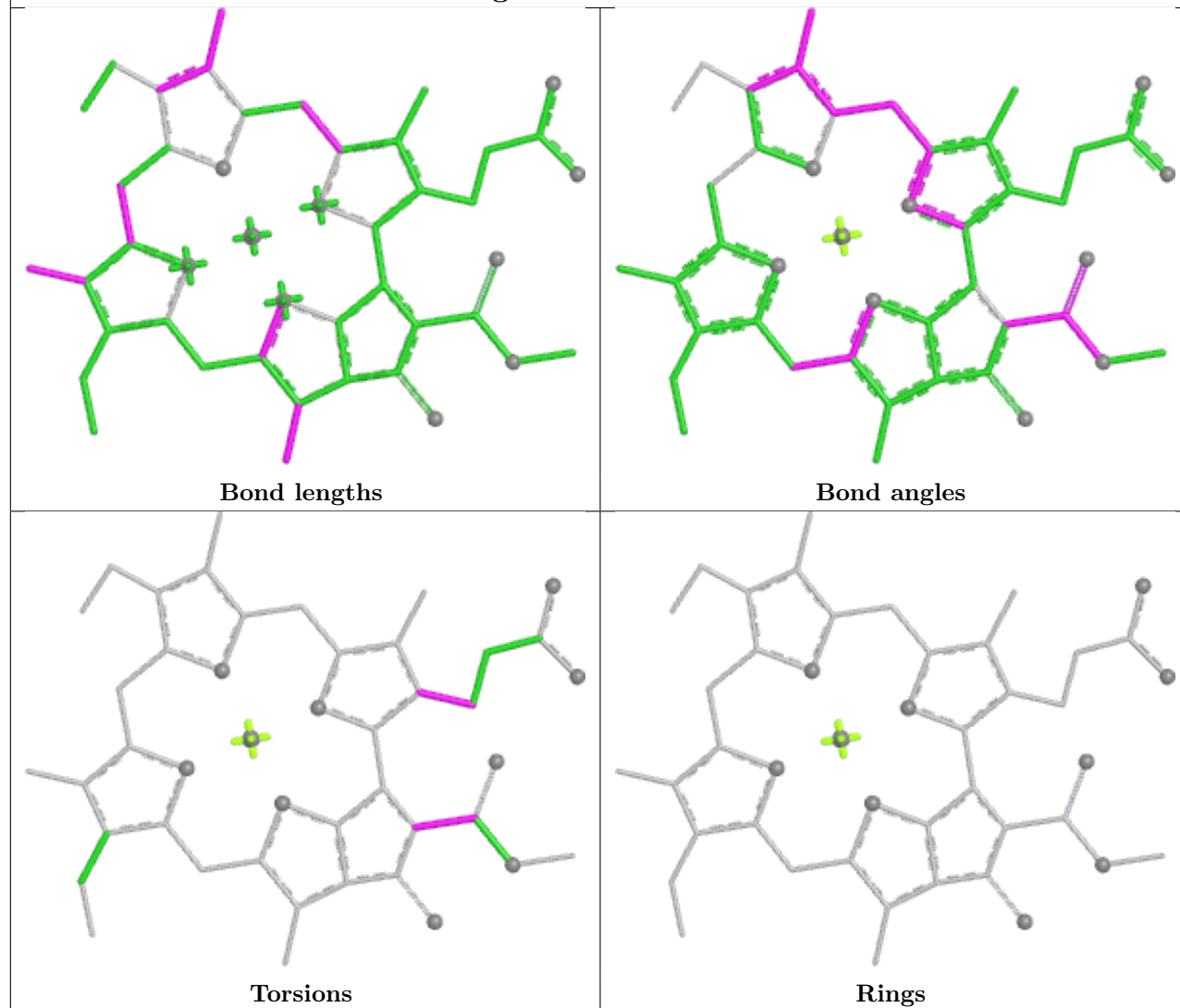
## Ligand CLA d 404

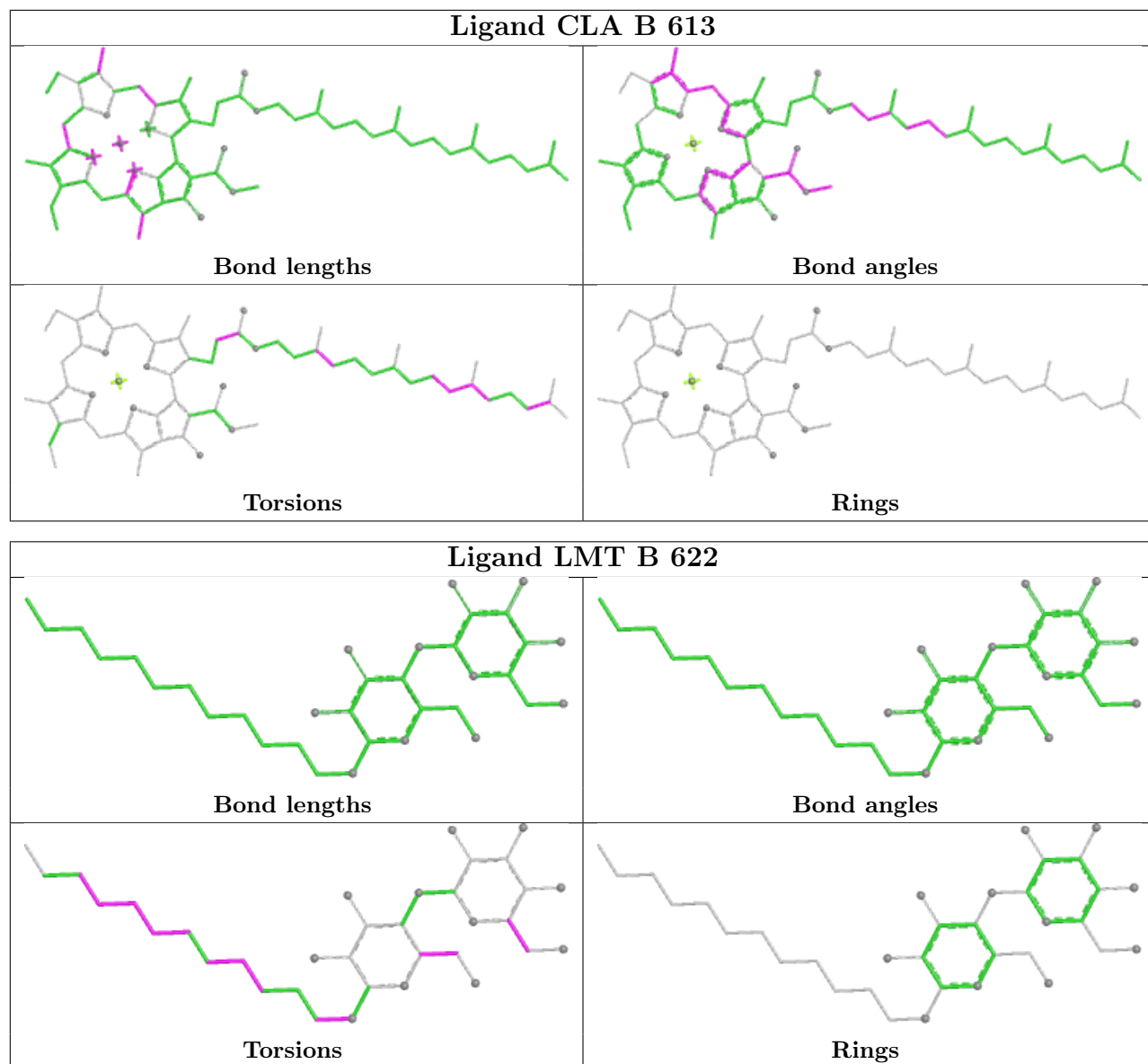


## Ligand CLA c 501

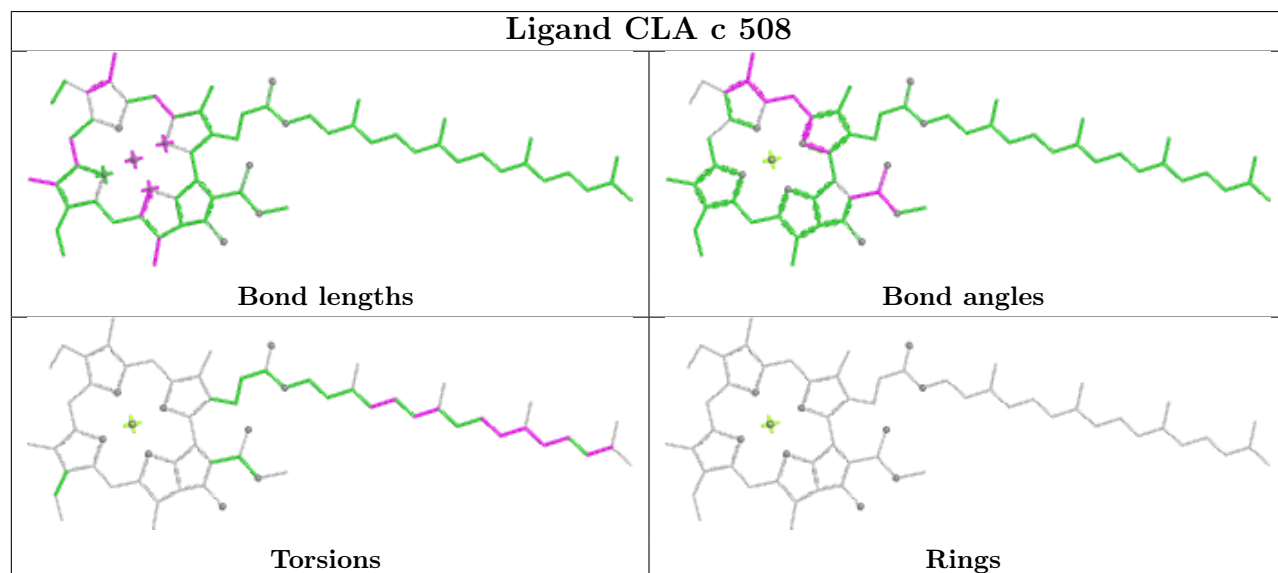
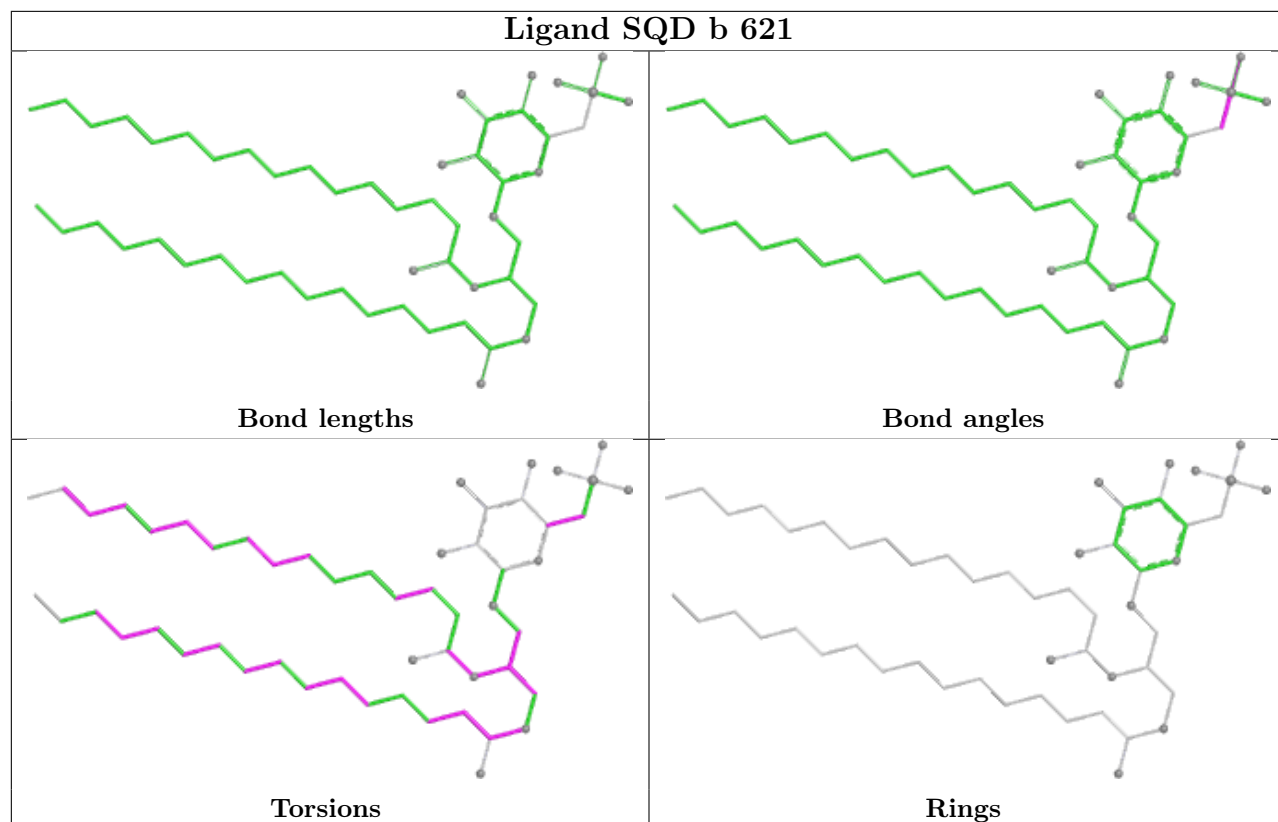


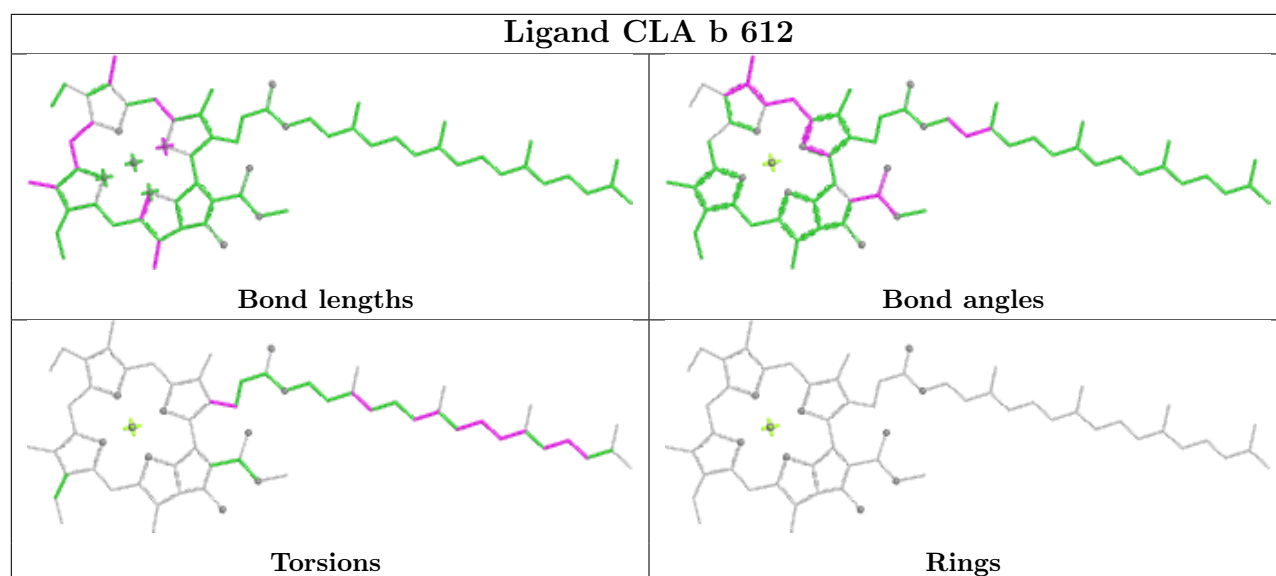
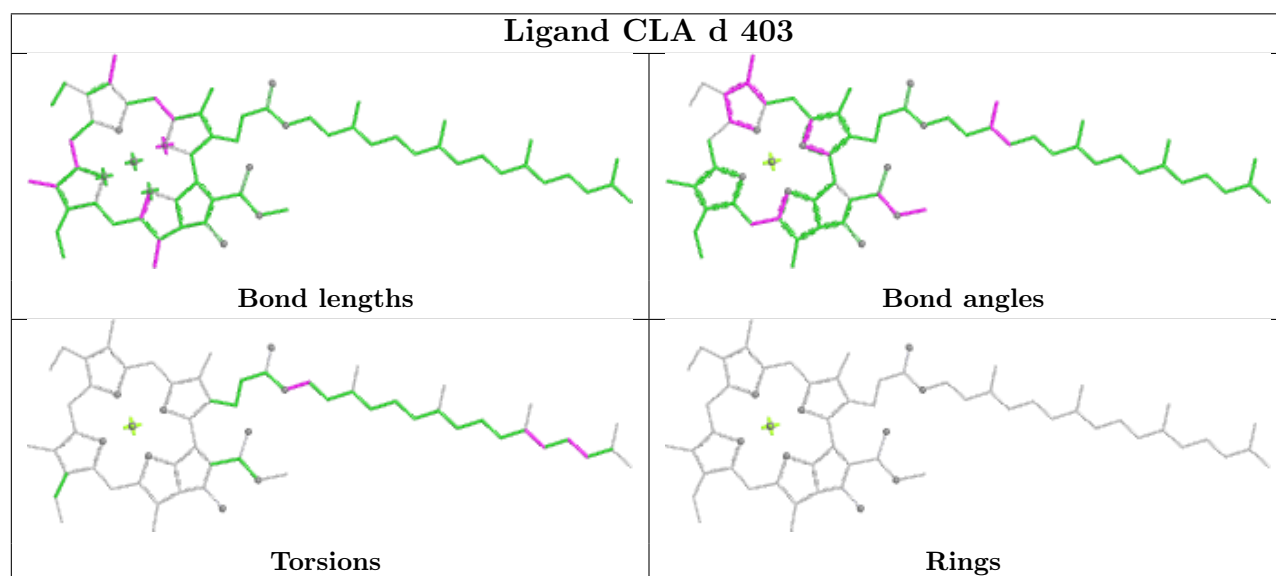
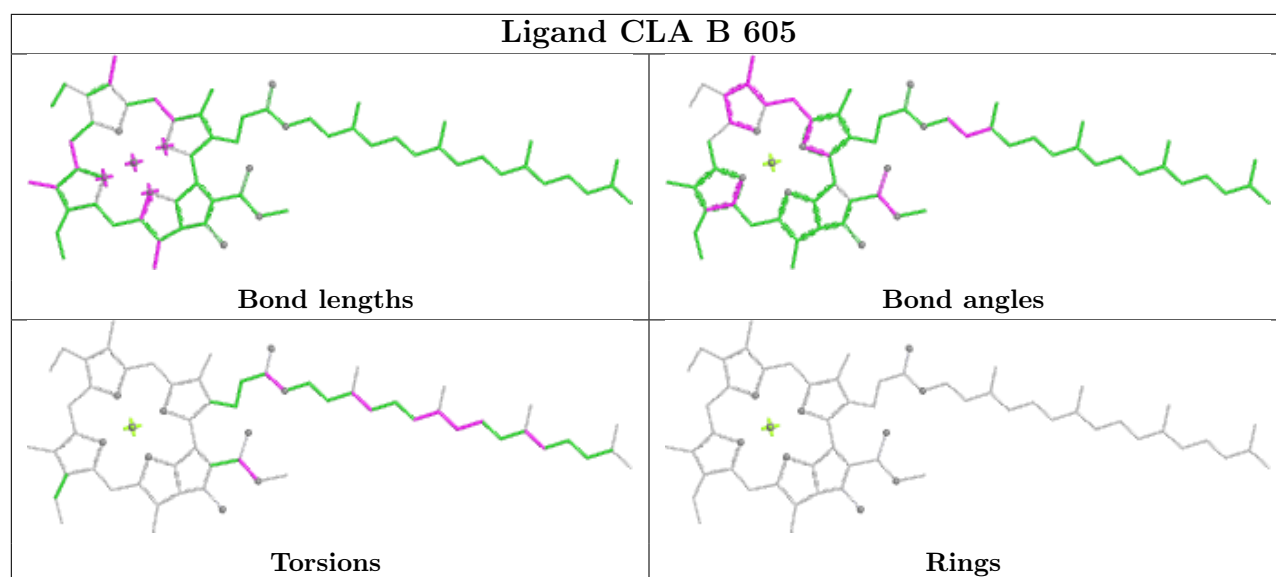
## Ligand CLA B 601

