



Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 09:38 AM EST

PDB ID : 7N8O
EMDB ID : EMD-24239
Title : High-resolution structure of photosystem II from the mesophilic cyanobacterium, *Synechocystis* sp. PCC 6803
Authors : Gisriel, C.J.; Brudvig, G.W.
Deposited on : 2021-06-15
Resolution : 1.93 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:

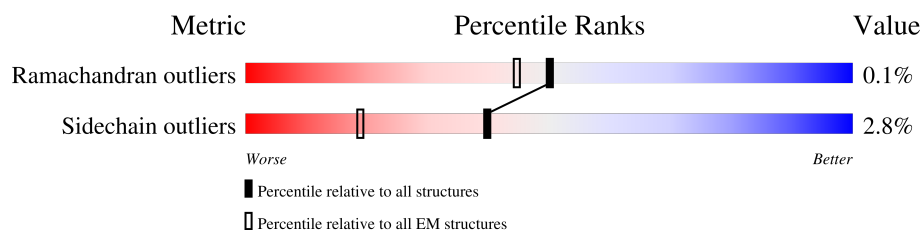
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 1.93 Å.

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



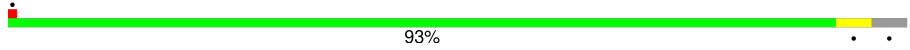


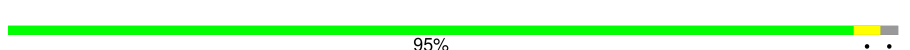

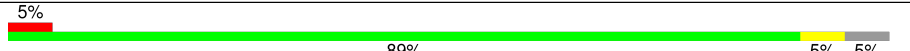
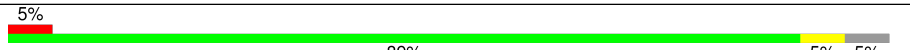

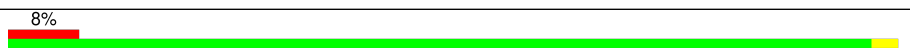
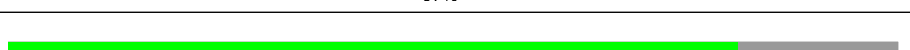
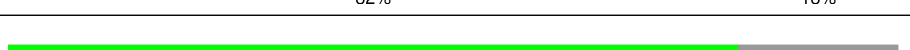
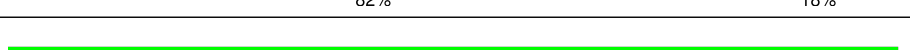
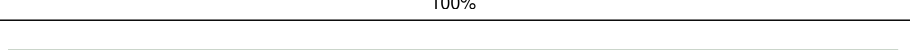
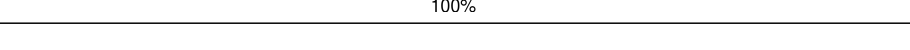
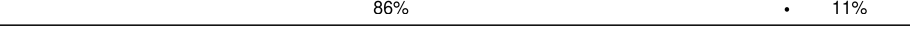
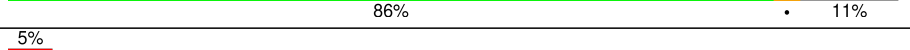
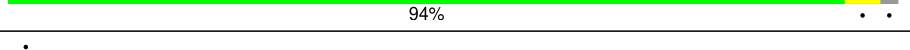
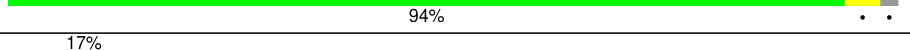



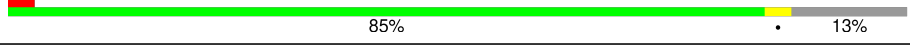
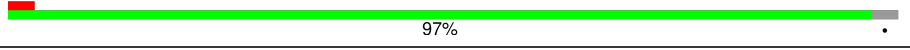
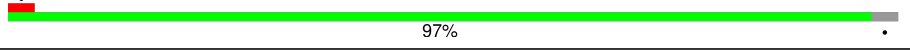

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	
1	a	360	
2	B	507	
2	b	507	
3	C	460	
3	c	460	
4	D	352	
4	d	352	
5	E	81	




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	81	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	45	
10	k	45	
11	L	39	
11	l	39	
12	M	35	
12	m	35	
13	O	247	
13	o	247	
14	Q	149	
14	q	149	
15	R	39	
15	r	39	
16	T	31	
16	t	31	
17	U	131	
17	u	131	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	V	160	
18	v	160	
19	X	39	
19	x	39	
20	Y	39	
20	y	39	
21	Z	62	
21	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	408	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	408	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
32	BCT	A	417	-	X	-	-
32	BCT	a	417	-	X	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 54656 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
			2624	1718	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2624	1718	429	462	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3935	2570	658	694	13		
2	b	503	Total	C	N	O	S	0	0
			3935	2570	658	694	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2726	1807	443	464	12		
4	d	341	Total	C	N	O	S	0	0
			2726	1807	443	464	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	35	Total	C	N	O	S	0	0
			279	189	46	43	1		
6	f	35	Total	C	N	O	S	0	0
			279	189	46	43	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			286	192	45	48	1		
8	i	36	Total	C	N	O	S	0	0
			286	192	45	48	1		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			299	210	42	47		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			299	210	42	47		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			245	169	36	39	1		
12	m	31	Total	C	N	O	S	0	0
			245	169	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1869	1183	304	379	3		
13	o	243	Total	C	N	O	S	0	0
			1869	1183	304	379	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	119	Total	C	N	O	S	0	0
			916	576	164	174	2		
14	q	119	Total	C	N	O	S	0	0
			916	576	164	174	2		

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

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

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

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

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

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

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

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

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

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

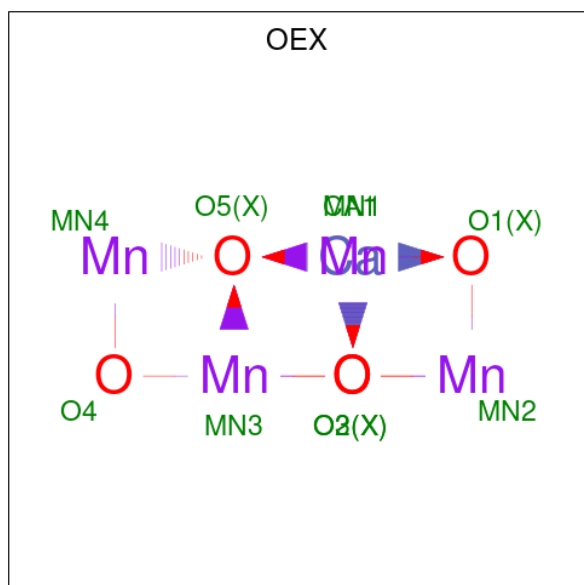
- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	32	Total	C	N	O		0	0
			242	165	37	40			
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 (three-letter code: 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 (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

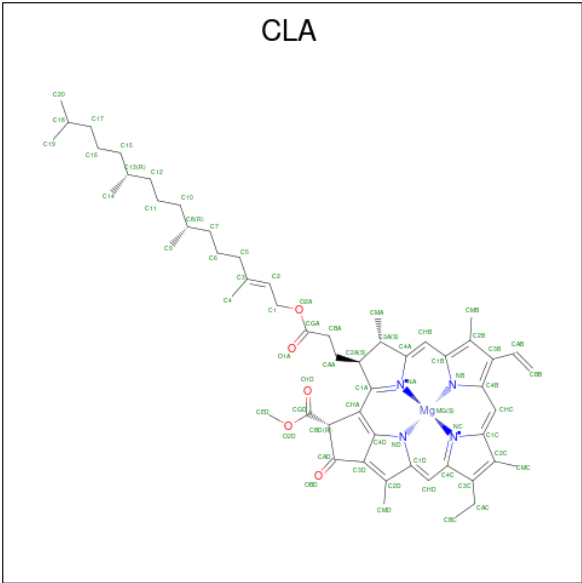
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	

Continued on next page...

Continued from previous page...

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: 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	

Continued on next page...

Continued from previous page...

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 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 55	C 45	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 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

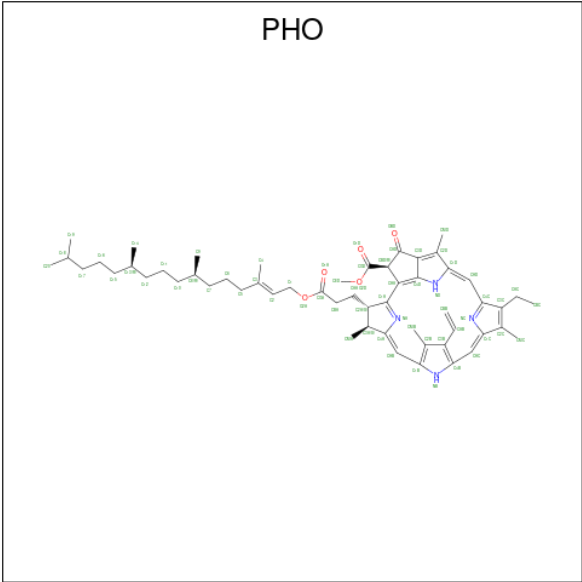
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total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

Continued on next page...

Continued from previous page...

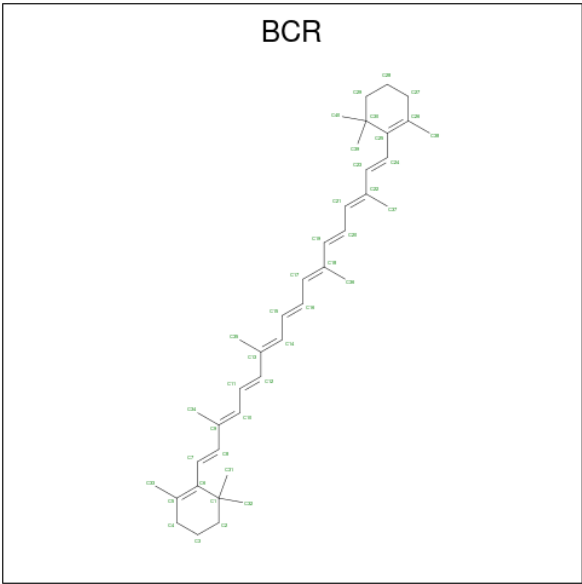
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			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
			50	40	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 (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



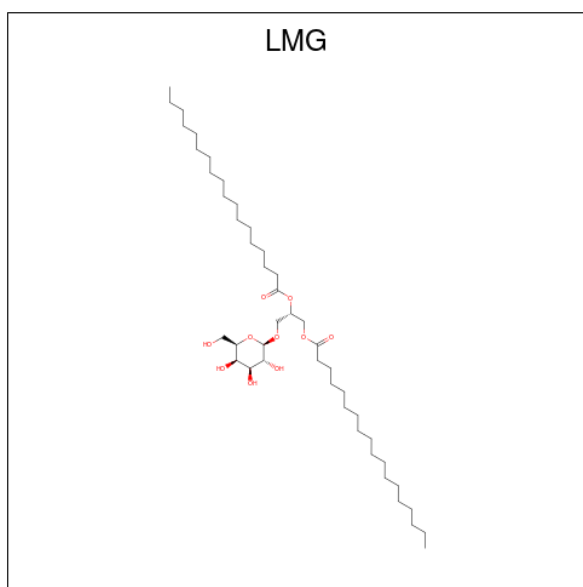
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: 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	k	1	Total C 40 40	0
27	z	1	Total C 40 40	0

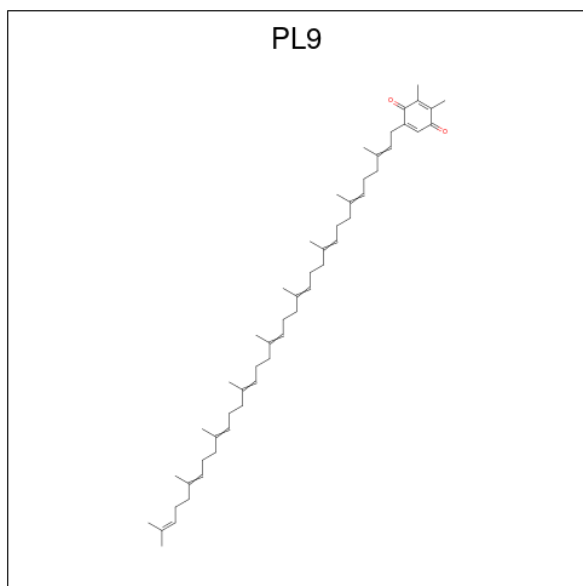
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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
			51	41	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
			51	41	10	

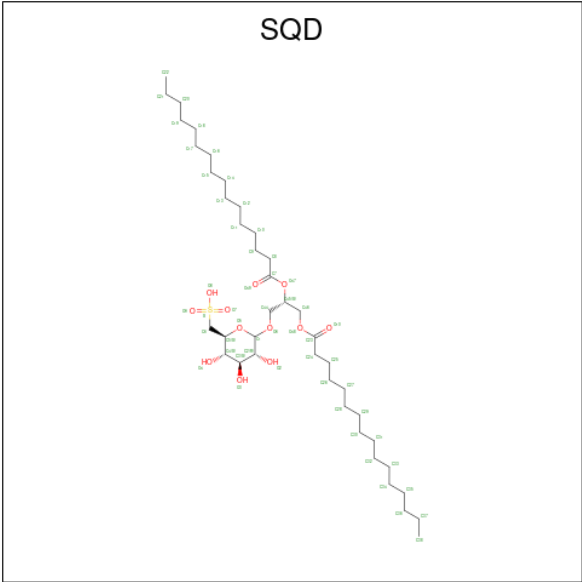
- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

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



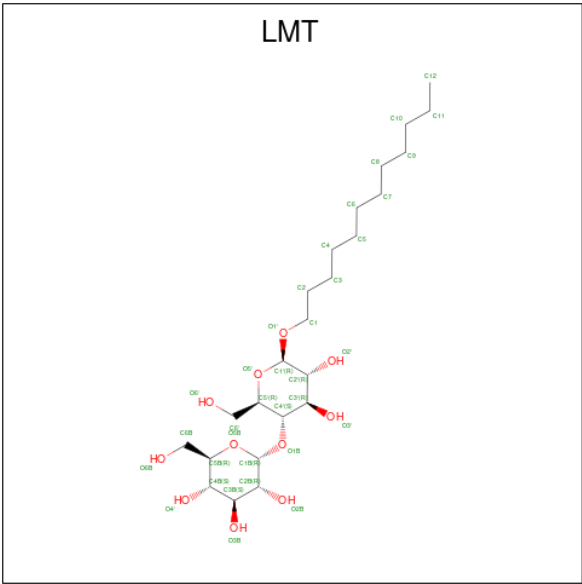
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			48	35	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
			45	36	9		
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			48	35	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
			45	36	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			24	18	6	
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
			25	19	6	
31	B	1	Total	C	O	0
			35	24	11	
31	C	1	Total	C	O	0
			28	17	11	
31	C	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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

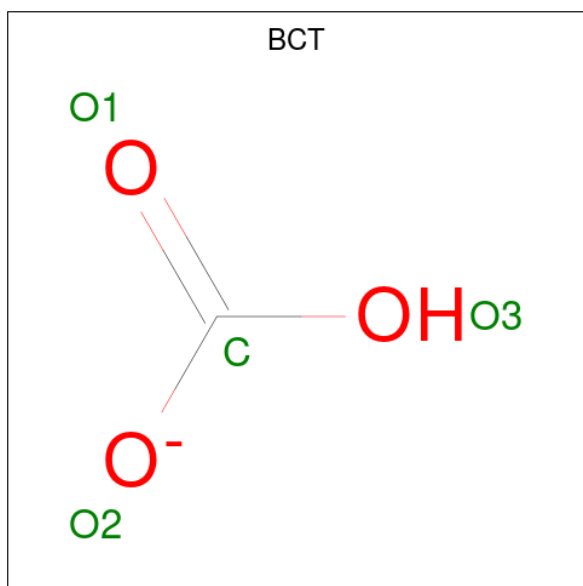
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			25	19	6	
31	b	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			28	17	11	
31	c	1	Total	C	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	d	1	Total	C	O	0
			24	18	6	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			35	24	11	
31	e	1	Total	C	O	0
			22	16	6	
31	e	1	Total	C	O	0
			35	24	11	
31	f	1	Total	C	O	0
			35	24	11	
31	h	1	Total	C	O	0
			24	18	6	
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	

Continued on next page...

Continued from previous page...

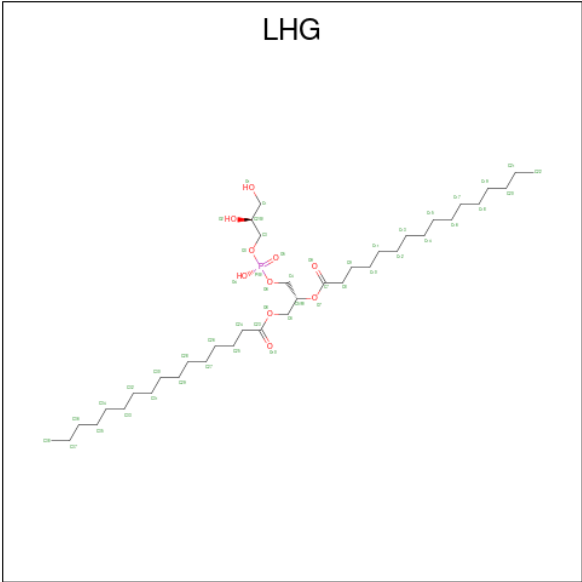
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			22	16	6	
31	j	1	Total	C	O	0
			24	18	6	
31	k	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			22	17	5	
31	y	1	Total	C	O	0
			21	15	6	

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



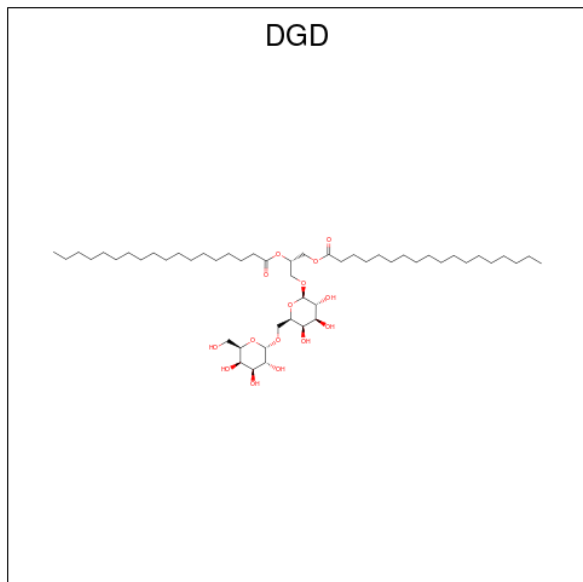
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

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



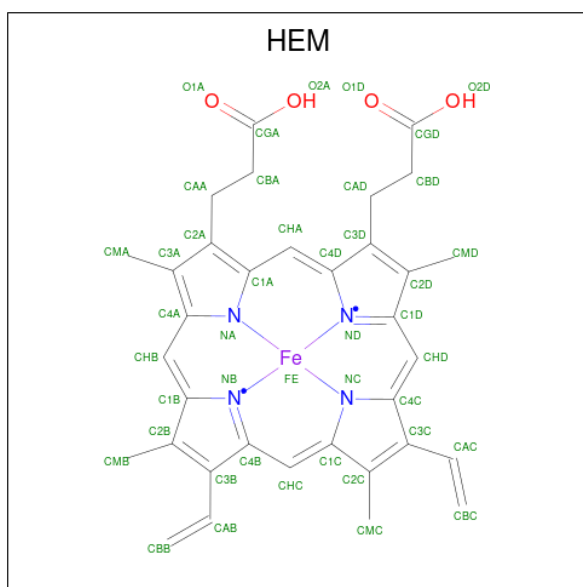
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			40	29	10	1	
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			46	35	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	b	1	Total	C	O	P	0
			40	29	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			46	35	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) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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

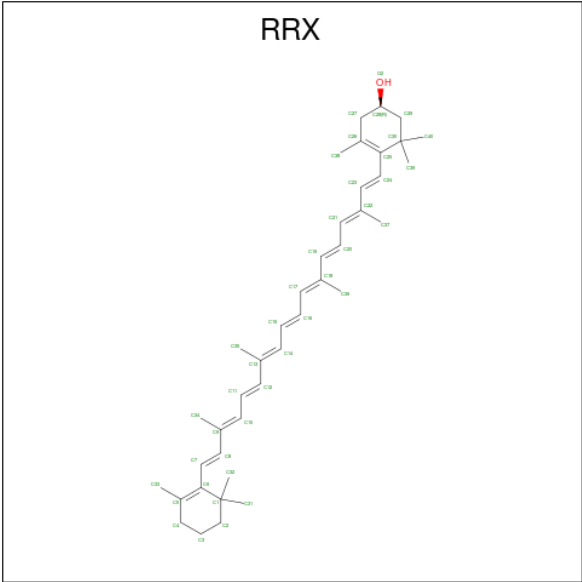


Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
37	X	1	Total	C	O	0
			41	40	1	
37	x	1	Total	C	O	0
			41	40	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	119	Total	O	0
			119	119	
38	B	114	Total	O	0
			114	114	
38	C	122	Total	O	0
			122	122	
38	D	120	Total	O	0
			120	120	
38	E	13	Total	O	0
			13	13	
38	F	4	Total	O	0
			4	4	
38	H	11	Total	O	0
			11	11	
38	I	2	Total	O	0
			2	2	
38	J	3	Total	O	0
			3	3	
38	K	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
38	L	9	Total 9	O 9	0
38	M	9	Total 9	O 9	0
38	O	40	Total 40	O 40	0
38	Q	2	Total 2	O 2	0
38	T	11	Total 11	O 11	0
38	U	11	Total 11	O 11	0
38	V	21	Total 21	O 21	0
38	X	7	Total 7	O 7	0
38	a	119	Total 119	O 119	0
38	b	114	Total 114	O 114	0
38	c	122	Total 122	O 122	0
38	d	120	Total 120	O 120	0
38	e	13	Total 13	O 13	0
38	f	4	Total 4	O 4	0
38	h	11	Total 11	O 11	0
38	i	2	Total 2	O 2	0
38	j	3	Total 3	O 3	0
38	k	1	Total 1	O 1	0
38	l	8	Total 8	O 8	0
38	m	8	Total 8	O 8	0
38	o	40	Total 40	O 40	0

Continued on next page...

Continued from previous page...

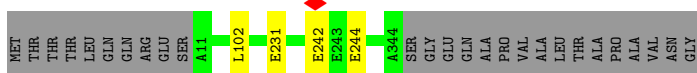
Mol	Chain	Residues	Atoms		AltConf
38	q	2	Total 2	O 2	0
38	t	11	Total 11	O 11	0
38	u	11	Total 11	O 11	0
38	v	21	Total 21	O 21	0
38	x	7	Total 7	O 7	0

3 Residue-property plots

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

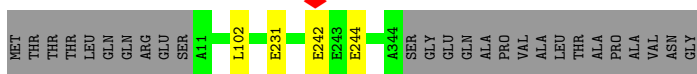
- Molecule 1: Photosystem II protein D1 2

Chain A:  92% 7%



- Molecule 1: Photosystem II protein D1 2

Chain a:  92% 7%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  97% ..



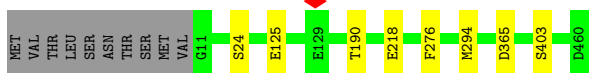
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  97% ..



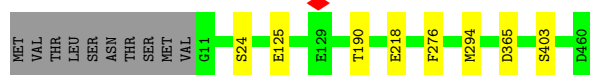
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  96% ..



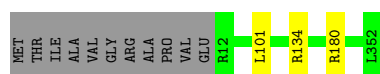
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96%



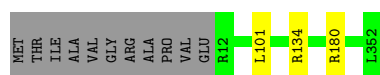
- Molecule 4: Photosystem II D2 protein

Chain D:  96%



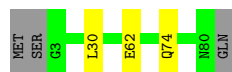
- Molecule 4: Photosystem II D2 protein

Chain d:  96%



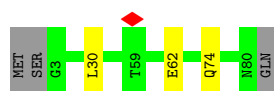
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  93%




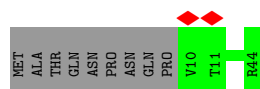
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  93%




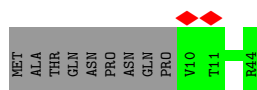
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  5% 80% 20%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  5% 80% 20%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 95%



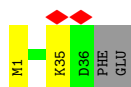
- Molecule 7: Photosystem II reaction center protein H

Chain h: 95%



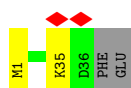
- Molecule 8: Photosystem II reaction center protein I

Chain I: 5% 89% 5% 5%



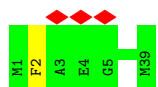
- Molecule 8: Photosystem II reaction center protein I

Chain i: 5% 89% 5% 5%



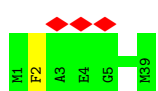
- Molecule 9: Photosystem II reaction center protein J

Chain J: 8% 97%




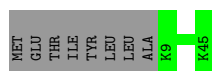
- Molecule 9: Photosystem II reaction center protein J

Chain j: 8% 97%




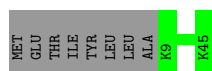
- Molecule 10: Photosystem II reaction center protein K

Chain K:  82% 18%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  82% 18%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

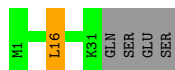
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%


There are no outlier residues recorded for this chain.

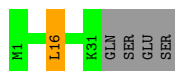
- Molecule 12: Photosystem II reaction center protein M

Chain M:  86% 11%



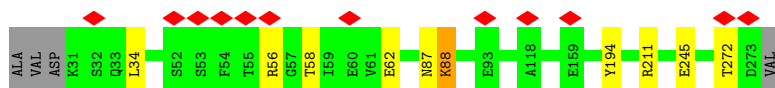
- Molecule 12: Photosystem II reaction center protein M

Chain m:  86% 11%



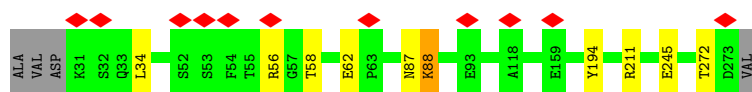
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  5% 94%

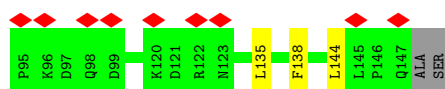
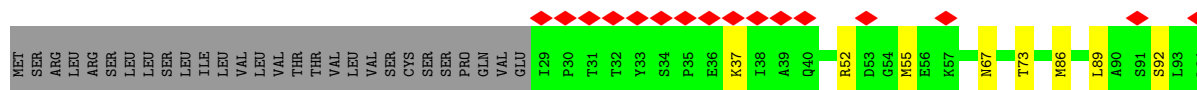
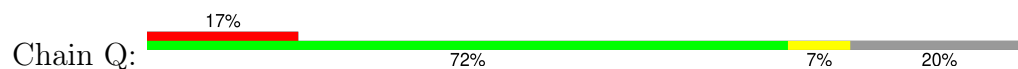


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

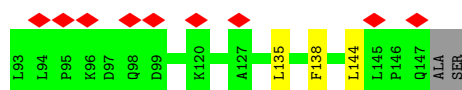
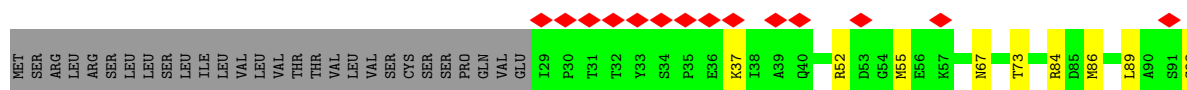
Chain o:  5% 94%



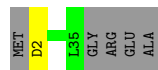
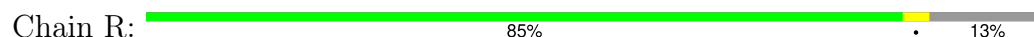
• Molecule 14: Sll1638 protein



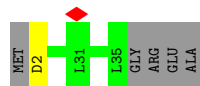
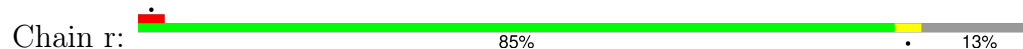
• Molecule 14: Sll1638 protein



• Molecule 15: Photosystem II protein Y



• Molecule 15: Photosystem II protein Y



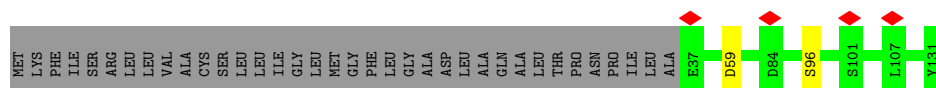
• Molecule 16: Photosystem II reaction center protein T



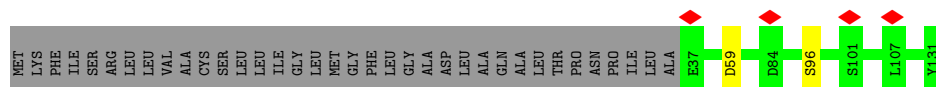
• Molecule 16: Photosystem II reaction center protein T



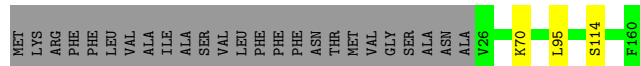
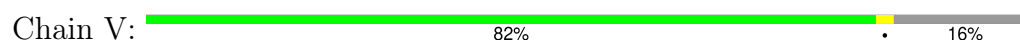
- Molecule 17: Photosystem II 12 kDa extrinsic protein



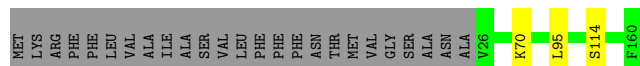
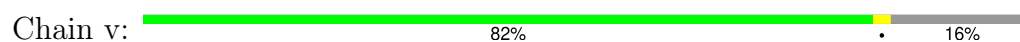
- Molecule 17: Photosystem II 12 kDa extrinsic protein



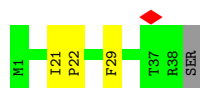
- Molecule 18: Cytochrome c-550



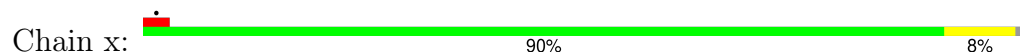
- Molecule 18: Cytochrome c-550



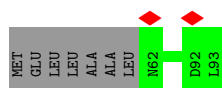
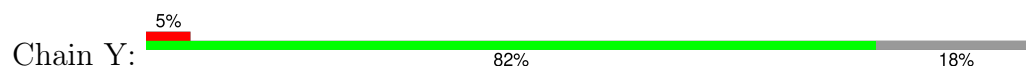
- Molecule 19: Photosystem II reaction center X protein



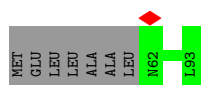
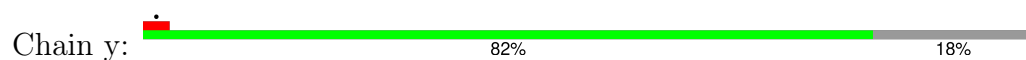
- Molecule 19: Photosystem II reaction center X protein



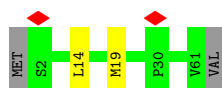
- Molecule 20: Photosystem II reaction center protein Ycf12



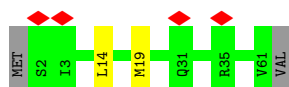
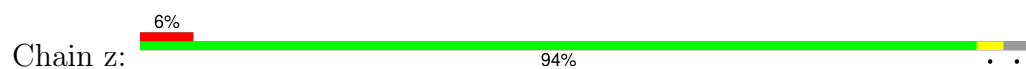
- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 21: Photosystem II reaction center protein Z



- Molecule 21: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/2709	0.51	0/3694
1	a	0.41	0/2709	0.51	0/3694
2	B	0.38	0/4068	0.51	1/5538 (0.0%)
2	b	0.38	0/4068	0.51	1/5538 (0.0%)
3	C	0.37	0/3608	0.50	0/4912
3	c	0.37	0/3608	0.50	0/4912
4	D	0.38	0/2823	0.50	0/3843
4	d	0.38	0/2823	0.50	0/3843
5	E	0.35	0/664	0.51	0/906
5	e	0.35	0/664	0.51	0/906
6	F	0.33	0/288	0.45	0/393
6	f	0.32	0/288	0.45	0/393
7	H	0.33	0/506	0.50	0/687
7	h	0.33	0/506	0.50	0/687
8	I	0.32	0/282	0.49	0/381
8	i	0.32	0/282	0.49	0/381
9	J	0.33	0/278	0.49	0/375
9	j	0.33	0/278	0.49	0/375
10	K	0.37	0/310	0.53	0/424
10	k	0.37	0/310	0.53	0/424
11	L	0.38	0/322	0.46	0/435
11	l	0.38	0/322	0.46	0/435
12	M	0.34	0/239	0.62	1/325 (0.3%)
12	m	0.34	0/239	0.62	1/325 (0.3%)
13	O	0.38	0/1907	0.59	0/2586
13	o	0.38	0/1907	0.59	0/2586
14	Q	0.28	0/930	0.44	0/1257
14	q	0.28	0/930	0.44	0/1257
15	R	0.26	0/262	0.45	0/361
15	r	0.26	0/262	0.45	0/361
16	T	0.33	0/236	0.46	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.34	0/236	0.46	0/321
17	U	0.34	0/751	0.48	0/1018
17	u	0.34	0/751	0.48	0/1018
18	V	0.31	0/1086	0.51	0/1476
18	v	0.31	0/1086	0.51	0/1476
19	X	0.31	0/293	0.53	0/399
19	x	0.31	0/293	0.53	0/399
20	Y	0.29	0/247	0.45	0/335
20	y	0.29	0/247	0.45	0/335
21	Z	0.32	0/472	0.45	0/649
21	z	0.32	0/472	0.45	0/649
All	All	0.37	0/44562	0.51	4/60630 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	1
13	o	0	1
19	X	0	1
19	x	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	121	GLU	CA-CB-CG	8.44	131.97	113.40
2	B	121	GLU	CA-CB-CG	8.43	131.95	113.40
12	M	16	LEU	CA-CB-CG	6.87	131.09	115.30
12	m	16	LEU	CA-CB-CG	6.86	131.07	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O	88	LYS	Peptide
19	X	21	ILE	Peptide
13	o	88	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
19	x	21	ILE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
1	a	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
2	B	501/507 (99%)	492 (98%)	9 (2%)	0	100	100
2	b	501/507 (99%)	492 (98%)	9 (2%)	0	100	100
3	C	448/460 (97%)	438 (98%)	10 (2%)	0	100	100
3	c	448/460 (97%)	438 (98%)	10 (2%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
5	e	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
6	F	33/44 (75%)	30 (91%)	3 (9%)	0	100	100
6	f	33/44 (75%)	30 (91%)	3 (9%)	0	100	100
7	H	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
7	h	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	34 (100%)	0	0	100	100
8	i	34/38 (90%)	34 (100%)	0	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
10	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/247 (98%)	219 (91%)	21 (9%)	1 (0%)	30	22
13	o	241/247 (98%)	219 (91%)	21 (9%)	1 (0%)	30	22
14	Q	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
14	q	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
16	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
17	U	93/131 (71%)	88 (95%)	5 (5%)	0	100	100
17	u	93/131 (71%)	88 (95%)	5 (5%)	0	100	100
18	V	133/160 (83%)	129 (97%)	4 (3%)	0	100	100
18	v	133/160 (83%)	129 (97%)	4 (3%)	0	100	100
19	X	36/39 (92%)	34 (94%)	1 (3%)	1 (3%)	4	0
19	x	36/39 (92%)	34 (94%)	1 (3%)	1 (3%)	4	0
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	54 (93%)	4 (7%)	0	100	100
21	z	58/62 (94%)	54 (93%)	4 (7%)	0	100	100
All	All	5460/5922 (92%)	5292 (97%)	164 (3%)	4 (0%)	50	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	87	ASN
13	o	87	ASN
19	X	22	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	x	22	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/293 (93%)	269 (98%)	4 (2%)	60	52
1	a	273/293 (93%)	269 (98%)	4 (2%)	60	52
2	B	401/404 (99%)	391 (98%)	10 (2%)	42	30
2	b	401/404 (99%)	391 (98%)	10 (2%)	42	30
3	C	351/361 (97%)	343 (98%)	8 (2%)	45	33
3	c	351/361 (97%)	343 (98%)	8 (2%)	45	33
4	D	277/285 (97%)	274 (99%)	3 (1%)	70	64
4	d	277/285 (97%)	274 (99%)	3 (1%)	70	64
5	E	70/73 (96%)	67 (96%)	3 (4%)	25	11
5	e	70/73 (96%)	67 (96%)	3 (4%)	25	11
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	51 (96%)	2 (4%)	28	14
7	h	53/54 (98%)	51 (96%)	2 (4%)	28	14
8	I	31/33 (94%)	30 (97%)	1 (3%)	34	22
8	i	31/33 (94%)	30 (97%)	1 (3%)	34	22
9	J	24/24 (100%)	23 (96%)	1 (4%)	25	12
9	j	24/24 (100%)	23 (96%)	1 (4%)	25	12
10	K	31/38 (82%)	31 (100%)	0	100	100
10	k	31/38 (82%)	31 (100%)	0	100	100
11	L	36/36 (100%)	36 (100%)	0	100	100
11	l	36/36 (100%)	36 (100%)	0	100	100
12	M	27/31 (87%)	26 (96%)	1 (4%)	29	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	27/31 (87%)	26 (96%)	1 (4%)	29	16
13	O	206/210 (98%)	197 (96%)	9 (4%)	24	11
13	o	206/210 (98%)	197 (96%)	9 (4%)	24	11
14	Q	93/128 (73%)	82 (88%)	11 (12%)	4	0
14	q	93/128 (73%)	81 (87%)	12 (13%)	3	0
15	R	26/29 (90%)	25 (96%)	1 (4%)	28	14
15	r	26/29 (90%)	25 (96%)	1 (4%)	28	14
16	T	24/25 (96%)	24 (100%)	0	100	100
16	t	24/25 (96%)	24 (100%)	0	100	100
17	U	83/111 (75%)	81 (98%)	2 (2%)	44	32
17	u	83/111 (75%)	81 (98%)	2 (2%)	44	32
18	V	117/137 (85%)	114 (97%)	3 (3%)	41	28
18	v	117/137 (85%)	114 (97%)	3 (3%)	41	28
19	X	32/33 (97%)	31 (97%)	1 (3%)	35	22
19	x	32/33 (97%)	31 (97%)	1 (3%)	35	22
20	Y	25/30 (83%)	25 (100%)	0	100	100
20	y	25/30 (83%)	25 (100%)	0	100	100
21	Z	49/52 (94%)	47 (96%)	2 (4%)	26	12
21	z	49/52 (94%)	47 (96%)	2 (4%)	26	12
All	All	4514/4848 (93%)	4389 (97%)	125 (3%)	40	25

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	231	GLU
1	A	242	GLU
1	A	244	GLU
2	B	79	SER
2	B	121	GLU
2	B	144	PHE
2	B	170	ASP
2	B	246	PHE
2	B	291	GLN
2	B	294	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	297	SER
2	B	298	LEU
2	B	419	LYS
3	C	24	SER
3	C	125	GLU
3	C	190	THR
3	C	218	GLU
3	C	276	PHE
3	C	294	MET
3	C	365	ASP
3	C	403	SER
4	D	101	LEU
4	D	134	ARG
4	D	180	ARG
5	E	30	LEU
5	E	62	GLU
5	E	74	GLN
7	H	6	ARG
7	H	49	TYR
8	I	35	LYS
9	J	2	PHE
12	M	16	LEU
13	O	34	LEU
13	O	56	ARG
13	O	58	THR
13	O	62	GLU
13	O	88	LYS
13	O	194	TYR
13	O	211	ARG
13	O	245	GLU
13	O	272	THR
14	Q	37	LYS
14	Q	52	ARG
14	Q	55	MET
14	Q	67	ASN
14	Q	73	THR
14	Q	86	MET
14	Q	89	LEU
14	Q	92	SER
14	Q	135	LEU
14	Q	138	PHE
14	Q	144	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	R	2	ASP
17	U	59	ASP
17	U	96	SER
18	V	70	LYS
18	V	95	LEU
18	V	114	SER
19	X	29	PHE
21	Z	14	LEU
21	Z	19	MET
1	a	102	LEU
1	a	231	GLU
1	a	242	GLU
1	a	244	GLU
2	b	79	SER
2	b	121	GLU
2	b	144	PHE
2	b	170	ASP
2	b	246	PHE
2	b	291	GLN
2	b	294	GLU
2	b	297	SER
2	b	298	LEU
2	b	419	LYS
3	c	24	SER
3	c	125	GLU
3	c	190	THR
3	c	218	GLU
3	c	276	PHE
3	c	294	MET
3	c	365	ASP
3	c	403	SER
4	d	101	LEU
4	d	134	ARG
4	d	180	ARG
5	e	30	LEU
5	e	62	GLU
5	e	74	GLN
7	h	6	ARG
7	h	49	TYR
8	i	35	LYS
9	j	2	PHE
12	m	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	o	34	LEU
13	o	56	ARG
13	o	58	THR
13	o	62	GLU
13	o	88	LYS
13	o	194	TYR
13	o	211	ARG
13	o	245	GLU
13	o	272	THR
14	q	37	LYS
14	q	52	ARG
14	q	55	MET
14	q	67	ASN
14	q	73	THR
14	q	84	ARG
14	q	86	MET
14	q	89	LEU
14	q	92	SER
14	q	135	LEU
14	q	138	PHE
14	q	144	LEU
15	r	2	ASP
17	u	59	ASP
17	u	96	SER
18	v	70	LYS
18	v	95	LEU
18	v	114	SER
19	x	29	PHE
21	z	14	LEU
21	z	19	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	25	ASN
1	A	130	GLN
1	A	234	ASN
1	A	261	GLN
1	A	338	ASN
2	B	216	HIS
2	B	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	285	GLN
2	B	291	GLN
2	B	343	HIS
2	B	409	GLN
2	B	489	GLN
3	C	142	ASN
3	C	309	GLN
3	C	314	ASN
3	C	375	GLN
3	C	405	ASN
4	D	129	GLN
5	E	23	HIS
5	E	73	ASN
5	E	74	GLN
7	H	3	GLN
7	H	50	ASN
8	I	31	ASN
11	L	10	GLN
13	O	109	GLN
13	O	166	ASN
13	O	176	ASN
13	O	199	ASN
13	O	246	GLN
14	Q	60	GLN
14	Q	67	ASN
14	Q	76	HIS
14	Q	143	ASN
17	U	106	ASN
18	V	50	GLN
18	V	55	GLN
18	V	93	ASN
18	V	119	ASN
19	X	7	ASN
20	Y	68	GLN
21	Z	32	ASN
1	a	19	GLN
1	a	25	ASN
1	a	130	GLN
1	a	234	ASN
1	a	261	GLN
1	a	338	ASN
2	b	216	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	260	ASN
2	b	285	GLN
2	b	291	GLN
2	b	343	HIS
2	b	409	GLN
2	b	489	GLN
3	c	142	ASN
3	c	309	GLN
3	c	314	ASN
3	c	375	GLN
4	d	129	GLN
5	e	23	HIS
5	e	73	ASN
5	e	74	GLN
7	h	3	GLN
7	h	50	ASN
8	i	31	ASN
11	l	8	ASN
11	l	10	GLN
13	o	109	GLN
13	o	166	ASN
13	o	176	ASN
13	o	199	ASN
13	o	246	GLN
14	q	60	GLN
14	q	67	ASN
14	q	76	HIS
14	q	143	ASN
17	u	57	ASN
17	u	106	ASN
18	v	50	GLN
18	v	93	ASN
18	v	119	ASN
19	x	7	ASN
20	y	68	GLN
21	z	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	FME	J	1	9	6,7,10	0.84	0	2,7,11	0.69	0
12	FME	M	1	12	8,9,10	0.99	0	8,9,11	0.90	0
16	FME	T	1	16	8,9,10	0.98	0	8,9,11	0.92	0
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.04	1 (12%)
16	FME	t	1	16	8,9,10	0.97	0	8,9,11	0.93	0
9	FME	j	1	9	6,7,10	0.84	0	2,7,11	0.69	0
12	FME	m	1	12	8,9,10	0.99	0	8,9,11	0.90	0
8	FME	i	1	8	8,9,10	0.98	0	8,9,11	1.04	1 (12%)

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
9	FME	J	1	9	-	1/5/6/11	-
12	FME	M	1	12	-	2/7/9/11	-
16	FME	T	1	16	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
16	FME	t	1	16	-	1/7/9/11	-
9	FME	j	1	9	-	1/5/6/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.27	113.88	109.50
8	I	1	FME	C-CA-N	2.27	113.87	109.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG
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
9	J	1	FME	C-CA-CB-CG
9	j	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 12 are monoatomic - leaving 216 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	D	411	-	36,36,36	1.05	4 (11%)	47,47,47	1.22	4 (8%)
28	LMG	C	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.16	3 (5%)
29	PL9	a	411	-	55,55,55	1.09	3 (5%)	68,69,69	1.56	12 (17%)
25	CLA	B	612	-	63,73,73	2.19	18 (28%)	74,113,113	2.53	23 (31%)
33	LHG	b	628	-	48,48,48	0.92	3 (6%)	51,54,54	0.98	3 (5%)
31	LMT	M	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	0
34	DGD	H	103	-	63,63,67	1.31	8 (12%)	77,77,81	0.97	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	511	-	63,73,73	2.26	19 (30%)	74,113,113	2.47	25 (33%)
25	CLA	a	406	38	63,73,73	2.19	18 (28%)	74,113,113	2.55	22 (29%)
26	PHO	d	402	-	50,69,69	1.02	5 (10%)	48,99,99	1.24	5 (10%)
28	LMG	a	410	-	51,51,55	1.45	8 (15%)	59,59,63	1.24	5 (8%)
31	LMT	B	626	-	24,24,36	1.03	2 (8%)	29,29,47	1.14	2 (6%)
31	LMT	f	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	3 (6%)
25	CLA	B	610	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	24 (32%)
25	CLA	D	404	-	63,73,73	2.21	19 (30%)	74,113,113	2.51	23 (31%)
30	SQD	H	102	-	52,54,54	0.98	5 (9%)	62,65,65	1.55	11 (17%)
31	LMT	a	415	-	36,36,36	1.22	6 (16%)	47,47,47	1.45	4 (8%)
33	LHG	e	102	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
35	HEM	e	104	6	42,50,50	1.56	4 (9%)	46,82,82	1.41	5 (10%)
25	CLA	c	509	-	63,73,73	2.21	19 (30%)	74,113,113	2.48	24 (32%)
33	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.11	3 (5%)
25	CLA	d	401	38	63,73,73	2.20	18 (28%)	74,113,113	2.44	22 (29%)
31	LMT	h	101	-	24,24,36	1.03	2 (8%)	29,29,47	1.02	2 (6%)
33	LHG	D	408	-	45,45,48	0.95	2 (4%)	48,51,54	1.00	2 (4%)
25	CLA	C	509	-	63,73,73	2.21	20 (31%)	74,113,113	2.48	24 (32%)
30	SQD	k	101	-	45,45,54	1.02	4 (8%)	53,53,65	1.39	7 (13%)
31	LMT	e	101	-	22,22,36	1.11	3 (13%)	27,27,47	1.11	1 (3%)
31	LMT	i	102	-	24,24,36	1.07	3 (12%)	29,29,47	1.37	3 (10%)
31	LMT	i	104	-	22,22,36	1.09	3 (13%)	27,27,47	1.14	2 (7%)
30	SQD	c	501	-	52,54,54	0.93	4 (7%)	62,65,65	1.58	10 (16%)
25	CLA	b	605	-	63,73,73	2.19	18 (28%)	74,113,113	2.50	22 (29%)
25	CLA	b	611	-	63,73,73	2.20	17 (26%)	74,113,113	2.41	23 (31%)
27	BCR	B	619	-	41,41,41	2.66	6 (14%)	56,56,56	6.62	23 (41%)
31	LMT	T	701	-	24,24,36	1.08	3 (12%)	29,29,47	1.27	3 (10%)
37	RRX	X	102	-	42,42,42	1.32	8 (19%)	56,58,58	1.46	10 (17%)
31	LMT	b	623	-	24,24,36	0.98	2 (8%)	29,29,47	1.29	3 (10%)
31	LMT	i	103	-	36,36,36	1.14	6 (16%)	47,47,47	1.11	3 (6%)
32	BCT	a	417	23	3,3,3	1.58	1 (33%)	2,3,3	4.03	2 (100%)
28	LMG	D	409	-	51,51,55	1.42	8 (15%)	59,59,63	1.15	4 (6%)
30	SQD	h	102	-	52,54,54	0.98	5 (9%)	62,65,65	1.55	11 (17%)
25	CLA	c	508	38	63,73,73	2.19	19 (30%)	74,113,113	2.54	26 (35%)
31	LMT	X	101	-	24,24,36	1.05	3 (12%)	29,29,47	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	c	523	-	49,49,55	0.20	0	57,57,63	0.22	0
31	LMT	C	520	-	29,29,36	1.25	5 (17%)	40,40,47	0.96	2 (5%)
26	PHO	A	407	-	50,69,69	1.05	3 (6%)	48,99,99	1.23	5 (10%)
30	SQD	A	413	-	46,48,54	1.01	4 (8%)	56,59,65	1.79	15 (26%)
25	CLA	D	403	-	63,73,73	2.22	19 (30%)	74,113,113	2.57	23 (31%)
31	LMT	E	101	-	22,22,36	1.11	3 (13%)	27,27,47	1.11	1 (3%)
27	BCR	Z	101	-	41,41,41	2.67	7 (17%)	56,56,56	6.48	19 (33%)
25	CLA	c	513	-	48,58,73	2.61	18 (37%)	56,95,113	2.74	22 (39%)
25	CLA	B	615	-	63,73,73	2.20	19 (30%)	74,113,113	2.45	25 (33%)
31	LMT	d	412	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	2 (4%)
25	CLA	B	606	-	58,68,73	2.31	18 (31%)	68,107,113	2.54	24 (35%)
28	LMG	B	621	-	51,51,55	1.45	8 (15%)	59,59,63	1.28	5 (8%)
31	LMT	b	626	-	24,24,36	1.04	2 (8%)	29,29,47	1.14	2 (6%)
29	PL9	d	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.50	13 (19%)
25	CLA	b	613	-	63,73,73	2.20	19 (30%)	74,113,113	2.54	20 (27%)
25	CLA	c	514	-	63,73,73	2.26	19 (30%)	74,113,113	2.50	24 (32%)
25	CLA	b	612	-	63,73,73	2.20	18 (28%)	74,113,113	2.53	23 (31%)
25	CLA	c	507	-	63,73,73	2.26	19 (30%)	74,113,113	2.46	24 (32%)
22	OEX	a	401	38,3,1	0,15,15	-	-	-	-	-
31	LMT	b	627	-	25,25,36	1.03	3 (12%)	30,30,47	1.15	2 (6%)
25	CLA	C	513	-	48,58,73	2.61	18 (37%)	56,95,113	2.74	22 (39%)
27	BCR	K	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.94	24 (42%)
31	LMT	c	520	-	29,29,36	1.25	5 (17%)	40,40,47	0.96	2 (5%)
25	CLA	c	505	38	63,73,73	2.26	20 (31%)	74,113,113	2.51	26 (35%)
25	CLA	c	512	3	63,73,73	2.22	17 (26%)	74,113,113	2.56	23 (31%)
28	LMG	A	410	-	51,51,55	1.45	8 (15%)	59,59,63	1.24	5 (8%)
31	LMT	D	410	-	24,24,36	1.02	3 (12%)	29,29,47	1.34	4 (13%)
34	DGD	c	517	-	63,63,67	1.32	8 (12%)	77,77,81	0.99	4 (5%)
33	LHG	z	102	-	35,35,48	1.11	2 (5%)	38,40,54	1.32	6 (15%)
33	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	3 (5%)
31	LMT	B	627	-	25,25,36	1.03	3 (12%)	30,30,47	1.15	2 (6%)
25	CLA	b	615	-	63,73,73	2.19	19 (30%)	74,113,113	2.45	25 (33%)
31	LMT	i	101	-	24,24,36	1.10	3 (12%)	29,29,47	1.16	2 (6%)
27	BCR	B	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	25 (44%)
25	CLA	C	507	-	63,73,73	2.26	19 (30%)	74,113,113	2.46	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	A	409	-	41,41,41	2.67	6 (14%)	56,56,56	6.57	19 (33%)
25	CLA	c	503	-	63,73,73	2.25	18 (28%)	74,113,113	2.47	24 (32%)
27	BCR	F	101	-	41,41,41	2.64	7 (17%)	56,56,56	6.65	20 (35%)
27	BCR	b	619	-	41,41,41	2.66	6 (14%)	56,56,56	6.61	23 (41%)
29	PL9	A	411	-	55,55,55	1.09	3 (5%)	68,69,69	1.56	12 (17%)
33	LHG	Z	102	-	35,35,48	1.11	2 (5%)	38,40,54	1.31	6 (15%)
31	LMT	x	103	-	22,22,36	1.10	4 (18%)	27,27,47	1.14	1 (3%)
25	CLA	B	613	-	63,73,73	2.20	19 (30%)	74,113,113	2.54	20 (27%)
31	LMT	X	103	-	22,22,36	1.11	4 (18%)	27,27,47	1.14	1 (3%)
31	LMT	I	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.11	3 (6%)
33	LHG	E	102	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
27	BCR	k	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.94	24 (42%)
25	CLA	B	616	-	58,68,73	2.27	18 (31%)	68,107,113	2.58	25 (36%)
25	CLA	d	404	-	63,73,73	2.21	19 (30%)	74,113,113	2.50	23 (31%)
35	HEM	E	104	6	42,50,50	1.57	4 (9%)	46,82,82	1.41	5 (10%)
25	CLA	C	512	3	63,73,73	2.22	17 (26%)	74,113,113	2.56	22 (29%)
31	LMT	C	522	-	24,24,36	1.02	2 (8%)	29,29,47	1.10	1 (3%)
31	LMT	B	624	-	24,24,36	1.04	1 (4%)	29,29,47	1.22	2 (6%)
25	CLA	D	401	38	63,73,73	2.20	18 (28%)	74,113,113	2.44	21 (28%)
31	LMT	c	521	-	24,24,36	1.03	3 (12%)	29,29,47	1.08	2 (6%)
25	CLA	b	614	-	63,73,73	2.22	18 (28%)	74,113,113	2.55	23 (31%)
25	CLA	C	504	-	63,73,73	2.26	20 (31%)	74,113,113	2.55	26 (35%)
31	LMT	B	625	-	36,36,36	1.21	6 (16%)	47,47,47	1.04	3 (6%)
30	SQD	A	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.59	10 (16%)
25	CLA	b	604	-	63,73,73	2.21	18 (28%)	74,113,113	2.54	23 (31%)
25	CLA	B	609	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	21 (28%)
25	CLA	c	510	-	63,73,73	2.28	18 (28%)	74,113,113	2.45	23 (31%)
27	BCR	k	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.69	22 (39%)
31	LMT	k	105	-	36,36,36	1.11	5 (13%)	47,47,47	0.99	2 (4%)
27	BCR	c	515	-	41,41,41	2.71	6 (14%)	56,56,56	6.65	19 (33%)
28	LMG	c	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.16	3 (5%)
25	CLA	B	601	38	43,53,73	2.54	17 (39%)	50,89,113	2.88	19 (38%)
28	LMG	b	621	-	51,51,55	1.45	8 (15%)	59,59,63	1.28	5 (8%)
27	BCR	K	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.69	22 (39%)
33	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	623	-	24,24,36	0.98	2 (8%)	29,29,47	1.29	3 (10%)
31	LMT	x	101	-	24,24,36	1.05	3 (12%)	29,29,47	1.11	2 (6%)
25	CLA	C	503	-	63,73,73	2.25	18 (28%)	74,113,113	2.47	24 (32%)
31	LMT	c	522	-	24,24,36	1.03	2 (8%)	29,29,47	1.10	1 (3%)
32	BCT	A	417	23	3,3,3	1.59	1 (33%)	2,3,3	4.03	2 (100%)
28	LMG	d	409	-	51,51,55	1.42	8 (15%)	59,59,63	1.15	4 (6%)
31	LMT	I	104	-	22,22,36	1.08	3 (13%)	27,27,47	1.15	2 (7%)
31	LMT	M	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	2 (6%)
25	CLA	b	608	-	63,73,73	2.24	19 (30%)	74,113,113	2.37	22 (29%)
29	PL9	D	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.50	13 (19%)
34	DGD	c	518	-	63,63,67	1.31	8 (12%)	77,77,81	1.02	3 (3%)
25	CLA	C	505	38	63,73,73	2.26	20 (31%)	74,113,113	2.51	26 (35%)
25	CLA	a	408	-	58,68,73	2.31	18 (31%)	68,107,113	2.64	24 (35%)
31	LMT	a	416	-	24,24,36	1.03	3 (12%)	29,29,47	0.95	0
25	CLA	b	610	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	24 (32%)
31	LMT	m	101	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	2 (6%)
31	LMT	b	629	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	1 (2%)
27	BCR	z	101	-	41,41,41	2.67	7 (17%)	56,56,56	6.48	21 (37%)
31	LMT	H	101	-	24,24,36	1.02	2 (8%)	29,29,47	1.02	2 (6%)
33	LHG	d	408	-	45,45,48	0.95	2 (4%)	48,51,54	1.00	2 (4%)
31	LMT	J	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.12	3 (10%)
31	LMT	C	524	-	36,36,36	1.11	5 (13%)	47,47,47	1.08	2 (4%)
31	LMT	A	416	-	24,24,36	1.03	3 (12%)	29,29,47	0.95	0
30	SQD	C	501	-	52,54,54	0.94	4 (7%)	62,65,65	1.58	10 (16%)
30	SQD	B	620	-	52,54,54	0.95	3 (5%)	62,65,65	1.64	11 (17%)
33	LHG	B	622	-	39,39,48	1.04	2 (5%)	42,45,54	1.10	3 (7%)
25	CLA	C	514	-	63,73,73	2.26	19 (30%)	74,113,113	2.51	24 (32%)
33	LHG	b	622	-	39,39,48	1.04	2 (5%)	42,45,54	1.10	3 (7%)
25	CLA	B	605	-	63,73,73	2.19	18 (28%)	74,113,113	2.50	23 (31%)
26	PHO	a	407	-	50,69,69	1.06	4 (8%)	48,99,99	1.23	5 (10%)
27	BCR	B	618	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	18 (32%)
31	LMT	A	415	-	36,36,36	1.23	6 (16%)	47,47,47	1.45	4 (8%)
25	CLA	C	511	-	63,73,73	2.26	19 (30%)	74,113,113	2.47	25 (33%)
30	SQD	K	101	-	45,45,54	1.02	4 (8%)	53,53,65	1.39	7 (13%)
31	LMT	K	105	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	601	38	43,53,73	2.54	17 (39%)	50,89,113	2.88	19 (38%)
31	LMT	L	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	2 (4%)
31	LMT	b	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.05	3 (6%)
25	CLA	C	508	38	63,73,73	2.19	19 (30%)	74,113,113	2.53	26 (35%)
25	CLA	B	611	-	63,73,73	2.20	17 (26%)	74,113,113	2.41	23 (31%)
30	SQD	F	102	-	32,34,54	1.23	5 (15%)	42,45,65	1.88	10 (23%)
28	LMG	C	523	-	49,49,55	0.20	0	57,57,63	0.22	0
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.11	3 (5%)
26	PHO	D	402	-	50,69,69	1.02	5 (10%)	48,99,99	1.24	5 (10%)
31	LMT	d	410	-	24,24,36	1.01	3 (12%)	29,29,47	1.34	4 (13%)
31	LMT	j	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.12	3 (10%)
31	LMT	b	624	-	24,24,36	1.04	1 (4%)	29,29,47	1.22	2 (6%)
30	SQD	a	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.59	10 (16%)
25	CLA	C	502	-	63,73,73	2.31	20 (31%)	74,113,113	2.34	25 (33%)
31	LMT	d	411	-	36,36,36	1.05	4 (11%)	47,47,47	1.22	4 (8%)
31	LMT	t	701	-	24,24,36	1.08	3 (12%)	29,29,47	1.26	3 (10%)
34	DGD	C	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.99	3 (3%)
25	CLA	B	614	-	63,73,73	2.22	18 (28%)	74,113,113	2.55	23 (31%)
31	LMT	I	101	-	24,24,36	1.10	3 (12%)	29,29,47	1.16	2 (6%)
28	LMG	a	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.17	4 (9%)
25	CLA	B	607	38	63,73,73	2.23	18 (28%)	74,113,113	2.43	24 (32%)
25	CLA	b	606	-	58,68,73	2.31	18 (31%)	68,107,113	2.54	24 (35%)
31	LMT	E	103	-	36,36,36	1.20	4 (11%)	47,47,47	1.14	4 (8%)
25	CLA	b	607	38	63,73,73	2.23	18 (28%)	74,113,113	2.43	24 (32%)
25	CLA	b	609	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	21 (28%)
25	CLA	b	602	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	25 (33%)
25	CLA	c	506	-	53,63,73	2.45	18 (33%)	62,101,113	2.62	22 (35%)
31	LMT	D	412	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	2 (4%)
22	OEX	A	401	38,3,1	0,15,15	-	-	-	-	-
25	CLA	A	406	38	63,73,73	2.19	18 (28%)	74,113,113	2.56	22 (29%)
33	LHG	B	628	-	48,48,48	0.92	3 (6%)	51,54,54	0.98	3 (5%)
25	CLA	c	504	-	63,73,73	2.26	20 (31%)	74,113,113	2.54	26 (35%)
25	CLA	a	405	-	63,73,73	2.16	18 (28%)	74,113,113	2.61	26 (35%)
25	CLA	C	506	-	53,63,73	2.45	18 (33%)	62,101,113	2.62	22 (35%)
25	CLA	b	603	-	63,73,73	2.28	18 (28%)	74,113,113	2.49	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	A	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.17	4 (9%)
27	BCR	b	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	25 (44%)
31	LMT	I	102	-	24,24,36	1.07	3 (12%)	29,29,47	1.38	3 (10%)
31	LMT	e	103	-	36,36,36	1.20	4 (11%)	47,47,47	1.15	4 (8%)
34	DGD	c	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.99	3 (3%)
25	CLA	d	403	-	63,73,73	2.22	19 (30%)	74,113,113	2.57	23 (31%)
27	BCR	a	409	-	41,41,41	2.67	6 (14%)	56,56,56	6.57	19 (33%)
25	CLA	B	603	-	63,73,73	2.28	18 (28%)	74,113,113	2.49	23 (31%)
25	CLA	B	608	-	63,73,73	2.24	19 (30%)	74,113,113	2.37	22 (29%)
25	CLA	A	405	-	63,73,73	2.15	18 (28%)	74,113,113	2.61	26 (35%)
25	CLA	b	616	-	58,68,73	2.28	18 (31%)	68,107,113	2.58	25 (36%)
27	BCR	f	101	-	41,41,41	2.64	7 (17%)	56,56,56	6.66	20 (35%)
31	LMT	C	521	-	24,24,36	1.02	3 (12%)	29,29,47	1.08	2 (6%)
25	CLA	A	408	-	58,68,73	2.31	18 (31%)	68,107,113	2.64	24 (35%)
31	LMT	F	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	3 (6%)
34	DGD	C	518	-	63,63,67	1.32	8 (12%)	77,77,81	1.02	3 (3%)
34	DGD	h	103	-	63,63,67	1.32	8 (12%)	77,77,81	0.97	4 (5%)
30	SQD	a	413	-	46,48,54	1.01	4 (8%)	56,59,65	1.78	15 (26%)
31	LMT	B	629	-	36,36,36	1.15	5 (13%)	47,47,47	0.94	1 (2%)
25	CLA	B	602	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	25 (33%)
34	DGD	C	517	-	63,63,67	1.32	8 (12%)	77,77,81	0.99	4 (5%)
25	CLA	C	510	-	63,73,73	2.28	18 (28%)	74,113,113	2.45	23 (31%)
31	LMT	Y	101	-	21,21,36	1.09	3 (14%)	26,26,47	1.15	2 (7%)
25	CLA	c	502	-	63,73,73	2.31	20 (31%)	74,113,113	2.35	25 (33%)
37	RRX	x	102	-	42,42,42	1.32	8 (19%)	56,58,58	1.46	10 (17%)
27	BCR	C	515	-	41,41,41	2.70	6 (14%)	56,56,56	6.65	19 (33%)
30	SQD	f	102	-	32,34,54	1.23	4 (12%)	42,45,65	1.88	10 (23%)
25	CLA	B	604	-	63,73,73	2.21	18 (28%)	74,113,113	2.54	23 (31%)
30	SQD	b	620	-	52,54,54	0.94	3 (5%)	62,65,65	1.63	11 (17%)
35	HEM	V	201	18	42,50,50	1.42	4 (9%)	46,82,82	1.43	7 (15%)
31	LMT	c	524	-	36,36,36	1.11	5 (13%)	47,47,47	1.08	2 (4%)
31	LMT	y	101	-	21,21,36	1.09	3 (14%)	26,26,47	1.15	2 (7%)
35	HEM	v	201	18	42,50,50	1.43	4 (9%)	46,82,82	1.43	7 (15%)
27	BCR	b	618	-	41,41,41	2.65	6 (14%)	56,56,56	6.57	19 (33%)

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	D	411	-	-	12/21/61/61	0/2/2/2
28	LMG	C	519	-	-	19/46/66/70	0/1/1/1
29	PL9	a	411	-	-	27/53/73/73	0/1/1/1
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
33	LHG	b	628	-	-	24/53/53/53	-
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
34	DGD	H	103	-	-	7/51/91/95	0/2/2/2
25	CLA	c	511	-	1/1/15/20	14/37/115/115	-
25	CLA	a	406	38	1/1/15/20	12/37/115/115	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
28	LMG	a	410	-	-	17/46/66/70	0/1/1/1
31	LMT	B	626	-	-	9/15/35/61	0/1/1/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	B	610	-	1/1/15/20	5/37/115/115	-
25	CLA	D	404	-	1/1/15/20	14/37/115/115	-
30	SQD	H	102	-	-	24/49/69/69	0/1/1/1
31	LMT	a	415	-	-	9/21/61/61	0/2/2/2
33	LHG	e	102	-	-	25/44/44/53	-
35	HEM	e	104	6	-	2/12/54/54	-
25	CLA	c	509	-	1/1/15/20	7/37/115/115	-
33	LHG	D	406	-	-	27/53/53/53	-
25	CLA	d	401	38	1/1/15/20	9/37/115/115	-
31	LMT	h	101	-	-	5/15/35/61	0/1/1/2
33	LHG	D	408	-	-	18/50/50/53	-
25	CLA	C	509	-	1/1/15/20	7/37/115/115	-
30	SQD	k	101	-	-	20/39/59/69	0/1/1/1
31	LMT	e	101	-	-	3/13/33/61	0/1/1/2
31	LMT	i	102	-	-	10/15/35/61	0/1/1/2
31	LMT	i	104	-	-	3/13/33/61	0/1/1/2
30	SQD	c	501	-	-	28/49/69/69	0/1/1/1
25	CLA	b	605	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	611	-	1/1/15/20	11/37/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
31	LMT	T	701	-	-	5/15/35/61	0/1/1/2
37	RRX	X	102	-	-	21/29/65/65	0/2/2/2
31	LMT	b	623	-	-	6/15/35/61	0/1/1/2
31	LMT	i	103	-	-	8/21/61/61	0/2/2/2
28	LMG	D	409	-	-	12/46/66/70	0/1/1/1
30	SQD	h	102	-	-	24/49/69/69	0/1/1/1
25	CLA	c	508	38	1/1/15/20	11/37/115/115	-
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
28	LMG	c	523	-	-	24/44/64/70	0/1/1/1
31	LMT	C	520	-	-	3/14/54/61	0/2/2/2
26	PHO	A	407	-	-	6/37/103/103	0/5/6/6
30	SQD	A	413	-	-	21/43/63/69	0/1/1/1
25	CLA	D	403	-	1/1/15/20	7/37/115/115	-
31	LMT	E	101	-	-	3/13/33/61	0/1/1/2
27	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	513	-	1/1/12/20	6/19/97/115	-
25	CLA	B	615	-	1/1/15/20	12/37/115/115	-
31	LMT	d	412	-	-	4/21/61/61	0/2/2/2
25	CLA	B	606	-	1/1/14/20	9/31/109/115	-
28	LMG	B	621	-	-	7/46/66/70	0/1/1/1
31	LMT	b	626	-	-	9/15/35/61	0/1/1/2
29	PL9	d	405	-	-	10/53/73/73	0/1/1/1
25	CLA	b	613	-	1/1/15/20	12/37/115/115	-
25	CLA	c	514	-	1/1/15/20	14/37/115/115	-
25	CLA	b	612	-	1/1/15/20	8/37/115/115	-
25	CLA	c	507	-	1/1/15/20	17/37/115/115	-
31	LMT	b	627	-	-	6/17/37/61	0/1/1/2
25	CLA	C	513	-	1/1/12/20	6/19/97/115	-
27	BCR	K	102	-	-	13/29/63/63	0/2/2/2
31	LMT	c	520	-	-	3/14/54/61	0/2/2/2
25	CLA	c	505	38	1/1/15/20	11/37/115/115	-
25	CLA	c	512	3	1/1/15/20	8/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	A	410	-	-	17/46/66/70	0/1/1/1
31	LMT	D	410	-	-	12/15/35/61	0/1/1/2
34	DGD	c	517	-	-	16/51/91/95	0/2/2/2
33	LHG	z	102	-	-	16/37/37/53	-
33	LHG	D	407	-	-	26/53/53/53	-
31	LMT	B	627	-	-	6/17/37/61	0/1/1/2
25	CLA	b	615	-	1/1/15/20	12/37/115/115	-
31	LMT	i	101	-	-	12/15/35/61	0/1/1/2
27	BCR	B	617	-	-	9/29/63/63	0/2/2/2
25	CLA	C	507	-	1/1/15/20	17/37/115/115	-
27	BCR	A	409	-	-	6/29/63/63	0/2/2/2
25	CLA	c	503	-	1/1/15/20	7/37/115/115	-
27	BCR	F	101	-	-	10/29/63/63	0/2/2/2
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
29	PL9	A	411	-	-	27/53/73/73	0/1/1/1
33	LHG	Z	102	-	-	16/37/37/53	-
31	LMT	x	103	-	-	10/12/32/61	0/1/1/2
25	CLA	B	613	-	1/1/15/20	12/37/115/115	-
31	LMT	X	103	-	-	10/12/32/61	0/1/1/2
31	LMT	I	103	-	-	8/21/61/61	0/2/2/2
33	LHG	E	102	-	-	25/44/44/53	-
27	BCR	k	102	-	-	13/29/63/63	0/2/2/2
25	CLA	B	616	-	1/1/14/20	16/31/109/115	-
25	CLA	d	404	-	1/1/15/20	14/37/115/115	-
35	HEM	E	104	6	-	2/12/54/54	-
25	CLA	C	512	3	1/1/15/20	8/37/115/115	-
31	LMT	C	522	-	-	9/15/35/61	0/1/1/2
31	LMT	B	624	-	-	8/15/35/61	0/1/1/2
25	CLA	D	401	38	1/1/15/20	9/37/115/115	-
31	LMT	c	521	-	-	11/15/35/61	0/1/1/2
25	CLA	b	614	-	1/1/15/20	17/37/115/115	-
25	CLA	C	504	-	1/1/15/20	10/37/115/115	-
31	LMT	B	625	-	-	5/21/61/61	0/2/2/2
30	SQD	A	412	-	-	25/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	604	-	1/1/15/20	14/37/115/115	-
25	CLA	B	609	-	1/1/15/20	13/37/115/115	-
25	CLA	c	510	-	1/1/15/20	15/37/115/115	-
27	BCR	k	103	-	-	6/29/63/63	0/2/2/2
31	LMT	k	105	-	-	12/21/61/61	0/2/2/2
27	BCR	c	515	-	-	7/29/63/63	0/2/2/2
28	LMG	c	519	-	-	19/46/66/70	0/1/1/1
25	CLA	B	601	38	1/1/11/20	4/13/91/115	-
28	LMG	b	621	-	-	7/46/66/70	0/1/1/1
27	BCR	K	103	-	-	6/29/63/63	0/2/2/2
33	LHG	d	407	-	-	26/53/53/53	-
31	LMT	B	623	-	-	6/15/35/61	0/1/1/2
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
25	CLA	C	503	-	1/1/15/20	7/37/115/115	-
31	LMT	c	522	-	-	9/15/35/61	0/1/1/2
28	LMG	d	409	-	-	12/46/66/70	0/1/1/1
31	LMT	I	104	-	-	3/13/33/61	0/1/1/2
31	LMT	M	102	-	-	7/15/35/61	0/1/1/2
25	CLA	b	608	-	1/1/15/20	11/37/115/115	-
29	PL9	D	405	-	-	10/53/73/73	0/1/1/1
34	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	CLA	C	505	38	1/1/15/20	11/37/115/115	-
25	CLA	a	408	-	1/1/14/20	14/31/109/115	-
31	LMT	a	416	-	-	8/15/35/61	0/1/1/2
25	CLA	b	610	-	1/1/15/20	6/37/115/115	-
31	LMT	m	101	-	-	7/15/35/61	0/1/1/2
31	LMT	b	629	-	-	10/21/61/61	0/2/2/2
27	BCR	z	101	-	-	8/29/63/63	0/2/2/2
31	LMT	H	101	-	-	5/15/35/61	0/1/1/2
33	LHG	d	408	-	-	18/50/50/53	-
31	LMT	J	101	-	-	10/15/35/61	0/1/1/2
31	LMT	C	524	-	-	9/21/61/61	0/2/2/2
31	LMT	A	416	-	-	8/15/35/61	0/1/1/2
30	SQD	C	501	-	-	28/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	B	620	-	-	21/49/69/69	0/1/1/1
33	LHG	B	622	-	-	28/44/44/53	-
25	CLA	C	514	-	1/1/15/20	14/37/115/115	-
33	LHG	b	622	-	-	28/44/44/53	-
25	CLA	B	605	-	1/1/15/20	13/37/115/115	-
26	PHO	a	407	-	-	6/37/103/103	0/5/6/6
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
31	LMT	A	415	-	-	9/21/61/61	0/2/2/2
25	CLA	C	511	-	1/1/15/20	14/37/115/115	-
30	SQD	K	101	-	-	20/39/59/69	0/1/1/1
31	LMT	K	105	-	-	12/21/61/61	0/2/2/2
25	CLA	b	601	38	1/1/11/20	4/13/91/115	-
31	LMT	L	101	-	-	13/21/61/61	0/2/2/2
31	LMT	b	625	-	-	5/21/61/61	0/2/2/2
25	CLA	C	508	38	1/1/15/20	11/37/115/115	-
25	CLA	B	611	-	1/1/15/20	11/37/115/115	-
30	SQD	F	102	-	-	16/29/49/69	0/1/1/1
28	LMG	C	523	-	-	24/44/64/70	0/1/1/1
33	LHG	d	406	-	-	27/53/53/53	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	LMT	d	410	-	-	12/15/35/61	0/1/1/2
31	LMT	j	101	-	-	10/15/35/61	0/1/1/2
31	LMT	b	624	-	-	8/15/35/61	0/1/1/2
30	SQD	a	412	-	-	25/49/69/69	0/1/1/1
25	CLA	C	502	-	1/1/15/20	14/37/115/115	-
31	LMT	d	411	-	-	12/21/61/61	0/2/2/2
31	LMT	t	701	-	-	5/15/35/61	0/1/1/2
34	DGD	C	516	-	-	20/51/91/95	0/2/2/2
25	CLA	B	614	-	1/1/15/20	17/37/115/115	-
31	LMT	I	101	-	-	12/15/35/61	0/1/1/2
28	LMG	a	414	-	-	7/31/51/70	0/1/1/1
25	CLA	B	607	38	1/1/15/20	9/37/115/115	-
25	CLA	b	606	-	1/1/14/20	9/31/109/115	-
31	LMT	E	103	-	-	12/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	607	38	1/1/15/20	9/37/115/115	-
25	CLA	b	609	-	1/1/15/20	13/37/115/115	-
25	CLA	b	602	-	1/1/15/20	12/37/115/115	-
25	CLA	c	506	-	1/1/13/20	4/25/103/115	-
31	LMT	D	412	-	-	4/21/61/61	0/2/2/2
25	CLA	A	406	38	1/1/15/20	12/37/115/115	-
33	LHG	B	628	-	-	24/53/53/53	-
25	CLA	c	504	-	1/1/15/20	10/37/115/115	-
25	CLA	a	405	-	1/1/15/20	8/37/115/115	-
25	CLA	C	506	-	1/1/13/20	4/25/103/115	-
25	CLA	b	603	-	1/1/15/20	10/37/115/115	-
28	LMG	A	414	-	-	7/31/51/70	0/1/1/1
27	BCR	b	617	-	-	9/29/63/63	0/2/2/2
31	LMT	I	102	-	-	10/15/35/61	0/1/1/2
31	LMT	e	103	-	-	12/21/61/61	0/2/2/2
34	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	CLA	d	403	-	1/1/15/20	7/37/115/115	-
27	BCR	a	409	-	-	6/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	10/37/115/115	-
25	CLA	B	608	-	1/1/15/20	11/37/115/115	-
25	CLA	A	405	-	1/1/15/20	8/37/115/115	-
25	CLA	b	616	-	1/1/14/20	16/31/109/115	-
27	BCR	f	101	-	-	10/29/63/63	0/2/2/2
31	LMT	C	521	-	-	11/15/35/61	0/1/1/2
25	CLA	A	408	-	1/1/14/20	14/31/109/115	-
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
34	DGD	C	518	-	-	15/51/91/95	0/2/2/2
34	DGD	h	103	-	-	7/51/91/95	0/2/2/2
30	SQD	a	413	-	-	21/43/63/69	0/1/1/1
31	LMT	B	629	-	-	10/21/61/61	0/2/2/2
25	CLA	B	602	-	1/1/15/20	12/37/115/115	-
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	CLA	C	510	-	1/1/15/20	15/37/115/115	-
31	LMT	Y	101	-	-	4/12/32/61	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	502	-	1/1/15/20	14/37/115/115	-
37	RRX	x	102	-	-	21/29/65/65	0/2/2/2
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
30	SQD	f	102	-	-	16/29/49/69	0/1/1/1
25	CLA	B	604	-	1/1/15/20	14/37/115/115	-
30	SQD	b	620	-	-	21/49/69/69	0/1/1/1
35	HEM	V	201	18	-	2/12/54/54	-
31	LMT	c	524	-	-	9/21/61/61	0/2/2/2
31	LMT	y	101	-	-	4/12/32/61	0/1/1/2
35	HEM	v	201	18	-	2/12/54/54	-
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2

