



# Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 04:40 AM EST

PDB ID : 7RCV  
EMDB ID : EMD-24407  
Title : High-resolution structure of photosystem II from the mesophilic cyanobacterium, *Synechocystis* sp. PCC 6803  
Authors : Gisriel, C.J.; Brudvig, G.W.  
Deposited on : 2021-07-08  
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

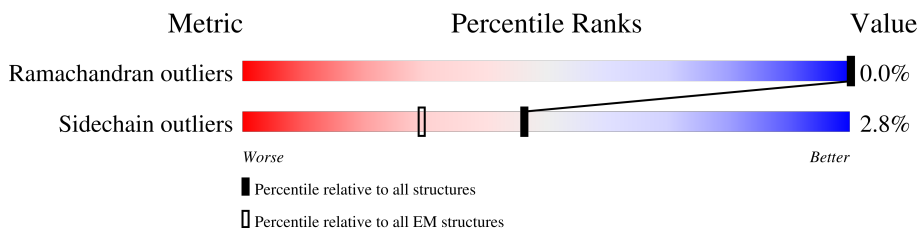
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.01 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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	360	93% 7%
1	a	360	93% 7%
2	B	507	97% ..
2	b	507	97% ..
3	C	460	97% ..
3	c	460	97% ..
4	D	352	96% ..
4	d	352	96% ..
5	E	81	90% 6% .



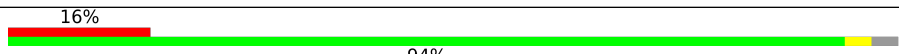
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Mol	Chain	Length	Quality of chain
5	e	81	90% 6% .
6	F	44	80% 20% .
6	f	44	80% 20% .
7	H	64	94% 5% .
7	h	64	94% 5% .
8	I	38	92% . 5%
8	i	38	92% . 5%
9	J	39	15% 97% .
9	j	39	15% 97% .
10	K	45	82% 18%
10	k	45	82% 18%
11	L	39	95% 5%
11	l	39	95% 5%
12	M	35	83% 6% 11%
12	m	35	83% 6% 11%
13	O	247	5% 94% . .
13	o	247	5% 95% . .
14	Q	149	36% 76% . 20%
14	q	149	36% 76% . 20%
15	R	39	82% 5% 13% .
15	r	39	5% 82% 5% 13%
16	T	31	90% 6% .
16	t	31	90% 6% .
17	U	131	70% . 27%
17	u	131	5% 70% . 27%

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Mol	Chain	Length	Quality of chain
18	V	160	 82% 16%
18	v	160	 82% 16%
19	X	39	 87% 10%
19	x	39	 87% 10%
20	Y	39	 82% 18%
20	y	39	 82% 18%
21	Z	62	 13% 94%
21	z	62	 16% 94%

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	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
25	CLA	C	513	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	501	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	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

## 2 Entry composition [i](#)

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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		

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

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

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

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

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

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

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

- Molecule 14 is a protein called Sll1638 protein.

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

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

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

- 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		

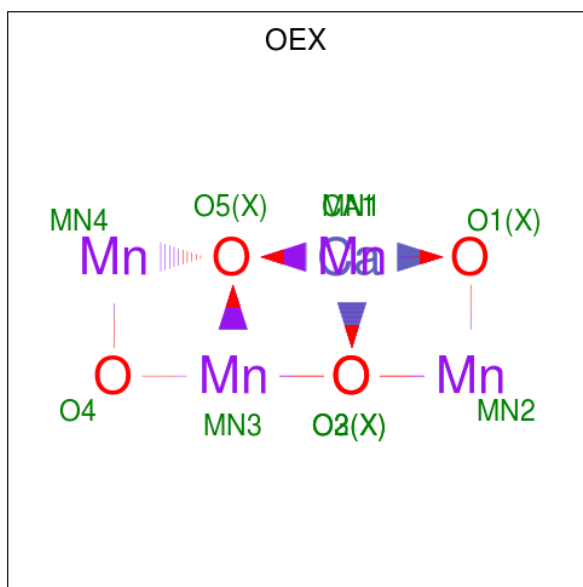
- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

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:  $\text{CaMn}_4\text{O}_5$ ) (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).

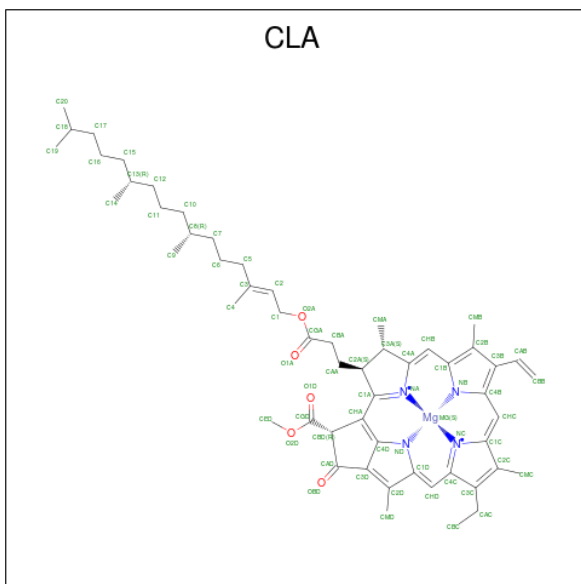
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C Mg N O 190 160 3 12 15	0
25	A	1	Total C Mg N O 190 160 3 12 15	0
25	A	1	Total C Mg N O 190 160 3 12 15	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0
25	B	1	Total C Mg N O 1010 850 16 64 80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	B	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0

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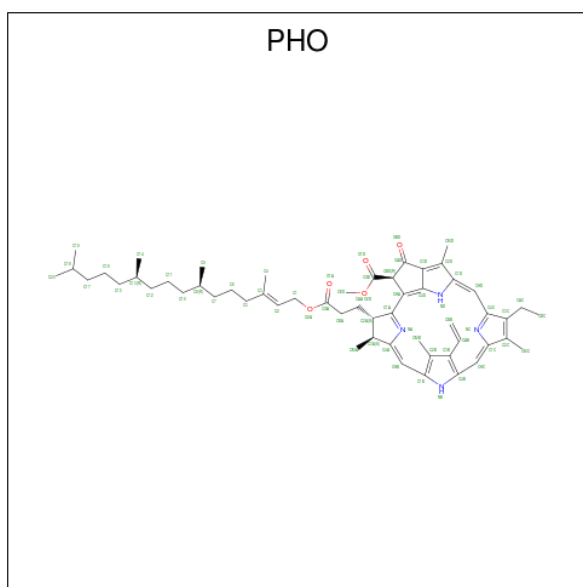
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	C	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
25	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
25	D	1	Total 195	C 165	Mg 3	N 12	O 15	0
25	a	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	a	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	a	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0

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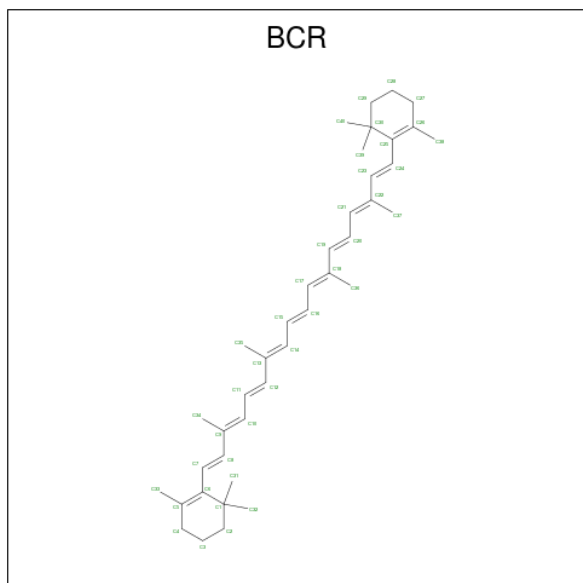
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	b	1	Total 1010	C 850	Mg 16	N 64	O 80	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	c	1	Total 820	C 690	Mg 13	N 52	O 65	0
25	d	1	Total 195	C 165	Mg 3	N 12	O 15	0
25	d	1	Total 195	C 165	Mg 3	N 12	O 15	0
25	d	1	Total 195	C 165	Mg 3	N 12	O 15	0

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



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

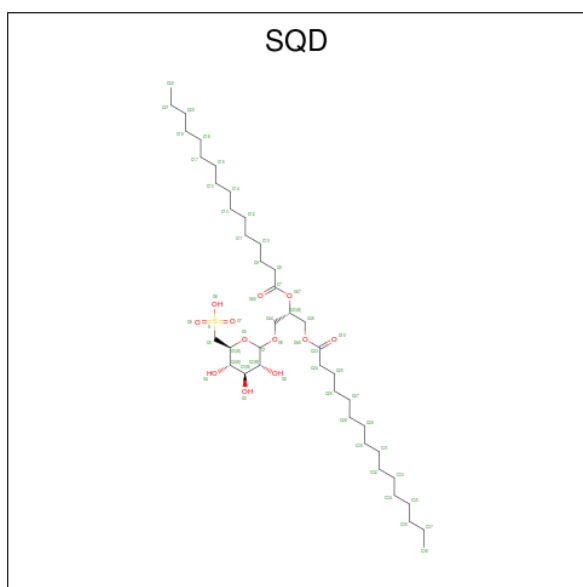
- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





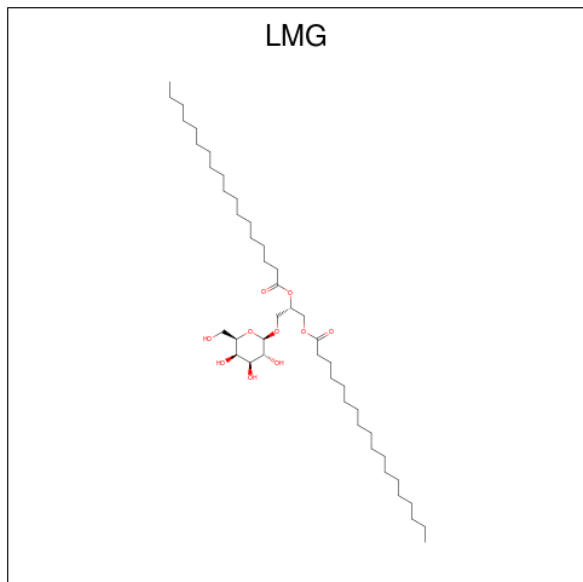
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 120 120	0
27	B	1	Total C 120 120	0
27	B	1	Total C 120 120	0
27	C	1	Total C 80 80	0
27	C	1	Total C 80 80	0
27	D	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	Z	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 120 120	0
27	b	1	Total C 120 120	0
27	b	1	Total C 120 120	0
27	c	1	Total C 80 80	0
27	c	1	Total C 80 80	0
27	d	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-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



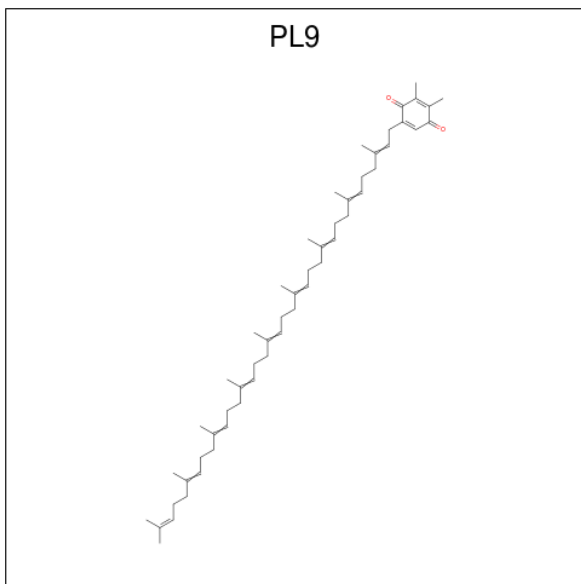
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
28	A	1	Total 156	C 117	O 36	S 3	0
28	A	1	Total 156	C 117	O 36	S 3	0
28	A	1	Total 156	C 117	O 36	S 3	0
28	B	1	Total 54	C 41	O 12	S 1	0
28	F	1	Total 34	C 21	O 12	S 1	0
28	H	1	Total 54	C 41	O 12	S 1	0
28	K	1	Total 45	C 36	O 9		0
28	T	1	Total 54	C 41	O 12	S 1	0
28	a	1	Total 156	C 117	O 36	S 3	0
28	a	1	Total 156	C 117	O 36	S 3	0
28	a	1	Total 156	C 117	O 36	S 3	0
28	f	1	Total 34	C 21	O 12	S 1	0
28	h	1	Total 54	C 41	O 12	S 1	0
28	k	1	Total 45	C 36	O 9		0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



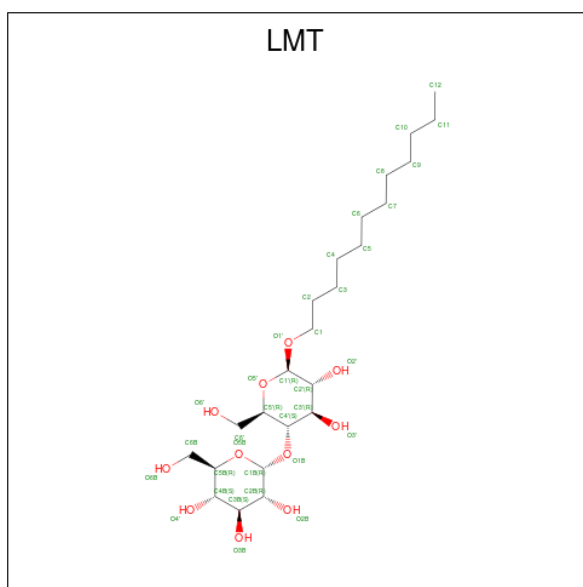
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	87	67	20	0
29	A	1	87	67	20	0
29	B	1	51	41	10	0
29	C	1	100	80	20	0
29	C	1	100	80	20	0
29	D	1	51	41	10	0
29	a	1	87	67	20	0
29	a	1	87	67	20	0
29	b	1	51	41	10	0
29	c	1	100	80	20	0
29	c	1	100	80	20	0
29	d	1	51	41	10	0

- Molecule 30 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
30	A	1	Total	C	O	0
			55	53	2	
30	D	1	Total	C	O	0
			55	53	2	
30	a	1	Total	C	O	0
			55	53	2	
30	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			59	42	17	
31	A	1	Total	C	O	0
			59	42	17	
31	B	1	Total	C	O	0
			107	78	29	
31	B	1	Total	C	O	0
			107	78	29	
31	B	1	Total	C	O	0
			107	78	29	
31	B	1	Total	C	O	0
			107	78	29	
31	C	1	Total	C	O	0
			111	77	34	
31	C	1	Total	C	O	0
			111	77	34	
31	C	1	Total	C	O	0
			111	77	34	
31	C	1	Total	C	O	0
			111	77	34	
31	D	1	Total	C	O	0
			84	61	23	
31	D	1	Total	C	O	0
			84	61	23	
31	D	1	Total	C	O	0
			84	61	23	
31	E	1	Total	C	O	0
			57	40	17	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	E	1	57	40	17	0
31	F	1	35	24	11	0
31	H	1	24	18	6	0
31	I	1	105	76	29	0
31	I	1	105	76	29	0
31	I	1	105	76	29	0
31	I	1	105	76	29	0
31	J	1	24	18	6	0
31	K	1	35	24	11	0
31	M	1	94	66	28	0
31	M	1	94	66	28	0
31	M	1	94	66	28	0
31	T	1	24	18	6	0
31	X	1	81	59	22	0
31	X	1	81	59	22	0
31	X	1	81	59	22	0
31	Y	1	21	15	6	0
31	a	1	59	42	17	0
31	a	1	59	42	17	0
31	b	1	107	78	29	0
31	b	1	107	78	29	0

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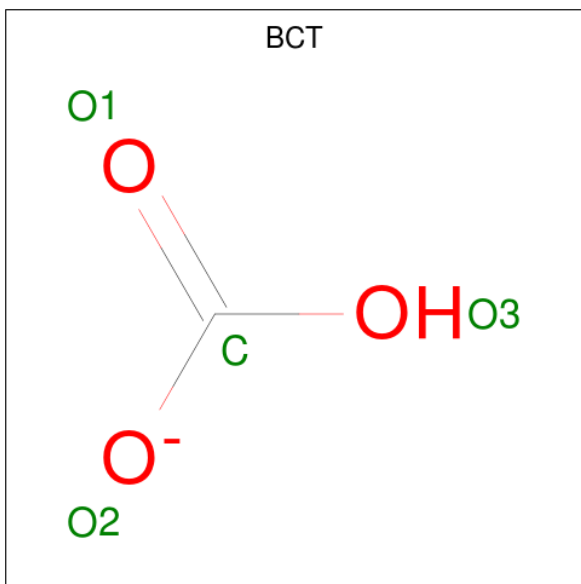
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	b	1	107	78	29	0
31	b	1	107	78	29	0
31	c	1	111	77	34	0
31	c	1	111	77	34	0
31	c	1	111	77	34	0
31	c	1	111	77	34	0
31	d	1	84	61	23	0
31	d	1	84	61	23	0
31	d	1	84	61	23	0
31	e	1	57	40	17	0
31	e	1	57	40	17	0
31	f	1	35	24	11	0
31	h	1	24	18	6	0
31	i	1	105	76	29	0
31	i	1	105	76	29	0
31	i	1	105	76	29	0
31	i	1	105	76	29	0
31	j	1	24	18	6	0
31	k	1	35	24	11	0
31	m	1	94	66	28	0
31	m	1	94	66	28	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	m	1	94	66	28	0
31	t	1	24	18	6	0
31	x	1	81	59	22	0
31	x	1	81	59	22	0
31	x	1	81	59	22	0
31	y	1	21	15	6	0

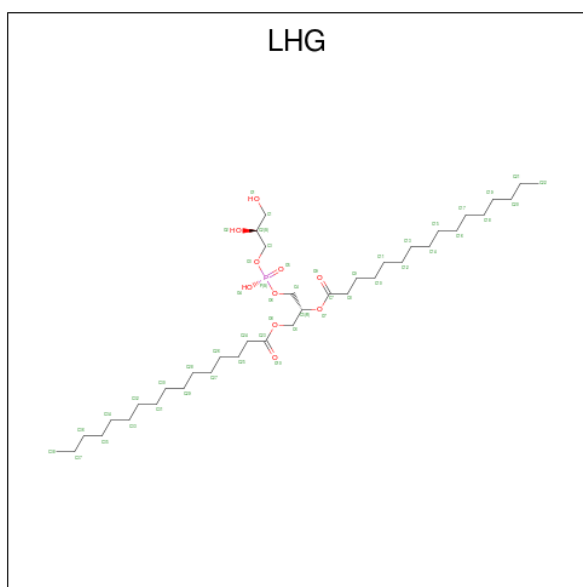
- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

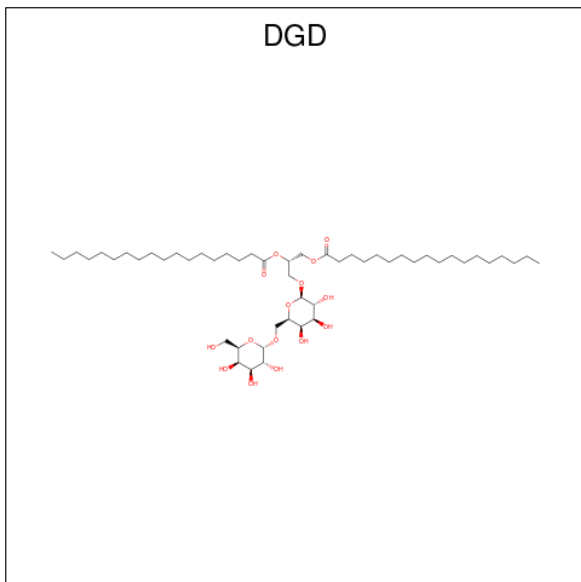
- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).





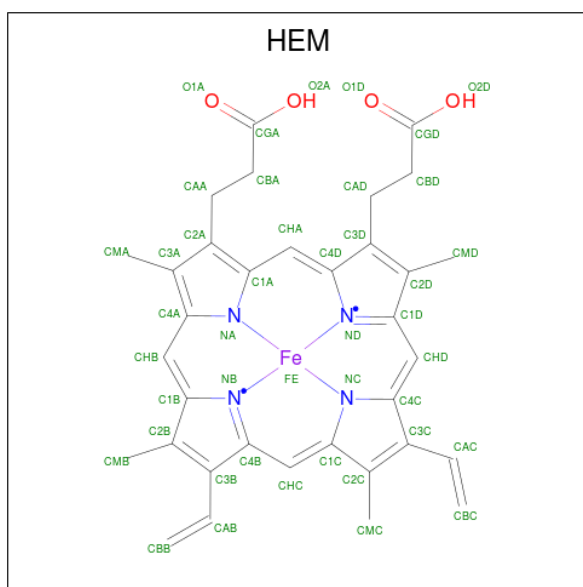
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	A	1	46	35	10	1	0
33	B	1	40	29	10	1	0
33	D	1	98	76	20	2	0
33	D	1	98	76	20	2	0
33	E	1	40	29	10	1	0
33	L	1	49	38	10	1	0
33	Z	1	36	27	8	1	0
33	a	1	46	35	10	1	0
33	b	1	40	29	10	1	0
33	d	1	98	76	20	2	0
33	d	1	98	76	20	2	0
33	e	1	40	29	10	1	0
33	l	1	49	38	10	1	0
33	z	1	36	27	8	1	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	C	1	186	141	45	0
34	C	1	186	141	45	0
34	C	1	186	141	45	0
34	H	1	62	47	15	0
34	c	1	186	141	45	0
34	c	1	186	141	45	0
34	c	1	186	141	45	0
34	h	1	62	47	15	0

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

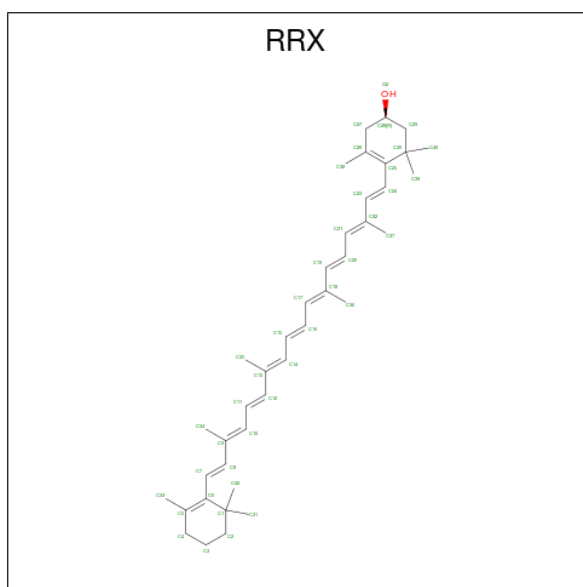


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
35	F	1	43	34	1	4	4	0
35	V	1	43	34	1	4	4	0
35	f	1	43	34	1	4	4	0
35	v	1	43	34	1	4	4	0

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

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

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>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	115	Total	O	0
			115	115	
38	B	119	Total	O	0
			119	119	
38	C	118	Total	O	0
			118	118	
38	D	119	Total	O	0
			119	119	
38	E	12	Total	O	0
			12	12	
38	F	5	Total	O	0
			5	5	
38	H	8	Total	O	0
			8	8	
38	I	4	Total	O	0
			4	4	
38	J	4	Total	O	0
			4	4	
38	K	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
38	L	11	Total 11	O 11	0
38	M	7	Total 7	O 7	0
38	O	39	Total 39	O 39	0
38	Q	1	Total 1	O 1	0
38	T	12	Total 12	O 12	0
38	U	15	Total 15	O 15	0
38	V	24	Total 24	O 24	0
38	X	7	Total 7	O 7	0
38	a	115	Total 115	O 115	0
38	b	116	Total 116	O 116	0
38	c	118	Total 118	O 118	0
38	d	119	Total 119	O 119	0
38	e	12	Total 12	O 12	0
38	f	5	Total 5	O 5	0
38	h	8	Total 8	O 8	0
38	i	4	Total 4	O 4	0
38	j	4	Total 4	O 4	0
38	k	1	Total 1	O 1	0
38	l	11	Total 11	O 11	0
38	m	7	Total 7	O 7	0
38	o	39	Total 39	O 39	0

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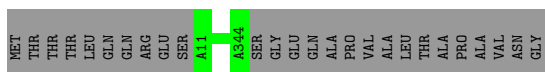
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
38	q	1	Total 1	O 1	0
38	t	9	Total 9	O 9	0
38	u	15	Total 15	O 15	0
38	v	24	Total 24	O 24	0
38	x	7	Total 7	O 7	0

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

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

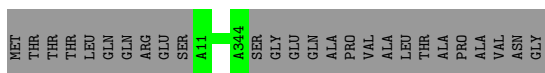
- Molecule 1: Photosystem II protein D1 2

Chain A:  93% 7%



- Molecule 1: Photosystem II protein D1 2

Chain a:  93% 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:  97% ..



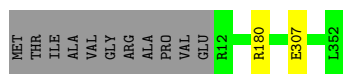
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  97% ..



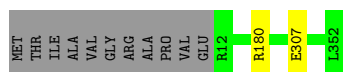
• Molecule 4: Photosystem II D2 protein

Chain D:  96% ..

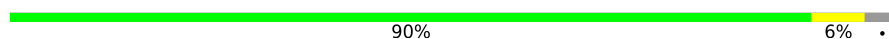


• Molecule 4: Photosystem II D2 protein

Chain d:  96% ..




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:  90% 6% .




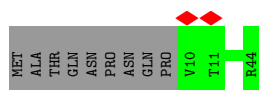
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:  90% 6% .




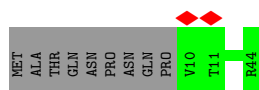
• Molecule 6: Cytochrome b559 subunit beta

Chain F:  5% 80% 20%



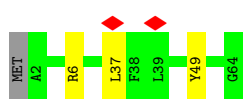
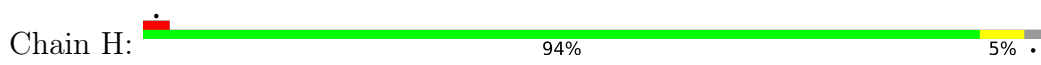
• Molecule 6: Cytochrome b559 subunit beta

Chain f:  5% 80% 20%

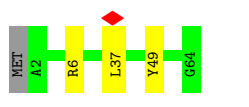
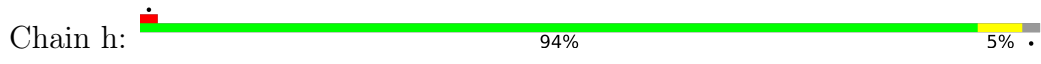


• Molecule 7: Photosystem II reaction center protein H

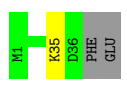
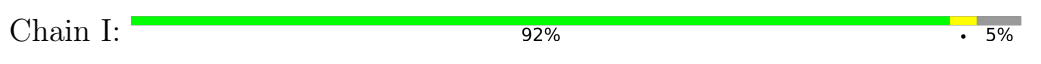




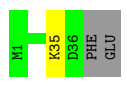
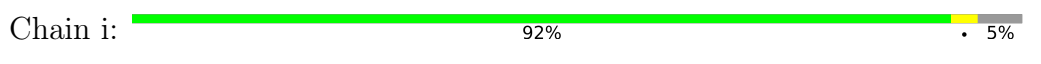
• Molecule 7: Photosystem II reaction center protein H



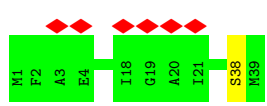
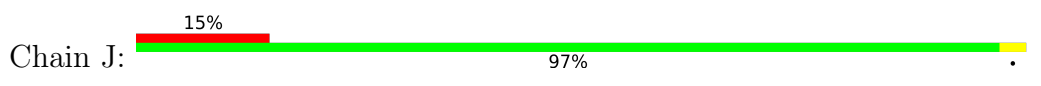
• Molecule 8: Photosystem II reaction center protein I



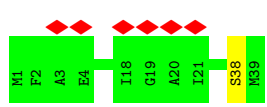
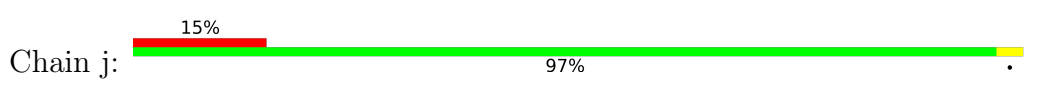
• Molecule 8: Photosystem II reaction center protein I



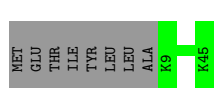
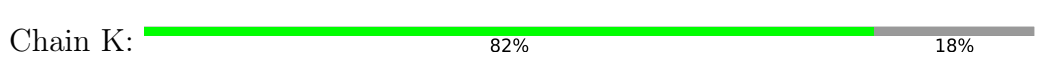
• Molecule 9: Photosystem II reaction center protein J



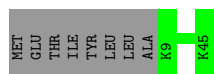
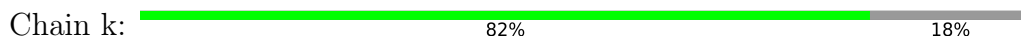
• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



• Molecule 10: Photosystem II reaction center protein K



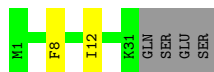
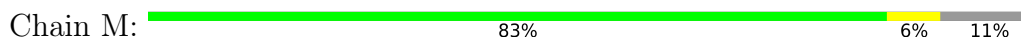
• Molecule 11: Photosystem II reaction center protein L



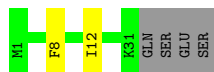
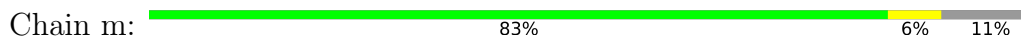
• Molecule 11: Photosystem II reaction center protein L



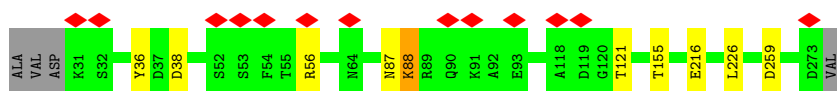
• Molecule 12: Photosystem II reaction center protein M



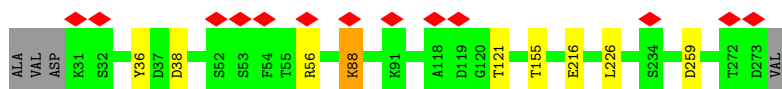
• Molecule 12: Photosystem II reaction center protein M