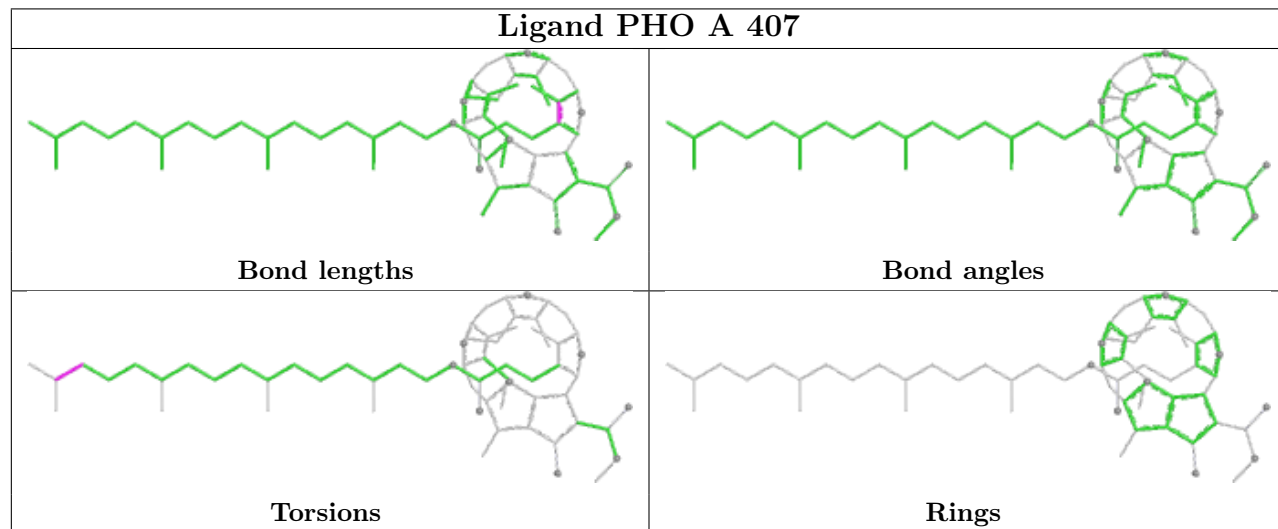
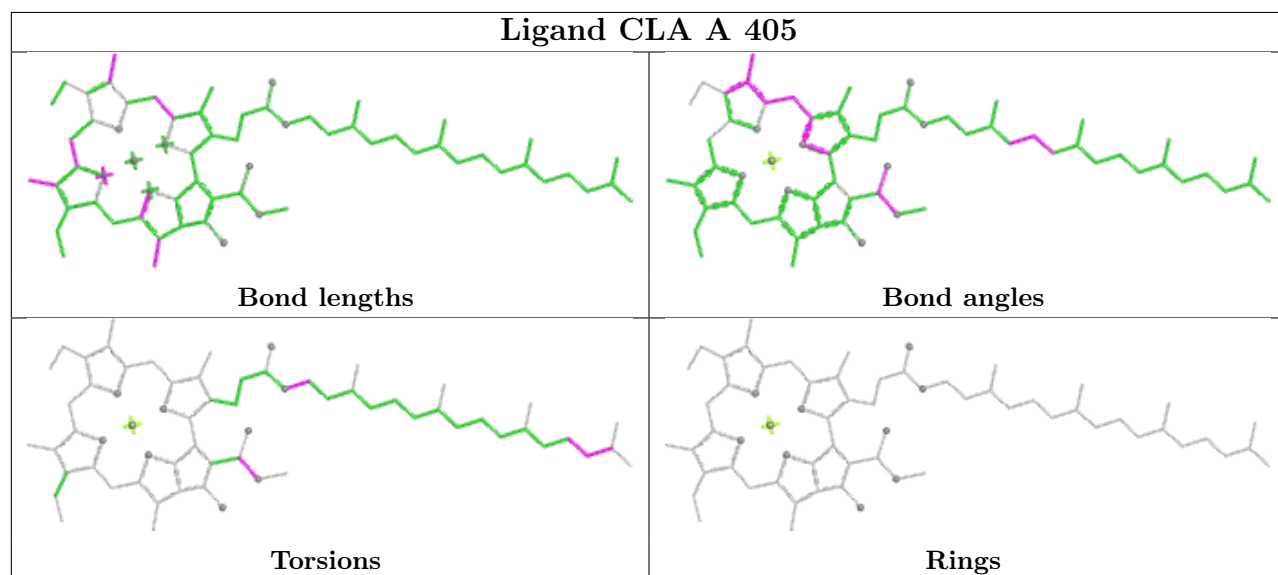
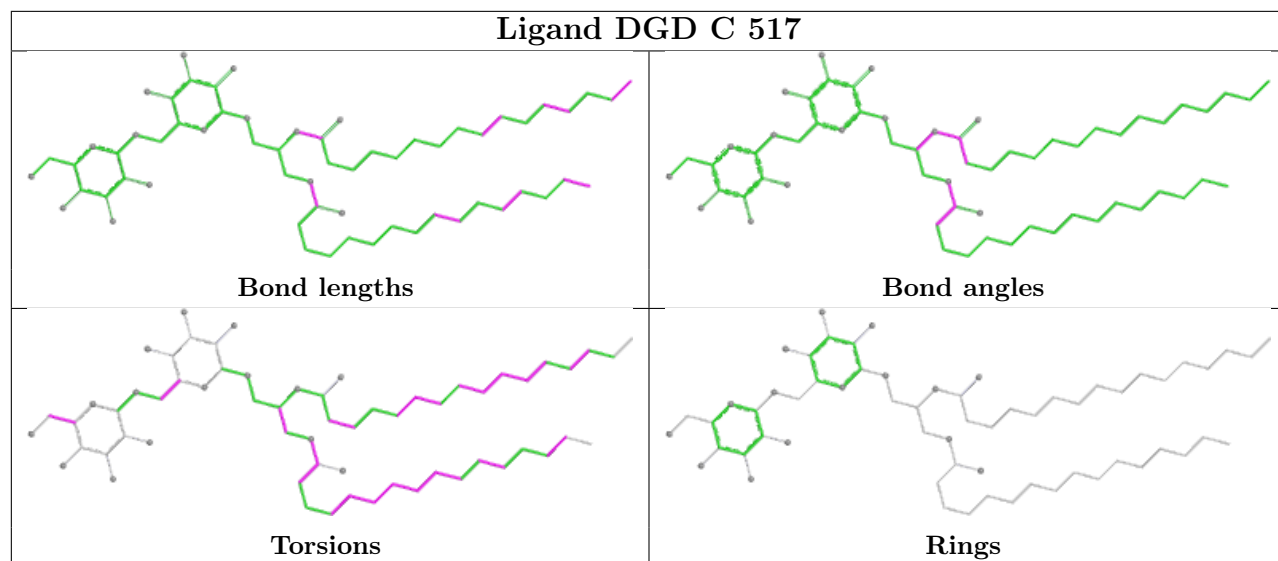


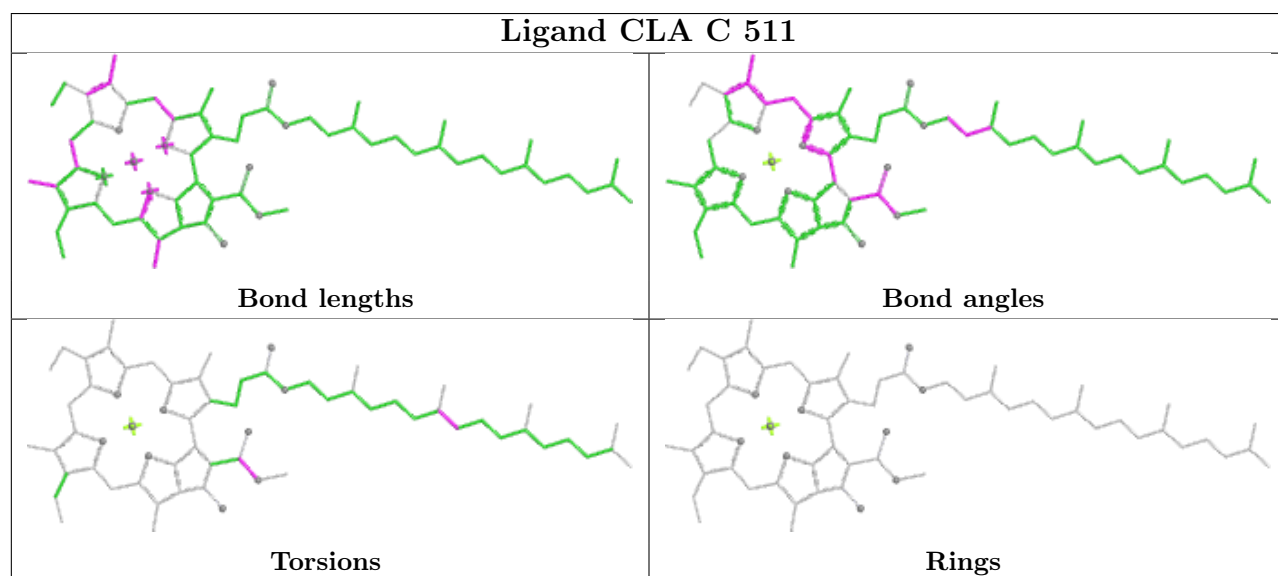
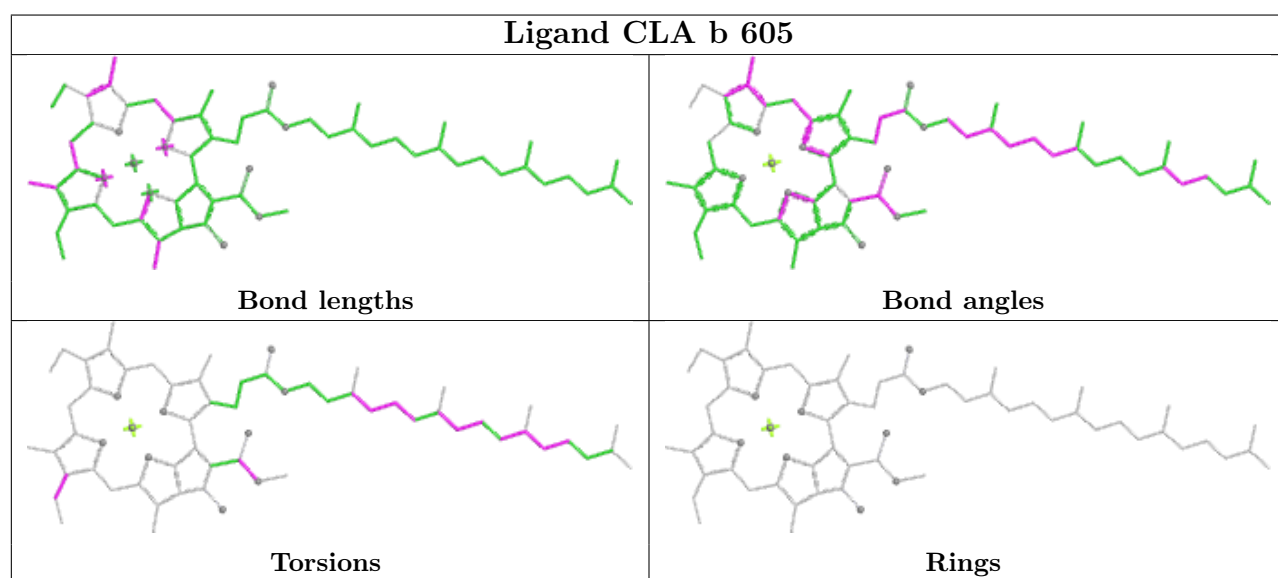
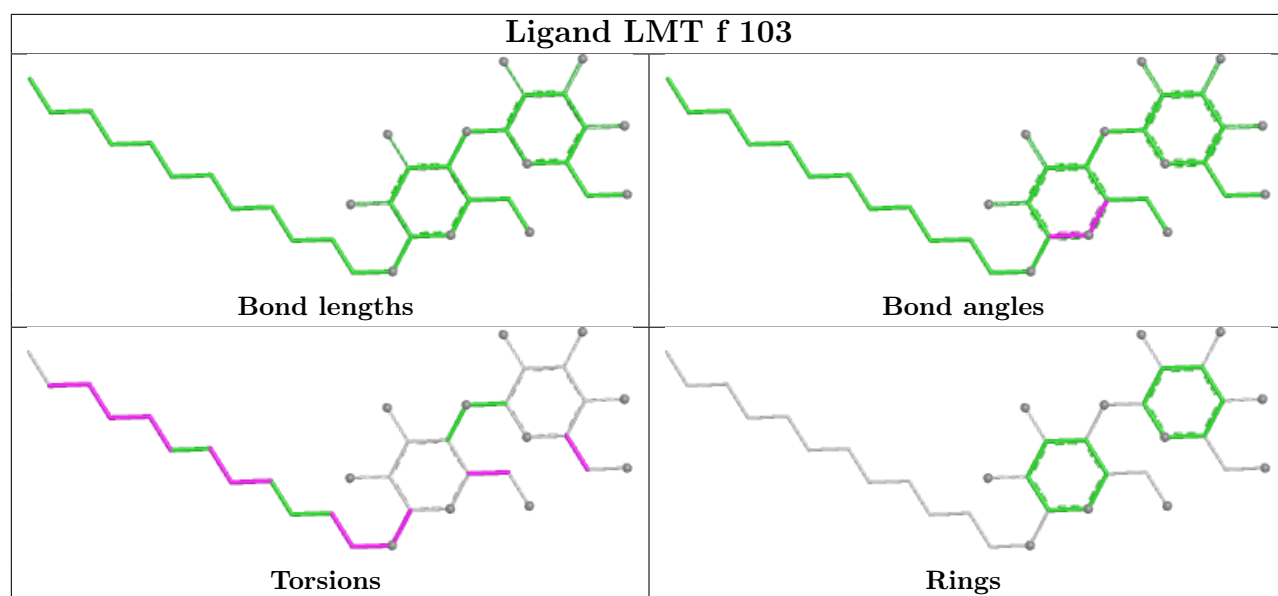


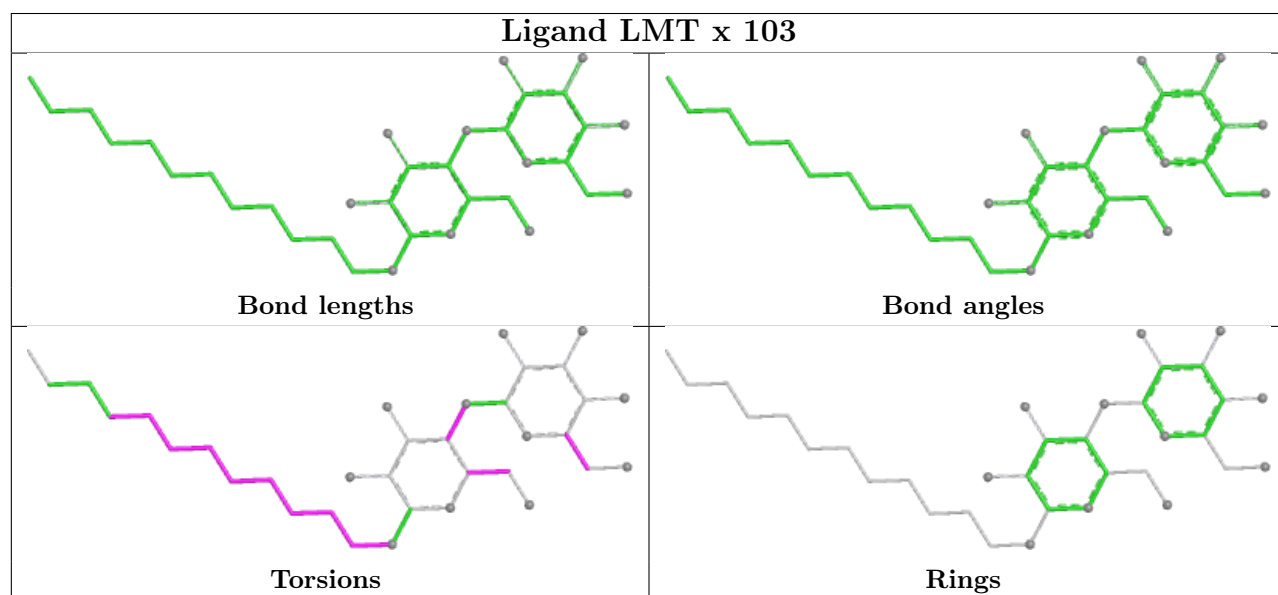
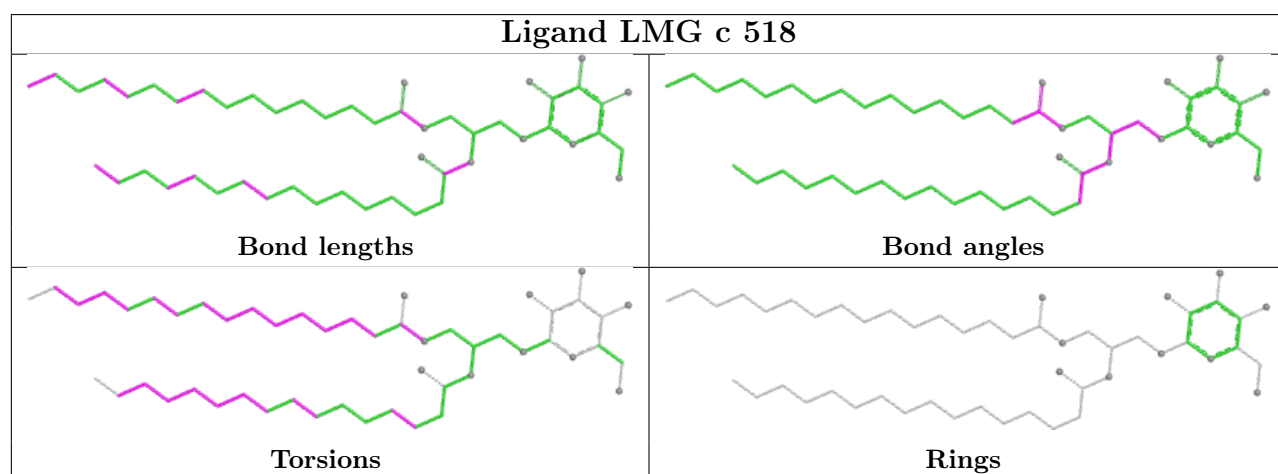
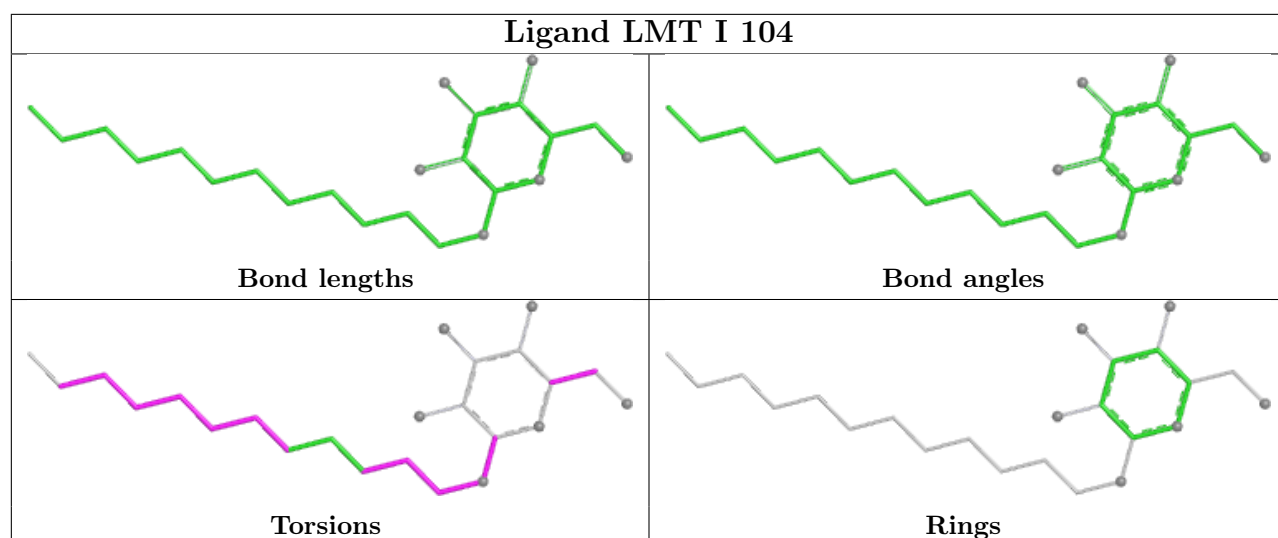


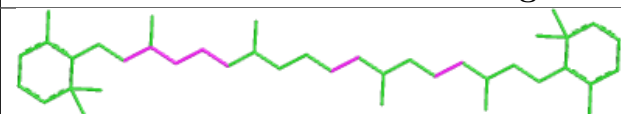
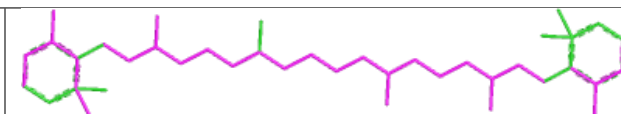
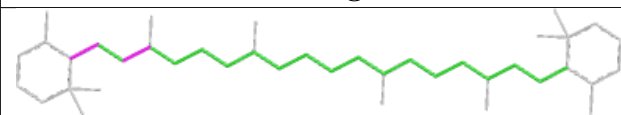
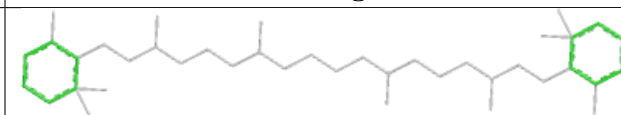

