



Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 08:54 PM EST

PDB ID : 9PHW / pdb_00009phw
EMDB ID : EMD-71652
Title : Structure of the D1-Val185Asn mutated photosystem II complex with slow O-O bond formation reveals changes in the Cl1 water channel
Authors : Flesher, D.A.; Debus, R.J.; Brudvig, G.W.
Deposited on : 2025-07-09
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

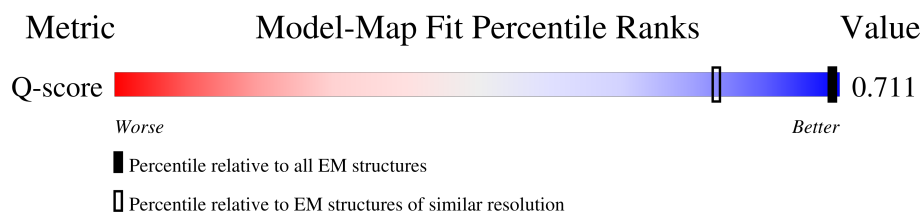
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.99 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	1416 (1.50 - 2.49)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 54592 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
			2626	1717	430	464	15		
1	a	334	Total	C	N	O	S	0	0
			2626	1717	430	464	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASN	VAL	engineered mutation	UNP P16033
a	185	ASN	VAL	engineered mutation	UNP P16033

- 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		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	508	HIS	-	expression tag	UNP P05429
B	509	HIS	-	expression tag	UNP P05429
B	510	HIS	-	expression tag	UNP P05429
B	511	HIS	-	expression tag	UNP P05429
B	512	HIS	-	expression tag	UNP P05429
B	513	HIS	-	expression tag	UNP P05429
b	508	HIS	-	expression tag	UNP P05429
b	509	HIS	-	expression tag	UNP P05429
b	510	HIS	-	expression tag	UNP P05429
b	511	HIS	-	expression tag	UNP P05429
b	512	HIS	-	expression tag	UNP P05429

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Chain	Residue	Modelled	Actual	Comment	Reference
b	513	HIS	-	expression tag	UNP P05429

- 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	1	0
			2735	1813	445	465	12		
4	d	341	Total	C	N	O	S	1	0
			2735	1813	445	465	12		

- 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	34	Total	C	N	O	S	0	0
			274	186	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			274	186	45	42	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	35	Total	C	N	O	S	0	0
			246	166	39	40	1		
9	j	35	Total	C	N	O	S	0	0
			246	166	39	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	N	O	S	0	0
			299	210	42	47			
10	k	37	Total	C	N	O	S	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	242	Total	C	N	O	S	0	0
			1865	1182	304	376	3		
13	o	242	Total	C	N	O	S	0	0
			1865	1182	304	376	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	114	Total	C	N	O	S	0	0
			891	561	159	169	2		
14	q	114	Total	C	N	O	S	0	0
			891	561	159	169	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		

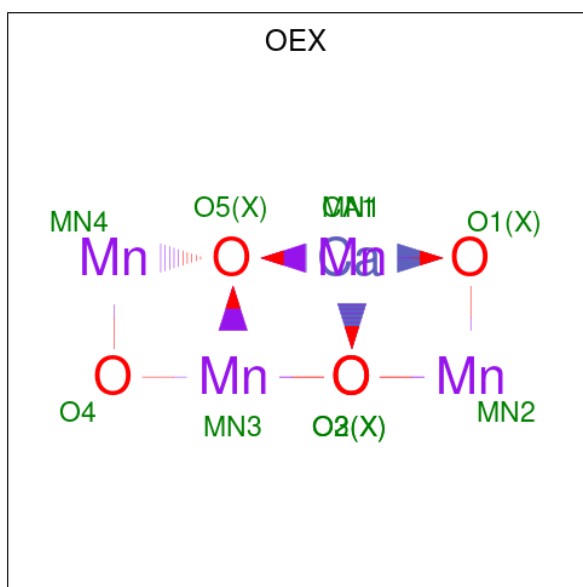
- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total	C	N	O	0	0
			242	165	37	40		
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	0
			460	317	70	72	1		
21	z	60	Total	C	N	O	S	0	0
			460	317	70	72	1		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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	

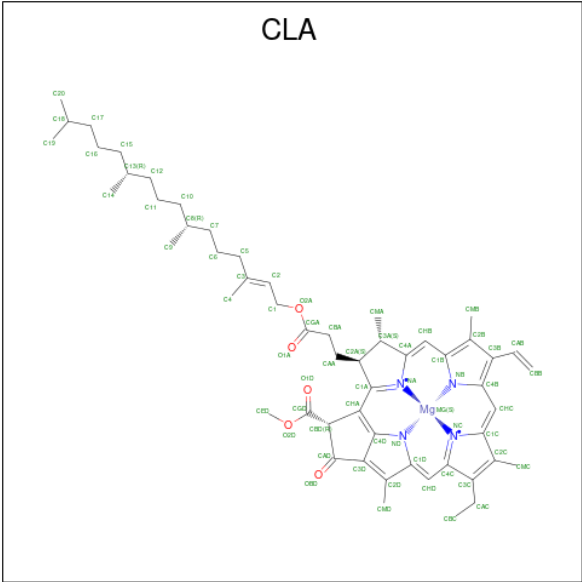
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: CL) (formula: Cl).

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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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	
25	B	1	Total	C	Mg	N	O	0
			60	50	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	
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 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
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

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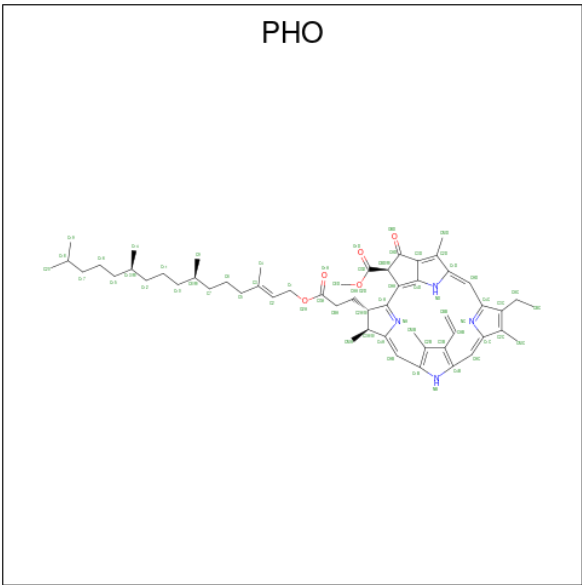
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total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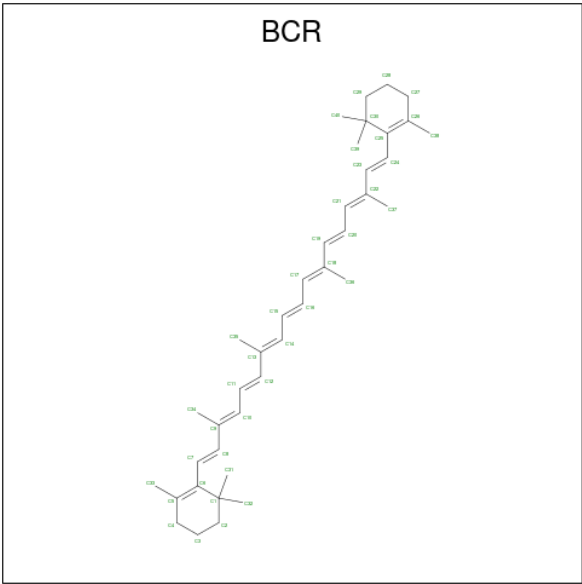
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0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

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



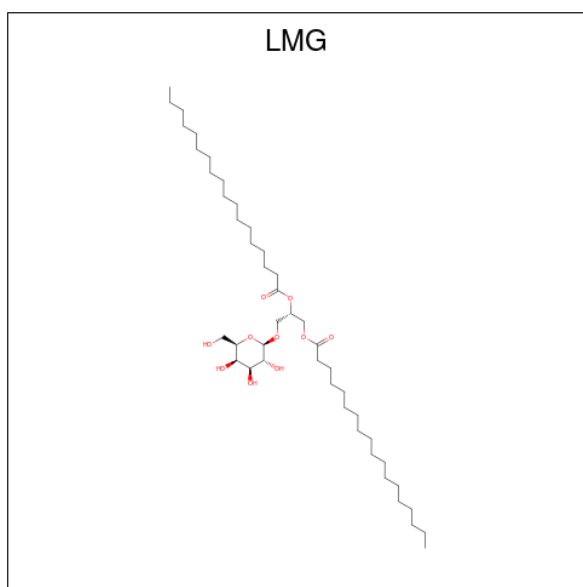
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



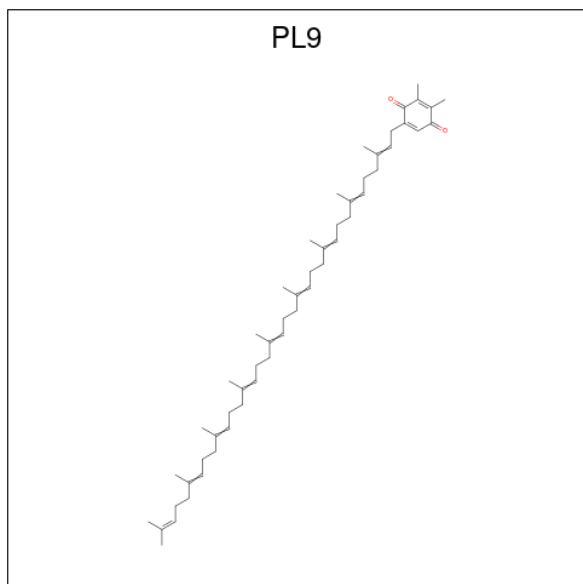
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	Z	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	f	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	z	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



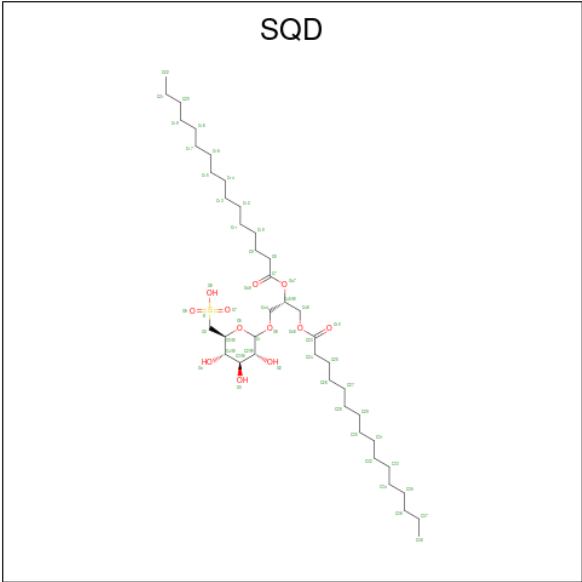
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	41	10	
28	A	1	Total	C	O	0
			36	26	10	
28	B	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			49	39	10	
28	D	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			55	45	10	
28	a	1	Total	C	O	0
			51	41	10	
28	a	1	Total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

- 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



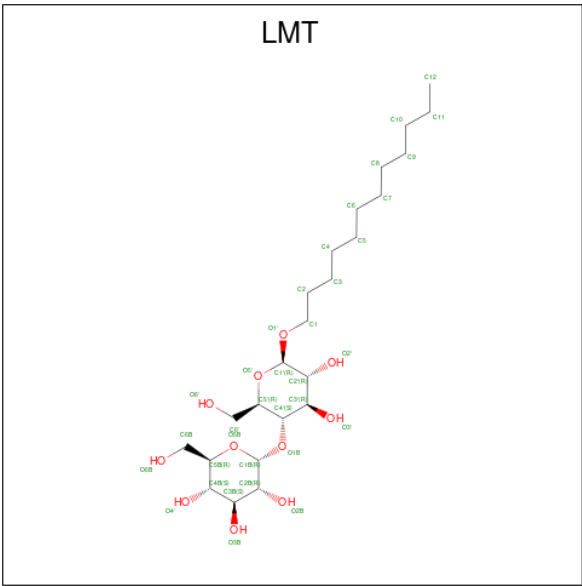
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			44	31	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	C	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
			54	41	12	1	
30	a	1	Total	C	O	S	0
			44	31	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	c	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-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
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	

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Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			35	24	11	
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	I	1	Total	C	O	0
			24	18	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	K	1	Total	C	O	0
			35	24	11	
31	L	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			24	18	6	
31	M	1	Total	C	O	0
			35	24	11	
31	T	1	Total	C	O	0
			24	18	6	
31	X	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	Y	1	Total	C	O	0
			21	15	6	
31	a	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			35	24	11	

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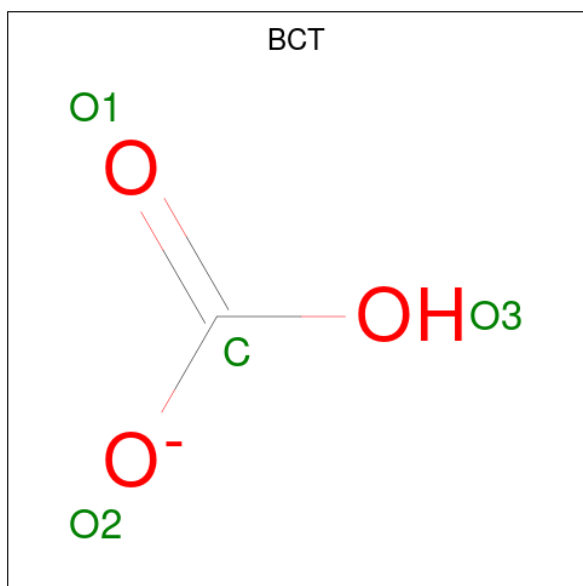
Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			21	15	6	
31	c	1	Total	C	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	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	i	1	Total	C	O	0
			24	18	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	k	1	Total	C	O	0
			35	24	11	

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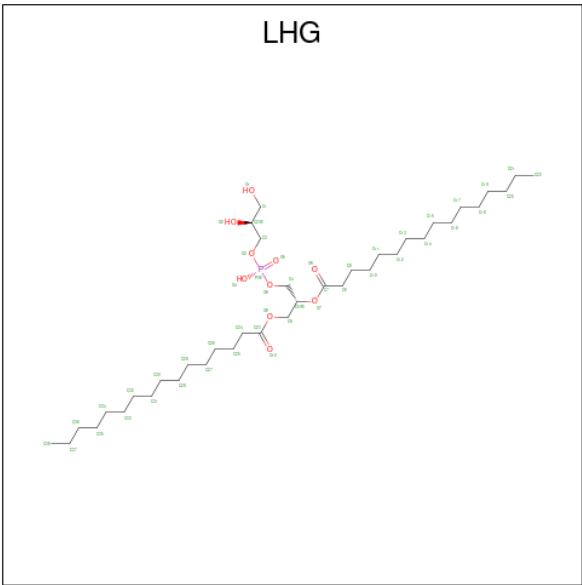
Mol	Chain	Residues	Atoms			AltConf
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			35	24	11	
31	x	1	Total	C	O	0
			22	17	5	
31	x	1	Total	C	O	0
			22	16	6	
31	y	1	Total	C	O	0
			21	15	6	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



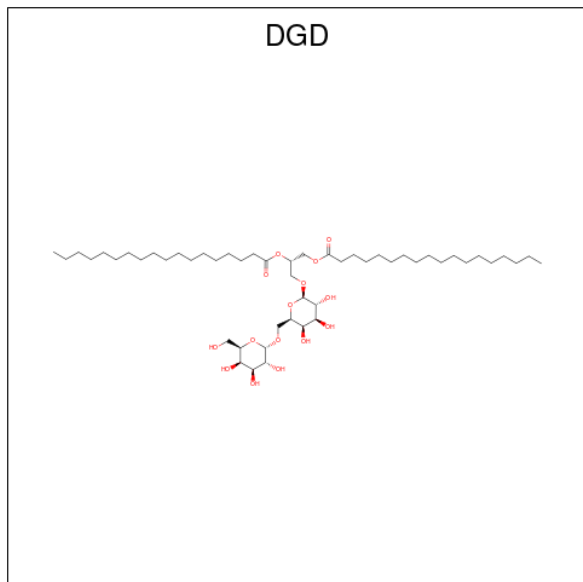
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



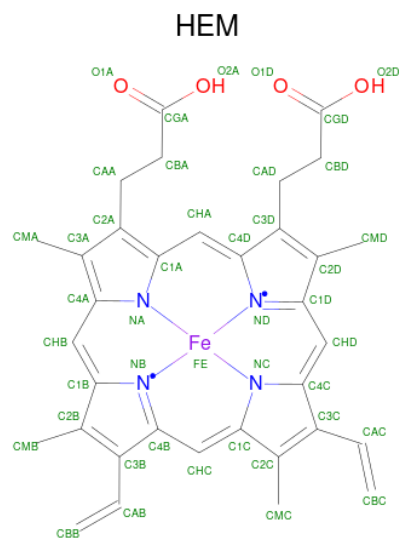
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	b	1	Total	C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

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



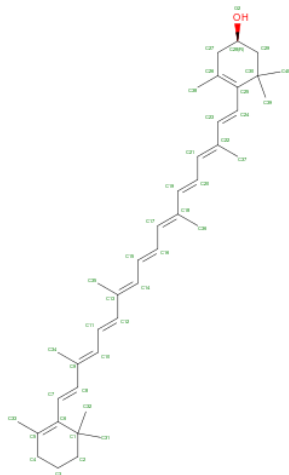
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

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



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

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (CCD ID: 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 (CCD ID: 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	114	Total	O	0
			114	114	
38	B	106	Total	O	0
			106	106	
38	C	91	Total	O	0
			91	91	
38	D	93	Total	O	0
			93	93	
38	E	8	Total	O	0
			8	8	
38	F	5	Total	O	0
			5	5	
38	H	9	Total	O	0
			9	9	
38	I	2	Total	O	0
			2	2	
38	J	6	Total	O	0
			6	6	
38	L	8	Total	O	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
38	M	2	Total 2	O 2	0
38	O	25	Total 25	O 25	0
38	T	5	Total 5	O 5	0
38	U	6	Total 6	O 6	0
38	V	26	Total 26	O 26	0
38	X	2	Total 2	O 2	0
38	a	114	Total 114	O 114	0
38	b	106	Total 106	O 106	0
38	c	91	Total 91	O 91	0
38	d	93	Total 93	O 93	0
38	e	8	Total 8	O 8	0
38	f	5	Total 5	O 5	0
38	h	9	Total 9	O 9	0
38	i	2	Total 2	O 2	0
38	j	6	Total 6	O 6	0
38	l	8	Total 8	O 8	0
38	m	2	Total 2	O 2	0
38	o	25	Total 25	O 25	0
38	t	5	Total 5	O 5	0
38	u	6	Total 6	O 6	0
38	v	26	Total 26	O 26	0

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Mol	Chain	Residues	Atoms		AltConf
38	x	2	Total	O	0
			2	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	72628	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 ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0022	Depositor
Map size (Å)	389.4, 389.4, 389.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.649, 0.649, 0.649	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

6 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	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.34	0	8,9,11	0.75	0
8	FME	i	1	8	8,9,10	0.40	0	8,9,11	0.62	0
16	FME	t	1	16	8,9,10	0.46	0	8,9,11	1.48	2 (25%)
8	FME	I	1	8	8,9,10	0.40	0	8,9,11	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.34	0	8,9,11	0.75	0
16	FME	T	1	16	8,9,10	0.45	0	8,9,11	1.48	2 (25%)

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
12	FME	m	1	12	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
16	FME	t	1	16	-	5/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-
16	FME	T	1	16	-	5/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	t	1	FME	O-C-CA	-2.89	117.34	124.77
16	T	1	FME	O-C-CA	-2.89	117.34	124.77
16	T	1	FME	CA-N-CN	2.24	126.27	122.82
16	t	1	FME	CA-N-CN	2.24	126.27	122.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
16	T	1	FME	O1-CN-N-CA
16	T	1	FME	C-CA-CB-CG
8	i	1	FME	O-C-CA-CB
16	t	1	FME	O1-CN-N-CA
16	t	1	FME	C-CA-CB-CG
16	T	1	FME	CA-CB-CG-SD
16	t	1	FME	CA-CB-CG-SD
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
12	M	1	FME	CB-CG-SD-CE
12	m	1	FME	CB-CG-SD-CE
16	T	1	FME	N-CA-CB-CG
16	t	1	FME	N-CA-CB-CG
12	M	1	FME	C-CA-CB-CG
12	m	1	FME	C-CA-CB-CG
8	I	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN
16	T	1	FME	CB-CG-SD-CE
16	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 230 ligands modelled in this entry, 12 are monoatomic - leaving 218 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	$\# Z > 2$
31	LMT	i	103	-	22,22,36	0.38	0	27,27,47	0.72	0
31	LMT	Y	101	-	21,21,36	0.35	0	26,26,47	0.73	0
30	SQD	A	413	-	42,44,54	0.45	1 (2%)	52,55,65	0.53	1 (1%)
31	LMT	x	102	-	22,22,36	0.49	0	27,27,47	0.90	0
36	RRX	H	101	-	42,42,42	1.44	6 (14%)	56,58,58	1.36	11 (19%)
30	SQD	a	413	-	42,44,54	0.45	1 (2%)	52,55,65	0.54	1 (1%)
28	LMG	c	518	-	51,51,55	0.33	0	59,59,63	0.48	1 (1%)
25	CLA	b	605	2	63,73,73	1.26	8 (12%)	74,113,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	i	102	-	36,36,36	0.35	0	47,47,47	0.85	1 (2%)
25	CLA	C	505	3	63,73,73	1.30	8 (12%)	74,113,113	1.35	6 (8%)
31	LMT	B	627	-	24,24,36	0.44	0	29,29,47	1.11	3 (10%)
25	CLA	b	602	2	63,73,73	1.20	7 (11%)	74,113,113	1.44	9 (12%)
31	LMT	i	101	-	24,24,36	0.33	0	29,29,47	0.70	0
34	DGD	H	104	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	3 (3%)
33	LHG	b	628	-	48,48,48	0.36	0	51,54,54	0.46	0
28	LMG	J	101	-	55,55,55	0.24	0	63,63,63	0.30	0
31	LMT	d	411	-	36,36,36	0.49	0	47,47,47	1.27	5 (10%)
27	BCR	b	618	-	41,41,41	1.46	6 (14%)	56,56,56	1.30	10 (17%)
35	HEM	E	104	6,5	42,50,50	1.46	5 (11%)	46,82,82	2.04	11 (23%)
31	LMT	C	521	-	36,36,36	0.35	0	47,47,47	0.90	2 (4%)
33	LHG	D	406	-	48,48,48	0.35	0	51,54,54	0.37	0
34	DGD	C	515	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	3 (3%)
29	PL9	A	411	-	55,55,55	0.78	1 (1%)	68,69,69	0.61	3 (4%)
25	CLA	B	606	2	58,68,73	1.40	10 (17%)	68,107,113	1.45	8 (11%)
31	LMT	A	415	-	36,36,36	0.19	0	47,47,47	0.39	0
31	LMT	I	103	-	22,22,36	0.39	0	27,27,47	0.73	0
31	LMT	M	101	-	36,36,36	0.43	0	47,47,47	1.27	4 (8%)
31	LMT	I	102	-	36,36,36	0.35	0	47,47,47	0.85	1 (2%)
25	CLA	b	609	2	63,73,73	1.32	10 (15%)	74,113,113	1.40	9 (12%)
25	CLA	C	513	3	63,73,73	1.25	6 (9%)	74,113,113	1.48	8 (10%)
25	CLA	B	608	2	63,73,73	1.34	9 (14%)	74,113,113	1.42	9 (12%)
25	CLA	b	606	2	58,68,73	1.40	10 (17%)	68,107,113	1.45	8 (11%)
27	BCR	k	103	-	41,41,41	1.41	5 (12%)	56,56,56	1.47	11 (19%)
25	CLA	b	610	38	63,73,73	1.24	7 (11%)	74,113,113	1.43	9 (12%)
27	BCR	C	514	-	41,41,41	1.44	4 (9%)	56,56,56	1.45	11 (19%)
31	LMT	d	410	-	24,24,36	0.38	0	29,29,47	0.73	0
31	LMT	m	102	-	24,24,36	0.38	0	29,29,47	0.84	1 (3%)
25	CLA	b	612	2	63,73,73	1.37	8 (12%)	74,113,113	1.43	8 (10%)
25	CLA	c	505	3	63,73,73	1.30	8 (12%)	74,113,113	1.35	6 (8%)
25	CLA	B	612	2	63,73,73	1.37	8 (12%)	74,113,113	1.43	8 (10%)
25	CLA	A	408	1	58,68,73	1.28	8 (13%)	68,107,113	1.49	8 (11%)
25	CLA	C	501	3	63,73,73	1.40	9 (14%)	74,113,113	1.45	9 (12%)
29	PL9	d	405	-	55,55,55	0.90	1 (1%)	68,69,69	0.60	1 (1%)
30	SQD	c	525	-	52,54,54	0.44	0	62,65,65	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	502	3	63,73,73	1.30	9 (14%)	74,113,113	1.51	9 (12%)
25	CLA	C	504	38	63,73,73	1.25	7 (11%)	74,113,113	1.40	6 (8%)
25	CLA	a	408	1	58,68,73	1.28	8 (13%)	68,107,113	1.48	8 (11%)
31	LMT	x	101	-	24,24,36	0.33	0	29,29,47	0.81	0
25	CLA	c	513	3	63,73,73	1.25	6 (9%)	74,113,113	1.48	8 (10%)
33	LHG	D	407	-	48,48,48	0.37	0	51,54,54	0.35	0
25	CLA	b	601	38	43,53,73	1.55	8 (18%)	50,89,113	1.59	6 (12%)
31	LMT	D	410	-	24,24,36	0.38	0	29,29,47	0.73	0
30	SQD	f	102	-	32,34,54	1.83	8 (25%)	42,45,65	1.80	11 (26%)
31	LMT	T	101	-	24,24,36	0.36	0	29,29,47	0.90	1 (3%)
31	LMT	E	101	-	22,22,36	0.35	0	27,27,47	0.69	0
31	LMT	x	103	-	22,22,36	0.44	0	27,27,47	0.98	4 (14%)
27	BCR	F	101	-	41,41,41	1.44	5 (12%)	56,56,56	1.39	10 (17%)
28	LMG	j	101	-	55,55,55	0.24	0	63,63,63	0.30	0
25	CLA	d	403	4	63,73,73	1.30	8 (12%)	74,113,113	1.31	7 (9%)
25	CLA	B	609	2	63,73,73	1.32	10 (15%)	74,113,113	1.40	9 (12%)
31	LMT	y	101	-	21,21,36	0.35	0	26,26,47	0.73	0
25	CLA	B	613	2	63,73,73	1.44	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	I	101	-	24,24,36	0.33	0	29,29,47	0.70	0
32	BCT	a	416	23	3,3,3	1.22	0	2,3,3	0.35	0
25	CLA	A	406	38	63,73,73	1.25	9 (14%)	74,113,113	1.45	9 (12%)
27	BCR	A	409	-	41,41,41	1.46	4 (9%)	56,56,56	1.30	8 (14%)
25	CLA	B	605	2	63,73,73	1.26	7 (11%)	74,113,113	1.41	8 (10%)
25	CLA	b	604	2	63,73,73	1.46	10 (15%)	74,113,113	1.57	11 (14%)
28	LMG	A	414	-	36,36,55	0.30	0	44,44,63	0.51	1 (2%)
27	BCR	b	617	-	41,41,41	1.47	6 (14%)	56,56,56	1.32	10 (17%)
27	BCR	Z	101	-	41,41,41	1.42	8 (19%)	56,56,56	1.41	9 (16%)
27	BCR	b	619	-	41,41,41	1.43	4 (9%)	56,56,56	1.34	10 (17%)
32	BCT	A	417	23	3,3,3	1.22	0	2,3,3	0.35	0
31	LMT	K	105	-	36,36,36	0.38	0	47,47,47	1.38	6 (12%)
28	LMG	B	621	-	51,51,55	0.32	0	59,59,63	0.47	1 (1%)
25	CLA	B	601	38	43,53,73	1.55	8 (18%)	50,89,113	1.59	6 (12%)
30	SQD	A	412	-	52,54,54	0.44	1 (1%)	62,65,65	0.42	0
25	CLA	B	602	2	63,73,73	1.20	6 (9%)	74,113,113	1.44	9 (12%)
25	CLA	b	611	2	63,73,73	1.35	7 (11%)	74,113,113	1.53	9 (12%)
25	CLA	c	507	38	63,73,73	1.31	9 (14%)	74,113,113	1.59	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DGD	C	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
28	LMG	a	410	-	51,51,55	0.27	0	59,59,63	0.33	0
31	LMT	B	626	-	24,24,36	0.36	0	29,29,47	0.77	0
25	CLA	c	504	38	63,73,73	1.25	7 (11%)	74,113,113	1.40	6 (8%)
33	LHG	Z	102	-	35,35,48	0.47	0	38,40,54	0.52	1 (2%)
25	CLA	b	607	38	63,73,73	1.36	9 (14%)	74,113,113	1.58	7 (9%)
27	BCR	z	101	-	41,41,41	1.42	8 (19%)	56,56,56	1.41	9 (16%)
25	CLA	a	405	1	63,73,73	1.33	9 (14%)	74,113,113	1.41	6 (8%)
34	DGD	c	515	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	3 (3%)
33	LHG	D	413	-	48,48,48	0.32	0	51,54,54	0.32	0
25	CLA	D	404	4	63,73,73	1.25	8 (12%)	74,113,113	1.51	8 (10%)
28	LMG	d	409	-	55,55,55	0.29	0	63,63,63	0.43	1 (1%)
25	CLA	D	401	38	63,73,73	1.32	11 (17%)	74,113,113	1.55	10 (13%)
31	LMT	B	624	-	24,24,36	0.47	0	29,29,47	0.71	0
31	LMT	E	103	-	36,36,36	0.46	0	47,47,47	1.23	4 (8%)
27	BCR	c	514	-	41,41,41	1.44	4 (9%)	56,56,56	1.44	11 (19%)
33	LHG	d	408	-	48,48,48	0.36	0	51,54,54	0.39	0
25	CLA	A	405	1	63,73,73	1.33	9 (14%)	74,113,113	1.41	6 (8%)
34	DGD	c	517	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	5 (6%)
25	CLA	b	613	2	63,73,73	1.44	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	x	104	-	36,36,36	0.32	0	47,47,47	0.80	0
33	LHG	B	628	-	48,48,48	0.36	0	51,54,54	0.46	0
33	LHG	e	102	-	39,39,48	0.33	0	42,45,54	0.41	0
31	LMT	C	524	-	36,36,36	0.41	0	47,47,47	1.05	3 (6%)
25	CLA	C	512	3	63,73,73	1.32	9 (14%)	74,113,113	1.37	8 (10%)
31	LMT	a	415	-	36,36,36	0.19	0	47,47,47	0.39	0
25	CLA	C	511	3	63,73,73	1.29	8 (12%)	74,113,113	1.49	8 (10%)
31	LMT	k	105	-	36,36,36	0.38	0	47,47,47	1.38	6 (12%)
27	BCR	B	617	-	41,41,41	1.47	6 (14%)	56,56,56	1.32	10 (17%)
30	SQD	h	103	-	52,54,54	0.43	0	62,65,65	0.52	0
25	CLA	b	615	2	63,73,73	1.32	10 (15%)	74,113,113	1.43	9 (12%)
28	LMG	D	409	-	55,55,55	0.29	0	63,63,63	0.43	1 (1%)
25	CLA	d	401	38	63,73,73	1.32	11 (17%)	74,113,113	1.55	10 (13%)
25	CLA	c	502	3	63,73,73	1.30	9 (14%)	74,113,113	1.51	9 (12%)
26	PHO	A	407	-	50,69,69	0.67	2 (4%)	48,99,99	0.66	0
25	CLA	b	603	2	63,73,73	1.35	9 (14%)	74,113,113	1.42	8 (10%)
31	LMT	c	520	-	24,24,36	0.37	0	29,29,47	0.99	2 (6%)

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	1.32	9 (14%)	74,113,113	1.38	8 (10%)
35	HEM	V	201	18	42,50,50	1.46	4 (9%)	46,82,82	1.36	7 (15%)
25	CLA	b	616	2	58,68,73	1.45	10 (17%)	68,107,113	1.46	6 (8%)
33	LHG	d	406	-	48,48,48	0.34	0	51,54,54	0.37	0
30	SQD	C	525	-	52,54,54	0.44	0	62,65,65	0.44	0
25	CLA	c	511	3	63,73,73	1.29	8 (12%)	74,113,113	1.49	8 (10%)
31	LMT	B	625	-	36,36,36	0.32	0	47,47,47	0.88	1 (2%)
33	LHG	D	408	-	48,48,48	0.36	0	51,54,54	0.39	0
31	LMT	i	104	-	24,24,36	0.42	0	29,29,47	0.92	1 (3%)
30	SQD	H	103	-	52,54,54	0.43	0	62,65,65	0.52	0
25	CLA	B	610	38	63,73,73	1.24	7 (11%)	74,113,113	1.43	9 (12%)
25	CLA	d	404	4	63,73,73	1.25	8 (12%)	74,113,113	1.51	8 (10%)
31	LMT	C	523	-	24,24,36	0.40	0	29,29,47	0.88	0
31	LMT	L	105	-	36,36,36	0.43	0	47,47,47	1.27	4 (8%)
33	LHG	d	407	-	48,48,48	0.37	0	51,54,54	0.35	0
25	CLA	C	506	3	63,73,73	1.31	9 (14%)	74,113,113	1.48	7 (9%)
25	CLA	c	501	3	63,73,73	1.40	9 (14%)	74,113,113	1.45	9 (12%)
31	LMT	X	101	-	24,24,36	0.33	0	29,29,47	0.81	0
25	CLA	B	611	2	63,73,73	1.34	7 (11%)	74,113,113	1.53	9 (12%)
25	CLA	B	603	2	63,73,73	1.34	9 (14%)	74,113,113	1.43	8 (10%)
34	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
25	CLA	C	509	3	63,73,73	1.44	8 (12%)	74,113,113	1.60	12 (16%)
25	CLA	C	510	3	63,73,73	1.42	8 (12%)	74,113,113	1.42	7 (9%)
25	CLA	b	614	2	63,73,73	1.33	8 (12%)	74,113,113	1.52	9 (12%)
26	PHO	a	407	-	50,69,69	0.67	2 (4%)	48,99,99	0.66	0
25	CLA	B	616	2	58,68,73	1.44	10 (17%)	68,107,113	1.46	6 (8%)
25	CLA	c	512	3	63,73,73	1.32	9 (14%)	74,113,113	1.38	8 (10%)
34	DGD	h	104	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	3 (3%)
22	OEX	A	401	1,38,3	0,15,15	-	-	-	-	-
31	LMT	f	103	-	36,36,36	0.55	0	47,47,47	0.82	1 (2%)
25	CLA	B	614	2	63,73,73	1.33	8 (12%)	74,113,113	1.52	9 (12%)
29	PL9	D	405	-	55,55,55	0.90	1 (1%)	68,69,69	0.60	1 (1%)
27	BCR	B	618	-	41,41,41	1.47	6 (14%)	56,56,56	1.30	10 (17%)
27	BCR	K	104	-	41,41,41	1.45	6 (14%)	56,56,56	1.35	10 (17%)
31	LMT	D	411	-	36,36,36	0.50	0	47,47,47	1.27	5 (10%)
31	LMT	c	523	-	24,24,36	0.40	0	29,29,47	0.88	0
31	LMT	i	105	-	24,24,36	0.22	0	29,29,47	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	d	412	-	48,48,48	0.32	0	51,54,54	0.32	0
25	CLA	c	503	3	63,73,73	1.32	9 (14%)	74,113,113	1.38	8 (10%)
25	CLA	c	509	3	63,73,73	1.44	8 (12%)	74,113,113	1.59	12 (16%)
30	SQD	F	102	-	32,34,54	1.83	8 (25%)	42,45,65	1.80	11 (26%)
31	LMT	e	103	-	36,36,36	0.46	1 (2%)	47,47,47	1.23	4 (8%)
27	BCR	K	103	-	41,41,41	1.41	5 (12%)	56,56,56	1.47	11 (19%)
31	LMT	c	521	-	36,36,36	0.35	0	47,47,47	0.90	2 (4%)
26	PHO	d	402	-	50,69,69	0.72	2 (4%)	48,99,99	0.78	1 (2%)
31	LMT	I	104	-	24,24,36	0.42	0	29,29,47	0.92	1 (3%)
25	CLA	c	506	3	63,73,73	1.31	9 (14%)	74,113,113	1.47	7 (9%)
31	LMT	t	101	-	24,24,36	0.36	0	29,29,47	0.90	1 (3%)
28	LMG	b	621	-	51,51,55	0.32	0	59,59,63	0.47	1 (1%)
35	HEM	v	201	18	42,50,50	1.46	4 (9%)	46,82,82	1.37	7 (15%)
31	LMT	b	624	-	24,24,36	0.47	0	29,29,47	0.71	0
25	CLA	C	508	3	63,73,73	1.36	9 (14%)	74,113,113	1.45	7 (9%)
25	CLA	B	604	2	63,73,73	1.46	10 (15%)	74,113,113	1.57	11 (14%)
25	CLA	B	607	38	63,73,73	1.36	9 (14%)	74,113,113	1.58	7 (9%)
30	SQD	k	102	-	41,41,54	0.28	0	49,49,65	0.30	0
31	LMT	b	629	-	36,36,36	0.33	0	47,47,47	0.79	1 (2%)
25	CLA	D	403	4	63,73,73	1.29	8 (12%)	74,113,113	1.31	7 (9%)
31	LMT	X	103	-	22,22,36	0.44	0	27,27,47	0.98	4 (14%)
30	SQD	a	412	-	52,54,54	0.44	1 (1%)	62,65,65	0.42	0
30	SQD	b	620	-	52,54,54	0.41	0	62,65,65	0.52	0
31	LMT	C	522	-	21,21,36	0.46	0	26,26,47	1.30	5 (19%)
29	PL9	a	411	-	55,55,55	0.78	1 (1%)	68,69,69	0.61	3 (4%)
31	LMT	B	629	-	36,36,36	0.33	0	47,47,47	0.79	1 (2%)
27	BCR	a	409	-	41,41,41	1.46	4 (9%)	56,56,56	1.30	8 (14%)
25	CLA	c	510	3	63,73,73	1.42	8 (12%)	74,113,113	1.42	7 (9%)
31	LMT	X	102	-	22,22,36	0.49	0	27,27,47	0.89	0
33	LHG	z	102	-	35,35,48	0.47	0	38,40,54	0.52	1 (2%)
25	CLA	c	508	3	63,73,73	1.36	9 (14%)	74,113,113	1.45	7 (9%)
31	LMT	D	412	-	36,36,36	0.32	0	47,47,47	0.80	0
25	CLA	b	608	2	63,73,73	1.34	9 (14%)	74,113,113	1.42	9 (12%)
28	LMG	C	518	-	51,51,55	0.33	0	59,59,63	0.48	1 (1%)
31	LMT	b	623	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
31	LMT	b	626	-	24,24,36	0.36	0	29,29,47	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	I	105	-	24,24,36	0.22	0	29,29,47	0.41	0
27	BCR	B	619	-	41,41,41	1.43	4 (9%)	56,56,56	1.34	10 (17%)
35	HEM	e	104	6,5	42,50,50	1.46	5 (11%)	46,82,82	2.04	11 (23%)
26	PHO	D	402	-	50,69,69	0.72	2 (4%)	48,99,99	0.78	1 (2%)
28	LMG	A	410	-	51,51,55	0.27	0	59,59,63	0.33	0
27	BCR	z	103	-	41,41,41	1.45	6 (14%)	56,56,56	1.35	10 (17%)
28	LMG	C	519	-	49,49,55	0.29	0	57,57,63	0.50	0
31	LMT	b	625	-	36,36,36	0.32	0	47,47,47	0.88	1 (2%)
31	LMT	c	524	-	36,36,36	0.41	0	47,47,47	1.05	3 (6%)
25	CLA	a	406	38	63,73,73	1.25	9 (14%)	74,113,113	1.46	10 (13%)
30	SQD	B	620	-	52,54,54	0.42	0	62,65,65	0.52	0
31	LMT	F	103	-	36,36,36	0.54	0	47,47,47	0.82	1 (2%)
33	LHG	E	102	-	39,39,48	0.33	0	42,45,54	0.41	0
22	OEX	a	401	1,38,3	0,15,15	-	-	-	-	-
28	LMG	a	414	-	36,36,55	0.30	0	44,44,63	0.51	1 (2%)
28	LMG	c	519	-	49,49,55	0.29	0	57,57,63	0.50	0
36	RRX	h	101	-	42,42,42	1.43	7 (16%)	56,58,58	1.35	11 (19%)
25	CLA	C	507	38	63,73,73	1.31	9 (14%)	74,113,113	1.58	9 (12%)
30	SQD	K	102	-	41,41,54	0.28	0	49,49,65	0.30	0
31	LMT	b	630	-	24,24,36	0.44	0	29,29,47	1.11	3 (10%)
31	LMT	B	623	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
31	LMT	M	102	-	24,24,36	0.38	0	29,29,47	0.84	1 (3%)
34	DGD	C	517	-	63,63,67	0.82	3 (4%)	77,77,81	1.08	5 (6%)
31	LMT	e	101	-	22,22,36	0.36	0	27,27,47	0.69	0
31	LMT	c	522	-	21,21,36	0.46	0	26,26,47	1.30	5 (19%)
27	BCR	f	101	-	41,41,41	1.44	5 (12%)	56,56,56	1.39	10 (17%)
25	CLA	B	615	2	63,73,73	1.31	10 (15%)	74,113,113	1.42	9 (12%)
31	LMT	C	520	-	24,24,36	0.37	0	29,29,47	0.99	2 (6%)

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
31	LMT	i	103	-	-	8/13/33/61	0/1/1/2
31	LMT	Y	101	-	-	8/12/32/61	0/1/1/2
30	SQD	A	413	-	-	21/39/59/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	x	102	-	-	8/12/32/61	0/1/1/2
36	RRX	H	101	-	-	13/29/65/65	0/2/2/2
30	SQD	a	413	-	-	21/39/59/69	0/1/1/1
28	LMG	c	518	-	-	19/46/66/70	0/1/1/1
25	CLA	b	605	2	1/1/15/20	12/37/115/115	-
31	LMT	i	102	-	-	12/21/61/61	0/2/2/2
25	CLA	C	505	3	1/1/15/20	9/37/115/115	-
31	LMT	B	627	-	-	7/15/35/61	0/1/1/2
25	CLA	b	602	2	1/1/15/20	9/37/115/115	-
31	LMT	i	101	-	-	9/15/35/61	0/1/1/2
34	DGD	H	104	-	-	16/51/91/95	0/2/2/2
33	LHG	b	628	-	-	30/53/53/53	-
28	LMG	J	101	-	-	33/50/70/70	0/1/1/1
31	LMT	d	411	-	-	14/21/61/61	0/2/2/2
27	BCR	b	618	-	-	11/29/63/63	0/2/2/2
35	HEM	E	104	6,5	-	2/12/54/54	-
31	LMT	C	521	-	-	10/21/61/61	0/2/2/2
33	LHG	D	406	-	-	20/53/53/53	-
34	DGD	C	515	-	-	24/51/91/95	0/2/2/2
29	PL9	A	411	-	-	23/53/73/73	0/1/1/1
25	CLA	B	606	2	1/1/14/20	5/31/109/115	-
31	LMT	A	415	-	-	15/21/61/61	0/2/2/2
31	LMT	I	103	-	-	8/13/33/61	0/1/1/2
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
31	LMT	I	102	-	-	12/21/61/61	0/2/2/2
25	CLA	b	609	2	1/1/15/20	7/37/115/115	-
25	CLA	C	513	3	1/1/15/20	19/37/115/115	-
25	CLA	B	608	2	1/1/15/20	2/37/115/115	-
25	CLA	b	606	2	1/1/14/20	5/31/109/115	-
27	BCR	k	103	-	-	19/29/63/63	0/2/2/2
25	CLA	b	610	38	1/1/15/20	11/37/115/115	-
27	BCR	C	514	-	-	11/29/63/63	0/2/2/2
31	LMT	d	410	-	-	9/15/35/61	0/1/1/2
31	LMT	m	102	-	-	10/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	612	2	1/1/15/20	9/37/115/115	-
25	CLA	c	505	3	1/1/15/20	9/37/115/115	-
25	CLA	B	612	2	1/1/15/20	9/37/115/115	-
25	CLA	A	408	1	1/1/14/20	13/31/109/115	-
25	CLA	C	501	3	1/1/15/20	5/37/115/115	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
30	SQD	c	525	-	-	22/49/69/69	0/1/1/1
25	CLA	C	504	38	1/1/15/20	9/37/115/115	-
25	CLA	C	502	3	-	8/37/115/115	-
25	CLA	a	408	1	-	13/31/109/115	-
31	LMT	x	101	-	-	7/15/35/61	0/1/1/2
25	CLA	c	513	3	1/1/15/20	19/37/115/115	-
33	LHG	D	407	-	-	19/53/53/53	-
25	CLA	b	601	38	1/1/11/20	4/13/91/115	-
31	LMT	D	410	-	-	9/15/35/61	0/1/1/2
30	SQD	f	102	-	-	14/29/49/69	0/1/1/1
31	LMT	T	101	-	-	9/15/35/61	0/1/1/2
31	LMT	E	101	-	-	7/13/33/61	0/1/1/2
31	LMT	x	103	-	-	5/13/33/61	0/1/1/2
27	BCR	F	101	-	-	11/29/63/63	0/2/2/2
28	LMG	j	101	-	-	34/50/70/70	0/1/1/1
25	CLA	d	403	4	1/1/15/20	5/37/115/115	-
25	CLA	B	609	2	1/1/15/20	7/37/115/115	-
31	LMT	y	101	-	-	8/12/32/61	0/1/1/2
25	CLA	B	613	2	1/1/15/20	9/37/115/115	-
31	LMT	I	101	-	-	9/15/35/61	0/1/1/2
25	CLA	A	406	38	1/1/15/20	9/37/115/115	-
27	BCR	A	409	-	-	10/29/63/63	0/2/2/2
25	CLA	B	605	2	1/1/15/20	12/37/115/115	-
25	CLA	b	604	2	1/1/15/20	10/37/115/115	-
28	LMG	A	414	-	-	14/31/51/70	0/1/1/1
27	BCR	b	617	-	-	13/29/63/63	0/2/2/2
27	BCR	Z	101	-	-	21/29/63/63	0/2/2/2
27	BCR	b	619	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	K	105	-	-	15/21/61/61	0/2/2/2
28	LMG	B	621	-	-	20/46/66/70	0/1/1/1
25	CLA	B	601	38	1/1/11/20	4/13/91/115	-
30	SQD	A	412	-	-	31/49/69/69	0/1/1/1
25	CLA	B	602	2	1/1/15/20	9/37/115/115	-
25	CLA	b	611	2	1/1/15/20	9/37/115/115	-
25	CLA	c	507	38	1/1/15/20	13/37/115/115	-
34	DGD	C	516	-	-	20/51/91/95	0/2/2/2
28	LMG	a	410	-	-	23/46/66/70	0/1/1/1
31	LMT	B	626	-	-	11/15/35/61	0/1/1/2
25	CLA	c	504	38	1/1/15/20	9/37/115/115	-
33	LHG	Z	102	-	-	18/37/37/53	-
25	CLA	b	607	38	1/1/15/20	7/37/115/115	-
27	BCR	z	101	-	-	21/29/63/63	0/2/2/2
25	CLA	a	405	1	1/1/15/20	7/37/115/115	-
34	DGD	c	515	-	-	24/51/91/95	0/2/2/2
33	LHG	D	413	-	-	44/53/53/53	-
25	CLA	D	404	4	-	11/37/115/115	-
28	LMG	d	409	-	-	28/50/70/70	0/1/1/1
25	CLA	D	401	38	1/1/15/20	7/37/115/115	-
31	LMT	B	624	-	-	11/15/35/61	0/1/1/2
31	LMT	E	103	-	-	12/21/61/61	0/2/2/2
27	BCR	c	514	-	-	11/29/63/63	0/2/2/2
33	LHG	d	408	-	-	24/53/53/53	-
25	CLA	A	405	1	1/1/15/20	7/37/115/115	-
34	DGD	c	517	-	-	16/51/91/95	0/2/2/2
25	CLA	b	613	2	1/1/15/20	9/37/115/115	-
31	LMT	x	104	-	-	7/21/61/61	0/2/2/2
33	LHG	B	628	-	-	30/53/53/53	-
33	LHG	e	102	-	-	21/44/44/53	-
31	LMT	C	524	-	-	12/21/61/61	0/2/2/2
25	CLA	C	512	3	1/1/15/20	16/37/115/115	-
31	LMT	a	415	-	-	15/21/61/61	0/2/2/2
25	CLA	C	511	3	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	k	105	-	-	15/21/61/61	0/2/2/2
27	BCR	B	617	-	-	13/29/63/63	0/2/2/2
30	SQD	h	103	-	-	28/49/69/69	0/1/1/1
25	CLA	b	615	2	1/1/15/20	11/37/115/115	-
28	LMG	D	409	-	-	28/50/70/70	0/1/1/1
25	CLA	d	401	38	1/1/15/20	7/37/115/115	-
25	CLA	c	502	3	-	8/37/115/115	-
26	PHO	A	407	-	-	13/37/103/103	0/5/6/6
25	CLA	b	603	2	1/1/15/20	13/37/115/115	-
31	LMT	c	520	-	-	9/15/35/61	0/1/1/2
25	CLA	C	503	3	1/1/15/20	6/37/115/115	-
35	HEM	V	201	18	-	0/12/54/54	-
25	CLA	b	616	2	1/1/14/20	11/31/109/115	-
33	LHG	d	406	-	-	20/53/53/53	-
30	SQD	C	525	-	-	22/49/69/69	0/1/1/1
25	CLA	c	511	3	1/1/15/20	5/37/115/115	-
31	LMT	B	625	-	-	16/21/61/61	0/2/2/2
33	LHG	D	408	-	-	24/53/53/53	-
31	LMT	i	104	-	-	7/15/35/61	0/1/1/2
30	SQD	H	103	-	-	28/49/69/69	0/1/1/1
25	CLA	B	610	38	1/1/15/20	11/37/115/115	-
25	CLA	d	404	4	-	11/37/115/115	-
31	LMT	C	523	-	-	10/15/35/61	0/1/1/2
31	LMT	L	105	-	-	13/21/61/61	0/2/2/2
33	LHG	d	407	-	-	19/53/53/53	-
25	CLA	C	506	3	1/1/15/20	11/37/115/115	-
25	CLA	c	501	3	1/1/15/20	5/37/115/115	-
31	LMT	X	101	-	-	7/15/35/61	0/1/1/2
25	CLA	B	611	2	1/1/15/20	9/37/115/115	-
25	CLA	B	603	2	1/1/15/20	13/37/115/115	-
34	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	CLA	C	509	3	1/1/15/20	9/37/115/115	-
25	CLA	C	510	3	1/1/15/20	10/37/115/115	-
25	CLA	b	614	2	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	a	407	-	-	13/37/103/103	0/5/6/6
25	CLA	B	616	2	1/1/14/20	11/31/109/115	-
25	CLA	c	512	3	1/1/15/20	16/37/115/115	-
34	DGD	h	104	-	-	16/51/91/95	0/2/2/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	B	614	2	1/1/15/20	16/37/115/115	-
29	PL9	D	405	-	-	7/53/73/73	0/1/1/1
27	BCR	B	618	-	-	11/29/63/63	0/2/2/2
27	BCR	K	104	-	-	12/29/63/63	0/2/2/2
31	LMT	D	411	-	-	14/21/61/61	0/2/2/2
31	LMT	c	523	-	-	10/15/35/61	0/1/1/2
31	LMT	i	105	-	-	10/15/35/61	0/1/1/2
33	LHG	d	412	-	-	44/53/53/53	-
25	CLA	c	503	3	1/1/15/20	6/37/115/115	-
25	CLA	c	509	3	1/1/15/20	9/37/115/115	-
30	SQD	F	102	-	-	14/29/49/69	0/1/1/1
31	LMT	e	103	-	-	12/21/61/61	0/2/2/2
27	BCR	K	103	-	-	19/29/63/63	0/2/2/2
31	LMT	c	521	-	-	10/21/61/61	0/2/2/2
26	PHO	d	402	-	-	2/37/103/103	0/5/6/6
31	LMT	I	104	-	-	7/15/35/61	0/1/1/2
25	CLA	c	506	3	1/1/15/20	11/37/115/115	-
31	LMT	t	101	-	-	9/15/35/61	0/1/1/2
28	LMG	b	621	-	-	20/46/66/70	0/1/1/1
35	HEM	v	201	18	-	0/12/54/54	-
31	LMT	b	624	-	-	11/15/35/61	0/1/1/2
25	CLA	C	508	3	1/1/15/20	10/37/115/115	-
25	CLA	B	604	2	1/1/15/20	10/37/115/115	-
25	CLA	B	607	38	1/1/15/20	7/37/115/115	-
30	SQD	k	102	-	-	27/35/55/69	0/1/1/1
31	LMT	b	629	-	-	9/21/61/61	0/2/2/2
25	CLA	D	403	4	1/1/15/20	5/37/115/115	-
31	LMT	X	103	-	-	5/13/33/61	0/1/1/2
30	SQD	a	412	-	-	31/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	b	620	-	-	24/49/69/69	0/1/1/1
31	LMT	C	522	-	-	8/12/32/61	0/1/1/2
29	PL9	a	411	-	-	23/53/73/73	0/1/1/1
31	LMT	B	629	-	-	9/21/61/61	0/2/2/2
27	BCR	a	409	-	-	10/29/63/63	0/2/2/2
25	CLA	c	510	3	1/1/15/20	10/37/115/115	-
31	LMT	X	102	-	-	8/12/32/61	0/1/1/2
33	LHG	z	102	-	-	18/37/37/53	-
25	CLA	c	508	3	1/1/15/20	10/37/115/115	-
31	LMT	D	412	-	-	7/21/61/61	0/2/2/2
25	CLA	b	608	2	1/1/15/20	2/37/115/115	-
28	LMG	C	518	-	-	19/46/66/70	0/1/1/1
31	LMT	b	623	-	-	8/21/61/61	0/2/2/2
31	LMT	b	626	-	-	11/15/35/61	0/1/1/2
31	LMT	I	105	-	-	10/15/35/61	0/1/1/2
27	BCR	B	619	-	-	9/29/63/63	0/2/2/2
35	HEM	e	104	6,5	-	2/12/54/54	-
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
28	LMG	A	410	-	-	23/46/66/70	0/1/1/1
27	BCR	z	103	-	-	12/29/63/63	0/2/2/2
28	LMG	C	519	-	-	26/44/64/70	0/1/1/1
31	LMT	b	625	-	-	16/21/61/61	0/2/2/2
31	LMT	c	524	-	-	12/21/61/61	0/2/2/2
25	CLA	a	406	38	1/1/15/20	9/37/115/115	-
30	SQD	B	620	-	-	24/49/69/69	0/1/1/1
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
33	LHG	E	102	-	-	21/44/44/53	-
28	LMG	a	414	-	-	14/31/51/70	0/1/1/1
28	LMG	c	519	-	-	26/44/64/70	0/1/1/1
36	RRX	h	101	-	-	13/29/65/65	0/2/2/2
25	CLA	C	507	38	1/1/15/20	13/37/115/115	-
30	SQD	K	102	-	-	27/35/55/69	0/1/1/1
31	LMT	b	630	-	-	7/15/35/61	0/1/1/2
31	LMT	B	623	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	M	102	-	-	10/15/35/61	0/1/1/2
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
31	LMT	e	101	-	-	7/13/33/61	0/1/1/2
31	LMT	c	522	-	-	8/12/32/61	0/1/1/2
27	BCR	f	101	-	-	11/29/63/63	0/2/2/2
25	CLA	B	615	2	1/1/15/20	11/37/115/115	-
31	LMT	C	520	-	-	9/15/35/61	0/1/1/2

All (780) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	405	PL9	C3-C4	-5.69	1.40	1.49
29	d	405	PL9	C3-C4	-5.69	1.40	1.49
25	b	615	CLA	CHB-C4A	5.38	1.38	1.33
25	b	611	CLA	CHB-C4A	5.35	1.38	1.33
25	c	511	CLA	CHB-C4A	5.34	1.38	1.33
25	C	506	CLA	CHB-C4A	5.33	1.38	1.33
25	c	506	CLA	CHB-C4A	5.33	1.38	1.33
25	C	511	CLA	CHB-C4A	5.31	1.38	1.33
25	B	611	CLA	CHB-C4A	5.29	1.38	1.33
25	A	405	CLA	CHB-C4A	5.29	1.38	1.33
25	a	405	CLA	CHB-C4A	5.29	1.38	1.33
25	B	615	CLA	CHB-C4A	5.27	1.37	1.33
25	C	504	CLA	CHB-C4A	5.25	1.37	1.33
25	c	504	CLA	CHB-C4A	5.25	1.37	1.33
25	B	606	CLA	CHB-C4A	5.23	1.37	1.33
25	b	606	CLA	CHB-C4A	5.23	1.37	1.33
25	B	604	CLA	CHB-C4A	5.21	1.37	1.33
25	b	604	CLA	CHB-C4A	5.21	1.37	1.33
25	B	614	CLA	CHB-C4A	5.16	1.37	1.33
25	b	614	CLA	CHB-C4A	5.16	1.37	1.33
25	B	607	CLA	CHB-C4A	5.15	1.37	1.33
25	b	607	CLA	CHB-C4A	5.15	1.37	1.33
25	C	505	CLA	CHB-C4A	5.15	1.37	1.33
25	D	403	CLA	CHB-C4A	5.15	1.37	1.33
25	d	403	CLA	CHB-C4A	5.15	1.37	1.33
25	C	501	CLA	CHB-C4A	5.13	1.37	1.33
25	c	501	CLA	CHB-C4A	5.13	1.37	1.33
25	C	510	CLA	MG-ND	-5.13	1.95	2.05
25	c	510	CLA	MG-ND	-5.13	1.95	2.05
25	B	613	CLA	MG-ND	-5.10	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	613	CLA	MG-ND	-5.10	1.95	2.05
25	A	408	CLA	CHB-C4A	5.09	1.37	1.33
25	a	408	CLA	CHB-C4A	5.09	1.37	1.33
25	c	505	CLA	CHB-C4A	5.08	1.37	1.33
29	A	411	PL9	C3-C4	-5.05	1.41	1.49
29	a	411	PL9	C3-C4	-5.05	1.41	1.49
25	c	509	CLA	MG-NA	5.03	2.18	2.06
25	C	509	CLA	MG-NA	5.03	2.18	2.06
25	C	507	CLA	CHB-C4A	5.02	1.37	1.33
25	c	507	CLA	CHB-C4A	5.02	1.37	1.33
25	C	512	CLA	CHB-C4A	4.99	1.37	1.33
25	c	512	CLA	CHB-C4A	4.99	1.37	1.33
25	B	603	CLA	CHB-C4A	4.94	1.37	1.33
25	b	603	CLA	CHB-C4A	4.94	1.37	1.33
25	C	509	CLA	CHB-C4A	4.90	1.37	1.33
25	b	609	CLA	CHB-C4A	4.88	1.37	1.33
25	C	513	CLA	CHB-C4A	4.87	1.37	1.33
25	c	513	CLA	CHB-C4A	4.87	1.37	1.33
25	B	609	CLA	CHB-C4A	4.85	1.37	1.33
25	c	508	CLA	MG-ND	-4.84	1.96	2.05
25	c	509	CLA	CHB-C4A	4.84	1.37	1.33
25	D	404	CLA	CHB-C4A	4.84	1.37	1.33
25	d	404	CLA	CHB-C4A	4.83	1.37	1.33
25	C	508	CLA	MG-ND	-4.83	1.96	2.05
25	B	604	CLA	MG-ND	-4.80	1.96	2.05
25	b	604	CLA	MG-ND	-4.80	1.96	2.05
25	c	501	CLA	MG-ND	-4.79	1.96	2.05
25	B	605	CLA	CHB-C4A	4.79	1.37	1.33
25	b	605	CLA	CHB-C4A	4.79	1.37	1.33
25	C	501	CLA	MG-ND	-4.78	1.96	2.05
25	B	613	CLA	CHB-C4A	4.77	1.37	1.33
25	b	613	CLA	CHB-C4A	4.77	1.37	1.33
25	B	612	CLA	CHB-C4A	4.77	1.37	1.33
25	b	612	CLA	CHB-C4A	4.77	1.37	1.33
25	C	510	CLA	CHB-C4A	4.73	1.37	1.33
25	A	406	CLA	CHB-C4A	4.73	1.37	1.33
25	a	406	CLA	CHB-C4A	4.73	1.37	1.33
25	b	608	CLA	MG-ND	-4.69	1.96	2.05
25	B	610	CLA	CHB-C4A	4.69	1.37	1.33
25	b	610	CLA	CHB-C4A	4.69	1.37	1.33
25	B	608	CLA	MG-ND	-4.68	1.96	2.05
25	c	510	CLA	CHB-C4A	4.67	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CHB-C4A	4.66	1.37	1.33
25	c	502	CLA	CHB-C4A	4.66	1.37	1.33
25	B	601	CLA	CHB-C4A	4.66	1.37	1.33
25	b	601	CLA	CHB-C4A	4.66	1.37	1.33
25	C	508	CLA	CHB-C4A	4.62	1.37	1.33
25	c	508	CLA	CHB-C4A	4.62	1.37	1.33
30	F	102	SQD	O48-C23	4.56	1.46	1.33
30	f	102	SQD	O48-C23	4.56	1.46	1.33
25	C	503	CLA	CHB-C4A	4.54	1.37	1.33
25	c	503	CLA	CHB-C4A	4.54	1.37	1.33
25	D	401	CLA	CHB-C4A	4.47	1.37	1.33
25	d	401	CLA	CHB-C4A	4.47	1.37	1.33
25	B	608	CLA	CHB-C4A	4.44	1.37	1.33
25	b	608	CLA	CHB-C4A	4.44	1.37	1.33
25	B	602	CLA	CHB-C4A	4.28	1.37	1.33
25	b	602	CLA	CHB-C4A	4.28	1.37	1.33
25	B	616	CLA	CHB-C4A	4.26	1.37	1.33
25	b	616	CLA	CHB-C4A	4.26	1.37	1.33
25	C	512	CLA	MG-ND	-4.23	1.97	2.05
25	c	512	CLA	MG-ND	-4.23	1.97	2.05
35	E	104	HEM	C1B-NB	-4.17	1.33	1.40
35	e	104	HEM	C1B-NB	-4.17	1.33	1.40
25	b	616	CLA	MG-NA	4.14	2.16	2.06
25	B	616	CLA	MG-NA	4.13	2.16	2.06
25	B	612	CLA	MG-ND	-4.09	1.97	2.05
25	b	612	CLA	MG-ND	-4.09	1.97	2.05
35	V	201	HEM	C3C-C2C	-4.06	1.34	1.40
35	v	201	HEM	C3C-C2C	-4.06	1.34	1.40
25	C	503	CLA	MG-ND	-4.05	1.97	2.05
25	c	503	CLA	MG-ND	-4.05	1.97	2.05
34	h	104	DGD	O1G-C1A	4.03	1.45	1.33
34	H	104	DGD	O1G-C1A	4.02	1.45	1.33
34	C	516	DGD	O1G-C1A	4.02	1.45	1.33
34	c	516	DGD	O1G-C1A	4.02	1.45	1.33
35	E	104	HEM	C4D-ND	-3.99	1.33	1.40
35	e	104	HEM	C4D-ND	-3.98	1.33	1.40
30	F	102	SQD	O47-C45	-3.83	1.37	1.46
30	f	102	SQD	O47-C45	-3.83	1.37	1.46
34	C	515	DGD	O1G-C1A	3.79	1.44	1.33
34	c	515	DGD	O1G-C1A	3.79	1.44	1.33
34	c	517	DGD	O1G-C1A	3.78	1.44	1.33
34	C	517	DGD	O1G-C1A	3.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	104	DGD	O2G-C1B	3.60	1.44	1.34
34	h	104	DGD	O2G-C1B	3.60	1.44	1.34
27	a	409	BCR	C23-C22	-3.58	1.38	1.46
34	C	517	DGD	O2G-C1B	3.58	1.44	1.34
34	c	517	DGD	O2G-C1B	3.58	1.44	1.34
27	A	409	BCR	C23-C22	-3.58	1.38	1.46
27	B	618	BCR	C23-C22	-3.55	1.38	1.46
27	b	618	BCR	C23-C22	-3.55	1.38	1.46
27	B	617	BCR	C23-C22	-3.54	1.38	1.46
27	b	617	BCR	C23-C22	-3.54	1.38	1.46
27	c	514	BCR	C23-C22	-3.53	1.38	1.46
27	C	514	BCR	C23-C22	-3.51	1.38	1.46
36	H	101	RRX	C23-C22	-3.51	1.38	1.46
36	h	101	RRX	C23-C22	-3.51	1.38	1.46
36	H	101	RRX	C8-C9	-3.50	1.38	1.46
36	h	101	RRX	C8-C9	-3.50	1.38	1.46
27	B	617	BCR	C8-C9	-3.50	1.38	1.46
27	b	617	BCR	C8-C9	-3.50	1.38	1.46
34	C	515	DGD	O2G-C1B	3.47	1.44	1.34
34	c	515	DGD	O2G-C1B	3.47	1.44	1.34
25	D	401	CLA	MG-ND	-3.46	1.98	2.05
25	d	401	CLA	MG-ND	-3.46	1.98	2.05
34	C	516	DGD	O2G-C1B	3.46	1.44	1.34
34	c	516	DGD	O2G-C1B	3.46	1.44	1.34
35	V	201	HEM	C3C-CAC	3.46	1.55	1.47
35	v	201	HEM	C3C-CAC	3.46	1.55	1.47
27	B	618	BCR	C8-C9	-3.44	1.38	1.46
30	F	102	SQD	O5-C1	3.44	1.50	1.41
30	f	102	SQD	O5-C1	3.44	1.50	1.41
25	B	607	CLA	MG-ND	-3.42	1.99	2.05
25	b	607	CLA	MG-ND	-3.42	1.99	2.05
27	b	618	BCR	C8-C9	-3.41	1.38	1.46
27	K	104	BCR	C23-C22	-3.41	1.38	1.46
27	z	103	BCR	C23-C22	-3.41	1.38	1.46
25	B	603	CLA	MG-ND	-3.39	1.99	2.05
25	b	603	CLA	MG-ND	-3.39	1.99	2.05
27	B	619	BCR	C23-C22	-3.38	1.38	1.46
27	b	619	BCR	C23-C22	-3.38	1.38	1.46
27	Z	101	BCR	C23-C22	-3.31	1.38	1.46
27	z	101	BCR	C23-C22	-3.31	1.38	1.46
25	C	505	CLA	CMD-C2D	-3.26	1.44	1.50
25	c	505	CLA	CMD-C2D	-3.26	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	409	BCR	C8-C9	-3.25	1.39	1.46
36	H	101	RRX	C19-C18	-3.24	1.39	1.46
27	a	409	BCR	C8-C9	-3.23	1.39	1.46
27	F	101	BCR	C23-C22	-3.22	1.39	1.46
27	f	101	BCR	C23-C22	-3.22	1.39	1.46
27	K	103	BCR	C23-C22	-3.22	1.39	1.46
27	k	103	BCR	C23-C22	-3.22	1.39	1.46
36	h	101	RRX	C19-C18	-3.20	1.39	1.46
25	C	513	CLA	CHC-C1C	3.20	1.42	1.34
25	c	513	CLA	CHC-C1C	3.20	1.42	1.34
27	B	619	BCR	C8-C9	-3.19	1.39	1.46
27	b	619	BCR	C8-C9	-3.19	1.39	1.46
27	B	617	BCR	C19-C18	-3.18	1.39	1.46
27	b	617	BCR	C19-C18	-3.18	1.39	1.46
25	B	611	CLA	CHC-C1C	3.18	1.42	1.34
27	K	104	BCR	C8-C9	-3.18	1.39	1.46
27	z	103	BCR	C8-C9	-3.18	1.39	1.46
27	Z	101	BCR	C8-C9	-3.17	1.39	1.46
27	z	101	BCR	C8-C9	-3.17	1.39	1.46
27	F	101	BCR	C8-C9	-3.17	1.39	1.46
27	f	101	BCR	C8-C9	-3.17	1.39	1.46
25	B	614	CLA	CHC-C1C	3.17	1.42	1.34
25	b	614	CLA	CHC-C1C	3.17	1.42	1.34
25	b	611	CLA	CHC-C1C	3.17	1.42	1.34
27	C	514	BCR	C8-C9	-3.16	1.39	1.46
27	c	514	BCR	C8-C9	-3.16	1.39	1.46
27	B	618	BCR	C19-C18	-3.14	1.39	1.46
27	b	618	BCR	C19-C18	-3.14	1.39	1.46
25	C	502	CLA	CMB-C2B	-3.12	1.45	1.51
25	c	502	CLA	CMB-C2B	-3.12	1.45	1.51
25	C	511	CLA	CHC-C1C	3.11	1.42	1.34
25	b	604	CLA	MG-NA	3.11	2.13	2.06
25	B	604	CLA	MG-NA	3.11	2.13	2.06
27	A	409	BCR	C19-C18	-3.11	1.39	1.46
27	a	409	BCR	C19-C18	-3.11	1.39	1.46
30	F	102	SQD	O47-C7	3.10	1.43	1.34
30	f	102	SQD	O47-C7	3.10	1.43	1.34
26	D	402	PHO	C3A-C2A	-3.09	1.52	1.54
26	d	402	PHO	C3A-C2A	-3.09	1.52	1.54
25	c	511	CLA	CHC-C1C	3.09	1.42	1.34
25	B	609	CLA	CMB-C2B	-3.09	1.45	1.51
25	b	609	CLA	CMB-C2B	-3.09	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	CLA	CHC-C1C	3.08	1.42	1.34
25	a	408	CLA	CHC-C1C	3.08	1.42	1.34
27	K	103	BCR	C8-C9	-3.08	1.39	1.46
27	k	103	BCR	C8-C9	-3.08	1.39	1.46
25	B	613	CLA	CHC-C1C	3.07	1.42	1.34
25	b	613	CLA	CHC-C1C	3.07	1.42	1.34
25	C	502	CLA	MG-ND	-3.06	1.99	2.05
25	c	502	CLA	MG-ND	-3.06	1.99	2.05
25	c	510	CLA	CMB-C2B	-3.05	1.45	1.51
25	A	406	CLA	CHC-C1C	3.04	1.42	1.34
25	B	609	CLA	MG-ND	-3.04	1.99	2.05
36	H	101	RRX	C12-C13	-3.04	1.39	1.46
36	h	101	RRX	C12-C13	-3.04	1.39	1.46
25	C	510	CLA	CMB-C2B	-3.02	1.45	1.51
25	a	406	CLA	CHC-C1C	3.02	1.42	1.34
25	B	607	CLA	MG-NA	3.02	2.13	2.06
25	b	607	CLA	MG-NA	3.02	2.13	2.06
27	b	617	BCR	C12-C13	-3.02	1.39	1.46
25	b	609	CLA	MG-ND	-3.02	1.99	2.05
25	D	401	CLA	CMB-C2B	-3.02	1.45	1.51
25	d	401	CLA	CMB-C2B	-3.02	1.45	1.51
27	F	101	BCR	C12-C13	-3.01	1.39	1.46
27	f	101	BCR	C12-C13	-3.01	1.39	1.46
35	V	201	HEM	CAB-C3B	3.01	1.55	1.47
35	v	201	HEM	CAB-C3B	3.01	1.55	1.47
25	A	405	CLA	CMB-C2B	-3.01	1.45	1.51
25	C	505	CLA	CHC-C1C	3.01	1.42	1.34
25	c	505	CLA	CHC-C1C	3.01	1.42	1.34
25	a	405	CLA	CMB-C2B	-2.99	1.45	1.51
27	B	617	BCR	C12-C13	-2.99	1.39	1.46
25	C	509	CLA	C1D-ND	2.98	1.41	1.37
25	c	509	CLA	C1D-ND	2.98	1.41	1.37
25	B	604	CLA	C1D-ND	2.97	1.41	1.37
27	a	409	BCR	C12-C13	-2.96	1.39	1.46
25	B	603	CLA	CHC-C1C	2.96	1.41	1.34
25	b	603	CLA	CHC-C1C	2.96	1.41	1.34
25	C	506	CLA	MG-ND	-2.96	1.99	2.05
25	c	506	CLA	MG-ND	-2.96	1.99	2.05
30	F	102	SQD	C24-C23	2.96	1.59	1.50
30	f	102	SQD	C24-C23	2.96	1.59	1.50
25	C	510	CLA	C1D-ND	2.96	1.41	1.37
25	c	510	CLA	C1D-ND	2.96	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	606	CLA	MG-ND	-2.96	1.99	2.05
25	b	606	CLA	MG-ND	-2.96	1.99	2.05
27	A	409	BCR	C12-C13	-2.94	1.39	1.46
25	B	605	CLA	CHC-C1C	2.94	1.41	1.34
25	b	605	CLA	CHC-C1C	2.94	1.41	1.34
25	C	508	CLA	CHC-C1C	2.94	1.41	1.34
25	c	508	CLA	CHC-C1C	2.94	1.41	1.34
25	A	405	CLA	CHC-C1C	2.93	1.41	1.34
25	a	405	CLA	CHC-C1C	2.93	1.41	1.34
25	B	602	CLA	CHC-C1C	2.93	1.41	1.34
25	b	602	CLA	CHC-C1C	2.93	1.41	1.34
25	C	509	CLA	CHC-C1C	2.93	1.41	1.34
25	c	509	CLA	CHC-C1C	2.93	1.41	1.34
27	B	619	BCR	C19-C18	-2.93	1.39	1.46
25	b	608	CLA	CHC-C1C	2.92	1.41	1.34
27	b	619	BCR	C19-C18	-2.92	1.39	1.46
25	B	601	CLA	CHC-C1C	2.92	1.41	1.34
25	b	601	CLA	CHC-C1C	2.92	1.41	1.34
25	B	612	CLA	CHC-C1C	2.92	1.41	1.34
25	b	612	CLA	CHC-C1C	2.92	1.41	1.34
25	d	403	CLA	CHC-C1C	2.91	1.41	1.34
25	b	604	CLA	C1D-ND	2.91	1.41	1.37
25	B	608	CLA	CMB-C2B	-2.91	1.45	1.51
25	C	506	CLA	CMB-C2B	-2.91	1.45	1.51
25	c	506	CLA	CMB-C2B	-2.91	1.45	1.51
25	B	603	CLA	CMB-C2B	-2.91	1.45	1.51
25	b	603	CLA	CMB-C2B	-2.91	1.45	1.51
25	B	608	CLA	CHC-C1C	2.91	1.41	1.34
27	B	618	BCR	C12-C13	-2.90	1.39	1.46
27	b	618	BCR	C12-C13	-2.90	1.39	1.46
25	B	613	CLA	MG-NA	2.90	2.13	2.06
25	b	612	CLA	CMD-C2D	-2.89	1.44	1.50
25	C	504	CLA	CHC-C1C	2.89	1.41	1.34
25	c	504	CLA	CHC-C1C	2.89	1.41	1.34
25	b	608	CLA	CMB-C2B	-2.89	1.45	1.51
25	C	510	CLA	CHC-C1C	2.88	1.41	1.34
25	c	510	CLA	CHC-C1C	2.88	1.41	1.34
25	b	613	CLA	MG-NA	2.88	2.13	2.06
25	D	403	CLA	CHC-C1C	2.88	1.41	1.34
25	C	502	CLA	CHC-C1C	2.88	1.41	1.34
25	D	404	CLA	CHC-C1C	2.88	1.41	1.34
25	c	502	CLA	CHC-C1C	2.88	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	CHC-C1C	2.88	1.41	1.34
25	B	604	CLA	CMD-C2D	-2.87	1.44	1.50
25	b	604	CLA	CMD-C2D	-2.87	1.44	1.50
25	B	613	CLA	CMB-C2B	-2.87	1.45	1.51
25	b	613	CLA	CMB-C2B	-2.87	1.45	1.51
25	b	606	CLA	CHC-C1C	2.87	1.41	1.34
25	B	616	CLA	C1D-ND	2.86	1.41	1.37
25	b	616	CLA	C1D-ND	2.86	1.41	1.37
25	B	609	CLA	CHC-C1C	2.86	1.41	1.34
25	A	408	CLA	CMB-C2B	-2.86	1.45	1.51
25	a	408	CLA	CMB-C2B	-2.86	1.45	1.51
25	B	612	CLA	CMD-C2D	-2.86	1.44	1.50
25	B	601	CLA	MG-ND	-2.86	2.00	2.05
25	b	601	CLA	MG-ND	-2.86	2.00	2.05
25	C	501	CLA	CHC-C1C	2.86	1.41	1.34
25	B	606	CLA	CHC-C1C	2.86	1.41	1.34
25	c	501	CLA	CHC-C1C	2.86	1.41	1.34
25	C	506	CLA	CHC-C1C	2.85	1.41	1.34
25	c	506	CLA	CHC-C1C	2.85	1.41	1.34
25	B	607	CLA	CMB-C2B	-2.85	1.45	1.51
25	b	607	CLA	CMB-C2B	-2.85	1.45	1.51
25	B	610	CLA	CHC-C1C	2.85	1.41	1.34
25	b	610	CLA	CHC-C1C	2.85	1.41	1.34
25	C	503	CLA	C1D-ND	2.85	1.41	1.37
25	B	610	CLA	CMB-C2B	-2.84	1.45	1.51
25	b	610	CLA	CMB-C2B	-2.84	1.45	1.51
25	b	609	CLA	CHC-C1C	2.84	1.41	1.34
25	B	605	CLA	CMB-C2B	-2.84	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.84	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.83	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.83	1.46	1.51
25	B	611	CLA	C1D-ND	2.83	1.41	1.37
25	B	603	CLA	MG-NA	2.83	2.13	2.06
25	B	604	CLA	CMB-C2B	-2.82	1.46	1.51
25	b	604	CLA	CMB-C2B	-2.82	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.82	1.46	1.51
27	K	104	BCR	C19-C18	-2.82	1.39	1.46
27	z	103	BCR	C19-C18	-2.82	1.39	1.46
25	B	607	CLA	CHC-C1C	2.82	1.41	1.34
25	b	607	CLA	CHC-C1C	2.82	1.41	1.34
25	B	606	CLA	C1D-ND	2.82	1.41	1.37
25	b	606	CLA	C1D-ND	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C1D-ND	2.81	1.41	1.37
25	B	606	CLA	CMB-C2B	-2.81	1.46	1.51
25	b	606	CLA	CMB-C2B	-2.81	1.46	1.51
25	C	503	CLA	CHC-C1C	2.81	1.41	1.34
25	c	503	CLA	CHC-C1C	2.81	1.41	1.34
25	b	616	CLA	CMB-C2B	-2.81	1.46	1.51
25	c	506	CLA	C1D-ND	2.80	1.41	1.37
25	C	512	CLA	CHC-C1C	2.80	1.41	1.34
25	B	615	CLA	CMB-C2B	-2.80	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.80	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.79	1.46	1.51
25	b	603	CLA	MG-NA	2.79	2.12	2.06
25	b	611	CLA	C1D-ND	2.79	1.41	1.37
25	c	503	CLA	C1D-ND	2.79	1.41	1.37
25	b	614	CLA	MG-ND	-2.79	2.00	2.05
25	B	614	CLA	CMB-C2B	-2.79	1.46	1.51
25	b	614	CLA	CMB-C2B	-2.79	1.46	1.51
25	b	601	CLA	CMB-C2B	-2.79	1.46	1.51
25	A	405	CLA	CMD-C2D	-2.79	1.45	1.50
25	c	512	CLA	CHC-C1C	2.78	1.41	1.34
25	c	507	CLA	CMB-C2B	-2.78	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.78	1.46	1.51
25	B	604	CLA	CHC-C1C	2.78	1.41	1.34
25	C	508	CLA	CMB-C2B	-2.78	1.46	1.51
27	C	514	BCR	C19-C18	-2.78	1.40	1.46
27	B	619	BCR	C12-C13	-2.77	1.40	1.46
27	b	619	BCR	C12-C13	-2.77	1.40	1.46
25	C	507	CLA	CMB-C2B	-2.77	1.46	1.51
25	B	608	CLA	CMD-C2D	-2.77	1.45	1.50
25	b	608	CLA	CMD-C2D	-2.77	1.45	1.50
25	B	611	CLA	MG-ND	-2.77	2.00	2.05
25	b	611	CLA	MG-ND	-2.77	2.00	2.05
27	K	103	BCR	C19-C18	-2.77	1.40	1.46
27	k	103	BCR	C19-C18	-2.77	1.40	1.46
25	D	401	CLA	CHC-C1C	2.77	1.41	1.34
25	d	401	CLA	CHC-C1C	2.77	1.41	1.34
25	C	507	CLA	C1D-ND	2.76	1.41	1.37
25	c	507	CLA	C1D-ND	2.76	1.41	1.37
25	B	602	CLA	C1D-ND	2.76	1.41	1.37
25	b	602	CLA	C1D-ND	2.76	1.41	1.37
25	a	405	CLA	CMD-C2D	-2.76	1.45	1.50
27	F	101	BCR	C19-C18	-2.76	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	BCR	C19-C18	-2.76	1.40	1.46
25	C	511	CLA	CMB-C2B	-2.76	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.76	1.46	1.51
27	c	514	BCR	C19-C18	-2.75	1.40	1.46
25	C	513	CLA	C1D-ND	2.75	1.41	1.37
25	c	513	CLA	C1D-ND	2.75	1.41	1.37
25	B	614	CLA	MG-ND	-2.75	2.00	2.05
25	b	604	CLA	CHC-C1C	2.75	1.41	1.34
35	E	104	HEM	C1D-ND	-2.74	1.33	1.38
35	e	104	HEM	C1D-ND	-2.74	1.33	1.38
25	B	603	CLA	CMD-C2D	-2.74	1.45	1.50
25	b	603	CLA	CMD-C2D	-2.74	1.45	1.50
25	C	502	CLA	C1D-ND	2.74	1.41	1.37
25	c	502	CLA	C1D-ND	2.74	1.41	1.37
25	B	615	CLA	CHC-C1C	2.73	1.41	1.34
25	b	615	CLA	CHC-C1C	2.73	1.41	1.34
25	B	616	CLA	CHC-C1C	2.73	1.41	1.34
25	b	616	CLA	CHC-C1C	2.73	1.41	1.34
25	C	504	CLA	CMB-C2B	-2.73	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.73	1.46	1.51
25	C	507	CLA	CHC-C1C	2.73	1.41	1.34
25	c	507	CLA	CHC-C1C	2.73	1.41	1.34
25	B	609	CLA	C1D-ND	2.71	1.41	1.37
25	b	609	CLA	C1D-ND	2.71	1.41	1.37
25	D	404	CLA	C1D-ND	2.71	1.41	1.37
25	A	406	CLA	CMB-C2B	-2.70	1.46	1.51
25	a	406	CLA	CMB-C2B	-2.70	1.46	1.51
25	D	403	CLA	MG-ND	-2.70	2.00	2.05
25	d	403	CLA	MG-ND	-2.70	2.00	2.05
25	d	404	CLA	C1D-ND	2.69	1.41	1.37
25	B	602	CLA	CMB-C2B	-2.69	1.46	1.51
25	B	612	CLA	C1D-ND	2.69	1.41	1.37
25	b	612	CLA	C1D-ND	2.69	1.41	1.37
25	B	601	CLA	C1D-ND	2.68	1.41	1.37
25	b	601	CLA	C1D-ND	2.68	1.41	1.37
25	B	610	CLA	C1D-ND	2.68	1.41	1.37
25	b	610	CLA	C1D-ND	2.68	1.41	1.37
25	C	507	CLA	C3B-C2B	-2.67	1.36	1.40
25	c	507	CLA	C3B-C2B	-2.67	1.36	1.40
25	C	512	CLA	CMB-C2B	-2.66	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.66	1.46	1.51
27	C	514	BCR	C12-C13	-2.66	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	514	BCR	C12-C13	-2.66	1.40	1.46
25	C	508	CLA	C1D-ND	2.66	1.41	1.37
25	c	508	CLA	C1D-ND	2.66	1.41	1.37
25	b	614	CLA	MG-NA	2.64	2.12	2.06
25	b	602	CLA	CMB-C2B	-2.64	1.46	1.51
25	B	605	CLA	C1D-ND	2.64	1.41	1.37
25	b	605	CLA	C1D-ND	2.64	1.41	1.37
25	C	505	CLA	CMB-C2B	-2.64	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.64	1.46	1.51
25	C	513	CLA	CMD-C2D	-2.64	1.45	1.50
25	c	513	CLA	CMD-C2D	-2.64	1.45	1.50
25	A	408	CLA	C1D-ND	2.63	1.41	1.37
25	a	408	CLA	C1D-ND	2.63	1.41	1.37
27	Z	101	BCR	C12-C13	-2.63	1.40	1.46
27	z	101	BCR	C12-C13	-2.63	1.40	1.46
25	A	405	CLA	CMC-C2C	-2.63	1.45	1.50
25	a	405	CLA	CMC-C2C	-2.63	1.45	1.50
25	C	501	CLA	CMB-C2B	-2.63	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.63	1.46	1.51
25	B	614	CLA	CMD-C2D	-2.62	1.45	1.50
25	b	614	CLA	CMD-C2D	-2.62	1.45	1.50
25	B	614	CLA	MG-NA	2.62	2.12	2.06
27	k	103	BCR	C12-C13	-2.62	1.40	1.46
25	C	501	CLA	C1D-ND	2.62	1.41	1.37
25	c	501	CLA	C1D-ND	2.62	1.41	1.37
25	C	510	CLA	CMD-C2D	-2.62	1.45	1.50
25	c	510	CLA	CMD-C2D	-2.62	1.45	1.50
25	B	608	CLA	C1D-ND	2.61	1.41	1.37
25	b	608	CLA	C1D-ND	2.61	1.41	1.37
25	D	404	CLA	CMB-C2B	-2.61	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.61	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.61	1.46	1.51
25	B	601	CLA	CMD-C2D	-2.61	1.45	1.50
25	b	601	CLA	CMD-C2D	-2.61	1.45	1.50
27	K	103	BCR	C12-C13	-2.61	1.40	1.46
25	B	612	CLA	CMB-C2B	-2.60	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.60	1.46	1.51
25	B	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.59	1.46	1.51
25	c	504	CLA	C1D-ND	2.59	1.41	1.37
26	A	407	PHO	C3A-C2A	-2.58	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	407	PHO	C3A-C2A	-2.58	1.52	1.54
25	d	404	CLA	MG-ND	-2.57	2.00	2.05
25	C	513	CLA	CMB-C2B	-2.56	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.56	1.46	1.51
25	D	404	CLA	MG-ND	-2.56	2.00	2.05
25	B	615	CLA	C1D-ND	2.56	1.41	1.37
25	b	615	CLA	C1D-ND	2.56	1.41	1.37
25	d	403	CLA	CMD-C2D	-2.56	1.45	1.50
25	C	503	CLA	CMB-C2B	-2.56	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.56	1.46	1.51
25	B	616	CLA	CMC-C2C	-2.56	1.45	1.50
25	b	616	CLA	CMC-C2C	-2.56	1.45	1.50
25	C	501	CLA	CMD-C2D	-2.54	1.45	1.50
25	c	501	CLA	CMD-C2D	-2.54	1.45	1.50
26	D	402	PHO	CBD-CGD	-2.54	1.49	1.52
26	d	402	PHO	CBD-CGD	-2.54	1.49	1.52
27	K	104	BCR	C12-C13	-2.54	1.40	1.46
27	z	103	BCR	C12-C13	-2.54	1.40	1.46
25	C	511	CLA	MG-NA	2.54	2.12	2.06
25	C	504	CLA	C1D-ND	2.54	1.41	1.37
25	D	403	CLA	CMD-C2D	-2.54	1.45	1.50
25	C	501	CLA	MG-NA	2.54	2.12	2.06
25	B	615	CLA	MG-ND	-2.52	2.00	2.05
25	c	501	CLA	MG-NA	2.51	2.12	2.06
25	c	511	CLA	MG-NA	2.51	2.12	2.06
27	Z	101	BCR	C19-C18	-2.51	1.40	1.46
27	z	101	BCR	C19-C18	-2.51	1.40	1.46
25	C	509	CLA	MG-ND	-2.51	2.00	2.05
25	c	509	CLA	MG-ND	-2.51	2.00	2.05
25	B	613	CLA	C1D-ND	2.50	1.41	1.37
25	b	613	CLA	C1D-ND	2.50	1.41	1.37
25	B	614	CLA	C1D-ND	2.50	1.41	1.37
25	b	614	CLA	C1D-ND	2.50	1.41	1.37
25	a	406	CLA	C1D-ND	2.50	1.41	1.37
25	b	615	CLA	MG-ND	-2.50	2.00	2.05
25	C	504	CLA	CMD-C2D	-2.50	1.45	1.50
25	c	504	CLA	CMD-C2D	-2.50	1.45	1.50
25	D	404	CLA	CMD-C2D	-2.49	1.45	1.50
25	d	404	CLA	CMD-C2D	-2.49	1.45	1.50
25	C	505	CLA	C1D-ND	2.49	1.41	1.37
25	c	505	CLA	C1D-ND	2.49	1.41	1.37
25	B	609	CLA	C3B-C2B	-2.49	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	609	CLA	C3B-C2B	-2.49	1.37	1.40
25	B	603	CLA	C1D-ND	2.48	1.41	1.37
25	b	603	CLA	C1D-ND	2.48	1.41	1.37
25	A	406	CLA	C1D-ND	2.48	1.41	1.37
35	e	104	HEM	C4B-NB	-2.48	1.34	1.38
25	A	406	CLA	CMD-C2D	-2.48	1.45	1.50
25	a	406	CLA	CMD-C2D	-2.48	1.45	1.50
25	C	509	CLA	CMD-C2D	-2.47	1.45	1.50
25	c	509	CLA	CMD-C2D	-2.47	1.45	1.50
25	b	601	CLA	C3B-C2B	-2.47	1.37	1.40
25	b	616	CLA	MG-ND	-2.47	2.00	2.05
25	B	601	CLA	C3B-C2B	-2.47	1.37	1.40
25	C	502	CLA	CMD-C2D	-2.46	1.45	1.50
25	c	502	CLA	CMD-C2D	-2.46	1.45	1.50
25	B	605	CLA	CMD-C2D	-2.46	1.45	1.50
25	B	608	CLA	C3B-C2B	-2.46	1.37	1.40
25	b	608	CLA	C3B-C2B	-2.46	1.37	1.40
25	A	408	CLA	CMD-C2D	-2.45	1.45	1.50
25	a	408	CLA	CMD-C2D	-2.45	1.45	1.50
25	c	512	CLA	CMD-C2D	-2.45	1.45	1.50
25	c	505	CLA	MG-ND	-2.45	2.00	2.05
25	B	602	CLA	CMD-C2D	-2.45	1.45	1.50
25	C	508	CLA	CMD-C2D	-2.44	1.45	1.50
25	b	605	CLA	CMD-C2D	-2.44	1.45	1.50
25	C	511	CLA	C1D-ND	2.44	1.41	1.37
25	c	511	CLA	C1D-ND	2.44	1.41	1.37
25	D	401	CLA	C1D-ND	2.44	1.41	1.37
25	d	401	CLA	C1D-ND	2.44	1.41	1.37
25	c	507	CLA	CMD-C2D	-2.44	1.45	1.50
25	B	611	CLA	CMD-C2D	-2.44	1.45	1.50
25	b	611	CLA	CMD-C2D	-2.44	1.45	1.50
25	c	508	CLA	CMD-C2D	-2.43	1.45	1.50
25	C	512	CLA	CMD-C2D	-2.43	1.45	1.50
25	A	405	CLA	C1D-ND	2.43	1.41	1.37
25	a	405	CLA	C1D-ND	2.43	1.41	1.37
35	E	104	HEM	C4B-NB	-2.43	1.34	1.38
25	b	602	CLA	CMD-C2D	-2.43	1.45	1.50
25	b	613	CLA	C3B-C2B	-2.43	1.37	1.40
25	B	603	CLA	C3B-C2B	-2.43	1.37	1.40
25	b	603	CLA	C3B-C2B	-2.43	1.37	1.40
25	C	505	CLA	MG-ND	-2.43	2.01	2.05
25	B	616	CLA	MG-ND	-2.43	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	C1D-ND	2.42	1.41	1.37
25	b	607	CLA	C1D-ND	2.42	1.41	1.37
25	B	616	CLA	C3B-C2B	-2.42	1.37	1.40
25	b	616	CLA	C3B-C2B	-2.42	1.37	1.40
25	C	507	CLA	CMD-C2D	-2.41	1.45	1.50
25	B	607	CLA	CMD-C2D	-2.41	1.45	1.50
25	b	607	CLA	CMD-C2D	-2.41	1.45	1.50
25	B	613	CLA	C3B-C2B	-2.40	1.37	1.40
25	B	612	CLA	CMC-C2C	-2.40	1.45	1.50
25	b	612	CLA	CMC-C2C	-2.40	1.45	1.50
25	B	606	CLA	MG-NA	2.40	2.12	2.06
25	b	606	CLA	MG-NA	2.40	2.12	2.06
25	B	613	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	613	CLA	CMD-C2D	-2.39	1.45	1.50
25	C	508	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	606	CLA	CMC-C2C	-2.38	1.45	1.50
25	c	508	CLA	CMC-C2C	-2.38	1.45	1.50
25	b	606	CLA	CMC-C2C	-2.38	1.45	1.50
25	C	506	CLA	CMD-C2D	-2.37	1.45	1.50
25	c	507	CLA	CMC-C2C	-2.37	1.45	1.50
25	C	502	CLA	C3B-C2B	-2.37	1.37	1.40
25	c	502	CLA	C3B-C2B	-2.37	1.37	1.40
25	B	616	CLA	CMD-C2D	-2.36	1.45	1.50
25	b	616	CLA	CMD-C2D	-2.36	1.45	1.50
30	A	412	SQD	O8-S	2.36	1.56	1.47
25	B	609	CLA	CMD-C2D	-2.36	1.45	1.50
25	b	609	CLA	CMD-C2D	-2.36	1.45	1.50
25	c	506	CLA	CMD-C2D	-2.36	1.45	1.50
25	C	507	CLA	CMC-C2C	-2.36	1.45	1.50
25	B	611	CLA	CMC-C2C	-2.35	1.45	1.50
25	b	611	CLA	CMC-C2C	-2.35	1.45	1.50
30	a	412	SQD	O8-S	2.34	1.56	1.47
25	C	512	CLA	C1D-ND	2.34	1.40	1.37
25	c	512	CLA	C1D-ND	2.34	1.40	1.37
25	B	610	CLA	CMD-C2D	-2.34	1.46	1.50
25	b	610	CLA	CMD-C2D	-2.34	1.46	1.50
25	B	613	CLA	CMC-C2C	-2.34	1.46	1.50
25	b	613	CLA	CMC-C2C	-2.34	1.46	1.50
25	C	512	CLA	C3B-C2B	-2.34	1.37	1.40
25	c	512	CLA	C3B-C2B	-2.34	1.37	1.40
25	B	610	CLA	C3B-C2B	-2.33	1.37	1.40
25	b	610	CLA	C3B-C2B	-2.33	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	606	CLA	CMD-C2D	-2.33	1.46	1.50
25	b	606	CLA	CMD-C2D	-2.33	1.46	1.50
25	B	615	CLA	MG-NC	2.33	2.11	2.06
25	b	615	CLA	MG-NC	2.33	2.11	2.06
25	A	406	CLA	C3B-C2B	-2.32	1.37	1.40
25	a	406	CLA	C3B-C2B	-2.32	1.37	1.40
25	b	602	CLA	CMC-C2C	-2.32	1.46	1.50
25	B	616	CLA	C4B-CHC	-2.32	1.34	1.41
25	b	616	CLA	C4B-CHC	-2.32	1.34	1.41
35	e	104	HEM	FE-NB	2.32	2.10	1.98
25	B	605	CLA	C3B-C2B	-2.32	1.37	1.40
25	b	605	CLA	C3B-C2B	-2.32	1.37	1.40
25	B	614	CLA	CMC-C2C	-2.31	1.46	1.50
25	b	614	CLA	CMC-C2C	-2.31	1.46	1.50
25	C	511	CLA	CMD-C2D	-2.31	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.31	1.46	1.50
35	E	104	HEM	FE-NB	2.31	2.10	1.98
25	B	615	CLA	CMD-C2D	-2.30	1.46	1.50
25	C	504	CLA	CMC-C2C	-2.30	1.46	1.50
25	b	615	CLA	CMD-C2D	-2.30	1.46	1.50
25	c	504	CLA	CMC-C2C	-2.30	1.46	1.50
25	B	602	CLA	CMC-C2C	-2.30	1.46	1.50
25	B	607	CLA	CMC-C2C	-2.30	1.46	1.50
25	b	607	CLA	CMC-C2C	-2.30	1.46	1.50
25	C	502	CLA	CMC-C2C	-2.30	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.30	1.46	1.50
25	C	505	CLA	CMC-C2C	-2.28	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.28	1.46	1.50
25	B	615	CLA	C3B-C2B	-2.27	1.37	1.40
25	b	615	CLA	C3B-C2B	-2.27	1.37	1.40
25	D	401	CLA	CMD-C2D	-2.26	1.46	1.50
25	d	401	CLA	CMD-C2D	-2.26	1.46	1.50
25	b	605	CLA	CMC-C2C	-2.25	1.46	1.50
25	C	503	CLA	C3B-C2B	-2.25	1.37	1.40
25	b	604	CLA	C3B-C2B	-2.25	1.37	1.40
25	D	403	CLA	C1D-ND	2.25	1.40	1.37
25	d	403	CLA	C1D-ND	2.25	1.40	1.37
25	c	503	CLA	C3B-C2B	-2.25	1.37	1.40
25	b	603	CLA	CMC-C2C	-2.24	1.46	1.50
25	C	507	CLA	MG-ND	-2.24	2.01	2.05
25	B	606	CLA	C4B-CHC	-2.24	1.34	1.41
25	b	606	CLA	C4B-CHC	-2.24	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CMC-C2C	-2.23	1.46	1.50
25	c	511	CLA	CMC-C2C	-2.23	1.46	1.50
25	B	603	CLA	CMC-C2C	-2.23	1.46	1.50
34	H	104	DGD	O2G-C2G	-2.22	1.41	1.46
25	c	507	CLA	MG-ND	-2.22	2.01	2.05
26	A	407	PHO	CBD-CGD	-2.22	1.49	1.52
26	a	407	PHO	CBD-CGD	-2.22	1.49	1.52
25	C	503	CLA	CMD-C2D	-2.22	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.22	1.46	1.50
25	B	608	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	604	CLA	C3B-C2B	-2.21	1.37	1.40
25	B	604	CLA	CMC-C2C	-2.21	1.46	1.50
25	b	604	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	605	CLA	CMC-C2C	-2.21	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.20	1.46	1.50
25	d	403	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	615	CLA	CMC-C2C	-2.20	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.20	1.46	1.50
34	h	104	DGD	O2G-C2G	-2.19	1.41	1.46
25	b	609	CLA	CMC-C2C	-2.19	1.46	1.50
25	A	406	CLA	MG-ND	-2.19	2.01	2.05
25	a	406	CLA	MG-ND	-2.19	2.01	2.05
25	C	512	CLA	C4B-CHC	-2.19	1.34	1.41
25	c	512	CLA	C4B-CHC	-2.19	1.34	1.41
27	K	104	BCR	C10-C9	2.19	1.40	1.35
27	z	103	BCR	C10-C9	2.19	1.40	1.35
25	D	403	CLA	CMC-C2C	-2.18	1.46	1.50
25	D	401	CLA	C4B-CHC	-2.18	1.34	1.41
25	d	401	CLA	C4B-CHC	-2.18	1.34	1.41
25	B	609	CLA	CMC-C2C	-2.18	1.46	1.50
25	D	401	CLA	C3B-C2B	-2.18	1.37	1.40
25	d	401	CLA	C3B-C2B	-2.18	1.37	1.40
25	c	505	CLA	C3B-C2B	-2.18	1.37	1.40
25	C	510	CLA	CMC-C2C	-2.17	1.46	1.50
25	C	512	CLA	CMC-C2C	-2.17	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.17	1.46	1.50
25	D	404	CLA	CMC-C2C	-2.17	1.46	1.50
25	d	404	CLA	CMC-C2C	-2.17	1.46	1.50
25	c	503	CLA	CMC-C2C	-2.16	1.46	1.50
30	F	102	SQD	O9-S	2.16	1.51	1.45
30	f	102	SQD	O9-S	2.16	1.51	1.45
25	C	509	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	CMC-C2C	-2.16	1.46	1.50
30	a	413	SQD	O8-S	2.16	1.55	1.47
25	C	513	CLA	CMC-C2C	-2.16	1.46	1.50
25	c	513	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	609	CLA	C4B-CHC	-2.15	1.35	1.41
25	b	609	CLA	C4B-CHC	-2.15	1.35	1.41
25	C	506	CLA	C4B-CHC	-2.14	1.35	1.41
30	A	413	SQD	O8-S	2.14	1.55	1.47
25	c	512	CLA	CMC-C2C	-2.14	1.46	1.50
25	C	503	CLA	CMC-C2C	-2.14	1.46	1.50
25	B	615	CLA	C4B-CHC	-2.14	1.35	1.41
25	b	615	CLA	C4B-CHC	-2.14	1.35	1.41
25	B	610	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.13	1.46	1.50
30	F	102	SQD	O7-S	2.13	1.51	1.45
30	f	102	SQD	O7-S	2.13	1.51	1.45
25	C	504	CLA	C4B-CHC	-2.13	1.35	1.41
25	c	504	CLA	C4B-CHC	-2.13	1.35	1.41
27	Z	101	BCR	C14-C13	2.13	1.40	1.35
27	z	101	BCR	C14-C13	2.13	1.40	1.35
25	D	403	CLA	C3B-C2B	-2.13	1.37	1.40
25	d	403	CLA	C3B-C2B	-2.13	1.37	1.40
25	C	506	CLA	CMC-C2C	-2.13	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.13	1.46	1.50
25	D	401	CLA	CMC-C2C	-2.13	1.46	1.50
25	d	401	CLA	CMC-C2C	-2.13	1.46	1.50
25	C	501	CLA	CMC-C2C	-2.12	1.46	1.50
27	K	104	BCR	C14-C13	2.12	1.40	1.35
27	z	103	BCR	C14-C13	2.12	1.40	1.35
25	c	501	CLA	CMC-C2C	-2.12	1.46	1.50
25	C	505	CLA	C3B-C2B	-2.12	1.37	1.40
25	c	506	CLA	C4B-CHC	-2.11	1.35	1.41
34	C	515	DGD	O1G-C1G	-2.11	1.40	1.45
34	c	515	DGD	O1G-C1G	-2.11	1.40	1.45
25	C	506	CLA	C3B-C2B	-2.11	1.37	1.40
25	c	506	CLA	C3B-C2B	-2.11	1.37	1.40
30	F	102	SQD	C8-C7	2.11	1.56	1.50
30	f	102	SQD	C8-C7	2.11	1.56	1.50
25	A	405	CLA	C4B-CHC	-2.10	1.35	1.41
25	a	405	CLA	C4B-CHC	-2.10	1.35	1.41
25	A	406	CLA	CMC-C2C	-2.10	1.46	1.50
25	a	406	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	101	RRX	C16-C17	-2.09	1.36	1.43
25	C	503	CLA	C4B-CHC	-2.09	1.35	1.41
25	c	503	CLA	C4B-CHC	-2.09	1.35	1.41
25	C	511	CLA	C3B-C2B	-2.09	1.37	1.40
25	c	511	CLA	C3B-C2B	-2.09	1.37	1.40
25	d	401	CLA	CAC-C3C	-2.09	1.45	1.51
27	z	101	BCR	C10-C9	2.08	1.40	1.35
36	h	101	RRX	C16-C17	-2.08	1.36	1.43
25	C	502	CLA	C4B-CHC	-2.07	1.35	1.41
25	c	502	CLA	C4B-CHC	-2.07	1.35	1.41
25	B	601	CLA	CMC-C2C	-2.07	1.46	1.50
25	b	601	CLA	CMC-C2C	-2.07	1.46	1.50
27	z	101	BCR	C17-C18	2.07	1.40	1.35
25	D	401	CLA	CAC-C3C	-2.07	1.45	1.51
25	A	408	CLA	CMC-C2C	-2.06	1.46	1.50
25	a	408	CLA	CMC-C2C	-2.06	1.46	1.50
25	b	608	CLA	C4B-CHC	-2.06	1.35	1.41
27	Z	101	BCR	C10-C9	2.06	1.40	1.35
25	A	408	CLA	C4B-CHC	-2.06	1.35	1.41
25	a	408	CLA	C4B-CHC	-2.06	1.35	1.41
25	B	608	CLA	C4B-CHC	-2.06	1.35	1.41
25	B	609	CLA	MG-NA	2.06	2.11	2.06
27	B	618	BCR	C11-C10	-2.06	1.36	1.43
25	A	405	CLA	C3B-C2B	-2.05	1.37	1.40
25	a	405	CLA	C3B-C2B	-2.05	1.37	1.40
25	b	602	CLA	C3B-C2B	-2.05	1.37	1.40
34	C	517	DGD	O2G-C2G	-2.05	1.41	1.46
34	c	517	DGD	O2G-C2G	-2.05	1.41	1.46
25	D	404	CLA	C4B-CHC	-2.05	1.35	1.41
27	b	618	BCR	C11-C10	-2.05	1.36	1.43
25	C	510	CLA	MG-NA	2.05	2.11	2.06
25	c	510	CLA	MG-NA	2.05	2.11	2.06
25	B	604	CLA	C4B-CHC	-2.04	1.35	1.41
25	b	604	CLA	C4B-CHC	-2.04	1.35	1.41
25	d	404	CLA	C4B-CHC	-2.04	1.35	1.41
27	B	617	BCR	C20-C21	-2.04	1.36	1.43
31	e	103	LMT	O1'-C1'	2.04	1.43	1.40
27	K	103	BCR	C10-C9	2.04	1.40	1.35
27	k	103	BCR	C10-C9	2.04	1.40	1.35
25	B	612	CLA	MG-NA	2.04	2.11	2.06
27	F	101	BCR	C21-C22	2.03	1.40	1.35
27	f	101	BCR	C21-C22	2.03	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEM	C3C-C4C	2.03	1.44	1.41
35	v	201	HEM	C3C-C4C	2.03	1.44	1.41
25	B	607	CLA	C4B-CHC	-2.03	1.35	1.41
25	b	607	CLA	C4B-CHC	-2.03	1.35	1.41
27	Z	101	BCR	C17-C18	2.03	1.40	1.35
25	b	612	CLA	MG-NA	2.03	2.11	2.06
25	b	609	CLA	MG-NA	2.02	2.11	2.06
27	B	617	BCR	C16-C17	-2.02	1.36	1.43
27	b	617	BCR	C16-C17	-2.02	1.36	1.43
25	b	605	CLA	C4B-CHC	-2.02	1.35	1.41
27	b	617	BCR	C20-C21	-2.02	1.36	1.43
36	H	101	RRX	C15-C14	-2.02	1.36	1.43
36	h	101	RRX	C15-C14	-2.02	1.36	1.43
25	a	405	CLA	MG-ND	-2.02	2.01	2.05
27	B	618	BCR	C15-C14	-2.01	1.36	1.43
25	A	405	CLA	MG-ND	-2.01	2.01	2.05
25	A	408	CLA	C3B-C2B	-2.01	1.37	1.40
25	a	408	CLA	C3B-C2B	-2.01	1.37	1.40
27	b	618	BCR	C20-C21	-2.01	1.37	1.43
25	C	508	CLA	C3B-C2B	-2.01	1.37	1.40
25	c	508	CLA	C3B-C2B	-2.01	1.37	1.40
36	h	101	RRX	C20-C21	-2.01	1.37	1.43
25	A	406	CLA	C4B-CHC	-2.01	1.35	1.41
25	C	501	CLA	C4B-CHC	-2.01	1.35	1.41
25	a	406	CLA	C4B-CHC	-2.01	1.35	1.41
25	c	501	CLA	C4B-CHC	-2.01	1.35	1.41
25	C	507	CLA	C4B-CHC	-2.01	1.35	1.41
25	c	507	CLA	C4B-CHC	-2.01	1.35	1.41
25	D	401	CLA	MG-NC	-2.00	2.01	2.06
25	d	401	CLA	MG-NC	-2.00	2.01	2.06
25	B	606	CLA	C3B-C2B	-2.00	1.37	1.40
25	b	606	CLA	C3B-C2B	-2.00	1.37	1.40
27	Z	101	BCR	C21-C22	2.00	1.40	1.35
27	z	101	BCR	C21-C22	2.00	1.40	1.35
25	C	508	CLA	C4B-CHC	-2.00	1.35	1.41
25	c	508	CLA	C4B-CHC	-2.00	1.35	1.41