All (1916) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	z	101	BCR	C8-C9	-8.57	1.27	1.46
27	Z	101	BCR	C8-C9	-8.57	1.27	1.46
27	C	515	BCR	C8-C9	-8.45	1.27	1.46
27	c	515	BCR	C8-C9	-8.44	1.27	1.46
27	b	619	BCR	C8-C9	-8.42	1.27	1.46
27	B	619	BCR	C8-C9	-8.42	1.27	1.46
27	k	103	BCR	C8-C9	-8.42	1.27	1.46
27	a	409	BCR	C8-C9	-8.41	1.27	1.46
27	A	409	BCR	C8-C9	-8.40	1.28	1.46
27	K	103	BCR	C8-C9	-8.40	1.28	1.46
27	B	617	BCR	C8-C9	-8.33	1.28	1.46
27	b	617	BCR	C8-C9	-8.32	1.28	1.46
27	F	101	BCR	C8-C9	-8.29	1.28	1.46
27	f	101	BCR	C8-C9	-8.28	1.28	1.46
27	K	102	BCR	C8-C9	-8.22	1.28	1.46
27	k	102	BCR	C8-C9	-8.22	1.28	1.46
27	B	618	BCR	C8-C9	-8.20	1.28	1.46
27	c	515	BCR	C11-C10	-8.20	1.17	1.43
27	b	618	BCR	C8-C9	-8.20	1.28	1.46
27	C	515	BCR	C11-C10	-8.19	1.17	1.43
27	b	617	BCR	C11-C10	-8.11	1.18	1.43
27	a	409	BCR	C11-C10	-8.09	1.18	1.43
27	B	617	BCR	C11-C10	-8.09	1.18	1.43
27	A	409	BCR	C11-C10	-8.08	1.18	1.43
27	F	101	BCR	C11-C10	-8.06	1.18	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	BCR	C11-C10	-8.05	1.18	1.43
27	b	619	BCR	C11-C10	-8.04	1.18	1.43
27	B	618	BCR	C11-C10	-8.03	1.18	1.43
27	B	619	BCR	C11-C10	-8.03	1.18	1.43
27	b	618	BCR	C11-C10	-8.03	1.18	1.43
27	Z	101	BCR	C11-C10	-7.99	1.18	1.43
27	z	101	BCR	C11-C10	-7.98	1.18	1.43
27	k	103	BCR	C11-C10	-7.94	1.18	1.43
27	K	103	BCR	C11-C10	-7.94	1.18	1.43
27	k	102	BCR	C11-C10	-7.84	1.18	1.43
27	K	102	BCR	C11-C10	-7.83	1.18	1.43
27	A	409	BCR	C20-C21	-7.51	1.19	1.43
27	a	409	BCR	C20-C21	-7.50	1.19	1.43
27	B	617	BCR	C20-C21	-7.49	1.20	1.43
27	b	617	BCR	C20-C21	-7.48	1.20	1.43
25	C	502	CLA	MG-NA	7.44	2.24	2.06
27	k	103	BCR	C20-C21	-7.44	1.20	1.43
27	c	515	BCR	C20-C21	-7.44	1.20	1.43
27	C	515	BCR	C20-C21	-7.44	1.20	1.43
27	K	103	BCR	C20-C21	-7.44	1.20	1.43
27	Z	101	BCR	C20-C21	-7.44	1.20	1.43
27	B	619	BCR	C20-C21	-7.43	1.20	1.43
27	b	618	BCR	C20-C21	-7.43	1.20	1.43
27	z	101	BCR	C20-C21	-7.43	1.20	1.43
25	B	604	CLA	MG-NA	7.42	2.23	2.06
27	b	619	BCR	C20-C21	-7.41	1.20	1.43
27	B	617	BCR	C16-C17	-7.41	1.20	1.43
27	B	618	BCR	C20-C21	-7.41	1.20	1.43
25	c	502	CLA	MG-NA	7.41	2.23	2.06
27	b	617	BCR	C16-C17	-7.40	1.20	1.43
27	c	515	BCR	C16-C17	-7.40	1.20	1.43
25	C	513	CLA	MG-NA	7.40	2.23	2.06
25	b	604	CLA	MG-NA	7.40	2.23	2.06
27	C	515	BCR	C16-C17	-7.39	1.20	1.43
25	c	513	CLA	MG-NA	7.39	2.23	2.06
25	B	613	CLA	MG-NA	7.39	2.23	2.06
25	C	510	CLA	MG-NA	7.39	2.23	2.06
25	c	510	CLA	MG-NA	7.39	2.23	2.06
25	b	613	CLA	MG-NA	7.39	2.23	2.06
27	a	409	BCR	C16-C17	-7.37	1.20	1.43
25	c	504	CLA	MG-NA	7.36	2.23	2.06
25	C	504	CLA	MG-NA	7.36	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	409	BCR	C16-C17	-7.36	1.20	1.43
25	b	603	CLA	MG-NA	7.32	2.23	2.06
25	B	603	CLA	MG-NA	7.31	2.23	2.06
25	c	508	CLA	MG-NA	7.30	2.23	2.06
27	b	618	BCR	C16-C17	-7.30	1.20	1.43
25	C	508	CLA	MG-NA	7.30	2.23	2.06
27	B	619	BCR	C16-C17	-7.29	1.20	1.43
27	b	619	BCR	C16-C17	-7.29	1.20	1.43
27	B	618	BCR	C16-C17	-7.29	1.20	1.43
27	K	103	BCR	C16-C17	-7.28	1.20	1.43
27	K	102	BCR	C20-C21	-7.28	1.20	1.43
27	k	102	BCR	C20-C21	-7.27	1.20	1.43
25	c	507	CLA	MG-NA	7.27	2.23	2.06
27	k	103	BCR	C16-C17	-7.26	1.20	1.43
25	C	503	CLA	MG-NA	7.26	2.23	2.06
25	C	507	CLA	MG-NA	7.25	2.23	2.06
25	C	511	CLA	MG-NA	7.25	2.23	2.06
25	c	511	CLA	MG-NA	7.25	2.23	2.06
27	F	101	BCR	C16-C17	-7.24	1.20	1.43
27	k	102	BCR	C16-C17	-7.24	1.20	1.43
27	f	101	BCR	C16-C17	-7.24	1.20	1.43
27	K	102	BCR	C16-C17	-7.24	1.20	1.43
25	c	503	CLA	MG-NA	7.22	2.23	2.06
27	Z	101	BCR	C16-C17	-7.19	1.20	1.43
27	f	101	BCR	C20-C21	-7.19	1.20	1.43
25	B	615	CLA	MG-NA	7.19	2.23	2.06
27	z	101	BCR	C16-C17	-7.19	1.20	1.43
25	b	615	CLA	MG-NA	7.17	2.23	2.06
27	F	101	BCR	C20-C21	-7.17	1.20	1.43
25	B	611	CLA	MG-NA	7.17	2.23	2.06
25	c	514	CLA	MG-NA	7.17	2.23	2.06
25	b	611	CLA	MG-NA	7.16	2.23	2.06
25	B	601	CLA	MG-NA	7.15	2.23	2.06
25	C	514	CLA	MG-NA	7.15	2.23	2.06
25	b	601	CLA	MG-NA	7.15	2.23	2.06
25	c	509	CLA	MG-NA	7.13	2.23	2.06
25	C	509	CLA	MG-NA	7.13	2.23	2.06
25	C	506	CLA	MG-NA	7.11	2.23	2.06
25	c	506	CLA	MG-NA	7.11	2.23	2.06
25	c	512	CLA	MG-NA	7.09	2.23	2.06
25	C	512	CLA	MG-NA	7.05	2.23	2.06
25	B	608	CLA	MG-NA	7.05	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	MG-NA	7.04	2.23	2.06
25	c	505	CLA	MG-NA	7.02	2.22	2.06
25	B	609	CLA	MG-NA	7.01	2.22	2.06
25	b	609	CLA	MG-NA	6.99	2.22	2.06
25	C	505	CLA	MG-NA	6.98	2.22	2.06
25	b	607	CLA	MG-NA	6.98	2.22	2.06
25	B	607	CLA	MG-NA	6.96	2.22	2.06
25	a	406	CLA	MG-NA	6.94	2.22	2.06
25	A	406	CLA	MG-NA	6.94	2.22	2.06
25	d	401	CLA	MG-NA	6.94	2.22	2.06
25	D	401	CLA	MG-NA	6.94	2.22	2.06
25	B	614	CLA	MG-NA	6.91	2.22	2.06
25	B	606	CLA	MG-NA	6.90	2.22	2.06
25	b	616	CLA	MG-NA	6.88	2.22	2.06
25	b	614	CLA	MG-NA	6.88	2.22	2.06
25	B	616	CLA	MG-NA	6.87	2.22	2.06
25	b	606	CLA	MG-NA	6.87	2.22	2.06
25	B	610	CLA	MG-NA	6.86	2.22	2.06
25	b	610	CLA	MG-NA	6.86	2.22	2.06
25	b	602	CLA	MG-NA	6.85	2.22	2.06
25	D	404	CLA	MG-NA	6.84	2.22	2.06
25	d	404	CLA	MG-NA	6.84	2.22	2.06
25	B	602	CLA	MG-NA	6.83	2.22	2.06
25	a	408	CLA	MG-NA	6.82	2.22	2.06
25	b	612	CLA	MG-NA	6.82	2.22	2.06
25	B	612	CLA	MG-NA	6.82	2.22	2.06
25	d	403	CLA	MG-NA	6.82	2.22	2.06
25	D	403	CLA	MG-NA	6.81	2.22	2.06
25	A	408	CLA	MG-NA	6.81	2.22	2.06
25	b	605	CLA	MG-NA	6.80	2.22	2.06
25	B	605	CLA	MG-NA	6.78	2.22	2.06
25	a	405	CLA	MG-NA	6.75	2.22	2.06
25	A	405	CLA	MG-NA	6.71	2.22	2.06
29	D	405	PL9	C7-C3	-5.60	1.43	1.51
29	d	405	PL9	C7-C3	-5.58	1.43	1.51
25	b	608	CLA	CHC-C1C	5.55	1.48	1.34
25	C	508	CLA	O2A-C1	5.54	1.61	1.46
29	d	405	PL9	C3-C4	-5.53	1.40	1.49
29	D	405	PL9	C3-C4	-5.53	1.40	1.49
25	c	508	CLA	O2A-C1	5.52	1.61	1.46
25	B	608	CLA	CHC-C1C	5.51	1.48	1.34
25	C	513	CLA	O2A-C1	5.51	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	O2A-C1	5.51	1.61	1.46
25	C	505	CLA	O2A-C1	5.48	1.60	1.46
25	c	505	CLA	O2A-C1	5.47	1.60	1.46
25	b	607	CLA	CHC-C1C	5.46	1.48	1.34
25	B	607	CLA	CHC-C1C	5.44	1.48	1.34
25	d	401	CLA	O2A-C1	5.43	1.60	1.46
25	D	401	CLA	O2A-C1	5.40	1.60	1.46
25	A	406	CLA	O2A-C1	5.39	1.60	1.46
25	a	406	CLA	O2A-C1	5.38	1.60	1.46
25	b	614	CLA	CHC-C1C	5.36	1.47	1.34
25	c	514	CLA	CHC-C1C	5.35	1.47	1.34
25	C	514	CLA	CHC-C1C	5.35	1.47	1.34
25	C	502	CLA	CHC-C1C	5.35	1.47	1.34
25	B	614	CLA	CHC-C1C	5.35	1.47	1.34
25	B	603	CLA	CHC-C1C	5.34	1.47	1.34
25	b	607	CLA	O2A-C1	5.34	1.60	1.46
25	b	603	CLA	CHC-C1C	5.34	1.47	1.34
25	B	607	CLA	O2A-C1	5.33	1.60	1.46
25	b	616	CLA	O2A-C1	5.33	1.60	1.46
25	c	502	CLA	CHC-C1C	5.33	1.47	1.34
25	b	603	CLA	O2A-C1	5.32	1.60	1.46
25	a	408	CLA	O2A-C1	5.32	1.60	1.46
25	A	408	CLA	O2A-C1	5.32	1.60	1.46
25	D	404	CLA	O2A-C1	5.31	1.60	1.46
25	B	615	CLA	O2A-C1	5.31	1.60	1.46
25	B	603	CLA	O2A-C1	5.31	1.60	1.46
35	E	104	HEM	C3C-C2C	-5.31	1.33	1.40
25	d	404	CLA	O2A-C1	5.29	1.60	1.46
25	B	616	CLA	O2A-C1	5.29	1.60	1.46
25	c	505	CLA	C3B-C2B	5.29	1.47	1.40
25	c	503	CLA	CHC-C1C	5.28	1.47	1.34
25	b	615	CLA	O2A-C1	5.28	1.60	1.46
25	C	506	CLA	CHC-C1C	5.28	1.47	1.34
25	c	510	CLA	CHC-C1C	5.28	1.47	1.34
25	C	510	CLA	CHC-C1C	5.28	1.47	1.34
25	C	503	CLA	CHC-C1C	5.28	1.47	1.34
25	c	506	CLA	CHC-C1C	5.27	1.47	1.34
25	C	505	CLA	C3B-C2B	5.27	1.47	1.40
25	b	601	CLA	CHC-C1C	5.26	1.47	1.34
25	B	602	CLA	O2A-C1	5.26	1.60	1.46
25	b	602	CLA	O2A-C1	5.26	1.60	1.46
35	e	104	HEM	C3C-C2C	-5.25	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	O2A-C1	5.25	1.60	1.46
25	B	601	CLA	CHC-C1C	5.25	1.47	1.34
25	b	612	CLA	O2A-C1	5.24	1.60	1.46
25	C	502	CLA	O2A-C1	5.24	1.60	1.46
25	B	608	CLA	O2A-C1	5.23	1.60	1.46
25	C	505	CLA	CHC-C1C	5.23	1.47	1.34
25	c	505	CLA	CHC-C1C	5.23	1.47	1.34
25	C	510	CLA	O2A-C1	5.22	1.60	1.46
25	c	502	CLA	O2A-C1	5.22	1.60	1.46
25	c	510	CLA	O2A-C1	5.22	1.60	1.46
25	C	507	CLA	O2A-C1	5.21	1.60	1.46
25	B	612	CLA	O2A-C1	5.21	1.60	1.46
25	c	507	CLA	O2A-C1	5.21	1.60	1.46
25	C	511	CLA	CHC-C1C	5.20	1.47	1.34
25	c	504	CLA	O2A-C1	5.18	1.60	1.46
25	c	514	CLA	O2A-C1	5.18	1.60	1.46
25	C	514	CLA	O2A-C1	5.18	1.60	1.46
25	C	504	CLA	O2A-C1	5.18	1.60	1.46
25	b	610	CLA	O2A-C1	5.17	1.60	1.46
25	B	610	CLA	O2A-C1	5.17	1.60	1.46
25	c	511	CLA	CHC-C1C	5.17	1.47	1.34
25	C	512	CLA	O2A-C1	5.17	1.60	1.46
25	a	406	CLA	CHC-C1C	5.17	1.47	1.34
25	b	602	CLA	CHC-C1C	5.16	1.47	1.34
25	B	612	CLA	CHC-C1C	5.16	1.47	1.34
25	b	614	CLA	O2A-C1	5.16	1.60	1.46
25	B	602	CLA	CHC-C1C	5.15	1.47	1.34
25	B	614	CLA	O2A-C1	5.15	1.60	1.46
25	c	512	CLA	O2A-C1	5.15	1.60	1.46
25	A	406	CLA	CHC-C1C	5.15	1.47	1.34
25	b	612	CLA	CHC-C1C	5.14	1.47	1.34
25	a	405	CLA	O2A-C1	5.14	1.60	1.46
25	B	615	CLA	CHC-C1C	5.14	1.47	1.34
25	A	405	CLA	O2A-C1	5.13	1.59	1.46
25	b	606	CLA	O2A-C1	5.13	1.59	1.46
25	b	615	CLA	CHC-C1C	5.13	1.47	1.34
25	B	606	CLA	O2A-C1	5.13	1.59	1.46
25	d	404	CLA	CHC-C1C	5.12	1.47	1.34
25	c	512	CLA	CHC-C1C	5.12	1.47	1.34
25	C	509	CLA	O2A-C1	5.12	1.59	1.46
25	c	509	CLA	O2A-C1	5.10	1.59	1.46
25	b	609	CLA	O2A-C1	5.10	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	CHC-C1C	5.10	1.47	1.34
25	C	512	CLA	CHC-C1C	5.10	1.47	1.34
25	B	609	CLA	O2A-C1	5.10	1.59	1.46
25	b	605	CLA	CHC-C1C	5.09	1.47	1.34
25	B	605	CLA	CHC-C1C	5.09	1.47	1.34
25	C	507	CLA	CHC-C1C	5.08	1.47	1.34
25	b	610	CLA	O2D-CGD	5.08	1.45	1.33
25	d	403	CLA	O2A-C1	5.08	1.59	1.46
25	c	507	CLA	CHC-C1C	5.07	1.47	1.34
25	d	401	CLA	CHC-C1C	5.07	1.47	1.34
25	B	610	CLA	O2D-CGD	5.07	1.45	1.33
25	D	403	CLA	O2A-C1	5.07	1.59	1.46
25	C	511	CLA	O2D-CGD	5.06	1.45	1.33
25	d	401	CLA	O2D-CGD	5.05	1.45	1.33
25	C	502	CLA	C3B-C2B	5.05	1.47	1.40
25	c	502	CLA	C3B-C2B	5.05	1.47	1.40
25	c	513	CLA	CHC-C1C	5.05	1.47	1.34
25	b	609	CLA	O2D-CGD	5.05	1.45	1.33
25	D	401	CLA	O2D-CGD	5.05	1.45	1.33
25	C	513	CLA	CHC-C1C	5.05	1.47	1.34
25	c	511	CLA	O2D-CGD	5.04	1.45	1.33
25	D	401	CLA	CHC-C1C	5.04	1.47	1.34
25	C	504	CLA	CHC-C1C	5.04	1.47	1.34
25	c	503	CLA	O2A-C1	5.04	1.59	1.46
25	c	504	CLA	CHC-C1C	5.04	1.47	1.34
25	B	609	CLA	O2D-CGD	5.03	1.45	1.33
25	D	403	CLA	CHC-C1C	5.03	1.47	1.34
25	b	615	CLA	O2D-CGD	5.03	1.45	1.33
25	B	605	CLA	O2D-CGD	5.02	1.45	1.33
25	B	615	CLA	O2D-CGD	5.02	1.45	1.33
25	b	605	CLA	O2A-C1	5.02	1.59	1.46
25	C	503	CLA	O2A-C1	5.02	1.59	1.46
25	d	403	CLA	CHC-C1C	5.01	1.46	1.34
25	b	613	CLA	O2A-C1	5.01	1.59	1.46
25	B	613	CLA	O2A-C1	5.00	1.59	1.46
25	b	606	CLA	CHC-C1C	5.00	1.46	1.34
25	C	507	CLA	O2D-CGD	5.00	1.45	1.33
25	B	605	CLA	O2A-C1	4.99	1.59	1.46
25	C	513	CLA	O2D-CGD	4.99	1.45	1.33
25	c	513	CLA	O2D-CGD	4.99	1.45	1.33
25	b	605	CLA	O2D-CGD	4.99	1.45	1.33
25	c	504	CLA	C3B-C2B	4.99	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	O2D-CGD	4.99	1.45	1.33
25	B	606	CLA	CHC-C1C	4.98	1.46	1.34
25	B	610	CLA	CHC-C1C	4.98	1.46	1.34
25	A	405	CLA	CHC-C1C	4.98	1.46	1.34
25	a	405	CLA	CHC-C1C	4.98	1.46	1.34
25	B	616	CLA	CHC-C1C	4.98	1.46	1.34
25	C	504	CLA	C3B-C2B	4.97	1.47	1.40
25	c	506	CLA	O2A-C1	4.97	1.59	1.46
25	a	408	CLA	CHC-C1C	4.97	1.46	1.34
25	b	616	CLA	CHC-C1C	4.97	1.46	1.34
25	c	514	CLA	O2D-CGD	4.96	1.45	1.33
25	C	506	CLA	O2A-C1	4.96	1.59	1.46
25	C	506	CLA	C3D-C4D	-4.96	1.33	1.44
25	C	514	CLA	O2D-CGD	4.95	1.45	1.33
25	b	610	CLA	CHC-C1C	4.95	1.46	1.34
25	A	408	CLA	CHC-C1C	4.95	1.46	1.34
25	c	509	CLA	CHC-C1C	4.94	1.46	1.34
25	b	611	CLA	O2A-C1	4.94	1.59	1.46
25	c	503	CLA	O2D-CGD	4.94	1.45	1.33
25	B	606	CLA	C3B-C2B	4.94	1.47	1.40
25	b	606	CLA	C3B-C2B	4.94	1.47	1.40
25	b	609	CLA	CHC-C1C	4.94	1.46	1.34
25	c	506	CLA	C3D-C4D	-4.93	1.33	1.44
25	B	611	CLA	O2A-C1	4.93	1.59	1.46
25	c	511	CLA	O2A-C1	4.93	1.59	1.46
25	C	509	CLA	CHC-C1C	4.93	1.46	1.34
25	C	503	CLA	O2D-CGD	4.92	1.45	1.33
25	B	609	CLA	CHC-C1C	4.92	1.46	1.34
25	c	506	CLA	O2D-CGD	4.91	1.45	1.33
25	C	511	CLA	O2A-C1	4.91	1.59	1.46
25	b	613	CLA	O2D-CGD	4.90	1.45	1.33
25	B	613	CLA	O2D-CGD	4.89	1.45	1.33
25	B	607	CLA	C3B-C2B	4.88	1.47	1.40
25	C	506	CLA	O2D-CGD	4.88	1.45	1.33
25	c	508	CLA	CHC-C1C	4.87	1.46	1.34
25	a	406	CLA	O2D-CGD	4.86	1.45	1.33
25	b	607	CLA	C3B-C2B	4.86	1.46	1.40
25	C	508	CLA	CHC-C1C	4.85	1.46	1.34
25	A	406	CLA	O2D-CGD	4.84	1.45	1.33
25	b	605	CLA	C3B-C2B	4.84	1.46	1.40
25	d	404	CLA	O2D-CGD	4.83	1.45	1.33
25	D	404	CLA	O2D-CGD	4.83	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	CHC-C1C	4.83	1.46	1.34
25	c	513	CLA	C3B-C2B	4.82	1.46	1.40
25	B	605	CLA	C3B-C2B	4.82	1.46	1.40
25	B	604	CLA	O2A-C1	4.82	1.59	1.46
25	c	510	CLA	C3D-C4D	-4.81	1.33	1.44
25	b	601	CLA	O2D-CGD	4.81	1.45	1.33
25	b	604	CLA	CHC-C1C	4.80	1.46	1.34
25	b	607	CLA	O2D-CGD	4.80	1.45	1.33
25	B	601	CLA	O2D-CGD	4.79	1.45	1.33
25	c	504	CLA	O2D-CGD	4.79	1.45	1.33
25	d	403	CLA	C3B-C2B	4.79	1.46	1.40
25	B	607	CLA	O2D-CGD	4.79	1.45	1.33
25	b	604	CLA	O2A-C1	4.79	1.59	1.46
25	C	504	CLA	O2D-CGD	4.78	1.45	1.33
25	B	611	CLA	CHC-C1C	4.78	1.46	1.34
25	c	509	CLA	O2D-CGD	4.78	1.45	1.33
25	B	606	CLA	O2D-CGD	4.78	1.45	1.33
25	C	510	CLA	C3D-C4D	-4.77	1.33	1.44
25	b	611	CLA	CHC-C1C	4.77	1.46	1.34
25	B	604	CLA	O2D-CGD	4.77	1.45	1.33
25	b	604	CLA	O2D-CGD	4.77	1.44	1.33
25	B	603	CLA	C3B-C2B	4.76	1.46	1.40
25	C	513	CLA	C3B-C2B	4.76	1.46	1.40
25	b	612	CLA	O2D-CGD	4.76	1.44	1.33
25	c	502	CLA	CHD-C1D	4.75	1.47	1.38
25	b	606	CLA	O2D-CGD	4.75	1.44	1.33
25	D	403	CLA	C3B-C2B	4.74	1.46	1.40
25	c	503	CLA	C3B-C2B	4.74	1.46	1.40
25	B	612	CLA	O2D-CGD	4.74	1.44	1.33
25	C	509	CLA	O2D-CGD	4.74	1.44	1.33
25	b	603	CLA	C3B-C2B	4.74	1.46	1.40
25	C	510	CLA	C3B-C2B	4.73	1.46	1.40
25	D	403	CLA	O2D-CGD	4.72	1.44	1.33
25	b	616	CLA	O2D-CGD	4.72	1.44	1.33
25	d	403	CLA	O2D-CGD	4.72	1.44	1.33
25	C	503	CLA	C3B-C2B	4.72	1.46	1.40
25	b	612	CLA	C3B-C2B	4.72	1.46	1.40
25	C	502	CLA	CHD-C1D	4.72	1.47	1.38
25	c	510	CLA	C3B-C2B	4.70	1.46	1.40
25	B	612	CLA	C3B-C2B	4.70	1.46	1.40
25	B	613	CLA	CHC-C1C	4.69	1.46	1.34
25	b	611	CLA	C3D-C4D	-4.69	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	O2D-CGD	4.69	1.44	1.33
25	B	611	CLA	C3D-C4D	-4.69	1.33	1.44
25	C	509	CLA	C3D-C4D	-4.69	1.33	1.44
25	b	613	CLA	CHC-C1C	4.68	1.46	1.34
25	c	509	CLA	C3D-C4D	-4.68	1.33	1.44
25	c	512	CLA	O2D-CGD	4.68	1.44	1.33
25	C	512	CLA	O2D-CGD	4.68	1.44	1.33
25	B	606	CLA	C3D-C4D	-4.67	1.33	1.44
25	b	606	CLA	C3D-C4D	-4.67	1.33	1.44
25	B	608	CLA	O2D-CGD	4.67	1.44	1.33
25	B	611	CLA	O2D-CGD	4.66	1.44	1.33
25	b	608	CLA	O2D-CGD	4.66	1.44	1.33
25	b	611	CLA	O2D-CGD	4.66	1.44	1.33
25	C	505	CLA	O2D-CGD	4.65	1.44	1.33
25	B	602	CLA	O2D-CGD	4.65	1.44	1.33
25	B	604	CLA	C3D-C4D	-4.64	1.33	1.44
25	a	408	CLA	O2D-CGD	4.63	1.44	1.33
25	D	403	CLA	C3D-C4D	-4.62	1.33	1.44
25	c	514	CLA	C3B-C2B	4.62	1.46	1.40
25	c	505	CLA	O2D-CGD	4.62	1.44	1.33
25	b	602	CLA	O2D-CGD	4.62	1.44	1.33
25	c	508	CLA	O2D-CGD	4.62	1.44	1.33
27	c	515	BCR	C10-C9	-4.62	1.25	1.35
25	b	604	CLA	C3D-C4D	-4.61	1.33	1.44
25	c	502	CLA	O2D-CGD	4.61	1.44	1.33
25	A	408	CLA	O2D-CGD	4.61	1.44	1.33
25	C	502	CLA	O2D-CGD	4.61	1.44	1.33
25	C	508	CLA	O2D-CGD	4.60	1.44	1.33
25	C	510	CLA	O2D-CGD	4.60	1.44	1.33
25	d	403	CLA	C3D-C4D	-4.59	1.33	1.44
27	C	515	BCR	C10-C9	-4.59	1.25	1.35
25	D	403	CLA	C1D-ND	-4.59	1.31	1.37
25	B	605	CLA	C3D-C4D	-4.59	1.33	1.44
25	c	507	CLA	C3D-C4D	-4.59	1.33	1.44
25	C	507	CLA	C3D-C4D	-4.59	1.33	1.44
25	C	514	CLA	C3B-C2B	4.59	1.46	1.40
25	c	510	CLA	O2D-CGD	4.59	1.44	1.33
25	B	609	CLA	C3D-C4D	-4.59	1.33	1.44
25	b	615	CLA	C3B-C2B	4.58	1.46	1.40
25	d	403	CLA	C1D-ND	-4.57	1.31	1.37
25	b	605	CLA	C3D-C4D	-4.57	1.33	1.44
25	b	612	CLA	C3D-C4D	-4.57	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	O2D-CGD	4.56	1.44	1.33
25	A	408	CLA	C3D-C4D	-4.56	1.33	1.44
25	a	408	CLA	C3D-C4D	-4.56	1.33	1.44
25	b	609	CLA	C3D-C4D	-4.56	1.33	1.44
25	a	405	CLA	C3B-C2B	4.56	1.46	1.40
25	B	616	CLA	C3D-C4D	-4.56	1.33	1.44
25	a	405	CLA	O2D-CGD	4.55	1.44	1.33
25	A	405	CLA	O2D-CGD	4.55	1.44	1.33
25	d	404	CLA	CHD-C1D	4.55	1.47	1.38
25	B	608	CLA	C3D-C4D	-4.55	1.34	1.44
25	b	614	CLA	O2D-CGD	4.55	1.44	1.33
25	b	610	CLA	C3D-C4D	-4.55	1.34	1.44
25	b	616	CLA	C3D-C4D	-4.55	1.34	1.44
25	b	608	CLA	C3D-C4D	-4.55	1.34	1.44
25	D	404	CLA	CHD-C1D	4.54	1.47	1.38
25	A	405	CLA	C3B-C2B	4.54	1.46	1.40
25	B	612	CLA	C3D-C4D	-4.54	1.34	1.44
25	C	511	CLA	C3B-C2B	4.54	1.46	1.40
25	B	601	CLA	C3D-C4D	-4.53	1.34	1.44
25	b	601	CLA	C3D-C4D	-4.53	1.34	1.44
25	B	610	CLA	C3D-C4D	-4.53	1.34	1.44
25	C	512	CLA	C3B-C2B	4.53	1.46	1.40
27	A	409	BCR	C10-C9	-4.52	1.25	1.35
25	B	615	CLA	C3B-C2B	4.52	1.46	1.40
25	c	514	CLA	C3C-C2C	4.51	1.46	1.36
27	a	409	BCR	C10-C9	-4.51	1.25	1.35
25	b	603	CLA	O2D-CGD	4.51	1.44	1.33
25	C	514	CLA	C3C-C2C	4.51	1.46	1.36
25	b	607	CLA	C3D-C4D	-4.50	1.34	1.44
25	B	603	CLA	O2D-CGD	4.50	1.44	1.33
25	c	512	CLA	C3B-C2B	4.50	1.46	1.40
25	B	607	CLA	C3D-C4D	-4.49	1.34	1.44
25	A	408	CLA	C3B-C2B	4.49	1.46	1.40
25	D	404	CLA	C3D-C4D	-4.49	1.34	1.44
25	B	608	CLA	C3C-C2C	4.49	1.46	1.36
28	a	414	LMG	O8-C28	4.49	1.46	1.33
25	d	404	CLA	C3D-C4D	-4.48	1.34	1.44
25	b	609	CLA	C3B-C2B	4.48	1.46	1.40
25	B	602	CLA	C3D-C4D	-4.48	1.34	1.44
25	c	511	CLA	C3B-C2B	4.48	1.46	1.40
25	b	608	CLA	C3C-C2C	4.48	1.46	1.36
28	A	414	LMG	O8-C28	4.48	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	C3D-C4D	-4.47	1.34	1.44
25	A	406	CLA	C3B-C2B	4.47	1.46	1.40
25	C	506	CLA	CHD-C1D	4.47	1.47	1.38
25	b	610	CLA	C1D-ND	-4.47	1.32	1.37
25	B	614	CLA	C3D-C4D	-4.47	1.34	1.44
25	b	608	CLA	CHD-C1D	4.47	1.47	1.38
25	b	614	CLA	C3D-C4D	-4.47	1.34	1.44
25	B	609	CLA	C3B-C2B	4.46	1.46	1.40
25	B	610	CLA	C1D-ND	-4.46	1.32	1.37
25	c	506	CLA	CHD-C1D	4.46	1.47	1.38
25	B	608	CLA	CHD-C1D	4.46	1.47	1.38
25	C	503	CLA	C3D-C4D	-4.45	1.34	1.44
25	d	401	CLA	C3C-C2C	4.45	1.46	1.36
25	c	505	CLA	C3D-C4D	-4.45	1.34	1.44
25	B	614	CLA	C3B-C2B	4.44	1.46	1.40
25	b	614	CLA	C3B-C2B	4.44	1.46	1.40
25	c	503	CLA	C3D-C4D	-4.44	1.34	1.44
25	a	408	CLA	C3B-C2B	4.44	1.46	1.40
25	C	508	CLA	C3D-C4D	-4.44	1.34	1.44
27	b	617	BCR	C10-C9	-4.44	1.25	1.35
25	a	406	CLA	C3B-C2B	4.44	1.46	1.40
25	b	603	CLA	C3C-C2C	4.44	1.46	1.36
27	B	617	BCR	C10-C9	-4.43	1.25	1.35
25	B	603	CLA	C3D-C4D	-4.43	1.34	1.44
25	c	512	CLA	C3D-C4D	-4.43	1.34	1.44
25	b	603	CLA	C3D-C4D	-4.43	1.34	1.44
25	D	401	CLA	C3C-C2C	4.43	1.46	1.36
25	b	604	CLA	C3B-C2B	4.43	1.46	1.40
25	C	512	CLA	C3D-C4D	-4.42	1.34	1.44
25	b	603	CLA	CHD-C1D	4.42	1.47	1.38
25	B	603	CLA	C3C-C2C	4.42	1.46	1.36
25	C	505	CLA	C3D-C4D	-4.42	1.34	1.44
25	c	511	CLA	CHD-C1D	4.42	1.47	1.38
25	c	508	CLA	C3D-C4D	-4.42	1.34	1.44
25	C	511	CLA	CHD-C1D	4.41	1.47	1.38
25	B	604	CLA	C3B-C2B	4.41	1.46	1.40
27	F	101	BCR	C10-C9	-4.41	1.25	1.35
25	B	603	CLA	CHD-C1D	4.40	1.47	1.38
27	B	619	BCR	C10-C9	-4.40	1.25	1.35
27	b	618	BCR	C10-C9	-4.40	1.25	1.35
25	c	506	CLA	C3C-C2C	4.40	1.46	1.36
25	B	616	CLA	C3B-C2B	4.40	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	BCR	C10-C9	-4.39	1.25	1.35
25	b	616	CLA	C3B-C2B	4.39	1.46	1.40
27	B	618	BCR	C10-C9	-4.39	1.25	1.35
25	b	612	CLA	C1D-ND	-4.39	1.32	1.37
25	C	513	CLA	C3D-C4D	-4.39	1.34	1.44
25	B	613	CLA	C3B-C2B	4.39	1.46	1.40
25	B	612	CLA	C1D-ND	-4.39	1.32	1.37
33	B	622	LHG	O8-C23	4.38	1.46	1.33
25	D	401	CLA	C3B-C2B	4.38	1.46	1.40
33	b	622	LHG	O8-C23	4.38	1.46	1.33
27	b	619	BCR	C10-C9	-4.38	1.25	1.35
25	b	613	CLA	C3B-C2B	4.37	1.46	1.40
25	c	513	CLA	C3D-C4D	-4.37	1.34	1.44
25	C	506	CLA	C3C-C2C	4.37	1.46	1.36
25	c	511	CLA	C3C-C2C	4.35	1.46	1.36
25	C	504	CLA	C3D-C4D	-4.35	1.34	1.44
25	b	602	CLA	C3B-C2B	4.35	1.46	1.40
25	d	401	CLA	C3B-C2B	4.35	1.46	1.40
25	b	611	CLA	C1D-ND	-4.34	1.32	1.37
25	c	502	CLA	C3C-C2C	4.34	1.46	1.36
25	C	511	CLA	C3D-C4D	-4.34	1.34	1.44
25	C	502	CLA	C3C-C2C	4.34	1.46	1.36
25	B	601	CLA	C3B-C2B	4.34	1.46	1.40
25	B	602	CLA	C3B-C2B	4.34	1.46	1.40
25	C	511	CLA	C3C-C2C	4.33	1.46	1.36
25	c	504	CLA	C3D-C4D	-4.33	1.34	1.44
25	B	614	CLA	CHD-C1D	4.33	1.46	1.38
25	d	404	CLA	C3C-C2C	4.33	1.46	1.36
25	A	405	CLA	C3D-C4D	-4.33	1.34	1.44
25	a	405	CLA	C3D-C4D	-4.33	1.34	1.44
25	c	511	CLA	C3D-C4D	-4.33	1.34	1.44
25	b	614	CLA	CHD-C1D	4.33	1.46	1.38
25	B	611	CLA	C1D-ND	-4.32	1.32	1.37
25	D	404	CLA	C3C-C2C	4.32	1.46	1.36
28	c	519	LMG	O8-C28	4.30	1.45	1.33
25	b	601	CLA	C3B-C2B	4.30	1.46	1.40
25	B	604	CLA	CHD-C1D	4.29	1.46	1.38
25	B	602	CLA	C3C-C2C	4.29	1.46	1.36
28	C	519	LMG	O8-C28	4.29	1.45	1.33
25	c	514	CLA	C3D-C4D	-4.28	1.34	1.44
25	d	404	CLA	C3B-C2B	4.28	1.46	1.40
25	b	604	CLA	CHD-C1D	4.28	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	C3C-C2C	4.28	1.46	1.36
25	B	608	CLA	C3B-C2B	4.27	1.46	1.40
27	z	101	BCR	C10-C9	-4.27	1.25	1.35
25	C	504	CLA	CHD-C1D	4.27	1.46	1.38
25	B	613	CLA	C3D-C4D	-4.27	1.34	1.44
25	C	514	CLA	C3D-C4D	-4.26	1.34	1.44
27	Z	101	BCR	C10-C9	-4.26	1.25	1.35
34	c	517	DGD	O1G-C1A	4.26	1.45	1.33
34	h	103	DGD	O1G-C1A	4.26	1.45	1.33
25	b	613	CLA	C3D-C4D	-4.25	1.34	1.44
25	b	615	CLA	CHD-C1D	4.25	1.46	1.38
25	c	504	CLA	CHD-C1D	4.25	1.46	1.38
25	C	505	CLA	C3C-C2C	4.25	1.45	1.36
25	C	510	CLA	CHD-C1D	4.25	1.46	1.38
25	B	615	CLA	CHD-C1D	4.25	1.46	1.38
25	A	406	CLA	C3C-C2C	4.25	1.45	1.36
25	b	608	CLA	C3B-C2B	4.25	1.46	1.40
25	D	404	CLA	C3B-C2B	4.24	1.46	1.40
34	H	103	DGD	O1G-C1A	4.24	1.45	1.33
34	C	517	DGD	O1G-C1A	4.24	1.45	1.33
25	B	607	CLA	C3C-C2C	4.24	1.45	1.36
25	A	408	CLA	CHD-C1D	4.24	1.46	1.38
25	b	607	CLA	C3C-C2C	4.24	1.45	1.36
25	c	505	CLA	C3C-C2C	4.23	1.45	1.36
25	a	406	CLA	C3C-C2C	4.23	1.45	1.36
25	a	408	CLA	CHD-C1D	4.23	1.46	1.38
25	c	510	CLA	CHD-C1D	4.23	1.46	1.38
25	c	502	CLA	C3D-C4D	-4.22	1.34	1.44
25	C	507	CLA	C3C-C2C	4.22	1.45	1.36
25	c	507	CLA	C3C-C2C	4.22	1.45	1.36
35	v	201	HEM	C3C-C2C	-4.21	1.34	1.40
25	a	405	CLA	C1D-ND	-4.21	1.32	1.37
25	C	502	CLA	C3D-C4D	-4.21	1.34	1.44
25	B	601	CLA	C3C-C2C	4.21	1.45	1.36
25	C	513	CLA	C3C-C2C	4.21	1.45	1.36
25	b	601	CLA	C3C-C2C	4.21	1.45	1.36
25	C	514	CLA	CHD-C1D	4.21	1.46	1.38
25	C	507	CLA	CHD-C1D	4.20	1.46	1.38
25	c	507	CLA	CHD-C1D	4.20	1.46	1.38
27	k	103	BCR	C10-C9	-4.20	1.26	1.35
25	c	513	CLA	C3C-C2C	4.20	1.45	1.36
27	K	103	BCR	C10-C9	-4.19	1.26	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	514	CLA	CHD-C1D	4.19	1.46	1.38
25	c	510	CLA	C3C-C2C	4.19	1.45	1.36
25	C	510	CLA	C3C-C2C	4.19	1.45	1.36
25	C	509	CLA	C3B-C2B	4.19	1.46	1.40
35	V	201	HEM	C3C-C2C	-4.19	1.34	1.40
25	c	509	CLA	C3C-C2C	4.18	1.45	1.36
25	c	509	CLA	C3B-C2B	4.17	1.46	1.40
25	C	504	CLA	C3C-C2C	4.17	1.45	1.36
25	A	405	CLA	C1D-ND	-4.17	1.32	1.37
33	E	102	LHG	O8-C23	4.16	1.45	1.33
25	C	509	CLA	C3C-C2C	4.16	1.45	1.36
28	C	519	LMG	O7-C10	4.16	1.46	1.34
25	D	403	CLA	C3C-C2C	4.16	1.45	1.36
25	B	609	CLA	C3C-C2C	4.16	1.45	1.36
25	C	512	CLA	C3C-C2C	4.16	1.45	1.36
25	b	609	CLA	C3C-C2C	4.16	1.45	1.36
25	c	504	CLA	C3C-C2C	4.15	1.45	1.36
25	B	607	CLA	CHD-C1D	4.15	1.46	1.38
25	d	403	CLA	C3C-C2C	4.15	1.45	1.36
25	c	512	CLA	C3C-C2C	4.15	1.45	1.36
28	c	519	LMG	O7-C10	4.15	1.46	1.34
33	e	102	LHG	O8-C23	4.15	1.45	1.33
28	B	621	LMG	O8-C28	4.14	1.45	1.33
28	b	621	LMG	O8-C28	4.14	1.45	1.33
27	k	102	BCR	C10-C9	-4.13	1.26	1.35
28	a	410	LMG	O8-C28	4.13	1.45	1.33
25	B	602	CLA	CHD-C1D	4.13	1.46	1.38
27	K	102	BCR	C10-C9	-4.13	1.26	1.35
25	B	606	CLA	C3C-C2C	4.13	1.45	1.36
25	b	607	CLA	CHD-C1D	4.13	1.46	1.38
33	D	406	LHG	O8-C23	4.13	1.45	1.33
28	A	410	LMG	O8-C28	4.12	1.45	1.33
33	Z	102	LHG	O8-C23	4.12	1.45	1.33
25	b	612	CLA	C3C-C2C	4.12	1.45	1.36
25	C	513	CLA	C1D-ND	-4.12	1.32	1.37
33	d	406	LHG	O8-C23	4.12	1.45	1.33
34	c	516	DGD	O2G-C1B	4.12	1.45	1.34
25	b	606	CLA	C3C-C2C	4.12	1.45	1.36
33	z	102	LHG	O8-C23	4.11	1.45	1.33
25	c	513	CLA	C1D-ND	-4.11	1.32	1.37
25	B	612	CLA	C3C-C2C	4.11	1.45	1.36
25	c	503	CLA	C3C-C2C	4.11	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C3C-C2C	4.11	1.45	1.36
34	C	516	DGD	O2G-C1B	4.10	1.45	1.34
25	A	408	CLA	C3C-C2C	4.10	1.45	1.36
25	b	610	CLA	CHD-C1D	4.10	1.46	1.38
25	c	508	CLA	CHD-C1D	4.10	1.46	1.38
25	b	602	CLA	CHD-C1D	4.10	1.46	1.38
25	c	503	CLA	CHD-C1D	4.10	1.46	1.38
25	a	408	CLA	C3C-C2C	4.09	1.45	1.36
25	B	610	CLA	C3C-C2C	4.09	1.45	1.36
25	C	503	CLA	C3C-C2C	4.09	1.45	1.36
33	b	628	LHG	O8-C23	4.09	1.45	1.33
25	A	406	CLA	C3D-C4D	-4.09	1.35	1.44
25	a	406	CLA	C3D-C4D	-4.09	1.35	1.44
25	C	503	CLA	CHD-C1D	4.08	1.46	1.38
33	D	408	LHG	O7-C7	4.08	1.45	1.34
34	c	516	DGD	O1G-C1A	4.08	1.45	1.33
25	C	508	CLA	CHD-C1D	4.08	1.46	1.38
25	B	614	CLA	C3C-C2C	4.07	1.45	1.36
33	z	102	LHG	O7-C7	4.07	1.45	1.34
25	C	505	CLA	CHD-C1D	4.07	1.46	1.38
33	B	628	LHG	O8-C23	4.07	1.45	1.33
33	Z	102	LHG	O7-C7	4.07	1.45	1.34
25	b	614	CLA	C3C-C2C	4.06	1.45	1.36
33	d	408	LHG	O7-C7	4.06	1.45	1.34
34	C	516	DGD	O1G-C1A	4.06	1.45	1.33
25	b	601	CLA	CHD-C1D	4.06	1.46	1.38
25	c	502	CLA	CHD-C4C	4.06	1.48	1.39
25	b	615	CLA	C3D-C4D	-4.06	1.35	1.44
25	B	610	CLA	CHD-C1D	4.06	1.46	1.38
25	B	601	CLA	CHD-C1D	4.06	1.46	1.38
25	B	615	CLA	C3D-C4D	-4.05	1.35	1.44
25	D	401	CLA	C3D-C4D	-4.05	1.35	1.44
25	c	505	CLA	CHD-C1D	4.05	1.46	1.38
25	C	502	CLA	CHD-C4C	4.04	1.48	1.39
25	C	507	CLA	C3B-C2B	4.04	1.45	1.40
34	C	518	DGD	O1G-C1A	4.04	1.45	1.33
25	d	401	CLA	C3D-C4D	-4.04	1.35	1.44
25	c	508	CLA	C3C-C2C	4.03	1.45	1.36
34	c	518	DGD	O1G-C1A	4.03	1.45	1.33
25	c	507	CLA	C3B-C2B	4.03	1.45	1.40
25	C	508	CLA	C3C-C2C	4.02	1.45	1.36
25	b	606	CLA	CHD-C1D	4.01	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	CHD-C1D	4.01	1.46	1.38
25	b	610	CLA	C3B-C2B	4.00	1.45	1.40
25	b	611	CLA	CHD-C1D	4.00	1.46	1.38
25	B	610	CLA	C3B-C2B	3.99	1.45	1.40
25	b	604	CLA	C3C-C2C	3.98	1.45	1.36
25	B	606	CLA	CHD-C1D	3.98	1.46	1.38
25	b	605	CLA	C3C-C2C	3.97	1.45	1.36
25	B	604	CLA	C3C-C2C	3.97	1.45	1.36
33	d	408	LHG	O8-C23	3.97	1.44	1.33
25	b	611	CLA	C3B-C2B	3.97	1.45	1.40
33	D	406	LHG	O7-C7	3.97	1.45	1.34
25	B	609	CLA	CHD-C1D	3.96	1.46	1.38
25	C	511	CLA	CHD-C4C	3.96	1.48	1.39
25	b	611	CLA	C3C-C2C	3.96	1.45	1.36
25	B	605	CLA	C3C-C2C	3.96	1.45	1.36
25	c	512	CLA	C1D-ND	-3.96	1.32	1.37
28	A	414	LMG	O7-C10	3.96	1.45	1.34
25	B	616	CLA	CHD-C1D	3.95	1.46	1.38
33	D	408	LHG	O8-C23	3.95	1.44	1.33
25	B	611	CLA	C3C-C2C	3.95	1.45	1.36
25	d	401	CLA	CHD-C1D	3.94	1.46	1.38
33	d	406	LHG	O7-C7	3.94	1.45	1.34
28	a	414	LMG	O7-C10	3.94	1.45	1.34
25	b	616	CLA	CHD-C1D	3.94	1.46	1.38
25	C	506	CLA	C3B-C2B	3.93	1.45	1.40
25	B	605	CLA	C1D-ND	-3.93	1.32	1.37
25	b	609	CLA	CHD-C1D	3.93	1.46	1.38
25	c	511	CLA	CHD-C4C	3.93	1.48	1.39
25	B	611	CLA	C3B-C2B	3.92	1.45	1.40
25	C	512	CLA	CHD-C1D	3.92	1.46	1.38
25	c	509	CLA	CHD-C1D	3.92	1.46	1.38
25	D	401	CLA	CHD-C1D	3.92	1.46	1.38
25	B	615	CLA	C3C-C2C	3.92	1.45	1.36
25	c	512	CLA	CHD-C1D	3.92	1.46	1.38
33	b	622	LHG	O7-C7	3.91	1.45	1.34
25	b	613	CLA	CHD-C1D	3.91	1.46	1.38
25	c	506	CLA	C3B-C2B	3.91	1.45	1.40
25	c	506	CLA	C1D-ND	-3.91	1.32	1.37
33	B	622	LHG	O7-C7	3.91	1.45	1.34
25	c	505	CLA	CHD-C4C	3.91	1.48	1.39
25	C	509	CLA	CHD-C1D	3.91	1.46	1.38
25	C	505	CLA	CHD-C4C	3.90	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	CHD-C1D	3.90	1.46	1.38
25	C	506	CLA	C1D-ND	-3.90	1.32	1.37
25	b	615	CLA	C3C-C2C	3.89	1.45	1.36
25	C	512	CLA	C1D-ND	-3.89	1.32	1.37
25	b	605	CLA	C1D-ND	-3.89	1.32	1.37
25	c	513	CLA	CHD-C1D	3.89	1.46	1.38
25	c	514	CLA	CHD-C4C	3.89	1.48	1.39
33	E	102	LHG	O7-C7	3.88	1.45	1.34
25	C	513	CLA	CHD-C1D	3.88	1.46	1.38
33	e	102	LHG	O7-C7	3.88	1.45	1.34
28	d	409	LMG	O8-C28	3.88	1.44	1.33
28	D	409	LMG	O8-C28	3.87	1.44	1.33
25	A	406	CLA	CHD-C1D	3.87	1.46	1.38
25	D	404	CLA	CHD-C4C	3.87	1.48	1.39
25	a	406	CLA	CHD-C1D	3.87	1.46	1.38
25	c	510	CLA	C1D-ND	-3.86	1.32	1.37
25	C	510	CLA	C1D-ND	-3.85	1.32	1.37
25	C	514	CLA	CHD-C4C	3.85	1.48	1.39
25	b	602	CLA	C1D-ND	-3.85	1.32	1.37
25	d	404	CLA	CHD-C4C	3.84	1.47	1.39
25	B	603	CLA	CHD-C4C	3.84	1.47	1.39
25	B	613	CLA	C3C-C2C	3.84	1.45	1.36
28	A	410	LMG	C19-C18	-3.84	1.32	1.51
28	a	410	LMG	C19-C18	-3.84	1.32	1.51
28	A	410	LMG	O7-C10	3.83	1.45	1.34
28	D	409	LMG	O7-C10	3.82	1.45	1.34
25	B	602	CLA	C1D-ND	-3.82	1.32	1.37
28	a	410	LMG	O7-C10	3.81	1.45	1.34
33	d	407	LHG	O8-C23	3.81	1.44	1.33
28	b	621	LMG	O7-C10	3.81	1.45	1.34
28	d	409	LMG	O7-C10	3.80	1.45	1.34
25	b	613	CLA	C3C-C2C	3.80	1.45	1.36
33	D	407	LHG	O8-C23	3.80	1.44	1.33
34	C	518	DGD	CAB-C9B	-3.80	1.32	1.51
29	a	411	PL9	C7-C3	-3.79	1.46	1.51
25	b	603	CLA	CHD-C4C	3.79	1.47	1.39
25	B	608	CLA	CHD-C4C	3.79	1.47	1.39
34	c	518	DGD	CAB-C9B	-3.79	1.32	1.51
34	C	518	DGD	O2G-C1B	3.79	1.45	1.34
25	a	408	CLA	CHD-C4C	3.79	1.47	1.39
28	B	621	LMG	O7-C10	3.79	1.45	1.34
28	B	621	LMG	C40-C39	-3.78	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	CHD-C4C	3.78	1.47	1.39
28	b	621	LMG	C40-C39	-3.78	1.33	1.51
34	c	518	DGD	O2G-C1B	3.78	1.44	1.34
29	A	411	PL9	C7-C3	-3.77	1.46	1.51
25	D	401	CLA	CHD-C4C	3.77	1.47	1.39
25	B	602	CLA	CHD-C4C	3.77	1.47	1.39
25	A	408	CLA	C1D-ND	-3.76	1.32	1.37
25	A	408	CLA	CHD-C4C	3.76	1.47	1.39
25	a	408	CLA	C1D-ND	-3.76	1.32	1.37
28	a	410	LMG	C22-C21	-3.76	1.33	1.51
25	b	602	CLA	OBD-CAD	3.76	1.29	1.22
25	d	401	CLA	CHD-C4C	3.76	1.47	1.39
28	A	410	LMG	C22-C21	-3.75	1.33	1.51
28	B	621	LMG	C19-C18	-3.75	1.33	1.51
25	a	405	CLA	CHD-C1D	3.75	1.45	1.38
28	b	621	LMG	C19-C18	-3.75	1.33	1.51
25	b	608	CLA	CHD-C4C	3.75	1.47	1.39
25	C	508	CLA	C3B-C2B	3.75	1.45	1.40
25	c	506	CLA	CHD-C4C	3.74	1.47	1.39
25	B	602	CLA	OBD-CAD	3.74	1.28	1.22
28	C	519	LMG	C19-C18	-3.74	1.33	1.51
34	C	518	DGD	CDB-CCB	-3.74	1.33	1.51
28	c	519	LMG	C19-C18	-3.74	1.33	1.51
25	b	614	CLA	CHD-C4C	3.74	1.47	1.39
25	C	506	CLA	CHD-C4C	3.73	1.47	1.39
28	b	621	LMG	C22-C21	-3.73	1.33	1.51
34	c	518	DGD	CDB-CCB	-3.73	1.33	1.51
34	c	517	DGD	CAA-C9A	-3.73	1.33	1.51
34	C	516	DGD	CAB-C9B	-3.73	1.33	1.51
34	c	518	DGD	CDA-CCA	-3.73	1.33	1.51
28	B	621	LMG	C37-C36	-3.73	1.33	1.51
33	D	407	LHG	O7-C7	3.73	1.44	1.34
34	C	517	DGD	CAA-C9A	-3.72	1.33	1.51
33	d	407	LHG	O7-C7	3.72	1.44	1.34
28	B	621	LMG	C22-C21	-3.72	1.33	1.51
34	C	517	DGD	CAB-C9B	-3.72	1.33	1.51
28	b	621	LMG	C37-C36	-3.72	1.33	1.51
34	c	517	DGD	CAB-C9B	-3.72	1.33	1.51
34	h	103	DGD	CDB-CCB	-3.72	1.33	1.51
25	B	616	CLA	C3C-C2C	3.72	1.44	1.36
34	C	516	DGD	CDB-CCB	-3.72	1.33	1.51
25	A	405	CLA	CHD-C1D	3.72	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	518	DGD	CAA-C9A	-3.72	1.33	1.51
25	c	502	CLA	OBD-CAD	3.72	1.28	1.22
28	D	409	LMG	C40-C39	-3.71	1.33	1.51
34	c	518	DGD	CAA-C9A	-3.71	1.33	1.51
25	B	614	CLA	CHD-C4C	3.71	1.47	1.39
34	C	518	DGD	CDA-CCA	-3.71	1.33	1.51
25	B	610	CLA	C1C-NC	-3.71	1.32	1.37
34	c	516	DGD	CAB-C9B	-3.71	1.33	1.51
34	H	103	DGD	CDB-CCB	-3.70	1.33	1.51
25	b	616	CLA	C3C-C2C	3.70	1.44	1.36
25	c	508	CLA	C3B-C2B	3.70	1.45	1.40
25	b	610	CLA	C1C-NC	-3.70	1.32	1.37
34	c	516	DGD	CDB-CCB	-3.70	1.33	1.51
28	d	409	LMG	C40-C39	-3.70	1.33	1.51
25	C	502	CLA	OBD-CAD	3.70	1.28	1.22
34	C	517	DGD	CDA-CCA	-3.70	1.33	1.51
28	d	409	LMG	C22-C21	-3.70	1.33	1.51
28	D	409	LMG	C37-C36	-3.69	1.33	1.51
28	d	409	LMG	C37-C36	-3.69	1.33	1.51
25	B	603	CLA	C1D-ND	-3.69	1.33	1.37
25	b	603	CLA	C1D-ND	-3.69	1.33	1.37
34	H	103	DGD	CAB-C9B	-3.69	1.33	1.51
34	H	103	DGD	CAA-C9A	-3.69	1.33	1.51
34	h	103	DGD	CAA-C9A	-3.69	1.33	1.51
34	C	517	DGD	CDB-CCB	-3.69	1.33	1.51
34	c	517	DGD	CDA-CCA	-3.69	1.33	1.51
28	D	409	LMG	C22-C21	-3.69	1.33	1.51
25	c	509	CLA	CHD-C4C	3.69	1.47	1.39
34	h	103	DGD	CAB-C9B	-3.69	1.33	1.51
28	C	519	LMG	C37-C36	-3.69	1.33	1.51
25	C	503	CLA	C1D-ND	-3.69	1.33	1.37
28	c	519	LMG	C37-C36	-3.69	1.33	1.51
34	c	517	DGD	CDB-CCB	-3.69	1.33	1.51
28	c	519	LMG	C22-C21	-3.68	1.33	1.51
28	A	410	LMG	C37-C36	-3.68	1.33	1.51
28	C	519	LMG	C22-C21	-3.68	1.33	1.51
25	C	509	CLA	CHD-C4C	3.68	1.47	1.39
28	a	410	LMG	C37-C36	-3.67	1.33	1.51
34	C	516	DGD	CAA-C9A	-3.67	1.33	1.51
28	a	410	LMG	C40-C39	-3.67	1.33	1.51
34	c	516	DGD	CAA-C9A	-3.66	1.33	1.51
28	A	410	LMG	C40-C39	-3.66	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	C1D-ND	-3.65	1.33	1.37
25	c	510	CLA	CHD-C4C	3.64	1.47	1.39
25	B	609	CLA	C1D-ND	-3.64	1.33	1.37
25	B	605	CLA	CHD-C1D	3.64	1.45	1.38
28	D	409	LMG	C19-C18	-3.64	1.33	1.51
25	C	504	CLA	CHD-C4C	3.64	1.47	1.39
25	B	616	CLA	C1C-NC	-3.64	1.32	1.37
25	b	616	CLA	C1C-NC	-3.64	1.32	1.37
28	d	409	LMG	C19-C18	-3.63	1.33	1.51
25	c	504	CLA	CHD-C4C	3.63	1.47	1.39
28	c	519	LMG	C40-C39	-3.63	1.33	1.51
25	b	605	CLA	CHD-C1D	3.63	1.45	1.38
25	C	510	CLA	CHD-C4C	3.63	1.47	1.39
28	C	519	LMG	C40-C39	-3.63	1.33	1.51
34	C	516	DGD	CDA-CCA	-3.63	1.33	1.51
25	a	405	CLA	C3C-C2C	3.63	1.44	1.36
25	C	509	CLA	C1D-ND	-3.62	1.33	1.37
25	b	613	CLA	C1D-ND	-3.62	1.33	1.37
25	B	601	CLA	CHD-C4C	3.62	1.47	1.39
34	H	103	DGD	CDA-CCA	-3.62	1.33	1.51
34	h	103	DGD	CDA-CCA	-3.62	1.33	1.51
25	c	505	CLA	C1D-ND	-3.62	1.33	1.37
34	c	516	DGD	CDA-CCA	-3.62	1.33	1.51
25	c	507	CLA	CHD-C4C	3.61	1.47	1.39
25	A	405	CLA	C3C-C2C	3.61	1.44	1.36
25	b	601	CLA	CHD-C4C	3.61	1.47	1.39
25	B	615	CLA	CHD-C4C	3.61	1.47	1.39
25	b	615	CLA	CHD-C4C	3.61	1.47	1.39
25	A	406	CLA	CHD-C4C	3.61	1.47	1.39
25	C	505	CLA	C1D-ND	-3.61	1.33	1.37
25	b	606	CLA	C1D-ND	-3.61	1.33	1.37
25	C	507	CLA	CHD-C4C	3.60	1.47	1.39
25	B	606	CLA	C1D-ND	-3.60	1.33	1.37
34	C	517	DGD	O2G-C1B	3.60	1.44	1.34
25	C	508	CLA	CHD-C4C	3.60	1.47	1.39
25	a	406	CLA	CHD-C4C	3.59	1.47	1.39
25	C	503	CLA	CHD-C4C	3.59	1.47	1.39
33	B	628	LHG	O7-C7	3.59	1.44	1.34
25	c	507	CLA	C1D-ND	-3.59	1.33	1.37
25	c	509	CLA	C1D-ND	-3.59	1.33	1.37
25	c	508	CLA	CHD-C4C	3.59	1.47	1.39
25	b	616	CLA	C1D-ND	-3.59	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	h	103	DGD	O2G-C1B	3.59	1.44	1.34
34	c	517	DGD	O2G-C1B	3.58	1.44	1.34
25	c	503	CLA	CHD-C4C	3.58	1.47	1.39
25	B	616	CLA	C1D-ND	-3.58	1.33	1.37
33	b	628	LHG	O7-C7	3.58	1.44	1.34
25	B	611	CLA	CHD-C4C	3.58	1.47	1.39
25	B	613	CLA	C1D-ND	-3.58	1.33	1.37
25	b	609	CLA	C1D-ND	-3.57	1.33	1.37
25	b	609	CLA	CHD-C4C	3.57	1.47	1.39
25	b	614	CLA	C1D-ND	-3.57	1.33	1.37
25	B	609	CLA	CHD-C4C	3.57	1.47	1.39
25	C	511	CLA	OBD-CAD	3.57	1.28	1.22
25	b	611	CLA	CHD-C4C	3.56	1.47	1.39
27	C	515	BCR	C11-C12	-3.56	1.25	1.34
25	C	507	CLA	C1D-ND	-3.56	1.33	1.37
25	c	513	CLA	CHD-C4C	3.56	1.47	1.39
34	H	103	DGD	O2G-C1B	3.56	1.44	1.34
25	B	614	CLA	C1D-ND	-3.55	1.33	1.37
25	C	514	CLA	C1D-ND	-3.55	1.33	1.37
25	c	511	CLA	OBD-CAD	3.55	1.28	1.22
25	C	513	CLA	CHD-C4C	3.55	1.47	1.39
25	B	601	CLA	C1D-ND	-3.54	1.33	1.37
25	b	604	CLA	C1C-NC	-3.54	1.32	1.37
25	B	606	CLA	CHD-C4C	3.54	1.47	1.39
25	b	606	CLA	CHD-C4C	3.54	1.47	1.39
27	c	515	BCR	C11-C12	-3.54	1.25	1.34
25	b	601	CLA	C1D-ND	-3.53	1.33	1.37
25	C	504	CLA	C1D-ND	-3.53	1.33	1.37
25	c	504	CLA	C1D-ND	-3.53	1.33	1.37
25	B	603	CLA	OBD-CAD	3.53	1.28	1.22
25	C	514	CLA	OBD-CAD	3.52	1.28	1.22
25	c	514	CLA	C1D-ND	-3.51	1.33	1.37
25	c	514	CLA	OBD-CAD	3.51	1.28	1.22
25	b	607	CLA	CHD-C4C	3.51	1.47	1.39
27	A	409	BCR	C11-C12	-3.51	1.25	1.34
25	A	406	CLA	OBD-CAD	3.51	1.28	1.22
25	a	406	CLA	OBD-CAD	3.51	1.28	1.22
25	b	603	CLA	OBD-CAD	3.51	1.28	1.22
25	B	604	CLA	C1C-NC	-3.50	1.32	1.37
27	B	618	BCR	C11-C12	-3.50	1.25	1.34
27	b	618	BCR	C11-C12	-3.50	1.25	1.34
25	B	607	CLA	CHD-C4C	3.50	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	OBD-CAD	3.49	1.28	1.22
27	a	409	BCR	C11-C12	-3.49	1.25	1.34
25	d	404	CLA	C1D-ND	-3.48	1.33	1.37
25	b	610	CLA	OBD-CAD	3.47	1.28	1.22
27	B	617	BCR	C11-C12	-3.47	1.25	1.34
25	C	503	CLA	OBD-CAD	3.47	1.28	1.22
25	c	503	CLA	OBD-CAD	3.47	1.28	1.22
25	b	604	CLA	CHD-C4C	3.46	1.47	1.39
25	b	604	CLA	C1D-ND	-3.46	1.33	1.37
25	B	613	CLA	CHD-C4C	3.46	1.47	1.39
25	D	404	CLA	C1D-ND	-3.46	1.33	1.37
27	b	617	BCR	C11-C12	-3.46	1.25	1.34
25	b	611	CLA	C1C-NC	-3.46	1.32	1.37
25	B	604	CLA	C1D-ND	-3.45	1.33	1.37
25	A	405	CLA	C1C-NC	-3.45	1.32	1.37
25	b	610	CLA	CHD-C4C	3.45	1.47	1.39
25	c	507	CLA	OBD-CAD	3.45	1.28	1.22
25	b	613	CLA	CHD-C4C	3.45	1.47	1.39
25	B	610	CLA	CHD-C4C	3.45	1.47	1.39
25	B	610	CLA	OBD-CAD	3.44	1.28	1.22
25	B	612	CLA	CHD-C1D	3.44	1.45	1.38
25	b	612	CLA	CHD-C1D	3.44	1.45	1.38
25	B	604	CLA	CHD-C4C	3.43	1.47	1.39
25	B	611	CLA	C1C-NC	-3.43	1.32	1.37
25	c	512	CLA	CHD-C4C	3.43	1.47	1.39
25	a	405	CLA	C1C-NC	-3.43	1.32	1.37
35	V	201	HEM	C3C-CAC	3.42	1.55	1.47
35	v	201	HEM	C3C-CAC	3.41	1.55	1.47
25	D	403	CLA	CHD-C1D	3.41	1.45	1.38
25	C	512	CLA	CHD-C4C	3.41	1.47	1.39
25	B	602	CLA	C1C-NC	-3.40	1.32	1.37
27	Z	101	BCR	C11-C12	-3.40	1.25	1.34
25	b	609	CLA	OBD-CAD	3.40	1.28	1.22
25	d	403	CLA	CHD-C1D	3.40	1.45	1.38
27	z	101	BCR	C11-C12	-3.39	1.25	1.34
25	a	406	CLA	C1D-ND	-3.39	1.33	1.37
25	b	616	CLA	CHD-C4C	3.39	1.46	1.39
25	A	406	CLA	C1D-ND	-3.39	1.33	1.37
25	B	611	CLA	MG-ND	-3.38	1.99	2.05
25	B	616	CLA	CHD-C4C	3.37	1.46	1.39
25	c	508	CLA	OBD-CAD	3.36	1.28	1.22
25	b	602	CLA	C1C-NC	-3.36	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	C1C-NC	-3.36	1.32	1.37
25	B	609	CLA	OBD-CAD	3.36	1.28	1.22
25	C	508	CLA	OBD-CAD	3.36	1.28	1.22
27	b	619	BCR	C11-C12	-3.36	1.25	1.34
25	B	605	CLA	CHD-C4C	3.35	1.46	1.39
25	b	605	CLA	CHD-C4C	3.35	1.46	1.39
25	C	512	CLA	C1C-NC	-3.35	1.32	1.37
27	F	101	BCR	C11-C12	-3.35	1.25	1.34
25	C	508	CLA	C1D-ND	-3.35	1.33	1.37
27	f	101	BCR	C11-C12	-3.35	1.25	1.34
27	B	619	BCR	C11-C12	-3.34	1.26	1.34
25	b	611	CLA	MG-ND	-3.34	1.99	2.05
25	d	403	CLA	C1C-NC	-3.34	1.32	1.37
25	c	508	CLA	MG-ND	-3.34	1.99	2.05
25	c	502	CLA	C3D-C2D	3.33	1.48	1.39
25	b	614	CLA	OBD-CAD	3.33	1.28	1.22
25	B	608	CLA	C1D-ND	-3.32	1.33	1.37
25	B	601	CLA	OBD-CAD	3.32	1.28	1.22
25	B	614	CLA	OBD-CAD	3.32	1.28	1.22
25	c	508	CLA	C1D-ND	-3.31	1.33	1.37
25	b	601	CLA	OBD-CAD	3.31	1.28	1.22
25	C	508	CLA	MG-ND	-3.30	1.99	2.05
25	D	403	CLA	C1C-NC	-3.30	1.32	1.37
25	C	502	CLA	C3D-C2D	3.30	1.48	1.39
25	a	408	CLA	OBD-CAD	3.29	1.28	1.22
25	b	609	CLA	MG-ND	-3.29	1.99	2.05
25	B	609	CLA	MG-ND	-3.28	1.99	2.05
25	A	408	CLA	OBD-CAD	3.28	1.28	1.22
27	k	103	BCR	C11-C12	-3.28	1.26	1.34
25	d	401	CLA	C1C-NC	-3.28	1.32	1.37
27	K	102	BCR	C11-C12	-3.28	1.26	1.34
25	B	615	CLA	OBD-CAD	3.28	1.28	1.22
27	k	102	BCR	C11-C12	-3.27	1.26	1.34
25	c	513	CLA	MG-ND	-3.27	1.99	2.05
27	K	103	BCR	C11-C12	-3.27	1.26	1.34
25	b	612	CLA	CHD-C4C	3.26	1.46	1.39
25	B	612	CLA	CHD-C4C	3.26	1.46	1.39
25	c	513	CLA	OBD-CAD	3.26	1.28	1.22
25	D	401	CLA	C1C-NC	-3.26	1.32	1.37
25	C	512	CLA	OBD-CAD	3.26	1.28	1.22
25	b	615	CLA	OBD-CAD	3.26	1.28	1.22
25	C	513	CLA	OBD-CAD	3.25	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	C1D-ND	-3.25	1.33	1.37
25	d	401	CLA	C1D-ND	-3.25	1.33	1.37
25	b	612	CLA	MG-ND	-3.25	1.99	2.05
25	C	513	CLA	MG-ND	-3.25	1.99	2.05
25	b	606	CLA	OBD-CAD	3.24	1.28	1.22
25	B	612	CLA	MG-ND	-3.23	1.99	2.05
25	c	512	CLA	OBD-CAD	3.23	1.28	1.22
25	D	401	CLA	C1D-ND	-3.22	1.33	1.37
25	a	405	CLA	CHD-C4C	3.22	1.46	1.39
25	A	405	CLA	CHD-C4C	3.22	1.46	1.39
25	c	509	CLA	C1C-NC	-3.22	1.32	1.37
25	c	506	CLA	MG-ND	-3.22	1.99	2.05
25	c	502	CLA	C1D-ND	-3.22	1.33	1.37
25	B	606	CLA	OBD-CAD	3.22	1.28	1.22
25	C	506	CLA	MG-ND	-3.22	1.99	2.05
25	b	612	CLA	C1C-NC	-3.21	1.32	1.37
25	b	608	CLA	OBD-CAD	3.21	1.28	1.22
25	b	606	CLA	C1C-NC	-3.21	1.32	1.37
25	b	613	CLA	MG-ND	-3.20	1.99	2.05
25	C	509	CLA	C1C-NC	-3.20	1.32	1.37
25	B	613	CLA	MG-ND	-3.19	1.99	2.05
25	c	510	CLA	OBD-CAD	3.19	1.28	1.22
25	B	608	CLA	OBD-CAD	3.19	1.28	1.22
25	C	502	CLA	C1D-ND	-3.19	1.33	1.37
25	C	506	CLA	OBD-CAD	3.19	1.28	1.22
25	c	509	CLA	MG-ND	-3.18	1.99	2.05
25	C	513	CLA	C3D-C2D	3.18	1.47	1.39
25	b	609	CLA	C1C-NC	-3.18	1.32	1.37
25	d	403	CLA	CHD-C4C	3.18	1.46	1.39
25	D	403	CLA	CHD-C4C	3.18	1.46	1.39
25	C	510	CLA	OBD-CAD	3.18	1.28	1.22
25	D	401	CLA	OBD-CAD	3.18	1.28	1.22
25	C	509	CLA	OBD-CAD	3.17	1.28	1.22
25	c	505	CLA	OBD-CAD	3.17	1.27	1.22
25	B	612	CLA	C1C-NC	-3.17	1.32	1.37
25	c	506	CLA	OBD-CAD	3.17	1.27	1.22
25	c	513	CLA	C3D-C2D	3.16	1.47	1.39
25	B	606	CLA	C1C-NC	-3.16	1.32	1.37
25	a	408	CLA	C1C-NC	-3.16	1.32	1.37
25	C	509	CLA	MG-ND	-3.16	1.99	2.05
25	D	404	CLA	OBD-CAD	3.16	1.27	1.22
25	C	505	CLA	OBD-CAD	3.16	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	MG-ND	-3.16	1.99	2.05
25	d	401	CLA	OBD-CAD	3.16	1.27	1.22
25	d	404	CLA	OBD-CAD	3.15	1.27	1.22
25	C	507	CLA	MG-ND	-3.15	1.99	2.05
25	a	408	CLA	C3D-C2D	3.14	1.47	1.39
25	c	503	CLA	C3D-C2D	3.14	1.47	1.39
25	B	609	CLA	C1C-NC	-3.13	1.33	1.37
25	B	604	CLA	OBD-CAD	3.13	1.27	1.22
25	A	408	CLA	C1C-NC	-3.13	1.33	1.37
25	b	604	CLA	OBD-CAD	3.12	1.27	1.22
25	A	408	CLA	C3D-C2D	3.12	1.47	1.39
25	c	509	CLA	OBD-CAD	3.12	1.27	1.22
25	C	503	CLA	C3D-C2D	3.12	1.47	1.39
30	F	102	SQD	O47-C7	3.11	1.43	1.34
25	c	508	CLA	C1C-NC	-3.09	1.33	1.37
30	f	102	SQD	O47-C7	3.09	1.43	1.34
30	A	412	SQD	O48-C23	3.09	1.42	1.33
30	a	412	SQD	O48-C23	3.09	1.42	1.33
29	d	405	PL9	C6-C1	-3.09	1.43	1.48
29	D	405	PL9	C6-C1	-3.08	1.43	1.48
30	f	102	SQD	O48-C23	3.08	1.42	1.33
25	c	511	CLA	MG-ND	-3.08	1.99	2.05
35	E	104	HEM	C3C-CAC	3.08	1.54	1.47
30	F	102	SQD	O48-C23	3.07	1.42	1.33
25	C	512	CLA	C3D-C2D	3.07	1.47	1.39
25	b	613	CLA	C1C-NC	-3.07	1.33	1.37
25	C	511	CLA	MG-ND	-3.07	1.99	2.05
25	B	613	CLA	C1C-NC	-3.07	1.33	1.37
35	e	104	HEM	C3C-CAC	3.07	1.54	1.47
25	d	401	CLA	C3D-C2D	3.06	1.47	1.39
25	C	508	CLA	C1C-NC	-3.06	1.33	1.37
25	c	512	CLA	C3D-C2D	3.06	1.47	1.39
25	D	401	CLA	C3D-C2D	3.05	1.47	1.39
30	k	101	SQD	O48-C23	3.04	1.42	1.33
25	C	511	CLA	C1C-NC	-3.03	1.33	1.37
25	b	605	CLA	MG-ND	-3.03	1.99	2.05
25	B	605	CLA	C1C-NC	-3.03	1.33	1.37
25	b	605	CLA	C1C-NC	-3.02	1.33	1.37
25	c	511	CLA	C1C-NC	-3.02	1.33	1.37
25	C	511	CLA	C1D-ND	-3.02	1.33	1.37
25	D	403	CLA	MG-ND	-3.02	1.99	2.05
25	B	604	CLA	MG-NC	3.02	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	C1D-ND	-3.01	1.33	1.37
30	K	101	SQD	O48-C23	3.01	1.42	1.33
25	d	403	CLA	MG-ND	-3.01	1.99	2.05
30	h	102	SQD	O48-C23	3.01	1.42	1.33
25	b	604	CLA	MG-NC	3.01	2.13	2.06
25	B	605	CLA	MG-ND	-3.01	1.99	2.05
25	B	610	CLA	C3D-C2D	3.00	1.47	1.39
30	H	102	SQD	O48-C23	3.00	1.42	1.33
25	b	615	CLA	C1D-ND	-3.00	1.33	1.37
25	b	613	CLA	OBD-CAD	3.00	1.27	1.22
25	B	616	CLA	OBD-CAD	2.99	1.27	1.22
25	b	610	CLA	C3D-C2D	2.99	1.47	1.39
25	B	613	CLA	OBD-CAD	2.99	1.27	1.22
35	e	104	HEM	C3C-C4C	2.99	1.45	1.41
30	B	620	SQD	O48-C23	2.99	1.42	1.33
30	b	620	SQD	O48-C23	2.99	1.42	1.33
25	c	504	CLA	MG-NC	2.99	2.13	2.06
25	B	606	CLA	C3D-C2D	2.98	1.47	1.39
25	b	614	CLA	MG-NC	2.98	2.13	2.06
25	c	511	CLA	C1D-ND	-2.98	1.33	1.37
25	b	616	CLA	OBD-CAD	2.98	1.27	1.22
25	b	606	CLA	C3D-C2D	2.97	1.47	1.39
25	c	504	CLA	OBD-CAD	2.97	1.27	1.22
25	B	614	CLA	MG-NC	2.97	2.13	2.06
25	C	504	CLA	MG-NC	2.97	2.13	2.06
25	C	510	CLA	MG-ND	-2.97	1.99	2.05
25	C	504	CLA	OBD-CAD	2.97	1.27	1.22
25	c	510	CLA	MG-ND	-2.97	1.99	2.05
25	B	607	CLA	C1D-ND	-2.97	1.34	1.37
25	b	602	CLA	C3D-C2D	2.96	1.47	1.39
25	b	607	CLA	C3D-C2D	2.96	1.47	1.39
25	B	602	CLA	C3D-C2D	2.96	1.47	1.39
35	E	104	HEM	C3C-C4C	2.96	1.45	1.41
25	C	511	CLA	MG-NC	2.95	2.13	2.06
25	C	510	CLA	C1C-NC	-2.95	1.33	1.37
25	c	510	CLA	C1C-NC	-2.95	1.33	1.37
25	B	607	CLA	C3D-C2D	2.95	1.47	1.39
29	A	411	PL9	C3-C4	-2.94	1.45	1.49
25	b	607	CLA	MG-ND	-2.94	2.00	2.05
25	C	503	CLA	MG-ND	-2.93	2.00	2.05
25	B	607	CLA	MG-ND	-2.93	2.00	2.05
25	B	615	CLA	C3D-C2D	2.92	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	MG-NC	2.92	2.13	2.06
25	b	609	CLA	C3D-C2D	2.92	1.47	1.39
25	A	406	CLA	C3D-C2D	2.92	1.47	1.39
25	B	607	CLA	MG-NC	2.92	2.13	2.06
25	c	503	CLA	MG-ND	-2.92	2.00	2.05
25	b	607	CLA	C1D-ND	-2.92	1.34	1.37
29	a	411	PL9	C3-C4	-2.91	1.45	1.49
25	a	406	CLA	C3D-C2D	2.91	1.46	1.39
25	C	510	CLA	MG-NC	2.91	2.13	2.06
25	c	508	CLA	C3D-C2D	2.91	1.46	1.39
25	d	404	CLA	C1C-NC	-2.91	1.33	1.37
31	m	101	LMT	O3'-C3'	-2.91	1.35	1.43
25	b	615	CLA	C3D-C2D	2.91	1.46	1.39
30	B	620	SQD	O47-C7	2.90	1.42	1.34
25	C	511	CLA	C3D-C2D	2.90	1.46	1.39
25	c	510	CLA	MG-NC	2.90	2.13	2.06
25	c	502	CLA	MG-NC	2.90	2.13	2.06
25	c	511	CLA	C3D-C2D	2.90	1.46	1.39
30	A	412	SQD	O47-C7	2.90	1.42	1.34
31	t	701	LMT	O3'-C3'	-2.90	1.35	1.43
25	C	504	CLA	C1C-NC	-2.90	1.33	1.37
25	b	607	CLA	MG-NC	2.90	2.13	2.06
30	a	412	SQD	O47-C7	2.90	1.42	1.34
25	C	508	CLA	C3D-C2D	2.90	1.46	1.39
25	B	609	CLA	C3D-C2D	2.89	1.46	1.39
30	b	620	SQD	O47-C7	2.89	1.42	1.34
31	M	102	LMT	O3'-C3'	-2.89	1.35	1.43
25	C	502	CLA	MG-NC	2.89	2.13	2.06
25	D	404	CLA	C1C-NC	-2.89	1.33	1.37
25	B	607	CLA	C1C-NC	-2.89	1.33	1.37
25	C	513	CLA	C1C-NC	-2.88	1.33	1.37
25	b	613	CLA	MG-NC	2.88	2.13	2.06
25	b	607	CLA	C1C-NC	-2.88	1.33	1.37
25	b	604	CLA	MG-ND	-2.87	2.00	2.05
25	c	513	CLA	C1C-NC	-2.87	1.33	1.37
25	C	514	CLA	C1C-NC	-2.87	1.33	1.37
25	c	504	CLA	C1C-NC	-2.87	1.33	1.37
25	C	507	CLA	C3D-C2D	2.87	1.46	1.39
25	C	512	CLA	MG-ND	-2.87	2.00	2.05
25	c	507	CLA	C3D-C2D	2.86	1.46	1.39
31	d	410	LMT	O3'-C3'	-2.86	1.35	1.43
25	c	514	CLA	C1C-NC	-2.86	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C4D-CHA	2.86	1.48	1.38
31	T	701	LMT	O3'-C3'	-2.86	1.35	1.43
26	D	402	PHO	CAC-C3C	-2.86	1.47	1.52
25	D	404	CLA	C3D-C2D	2.86	1.46	1.39
25	c	512	CLA	MG-ND	-2.86	2.00	2.05
25	c	513	CLA	C4D-CHA	2.85	1.48	1.38
35	e	104	HEM	CAB-C3B	2.85	1.55	1.47
25	B	613	CLA	MG-NC	2.85	2.13	2.06
31	D	410	LMT	O3'-C3'	-2.85	1.35	1.43
25	B	605	CLA	C3D-C2D	2.85	1.46	1.39
35	E	104	HEM	CAB-C3B	2.85	1.55	1.47
25	B	604	CLA	MG-ND	-2.85	2.00	2.05
25	d	404	CLA	C3D-C2D	2.85	1.46	1.39
25	b	605	CLA	C3D-C2D	2.85	1.46	1.39
25	b	616	CLA	C3D-C2D	2.84	1.46	1.39
25	B	610	CLA	MG-ND	-2.84	2.00	2.05
25	C	507	CLA	C1C-NC	-2.84	1.33	1.37
31	E	103	LMT	O3'-C3'	-2.84	1.35	1.43
31	e	103	LMT	O3'-C3'	-2.84	1.35	1.43
25	C	506	CLA	MG-NC	2.84	2.13	2.06
25	B	616	CLA	C3D-C2D	2.84	1.46	1.39
25	b	608	CLA	MG-ND	-2.84	2.00	2.05
25	b	610	CLA	MG-ND	-2.84	2.00	2.05
26	d	402	PHO	CAC-C3C	-2.84	1.47	1.52
25	C	502	CLA	C4D-CHA	2.83	1.48	1.38
25	C	504	CLA	MG-ND	-2.83	2.00	2.05
30	C	501	SQD	O48-C23	2.83	1.41	1.33
30	c	501	SQD	O48-C23	2.83	1.41	1.33
35	v	201	HEM	CAB-C3B	2.83	1.54	1.47
25	C	514	CLA	C3D-C2D	2.83	1.46	1.39
30	h	102	SQD	O47-C7	2.82	1.42	1.34
25	b	616	CLA	MG-ND	-2.82	2.00	2.05
25	c	504	CLA	MG-ND	-2.82	2.00	2.05
25	B	615	CLA	C1C-NC	-2.82	1.33	1.37
25	C	510	CLA	C3D-C2D	2.82	1.46	1.39
25	B	614	CLA	C3D-C2D	2.82	1.46	1.39
25	c	502	CLA	C4D-CHA	2.82	1.48	1.38
25	c	506	CLA	MG-NC	2.82	2.13	2.06
25	b	614	CLA	C3D-C2D	2.82	1.46	1.39
25	b	608	CLA	C1C-NC	-2.82	1.33	1.37
25	c	509	CLA	C3D-C2D	2.82	1.46	1.39
25	c	510	CLA	C3D-C2D	2.82	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	C4D-CHA	2.82	1.48	1.38
25	B	603	CLA	C3D-C2D	2.81	1.46	1.39
30	H	102	SQD	O47-C7	2.81	1.42	1.34
25	B	616	CLA	MG-ND	-2.81	2.00	2.05
25	b	603	CLA	C3D-C2D	2.81	1.46	1.39
25	C	506	CLA	C1C-NC	-2.81	1.33	1.37
25	b	612	CLA	OBD-CAD	2.81	1.27	1.22
25	b	604	CLA	C4D-CHA	2.81	1.48	1.38
25	C	509	CLA	C3D-C2D	2.81	1.46	1.39
25	c	507	CLA	C1C-NC	-2.81	1.33	1.37
35	V	201	HEM	CAB-C3B	2.81	1.54	1.47
25	c	514	CLA	C3D-C2D	2.81	1.46	1.39
25	B	608	CLA	C1C-NC	-2.80	1.33	1.37
25	b	615	CLA	C1C-NC	-2.80	1.33	1.37
25	b	615	CLA	MG-NC	2.80	2.12	2.06
26	a	407	PHO	CAC-C3C	-2.80	1.47	1.52
25	b	608	CLA	C3D-C2D	2.80	1.46	1.39
25	B	605	CLA	OBD-CAD	2.80	1.27	1.22
25	B	602	CLA	MG-ND	-2.79	2.00	2.05
25	A	405	CLA	OBD-CAD	2.79	1.27	1.22
25	B	612	CLA	OBD-CAD	2.79	1.27	1.22
25	a	406	CLA	C4D-CHA	2.79	1.48	1.38
25	B	608	CLA	MG-ND	-2.79	2.00	2.05
25	c	502	CLA	MG-ND	-2.79	2.00	2.05
30	a	413	SQD	O48-C23	2.79	1.41	1.33
29	D	405	PL9	C52-C5	-2.79	1.45	1.50
25	A	406	CLA	C4D-CHA	2.79	1.48	1.38
25	c	506	CLA	C1C-NC	-2.79	1.33	1.37
25	C	502	CLA	MG-ND	-2.79	2.00	2.05
25	B	615	CLA	MG-NC	2.78	2.12	2.06
25	B	601	CLA	C3D-C2D	2.78	1.46	1.39
25	b	605	CLA	OBD-CAD	2.78	1.27	1.22
25	b	601	CLA	C3D-C2D	2.78	1.46	1.39
30	A	413	SQD	O48-C23	2.78	1.41	1.33
25	a	405	CLA	OBD-CAD	2.78	1.27	1.22
25	B	608	CLA	C3D-C2D	2.78	1.46	1.39
30	a	413	SQD	O47-C7	2.77	1.42	1.34
25	b	602	CLA	MG-ND	-2.77	2.00	2.05
29	d	405	PL9	C52-C5	-2.77	1.45	1.50
25	b	606	CLA	MG-ND	-2.77	2.00	2.05
25	B	607	CLA	OBD-CAD	2.77	1.27	1.22
25	B	606	CLA	MG-ND	-2.77	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	407	PHO	CAC-C3C	-2.77	1.47	1.52
25	D	401	CLA	C4D-CHA	2.77	1.47	1.38
25	C	505	CLA	C3D-C2D	2.77	1.46	1.39
30	A	413	SQD	O47-C7	2.76	1.42	1.34
25	c	505	CLA	C3D-C2D	2.76	1.46	1.39
25	d	401	CLA	C4D-CHA	2.76	1.47	1.38
37	x	102	RRX	C8-C9	-2.76	1.40	1.46
37	X	102	RRX	C8-C9	-2.76	1.40	1.46
25	B	603	CLA	MG-ND	-2.76	2.00	2.05
25	b	607	CLA	OBD-CAD	2.76	1.27	1.22
25	c	514	CLA	MG-ND	-2.76	2.00	2.05
25	C	505	CLA	MG-NC	2.76	2.12	2.06
37	X	102	RRX	C23-C22	-2.75	1.40	1.46
25	c	503	CLA	MG-NC	2.75	2.12	2.06
25	B	608	CLA	MG-NC	2.75	2.12	2.06
25	c	505	CLA	MG-NC	2.75	2.12	2.06
37	x	102	RRX	C23-C22	-2.75	1.40	1.46
25	a	406	CLA	C1C-NC	-2.75	1.33	1.37
25	b	603	CLA	MG-ND	-2.74	2.00	2.05
25	C	514	CLA	MG-ND	-2.74	2.00	2.05
25	b	607	CLA	C4B-CHC	2.73	1.48	1.41
25	A	408	CLA	MG-ND	-2.73	2.00	2.05
30	k	101	SQD	O47-C7	2.73	1.42	1.34
25	C	503	CLA	MG-NC	2.73	2.12	2.06
25	C	503	CLA	C1C-NC	-2.73	1.33	1.37
25	c	503	CLA	C1C-NC	-2.73	1.33	1.37
25	b	608	CLA	MG-NC	2.73	2.12	2.06
25	c	509	CLA	MG-NC	2.72	2.12	2.06
25	C	509	CLA	MG-NC	2.72	2.12	2.06
30	K	101	SQD	O47-C7	2.72	1.42	1.34
25	a	408	CLA	MG-ND	-2.72	2.00	2.05
25	A	406	CLA	C1C-NC	-2.72	1.33	1.37
25	C	507	CLA	MG-NC	2.72	2.12	2.06
25	B	615	CLA	MG-ND	-2.72	2.00	2.05
25	B	613	CLA	C3D-C2D	2.72	1.46	1.39
25	b	613	CLA	C3D-C2D	2.72	1.46	1.39
25	b	603	CLA	MG-NC	2.72	2.12	2.06
25	B	607	CLA	C4B-CHC	2.71	1.48	1.41
25	C	512	CLA	MG-NC	2.71	2.12	2.06
25	b	610	CLA	MG-NC	2.71	2.12	2.06
25	b	615	CLA	MG-ND	-2.71	2.00	2.05
25	C	513	CLA	MG-NC	2.71	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	MG-NC	2.70	2.12	2.06
25	D	403	CLA	OBD-CAD	2.70	1.27	1.22
25	B	610	CLA	MG-NC	2.70	2.12	2.06
25	b	601	CLA	MG-ND	-2.70	2.00	2.05
25	c	513	CLA	MG-NC	2.70	2.12	2.06
25	C	510	CLA	C4D-CHA	2.70	1.47	1.38
25	b	609	CLA	MG-NC	2.70	2.12	2.06
25	c	510	CLA	C4D-CHA	2.70	1.47	1.38
25	B	611	CLA	C3D-C2D	2.70	1.46	1.39
31	I	102	LMT	O3'-C3'	-2.69	1.36	1.43
25	c	507	CLA	MG-NC	2.69	2.12	2.06
25	b	613	CLA	C4D-CHA	2.69	1.47	1.38
25	B	601	CLA	MG-ND	-2.69	2.00	2.05
25	b	611	CLA	C3D-C2D	2.68	1.46	1.39
25	d	403	CLA	OBD-CAD	2.68	1.27	1.22
25	c	512	CLA	MG-NC	2.68	2.12	2.06
25	B	613	CLA	C4D-CHA	2.68	1.47	1.38
25	A	405	CLA	C3D-C2D	2.68	1.46	1.39
25	a	405	CLA	C3D-C2D	2.68	1.46	1.39
30	C	501	SQD	O47-C7	2.67	1.41	1.34
25	B	609	CLA	MG-NC	2.67	2.12	2.06
25	C	514	CLA	C4D-CHA	2.67	1.47	1.38
25	b	603	CLA	C4D-CHA	2.66	1.47	1.38
25	B	604	CLA	C3D-C2D	2.66	1.46	1.39
25	B	603	CLA	C4D-CHA	2.66	1.47	1.38
25	C	503	CLA	C4D-CHA	2.66	1.47	1.38
25	C	504	CLA	C3D-C2D	2.66	1.46	1.39
25	C	514	CLA	MG-NC	2.66	2.12	2.06
30	c	501	SQD	O47-C7	2.66	1.41	1.34
31	c	522	LMT	O3'-C3'	-2.66	1.36	1.43
31	i	102	LMT	O3'-C3'	-2.66	1.36	1.43
25	c	508	CLA	C4D-CHA	2.66	1.47	1.38
25	d	403	CLA	MG-NC	2.66	2.12	2.06
31	i	101	LMT	O3'-C3'	-2.66	1.36	1.43
25	C	507	CLA	C4D-CHA	2.66	1.47	1.38
25	b	609	CLA	C4D-CHA	2.66	1.47	1.38
25	b	611	CLA	MG-NC	2.65	2.12	2.06
25	b	612	CLA	MG-NC	2.65	2.12	2.06
31	I	101	LMT	O3'-C3'	-2.65	1.36	1.43
25	B	611	CLA	MG-NC	2.65	2.12	2.06
25	c	514	CLA	C4D-CHA	2.65	1.47	1.38
25	c	514	CLA	MG-NC	2.65	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	C4D-CHA	2.65	1.47	1.38
25	c	507	CLA	C4D-CHA	2.65	1.47	1.38
31	C	522	LMT	O3'-C3'	-2.65	1.36	1.43
25	c	505	CLA	MG-ND	-2.65	2.00	2.05
25	B	609	CLA	C4D-CHA	2.65	1.47	1.38
25	C	508	CLA	C4D-CHA	2.65	1.47	1.38
25	B	606	CLA	C4D-CHA	2.65	1.47	1.38
25	b	606	CLA	C4D-CHA	2.65	1.47	1.38
25	c	504	CLA	C3D-C2D	2.64	1.46	1.39
31	a	415	LMT	O3'-C3'	-2.64	1.36	1.43
25	B	603	CLA	C1C-NC	-2.64	1.33	1.37
25	B	612	CLA	MG-NC	2.64	2.12	2.06
25	b	601	CLA	C1C-NC	-2.64	1.33	1.37
25	b	605	CLA	MG-NC	2.64	2.12	2.06
25	C	504	CLA	C4D-CHA	2.64	1.47	1.38
25	B	605	CLA	MG-NC	2.64	2.12	2.06
25	b	604	CLA	C3D-C2D	2.63	1.46	1.39
25	C	505	CLA	MG-ND	-2.63	2.00	2.05
31	A	415	LMT	O3'-C3'	-2.63	1.36	1.43
25	D	403	CLA	MG-NC	2.63	2.12	2.06
31	A	416	LMT	O3'-C3'	-2.63	1.36	1.43
25	B	614	CLA	C4B-CHC	2.62	1.48	1.41
25	B	601	CLA	C1C-NC	-2.62	1.33	1.37
25	c	504	CLA	C4D-CHA	2.62	1.47	1.38
25	c	512	CLA	C4D-CHA	2.62	1.47	1.38
25	A	408	CLA	MG-NC	2.62	2.12	2.06
25	b	614	CLA	C4B-CHC	2.62	1.48	1.41
25	D	403	CLA	C3D-C2D	2.62	1.46	1.39
25	c	511	CLA	C4D-CHA	2.62	1.47	1.38
25	C	512	CLA	C4D-CHA	2.62	1.47	1.38
25	B	601	CLA	C4D-CHA	2.61	1.47	1.38
25	b	601	CLA	C4D-CHA	2.61	1.47	1.38
31	D	412	LMT	O3'-C3'	-2.61	1.36	1.43
31	X	101	LMT	O3'-C3'	-2.61	1.36	1.43
31	a	416	LMT	O3'-C3'	-2.61	1.36	1.43
31	x	101	LMT	O3'-C3'	-2.61	1.36	1.43
25	a	408	CLA	MG-NC	2.60	2.12	2.06
25	d	403	CLA	C3D-C2D	2.60	1.46	1.39
31	d	412	LMT	O3'-C3'	-2.60	1.36	1.43
25	b	603	CLA	C1C-NC	-2.60	1.33	1.37
25	D	403	CLA	C1B-CHB	2.60	1.48	1.41
25	d	403	CLA	C1B-CHB	2.60	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	J	101	LMT	O3'-C3'	-2.59	1.36	1.43
25	c	505	CLA	C1C-NC	-2.59	1.33	1.37
25	C	511	CLA	C4D-CHA	2.59	1.47	1.38
25	C	506	CLA	C4D-CHA	2.58	1.47	1.38
25	b	608	CLA	C4D-CHA	2.58	1.47	1.38
25	B	608	CLA	C4D-CHA	2.58	1.47	1.38
25	c	505	CLA	C4D-CHA	2.58	1.47	1.38
25	b	606	CLA	MG-NC	2.57	2.12	2.06
31	j	101	LMT	O3'-C3'	-2.57	1.36	1.43
25	c	502	CLA	C4B-CHC	2.57	1.48	1.41
25	C	505	CLA	C4D-CHA	2.57	1.47	1.38
31	c	524	LMT	O3'-C3'	-2.57	1.36	1.43
25	C	505	CLA	C1C-NC	-2.57	1.33	1.37
25	b	616	CLA	C4D-CHA	2.57	1.47	1.38
31	C	524	LMT	O3'-C3'	-2.57	1.36	1.43
31	B	624	LMT	O3'-C3'	-2.56	1.36	1.43
25	B	616	CLA	C4D-CHA	2.56	1.47	1.38
25	c	506	CLA	C4D-CHA	2.56	1.47	1.38
25	b	610	CLA	C4D-CHA	2.56	1.47	1.38
31	B	627	LMT	O3'-C3'	-2.56	1.36	1.43
31	X	103	LMT	O3'-C3'	-2.56	1.36	1.43
25	C	508	CLA	MG-NC	2.56	2.12	2.06
31	e	101	LMT	O3'-C3'	-2.56	1.36	1.43
25	d	401	CLA	MG-NC	2.56	2.12	2.06
31	M	101	LMT	O2B-C2B	-2.55	1.36	1.43
25	D	401	CLA	MG-NC	2.55	2.12	2.06
25	B	606	CLA	MG-NC	2.55	2.12	2.06
31	L	101	LMT	O3'-C3'	-2.55	1.36	1.43
31	b	627	LMT	O3'-C3'	-2.55	1.36	1.43
25	C	502	CLA	C4B-CHC	2.55	1.48	1.41
25	b	614	CLA	C4D-CHA	2.55	1.47	1.38
31	E	101	LMT	O3'-C3'	-2.55	1.36	1.43
25	c	508	CLA	MG-NC	2.55	2.12	2.06
31	L	101	LMT	O2'-C2'	-2.55	1.36	1.43
31	M	101	LMT	O3'-C3'	-2.54	1.36	1.43
25	B	614	CLA	C4D-CHA	2.54	1.47	1.38
31	M	101	LMT	O2'-C2'	-2.54	1.36	1.43
25	B	610	CLA	C4D-CHA	2.54	1.47	1.38
31	b	624	LMT	O3'-C3'	-2.54	1.36	1.43
31	h	101	LMT	O3'-C3'	-2.54	1.36	1.43
25	B	608	CLA	C4B-CHC	2.54	1.48	1.41
25	D	401	CLA	MG-ND	-2.54	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	C4D-CHA	2.53	1.47	1.38
25	b	608	CLA	C4B-CHC	2.53	1.48	1.41
25	B	615	CLA	C4D-CHA	2.53	1.47	1.38
25	B	602	CLA	C4D-CHA	2.53	1.47	1.38
25	d	401	CLA	MG-ND	-2.52	2.00	2.05
31	b	626	LMT	O3'-C3'	-2.52	1.36	1.43
31	d	411	LMT	O3'-C3'	-2.52	1.36	1.43
25	A	408	CLA	C4D-CHA	2.52	1.47	1.38
31	H	101	LMT	O3'-C3'	-2.52	1.36	1.43
31	D	411	LMT	O3'-C3'	-2.52	1.36	1.43
31	d	412	LMT	O2'-C2'	-2.52	1.36	1.43
31	x	103	LMT	O3'-C3'	-2.52	1.36	1.43
31	L	101	LMT	O2B-C2B	-2.52	1.36	1.43
25	a	408	CLA	C4D-CHA	2.51	1.47	1.38
25	B	616	CLA	MG-NC	2.51	2.12	2.06
25	b	615	CLA	C4D-CHA	2.51	1.47	1.38
25	B	605	CLA	C4B-CHC	2.51	1.48	1.41
31	B	623	LMT	O3'-C3'	-2.51	1.36	1.43
31	D	412	LMT	O2'-C2'	-2.50	1.36	1.43
31	B	626	LMT	O3'-C3'	-2.50	1.36	1.43
31	b	625	LMT	O1'-C1'	-2.50	1.36	1.40
31	c	521	LMT	O3'-C3'	-2.50	1.36	1.43
25	b	616	CLA	MG-NC	2.50	2.12	2.06
25	b	613	CLA	C1B-CHB	2.50	1.47	1.41
25	C	502	CLA	C1C-NC	-2.50	1.34	1.37
31	b	623	LMT	O3'-C3'	-2.50	1.36	1.43
31	C	521	LMT	O3'-C3'	-2.50	1.36	1.43
31	I	104	LMT	O3'-C3'	-2.50	1.36	1.43
25	b	605	CLA	C4B-CHC	2.50	1.47	1.41
31	C	520	LMT	O3'-C3'	-2.50	1.36	1.43
25	B	601	CLA	C4B-CHC	2.49	1.47	1.41
31	x	101	LMT	O2'-C2'	-2.49	1.36	1.43
25	d	404	CLA	MG-NC	2.49	2.12	2.06
25	b	614	CLA	C1C-NC	-2.49	1.34	1.37
25	b	601	CLA	C4B-CHC	2.48	1.47	1.41
31	i	104	LMT	O3'-C3'	-2.48	1.36	1.43
25	D	404	CLA	MG-ND	-2.48	2.00	2.05
31	f	103	LMT	O3'-C3'	-2.48	1.36	1.43
25	c	502	CLA	C1C-NC	-2.48	1.34	1.37
31	X	101	LMT	O2'-C2'	-2.48	1.36	1.43
31	c	520	LMT	O3'-C3'	-2.48	1.36	1.43
25	b	601	CLA	MG-NC	2.48	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	103	LMT	O3'-C3'	-2.48	1.36	1.43
26	D	402	PHO	CMC-C2C	-2.48	1.45	1.51
26	d	402	PHO	CMC-C2C	-2.48	1.45	1.51
31	k	105	LMT	O3'-C3'	-2.48	1.36	1.43
31	B	625	LMT	O1'-C1'	-2.48	1.36	1.40
25	B	614	CLA	C1C-NC	-2.47	1.34	1.37
25	B	613	CLA	C1B-CHB	2.47	1.47	1.41
25	D	404	CLA	MG-NC	2.47	2.12	2.06
31	y	101	LMT	O3'-C3'	-2.47	1.36	1.43
31	F	103	LMT	O3'-C3'	-2.47	1.36	1.43
25	B	612	CLA	C3D-C2D	2.47	1.45	1.39
25	A	406	CLA	MG-NC	2.47	2.12	2.06
25	a	406	CLA	MG-NC	2.47	2.12	2.06
25	B	602	CLA	MG-NC	2.46	2.12	2.06
25	b	602	CLA	MG-NC	2.46	2.12	2.06
31	K	105	LMT	O3'-C3'	-2.46	1.36	1.43
31	B	625	LMT	O3'-C3'	-2.45	1.36	1.43
25	B	601	CLA	MG-NC	2.45	2.12	2.06
31	Y	101	LMT	O3'-C3'	-2.45	1.36	1.43
25	b	611	CLA	C4D-CHA	2.45	1.46	1.38
25	d	404	CLA	MG-ND	-2.45	2.00	2.05
25	B	614	CLA	MG-ND	-2.45	2.00	2.05
25	b	612	CLA	C3D-C2D	2.45	1.45	1.39
25	A	405	CLA	MG-ND	-2.45	2.00	2.05
31	b	625	LMT	O3'-C3'	-2.45	1.36	1.43
31	b	629	LMT	O1'-C1'	-2.44	1.36	1.40
31	B	626	LMT	O2'-C2'	-2.44	1.36	1.43
31	b	626	LMT	O2'-C2'	-2.44	1.36	1.43
25	a	405	CLA	MG-ND	-2.44	2.01	2.05
25	B	611	CLA	C4D-CHA	2.44	1.46	1.38
25	c	503	CLA	C1B-CHB	2.44	1.47	1.41
31	i	103	LMT	O3'-C3'	-2.43	1.36	1.43
25	b	614	CLA	MG-ND	-2.43	2.01	2.05
25	d	404	CLA	C1D-C2D	2.43	1.50	1.45
31	b	625	LMT	O2B-C2B	-2.43	1.36	1.43
25	B	603	CLA	C4B-CHC	2.43	1.47	1.41
25	C	503	CLA	C1B-CHB	2.43	1.47	1.41
25	D	404	CLA	C1D-C2D	2.42	1.50	1.45
31	B	629	LMT	O1'-C1'	-2.42	1.36	1.40
31	B	625	LMT	O2B-C2B	-2.42	1.37	1.43
28	b	621	LMG	C25-C24	-2.42	1.33	1.50
25	C	507	CLA	C1B-CHB	2.42	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C4B-CHC	2.42	1.47	1.41
28	B	621	LMG	C25-C24	-2.42	1.33	1.50
34	H	103	DGD	CGB-CFB	-2.41	1.33	1.50
25	b	603	CLA	C4B-CHC	2.41	1.47	1.41
33	B	628	LHG	O7-C5	-2.41	1.40	1.46
25	c	509	CLA	C4D-CHA	2.41	1.46	1.38
34	H	103	DGD	CGA-CFA	-2.41	1.33	1.50
34	h	103	DGD	CGB-CFB	-2.41	1.33	1.50
34	h	103	DGD	CGA-CFA	-2.41	1.33	1.50
31	B	629	LMT	O2B-C2B	-2.41	1.37	1.43
25	C	506	CLA	C4B-CHC	2.41	1.47	1.41
25	b	611	CLA	OBD-CAD	2.41	1.26	1.22
33	b	628	LHG	O7-C5	-2.41	1.40	1.46
28	C	519	LMG	C25-C24	-2.40	1.33	1.50
25	C	509	CLA	C4D-CHA	2.40	1.46	1.38
34	c	518	DGD	CGB-CFB	-2.40	1.33	1.50
34	C	518	DGD	CGB-CFB	-2.40	1.33	1.50
28	a	410	LMG	C43-C42	-2.40	1.33	1.50
25	c	507	CLA	C1B-CHB	2.40	1.47	1.41
34	c	517	DGD	CGB-CFB	-2.40	1.33	1.50
29	D	405	PL9	C53-C6	-2.40	1.45	1.50
25	B	611	CLA	OBD-CAD	2.39	1.26	1.22
28	c	519	LMG	C25-C24	-2.39	1.33	1.50
34	C	517	DGD	CGB-CFB	-2.39	1.33	1.50
25	C	512	CLA	C1B-CHB	2.39	1.47	1.41
25	c	504	CLA	C4B-CHC	2.39	1.47	1.41
28	A	410	LMG	C43-C42	-2.39	1.33	1.50
28	a	410	LMG	C25-C24	-2.39	1.33	1.50
29	d	405	PL9	C53-C6	-2.39	1.45	1.50
31	b	629	LMT	O2B-C2B	-2.39	1.37	1.43
25	c	512	CLA	C1B-CHB	2.39	1.47	1.41
28	A	410	LMG	C25-C24	-2.38	1.33	1.50
29	d	405	PL9	C7-C8	-2.38	1.46	1.50
34	c	518	DGD	CGA-CFA	-2.38	1.33	1.50
28	b	621	LMG	C43-C42	-2.38	1.33	1.50
29	D	405	PL9	C7-C8	-2.38	1.46	1.50
25	b	604	CLA	C4B-CHC	2.38	1.47	1.41
25	c	504	CLA	C1B-CHB	2.38	1.47	1.41
25	C	504	CLA	C4B-CHC	2.38	1.47	1.41
34	C	518	DGD	CGA-CFA	-2.38	1.33	1.50
34	C	516	DGD	CGB-CFB	-2.38	1.33	1.50
28	D	409	LMG	C43-C42	-2.38	1.33	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	405	CLA	C4D-CHA	2.38	1.46	1.38
25	a	405	CLA	C4D-CHA	2.38	1.46	1.38
25	c	502	CLA	C1D-C2D	2.38	1.50	1.45
34	c	516	DGD	CGB-CFB	-2.38	1.33	1.50
28	D	409	LMG	C25-C24	-2.38	1.33	1.50
28	d	409	LMG	C43-C42	-2.38	1.33	1.50
28	B	621	LMG	C43-C42	-2.37	1.33	1.50
34	C	517	DGD	CGA-CFA	-2.37	1.33	1.50
34	c	517	DGD	CGA-CFA	-2.37	1.33	1.50
28	d	409	LMG	C25-C24	-2.37	1.33	1.50
25	C	506	CLA	C3D-C2D	2.37	1.45	1.39
25	C	504	CLA	C1B-CHB	2.37	1.47	1.41
25	C	502	CLA	C1D-C2D	2.37	1.50	1.45
31	I	101	LMT	O2'-C2'	-2.37	1.37	1.43
25	B	605	CLA	C4D-CHA	2.36	1.46	1.38
25	a	408	CLA	C1B-CHB	2.36	1.47	1.41
34	c	516	DGD	CGA-CFA	-2.36	1.33	1.50
28	C	519	LMG	C43-C42	-2.36	1.33	1.50
25	b	605	CLA	C4D-CHA	2.36	1.46	1.38
28	c	519	LMG	C43-C42	-2.36	1.33	1.50
25	B	604	CLA	C4B-CHC	2.36	1.47	1.41
25	C	514	CLA	C4B-CHC	2.36	1.47	1.41
25	A	408	CLA	C1B-CHB	2.36	1.47	1.41
31	A	415	LMT	O5'-C5'	-2.36	1.38	1.44
34	C	516	DGD	CGA-CFA	-2.36	1.33	1.50
31	i	101	LMT	O2'-C2'	-2.36	1.37	1.43
25	A	406	CLA	MG-ND	-2.35	2.01	2.05
25	a	406	CLA	MG-ND	-2.35	2.01	2.05
25	B	616	CLA	C1B-CHB	2.35	1.47	1.41
25	d	404	CLA	C4D-CHA	2.35	1.46	1.38
31	i	101	LMT	O1'-C1'	-2.35	1.36	1.40
25	D	404	CLA	C4D-CHA	2.35	1.46	1.38
25	c	514	CLA	C4B-CHC	2.35	1.47	1.41
31	a	415	LMT	O5'-C5'	-2.34	1.38	1.44
31	I	101	LMT	O1'-C1'	-2.34	1.36	1.40
25	c	506	CLA	C3D-C2D	2.34	1.45	1.39
25	b	616	CLA	C1B-CHB	2.33	1.47	1.41
31	D	410	LMT	O1'-C1'	-2.33	1.36	1.40
31	b	629	LMT	O3'-C3'	-2.33	1.37	1.43
31	D	411	LMT	O2'-C2'	-2.33	1.37	1.43
25	b	612	CLA	C4D-CHA	2.33	1.46	1.38
37	x	102	RRX	C10-C9	2.33	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	102	RRX	C10-C9	2.33	1.41	1.35
31	B	629	LMT	O3'-C3'	-2.33	1.37	1.43
31	E	103	LMT	O2B-C2B	-2.33	1.37	1.43
25	b	611	CLA	C1B-CHB	2.33	1.47	1.41
25	d	403	CLA	CHB-C4A	2.33	1.35	1.33
31	E	101	LMT	O2'-C2'	-2.32	1.37	1.43
31	e	101	LMT	O2'-C2'	-2.32	1.37	1.43
25	c	505	CLA	C4B-CHC	2.32	1.47	1.41
31	A	415	LMT	O1'-C1'	-2.32	1.36	1.40
29	a	411	PL9	C53-C6	-2.32	1.46	1.50
25	B	612	CLA	C4D-CHA	2.32	1.46	1.38
31	e	103	LMT	O2B-C2B	-2.32	1.37	1.43
25	C	505	CLA	C4B-CHC	2.32	1.47	1.41
25	B	607	CLA	C4D-CHA	2.32	1.46	1.38
25	a	405	CLA	C1B-CHB	2.32	1.47	1.41
31	a	415	LMT	O1'-C1'	-2.32	1.36	1.40
31	K	105	LMT	O2B-C2B	-2.31	1.37	1.43
31	K	105	LMT	O2'-C2'	-2.31	1.37	1.43
31	k	105	LMT	O2'-C2'	-2.31	1.37	1.43
31	k	105	LMT	O2B-C2B	-2.31	1.37	1.43
25	C	505	CLA	C4C-C3C	2.30	1.48	1.45
31	d	411	LMT	O2'-C2'	-2.30	1.37	1.43
25	c	503	CLA	C4B-CHC	2.30	1.47	1.41
25	c	505	CLA	C4C-C3C	2.30	1.48	1.45
29	A	411	PL9	C53-C6	-2.30	1.46	1.50
31	d	410	LMT	O1'-C1'	-2.30	1.36	1.40
25	B	611	CLA	C1B-CHB	2.30	1.47	1.41
25	A	405	CLA	C1B-CHB	2.30	1.47	1.41
37	x	102	RRX	C21-C22	2.30	1.41	1.35
25	b	607	CLA	C4D-CHA	2.30	1.46	1.38
25	C	503	CLA	C4B-CHC	2.30	1.47	1.41
31	D	412	LMT	O2B-C2B	-2.30	1.37	1.43
31	d	412	LMT	O2B-C2B	-2.30	1.37	1.43
37	X	102	RRX	C17-C18	2.29	1.41	1.35
33	D	407	LHG	O7-C5	-2.29	1.41	1.46
25	B	606	CLA	C4B-CHC	2.29	1.47	1.41
25	b	606	CLA	C4B-CHC	2.29	1.47	1.41
37	X	102	RRX	C21-C22	2.29	1.41	1.35
31	e	103	LMT	O3B-C3B	-2.29	1.37	1.43
25	b	615	CLA	C4B-CHC	2.29	1.47	1.41
31	E	103	LMT	O3B-C3B	-2.29	1.37	1.43
37	x	102	RRX	C17-C18	2.28	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	415	LMT	O2B-C2B	-2.28	1.37	1.43
25	B	615	CLA	C4B-CHC	2.28	1.47	1.41
25	D	403	CLA	CHB-C4A	2.28	1.35	1.33
31	m	101	LMT	O1'-C1'	-2.28	1.36	1.40
31	E	101	LMT	O1'-C1'	-2.27	1.36	1.40
25	c	509	CLA	C1B-CHB	2.27	1.47	1.41
37	X	102	RRX	C14-C13	2.27	1.41	1.35
33	d	407	LHG	O7-C5	-2.27	1.41	1.46
25	C	511	CLA	C1D-C2D	2.27	1.49	1.45
25	C	505	CLA	C1D-C2D	2.26	1.49	1.45
27	Z	101	BCR	C30-C25	-2.26	1.50	1.53
37	x	102	RRX	C12-C13	-2.26	1.41	1.46
25	c	505	CLA	C1D-C2D	2.26	1.49	1.45
37	X	102	RRX	C12-C13	-2.26	1.41	1.46
25	C	509	CLA	C1B-CHB	2.25	1.47	1.41
25	c	511	CLA	C1B-CHB	2.25	1.47	1.41
25	D	403	CLA	C4D-CHA	2.25	1.46	1.38
31	a	415	LMT	O3B-C3B	-2.25	1.37	1.43
26	a	407	PHO	CMC-C2C	-2.25	1.46	1.51
31	a	415	LMT	O2B-C2B	-2.25	1.37	1.43
27	z	101	BCR	C30-C25	-2.25	1.50	1.53
25	b	612	CLA	C1B-CHB	2.25	1.47	1.41
25	A	406	CLA	C4B-CHC	2.24	1.47	1.41
31	K	105	LMT	O3B-C3B	-2.24	1.37	1.43
25	c	513	CLA	C1B-CHB	2.24	1.47	1.41
31	h	101	LMT	O2'-C2'	-2.24	1.37	1.43
25	C	511	CLA	C1B-CHB	2.24	1.47	1.41
31	M	102	LMT	O1'-C1'	-2.24	1.36	1.40
25	C	513	CLA	C1B-CHB	2.24	1.47	1.41
30	C	501	SQD	O47-C45	-2.24	1.41	1.46
31	i	103	LMT	O1'-C1'	-2.24	1.36	1.40
25	d	403	CLA	C4D-CHA	2.24	1.46	1.38
25	C	513	CLA	C4B-CHC	2.24	1.47	1.41
31	H	101	LMT	O2'-C2'	-2.24	1.37	1.43
31	b	627	LMT	O2'-C2'	-2.24	1.37	1.43
30	c	501	SQD	O47-C45	-2.23	1.41	1.46
25	D	404	CLA	C4B-CHC	2.23	1.47	1.41
31	I	103	LMT	O2'-C2'	-2.23	1.37	1.43
25	c	513	CLA	C4B-CHC	2.23	1.47	1.41
25	b	602	CLA	C1D-C2D	2.23	1.49	1.45
25	c	502	CLA	C1B-CHB	2.23	1.47	1.41
25	C	507	CLA	C4B-CHC	2.23	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	627	LMT	O2'-C2'	-2.23	1.37	1.43
31	k	105	LMT	O3B-C3B	-2.23	1.37	1.43
31	A	415	LMT	O3B-C3B	-2.23	1.37	1.43
31	c	520	LMT	O2'-C2'	-2.23	1.37	1.43
37	x	102	RRX	C14-C13	2.23	1.41	1.35
31	e	101	LMT	O1'-C1'	-2.23	1.36	1.40
25	d	404	CLA	C1B-CHB	2.23	1.47	1.41
31	I	103	LMT	O1'-C1'	-2.23	1.36	1.40
31	D	410	LMT	O2'-C2'	-2.23	1.37	1.43
27	F	101	BCR	C30-C25	-2.23	1.50	1.53
25	c	511	CLA	C1D-C2D	2.23	1.49	1.45
25	c	507	CLA	C4B-CHC	2.23	1.47	1.41
31	x	103	LMT	O2'-C2'	-2.22	1.37	1.43
25	c	502	CLA	C4C-C3C	2.22	1.48	1.45
25	B	602	CLA	C1D-C2D	2.22	1.49	1.45
31	X	103	LMT	O2'-C2'	-2.22	1.37	1.43
31	T	701	LMT	O2'-C2'	-2.22	1.37	1.43
31	f	103	LMT	O2B-C2B	-2.21	1.37	1.43
31	d	412	LMT	O3B-C3B	-2.21	1.37	1.43
31	c	520	LMT	O2B-C2B	-2.21	1.37	1.43
26	A	407	PHO	CMC-C2C	-2.21	1.46	1.51
31	i	103	LMT	O2'-C2'	-2.21	1.37	1.43
31	X	103	LMT	O1'-C1'	-2.21	1.36	1.40
25	B	612	CLA	C1B-CHB	2.21	1.47	1.41
25	C	514	CLA	C1D-C2D	2.21	1.49	1.45
25	C	510	CLA	C4B-CHC	2.21	1.47	1.41
25	c	510	CLA	C1B-CHB	2.21	1.47	1.41
25	d	404	CLA	C4B-CHC	2.21	1.47	1.41
25	b	609	CLA	C4B-CHC	2.21	1.47	1.41
31	b	625	LMT	O3B-C3B	-2.21	1.37	1.43
31	x	103	LMT	O1'-C1'	-2.21	1.36	1.40
25	D	404	CLA	C1B-CHB	2.20	1.47	1.41
31	C	520	LMT	O2B-C2B	-2.20	1.37	1.43
25	c	514	CLA	C1D-C2D	2.20	1.49	1.45
25	C	502	CLA	C1B-CHB	2.20	1.47	1.41
31	D	412	LMT	O3B-C3B	-2.20	1.37	1.43
25	a	406	CLA	C4B-CHC	2.20	1.47	1.41
37	x	102	RRX	C19-C18	-2.20	1.41	1.46
31	x	101	LMT	O1'-C1'	-2.20	1.36	1.40
25	a	406	CLA	C1B-CHB	2.20	1.47	1.41
37	X	102	RRX	C19-C18	-2.20	1.41	1.46
25	c	510	CLA	C4B-CHC	2.20	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	103	LMT	O2B-C2B	-2.20	1.37	1.43
25	C	510	CLA	C1B-CHB	2.20	1.47	1.41
31	B	629	LMT	O2'-C2'	-2.20	1.37	1.43
31	M	101	LMT	O3B-C3B	-2.20	1.37	1.43
31	C	520	LMT	O2'-C2'	-2.20	1.37	1.43
31	i	103	LMT	O2B-C2B	-2.20	1.37	1.43
25	B	609	CLA	C4B-CHC	2.20	1.47	1.41
31	F	103	LMT	O2B-C2B	-2.19	1.37	1.43
31	t	701	LMT	O2'-C2'	-2.19	1.37	1.43
25	B	614	CLA	C1B-CHB	2.19	1.47	1.41
25	B	613	CLA	C1D-C2D	2.19	1.49	1.45
31	d	410	LMT	O2'-C2'	-2.19	1.37	1.43
25	b	606	CLA	C1B-CHB	2.19	1.47	1.41
31	I	103	LMT	O3B-C3B	-2.19	1.37	1.43
25	B	606	CLA	C1B-CHB	2.19	1.47	1.41
25	c	504	CLA	C1D-C2D	2.19	1.49	1.45
31	b	629	LMT	O2'-C2'	-2.19	1.37	1.43
25	B	605	CLA	C1B-CHB	2.19	1.47	1.41
25	c	511	CLA	C4B-CHC	2.19	1.47	1.41
25	C	502	CLA	C4C-C3C	2.19	1.48	1.45
25	b	614	CLA	C1B-CHB	2.18	1.47	1.41
31	J	101	LMT	O2'-C2'	-2.18	1.37	1.43
31	c	524	LMT	O3B-C3B	-2.18	1.37	1.43
25	b	613	CLA	C1D-C2D	2.18	1.49	1.45
31	B	625	LMT	O3B-C3B	-2.18	1.37	1.43
30	f	102	SQD	O3-C3	-2.18	1.37	1.43
25	C	505	CLA	C1B-CHB	2.18	1.47	1.41
31	D	411	LMT	O2B-C2B	-2.18	1.37	1.43
25	d	401	CLA	C1B-CHB	2.18	1.47	1.41
30	F	102	SQD	O3-C3	-2.18	1.37	1.43
31	L	101	LMT	O3B-C3B	-2.18	1.37	1.43
32	A	417	BCT	O1-C	-2.18	1.18	1.25
31	j	101	LMT	O2'-C2'	-2.18	1.37	1.43
25	A	406	CLA	C1B-CHB	2.17	1.47	1.41
25	d	403	CLA	C4B-CHC	2.17	1.47	1.41
30	c	501	SQD	O2-C2	-2.17	1.37	1.43
25	c	505	CLA	C1B-CHB	2.17	1.47	1.41
25	B	608	CLA	C1D-C2D	2.17	1.49	1.45
25	A	405	CLA	MG-NC	2.17	2.11	2.06
27	f	101	BCR	C30-C25	-2.17	1.51	1.53
31	C	524	LMT	O2B-C2B	-2.17	1.37	1.43
25	C	511	CLA	C4B-CHC	2.17	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	612	CLA	C4B-CHC	2.17	1.47	1.41
30	C	501	SQD	O2-C2	-2.17	1.37	1.43
25	b	605	CLA	C1B-CHB	2.17	1.47	1.41
25	b	608	CLA	C1D-C2D	2.17	1.49	1.45
31	c	524	LMT	O2B-C2B	-2.17	1.37	1.43
31	d	411	LMT	O2B-C2B	-2.17	1.37	1.43
25	D	403	CLA	C4B-CHC	2.17	1.47	1.41
31	C	524	LMT	O3B-C3B	-2.17	1.37	1.43
25	D	401	CLA	C1B-CHB	2.17	1.47	1.41
25	B	612	CLA	C4B-CHC	2.17	1.47	1.41
25	c	514	CLA	C1B-CHB	2.16	1.47	1.41
31	X	101	LMT	O1'-C1'	-2.16	1.36	1.40
31	i	103	LMT	O3B-C3B	-2.16	1.37	1.43
31	C	520	LMT	O3B-C3B	-2.16	1.37	1.43
32	a	417	BCT	O1-C	-2.16	1.18	1.25
31	a	416	LMT	O1'-C1'	-2.16	1.36	1.40
31	e	103	LMT	O1'-C1'	-2.16	1.36	1.40
31	y	101	LMT	O2'-C2'	-2.16	1.37	1.43
31	L	101	LMT	O1'-C1'	-2.15	1.36	1.40
31	i	104	LMT	O2'-C2'	-2.15	1.37	1.43
25	a	405	CLA	MG-NC	2.15	2.11	2.06
31	b	625	LMT	O2'-C2'	-2.15	1.37	1.43
31	B	625	LMT	O2'-C2'	-2.15	1.37	1.43
31	c	520	LMT	O3B-C3B	-2.15	1.37	1.43
25	C	504	CLA	C1D-C2D	2.15	1.49	1.45
31	Y	101	LMT	O2'-C2'	-2.15	1.37	1.43
25	B	603	CLA	C1B-CHB	2.15	1.47	1.41
25	b	601	CLA	C1B-CHB	2.15	1.47	1.41
31	E	103	LMT	O1'-C1'	-2.15	1.36	1.40
25	C	514	CLA	C1B-CHB	2.15	1.47	1.41
31	A	416	LMT	O1'-C1'	-2.14	1.36	1.40
25	B	607	CLA	C1B-CHB	2.14	1.46	1.41
31	C	521	LMT	O2'-C2'	-2.14	1.37	1.43
31	c	521	LMT	O2'-C2'	-2.14	1.37	1.43
25	b	610	CLA	C4B-CHC	2.14	1.46	1.41
31	I	104	LMT	O1'-C1'	-2.14	1.36	1.40
31	i	104	LMT	O1'-C1'	-2.14	1.36	1.40
31	M	101	LMT	O1'-C1'	-2.14	1.36	1.40
25	c	507	CLA	C1D-C2D	2.14	1.49	1.45
25	B	610	CLA	C4B-CHC	2.14	1.46	1.41
31	F	103	LMT	O2'-C2'	-2.14	1.37	1.43
25	b	603	CLA	C1B-CHB	2.14	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C1B-CHB	2.14	1.46	1.41
25	b	604	CLA	C1B-CHB	2.14	1.46	1.41
25	C	507	CLA	C1D-C2D	2.13	1.49	1.45
25	b	602	CLA	C1B-CHB	2.13	1.46	1.41
25	b	609	CLA	C1B-CHB	2.13	1.46	1.41
31	f	103	LMT	O2'-C2'	-2.12	1.37	1.43
25	b	607	CLA	C1B-CHB	2.12	1.46	1.41
25	b	615	CLA	C1B-CHB	2.12	1.46	1.41
25	B	602	CLA	C1B-CHB	2.12	1.46	1.41
25	B	604	CLA	C1B-CHB	2.12	1.46	1.41
31	D	412	LMT	O4'-C4B	-2.12	1.37	1.43
25	c	508	CLA	C4B-CHC	2.12	1.46	1.41
29	D	405	PL9	C46-C44	-2.12	1.46	1.51
26	d	402	PHO	CMD-C2D	-2.12	1.46	1.51
31	I	104	LMT	O2'-C2'	-2.12	1.37	1.43
25	C	508	CLA	C4B-CHC	2.12	1.46	1.41
31	d	411	LMT	O3B-C3B	-2.12	1.37	1.43
31	A	415	LMT	O2'-C2'	-2.12	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.12	1.37	1.43
30	b	620	SQD	O4-C4	-2.12	1.37	1.43
26	A	407	PHO	CMB-C2B	-2.12	1.46	1.51
29	d	405	PL9	C46-C44	-2.12	1.46	1.51
25	B	615	CLA	C1B-CHB	2.11	1.46	1.41
31	D	412	LMT	O1'-C1'	-2.11	1.36	1.40
31	d	412	LMT	O4'-C4B	-2.11	1.37	1.43
26	D	402	PHO	C1C-NC	-2.11	1.32	1.38
25	B	609	CLA	C1B-CHB	2.11	1.46	1.41
25	B	610	CLA	C1B-CHB	2.11	1.46	1.41
25	C	506	CLA	C1B-CHB	2.11	1.46	1.41
25	C	509	CLA	C4C-C3C	2.11	1.48	1.45
26	d	402	PHO	C1C-NC	-2.11	1.32	1.38
30	B	620	SQD	O4-C4	-2.10	1.37	1.43
26	D	402	PHO	CMD-C2D	-2.10	1.46	1.51
30	a	412	SQD	O2-C2	-2.10	1.37	1.43
31	D	411	LMT	O3B-C3B	-2.10	1.37	1.43
25	c	506	CLA	C1B-CHB	2.10	1.46	1.41
31	d	412	LMT	O1'-C1'	-2.09	1.36	1.40
31	a	415	LMT	O2'-C2'	-2.09	1.37	1.43
26	a	407	PHO	CMB-C2B	-2.09	1.46	1.51
31	F	103	LMT	O3B-C3B	-2.09	1.37	1.43
31	b	623	LMT	O2'-C2'	-2.09	1.37	1.43
31	f	103	LMT	O3B-C3B	-2.09	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	524	LMT	O2'-C2'	-2.09	1.37	1.43
26	d	402	PHO	CMB-C2B	-2.09	1.46	1.51
31	i	102	LMT	O5'-C5'	-2.09	1.39	1.44
31	c	524	LMT	O2'-C2'	-2.09	1.37	1.43
31	f	103	LMT	O4'-C4B	-2.08	1.37	1.43
31	F	103	LMT	O4'-C4B	-2.08	1.37	1.43
26	D	402	PHO	CMB-C2B	-2.08	1.46	1.51
31	b	629	LMT	O3B-C3B	-2.08	1.37	1.43
25	c	509	CLA	C4C-C3C	2.08	1.48	1.45
25	b	610	CLA	C1B-CHB	2.07	1.46	1.41
31	T	701	LMT	O1'-C1'	-2.07	1.36	1.40
31	X	103	LMT	O5'-C5'	-2.07	1.39	1.44
30	A	412	SQD	O2-C2	-2.07	1.37	1.43
30	K	101	SQD	O4-C4	-2.07	1.37	1.43
30	k	101	SQD	O4-C4	-2.07	1.37	1.43
31	x	103	LMT	O5'-C5'	-2.07	1.39	1.44
31	I	102	LMT	O5'-C5'	-2.07	1.39	1.44
31	t	701	LMT	O1'-C1'	-2.07	1.36	1.40
25	b	615	CLA	C1D-C2D	2.06	1.49	1.45
25	B	616	CLA	C4B-CHC	2.06	1.46	1.41
30	A	413	SQD	O2-C2	-2.06	1.37	1.43
25	D	401	CLA	C4B-CHC	2.06	1.46	1.41
31	L	101	LMT	O4'-C4B	-2.06	1.37	1.43
30	a	412	SQD	O4-C4	-2.06	1.37	1.43
31	c	520	LMT	O1'-C1'	-2.06	1.36	1.40
30	H	102	SQD	O3-C3	-2.06	1.37	1.43
25	b	616	CLA	C4B-CHC	2.06	1.46	1.41
30	A	412	SQD	O4-C4	-2.06	1.37	1.43
30	k	101	SQD	O47-C45	-2.05	1.41	1.46
31	c	524	LMT	O4'-C4B	-2.05	1.37	1.43
35	v	201	HEM	C3C-C4C	2.05	1.44	1.41
25	b	613	CLA	C4B-CHC	2.05	1.46	1.41
25	B	615	CLA	C1D-C2D	2.05	1.49	1.45
30	h	102	SQD	O3-C3	-2.05	1.37	1.43
31	B	629	LMT	O3B-C3B	-2.05	1.37	1.43
31	M	101	LMT	O4'-C4B	-2.05	1.37	1.43
25	C	509	CLA	C4B-CHC	2.05	1.46	1.41
25	c	509	CLA	C4B-CHC	2.05	1.46	1.41
25	B	613	CLA	C4B-CHC	2.05	1.46	1.41
31	C	524	LMT	O4'-C4B	-2.05	1.37	1.43
25	A	405	CLA	C4B-CHC	2.05	1.46	1.41
25	a	405	CLA	C4B-CHC	2.04	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	102	LMT	O1'-C1'	-2.04	1.36	1.40
35	V	201	HEM	C3C-C4C	2.04	1.44	1.41
25	d	401	CLA	C4B-CHC	2.04	1.46	1.41
30	F	102	SQD	O2-C2	-2.04	1.37	1.43
31	C	520	LMT	O1'-C1'	-2.04	1.36	1.40
29	d	405	PL9	C41-C39	-2.04	1.47	1.51
31	c	522	LMT	O1'-C1'	-2.04	1.36	1.40
31	c	521	LMT	O1'-C1'	-2.03	1.36	1.40
25	C	508	CLA	C1D-C2D	2.03	1.49	1.45
26	a	407	PHO	C3B-C2B	-2.03	1.37	1.40
31	b	627	LMT	O5'-C5'	-2.03	1.39	1.44
30	a	413	SQD	O2-C2	-2.03	1.37	1.43
25	B	608	CLA	C1B-CHB	2.03	1.46	1.41
31	a	416	LMT	O2'-C2'	-2.03	1.37	1.43
31	Y	101	LMT	O1'-C1'	-2.03	1.36	1.40
30	h	102	SQD	O47-C45	-2.03	1.41	1.46
25	C	504	CLA	C4C-C3C	2.02	1.48	1.45
29	D	405	PL9	C41-C39	-2.02	1.47	1.51
31	C	521	LMT	O1'-C1'	-2.02	1.36	1.40
31	y	101	LMT	O1'-C1'	-2.02	1.36	1.40
30	h	102	SQD	O2-C2	-2.02	1.37	1.43
25	C	509	CLA	C1D-C2D	2.02	1.49	1.45
30	K	101	SQD	O47-C45	-2.02	1.41	1.46
25	c	508	CLA	C1B-CHB	2.02	1.46	1.41
30	H	102	SQD	O2-C2	-2.02	1.38	1.43
30	f	102	SQD	O2-C2	-2.02	1.38	1.43
31	B	627	LMT	O5'-C5'	-2.02	1.39	1.44
31	I	102	LMT	O1'-C1'	-2.02	1.36	1.40
25	A	408	CLA	C4B-CHC	2.01	1.46	1.41
31	B	625	LMT	O5'-C5'	-2.01	1.39	1.44
25	a	408	CLA	C4B-CHC	2.01	1.46	1.41
25	c	504	CLA	C4C-C3C	2.01	1.48	1.45
30	a	413	SQD	O3-C3	-2.01	1.38	1.43
25	c	508	CLA	C1D-C2D	2.01	1.49	1.45
31	C	522	LMT	O1'-C1'	-2.01	1.36	1.40
31	i	103	LMT	O4'-C4B	-2.01	1.38	1.43
30	H	102	SQD	O47-C45	-2.01	1.41	1.46
25	b	608	CLA	C1B-CHB	2.01	1.46	1.41
30	F	102	SQD	O4-C4	-2.01	1.38	1.43
30	A	413	SQD	O3-C3	-2.01	1.38	1.43
31	A	416	LMT	O2'-C2'	-2.01	1.38	1.43
31	k	105	LMT	O1'-C1'	-2.00	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	C1B-CHB	2.00	1.46	1.41