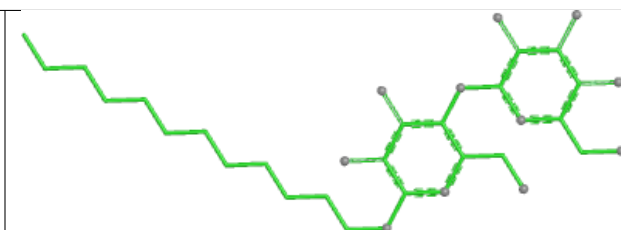
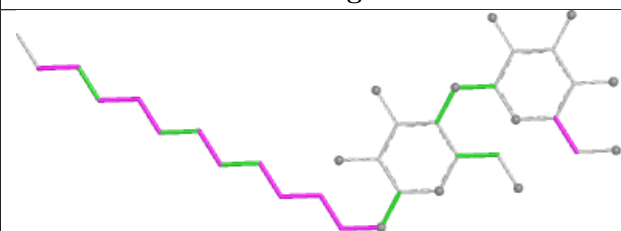
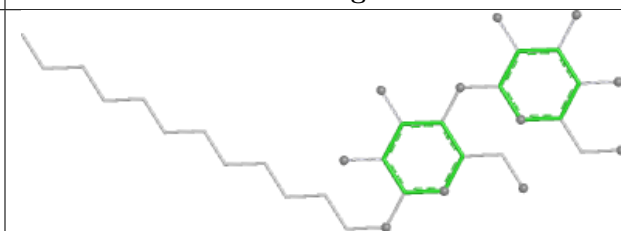
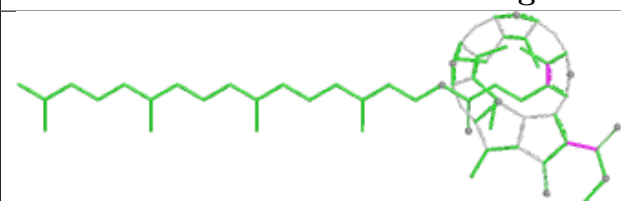
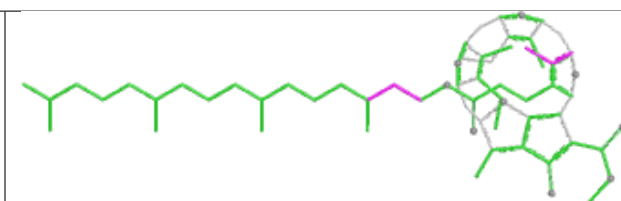
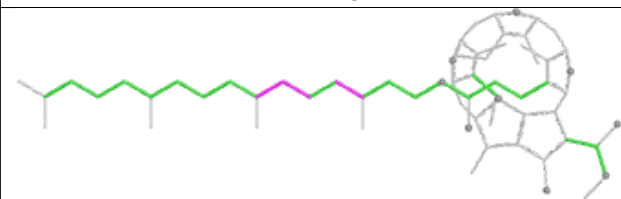
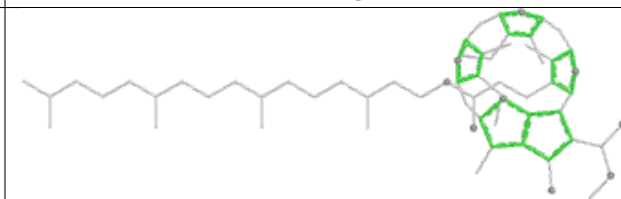


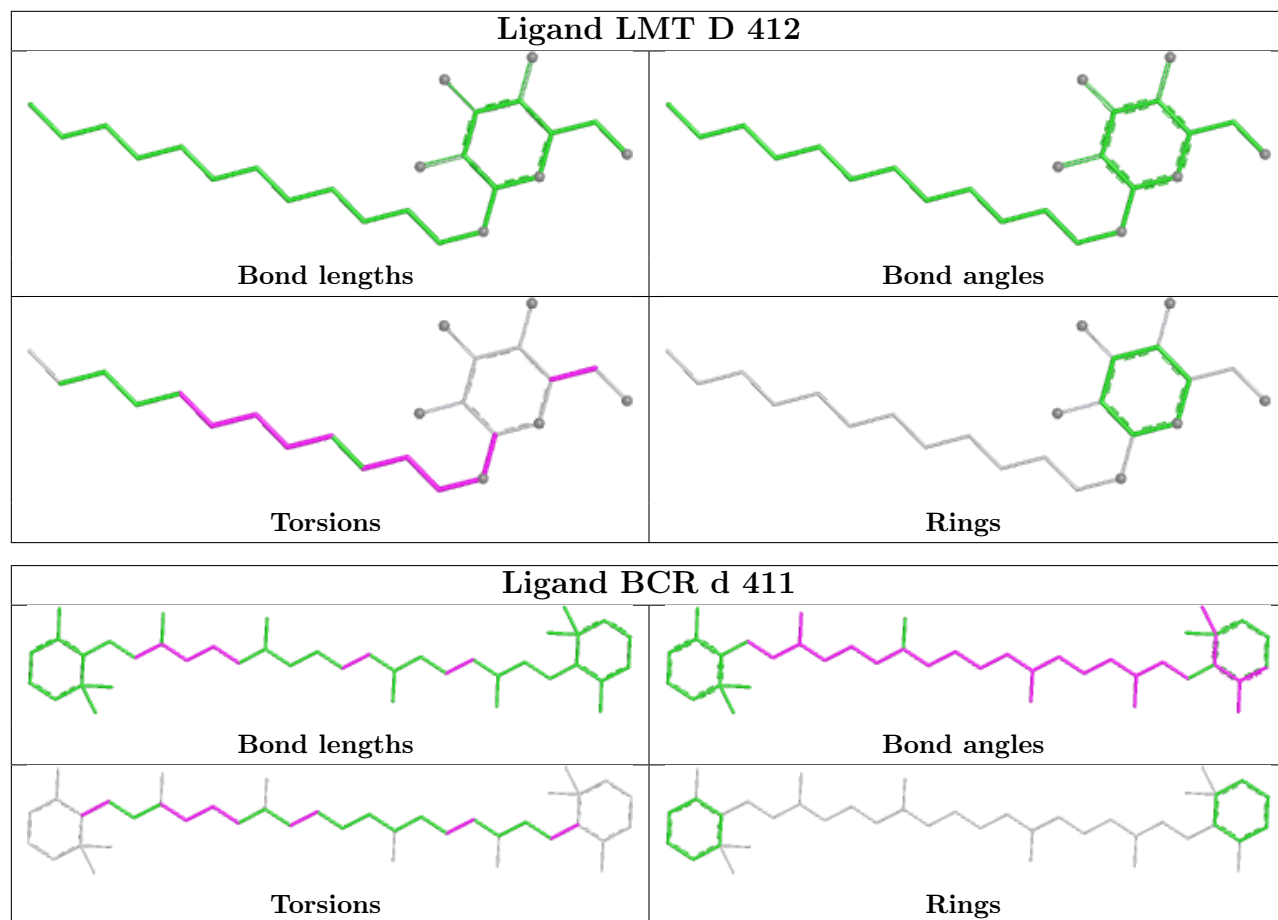




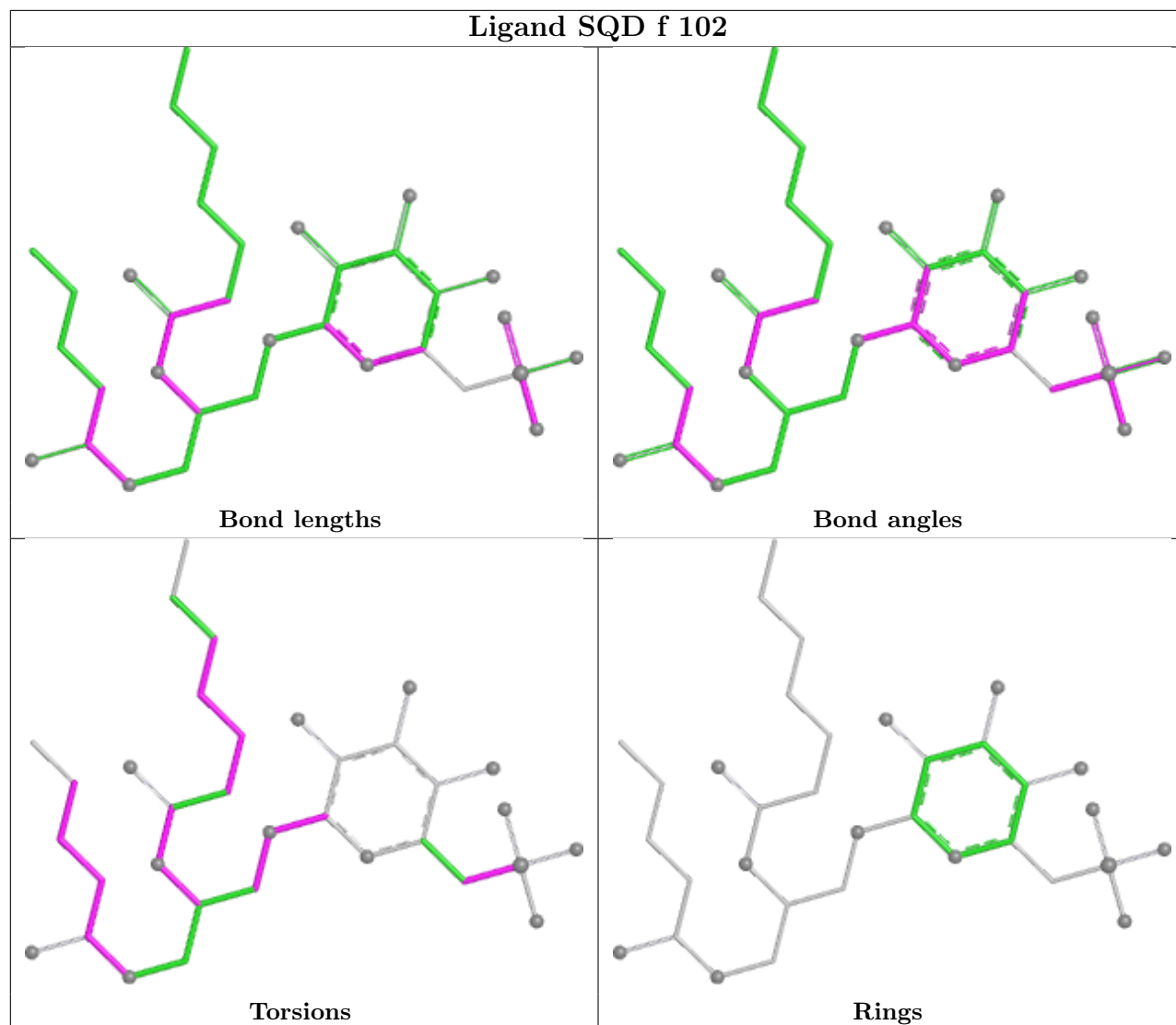




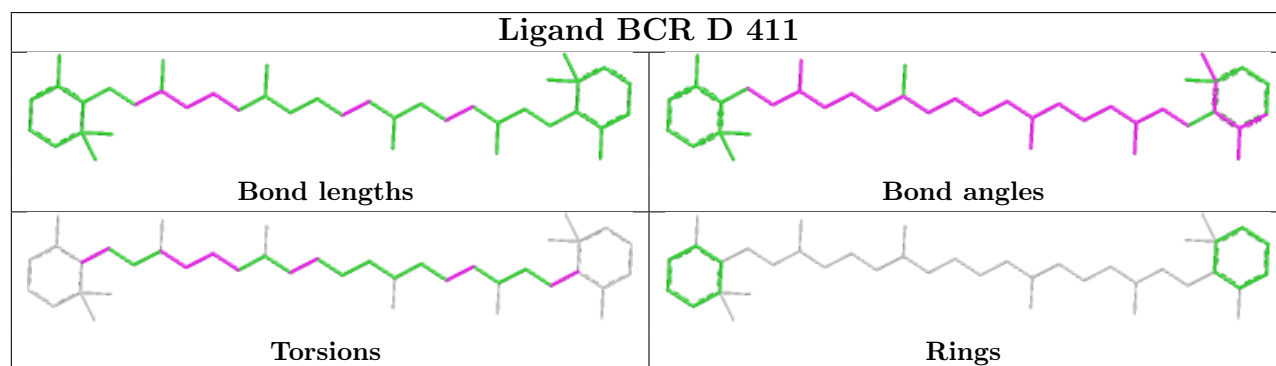
Ligand BCR C 527	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT A 414	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO D 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



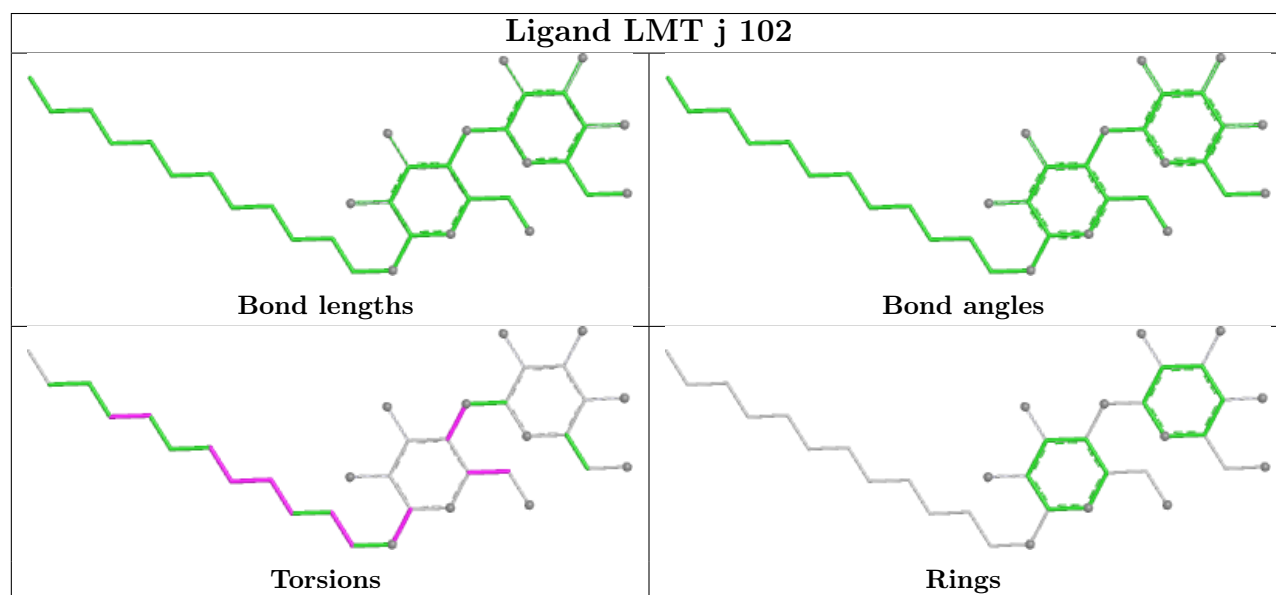
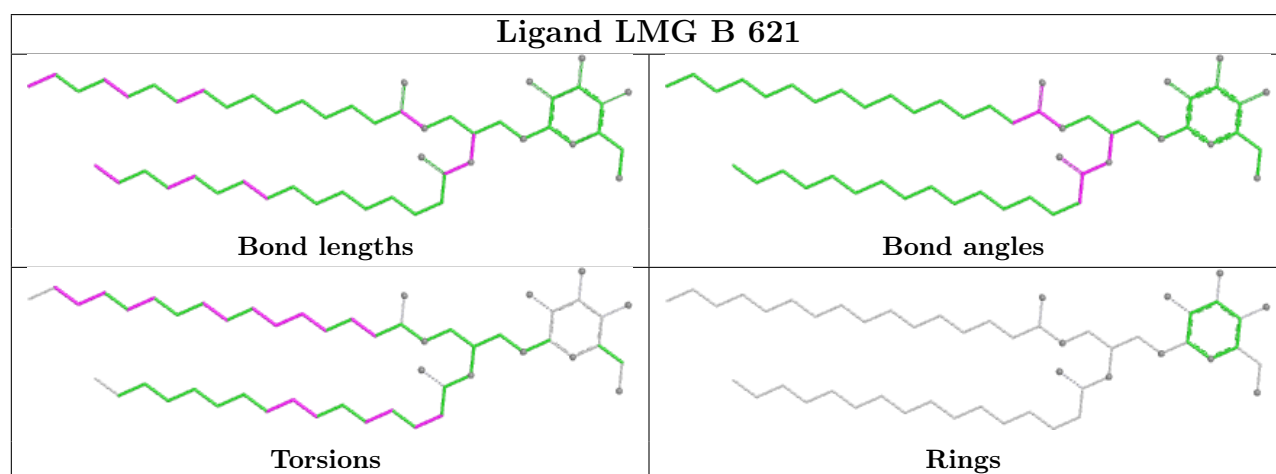
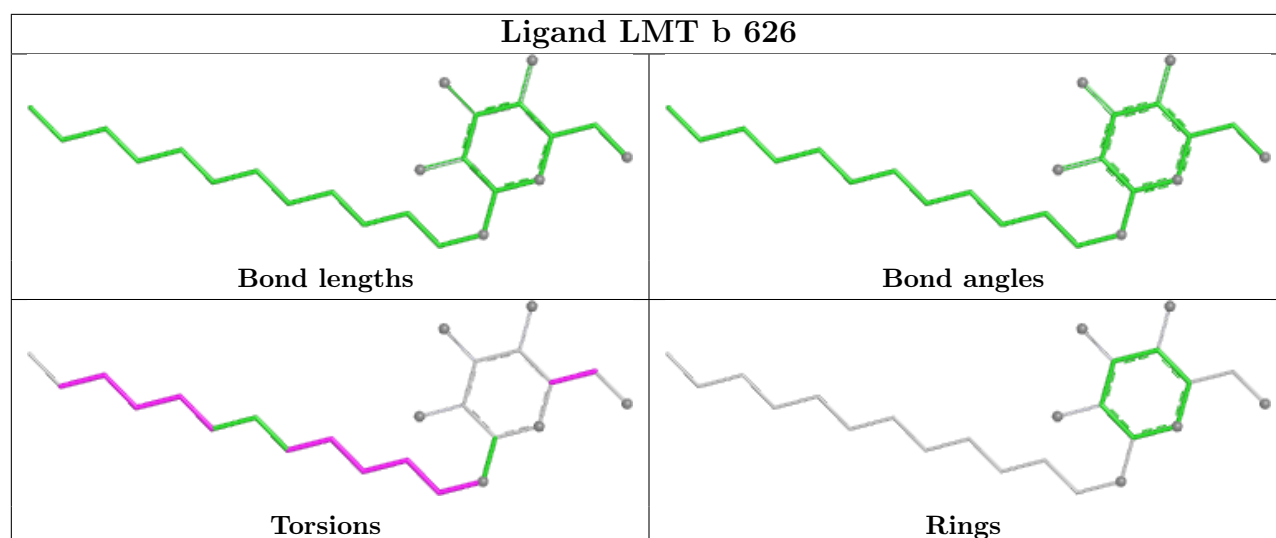
## Ligand SQD f 102