All (975) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	C4A-NA-C1A	8.74	110.67	106.68
25	C	507	CLA	C4A-NA-C1A	8.66	110.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	b	607	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	C	506	CLA	C4A-NA-C1A	7.12	109.93	106.68
25	c	506	CLA	C4A-NA-C1A	7.12	109.93	106.68
25	B	611	CLA	C4A-NA-C1A	7.09	109.91	106.68
25	b	611	CLA	C4A-NA-C1A	7.09	109.91	106.68
25	C	509	CLA	C4A-NA-C1A	7.02	109.88	106.68
25	C	511	CLA	C4A-NA-C1A	7.02	109.88	106.68
25	c	511	CLA	C4A-NA-C1A	7.02	109.88	106.68
25	c	509	CLA	C4A-NA-C1A	6.98	109.86	106.68
25	C	502	CLA	C4A-NA-C1A	6.82	109.79	106.68
25	c	502	CLA	C4A-NA-C1A	6.82	109.79	106.68
25	B	612	CLA	C4A-NA-C1A	6.79	109.78	106.68
25	b	612	CLA	C4A-NA-C1A	6.79	109.78	106.68
25	B	604	CLA	C4A-NA-C1A	6.77	109.77	106.68
25	b	604	CLA	C4A-NA-C1A	6.77	109.77	106.68
25	a	405	CLA	C4A-NA-C1A	6.61	109.69	106.68
25	A	405	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	b	614	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	d	401	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	B	614	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	D	404	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	d	404	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	D	401	CLA	C4A-NA-C1A	6.26	109.53	106.68
25	C	513	CLA	C4A-NA-C1A	6.19	109.50	106.68
25	c	513	CLA	C4A-NA-C1A	6.19	109.50	106.68
25	b	615	CLA	C4A-NA-C1A	6.17	109.49	106.68
25	B	615	CLA	C4A-NA-C1A	6.15	109.49	106.68
35	E	104	HEM	CBD-CAD-C3D	-6.01	95.92	112.53
35	e	104	HEM	CBD-CAD-C3D	-6.00	95.93	112.53
25	B	605	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	a	406	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	C	504	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	c	504	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	B	601	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	b	601	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	B	610	CLA	C4A-NA-C1A	5.94	109.39	106.68
25	b	610	CLA	C4A-NA-C1A	5.94	109.39	106.68
25	A	406	CLA	C4A-NA-C1A	5.93	109.39	106.68
25	B	613	CLA	C4A-NA-C1A	5.91	109.38	106.68
25	b	613	CLA	C4A-NA-C1A	5.91	109.38	106.68
25	b	605	CLA	C4A-NA-C1A	5.89	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	c	510	CLA	C4A-NA-C1A	5.84	109.34	106.68
25	b	603	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	D	403	CLA	C4A-NA-C1A	5.80	109.33	106.68
25	d	403	CLA	C4A-NA-C1A	5.80	109.33	106.68
25	C	510	CLA	C4A-NA-C1A	5.80	109.32	106.68
25	B	606	CLA	C4A-NA-C1A	5.78	109.31	106.68
25	b	606	CLA	C4A-NA-C1A	5.75	109.30	106.68
25	C	508	CLA	C4A-NA-C1A	5.63	109.25	106.68
25	c	508	CLA	C4A-NA-C1A	5.63	109.25	106.68
25	B	609	CLA	C4A-NA-C1A	5.55	109.21	106.68
25	b	609	CLA	C4A-NA-C1A	5.55	109.21	106.68
25	A	408	CLA	C4A-NA-C1A	5.55	109.21	106.68
25	C	505	CLA	C4A-NA-C1A	5.54	109.21	106.68
25	c	505	CLA	C4A-NA-C1A	5.54	109.21	106.68
35	E	104	HEM	CHC-C4B-NB	5.52	130.38	124.44
35	e	104	HEM	CHC-C4B-NB	5.50	130.36	124.44
25	a	408	CLA	C4A-NA-C1A	5.45	109.16	106.68
25	B	608	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	b	608	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	C	501	CLA	C4A-NA-C1A	5.41	109.15	106.68
25	c	501	CLA	C4A-NA-C1A	5.41	109.15	106.68
25	b	616	CLA	C4A-NA-C1A	5.30	109.10	106.68
25	B	616	CLA	C4A-NA-C1A	5.28	109.09	106.68
25	C	503	CLA	C4A-NA-C1A	4.96	108.94	106.68
25	c	503	CLA	C4A-NA-C1A	4.96	108.94	106.68
25	c	510	CLA	CMB-C2B-C1B	-4.95	121.20	128.46
25	C	510	CLA	CMB-C2B-C1B	-4.94	121.22	128.46
25	C	501	CLA	CMB-C2B-C1B	-4.88	121.31	128.46
25	c	501	CLA	CMB-C2B-C1B	-4.88	121.31	128.46
25	B	604	CLA	C1-C2-C3	-4.73	118.44	126.20
25	b	604	CLA	C1-C2-C3	-4.73	118.44	126.20
25	c	512	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	c	508	CLA	CMB-C2B-C1B	-4.70	121.57	128.46
25	b	608	CLA	CMB-C2B-C1B	-4.67	121.61	128.46
25	C	508	CLA	CMB-C2B-C1B	-4.66	121.63	128.46
25	B	608	CLA	CMB-C2B-C1B	-4.65	121.65	128.46
25	B	607	CLA	CMB-C2B-C1B	-4.64	121.66	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.64	121.66	128.46
25	C	512	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	B	606	CLA	CMB-C2B-C1B	-4.58	121.74	128.46
25	b	606	CLA	CMB-C2B-C1B	-4.58	121.74	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	CMB-C2B-C1B	-4.57	121.76	128.46
25	c	509	CLA	CMB-C2B-C1B	-4.57	121.76	128.46
30	F	102	SQD	O47-C7-C8	4.57	121.37	111.48
30	f	102	SQD	O47-C7-C8	4.57	121.37	111.48
25	B	602	CLA	C4A-NA-C1A	4.56	108.76	106.68
25	b	602	CLA	C4A-NA-C1A	4.56	108.76	106.68
25	c	503	CLA	CMB-C2B-C1B	-4.53	121.82	128.46
25	C	503	CLA	CMB-C2B-C1B	-4.51	121.85	128.46
25	B	616	CLA	CMB-C2B-C1B	-4.49	121.88	128.46
25	C	513	CLA	CMB-C2B-C1B	-4.48	121.89	128.46
25	b	616	CLA	CMB-C2B-C1B	-4.47	121.91	128.46
25	c	513	CLA	CMB-C2B-C1B	-4.46	121.92	128.46
25	C	504	CLA	CMB-C2B-C1B	-4.44	121.96	128.46
25	c	504	CLA	CMB-C2B-C1B	-4.44	121.96	128.46
25	A	405	CLA	CMB-C2B-C1B	-4.42	121.98	128.46
25	B	614	CLA	CMB-C2B-C1B	-4.40	122.01	128.46
25	b	614	CLA	CMB-C2B-C1B	-4.40	122.01	128.46
25	a	405	CLA	CMB-C2B-C1B	-4.40	122.01	128.46
25	B	611	CLA	CMB-C2B-C1B	-4.39	122.03	128.46
25	b	611	CLA	CMB-C2B-C1B	-4.39	122.03	128.46
25	B	615	CLA	CMB-C2B-C1B	-4.38	122.04	128.46
25	b	615	CLA	CMB-C2B-C1B	-4.38	122.04	128.46
34	C	516	DGD	O2G-C1B-C2B	4.36	120.92	111.48
34	c	516	DGD	O2G-C1B-C2B	4.36	120.92	111.48
25	B	612	CLA	CMB-C2B-C1B	-4.35	122.08	128.46
25	b	612	CLA	CMB-C2B-C1B	-4.35	122.08	128.46
25	b	609	CLA	CMB-C2B-C1B	-4.34	122.10	128.46
25	B	609	CLA	CMB-C2B-C1B	-4.33	122.11	128.46
25	b	602	CLA	CMB-C2B-C1B	-4.32	122.13	128.46
25	B	602	CLA	CMB-C2B-C1B	-4.31	122.15	128.46
25	C	506	CLA	CMB-C2B-C1B	-4.25	122.23	128.46
25	c	506	CLA	CMB-C2B-C1B	-4.25	122.23	128.46
25	B	613	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
25	b	613	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
25	A	408	CLA	CMB-C2B-C1B	-4.21	122.28	128.46
25	a	408	CLA	CMB-C2B-C1B	-4.21	122.28	128.46
25	B	610	CLA	CMB-C2B-C1B	-4.19	122.32	128.46
25	b	610	CLA	CMB-C2B-C1B	-4.19	122.32	128.46
31	k	105	LMT	C1'-C2'-C3'	4.13	118.69	110.01
25	D	404	CLA	O2D-CGD-O1D	-4.12	115.82	123.85
25	d	404	CLA	O2D-CGD-O1D	-4.12	115.82	123.85
31	K	105	LMT	C1'-C2'-C3'	4.11	118.67	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	517	DGD	O2G-C1B-C2B	4.00	120.14	111.48
25	B	603	CLA	CMB-C2B-C1B	-4.00	122.60	128.46
25	b	603	CLA	CMB-C2B-C1B	-4.00	122.60	128.46
34	c	517	DGD	O2G-C1B-C2B	3.99	120.10	111.48
25	D	404	CLA	CMB-C2B-C1B	-3.98	122.63	128.46
25	d	404	CLA	CMB-C2B-C1B	-3.98	122.63	128.46
25	D	403	CLA	CMB-C2B-C1B	-3.97	122.65	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.96	122.65	128.46
25	B	614	CLA	C1-C2-C3	-3.95	119.72	126.20
25	b	614	CLA	C1-C2-C3	-3.95	119.72	126.20
25	C	502	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
25	c	502	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
25	C	512	CLA	CMB-C2B-C1B	-3.94	122.68	128.46
25	c	512	CLA	CMB-C2B-C1B	-3.94	122.68	128.46
25	C	511	CLA	CMB-C2B-C1B	-3.92	122.71	128.46
25	c	511	CLA	CMB-C2B-C1B	-3.92	122.71	128.46
31	E	103	LMT	C1'-C2'-C3'	3.92	118.25	110.01
25	c	505	CLA	CMB-C2B-C1B	-3.92	122.72	128.46
27	K	104	BCR	C16-C15-C14	3.91	131.52	123.52
27	z	103	BCR	C16-C15-C14	3.91	131.52	123.52
31	e	103	LMT	C1'-C2'-C3'	3.91	118.23	110.01
25	B	601	CLA	CMB-C2B-C1B	-3.90	122.74	128.46
25	C	505	CLA	CMB-C2B-C1B	-3.90	122.74	128.46
25	b	601	CLA	CMB-C2B-C1B	-3.90	122.74	128.46
25	C	502	CLA	CMB-C2B-C1B	-3.90	122.75	128.46
25	c	502	CLA	CMB-C2B-C1B	-3.90	122.75	128.46
25	B	611	CLA	C1-C2-C3	-3.88	119.84	126.20
25	b	611	CLA	C1-C2-C3	-3.86	119.87	126.20
25	D	401	CLA	CMB-C2B-C1B	-3.85	122.82	128.46
25	d	401	CLA	CMB-C2B-C1B	-3.85	122.82	128.46
25	B	605	CLA	CMB-C2B-C1B	-3.83	122.85	128.46
25	b	605	CLA	CMB-C2B-C1B	-3.83	122.85	128.46
34	C	515	DGD	O2G-C1B-C2B	3.80	119.69	111.48
34	c	515	DGD	O2G-C1B-C2B	3.80	119.69	111.48
25	C	501	CLA	CMB-C2B-C3B	3.77	132.22	124.68
25	c	501	CLA	CMB-C2B-C3B	3.77	132.22	124.68
27	F	101	BCR	C15-C16-C17	3.77	131.24	123.52
27	f	101	BCR	C15-C16-C17	3.77	131.24	123.52
25	a	406	CLA	CMB-C2B-C1B	-3.77	122.94	128.46
30	F	102	SQD	O9-S-O7	-3.76	101.60	113.82
30	f	102	SQD	O9-S-O7	-3.76	101.60	113.82
25	A	406	CLA	CMB-C2B-C1B	-3.75	122.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
25	c	513	CLA	C1-C2-C3	-3.74	120.07	126.20
25	C	513	CLA	C1-C2-C3	-3.73	120.08	126.20
25	b	602	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
25	B	603	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
25	b	603	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
25	B	604	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
25	b	604	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
25	B	614	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
25	b	614	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
31	e	103	LMT	C1B-O1B-C4'	-3.67	109.27	117.98
31	E	103	LMT	C1B-O1B-C4'	-3.66	109.29	117.98
25	c	508	CLA	CMB-C2B-C3B	3.66	131.99	124.68
25	b	608	CLA	C1-C2-C3	-3.63	120.25	126.20
25	C	508	CLA	CMB-C2B-C3B	3.63	131.94	124.68
25	C	508	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
25	c	508	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
31	d	411	LMT	C2'-C3'-C4'	3.62	117.90	109.68
25	B	608	CLA	C1-C2-C3	-3.62	120.27	126.20
36	H	101	RRX	C37-C22-C21	-3.62	116.95	122.82
31	D	411	LMT	C2'-C3'-C4'	3.62	117.89	109.68
36	h	101	RRX	C37-C22-C21	-3.61	116.96	122.82
25	B	616	CLA	CMB-C2B-C3B	3.61	131.89	124.68
25	b	616	CLA	CMB-C2B-C3B	3.59	131.86	124.68
35	E	104	HEM	CHD-C1D-ND	3.58	128.29	124.44
35	e	104	HEM	CHD-C1D-ND	3.58	128.29	124.44
25	c	513	CLA	CMB-C2B-C3B	3.58	131.83	124.68
34	H	104	DGD	O2G-C1B-C2B	3.57	119.20	111.48
34	h	104	DGD	O2G-C1B-C2B	3.57	119.20	111.48
27	Z	101	BCR	C15-C16-C17	3.56	130.80	123.52
25	C	513	CLA	CMB-C2B-C3B	3.56	131.79	124.68
27	K	103	BCR	C37-C22-C21	-3.55	117.06	122.82
27	z	101	BCR	C15-C16-C17	3.55	130.78	123.52
27	f	101	BCR	C34-C9-C10	-3.54	117.08	122.82
30	F	102	SQD	C3-C4-C5	3.54	116.66	110.23
30	f	102	SQD	C3-C4-C5	3.54	116.66	110.23
25	B	611	CLA	CMB-C2B-C3B	3.54	131.76	124.68
25	b	611	CLA	CMB-C2B-C3B	3.54	131.76	124.68
27	k	103	BCR	C15-C16-C17	3.54	130.76	123.52
27	k	103	BCR	C37-C22-C21	-3.54	117.09	122.82
27	C	514	BCR	C34-C9-C10	-3.53	117.10	122.82
27	c	514	BCR	C34-C9-C10	-3.53	117.10	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	101	BCR	C34-C9-C10	-3.53	117.10	122.82
25	A	406	CLA	O2D-CGD-CBD	3.52	117.39	111.23
25	a	406	CLA	O2D-CGD-CBD	3.52	117.39	111.23
27	K	103	BCR	C15-C16-C17	3.52	130.73	123.52
36	H	101	RRX	C34-C9-C10	-3.52	117.12	122.82
27	Z	101	BCR	C34-C9-C10	-3.51	117.13	122.82
36	h	101	RRX	C34-C9-C10	-3.50	117.15	122.82
25	a	408	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
25	A	408	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
27	A	409	BCR	C34-C9-C10	-3.49	117.16	122.82
27	a	409	BCR	C34-C9-C10	-3.49	117.16	122.82
27	K	104	BCR	C37-C22-C21	-3.49	117.17	122.82
27	z	103	BCR	C37-C22-C21	-3.49	117.17	122.82
27	z	101	BCR	C34-C9-C10	-3.49	117.17	122.82
30	F	102	SQD	O5-C5-C4	3.49	115.98	109.70
25	c	503	CLA	CMB-C2B-C3B	3.48	131.64	124.68
25	C	503	CLA	CMB-C2B-C3B	3.47	131.63	124.68
25	b	608	CLA	CMB-C2B-C3B	3.47	131.62	124.68
30	f	102	SQD	O5-C5-C4	3.47	115.95	109.70
25	B	606	CLA	CMB-C2B-C3B	3.46	131.60	124.68
25	b	606	CLA	CMB-C2B-C3B	3.46	131.60	124.68
25	b	612	CLA	CMB-C2B-C3B	3.46	131.59	124.68
25	B	608	CLA	CMB-C2B-C3B	3.46	131.59	124.68
25	D	404	CLA	O2D-CGD-CBD	3.45	117.26	111.23
25	d	404	CLA	O2D-CGD-CBD	3.45	117.26	111.23
25	C	509	CLA	CMB-C2B-C3B	3.45	131.57	124.68
25	c	509	CLA	CMB-C2B-C3B	3.45	131.57	124.68
25	B	612	CLA	CMB-C2B-C3B	3.44	131.56	124.68
25	C	501	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
25	B	602	CLA	CMB-C2B-C3B	3.43	131.53	124.68
25	b	602	CLA	CMB-C2B-C3B	3.43	131.53	124.68
27	B	618	BCR	C34-C9-C10	-3.41	117.29	122.82
29	D	405	PL9	C7-C3-C4	3.40	119.71	116.91
29	d	405	PL9	C7-C3-C4	3.40	119.71	116.91
25	c	501	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
25	c	510	CLA	CMB-C2B-C3B	3.40	131.48	124.68
27	b	618	BCR	C34-C9-C10	-3.40	117.31	122.82
31	M	101	LMT	C1B-C2B-C3B	3.39	117.15	110.01
27	B	618	BCR	C37-C22-C21	-3.39	117.32	122.82
27	b	618	BCR	C37-C22-C21	-3.39	117.32	122.82
25	C	510	CLA	CMB-C2B-C3B	3.39	131.45	124.68
25	c	505	CLA	O2D-CGD-CBD	3.38	117.15	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	105	LMT	C1B-C2B-C3B	3.38	117.13	110.01
27	K	103	BCR	C34-C9-C10	-3.38	117.34	122.82
27	k	103	BCR	C34-C9-C10	-3.38	117.34	122.82
27	a	409	BCR	C37-C22-C21	-3.38	117.35	122.82
27	A	409	BCR	C37-C22-C21	-3.37	117.36	122.82
27	Z	101	BCR	C37-C22-C21	-3.36	117.36	122.82
27	z	101	BCR	C37-C22-C21	-3.36	117.36	122.82
25	C	505	CLA	O2D-CGD-CBD	3.36	117.11	111.23
27	B	618	BCR	C16-C15-C14	3.35	130.38	123.52
27	C	514	BCR	C16-C15-C14	3.35	130.37	123.52
27	c	514	BCR	C16-C15-C14	3.35	130.37	123.52
27	B	619	BCR	C34-C9-C10	-3.35	117.39	122.82
27	F	101	BCR	C37-C22-C21	-3.35	117.39	122.82
27	b	619	BCR	C34-C9-C10	-3.35	117.39	122.82
27	f	101	BCR	C37-C22-C21	-3.35	117.39	122.82
27	b	618	BCR	C16-C15-C14	3.35	130.37	123.52
35	E	104	HEM	C1B-NB-C4B	3.35	109.17	105.21
27	B	617	BCR	C37-C22-C21	-3.35	117.39	122.82
27	b	617	BCR	C37-C22-C21	-3.35	117.39	122.82
31	K	105	LMT	O5'-C5'-C4'	-3.35	102.81	109.72
35	e	104	HEM	CBA-CAA-C2A	-3.34	106.92	112.54
31	k	105	LMT	O5'-C5'-C4'	-3.34	102.82	109.72
25	A	406	CLA	C1-C2-C3	-3.34	120.73	126.20
25	a	406	CLA	C1-C2-C3	-3.34	120.73	126.20
35	E	104	HEM	CBA-CAA-C2A	-3.34	106.93	112.54
25	B	604	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
25	b	604	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
35	e	104	HEM	C1B-NB-C4B	3.33	109.15	105.21
25	C	504	CLA	CMB-C2B-C3B	3.33	131.33	124.68
25	c	504	CLA	CMB-C2B-C3B	3.33	131.33	124.68
27	Z	101	BCR	C16-C15-C14	3.32	130.31	123.52
25	A	408	CLA	CMB-C2B-C3B	3.32	131.31	124.68
25	a	408	CLA	CMB-C2B-C3B	3.32	131.31	124.68
31	M	101	LMT	C1B-O5B-C5B	-3.31	107.25	113.72
25	B	614	CLA	CMB-C2B-C3B	3.31	131.29	124.68
25	b	614	CLA	CMB-C2B-C3B	3.31	131.29	124.68
31	L	105	LMT	C1B-O5B-C5B	-3.31	107.26	113.72
27	z	101	BCR	C16-C15-C14	3.30	130.28	123.52
27	B	617	BCR	C34-C9-C10	-3.30	117.47	122.82
27	b	617	BCR	C34-C9-C10	-3.30	117.47	122.82
31	K	105	LMT	O1B-C4'-C3'	3.30	115.61	107.23
31	k	105	LMT	O1B-C4'-C3'	3.30	115.61	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C30-C25-C26	-3.28	118.16	122.64
27	k	103	BCR	C30-C25-C26	-3.28	118.16	122.64
25	B	602	CLA	C1B-CHB-C4A	-3.27	123.80	130.04
25	b	602	CLA	C1B-CHB-C4A	-3.27	123.80	130.04
30	F	102	SQD	O7-S-C6	3.27	111.64	106.76
30	f	102	SQD	O7-S-C6	3.27	111.64	106.76
25	A	405	CLA	CMB-C2B-C3B	3.27	131.21	124.68
25	a	405	CLA	CMB-C2B-C3B	3.25	131.18	124.68
25	c	512	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
35	E	104	HEM	CHA-C4D-ND	3.25	128.40	124.37
35	e	104	HEM	CHA-C4D-ND	3.24	128.39	124.37
27	B	619	BCR	C37-C22-C21	-3.24	117.56	122.82
27	b	619	BCR	C37-C22-C21	-3.24	117.56	122.82
25	C	512	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
31	C	522	LMT	C1'-O5'-C5'	-3.24	107.40	113.72
31	c	522	LMT	C1'-O5'-C5'	-3.24	107.40	113.72
25	B	610	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	C	511	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	b	610	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	c	511	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
29	A	411	PL9	C7-C3-C4	3.22	119.56	116.91
29	a	411	PL9	C7-C3-C4	3.22	119.56	116.91
25	D	401	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
25	d	401	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
25	b	607	CLA	CMB-C2B-C3B	3.21	131.10	124.68
25	C	507	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
25	c	507	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
27	B	619	BCR	C15-C16-C17	3.20	130.07	123.52
27	b	619	BCR	C15-C16-C17	3.20	130.07	123.52
25	B	607	CLA	CMB-C2B-C3B	3.19	131.06	124.68
27	K	104	BCR	C34-C9-C10	-3.18	117.66	122.82
27	z	103	BCR	C34-C9-C10	-3.18	117.66	122.82
31	D	411	LMT	C1B-O1B-C4'	-3.18	110.44	117.98
31	d	411	LMT	C1B-O1B-C4'	-3.18	110.44	117.98
25	D	401	CLA	CHB-C4A-NA	3.18	128.98	124.40
25	d	401	CLA	CHB-C4A-NA	3.18	128.98	124.40
25	B	615	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
25	b	615	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
35	E	104	HEM	CHB-C1B-NB	3.16	128.28	124.37
35	e	104	HEM	CHB-C1B-NB	3.16	128.28	124.37
25	B	615	CLA	CMB-C2B-C3B	3.15	130.98	124.68
25	b	615	CLA	CMB-C2B-C3B	3.15	130.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	d	403	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	L	105	LMT	C4B-C3B-C2B	3.13	116.33	110.83
31	M	101	LMT	C4B-C3B-C2B	3.13	116.33	110.83
25	a	406	CLA	CHB-C4A-NA	3.13	128.92	124.40
31	K	105	LMT	C1'-O5'-C5'	-3.13	107.61	113.72
31	k	105	LMT	C1'-O5'-C5'	-3.13	107.61	113.72
25	C	506	CLA	CMB-C2B-C3B	3.13	130.94	124.68
25	c	506	CLA	CMB-C2B-C3B	3.13	130.94	124.68
27	C	514	BCR	C15-C16-C17	3.13	129.92	123.52
27	c	514	BCR	C15-C16-C17	3.13	129.92	123.52
25	A	406	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	a	406	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
27	a	409	BCR	C15-C16-C17	3.13	129.91	123.52
25	C	508	CLA	O2D-CGD-CBD	3.13	116.69	111.23
25	c	508	CLA	O2D-CGD-CBD	3.13	116.69	111.23
25	B	603	CLA	CMB-C2B-C3B	3.12	130.93	124.68
25	b	603	CLA	CMB-C2B-C3B	3.12	130.93	124.68
25	B	601	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	A	406	CLA	CHB-C4A-NA	3.12	128.90	124.40
25	c	505	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
27	A	409	BCR	C15-C16-C17	3.11	129.89	123.52
25	B	608	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
25	B	606	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
25	b	606	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
31	C	524	LMT	C1'-C2'-C3'	3.11	116.55	110.01
31	c	524	LMT	C1'-C2'-C3'	3.11	116.55	110.01
25	C	509	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
25	c	509	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
25	c	503	CLA	C1B-CHB-C4A	-3.11	124.12	130.04
25	b	601	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
25	b	608	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
25	C	511	CLA	C1-C2-C3	-3.10	121.12	126.20
25	c	511	CLA	C1-C2-C3	-3.10	121.12	126.20
25	C	512	CLA	CMB-C2B-C3B	3.10	130.87	124.68
25	c	512	CLA	CMB-C2B-C3B	3.10	130.87	124.68
25	C	505	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
25	B	605	CLA	CMB-C2B-C3B	3.09	130.85	124.68
25	b	605	CLA	CMB-C2B-C3B	3.09	130.85	124.68
25	C	503	CLA	C1B-CHB-C4A	-3.09	124.15	130.04
25	C	504	CLA	CHB-C4A-NA	3.08	128.85	124.40
25	c	504	CLA	CHB-C4A-NA	3.08	128.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	CMB-C2B-C3B	3.08	130.84	124.68
25	c	505	CLA	CMB-C2B-C3B	3.08	130.84	124.68
25	B	613	CLA	C1-C2-C3	-3.07	121.17	126.20
25	B	613	CLA	CMB-C2B-C3B	3.07	130.82	124.68
25	C	505	CLA	CMB-C2B-C3B	3.07	130.82	124.68
25	D	401	CLA	CMB-C2B-C3B	3.06	130.80	124.68
25	d	401	CLA	CMB-C2B-C3B	3.06	130.80	124.68
25	A	408	CLA	C1-C2-C3	-3.06	121.18	126.20
25	a	408	CLA	C1-C2-C3	-3.06	121.18	126.20
25	A	406	CLA	CMB-C2B-C3B	3.06	130.79	124.68
25	a	406	CLA	CMB-C2B-C3B	3.06	130.79	124.68
25	D	404	CLA	CMB-C2B-C3B	3.06	130.79	124.68
25	d	404	CLA	CMB-C2B-C3B	3.06	130.79	124.68
25	b	616	CLA	C1B-CHB-C4A	-3.05	124.21	130.04
36	H	101	RRX	C35-C13-C14	-3.05	117.88	122.82
36	h	101	RRX	C35-C13-C14	-3.05	117.88	122.82
25	b	613	CLA	C1-C2-C3	-3.05	121.20	126.20
26	d	402	PHO	C1-C2-C3	-3.04	121.21	126.20
25	C	511	CLA	CMB-C2B-C3B	3.04	130.75	124.68
25	c	511	CLA	CMB-C2B-C3B	3.04	130.75	124.68
25	B	616	CLA	C1B-CHB-C4A	-3.03	124.25	130.04
25	D	401	CLA	C1-C2-C3	-3.03	121.23	126.20
26	D	402	PHO	C1-C2-C3	-3.03	121.23	126.20
25	d	401	CLA	C1-C2-C3	-3.03	121.23	126.20
25	b	609	CLA	C1B-CHB-C4A	-3.02	124.28	130.04
25	d	403	CLA	CMB-C2B-C3B	3.02	130.71	124.68
25	B	609	CLA	C1B-CHB-C4A	-3.00	124.31	130.04
25	D	403	CLA	CMB-C2B-C3B	3.00	130.68	124.68
25	B	610	CLA	CMB-C2B-C3B	3.00	130.67	124.68
25	b	610	CLA	CMB-C2B-C3B	3.00	130.67	124.68
25	B	604	CLA	O2D-CGD-CBD	3.00	116.47	111.23
25	b	604	CLA	O2D-CGD-CBD	3.00	116.47	111.23
25	c	509	CLA	C1-C2-C3	-2.99	121.29	126.20
25	c	512	CLA	CHB-C4A-NA	2.99	128.72	124.40
25	C	506	CLA	C1-C2-C3	-2.98	121.31	126.20
25	c	506	CLA	C1-C2-C3	-2.98	121.31	126.20
28	C	518	LMG	O1-C7-C8	-2.98	103.57	110.82
28	c	518	LMG	O1-C7-C8	-2.98	103.57	110.82
27	K	103	BCR	C19-C18-C17	2.98	123.69	119.01
27	k	103	BCR	C19-C18-C17	2.98	123.69	119.01
34	H	104	DGD	O1G-C1A-C2A	2.97	120.89	111.83
25	C	509	CLA	C1-C2-C3	-2.97	121.33	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	609	CLA	CMB-C2B-C3B	2.97	130.61	124.68
25	b	609	CLA	CMB-C2B-C3B	2.97	130.61	124.68
27	c	514	BCR	C1-C6-C5	-2.96	118.59	122.64
27	C	514	BCR	C1-C6-C5	-2.96	118.59	122.64
27	Z	101	BCR	C19-C18-C17	2.96	123.66	119.01
34	h	104	DGD	O1G-C1A-C2A	2.96	120.85	111.83
27	K	103	BCR	C36-C18-C17	-2.96	118.03	122.82
27	k	103	BCR	C36-C18-C17	-2.96	118.03	122.82
25	C	512	CLA	CHB-C4A-NA	2.95	128.66	124.40
27	z	101	BCR	C19-C18-C17	2.95	123.65	119.01
25	D	401	CLA	O2D-CGD-CBD	2.95	116.38	111.23
25	d	401	CLA	O2D-CGD-CBD	2.95	116.38	111.23
27	B	617	BCR	C15-C16-C17	2.94	129.54	123.52
27	b	617	BCR	C15-C16-C17	2.94	129.54	123.52
25	C	513	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	c	513	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	A	408	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	a	408	CLA	CHB-C4A-NA	2.93	128.63	124.40
30	F	102	SQD	O9-S-C6	2.93	111.13	106.76
30	f	102	SQD	O9-S-C6	2.93	111.13	106.76
25	B	603	CLA	C1B-CHB-C4A	-2.93	124.46	130.04
25	b	603	CLA	C1B-CHB-C4A	-2.93	124.46	130.04
25	D	401	CLA	C1B-CHB-C4A	-2.92	124.46	130.04
25	d	401	CLA	C1B-CHB-C4A	-2.92	124.46	130.04
25	a	408	CLA	O2D-CGD-CBD	2.92	116.34	111.23
25	B	602	CLA	O2D-CGD-CBD	2.92	116.33	111.23
27	C	514	BCR	C8-C9-C10	2.92	123.60	119.01
27	c	514	BCR	C8-C9-C10	2.92	123.60	119.01
25	b	602	CLA	O2D-CGD-CBD	2.92	116.33	111.23
35	E	104	HEM	CAD-CBD-CGD	2.91	121.39	113.67
35	e	104	HEM	CAD-CBD-CGD	2.91	121.39	113.67
25	c	512	CLA	C1B-CHB-C4A	-2.91	124.49	130.04
27	z	103	BCR	C15-C16-C17	2.90	129.46	123.52
25	A	408	CLA	O2D-CGD-CBD	2.90	116.31	111.23
36	H	101	RRX	C16-C15-C14	2.90	129.46	123.52
36	h	101	RRX	C16-C15-C14	2.90	129.46	123.52
27	C	514	BCR	C37-C22-C21	-2.90	118.11	122.82
27	c	514	BCR	C37-C22-C21	-2.90	118.11	122.82
25	C	502	CLA	CMB-C2B-C3B	2.90	130.48	124.68
25	c	502	CLA	CMB-C2B-C3B	2.90	130.48	124.68
27	K	104	BCR	C15-C16-C17	2.90	129.46	123.52
36	h	101	RRX	C15-C16-C17	2.90	129.45	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	c	513	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	C	512	CLA	C1B-CHB-C4A	-2.89	124.53	130.04
25	b	616	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
25	C	510	CLA	C1-C2-C3	-2.89	121.47	126.20
27	C	514	BCR	C35-C13-C14	-2.89	118.14	122.82
36	H	101	RRX	C15-C16-C17	2.89	129.42	123.52
31	b	630	LMT	C1'-O5'-C5'	2.89	119.36	113.72
25	B	616	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
31	B	627	LMT	C1'-O5'-C5'	2.88	119.34	113.72
27	c	514	BCR	C35-C13-C14	-2.87	118.16	122.82
27	b	618	BCR	C35-C13-C14	-2.87	118.17	122.82
25	b	604	CLA	CMB-C2B-C3B	2.87	130.42	124.68
25	A	406	CLA	C1B-CHB-C4A	-2.87	124.57	130.04
25	a	406	CLA	C1B-CHB-C4A	-2.87	124.57	130.04
25	c	510	CLA	C1-C2-C3	-2.86	121.51	126.20
25	B	604	CLA	CMB-C2B-C3B	2.85	130.39	124.68
25	B	601	CLA	CMB-C2B-C3B	2.85	130.38	124.68
27	Z	101	BCR	C36-C18-C17	-2.85	118.20	122.82
27	A	409	BCR	C16-C15-C14	2.85	129.34	123.52
27	a	409	BCR	C16-C15-C14	2.85	129.34	123.52
27	z	101	BCR	C36-C18-C17	-2.84	118.21	122.82
28	A	414	LMG	O1-C7-C8	-2.84	103.90	110.82
27	Z	101	BCR	C12-C13-C14	2.84	123.48	119.01
27	z	101	BCR	C12-C13-C14	2.84	123.48	119.01
28	a	414	LMG	O1-C7-C8	-2.84	103.91	110.82
25	B	608	CLA	C1B-CHB-C4A	-2.84	124.63	130.04
25	b	601	CLA	CMB-C2B-C3B	2.84	130.35	124.68
27	B	618	BCR	C35-C13-C14	-2.84	118.22	122.82
25	B	612	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	d	404	CLA	C1B-CHB-C4A	-2.83	124.64	130.04
25	D	404	CLA	C1B-CHB-C4A	-2.83	124.64	130.04
27	F	101	BCR	C19-C18-C17	2.83	123.46	119.01
27	f	101	BCR	C19-C18-C17	2.83	123.46	119.01
25	B	603	CLA	O2D-CGD-CBD	2.83	116.17	111.23
25	b	603	CLA	O2D-CGD-CBD	2.83	116.17	111.23
27	a	409	BCR	C12-C13-C14	2.82	123.45	119.01
25	b	608	CLA	C1B-CHB-C4A	-2.82	124.66	130.04
25	C	506	CLA	CHB-C4A-NA	2.82	128.47	124.40
25	c	506	CLA	CHB-C4A-NA	2.82	128.47	124.40
25	c	509	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
31	D	411	LMT	C1'-C2'-C3'	2.81	115.93	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	411	LMT	C1'-C2'-C3'	2.81	115.93	110.01
25	b	612	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	C	510	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	c	510	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	C	507	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	c	507	CLA	CHB-C4A-NA	2.81	128.46	124.40
27	K	103	BCR	C35-C13-C14	-2.81	118.26	122.82
27	k	103	BCR	C35-C13-C14	-2.81	118.26	122.82
27	K	104	BCR	C12-C13-C14	2.81	123.42	119.01
27	z	103	BCR	C12-C13-C14	2.81	123.42	119.01
27	F	101	BCR	C16-C15-C14	2.80	129.26	123.52
27	A	409	BCR	C12-C13-C14	2.80	123.42	119.01
27	C	514	BCR	C12-C13-C14	2.80	123.42	119.01
25	C	509	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
35	V	201	HEM	CBA-CAA-C2A	-2.80	107.83	112.54
35	v	201	HEM	CBA-CAA-C2A	-2.80	107.83	112.54
25	c	502	CLA	C1-C2-C3	-2.79	121.62	126.20
27	a	409	BCR	C35-C13-C14	-2.79	118.29	122.82
27	A	409	BCR	C35-C13-C14	-2.79	118.30	122.82
27	c	514	BCR	C12-C13-C14	2.79	123.39	119.01
27	f	101	BCR	C16-C15-C14	2.79	129.22	123.52
27	F	101	BCR	C36-C18-C17	-2.79	118.30	122.82
27	f	101	BCR	C36-C18-C17	-2.79	118.30	122.82
34	c	517	DGD	C3A-C2A-C1A	-2.79	103.49	113.69
27	b	619	BCR	C16-C15-C14	2.78	129.22	123.52
27	C	514	BCR	C19-C18-C17	2.78	123.39	119.01
25	C	502	CLA	C1-C2-C3	-2.78	121.64	126.20
34	C	517	DGD	C3A-C2A-C1A	-2.78	103.50	113.69
27	B	619	BCR	C16-C15-C14	2.77	129.19	123.52
27	K	104	BCR	C35-C13-C14	-2.76	118.34	122.82
27	z	103	BCR	C35-C13-C14	-2.76	118.34	122.82
27	c	514	BCR	C19-C18-C17	2.76	123.36	119.01
25	B	605	CLA	C1B-CHB-C4A	-2.76	124.78	130.04
25	b	605	CLA	C1B-CHB-C4A	-2.76	124.78	130.04
36	H	101	RRX	C12-C13-C14	2.75	123.34	119.01
36	h	101	RRX	C12-C13-C14	2.75	123.34	119.01
25	C	508	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	c	508	CLA	CHB-C4A-NA	2.75	128.37	124.40
27	Z	101	BCR	C35-C13-C14	-2.75	118.36	122.82
27	z	101	BCR	C35-C13-C14	-2.75	118.36	122.82
27	K	103	BCR	C16-C15-C14	2.74	129.13	123.52
27	k	103	BCR	C16-C15-C14	2.74	129.13	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	617	BCR	C35-C13-C14	-2.74	118.38	122.82
27	B	618	BCR	C12-C13-C14	2.73	123.31	119.01
27	b	618	BCR	C12-C13-C14	2.73	123.31	119.01
25	C	503	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	c	503	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	C	504	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
25	B	612	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	b	612	CLA	CHB-C4A-NA	2.72	128.33	124.40
27	B	617	BCR	C35-C13-C14	-2.72	118.40	122.82
25	a	405	CLA	CHB-C4A-NA	2.71	128.32	124.40
31	C	524	LMT	C1B-O1B-C4'	-2.71	111.56	117.98
31	c	524	LMT	C1B-O1B-C4'	-2.71	111.56	117.98
25	B	611	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	c	504	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
25	A	405	CLA	CHB-C4A-NA	2.70	128.30	124.40
36	H	101	RRX	C36-C18-C17	-2.70	118.45	122.82
27	A	409	BCR	C36-C18-C17	-2.69	118.45	122.82
27	a	409	BCR	C36-C18-C17	-2.69	118.45	122.82
25	C	502	CLA	C1B-CHB-C4A	-2.69	124.91	130.04
25	c	502	CLA	C1B-CHB-C4A	-2.69	124.91	130.04
25	b	611	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	C	513	CLA	C1B-CHB-C4A	-2.69	124.92	130.04
25	c	513	CLA	C1B-CHB-C4A	-2.69	124.92	130.04
25	B	607	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	b	607	CLA	CHB-C4A-NA	2.69	128.28	124.40
27	B	619	BCR	C35-C13-C14	-2.68	118.47	122.82
27	b	619	BCR	C35-C13-C14	-2.68	118.47	122.82
36	h	101	RRX	C36-C18-C17	-2.68	118.48	122.82
27	A	409	BCR	C19-C18-C17	2.68	123.22	119.01
27	a	409	BCR	C19-C18-C17	2.68	123.22	119.01
25	B	607	CLA	C16-C15-C13	-2.68	107.07	115.97
25	b	607	CLA	C16-C15-C13	-2.68	107.07	115.97
25	C	507	CLA	CMB-C2B-C1B	-2.67	124.54	128.46
25	B	604	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
27	C	514	BCR	C36-C18-C17	-2.67	118.49	122.82
25	c	507	CLA	CMB-C2B-C1B	-2.67	124.55	128.46
25	B	601	CLA	C1B-CHB-C4A	-2.67	124.95	130.04
25	b	601	CLA	C1B-CHB-C4A	-2.67	124.95	130.04
27	F	101	BCR	C35-C13-C14	-2.67	118.49	122.82
27	f	101	BCR	C35-C13-C14	-2.67	118.49	122.82
27	b	617	BCR	C12-C13-C14	2.67	123.20	119.01
25	b	604	CLA	O2A-CGA-O1A	-2.66	116.96	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	BCR	C12-C13-C14	2.66	123.20	119.01
27	c	514	BCR	C36-C18-C17	-2.66	118.51	122.82
25	B	604	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	b	604	CLA	CHB-C4A-NA	2.65	128.23	124.40
27	B	619	BCR	C36-C18-C17	-2.64	118.53	122.82
36	H	101	RRX	C19-C18-C17	2.64	123.16	119.01
27	b	619	BCR	C36-C18-C17	-2.63	118.55	122.82
25	B	611	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	b	611	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
31	K	105	LMT	C1-O1'-C1'	-2.63	109.20	113.68
31	k	105	LMT	C1-O1'-C1'	-2.63	109.20	113.68
36	h	101	RRX	C19-C18-C17	2.62	123.13	119.01
25	B	602	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	b	602	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	C	506	CLA	C1B-CHB-C4A	-2.59	125.10	130.04
25	c	506	CLA	C1B-CHB-C4A	-2.59	125.10	130.04
25	C	509	CLA	O1D-CGD-CBD	2.59	129.62	124.52
25	c	509	CLA	O1D-CGD-CBD	2.59	129.62	124.52
31	C	520	LMT	C6'-C5'-C4'	-2.59	106.67	113.02
31	c	520	LMT	C6'-C5'-C4'	-2.59	106.67	113.02
31	B	627	LMT	O1'-C1'-C2'	2.58	112.20	108.27
31	b	630	LMT	O1'-C1'-C2'	2.58	112.20	108.27
31	C	520	LMT	C4'-C3'-C2'	-2.58	106.30	110.83
31	c	520	LMT	C4'-C3'-C2'	-2.58	106.30	110.83
31	M	101	LMT	C1B-O1B-C4'	-2.57	111.88	117.98
25	B	607	CLA	C1B-CHB-C4A	-2.57	125.15	130.04
27	z	103	BCR	C36-C18-C17	-2.56	118.67	122.82
25	D	404	CLA	C1-C2-C3	-2.56	122.00	126.20
25	B	609	CLA	C1-C2-C3	-2.56	122.00	126.20
25	b	609	CLA	C1-C2-C3	-2.56	122.00	126.20
25	b	607	CLA	C1B-CHB-C4A	-2.56	125.16	130.04
31	L	105	LMT	C1B-O1B-C4'	-2.56	111.92	117.98
25	B	609	CLA	C7-C6-C5	-2.56	106.45	113.26
31	E	103	LMT	O5'-C5'-C4'	-2.55	104.44	109.72
31	e	103	LMT	O5'-C5'-C4'	-2.55	104.44	109.72
27	K	104	BCR	C36-C18-C17	-2.55	118.68	122.82
25	d	404	CLA	C1-C2-C3	-2.55	122.02	126.20
25	B	611	CLA	O2D-CGD-CBD	2.55	115.68	111.23
25	C	508	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
30	F	102	SQD	O5-C1-C2	2.55	115.60	110.37
25	C	502	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	c	502	CLA	CHB-C4A-NA	2.54	128.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
25	c	507	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
31	B	625	LMT	O1B-C4'-C3'	2.54	113.69	107.23
31	b	625	LMT	O1B-C4'-C3'	2.54	113.69	107.23
25	b	609	CLA	C7-C6-C5	-2.54	106.49	113.26
25	b	611	CLA	O2D-CGD-CBD	2.54	115.67	111.23
34	C	516	DGD	O1G-C1A-C2A	2.53	119.56	111.83
34	c	516	DGD	O1G-C1A-C2A	2.53	119.56	111.83
27	k	103	BCR	C12-C13-C14	2.53	123.00	119.01
25	b	605	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	B	612	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
25	b	612	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
27	F	101	BCR	C12-C13-C14	2.53	123.00	119.01
27	f	101	BCR	C12-C13-C14	2.53	123.00	119.01
25	B	609	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
25	b	609	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
27	K	103	BCR	C12-C13-C14	2.53	122.99	119.01
27	B	617	BCR	C16-C15-C14	2.53	128.70	123.52
25	c	508	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
25	B	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	b	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	C	501	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
25	c	501	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
30	F	102	SQD	O48-C23-C24	2.53	119.53	111.83
30	f	102	SQD	O48-C23-C24	2.53	119.53	111.83
30	f	102	SQD	O5-C1-C2	2.52	115.56	110.37
25	B	605	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
27	Z	101	BCR	C8-C9-C10	2.52	122.97	119.01
27	b	617	BCR	C16-C15-C14	2.51	128.66	123.52
27	B	617	BCR	C36-C18-C17	-2.51	118.74	122.82
25	d	404	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	D	404	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	B	610	CLA	C1B-CHB-C4A	-2.50	125.28	130.04
25	D	401	CLA	CHD-C1D-ND	-2.49	121.29	124.80
25	d	401	CLA	CHD-C1D-ND	-2.49	121.29	124.80
27	z	101	BCR	C8-C9-C10	2.49	122.93	119.01
27	z	103	BCR	C19-C18-C17	2.49	122.93	119.01
25	B	605	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
27	b	617	BCR	C36-C18-C17	-2.49	118.78	122.82
27	K	104	BCR	C19-C18-C17	2.48	122.91	119.01
27	B	619	BCR	C2-C1-C6	2.48	114.04	110.44
25	C	506	CLA	O2D-CGD-O1D	-2.48	119.02	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
27	b	618	BCR	C36-C18-C17	-2.48	118.80	122.82
25	b	605	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
27	b	619	BCR	C2-C1-C6	2.48	114.04	110.44
25	B	610	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	b	610	CLA	C1B-CHB-C4A	-2.47	125.32	130.04
25	b	614	CLA	CHB-C4A-NA	2.47	127.97	124.40
34	C	516	DGD	C2G-O2G-C1B	-2.47	111.89	117.80
34	c	516	DGD	C2G-O2G-C1B	-2.47	111.89	117.80
27	B	618	BCR	C36-C18-C17	-2.46	118.83	122.82
25	C	509	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	K	104	BCR	C23-C22-C21	2.46	122.88	119.01
27	z	103	BCR	C23-C22-C21	2.46	122.88	119.01
25	c	503	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
25	B	610	CLA	CAA-CBA-CGA	-2.46	106.24	113.21
25	b	610	CLA	CAA-CBA-CGA	-2.46	106.24	113.21
25	B	613	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
25	b	613	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
25	c	509	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	B	606	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
25	b	606	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
25	C	501	CLA	C1-C2-C3	-2.45	122.18	126.20
25	c	501	CLA	C1-C2-C3	-2.45	122.18	126.20
25	C	503	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
27	B	619	BCR	C12-C13-C14	2.45	122.86	119.01
27	b	619	BCR	C12-C13-C14	2.45	122.86	119.01
35	v	201	HEM	C4C-CHD-C1D	2.45	125.79	122.56
28	B	621	LMG	O1-C7-C8	-2.45	104.87	110.82
27	b	619	BCR	C19-C18-C17	2.45	122.86	119.01
25	b	610	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	b	621	LMG	O1-C7-C8	-2.45	104.87	110.82
25	B	614	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	A	405	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
25	a	405	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
27	B	619	BCR	C19-C18-C17	2.43	122.83	119.01
27	b	618	BCR	C34-C9-C8	2.43	121.80	118.09
27	B	618	BCR	C34-C9-C8	2.43	121.79	118.09
35	V	201	HEM	C4C-CHD-C1D	2.42	125.76	122.56
25	b	603	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
31	C	521	LMT	C1B-O1B-C4'	-2.42	112.24	117.98
25	C	509	CLA	CED-O2D-CGD	2.41	121.39	115.92
25	c	509	CLA	CED-O2D-CGD	2.41	121.39	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C1-C2-C3	-2.41	122.25	126.20
25	b	602	CLA	C1-C2-C3	-2.41	122.25	126.20
25	C	507	CLA	C2A-C1A-CHA	2.41	128.05	123.87
25	c	507	CLA	C2A-C1A-CHA	2.41	128.05	123.87
25	B	603	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
25	b	614	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
25	B	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	b	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
27	b	617	BCR	C2-C1-C6	2.41	113.93	110.44
31	c	521	LMT	C1B-O1B-C4'	-2.41	112.28	117.98
25	A	408	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
25	a	408	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
25	B	613	CLA	C7-C6-C5	-2.40	106.87	113.26
25	b	613	CLA	C7-C6-C5	-2.40	106.87	113.26
28	D	409	LMG	O7-C10-C11	2.40	116.67	111.48
28	d	409	LMG	O7-C10-C11	2.40	116.67	111.48
25	C	510	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	C	501	CLA	O2D-CGD-CBD	2.40	115.42	111.23
35	E	104	HEM	O2A-CGA-CBA	2.40	121.57	114.00
27	B	617	BCR	C2-C1-C6	2.39	113.91	110.44
35	V	201	HEM	C4D-ND-C1D	2.39	108.04	105.21
35	v	201	HEM	C4D-ND-C1D	2.39	108.04	105.21
25	B	614	CLA	C1B-CHB-C4A	-2.39	125.48	130.04
35	V	201	HEM	C4B-CHC-C1C	2.39	125.71	122.56
35	v	201	HEM	C4B-CHC-C1C	2.39	125.71	122.56
25	B	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
25	b	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
25	c	501	CLA	O2D-CGD-CBD	2.39	115.40	111.23
35	e	104	HEM	O2A-CGA-CBA	2.39	121.54	114.00
25	c	510	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
31	D	411	LMT	C3B-C4B-C5B	-2.38	105.92	110.23
25	D	403	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
25	d	403	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
25	C	511	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	c	511	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	C	504	CLA	C1B-CHB-C4A	-2.38	125.51	130.04
25	c	504	CLA	C1B-CHB-C4A	-2.38	125.51	130.04
35	V	201	HEM	C3D-C4D-ND	-2.38	107.56	110.17
35	v	201	HEM	C3D-C4D-ND	-2.38	107.56	110.17
31	d	411	LMT	C3B-C4B-C5B	-2.38	105.92	110.23
25	B	608	CLA	CHB-C4A-NA	2.37	127.83	124.40
25	b	608	CLA	CHB-C4A-NA	2.37	127.83	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
25	b	610	CLA	O2D-CGD-CBD	2.37	115.37	111.23
36	H	101	RRX	C37-C22-C23	2.36	121.70	118.09
33	Z	102	LHG	O4-P-O5	2.36	120.03	110.83
33	z	102	LHG	O4-P-O5	2.36	120.03	110.83
36	h	101	RRX	C37-C22-C23	2.36	121.69	118.09
34	C	517	DGD	O1G-C1A-C2A	2.36	119.02	111.83
34	C	516	DGD	O2G-C1B-O1B	-2.35	118.20	123.70
34	c	516	DGD	O2G-C1B-O1B	-2.35	118.20	123.70
34	c	517	DGD	O1G-C1A-C2A	2.35	119.01	111.83
25	B	610	CLA	O2D-CGD-CBD	2.35	115.33	111.23
25	C	503	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	c	503	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	B	609	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
25	C	512	CLA	CBA-CAA-C2A	-2.34	106.83	113.79
25	c	512	CLA	CBA-CAA-C2A	-2.34	106.83	113.79
25	c	511	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	B	606	CLA	O2D-CGD-CBD	2.34	115.32	111.23
25	b	606	CLA	O2D-CGD-CBD	2.34	115.32	111.23
25	C	509	CLA	C1B-CHB-C4A	-2.34	125.58	130.04
30	F	102	SQD	O8-S-C6	2.33	110.48	105.97
30	f	102	SQD	O8-S-C6	2.33	110.48	105.97
25	b	605	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	c	512	CLA	O2D-CGD-CBD	2.33	115.31	111.23
25	b	606	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
25	B	605	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	c	501	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
27	B	618	BCR	C15-C16-C17	2.33	128.28	123.52
25	C	512	CLA	O2D-CGD-CBD	2.32	115.29	111.23
25	b	606	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	B	606	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
25	C	501	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
27	b	618	BCR	C15-C16-C17	2.32	128.26	123.52
25	c	509	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
25	C	505	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
25	B	615	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
25	c	509	CLA	CHA-C1A-NA	-2.31	121.16	126.39
25	b	615	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
25	c	505	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
25	b	616	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	B	618	BCR	C37-C22-C23	2.31	121.61	118.09
27	b	618	BCR	C37-C22-C23	2.31	121.61	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	411	LMT	C1B-C2B-C3B	2.31	114.86	110.01
31	d	411	LMT	C1B-C2B-C3B	2.31	114.86	110.01
25	c	510	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
25	B	605	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	b	605	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	B	616	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	C	511	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	B	606	CLA	CHB-C4A-NA	2.30	127.72	124.40
25	C	509	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	C	522	LMT	C4'-C3'-C2'	2.30	114.86	110.83
31	c	522	LMT	C4'-C3'-C2'	2.30	114.86	110.83
25	B	615	CLA	CHB-C4A-NA	2.30	127.71	124.40
25	C	507	CLA	CMB-C2B-C3B	2.29	129.26	124.68
25	C	510	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
25	c	507	CLA	CMB-C2B-C3B	2.29	129.25	124.68
25	b	615	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	B	614	CLA	O2D-CGD-CBD	2.27	115.20	111.23
25	b	614	CLA	O2D-CGD-CBD	2.27	115.20	111.23
31	I	104	LMT	O5'-C1'-C2'	-2.26	105.72	110.37
31	i	104	LMT	O5'-C1'-C2'	-2.26	105.72	110.37
27	C	514	BCR	C20-C21-C22	2.26	130.45	127.28
27	c	514	BCR	C20-C21-C22	2.26	130.45	127.28
27	B	618	BCR	C19-C18-C17	2.26	122.56	119.01
27	b	618	BCR	C19-C18-C17	2.26	122.56	119.01
25	B	607	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	B	604	CLA	CHA-C1A-NA	-2.24	121.33	126.39
25	b	604	CLA	CHA-C1A-NA	-2.24	121.33	126.39
25	b	607	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
27	B	617	BCR	C19-C18-C17	2.23	122.51	119.01
27	b	617	BCR	C19-C18-C17	2.23	122.51	119.01
30	F	102	SQD	C45-O47-C7	-2.22	112.47	117.80
30	f	102	SQD	C45-O47-C7	-2.22	112.47	117.80
25	C	509	CLA	CHA-C4D-ND	2.22	137.12	132.55
31	X	103	LMT	O5'-C1'-C2'	-2.22	105.82	110.37
31	x	103	LMT	O5'-C1'-C2'	-2.22	105.82	110.37
34	H	104	DGD	O1G-C1A-O1A	-2.21	118.09	123.63
27	K	103	BCR	C23-C22-C21	2.21	122.49	119.01
31	T	101	LMT	C1'-O5'-C5'	-2.21	109.40	113.72
31	t	101	LMT	C1'-O5'-C5'	-2.21	109.40	113.72
35	E	104	HEM	CHD-C1D-C2D	-2.21	121.54	125.03
35	e	104	HEM	CHD-C1D-C2D	-2.21	121.54	125.03
25	D	401	CLA	CHC-C1C-NC	2.21	127.64	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	CHC-C1C-NC	2.21	127.64	124.31
25	b	614	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
25	C	513	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
25	c	513	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
25	A	405	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	a	405	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	B	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
25	b	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
25	c	511	CLA	C1B-CHB-C4A	-2.20	125.85	130.04
30	A	413	SQD	O7-S-C6	2.20	110.04	106.76
27	k	103	BCR	C23-C22-C21	2.20	122.47	119.01
25	C	502	CLA	O2D-CGD-CBD	2.20	115.07	111.23
25	c	502	CLA	O2D-CGD-CBD	2.20	115.07	111.23
25	c	509	CLA	CHA-C4D-ND	2.19	137.08	132.55
34	h	104	DGD	O1G-C1A-O1A	-2.19	118.14	123.63
25	D	403	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	d	403	CLA	CHB-C4A-NA	2.19	127.56	124.40
30	a	413	SQD	O7-S-C6	2.19	110.03	106.76
25	B	614	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
31	I	102	LMT	C1B-O1B-C4'	-2.18	112.80	117.98
31	i	102	LMT	C1B-O1B-C4'	-2.18	112.80	117.98
31	C	521	LMT	C1-O1'-C1'	-2.18	109.96	113.68
31	c	521	LMT	C1-O1'-C1'	-2.18	109.96	113.68
25	B	601	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	b	601	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	D	403	CLA	O2D-CGD-CBD	2.17	115.03	111.23
25	C	511	CLA	C1B-CHB-C4A	-2.17	125.90	130.04
25	B	615	CLA	O1D-CGD-CBD	2.17	128.79	124.52
27	K	104	BCR	C8-C9-C10	2.16	122.41	119.01
27	z	103	BCR	C8-C9-C10	2.16	122.41	119.01
25	B	611	CLA	C1B-CHB-C4A	-2.16	125.92	130.04
31	F	103	LMT	C1'-O5'-C5'	2.16	117.94	113.72
25	d	403	CLA	O2D-CGD-CBD	2.16	115.01	111.23
34	C	517	DGD	C2G-O2G-C1B	-2.16	112.63	117.80
34	c	517	DGD	C2G-O2G-C1B	-2.16	112.63	117.80
25	b	609	CLA	CHB-C4A-NA	2.16	127.52	124.40
25	B	612	CLA	C1-C2-C3	-2.16	122.66	126.20
25	b	612	CLA	C1-C2-C3	-2.16	122.66	126.20
31	f	103	LMT	C1'-O5'-C5'	2.16	117.93	113.72
25	B	604	CLA	C6-C7-C8	-2.15	108.80	115.97
25	b	611	CLA	C1B-CHB-C4A	-2.15	125.94	130.04
25	b	615	CLA	O1D-CGD-CBD	2.15	128.75	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C6-C7-C8	-2.14	108.84	115.97
34	C	515	DGD	O1G-C1A-C2A	2.14	118.37	111.83
34	c	515	DGD	O1G-C1A-C2A	2.14	118.37	111.83
25	C	502	CLA	O1D-CGD-CBD	2.14	128.74	124.52
25	c	502	CLA	O1D-CGD-CBD	2.14	128.74	124.52
31	X	103	LMT	C3'-C4'-C5'	2.14	114.12	110.23
31	x	103	LMT	C3'-C4'-C5'	2.14	114.12	110.23
25	B	608	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	b	608	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
27	F	101	BCR	C2-C1-C6	2.14	113.55	110.44
25	B	609	CLA	CHB-C4A-NA	2.14	127.48	124.40
31	b	629	LMT	C1B-O1B-C4'	-2.14	112.92	117.98
31	M	102	LMT	C6'-C5'-C4'	-2.13	107.78	113.02
31	m	102	LMT	C6'-C5'-C4'	-2.13	107.78	113.02
31	B	629	LMT	C1B-O1B-C4'	-2.13	112.93	117.98
25	C	507	CLA	CHA-C1A-NA	-2.13	121.57	126.39
35	V	201	HEM	CAD-CBD-CGD	-2.13	108.03	113.67
30	F	102	SQD	O47-C7-O49	-2.12	118.74	123.70
30	f	102	SQD	O47-C7-O49	-2.12	118.74	123.70
27	f	101	BCR	C2-C1-C6	2.12	113.52	110.44
35	v	201	HEM	CAD-CBD-CGD	-2.12	108.05	113.67
31	B	623	LMT	C1'-O5'-C5'	2.11	117.85	113.72
31	b	623	LMT	C1'-O5'-C5'	2.11	117.85	113.72
27	B	617	BCR	C37-C22-C23	2.11	121.32	118.09
27	b	617	BCR	C37-C22-C23	2.11	121.32	118.09
25	c	507	CLA	CHA-C1A-NA	-2.11	121.61	126.39
36	H	101	RRX	C8-C9-C10	2.11	122.33	119.01
36	h	101	RRX	C8-C9-C10	2.11	122.33	119.01
25	b	615	CLA	C1B-CHB-C4A	-2.10	126.03	130.04
25	B	615	CLA	C1B-CHB-C4A	-2.10	126.03	130.04
31	E	103	LMT	O5'-C5'-C6'	2.10	111.65	106.44
31	e	103	LMT	O5'-C5'-C6'	2.10	111.65	106.44
25	C	507	CLA	O2D-CGD-CBD	2.10	114.90	111.23
25	c	507	CLA	O2D-CGD-CBD	2.10	114.90	111.23
25	C	501	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	c	501	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	C	522	LMT	O5'-C5'-C4'	-2.10	105.92	109.70
31	c	522	LMT	O5'-C5'-C4'	-2.10	105.92	109.70
25	b	604	CLA	C1B-CHB-C4A	-2.10	126.04	130.04
25	B	615	CLA	CHA-C1A-NA	-2.09	121.65	126.39
27	K	103	BCR	C8-C9-C10	2.09	122.30	119.01
27	k	103	BCR	C8-C9-C10	2.09	122.30	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C1B-CHB-C4A	-2.09	126.06	130.04
35	V	201	HEM	C1B-NB-C4B	2.09	107.68	105.21
35	v	201	HEM	C1B-NB-C4B	2.09	107.68	105.21
25	a	406	CLA	C16-C15-C13	-2.08	109.04	115.97
25	A	406	CLA	C16-C15-C13	-2.08	109.04	115.97
31	k	105	LMT	O5'-C5'-C6'	2.08	111.60	106.44
31	C	522	LMT	C1'-C2'-C3'	2.08	114.39	110.01
31	c	522	LMT	C1'-C2'-C3'	2.08	114.39	110.01
25	b	615	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	B	627	LMT	C1-O1'-C1'	-2.08	110.13	113.68
31	b	630	LMT	C1-O1'-C1'	-2.08	110.13	113.68
34	C	515	DGD	C3G-C2G-C1G	-2.08	106.94	111.78
34	C	517	DGD	C3G-C2G-C1G	-2.08	106.94	111.78
34	c	517	DGD	C3G-C2G-C1G	-2.08	106.94	111.78
25	c	503	CLA	CED-O2D-CGD	2.08	120.62	115.92
35	E	104	HEM	CHA-C4D-C3D	-2.08	121.40	125.23
31	K	105	LMT	O5'-C5'-C6'	2.07	111.58	106.44
31	c	522	LMT	C1-O1'-C1'	-2.07	110.14	113.68
25	B	608	CLA	O2D-CGD-CBD	2.07	114.85	111.23
34	c	515	DGD	C3G-C2G-C1G	-2.07	106.96	111.78
27	f	101	BCR	C8-C9-C10	2.07	122.26	119.01
25	B	613	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	C	503	CLA	CED-O2D-CGD	2.07	120.61	115.92
25	b	602	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	b	608	CLA	O2D-CGD-CBD	2.06	114.84	111.23
35	e	104	HEM	CHA-C4D-C3D	-2.06	121.43	125.23
25	b	613	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
31	c	524	LMT	C4B-C3B-C2B	-2.05	107.24	110.83
27	F	101	BCR	C8-C9-C10	2.05	122.23	119.01
25	B	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	C	522	LMT	C1-O1'-C1'	-2.04	110.19	113.68
25	B	612	CLA	C2A-C3A-C4A	2.04	105.16	101.87
25	b	612	CLA	C2A-C3A-C4A	2.04	105.16	101.87
36	H	101	RRX	C2-C1-C6	2.04	113.40	110.44
36	h	101	RRX	C2-C1-C6	2.04	113.40	110.44
29	A	411	PL9	C7-C3-C2	-2.04	120.98	123.39
29	a	411	PL9	C7-C3-C2	-2.04	120.98	123.39
31	C	524	LMT	C4B-C3B-C2B	-2.03	107.27	110.83
29	A	411	PL9	C3-C4-C5	2.02	121.09	118.57
29	a	411	PL9	C3-C4-C5	2.02	121.09	118.57
25	a	406	CLA	CHD-C1D-ND	-2.01	121.97	124.80
27	B	619	BCR	C8-C9-C10	2.01	122.17	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	619	BCR	C8-C9-C10	2.01	122.17	119.01
31	X	103	LMT	O5'-C5'-C4'	2.01	113.31	109.70
31	x	103	LMT	O5'-C5'-C4'	2.01	113.31	109.70
25	B	610	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	b	610	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
31	X	103	LMT	C6'-C5'-C4'	-2.00	108.11	113.02
31	x	103	LMT	C6'-C5'-C4'	-2.00	108.11	113.02

All (65) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	408	CLA	ND
25	B	601	CLA	ND
25	B	602	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	609	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	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND

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Mol	Chain	Res	Type	Atom
25	D	401	CLA	ND
25	D	403	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	b	601	CLA	ND
25	b	602	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	609	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	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND

All (2787) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C12-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C4-C3-C5-C6
25	C	509	CLA	C6-C7-C8-C9
25	C	513	CLA	C2-C1-O2A-CGA
25	b	613	CLA	C12-C13-C15-C16
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C4-C3-C5-C6
25	c	509	CLA	C6-C7-C8-C9
25	c	513	CLA	C2-C1-O2A-CGA
27	A	409	BCR	C17-C18-C19-C20
27	B	617	BCR	C14-C15-C16-C17
27	B	617	BCR	C16-C17-C18-C19
27	B	617	BCR	C16-C17-C18-C36
27	B	617	BCR	C17-C18-C19-C20
27	B	617	BCR	C21-C22-C23-C24
27	B	618	BCR	C21-C22-C23-C24
27	B	618	BCR	C37-C22-C23-C24
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	C	514	BCR	C35-C13-C14-C15
27	C	514	BCR	C21-C22-C23-C24
27	F	101	BCR	C7-C8-C9-C10
27	F	101	BCR	C16-C17-C18-C19
27	F	101	BCR	C16-C17-C18-C36
27	K	103	BCR	C1-C6-C7-C8
27	K	103	BCR	C5-C6-C7-C8
27	K	103	BCR	C7-C8-C9-C10
27	K	103	BCR	C11-C10-C9-C8
27	K	103	BCR	C11-C10-C9-C34
27	K	104	BCR	C11-C12-C13-C14
27	K	104	BCR	C12-C13-C14-C15
27	K	104	BCR	C35-C13-C14-C15
27	K	104	BCR	C14-C15-C16-C17
27	Z	101	BCR	C12-C13-C14-C15
27	Z	101	BCR	C35-C13-C14-C15
27	Z	101	BCR	C37-C22-C23-C24
27	a	409	BCR	C17-C18-C19-C20
27	b	617	BCR	C14-C15-C16-C17
27	b	617	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	b	617	BCR	C16-C17-C18-C36
27	b	617	BCR	C17-C18-C19-C20
27	b	617	BCR	C21-C22-C23-C24
27	b	618	BCR	C21-C22-C23-C24
27	b	618	BCR	C37-C22-C23-C24
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	c	514	BCR	C35-C13-C14-C15
27	c	514	BCR	C21-C22-C23-C24
27	f	101	BCR	C7-C8-C9-C10
27	f	101	BCR	C16-C17-C18-C19
27	f	101	BCR	C16-C17-C18-C36
27	k	103	BCR	C1-C6-C7-C8
27	k	103	BCR	C5-C6-C7-C8
27	k	103	BCR	C7-C8-C9-C10
27	k	103	BCR	C11-C10-C9-C8
27	k	103	BCR	C11-C10-C9-C34
27	z	101	BCR	C12-C13-C14-C15
27	z	101	BCR	C35-C13-C14-C15
27	z	101	BCR	C37-C22-C23-C24
27	z	103	BCR	C11-C12-C13-C14
27	z	103	BCR	C12-C13-C14-C15
27	z	103	BCR	C35-C13-C14-C15
27	z	103	BCR	C14-C15-C16-C17
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	409	LMG	O9-C10-O7-C8
28	D	409	LMG	C11-C10-O7-C8
28	J	101	LMG	O6-C1-O1-C7
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	409	LMG	O9-C10-O7-C8
28	d	409	LMG	C11-C10-O7-C8
28	j	101	LMG	O6-C1-O1-C7
29	A	411	PL9	C11-C12-C13-C14
29	A	411	PL9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	A	411	PL9	C12-C13-C14-C16
29	A	411	PL9	C20-C19-C21-C22
29	A	411	PL9	C47-C48-C49-C50
29	A	411	PL9	C47-C48-C49-C51
29	a	411	PL9	C11-C12-C13-C14
29	a	411	PL9	C12-C13-C14-C15
29	a	411	PL9	C12-C13-C14-C16
29	a	411	PL9	C20-C19-C21-C22
29	a	411	PL9	C47-C48-C49-C50
29	a	411	PL9	C47-C48-C49-C51
30	A	412	SQD	C2-C1-O6-C44
30	A	412	SQD	O10-C23-O48-C46
30	A	412	SQD	C24-C23-O48-C46
30	A	412	SQD	C4-C5-C6-S
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	O5-C1-O6-C44
30	A	413	SQD	C8-C7-O47-C45
30	B	620	SQD	C8-C7-O47-C45
30	B	620	SQD	O5-C5-C6-S
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	103	SQD	C5-C6-S-O7
30	H	103	SQD	C5-C6-S-O8
30	H	103	SQD	C5-C6-S-O9
30	K	102	SQD	C8-C7-O47-C45
30	a	412	SQD	C2-C1-O6-C44
30	a	412	SQD	O10-C23-O48-C46
30	a	412	SQD	C24-C23-O48-C46
30	a	412	SQD	C4-C5-C6-S
30	a	413	SQD	C2-C1-O6-C44
30	a	413	SQD	O5-C1-O6-C44
30	a	413	SQD	C8-C7-O47-C45
30	b	620	SQD	C8-C7-O47-C45
30	b	620	SQD	O5-C5-C6-S
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	103	SQD	C5-C6-S-O7
30	h	103	SQD	C5-C6-S-O8
30	h	103	SQD	C5-C6-S-O9
30	k	102	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
31	A	415	LMT	O5'-C1'-O1'-C1
31	B	624	LMT	C2'-C1'-O1'-C1
31	B	624	LMT	O5'-C1'-O1'-C1
31	B	625	LMT	C3'-C4'-O1B-C1B
31	B	626	LMT	O5'-C1'-O1'-C1
31	C	520	LMT	C2-C1-O1'-C1'
31	C	524	LMT	C2'-C1'-O1'-C1
31	C	524	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	C2-C1-O1'-C1'
31	D	411	LMT	O5'-C1'-O1'-C1
31	E	101	LMT	C2-C1-O1'-C1'
31	K	105	LMT	C3'-C4'-O1B-C1B
31	K	105	LMT	C2'-C1'-O1'-C1
31	K	105	LMT	C2-C1-O1'-C1'
31	L	105	LMT	C2'-C1'-O1'-C1
31	L	105	LMT	O5'-C1'-O1'-C1
31	L	105	LMT	C2-C1-O1'-C1'
31	M	101	LMT	C2'-C1'-O1'-C1
31	M	101	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	C2-C1-O1'-C1'
31	a	415	LMT	O5'-C1'-O1'-C1
31	b	624	LMT	C2'-C1'-O1'-C1
31	b	624	LMT	O5'-C1'-O1'-C1
31	b	625	LMT	C3'-C4'-O1B-C1B
31	b	626	LMT	O5'-C1'-O1'-C1
31	c	520	LMT	C2-C1-O1'-C1'
31	c	524	LMT	C2'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	C2-C1-O1'-C1'
31	d	411	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	C2-C1-O1'-C1'
31	k	105	LMT	C3'-C4'-O1B-C1B
31	k	105	LMT	C2'-C1'-O1'-C1
31	k	105	LMT	C2-C1-O1'-C1'
33	B	628	LHG	C3-O3-P-O4
33	B	628	LHG	C3-O3-P-O6
33	D	406	LHG	O1-C1-C2-C3
33	D	406	LHG	C3-O3-P-O5
33	D	413	LHG	O1-C1-C2-C3
33	D	413	LHG	C3-O3-P-O4
33	D	413	LHG	C3-O3-P-O6
33	D	413	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	D	407	LHG	C3-O3-P-O4
33	D	407	LHG	C3-O3-P-O5
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O4
33	E	102	LHG	C4-O6-P-O3
33	Z	102	LHG	C8-C7-O7-C5
33	b	628	LHG	C3-O3-P-O4
33	b	628	LHG	C3-O3-P-O6
33	d	406	LHG	O1-C1-C2-C3
33	d	406	LHG	C3-O3-P-O5
33	d	412	LHG	O1-C1-C2-C3
33	d	412	LHG	C3-O3-P-O4
33	d	412	LHG	C3-O3-P-O6
33	d	412	LHG	C4-O6-P-O5
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O5
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O4
33	e	102	LHG	C4-O6-P-O3
33	z	102	LHG	C8-C7-O7-C5
34	C	515	DGD	C2A-C1A-O1G-C1G
34	c	515	DGD	C2A-C1A-O1G-C1G
36	H	101	RRX	C16-C17-C18-C19
36	H	101	RRX	C16-C17-C18-C36
36	H	101	RRX	C14-C15-C16-C17
36	H	101	RRX	C11-C12-C13-C14
36	h	101	RRX	C16-C17-C18-C19
36	h	101	RRX	C16-C17-C18-C36
36	h	101	RRX	C14-C15-C16-C17
36	h	101	RRX	C11-C12-C13-C14
25	C	503	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	C	509	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	O1D-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
30	H	103	SQD	O10-C23-O48-C46
30	h	103	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
33	D	413	LHG	O10-C23-O8-C6
33	d	412	LHG	O10-C23-O8-C6
34	C	515	DGD	O1A-C1A-O1G-C1G
34	c	515	DGD	O1A-C1A-O1G-C1G
33	B	628	LHG	C5-C6-O8-C23
33	b	628	LHG	C5-C6-O8-C23
30	H	103	SQD	C24-C23-O48-C46
30	h	103	SQD	C24-C23-O48-C46
33	D	413	LHG	C24-C23-O8-C6
33	d	412	LHG	C24-C23-O8-C6
28	A	410	LMG	O10-C28-O8-C9
28	J	101	LMG	O10-C28-O8-C9
28	a	410	LMG	O10-C28-O8-C9
28	j	101	LMG	O10-C28-O8-C9
30	K	102	SQD	O10-C23-O48-C46
30	k	102	SQD	O10-C23-O48-C46
25	C	513	CLA	C13-C15-C16-C17
25	c	513	CLA	C13-C15-C16-C17
30	A	413	SQD	O49-C7-O47-C45
30	B	620	SQD	O49-C7-O47-C45
30	K	102	SQD	O49-C7-O47-C45
30	a	413	SQD	O49-C7-O47-C45
30	b	620	SQD	O49-C7-O47-C45
30	k	102	SQD	O49-C7-O47-C45
25	C	506	CLA	C3-C5-C6-C7
25	c	506	CLA	C3-C5-C6-C7
28	A	410	LMG	C29-C28-O8-C9
28	a	410	LMG	C29-C28-O8-C9
30	K	102	SQD	C24-C23-O48-C46
30	k	102	SQD	C24-C23-O48-C46
25	B	614	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
31	A	415	LMT	C4'-C5'-C6'-O6'
31	L	105	LMT	C4B-C5B-C6B-O6B
31	M	101	LMT	C4B-C5B-C6B-O6B
31	a	415	LMT	C4'-C5'-C6'-O6'
25	C	512	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