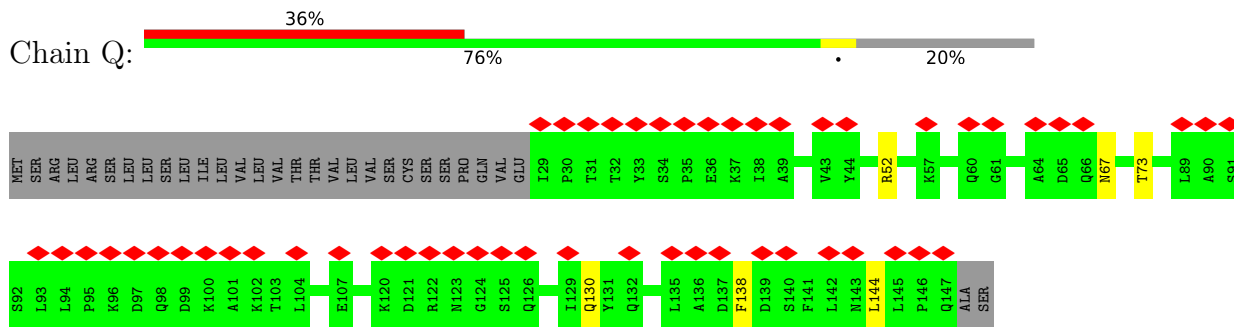
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 13: Photosystem II manganese-stabilizing polypeptide



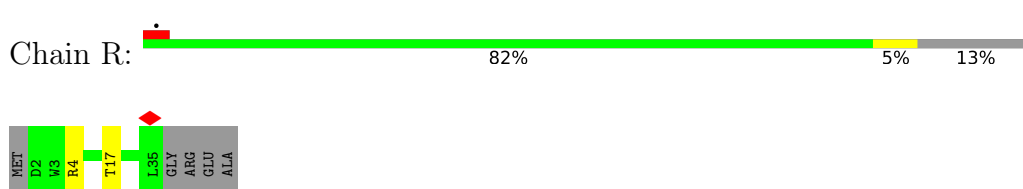
• Molecule 14: Sll1638 protein



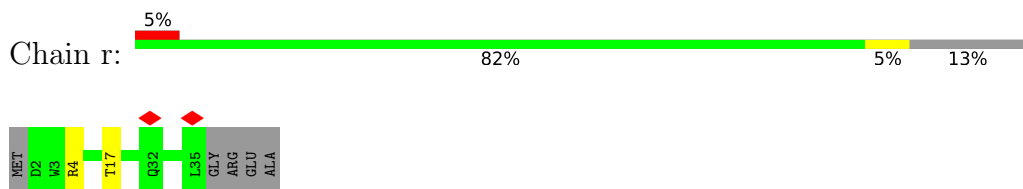
• Molecule 14: Sll1638 protein



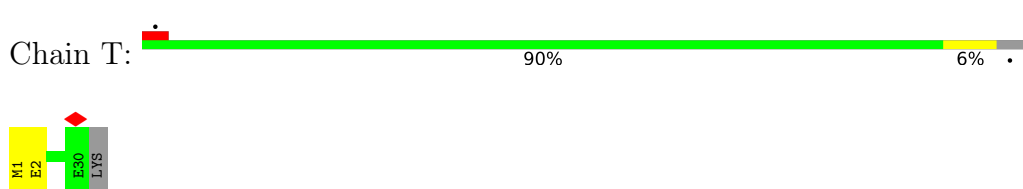
• Molecule 15: Photosystem II protein Y



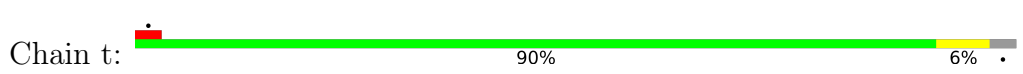
• Molecule 15: Photosystem II protein Y

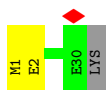


• Molecule 16: Photosystem II reaction center protein T

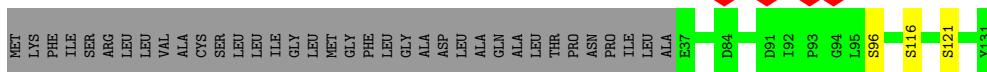


• Molecule 16: Photosystem II reaction center protein T

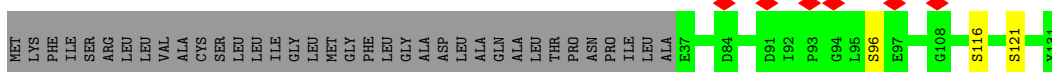




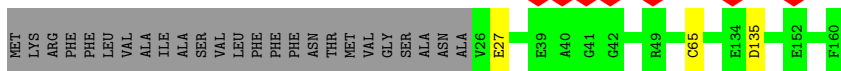
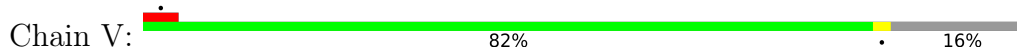
• Molecule 17: Photosystem II 12 kDa extrinsic protein



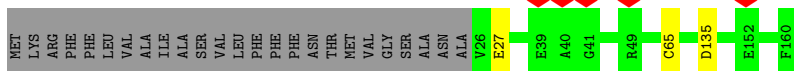
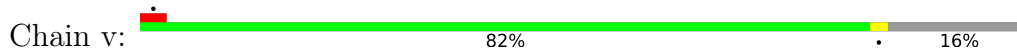
• Molecule 17: Photosystem II 12 kDa extrinsic protein



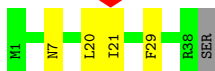
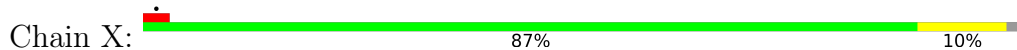
• Molecule 18: Cytochrome c-550



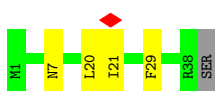
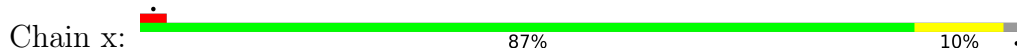
• Molecule 18: Cytochrome c-550




• Molecule 19: Photosystem II reaction center X protein

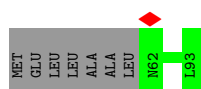


• Molecule 19: Photosystem II reaction center X protein




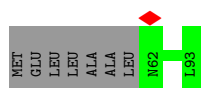
• Molecule 20: Photosystem II reaction center protein Ycf12

Chain Y:  82% 18%




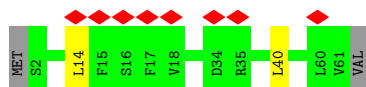
- Molecule 20: Photosystem II reaction center protein Ycf12

Chain y:  82% 18%




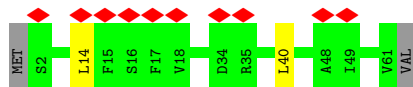
- Molecule 21: Photosystem II reaction center protein Z

Chain Z:  13% 94% ..



- Molecule 21: Photosystem II reaction center protein Z

Chain z:  16% 94% ..



## 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	0.101	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.33	0/2709	0.47	0/3694
1	a	0.33	0/2709	0.47	0/3694
2	B	0.32	0/4068	0.48	1/5538 (0.0%)
2	b	0.32	0/4068	0.48	1/5538 (0.0%)
3	C	0.31	0/3608	0.47	0/4912
3	c	0.31	0/3608	0.47	0/4912
4	D	0.32	0/2823	0.47	0/3843
4	d	0.32	0/2823	0.47	0/3843
5	E	0.30	0/664	0.50	0/906
5	e	0.31	0/664	0.50	0/906
6	F	0.29	0/288	0.41	0/393
6	f	0.29	0/288	0.41	0/393
7	H	0.29	0/506	0.48	0/687
7	h	0.30	0/506	0.48	0/687
8	I	0.28	0/282	0.44	0/381
8	i	0.28	0/282	0.44	0/381
9	J	0.29	0/278	0.46	0/375
9	j	0.29	0/278	0.46	0/375
10	K	0.32	0/310	0.48	0/424
10	k	0.32	0/310	0.48	0/424
11	L	0.30	0/322	0.45	0/435
11	l	0.30	0/322	0.45	0/435
12	M	0.30	0/239	0.47	0/325
12	m	0.30	0/239	0.47	0/325
13	O	0.34	0/1907	0.55	0/2586
13	o	0.34	0/1907	0.55	0/2586
14	Q	0.27	0/930	0.43	0/1257
14	q	0.27	0/930	0.43	0/1257
15	R	0.26	0/262	0.45	0/361
15	r	0.26	0/262	0.45	0/361
16	T	0.34	0/236	0.47	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	t	0.34	0/236	0.47	0/321
17	U	0.28	0/751	0.46	0/1018
17	u	0.28	0/751	0.46	0/1018
18	V	0.34	0/1086	0.54	0/1476
18	v	0.34	0/1086	0.54	0/1476
19	X	0.27	0/293	0.54	0/399
19	x	0.27	0/293	0.54	0/399
20	Y	0.28	0/247	0.44	0/335
20	y	0.28	0/247	0.44	0/335
21	Z	0.28	0/472	0.42	0/649
21	z	0.28	0/472	0.42	0/649
All	All	0.31	0/44562	0.48	2/60630 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	389	LYS	CD-CE-NZ	6.39	126.40	111.70
2	b	389	LYS	CD-CE-NZ	6.39	126.40	111.70

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
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%)	491 (98%)	10 (2%)	0	100	100
2	b	501/507 (99%)	491 (98%)	10 (2%)	0	100	100
3	C	448/460 (97%)	437 (98%)	11 (2%)	0	100	100
3	c	448/460 (97%)	437 (98%)	11 (2%)	0	100	100
4	D	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
5	e	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	33/44 (75%)	33 (100%)	0	0	100	100
7	H	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
7	h	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
8	I	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
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	35 (100%)	0	0	100	100
10	k	35/45 (78%)	35 (100%)	0	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	224 (93%)	16 (7%)	1 (0%)	34	30
13	o	241/247 (98%)	224 (93%)	17 (7%)	0	100	100
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%)	27 (96%)	1 (4%)	0	100	100
16	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
17	U	93/131 (71%)	89 (96%)	4 (4%)	0	100	100
17	u	93/131 (71%)	89 (96%)	4 (4%)	0	100	100
18	V	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
18	v	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
19	X	36/39 (92%)	32 (89%)	4 (11%)	0	100	100
19	x	36/39 (92%)	32 (89%)	4 (11%)	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
21	z	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
All	All	5460/5922 (92%)	5318 (97%)	141 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	87	ASN

### 5.3.2 Protein sidechains [i](#)

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%)	273 (100%)	0	100	100
1	a	273/293 (93%)	273 (100%)	0	100	100
2	B	401/404 (99%)	389 (97%)	12 (3%)	41	41
2	b	401/404 (99%)	389 (97%)	12 (3%)	41	41
3	C	351/361 (97%)	345 (98%)	6 (2%)	60	65
3	c	351/361 (97%)	345 (98%)	6 (2%)	60	65
4	D	277/285 (97%)	275 (99%)	2 (1%)	84	88
4	d	277/285 (97%)	275 (99%)	2 (1%)	84	88
5	E	70/73 (96%)	65 (93%)	5 (7%)	14	10
5	e	70/73 (96%)	65 (93%)	5 (7%)	14	10
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%)	50 (94%)	3 (6%)	20	16
7	h	53/54 (98%)	50 (94%)	3 (6%)	20	16
8	I	31/33 (94%)	30 (97%)	1 (3%)	39	38
8	i	31/33 (94%)	30 (97%)	1 (3%)	39	38
9	J	24/24 (100%)	23 (96%)	1 (4%)	30	27
9	j	24/24 (100%)	23 (96%)	1 (4%)	30	27
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%)	34 (94%)	2 (6%)	21	17
11	l	36/36 (100%)	34 (94%)	2 (6%)	21	17
12	M	27/31 (87%)	25 (93%)	2 (7%)	13	9
12	m	27/31 (87%)	25 (93%)	2 (7%)	13	9
13	O	206/210 (98%)	197 (96%)	9 (4%)	28	25
13	o	206/210 (98%)	197 (96%)	9 (4%)	28	25
14	Q	93/128 (73%)	87 (94%)	6 (6%)	17	12
14	q	93/128 (73%)	87 (94%)	6 (6%)	17	12
15	R	26/29 (90%)	24 (92%)	2 (8%)	13	8
15	r	26/29 (90%)	24 (92%)	2 (8%)	13	8
16	T	24/25 (96%)	23 (96%)	1 (4%)	30	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	t	24/25 (96%)	23 (96%)	1 (4%)	30	27
17	U	83/111 (75%)	80 (96%)	3 (4%)	35	34
17	u	83/111 (75%)	80 (96%)	3 (4%)	35	34
18	V	117/137 (85%)	114 (97%)	3 (3%)	46	48
18	v	117/137 (85%)	114 (97%)	3 (3%)	46	48
19	X	32/33 (97%)	29 (91%)	3 (9%)	8	5
19	x	32/33 (97%)	29 (91%)	3 (9%)	8	5
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%)	30	28
21	z	49/52 (94%)	47 (96%)	2 (4%)	30	28
All	All	4514/4848 (93%)	4388 (97%)	126 (3%)	46	44

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
2	B	137	LYS
2	B	156	PHE
2	B	177	HIS
2	B	246	PHE
2	B	290	SER
2	B	297	SER
2	B	347	LYS
2	B	362	PHE
2	B	378	ARG
2	B	385	ARG
2	B	389	LYS
3	C	168	PHE
3	C	169	PHE
3	C	190	THR
3	C	202	LYS
3	C	276	PHE
3	C	294	MET
4	D	180	ARG
4	D	307	GLU
5	E	12	ASP
5	E	61	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	62	GLU
5	E	74	GLN
5	E	80	ASN
7	H	6	ARG
7	H	37	LEU
7	H	49	TYR
8	I	35	LYS
9	J	38	SER
11	L	2	ASP
11	L	4	ASN
12	M	8	PHE
12	M	12	ILE
13	O	36	TYR
13	O	38	ASP
13	O	56	ARG
13	O	88	LYS
13	O	121	THR
13	O	155	THR
13	O	216	GLU
13	O	226	LEU
13	O	259	ASP
14	Q	52	ARG
14	Q	67	ASN
14	Q	73	THR
14	Q	130	GLN
14	Q	138	PHE
14	Q	144	LEU
15	R	4	ARG
15	R	17	THR
16	T	2	GLU
17	U	96	SER
17	U	116	SER
17	U	121	SER
18	V	27	GLU
18	V	65	CYS
18	V	135	ASP
19	X	7	ASN
19	X	20	LEU
19	X	29	PHE
21	Z	14	LEU
21	Z	40	LEU
2	b	76	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	137	LYS
2	b	156	PHE
2	b	177	HIS
2	b	246	PHE
2	b	290	SER
2	b	297	SER
2	b	347	LYS
2	b	362	PHE
2	b	378	ARG
2	b	385	ARG
2	b	389	LYS
3	c	168	PHE
3	c	169	PHE
3	c	190	THR
3	c	202	LYS
3	c	276	PHE
3	c	294	MET
4	d	180	ARG
4	d	307	GLU
5	e	12	ASP
5	e	61	GLN
5	e	62	GLU
5	e	74	GLN
5	e	80	ASN
7	h	6	ARG
7	h	37	LEU
7	h	49	TYR
8	i	35	LYS
9	j	38	SER
11	l	2	ASP
11	l	4	ASN
12	m	8	PHE
12	m	12	ILE
13	o	36	TYR
13	o	38	ASP
13	o	56	ARG
13	o	88	LYS
13	o	121	THR
13	o	155	THR
13	o	216	GLU
13	o	226	LEU
13	o	259	ASP

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Mol	Chain	Res	Type
14	q	52	ARG
14	q	67	ASN
14	q	73	THR
14	q	130	GLN
14	q	138	PHE
14	q	144	LEU
15	r	4	ARG
15	r	17	THR
16	t	2	GLU
17	u	96	SER
17	u	116	SER
17	u	121	SER
18	v	27	GLU
18	v	65	CYS
18	v	135	ASP
19	x	7	ASN
19	x	20	LEU
19	x	29	PHE
21	z	14	LEU
21	z	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	130	GLN
1	A	234	ASN
1	A	261	GLN
1	A	310	GLN
1	A	338	ASN
2	B	76	ASN
2	B	179	GLN
2	B	216	HIS
2	B	281	GLN
2	B	343	HIS
2	B	489	GLN
3	C	142	ASN
3	C	314	ASN
3	C	375	GLN
3	C	405	ASN
4	D	98	GLN
4	D	129	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	23	HIS
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	199	ASN
13	O	227	GLN
13	O	230	GLN
13	O	246	GLN
14	Q	67	ASN
14	Q	76	HIS
14	Q	130	GLN
14	Q	143	ASN
17	U	80	ASN
17	U	106	ASN
18	V	50	GLN
18	V	53	ASN
18	V	119	ASN
19	X	7	ASN
20	Y	68	GLN
21	Z	32	ASN
1	a	16	GLN
1	a	130	GLN
1	a	234	ASN
1	a	261	GLN
1	a	310	GLN
1	a	338	ASN
2	b	76	ASN
2	b	179	GLN
2	b	216	HIS
2	b	260	ASN
2	b	281	GLN
2	b	343	HIS
2	b	409	GLN
2	b	489	GLN
3	c	142	ASN
3	c	314	ASN
3	c	375	GLN
4	d	98	GLN
4	d	129	GLN

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Mol	Chain	Res	Type
5	e	23	HIS
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	199	ASN
13	o	227	GLN
13	o	230	GLN
13	o	246	GLN
14	q	67	ASN
14	q	76	HIS
14	q	130	GLN
14	q	143	ASN
17	u	80	ASN
17	u	106	ASN
18	v	50	GLN
18	v	53	ASN
18	v	119	ASN
19	x	7	ASN
20	y	68	GLN
21	z	32	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
12	FME	m	1	12	8,9,10	0.98	0	7,9,11	0.92	0

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	0.79	0	2,7,11	0.91	0
16	FME	t	1	16	8,9,10	0.99	0	7,9,11	1.29	1 (14%)
8	FME	i	1	8	8,9,10	0.96	0	7,9,11	0.98	0
16	FME	T	1	16	8,9,10	0.99	0	7,9,11	1.29	1 (14%)
8	FME	I	1	8	8,9,10	0.95	0	7,9,11	0.97	0
12	FME	M	1	12	8,9,10	0.98	0	7,9,11	0.92	0
9	FME	j	1	9	6,7,10	0.78	0	2,7,11	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	2/7/9/11	-
9	FME	J	1	9	-	0/5/6/11	-
16	FME	t	1	16	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
16	FME	T	1	16	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
9	FME	j	1	9	-	0/5/6/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	1	FME	C-CA-N	2.87	114.91	109.73
16	t	1	FME	C-CA-N	2.85	114.87	109.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