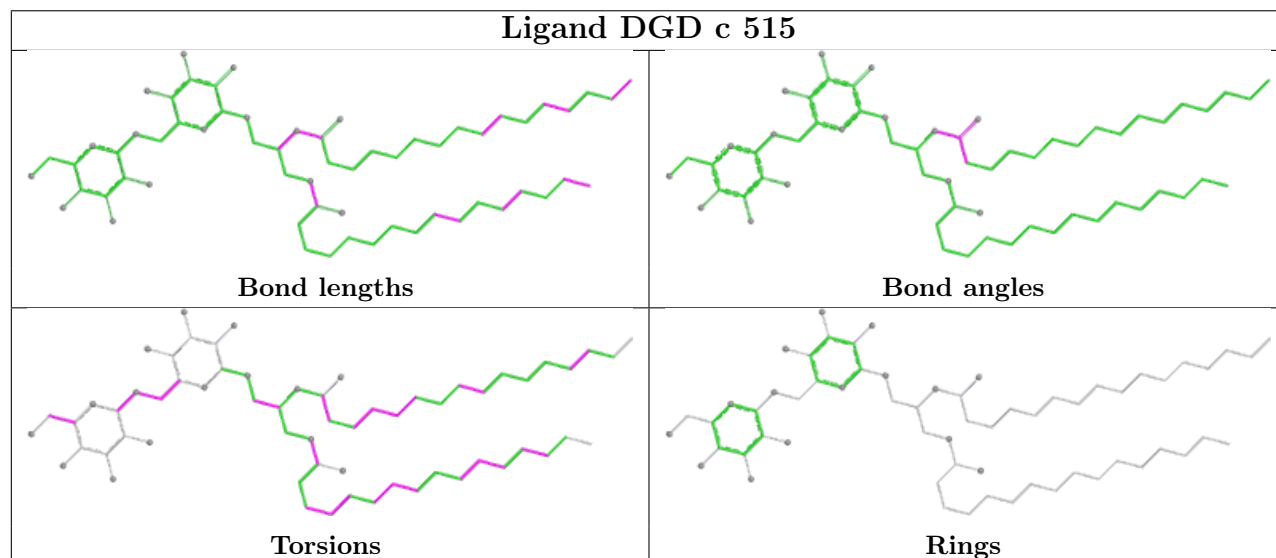
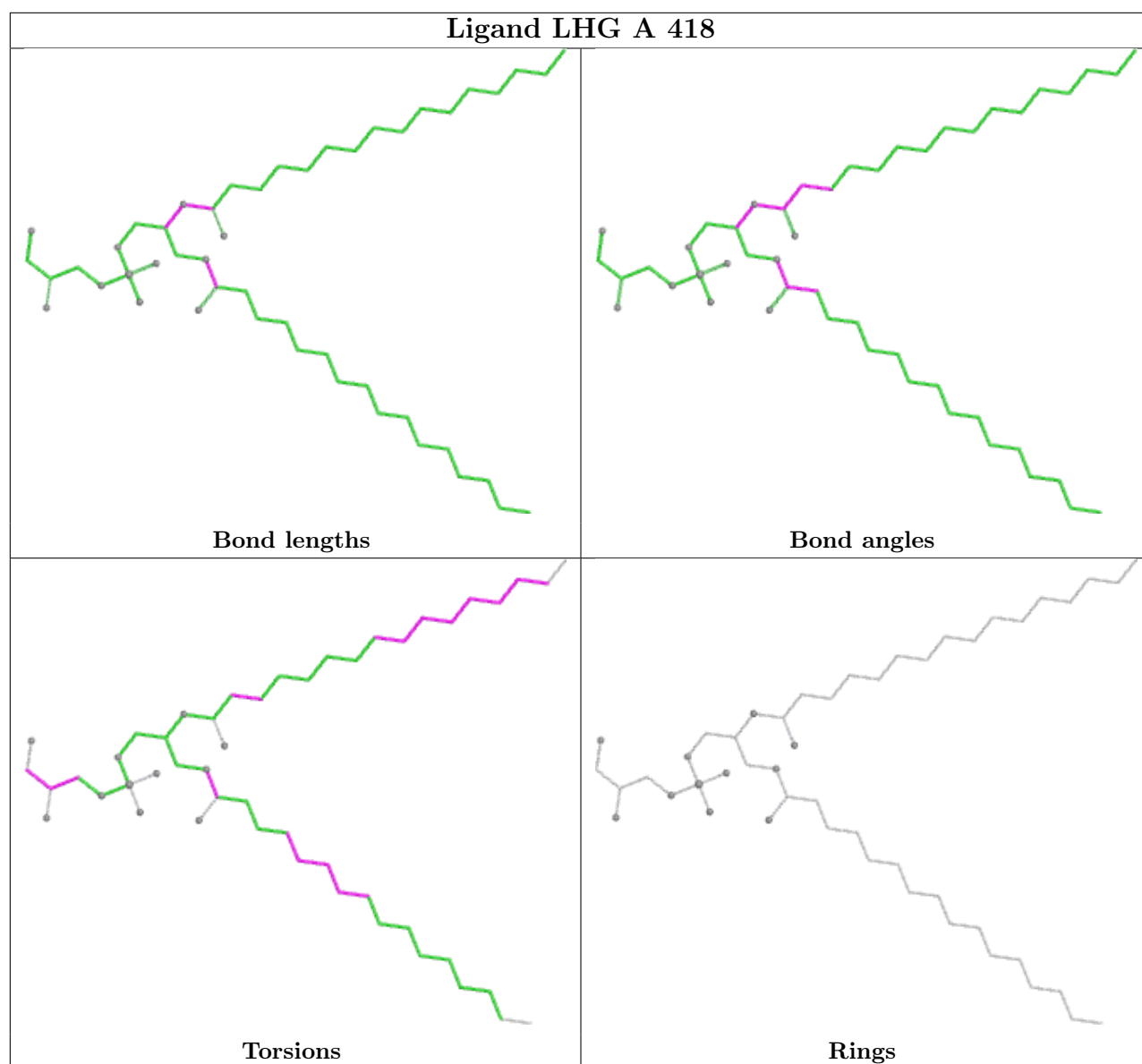


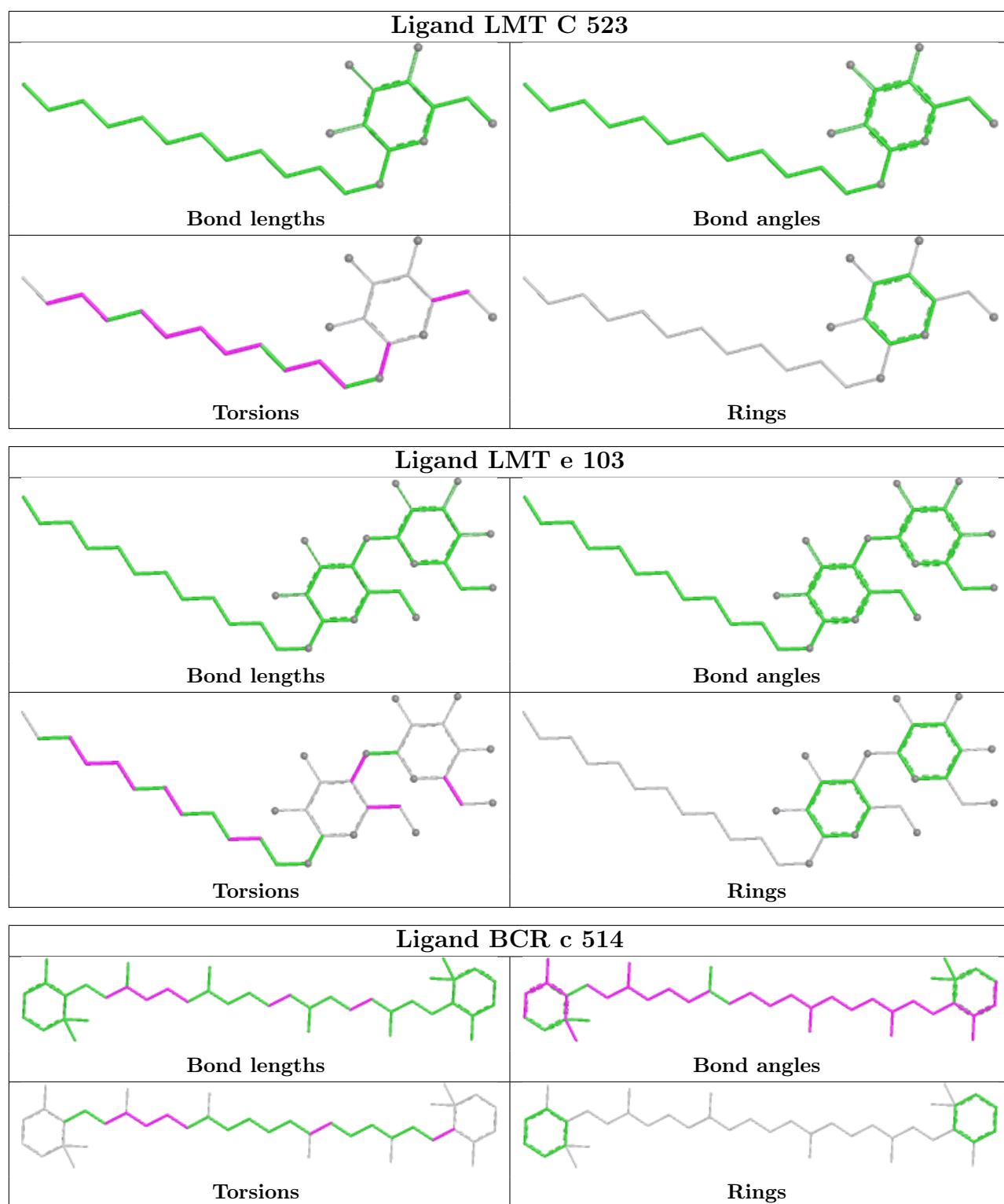
## Ligand BCR D 411

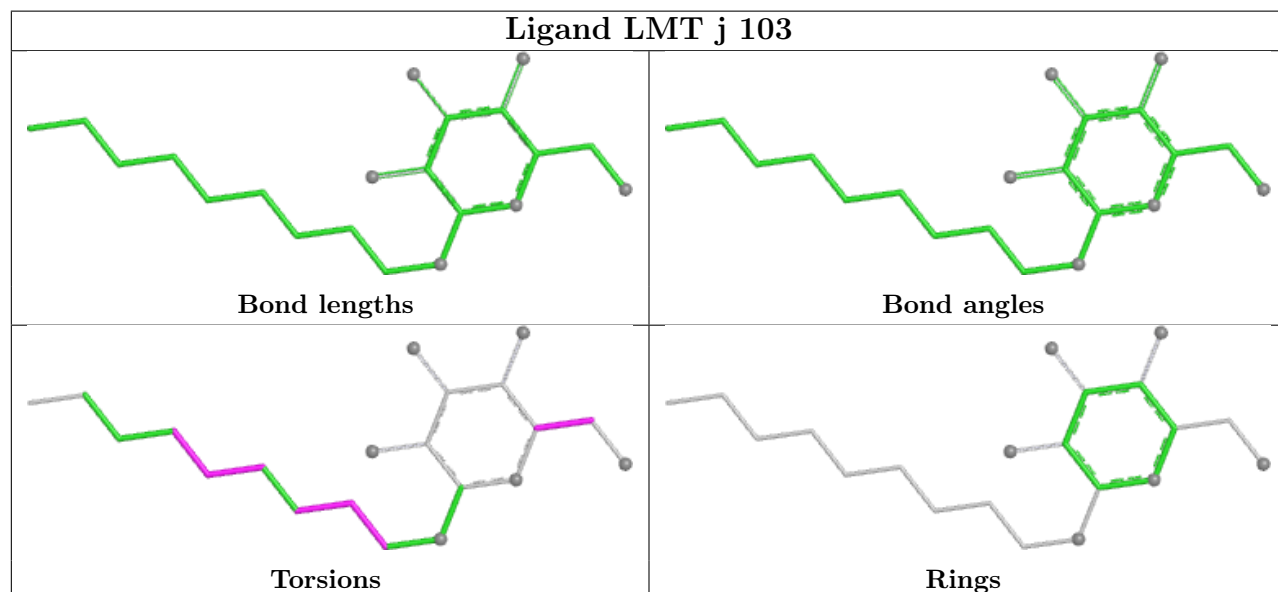
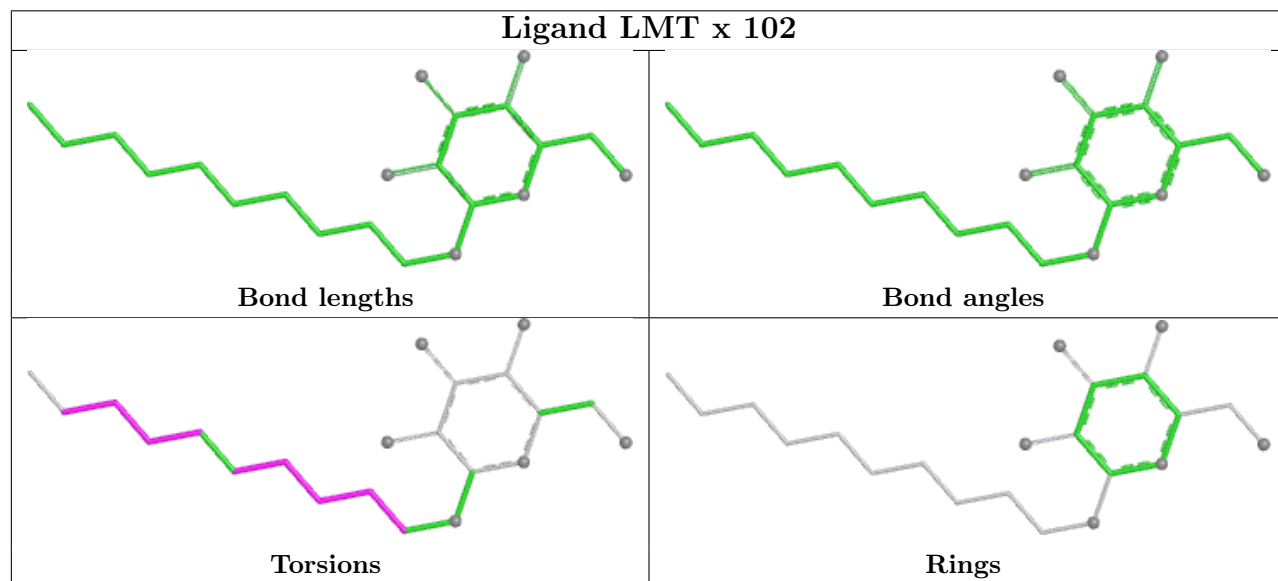
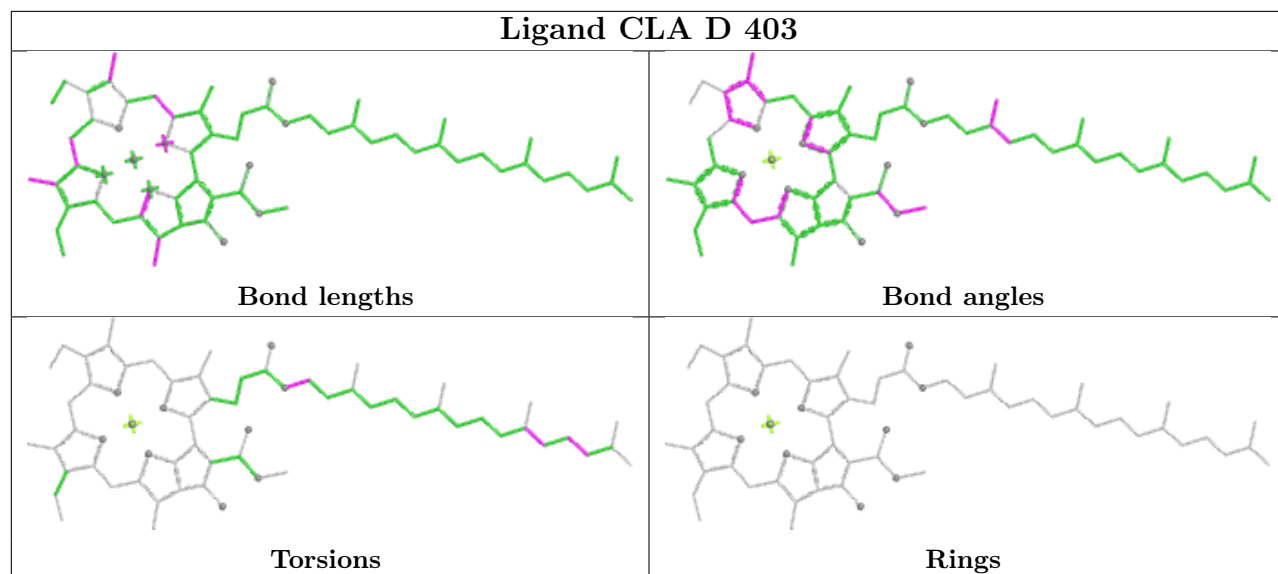