All (2542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C20-C21-C22	24.77	162.02	127.28
27	k	102	BCR	C20-C21-C22	24.74	161.98	127.28
27	k	103	BCR	C20-C21-C22	22.03	158.18	127.28
27	K	103	BCR	C20-C21-C22	22.03	158.17	127.28
27	f	101	BCR	C20-C21-C22	21.95	158.06	127.28
27	F	101	BCR	C20-C21-C22	21.92	158.03	127.28
27	c	515	BCR	C16-C17-C18	21.41	157.30	127.28
27	C	515	BCR	C16-C17-C18	21.39	157.28	127.28
27	a	409	BCR	C15-C16-C17	21.24	166.97	123.52
27	A	409	BCR	C15-C16-C17	21.23	166.95	123.52
27	z	101	BCR	C20-C21-C22	20.98	156.71	127.28
27	Z	101	BCR	C20-C21-C22	20.96	156.67	127.28
27	c	515	BCR	C20-C21-C22	20.88	156.56	127.28
27	C	515	BCR	C20-C21-C22	20.88	156.55	127.28
27	k	102	BCR	C16-C17-C18	20.87	156.54	127.28
27	K	102	BCR	C16-C17-C18	20.84	156.50	127.28
27	f	101	BCR	C15-C16-C17	20.82	166.12	123.52
27	F	101	BCR	C15-C16-C17	20.80	166.07	123.52
27	a	409	BCR	C20-C21-C22	20.78	156.42	127.28
27	A	409	BCR	C20-C21-C22	20.77	156.40	127.28
27	B	618	BCR	C20-C21-C22	20.75	156.38	127.28
27	b	618	BCR	C20-C21-C22	20.75	156.37	127.28
27	k	103	BCR	C15-C16-C17	20.72	165.92	123.52
27	K	103	BCR	C15-C16-C17	20.72	165.91	123.52
27	B	617	BCR	C20-C21-C22	20.60	156.16	127.28
27	b	617	BCR	C20-C21-C22	20.57	156.13	127.28
27	b	617	BCR	C15-C16-C17	20.55	165.56	123.52
27	B	617	BCR	C15-C16-C17	20.53	165.53	123.52
27	b	619	BCR	C20-C21-C22	20.50	156.03	127.28
27	B	619	BCR	C20-C21-C22	20.49	156.02	127.28
27	z	101	BCR	C16-C17-C18	20.42	155.91	127.28
27	Z	101	BCR	C16-C17-C18	20.41	155.91	127.28
27	B	618	BCR	C15-C16-C17	20.38	165.23	123.52
27	b	618	BCR	C15-C16-C17	20.37	165.20	123.52
27	B	618	BCR	C16-C17-C18	19.99	155.31	127.28
27	b	618	BCR	C16-C17-C18	19.98	155.29	127.28
27	C	515	BCR	C15-C16-C17	19.93	164.30	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	515	BCR	C15-C16-C17	19.93	164.29	123.52
27	b	619	BCR	C15-C16-C17	19.79	164.02	123.52
27	B	619	BCR	C15-C16-C17	19.79	164.01	123.52
27	b	619	BCR	C16-C17-C18	19.71	154.93	127.28
27	B	619	BCR	C16-C17-C18	19.71	154.92	127.28
27	K	102	BCR	C15-C16-C17	19.62	163.66	123.52
27	k	102	BCR	C15-C16-C17	19.61	163.65	123.52
27	b	617	BCR	C16-C17-C18	19.36	154.43	127.28
27	B	617	BCR	C16-C17-C18	19.34	154.40	127.28
27	z	101	BCR	C15-C16-C17	19.17	162.74	123.52
27	Z	101	BCR	C15-C16-C17	19.17	162.74	123.52
27	a	409	BCR	C16-C17-C18	19.12	154.09	127.28
27	A	409	BCR	C16-C17-C18	19.11	154.07	127.28
27	k	103	BCR	C16-C17-C18	18.97	153.89	127.28
27	K	103	BCR	C16-C17-C18	18.97	153.88	127.28
27	k	103	BCR	C10-C11-C12	18.76	177.56	123.20
27	K	103	BCR	C10-C11-C12	18.74	177.50	123.20
27	f	101	BCR	C16-C17-C18	18.61	153.37	127.28
27	F	101	BCR	C16-C17-C18	18.57	153.32	127.28
27	c	515	BCR	C10-C11-C12	18.57	177.01	123.20
27	z	101	BCR	C10-C11-C12	18.56	176.99	123.20
27	Z	101	BCR	C10-C11-C12	18.56	176.99	123.20
27	C	515	BCR	C10-C11-C12	18.55	176.96	123.20
27	K	102	BCR	C10-C11-C12	18.46	176.69	123.20
27	k	102	BCR	C10-C11-C12	18.46	176.68	123.20
27	A	409	BCR	C10-C11-C12	18.31	176.25	123.20
27	a	409	BCR	C10-C11-C12	18.30	176.23	123.20
27	F	101	BCR	C10-C11-C12	18.21	175.96	123.20
27	f	101	BCR	C10-C11-C12	18.21	175.95	123.20
27	B	619	BCR	C10-C11-C12	18.12	175.71	123.20
27	B	617	BCR	C10-C11-C12	18.11	175.69	123.20
27	b	619	BCR	C10-C11-C12	18.11	175.68	123.20
27	b	617	BCR	C10-C11-C12	18.11	175.66	123.20
27	b	618	BCR	C10-C11-C12	18.03	175.44	123.20
27	B	618	BCR	C10-C11-C12	18.02	175.41	123.20
27	k	102	BCR	C11-C10-C9	15.01	148.33	127.28
27	K	102	BCR	C11-C10-C9	15.01	148.32	127.28
27	B	619	BCR	C21-C20-C19	14.46	165.10	123.20
27	b	619	BCR	C21-C20-C19	14.45	165.07	123.20
27	F	101	BCR	C11-C10-C9	14.28	147.31	127.28
27	f	101	BCR	C11-C10-C9	14.26	147.28	127.28
27	b	617	BCR	C11-C10-C9	14.16	147.14	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	BCR	C11-C10-C9	14.15	147.13	127.28
27	B	619	BCR	C11-C10-C9	14.13	147.10	127.28
27	b	619	BCR	C11-C10-C9	14.11	147.07	127.28
27	Z	101	BCR	C21-C20-C19	13.84	163.29	123.20
27	z	101	BCR	C21-C20-C19	13.84	163.29	123.20
27	a	409	BCR	C21-C20-C19	13.79	163.16	123.20
27	A	409	BCR	C21-C20-C19	13.78	163.14	123.20
27	f	101	BCR	C21-C20-C19	13.74	163.01	123.20
27	F	101	BCR	C21-C20-C19	13.73	162.99	123.20
27	K	103	BCR	C21-C20-C19	13.68	162.85	123.20
27	k	103	BCR	C21-C20-C19	13.68	162.83	123.20
27	B	618	BCR	C21-C20-C19	13.67	162.81	123.20
27	b	618	BCR	C21-C20-C19	13.67	162.81	123.20
27	z	101	BCR	C16-C15-C14	13.67	151.48	123.52
27	Z	101	BCR	C16-C15-C14	13.66	151.46	123.52
27	k	103	BCR	C11-C10-C9	13.52	146.24	127.28
27	B	617	BCR	C21-C20-C19	13.49	162.29	123.20
27	b	617	BCR	C21-C20-C19	13.49	162.28	123.20
27	B	618	BCR	C11-C10-C9	13.48	146.19	127.28
27	b	618	BCR	C11-C10-C9	13.48	146.19	127.28
27	K	103	BCR	C11-C10-C9	13.47	146.17	127.28
27	A	409	BCR	C11-C10-C9	13.26	145.87	127.28
27	a	409	BCR	C11-C10-C9	13.26	145.87	127.28
27	c	515	BCR	C21-C20-C19	13.19	161.42	123.20
27	K	102	BCR	C16-C15-C14	13.18	150.48	123.52
27	C	515	BCR	C21-C20-C19	13.18	161.38	123.20
27	k	102	BCR	C16-C15-C14	13.17	150.46	123.52
27	K	102	BCR	C21-C20-C19	13.02	160.94	123.20
27	k	102	BCR	C21-C20-C19	13.02	160.93	123.20
27	c	515	BCR	C11-C10-C9	12.86	145.31	127.28
27	C	515	BCR	C11-C10-C9	12.84	145.28	127.28
27	b	618	BCR	C16-C15-C14	12.60	149.30	123.52
27	B	618	BCR	C16-C15-C14	12.60	149.30	123.52
27	b	619	BCR	C16-C15-C14	12.59	149.28	123.52
27	B	619	BCR	C16-C15-C14	12.58	149.26	123.52
27	f	101	BCR	C16-C15-C14	12.29	148.67	123.52
27	F	101	BCR	C16-C15-C14	12.29	148.66	123.52
27	k	103	BCR	C16-C15-C14	12.27	148.63	123.52
27	K	103	BCR	C16-C15-C14	12.27	148.62	123.52
27	C	515	BCR	C16-C15-C14	11.99	148.04	123.52
27	c	515	BCR	C16-C15-C14	11.97	148.02	123.52
27	b	617	BCR	C16-C15-C14	11.79	147.65	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	BCR	C16-C15-C14	11.78	147.63	123.52
27	A	409	BCR	C11-C12-C13	11.64	158.29	126.36
27	a	409	BCR	C11-C12-C13	11.64	158.28	126.36
27	B	619	BCR	C11-C12-C13	11.38	157.58	126.36
27	b	619	BCR	C11-C12-C13	11.37	157.53	126.36
27	F	101	BCR	C11-C12-C13	11.28	157.29	126.36
27	f	101	BCR	C11-C12-C13	11.27	157.28	126.36
27	a	409	BCR	C16-C15-C14	11.24	146.51	123.52
27	A	409	BCR	C16-C15-C14	11.22	146.47	123.52
27	B	617	BCR	C11-C12-C13	11.17	156.99	126.36
27	b	617	BCR	C11-C12-C13	11.17	156.99	126.36
27	C	515	BCR	C11-C12-C13	11.16	156.96	126.36
27	c	515	BCR	C11-C12-C13	11.16	156.96	126.36
27	b	618	BCR	C11-C12-C13	10.87	156.16	126.36
27	B	618	BCR	C11-C12-C13	10.85	156.11	126.36
27	k	103	BCR	C11-C12-C13	10.73	155.78	126.36
27	K	103	BCR	C11-C12-C13	10.72	155.76	126.36
27	z	101	BCR	C11-C10-C9	10.36	141.81	127.28
27	Z	101	BCR	C11-C10-C9	10.36	141.80	127.28
27	k	102	BCR	C11-C12-C13	10.32	154.66	126.36
27	K	102	BCR	C11-C12-C13	10.32	154.66	126.36
27	z	101	BCR	C11-C12-C13	9.77	153.15	126.36
27	Z	101	BCR	C11-C12-C13	9.76	153.12	126.36
25	a	405	CLA	C4A-NA-C1A	8.58	110.59	106.68
25	A	405	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	b	602	CLA	CMD-C2D-C1D	8.42	139.56	124.73
25	B	602	CLA	CMD-C2D-C1D	8.42	139.55	124.73
25	C	506	CLA	CMD-C2D-C1D	8.39	139.51	124.73
25	c	506	CLA	CMD-C2D-C1D	8.39	139.50	124.73
25	b	601	CLA	CMD-C2D-C1D	8.25	139.26	124.73
25	B	601	CLA	CMD-C2D-C1D	8.25	139.26	124.73
25	c	511	CLA	CMD-C2D-C1D	8.21	139.18	124.73
27	K	102	BCR	C20-C19-C18	8.21	148.86	126.36
27	k	102	BCR	C20-C19-C18	8.20	148.85	126.36
25	C	511	CLA	CMD-C2D-C1D	8.19	139.16	124.73
25	C	504	CLA	CMD-C2D-C1D	8.16	139.10	124.73
25	c	504	CLA	CMD-C2D-C1D	8.14	139.06	124.73
25	B	613	CLA	CMD-C2D-C1D	7.98	138.77	124.73
25	b	613	CLA	CMD-C2D-C1D	7.98	138.77	124.73
25	C	514	CLA	CMD-C2D-C1D	7.92	138.68	124.73
25	d	403	CLA	C4A-NA-C1A	7.90	110.28	106.68
25	c	514	CLA	CMD-C2D-C1D	7.90	138.64	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	CMD-C2D-C1D	7.90	138.64	124.73
25	b	608	CLA	CMD-C2D-C1D	7.90	138.64	124.73
25	B	608	CLA	CMD-C2D-C1D	7.87	138.59	124.73
25	d	404	CLA	CMD-C2D-C1D	7.87	138.58	124.73
25	C	505	CLA	CMD-C2D-C1D	7.82	138.51	124.73
25	a	405	CLA	CMD-C2D-C1D	7.82	138.51	124.73
25	c	507	CLA	CMD-C2D-C1D	7.82	138.50	124.73
25	D	403	CLA	C4A-NA-C1A	7.82	110.25	106.68
25	C	507	CLA	CMD-C2D-C1D	7.81	138.49	124.73
25	c	505	CLA	CMD-C2D-C1D	7.81	138.48	124.73
25	A	405	CLA	CMD-C2D-C1D	7.80	138.47	124.73
25	B	603	CLA	CMD-C2D-C1D	7.77	138.42	124.73
25	b	603	CLA	CMD-C2D-C1D	7.77	138.41	124.73
25	c	508	CLA	CMD-C2D-C1D	7.77	138.40	124.73
25	C	508	CLA	CMD-C2D-C1D	7.76	138.40	124.73
25	C	510	CLA	CMD-C2D-C1D	7.70	138.29	124.73
25	c	510	CLA	CMD-C2D-C1D	7.70	138.28	124.73
25	b	609	CLA	CMD-C2D-C1D	7.65	138.21	124.73
25	B	609	CLA	CMD-C2D-C1D	7.64	138.19	124.73
25	B	606	CLA	CMD-C2D-C1D	7.60	138.12	124.73
25	b	606	CLA	CMD-C2D-C1D	7.60	138.11	124.73
27	c	515	BCR	C20-C19-C18	7.56	147.09	126.36
27	C	515	BCR	C20-C19-C18	7.54	147.04	126.36
25	B	611	CLA	CMD-C2D-C1D	7.50	137.94	124.73
25	D	403	CLA	CMD-C2D-C1D	7.50	137.94	124.73
25	B	614	CLA	CMD-C2D-C1D	7.49	137.92	124.73
25	d	403	CLA	CMD-C2D-C1D	7.49	137.92	124.73
25	b	614	CLA	CMD-C2D-C1D	7.48	137.91	124.73
27	b	617	BCR	C20-C19-C18	7.48	146.89	126.36
25	b	611	CLA	CMD-C2D-C1D	7.48	137.91	124.73
27	B	617	BCR	C20-C19-C18	7.48	146.86	126.36
25	B	615	CLA	CMD-C2D-C1D	7.44	137.84	124.73
25	b	615	CLA	CMD-C2D-C1D	7.42	137.80	124.73
25	c	512	CLA	C4A-NA-C1A	7.35	110.03	106.68
27	K	103	BCR	C20-C19-C18	7.33	146.45	126.36
27	k	103	BCR	C20-C19-C18	7.32	146.44	126.36
25	B	616	CLA	CMD-C2D-C1D	7.32	137.62	124.73
25	b	616	CLA	CMD-C2D-C1D	7.31	137.60	124.73
25	c	502	CLA	CMD-C2D-C1D	7.29	137.56	124.73
25	C	502	CLA	CMD-C2D-C1D	7.27	137.53	124.73
25	C	512	CLA	C4A-NA-C1A	7.26	109.99	106.68
25	B	604	CLA	CMD-C2D-C1D	7.24	137.48	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	CMD-C2D-C1D	7.23	137.47	124.73
25	C	509	CLA	CMD-C2D-C1D	7.21	137.43	124.73
25	A	406	CLA	CMD-C2D-C1D	7.21	137.43	124.73
25	c	509	CLA	CMD-C2D-C1D	7.21	137.43	124.73
25	a	406	CLA	CMD-C2D-C1D	7.20	137.41	124.73
27	f	101	BCR	C20-C19-C18	7.13	145.91	126.36
27	F	101	BCR	C20-C19-C18	7.13	145.91	126.36
25	a	408	CLA	CMD-C2D-C1D	7.12	137.26	124.73
27	B	618	BCR	C20-C19-C18	7.12	145.88	126.36
27	b	618	BCR	C20-C19-C18	7.12	145.88	126.36
25	A	408	CLA	CMD-C2D-C1D	7.11	137.26	124.73
27	a	409	BCR	C20-C19-C18	7.07	145.74	126.36
27	A	409	BCR	C20-C19-C18	7.07	145.74	126.36
25	B	605	CLA	CMD-C2D-C1D	7.00	137.05	124.73
25	B	612	CLA	CMD-C2D-C1D	7.00	137.05	124.73
25	b	605	CLA	CMD-C2D-C1D	6.98	137.01	124.73
25	b	612	CLA	CMD-C2D-C1D	6.96	136.99	124.73
25	b	610	CLA	CMD-C2D-C1D	6.90	136.88	124.73
25	b	607	CLA	CMD-C2D-C1D	6.90	136.87	124.73
25	B	610	CLA	CMD-C2D-C1D	6.89	136.87	124.73
25	B	607	CLA	CMD-C2D-C1D	6.89	136.86	124.73
25	B	614	CLA	C4A-NA-C1A	6.80	109.78	106.68
25	c	503	CLA	CMD-C2D-C1D	6.78	136.68	124.73
25	a	408	CLA	C4A-NA-C1A	6.78	109.77	106.68
25	b	614	CLA	C4A-NA-C1A	6.78	109.77	106.68
25	C	503	CLA	CMD-C2D-C1D	6.77	136.65	124.73
25	d	401	CLA	CMD-C2D-C1D	6.75	136.62	124.73
25	D	401	CLA	CMD-C2D-C1D	6.74	136.60	124.73
25	A	408	CLA	C4A-NA-C1A	6.73	109.75	106.68
25	B	604	CLA	C4A-NA-C1A	6.69	109.73	106.68
25	B	605	CLA	C4A-NA-C1A	6.62	109.70	106.68
25	b	604	CLA	C4A-NA-C1A	6.62	109.70	106.68
25	C	512	CLA	CMD-C2D-C1D	6.60	136.35	124.73
25	c	512	CLA	CMD-C2D-C1D	6.59	136.33	124.73
25	b	605	CLA	C4A-NA-C1A	6.58	109.68	106.68
27	Z	101	BCR	C20-C19-C18	6.56	144.34	126.36
27	z	101	BCR	C20-C19-C18	6.56	144.34	126.36
30	c	501	SQD	O6-C1-C2	6.52	118.17	108.27
30	C	501	SQD	O6-C1-C2	6.51	118.16	108.27
25	C	513	CLA	CMD-C2D-C1D	6.42	136.04	124.73
25	c	513	CLA	CMD-C2D-C1D	6.42	136.04	124.73
25	c	508	CLA	C2C-C1C-NC	6.41	116.71	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	619	BCR	C20-C19-C18	6.40	143.92	126.36
27	b	619	BCR	C20-C19-C18	6.40	143.90	126.36
25	C	508	CLA	C2C-C1C-NC	6.39	116.70	109.98
25	b	612	CLA	C4A-NA-C1A	6.39	109.59	106.68
25	B	613	CLA	C2C-C1C-NC	6.34	116.64	109.98
25	B	611	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	B	612	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	C	509	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	c	509	CLA	C4A-NA-C1A	6.31	109.56	106.68
25	b	613	CLA	C2C-C1C-NC	6.29	116.59	109.98
25	b	604	CLA	C2C-C1C-NC	6.28	116.58	109.98
25	A	406	CLA	C4A-NA-C1A	6.26	109.54	106.68
25	C	513	CLA	C2C-C1C-NC	6.26	116.56	109.98
25	B	604	CLA	C2C-C1C-NC	6.25	116.55	109.98
25	b	611	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	C	506	CLA	O2D-CGD-CBD	6.25	122.15	111.23
25	c	513	CLA	C2C-C1C-NC	6.24	116.54	109.98
25	c	506	CLA	O2D-CGD-CBD	6.24	122.14	111.23
25	c	508	CLA	C1C-C2C-C3C	-6.24	100.42	106.98
25	B	610	CLA	C2C-C1C-NC	6.23	116.53	109.98
25	b	610	CLA	C4A-NA-C1A	6.23	109.52	106.68
27	C	515	BCR	C7-C8-C9	-6.23	117.02	126.23
25	a	406	CLA	C4A-NA-C1A	6.23	109.52	106.68
25	b	610	CLA	C2C-C1C-NC	6.23	116.52	109.98
25	D	401	CLA	C4A-NA-C1A	6.22	109.52	106.68
27	c	515	BCR	C7-C8-C9	-6.22	117.04	126.23
25	d	401	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	C	508	CLA	C1C-C2C-C3C	-6.21	100.45	106.98
27	K	103	BCR	C24-C23-C22	-6.18	117.09	126.23
25	B	610	CLA	C4A-NA-C1A	6.18	109.50	106.68
25	a	408	CLA	C2C-C1C-NC	6.18	116.47	109.98
25	B	607	CLA	C4A-NA-C1A	6.17	109.49	106.68
27	k	103	BCR	C24-C23-C22	-6.17	117.11	126.23
25	C	504	CLA	C2C-C1C-NC	6.15	116.44	109.98
25	A	408	CLA	C2C-C1C-NC	6.14	116.44	109.98
25	C	511	CLA	C2C-C1C-NC	6.14	116.43	109.98
25	c	511	CLA	C2C-C1C-NC	6.14	116.43	109.98
25	b	604	CLA	O2D-CGD-CBD	6.13	121.95	111.23
25	A	406	CLA	C2D-C1D-ND	6.13	116.19	110.13
25	b	607	CLA	C4A-NA-C1A	6.13	109.47	106.68
25	B	604	CLA	O2D-CGD-CBD	6.12	121.94	111.23
25	a	406	CLA	C2D-C1D-ND	6.11	116.17	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C2C-C1C-NC	6.11	116.40	109.98
25	b	613	CLA	C1C-C2C-C3C	-6.11	100.56	106.98
25	C	509	CLA	C2C-C1C-NC	6.10	116.39	109.98
25	B	616	CLA	C4A-NA-C1A	6.09	109.46	106.68
25	B	613	CLA	C1C-C2C-C3C	-6.09	100.57	106.98
25	c	504	CLA	C2C-C1C-NC	6.09	116.38	109.98
25	c	505	CLA	C4A-NA-C1A	6.09	109.46	106.68
25	a	405	CLA	C2D-C1D-ND	6.08	116.14	110.13
25	b	616	CLA	C4A-NA-C1A	6.07	109.45	106.68
25	C	508	CLA	O2D-CGD-CBD	6.06	121.83	111.23
25	c	508	CLA	O2D-CGD-CBD	6.05	121.81	111.23
25	b	609	CLA	C2C-C1C-NC	6.03	116.31	109.98
25	B	601	CLA	O2D-CGD-CBD	6.03	121.76	111.23
25	A	405	CLA	C2D-C1D-ND	6.02	116.09	110.13
25	b	601	CLA	O2D-CGD-CBD	6.01	121.74	111.23
25	B	609	CLA	C2C-C1C-NC	6.01	116.29	109.98
25	C	505	CLA	C4A-NA-C1A	6.00	109.42	106.68
27	z	101	BCR	C24-C23-C22	-5.99	117.38	126.23
27	Z	101	BCR	C24-C23-C22	-5.98	117.39	126.23
25	c	505	CLA	C2C-C1C-NC	5.96	116.24	109.98
25	C	505	CLA	C2C-C1C-NC	5.95	116.23	109.98
25	c	503	CLA	C2C-C1C-NC	5.95	116.23	109.98
25	B	615	CLA	C4A-NA-C1A	5.93	109.39	106.68
25	C	503	CLA	C2C-C1C-NC	5.93	116.21	109.98
25	b	615	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	A	406	CLA	C1D-ND-C4D	-5.92	102.16	106.31
25	c	512	CLA	C2C-C1C-NC	5.91	116.19	109.98
27	f	101	BCR	C24-C23-C22	-5.91	117.50	126.23
27	F	101	BCR	C24-C23-C22	-5.90	117.51	126.23
25	C	512	CLA	C2C-C1C-NC	5.89	116.17	109.98
25	C	510	CLA	C2C-C1C-NC	5.88	116.16	109.98
25	c	506	CLA	C2C-C1C-NC	5.88	116.16	109.98
25	c	510	CLA	C2C-C1C-NC	5.88	116.16	109.98
25	a	406	CLA	C1D-ND-C4D	-5.87	102.19	106.31
25	b	612	CLA	C2C-C1C-NC	5.87	116.15	109.98
25	B	614	CLA	C3D-C2D-C1D	-5.86	97.83	105.83
25	B	612	CLA	C2C-C1C-NC	5.86	116.14	109.98
25	B	612	CLA	O2D-CGD-CBD	5.85	121.46	111.23
25	b	612	CLA	O2D-CGD-CBD	5.85	121.45	111.23
25	C	506	CLA	C2C-C1C-NC	5.84	116.12	109.98
25	b	614	CLA	C3D-C2D-C1D	-5.84	97.85	105.83
25	B	612	CLA	C2D-C1D-ND	5.82	115.89	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	CLA	C2D-C1D-ND	5.81	115.88	110.13
25	D	403	CLA	C2D-C1D-ND	5.81	115.88	110.13
25	B	609	CLA	C4A-NA-C1A	5.80	109.33	106.68
25	C	507	CLA	C2C-C1C-NC	5.80	116.07	109.98
25	c	507	CLA	C2C-C1C-NC	5.80	116.07	109.98
25	C	513	CLA	O2D-CGD-CBD	5.79	121.35	111.23
25	c	513	CLA	O2D-CGD-CBD	5.79	121.35	111.23
25	b	612	CLA	C2D-C1D-ND	5.79	115.85	110.13
25	B	606	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	c	504	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	b	613	CLA	C3D-C2D-C1D	-5.78	97.95	105.83
25	B	613	CLA	C3D-C2D-C1D	-5.78	97.95	105.83
25	B	605	CLA	C2D-C1D-ND	5.76	115.83	110.13
25	C	503	CLA	O2D-CGD-CBD	5.76	121.30	111.23
25	b	605	CLA	C2D-C1D-ND	5.76	115.82	110.13
25	b	609	CLA	C4A-NA-C1A	5.76	109.31	106.68
25	c	503	CLA	O2D-CGD-CBD	5.75	121.29	111.23
25	C	504	CLA	C4A-NA-C1A	5.75	109.30	106.68
25	B	603	CLA	O2A-CGA-O1A	-5.75	109.24	123.63
25	b	606	CLA	C4A-NA-C1A	5.74	109.30	106.68
25	b	603	CLA	O2A-CGA-O1A	-5.74	109.28	123.63
25	b	603	CLA	C4A-NA-C1A	5.73	109.29	106.68
25	b	610	CLA	C1C-C2C-C3C	-5.73	100.95	106.98
25	b	613	CLA	C4A-NA-C1A	5.73	109.29	106.68
25	C	513	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
25	b	604	CLA	C1C-C2C-C3C	-5.71	100.98	106.98
25	b	609	CLA	C1C-C2C-C3C	-5.70	100.98	106.98
25	B	603	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	B	613	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	B	610	CLA	C1C-C2C-C3C	-5.70	100.98	106.98
25	C	504	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
25	C	512	CLA	C2D-C1D-ND	5.69	115.75	110.13
25	c	512	CLA	C2D-C1D-ND	5.68	115.75	110.13
25	B	604	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
25	c	513	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
25	c	504	CLA	C3D-C2D-C1D	-5.68	98.09	105.83
25	B	605	CLA	O2D-CGD-CBD	5.67	121.14	111.23
25	C	509	CLA	C1C-C2C-C3C	-5.67	101.02	106.98
25	C	504	CLA	C3D-C2D-C1D	-5.67	98.10	105.83
25	d	404	CLA	O2D-CGD-CBD	5.66	121.13	111.23
25	B	609	CLA	C1C-C2C-C3C	-5.66	101.02	106.98
25	b	607	CLA	C3D-C2D-C1D	-5.66	98.10	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	O2D-CGD-CBD	5.66	121.13	111.23
25	c	509	CLA	C1C-C2C-C3C	-5.66	101.03	106.98
25	D	404	CLA	O2D-CGD-CBD	5.66	121.12	111.23
25	B	607	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
25	c	504	CLA	C1C-C2C-C3C	-5.63	101.05	106.98
25	a	405	CLA	C3D-C2D-C1D	-5.63	98.14	105.83
25	B	611	CLA	C2C-C1C-NC	5.63	115.89	109.98
25	c	514	CLA	C4A-NA-C1A	5.62	109.25	106.68
25	b	611	CLA	C2C-C1C-NC	5.62	115.88	109.98
25	A	405	CLA	C3D-C2D-C1D	-5.61	98.17	105.83
25	b	612	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
25	B	615	CLA	C2C-C1C-NC	5.60	115.86	109.98
25	B	616	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
25	c	502	CLA	C2C-C1C-NC	5.59	115.85	109.98
25	C	510	CLA	O2A-CGA-O1A	-5.59	109.64	123.63
25	C	502	CLA	C2C-C1C-NC	5.59	115.85	109.98
25	b	616	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
25	b	605	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
25	c	508	CLA	C4A-NA-C1A	5.59	109.23	106.68
25	c	510	CLA	O2A-CGA-O1A	-5.59	109.65	123.63
25	d	404	CLA	C2C-C1C-NC	5.59	115.85	109.98
29	a	411	PL9	C7-C3-C4	5.58	121.51	116.91
25	c	505	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
25	b	615	CLA	C2C-C1C-NC	5.58	115.84	109.98
25	a	408	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
25	C	508	CLA	C4A-NA-C1A	5.58	109.22	106.68
25	D	404	CLA	C2C-C1C-NC	5.58	115.84	109.98
25	B	614	CLA	C2D-C1D-ND	5.58	115.64	110.13
25	C	514	CLA	C4A-NA-C1A	5.57	109.22	106.68
29	A	411	PL9	C7-C3-C4	5.57	121.50	116.91
25	D	403	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
25	B	612	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
25	B	605	CLA	C1C-C2C-C3C	-5.57	101.13	106.98
25	A	408	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
25	C	505	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
25	a	406	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
25	b	602	CLA	C4A-NA-C1A	5.56	109.22	106.68
25	b	614	CLA	C2D-C1D-ND	5.56	115.62	110.13
25	d	403	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
25	C	511	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
25	A	406	CLA	C3D-C2D-C1D	-5.54	98.26	105.83
25	B	605	CLA	C3D-C2D-C1D	-5.54	98.27	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
25	c	510	CLA	C1C-C2C-C3C	-5.53	101.17	106.98
25	b	605	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
27	C	515	BCR	C24-C23-C22	-5.52	118.07	126.23
25	C	510	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
27	B	619	BCR	C24-C23-C22	-5.51	118.09	126.23
27	b	619	BCR	C24-C23-C22	-5.50	118.09	126.23
25	A	406	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
27	c	515	BCR	C24-C23-C22	-5.50	118.10	126.23
25	d	401	CLA	C2C-C1C-NC	5.50	115.75	109.98
25	C	512	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
27	a	409	BCR	C24-C23-C22	-5.49	118.11	126.23
25	B	602	CLA	C4A-NA-C1A	5.49	109.18	106.68
25	c	512	CLA	C3D-C2D-C1D	-5.49	98.35	105.83
25	b	601	CLA	C2D-C1D-ND	5.48	115.55	110.13
25	D	401	CLA	C2C-C1C-NC	5.48	115.74	109.98
25	c	513	CLA	C2D-C1D-ND	5.48	115.55	110.13
25	b	613	CLA	C2D-C1D-ND	5.48	115.55	110.13
25	a	406	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
25	a	405	CLA	C1D-ND-C4D	-5.47	102.47	106.31
25	C	513	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
25	C	513	CLA	C2D-C1D-ND	5.47	115.54	110.13
25	A	408	CLA	O2D-CGD-CBD	5.47	120.79	111.23
25	B	602	CLA	C2C-C1C-NC	5.47	115.73	109.98
27	A	409	BCR	C24-C23-C22	-5.47	118.14	126.23
25	b	616	CLA	C2C-C1C-NC	5.47	115.73	109.98
25	c	513	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	B	607	CLA	C2D-C1D-ND	5.47	115.54	110.13
25	b	610	CLA	C2D-C1D-ND	5.47	115.54	110.13
25	B	616	CLA	C2D-C1D-ND	5.47	115.53	110.13
25	b	616	CLA	C2D-C1D-ND	5.46	115.53	110.13
25	C	506	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
25	c	506	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
25	B	601	CLA	C2D-C1D-ND	5.46	115.53	110.13
25	B	616	CLA	C2C-C1C-NC	5.46	115.72	109.98
25	b	607	CLA	C2D-C1D-ND	5.46	115.53	110.13
25	B	615	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
25	b	614	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
25	A	405	CLA	C1D-ND-C4D	-5.46	102.48	106.31
25	b	606	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
25	a	406	CLA	O2A-CGA-O1A	-5.45	109.98	123.63
25	B	610	CLA	C2D-C1D-ND	5.45	115.52	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
25	D	404	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
25	b	612	CLA	C1D-ND-C4D	-5.45	102.49	106.31
25	b	614	CLA	C2C-C1C-NC	5.45	115.70	109.98
25	d	404	CLA	C1C-C2C-C3C	-5.44	101.25	106.98
25	A	406	CLA	O2A-CGA-O1A	-5.44	110.02	123.63
25	a	408	CLA	O2D-CGD-CBD	5.44	120.74	111.23
25	B	612	CLA	C1D-ND-C4D	-5.44	102.50	106.31
25	b	615	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
25	C	509	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
25	B	613	CLA	C2D-C1D-ND	5.44	115.51	110.13
25	B	606	CLA	O2D-CGD-CBD	5.43	120.73	111.23
25	b	606	CLA	C2C-C1C-NC	5.43	115.69	109.98
25	b	606	CLA	O2D-CGD-CBD	5.42	120.71	111.23
25	c	509	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
25	B	614	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
25	B	609	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
25	b	602	CLA	C2C-C1C-NC	5.42	115.67	109.98
25	d	403	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
25	b	609	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
25	B	614	CLA	C2C-C1C-NC	5.40	115.65	109.98
25	B	606	CLA	C2C-C1C-NC	5.40	115.65	109.98
25	C	505	CLA	O2D-CGD-CBD	5.40	120.67	111.23
25	c	505	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	b	608	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	c	511	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	B	608	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	D	403	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
25	b	616	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
25	B	616	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
25	b	607	CLA	C2C-C1C-NC	5.36	115.61	109.98
25	B	615	CLA	C2D-C1D-ND	5.36	115.43	110.13
25	b	609	CLA	O2A-CGA-O1A	-5.36	110.23	123.63
25	c	507	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
25	b	601	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
25	d	401	CLA	C2D-C1D-ND	5.35	115.42	110.13
25	B	609	CLA	O2A-CGA-O1A	-5.35	110.24	123.63
25	B	607	CLA	C2C-C1C-NC	5.35	115.60	109.98
25	C	507	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
25	C	511	CLA	O2D-CGD-CBD	5.35	120.58	111.23
25	B	601	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
25	B	603	CLA	C1C-C2C-C3C	-5.35	101.36	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	C1D-ND-C4D	-5.35	102.56	106.31
25	D	401	CLA	C2D-C1D-ND	5.34	115.41	110.13
25	C	504	CLA	C2D-C1D-ND	5.34	115.41	110.13
25	B	612	CLA	O2A-CGA-O1A	-5.34	110.28	123.63
25	c	502	CLA	O2A-CGA-O1A	-5.34	110.28	123.63
25	c	504	CLA	C2D-C1D-ND	5.33	115.41	110.13
25	B	603	CLA	O2D-CGD-CBD	5.33	120.55	111.23
25	b	612	CLA	O2A-CGA-O1A	-5.33	110.30	123.63
25	C	502	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
25	b	603	CLA	O2D-CGD-CBD	5.33	120.55	111.23
25	D	404	CLA	C1D-ND-C4D	-5.33	102.57	106.31
25	c	502	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
25	b	615	CLA	C2D-C1D-ND	5.33	115.40	110.13
25	c	509	CLA	C2D-C1D-ND	5.32	115.40	110.13
25	b	603	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
27	k	103	BCR	C7-C8-C9	-5.32	118.36	126.23
25	D	401	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
25	B	605	CLA	C1D-ND-C4D	-5.32	102.58	106.31
25	d	401	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
25	c	507	CLA	O2D-CGD-CBD	5.31	120.52	111.23
25	C	502	CLA	O2A-CGA-O1A	-5.31	110.34	123.63
27	K	103	BCR	C7-C8-C9	-5.31	118.38	126.23
25	B	613	CLA	C1-C2-C3	-5.31	117.50	126.20
25	C	514	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
25	b	613	CLA	C1-C2-C3	-5.30	117.52	126.20
25	C	507	CLA	O2D-CGD-CBD	5.30	120.49	111.23
25	d	404	CLA	C1D-ND-C4D	-5.29	102.60	106.31
25	C	509	CLA	C2D-C1D-ND	5.29	115.36	110.13
25	c	514	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
25	C	503	CLA	C4A-NA-C1A	5.29	109.09	106.68
25	B	612	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
25	c	503	CLA	C4A-NA-C1A	5.28	109.09	106.68
25	B	603	CLA	C2C-C1C-NC	5.28	115.53	109.98
25	a	406	CLA	O2D-CGD-CBD	5.28	120.45	111.23
25	c	503	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
25	b	612	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
25	B	605	CLA	C2C-C1C-NC	5.26	115.51	109.98
25	b	605	CLA	C2C-C1C-NC	5.26	115.51	109.98
25	A	406	CLA	O2D-CGD-CBD	5.26	120.43	111.23
25	c	512	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
25	C	512	CLA	O2A-CGA-O1A	-5.25	110.50	123.63
25	C	514	CLA	C2C-C1C-NC	5.25	115.50	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
25	D	403	CLA	C2C-C1C-NC	5.25	115.49	109.98
25	b	603	CLA	C2C-C1C-NC	5.25	115.49	109.98
25	c	514	CLA	C2C-C1C-NC	5.25	115.49	109.98
25	B	616	CLA	O2D-CGD-CBD	5.24	120.40	111.23
25	d	403	CLA	C2C-C1C-NC	5.24	115.49	109.98
25	C	503	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
25	C	512	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
25	D	401	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
27	b	618	BCR	C24-C23-C22	-5.24	118.49	126.23
25	B	606	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	d	401	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	C	510	CLA	O2D-CGD-CBD	5.22	120.36	111.23
25	B	611	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
27	B	618	BCR	C24-C23-C22	-5.22	118.51	126.23
25	b	601	CLA	C1D-ND-C4D	-5.22	102.65	106.31
25	b	611	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
25	B	602	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
25	b	606	CLA	C3D-C2D-C1D	-5.21	98.71	105.83
25	b	616	CLA	O2D-CGD-CBD	5.21	120.34	111.23
25	B	601	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
25	c	510	CLA	O2D-CGD-CBD	5.21	120.33	111.23
25	C	514	CLA	C2D-C1D-ND	5.21	115.28	110.13
25	C	510	CLA	C4A-NA-C1A	5.21	109.05	106.68
25	b	602	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
25	b	610	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
25	a	408	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
25	b	602	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
25	A	408	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
25	b	601	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
25	B	610	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
25	B	601	CLA	C1D-ND-C4D	-5.18	102.67	106.31
25	B	602	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
25	C	505	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
25	c	505	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
25	b	606	CLA	C2D-C1D-ND	5.17	115.25	110.13
25	c	514	CLA	C2D-C1D-ND	5.17	115.24	110.13
25	D	404	CLA	C4A-NA-C1A	5.16	109.03	106.68
25	C	504	CLA	O2D-CGD-CBD	5.15	120.24	111.23
25	b	608	CLA	C2C-C1C-NC	5.15	115.39	109.98
25	b	611	CLA	C1C-C2C-C3C	-5.15	101.57	106.98
25	b	607	CLA	O2D-CGD-CBD	5.15	120.23	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	C4A-NA-C1A	5.15	109.03	106.68
25	c	502	CLA	O2D-CGD-CBD	5.15	120.23	111.23
25	d	404	CLA	C4A-NA-C1A	5.14	109.03	106.68
25	c	510	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
25	C	502	CLA	O2D-CGD-CBD	5.14	120.21	111.23
25	c	504	CLA	O2D-CGD-CBD	5.14	120.21	111.23
25	B	607	CLA	O2D-CGD-CBD	5.14	120.21	111.23
25	B	606	CLA	C2D-C1D-ND	5.14	115.21	110.13
25	c	514	CLA	O2A-CGA-O1A	-5.13	110.79	123.63
25	B	611	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
25	c	507	CLA	O2A-CGA-O1A	-5.12	110.81	123.63
25	C	507	CLA	O2A-CGA-O1A	-5.12	110.81	123.63
25	A	406	CLA	C2C-C1C-NC	5.12	115.36	109.98
25	C	510	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
25	C	514	CLA	O2A-CGA-O1A	-5.12	110.82	123.63
25	B	601	CLA	C2C-C1C-NC	5.12	115.36	109.98
25	C	514	CLA	O2D-CGD-CBD	5.12	120.18	111.23
25	C	511	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
25	B	608	CLA	C2C-C1C-NC	5.11	115.35	109.98
25	c	514	CLA	O2D-CGD-CBD	5.11	120.16	111.23
25	C	507	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
25	c	505	CLA	O2A-CGA-O1A	-5.11	110.86	123.63
25	a	406	CLA	C2C-C1C-NC	5.10	115.34	109.98
25	c	507	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	B	614	CLA	O2D-CGD-CBD	5.10	120.14	111.23
25	b	614	CLA	O2D-CGD-CBD	5.10	120.14	111.23
25	b	601	CLA	C2C-C1C-NC	5.09	115.33	109.98
25	C	505	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
25	c	509	CLA	C1D-ND-C4D	-5.09	102.74	106.31
25	a	408	CLA	C2D-C1D-ND	5.09	115.16	110.13
25	A	408	CLA	C2D-C1D-ND	5.08	115.16	110.13
25	c	511	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
25	b	608	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
25	B	609	CLA	C2D-C1D-ND	5.07	115.15	110.13
25	B	611	CLA	O2D-CGD-CBD	5.07	120.10	111.23
25	d	401	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
25	D	401	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
25	C	512	CLA	O2D-CGD-CBD	5.07	120.09	111.23
25	b	611	CLA	O2D-CGD-CBD	5.07	120.09	111.23
25	b	607	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
25	B	604	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
25	b	611	CLA	O2A-CGA-O1A	-5.06	110.96	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
25	C	503	CLA	C2D-C1D-ND	5.06	115.14	110.13
25	c	508	CLA	O2A-CGA-O1A	-5.06	110.97	123.63
25	B	608	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
25	c	512	CLA	O2D-CGD-CBD	5.05	120.06	111.23
25	b	609	CLA	C2D-C1D-ND	5.05	115.12	110.13
25	B	607	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
25	b	604	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
25	C	508	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
25	c	503	CLA	C2D-C1D-ND	5.04	115.12	110.13
25	c	508	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
25	C	508	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
25	B	601	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	c	514	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
27	K	102	BCR	C24-C23-C22	-5.03	118.80	126.23
25	b	608	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
25	c	506	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	C	509	CLA	C1D-ND-C4D	-5.02	102.79	106.31
25	C	514	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
25	B	606	CLA	O2A-CGA-O1A	-5.01	111.09	123.63
25	B	608	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
25	b	606	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
25	C	504	CLA	O2A-CGA-O1A	-5.00	111.11	123.63
27	k	102	BCR	C24-C23-C22	-5.00	118.84	126.23
25	c	513	CLA	O2A-CGA-O1A	-5.00	111.12	123.63
25	C	506	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	c	504	CLA	O2A-CGA-O1A	-5.00	111.13	123.63
25	b	607	CLA	O2A-CGA-O1A	-4.99	111.14	123.63
25	B	607	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
25	b	601	CLA	C4A-NA-C1A	4.99	108.95	106.68
25	C	503	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	C	513	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
25	d	404	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
32	A	417	BCT	O2-C-O1	4.98	132.41	119.68
25	D	403	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
25	D	404	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
25	C	509	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	c	509	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	d	403	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
27	B	619	BCR	C7-C8-C9	-4.97	118.89	126.23
32	a	417	BCT	O2-C-O1	4.97	132.38	119.68
25	c	503	CLA	C3D-C2D-C1D	-4.95	99.08	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	C2D-C1D-ND	4.95	115.02	110.13
27	b	619	BCR	C7-C8-C9	-4.94	118.93	126.23
25	D	404	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
25	b	616	CLA	C1D-ND-C4D	-4.93	102.86	106.31
25	B	615	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
25	b	615	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
25	d	404	CLA	C2D-C1D-ND	4.92	114.99	110.13
25	d	404	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
25	B	616	CLA	C1D-ND-C4D	-4.91	102.86	106.31
25	C	513	CLA	C4A-NA-C1A	4.90	108.92	106.68
25	B	614	CLA	O2A-CGA-O1A	-4.90	111.38	123.63
25	b	614	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
25	C	510	CLA	C2D-C1D-ND	4.89	114.97	110.13
25	c	510	CLA	C2D-C1D-ND	4.89	114.96	110.13
25	c	509	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
25	c	505	CLA	C2D-C1D-ND	4.88	114.95	110.13
25	C	509	CLA	O2A-CGA-O1A	-4.88	111.43	123.63
25	c	513	CLA	C4A-NA-C1A	4.88	108.90	106.68
25	C	505	CLA	C2D-C1D-ND	4.88	114.95	110.13
25	B	608	CLA	C1D-ND-C4D	-4.87	102.89	106.31
25	d	403	CLA	C1D-ND-C4D	-4.87	102.89	106.31
25	b	608	CLA	C1D-ND-C4D	-4.87	102.89	106.31
25	B	607	CLA	C1D-ND-C4D	-4.87	102.90	106.31
25	b	607	CLA	C1D-ND-C4D	-4.86	102.90	106.31
25	a	405	CLA	C2C-C1C-NC	4.86	115.09	109.98
25	A	405	CLA	C2C-C1C-NC	4.86	115.08	109.98
25	D	403	CLA	C1D-ND-C4D	-4.85	102.91	106.31
25	B	610	CLA	O2D-CGD-CBD	4.85	119.70	111.23
25	B	615	CLA	O2D-CGD-CBD	4.84	119.70	111.23
25	c	503	CLA	C1-C2-C3	-4.84	118.26	126.20
25	C	503	CLA	C1-C2-C3	-4.84	118.27	126.20
25	b	615	CLA	O2D-CGD-CBD	4.84	119.69	111.23
25	b	609	CLA	O2D-CGD-CBD	4.83	119.68	111.23
25	b	610	CLA	O2D-CGD-CBD	4.83	119.67	111.23
25	B	609	CLA	O2D-CGD-CBD	4.82	119.66	111.23
25	d	403	CLA	O2D-CGD-CBD	4.82	119.66	111.23
25	D	403	CLA	O2D-CGD-CBD	4.82	119.65	111.23
25	b	608	CLA	C2D-C1D-ND	4.81	114.89	110.13
25	B	608	CLA	C2D-C1D-ND	4.81	114.88	110.13
25	a	405	CLA	O2A-CGA-O1A	-4.80	111.61	123.63
25	A	405	CLA	O2A-CGA-O1A	-4.80	111.61	123.63
25	B	604	CLA	C1-C2-C3	-4.79	118.35	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
25	B	602	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
25	c	507	CLA	C4A-NA-C1A	4.78	108.86	106.68
25	b	604	CLA	C1-C2-C3	-4.77	118.37	126.20
25	b	606	CLA	C1D-ND-C4D	-4.75	102.98	106.31
30	a	412	SQD	O7-S-C6	4.74	113.83	106.76
25	b	610	CLA	C1D-ND-C4D	-4.73	102.99	106.31
25	A	408	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
25	C	507	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	a	405	CLA	C1C-C2C-C3C	-4.73	102.01	106.98
25	a	408	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
30	A	412	SQD	O7-S-C6	4.73	113.81	106.76
25	b	603	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
25	B	603	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
25	A	405	CLA	C1C-C2C-C3C	-4.71	102.02	106.98
25	B	602	CLA	C2D-C1D-ND	4.71	114.79	110.13
25	C	511	CLA	C2D-C1D-ND	4.71	114.79	110.13
25	b	602	CLA	C2D-C1D-ND	4.71	114.79	110.13
25	C	511	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
25	B	610	CLA	C1D-ND-C4D	-4.70	103.01	106.31
30	a	413	SQD	C1-O5-C5	4.70	122.89	113.72
25	c	511	CLA	O2A-CGA-O1A	-4.69	111.88	123.63
25	B	611	CLA	C2D-C1D-ND	4.69	114.77	110.13
25	c	511	CLA	C2D-C1D-ND	4.69	114.77	110.13
30	A	413	SQD	C1-O5-C5	4.67	122.85	113.72
25	B	606	CLA	C1D-ND-C4D	-4.67	103.04	106.31
27	b	617	BCR	C24-C23-C22	-4.66	119.33	126.23
25	B	604	CLA	C2D-C1D-ND	4.66	114.74	110.13
25	b	604	CLA	C2D-C1D-ND	4.66	114.74	110.13
25	c	502	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
25	B	610	CLA	O2A-CGA-O1A	-4.66	111.97	123.63
25	D	401	CLA	C1D-ND-C4D	-4.66	103.04	106.31
27	B	617	BCR	C24-C23-C22	-4.66	119.34	126.23
25	B	613	CLA	O2A-CGA-O1A	-4.66	111.97	123.63
25	b	613	CLA	O2D-CGD-CBD	4.66	119.37	111.23
25	b	610	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
25	B	602	CLA	O2D-CGD-CBD	4.64	119.34	111.23
25	b	613	CLA	O2A-CGA-O1A	-4.64	112.03	123.63
25	B	613	CLA	O2D-CGD-CBD	4.64	119.33	111.23
25	b	611	CLA	C2D-C1D-ND	4.63	114.71	110.13
25	C	514	CLA	C1D-ND-C4D	-4.63	103.06	106.31
25	d	401	CLA	C1D-ND-C4D	-4.63	103.06	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	CLA	C1D-ND-C4D	-4.63	103.07	106.31
25	C	506	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
25	C	502	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
25	c	507	CLA	C2D-C1D-ND	4.62	114.70	110.13
25	C	511	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	C	507	CLA	C2D-C1D-ND	4.62	114.70	110.13
25	B	603	CLA	C2D-C1D-ND	4.61	114.69	110.13
25	b	602	CLA	O2D-CGD-CBD	4.61	119.29	111.23
25	b	603	CLA	C2D-C1D-ND	4.61	114.69	110.13
25	B	608	CLA	O2A-CGA-O1A	-4.61	112.11	123.63
25	b	608	CLA	O2A-CGA-O1A	-4.60	112.12	123.63
25	C	512	CLA	C1D-ND-C4D	-4.60	103.08	106.31
25	c	506	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
25	c	508	CLA	C2D-C1D-ND	4.59	114.67	110.13
25	c	512	CLA	C1D-ND-C4D	-4.59	103.09	106.31
25	B	614	CLA	C1D-ND-C4D	-4.57	103.10	106.31
25	c	511	CLA	C4A-NA-C1A	4.57	108.76	106.68
25	b	601	CLA	O2A-CGA-O1A	-4.57	111.58	123.33
25	B	601	CLA	O2A-CGA-O1A	-4.57	111.58	123.33
33	z	102	LHG	O7-C7-C8	4.55	121.33	111.48
25	b	614	CLA	C1D-ND-C4D	-4.55	103.12	106.31
25	C	508	CLA	C2D-C1D-ND	4.54	114.62	110.13
33	Z	102	LHG	O7-C7-C8	4.54	121.31	111.48
25	c	505	CLA	C1D-ND-C4D	-4.54	103.13	106.31
27	K	102	BCR	C3-C4-C5	-4.54	105.97	114.06
27	b	619	BCR	C28-C27-C26	-4.53	105.98	114.06
25	b	615	CLA	O2A-CGA-O1A	-4.53	112.31	123.63
27	k	102	BCR	C3-C4-C5	-4.53	105.98	114.06
25	D	401	CLA	O2D-CGD-CBD	4.52	119.14	111.23
25	d	401	CLA	O2D-CGD-CBD	4.52	119.14	111.23
27	C	515	BCR	C33-C5-C6	-4.52	119.55	124.48
25	A	408	CLA	C1D-ND-C4D	-4.52	103.14	106.31
25	B	615	CLA	O2A-CGA-O1A	-4.52	112.32	123.63
27	B	619	BCR	C28-C27-C26	-4.52	106.00	114.06
27	c	515	BCR	C33-C5-C6	-4.51	119.56	124.48
30	A	413	SQD	O5-C5-C4	4.51	117.82	109.70
30	a	413	SQD	O5-C5-C4	4.50	117.81	109.70
25	C	505	CLA	C1D-ND-C4D	-4.50	103.16	106.31
25	C	504	CLA	C1D-ND-C4D	-4.49	103.16	106.31
25	a	408	CLA	C1D-ND-C4D	-4.49	103.16	106.31
25	c	504	CLA	C1D-ND-C4D	-4.48	103.17	106.31
25	b	616	CLA	C1C-C2C-C3C	-4.48	102.27	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	O2A-CGA-CBA	4.48	125.48	111.83
25	B	615	CLA	C1D-ND-C4D	-4.47	103.17	106.31
25	B	616	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
25	b	609	CLA	C1-C2-C3	-4.47	118.87	126.20
25	B	609	CLA	C1-C2-C3	-4.47	118.87	126.20
25	b	615	CLA	C1D-ND-C4D	-4.47	103.18	106.31
25	B	616	CLA	O2A-CGA-CBA	4.46	125.43	111.83
25	c	506	CLA	O2A-CGA-O1A	-4.45	112.49	123.63
25	c	513	CLA	O2A-CGA-CBA	4.45	125.40	111.83
25	C	513	CLA	O2A-CGA-CBA	4.45	125.40	111.83
25	C	506	CLA	O2A-CGA-O1A	-4.45	112.51	123.63
25	B	608	CLA	C4A-NA-C1A	4.44	108.70	106.68
25	b	608	CLA	C4A-NA-C1A	4.43	108.70	106.68
27	K	102	BCR	C7-C8-C9	-4.43	119.68	126.23
25	C	506	CLA	C1D-ND-C4D	-4.43	103.21	106.31
27	k	102	BCR	C7-C8-C9	-4.42	119.69	126.23
25	C	503	CLA	C1D-ND-C4D	-4.41	103.22	106.31
25	C	503	CLA	O2A-CGA-O1A	-4.40	112.61	123.63
25	b	614	CLA	C1-C2-C3	-4.40	118.99	126.20
25	c	506	CLA	C1D-ND-C4D	-4.40	103.23	106.31
25	c	503	CLA	O2A-CGA-O1A	-4.40	112.63	123.63
29	A	411	PL9	C7-C3-C2	-4.39	118.21	123.39
25	b	602	CLA	C1-C2-C3	-4.39	119.01	126.20
25	c	503	CLA	C1D-ND-C4D	-4.39	103.23	106.31
25	B	602	CLA	C1-C2-C3	-4.38	119.02	126.20
25	B	614	CLA	C1-C2-C3	-4.38	119.03	126.20
25	C	511	CLA	C1D-ND-C4D	-4.37	103.25	106.31
29	a	411	PL9	C7-C3-C2	-4.37	118.24	123.39
27	b	618	BCR	C7-C8-C9	-4.37	119.78	126.23
25	c	511	CLA	C1D-ND-C4D	-4.36	103.25	106.31
25	C	510	CLA	O2A-CGA-CBA	4.36	125.12	111.83
25	B	604	CLA	O2A-CGA-O1A	-4.36	112.73	123.63
25	B	609	CLA	C1D-ND-C4D	-4.36	103.25	106.31
25	b	604	CLA	O2A-CGA-O1A	-4.35	112.74	123.63
25	c	510	CLA	O2A-CGA-CBA	4.35	125.10	111.83
25	b	609	CLA	C1D-ND-C4D	-4.34	103.27	106.31
31	a	415	LMT	O5B-C5B-C4B	4.34	117.52	109.70
27	B	618	BCR	C7-C8-C9	-4.33	119.83	126.23
28	d	409	LMG	O7-C10-C11	4.33	120.84	111.48
28	D	409	LMG	O7-C10-C11	4.32	120.84	111.48
25	B	603	CLA	O2A-CGA-CBA	4.32	125.01	111.83
25	c	514	CLA	C1-C2-C3	-4.32	119.12	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	621	LMG	O7-C10-C11	4.32	120.82	111.48
25	C	514	CLA	C1-C2-C3	-4.32	119.13	126.20
31	A	415	LMT	O5B-C5B-C4B	4.31	117.47	109.70
25	c	510	CLA	C1D-ND-C4D	-4.31	103.29	106.31
28	b	621	LMG	O7-C10-C11	4.30	120.79	111.48
25	b	609	CLA	O2A-CGA-CBA	4.30	124.96	111.83
25	b	603	CLA	O2A-CGA-CBA	4.30	124.95	111.83
28	a	410	LMG	O7-C10-C11	4.30	120.79	111.48
25	C	512	CLA	C1-C2-C3	-4.30	119.15	126.20
25	C	510	CLA	C1D-ND-C4D	-4.30	103.30	106.31
27	B	617	BCR	C3-C4-C5	-4.30	106.39	114.06
28	A	410	LMG	O7-C10-C11	4.30	120.78	111.48
25	c	502	CLA	C2D-C1D-ND	4.30	114.38	110.13
25	b	613	CLA	C1D-ND-C4D	-4.29	103.30	106.31
25	B	609	CLA	O2A-CGA-CBA	4.29	124.92	111.83
33	d	406	LHG	O7-C7-C8	4.29	120.76	111.48
27	b	617	BCR	C3-C4-C5	-4.29	106.41	114.06
33	D	406	LHG	O7-C7-C8	4.28	120.73	111.48
30	b	620	SQD	O5-C5-C4	4.27	117.40	109.70
25	B	613	CLA	C1D-ND-C4D	-4.27	103.32	106.31
25	c	512	CLA	C1-C2-C3	-4.27	119.21	126.20
30	B	620	SQD	O5-C5-C4	4.26	117.38	109.70
25	C	502	CLA	C2D-C1D-ND	4.26	114.34	110.13
29	d	405	PL9	C7-C3-C4	4.25	120.41	116.91
28	A	414	LMG	O7-C10-C11	4.25	120.68	111.48
28	a	414	LMG	O7-C10-C11	4.25	120.68	111.48
25	C	506	CLA	C2D-C1D-ND	4.25	114.33	110.13
31	A	415	LMT	C3'-C4'-C5'	-4.24	101.54	110.93
25	b	612	CLA	O2A-CGA-CBA	4.23	124.75	111.83
25	c	506	CLA	C2D-C1D-ND	4.23	114.32	110.13
25	B	612	CLA	O2A-CGA-CBA	4.23	124.75	111.83
31	a	415	LMT	C3'-C4'-C5'	-4.23	101.54	110.93
25	B	605	CLA	O2A-CGA-O1A	-4.23	113.05	123.63
25	b	605	CLA	O2A-CGA-O1A	-4.22	113.06	123.63
25	d	404	CLA	CHD-C1D-ND	-4.21	118.88	124.80
29	D	405	PL9	C7-C3-C4	4.21	120.38	116.91
34	C	518	DGD	O2G-C1B-C2B	4.21	120.58	111.48
34	c	518	DGD	O2G-C1B-C2B	4.20	120.58	111.48
33	d	408	LHG	O7-C7-C8	4.20	120.57	111.48
25	c	512	CLA	O2A-CGA-CBA	4.20	124.64	111.83
25	C	512	CLA	O2A-CGA-CBA	4.20	124.64	111.83
25	D	404	CLA	CHD-C1D-ND	-4.20	118.89	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	408	LHG	O7-C7-C8	4.19	120.55	111.48
25	D	403	CLA	O2A-CGA-CBA	4.17	124.55	111.83
25	d	403	CLA	O2A-CGA-CBA	4.16	124.53	111.83
25	B	603	CLA	C1D-ND-C4D	-4.15	103.40	106.31
25	b	603	CLA	C1D-ND-C4D	-4.13	103.42	106.31
25	c	514	CLA	O2A-CGA-CBA	4.13	124.42	111.83
30	f	102	SQD	C1-O5-C5	4.12	121.77	113.72
30	F	102	SQD	C1-O5-C5	4.12	121.76	113.72
25	C	514	CLA	O2A-CGA-CBA	4.12	124.39	111.83
30	a	412	SQD	O9-S-O7	-4.11	100.45	113.82
34	C	516	DGD	O2G-C1B-C2B	4.11	120.37	111.48
30	A	412	SQD	O9-S-O7	-4.11	100.46	113.82
25	C	502	CLA	C4A-NA-C1A	4.11	108.55	106.68
30	f	102	SQD	O5-C5-C4	4.10	117.09	109.70
25	c	502	CLA	O2A-CGA-CBA	4.10	124.34	111.83
25	C	502	CLA	O2A-CGA-CBA	4.10	124.33	111.83
25	c	502	CLA	C4A-NA-C1A	4.10	108.55	106.68
30	F	102	SQD	O5-C5-C4	4.10	117.08	109.70
34	c	516	DGD	O2G-C1B-C2B	4.10	120.34	111.48
27	A	409	BCR	C7-C8-C9	-4.09	120.18	126.23
25	b	610	CLA	O2A-CGA-CBA	4.09	124.31	111.83
25	c	507	CLA	C1D-ND-C4D	-4.09	103.44	106.31
25	D	401	CLA	C1-C2-C3	-4.08	119.51	126.20
25	B	610	CLA	O2A-CGA-CBA	4.08	124.27	111.83
25	C	507	CLA	C1D-ND-C4D	-4.07	103.45	106.31
27	k	103	BCR	C33-C5-C6	-4.05	120.06	124.48
27	a	409	BCR	C7-C8-C9	-4.05	120.24	126.23
25	d	401	CLA	C1-C2-C3	-4.05	119.56	126.20
27	f	101	BCR	C38-C26-C25	-4.05	120.07	124.48
27	F	101	BCR	C38-C26-C25	-4.04	120.07	124.48
27	K	103	BCR	C33-C5-C6	-4.04	120.07	124.48
25	a	405	CLA	O2A-CGA-CBA	4.04	124.16	111.83
25	A	405	CLA	O2A-CGA-CBA	4.02	124.10	111.83
25	a	406	CLA	O2A-CGA-CBA	4.02	124.10	111.83
25	A	406	CLA	O2A-CGA-CBA	4.02	124.09	111.83
30	h	102	SQD	O9-S-C6	4.02	112.75	106.76
28	b	621	LMG	C8-O7-C10	-4.01	108.19	117.80
27	Z	101	BCR	C38-C26-C25	-4.01	120.11	124.48
30	H	102	SQD	O9-S-C6	4.01	112.75	106.76
27	z	101	BCR	C38-C26-C25	-4.01	120.11	124.48
28	B	621	LMG	C8-O7-C10	-4.01	108.21	117.80
31	D	411	LMT	O1'-C1'-C2'	3.99	114.33	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C7-C3-C2	-3.98	118.70	123.39
31	C	522	LMT	O5'-C5'-C4'	3.98	116.86	109.70
31	c	522	LMT	O5'-C5'-C4'	3.97	116.85	109.70
31	d	411	LMT	O1'-C1'-C2'	3.96	114.29	108.27
25	a	405	CLA	CMC-C2C-C1C	3.95	131.21	125.03
25	A	405	CLA	CMC-C2C-C1C	3.95	131.20	125.03
25	c	507	CLA	O2A-CGA-CBA	3.94	123.86	111.83
30	A	412	SQD	C44-O6-C1	3.94	122.25	113.80
25	C	503	CLA	O2A-C1-C2	3.94	123.26	108.11
25	C	507	CLA	O2A-CGA-CBA	3.94	123.84	111.83
25	B	602	CLA	CHD-C1D-ND	-3.94	119.26	124.80
29	D	405	PL9	C7-C3-C2	-3.93	118.75	123.39
25	a	408	CLA	C1-C2-C3	-3.93	119.75	126.20
25	A	408	CLA	C1-C2-C3	-3.93	119.76	126.20
25	b	602	CLA	CHD-C1D-ND	-3.93	119.27	124.80
30	a	412	SQD	C44-O6-C1	3.93	122.22	113.80
25	c	503	CLA	O2A-C1-C2	3.93	123.22	108.11
25	D	401	CLA	O2A-CGA-CBA	3.92	123.79	111.83
25	b	606	CLA	CHD-C1D-ND	-3.92	119.28	124.80
30	A	413	SQD	O9-S-O7	-3.92	101.07	113.82
30	a	413	SQD	O9-S-O7	-3.92	101.07	113.82
25	d	401	CLA	O2A-CGA-CBA	3.92	123.78	111.83
27	Z	101	BCR	C15-C14-C13	-3.92	121.78	127.28
27	z	101	BCR	C15-C14-C13	-3.92	121.79	127.28
25	C	507	CLA	CHD-C1D-ND	-3.91	119.30	124.80
25	c	504	CLA	CHD-C1D-ND	-3.90	119.31	124.80
30	H	102	SQD	O9-S-O7	-3.90	101.14	113.82
25	C	504	CLA	CHD-C1D-ND	-3.90	119.32	124.80
25	B	606	CLA	CHD-C1D-ND	-3.89	119.32	124.80
30	h	102	SQD	O9-S-O7	-3.89	101.17	113.82
25	c	507	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	A	406	CLA	CHD-C1D-ND	-3.88	119.34	124.80
25	B	602	CLA	C1D-ND-C4D	-3.88	103.59	106.31
25	c	508	CLA	C1D-ND-C4D	-3.88	103.59	106.31
25	B	604	CLA	C1D-ND-C4D	-3.87	103.60	106.31
25	b	604	CLA	C1D-ND-C4D	-3.87	103.60	106.31
25	a	406	CLA	CHD-C1D-ND	-3.86	119.37	124.80
25	b	602	CLA	CAA-C2A-C3A	-3.85	102.59	113.00
25	B	602	CLA	CAA-C2A-C3A	-3.85	102.60	113.00
25	b	608	CLA	CHD-C1D-ND	-3.84	119.39	124.80
25	C	514	CLA	CMB-C2B-C3B	3.84	132.36	124.68
25	a	405	CLA	CHD-C1D-ND	-3.84	119.39	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	CLA	CMB-C2B-C3B	3.84	132.36	124.68
25	C	507	CLA	O2A-C1-C2	3.84	122.87	108.11
25	c	505	CLA	CHD-C1D-ND	-3.84	119.41	124.80
30	f	102	SQD	C44-O6-C1	3.83	122.01	113.80
30	f	102	SQD	O9-S-O7	-3.83	101.36	113.82
30	F	102	SQD	C44-O6-C1	3.83	122.01	113.80
25	C	511	CLA	C1-C2-C3	-3.83	119.92	126.20
25	b	611	CLA	C1-C2-C3	-3.83	119.92	126.20
25	B	608	CLA	CHD-C1D-ND	-3.83	119.42	124.80
25	c	507	CLA	O2A-C1-C2	3.83	122.84	108.11
25	A	405	CLA	CHD-C1D-ND	-3.83	119.42	124.80
25	c	511	CLA	C1-C2-C3	-3.83	119.93	126.20
25	C	505	CLA	CHD-C1D-ND	-3.82	119.43	124.80
25	b	602	CLA	C1D-ND-C4D	-3.82	103.63	106.31
25	C	508	CLA	C1D-ND-C4D	-3.82	103.64	106.31
30	F	102	SQD	O9-S-O7	-3.81	101.42	113.82
34	H	103	DGD	O2G-C1B-C2B	3.81	119.73	111.48
34	h	103	DGD	O2G-C1B-C2B	3.81	119.73	111.48
25	B	611	CLA	C1-C2-C3	-3.81	119.96	126.20
25	A	408	CLA	O2A-CGA-CBA	3.80	123.42	111.83
25	a	408	CLA	O2A-CGA-CBA	3.80	123.41	111.83
30	H	102	SQD	O47-C7-C8	3.79	119.69	111.48
25	c	512	CLA	O2A-C1-C2	3.79	122.69	108.11
25	c	509	CLA	CHD-C1D-ND	-3.79	119.47	124.80
30	h	102	SQD	O47-C7-C8	3.78	119.67	111.48
25	C	512	CLA	O2A-C1-C2	3.78	122.66	108.11
34	c	517	DGD	O2G-C1B-C2B	3.78	119.65	111.48
25	c	513	CLA	C1D-ND-C4D	-3.78	103.66	106.31
25	B	615	CLA	C1-C2-C3	-3.77	120.02	126.20
27	k	103	BCR	C3-C4-C5	-3.77	107.33	114.06
25	C	513	CLA	C1D-ND-C4D	-3.77	103.67	106.31
25	d	403	CLA	CMC-C2C-C1C	3.77	130.92	125.03
27	K	103	BCR	C3-C4-C5	-3.77	107.34	114.06
25	D	403	CLA	CMC-C2C-C1C	3.77	130.92	125.03
25	b	614	CLA	CMC-C2C-C1C	3.76	130.91	125.03
34	C	517	DGD	O2G-C1B-C2B	3.76	119.62	111.48
25	b	615	CLA	C1-C2-C3	-3.76	120.04	126.20
25	B	614	CLA	CMC-C2C-C1C	3.76	130.90	125.03
25	C	509	CLA	CHD-C1D-ND	-3.75	119.52	124.80
25	C	504	CLA	O2A-CGA-CBA	3.75	123.28	111.83
37	x	102	RRX	C16-C15-C14	3.75	131.20	123.52
37	X	102	RRX	C16-C15-C14	3.75	131.19	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	C1-C2-C3	-3.75	120.06	126.20
28	C	519	LMG	O7-C10-C11	3.75	119.59	111.48
25	D	404	CLA	C1-C2-C3	-3.75	120.06	126.20
25	c	504	CLA	O2A-CGA-CBA	3.75	123.25	111.83
25	B	614	CLA	O2A-CGA-CBA	3.74	123.25	111.83
25	b	603	CLA	CAA-C2A-C3A	-3.74	102.88	113.00
25	B	610	CLA	C1-C2-C3	-3.74	120.06	126.20
25	d	404	CLA	C1-C2-C3	-3.74	120.06	126.20
25	B	603	CLA	CAA-C2A-C3A	-3.74	102.89	113.00
28	c	519	LMG	O7-C10-C11	3.74	119.57	111.48
25	b	614	CLA	O2A-CGA-CBA	3.73	123.22	111.83
25	C	505	CLA	O2A-C1-C2	3.73	122.45	108.11
25	c	505	CLA	C1-C2-C3	-3.72	120.09	126.20
25	c	505	CLA	O2A-C1-C2	3.72	122.44	108.11
25	B	602	CLA	O2A-CGA-CBA	3.72	123.19	111.83
31	b	623	LMT	O1'-C1'-C2'	3.72	113.93	108.27
27	Z	101	BCR	C7-C8-C9	-3.72	120.73	126.23
25	C	505	CLA	C1-C2-C3	-3.72	120.10	126.20
25	c	513	CLA	C1-C2-C3	-3.71	120.76	126.76
25	b	602	CLA	O2A-CGA-CBA	3.71	123.14	111.83
31	B	623	LMT	O1'-C1'-C2'	3.70	113.90	108.27
25	C	513	CLA	C1-C2-C3	-3.70	120.77	126.76
25	C	511	CLA	O2A-CGA-CBA	3.70	123.11	111.83
25	C	502	CLA	C1D-ND-C4D	-3.69	103.72	106.31
30	k	101	SQD	C1-O5-C5	3.69	119.94	113.63
25	b	609	CLA	O2A-C1-C2	3.69	122.32	108.11
27	z	101	BCR	C7-C8-C9	-3.69	120.78	126.23
30	K	101	SQD	C1-O5-C5	3.69	119.92	113.63
25	B	611	CLA	CHD-C1D-ND	-3.69	119.61	124.80
25	c	511	CLA	O2A-CGA-CBA	3.69	123.08	111.83
25	B	609	CLA	O2A-C1-C2	3.68	122.29	108.11
25	c	502	CLA	C1D-ND-C4D	-3.68	103.73	106.31
30	B	620	SQD	O9-S-O7	-3.68	101.87	113.82
25	b	601	CLA	CHD-C1D-ND	-3.67	119.63	124.80
25	b	610	CLA	O2A-C1-C2	3.67	122.24	108.11
25	B	610	CLA	O2A-C1-C2	3.67	122.23	108.11
30	b	620	SQD	O9-S-O7	-3.66	101.91	113.82
25	B	601	CLA	CHD-C1D-ND	-3.66	119.65	124.80
27	C	515	BCR	C38-C26-C25	-3.66	120.49	124.48
25	b	611	CLA	CHD-C1D-ND	-3.65	119.67	124.80
25	C	503	CLA	O2A-CGA-CBA	3.65	122.95	111.83
25	B	611	CLA	C1D-ND-C4D	-3.64	103.76	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	620	SQD	C4-C3-C2	3.64	117.22	110.83
25	B	605	CLA	C4-C3-C5	3.64	121.54	115.23
27	c	515	BCR	C38-C26-C25	-3.64	120.52	124.48
30	b	620	SQD	C4-C3-C2	3.63	117.20	110.83
25	c	503	CLA	O2A-CGA-CBA	3.63	122.90	111.83
25	B	606	CLA	O2A-CGA-CBA	3.63	122.89	111.83
25	b	605	CLA	C4-C3-C5	3.63	121.52	115.23
25	B	614	CLA	CHD-C1D-ND	-3.62	119.70	124.80
25	b	606	CLA	O2A-CGA-CBA	3.62	122.88	111.83
31	T	701	LMT	C3'-C4'-C5'	-3.62	103.67	110.23
25	b	614	CLA	CHD-C1D-ND	-3.61	119.72	124.80
25	A	408	CLA	CHD-C1D-ND	-3.61	119.72	124.80
27	A	409	BCR	C33-C5-C6	-3.61	120.55	124.48
25	d	404	CLA	O2A-CGA-CBA	3.61	122.83	111.83
37	X	102	RRX	C15-C16-C17	3.60	130.89	123.52
25	a	408	CLA	CHD-C1D-ND	-3.60	119.74	124.80
35	e	104	HEM	CBD-CAD-C3D	-3.60	102.58	112.53
35	E	104	HEM	CBD-CAD-C3D	-3.60	102.59	112.53
25	d	404	CLA	O2A-C1-C2	3.59	121.94	108.11
25	D	404	CLA	O2A-CGA-CBA	3.59	122.79	111.83
31	t	701	LMT	C3'-C4'-C5'	-3.59	103.72	110.23
25	c	511	CLA	CHD-C1D-ND	-3.59	119.75	124.80
27	a	409	BCR	C33-C5-C6	-3.59	120.57	124.48
37	x	102	RRX	C15-C16-C17	3.59	130.86	123.52
25	D	404	CLA	O2A-C1-C2	3.58	121.90	108.11
25	B	611	CLA	O2A-CGA-CBA	3.58	122.77	111.83
25	b	611	CLA	O2A-CGA-CBA	3.58	122.76	111.83
25	C	502	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
25	c	508	CLA	CHD-C1D-ND	-3.58	119.77	124.80
25	c	502	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
25	b	608	CLA	CMB-C2B-C3B	3.58	131.84	124.68
25	B	608	CLA	CMB-C2B-C3B	3.58	131.83	124.68
25	b	611	CLA	C1D-ND-C4D	-3.58	103.80	106.31
25	C	511	CLA	CHD-C1D-ND	-3.57	119.77	124.80
25	C	514	CLA	CHD-C1D-ND	-3.57	119.77	124.80
25	c	514	CLA	CHD-C1D-ND	-3.56	119.79	124.80
25	b	607	CLA	O2A-CGA-CBA	3.56	122.68	111.83
33	b	622	LHG	O7-C7-C8	3.55	119.17	111.48
25	C	508	CLA	CHD-C1D-ND	-3.55	119.80	124.80
25	c	505	CLA	O2A-CGA-CBA	3.55	122.66	111.83
25	B	607	CLA	O2A-CGA-CBA	3.55	122.66	111.83
33	e	102	LHG	O7-C7-C8	3.55	119.16	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	622	LHG	O7-C7-C8	3.55	119.15	111.48
33	E	102	LHG	O7-C7-C8	3.55	119.15	111.48
25	C	505	CLA	O2A-CGA-CBA	3.55	122.65	111.83
30	a	413	SQD	O7-S-C6	3.54	112.05	106.76
31	b	624	LMT	C3'-C4'-C5'	-3.54	103.81	110.23
30	C	501	SQD	O9-S-O7	-3.54	102.30	113.82
30	c	501	SQD	O9-S-O7	-3.54	102.31	113.82
25	c	508	CLA	O2A-CGA-CBA	3.54	122.63	111.83
25	d	403	CLA	CHD-C1D-ND	-3.54	119.82	124.80
31	B	624	LMT	C3'-C4'-C5'	-3.53	103.83	110.23
30	A	413	SQD	O7-S-C6	3.53	112.03	106.76
25	C	508	CLA	O2A-CGA-CBA	3.53	122.60	111.83
25	D	403	CLA	CHD-C1D-ND	-3.51	119.86	124.80
25	c	508	CLA	O2A-C1-C2	3.51	121.62	108.11
31	e	103	LMT	C3'-C4'-C5'	-3.51	103.15	110.93
25	C	508	CLA	O2A-C1-C2	3.51	121.60	108.11
25	c	510	CLA	CHD-C1D-ND	-3.50	119.87	124.80
31	E	103	LMT	C3'-C4'-C5'	-3.50	103.17	110.93
25	C	510	CLA	CHD-C1D-ND	-3.49	119.88	124.80
30	a	412	SQD	O5-C1-C2	3.49	117.54	110.37
25	B	612	CLA	CHD-C1D-ND	-3.49	119.89	124.80
25	b	612	CLA	CHD-C1D-ND	-3.49	119.89	124.80
30	A	412	SQD	O5-C1-C2	3.48	117.53	110.37
37	X	102	RRX	C37-C22-C21	-3.48	117.17	122.82
31	x	103	LMT	C1'-O5'-C5'	-3.48	107.69	113.63
31	X	103	LMT	C1'-O5'-C5'	-3.48	107.70	113.63
37	x	102	RRX	C37-C22-C21	-3.48	117.19	122.82
30	B	620	SQD	C3-C4-C5	3.47	116.52	110.23
30	b	620	SQD	C3-C4-C5	3.46	116.51	110.23
25	B	608	CLA	O2A-CGA-CBA	3.46	122.37	111.83
25	b	608	CLA	O2A-CGA-CBA	3.45	122.36	111.83
37	x	102	RRX	C34-C9-C10	-3.45	117.22	122.82
27	B	618	BCR	C38-C26-C25	-3.45	120.72	124.48
37	X	102	RRX	C34-C9-C10	-3.45	117.23	122.82
25	d	403	CLA	C4-C3-C5	3.45	121.21	115.23
27	B	618	BCR	C33-C5-C6	-3.44	120.73	124.48
25	b	605	CLA	CMC-C2C-C1C	3.44	130.41	125.03
27	k	102	BCR	C33-C5-C6	-3.44	120.73	124.48
25	C	502	CLA	CHD-C1D-ND	-3.44	119.96	124.80
25	b	613	CLA	O2A-CGA-CBA	3.44	122.32	111.83
27	b	618	BCR	C38-C26-C25	-3.44	120.73	124.48
27	K	102	BCR	C33-C5-C6	-3.44	120.73	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	i	103	LMT	C1'-O5'-C5'	-3.44	107.01	113.72
25	B	613	CLA	O2A-CGA-CBA	3.44	122.31	111.83
27	z	101	BCR	C19-C18-C17	3.43	124.41	119.01
25	B	614	CLA	O2A-C1-C2	3.43	121.31	108.11
25	c	502	CLA	CHD-C1D-ND	-3.43	119.97	124.80
25	D	403	CLA	C4-C3-C5	3.43	121.18	115.23
25	b	605	CLA	CHD-C1D-ND	-3.43	119.98	124.80
30	F	102	SQD	O7-S-C6	3.42	111.87	106.76
25	B	605	CLA	CMC-C2C-C1C	3.42	130.38	125.03
25	b	614	CLA	O2A-C1-C2	3.42	121.28	108.11
31	I	103	LMT	C1'-O5'-C5'	-3.42	107.04	113.72
27	Z	101	BCR	C19-C18-C17	3.42	124.39	119.01
30	f	102	SQD	O7-S-C6	3.41	111.85	106.76
27	f	101	BCR	C19-C18-C17	3.41	124.38	119.01
27	F	101	BCR	C19-C18-C17	3.41	124.37	119.01
31	X	101	LMT	C3'-C4'-C5'	-3.41	104.05	110.23
25	B	605	CLA	CHD-C1D-ND	-3.41	120.00	124.80
25	c	506	CLA	CHD-C1D-ND	-3.41	120.01	124.80
25	c	503	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
27	b	618	BCR	C33-C5-C6	-3.41	120.77	124.48
25	A	405	CLA	O2D-CGD-CBD	3.41	117.18	111.23
25	B	609	CLA	CHD-C1D-ND	-3.40	120.01	124.80
25	C	503	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
31	x	101	LMT	C3'-C4'-C5'	-3.40	104.06	110.23
29	a	411	PL9	C40-C39-C41	3.40	121.13	115.23
25	C	506	CLA	CHD-C1D-ND	-3.39	120.03	124.80
29	A	411	PL9	C40-C39-C41	3.39	121.11	115.23
25	c	511	CLA	O2A-C1-C2	3.39	121.14	108.11
25	B	616	CLA	CHD-C1D-ND	-3.39	120.04	124.80
25	b	609	CLA	CHD-C1D-ND	-3.38	120.04	124.80
25	A	406	CLA	CMB-C2B-C3B	3.38	131.44	124.68
25	D	404	CLA	C3D-C4D-ND	3.38	115.49	109.99
25	a	406	CLA	CMB-C2B-C3B	3.38	131.44	124.68
25	a	408	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
25	C	511	CLA	O2A-C1-C2	3.38	121.12	108.11
25	b	603	CLA	CMB-C2B-C3B	3.38	131.44	124.68
25	A	405	CLA	O2A-C1-C2	3.38	121.11	108.11
25	b	616	CLA	CHD-C1D-ND	-3.38	120.05	124.80
25	a	405	CLA	O2A-C1-C2	3.37	121.09	108.11
25	a	405	CLA	O2D-CGD-CBD	3.37	117.13	111.23
25	b	613	CLA	CHD-C1D-ND	-3.37	120.05	124.80
28	c	519	LMG	O8-C28-C29	3.37	122.12	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	CLA	C3D-C4D-ND	3.37	115.47	109.99
25	b	613	CLA	O2A-C1-C2	3.37	121.08	108.11
25	B	613	CLA	CHD-C1D-ND	-3.37	120.06	124.80
25	B	613	CLA	O2A-C1-C2	3.37	121.07	108.11
25	A	408	CLA	CAA-C2A-C3A	-3.37	103.90	113.00
28	C	519	LMG	O8-C28-C29	3.36	122.09	111.83
25	B	603	CLA	CMB-C2B-C3B	3.36	131.39	124.68
25	B	610	CLA	CHD-C1D-ND	-3.35	120.08	124.80
25	b	610	CLA	CHD-C1D-ND	-3.35	120.08	124.80
26	d	402	PHO	CMB-C2B-C3B	3.35	131.38	124.68
28	A	410	LMG	C8-O7-C10	-3.35	109.78	117.80
26	D	402	PHO	CMB-C2B-C3B	3.35	131.38	124.68
25	C	514	CLA	O2A-C1-C2	3.35	120.99	108.11
25	b	606	CLA	CMB-C2B-C3B	3.35	131.37	124.68
25	c	514	CLA	O2A-C1-C2	3.35	120.99	108.11
28	a	410	LMG	C8-O7-C10	-3.35	109.79	117.80
25	B	606	CLA	CMB-C2B-C3B	3.34	131.37	124.68
30	F	102	SQD	O9-S-C6	3.33	111.73	106.76
30	f	102	SQD	O9-S-C6	3.33	111.73	106.76
31	I	101	LMT	C3'-C4'-C5'	-3.33	104.20	110.23
31	i	101	LMT	C3'-C4'-C5'	-3.32	104.21	110.23
30	H	102	SQD	C4-C3-C2	3.31	116.64	110.83
30	h	102	SQD	C4-C3-C2	3.30	116.63	110.83
25	A	408	CLA	O2A-C1-C2	3.30	120.82	108.11
27	F	101	BCR	C3-C4-C5	-3.30	108.17	114.06
30	a	412	SQD	O47-C7-C8	3.30	118.61	111.48
25	C	504	CLA	CMC-C2C-C1C	3.30	130.19	125.03
25	a	408	CLA	O2A-C1-C2	3.30	120.79	108.11
25	b	603	CLA	C4-C3-C5	3.29	120.94	115.23
30	A	412	SQD	O47-C7-C8	3.29	118.59	111.48
25	B	605	CLA	CMB-C2B-C3B	3.29	131.25	124.68
25	B	603	CLA	C4-C3-C5	3.29	120.93	115.23
27	f	101	BCR	C3-C4-C5	-3.29	108.20	114.06
25	b	605	CLA	CMB-C2B-C3B	3.28	131.25	124.68
27	K	102	BCR	C30-C25-C26	-3.28	118.15	122.64
25	C	509	CLA	CMB-C2B-C3B	3.28	131.23	124.68
25	b	603	CLA	CHD-C1D-ND	-3.27	120.20	124.80
27	k	102	BCR	C30-C25-C26	-3.27	118.17	122.64
25	B	601	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
25	c	509	CLA	CMB-C2B-C3B	3.27	131.21	124.68
30	b	620	SQD	O47-C7-C8	3.26	118.54	111.48
25	b	601	CLA	O2D-CGD-O1D	-3.26	117.50	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	CMC-C2C-C1C	3.26	130.13	125.03
27	B	618	BCR	C15-C14-C13	-3.26	122.71	127.28
25	c	507	CLA	C1-C2-C3	-3.26	120.86	126.20
25	B	603	CLA	CHD-C1D-ND	-3.25	120.22	124.80
27	b	618	BCR	C15-C14-C13	-3.25	122.72	127.28
25	C	512	CLA	CHD-C1D-ND	-3.25	120.23	124.80
25	b	604	CLA	O2A-C1-C2	3.25	120.61	108.11
30	B	620	SQD	O47-C7-C8	3.25	118.51	111.48
25	B	615	CLA	CMB-C2B-C3B	3.25	131.17	124.68
25	b	615	CLA	CMB-C2B-C3B	3.25	131.17	124.68
25	B	604	CLA	O2A-CGA-CBA	3.24	121.73	111.83
25	A	406	CLA	C3D-C4D-ND	3.24	115.26	109.99
25	B	601	CLA	CMC-C2C-C1C	3.24	130.10	125.03
25	C	507	CLA	C1-C2-C3	-3.24	120.88	126.20
25	b	604	CLA	O2A-CGA-CBA	3.24	121.72	111.83
25	c	504	CLA	CMA-C3A-C4A	3.24	120.48	111.77
25	b	601	CLA	CMC-C2C-C1C	3.24	130.10	125.03
25	B	604	CLA	O2A-C1-C2	3.24	120.56	108.11
25	a	406	CLA	C3D-C4D-ND	3.23	115.25	109.99
25	C	504	CLA	CMA-C3A-C4A	3.23	120.47	111.77
25	c	512	CLA	CHD-C1D-ND	-3.23	120.25	124.80
25	C	510	CLA	C1-C2-C3	-3.23	120.90	126.20
30	F	102	SQD	O6-C1-C2	3.23	113.18	108.27
27	B	619	BCR	C3-C4-C5	-3.23	108.30	114.06
25	b	604	CLA	CMA-C3A-C4A	3.23	120.45	111.77
28	a	414	LMG	C8-O7-C10	-3.23	110.07	117.80
27	b	619	BCR	C3-C4-C5	-3.22	108.31	114.06
28	A	414	LMG	C8-O7-C10	-3.22	110.09	117.80
30	A	413	SQD	O9-S-C6	3.22	111.56	106.76
25	c	513	CLA	CHD-C1D-ND	-3.22	120.27	124.80
25	B	604	CLA	CMA-C3A-C4A	3.22	120.42	111.77
30	c	501	SQD	C4-C3-C2	3.22	116.48	110.83
25	D	403	CLA	O2A-C1-C2	3.22	120.48	108.11
25	C	513	CLA	CHD-C1D-ND	-3.21	120.28	124.80
25	c	510	CLA	C1-C2-C3	-3.21	120.93	126.20
30	a	413	SQD	O9-S-C6	3.21	111.55	106.76
30	C	501	SQD	C4-C3-C2	3.21	116.47	110.83
25	d	403	CLA	O2A-C1-C2	3.21	120.46	108.11
25	C	506	CLA	C4D-C3D-CAD	3.20	111.58	108.11
31	C	524	LMT	C3'-C4'-C5'	-3.20	103.84	110.93
30	B	620	SQD	O9-S-C6	3.20	111.53	106.76
30	f	102	SQD	O6-C1-C2	3.20	113.13	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	O1-C4-C3	-3.19	117.36	120.73
25	a	405	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
25	c	509	CLA	O2A-CGA-CBA	3.19	121.56	111.83
25	A	405	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
30	b	620	SQD	O9-S-C6	3.18	111.51	106.76
31	c	524	LMT	C3'-C4'-C5'	-3.18	103.88	110.93
25	C	511	CLA	CMB-C2B-C3B	3.18	131.04	124.68
30	A	413	SQD	O5-C1-C2	3.18	116.90	110.37
25	C	509	CLA	O2A-CGA-CBA	3.18	121.52	111.83
25	c	511	CLA	CMB-C2B-C3B	3.18	131.03	124.68
25	a	405	CLA	CAA-C2A-C1A	-3.17	101.57	111.97
25	A	405	CLA	CAA-C2A-C1A	-3.17	101.58	111.97
25	b	603	CLA	C4D-C3D-CAD	3.17	111.55	108.11
30	a	413	SQD	C3-C4-C5	3.17	115.98	110.23
30	A	413	SQD	C3-C4-C5	3.17	115.98	110.23
25	c	506	CLA	C4D-C3D-CAD	3.17	111.54	108.11
31	F	103	LMT	C1'-O5'-C5'	-3.16	107.55	113.72
29	D	405	PL9	O1-C4-C3	-3.16	117.39	120.73
27	C	515	BCR	C3-C4-C5	-3.16	108.42	114.06
27	c	515	BCR	C3-C4-C5	-3.16	108.42	114.06
25	C	502	CLA	CMB-C2B-C3B	3.16	131.00	124.68
25	A	406	CLA	O2A-C1-C2	3.16	120.26	108.11
31	f	103	LMT	C1'-O5'-C5'	-3.16	107.56	113.72
30	a	413	SQD	O5-C1-C2	3.15	116.85	110.37
27	B	617	BCR	C37-C22-C21	-3.15	117.71	122.82
25	a	406	CLA	O2A-C1-C2	3.15	120.24	108.11
27	b	617	BCR	C37-C22-C21	-3.15	117.71	122.82
27	a	409	BCR	C38-C26-C25	-3.15	121.05	124.48
25	C	512	CLA	C4-C3-C5	3.14	120.69	115.23
25	B	608	CLA	C3D-C4D-ND	3.14	115.10	109.99
25	B	603	CLA	C4D-C3D-CAD	3.14	111.52	108.11
25	b	605	CLA	C3D-C4D-ND	3.14	115.10	109.99
25	D	401	CLA	CMB-C2B-C3B	3.14	130.97	124.68
25	d	404	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
25	c	502	CLA	CMB-C2B-C3B	3.14	130.96	124.68
27	f	101	BCR	C36-C18-C17	-3.14	117.72	122.82
25	b	608	CLA	C3D-C4D-ND	3.14	115.09	109.99
30	k	101	SQD	O5-C5-C4	3.14	115.21	109.55
25	c	512	CLA	C4-C3-C5	3.14	120.68	115.23
31	I	102	LMT	C1'-C2'-C3'	3.14	116.61	110.01
25	b	615	CLA	CMC-C2C-C1C	3.14	129.94	125.03
30	K	101	SQD	O5-C5-C4	3.14	115.20	109.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	CMC-C2C-C1C	3.13	129.93	125.03
25	d	401	CLA	CMB-C2B-C3B	3.13	130.95	124.68
25	b	615	CLA	O2A-CGA-CBA	3.13	121.39	111.83
25	B	615	CLA	O2A-CGA-CBA	3.13	121.38	111.83
30	f	102	SQD	O47-C7-C8	3.13	118.25	111.48
25	B	605	CLA	C3D-C4D-ND	3.13	115.08	109.99
25	D	404	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	B	610	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
25	b	610	CLA	CAA-C2A-C3A	-3.12	104.56	113.00
27	F	101	BCR	C36-C18-C17	-3.12	117.75	122.82
27	A	409	BCR	C38-C26-C25	-3.12	121.08	124.48
25	a	405	CLA	CMB-C2B-C3B	3.12	130.92	124.68
30	F	102	SQD	O47-C7-C8	3.12	118.23	111.48
25	B	615	CLA	CMC-C2C-C1C	3.12	129.91	125.03
31	i	102	LMT	C1'-C2'-C3'	3.12	116.57	110.01
25	b	610	CLA	C3D-C4D-ND	3.12	115.06	109.99
25	D	401	CLA	CAA-C2A-C3A	-3.12	104.58	113.00
30	H	102	SQD	C44-O6-C1	3.12	120.47	113.80
25	d	401	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
25	B	610	CLA	C3D-C4D-ND	3.11	115.04	109.99
25	c	507	CLA	CMC-C2C-C1C	3.11	129.89	125.03
25	C	510	CLA	O2A-C1-C2	3.11	120.06	108.11
25	D	403	CLA	C1-C2-C3	-3.11	121.11	126.20
25	B	615	CLA	CHD-C1D-ND	-3.11	120.43	124.80
25	b	615	CLA	CHD-C1D-ND	-3.11	120.43	124.80
25	b	602	CLA	O2A-C1-C2	3.11	120.06	108.11
25	A	408	CLA	C3D-C4D-ND	3.11	115.03	109.99
25	c	510	CLA	O2A-C1-C2	3.10	120.06	108.11
30	h	102	SQD	C44-O6-C1	3.10	120.45	113.80
25	B	602	CLA	O2A-C1-C2	3.10	120.04	108.11
25	c	503	CLA	CHD-C1D-ND	-3.10	120.45	124.80
29	D	405	PL9	C7-C8-C9	-3.09	121.50	126.83
25	C	508	CLA	CBC-CAC-C3C	-3.09	104.04	112.42
27	b	617	BCR	C28-C27-C26	-3.09	108.55	114.06
25	b	604	CLA	C3C-C4C-NC	3.09	114.39	110.43
25	c	510	CLA	CMB-C2B-C3B	3.09	130.85	124.68
33	d	407	LHG	O7-C7-C8	3.09	118.16	111.48
25	C	510	CLA	CMB-C2B-C3B	3.09	130.85	124.68
27	B	617	BCR	C28-C27-C26	-3.09	108.55	114.06
25	A	405	CLA	CMB-C2B-C3B	3.09	130.85	124.68
25	c	508	CLA	CBC-CAC-C3C	-3.08	104.06	112.42
25	B	615	CLA	O2A-C1-C2	3.08	119.97	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	O2A-C1-C2	3.08	119.97	108.11
25	b	607	CLA	CMB-C2B-C3B	3.08	130.84	124.68
25	a	408	CLA	C3D-C4D-ND	3.08	115.00	109.99
31	D	410	LMT	C3'-C4'-C5'	-3.08	104.65	110.23
25	B	604	CLA	C3C-C4C-NC	3.08	114.37	110.43
33	D	407	LHG	O7-C7-C8	3.08	118.14	111.48
25	C	503	CLA	CHD-C1D-ND	-3.08	120.47	124.80
30	k	101	SQD	O47-C7-C8	3.08	118.14	111.48
25	B	604	CLA	CHD-C1D-ND	-3.08	120.47	124.80
29	d	405	PL9	C7-C8-C9	-3.08	121.53	126.83
25	b	604	CLA	CHD-C1D-ND	-3.07	120.48	124.80
30	K	101	SQD	O47-C7-C8	3.07	118.12	111.48
25	d	403	CLA	C1-C2-C3	-3.07	121.17	126.20
25	b	602	CLA	CMB-C2B-C3B	3.07	130.82	124.68
25	B	607	CLA	CMB-C2B-C3B	3.07	130.82	124.68
25	C	512	CLA	CMA-C3A-C4A	3.07	120.02	111.77
25	B	607	CLA	CHD-C1D-ND	-3.07	120.48	124.80
25	b	607	CLA	CHD-C1D-ND	-3.07	120.48	124.80
25	B	602	CLA	CMB-C2B-C3B	3.07	130.81	124.68
25	c	512	CLA	CMA-C3A-C4A	3.06	120.01	111.77
31	d	410	LMT	C3'-C4'-C5'	-3.06	104.68	110.23
25	d	401	CLA	CHD-C1D-ND	-3.06	120.49	124.80
25	B	613	CLA	CMC-C2C-C1C	3.06	129.82	125.03
25	c	513	CLA	O2A-C1-C2	3.06	119.89	108.11
25	B	601	CLA	O2A-CGA-CBA	3.06	123.66	114.00
25	C	513	CLA	O2A-C1-C2	3.05	119.86	108.11
25	a	408	CLA	CMC-C2C-C1C	3.05	129.80	125.03
25	b	608	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
25	A	405	CLA	C3D-C4D-ND	3.05	114.95	109.99
27	A	409	BCR	C28-C27-C26	-3.05	108.62	114.06
25	b	613	CLA	CMC-C2C-C1C	3.05	129.80	125.03
25	c	506	CLA	O2A-CGA-CBA	3.04	121.11	111.83
25	b	601	CLA	O2A-CGA-CBA	3.04	123.61	114.00
26	D	402	PHO	O1D-CGD-CBD	3.04	129.34	124.72
25	D	401	CLA	CHD-C1D-ND	-3.04	120.52	124.80
25	B	608	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	c	509	CLA	C3D-C4D-ND	3.04	114.92	109.99
25	C	506	CLA	O2A-CGA-CBA	3.04	121.09	111.83
27	a	409	BCR	C28-C27-C26	-3.03	108.64	114.06
26	d	402	PHO	O1D-CGD-CBD	3.03	129.31	124.72
31	e	101	LMT	C1'-O5'-C5'	-3.03	107.81	113.72
25	a	405	CLA	C3D-C4D-ND	3.03	114.90	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	CLA	CMC-C2C-C1C	3.02	129.76	125.03
33	z	102	LHG	C5-O7-C7	-3.02	110.56	117.80
25	C	504	CLA	CMB-C2B-C3B	3.02	130.72	124.68
33	Z	102	LHG	C5-O7-C7	-3.02	110.56	117.80
25	B	604	CLA	CMC-C2C-C1C	3.02	129.75	125.03
25	b	604	CLA	CMC-C2C-C1C	3.02	129.75	125.03
26	D	402	PHO	C1-C2-C3	-3.02	121.25	126.20
25	b	609	CLA	CMC-C2C-C1C	3.01	129.75	125.03
25	b	615	CLA	C1-O2A-CGA	3.01	123.95	116.65
31	E	101	LMT	C1'-O5'-C5'	-3.01	107.83	113.72
25	c	504	CLA	CMB-C2B-C3B	3.01	130.70	124.68
25	D	401	CLA	O2A-C1-C2	3.01	119.69	108.11
26	d	402	PHO	C1-C2-C3	-3.01	121.27	126.20
25	C	509	CLA	C3D-C4D-ND	3.01	114.88	109.99
25	B	615	CLA	C1-O2A-CGA	3.01	123.92	116.65
25	d	401	CLA	O2A-C1-C2	3.00	119.66	108.11
25	B	609	CLA	CMC-C2C-C1C	3.00	129.72	125.03
25	b	616	CLA	O2A-C1-C2	3.00	119.65	108.11
25	B	616	CLA	O2A-C1-C2	3.00	119.65	108.11
27	k	103	BCR	C19-C18-C17	2.99	123.72	119.01
27	K	103	BCR	C19-C18-C17	2.99	123.71	119.01
30	k	101	SQD	O6-C1-C2	2.99	112.81	108.27
25	b	612	CLA	C3D-C4D-ND	2.98	114.84	109.99
25	c	505	CLA	CMB-C2B-C3B	2.98	130.64	124.68
30	K	101	SQD	O6-C1-C2	2.98	112.80	108.27
37	x	102	RRX	C12-C13-C14	2.98	123.69	119.01
31	b	626	LMT	C1'-O5'-C5'	-2.98	107.91	113.72
25	C	504	CLA	C1-C2-C3	-2.98	121.32	126.20
25	B	612	CLA	C3D-C4D-ND	2.98	114.82	109.99
27	b	619	BCR	C19-C18-C17	2.97	123.69	119.01
31	i	102	LMT	C3'-C4'-C5'	-2.97	104.84	110.23
26	A	407	PHO	CMB-C2B-C3B	2.97	130.62	124.68
27	B	619	BCR	C19-C18-C17	2.97	123.68	119.01
37	X	102	RRX	C12-C13-C14	2.97	123.68	119.01
25	C	505	CLA	CMB-C2B-C3B	2.96	130.61	124.68
25	c	504	CLA	C1-C2-C3	-2.96	121.34	126.20
25	C	504	CLA	C6-C5-C3	-2.96	106.26	113.47
31	B	626	LMT	C1'-O5'-C5'	-2.96	107.94	113.72
25	c	504	CLA	C6-C5-C3	-2.96	106.27	113.47
35	e	104	HEM	CBA-CAA-C2A	-2.96	107.57	112.54
25	B	612	CLA	CMB-C2B-C3B	2.96	130.59	124.68
26	a	407	PHO	CMB-C2B-C3B	2.95	130.59	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	102	LMT	C3'-C4'-C5'	-2.95	104.88	110.23
25	b	612	CLA	CMB-C2B-C3B	2.95	130.58	124.68
25	c	505	CLA	C3D-C4D-ND	2.95	114.78	109.99
25	c	506	CLA	CMD-C2D-C3D	-2.94	120.94	127.69
25	C	503	CLA	C3D-C4D-ND	2.94	114.77	109.99
35	E	104	HEM	CBA-CAA-C2A	-2.94	107.59	112.54
25	c	502	CLA	O2A-C1-C2	2.94	119.43	108.11
25	c	503	CLA	C3D-C4D-ND	2.94	114.77	109.99
25	B	611	CLA	O2A-C1-C2	2.94	119.41	108.11
31	m	101	LMT	C1'-O5'-C5'	-2.94	107.99	113.72
25	b	611	CLA	O2A-C1-C2	2.94	119.40	108.11
25	C	502	CLA	O2A-C1-C2	2.93	119.40	108.11
25	C	503	CLA	CMB-C2B-C3B	2.93	130.55	124.68
25	B	609	CLA	CMB-C2B-C3B	2.93	130.54	124.68
25	C	513	CLA	CMB-C2B-C3B	2.93	130.54	124.68
25	C	506	CLA	CMD-C2D-C3D	-2.93	120.96	127.69
25	B	616	CLA	C4-C3-C5	2.93	120.32	115.23
25	C	505	CLA	C3D-C4D-ND	2.93	114.75	109.99
31	y	101	LMT	C3'-C4'-C5'	-2.93	104.92	110.23
37	x	102	RRX	C19-C18-C17	2.93	123.62	119.01
25	c	510	CLA	CMC-C2C-C1C	2.93	129.61	125.03
31	Y	101	LMT	C3'-C4'-C5'	-2.93	104.93	110.23
31	M	102	LMT	C1'-O5'-C5'	-2.93	108.01	113.72
25	c	503	CLA	CMB-C2B-C3B	2.93	130.53	124.68
37	X	102	RRX	C19-C18-C17	2.92	123.61	119.01
25	B	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	b	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	c	513	CLA	CMB-C2B-C3B	2.92	130.52	124.68
27	Z	101	BCR	C36-C18-C17	-2.92	118.08	122.82
25	c	506	CLA	C4-C3-C5	2.92	120.30	115.23
25	b	616	CLA	C4-C3-C5	2.92	120.30	115.23
25	C	506	CLA	C4-C3-C5	2.92	120.29	115.23
25	C	506	CLA	C3D-C4D-ND	2.92	114.73	109.99
25	b	605	CLA	C1-O2A-CGA	2.92	123.71	116.65
25	b	609	CLA	CMB-C2B-C3B	2.92	130.51	124.68
25	B	605	CLA	C1-O2A-CGA	2.92	123.71	116.65
25	A	408	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
25	b	613	CLA	C4-C3-C5	2.91	120.28	115.23
27	z	101	BCR	C36-C18-C17	-2.91	118.10	122.82
25	b	614	CLA	C1-O2A-CGA	2.91	123.70	116.65
25	D	401	CLA	C3D-C4D-ND	2.91	114.72	109.99
25	B	614	CLA	C1-O2A-CGA	2.91	123.69	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	C3D-C4D-ND	2.91	114.71	109.99
33	B	622	LHG	C5-O7-C7	-2.91	110.84	117.80
25	C	510	CLA	CMC-C2C-C1C	2.91	129.57	125.03
25	B	616	CLA	C1-C2-C3	-2.90	121.44	126.20
33	b	622	LHG	C5-O7-C7	-2.90	110.86	117.80
25	b	616	CLA	C1-C2-C3	-2.90	121.45	126.20
25	b	602	CLA	C6-C5-C3	-2.90	106.41	113.47
30	c	501	SQD	O9-S-C6	2.90	111.08	106.76
25	B	613	CLA	C4-C3-C5	2.90	120.26	115.23
25	b	611	CLA	CMB-C2B-C3B	2.90	130.47	124.68
25	b	606	CLA	C1-O2A-CGA	2.89	123.66	116.65
25	d	401	CLA	C3D-C4D-ND	2.89	114.69	109.99
25	D	403	CLA	C3C-C4C-NC	2.89	114.13	110.43
25	c	510	CLA	C4-C3-C5	2.89	120.25	115.23
25	B	602	CLA	C6-C5-C3	-2.89	106.43	113.47
25	C	511	CLA	C4D-C3D-CAD	2.89	111.25	108.11
30	B	620	SQD	C44-O6-C1	2.89	119.99	113.80
37	X	102	RRX	C35-C13-C14	-2.89	118.14	122.82
30	C	501	SQD	O9-S-C6	2.89	111.07	106.76
25	c	506	CLA	C3D-C4D-ND	2.89	114.68	109.99
25	B	616	CLA	C3D-C4D-ND	2.89	114.68	109.99
25	B	611	CLA	CMB-C2B-C3B	2.88	130.45	124.68
25	c	511	CLA	C4D-C3D-CAD	2.88	111.24	108.11
25	C	508	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
31	d	410	LMT	O1'-C1'-C2'	2.88	112.65	108.27
25	c	508	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	B	610	CLA	CMA-C3A-C4A	2.88	119.52	111.77
31	D	410	LMT	O1'-C1'-C2'	2.88	112.65	108.27
25	B	606	CLA	C1-O2A-CGA	2.88	123.62	116.65
25	a	408	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	C	510	CLA	C4-C3-C5	2.88	120.23	115.23
25	b	607	CLA	C1-O2A-CGA	2.88	123.62	116.65
30	b	620	SQD	C44-O6-C1	2.87	119.96	113.80
25	b	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
27	f	101	BCR	C7-C8-C9	-2.87	121.98	126.23
25	B	607	CLA	C1-O2A-CGA	2.87	123.59	116.65
37	x	102	RRX	C35-C13-C14	-2.87	118.17	122.82
25	b	610	CLA	CMB-C2B-C3B	2.86	130.41	124.68
25	d	403	CLA	C3C-C4C-NC	2.86	114.10	110.43
25	B	610	CLA	CMB-C2B-C3B	2.86	130.41	124.68
25	B	608	CLA	C1-O2A-CGA	2.86	123.58	116.65
31	b	627	LMT	C1'-O5'-C5'	-2.86	108.13	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	k	102	BCR	C37-C22-C21	-2.86	118.18	122.82
25	B	615	CLA	C4-C3-C5	2.86	120.19	115.23
25	b	608	CLA	C1-O2A-CGA	2.86	123.58	116.65
31	B	627	LMT	C1'-O5'-C5'	-2.86	108.13	113.72
27	K	103	BCR	C36-C18-C17	-2.86	118.18	122.82
25	c	508	CLA	CMC-C2C-C1C	2.86	129.50	125.03
25	A	406	CLA	C1-C2-C3	-2.86	121.52	126.20
27	k	103	BCR	C36-C18-C17	-2.86	118.19	122.82
25	b	612	CLA	CMC-C2C-C1C	2.86	129.50	125.03
25	b	601	CLA	C3D-C4D-ND	2.86	114.63	109.99
30	B	620	SQD	C1-O5-C5	2.85	119.29	113.72
27	F	101	BCR	C7-C8-C9	-2.85	122.02	126.23
25	A	408	CLA	CMB-C2B-C3B	2.85	130.38	124.68
25	C	508	CLA	CMC-C2C-C1C	2.85	129.49	125.03
25	a	408	CLA	CMB-C2B-C3B	2.85	130.37	124.68
25	b	615	CLA	C4-C3-C5	2.85	120.17	115.23
37	X	102	RRX	C36-C18-C17	-2.85	118.20	122.82
25	a	406	CLA	C1-C2-C3	-2.85	121.53	126.20
27	K	102	BCR	C37-C22-C21	-2.84	118.21	122.82
25	b	614	CLA	CMB-C2B-C3B	2.84	130.37	124.68
25	B	601	CLA	C3D-C4D-ND	2.84	114.61	109.99
25	D	403	CLA	C3D-C4D-ND	2.84	114.61	109.99
37	x	102	RRX	C36-C18-C17	-2.84	118.21	122.82
25	c	514	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
31	T	701	LMT	C1'-O5'-C5'	-2.84	108.17	113.72
30	b	620	SQD	C1-O5-C5	2.84	119.27	113.72
25	B	614	CLA	CMB-C2B-C3B	2.84	130.35	124.68
30	a	412	SQD	C1-C2-C3	2.83	115.97	110.01
25	b	601	CLA	C4D-C3D-CAD	2.83	111.18	108.11
28	A	410	LMG	O8-C28-C29	2.83	120.47	111.83
25	B	609	CLA	C3D-C4D-ND	2.83	114.59	109.99
25	b	609	CLA	C3D-C4D-ND	2.83	114.59	109.99
25	C	514	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
28	a	410	LMG	O8-C28-C29	2.83	120.46	111.83
25	d	403	CLA	C3D-C4D-ND	2.83	114.58	109.99
30	A	412	SQD	C1-C2-C3	2.82	115.95	110.01
25	b	606	CLA	C3D-C4D-ND	2.82	114.57	109.99
29	d	405	PL9	C22-C23-C24	-2.82	121.17	127.62
25	c	511	CLA	C3D-C4D-ND	2.82	114.57	109.99
25	B	601	CLA	C4D-C3D-CAD	2.82	111.17	108.11
25	B	612	CLA	CMC-C2C-C1C	2.82	129.44	125.03
29	D	405	PL9	C22-C23-C24	-2.82	121.17	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
31	t	701	LMT	C1'-O5'-C5'	-2.82	108.22	113.72
25	C	511	CLA	C3D-C4D-ND	2.82	114.57	109.99
25	C	502	CLA	C4-C3-C5	2.82	120.11	115.23
35	e	104	HEM	C4B-CHC-C1C	2.81	126.27	122.56
25	A	406	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	b	628	LHG	O7-C7-C8	2.81	117.55	111.48
25	c	508	CLA	C1-O2A-CGA	2.81	123.44	116.65
25	c	502	CLA	C4-C3-C5	2.81	120.10	115.23
25	C	502	CLA	C3D-C4D-ND	2.81	114.55	109.99
25	b	607	CLA	O2A-C1-C2	2.81	118.90	108.11
30	c	501	SQD	O7-S-C6	2.80	110.94	106.76
25	C	508	CLA	C1-O2A-CGA	2.80	123.44	116.65
25	B	607	CLA	O2A-C1-C2	2.80	118.88	108.11
33	B	628	LHG	O7-C7-C8	2.80	117.54	111.48
25	B	603	CLA	CMC-C2C-C1C	2.80	129.41	125.03
25	c	502	CLA	C3D-C4D-ND	2.80	114.53	109.99
33	B	628	LHG	O8-C23-C24	2.80	120.36	111.83
27	k	102	BCR	C2-C1-C6	2.79	114.50	110.44
25	B	606	CLA	C3D-C4D-ND	2.79	114.53	109.99
25	B	614	CLA	C4-C3-C5	2.79	120.08	115.23
25	b	602	CLA	C4D-C3D-CAD	2.79	111.14	108.11
25	C	506	CLA	C1-O2A-CGA	2.79	123.41	116.65
25	C	514	CLA	C3D-C4D-ND	2.79	114.53	109.99
25	c	506	CLA	C1-O2A-CGA	2.79	123.41	116.65
25	C	513	CLA	C3C-C4C-NC	2.79	114.00	110.43
25	B	615	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	C	501	SQD	O7-S-C6	2.79	110.92	106.76
25	B	611	CLA	CAC-C3C-C4C	2.79	128.41	124.79
25	b	611	CLA	CAC-C3C-C4C	2.79	128.41	124.79
35	E	104	HEM	C4B-CHC-C1C	2.79	126.23	122.56
25	B	602	CLA	C4D-C3D-CAD	2.79	111.13	108.11
25	c	507	CLA	C3D-C4D-ND	2.79	114.51	109.99
32	a	417	BCT	O3-C-O1	-2.78	112.56	119.68
25	c	513	CLA	C3C-C4C-NC	2.78	113.99	110.43
33	b	628	LHG	O8-C23-C24	2.78	120.32	111.83
25	c	514	CLA	C3D-C4D-ND	2.78	114.50	109.99
28	B	621	LMG	O1-C7-C8	-2.78	104.06	110.82
33	b	622	LHG	O8-C23-C24	2.78	120.31	111.83
31	j	101	LMT	O1'-C1'-C2'	2.78	112.49	108.27
25	C	507	CLA	C3D-C4D-ND	2.78	114.50	109.99
32	A	417	BCT	O3-C-O1	-2.77	112.58	119.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	501	SQD	O47-C7-C8	2.77	117.48	111.48
25	b	603	CLA	CMC-C2C-C1C	2.77	129.37	125.03
31	i	104	LMT	C3'-C4'-C5'	-2.77	105.21	110.23
25	b	614	CLA	C4-C3-C5	2.77	120.04	115.23
25	B	612	CLA	C3C-C4C-NC	2.77	113.98	110.43
25	b	615	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
27	K	103	BCR	C28-C27-C26	-2.77	109.12	114.06
27	b	617	BCR	C38-C26-C25	-2.77	121.46	124.48
25	b	612	CLA	C3C-C4C-NC	2.77	113.98	110.43
31	I	104	LMT	C3'-C4'-C5'	-2.77	105.22	110.23
25	b	604	CLA	C4-C3-C5	2.77	120.03	115.23
33	D	406	LHG	O8-C23-C24	2.77	120.27	111.83
30	c	501	SQD	O47-C7-C8	2.77	117.46	111.48
33	B	622	LHG	O8-C23-C24	2.76	120.27	111.83
27	B	619	BCR	C36-C18-C17	-2.76	118.34	122.82
25	B	604	CLA	C4-C3-C5	2.76	120.03	115.23
28	b	621	LMG	O1-C7-C8	-2.76	104.10	110.82
25	c	512	CLA	C3D-C4D-ND	2.76	114.48	109.99
27	k	103	BCR	C28-C27-C26	-2.76	109.13	114.06
27	b	619	BCR	C36-C18-C17	-2.76	118.34	122.82
27	K	102	BCR	C2-C1-C6	2.76	114.45	110.44
31	J	101	LMT	O1'-C1'-C2'	2.76	112.46	108.27
25	B	602	CLA	C3D-C4D-ND	2.76	114.47	109.99
33	d	406	LHG	O8-C23-C24	2.76	120.24	111.83
25	C	512	CLA	C3D-C4D-ND	2.76	114.47	109.99
25	B	607	CLA	C3D-C4D-ND	2.75	114.46	109.99
27	B	617	BCR	C38-C26-C25	-2.75	121.48	124.48
27	b	617	BCR	C33-C5-C6	-2.75	121.48	124.48
27	k	102	BCR	C27-C26-C25	-2.75	118.99	122.70
27	K	102	BCR	C27-C26-C25	-2.75	118.99	122.70
28	B	621	LMG	O7-C10-O9	-2.75	117.28	123.70
25	C	509	CLA	C4-C3-C5	2.75	120.00	115.23
25	B	607	CLA	CAA-C2A-C1A	-2.75	102.97	111.97
25	b	607	CLA	C3D-C4D-ND	2.75	114.45	109.99
27	b	617	BCR	C29-C30-C25	2.75	114.43	110.44
30	H	102	SQD	O7-S-C6	2.74	110.85	106.76
27	b	618	BCR	C19-C18-C17	2.74	123.32	119.01
27	B	618	BCR	C19-C18-C17	2.74	123.32	119.01
25	b	610	CLA	CMC-C2C-C1C	2.74	129.31	125.03
25	b	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
28	A	414	LMG	O8-C28-C29	2.74	120.18	111.83
28	b	621	LMG	O7-C10-O9	-2.74	117.30	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	505	CLA	CAC-C3C-C4C	2.74	128.35	124.79
25	B	610	CLA	CMC-C2C-C1C	2.74	129.31	125.03
28	a	414	LMG	O8-C28-C29	2.74	120.18	111.83
27	B	617	BCR	C33-C5-C6	-2.73	121.50	124.48
29	A	411	PL9	O2-C1-C6	2.73	124.83	120.48
25	c	505	CLA	CAC-C3C-C4C	2.73	128.34	124.79
30	h	102	SQD	O7-S-C6	2.73	110.83	106.76
25	b	602	CLA	C3D-C4D-ND	2.73	114.43	109.99
25	A	406	CLA	CMC-C2C-C1C	2.73	129.30	125.03
30	a	412	SQD	O8-S-C6	2.73	111.24	105.97
25	C	507	CLA	C6-C5-C3	-2.73	106.83	113.47
25	B	603	CLA	C3D-C4D-ND	2.72	114.42	109.99
30	A	412	SQD	O8-S-C6	2.72	111.23	105.97
25	b	603	CLA	C3D-C4D-ND	2.72	114.41	109.99
27	B	617	BCR	C29-C30-C25	2.72	114.39	110.44
25	c	507	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	c	502	CLA	C1-O2A-CGA	2.72	123.24	116.65
33	z	102	LHG	O8-C23-C24	2.72	120.13	111.83
31	I	104	LMT	C1'-O5'-C5'	-2.72	108.41	113.72
25	c	507	CLA	C6-C5-C3	-2.72	106.84	113.47
25	a	406	CLA	CMC-C2C-C1C	2.72	129.28	125.03
31	C	521	LMT	C3'-C4'-C5'	-2.72	105.31	110.23
25	b	612	CLA	C1-C2-C3	-2.72	121.75	126.20
31	c	521	LMT	C3'-C4'-C5'	-2.72	105.31	110.23
29	a	411	PL9	O2-C1-C6	2.72	124.80	120.48
33	Z	102	LHG	O8-C23-C24	2.71	120.11	111.83
31	i	104	LMT	C1'-O5'-C5'	-2.71	108.42	113.72
33	D	406	LHG	C5-O7-C7	-2.71	111.31	117.80
25	c	509	CLA	C4-C3-C5	2.71	119.94	115.23
25	B	616	CLA	CAC-C3C-C4C	2.71	128.32	124.79
25	c	509	CLA	O2A-C1-C2	2.71	118.54	108.11
25	C	507	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	C	509	CLA	O2A-C1-C2	2.70	118.51	108.11
25	B	614	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
25	C	512	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	c	506	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	C	502	CLA	C1-O2A-CGA	2.70	123.18	116.65
25	B	612	CLA	C1-C2-C3	-2.70	121.78	126.20
25	C	506	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	b	614	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
33	d	406	LHG	C5-O7-C7	-2.69	111.35	117.80
29	a	411	PL9	C32-C33-C34	-2.69	121.46	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	CMC-C2C-C1C	2.69	129.24	125.03
25	C	512	CLA	CMC-C2C-C1C	2.69	129.24	125.03
34	c	517	DGD	O1G-C1A-C2A	2.69	120.04	111.83
29	A	411	PL9	C32-C33-C34	-2.69	121.46	127.62
25	c	512	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
25	b	616	CLA	CAC-C3C-C4C	2.69	128.29	124.79
31	d	411	LMT	O5'-C5'-C6'	2.69	113.11	106.44
34	c	518	DGD	O1G-C1A-C2A	2.69	120.03	111.83
25	C	502	CLA	CMC-C2C-C1C	2.69	129.24	125.03
34	C	517	DGD	O1G-C1A-C2A	2.68	120.02	111.83
25	b	604	CLA	O1D-CGD-CBD	-2.68	119.22	124.52
25	C	506	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
31	D	411	LMT	O5'-C5'-C6'	2.68	113.08	106.44
27	K	103	BCR	C38-C26-C25	-2.68	121.56	124.48
25	C	505	CLA	CMC-C2C-C1C	2.68	129.22	125.03
25	c	506	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
25	C	514	CLA	C4-C3-C5	2.68	119.88	115.23
27	B	618	BCR	C36-C18-C17	-2.68	118.48	122.82
25	c	502	CLA	CMC-C2C-C1C	2.68	129.22	125.03
27	k	103	BCR	C38-C26-C25	-2.68	121.56	124.48
25	c	505	CLA	C1-O2A-CGA	2.67	123.12	116.65
27	C	515	BCR	C33-C5-C4	2.67	119.30	113.60
34	C	518	DGD	O1G-C1A-C2A	2.67	119.98	111.83
25	C	505	CLA	C1-O2A-CGA	2.67	123.11	116.65
30	A	412	SQD	O9-S-C6	2.67	110.74	106.76
27	b	618	BCR	C36-C18-C17	-2.67	118.49	122.82
25	c	514	CLA	C4-C3-C5	2.67	119.86	115.23
25	B	604	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
25	c	510	CLA	C3D-C4D-ND	2.67	114.32	109.99
30	a	412	SQD	O9-S-C6	2.67	110.74	106.76
25	C	510	CLA	C3D-C4D-ND	2.67	114.32	109.99
25	c	505	CLA	CMC-C2C-C1C	2.66	129.20	125.03
34	H	103	DGD	C2G-O2G-C1B	-2.66	111.42	117.80
27	c	515	BCR	C33-C5-C4	2.66	119.28	113.60
25	b	610	CLA	C4-C3-C5	2.66	119.85	115.23
25	A	408	CLA	C4-C3-C5	2.66	119.85	115.23
33	d	407	LHG	O8-C23-C24	2.66	119.95	111.83
25	a	408	CLA	C4-C3-C5	2.66	119.84	115.23
25	b	611	CLA	C4-C3-C5	2.66	119.84	115.23
25	b	605	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
25	B	605	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
34	h	103	DGD	C2G-O2G-C1B	-2.66	111.44	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	CLA	CAC-C3C-C4C	2.65	128.24	124.79
33	D	407	LHG	O8-C23-C24	2.65	119.92	111.83
31	B	627	LMT	C3'-C4'-C5'	-2.65	105.05	110.93
25	B	611	CLA	C4-C3-C5	2.65	119.83	115.23
26	a	407	PHO	O2D-CGD-O1D	-2.65	118.69	123.85
31	y	101	LMT	C1'-O5'-C5'	-2.65	108.55	113.72
25	c	503	CLA	C3C-C4C-NC	2.65	113.82	110.43
25	C	513	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
31	Y	101	LMT	C1'-O5'-C5'	-2.65	108.55	113.72
27	K	102	BCR	C38-C26-C27	2.65	119.24	113.60
25	B	610	CLA	C4-C3-C5	2.65	119.82	115.23
25	a	408	CLA	CAC-C3C-C4C	2.65	128.23	124.79
31	M	102	LMT	C3'-C4'-C5'	-2.65	105.44	110.23
26	A	407	PHO	O2D-CGD-O1D	-2.64	118.70	123.85
27	k	102	BCR	C38-C26-C27	2.64	119.23	113.60
31	b	627	LMT	C3'-C4'-C5'	-2.64	105.07	110.93
25	A	405	CLA	CAC-C3C-C4C	2.64	128.23	124.79
25	C	510	CLA	C3C-C4C-NC	2.64	113.82	110.43
34	h	103	DGD	O1G-C1A-C2A	2.64	119.89	111.83
25	C	509	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
25	B	604	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	B	613	CLA	C3C-C4C-NC	2.64	113.81	110.43
34	H	103	DGD	O1G-C1A-C2A	2.64	119.88	111.83
25	c	509	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
31	I	102	LMT	C1'-O5'-C5'	-2.64	108.57	113.72
25	c	510	CLA	C3C-C4C-NC	2.64	113.81	110.43
25	A	408	CLA	CAC-C3C-C4C	2.64	128.22	124.79
25	b	604	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
25	C	503	CLA	C3C-C4C-NC	2.63	113.80	110.43
27	b	619	BCR	C33-C5-C6	-2.63	121.62	124.48
27	f	101	BCR	C33-C5-C6	-2.63	121.62	124.48
25	d	404	CLA	C4D-C3D-CAD	2.62	110.96	108.11
27	B	619	BCR	C33-C5-C6	-2.62	121.62	124.48
31	m	101	LMT	C3'-C4'-C5'	-2.62	105.47	110.23
25	c	513	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
25	b	614	CLA	C3D-C4D-ND	2.62	114.25	109.99
30	A	413	SQD	O6-C44-C45	-2.62	104.44	110.82
25	D	404	CLA	C4D-C3D-CAD	2.62	110.95	108.11
27	F	101	BCR	C33-C5-C6	-2.62	121.63	124.48
31	D	412	LMT	C3'-C4'-C5'	-2.62	105.13	110.93
25	A	405	CLA	C4D-C3D-CAD	2.62	110.95	108.11
25	B	602	CLA	CMD-C2D-C3D	-2.62	121.69	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	C3D-C4D-ND	2.62	114.24	109.99
30	a	413	SQD	O6-C44-C45	-2.61	104.46	110.82
31	i	102	LMT	C1'-O5'-C5'	-2.61	108.61	113.72
25	b	612	CLA	C4D-C3D-CAD	2.61	110.94	108.11
25	b	602	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
25	b	608	CLA	CMC-C2C-C1C	2.61	129.11	125.03
25	c	504	CLA	O2A-C1-C2	2.61	118.16	108.11
25	C	508	CLA	CMA-C3A-C4A	2.61	118.79	111.77
25	c	508	CLA	CMA-C3A-C4A	2.61	118.79	111.77
26	D	402	PHO	O2D-CGD-O1D	-2.61	118.77	123.85
31	d	412	LMT	C3'-C4'-C5'	-2.60	105.16	110.93
25	C	504	CLA	O2A-C1-C2	2.60	118.13	108.11
25	B	612	CLA	C4D-C3D-CAD	2.60	110.93	108.11
27	F	101	BCR	C38-C26-C27	2.60	119.14	113.60
26	d	402	PHO	O2D-CGD-O1D	-2.60	118.78	123.85
27	f	101	BCR	C38-C26-C27	2.60	119.14	113.60
25	b	611	CLA	C3D-C4D-ND	2.60	114.21	109.99
25	C	510	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
25	b	613	CLA	C3C-C4C-NC	2.60	113.76	110.43
25	B	611	CLA	C3D-C4D-ND	2.60	114.21	109.99
25	c	512	CLA	C3C-C4C-NC	2.60	113.76	110.43
25	B	608	CLA	CMC-C2C-C1C	2.60	129.09	125.03
25	b	613	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
31	C	521	LMT	C1'-O5'-C5'	-2.59	108.65	113.72
25	C	507	CLA	CMB-C2B-C3B	2.59	129.87	124.68
30	H	102	SQD	C1-C2-C3	2.59	115.47	110.01
25	b	610	CLA	CAC-C3C-C4C	2.59	128.16	124.79
31	c	521	LMT	C1'-O5'-C5'	-2.59	108.66	113.72
30	h	102	SQD	C1-C2-C3	2.59	115.46	110.01
31	a	415	LMT	C1'-C2'-C3'	2.59	115.45	110.01
27	K	103	BCR	C33-C5-C4	2.59	119.11	113.60
25	c	508	CLA	C3D-C4D-ND	2.59	114.19	109.99
25	c	510	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
29	d	405	PL9	O2-C1-C6	2.58	124.59	120.48
30	C	501	SQD	O8-S-C6	2.58	110.96	105.97
25	c	507	CLA	CMB-C2B-C3B	2.58	129.84	124.68
25	B	616	CLA	CMB-C2B-C3B	2.58	129.84	124.68
25	a	405	CLA	C4D-C3D-CAD	2.58	110.91	108.11
25	c	503	CLA	C6-C5-C3	-2.58	107.19	113.47
31	c	520	LMT	C1'-O5'-C5'	-2.58	108.68	113.72
31	C	520	LMT	C1'-O5'-C5'	-2.58	108.68	113.72
35	v	201	HEM	CBA-CAA-C2A	-2.58	108.20	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	415	LMT	C1'-C2'-C3'	2.58	115.43	110.01
25	B	613	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
29	D	405	PL9	O2-C1-C6	2.58	124.58	120.48
25	C	503	CLA	C6-C5-C3	-2.58	107.19	113.47
33	e	102	LHG	C5-O7-C7	-2.58	111.63	117.80
35	V	201	HEM	CBA-CAA-C2A	-2.57	108.21	112.54
33	E	102	LHG	C5-O7-C7	-2.57	111.64	117.80
27	k	103	BCR	C33-C5-C4	2.57	119.08	113.60
25	c	502	CLA	CMA-C3A-C4A	2.57	118.69	111.77
25	A	406	CLA	CBC-CAC-C3C	-2.57	105.44	112.42
30	c	501	SQD	O8-S-C6	2.57	110.94	105.97
25	A	406	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
25	a	406	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
25	b	616	CLA	CMB-C2B-C3B	2.57	129.82	124.68
25	C	508	CLA	C3D-C4D-ND	2.57	114.17	109.99
25	B	611	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
25	C	512	CLA	C3C-C4C-NC	2.57	113.72	110.43
25	B	610	CLA	CAC-C3C-C4C	2.57	128.13	124.79
25	a	406	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
25	b	611	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	C	502	CLA	CMA-C3A-C4A	2.57	118.67	111.77
25	B	606	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
31	B	624	LMT	C1'-O5'-C5'	-2.56	108.72	113.72
28	D	409	LMG	C8-O7-C10	-2.56	111.67	117.80
30	B	620	SQD	O8-S-C6	2.56	110.91	105.97
28	d	409	LMG	C8-O7-C10	-2.56	111.68	117.80
25	C	504	CLA	C3D-C4D-ND	2.55	114.14	109.99
27	b	618	BCR	C37-C22-C21	-2.55	118.68	122.82
27	B	618	BCR	C37-C22-C21	-2.55	118.69	122.82
25	B	601	CLA	CMA-C3A-C4A	2.54	118.61	111.77
31	J	101	LMT	O5'-C5'-C6'	2.54	112.74	106.44
25	b	601	CLA	CMB-C2B-C3B	2.54	129.76	124.68
25	b	603	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	B	603	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	C	507	CLA	C3C-C4C-NC	2.54	113.68	110.43
25	B	603	CLA	O2A-C1-C2	2.54	117.88	108.11
25	b	601	CLA	CMA-C3A-C4A	2.54	118.60	111.77
31	j	101	LMT	O5'-C5'-C6'	2.54	112.73	106.44
25	c	504	CLA	C3D-C4D-ND	2.54	114.11	109.99
25	B	601	CLA	CMB-C2B-C3B	2.54	129.75	124.68
25	b	603	CLA	O2A-C1-C2	2.54	117.87	108.11
30	b	620	SQD	O8-S-C6	2.53	110.86	105.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	C3C-C4C-NC	2.53	113.67	110.43
25	B	602	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	b	624	LMT	C1'-O5'-C5'	-2.53	108.78	113.72
31	d	410	LMT	O5'-C5'-C4'	2.53	114.26	109.70
25	b	606	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	b	626	LMT	C3'-C4'-C5'	-2.53	105.65	110.23
25	b	605	CLA	O2A-CGA-CBA	2.53	119.54	111.83
27	b	619	BCR	C38-C26-C25	-2.52	121.73	124.48
25	D	403	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	d	410	LMT	C4'-C3'-C2'	-2.52	106.40	110.83
31	D	410	LMT	C4'-C3'-C2'	-2.52	106.41	110.83
25	b	606	CLA	CMC-C2C-C1C	2.52	128.97	125.03
25	c	511	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
25	B	616	CLA	C3C-C4C-NC	2.52	113.65	110.43
31	D	410	LMT	O5'-C5'-C4'	2.52	114.23	109.70
27	B	617	BCR	C34-C9-C8	2.52	121.93	118.09
25	b	607	CLA	C4-C3-C5	2.52	119.59	115.23
25	B	605	CLA	O2A-CGA-CBA	2.52	119.50	111.83
25	d	404	CLA	CMB-C2B-C3B	2.52	129.71	124.68
25	B	606	CLA	CMC-C2C-C1C	2.51	128.96	125.03
25	B	608	CLA	C4D-C3D-CAD	2.51	110.84	108.11
25	C	514	CLA	C4D-C3D-CAD	2.51	110.84	108.11
31	B	626	LMT	C3'-C4'-C5'	-2.51	105.67	110.23
27	k	103	BCR	C31-C1-C6	-2.51	106.30	110.24
25	b	613	CLA	CMB-C2B-C3B	2.51	129.70	124.68
25	d	403	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
25	D	404	CLA	CMB-C2B-C3B	2.51	129.70	124.68
25	b	616	CLA	C3C-C4C-NC	2.51	113.64	110.43
27	K	103	BCR	C31-C1-C6	-2.51	106.31	110.24
25	B	616	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
25	b	606	CLA	C4-C3-C5	2.50	119.58	115.23
27	B	619	BCR	C38-C26-C25	-2.50	121.75	124.48
25	b	610	CLA	C3C-C4C-NC	2.50	113.64	110.43
25	B	606	CLA	C4-C3-C5	2.50	119.57	115.23
25	c	503	CLA	CMC-C2C-C1C	2.50	128.94	125.03
25	c	514	CLA	C4D-C3D-CAD	2.50	110.82	108.11
25	B	613	CLA	CMB-C2B-C3B	2.50	129.68	124.68
27	b	617	BCR	C34-C9-C8	2.50	121.91	118.09
31	b	629	LMT	C3'-C4'-C5'	-2.50	105.39	110.93
27	K	103	BCR	C15-C14-C13	-2.50	123.77	127.28
27	k	103	BCR	C15-C14-C13	-2.50	123.77	127.28
25	b	616	CLA	O2D-CGD-O1D	-2.50	118.98	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	621	LMG	O8-C28-C29	2.50	119.45	111.83
25	D	401	CLA	C4-C3-C5	2.50	119.56	115.23
25	B	610	CLA	C3C-C4C-NC	2.50	113.63	110.43
25	b	608	CLA	C4D-C3D-CAD	2.50	110.82	108.11
25	B	607	CLA	C4-C3-C5	2.50	119.56	115.23
25	B	602	CLA	CAA-CBA-CGA	-2.50	106.12	113.21
25	d	404	CLA	C4-C3-C5	2.50	119.56	115.23
28	B	621	LMG	O8-C28-C29	2.49	119.44	111.83
25	d	401	CLA	C4-C3-C5	2.49	119.56	115.23
31	e	103	LMT	O5B-C5B-C4B	2.49	114.19	109.70
34	C	517	DGD	C2G-O2G-C1B	-2.49	111.83	117.80
25	b	602	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
31	H	101	LMT	C3'-C4'-C5'	-2.49	105.72	110.23
33	e	102	LHG	O8-C23-C24	2.49	119.42	111.83
25	b	614	CLA	C3C-C4C-NC	2.49	113.62	110.43
25	C	511	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
31	h	101	LMT	C3'-C4'-C5'	-2.49	105.72	110.23
33	E	102	LHG	O8-C23-C24	2.49	119.42	111.83
34	c	517	DGD	C2G-O2G-C1B	-2.49	111.84	117.80
27	K	102	BCR	C38-C26-C25	-2.49	121.77	124.48
25	b	606	CLA	CBC-CAC-C3C	-2.49	105.68	112.42
25	B	614	CLA	C3C-C4C-NC	2.48	113.61	110.43
30	H	102	SQD	O48-C23-C24	2.48	119.41	111.83
31	B	629	LMT	C3'-C4'-C5'	-2.48	105.42	110.93
25	c	508	CLA	C4D-C3D-CAD	2.48	110.80	108.11
25	B	612	CLA	C4-C3-C5	2.48	119.54	115.23
25	C	503	CLA	CMC-C2C-C1C	2.48	128.91	125.03
25	B	606	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
30	h	102	SQD	O48-C23-C24	2.48	119.40	111.83
31	E	103	LMT	O5B-C5B-C4B	2.48	114.17	109.70
25	c	506	CLA	CMC-C2C-C1C	2.48	128.91	125.03
27	k	102	BCR	C38-C26-C25	-2.48	121.78	124.48
25	C	504	CLA	C4-C3-C5	2.48	119.53	115.23
25	b	602	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
29	D	405	PL9	C27-C28-C29	-2.48	121.95	127.62
35	V	201	HEM	C4B-CHC-C1C	2.48	125.83	122.56
35	v	201	HEM	C4B-CHC-C1C	2.48	125.83	122.56
31	c	520	LMT	C3'-C4'-C5'	-2.48	105.44	110.93
25	C	506	CLA	CMC-C2C-C1C	2.47	128.90	125.03
27	a	409	BCR	C3-C4-C5	-2.47	109.64	114.06
25	C	508	CLA	C4D-C3D-CAD	2.47	110.79	108.11
25	c	504	CLA	C4-C3-C5	2.47	119.52	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C27-C28-C29	-2.47	121.97	127.62
25	B	607	CLA	C4D-C3D-CAD	2.47	110.79	108.11
27	a	409	BCR	C35-C13-C12	2.47	121.86	118.09
25	D	404	CLA	C4-C3-C5	2.47	119.52	115.23
25	c	511	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
27	A	409	BCR	C3-C4-C5	-2.47	109.65	114.06
25	C	504	CLA	C1-O2A-CGA	2.47	122.63	116.65
25	C	511	CLA	C1-O2A-CGA	2.47	122.63	116.65
25	C	502	CLA	C1-C2-C3	-2.47	122.15	126.20
25	B	615	CLA	C3D-C4D-ND	2.47	114.00	109.99
27	A	409	BCR	C35-C13-C12	2.47	121.86	118.09
30	F	102	SQD	O48-C23-C24	2.47	119.36	111.83
25	A	408	CLA	CMA-C3A-C4A	2.47	118.40	111.77
25	b	615	CLA	C3D-C4D-ND	2.47	113.99	109.99
25	B	602	CLA	C4-C3-C5	2.46	119.50	115.23
25	B	608	CLA	C4-C3-C5	2.46	119.50	115.23
25	b	607	CLA	C4D-C3D-CAD	2.46	110.78	108.11
25	b	608	CLA	C4-C3-C5	2.46	119.50	115.23
31	C	520	LMT	C3'-C4'-C5'	-2.46	105.48	110.93
31	B	625	LMT	C1'-O5'-C5'	-2.46	108.92	113.72
25	c	502	CLA	C1-C2-C3	-2.46	122.17	126.20
25	C	511	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
25	B	609	CLA	C3C-C4C-NC	2.46	113.58	110.43
25	c	511	CLA	C1-O2A-CGA	2.46	122.60	116.65
30	f	102	SQD	O48-C23-C24	2.46	119.33	111.83
25	a	408	CLA	CMA-C3A-C4A	2.46	118.37	111.77
25	b	602	CLA	C4-C3-C5	2.46	119.49	115.23
25	c	504	CLA	C1-O2A-CGA	2.45	122.59	116.65
31	b	625	LMT	C1'-O5'-C5'	-2.45	108.93	113.72
33	B	628	LHG	C5-O7-C7	-2.45	111.93	117.80
25	b	612	CLA	C4-C3-C5	2.45	119.48	115.23
25	c	511	CLA	C4-C3-C5	2.45	119.48	115.23
25	C	506	CLA	CMB-C2B-C3B	2.45	129.58	124.68
25	c	509	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
35	e	104	HEM	C4D-ND-C1D	2.44	108.10	105.21
25	C	514	CLA	CMA-C3A-C4A	2.44	118.34	111.77
25	B	605	CLA	C3C-C4C-NC	2.44	113.56	110.43
31	H	101	LMT	C1'-O5'-C5'	-2.44	108.95	113.72
33	b	628	LHG	C5-O7-C7	-2.44	111.95	117.80
25	C	504	CLA	C4D-C3D-CAD	2.44	110.76	108.11
25	a	405	CLA	C3C-C4C-NC	2.44	113.56	110.43
25	a	406	CLA	CMA-C3A-C4A	2.44	118.32	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	CMA-C3A-C4A	2.44	118.32	111.77
35	E	104	HEM	C4D-ND-C1D	2.43	108.09	105.21
25	A	405	CLA	C3C-C4C-NC	2.43	113.55	110.43
29	a	411	PL9	C27-C28-C29	-2.43	122.05	127.62
25	b	609	CLA	C3C-C4C-NC	2.43	113.55	110.43
25	b	609	CLA	C4-C3-C5	2.43	119.45	115.23
35	V	201	HEM	C3B-C2B-C1B	2.43	108.24	106.41
25	c	514	CLA	CMA-C3A-C4A	2.43	118.31	111.77
25	c	506	CLA	CMB-C2B-C3B	2.43	129.54	124.68
25	c	503	CLA	CMA-C3A-C4A	2.43	118.31	111.77
35	v	201	HEM	C3B-C2B-C1B	2.43	108.24	106.41
25	B	609	CLA	C4-C3-C5	2.43	119.45	115.23
25	B	615	CLA	C4D-C3D-CAD	2.43	110.75	108.11
25	A	406	CLA	CMA-C3A-C4A	2.43	118.30	111.77
25	C	509	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
30	K	101	SQD	O48-C23-C24	2.43	119.24	111.83
27	k	102	BCR	C23-C22-C21	2.43	122.83	119.01
31	i	103	LMT	C3'-C4'-C5'	-2.43	105.55	110.93
31	I	103	LMT	C3B-C4B-C5B	-2.43	105.83	110.23
25	C	511	CLA	C4-C3-C5	2.43	119.44	115.23
25	D	403	CLA	CMB-C2B-C3B	2.43	129.53	124.68
31	i	103	LMT	C3B-C4B-C5B	-2.43	105.83	110.23
25	c	506	CLA	C3C-C4C-NC	2.42	113.54	110.43
25	A	408	CLA	C1-O2A-CGA	2.42	122.52	116.65
25	c	507	CLA	C4-C3-C5	2.42	119.43	115.23
30	k	101	SQD	O48-C23-C24	2.42	119.22	111.83
25	b	606	CLA	O2A-C1-C2	2.42	117.43	108.11
26	D	402	PHO	CMC-C2C-C3C	2.42	129.51	124.94
31	I	103	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
25	C	510	CLA	C4D-C3D-CAD	2.42	110.73	108.11
25	C	507	CLA	C4-C3-C5	2.42	119.42	115.23
25	a	408	CLA	C1-O2A-CGA	2.42	122.50	116.65
30	f	102	SQD	O8-S-C6	2.42	110.64	105.97
31	h	101	LMT	C1'-O5'-C5'	-2.42	109.00	113.72
25	c	510	CLA	C4D-C3D-CAD	2.42	110.73	108.11
31	a	415	LMT	C1'-O5'-C5'	-2.41	109.00	113.72
25	B	606	CLA	O2A-C1-C2	2.41	117.40	108.11
25	d	403	CLA	CMB-C2B-C3B	2.41	129.51	124.68
30	A	413	SQD	O47-C7-C8	2.41	116.70	111.48
29	A	411	PL9	C27-C28-C29	-2.41	122.10	127.62
27	b	619	BCR	C29-C30-C25	2.41	113.94	110.44
25	b	605	CLA	C3C-C4C-NC	2.41	113.52	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	C3C-C4C-NC	2.41	113.52	110.43
25	b	615	CLA	C4D-C3D-CAD	2.41	110.72	108.11
27	B	619	BCR	C29-C30-C25	2.40	113.93	110.44
27	K	102	BCR	C23-C22-C21	2.40	122.79	119.01
31	A	415	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
26	d	402	PHO	CMC-C2C-C3C	2.40	129.47	124.94
25	c	511	CLA	C3C-C4C-NC	2.40	113.51	110.43
25	B	603	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
25	c	507	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
25	c	508	CLA	C1-C2-C3	-2.40	122.26	126.20
30	b	620	SQD	O7-S-C6	2.40	110.34	106.76
25	b	607	CLA	C3C-C4C-NC	2.40	113.50	110.43
31	B	623	LMT	O5'-C5'-C4'	2.40	114.02	109.70
25	C	507	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
28	D	409	LMG	O8-C28-C29	2.40	119.14	111.83
25	B	609	CLA	C4D-C3D-CAD	2.40	110.71	108.11
25	C	508	CLA	C1-C2-C3	-2.40	122.27	126.20
27	K	102	BCR	C34-C9-C10	-2.40	118.94	122.82
30	a	413	SQD	O47-C7-C8	2.40	116.66	111.48
30	F	102	SQD	O8-S-C6	2.40	110.60	105.97
25	c	504	CLA	C3C-C4C-NC	2.39	113.50	110.43
26	a	407	PHO	O1D-CGD-CBD	2.39	128.35	124.72
25	b	603	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
25	B	601	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
25	c	504	CLA	C4D-C3D-CAD	2.39	110.70	108.11
25	C	511	CLA	C3C-C4C-NC	2.39	113.49	110.43
28	d	409	LMG	O8-C28-C29	2.39	119.12	111.83
27	k	102	BCR	C34-C9-C10	-2.39	118.94	122.82
25	b	601	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
27	a	409	BCR	C19-C18-C17	2.39	122.77	119.01
25	b	611	CLA	CMC-C2C-C1C	2.39	128.77	125.03
25	b	609	CLA	CED-O2D-CGD	2.39	121.33	115.92
25	C	509	CLA	C1-C2-C3	-2.39	122.29	126.20
27	A	409	BCR	C19-C18-C17	2.38	122.76	119.01
25	B	609	CLA	CED-O2D-CGD	2.38	121.32	115.92
34	h	103	DGD	O2G-C1B-O1B	-2.38	118.13	123.70
25	D	403	CLA	C4D-C3D-CAD	2.38	110.69	108.11
25	b	612	CLA	C6-C5-C3	-2.38	107.67	113.47
25	B	601	CLA	C3C-C4C-NC	2.38	113.48	110.43
26	A	407	PHO	O1D-CGD-CBD	2.38	128.33	124.72
30	B	620	SQD	O7-S-C6	2.38	110.31	106.76
31	b	623	LMT	O5'-C5'-C4'	2.38	113.98	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	CMC-C2C-C1C	2.38	128.75	125.03
27	c	515	BCR	C35-C13-C12	2.37	121.71	118.09
25	B	612	CLA	C6-C5-C3	-2.37	107.70	113.47
25	c	508	CLA	CMB-C2B-C3B	2.37	129.42	124.68
25	c	509	CLA	C1-C2-C3	-2.37	122.32	126.20
34	H	103	DGD	O2G-C1B-O1B	-2.37	118.17	123.70
25	B	607	CLA	C3C-C4C-NC	2.37	113.46	110.43
25	C	504	CLA	C3C-C4C-NC	2.37	113.46	110.43
25	D	404	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
25	b	601	CLA	C3C-C4C-NC	2.36	113.46	110.43
25	B	607	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
27	b	617	BCR	C36-C18-C17	-2.36	118.99	122.82
27	B	617	BCR	C36-C18-C17	-2.36	118.99	122.82
25	C	512	CLA	CMB-C2B-C3B	2.36	129.40	124.68
31	k	105	LMT	C1'-O5'-C5'	-2.36	109.11	113.72
25	C	508	CLA	CMB-C2B-C3B	2.36	129.40	124.68
25	C	513	CLA	C3D-C4D-ND	2.36	113.82	109.99
27	C	515	BCR	C35-C13-C12	2.36	121.69	118.09
25	b	609	CLA	C4D-C3D-CAD	2.35	110.66	108.11
25	b	607	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
25	d	404	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
25	c	514	CLA	C3C-C4C-NC	2.35	113.44	110.43
31	K	105	LMT	C1'-O5'-C5'	-2.35	109.13	113.72
25	c	513	CLA	C3D-C4D-ND	2.35	113.81	109.99
25	B	607	CLA	CMC-C2C-C1C	2.35	128.70	125.03
27	b	617	BCR	C19-C18-C17	2.35	122.70	119.01
25	B	612	CLA	O2A-C1-C2	2.35	117.13	108.11
25	b	608	CLA	C1-C2-C3	-2.34	122.36	126.20
35	E	104	HEM	C4C-CHD-C1D	2.34	125.65	122.56
25	d	403	CLA	C4D-C3D-CAD	2.34	110.65	108.11
27	b	617	BCR	C8-C7-C6	-2.34	120.75	127.00
25	B	615	CLA	CAC-C3C-C4C	2.34	127.83	124.79
25	b	612	CLA	O2A-C1-C2	2.34	117.10	108.11
25	c	513	CLA	O1D-CGD-CBD	-2.33	119.91	124.52
25	b	604	CLA	CMB-C2B-C3B	2.33	129.34	124.68
25	b	613	CLA	C3D-C4D-ND	2.33	113.78	109.99
30	C	501	SQD	O47-C7-O49	-2.33	118.25	123.70
27	B	617	BCR	C8-C7-C6	-2.33	120.77	127.00
25	c	512	CLA	CMB-C2B-C3B	2.33	129.34	124.68
34	C	516	DGD	O1G-C1A-C2A	2.33	118.94	111.83
25	B	604	CLA	CMB-C2B-C3B	2.33	129.34	124.68
27	B	617	BCR	C19-C18-C17	2.33	122.67	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	410	LMG	C7-O1-C1	-2.33	108.80	113.80
25	B	608	CLA	C1-C2-C3	-2.33	122.38	126.20
25	C	508	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
25	B	610	CLA	CAA-CBA-CGA	-2.33	106.60	113.21
30	c	501	SQD	O47-C7-O49	-2.33	118.27	123.70
25	c	505	CLA	C4D-C3D-CAD	2.33	110.63	108.11
25	c	505	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
25	c	509	CLA	C4D-C3D-CAD	2.32	110.63	108.11
25	B	613	CLA	C3D-C4D-ND	2.32	113.76	109.99
25	C	503	CLA	C1-O2A-CGA	2.32	122.27	116.65
25	D	403	CLA	CHD-C4C-C3C	-2.32	121.39	124.77
29	A	411	PL9	O2-C1-C2	-2.32	116.55	121.83
27	F	101	BCR	C15-C14-C13	-2.32	124.02	127.28
25	c	509	CLA	C1-O2A-CGA	2.32	122.27	116.65
28	a	410	LMG	C7-O1-C1	-2.32	108.82	113.80
29	a	411	PL9	O2-C1-C2	-2.32	116.55	121.83
25	C	509	CLA	C1-O2A-CGA	2.32	122.27	116.65
25	c	502	CLA	CAC-C3C-C4C	2.32	127.81	124.79
25	b	610	CLA	CAA-CBA-CGA	-2.32	106.62	113.21
25	C	502	CLA	CAC-C3C-C4C	2.32	127.81	124.79
29	A	411	PL9	C7-C8-C9	-2.32	122.84	126.83
25	b	607	CLA	CMC-C2C-C1C	2.32	128.66	125.03
25	B	604	CLA	C3D-C4D-ND	2.32	113.75	109.99
25	C	514	CLA	C3C-C4C-NC	2.31	113.39	110.43
25	C	513	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
25	c	508	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
25	C	505	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
34	c	516	DGD	O1G-C1A-C2A	2.31	118.88	111.83
31	B	623	LMT	C3'-C4'-C5'	-2.31	106.04	110.23
35	e	104	HEM	C4C-CHD-C1D	2.31	125.61	122.56
31	b	623	LMT	C3'-C4'-C5'	-2.31	106.05	110.23
25	B	606	CLA	C3C-C4C-NC	2.31	113.38	110.43
26	a	407	PHO	CMC-C2C-C3C	2.31	129.29	124.94
29	a	411	PL9	C7-C8-C9	-2.31	122.86	126.83
26	A	407	PHO	CMC-C2C-C3C	2.30	129.29	124.94
33	d	408	LHG	O8-C23-C24	2.30	118.86	111.83
25	c	503	CLA	C1-O2A-CGA	2.30	122.23	116.65
25	d	403	CLA	CHD-C4C-C3C	-2.30	121.42	124.77
33	D	408	LHG	O8-C23-C24	2.30	118.85	111.83
25	B	604	CLA	C4D-C3D-CAD	2.30	110.60	108.11
25	C	505	CLA	C4D-C3D-CAD	2.30	110.60	108.11
25	C	505	CLA	O1D-CGD-CBD	-2.30	119.98	124.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	101	BCR	C15-C14-C13	-2.30	124.06	127.28
25	b	607	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
25	b	606	CLA	C3C-C4C-NC	2.29	113.37	110.43
25	b	604	CLA	C3D-C4D-ND	2.29	113.72	109.99
27	a	409	BCR	C37-C22-C21	-2.29	119.11	122.82
25	B	606	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
25	b	606	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
25	B	607	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
25	C	503	CLA	C4-C3-C5	2.29	119.20	115.23
25	b	615	CLA	CAC-C3C-C4C	2.29	127.76	124.79
25	c	503	CLA	C4-C3-C5	2.28	119.19	115.23
31	d	411	LMT	C1-O1'-C1'	2.28	117.58	113.68
25	C	504	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
25	b	608	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
25	C	509	CLA	C4D-C3D-CAD	2.28	110.58	108.11
25	c	505	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
27	A	409	BCR	C37-C22-C21	-2.28	119.12	122.82
27	K	103	BCR	C37-C22-C21	-2.28	119.12	122.82
25	B	610	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
29	A	411	PL9	C22-C23-C24	-2.28	122.41	127.62
27	C	515	BCR	C31-C1-C6	-2.28	106.67	110.24
27	k	103	BCR	C37-C22-C21	-2.28	119.13	122.82
31	D	411	LMT	C1-O1'-C1'	2.27	117.57	113.68
27	c	515	BCR	C31-C1-C6	-2.27	106.68	110.24
29	a	411	PL9	C22-C23-C24	-2.27	122.42	127.62
25	B	608	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
25	c	504	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
25	b	608	CLA	O2A-C1-C2	2.27	116.84	108.11
25	B	608	CLA	O2A-C1-C2	2.27	116.84	108.11
25	C	506	CLA	C6-C5-C3	-2.27	107.95	113.47
25	b	610	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
25	B	615	CLA	C3C-C4C-NC	2.27	113.33	110.43
25	c	506	CLA	C6-C5-C3	-2.26	107.95	113.47
29	D	405	PL9	C12-C13-C14	-2.26	122.44	127.62
25	b	604	CLA	C4D-C3D-CAD	2.26	110.56	108.11
37	X	102	RRX	C23-C22-C21	2.26	122.57	119.01
28	c	519	LMG	O8-C28-O10	-2.26	117.97	123.63
25	B	616	CLA	CMC-C2C-C1C	2.26	128.56	125.03
30	A	413	SQD	C45-O47-C7	2.26	123.20	117.80
35	v	201	HEM	C1B-NB-C4B	2.26	107.88	105.21
31	J	101	LMT	O5'-C5'-C4'	2.26	113.77	109.70
29	d	405	PL9	C12-C13-C14	-2.26	122.46	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	C4-C3-C5	2.25	119.14	115.23
25	b	616	CLA	CMC-C2C-C1C	2.25	128.55	125.03
27	b	617	BCR	C33-C5-C4	2.25	118.40	113.60
27	b	619	BCR	C35-C13-C12	2.25	121.53	118.09
31	j	101	LMT	O5'-C5'-C4'	2.25	113.75	109.70
25	c	502	CLA	CAA-C2A-C3A	-2.25	106.93	113.00
25	B	616	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
31	C	524	LMT	O5B-C5B-C4B	2.25	113.75	109.70
31	c	524	LMT	O5B-C5B-C4B	2.25	113.75	109.70
25	c	505	CLA	C4-C3-C5	2.25	119.12	115.23
28	C	519	LMG	O8-C28-O10	-2.24	118.01	123.63
31	T	701	LMT	O1'-C1'-C2'	2.24	111.68	108.27
27	B	617	BCR	C33-C5-C4	2.24	118.38	113.60
30	a	413	SQD	C45-O47-C7	2.24	123.17	117.80
25	C	511	CLA	CED-O2D-CGD	2.24	121.00	115.92
25	c	509	CLA	CMC-C2C-C1C	2.24	128.54	125.03
37	x	102	RRX	C23-C22-C21	2.24	122.53	119.01
25	A	406	CLA	C4-C3-C5	2.24	119.12	115.23
27	a	409	BCR	C36-C18-C17	-2.24	119.19	122.82
25	C	513	CLA	CMC-C2C-C1C	2.24	128.53	125.03
25	b	615	CLA	C3C-C4C-NC	2.24	113.30	110.43
25	C	502	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
25	b	614	CLA	C4D-C3D-CAD	2.24	110.54	108.11
35	V	201	HEM	C1B-NB-C4B	2.24	107.86	105.21
25	b	616	CLA	C4C-C3C-C2C	-2.24	103.64	106.89
25	c	511	CLA	CED-O2D-CGD	2.24	120.99	115.92
27	B	619	BCR	C38-C26-C27	2.24	118.36	113.60
25	B	603	CLA	CMA-C3A-C4A	2.23	117.78	111.77
25	b	604	CLA	C6-C5-C3	-2.23	108.02	113.47
27	b	619	BCR	C38-C26-C27	2.23	118.36	113.60
31	d	411	LMT	O5B-C5B-C4B	2.23	113.73	109.70
25	C	505	CLA	C4-C3-C5	2.23	119.11	115.23
37	x	102	RRX	C8-C9-C10	2.23	122.52	119.01
27	A	409	BCR	C36-C18-C17	-2.23	119.20	122.82
25	B	604	CLA	C6-C5-C3	-2.23	108.03	113.47
30	A	413	SQD	O8-S-C6	2.23	110.28	105.97
25	C	514	CLA	CMC-C2C-C1C	2.23	128.52	125.03
25	b	605	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
25	b	603	CLA	CMA-C3A-C4A	2.23	117.77	111.77
30	a	413	SQD	O8-S-C6	2.23	110.28	105.97
25	c	514	CLA	CMC-C2C-C1C	2.23	128.52	125.03
25	A	405	CLA	CAA-CBA-CGA	-2.23	106.88	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	411	LMT	O5B-C5B-C4B	2.23	113.72	109.70
31	b	625	LMT	C3'-C4'-C5'	-2.23	105.99	110.93
35	v	201	HEM	CHC-C4B-NB	2.23	126.83	124.44
37	X	102	RRX	C8-C9-C10	2.22	122.51	119.01
25	c	513	CLA	CMC-C2C-C1C	2.22	128.51	125.03
25	B	614	CLA	C4D-C3D-CAD	2.22	110.52	108.11
27	B	619	BCR	C35-C13-C12	2.22	121.48	118.09
28	A	410	LMG	O7-C10-O9	-2.22	118.51	123.70
25	C	503	CLA	CAC-C3C-C4C	2.22	127.68	124.79
25	B	605	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
25	b	606	CLA	C4D-C3D-CAD	2.22	110.52	108.11
25	d	404	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
25	C	509	CLA	CMC-C2C-C1C	2.22	128.50	125.03
25	d	404	CLA	CMC-C2C-C1C	2.22	128.50	125.03
25	c	513	CLA	C1-O2A-CGA	2.22	122.02	116.65
25	B	615	CLA	C6-C5-C3	-2.22	108.07	113.47
31	t	701	LMT	O1'-C1'-C2'	2.22	111.64	108.27
25	D	404	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
25	a	405	CLA	CAA-CBA-CGA	-2.22	106.92	113.21
25	c	508	CLA	C4-C3-C5	2.22	119.07	115.23
30	A	413	SQD	O48-C23-C24	2.21	118.58	111.83
31	B	625	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
29	d	405	PL9	O2-C1-C2	-2.21	116.80	121.83
25	D	404	CLA	CMC-C2C-C1C	2.21	128.49	125.03
25	c	503	CLA	CAC-C3C-C4C	2.21	127.67	124.79
25	B	606	CLA	C4D-C3D-CAD	2.21	110.51	108.11
25	A	405	CLA	CED-O2D-CGD	2.21	120.93	115.92
25	C	513	CLA	C1-O2A-CGA	2.21	122.00	116.65
33	z	102	LHG	O7-C7-O9	-2.21	118.54	123.70
29	D	405	PL9	C37-C38-C39	-2.21	122.57	127.62
25	c	510	CLA	CED-O2D-CGD	2.21	120.92	115.92
25	c	507	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
25	b	615	CLA	C6-C5-C3	-2.21	108.09	113.47
25	c	508	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
27	B	617	BCR	C23-C22-C21	2.20	122.47	119.01
25	C	508	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
27	k	102	BCR	C15-C14-C13	-2.20	124.19	127.28
25	C	507	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
30	a	413	SQD	O48-C23-C24	2.20	118.54	111.83
25	c	503	CLA	CED-O2D-CGD	2.20	120.90	115.92
28	a	410	LMG	O7-C10-O9	-2.20	118.56	123.70
29	D	405	PL9	O2-C1-C2	-2.20	116.83	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	516	DGD	O3G-C3G-C2G	-2.20	105.47	110.82
31	k	105	LMT	C3'-C4'-C5'	-2.20	106.06	110.93
25	B	605	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
25	b	605	CLA	CED-O2D-CGD	2.20	120.90	115.92
27	K	102	BCR	C15-C14-C13	-2.20	124.20	127.28
25	b	616	CLA	C4D-C3D-CAD	2.20	110.49	108.11
33	Z	102	LHG	O7-C7-O9	-2.19	118.58	123.70
25	C	508	CLA	C4-C3-C5	2.19	119.03	115.23
34	c	516	DGD	O3G-C3G-C2G	-2.19	105.48	110.82
31	K	105	LMT	C3'-C4'-C5'	-2.19	106.07	110.93
25	A	408	CLA	C3C-C4C-NC	2.19	113.24	110.43
27	b	617	BCR	C23-C22-C21	2.19	122.46	119.01
25	a	405	CLA	CED-O2D-CGD	2.19	120.89	115.92
25	a	408	CLA	C3C-C4C-NC	2.19	113.24	110.43
25	c	507	CLA	C4D-C3D-CAD	2.19	110.48	108.11
25	c	512	CLA	C1-O2A-CGA	2.19	121.95	116.65
29	d	405	PL9	C37-C38-C39	-2.19	122.61	127.62
25	b	605	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
30	A	412	SQD	O48-C23-O10	-2.19	118.16	123.63
25	B	605	CLA	CED-O2D-CGD	2.19	120.88	115.92
25	C	503	CLA	CED-O2D-CGD	2.19	120.88	115.92
25	C	510	CLA	CED-O2D-CGD	2.19	120.88	115.92
30	a	412	SQD	O48-C23-O10	-2.19	118.16	123.63
25	b	611	CLA	C4D-C3D-CAD	2.19	110.48	108.11
27	c	515	BCR	C37-C22-C21	-2.18	119.28	122.82
25	B	611	CLA	C4D-C3D-CAD	2.18	110.48	108.11
25	b	613	CLA	C4D-C3D-CAD	2.18	110.47	108.11
25	d	401	CLA	C3C-C4C-NC	2.18	113.22	110.43
25	c	507	CLA	CED-O2D-CGD	2.18	120.86	115.92
35	V	201	HEM	CHC-C4B-NB	2.18	126.78	124.44
25	B	609	CLA	O2D-CGD-O1D	-2.17	119.61	123.85
27	C	515	BCR	C37-C22-C21	-2.17	119.30	122.82
25	C	512	CLA	C1-O2A-CGA	2.17	121.91	116.65
25	d	403	CLA	CAA-C2A-C1A	-2.17	104.85	111.97
25	b	609	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
25	D	401	CLA	C3C-C4C-NC	2.17	113.21	110.43
34	C	518	DGD	C2G-O2G-C1B	-2.17	112.60	117.80
25	C	507	CLA	CED-O2D-CGD	2.17	120.84	115.92
31	F	103	LMT	O5B-C5B-C6B	2.17	111.82	106.44
30	B	620	SQD	O48-C23-C24	2.17	118.45	111.83
25	B	613	CLA	C4D-C3D-CAD	2.17	110.46	108.11
25	C	507	CLA	C4D-C3D-CAD	2.17	110.46	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C20-C19-C21	2.17	118.99	115.23
25	c	509	CLA	CHC-C1C-C2C	-2.17	120.80	126.94
35	V	201	HEM	CMC-C2C-C3C	2.17	129.01	124.68
25	D	403	CLA	CAA-C2A-C1A	-2.16	104.88	111.97
25	C	505	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
25	B	611	CLA	C3C-C4C-NC	2.16	113.20	110.43
25	b	611	CLA	C3C-C4C-NC	2.16	113.20	110.43
25	c	509	CLA	CAC-C3C-C4C	2.16	127.61	124.79
34	c	518	DGD	C2G-O2G-C1B	-2.16	112.62	117.80
25	C	509	CLA	CHC-C1C-C2C	-2.16	120.81	126.94
27	Z	101	BCR	C38-C26-C27	2.16	118.21	113.60
31	f	103	LMT	O5B-C5B-C6B	2.16	111.80	106.44
27	k	102	BCR	C36-C18-C17	-2.16	119.31	122.82
25	B	603	CLA	C1-O2A-CGA	2.16	121.88	116.65
30	a	413	SQD	O47-C45-C44	2.16	116.09	108.34
25	C	514	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
30	b	620	SQD	O48-C23-C24	2.16	118.42	111.83
25	B	602	CLA	CAA-C2A-C1A	-2.16	104.91	111.97
30	A	413	SQD	O47-C45-C44	2.16	116.08	108.34
25	c	514	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
25	b	614	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
25	c	505	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
25	C	509	CLA	CAC-C3C-C4C	2.15	127.59	124.79
29	D	405	PL9	C20-C19-C21	2.15	118.97	115.23
27	b	619	BCR	C37-C22-C21	-2.15	119.33	122.82
25	b	602	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
31	I	101	LMT	C1'-O5'-C5'	-2.15	109.52	113.72
25	A	405	CLA	CHD-C4C-C3C	-2.15	121.64	124.77
25	B	614	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
30	H	102	SQD	O47-C7-O49	-2.15	118.69	123.70
35	v	201	HEM	CMC-C2C-C3C	2.14	128.97	124.68
25	A	405	CLA	C4-C3-C5	2.14	118.95	115.23
25	B	616	CLA	C4D-C3D-CAD	2.14	110.43	108.11
25	a	405	CLA	C4-C3-C5	2.14	118.95	115.23
27	z	101	BCR	C38-C26-C27	2.14	118.17	113.60
30	H	102	SQD	O8-S-C6	2.14	110.11	105.97
30	C	501	SQD	O5-C5-C4	2.14	113.56	109.70
27	B	619	BCR	C37-C22-C21	-2.14	119.35	122.82
25	a	405	CLA	CHD-C4C-C3C	-2.14	121.65	124.77
30	h	102	SQD	O47-C7-O49	-2.14	118.70	123.70
25	C	514	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
25	b	603	CLA	C1-O2A-CGA	2.14	121.83	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	611	CLA	CHC-C1C-C2C	-2.14	120.89	126.94
25	c	513	CLA	C5-C3-C4	2.14	119.51	114.59
31	i	101	LMT	C1'-O5'-C5'	-2.14	109.55	113.72
25	D	401	CLA	CBC-CAC-C3C	-2.14	106.63	112.42
30	A	412	SQD	O47-C7-O49	-2.14	118.71	123.70
29	a	411	PL9	C36-C34-C33	-2.14	116.37	121.17
30	c	501	SQD	O5-C5-C4	2.14	113.55	109.70
30	a	412	SQD	O47-C7-O49	-2.14	118.71	123.70
30	h	102	SQD	O8-S-C6	2.13	110.09	105.97
25	d	401	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
29	A	411	PL9	C36-C34-C33	-2.13	116.38	121.17
25	c	511	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
25	C	505	CLA	CAA-C2A-C1A	-2.13	104.99	111.97
25	c	514	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
25	C	513	CLA	C5-C3-C4	2.13	119.49	114.59
30	h	102	SQD	O5-C1-C2	2.13	114.75	110.37
25	C	504	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
25	c	505	CLA	CAA-C2A-C1A	-2.13	104.99	111.97
27	K	102	BCR	C36-C18-C17	-2.13	119.37	122.82
25	B	611	CLA	CHC-C1C-C2C	-2.13	120.91	126.94
29	A	411	PL9	C50-C49-C48	-2.13	116.27	122.66
28	D	409	LMG	O7-C10-O9	-2.13	118.73	123.70
27	b	617	BCR	C7-C8-C9	-2.13	123.09	126.23
34	C	517	DGD	O2G-C1B-O1B	-2.13	118.73	123.70
25	B	607	CLA	C1-C2-C3	-2.12	122.72	126.20
25	c	508	CLA	CHC-C1C-C2C	-2.12	120.93	126.94
25	c	502	CLA	C3C-C4C-NC	2.12	113.15	110.43
34	c	517	DGD	O2G-C1B-O1B	-2.12	118.75	123.70
27	c	515	BCR	C36-C18-C17	-2.12	119.38	122.82
25	c	510	CLA	C6-C5-C3	-2.12	108.31	113.47
25	D	403	CLA	CHC-C1C-NC	-2.12	121.12	124.31
27	B	617	BCR	C7-C8-C9	-2.12	123.10	126.23
33	z	102	LHG	O4-P-O5	2.12	119.08	110.83
30	H	102	SQD	O5-C1-C2	2.12	114.72	110.37
28	d	409	LMG	O7-C10-O9	-2.12	118.76	123.70
25	c	502	CLA	C4D-C3D-CAD	2.11	110.40	108.11
25	b	607	CLA	C1-C2-C3	-2.11	122.73	126.20
25	C	508	CLA	CHC-C1C-C2C	-2.11	120.95	126.94
33	Z	102	LHG	O4-P-O5	2.11	119.06	110.83
29	a	411	PL9	C50-C49-C48	-2.11	116.32	122.66
25	C	511	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
25	c	504	CLA	CMD-C2D-C3D	-2.11	122.85	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	515	BCR	C36-C18-C17	-2.11	119.40	122.82
25	d	401	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
25	b	605	CLA	C4D-C3D-CAD	2.11	110.40	108.11
25	C	504	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
25	c	504	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
27	Z	101	BCR	C37-C22-C21	-2.11	119.40	122.82
25	D	401	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
25	d	403	CLA	CHC-C1C-NC	-2.11	121.14	124.31
25	b	606	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
25	C	510	CLA	C6-C5-C3	-2.10	108.34	113.47
25	a	405	CLA	C11-C12-C13	-2.10	108.97	115.97
25	b	616	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
25	C	510	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
25	C	502	CLA	C4D-C3D-CAD	2.10	110.39	108.11
25	c	509	CLA	C3C-C4C-NC	2.10	113.12	110.43
27	b	617	BCR	C40-C30-C25	-2.10	106.95	110.24
27	Z	101	BCR	C3-C4-C5	-2.10	110.31	114.06
25	B	612	CLA	CHD-C4C-C3C	-2.10	121.71	124.77
25	b	612	CLA	CHD-C4C-C3C	-2.10	121.71	124.77
27	B	617	BCR	C40-C30-C25	-2.10	106.95	110.24
25	A	405	CLA	C11-C12-C13	-2.10	108.99	115.97
25	C	502	CLA	C3C-C4C-NC	2.10	113.12	110.43
25	C	509	CLA	C3C-C4C-NC	2.10	113.12	110.43
27	z	101	BCR	C37-C22-C21	-2.10	119.42	122.82
25	B	612	CLA	O1D-CGD-CBD	-2.10	120.39	124.52
25	D	401	CLA	C6-C5-C3	-2.09	108.36	113.47
25	B	616	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
27	B	617	BCR	C35-C13-C12	2.09	121.29	118.09
25	B	607	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
25	B	605	CLA	C4D-C3D-CAD	2.09	110.38	108.11
25	b	607	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
25	b	612	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
27	B	619	BCR	C27-C26-C25	-2.09	119.88	122.70
30	K	101	SQD	O5-C1-C2	2.09	114.66	110.37
26	A	407	PHO	OBD-CAD-CBD	-2.09	122.76	125.82
27	F	101	BCR	C35-C13-C12	2.09	121.28	118.09
25	C	511	CLA	CHC-C1C-C2C	-2.09	121.03	126.94
25	a	405	CLA	C1-C2-C3	-2.09	122.78	126.20
25	c	510	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
25	c	511	CLA	CHC-C1C-C2C	-2.09	121.03	126.94
27	z	101	BCR	C3-C4-C5	-2.08	110.34	114.06
35	V	201	HEM	C4D-ND-C1D	2.08	107.67	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	k	101	SQD	O5-C1-C2	2.08	114.65	110.37
25	B	606	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
27	F	101	BCR	C34-C9-C10	-2.08	119.44	122.82
25	B	608	CLA	C3C-C4C-NC	2.08	113.10	110.43
27	f	101	BCR	C35-C13-C12	2.08	121.27	118.09
25	b	616	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
25	d	401	CLA	C6-C5-C3	-2.08	108.40	113.47
27	k	102	BCR	C33-C5-C4	2.08	118.03	113.60
31	x	101	LMT	C1'-O5'-C5'	-2.08	109.66	113.72
25	B	616	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
31	X	101	LMT	C1'-O5'-C5'	-2.08	109.66	113.72
30	k	101	SQD	O48-C23-O10	-2.08	118.43	123.63
27	K	102	BCR	C33-C5-C4	2.08	118.02	113.60
29	d	405	PL9	C32-C33-C34	-2.08	122.87	127.62
29	D	405	PL9	C32-C33-C34	-2.08	122.87	127.62
26	a	407	PHO	OBD-CAD-CBD	-2.07	122.78	125.82
27	b	617	BCR	C35-C13-C12	2.07	121.26	118.09
25	b	611	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
27	B	618	BCR	C34-C9-C10	-2.07	119.46	122.82
31	B	625	LMT	O1B-C4'-C3'	2.07	112.50	107.23
25	B	602	CLA	C6-C7-C8	-2.07	109.08	115.97
27	b	619	BCR	C27-C26-C25	-2.07	119.91	122.70
25	A	405	CLA	C1-C2-C3	-2.07	122.81	126.20
27	b	618	BCR	C34-C9-C10	-2.07	119.46	122.82
25	C	512	CLA	C3B-C4B-NB	2.07	111.88	109.21
25	b	608	CLA	C3C-C4C-NC	2.07	113.08	110.43
35	v	201	HEM	C4D-ND-C1D	2.07	107.65	105.21
25	C	502	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
29	d	405	PL9	C42-C43-C44	-2.06	122.90	127.62
31	b	625	LMT	O1B-C4'-C3'	2.06	112.48	107.23
25	B	611	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
25	a	408	CLA	CHC-C1C-C2C	-2.06	121.10	126.94
25	c	502	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
25	A	408	CLA	CHC-C1C-C2C	-2.06	121.11	126.94
30	K	101	SQD	O48-C23-O10	-2.06	118.48	123.63
25	c	512	CLA	C3B-C4B-NB	2.06	111.87	109.21
25	b	602	CLA	C6-C7-C8	-2.06	109.13	115.97
25	B	614	CLA	CBC-CAC-C3C	-2.05	106.85	112.42
29	D	405	PL9	C42-C43-C44	-2.05	122.92	127.62
25	A	406	CLA	C3C-C4C-NC	2.05	113.06	110.43
33	Z	102	LHG	O8-C23-O10	-2.05	118.49	123.63
30	a	413	SQD	C46-C45-C44	-2.05	107.00	111.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	101	BCR	C34-C9-C10	-2.05	119.49	122.82
31	f	103	LMT	C3'-C4'-C5'	-2.05	106.39	110.93
31	E	103	LMT	O5'-C1'-C2'	2.05	114.58	110.37
33	z	102	LHG	O8-C23-O10	-2.05	118.50	123.63
25	c	508	CLA	C3C-C4C-NC	2.05	113.05	110.43
25	b	614	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
31	F	103	LMT	C3'-C4'-C5'	-2.05	106.39	110.93
30	A	413	SQD	C46-C45-C44	-2.05	107.01	111.78
25	C	514	CLA	C6-C5-C3	-2.05	108.48	113.47
30	a	413	SQD	O47-C7-O49	-2.04	118.92	123.70
30	A	413	SQD	O47-C7-O49	-2.04	118.93	123.70
25	B	602	CLA	CED-O2D-CGD	2.04	120.55	115.92
25	c	514	CLA	C6-C5-C3	-2.04	108.49	113.47
31	d	412	LMT	O5'-C1'-O1'	-2.04	105.22	110.04
31	e	103	LMT	O5'-C1'-C2'	2.04	114.56	110.37
25	C	504	CLA	CAC-C3C-C4C	2.04	127.44	124.79
28	A	414	LMG	O7-C10-O9	-2.04	118.93	123.70
28	a	414	LMG	O7-C10-O9	-2.04	118.93	123.70
25	c	504	CLA	CAC-C3C-C4C	2.04	127.44	124.79
27	B	619	BCR	C15-C14-C13	-2.04	124.42	127.28
25	D	404	CLA	CHC-C1C-C2C	-2.04	121.17	126.94
30	C	501	SQD	O48-C23-C24	2.04	118.05	111.83
25	B	603	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
25	c	505	CLA	C7-C6-C5	-2.04	107.83	113.26
27	z	101	BCR	C29-C28-C27	2.03	115.75	111.28
25	C	508	CLA	C3C-C4C-NC	2.03	113.04	110.43
31	D	412	LMT	O5'-C1'-O1'	-2.03	105.24	110.04
25	C	505	CLA	C7-C6-C5	-2.03	107.84	113.26
25	b	603	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
27	Z	101	BCR	C29-C28-C27	2.03	115.75	111.28
25	b	615	CLA	CMA-C3A-C4A	2.03	117.23	111.77
25	d	404	CLA	CHC-C1C-C2C	-2.03	121.19	126.94
25	a	406	CLA	C3C-C4C-NC	2.03	113.03	110.43
29	A	411	PL9	C42-C43-C44	-2.03	122.99	127.62
30	c	501	SQD	O48-C23-C24	2.03	118.01	111.83
33	d	407	LHG	O8-C23-O10	-2.03	118.56	123.63
25	B	615	CLA	CMA-C3A-C4A	2.02	117.22	111.77
25	B	606	CLA	CED-O2D-CGD	2.02	120.51	115.92
25	d	404	CLA	CED-O2D-CGD	2.02	120.50	115.92
25	b	602	CLA	CED-O2D-CGD	2.02	120.50	115.92
25	B	616	CLA	CMA-C3A-C4A	2.02	117.21	111.77
25	C	511	CLA	CMC-C2C-C1C	2.02	128.19	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	CMC-C2C-C1C	2.02	128.19	125.03
31	E	103	LMT	C1'-C2'-C3'	2.02	114.26	110.01
31	e	103	LMT	C1'-C2'-C3'	2.02	114.26	110.01
29	a	411	PL9	C42-C43-C44	-2.02	123.01	127.62
25	b	606	CLA	CED-O2D-CGD	2.02	120.49	115.92
25	C	513	CLA	CHC-C1C-C2C	-2.02	121.23	126.94
25	C	505	CLA	CHC-C1C-C2C	-2.02	121.23	126.94
27	k	103	BCR	C2-C1-C6	2.01	113.36	110.44
25	B	610	CLA	CHC-C1C-C2C	-2.01	121.24	126.94
27	z	101	BCR	C31-C1-C6	-2.01	107.09	110.24
25	c	505	CLA	CHC-C1C-C2C	-2.01	121.25	126.94
27	b	619	BCR	C15-C14-C13	-2.01	124.46	127.28
27	b	618	BCR	C32-C1-C6	-2.01	107.09	110.24
27	z	101	BCR	C33-C5-C6	-2.01	122.29	124.48
33	D	407	LHG	O8-C23-O10	-2.01	118.61	123.63
31	L	101	LMT	O5B-C5B-C4B	2.01	113.31	109.70
25	b	615	CLA	OBD-CAD-C3D	-2.01	123.73	128.42
25	B	615	CLA	OBD-CAD-C3D	-2.00	123.73	128.42
25	c	512	CLA	CAC-C3C-C4C	2.00	127.40	124.79
25	c	513	CLA	CHC-C1C-C2C	-2.00	121.27	126.94
25	b	610	CLA	CHC-C1C-C2C	-2.00	121.27	126.94
25	D	404	CLA	CED-O2D-CGD	2.00	120.46	115.92
27	K	103	BCR	C2-C1-C6	2.00	113.35	110.44
25	d	401	CLA	CAC-C3C-C4C	2.00	127.39	124.79
31	L	101	LMT	O5B-C5B-C6B	2.00	111.40	106.44
25	b	616	CLA	CMA-C3A-C4A	2.00	117.15	111.77
25	B	605	CLA	CAA-C2A-C3A	-2.00	107.59	113.00