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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	CB-CG-SD-CE
16	t	1	FME	CB-CG-SD-CE
16	T	1	FME	CB-CA-N-CN
16	t	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z  > 2$
25	CLA	b	603	-	65,73,73	2.22	18 (27%)	76,113,113	2.55	21 (27%)
28	SQD	H	102	-	53,54,54	0.98	5 (9%)	62,65,65	1.66	12 (19%)
27	BCR	C	514	-	41,41,41	2.87	6 (14%)	56,56,56	6.49	22 (39%)
25	CLA	C	509	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	21 (27%)
25	CLA	C	512	-	50,58,73	2.53	18 (36%)	58,95,113	2.86	21 (36%)
25	CLA	B	602	-	65,73,73	2.21	19 (29%)	76,113,113	2.57	24 (31%)
33	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
35	HEM	v	201	18	41,50,50	1.42	3 (7%)	45,82,82	1.41	8 (17%)
29	LMG	D	409	-	51,51,55	1.32	8 (15%)	59,59,63	1.05	3 (5%)
31	LMT	d	411	-	25,25,36	1.06	2 (8%)	30,30,47	1.10	2 (6%)
35	HEM	f	102	6	41,50,50	1.52	4 (9%)	45,82,82	1.47	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	a	417	-	24,24,36	1.12	3 (12%)	29,29,47	1.45	4 (13%)
25	CLA	D	403	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	22 (28%)
28	SQD	F	101	-	33,34,54	1.21	5 (15%)	42,45,65	1.97	10 (23%)
25	CLA	B	615	-	65,73,73	2.21	19 (29%)	76,113,113	2.56	24 (31%)
31	LMT	D	411	-	25,25,36	1.06	2 (8%)	30,30,47	1.10	2 (6%)
31	LMT	i	104	-	22,22,36	1.10	3 (13%)	27,27,47	1.12	2 (7%)
25	CLA	C	510	-	65,73,73	2.22	19 (29%)	76,113,113	2.55	22 (28%)
33	LHG	z	102	-	35,35,48	1.12	2 (5%)	39,40,54	1.29	6 (15%)
31	LMT	b	624	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	1 (2%)
31	LMT	x	103	-	36,36,36	1.19	6 (16%)	47,47,47	0.96	2 (4%)
25	CLA	b	608	-	65,73,73	2.22	19 (29%)	76,113,113	2.55	22 (28%)
27	BCR	c	522	-	41,41,41	2.84	6 (14%)	56,56,56	6.49	25 (44%)
25	CLA	c	512	-	50,58,73	2.53	19 (38%)	58,95,113	2.85	21 (36%)
31	LMT	f	103	-	36,36,36	1.21	6 (16%)	47,47,47	0.98	1 (2%)
25	CLA	c	505	-	55,63,73	2.38	18 (32%)	64,101,113	2.73	23 (35%)
25	CLA	A	406	38	65,73,73	2.19	19 (29%)	76,113,113	2.63	23 (30%)
25	CLA	C	503	-	65,73,73	2.23	20 (30%)	76,113,113	2.58	24 (31%)
25	CLA	A	408	-	60,68,73	2.30	19 (31%)	70,107,113	2.67	23 (32%)
33	LHG	D	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
31	LMT	M	101	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	1 (2%)
26	PHO	D	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.24	5 (10%)
28	SQD	a	414	-	47,48,54	1.00	5 (10%)	56,59,65	1.81	12 (21%)
33	LHG	Z	102	-	35,35,48	1.12	2 (5%)	39,40,54	1.29	6 (15%)
33	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
29	LMG	A	411	-	51,51,55	1.34	8 (15%)	59,59,63	1.20	4 (6%)
27	BCR	d	405	-	41,41,41	2.79	6 (14%)	56,56,56	6.49	20 (35%)
28	SQD	K	101	-	45,45,54	1.04	5 (11%)	53,53,65	1.35	7 (13%)
25	CLA	b	610	-	65,73,73	2.19	20 (30%)	76,113,113	2.63	24 (31%)
31	LMT	B	624	-	24,24,36	1.04	2 (8%)	29,29,47	1.24	2 (6%)
31	LMT	C	524	-	36,36,36	1.16	5 (13%)	47,47,47	1.17	2 (4%)
25	CLA	b	605	-	65,73,73	2.20	18 (27%)	76,113,113	2.54	24 (31%)
37	RRX	X	102	-	42,42,42	1.66	8 (19%)	57,58,58	1.64	10 (17%)
22	OEX	A	401	38,1,3	0,15,15	-	-	-	-	-
25	CLA	C	506	-	65,73,73	2.25	20 (30%)	76,113,113	2.53	24 (31%)
28	SQD	h	102	-	53,54,54	0.97	5 (9%)	62,65,65	1.66	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	E	101	-	22,22,36	1.10	3 (13%)	27,27,47	1.11	1 (3%)
31	LMT	c	520	-	24,24,36	1.03	2 (8%)	29,29,47	1.12	2 (6%)
34	DGD	c	515	-	63,63,67	1.22	8 (12%)	77,77,81	0.99	3 (3%)
27	BCR	k	102	-	41,41,41	2.81	6 (14%)	56,56,56	6.68	24 (42%)
25	CLA	B	607	38	65,73,73	2.19	19 (29%)	76,113,113	2.62	24 (31%)
31	LMT	I	104	-	22,22,36	1.10	3 (13%)	27,27,47	1.11	2 (7%)
28	SQD	A	413	-	53,54,54	0.97	5 (9%)	62,65,65	1.58	10 (16%)
31	LMT	C	520	-	24,24,36	1.04	2 (8%)	29,29,47	1.13	2 (6%)
25	CLA	A	405	-	65,73,73	2.14	18 (27%)	76,113,113	2.71	26 (34%)
27	BCR	b	617	-	41,41,41	2.82	6 (14%)	56,56,56	6.41	22 (39%)
30	PL9	a	412	-	55,55,55	1.16	3 (5%)	68,69,69	1.57	14 (20%)
31	LMT	B	623	-	24,24,36	0.98	2 (8%)	29,29,47	1.22	3 (10%)
31	LMT	E	103	-	36,36,36	1.17	4 (11%)	47,47,47	1.10	4 (8%)
25	CLA	C	508	-	65,73,73	2.22	19 (29%)	76,113,113	2.50	22 (28%)
25	CLA	b	614	-	65,73,73	2.19	18 (27%)	76,113,113	2.61	21 (27%)
25	CLA	c	506	-	65,73,73	2.25	20 (30%)	76,113,113	2.53	24 (31%)
25	CLA	B	616	-	60,68,73	2.26	19 (31%)	70,107,113	2.66	23 (32%)
31	LMT	t	701	-	24,24,36	1.09	2 (8%)	29,29,47	1.22	2 (6%)
25	CLA	c	503	-	65,73,73	2.23	20 (30%)	76,113,113	2.58	23 (30%)
25	CLA	d	404	-	65,73,73	2.22	20 (30%)	76,113,113	2.60	23 (30%)
31	LMT	A	417	-	24,24,36	1.13	3 (12%)	29,29,47	1.45	4 (13%)
31	LMT	h	101	-	24,24,36	1.02	2 (8%)	29,29,47	1.03	2 (6%)
25	CLA	a	408	-	60,68,73	2.29	19 (31%)	70,107,113	2.68	23 (32%)
29	LMG	C	518	-	51,51,55	1.35	7 (13%)	59,59,63	1.17	4 (6%)
28	SQD	a	413	-	53,54,54	0.97	5 (9%)	62,65,65	1.58	10 (16%)
29	LMG	B	621	-	51,51,55	1.32	8 (15%)	59,59,63	1.14	4 (6%)
31	LMT	m	102	-	36,36,36	1.21	6 (16%)	47,47,47	1.00	1 (2%)
31	LMT	e	103	-	36,36,36	1.17	4 (11%)	47,47,47	1.10	4 (8%)
31	LMT	M	103	-	24,24,36	1.07	3 (12%)	29,29,47	1.08	2 (6%)
29	LMG	A	415	-	36,36,55	1.09	2 (5%)	44,44,63	1.14	3 (6%)
25	CLA	b	616	-	60,68,73	2.26	19 (31%)	70,107,113	2.66	24 (34%)
25	CLA	a	405	-	65,73,73	2.14	18 (27%)	76,113,113	2.71	26 (34%)
25	CLA	b	615	-	65,73,73	2.21	19 (29%)	76,113,113	2.56	24 (31%)
25	CLA	c	511	3	65,73,73	2.23	18 (27%)	76,113,113	2.58	21 (27%)
33	LHG	e	102	-	39,39,48	1.01	2 (5%)	42,45,54	1.06	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	C	521	-	24,24,36	1.00	2 (8%)	29,29,47	1.09	1 (3%)
31	LMT	M	102	-	36,36,36	1.22	6 (16%)	47,47,47	1.00	1 (2%)
31	LMT	d	412	-	36,36,36	1.15	5 (13%)	47,47,47	1.16	3 (6%)
34	DGD	C	515	-	63,63,67	1.22	8 (12%)	77,77,81	0.99	3 (3%)
25	CLA	D	404	-	65,73,73	2.22	20 (30%)	76,113,113	2.59	23 (30%)
30	PL9	A	412	-	55,55,55	1.17	3 (5%)	68,69,69	1.57	14 (20%)
28	SQD	A	410	-	53,54,54	0.94	3 (5%)	62,65,65	1.54	9 (14%)
34	DGD	C	516	-	63,63,67	1.21	8 (12%)	77,77,81	1.00	5 (6%)
31	LMT	D	410	-	24,24,36	1.00	3 (12%)	29,29,47	1.30	4 (13%)
27	BCR	b	618	-	41,41,41	2.80	6 (14%)	56,56,56	6.43	19 (33%)
25	CLA	b	606	-	60,68,73	2.30	19 (31%)	70,107,113	2.64	26 (37%)
31	LMT	B	626	-	24,24,36	1.09	2 (8%)	29,29,47	1.10	2 (6%)
31	LMT	j	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.09	3 (10%)
31	LMT	x	104	-	22,22,36	1.09	3 (13%)	27,27,47	1.14	1 (3%)
25	CLA	b	604	-	65,73,73	2.17	18 (27%)	76,113,113	2.71	26 (34%)
29	LMG	a	415	-	36,36,55	1.09	2 (5%)	44,44,63	1.13	3 (6%)
31	LMT	b	625	-	24,24,36	1.09	2 (8%)	29,29,47	1.10	2 (6%)
31	LMT	y	101	-	21,21,36	1.12	3 (14%)	26,26,47	1.27	2 (7%)
33	LHG	A	419	-	45,45,48	0.95	2 (4%)	48,51,54	1.05	2 (4%)
31	LMT	X	101	-	24,24,36	1.07	3 (12%)	29,29,47	1.15	2 (6%)
31	LMT	I	101	-	24,24,36	1.04	2 (8%)	29,29,47	1.01	1 (3%)
31	LMT	i	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.15	2 (6%)
27	BCR	D	405	-	41,41,41	2.79	6 (14%)	56,56,56	6.49	20 (35%)
25	CLA	c	508	-	65,73,73	2.22	19 (29%)	76,113,113	2.49	22 (28%)
27	BCR	B	618	-	41,41,41	2.80	6 (14%)	56,56,56	6.43	19 (33%)
25	CLA	c	507	38	65,73,73	2.19	18 (27%)	76,113,113	2.62	25 (32%)
29	LMG	d	409	-	51,51,55	1.33	8 (15%)	59,59,63	1.05	3 (5%)
25	CLA	B	609	-	65,73,73	2.23	19 (29%)	76,113,113	2.55	22 (28%)
31	LMT	c	524	-	36,36,36	1.16	5 (13%)	47,47,47	1.17	2 (4%)
29	LMG	c	518	-	51,51,55	1.35	7 (13%)	59,59,63	1.17	4 (6%)
25	CLA	b	601	38	45,53,73	2.51	18 (40%)	52,89,113	2.96	19 (36%)
31	LMT	b	623	-	24,24,36	1.04	2 (8%)	29,29,47	1.24	2 (6%)
25	CLA	d	401	38	65,73,73	2.20	19 (29%)	76,113,113	2.59	27 (35%)
26	PHO	a	407	-	51,69,69	1.01	4 (7%)	47,99,99	1.12	4 (8%)
22	OEX	a	401	38,1,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	603	-	65,73,73	2.22	18 (27%)	76,113,113	2.55	21 (27%)
25	CLA	B	606	-	60,68,73	2.30	19 (31%)	70,107,113	2.64	26 (37%)
25	CLA	B	614	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	21 (27%)
25	CLA	B	611	-	65,73,73	2.19	20 (30%)	76,113,113	2.52	22 (28%)
25	CLA	B	605	-	65,73,73	2.20	18 (27%)	76,113,113	2.54	24 (31%)
31	LMT	J	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.09	3 (10%)
31	LMT	Y	101	-	21,21,36	1.12	3 (14%)	26,26,47	1.27	2 (7%)
25	CLA	c	509	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	21 (27%)
31	LMT	m	103	-	24,24,36	1.07	3 (12%)	29,29,47	1.08	2 (6%)
27	BCR	a	409	-	41,41,41	2.84	6 (14%)	56,56,56	6.42	17 (30%)
25	CLA	C	507	38	65,73,73	2.18	18 (27%)	76,113,113	2.62	25 (32%)
31	LMT	x	101	-	24,24,36	1.06	3 (12%)	29,29,47	1.15	2 (6%)
31	LMT	a	416	-	36,36,36	1.22	7 (19%)	47,47,47	1.38	5 (10%)
27	BCR	z	101	-	41,41,41	2.82	7 (17%)	56,56,56	6.44	20 (35%)
32	BCT	a	418	23	2,3,3	1.15	0	2,3,3	4.20	2 (100%)
34	DGD	c	516	-	63,63,67	1.21	8 (12%)	77,77,81	1.00	4 (5%)
31	LMT	H	101	-	24,24,36	1.02	2 (8%)	29,29,47	1.03	2 (6%)
25	CLA	C	511	3	65,73,73	2.22	19 (29%)	76,113,113	2.58	21 (27%)
31	LMT	m	101	-	36,36,36	1.16	6 (16%)	47,47,47	0.92	1 (2%)
25	CLA	C	504	38	65,73,73	2.21	20 (30%)	76,113,113	2.63	23 (30%)
25	CLA	c	501	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	24 (31%)
25	CLA	c	510	-	65,73,73	2.22	19 (29%)	76,113,113	2.56	23 (30%)
33	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
25	CLA	B	608	-	65,73,73	2.22	19 (29%)	76,113,113	2.55	22 (28%)
25	CLA	b	611	-	65,73,73	2.19	20 (30%)	76,113,113	2.52	22 (28%)
31	LMT	X	103	-	36,36,36	1.19	5 (13%)	47,47,47	0.96	2 (4%)
33	LHG	b	621	-	39,39,48	1.04	2 (5%)	42,45,54	1.06	3 (7%)
25	CLA	B	601	38	45,53,73	2.51	18 (40%)	52,89,113	2.96	19 (36%)
33	LHG	D	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
35	HEM	V	201	18	41,50,50	1.42	3 (7%)	45,82,82	1.42	8 (17%)
30	PL9	d	406	-	55,55,55	1.30	6 (10%)	68,69,69	1.52	15 (22%)
25	CLA	B	613	-	65,73,73	2.19	19 (29%)	76,113,113	2.59	21 (27%)
25	CLA	C	505	-	55,63,73	2.38	18 (32%)	64,101,113	2.72	23 (35%)
28	SQD	T	101	-	53,54,54	0.94	4 (7%)	62,65,65	1.60	12 (19%)
29	LMG	c	523	-	49,49,55	1.33	6 (12%)	57,57,63	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	I	103	-	36,36,36	1.18	6 (16%)	47,47,47	1.10	2 (4%)
25	CLA	d	403	-	65,73,73	2.18	19 (29%)	76,113,113	2.63	23 (30%)
25	CLA	b	613	-	65,73,73	2.19	19 (29%)	76,113,113	2.59	21 (27%)
33	LHG	B	622	-	39,39,48	1.04	2 (5%)	42,45,54	1.06	3 (7%)
27	BCR	Z	101	-	41,41,41	2.82	7 (17%)	56,56,56	6.44	20 (35%)
35	HEM	F	102	6	41,50,50	1.52	4 (9%)	45,82,82	1.46	8 (17%)
31	LMT	C	519	-	29,29,36	1.31	5 (17%)	40,40,47	0.96	2 (5%)
31	LMT	I	102	-	24,24,36	1.06	2 (8%)	29,29,47	1.15	2 (6%)
34	DGD	c	517	-	63,63,67	1.22	7 (11%)	77,77,81	1.02	3 (3%)
34	DGD	C	517	-	63,63,67	1.22	7 (11%)	77,77,81	1.02	3 (3%)
25	CLA	C	501	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	24 (31%)
32	BCT	A	418	23	2,3,3	1.15	0	2,3,3	4.22	2 (100%)
31	LMT	D	412	-	36,36,36	1.15	5 (13%)	47,47,47	1.16	3 (6%)
25	CLA	b	607	38	65,73,73	2.19	19 (29%)	76,113,113	2.62	24 (31%)
28	SQD	B	620	-	53,54,54	0.95	4 (7%)	62,65,65	1.60	12 (19%)
27	BCR	K	102	-	41,41,41	2.81	6 (14%)	56,56,56	6.68	24 (42%)
31	LMT	e	101	-	22,22,36	1.10	2 (9%)	27,27,47	1.11	1 (3%)
31	LMT	T	102	-	24,24,36	1.09	2 (8%)	29,29,47	1.22	2 (6%)
27	BCR	A	409	-	41,41,41	2.84	6 (14%)	56,56,56	6.42	17 (30%)
27	BCR	B	617	-	41,41,41	2.82	6 (14%)	56,56,56	6.41	22 (39%)
29	LMG	a	411	-	51,51,55	1.34	8 (15%)	59,59,63	1.20	4 (6%)
25	CLA	B	610	-	65,73,73	2.19	20 (30%)	76,113,113	2.63	24 (31%)
25	CLA	c	504	38	65,73,73	2.21	20 (30%)	76,113,113	2.63	23 (30%)
25	CLA	b	612	-	65,73,73	2.20	19 (29%)	76,113,113	2.58	21 (27%)
26	PHO	d	402	-	51,69,69	1.02	4 (7%)	47,99,99	1.24	5 (10%)
28	SQD	f	101	-	33,34,54	1.21	5 (15%)	42,45,65	1.98	10 (23%)
27	BCR	c	514	-	41,41,41	2.87	6 (14%)	56,56,56	6.50	22 (39%)
31	LMT	i	101	-	24,24,36	1.03	2 (8%)	29,29,47	1.01	1 (3%)
25	CLA	c	502	-	65,73,73	2.21	20 (30%)	76,113,113	2.56	22 (28%)
26	PHO	A	407	-	51,69,69	1.01	4 (7%)	47,99,99	1.12	4 (8%)
28	SQD	A	414	-	47,48,54	1.00	5 (10%)	56,59,65	1.81	12 (21%)
29	LMG	b	620	-	51,51,55	1.32	8 (15%)	59,59,63	1.14	4 (6%)
25	CLA	B	604	-	65,73,73	2.17	18 (27%)	76,113,113	2.71	26 (34%)
31	LMT	b	622	-	24,24,36	0.98	2 (8%)	29,29,47	1.23	3 (10%)
31	LMT	i	103	-	36,36,36	1.18	6 (16%)	47,47,47	1.10	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	K	104	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	2 (4%)
31	LMT	F	103	-	36,36,36	1.21	6 (16%)	47,47,47	0.98	1 (2%)
31	LMT	k	104	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	2 (4%)
33	LHG	E	102	-	39,39,48	1.01	2 (5%)	42,45,54	1.07	3 (7%)
25	CLA	C	502	-	65,73,73	2.21	20 (30%)	76,113,113	2.56	22 (28%)
31	LMT	A	416	-	36,36,36	1.22	7 (19%)	47,47,47	1.38	5 (10%)
34	DGD	H	103	-	63,63,67	1.23	8 (12%)	77,77,81	0.93	3 (3%)
25	CLA	a	406	38	65,73,73	2.19	19 (29%)	76,113,113	2.62	23 (30%)
37	RRX	x	102	-	42,42,42	1.67	8 (19%)	57,58,58	1.64	10 (17%)
33	LHG	a	419	-	45,45,48	0.95	2 (4%)	48,51,54	1.05	2 (4%)
34	DGD	h	103	-	63,63,67	1.23	8 (12%)	77,77,81	0.93	3 (3%)
27	BCR	C	522	-	41,41,41	2.84	6 (14%)	56,56,56	6.49	25 (44%)
27	BCR	b	619	-	41,41,41	2.81	6 (14%)	56,56,56	6.48	22 (39%)
28	SQD	k	101	-	45,45,54	1.04	5 (11%)	53,53,65	1.35	7 (13%)
29	LMG	C	523	-	49,49,55	1.33	6 (12%)	57,57,63	1.06	3 (5%)
28	SQD	a	410	-	53,54,54	0.94	3 (5%)	62,65,65	1.54	9 (14%)
31	LMT	B	625	-	36,36,36	1.16	6 (16%)	47,47,47	1.01	1 (2%)
31	LMT	c	519	-	29,29,36	1.31	5 (17%)	40,40,47	0.95	2 (5%)
25	CLA	D	401	38	65,73,73	2.20	19 (29%)	76,113,113	2.59	27 (35%)
25	CLA	B	612	-	65,73,73	2.20	19 (29%)	76,113,113	2.58	21 (27%)
25	CLA	c	513	-	65,73,73	2.25	19 (29%)	76,113,113	2.51	24 (31%)
31	LMT	X	104	-	22,22,36	1.08	3 (13%)	27,27,47	1.14	1 (3%)
25	CLA	C	513	-	65,73,73	2.25	19 (29%)	76,113,113	2.51	24 (31%)
30	PL9	D	406	-	55,55,55	1.30	6 (10%)	68,69,69	1.52	15 (22%)
33	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
31	LMT	d	410	-	24,24,36	1.00	3 (12%)	29,29,47	1.30	4 (13%)
25	CLA	b	602	-	65,73,73	2.22	19 (29%)	76,113,113	2.57	24 (31%)
27	BCR	B	619	-	41,41,41	2.81	6 (14%)	56,56,56	6.48	22 (39%)
25	CLA	b	609	-	65,73,73	2.23	19 (29%)	76,113,113	2.55	22 (28%)
31	LMT	c	521	-	24,24,36	1.00	2 (8%)	29,29,47	1.09	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	603	-	1/1/15/20	7/37/115/115	-
28	SQD	H	102	-	-	24/49/69/69	0/1/1/1
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	14/37/115/115	-
25	CLA	C	512	-	1/1/12/20	7/19/97/115	-
25	CLA	B	602	-	1/1/15/20	21/37/115/115	-
33	LHG	d	407	-	-	23/53/53/53	-
35	HEM	v	201	18	-	2/12/54/54	-
29	LMG	D	409	-	-	12/46/66/70	0/1/1/1
31	LMT	d	411	-	-	5/17/37/61	0/1/1/2
35	HEM	f	102	6	-	3/12/54/54	-
31	LMT	a	417	-	-	6/15/35/61	0/1/1/2
25	CLA	D	403	-	1/1/15/20	7/37/115/115	-
28	SQD	F	101	-	-	16/29/49/69	0/1/1/1
25	CLA	B	615	-	1/1/15/20	10/37/115/115	-
31	LMT	D	411	-	-	5/17/37/61	0/1/1/2
31	LMT	i	104	-	-	2/13/33/61	0/1/1/2
25	CLA	C	510	-	1/1/15/20	14/37/115/115	-
33	LHG	z	102	-	-	19/37/37/53	-
31	LMT	b	624	-	-	6/21/61/61	0/2/2/2
31	LMT	x	103	-	-	6/21/61/61	0/2/2/2
25	CLA	b	608	-	1/1/15/20	11/37/115/115	-
27	BCR	c	522	-	-	10/29/63/63	0/2/2/2
25	CLA	c	512	-	1/1/12/20	7/19/97/115	-
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	c	505	-	1/1/13/20	2/25/103/115	-
25	CLA	A	406	38	1/1/15/20	11/37/115/115	-
25	CLA	C	503	-	1/1/15/20	8/37/115/115	-
25	CLA	A	408	-	1/1/14/20	11/31/109/115	-
33	LHG	D	407	-	-	23/53/53/53	-
31	LMT	M	101	-	-	9/21/61/61	0/2/2/2
26	PHO	D	402	-	-	5/37/103/103	0/5/6/6
28	SQD	a	414	-	-	21/43/63/69	0/1/1/1
33	LHG	Z	102	-	-	19/37/37/53	-
33	LHG	l	101	-	-	28/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	A	411	-	-	16/46/66/70	0/1/1/1
27	BCR	d	405	-	-	11/29/63/63	0/2/2/2
28	SQD	K	101	-	-	18/39/59/69	0/1/1/1
25	CLA	b	610	-	1/1/15/20	7/37/115/115	-
31	LMT	B	624	-	-	8/15/35/61	0/1/1/2
31	LMT	C	524	-	-	9/21/61/61	0/2/2/2
25	CLA	b	605	-	1/1/15/20	16/37/115/115	-
37	RRX	X	102	-	-	5/29/65/65	0/2/2/2
25	CLA	C	506	-	1/1/15/20	16/37/115/115	-
28	SQD	h	102	-	-	24/49/69/69	0/1/1/1
31	LMT	E	101	-	-	5/13/33/61	0/1/1/2
31	LMT	c	520	-	-	11/15/35/61	0/1/1/2
34	DGD	c	515	-	-	20/51/91/95	0/2/2/2
27	BCR	k	102	-	-	13/29/63/63	0/2/2/2
25	CLA	B	607	38	1/1/15/20	12/37/115/115	-
31	LMT	I	104	-	-	2/13/33/61	0/1/1/2
28	SQD	A	413	-	-	25/49/69/69	0/1/1/1
31	LMT	C	520	-	-	11/15/35/61	0/1/1/2
25	CLA	A	405	-	1/1/15/20	8/37/115/115	-
27	BCR	b	617	-	-	4/29/63/63	0/2/2/2
30	PL9	a	412	-	-	25/53/73/73	0/1/1/1
31	LMT	B	623	-	-	8/15/35/61	0/1/1/2
31	LMT	E	103	-	-	12/21/61/61	0/2/2/2
25	CLA	C	508	-	1/1/15/20	11/37/115/115	-
25	CLA	b	614	-	1/1/15/20	22/37/115/115	-
25	CLA	c	506	-	1/1/15/20	16/37/115/115	-
25	CLA	B	616	-	1/1/14/20	15/31/109/115	-
31	LMT	t	701	-	-	7/15/35/61	0/1/1/2
25	CLA	c	503	-	1/1/15/20	8/37/115/115	-
25	CLA	d	404	-	1/1/15/20	15/37/115/115	-
31	LMT	A	417	-	-	6/15/35/61	0/1/1/2
31	LMT	h	101	-	-	6/15/35/61	0/1/1/2
25	CLA	a	408	-	1/1/14/20	11/31/109/115	-
29	LMG	C	518	-	-	16/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	a	413	-	-	25/49/69/69	0/1/1/1
29	LMG	B	621	-	-	8/46/66/70	0/1/1/1
31	LMT	m	102	-	-	11/21/61/61	0/2/2/2
31	LMT	e	103	-	-	12/21/61/61	0/2/2/2
31	LMT	M	103	-	-	7/15/35/61	0/1/1/2
29	LMG	A	415	-	-	10/31/51/70	0/1/1/1
25	CLA	b	616	-	1/1/14/20	15/31/109/115	-
25	CLA	a	405	-	1/1/15/20	8/37/115/115	-
25	CLA	b	615	-	1/1/15/20	10/37/115/115	-
25	CLA	c	511	3	1/1/15/20	11/37/115/115	-
33	LHG	e	102	-	-	26/44/44/53	-
31	LMT	C	521	-	-	10/15/35/61	0/1/1/2
31	LMT	M	102	-	-	11/21/61/61	0/2/2/2
31	LMT	d	412	-	-	11/21/61/61	0/2/2/2
34	DGD	C	515	-	-	20/51/91/95	0/2/2/2
25	CLA	D	404	-	1/1/15/20	15/37/115/115	-
30	PL9	A	412	-	-	25/53/73/73	0/1/1/1
28	SQD	A	410	-	-	28/49/69/69	0/1/1/1
34	DGD	C	516	-	-	15/51/91/95	0/2/2/2
31	LMT	D	410	-	-	11/15/35/61	0/1/1/2
27	BCR	b	618	-	-	12/29/63/63	0/2/2/2
25	CLA	b	606	-	1/1/14/20	11/31/109/115	-
31	LMT	B	626	-	-	6/15/35/61	0/1/1/2
31	LMT	j	101	-	-	10/15/35/61	0/1/1/2
31	LMT	x	104	-	-	9/12/32/61	0/1/1/2
25	CLA	b	604	-	1/1/15/20	16/37/115/115	-
29	LMG	a	415	-	-	10/31/51/70	0/1/1/1
31	LMT	b	625	-	-	6/15/35/61	0/1/1/2
31	LMT	y	101	-	-	4/12/32/61	0/1/1/2
33	LHG	A	419	-	-	17/50/50/53	-
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
31	LMT	I	101	-	-	9/15/35/61	0/1/1/2
31	LMT	i	102	-	-	11/15/35/61	0/1/1/2
27	BCR	D	405	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	508	-	1/1/15/20	11/37/115/115	-
27	BCR	B	618	-	-	12/29/63/63	0/2/2/2
25	CLA	c	507	38	1/1/15/20	10/37/115/115	-
29	LMG	d	409	-	-	12/46/66/70	0/1/1/1
25	CLA	B	609	-	1/1/15/20	14/37/115/115	-
31	LMT	c	524	-	-	9/21/61/61	0/2/2/2
29	LMG	c	518	-	-	16/46/66/70	0/1/1/1
25	CLA	b	601	38	1/1/11/20	7/13/91/115	-
31	LMT	b	623	-	-	8/15/35/61	0/1/1/2
25	CLA	d	401	38	1/1/15/20	9/37/115/115	-
26	PHO	a	407	-	-	4/37/103/103	0/5/6/6
25	CLA	B	603	-	1/1/15/20	7/37/115/115	-
25	CLA	B	606	-	1/1/14/20	11/31/109/115	-
25	CLA	B	614	-	1/1/15/20	22/37/115/115	-
25	CLA	B	611	-	1/1/15/20	13/37/115/115	-
25	CLA	B	605	-	1/1/15/20	16/37/115/115	-
31	LMT	J	101	-	-	10/15/35/61	0/1/1/2
31	LMT	Y	101	-	-	4/12/32/61	0/1/1/2
25	CLA	c	509	-	1/1/15/20	14/37/115/115	-
31	LMT	m	103	-	-	7/15/35/61	0/1/1/2
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	507	38	1/1/15/20	10/37/115/115	-
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
31	LMT	a	416	-	-	11/21/61/61	0/2/2/2
27	BCR	z	101	-	-	9/29/63/63	0/2/2/2
34	DGD	c	516	-	-	15/51/91/95	0/2/2/2
31	LMT	H	101	-	-	6/15/35/61	0/1/1/2
25	CLA	C	511	3	1/1/15/20	11/37/115/115	-
31	LMT	m	101	-	-	9/21/61/61	0/2/2/2
25	CLA	C	504	38	1/1/15/20	12/37/115/115	-
25	CLA	c	501	-	1/1/15/20	14/37/115/115	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
33	LHG	L	101	-	-	27/53/53/53	-
25	CLA	B	608	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	611	-	1/1/15/20	13/37/115/115	-
31	LMT	X	103	-	-	6/21/61/61	0/2/2/2
33	LHG	b	621	-	-	30/44/44/53	-
25	CLA	B	601	38	1/1/11/20	7/13/91/115	-
33	LHG	D	408	-	-	22/53/53/53	-
35	HEM	V	201	18	-	2/12/54/54	-
30	PL9	d	406	-	-	10/53/73/73	0/1/1/1
25	CLA	B	613	-	1/1/15/20	13/37/115/115	-
25	CLA	C	505	-	1/1/13/20	2/25/103/115	-
28	SQD	T	101	-	-	23/49/69/69	0/1/1/1
29	LMG	c	523	-	-	24/44/64/70	0/1/1/1
31	LMT	I	103	-	-	10/21/61/61	0/2/2/2
25	CLA	d	403	-	1/1/15/20	7/37/115/115	-
25	CLA	b	613	-	1/1/15/20	13/37/115/115	-
33	LHG	B	622	-	-	30/44/44/53	-
27	BCR	Z	101	-	-	9/29/63/63	0/2/2/2
35	HEM	F	102	6	-	3/12/54/54	-
31	LMT	C	519	-	-	3/14/54/61	0/2/2/2
31	LMT	I	102	-	-	11/15/35/61	0/1/1/2
34	DGD	c	517	-	-	14/51/91/95	0/2/2/2
34	DGD	C	517	-	-	14/51/91/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	14/37/115/115	-
31	LMT	D	412	-	-	11/21/61/61	0/2/2/2
25	CLA	b	607	38	1/1/15/20	12/37/115/115	-
28	SQD	B	620	-	-	23/49/69/69	0/1/1/1
27	BCR	K	102	-	-	13/29/63/63	0/2/2/2
31	LMT	e	101	-	-	5/13/33/61	0/1/1/2
31	LMT	T	102	-	-	7/15/35/61	0/1/1/2
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
29	LMG	a	411	-	-	16/46/66/70	0/1/1/1
25	CLA	B	610	-	1/1/15/20	7/37/115/115	-
25	CLA	c	504	38	1/1/15/20	12/37/115/115	-
25	CLA	b	612	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
28	SQD	f	101	-	-	16/29/49/69	0/1/1/1
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
31	LMT	i	101	-	-	9/15/35/61	0/1/1/2
25	CLA	c	502	-	1/1/15/20	10/37/115/115	-
26	PHO	A	407	-	-	4/37/103/103	0/5/6/6
28	SQD	A	414	-	-	21/43/63/69	0/1/1/1
29	LMG	b	620	-	-	8/46/66/70	0/1/1/1
25	CLA	B	604	-	1/1/15/20	16/37/115/115	-
31	LMT	b	622	-	-	8/15/35/61	0/1/1/2
31	LMT	i	103	-	-	10/21/61/61	0/2/2/2
31	LMT	K	104	-	-	13/21/61/61	0/2/2/2
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
31	LMT	k	104	-	-	13/21/61/61	0/2/2/2
33	LHG	E	102	-	-	26/44/44/53	-
25	CLA	C	502	-	1/1/15/20	10/37/115/115	-
31	LMT	A	416	-	-	11/21/61/61	0/2/2/2
34	DGD	H	103	-	-	8/51/91/95	0/2/2/2
25	CLA	a	406	38	1/1/15/20	11/37/115/115	-
37	RRX	x	102	-	-	5/29/65/65	0/2/2/2
33	LHG	a	419	-	-	17/50/50/53	-
34	DGD	h	103	-	-	8/51/91/95	0/2/2/2
27	BCR	C	522	-	-	10/29/63/63	0/2/2/2
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
28	SQD	k	101	-	-	18/39/59/69	0/1/1/1
29	LMG	C	523	-	-	24/44/64/70	0/1/1/1
28	SQD	a	410	-	-	28/49/69/69	0/1/1/1
31	LMT	B	625	-	-	6/21/61/61	0/2/2/2
31	LMT	c	519	-	-	3/14/54/61	0/2/2/2
25	CLA	D	401	38	1/1/15/20	9/37/115/115	-
25	CLA	B	612	-	1/1/15/20	9/37/115/115	-
25	CLA	c	513	-	1/1/15/20	19/37/115/115	-
31	LMT	X	104	-	-	9/12/32/61	0/1/1/2
25	CLA	C	513	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PL9	D	406	-	-	10/53/73/73	0/1/1/1
33	LHG	d	408	-	-	22/53/53/53	-
31	LMT	d	410	-	-	11/15/35/61	0/1/1/2
25	CLA	b	602	-	1/1/15/20	21/37/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
25	CLA	b	609	-	1/1/15/20	14/37/115/115	-
31	LMT	c	521	-	-	10/15/35/61	0/1/1/2