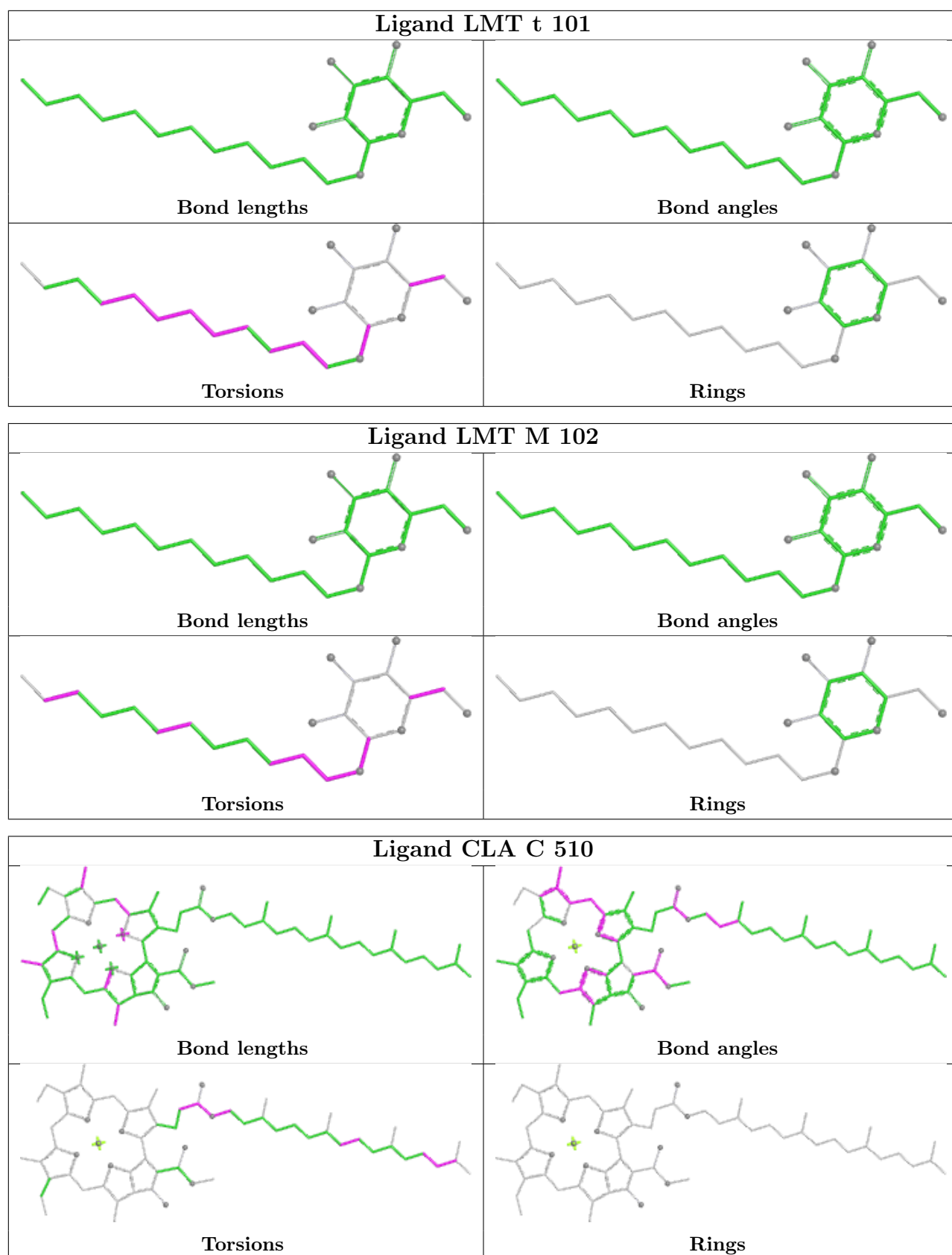


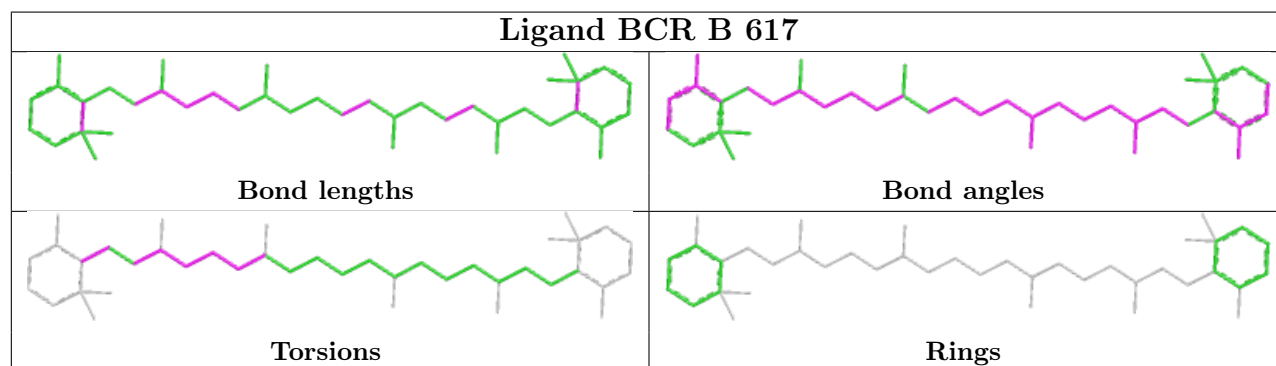
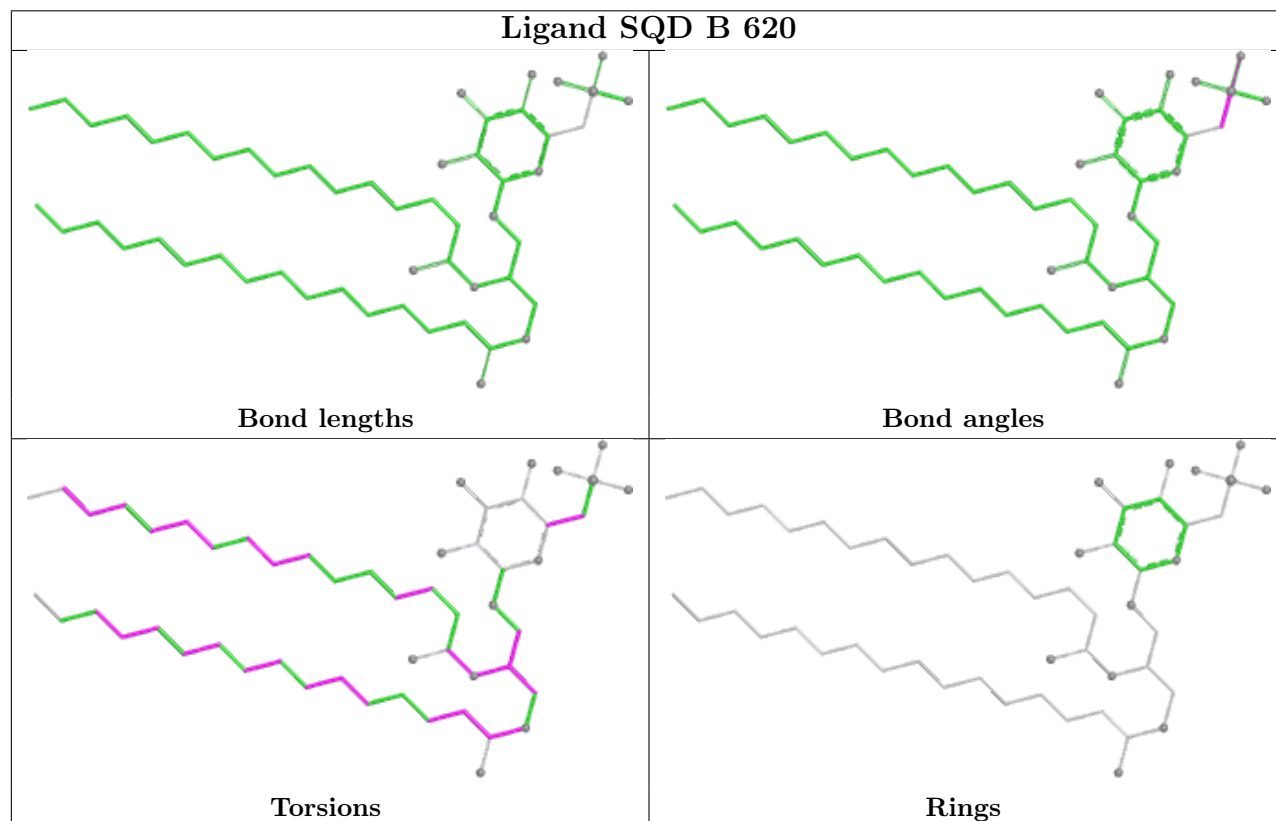
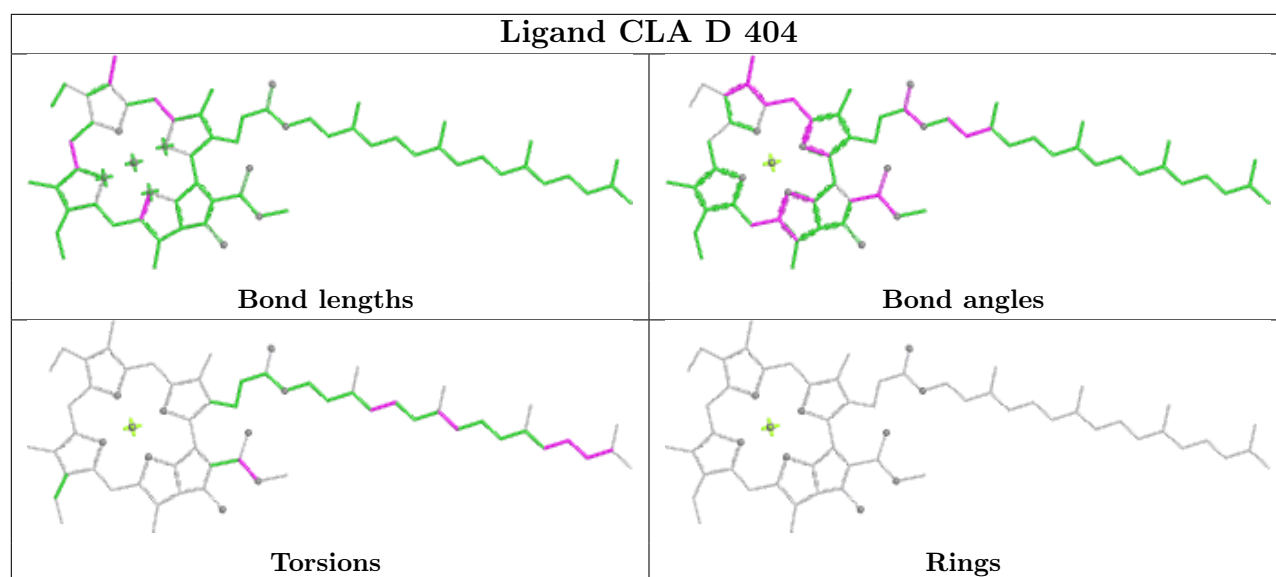


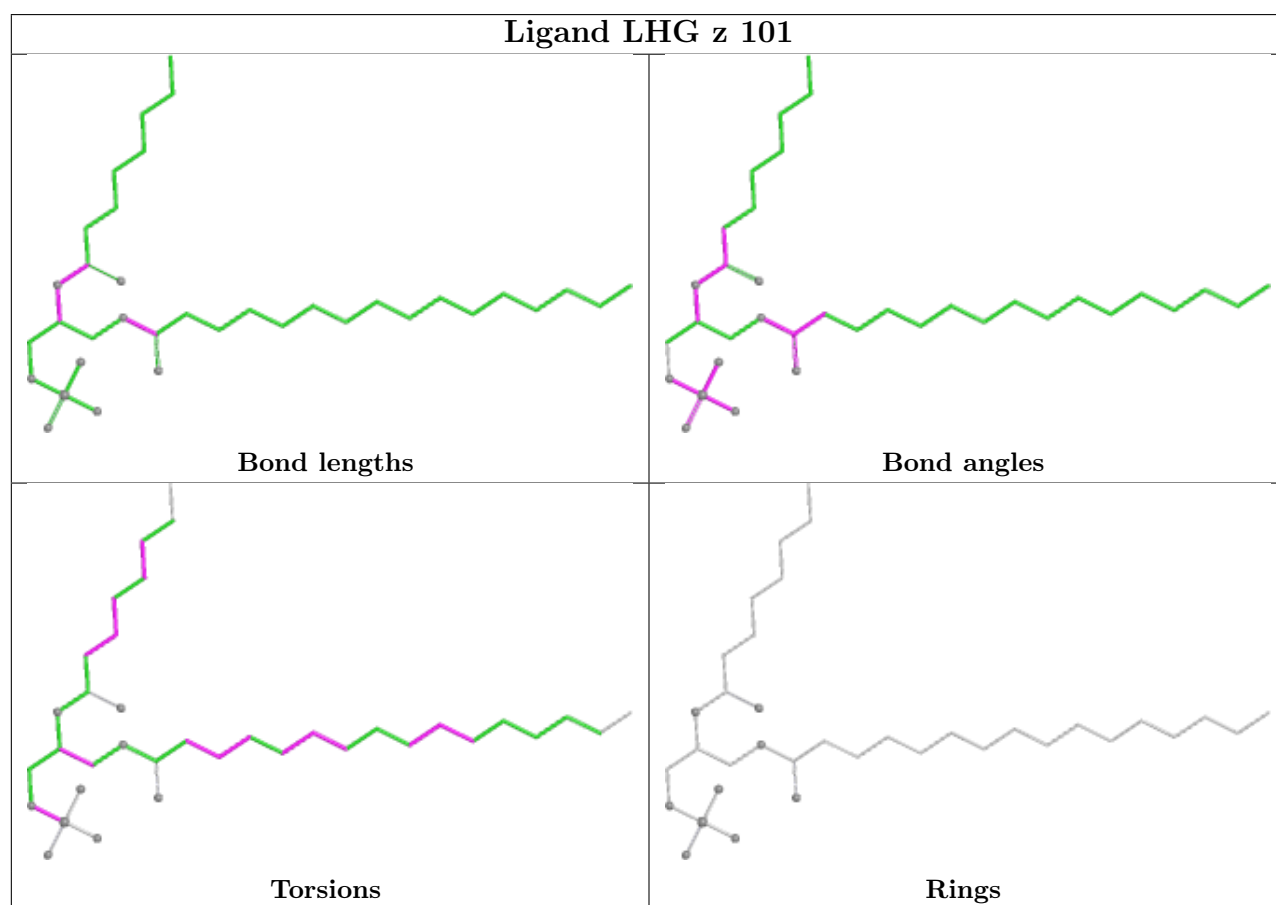
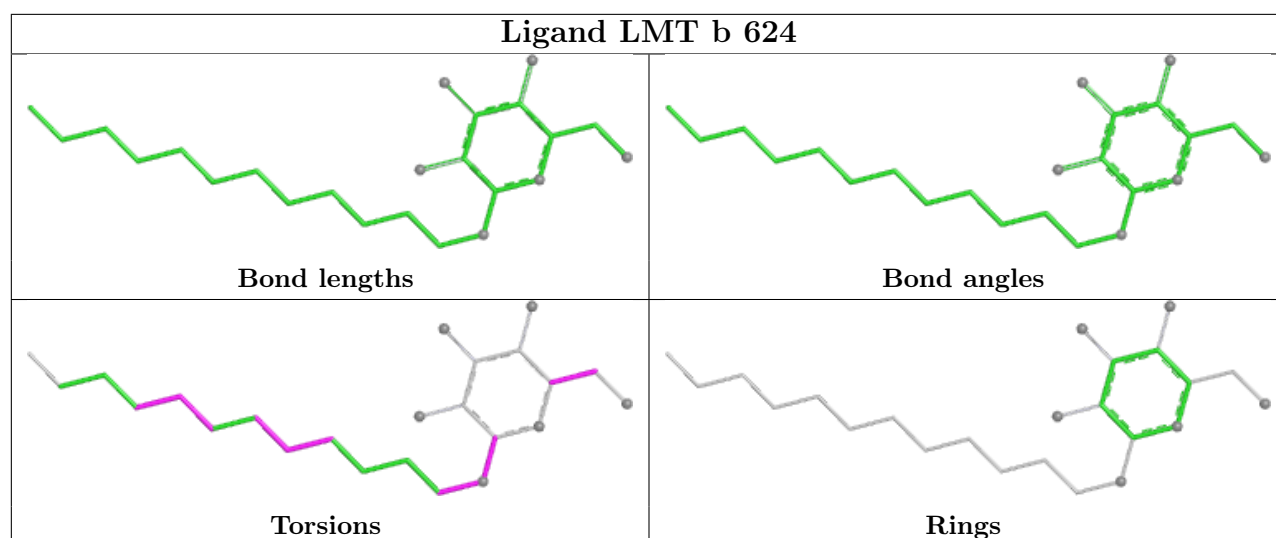


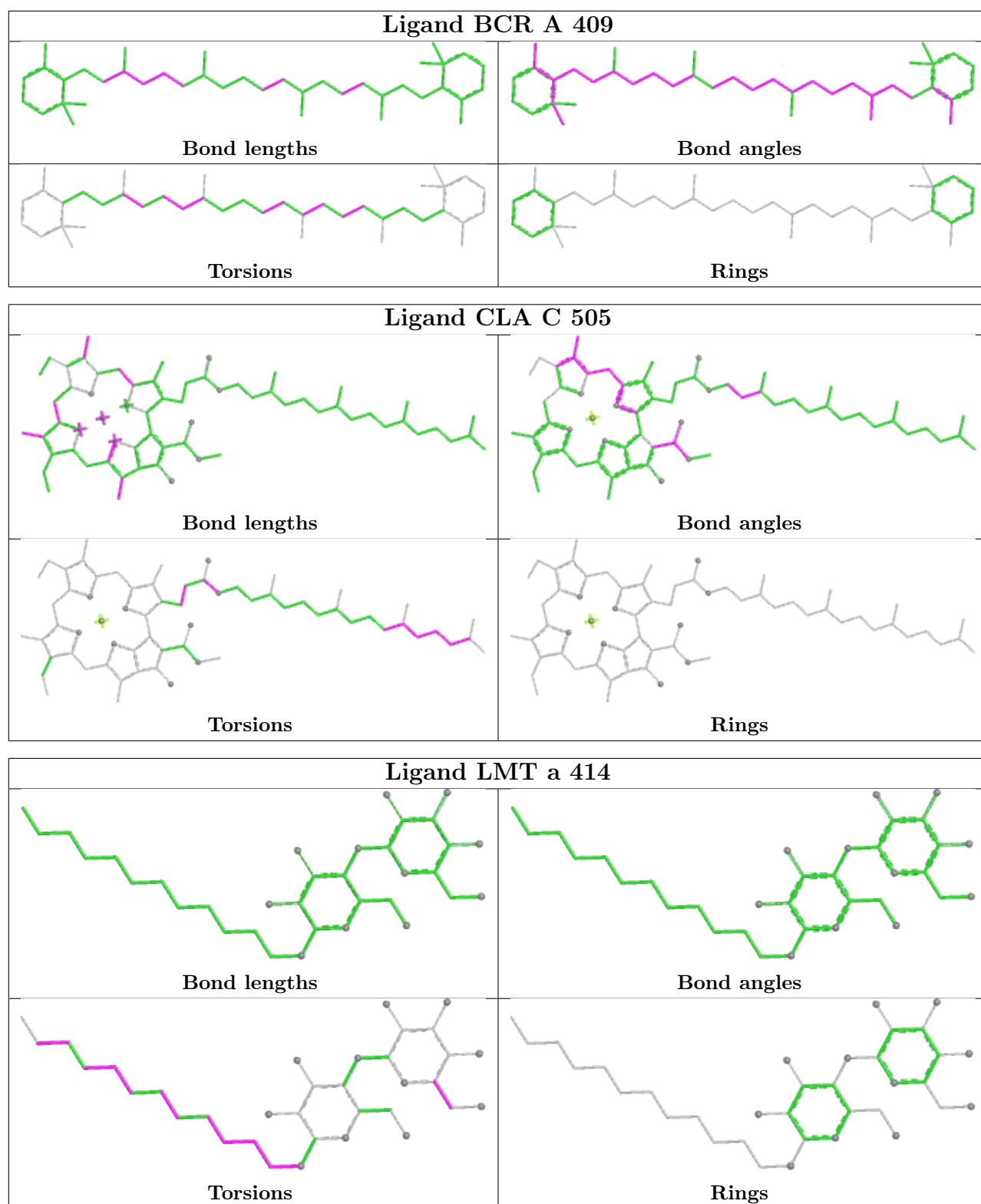




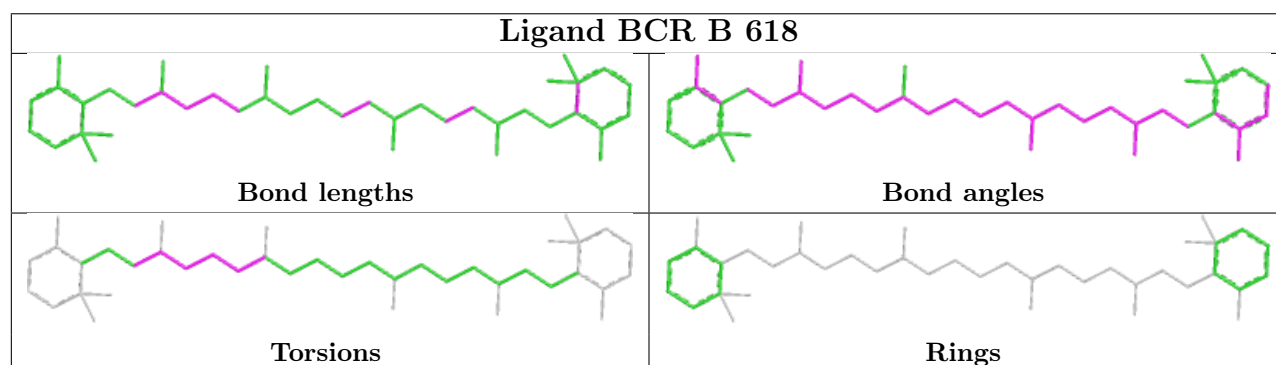
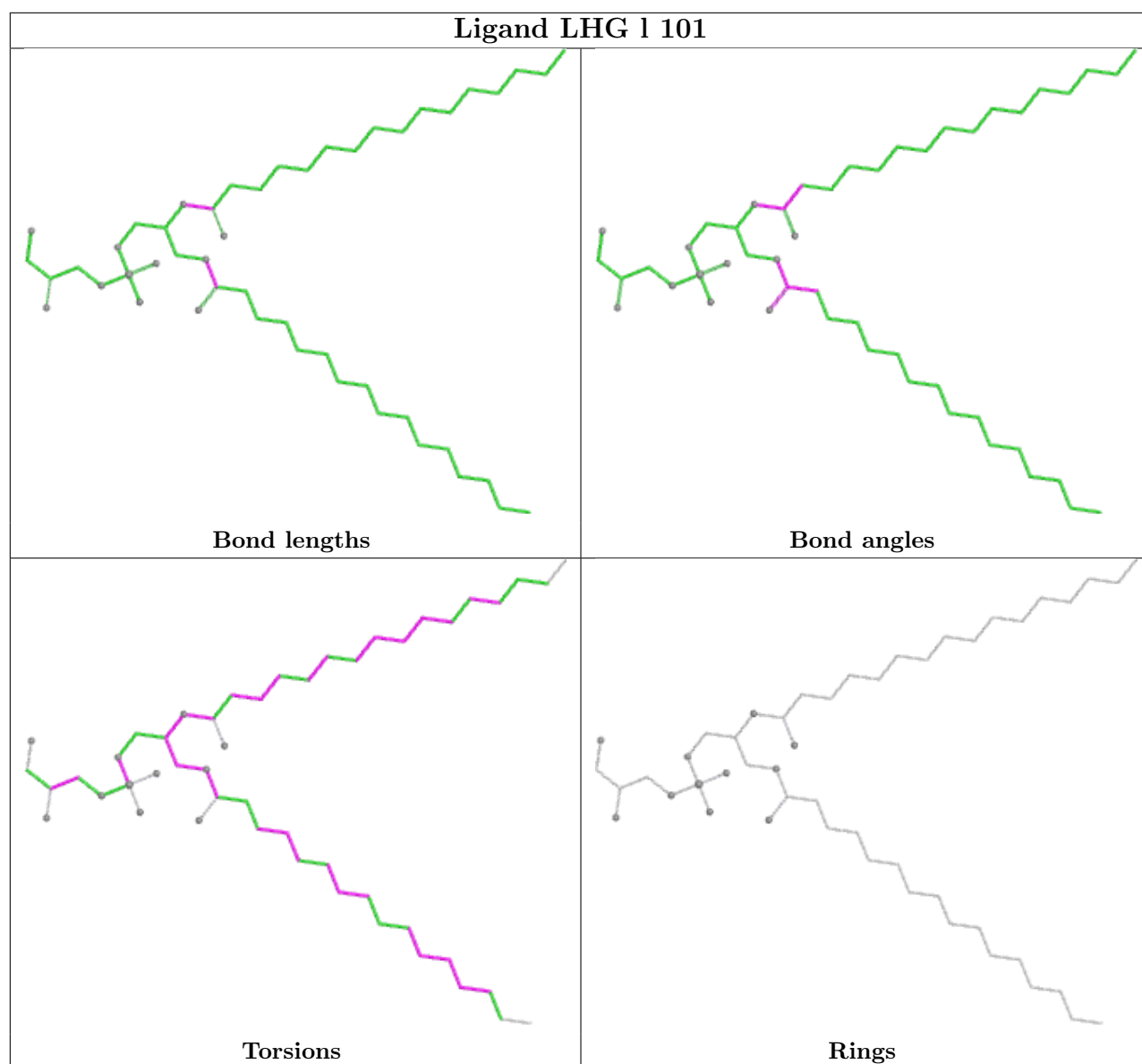