All (70) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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	502	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	C	514	CLA	ND
25	D	401	CLA	ND
25	D	403	CLA	ND
25	D	404	CLA	ND
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	b	616	CLA	ND
25	c	502	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	c	514	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND

All (2477) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	C3A-C2A-CAA-CBA
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	C2-C1-O2A-CGA
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	C4-C3-C5-C6
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	C3A-C2A-CAA-CBA
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	507	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	510	CLA	C2-C1-O2A-CGA
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	C4-C3-C5-C6
27	A	409	BCR	C7-C8-C9-C10
27	B	617	BCR	C7-C8-C9-C10
27	B	617	BCR	C10-C11-C12-C13
27	B	618	BCR	C11-C10-C9-C8
27	B	618	BCR	C11-C10-C9-C34
27	B	618	BCR	C10-C11-C12-C13
27	B	619	BCR	C7-C8-C9-C10
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C10-C9-C8
27	B	619	BCR	C11-C10-C9-C34
27	B	619	BCR	C10-C11-C12-C13
27	C	515	BCR	C7-C8-C9-C10
27	C	515	BCR	C11-C10-C9-C8
27	C	515	BCR	C11-C10-C9-C34
27	C	515	BCR	C10-C11-C12-C13
27	F	101	BCR	C11-C10-C9-C8
27	F	101	BCR	C11-C10-C9-C34
27	F	101	BCR	C10-C11-C12-C13
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	K	102	BCR	C7-C8-C9-C10
27	K	102	BCR	C11-C10-C9-C8
27	K	102	BCR	C11-C10-C9-C34
27	K	102	BCR	C10-C11-C12-C13
27	K	103	BCR	C11-C10-C9-C8
27	K	103	BCR	C11-C10-C9-C34
27	K	103	BCR	C10-C11-C12-C13
27	K	103	BCR	C17-C18-C19-C20
27	Z	101	BCR	C7-C8-C9-C10
27	Z	101	BCR	C7-C8-C9-C34
27	Z	101	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	409	BCR	C7-C8-C9-C10
27	b	617	BCR	C7-C8-C9-C10
27	b	617	BCR	C10-C11-C12-C13
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C7-C8-C9-C10
27	b	619	BCR	C7-C8-C9-C34
27	b	619	BCR	C11-C10-C9-C8
27	b	619	BCR	C11-C10-C9-C34
27	b	619	BCR	C10-C11-C12-C13
27	c	515	BCR	C7-C8-C9-C10
27	c	515	BCR	C11-C10-C9-C8
27	c	515	BCR	C11-C10-C9-C34
27	c	515	BCR	C10-C11-C12-C13
27	f	101	BCR	C11-C10-C9-C8
27	f	101	BCR	C11-C10-C9-C34
27	f	101	BCR	C10-C11-C12-C13
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C11-C10-C9-C8
27	k	102	BCR	C11-C10-C9-C34
27	k	102	BCR	C10-C11-C12-C13
27	k	103	BCR	C11-C10-C9-C8
27	k	103	BCR	C11-C10-C9-C34
27	k	103	BCR	C10-C11-C12-C13
27	k	103	BCR	C17-C18-C19-C20
27	z	101	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C34
27	z	101	BCR	C11-C10-C9-C34
29	A	411	PL9	C12-C13-C14-C16
29	A	411	PL9	C17-C18-C19-C20
29	A	411	PL9	C17-C18-C19-C21
29	A	411	PL9	C22-C23-C24-C25
29	A	411	PL9	C22-C23-C24-C26
29	A	411	PL9	C37-C38-C39-C40
29	A	411	PL9	C37-C38-C39-C41
29	A	411	PL9	C42-C43-C44-C46
29	A	411	PL9	C46-C47-C48-C49
29	A	411	PL9	C47-C48-C49-C51
29	D	405	PL9	C42-C43-C44-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C42-C43-C44-C46
29	a	411	PL9	C12-C13-C14-C16
29	a	411	PL9	C17-C18-C19-C20
29	a	411	PL9	C17-C18-C19-C21
29	a	411	PL9	C22-C23-C24-C25
29	a	411	PL9	C22-C23-C24-C26
29	a	411	PL9	C37-C38-C39-C40
29	a	411	PL9	C37-C38-C39-C41
29	a	411	PL9	C42-C43-C44-C46
29	a	411	PL9	C46-C47-C48-C49
29	a	411	PL9	C47-C48-C49-C51
29	d	405	PL9	C42-C43-C44-C45
29	d	405	PL9	C42-C43-C44-C46
30	A	412	SQD	O49-C7-O47-C45
30	A	412	SQD	C8-C7-O47-C45
30	A	412	SQD	C5-C6-S-O8
30	A	412	SQD	C5-C6-S-O9
30	A	413	SQD	C5-C6-S-O9
30	B	620	SQD	O5-C1-O6-C44
30	B	620	SQD	C46-C45-O47-C7
30	F	102	SQD	O5-C1-O6-C44
30	H	102	SQD	C2-C1-O6-C44
30	H	102	SQD	O5-C1-O6-C44
30	H	102	SQD	O6-C44-C45-O47
30	H	102	SQD	O49-C7-O47-C45
30	H	102	SQD	C8-C7-O47-C45
30	H	102	SQD	O10-C23-O48-C46
30	H	102	SQD	C5-C6-S-O7
30	H	102	SQD	C5-C6-S-O8
30	H	102	SQD	C5-C6-S-O9
30	K	101	SQD	O5-C1-O6-C44
30	a	412	SQD	O49-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
30	a	412	SQD	C5-C6-S-O8
30	a	412	SQD	C5-C6-S-O9
30	a	413	SQD	C5-C6-S-O9
30	b	620	SQD	O5-C1-O6-C44
30	b	620	SQD	C46-C45-O47-C7
30	f	102	SQD	O5-C1-O6-C44
30	h	102	SQD	C2-C1-O6-C44
30	h	102	SQD	O5-C1-O6-C44
30	h	102	SQD	O6-C44-C45-O47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	102	SQD	O49-C7-O47-C45
30	h	102	SQD	C8-C7-O47-C45
30	h	102	SQD	O10-C23-O48-C46
30	h	102	SQD	C5-C6-S-O7
30	h	102	SQD	C5-C6-S-O8
30	h	102	SQD	C5-C6-S-O9
30	k	101	SQD	O5-C1-O6-C44
31	A	415	LMT	C2'-C1'-O1'-C1
31	B	623	LMT	C2-C1-O1'-C1'
31	B	624	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	C2'-C1'-O1'-C1
31	D	410	LMT	C2'-C1'-O1'-C1
31	D	411	LMT	C2'-C1'-O1'-C1
31	D	411	LMT	O5'-C1'-O1'-C1
31	E	101	LMT	O5'-C1'-O1'-C1
31	H	101	LMT	C2'-C1'-O1'-C1
31	H	101	LMT	O5'-C1'-O1'-C1
31	I	101	LMT	C2'-C1'-O1'-C1
31	I	101	LMT	O5'-C1'-O1'-C1
31	I	101	LMT	C2-C1-O1'-C1'
31	J	101	LMT	C2'-C1'-O1'-C1
31	J	101	LMT	C2-C1-O1'-C1'
31	M	102	LMT	O5'-C1'-O1'-C1
31	a	415	LMT	C2'-C1'-O1'-C1
31	b	623	LMT	C2-C1-O1'-C1'
31	b	624	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	C2'-C1'-O1'-C1
31	d	410	LMT	C2'-C1'-O1'-C1
31	d	411	LMT	C2'-C1'-O1'-C1
31	d	411	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	h	101	LMT	C2'-C1'-O1'-C1
31	h	101	LMT	O5'-C1'-O1'-C1
31	i	101	LMT	C2'-C1'-O1'-C1
31	i	101	LMT	O5'-C1'-O1'-C1
31	i	101	LMT	C2-C1-O1'-C1'
31	j	101	LMT	C2'-C1'-O1'-C1
31	j	101	LMT	C2-C1-O1'-C1'
31	m	101	LMT	O5'-C1'-O1'-C1
33	B	622	LHG	O1-C1-C2-C3
33	B	622	LHG	C2-C3-O3-P
33	B	622	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	628	LHG	C4-O6-P-O3
33	B	628	LHG	C4-O6-P-O4
33	B	628	LHG	C4-O6-P-O5
33	D	406	LHG	C3-O3-P-O4
33	D	406	LHG	C3-O3-P-O6
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C3-O3-P-O4
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O4
33	D	407	LHG	C4-O6-P-O5
33	E	102	LHG	O1-C1-C2-O2
33	E	102	LHG	O1-C1-C2-C3
33	E	102	LHG	C3-O3-P-O5
33	E	102	LHG	C4-O6-P-O3
33	E	102	LHG	C4-O6-P-O4
33	E	102	LHG	O7-C5-C6-O8
33	b	622	LHG	O1-C1-C2-C3
33	b	622	LHG	C2-C3-O3-P
33	b	622	LHG	C3-O3-P-O5
33	b	628	LHG	C4-O6-P-O3
33	b	628	LHG	C4-O6-P-O4
33	b	628	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O4
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	d	407	LHG	C4-O6-P-O5
33	e	102	LHG	O1-C1-C2-O2
33	e	102	LHG	O1-C1-C2-C3
33	e	102	LHG	C3-O3-P-O5
33	e	102	LHG	C4-O6-P-O3
33	e	102	LHG	C4-O6-P-O4
33	e	102	LHG	O7-C5-C6-O8
37	X	102	RRX	C37-C22-C23-C24
37	X	102	RRX	C21-C22-C23-C24
37	X	102	RRX	C20-C21-C22-C23
37	X	102	RRX	C20-C21-C22-C37
37	X	102	RRX	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	X	102	RRX	C11-C12-C13-C14
37	X	102	RRX	C11-C12-C13-C35
37	X	102	RRX	C9-C10-C11-C12
37	X	102	RRX	C11-C10-C9-C34
37	x	102	RRX	C37-C22-C23-C24
37	x	102	RRX	C21-C22-C23-C24
37	x	102	RRX	C20-C21-C22-C23
37	x	102	RRX	C20-C21-C22-C37
37	x	102	RRX	C18-C19-C20-C21
37	x	102	RRX	C11-C12-C13-C14
37	x	102	RRX	C11-C12-C13-C35
37	x	102	RRX	C9-C10-C11-C12
37	x	102	RRX	C11-C10-C9-C34
31	B	625	LMT	C3'-C4'-O1B-C1B
31	b	625	LMT	C3'-C4'-O1B-C1B
25	A	405	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
28	C	523	LMG	O10-C28-O8-C9
28	c	523	LMG	O10-C28-O8-C9
34	C	516	DGD	O1A-C1A-O1G-C1G
34	c	516	DGD	O1A-C1A-O1G-C1G
25	C	510	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C47-C48-C49-C50
29	a	411	PL9	C47-C48-C49-C50
33	B	628	LHG	C5-C6-O8-C23
33	b	628	LHG	C5-C6-O8-C23
25	C	513	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C29-C28-O8-C9
28	C	523	LMG	C29-C28-O8-C9
28	a	410	LMG	C29-C28-O8-C9
28	c	523	LMG	C29-C28-O8-C9
30	A	412	SQD	C24-C23-O48-C46
30	F	102	SQD	C24-C23-O48-C46
30	H	102	SQD	C24-C23-O48-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
30	h	102	SQD	C24-C23-O48-C46
34	C	516	DGD	C2A-C1A-O1G-C1G
34	c	516	DGD	C2A-C1A-O1G-C1G
28	A	410	LMG	O10-C28-O8-C9
28	A	414	LMG	O10-C28-O8-C9
28	a	410	LMG	O10-C28-O8-C9
28	a	414	LMG	O10-C28-O8-C9
30	A	412	SQD	O10-C23-O48-C46
30	B	620	SQD	O10-C23-O48-C46
30	F	102	SQD	O10-C23-O48-C46
30	a	412	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
25	C	510	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
31	I	102	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4'-C5'-C6'-O6'
25	C	511	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
31	L	101	LMT	C3'-C4'-O1B-C1B
31	M	101	LMT	C3'-C4'-O1B-C1B
31	K	105	LMT	O5B-C1B-O1B-C4'
31	k	105	LMT	O5B-C1B-O1B-C4'
30	F	102	SQD	O49-C7-O47-C45
30	f	102	SQD	O49-C7-O47-C45
25	D	404	CLA	C3-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
25	B	604	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	b	604	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
28	A	414	LMG	C29-C28-O8-C9
28	a	414	LMG	C29-C28-O8-C9
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	C4-C3-C5-C6
25	C	508	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	c	508	CLA	C4-C3-C5-C6
29	D	405	PL9	C20-C19-C21-C22
29	d	405	PL9	C20-C19-C21-C22
25	C	508	CLA	C2-C3-C5-C6
25	D	404	CLA	C2-C3-C5-C6
25	c	508	CLA	C2-C3-C5-C6
25	d	404	CLA	C2-C3-C5-C6
29	A	411	PL9	C33-C34-C36-C37
29	A	411	PL9	C38-C39-C41-C42
29	a	411	PL9	C33-C34-C36-C37
29	a	411	PL9	C38-C39-C41-C42
25	A	408	CLA	CBD-CGD-O2D-CED
25	a	408	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	D	404	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C17-C18-C19-C20
28	C	519	LMG	C17-C18-C19-C20
28	C	519	LMG	C20-C21-C22-C23
28	C	519	LMG	C38-C39-C40-C41
28	a	410	LMG	C17-C18-C19-C20
28	c	519	LMG	C17-C18-C19-C20
31	H	101	LMT	C4'-C5'-C6'-O6'
31	h	101	LMT	C4'-C5'-C6'-O6'
29	A	411	PL9	C12-C13-C14-C15
29	A	411	PL9	C27-C28-C29-C30
29	a	411	PL9	C12-C13-C14-C15
29	a	411	PL9	C27-C28-C29-C30
29	A	411	PL9	C27-C28-C29-C31
29	a	411	PL9	C27-C28-C29-C31
28	c	519	LMG	C38-C39-C40-C41
34	C	518	DGD	C8A-C9A-CAA-CBA
34	c	518	DGD	C8A-C9A-CAA-CBA
31	B	624	LMT	O5'-C5'-C6'-O6'
31	I	102	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	624	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
31	B	624	LMT	C4'-C5'-C6'-O6'
31	b	624	LMT	C4'-C5'-C6'-O6'
25	B	604	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	O1A-CGA-O2A-C1
25	b	604	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1A-CGA-O2A-C1
28	c	519	LMG	C20-C21-C22-C23
34	c	518	DGD	C8B-C9B-CAB-CBB
34	C	517	DGD	C8B-C9B-CAB-CBB
34	C	517	DGD	CBB-CCB-CDB-CEB
34	C	518	DGD	C8B-C9B-CAB-CBB
34	H	103	DGD	CBB-CCB-CDB-CEB
34	c	517	DGD	C8B-C9B-CAB-CBB
34	c	517	DGD	CBB-CCB-CDB-CEB
34	h	103	DGD	CBB-CCB-CDB-CEB
31	K	105	LMT	O5'-C5'-C6'-O6'
31	k	105	LMT	O5'-C5'-C6'-O6'
25	C	504	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
28	A	410	LMG	C20-C21-C22-C23
28	a	410	LMG	C20-C21-C22-C23
33	D	406	LHG	O2-C2-C3-O3
33	D	407	LHG	O2-C2-C3-O3
33	d	406	LHG	O2-C2-C3-O3
33	d	407	LHG	O2-C2-C3-O3
25	A	405	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
30	B	620	SQD	C24-C23-O48-C46
30	b	620	SQD	C24-C23-O48-C46
33	B	628	LHG	C24-C23-O8-C6
33	b	628	LHG	C24-C23-O8-C6
28	C	523	LMG	O6-C5-C6-O5
28	c	523	LMG	O6-C5-C6-O5
31	B	626	LMT	O5'-C5'-C6'-O6'
31	C	524	LMT	O5B-C5B-C6B-O6B
31	D	412	LMT	O5B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	H	101	LMT	O5'-C5'-C6'-O6'
31	Y	101	LMT	O5'-C5'-C6'-O6'
31	b	626	LMT	O5'-C5'-C6'-O6'
31	c	524	LMT	O5B-C5B-C6B-O6B
31	d	412	LMT	O5B-C5B-C6B-O6B
31	h	101	LMT	O5'-C5'-C6'-O6'
31	y	101	LMT	O5'-C5'-C6'-O6'
31	K	105	LMT	O5B-C5B-C6B-O6B
31	k	105	LMT	O5B-C5B-C6B-O6B
31	A	415	LMT	C4B-C5B-C6B-O6B
31	K	105	LMT	C4B-C5B-C6B-O6B
31	a	415	LMT	C4B-C5B-C6B-O6B
31	k	105	LMT	C4B-C5B-C6B-O6B
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
33	E	102	LHG	C8-C7-O7-C5
33	e	102	LHG	C8-C7-O7-C5
31	I	104	LMT	O5'-C5'-C6'-O6'
31	J	101	LMT	O5'-C5'-C6'-O6'
31	L	101	LMT	O5'-C5'-C6'-O6'
31	M	101	LMT	O5'-C5'-C6'-O6'
31	i	104	LMT	O5'-C5'-C6'-O6'
31	j	101	LMT	O5'-C5'-C6'-O6'
31	E	103	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4'-C5'-C6'-O6'
31	B	629	LMT	O5'-C5'-C6'-O6'
31	b	629	LMT	O5'-C5'-C6'-O6'
25	C	507	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
31	C	521	LMT	O5'-C5'-C6'-O6'
31	F	103	LMT	O5'-C5'-C6'-O6'
31	c	521	LMT	O5'-C5'-C6'-O6'
31	f	103	LMT	O5'-C5'-C6'-O6'
29	A	411	PL9	C9-C11-C12-C13
29	A	411	PL9	C24-C26-C27-C28
29	A	411	PL9	C34-C36-C37-C38
29	A	411	PL9	C44-C46-C47-C48
29	D	405	PL9	C39-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C44-C46-C47-C48
29	a	411	PL9	C9-C11-C12-C13
29	a	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C34-C36-C37-C38
29	a	411	PL9	C44-C46-C47-C48
29	d	405	PL9	C39-C41-C42-C43
29	d	405	PL9	C44-C46-C47-C48
31	E	103	LMT	O5B-C5B-C6B-O6B
31	E	103	LMT	O5'-C5'-C6'-O6'
31	L	101	LMT	O5B-C5B-C6B-O6B
31	M	101	LMT	O5B-C5B-C6B-O6B
31	e	103	LMT	O5B-C5B-C6B-O6B
31	e	103	LMT	O5'-C5'-C6'-O6'
31	D	412	LMT	C4B-C5B-C6B-O6B
31	J	101	LMT	C4'-C5'-C6'-O6'
31	d	412	LMT	C4B-C5B-C6B-O6B
31	j	101	LMT	C4'-C5'-C6'-O6'
30	K	101	SQD	O10-C23-O48-C46
30	k	101	SQD	O10-C23-O48-C46
33	B	628	LHG	O10-C23-O8-C6
33	b	628	LHG	O10-C23-O8-C6
28	C	523	LMG	O6-C1-O1-C7
28	c	523	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
30	a	413	SQD	O5-C1-O6-C44
31	C	522	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	O5'-C1'-O1'-C1
31	D	410	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	X	101	LMT	O5'-C1'-O1'-C1
31	X	103	LMT	O5'-C1'-O1'-C1
31	c	522	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	d	410	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
31	x	103	LMT	O5'-C1'-O1'-C1
31	D	410	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5'-C5'-C6'-O6'
25	C	512	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	C	503	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	401	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	d	401	CLA	CBD-CGD-O2D-CED
31	I	103	LMT	O5'-C5'-C6'-O6'
31	M	102	LMT	O5'-C5'-C6'-O6'
31	i	103	LMT	O5'-C5'-C6'-O6'
31	m	101	LMT	O5'-C5'-C6'-O6'
25	C	514	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
33	B	622	LHG	C1-C2-C3-O3
33	D	406	LHG	C1-C2-C3-O3
33	b	622	LHG	C1-C2-C3-O3
33	d	406	LHG	C1-C2-C3-O3
25	B	616	CLA	CBA-CGA-O2A-C1
25	C	514	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	c	514	CLA	CBA-CGA-O2A-C1
28	C	523	LMG	C36-C37-C38-C39
28	c	523	LMG	C36-C37-C38-C39
31	A	416	LMT	O5'-C5'-C6'-O6'
31	a	416	LMT	O5'-C5'-C6'-O6'
25	B	613	CLA	CBD-CGD-O2D-CED
31	B	626	LMT	C4'-C5'-C6'-O6'
31	K	105	LMT	C4'-C5'-C6'-O6'
31	b	626	LMT	C4'-C5'-C6'-O6'
31	k	105	LMT	C4'-C5'-C6'-O6'
29	A	411	PL9	C40-C39-C41-C42
29	a	411	PL9	C40-C39-C41-C42
25	B	604	CLA	C11-C10-C8-C9
25	B	609	CLA	C6-C7-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	502	CLA	C6-C7-C8-C9
25	C	507	CLA	C6-C7-C8-C9
25	C	514	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	616	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	502	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
25	c	514	CLA	C6-C7-C8-C9
28	C	523	LMG	C2-C1-O1-C7
28	c	523	LMG	C2-C1-O1-C7
30	A	413	SQD	C2-C1-O6-C44
30	a	413	SQD	C2-C1-O6-C44
31	C	522	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	X	101	LMT	C2'-C1'-O1'-C1
31	X	103	LMT	C2'-C1'-O1'-C1
31	c	522	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	C2'-C1'-O1'-C1
31	m	101	LMT	C2'-C1'-O1'-C1
31	x	101	LMT	C2'-C1'-O1'-C1
31	x	103	LMT	C2'-C1'-O1'-C1
33	B	622	LHG	C11-C10-C9-C8
33	b	622	LHG	C11-C10-C9-C8
25	b	616	CLA	O1A-CGA-O2A-C1
27	A	409	BCR	C7-C8-C9-C34
27	B	617	BCR	C7-C8-C9-C34
27	B	618	BCR	C7-C8-C9-C34
27	C	515	BCR	C7-C8-C9-C34
27	K	102	BCR	C7-C8-C9-C34
27	K	103	BCR	C36-C18-C19-C20
27	a	409	BCR	C7-C8-C9-C34
27	b	617	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
27	c	515	BCR	C7-C8-C9-C34
27	k	102	BCR	C7-C8-C9-C34
27	k	103	BCR	C36-C18-C19-C20
37	X	102	RRX	C36-C18-C19-C20
37	X	102	RRX	C7-C8-C9-C34
37	x	102	RRX	C36-C18-C19-C20
37	x	102	RRX	C7-C8-C9-C34
31	A	415	LMT	O5B-C5B-C6B-O6B
31	a	415	LMT	O5B-C5B-C6B-O6B
37	X	102	RRX	C17-C18-C19-C20
37	x	102	RRX	C17-C18-C19-C20
33	E	102	LHG	C16-C17-C18-C19
33	e	102	LHG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	622	LHG	C23-C24-C25-C26
33	b	622	LHG	C23-C24-C25-C26
25	B	616	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
28	C	523	LMG	C4-C5-C6-O5
28	c	523	LMG	C4-C5-C6-O5
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
30	K	101	SQD	C24-C23-O48-C46
30	k	101	SQD	C24-C23-O48-C46
25	B	614	CLA	C8-C10-C11-C12
25	C	504	CLA	C15-C16-C17-C18
25	b	614	CLA	C8-C10-C11-C12
25	c	504	CLA	C15-C16-C17-C18
25	B	612	CLA	C2-C1-O2A-CGA
25	b	612	CLA	C2-C1-O2A-CGA
25	B	609	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	C	511	CLA	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
25	B	606	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
31	C	522	LMT	O5'-C5'-C6'-O6'
31	c	522	LMT	O5'-C5'-C6'-O6'
33	D	407	LHG	O1-C1-C2-O2
33	d	407	LHG	O1-C1-C2-O2
31	L	101	LMT	C4'-C5'-C6'-O6'
31	M	101	LMT	C4'-C5'-C6'-O6'
30	K	101	SQD	C23-C24-C25-C26
33	Z	102	LHG	C7-C8-C9-C10
33	z	102	LHG	C7-C8-C9-C10
25	B	616	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
31	B	625	LMT	O1'-C1-C2-C3
31	X	103	LMT	O1'-C1-C2-C3
31	b	625	LMT	O1'-C1-C2-C3
31	x	103	LMT	O1'-C1-C2-C3
31	K	105	LMT	C3'-C4'-O1B-C1B
31	k	105	LMT	C3'-C4'-O1B-C1B
31	D	411	LMT	O5'-C5'-C6'-O6'
31	d	411	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	507	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
33	B	628	LHG	C11-C10-C9-C8
33	b	628	LHG	C11-C10-C9-C8
25	C	510	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
28	C	519	LMG	C28-C29-C30-C31
28	c	519	LMG	C28-C29-C30-C31
30	k	101	SQD	C23-C24-C25-C26
30	B	620	SQD	O49-C7-O47-C45
30	b	620	SQD	O49-C7-O47-C45
31	I	101	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
25	B	610	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
31	B	629	LMT	C4B-C5B-C6B-O6B
31	B	629	LMT	C4'-C5'-C6'-O6'
31	C	520	LMT	C4'-C5'-C6'-O6'
31	b	629	LMT	C4B-C5B-C6B-O6B
31	b	629	LMT	C4'-C5'-C6'-O6'
31	c	520	LMT	C4'-C5'-C6'-O6'
31	L	101	LMT	O1'-C1-C2-C3
31	M	101	LMT	O1'-C1-C2-C3
31	T	701	LMT	O1'-C1-C2-C3
31	t	701	LMT	O1'-C1-C2-C3
25	B	613	CLA	C10-C11-C12-C13
31	C	521	LMT	C4'-C5'-C6'-O6'
31	c	521	LMT	C4'-C5'-C6'-O6'
30	K	101	SQD	C7-C8-C9-C10
30	k	101	SQD	C7-C8-C9-C10
33	D	407	LHG	C23-C24-C25-C26
33	Z	102	LHG	C23-C24-C25-C26
33	d	407	LHG	C23-C24-C25-C26
33	z	102	LHG	C23-C24-C25-C26
25	C	505	CLA	C15-C16-C17-C18
25	C	507	CLA	C15-C16-C17-C18
25	a	406	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
31	L	101	LMT	C4B-C5B-C6B-O6B
31	M	101	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
27	Z	101	BCR	C10-C11-C12-C13
27	z	101	BCR	C10-C11-C12-C13
25	A	406	CLA	C15-C16-C17-C18
25	B	604	CLA	C8-C10-C11-C12
25	B	607	CLA	C15-C16-C17-C18
25	B	614	CLA	C13-C15-C16-C17
25	D	404	CLA	C13-C15-C16-C17
25	b	607	CLA	C15-C16-C17-C18
25	b	614	CLA	C13-C15-C16-C17
25	d	404	CLA	C13-C15-C16-C17
28	A	410	LMG	C10-C11-C12-C13
28	a	410	LMG	C10-C11-C12-C13
30	C	501	SQD	C7-C8-C9-C10
30	c	501	SQD	C7-C8-C9-C10
33	D	408	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
31	A	415	LMT	O5'-C1'-O1'-C1
31	J	101	LMT	O5'-C1'-O1'-C1
31	a	415	LMT	O5'-C1'-O1'-C1
31	j	101	LMT	O5'-C1'-O1'-C1
33	Z	102	LHG	C11-C10-C9-C8
33	z	102	LHG	C11-C10-C9-C8
25	A	408	CLA	O1D-CGD-O2D-CED
25	a	408	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	C5-C6-C7-C8
25	C	507	CLA	C8-C10-C11-C12
25	b	604	CLA	C8-C10-C11-C12
25	c	506	CLA	C5-C6-C7-C8
25	c	507	CLA	C8-C10-C11-C12
25	d	404	CLA	C15-C16-C17-C18
33	B	622	LHG	O2-C2-C3-O3
33	b	622	LHG	O2-C2-C3-O3
25	B	609	CLA	CBA-CGA-O2A-C1
25	b	609	CLA	CBA-CGA-O2A-C1
25	C	514	CLA	O1A-CGA-O2A-C1
25	c	514	CLA	O1A-CGA-O2A-C1
31	Y	101	LMT	C4'-C5'-C6'-O6'
31	y	101	LMT	C4'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	A	406	CLA	C8-C10-C11-C12
25	D	404	CLA	C15-C16-C17-C18
31	B	629	LMT	O1'-C1-C2-C3
31	b	629	LMT	O1'-C1-C2-C3
25	C	504	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
31	C	524	LMT	O1'-C1-C2-C3
31	c	524	LMT	O1'-C1-C2-C3
25	B	611	CLA	C15-C16-C17-C18
25	C	507	CLA	C13-C15-C16-C17
25	a	406	CLA	C8-C10-C11-C12
25	b	611	CLA	C15-C16-C17-C18
25	c	507	CLA	C13-C15-C16-C17
25	C	502	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
30	F	102	SQD	C7-C8-C9-C10
30	f	102	SQD	C7-C8-C9-C10
33	D	406	LHG	C17-C18-C19-C20
33	d	406	LHG	C17-C18-C19-C20
25	B	608	CLA	C15-C16-C17-C18
25	C	502	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	c	502	CLA	C15-C16-C17-C18
25	B	612	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	CBA-CGA-O2A-C1
33	B	622	LHG	C8-C7-O7-C5
33	b	622	LHG	C8-C7-O7-C5
33	D	406	LHG	C26-C27-C28-C29
33	d	406	LHG	C26-C27-C28-C29
28	B	621	LMG	C28-C29-C30-C31
28	b	621	LMG	C28-C29-C30-C31
33	E	102	LHG	C23-C24-C25-C26
33	e	102	LHG	C23-C24-C25-C26
30	C	501	SQD	O49-C7-O47-C45
30	a	413	SQD	O49-C7-O47-C45
30	c	501	SQD	O49-C7-O47-C45
33	B	622	LHG	O9-C7-O7-C5
33	b	622	LHG	O9-C7-O7-C5
33	D	408	LHG	C24-C25-C26-C27
33	d	408	LHG	C24-C25-C26-C27
25	A	408	CLA	C8-C10-C11-C12
25	B	604	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C10-C11-C12-C13
25	C	503	CLA	C13-C15-C16-C17
25	C	504	CLA	C5-C6-C7-C8
25	a	408	CLA	C8-C10-C11-C12
25	b	604	CLA	C13-C15-C16-C17
25	b	614	CLA	C10-C11-C12-C13
25	c	503	CLA	C13-C15-C16-C17
25	c	504	CLA	C5-C6-C7-C8
30	A	412	SQD	C11-C10-C9-C8
30	a	412	SQD	C11-C10-C9-C8
25	B	602	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
31	E	101	LMT	O5'-C5'-C6'-O6'
31	e	101	LMT	O5'-C5'-C6'-O6'
31	E	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	O1'-C1-C2-C3
31	E	103	LMT	C4B-C5B-C6B-O6B
25	B	612	CLA	C13-C15-C16-C17
25	B	614	CLA	C15-C16-C17-C18
25	B	615	CLA	C5-C6-C7-C8
25	B	616	CLA	C5-C6-C7-C8
25	b	612	CLA	C13-C15-C16-C17
25	b	614	CLA	C15-C16-C17-C18
25	b	615	CLA	C5-C6-C7-C8
25	b	616	CLA	C5-C6-C7-C8
25	D	404	CLA	O1D-CGD-O2D-CED
25	d	404	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	C10-C11-C12-C13
25	b	616	CLA	C10-C11-C12-C13
31	e	103	LMT	C4B-C5B-C6B-O6B
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	O49-C7-O47-C45
30	F	102	SQD	C2-C1-O6-C44
30	f	102	SQD	C2-C1-O6-C44
31	L	101	LMT	C2'-C1'-O1'-C1
31	M	101	LMT	C2'-C1'-O1'-C1
25	C	508	CLA	C13-C15-C16-C17
25	c	508	CLA	C13-C15-C16-C17
29	A	411	PL9	C39-C41-C42-C43
29	a	411	PL9	C39-C41-C42-C43
25	A	406	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	406	CLA	CBA-CGA-O2A-C1
25	B	604	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
27	A	409	BCR	C11-C10-C9-C34
27	B	617	BCR	C11-C10-C9-C34
27	a	409	BCR	C11-C10-C9-C34
27	b	617	BCR	C11-C10-C9-C34
37	X	102	RRX	C16-C17-C18-C36
37	x	102	RRX	C16-C17-C18-C36
28	C	519	LMG	C10-C11-C12-C13
28	c	519	LMG	C10-C11-C12-C13
25	C	514	CLA	C15-C16-C17-C18
25	c	514	CLA	C15-C16-C17-C18
27	B	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C7-C8-C9-C10
37	X	102	RRX	C7-C8-C9-C10
37	x	102	RRX	C7-C8-C9-C10
25	B	609	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	O1A-CGA-O2A-C1
25	C	507	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
33	B	622	LHG	C7-C8-C9-C10
33	b	622	LHG	C7-C8-C9-C10
30	A	412	SQD	C44-C45-O47-C7
30	A	413	SQD	C44-C45-O47-C7
30	F	102	SQD	C44-C45-O47-C7
30	a	412	SQD	C44-C45-O47-C7
30	a	413	SQD	C44-C45-O47-C7
30	f	102	SQD	C44-C45-O47-C7
31	K	105	LMT	C5'-C4'-O1B-C1B
31	k	105	LMT	C5'-C4'-O1B-C1B
31	E	103	LMT	O1'-C1-C2-C3
31	e	103	LMT	O1'-C1-C2-C3
25	B	612	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
31	I	104	LMT	C4'-C5'-C6'-O6'
31	i	104	LMT	C4'-C5'-C6'-O6'
27	A	409	BCR	C11-C10-C9-C8
27	B	617	BCR	C11-C10-C9-C8
27	Z	101	BCR	C11-C10-C9-C8
27	a	409	BCR	C11-C10-C9-C8
27	b	617	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	z	101	BCR	C11-C10-C9-C8
37	X	102	RRX	C16-C17-C18-C19
37	X	102	RRX	C11-C10-C9-C8
37	x	102	RRX	C16-C17-C18-C19
37	x	102	RRX	C11-C10-C9-C8
31	L	101	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	O5'-C1'-O1'-C1
28	D	409	LMG	C28-C29-C30-C31
28	d	409	LMG	C28-C29-C30-C31
31	I	103	LMT	O1'-C1-C2-C3
31	i	103	LMT	O1'-C1-C2-C3
25	C	513	CLA	O1D-CGD-O2D-CED
25	A	406	CLA	C2-C1-O2A-CGA
25	B	610	CLA	C2-C1-O2A-CGA
25	B	616	CLA	C2-C1-O2A-CGA
25	C	507	CLA	C2-C1-O2A-CGA
25	D	401	CLA	C2-C1-O2A-CGA
25	a	406	CLA	C2-C1-O2A-CGA
25	b	610	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
25	c	507	CLA	C2-C1-O2A-CGA
25	d	401	CLA	C2-C1-O2A-CGA
25	B	615	CLA	C10-C11-C12-C13
25	B	615	CLA	C13-C15-C16-C17
25	b	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C13-C15-C16-C17
25	c	513	CLA	O1D-CGD-O2D-CED
31	B	623	LMT	O5'-C5'-C6'-O6'
31	b	623	LMT	O5'-C5'-C6'-O6'
30	b	620	SQD	C34-C35-C36-C37
31	I	102	LMT	C5-C6-C7-C8
31	i	102	LMT	C5-C6-C7-C8
31	I	102	LMT	O1'-C1-C2-C3
31	i	102	LMT	O1'-C1-C2-C3
28	C	523	LMG	C11-C12-C13-C14
28	c	523	LMG	C11-C12-C13-C14
30	A	413	SQD	C26-C27-C28-C29
30	B	620	SQD	C34-C35-C36-C37
30	F	102	SQD	C11-C10-C9-C8
30	K	101	SQD	C25-C26-C27-C28
30	a	413	SQD	C9-C10-C11-C12
30	a	413	SQD	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C11-C10-C9-C8
30	k	101	SQD	C25-C26-C27-C28
31	A	416	LMT	C6-C7-C8-C9
31	B	627	LMT	C6-C7-C8-C9
31	a	416	LMT	C6-C7-C8-C9
31	b	627	LMT	C6-C7-C8-C9
33	D	408	LHG	C26-C27-C28-C29
33	d	408	LHG	C26-C27-C28-C29
30	A	413	SQD	C9-C10-C11-C12
30	C	501	SQD	C26-C27-C28-C29
30	c	501	SQD	C26-C27-C28-C29
33	B	628	LHG	C12-C13-C14-C15
25	D	401	CLA	O1D-CGD-O2D-CED
30	H	102	SQD	C25-C26-C27-C28
30	h	102	SQD	C25-C26-C27-C28
31	B	624	LMT	C3-C4-C5-C6
31	B	626	LMT	C2-C3-C4-C5
31	b	624	LMT	C3-C4-C5-C6
31	b	626	LMT	C2-C3-C4-C5
33	D	407	LHG	C26-C27-C28-C29
33	Z	102	LHG	C33-C34-C35-C36
33	b	628	LHG	C12-C13-C14-C15
33	d	407	LHG	C26-C27-C28-C29
33	z	102	LHG	C33-C34-C35-C36
34	C	518	DGD	C7B-C8B-C9B-CAB
34	c	518	DGD	C7B-C8B-C9B-CAB
31	A	416	LMT	C2-C1-O1'-C1'
31	B	626	LMT	C2-C1-O1'-C1'
31	C	522	LMT	C2-C1-O1'-C1'
31	K	105	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2-C1-O1'-C1'
31	a	416	LMT	C2-C1-O1'-C1'
31	b	626	LMT	C2-C1-O1'-C1'
31	c	522	LMT	C2-C1-O1'-C1'
31	k	105	LMT	C2-C1-O1'-C1'
31	m	101	LMT	C2-C1-O1'-C1'
33	B	622	LHG	O1-C1-C2-O2
33	b	622	LHG	O1-C1-C2-O2
28	C	523	LMG	C18-C19-C20-C21
25	d	401	CLA	O1D-CGD-O2D-CED
30	H	102	SQD	C23-C24-C25-C26
30	h	102	SQD	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	523	LMG	C18-C19-C20-C21
25	C	509	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C20
25	c	509	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C20
28	C	519	LMG	C34-C35-C36-C37
28	c	519	LMG	C34-C35-C36-C37
31	B	627	LMT	C5-C6-C7-C8
31	b	627	LMT	C5-C6-C7-C8
33	B	628	LHG	C8-C7-O7-C5
33	b	628	LHG	C8-C7-O7-C5
31	B	629	LMT	C11-C10-C9-C8
31	b	629	LMT	C11-C10-C9-C8
25	A	406	CLA	C6-C7-C8-C10
25	a	406	CLA	C6-C7-C8-C10
30	K	101	SQD	C9-C10-C11-C12
30	K	101	SQD	C12-C13-C14-C15
30	k	101	SQD	C9-C10-C11-C12
30	k	101	SQD	C12-C13-C14-C15
34	c	518	DGD	C6B-C7B-C8B-C9B
28	C	523	LMG	C10-C11-C12-C13
28	c	523	LMG	C10-C11-C12-C13
34	C	518	DGD	C1A-C2A-C3A-C4A
34	c	518	DGD	C1A-C2A-C3A-C4A
28	d	409	LMG	C33-C34-C35-C36
30	C	501	SQD	C29-C30-C31-C32
31	I	103	LMT	C6-C7-C8-C9
31	i	103	LMT	C6-C7-C8-C9
33	D	407	LHG	C28-C29-C30-C31
33	d	407	LHG	C28-C29-C30-C31
34	C	518	DGD	CCA-CDA-CEA-CFA
34	C	518	DGD	C6B-C7B-C8B-C9B
34	c	518	DGD	CCA-CDA-CEA-CFA
31	C	524	LMT	C4B-C5B-C6B-O6B
31	c	524	LMT	C4B-C5B-C6B-O6B
26	D	402	PHO	C3A-C2A-CAA-CBA
26	d	402	PHO	C3A-C2A-CAA-CBA
28	D	409	LMG	C33-C34-C35-C36
33	d	406	LHG	C28-C29-C30-C31
30	c	501	SQD	C29-C30-C31-C32
33	D	406	LHG	C28-C29-C30-C31
25	b	602	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	102	SQD	C12-C13-C14-C15
25	A	405	CLA	C16-C17-C18-C20
25	B	603	CLA	C16-C17-C18-C20
25	B	604	CLA	C16-C17-C18-C19
25	B	613	CLA	C16-C17-C18-C19
25	B	613	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
25	b	603	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C20
30	B	620	SQD	C27-C28-C29-C30
30	H	102	SQD	C12-C13-C14-C15
30	b	620	SQD	C27-C28-C29-C30
34	C	517	DGD	C3A-C4A-C5A-C6A
34	c	517	DGD	C3A-C4A-C5A-C6A
25	B	602	CLA	C15-C16-C17-C18
25	B	608	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
31	D	410	LMT	C5-C6-C7-C8
31	d	410	LMT	C5-C6-C7-C8
33	D	407	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
31	M	102	LMT	C1-C2-C3-C4
31	m	101	LMT	C1-C2-C3-C4
30	C	501	SQD	C17-C18-C19-C20
30	K	101	SQD	C10-C11-C12-C13
30	c	501	SQD	C17-C18-C19-C20
30	k	101	SQD	C10-C11-C12-C13
30	C	501	SQD	C11-C12-C13-C14
30	C	501	SQD	C16-C17-C18-C19
30	c	501	SQD	C11-C12-C13-C14
30	c	501	SQD	C16-C17-C18-C19
31	B	624	LMT	C2-C3-C4-C5
31	D	410	LMT	C7-C8-C9-C10
31	b	624	LMT	C2-C3-C4-C5
31	d	410	LMT	C7-C8-C9-C10
31	M	102	LMT	C4'-C5'-C6'-O6'
31	m	101	LMT	C4'-C5'-C6'-O6'
31	B	623	LMT	C11-C10-C9-C8
31	b	623	LMT	C11-C10-C9-C8
25	C	503	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	503	CLA	O1D-CGD-O2D-CED
33	b	622	LHG	C11-C12-C13-C14
25	B	616	CLA	C8-C10-C11-C12
25	b	605	CLA	C8-C10-C11-C12
25	b	616	CLA	C8-C10-C11-C12
28	C	519	LMG	C11-C12-C13-C14
28	C	523	LMG	C16-C17-C18-C19
28	c	519	LMG	C11-C12-C13-C14
28	c	523	LMG	C16-C17-C18-C19
30	A	412	SQD	C27-C28-C29-C30
30	a	412	SQD	C27-C28-C29-C30
31	B	625	LMT	C7-C8-C9-C10
31	b	625	LMT	C7-C8-C9-C10
33	B	622	LHG	C11-C12-C13-C14
33	B	622	LHG	C24-C25-C26-C27
33	D	408	LHG	C9-C10-C11-C12
33	d	408	LHG	C9-C10-C11-C12
27	B	617	BCR	C1-C6-C7-C8
27	F	101	BCR	C23-C24-C25-C26
27	F	101	BCR	C23-C24-C25-C30
27	b	617	BCR	C1-C6-C7-C8
27	f	101	BCR	C23-C24-C25-C26
27	f	101	BCR	C23-C24-C25-C30
37	X	102	RRX	C1-C6-C7-C8
37	X	102	RRX	C5-C6-C7-C8
37	x	102	RRX	C1-C6-C7-C8
37	x	102	RRX	C5-C6-C7-C8
30	a	412	SQD	C32-C33-C34-C35
33	b	622	LHG	C24-C25-C26-C27
33	b	628	LHG	C15-C16-C17-C18
25	C	509	CLA	CBA-CGA-O2A-C1
25	D	401	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CBA-CGA-O2A-C1
25	d	401	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	C8-C10-C11-C12
30	A	412	SQD	C32-C33-C34-C35
30	H	102	SQD	C14-C15-C16-C17
30	h	102	SQD	C14-C15-C16-C17
25	C	514	CLA	O1D-CGD-O2D-CED
25	c	514	CLA	O1D-CGD-O2D-CED
33	B	628	LHG	C15-C16-C17-C18
33	D	408	LHG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	628	LHG	C13-C14-C15-C16
33	d	408	LHG	C14-C15-C16-C17
25	C	508	CLA	C5-C6-C7-C8
25	c	508	CLA	C5-C6-C7-C8
28	a	410	LMG	C14-C15-C16-C17
33	B	628	LHG	C13-C14-C15-C16
33	D	406	LHG	C11-C10-C9-C8
33	B	628	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
31	C	524	LMT	C2-C3-C4-C5
31	c	524	LMT	C2-C3-C4-C5
33	B	628	LHG	C31-C32-C33-C34
33	b	628	LHG	C31-C32-C33-C34
33	d	406	LHG	C11-C10-C9-C8
25	B	604	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
28	A	410	LMG	C14-C15-C16-C17
28	C	523	LMG	C19-C20-C21-C22
30	A	413	SQD	C28-C29-C30-C31
30	a	413	SQD	C28-C29-C30-C31
31	E	103	LMT	C4-C5-C6-C7
31	J	101	LMT	C5-C6-C7-C8
31	e	103	LMT	C4-C5-C6-C7
31	j	101	LMT	C5-C6-C7-C8
28	c	523	LMG	C19-C20-C21-C22
33	D	406	LHG	C24-C25-C26-C27
33	d	406	LHG	C24-C25-C26-C27
31	E	103	LMT	C7-C8-C9-C10
31	J	101	LMT	C7-C8-C9-C10
31	e	103	LMT	C7-C8-C9-C10
31	j	101	LMT	C7-C8-C9-C10
33	D	407	LHG	C31-C32-C33-C34
33	d	407	LHG	C31-C32-C33-C34
31	C	521	LMT	O5'-C1'-O1'-C1
31	c	521	LMT	O5'-C1'-O1'-C1
28	C	519	LMG	C18-C19-C20-C21
28	c	519	LMG	C18-C19-C20-C21
33	E	102	LHG	C11-C12-C13-C14
33	e	102	LHG	C11-C12-C13-C14
30	C	501	SQD	C24-C25-C26-C27
33	B	622	LHG	C30-C31-C32-C33
33	Z	102	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	622	LHG	C30-C31-C32-C33
31	c	521	LMT	O1'-C1-C2-C3
30	c	501	SQD	C24-C25-C26-C27
31	F	103	LMT	C6-C7-C8-C9
31	I	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
33	B	622	LHG	C28-C29-C30-C31
33	b	622	LHG	C28-C29-C30-C31
33	z	102	LHG	C28-C29-C30-C31
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
31	f	103	LMT	C6-C7-C8-C9
31	C	521	LMT	O1'-C1-C2-C3
31	C	520	LMT	O5'-C5'-C6'-O6'
31	c	520	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	C4-C5-C6-C7
31	b	629	LMT	C4-C5-C6-C7
28	C	519	LMG	C11-C10-O7-C8
28	c	519	LMG	C11-C10-O7-C8
30	B	620	SQD	C8-C7-O47-C45
30	K	101	SQD	C8-C7-O47-C45
30	b	620	SQD	C8-C7-O47-C45
30	k	101	SQD	C8-C7-O47-C45
34	C	516	DGD	C2B-C1B-O2G-C2G
34	c	516	DGD	C2B-C1B-O2G-C2G
31	D	410	LMT	C3-C4-C5-C6
31	d	410	LMT	C3-C4-C5-C6
28	c	519	LMG	O9-C10-O7-C8
28	C	523	LMG	C30-C31-C32-C33
28	c	523	LMG	C30-C31-C32-C33
30	H	102	SQD	C31-C32-C33-C34
30	h	102	SQD	C31-C32-C33-C34
33	b	622	LHG	C25-C26-C27-C28
33	B	622	LHG	C25-C26-C27-C28
34	C	517	DGD	C2G-C3G-O3G-C1D
34	C	517	DGD	C5D-C6D-O5D-C1E
34	c	517	DGD	C2G-C3G-O3G-C1D
34	c	517	DGD	C5D-C6D-O5D-C1E
28	C	523	LMG	C34-C35-C36-C37
28	c	523	LMG	C34-C35-C36-C37
31	D	411	LMT	C3-C4-C5-C6
31	T	701	LMT	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	d	411	LMT	C3-C4-C5-C6
31	t	701	LMT	C4-C5-C6-C7
30	A	412	SQD	C28-C29-C30-C31
30	a	412	SQD	C28-C29-C30-C31
25	A	406	CLA	C13-C15-C16-C17
25	a	406	CLA	C13-C15-C16-C17
31	K	105	LMT	C2-C3-C4-C5
31	k	105	LMT	C2-C3-C4-C5
25	A	406	CLA	O1A-CGA-O2A-C1
25	a	406	CLA	O1A-CGA-O2A-C1
28	D	409	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
25	B	611	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
33	D	408	LHG	C16-C17-C18-C19
33	d	408	LHG	C16-C17-C18-C19
34	C	517	DGD	CCA-CDA-CEA-CFA
34	c	517	DGD	CCA-CDA-CEA-CFA
31	I	101	LMT	C11-C10-C9-C8
31	i	101	LMT	C11-C10-C9-C8
34	C	518	DGD	C2A-C3A-C4A-C5A
34	c	518	DGD	C2A-C3A-C4A-C5A
34	h	103	DGD	CCB-CDB-CEB-CFB
28	C	519	LMG	O9-C10-O7-C8
34	H	103	DGD	CCB-CDB-CEB-CFB
25	B	614	CLA	C5-C6-C7-C8
25	D	401	CLA	C15-C16-C17-C18
25	b	614	CLA	C5-C6-C7-C8
25	d	401	CLA	C15-C16-C17-C18
30	c	501	SQD	C27-C28-C29-C30
31	t	701	LMT	C3-C4-C5-C6
33	B	628	LHG	C25-C26-C27-C28
33	b	628	LHG	C25-C26-C27-C28
31	B	629	LMT	O5B-C5B-C6B-O6B
30	C	501	SQD	C27-C28-C29-C30
31	T	701	LMT	C3-C4-C5-C6
34	H	103	DGD	C6A-C7A-C8A-C9A
34	h	103	DGD	C6A-C7A-C8A-C9A
33	E	102	LHG	C7-C8-C9-C10
33	e	102	LHG	C7-C8-C9-C10
31	T	701	LMT	O5'-C5'-C6'-O6'
31	t	701	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	502	CLA	C3-C5-C6-C7
25	c	502	CLA	C3-C5-C6-C7
30	A	413	SQD	O47-C45-C46-O48
30	C	501	SQD	O47-C45-C46-O48
30	a	413	SQD	O47-C45-C46-O48
30	c	501	SQD	O47-C45-C46-O48
31	B	627	LMT	C2-C3-C4-C5
31	b	627	LMT	C2-C3-C4-C5
33	B	628	LHG	C16-C17-C18-C19
33	b	628	LHG	C16-C17-C18-C19
34	C	518	DGD	C5A-C6A-C7A-C8A
34	c	518	DGD	C5A-C6A-C7A-C8A
31	D	411	LMT	O5B-C5B-C6B-O6B
31	b	629	LMT	O5B-C5B-C6B-O6B
31	d	411	LMT	O5B-C5B-C6B-O6B
31	L	101	LMT	C2-C3-C4-C5
31	M	101	LMT	C2-C3-C4-C5
30	a	412	SQD	C12-C13-C14-C15
31	I	103	LMT	C7-C8-C9-C10
31	X	103	LMT	C2-C3-C4-C5
31	i	103	LMT	C7-C8-C9-C10
31	x	103	LMT	C2-C3-C4-C5
30	A	412	SQD	C12-C13-C14-C15
30	A	413	SQD	C11-C12-C13-C14
30	a	413	SQD	C11-C12-C13-C14
31	F	103	LMT	C5-C6-C7-C8
31	f	103	LMT	C5-C6-C7-C8
31	C	522	LMT	C4-C5-C6-C7
31	c	522	LMT	C4-C5-C6-C7
25	C	502	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	C2A-CAA-CBA-CGA
31	B	626	LMT	C11-C10-C9-C8
31	b	626	LMT	C11-C10-C9-C8
34	C	516	DGD	O6E-C5E-C6E-O5E
34	c	516	DGD	O6E-C5E-C6E-O5E
31	C	521	LMT	C11-C10-C9-C8
31	c	521	LMT	C11-C10-C9-C8
33	Z	102	LHG	C25-C26-C27-C28
33	z	102	LHG	C25-C26-C27-C28
28	C	523	LMG	C14-C15-C16-C17
28	c	523	LMG	C14-C15-C16-C17
30	A	413	SQD	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	413	SQD	C12-C13-C14-C15
31	D	410	LMT	C4-C5-C6-C7
31	d	410	LMT	C4-C5-C6-C7
25	C	509	CLA	O1A-CGA-O2A-C1
25	D	401	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
25	d	401	CLA	O1A-CGA-O2A-C1
28	D	409	LMG	C32-C33-C34-C35
28	d	409	LMG	C32-C33-C34-C35
30	B	620	SQD	C18-C19-C20-C21
30	C	501	SQD	C12-C13-C14-C15
30	b	620	SQD	C18-C19-C20-C21
30	c	501	SQD	C12-C13-C14-C15
30	h	102	SQD	C13-C14-C15-C16
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C1A-C2A-CAA-CBA
25	C	509	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	509	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C15-C16-C17-C18
25	d	403	CLA	C15-C16-C17-C18
30	H	102	SQD	C13-C14-C15-C16
31	E	103	LMT	C11-C10-C9-C8
31	e	103	LMT	C11-C10-C9-C8
33	B	628	LHG	C11-C12-C13-C14
33	b	628	LHG	C11-C12-C13-C14
25	B	602	CLA	C11-C12-C13-C15
25	B	602	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C10-C8-C7
25	B	605	CLA	C12-C13-C15-C16
25	B	606	CLA	C11-C10-C8-C7
25	B	611	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	C	508	CLA	C11-C10-C8-C7
25	C	514	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C10-C8-C7
25	b	605	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C11-C10-C8-C7
25	b	611	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C10-C8-C7
25	c	514	CLA	C11-C10-C8-C7
30	K	101	SQD	C27-C28-C29-C30
30	k	101	SQD	C27-C28-C29-C30
33	D	406	LHG	C34-C35-C36-C37
33	D	407	LHG	C27-C28-C29-C30
33	d	406	LHG	C34-C35-C36-C37
33	d	407	LHG	C27-C28-C29-C30
30	a	413	SQD	C14-C15-C16-C17
30	F	102	SQD	C23-C24-C25-C26
30	f	102	SQD	C23-C24-C25-C26
34	C	516	DGD	C1B-C2B-C3B-C4B
34	c	516	DGD	C1B-C2B-C3B-C4B
30	A	413	SQD	C14-C15-C16-C17
31	C	522	LMT	C7-C8-C9-C10
31	c	522	LMT	C7-C8-C9-C10
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C11-C10-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	C	514	CLA	C11-C10-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C9
25	b	608	CLA	C14-C13-C15-C16
25	c	514	CLA	C11-C10-C8-C9
31	A	415	LMT	C6-C7-C8-C9
31	A	416	LMT	C4-C5-C6-C7
31	a	416	LMT	C4-C5-C6-C7
31	e	103	LMT	C3-C4-C5-C6
33	Z	102	LHG	C34-C35-C36-C37
33	z	102	LHG	C34-C35-C36-C37
31	a	415	LMT	C6-C7-C8-C9
34	C	516	DGD	C4B-C5B-C6B-C7B
34	c	516	DGD	C4B-C5B-C6B-C7B
33	E	102	LHG	C24-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
31	E	103	LMT	C3-C4-C5-C6
31	i	101	LMT	C2-C3-C4-C5
31	I	101	LMT	C2-C3-C4-C5
30	A	412	SQD	C2-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C2-C1-O6-C44
31	C	521	LMT	C2'-C1'-O1'-C1
31	c	521	LMT	C2'-C1'-O1'-C1
34	C	516	DGD	CAA-CBA-CCA-CDA
31	f	103	LMT	C1-C2-C3-C4
30	A	413	SQD	C44-C45-C46-O48
30	C	501	SQD	C44-C45-C46-O48
30	H	102	SQD	O6-C44-C45-C46
30	a	413	SQD	C44-C45-C46-O48
30	c	501	SQD	C44-C45-C46-O48
30	h	102	SQD	O6-C44-C45-C46
34	C	517	DGD	C2B-C3B-C4B-C5B
34	c	516	DGD	CAA-CBA-CCA-CDA
34	c	517	DGD	C2B-C3B-C4B-C5B
25	B	609	CLA	C5-C6-C7-C8
25	b	609	CLA	C5-C6-C7-C8
31	F	103	LMT	C1-C2-C3-C4
25	C	502	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	CBA-CGA-O2A-C1
25	B	611	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
28	B	621	LMG	C13-C14-C15-C16
28	b	621	LMG	C13-C14-C15-C16
34	C	516	DGD	C6B-C7B-C8B-C9B
34	c	516	DGD	C6B-C7B-C8B-C9B
28	C	523	LMG	C13-C14-C15-C16
28	c	523	LMG	C13-C14-C15-C16
31	B	624	LMT	C4-C5-C6-C7
31	b	624	LMT	C4-C5-C6-C7
29	A	411	PL9	C43-C44-C46-C47
29	a	411	PL9	C43-C44-C46-C47
31	D	411	LMT	C4B-C5B-C6B-O6B
31	d	411	LMT	C4B-C5B-C6B-O6B
30	B	620	SQD	C9-C10-C11-C12
30	C	501	SQD	C30-C31-C32-C33
30	b	620	SQD	C9-C10-C11-C12
30	c	501	SQD	C30-C31-C32-C33
28	A	414	LMG	O6-C5-C6-O5
28	a	414	LMG	O6-C5-C6-O5
25	A	405	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	405	CLA	C15-C16-C17-C18
31	J	101	LMT	C4-C5-C6-C7
31	j	101	LMT	C4-C5-C6-C7
33	B	628	LHG	C14-C15-C16-C17
33	D	406	LHG	C13-C14-C15-C16
33	b	628	LHG	C14-C15-C16-C17
33	d	406	LHG	C13-C14-C15-C16
31	B	623	LMT	C6-C7-C8-C9
31	b	623	LMT	C6-C7-C8-C9
25	B	608	CLA	CBA-CGA-O2A-C1
25	b	608	CLA	CBA-CGA-O2A-C1
33	D	408	LHG	C10-C11-C12-C13
33	d	408	LHG	C10-C11-C12-C13
34	C	518	DGD	C6A-C7A-C8A-C9A
34	c	518	DGD	C6A-C7A-C8A-C9A
28	D	409	LMG	C19-C20-C21-C22
31	X	103	LMT	C6-C7-C8-C9
27	K	102	BCR	C9-C10-C11-C12
27	k	102	BCR	C9-C10-C11-C12
37	X	102	RRX	C13-C14-C15-C16
37	x	102	RRX	C13-C14-C15-C16
31	x	103	LMT	C6-C7-C8-C9
28	a	410	LMG	C11-C12-C13-C14
25	B	613	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
28	A	410	LMG	C11-C12-C13-C14
28	d	409	LMG	C19-C20-C21-C22
25	c	511	CLA	CBA-CGA-O2A-C1
31	F	103	LMT	C4'-C5'-C6'-O6'
30	C	501	SQD	C45-C46-O48-C23
30	c	501	SQD	C45-C46-O48-C23
28	C	523	LMG	C32-C33-C34-C35
28	c	523	LMG	C32-C33-C34-C35
31	f	103	LMT	C4'-C5'-C6'-O6'
25	b	603	CLA	C4-C3-C5-C6
25	C	511	CLA	C2-C3-C5-C6
25	c	511	CLA	C2-C3-C5-C6
30	A	412	SQD	C14-C15-C16-C17
30	a	412	SQD	C14-C15-C16-C17
25	C	504	CLA	C16-C17-C18-C20
25	c	504	CLA	C16-C17-C18-C20
30	H	102	SQD	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	102	SQD	C34-C35-C36-C37
31	I	103	LMT	C2-C3-C4-C5
31	i	103	LMT	C2-C3-C4-C5
33	D	406	LHG	C25-C26-C27-C28
33	d	406	LHG	C25-C26-C27-C28
33	d	407	LHG	C29-C30-C31-C32
34	c	518	DGD	C4B-C5B-C6B-C7B
31	A	415	LMT	C7-C8-C9-C10
31	F	103	LMT	C11-C10-C9-C8
31	a	415	LMT	C7-C8-C9-C10
31	f	103	LMT	C11-C10-C9-C8
33	D	407	LHG	C29-C30-C31-C32
34	C	518	DGD	C9A-CAA-CBA-CCA
34	C	518	DGD	C4B-C5B-C6B-C7B
34	c	518	DGD	C9A-CAA-CBA-CCA
33	B	622	LHG	C32-C33-C34-C35
33	b	622	LHG	C32-C33-C34-C35
31	B	624	LMT	C7-C8-C9-C10
25	C	511	CLA	CBA-CGA-O2A-C1
31	I	102	LMT	C2-C3-C4-C5
31	b	624	LMT	C7-C8-C9-C10
31	i	102	LMT	C2-C3-C4-C5
33	b	622	LHG	C13-C14-C15-C16
31	C	521	LMT	C2-C3-C4-C5
31	X	101	LMT	C6-C7-C8-C9
31	x	101	LMT	C6-C7-C8-C9
25	B	614	CLA	C3-C5-C6-C7
25	C	507	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	c	507	CLA	C3-C5-C6-C7
31	c	521	LMT	C2-C3-C4-C5
33	B	622	LHG	C13-C14-C15-C16
25	B	614	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	CBA-CGA-O2A-C1
25	C	505	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C11-C10-O7-C8
28	a	410	LMG	C11-C10-O7-C8
29	D	405	PL9	C7-C8-C9-C10
29	d	405	PL9	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	624	LMT	C11-C10-C9-C8
31	b	624	LMT	C11-C10-C9-C8
33	E	102	LHG	C12-C13-C14-C15
33	e	102	LHG	C12-C13-C14-C15
33	B	622	LHG	C9-C10-C11-C12
33	b	622	LHG	C9-C10-C11-C12
25	B	603	CLA	C4-C3-C5-C6
33	E	102	LHG	O10-C23-O8-C6
33	e	102	LHG	O10-C23-O8-C6
33	D	407	LHG	C30-C31-C32-C33
33	d	407	LHG	C30-C31-C32-C33
33	Z	102	LHG	C31-C32-C33-C34
33	z	102	LHG	C31-C32-C33-C34
25	D	401	CLA	C2C-C3C-CAC-CBC
34	C	516	DGD	O1B-C1B-O2G-C2G
34	c	516	DGD	O1B-C1B-O2G-C2G
31	B	629	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2-C1-O1'-C1'
31	b	629	LMT	C2-C1-O1'-C1'
31	d	410	LMT	C2-C1-O1'-C1'
25	A	406	CLA	C6-C7-C8-C9
25	A	408	CLA	C11-C10-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	B	611	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C9
25	C	511	CLA	C11-C12-C13-C14
25	a	406	CLA	C6-C7-C8-C9
25	a	408	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	611	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C10-C8-C9
25	c	507	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C10-C8-C9
25	c	511	CLA	C11-C12-C13-C14
25	B	605	CLA	C5-C6-C7-C8
25	C	509	CLA	C8-C10-C11-C12
25	b	605	CLA	C5-C6-C7-C8
25	c	509	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C31-C32-C33-C34
33	D	406	LHG	C31-C32-C33-C34
25	d	401	CLA	C2C-C3C-CAC-CBC
31	E	103	LMT	C1-C2-C3-C4
31	B	627	LMT	C7-C8-C9-C10
31	D	410	LMT	C2-C3-C4-C5
31	X	103	LMT	C3-C4-C5-C6
31	b	627	LMT	C7-C8-C9-C10
31	d	410	LMT	C2-C3-C4-C5
31	x	103	LMT	C3-C4-C5-C6
25	a	406	CLA	C3-C5-C6-C7
31	e	103	LMT	C1-C2-C3-C4
25	A	408	CLA	C11-C10-C8-C7
25	B	608	CLA	C12-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C10
25	C	507	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C15
25	a	408	CLA	C11-C10-C8-C7
25	b	608	CLA	C12-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C10
25	c	507	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C15
31	M	101	LMT	C11-C10-C9-C8
31	L	101	LMT	C11-C10-C9-C8
25	B	616	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C12-C13-C15
25	A	406	CLA	C3-C5-C6-C7
25	C	505	CLA	C3A-C2A-CAA-CBA
25	C	511	CLA	C4-C3-C5-C6
25	c	505	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	C4-C3-C5-C6
33	D	407	LHG	C32-C33-C34-C35
33	d	407	LHG	C32-C33-C34-C35
31	B	629	LMT	O5'-C1'-O1'-C1
31	b	629	LMT	O5'-C1'-O1'-C1
31	A	416	LMT	C7-C8-C9-C10
25	B	608	CLA	O1A-CGA-O2A-C1
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
31	a	416	LMT	C7-C8-C9-C10
27	k	103	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	X	102	RRX	C19-C20-C21-C22
37	x	102	RRX	C19-C20-C21-C22
33	B	628	LHG	C24-C25-C26-C27
33	b	628	LHG	C24-C25-C26-C27
33	z	102	LHG	C11-C12-C13-C14
25	C	502	CLA	O1A-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
30	B	620	SQD	C35-C36-C37-C38
33	Z	102	LHG	C11-C12-C13-C14
30	B	620	SQD	C13-C14-C15-C16
30	b	620	SQD	C13-C14-C15-C16
31	i	101	LMT	C4-C5-C6-C7
30	b	620	SQD	C35-C36-C37-C38
31	I	101	LMT	C4-C5-C6-C7
33	D	408	LHG	C30-C31-C32-C33
33	d	408	LHG	C30-C31-C32-C33
30	B	620	SQD	C44-C45-C46-O48
30	b	620	SQD	C44-C45-C46-O48
33	B	628	LHG	C4-C5-C6-O8
33	E	102	LHG	C4-C5-C6-O8
33	b	628	LHG	C4-C5-C6-O8
33	e	102	LHG	C4-C5-C6-O8
31	C	521	LMT	C6-C7-C8-C9
31	c	521	LMT	C6-C7-C8-C9
30	A	412	SQD	C7-C8-C9-C10
30	a	412	SQD	C7-C8-C9-C10
30	f	102	SQD	C24-C25-C26-C27
28	C	519	LMG	C29-C30-C31-C32
28	c	519	LMG	C29-C30-C31-C32
30	C	501	SQD	C13-C14-C15-C16
26	D	402	PHO	C1A-C2A-CAA-CBA
26	d	402	PHO	C1A-C2A-CAA-CBA
30	F	102	SQD	C10-C11-C12-C13
30	F	102	SQD	C24-C25-C26-C27
30	f	102	SQD	C10-C11-C12-C13
34	c	516	DGD	C2G-C1G-O1G-C1A
30	c	501	SQD	C13-C14-C15-C16
31	X	103	LMT	C1-C2-C3-C4
31	A	415	LMT	C11-C10-C9-C8
31	x	103	LMT	C1-C2-C3-C4
33	d	406	LHG	C35-C36-C37-C38
31	a	415	LMT	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C19
33	D	406	LHG	C35-C36-C37-C38
27	A	409	BCR	C23-C24-C25-C30
27	B	619	BCR	C1-C6-C7-C8
27	a	409	BCR	C23-C24-C25-C30
27	b	619	BCR	C1-C6-C7-C8
31	D	411	LMT	C11-C10-C9-C8
25	B	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C8-C10-C11-C12
31	d	411	LMT	C11-C10-C9-C8
25	B	602	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	O1D-CGD-O2D-CED
28	c	519	LMG	C19-C20-C21-C22
31	D	411	LMT	C5-C6-C7-C8
28	B	621	LMG	C12-C13-C14-C15
28	C	519	LMG	C19-C20-C21-C22
25	B	616	CLA	C11-C12-C13-C14
25	C	504	CLA	C16-C17-C18-C19
25	c	504	CLA	C16-C17-C18-C19
34	C	516	DGD	C2G-C1G-O1G-C1A
28	A	410	LMG	O7-C8-C9-O8
28	a	410	LMG	O7-C8-C9-O8
30	B	620	SQD	O47-C45-C46-O48
30	H	102	SQD	O47-C45-C46-O48
30	K	101	SQD	O47-C45-C46-O48
30	b	620	SQD	O47-C45-C46-O48
30	h	102	SQD	O47-C45-C46-O48
30	k	101	SQD	O47-C45-C46-O48
33	B	622	LHG	O7-C5-C6-O8
33	B	628	LHG	O7-C5-C6-O8
33	Z	102	LHG	O7-C5-C6-O8
33	b	622	LHG	O7-C5-C6-O8
33	b	628	LHG	O7-C5-C6-O8
33	z	102	LHG	O7-C5-C6-O8
30	C	501	SQD	C32-C33-C34-C35
30	c	501	SQD	C32-C33-C34-C35
31	A	415	LMT	C5-C6-C7-C8
31	C	524	LMT	C3-C4-C5-C6
31	a	415	LMT	C5-C6-C7-C8
31	d	411	LMT	C5-C6-C7-C8
28	b	621	LMG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	524	LMT	C3-C4-C5-C6
34	C	517	DGD	CAA-CBA-CCA-CDA
34	c	517	DGD	CAA-CBA-CCA-CDA
33	D	407	LHG	C35-C36-C37-C38
33	d	407	LHG	C35-C36-C37-C38
25	C	514	CLA	C13-C15-C16-C17
25	c	514	CLA	C13-C15-C16-C17
31	F	103	LMT	O1'-C1-C2-C3
31	f	103	LMT	O1'-C1-C2-C3
25	b	616	CLA	C11-C12-C13-C14
31	C	522	LMT	C2-C3-C4-C5
31	L	101	LMT	C3-C4-C5-C6
31	M	101	LMT	C3-C4-C5-C6
31	X	103	LMT	C7-C8-C9-C10
31	c	522	LMT	C2-C3-C4-C5
31	x	103	LMT	C7-C8-C9-C10
33	z	102	LHG	C24-C25-C26-C27
30	C	501	SQD	C23-C24-C25-C26
30	c	501	SQD	C23-C24-C25-C26
33	Z	102	LHG	C24-C25-C26-C27
25	B	605	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	D	403	CLA	C6-C7-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C9
25	d	403	CLA	C6-C7-C8-C9
31	X	101	LMT	C7-C8-C9-C10
31	x	101	LMT	C7-C8-C9-C10
31	B	626	LMT	O5'-C1'-O1'-C1
31	b	626	LMT	O5'-C1'-O1'-C1
31	y	101	LMT	O5'-C1'-O1'-C1
25	B	614	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
34	C	517	DGD	C4A-C5A-C6A-C7A
30	H	102	SQD	C11-C10-C9-C8
30	h	102	SQD	C11-C10-C9-C8
31	X	101	LMT	C5-C6-C7-C8
31	x	101	LMT	C5-C6-C7-C8
34	c	517	DGD	C4A-C5A-C6A-C7A
31	E	103	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	103	LMT	C5'-C4'-O1B-C1B
33	D	406	LHG	C19-C20-C21-C22
33	d	406	LHG	C19-C20-C21-C22
33	D	406	LHG	O1-C1-C2-O2
33	d	406	LHG	O1-C1-C2-O2
25	C	506	CLA	C4-C3-C5-C6
34	H	103	DGD	C9A-CAA-CBA-CCA
34	h	103	DGD	C9A-CAA-CBA-CCA
27	K	103	BCR	C9-C10-C11-C12
25	A	405	CLA	C16-C17-C18-C19
25	B	603	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
30	a	413	SQD	C23-C24-C25-C26
28	A	410	LMG	O9-C10-O7-C8
28	a	410	LMG	O9-C10-O7-C8
30	C	501	SQD	C14-C15-C16-C17
30	c	501	SQD	C14-C15-C16-C17
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
33	D	407	LHG	O6-C4-C5-C6
33	Z	102	LHG	O6-C4-C5-C6
33	d	407	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
25	C	510	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
25	c	510	CLA	C16-C17-C18-C19
25	B	602	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10
25	C	510	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C10-C8-C7
25	b	616	CLA	C6-C7-C8-C10
25	c	510	CLA	C11-C10-C8-C7
30	A	413	SQD	C23-C24-C25-C26
31	J	101	LMT	C6-C7-C8-C9
31	j	101	LMT	C6-C7-C8-C9
33	E	102	LHG	C25-C26-C27-C28
33	e	102	LHG	C25-C26-C27-C28
25	B	608	CLA	CBD-CGD-O2D-CED
33	B	628	LHG	C7-C8-C9-C10
33	b	628	LHG	C7-C8-C9-C10
25	C	505	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	608	CLA	CBD-CGD-O2D-CED
31	I	103	LMT	C4'-C5'-C6'-O6'
31	i	103	LMT	C4'-C5'-C6'-O6'
33	D	408	LHG	C28-C29-C30-C31
25	c	506	CLA	C4-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
33	d	408	LHG	C28-C29-C30-C31
33	B	622	LHG	C27-C28-C29-C30
33	b	622	LHG	C27-C28-C29-C30
25	C	505	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
25	C	504	CLA	C8-C10-C11-C12
25	c	504	CLA	C8-C10-C11-C12
25	B	607	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
33	B	628	LHG	C34-C35-C36-C37
33	b	628	LHG	C34-C35-C36-C37
25	B	609	CLA	C15-C16-C17-C18
25	B	615	CLA	C8-C10-C11-C12
25	b	609	CLA	C15-C16-C17-C18
25	b	615	CLA	C8-C10-C11-C12
33	B	622	LHG	O6-C4-C5-O7
33	D	407	LHG	O6-C4-C5-O7
33	b	622	LHG	O6-C4-C5-O7
33	d	407	LHG	O6-C4-C5-O7
30	C	501	SQD	C25-C26-C27-C28
30	c	501	SQD	C25-C26-C27-C28
31	Y	101	LMT	O5'-C1'-O1'-C1
31	C	521	LMT	C1-C2-C3-C4
31	c	521	LMT	C1-C2-C3-C4
28	A	410	LMG	C7-C8-C9-O8
28	a	410	LMG	C7-C8-C9-O8
33	B	622	LHG	C4-C5-C6-O8
33	b	622	LHG	C4-C5-C6-O8
34	C	516	DGD	C5B-C6B-C7B-C8B
34	c	516	DGD	C5B-C6B-C7B-C8B
31	I	101	LMT	C4'-C5'-C6'-O6'
31	i	101	LMT	C4'-C5'-C6'-O6'
29	D	405	PL9	C47-C48-C49-C51
29	d	405	PL9	C47-C48-C49-C51
33	E	102	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C13-C14-C15-C16
31	L	101	LMT	C5'-C4'-O1B-C1B
31	M	101	LMT	C5'-C4'-O1B-C1B
25	A	408	CLA	C3-C5-C6-C7
33	d	406	LHG	C9-C10-C11-C12
30	A	412	SQD	O47-C45-C46-O48
30	a	412	SQD	O47-C45-C46-O48
25	B	602	CLA	C11-C10-C8-C9
25	B	610	CLA	C11-C12-C13-C14
25	b	602	CLA	C11-C10-C8-C9
25	b	610	CLA	C11-C12-C13-C14
33	D	406	LHG	C9-C10-C11-C12
31	D	410	LMT	C6-C7-C8-C9
31	d	410	LMT	C6-C7-C8-C9
30	F	102	SQD	C9-C10-C11-C12
30	f	102	SQD	C9-C10-C11-C12
33	d	406	LHG	C29-C30-C31-C32
25	a	408	CLA	C3-C5-C6-C7
33	D	406	LHG	C29-C30-C31-C32
33	d	406	LHG	C8-C7-O7-C5
30	C	501	SQD	C2-C1-O6-C44
30	c	501	SQD	C2-C1-O6-C44
33	D	406	LHG	C11-C12-C13-C14
33	d	406	LHG	C11-C12-C13-C14
30	C	501	SQD	C9-C10-C11-C12
30	c	501	SQD	C9-C10-C11-C12
31	I	101	LMT	O1'-C1-C2-C3
25	B	614	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
33	D	407	LHG	C13-C14-C15-C16
33	d	407	LHG	C13-C14-C15-C16
31	i	101	LMT	O1'-C1-C2-C3
30	A	412	SQD	C23-C24-C25-C26
30	a	412	SQD	C23-C24-C25-C26
28	d	409	LMG	C39-C40-C41-C42
25	b	611	CLA	CBD-CGD-O2D-CED
25	C	514	CLA	C3-C5-C6-C7
25	c	514	CLA	C3-C5-C6-C7
28	D	409	LMG	C39-C40-C41-C42
33	D	406	LHG	C8-C7-O7-C5
31	A	415	LMT	C2-C1-O1'-C1'
31	B	625	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	C	521	LMT	C2-C1-O1'-C1'
31	a	415	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
31	c	521	LMT	C2-C1-O1'-C1'
30	b	620	SQD	C10-C11-C12-C13
33	E	102	LHG	C10-C11-C12-C13
25	B	607	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
30	B	620	SQD	C10-C11-C12-C13
31	I	101	LMT	C1-C2-C3-C4
31	i	101	LMT	C1-C2-C3-C4
33	e	102	LHG	C10-C11-C12-C13
30	h	102	SQD	C10-C11-C12-C13
28	b	621	LMG	C40-C41-C42-C43
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
30	H	102	SQD	C10-C11-C12-C13
33	D	408	LHG	C31-C32-C33-C34
33	B	622	LHG	O6-C4-C5-C6
33	b	622	LHG	O6-C4-C5-C6
28	D	409	LMG	C13-C14-C15-C16
28	d	409	LMG	C13-C14-C15-C16
33	d	408	LHG	C31-C32-C33-C34
28	B	621	LMG	C40-C41-C42-C43
25	B	611	CLA	CBD-CGD-O2D-CED
31	D	411	LMT	C6-C7-C8-C9
30	A	412	SQD	C5-C6-S-O7
30	a	412	SQD	C5-C6-S-O7
31	d	411	LMT	C6-C7-C8-C9
31	A	416	LMT	C4'-C5'-C6'-O6'
25	B	603	CLA	C11-C12-C13-C15
25	B	608	CLA	C11-C12-C13-C15
25	B	615	CLA	C12-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C7
25	b	603	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C12-C13-C15
25	b	615	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C7
34	c	517	DGD	C3B-C4B-C5B-C6B
31	a	416	LMT	C4'-C5'-C6'-O6'
34	C	517	DGD	C3B-C4B-C5B-C6B
31	D	411	LMT	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	d	411	LMT	C4-C5-C6-C7
28	A	410	LMG	C31-C32-C33-C34
28	a	410	LMG	C31-C32-C33-C34
31	K	105	LMT	C11-C10-C9-C8
25	B	608	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
25	B	615	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
31	k	105	LMT	C11-C10-C9-C8
33	Z	102	LHG	O6-C4-C5-O7
33	z	102	LHG	O6-C4-C5-O7
26	A	407	PHO	C3-C5-C6-C7
25	B	604	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	b	604	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C12-C13-C14
28	d	409	LMG	C18-C19-C20-C21
28	D	409	LMG	C18-C19-C20-C21
27	c	515	BCR	C9-C10-C11-C12
31	b	627	LMT	C3-C4-C5-C6
30	H	102	SQD	O5-C5-C6-S
30	h	102	SQD	O5-C5-C6-S
31	B	627	LMT	C3-C4-C5-C6
26	a	407	PHO	C3-C5-C6-C7
25	C	511	CLA	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C20
30	H	102	SQD	C44-C45-C46-O48
30	h	102	SQD	C44-C45-C46-O48
25	A	405	CLA	O1A-CGA-O2A-C1
33	D	406	LHG	C15-C16-C17-C18
33	d	406	LHG	C15-C16-C17-C18
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	C	511	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	511	CLA	CAD-CBD-CGD-O2D
25	D	404	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	d	404	CLA	C5-C6-C7-C8
25	a	405	CLA	O1A-CGA-O2A-C1
30	C	501	SQD	C24-C23-O48-C46
30	c	501	SQD	C24-C23-O48-C46
33	d	407	LHG	C17-C18-C19-C20
34	h	103	DGD	CCA-CDA-CEA-CFA
33	D	407	LHG	C17-C18-C19-C20
34	H	103	DGD	CCA-CDA-CEA-CFA
25	a	408	CLA	C10-C11-C12-C13
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CAD-CBD-CGD-O1D
25	C	510	CLA	CAD-CBD-CGD-O1D
25	C	511	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	b	612	CLA	CAD-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CAD-CBD-CGD-O1D
25	c	510	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	C	515	BCR	C9-C10-C11-C12
27	F	101	BCR	C13-C14-C15-C16
27	F	101	BCR	C19-C20-C21-C22
27	Z	101	BCR	C19-C20-C21-C22
27	f	101	BCR	C13-C14-C15-C16
27	f	101	BCR	C19-C20-C21-C22
27	z	101	BCR	C19-C20-C21-C22
33	B	622	LHG	C3-O3-P-O6
33	E	102	LHG	C4-O6-P-O5
33	b	622	LHG	C3-O3-P-O6
33	e	102	LHG	C4-O6-P-O5
25	D	401	CLA	C3-C5-C6-C7
25	d	401	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C16-C17-C18-C19
28	c	519	LMG	C33-C34-C35-C36
34	c	516	DGD	C6A-C7A-C8A-C9A
34	C	516	DGD	C6A-C7A-C8A-C9A
31	d	410	LMT	C9-C10-C11-C12
29	A	411	PL9	C23-C24-C26-C27
29	a	411	PL9	C23-C24-C26-C27
28	C	519	LMG	C33-C34-C35-C36
25	c	503	CLA	C15-C16-C17-C18
33	D	408	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
33	D	406	LHG	O9-C7-O7-C5
33	d	406	LHG	O9-C7-O7-C5
31	D	410	LMT	C9-C10-C11-C12
25	A	408	CLA	C10-C11-C12-C13
25	C	503	CLA	C15-C16-C17-C18
25	B	607	CLA	C16-C17-C18-C19
25	B	609	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C19
25	b	609	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
31	D	412	LMT	C2-C3-C4-C5
34	H	103	DGD	O2G-C1B-C2B-C3B
34	h	103	DGD	O2G-C1B-C2B-C3B
31	d	412	LMT	C2-C3-C4-C5
33	Z	102	LHG	C4-O6-P-O5
33	z	102	LHG	C4-O6-P-O5
31	m	101	LMT	C3-C4-C5-C6
34	c	516	DGD	C5A-C6A-C7A-C8A
25	C	504	CLA	C2A-CAA-CBA-CGA
25	c	504	CLA	C2A-CAA-CBA-CGA
31	M	102	LMT	C3-C4-C5-C6
34	C	516	DGD	C5A-C6A-C7A-C8A
29	A	411	PL9	C4-C3-C7-C8
29	a	411	PL9	C4-C3-C7-C8
30	C	501	SQD	C44-C45-O47-C7
30	c	501	SQD	C44-C45-O47-C7
25	B	604	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
27	K	102	BCR	C18-C19-C20-C21
27	k	102	BCR	C18-C19-C20-C21
28	a	410	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	501	SQD	C15-C16-C17-C18
30	c	501	SQD	C15-C16-C17-C18
33	D	408	LHG	C18-C19-C20-C21
28	A	410	LMG	C39-C40-C41-C42
33	E	102	LHG	C26-C27-C28-C29
33	e	102	LHG	C26-C27-C28-C29
31	B	625	LMT	C4B-C5B-C6B-O6B
31	b	625	LMT	C4B-C5B-C6B-O6B
31	C	522	LMT	C9-C10-C11-C12
33	d	408	LHG	C18-C19-C20-C21
34	C	518	DGD	O6D-C5D-C6D-O5D
34	c	518	DGD	O6D-C5D-C6D-O5D
31	c	522	LMT	C9-C10-C11-C12
33	B	628	LHG	C35-C36-C37-C38
33	b	628	LHG	C35-C36-C37-C38
25	B	603	CLA	C11-C12-C13-C14
25	B	605	CLA	C11-C10-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	b	605	CLA	C11-C10-C8-C9
25	b	613	CLA	C6-C7-C8-C9
31	A	416	LMT	C5-C6-C7-C8
25	B	604	CLA	C6-C7-C8-C10
25	B	605	CLA	C11-C10-C8-C7
25	b	604	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C10-C8-C7
28	B	621	LMG	C33-C34-C35-C36
28	b	621	LMG	C33-C34-C35-C36
31	a	416	LMT	C5-C6-C7-C8
33	D	408	LHG	C29-C30-C31-C32
33	d	408	LHG	C29-C30-C31-C32
33	E	102	LHG	C11-C10-C9-C8
31	B	626	LMT	C2'-C1'-O1'-C1
31	b	626	LMT	C2'-C1'-O1'-C1
25	B	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
33	e	102	LHG	C11-C10-C9-C8
25	B	614	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
30	k	101	SQD	C13-C14-C15-C16
30	K	101	SQD	C13-C14-C15-C16
31	I	104	LMT	O1'-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	i	104	LMT	O1'-C1-C2-C3
25	B	612	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C19
25	A	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	C2-C1-O2A-CGA
25	c	508	CLA	C2-C1-O2A-CGA
25	B	606	CLA	C11-C12-C13-C15
25	C	510	CLA	C16-C17-C18-C20
25	c	510	CLA	C16-C17-C18-C20
31	I	103	LMT	C1-C2-C3-C4
31	i	103	LMT	C1-C2-C3-C4
25	b	606	CLA	C11-C12-C13-C15
34	C	518	DGD	CDA-CEA-CFA-CGA
34	C	516	DGD	C5D-C6D-O5D-C1E
34	c	516	DGD	C5D-C6D-O5D-C1E
34	C	516	DGD	C2A-C3A-C4A-C5A
34	c	516	DGD	C2A-C3A-C4A-C5A
34	c	518	DGD	CDA-CEA-CFA-CGA
28	C	519	LMG	C37-C38-C39-C40
28	c	519	LMG	C37-C38-C39-C40
25	c	508	CLA	C2A-CAA-CBA-CGA
27	B	617	BCR	C9-C10-C11-C12
27	C	515	BCR	C19-C20-C21-C22
27	b	617	BCR	C9-C10-C11-C12
27	c	515	BCR	C19-C20-C21-C22
25	b	608	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
31	C	524	LMT	C2-C1-O1'-C1'
31	c	524	LMT	C2-C1-O1'-C1'
25	B	616	CLA	C11-C10-C8-C9
25	b	616	CLA	C11-C10-C8-C9
25	b	602	CLA	CBA-CGA-O2A-C1
25	A	408	CLA	O1A-CGA-O2A-C1
25	C	502	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20
25	B	602	CLA	CBA-CGA-O2A-C1
25	a	408	CLA	O1A-CGA-O2A-C1
25	C	508	CLA	C2A-CAA-CBA-CGA
29	D	405	PL9	C40-C39-C41-C42
29	d	405	PL9	C40-C39-C41-C42
31	F	103	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	f	103	LMT	C4B-C5B-C6B-O6B
28	a	414	LMG	C30-C31-C32-C33
31	D	411	LMT	C2-C3-C4-C5
31	d	411	LMT	C2-C3-C4-C5
25	C	504	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
28	A	414	LMG	C30-C31-C32-C33
28	C	523	LMG	C35-C36-C37-C38
28	c	523	LMG	C35-C36-C37-C38
34	C	517	DGD	C9A-CAA-CBA-CCA
34	c	517	DGD	C9A-CAA-CBA-CCA
31	B	623	LMT	C1-C2-C3-C4
31	b	623	LMT	C1-C2-C3-C4
31	K	105	LMT	C4-C5-C6-C7
31	c	524	LMT	C6-C7-C8-C9
31	k	105	LMT	C4-C5-C6-C7
33	D	406	LHG	C33-C34-C35-C36
33	d	406	LHG	C33-C34-C35-C36
34	C	517	DGD	C1A-C2A-C3A-C4A
33	D	406	LHG	C14-C15-C16-C17
33	d	406	LHG	C14-C15-C16-C17
31	C	524	LMT	C6-C7-C8-C9
25	b	603	CLA	C15-C16-C17-C18
27	K	102	BCR	C20-C21-C22-C37
27	k	102	BCR	C20-C21-C22-C37
34	c	517	DGD	C1A-C2A-C3A-C4A
25	B	603	CLA	C15-C16-C17-C18
25	D	404	CLA	C2-C1-O2A-CGA
25	d	404	CLA	C2-C1-O2A-CGA
25	A	408	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
25	B	608	CLA	C11-C12-C13-C14
25	C	512	CLA	C11-C10-C8-C9
25	b	608	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C10-C8-C9
25	B	611	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
25	a	408	CLA	CBA-CGA-O2A-C1
28	C	523	LMG	C12-C13-C14-C15
28	c	523	LMG	C12-C13-C14-C15
25	A	408	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	408	CLA	C1A-C2A-CAA-CBA
27	K	102	BCR	C20-C21-C22-C23
27	k	102	BCR	C20-C21-C22-C23
31	D	411	LMT	C5'-C4'-O1B-C1B
27	A	409	BCR	C23-C24-C25-C26
27	B	617	BCR	C5-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	F	101	BCR	C1-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C30
27	a	409	BCR	C23-C24-C25-C26
27	b	617	BCR	C5-C6-C7-C8
27	b	619	BCR	C5-C6-C7-C8
27	f	101	BCR	C1-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
31	d	411	LMT	C5'-C4'-O1B-C1B
35	E	104	HEM	CAD-CBD-CGD-O1D
35	e	104	HEM	CAD-CBD-CGD-O1D
31	J	101	LMT	C3-C4-C5-C6
28	C	519	LMG	C15-C16-C17-C18
31	j	101	LMT	C3-C4-C5-C6
28	c	519	LMG	C15-C16-C17-C18
33	D	408	LHG	C15-C16-C17-C18
33	d	408	LHG	C15-C16-C17-C18
27	b	619	BCR	C9-C10-C11-C12
25	B	609	CLA	C6-C7-C8-C10
25	C	505	CLA	C6-C7-C8-C10
25	b	609	CLA	C6-C7-C8-C10
25	c	505	CLA	C6-C7-C8-C10
30	A	413	SQD	C30-C31-C32-C33
31	I	102	LMT	C4-C5-C6-C7
25	A	408	CLA	C11-C12-C13-C15
25	a	408	CLA	C11-C12-C13-C15
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
30	a	413	SQD	C30-C31-C32-C33
31	i	102	LMT	C4-C5-C6-C7
28	D	409	LMG	C22-C23-C24-C25
31	B	627	LMT	C4-C5-C6-C7
28	d	409	LMG	C22-C23-C24-C25
31	b	627	LMT	C4-C5-C6-C7
27	b	617	BCR	C36-C18-C19-C20
26	A	407	PHO	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C18-C19-C21-C22
29	d	405	PL9	C18-C19-C21-C22
26	a	407	PHO	CBA-CGA-O2A-C1
28	A	410	LMG	C21-C22-C23-C24
25	B	615	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C10-C8-C9
28	a	410	LMG	C21-C22-C23-C24
33	e	102	LHG	C24-C25-C26-C27
33	E	102	LHG	C24-C25-C26-C27
31	B	629	LMT	C6-C7-C8-C9
31	b	629	LMT	C6-C7-C8-C9
31	b	623	LMT	C9-C10-C11-C12
30	a	413	SQD	C32-C33-C34-C35
37	X	102	RRX	C6-C7-C8-C9
37	x	102	RRX	C6-C7-C8-C9
30	A	413	SQD	C32-C33-C34-C35
31	B	623	LMT	C9-C10-C11-C12
25	A	408	CLA	C4-C3-C5-C6
25	B	606	CLA	C4-C3-C5-C6
25	a	408	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
31	F	103	LMT	C5'-C4'-O1B-C1B
31	f	103	LMT	C5'-C4'-O1B-C1B
33	E	102	LHG	C2-C3-O3-P
33	e	102	LHG	C2-C3-O3-P
25	B	607	CLA	C13-C15-C16-C17
25	b	607	CLA	C13-C15-C16-C17
25	B	606	CLA	C11-C12-C13-C14
25	b	606	CLA	C11-C12-C13-C14
31	I	102	LMT	C1-C2-C3-C4
31	L	101	LMT	C1-C2-C3-C4
31	M	101	LMT	C1-C2-C3-C4
31	i	102	LMT	C1-C2-C3-C4
25	D	401	CLA	C4C-C3C-CAC-CBC
33	Z	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C4-C5-C6-O8
25	d	401	CLA	C4C-C3C-CAC-CBC
25	B	610	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	X	103	LMT	C11-C10-C9-C8
31	x	103	LMT	C11-C10-C9-C8
31	C	522	LMT	C1-C2-C3-C4
31	c	522	LMT	C1-C2-C3-C4
25	B	607	CLA	C10-C11-C12-C13
31	T	701	LMT	C2-C1-O1'-C1'
31	t	701	LMT	C2-C1-O1'-C1'
27	B	619	BCR	C9-C10-C11-C12
34	C	516	DGD	O2G-C1B-C2B-C3B
34	C	518	DGD	O1G-C1A-C2A-C3A
34	c	516	DGD	O2G-C1B-C2B-C3B
34	c	518	DGD	O1G-C1A-C2A-C3A
25	B	602	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
35	E	104	HEM	CAD-CBD-CGD-O2D
25	B	611	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
35	e	104	HEM	CAD-CBD-CGD-O2D
26	D	402	PHO	CHA-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O1D
30	a	412	SQD	C25-C26-C27-C28
25	B	601	CLA	CAA-CBA-CGA-O2A
25	b	601	CLA	CAA-CBA-CGA-O2A
30	A	412	SQD	C25-C26-C27-C28
33	d	407	LHG	C34-C35-C36-C37
33	D	407	LHG	C34-C35-C36-C37
30	K	101	SQD	C33-C34-C35-C36
25	B	606	CLA	C2-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
31	I	102	LMT	C9-C10-C11-C12
25	C	514	CLA	C11-C12-C13-C15
25	c	514	CLA	C11-C12-C13-C15
30	k	101	SQD	C33-C34-C35-C36
31	i	102	LMT	C9-C10-C11-C12
27	B	618	BCR	C9-C10-C11-C12
25	D	403	CLA	CAA-CBA-CGA-O2A
25	d	403	CLA	CAA-CBA-CGA-O2A
25	B	613	CLA	C11-C10-C8-C9
25	C	508	CLA	C14-C13-C15-C16
25	b	605	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C10-C8-C9
25	c	508	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	413	SQD	C5-C6-S-O8
30	B	620	SQD	C45-C44-O6-C1
30	F	102	SQD	C45-C44-O6-C1
30	a	413	SQD	C5-C6-S-O8
30	b	620	SQD	C45-C44-O6-C1
30	f	102	SQD	C45-C44-O6-C1
26	A	407	PHO	C2A-CAA-CBA-CGA
26	a	407	PHO	C2A-CAA-CBA-CGA
25	B	609	CLA	C2-C1-O2A-CGA
25	C	502	CLA	C2-C1-O2A-CGA
25	C	512	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
34	C	517	DGD	CDA-CEA-CFA-CGA
25	A	406	CLA	C3A-C2A-CAA-CBA
25	a	406	CLA	C3A-C2A-CAA-CBA
34	c	517	DGD	CDA-CEA-CFA-CGA
26	A	407	PHO	O1A-CGA-O2A-C1
26	a	407	PHO	O1A-CGA-O2A-C1
29	A	411	PL9	C18-C19-C21-C22
31	b	626	LMT	O1'-C1-C2-C3
31	B	626	LMT	O1'-C1-C2-C3
30	K	101	SQD	C2-C1-O6-C44
30	k	101	SQD	C2-C1-O6-C44
31	I	102	LMT	C2'-C1'-O1'-C1
31	i	102	LMT	C2'-C1'-O1'-C1
34	C	517	DGD	C2E-C1E-O5D-C6D
34	c	517	DGD	C2E-C1E-O5D-C6D
30	B	620	SQD	C11-C12-C13-C14
25	B	601	CLA	CAA-CBA-CGA-O1A
25	b	601	CLA	CAA-CBA-CGA-O1A
30	b	620	SQD	C11-C12-C13-C14
28	a	414	LMG	C28-C29-C30-C31
29	a	411	PL9	C18-C19-C21-C22
28	A	414	LMG	C28-C29-C30-C31
31	C	521	LMT	C7-C8-C9-C10
31	c	521	LMT	C7-C8-C9-C10
26	a	407	PHO	C8-C10-C11-C12
34	C	517	DGD	O6E-C1E-O5D-C6D
34	c	517	DGD	O6E-C1E-O5D-C6D
26	A	407	PHO	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C13-C15-C16-C17
30	K	101	SQD	C11-C12-C13-C14
33	d	408	LHG	C19-C20-C21-C22
28	c	519	LMG	C30-C31-C32-C33
34	C	517	DGD	C5A-C6A-C7A-C8A
34	c	517	DGD	C5A-C6A-C7A-C8A
33	D	408	LHG	C19-C20-C21-C22
25	A	408	CLA	C2A-CAA-CBA-CGA
25	a	408	CLA	C2A-CAA-CBA-CGA
28	C	519	LMG	C30-C31-C32-C33
28	a	410	LMG	C30-C31-C32-C33
30	k	101	SQD	C11-C12-C13-C14
28	A	410	LMG	C30-C31-C32-C33
25	c	512	CLA	C13-C15-C16-C17
25	b	611	CLA	C8-C10-C11-C12
29	A	411	PL9	C32-C33-C34-C36
30	k	101	SQD	C34-C35-C36-C37
34	c	516	DGD	C3B-C4B-C5B-C6B
30	B	620	SQD	O6-C44-C45-O47
30	b	620	SQD	O6-C44-C45-O47
34	C	516	DGD	C3B-C4B-C5B-C6B
25	B	611	CLA	C8-C10-C11-C12
25	B	605	CLA	C6-C7-C8-C9
30	K	101	SQD	C34-C35-C36-C37
33	B	622	LHG	O8-C23-C24-C25
33	D	406	LHG	O8-C23-C24-C25
33	d	406	LHG	O8-C23-C24-C25
33	E	102	LHG	O6-C4-C5-C6
33	e	102	LHG	O6-C4-C5-C6
30	K	101	SQD	C30-C31-C32-C33
30	b	620	SQD	O47-C7-C8-C9
25	b	604	CLA	C2-C3-C5-C6
31	x	101	LMT	O1'-C1-C2-C3
25	B	613	CLA	C11-C10-C8-C7
25	B	615	CLA	C6-C7-C8-C10
25	C	507	CLA	C6-C7-C8-C10
25	C	514	CLA	C6-C7-C8-C10
25	D	403	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	b	615	CLA	C6-C7-C8-C10
25	c	507	CLA	C6-C7-C8-C10
25	c	514	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C12-C13-C15-C16
27	F	101	BCR	C5-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C30
27	f	101	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C30
30	B	620	SQD	O47-C7-C8-C9
28	C	519	LMG	C21-C22-C23-C24
30	k	101	SQD	C30-C31-C32-C33
25	A	408	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
25	a	408	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
26	A	407	PHO	C2-C1-O2A-CGA
26	a	407	PHO	C2-C1-O2A-CGA
31	X	101	LMT	O1'-C1-C2-C3
28	c	519	LMG	C21-C22-C23-C24
25	B	613	CLA	CAA-CBA-CGA-O2A
33	b	622	LHG	O8-C23-C24-C25
31	D	412	LMT	O5'-C1'-O1'-C1
31	d	412	LMT	O5'-C1'-O1'-C1
30	C	501	SQD	C10-C11-C12-C13
30	c	501	SQD	C10-C11-C12-C13
34	c	516	DGD	O6D-C5D-C6D-O5D
25	b	613	CLA	CAA-CBA-CGA-O2A
28	A	414	LMG	O8-C28-C29-C30
28	a	414	LMG	O8-C28-C29-C30
25	C	505	CLA	C10-C11-C12-C13
25	c	505	CLA	C10-C11-C12-C13
25	B	612	CLA	CAA-CBA-CGA-O2A
28	C	523	LMG	O7-C10-C11-C12
34	C	516	DGD	O6D-C5D-C6D-O5D
25	B	609	CLA	C13-C15-C16-C17
25	b	609	CLA	C13-C15-C16-C17
25	b	612	CLA	CAA-CBA-CGA-O2A
28	c	523	LMG	O7-C10-C11-C12
31	D	410	LMT	C4'-C5'-C6'-O6'
31	d	410	LMT	C4'-C5'-C6'-O6'
31	H	101	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	h	101	LMT	C7-C8-C9-C10
28	b	621	LMG	C34-C35-C36-C37
30	A	412	SQD	C4-C5-C6-S
30	A	413	SQD	C4-C5-C6-S
30	a	412	SQD	C4-C5-C6-S
30	a	413	SQD	C4-C5-C6-S
28	B	621	LMG	C34-C35-C36-C37
29	a	411	PL9	C32-C33-C34-C36
25	B	604	CLA	C2-C3-C5-C6
30	c	501	SQD	C8-C7-O47-C45
31	I	101	LMT	C7-C8-C9-C10
25	B	603	CLA	O1A-CGA-O2A-C1
25	b	603	CLA	O1A-CGA-O2A-C1
30	a	413	SQD	C25-C26-C27-C28
31	i	101	LMT	C7-C8-C9-C10
35	V	201	HEM	CAD-CBD-CGD-O1D
35	v	201	HEM	CAD-CBD-CGD-O1D
25	A	406	CLA	C11-C12-C13-C14
25	B	611	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C12-C13-C14
25	b	611	CLA	C11-C12-C13-C14
30	A	413	SQD	C25-C26-C27-C28
27	B	617	BCR	C36-C18-C19-C20
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	506	CLA	CAA-CBA-CGA-O2A
25	c	506	CLA	CAA-CBA-CGA-O2A
28	A	410	LMG	O7-C10-C11-C12
28	D	409	LMG	O7-C10-C11-C12
28	a	410	LMG	O7-C10-C11-C12
28	d	409	LMG	O7-C10-C11-C12
30	A	412	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48
30	A	412	SQD	C31-C32-C33-C34
25	B	603	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
33	D	408	LHG	C24-C23-O8-C6
33	d	408	LHG	C24-C23-O8-C6
25	C	504	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C3-C5-C6-C7
30	a	412	SQD	C31-C32-C33-C34
30	C	501	SQD	C8-C7-O47-C45
31	A	416	LMT	O5'-C1'-O1'-C1
31	I	102	LMT	O5'-C1'-O1'-C1
31	K	105	LMT	O5'-C1'-O1'-C1
31	a	416	LMT	O5'-C1'-O1'-C1
31	i	102	LMT	O5'-C1'-O1'-C1
31	k	105	LMT	O5'-C1'-O1'-C1
25	C	511	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
27	F	101	BCR	C9-C10-C11-C12
27	b	618	BCR	C9-C10-C11-C12
27	f	101	BCR	C9-C10-C11-C12
30	b	620	SQD	C30-C31-C32-C33
25	C	503	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
25	C	511	CLA	C15-C16-C17-C18
30	B	620	SQD	C30-C31-C32-C33
25	c	511	CLA	CAA-CBA-CGA-O2A
30	K	101	SQD	O47-C7-C8-C9
30	k	101	SQD	O47-C7-C8-C9
33	B	622	LHG	C12-C13-C14-C15
33	d	408	LHG	C25-C26-C27-C28
25	c	511	CLA	C15-C16-C17-C18
28	C	523	LMG	C38-C39-C40-C41
33	D	408	LHG	C25-C26-C27-C28
33	b	622	LHG	C12-C13-C14-C15
25	a	405	CLA	C13-C15-C16-C17
25	C	512	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
30	B	620	SQD	C25-C26-C27-C28
30	C	501	SQD	C5-C6-S-O7
30	c	501	SQD	C5-C6-S-O7
28	c	523	LMG	C38-C39-C40-C41
25	A	405	CLA	C13-C15-C16-C17
30	b	620	SQD	C25-C26-C27-C28
31	X	103	LMT	C4-C5-C6-C7
31	x	103	LMT	C4-C5-C6-C7
25	B	604	CLA	C2-C1-O2A-CGA
25	b	604	CLA	C2-C1-O2A-CGA
25	C	502	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	514	CLA	C12-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C15
25	c	502	CLA	C6-C7-C8-C10
25	c	514	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
35	V	201	HEM	CAD-CBD-CGD-O2D
35	v	201	HEM	CAD-CBD-CGD-O2D
31	i	103	LMT	C5'-C4'-O1B-C1B
33	D	406	LHG	O10-C23-C24-C25
33	d	406	LHG	O10-C23-C24-C25
28	C	523	LMG	C15-C16-C17-C18
28	c	523	LMG	C15-C16-C17-C18
31	I	103	LMT	C5'-C4'-O1B-C1B
33	d	406	LHG	C16-C17-C18-C19
31	E	103	LMT	C3'-C4'-O1B-C1B
33	D	407	LHG	C25-C26-C27-C28
33	d	407	LHG	C25-C26-C27-C28
31	e	103	LMT	C3'-C4'-O1B-C1B
33	D	406	LHG	C16-C17-C18-C19
25	A	406	CLA	C4-C3-C5-C6
25	a	406	CLA	C4-C3-C5-C6
25	B	613	CLA	CAA-CBA-CGA-O1A
31	Y	101	LMT	C5-C6-C7-C8
31	y	101	LMT	C5-C6-C7-C8
33	d	407	LHG	C18-C19-C20-C21
33	D	407	LHG	C18-C19-C20-C21
25	b	613	CLA	CAA-CBA-CGA-O1A
28	A	414	LMG	O10-C28-C29-C30
28	a	414	LMG	O10-C28-C29-C30
31	C	520	LMT	C4B-C5B-C6B-O6B
31	c	520	LMT	C4B-C5B-C6B-O6B
30	A	412	SQD	O49-C7-C8-C9
30	a	412	SQD	O49-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	b	615	CLA	C14-C13-C15-C16
28	C	523	LMG	O9-C10-C11-C12
30	h	102	SQD	O49-C7-C8-C9
34	c	516	DGD	C7A-C8A-C9A-CAA
34	C	516	DGD	C7A-C8A-C9A-CAA
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
30	H	102	SQD	O49-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	514	CLA	CAA-CBA-CGA-O2A
30	A	412	SQD	O5-C5-C6-S
30	A	413	SQD	O5-C5-C6-S
30	F	102	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C5-C6-S
30	a	413	SQD	O5-C5-C6-S
30	f	102	SQD	O5-C5-C6-S
33	D	408	LHG	O10-C23-O8-C6
33	d	408	LHG	O10-C23-O8-C6
28	D	409	LMG	C30-C31-C32-C33
28	c	523	LMG	O9-C10-C11-C12
30	K	101	SQD	O49-C7-C8-C9
30	k	101	SQD	O49-C7-C8-C9
28	d	409	LMG	C30-C31-C32-C33
25	c	514	CLA	CAA-CBA-CGA-O2A
28	C	519	LMG	C13-C14-C15-C16
33	b	622	LHG	O10-C23-C24-C25
30	C	501	SQD	C45-C44-O6-C1
30	c	501	SQD	C45-C44-O6-C1
34	H	103	DGD	C2G-C3G-O3G-C1D
34	h	103	DGD	C2G-C3G-O3G-C1D
30	F	102	SQD	O6-C44-C45-O47
30	f	102	SQD	O6-C44-C45-O47
28	c	519	LMG	C13-C14-C15-C16
28	d	409	LMG	O9-C10-C11-C12
33	B	622	LHG	O10-C23-C24-C25
30	A	413	SQD	O47-C7-C8-C9
30	a	413	SQD	O47-C7-C8-C9
33	b	628	LHG	C23-C24-C25-C26
31	b	626	LMT	C7-C8-C9-C10
34	c	518	DGD	CAA-CBA-CCA-CDA
28	D	409	LMG	O9-C10-C11-C12
29	D	405	PL9	C11-C12-C13-C14
29	d	405	PL9	C11-C12-C13-C14
33	B	628	LHG	C23-C24-C25-C26
28	B	621	LMG	O8-C28-C29-C30
28	b	621	LMG	O8-C28-C29-C30
31	B	626	LMT	C7-C8-C9-C10
34	C	518	DGD	CAA-CBA-CCA-CDA
33	D	407	LHG	C16-C17-C18-C19
33	d	407	LHG	C16-C17-C18-C19
25	B	607	CLA	CAD-CBD-CGD-O2D

Continued on next page...