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C2-C3-C5-C6
25	C	512	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
29	A	411	PL9	C18-C19-C21-C22
29	A	411	PL9	C28-C29-C31-C32
29	a	411	PL9	C18-C19-C21-C22
29	a	411	PL9	C28-C29-C31-C32
31	E	103	LMT	O5'-C5'-C6'-O6'
31	e	103	LMT	O5'-C5'-C6'-O6'
28	J	101	LMG	C29-C28-O8-C9
28	j	101	LMG	C29-C28-O8-C9
33	B	628	LHG	C24-C23-O8-C6
33	b	628	LHG	C24-C23-O8-C6
29	A	411	PL9	C27-C28-C29-C30
29	A	411	PL9	C42-C43-C44-C45
29	a	411	PL9	C27-C28-C29-C30
29	a	411	PL9	C42-C43-C44-C45
29	A	411	PL9	C27-C28-C29-C31
29	a	411	PL9	C27-C28-C29-C31
31	C	522	LMT	O5'-C5'-C6'-O6'
31	I	105	LMT	O5'-C5'-C6'-O6'
31	c	522	LMT	O5'-C5'-C6'-O6'
31	i	105	LMT	O5'-C5'-C6'-O6'
36	H	101	RRX	C9-C10-C11-C12
36	h	101	RRX	C9-C10-C11-C12
25	C	509	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
33	B	628	LHG	O10-C23-O8-C6
33	b	628	LHG	O10-C23-O8-C6
33	Z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	O9-C7-O7-C5
28	B	621	LMG	C31-C32-C33-C34
28	b	621	LMG	C31-C32-C33-C34
31	I	102	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
25	B	614	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	B	605	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	I	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
25	C	509	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
31	A	415	LMT	O5B-C5B-C6B-O6B
31	B	625	LMT	O5'-C5'-C6'-O6'
31	I	102	LMT	O5B-C5B-C6B-O6B
31	a	415	LMT	O5B-C5B-C6B-O6B
31	b	625	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5B-C5B-C6B-O6B
31	D	411	LMT	C4B-C5B-C6B-O6B
31	d	411	LMT	C4B-C5B-C6B-O6B
31	D	410	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5'-C5'-C6'-O6'
31	C	522	LMT	C4'-C5'-C6'-O6'
31	E	103	LMT	C4'-C5'-C6'-O6'
31	I	102	LMT	C4'-C5'-C6'-O6'
31	c	522	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4'-C5'-C6'-O6'
31	D	411	LMT	O5'-C5'-C6'-O6'
31	b	629	LMT	O5'-C5'-C6'-O6'
31	d	411	LMT	O5'-C5'-C6'-O6'
29	D	405	PL9	C47-C48-C49-C51
29	d	405	PL9	C47-C48-C49-C51
25	C	501	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
30	A	412	SQD	C7-C8-C9-C10
30	a	412	SQD	C7-C8-C9-C10
31	B	629	LMT	O5'-C5'-C6'-O6'
31	I	105	LMT	C4'-C5'-C6'-O6'
31	I	102	LMT	C4B-C5B-C6B-O6B
31	i	105	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4B-C5B-C6B-O6B
25	B	604	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
31	A	415	LMT	O5'-C5'-C6'-O6'
31	F	103	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5'-C5'-C6'-O6'
31	f	103	LMT	O5'-C5'-C6'-O6'
31	D	411	LMT	C4'-C5'-C6'-O6'
31	d	411	LMT	C4'-C5'-C6'-O6'
28	C	518	LMG	C19-C20-C21-C22
28	c	518	LMG	C19-C20-C21-C22
31	L	105	LMT	O5B-C5B-C6B-O6B
31	M	101	LMT	O5B-C5B-C6B-O6B
25	C	507	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
28	C	519	LMG	C38-C39-C40-C41
28	c	519	LMG	C38-C39-C40-C41
33	D	407	LHG	C31-C32-C33-C34
33	d	407	LHG	C31-C32-C33-C34
33	E	102	LHG	O10-C23-O8-C6
33	e	102	LHG	O10-C23-O8-C6
31	C	523	LMT	O5'-C1'-O1'-C1
31	K	105	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	X	101	LMT	O5'-C1'-O1'-C1
31	c	523	LMT	O5'-C1'-O1'-C1
31	k	105	LMT	O5'-C1'-O1'-C1
31	m	102	LMT	O5'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
30	B	620	SQD	C11-C10-C9-C8
30	b	620	SQD	C11-C10-C9-C8
31	T	101	LMT	C4-C5-C6-C7
31	t	101	LMT	C4-C5-C6-C7
33	Z	102	LHG	C9-C10-C11-C12
33	z	102	LHG	C9-C10-C11-C12
28	A	414	LMG	C29-C28-O8-C9
28	a	414	LMG	C29-C28-O8-C9
30	B	620	SQD	C24-C23-O48-C46
30	b	620	SQD	C24-C23-O48-C46
33	E	102	LHG	C24-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
33	Z	102	LHG	C29-C30-C31-C32
33	z	102	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	C6A-C7A-C8A-C9A
34	c	517	DGD	C6A-C7A-C8A-C9A
25	A	405	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
34	C	517	DGD	C4A-C5A-C6A-C7A
34	c	517	DGD	C4A-C5A-C6A-C7A
30	C	525	SQD	C17-C18-C19-C20
30	c	525	SQD	C17-C18-C19-C20
31	K	105	LMT	O5'-C5'-C6'-O6'
31	k	105	LMT	O5'-C5'-C6'-O6'
28	C	519	LMG	C17-C18-C19-C20
28	c	519	LMG	C17-C18-C19-C20
31	C	524	LMT	C5-C6-C7-C8
31	c	524	LMT	C5-C6-C7-C8
31	K	105	LMT	C1-C2-C3-C4
31	k	105	LMT	C1-C2-C3-C4
25	B	603	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
31	M	102	LMT	C2-C3-C4-C5
31	m	102	LMT	C2-C3-C4-C5
28	J	101	LMG	C37-C38-C39-C40
28	d	409	LMG	C20-C21-C22-C23
28	j	101	LMG	C37-C38-C39-C40
33	E	102	LHG	C10-C11-C12-C13
33	e	102	LHG	C10-C11-C12-C13
27	Z	101	BCR	C19-C20-C21-C22
27	z	101	BCR	C19-C20-C21-C22
33	D	406	LHG	C1-C2-C3-O3
33	d	406	LHG	C1-C2-C3-O3
28	C	518	LMG	C29-C28-O8-C9
28	c	518	LMG	C29-C28-O8-C9
28	D	409	LMG	C20-C21-C22-C23
31	C	520	LMT	C5-C6-C7-C8
31	c	520	LMT	C5-C6-C7-C8
25	B	609	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
30	A	412	SQD	C13-C14-C15-C16
30	A	413	SQD	C24-C25-C26-C27
30	a	412	SQD	C13-C14-C15-C16
30	a	413	SQD	C24-C25-C26-C27
31	D	410	LMT	C2-C3-C4-C5
31	d	410	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	C	520	LMT	C1-C2-C3-C4
31	c	520	LMT	C1-C2-C3-C4
25	B	614	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
28	A	410	LMG	C17-C18-C19-C20
28	a	410	LMG	C17-C18-C19-C20
30	C	525	SQD	C11-C12-C13-C14
30	c	525	SQD	C11-C12-C13-C14
28	D	409	LMG	C40-C41-C42-C43
28	d	409	LMG	C40-C41-C42-C43
33	D	408	LHG	C13-C14-C15-C16
33	D	408	LHG	C15-C16-C17-C18
33	d	408	LHG	C13-C14-C15-C16
33	d	408	LHG	C15-C16-C17-C18
34	C	515	DGD	CAA-CBA-CCA-CDA
34	c	515	DGD	CAA-CBA-CCA-CDA
25	B	605	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	B	602	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	B	616	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	A	408	CLA	C6-C7-C8-C9
25	B	607	CLA	C11-C12-C13-C14
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	B	614	CLA	C11-C10-C8-C9
25	C	502	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14
25	C	513	CLA	C6-C7-C8-C9
25	a	408	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
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	b	614	CLA	C11-C10-C8-C9
25	c	502	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C14
25	c	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	D	409	LMG	C32-C33-C34-C35
31	B	625	LMT	C6-C7-C8-C9
31	b	625	LMT	C6-C7-C8-C9
31	B	625	LMT	O5B-C5B-C6B-O6B
31	b	625	LMT	O5B-C5B-C6B-O6B
31	A	415	LMT	C4B-C5B-C6B-O6B
31	D	410	LMT	C4'-C5'-C6'-O6'
31	K	105	LMT	C4'-C5'-C6'-O6'
31	a	415	LMT	C4B-C5B-C6B-O6B
31	d	410	LMT	C4'-C5'-C6'-O6'
31	k	105	LMT	C4'-C5'-C6'-O6'
30	F	102	SQD	C2-C1-O6-C44
30	f	102	SQD	C2-C1-O6-C44
31	A	415	LMT	C2'-C1'-O1'-C1
31	C	523	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	a	415	LMT	C2'-C1'-O1'-C1
31	c	523	LMT	C2'-C1'-O1'-C1
31	m	102	LMT	C2'-C1'-O1'-C1
28	d	409	LMG	C32-C33-C34-C35
31	I	105	LMT	C6-C7-C8-C9
31	i	105	LMT	C6-C7-C8-C9
33	D	406	LHG	O2-C2-C3-O3
33	d	406	LHG	O2-C2-C3-O3
31	B	623	LMT	O5B-C5B-C6B-O6B
31	b	623	LMT	O5B-C5B-C6B-O6B
31	X	102	LMT	C6-C7-C8-C9
31	x	102	LMT	C6-C7-C8-C9
27	A	409	BCR	C36-C18-C19-C20
27	A	409	BCR	C37-C22-C23-C24
27	B	617	BCR	C36-C18-C19-C20
27	B	617	BCR	C37-C22-C23-C24
27	C	514	BCR	C37-C22-C23-C24
27	F	101	BCR	C7-C8-C9-C34
27	F	101	BCR	C36-C18-C19-C20
27	K	103	BCR	C7-C8-C9-C34
27	K	104	BCR	C11-C12-C13-C35
27	Z	101	BCR	C11-C12-C13-C35
27	Z	101	BCR	C36-C18-C19-C20
27	a	409	BCR	C36-C18-C19-C20
27	a	409	BCR	C37-C22-C23-C24
27	b	617	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	b	617	BCR	C37-C22-C23-C24
27	c	514	BCR	C37-C22-C23-C24
27	f	101	BCR	C7-C8-C9-C34
27	f	101	BCR	C36-C18-C19-C20
27	k	103	BCR	C7-C8-C9-C34
27	z	101	BCR	C11-C12-C13-C35
27	z	101	BCR	C36-C18-C19-C20
27	z	103	BCR	C11-C12-C13-C35
36	H	101	RRX	C11-C12-C13-C35
36	H	101	RRX	C7-C8-C9-C34
36	h	101	RRX	C11-C12-C13-C35
36	h	101	RRX	C7-C8-C9-C34
27	Z	101	BCR	C11-C12-C13-C14
27	Z	101	BCR	C21-C22-C23-C24
27	z	101	BCR	C11-C12-C13-C14
27	z	101	BCR	C21-C22-C23-C24
31	C	523	LMT	C4-C5-C6-C7
31	c	523	LMT	C4-C5-C6-C7
30	C	525	SQD	C13-C14-C15-C16
30	c	525	SQD	C13-C14-C15-C16
25	A	408	CLA	C8-C10-C11-C12
25	a	408	CLA	C8-C10-C11-C12
25	C	509	CLA	C2-C1-O2A-CGA
25	c	509	CLA	C2-C1-O2A-CGA
31	X	103	LMT	C1-C2-C3-C4
31	x	103	LMT	C1-C2-C3-C4
28	C	518	LMG	C21-C22-C23-C24
28	C	518	LMG	C36-C37-C38-C39
28	c	518	LMG	C21-C22-C23-C24
28	c	518	LMG	C36-C37-C38-C39
31	B	625	LMT	C2-C3-C4-C5
31	C	521	LMT	C2-C3-C4-C5
31	b	625	LMT	C2-C3-C4-C5
31	c	521	LMT	C2-C3-C4-C5
25	C	506	CLA	C10-C11-C12-C13
25	c	506	CLA	C10-C11-C12-C13
29	D	405	PL9	C47-C48-C49-C50
29	d	405	PL9	C47-C48-C49-C50
30	F	102	SQD	C7-C8-C9-C10
30	f	102	SQD	C7-C8-C9-C10
29	A	411	PL9	C42-C43-C44-C46
29	a	411	PL9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
25	C	511	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
31	D	411	LMT	O5B-C5B-C6B-O6B
31	d	411	LMT	O5B-C5B-C6B-O6B
33	D	413	LHG	C9-C10-C11-C12
33	d	412	LHG	C9-C10-C11-C12
25	A	406	CLA	C11-C12-C13-C15
25	a	406	CLA	C11-C12-C13-C15
30	C	525	SQD	C27-C28-C29-C30
30	c	525	SQD	C27-C28-C29-C30
31	L	105	LMT	O1'-C1-C2-C3
31	M	101	LMT	O1'-C1-C2-C3
25	C	506	CLA	C15-C16-C17-C18
25	c	506	CLA	C15-C16-C17-C18
31	B	629	LMT	C4'-C5'-C6'-O6'
31	b	629	LMT	C4'-C5'-C6'-O6'
33	D	408	LHG	C7-C8-C9-C10
33	d	408	LHG	C7-C8-C9-C10
25	C	506	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C29-C31-C32-C33
29	a	411	PL9	C29-C31-C32-C33
31	F	103	LMT	O1'-C1-C2-C3
31	f	103	LMT	O1'-C1-C2-C3
31	X	103	LMT	C5-C6-C7-C8
31	x	103	LMT	C5-C6-C7-C8
25	A	405	CLA	C13-C15-C16-C17
25	D	401	CLA	C13-C15-C16-C17
25	a	405	CLA	C13-C15-C16-C17
25	d	401	CLA	C13-C15-C16-C17
28	D	409	LMG	C34-C35-C36-C37
28	d	409	LMG	C34-C35-C36-C37
28	j	101	LMG	C17-C18-C19-C20
31	Y	101	LMT	C5-C6-C7-C8
31	y	101	LMT	C5-C6-C7-C8
34	H	104	DGD	CBB-CCB-CDB-CEB
34	h	104	DGD	CBB-CCB-CDB-CEB
28	J	101	LMG	C17-C18-C19-C20
28	J	101	LMG	C39-C40-C41-C42
28	j	101	LMG	C39-C40-C41-C42
31	T	101	LMT	C6-C7-C8-C9
31	t	101	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	519	LMG	C10-C11-C12-C13
28	J	101	LMG	C28-C29-C30-C31
28	c	519	LMG	C10-C11-C12-C13
28	j	101	LMG	C28-C29-C30-C31
30	F	102	SQD	C23-C24-C25-C26
30	f	102	SQD	C23-C24-C25-C26
33	D	413	LHG	C23-C24-C25-C26
33	d	412	LHG	C23-C24-C25-C26
28	C	518	LMG	O10-C28-O8-C9
28	c	518	LMG	O10-C28-O8-C9
25	A	405	CLA	C15-C16-C17-C18
25	B	607	CLA	C13-C15-C16-C17
25	C	512	CLA	C15-C16-C17-C18
25	a	405	CLA	C15-C16-C17-C18
25	b	607	CLA	C13-C15-C16-C17
25	c	512	CLA	C15-C16-C17-C18
31	I	104	LMT	O1'-C1-C2-C3
31	i	104	LMT	O1'-C1-C2-C3
31	M	102	LMT	O5'-C5'-C6'-O6'
31	m	102	LMT	O5'-C5'-C6'-O6'
25	B	603	CLA	C5-C6-C7-C8
25	B	604	CLA	C13-C15-C16-C17
25	C	512	CLA	C13-C15-C16-C17
25	b	603	CLA	C5-C6-C7-C8
25	b	604	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
31	B	625	LMT	C4'-C5'-C6'-O6'
31	b	625	LMT	C4'-C5'-C6'-O6'
30	K	102	SQD	C23-C24-C25-C26
30	k	102	SQD	C23-C24-C25-C26
33	D	406	LHG	C23-C24-C25-C26
33	D	408	LHG	C23-C24-C25-C26
33	d	406	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
28	A	414	LMG	O10-C28-O8-C9
28	a	414	LMG	O10-C28-O8-C9
30	F	102	SQD	O5-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	X	102	LMT	O5'-C1'-O1'-C1
31	x	102	LMT	O5'-C1'-O1'-C1
25	B	603	CLA	C15-C16-C17-C18
25	C	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C15-C16-C17-C18
25	b	603	CLA	C15-C16-C17-C18
25	c	503	CLA	C15-C16-C17-C18
25	c	513	CLA	C15-C16-C17-C18
33	D	413	LHG	O2-C2-C3-O3
33	d	412	LHG	O2-C2-C3-O3
31	L	105	LMT	C5'-C4'-O1B-C1B
31	M	101	LMT	C5'-C4'-O1B-C1B
30	B	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
28	C	519	LMG	C28-C29-C30-C31
28	D	409	LMG	C28-C29-C30-C31
28	c	519	LMG	C28-C29-C30-C31
28	d	409	LMG	C28-C29-C30-C31
25	B	604	CLA	C8-C10-C11-C12
25	b	604	CLA	C8-C10-C11-C12
31	C	524	LMT	O1'-C1-C2-C3
31	c	524	LMT	O1'-C1-C2-C3
31	I	104	LMT	C5-C6-C7-C8
31	i	104	LMT	C5-C6-C7-C8
31	y	101	LMT	C3-C4-C5-C6
31	C	523	LMT	O1'-C1-C2-C3
31	I	103	LMT	O1'-C1-C2-C3
31	c	523	LMT	O1'-C1-C2-C3
31	i	103	LMT	O1'-C1-C2-C3
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
31	Y	101	LMT	C3-C4-C5-C6
28	C	519	LMG	C8-C9-O8-C28
28	a	410	LMG	C8-C9-O8-C28
28	c	519	LMG	C8-C9-O8-C28
28	A	414	LMG	C28-C29-C30-C31
28	a	414	LMG	C28-C29-C30-C31
34	C	515	DGD	CCA-CDA-CEA-CFA
34	c	515	DGD	CCA-CDA-CEA-CFA
25	B	613	CLA	C10-C11-C12-C13
25	C	513	CLA	C10-C11-C12-C13
25	b	613	CLA	C10-C11-C12-C13
25	c	513	CLA	C10-C11-C12-C13
33	D	413	LHG	C8-C7-O7-C5
33	d	412	LHG	C8-C7-O7-C5
31	X	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	x	101	LMT	O1'-C1-C2-C3
25	B	604	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
28	A	410	LMG	C8-C9-O8-C28
27	Z	101	BCR	C9-C10-C11-C12
27	z	101	BCR	C9-C10-C11-C12
25	A	406	CLA	C10-C11-C12-C13
25	C	502	CLA	C15-C16-C17-C18
25	a	406	CLA	C10-C11-C12-C13
25	c	502	CLA	C15-C16-C17-C18
28	D	409	LMG	C37-C38-C39-C40
28	d	409	LMG	C37-C38-C39-C40
30	H	103	SQD	C12-C13-C14-C15
30	h	103	SQD	C12-C13-C14-C15
33	D	413	LHG	O9-C7-O7-C5
33	d	412	LHG	O9-C7-O7-C5
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	B	616	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	C15-C16-C17-C18
25	B	615	CLA	C5-C6-C7-C8
25	C	507	CLA	C15-C16-C17-C18
25	C	509	CLA	C8-C10-C11-C12
25	D	404	CLA	C13-C15-C16-C17
25	b	602	CLA	C15-C16-C17-C18
25	b	615	CLA	C5-C6-C7-C8
25	c	507	CLA	C15-C16-C17-C18
25	c	509	CLA	C8-C10-C11-C12
25	d	404	CLA	C13-C15-C16-C17
28	b	621	LMG	C15-C16-C17-C18
34	C	515	DGD	C2A-C3A-C4A-C5A
34	c	515	DGD	C2A-C3A-C4A-C5A
25	B	610	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
28	B	621	LMG	C15-C16-C17-C18
33	D	413	LHG	C7-C8-C9-C10
33	E	102	LHG	C23-C24-C25-C26
33	d	412	LHG	C7-C8-C9-C10
33	e	102	LHG	C23-C24-C25-C26
25	B	602	CLA	C13-C15-C16-C17
25	B	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	c	505	CLA	C13-C15-C16-C17
31	D	412	LMT	C4'-C5'-C6'-O6'
31	x	104	LMT	C4'-C5'-C6'-O6'
30	B	620	SQD	C19-C20-C21-C22
30	b	620	SQD	C19-C20-C21-C22
25	A	408	CLA	C5-C6-C7-C8
25	B	606	CLA	C10-C11-C12-C13
25	B	616	CLA	C10-C11-C12-C13
25	C	508	CLA	C15-C16-C17-C18
25	b	606	CLA	C10-C11-C12-C13
25	b	616	CLA	C10-C11-C12-C13
25	c	508	CLA	C15-C16-C17-C18
31	e	101	LMT	O1'-C1-C2-C3
29	A	411	PL9	C35-C34-C36-C37
29	a	411	PL9	C35-C34-C36-C37
30	K	102	SQD	C30-C31-C32-C33
30	k	102	SQD	C30-C31-C32-C33
25	B	604	CLA	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
25	a	408	CLA	C5-C6-C7-C8
25	b	604	CLA	C10-C11-C12-C13
25	c	507	CLA	C13-C15-C16-C17
31	E	101	LMT	O1'-C1-C2-C3
30	H	103	SQD	C8-C7-O47-C45
30	h	103	SQD	C8-C7-O47-C45
31	C	522	LMT	C3-C4-C5-C6
31	c	522	LMT	C3-C4-C5-C6
34	C	517	DGD	CAA-CBA-CCA-CDA
34	c	517	DGD	CAA-CBA-CCA-CDA
30	H	103	SQD	O49-C7-O47-C45
30	h	103	SQD	O49-C7-O47-C45
31	X	101	LMT	C2'-C1'-O1'-C1
31	X	102	LMT	C2'-C1'-O1'-C1
31	x	101	LMT	C2'-C1'-O1'-C1
31	x	102	LMT	C2'-C1'-O1'-C1
30	B	620	SQD	C23-C24-C25-C26
30	b	620	SQD	C23-C24-C25-C26
31	C	521	LMT	C4B-C5B-C6B-O6B
31	c	521	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C8-C10-C11-C12
27	A	409	BCR	C20-C21-C22-C37
27	B	617	BCR	C35-C13-C14-C15
27	B	617	BCR	C20-C21-C22-C37
27	B	619	BCR	C35-C13-C14-C15
27	C	514	BCR	C16-C17-C18-C36
27	C	514	BCR	C20-C21-C22-C37
27	F	101	BCR	C20-C21-C22-C37
27	K	103	BCR	C35-C13-C14-C15
27	K	104	BCR	C16-C17-C18-C36
27	Z	101	BCR	C11-C10-C9-C34
27	a	409	BCR	C20-C21-C22-C37
27	b	617	BCR	C35-C13-C14-C15
27	b	617	BCR	C20-C21-C22-C37
27	b	619	BCR	C35-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C36
27	c	514	BCR	C20-C21-C22-C37
27	f	101	BCR	C20-C21-C22-C37
27	k	103	BCR	C35-C13-C14-C15
27	z	101	BCR	C11-C10-C9-C34
27	z	103	BCR	C16-C17-C18-C36
36	H	101	RRX	C11-C10-C9-C34
36	h	101	RRX	C11-C10-C9-C34
30	C	525	SQD	C23-C24-C25-C26
30	c	525	SQD	C23-C24-C25-C26
31	B	625	LMT	C4B-C5B-C6B-O6B
31	b	625	LMT	C4B-C5B-C6B-O6B
27	B	618	BCR	C7-C8-C9-C34
27	F	101	BCR	C37-C22-C23-C24
27	K	103	BCR	C36-C18-C19-C20
27	b	618	BCR	C7-C8-C9-C34
27	f	101	BCR	C37-C22-C23-C24
27	k	103	BCR	C36-C18-C19-C20
31	B	625	LMT	C4-C5-C6-C7
31	b	625	LMT	C4-C5-C6-C7
27	F	101	BCR	C17-C18-C19-C20
27	Z	101	BCR	C17-C18-C19-C20
27	f	101	BCR	C17-C18-C19-C20
27	z	101	BCR	C17-C18-C19-C20
36	H	101	RRX	C7-C8-C9-C10
36	h	101	RRX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	c	522	LMT	O1'-C1-C2-C3
33	D	408	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
31	C	522	LMT	O1'-C1-C2-C3
30	B	620	SQD	C46-C45-O47-C7
30	b	620	SQD	C46-C45-O47-C7
25	A	406	CLA	C16-C17-C18-C20
25	C	506	CLA	C16-C17-C18-C20
25	a	406	CLA	C16-C17-C18-C20
25	c	506	CLA	C16-C17-C18-C20
27	A	409	BCR	C20-C21-C22-C23
27	B	617	BCR	C12-C13-C14-C15
27	B	617	BCR	C20-C21-C22-C23
27	B	619	BCR	C12-C13-C14-C15
27	C	514	BCR	C12-C13-C14-C15
27	C	514	BCR	C16-C17-C18-C19
27	C	514	BCR	C20-C21-C22-C23
27	F	101	BCR	C20-C21-C22-C23
27	K	103	BCR	C12-C13-C14-C15
27	K	104	BCR	C16-C17-C18-C19
27	Z	101	BCR	C11-C10-C9-C8
27	a	409	BCR	C20-C21-C22-C23
27	b	617	BCR	C12-C13-C14-C15
27	b	617	BCR	C20-C21-C22-C23
27	b	619	BCR	C12-C13-C14-C15
27	c	514	BCR	C12-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C19
27	c	514	BCR	C20-C21-C22-C23
27	f	101	BCR	C20-C21-C22-C23
27	k	103	BCR	C12-C13-C14-C15
27	z	101	BCR	C11-C10-C9-C8
27	z	103	BCR	C16-C17-C18-C19
36	H	101	RRX	C11-C10-C9-C8
36	h	101	RRX	C11-C10-C9-C8
31	E	101	LMT	C1-C2-C3-C4
31	e	101	LMT	C1-C2-C3-C4
28	A	410	LMG	C11-C10-O7-C8
28	a	410	LMG	C11-C10-O7-C8
31	B	629	LMT	C3-C4-C5-C6
28	J	101	LMG	C13-C14-C15-C16
28	j	101	LMG	C13-C14-C15-C16
31	b	629	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	K	102	SQD	O6-C44-C45-O47
30	K	102	SQD	O47-C45-C46-O48
30	k	102	SQD	O6-C44-C45-O47
30	k	102	SQD	O47-C45-C46-O48
25	B	611	CLA	C8-C10-C11-C12
25	D	404	CLA	C10-C11-C12-C13
25	b	611	CLA	C8-C10-C11-C12
25	d	404	CLA	C10-C11-C12-C13
31	B	625	LMT	O1'-C1-C2-C3
31	b	625	LMT	O1'-C1-C2-C3
25	B	614	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C19
25	C	504	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C19
25	D	404	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
25	c	504	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C19
25	d	404	CLA	C16-C17-C18-C19
31	T	101	LMT	C1-C2-C3-C4
31	t	101	LMT	C1-C2-C3-C4
25	B	610	CLA	C13-C15-C16-C17
25	B	616	CLA	C8-C10-C11-C12
25	b	610	CLA	C13-C15-C16-C17
25	b	616	CLA	C8-C10-C11-C12
28	C	518	LMG	C13-C14-C15-C16
31	B	626	LMT	C2-C3-C4-C5
31	X	102	LMT	C2-C3-C4-C5
31	b	626	LMT	C2-C3-C4-C5
33	D	406	LHG	C13-C14-C15-C16
33	D	413	LHG	C17-C18-C19-C20
33	d	406	LHG	C13-C14-C15-C16
25	D	404	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
31	I	102	LMT	C1-C2-C3-C4
31	i	102	LMT	C1-C2-C3-C4
28	A	410	LMG	C36-C37-C38-C39
28	B	621	LMG	C33-C34-C35-C36
28	C	518	LMG	C29-C30-C31-C32
28	J	101	LMG	C33-C34-C35-C36
28	a	410	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
28	b	621	LMG	C33-C34-C35-C36
28	c	518	LMG	C13-C14-C15-C16
28	c	518	LMG	C29-C30-C31-C32
28	j	101	LMG	C33-C34-C35-C36
30	H	103	SQD	C17-C18-C19-C20
30	h	103	SQD	C17-C18-C19-C20
31	B	626	LMT	C6-C7-C8-C9
31	K	105	LMT	C4-C5-C6-C7
31	b	626	LMT	C6-C7-C8-C9
31	k	105	LMT	C4-C5-C6-C7
31	x	102	LMT	C2-C3-C4-C5
31	x	102	LMT	C3-C4-C5-C6
33	D	406	LHG	C14-C15-C16-C17
33	D	408	LHG	C9-C10-C11-C12
33	D	413	LHG	C10-C11-C12-C13
33	d	406	LHG	C14-C15-C16-C17
33	d	408	LHG	C9-C10-C11-C12
33	d	412	LHG	C10-C11-C12-C13
33	d	412	LHG	C17-C18-C19-C20
34	C	515	DGD	C9A-CAA-CBA-CCA
34	C	517	DGD	C5B-C6B-C7B-C8B
34	c	517	DGD	C5B-C6B-C7B-C8B
25	B	610	CLA	C15-C16-C17-C18
25	b	610	CLA	C15-C16-C17-C18
28	C	518	LMG	C20-C21-C22-C23
28	C	518	LMG	C34-C35-C36-C37
28	c	518	LMG	C34-C35-C36-C37
30	B	620	SQD	C18-C19-C20-C21
30	K	102	SQD	C28-C29-C30-C31
30	b	620	SQD	C18-C19-C20-C21
30	k	102	SQD	C28-C29-C30-C31
31	E	103	LMT	C2-C3-C4-C5
31	X	102	LMT	C3-C4-C5-C6
31	e	103	LMT	C2-C3-C4-C5
33	D	413	LHG	C31-C32-C33-C34
33	d	412	LHG	C31-C32-C33-C34
34	c	515	DGD	C9A-CAA-CBA-CCA
30	F	102	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
28	C	519	LMG	C19-C20-C21-C22
28	C	519	LMG	C35-C36-C37-C38
28	D	409	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	J	101	LMG	C12-C13-C14-C15
28	J	101	LMG	C35-C36-C37-C38
28	c	518	LMG	C20-C21-C22-C23
28	c	519	LMG	C19-C20-C21-C22
28	c	519	LMG	C20-C21-C22-C23
28	c	519	LMG	C35-C36-C37-C38
28	j	101	LMG	C12-C13-C14-C15
28	j	101	LMG	C35-C36-C37-C38
31	C	523	LMT	C5-C6-C7-C8
33	D	408	LHG	C10-C11-C12-C13
33	D	408	LHG	C26-C27-C28-C29
33	D	408	LHG	C31-C32-C33-C34
33	d	408	LHG	C10-C11-C12-C13
33	d	408	LHG	C26-C27-C28-C29
33	d	408	LHG	C31-C32-C33-C34
34	C	516	DGD	C5A-C6A-C7A-C8A
34	C	516	DGD	CBA-CCA-CDA-CEA
34	H	104	DGD	C9A-CAA-CBA-CCA
34	H	104	DGD	CCB-CDB-CEB-CFB
34	c	516	DGD	C5A-C6A-C7A-C8A
34	c	516	DGD	CBA-CCA-CDA-CEA
34	h	104	DGD	C9A-CAA-CBA-CCA
34	h	104	DGD	CCB-CDB-CEB-CFB
28	A	410	LMG	O9-C10-O7-C8
28	a	410	LMG	O9-C10-O7-C8
31	B	625	LMT	C2-C1-O1'-C1'
31	E	103	LMT	C2-C1-O1'-C1'
31	X	103	LMT	C2-C1-O1'-C1'
31	Y	101	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
31	e	103	LMT	C2-C1-O1'-C1'
31	x	103	LMT	C2-C1-O1'-C1'
31	y	101	LMT	C2-C1-O1'-C1'
33	D	406	LHG	O1-C1-C2-O2
33	D	413	LHG	O1-C1-C2-O2
33	d	406	LHG	O1-C1-C2-O2
33	d	412	LHG	O1-C1-C2-O2
28	C	519	LMG	C20-C21-C22-C23
28	d	409	LMG	C13-C14-C15-C16
30	h	103	SQD	C27-C28-C29-C30
31	B	625	LMT	C7-C8-C9-C10
31	c	523	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	D	409	LMG	C10-C11-C12-C13
28	d	409	LMG	C10-C11-C12-C13
33	z	102	LHG	C23-C24-C25-C26
28	D	409	LMG	C18-C19-C20-C21
30	C	525	SQD	C31-C32-C33-C34
30	H	103	SQD	C27-C28-C29-C30
30	c	525	SQD	C31-C32-C33-C34
31	A	415	LMT	C5-C6-C7-C8
31	a	415	LMT	C5-C6-C7-C8
31	b	625	LMT	C7-C8-C9-C10
25	A	405	CLA	C16-C17-C18-C20
25	C	512	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
25	B	616	CLA	O1A-CGA-O2A-C1
28	d	409	LMG	C18-C19-C20-C21
30	C	525	SQD	C29-C30-C31-C32
30	c	525	SQD	C29-C30-C31-C32
33	E	102	LHG	C13-C14-C15-C16
33	e	102	LHG	C13-C14-C15-C16
34	C	517	DGD	C9A-CAA-CBA-CCA
34	c	517	DGD	C9A-CAA-CBA-CCA
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
33	B	628	LHG	C8-C7-O7-C5
33	b	628	LHG	C8-C7-O7-C5
31	X	103	LMT	O1'-C1-C2-C3
31	x	103	LMT	O1'-C1-C2-C3
30	A	412	SQD	C27-C28-C29-C30
30	a	412	SQD	C27-C28-C29-C30
31	I	103	LMT	C2-C3-C4-C5
31	a	415	LMT	C4-C5-C6-C7
31	i	103	LMT	C2-C3-C4-C5
34	H	104	DGD	C6A-C7A-C8A-C9A
31	L	105	LMT	C3'-C4'-O1B-C1B
31	M	101	LMT	C3'-C4'-O1B-C1B
33	Z	102	LHG	C7-C8-C9-C10
33	Z	102	LHG	C23-C24-C25-C26
33	z	102	LHG	C7-C8-C9-C10
25	B	609	CLA	C15-C16-C17-C18
25	D	403	CLA	C13-C15-C16-C17
25	b	609	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C13-C15-C16-C17
31	D	412	LMT	O5'-C5'-C6'-O6'
28	J	101	LMG	C30-C31-C32-C33
28	j	101	LMG	C30-C31-C32-C33
30	A	412	SQD	C15-C16-C17-C18
30	A	412	SQD	C31-C32-C33-C34
30	H	103	SQD	C11-C12-C13-C14
30	a	412	SQD	C15-C16-C17-C18
30	a	412	SQD	C31-C32-C33-C34
30	h	103	SQD	C11-C12-C13-C14
31	A	415	LMT	C4-C5-C6-C7
31	I	101	LMT	C11-C10-C9-C8
31	I	104	LMT	C7-C8-C9-C10
31	K	105	LMT	C3-C4-C5-C6
31	i	101	LMT	C2-C3-C4-C5
31	i	101	LMT	C11-C10-C9-C8
31	i	104	LMT	C7-C8-C9-C10
31	k	105	LMT	C3-C4-C5-C6
33	D	408	LHG	C17-C18-C19-C20
33	d	408	LHG	C17-C18-C19-C20
34	H	104	DGD	C7A-C8A-C9A-CAA
34	h	104	DGD	C6A-C7A-C8A-C9A
34	h	104	DGD	C7A-C8A-C9A-CAA
25	b	616	CLA	O1A-CGA-O2A-C1
31	I	101	LMT	C2-C3-C4-C5
31	I	102	LMT	C6-C7-C8-C9
31	i	102	LMT	C6-C7-C8-C9
33	D	413	LHG	C13-C14-C15-C16
33	D	413	LHG	C30-C31-C32-C33
33	d	412	LHG	C13-C14-C15-C16
33	d	412	LHG	C30-C31-C32-C33
31	C	522	LMT	C1-C2-C3-C4
31	E	103	LMT	C1-C2-C3-C4
31	c	522	LMT	C1-C2-C3-C4
31	e	103	LMT	C1-C2-C3-C4
33	Z	102	LHG	C11-C12-C13-C14
33	z	102	LHG	C11-C12-C13-C14
30	C	525	SQD	C11-C10-C9-C8
30	c	525	SQD	C11-C10-C9-C8
34	C	517	DGD	CAB-CBB-CCB-CDB
34	c	517	DGD	CAB-CBB-CCB-CDB
25	B	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C8-C10-C11-C12
25	b	616	CLA	C5-C6-C7-C8
25	c	504	CLA	C8-C10-C11-C12
28	C	518	LMG	C28-C29-C30-C31
28	c	518	LMG	C28-C29-C30-C31
31	D	411	LMT	C4-C5-C6-C7
31	d	411	LMT	C4-C5-C6-C7
36	H	101	RRX	C13-C14-C15-C16
36	h	101	RRX	C13-C14-C15-C16
31	D	410	LMT	O1'-C1-C2-C3
31	x	104	LMT	O5'-C5'-C6'-O6'
31	I	101	LMT	C1-C2-C3-C4
31	i	101	LMT	C1-C2-C3-C4
28	D	409	LMG	C15-C16-C17-C18
28	d	409	LMG	C15-C16-C17-C18
34	C	515	DGD	C5B-C6B-C7B-C8B
34	C	516	DGD	CAA-CBA-CCA-CDA
34	c	515	DGD	C5B-C6B-C7B-C8B
34	c	516	DGD	CAA-CBA-CCA-CDA
31	d	410	LMT	O1'-C1-C2-C3
30	A	412	SQD	C14-C15-C16-C17
30	a	412	SQD	C14-C15-C16-C17
28	C	519	LMG	C29-C28-O8-C9
28	c	519	LMG	C29-C28-O8-C9
28	B	621	LMG	C34-C35-C36-C37
28	J	101	LMG	C20-C21-C22-C23
28	b	621	LMG	C34-C35-C36-C37
28	j	101	LMG	C20-C21-C22-C23
28	B	621	LMG	C10-C11-C12-C13
28	b	621	LMG	C10-C11-C12-C13
30	B	620	SQD	C14-C15-C16-C17
30	C	525	SQD	C33-C34-C35-C36
30	H	103	SQD	C16-C17-C18-C19
30	K	102	SQD	C11-C10-C9-C8
30	b	620	SQD	C14-C15-C16-C17
30	c	525	SQD	C33-C34-C35-C36
30	h	103	SQD	C16-C17-C18-C19
30	k	102	SQD	C11-C10-C9-C8
31	E	101	LMT	C4-C5-C6-C7
31	E	101	LMT	C5-C6-C7-C8
31	e	101	LMT	C4-C5-C6-C7
31	e	101	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C11-C12-C13-C14
33	D	413	LHG	C11-C12-C13-C14
33	D	407	LHG	C16-C17-C18-C19
33	d	408	LHG	C11-C12-C13-C14
33	d	412	LHG	C11-C12-C13-C14
33	d	407	LHG	C16-C17-C18-C19
31	Y	101	LMT	C4'-C5'-C6'-O6'
33	B	628	LHG	C35-C36-C37-C38
33	b	628	LHG	C35-C36-C37-C38
30	B	620	SQD	C31-C32-C33-C34
30	K	102	SQD	C10-C11-C12-C13
30	b	620	SQD	C31-C32-C33-C34
30	k	102	SQD	C10-C11-C12-C13
31	A	415	LMT	C2-C3-C4-C5
31	E	101	LMT	C3-C4-C5-C6
31	I	105	LMT	C2-C3-C4-C5
31	a	415	LMT	C2-C3-C4-C5
31	e	101	LMT	C3-C4-C5-C6
31	i	105	LMT	C2-C3-C4-C5
28	C	519	LMG	C32-C33-C34-C35
28	J	101	LMG	C18-C19-C20-C21
28	c	519	LMG	C32-C33-C34-C35
28	j	101	LMG	C18-C19-C20-C21
31	y	101	LMT	C4'-C5'-C6'-O6'
31	B	629	LMT	C6-C7-C8-C9
31	b	629	LMT	C6-C7-C8-C9
33	D	408	LHG	C33-C34-C35-C36
33	d	408	LHG	C33-C34-C35-C36
28	A	410	LMG	C28-C29-C30-C31
28	a	410	LMG	C28-C29-C30-C31
34	C	516	DGD	C1A-C2A-C3A-C4A
34	c	516	DGD	C1A-C2A-C3A-C4A
33	D	413	LHG	C19-C20-C21-C22
33	d	412	LHG	C19-C20-C21-C22
28	A	410	LMG	C21-C22-C23-C24
28	a	410	LMG	C21-C22-C23-C24
33	E	102	LHG	C8-C7-O7-C5
33	e	102	LHG	C8-C7-O7-C5
28	A	410	LMG	C22-C23-C24-C25
28	a	410	LMG	C22-C23-C24-C25
30	B	620	SQD	C16-C17-C18-C19
30	b	620	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	I	101	LMT	C4-C5-C6-C7
31	I	103	LMT	C6-C7-C8-C9
31	a	415	LMT	C11-C10-C9-C8
31	i	101	LMT	C4-C5-C6-C7
31	i	103	LMT	C6-C7-C8-C9
33	D	413	LHG	C12-C13-C14-C15
33	d	412	LHG	C12-C13-C14-C15
30	k	102	SQD	C9-C10-C11-C12
31	A	415	LMT	C11-C10-C9-C8
33	D	406	LHG	C15-C16-C17-C18
30	F	102	SQD	C10-C11-C12-C13
30	f	102	SQD	C10-C11-C12-C13
30	K	102	SQD	C9-C10-C11-C12
33	d	406	LHG	C15-C16-C17-C18
30	F	102	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
33	B	628	LHG	C12-C13-C14-C15
33	Z	102	LHG	C24-C25-C26-C27
33	b	628	LHG	C12-C13-C14-C15
33	z	102	LHG	C24-C25-C26-C27
28	A	414	LMG	C33-C34-C35-C36
28	a	414	LMG	C33-C34-C35-C36
30	F	102	SQD	O49-C7-O47-C45
30	f	102	SQD	O49-C7-O47-C45
33	B	628	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
28	B	621	LMG	C36-C37-C38-C39
28	b	621	LMG	C36-C37-C38-C39
30	k	102	SQD	C27-C28-C29-C30
31	D	410	LMT	C4-C5-C6-C7
31	d	410	LMT	C4-C5-C6-C7
27	A	409	BCR	C10-C11-C12-C13
27	B	618	BCR	C18-C19-C20-C21
27	K	103	BCR	C18-C19-C20-C21
27	K	104	BCR	C18-C19-C20-C21
27	Z	101	BCR	C10-C11-C12-C13
27	a	409	BCR	C10-C11-C12-C13
27	b	618	BCR	C18-C19-C20-C21
27	k	103	BCR	C18-C19-C20-C21
27	z	101	BCR	C10-C11-C12-C13
27	z	103	BCR	C18-C19-C20-C21
29	A	411	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
29	a	411	PL9	C33-C34-C36-C37
28	B	621	LMG	C40-C41-C42-C43
28	b	621	LMG	C40-C41-C42-C43
28	B	621	LMG	C16-C17-C18-C19
28	b	621	LMG	C16-C17-C18-C19
30	C	525	SQD	C25-C26-C27-C28
30	K	102	SQD	C27-C28-C29-C30
30	c	525	SQD	C25-C26-C27-C28
31	B	626	LMT	C7-C8-C9-C10
31	C	520	LMT	C6-C7-C8-C9
31	D	411	LMT	C3-C4-C5-C6
31	b	626	LMT	C7-C8-C9-C10
31	c	520	LMT	C6-C7-C8-C9
31	d	411	LMT	C3-C4-C5-C6
33	E	102	LHG	C17-C18-C19-C20
33	e	102	LHG	C17-C18-C19-C20
34	C	515	DGD	CCB-CDB-CEB-CFB
34	c	515	DGD	CCB-CDB-CEB-CFB
25	D	404	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	C14-C13-C15-C16
25	b	614	CLA	C14-C13-C15-C16
28	j	101	LMG	C23-C24-C25-C26
30	A	412	SQD	C34-C35-C36-C37
30	H	103	SQD	C25-C26-C27-C28
30	a	412	SQD	C34-C35-C36-C37
30	h	103	SQD	C25-C26-C27-C28
31	C	521	LMT	O5B-C5B-C6B-O6B
31	c	521	LMT	O5B-C5B-C6B-O6B
28	D	409	LMG	C23-C24-C25-C26
28	J	101	LMG	C23-C24-C25-C26
28	d	409	LMG	C23-C24-C25-C26
31	B	624	LMT	C11-C10-C9-C8
31	I	103	LMT	C5-C6-C7-C8
31	b	624	LMT	C11-C10-C9-C8
31	i	103	LMT	C5-C6-C7-C8
33	D	406	LHG	C28-C29-C30-C31
33	d	406	LHG	C28-C29-C30-C31
34	C	517	DGD	C7A-C8A-C9A-CAA
34	c	517	DGD	C7A-C8A-C9A-CAA
27	K	103	BCR	C22-C23-C24-C25
27	k	103	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
31	F	103	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
33	D	413	LHG	C15-C16-C17-C18
33	d	412	LHG	C15-C16-C17-C18
28	A	414	LMG	O6-C5-C6-O5
28	a	414	LMG	O6-C5-C6-O5
30	K	102	SQD	C2-C1-O6-C44
30	k	102	SQD	C2-C1-O6-C44
28	C	519	LMG	O10-C28-O8-C9
28	c	519	LMG	O10-C28-O8-C9
30	A	413	SQD	C27-C28-C29-C30
31	C	521	LMT	C11-C10-C9-C8
31	c	521	LMT	C11-C10-C9-C8
34	H	104	DGD	C5B-C6B-C7B-C8B
34	h	104	DGD	C5B-C6B-C7B-C8B
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
28	d	409	LMG	C12-C13-C14-C15
30	a	413	SQD	C27-C28-C29-C30
31	C	524	LMT	C6-C7-C8-C9
31	c	524	LMT	C6-C7-C8-C9
34	C	516	DGD	C5B-C6B-C7B-C8B
34	C	517	DGD	C3A-C4A-C5A-C6A
34	c	516	DGD	C5B-C6B-C7B-C8B
34	c	517	DGD	C3A-C4A-C5A-C6A
31	I	103	LMT	C7-C8-C9-C10
31	i	103	LMT	C7-C8-C9-C10
28	C	518	LMG	C33-C34-C35-C36
28	D	409	LMG	C12-C13-C14-C15
28	c	518	LMG	C33-C34-C35-C36
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
31	B	629	LMT	C4-C5-C6-C7
31	b	625	LMT	C3-C4-C5-C6
31	b	629	LMT	C4-C5-C6-C7
33	D	406	LHG	C25-C26-C27-C28
33	D	413	LHG	C28-C29-C30-C31
33	d	406	LHG	C25-C26-C27-C28
33	d	412	LHG	C28-C29-C30-C31
34	C	515	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
34	c	515	DGD	CBA-CCA-CDA-CEA
25	B	616	CLA	C11-C12-C13-C15
25	C	508	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C20
31	B	625	LMT	C3-C4-C5-C6
31	B	626	LMT	O1'-C1-C2-C3
31	b	626	LMT	O1'-C1-C2-C3
34	C	515	DGD	C1B-C2B-C3B-C4B
34	c	515	DGD	C1B-C2B-C3B-C4B
30	A	412	SQD	C19-C20-C21-C22
30	a	412	SQD	C19-C20-C21-C22
28	C	518	LMG	C37-C38-C39-C40
28	c	518	LMG	C37-C38-C39-C40
31	I	105	LMT	C1-C2-C3-C4
31	i	105	LMT	C1-C2-C3-C4
28	C	519	LMG	C34-C35-C36-C37
28	c	519	LMG	C34-C35-C36-C37
31	M	102	LMT	C11-C10-C9-C8
31	m	102	LMT	C11-C10-C9-C8
33	D	413	LHG	C33-C34-C35-C36
33	d	412	LHG	C33-C34-C35-C36
27	B	619	BCR	C37-C22-C23-C24
27	Z	101	BCR	C7-C8-C9-C34
27	b	619	BCR	C37-C22-C23-C24
27	z	101	BCR	C7-C8-C9-C34
30	H	103	SQD	C28-C29-C30-C31
30	h	103	SQD	C28-C29-C30-C31
33	D	408	LHG	C32-C33-C34-C35
33	d	408	LHG	C32-C33-C34-C35
27	Z	101	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C10
30	F	102	SQD	C45-C44-O6-C1
30	f	102	SQD	C45-C44-O6-C1
28	C	519	LMG	C18-C19-C20-C21
28	c	519	LMG	C18-C19-C20-C21
30	A	412	SQD	C29-C30-C31-C32
30	a	412	SQD	C29-C30-C31-C32
33	E	102	LHG	C15-C16-C17-C18
33	e	102	LHG	C15-C16-C17-C18
25	B	614	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	b	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	A	407	PHO	C16-C17-C18-C20
26	a	407	PHO	C16-C17-C18-C20
28	D	409	LMG	C22-C23-C24-C25
28	d	409	LMG	C22-C23-C24-C25
30	C	525	SQD	C28-C29-C30-C31
30	c	525	SQD	C28-C29-C30-C31
33	D	413	LHG	C32-C33-C34-C35
33	d	412	LHG	C32-C33-C34-C35
29	D	405	PL9	C30-C29-C31-C32
29	d	405	PL9	C30-C29-C31-C32
31	C	521	LMT	C4-C5-C6-C7
31	c	521	LMT	C4-C5-C6-C7
30	A	413	SQD	C32-C33-C34-C35
30	C	525	SQD	C30-C31-C32-C33
30	a	413	SQD	C32-C33-C34-C35
30	c	525	SQD	C30-C31-C32-C33
33	D	408	LHG	C28-C29-C30-C31
33	E	102	LHG	C11-C10-C9-C8
33	d	408	LHG	C28-C29-C30-C31
33	e	102	LHG	C11-C10-C9-C8
30	F	102	SQD	C11-C10-C9-C8
30	f	102	SQD	C11-C10-C9-C8
25	B	605	CLA	C13-C15-C16-C17
25	b	605	CLA	C13-C15-C16-C17
25	B	609	CLA	O1D-CGD-O2D-CED
31	E	103	LMT	O1'-C1-C2-C3
25	b	609	CLA	O1D-CGD-O2D-CED
28	C	518	LMG	C15-C16-C17-C18
28	c	518	LMG	C15-C16-C17-C18
28	d	409	LMG	C30-C31-C32-C33
30	K	102	SQD	C11-C12-C13-C14
30	k	102	SQD	C11-C12-C13-C14
31	B	626	LMT	C11-C10-C9-C8
31	b	626	LMT	C11-C10-C9-C8
33	B	628	LHG	C25-C26-C27-C28
33	B	628	LHG	C32-C33-C34-C35
33	b	628	LHG	C25-C26-C27-C28
33	b	628	LHG	C32-C33-C34-C35
25	A	406	CLA	C16-C17-C18-C19
25	C	507	CLA	C16-C17-C18-C20
25	a	406	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	D	409	LMG	C30-C31-C32-C33
30	B	620	SQD	C11-C12-C13-C14
31	X	101	LMT	C3-C4-C5-C6
31	x	101	LMT	C3-C4-C5-C6
33	D	406	LHG	C11-C10-C9-C8
31	e	103	LMT	O1'-C1-C2-C3
31	B	629	LMT	C11-C10-C9-C8
31	C	521	LMT	C7-C8-C9-C10
31	L	105	LMT	C3-C4-C5-C6
31	M	101	LMT	C3-C4-C5-C6
31	b	629	LMT	C11-C10-C9-C8
31	c	521	LMT	C7-C8-C9-C10
33	d	406	LHG	C11-C10-C9-C8
25	A	405	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
30	b	620	SQD	C11-C12-C13-C14
31	m	102	LMT	C4-C5-C6-C7
31	D	412	LMT	O5B-C5B-C6B-O6B
31	x	104	LMT	O5B-C5B-C6B-O6B
30	K	102	SQD	C26-C27-C28-C29
30	h	103	SQD	C15-C16-C17-C18
30	k	102	SQD	C26-C27-C28-C29
31	M	102	LMT	C4-C5-C6-C7
31	Y	101	LMT	O1'-C1-C2-C3
31	y	101	LMT	O1'-C1-C2-C3
30	H	103	SQD	C15-C16-C17-C18
31	I	102	LMT	C7-C8-C9-C10
31	L	105	LMT	O5'-C5'-C6'-O6'
31	M	101	LMT	O5'-C5'-C6'-O6'
28	A	410	LMG	C19-C20-C21-C22
31	i	102	LMT	C7-C8-C9-C10
34	H	104	DGD	C7B-C8B-C9B-CAB
34	h	104	DGD	C7B-C8B-C9B-CAB
28	A	410	LMG	C30-C31-C32-C33
28	a	410	LMG	C19-C20-C21-C22
28	a	410	LMG	C30-C31-C32-C33
31	C	520	LMT	C11-C10-C9-C8
31	K	105	LMT	C2-C3-C4-C5
31	c	520	LMT	C11-C10-C9-C8
31	k	105	LMT	C2-C3-C4-C5
33	D	407	LHG	C18-C19-C20-C21
33	E	102	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	d	407	LHG	C18-C19-C20-C21
33	e	102	LHG	C9-C10-C11-C12
34	C	516	DGD	C7B-C8B-C9B-CAB
34	c	516	DGD	C7B-C8B-C9B-CAB
25	B	611	CLA	C16-C17-C18-C20
25	C	512	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
31	B	623	LMT	C4B-C5B-C6B-O6B
31	b	623	LMT	C4B-C5B-C6B-O6B
28	A	410	LMG	C34-C35-C36-C37
28	a	410	LMG	C34-C35-C36-C37
30	H	103	SQD	C18-C19-C20-C21
30	h	103	SQD	C18-C19-C20-C21
33	D	407	LHG	C30-C31-C32-C33
33	d	407	LHG	C30-C31-C32-C33
31	I	101	LMT	O1'-C1-C2-C3
31	i	101	LMT	O1'-C1-C2-C3
26	A	407	PHO	C4-C3-C5-C6
26	a	407	PHO	C4-C3-C5-C6
28	A	410	LMG	C29-C30-C31-C32
28	B	621	LMG	C21-C22-C23-C24
28	a	410	LMG	C29-C30-C31-C32
28	b	621	LMG	C21-C22-C23-C24
33	D	407	LHG	C15-C16-C17-C18
33	d	407	LHG	C15-C16-C17-C18
25	B	616	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
28	C	519	LMG	C13-C14-C15-C16
28	c	519	LMG	C13-C14-C15-C16
31	C	523	LMT	C1-C2-C3-C4
31	c	523	LMT	C1-C2-C3-C4
31	X	101	LMT	C4-C5-C6-C7
31	x	101	LMT	C4-C5-C6-C7
25	D	404	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1A-CGA-O2A-C1
28	D	409	LMG	C38-C39-C40-C41
28	d	409	LMG	C38-C39-C40-C41
25	C	506	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
31	d	411	LMT	C5-C6-C7-C8
33	B	628	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	b	628	LHG	C30-C31-C32-C33
28	A	414	LMG	C13-C14-C15-C16
28	a	414	LMG	C13-C14-C15-C16
28	j	101	LMG	C38-C39-C40-C41
31	D	411	LMT	C5-C6-C7-C8
33	D	408	LHG	C25-C26-C27-C28
25	a	408	CLA	C10-C11-C12-C13
33	D	413	LHG	O6-C4-C5-C6
33	d	412	LHG	O6-C4-C5-C6
31	F	103	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5B-C5B-C6B-O6B
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
28	J	101	LMG	C38-C39-C40-C41
31	I	103	LMT	C3-C4-C5-C6
33	d	408	LHG	C25-C26-C27-C28
26	A	407	PHO	C3-C5-C6-C7
26	a	407	PHO	C3-C5-C6-C7
25	A	406	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C10-C8-C7
25	B	607	CLA	C11-C12-C13-C15
25	B	613	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	509	CLA	C6-C7-C8-C10
25	D	404	CLA	C6-C7-C8-C10
25	a	406	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C10-C8-C7
25	b	607	CLA	C11-C12-C13-C15
25	b	613	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
25	d	404	CLA	C6-C7-C8-C10
31	i	103	LMT	C3-C4-C5-C6
31	Y	101	LMT	O5'-C5'-C6'-O6'
31	y	101	LMT	O5'-C5'-C6'-O6'
31	C	524	LMT	C11-C10-C9-C8
31	c	524	LMT	C11-C10-C9-C8
31	C	524	LMT	C9-C10-C11-C12
31	c	524	LMT	C9-C10-C11-C12
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
33	D	406	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C26-C27-C28-C29
25	A	408	CLA	C10-C11-C12-C13
26	A	407	PHO	C2-C3-C5-C6
26	a	407	PHO	C2-C3-C5-C6
31	E	103	LMT	C4-C5-C6-C7
31	e	103	LMT	C4-C5-C6-C7
25	B	612	CLA	C10-C11-C12-C13
25	b	612	CLA	C10-C11-C12-C13
25	B	603	CLA	C6-C7-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	C	508	CLA	C11-C12-C13-C14
25	b	603	CLA	C6-C7-C8-C9
25	b	610	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	c	508	CLA	C11-C12-C13-C14
33	B	628	LHG	C15-C16-C17-C18
33	b	628	LHG	C15-C16-C17-C18
31	I	101	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
25	C	510	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C19
30	H	103	SQD	C30-C31-C32-C33
30	h	103	SQD	C30-C31-C32-C33
33	B	628	LHG	C27-C28-C29-C30
33	b	628	LHG	C27-C28-C29-C30
31	B	625	LMT	C9-C10-C11-C12
31	b	625	LMT	C9-C10-C11-C12
33	d	412	LHG	C29-C30-C31-C32
30	A	413	SQD	C23-C24-C25-C26
30	a	413	SQD	C23-C24-C25-C26
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	O1D-CGD-O2D-CED
28	A	414	LMG	C7-C8-C9-O8
28	C	519	LMG	C7-C8-C9-O8
28	D	409	LMG	C7-C8-C9-O8
28	a	414	LMG	C7-C8-C9-O8
28	c	519	LMG	C7-C8-C9-O8
28	d	409	LMG	C7-C8-C9-O8
30	B	620	SQD	C44-C45-C46-O48
30	K	102	SQD	O6-C44-C45-C46
30	K	102	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	C44-C45-C46-O48
30	k	102	SQD	O6-C44-C45-C46
30	k	102	SQD	C44-C45-C46-O48
33	B	628	LHG	C4-C5-C6-O8
33	b	628	LHG	C4-C5-C6-O8
28	B	621	LMG	C4-C5-C6-O5
28	b	621	LMG	C4-C5-C6-O5
31	C	520	LMT	O1'-C1-C2-C3
31	c	520	LMT	O1'-C1-C2-C3
28	j	101	LMG	C31-C32-C33-C34
31	B	627	LMT	C5-C6-C7-C8
31	b	630	LMT	C5-C6-C7-C8
33	D	413	LHG	C29-C30-C31-C32
28	J	101	LMG	C31-C32-C33-C34
25	B	614	CLA	C5-C6-C7-C8
25	b	614	CLA	C5-C6-C7-C8
28	A	414	LMG	C29-C30-C31-C32
28	B	621	LMG	C37-C38-C39-C40
28	J	101	LMG	C40-C41-C42-C43
28	a	414	LMG	C29-C30-C31-C32
28	b	621	LMG	C37-C38-C39-C40
28	j	101	LMG	C40-C41-C42-C43
31	B	624	LMT	C4-C5-C6-C7
31	B	629	LMT	C5-C6-C7-C8
31	X	101	LMT	C2-C3-C4-C5
31	b	624	LMT	C4-C5-C6-C7
31	b	629	LMT	C5-C6-C7-C8
31	x	101	LMT	C2-C3-C4-C5
27	B	618	BCR	C20-C21-C22-C37
27	K	103	BCR	C20-C21-C22-C37
27	b	618	BCR	C20-C21-C22-C37
27	k	103	BCR	C20-C21-C22-C37
31	e	101	LMT	C6-C7-C8-C9
33	Z	102	LHG	C11-C10-C9-C8
33	z	102	LHG	C11-C10-C9-C8
34	C	515	DGD	O6E-C5E-C6E-O5E
34	c	515	DGD	O6E-C5E-C6E-O5E
31	E	101	LMT	C6-C7-C8-C9
29	D	405	PL9	C28-C29-C31-C32
29	d	405	PL9	C28-C29-C31-C32
31	B	625	LMT	C11-C10-C9-C8
31	I	101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
31	b	625	LMT	C11-C10-C9-C8
31	i	101	LMT	C3-C4-C5-C6
30	A	413	SQD	C9-C10-C11-C12
30	a	413	SQD	C9-C10-C11-C12
28	D	409	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
27	A	409	BCR	C21-C22-C23-C24
27	F	101	BCR	C21-C22-C23-C24
27	K	103	BCR	C17-C18-C19-C20
27	a	409	BCR	C21-C22-C23-C24
27	f	101	BCR	C21-C22-C23-C24
27	k	103	BCR	C17-C18-C19-C20
25	B	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
31	B	624	LMT	O5'-C5'-C6'-O6'
31	b	624	LMT	O5'-C5'-C6'-O6'
31	Y	101	LMT	C4-C5-C6-C7
31	y	101	LMT	C4-C5-C6-C7
31	E	103	LMT	C7-C8-C9-C10
30	A	412	SQD	C23-C24-C25-C26
30	K	102	SQD	C7-C8-C9-C10
30	a	412	SQD	C23-C24-C25-C26
30	k	102	SQD	C7-C8-C9-C10
30	A	413	SQD	C25-C26-C27-C28
31	L	105	LMT	C11-C10-C9-C8
31	M	101	LMT	C11-C10-C9-C8
31	e	103	LMT	C7-C8-C9-C10
25	A	408	CLA	CBA-CGA-O2A-C1
25	B	612	CLA	CBA-CGA-O2A-C1
25	a	408	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	CBA-CGA-O2A-C1
31	B	626	LMT	C4'-C5'-C6'-O6'
31	b	626	LMT	C4'-C5'-C6'-O6'
28	B	621	LMG	C13-C14-C15-C16
28	b	621	LMG	C13-C14-C15-C16
30	a	413	SQD	C25-C26-C27-C28
31	X	102	LMT	C1-C2-C3-C4
31	x	102	LMT	C1-C2-C3-C4
31	D	410	LMT	C3-C4-C5-C6
31	L	105	LMT	C2-C3-C4-C5
31	M	101	LMT	C2-C3-C4-C5
31	d	410	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	K	103	BCR	C19-C20-C21-C22
27	k	103	BCR	C19-C20-C21-C22
28	A	410	LMG	C37-C38-C39-C40
28	J	101	LMG	C36-C37-C38-C39
28	j	101	LMG	C36-C37-C38-C39
27	B	618	BCR	C20-C21-C22-C23
27	K	103	BCR	C20-C21-C22-C23
27	b	618	BCR	C20-C21-C22-C23
27	k	103	BCR	C20-C21-C22-C23
28	a	410	LMG	C37-C38-C39-C40
31	b	626	LMT	O5'-C5'-C6'-O6'
28	B	621	LMG	C30-C31-C32-C33
28	b	621	LMG	C30-C31-C32-C33
28	c	519	LMG	C36-C37-C38-C39
31	D	412	LMT	C6-C7-C8-C9
31	x	104	LMT	C6-C7-C8-C9
31	B	626	LMT	O5'-C5'-C6'-O6'
31	d	411	LMT	C9-C10-C11-C12
28	C	519	LMG	C36-C37-C38-C39
30	K	102	SQD	C25-C26-C27-C28
30	k	102	SQD	C25-C26-C27-C28
31	D	411	LMT	C9-C10-C11-C12
30	H	103	SQD	C24-C25-C26-C27
30	h	103	SQD	C24-C25-C26-C27
31	I	102	LMT	C2-C3-C4-C5
31	T	101	LMT	C2-C3-C4-C5
31	i	102	LMT	C2-C3-C4-C5
31	t	101	LMT	C2-C3-C4-C5
33	B	628	LHG	C16-C17-C18-C19
33	D	408	LHG	C34-C35-C36-C37
33	b	628	LHG	C16-C17-C18-C19
33	d	408	LHG	C34-C35-C36-C37
25	D	403	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
33	B	628	LHG	C14-C15-C16-C17
33	b	628	LHG	C14-C15-C16-C17
30	B	620	SQD	C13-C14-C15-C16
30	b	620	SQD	C13-C14-C15-C16
34	C	515	DGD	O2G-C2G-C3G-O3G
34	c	515	DGD	O2G-C2G-C3G-O3G
31	B	626	LMT	C9-C10-C11-C12
31	b	626	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	Z	102	LHG	C32-C33-C34-C35
33	z	102	LHG	C32-C33-C34-C35
31	f	103	LMT	C4'-C5'-C6'-O6'
34	C	517	DGD	CDB-CEB-CFB-CGB
34	c	517	DGD	CDB-CEB-CFB-CGB
28	D	409	LMG	C11-C12-C13-C14
28	d	409	LMG	C11-C12-C13-C14
30	B	620	SQD	C17-C18-C19-C20
30	b	620	SQD	C17-C18-C19-C20
25	c	511	CLA	O1D-CGD-O2D-CED
31	F	103	LMT	C4'-C5'-C6'-O6'
25	B	615	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
31	X	102	LMT	C11-C10-C9-C8
31	x	102	LMT	C11-C10-C9-C8
25	C	505	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
30	A	412	SQD	C9-C10-C11-C12
30	H	103	SQD	C29-C30-C31-C32
30	a	412	SQD	C9-C10-C11-C12
30	h	103	SQD	C29-C30-C31-C32
25	C	511	CLA	O1D-CGD-O2D-CED
26	A	407	PHO	CBA-CGA-O2A-C1
26	a	407	PHO	CBA-CGA-O2A-C1
33	D	406	LHG	C24-C23-O8-C6
33	d	406	LHG	C24-C23-O8-C6
28	B	621	LMG	C22-C23-C24-C25
28	b	621	LMG	C22-C23-C24-C25
31	T	101	LMT	C3-C4-C5-C6
31	t	101	LMT	C3-C4-C5-C6
30	A	412	SQD	C35-C36-C37-C38
30	a	412	SQD	C35-C36-C37-C38
31	C	520	LMT	C9-C10-C11-C12
31	c	520	LMT	C9-C10-C11-C12
28	B	621	LMG	C38-C39-C40-C41
28	b	621	LMG	C38-C39-C40-C41
31	e	103	LMT	C5-C6-C7-C8
25	D	401	CLA	C15-C16-C17-C18
25	d	401	CLA	C15-C16-C17-C18
31	E	103	LMT	C5-C6-C7-C8
30	H	103	SQD	C35-C36-C37-C38
30	h	103	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	I	102	LMT	C9-C10-C11-C12
31	X	103	LMT	C7-C8-C9-C10
31	i	102	LMT	C9-C10-C11-C12
31	x	103	LMT	C7-C8-C9-C10
31	K	105	LMT	C9-C10-C11-C12
31	k	105	LMT	C9-C10-C11-C12
30	C	525	SQD	C19-C20-C21-C22
30	c	525	SQD	C19-C20-C21-C22
28	C	518	LMG	C17-C18-C19-C20
28	c	518	LMG	C17-C18-C19-C20
28	C	518	LMG	C11-C12-C13-C14
28	c	518	LMG	C11-C12-C13-C14
31	A	415	LMT	C2-C1-O1'-C1'
31	B	624	LMT	C2-C1-O1'-C1'
31	C	522	LMT	C2-C1-O1'-C1'
31	a	415	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C2-C1-O1'-C1'
31	c	522	LMT	C2-C1-O1'-C1'
25	B	605	CLA	C6-C7-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C12-C13-C14
25	b	605	CLA	C6-C7-C8-C9
25	b	607	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C14
25	B	610	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
33	D	413	LHG	C5-C4-O6-P
33	d	412	LHG	C5-C4-O6-P
31	A	415	LMT	C3-C4-C5-C6
31	a	415	LMT	C3-C4-C5-C6
34	C	516	DGD	C2A-C3A-C4A-C5A
34	c	516	DGD	C2A-C3A-C4A-C5A
25	C	505	CLA	C8-C10-C11-C12
25	b	611	CLA	C10-C11-C12-C13
25	c	505	CLA	C8-C10-C11-C12
31	E	103	LMT	C2'-C1'-O1'-C1
31	e	103	LMT	C2'-C1'-O1'-C1
25	B	611	CLA	C10-C11-C12-C13
28	A	410	LMG	C15-C16-C17-C18
28	a	410	LMG	C15-C16-C17-C18
30	K	102	SQD	C14-C15-C16-C17
30	k	102	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	d	412	LHG	C35-C36-C37-C38
28	J	101	LMG	C32-C33-C34-C35
28	j	101	LMG	C32-C33-C34-C35
31	C	524	LMT	C7-C8-C9-C10
31	c	524	LMT	C7-C8-C9-C10
25	B	603	CLA	C6-C7-C8-C10
25	B	607	CLA	C12-C13-C15-C16
25	B	610	CLA	C12-C13-C15-C16
25	B	615	CLA	C12-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
25	C	508	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C12-C13-C15
25	C	512	CLA	C11-C10-C8-C7
25	C	513	CLA	C6-C7-C8-C10
25	b	603	CLA	C6-C7-C8-C10
25	b	607	CLA	C12-C13-C15-C16
25	b	610	CLA	C12-C13-C15-C16
25	b	615	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	c	508	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C12-C13-C15
25	c	512	CLA	C11-C10-C8-C7
25	c	513	CLA	C6-C7-C8-C10
25	C	504	CLA	C13-C15-C16-C17
25	c	504	CLA	C13-C15-C16-C17
25	B	612	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
33	D	413	LHG	C35-C36-C37-C38
31	F	103	LMT	C9-C10-C11-C12
31	f	103	LMT	C9-C10-C11-C12
25	C	506	CLA	C16-C17-C18-C19
25	c	506	CLA	C16-C17-C18-C19
29	A	411	PL9	C15-C14-C16-C17
29	a	411	PL9	C15-C14-C16-C17
34	C	516	DGD	O6E-C1E-O5D-C6D
34	c	516	DGD	O6E-C1E-O5D-C6D
27	A	409	BCR	C9-C10-C11-C12
27	a	409	BCR	C9-C10-C11-C12
25	C	504	CLA	C16-C17-C18-C19
25	c	504	CLA	C16-C17-C18-C19
27	z	103	BCR	C36-C18-C19-C20
34	C	516	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
34	c	516	DGD	C4A-C5A-C6A-C7A
31	T	101	LMT	C9-C10-C11-C12
31	t	101	LMT	C9-C10-C11-C12
30	A	412	SQD	C24-C25-C26-C27
30	a	412	SQD	C24-C25-C26-C27
25	B	614	CLA	C8-C10-C11-C12
34	C	516	DGD	C3B-C4B-C5B-C6B
34	c	516	DGD	C3B-C4B-C5B-C6B
31	K	105	LMT	C7-C8-C9-C10
31	k	105	LMT	C7-C8-C9-C10
33	D	407	LHG	C27-C28-C29-C30
25	b	614	CLA	C8-C10-C11-C12
30	A	412	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48
33	Z	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C4-C5-C6-O8
34	C	515	DGD	C1G-C2G-C3G-O3G
34	c	515	DGD	C1G-C2G-C3G-O3G
33	d	407	LHG	C27-C28-C29-C30
34	C	516	DGD	CDA-CEA-CFA-CGA
34	c	516	DGD	CDA-CEA-CFA-CGA
25	C	507	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	D	403	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
31	I	105	LMT	C7-C8-C9-C10
31	i	105	LMT	C7-C8-C9-C10
28	A	410	LMG	C18-C19-C20-C21
28	a	410	LMG	C18-C19-C20-C21
30	h	103	SQD	C10-C11-C12-C13
33	B	628	LHG	C17-C18-C19-C20
33	b	628	LHG	C17-C18-C19-C20
30	H	103	SQD	C10-C11-C12-C13
25	B	609	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
29	A	411	PL9	C13-C14-C16-C17
29	a	411	PL9	C13-C14-C16-C17
30	A	413	SQD	C33-C34-C35-C36
30	a	413	SQD	C33-C34-C35-C36
25	B	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
33	D	413	LHG	O6-C4-C5-O7
33	d	412	LHG	O6-C4-C5-O7
27	A	409	BCR	C23-C24-C25-C30
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C30
27	a	409	BCR	C23-C24-C25-C30
27	b	618	BCR	C23-C24-C25-C30
27	c	514	BCR	C23-C24-C25-C30
36	H	101	RRX	C23-C24-C25-C30
36	h	101	RRX	C23-C24-C25-C30
34	C	515	DGD	O2G-C1B-C2B-C3B
34	c	515	DGD	O2G-C1B-C2B-C3B
28	D	409	LMG	C29-C30-C31-C32
28	d	409	LMG	C29-C30-C31-C32
30	H	103	SQD	C26-C27-C28-C29
30	h	103	SQD	C26-C27-C28-C29
31	I	104	LMT	C2-C3-C4-C5
31	i	104	LMT	C2-C3-C4-C5
25	A	408	CLA	O1A-CGA-O2A-C1
25	B	608	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
33	B	628	LHG	C24-C25-C26-C27
33	b	628	LHG	C24-C25-C26-C27
31	C	522	LMT	C2-C3-C4-C5
31	c	522	LMT	C2-C3-C4-C5
34	C	515	DGD	C4B-C5B-C6B-C7B
34	c	515	DGD	C4B-C5B-C6B-C7B
25	c	503	CLA	C16-C17-C18-C19
28	C	519	LMG	O7-C8-C9-O8
28	J	101	LMG	O7-C8-C9-O8
28	c	519	LMG	O7-C8-C9-O8
28	j	101	LMG	O7-C8-C9-O8
30	B	620	SQD	O47-C45-C46-O48
30	C	525	SQD	O6-C44-C45-O47
30	b	620	SQD	O47-C45-C46-O48
30	c	525	SQD	O6-C44-C45-O47
33	B	628	LHG	O7-C5-C6-O8
33	D	413	LHG	O7-C5-C6-O8
33	b	628	LHG	O7-C5-C6-O8
33	d	412	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	a	408	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	C31-C32-C33-C34
30	a	413	SQD	C31-C32-C33-C34
31	B	623	LMT	C7-C8-C9-C10
31	b	623	LMT	C7-C8-C9-C10
25	B	603	CLA	C4-C3-C5-C6
25	C	510	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
25	B	609	CLA	C2-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
33	D	406	LHG	C30-C31-C32-C33
33	d	406	LHG	C30-C31-C32-C33
26	A	407	PHO	C1-C2-C3-C5
26	a	407	PHO	C1-C2-C3-C5
31	C	524	LMT	C4-C5-C6-C7
31	c	524	LMT	C4-C5-C6-C7
33	B	628	LHG	C33-C34-C35-C36
33	D	413	LHG	C34-C35-C36-C37
33	b	628	LHG	C33-C34-C35-C36
33	d	412	LHG	C34-C35-C36-C37
25	C	512	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C10-C8-C9
30	B	620	SQD	C28-C29-C30-C31
30	b	620	SQD	C28-C29-C30-C31
28	B	621	LMG	O6-C5-C6-O5
28	b	621	LMG	O6-C5-C6-O5
27	Z	101	BCR	C6-C7-C8-C9
27	z	101	BCR	C6-C7-C8-C9
31	C	524	LMT	C1-C2-C3-C4
30	H	103	SQD	C9-C10-C11-C12
30	h	103	SQD	C9-C10-C11-C12
31	I	104	LMT	C9-C10-C11-C12
31	i	104	LMT	C9-C10-C11-C12
25	A	405	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C14
25	C	503	CLA	C16-C17-C18-C20
25	D	404	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
25	d	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	c	524	LMT	C1-C2-C3-C4
29	A	411	PL9	C14-C16-C17-C18
29	a	411	PL9	C14-C16-C17-C18
31	i	102	LMT	C4-C5-C6-C7
31	I	102	LMT	C4-C5-C6-C7
27	K	103	BCR	C13-C14-C15-C16
27	k	103	BCR	C13-C14-C15-C16
25	b	616	CLA	C11-C12-C13-C14
31	M	102	LMT	O1'-C1-C2-C3
28	D	409	LMG	C31-C32-C33-C34
28	d	409	LMG	C31-C32-C33-C34
31	m	102	LMT	O1'-C1-C2-C3
33	D	413	LHG	C1-C2-C3-O3
33	d	412	LHG	C1-C2-C3-O3
30	B	620	SQD	C27-C28-C29-C30
30	C	525	SQD	C15-C16-C17-C18
30	b	620	SQD	C27-C28-C29-C30
30	c	525	SQD	C15-C16-C17-C18
34	H	104	DGD	CAA-CBA-CCA-CDA
34	h	104	DGD	CAA-CBA-CCA-CDA
27	B	618	BCR	C16-C17-C18-C36
27	K	104	BCR	C11-C10-C9-C34
27	b	618	BCR	C16-C17-C18-C36
27	z	103	BCR	C11-C10-C9-C34
34	H	104	DGD	O2G-C1B-C2B-C3B
34	h	104	DGD	O2G-C1B-C2B-C3B
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
26	A	407	PHO	C16-C17-C18-C19
26	a	407	PHO	C16-C17-C18-C19
31	I	103	LMT	C1-C2-C3-C4
31	i	103	LMT	C1-C2-C3-C4
25	B	613	CLA	C13-C15-C16-C17
25	b	613	CLA	C13-C15-C16-C17
27	K	104	BCR	C36-C18-C19-C20
28	J	101	LMG	C29-C30-C31-C32
28	j	101	LMG	C29-C30-C31-C32
25	B	602	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	603	CLA	C11-C12-C13-C15
25	B	605	CLA	C11-C10-C8-C7
25	B	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C11-C10-C8-C7
25	C	502	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	b	602	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	603	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C10-C8-C7
25	b	606	CLA	C11-C10-C8-C7
25	b	614	CLA	C11-C10-C8-C7
25	c	502	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C15
27	B	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C7-C8-C9-C10
33	Z	102	LHG	C24-C23-O8-C6
33	z	102	LHG	C24-C23-O8-C6
28	A	410	LMG	C39-C40-C41-C42
28	a	410	LMG	C39-C40-C41-C42
33	D	406	LHG	O10-C23-O8-C6
33	d	406	LHG	O10-C23-O8-C6
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
30	H	103	SQD	C23-C24-C25-C26
30	h	103	SQD	C23-C24-C25-C26
25	B	609	CLA	C16-C17-C18-C19
25	b	609	CLA	C16-C17-C18-C19
31	T	101	LMT	C7-C8-C9-C10
31	t	101	LMT	C7-C8-C9-C10
25	b	603	CLA	C4-C3-C5-C6
26	A	407	PHO	O1A-CGA-O2A-C1
26	a	407	PHO	O1A-CGA-O2A-C1
35	E	104	HEM	C2B-C3B-CAB-CBB
35	e	104	HEM	C2B-C3B-CAB-CBB
33	d	408	LHG	C29-C30-C31-C32
34	h	104	DGD	CDA-CEA-CFA-CGA
33	D	408	LHG	C29-C30-C31-C32
34	H	104	DGD	CDA-CEA-CFA-CGA
28	J	101	LMG	C16-C17-C18-C19
28	j	101	LMG	C16-C17-C18-C19
31	B	627	LMT	C7-C8-C9-C10
31	T	101	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	b	630	LMT	C7-C8-C9-C10
31	t	101	LMT	C11-C10-C9-C8
33	D	407	LHG	C12-C13-C14-C15
33	d	407	LHG	C12-C13-C14-C15
25	D	401	CLA	C16-C17-C18-C19
25	d	401	CLA	C16-C17-C18-C19
25	B	612	CLA	C13-C15-C16-C17
25	C	513	CLA	C5-C6-C7-C8
25	b	612	CLA	C13-C15-C16-C17
25	c	513	CLA	C5-C6-C7-C8
33	D	407	LHG	C34-C35-C36-C37
33	d	407	LHG	C34-C35-C36-C37
27	B	618	BCR	C16-C17-C18-C19
27	b	618	BCR	C16-C17-C18-C19
34	C	515	DGD	C6B-C7B-C8B-C9B
34	c	515	DGD	C6B-C7B-C8B-C9B
31	b	630	LMT	C4-C5-C6-C7
31	B	623	LMT	C9-C10-C11-C12
31	b	623	LMT	C9-C10-C11-C12
31	B	627	LMT	C4-C5-C6-C7
30	A	412	SQD	O6-C44-C45-C46
30	a	412	SQD	O6-C44-C45-C46
34	C	517	DGD	O1G-C1G-C2G-C3G
34	c	517	DGD	O1G-C1G-C2G-C3G
25	B	616	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
33	D	413	LHG	C14-C15-C16-C17
33	d	412	LHG	C14-C15-C16-C17
30	A	412	SQD	C12-C13-C14-C15
30	a	412	SQD	C12-C13-C14-C15
30	a	412	SQD	C33-C34-C35-C36
30	A	412	SQD	C33-C34-C35-C36
28	J	101	LMG	C34-C35-C36-C37
28	j	101	LMG	C34-C35-C36-C37
30	A	412	SQD	C28-C29-C30-C31
30	a	412	SQD	C28-C29-C30-C31
28	A	414	LMG	O7-C8-C9-O8
28	a	414	LMG	O7-C8-C9-O8
30	A	412	SQD	O47-C45-C46-O48
30	a	412	SQD	O47-C45-C46-O48
30	a	413	SQD	O6-C44-C45-O47
28	C	519	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C6-C7-C8-C9
25	B	603	CLA	C11-C12-C13-C14
25	C	505	CLA	C14-C13-C15-C16
25	b	602	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	c	505	CLA	C14-C13-C15-C16
28	J	101	LMG	C21-C22-C23-C24
28	j	101	LMG	C21-C22-C23-C24
31	B	626	LMT	C5-C6-C7-C8
31	b	626	LMT	C5-C6-C7-C8
28	c	519	LMG	C21-C22-C23-C24
30	A	413	SQD	C26-C27-C28-C29
30	a	413	SQD	C26-C27-C28-C29
33	D	407	LHG	C13-C14-C15-C16
33	d	407	LHG	C13-C14-C15-C16
33	Z	102	LHG	O10-C23-O8-C6
33	z	102	LHG	O10-C23-O8-C6
31	B	623	LMT	C1-C2-C3-C4
26	D	402	PHO	C2C-C3C-CAC-CBC
26	d	402	PHO	C2C-C3C-CAC-CBC
31	a	415	LMT	C6-C7-C8-C9
34	C	516	DGD	C9B-CAB-CBB-CCB
34	c	516	DGD	C9B-CAB-CBB-CCB
31	A	415	LMT	C9-C10-C11-C12
31	a	415	LMT	C9-C10-C11-C12
31	b	623	LMT	C1-C2-C3-C4
30	C	525	SQD	C24-C25-C26-C27
30	c	525	SQD	C24-C25-C26-C27
31	A	415	LMT	C6-C7-C8-C9
31	C	523	LMT	C3-C4-C5-C6
31	c	523	LMT	C3-C4-C5-C6
25	D	404	CLA	O1D-CGD-O2D-CED
25	d	404	CLA	O1D-CGD-O2D-CED
34	C	516	DGD	C2E-C1E-O5D-C6D
34	c	516	DGD	C2E-C1E-O5D-C6D
25	D	401	CLA	C16-C17-C18-C20
25	d	401	CLA	C16-C17-C18-C20
25	B	612	CLA	C8-C10-C11-C12
33	E	102	LHG	C5-C4-O6-P
33	e	102	LHG	C5-C4-O6-P
31	D	410	LMT	C5-C6-C7-C8
31	d	410	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	f	103	LMT	C1-C2-C3-C4
25	b	612	CLA	C8-C10-C11-C12
31	F	103	LMT	C5-C6-C7-C8
31	f	103	LMT	C5-C6-C7-C8
25	B	612	CLA	C15-C16-C17-C18
25	b	612	CLA	C15-C16-C17-C18
27	F	101	BCR	C14-C15-C16-C17
27	f	101	BCR	C14-C15-C16-C17
31	F	103	LMT	C1-C2-C3-C4
28	C	519	LMG	C30-C31-C32-C33
31	D	410	LMT	C11-C10-C9-C8
31	L	105	LMT	C4-C5-C6-C7
31	b	624	LMT	C2-C3-C4-C5
31	d	410	LMT	C11-C10-C9-C8
28	c	519	LMG	C30-C31-C32-C33
31	M	101	LMT	C4-C5-C6-C7
31	B	624	LMT	C2-C3-C4-C5
31	F	103	LMT	C2-C1-O1'-C1'
31	f	103	LMT	C2-C1-O1'-C1'
27	K	103	BCR	C11-C12-C13-C35
27	k	103	BCR	C11-C12-C13-C35
31	D	411	LMT	C7-C8-C9-C10
31	Y	101	LMT	C2-C3-C4-C5
31	d	411	LMT	C7-C8-C9-C10
31	y	101	LMT	C2-C3-C4-C5
27	B	619	BCR	C21-C22-C23-C24
27	K	104	BCR	C17-C18-C19-C20
27	b	619	BCR	C21-C22-C23-C24
27	z	103	BCR	C17-C18-C19-C20
31	E	103	LMT	C9-C10-C11-C12
31	e	103	LMT	C9-C10-C11-C12
28	C	518	LMG	C16-C17-C18-C19
28	c	518	LMG	C16-C17-C18-C19
30	K	102	SQD	C31-C32-C33-C34
30	k	102	SQD	C31-C32-C33-C34
28	A	410	LMG	C40-C41-C42-C43
28	a	410	LMG	C40-C41-C42-C43
25	A	408	CLA	C11-C10-C8-C7
25	B	611	CLA	C11-C12-C13-C15
25	B	615	CLA	C6-C7-C8-C10
25	C	505	CLA	C12-C13-C15-C16
25	a	408	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	C11-C12-C13-C15
25	b	615	CLA	C6-C7-C8-C10
25	c	505	CLA	C12-C13-C15-C16
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
33	E	102	LHG	C16-C17-C18-C19
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
33	e	102	LHG	C16-C17-C18-C19
31	B	629	LMT	C9-C10-C11-C12
33	D	408	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
31	b	629	LMT	C9-C10-C11-C12
25	B	609	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C20
34	C	515	DGD	O6D-C5D-C6D-O5D
34	c	515	DGD	O6D-C5D-C6D-O5D
28	C	519	LMG	O6-C5-C6-O5
28	c	519	LMG	O6-C5-C6-O5
25	A	408	CLA	C11-C10-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	508	CLA	C6-C7-C8-C9
25	a	408	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	615	CLA	C14-C13-C15-C16
25	c	508	CLA	C6-C7-C8-C9
33	D	406	LHG	C31-C32-C33-C34
33	Z	102	LHG	C34-C35-C36-C37
33	d	406	LHG	C31-C32-C33-C34
33	z	102	LHG	C34-C35-C36-C37
34	H	104	DGD	CCA-CDA-CEA-CFA
34	h	104	DGD	CCA-CDA-CEA-CFA
27	C	514	BCR	C19-C20-C21-C22
27	c	514	BCR	C19-C20-C21-C22
33	B	628	LHG	C11-C12-C13-C14
31	T	101	LMT	C5-C6-C7-C8
31	t	101	LMT	C5-C6-C7-C8
33	b	628	LHG	C11-C12-C13-C14
34	C	515	DGD	C9B-CAB-CBB-CCB
34	c	515	DGD	C9B-CAB-CBB-CCB
28	D	409	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
28	d	409	LMG	O1-C7-C8-O7
30	A	412	SQD	O6-C44-C45-O47
30	A	413	SQD	O6-C44-C45-O47
30	B	620	SQD	O6-C44-C45-O47
30	a	412	SQD	O6-C44-C45-O47
30	b	620	SQD	O6-C44-C45-O47
33	Z	102	LHG	O7-C5-C6-O8
33	z	102	LHG	O7-C5-C6-O8
30	C	525	SQD	O6-C44-C45-C46
30	c	525	SQD	O6-C44-C45-C46
33	D	413	LHG	C4-C5-C6-O8
33	d	412	LHG	C4-C5-C6-O8
31	x	102	LMT	C4-C5-C6-C7
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
31	X	102	LMT	C4-C5-C6-C7
31	C	521	LMT	C9-C10-C11-C12
31	c	521	LMT	C9-C10-C11-C12
33	d	408	LHG	C12-C13-C14-C15
31	C	521	LMT	C3-C4-C5-C6
33	D	408	LHG	C12-C13-C14-C15
30	H	103	SQD	C34-C35-C36-C37
30	h	103	SQD	C34-C35-C36-C37
31	B	627	LMT	C6-C7-C8-C9
31	b	630	LMT	C6-C7-C8-C9
31	c	521	LMT	C3-C4-C5-C6
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
27	Z	101	BCR	C15-C16-C17-C18
27	z	101	BCR	C15-C16-C17-C18
33	B	628	LHG	C3-O3-P-O5
33	D	413	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O3
33	E	102	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O5
33	d	412	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O3
33	e	102	LHG	C4-O6-P-O5
28	C	518	LMG	C22-C23-C24-C25
28	c	518	LMG	C22-C23-C24-C25
25	A	408	CLA	C4-C3-C5-C6
25	a	408	CLA	C4-C3-C5-C6
28	D	409	LMG	C14-C15-C16-C17
28	d	409	LMG	C14-C15-C16-C17
25	B	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
33	D	413	LHG	C2-C3-O3-P
33	d	412	LHG	C2-C3-O3-P
31	D	412	LMT	C7-C8-C9-C10
31	x	104	LMT	C7-C8-C9-C10
28	A	414	LMG	C14-C15-C16-C17
25	B	615	CLA	C13-C15-C16-C17
28	a	414	LMG	C14-C15-C16-C17
34	C	515	DGD	C4D-C5D-C6D-O5D
34	c	515	DGD	C4D-C5D-C6D-O5D
34	C	517	DGD	C5A-C6A-C7A-C8A
34	H	104	DGD	CBA-CCA-CDA-CEA
34	c	517	DGD	C5A-C6A-C7A-C8A
34	h	104	DGD	CBA-CCA-CDA-CEA
33	E	102	LHG	C14-C15-C16-C17
33	e	102	LHG	C14-C15-C16-C17
31	b	624	LMT	O1'-C1-C2-C3
33	B	628	LHG	C11-C10-C9-C8
33	b	628	LHG	C11-C10-C9-C8
31	B	624	LMT	O1'-C1-C2-C3
25	b	615	CLA	C13-C15-C16-C17
28	B	621	LMG	C11-C12-C13-C14
28	a	410	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	b	621	LMG	C11-C12-C13-C14
33	b	628	LHG	C34-C35-C36-C37
34	C	515	DGD	C3B-C4B-C5B-C6B
28	A	410	LMG	C12-C13-C14-C15
31	D	411	LMT	C11-C10-C9-C8
31	d	411	LMT	C11-C10-C9-C8
33	B	628	LHG	C34-C35-C36-C37
34	c	515	DGD	C3B-C4B-C5B-C6B
31	D	412	LMT	C9-C10-C11-C12
31	x	104	LMT	C9-C10-C11-C12
31	b	629	LMT	C1-C2-C3-C4
31	B	629	LMT	C1-C2-C3-C4
25	B	610	CLA	C16-C17-C18-C20
25	C	501	CLA	C16-C17-C18-C20
25	b	610	CLA	C16-C17-C18-C20
25	c	501	CLA	C16-C17-C18-C20
30	A	413	SQD	C29-C30-C31-C32
30	a	413	SQD	C29-C30-C31-C32
34	H	104	DGD	C3B-C4B-C5B-C6B
30	A	413	SQD	C30-C31-C32-C33
30	a	413	SQD	C30-C31-C32-C33
34	h	104	DGD	C3B-C4B-C5B-C6B
25	A	406	CLA	C11-C10-C8-C9
25	a	406	CLA	C11-C10-C8-C9
28	D	409	LMG	C19-C20-C21-C22
25	B	613	CLA	C11-C10-C8-C7
25	b	613	CLA	C11-C10-C8-C7
28	d	409	LMG	C19-C20-C21-C22
31	e	103	LMT	C11-C10-C9-C8
27	K	104	BCR	C11-C10-C9-C8
27	z	103	BCR	C11-C10-C9-C8
31	E	103	LMT	C11-C10-C9-C8
33	D	413	LHG	C24-C25-C26-C27
25	C	502	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20
33	d	412	LHG	C24-C25-C26-C27
28	A	414	LMG	O8-C28-C29-C30
28	a	414	LMG	O8-C28-C29-C30
31	F	103	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	C2'-C1'-O1'-C1
28	D	409	LMG	O7-C8-C9-O8
28	d	409	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	O1G-C1G-C2G-O2G
34	c	517	DGD	O1G-C1G-C2G-O2G
30	A	413	SQD	O48-C23-C24-C25
30	a	413	SQD	O48-C23-C24-C25
28	a	414	LMG	C11-C12-C13-C14
28	A	414	LMG	C11-C12-C13-C14
31	B	625	LMT	C5-C6-C7-C8
31	b	625	LMT	C5-C6-C7-C8
30	K	102	SQD	C13-C14-C15-C16
30	k	102	SQD	C13-C14-C15-C16
28	J	101	LMG	C7-C8-C9-O8
28	j	101	LMG	C7-C8-C9-O8
30	A	413	SQD	O6-C44-C45-C46
30	a	413	SQD	O6-C44-C45-C46
33	D	407	LHG	C23-C24-C25-C26
33	d	407	LHG	C23-C24-C25-C26
30	H	103	SQD	C45-C44-O6-C1
31	b	623	LMT	C2-C3-C4-C5
31	I	103	LMT	O5'-C1'-O1'-C1
31	i	103	LMT	O5'-C1'-O1'-C1
33	B	628	LHG	O2-C2-C3-O3
33	b	628	LHG	O2-C2-C3-O3
31	B	623	LMT	C2-C3-C4-C5
30	C	525	SQD	C12-C13-C14-C15
30	c	525	SQD	C12-C13-C14-C15
31	B	623	LMT	C2-C1-O1'-C1'
31	D	411	LMT	C2-C1-O1'-C1'
31	I	104	LMT	C2-C1-O1'-C1'
31	b	623	LMT	C2-C1-O1'-C1'
31	d	411	LMT	C2-C1-O1'-C1'
31	i	104	LMT	C2-C1-O1'-C1'
33	B	628	LHG	C1-C2-C3-O3
33	b	628	LHG	C1-C2-C3-O3
25	A	406	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C12-C13-C14
25	c	513	CLA	C14-C13-C15-C16
34	C	517	DGD	C8B-C9B-CAB-CBB
34	c	517	DGD	C8B-C9B-CAB-CBB
34	C	517	DGD	O6D-C5D-C6D-O5D
34	c	517	DGD	O6D-C5D-C6D-O5D
28	D	409	LMG	C35-C36-C37-C38
28	d	409	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
35	E	104	HEM	C4B-C3B-CAB-CBB
35	e	104	HEM	C4B-C3B-CAB-CBB
25	B	610	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C19
25	C	504	CLA	C11-C12-C13-C15
25	c	504	CLA	C11-C12-C13-C15
31	M	102	LMT	C3-C4-C5-C6
31	m	102	LMT	C3-C4-C5-C6
31	i	102	LMT	C11-C10-C9-C8
31	I	102	LMT	C11-C10-C9-C8
25	B	602	CLA	C16-C17-C18-C19
25	B	603	CLA	C8-C10-C11-C12
25	b	603	CLA	C8-C10-C11-C12
25	C	510	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
28	A	410	LMG	C11-C12-C13-C14
30	H	103	SQD	O6-C44-C45-O47
30	h	103	SQD	O6-C44-C45-O47
28	a	410	LMG	C11-C12-C13-C14
25	C	513	CLA	C4-C3-C5-C6
25	c	513	CLA	C4-C3-C5-C6
25	c	502	CLA	O1A-CGA-O2A-C1
34	C	515	DGD	C4A-C5A-C6A-C7A
34	c	515	DGD	C4A-C5A-C6A-C7A
25	A	405	CLA	C2-C1-O2A-CGA
25	a	405	CLA	C2-C1-O2A-CGA
27	K	103	BCR	C15-C16-C17-C18
27	k	103	BCR	C15-C16-C17-C18
25	C	510	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
31	F	103	LMT	C3-C4-C5-C6
31	f	103	LMT	C3-C4-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
30	c	525	SQD	C26-C27-C28-C29
33	Z	102	LHG	C26-C27-C28-C29
31	k	105	LMT	C5-C6-C7-C8
25	C	501	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
33	z	102	LHG	C26-C27-C28-C29
29	D	405	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
29	d	405	PL9	C39-C41-C42-C43
30	C	525	SQD	C26-C27-C28-C29
31	K	105	LMT	C5-C6-C7-C8
25	C	503	CLA	C8-C10-C11-C12
25	c	503	CLA	C8-C10-C11-C12
25	C	502	CLA	O1A-CGA-O2A-C1
25	B	607	CLA	C6-C7-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C9
25	c	512	CLA	C6-C7-C8-C9
33	B	628	LHG	O1-C1-C2-C3
33	b	628	LHG	O1-C1-C2-C3
31	K	105	LMT	C11-C10-C9-C8
31	k	105	LMT	C11-C10-C9-C8
25	C	513	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
31	C	523	LMT	C11-C10-C9-C8
31	c	523	LMT	C11-C10-C9-C8
25	a	408	CLA	O1D-CGD-O2D-CED
33	D	408	LHG	C18-C19-C20-C21
33	d	408	LHG	C18-C19-C20-C21
25	B	604	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C19
33	B	628	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
27	A	409	BCR	C23-C24-C25-C26
27	B	617	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C30
27	a	409	BCR	C23-C24-C25-C26
27	b	617	BCR	C1-C6-C7-C8
27	b	618	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C30
36	H	101	RRX	C23-C24-C25-C26
36	h	101	RRX	C23-C24-C25-C26
28	B	621	LMG	C19-C20-C21-C22
28	b	621	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	K	102	SQD	C12-C13-C14-C15
30	k	102	SQD	C12-C13-C14-C15
31	B	624	LMT	C3-C4-C5-C6
31	b	624	LMT	C3-C4-C5-C6
33	E	102	LHG	C26-C27-C28-C29
33	e	102	LHG	C26-C27-C28-C29
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C45-C44-C46-C47
25	A	408	CLA	O1D-CGD-O2D-CED
31	C	520	LMT	C2-C3-C4-C5
31	c	520	LMT	C2-C3-C4-C5
30	a	413	SQD	C10-C11-C12-C13
25	A	408	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	D	403	CLA	C12-C13-C15-C16
25	a	408	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
25	d	403	CLA	C12-C13-C15-C16
25	C	505	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
31	I	105	LMT	C5-C6-C7-C8
31	i	105	LMT	C5-C6-C7-C8
30	A	413	SQD	C10-C11-C12-C13
31	M	102	LMT	C5-C6-C7-C8
31	m	102	LMT	C5-C6-C7-C8
28	C	518	LMG	C12-C13-C14-C15
28	c	518	LMG	C12-C13-C14-C15
34	C	516	DGD	CCA-CDA-CEA-CFA
33	E	102	LHG	C7-C8-C9-C10
33	e	102	LHG	C7-C8-C9-C10
34	c	516	DGD	CCA-CDA-CEA-CFA
33	D	406	LHG	C11-C12-C13-C14
33	d	406	LHG	C11-C12-C13-C14
25	C	513	CLA	C2-C3-C5-C6
25	c	513	CLA	C2-C3-C5-C6
28	D	409	LMG	C17-C18-C19-C20
28	d	409	LMG	C17-C18-C19-C20
33	Z	102	LHG	C33-C34-C35-C36
33	z	102	LHG	C33-C34-C35-C36
30	C	525	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	c	525	SQD	C10-C11-C12-C13
31	M	102	LMT	C4'-C5'-C6'-O6'
31	m	102	LMT	C4'-C5'-C6'-O6'
25	B	606	CLA	C8-C10-C11-C12
25	b	606	CLA	C8-C10-C11-C12
33	E	102	LHG	C11-C12-C13-C14
33	e	102	LHG	C11-C12-C13-C14
25	C	502	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
31	I	104	LMT	O5'-C1'-O1'-C1
31	i	104	LMT	O5'-C1'-O1'-C1
25	B	602	CLA	C4-C3-C5-C6
25	b	602	CLA	C4-C3-C5-C6
33	E	102	LHG	C2-C3-O3-P
33	e	102	LHG	C2-C3-O3-P
33	D	413	LHG	C27-C28-C29-C30
33	d	412	LHG	C27-C28-C29-C30
28	C	519	LMG	O1-C7-C8-C9
28	c	519	LMG	O1-C7-C8-C9
29	a	411	PL9	C24-C26-C27-C28
33	D	407	LHG	C35-C36-C37-C38
33	d	407	LHG	C35-C36-C37-C38
28	b	621	LMG	C20-C21-C22-C23
33	B	628	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-O2
28	B	621	LMG	C20-C21-C22-C23
29	A	411	PL9	C25-C24-C26-C27
29	a	411	PL9	C25-C24-C26-C27
26	A	407	PHO	CHA-CBD-CGD-O1D
26	a	407	PHO	CHA-CBD-CGD-O1D
27	B	619	BCR	C16-C17-C18-C36
27	b	619	BCR	C16-C17-C18-C36
31	B	624	LMT	C9-C10-C11-C12
31	b	624	LMT	C9-C10-C11-C12
28	A	410	LMG	C32-C33-C34-C35
28	a	410	LMG	C32-C33-C34-C35
33	e	102	LHG	C12-C13-C14-C15
33	E	102	LHG	C12-C13-C14-C15
34	H	104	DGD	O1G-C1G-C2G-O2G
34	h	104	DGD	O1G-C1G-C2G-O2G
25	C	507	CLA	C5-C6-C7-C8
25	c	507	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	H	104	DGD	C6B-C7B-C8B-C9B
34	h	104	DGD	C6B-C7B-C8B-C9B
31	C	521	LMT	O5'-C1'-O1'-C1
31	c	521	LMT	O5'-C1'-O1'-C1
31	D	412	LMT	C11-C10-C9-C8
31	x	104	LMT	C11-C10-C9-C8
26	a	407	PHO	C15-C16-C17-C18
31	b	630	LMT	C3-C4-C5-C6
29	A	411	PL9	C24-C26-C27-C28
25	A	406	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	613	CLA	C14-C13-C15-C16
25	C	512	CLA	C14-C13-C15-C16
25	a	406	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	613	CLA	C14-C13-C15-C16
25	c	512	CLA	C14-C13-C15-C16
31	B	627	LMT	C3-C4-C5-C6
31	B	626	LMT	C1-C2-C3-C4
31	b	626	LMT	C1-C2-C3-C4
30	K	102	SQD	C45-C44-O6-C1
30	h	103	SQD	C45-C44-O6-C1
30	k	102	SQD	C45-C44-O6-C1
25	B	610	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
26	A	407	PHO	C15-C16-C17-C18
25	C	510	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
31	K	105	LMT	C6-C7-C8-C9
31	k	105	LMT	C6-C7-C8-C9
25	A	408	CLA	C2-C3-C5-C6
25	a	408	CLA	C2-C3-C5-C6
31	C	523	LMT	C9-C10-C11-C12
34	C	515	DGD	O1B-C1B-C2B-C3B
34	c	515	DGD	O1B-C1B-C2B-C3B
33	Z	102	LHG	C25-C26-C27-C28
33	z	102	LHG	C25-C26-C27-C28
31	c	523	LMT	C9-C10-C11-C12
25	C	512	CLA	O2A-C1-C2-C3
25	c	512	CLA	O2A-C1-C2-C3
31	C	522	LMT	C4-C5-C6-C7
31	c	522	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	I	101	LMT	C7-C8-C9-C10
31	X	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C7-C8-C9-C10
31	x	101	LMT	C6-C7-C8-C9
28	C	518	LMG	C18-C19-C20-C21
28	c	518	LMG	C18-C19-C20-C21
31	D	411	LMT	C6-C7-C8-C9
25	c	507	CLA	CBA-CGA-O2A-C1
31	b	624	LMT	C7-C8-C9-C10
31	d	411	LMT	C6-C7-C8-C9
31	B	624	LMT	C7-C8-C9-C10
31	D	410	LMT	C9-C10-C11-C12
31	d	410	LMT	C9-C10-C11-C12
25	B	605	CLA	C8-C10-C11-C12
25	b	605	CLA	C8-C10-C11-C12
25	C	507	CLA	CBA-CGA-O2A-C1
30	B	620	SQD	O6-C44-C45-C46
30	b	620	SQD	O6-C44-C45-C46
25	A	408	CLA	CBD-CGD-O2D-CED
25	a	408	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
30	B	620	SQD	C25-C26-C27-C28
30	b	620	SQD	C25-C26-C27-C28
33	d	412	LHG	O8-C23-C24-C25
33	D	408	LHG	C14-C15-C16-C17
33	d	408	LHG	C14-C15-C16-C17
25	B	615	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	D	401	CLA	C14-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C9
25	c	513	CLA	C11-C10-C8-C9
25	d	401	CLA	C14-C13-C15-C16
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
30	K	102	SQD	O47-C7-C8-C9
30	k	102	SQD	O47-C7-C8-C9
33	D	413	LHG	O8-C23-C24-C25
28	j	101	LMG	C11-C12-C13-C14
31	C	520	LMT	C7-C8-C9-C10
31	c	520	LMT	C7-C8-C9-C10
28	J	101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	A	406	CLA	C6-C7-C8-C10
25	B	611	CLA	C6-C7-C8-C10
25	C	501	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C10-C8-C7
25	a	406	CLA	C6-C7-C8-C10
25	b	611	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C10-C8-C7
25	d	404	CLA	C11-C10-C8-C7
27	B	617	BCR	C5-C6-C7-C8
27	Z	101	BCR	C1-C6-C7-C8
27	Z	101	BCR	C5-C6-C7-C8
27	Z	101	BCR	C23-C24-C25-C26
27	b	617	BCR	C5-C6-C7-C8
27	z	101	BCR	C1-C6-C7-C8
27	z	101	BCR	C5-C6-C7-C8
27	z	101	BCR	C23-C24-C25-C26
30	A	412	SQD	C8-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
33	D	407	LHG	O9-C7-O7-C5
33	d	407	LHG	O9-C7-O7-C5
28	C	519	LMG	C11-C12-C13-C14
33	D	406	LHG	C18-C19-C20-C21
33	d	406	LHG	C18-C19-C20-C21
25	B	608	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C1-O2A-CGA
25	B	616	CLA	C2-C1-O2A-CGA
25	b	608	CLA	C2-C1-O2A-CGA
25	b	612	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
28	c	519	LMG	C11-C12-C13-C14
28	J	101	LMG	C22-C23-C24-C25
28	C	519	LMG	C4-C5-C6-O5
28	j	101	LMG	C22-C23-C24-C25
31	B	627	LMT	C11-C10-C9-C8
31	b	630	LMT	C11-C10-C9-C8
25	B	613	CLA	CAA-CBA-CGA-O2A
25	b	613	CLA	CAA-CBA-CGA-O2A
31	d	411	LMT	O1'-C1-C2-C3
28	J	101	LMG	C42-C43-C44-C45
28	j	101	LMG	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
31	B	627	LMT	O1'-C1-C2-C3
31	b	630	LMT	O1'-C1-C2-C3
28	c	519	LMG	C4-C5-C6-O5
26	A	407	PHO	C8-C10-C11-C12
26	a	407	PHO	C8-C10-C11-C12
25	C	505	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
31	D	411	LMT	O1'-C1-C2-C3
25	C	513	CLA	CAA-CBA-CGA-O2A
25	c	513	CLA	CAA-CBA-CGA-O2A
25	C	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
30	A	412	SQD	O49-C7-O47-C45
30	a	412	SQD	O49-C7-O47-C45
33	D	407	LHG	C8-C7-O7-C5
33	d	407	LHG	C8-C7-O7-C5
30	A	412	SQD	C32-C33-C34-C35
30	a	412	SQD	C32-C33-C34-C35
29	A	411	PL9	C4-C3-C7-C8
29	a	411	PL9	C4-C3-C7-C8
25	C	507	CLA	C10-C11-C12-C13
25	c	507	CLA	C10-C11-C12-C13
25	C	510	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
34	c	516	DGD	C3A-C4A-C5A-C6A
31	I	105	LMT	C9-C10-C11-C12
31	i	105	LMT	C9-C10-C11-C12
34	C	516	DGD	C3A-C4A-C5A-C6A
33	D	407	LHG	C33-C34-C35-C36
33	d	407	LHG	C33-C34-C35-C36
33	D	408	LHG	C30-C31-C32-C33
33	d	408	LHG	C30-C31-C32-C33
25	C	508	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	C	510	CLA	C15-C16-C17-C18
25	c	510	CLA	C15-C16-C17-C18
31	i	102	LMT	O1'-C1-C2-C3
31	I	102	LMT	O1'-C1-C2-C3
34	C	515	DGD	O6E-C1E-O5D-C6D
34	c	515	DGD	O6E-C1E-O5D-C6D
30	C	525	SQD	O47-C7-C8-C9
30	c	525	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	K	103	BCR	C11-C12-C13-C14
27	k	103	BCR	C11-C12-C13-C14
31	c	524	LMT	C3-C4-C5-C6
31	C	524	LMT	C3-C4-C5-C6
33	D	408	LHG	C24-C25-C26-C27
31	B	623	LMT	O1'-C1-C2-C3
31	b	623	LMT	O1'-C1-C2-C3
33	d	408	LHG	C24-C25-C26-C27
25	c	512	CLA	O1A-CGA-O2A-C1
28	J	101	LMG	C11-C10-O7-C8
28	j	101	LMG	C11-C10-O7-C8
29	D	405	PL9	C16-C17-C18-C19
29	d	405	PL9	C16-C17-C18-C19
30	A	412	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O9
30	a	412	SQD	C5-C6-S-O7
30	a	413	SQD	C5-C6-S-O9
25	B	614	CLA	C2-C1-O2A-CGA
25	b	614	CLA	C2-C1-O2A-CGA
25	B	604	CLA	C11-C12-C13-C15
25	B	610	CLA	C11-C12-C13-C15
25	C	512	CLA	C12-C13-C15-C16
25	D	401	CLA	C6-C7-C8-C10
25	b	604	CLA	C11-C12-C13-C15
25	b	610	CLA	C11-C12-C13-C15
25	c	512	CLA	C12-C13-C15-C16
25	d	401	CLA	C6-C7-C8-C10
34	C	516	DGD	C4B-C5B-C6B-C7B
34	c	516	DGD	C4B-C5B-C6B-C7B
34	C	517	DGD	C8A-C9A-CAA-CBA
34	c	517	DGD	C8A-C9A-CAA-CBA
25	C	512	CLA	O1A-CGA-O2A-C1
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C16-C17-C18-C19
25	C	513	CLA	C16-C17-C18-C20
25	b	603	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
26	D	402	PHO	C16-C17-C18-C20
26	d	402	PHO	C16-C17-C18-C20
30	B	620	SQD	C15-C16-C17-C18
30	b	620	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	B	621	LMG	C12-C13-C14-C15
25	B	613	CLA	CAA-CBA-CGA-O1A
25	b	613	CLA	CAA-CBA-CGA-O1A
25	C	512	CLA	C8-C10-C11-C12
33	D	413	LHG	O10-C23-C24-C25
33	d	412	LHG	O10-C23-C24-C25
28	b	621	LMG	C12-C13-C14-C15
25	B	605	CLA	C10-C11-C12-C13
25	b	605	CLA	C10-C11-C12-C13
25	c	512	CLA	C8-C10-C11-C12
33	D	413	LHG	C25-C26-C27-C28
33	d	412	LHG	C25-C26-C27-C28
34	C	516	DGD	C6A-C7A-C8A-C9A
34	c	516	DGD	C6A-C7A-C8A-C9A
28	J	101	LMG	O8-C28-C29-C30
28	j	101	LMG	O8-C28-C29-C30
25	B	614	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C11-C12-C13-C14
25	B	611	CLA	C6-C7-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	D	401	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	611	CLA	C6-C7-C8-C9
25	c	506	CLA	C14-C13-C15-C16
25	d	401	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C10-C8-C9
28	a	414	LMG	C12-C13-C14-C15
34	H	104	DGD	O1B-C1B-C2B-C3B
34	h	104	DGD	O1B-C1B-C2B-C3B
31	B	625	LMT	C1-C2-C3-C4
31	b	625	LMT	C1-C2-C3-C4
28	A	414	LMG	C12-C13-C14-C15
34	c	517	DGD	CDA-CEA-CFA-CGA
25	C	504	CLA	C2-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
30	A	412	SQD	O5-C5-C6-S
30	A	413	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C5-C6-S
30	a	413	SQD	O5-C5-C6-S
25	B	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	CDA-CEA-CFA-CGA
31	I	105	LMT	C4-C5-C6-C7
25	C	513	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
25	c	513	CLA	CAA-CBA-CGA-O1A
30	K	102	SQD	O49-C7-C8-C9
30	k	102	SQD	O49-C7-C8-C9
31	C	523	LMT	C7-C8-C9-C10
31	c	523	LMT	C7-C8-C9-C10
28	j	101	LMG	C8-C7-O1-C1
34	C	515	DGD	C5D-C6D-O5D-C1E
34	c	515	DGD	C5D-C6D-O5D-C1E
28	J	101	LMG	O9-C10-O7-C8
28	j	101	LMG	O9-C10-O7-C8
33	D	408	LHG	C35-C36-C37-C38
33	d	408	LHG	C35-C36-C37-C38
25	B	601	CLA	CAA-CBA-CGA-O2A
25	b	601	CLA	CAA-CBA-CGA-O2A
31	i	105	LMT	C4-C5-C6-C7
33	D	413	LHG	O7-C7-C8-C9
33	d	412	LHG	O7-C7-C8-C9
30	H	103	SQD	C44-C45-C46-O48
30	h	103	SQD	C44-C45-C46-O48
28	a	414	LMG	C31-C32-C33-C34
31	I	105	LMT	O1'-C1-C2-C3
31	i	105	LMT	O1'-C1-C2-C3
25	C	510	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
30	C	525	SQD	O49-C7-C8-C9
30	c	525	SQD	O49-C7-C8-C9
28	A	414	LMG	C31-C32-C33-C34
26	A	407	PHO	CAD-CBD-CGD-O2D
26	a	407	PHO	CAD-CBD-CGD-O2D
34	c	516	DGD	C8A-C9A-CAA-CBA
30	A	412	SQD	O5-C1-O6-C44
30	a	412	SQD	O5-C1-O6-C44
25	D	403	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
26	A	407	PHO	C1-C2-C3-C4
26	a	407	PHO	C1-C2-C3-C4
34	C	516	DGD	C8A-C9A-CAA-CBA
25	c	508	CLA	C3-C5-C6-C7

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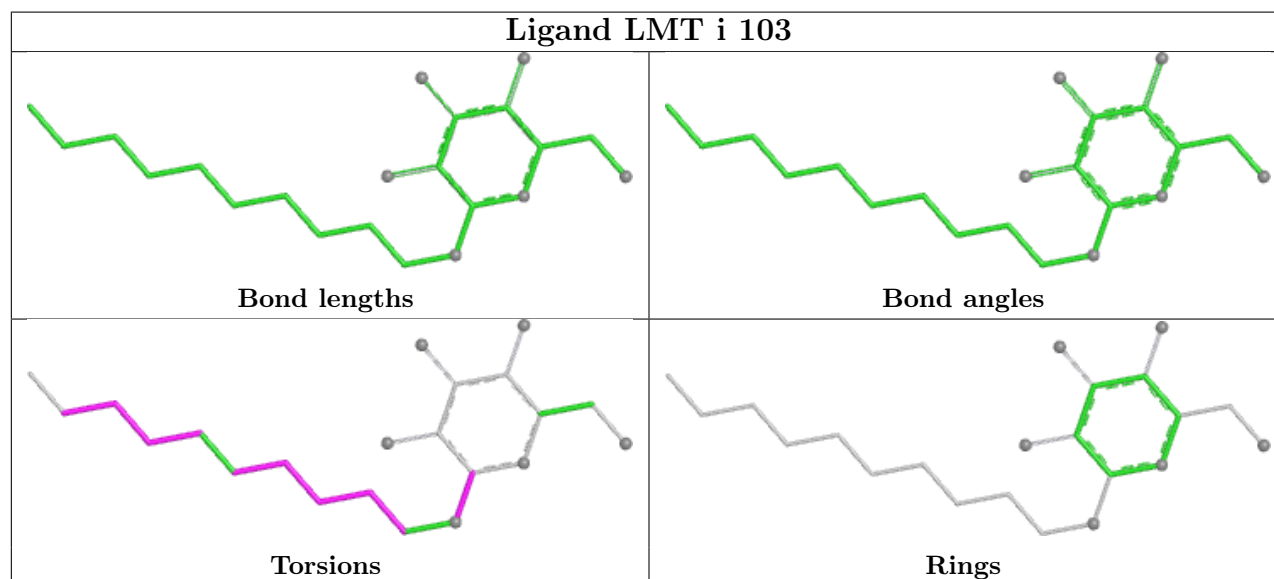
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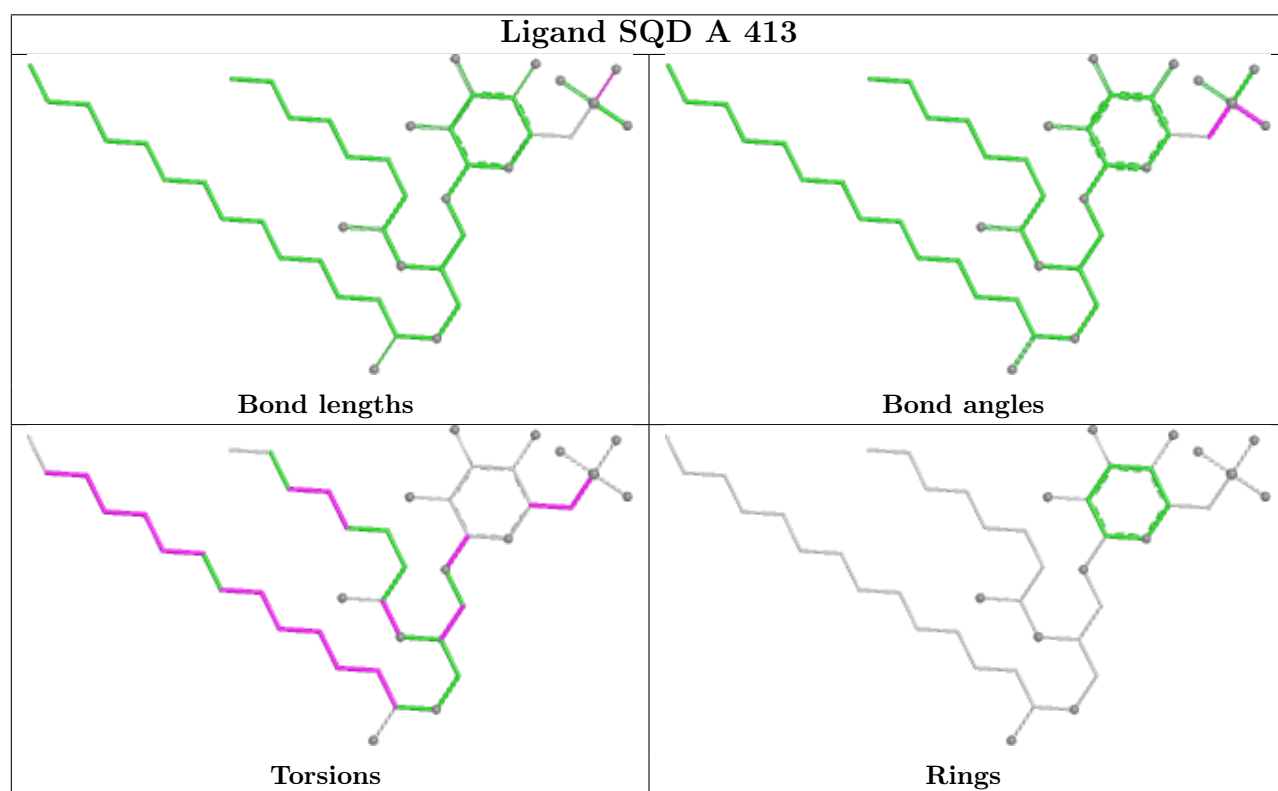
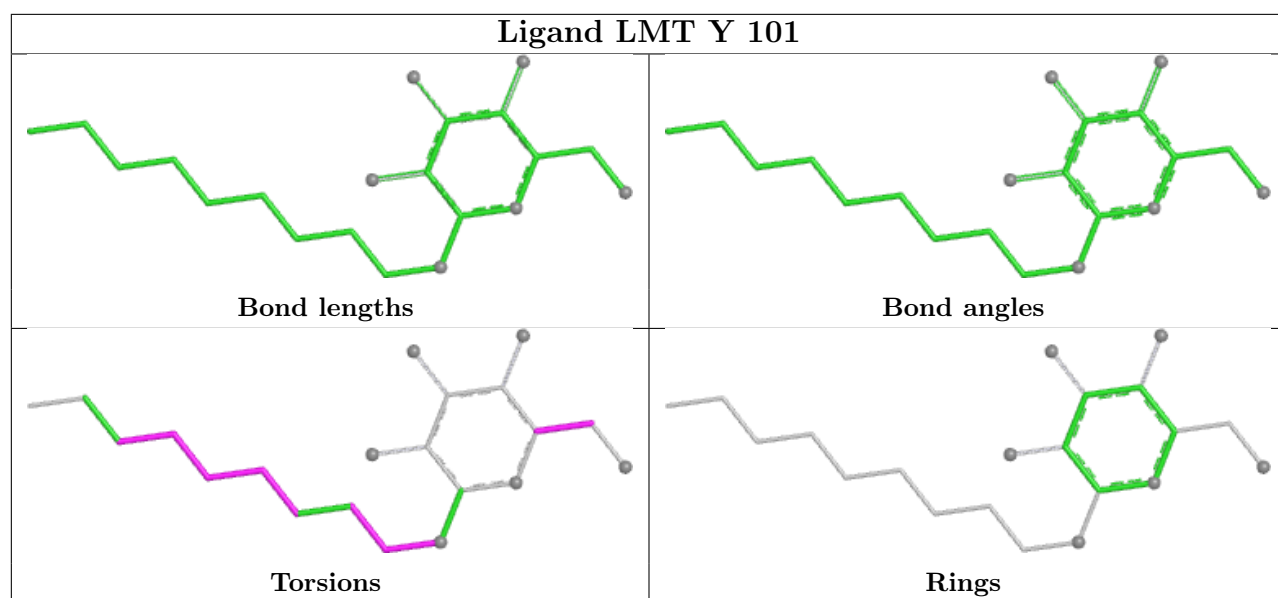
Mol	Chain	Res	Type	Atoms
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29	d	405	PL9	C13-C14-C16-C17
25	B	601	CLA	CAA-CBA-CGA-O1A
25	b	601	CLA	CAA-CBA-CGA-O1A
33	D	413	LHG	O9-C7-C8-C9
33	d	412	LHG	O9-C7-C8-C9
25	C	508	CLA	C3-C5-C6-C7
33	D	406	LHG	O8-C23-C24-C25
33	d	406	LHG	O8-C23-C24-C25
28	J	101	LMG	O10-C28-C29-C30
28	j	101	LMG	O10-C28-C29-C30

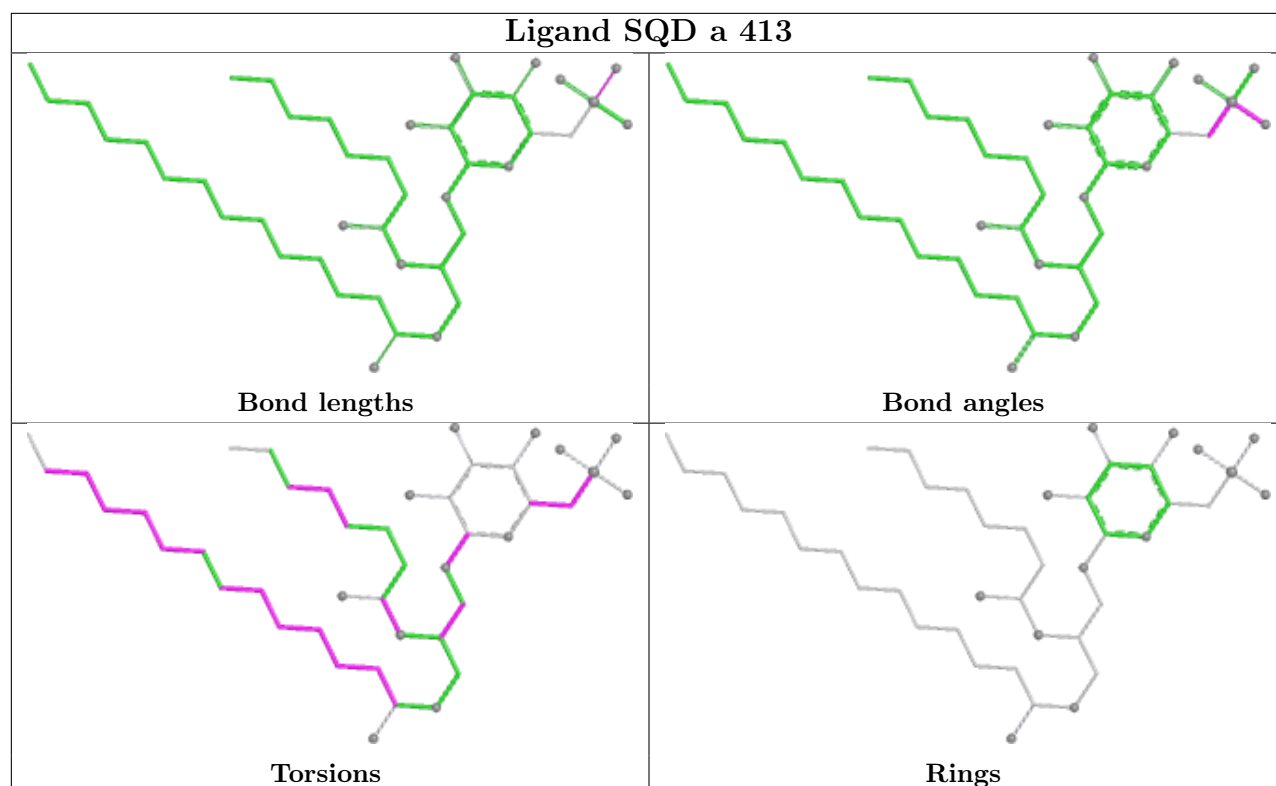
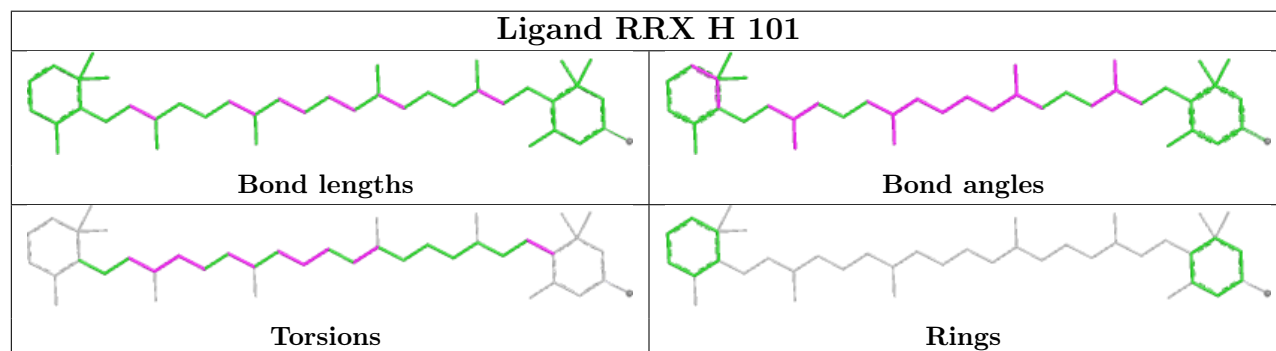
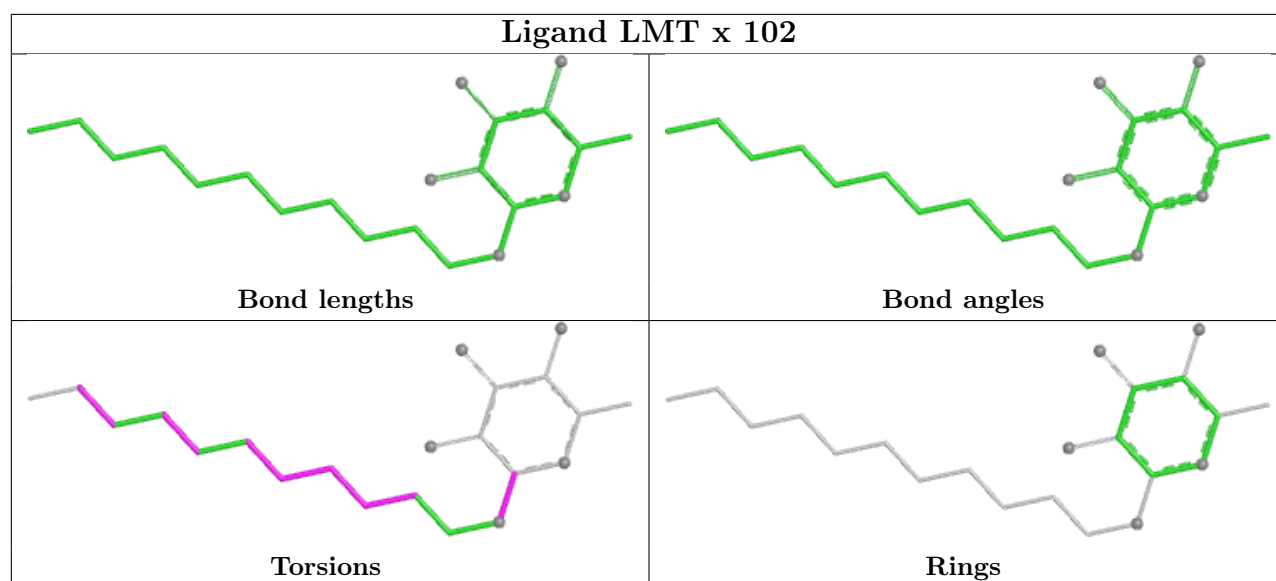
There are no ring outliers.