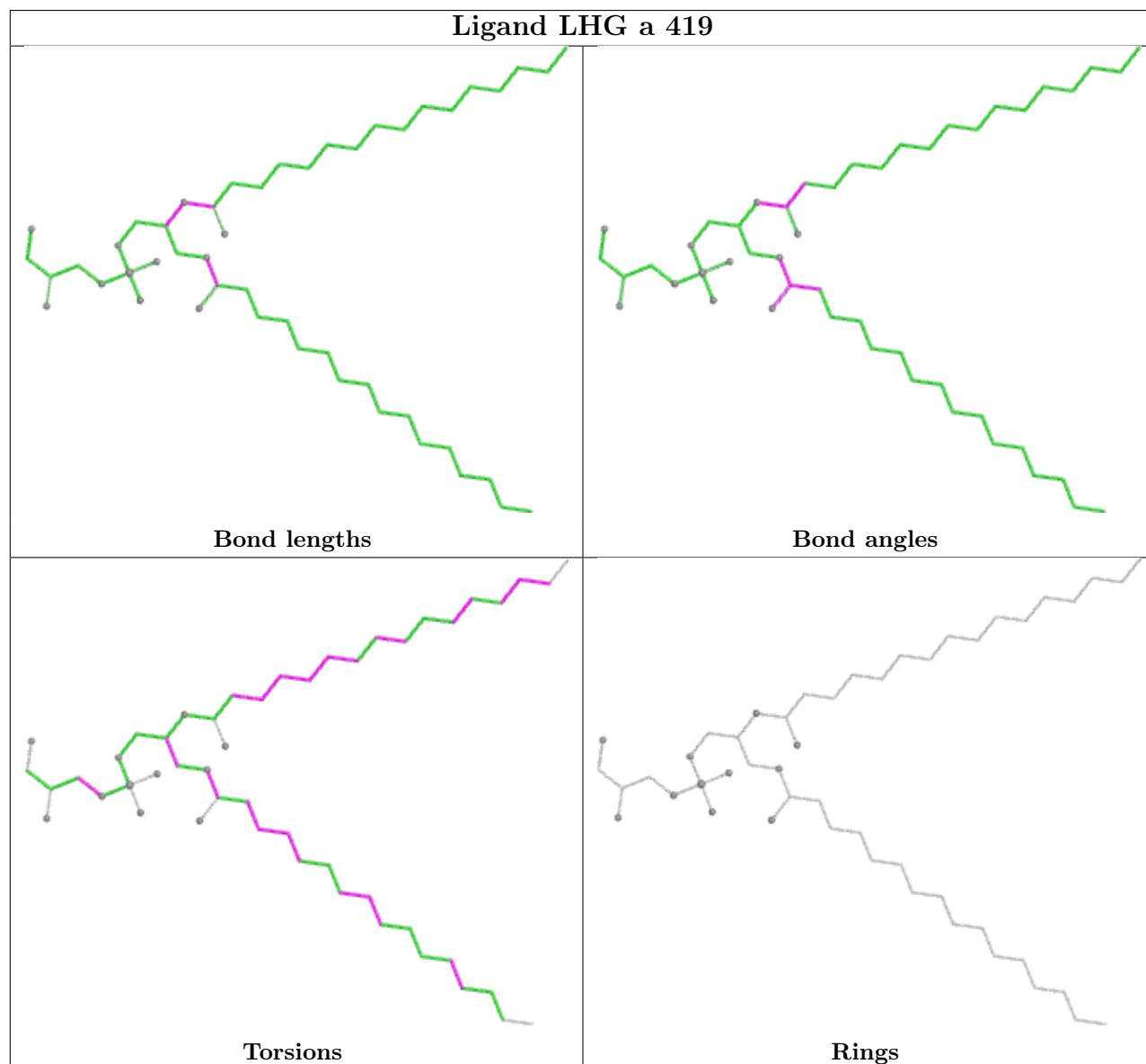
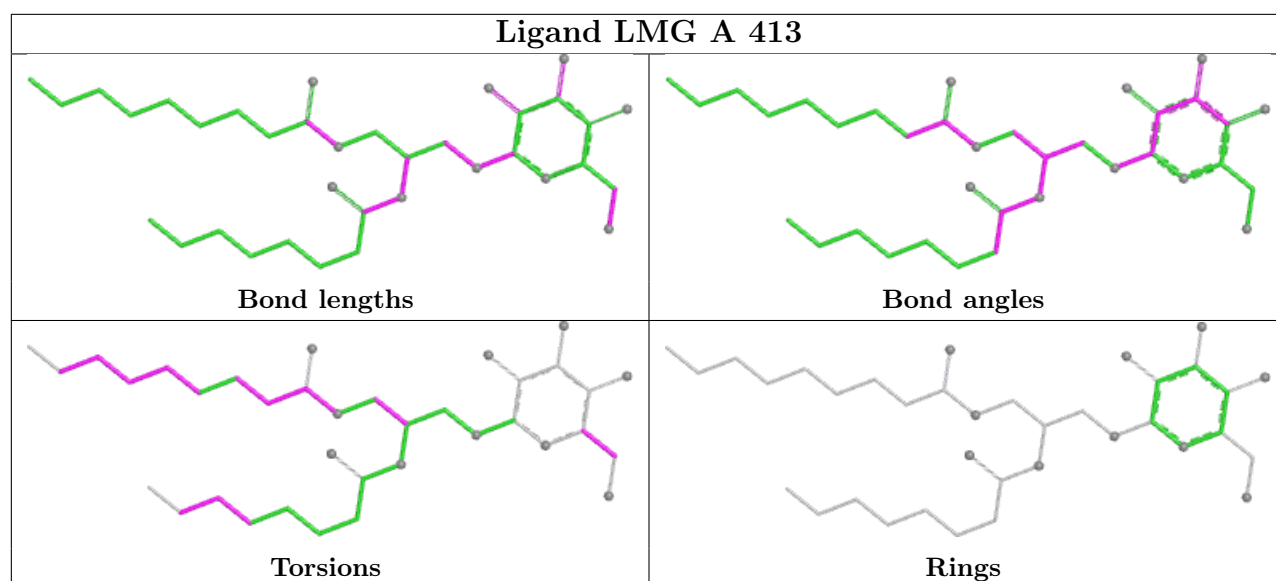


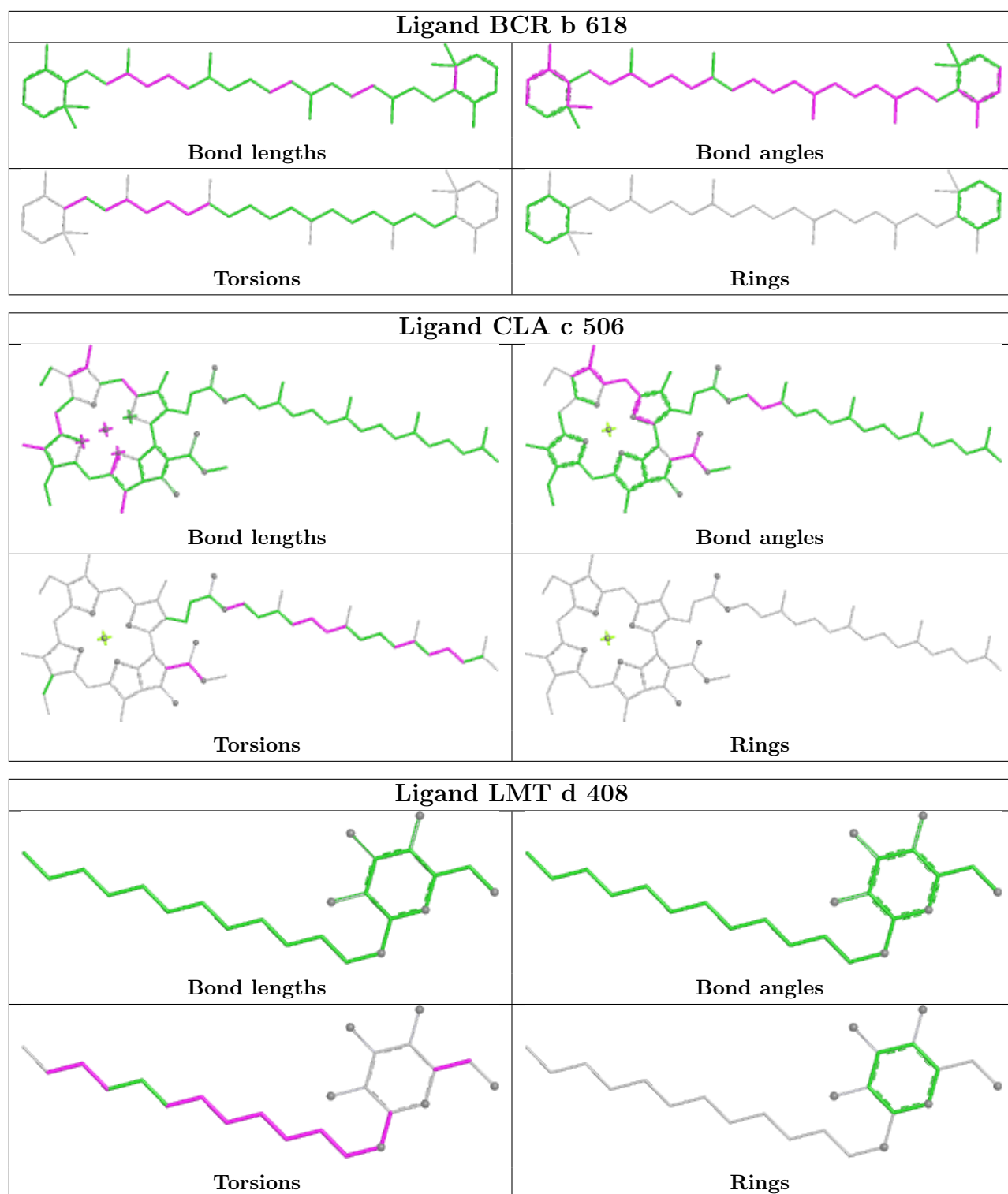


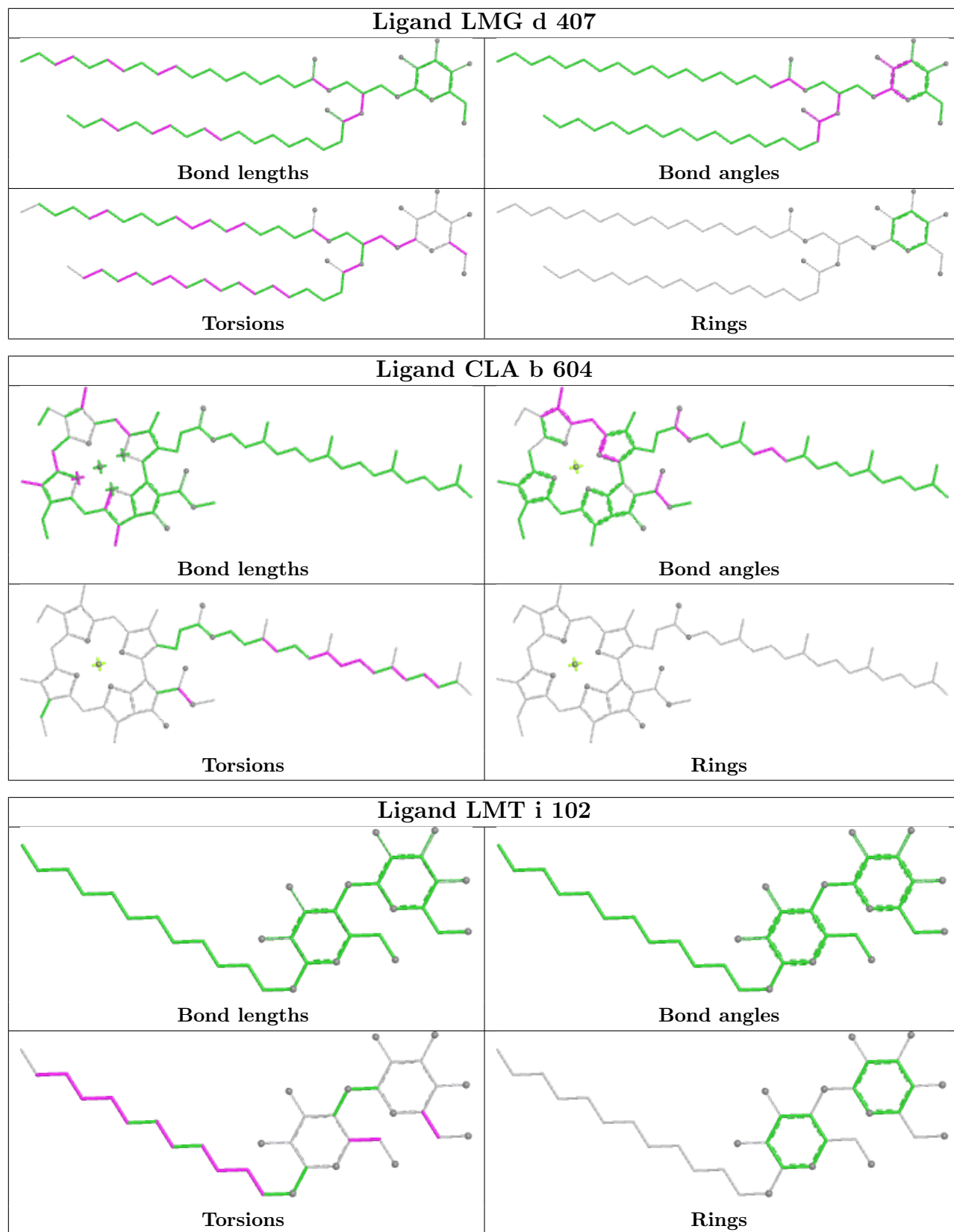




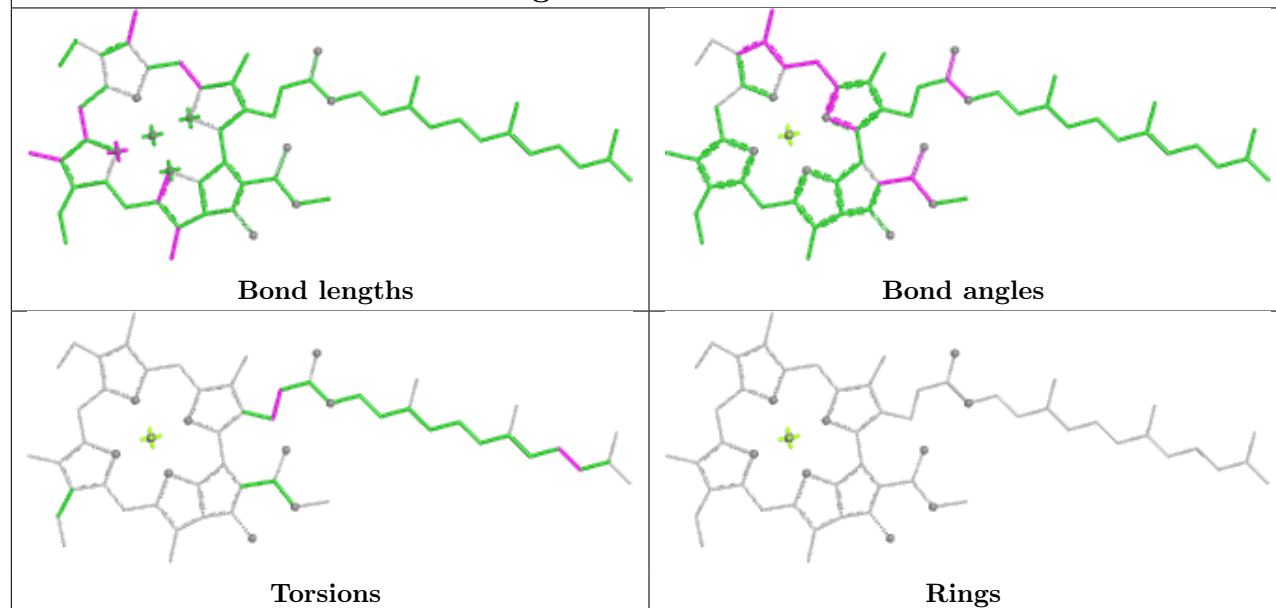




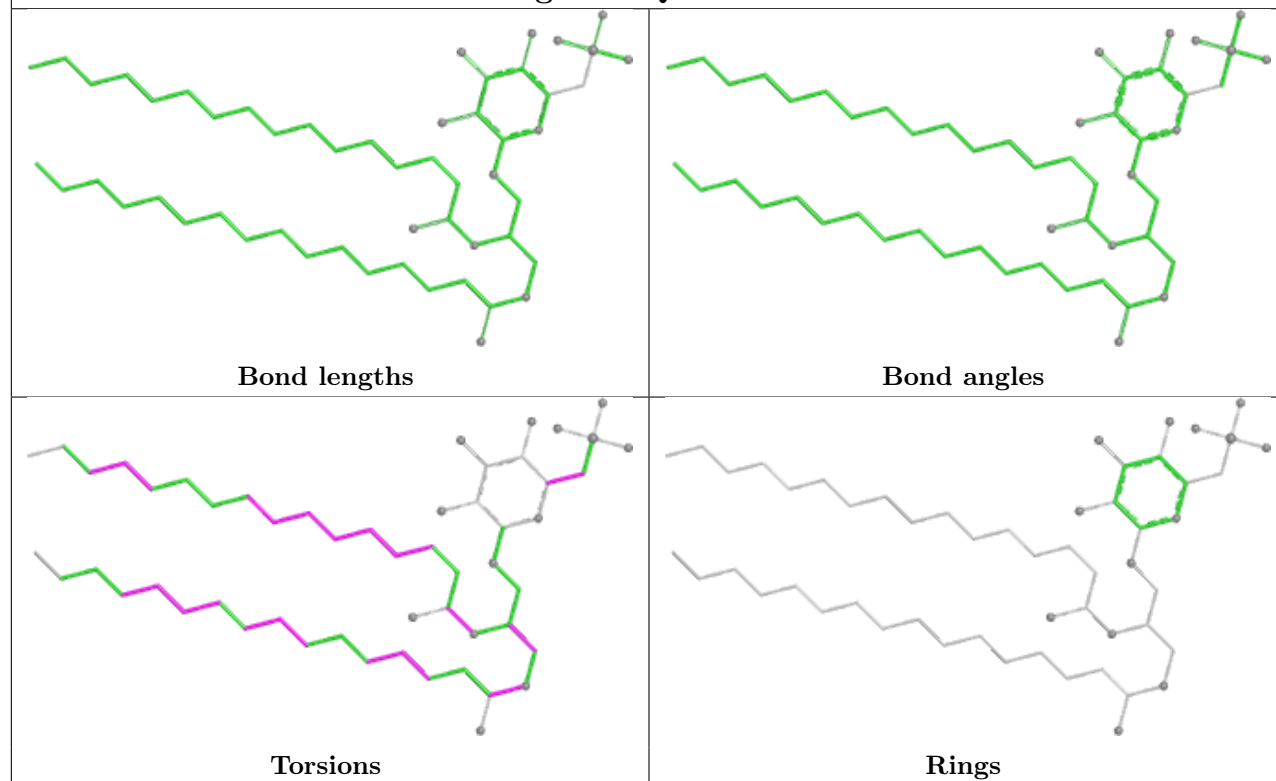


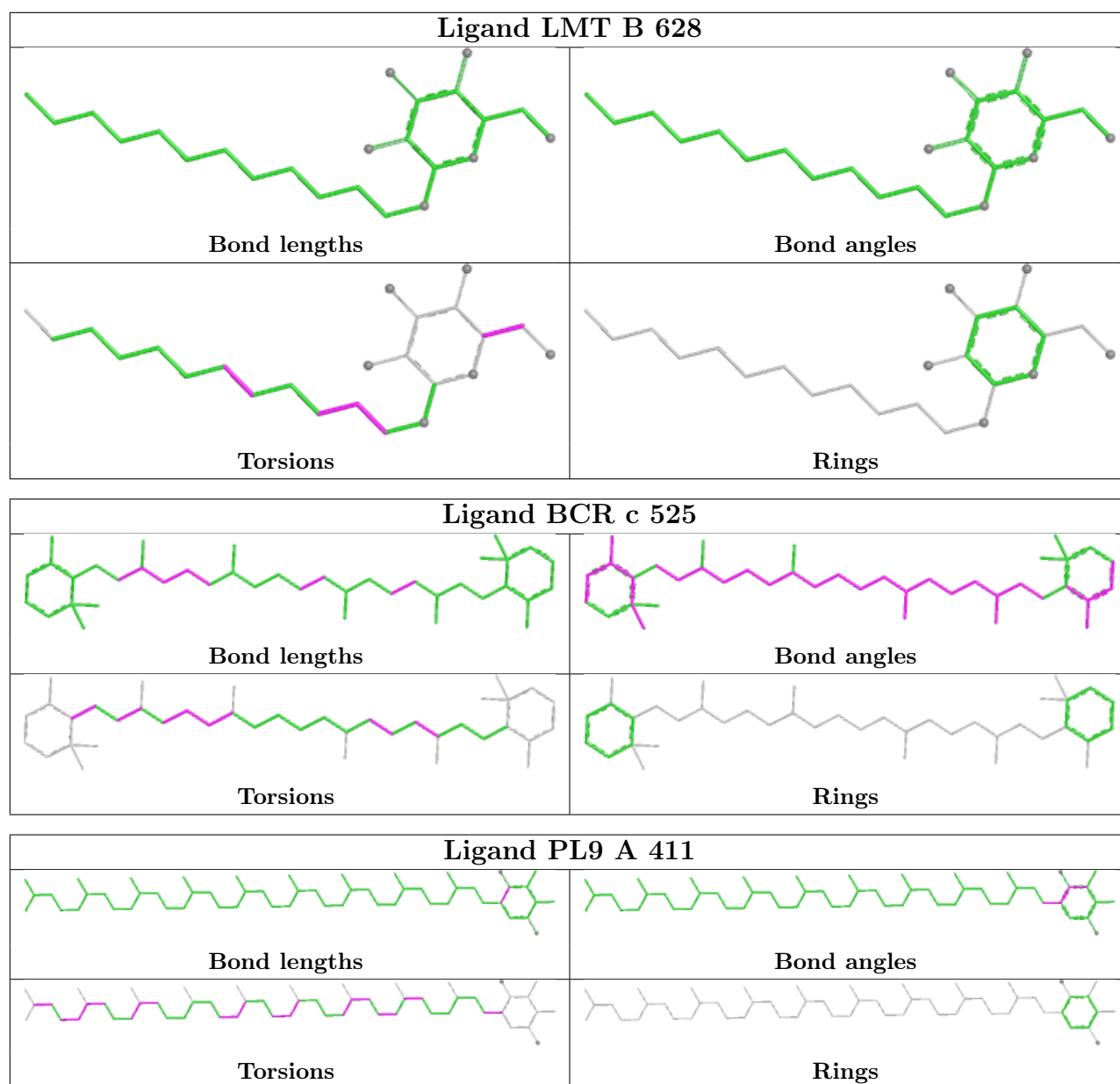


## Ligand CLA B 606



## Ligand SQD h 102





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

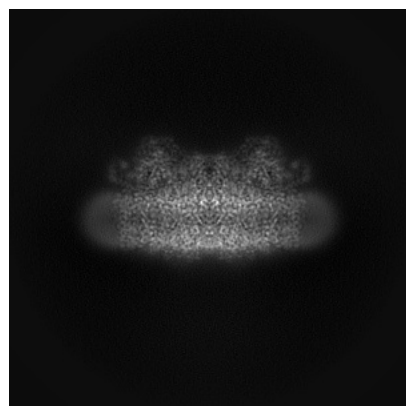
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48046. These allow visual inspection of the internal detail of the map and identification of artifacts.