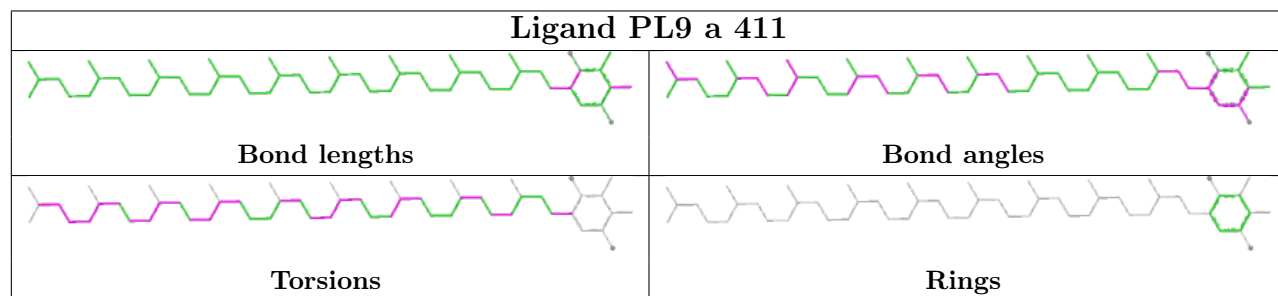
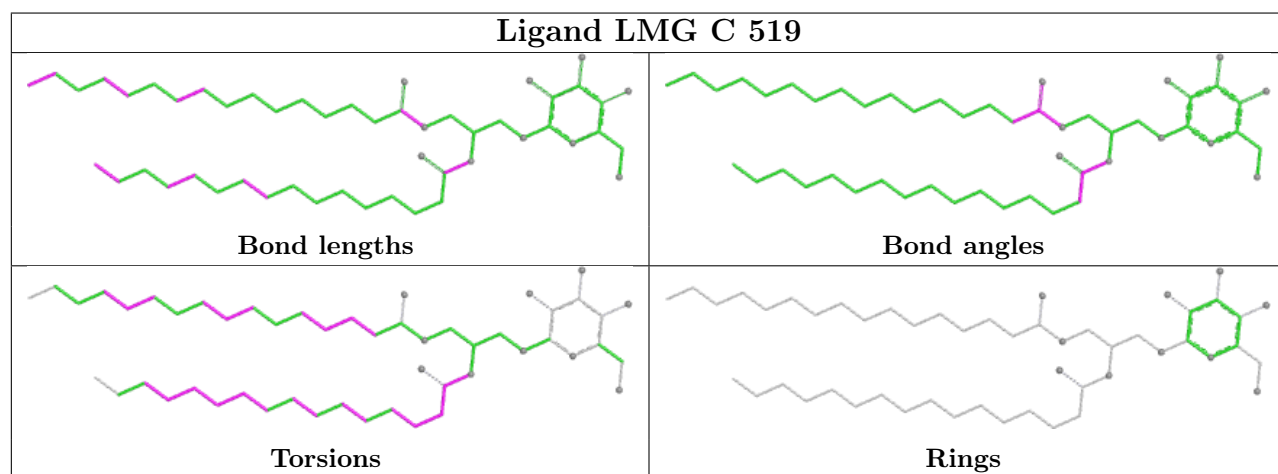
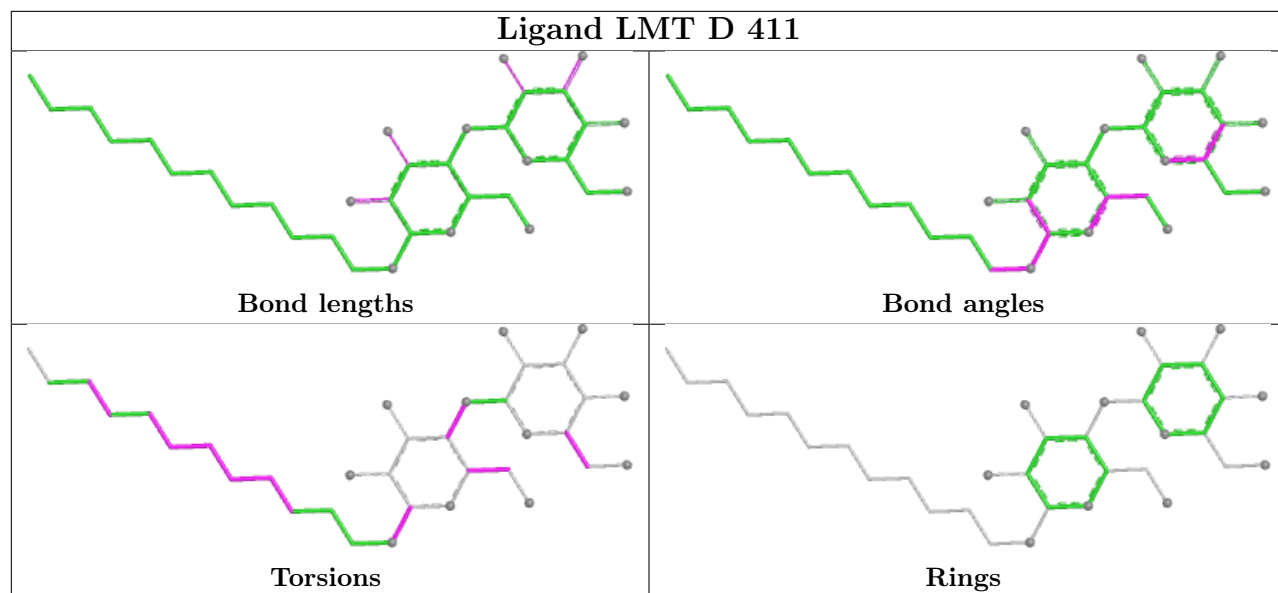
Continued from previous page...

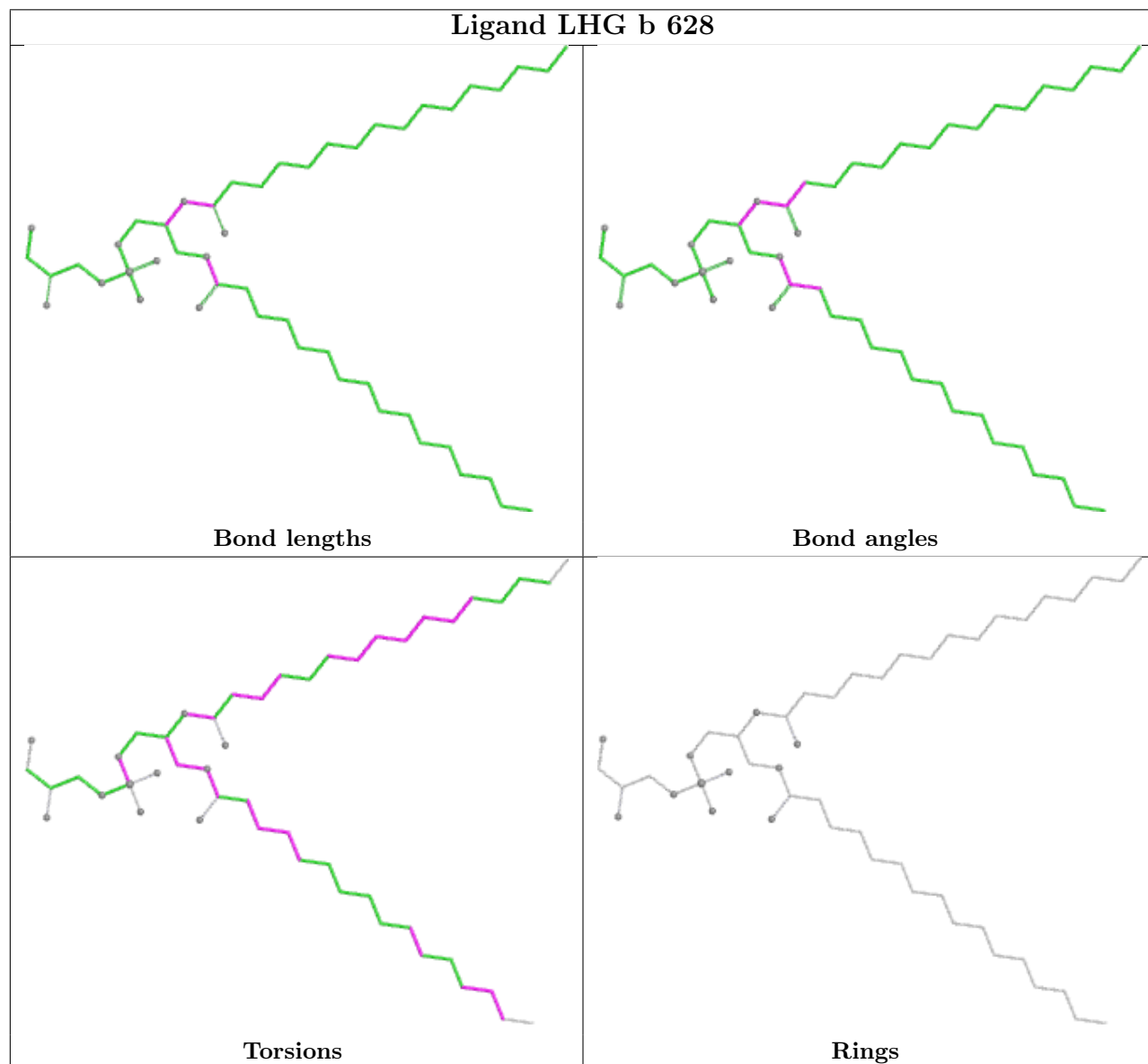
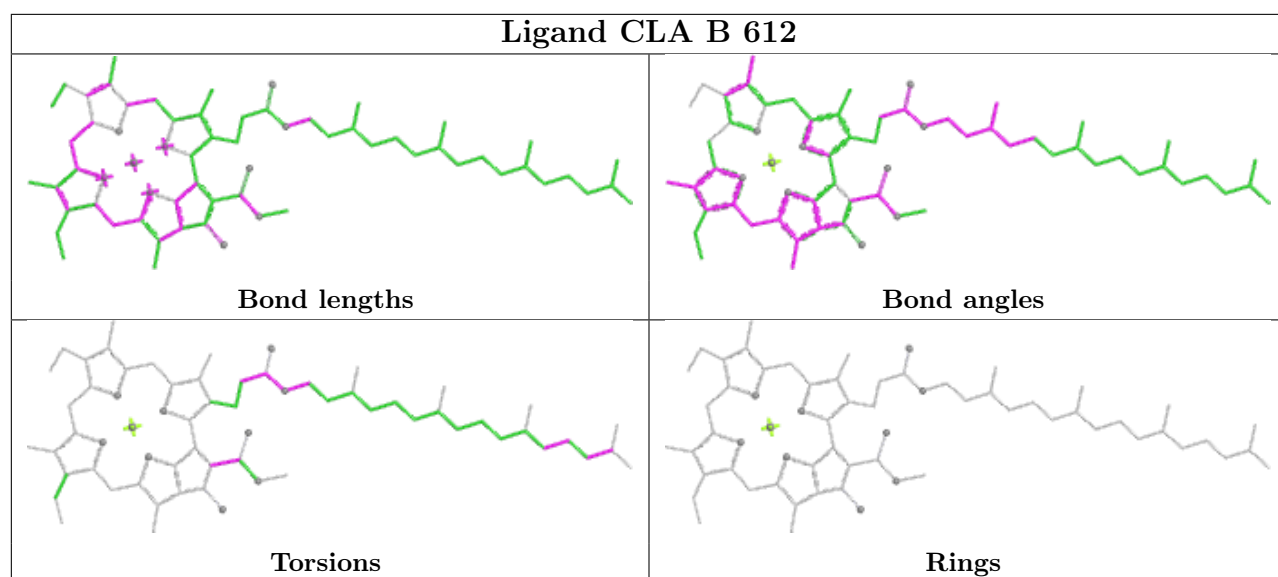
Mol	Chain	Res	Type	Atoms
25	b	607	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	C5-C6-C7-C8
25	B	602	CLA	C2-C1-O2A-CGA
25	b	602	CLA	C2-C1-O2A-CGA
33	Z	102	LHG	O8-C23-C24-C25
33	z	102	LHG	O8-C23-C24-C25
34	c	516	DGD	C9A-CAA-CBA-CCA
25	c	510	CLA	C5-C6-C7-C8
34	C	516	DGD	C9A-CAA-CBA-CCA
28	C	519	LMG	O7-C10-C11-C12
28	C	523	LMG	O8-C28-C29-C30
28	c	519	LMG	O7-C10-C11-C12
28	c	523	LMG	O8-C28-C29-C30
25	b	610	CLA	C5-C6-C7-C8
25	B	614	CLA	CAA-CBA-CGA-O1A
25	C	511	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A
25	c	511	CLA	CAA-CBA-CGA-O1A
28	A	410	LMG	O9-C10-C11-C12
28	a	410	LMG	O9-C10-C11-C12

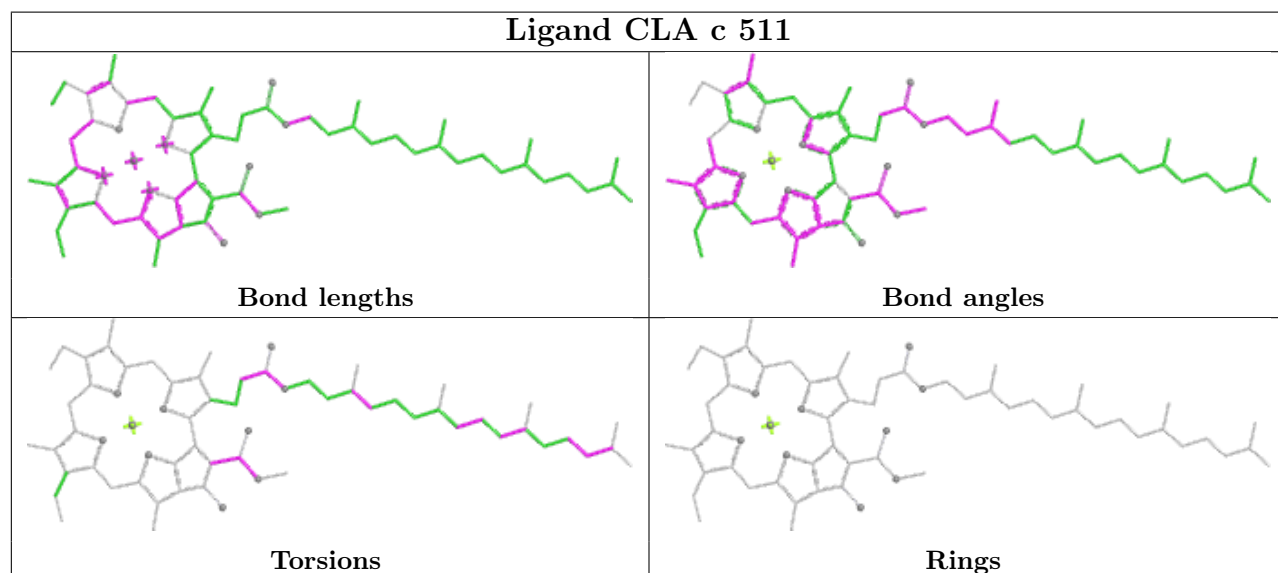
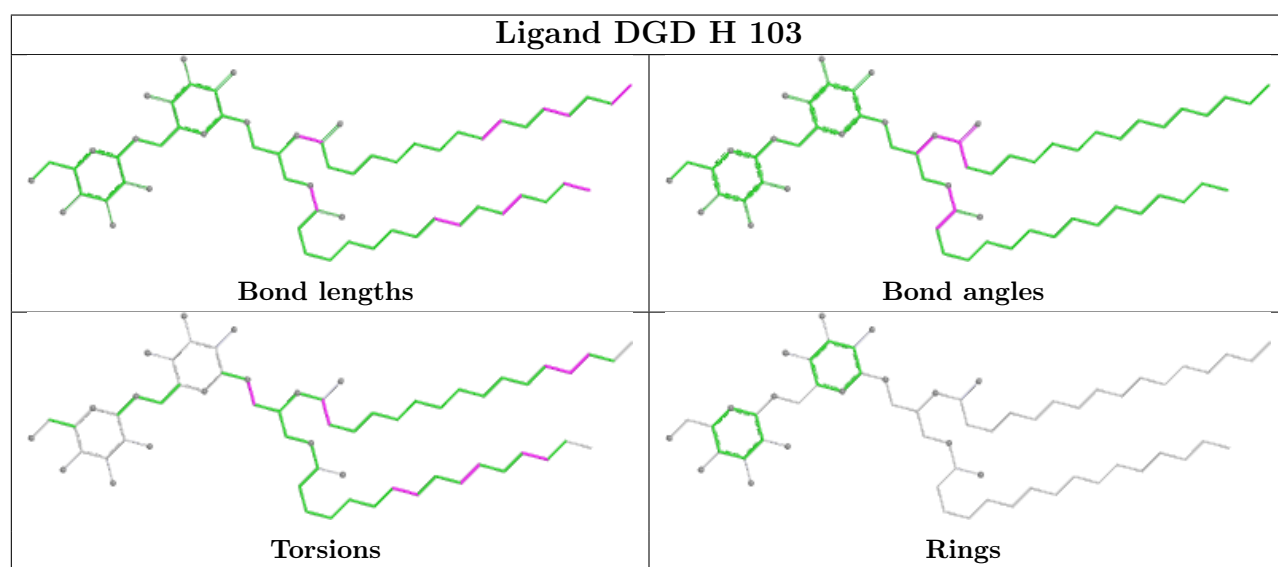
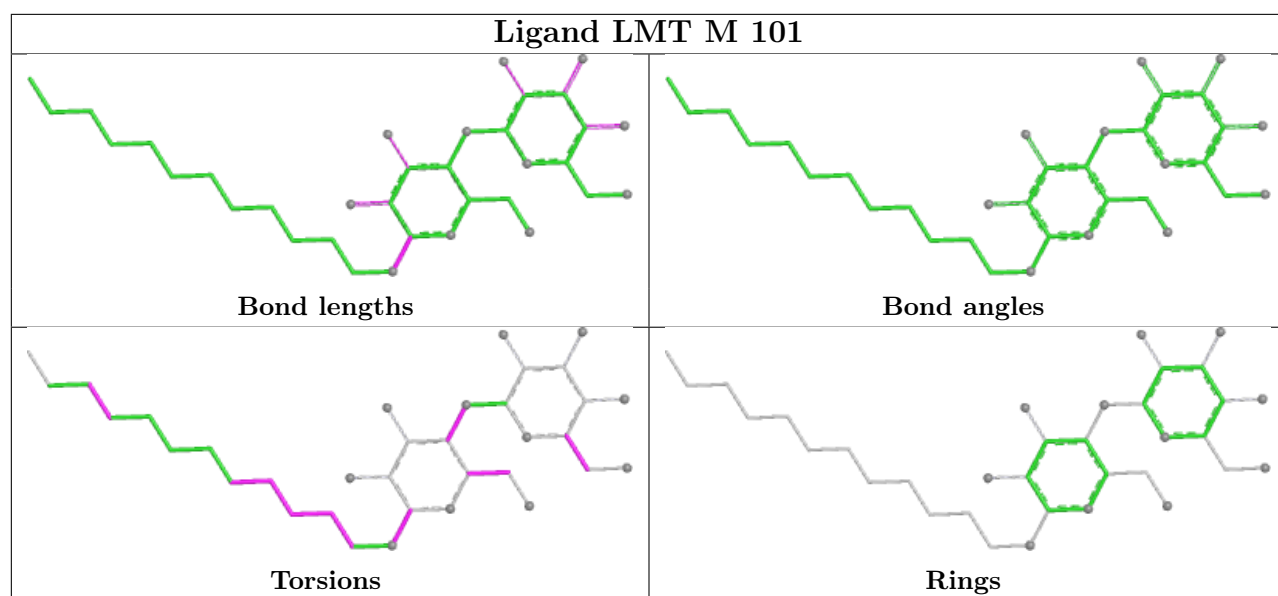
There are no ring outliers.

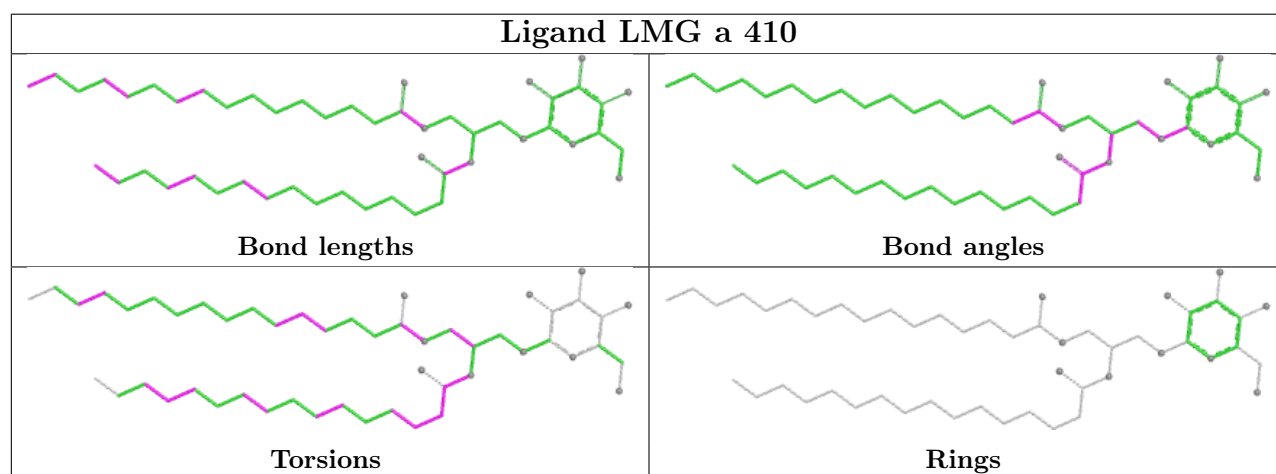
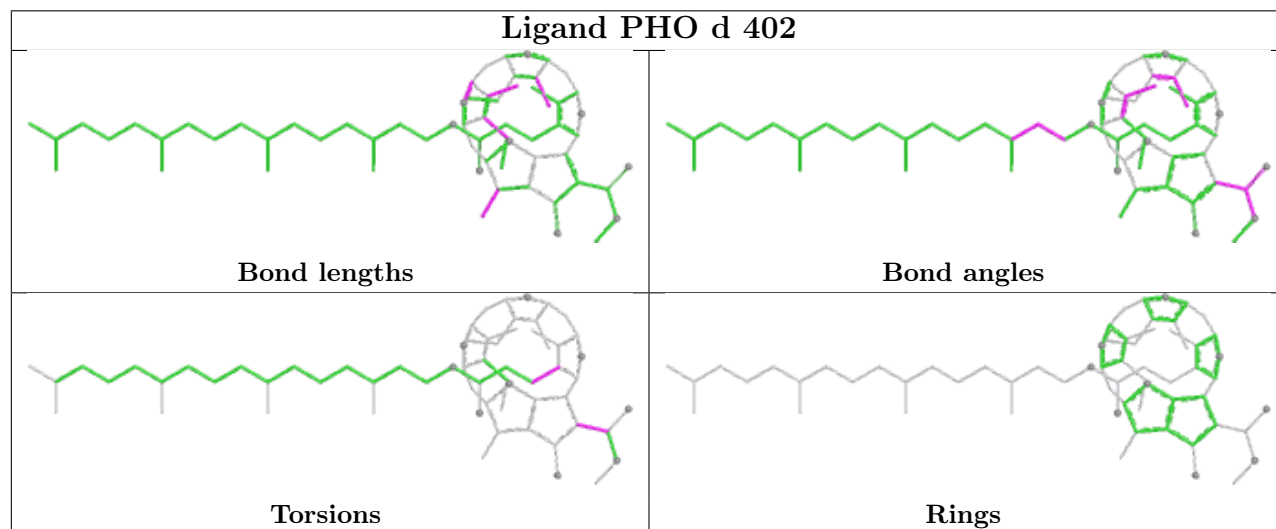
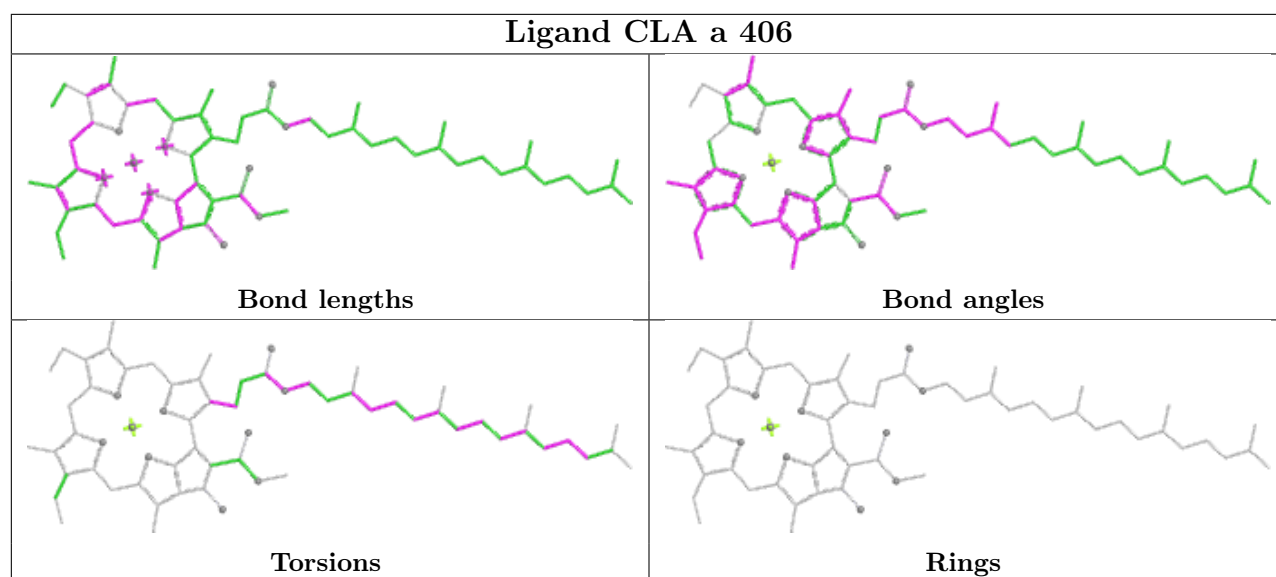
No monomer is involved in short contacts.

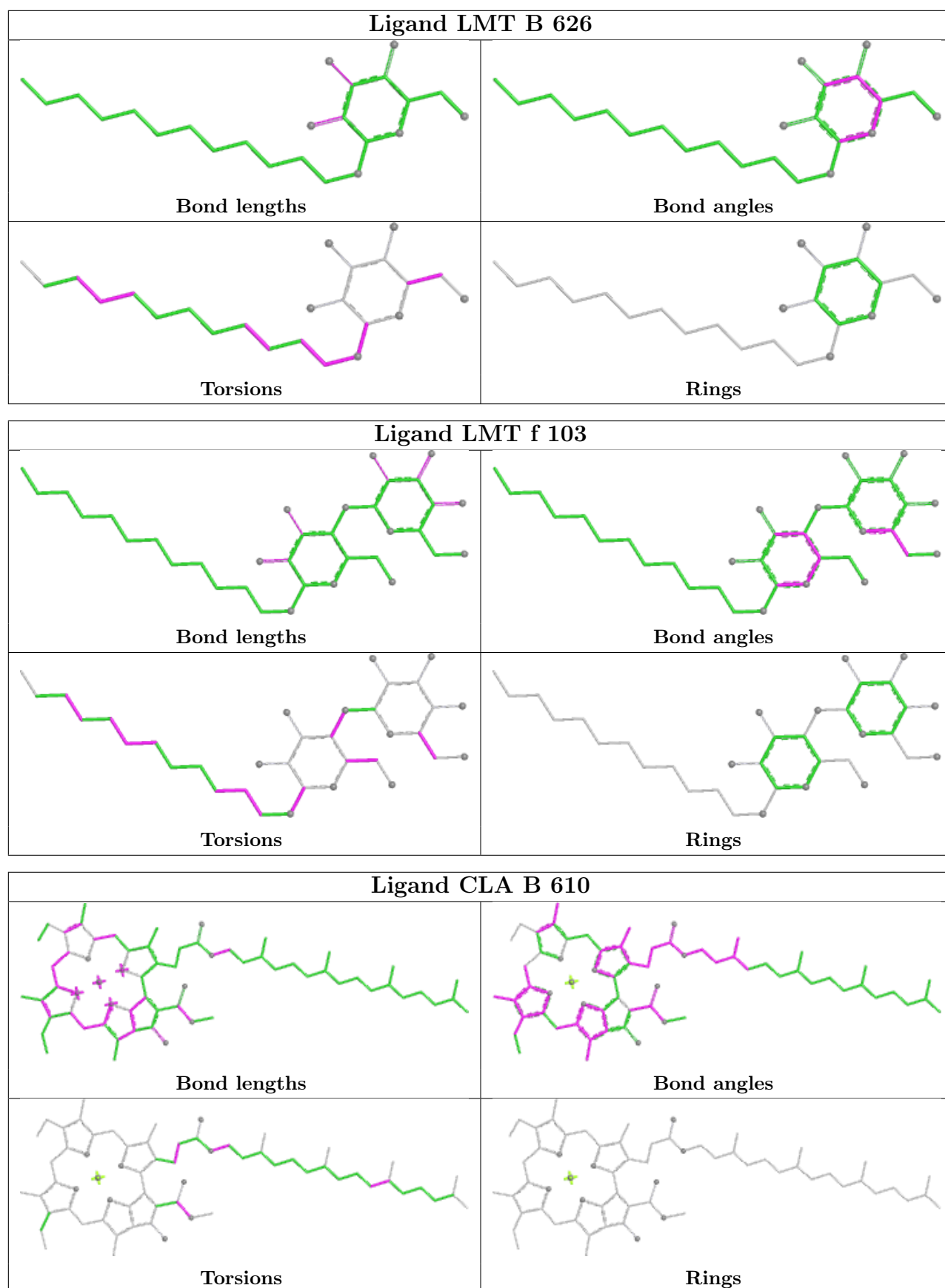
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

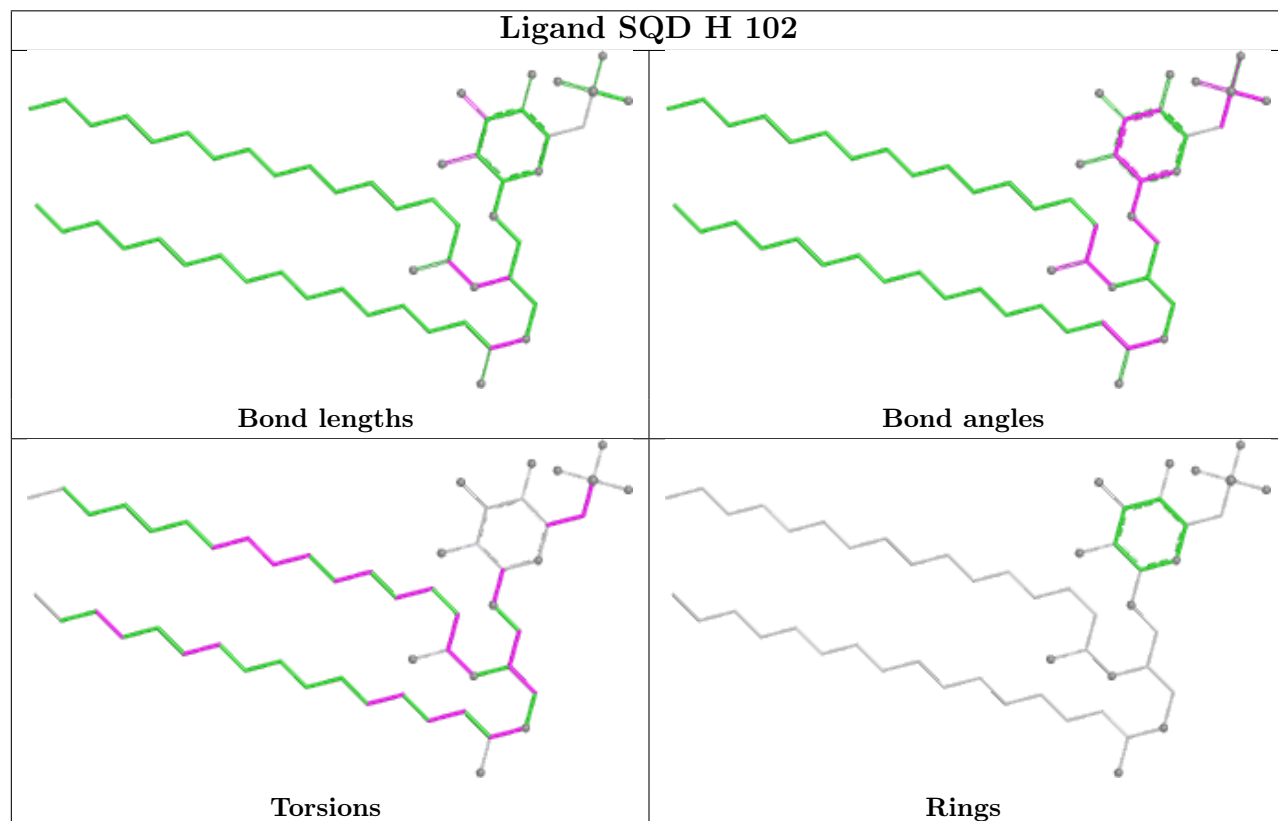
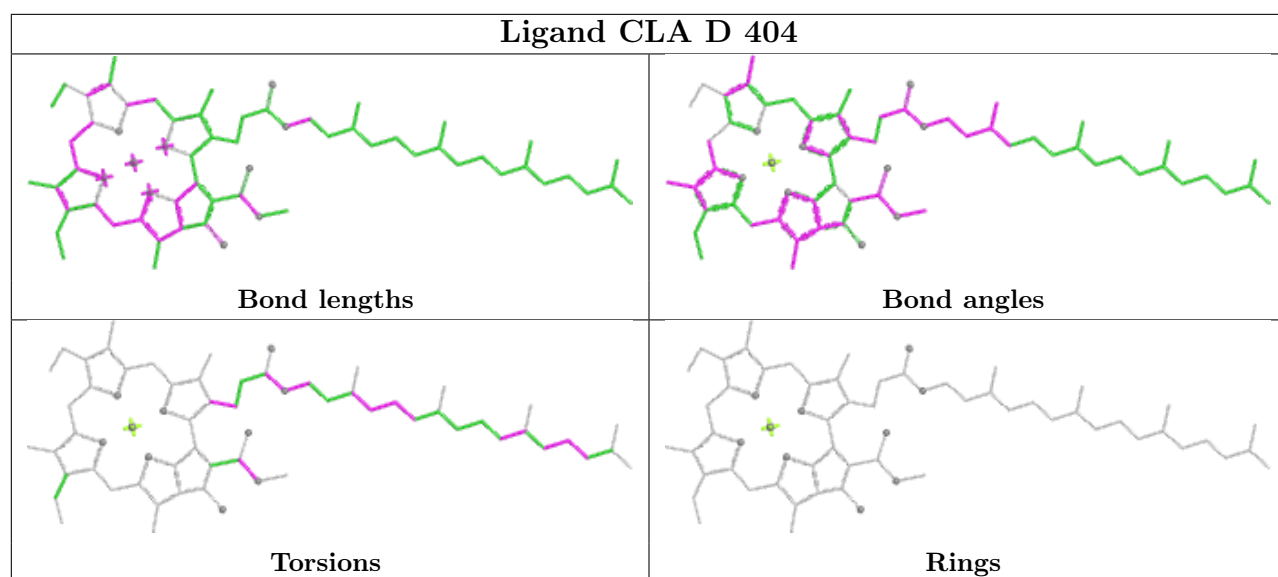


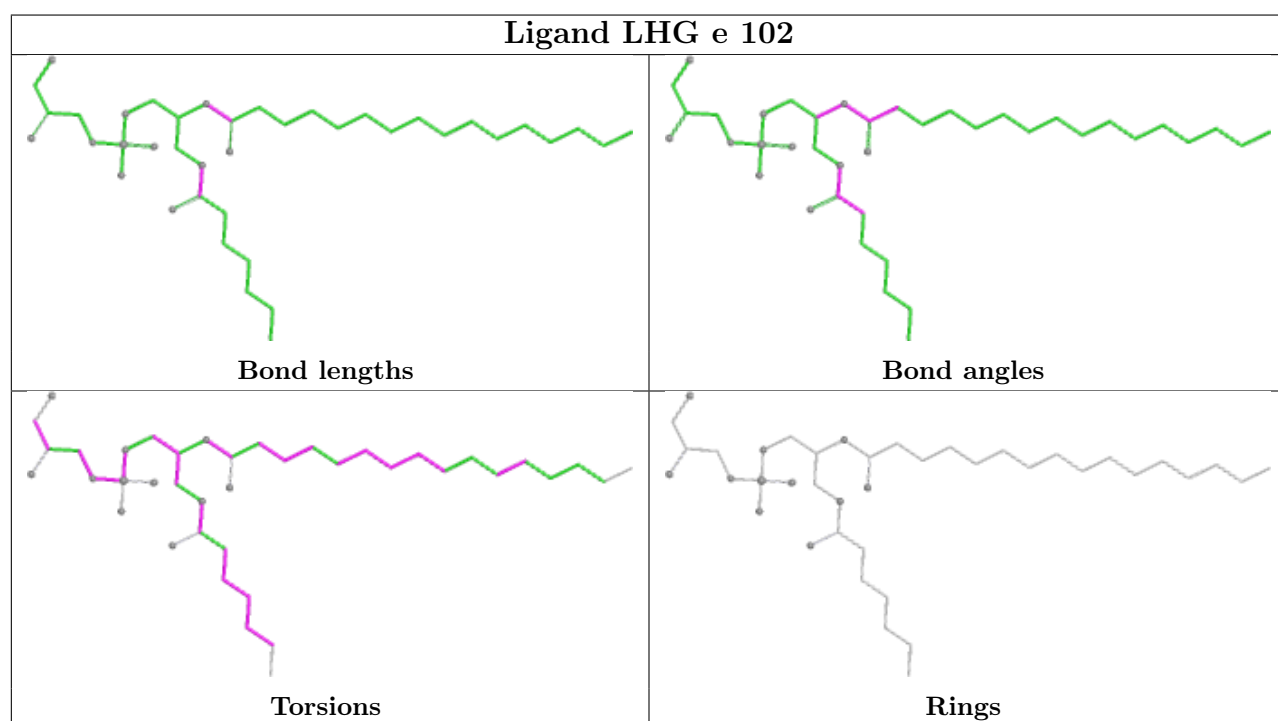
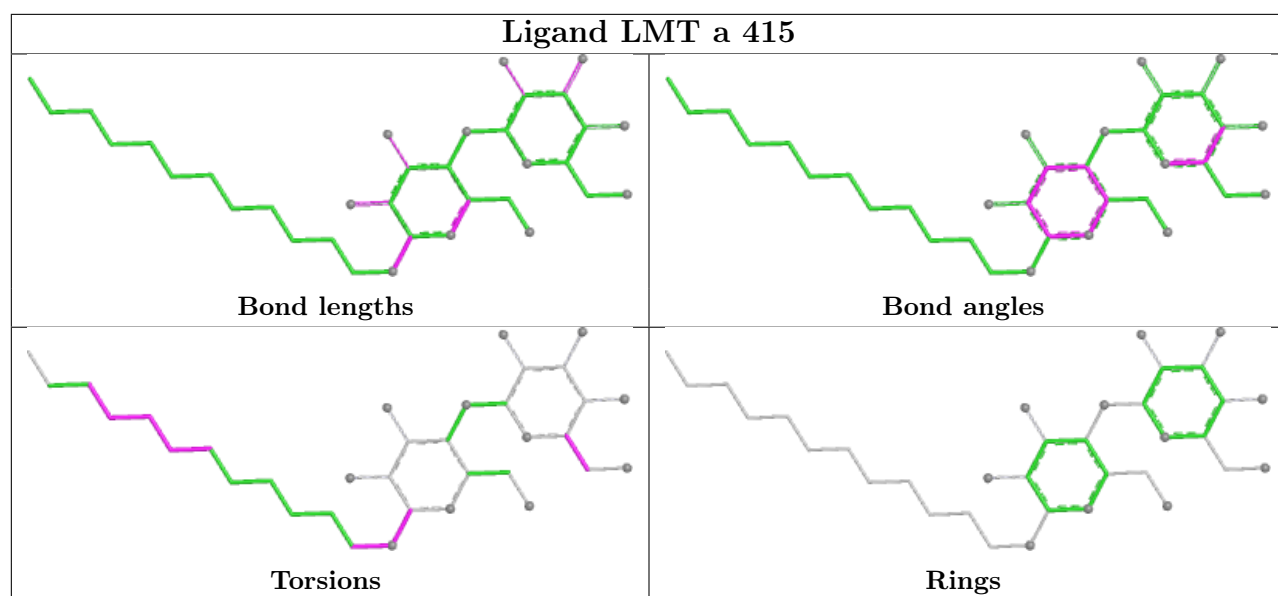


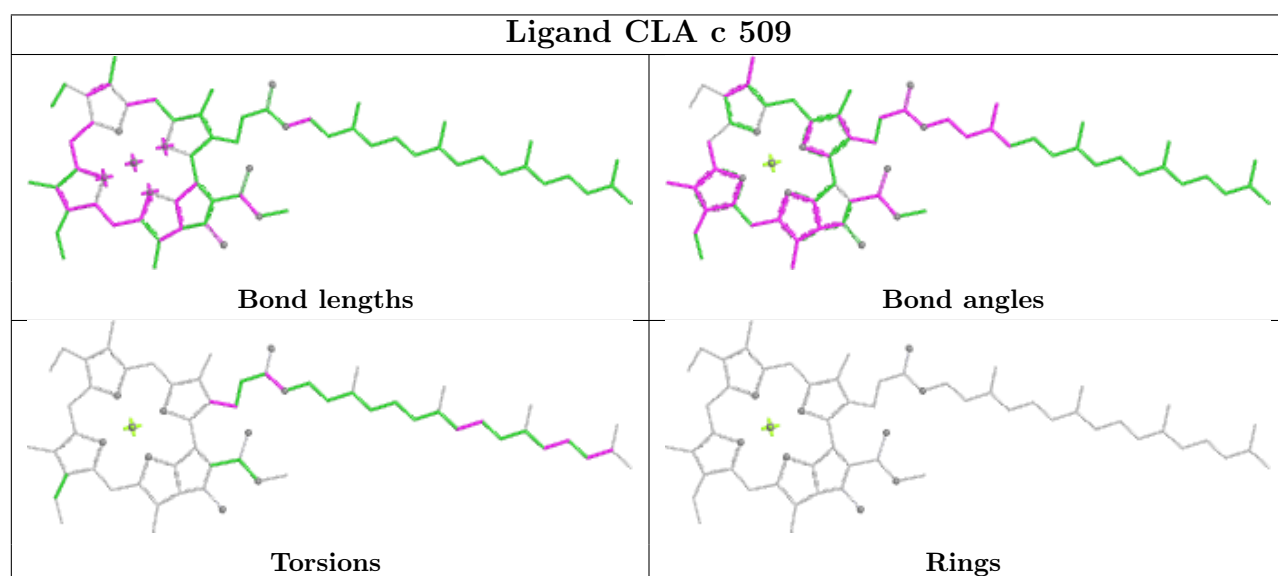
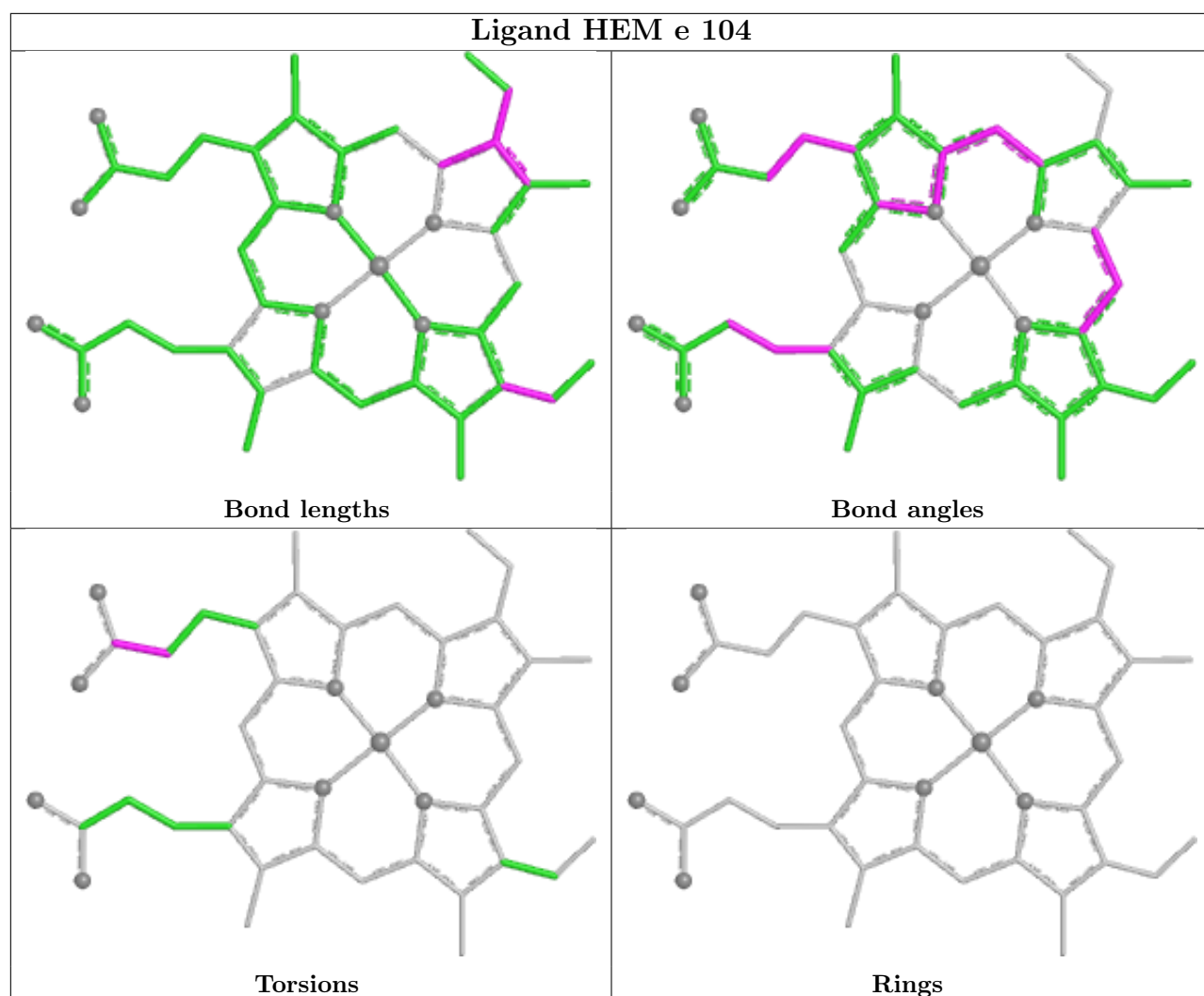


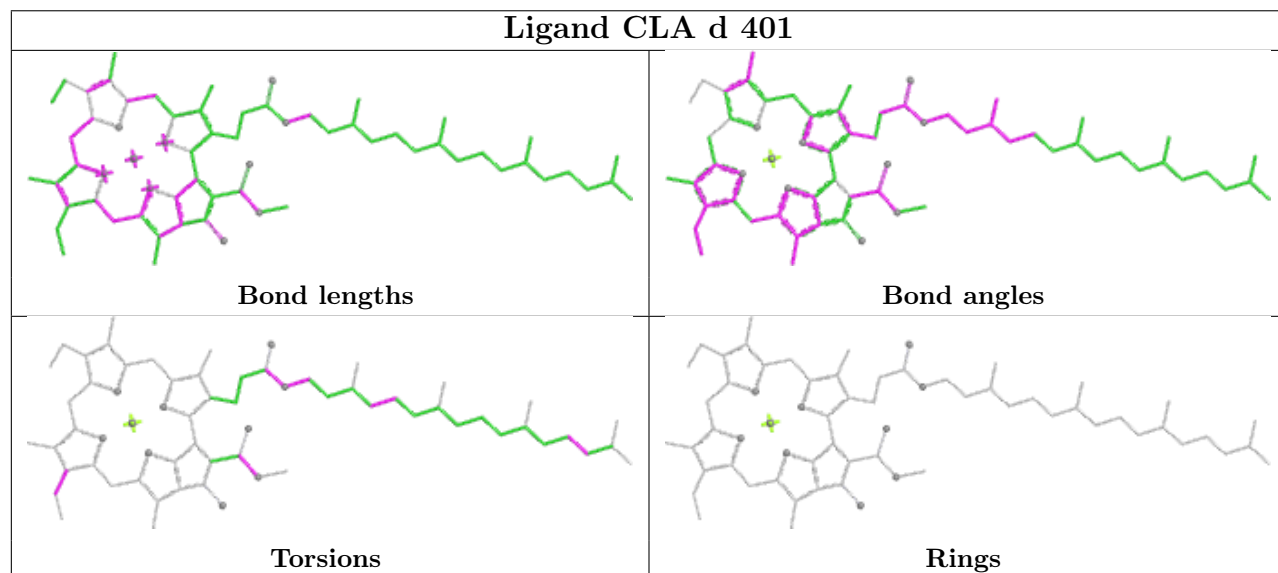
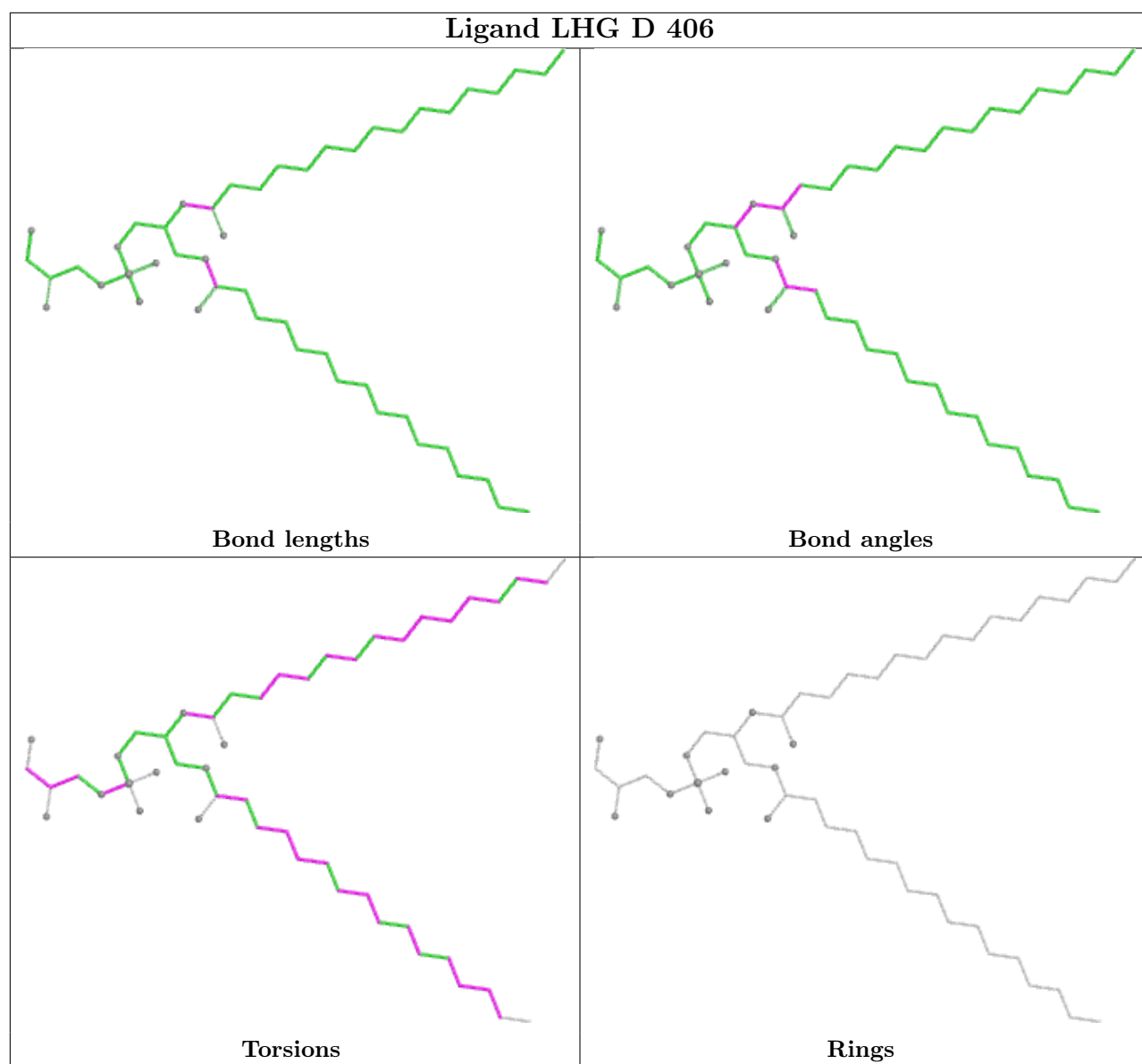


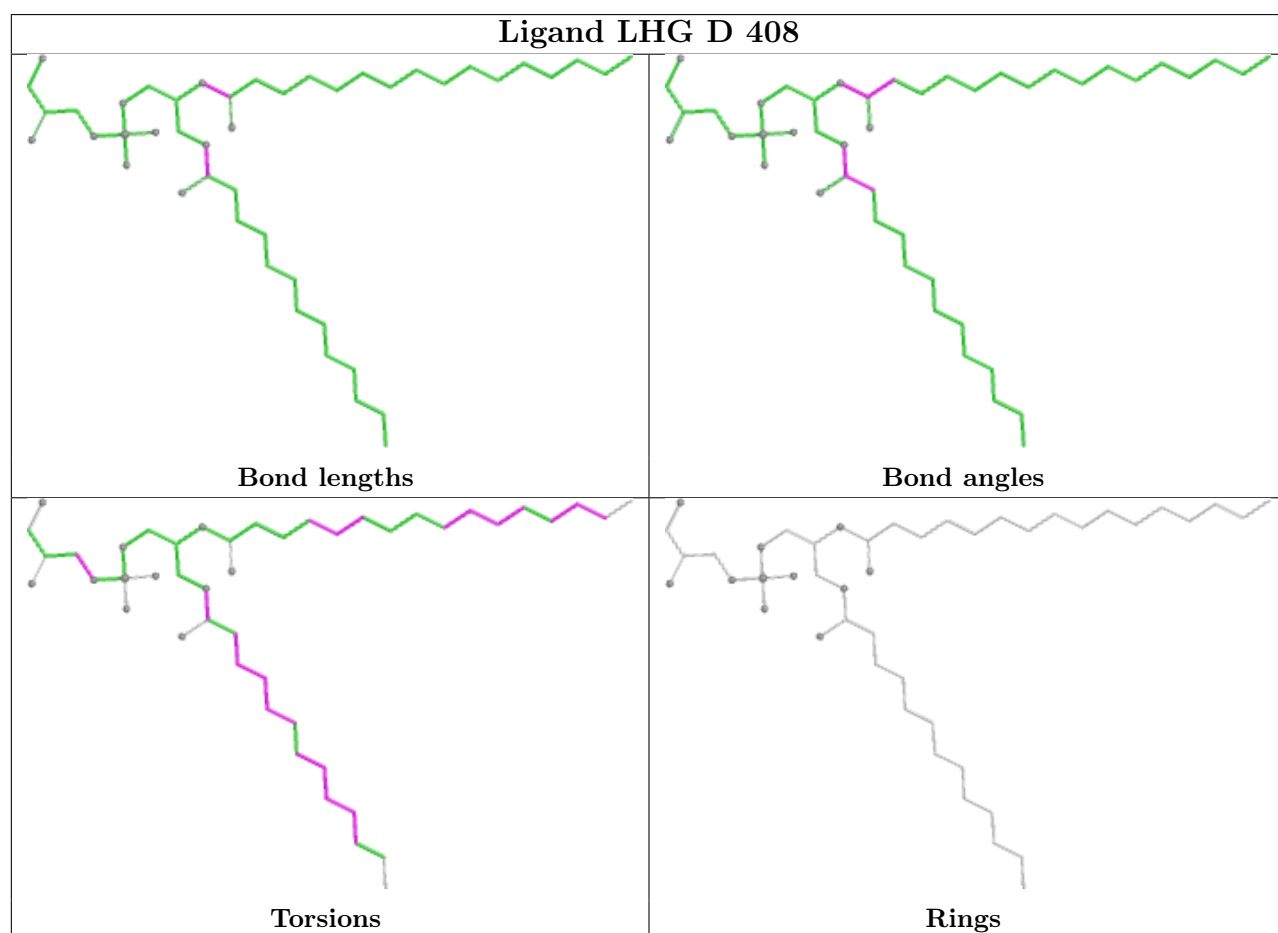
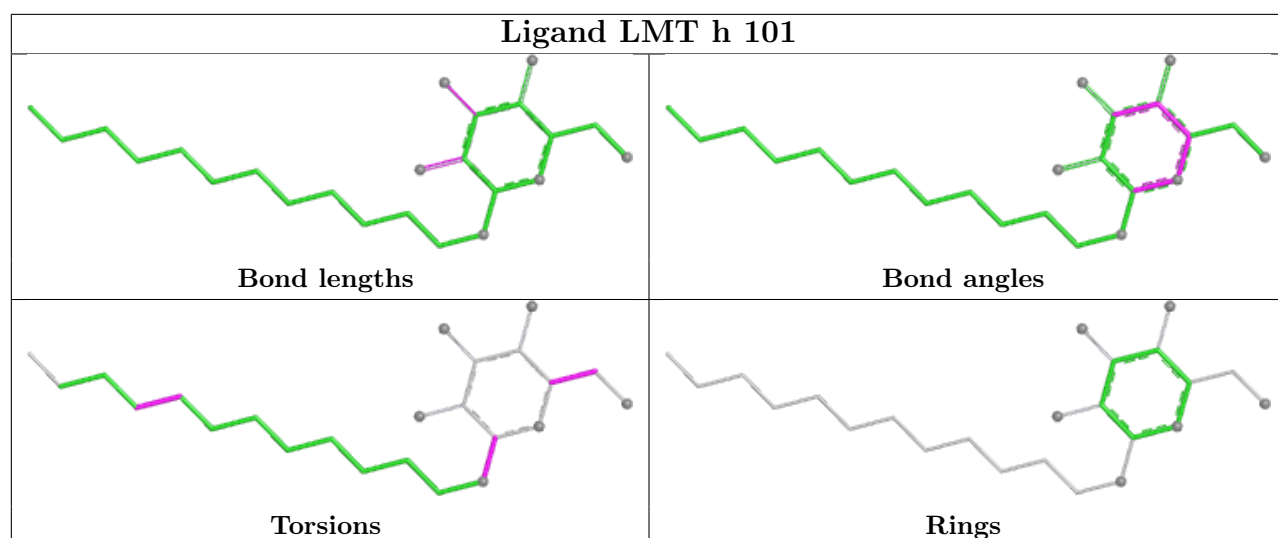


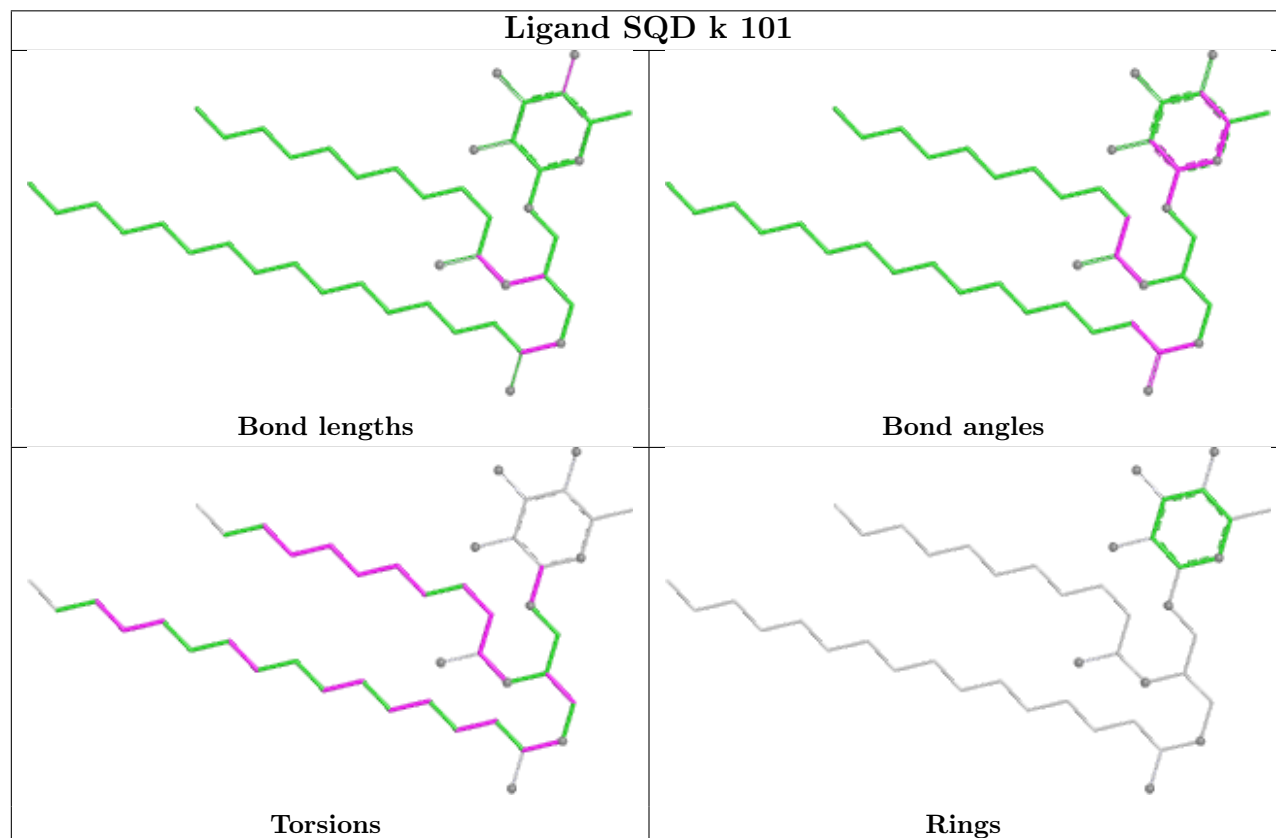
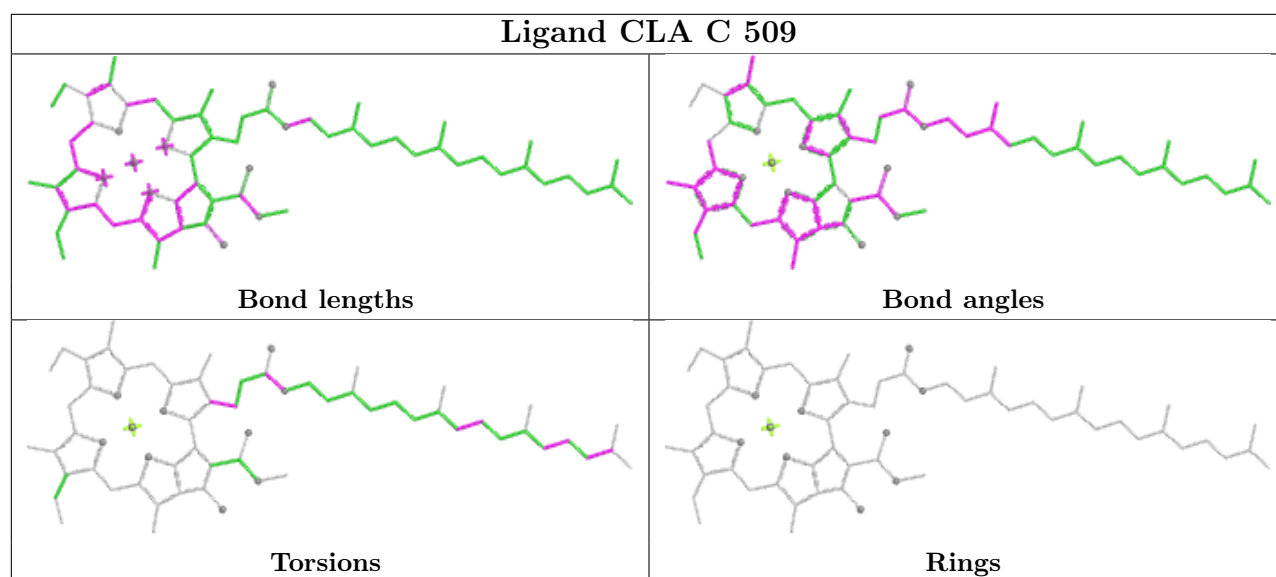


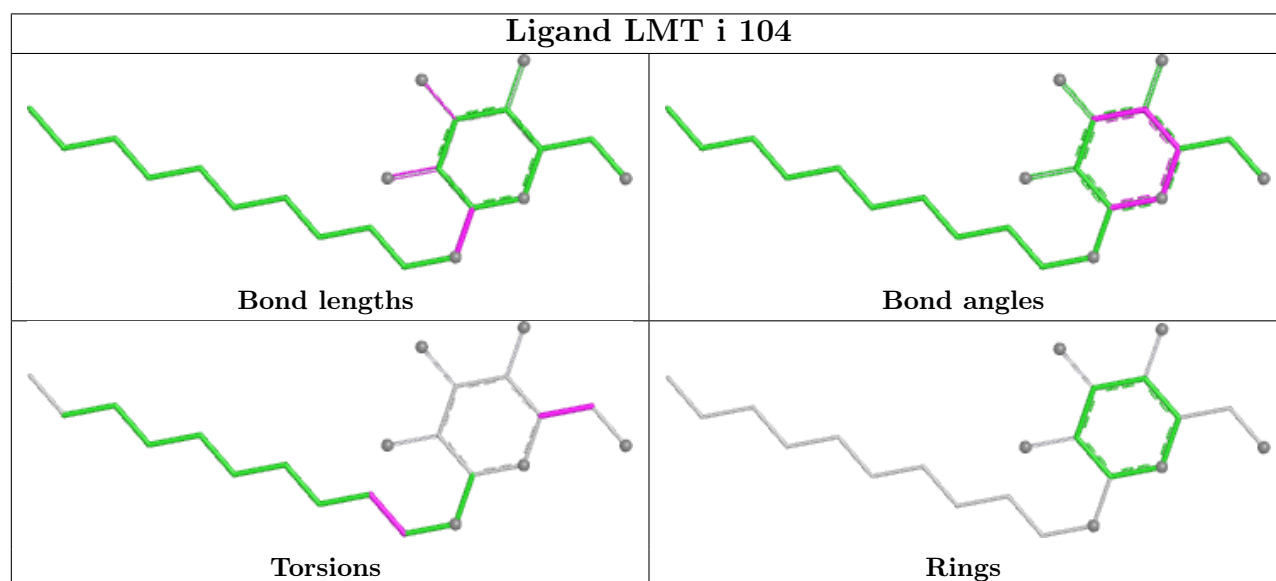
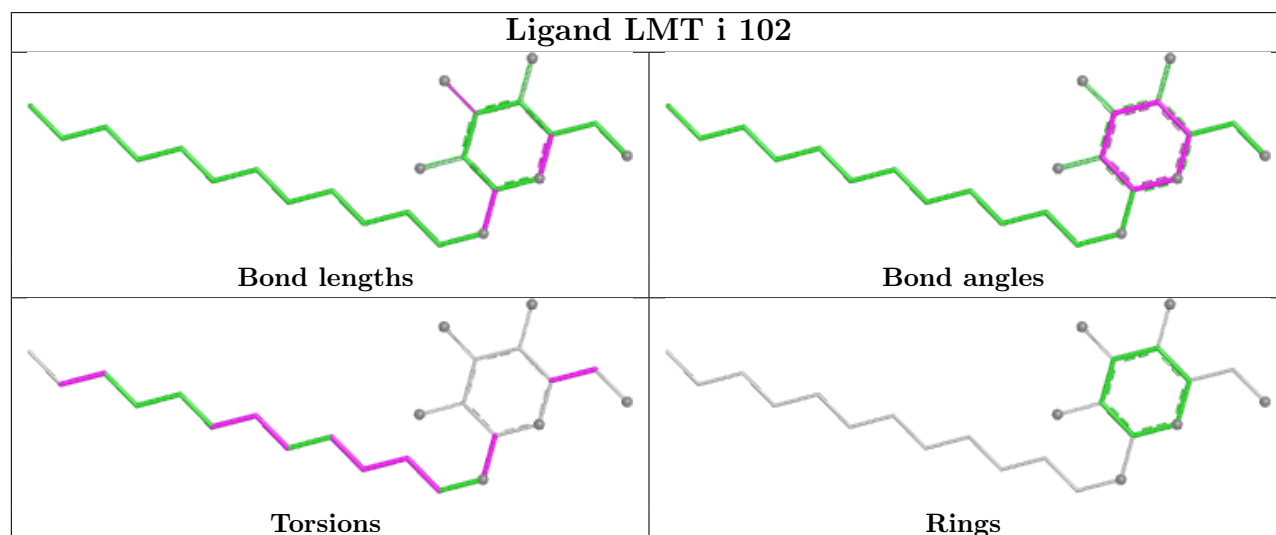
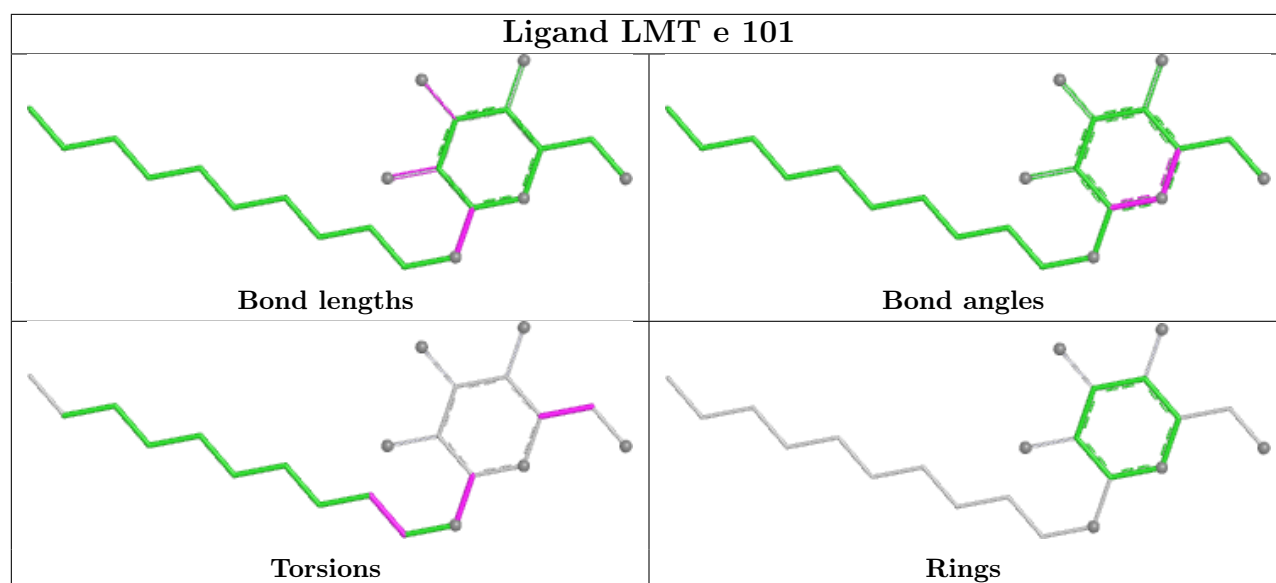


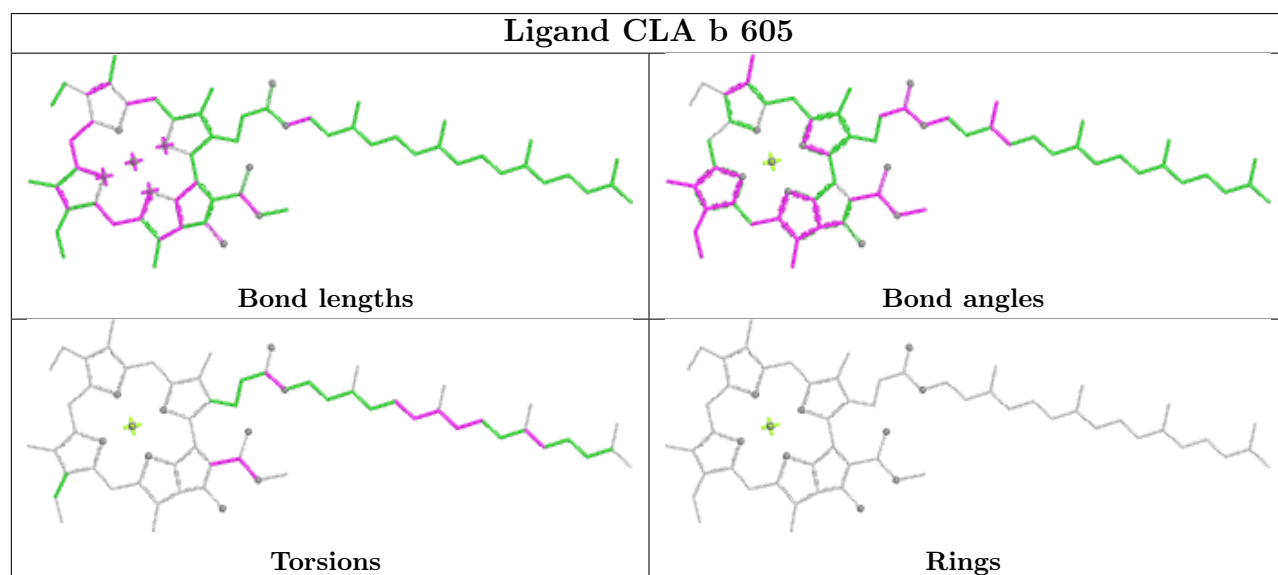
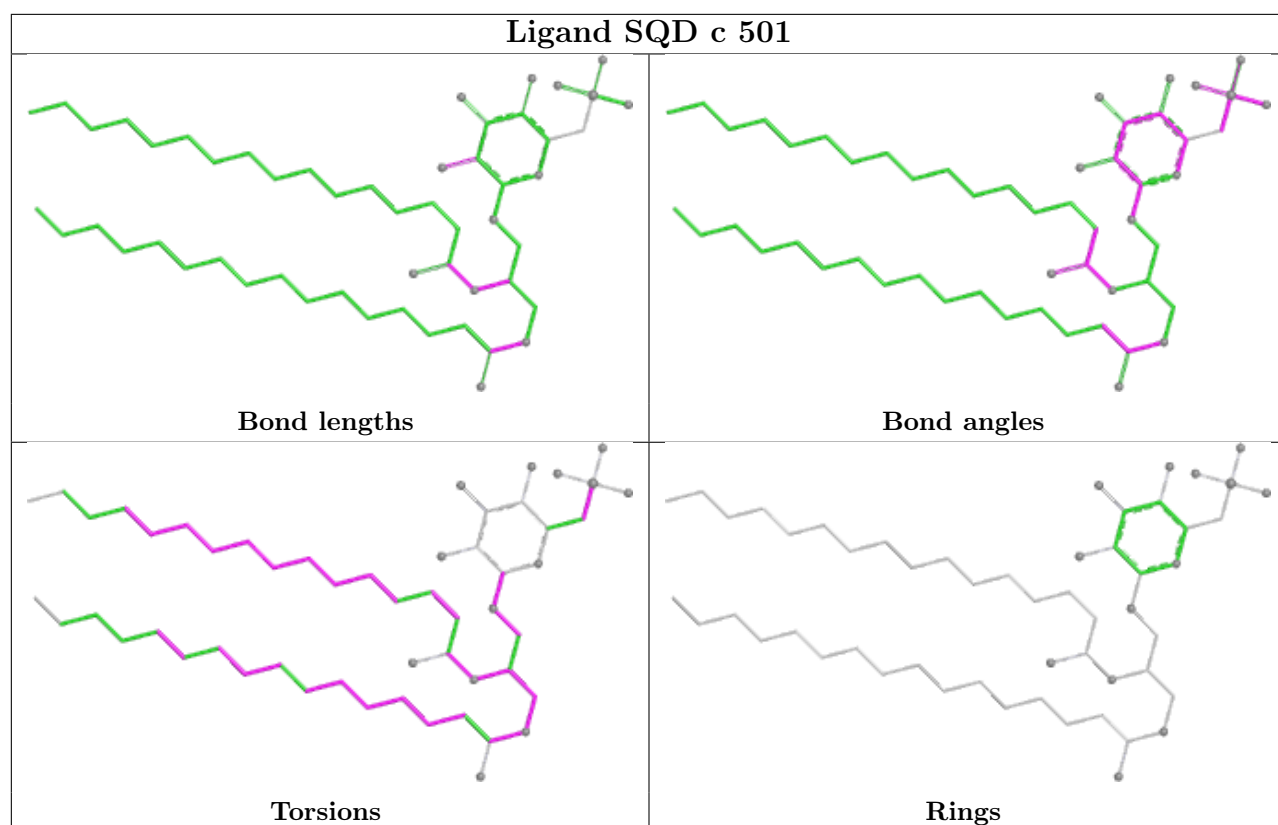


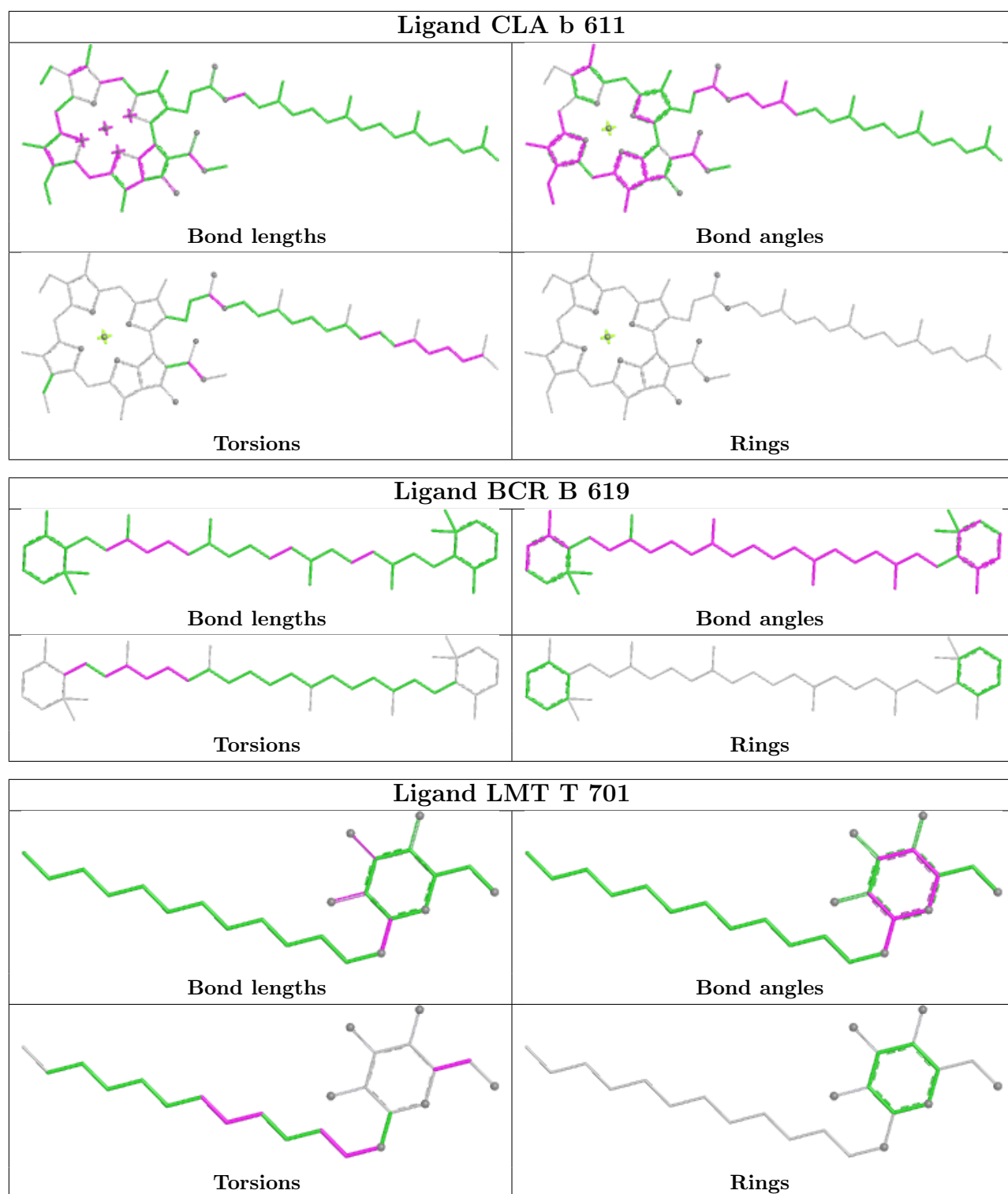


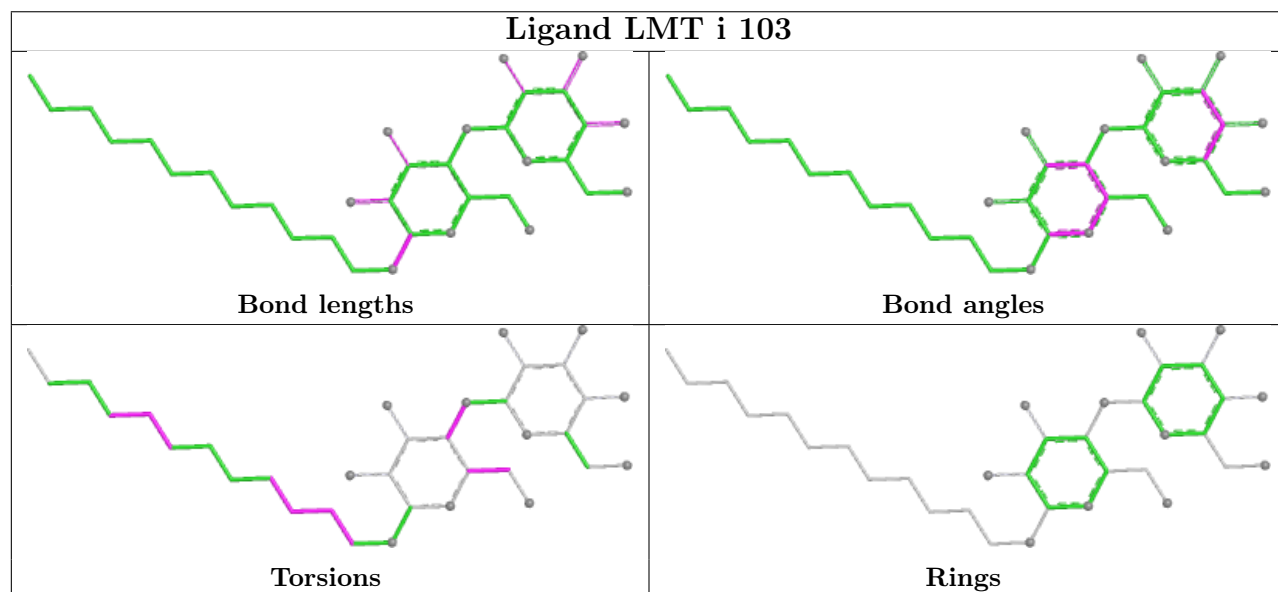
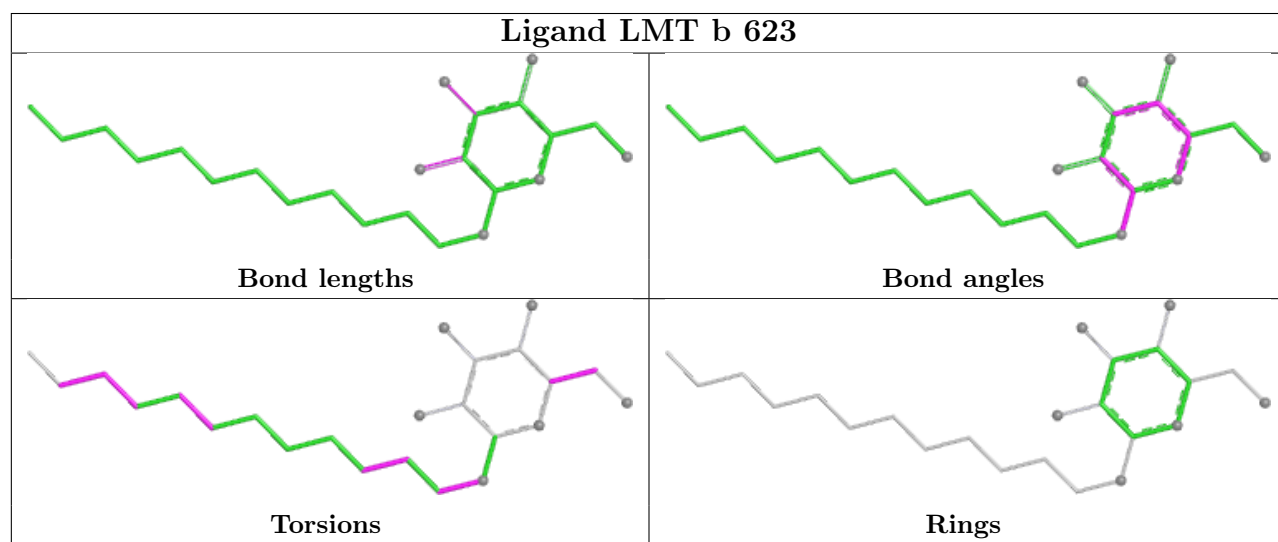
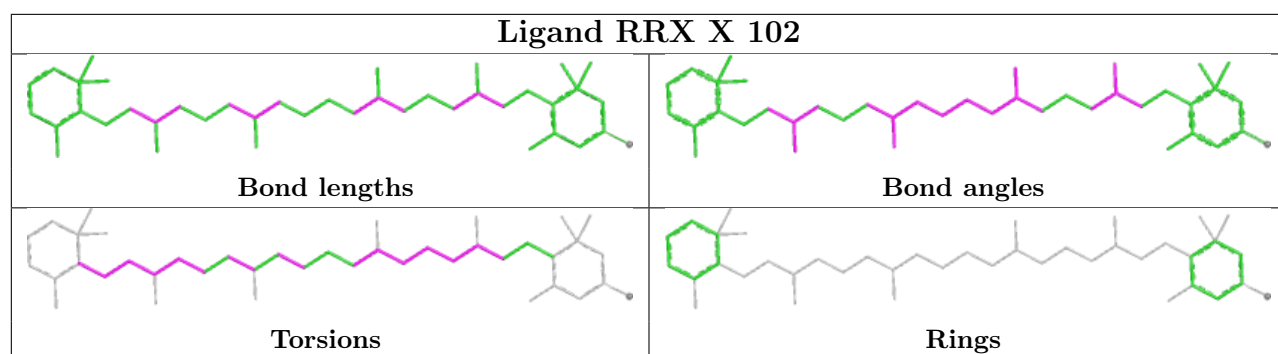


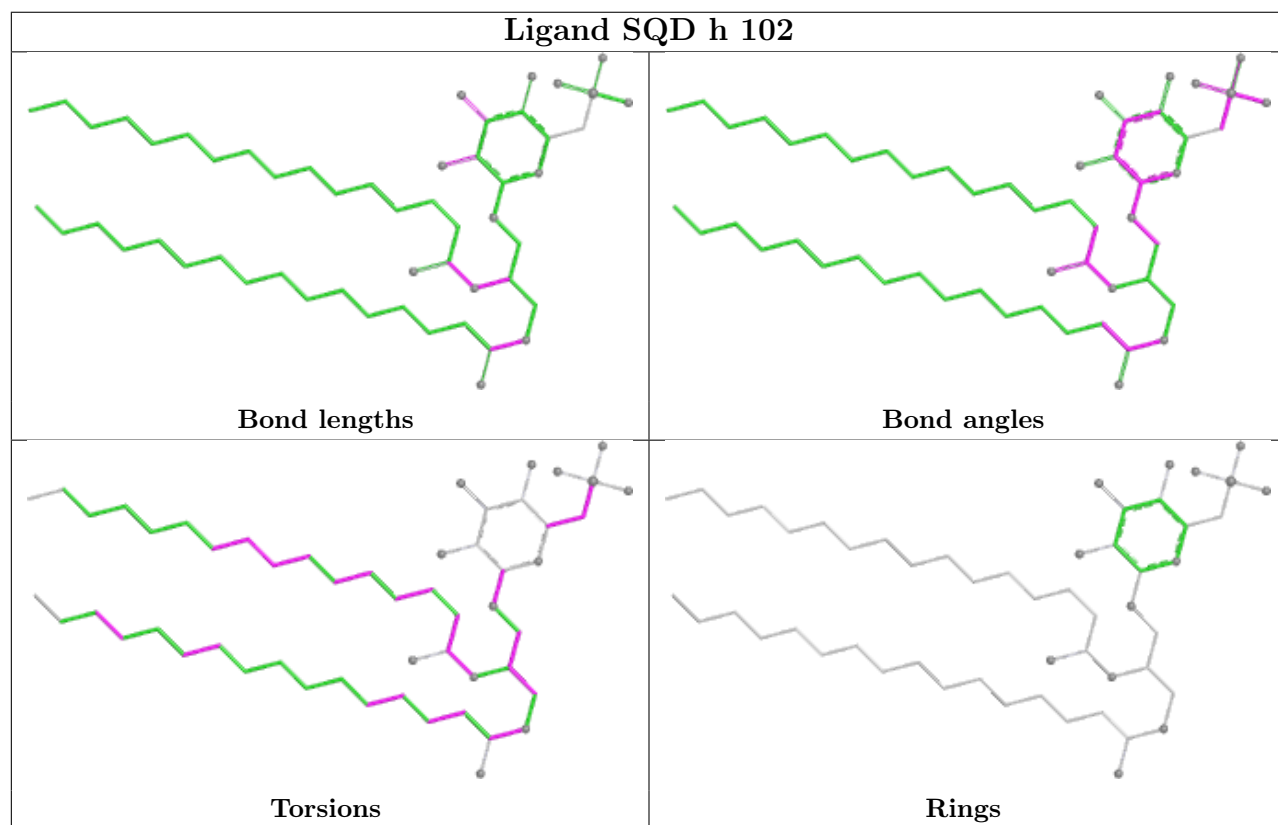
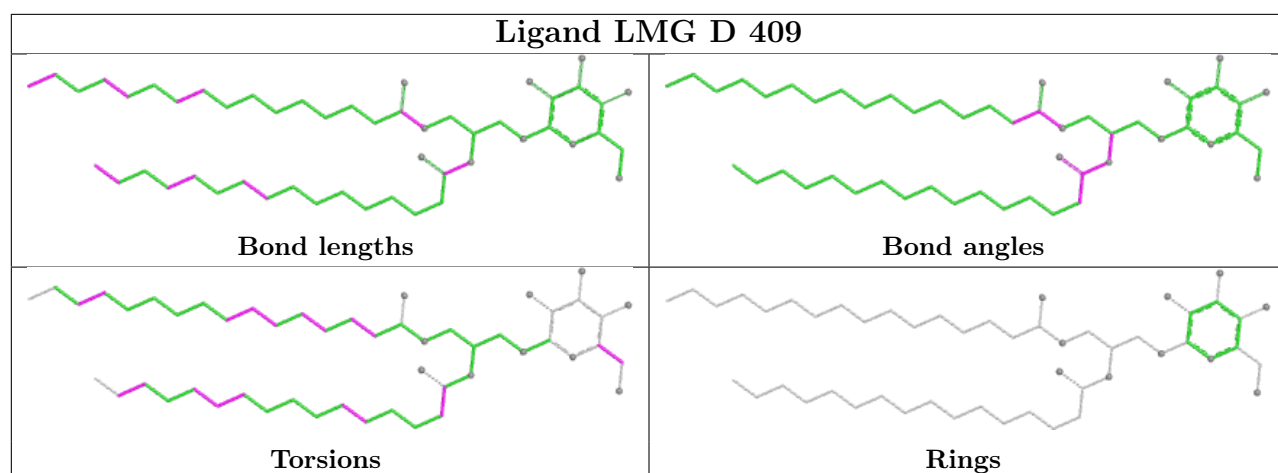


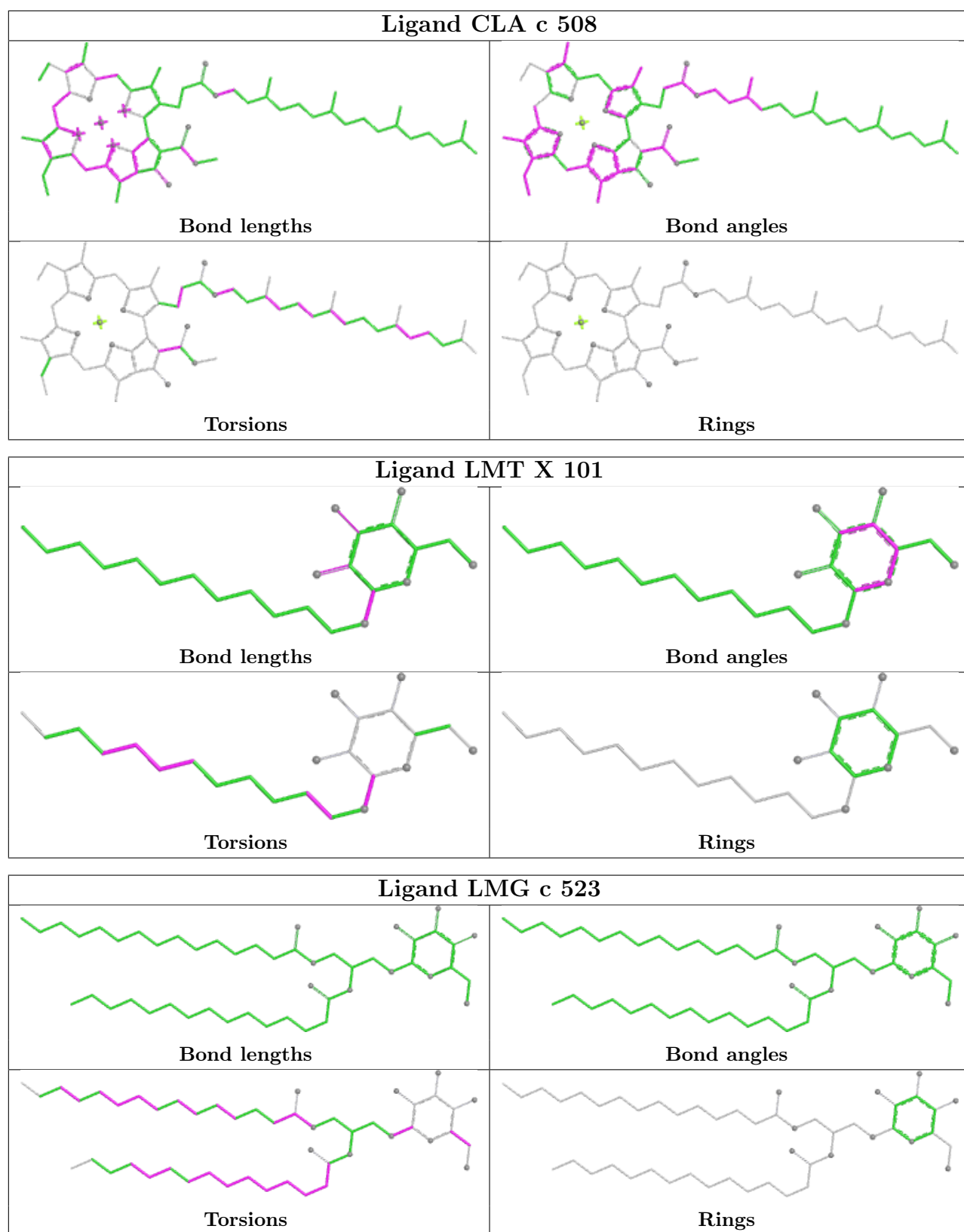


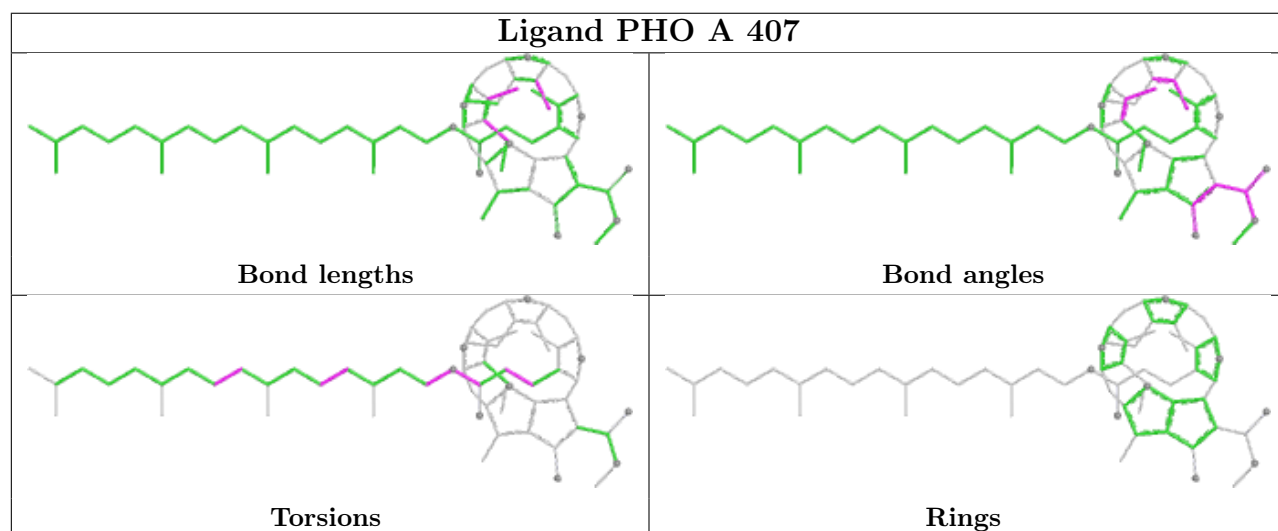
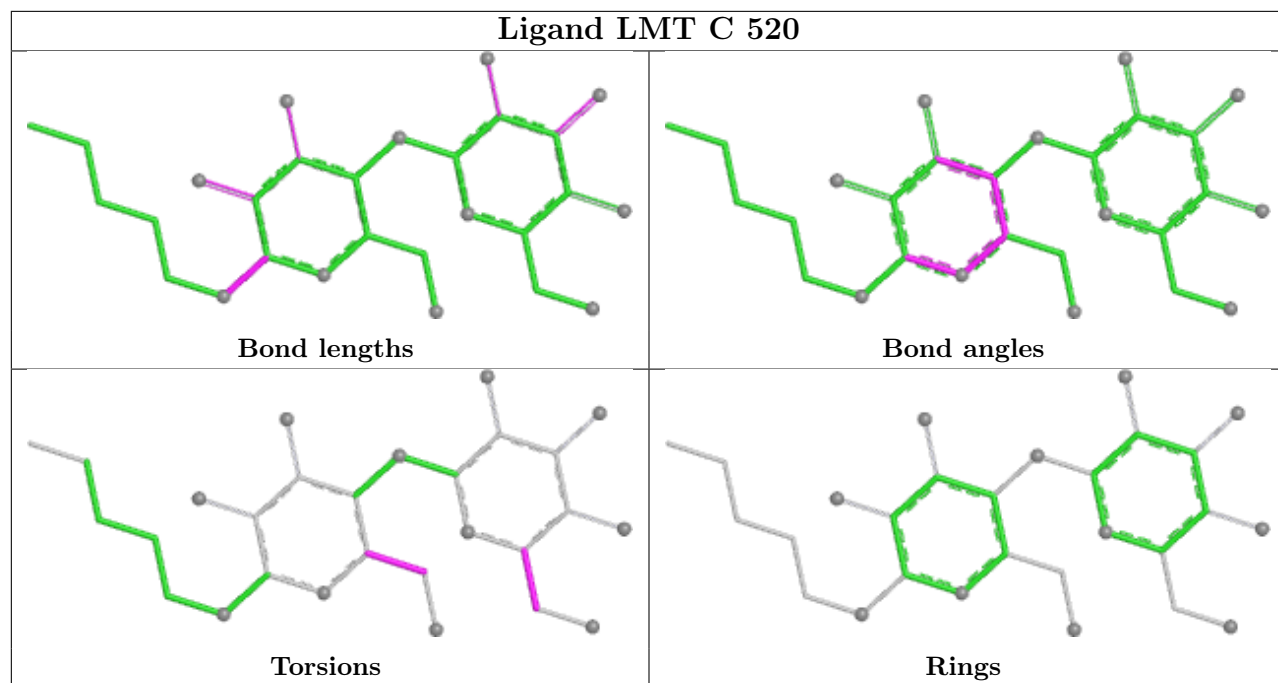


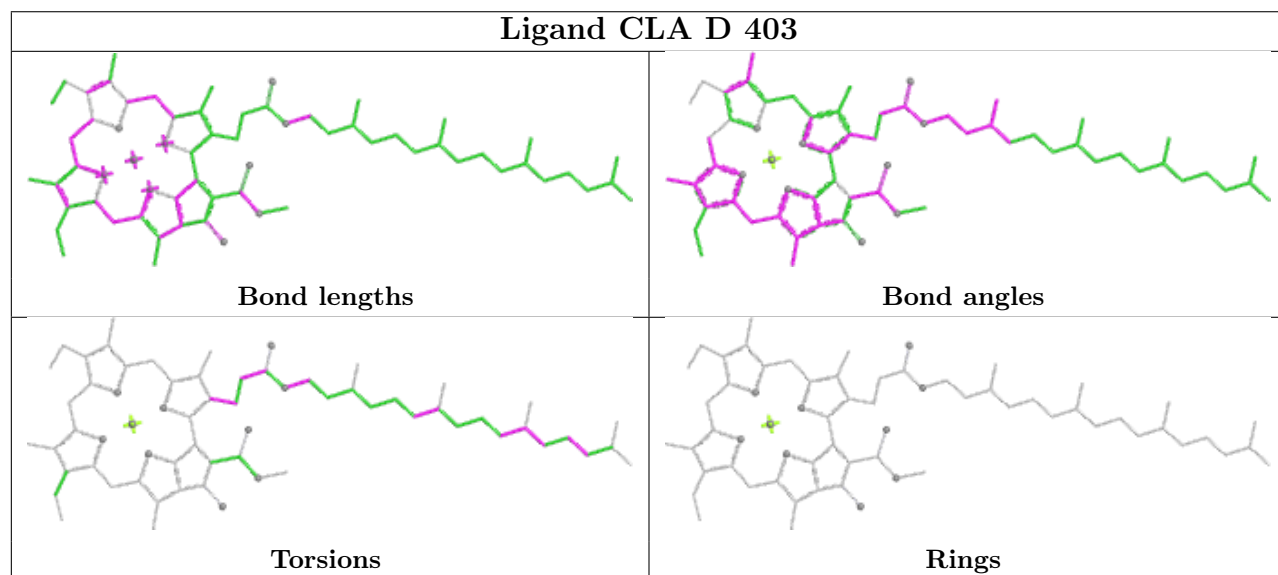
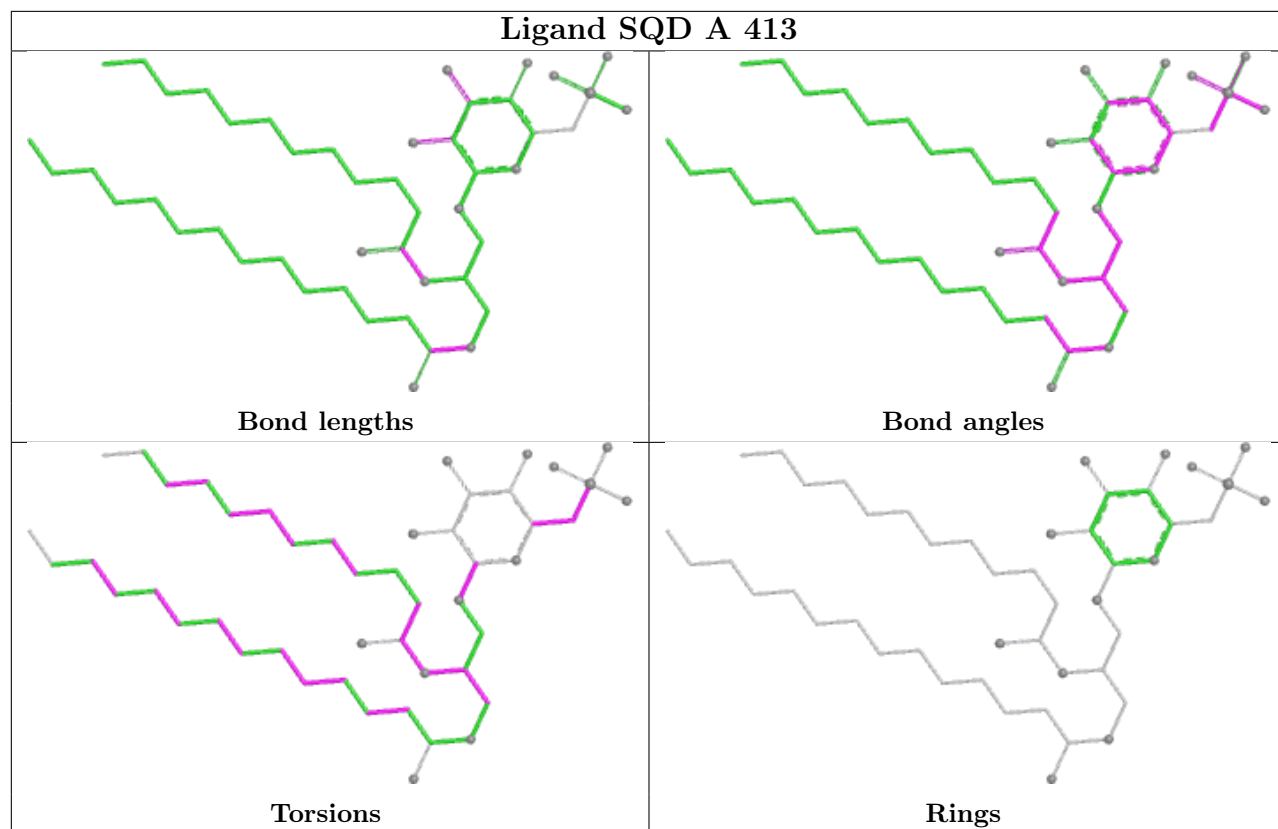


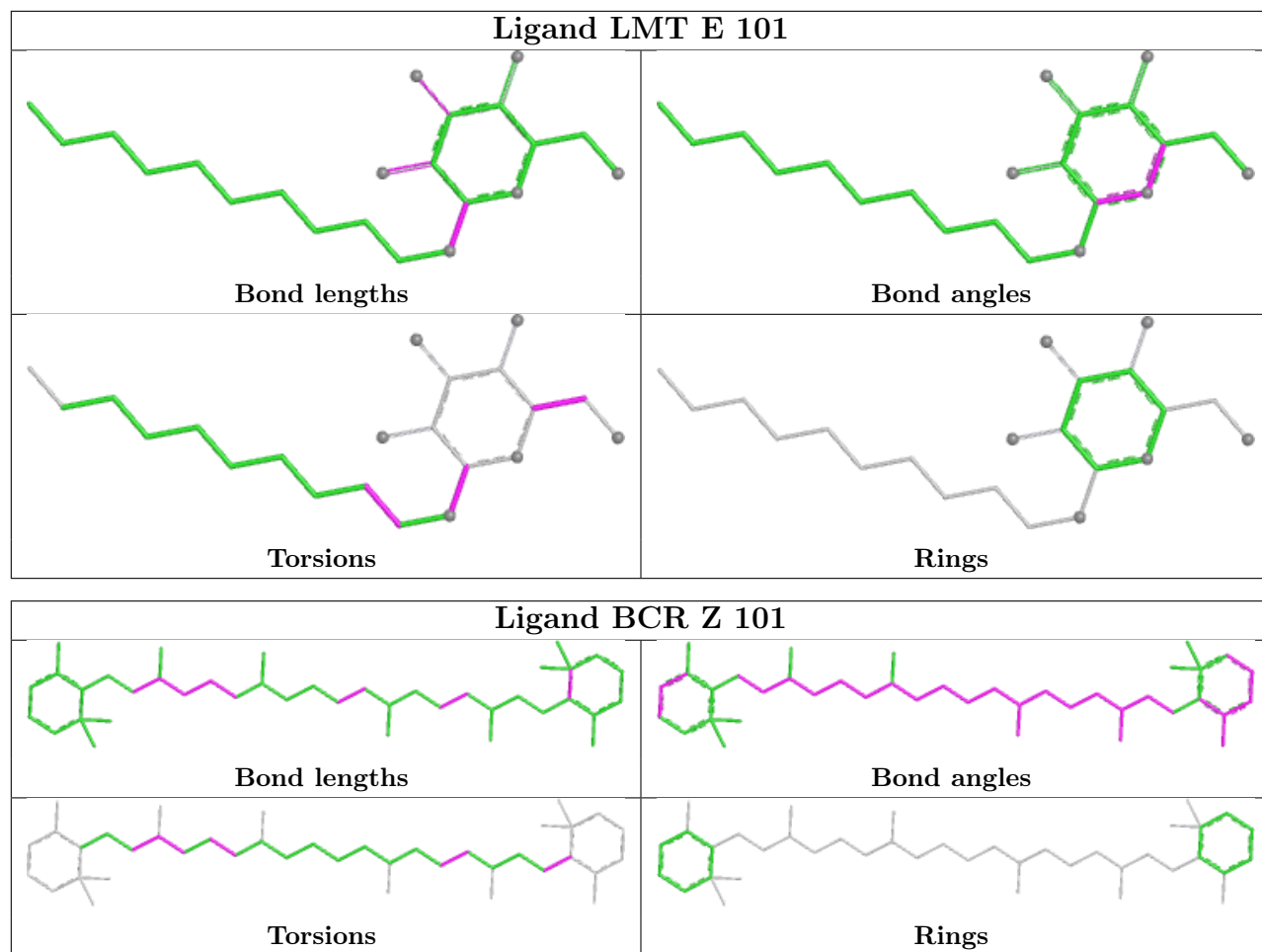




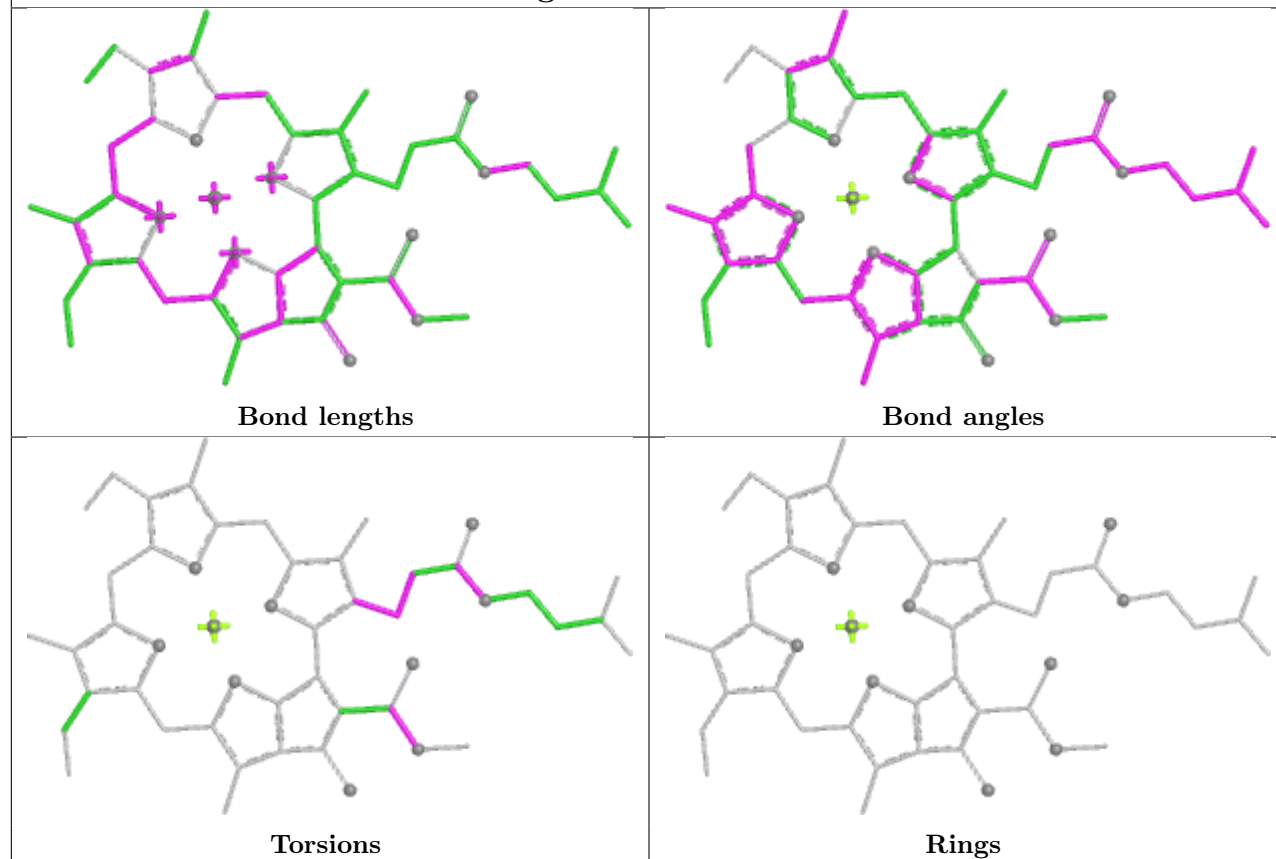




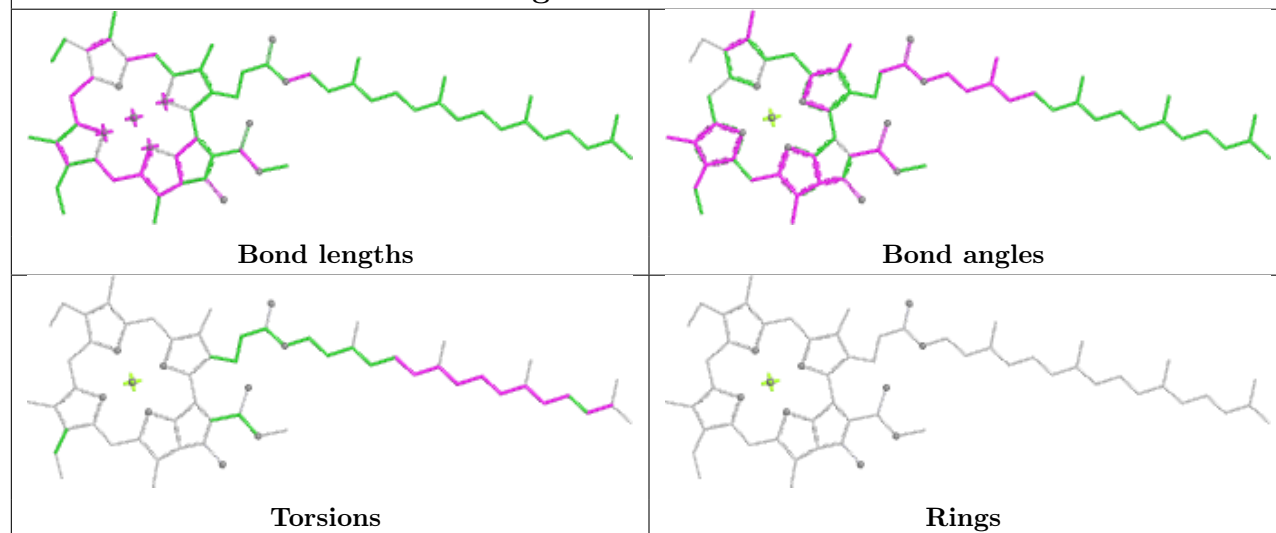


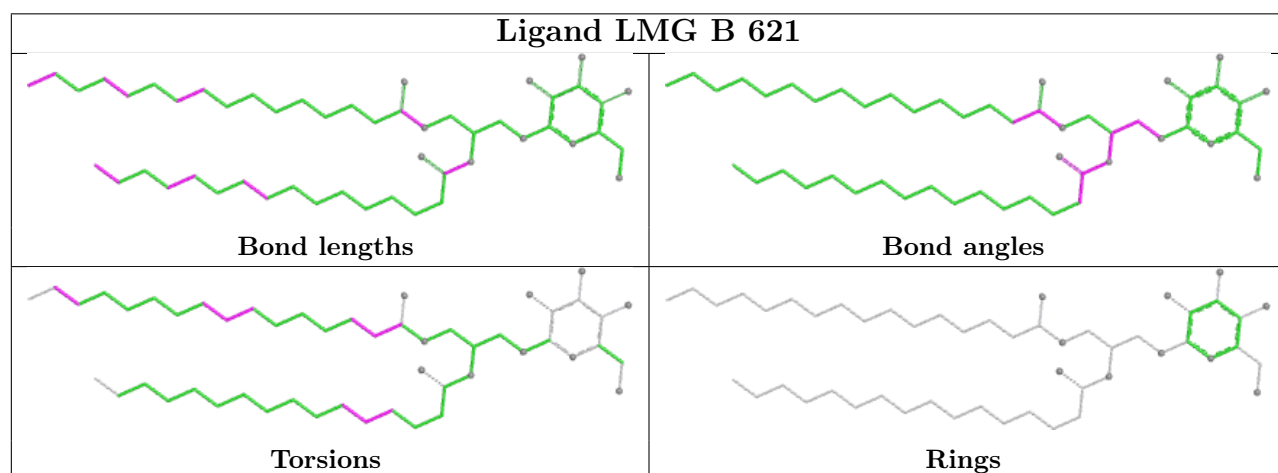
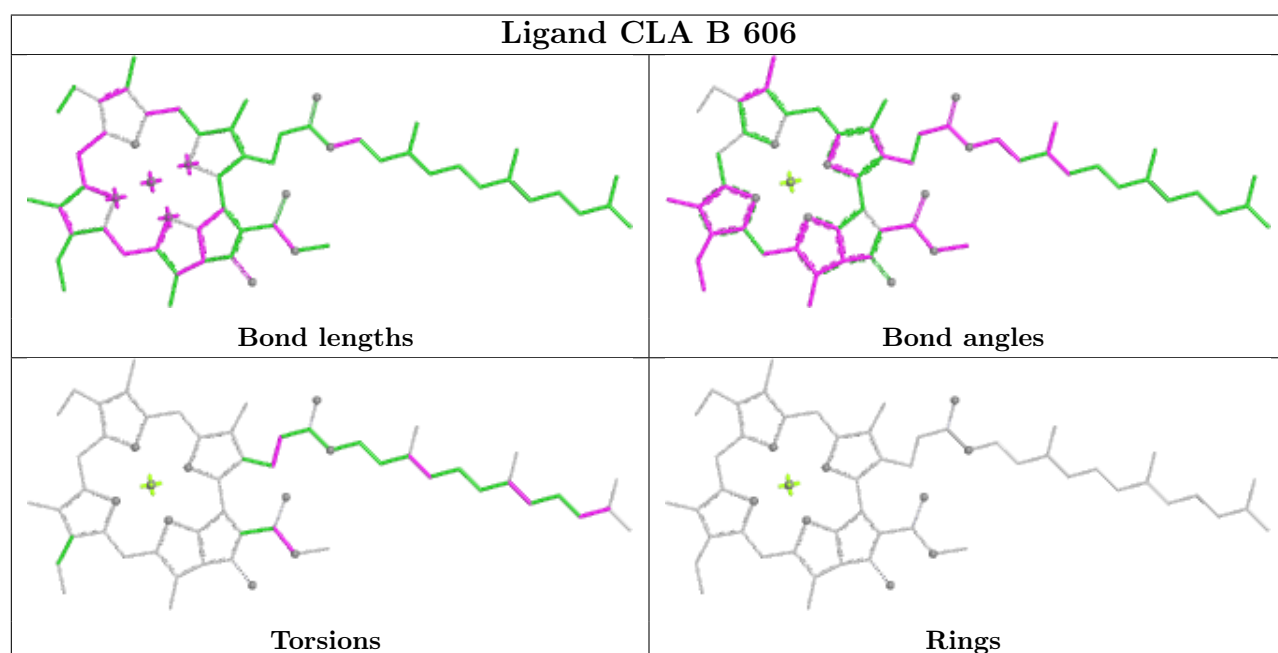
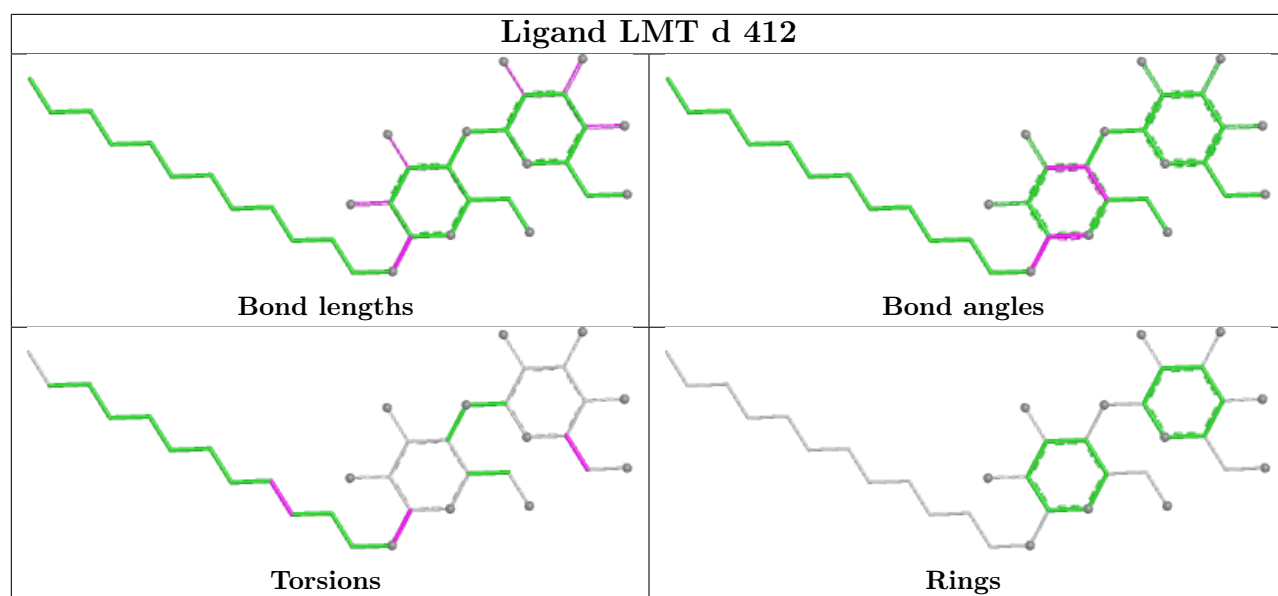