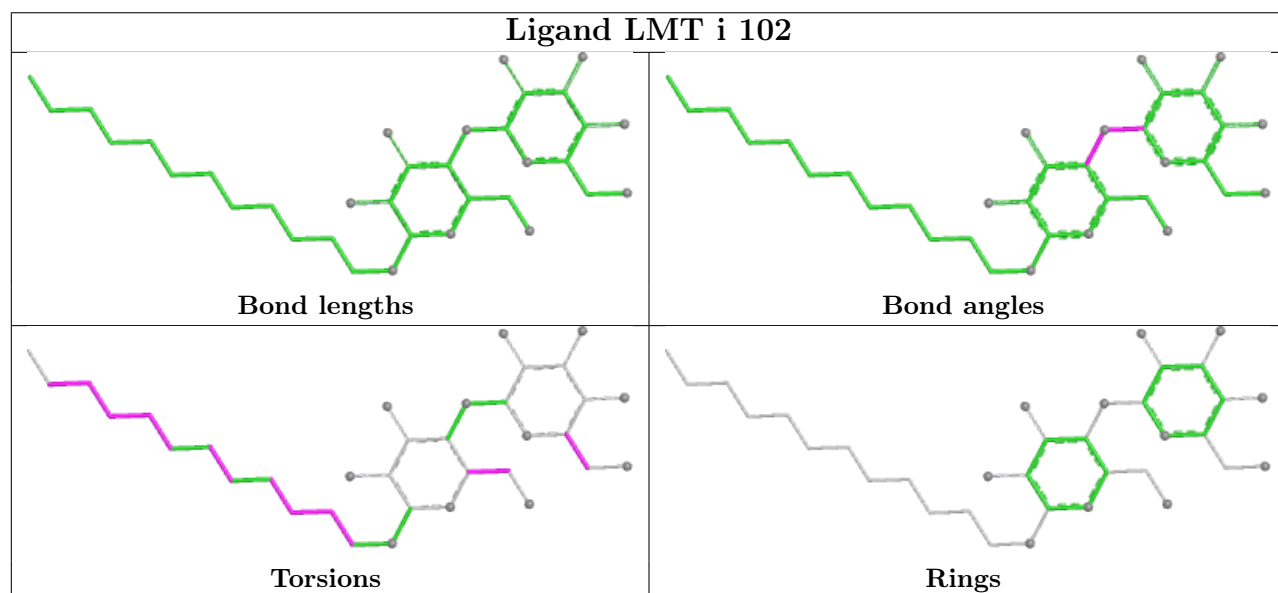
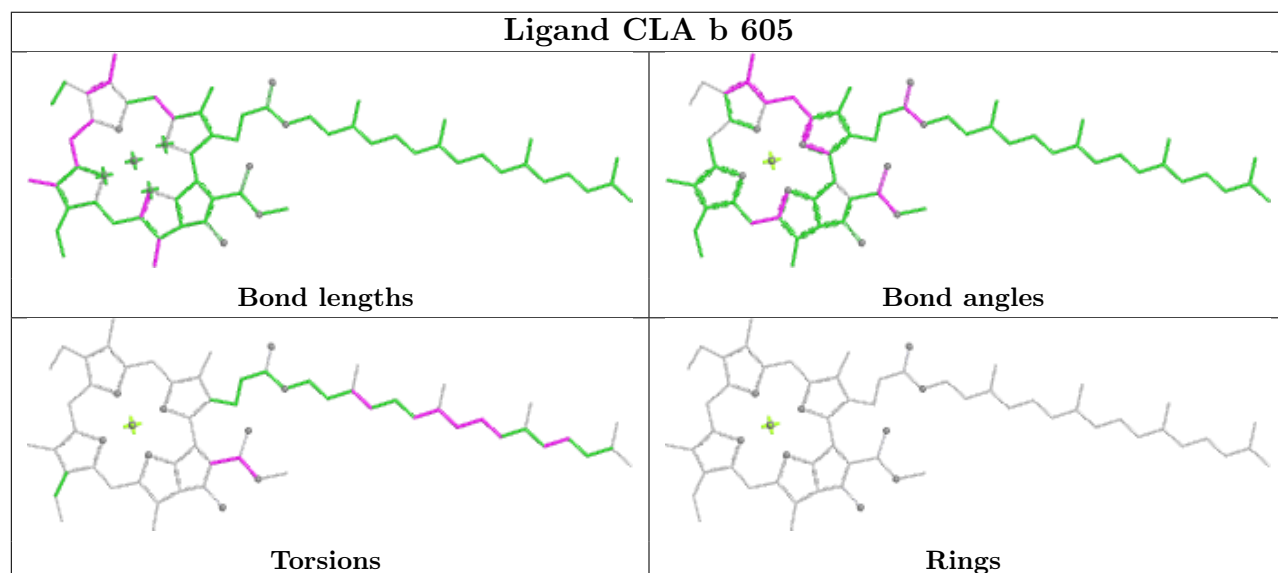
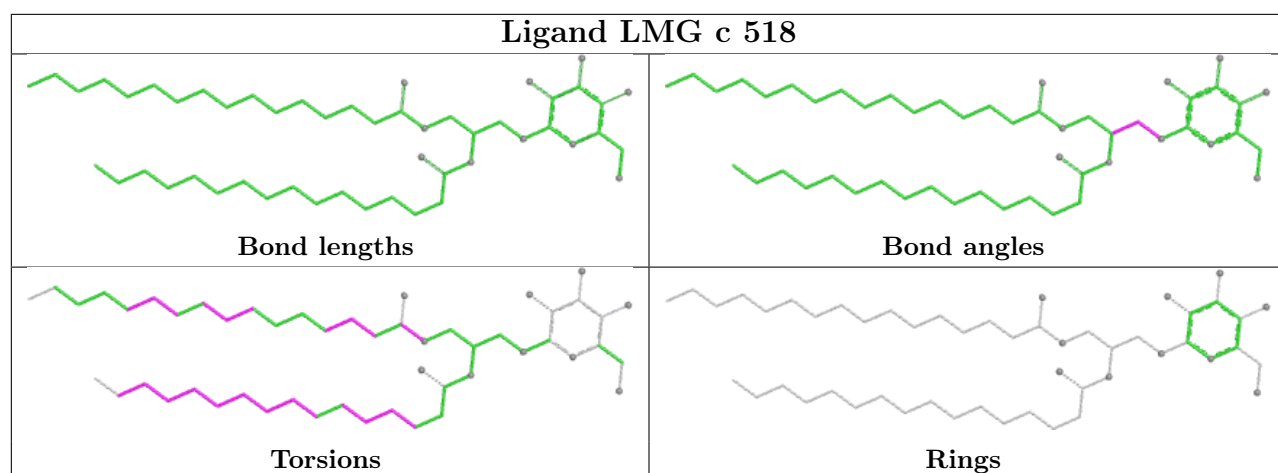
No monomer is involved in short contacts.

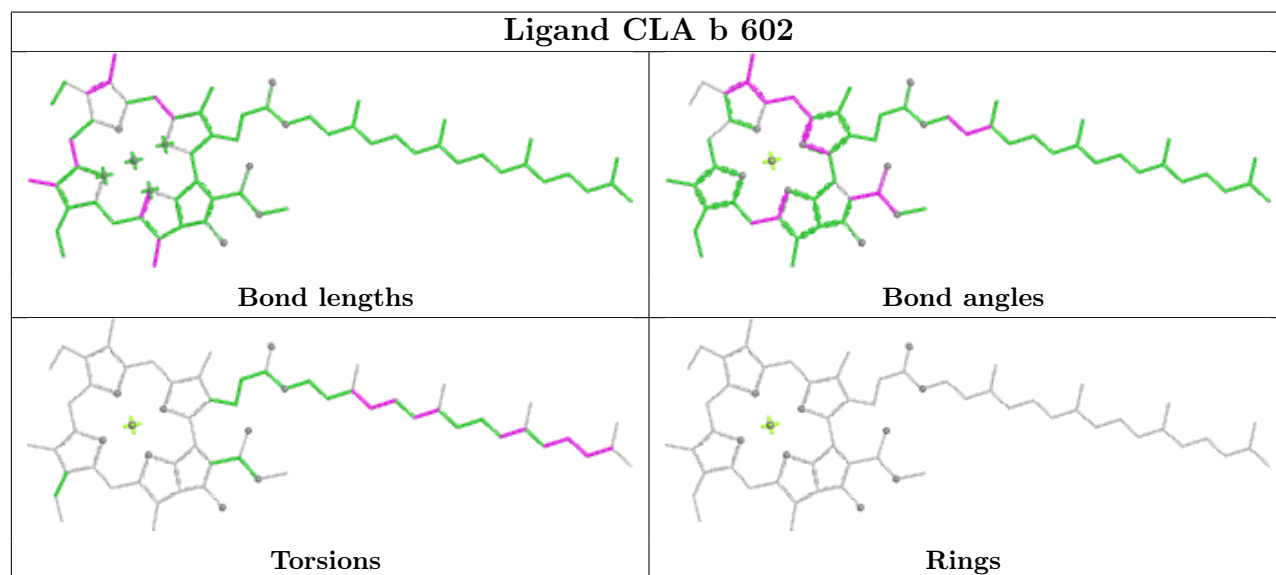
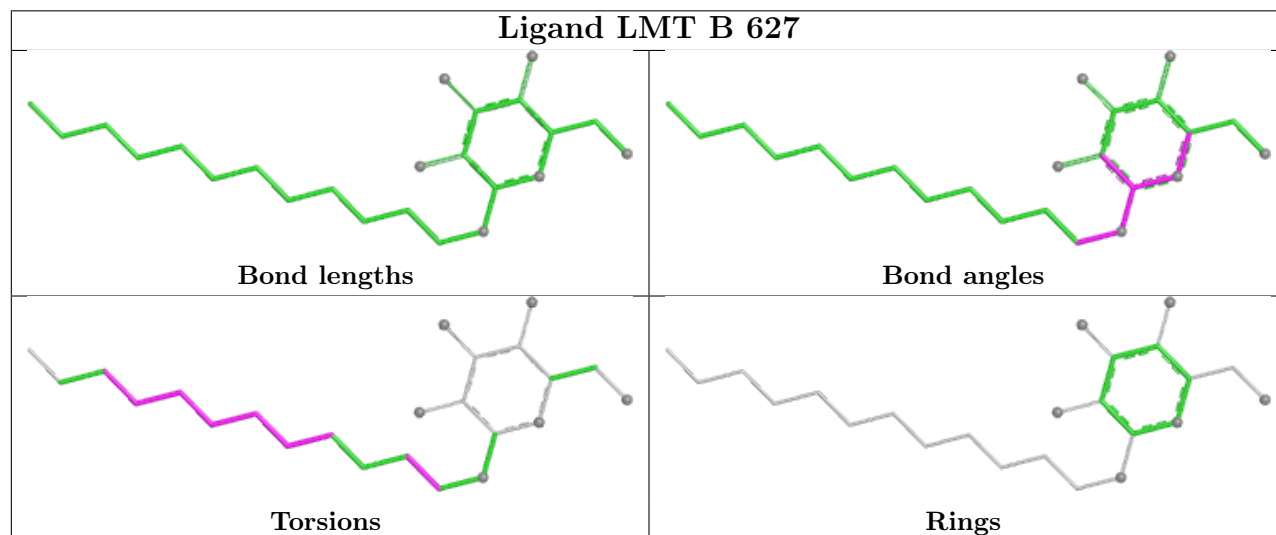
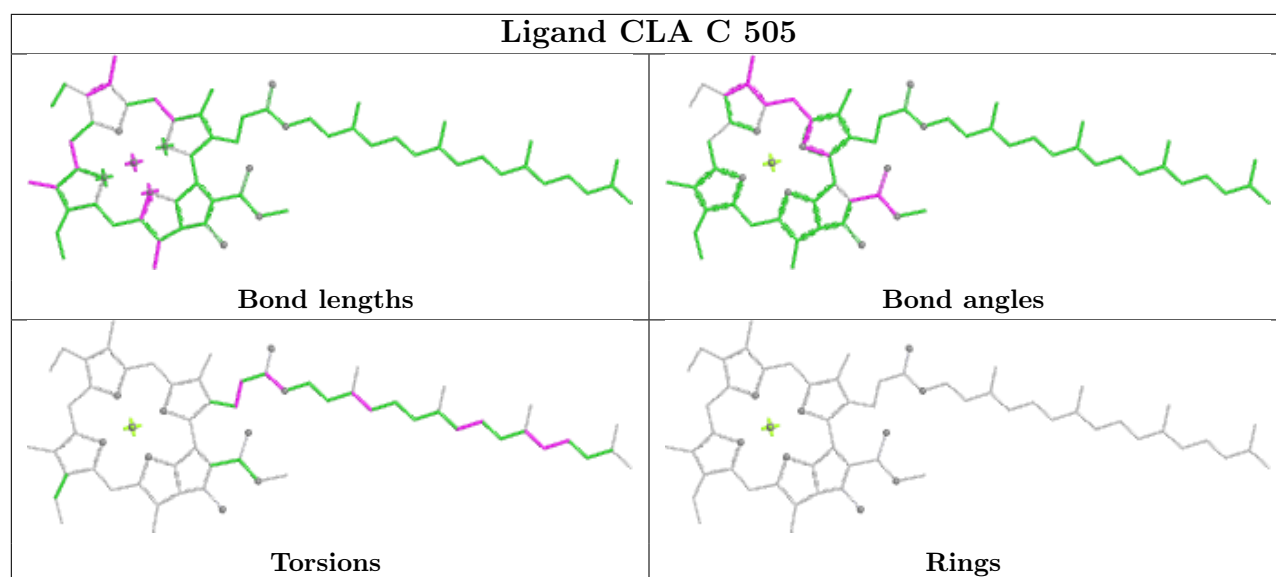
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

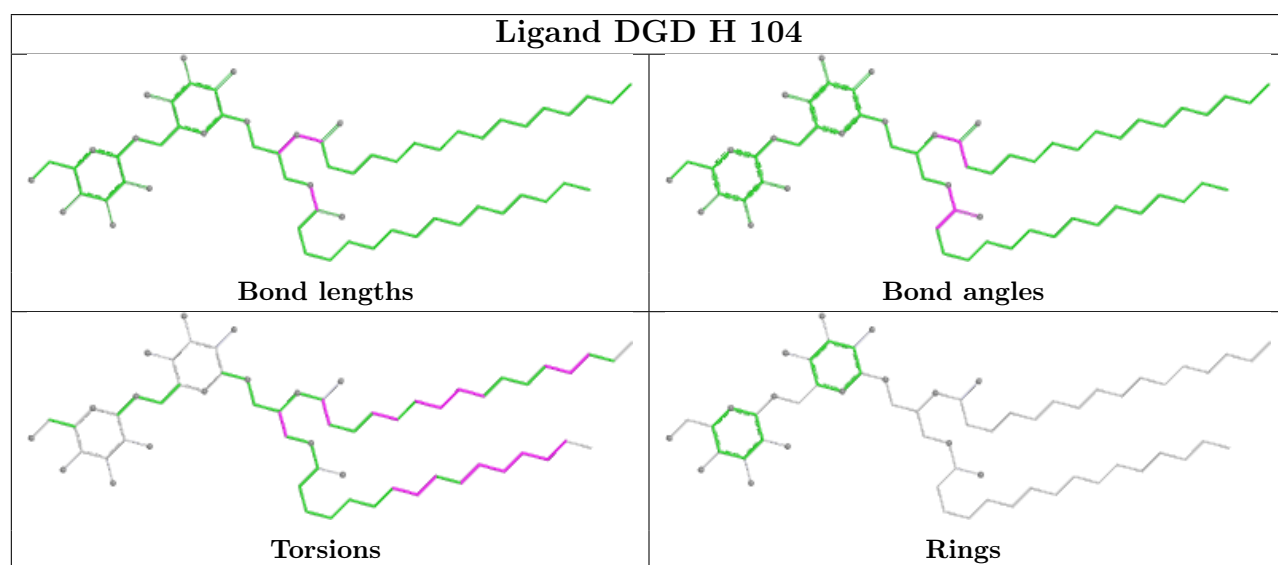
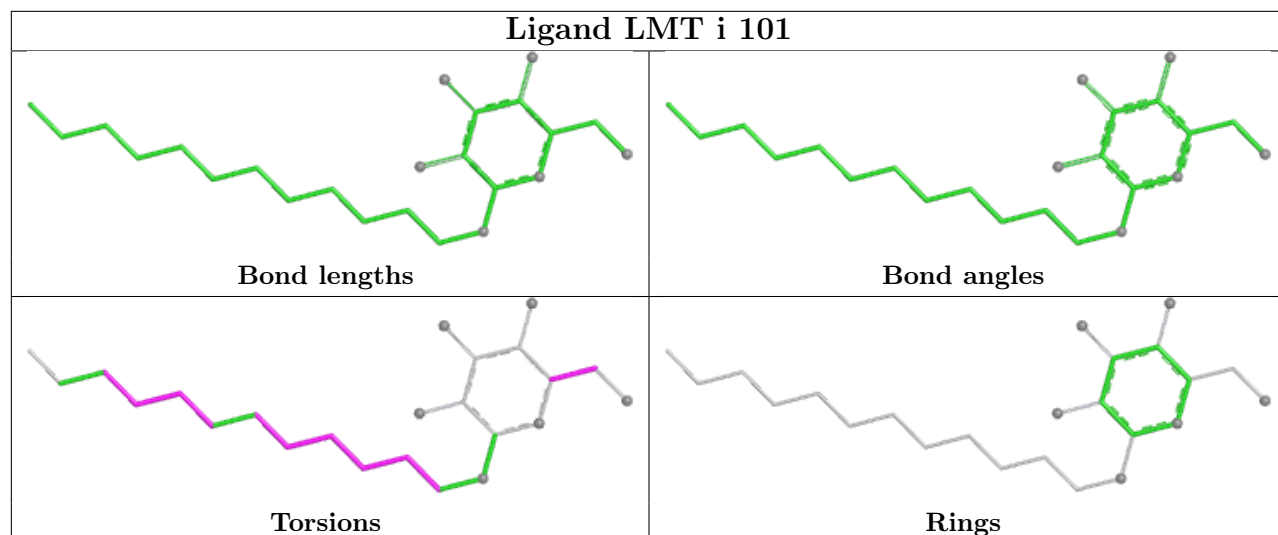


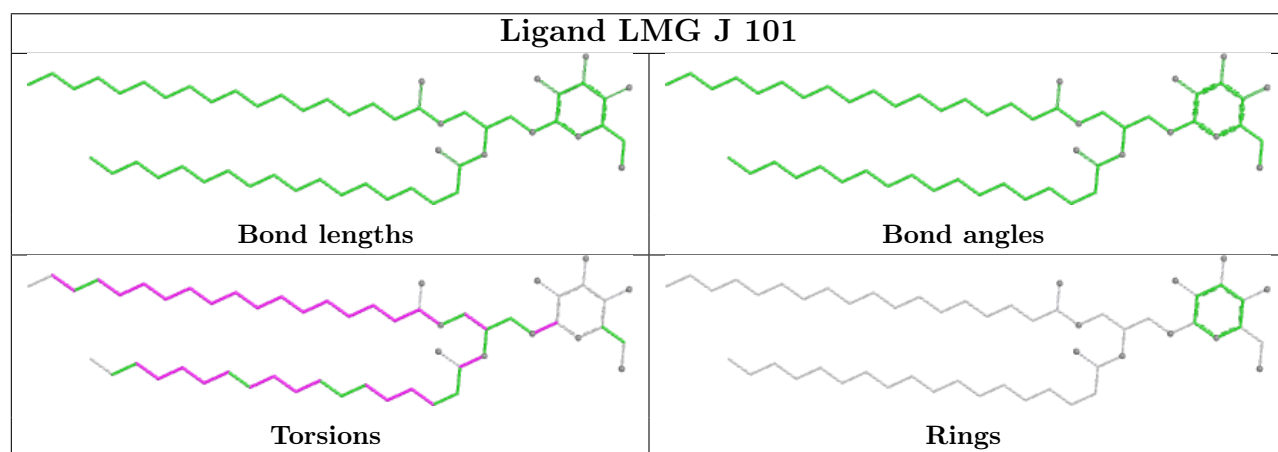
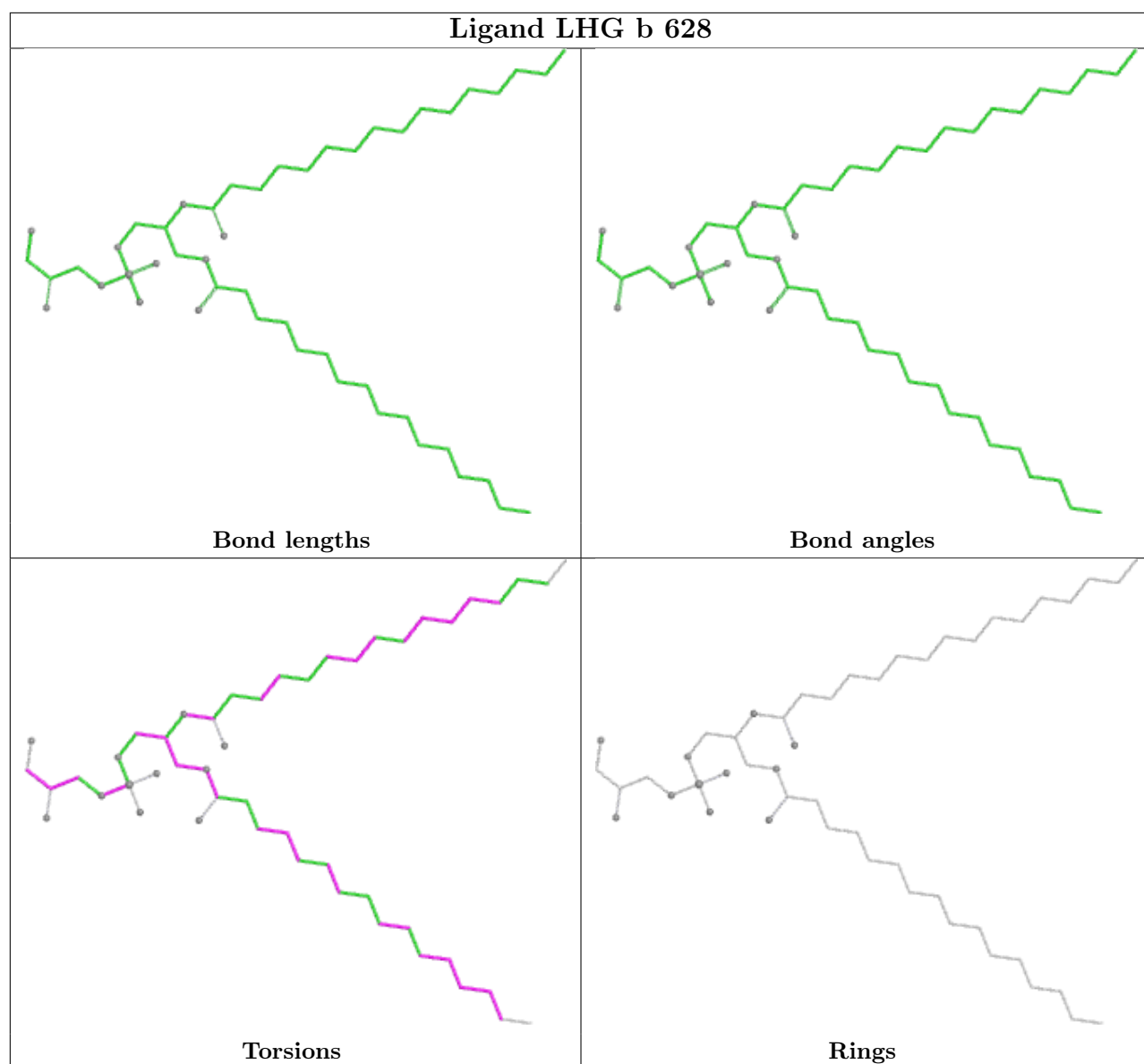


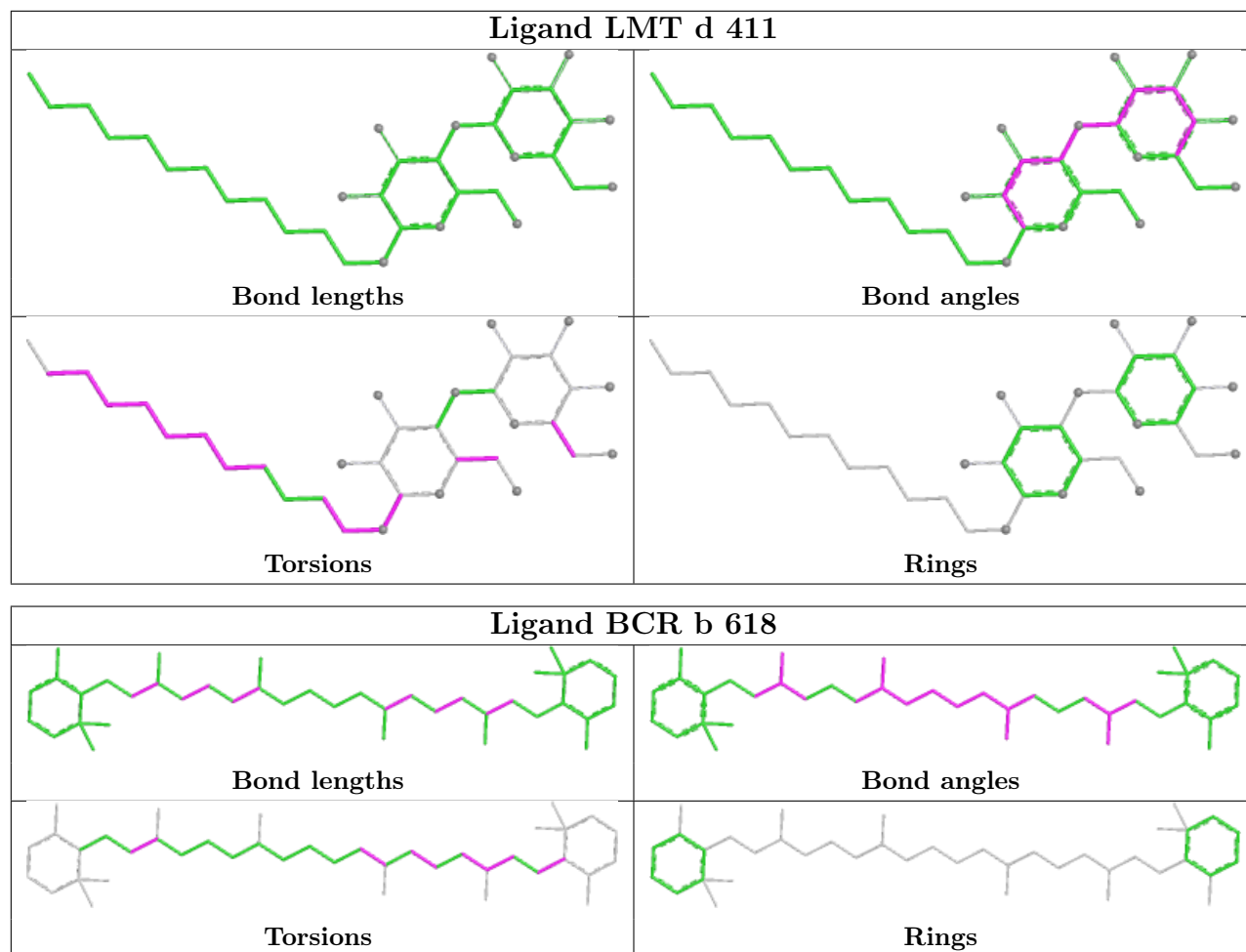


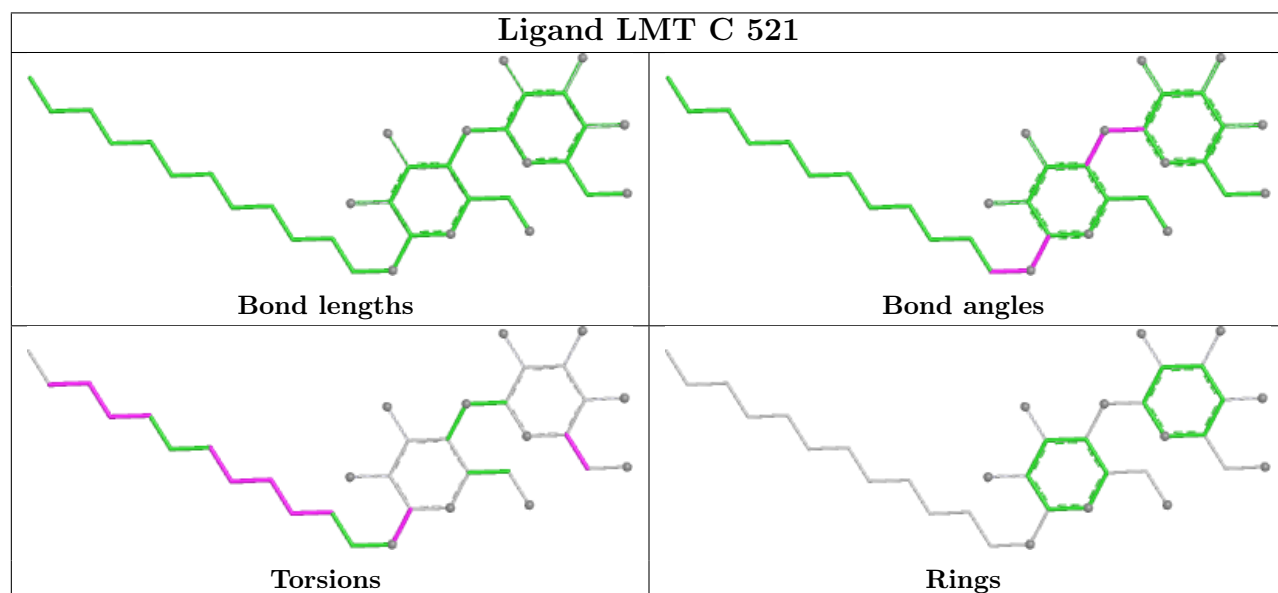
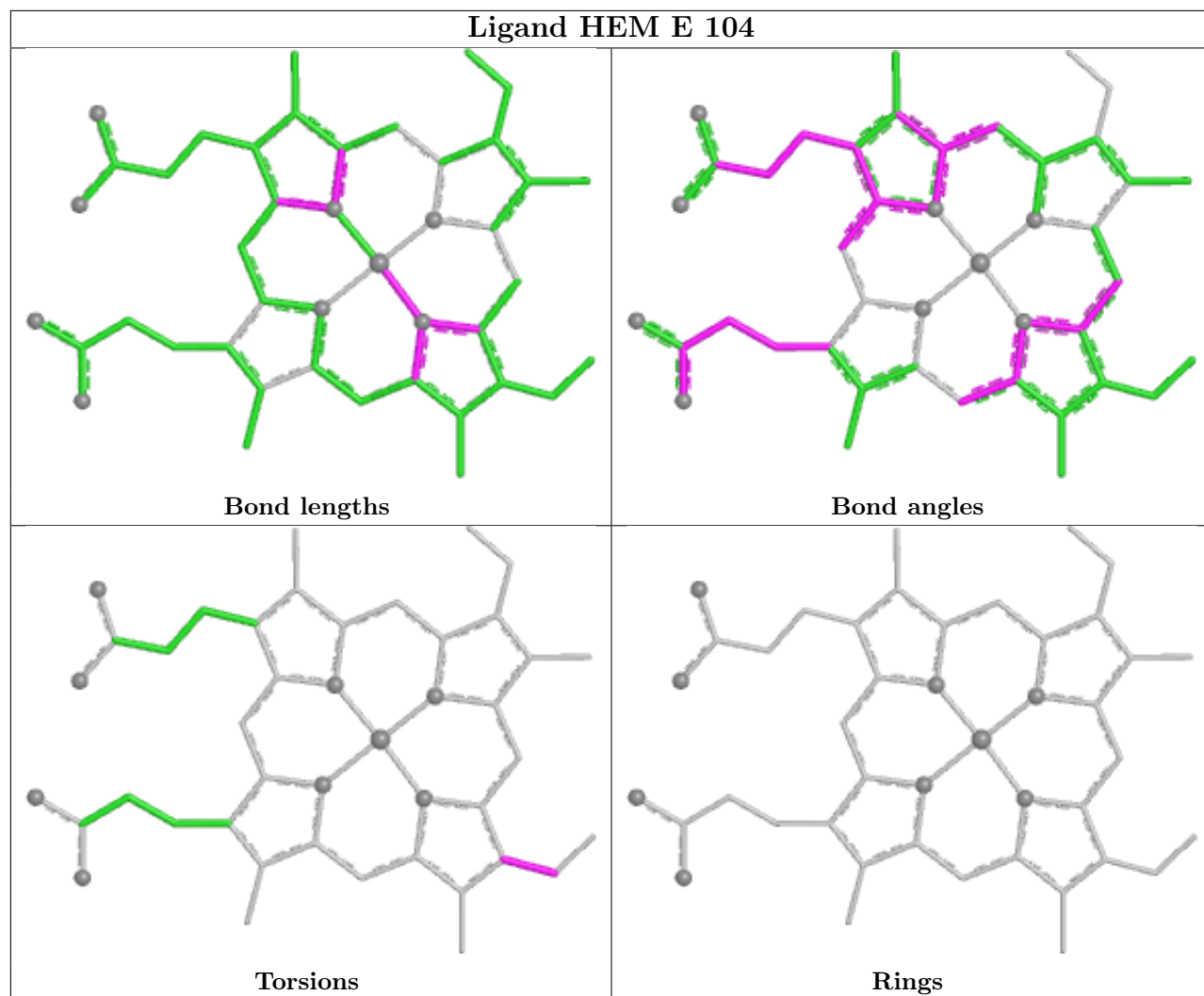


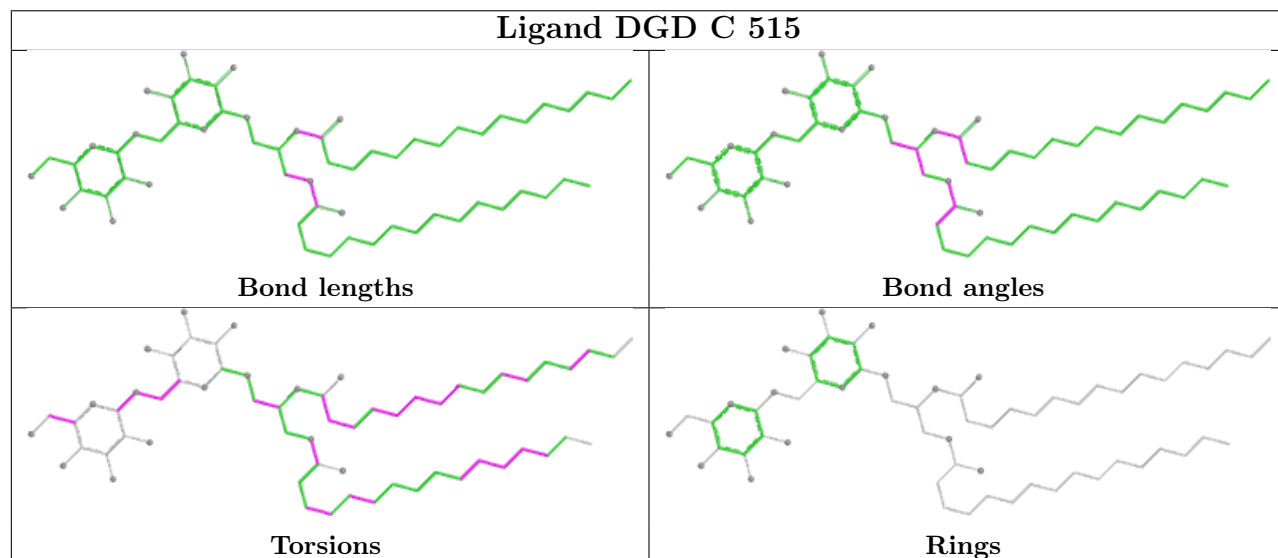
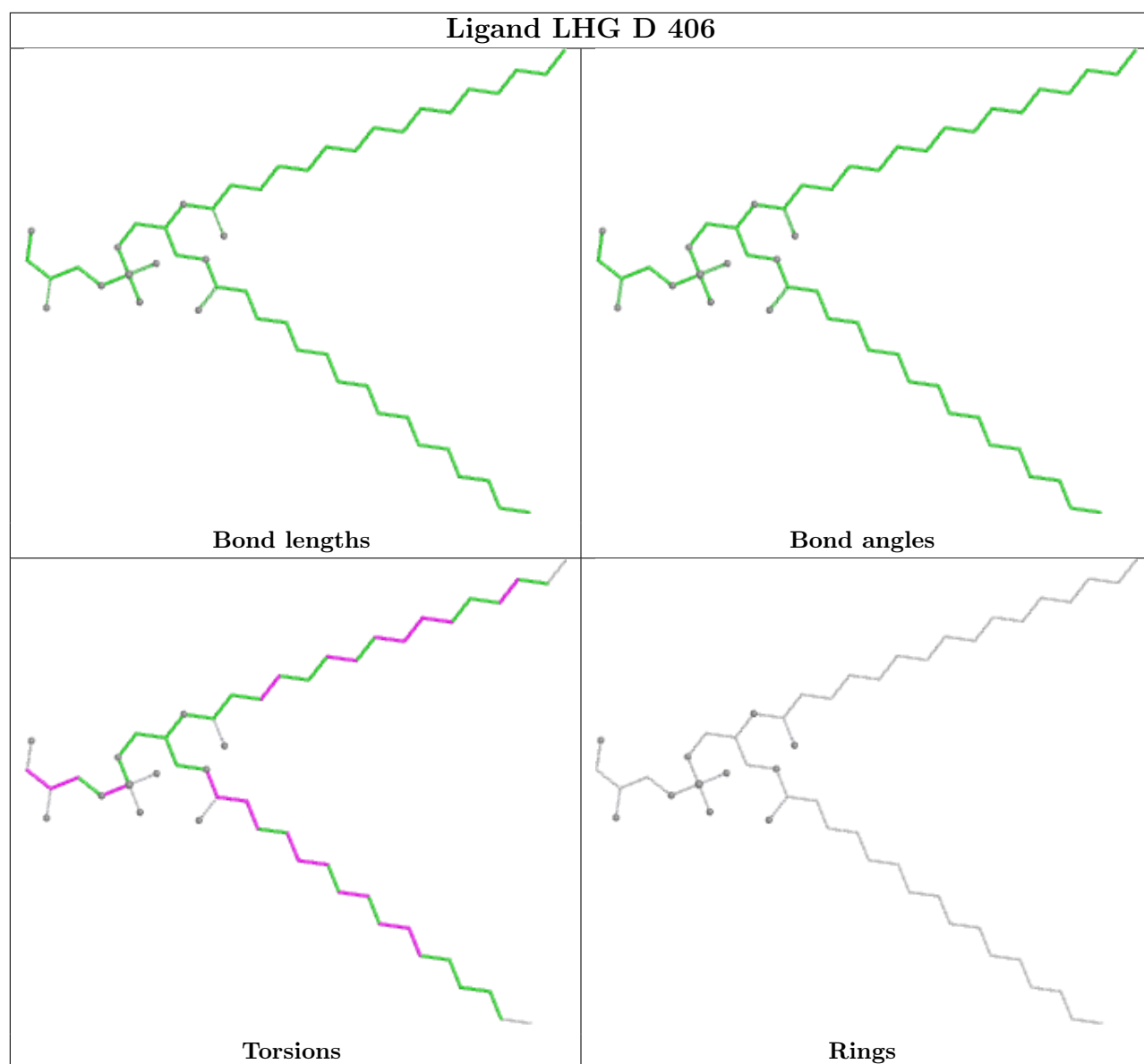


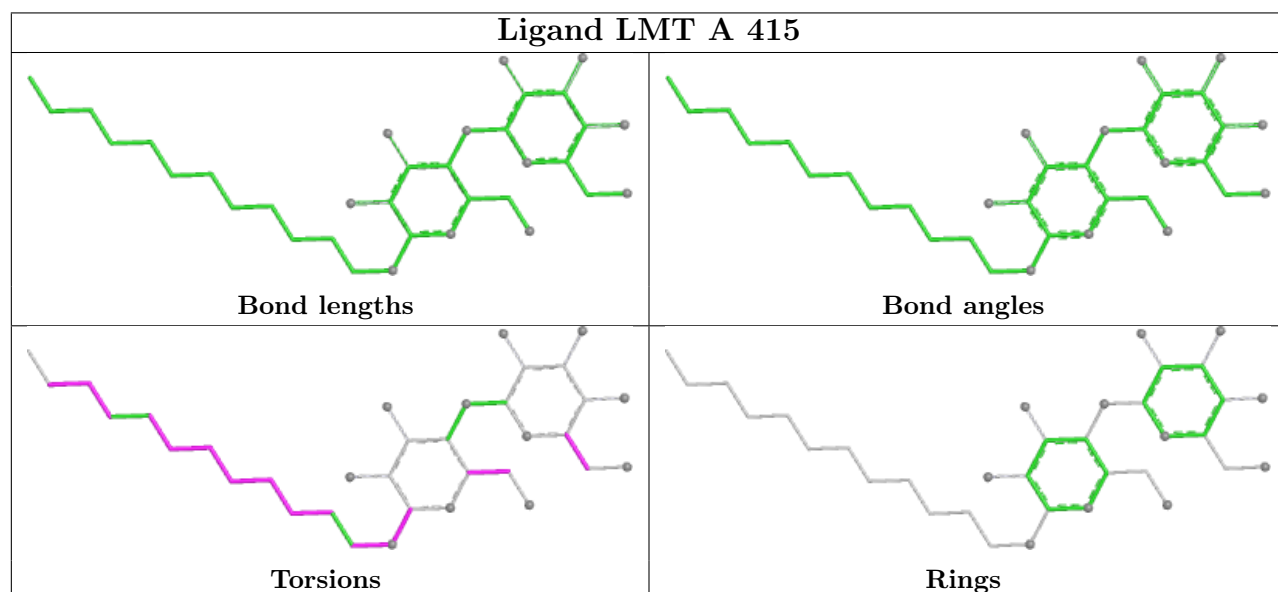
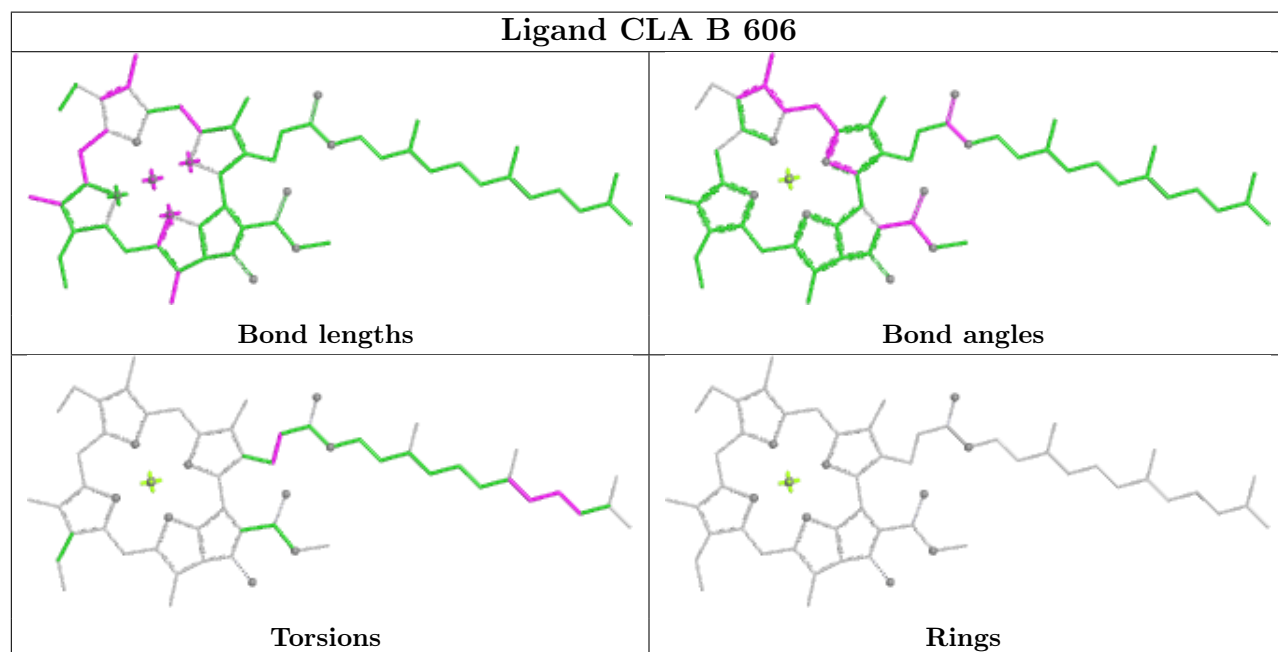
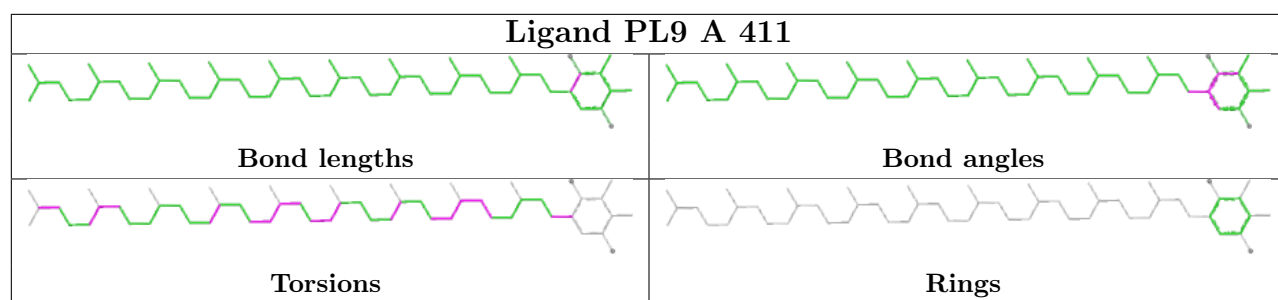


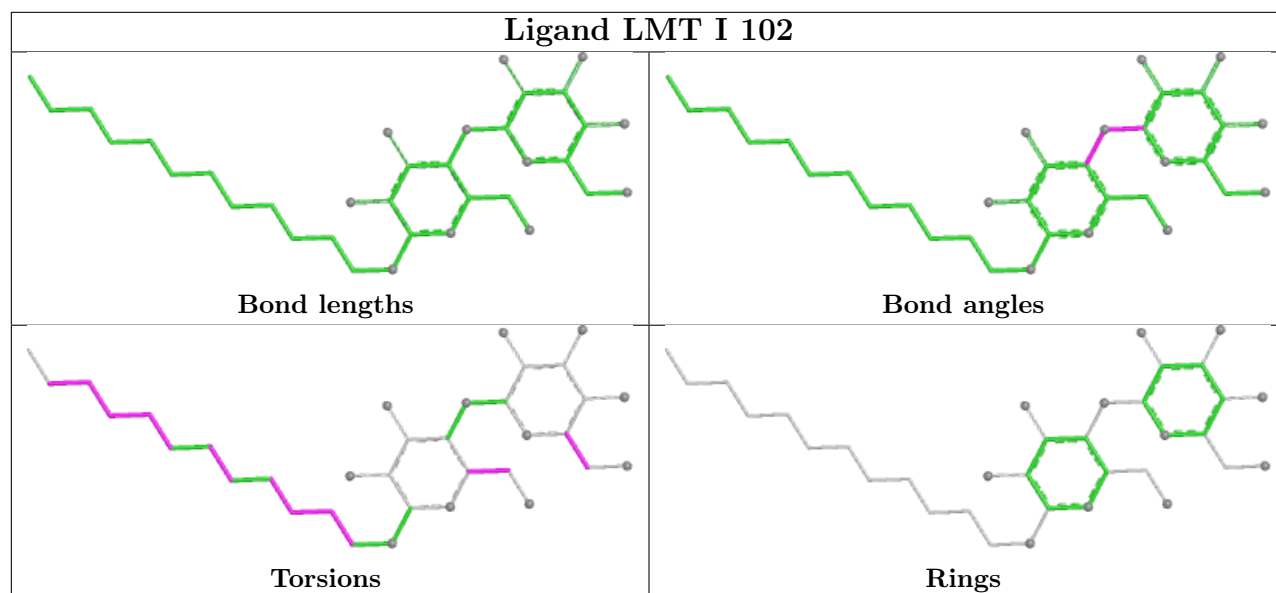
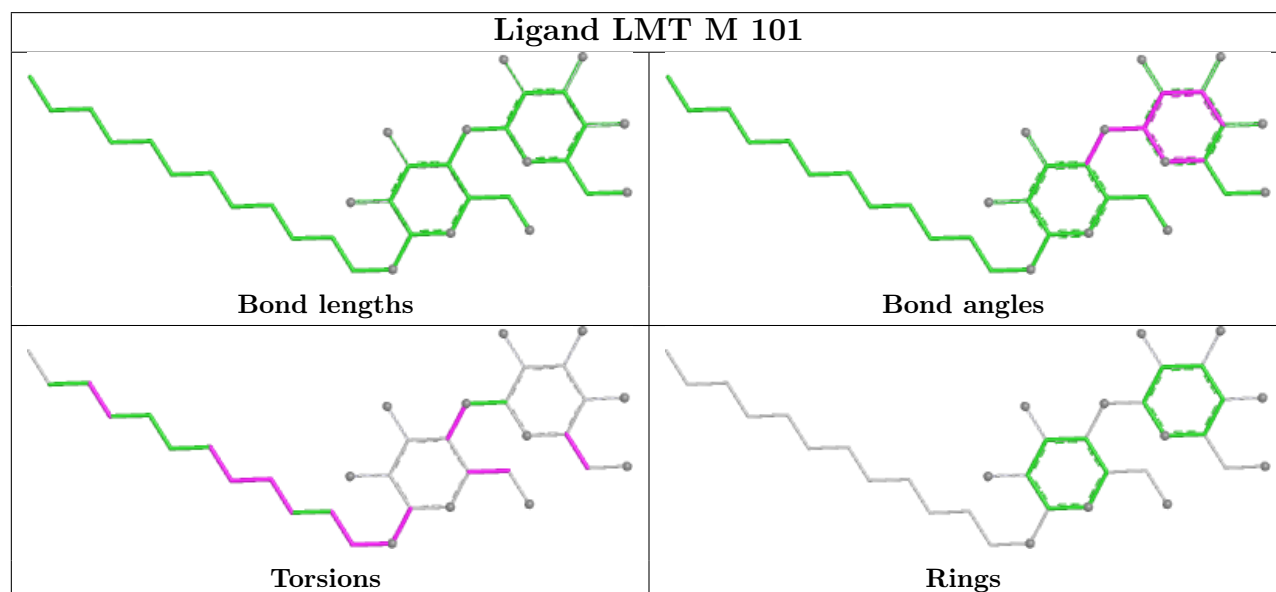
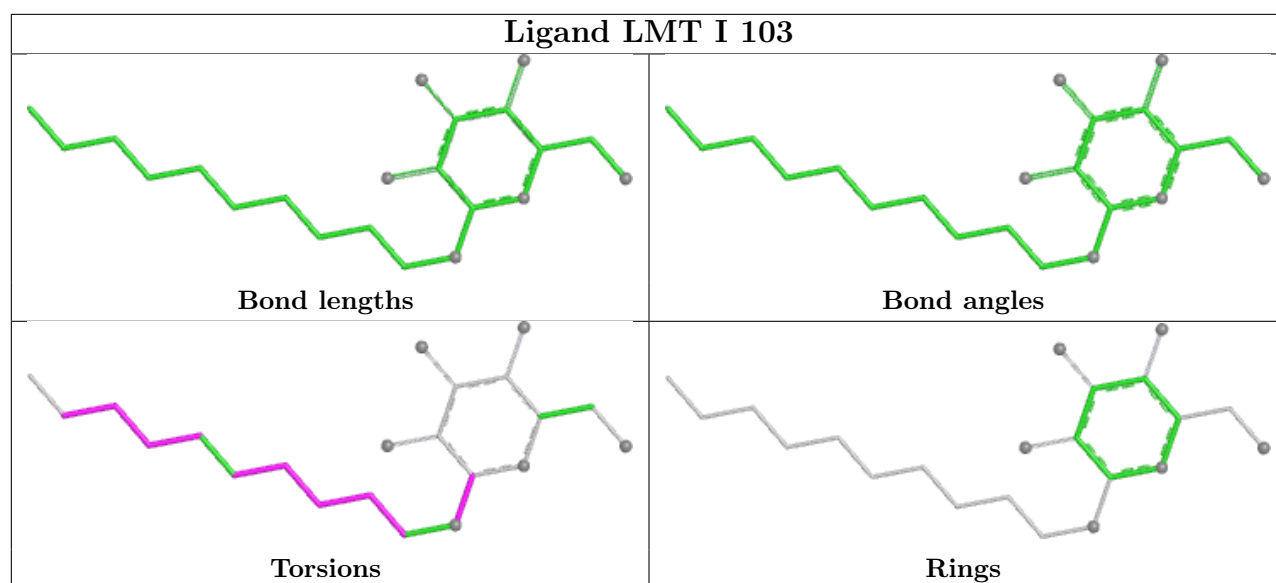


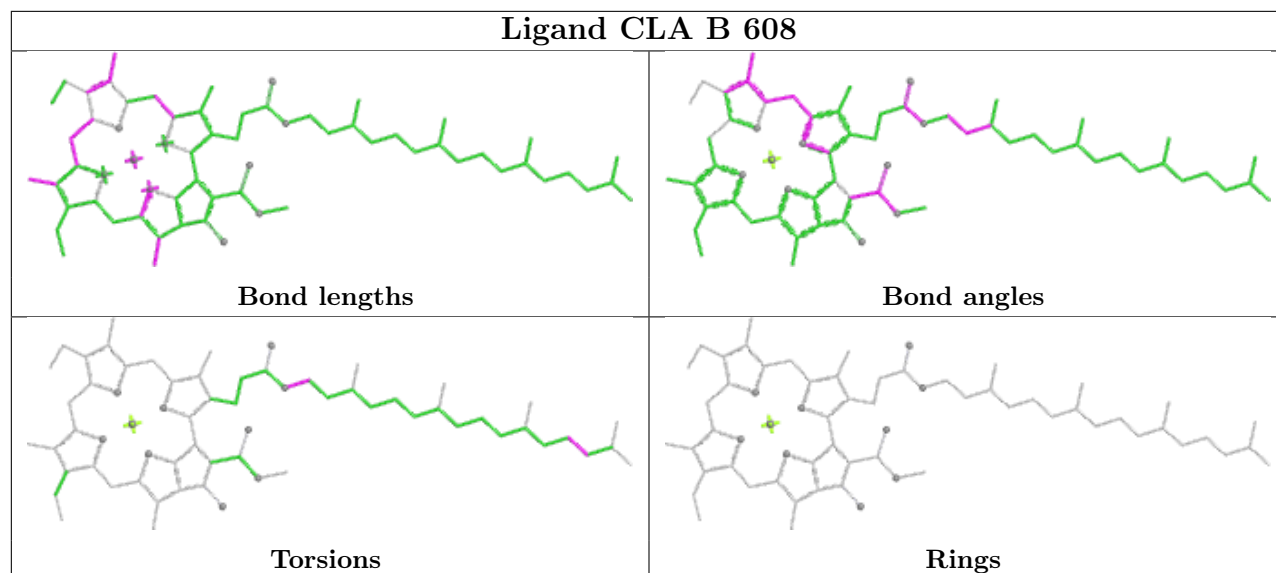
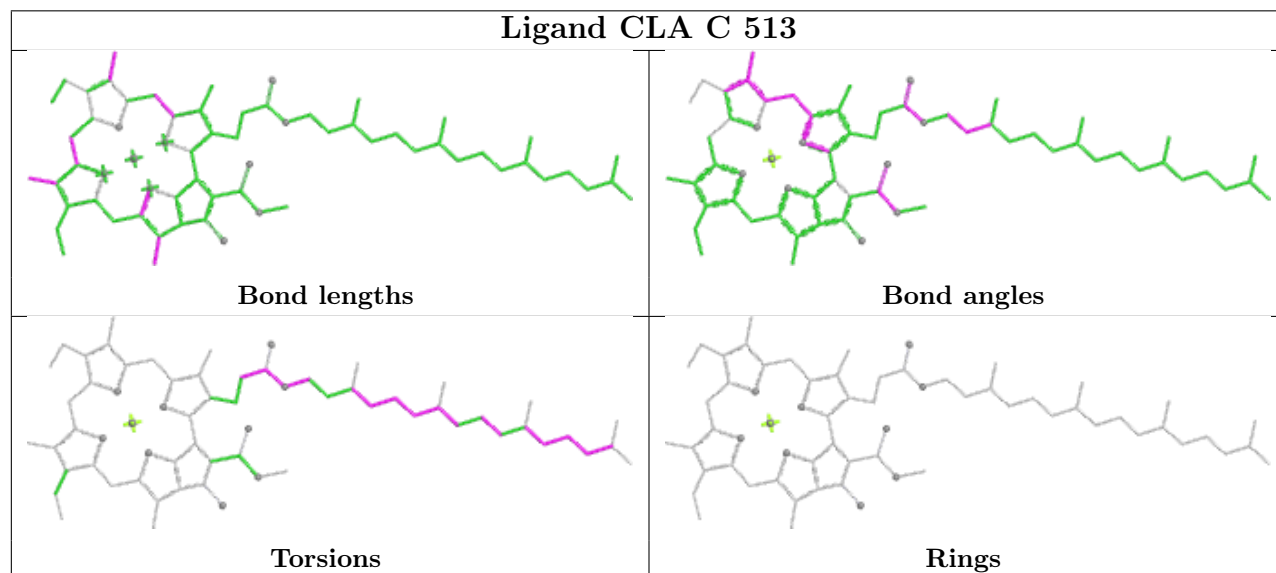
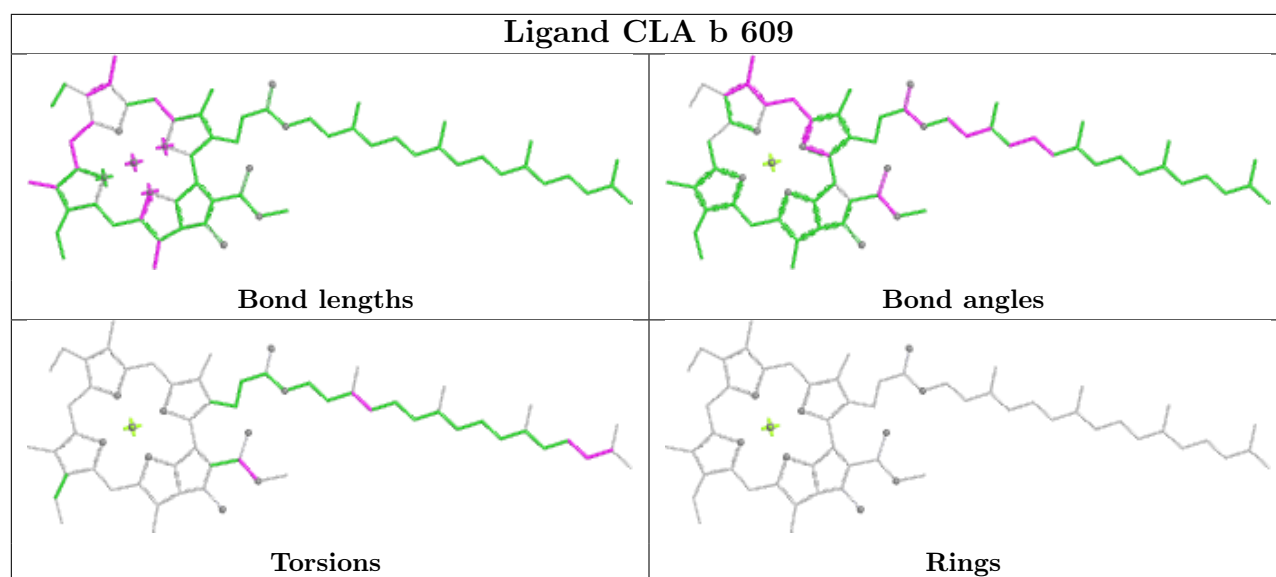


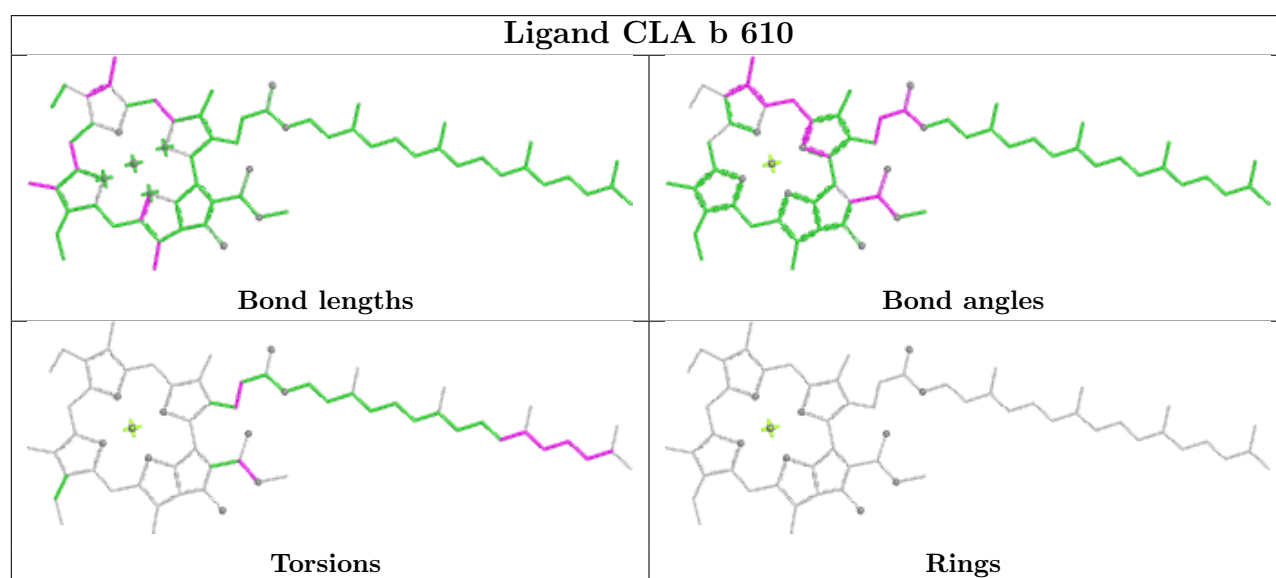
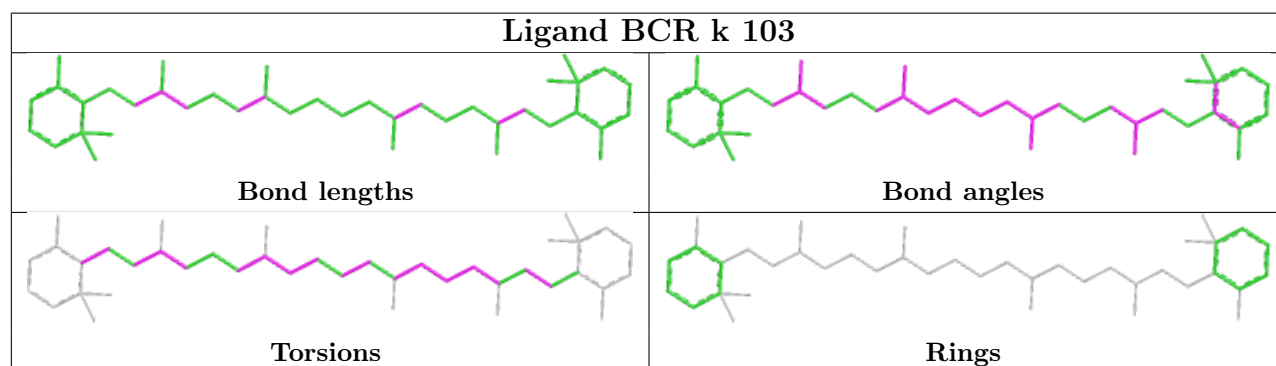
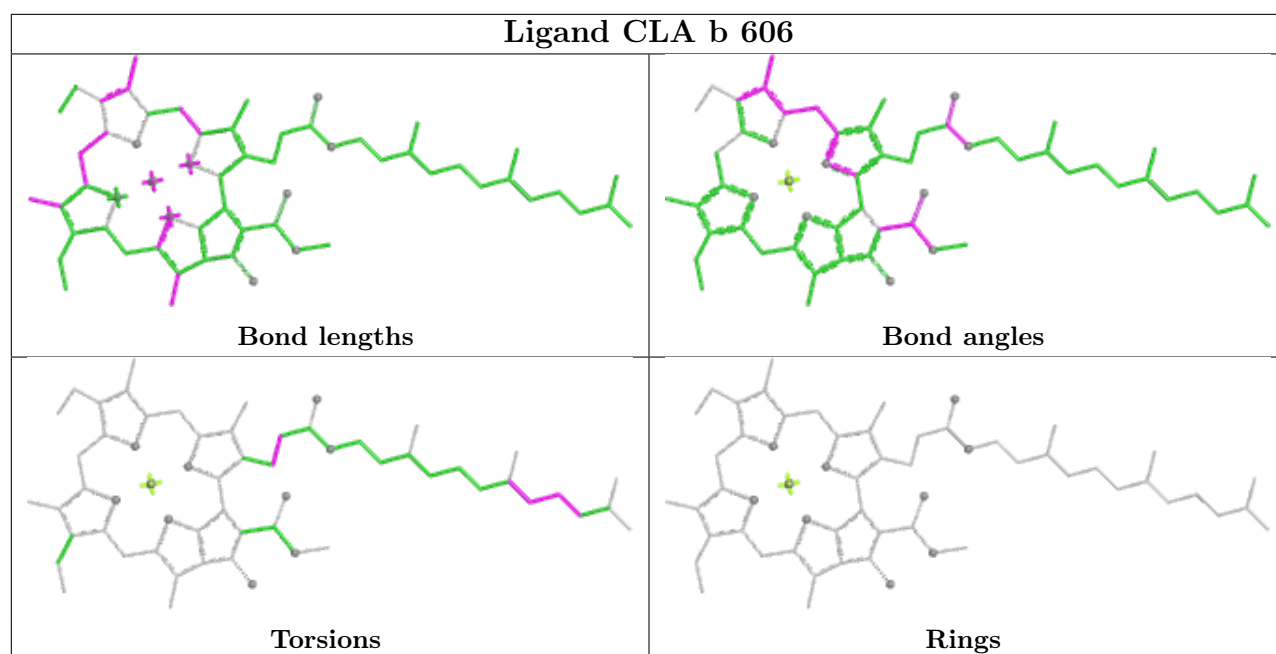


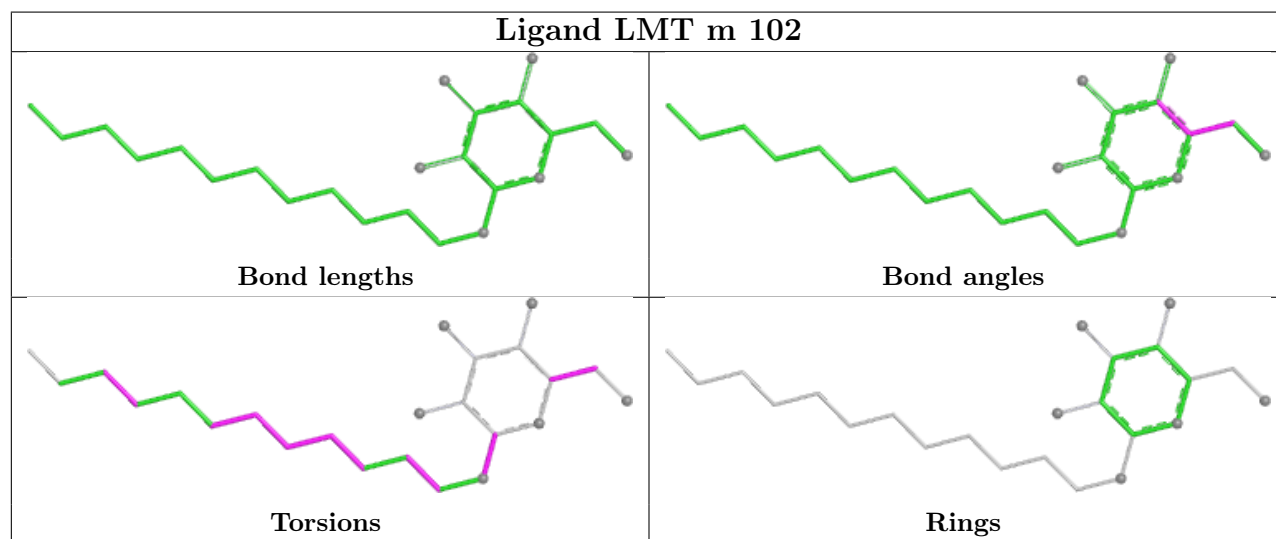
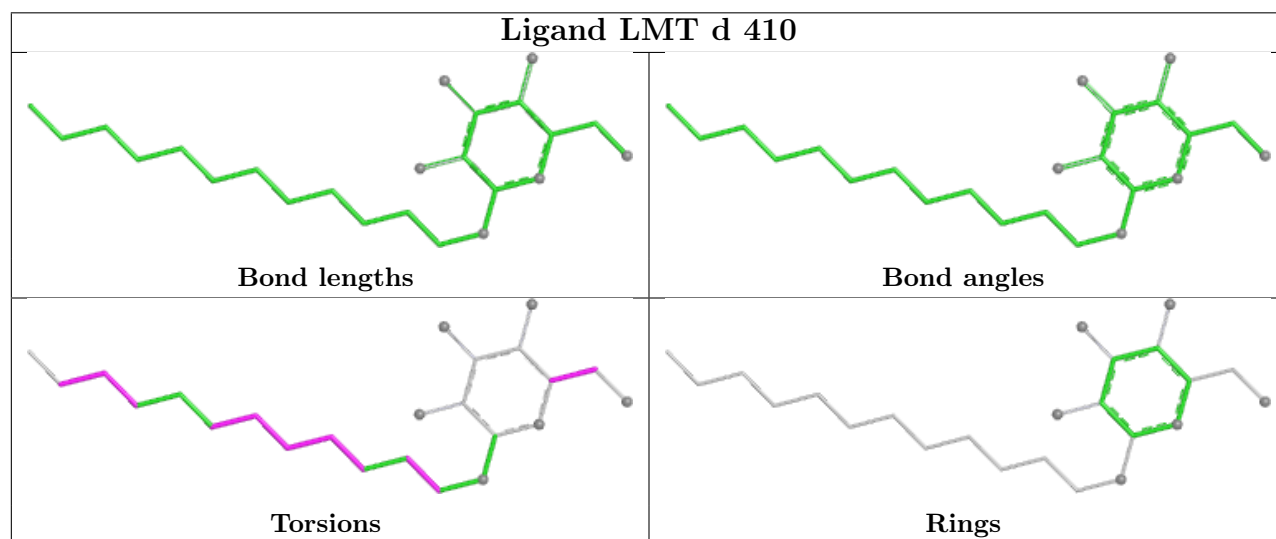
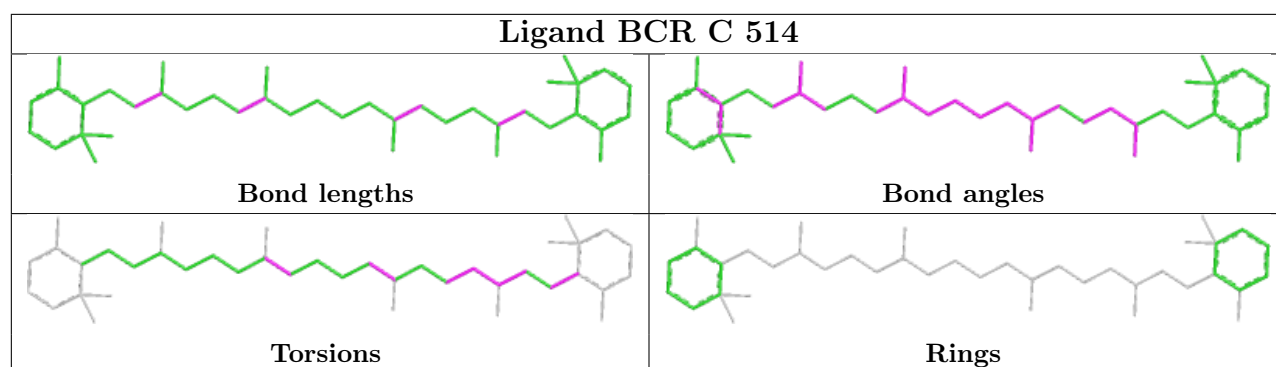


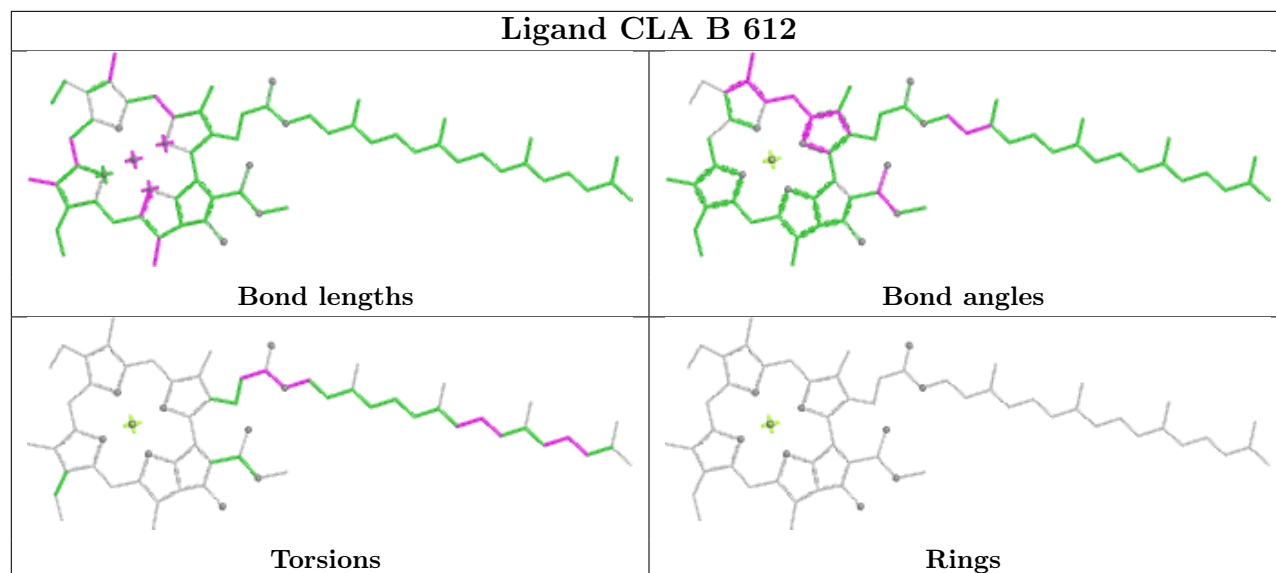
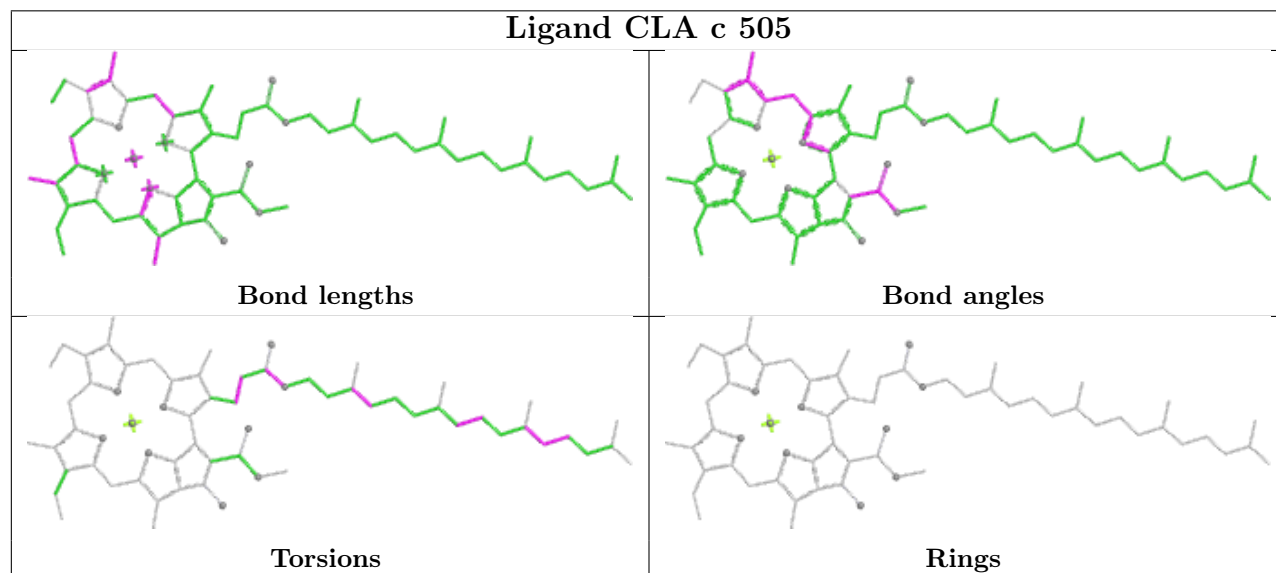
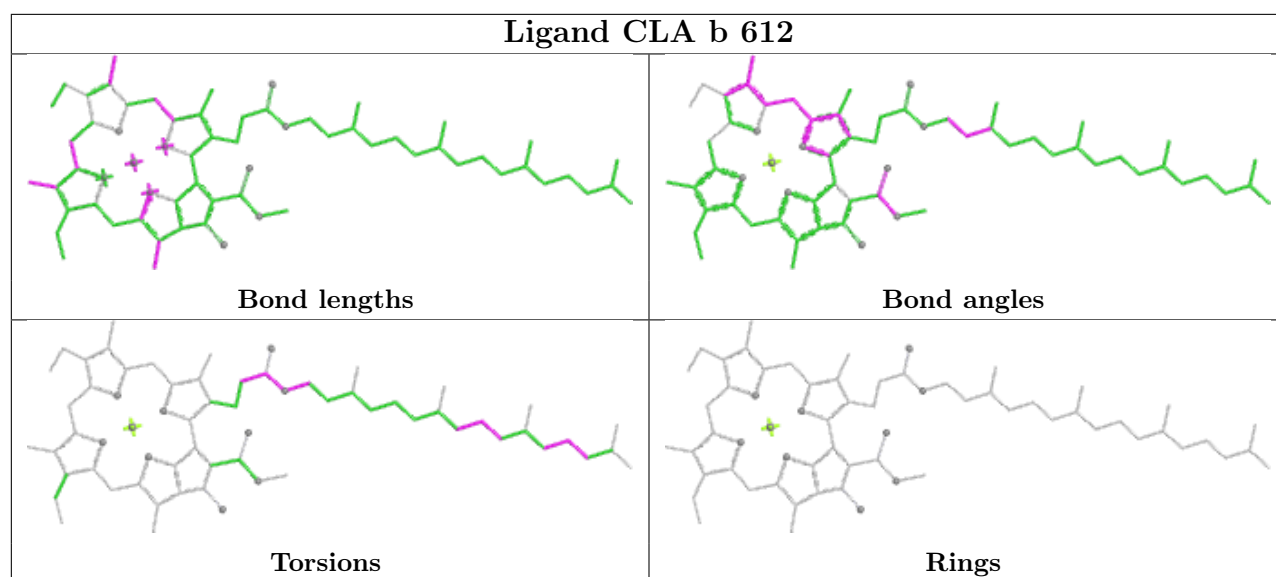


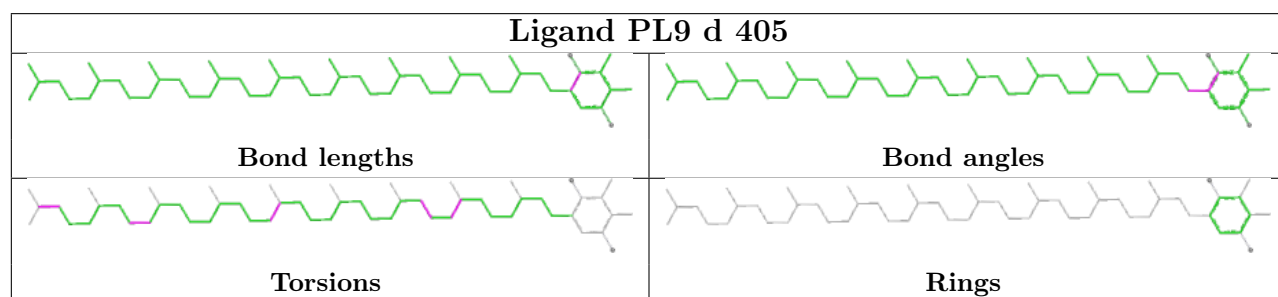
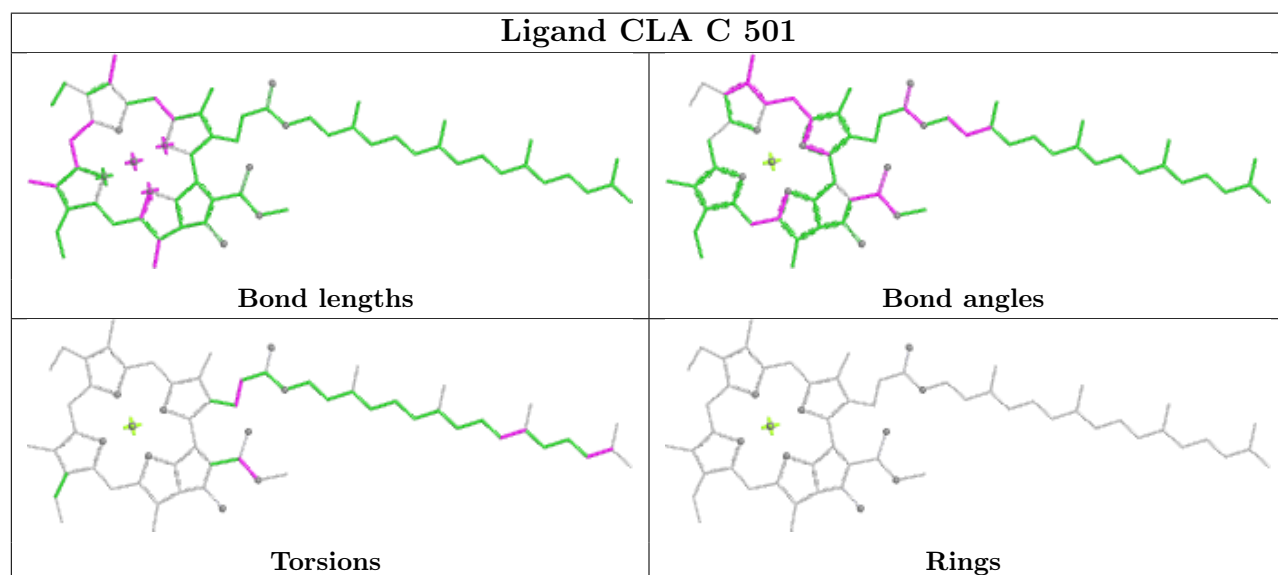
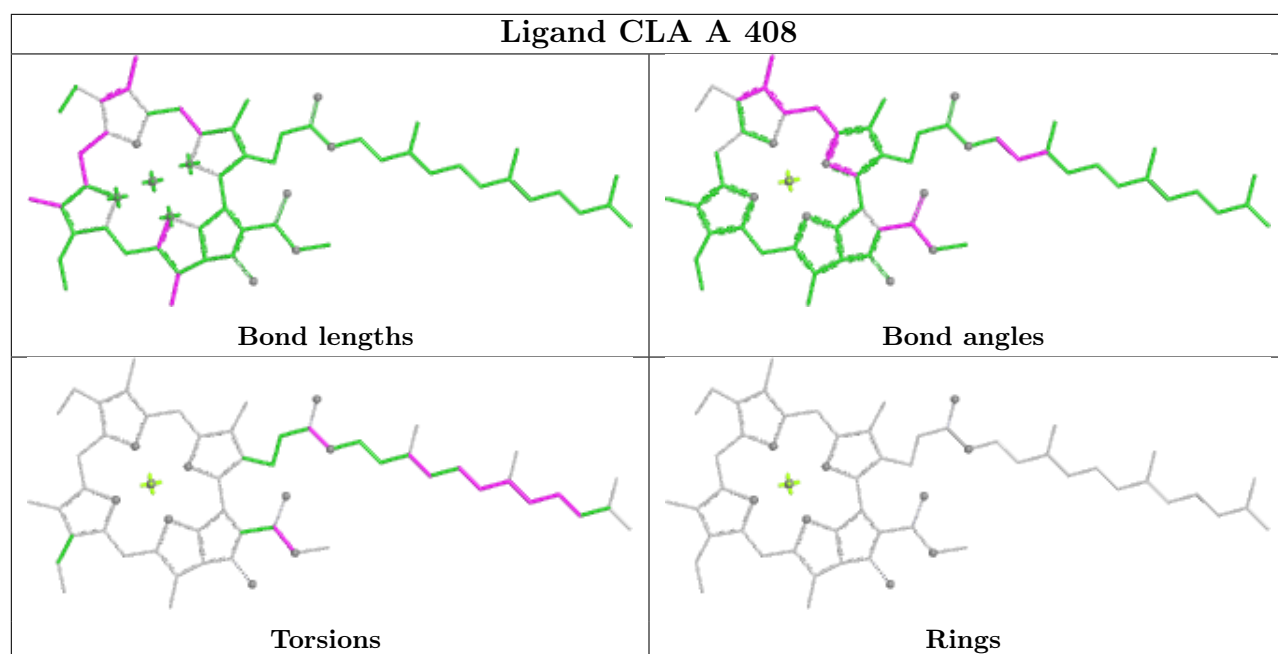


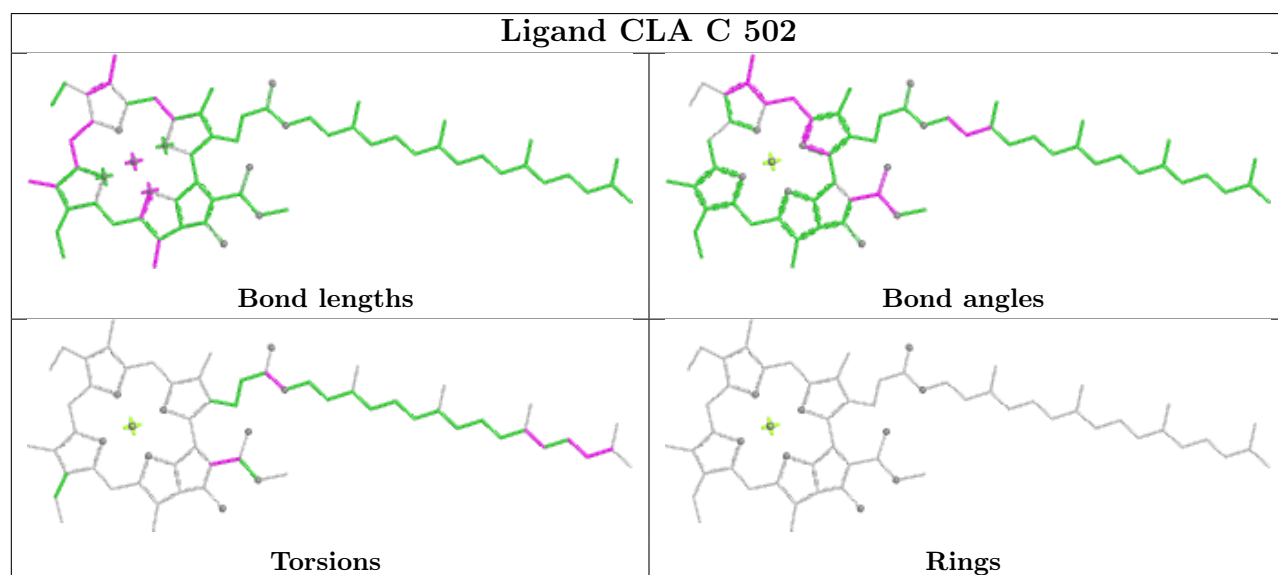
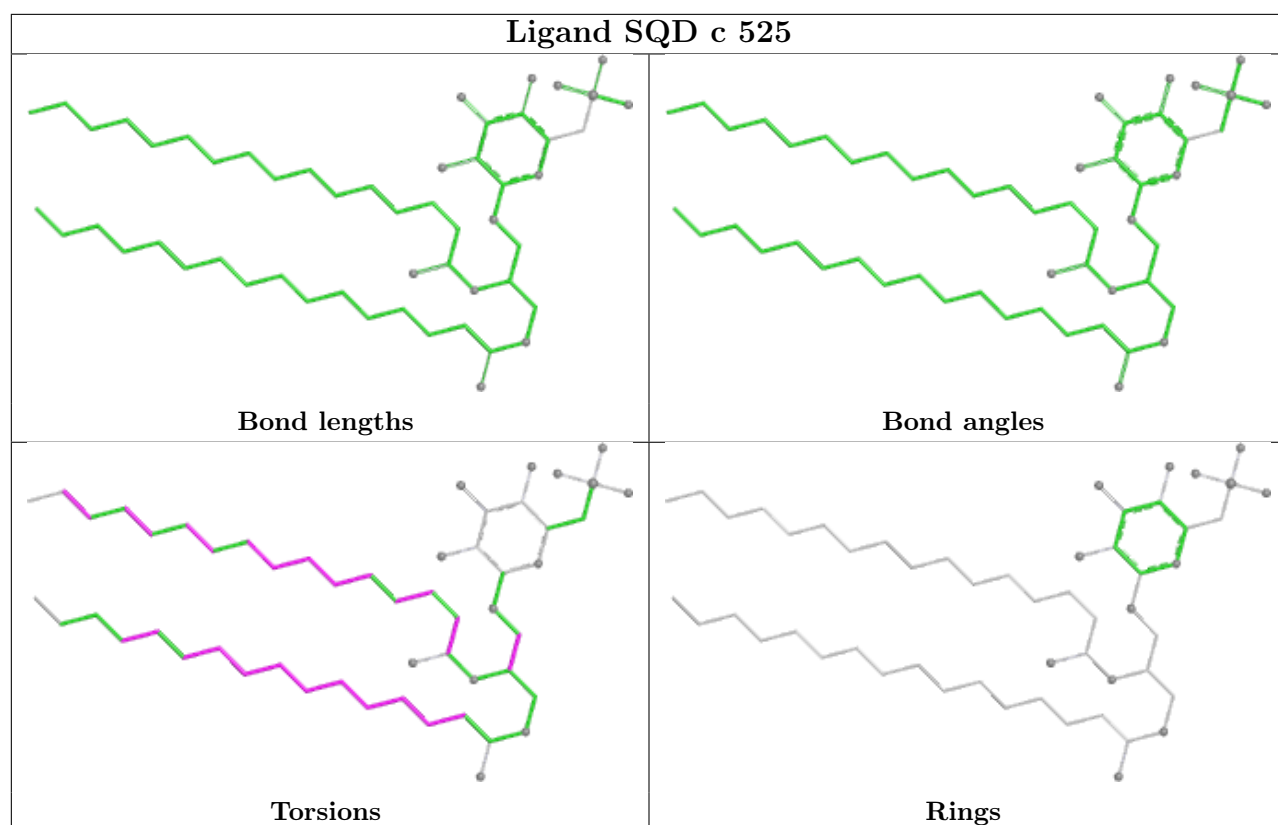


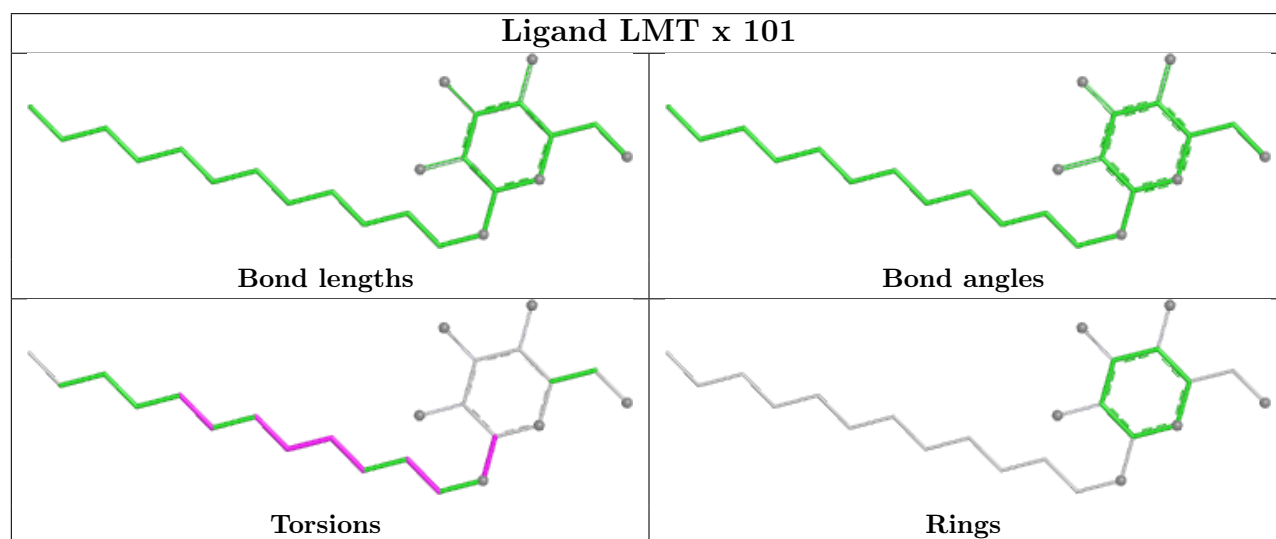
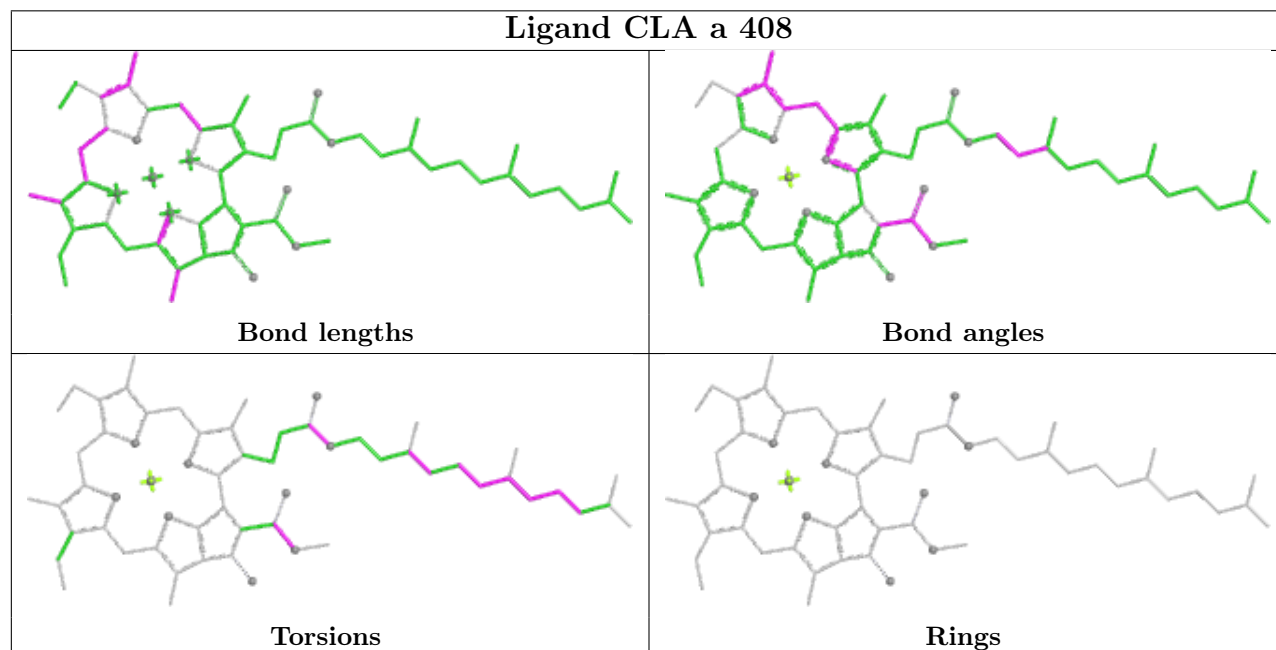
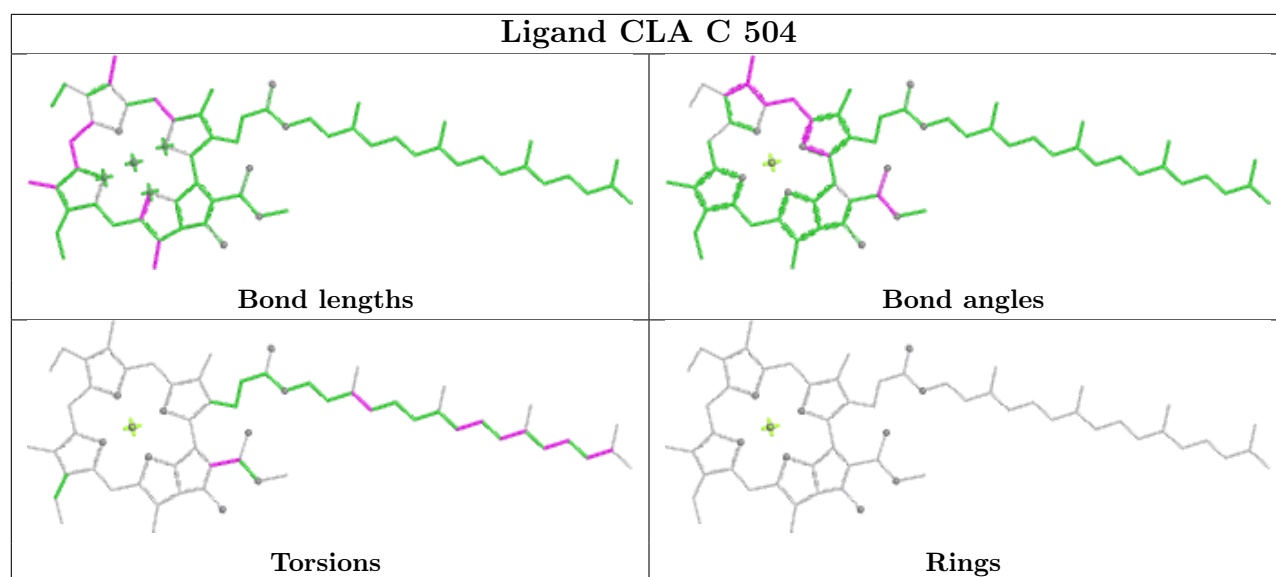


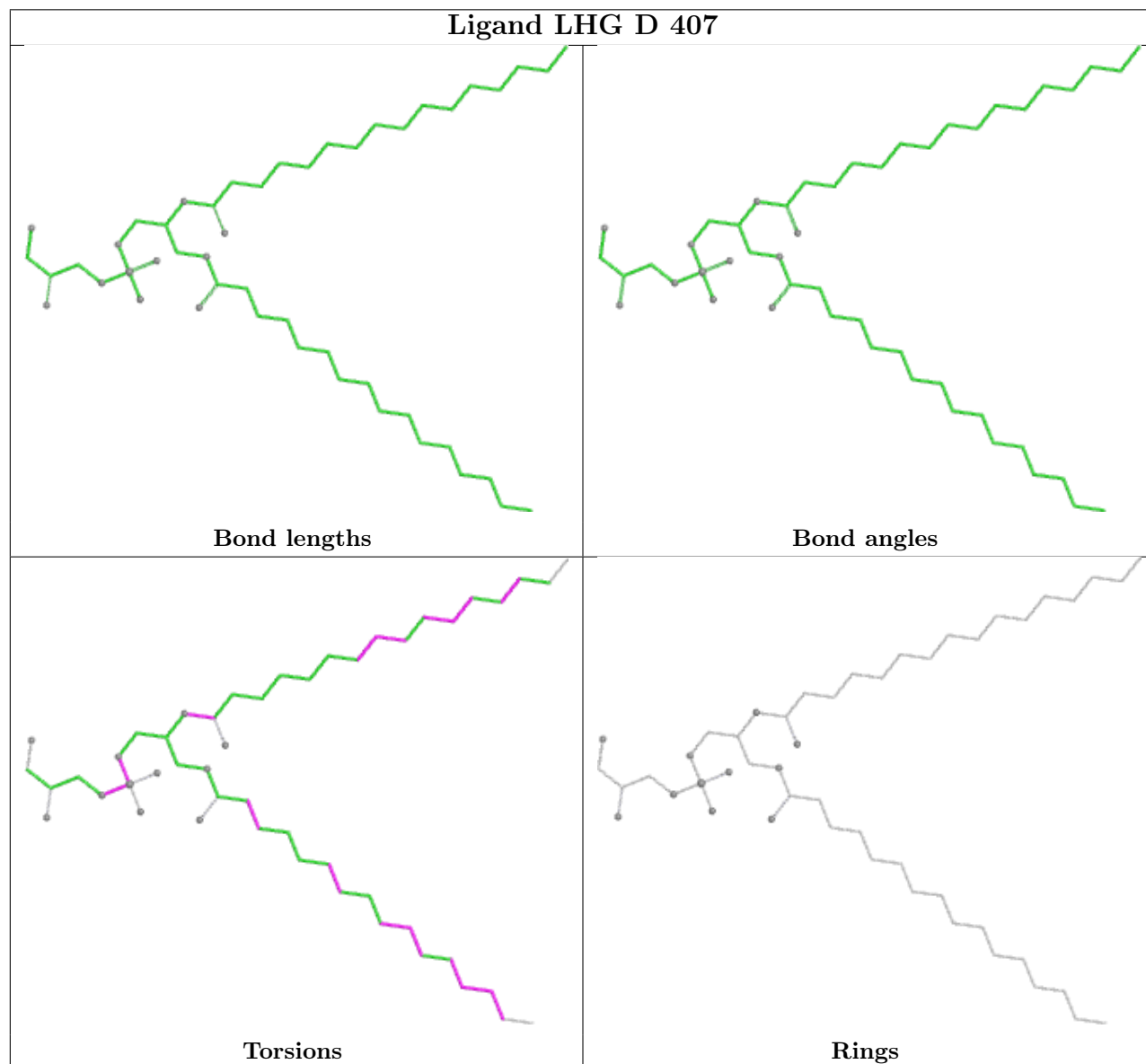
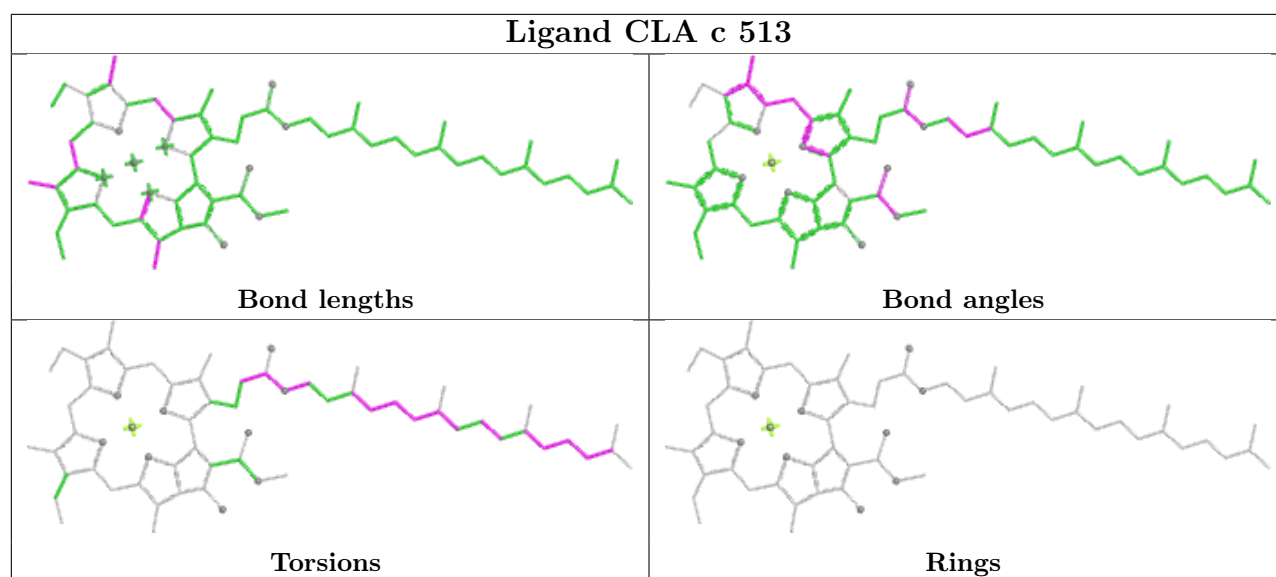