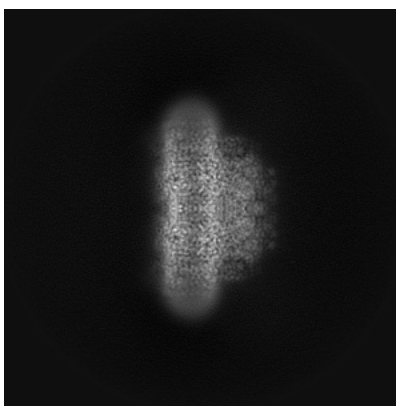
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

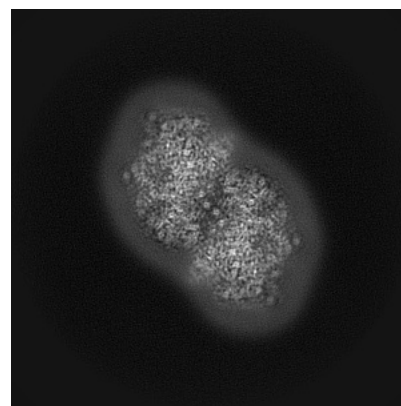
#### 6.1.1 Primary map



X

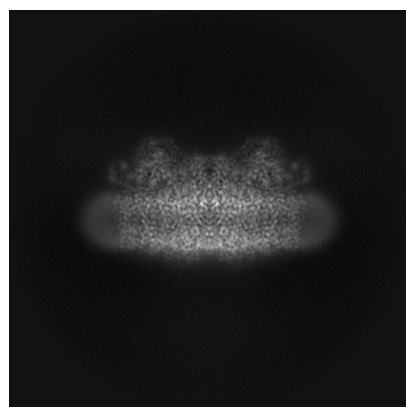


Y

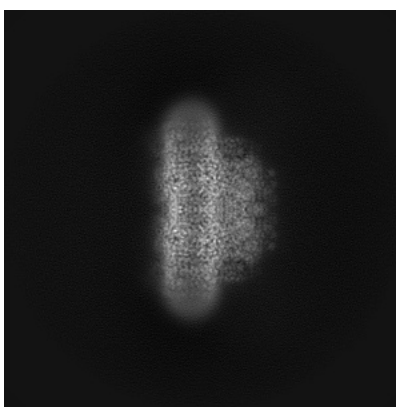


Z

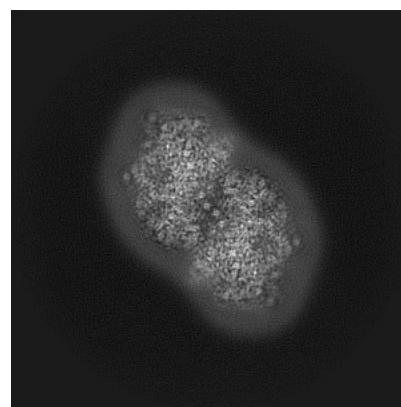
#### 6.1.2 Raw map



X



Y

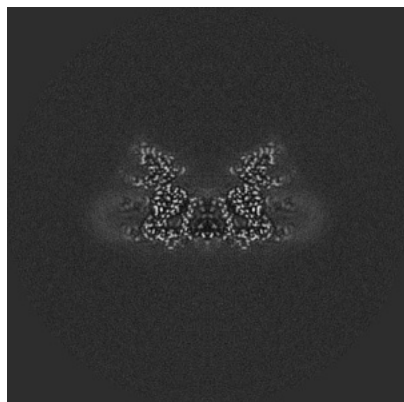


Z

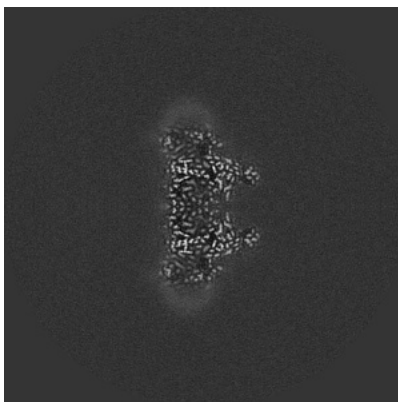
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

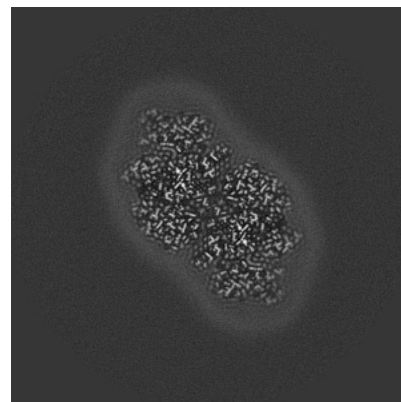
### 6.2.1 Primary map



X Index: 208

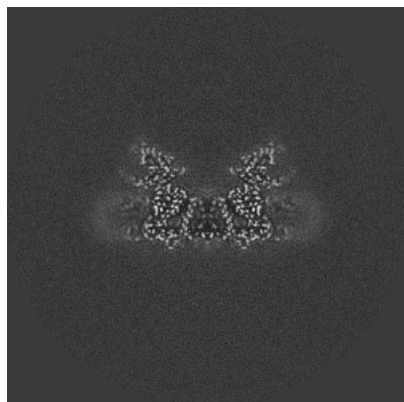


Y Index: 208

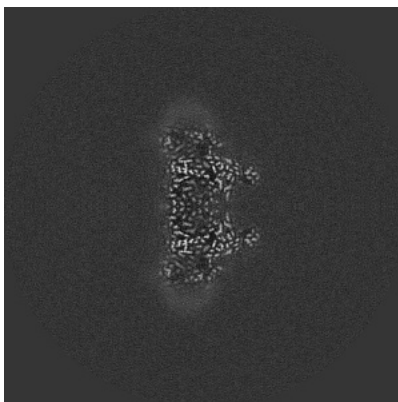


Z Index: 208

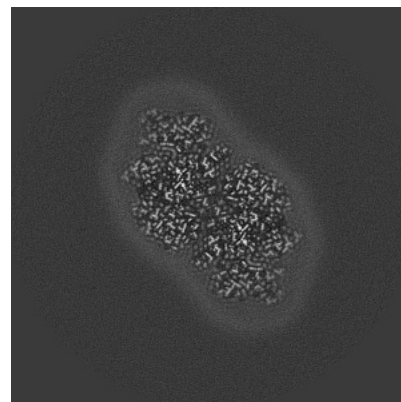
### 6.2.2 Raw map



X Index: 208



Y Index: 208



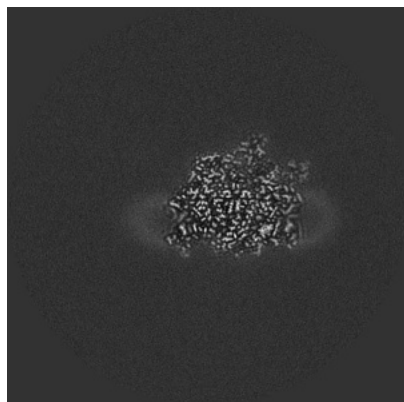
Z Index: 208

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

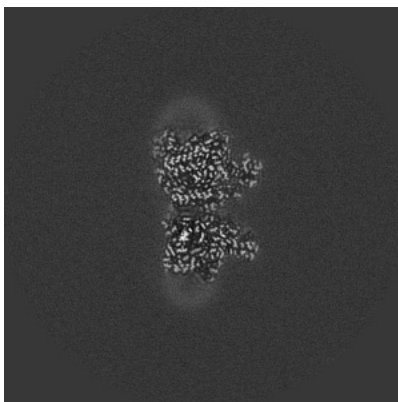


## 6.3 Largest variance slices [i](#)

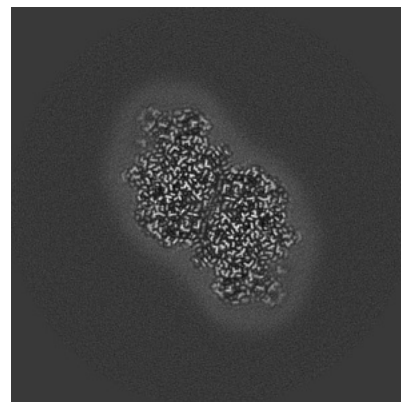
### 6.3.1 Primary map



X Index: 175

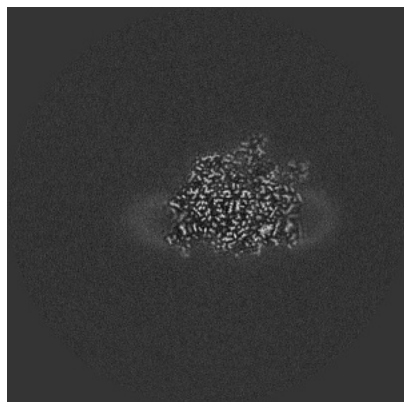


Y Index: 195

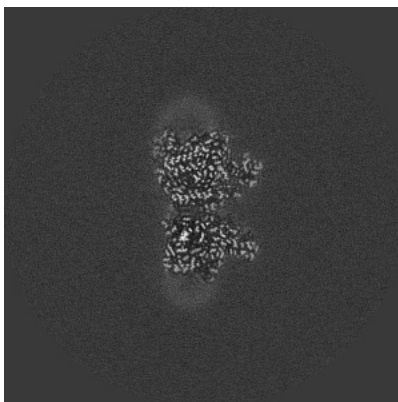


Z Index: 214

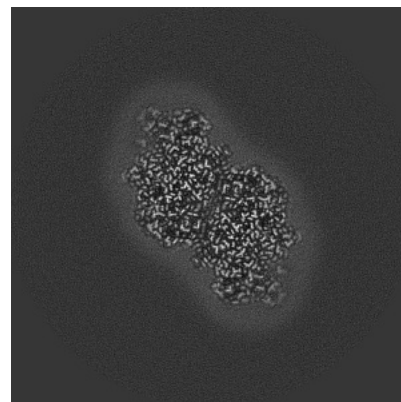
### 6.3.2 Raw map



X Index: 175



Y Index: 195

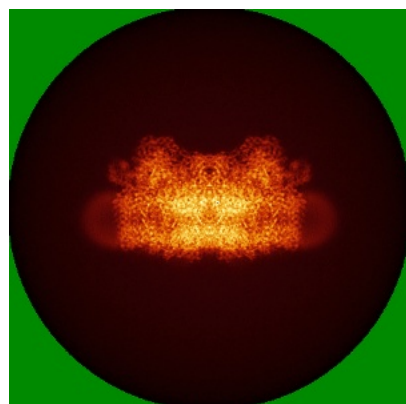


Z Index: 214

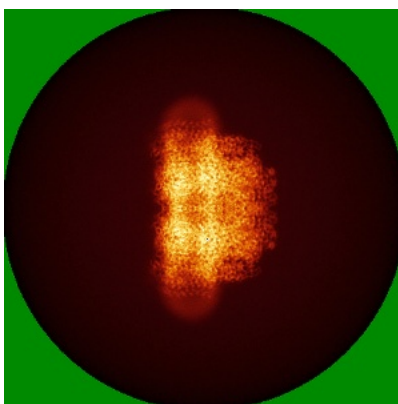
The images above show the largest variance slices of the map in three orthogonal directions.

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

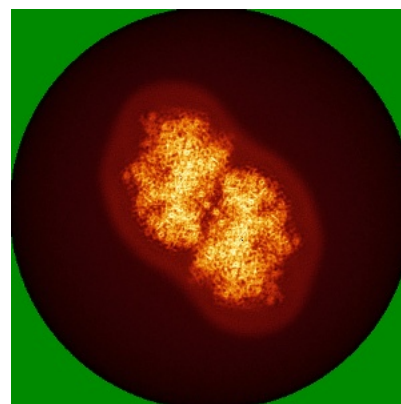
### 6.4.1 Primary map



X

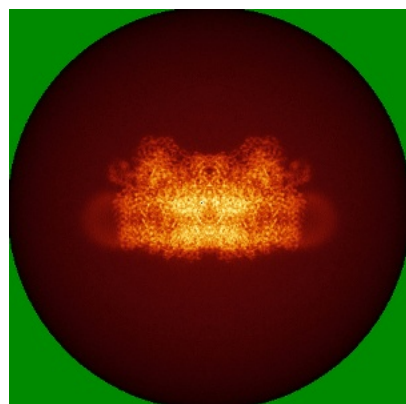


Y

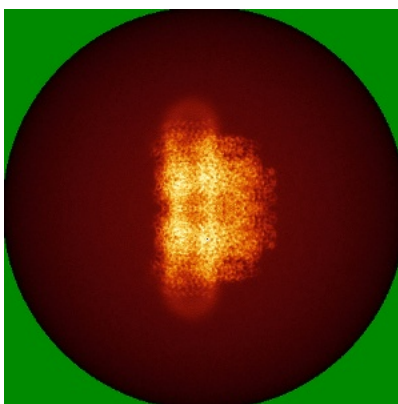


Z

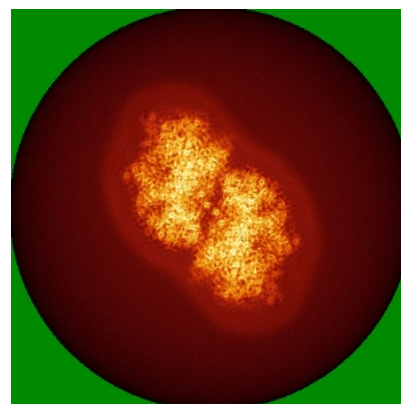
### 6.4.2 Raw map



X



Y

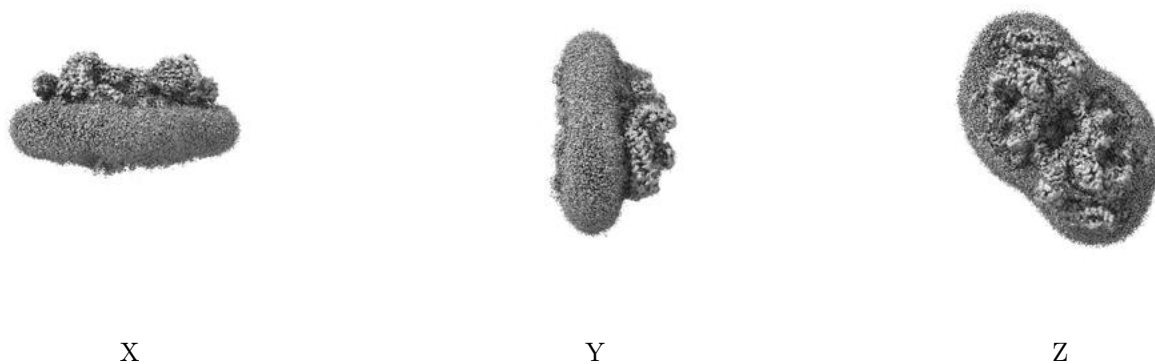


Z

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.

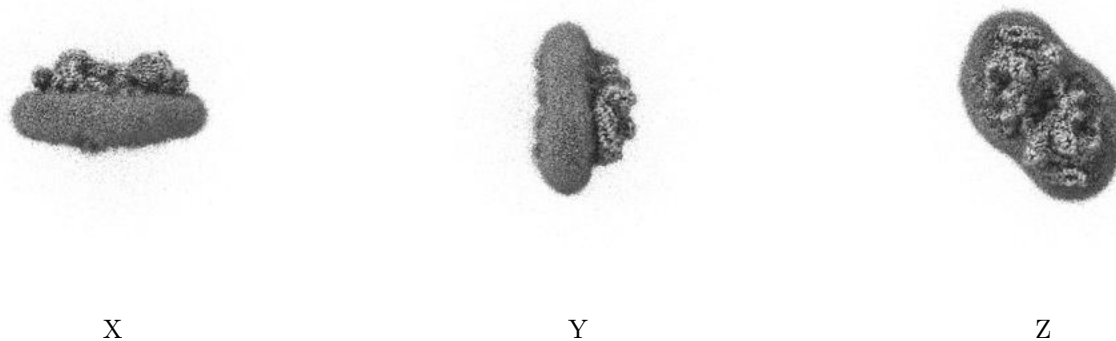
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

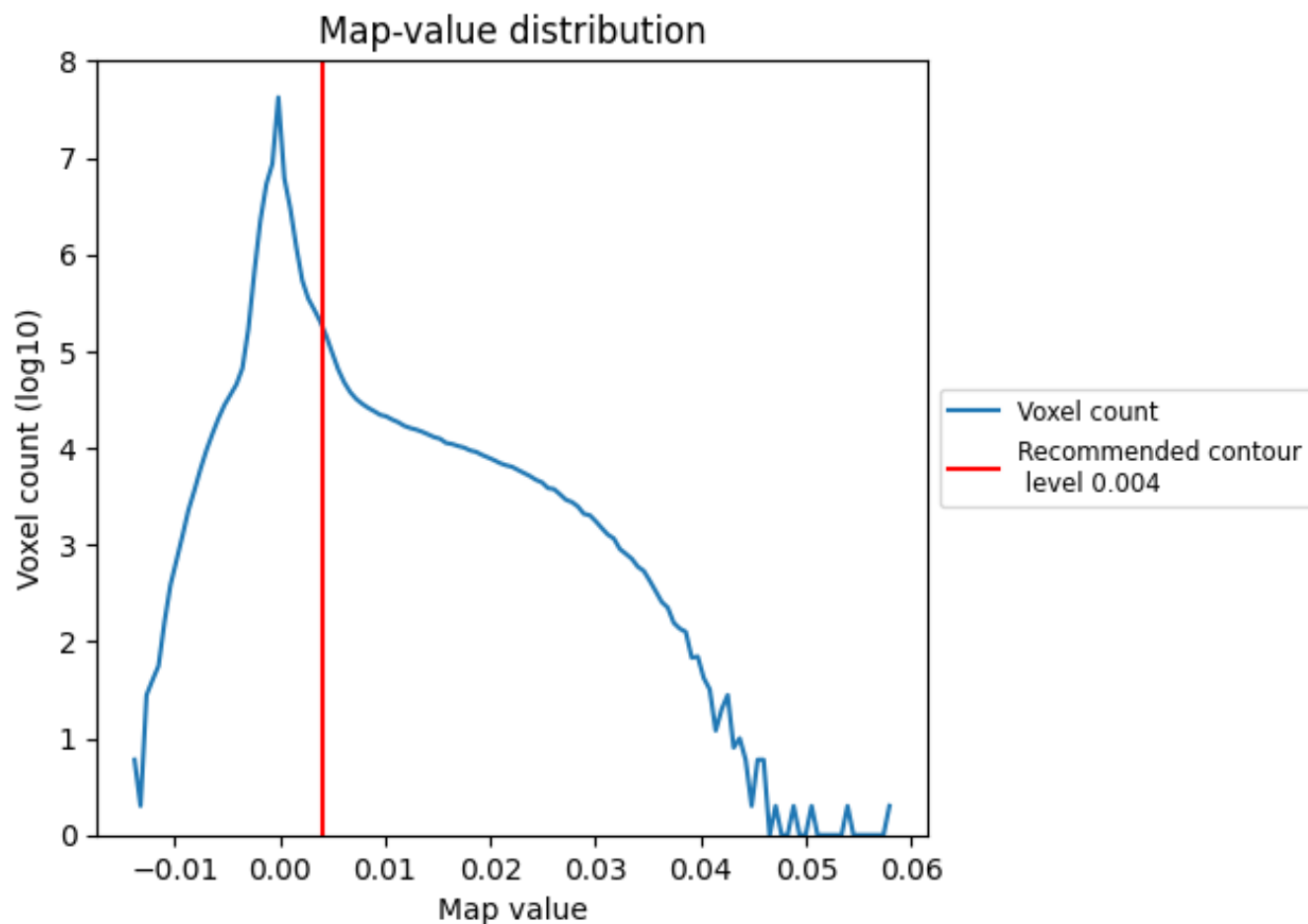
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

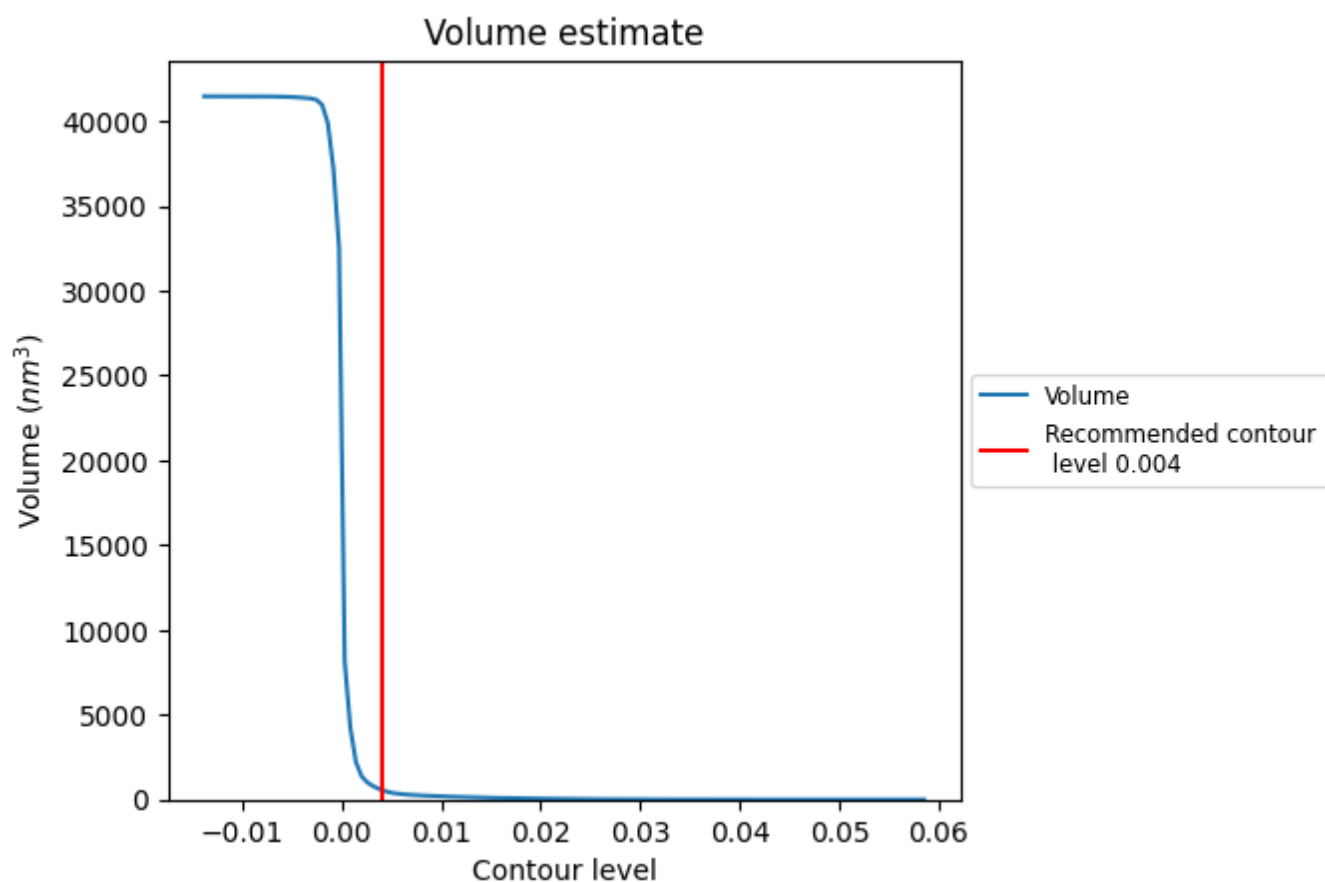
This section contains the results of statistical analysis of the map.