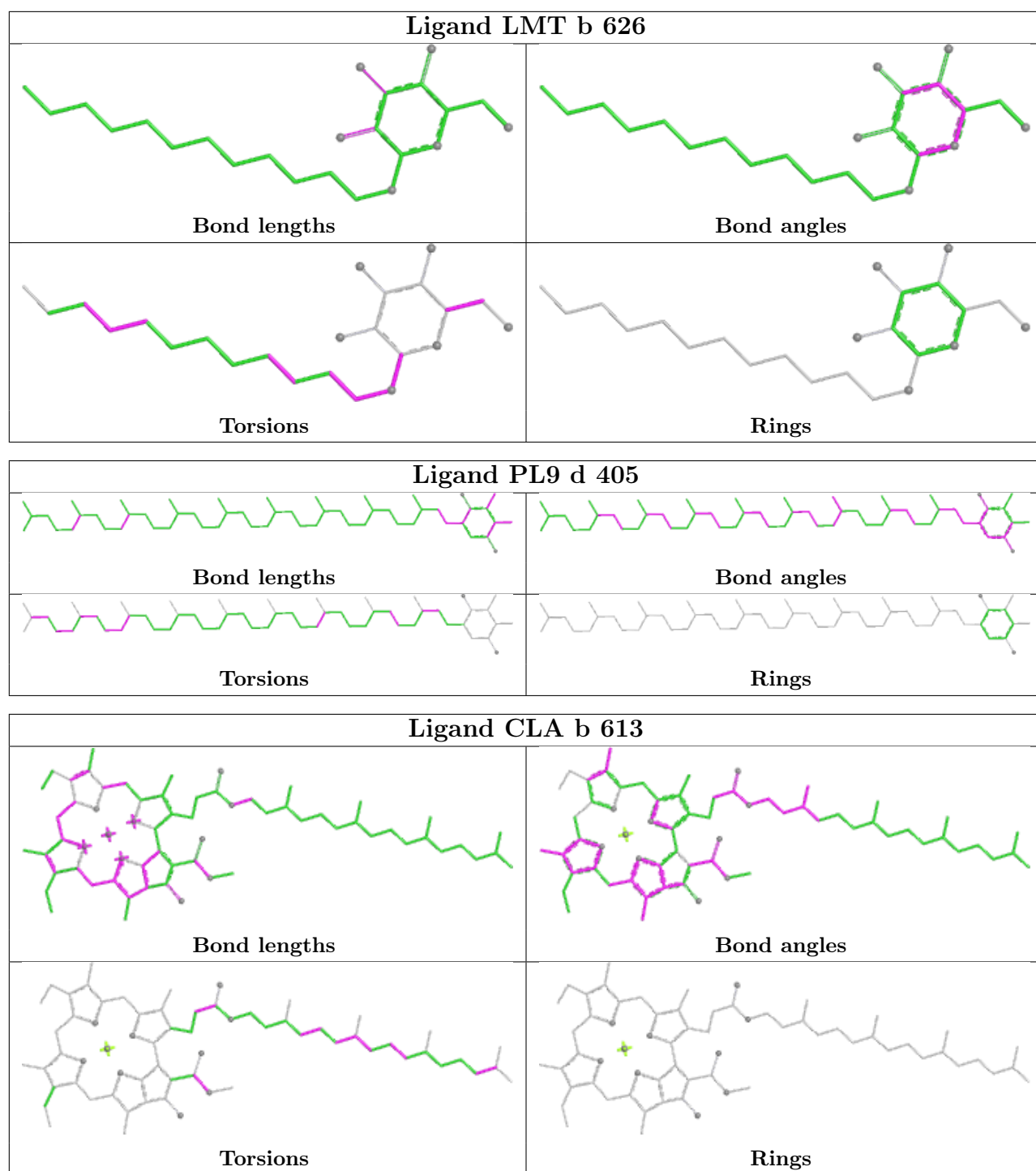
Ligand CLA c 513

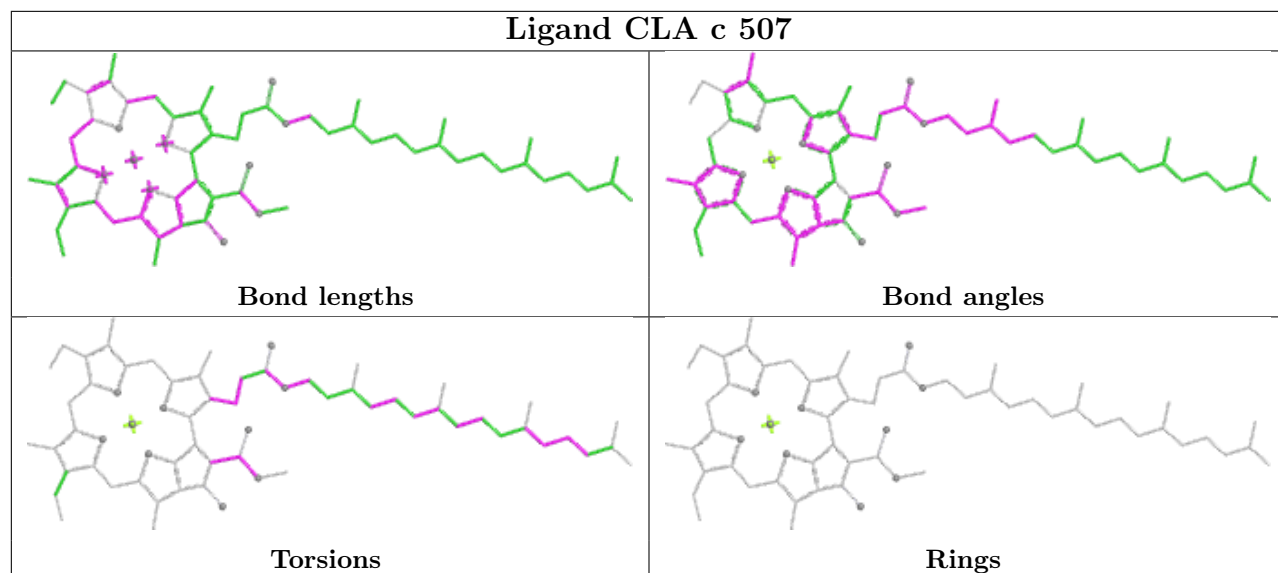
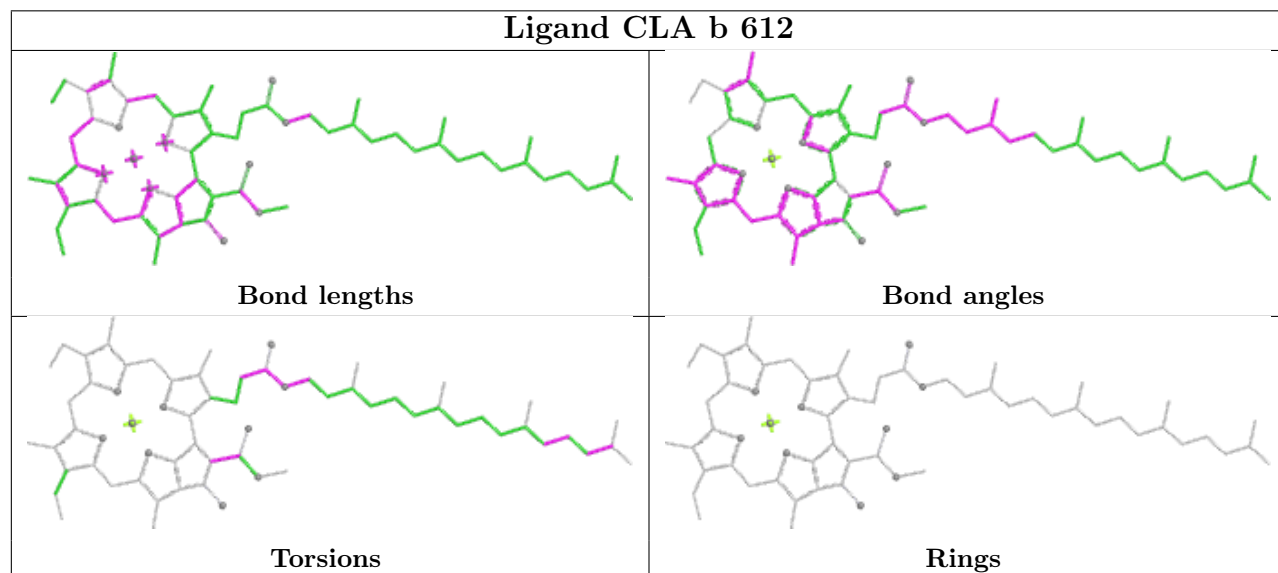
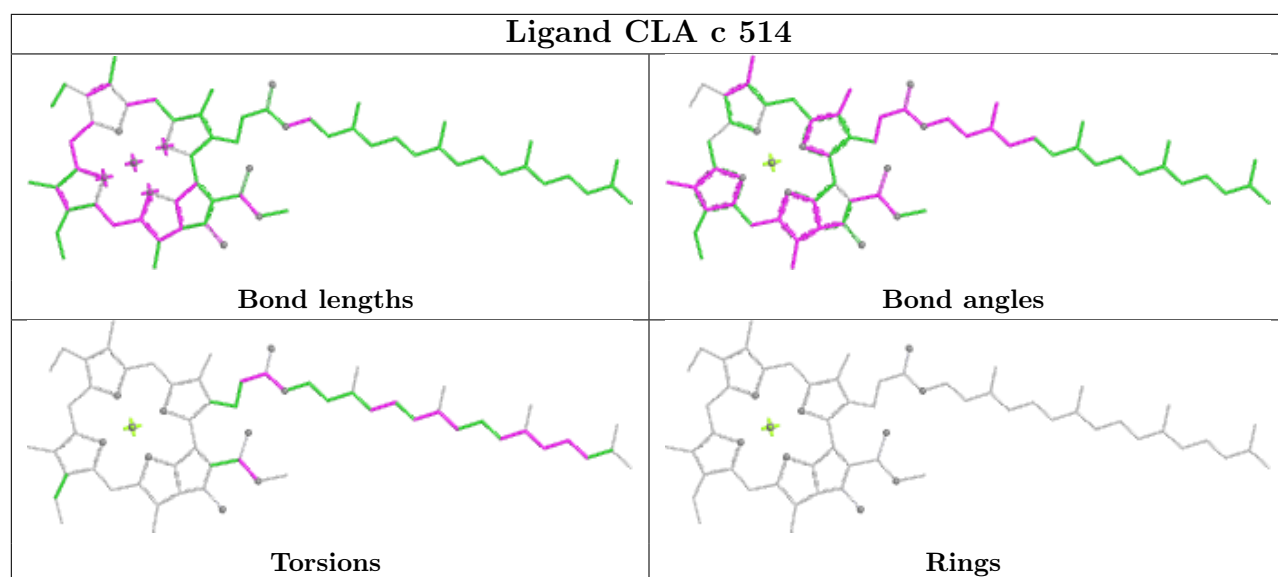


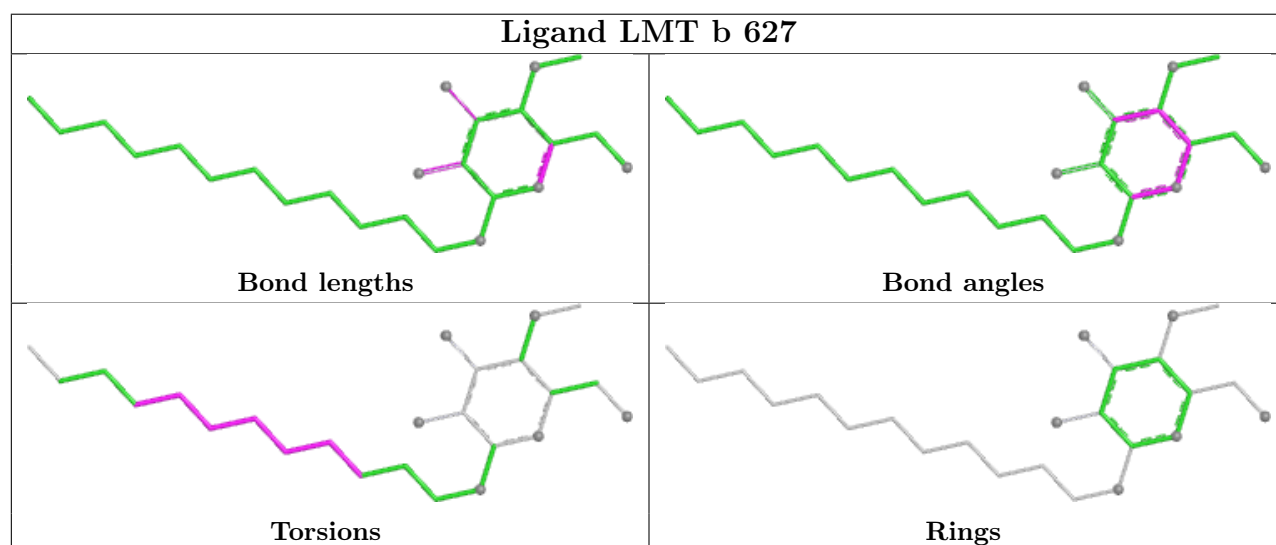
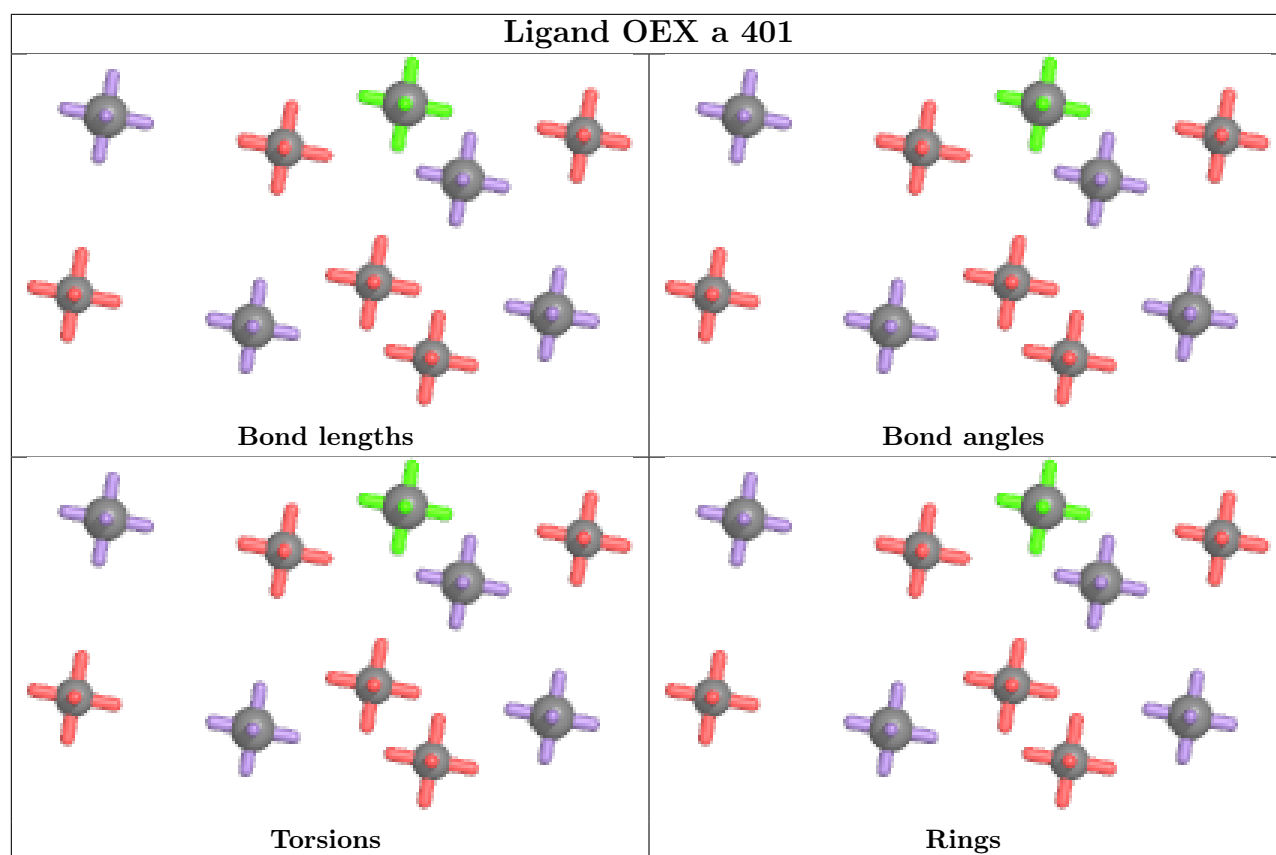
Ligand CLA B 615

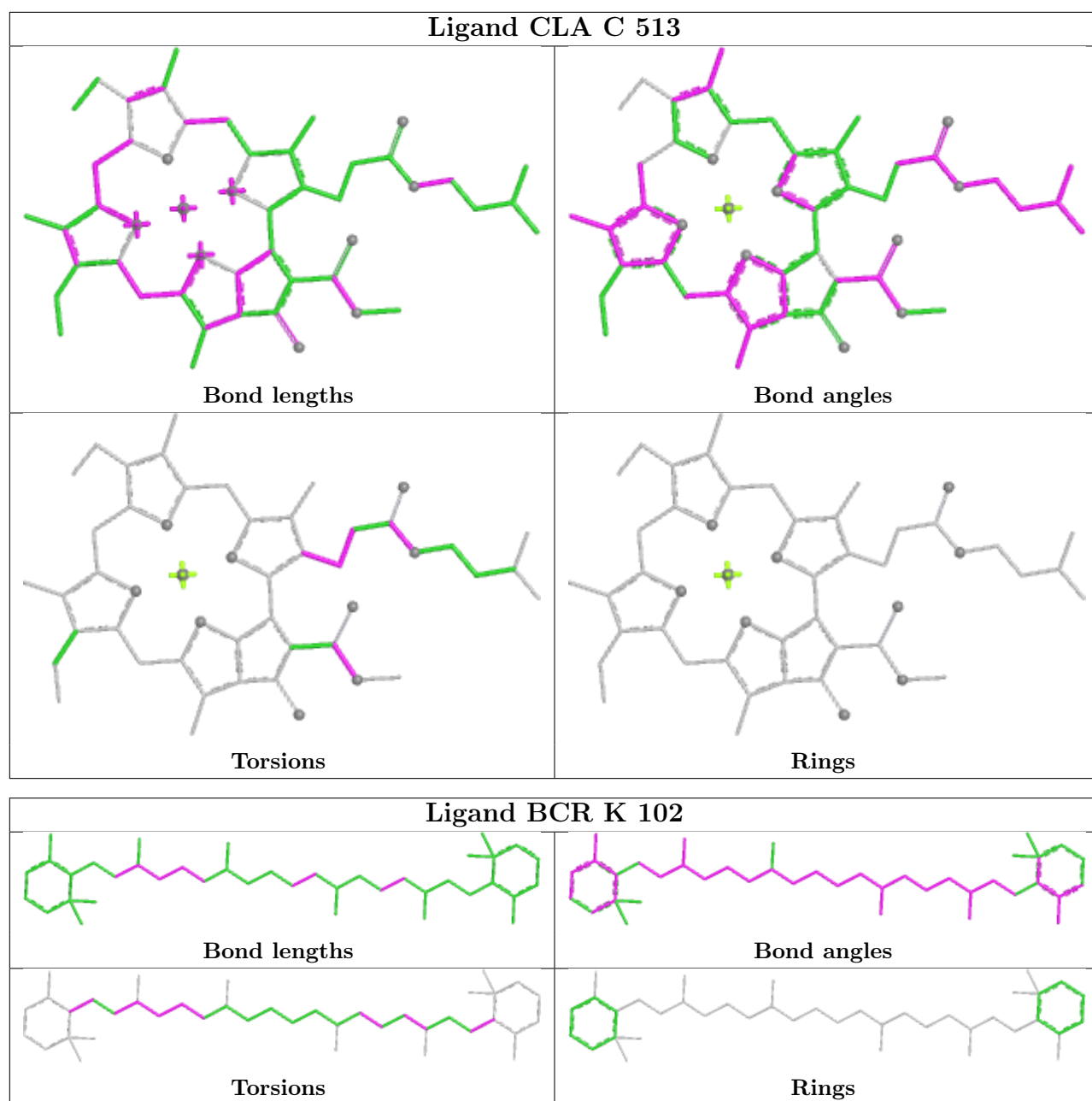


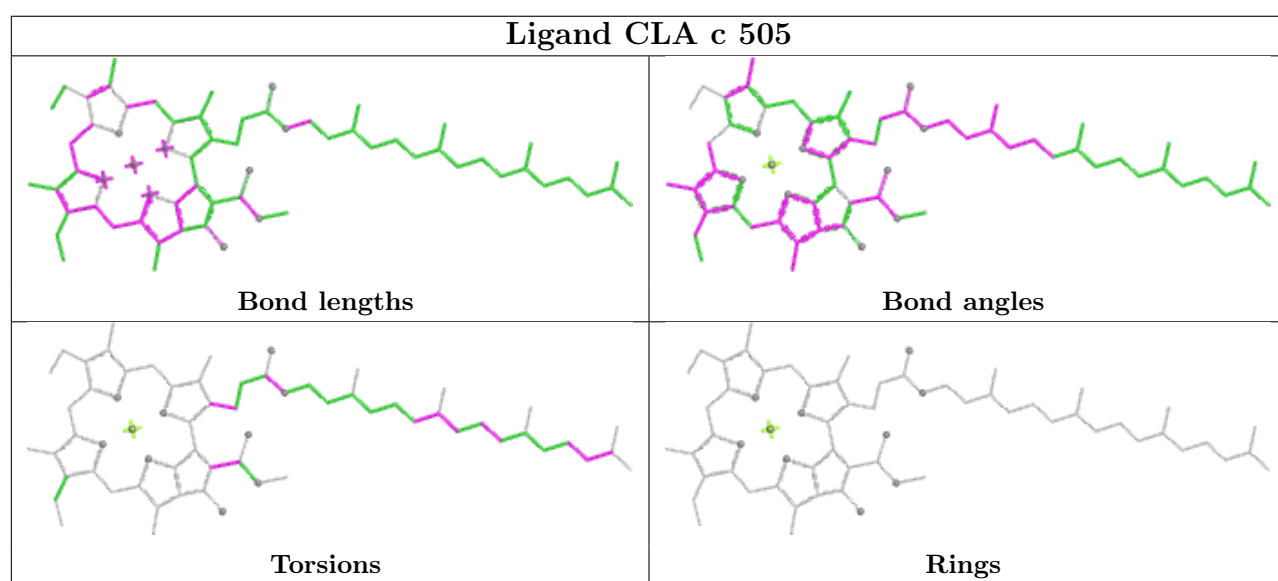
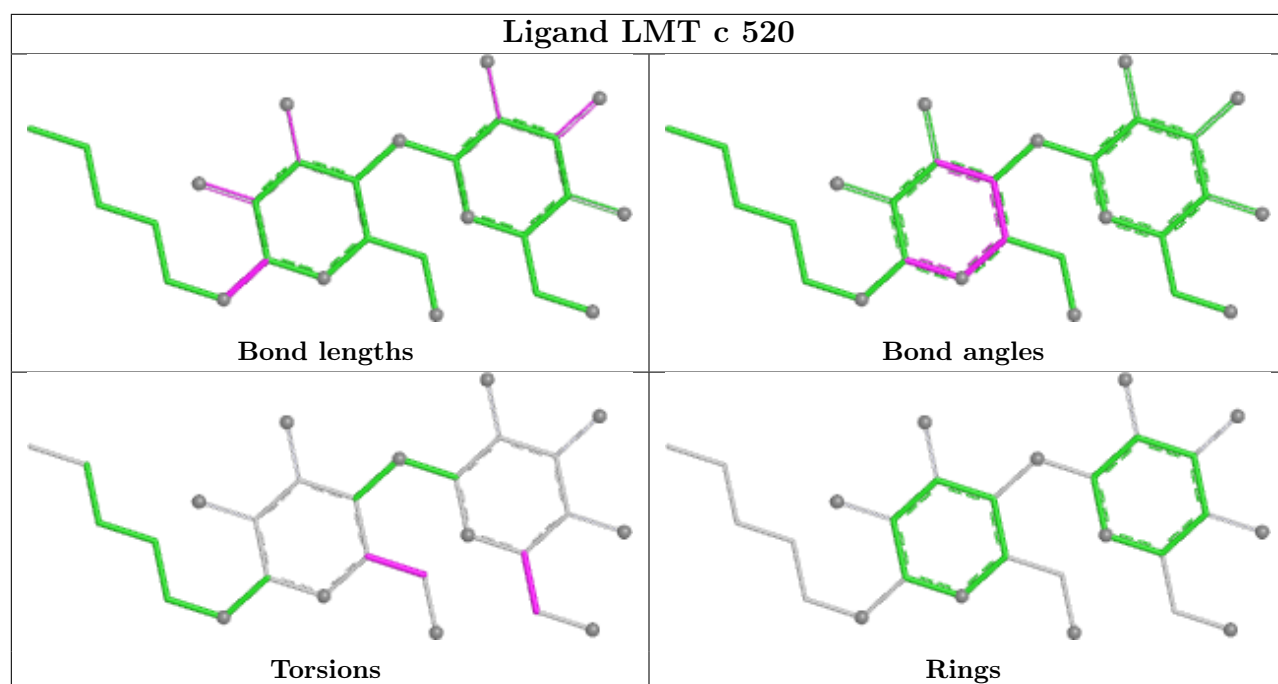


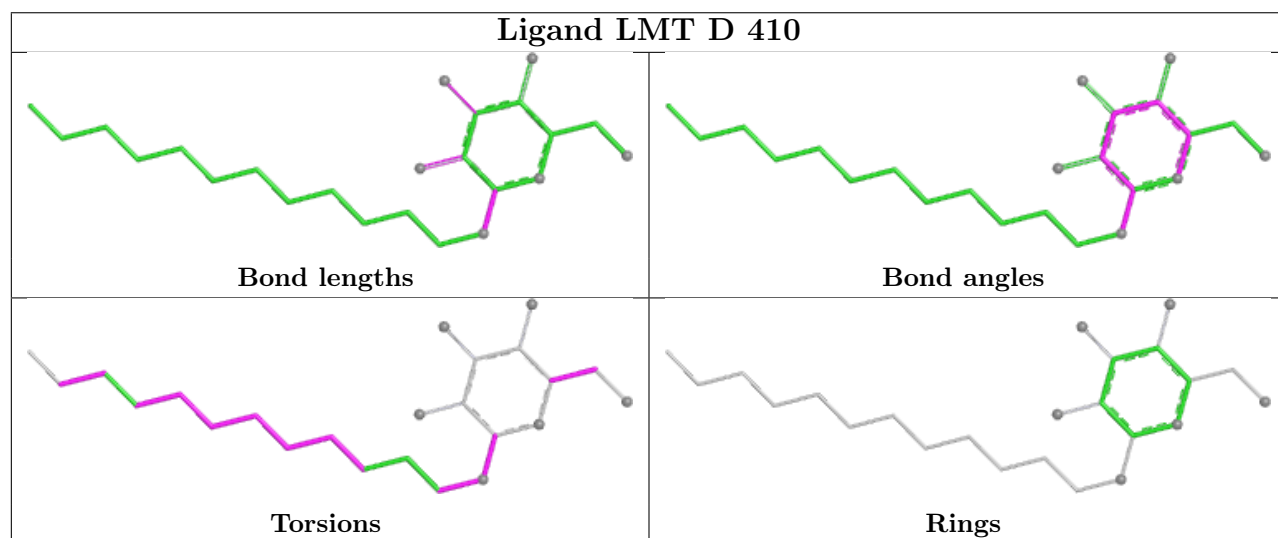
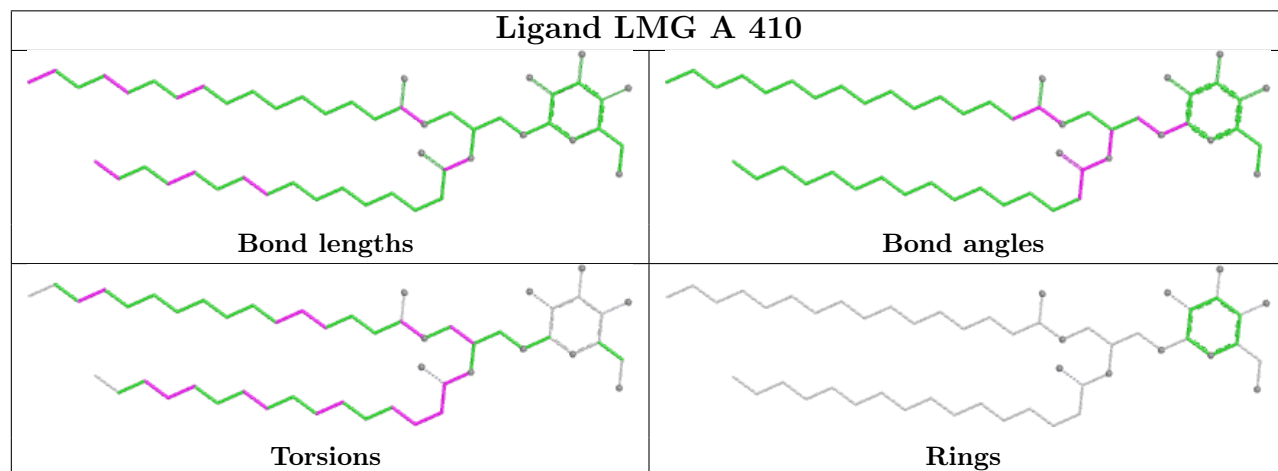
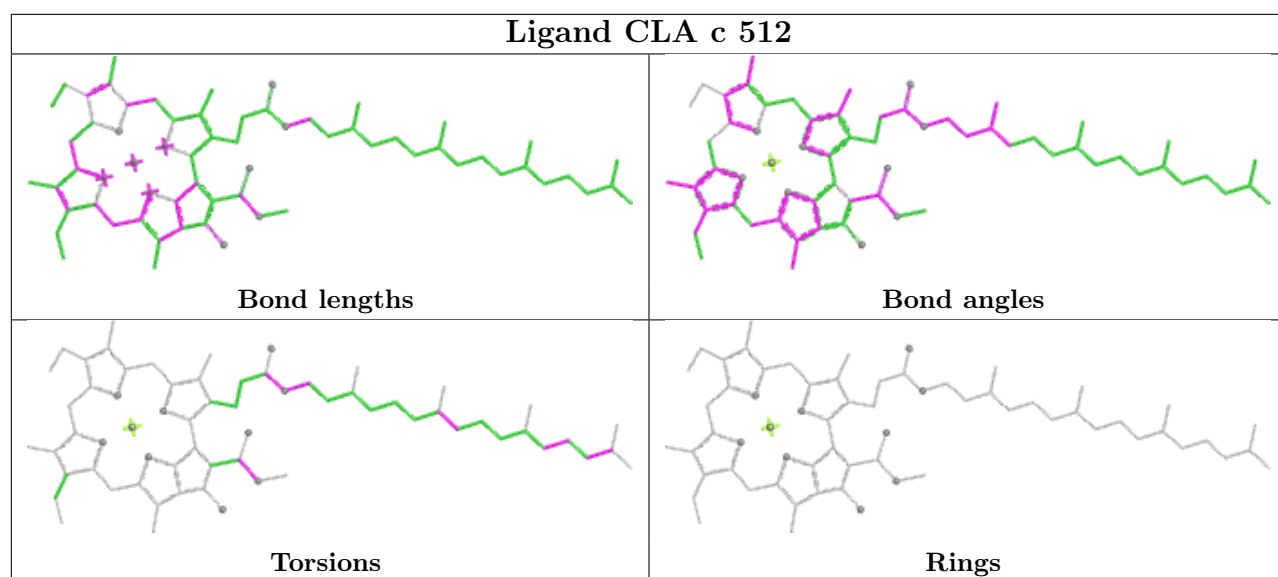


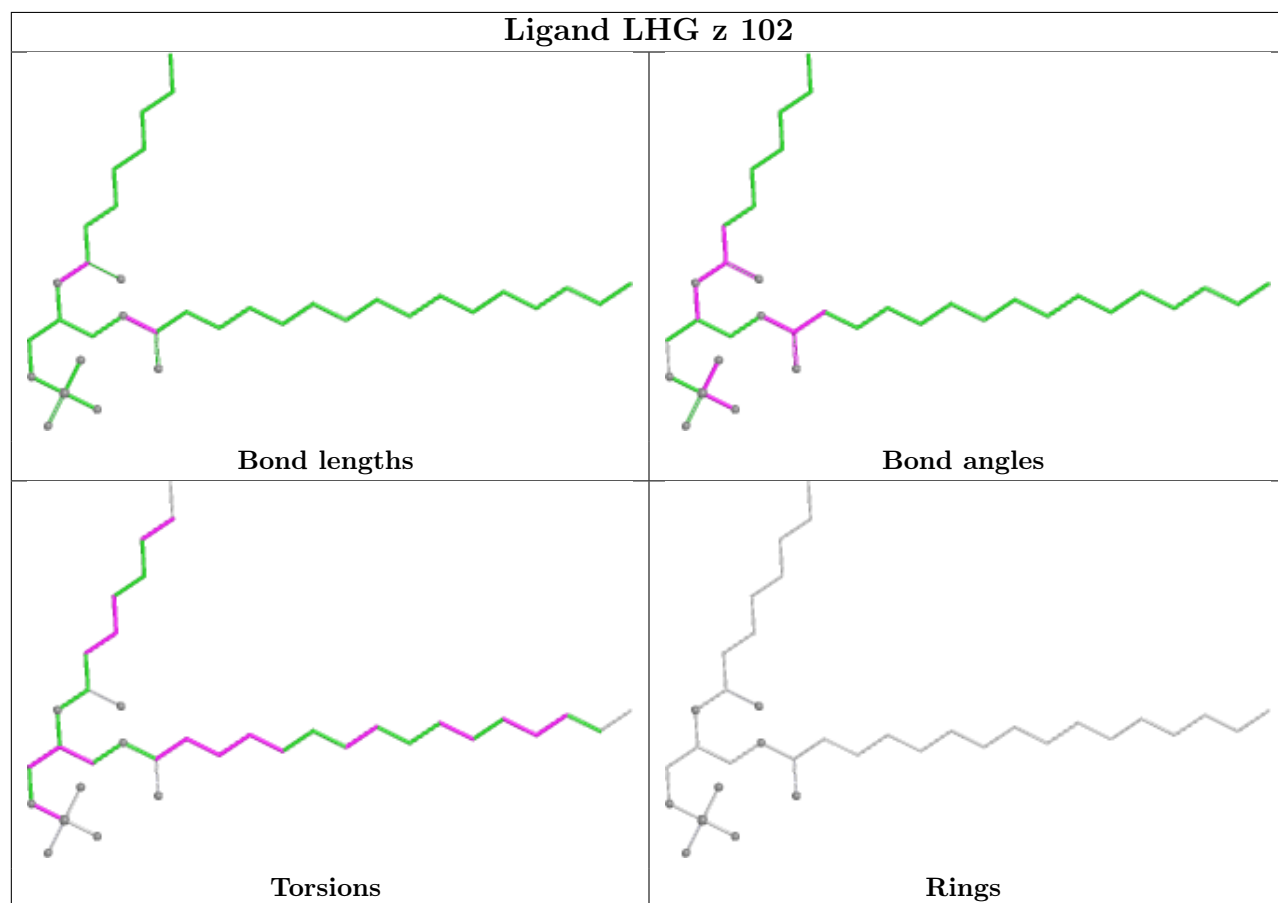
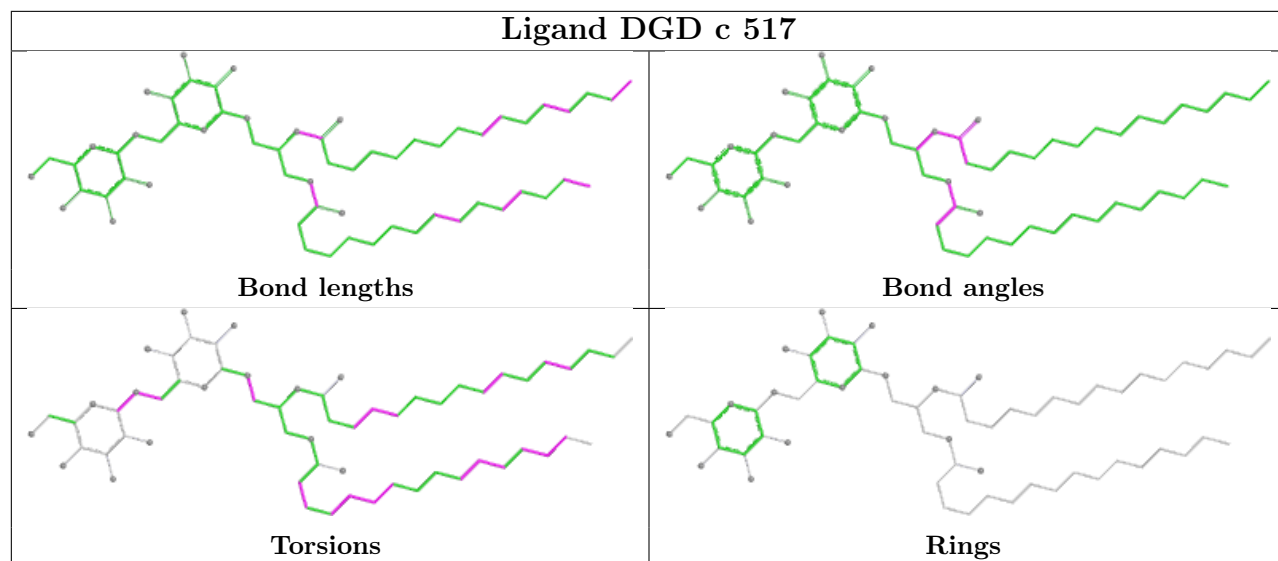


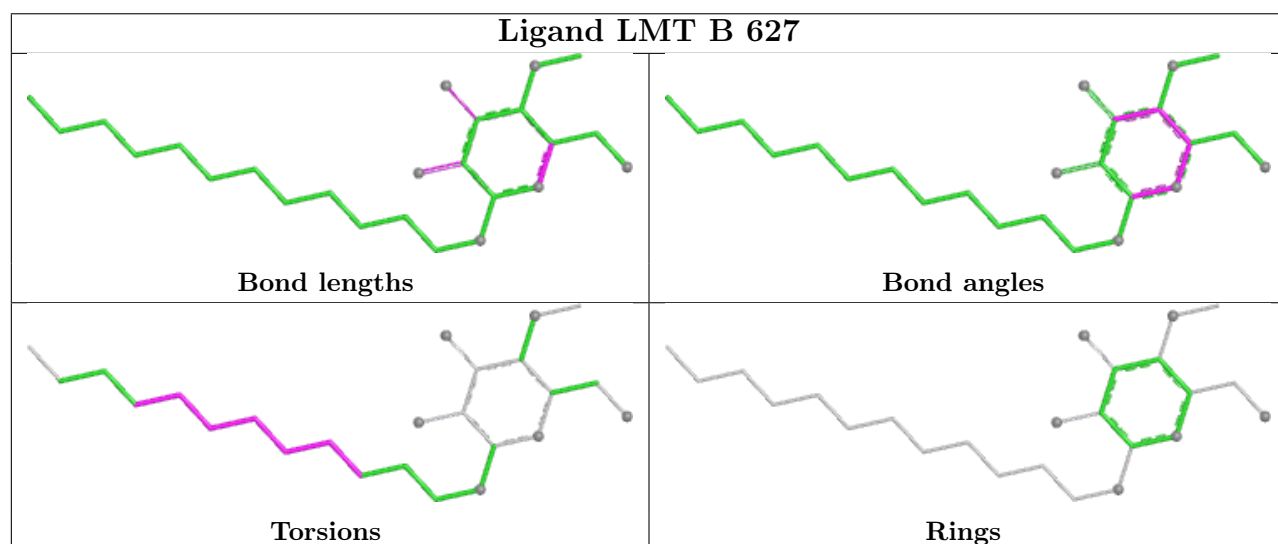
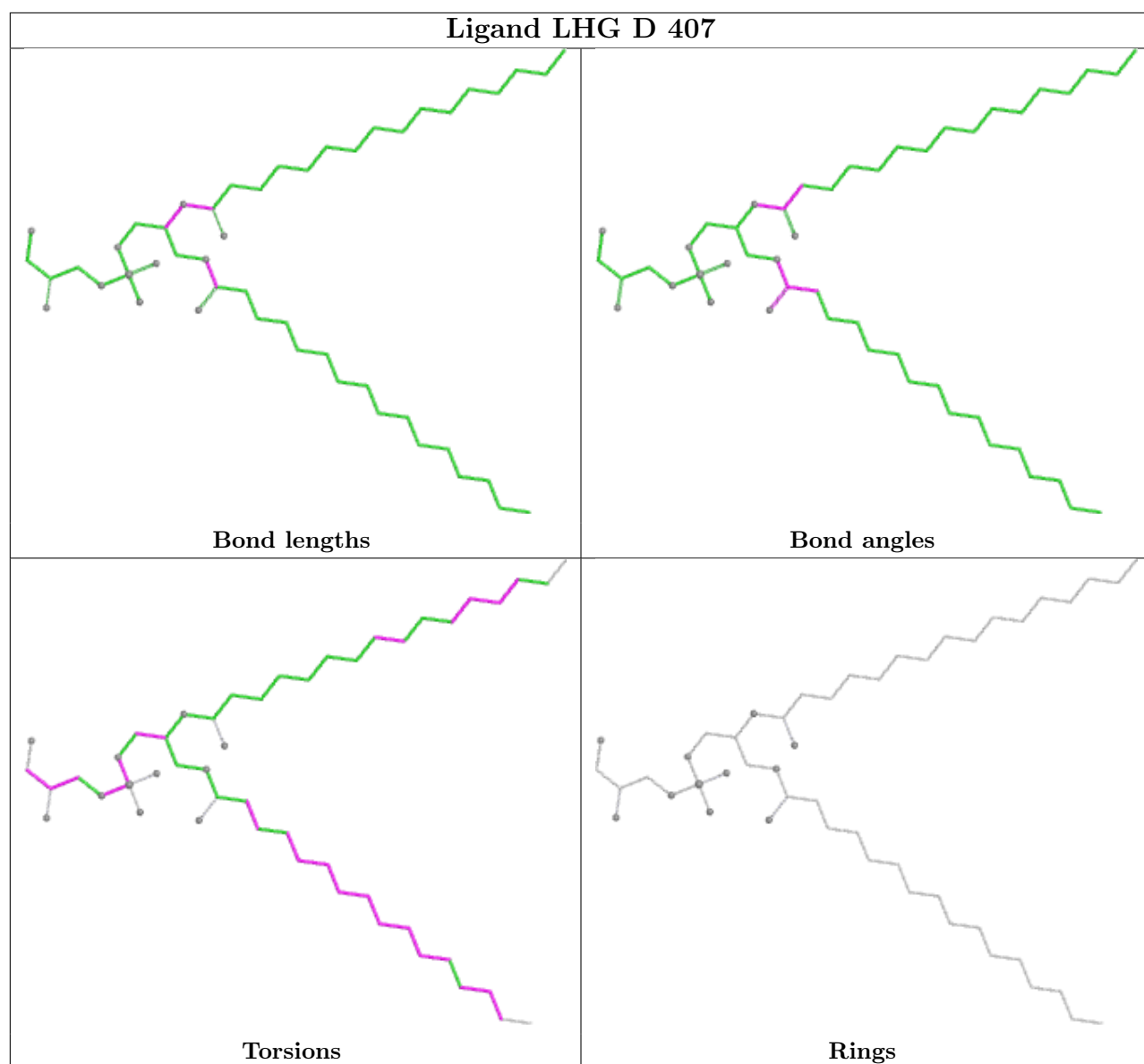


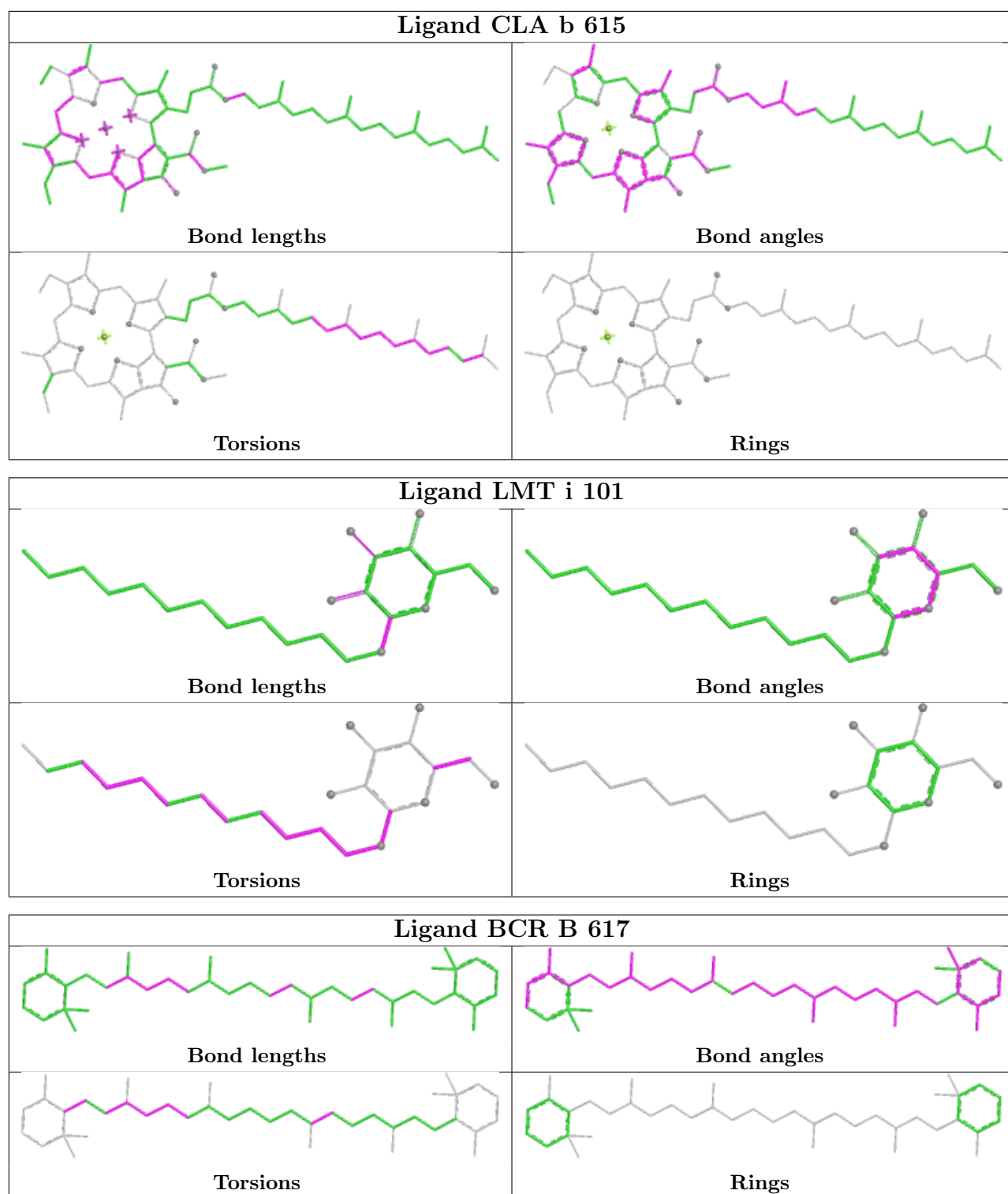


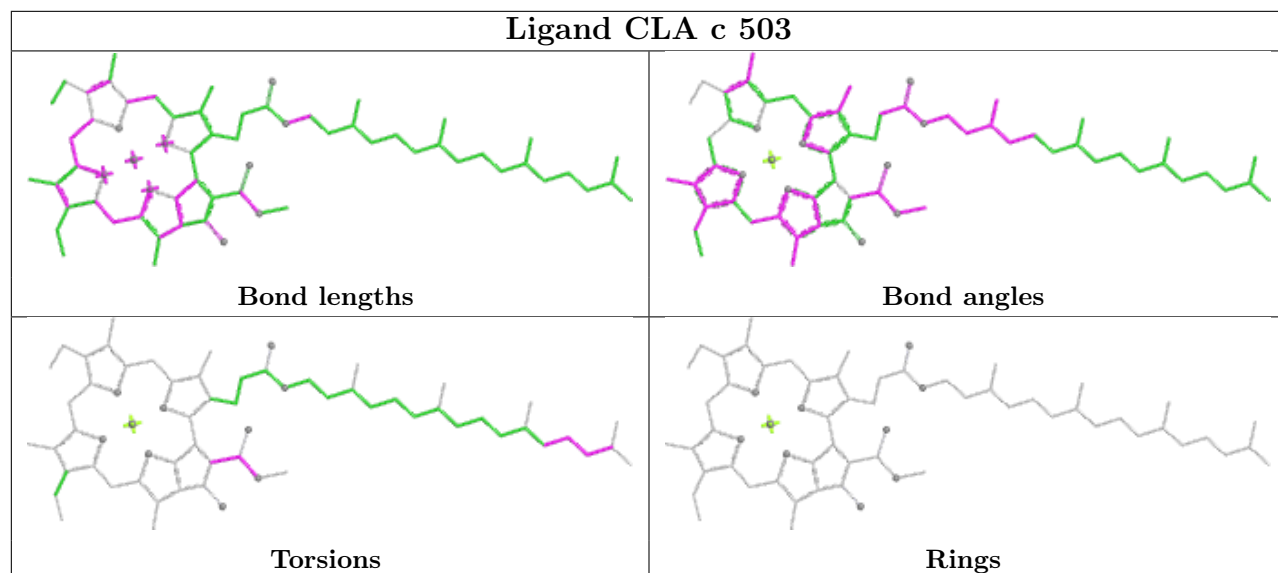
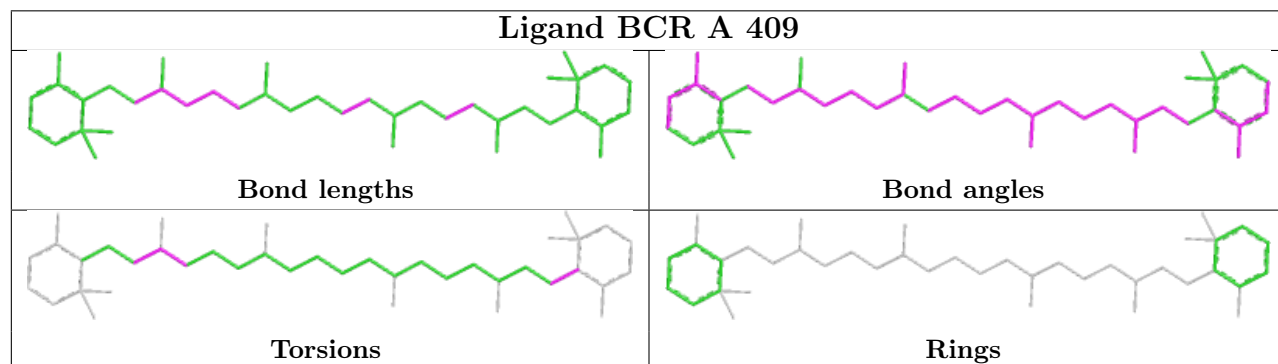
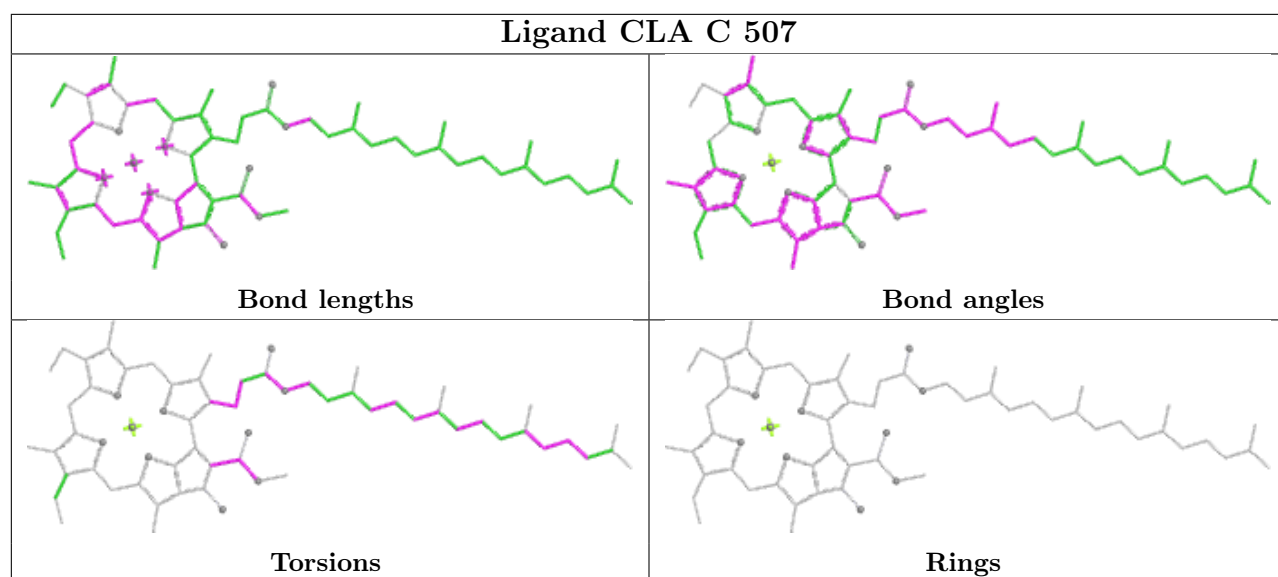


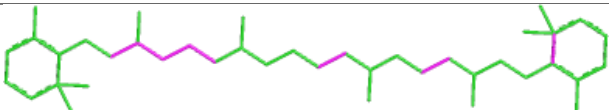
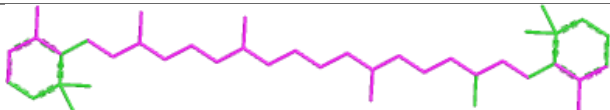
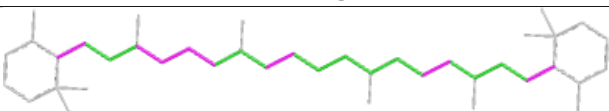
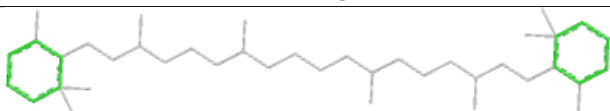




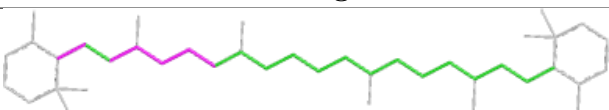
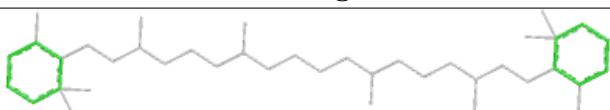



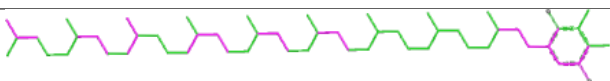
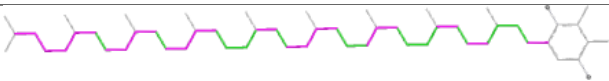
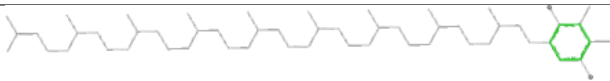




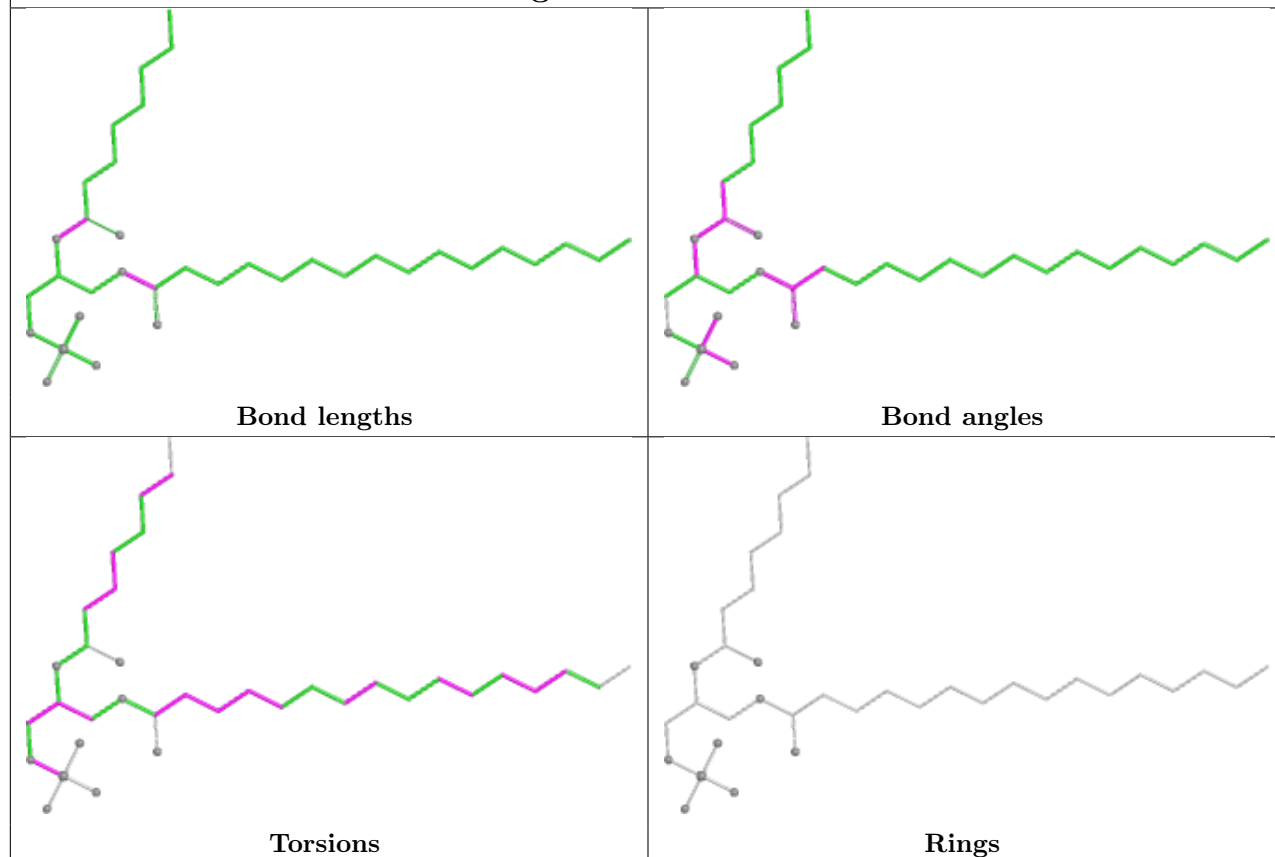


Ligand BCR F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

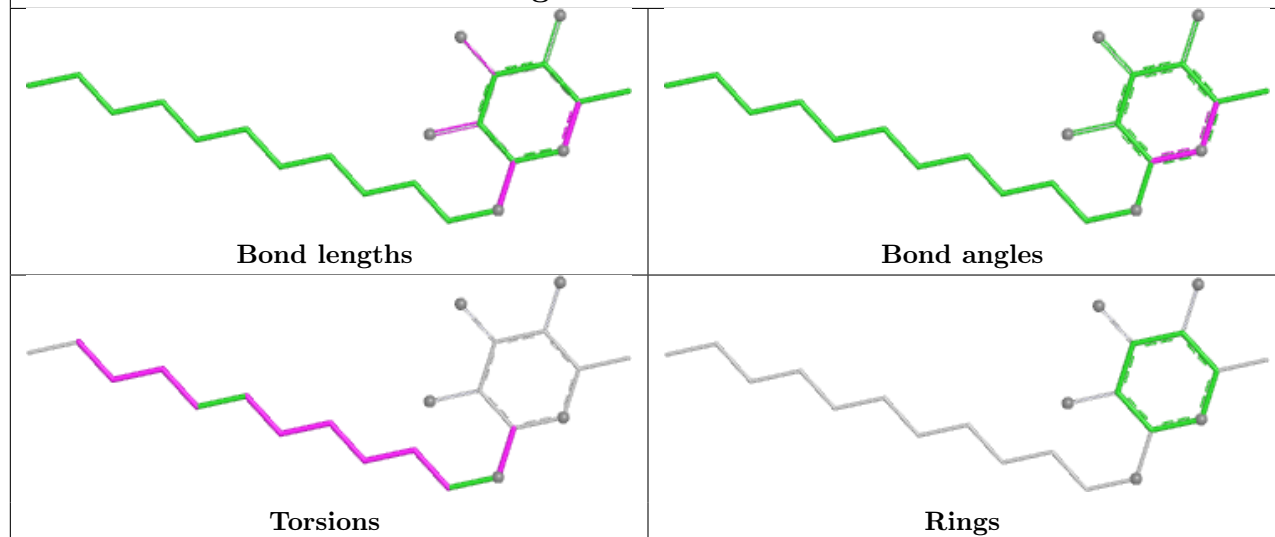
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

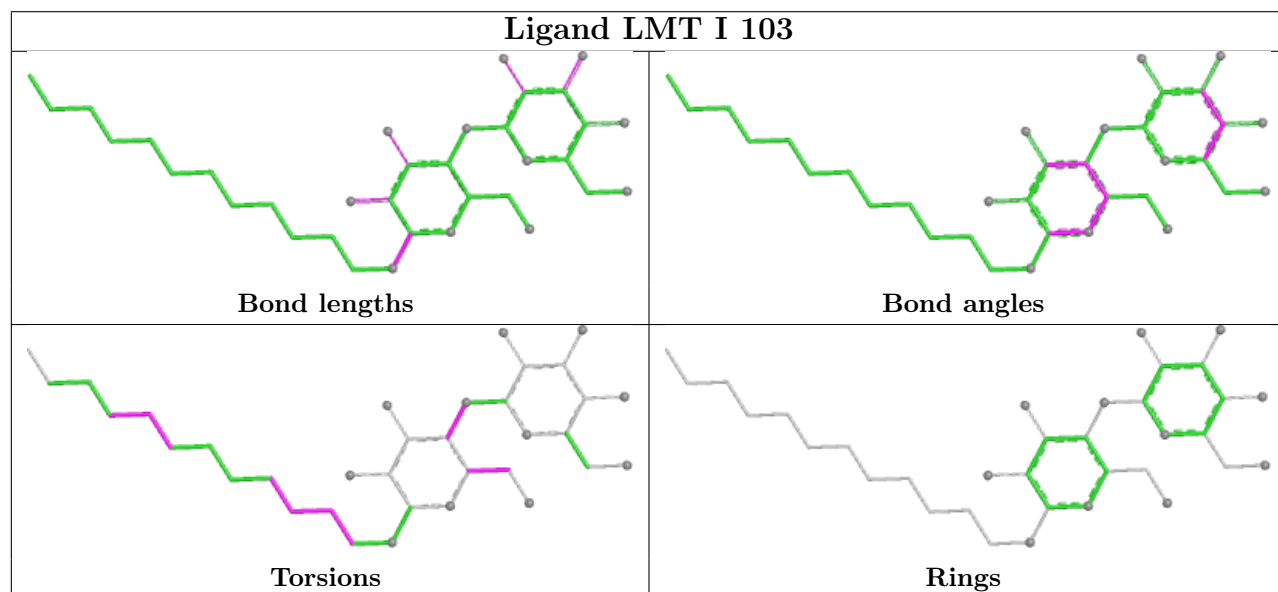
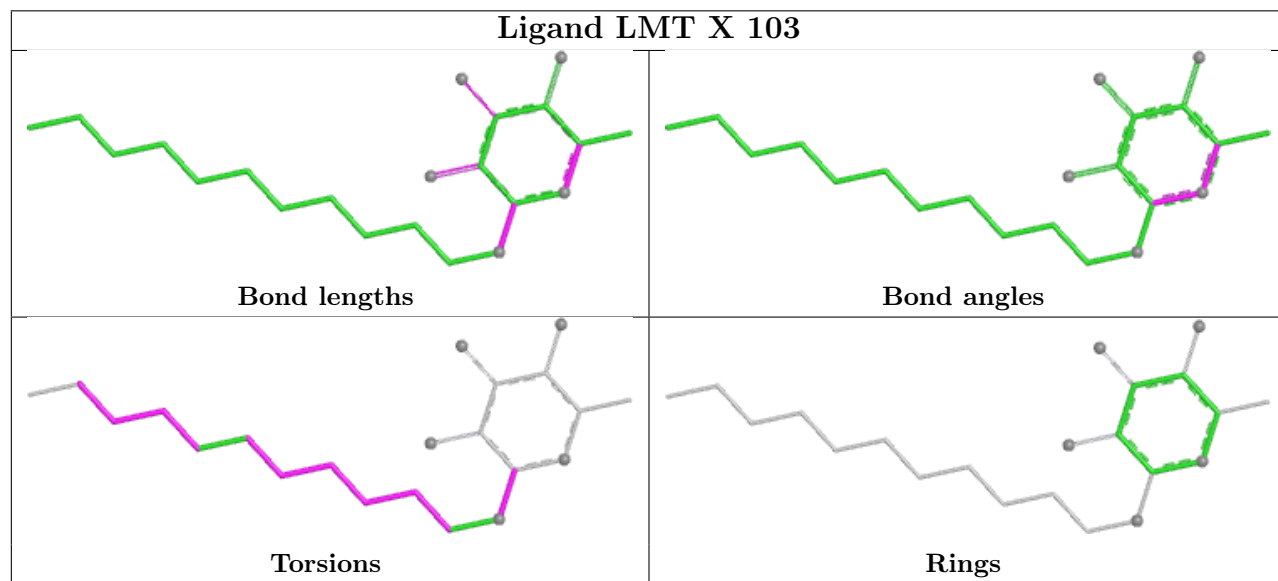
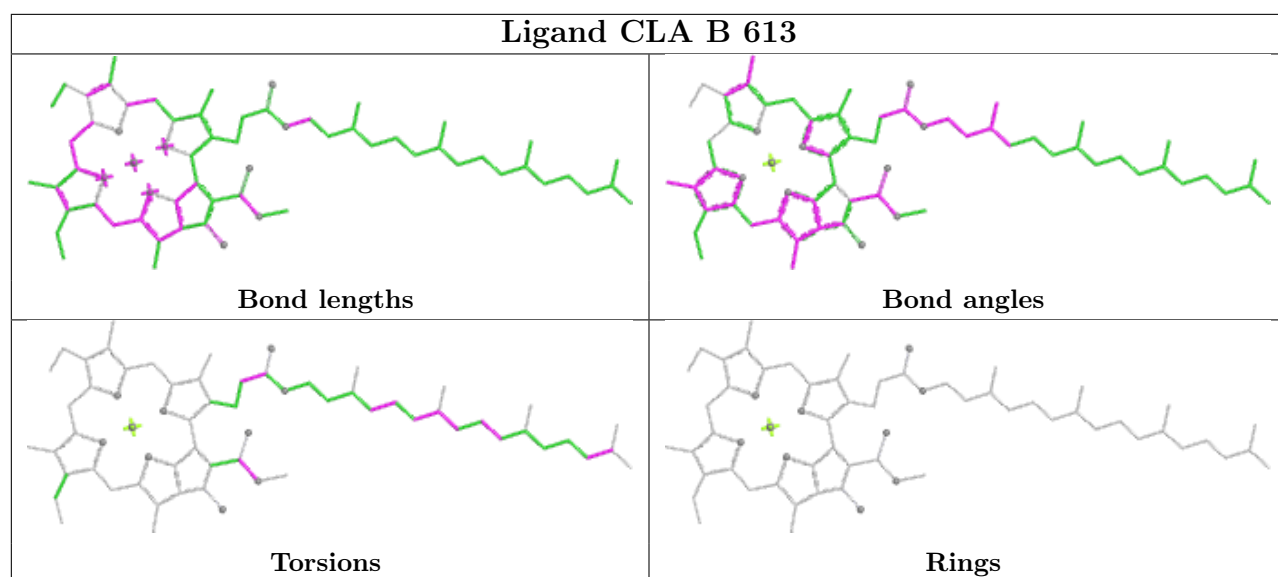
Ligand PL9 A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

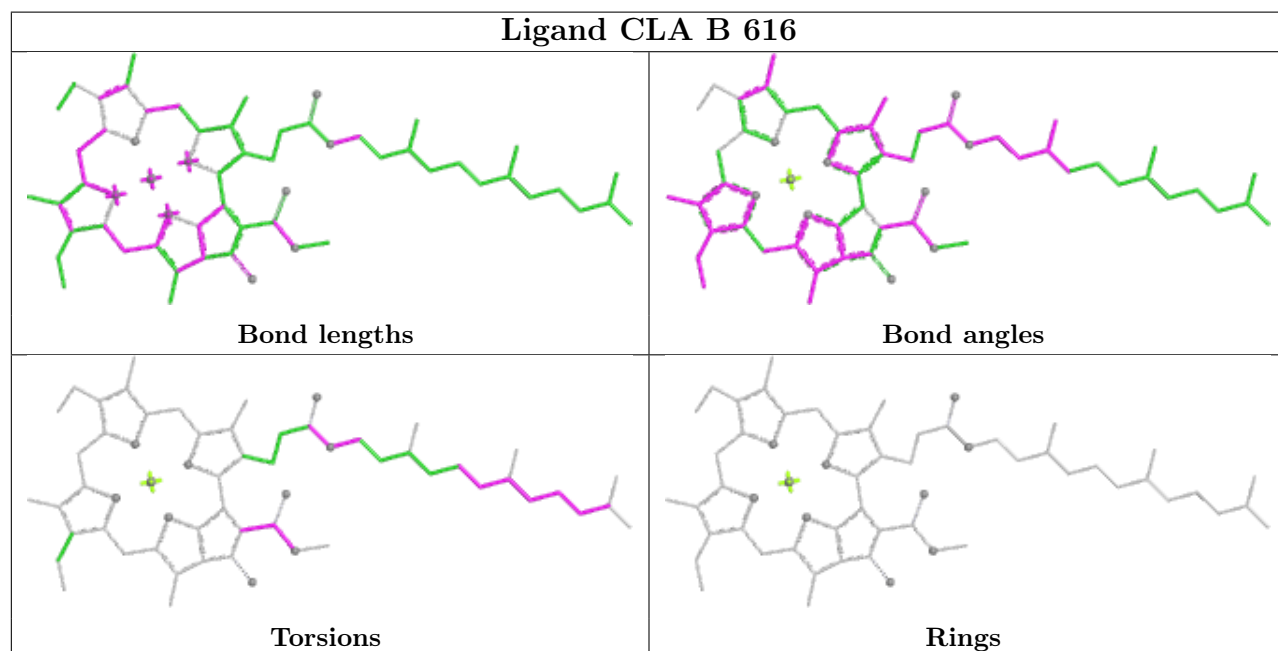
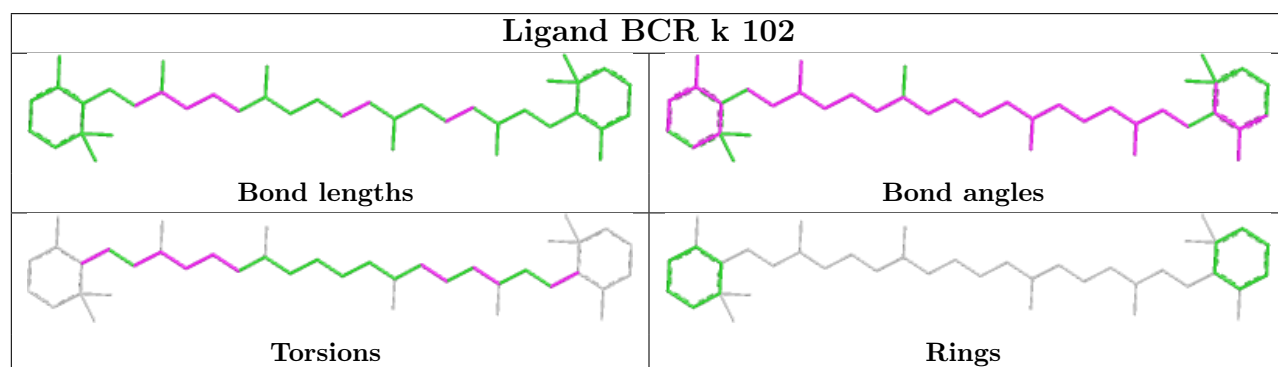
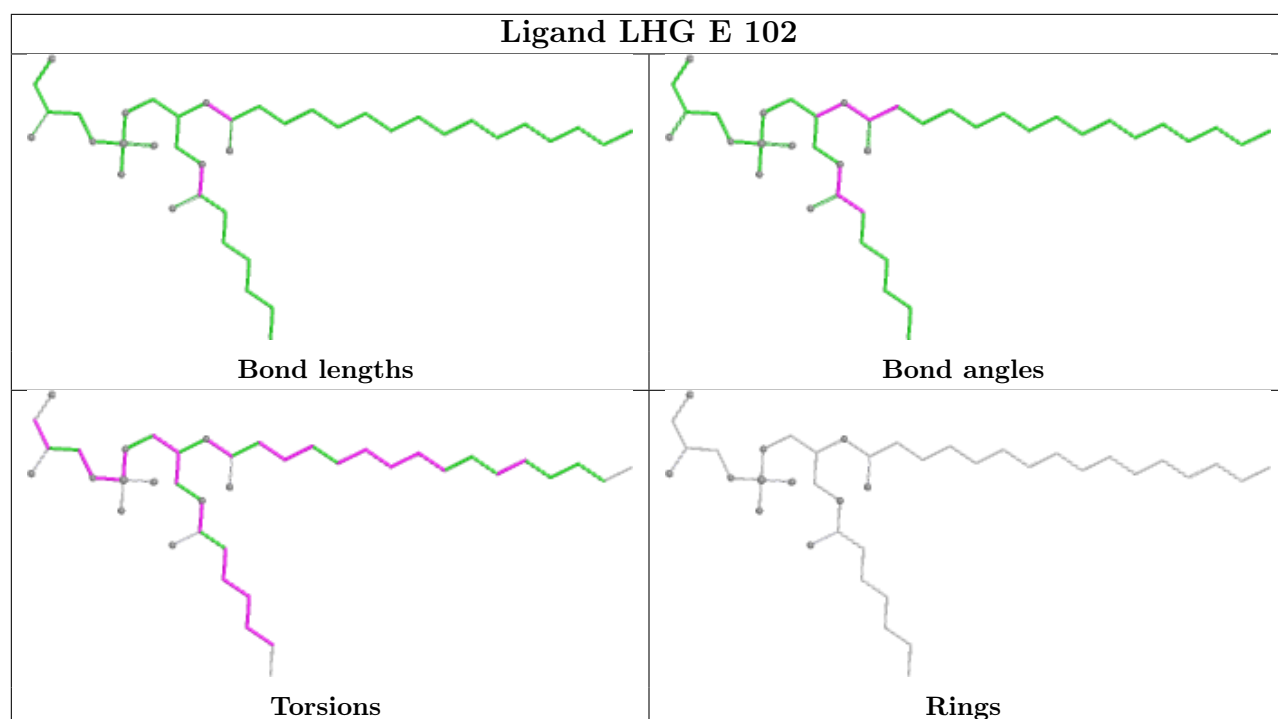
Ligand LHG Z 102



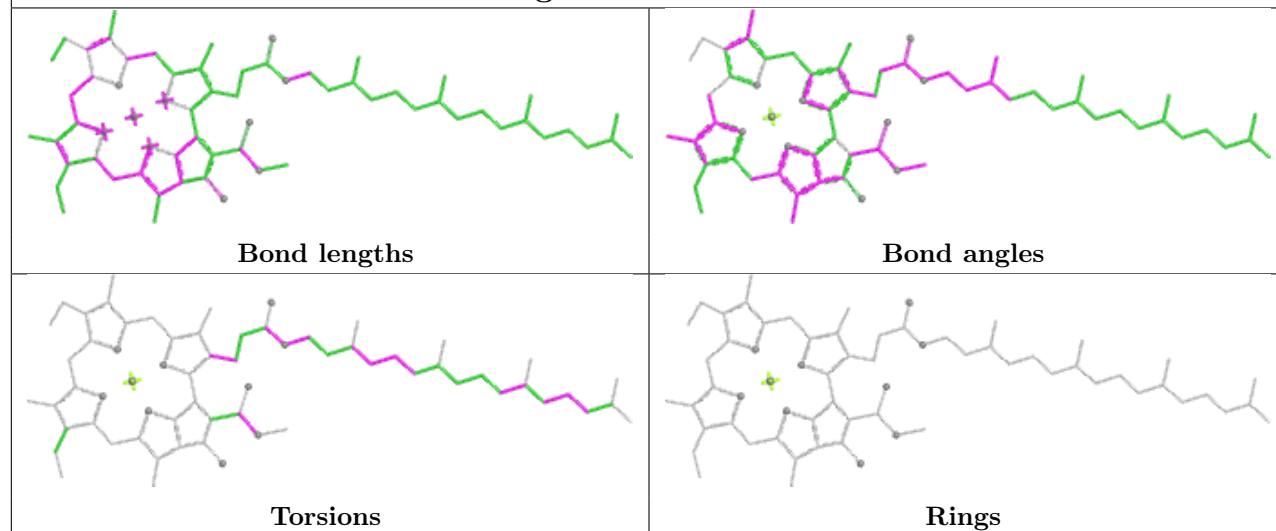
Ligand LMT x 103



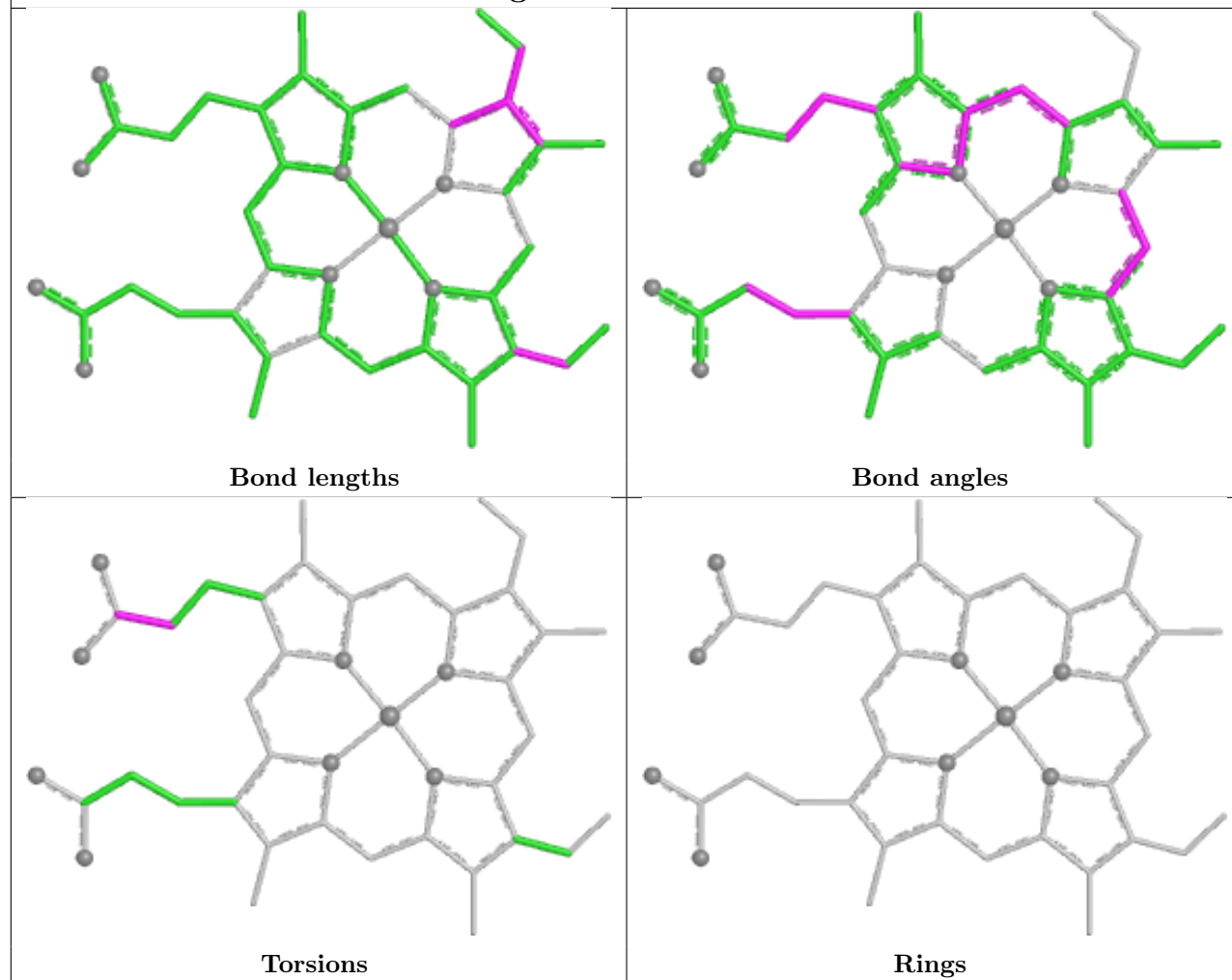


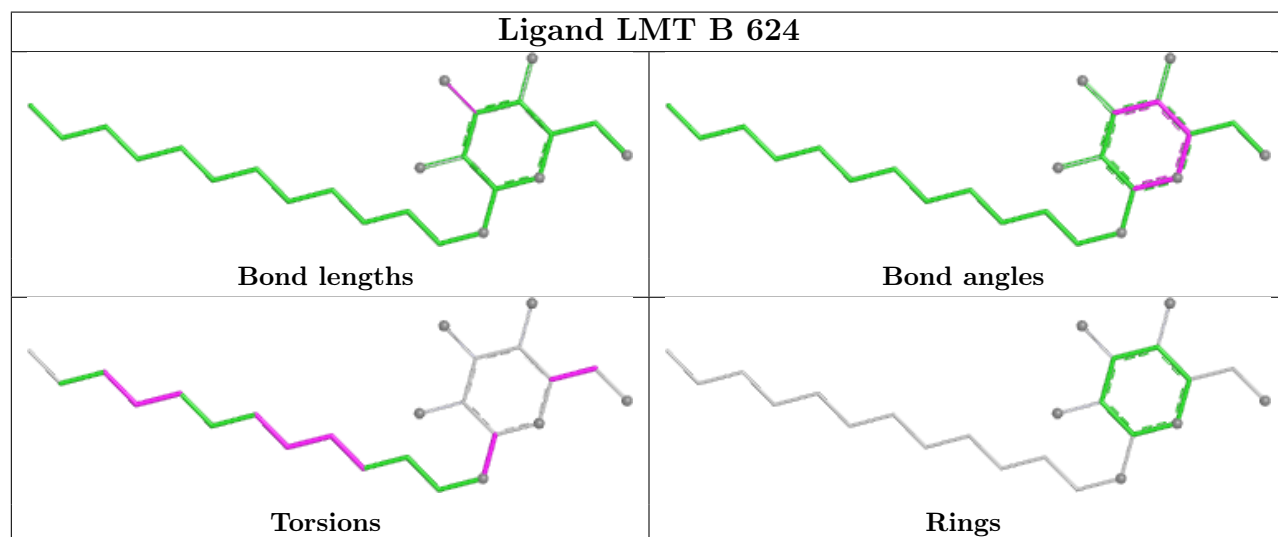
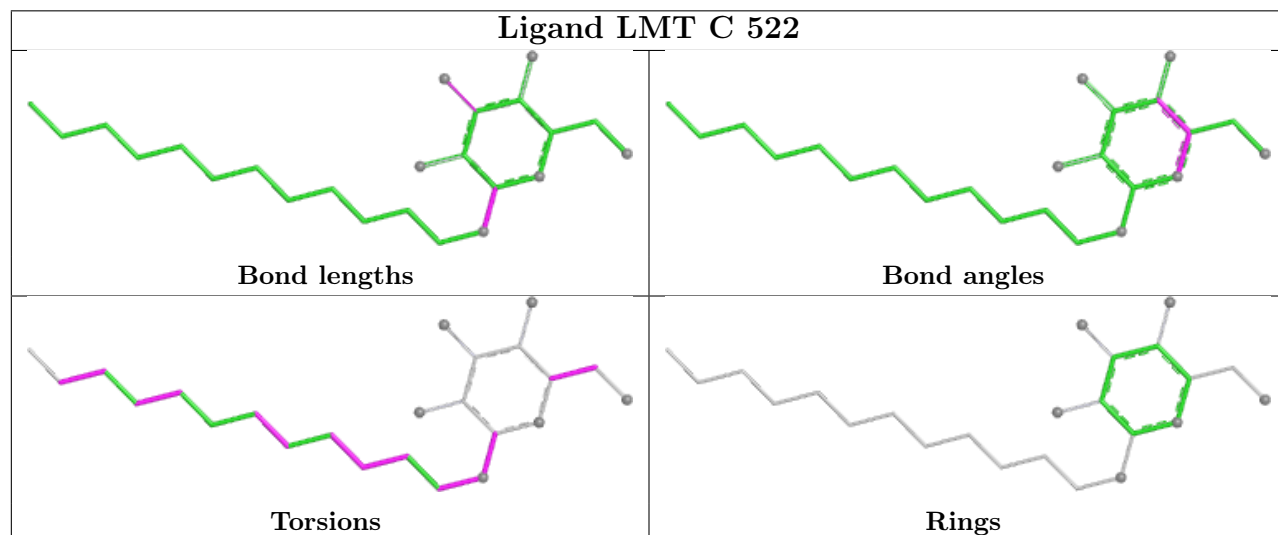
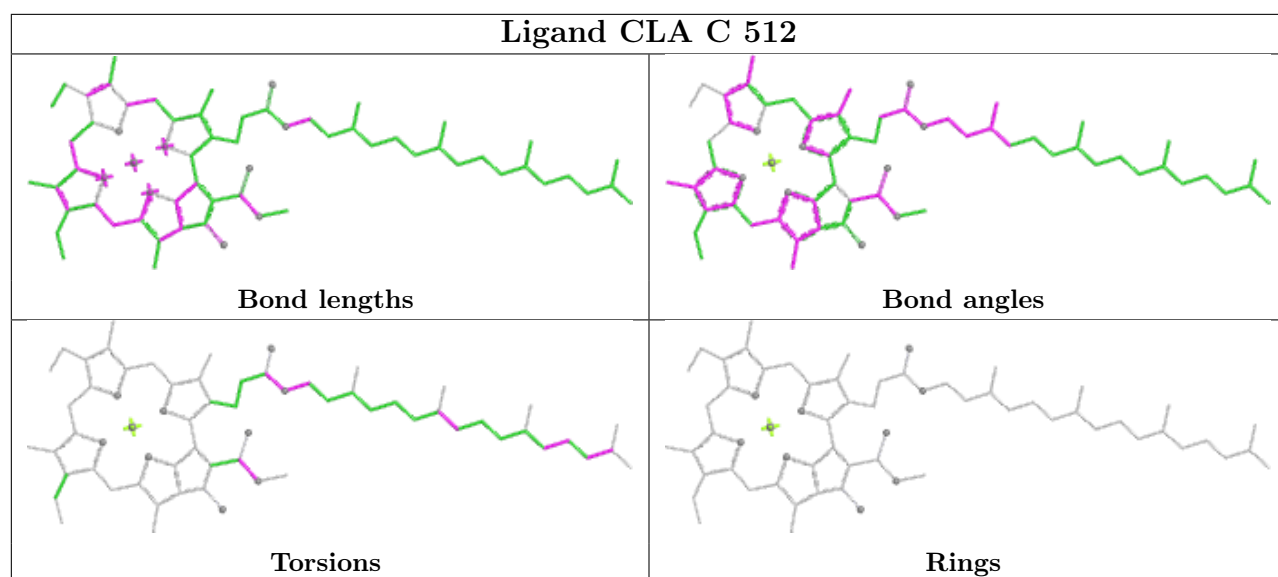


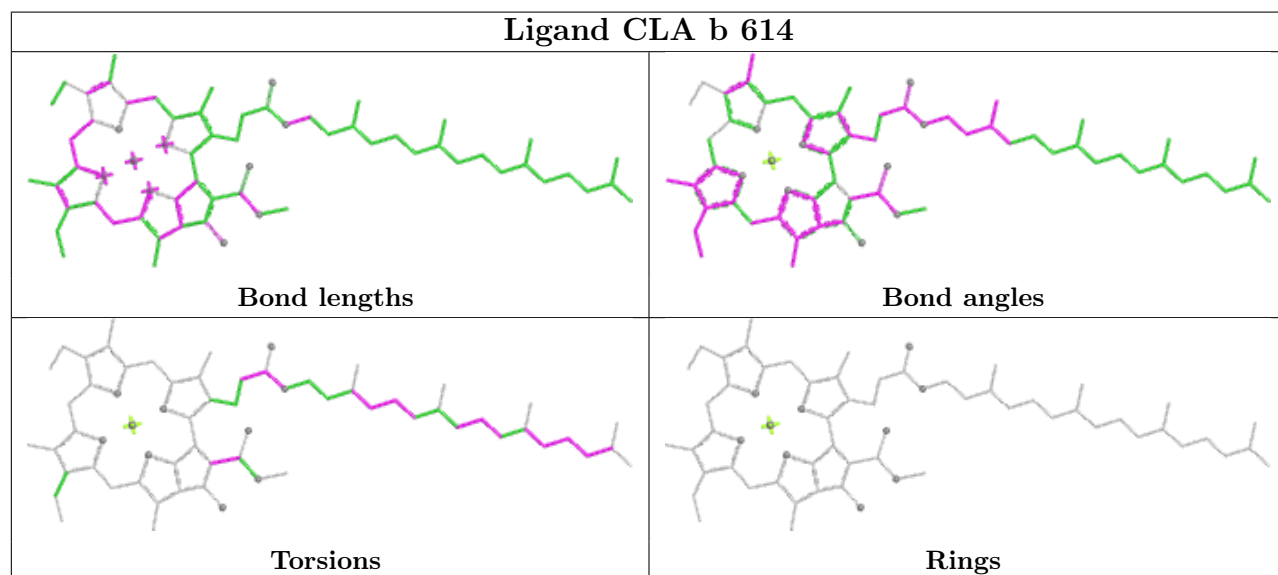
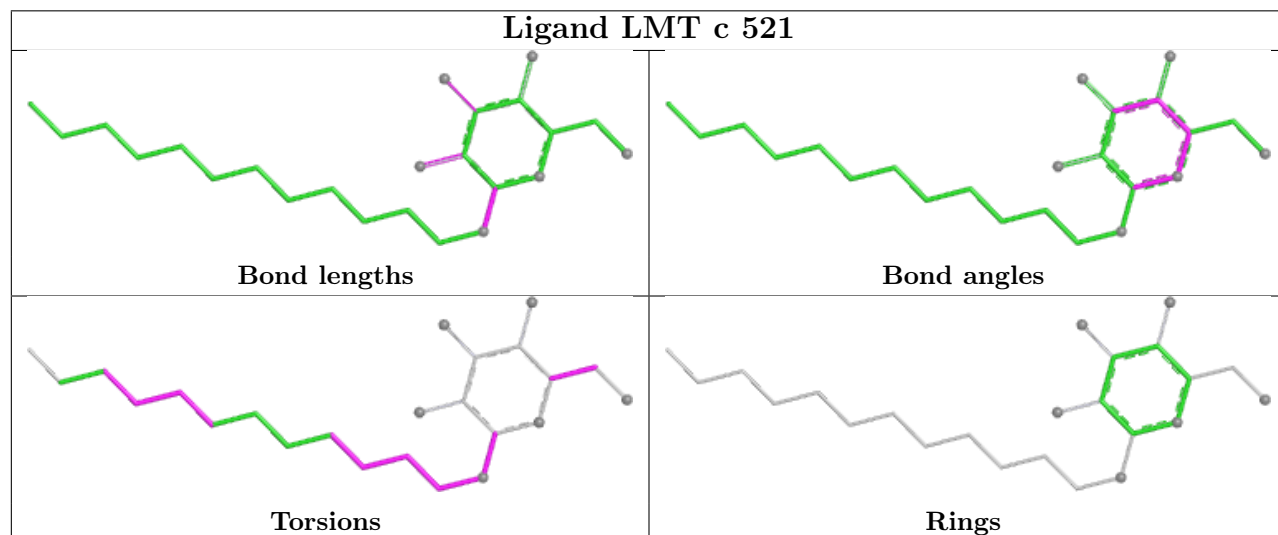
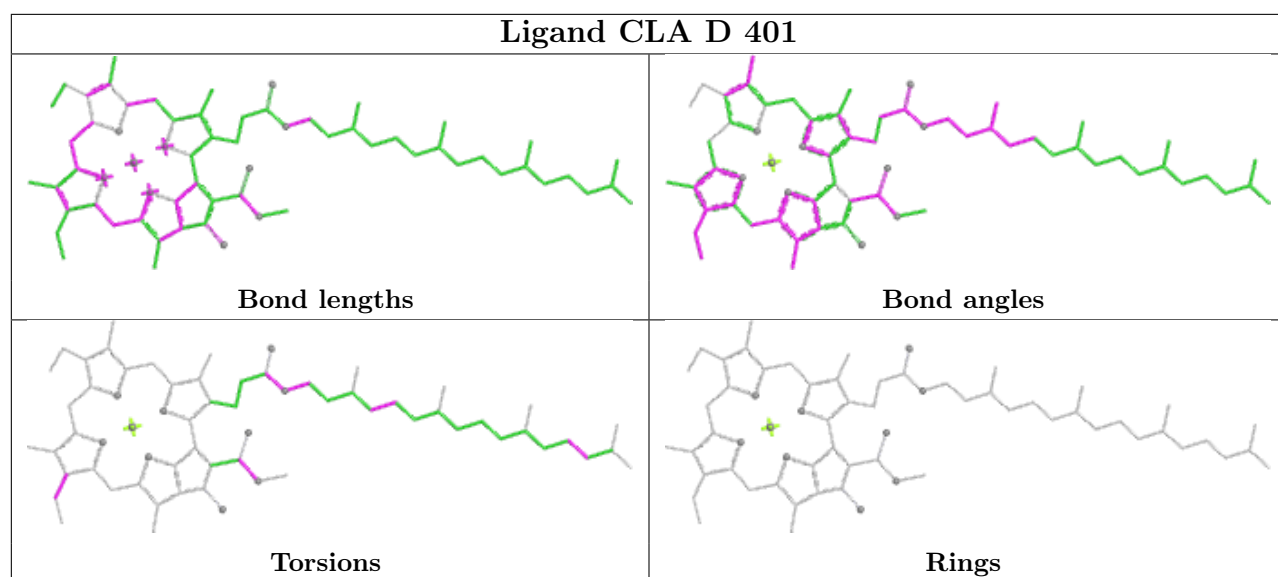
Ligand CLA d 404

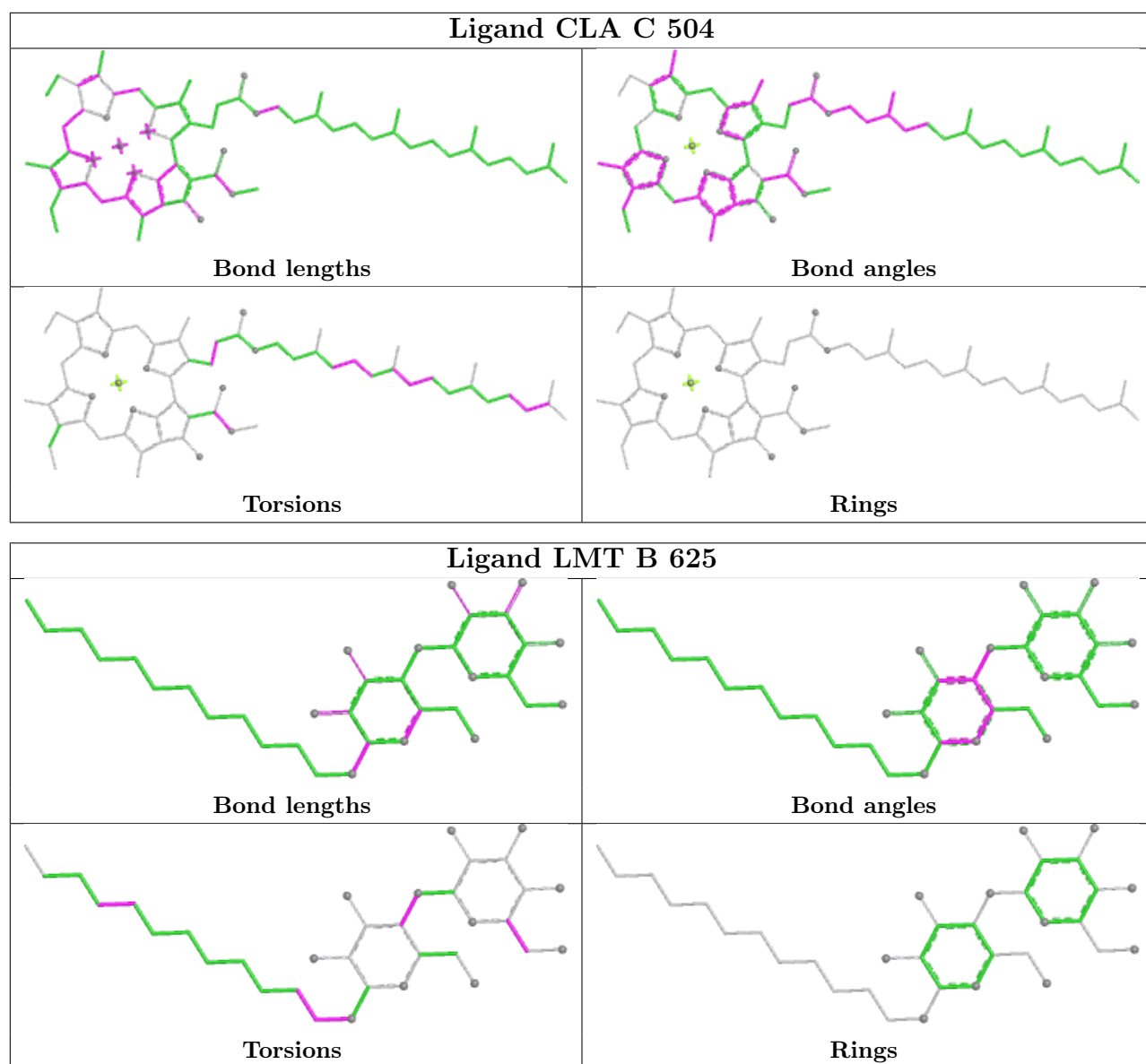


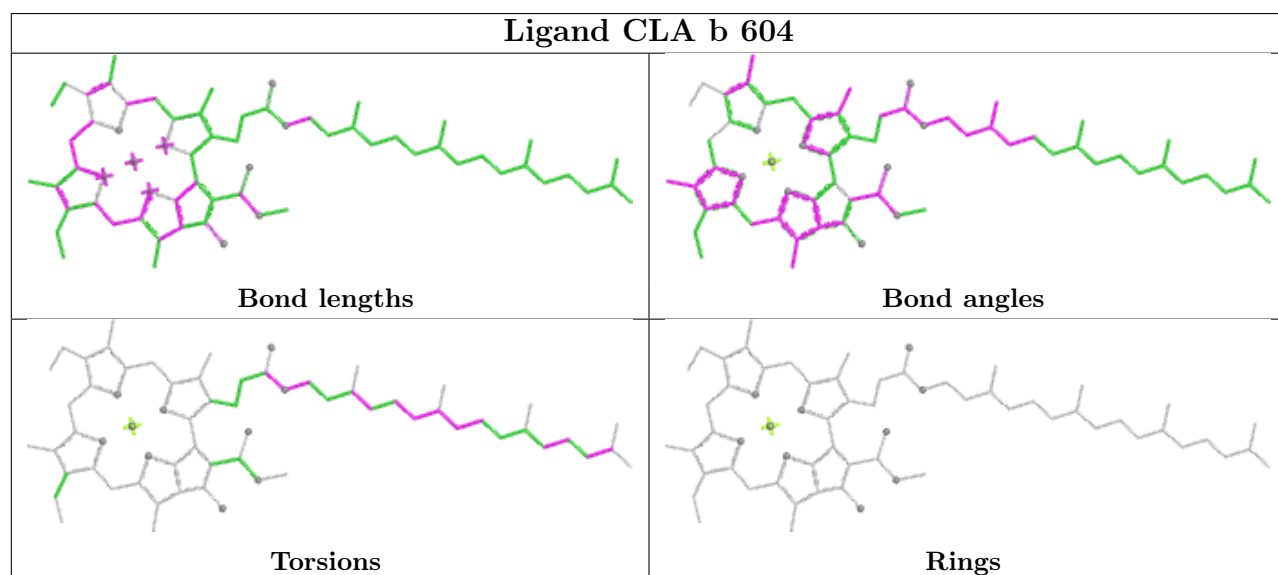
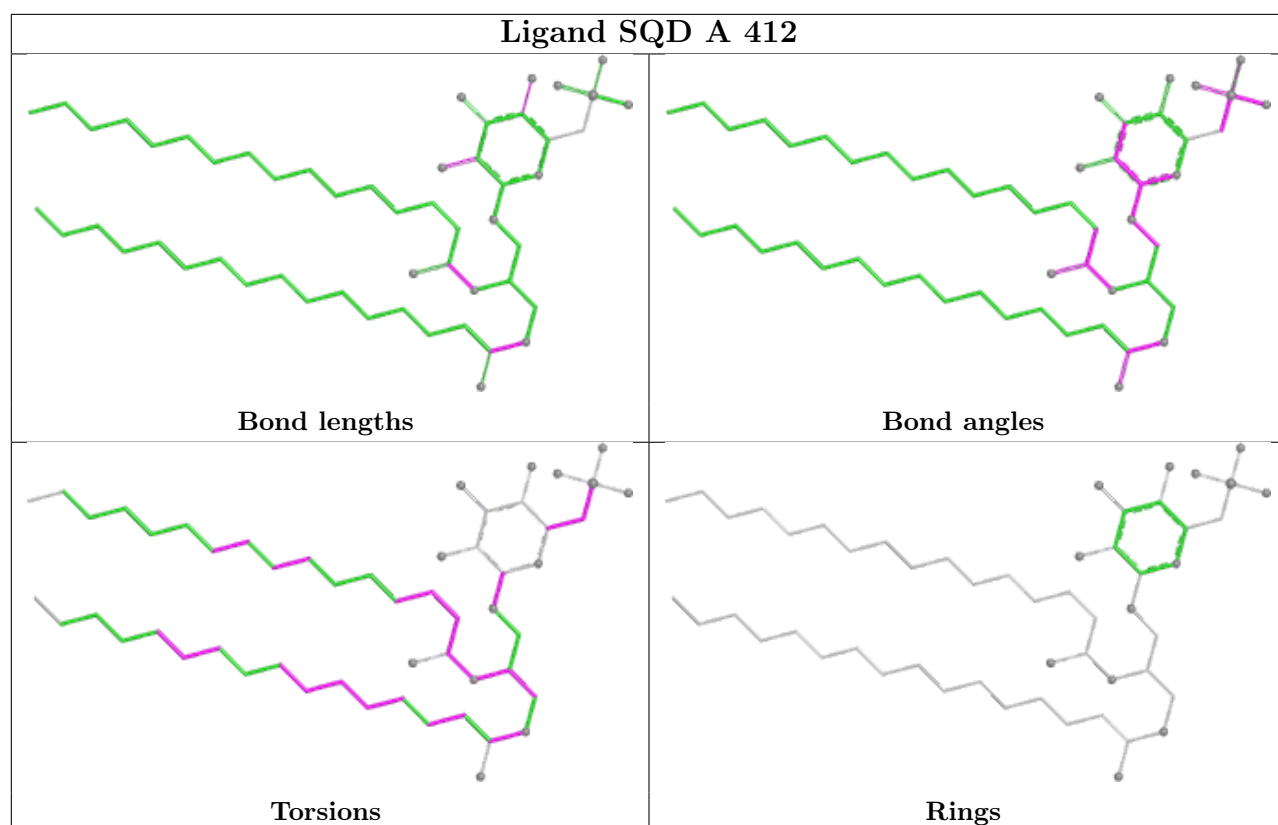
Ligand HEM E 104

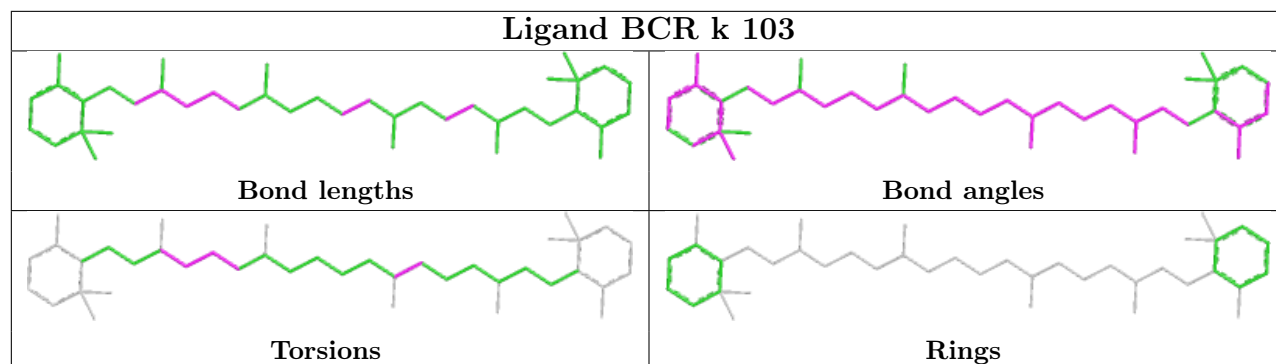
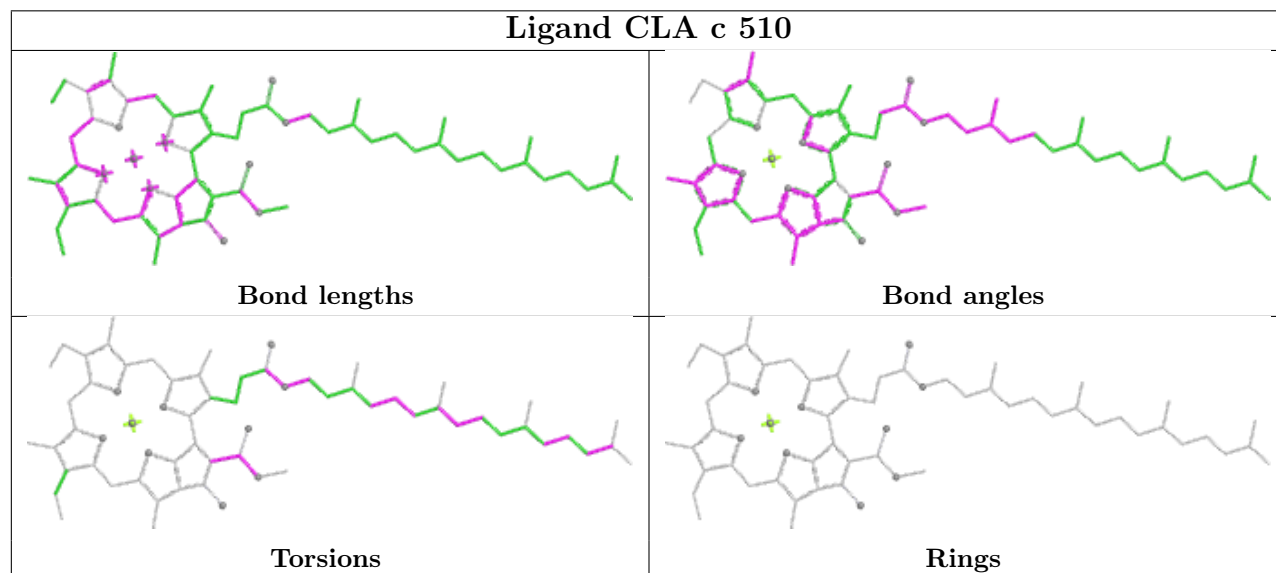
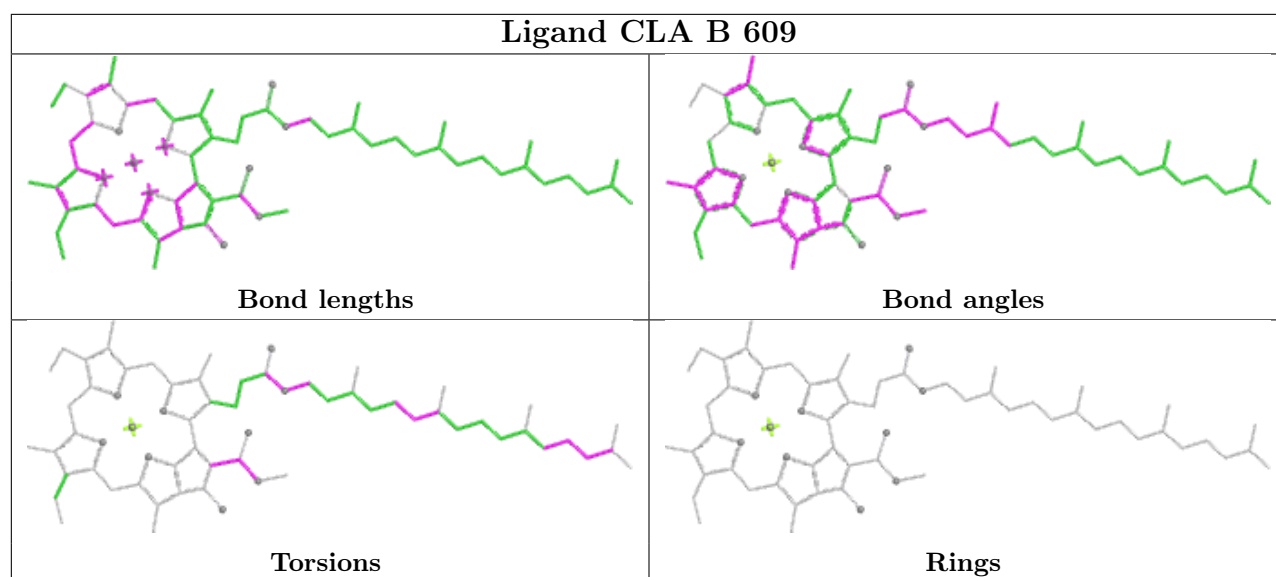


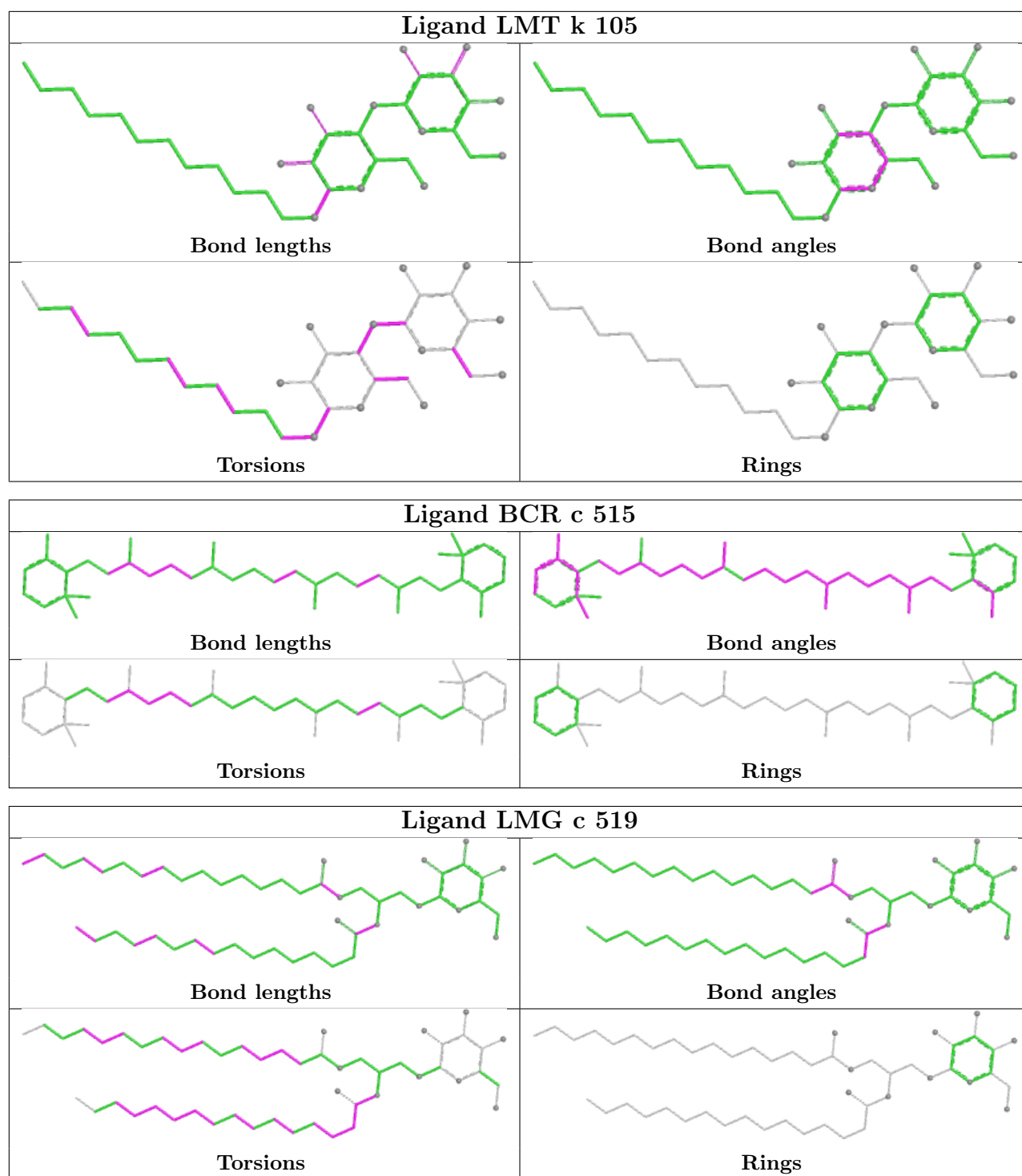


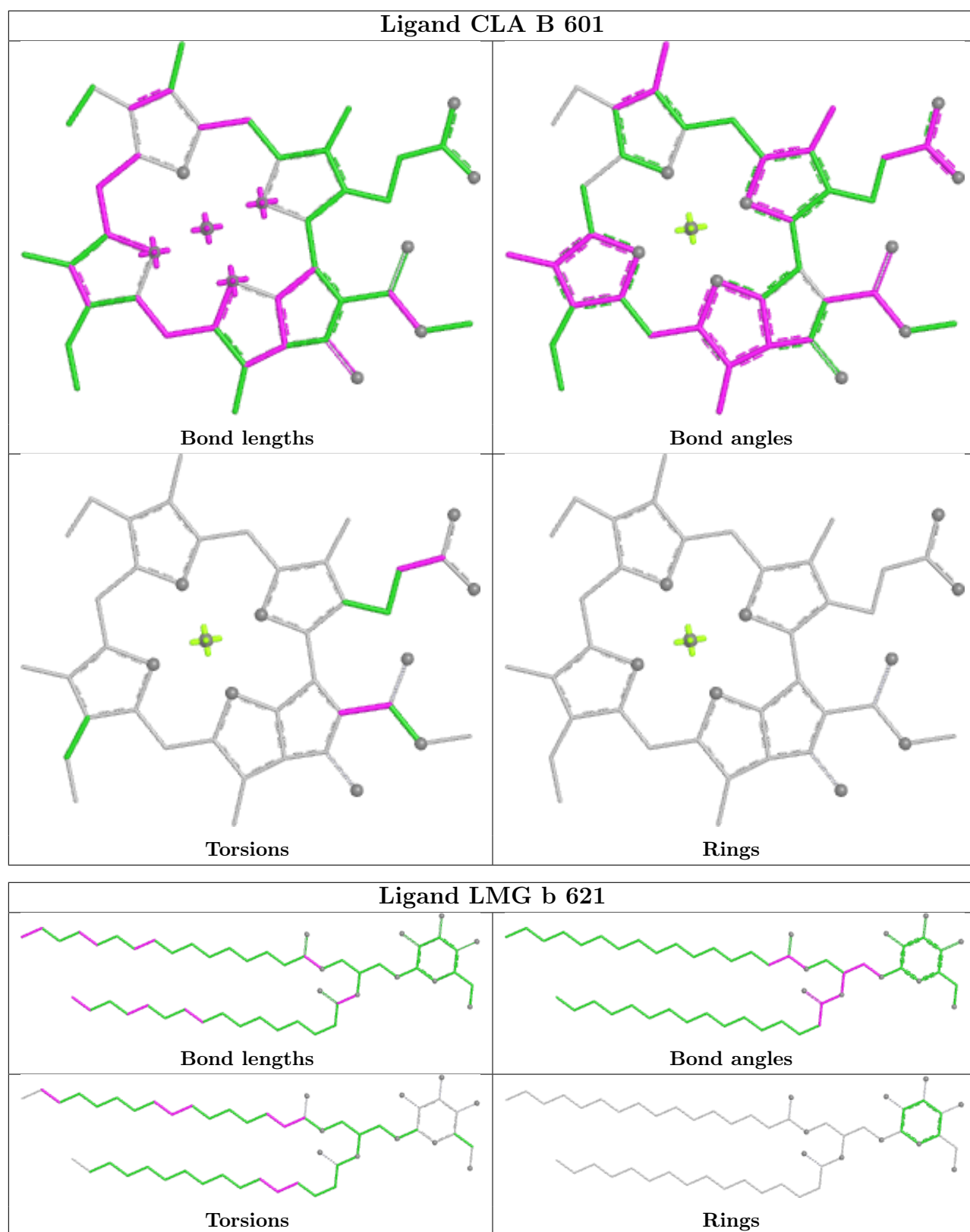


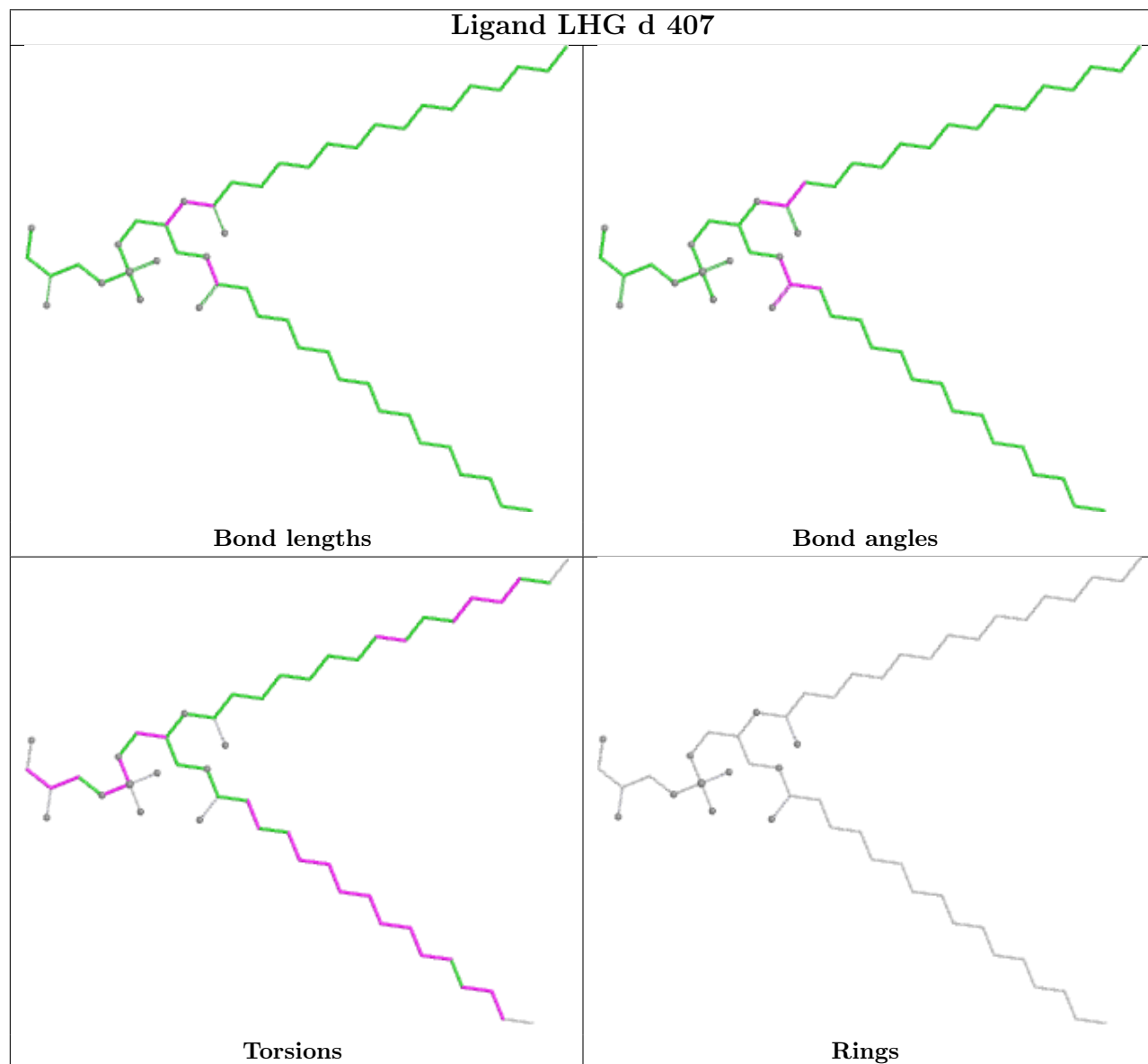
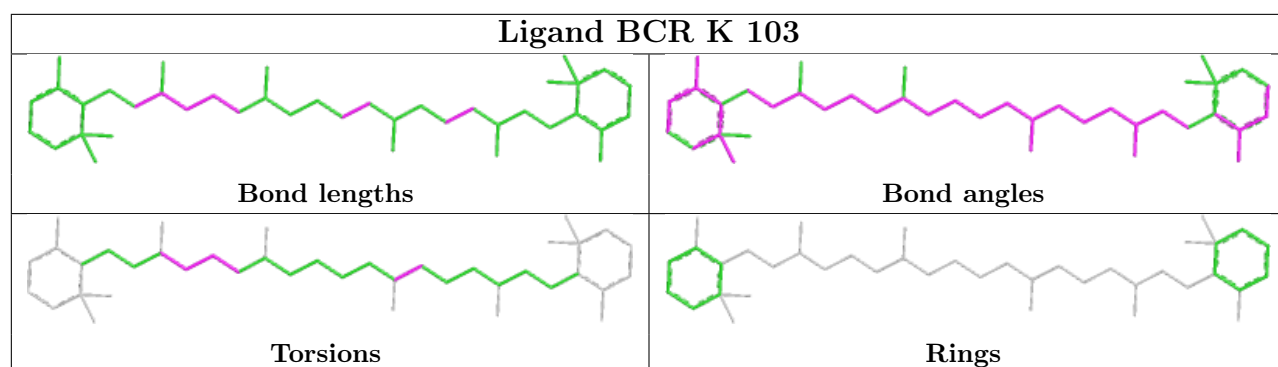


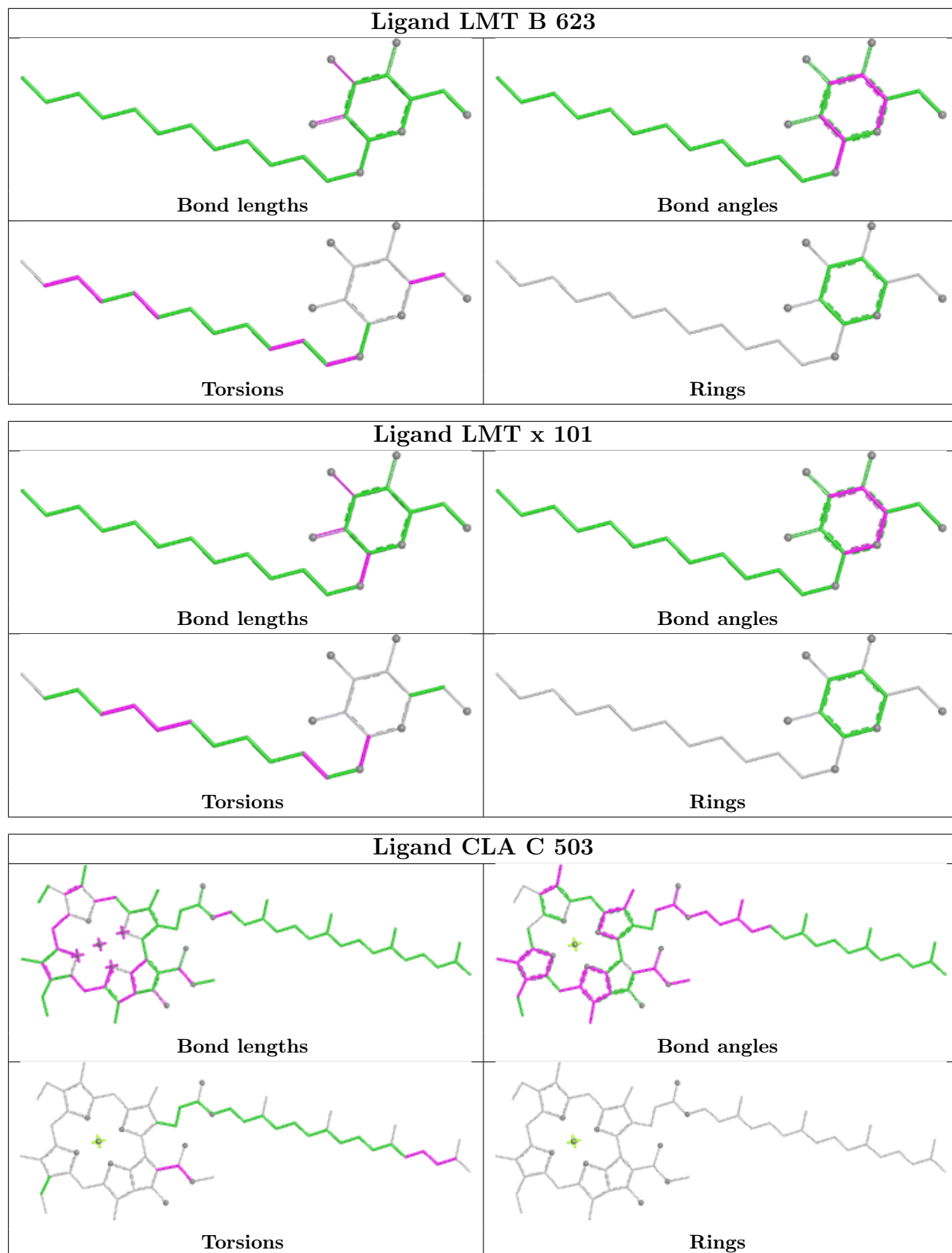


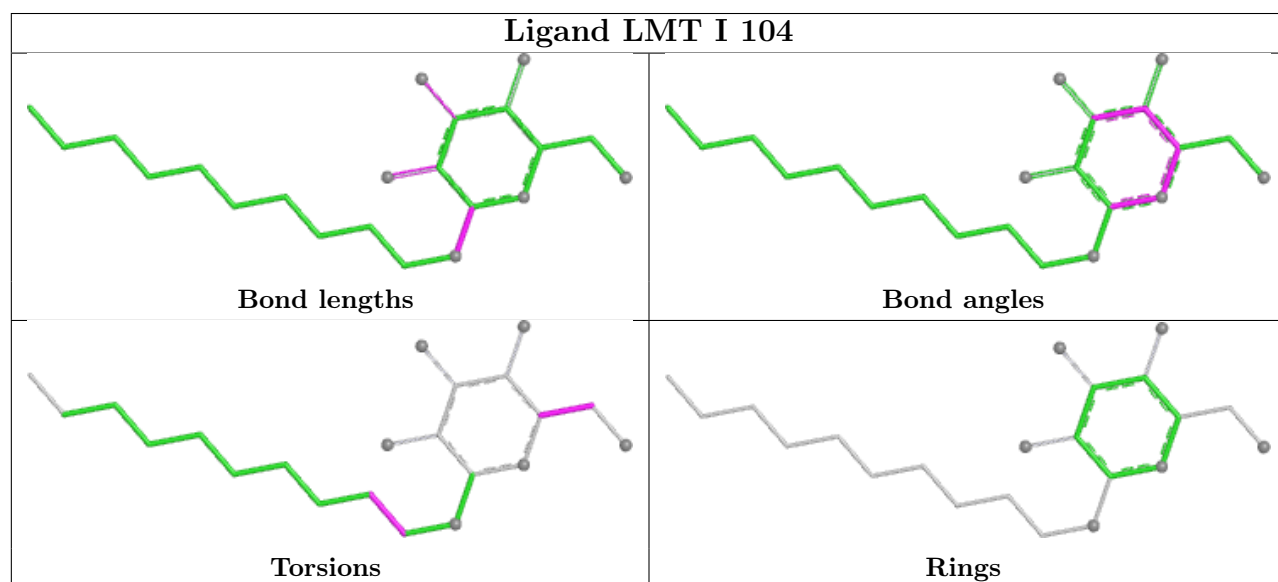
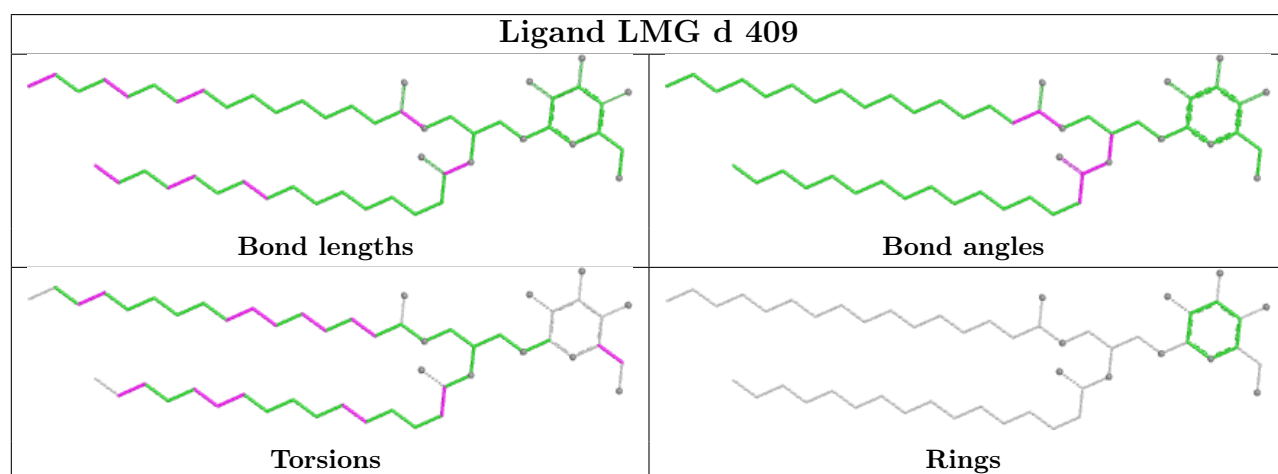
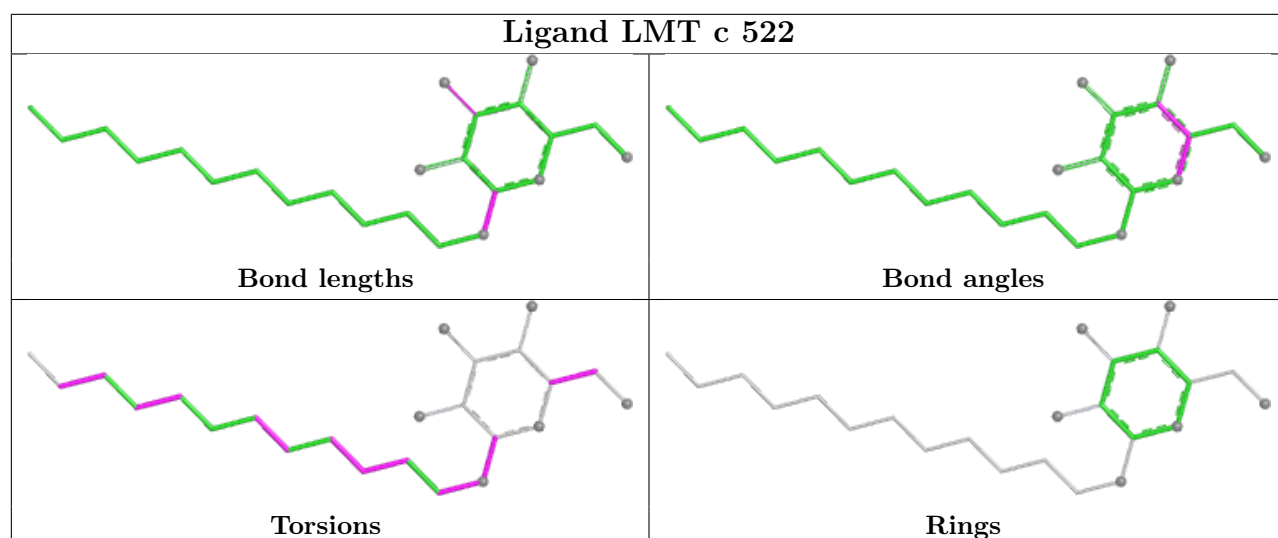