All (1953) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	522	BCR	C8-C9	-8.36	1.28	1.45
27	c	522	BCR	C8-C9	-8.35	1.28	1.45
27	A	409	BCR	C8-C9	-8.33	1.28	1.45
27	a	409	BCR	C8-C9	-8.32	1.28	1.45
27	z	101	BCR	C8-C9	-8.30	1.28	1.45
27	Z	101	BCR	C8-C9	-8.28	1.28	1.45
27	c	514	BCR	C8-C9	-8.28	1.28	1.45
27	C	514	BCR	C8-C9	-8.27	1.28	1.45
27	b	617	BCR	C8-C9	-8.26	1.28	1.45
27	k	102	BCR	C8-C9	-8.26	1.28	1.45
27	K	102	BCR	C8-C9	-8.24	1.28	1.45
27	B	619	BCR	C8-C9	-8.22	1.28	1.45
27	b	619	BCR	C8-C9	-8.22	1.28	1.45
27	B	617	BCR	C8-C9	-8.21	1.28	1.45
27	B	618	BCR	C8-C9	-8.18	1.28	1.45
27	b	618	BCR	C8-C9	-8.18	1.28	1.45
27	D	405	BCR	C8-C9	-8.16	1.28	1.45
27	d	405	BCR	C8-C9	-8.13	1.28	1.45
27	Z	101	BCR	C11-C10	-8.10	1.18	1.43
27	z	101	BCR	C11-C10	-8.10	1.18	1.43
27	C	514	BCR	C11-C10	-8.09	1.18	1.43
27	a	409	BCR	C11-C10	-8.09	1.18	1.43
27	A	409	BCR	C11-C10	-8.09	1.18	1.43
27	c	514	BCR	C11-C10	-8.08	1.18	1.43
27	c	522	BCR	C11-C10	-8.06	1.18	1.43
27	C	522	BCR	C11-C10	-8.06	1.18	1.43
27	B	617	BCR	C11-C10	-8.06	1.18	1.43
27	b	617	BCR	C11-C10	-8.05	1.18	1.43
27	b	619	BCR	C11-C10	-8.04	1.18	1.43
27	B	619	BCR	C11-C10	-8.03	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	405	BCR	C11-C10	-8.01	1.18	1.43
27	D	405	BCR	C11-C10	-8.00	1.18	1.43
27	K	102	BCR	C11-C10	-7.96	1.18	1.43
27	k	102	BCR	C11-C10	-7.94	1.18	1.43
27	b	618	BCR	C11-C10	-7.92	1.18	1.43
27	B	618	BCR	C11-C10	-7.89	1.19	1.43
27	A	409	BCR	C10-C9	-7.61	1.25	1.35
27	a	409	BCR	C10-C9	-7.56	1.25	1.35
27	C	514	BCR	C20-C21	-7.56	1.20	1.43
27	b	619	BCR	C20-C21	-7.56	1.20	1.43
27	B	619	BCR	C20-C21	-7.56	1.20	1.43
27	c	514	BCR	C20-C21	-7.55	1.20	1.43
27	b	617	BCR	C20-C21	-7.55	1.20	1.43
27	B	617	BCR	C20-C21	-7.54	1.20	1.43
27	B	617	BCR	C10-C9	-7.54	1.25	1.35
27	K	102	BCR	C20-C21	-7.53	1.20	1.43
27	k	102	BCR	C20-C21	-7.53	1.20	1.43
25	B	604	CLA	MG-NA	7.53	2.24	2.06
25	b	604	CLA	MG-NA	7.53	2.24	2.06
27	C	514	BCR	C10-C9	-7.53	1.25	1.35
27	c	514	BCR	C10-C9	-7.53	1.25	1.35
27	B	618	BCR	C20-C21	-7.52	1.20	1.43
27	b	617	BCR	C10-C9	-7.51	1.25	1.35
27	b	618	BCR	C20-C21	-7.51	1.20	1.43
25	C	503	CLA	MG-NA	7.50	2.24	2.06
27	C	522	BCR	C20-C21	-7.49	1.20	1.43
25	c	503	CLA	MG-NA	7.49	2.24	2.06
27	B	618	BCR	C16-C17	-7.47	1.20	1.43
27	c	522	BCR	C10-C9	-7.47	1.25	1.35
27	c	522	BCR	C20-C21	-7.47	1.20	1.43
27	c	514	BCR	C16-C17	-7.47	1.20	1.43
27	C	514	BCR	C16-C17	-7.47	1.20	1.43
27	b	618	BCR	C16-C17	-7.46	1.20	1.43
27	C	522	BCR	C10-C9	-7.45	1.25	1.35
25	c	509	CLA	MG-NA	7.45	2.24	2.06
25	C	509	CLA	MG-NA	7.44	2.23	2.06
27	D	405	BCR	C10-C9	-7.43	1.25	1.35
25	c	506	CLA	MG-NA	7.43	2.23	2.06
27	d	405	BCR	C10-C9	-7.42	1.25	1.35
25	c	507	CLA	MG-NA	7.42	2.23	2.06
27	a	409	BCR	C20-C21	-7.42	1.20	1.43
25	C	506	CLA	MG-NA	7.41	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	MG-NA	7.40	2.23	2.06
27	A	409	BCR	C20-C21	-7.40	1.20	1.43
25	B	615	CLA	MG-NA	7.39	2.23	2.06
27	b	619	BCR	C16-C17	-7.39	1.20	1.43
27	C	522	BCR	C16-C17	-7.38	1.20	1.43
25	C	512	CLA	MG-NA	7.38	2.23	2.06
27	c	522	BCR	C16-C17	-7.38	1.20	1.43
25	c	511	CLA	MG-NA	7.38	2.23	2.06
27	z	101	BCR	C20-C21	-7.37	1.20	1.43
27	Z	101	BCR	C10-C9	-7.37	1.26	1.35
25	C	511	CLA	MG-NA	7.37	2.23	2.06
27	B	619	BCR	C16-C17	-7.37	1.20	1.43
25	c	512	CLA	MG-NA	7.37	2.23	2.06
25	b	615	CLA	MG-NA	7.36	2.23	2.06
27	Z	101	BCR	C20-C21	-7.35	1.20	1.43
27	k	102	BCR	C16-C17	-7.35	1.20	1.43
27	K	102	BCR	C16-C17	-7.34	1.20	1.43
27	a	409	BCR	C16-C17	-7.34	1.20	1.43
27	B	619	BCR	C10-C9	-7.33	1.26	1.35
25	B	608	CLA	MG-NA	7.33	2.23	2.06
27	A	409	BCR	C16-C17	-7.33	1.20	1.43
27	z	101	BCR	C10-C9	-7.32	1.26	1.35
25	b	608	CLA	MG-NA	7.32	2.23	2.06
27	D	405	BCR	C20-C21	-7.32	1.20	1.43
27	b	619	BCR	C10-C9	-7.32	1.26	1.35
25	b	613	CLA	MG-NA	7.31	2.23	2.06
25	B	613	CLA	MG-NA	7.31	2.23	2.06
27	d	405	BCR	C20-C21	-7.31	1.20	1.43
27	k	102	BCR	C10-C9	-7.31	1.26	1.35
25	B	601	CLA	MG-NA	7.29	2.23	2.06
27	D	405	BCR	C16-C17	-7.29	1.20	1.43
25	c	513	CLA	MG-NA	7.28	2.23	2.06
27	d	405	BCR	C16-C17	-7.28	1.20	1.43
25	c	508	CLA	MG-NA	7.27	2.23	2.06
25	c	510	CLA	MG-NA	7.27	2.23	2.06
25	C	510	CLA	MG-NA	7.27	2.23	2.06
27	K	102	BCR	C10-C9	-7.27	1.26	1.35
25	b	603	CLA	MG-NA	7.27	2.23	2.06
25	C	501	CLA	MG-NA	7.27	2.23	2.06
25	C	513	CLA	MG-NA	7.27	2.23	2.06
25	b	601	CLA	MG-NA	7.26	2.23	2.06
25	B	603	CLA	MG-NA	7.26	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	MG-NA	7.26	2.23	2.06
25	c	501	CLA	MG-NA	7.25	2.23	2.06
25	C	508	CLA	MG-NA	7.25	2.23	2.06
27	B	617	BCR	C16-C17	-7.24	1.21	1.43
27	b	617	BCR	C16-C17	-7.24	1.21	1.43
25	C	505	CLA	MG-NA	7.23	2.23	2.06
27	B	618	BCR	C10-C9	-7.23	1.26	1.35
27	b	618	BCR	C10-C9	-7.22	1.26	1.35
25	c	502	CLA	MG-NA	7.22	2.23	2.06
27	z	101	BCR	C16-C17	-7.21	1.21	1.43
27	Z	101	BCR	C16-C17	-7.20	1.21	1.43
25	c	505	CLA	MG-NA	7.19	2.23	2.06
25	B	611	CLA	MG-NA	7.17	2.23	2.06
25	b	611	CLA	MG-NA	7.16	2.23	2.06
25	D	404	CLA	MG-NA	7.15	2.23	2.06
25	B	609	CLA	MG-NA	7.15	2.23	2.06
25	d	404	CLA	MG-NA	7.15	2.23	2.06
25	b	609	CLA	MG-NA	7.14	2.23	2.06
25	c	504	CLA	MG-NA	7.12	2.23	2.06
25	C	504	CLA	MG-NA	7.10	2.23	2.06
25	B	610	CLA	MG-NA	7.08	2.23	2.06
25	b	602	CLA	MG-NA	7.07	2.23	2.06
25	B	612	CLA	MG-NA	7.07	2.23	2.06
25	b	610	CLA	MG-NA	7.07	2.23	2.06
25	b	606	CLA	MG-NA	7.06	2.23	2.06
25	B	606	CLA	MG-NA	7.06	2.23	2.06
25	B	602	CLA	MG-NA	7.06	2.23	2.06
25	b	612	CLA	MG-NA	7.06	2.23	2.06
25	b	616	CLA	MG-NA	7.06	2.23	2.06
25	b	605	CLA	MG-NA	7.04	2.23	2.06
25	B	605	CLA	MG-NA	7.03	2.23	2.06
25	D	401	CLA	MG-NA	7.03	2.23	2.06
25	B	614	CLA	MG-NA	7.02	2.22	2.06
25	B	616	CLA	MG-NA	7.02	2.22	2.06
25	d	401	CLA	MG-NA	7.01	2.22	2.06
25	A	408	CLA	MG-NA	7.01	2.22	2.06
25	a	408	CLA	MG-NA	7.00	2.22	2.06
25	D	403	CLA	MG-NA	7.00	2.22	2.06
25	b	614	CLA	MG-NA	7.00	2.22	2.06
25	d	403	CLA	MG-NA	7.00	2.22	2.06
25	b	607	CLA	MG-NA	6.97	2.22	2.06
25	B	607	CLA	MG-NA	6.95	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	406	CLA	MG-NA	6.93	2.22	2.06
25	a	406	CLA	MG-NA	6.90	2.22	2.06
25	A	405	CLA	MG-NA	6.89	2.22	2.06
25	a	405	CLA	MG-NA	6.88	2.22	2.06
25	C	504	CLA	O2A-C1	5.25	1.60	1.46
25	c	504	CLA	O2A-C1	5.23	1.60	1.46
25	b	607	CLA	O2A-C1	5.20	1.60	1.46
25	B	607	CLA	O2A-C1	5.18	1.60	1.46
25	B	603	CLA	O2A-C1	5.18	1.60	1.46
25	b	603	CLA	O2A-C1	5.16	1.60	1.46
25	B	609	CLA	O2D-CGD	5.15	1.45	1.33
25	b	609	CLA	O2D-CGD	5.14	1.45	1.33
25	c	512	CLA	O2A-C1	5.14	1.60	1.46
25	c	513	CLA	CHC-C1C	5.13	1.48	1.35
25	d	401	CLA	O2A-C1	5.13	1.60	1.46
25	C	512	CLA	O2A-C1	5.13	1.60	1.46
25	C	507	CLA	O2A-C1	5.12	1.60	1.46
25	c	507	CLA	O2A-C1	5.12	1.60	1.46
25	C	513	CLA	CHC-C1C	5.12	1.48	1.35
25	B	605	CLA	O2D-CGD	5.10	1.45	1.33
25	b	605	CLA	O2D-CGD	5.10	1.45	1.33
25	D	401	CLA	O2A-C1	5.10	1.60	1.46
25	b	615	CLA	O2A-C1	5.10	1.60	1.46
25	B	615	CLA	O2A-C1	5.09	1.60	1.46
25	c	513	CLA	O2D-CGD	5.09	1.45	1.33
25	C	513	CLA	O2D-CGD	5.09	1.45	1.33
25	D	401	CLA	O2D-CGD	5.08	1.45	1.33
25	b	609	CLA	O2A-C1	5.08	1.60	1.46
25	C	505	CLA	O2D-CGD	5.08	1.45	1.33
25	c	505	CLA	O2D-CGD	5.08	1.45	1.33
25	C	502	CLA	O2D-CGD	5.07	1.45	1.33
25	B	615	CLA	O2D-CGD	5.07	1.45	1.33
25	c	502	CLA	O2D-CGD	5.07	1.45	1.33
25	C	503	CLA	O2A-C1	5.06	1.60	1.46
25	b	610	CLA	O2A-C1	5.06	1.60	1.46
25	c	503	CLA	O2A-C1	5.06	1.60	1.46
25	B	602	CLA	O2A-C1	5.06	1.60	1.46
25	b	615	CLA	O2D-CGD	5.06	1.45	1.33
25	B	610	CLA	O2A-C1	5.05	1.60	1.46
25	d	401	CLA	O2D-CGD	5.05	1.45	1.33
25	D	404	CLA	O2A-C1	5.05	1.60	1.46
25	a	405	CLA	O2A-C1	5.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	CHC-C1C	5.05	1.47	1.35
25	d	404	CLA	O2A-C1	5.05	1.60	1.46
25	b	602	CLA	O2A-C1	5.04	1.60	1.46
25	B	609	CLA	O2A-C1	5.04	1.60	1.46
25	c	508	CLA	O2A-C1	5.04	1.60	1.46
25	D	404	CLA	CHC-C1C	5.04	1.47	1.35
25	B	616	CLA	O2A-C1	5.04	1.60	1.46
25	b	616	CLA	O2A-C1	5.04	1.60	1.46
25	C	508	CLA	O2A-C1	5.04	1.60	1.46
25	C	509	CLA	CHC-C1C	5.03	1.47	1.35
25	a	408	CLA	O2A-C1	5.03	1.60	1.46
25	B	601	CLA	O2D-CGD	5.03	1.45	1.33
25	b	601	CLA	O2D-CGD	5.03	1.45	1.33
25	b	613	CLA	O2D-CGD	5.03	1.45	1.33
25	c	511	CLA	O2A-C1	5.03	1.60	1.46
25	d	404	CLA	O2D-CGD	5.02	1.45	1.33
25	A	408	CLA	O2A-C1	5.02	1.60	1.46
25	c	510	CLA	O2D-CGD	5.02	1.45	1.33
25	A	405	CLA	O2A-C1	5.02	1.60	1.46
25	D	404	CLA	O2D-CGD	5.02	1.45	1.33
25	c	506	CLA	O2A-C1	5.02	1.60	1.46
25	c	509	CLA	O2A-C1	5.02	1.60	1.46
25	C	511	CLA	O2A-C1	5.02	1.60	1.46
25	C	501	CLA	O2A-C1	5.02	1.60	1.46
25	C	506	CLA	O2A-C1	5.02	1.60	1.46
25	c	501	CLA	O2A-C1	5.02	1.60	1.46
25	b	612	CLA	O2A-C1	5.02	1.60	1.46
25	B	612	CLA	O2A-C1	5.01	1.60	1.46
25	B	613	CLA	O2D-CGD	5.01	1.45	1.33
25	c	512	CLA	O2D-CGD	5.01	1.45	1.33
25	C	512	CLA	O2D-CGD	5.00	1.45	1.33
25	c	509	CLA	CHC-C1C	5.00	1.47	1.35
25	c	513	CLA	O2A-C1	5.00	1.60	1.46
25	C	508	CLA	O2D-CGD	5.00	1.45	1.33
25	A	405	CLA	O2D-CGD	4.99	1.45	1.33
25	b	611	CLA	O2A-C1	4.99	1.60	1.46
25	C	513	CLA	O2A-C1	4.99	1.60	1.46
25	B	611	CLA	O2A-C1	4.99	1.60	1.46
25	C	510	CLA	O2D-CGD	4.99	1.45	1.33
25	B	614	CLA	O2A-C1	4.99	1.60	1.46
25	b	607	CLA	O2D-CGD	4.98	1.45	1.33
25	b	614	CLA	O2A-C1	4.98	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	O2D-CGD	4.98	1.45	1.33
25	C	509	CLA	O2A-C1	4.98	1.60	1.46
25	a	405	CLA	O2D-CGD	4.98	1.45	1.33
25	C	507	CLA	O2D-CGD	4.98	1.45	1.33
25	a	406	CLA	O2A-C1	4.98	1.60	1.46
25	b	608	CLA	O2A-C1	4.98	1.60	1.46
25	c	507	CLA	O2D-CGD	4.97	1.45	1.33
25	B	608	CLA	O2A-C1	4.97	1.60	1.46
25	C	506	CLA	O2D-CGD	4.97	1.45	1.33
25	c	508	CLA	O2D-CGD	4.96	1.45	1.33
25	b	608	CLA	CHC-C1C	4.96	1.47	1.35
25	a	406	CLA	O2D-CGD	4.96	1.45	1.33
25	B	616	CLA	O2D-CGD	4.96	1.45	1.33
25	b	616	CLA	O2D-CGD	4.96	1.45	1.33
25	B	611	CLA	O2D-CGD	4.95	1.45	1.33
25	b	611	CLA	O2D-CGD	4.95	1.45	1.33
25	c	506	CLA	O2D-CGD	4.95	1.45	1.33
25	A	406	CLA	O2A-C1	4.95	1.60	1.46
25	B	608	CLA	CHC-C1C	4.95	1.47	1.35
25	b	606	CLA	O2D-CGD	4.95	1.45	1.33
25	A	406	CLA	O2D-CGD	4.94	1.45	1.33
25	b	602	CLA	O2D-CGD	4.94	1.45	1.33
25	b	602	CLA	CHC-C1C	4.94	1.47	1.35
25	B	608	CLA	O2D-CGD	4.94	1.45	1.33
25	b	608	CLA	O2D-CGD	4.93	1.45	1.33
25	b	612	CLA	O2D-CGD	4.93	1.45	1.33
25	A	405	CLA	CHC-C1C	4.93	1.47	1.35
25	B	602	CLA	CHC-C1C	4.92	1.47	1.35
25	B	612	CLA	O2D-CGD	4.92	1.45	1.33
25	C	504	CLA	O2D-CGD	4.92	1.45	1.33
25	B	613	CLA	O2A-C1	4.92	1.60	1.46
25	B	602	CLA	O2D-CGD	4.91	1.45	1.33
25	B	606	CLA	O2D-CGD	4.91	1.45	1.33
25	c	504	CLA	O2D-CGD	4.91	1.45	1.33
25	B	606	CLA	O2A-C1	4.91	1.60	1.46
25	b	613	CLA	O2A-C1	4.90	1.60	1.46
25	c	502	CLA	O2A-C1	4.90	1.60	1.46
25	B	614	CLA	CHC-C1C	4.90	1.47	1.35
25	c	502	CLA	CHC-C1C	4.90	1.47	1.35
25	b	606	CLA	O2A-C1	4.90	1.59	1.46
25	a	405	CLA	CHC-C1C	4.90	1.47	1.35
25	C	502	CLA	O2A-C1	4.89	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	CHC-C1C	4.88	1.47	1.35
25	C	510	CLA	O2A-C1	4.88	1.59	1.46
25	c	510	CLA	O2A-C1	4.88	1.59	1.46
25	b	612	CLA	CHC-C1C	4.88	1.47	1.35
25	c	511	CLA	O2D-CGD	4.88	1.45	1.33
25	b	614	CLA	CHC-C1C	4.88	1.47	1.35
25	C	511	CLA	O2D-CGD	4.88	1.45	1.33
25	c	510	CLA	CHC-C1C	4.88	1.47	1.35
25	C	510	CLA	CHC-C1C	4.88	1.47	1.35
25	c	504	CLA	CHC-C1C	4.88	1.47	1.35
25	d	403	CLA	O2A-C1	4.87	1.59	1.46
25	B	605	CLA	CHC-C1C	4.87	1.47	1.35
25	C	501	CLA	CHC-C1C	4.87	1.47	1.35
25	b	605	CLA	CHC-C1C	4.87	1.47	1.35
25	C	502	CLA	CHC-C1C	4.87	1.47	1.35
25	B	605	CLA	O2A-C1	4.87	1.59	1.46
25	b	605	CLA	O2A-C1	4.86	1.59	1.46
25	D	403	CLA	O2A-C1	4.86	1.59	1.46
25	B	614	CLA	C3B-C2B	4.86	1.47	1.40
25	C	504	CLA	CHC-C1C	4.86	1.47	1.35
25	b	615	CLA	CHC-C1C	4.86	1.47	1.35
25	c	503	CLA	O2D-CGD	4.86	1.45	1.33
25	B	615	CLA	CHC-C1C	4.86	1.47	1.35
25	B	612	CLA	CHC-C1C	4.86	1.47	1.35
25	b	614	CLA	O2D-CGD	4.86	1.45	1.33
25	B	601	CLA	CHC-C1C	4.86	1.47	1.35
25	C	501	CLA	O2D-CGD	4.86	1.45	1.33
25	a	408	CLA	O2D-CGD	4.85	1.45	1.33
25	B	614	CLA	O2D-CGD	4.85	1.45	1.33
25	c	503	CLA	C3B-C2B	4.85	1.47	1.40
25	C	503	CLA	O2D-CGD	4.85	1.45	1.33
25	C	503	CLA	C3B-C2B	4.85	1.47	1.40
25	b	601	CLA	CHC-C1C	4.85	1.47	1.35
25	b	614	CLA	C3B-C2B	4.84	1.47	1.40
25	c	501	CLA	O2D-CGD	4.84	1.45	1.33
30	A	412	PL9	C7-C3	-4.84	1.46	1.51
25	C	511	CLA	CHC-C1C	4.84	1.47	1.35
25	C	503	CLA	CHC-C1C	4.83	1.47	1.35
25	b	603	CLA	CHC-C1C	4.83	1.47	1.35
25	B	610	CLA	O2D-CGD	4.83	1.45	1.33
25	A	408	CLA	O2D-CGD	4.83	1.45	1.33
25	b	610	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	CHC-C1C	4.83	1.47	1.35
25	c	513	CLA	C3B-C2B	4.83	1.47	1.40
25	C	513	CLA	C3B-C2B	4.82	1.47	1.40
30	a	412	PL9	C7-C3	-4.82	1.46	1.51
25	b	607	CLA	CHC-C1C	4.82	1.47	1.35
25	b	606	CLA	CHC-C1C	4.82	1.47	1.35
25	a	406	CLA	CHC-C1C	4.81	1.47	1.35
25	B	606	CLA	CHC-C1C	4.81	1.47	1.35
25	C	512	CLA	CHC-C1C	4.81	1.47	1.35
25	D	403	CLA	CHC-C1C	4.81	1.47	1.35
25	d	403	CLA	CHC-C1C	4.81	1.47	1.35
25	C	505	CLA	C3D-C4D	-4.81	1.33	1.44
25	C	509	CLA	O2D-CGD	4.81	1.44	1.33
25	c	503	CLA	CHC-C1C	4.81	1.47	1.35
25	c	511	CLA	CHC-C1C	4.81	1.47	1.35
25	d	403	CLA	O2D-CGD	4.80	1.44	1.33
25	B	603	CLA	CHC-C1C	4.80	1.47	1.35
25	c	512	CLA	CHC-C1C	4.80	1.47	1.35
25	b	609	CLA	CHC-C1C	4.80	1.47	1.35
25	c	509	CLA	O2D-CGD	4.80	1.44	1.33
25	D	403	CLA	O2D-CGD	4.80	1.44	1.33
25	A	406	CLA	CHC-C1C	4.80	1.47	1.35
25	B	609	CLA	CHC-C1C	4.80	1.47	1.35
25	a	408	CLA	CHC-C1C	4.80	1.47	1.35
25	A	408	CLA	CHC-C1C	4.79	1.47	1.35
25	b	611	CLA	CHC-C1C	4.78	1.47	1.35
25	c	505	CLA	C3D-C4D	-4.78	1.33	1.44
25	b	604	CLA	O2D-CGD	4.77	1.44	1.33
25	B	604	CLA	O2D-CGD	4.76	1.44	1.33
25	B	616	CLA	CHC-C1C	4.76	1.47	1.35
25	C	506	CLA	CHC-C1C	4.76	1.47	1.35
25	b	616	CLA	CHC-C1C	4.76	1.47	1.35
25	D	403	CLA	C3B-C2B	4.76	1.47	1.40
25	d	403	CLA	C3B-C2B	4.76	1.47	1.40
25	B	611	CLA	CHC-C1C	4.75	1.47	1.35
25	c	505	CLA	CHC-C1C	4.75	1.47	1.35
25	c	509	CLA	C3B-C2B	4.75	1.47	1.40
25	c	506	CLA	CHC-C1C	4.74	1.47	1.35
25	b	610	CLA	CHC-C1C	4.74	1.47	1.35
25	B	610	CLA	CHC-C1C	4.73	1.47	1.35
25	C	505	CLA	CHC-C1C	4.73	1.47	1.35
25	B	603	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	O2D-CGD	4.72	1.44	1.33
25	B	603	CLA	C3B-C2B	4.72	1.46	1.40
25	D	401	CLA	C3B-C2B	4.71	1.46	1.40
25	B	612	CLA	C3B-C2B	4.71	1.46	1.40
25	b	612	CLA	C3B-C2B	4.71	1.46	1.40
25	C	501	CLA	C3B-C2B	4.70	1.46	1.40
25	C	509	CLA	C3B-C2B	4.70	1.46	1.40
25	d	401	CLA	C3B-C2B	4.70	1.46	1.40
25	C	507	CLA	CHC-C1C	4.70	1.47	1.35
25	A	405	CLA	C3B-C2B	4.70	1.46	1.40
25	A	408	CLA	C3B-C2B	4.70	1.46	1.40
25	b	603	CLA	C3B-C2B	4.70	1.46	1.40
25	C	508	CLA	CHC-C1C	4.69	1.47	1.35
25	c	501	CLA	C3B-C2B	4.69	1.46	1.40
25	B	605	CLA	C3B-C2B	4.68	1.46	1.40
25	c	507	CLA	CHC-C1C	4.68	1.47	1.35
25	C	506	CLA	CHD-C1D	4.68	1.47	1.38
25	c	508	CLA	CHC-C1C	4.67	1.47	1.35
25	d	401	CLA	CHC-C1C	4.67	1.46	1.35
25	B	606	CLA	C3B-C2B	4.67	1.46	1.40
25	c	506	CLA	CHD-C1D	4.67	1.47	1.38
25	C	505	CLA	O2A-C1	4.67	1.59	1.46
25	C	504	CLA	C3B-C2B	4.67	1.46	1.40
25	a	408	CLA	C3B-C2B	4.67	1.46	1.40
25	b	605	CLA	C3B-C2B	4.67	1.46	1.40
25	a	405	CLA	C3B-C2B	4.66	1.46	1.40
25	D	401	CLA	CHC-C1C	4.66	1.46	1.35
25	b	604	CLA	CHC-C1C	4.66	1.46	1.35
25	c	504	CLA	C3B-C2B	4.66	1.46	1.40
25	c	505	CLA	O2A-C1	4.66	1.59	1.46
25	B	604	CLA	CHC-C1C	4.65	1.46	1.35
25	B	613	CLA	CHC-C1C	4.65	1.46	1.35
25	c	512	CLA	C3B-C2B	4.64	1.46	1.40
25	b	613	CLA	C3B-C2B	4.64	1.46	1.40
25	c	511	CLA	C3B-C2B	4.64	1.46	1.40
35	F	102	HEM	C3C-C2C	-4.64	1.33	1.40
25	b	613	CLA	CHC-C1C	4.63	1.46	1.35
25	C	512	CLA	C3B-C2B	4.62	1.46	1.40
25	b	606	CLA	C3B-C2B	4.61	1.46	1.40
25	B	607	CLA	C3B-C2B	4.61	1.46	1.40
35	f	102	HEM	C3C-C2C	-4.61	1.34	1.40
25	C	501	CLA	CHD-C1D	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	CHD-C1D	4.60	1.47	1.38
25	C	511	CLA	C3B-C2B	4.59	1.46	1.40
25	B	613	CLA	C3B-C2B	4.59	1.46	1.40
25	b	616	CLA	C3B-C2B	4.59	1.46	1.40
25	b	608	CLA	C3D-C4D	-4.58	1.33	1.44
25	b	607	CLA	C3B-C2B	4.58	1.46	1.40
25	B	616	CLA	C3B-C2B	4.57	1.46	1.40
25	c	502	CLA	C3B-C2B	4.57	1.46	1.40
25	B	608	CLA	C3D-C4D	-4.57	1.33	1.44
25	b	604	CLA	O2A-C1	4.57	1.59	1.46
25	c	510	CLA	C3B-C2B	4.56	1.46	1.40
25	C	513	CLA	C3C-C2C	4.56	1.46	1.36
25	B	604	CLA	O2A-C1	4.55	1.59	1.46
25	B	613	CLA	C3D-C4D	-4.55	1.33	1.44
25	b	613	CLA	C3D-C4D	-4.55	1.33	1.44
25	c	509	CLA	C3D-C4D	-4.55	1.33	1.44
25	c	513	CLA	C3C-C2C	4.55	1.46	1.36
25	d	404	CLA	C3D-C4D	-4.55	1.33	1.44
25	C	508	CLA	C3D-C4D	-4.55	1.33	1.44
25	b	611	CLA	C3D-C4D	-4.55	1.33	1.44
25	C	502	CLA	C3B-C2B	4.54	1.46	1.40
25	B	611	CLA	C3D-C4D	-4.54	1.33	1.44
25	B	602	CLA	C3C-C2C	4.54	1.46	1.36
25	D	404	CLA	CHD-C1D	4.54	1.47	1.38
25	d	404	CLA	CHD-C1D	4.54	1.47	1.38
25	D	404	CLA	C3D-C4D	-4.54	1.33	1.44
25	b	609	CLA	C3B-C2B	4.54	1.46	1.40
25	c	510	CLA	C3D-C4D	-4.54	1.33	1.44
25	B	615	CLA	C3B-C2B	4.53	1.46	1.40
25	B	604	CLA	C3D-C4D	-4.53	1.33	1.44
25	C	510	CLA	C3B-C2B	4.53	1.46	1.40
25	c	508	CLA	C3D-C4D	-4.53	1.33	1.44
25	B	609	CLA	C3B-C2B	4.53	1.46	1.40
25	C	513	CLA	CHD-C1D	4.53	1.47	1.38
25	d	404	CLA	C3C-C2C	4.53	1.46	1.36
25	C	509	CLA	C3D-C4D	-4.53	1.34	1.44
25	a	408	CLA	CHD-C1D	4.53	1.47	1.38
25	a	406	CLA	C3B-C2B	4.52	1.46	1.40
25	D	404	CLA	C3C-C2C	4.52	1.46	1.36
25	c	510	CLA	CHD-C1D	4.52	1.47	1.38
25	c	510	CLA	C3C-C2C	4.52	1.46	1.36
25	b	609	CLA	C3D-C4D	-4.52	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	CLA	C3D-C4D	-4.52	1.34	1.44
25	b	602	CLA	C3C-C2C	4.52	1.46	1.36
25	b	605	CLA	C3D-C4D	-4.51	1.34	1.44
25	C	510	CLA	CHD-C1D	4.51	1.47	1.38
25	C	510	CLA	C3D-C4D	-4.51	1.34	1.44
25	A	406	CLA	C3D-C4D	-4.51	1.34	1.44
25	c	503	CLA	C3C-C2C	4.51	1.46	1.36
25	C	503	CLA	C3C-C2C	4.51	1.46	1.36
25	c	513	CLA	CHD-C1D	4.51	1.47	1.38
25	b	615	CLA	C3B-C2B	4.50	1.46	1.40
25	A	408	CLA	CHD-C1D	4.50	1.47	1.38
25	b	604	CLA	C3D-C4D	-4.50	1.34	1.44
25	B	606	CLA	C3D-C4D	-4.50	1.34	1.44
25	B	605	CLA	C3D-C4D	-4.49	1.34	1.44
25	C	510	CLA	C3C-C2C	4.49	1.46	1.36
25	C	506	CLA	C3D-C4D	-4.49	1.34	1.44
25	A	406	CLA	C3B-C2B	4.49	1.46	1.40
25	B	609	CLA	C3D-C4D	-4.49	1.34	1.44
25	d	401	CLA	C3D-C4D	-4.49	1.34	1.44
25	b	606	CLA	C3D-C4D	-4.49	1.34	1.44
25	B	603	CLA	C3D-C4D	-4.49	1.34	1.44
25	b	608	CLA	C3C-C2C	4.48	1.46	1.36
25	C	511	CLA	C3C-C2C	4.48	1.46	1.36
25	B	612	CLA	C3D-C4D	-4.48	1.34	1.44
25	b	603	CLA	C3D-C4D	-4.48	1.34	1.44
25	b	612	CLA	C3D-C4D	-4.48	1.34	1.44
25	B	608	CLA	C3B-C2B	4.48	1.46	1.40
25	A	408	CLA	C3D-C4D	-4.47	1.34	1.44
25	b	608	CLA	C3B-C2B	4.47	1.46	1.40
25	B	608	CLA	C3C-C2C	4.47	1.46	1.36
25	c	506	CLA	C3D-C4D	-4.47	1.34	1.44
25	a	408	CLA	C3D-C4D	-4.47	1.34	1.44
25	b	602	CLA	C3D-C4D	-4.47	1.34	1.44
25	B	601	CLA	C3C-C2C	4.46	1.46	1.36
25	b	601	CLA	C3C-C2C	4.46	1.46	1.36
25	b	606	CLA	CHD-C1D	4.46	1.47	1.38
25	C	501	CLA	C3C-C2C	4.46	1.46	1.36
25	c	511	CLA	C3C-C2C	4.46	1.46	1.36
25	b	615	CLA	C3D-C4D	-4.45	1.34	1.44
25	D	401	CLA	C3D-C4D	-4.45	1.34	1.44
25	D	403	CLA	C3D-C4D	-4.45	1.34	1.44