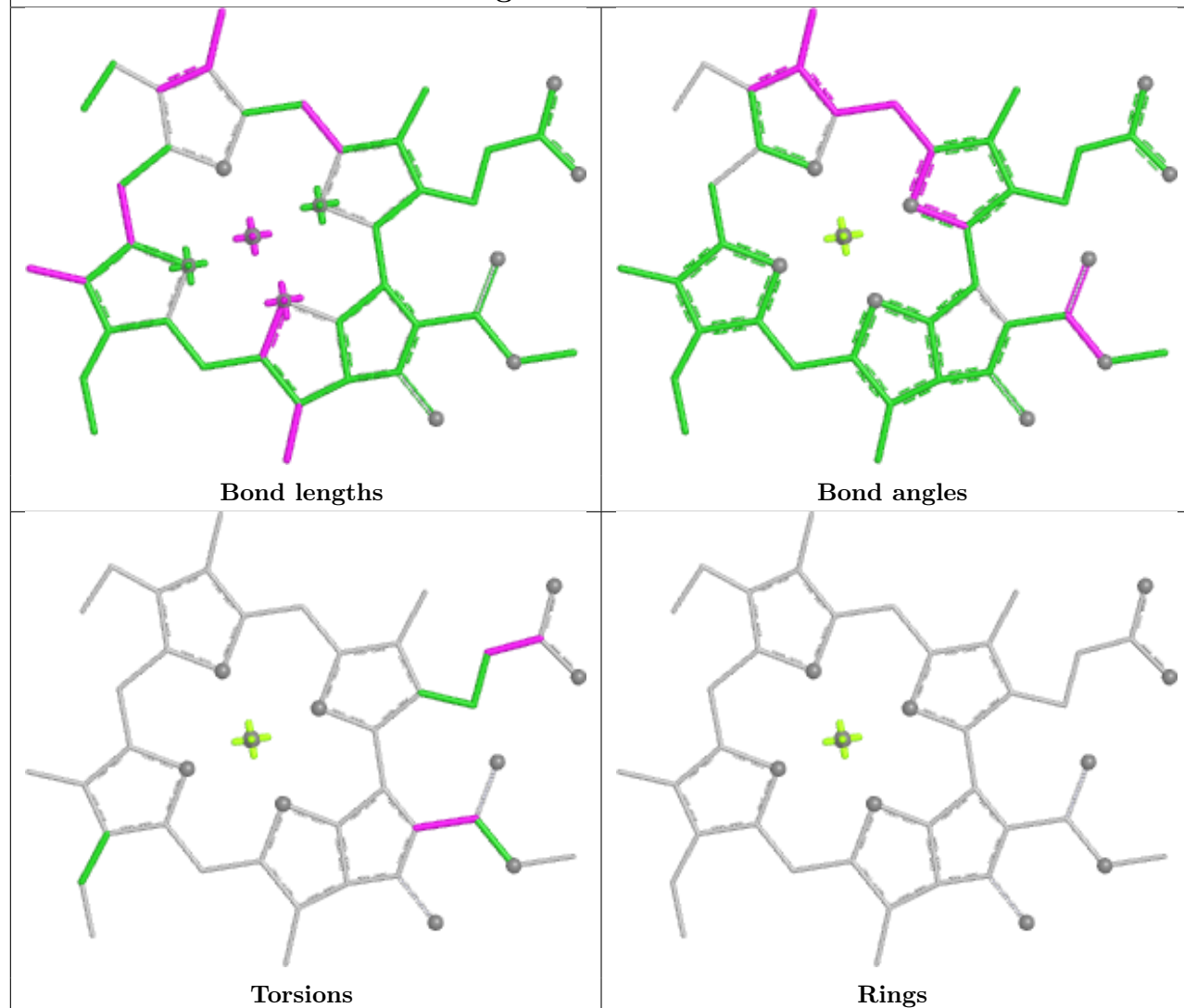




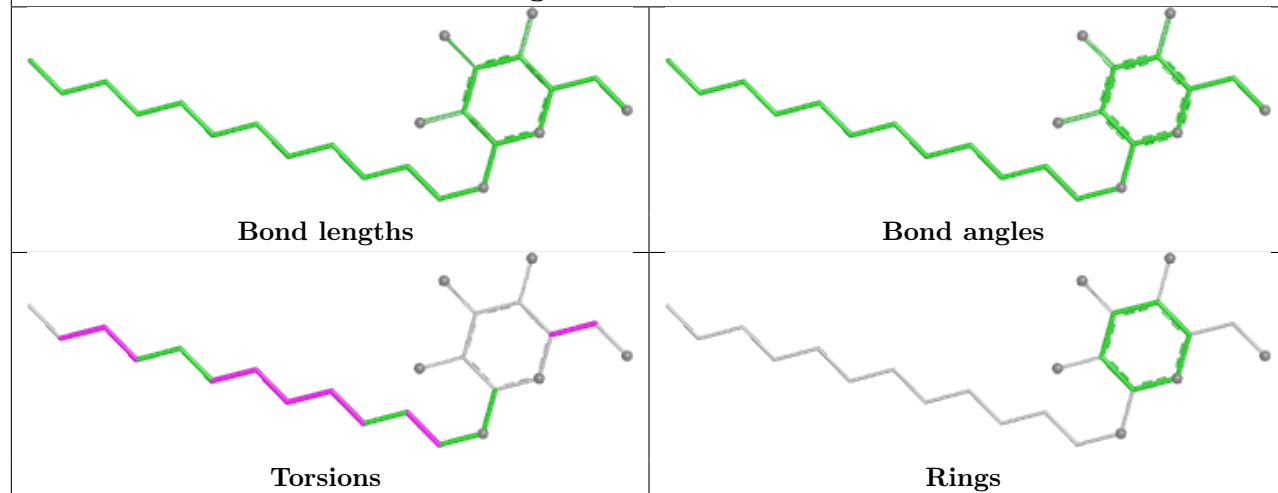




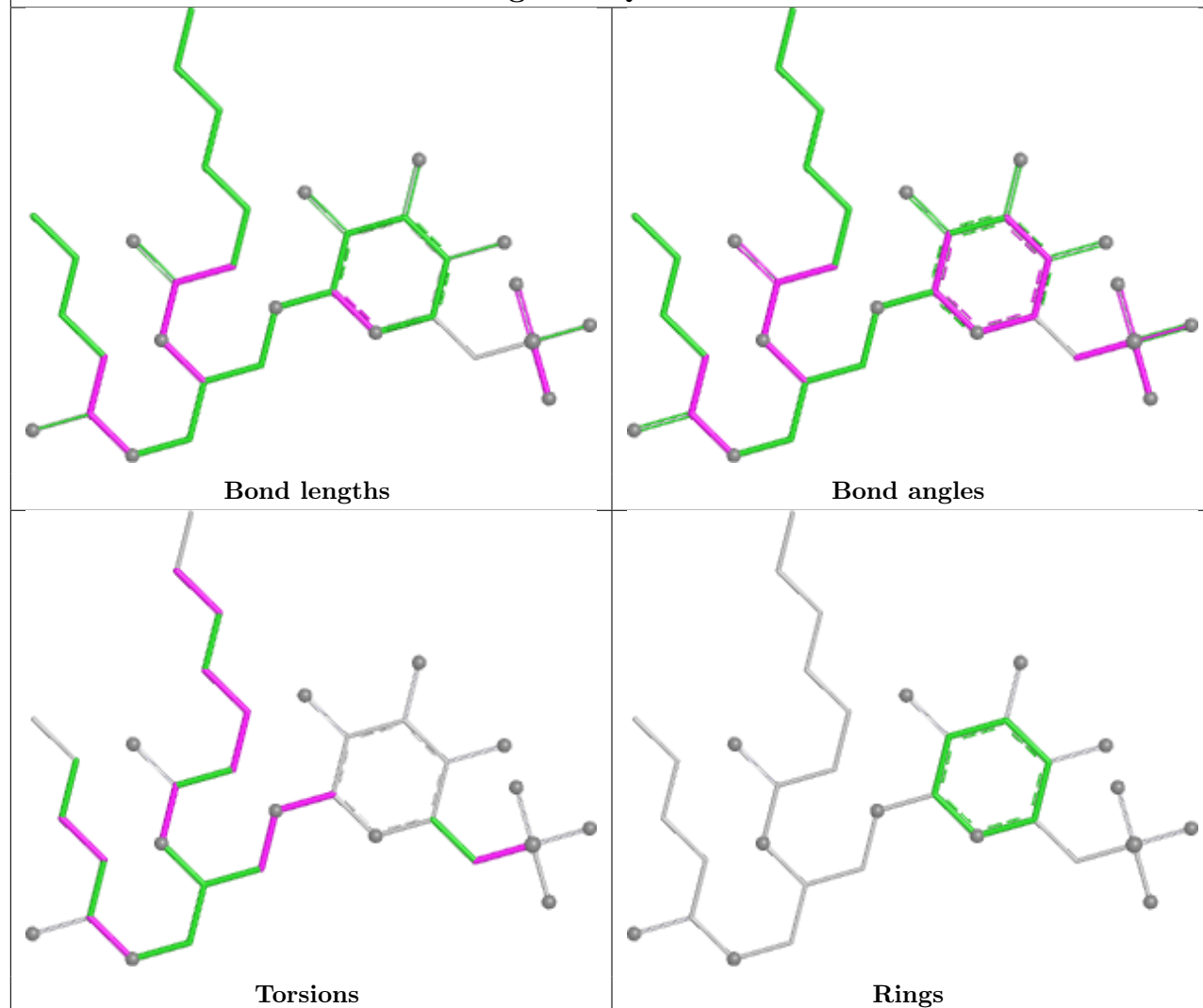
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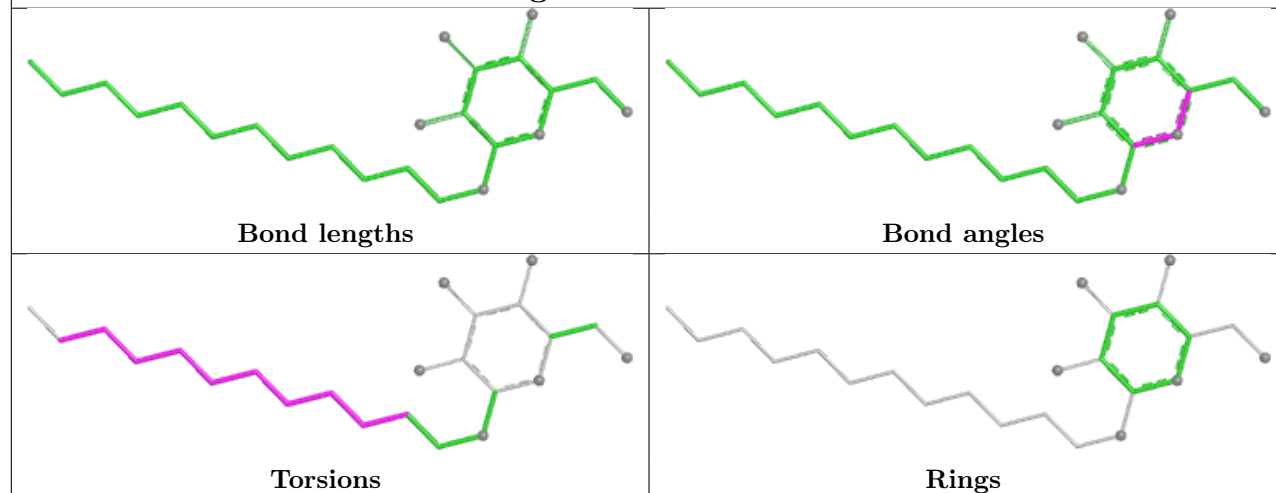
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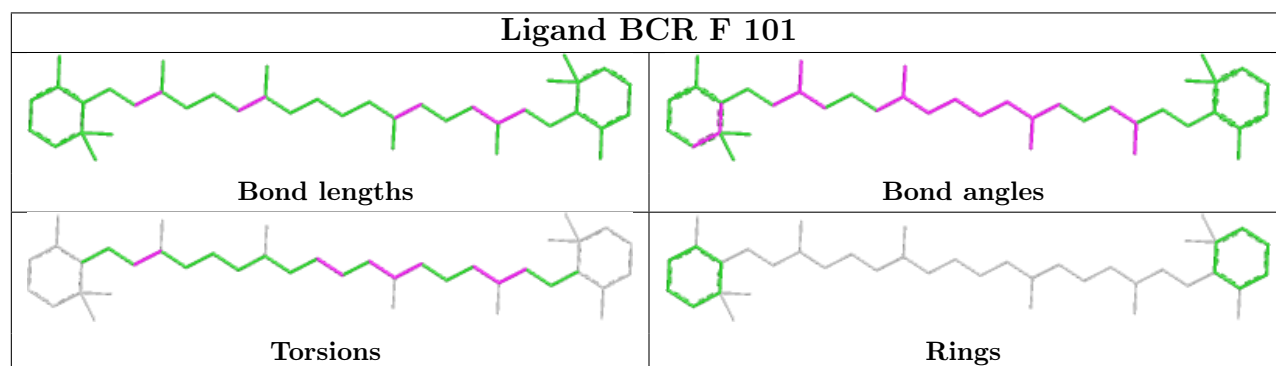
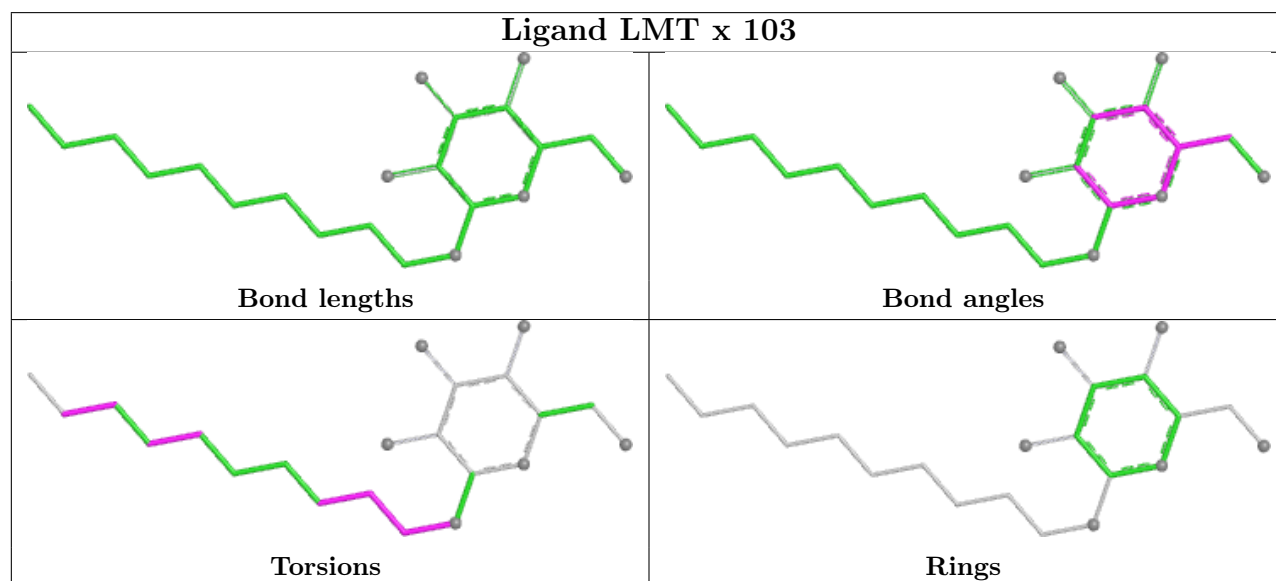
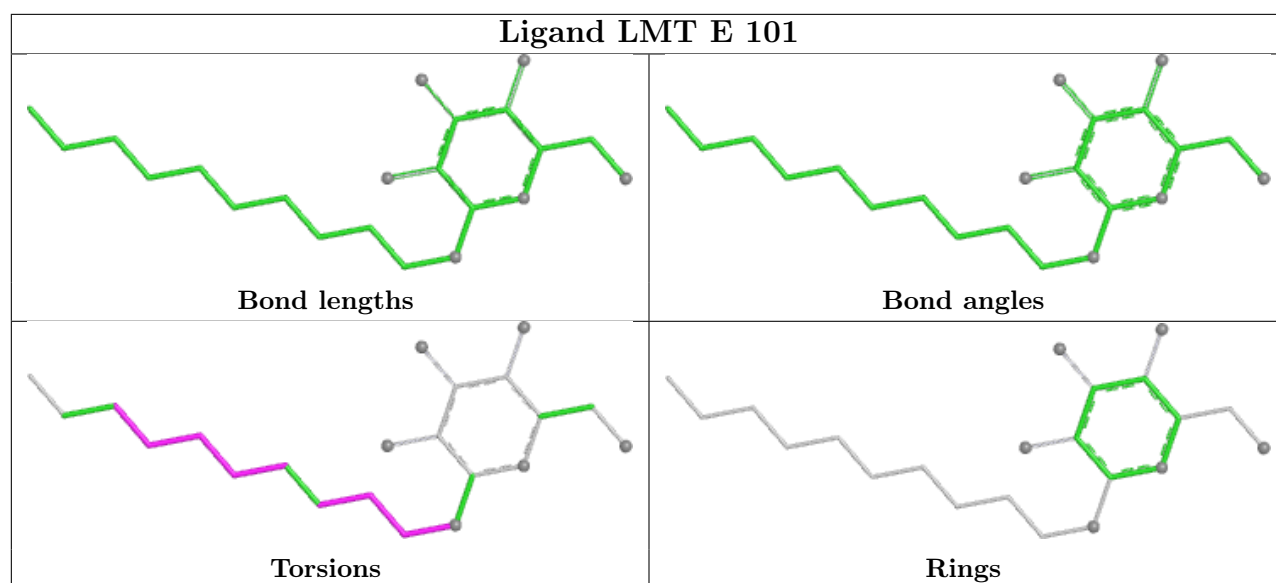


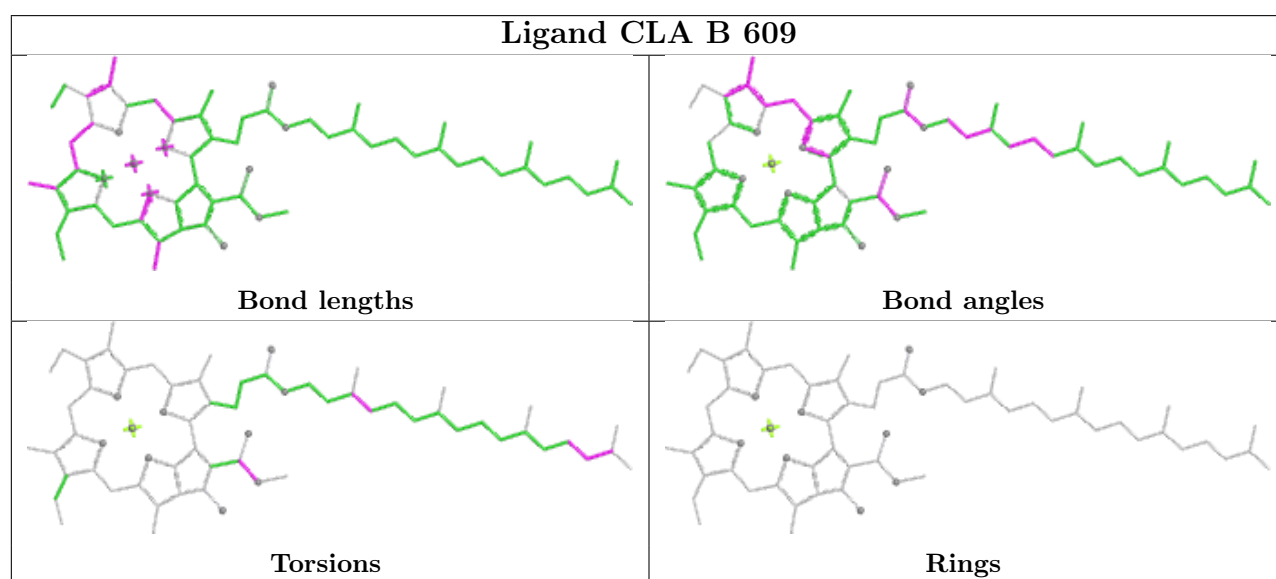
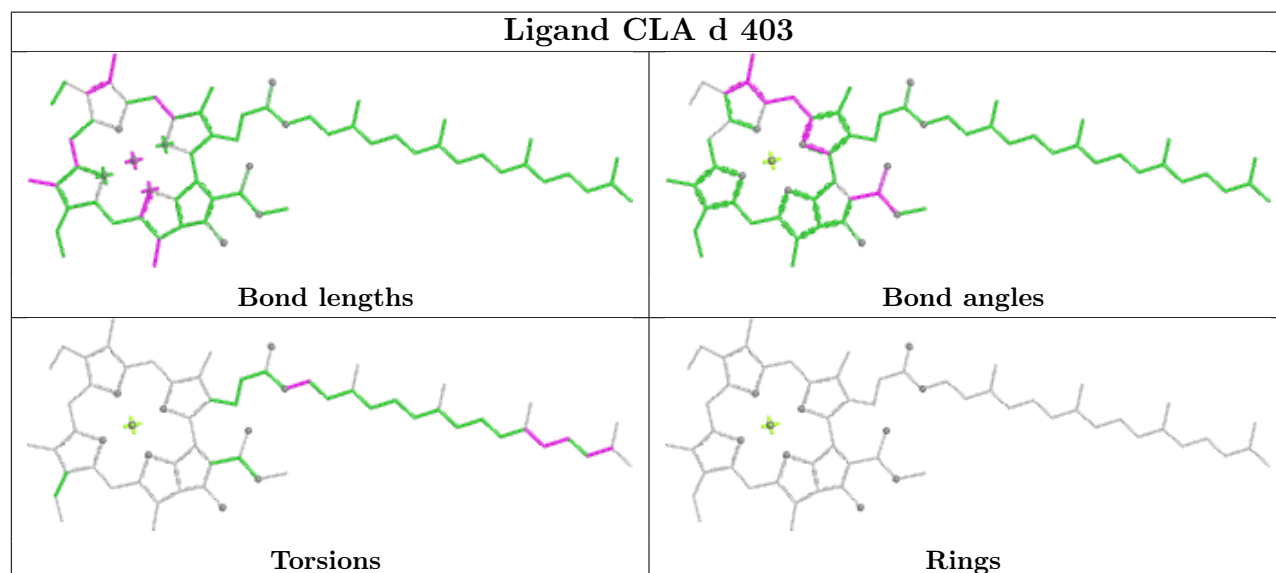
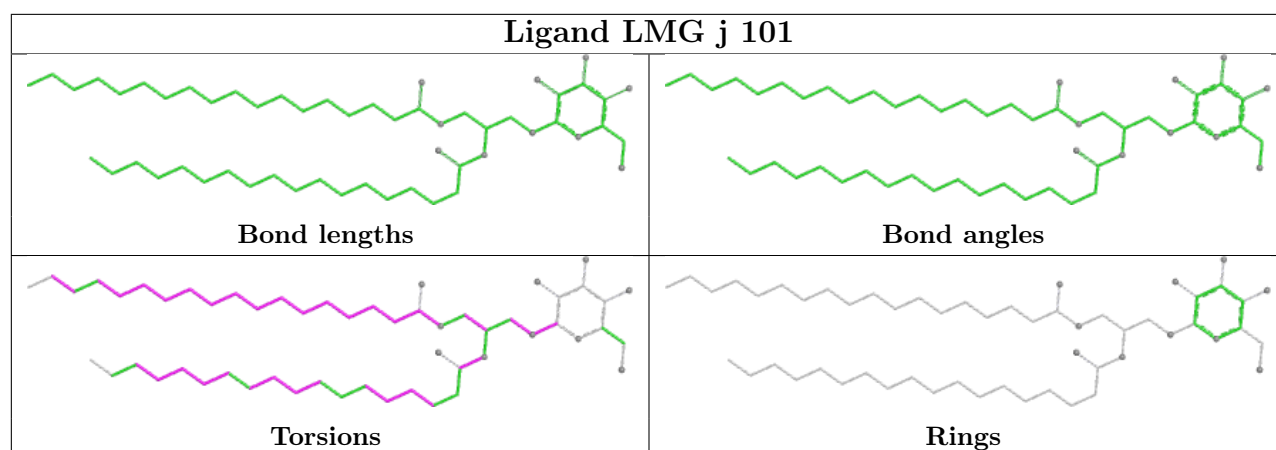
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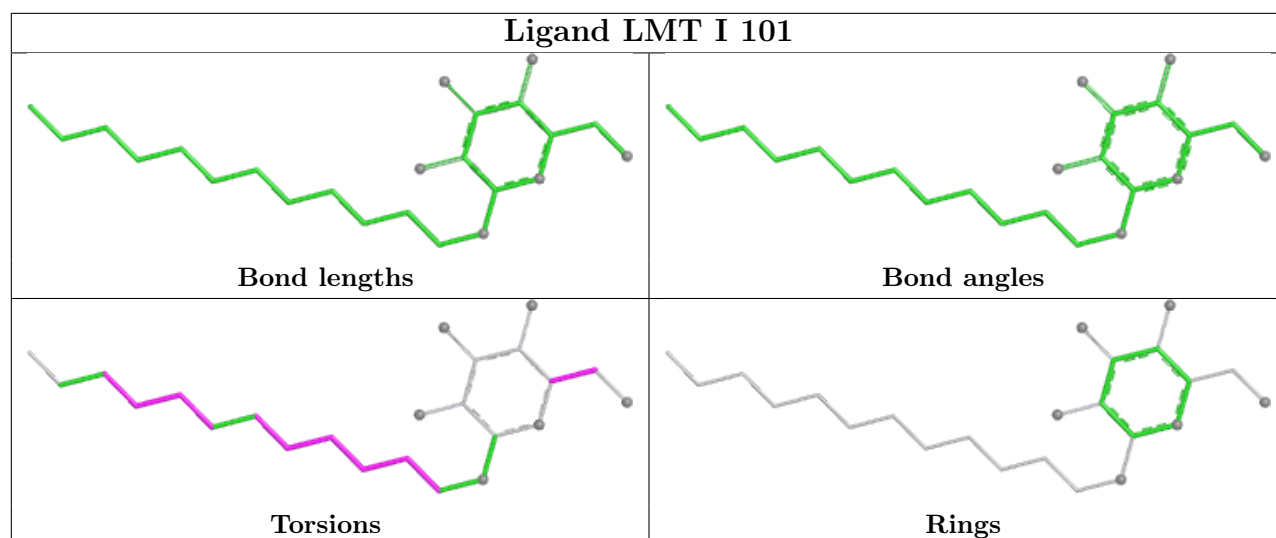
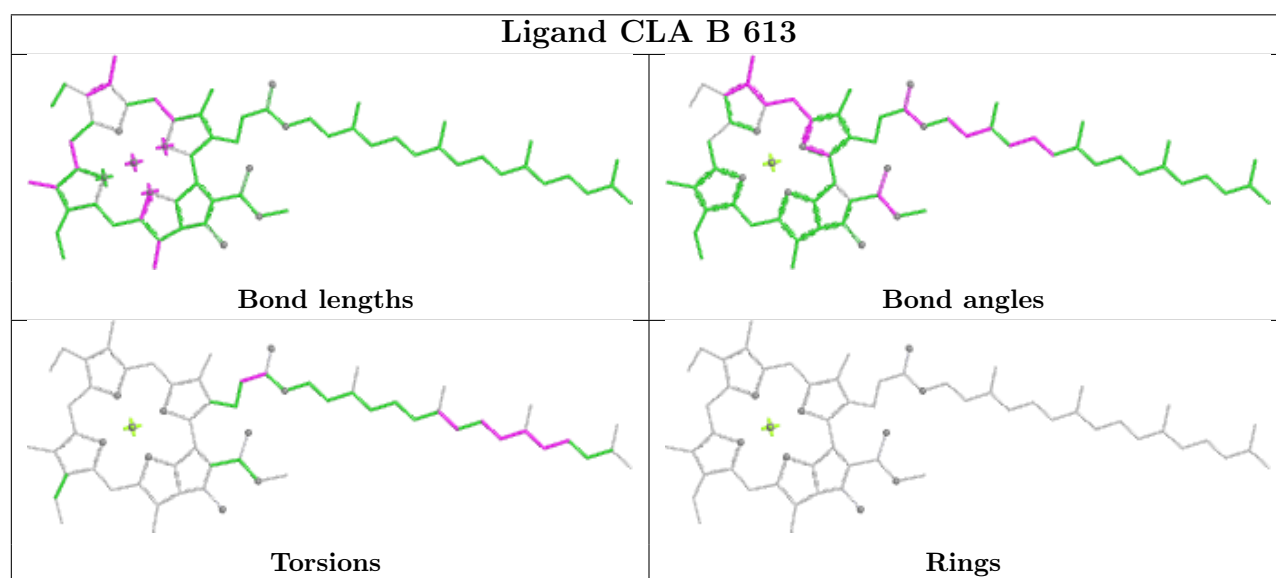
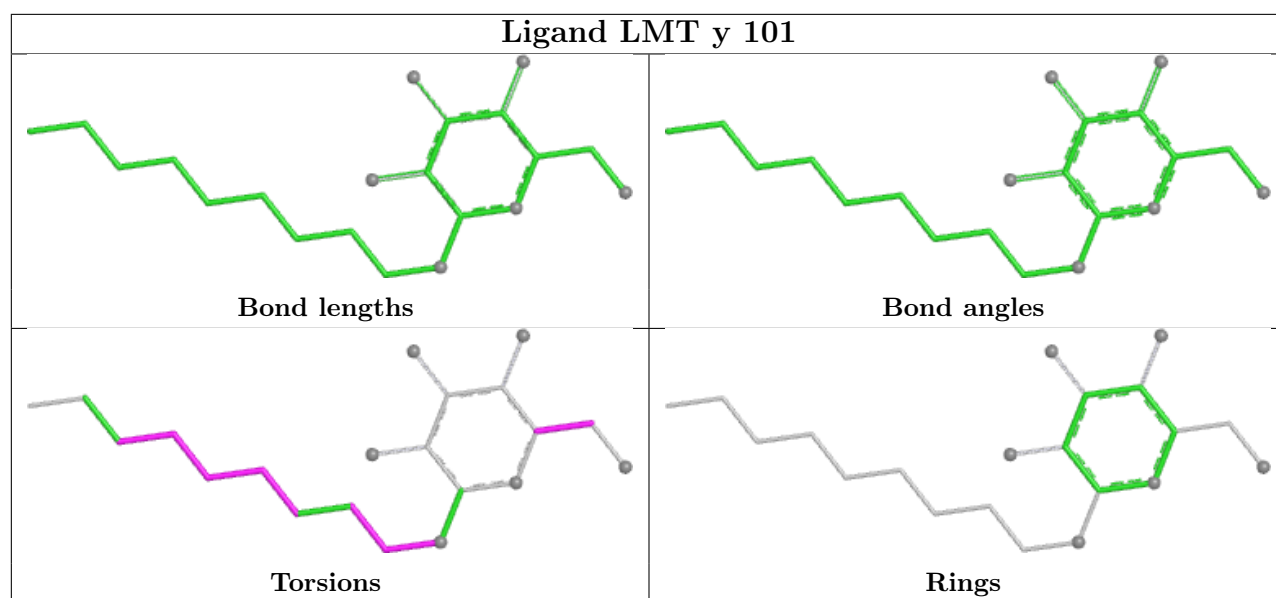


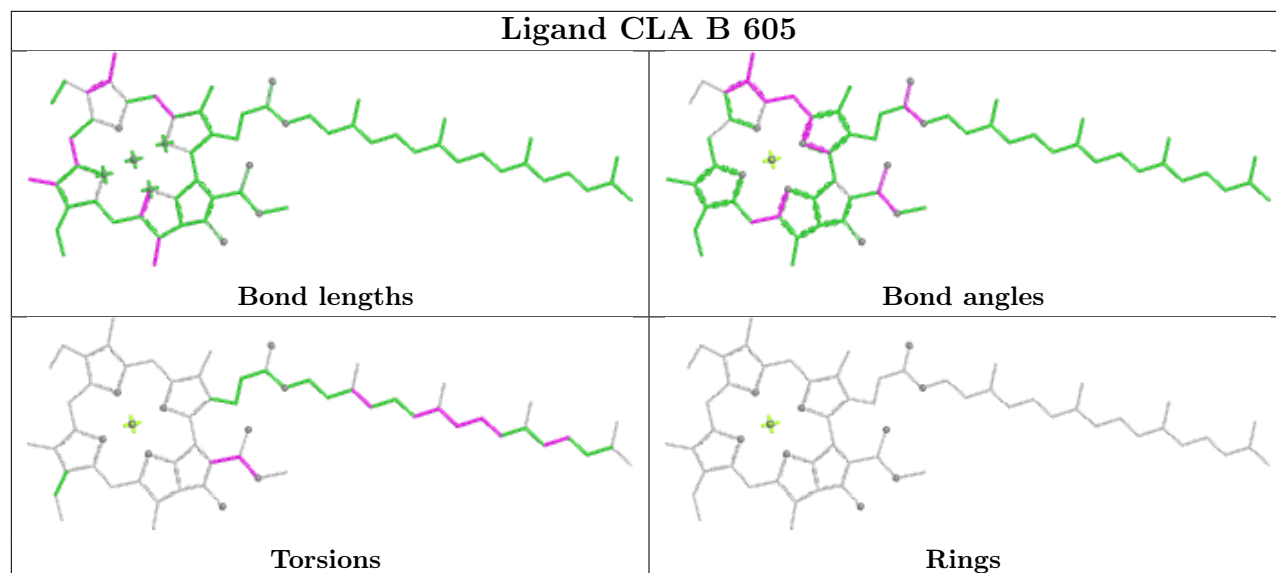
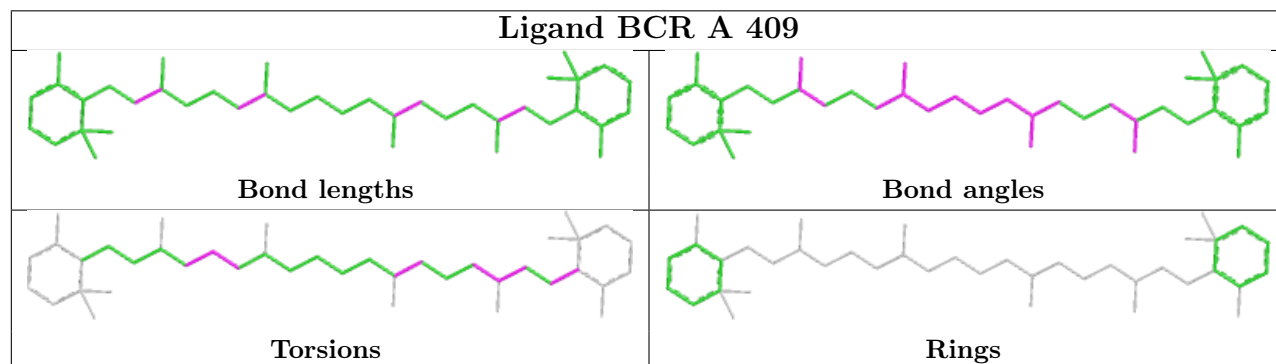
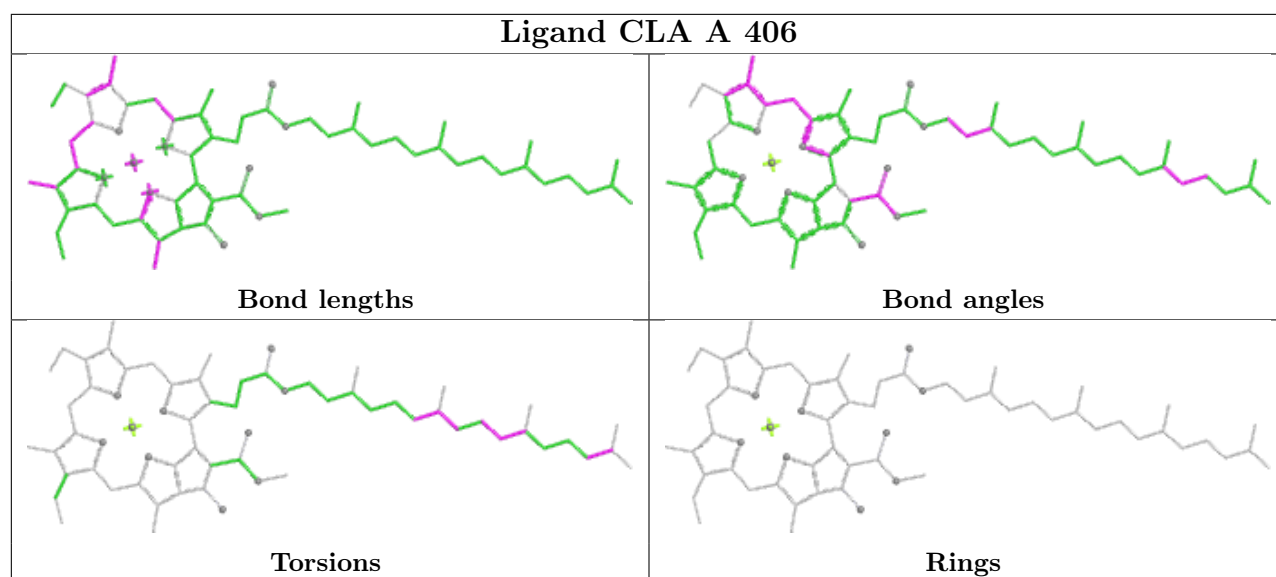
Ligand LMT T 101

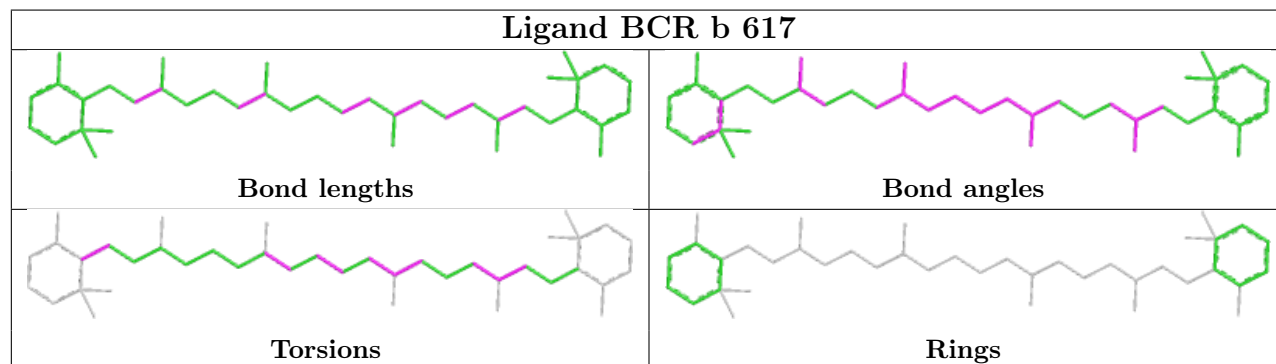
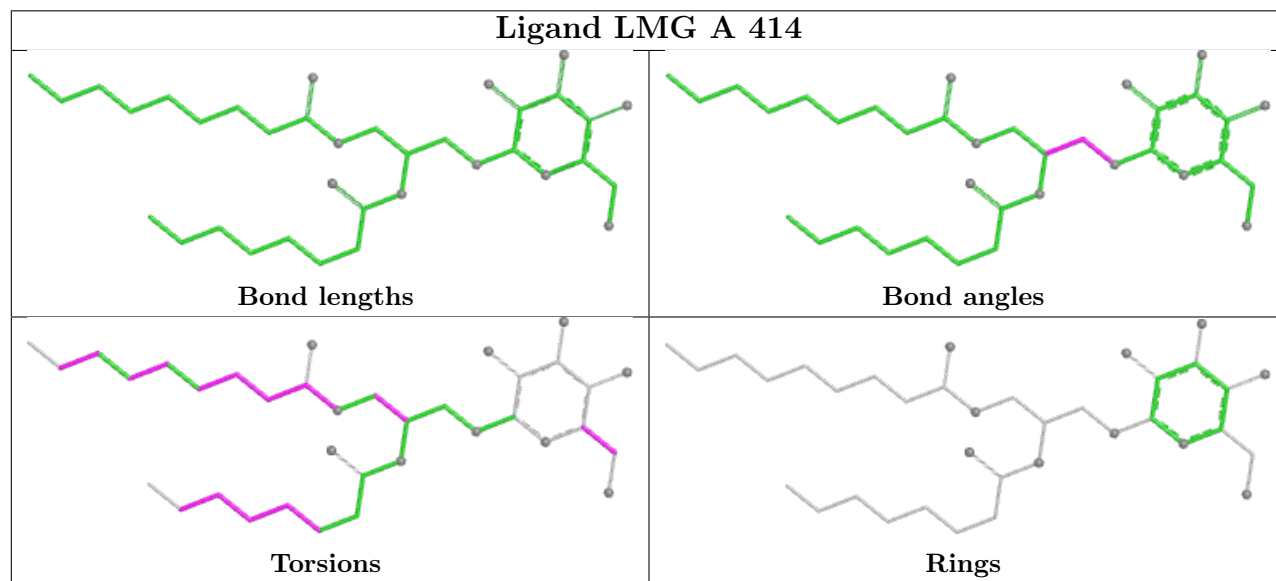
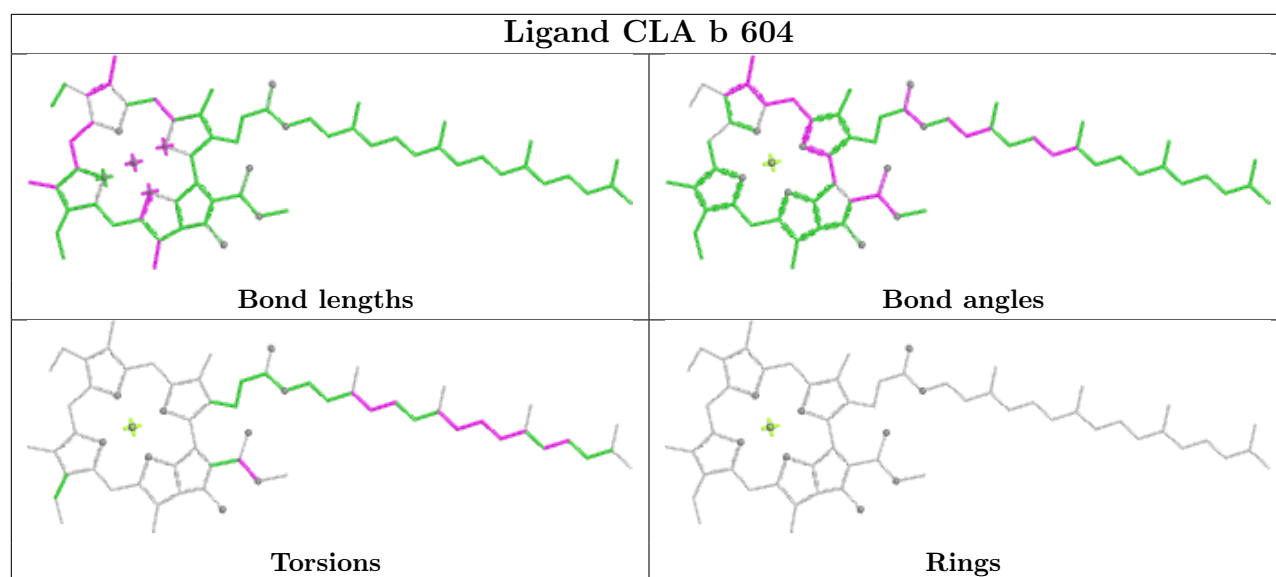


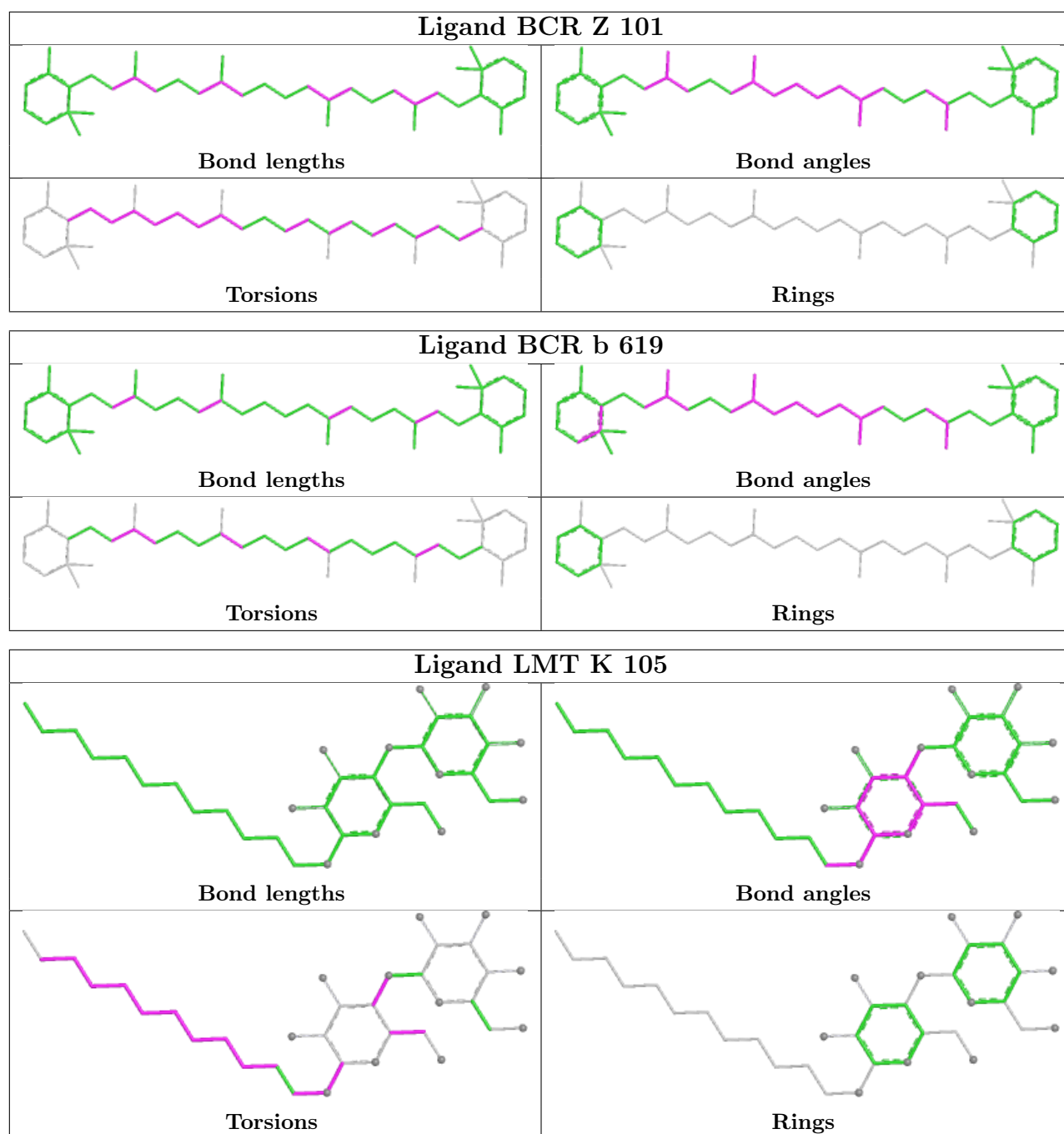


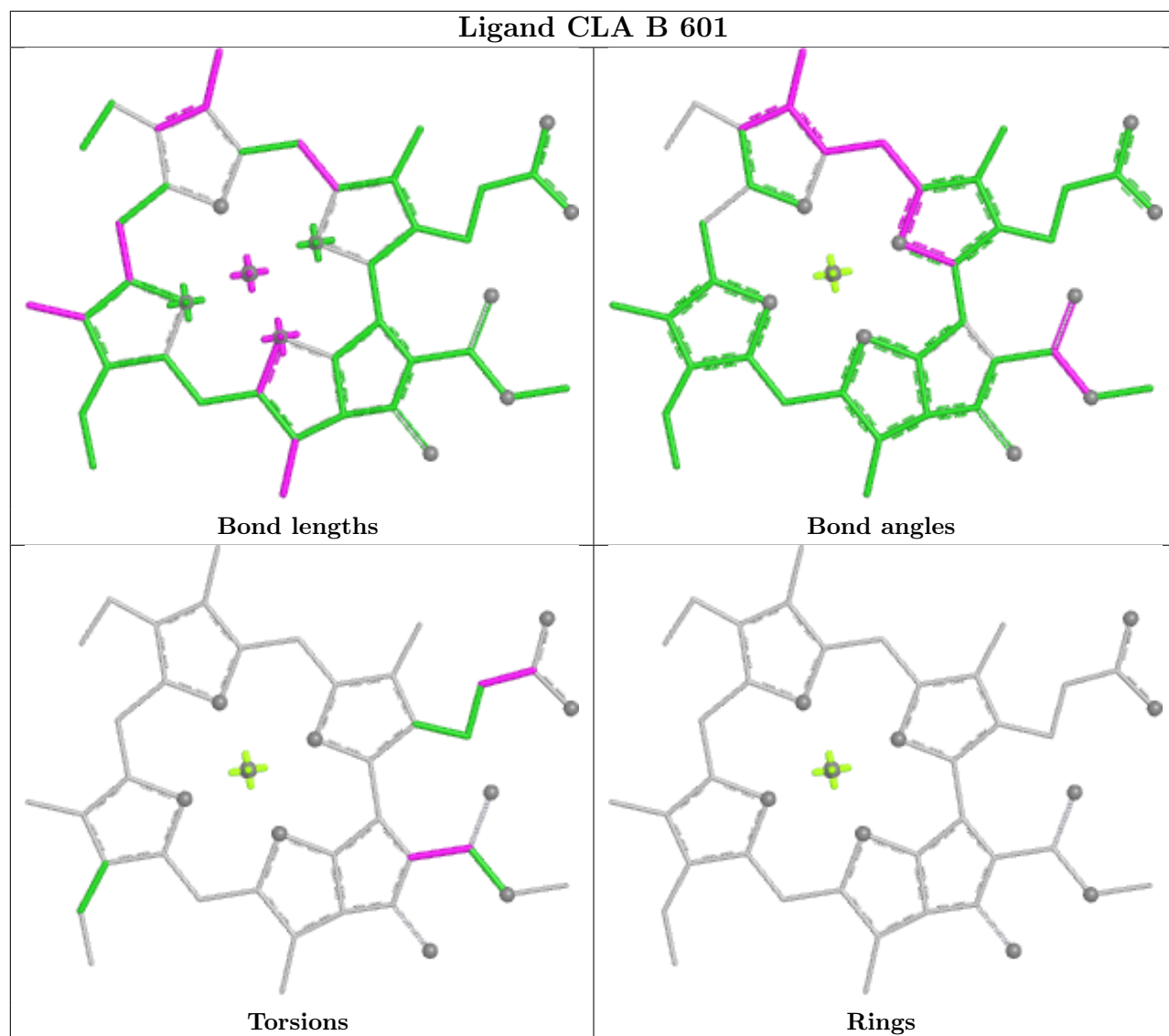
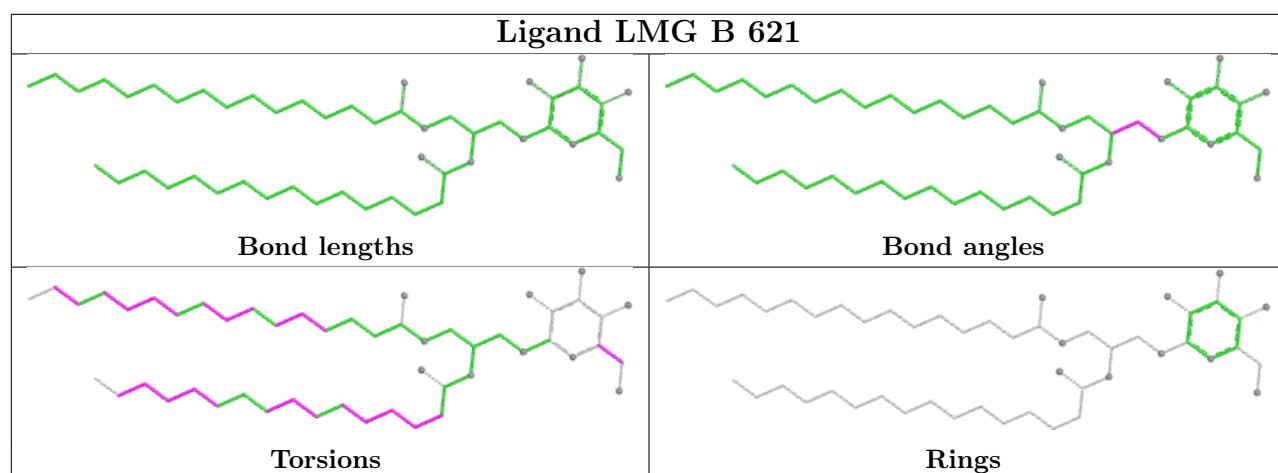


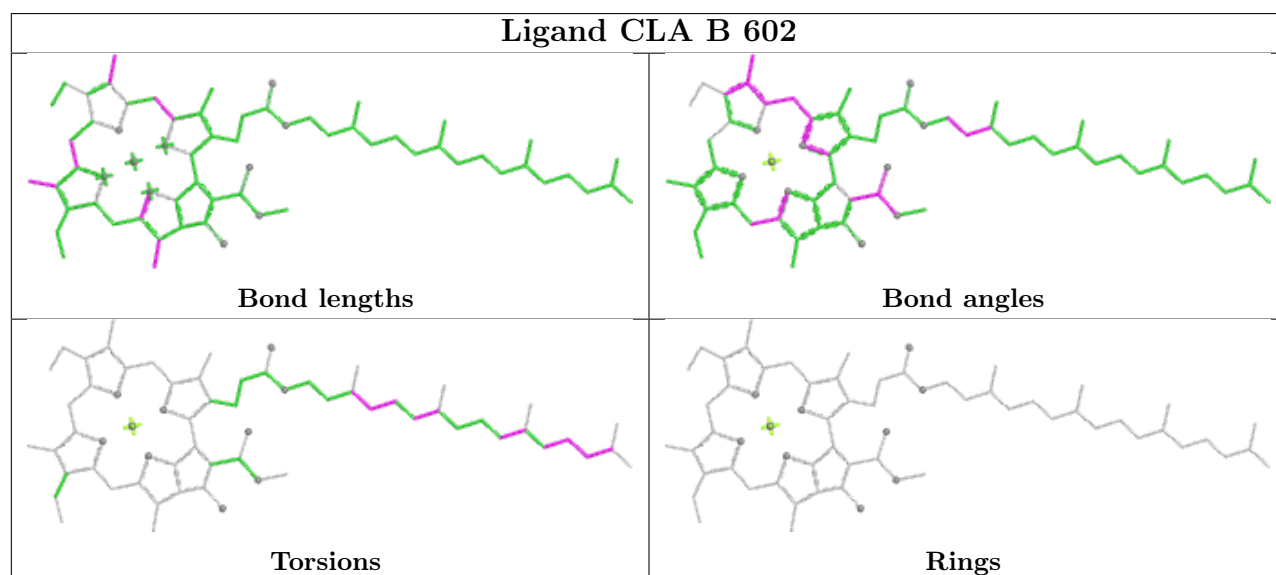
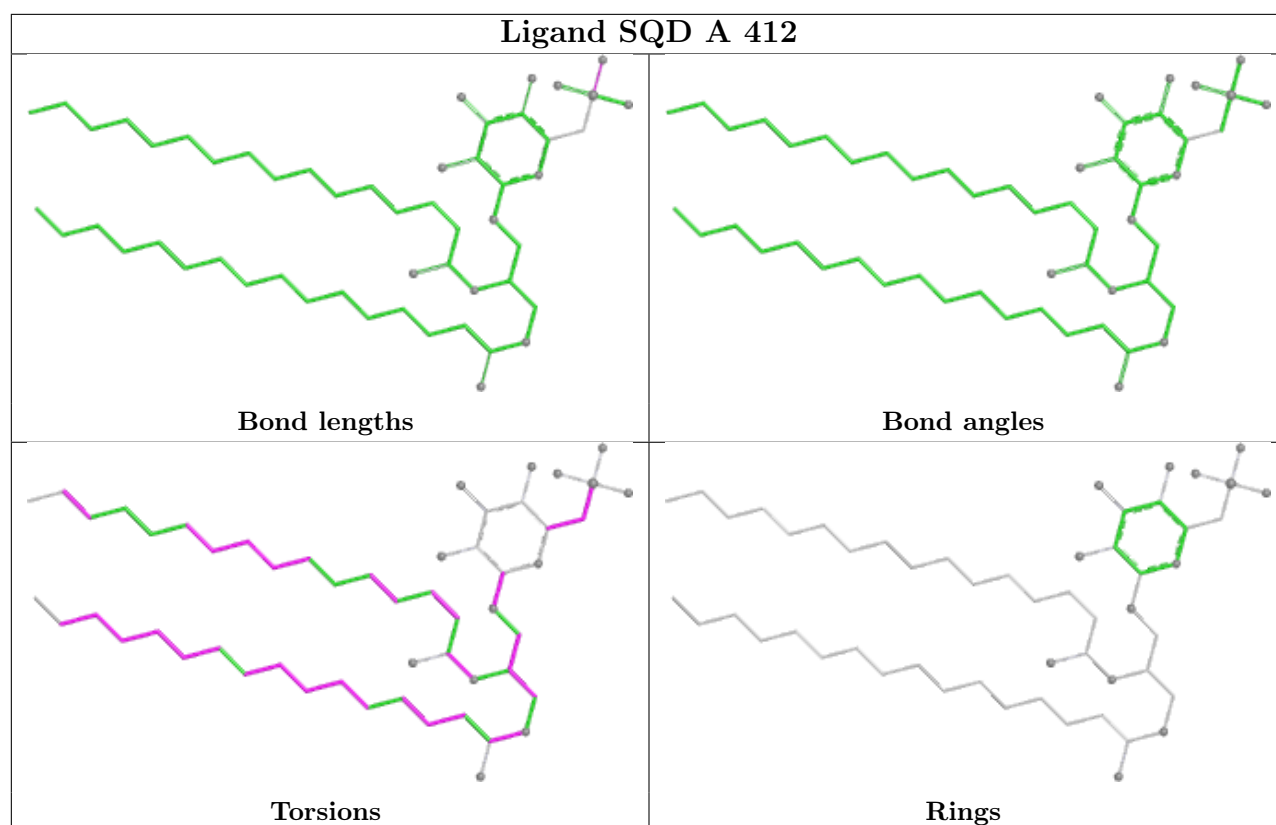


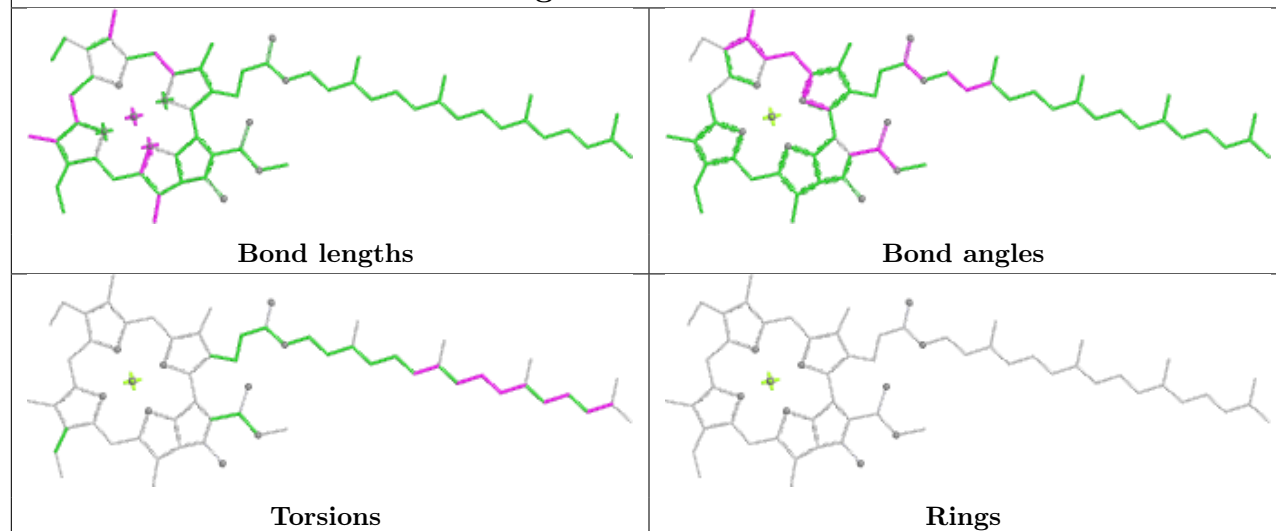
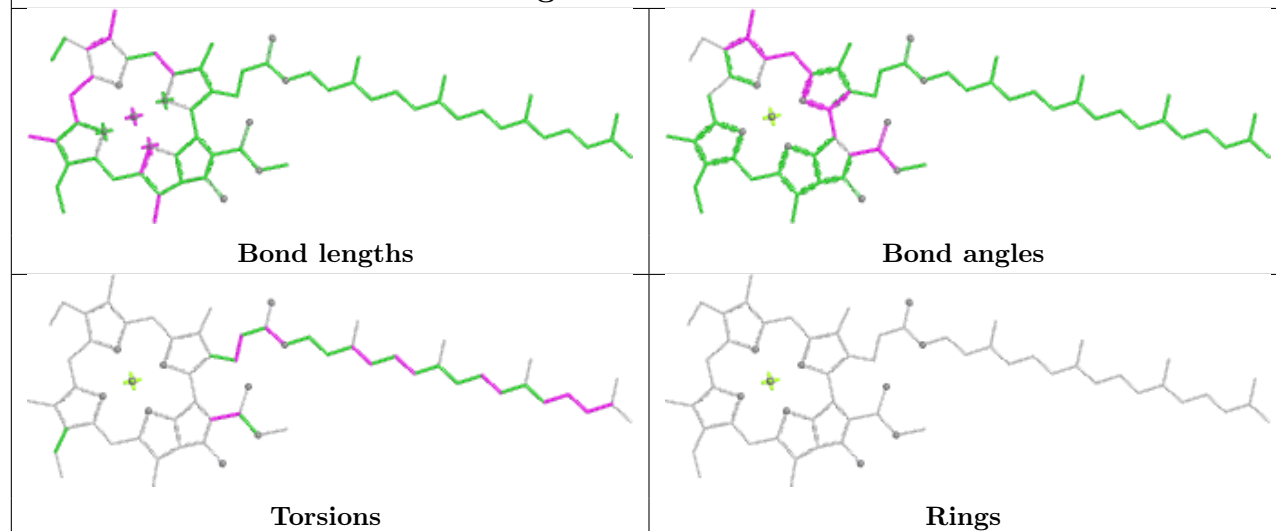
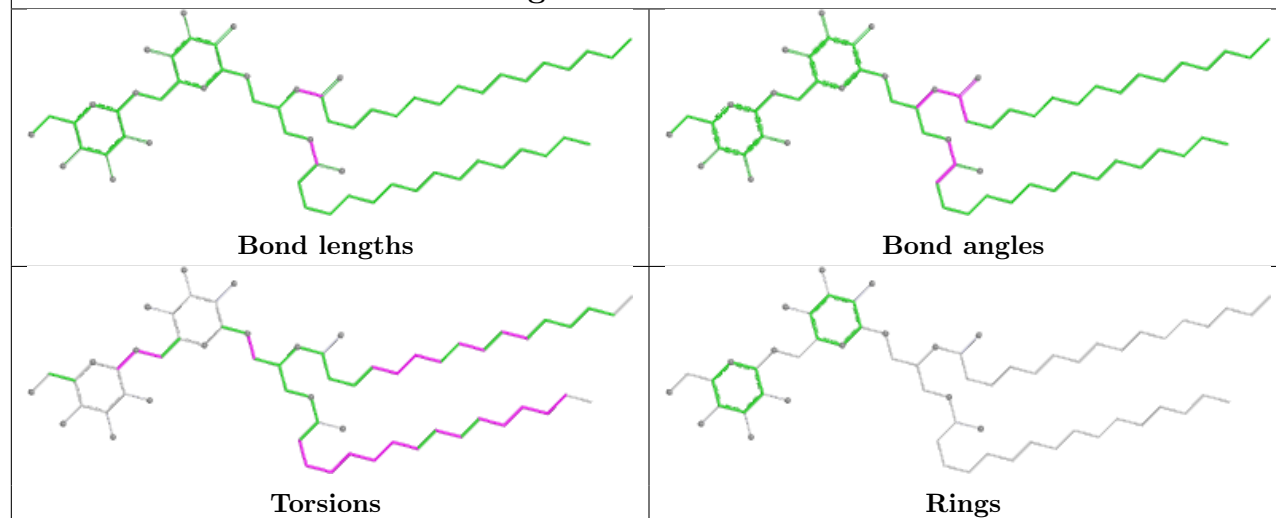


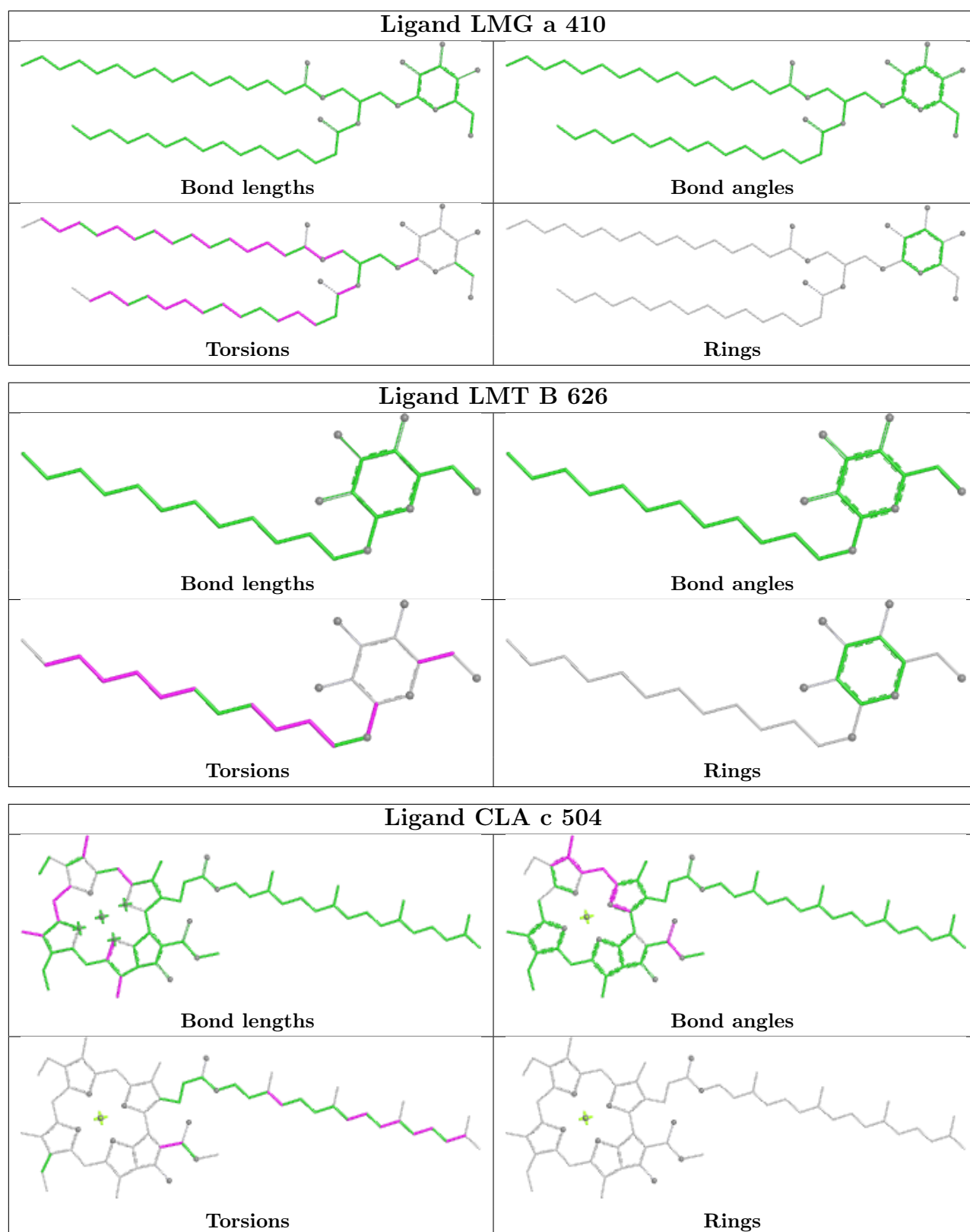




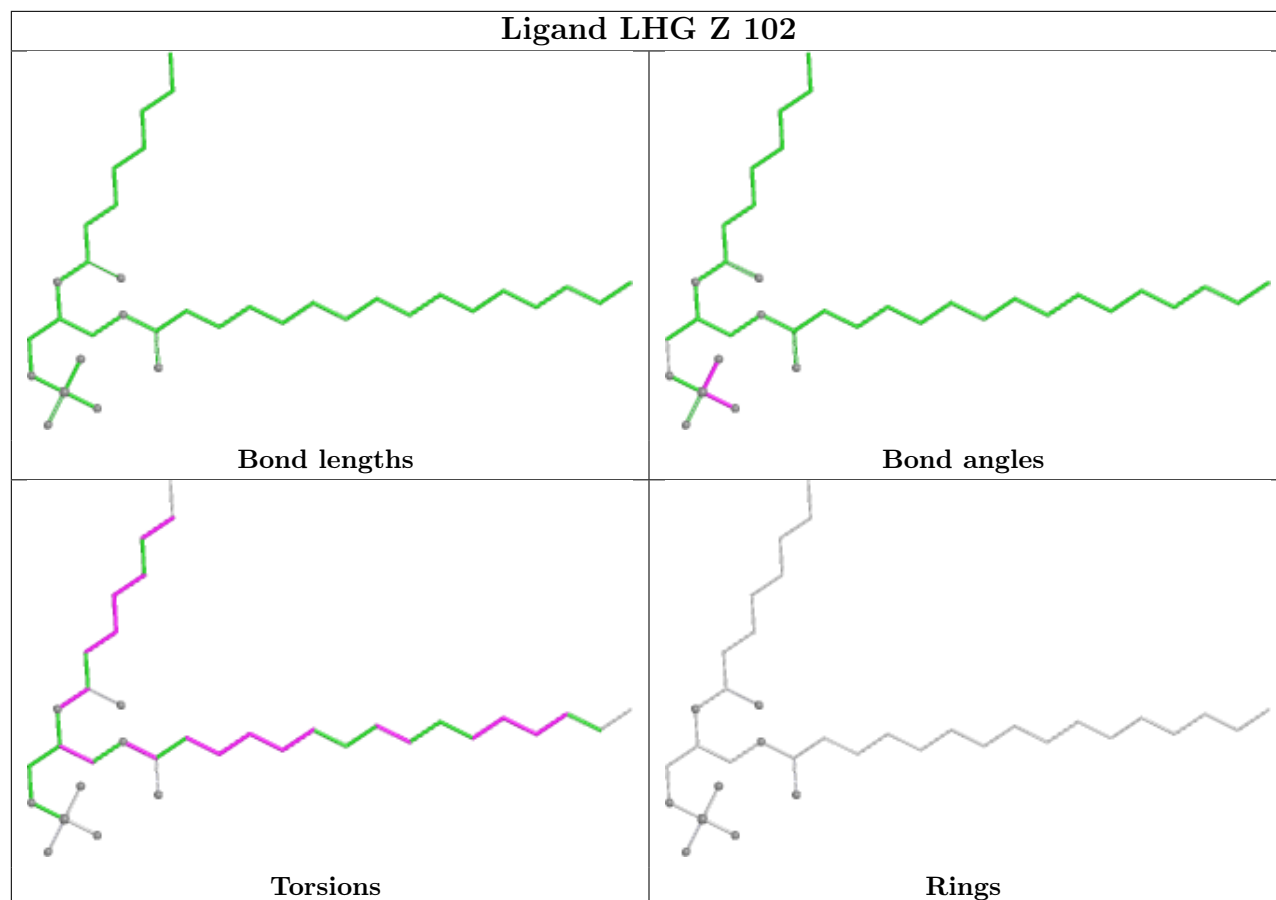




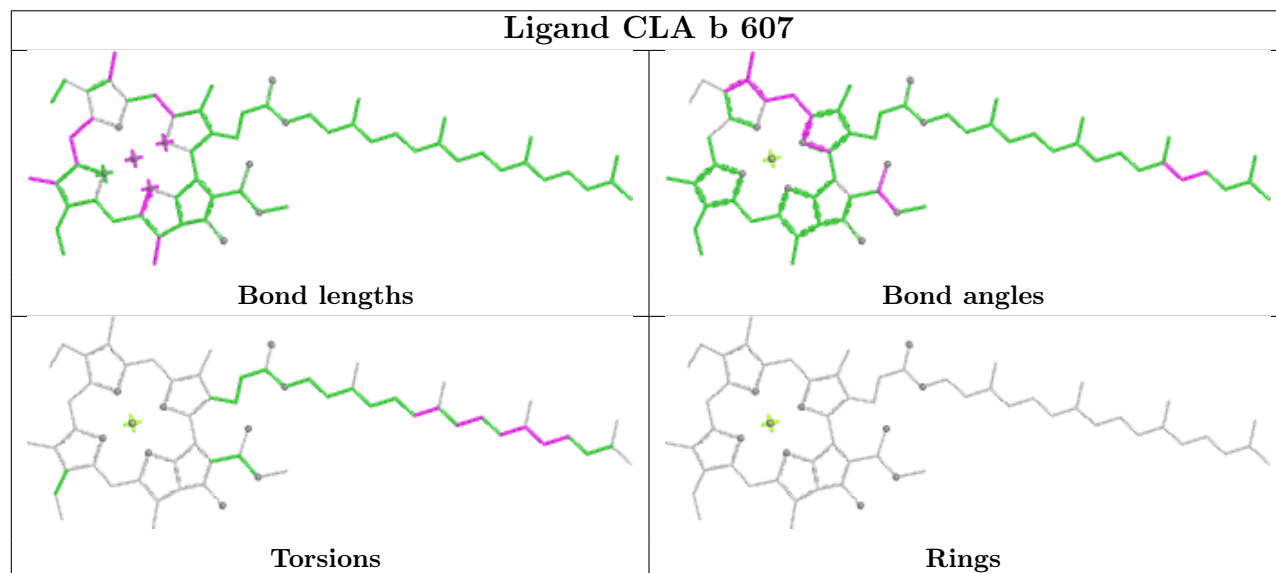
Ligand CLA b 611**Ligand CLA c 507****Ligand DGD C 516**

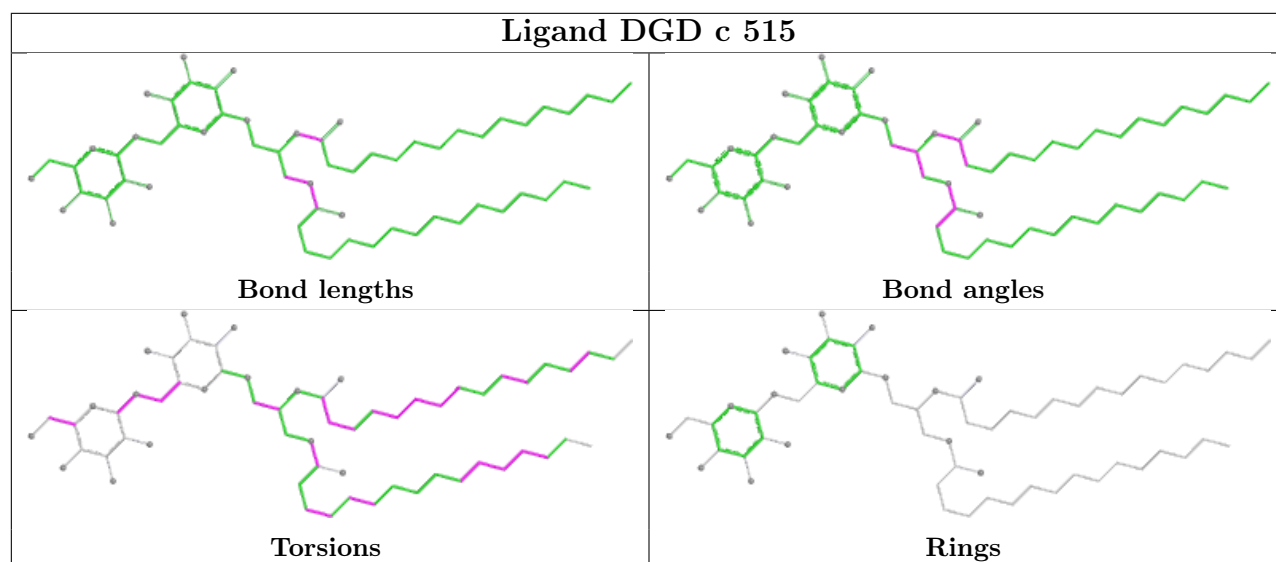
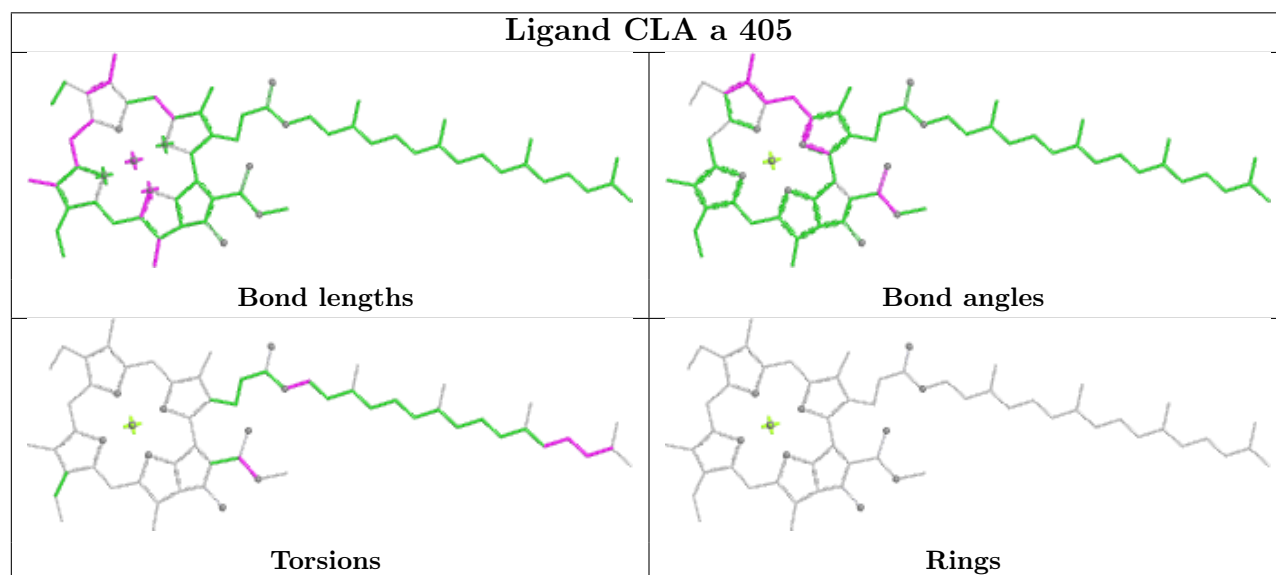
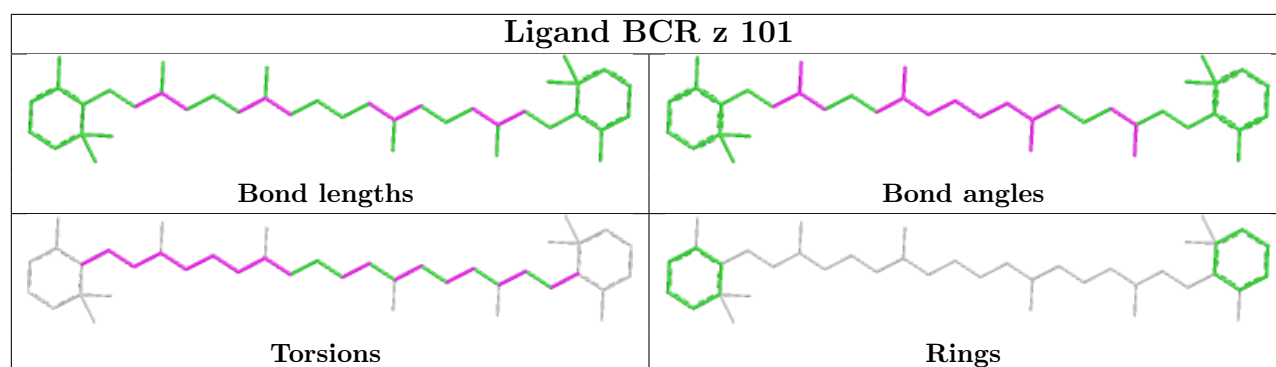


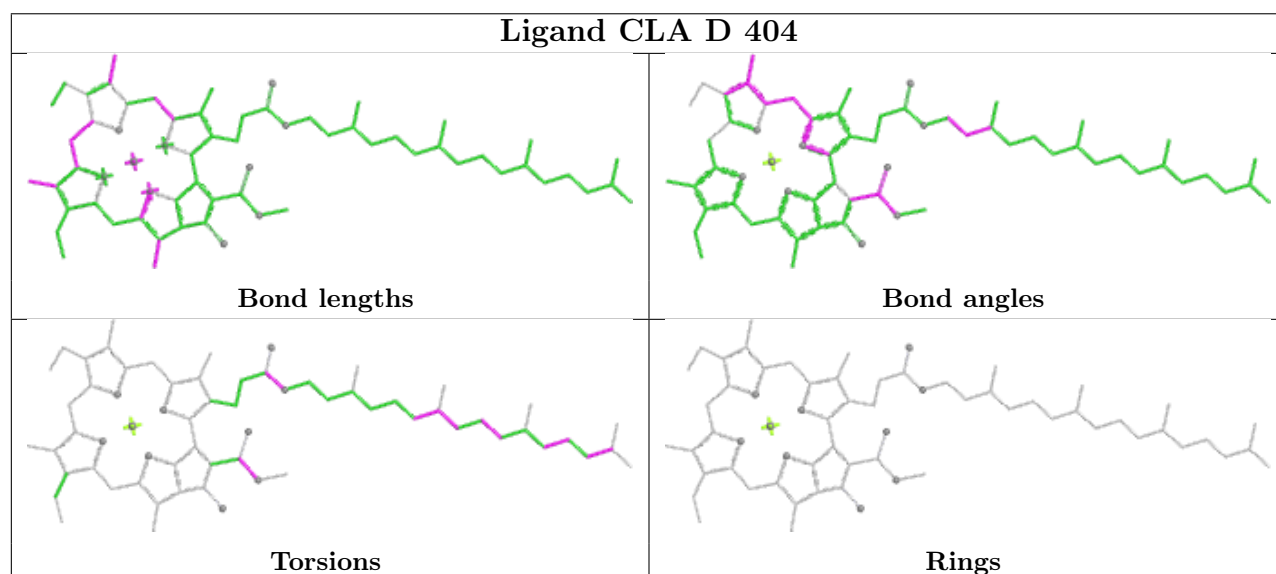
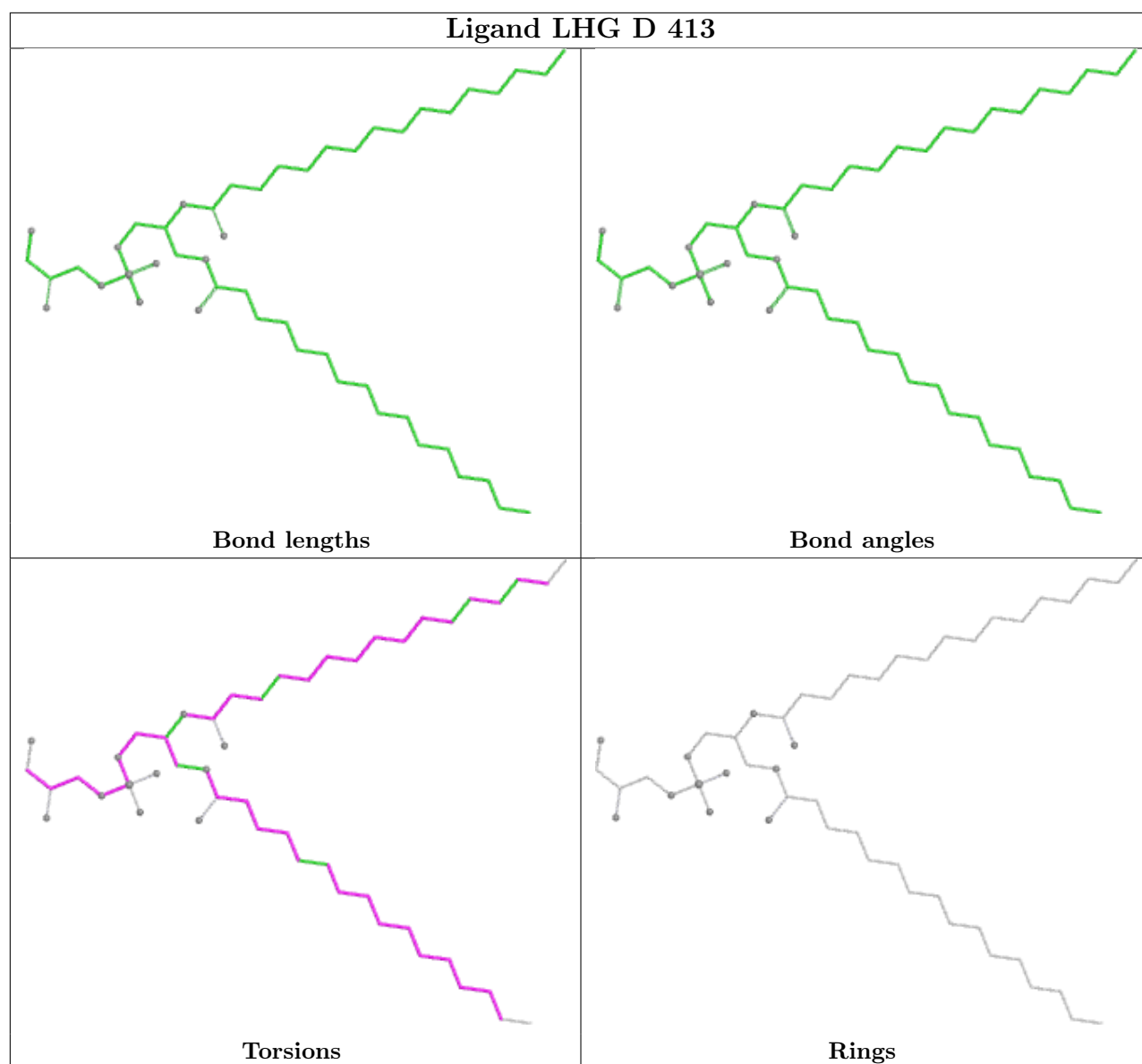
Ligand LHG Z 102

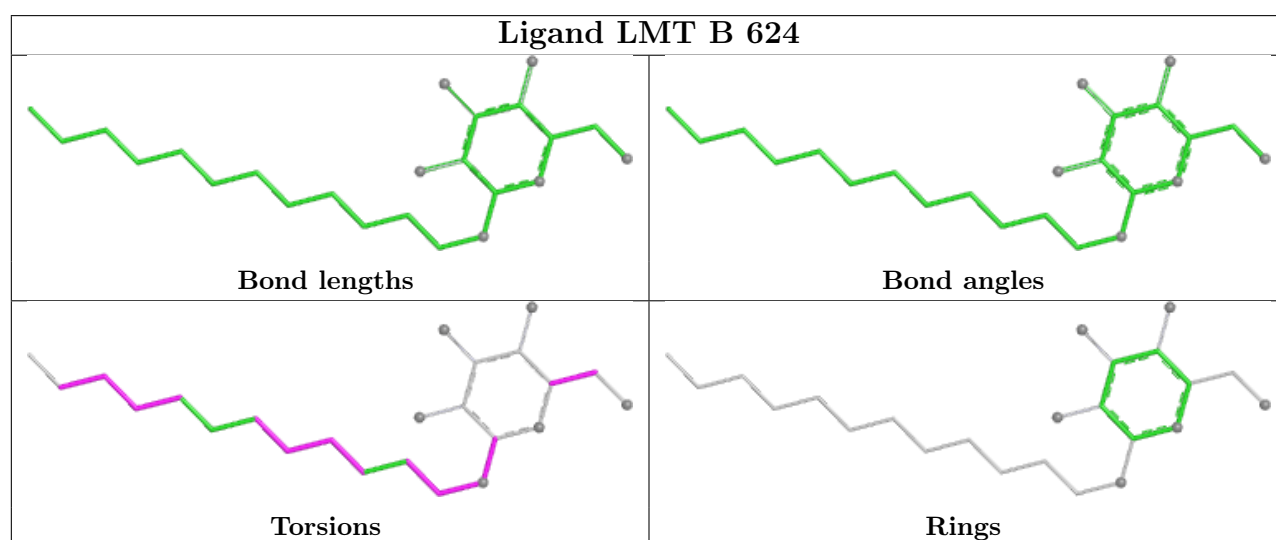
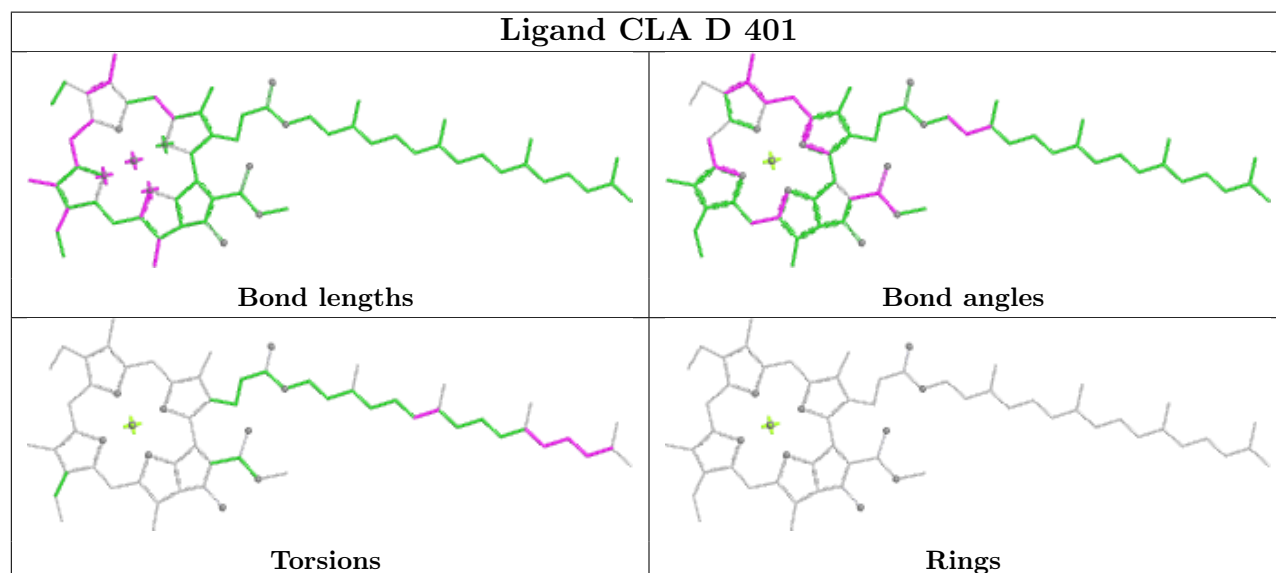
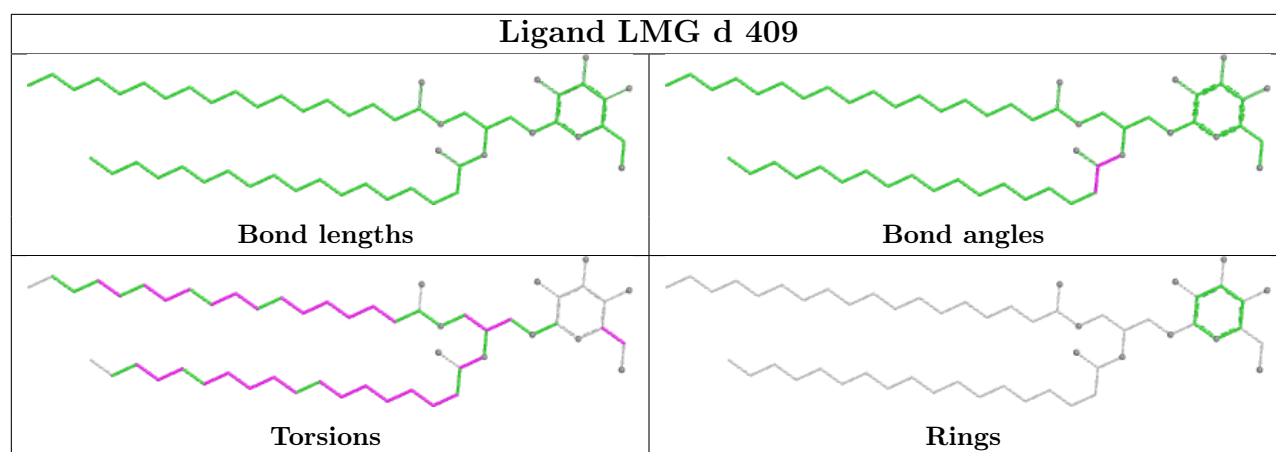


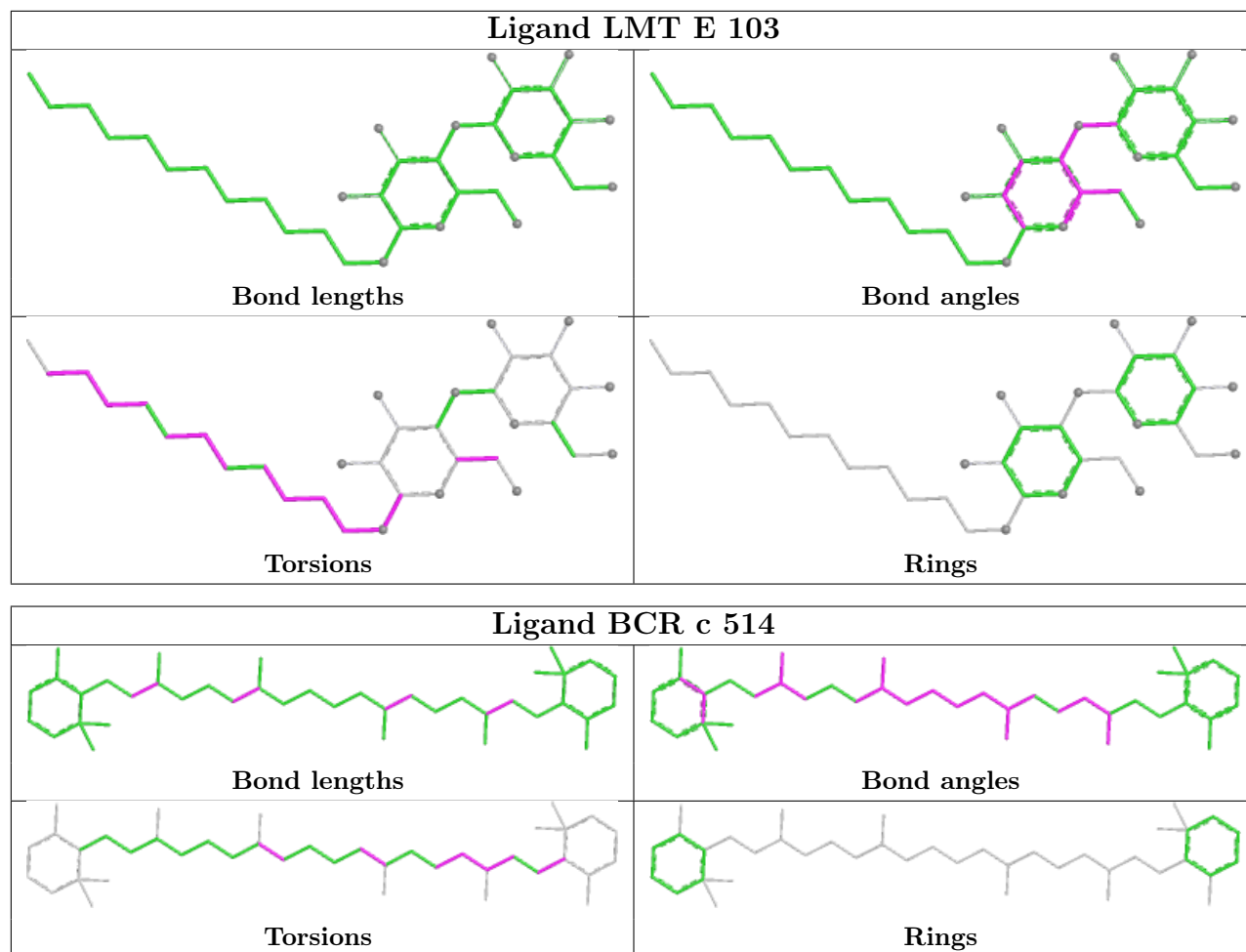
Ligand CLA b 607

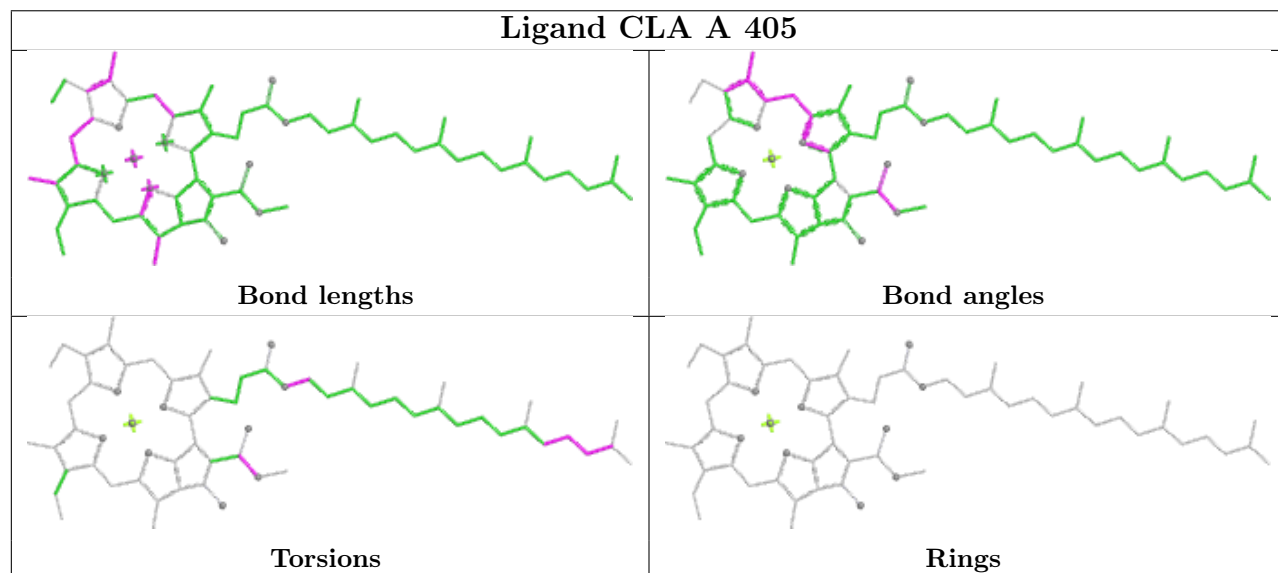
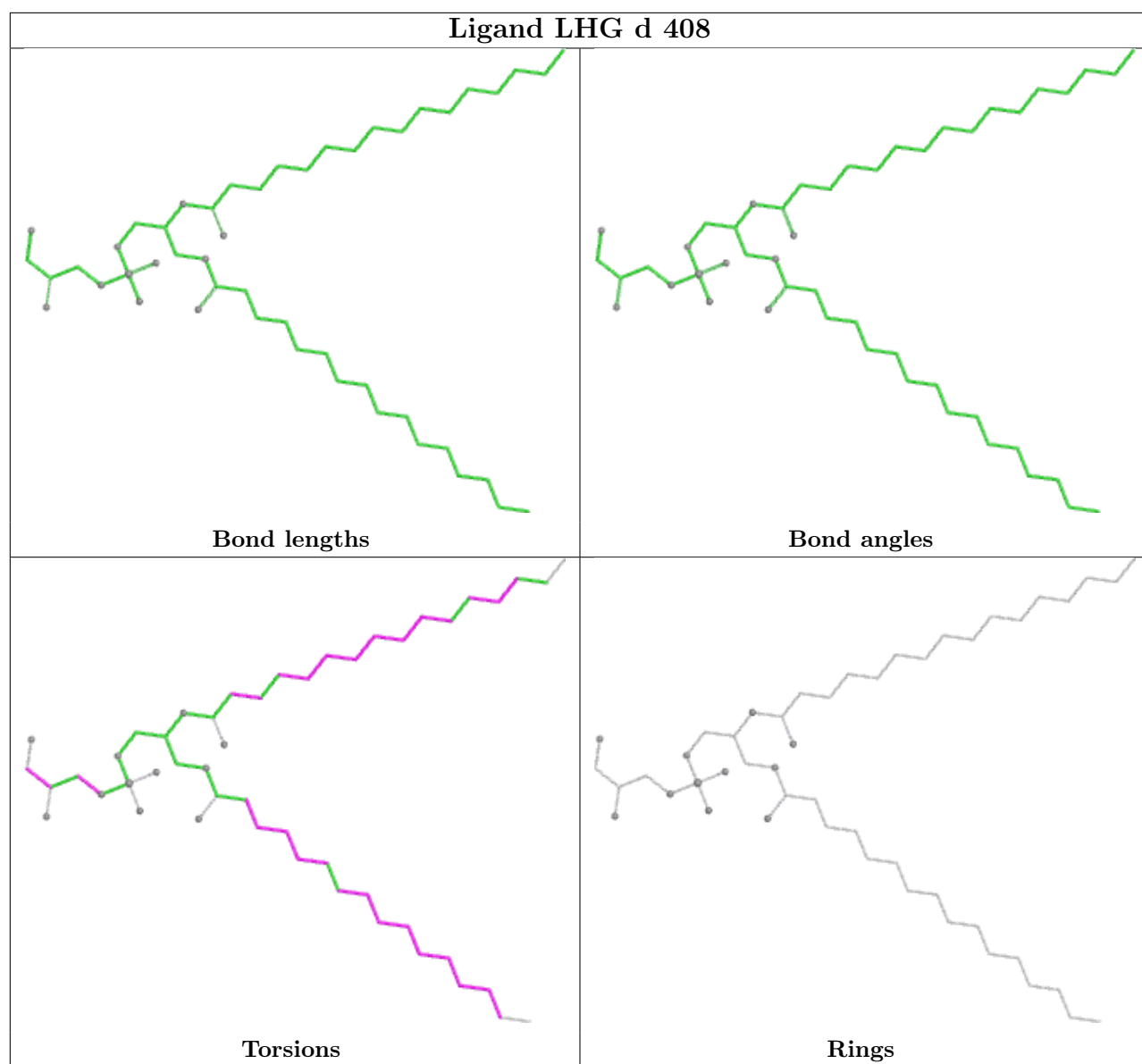