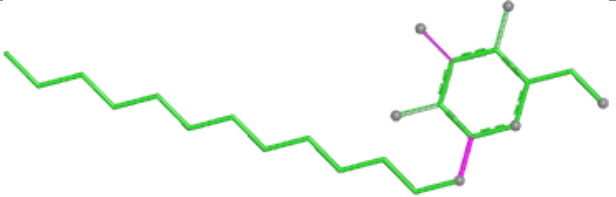
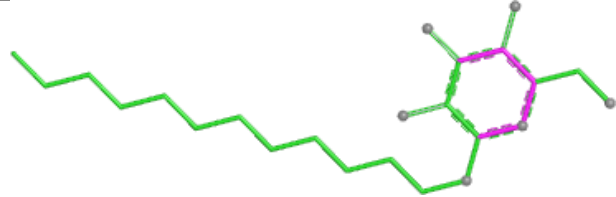
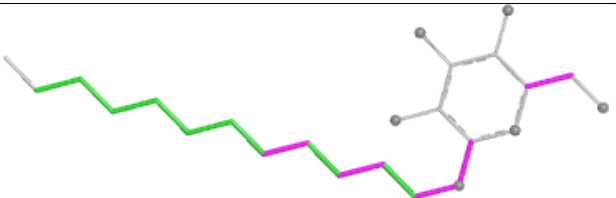



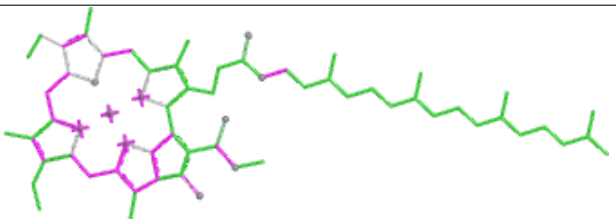
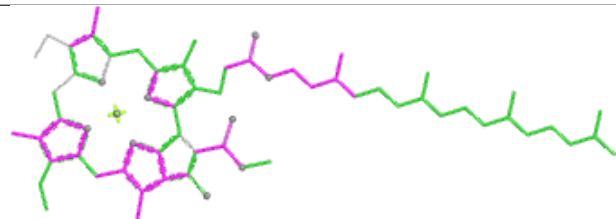
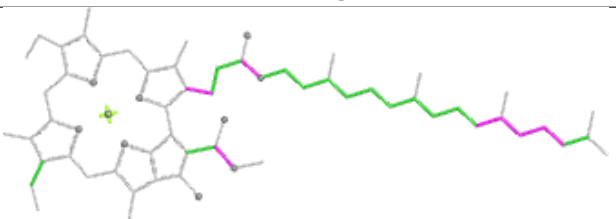
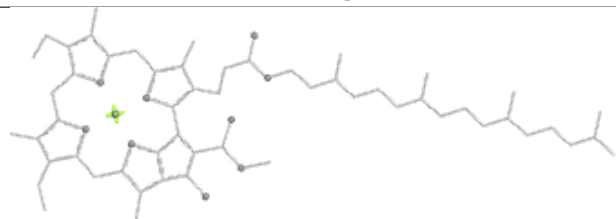


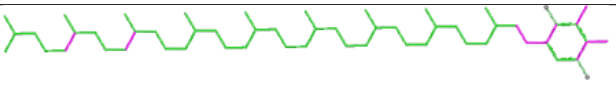
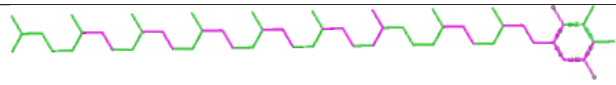
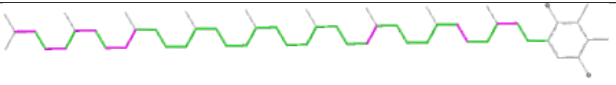
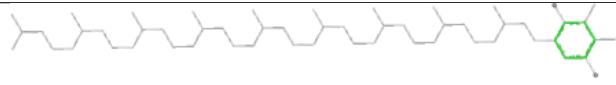


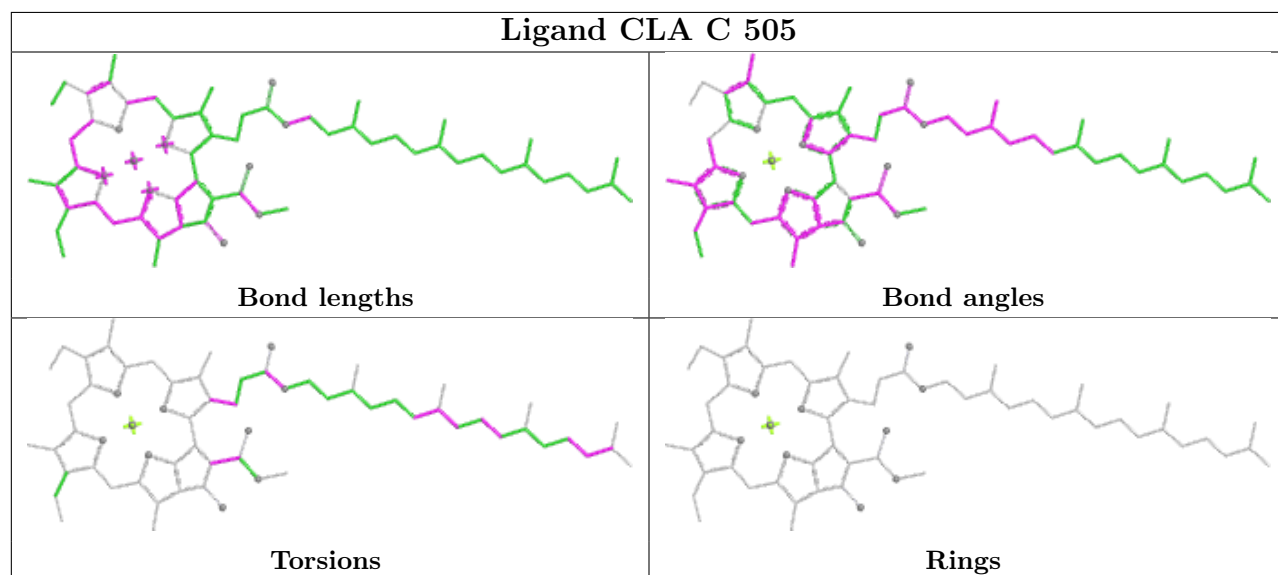
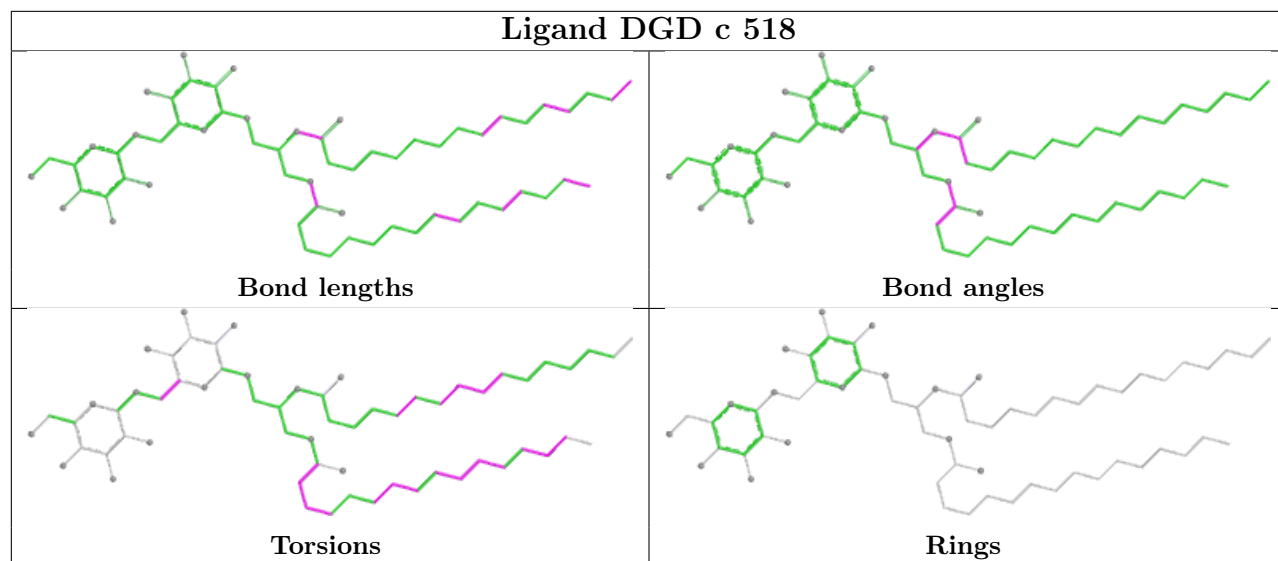


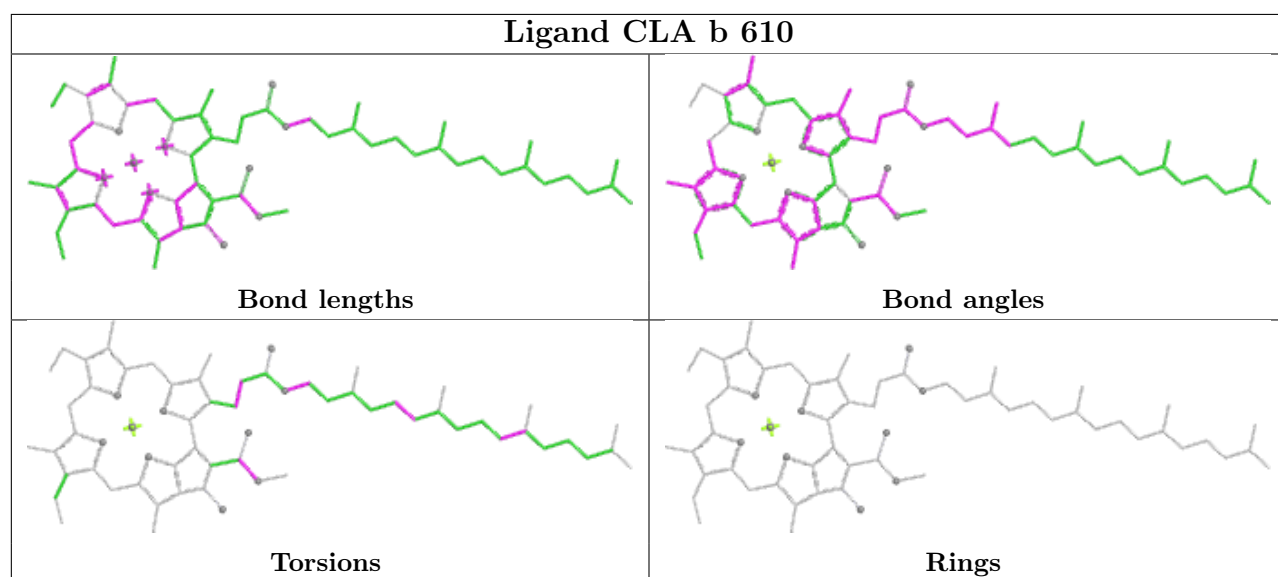
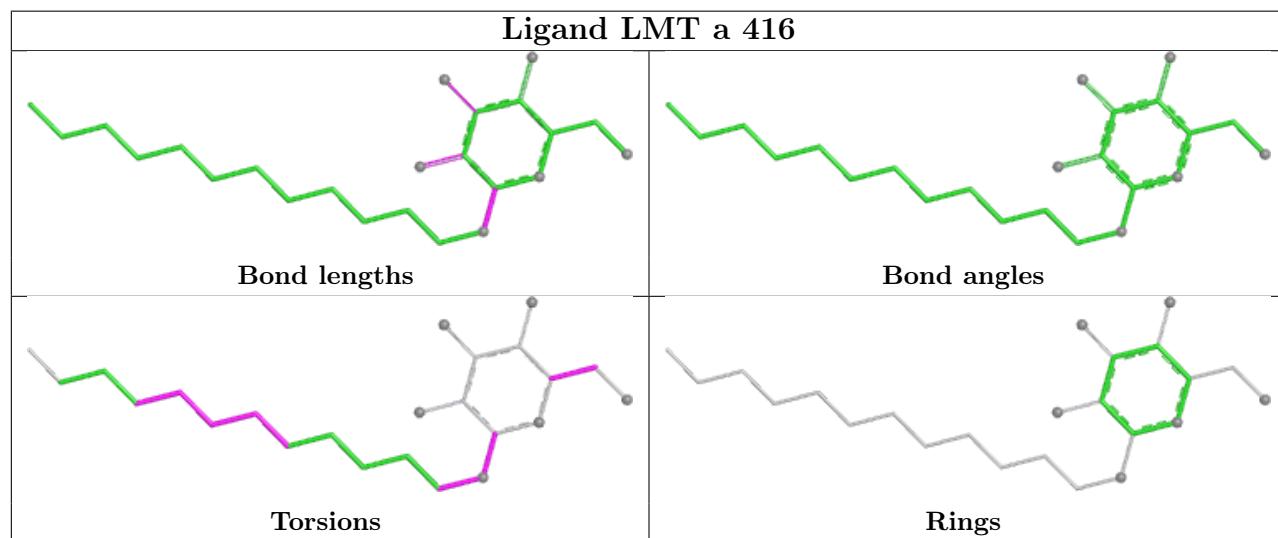
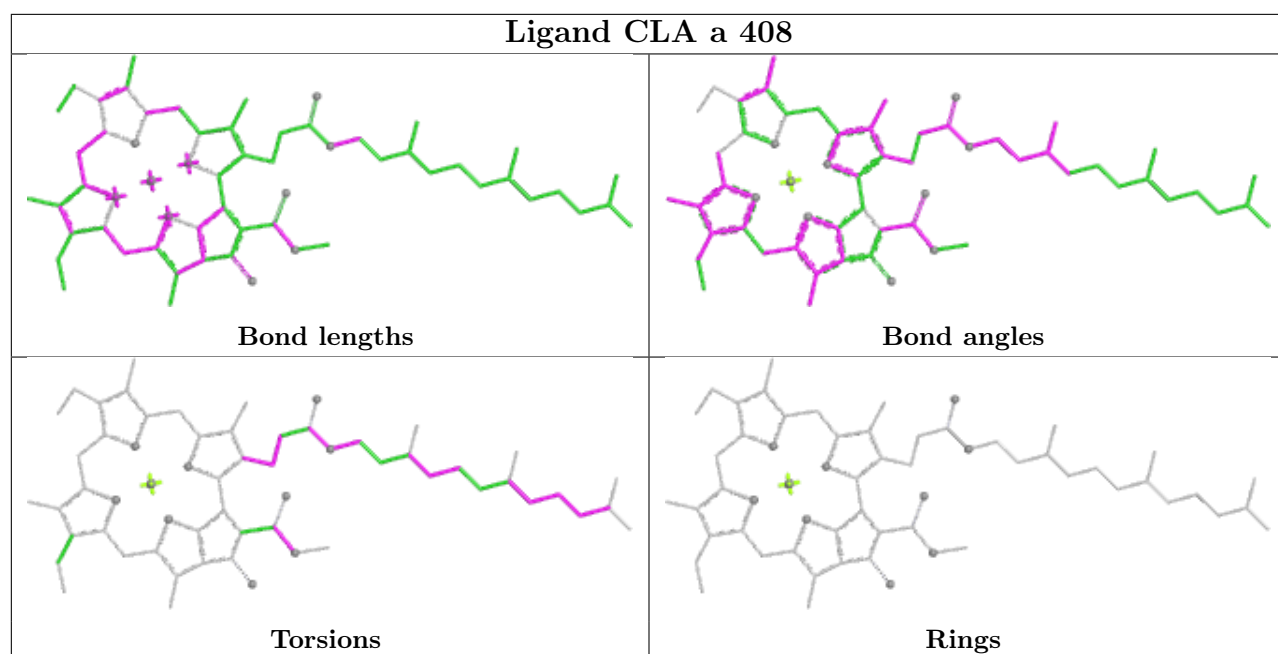


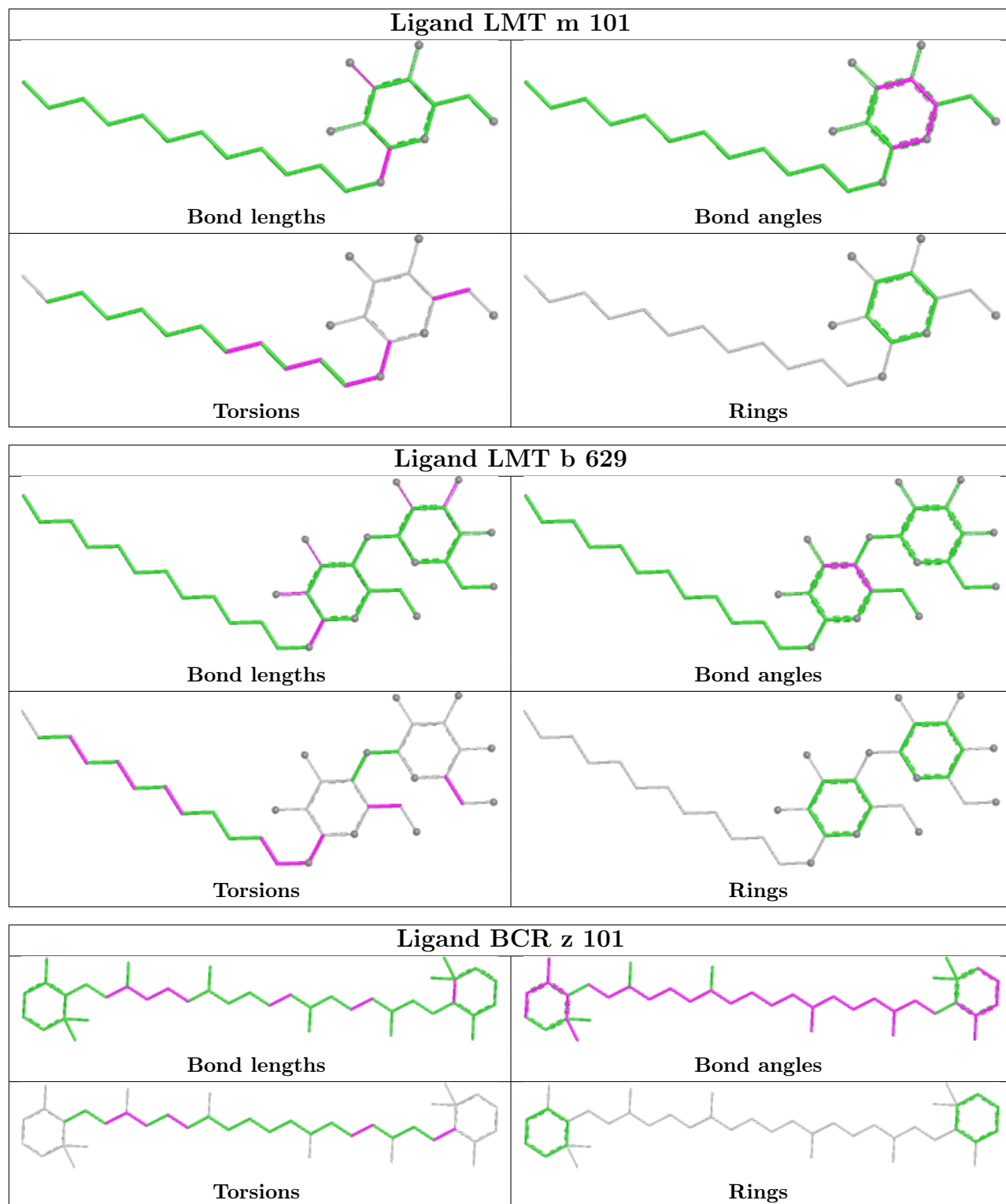
Ligand LMT M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

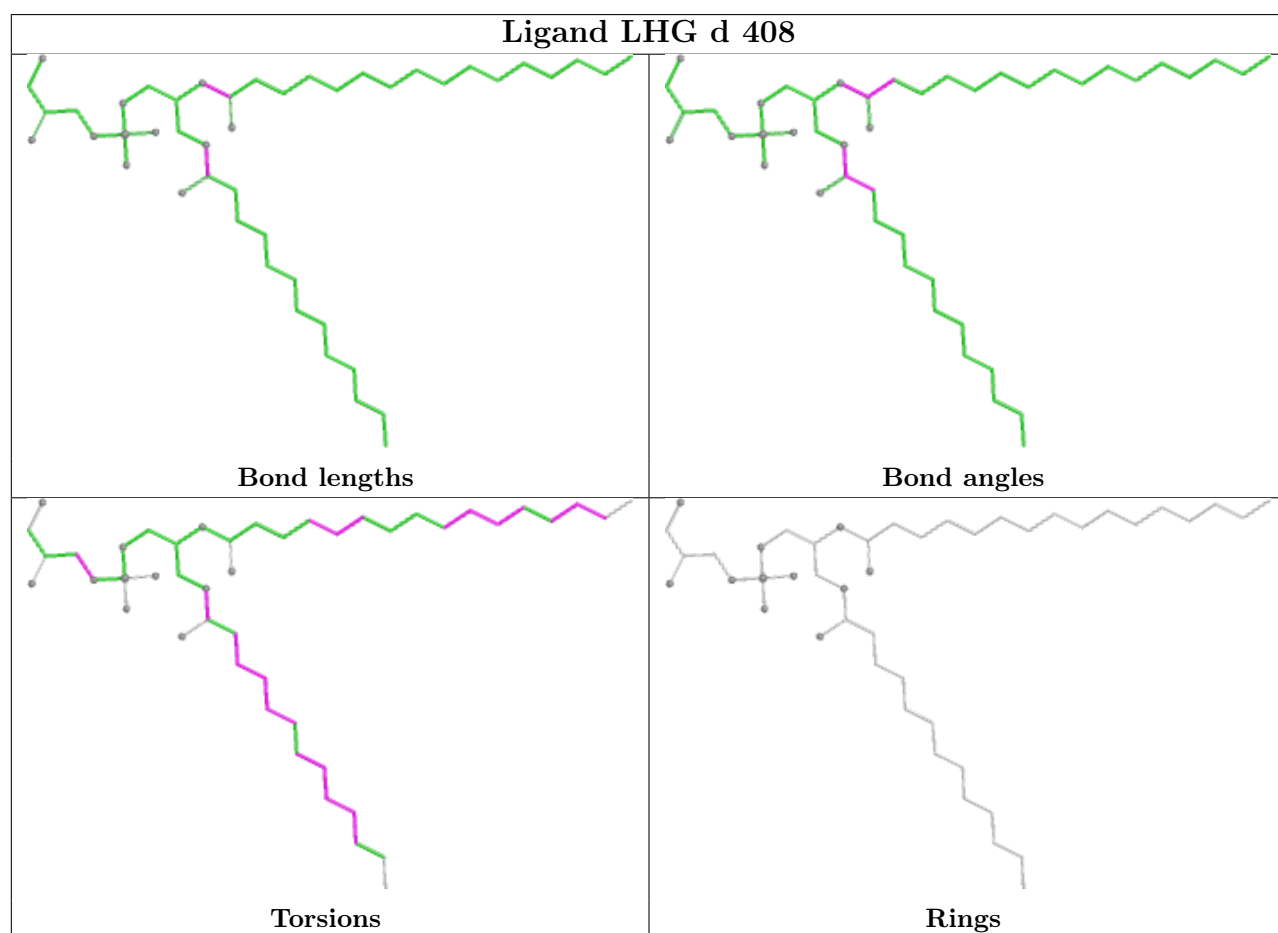
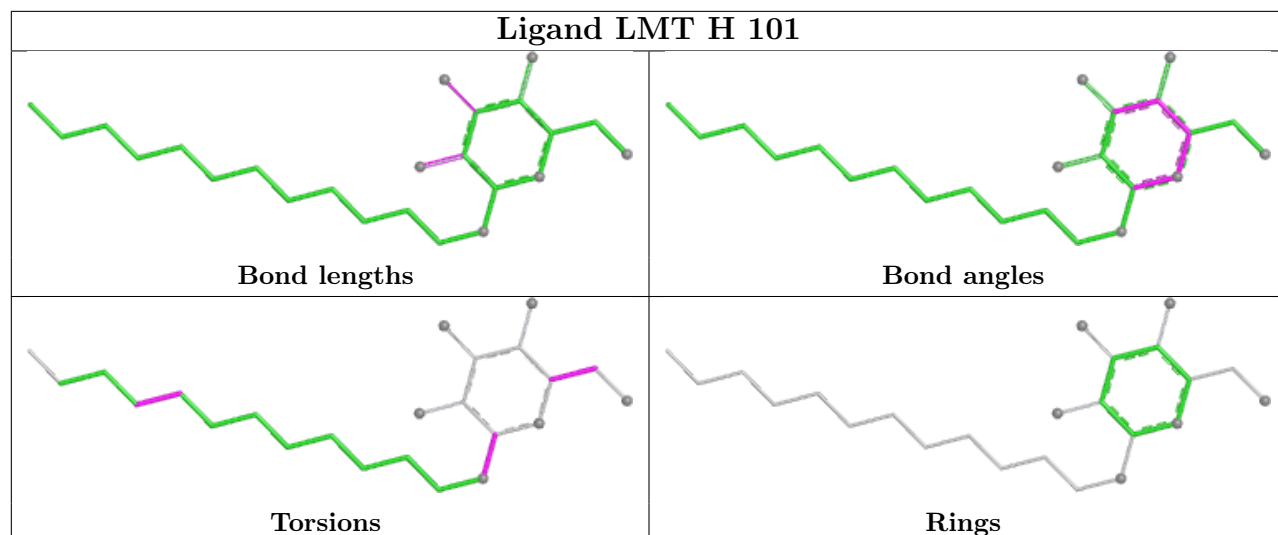
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

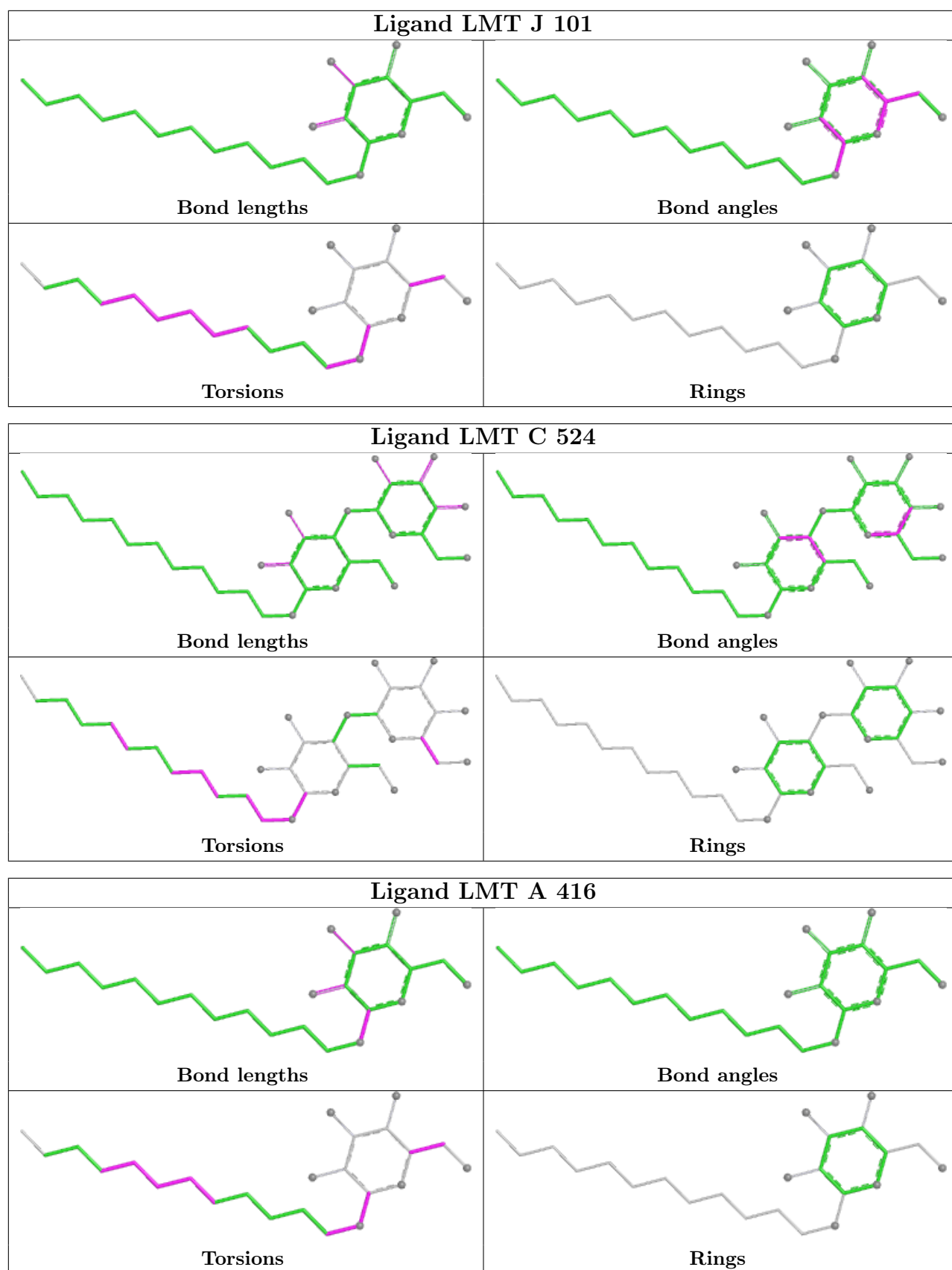
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

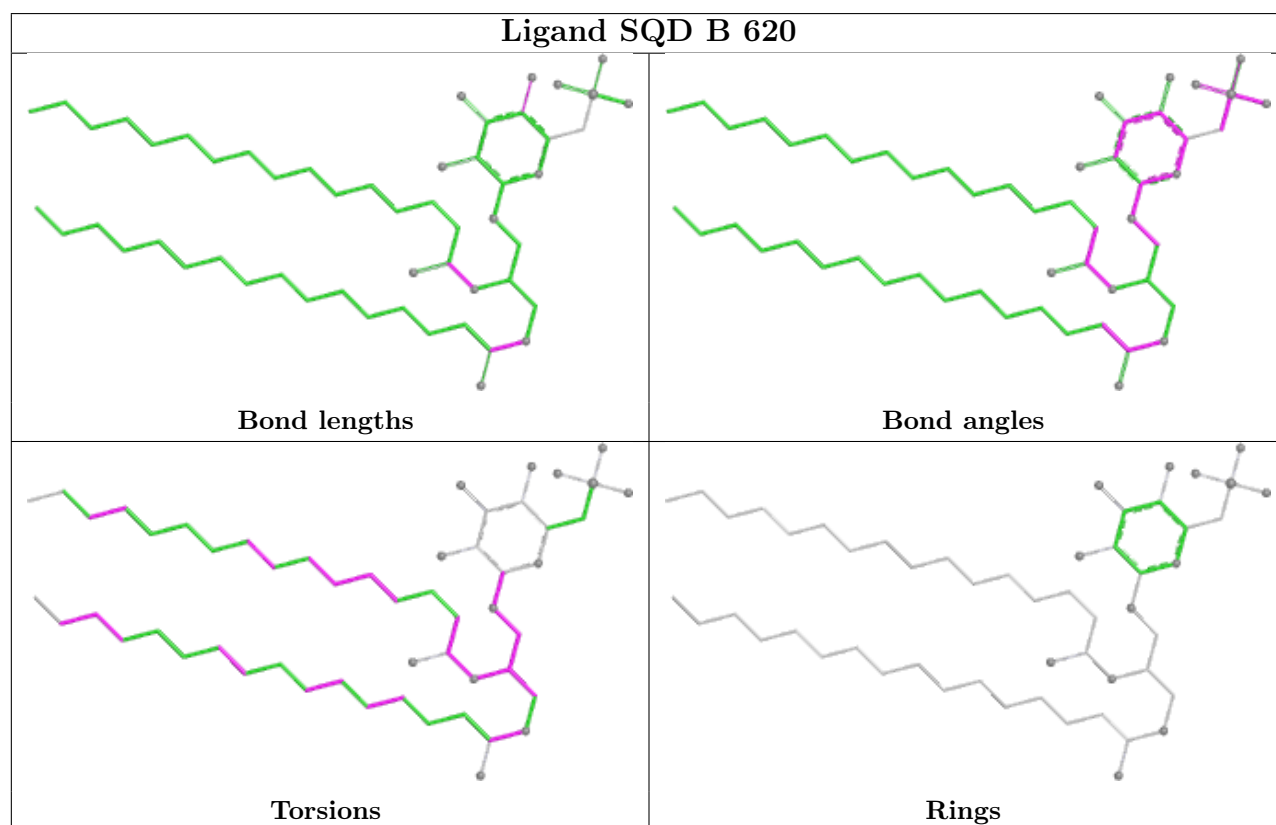
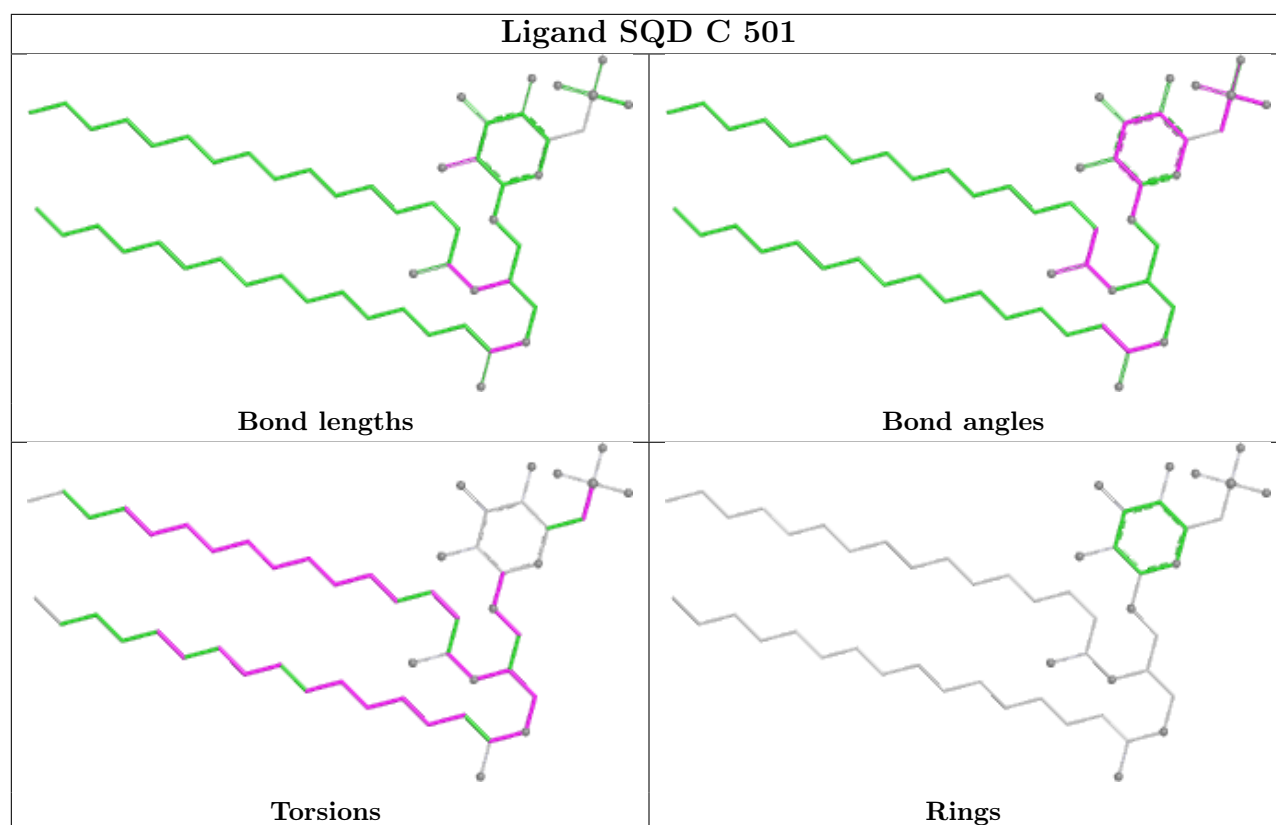


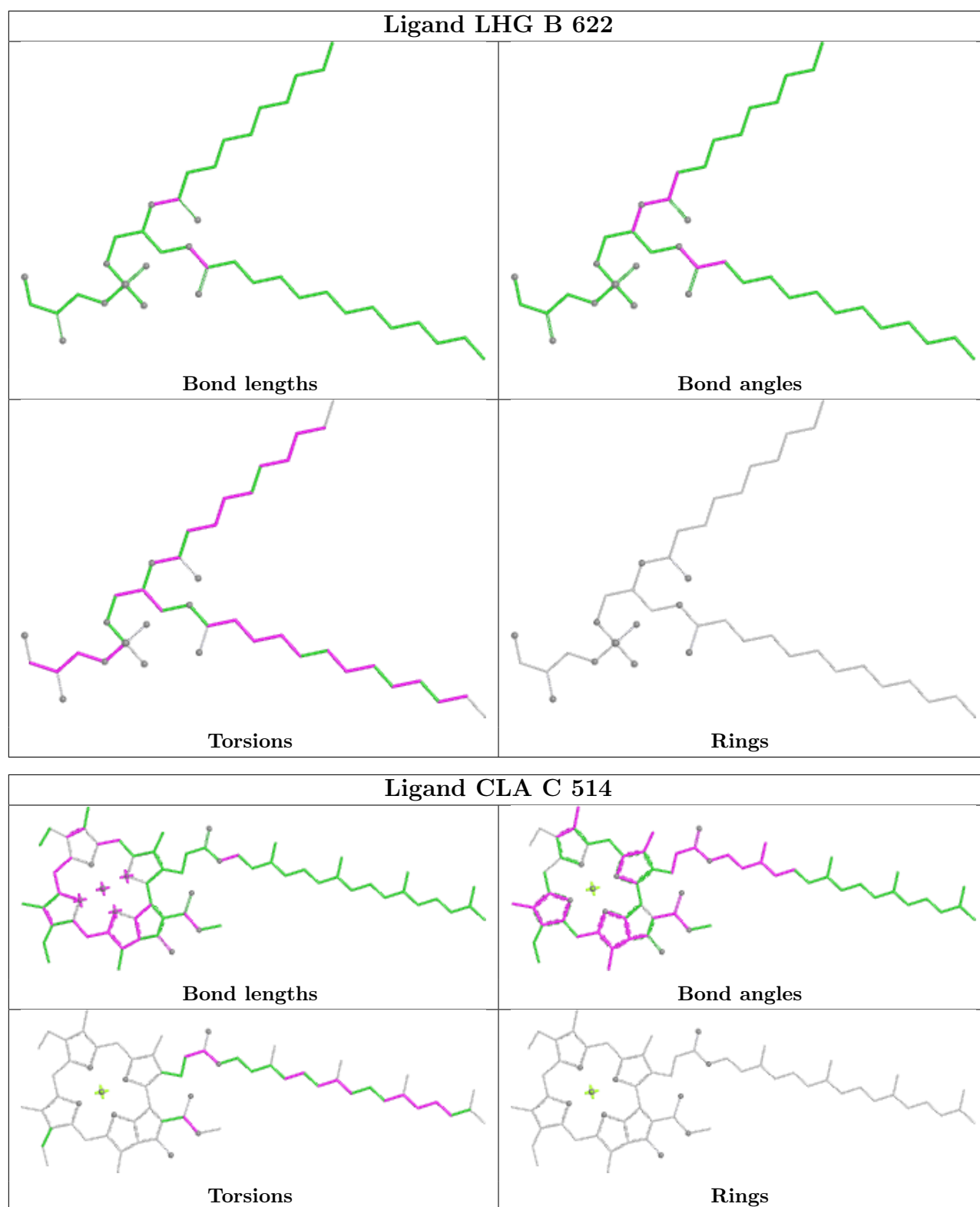


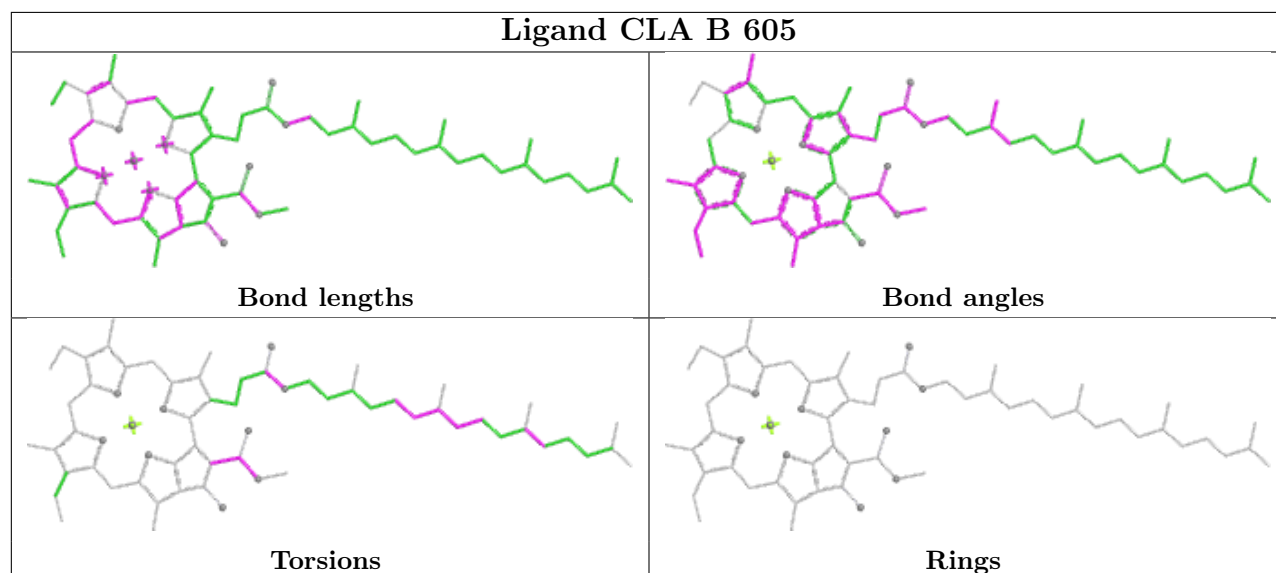
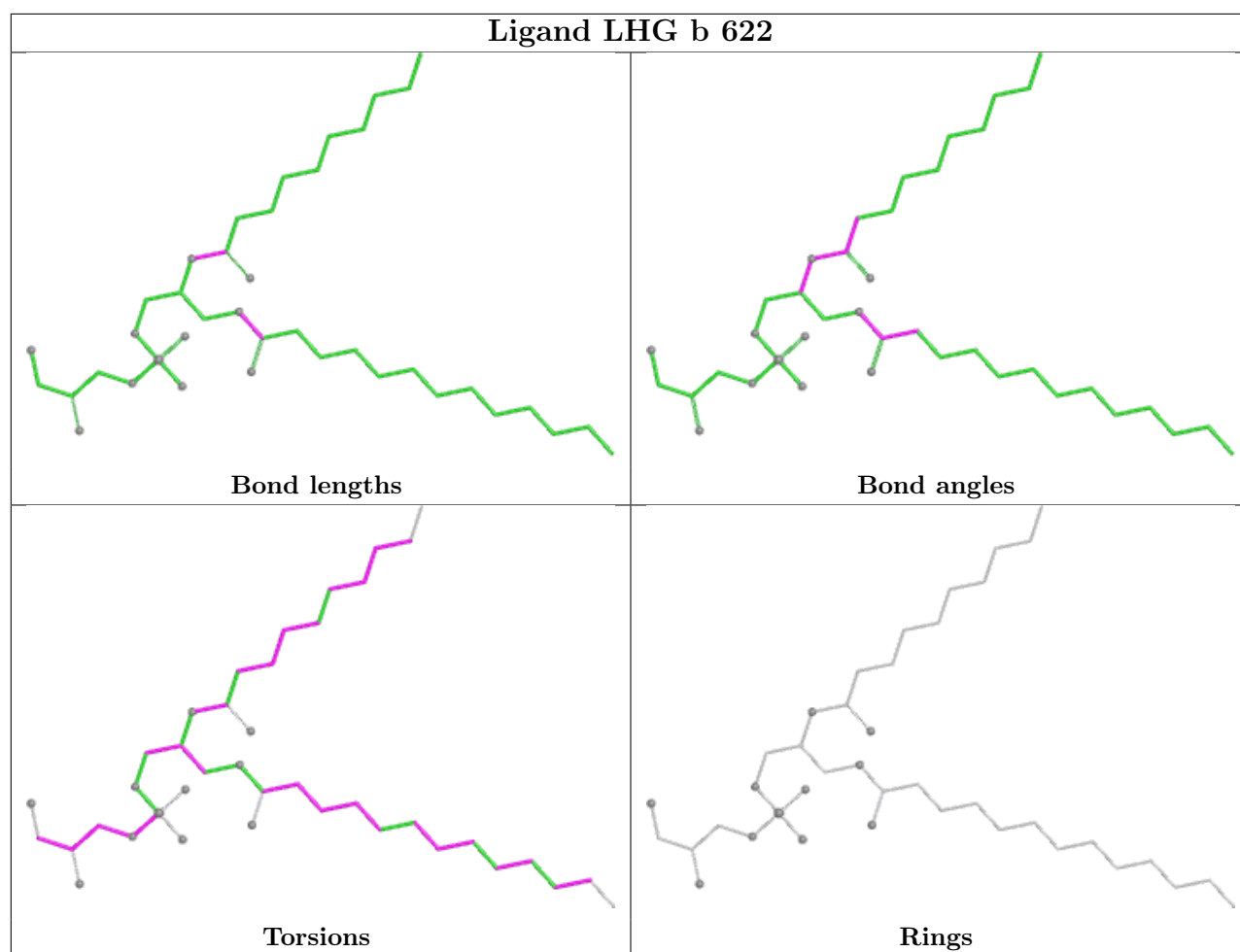


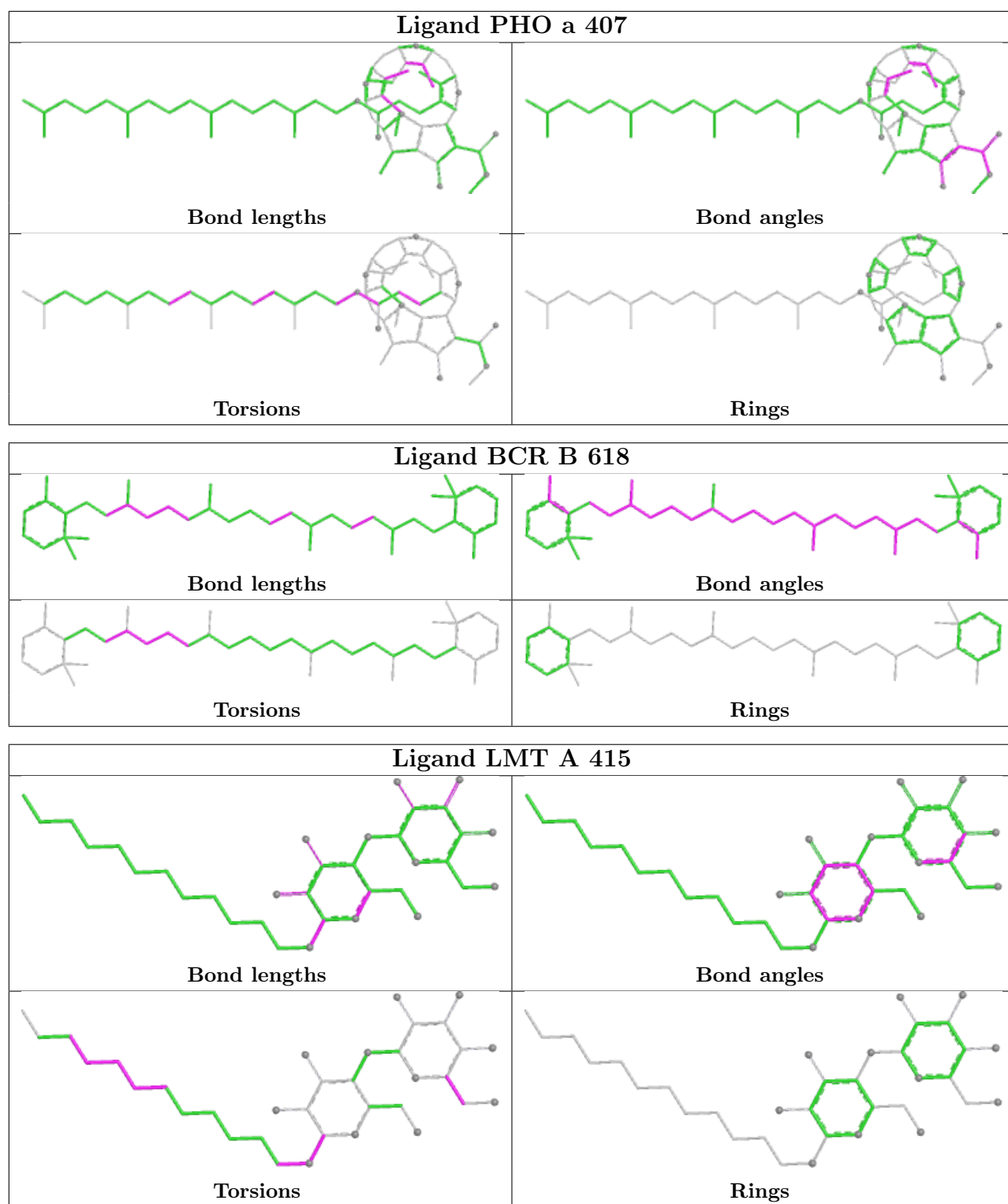


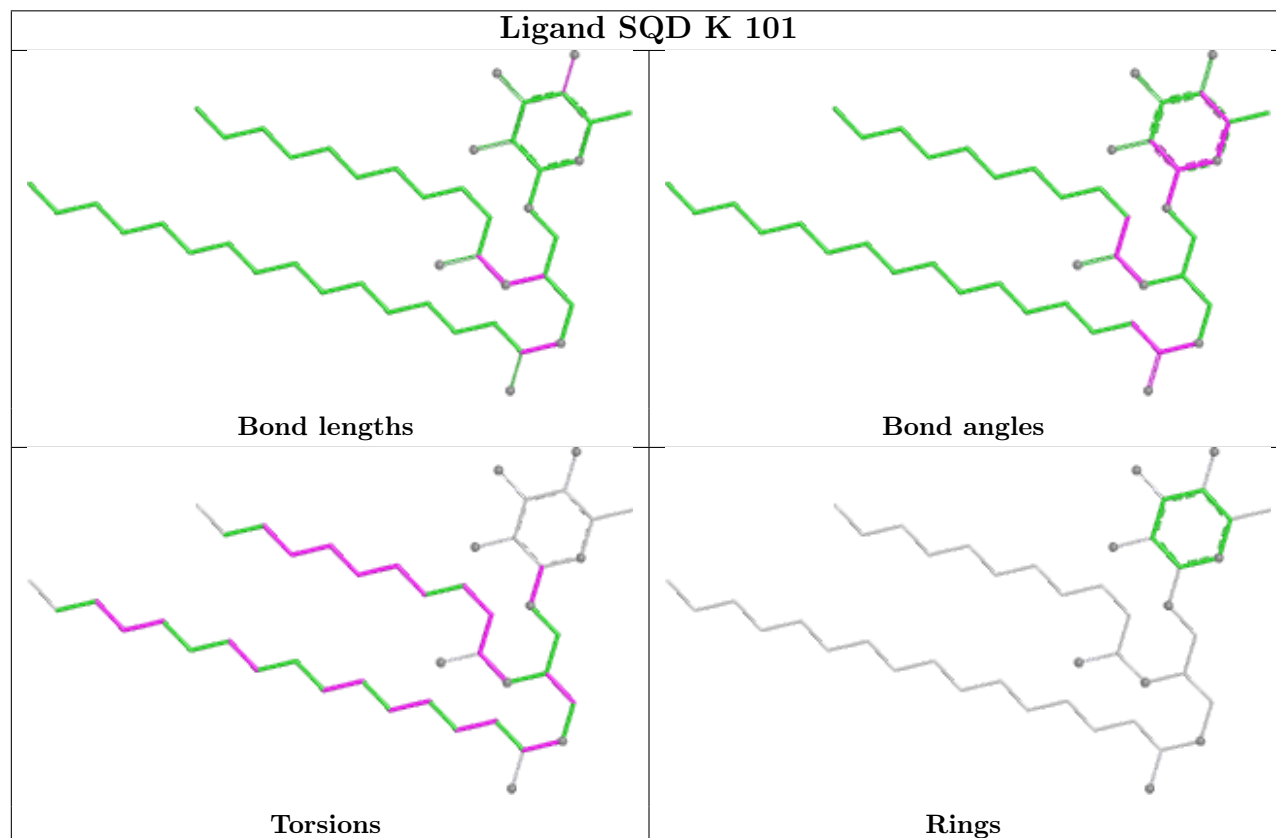
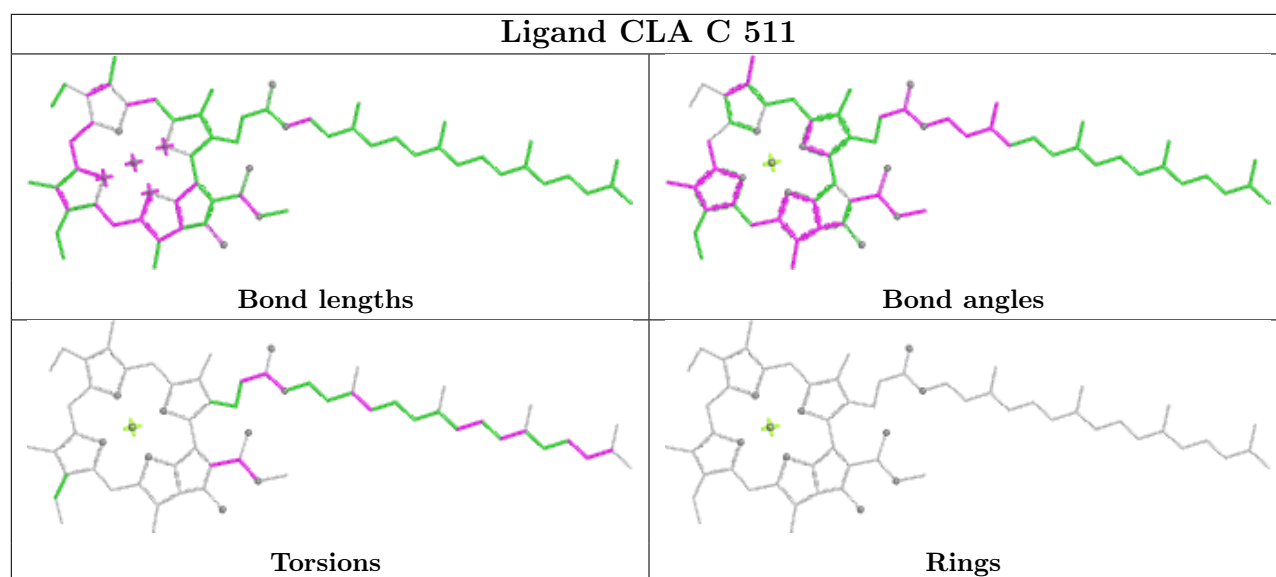


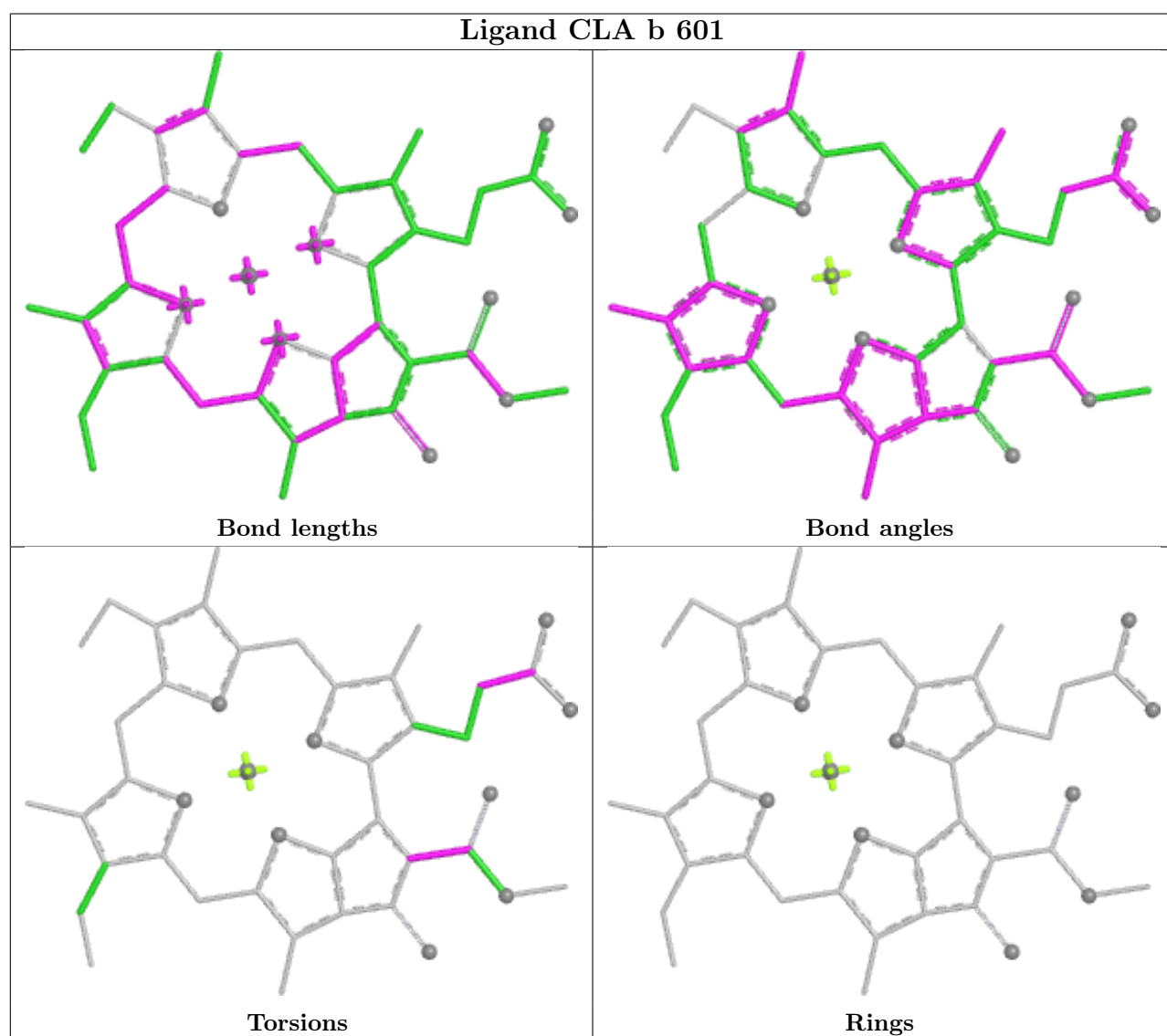
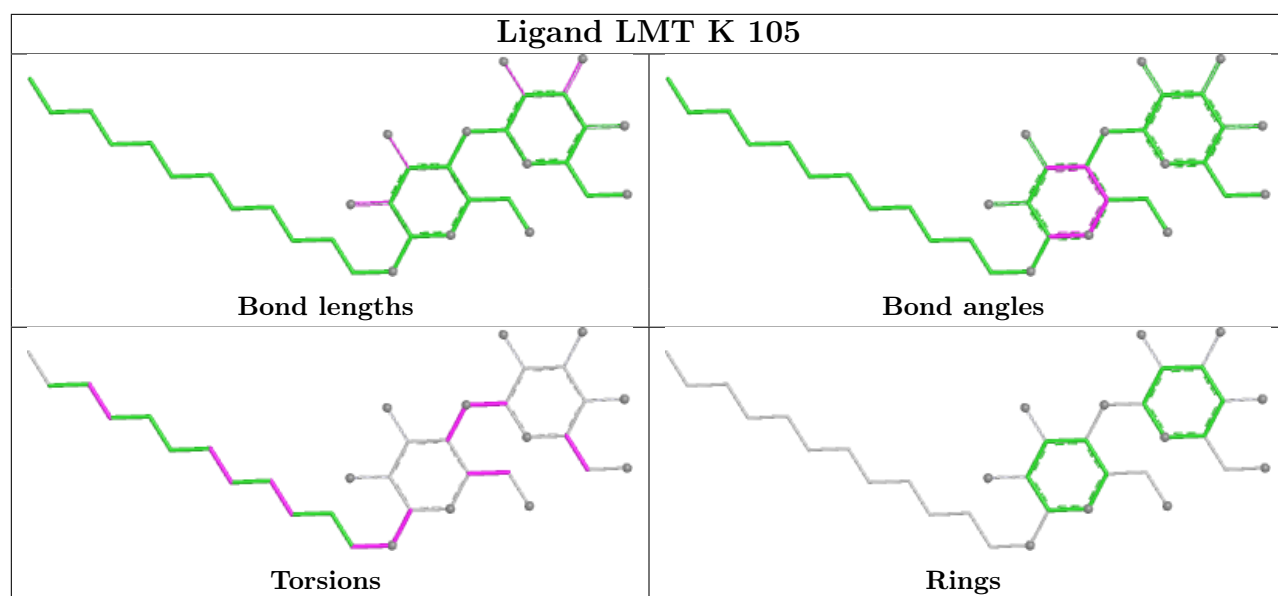


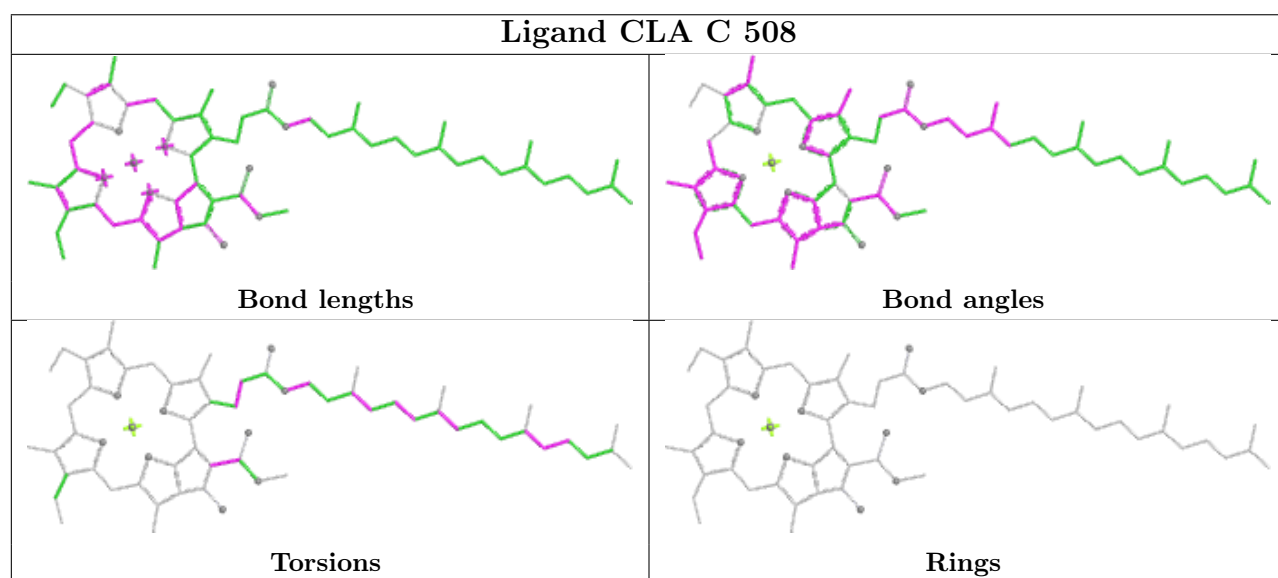
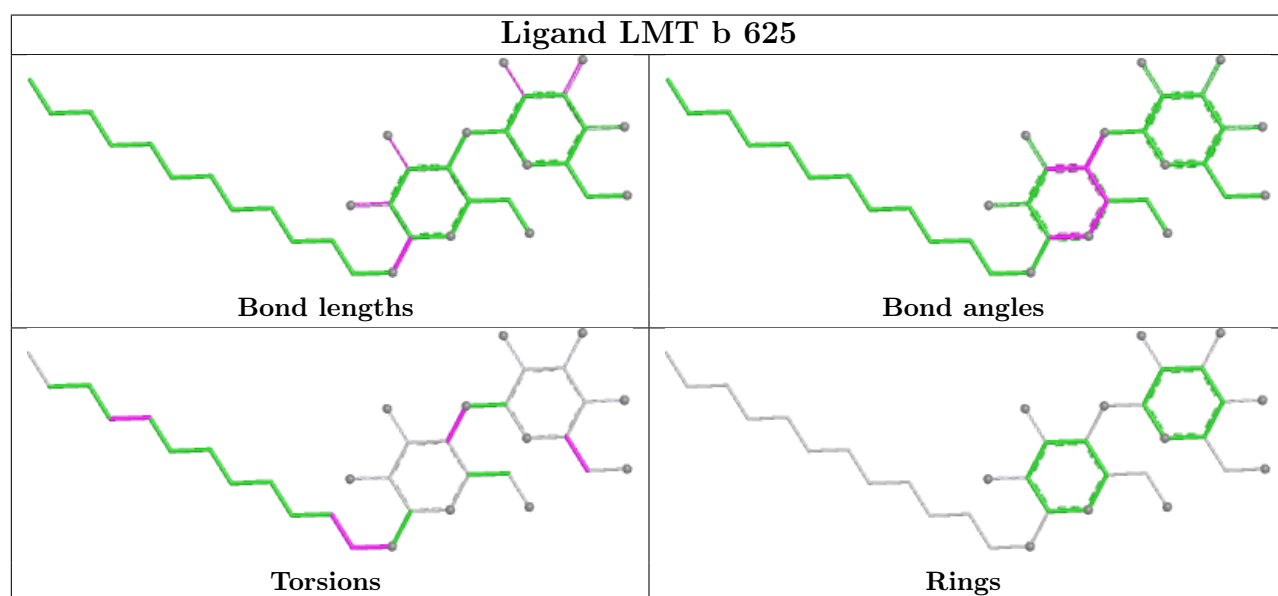
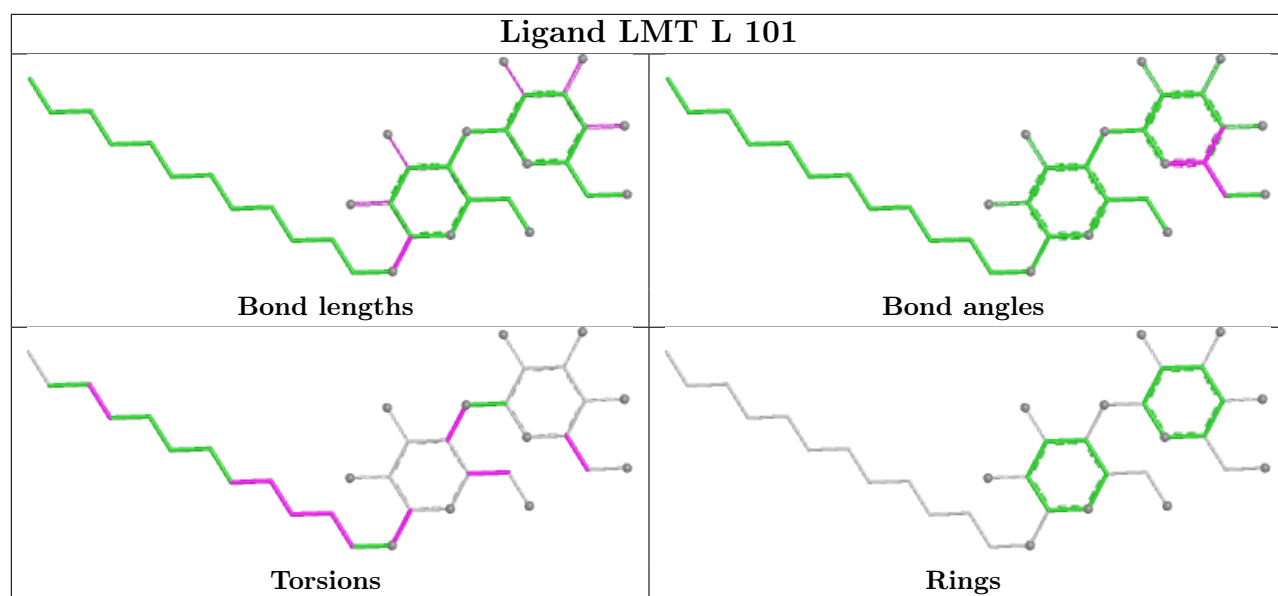


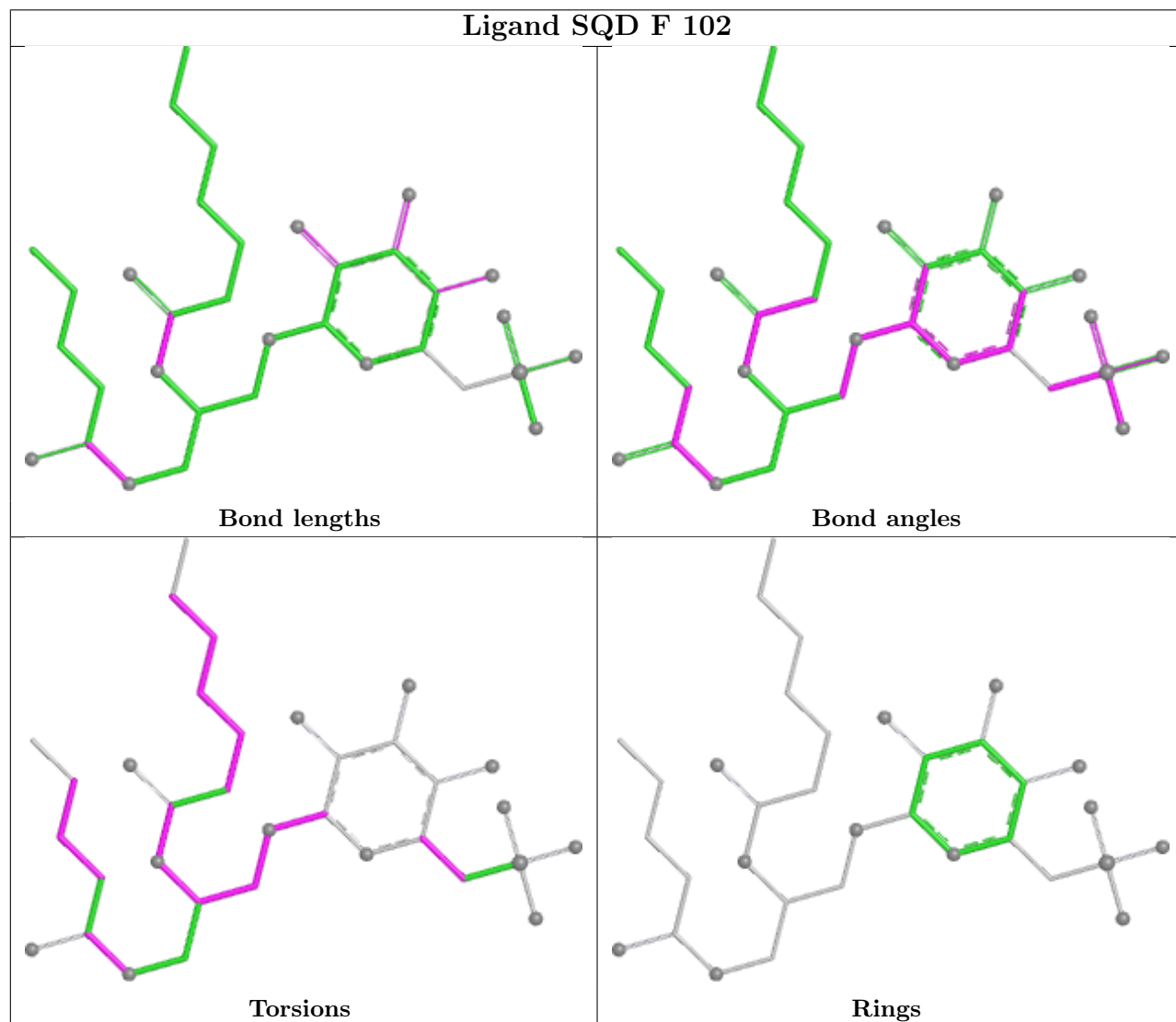
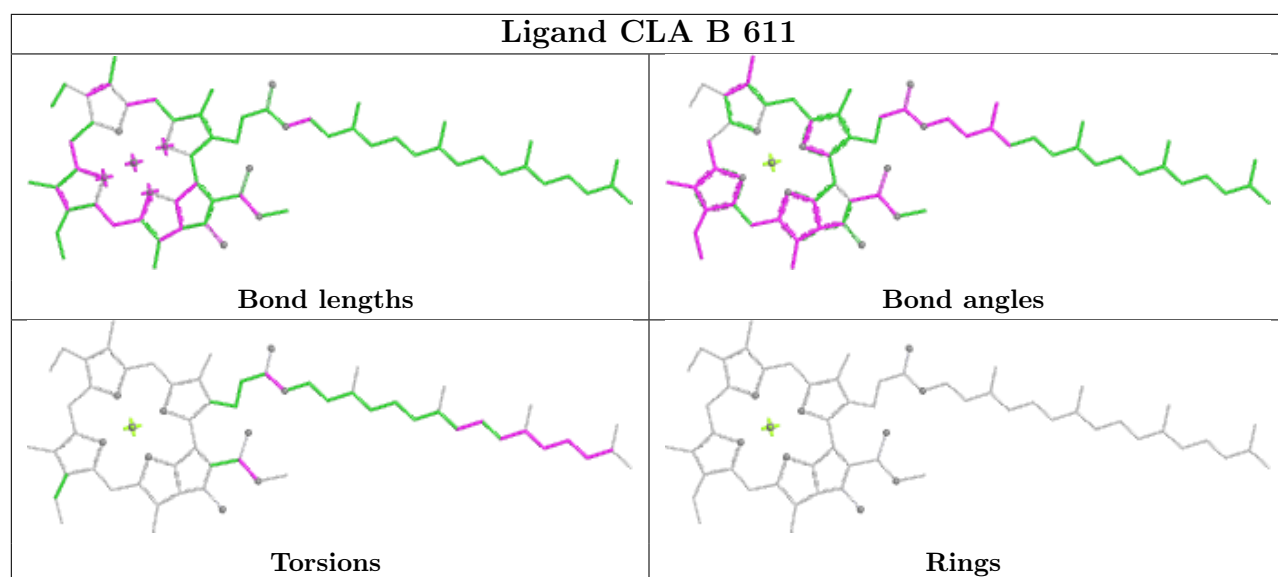


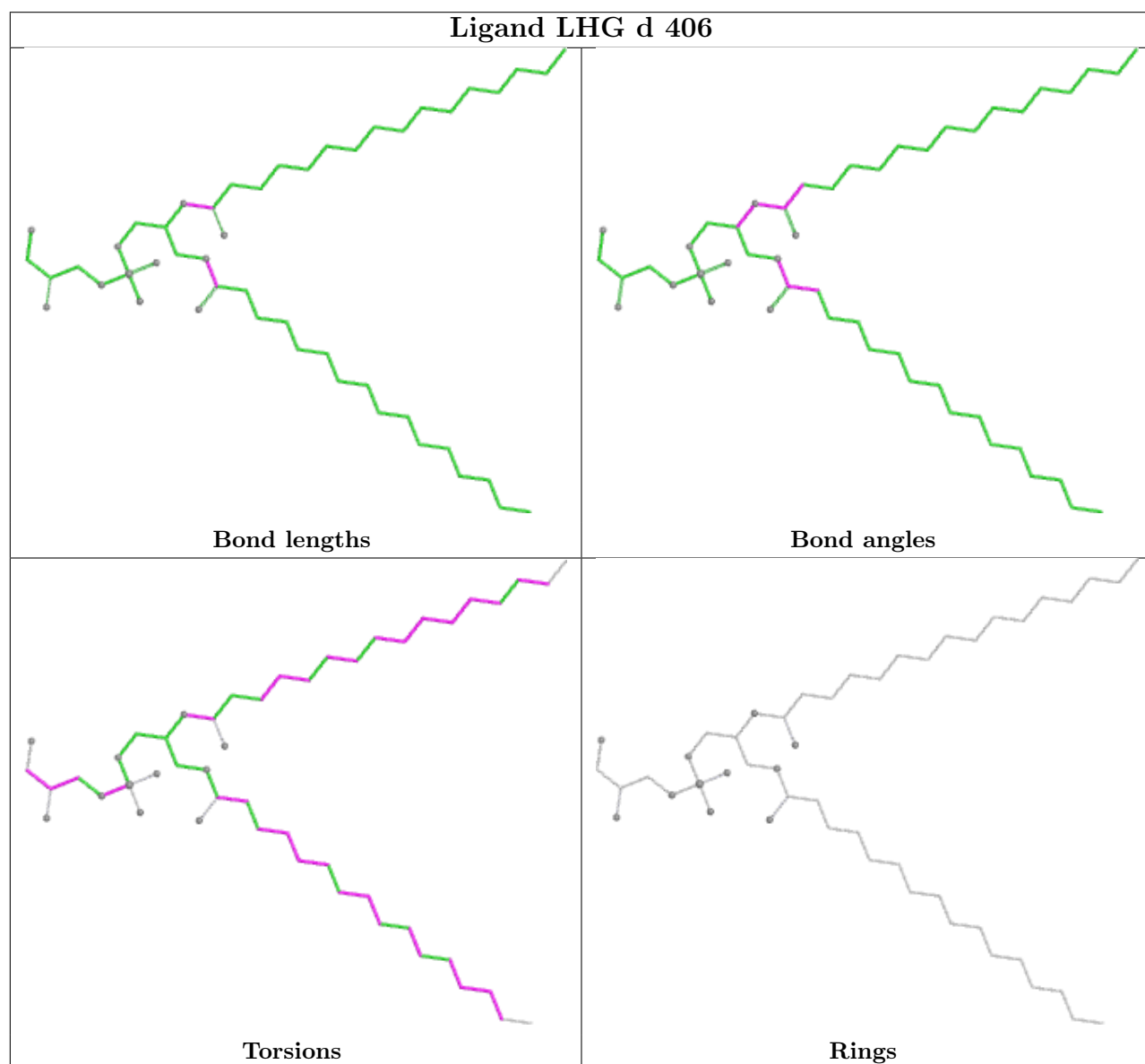
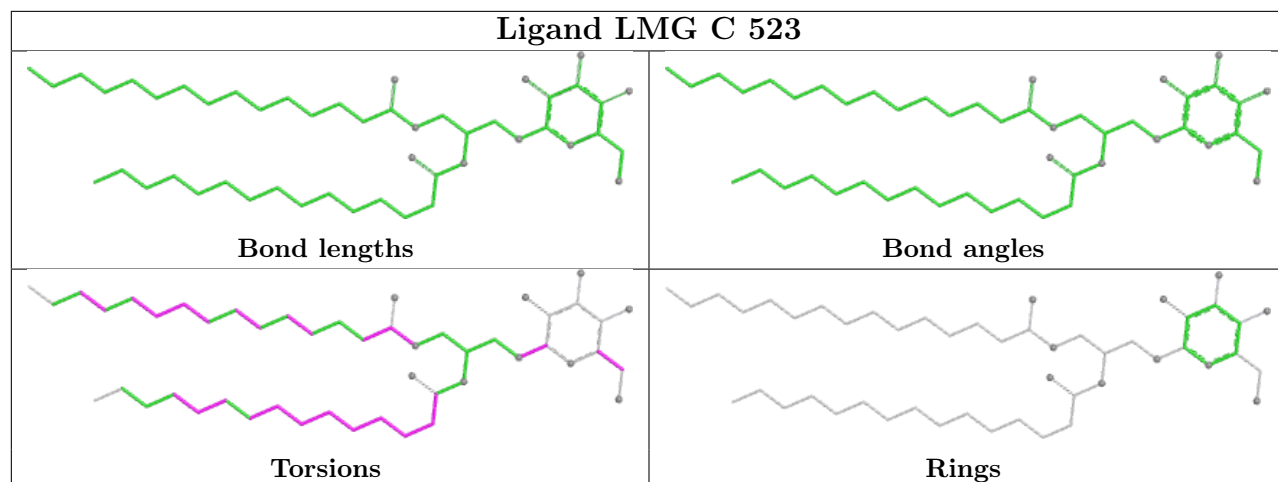


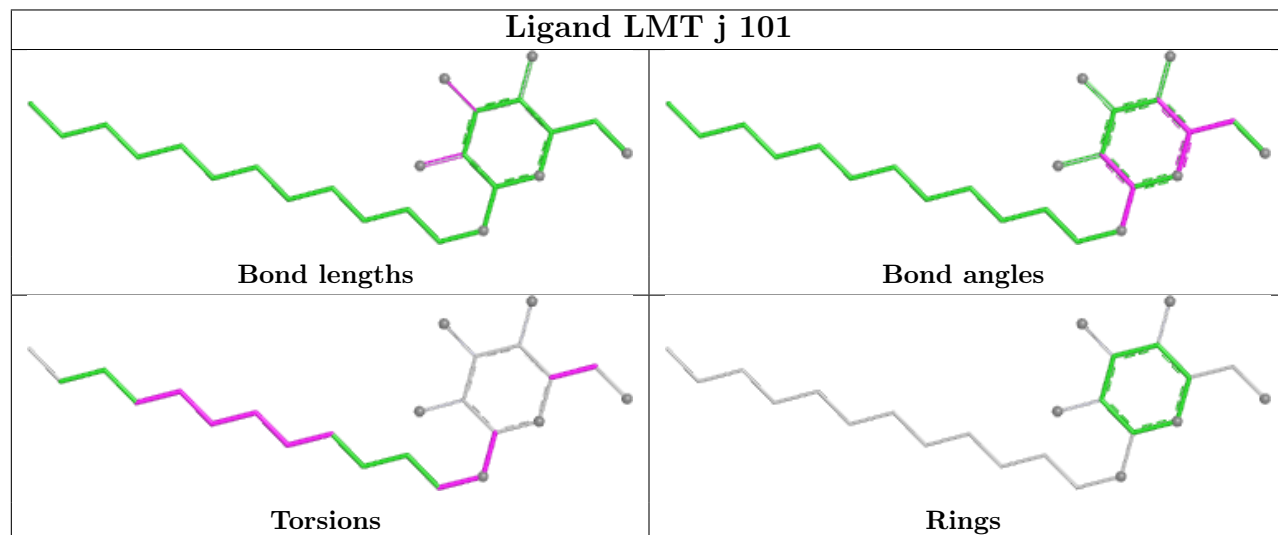
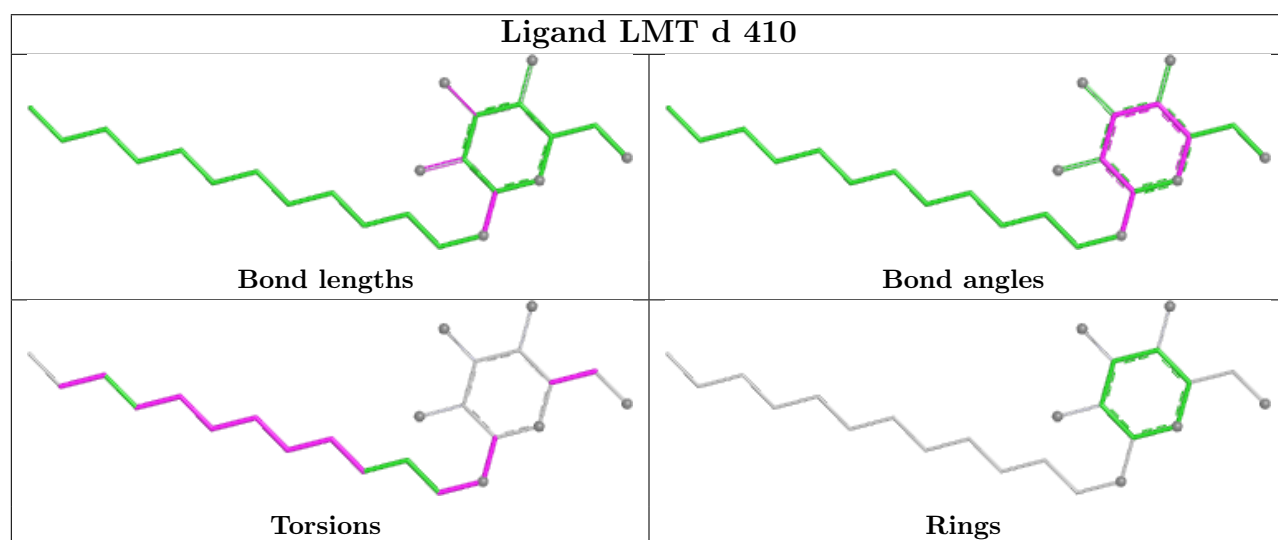
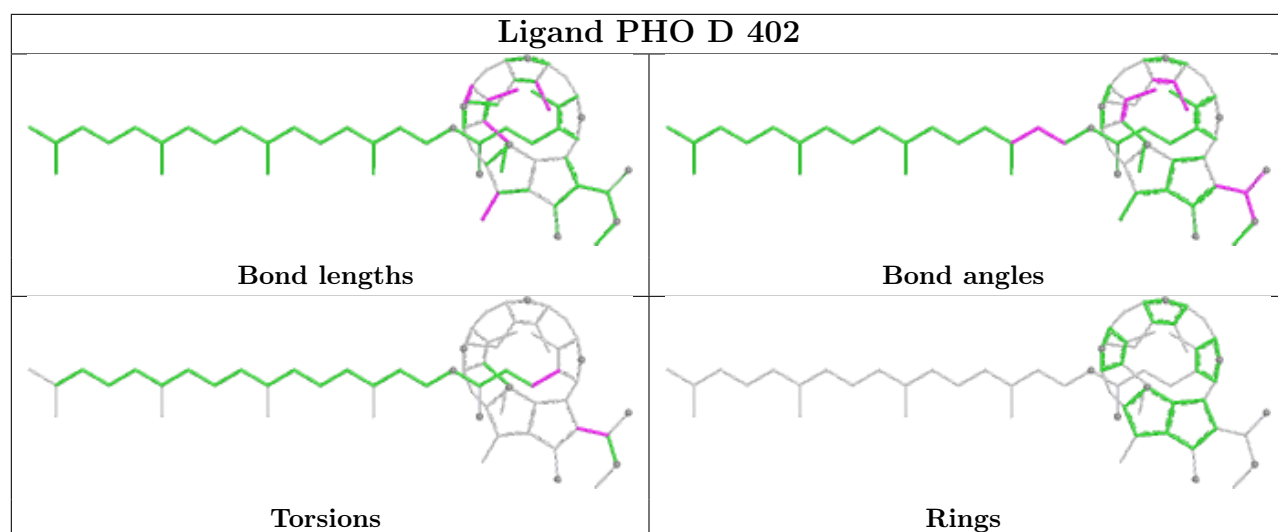


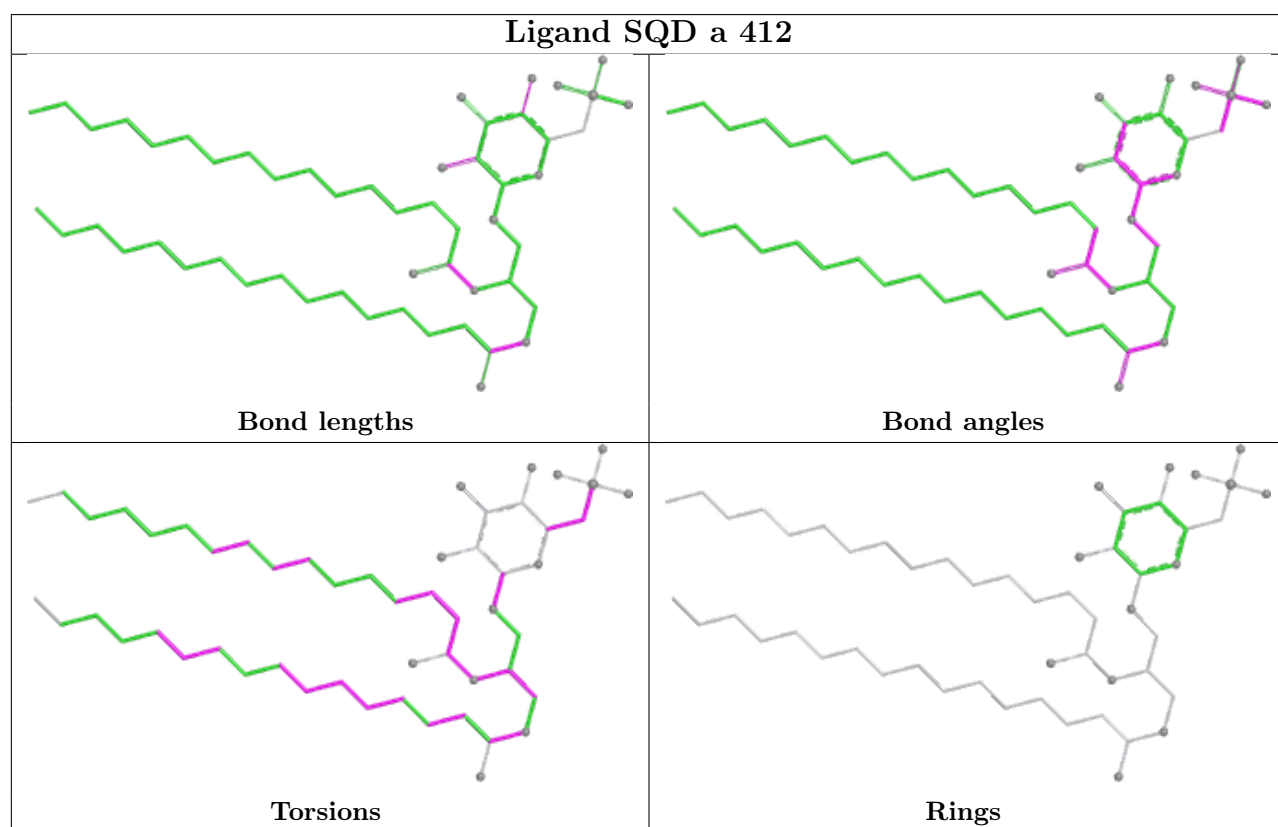
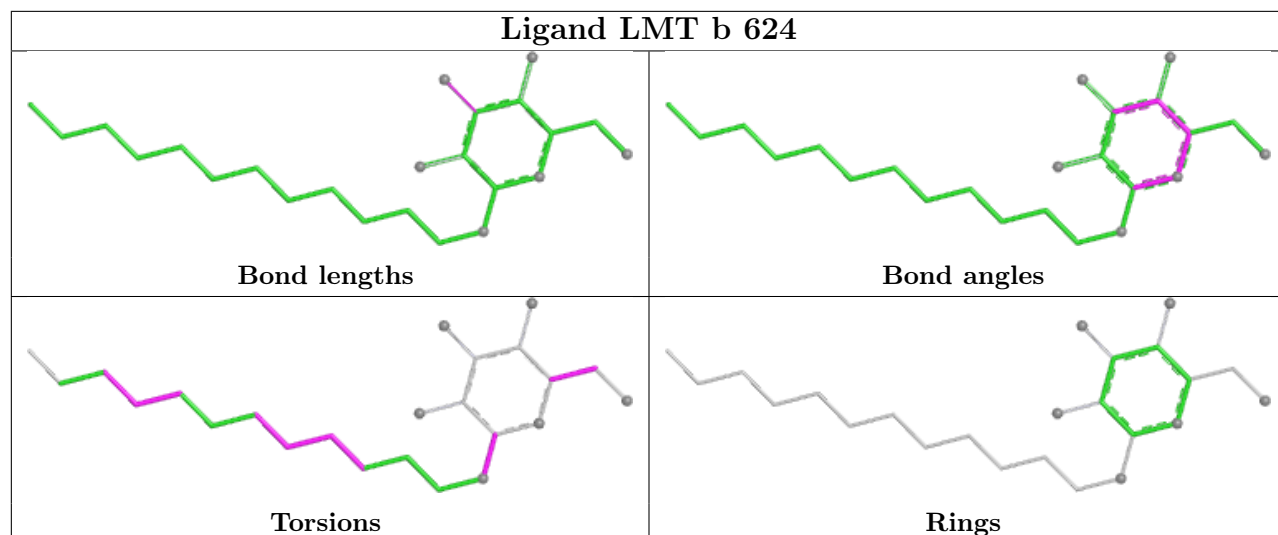


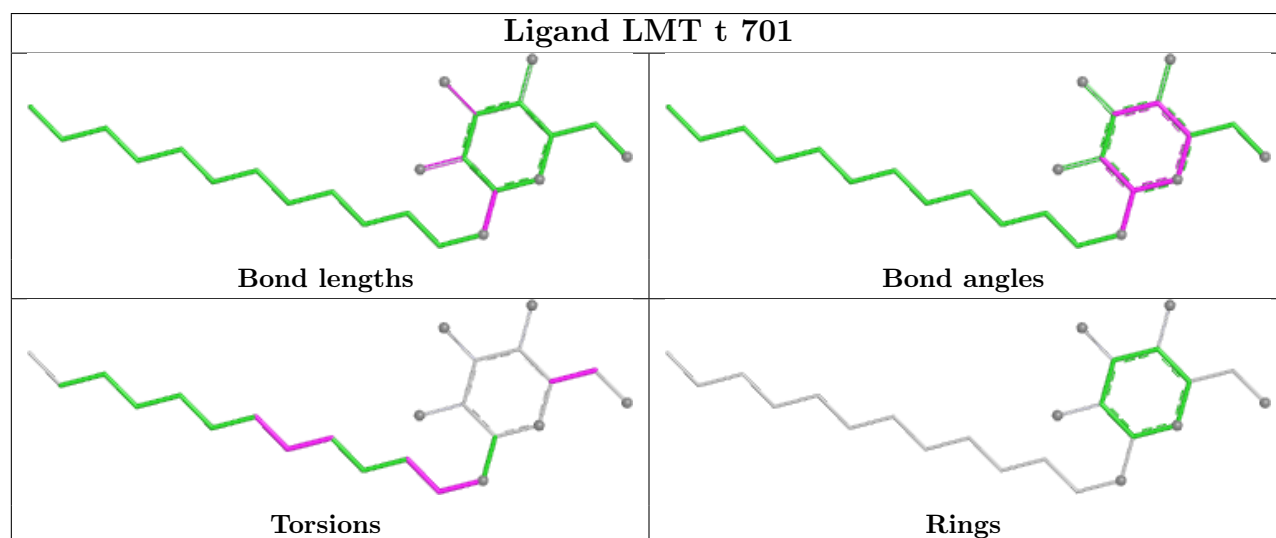
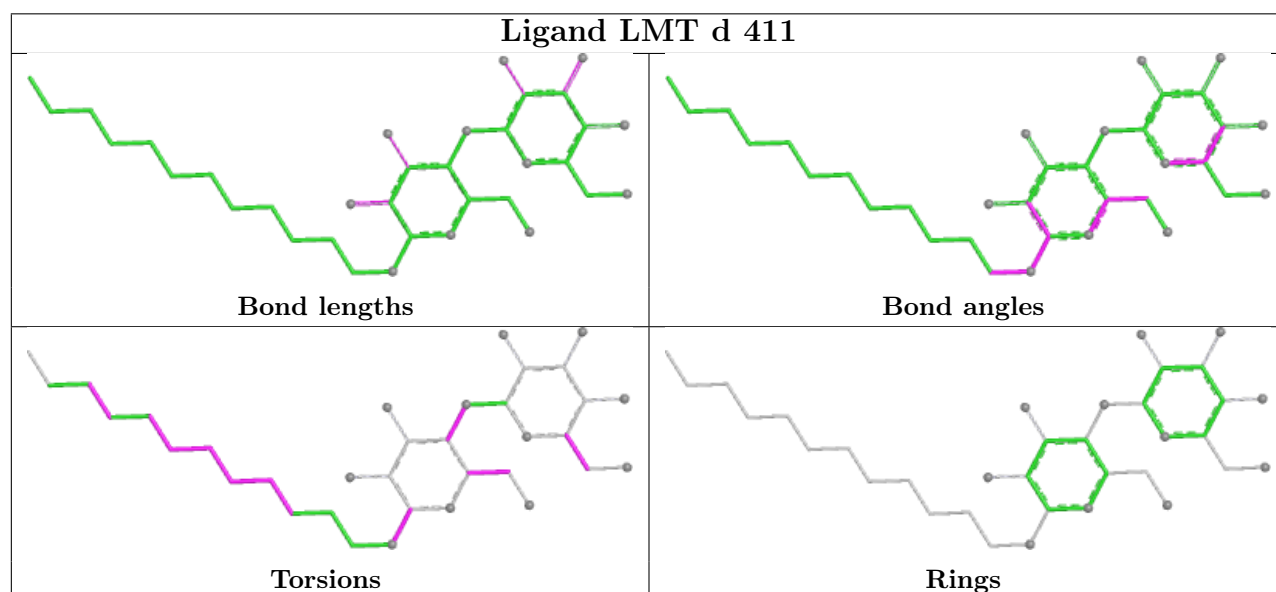
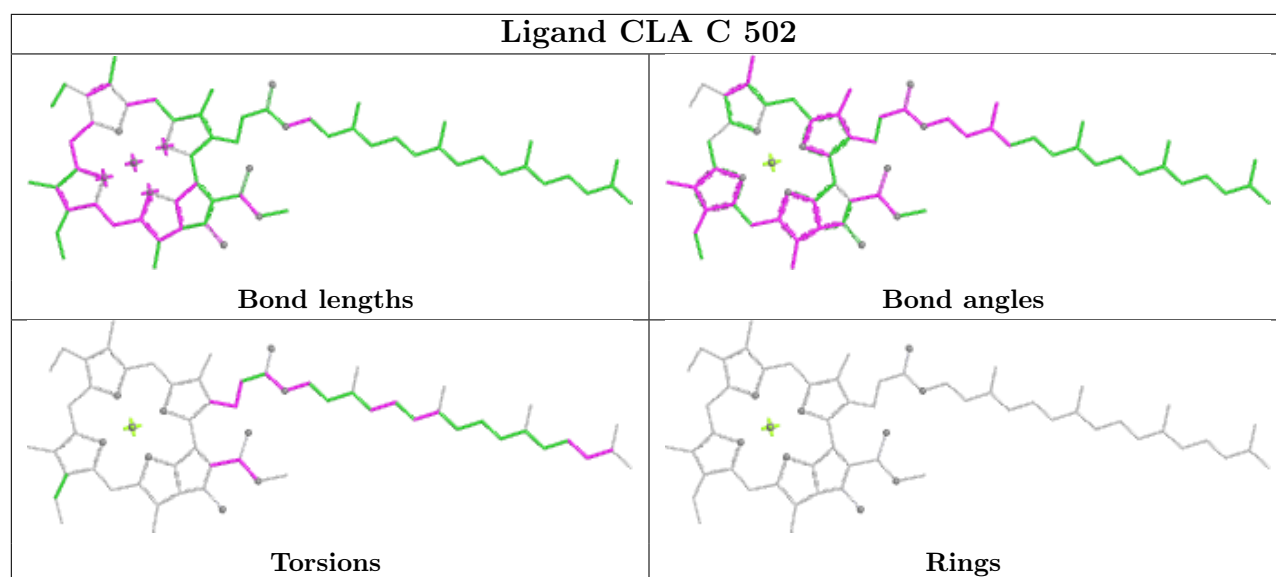


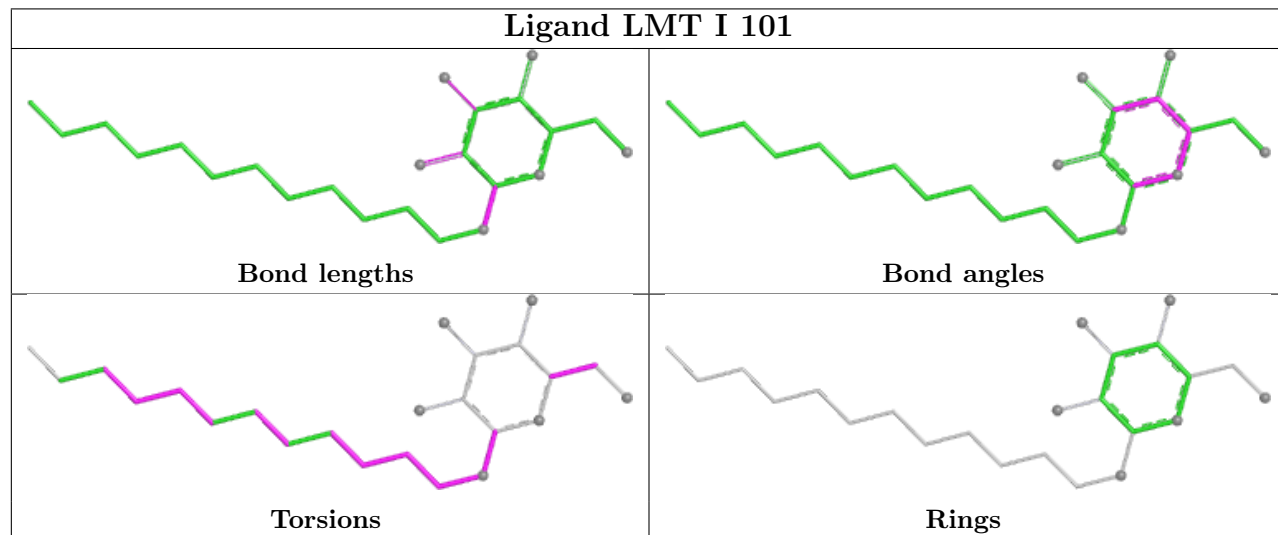
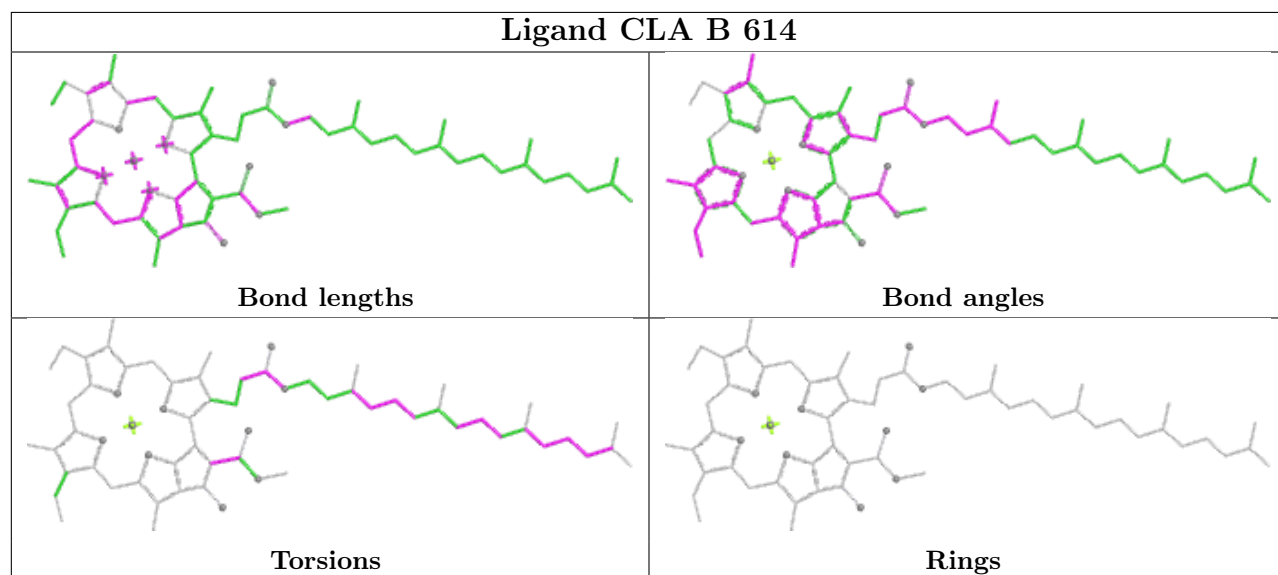
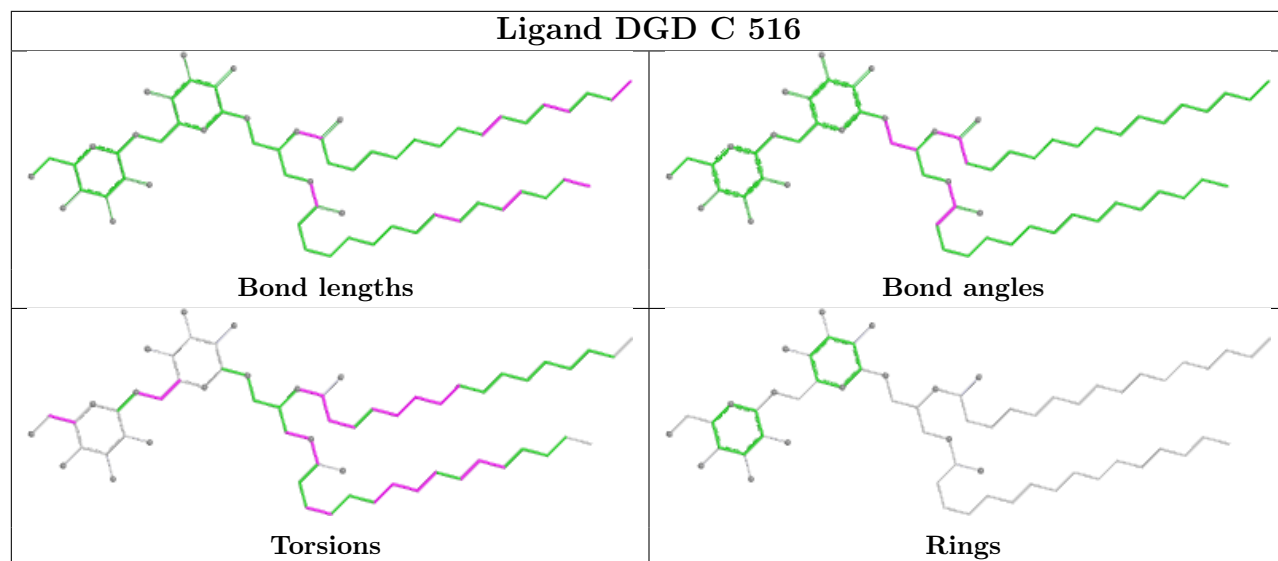


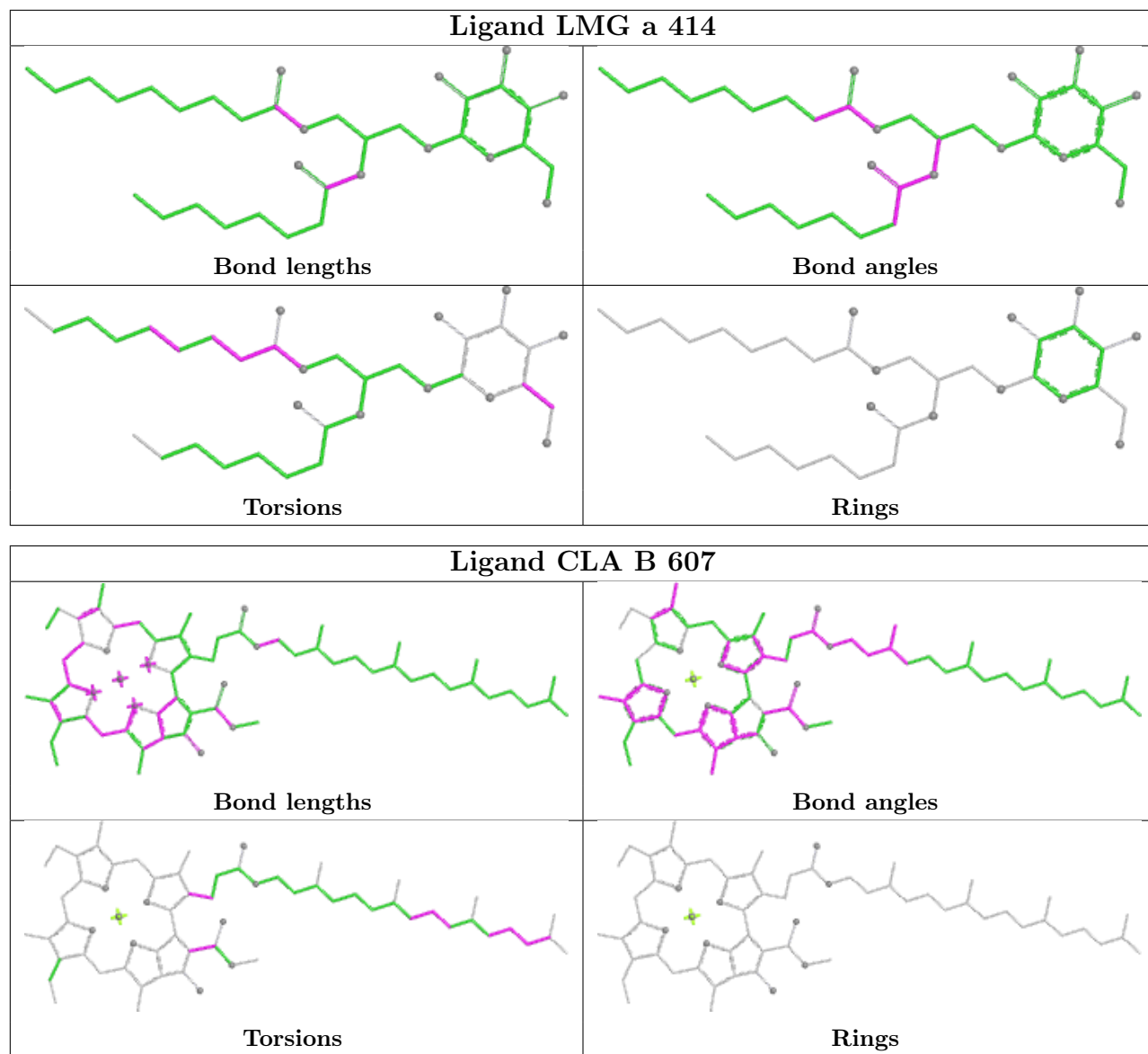


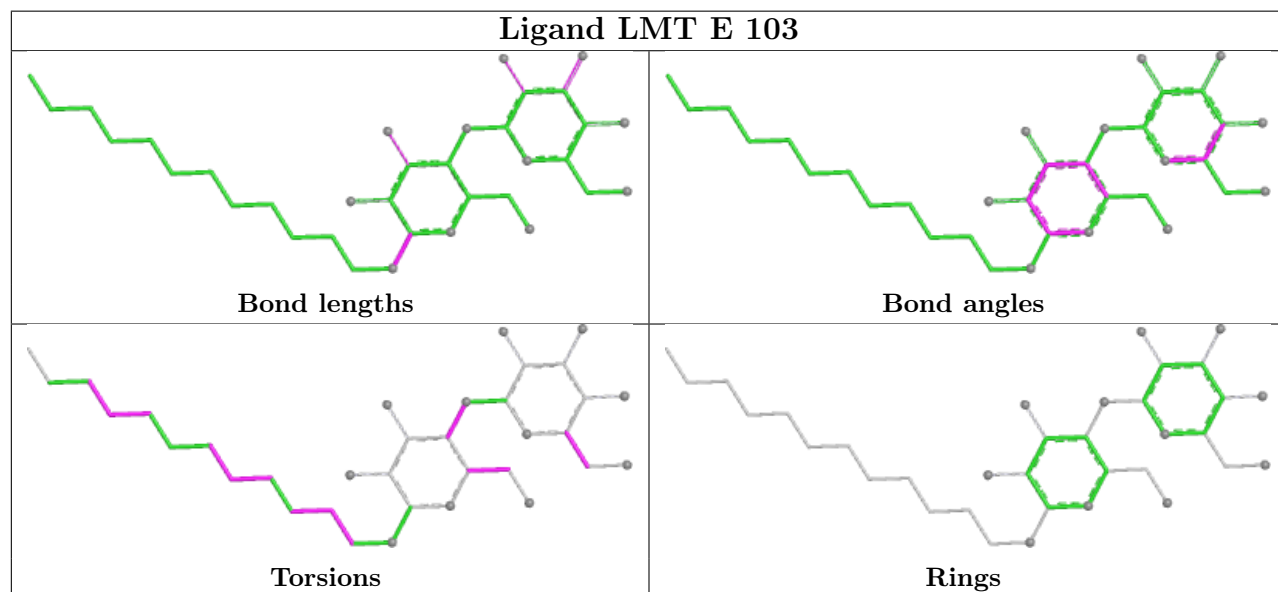
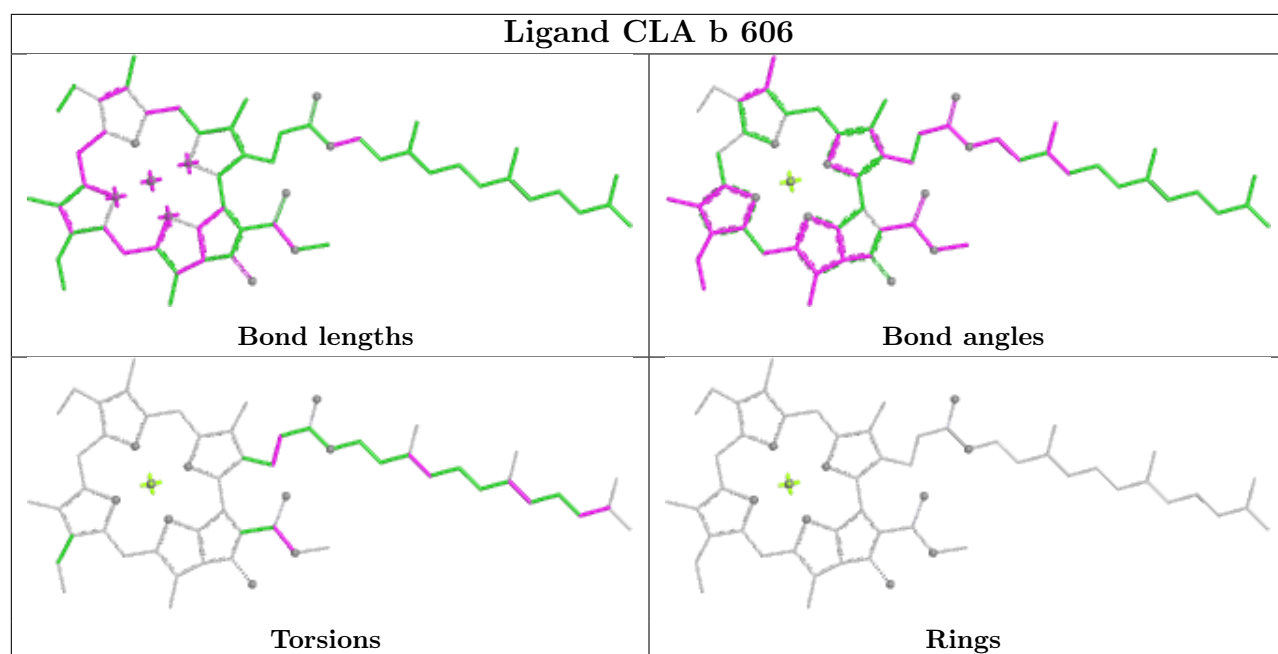


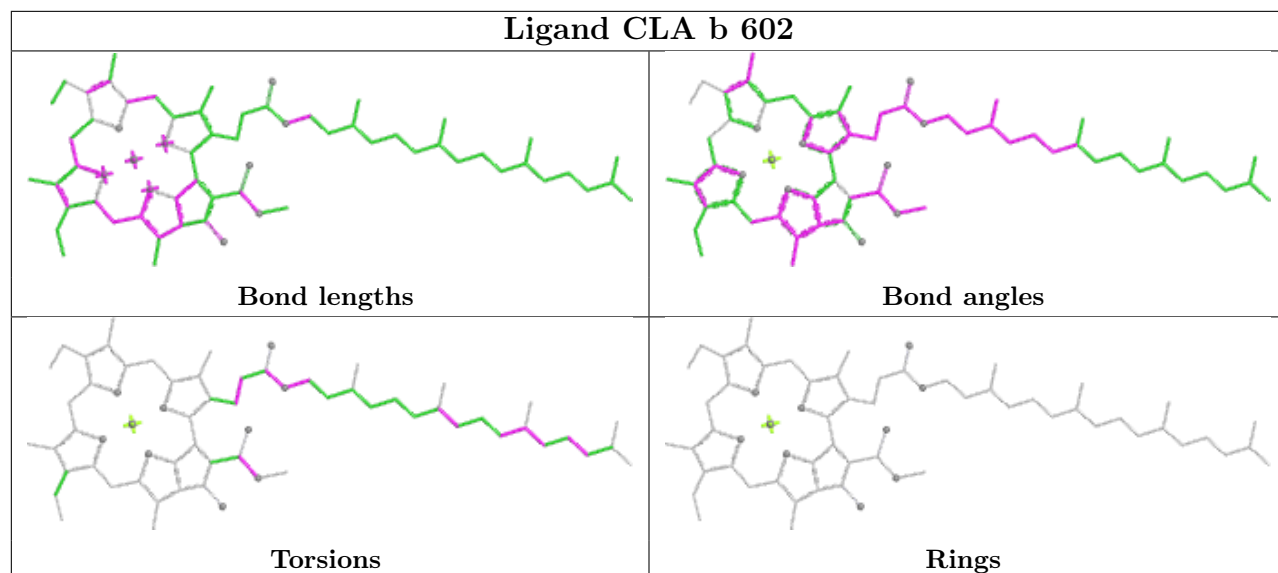
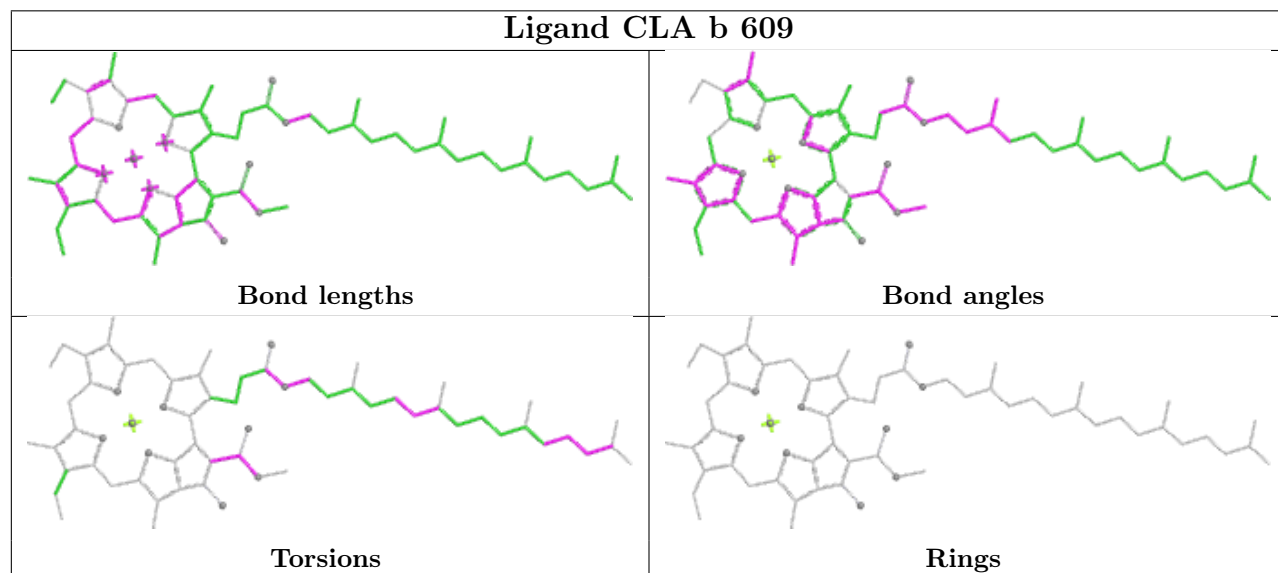
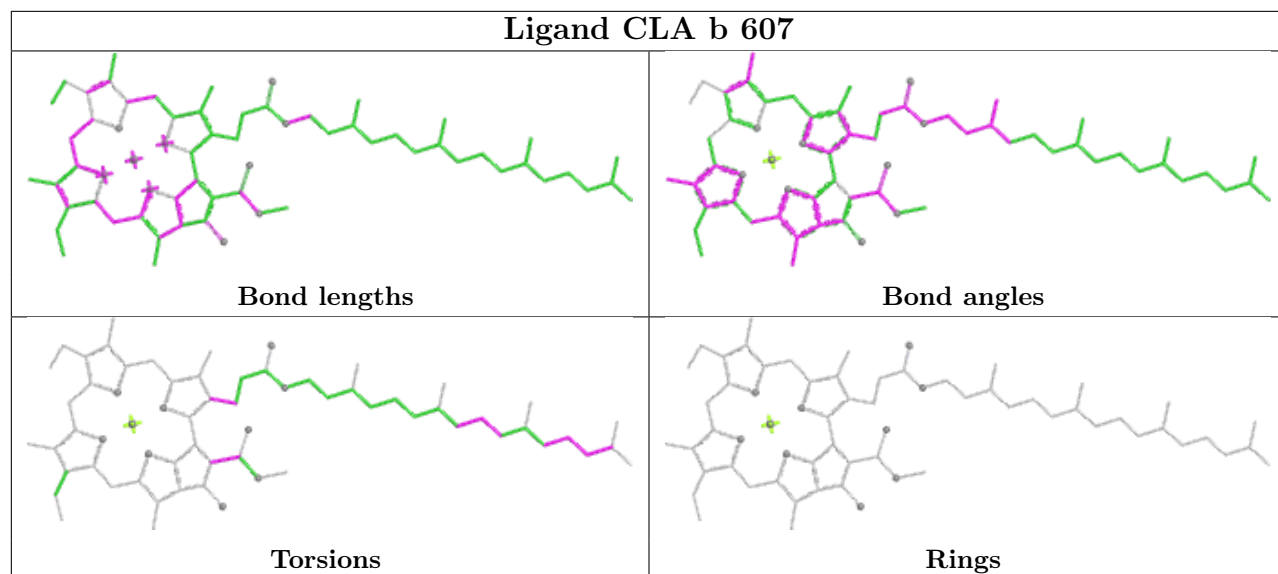