25	C	512	CLA	C3C-C2C	4.45	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	C3D-C4D	-4.45	1.34	1.44
25	B	602	CLA	C3D-C4D	-4.44	1.34	1.44
25	B	603	CLA	C3C-C2C	4.44	1.46	1.36
25	b	603	CLA	C3C-C2C	4.44	1.46	1.36
25	B	606	CLA	CHD-C1D	4.44	1.47	1.38
25	C	508	CLA	C3C-C2C	4.44	1.46	1.36
25	c	501	CLA	C3C-C2C	4.44	1.46	1.36
25	b	601	CLA	C3D-C4D	-4.43	1.34	1.44
25	b	616	CLA	C3D-C4D	-4.43	1.34	1.44
25	d	403	CLA	C3D-C4D	-4.43	1.34	1.44
25	b	607	CLA	C3D-C4D	-4.43	1.34	1.44
25	b	602	CLA	C3B-C2B	4.42	1.46	1.40
25	B	601	CLA	C3D-C4D	-4.42	1.34	1.44
25	B	616	CLA	C3D-C4D	-4.42	1.34	1.44
25	B	614	CLA	C3C-C2C	4.42	1.46	1.36
25	B	615	CLA	C3D-C4D	-4.42	1.34	1.44
25	C	509	CLA	C3C-C2C	4.42	1.46	1.36
25	d	401	CLA	C3C-C2C	4.42	1.46	1.36
25	c	512	CLA	C3C-C2C	4.42	1.46	1.36
25	b	614	CLA	C3C-C2C	4.42	1.46	1.36
25	b	602	CLA	CHD-C1D	4.41	1.47	1.38
25	c	507	CLA	C3D-C4D	-4.41	1.34	1.44
25	D	401	CLA	C3C-C2C	4.41	1.46	1.36
25	c	504	CLA	C3D-C4D	-4.40	1.34	1.44
25	C	502	CLA	C3D-C4D	-4.40	1.34	1.44
25	a	408	CLA	C3C-C2C	4.40	1.46	1.36
25	b	614	CLA	C3D-C4D	-4.40	1.34	1.44
25	C	507	CLA	C3D-C4D	-4.40	1.34	1.44
25	b	607	CLA	C3C-C2C	4.40	1.46	1.36
25	c	508	CLA	C3C-C2C	4.40	1.46	1.36
25	b	610	CLA	C3D-C4D	-4.40	1.34	1.44
25	c	502	CLA	C3D-C4D	-4.40	1.34	1.44
25	A	408	CLA	C3C-C2C	4.40	1.46	1.36
25	B	614	CLA	C3D-C4D	-4.40	1.34	1.44
25	B	607	CLA	C3C-C2C	4.39	1.46	1.36
25	C	506	CLA	C3C-C2C	4.39	1.46	1.36
25	B	602	CLA	C3B-C2B	4.39	1.46	1.40
25	c	505	CLA	CHD-C1D	4.39	1.46	1.38
25	c	509	CLA	C3C-C2C	4.39	1.46	1.36
25	B	602	CLA	CHD-C1D	4.39	1.46	1.38
25	a	405	CLA	C3D-C4D	-4.38	1.34	1.44
25	B	610	CLA	C3D-C4D	-4.38	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C3C-C2C	4.38	1.46	1.36
25	C	505	CLA	CHD-C1D	4.38	1.46	1.38
25	B	606	CLA	C3C-C2C	4.38	1.46	1.36
25	C	504	CLA	C3D-C4D	-4.38	1.34	1.44
25	B	609	CLA	CHD-C1D	4.38	1.46	1.38
29	a	415	LMG	O8-C28	4.38	1.46	1.33
33	b	621	LHG	O8-C23	4.37	1.46	1.33
25	b	609	CLA	CHD-C1D	4.37	1.46	1.38
29	A	415	LMG	O8-C28	4.37	1.46	1.33
33	B	622	LHG	O8-C23	4.37	1.46	1.33
25	A	405	CLA	C3D-C4D	-4.36	1.34	1.44
25	A	406	CLA	C3C-C2C	4.36	1.46	1.36
25	B	610	CLA	C3B-C2B	4.36	1.46	1.40
25	c	502	CLA	CHD-C1D	4.36	1.46	1.38
25	c	506	CLA	C3C-C2C	4.36	1.46	1.36
25	c	503	CLA	C3D-C4D	-4.36	1.34	1.44
25	C	503	CLA	C3D-C4D	-4.36	1.34	1.44
25	b	610	CLA	C3B-C2B	4.35	1.46	1.40
25	b	605	CLA	C3C-C2C	4.35	1.46	1.36
25	C	502	CLA	C3C-C2C	4.35	1.46	1.36
25	C	507	CLA	C3C-C2C	4.35	1.46	1.36
25	b	606	CLA	C3C-C2C	4.35	1.46	1.36
25	C	502	CLA	CHD-C1D	4.35	1.46	1.38
25	B	605	CLA	C3C-C2C	4.35	1.46	1.36
25	D	404	CLA	C3B-C2B	4.34	1.46	1.40
25	c	504	CLA	C3C-C2C	4.34	1.45	1.36
25	C	501	CLA	C3D-C4D	-4.34	1.34	1.44
25	B	609	CLA	C3C-C2C	4.34	1.45	1.36
25	B	601	CLA	CHD-C1D	4.33	1.46	1.38
25	d	404	CLA	C3B-C2B	4.33	1.46	1.40
25	c	501	CLA	C3D-C4D	-4.33	1.34	1.44
25	a	406	CLA	C3C-C2C	4.33	1.45	1.36
25	C	505	CLA	C3C-C2C	4.33	1.45	1.36
25	C	504	CLA	C3C-C2C	4.33	1.45	1.36
25	c	505	CLA	C3C-C2C	4.33	1.45	1.36
25	b	609	CLA	C3C-C2C	4.32	1.45	1.36
25	D	401	CLA	CHD-C1D	4.32	1.46	1.38
25	c	511	CLA	C3D-C4D	-4.32	1.34	1.44
29	a	411	LMG	O8-C28	4.32	1.46	1.33
25	b	601	CLA	CHD-C1D	4.31	1.46	1.38
25	c	502	CLA	C3C-C2C	4.31	1.45	1.36
25	b	612	CLA	C1D-ND	-4.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	411	LMG	O8-C28	4.30	1.45	1.33
25	c	504	CLA	CHD-C1D	4.30	1.46	1.38
25	b	610	CLA	C3C-C2C	4.30	1.45	1.36
25	D	403	CLA	C3C-C2C	4.30	1.45	1.36
25	B	601	CLA	C3B-C2B	4.30	1.46	1.40
25	c	509	CLA	CHD-C1D	4.30	1.46	1.38
25	C	509	CLA	CHD-C1D	4.30	1.46	1.38
25	C	504	CLA	CHD-C1D	4.29	1.46	1.38
25	C	511	CLA	C3D-C4D	-4.29	1.34	1.44
25	B	615	CLA	C3C-C2C	4.29	1.45	1.36
25	d	401	CLA	CHD-C1D	4.29	1.46	1.38
25	C	508	CLA	C3B-C2B	4.29	1.46	1.40
25	B	612	CLA	C1D-ND	-4.28	1.32	1.37
25	B	610	CLA	C3C-C2C	4.28	1.45	1.36
25	C	508	CLA	CHD-C1D	4.28	1.46	1.38
29	C	523	LMG	O8-C28	4.28	1.45	1.33
25	C	506	CLA	C3B-C2B	4.28	1.46	1.40
25	c	506	CLA	C3B-C2B	4.28	1.46	1.40
25	b	612	CLA	C3C-C2C	4.28	1.45	1.36
25	d	403	CLA	C3C-C2C	4.28	1.45	1.36
25	a	406	CLA	CHD-C1D	4.28	1.46	1.38
25	b	601	CLA	C3B-C2B	4.27	1.46	1.40
25	b	615	CLA	C3C-C2C	4.27	1.45	1.36
30	D	406	PL9	C7-C3	-4.27	1.46	1.51
29	c	523	LMG	O8-C28	4.27	1.45	1.33
25	c	513	CLA	C3D-C4D	-4.27	1.34	1.44
29	C	518	LMG	O8-C28	4.27	1.45	1.33
25	C	503	CLA	CHD-C1D	4.27	1.46	1.38
25	c	508	CLA	CHD-C1D	4.27	1.46	1.38
25	c	505	CLA	C3B-C2B	4.26	1.46	1.40
29	b	620	LMG	O8-C28	4.26	1.45	1.33
29	c	518	LMG	O8-C28	4.26	1.45	1.33
25	b	604	CLA	CHD-C1D	4.26	1.46	1.38
25	B	615	CLA	CHD-C1D	4.26	1.46	1.38
29	B	621	LMG	O8-C28	4.25	1.45	1.33
25	C	513	CLA	C3D-C4D	-4.25	1.34	1.44
25	c	508	CLA	C3B-C2B	4.25	1.46	1.40
25	B	612	CLA	C3C-C2C	4.25	1.45	1.36
25	c	512	CLA	C3D-C4D	-4.25	1.34	1.44
25	B	613	CLA	C3C-C2C	4.25	1.45	1.36
25	A	406	CLA	CHD-C1D	4.25	1.46	1.38
25	c	503	CLA	CHD-C1D	4.25	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C3B-C2B	4.24	1.46	1.40
33	Z	102	LHG	O8-C23	4.24	1.45	1.33
25	B	604	CLA	CHD-C1D	4.24	1.46	1.38
25	b	615	CLA	CHD-C1D	4.24	1.46	1.38
25	d	403	CLA	C1D-ND	-4.24	1.32	1.37
25	b	613	CLA	C3C-C2C	4.24	1.45	1.36
25	D	403	CLA	C1D-ND	-4.23	1.32	1.37
33	l	101	LHG	O8-C23	4.23	1.45	1.33
33	z	102	LHG	O8-C23	4.23	1.45	1.33
25	B	604	CLA	C3B-C2B	4.22	1.46	1.40
33	L	101	LHG	O8-C23	4.22	1.45	1.33
25	b	604	CLA	C3B-C2B	4.22	1.46	1.40
25	C	511	CLA	CHD-C1D	4.22	1.46	1.38
25	C	512	CLA	C3D-C4D	-4.22	1.34	1.44
34	C	516	DGD	O1G-C1A	4.22	1.45	1.33
34	c	516	DGD	O1G-C1A	4.21	1.45	1.33
30	d	406	PL9	C7-C3	-4.21	1.47	1.51
25	b	610	CLA	CHD-C1D	4.20	1.46	1.38
25	b	608	CLA	CHD-C1D	4.20	1.46	1.38
34	h	103	DGD	O1G-C1A	4.20	1.45	1.33
34	H	103	DGD	O1G-C1A	4.19	1.45	1.33
25	c	511	CLA	CHD-C1D	4.19	1.46	1.38
25	B	610	CLA	CHD-C1D	4.18	1.46	1.38
25	B	608	CLA	CHD-C1D	4.18	1.46	1.38
34	c	517	DGD	O1G-C1A	4.16	1.45	1.33
29	C	518	LMG	O7-C10	4.16	1.46	1.34
25	B	611	CLA	CHD-C1D	4.16	1.46	1.38
34	C	517	DGD	O1G-C1A	4.16	1.45	1.33
25	B	611	CLA	C3C-C2C	4.16	1.45	1.36
25	b	605	CLA	CHD-C1D	4.15	1.46	1.38
33	E	102	LHG	O8-C23	4.15	1.45	1.33
25	b	604	CLA	C3C-C2C	4.15	1.45	1.36
33	e	102	LHG	O8-C23	4.15	1.45	1.33
25	B	613	CLA	CHD-C1D	4.15	1.46	1.38
25	B	604	CLA	C3C-C2C	4.15	1.45	1.36
25	b	611	CLA	CHD-C1D	4.15	1.46	1.38
29	c	518	LMG	O7-C10	4.15	1.46	1.34
25	b	611	CLA	C3C-C2C	4.15	1.45	1.36
25	B	605	CLA	CHD-C1D	4.14	1.46	1.38
25	B	616	CLA	C3C-C2C	4.14	1.45	1.36
33	Z	102	LHG	O7-C7	4.14	1.46	1.34
30	d	406	PL9	C3-C4	-4.14	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	CHD-C1D	4.13	1.46	1.38
30	D	406	PL9	C3-C4	-4.13	1.42	1.49
25	c	507	CLA	CHD-C1D	4.13	1.46	1.38
33	d	407	LHG	O8-C23	4.13	1.45	1.33
25	b	613	CLA	CHD-C1D	4.12	1.46	1.38
33	z	102	LHG	O7-C7	4.11	1.45	1.34
25	b	616	CLA	CHD-C1D	4.11	1.46	1.38
33	D	407	LHG	O8-C23	4.11	1.45	1.33
33	A	419	LHG	O7-C7	4.11	1.45	1.34
25	b	616	CLA	C3C-C2C	4.10	1.45	1.36
25	C	512	CLA	CHD-C1D	4.10	1.46	1.38
25	B	616	CLA	CHD-C1D	4.10	1.46	1.38
25	c	512	CLA	CHD-C1D	4.10	1.46	1.38
33	a	419	LHG	O7-C7	4.09	1.45	1.34
33	D	407	LHG	O7-C7	4.09	1.45	1.34
33	d	407	LHG	O7-C7	4.08	1.45	1.34
29	c	523	LMG	O7-C10	4.08	1.45	1.34
25	B	611	CLA	C3B-C2B	4.08	1.46	1.40
25	B	607	CLA	CHD-C1D	4.08	1.46	1.38
25	b	611	CLA	C3B-C2B	4.08	1.46	1.40
25	b	603	CLA	CHD-C1D	4.07	1.46	1.38
29	C	523	LMG	O7-C10	4.07	1.45	1.34
25	B	603	CLA	CHD-C1D	4.06	1.46	1.38
34	C	515	DGD	O1G-C1A	4.06	1.45	1.33
25	b	607	CLA	CHD-C1D	4.05	1.46	1.38
35	V	201	HEM	C3C-C2C	-4.05	1.34	1.40
34	c	515	DGD	O1G-C1A	4.04	1.45	1.33
29	d	409	LMG	O8-C28	4.04	1.45	1.33
29	D	409	LMG	O8-C28	4.04	1.45	1.33
33	d	408	LHG	O8-C23	4.03	1.45	1.33
29	d	409	LMG	O7-C10	4.03	1.45	1.34
35	v	201	HEM	C3C-C2C	-4.02	1.34	1.40
33	D	408	LHG	O8-C23	4.02	1.45	1.33
29	D	409	LMG	O7-C10	4.02	1.45	1.34
25	C	507	CLA	C3B-C2B	4.01	1.45	1.40
29	A	415	LMG	O7-C10	4.01	1.45	1.34
33	B	622	LHG	O7-C7	4.01	1.45	1.34
33	b	621	LHG	O7-C7	4.00	1.45	1.34
29	A	411	LMG	O7-C10	4.00	1.45	1.34
29	a	411	LMG	O7-C10	4.00	1.45	1.34
29	a	415	LMG	O7-C10	4.00	1.45	1.34
25	b	614	CLA	CHD-C1D	3.99	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C3B-C2B	3.99	1.45	1.40
25	C	501	CLA	CHD-C4C	3.98	1.48	1.39
25	c	506	CLA	CHD-C4C	3.98	1.48	1.39
33	a	419	LHG	O8-C23	3.98	1.45	1.33
25	B	614	CLA	CHD-C1D	3.97	1.46	1.38
25	c	501	CLA	CHD-C4C	3.97	1.48	1.39
34	C	515	DGD	O2G-C1B	3.97	1.45	1.34
34	c	515	DGD	O2G-C1B	3.97	1.45	1.34
33	A	419	LHG	O8-C23	3.96	1.44	1.33
25	C	513	CLA	CHD-C4C	3.96	1.48	1.39
25	b	603	CLA	C1D-ND	-3.95	1.32	1.37
25	c	513	CLA	CHD-C4C	3.95	1.48	1.39
25	B	603	CLA	C1D-ND	-3.95	1.32	1.37
25	C	506	CLA	CHD-C4C	3.95	1.48	1.39
37	x	102	RRX	C21-C22	3.92	1.41	1.35
25	C	504	CLA	CHD-C4C	3.91	1.48	1.39
25	D	404	CLA	CHD-C4C	3.90	1.48	1.39
37	x	102	RRX	C17-C18	3.90	1.41	1.35
33	D	408	LHG	O7-C7	3.90	1.45	1.34
25	c	504	CLA	CHD-C4C	3.90	1.48	1.39
33	d	408	LHG	O7-C7	3.89	1.45	1.34
37	X	102	RRX	C21-C22	3.89	1.40	1.35
34	H	103	DGD	O2G-C1B	3.88	1.45	1.34
25	d	404	CLA	CHD-C4C	3.88	1.48	1.39
25	B	605	CLA	C1D-ND	-3.88	1.33	1.37
25	b	605	CLA	C1D-ND	-3.88	1.33	1.37
34	h	103	DGD	O2G-C1B	3.88	1.45	1.34
25	b	606	CLA	CHD-C4C	3.88	1.48	1.39
25	B	606	CLA	CHD-C4C	3.86	1.48	1.39
25	A	408	CLA	CHD-C4C	3.85	1.48	1.39
37	X	102	RRX	C17-C18	3.84	1.40	1.35
25	b	612	CLA	CHD-C1D	3.84	1.45	1.38
25	C	508	CLA	CHD-C4C	3.84	1.48	1.39
34	C	517	DGD	O2G-C1B	3.84	1.45	1.34
33	E	102	LHG	O7-C7	3.84	1.45	1.34
37	x	102	RRX	C14-C13	3.84	1.40	1.35
33	e	102	LHG	O7-C7	3.84	1.45	1.34
25	B	608	CLA	C1D-ND	-3.84	1.33	1.37
37	x	102	RRX	C10-C9	3.83	1.40	1.35
25	B	612	CLA	CHD-C1D	3.83	1.45	1.38
25	a	408	CLA	CHD-C4C	3.83	1.48	1.39
37	X	102	RRX	C10-C9	3.83	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	517	DGD	O2G-C1B	3.82	1.45	1.34
37	X	102	RRX	C14-C13	3.82	1.40	1.35
25	c	508	CLA	CHD-C4C	3.82	1.48	1.39
25	B	602	CLA	CHD-C4C	3.82	1.48	1.39
25	b	611	CLA	C1D-ND	-3.82	1.33	1.37
25	b	602	CLA	CHD-C4C	3.81	1.47	1.39
25	b	608	CLA	C1D-ND	-3.81	1.33	1.37
25	a	405	CLA	CHD-C1D	3.81	1.45	1.38
25	B	611	CLA	C1D-ND	-3.80	1.33	1.37
25	c	505	CLA	CHD-C4C	3.80	1.47	1.39
25	A	405	CLA	CHD-C1D	3.80	1.45	1.38
25	C	510	CLA	CHD-C4C	3.79	1.47	1.39
25	C	505	CLA	CHD-C4C	3.79	1.47	1.39
25	c	510	CLA	CHD-C4C	3.78	1.47	1.39
25	B	610	CLA	C1D-ND	-3.78	1.33	1.37
34	c	516	DGD	O2G-C1B	3.78	1.45	1.34
25	C	512	CLA	C1D-ND	-3.78	1.33	1.37
25	b	615	CLA	C1D-ND	-3.77	1.33	1.37
25	d	401	CLA	CHD-C4C	3.77	1.47	1.39
25	d	403	CLA	CHD-C1D	3.76	1.45	1.38
25	D	401	CLA	CHD-C4C	3.75	1.47	1.39
34	C	516	DGD	O2G-C1B	3.75	1.44	1.34
25	b	610	CLA	C1D-ND	-3.75	1.33	1.37
25	a	406	CLA	CHD-C4C	3.74	1.47	1.39
25	D	403	CLA	CHD-C1D	3.74	1.45	1.38
25	A	405	CLA	C3C-C2C	3.74	1.44	1.36
25	a	405	CLA	C3C-C2C	3.73	1.44	1.36
25	A	406	CLA	CHD-C4C	3.73	1.47	1.39
25	B	609	CLA	CHD-C4C	3.73	1.47	1.39
25	B	608	CLA	CHD-C4C	3.73	1.47	1.39
25	B	601	CLA	CHD-C4C	3.72	1.47	1.39
25	b	608	CLA	CHD-C4C	3.72	1.47	1.39
25	B	615	CLA	C1D-ND	-3.72	1.33	1.37
25	B	607	CLA	C1D-ND	-3.72	1.33	1.37
25	b	609	CLA	CHD-C4C	3.72	1.47	1.39
25	c	502	CLA	CHD-C4C	3.72	1.47	1.39
33	L	101	LHG	O7-C7	3.71	1.44	1.34
25	C	502	CLA	CHD-C4C	3.71	1.47	1.39
25	b	601	CLA	CHD-C4C	3.70	1.47	1.39
25	C	508	CLA	C1D-ND	-3.70	1.33	1.37
25	C	503	CLA	CHD-C4C	3.70	1.47	1.39
33	l	101	LHG	O7-C7	3.70	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	C1D-ND	-3.69	1.33	1.37
25	b	614	CLA	C1D-ND	-3.69	1.33	1.37
25	B	605	CLA	CHD-C4C	3.69	1.47	1.39
35	V	201	HEM	C3C-CAC	3.69	1.55	1.47
25	c	503	CLA	CHD-C4C	3.69	1.47	1.39
25	B	606	CLA	C1D-ND	-3.69	1.33	1.37
25	b	605	CLA	CHD-C4C	3.69	1.47	1.39
25	c	512	CLA	C1D-ND	-3.69	1.33	1.37
25	c	511	CLA	C1D-ND	-3.68	1.33	1.37
25	C	507	CLA	CHD-C4C	3.68	1.47	1.39
25	c	507	CLA	CHD-C4C	3.68	1.47	1.39
35	v	201	HEM	C3C-CAC	3.68	1.55	1.47
25	b	606	CLA	C1D-ND	-3.68	1.33	1.37
25	b	607	CLA	C1D-ND	-3.67	1.33	1.37
25	b	609	CLA	C1D-ND	-3.67	1.33	1.37
25	B	603	CLA	CHD-C4C	3.67	1.47	1.39
25	B	614	CLA	C1D-ND	-3.67	1.33	1.37
25	C	512	CLA	CHD-C4C	3.67	1.47	1.39
25	b	603	CLA	CHD-C4C	3.67	1.47	1.39
25	C	505	CLA	C1D-ND	-3.66	1.33	1.37
29	B	621	LMG	O7-C10	3.66	1.44	1.34
25	c	512	CLA	CHD-C4C	3.66	1.47	1.39
25	c	508	CLA	C1D-ND	-3.66	1.33	1.37
29	b	620	LMG	O7-C10	3.66	1.44	1.34
25	A	406	CLA	C1D-ND	-3.66	1.33	1.37
25	a	406	CLA	C1D-ND	-3.66	1.33	1.37
25	b	613	CLA	C1D-ND	-3.66	1.33	1.37
25	c	505	CLA	C1D-ND	-3.66	1.33	1.37
25	B	613	CLA	C1D-ND	-3.65	1.33	1.37
25	b	607	CLA	CHD-C4C	3.65	1.47	1.39
25	b	615	CLA	CHD-C4C	3.65	1.47	1.39
25	C	509	CLA	CHD-C4C	3.65	1.47	1.39
25	b	613	CLA	CHD-C4C	3.64	1.47	1.39
25	B	611	CLA	CHD-C4C	3.64	1.47	1.39
25	B	613	CLA	CHD-C4C	3.64	1.47	1.39
25	B	615	CLA	CHD-C4C	3.63	1.47	1.39
25	c	509	CLA	CHD-C4C	3.63	1.47	1.39
25	B	607	CLA	CHD-C4C	3.63	1.47	1.39
25	B	609	CLA	C1D-ND	-3.62	1.33	1.37
25	C	511	CLA	CHD-C4C	3.62	1.47	1.39
25	C	509	CLA	C1D-ND	-3.62	1.33	1.37
25	c	511	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	CHD-C4C	3.62	1.47	1.39
25	C	501	CLA	C1D-ND	-3.61	1.33	1.37
25	C	513	CLA	OBD-CAD	3.61	1.28	1.22
25	c	509	CLA	C1D-ND	-3.60	1.33	1.37
25	c	502	CLA	C1D-ND	-3.60	1.33	1.37
25	c	513	CLA	OBD-CAD	3.57	1.28	1.22
25	B	604	CLA	CHD-C4C	3.57	1.47	1.39
25	c	501	CLA	C1D-ND	-3.57	1.33	1.37
25	B	610	CLA	CHD-C4C	3.57	1.47	1.39
25	b	604	CLA	CHD-C4C	3.57	1.47	1.39
25	C	502	CLA	C1D-ND	-3.57	1.33	1.37
25	B	602	CLA	C1D-ND	-3.56	1.33	1.37
25	A	408	CLA	C1D-ND	-3.56	1.33	1.37
25	b	603	CLA	OBD-CAD	3.56	1.28	1.22
25	b	606	CLA	OBD-CAD	3.56	1.28	1.22
25	B	603	CLA	OBD-CAD	3.55	1.28	1.22
25	b	610	CLA	CHD-C4C	3.55	1.47	1.39
25	b	614	CLA	CHD-C4C	3.55	1.47	1.39
35	F	102	HEM	C3C-CAC	3.55	1.55	1.47
25	c	506	CLA	OBD-CAD	3.55	1.28	1.22
25	c	512	CLA	OBD-CAD	3.54	1.28	1.22
25	b	602	CLA	C1D-ND	-3.54	1.33	1.37
25	B	614	CLA	CHD-C4C	3.53	1.47	1.39
25	B	606	CLA	OBD-CAD	3.52	1.28	1.22
35	f	102	HEM	C3C-CAC	3.52	1.55	1.47
25	C	506	CLA	OBD-CAD	3.52	1.28	1.22
25	a	408	CLA	C1D-ND	-3.52	1.33	1.37
25	C	512	CLA	OBD-CAD	3.52	1.28	1.22
25	a	405	CLA	C1D-ND	-3.52	1.33	1.37
25	B	602	CLA	OBD-CAD	3.51	1.28	1.22
25	B	616	CLA	CHD-C4C	3.51	1.47	1.39
25	C	501	CLA	OBD-CAD	3.50	1.28	1.22
25	b	602	CLA	OBD-CAD	3.50	1.28	1.22
25	c	507	CLA	OBD-CAD	3.50	1.28	1.22
25	b	609	CLA	OBD-CAD	3.50	1.28	1.22
25	C	506	CLA	C1D-ND	-3.50	1.33	1.37
25	A	405	CLA	C1D-ND	-3.49	1.33	1.37
25	C	511	CLA	OBD-CAD	3.49	1.28	1.22
25	c	511	CLA	OBD-CAD	3.49	1.28	1.22
25	c	501	CLA	OBD-CAD	3.49	1.28	1.22
25	B	614	CLA	OBD-CAD	3.49	1.28	1.22
25	B	609	CLA	OBD-CAD	3.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	616	CLA	CHD-C4C	3.49	1.47	1.39
27	Z	101	BCR	C11-C12	-3.48	1.25	1.34
25	D	404	CLA	C1D-ND	-3.48	1.33	1.37
25	C	507	CLA	OBD-CAD	3.48	1.28	1.22
25	b	616	CLA	C1D-ND	-3.48	1.33	1.37
27	z	101	BCR	C11-C12	-3.48	1.25	1.34
25	B	601	CLA	OBD-CAD	3.47	1.28	1.22
25	B	604	CLA	C1D-ND	-3.47	1.33	1.37
25	b	601	CLA	OBD-CAD	3.47	1.28	1.22
25	B	616	CLA	C1D-ND	-3.47	1.33	1.37
25	b	614	CLA	OBD-CAD	3.47	1.28	1.22
25	d	404	CLA	C1D-ND	-3.47	1.33	1.37
25	C	504	CLA	OBD-CAD	3.46	1.28	1.22
25	c	506	CLA	C1D-ND	-3.45	1.33	1.37
25	b	610	CLA	OBD-CAD	3.45	1.28	1.22
25	B	610	CLA	OBD-CAD	3.45	1.28	1.22
25	b	604	CLA	C1D-ND	-3.44	1.33	1.37
25	c	503	CLA	C1D-ND	-3.44	1.33	1.37
27	c	514	BCR	C11-C12	-3.44	1.25	1.34
25	c	510	CLA	OBD-CAD	3.44	1.28	1.22
25	c	504	CLA	OBD-CAD	3.44	1.28	1.22
27	C	514	BCR	C11-C12	-3.43	1.25	1.34
25	C	503	CLA	C1D-ND	-3.42	1.33	1.37
25	d	403	CLA	CHD-C4C	3.42	1.47	1.39
25	C	510	CLA	OBD-CAD	3.41	1.28	1.22
25	D	401	CLA	OBD-CAD	3.41	1.28	1.22
25	D	401	CLA	C1D-ND	-3.41	1.33	1.37
25	D	403	CLA	CHD-C4C	3.41	1.47	1.39
25	c	508	CLA	OBD-CAD	3.41	1.28	1.22
25	B	612	CLA	CHD-C4C	3.40	1.47	1.39
25	B	616	CLA	C1C-NC	-3.40	1.32	1.37
25	C	502	CLA	OBD-CAD	3.40	1.28	1.22
25	d	401	CLA	C1D-ND	-3.40	1.33	1.37
25	a	406	CLA	OBD-CAD	3.40	1.28	1.22
27	b	617	BCR	C11-C12	-3.40	1.25	1.34
25	C	508	CLA	OBD-CAD	3.40	1.28	1.22
25	b	615	CLA	OBD-CAD	3.39	1.28	1.22
25	c	509	CLA	OBD-CAD	3.39	1.28	1.22
27	a	409	BCR	C11-C12	-3.39	1.25	1.34
25	C	509	CLA	OBD-CAD	3.39	1.28	1.22
25	b	616	CLA	C1C-NC	-3.39	1.32	1.37
25	c	502	CLA	OBD-CAD	3.39	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	406	CLA	OBD-CAD	3.39	1.28	1.22
25	B	615	CLA	OBD-CAD	3.39	1.28	1.22
27	B	617	BCR	C11-C12	-3.38	1.25	1.34
25	b	608	CLA	OBD-CAD	3.38	1.28	1.22
27	c	522	BCR	C11-C12	-3.38	1.25	1.34
25	d	401	CLA	OBD-CAD	3.38	1.28	1.22
25	c	505	CLA	OBD-CAD	3.37	1.28	1.22
27	C	522	BCR	C11-C12	-3.37	1.25	1.34
25	c	507	CLA	C1D-ND	-3.37	1.33	1.37
25	C	505	CLA	OBD-CAD	3.37	1.28	1.22
25	C	507	CLA	C1D-ND	-3.37	1.33	1.37
25	a	408	CLA	OBD-CAD	3.37	1.28	1.22
25	c	510	CLA	C1D-ND	-3.37	1.33	1.37
25	d	404	CLA	OBD-CAD	3.37	1.28	1.22
25	c	504	CLA	C1D-ND	-3.37	1.33	1.37
25	D	404	CLA	OBD-CAD	3.37	1.28	1.22
25	b	612	CLA	CHD-C4C	3.36	1.46	1.39
25	A	405	CLA	CHD-C4C	3.36	1.46	1.39
25	b	610	CLA	C1C-NC	-3.36	1.32	1.37
27	A	409	BCR	C11-C12	-3.36	1.25	1.34
25	A	408	CLA	OBD-CAD	3.36	1.28	1.22
25	B	608	CLA	OBD-CAD	3.35	1.28	1.22
25	B	610	CLA	C1C-NC	-3.35	1.32	1.37
25	C	510	CLA	C1D-ND	-3.33	1.33	1.37
25	a	405	CLA	CHD-C4C	3.33	1.46	1.39
27	B	618	BCR	C11-C12	-3.32	1.26	1.34
27	b	618	BCR	C11-C12	-3.31	1.26	1.34
25	c	503	CLA	OBD-CAD	3.30	1.28	1.22
34	C	517	DGD	CAB-C9B	-3.29	1.33	1.51
34	c	517	DGD	CAB-C9B	-3.29	1.33	1.51
34	H	103	DGD	CAB-C9B	-3.29	1.33	1.51
25	C	504	CLA	C1D-ND	-3.29	1.33	1.37
29	C	523	LMG	C22-C21	-3.29	1.33	1.51
29	C	518	LMG	C19-C18	-3.29	1.33	1.51
25	C	503	CLA	OBD-CAD	3.28	1.28	1.22
29	c	523	LMG	C22-C21	-3.28	1.33	1.51
25	B	611	CLA	C1C-NC	-3.28	1.32	1.37
29	c	518	LMG	C19-C18	-3.28	1.33	1.51
34	c	517	DGD	CAA-C9A	-3.28	1.33	1.51
27	k	102	BCR	C11-C12	-3.28	1.26	1.34
29	a	411	LMG	C19-C18	-3.28	1.33	1.51
34	h	103	DGD	CAB-C9B	-3.28	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	411	LMG	C19-C18	-3.27	1.33	1.51
25	c	513	CLA	C1D-ND	-3.27	1.33	1.37
34	C	517	DGD	CAA-C9A	-3.27	1.33	1.51
34	C	517	DGD	CDA-CCA	-3.27	1.33	1.51
34	c	517	DGD	CDA-CCA	-3.27	1.33	1.51
34	c	515	DGD	CDB-CCB	-3.27	1.33	1.51
34	c	515	DGD	CAB-C9B	-3.27	1.33	1.51
27	K	102	BCR	C11-C12	-3.27	1.26	1.34
34	C	515	DGD	CDB-CCB	-3.26	1.33	1.51
29	c	523	LMG	C19-C18	-3.26	1.33	1.51
25	B	612	CLA	OBD-CAD	3.26	1.28	1.22
29	b	620	LMG	C19-C18	-3.26	1.33	1.51
34	C	515	DGD	CAB-C9B	-3.26	1.33	1.51
34	c	516	DGD	CAB-C9B	-3.26	1.33	1.51
25	C	513	CLA	C1D-ND	-3.26	1.33	1.37
29	C	523	LMG	C19-C18	-3.25	1.33	1.51
34	C	516	DGD	CDA-CCA	-3.25	1.33	1.51
34	h	103	DGD	CDB-CCB	-3.25	1.33	1.51
34	c	515	DGD	CAA-C9A	-3.25	1.33	1.51
34	c	517	DGD	CDB-CCB	-3.25	1.33	1.51
25	b	611	CLA	C1C-NC	-3.25	1.33	1.37
25	B	604	CLA	OBD-CAD	3.25	1.28	1.22
29	B	621	LMG	C19-C18	-3.25	1.33	1.51
34	C	517	DGD	CDB-CCB	-3.25	1.33	1.51
29	B	621	LMG	C40-C39	-3.25	1.33	1.51