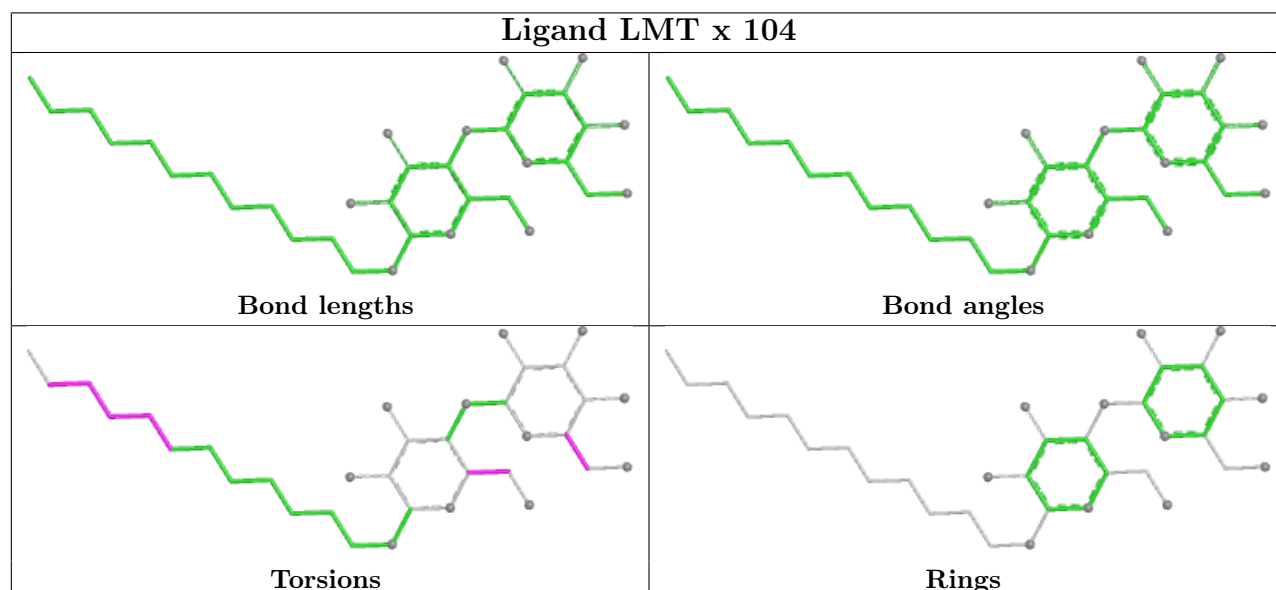
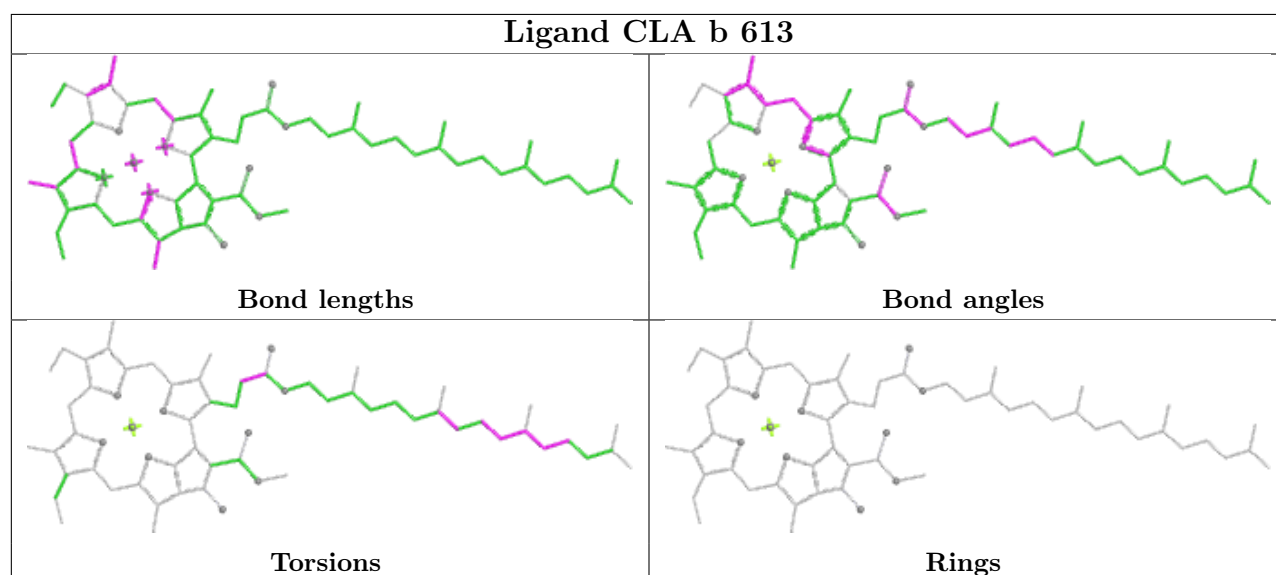
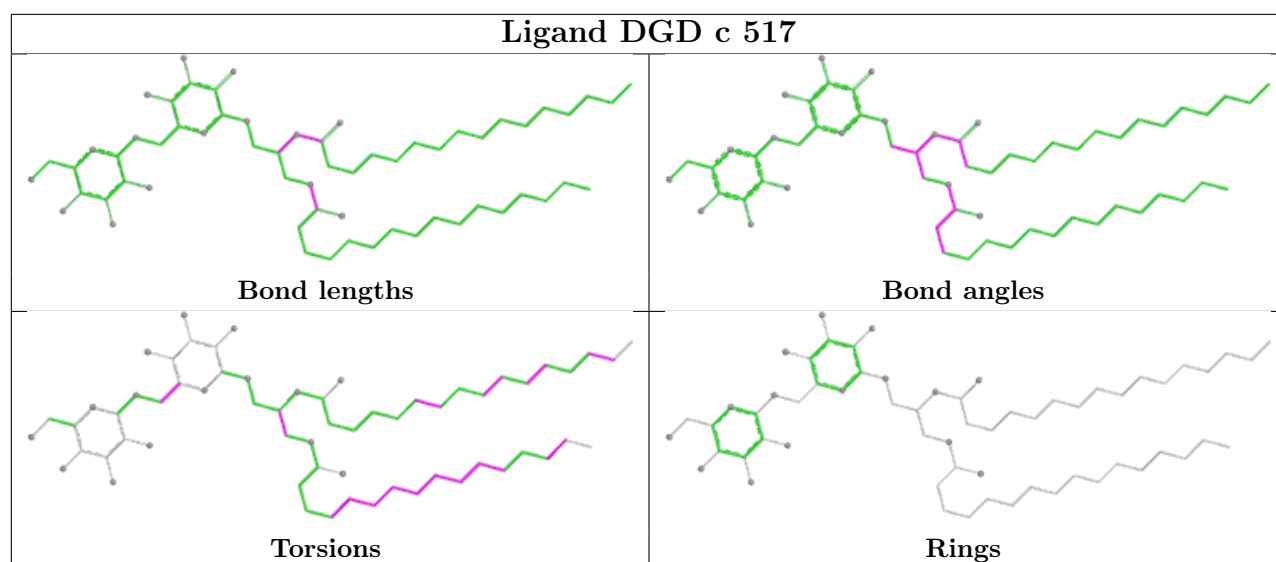


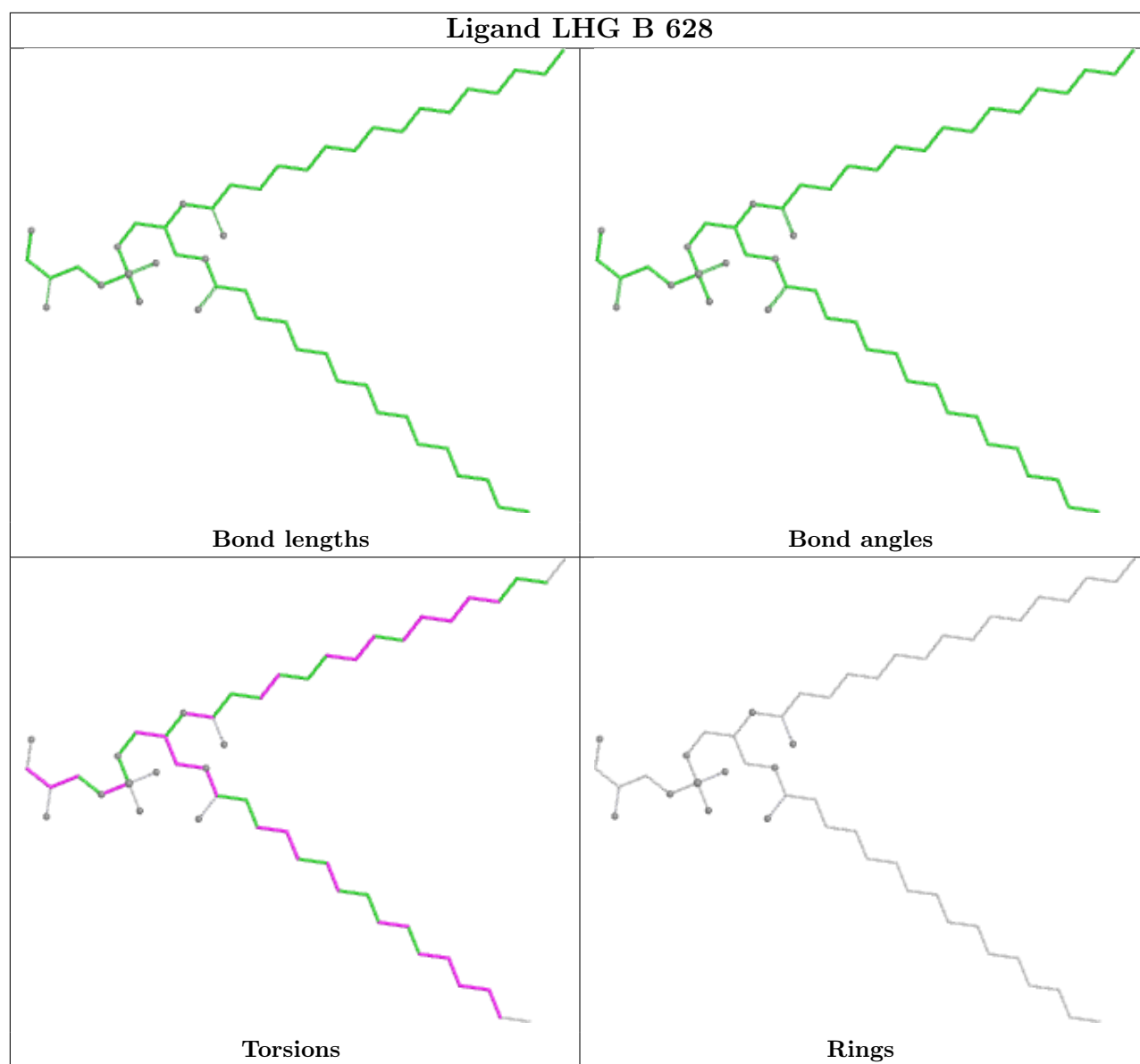


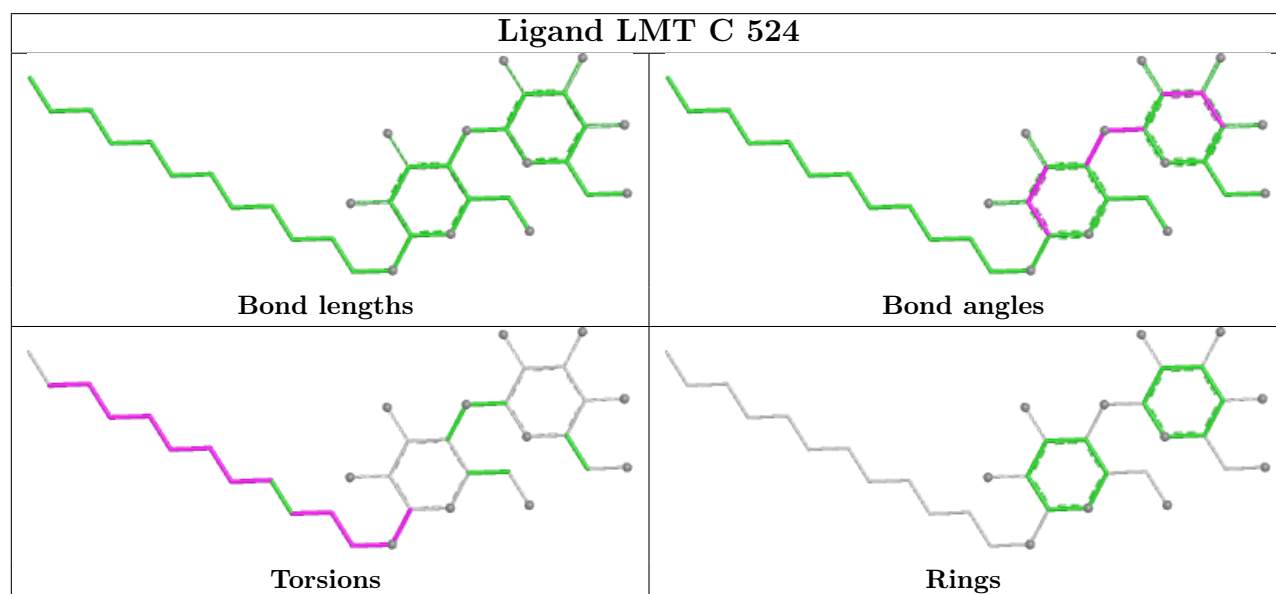
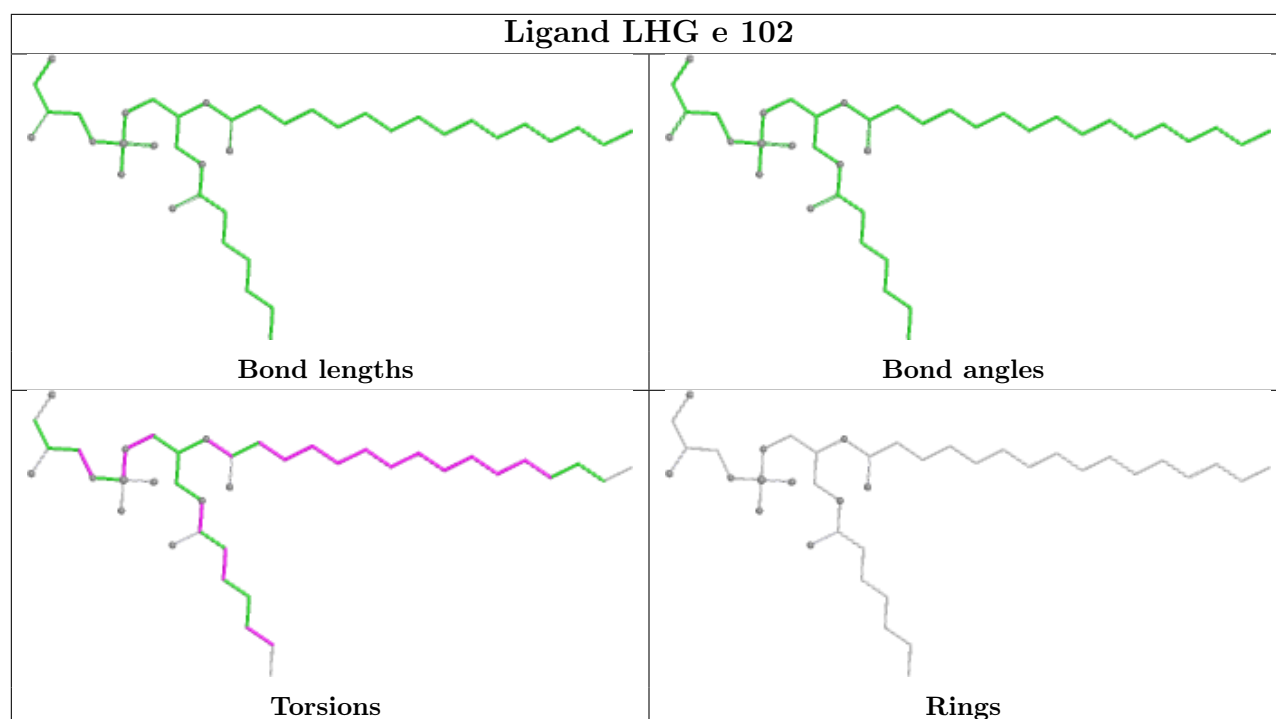


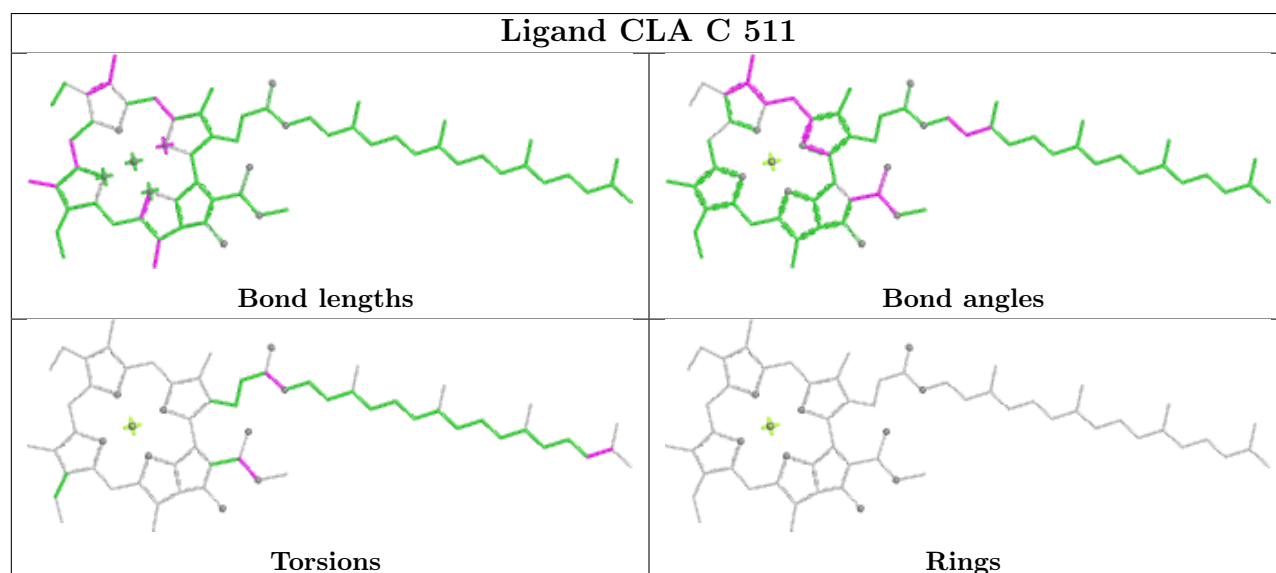
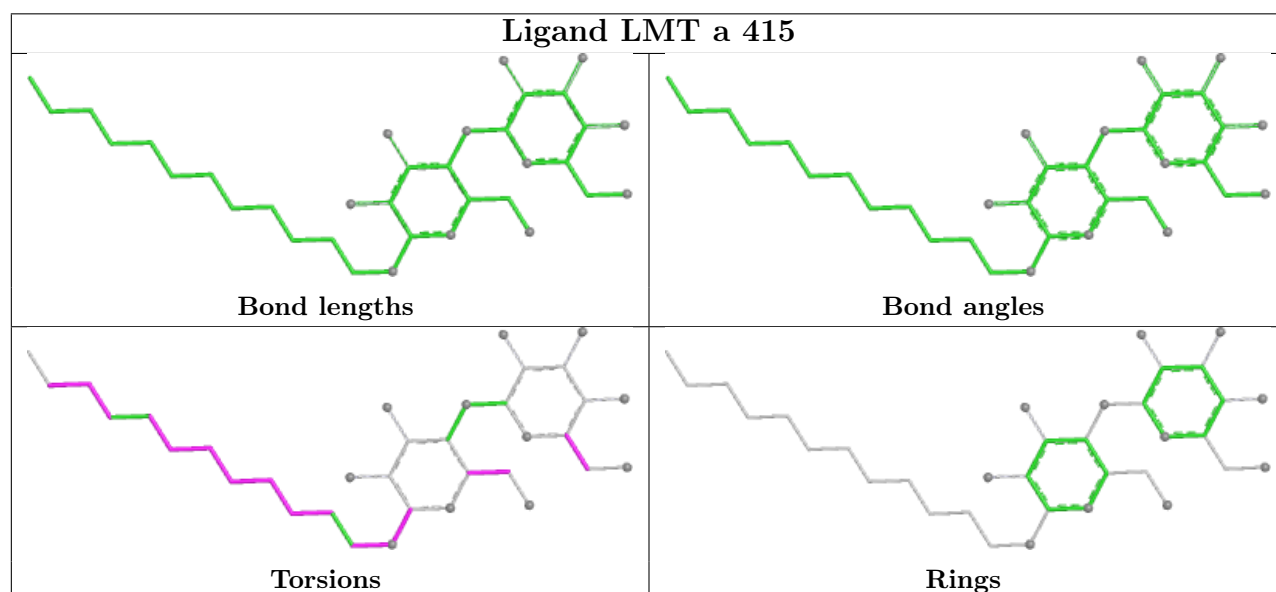
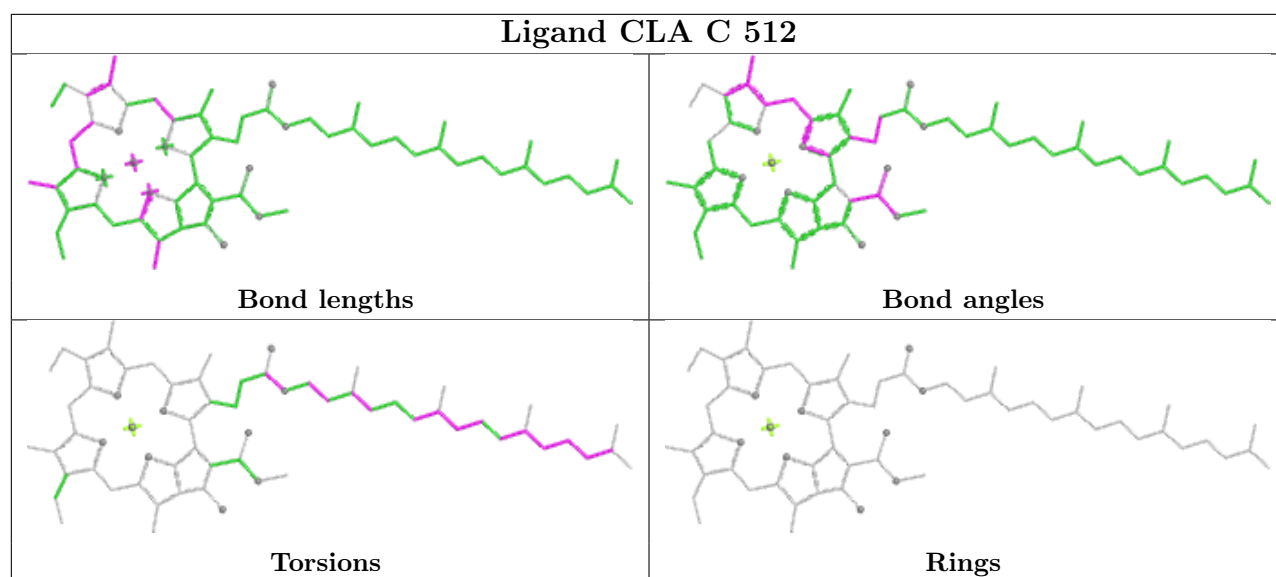


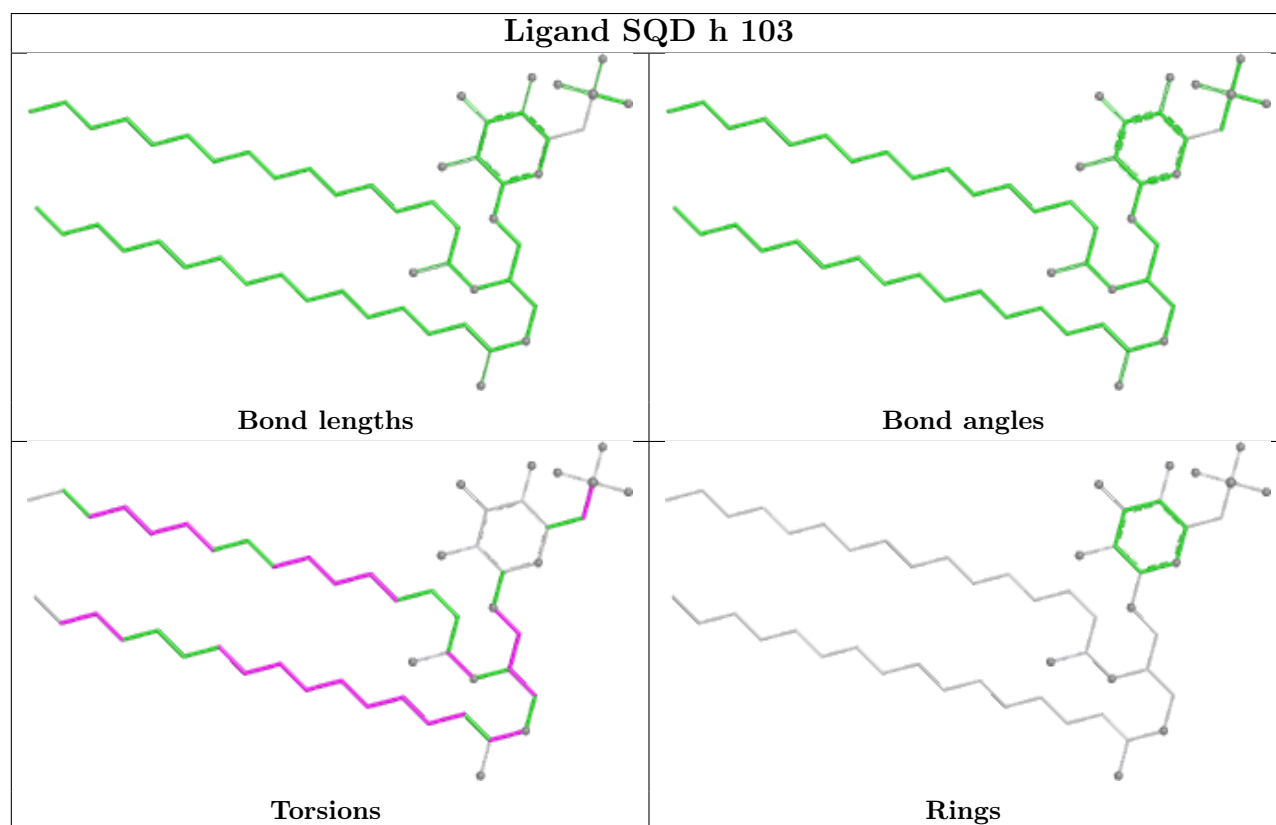
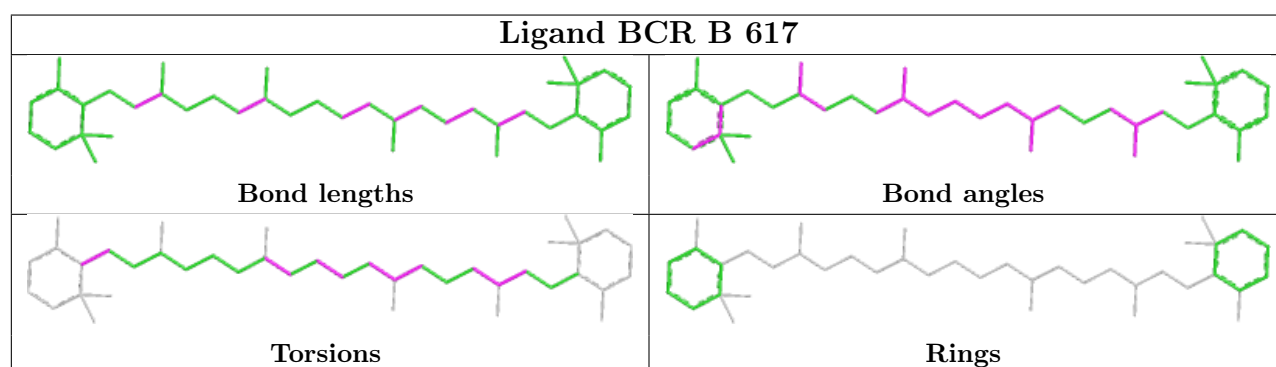
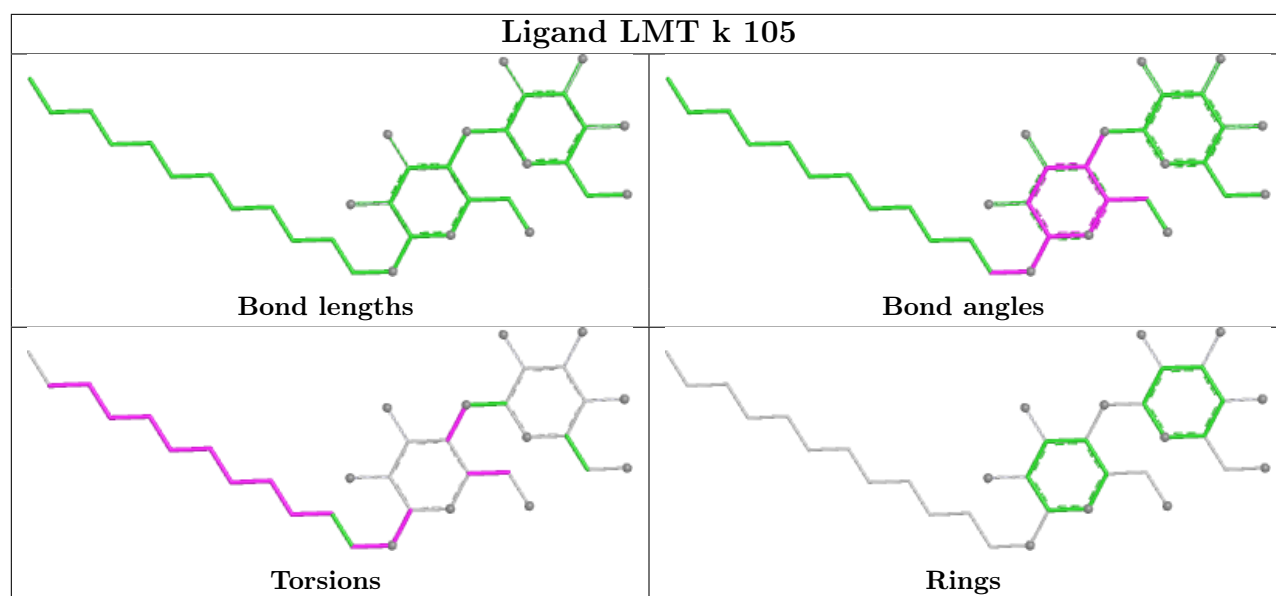




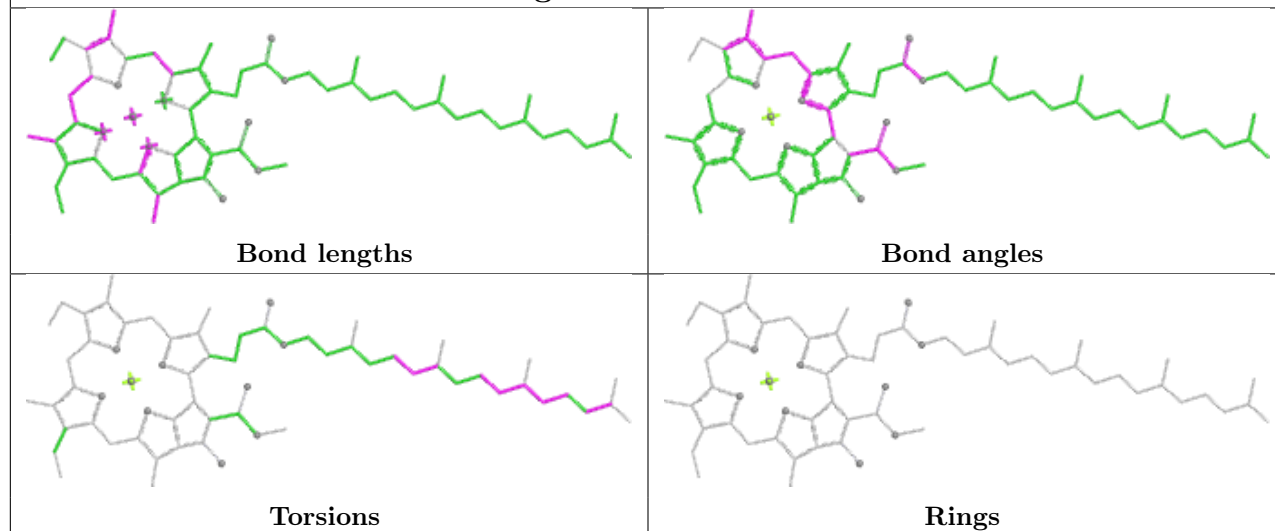




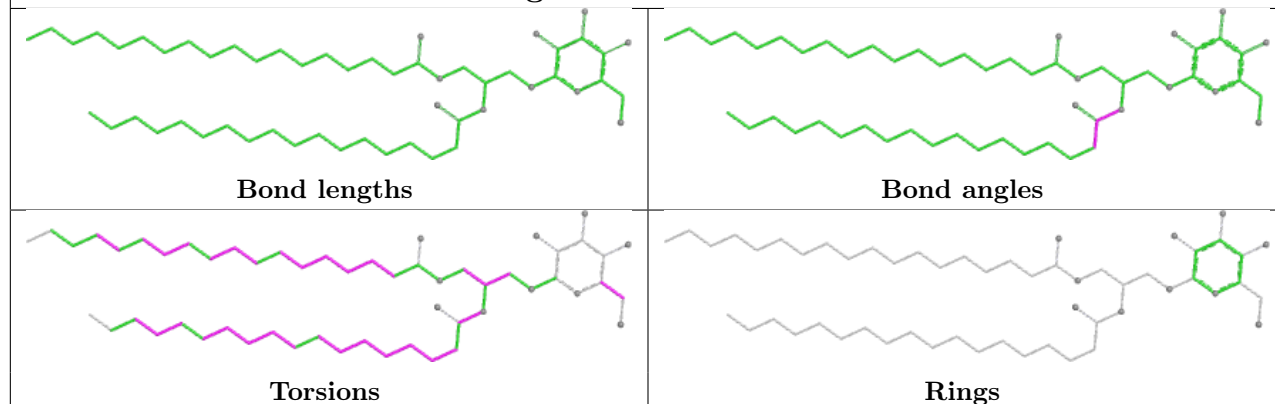




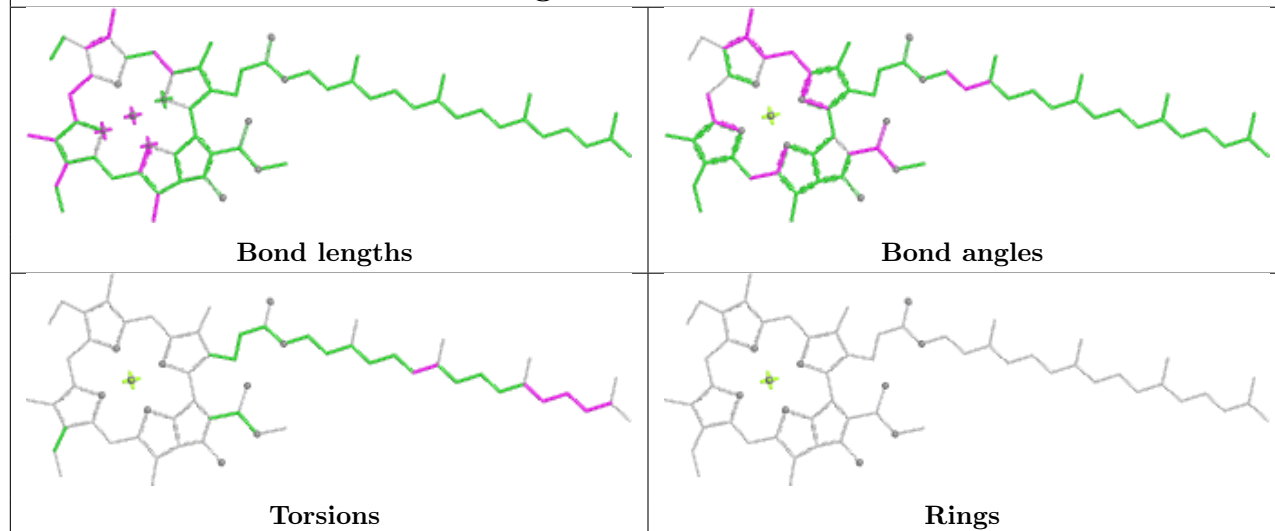
Ligand CLA b 615



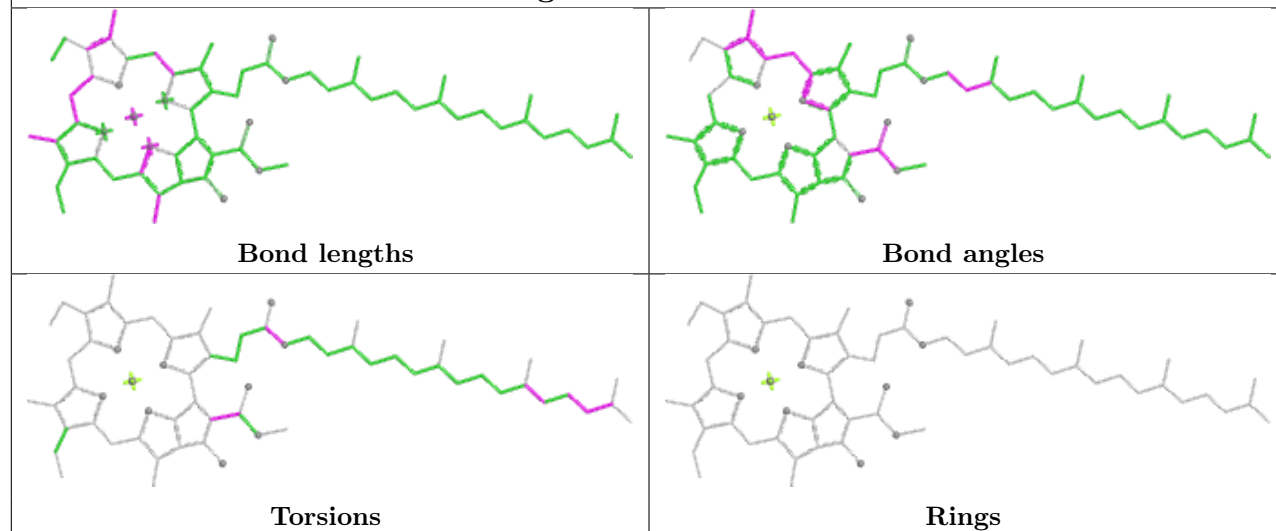
Ligand LMG D 409



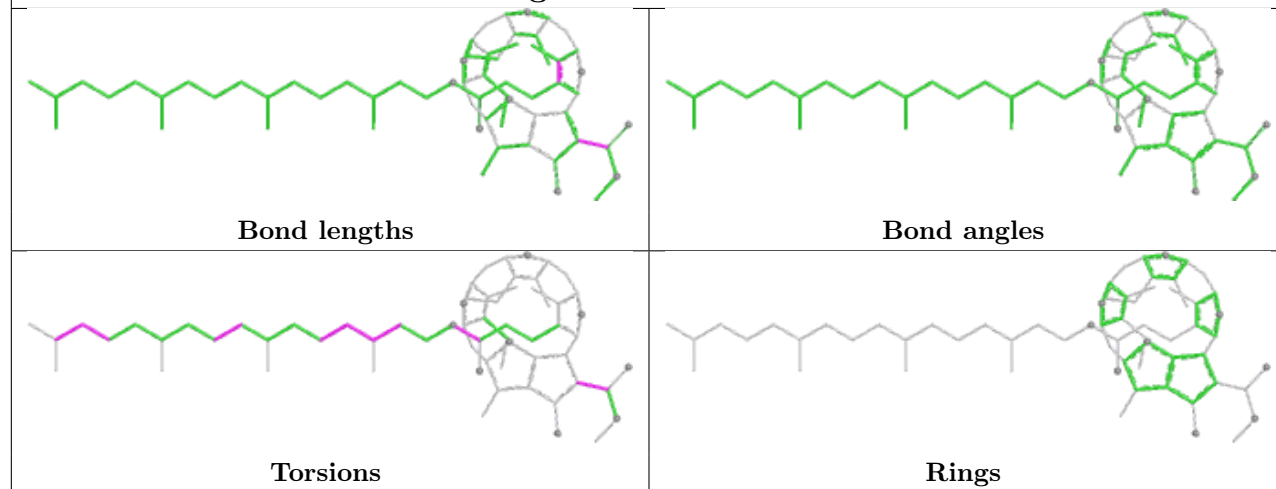
Ligand CLA d 401



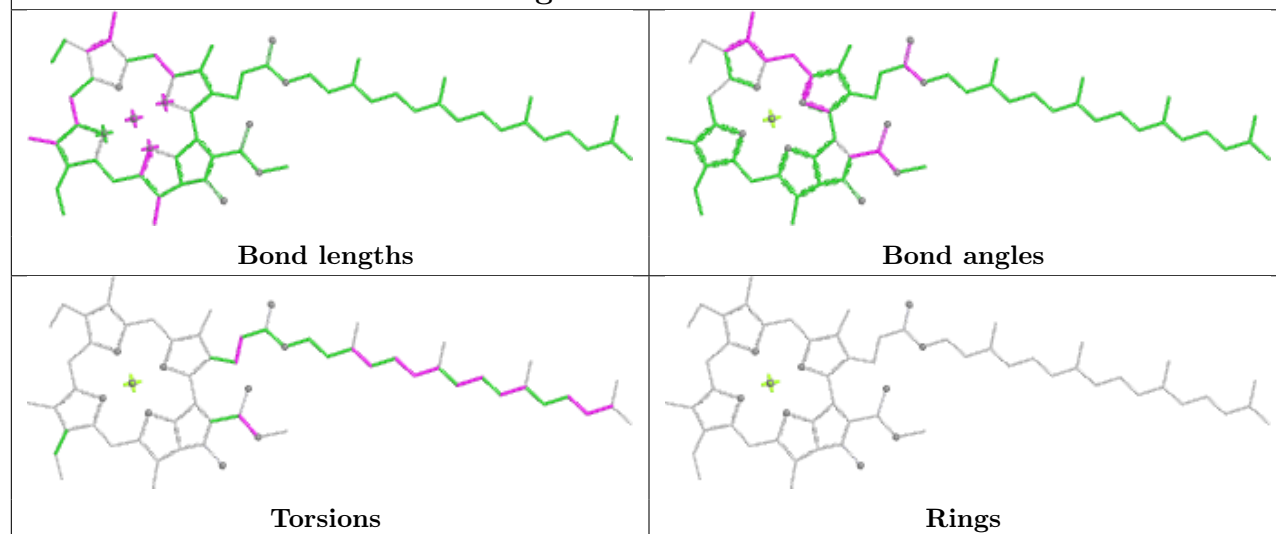
Ligand CLA c 502

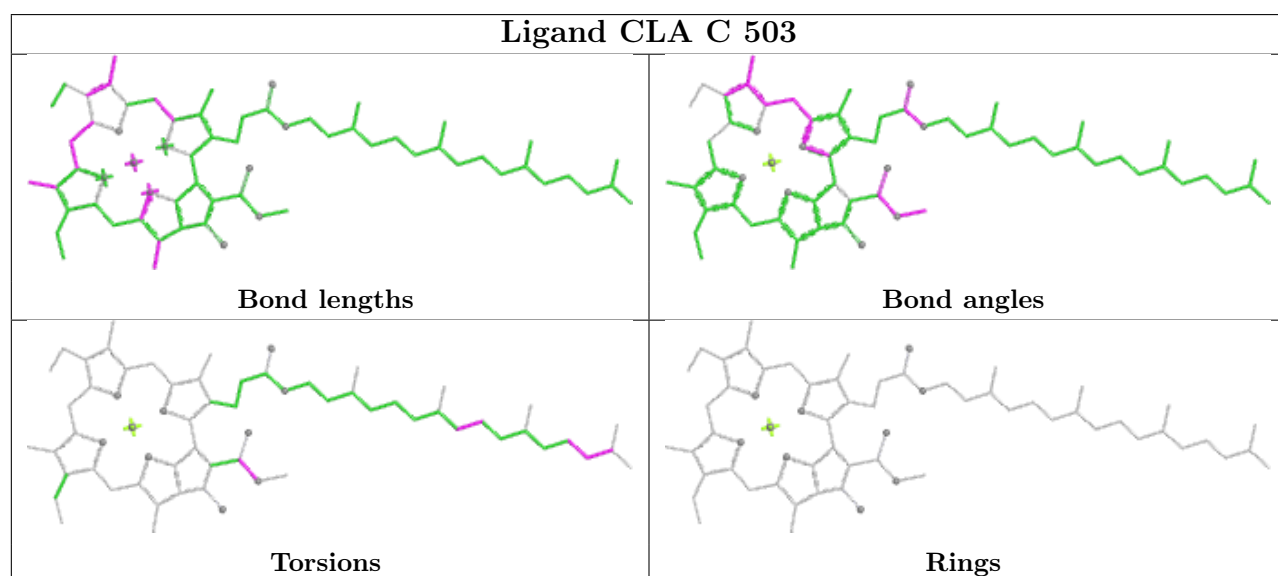
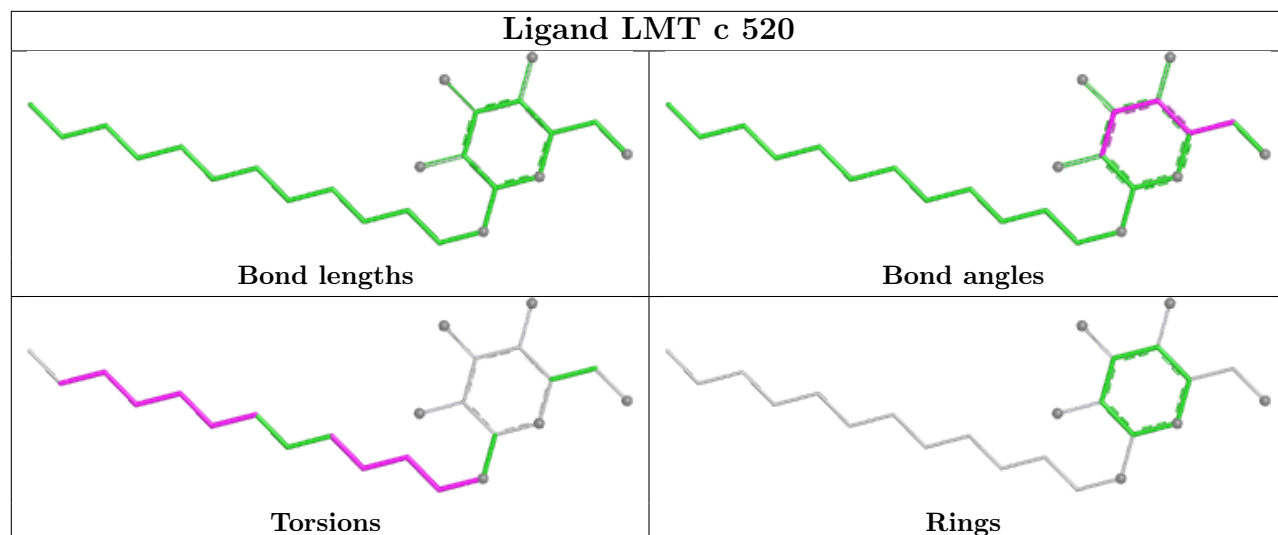


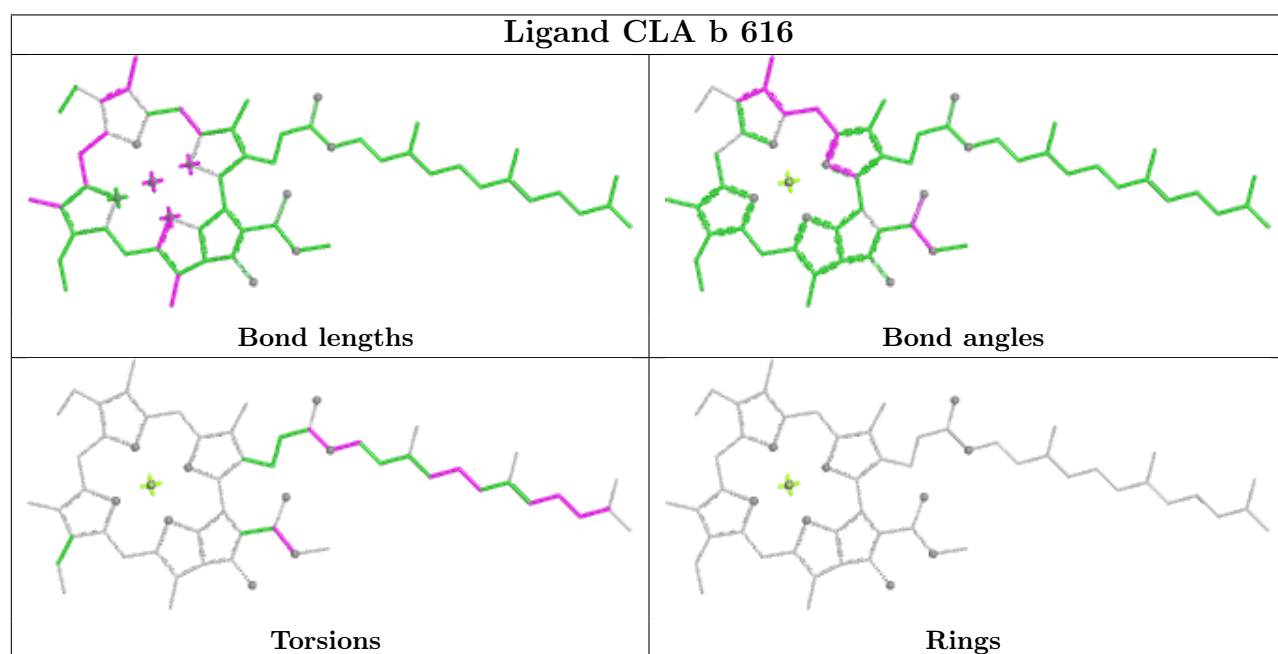
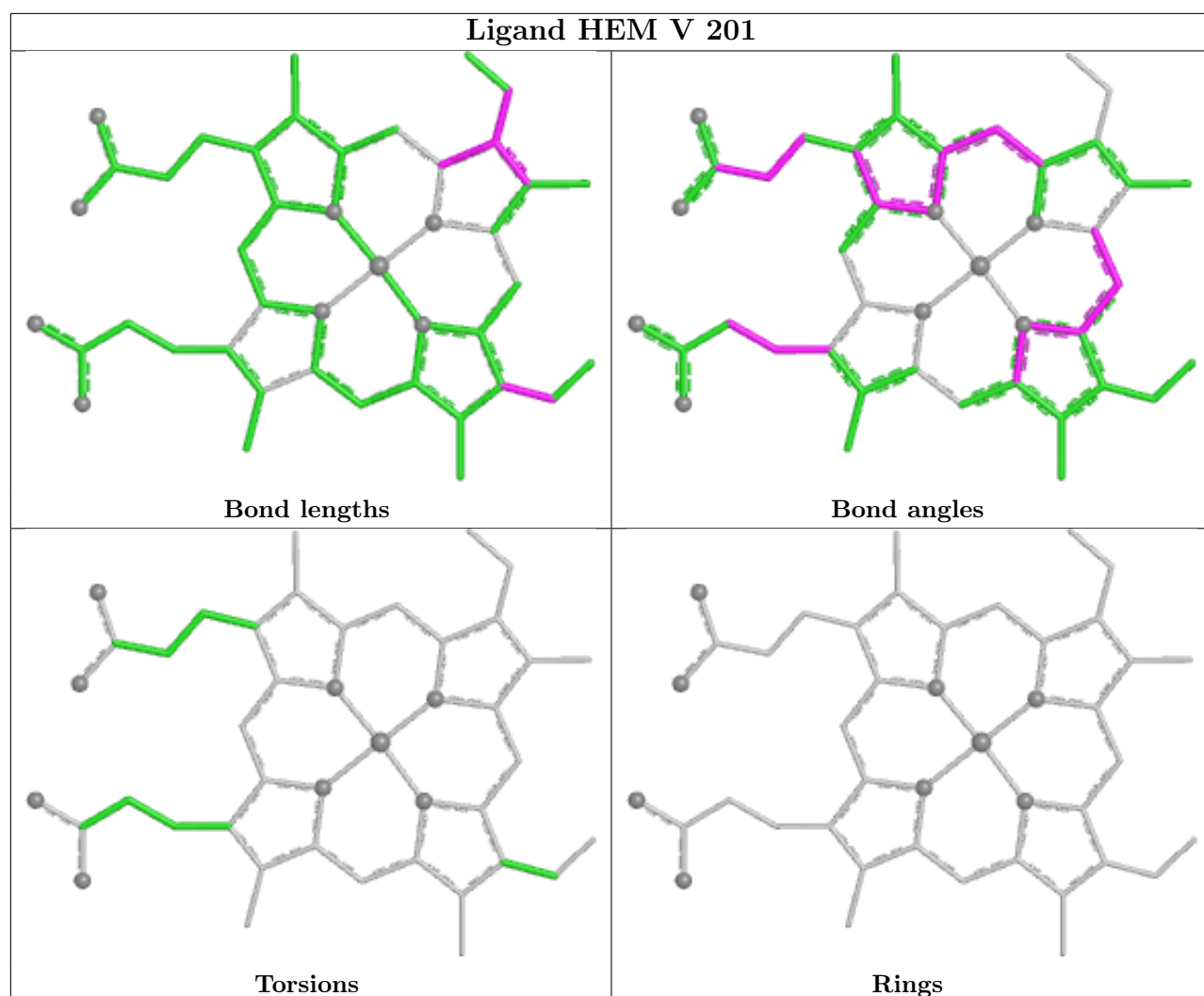
Ligand PHO A 407

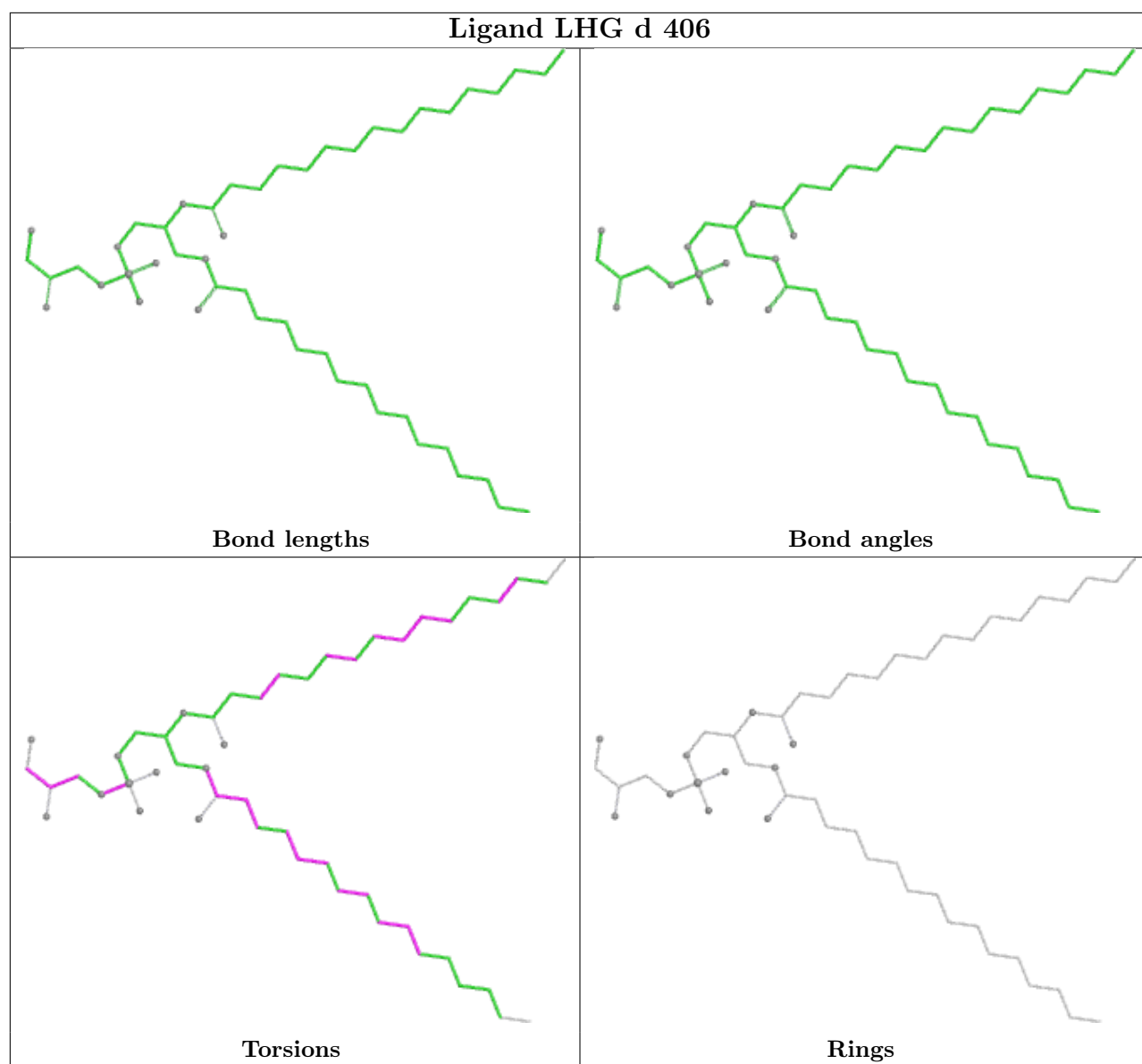


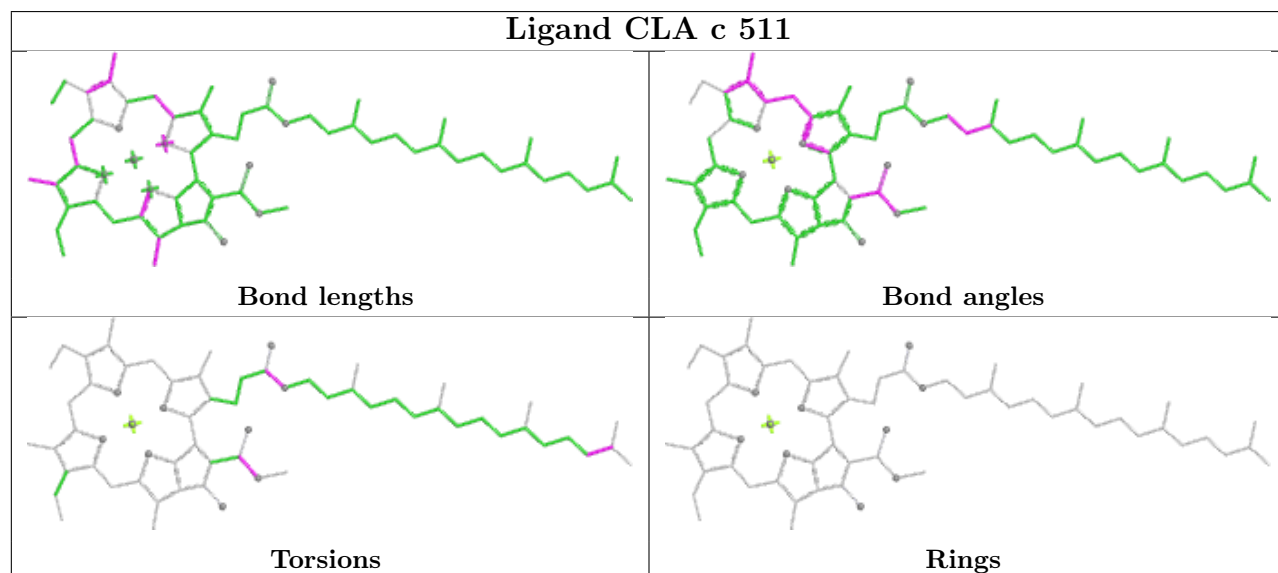
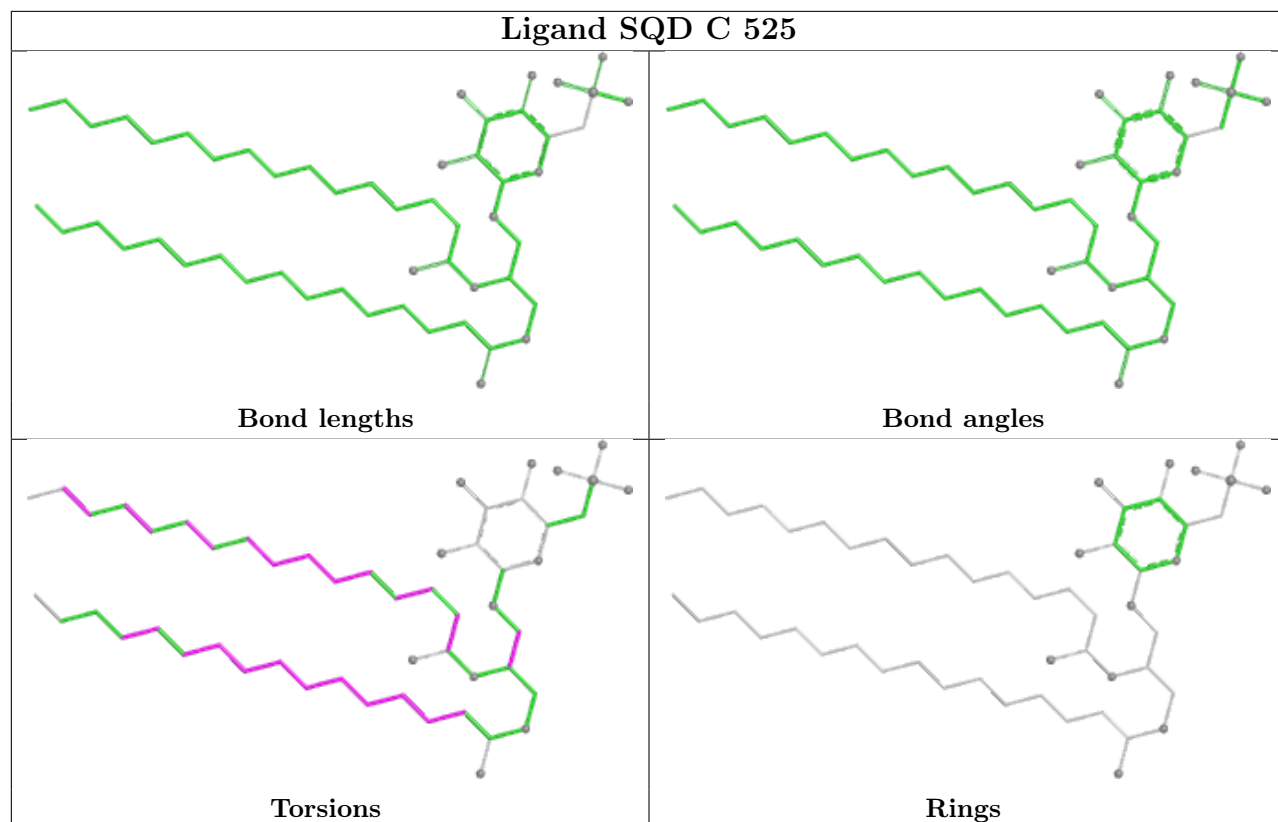
Ligand CLA b 603

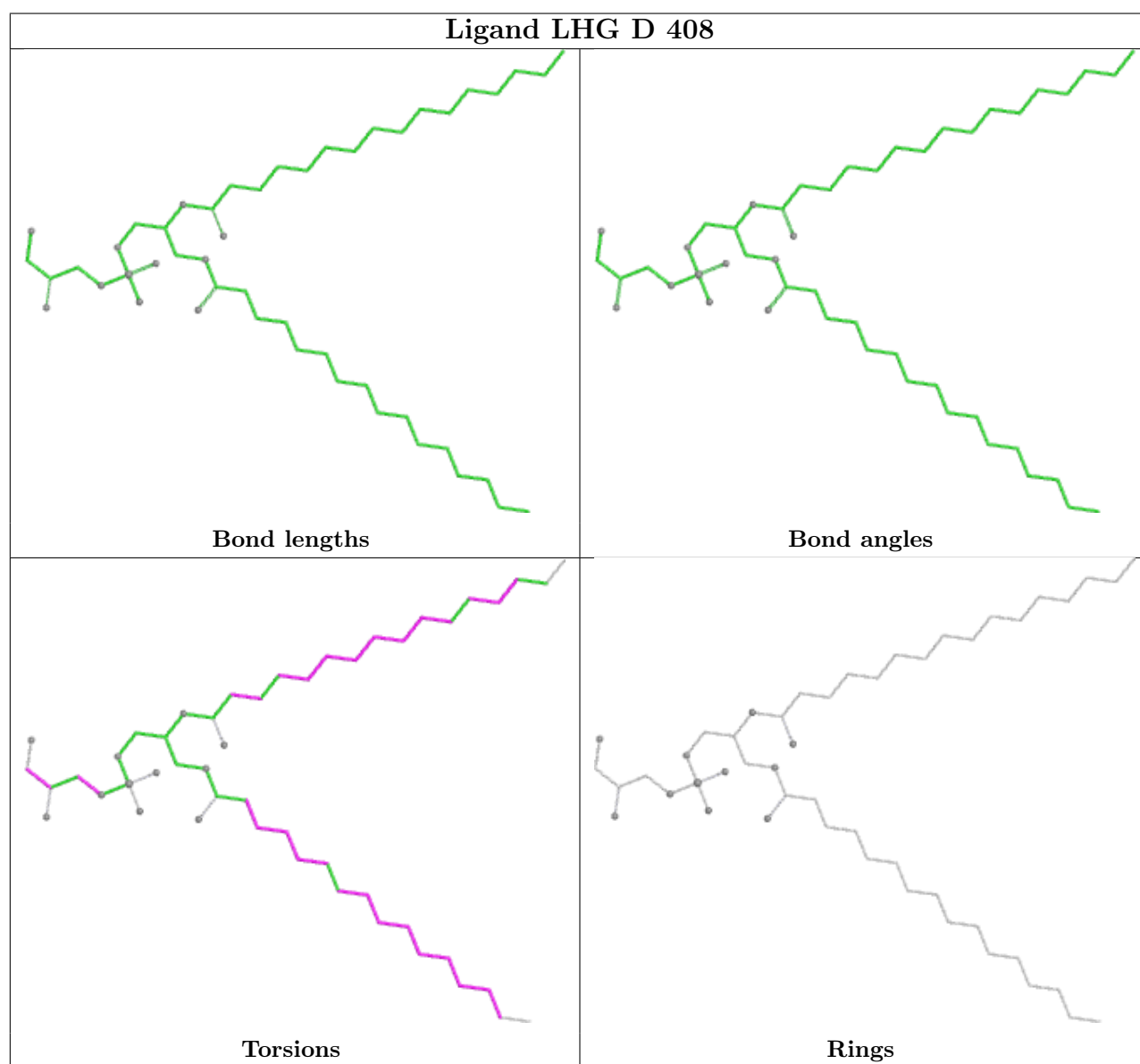
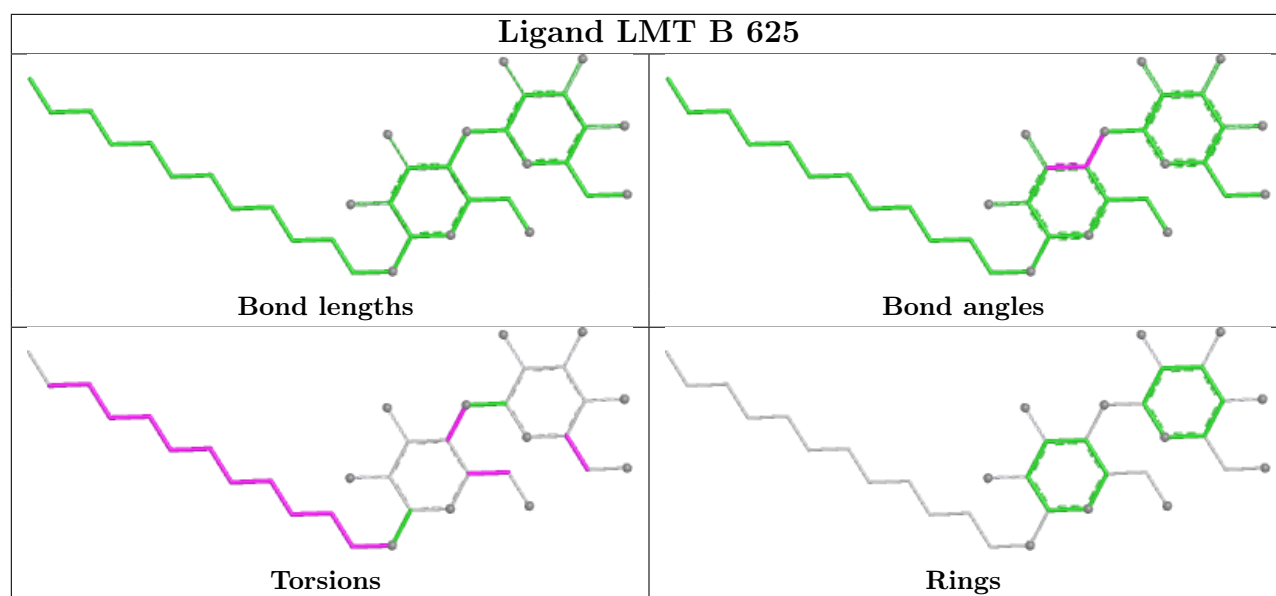


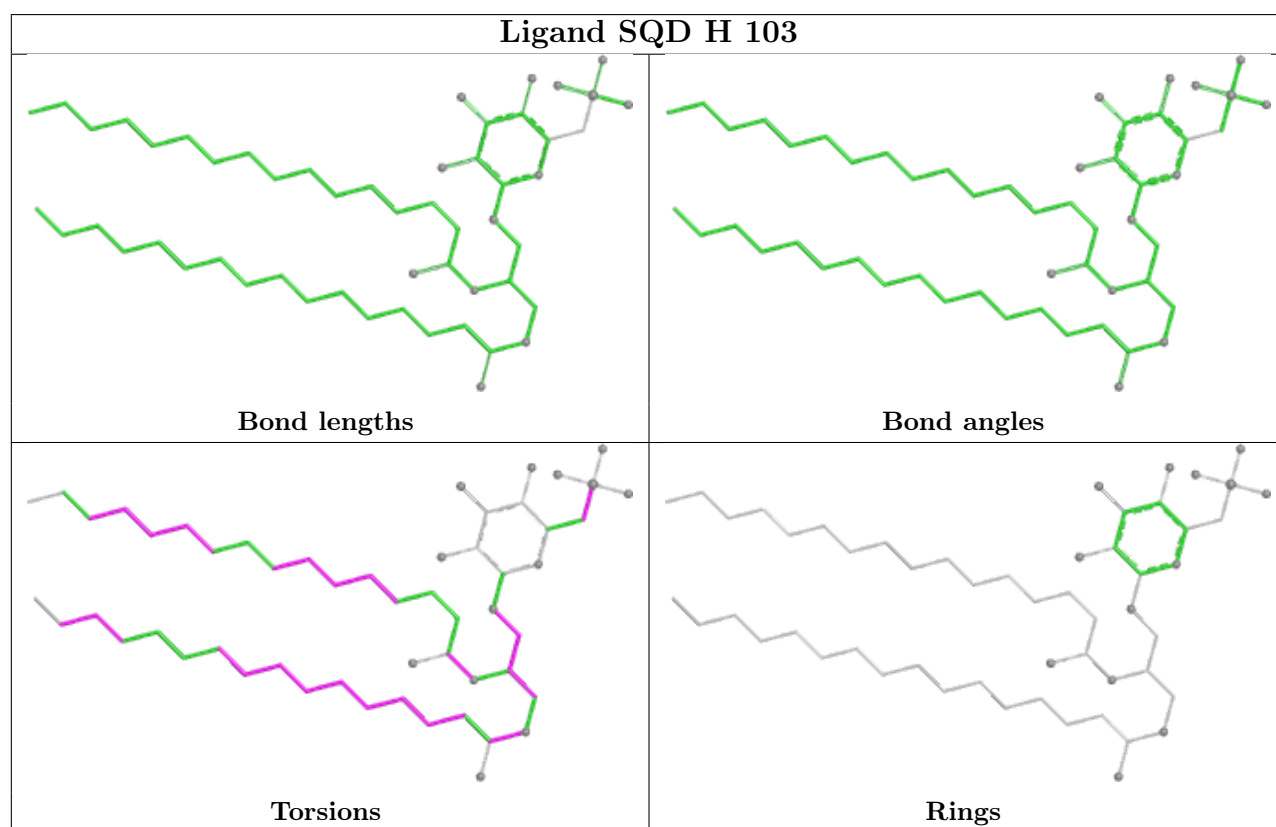
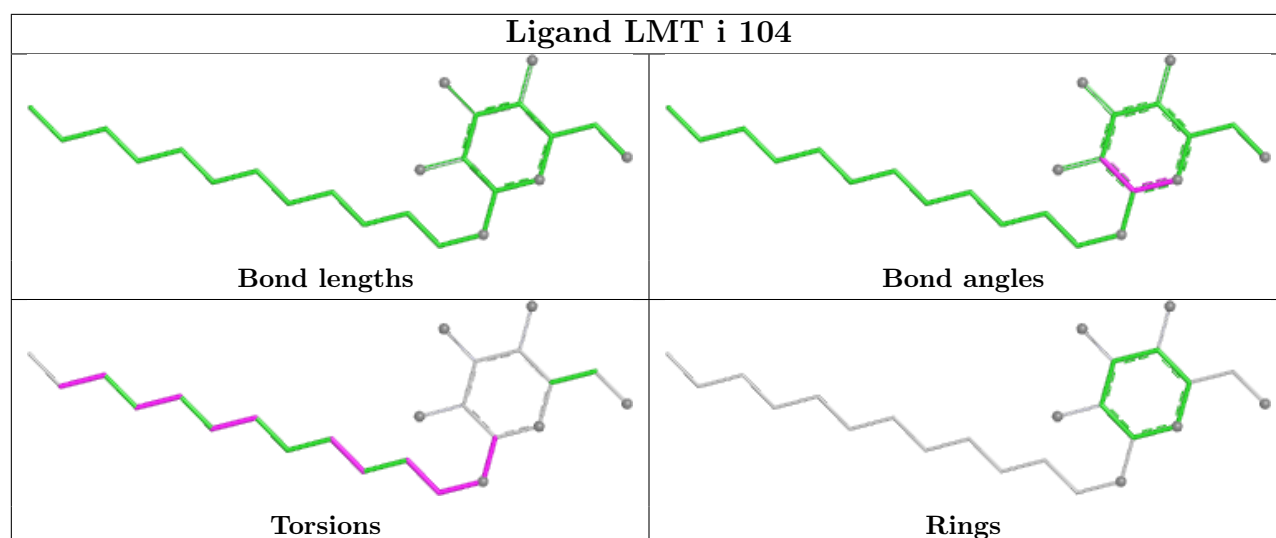


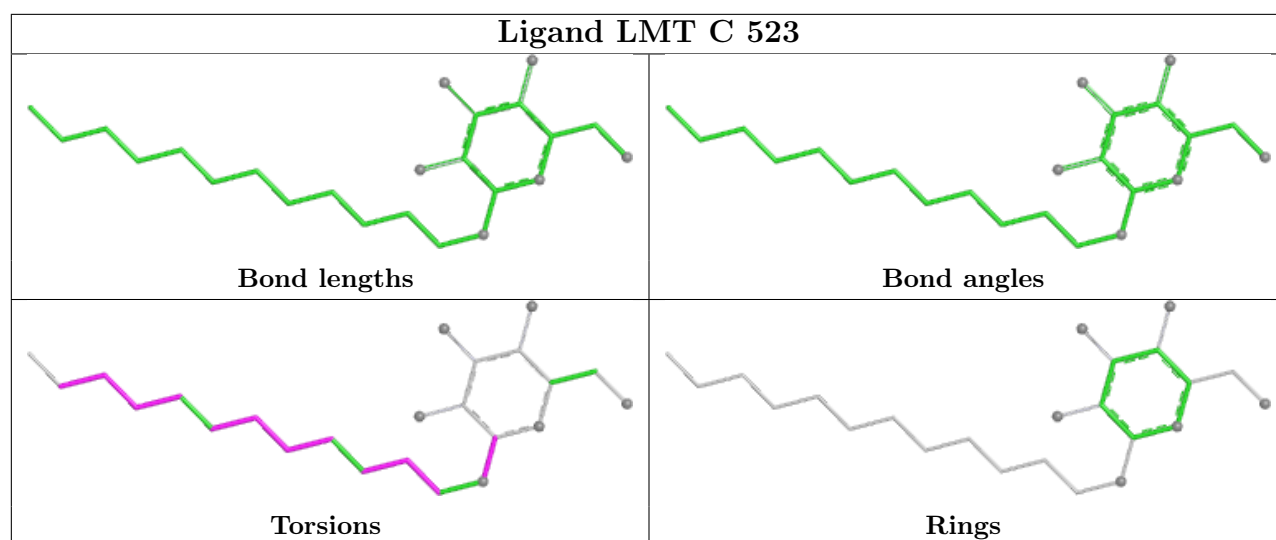
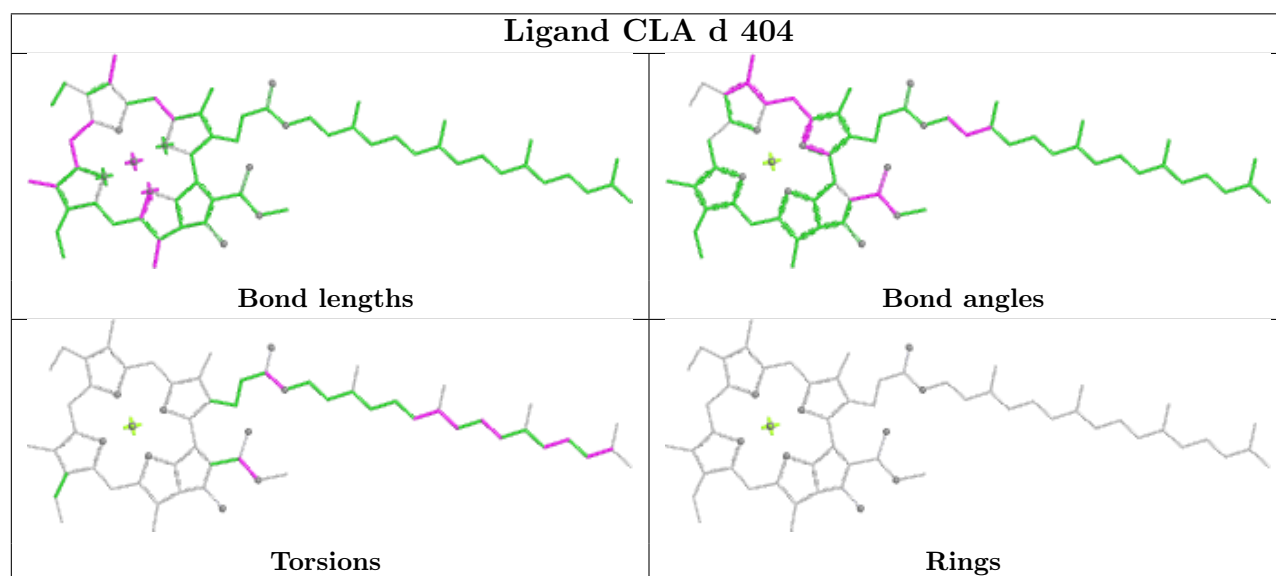
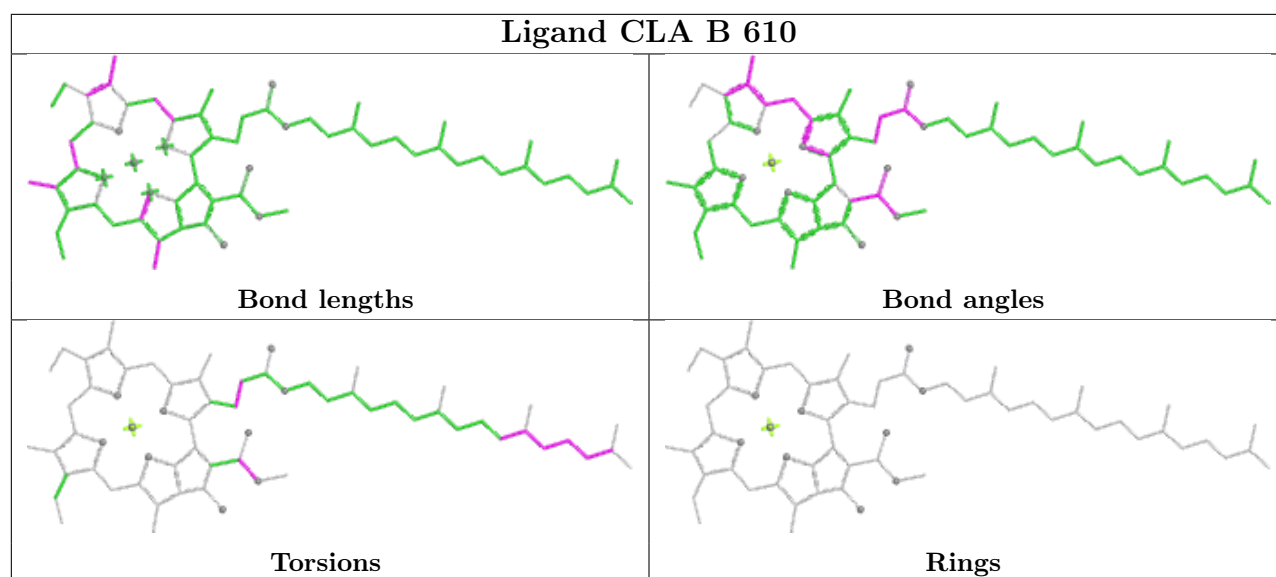


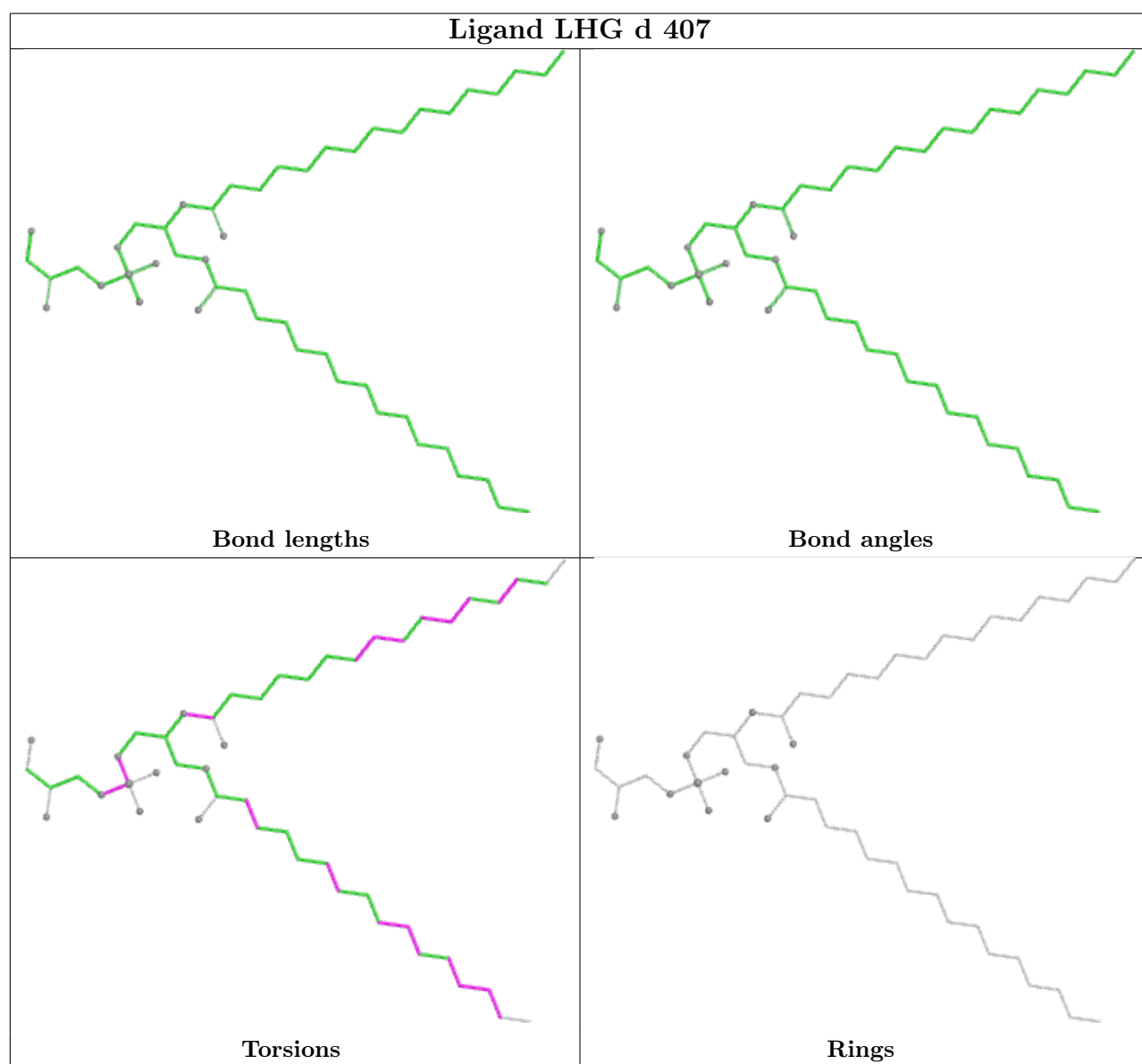
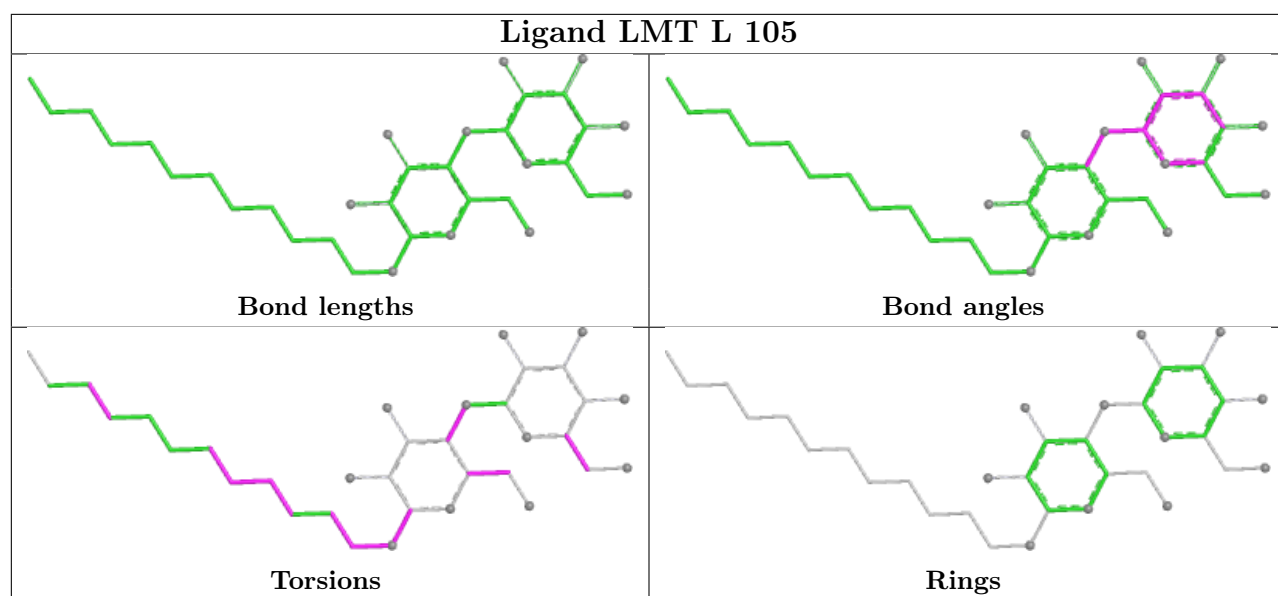


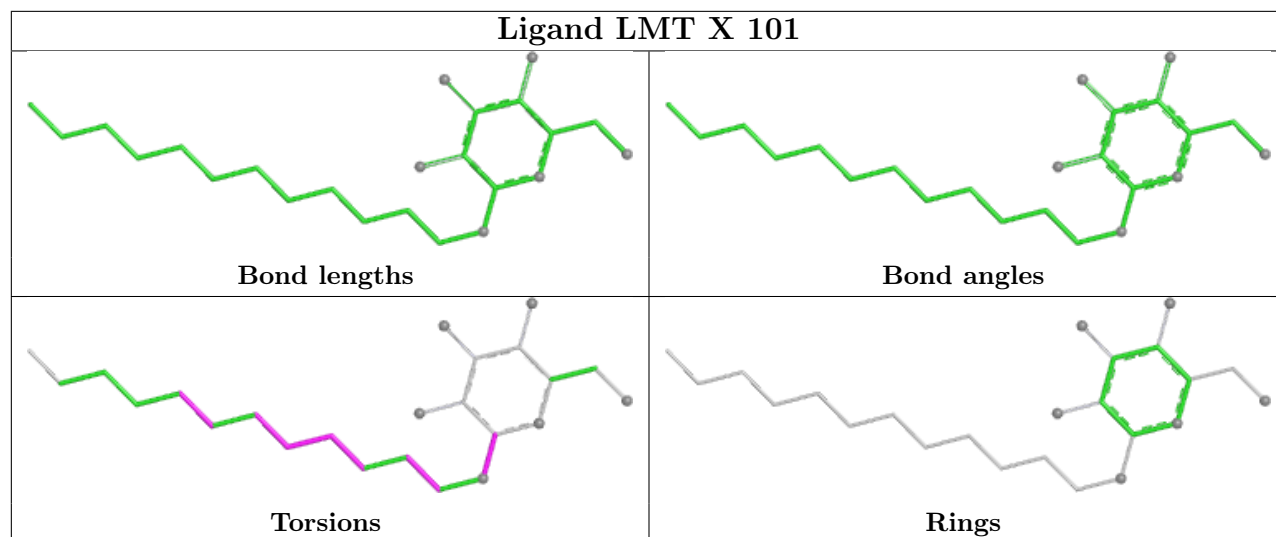
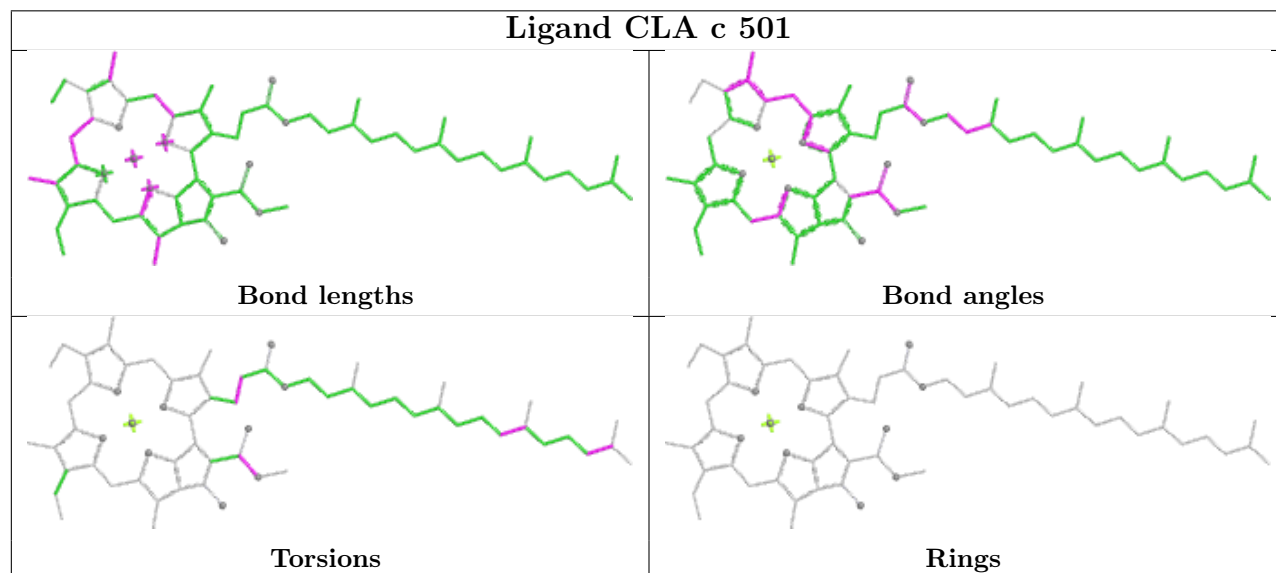
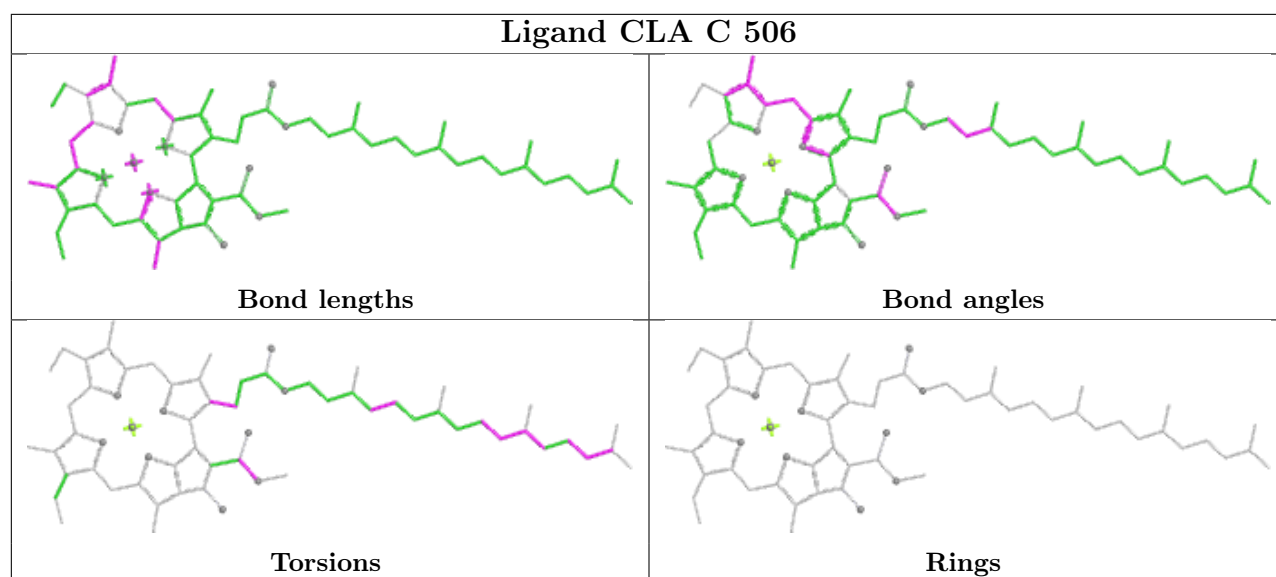


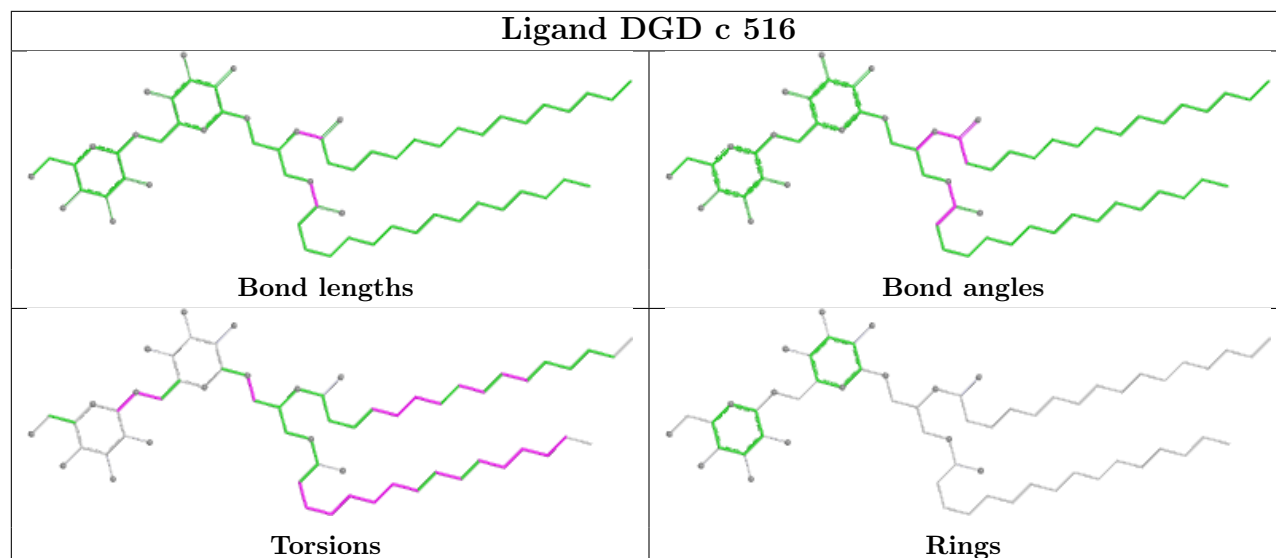
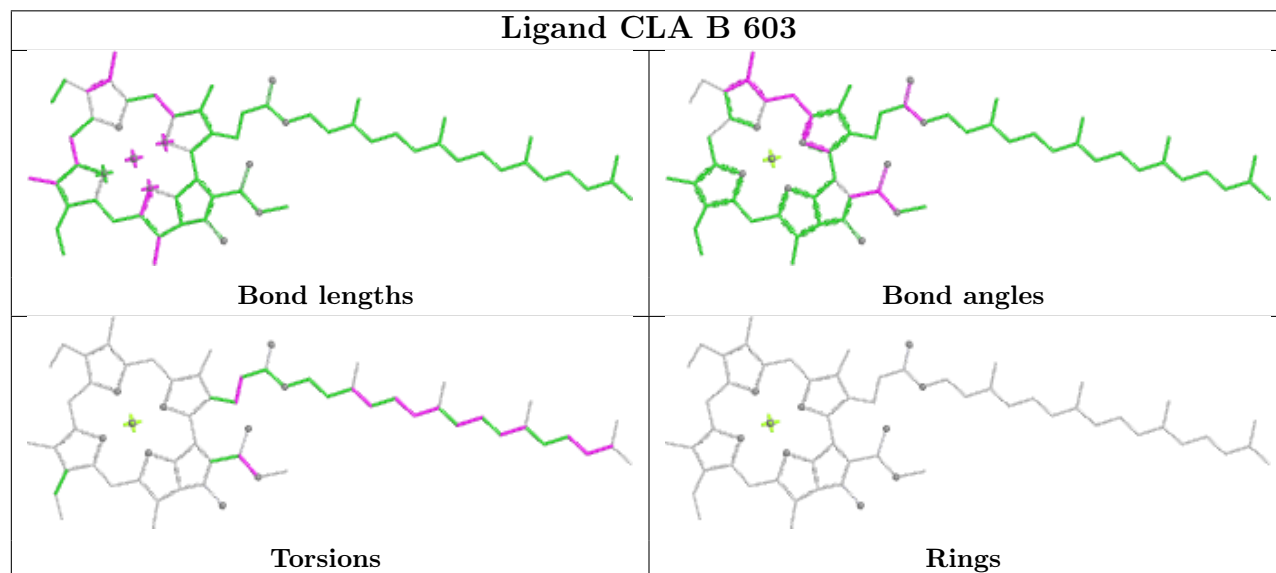
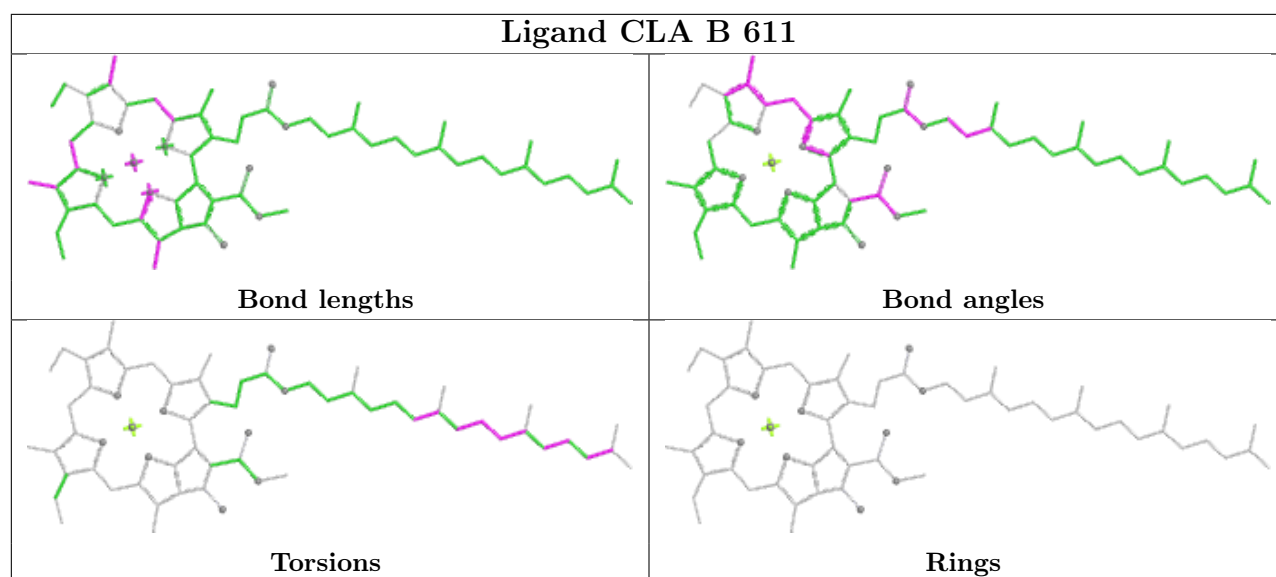


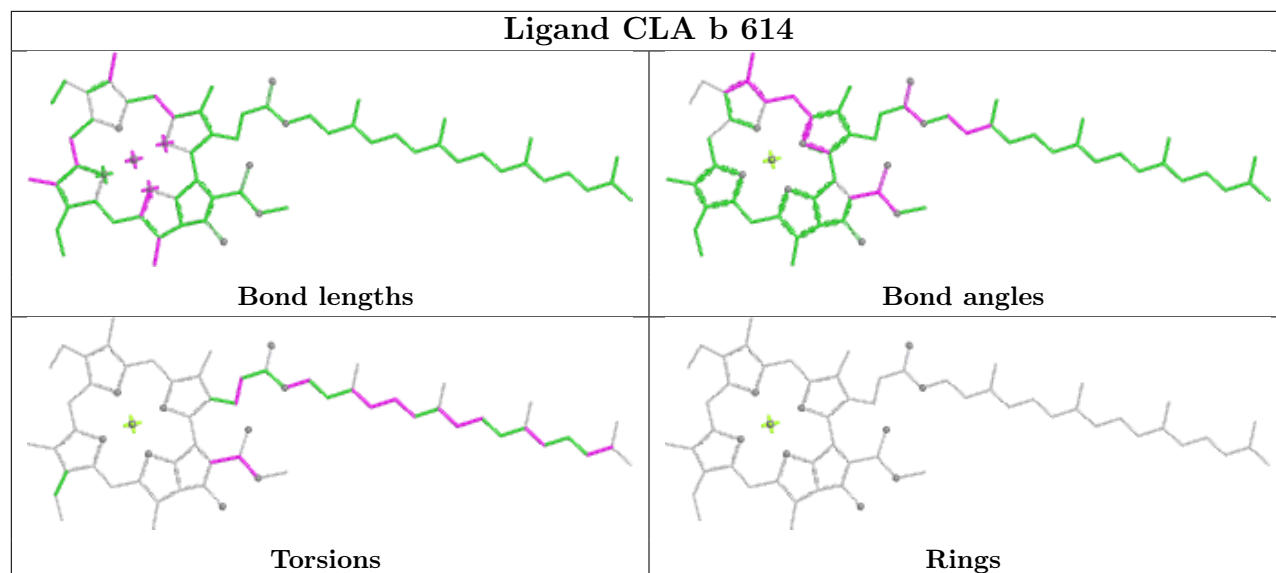
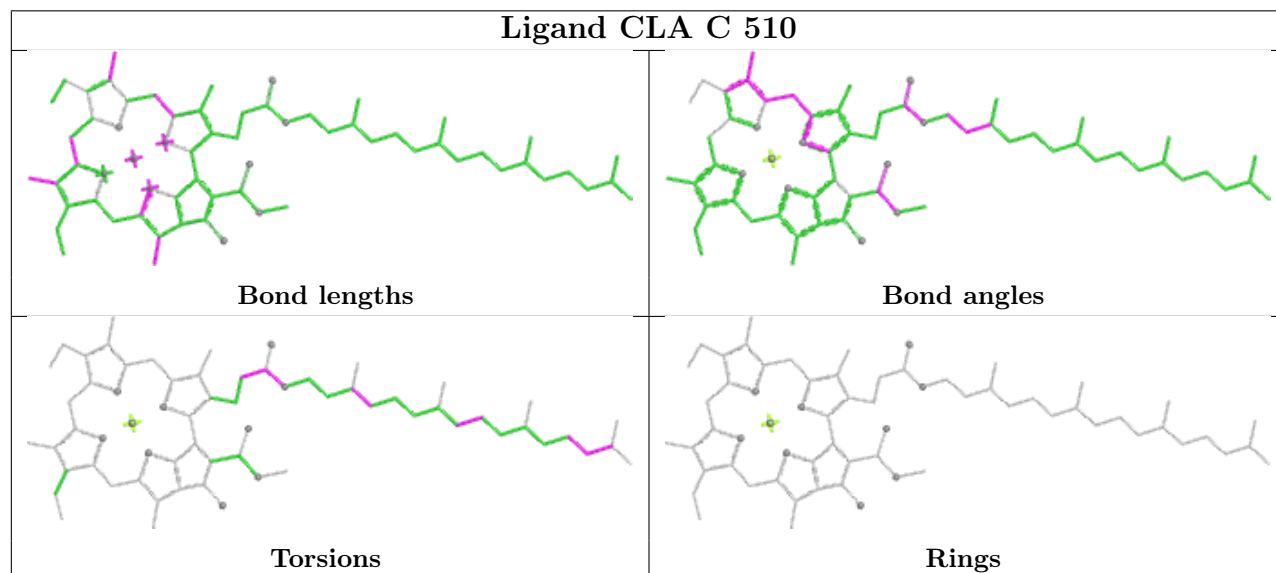
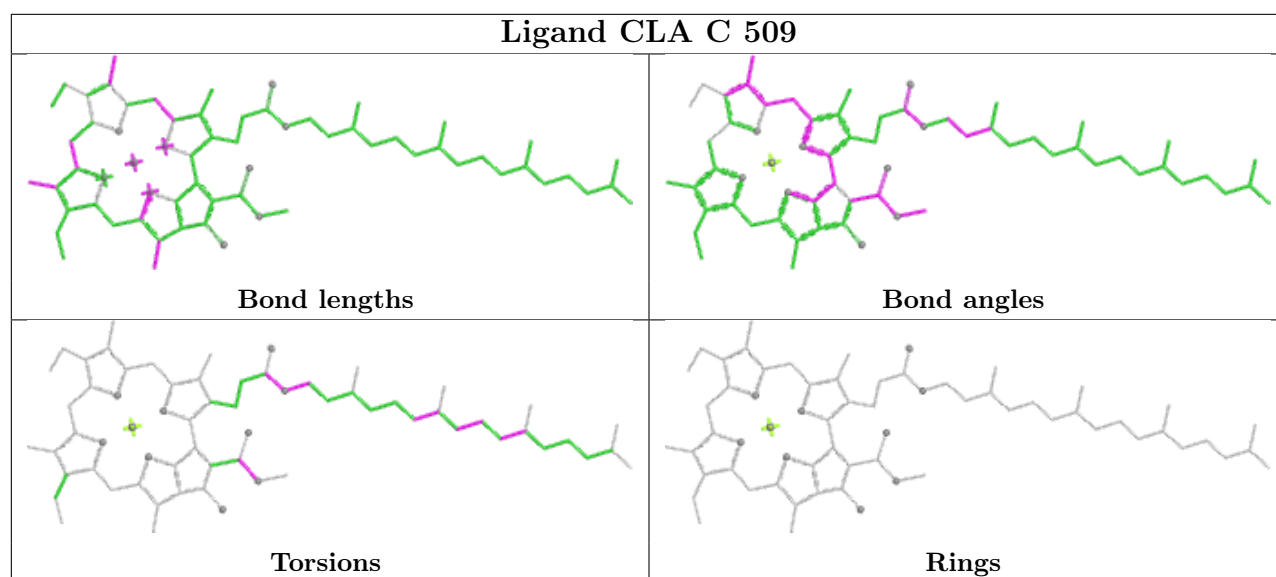