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



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

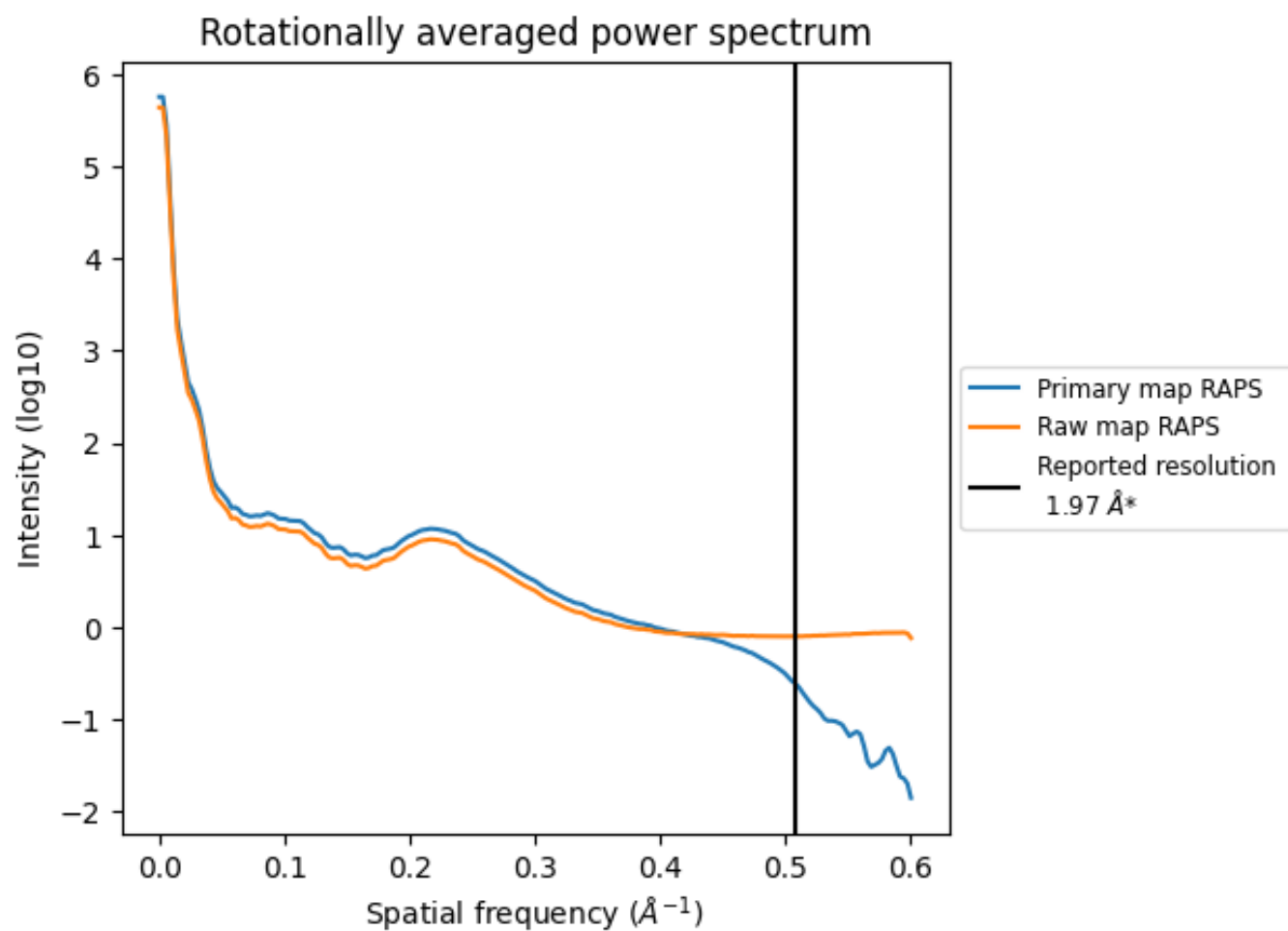
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 576 nm<sup>3</sup>; this corresponds to an approximate mass of 520 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 ⓘ

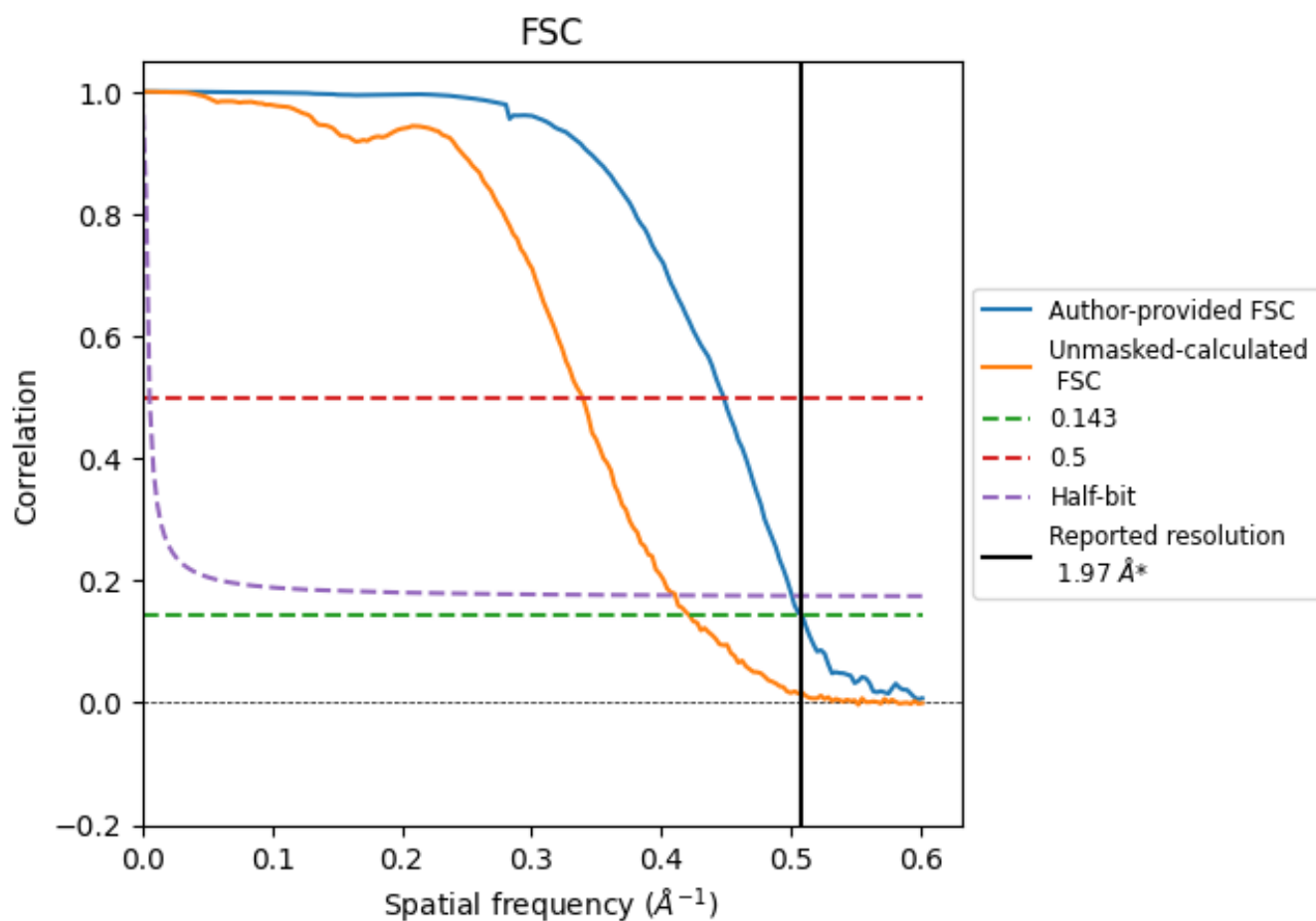


\*Reported resolution corresponds to spatial frequency of 0.508 Å<sup>-1</sup>

## 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 0.508  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.97	-	-
Author-provided FSC curve	1.97	2.23	2.00
Unmasked-calculated*	2.37	2.95	2.43

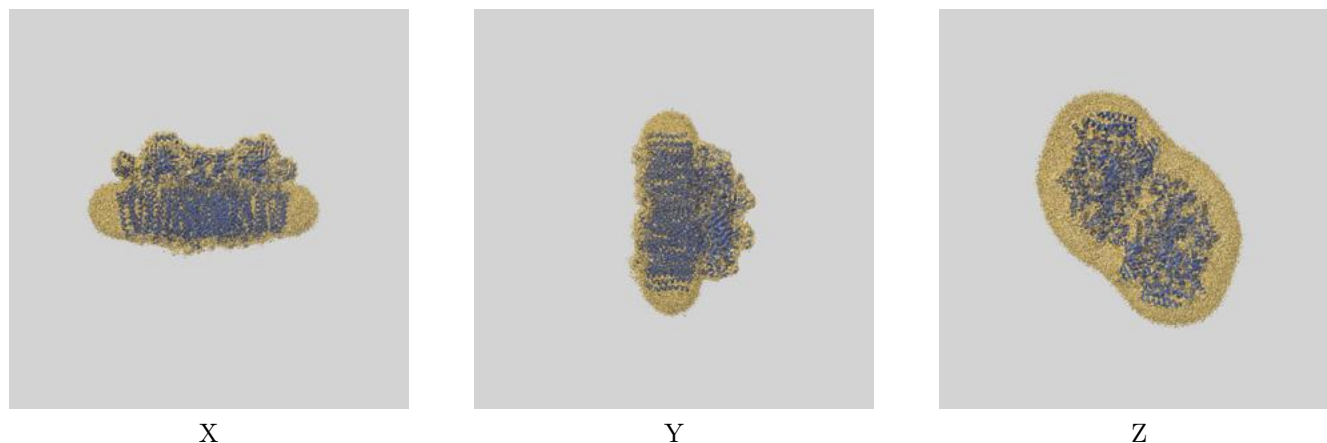
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.37 differs from the reported value 1.97 by more than 10 %



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

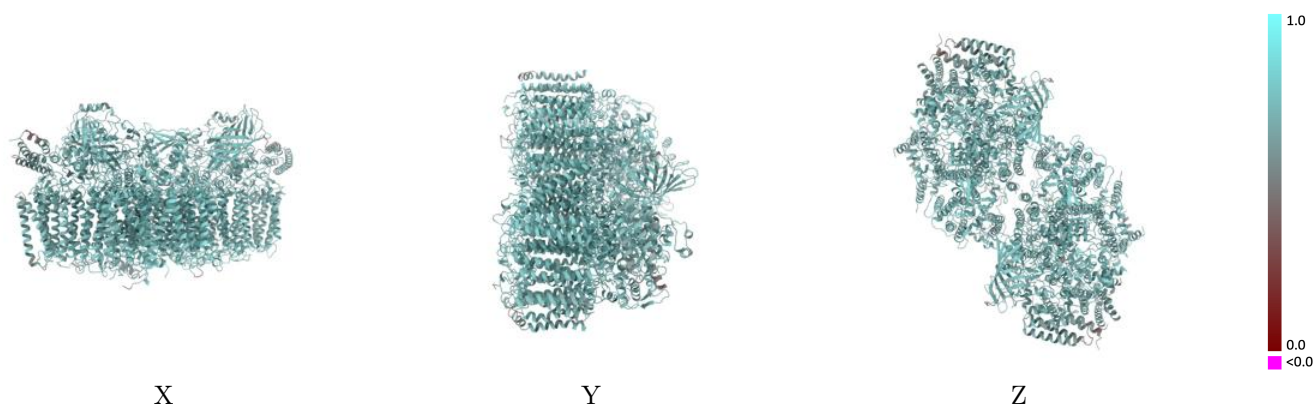
This section contains information regarding the fit between EMDB map EMD-48046 and PDB model 9EH5. Per-residue inclusion information can be found in [section 3](#) on [page 30](#).

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



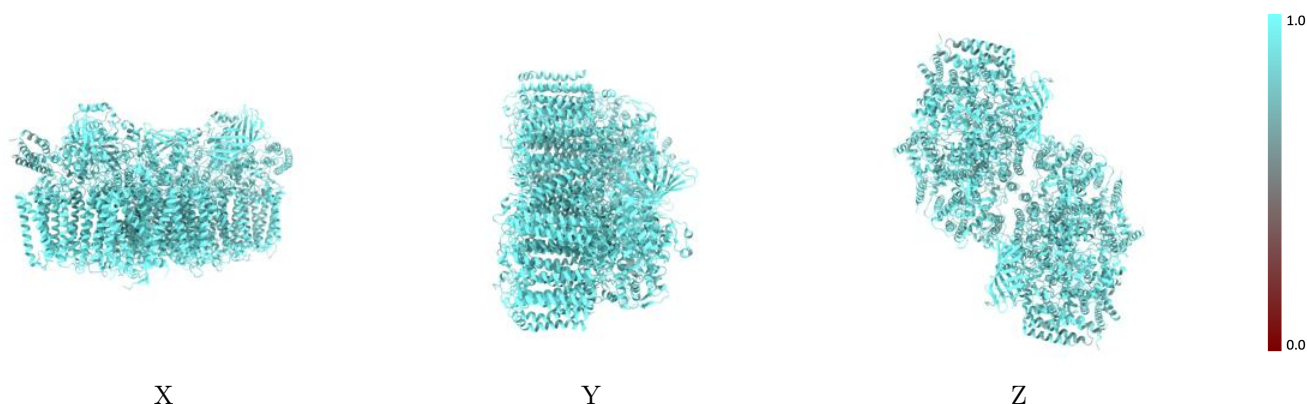
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



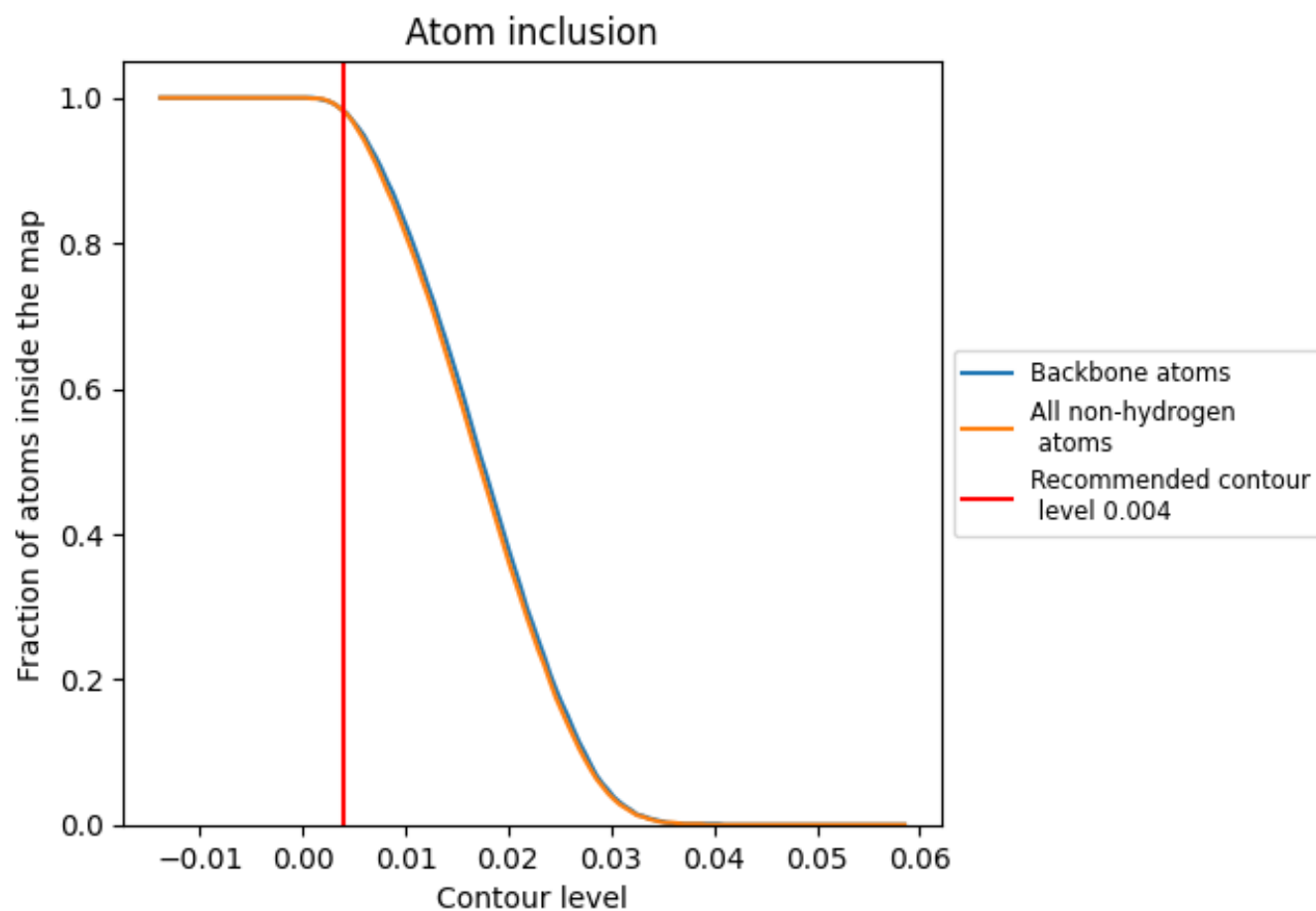
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.7030
A	 0.9870	 0.7320
B	 0.9860	 0.7180
C	 0.9900	 0.7090
D	 0.9900	 0.7350
E	 0.9750	 0.6780
F	 0.9950	 0.6820
H	 0.9830	 0.7030
I	 0.9850	 0.6800
J	 0.9790	 0.6510
K	 0.9710	 0.6660
L	 0.9940	 0.7360
M	 0.9900	 0.6860
O	 0.9700	 0.6770
Q	 0.8780	 0.6050
R	 0.9680	 0.6240
T	 0.9850	 0.7150
U	 0.9640	 0.6820
V	 0.9820	 0.6970
X	 0.9780	 0.6510
Y	 0.9880	 0.6500
Z	 0.9800	 0.6330
a	 0.9870	 0.7310
b	 0.9860	 0.7180
c	 0.9900	 0.7090
d	 0.9900	 0.7350
e	 0.9750	 0.6760
f	 0.9950	 0.6810
h	 0.9830	 0.7010
i	 0.9850	 0.6750
j	 0.9790	 0.6550
k	 0.9740	 0.6620
l	 0.9940	 0.7330
m	 0.9900	 0.6880
o	 0.9700	 0.6770



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Chain	Atom inclusion	Q-score
q	 0.8780	 0.6020
r	 0.9680	 0.6200
t	 0.9850	 0.7170
u	 0.9640	 0.6820
v	 0.9820	 0.6960
x	 0.9780	 0.6500
y	 0.9880	 0.6530
z	 0.9800	 0.6390