25	b	612	CLA	OBD-CAD	3.25	1.28	1.22
34	C	516	DGD	CDB-CCB	-3.24	1.33	1.51
27	B	619	BCR	C11-C12	-3.24	1.26	1.34
29	D	409	LMG	C37-C36	-3.24	1.33	1.51
29	D	409	LMG	C40-C39	-3.24	1.33	1.51
34	C	516	DGD	CAB-C9B	-3.24	1.33	1.51
34	c	516	DGD	CDB-CCB	-3.24	1.33	1.51
29	b	620	LMG	C40-C39	-3.24	1.33	1.51
34	H	103	DGD	CDB-CCB	-3.24	1.33	1.51
25	b	604	CLA	OBD-CAD	3.24	1.28	1.22
29	d	409	LMG	C37-C36	-3.24	1.33	1.51
34	H	103	DGD	CAA-C9A	-3.24	1.33	1.51
25	D	401	CLA	C1C-NC	-3.24	1.33	1.37
34	c	516	DGD	CDA-CCA	-3.24	1.33	1.51
29	d	409	LMG	C40-C39	-3.24	1.33	1.51
34	C	515	DGD	CAA-C9A	-3.24	1.33	1.51
29	b	620	LMG	C22-C21	-3.23	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	621	LMG	C22-C21	-3.23	1.33	1.51
34	h	103	DGD	CAA-C9A	-3.23	1.33	1.51
25	d	401	CLA	C1C-NC	-3.23	1.33	1.37
30	A	412	PL9	C3-C4	-3.23	1.44	1.49
25	b	605	CLA	OBD-CAD	3.23	1.28	1.22
25	b	607	CLA	C1C-NC	-3.23	1.33	1.37
29	b	620	LMG	C37-C36	-3.23	1.33	1.51
29	D	409	LMG	C22-C21	-3.23	1.33	1.51
30	a	412	PL9	C3-C4	-3.22	1.44	1.49
29	a	411	LMG	C40-C39	-3.22	1.33	1.51
25	d	403	CLA	OBD-CAD	3.22	1.28	1.22
29	a	411	LMG	C37-C36	-3.22	1.33	1.51
29	d	409	LMG	C22-C21	-3.22	1.33	1.51
25	B	605	CLA	OBD-CAD	3.22	1.28	1.22
29	B	621	LMG	C37-C36	-3.22	1.33	1.51
25	c	507	CLA	MG-ND	-3.22	1.99	2.05
29	C	523	LMG	C37-C36	-3.22	1.33	1.51
29	c	518	LMG	C37-C36	-3.22	1.33	1.51
29	A	411	LMG	C37-C36	-3.22	1.33	1.51
29	C	518	LMG	C37-C36	-3.22	1.33	1.51
29	C	518	LMG	C22-C21	-3.22	1.33	1.51
29	c	518	LMG	C22-C21	-3.22	1.33	1.51
34	c	515	DGD	CDA-CCA	-3.22	1.33	1.51
29	A	411	LMG	C22-C21	-3.21	1.33	1.51
34	C	516	DGD	CAA-C9A	-3.21	1.33	1.51
29	A	411	LMG	C40-C39	-3.21	1.33	1.51
25	D	403	CLA	OBD-CAD	3.21	1.28	1.22
27	b	619	BCR	C11-C12	-3.21	1.26	1.34
29	c	523	LMG	C37-C36	-3.21	1.33	1.51
34	C	515	DGD	CDA-CCA	-3.21	1.33	1.51
29	d	409	LMG	C19-C18	-3.21	1.33	1.51
29	C	523	LMG	C40-C39	-3.21	1.33	1.51
29	a	411	LMG	C22-C21	-3.21	1.33	1.51
25	B	601	CLA	C1D-ND	-3.21	1.33	1.37
29	D	409	LMG	C19-C18	-3.21	1.33	1.51
34	c	516	DGD	CAA-C9A	-3.20	1.33	1.51
25	B	607	CLA	C1C-NC	-3.20	1.33	1.37
25	a	405	CLA	OBD-CAD	3.20	1.28	1.22
29	c	523	LMG	C40-C39	-3.20	1.33	1.51
28	K	101	SQD	O48-C23	3.20	1.42	1.33
25	B	616	CLA	OBD-CAD	3.19	1.28	1.22
25	C	507	CLA	MG-ND	-3.19	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	405	CLA	OBD-CAD	3.19	1.28	1.22
27	D	405	BCR	C11-C12	-3.19	1.26	1.34
27	d	405	BCR	C11-C12	-3.19	1.26	1.34
28	k	101	SQD	O48-C23	3.19	1.42	1.33
25	b	616	CLA	OBD-CAD	3.19	1.28	1.22
25	a	405	CLA	C1C-NC	-3.18	1.33	1.37
29	c	518	LMG	C40-C39	-3.18	1.33	1.51
25	c	511	CLA	C1C-NC	-3.18	1.33	1.37
25	B	612	CLA	MG-ND	-3.18	1.99	2.05
34	h	103	DGD	CDA-CCA	-3.18	1.33	1.51
34	H	103	DGD	CDA-CCA	-3.17	1.33	1.51
29	C	518	LMG	C40-C39	-3.17	1.33	1.51
28	h	102	SQD	O48-C23	3.17	1.42	1.33
25	A	405	CLA	C1C-NC	-3.17	1.33	1.37
28	H	102	SQD	O48-C23	3.17	1.42	1.33
25	b	607	CLA	OBD-CAD	3.16	1.27	1.22
25	C	511	CLA	C1C-NC	-3.16	1.33	1.37
25	B	607	CLA	OBD-CAD	3.15	1.27	1.22
25	c	506	CLA	MG-ND	-3.14	1.99	2.05
25	b	601	CLA	C1D-ND	-3.14	1.33	1.37
25	b	612	CLA	MG-ND	-3.14	1.99	2.05
25	b	611	CLA	OBD-CAD	3.13	1.27	1.22
28	f	101	SQD	O48-C23	3.13	1.42	1.33
28	F	101	SQD	O48-C23	3.13	1.42	1.33
25	B	611	CLA	OBD-CAD	3.13	1.27	1.22
25	C	506	CLA	MG-ND	-3.13	1.99	2.05
28	a	413	SQD	O48-C23	3.12	1.42	1.33
25	C	508	CLA	C1C-NC	-3.11	1.33	1.37
25	c	512	CLA	C3D-C2D	3.10	1.47	1.39
25	c	512	CLA	MG-ND	-3.10	1.99	2.05
28	A	413	SQD	O48-C23	3.10	1.42	1.33
25	C	512	CLA	MG-ND	-3.10	1.99	2.05
25	C	512	CLA	C3D-C2D	3.09	1.47	1.39
25	b	604	CLA	MG-NC	3.09	2.13	2.06
25	c	508	CLA	MG-ND	-3.09	1.99	2.05
25	c	508	CLA	C1C-NC	-3.09	1.33	1.37
25	C	508	CLA	MG-ND	-3.08	1.99	2.05
25	a	408	CLA	C3D-C2D	3.08	1.47	1.39
25	B	604	CLA	MG-NC	3.08	2.13	2.06
28	B	620	SQD	O48-C23	3.06	1.42	1.33
25	A	408	CLA	C3D-C2D	3.06	1.47	1.39
28	T	101	SQD	O48-C23	3.06	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	406	CLA	C1C-NC	-3.06	1.33	1.37
25	a	406	CLA	C1C-NC	-3.06	1.33	1.37
25	c	508	CLA	C3D-C2D	3.05	1.47	1.39
25	c	503	CLA	MG-NC	3.05	2.13	2.06
25	d	401	CLA	C3D-C2D	3.04	1.47	1.39
25	B	613	CLA	OBD-CAD	3.04	1.27	1.22
25	b	604	CLA	MG-ND	-3.04	1.99	2.05
25	C	508	CLA	C3D-C2D	3.04	1.47	1.39
25	D	403	CLA	C1C-NC	-3.04	1.33	1.37
25	b	603	CLA	C1C-NC	-3.04	1.33	1.37
25	C	503	CLA	MG-NC	3.04	2.13	2.06
25	B	604	CLA	MG-ND	-3.03	1.99	2.05
25	B	609	CLA	C1C-NC	-3.03	1.33	1.37
25	b	613	CLA	OBD-CAD	3.03	1.27	1.22
28	f	101	SQD	O47-C7	3.03	1.42	1.34
25	D	401	CLA	C3D-C2D	3.03	1.47	1.39
28	F	101	SQD	O47-C7	3.03	1.42	1.34
25	B	612	CLA	C1C-NC	-3.03	1.33	1.37
25	C	502	CLA	C3D-C2D	3.02	1.47	1.39
25	d	403	CLA	C1C-NC	-3.02	1.33	1.37
25	b	612	CLA	C1C-NC	-3.02	1.33	1.37
25	c	511	CLA	C3D-C2D	3.01	1.47	1.39
25	c	502	CLA	C3D-C2D	3.01	1.47	1.39
25	b	602	CLA	C1C-NC	-3.01	1.33	1.37
25	b	609	CLA	C1C-NC	-3.01	1.33	1.37
28	a	410	SQD	O48-C23	3.01	1.42	1.33
25	B	614	CLA	C1C-NC	-3.00	1.33	1.37
25	C	511	CLA	C3D-C2D	3.00	1.47	1.39
25	b	604	CLA	C1C-NC	-3.00	1.33	1.37
25	c	512	CLA	MG-NC	3.00	2.13	2.06
25	B	604	CLA	C1C-NC	-3.00	1.33	1.37
25	C	512	CLA	MG-NC	3.00	2.13	2.06
25	c	505	CLA	MG-ND	-3.00	1.99	2.05
25	D	403	CLA	MG-ND	-2.99	1.99	2.05
28	A	410	SQD	O48-C23	2.99	1.42	1.33
25	B	611	CLA	MG-ND	-2.99	1.99	2.05
25	b	611	CLA	MG-ND	-2.99	1.99	2.05
31	T	102	LMT	O3'-C3'	-2.99	1.35	1.43
25	B	602	CLA	C1C-NC	-2.99	1.33	1.37
25	c	502	CLA	C1C-NC	-2.99	1.33	1.37
25	c	511	CLA	MG-ND	-2.98	1.99	2.05
25	B	603	CLA	C1C-NC	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	t	701	LMT	O3'-C3'	-2.98	1.36	1.43
25	b	605	CLA	C1C-NC	-2.98	1.33	1.37
28	A	414	SQD	O48-C23	2.97	1.42	1.33
25	C	505	CLA	MG-ND	-2.97	1.99	2.05
25	C	511	CLA	MG-ND	-2.97	1.99	2.05
25	d	403	CLA	MG-ND	-2.97	1.99	2.05
25	C	502	CLA	C1C-NC	-2.97	1.33	1.37
25	B	605	CLA	C1C-NC	-2.96	1.33	1.37
25	A	406	CLA	C3D-C2D	2.96	1.47	1.39
28	a	414	SQD	O48-C23	2.96	1.42	1.33
25	C	506	CLA	C1C-NC	-2.96	1.33	1.37
25	B	602	CLA	C3D-C2D	2.96	1.47	1.39
25	C	504	CLA	C1C-NC	-2.95	1.33	1.37
25	a	406	CLA	C3D-C2D	2.95	1.47	1.39
25	b	605	CLA	C3D-C2D	2.95	1.47	1.39
25	c	504	CLA	C1C-NC	-2.95	1.33	1.37
25	C	501	CLA	C3D-C2D	2.95	1.47	1.39
25	b	614	CLA	C1C-NC	-2.95	1.33	1.37
25	c	511	CLA	MG-NC	2.95	2.13	2.06
25	C	506	CLA	C3D-C2D	2.94	1.47	1.39
25	c	501	CLA	MG-ND	-2.94	2.00	2.05
31	m	103	LMT	O3'-C3'	-2.94	1.36	1.43
25	b	602	CLA	C3D-C2D	2.94	1.47	1.39
25	C	511	CLA	MG-NC	2.94	2.13	2.06
31	M	103	LMT	O3'-C3'	-2.93	1.36	1.43
25	C	506	CLA	MG-NC	2.93	2.13	2.06
25	D	404	CLA	C3D-C2D	2.93	1.47	1.39
25	b	609	CLA	C3D-C2D	2.93	1.47	1.39
25	d	404	CLA	C3D-C2D	2.93	1.47	1.39
25	B	611	CLA	C3D-C2D	2.93	1.47	1.39
25	C	501	CLA	MG-ND	-2.93	2.00	2.05
25	b	611	CLA	C3D-C2D	2.93	1.47	1.39
25	c	506	CLA	C3D-C2D	2.93	1.47	1.39
25	c	501	CLA	C3D-C2D	2.93	1.47	1.39
25	B	605	CLA	C3D-C2D	2.92	1.47	1.39
25	B	610	CLA	C3D-C2D	2.92	1.47	1.39
25	c	505	CLA	MG-NC	2.92	2.13	2.06
25	c	509	CLA	MG-NC	2.92	2.13	2.06
25	B	605	CLA	MG-ND	-2.92	2.00	2.05
25	b	609	CLA	MG-ND	-2.92	2.00	2.05
25	c	513	CLA	C3D-C2D	2.92	1.47	1.39
25	B	609	CLA	C3D-C2D	2.92	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEM	CAB-C3B	2.92	1.55	1.47
25	b	605	CLA	MG-ND	-2.92	2.00	2.05
28	B	620	SQD	O47-C7	2.92	1.42	1.34
25	C	509	CLA	MG-NC	2.91	2.13	2.06
28	A	413	SQD	O47-C7	2.91	1.42	1.34
35	v	201	HEM	CAB-C3B	2.91	1.55	1.47
25	b	613	CLA	MG-NC	2.91	2.13	2.06
25	B	606	CLA	C3D-C2D	2.91	1.47	1.39
31	D	410	LMT	O3'-C3'	-2.91	1.36	1.43
25	B	613	CLA	MG-NC	2.91	2.13	2.06
25	c	505	CLA	C1C-NC	-2.91	1.33	1.37
28	T	101	SQD	O47-C7	2.91	1.42	1.34
31	d	410	LMT	O3'-C3'	-2.91	1.36	1.43
25	b	606	CLA	C3D-C2D	2.91	1.47	1.39
25	C	505	CLA	MG-NC	2.90	2.13	2.06
25	C	513	CLA	C3D-C2D	2.90	1.47	1.39
25	c	503	CLA	MG-ND	-2.90	2.00	2.05
25	c	506	CLA	C1C-NC	-2.90	1.33	1.37
28	a	413	SQD	O47-C7	2.90	1.42	1.34
25	b	610	CLA	C3D-C2D	2.90	1.47	1.39
25	c	509	CLA	MG-ND	-2.90	2.00	2.05
37	x	102	RRX	C8-C9	-2.90	1.39	1.45
25	c	506	CLA	MG-NC	2.90	2.13	2.06
25	B	603	CLA	MG-ND	-2.90	2.00	2.05
25	B	609	CLA	MG-ND	-2.89	2.00	2.05
28	H	102	SQD	O47-C7	2.89	1.42	1.34
25	b	606	CLA	C1C-NC	-2.89	1.33	1.37
35	F	102	HEM	CAB-C3B	2.88	1.55	1.47
25	b	615	CLA	MG-NC	2.88	2.13	2.06
37	X	102	RRX	C8-C9	-2.88	1.39	1.45
25	B	615	CLA	MG-NC	2.88	2.13	2.06
25	C	513	CLA	MG-NC	2.88	2.13	2.06
25	C	510	CLA	MG-ND	-2.87	2.00	2.05
25	C	503	CLA	MG-ND	-2.87	2.00	2.05
25	B	606	CLA	C1C-NC	-2.87	1.33	1.37
25	C	509	CLA	MG-ND	-2.87	2.00	2.05
25	A	408	CLA	C1C-NC	-2.87	1.33	1.37
37	X	102	RRX	C23-C22	-2.86	1.39	1.45
25	b	616	CLA	MG-ND	-2.86	2.00	2.05
25	B	614	CLA	C3D-C2D	2.86	1.46	1.39
35	f	102	HEM	CAB-C3B	2.86	1.55	1.47
25	b	616	CLA	C3D-C2D	2.86	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C1C-NC	-2.86	1.33	1.37
25	b	603	CLA	MG-ND	-2.86	2.00	2.05
25	C	505	CLA	C1C-NC	-2.86	1.33	1.37
25	c	509	CLA	C3D-C2D	2.86	1.46	1.39
25	c	513	CLA	MG-NC	2.86	2.13	2.06
25	c	510	CLA	MG-ND	-2.85	2.00	2.05
37	x	102	RRX	C23-C22	-2.85	1.39	1.45
28	K	101	SQD	O47-C7	2.85	1.42	1.34
25	B	616	CLA	C3D-C2D	2.85	1.46	1.39
28	h	102	SQD	O47-C7	2.85	1.42	1.34
25	B	615	CLA	C3D-C2D	2.85	1.46	1.39
25	b	615	CLA	C3D-C2D	2.85	1.46	1.39
25	B	613	CLA	MG-ND	-2.85	2.00	2.05
25	C	507	CLA	C1C-NC	-2.85	1.33	1.37
25	b	607	CLA	MG-ND	-2.85	2.00	2.05
25	B	615	CLA	C1C-NC	-2.84	1.33	1.37
25	C	507	CLA	C3D-C2D	2.84	1.46	1.39
25	C	504	CLA	C3D-C2D	2.84	1.46	1.39
25	b	614	CLA	C3D-C2D	2.84	1.46	1.39
25	B	607	CLA	MG-ND	-2.84	2.00	2.05
25	C	509	CLA	C3D-C2D	2.84	1.46	1.39
25	c	503	CLA	C3D-C2D	2.84	1.46	1.39
25	c	507	CLA	C3D-C2D	2.84	1.46	1.39
28	k	101	SQD	O47-C7	2.84	1.42	1.34
25	a	408	CLA	C1C-NC	-2.84	1.33	1.37
25	C	508	CLA	MG-NC	2.83	2.13	2.06
25	c	504	CLA	C3D-C2D	2.83	1.46	1.39
25	c	502	CLA	MG-NC	2.83	2.13	2.06
31	X	101	LMT	O3'-C3'	-2.83	1.36	1.43
25	b	613	CLA	C3D-C2D	2.83	1.46	1.39
25	C	509	CLA	C1C-NC	-2.83	1.33	1.37
31	x	101	LMT	O3'-C3'	-2.83	1.36	1.43
25	b	615	CLA	C1C-NC	-2.83	1.33	1.37
25	B	613	CLA	C3D-C2D	2.83	1.46	1.39
25	c	509	CLA	C1C-NC	-2.83	1.33	1.37
25	B	616	CLA	MG-ND	-2.83	2.00	2.05
25	C	503	CLA	C3D-C2D	2.83	1.46	1.39
25	C	502	CLA	MG-NC	2.82	2.13	2.06
25	a	408	CLA	MG-ND	-2.82	2.00	2.05
25	c	508	CLA	MG-NC	2.82	2.13	2.06
25	C	501	CLA	C1C-NC	-2.82	1.33	1.37
31	k	104	LMT	O3'-C3'	-2.81	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	CLA	MG-ND	-2.81	2.00	2.05
25	c	501	CLA	C1C-NC	-2.80	1.33	1.37
25	b	613	CLA	MG-ND	-2.80	2.00	2.05
25	b	601	CLA	C3D-C2D	2.80	1.46	1.39
25	C	510	CLA	C1C-NC	-2.80	1.33	1.37
31	B	626	LMT	O2'-C2'	-2.80	1.36	1.43
25	B	608	CLA	MG-ND	-2.80	2.00	2.05
31	K	104	LMT	O3'-C3'	-2.80	1.36	1.43
31	X	103	LMT	O3'-C3'	-2.80	1.36	1.43
25	B	608	CLA	C3D-C2D	2.80	1.46	1.39
31	M	102	LMT	O2B-C2B	-2.79	1.36	1.43
25	B	608	CLA	C1C-NC	-2.79	1.33	1.37
25	B	608	CLA	MG-NC	2.79	2.12	2.06
25	b	612	CLA	MG-NC	2.79	2.12	2.06
25	b	608	CLA	C3D-C2D	2.79	1.46	1.39
25	C	503	CLA	C1C-NC	-2.79	1.33	1.37
25	C	513	CLA	MG-ND	-2.79	2.00	2.05
31	b	625	LMT	O2'-C2'	-2.78	1.36	1.43
25	c	510	CLA	C1C-NC	-2.78	1.33	1.37
25	b	608	CLA	MG-ND	-2.78	2.00	2.05
28	A	410	SQD	O47-C7	2.78	1.42	1.34
25	b	614	CLA	MG-ND	-2.77	2.00	2.05
31	x	103	LMT	O3'-C3'	-2.77	1.36	1.43
25	b	602	CLA	MG-ND	-2.77	2.00	2.05
25	c	503	CLA	C1C-NC	-2.77	1.33	1.37
28	a	410	SQD	O47-C7	2.77	1.42	1.34
25	d	401	CLA	MG-ND	-2.77	2.00	2.05
25	a	408	CLA	MG-NC	2.77	2.12	2.06
25	B	601	CLA	C3D-C2D	2.77	1.46	1.39
25	B	610	CLA	MG-NC	2.77	2.12	2.06
31	m	102	LMT	O2B-C2B	-2.77	1.36	1.43
31	D	412	LMT	O3'-C3'	-2.77	1.36	1.43
25	b	608	CLA	MG-NC	2.77	2.12	2.06
25	C	510	CLA	C3D-C2D	2.77	1.46	1.39
25	B	609	CLA	MG-NC	2.76	2.12	2.06
25	c	513	CLA	MG-ND	-2.76	2.00	2.05
25	D	401	CLA	MG-ND	-2.76	2.00	2.05
25	B	607	CLA	C3D-C2D	2.76	1.46	1.39
25	B	612	CLA	MG-NC	2.76	2.12	2.06
31	i	102	LMT	O3'-C3'	-2.76	1.36	1.43
25	B	614	CLA	MG-ND	-2.76	2.00	2.05
25	b	601	CLA	MG-NC	2.76	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	MG-NC	2.76	2.12	2.06
25	b	605	CLA	MG-NC	2.76	2.12	2.06
25	b	610	CLA	MG-NC	2.76	2.12	2.06
25	c	512	CLA	C4D-CHA	2.76	1.48	1.38
25	B	602	CLA	MG-ND	-2.76	2.00	2.05
31	I	102	LMT	O3'-C3'	-2.75	1.36	1.43
25	b	606	CLA	MG-ND	-2.75	2.00	2.05
25	b	607	CLA	C3D-C2D	2.75	1.46	1.39
25	C	512	CLA	C4D-CHA	2.75	1.48	1.38
25	C	507	CLA	MG-NC	2.75	2.12	2.06
25	A	408	CLA	MG-NC	2.75	2.12	2.06
25	B	605	CLA	MG-NC	2.75	2.12	2.06
28	A	414	SQD	O47-C7	2.75	1.42	1.34
31	a	416	LMT	O3'-C3'	-2.75	1.36	1.43
25	B	606	CLA	MG-ND	-2.75	2.00	2.05
31	d	412	LMT	O3'-C3'	-2.74	1.36	1.43
25	B	601	CLA	MG-NC	2.74	2.12	2.06
25	b	609	CLA	MG-NC	2.74	2.12	2.06
25	b	608	CLA	C1C-NC	-2.74	1.33	1.37
31	b	622	LMT	O3'-C3'	-2.74	1.36	1.43
25	c	510	CLA	C3D-C2D	2.74	1.46	1.39
25	C	504	CLA	MG-NC	2.73	2.12	2.06
25	B	614	CLA	MG-NC	2.73	2.12	2.06
28	a	414	SQD	O47-C7	2.73	1.42	1.34
25	C	502	CLA	MG-ND	-2.73	2.00	2.05
31	B	623	LMT	O3'-C3'	-2.73	1.36	1.43
31	I	101	LMT	O3'-C3'	-2.73	1.36	1.43
25	b	602	CLA	MG-NC	2.73	2.12	2.06
31	A	416	LMT	O3'-C3'	-2.72	1.36	1.43
25	b	614	CLA	MG-NC	2.72	2.12	2.06
25	B	602	CLA	MG-NC	2.72	2.12	2.06
25	c	501	CLA	MG-NC	2.72	2.12	2.06
25	C	510	CLA	MG-NC	2.72	2.12	2.06
25	c	510	CLA	MG-NC	2.72	2.12	2.06
25	c	504	CLA	MG-NC	2.72	2.12	2.06
25	D	404	CLA	MG-NC	2.72	2.12	2.06
25	B	601	CLA	C1C-NC	-2.71	1.33	1.37
26	a	407	PHO	CAC-C3C	-2.71	1.47	1.52
25	d	404	CLA	MG-NC	2.71	2.12	2.06
25	C	501	CLA	MG-NC	2.71	2.12	2.06
31	m	101	LMT	O3'-C3'	-2.71	1.36	1.43
25	B	606	CLA	MG-NC	2.71	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	J	101	LMT	O3'-C3'	-2.70	1.36	1.43
25	c	502	CLA	MG-ND	-2.70	2.00	2.05
31	F	103	LMT	O3'-C3'	-2.70	1.36	1.43
31	C	520	LMT	O3'-C3'	-2.70	1.36	1.43
25	b	606	CLA	MG-NC	2.70	2.12	2.06
31	M	101	LMT	O3'-C3'	-2.70	1.36	1.43
25	c	511	CLA	C4D-CHA	2.69	1.48	1.38
31	f	103	LMT	O3'-C3'	-2.69	1.36	1.43
25	C	511	CLA	C4D-CHA	2.69	1.48	1.38
31	i	101	LMT	O3'-C3'	-2.69	1.36	1.43
31	j	101	LMT	O3'-C3'	-2.69	1.36	1.43
25	d	403	CLA	C3D-C2D	2.69	1.46	1.39
31	M	102	LMT	O3'-C3'	-2.69	1.36	1.43
25	C	513	CLA	C4D-CHA	2.69	1.48	1.38
25	b	601	CLA	C1C-NC	-2.69	1.33	1.37
31	I	104	LMT	O3'-C3'	-2.69	1.36	1.43
25	d	404	CLA	MG-ND	-2.69	2.00	2.05
25	d	404	CLA	C1C-NC	-2.69	1.33	1.37
25	D	404	CLA	MG-ND	-2.68	2.00	2.05
25	D	403	CLA	C3D-C2D	2.68	1.46	1.39
25	C	513	CLA	C1C-NC	-2.68	1.33	1.37
31	i	104	LMT	O3'-C3'	-2.68	1.36	1.43
26	d	402	PHO	CAC-C3C	-2.68	1.47	1.52
31	c	519	LMT	O3'-C3'	-2.68	1.36	1.43
25	C	501	CLA	C4D-CHA	2.68	1.47	1.38
31	x	104	LMT	O3'-C3'	-2.68	1.36	1.43
25	b	613	CLA	C1C-NC	-2.68	1.33	1.37
31	E	103	LMT	O3'-C3'	-2.68	1.36	1.43
31	m	102	LMT	O3'-C3'	-2.68	1.36	1.43
25	a	405	CLA	C3D-C2D	2.68	1.46	1.39
25	D	404	CLA	C1C-NC	-2.67	1.33	1.37
25	A	406	CLA	MG-ND	-2.67	2.00	2.05
31	H	101	LMT	O3'-C3'	-2.67	1.36	1.43
25	D	403	CLA	MG-NC	2.67	2.12	2.06
26	A	407	PHO	CAC-C3C	-2.67	1.47	1.52
25	c	504	CLA	MG-ND	-2.67	2.00	2.05
25	b	604	CLA	C4D-CHA	2.67	1.47	1.38
31	E	101	LMT	O3'-C3'	-2.67	1.36	1.43
31	e	103	LMT	O3'-C3'	-2.67	1.36	1.43
31	C	519	LMT	O3'-C3'	-2.67	1.36	1.43
25	c	513	CLA	C4D-CHA	2.67	1.47	1.38
25	B	604	CLA	C4D-CHA	2.67	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	101	LMT	O3'-C3'	-2.67	1.36	1.43
25	B	613	CLA	C1C-NC	-2.67	1.33	1.37
26	D	402	PHO	CAC-C3C	-2.67	1.47	1.52
25	C	504	CLA	MG-ND	-2.67	2.00	2.05
25	C	509	CLA	C4D-CHA	2.67	1.47	1.38
31	c	520	LMT	O3'-C3'	-2.66	1.36	1.43
25	b	610	CLA	MG-ND	-2.66	2.00	2.05
25	a	406	CLA	MG-ND	-2.66	2.00	2.05
25	A	405	CLA	C3D-C2D	2.66	1.46	1.39
25	d	403	CLA	MG-NC	2.66	2.12	2.06
25	c	501	CLA	C4D-CHA	2.66	1.47	1.38
25	C	506	CLA	C4D-CHA	2.66	1.47	1.38
25	B	604	CLA	C3D-C2D	2.66	1.46	1.39
31	X	104	LMT	O3'-C3'	-2.66	1.36	1.43
25	c	509	CLA	C4D-CHA	2.65	1.47	1.38
25	B	603	CLA	C3D-C2D	2.65	1.46	1.39
25	B	615	CLA	MG-ND	-2.65	2.00	2.05
31	h	101	LMT	O3'-C3'	-2.65	1.36	1.43
25	b	603	CLA	C3D-C2D	2.65	1.46	1.39
25	c	506	CLA	C4D-CHA	2.64	1.47	1.38
25	c	513	CLA	C1C-NC	-2.64	1.33	1.37
25	c	503	CLA	C4D-CHA	2.64	1.47	1.38
25	C	503	CLA	C4D-CHA	2.64	1.47	1.38
25	b	607	CLA	MG-NC	2.64	2.12	2.06
25	b	613	CLA	C4D-CHA	2.64	1.47	1.38
25	b	604	CLA	C3D-C2D	2.64	1.46	1.39
31	B	624	LMT	O3'-C3'	-2.64	1.36	1.43
25	B	613	CLA	C4D-CHA	2.64	1.47	1.38
25	b	614	CLA	C4D-CHA	2.63	1.47	1.38
25	B	607	CLA	MG-NC	2.63	2.12	2.06
25	c	502	CLA	C4D-CHA	2.63	1.47	1.38
25	B	610	CLA	MG-ND	-2.63	2.00	2.05
31	b	623	LMT	O3'-C3'	-2.63	1.36	1.43
25	b	615	CLA	MG-ND	-2.63	2.00	2.05
31	C	524	LMT	O3'-C3'	-2.62	1.36	1.43
25	B	614	CLA	C4D-CHA	2.62	1.47	1.38
31	D	411	LMT	O3'-C3'	-2.62	1.36	1.43
25	C	502	CLA	C4D-CHA	2.62	1.47	1.38
25	B	616	CLA	MG-NC	2.62	2.12	2.06
25	b	601	CLA	C4D-CHA	2.62	1.47	1.38
25	b	603	CLA	MG-NC	2.61	2.12	2.06
25	b	602	CLA	C4D-CHA	2.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	103	LMT	O3'-C3'	-2.61	1.36	1.43
31	a	417	LMT	O3'-C3'	-2.61	1.36	1.43
31	A	417	LMT	O3'-C3'	-2.61	1.36	1.43
31	d	411	LMT	O3'-C3'	-2.61	1.36	1.43
25	B	603	CLA	C4D-CHA	2.61	1.47	1.38
31	c	524	LMT	O3'-C3'	-2.61	1.36	1.43
25	b	603	CLA	C4D-CHA	2.61	1.47	1.38
25	b	612	CLA	C3D-C2D	2.60	1.46	1.39
31	I	103	LMT	O3'-C3'	-2.60	1.36	1.43
31	y	101	LMT	O3'-C3'	-2.60	1.36	1.43
25	B	603	CLA	MG-NC	2.60	2.12	2.06
25	B	601	CLA	C4D-CHA	2.60	1.47	1.38
31	c	521	LMT	O3'-C3'	-2.60	1.36	1.43
31	C	521	LMT	O3'-C3'	-2.60	1.36	1.43
25	B	602	CLA	C4D-CHA	2.60	1.47	1.38
25	b	616	CLA	MG-NC	2.60	2.12	2.06
31	Y	101	LMT	O3'-C3'	-2.60	1.36	1.43
25	B	601	CLA	MG-ND	-2.59	2.00	2.05
25	C	512	CLA	C1C-NC	-2.59	1.33	1.37
31	b	625	LMT	O3'-C3'	-2.59	1.36	1.43
25	b	601	CLA	MG-ND	-2.59	2.00	2.05
25	B	612	CLA	C3D-C2D	2.59	1.46	1.39
25	B	611	CLA	MG-NC	2.59	2.12	2.06
25	b	609	CLA	C4D-CHA	2.58	1.47	1.38
25	b	611	CLA	MG-NC	2.58	2.12	2.06
25	C	507	CLA	C4D-CHA	2.58	1.47	1.38
25	B	609	CLA	C4D-CHA	2.58	1.47	1.38
31	B	626	LMT	O3'-C3'	-2.58	1.36	1.43
25	B	616	CLA	C4D-CHA	2.58	1.47	1.38
25	b	616	CLA	C4D-CHA	2.58	1.47	1.38
25	c	507	CLA	C4D-CHA	2.58	1.47	1.38
25	b	606	CLA	C4D-CHA	2.57	1.47	1.38
25	c	505	CLA	C4D-CHA	2.57	1.47	1.38
31	m	102	LMT	O2'-C2'	-2.57	1.36	1.43
25	c	512	CLA	C1C-NC	-2.57	1.34	1.37
25	C	505	CLA	C4D-CHA	2.57	1.47	1.38
25	D	403	CLA	C1B-CHB	2.57	1.48	1.41
31	M	102	LMT	O2'-C2'	-2.57	1.36	1.43
25	B	606	CLA	C4D-CHA	2.56	1.47	1.38
25	c	504	CLA	C4D-CHA	2.56	1.47	1.38
25	c	510	CLA	C4D-CHA	2.56	1.47	1.38
25	C	504	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	C1B-CHB	2.56	1.48	1.41
25	B	615	CLA	C4D-CHA	2.56	1.47	1.38
25	b	615	CLA	C4D-CHA	2.56	1.47	1.38
30	d	406	PL9	C6-C1	-2.56	1.44	1.48
25	C	510	CLA	C4D-CHA	2.56	1.47	1.38
31	d	412	LMT	O4'-C4B	-2.55	1.37	1.43
25	A	405	CLA	MG-ND	-2.55	2.00	2.05
31	D	412	LMT	O4'-C4B	-2.55	1.37	1.43
30	D	406	PL9	C6-C1	-2.55	1.44	1.48
31	k	104	LMT	O2B-C2B	-2.55	1.37	1.43
25	a	405	CLA	MG-ND	-2.55	2.00	2.05