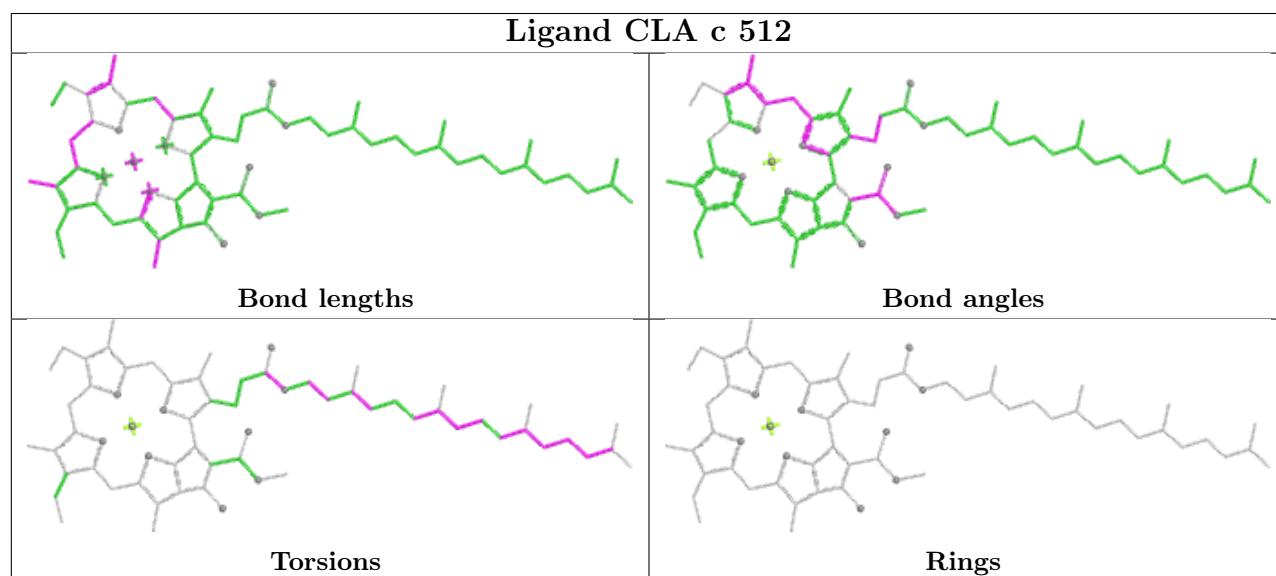
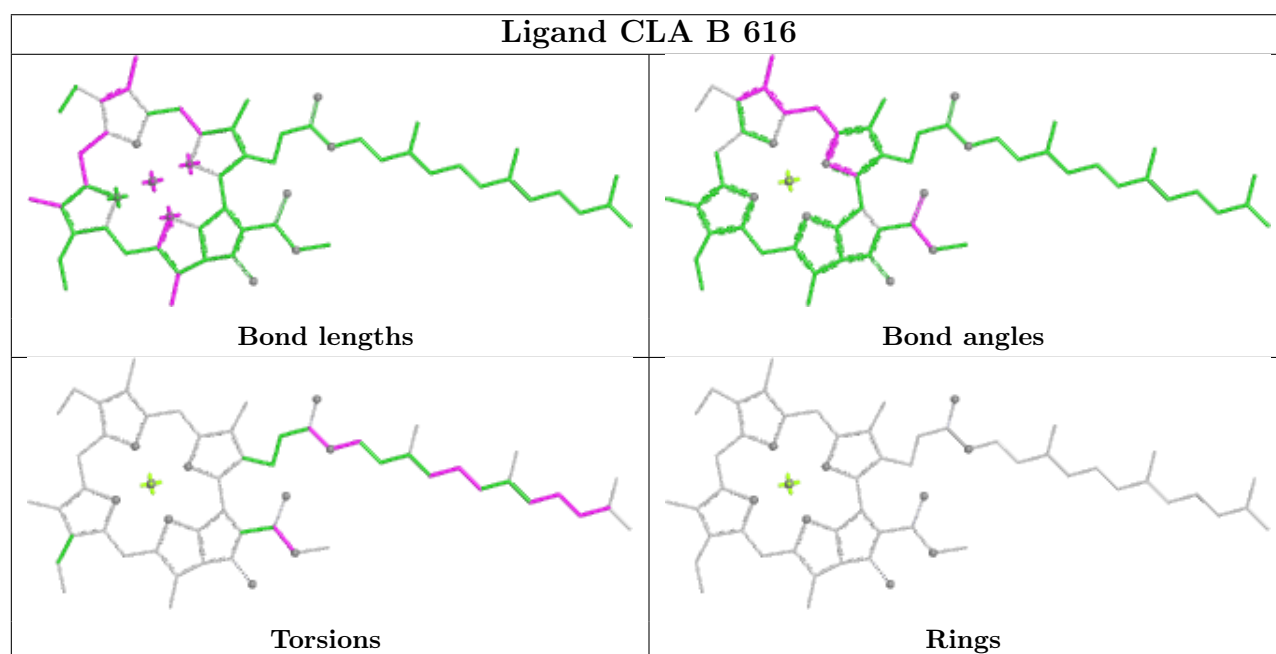
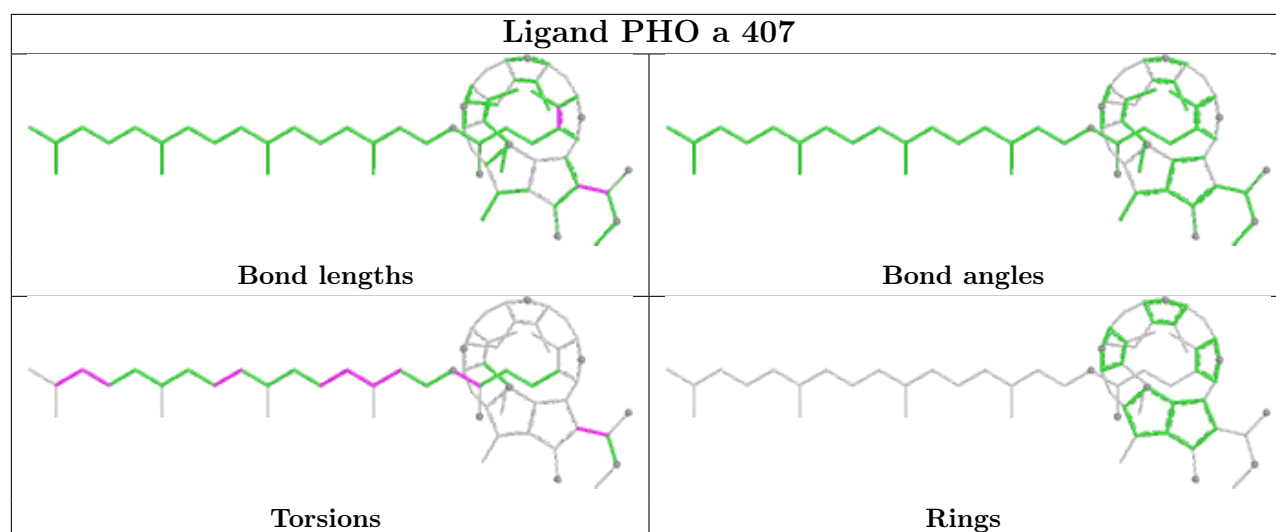


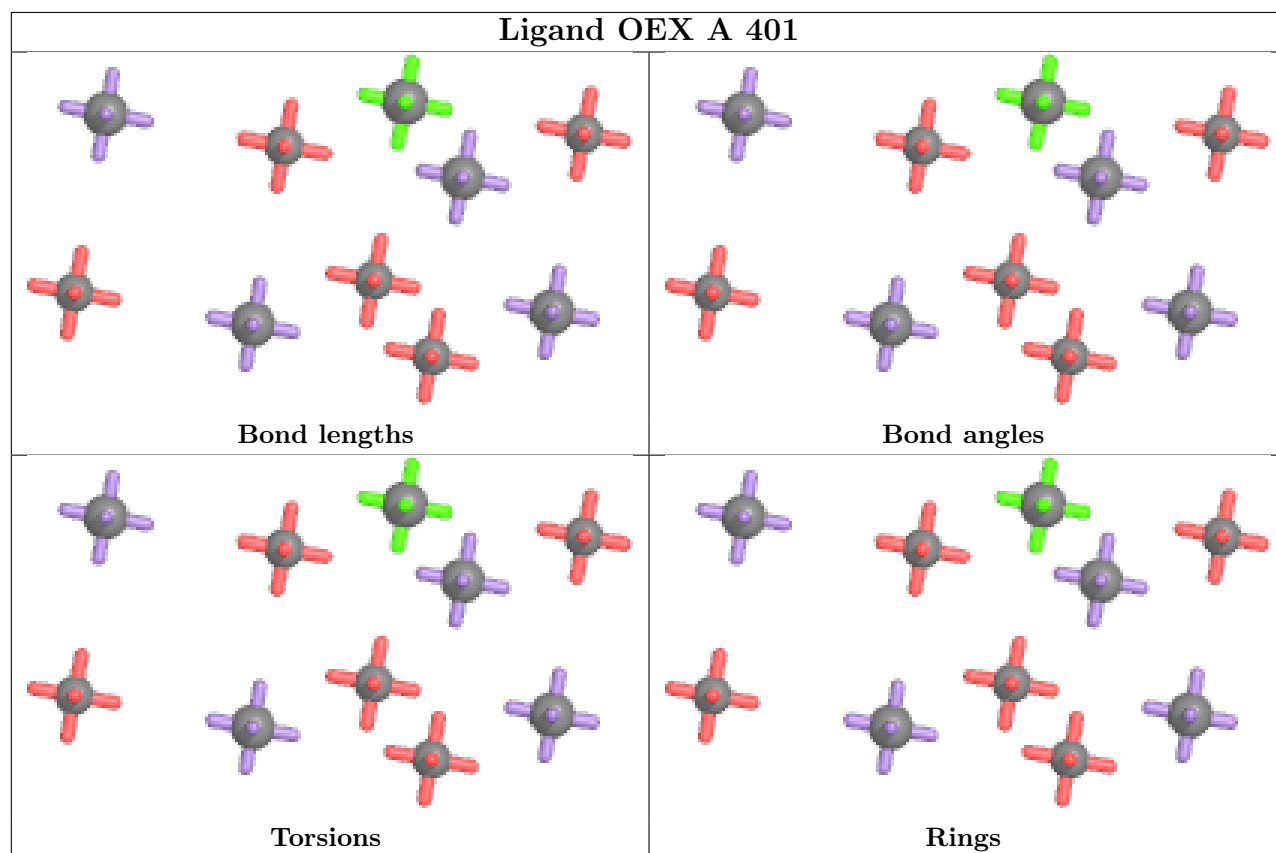
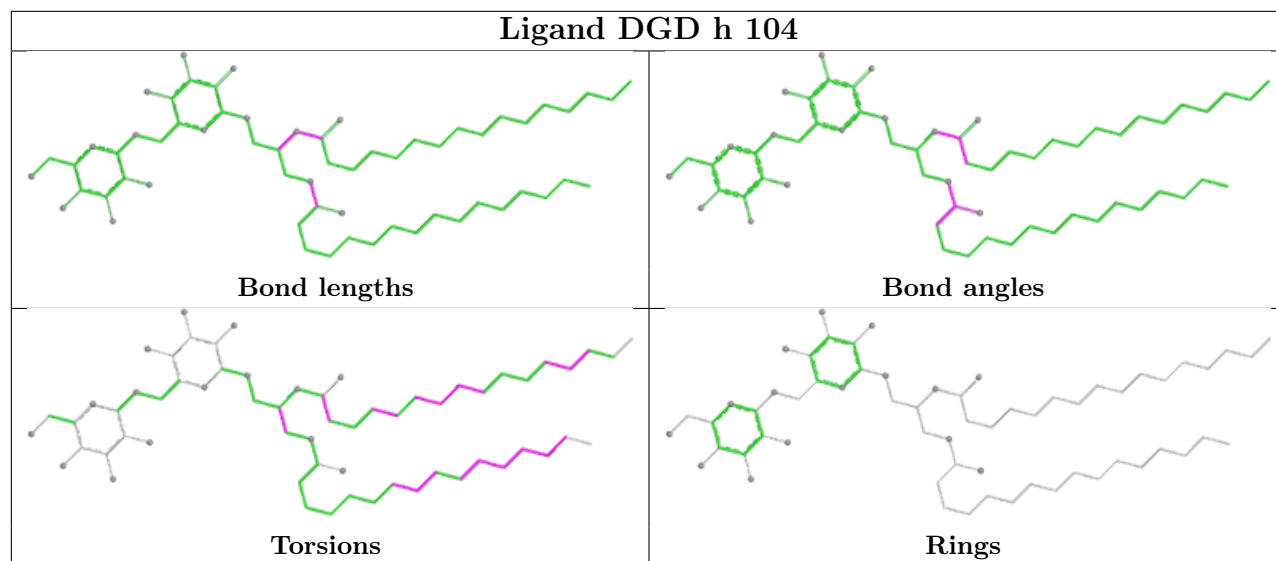


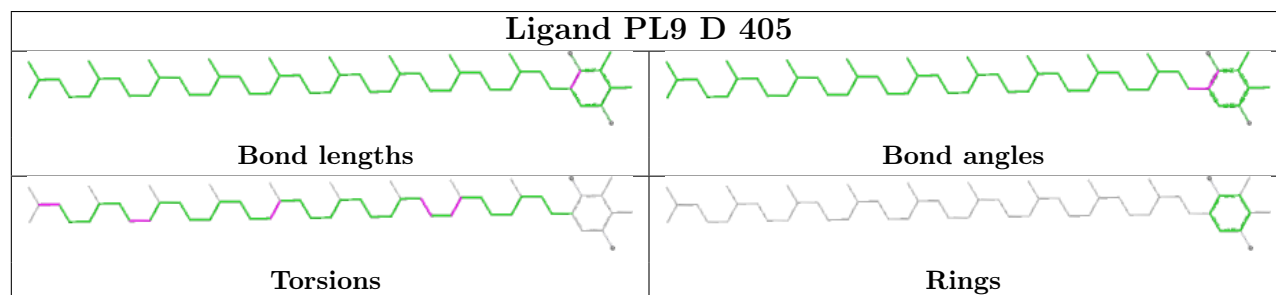
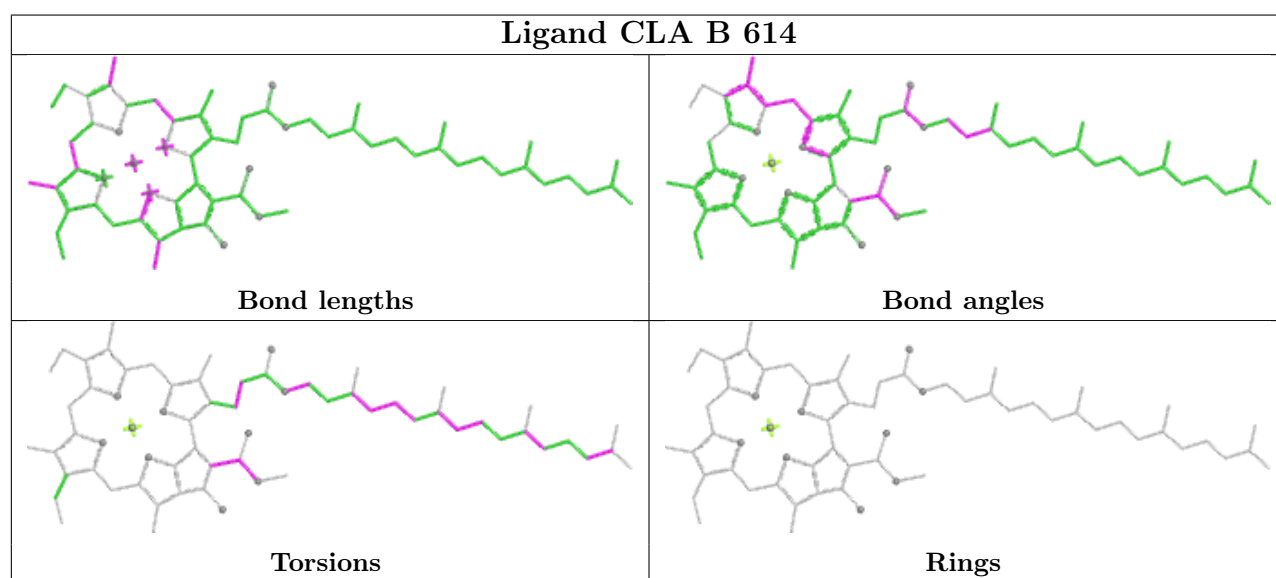
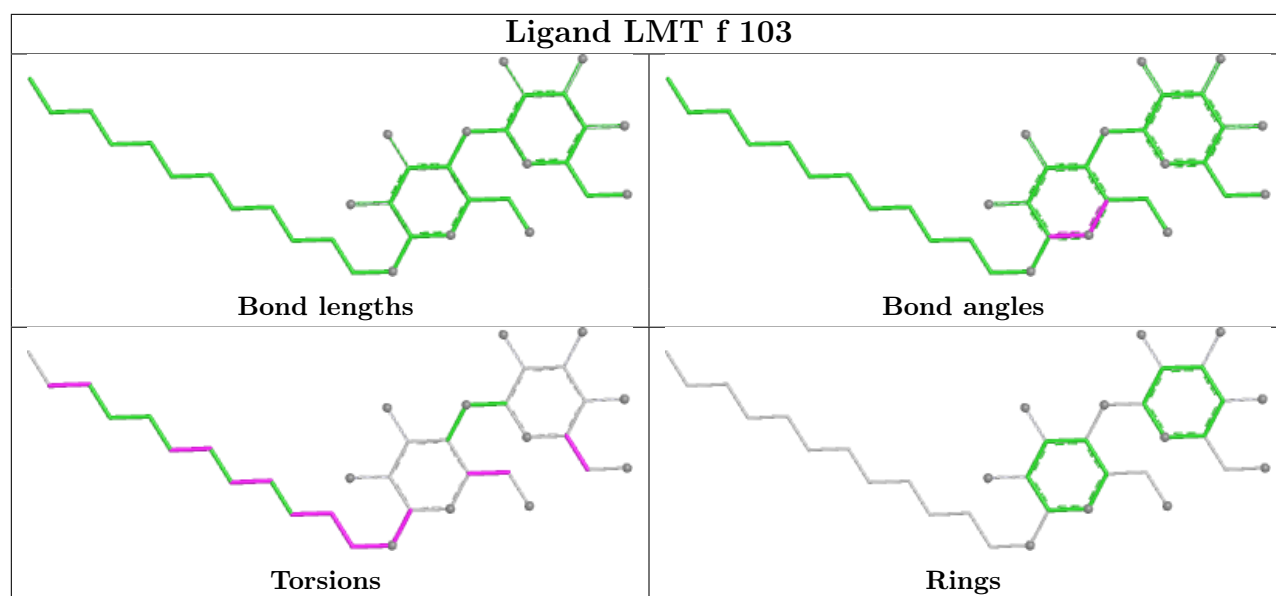


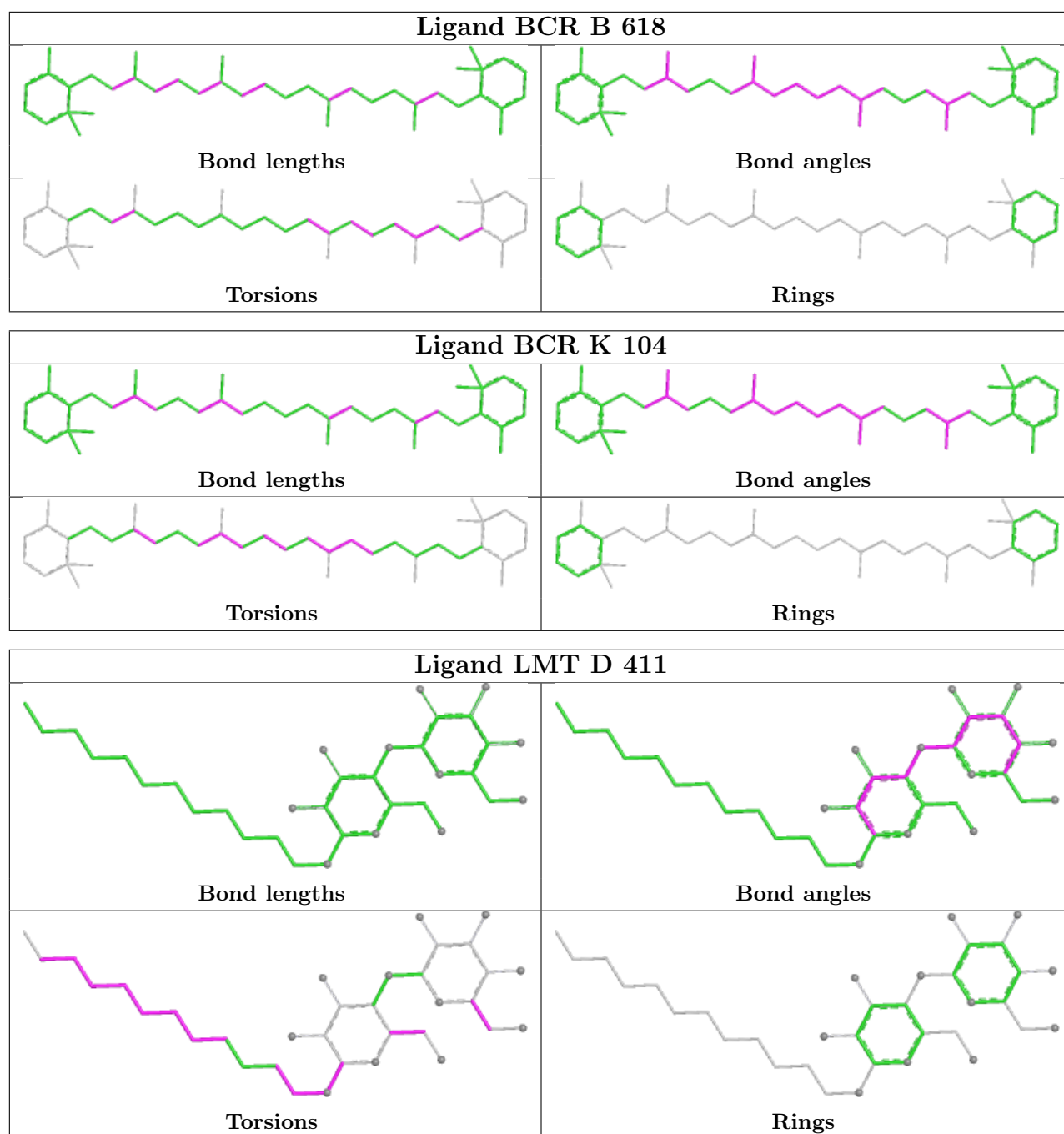


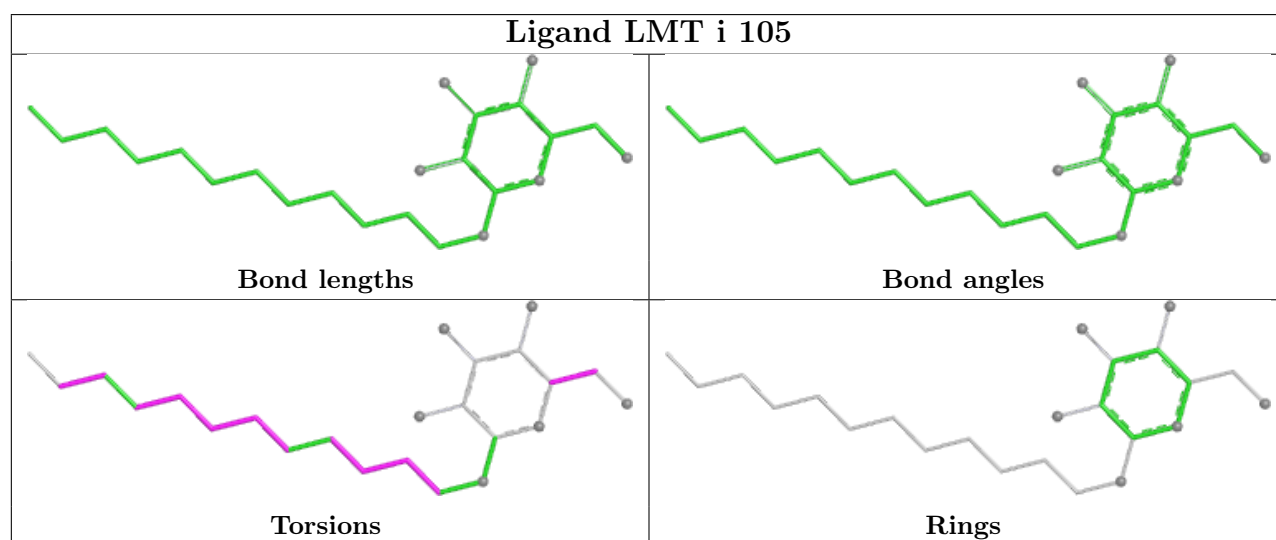
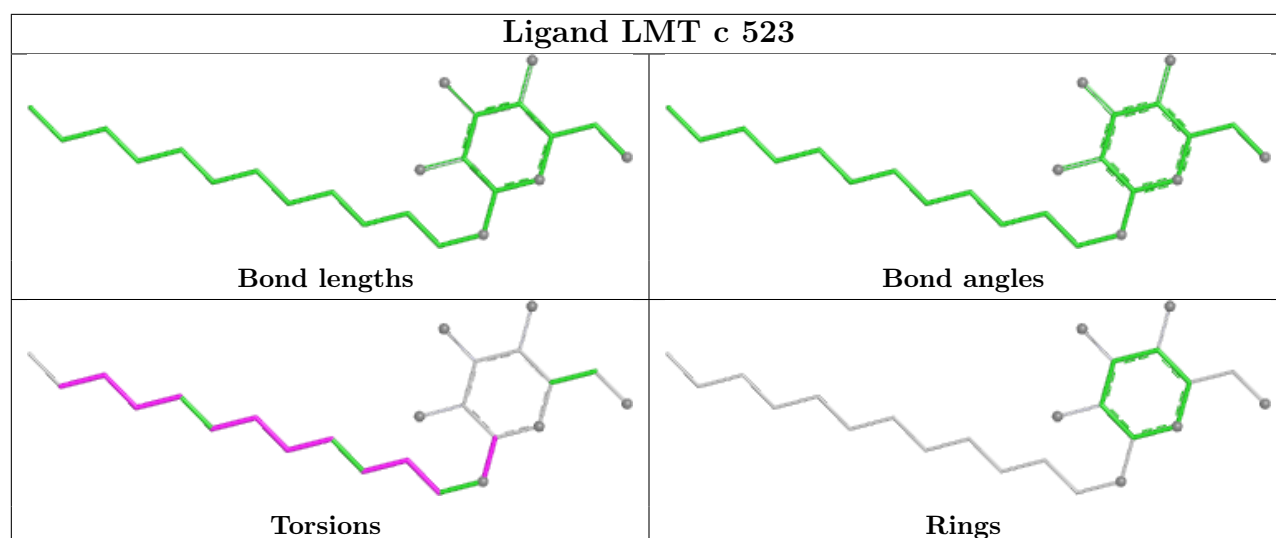


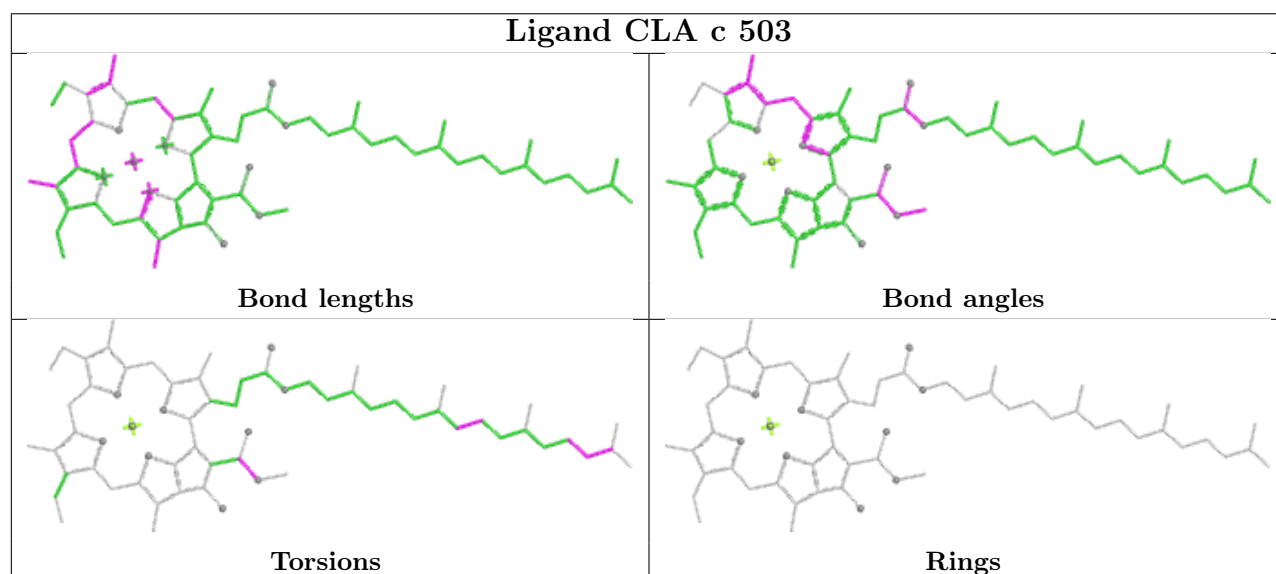
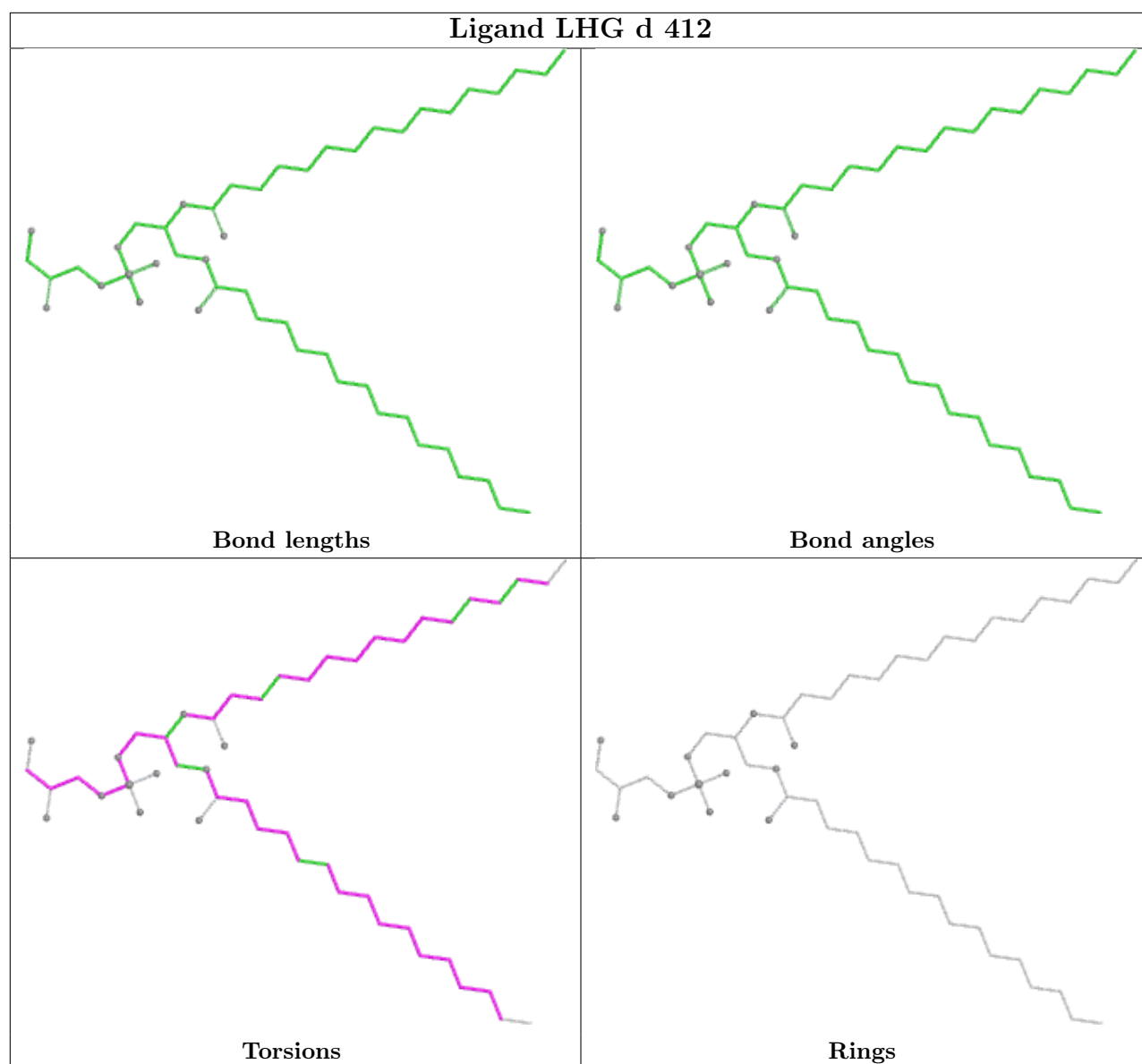




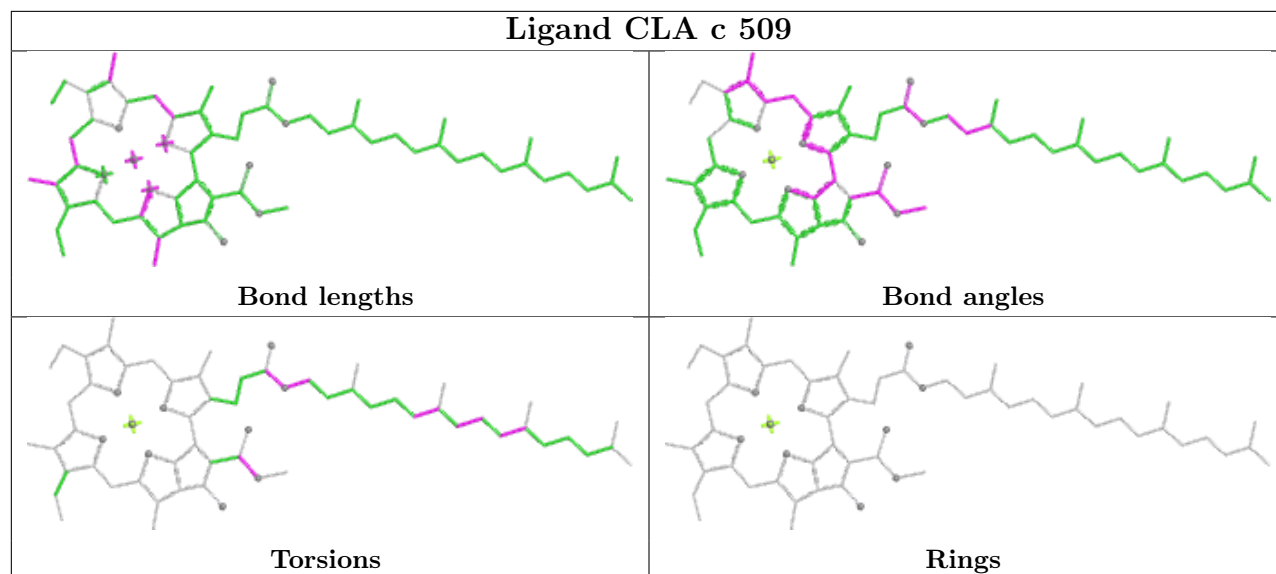




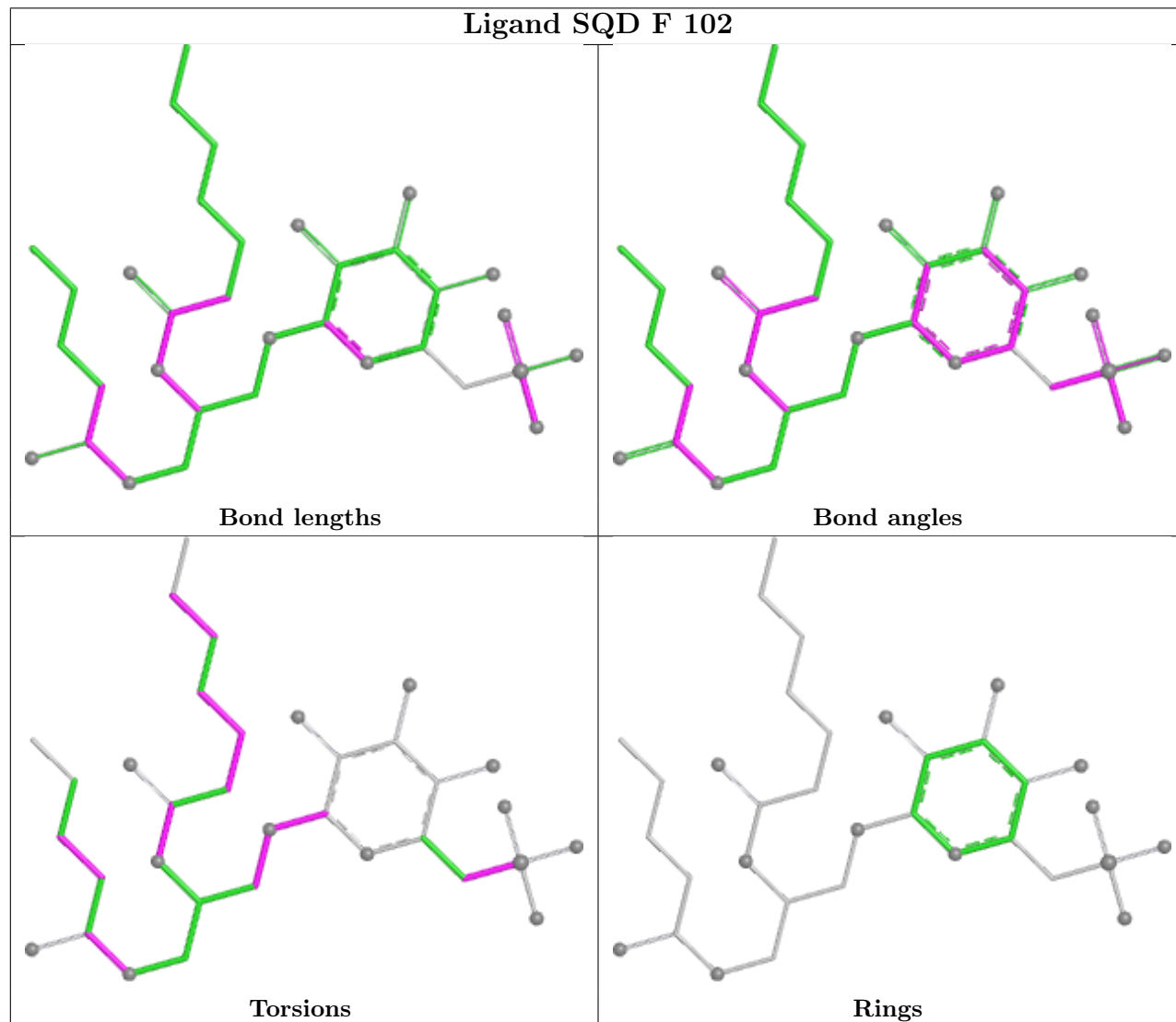


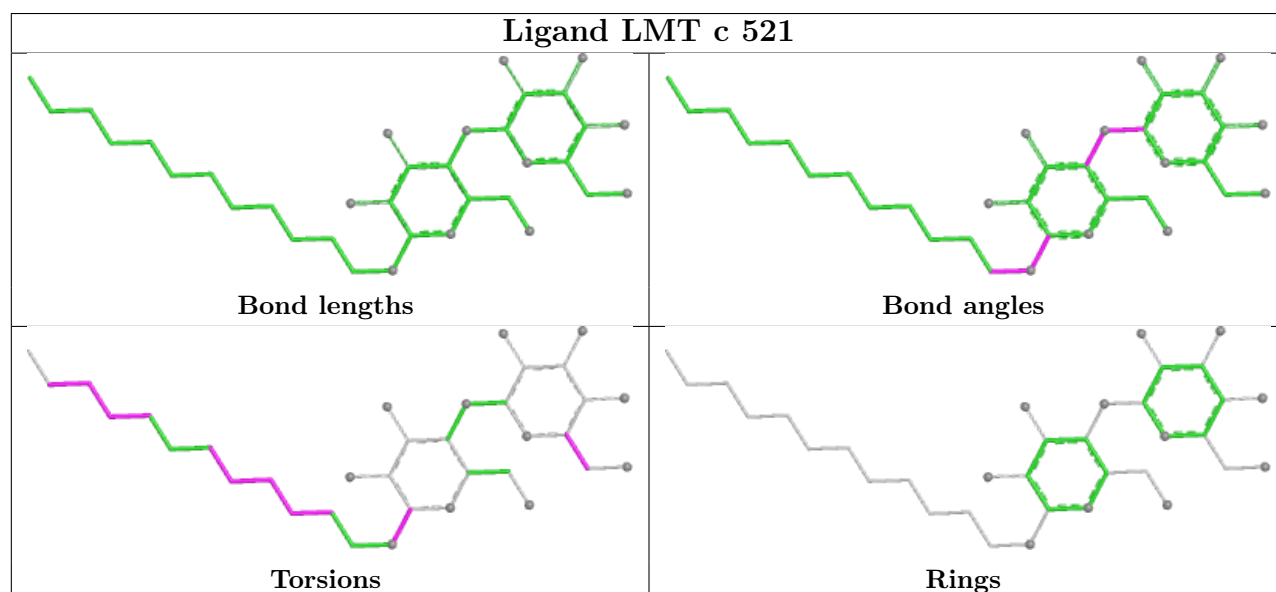
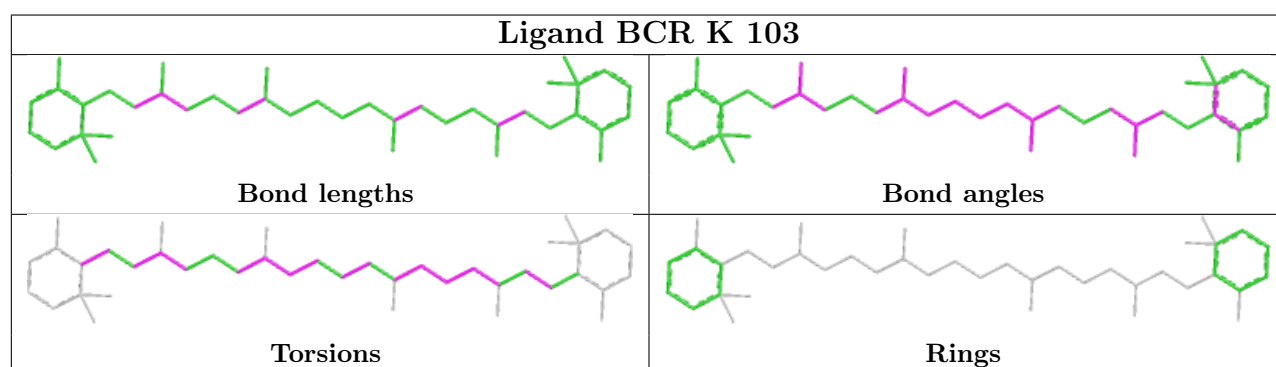
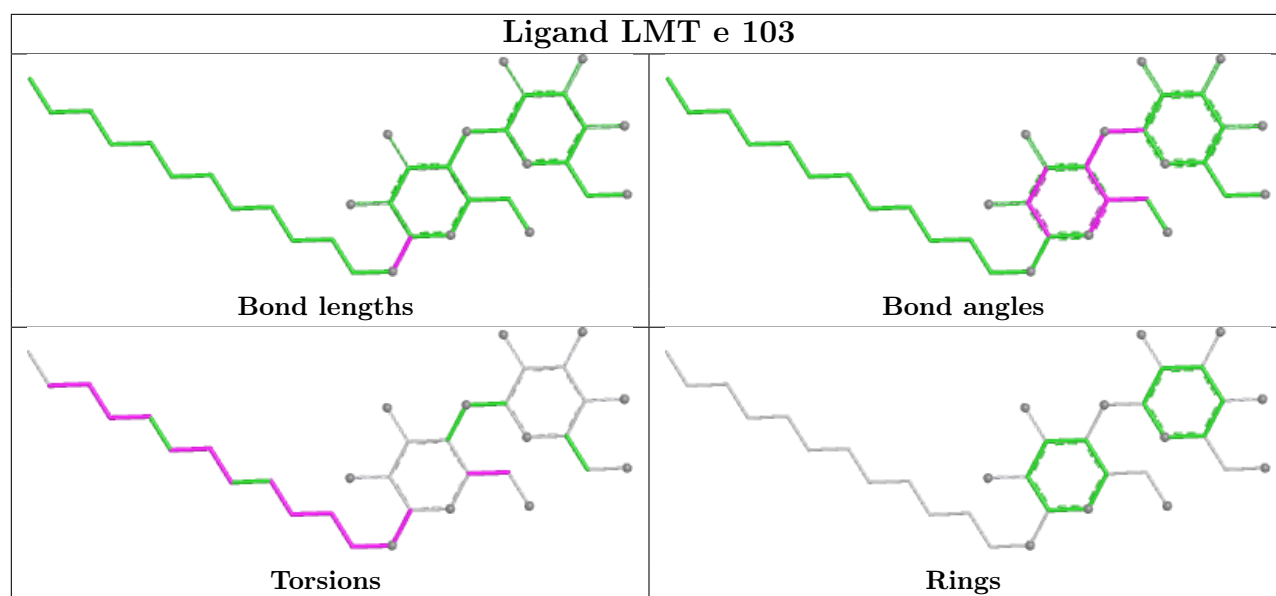


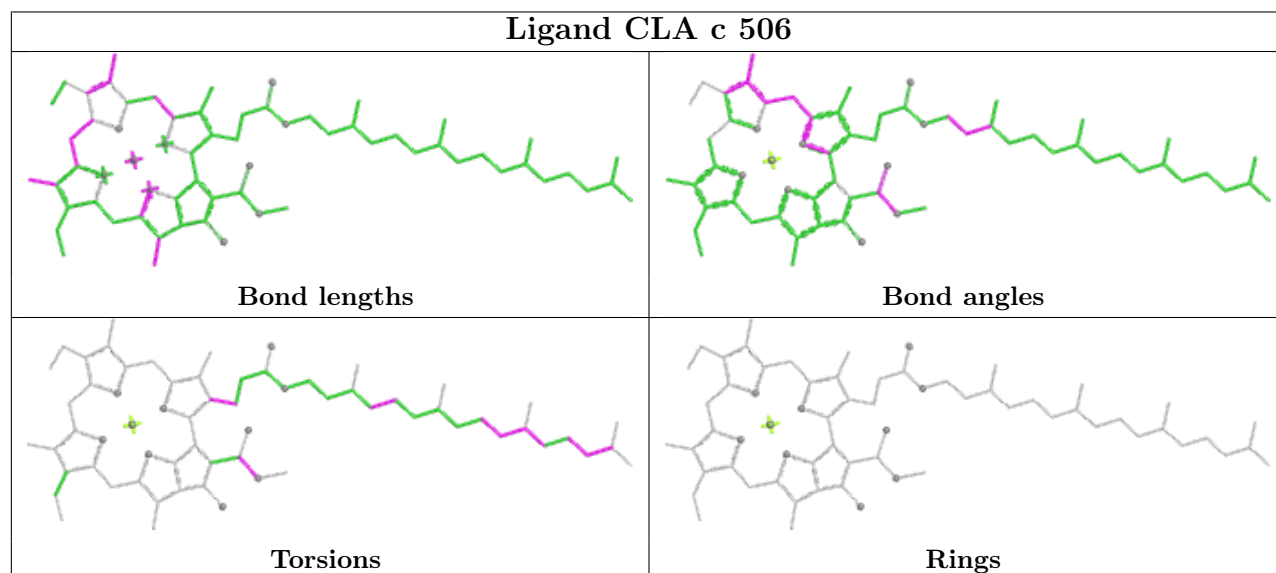
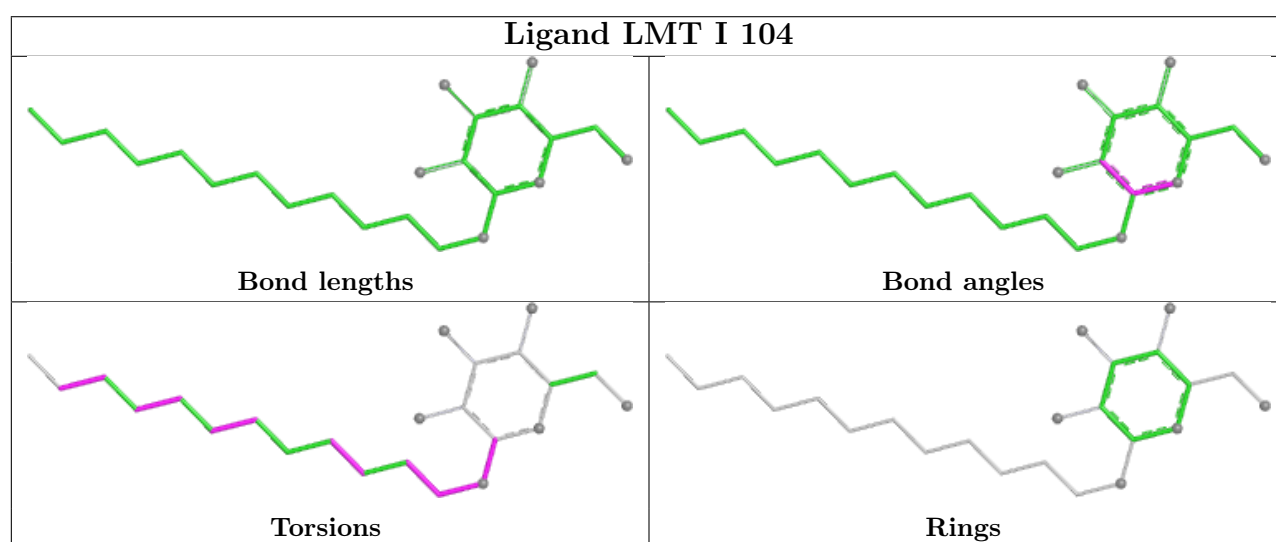
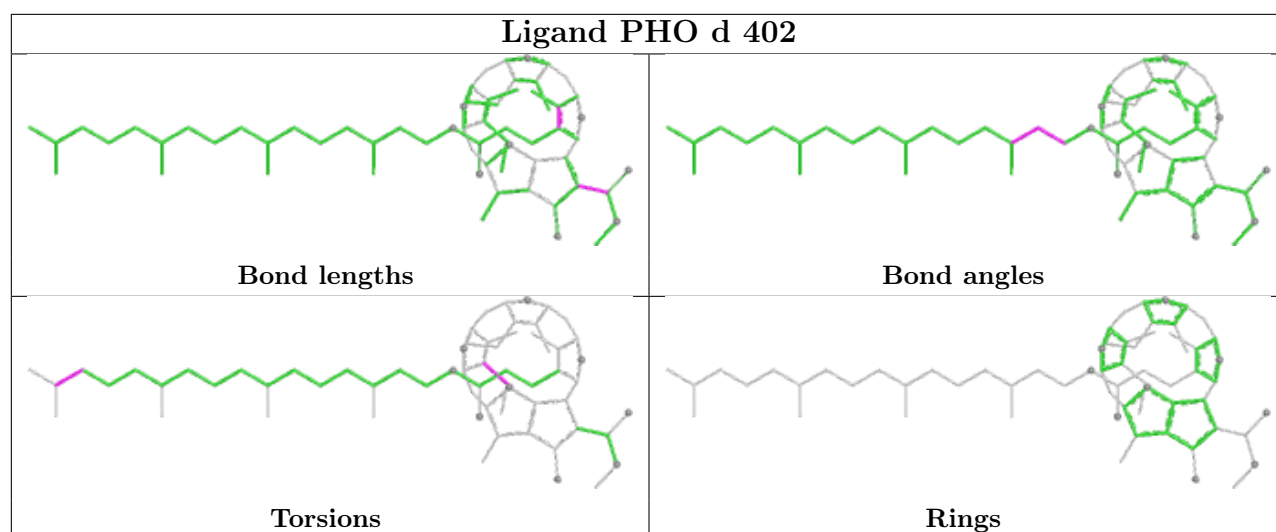
Ligand CLA c 509

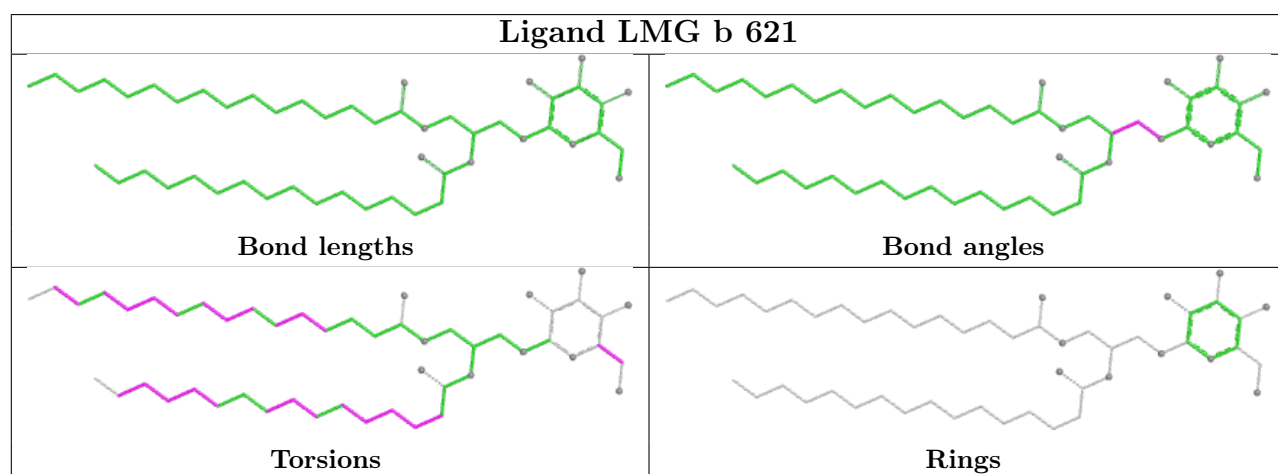
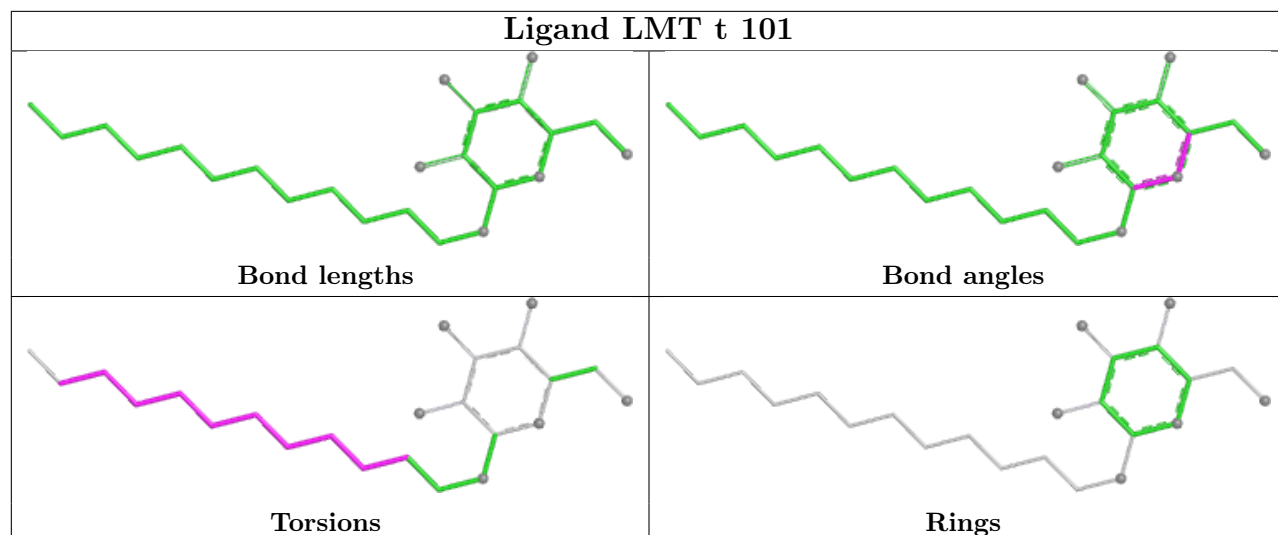


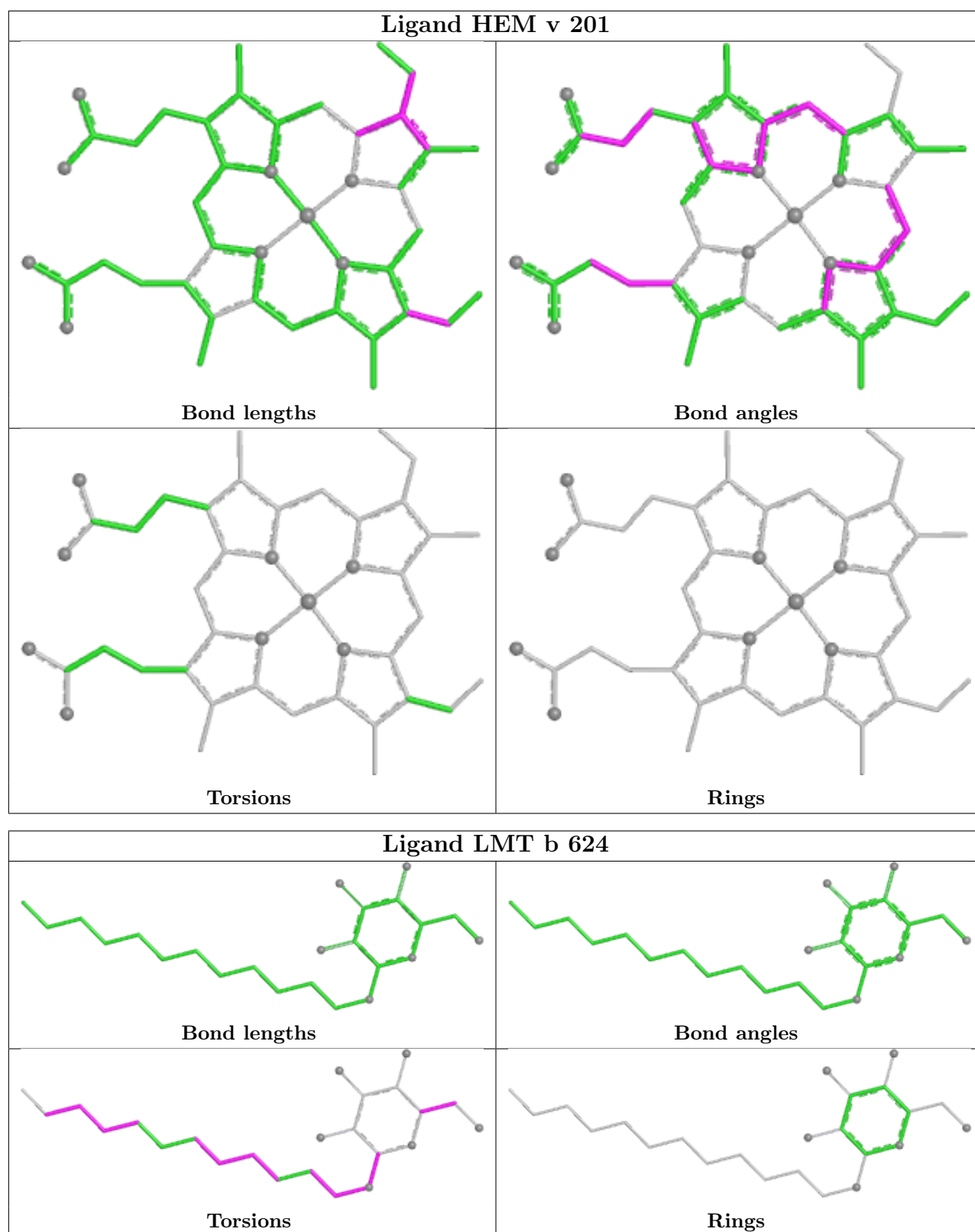
Ligand SQD F 102



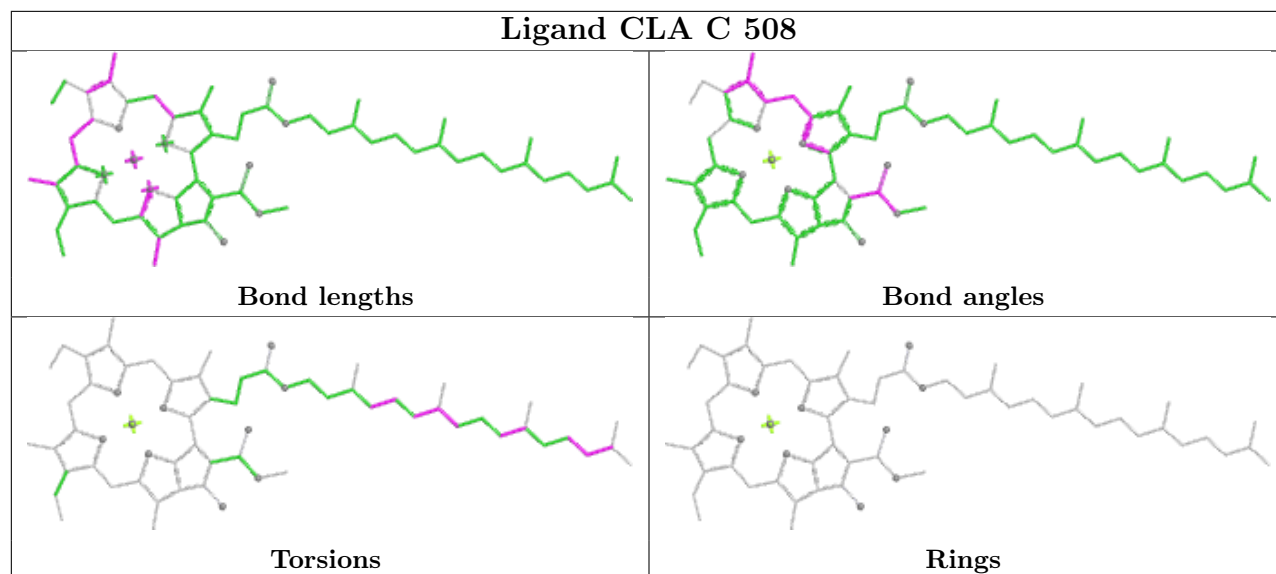




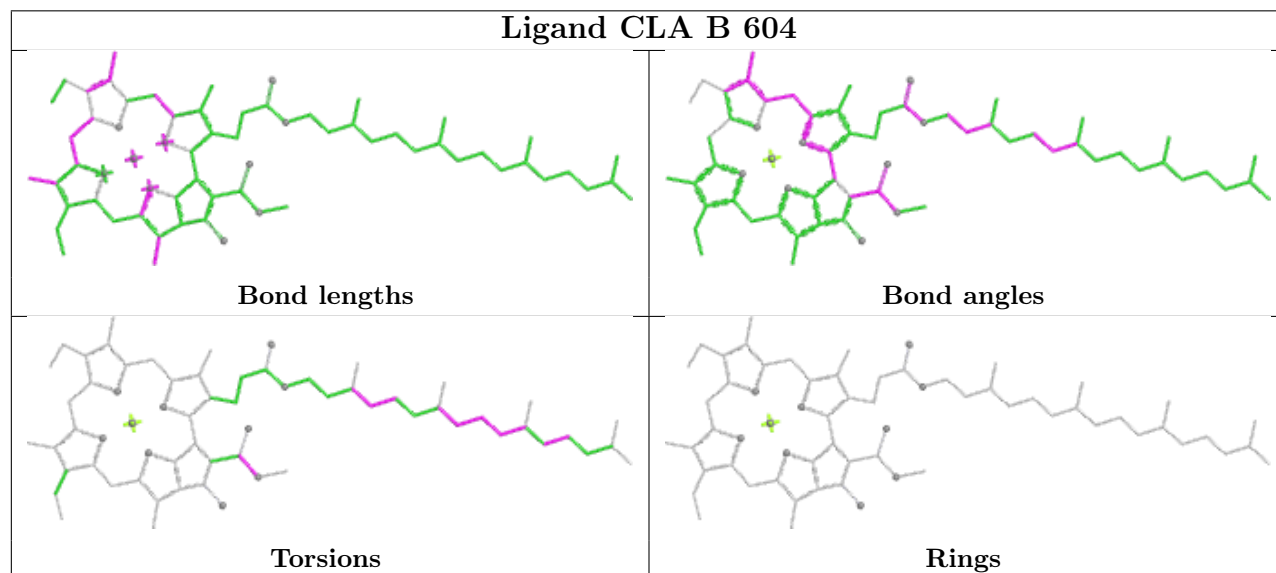




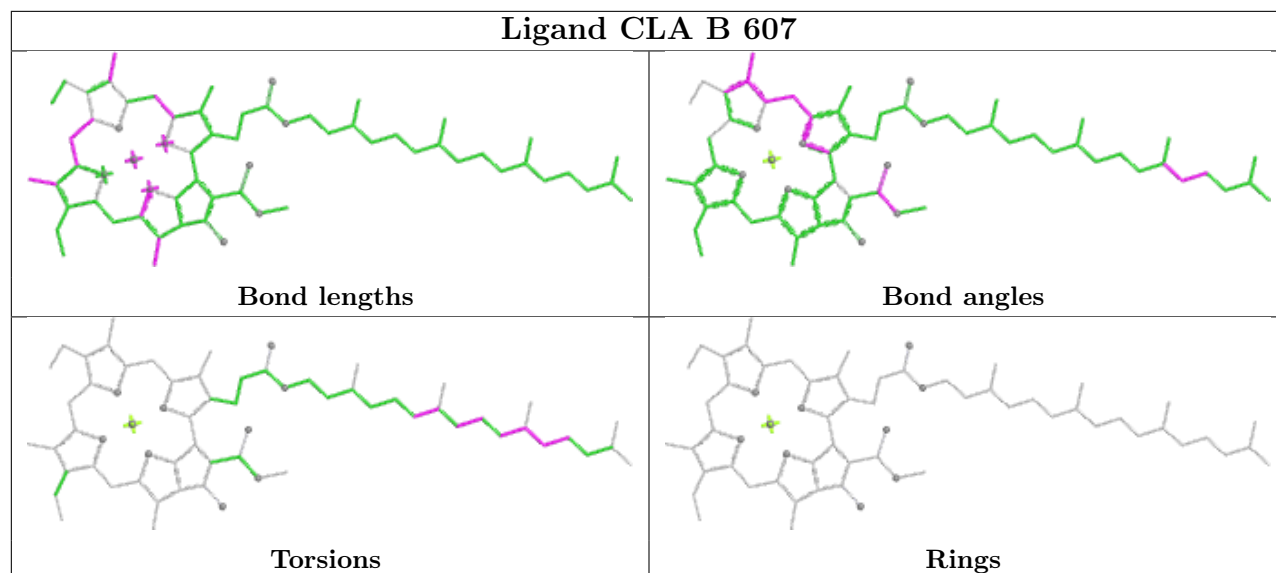
Ligand CLA C 508

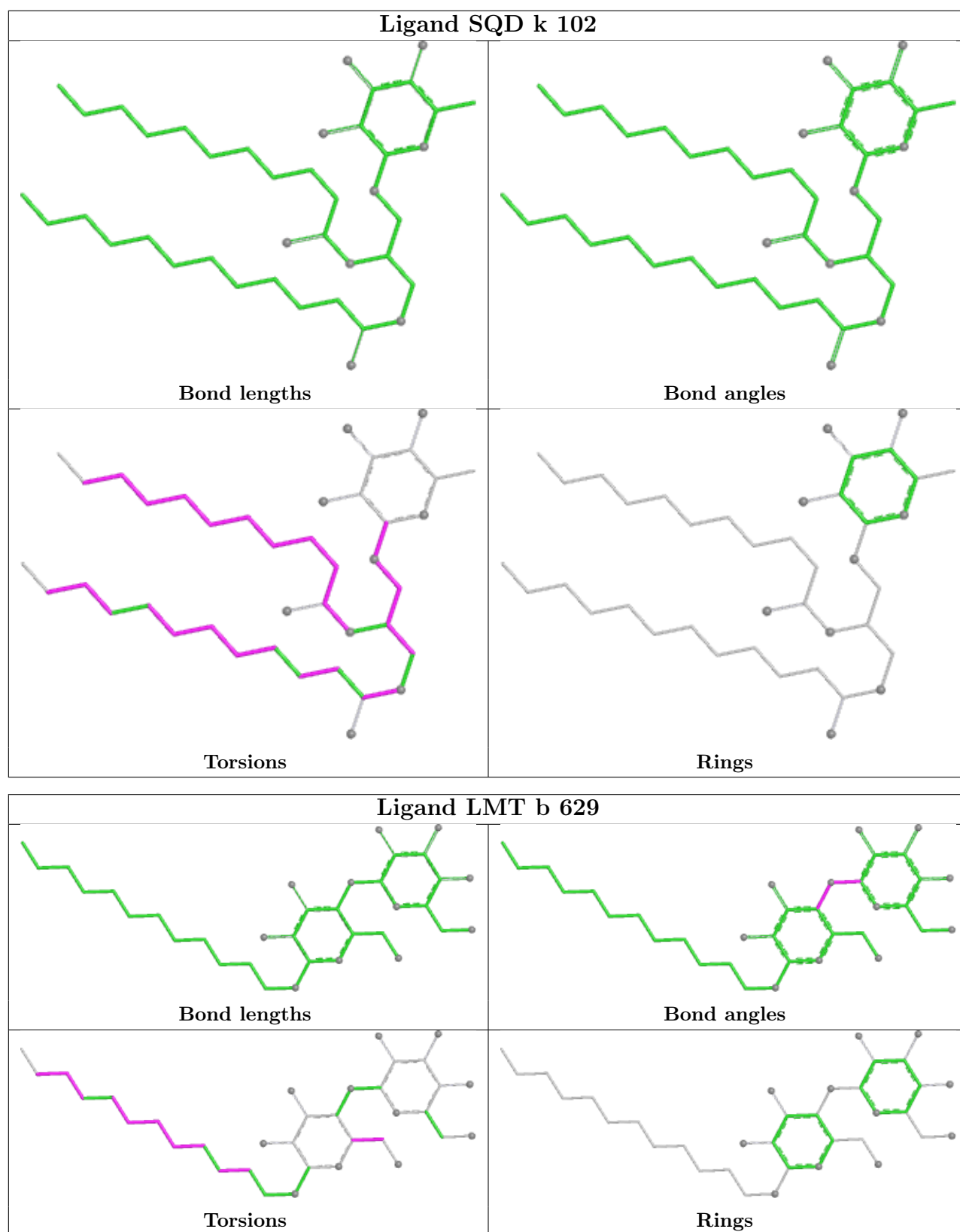


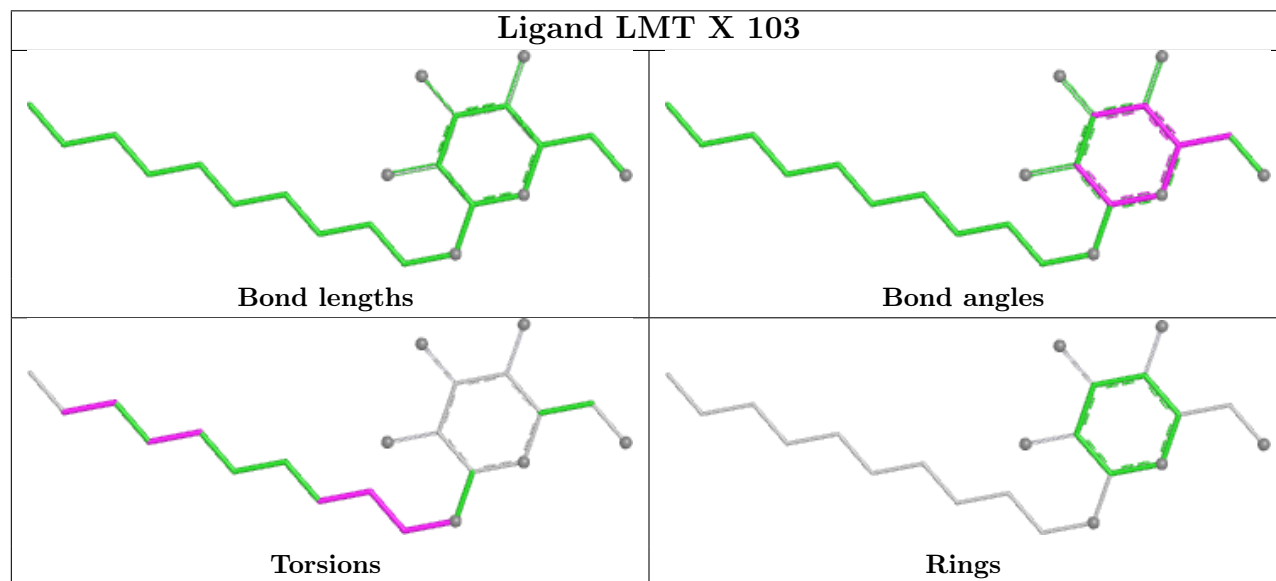
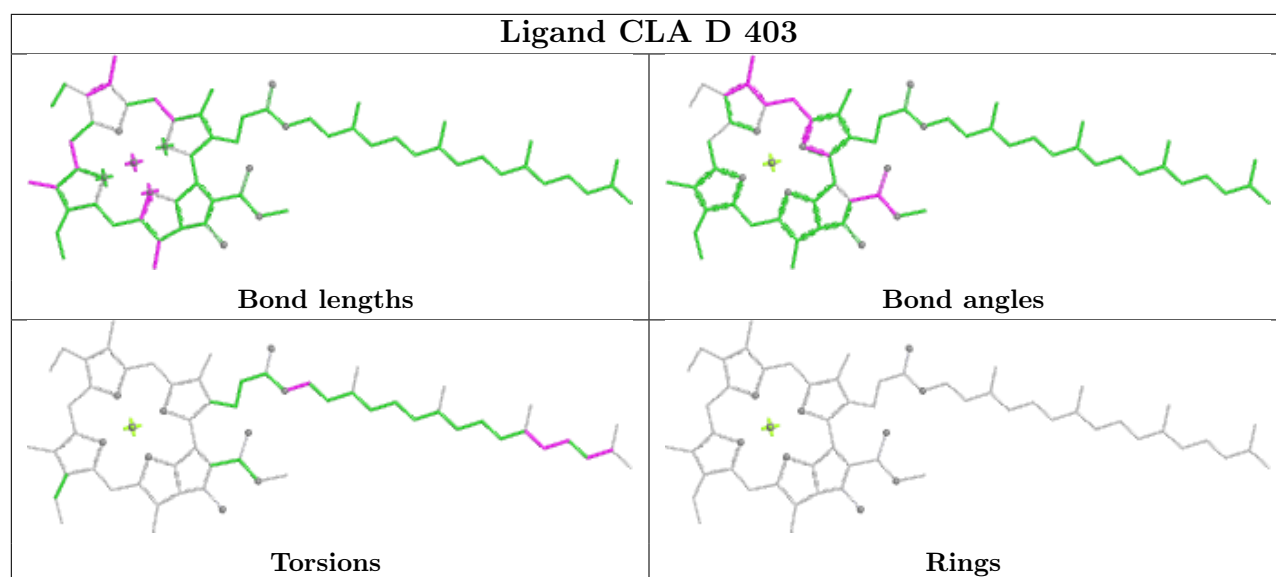
Ligand CLA B 604

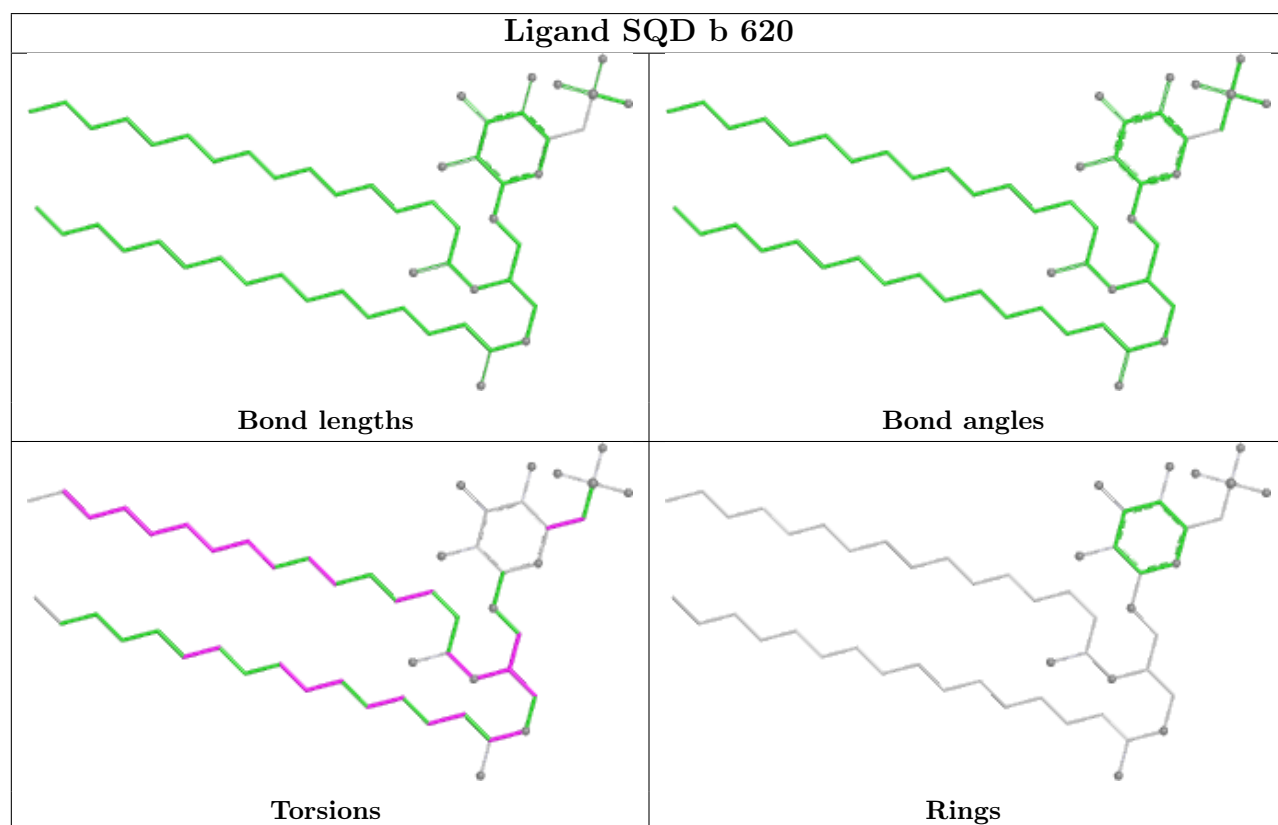
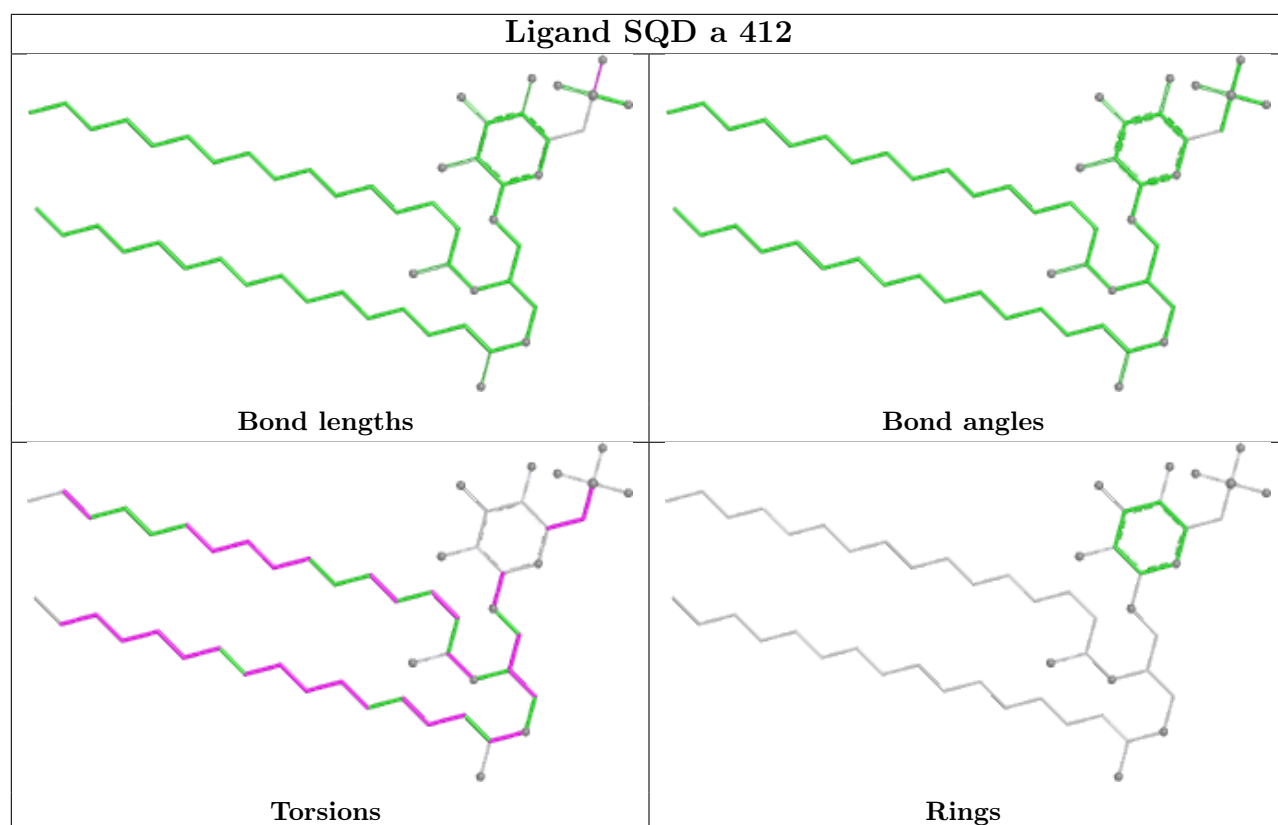


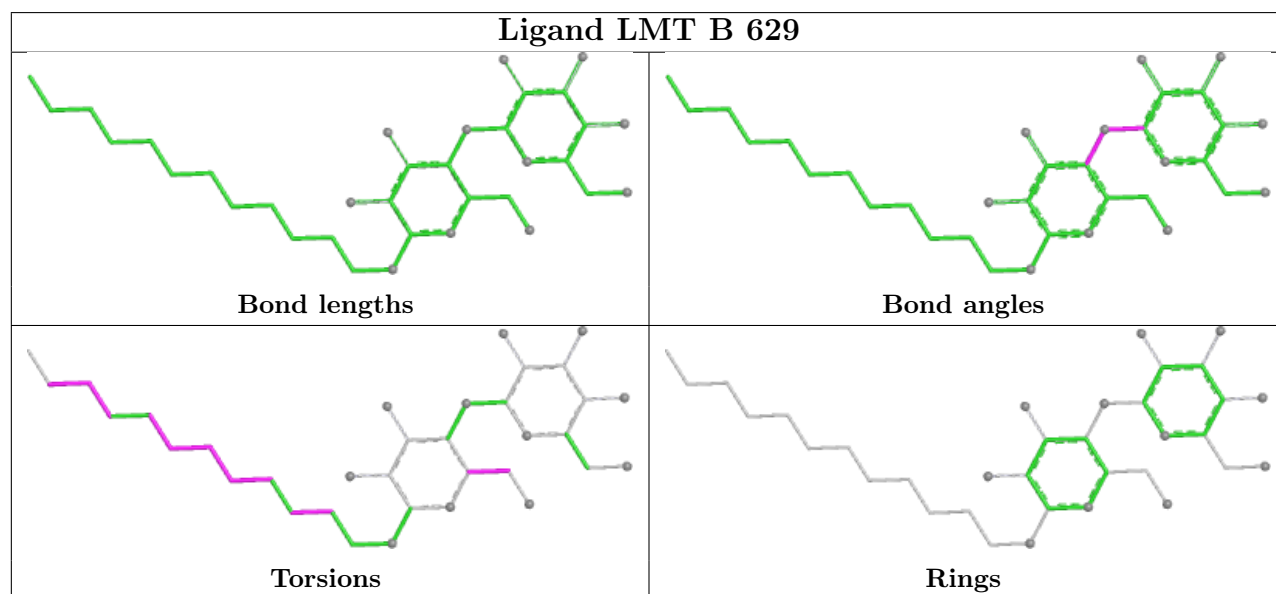
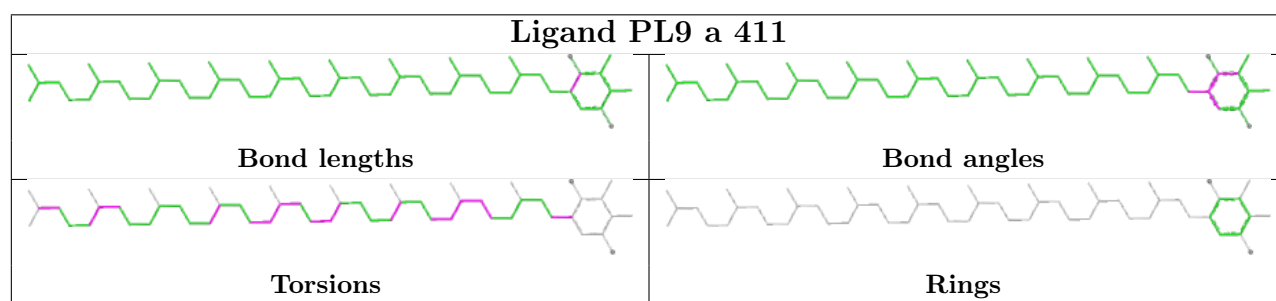
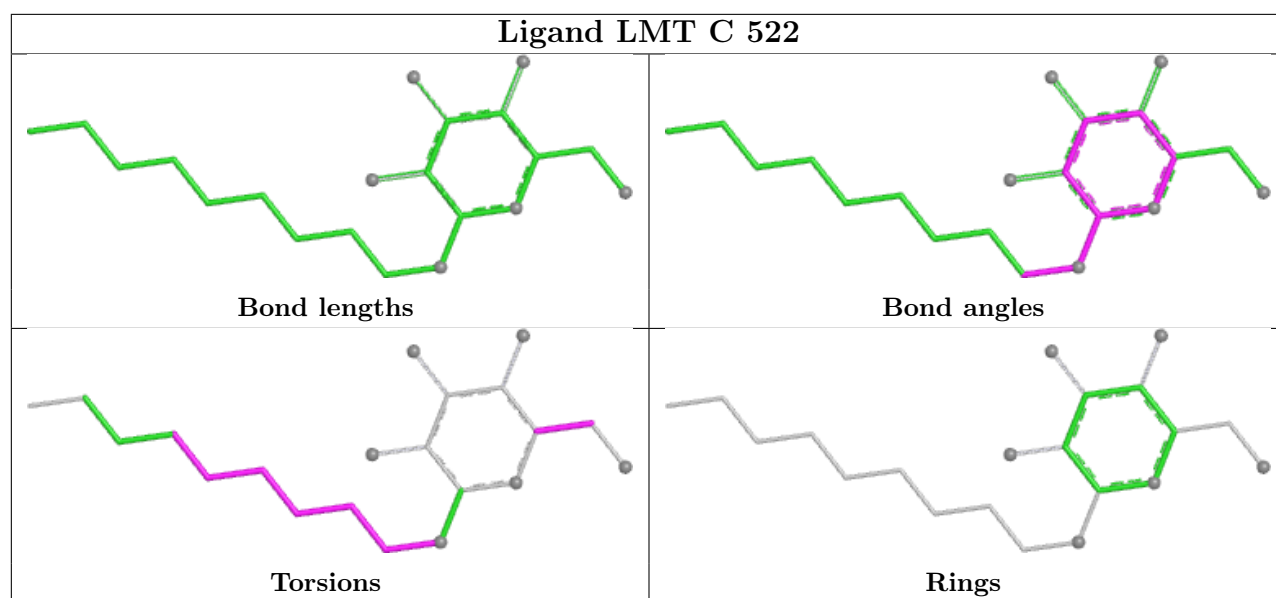
Ligand CLA B 607

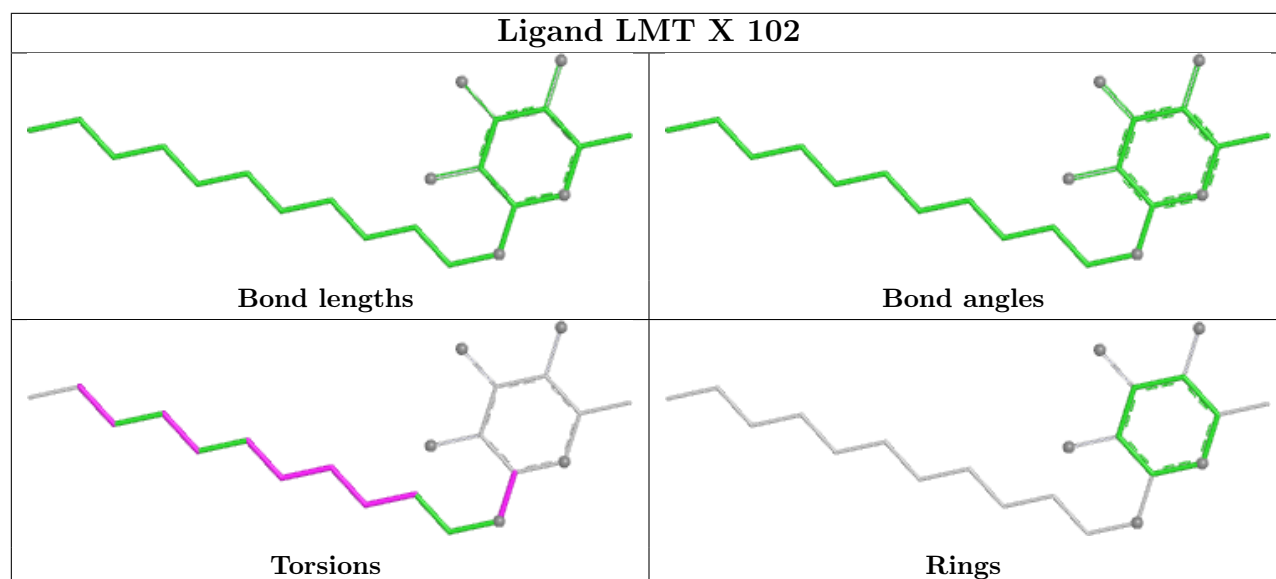
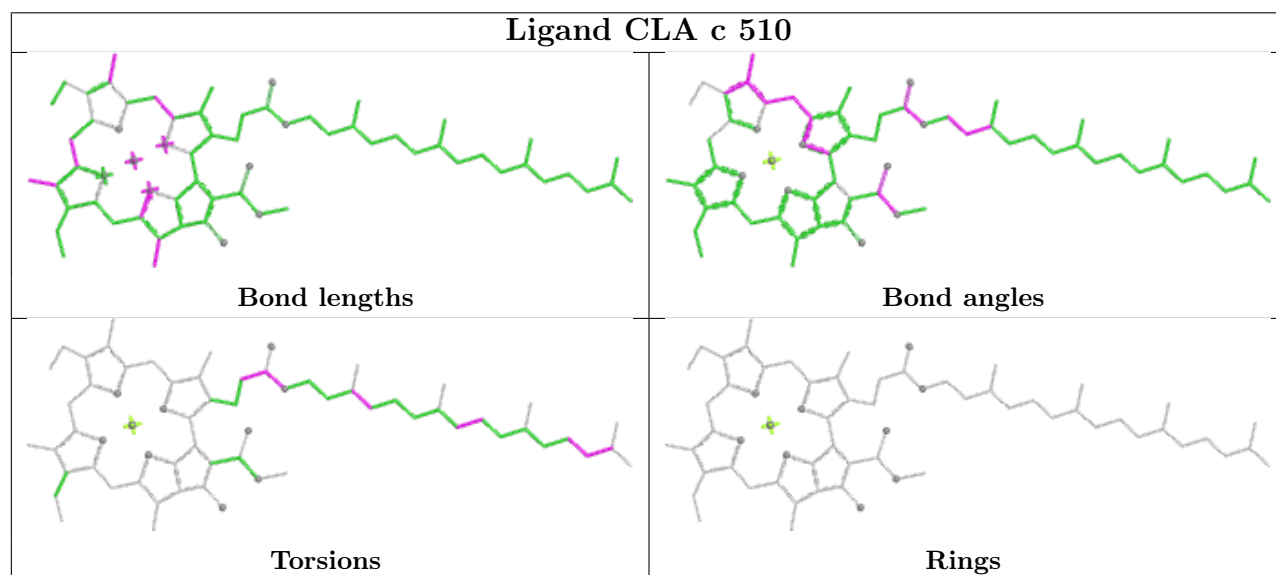
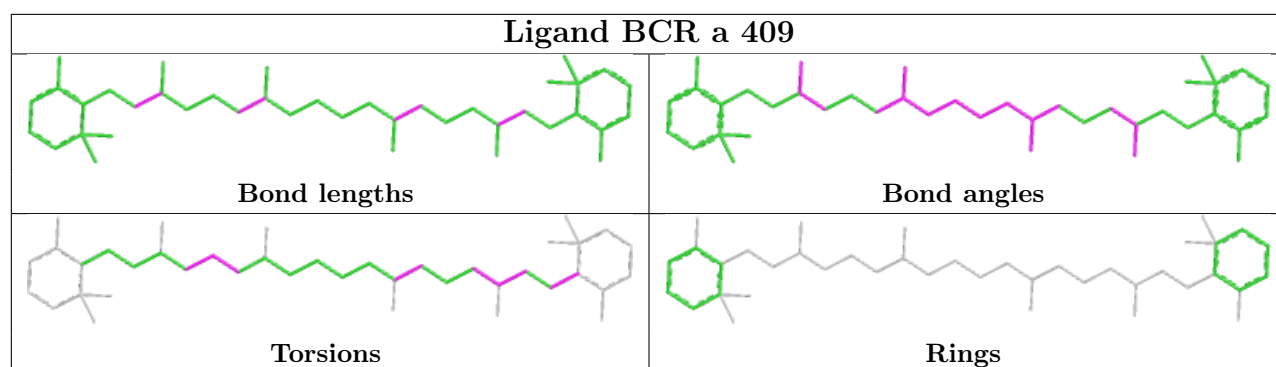




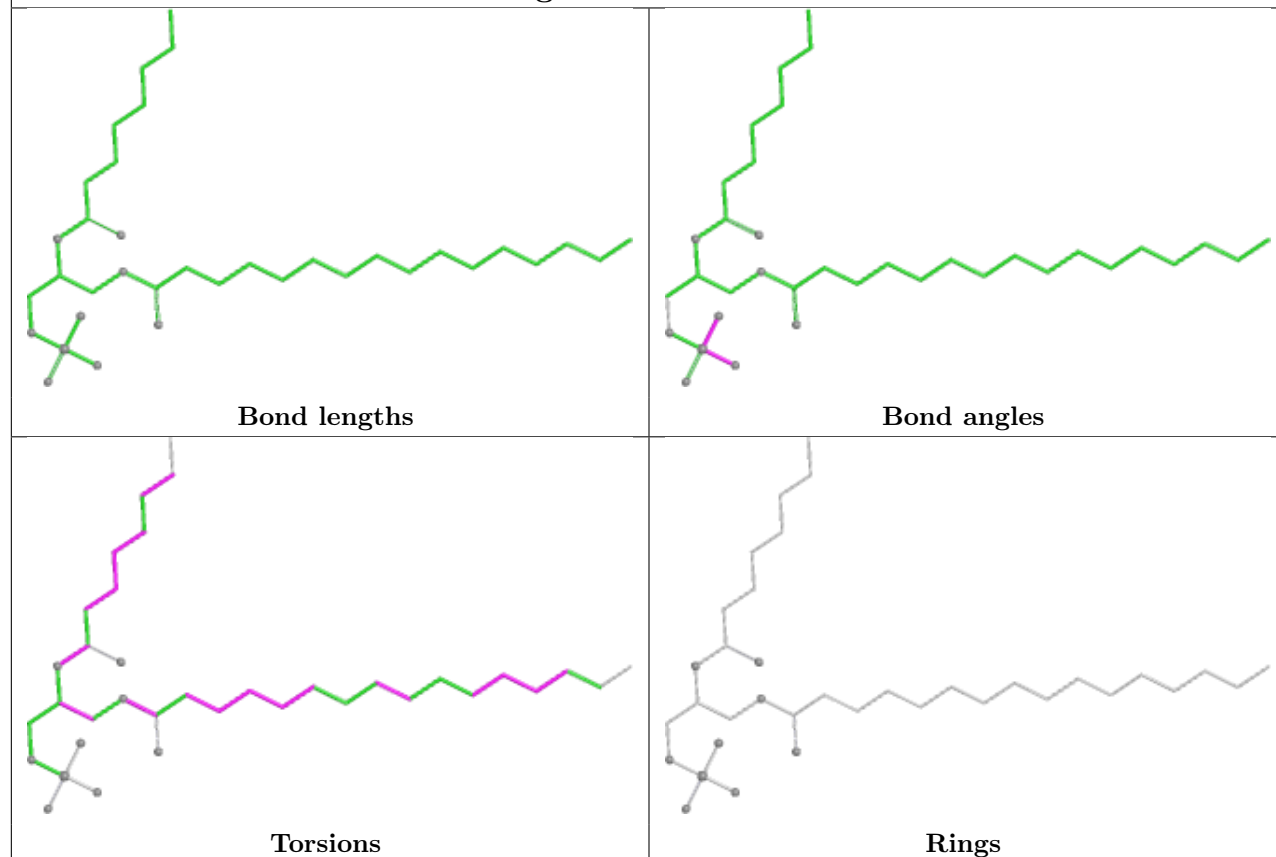




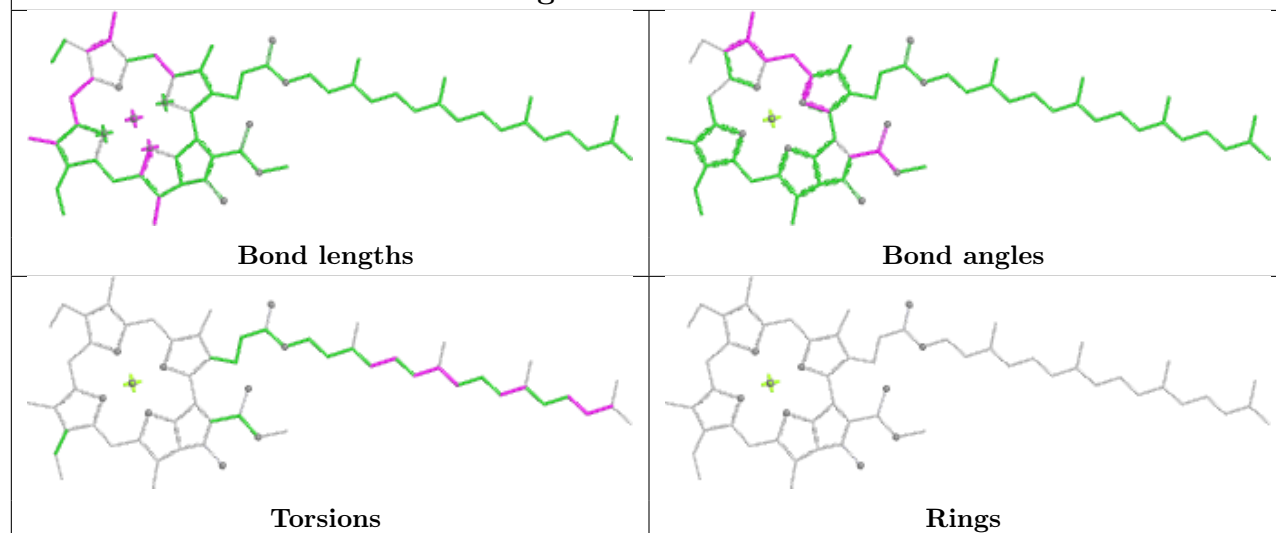


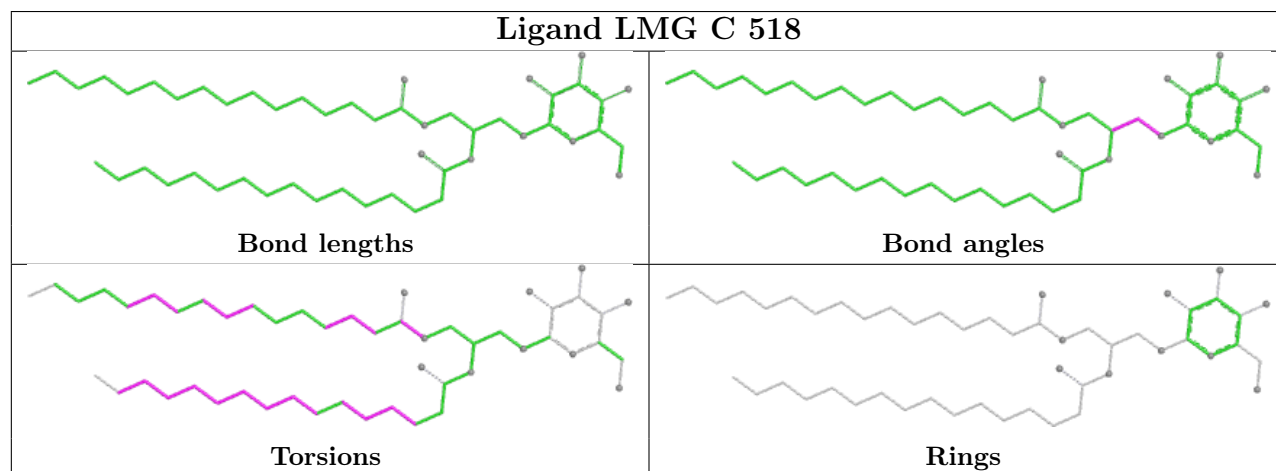
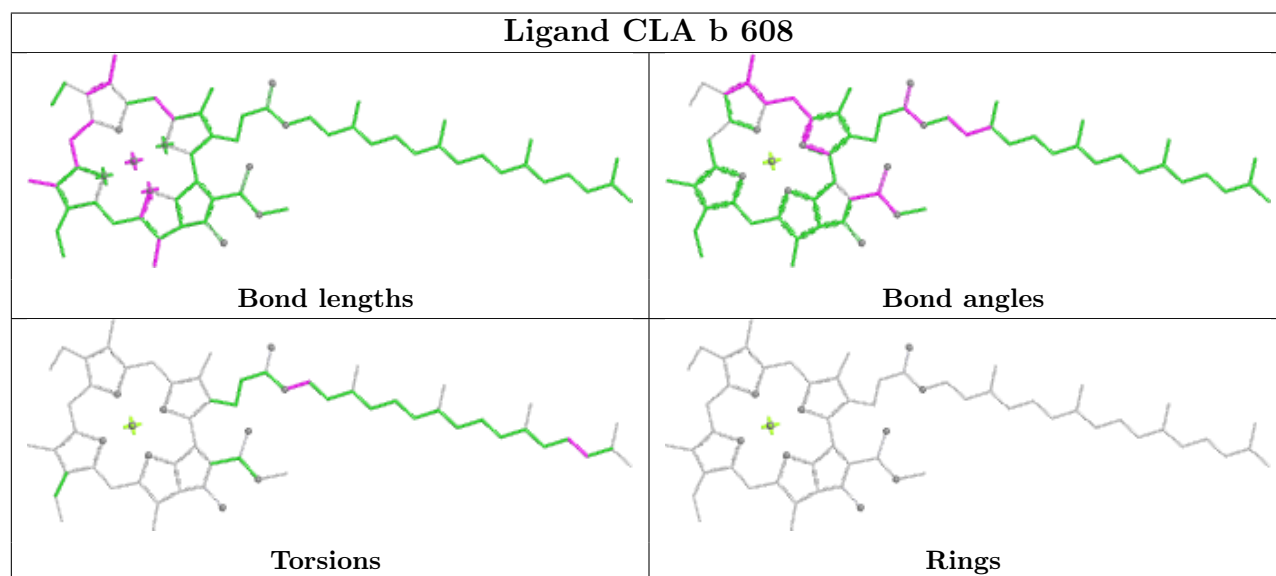
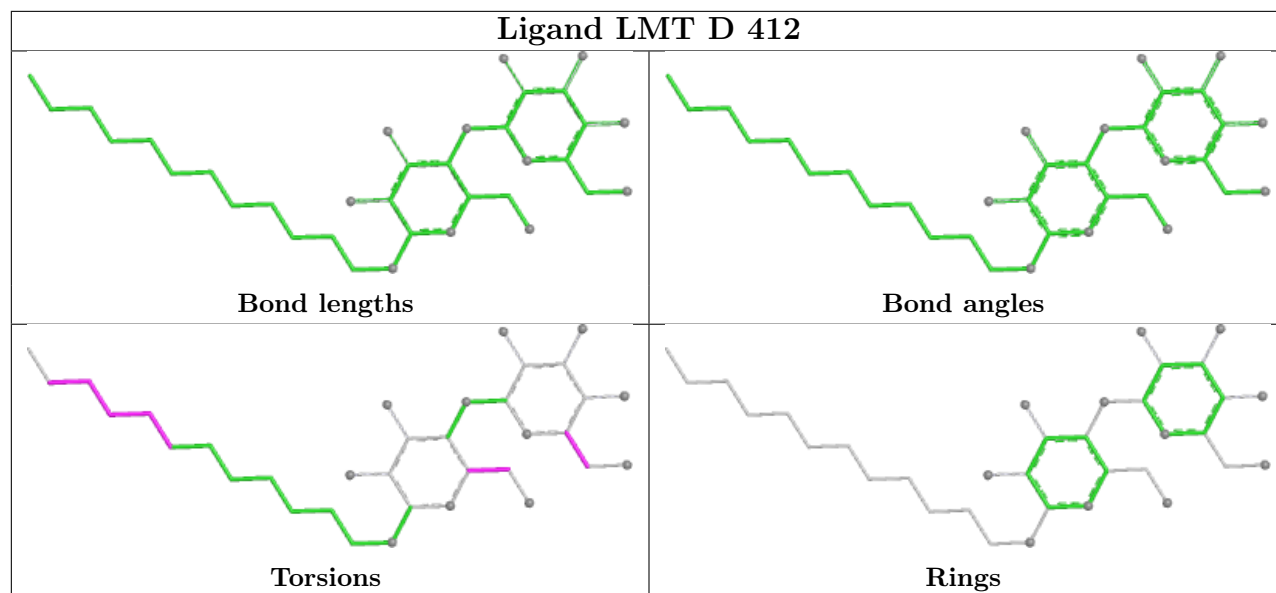