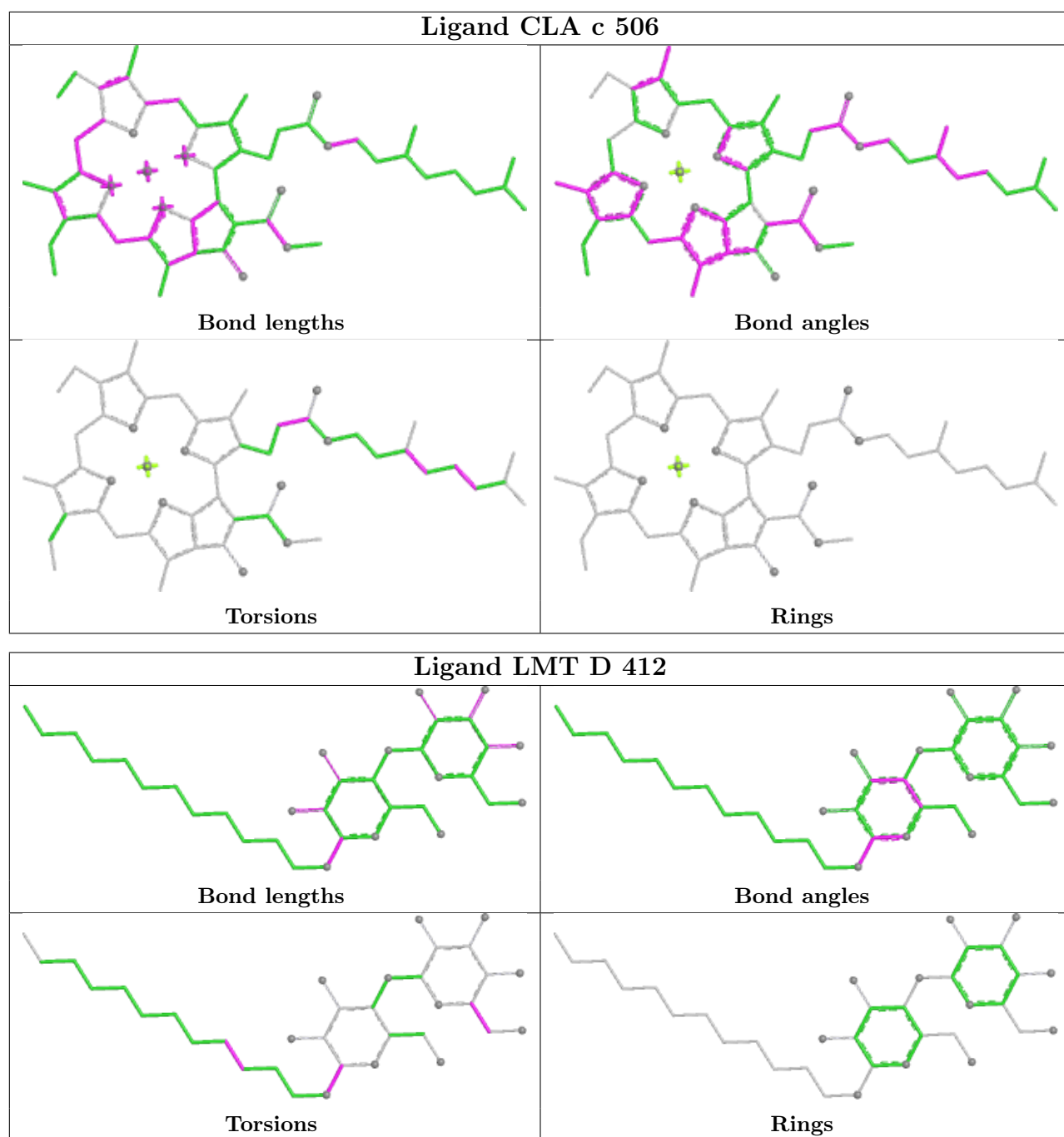


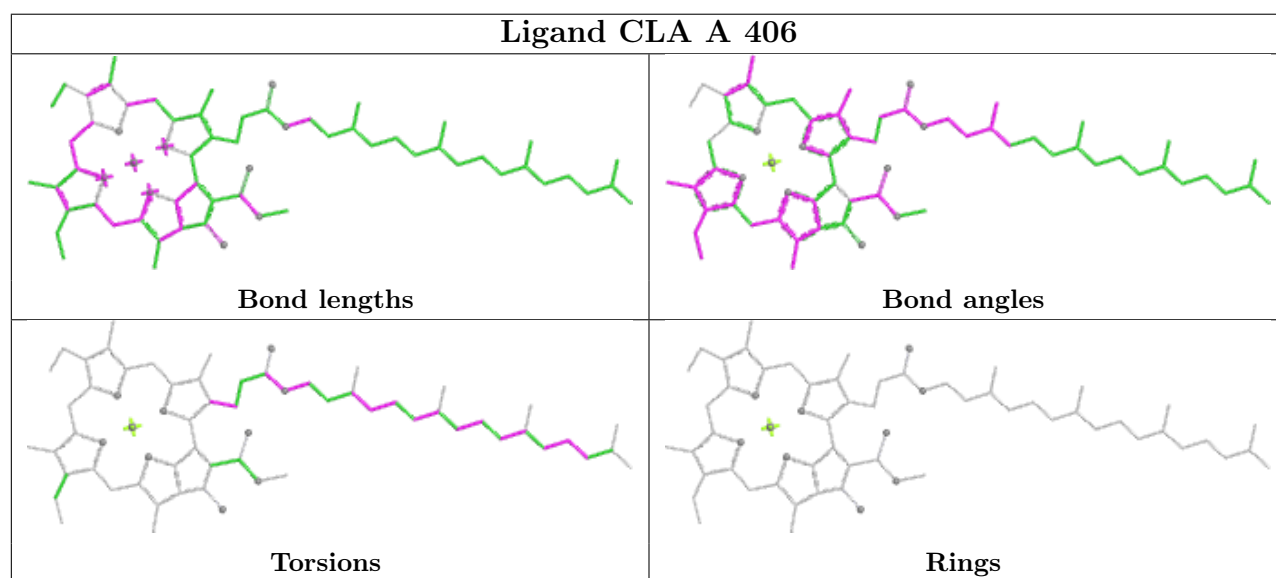
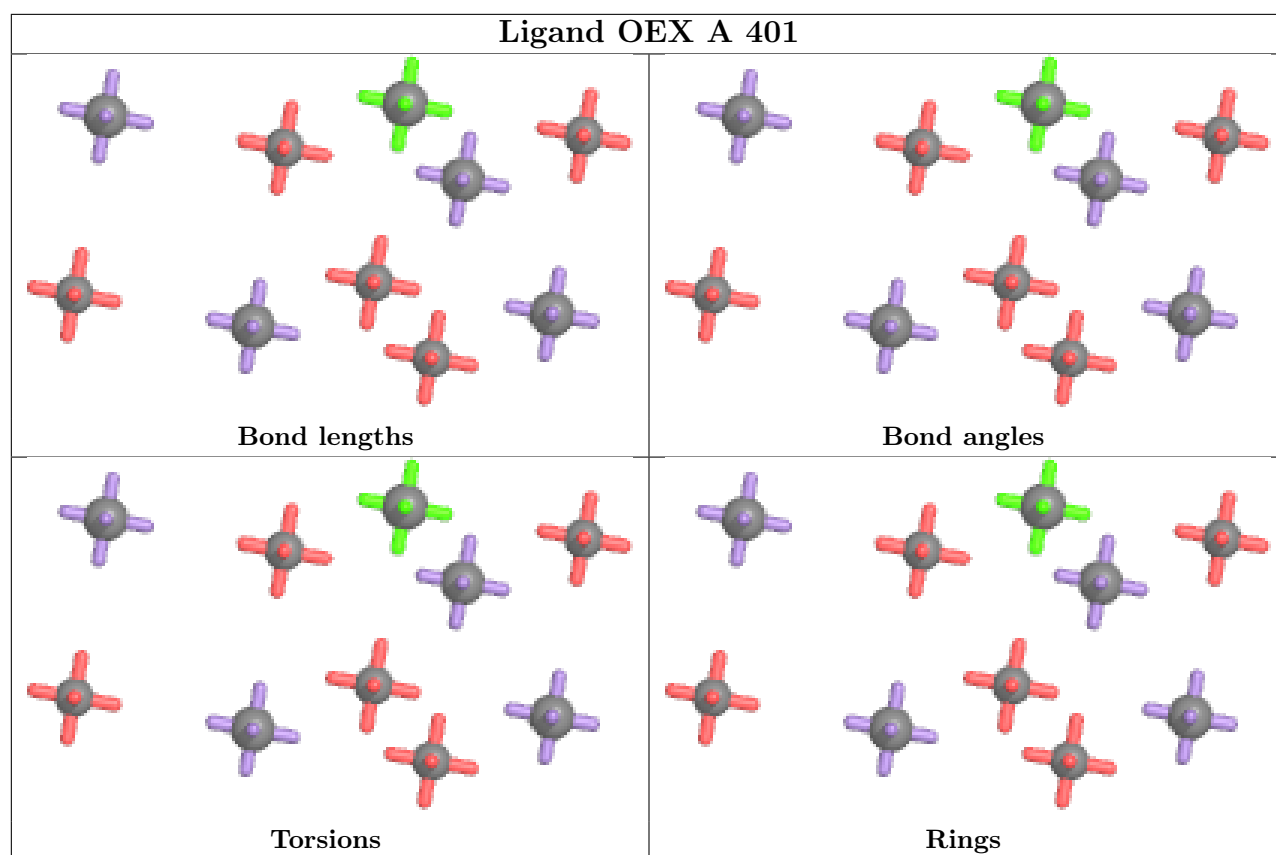


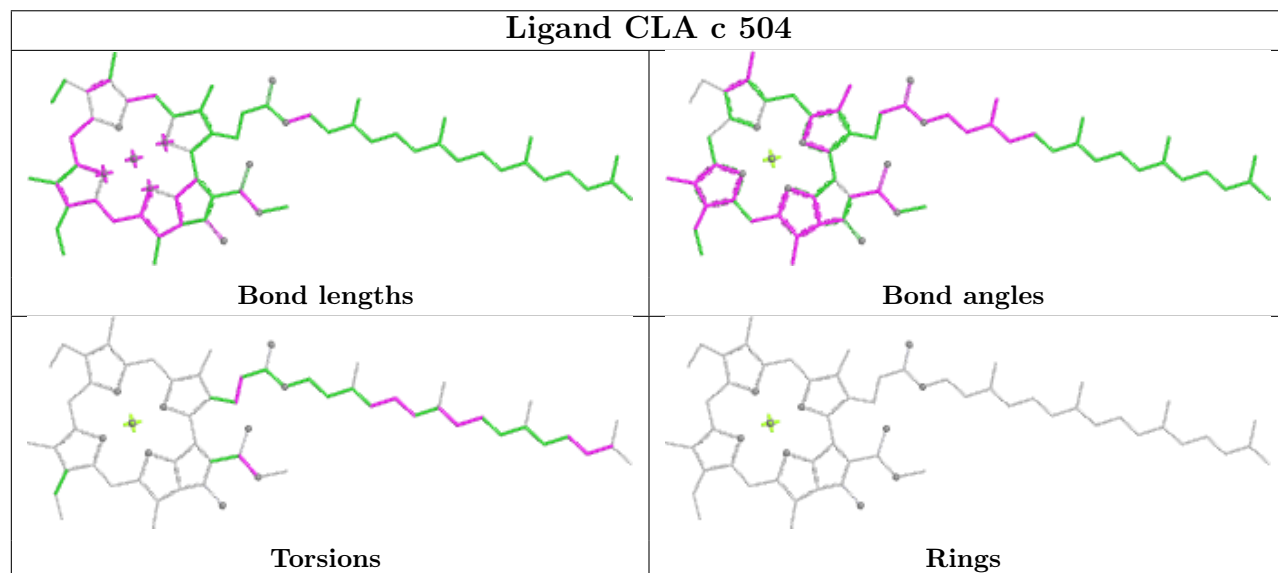
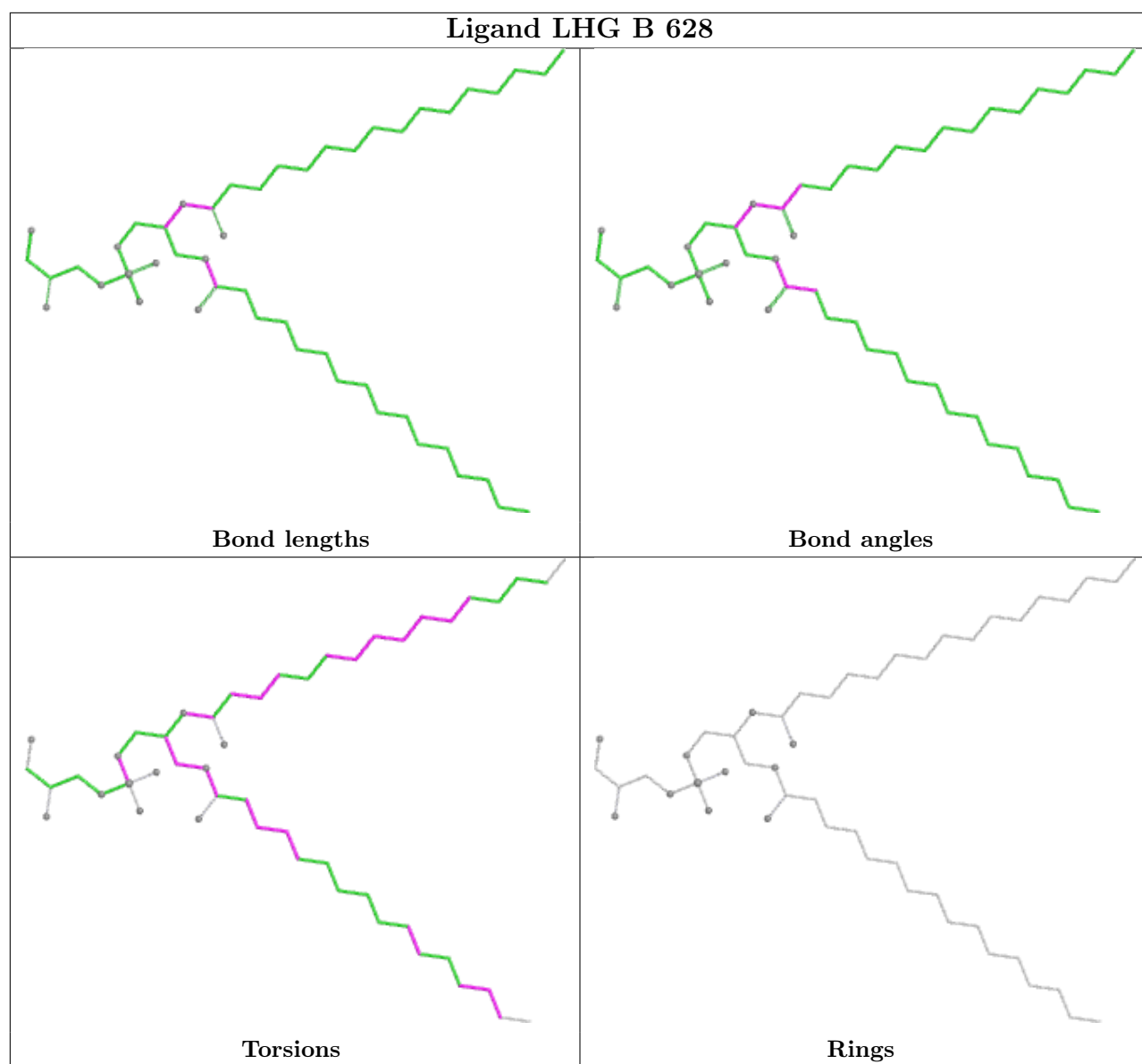




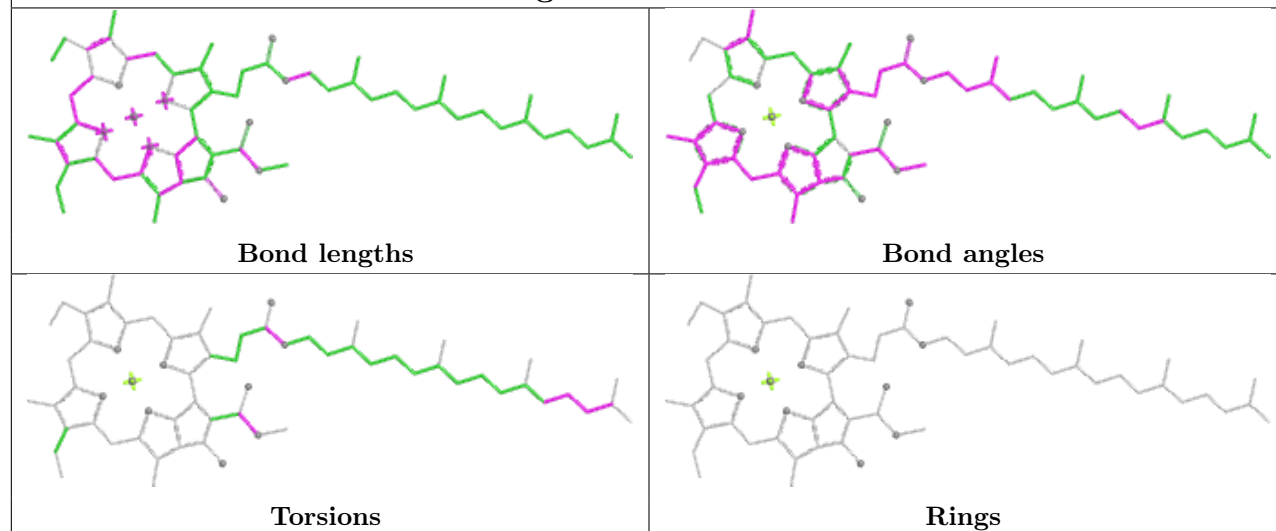




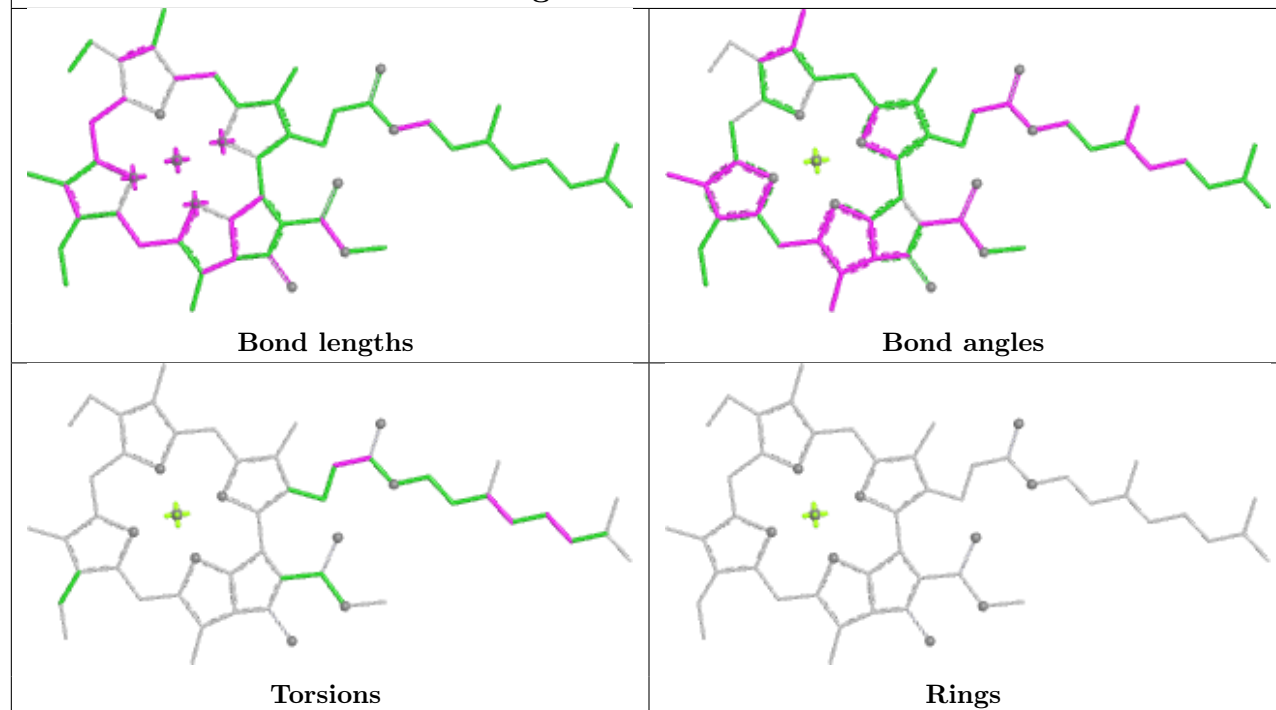


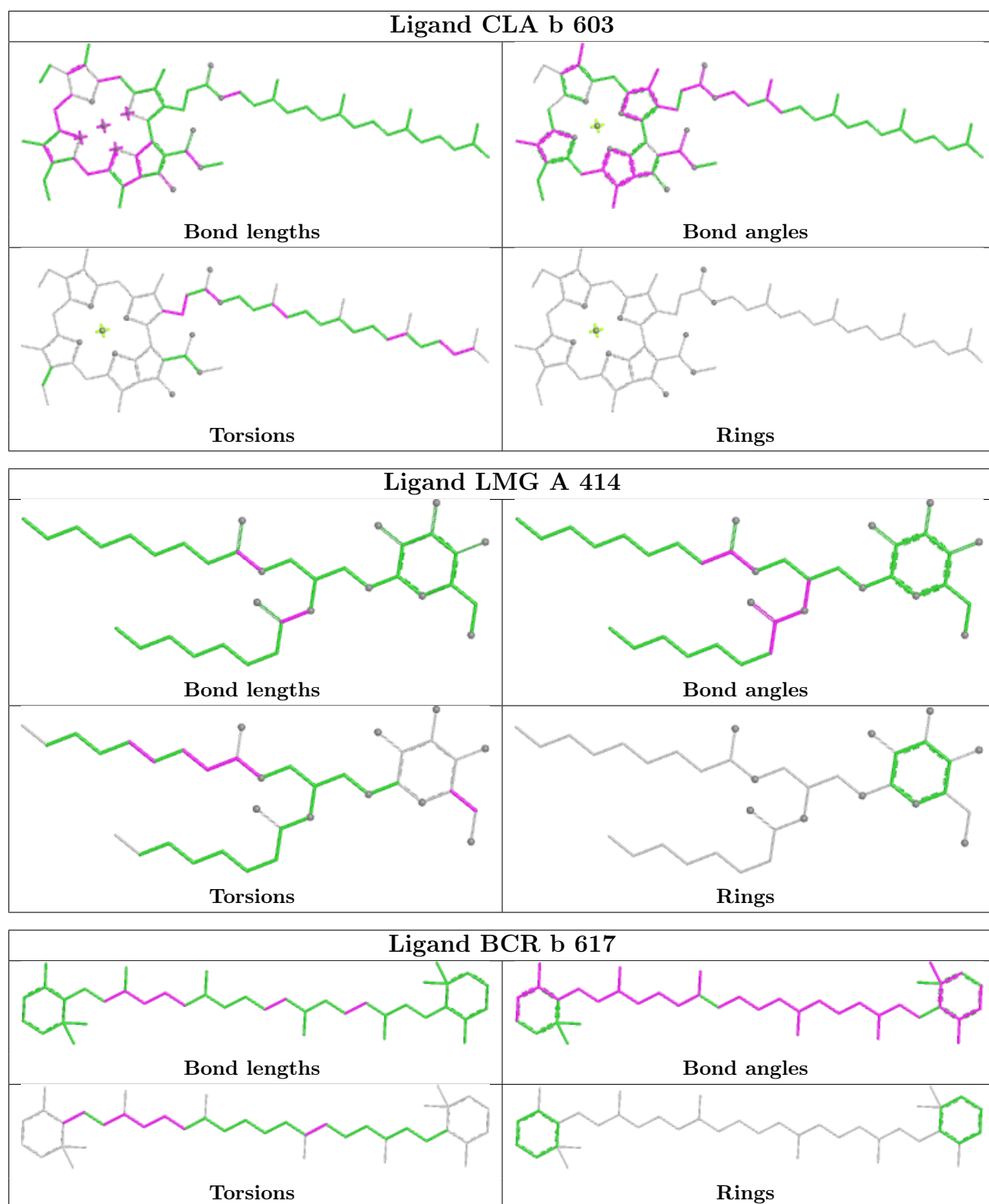


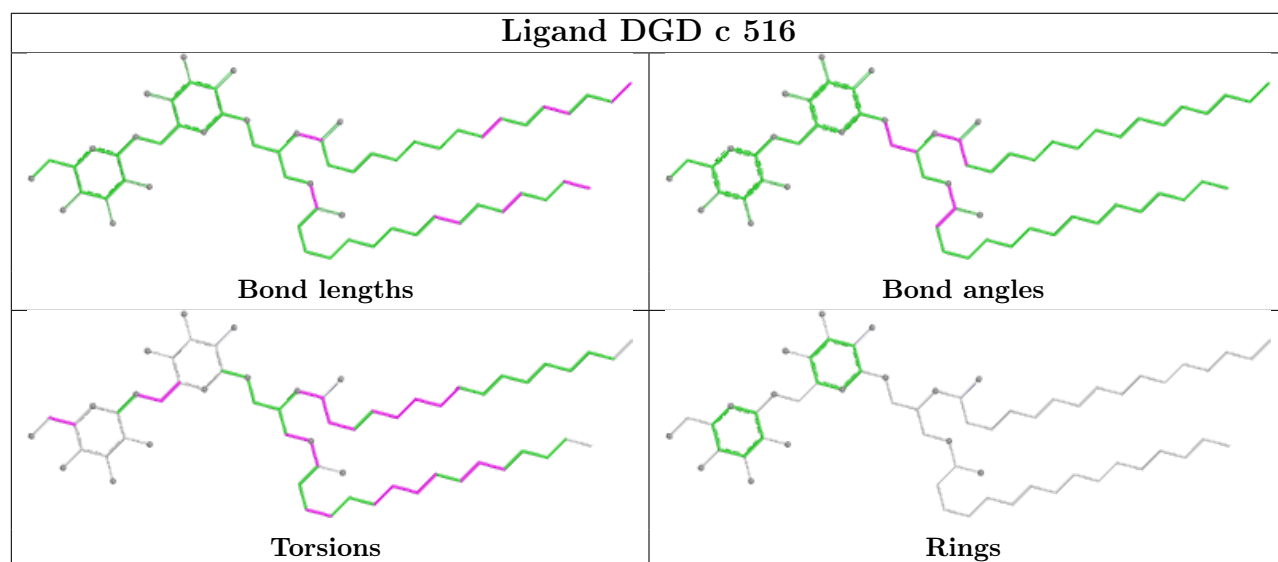
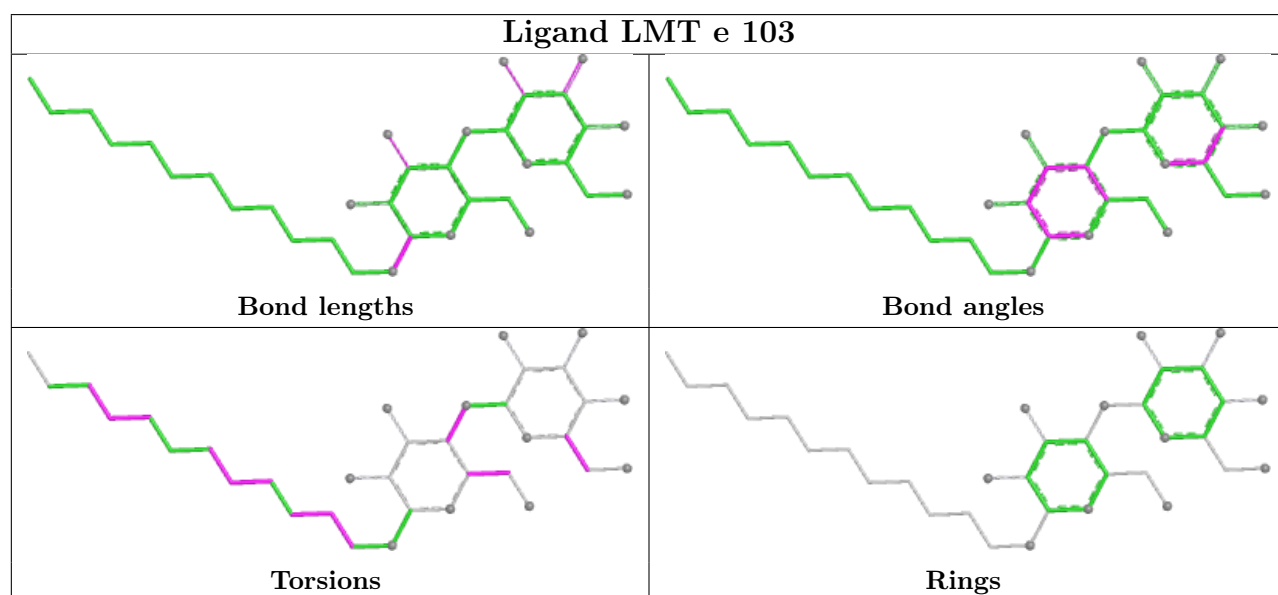
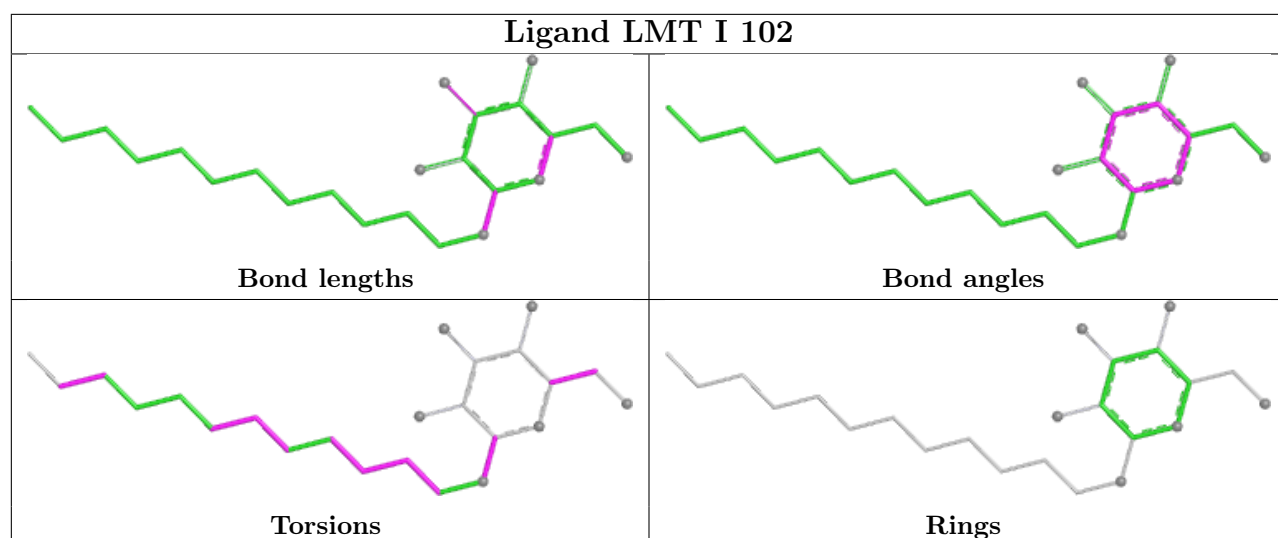
Ligand CLA a 405

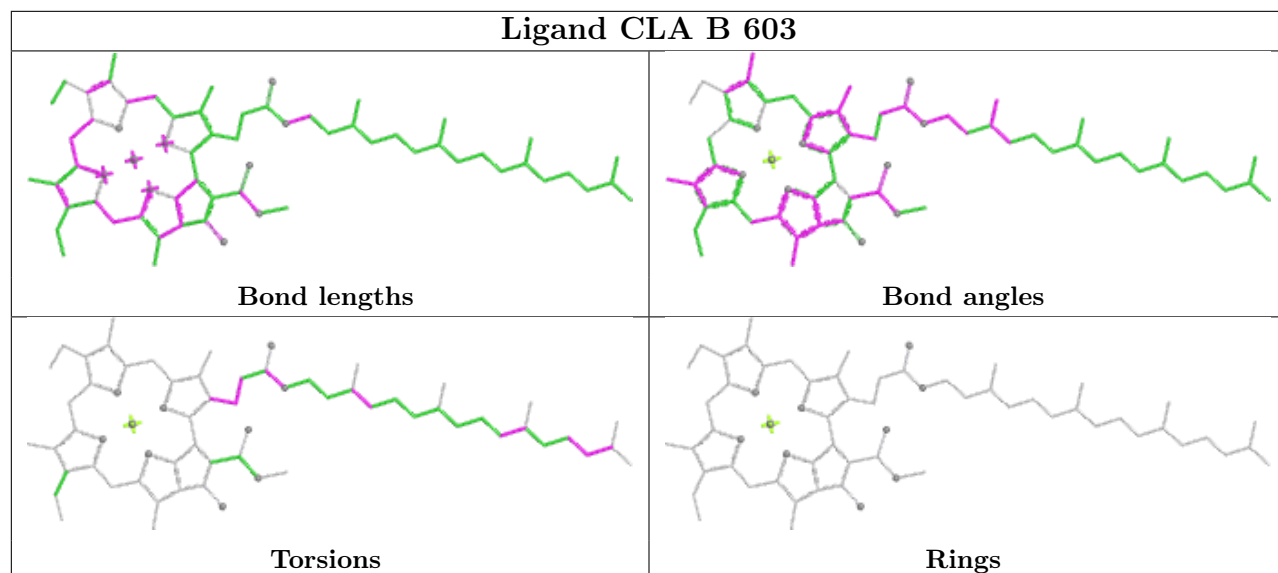
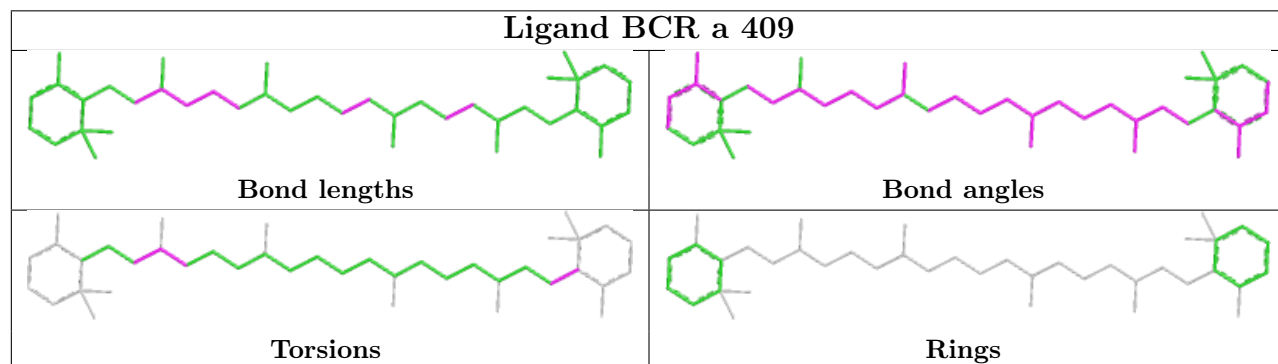
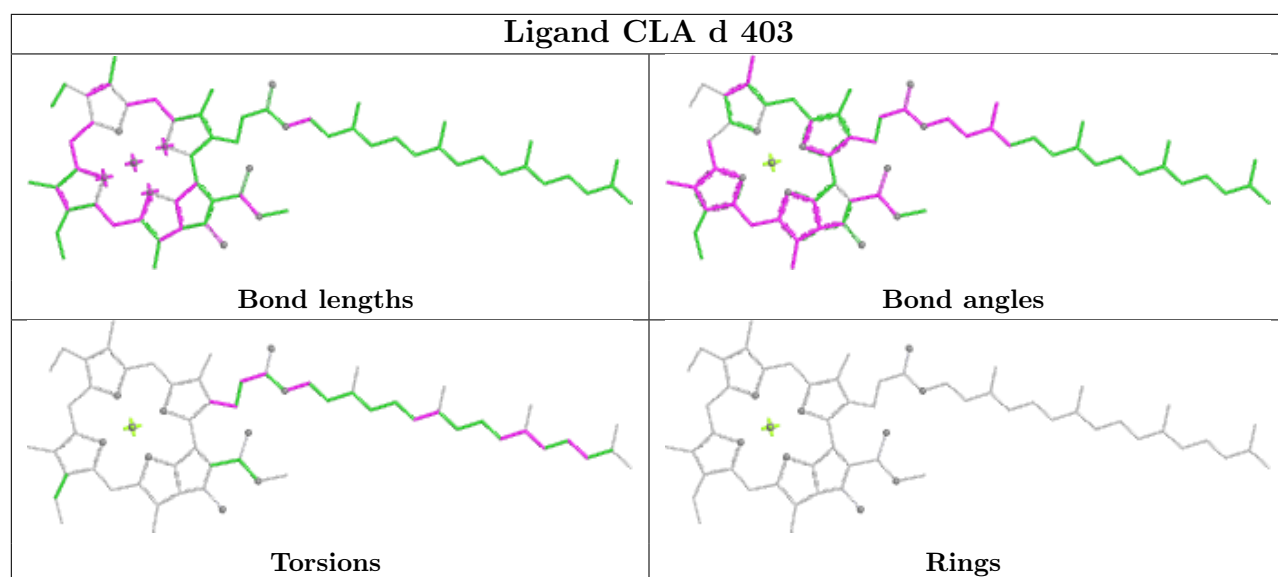


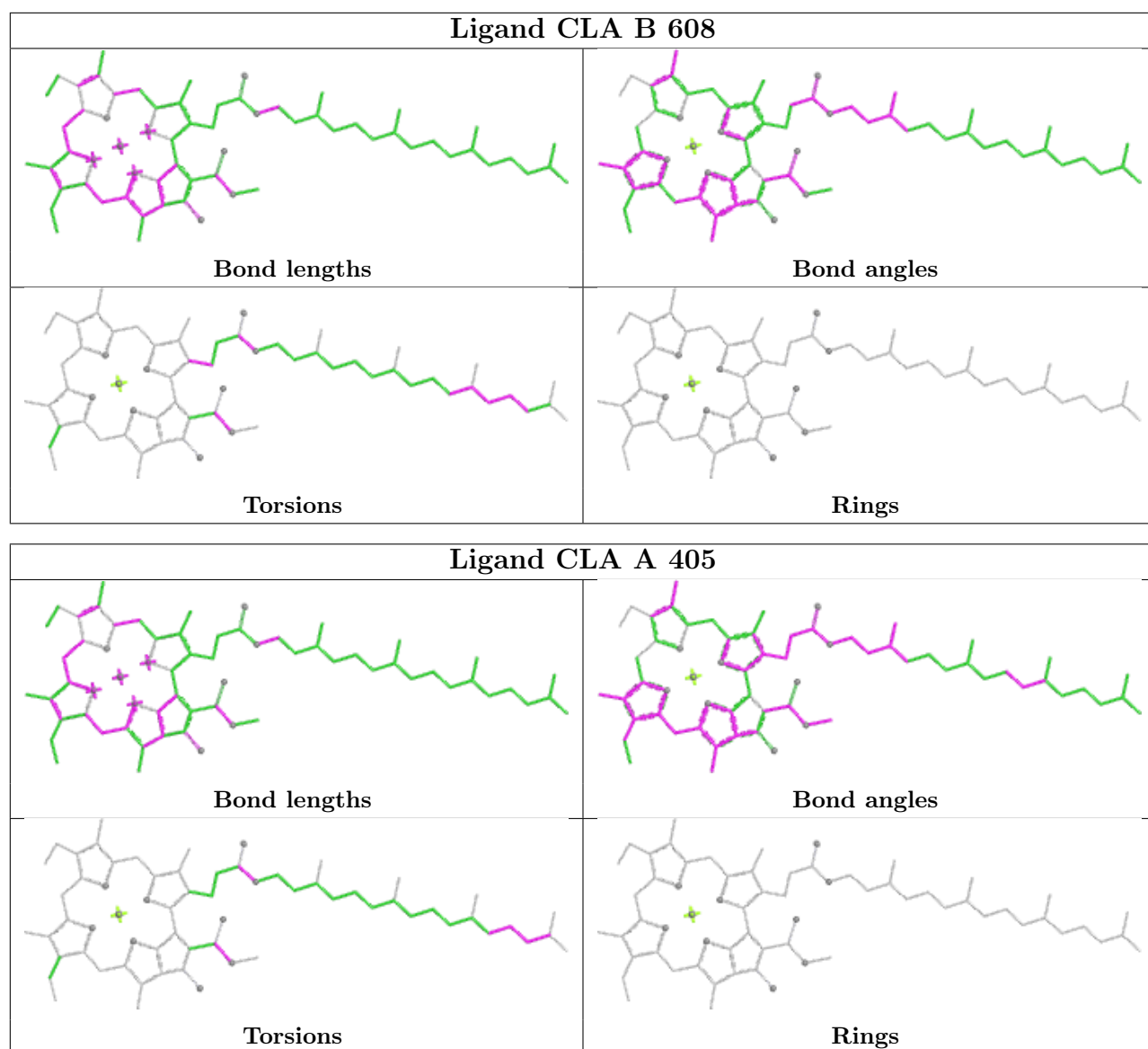
Ligand CLA C 506

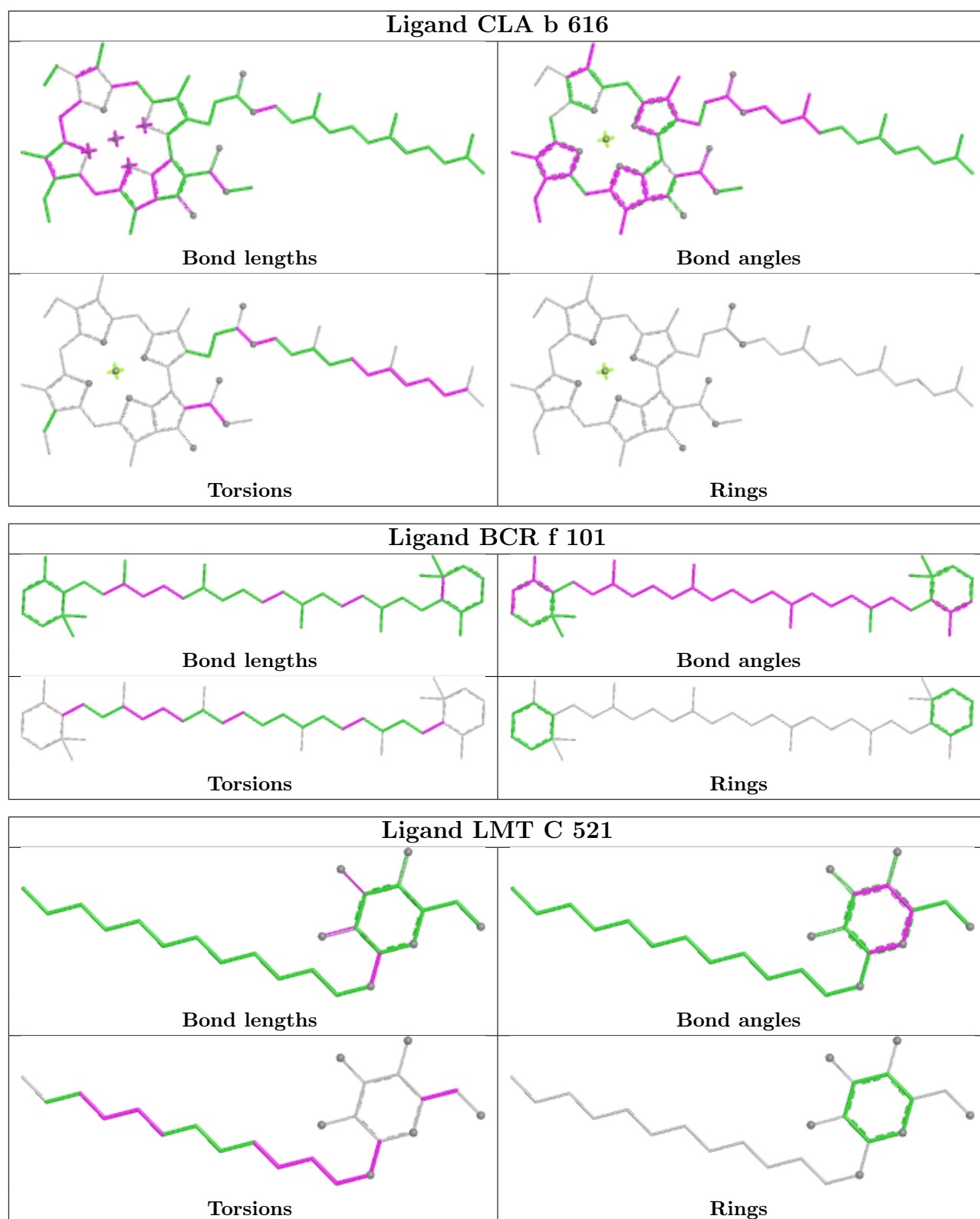


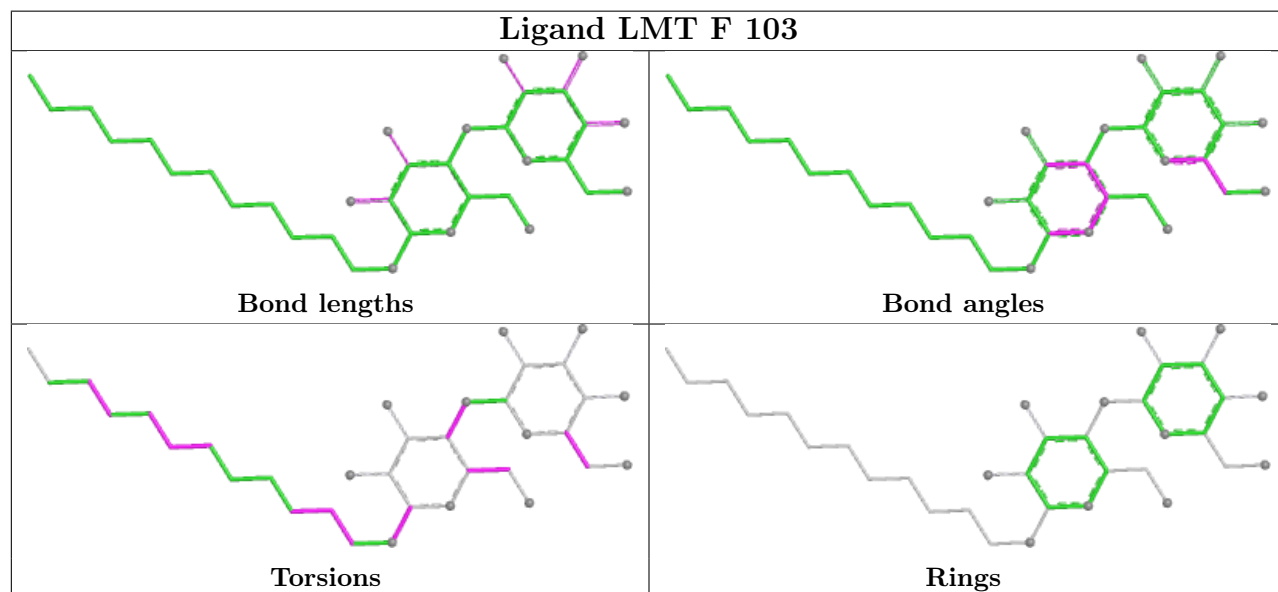
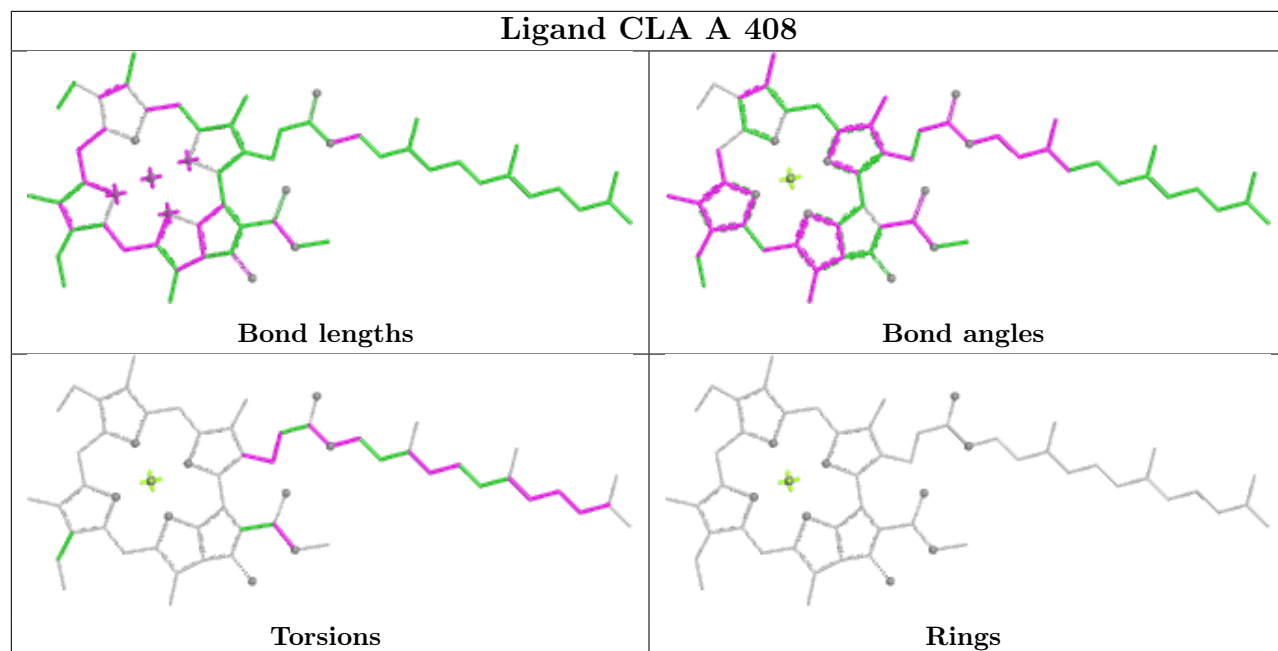


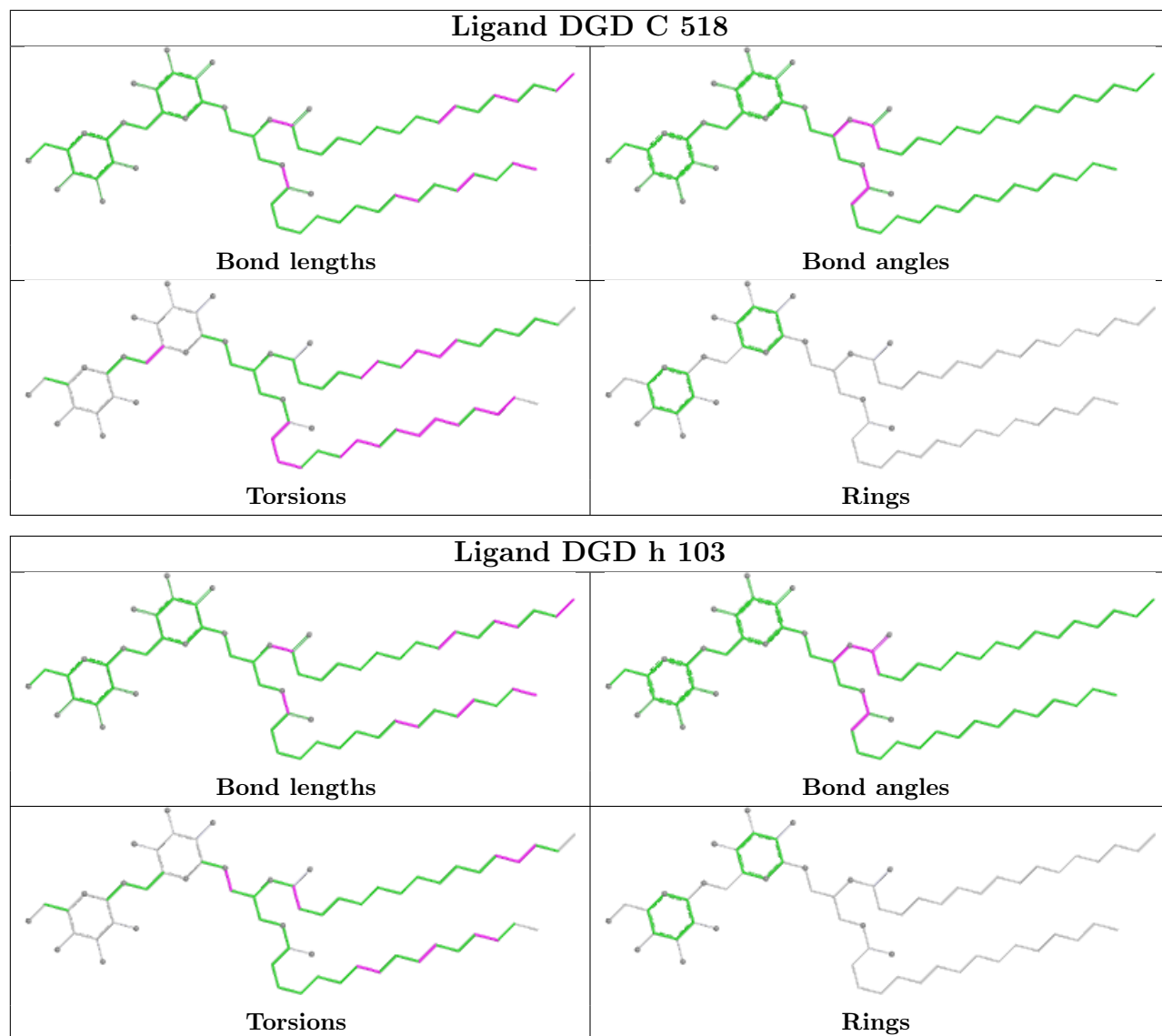


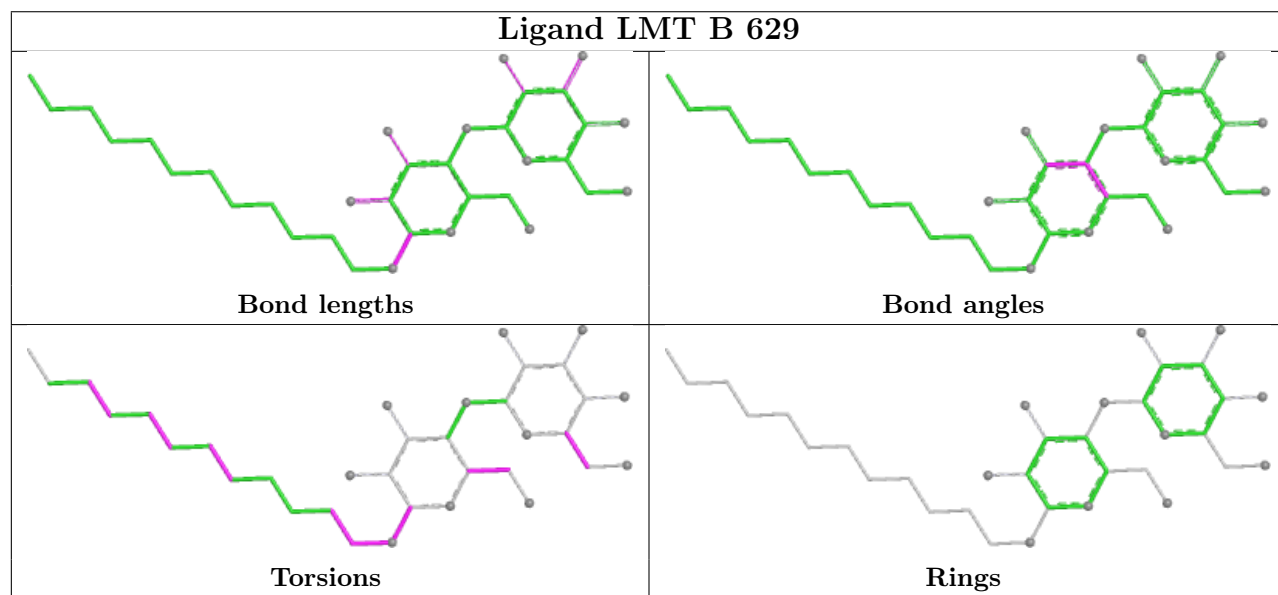
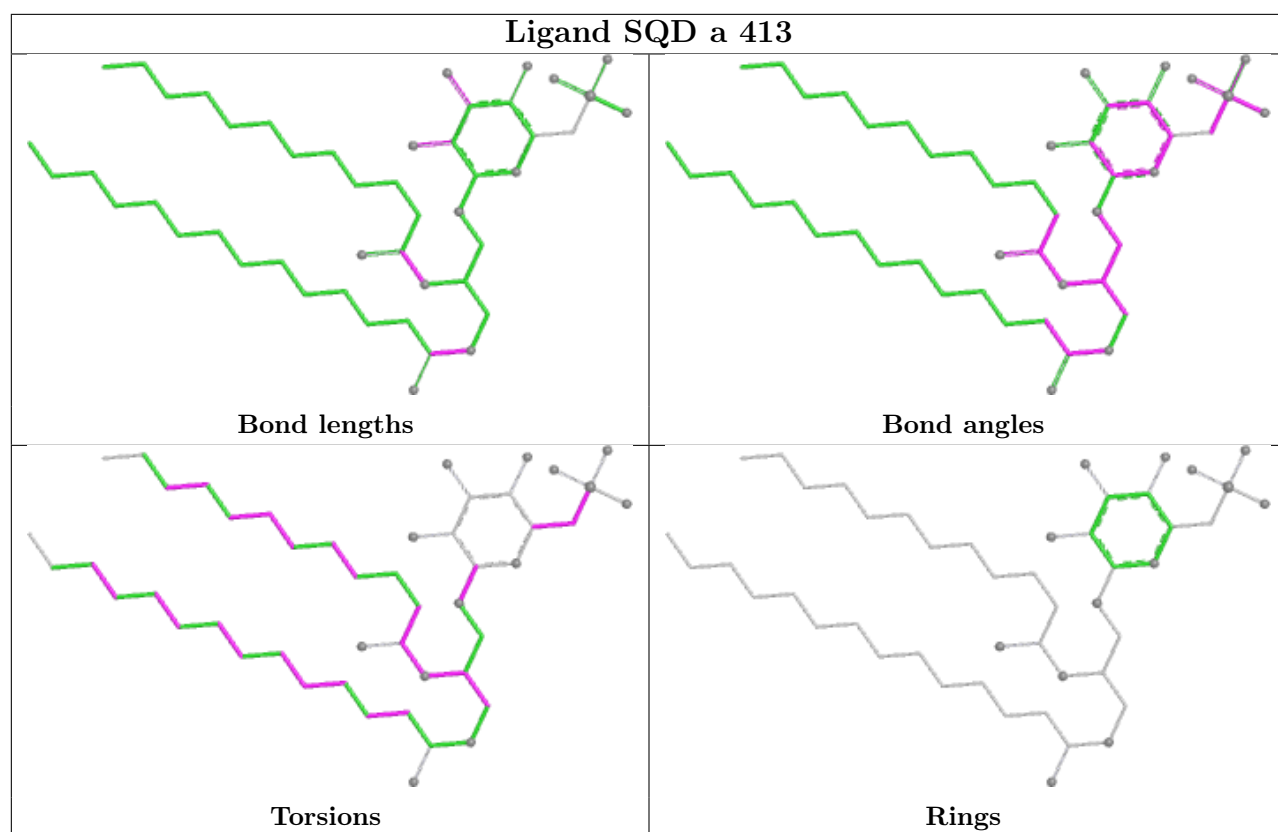


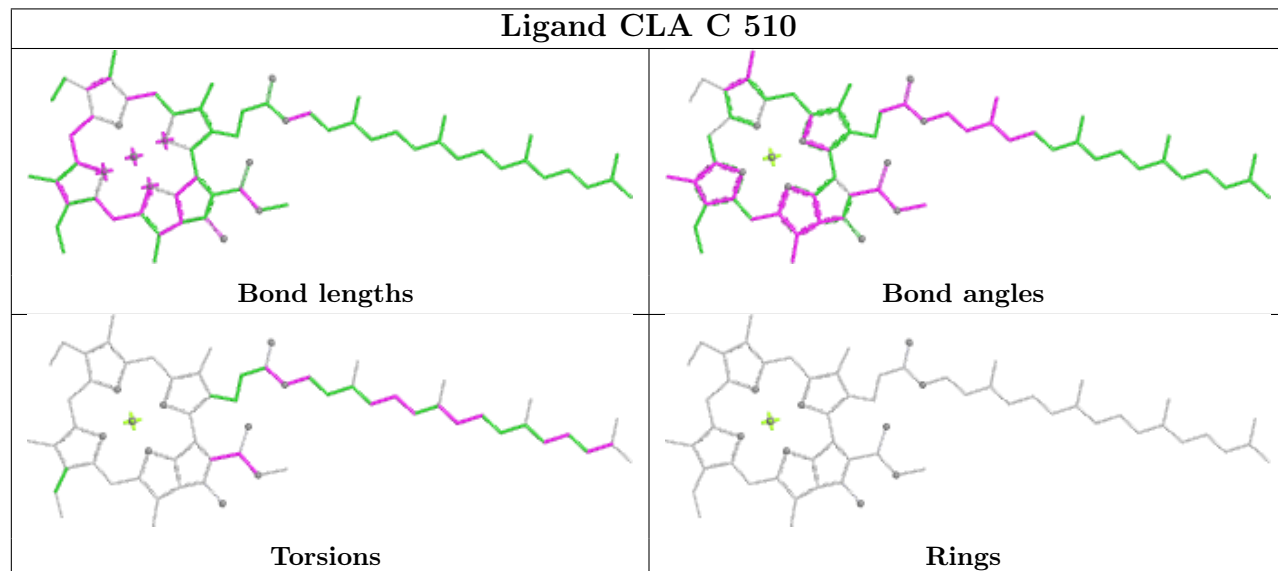
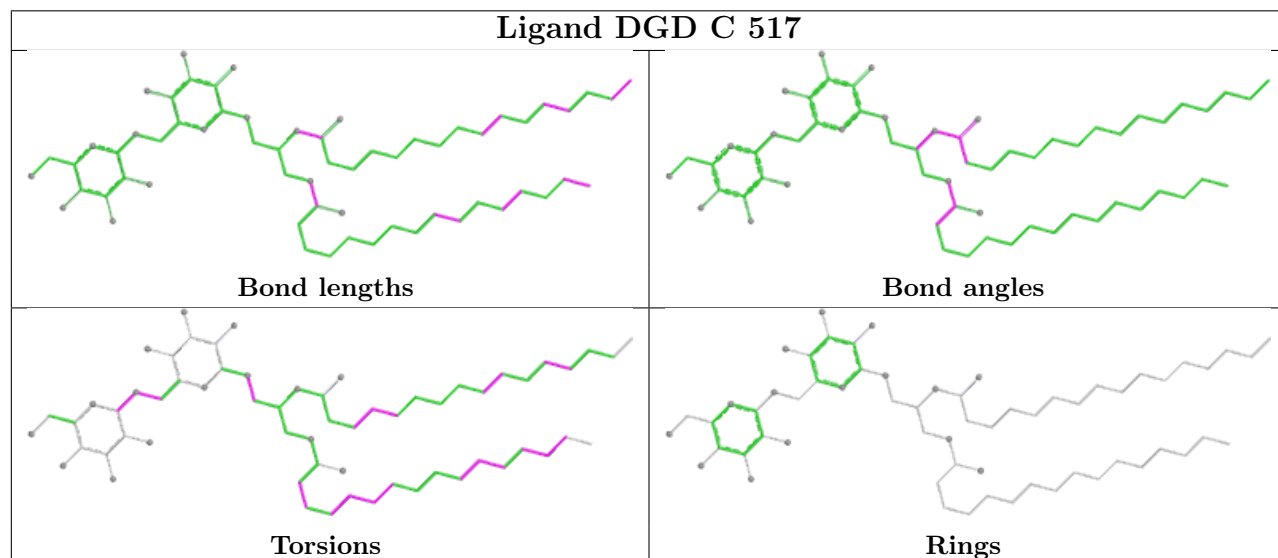
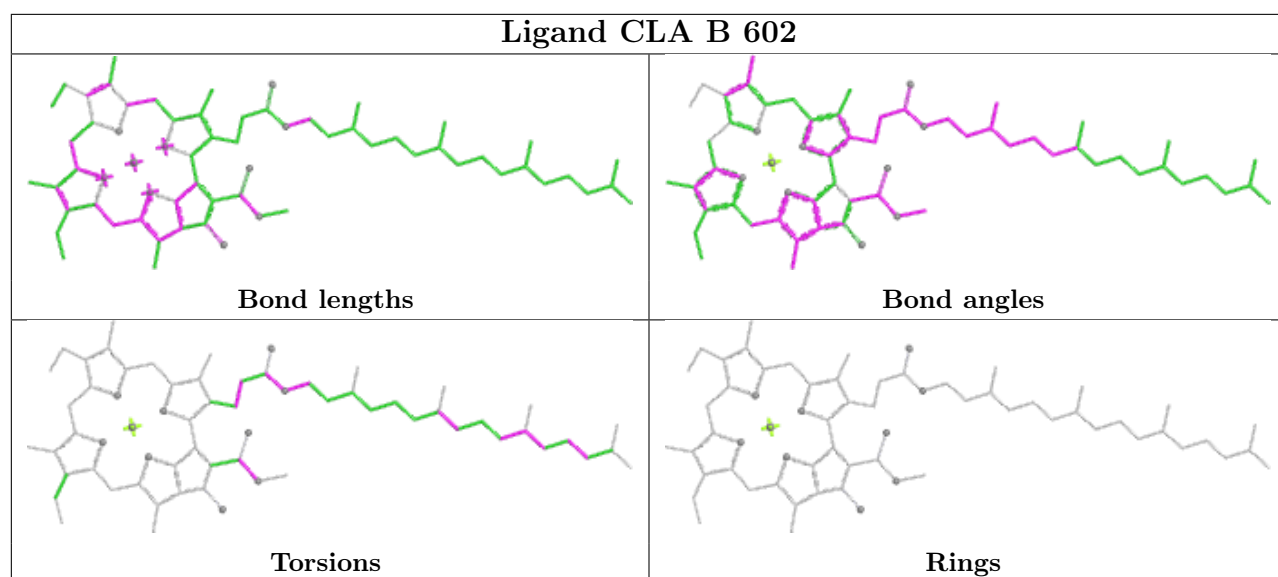


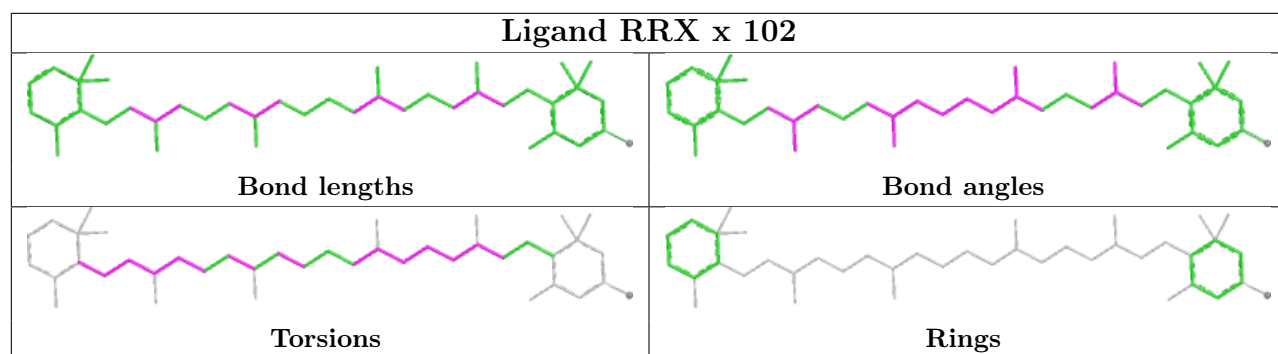
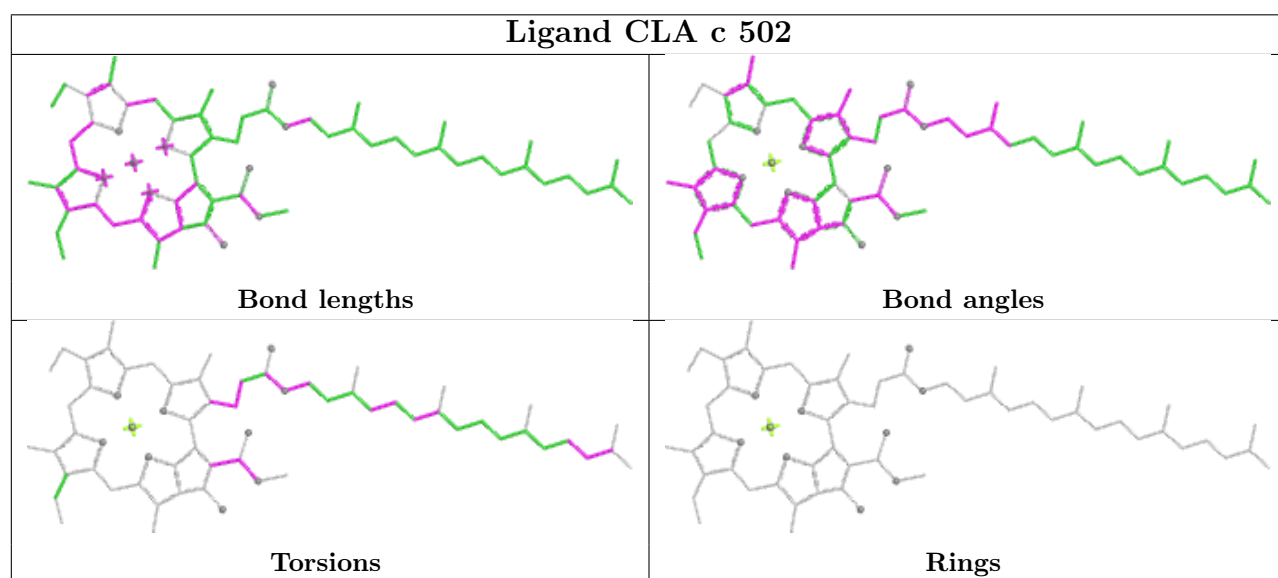
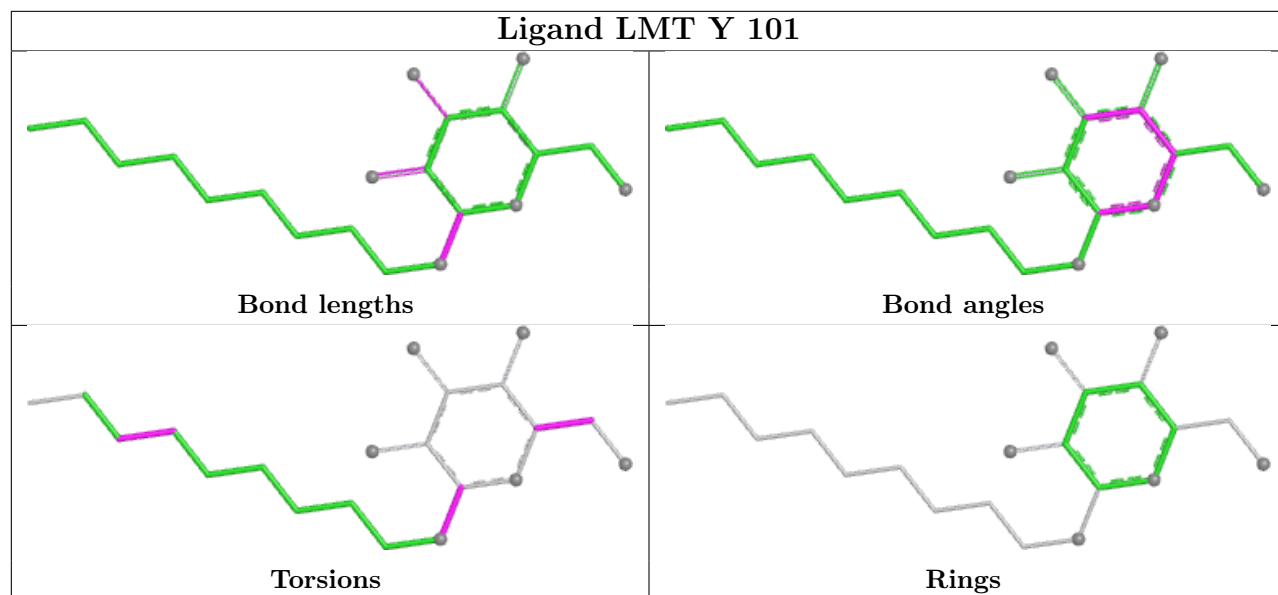


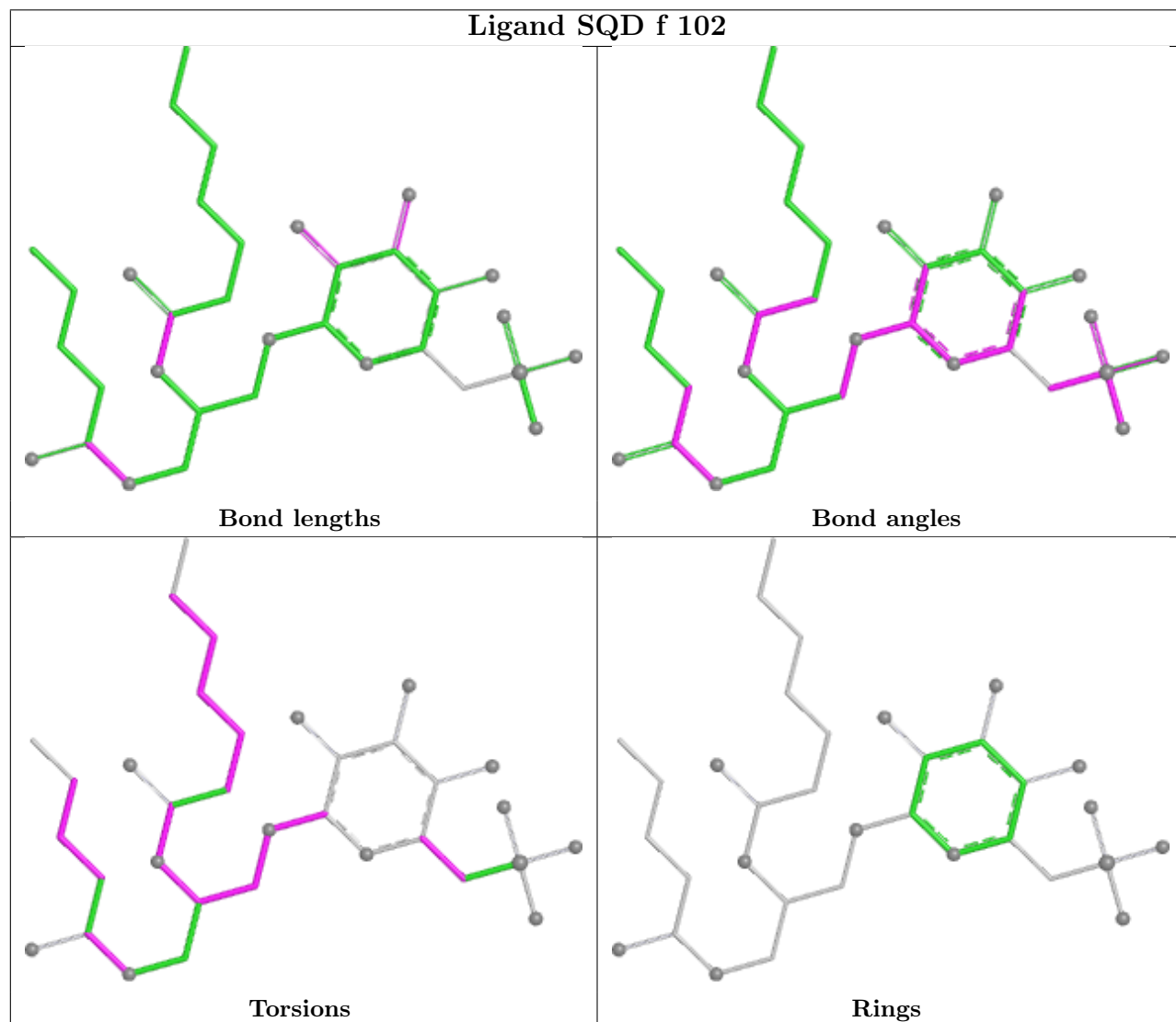
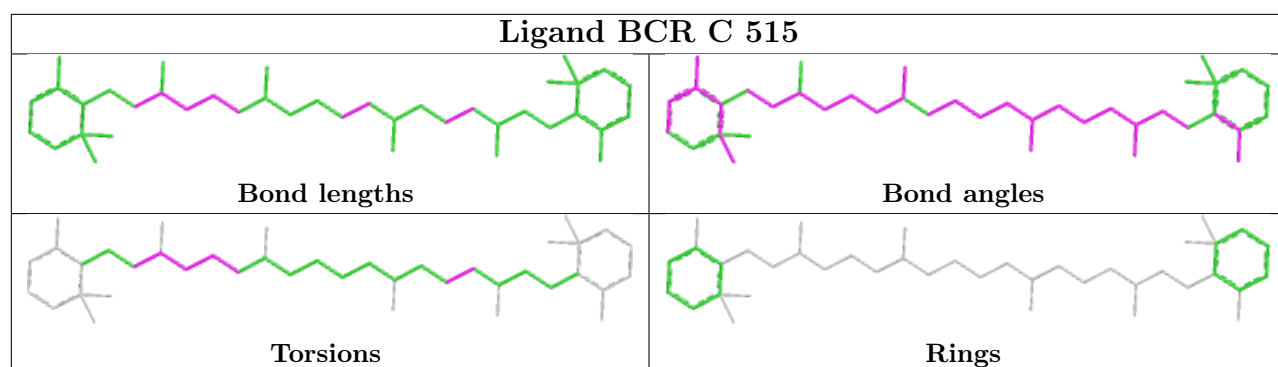


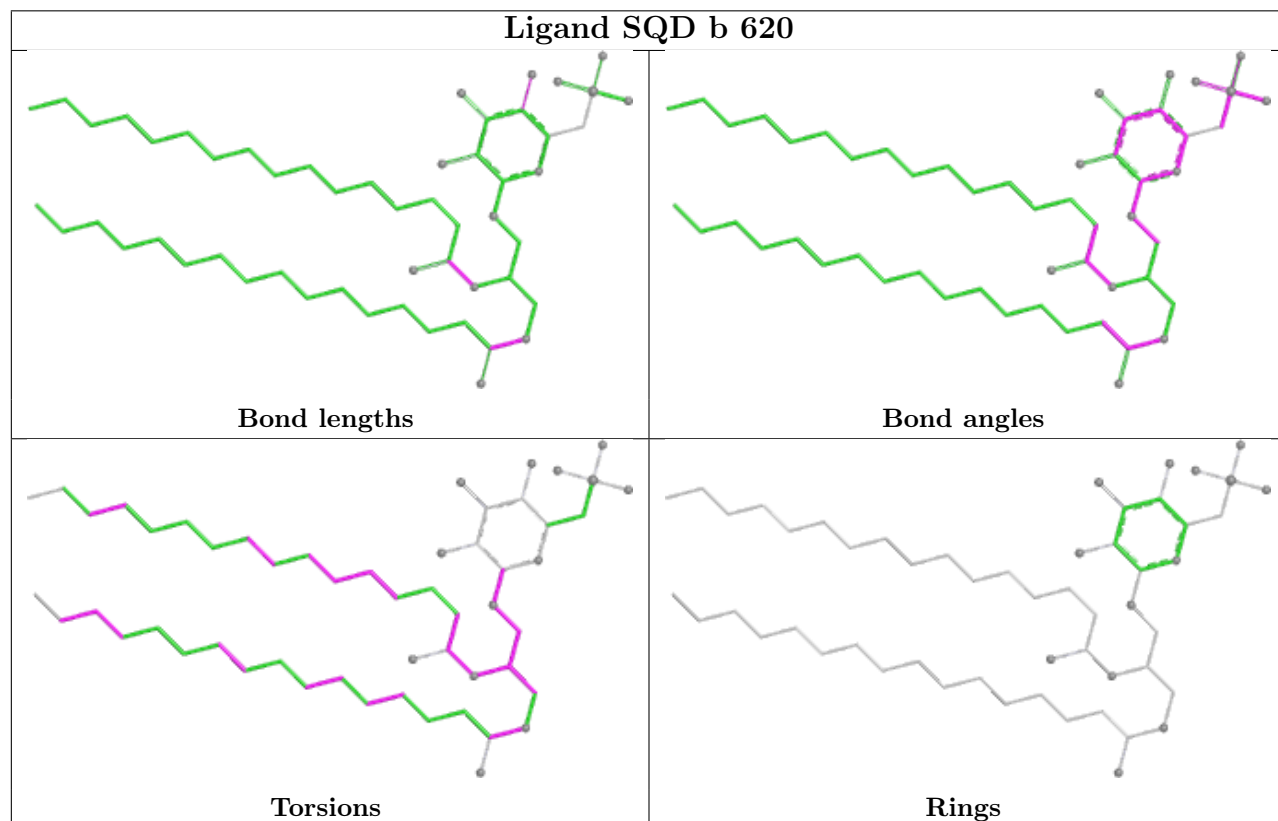
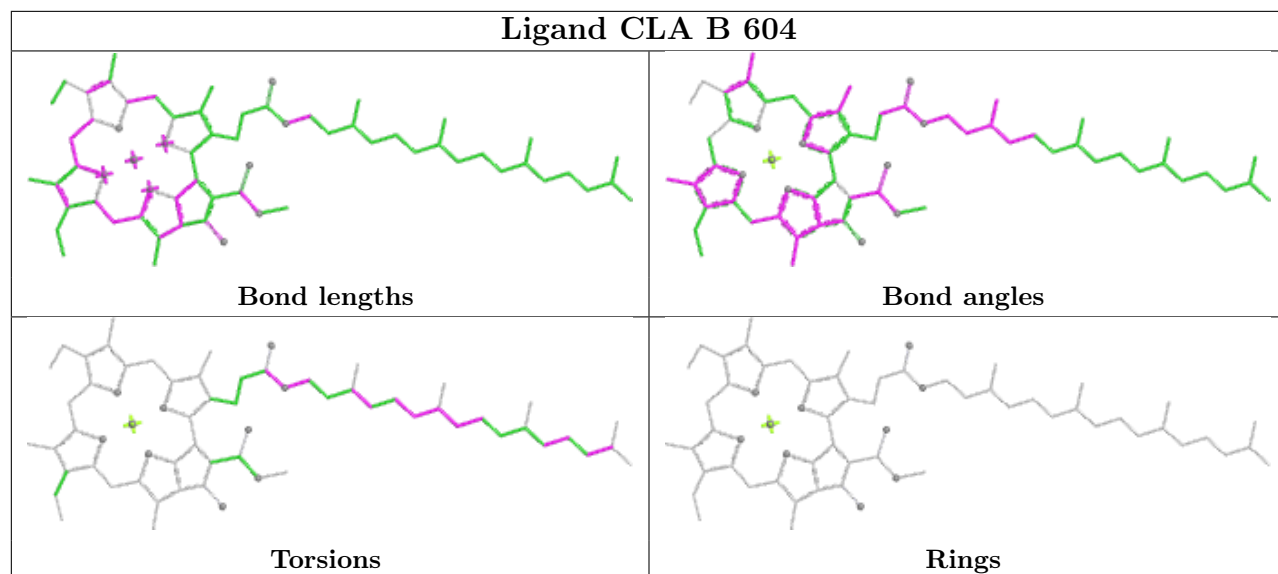


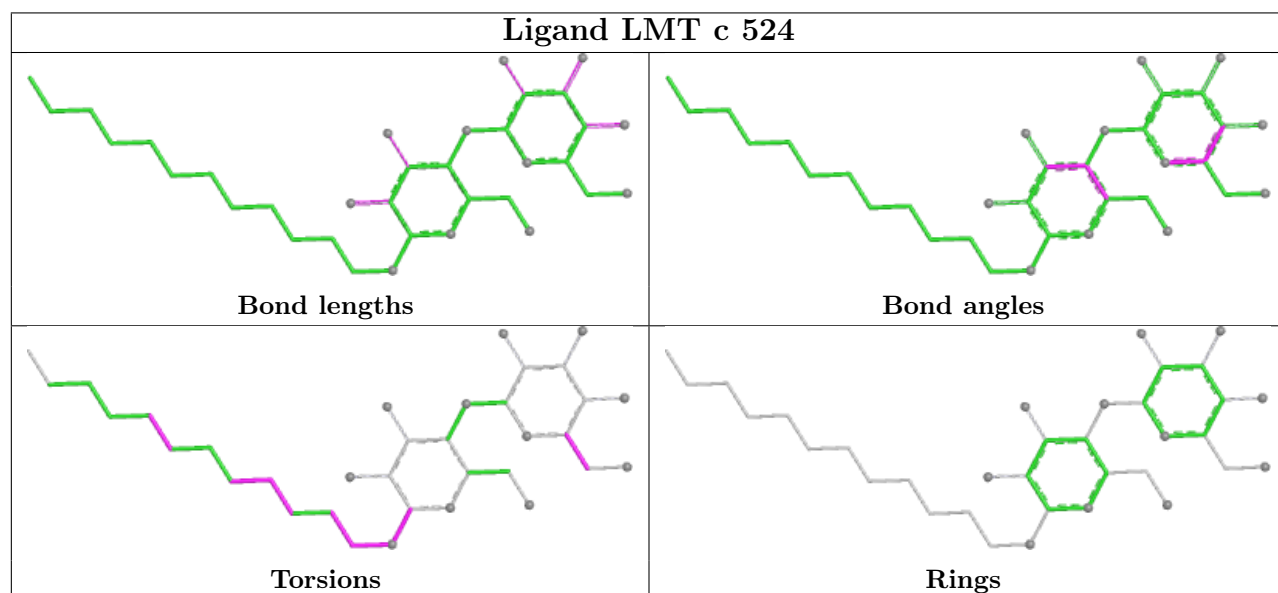
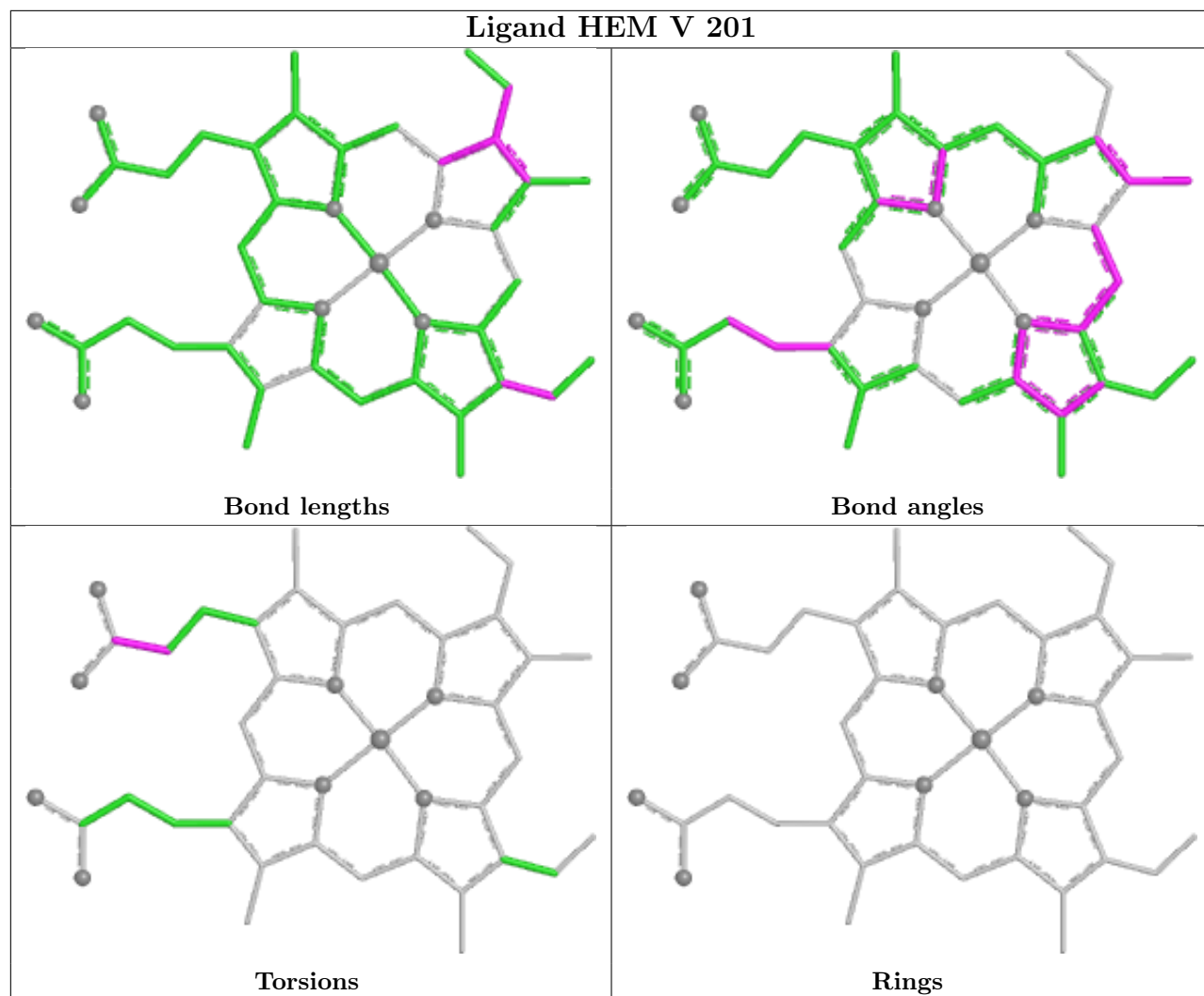


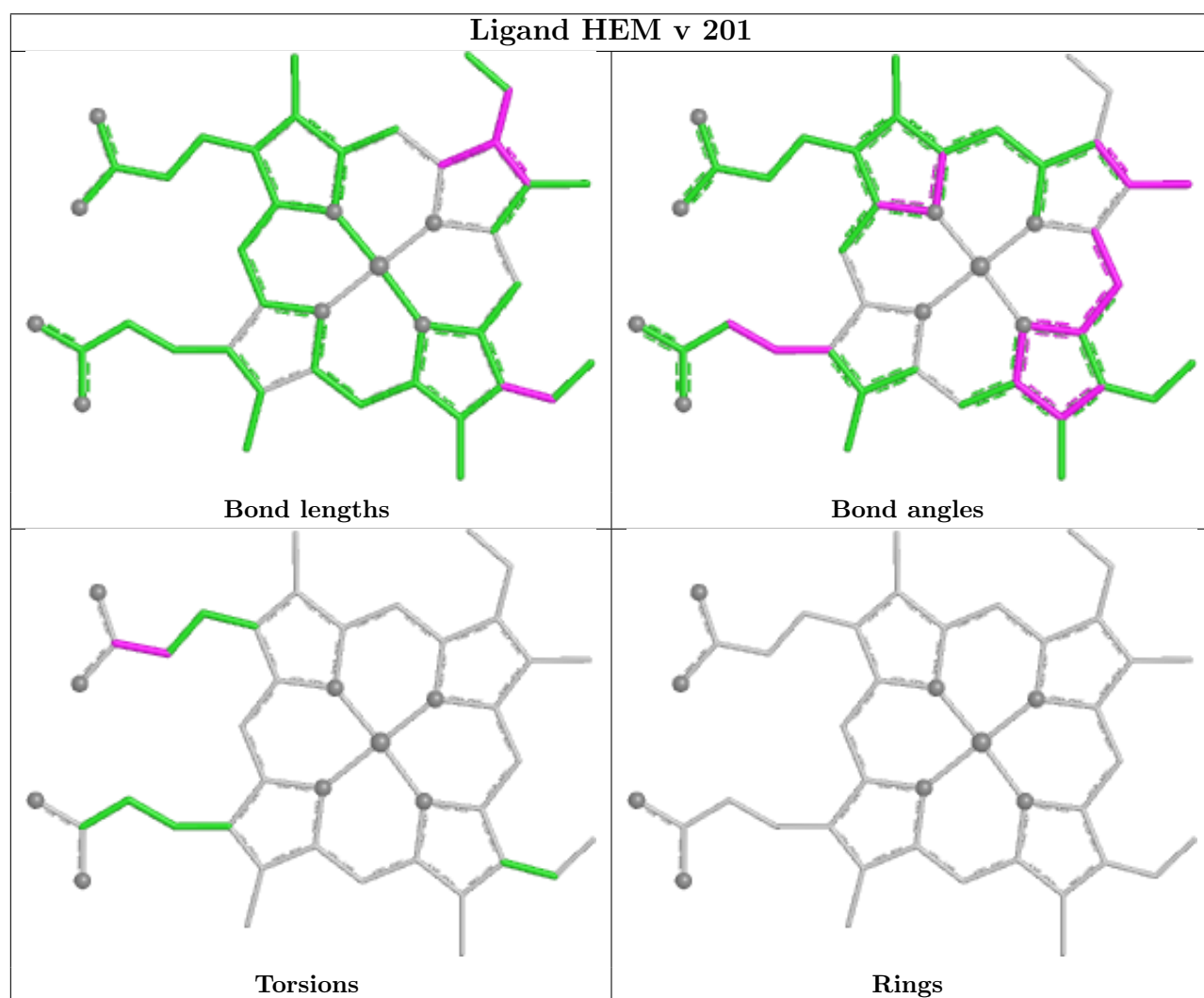
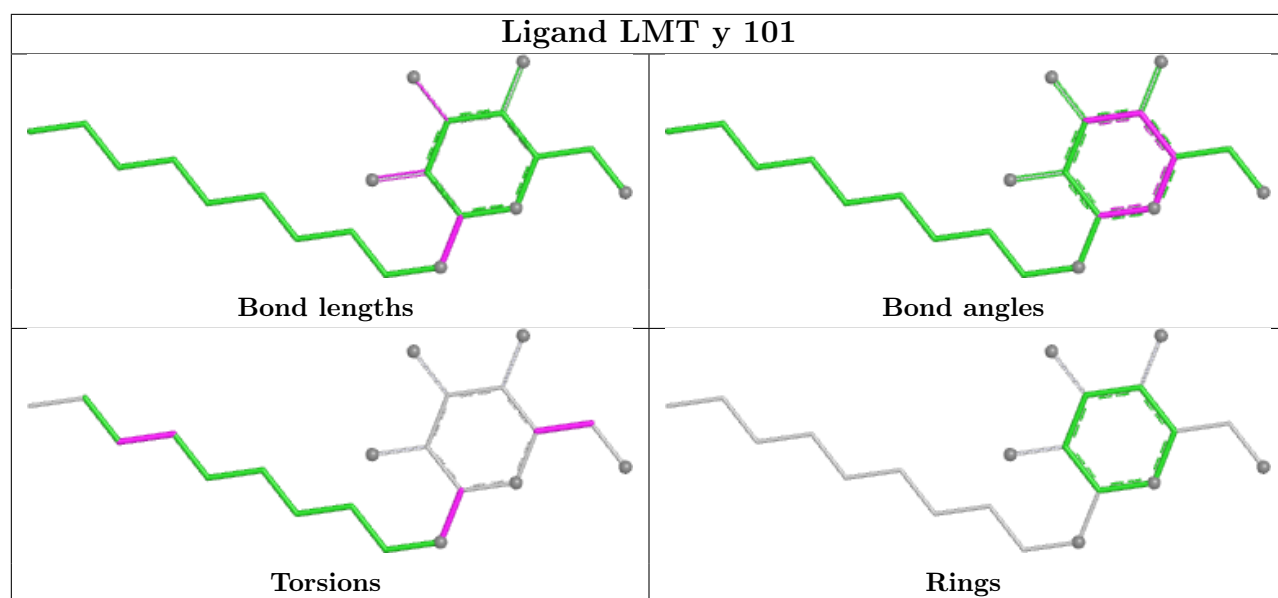


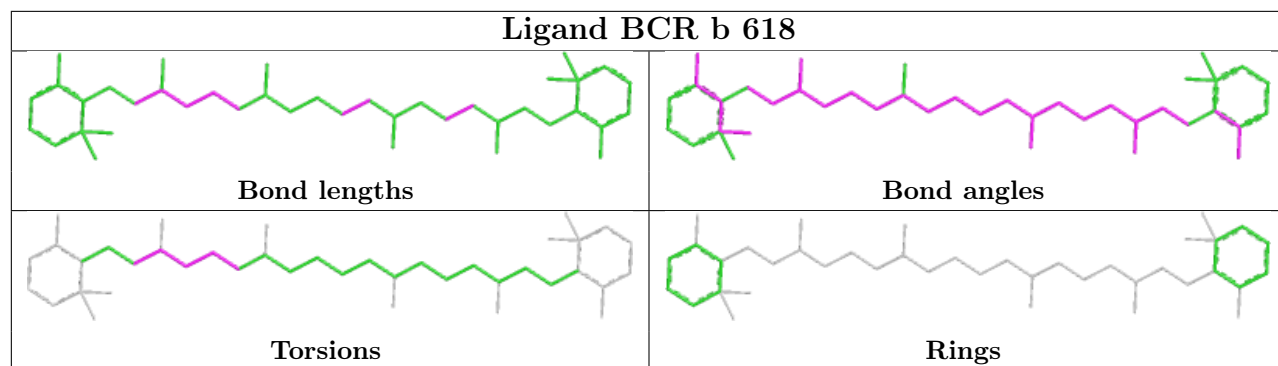












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

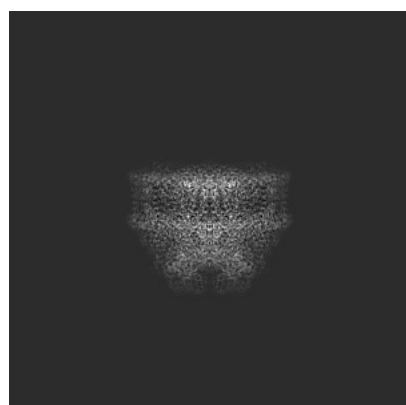
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24239. These allow visual inspection of the internal detail of the map and identification of artifacts.

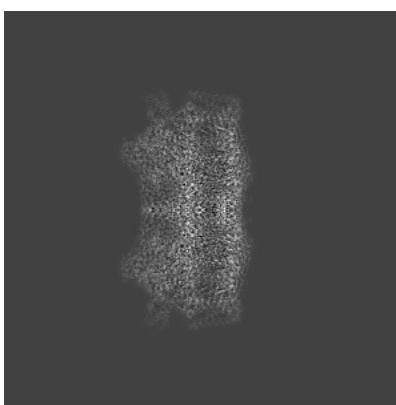
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

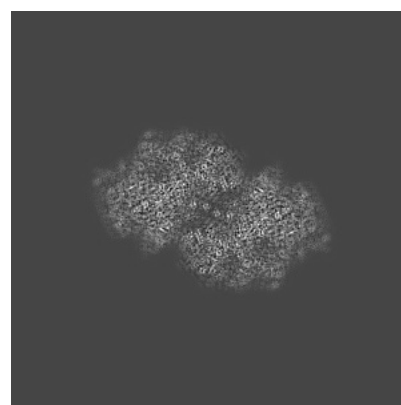
6.1.1 Primary map



X



Y

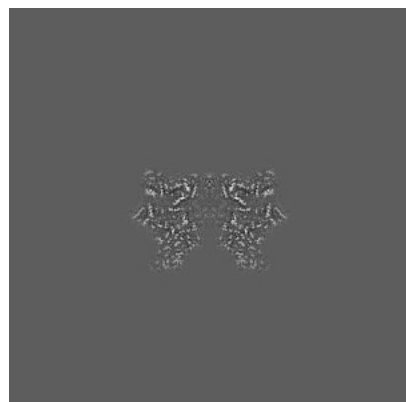


Z

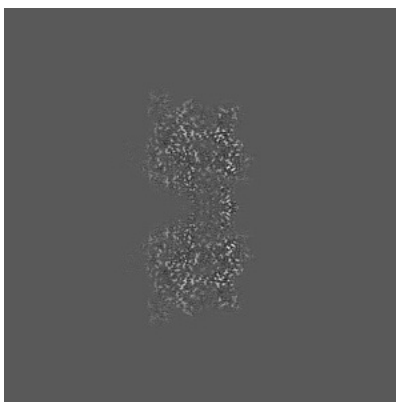
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

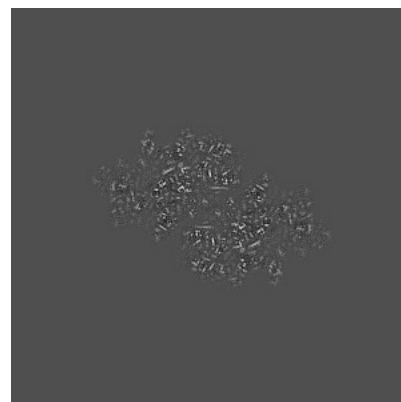
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

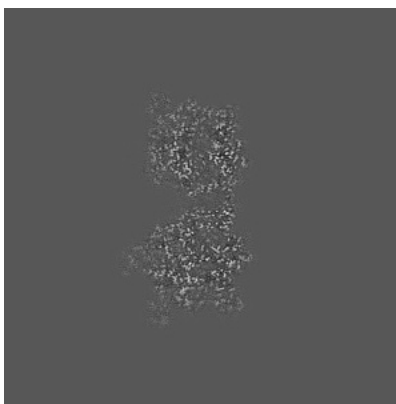
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

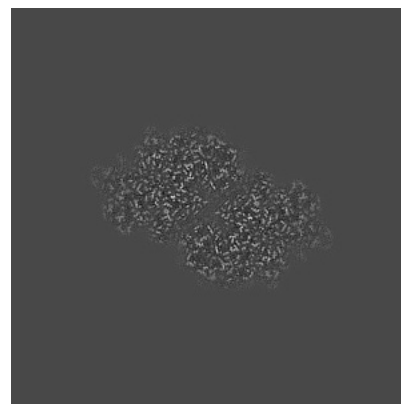
6.3.1 Primary map



X Index: 194



Y Index: 196

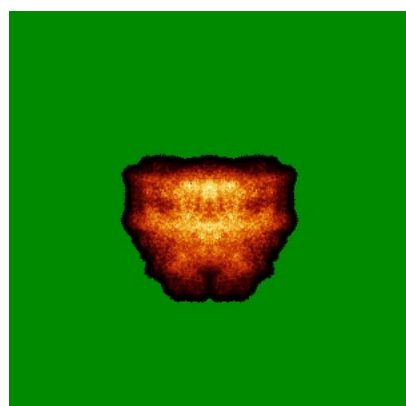


Z Index: 179

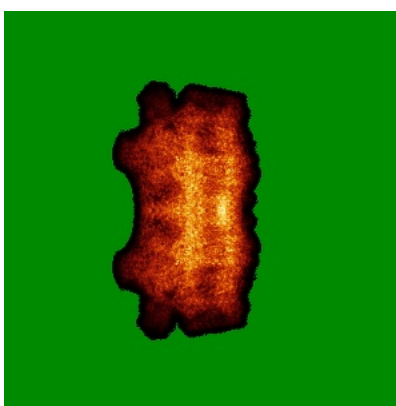
The images above show the largest variance slices of the map in three orthogonal directions.

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

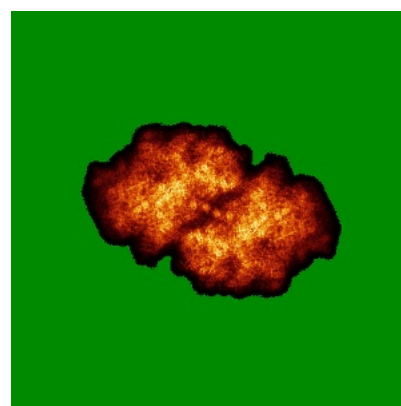
6.4.1 Primary map



X



Y

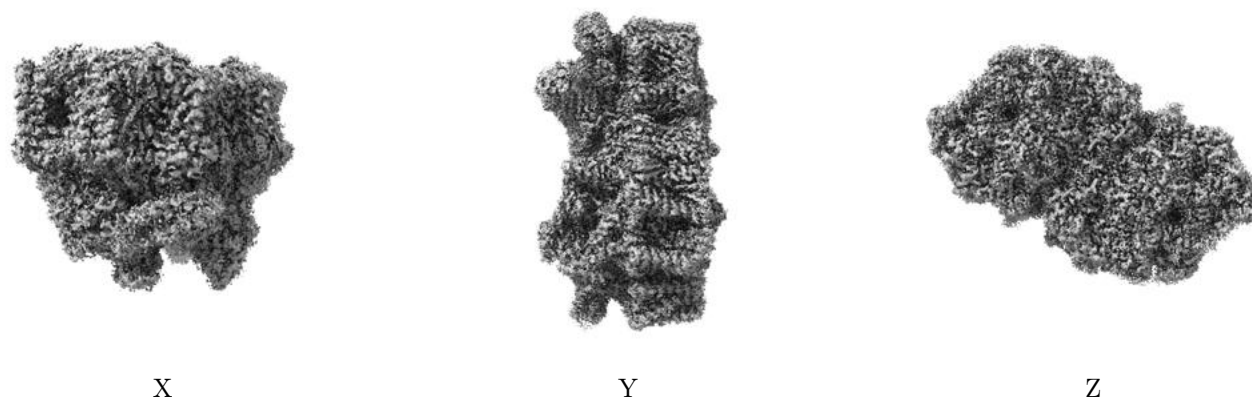


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

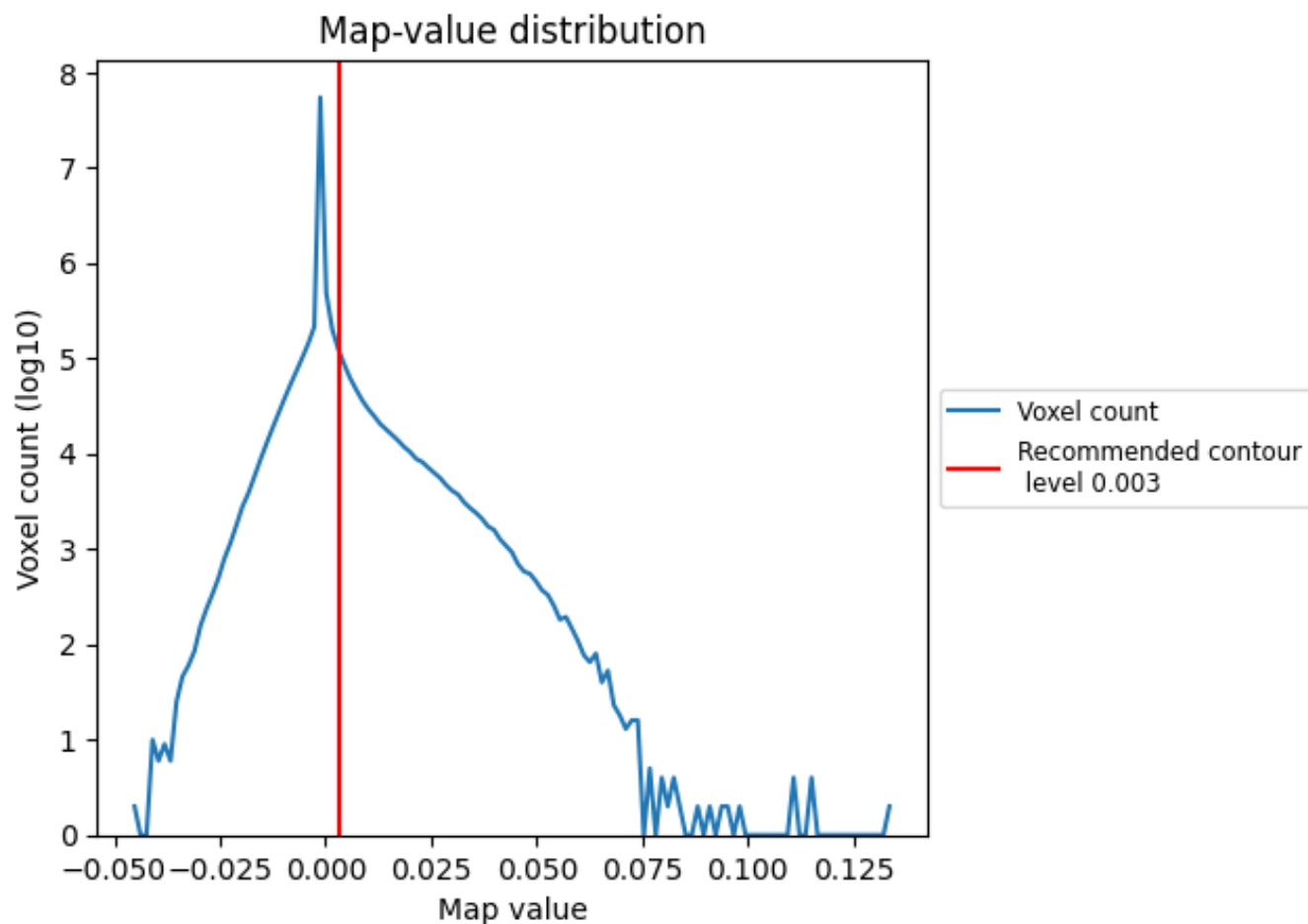
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

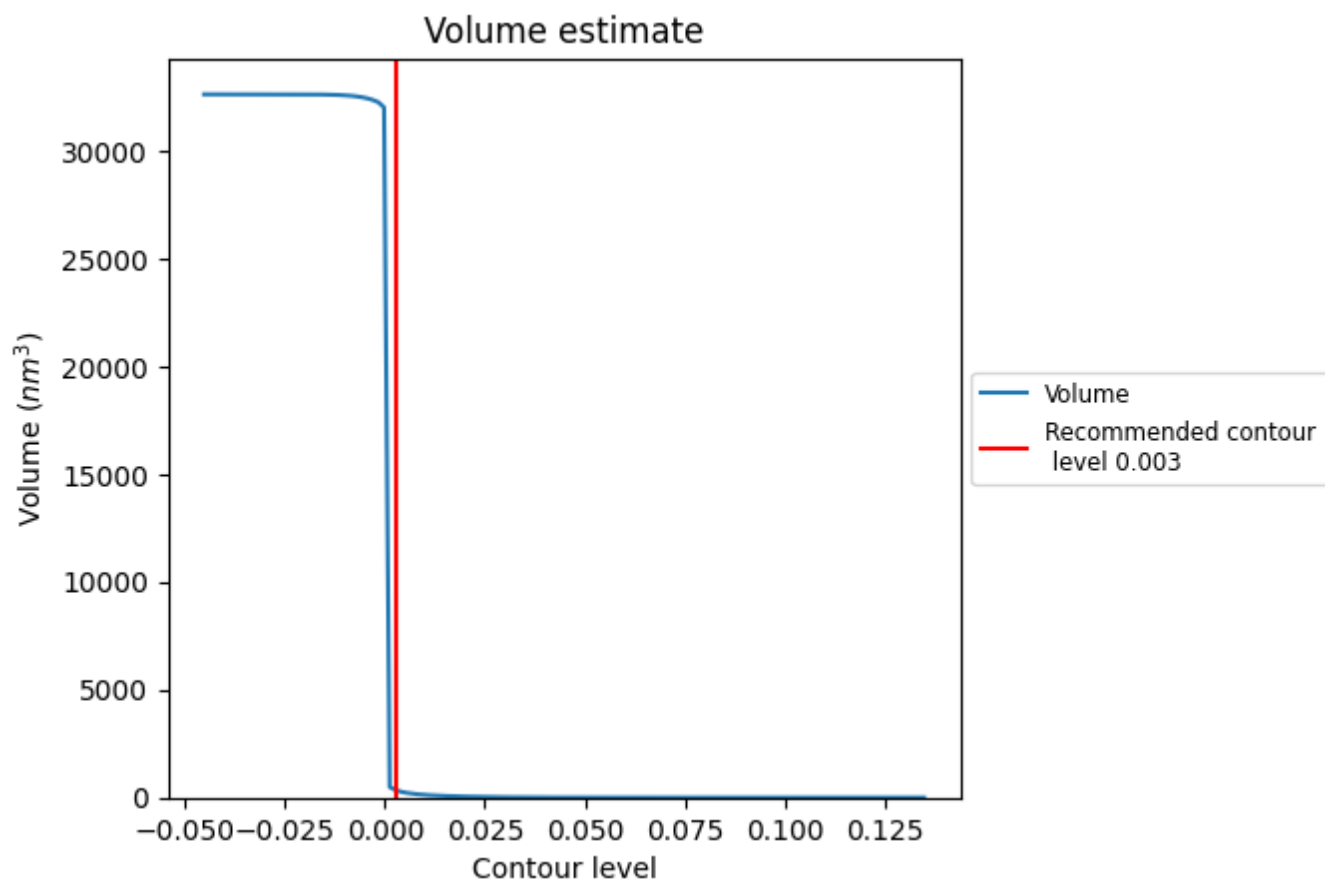
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

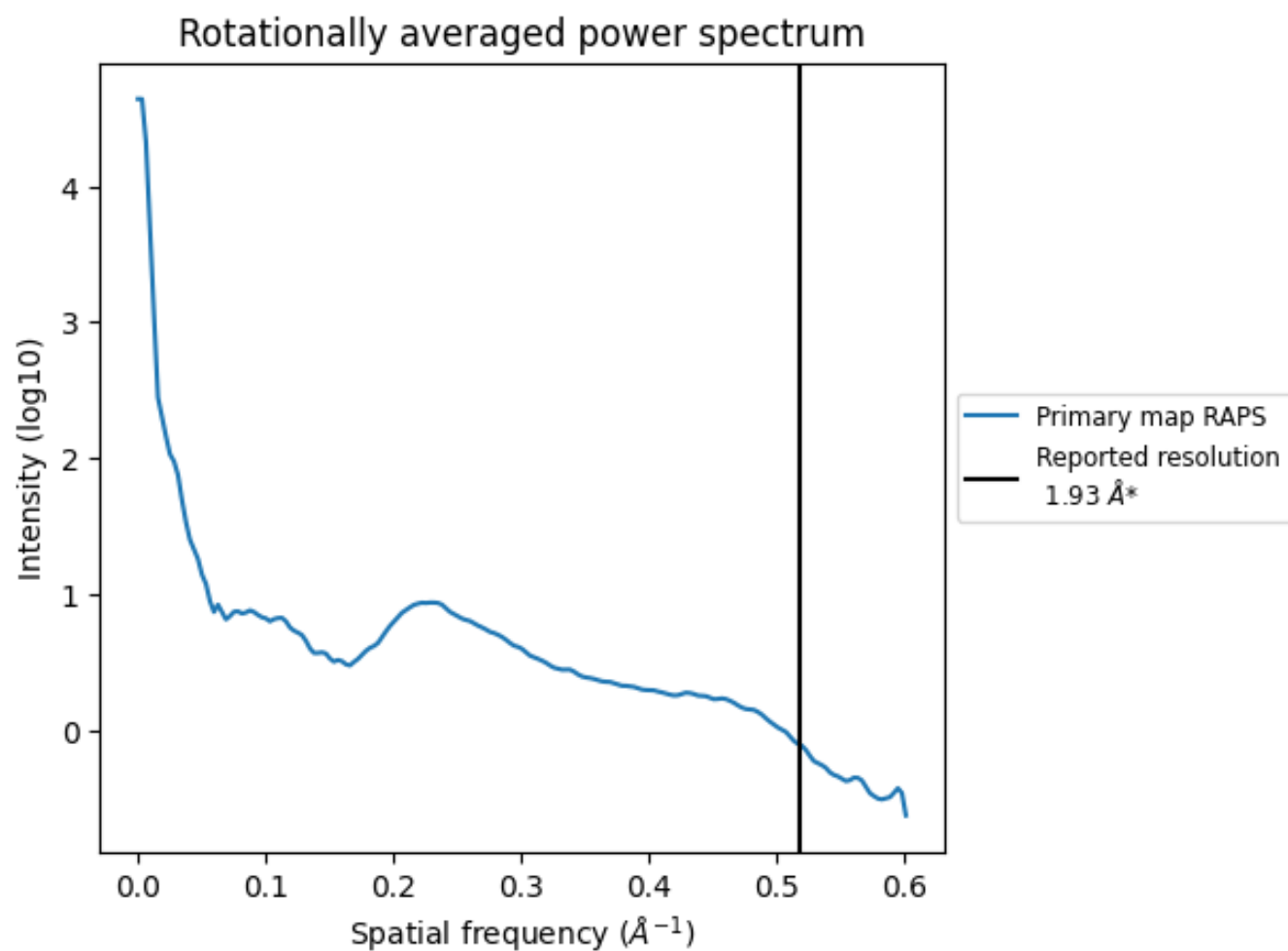
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

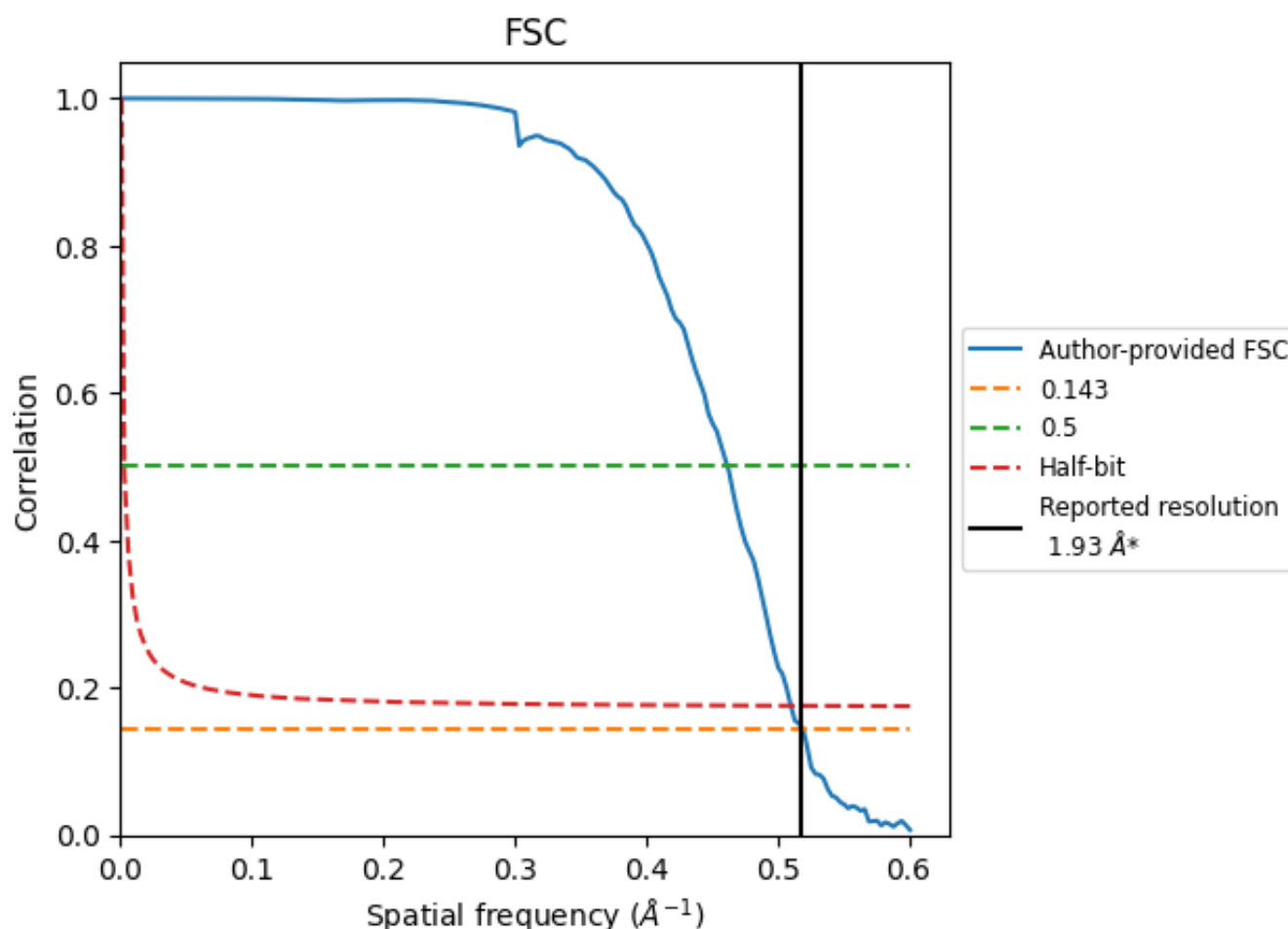


*Reported resolution corresponds to spatial frequency of 0.518 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.518 Å⁻¹

8.2 Resolution estimates [i](#)

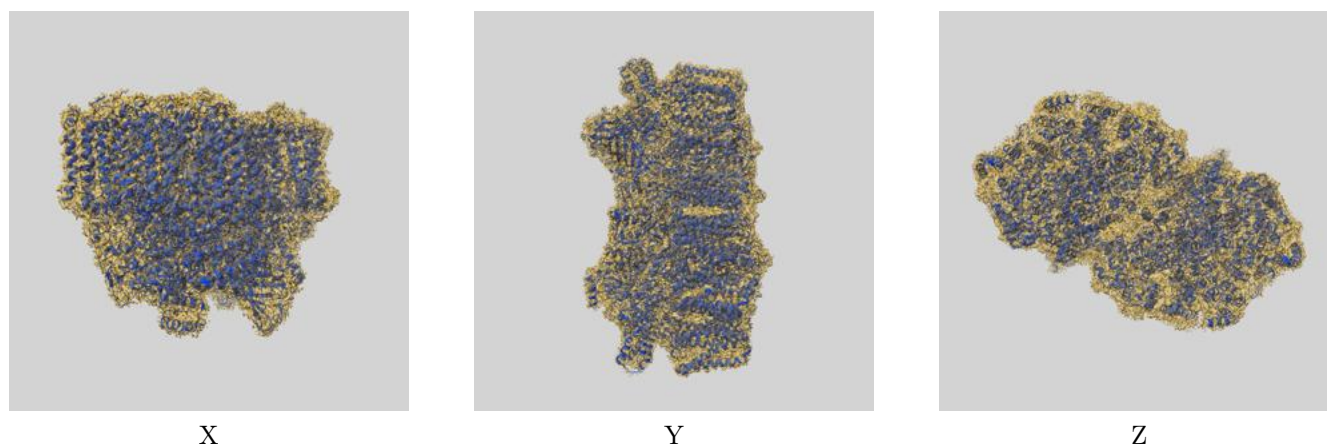
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.93	-	-
Author-provided FSC curve	1.92	2.16	1.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

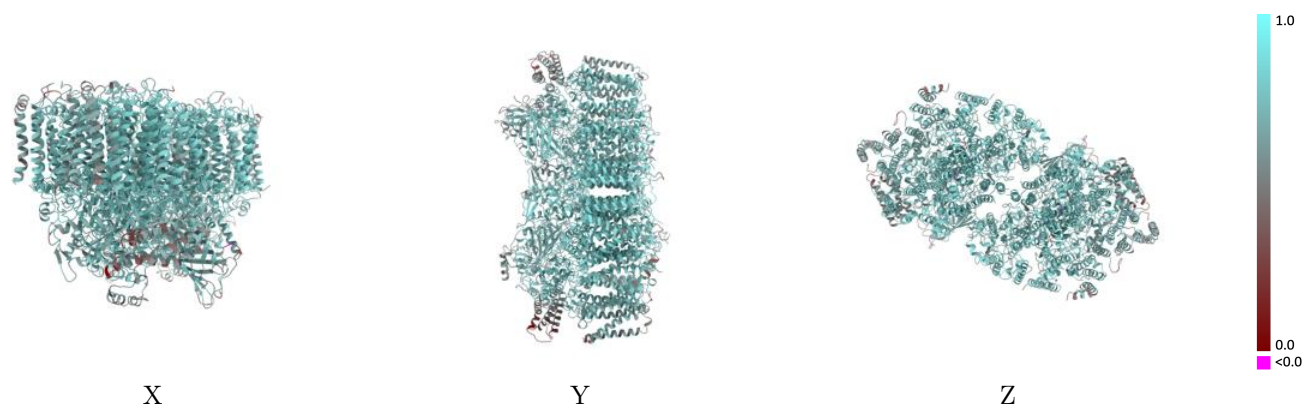
This section contains information regarding the fit between EMDB map EMD-24239 and PDB model 7N8O. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



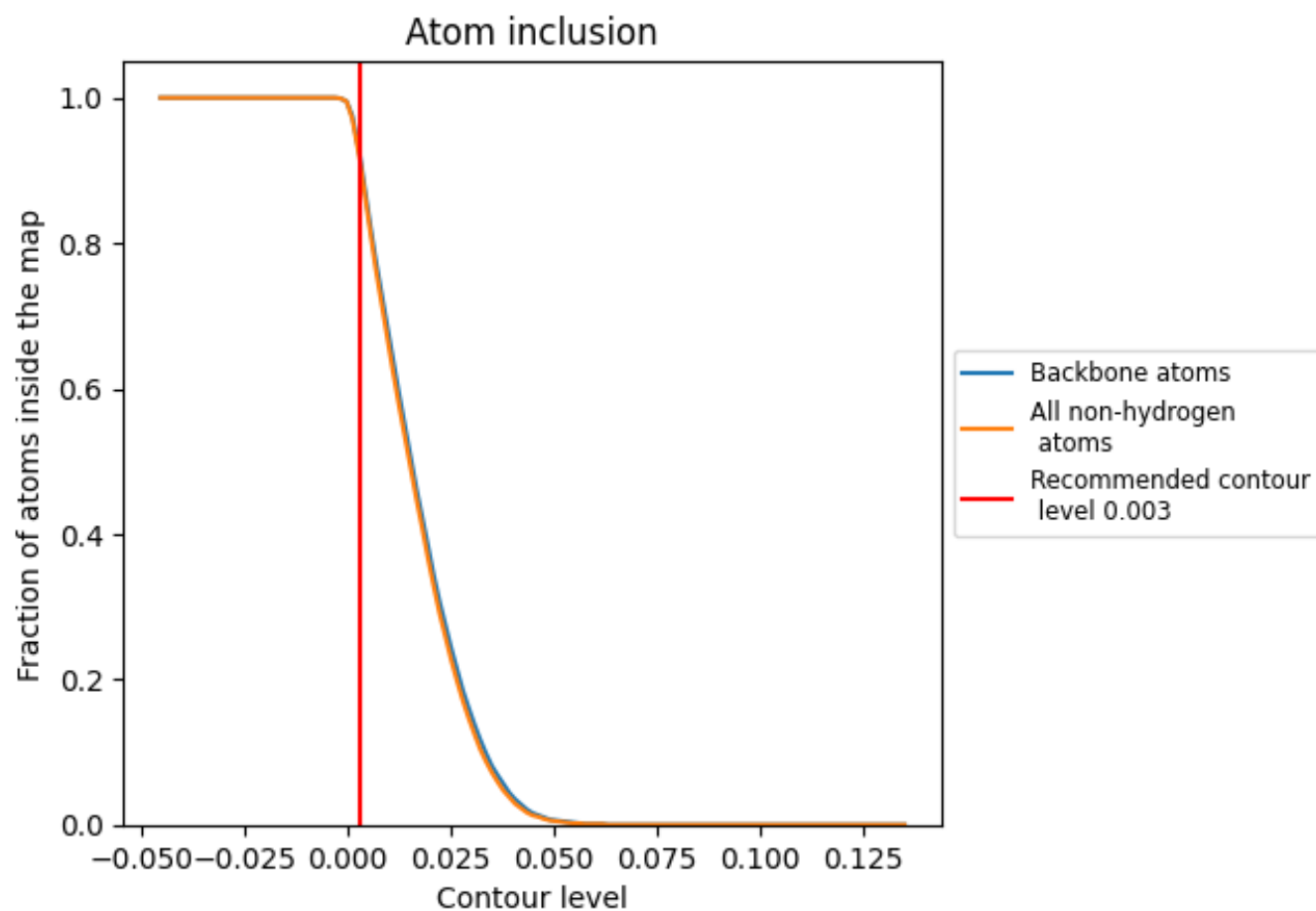
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.7080
A	 0.9580	 0.7680
B	 0.9500	 0.7380
C	 0.9360	 0.7280
D	 0.9740	 0.7760
E	 0.9030	 0.6830
F	 0.8510	 0.6520
H	 0.9250	 0.7270
I	 0.8260	 0.6760
J	 0.8620	 0.6430
K	 0.8620	 0.6330
L	 0.9360	 0.7290
M	 0.9310	 0.7060
O	 0.8630	 0.6610
Q	 0.6410	 0.4550
R	 0.8210	 0.5670
T	 0.9390	 0.7180
U	 0.8490	 0.6340
V	 0.8960	 0.6770
X	 0.9060	 0.6630
Y	 0.7620	 0.5800
Z	 0.8320	 0.5730
a	 0.9620	 0.7710
b	 0.9470	 0.7310
c	 0.9390	 0.7240
d	 0.9720	 0.7750
e	 0.9010	 0.6780
f	 0.8590	 0.6480
h	 0.9260	 0.7220
i	 0.8290	 0.6780
j	 0.8760	 0.6510
k	 0.8540	 0.6360
l	 0.9550	 0.7510
m	 0.9480	 0.7280
o	 0.8640	 0.6580



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.6460	 0.4600
r	 0.8330	 0.5720
t	 0.9310	 0.7170
u	 0.8480	 0.6310
v	 0.8980	 0.6760
x	 0.8950	 0.6560
y	 0.7620	 0.5840
z	 0.8280	 0.5720