25	b	611	CLA	C4D-CHA	2.55	1.47	1.38
25	A	406	CLA	C4D-CHA	2.54	1.47	1.38
31	m	101	LMT	O2B-C2B	-2.54	1.37	1.43
25	B	611	CLA	C4D-CHA	2.53	1.47	1.38
25	A	408	CLA	C4D-CHA	2.53	1.47	1.38
25	a	406	CLA	MG-NC	2.53	2.12	2.06
25	a	406	CLA	C4D-CHA	2.53	1.47	1.38
25	b	607	CLA	C4D-CHA	2.52	1.47	1.38
31	K	104	LMT	O2B-C2B	-2.52	1.37	1.43
25	c	508	CLA	C4D-CHA	2.52	1.47	1.38
25	a	408	CLA	C4D-CHA	2.52	1.47	1.38
25	B	607	CLA	C4D-CHA	2.51	1.47	1.38
25	C	508	CLA	C4D-CHA	2.51	1.47	1.38
31	M	101	LMT	O2B-C2B	-2.51	1.37	1.43
26	d	402	PHO	CMC-C2C	-2.51	1.45	1.51
25	d	404	CLA	C4D-CHA	2.51	1.47	1.38
31	D	411	LMT	O2'-C2'	-2.50	1.37	1.43
25	A	406	CLA	MG-NC	2.50	2.12	2.06
25	B	608	CLA	C4D-CHA	2.50	1.47	1.38
31	d	411	LMT	O2'-C2'	-2.49	1.37	1.43
25	d	404	CLA	C4B-CHC	2.49	1.47	1.41
25	c	513	CLA	C4B-CHC	2.49	1.47	1.41
25	C	513	CLA	C4B-CHC	2.49	1.47	1.41
25	b	608	CLA	C4D-CHA	2.49	1.47	1.38
25	b	610	CLA	C4D-CHA	2.49	1.47	1.38
25	d	401	CLA	C4D-CHA	2.49	1.47	1.38
25	D	404	CLA	C4D-CHA	2.49	1.47	1.38
25	D	401	CLA	C4D-CHA	2.49	1.47	1.38
25	D	401	CLA	MG-NC	2.48	2.12	2.06
25	b	614	CLA	C1B-CHB	2.48	1.47	1.41
25	B	610	CLA	C4D-CHA	2.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	CLA	MG-NC	2.47	2.12	2.06
26	D	402	PHO	CMC-C2C	-2.47	1.45	1.51
25	D	404	CLA	C4B-CHC	2.47	1.47	1.41
25	B	613	CLA	C1B-CHB	2.46	1.47	1.41
25	B	614	CLA	C1B-CHB	2.46	1.47	1.41
31	M	101	LMT	O2'-C2'	-2.46	1.37	1.43
31	X	103	LMT	O2B-C2B	-2.45	1.37	1.43
31	C	524	LMT	O2'-C2'	-2.45	1.37	1.43
25	C	505	CLA	C3D-C2D	2.45	1.45	1.39
25	b	601	CLA	C4B-CHC	2.45	1.47	1.41
25	a	405	CLA	C1B-CHB	2.44	1.47	1.41
31	x	103	LMT	O2B-C2B	-2.44	1.37	1.43
25	a	405	CLA	C4D-CHA	2.44	1.47	1.38
25	A	405	CLA	C1B-CHB	2.44	1.47	1.41
31	m	101	LMT	O2'-C2'	-2.44	1.37	1.43
25	b	613	CLA	C1B-CHB	2.44	1.47	1.41
25	B	601	CLA	C4B-CHC	2.44	1.47	1.41
25	B	604	CLA	C1B-CHB	2.44	1.47	1.41
25	A	405	CLA	MG-NC	2.44	2.12	2.06
25	b	612	CLA	C4D-CHA	2.43	1.47	1.38
25	c	503	CLA	C4B-CHC	2.43	1.47	1.41
25	B	615	CLA	C1B-CHB	2.43	1.47	1.41
25	c	505	CLA	C3D-C2D	2.43	1.45	1.39
25	b	604	CLA	C1B-CHB	2.43	1.47	1.41
25	A	405	CLA	C4D-CHA	2.43	1.47	1.38
25	b	615	CLA	C1B-CHB	2.43	1.47	1.41
25	a	405	CLA	MG-NC	2.43	2.12	2.06
25	B	612	CLA	C4D-CHA	2.43	1.47	1.38
31	x	103	LMT	O2'-C2'	-2.42	1.37	1.43
25	C	503	CLA	C4B-CHC	2.42	1.47	1.41
25	B	605	CLA	C4D-CHA	2.42	1.47	1.38
31	X	103	LMT	O2'-C2'	-2.42	1.37	1.43
25	c	502	CLA	C1B-CHB	2.42	1.47	1.41
31	c	519	LMT	O2'-C2'	-2.42	1.37	1.43
31	c	524	LMT	O2'-C2'	-2.42	1.37	1.43
31	D	412	LMT	O2'-C2'	-2.41	1.37	1.43
25	C	503	CLA	C1B-CHB	2.41	1.47	1.41
25	b	610	CLA	C4B-CHC	2.41	1.47	1.41
25	B	610	CLA	C4B-CHC	2.41	1.47	1.41
25	d	403	CLA	C4B-CHC	2.41	1.47	1.41
25	b	605	CLA	C4D-CHA	2.40	1.46	1.38
25	B	614	CLA	C4B-CHC	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C1D-C2D	2.40	1.50	1.45
25	B	605	CLA	C1B-CHB	2.40	1.47	1.41
31	b	624	LMT	O2'-C2'	-2.40	1.37	1.43
31	C	519	LMT	O2'-C2'	-2.40	1.37	1.43
31	d	412	LMT	O2'-C2'	-2.40	1.37	1.43
25	D	403	CLA	C4B-CHC	2.40	1.47	1.41
31	I	102	LMT	O2'-C2'	-2.39	1.37	1.43
31	b	624	LMT	O3'-C3'	-2.39	1.37	1.43
25	B	608	CLA	C4B-CHC	2.39	1.47	1.41
25	c	505	CLA	C1B-CHB	2.39	1.47	1.41
25	b	605	CLA	C1B-CHB	2.39	1.47	1.41
31	B	625	LMT	O2'-C2'	-2.39	1.37	1.43
25	c	503	CLA	C1B-CHB	2.39	1.47	1.41
25	D	401	CLA	C1B-CHB	2.39	1.47	1.41
31	h	101	LMT	O2'-C2'	-2.39	1.37	1.43
25	b	608	CLA	C4B-CHC	2.39	1.47	1.41
31	H	101	LMT	O2'-C2'	-2.39	1.37	1.43
31	c	519	LMT	O3B-C3B	-2.39	1.37	1.43
25	d	401	CLA	C1B-CHB	2.39	1.47	1.41
31	x	103	LMT	O3B-C3B	-2.38	1.37	1.43
25	b	614	CLA	C4B-CHC	2.38	1.47	1.41
25	c	509	CLA	C1B-CHB	2.38	1.47	1.41
25	b	605	CLA	C4B-CHC	2.38	1.47	1.41
25	C	502	CLA	C1B-CHB	2.38	1.47	1.41
37	x	102	RRX	C12-C13	-2.38	1.40	1.45
25	a	405	CLA	C4B-CHC	2.38	1.47	1.41
31	e	101	LMT	O2'-C2'	-2.38	1.37	1.43
31	X	103	LMT	O3B-C3B	-2.37	1.37	1.43
31	D	412	LMT	O3B-C3B	-2.37	1.37	1.43
31	M	102	LMT	O3B-C3B	-2.37	1.37	1.43
31	B	625	LMT	O3'-C3'	-2.37	1.37	1.43
31	d	412	LMT	O3B-C3B	-2.37	1.37	1.43
31	i	102	LMT	O2'-C2'	-2.37	1.37	1.43
25	A	405	CLA	C4B-CHC	2.37	1.47	1.41
31	c	524	LMT	O3B-C3B	-2.37	1.37	1.43
25	c	506	CLA	C1D-C2D	2.37	1.50	1.45
37	X	102	RRX	C12-C13	-2.37	1.40	1.45
25	b	611	CLA	C1B-CHB	2.37	1.47	1.41
25	C	505	CLA	C1B-CHB	2.36	1.47	1.41
31	E	101	LMT	O2'-C2'	-2.36	1.37	1.43
25	c	504	CLA	C1D-C2D	2.36	1.50	1.45
31	C	519	LMT	O3B-C3B	-2.36	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	104	LMT	O2'-C2'	-2.36	1.37	1.43
31	M	101	LMT	O3B-C3B	-2.36	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.36	1.37	1.43
31	b	622	LMT	O2'-C2'	-2.36	1.37	1.43
31	I	103	LMT	O2'-C2'	-2.36	1.37	1.43
25	B	609	CLA	C4B-CHC	2.36	1.47	1.41
25	c	512	CLA	C4B-CHC	2.36	1.47	1.41
31	I	103	LMT	O3B-C3B	-2.35	1.37	1.43
31	b	624	LMT	O3B-C3B	-2.35	1.37	1.43
25	C	505	CLA	C4B-CHC	2.35	1.47	1.41
25	D	404	CLA	C1D-C2D	2.35	1.50	1.45
31	C	519	LMT	O2B-C2B	-2.35	1.37	1.43
31	e	103	LMT	O3B-C3B	-2.35	1.37	1.43
31	m	102	LMT	O3B-C3B	-2.35	1.37	1.43
37	x	102	RRX	C19-C18	-2.35	1.40	1.45
25	b	609	CLA	C4B-CHC	2.35	1.47	1.41
25	B	603	CLA	C4B-CHC	2.35	1.47	1.41
25	c	510	CLA	C1B-CHB	2.35	1.47	1.41
31	i	103	LMT	O3B-C3B	-2.35	1.37	1.43
25	B	610	CLA	C1B-CHB	2.35	1.47	1.41
31	m	101	LMT	O3B-C3B	-2.35	1.37	1.43
31	A	417	LMT	O2'-C2'	-2.35	1.37	1.43
31	D	412	LMT	O2B-C2B	-2.35	1.37	1.43
25	B	616	CLA	C1B-CHB	2.35	1.47	1.41
25	c	505	CLA	C4B-CHC	2.35	1.47	1.41
25	C	509	CLA	C1B-CHB	2.35	1.47	1.41
25	b	603	CLA	C1B-CHB	2.35	1.47	1.41
25	B	605	CLA	C4B-CHC	2.35	1.47	1.41
31	a	417	LMT	O2'-C2'	-2.35	1.37	1.43
25	C	512	CLA	C4B-CHC	2.35	1.47	1.41
25	C	504	CLA	C1D-C2D	2.34	1.50	1.45
31	K	104	LMT	O2'-C2'	-2.34	1.37	1.43
31	i	103	LMT	O2'-C2'	-2.34	1.37	1.43
25	C	510	CLA	C1B-CHB	2.34	1.47	1.41
31	B	625	LMT	O3B-C3B	-2.34	1.37	1.43
25	b	602	CLA	C1D-C2D	2.34	1.49	1.45
31	E	103	LMT	O3B-C3B	-2.34	1.37	1.43
25	d	404	CLA	C1D-C2D	2.34	1.49	1.45
37	X	102	RRX	C19-C18	-2.34	1.40	1.45
25	d	403	CLA	C4D-CHA	2.34	1.46	1.38
25	C	502	CLA	C4B-CHC	2.34	1.47	1.41
25	D	403	CLA	C4D-CHA	2.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C1B-CHB	2.34	1.47	1.41
31	c	519	LMT	O2B-C2B	-2.33	1.37	1.43
25	b	612	CLA	C1B-CHB	2.33	1.47	1.41
31	d	412	LMT	O2B-C2B	-2.33	1.37	1.43
31	C	524	LMT	O3B-C3B	-2.33	1.37	1.43
31	B	625	LMT	O2B-C2B	-2.33	1.37	1.43
25	B	611	CLA	C1B-CHB	2.33	1.47	1.41
25	c	511	CLA	C1B-CHB	2.33	1.47	1.41
25	c	507	CLA	C4B-CHC	2.33	1.47	1.41
25	b	610	CLA	C1B-CHB	2.33	1.47	1.41
25	B	602	CLA	C1D-C2D	2.33	1.49	1.45
25	c	504	CLA	C4B-CHC	2.33	1.47	1.41
25	C	511	CLA	C1B-CHB	2.33	1.47	1.41
25	B	612	CLA	C1B-CHB	2.33	1.47	1.41
25	b	601	CLA	C1B-CHB	2.33	1.47	1.41
25	c	513	CLA	C1D-C2D	2.33	1.49	1.45
30	d	406	PL9	C52-C5	-2.33	1.45	1.50
25	C	513	CLA	C1D-C2D	2.33	1.49	1.45
30	d	406	PL9	C53-C6	-2.33	1.45	1.50
31	X	104	LMT	O2'-C2'	-2.33	1.37	1.43
31	k	104	LMT	O3B-C3B	-2.32	1.37	1.43
31	b	624	LMT	O2B-C2B	-2.32	1.37	1.43
30	D	406	PL9	C53-C6	-2.32	1.45	1.50
25	b	603	CLA	C4B-CHC	2.32	1.47	1.41
30	D	406	PL9	C52-C5	-2.32	1.45	1.50
25	b	613	CLA	C4B-CHC	2.32	1.47	1.41
25	c	502	CLA	C4B-CHC	2.32	1.47	1.41
25	C	510	CLA	C4B-CHC	2.32	1.47	1.41
25	C	504	CLA	C4B-CHC	2.32	1.47	1.41
31	T	102	LMT	O2'-C2'	-2.32	1.37	1.43
25	b	616	CLA	C1B-CHB	2.32	1.47	1.41
31	x	104	LMT	O2'-C2'	-2.32	1.37	1.43
25	B	606	CLA	C4B-CHC	2.32	1.47	1.41
31	x	101	LMT	O2'-C2'	-2.32	1.37	1.43
25	C	501	CLA	C1D-C2D	2.32	1.49	1.45
31	e	103	LMT	O2B-C2B	-2.32	1.37	1.43
25	C	507	CLA	C4B-CHC	2.32	1.47	1.41
31	t	701	LMT	O2'-C2'	-2.32	1.37	1.43
31	K	104	LMT	O3B-C3B	-2.31	1.37	1.43
31	I	103	LMT	O2B-C2B	-2.31	1.37	1.43
31	X	101	LMT	O2'-C2'	-2.31	1.37	1.43
25	B	601	CLA	C1B-CHB	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	C4B-CHC	2.31	1.47	1.41
25	b	606	CLA	C1B-CHB	2.31	1.47	1.41
25	c	510	CLA	C4B-CHC	2.31	1.47	1.41
31	i	103	LMT	O2B-C2B	-2.31	1.37	1.43
25	C	501	CLA	C4B-CHC	2.31	1.47	1.41
25	d	401	CLA	C1D-C2D	2.30	1.49	1.45
25	c	501	CLA	C4B-CHC	2.30	1.47	1.41
25	B	613	CLA	C4B-CHC	2.30	1.47	1.41
31	f	103	LMT	O3B-C3B	-2.30	1.37	1.43
25	B	607	CLA	C4B-CHC	2.30	1.47	1.41
31	c	524	LMT	O4'-C4B	-2.29	1.37	1.43
31	E	103	LMT	O2B-C2B	-2.29	1.37	1.43
31	F	103	LMT	O3B-C3B	-2.29	1.37	1.43
25	b	606	CLA	C4B-CHC	2.29	1.47	1.41
25	B	606	CLA	C1B-CHB	2.29	1.47	1.41
25	c	501	CLA	C1D-C2D	2.29	1.49	1.45
25	C	509	CLA	C4B-CHC	2.29	1.47	1.41
25	B	612	CLA	C4B-CHC	2.29	1.47	1.41
31	F	103	LMT	O2'-C2'	-2.28	1.37	1.43
25	b	612	CLA	C4B-CHC	2.28	1.47	1.41
25	A	406	CLA	C1D-C2D	2.28	1.49	1.45
25	a	406	CLA	C1D-C2D	2.28	1.49	1.45
25	b	607	CLA	C4B-CHC	2.28	1.47	1.41
25	B	615	CLA	C4B-CHC	2.28	1.47	1.41
25	C	506	CLA	C1B-CHB	2.28	1.47	1.41
25	A	408	CLA	C1B-CHB	2.28	1.47	1.41
31	f	103	LMT	O2'-C2'	-2.27	1.37	1.43
25	b	607	CLA	C1B-CHB	2.27	1.47	1.41
31	M	102	LMT	O1'-C1'	-2.27	1.36	1.40
25	a	408	CLA	C1B-CHB	2.27	1.47	1.41
31	A	416	LMT	O3B-C3B	-2.27	1.37	1.43
25	b	609	CLA	C1B-CHB	2.27	1.47	1.41
25	c	511	CLA	C4B-CHC	2.27	1.47	1.41
25	B	608	CLA	C1B-CHB	2.27	1.47	1.41
31	C	524	LMT	O4'-C4B	-2.27	1.37	1.43
25	b	615	CLA	C4B-CHC	2.27	1.47	1.41
25	C	511	CLA	C4B-CHC	2.27	1.47	1.41
31	A	416	LMT	O2B-C2B	-2.27	1.37	1.43
31	a	416	LMT	O2'-C2'	-2.27	1.37	1.43
25	B	607	CLA	C1B-CHB	2.27	1.47	1.41
31	m	102	LMT	O1'-C1'	-2.26	1.36	1.40
25	B	609	CLA	C1B-CHB	2.26	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C1B-CHB	2.26	1.47	1.41
25	c	503	CLA	C1D-C2D	2.26	1.49	1.45
25	D	401	CLA	C1D-C2D	2.26	1.49	1.45
31	a	416	LMT	O3B-C3B	-2.25	1.37	1.43
31	f	103	LMT	O2B-C2B	-2.25	1.37	1.43
25	b	608	CLA	C1B-CHB	2.25	1.47	1.41
25	a	406	CLA	C4B-CHC	2.25	1.47	1.41
25	A	406	CLA	C4B-CHC	2.25	1.47	1.41
31	A	416	LMT	O2'-C2'	-2.24	1.37	1.43
25	B	602	CLA	C4B-CHC	2.24	1.47	1.41
31	i	101	LMT	O2'-C2'	-2.24	1.37	1.43
31	I	101	LMT	O2'-C2'	-2.24	1.37	1.43
31	F	103	LMT	O2B-C2B	-2.24	1.37	1.43
31	a	416	LMT	O2B-C2B	-2.24	1.37	1.43
31	d	410	LMT	O2'-C2'	-2.24	1.37	1.43
25	c	508	CLA	C4B-CHC	2.23	1.47	1.41
31	i	104	LMT	O2'-C2'	-2.23	1.37	1.43
25	b	602	CLA	C4B-CHC	2.23	1.47	1.41
25	b	609	CLA	C1D-C2D	2.23	1.49	1.45
25	C	512	CLA	C1B-CHB	2.23	1.47	1.41
25	C	503	CLA	C1D-C2D	2.22	1.49	1.45
31	b	623	LMT	O2'-C2'	-2.22	1.37	1.43
25	C	508	CLA	C4B-CHC	2.22	1.47	1.41
28	F	101	SQD	O3-C3	-2.22	1.37	1.43
25	b	611	CLA	C1B-NB	-2.22	1.33	1.35
31	I	104	LMT	O2'-C2'	-2.22	1.37	1.43
25	B	609	CLA	C1D-C2D	2.22	1.49	1.45
25	c	512	CLA	C1B-CHB	2.22	1.47	1.41
25	c	504	CLA	C1B-CHB	2.22	1.47	1.41
25	C	508	CLA	C1B-CHB	2.22	1.47	1.41
31	D	410	LMT	O2'-C2'	-2.22	1.37	1.43
25	C	501	CLA	C1B-CHB	2.22	1.47	1.41
25	b	602	CLA	C1B-CHB	2.22	1.47	1.41
28	F	101	SQD	O2-C2	-2.22	1.37	1.43
25	B	604	CLA	C4B-CHC	2.22	1.47	1.41
31	J	101	LMT	O2'-C2'	-2.21	1.37	1.43
25	b	604	CLA	C4B-CHC	2.21	1.47	1.41
25	c	508	CLA	C1B-CHB	2.21	1.47	1.41
25	B	602	CLA	C1B-CHB	2.21	1.47	1.41
31	A	417	LMT	O5'-C5'	-2.21	1.39	1.44
31	M	102	LMT	O4'-C4B	-2.21	1.37	1.43
25	B	601	CLA	C1D-C2D	2.21	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	101	LMT	O2'-C2'	-2.21	1.37	1.43
28	f	101	SQD	O3-C3	-2.21	1.37	1.43
31	B	624	LMT	O2'-C2'	-2.21	1.37	1.43
25	C	506	CLA	C4C-C3C	2.21	1.48	1.45
25	C	504	CLA	C1B-CHB	2.21	1.47	1.41
31	m	102	LMT	O4'-C4B	-2.20	1.37	1.43
25	B	606	CLA	C1D-C2D	2.20	1.49	1.45
28	f	101	SQD	O2-C2	-2.20	1.37	1.43
25	c	507	CLA	C1B-CHB	2.20	1.47	1.41
31	f	103	LMT	O4'-C4B	-2.20	1.37	1.43
28	a	414	SQD	O2-C2	-2.20	1.37	1.43
25	c	506	CLA	C4C-C3C	2.20	1.48	1.45
31	a	417	LMT	O5'-C5'	-2.20	1.39	1.44
25	b	601	CLA	C1D-C2D	2.20	1.49	1.45
31	a	416	LMT	O5'-C5'	-2.19	1.39	1.44
31	A	416	LMT	O5'-C5'	-2.19	1.39	1.44
31	C	520	LMT	O2'-C2'	-2.19	1.37	1.43
31	F	103	LMT	O4'-C4B	-2.19	1.37	1.43
28	A	414	SQD	O2-C2	-2.19	1.37	1.43
25	b	606	CLA	C1D-C2D	2.19	1.49	1.45
31	C	524	LMT	O2B-C2B	-2.19	1.37	1.43
25	c	501	CLA	C1B-CHB	2.19	1.47	1.41
31	M	103	LMT	O2'-C2'	-2.18	1.37	1.43
25	C	507	CLA	C1B-CHB	2.18	1.47	1.41
25	C	510	CLA	C1D-C2D	2.18	1.49	1.45
31	k	104	LMT	O4'-C4B	-2.17	1.37	1.43
25	c	513	CLA	C1B-CHB	2.17	1.47	1.41
25	A	408	CLA	C4B-CHC	2.17	1.47	1.41
31	f	103	LMT	O1'-C1'	-2.17	1.36	1.40
25	c	509	CLA	C1D-C2D	2.17	1.49	1.45
31	m	103	LMT	O1'-C1'	-2.17	1.36	1.40
28	A	410	SQD	O2-C2	-2.17	1.37	1.43
31	c	524	LMT	O2B-C2B	-2.17	1.37	1.43
25	c	510	CLA	C1D-C2D	2.17	1.49	1.45
31	X	103	LMT	O4'-C4B	-2.17	1.37	1.43
25	c	502	CLA	C1D-C2D	2.16	1.49	1.45
25	C	513	CLA	C1B-CHB	2.16	1.47	1.41
25	c	508	CLA	C1D-C2D	2.16	1.49	1.45
25	D	404	CLA	C1B-CHB	2.16	1.47	1.41
25	C	506	CLA	C4B-CHC	2.16	1.47	1.41
25	c	504	CLA	C4C-C3C	2.16	1.48	1.45
30	A	412	PL9	C53-C6	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	CLA	C1B-CHB	2.16	1.47	1.41
30	a	412	PL9	C53-C6	-2.16	1.46	1.50
25	c	506	CLA	C4B-CHC	2.16	1.47	1.41
31	c	520	LMT	O2'-C2'	-2.16	1.37	1.43
31	K	104	LMT	O4'-C4B	-2.16	1.37	1.43
25	a	408	CLA	C4B-CHC	2.15	1.47	1.41
25	C	504	CLA	C4C-C3C	2.15	1.48	1.45
31	e	103	LMT	O4'-C4B	-2.15	1.37	1.43
31	x	103	LMT	O4'-C4B	-2.15	1.37	1.43
31	y	101	LMT	O2'-C2'	-2.15	1.37	1.43
28	K	101	SQD	O4-C4	-2.15	1.37	1.43
31	m	103	LMT	O2'-C2'	-2.15	1.37	1.43
31	i	104	LMT	O1'-C1'	-2.15	1.36	1.40
25	b	616	CLA	C1D-C2D	2.15	1.49	1.45
25	B	616	CLA	C4B-CHC	2.15	1.47	1.41
31	Y	101	LMT	O2'-C2'	-2.15	1.37	1.43
25	A	406	CLA	C1B-CHB	2.15	1.47	1.41
28	k	101	SQD	O4-C4	-2.15	1.37	1.43
25	d	404	CLA	C1B-CHB	2.15	1.47	1.41
26	A	407	PHO	CMC-C2C	-2.15	1.46	1.51
31	F	103	LMT	O1'-C1'	-2.15	1.36	1.40
31	E	103	LMT	O4'-C4B	-2.15	1.37	1.43
31	M	103	LMT	O1'-C1'	-2.14	1.36	1.40
28	a	410	SQD	O2-C2	-2.14	1.37	1.43
25	C	502	CLA	C1D-C2D	2.14	1.49	1.45
25	b	616	CLA	C4B-CHC	2.14	1.46	1.41
25	C	508	CLA	C1D-C2D	2.14	1.49	1.45
31	A	416	LMT	O1'-C1'	-2.14	1.36	1.40
28	H	102	SQD	O2-C2	-2.14	1.37	1.43
25	B	616	CLA	C1D-C2D	2.14	1.49	1.45
25	B	611	CLA	C1B-NB	-2.13	1.33	1.35
26	a	407	PHO	CMC-C2C	-2.13	1.46	1.51
25	B	611	CLA	C4B-CHC	2.13	1.46	1.41
25	C	509	CLA	C1D-C2D	2.13	1.49	1.45
28	A	413	SQD	O4-C4	-2.12	1.38	1.43
28	H	102	SQD	O3-C3	-2.12	1.38	1.43
31	C	519	LMT	O4'-C4B	-2.12	1.38	1.43
28	a	413	SQD	O2-C2	-2.12	1.38	1.43
31	c	519	LMT	O4'-C4B	-2.12	1.38	1.43
31	I	104	LMT	O1'-C1'	-2.12	1.36	1.40
25	b	611	CLA	C4B-CHC	2.12	1.46	1.41
26	A	407	PHO	CMD-C2D	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	C4C-C3C	2.11	1.48	1.45
31	b	624	LMT	O4'-C4B	-2.11	1.38	1.43
28	h	102	SQD	O2-C2	-2.11	1.38	1.43
28	A	413	SQD	O2-C2	-2.11	1.38	1.43
26	a	407	PHO	CMB-C2B	-2.11	1.46	1.51
28	A	414	SQD	O3-C3	-2.11	1.38	1.43
31	a	416	LMT	O1'-C1'	-2.11	1.36	1.40
25	C	503	CLA	C4C-C3C	2.10	1.48	1.45
28	h	102	SQD	O3-C3	-2.10	1.38	1.43
31	X	101	LMT	O1'-C1'	-2.10	1.36	1.40
31	x	104	LMT	O1'-C1'	-2.10	1.36	1.40
28	a	413	SQD	O4-C4	-2.10	1.38	1.43
31	C	521	LMT	O2'-C2'	-2.10	1.38	1.43
31	c	521	LMT	O2'-C2'	-2.10	1.38	1.43
25	A	408	CLA	C1D-C2D	2.10	1.49	1.45
31	B	625	LMT	O4'-C4B	-2.09	1.38	1.43
28	a	414	SQD	O3-C3	-2.09	1.38	1.43
26	a	407	PHO	CMD-C2D	-2.09	1.46	1.51
25	D	404	CLA	C4C-C3C	2.09	1.48	1.45
25	d	404	CLA	C4C-C3C	2.09	1.48	1.45
28	k	101	SQD	O3-C3	-2.08	1.38	1.43
26	A	407	PHO	CMB-C2B	-2.08	1.46	1.51
25	B	612	CLA	C1B-NB	-2.08	1.33	1.35
25	b	612	CLA	C1B-NB	-2.08	1.33	1.35
26	D	402	PHO	CMD-C2D	-2.08	1.46	1.51
25	c	502	CLA	C4C-C3C	2.08	1.48	1.45
35	f	102	HEM	FE-ND	2.08	2.07	1.96
25	B	610	CLA	C1D-C2D	2.08	1.49	1.45
25	B	613	CLA	C1D-C2D	2.08	1.49	1.45
31	I	103	LMT	O4'-C4B	-2.07	1.38	1.43
28	B	620	SQD	O2-C2	-2.07	1.38	1.43
31	I	103	LMT	O1'-C1'	-2.07	1.36	1.40
31	x	101	LMT	O1'-C1'	-2.07	1.36	1.40
25	a	408	CLA	C1D-C2D	2.07	1.49	1.45
28	h	102	SQD	O4-C4	-2.07	1.38	1.43
28	T	101	SQD	O2-C2	-2.07	1.38	1.43
28	K	101	SQD	O3-C3	-2.07	1.38	1.43
31	m	101	LMT	O4'-C4B	-2.07	1.38	1.43
31	D	410	LMT	O1'-C1'	-2.07	1.36	1.40
28	f	101	SQD	O4-C4	-2.07	1.38	1.43
31	i	103	LMT	O1'-C1'	-2.06	1.36	1.40
31	y	101	LMT	O1'-C1'	-2.06	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	620	SQD	O4-C4	-2.06	1.38	1.43
25	D	401	CLA	C4B-CHC	2.06	1.46	1.41
26	d	402	PHO	CMD-C2D	-2.06	1.46	1.51
28	H	102	SQD	O4-C4	-2.06	1.38	1.43
28	F	101	SQD	O4-C4	-2.06	1.38	1.43
31	i	103	LMT	O4'-C4B	-2.06	1.38	1.43
31	M	101	LMT	O4'-C4B	-2.06	1.38	1.43
25	B	610	CLA	C4C-C3C	2.06	1.48	1.45
35	F	102	HEM	FE-ND	2.06	2.07	1.96
28	K	101	SQD	O2-C2	-2.06	1.38	1.43
25	b	608	CLA	C1D-C2D	2.06	1.49	1.45
25	b	610	CLA	C4C-C3C	2.05	1.48	1.45
25	C	502	CLA	C4C-C3C	2.05	1.48	1.45
25	b	610	CLA	C1D-C2D	2.05	1.49	1.45
28	T	101	SQD	O4-C4	-2.05	1.38	1.43
25	B	607	CLA	C1D-C2D	2.05	1.49	1.45
28	k	101	SQD	O2-C2	-2.05	1.38	1.43
31	X	104	LMT	O1'-C1'	-2.05	1.36	1.40
31	Y	101	LMT	O1'-C1'	-2.04	1.36	1.40
31	A	416	LMT	O4'-C4B	-2.04	1.38	1.43
25	b	613	CLA	C1D-C2D	2.04	1.49	1.45
25	B	611	CLA	C1D-C2D	2.04	1.49	1.45
31	d	410	LMT	O1'-C1'	-2.04	1.36	1.40
31	a	416	LMT	O4'-C4B	-2.04	1.38	1.43
25	b	611	CLA	C1D-C2D	2.04	1.49	1.45
25	B	608	CLA	C1D-C2D	2.04	1.49	1.45
27	z	101	BCR	C30-C25	-2.04	1.51	1.53
28	A	414	SQD	O4-C4	-2.03	1.38	1.43
28	a	413	SQD	O3-C3	-2.03	1.38	1.43
31	E	101	LMT	O1'-C1'	-2.03	1.36	1.40
26	D	402	PHO	CMB-C2B	-2.03	1.46	1.51
29	b	620	LMG	C43-C42	-2.03	1.33	1.49
30	D	406	PL9	C7-C8	-2.03	1.47	1.50
25	B	615	CLA	C1D-C2D	2.03	1.49	1.45
25	b	607	CLA	C1D-C2D	2.03	1.49	1.45
26	d	402	PHO	CMB-C2B	-2.03	1.46	1.51
30	d	406	PL9	C7-C8	-2.03	1.47	1.50
25	d	401	CLA	C4B-CHC	2.03	1.46	1.41
29	d	409	LMG	C43-C42	-2.03	1.33	1.49
29	D	409	LMG	C43-C42	-2.02	1.33	1.49
29	B	621	LMG	C43-C42	-2.02	1.33	1.49
28	A	413	SQD	O3-C3	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	C1D-C2D	2.02	1.49	1.45
34	c	516	DGD	CGB-CFB	-2.02	1.33	1.49
29	B	621	LMG	C25-C24	-2.02	1.33	1.49
34	C	517	DGD	CGB-CFB	-2.02	1.33	1.49
25	d	403	CLA	C1C-C2C	2.02	1.48	1.44
34	H	103	DGD	CGA-CFA	-2.02	1.33	1.49
34	c	515	DGD	CGB-CFB	-2.02	1.33	1.49
29	b	620	LMG	C25-C24	-2.01	1.33	1.49
34	c	517	DGD	CGB-CFB	-2.01	1.33	1.49
34	C	516	DGD	CGB-CFB	-2.01	1.33	1.49
34	H	103	DGD	CGB-CFB	-2.01	1.33	1.49
27	Z	101	BCR	C30-C25	-2.01	1.51	1.53
29	d	409	LMG	C25-C24	-2.01	1.33	1.49
29	A	411	LMG	C43-C42	-2.01	1.33	1.49
28	a	414	SQD	O4-C4	-2.01	1.38	1.43
29	a	411	LMG	C25-C24	-2.01	1.33	1.49
34	h	103	DGD	CGA-CFA	-2.01	1.33	1.49
25	c	512	CLA	C4C-C3C	2.01	1.48	1.45
29	A	411	LMG	C25-C24	-2.01	1.33	1.49
34	h	103	DGD	CGB-CFB	-2.01	1.33	1.49
34	C	515	DGD	CGB-CFB	-2.01	1.33	1.49
31	B	625	LMT	O1'-C1'	-2.01	1.36	1.40
29	a	411	LMG	C43-C42	-2.01	1.33	1.49
29	D	409	LMG	C25-C24	-2.01	1.33	1.49
34	C	516	DGD	CGA-CFA	-2.01	1.33	1.49
34	c	516	DGD	CGA-CFA	-2.01	1.33	1.49
34	c	515	DGD	CGA-CFA	-2.00	1.33	1.49
29	c	518	LMG	C25-C24	-2.00	1.33	1.49
31	x	103	LMT	O1'-C1'	-2.00	1.36	1.40
25	C	511	CLA	C1D-C2D	2.00	1.49	1.45
31	m	101	LMT	O1'-C1'	-2.00	1.36	1.40
29	C	518	LMG	C25-C24	-2.00	1.33	1.49
34	C	515	DGD	CGA-CFA	-2.00	1.33	1.49