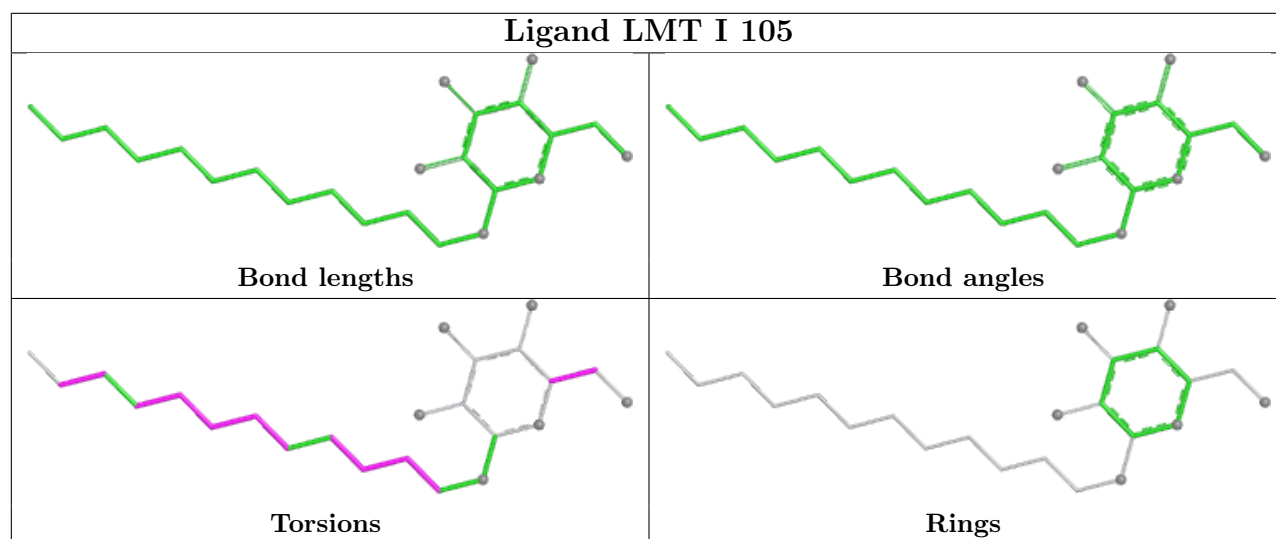
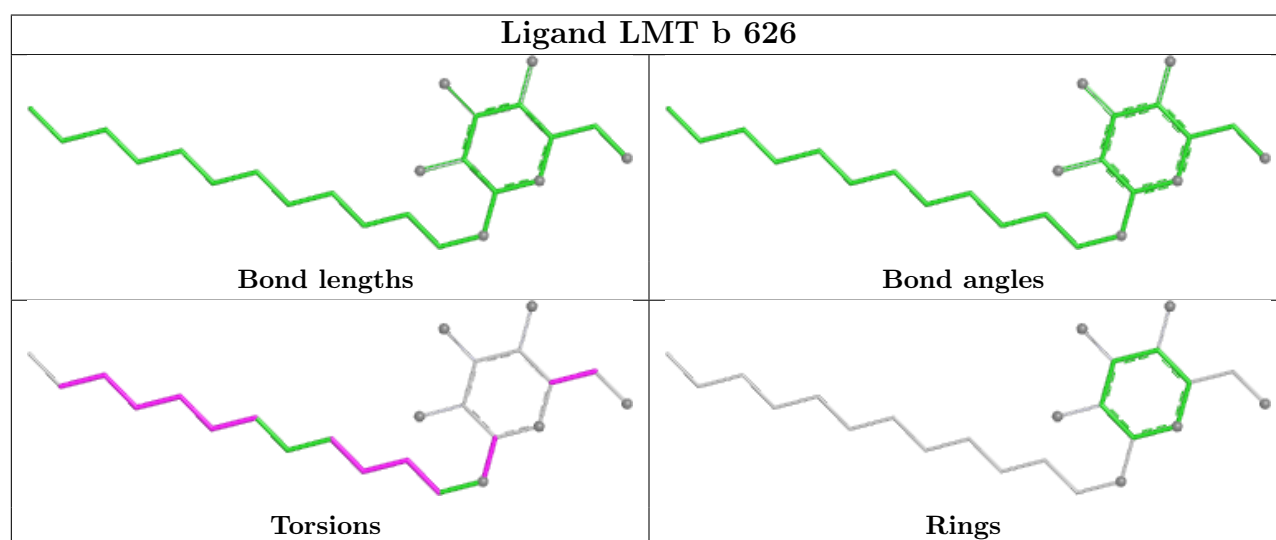
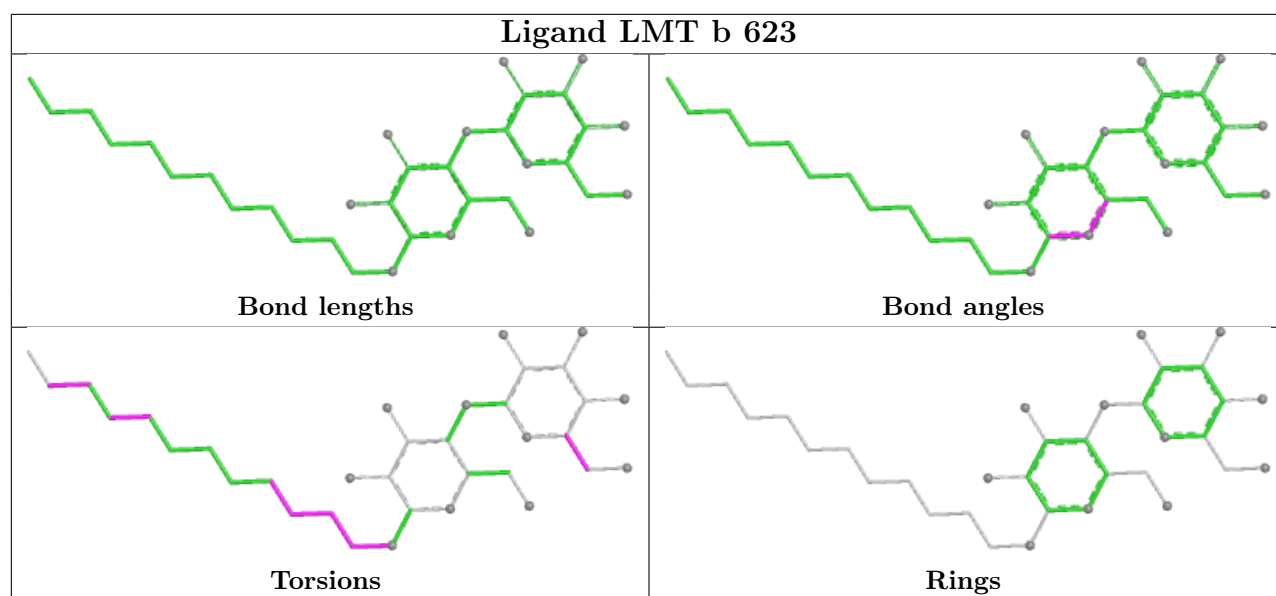
Ligand LHG z 102

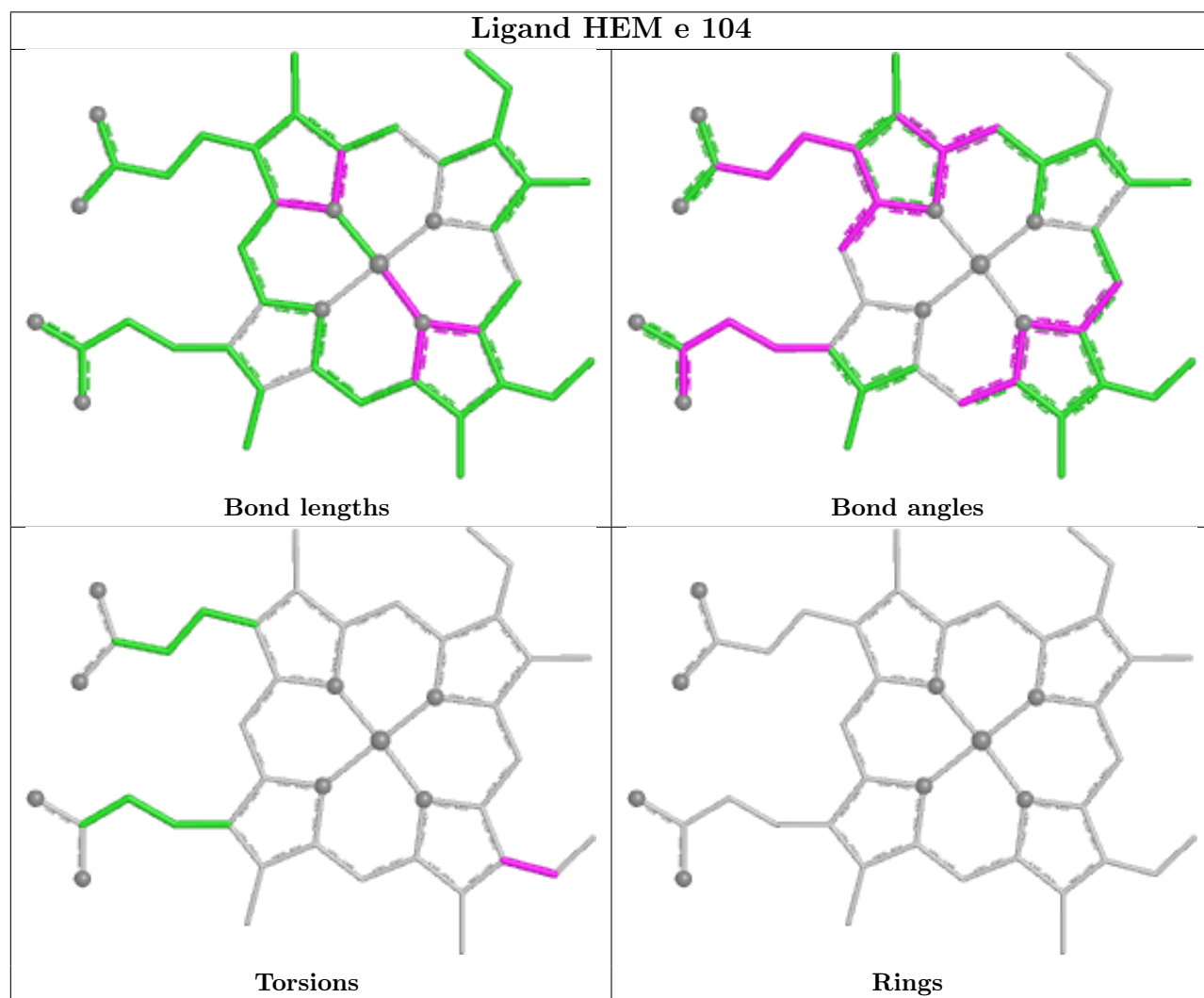
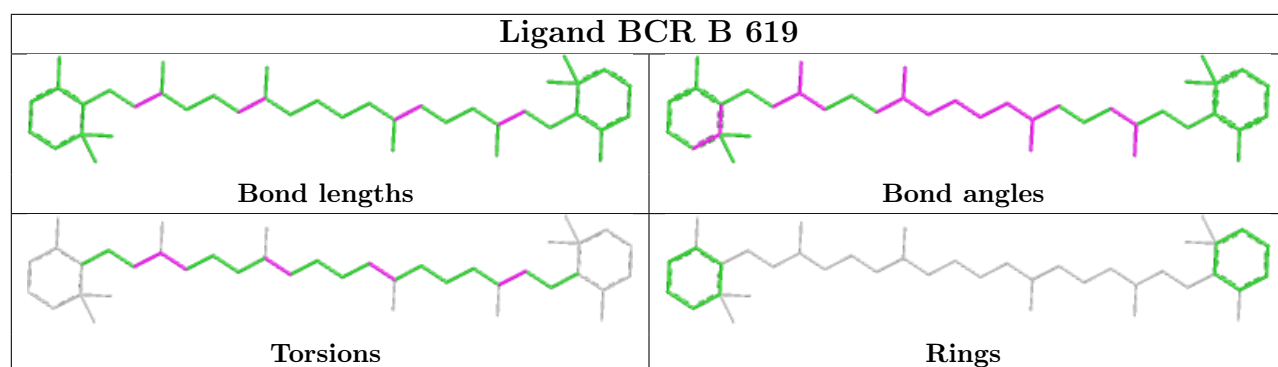


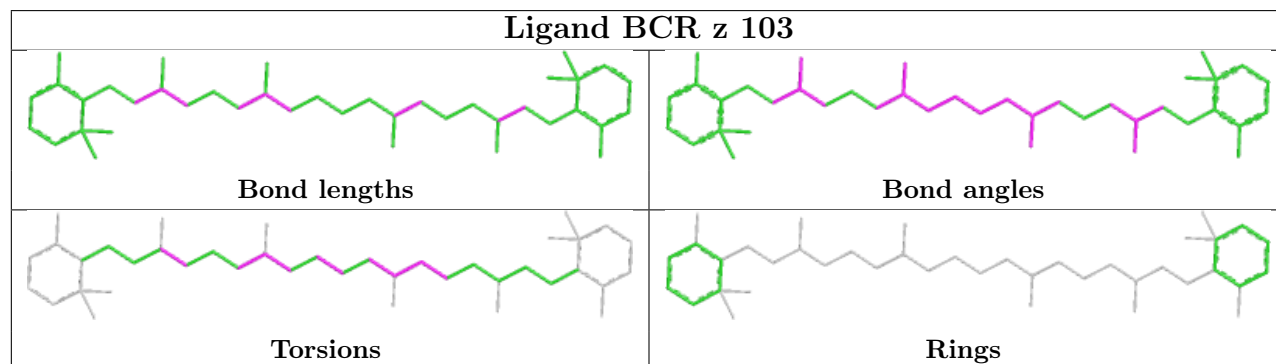
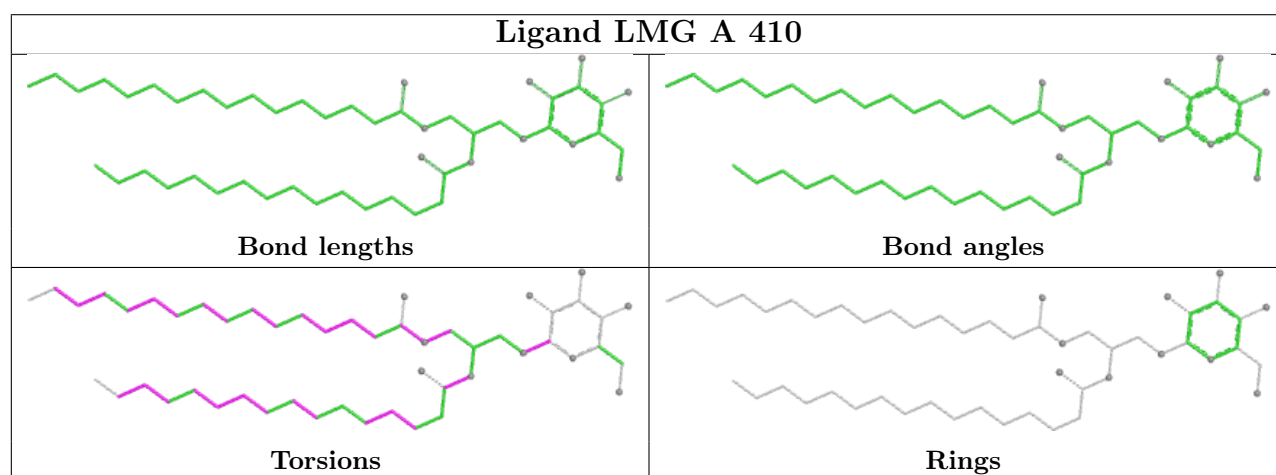
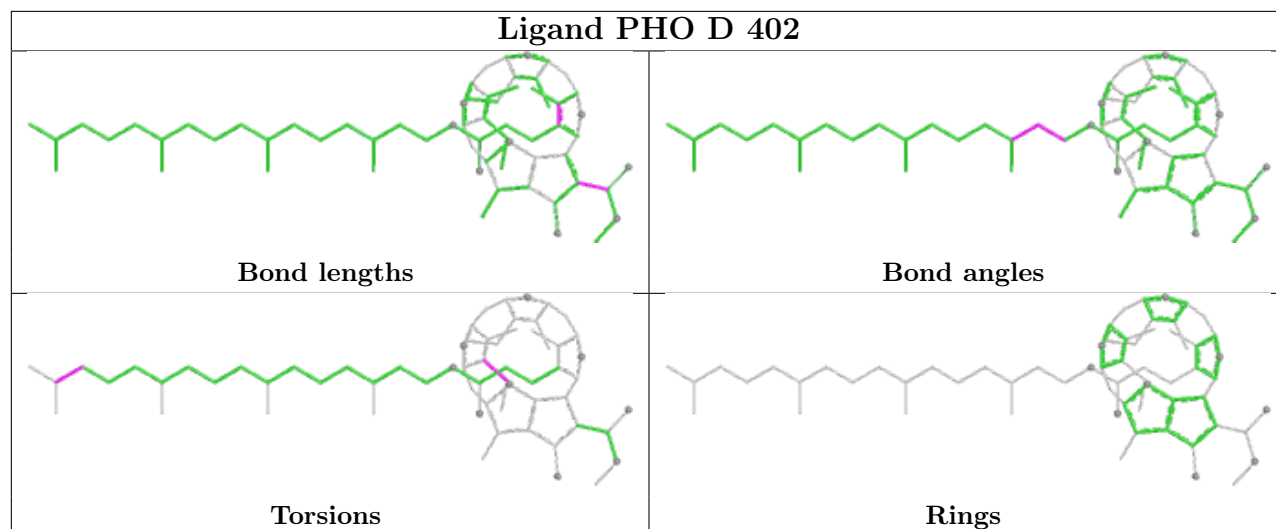
Ligand CLA c 508

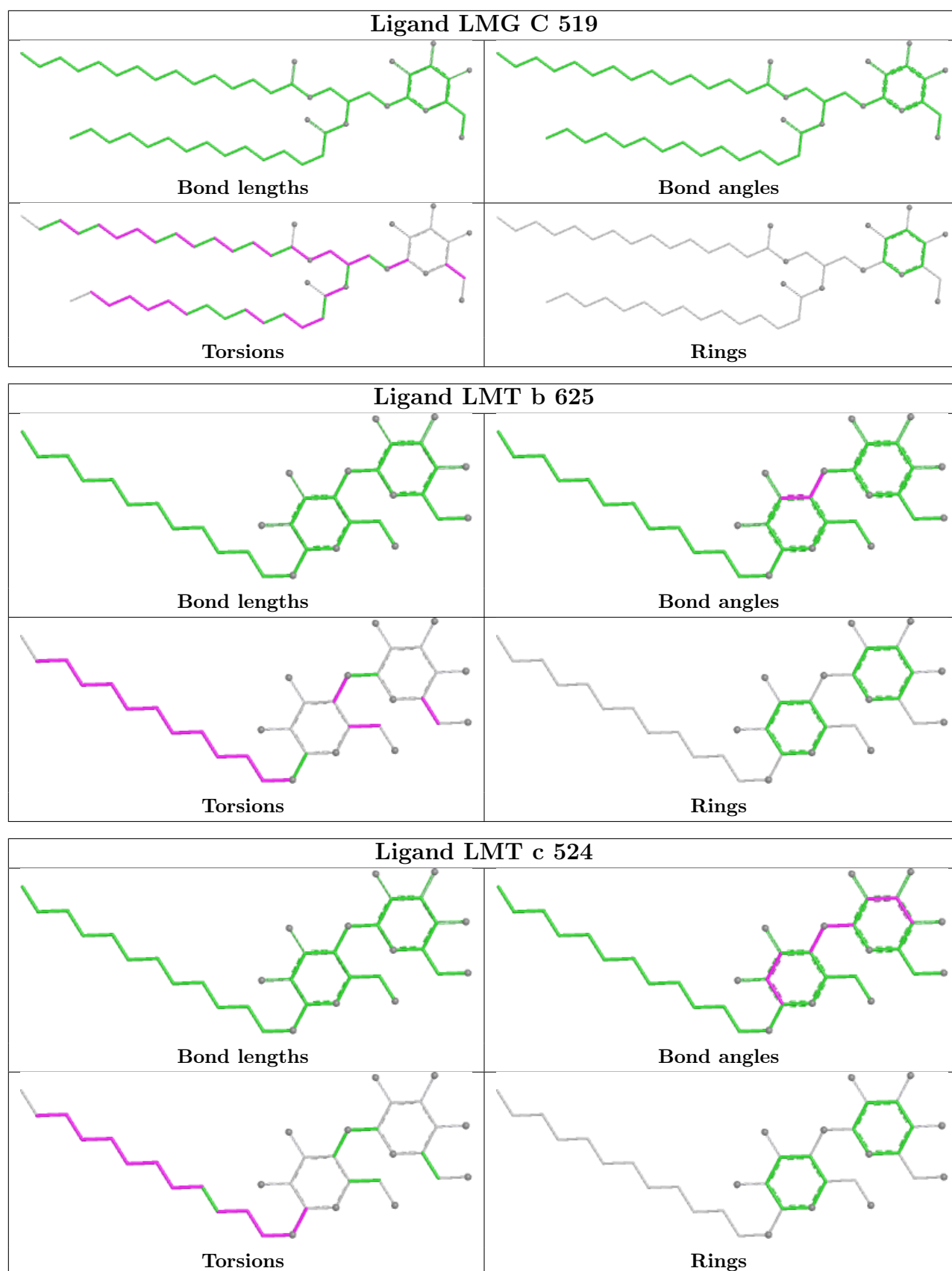


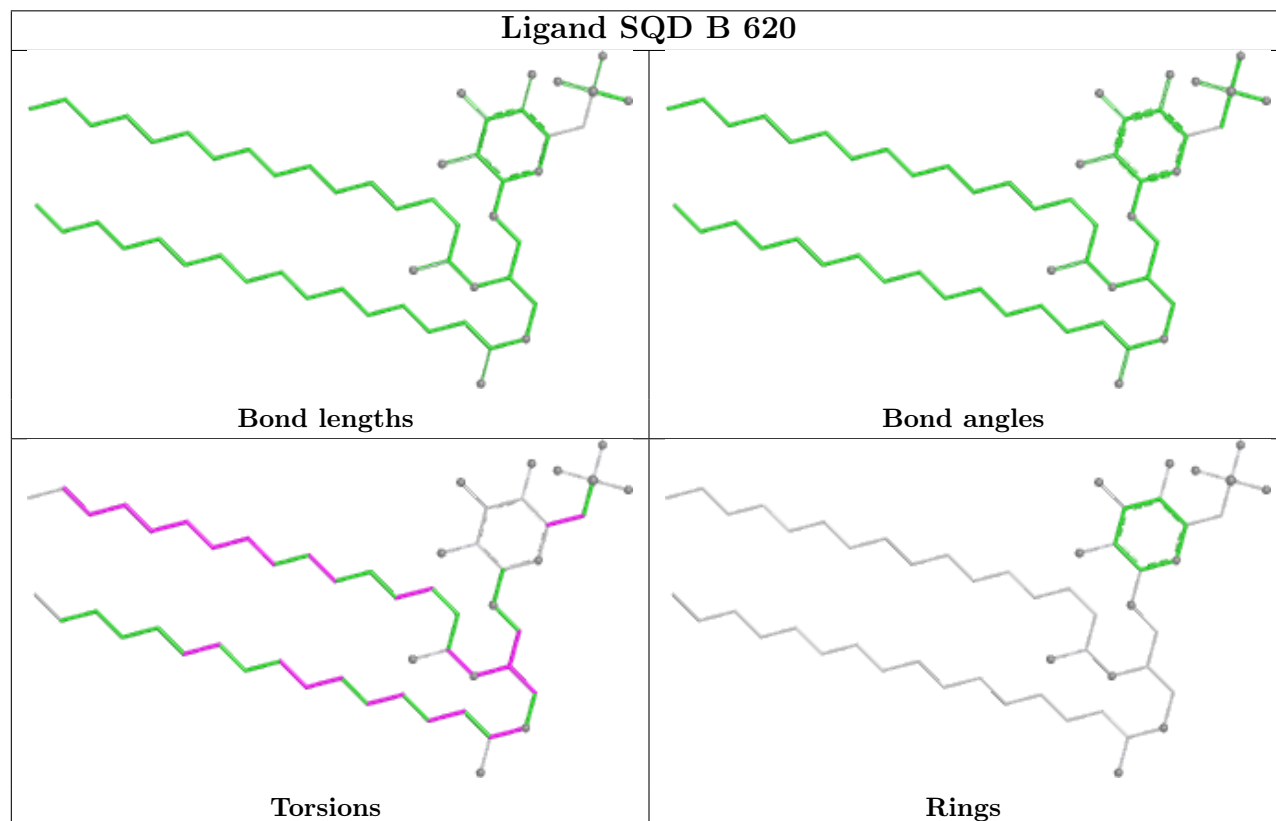
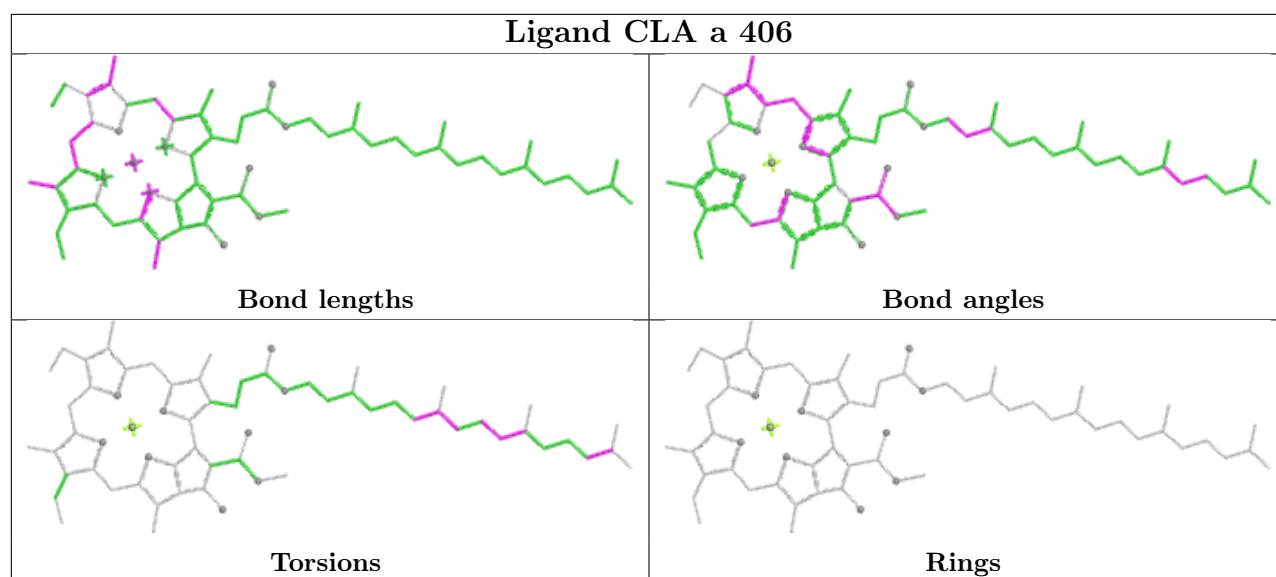


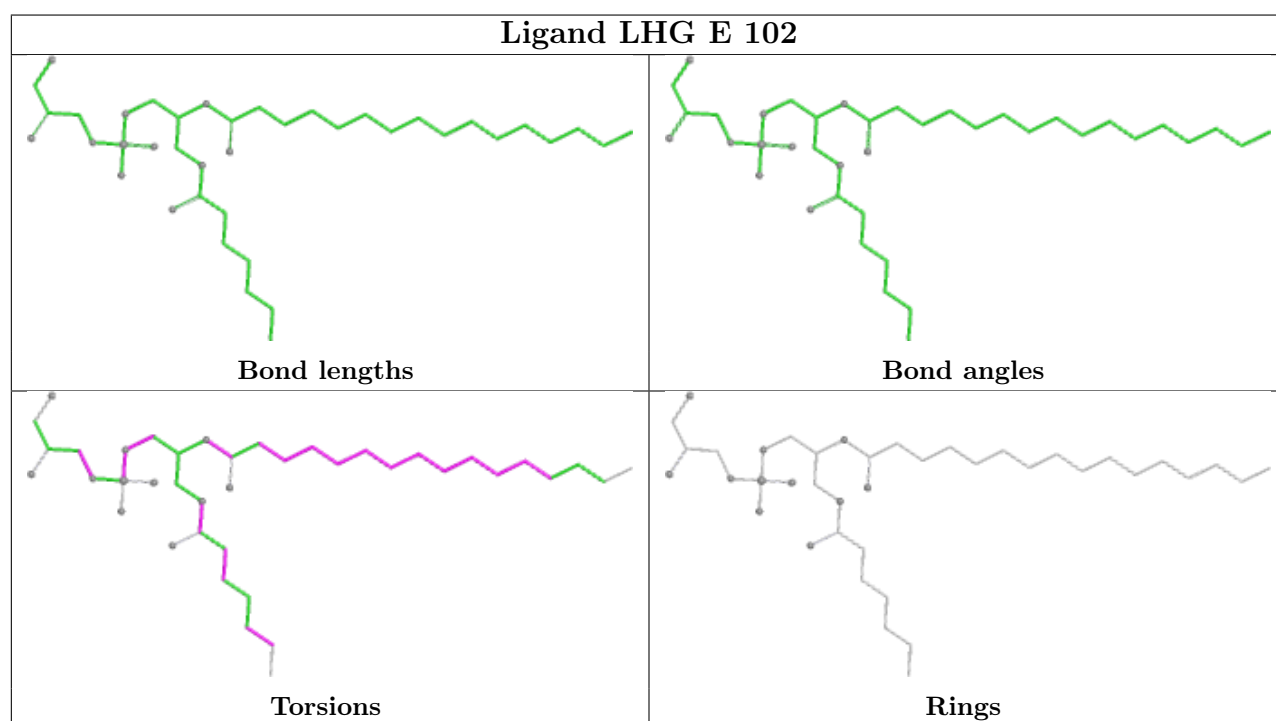
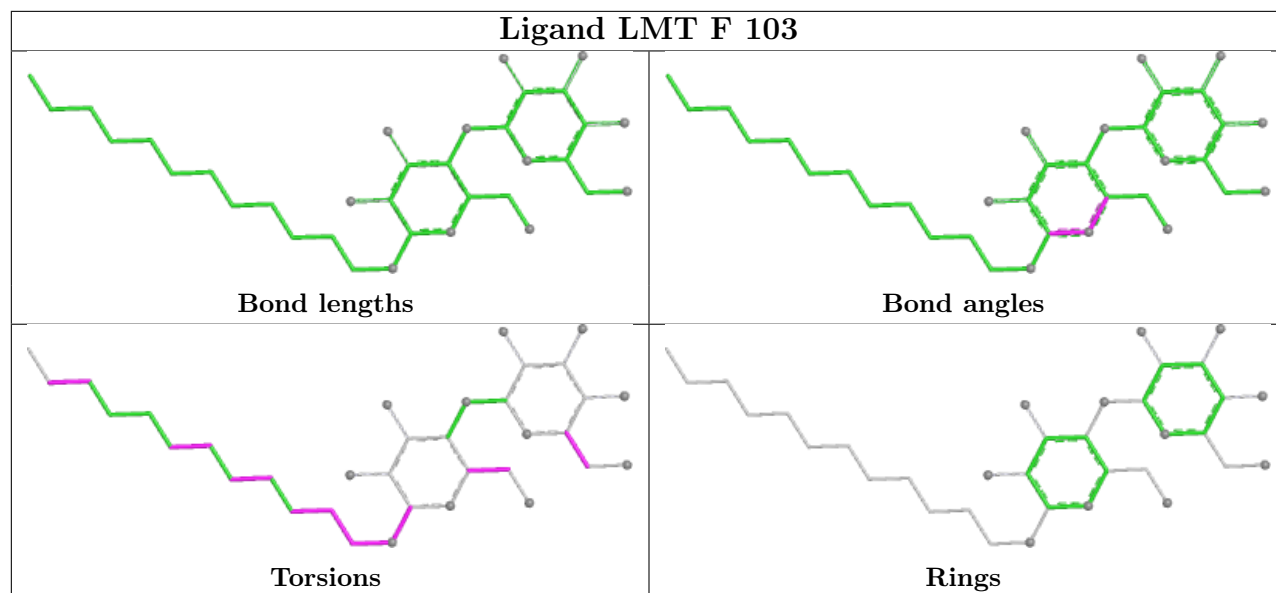


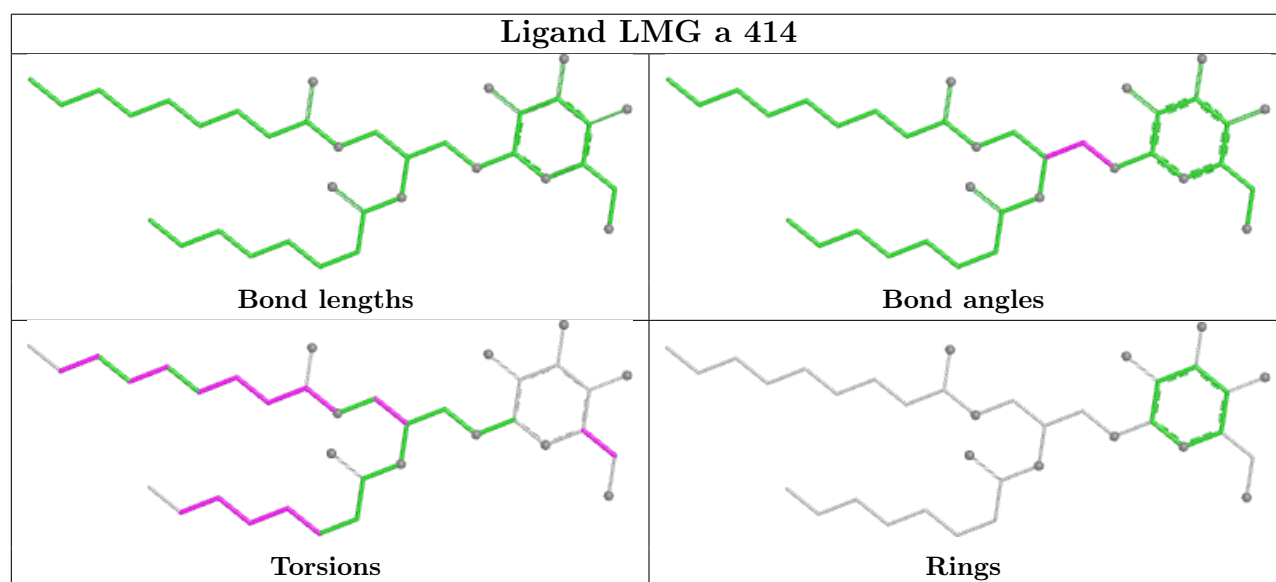
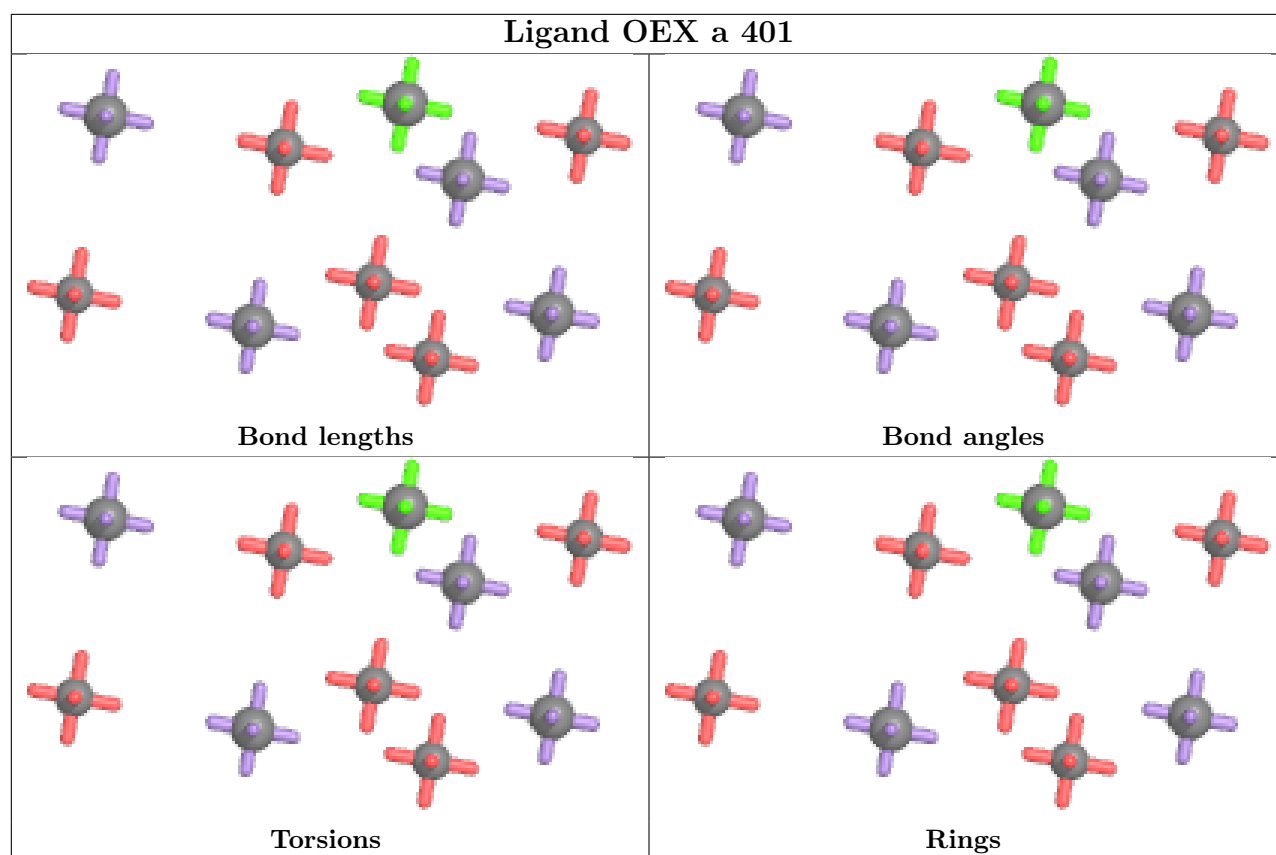


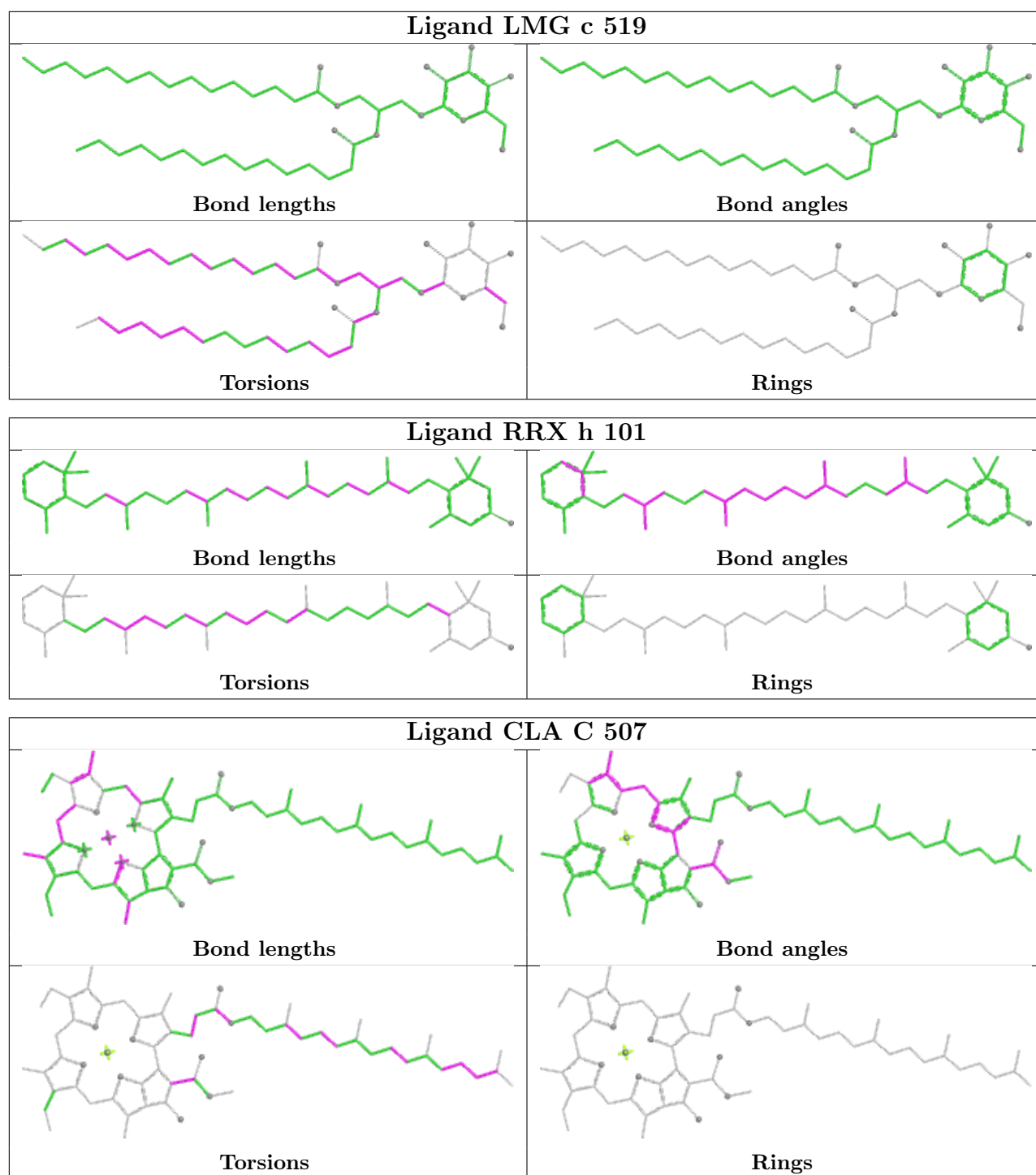


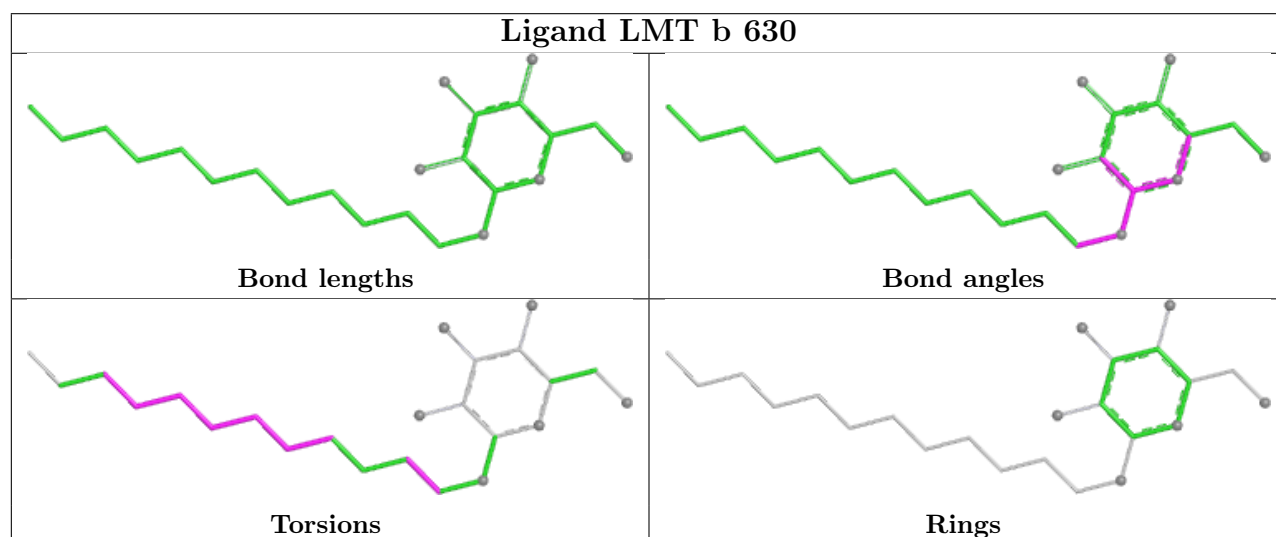
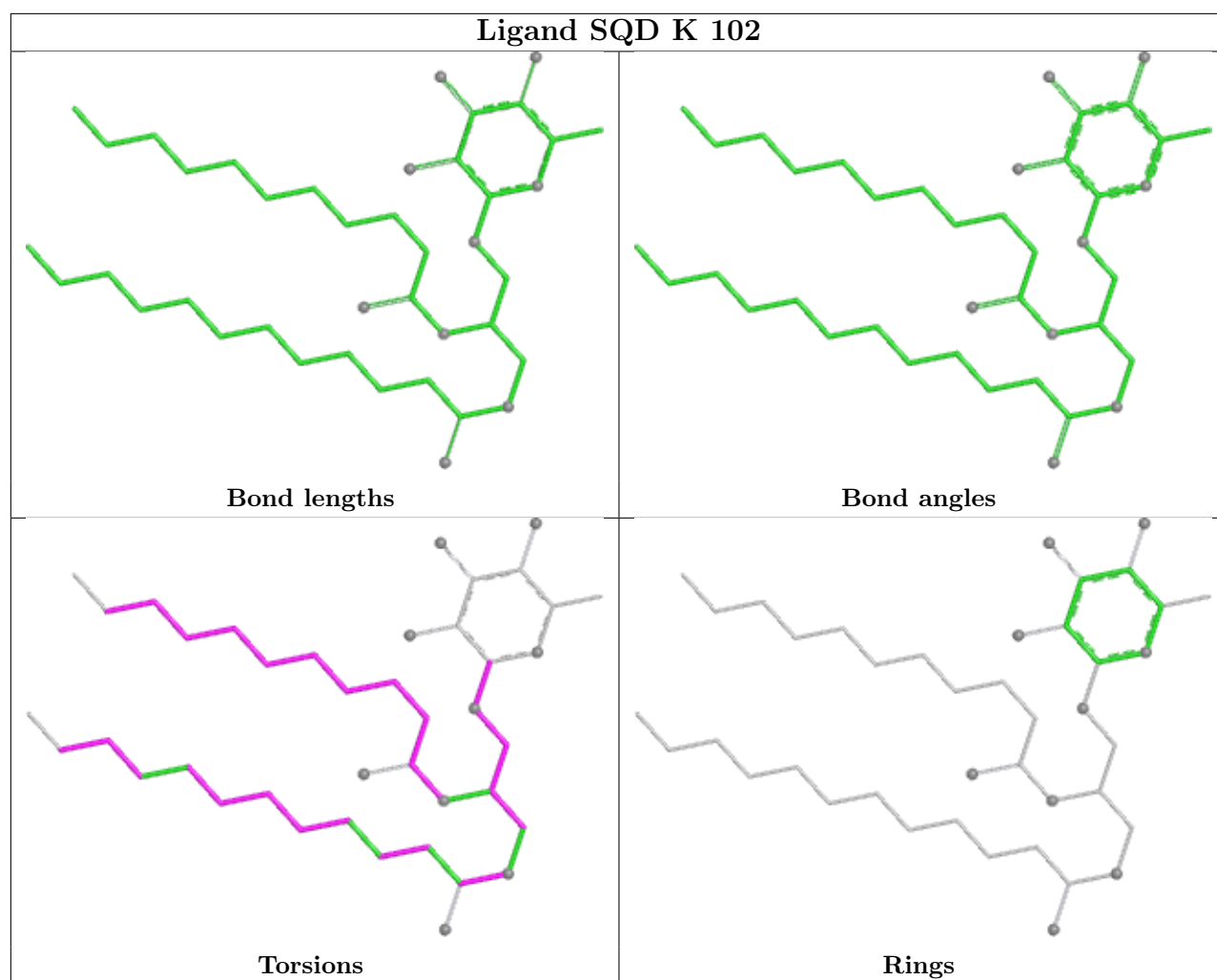


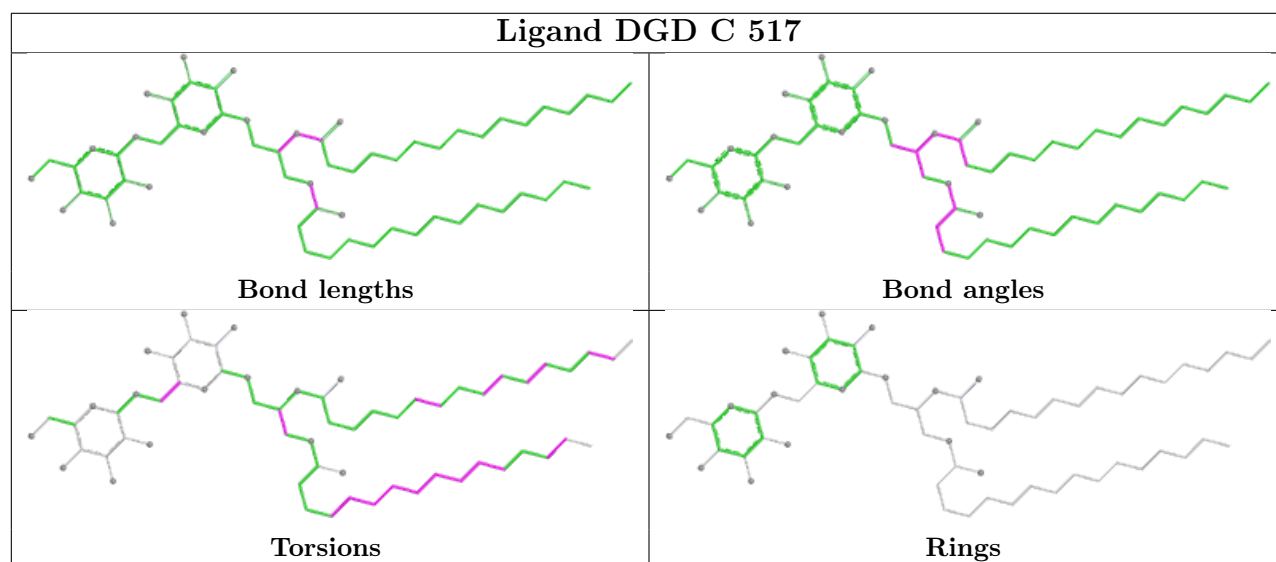
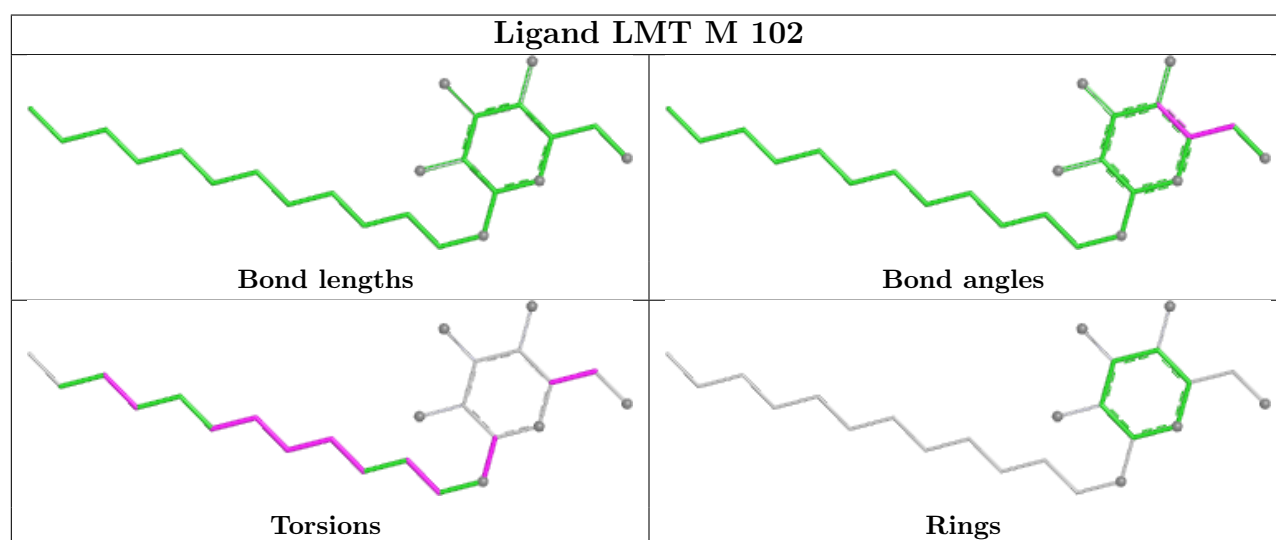
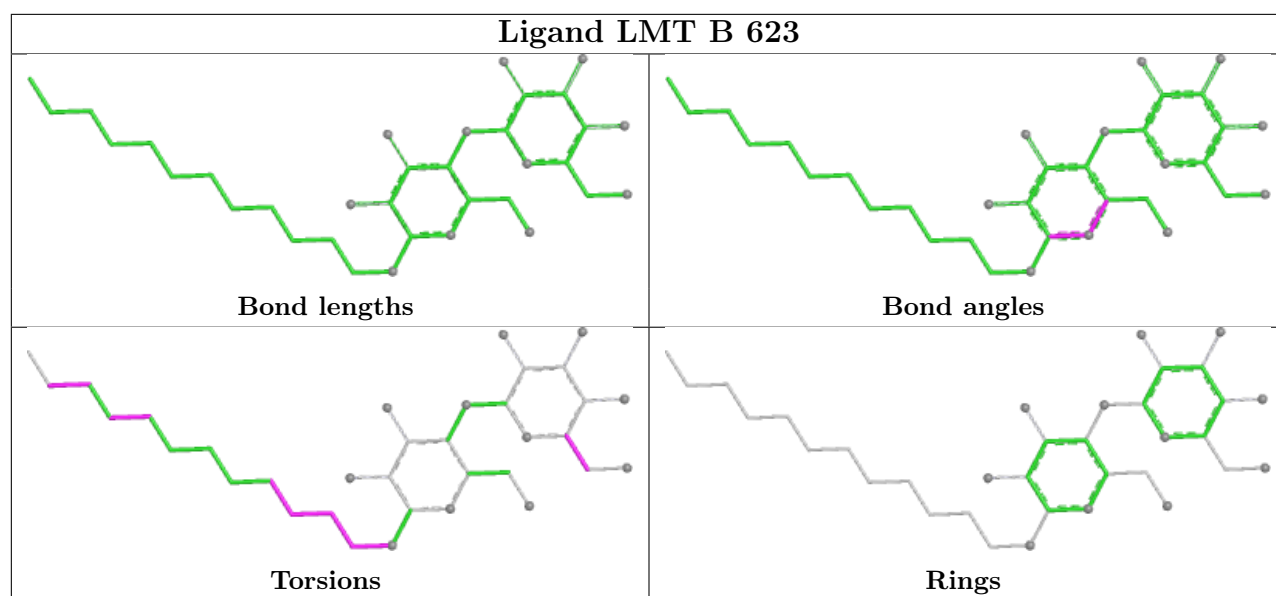


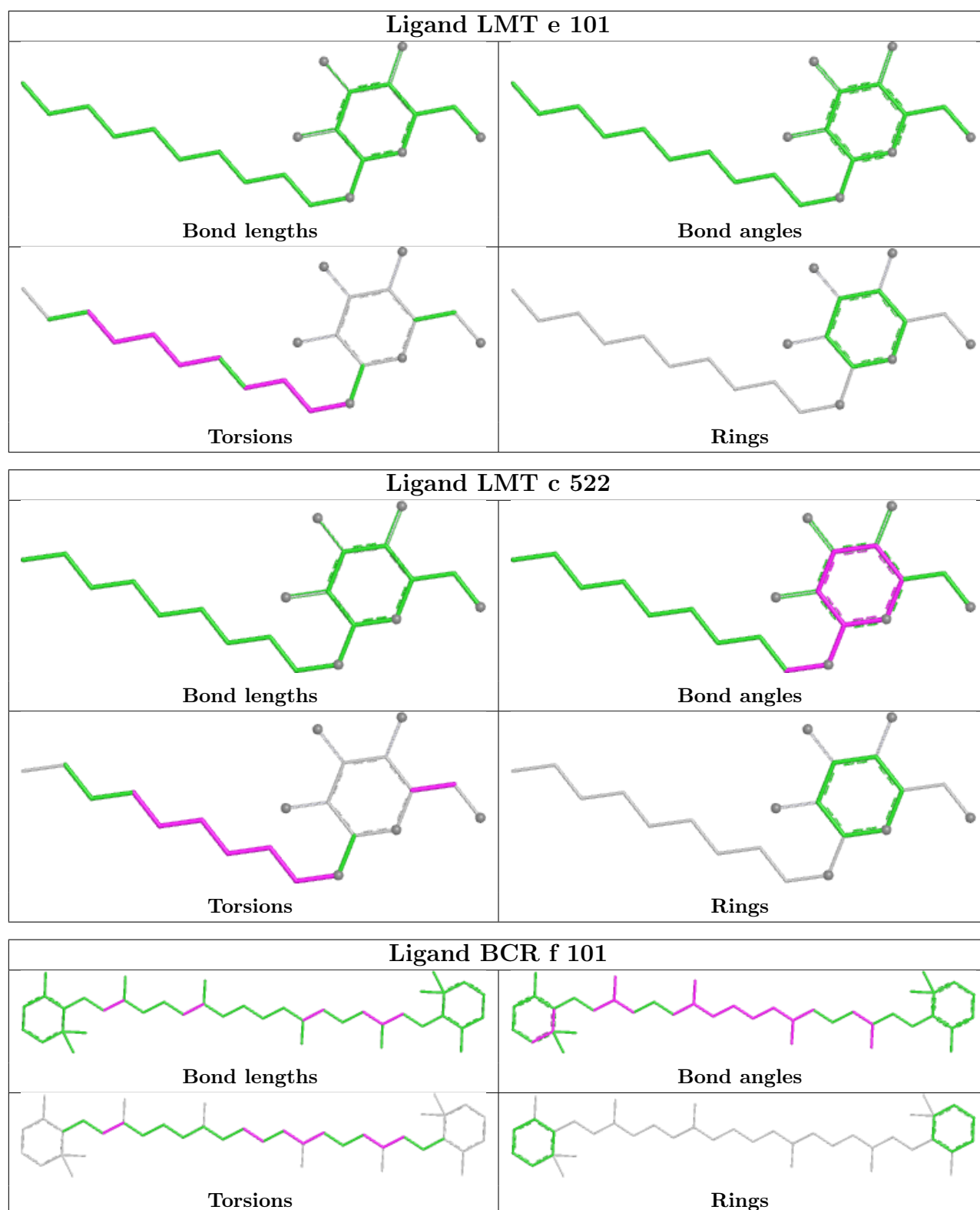


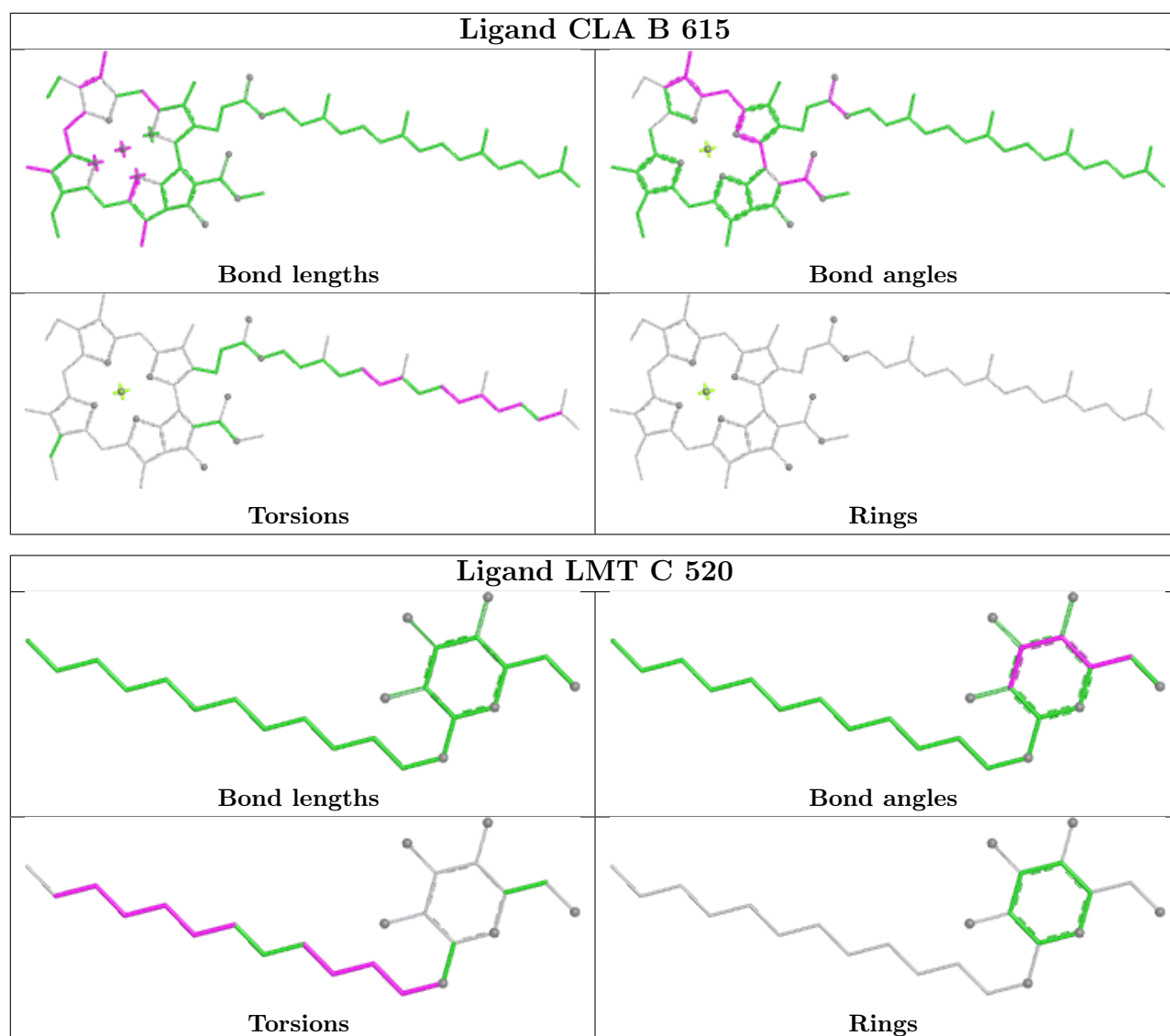












4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

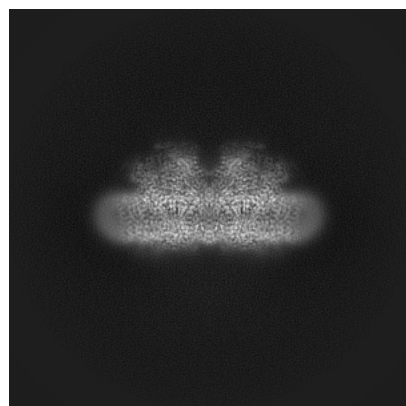
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71652. These allow visual inspection of the internal detail of the map and identification of artifacts.

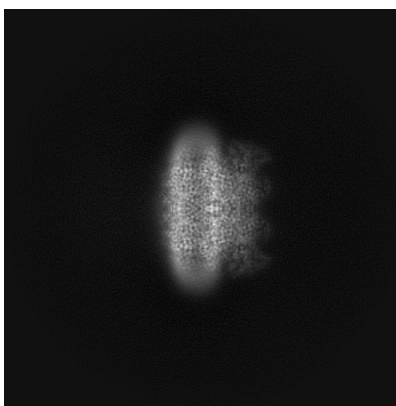
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

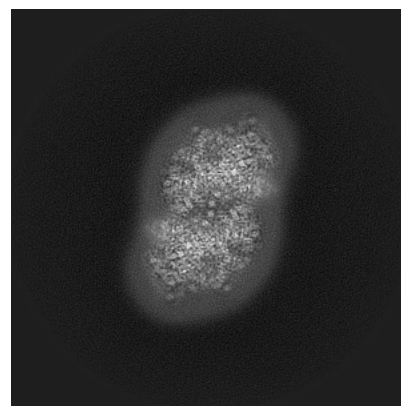
5.1.1 Primary map



X

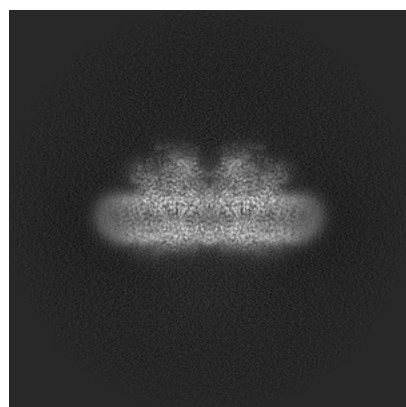


Y

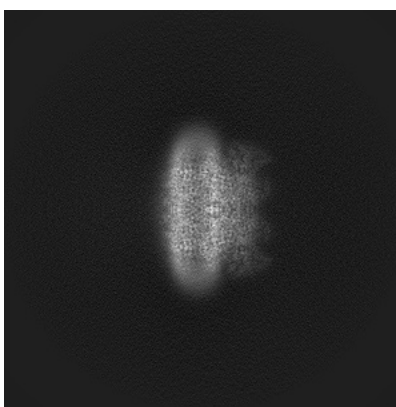


Z

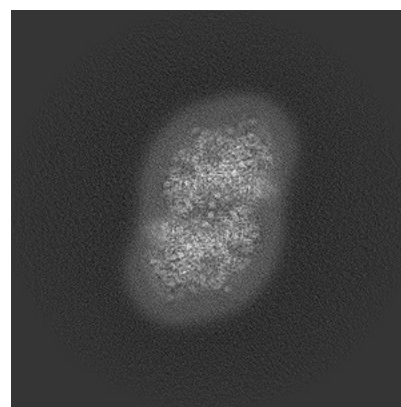
5.1.2 Raw map



X



Y

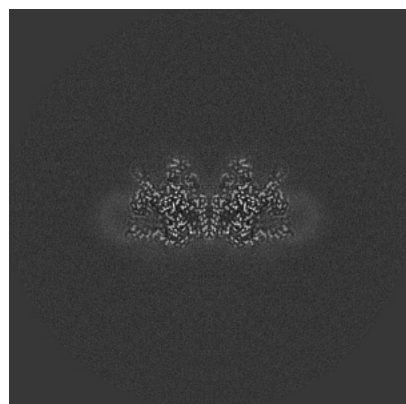


Z

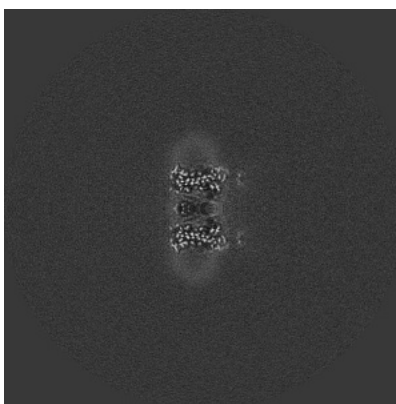
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

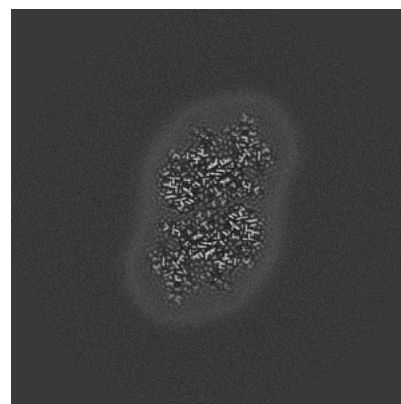
5.2.1 Primary map



X Index: 300

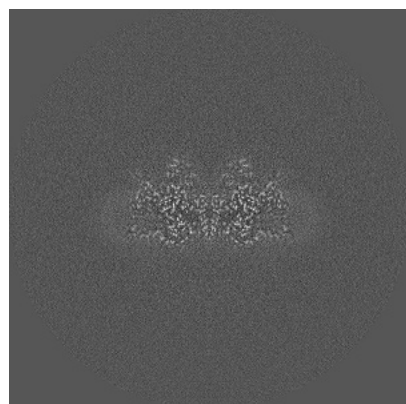


Y Index: 300

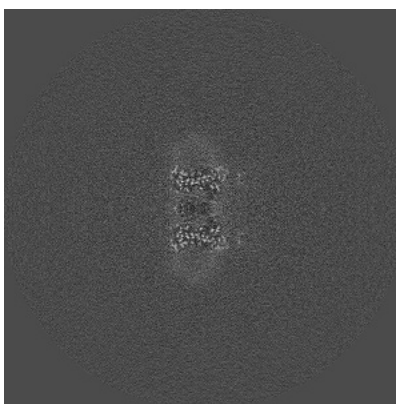


Z Index: 300

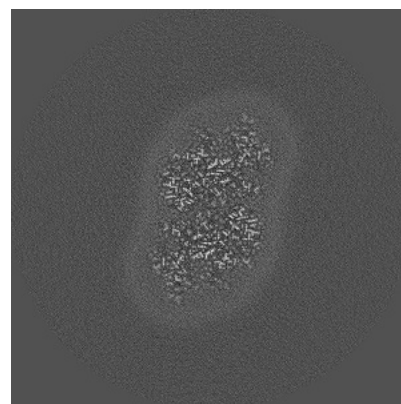
5.2.2 Raw map



X Index: 300



Y Index: 300

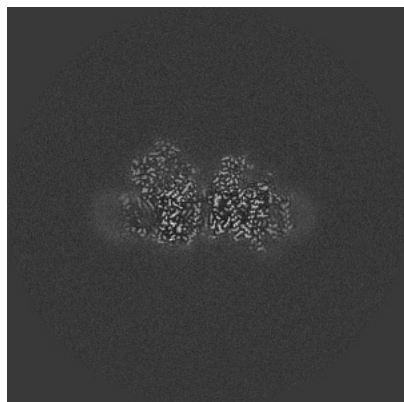


Z Index: 300

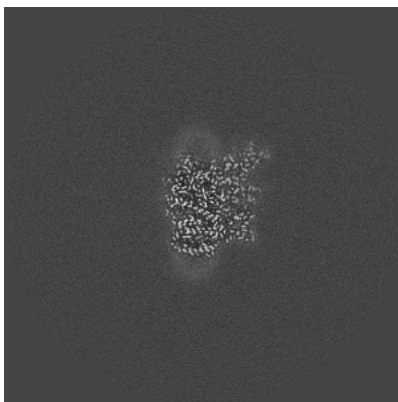
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

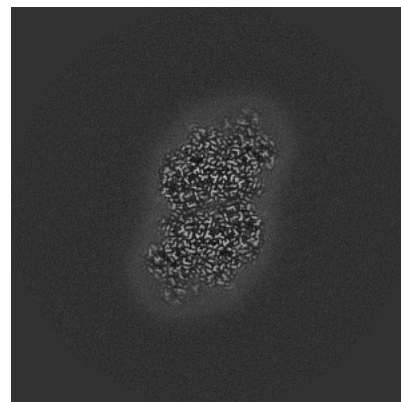
5.3.1 Primary map



X Index: 278

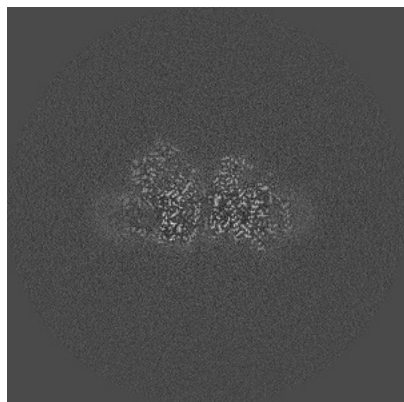


Y Index: 341

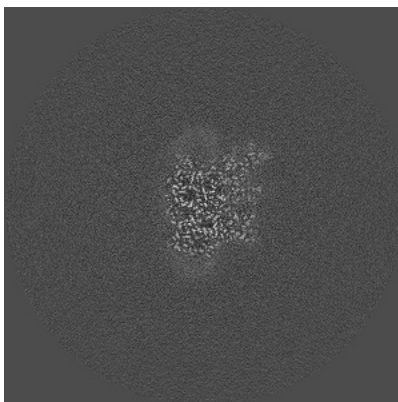


Z Index: 312

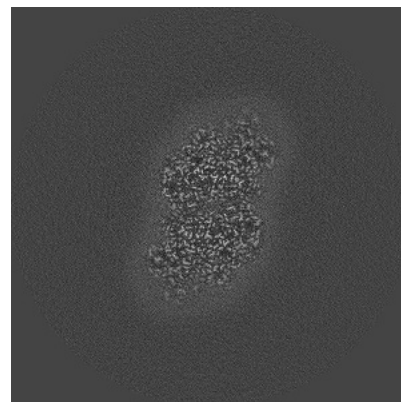
5.3.2 Raw map



X Index: 278



Y Index: 342

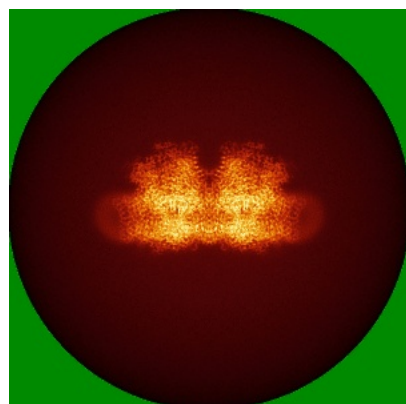


Z Index: 312

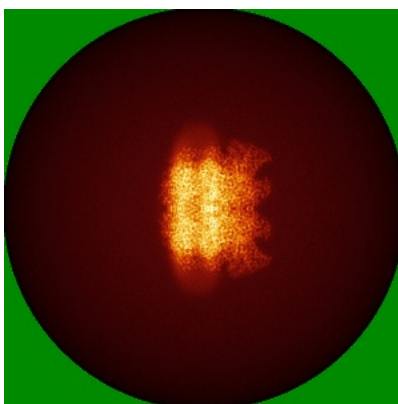
The images above show the largest variance slices of the map in three orthogonal directions.

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

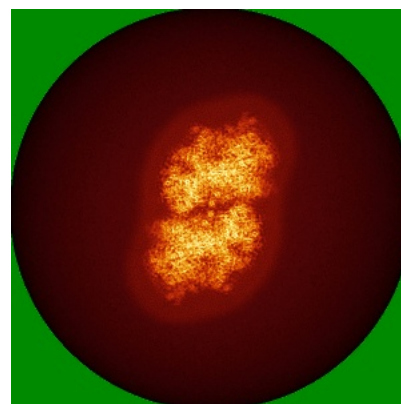
5.4.1 Primary map



X

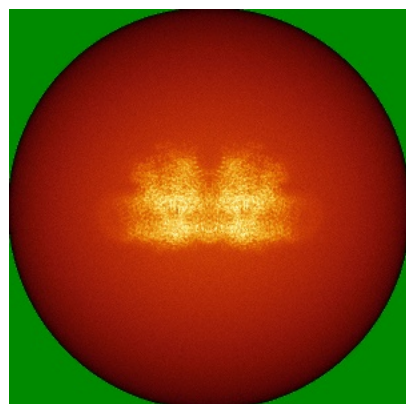


Y

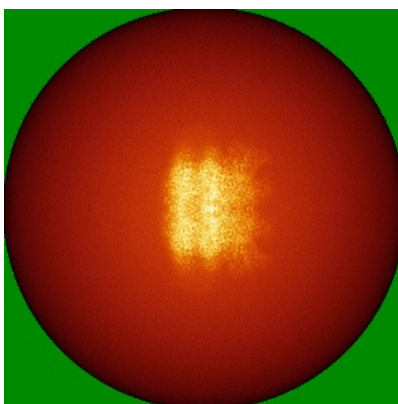


Z

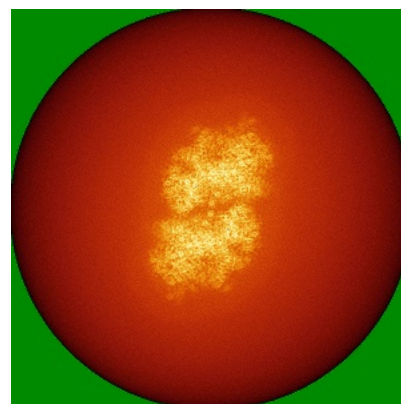
5.4.2 Raw map



X



Y

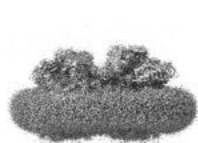


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



X



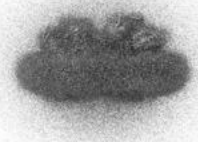
Y



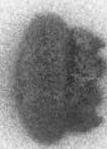
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



X



Y



Z

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.

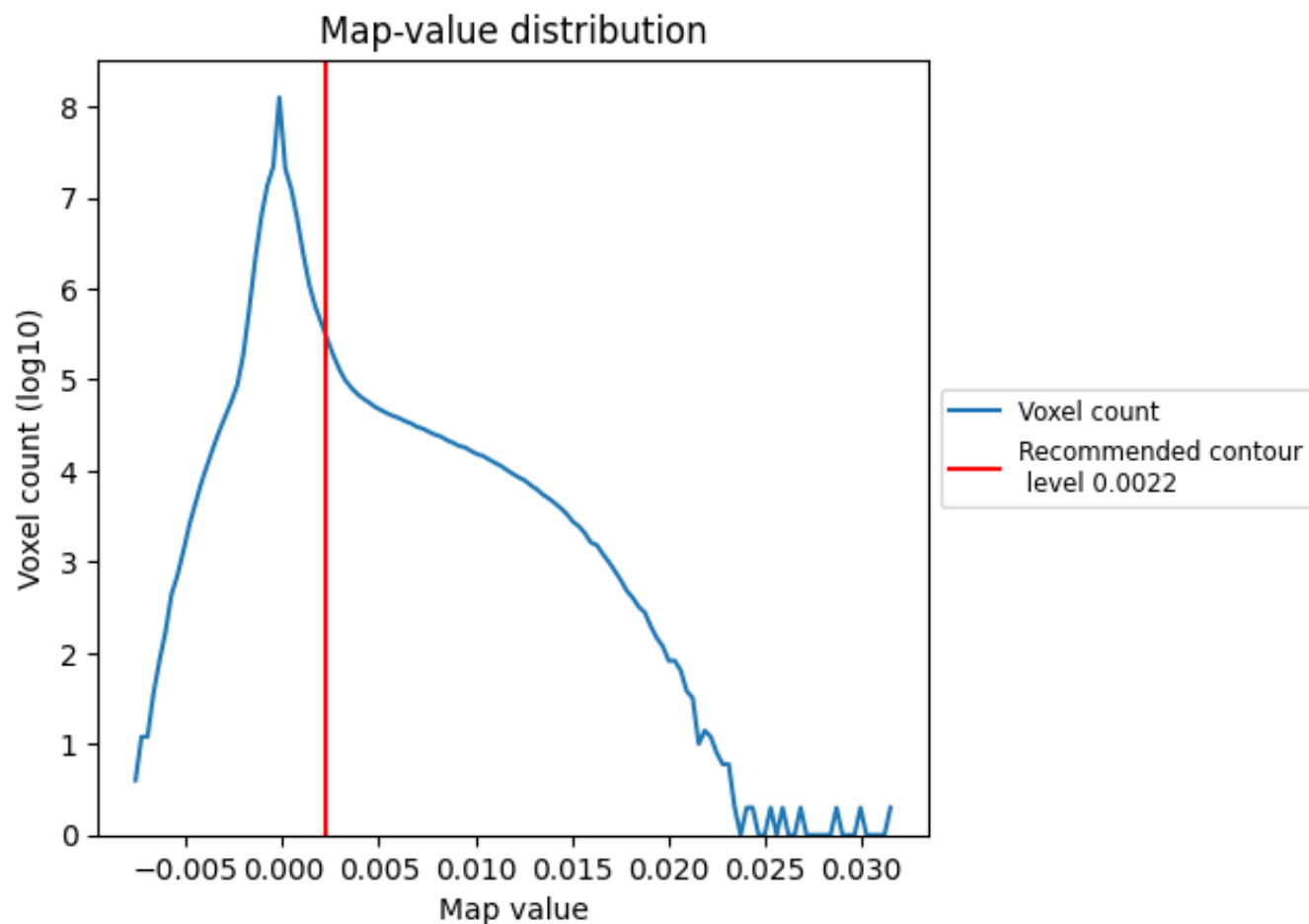
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

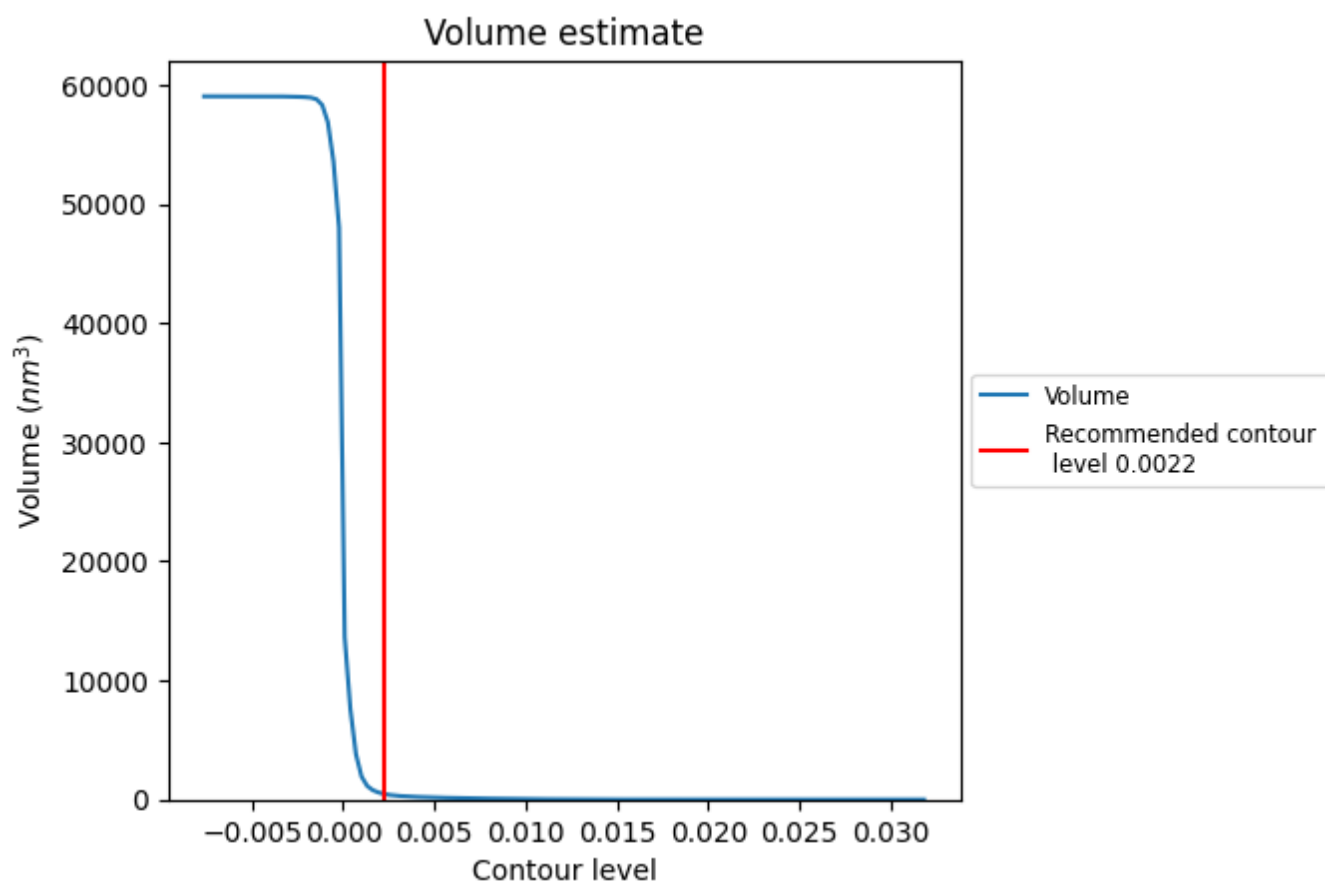
This section contains the results of statistical analysis of the map.

6.1 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.

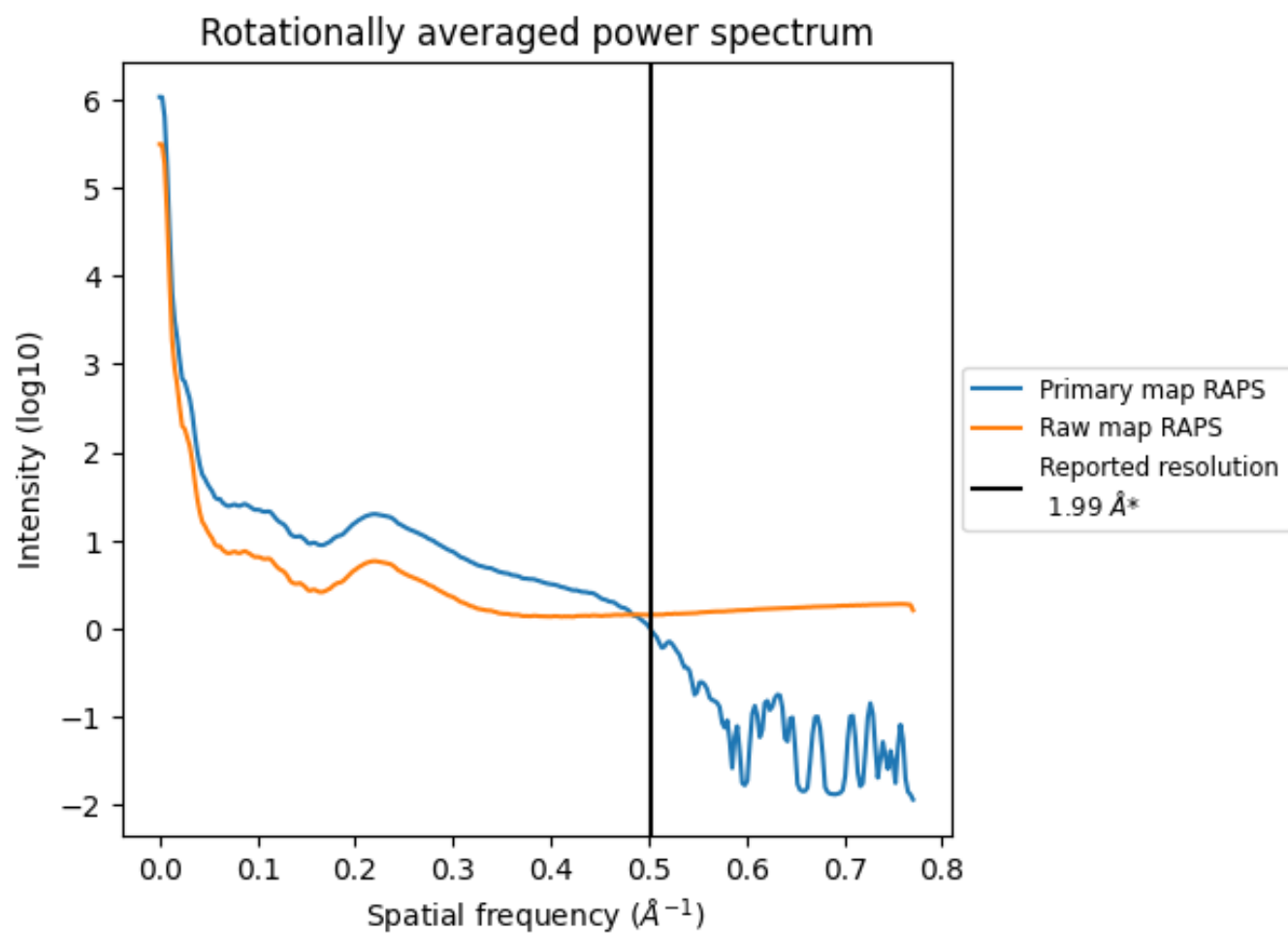
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; this corresponds to an approximate mass of 443 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.

6.3 Rotationally averaged power spectrum ⓘ

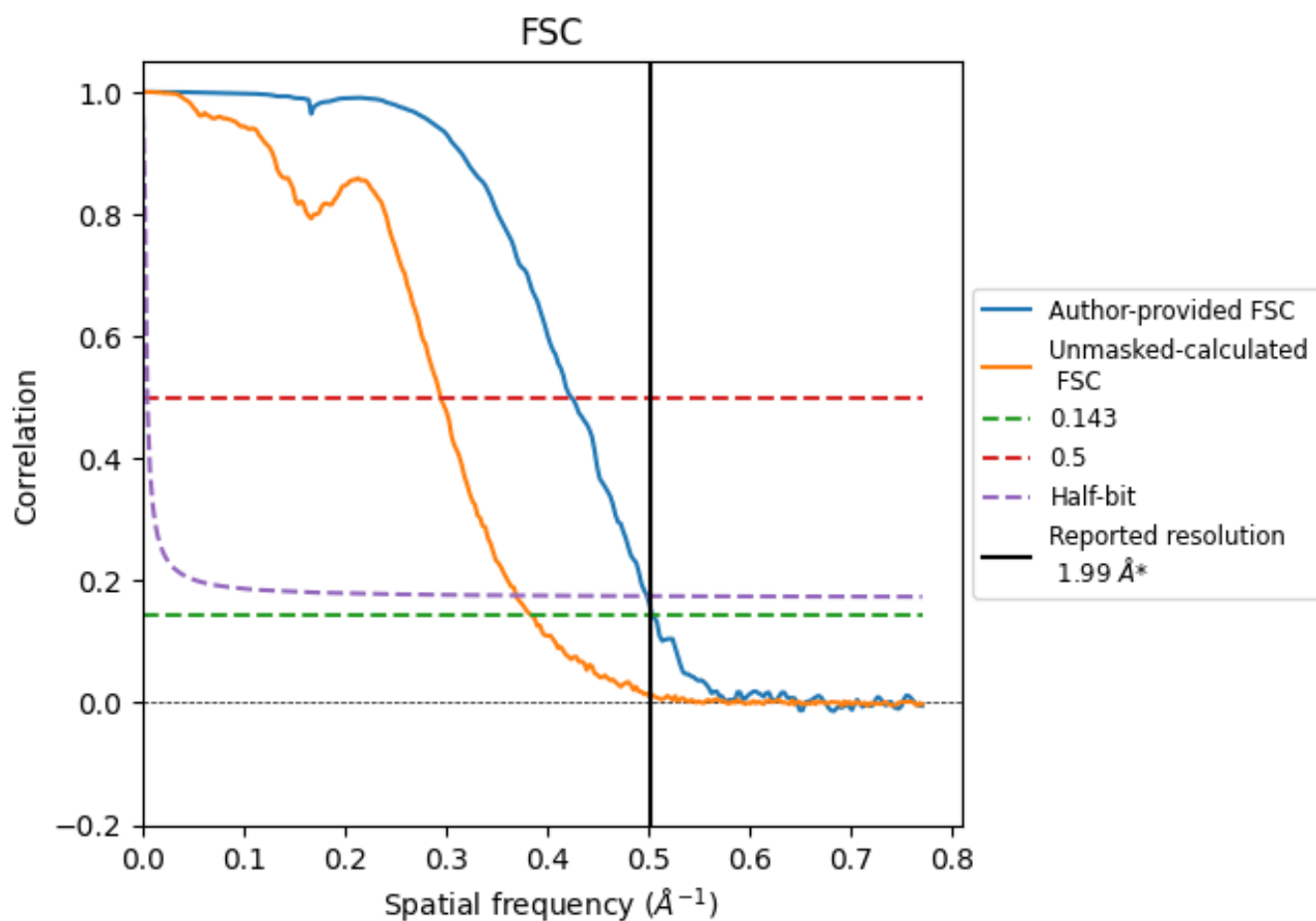


*Reported resolution corresponds to spatial frequency of 0.503 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.503 \AA^{-1}

7.2 Resolution estimates [i](#)

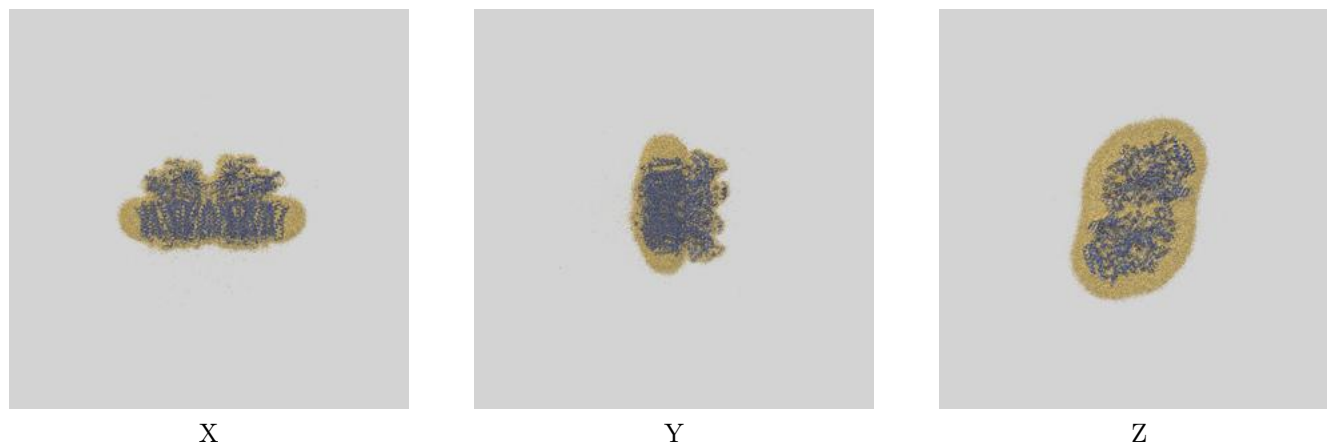
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.99	-	-
Author-provided FSC curve	1.98	2.36	2.01
Unmasked-calculated*	2.60	3.39	2.71

*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 2.60 differs from the reported value 1.99 by more than 10 %

8 Map-model fit [i](#)

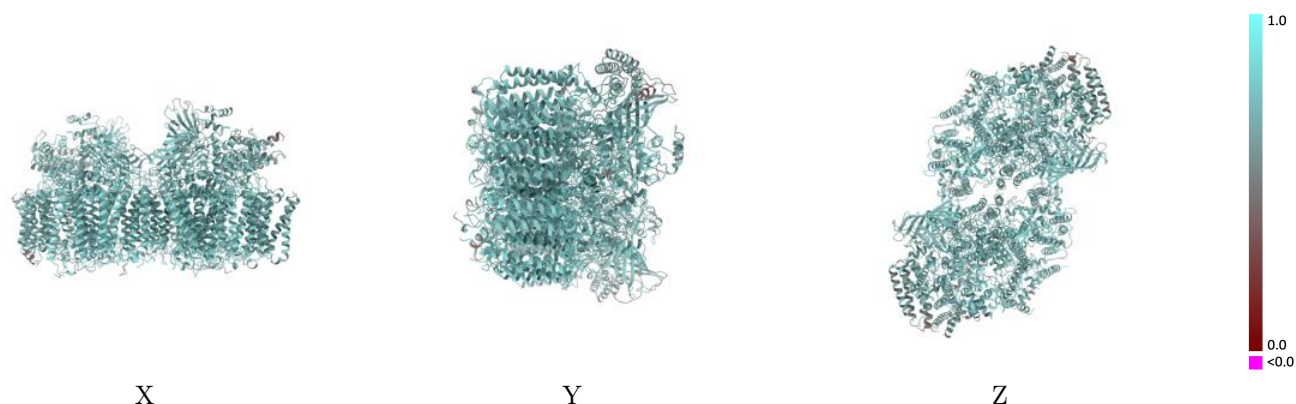
This section contains information regarding the fit between EMDB map EMD-71652 and PDB model 9PHW. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



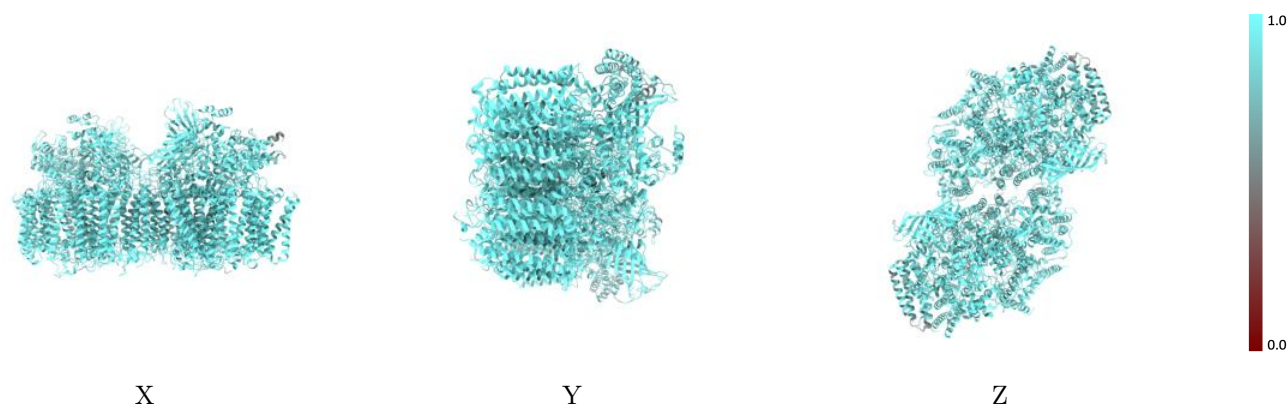
The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



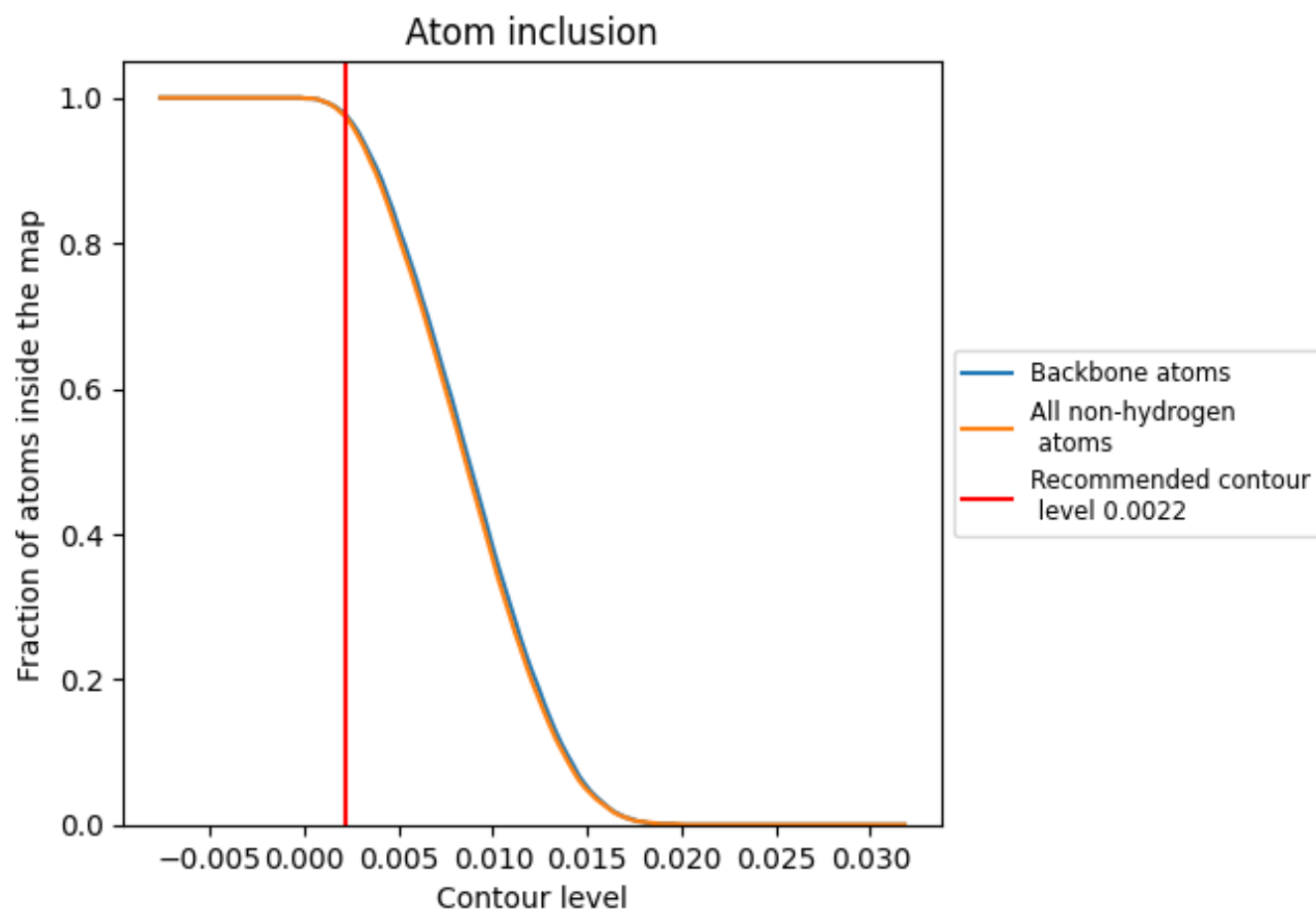
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.0022).







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.7110
A	 0.9900	 0.7480
B	 0.9850	 0.7270
C	 0.9860	 0.7190
D	 0.9900	 0.7480
E	 0.9650	 0.6820
F	 0.9680	 0.6830
H	 0.9880	 0.7120
I	 0.9740	 0.6720
J	 0.9630	 0.6790
K	 0.9320	 0.6600
L	 0.9830	 0.7250
M	 0.9740	 0.7100
O	 0.9550	 0.6700
Q	 0.8460	 0.5980
R	 0.9760	 0.6260
T	 0.9690	 0.7090
U	 0.9450	 0.6700
V	 0.9630	 0.6930
X	 0.9890	 0.6870
Y	 0.9620	 0.6460
Z	 0.9720	 0.6500
a	 0.9900	 0.7490
b	 0.9850	 0.7280
c	 0.9860	 0.7190
d	 0.9900	 0.7490
e	 0.9650	 0.6820
f	 0.9680	 0.6860
h	 0.9880	 0.7130
i	 0.9740	 0.6730
j	 0.9630	 0.6810
k	 0.9250	 0.6490
l	 0.9900	 0.7430
m	 0.9810	 0.7260
o	 0.9540	 0.6710



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Chain	Atom inclusion	Q-score
q	 0.8450	 0.5980
r	 0.9760	 0.6260
t	 0.9690	 0.7110
u	 0.9460	 0.6720
v	 0.9650	 0.6920
x	 0.9850	 0.6820
y	 0.9660	 0.6470
z	 0.9770	 0.6580