All (2515) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C20-C21-C22	23.68	161.10	127.31
27	k	102	BCR	C20-C21-C22	23.65	161.07	127.31
27	z	101	BCR	C20-C21-C22	21.36	157.80	127.31
27	Z	101	BCR	C20-C21-C22	21.31	157.72	127.31
27	D	405	BCR	C20-C21-C22	21.03	157.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	BCR	C20-C21-C22	21.02	157.31	127.31
27	D	405	BCR	C15-C16-C17	20.80	166.08	123.47
27	d	405	BCR	C15-C16-C17	20.80	166.08	123.47
27	c	514	BCR	C20-C21-C22	20.71	156.87	127.31
27	C	514	BCR	C20-C21-C22	20.68	156.83	127.31
27	C	514	BCR	C15-C16-C17	20.68	165.84	123.47
27	c	514	BCR	C15-C16-C17	20.67	165.82	123.47
27	b	619	BCR	C20-C21-C22	20.61	156.73	127.31
27	B	619	BCR	C20-C21-C22	20.59	156.69	127.31
27	a	409	BCR	C15-C16-C17	20.49	165.44	123.47
27	A	409	BCR	C15-C16-C17	20.48	165.43	123.47
27	C	522	BCR	C20-C21-C22	20.45	156.50	127.31
27	c	522	BCR	C20-C21-C22	20.45	156.50	127.31
27	c	514	BCR	C16-C17-C18	20.45	156.49	127.31
27	C	514	BCR	C16-C17-C18	20.44	156.49	127.31
27	B	617	BCR	C15-C16-C17	20.43	165.32	123.47
27	B	618	BCR	C15-C16-C17	20.43	165.32	123.47
27	b	618	BCR	C15-C16-C17	20.42	165.31	123.47
27	b	617	BCR	C15-C16-C17	20.40	165.27	123.47
27	c	522	BCR	C15-C16-C17	20.27	165.00	123.47
27	B	617	BCR	C20-C21-C22	20.26	156.23	127.31
27	C	522	BCR	C15-C16-C17	20.25	164.96	123.47
27	b	617	BCR	C20-C21-C22	20.24	156.20	127.31
27	B	619	BCR	C15-C16-C17	20.24	164.93	123.47
27	b	619	BCR	C15-C16-C17	20.23	164.91	123.47
27	K	102	BCR	C16-C17-C18	20.17	156.09	127.31
27	A	409	BCR	C20-C21-C22	20.15	156.07	127.31
27	a	409	BCR	C20-C21-C22	20.14	156.06	127.31
27	k	102	BCR	C16-C17-C18	20.14	156.05	127.31
27	z	101	BCR	C15-C16-C17	19.98	164.40	123.47
27	Z	101	BCR	C16-C17-C18	19.98	155.82	127.31
27	Z	101	BCR	C15-C16-C17	19.97	164.38	123.47
27	z	101	BCR	C16-C17-C18	19.97	155.81	127.31
27	b	618	BCR	C20-C21-C22	19.76	155.51	127.31
27	B	618	BCR	C20-C21-C22	19.75	155.49	127.31
27	K	102	BCR	C15-C16-C17	19.74	163.92	123.47
27	k	102	BCR	C15-C16-C17	19.74	163.91	123.47
27	B	619	BCR	C16-C17-C18	19.69	155.41	127.31
27	b	619	BCR	C16-C17-C18	19.67	155.39	127.31
27	b	618	BCR	C16-C17-C18	19.61	155.30	127.31
27	B	618	BCR	C16-C17-C18	19.61	155.29	127.31
27	D	405	BCR	C16-C17-C18	19.07	154.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	BCR	C16-C17-C18	19.06	154.52	127.31
27	c	522	BCR	C16-C17-C18	19.04	154.49	127.31
27	B	617	BCR	C16-C17-C18	19.00	154.43	127.31
27	C	522	BCR	C16-C17-C18	19.00	154.43	127.31
27	b	617	BCR	C16-C17-C18	18.99	154.42	127.31
27	a	409	BCR	C16-C17-C18	18.96	154.37	127.31
27	A	409	BCR	C16-C17-C18	18.93	154.33	127.31
27	k	102	BCR	C10-C11-C12	17.61	178.19	123.22
27	K	102	BCR	C10-C11-C12	17.61	178.18	123.22
27	c	514	BCR	C10-C11-C12	17.52	177.91	123.22
27	C	514	BCR	C10-C11-C12	17.52	177.90	123.22
27	C	522	BCR	C10-C11-C12	17.39	177.47	123.22
27	c	522	BCR	C10-C11-C12	17.38	177.47	123.22
27	Z	101	BCR	C10-C11-C12	17.17	176.81	123.22
27	z	101	BCR	C10-C11-C12	17.16	176.76	123.22
27	B	618	BCR	C10-C11-C12	17.08	176.51	123.22
27	b	618	BCR	C10-C11-C12	17.07	176.49	123.22
27	a	409	BCR	C10-C11-C12	16.99	176.25	123.22
27	A	409	BCR	C10-C11-C12	16.98	176.22	123.22
27	d	405	BCR	C10-C11-C12	16.93	176.06	123.22
27	D	405	BCR	C10-C11-C12	16.93	176.05	123.22
27	b	619	BCR	C10-C11-C12	16.67	175.23	123.22
27	B	619	BCR	C10-C11-C12	16.66	175.21	123.22
27	B	617	BCR	C10-C11-C12	16.57	174.92	123.22
27	b	617	BCR	C10-C11-C12	16.57	174.91	123.22
27	a	409	BCR	C11-C10-C9	13.91	147.17	127.31
27	A	409	BCR	C11-C10-C9	13.90	147.15	127.31
27	B	617	BCR	C11-C10-C9	13.86	147.09	127.31
27	b	617	BCR	C11-C10-C9	13.84	147.07	127.31
27	d	405	BCR	C11-C10-C9	13.76	146.94	127.31
27	D	405	BCR	C11-C10-C9	13.74	146.93	127.31
27	b	618	BCR	C11-C10-C9	13.56	146.66	127.31
27	B	618	BCR	C11-C10-C9	13.54	146.64	127.31
27	K	102	BCR	C11-C10-C9	13.46	146.52	127.31
27	k	102	BCR	C11-C10-C9	13.46	146.52	127.31
27	B	619	BCR	C11-C10-C9	13.43	146.48	127.31
27	b	619	BCR	C11-C10-C9	13.41	146.44	127.31
27	z	101	BCR	C16-C15-C14	13.41	150.94	123.47
27	Z	101	BCR	C16-C15-C14	13.39	150.90	123.47
27	C	522	BCR	C21-C20-C19	13.22	164.46	123.22
27	c	522	BCR	C21-C20-C19	13.21	164.45	123.22
27	k	102	BCR	C16-C15-C14	13.20	150.50	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C16-C15-C14	13.18	150.48	123.47
27	B	619	BCR	C21-C20-C19	13.16	164.30	123.22
27	b	619	BCR	C21-C20-C19	13.16	164.29	123.22
27	B	618	BCR	C21-C20-C19	13.07	164.00	123.22
27	b	618	BCR	C21-C20-C19	13.07	164.00	123.22
27	b	617	BCR	C21-C20-C19	12.90	163.49	123.22
27	B	617	BCR	C21-C20-C19	12.90	163.47	123.22
27	a	409	BCR	C21-C20-C19	12.88	163.40	123.22
27	A	409	BCR	C21-C20-C19	12.88	163.40	123.22
27	B	618	BCR	C16-C15-C14	12.80	149.70	123.47
27	b	618	BCR	C16-C15-C14	12.78	149.66	123.47
27	c	514	BCR	C21-C20-C19	12.72	162.91	123.22
27	C	514	BCR	C21-C20-C19	12.72	162.91	123.22
27	d	405	BCR	C21-C20-C19	12.69	162.83	123.22
27	D	405	BCR	C21-C20-C19	12.69	162.81	123.22
27	C	522	BCR	C16-C15-C14	12.63	149.34	123.47
27	c	522	BCR	C16-C15-C14	12.62	149.33	123.47
27	c	522	BCR	C11-C10-C9	12.62	145.32	127.31
27	C	522	BCR	C11-C10-C9	12.60	145.29	127.31
27	z	101	BCR	C21-C20-C19	12.54	162.34	123.22
27	Z	101	BCR	C21-C20-C19	12.51	162.26	123.22
27	A	409	BCR	C16-C15-C14	12.32	148.72	123.47
27	a	409	BCR	C16-C15-C14	12.31	148.70	123.47
27	d	405	BCR	C16-C15-C14	12.26	148.59	123.47
27	D	405	BCR	C16-C15-C14	12.25	148.56	123.47
27	B	617	BCR	C16-C15-C14	12.20	148.46	123.47
27	B	619	BCR	C16-C15-C14	12.19	148.44	123.47
27	b	619	BCR	C16-C15-C14	12.18	148.43	123.47
27	c	514	BCR	C11-C10-C9	12.16	144.67	127.31
27	b	617	BCR	C16-C15-C14	12.16	148.39	123.47
27	C	514	BCR	C11-C10-C9	12.14	144.64	127.31
27	b	619	BCR	C11-C12-C13	11.91	159.86	126.42
27	B	619	BCR	C11-C12-C13	11.90	159.84	126.42
27	C	514	BCR	C16-C15-C14	11.74	147.52	123.47
27	c	514	BCR	C16-C15-C14	11.74	147.52	123.47
27	K	102	BCR	C21-C20-C19	11.62	159.49	123.22
27	k	102	BCR	C21-C20-C19	11.61	159.44	123.22
27	b	617	BCR	C11-C12-C13	11.51	158.74	126.42
27	B	617	BCR	C11-C12-C13	11.50	158.72	126.42
27	Z	101	BCR	C11-C10-C9	11.19	143.27	127.31
27	D	405	BCR	C11-C12-C13	11.18	157.83	126.42
27	d	405	BCR	C11-C12-C13	11.18	157.82	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	z	101	BCR	C11-C10-C9	11.16	143.24	127.31
27	Z	101	BCR	C11-C12-C13	10.91	157.06	126.42
27	z	101	BCR	C11-C12-C13	10.89	157.01	126.42
27	c	522	BCR	C11-C12-C13	10.83	156.84	126.42
27	C	522	BCR	C11-C12-C13	10.82	156.82	126.42
27	C	514	BCR	C11-C12-C13	10.82	156.82	126.42
27	c	514	BCR	C11-C12-C13	10.81	156.78	126.42
27	a	409	BCR	C11-C12-C13	10.78	156.69	126.42
27	A	409	BCR	C11-C12-C13	10.76	156.65	126.42
27	k	102	BCR	C11-C12-C13	10.11	154.81	126.42
27	K	102	BCR	C11-C12-C13	10.10	154.79	126.42
27	b	618	BCR	C11-C12-C13	10.07	154.71	126.42
27	B	618	BCR	C11-C12-C13	10.07	154.71	126.42
25	c	505	CLA	CMD-C2D-C1D	8.64	139.93	124.71
25	C	505	CLA	CMD-C2D-C1D	8.63	139.93	124.71
25	b	601	CLA	CMD-C2D-C1D	8.37	139.47	124.71
25	B	601	CLA	CMD-C2D-C1D	8.37	139.47	124.71
25	c	503	CLA	CMD-C2D-C1D	8.30	139.34	124.71
25	C	503	CLA	CMD-C2D-C1D	8.30	139.34	124.71
25	A	405	CLA	CMD-C2D-C1D	8.20	139.17	124.71
25	a	405	CLA	CMD-C2D-C1D	8.20	139.16	124.71
25	B	604	CLA	CMD-C2D-C1D	8.07	138.94	124.71
25	b	604	CLA	CMD-C2D-C1D	8.07	138.93	124.71
25	C	510	CLA	CMD-C2D-C1D	8.06	138.92	124.71
25	c	510	CLA	CMD-C2D-C1D	8.05	138.89	124.71
25	D	404	CLA	CMD-C2D-C1D	8.04	138.89	124.71
25	d	404	CLA	CMD-C2D-C1D	8.04	138.88	124.71
25	B	602	CLA	CMD-C2D-C1D	8.04	138.88	124.71
25	b	602	CLA	CMD-C2D-C1D	8.02	138.84	124.71
25	C	504	CLA	CMD-C2D-C1D	7.98	138.78	124.71
25	c	504	CLA	CMD-C2D-C1D	7.98	138.77	124.71
25	A	405	CLA	C2D-C1D-ND	7.90	115.93	110.10
25	a	405	CLA	C2D-C1D-ND	7.90	115.92	110.10
25	C	506	CLA	CMD-C2D-C1D	7.89	138.62	124.71
25	c	506	CLA	CMD-C2D-C1D	7.88	138.60	124.71
25	C	501	CLA	CMD-C2D-C1D	7.88	138.60	124.71
25	B	607	CLA	CMD-C2D-C1D	7.88	138.59	124.71
25	b	607	CLA	CMD-C2D-C1D	7.87	138.58	124.71
25	c	501	CLA	CMD-C2D-C1D	7.86	138.57	124.71
25	d	403	CLA	C2D-C1D-ND	7.85	115.89	110.10
25	D	403	CLA	C2D-C1D-ND	7.81	115.86	110.10
25	C	513	CLA	CMD-C2D-C1D	7.79	138.43	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMD-C2D-C1D	7.79	138.43	124.71
25	B	606	CLA	CMD-C2D-C1D	7.76	138.40	124.71
25	c	507	CLA	CMD-C2D-C1D	7.76	138.39	124.71
25	b	606	CLA	CMD-C2D-C1D	7.75	138.38	124.71
25	C	509	CLA	CMD-C2D-C1D	7.75	138.37	124.71
25	C	507	CLA	CMD-C2D-C1D	7.74	138.36	124.71
25	c	509	CLA	CMD-C2D-C1D	7.74	138.36	124.71
25	b	609	CLA	CMD-C2D-C1D	7.74	138.35	124.71
25	b	613	CLA	CMD-C2D-C1D	7.74	138.35	124.71
25	B	613	CLA	CMD-C2D-C1D	7.73	138.33	124.71
25	B	608	CLA	CMD-C2D-C1D	7.72	138.32	124.71
25	B	609	CLA	CMD-C2D-C1D	7.72	138.31	124.71
25	b	608	CLA	CMD-C2D-C1D	7.70	138.29	124.71
25	b	603	CLA	CMD-C2D-C1D	7.68	138.24	124.71
25	B	603	CLA	CMD-C2D-C1D	7.67	138.24	124.71
25	B	614	CLA	CMD-C2D-C1D	7.62	138.14	124.71
25	D	403	CLA	CMD-C2D-C1D	7.60	138.11	124.71
25	b	614	CLA	CMD-C2D-C1D	7.60	138.11	124.71
25	d	403	CLA	CMD-C2D-C1D	7.60	138.11	124.71
25	B	615	CLA	CMD-C2D-C1D	7.59	138.09	124.71
25	b	615	CLA	CMD-C2D-C1D	7.58	138.07	124.71
25	b	611	CLA	CMD-C2D-C1D	7.58	138.06	124.71
25	B	611	CLA	CMD-C2D-C1D	7.56	138.04	124.71
25	b	616	CLA	CMD-C2D-C1D	7.56	138.04	124.71
25	B	616	CLA	CMD-C2D-C1D	7.54	138.00	124.71
25	B	610	CLA	CMD-C2D-C1D	7.45	137.85	124.71
27	k	102	BCR	C20-C19-C18	7.44	147.32	126.42
25	b	610	CLA	CMD-C2D-C1D	7.44	137.82	124.71
27	K	102	BCR	C20-C19-C18	7.44	147.31	126.42
25	B	614	CLA	C2D-C1D-ND	7.42	115.57	110.10
25	b	614	CLA	C2D-C1D-ND	7.42	115.57	110.10
25	a	408	CLA	CMD-C2D-C1D	7.41	137.78	124.71
25	A	406	CLA	CMD-C2D-C1D	7.41	137.77	124.71
27	z	101	BCR	C20-C19-C18	7.40	147.21	126.42
25	A	408	CLA	CMD-C2D-C1D	7.40	137.76	124.71
25	a	406	CLA	CMD-C2D-C1D	7.40	137.75	124.71
27	Z	101	BCR	C20-C19-C18	7.39	147.17	126.42
25	B	605	CLA	C2D-C1D-ND	7.37	115.54	110.10
25	b	605	CLA	C2D-C1D-ND	7.36	115.53	110.10
25	D	401	CLA	CMD-C2D-C1D	7.36	137.69	124.71
25	d	401	CLA	CMD-C2D-C1D	7.35	137.67	124.71
25	C	508	CLA	CMD-C2D-C1D	7.34	137.65	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	CMD-C2D-C1D	7.33	137.62	124.71
25	B	607	CLA	C2D-C1D-ND	7.30	115.49	110.10
25	b	607	CLA	C2D-C1D-ND	7.27	115.46	110.10
25	b	612	CLA	C2D-C1D-ND	7.27	115.46	110.10
25	B	612	CLA	C2D-C1D-ND	7.26	115.45	110.10
25	C	502	CLA	CMD-C2D-C1D	7.25	137.48	124.71
25	b	605	CLA	CMD-C2D-C1D	7.23	137.45	124.71
25	c	502	CLA	CMD-C2D-C1D	7.22	137.45	124.71
25	B	605	CLA	CMD-C2D-C1D	7.22	137.44	124.71
25	A	405	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	b	616	CLA	C2D-C1D-ND	7.17	115.39	110.10
25	C	512	CLA	C2D-C1D-ND	7.16	115.38	110.10
25	a	405	CLA	C4A-NA-C1A	7.16	109.92	106.71
25	B	615	CLA	C2D-C1D-ND	7.15	115.37	110.10
25	b	612	CLA	CMD-C2D-C1D	7.14	137.30	124.71
25	B	612	CLA	CMD-C2D-C1D	7.13	137.28	124.71
25	B	616	CLA	C2D-C1D-ND	7.13	115.36	110.10
25	c	512	CLA	C2D-C1D-ND	7.13	115.36	110.10
25	b	615	CLA	C2D-C1D-ND	7.12	115.35	110.10
25	C	506	CLA	C2C-C1C-NC	7.11	116.64	109.97
25	C	511	CLA	CMD-C2D-C1D	7.11	137.24	124.71
25	c	511	CLA	CMD-C2D-C1D	7.10	137.23	124.71
25	c	506	CLA	C2C-C1C-NC	7.07	116.60	109.97
25	b	604	CLA	C2C-C1C-NC	7.06	116.59	109.97
25	B	604	CLA	C2C-C1C-NC	7.06	116.59	109.97
27	b	617	BCR	C20-C19-C18	7.04	146.19	126.42
25	B	610	CLA	C2D-C1D-ND	7.03	115.28	110.10
27	B	617	BCR	C20-C19-C18	7.02	146.15	126.42
25	b	610	CLA	C2D-C1D-ND	7.02	115.28	110.10
25	d	401	CLA	C2C-C1C-NC	7.01	116.54	109.97
27	C	514	BCR	C20-C19-C18	6.97	146.01	126.42
25	D	401	CLA	C2C-C1C-NC	6.97	116.50	109.97
27	c	514	BCR	C20-C19-C18	6.97	146.00	126.42
25	A	406	CLA	C2D-C1D-ND	6.97	115.24	110.10
25	a	406	CLA	C2D-C1D-ND	6.97	115.24	110.10
25	c	505	CLA	C2C-C1C-NC	6.97	116.50	109.97
27	d	405	BCR	C20-C19-C18	6.96	145.96	126.42
27	D	405	BCR	C20-C19-C18	6.95	145.94	126.42
25	C	505	CLA	C2C-C1C-NC	6.94	116.48	109.97
25	c	503	CLA	C2D-C1D-ND	6.94	115.22	110.10
25	C	503	CLA	C2D-C1D-ND	6.91	115.19	110.10
25	b	603	CLA	C2C-C1C-NC	6.90	116.44	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C2D-C1D-ND	6.89	115.19	110.10
25	B	613	CLA	C2D-C1D-ND	6.88	115.17	110.10
25	B	603	CLA	C2C-C1C-NC	6.88	116.42	109.97
25	C	512	CLA	C2C-C1C-NC	6.86	116.40	109.97
25	C	504	CLA	C2D-C1D-ND	6.86	115.16	110.10
25	b	613	CLA	C2D-C1D-ND	6.85	115.15	110.10
25	c	512	CLA	C2C-C1C-NC	6.84	116.38	109.97
25	b	610	CLA	C2C-C1C-NC	6.81	116.35	109.97
25	B	610	CLA	C2C-C1C-NC	6.80	116.34	109.97
25	C	507	CLA	C2C-C1C-NC	6.79	116.34	109.97
25	c	507	CLA	C2C-C1C-NC	6.79	116.33	109.97
27	C	522	BCR	C24-C23-C22	-6.77	116.00	126.23
25	B	601	CLA	C2D-C1D-ND	6.77	115.09	110.10
27	c	522	BCR	C24-C23-C22	-6.76	116.02	126.23
25	b	601	CLA	C2D-C1D-ND	6.76	115.08	110.10
25	b	611	CLA	C2D-C1D-ND	6.75	115.08	110.10
25	b	613	CLA	C2C-C1C-NC	6.74	116.29	109.97
25	C	511	CLA	C2C-C1C-NC	6.74	116.28	109.97
27	A	409	BCR	C20-C19-C18	6.74	145.34	126.42
25	a	408	CLA	C2D-C1D-ND	6.73	115.07	110.10
27	a	409	BCR	C20-C19-C18	6.73	145.33	126.42
25	B	613	CLA	C2C-C1C-NC	6.73	116.28	109.97
25	C	511	CLA	C2D-C1D-ND	6.73	115.07	110.10
25	B	611	CLA	C2D-C1D-ND	6.73	115.06	110.10
25	c	507	CLA	C2D-C1D-ND	6.72	115.05	110.10
25	c	511	CLA	C2D-C1D-ND	6.71	115.05	110.10
25	C	503	CLA	C2C-C1C-NC	6.70	116.25	109.97
25	C	507	CLA	C2D-C1D-ND	6.70	115.04	110.10
25	A	408	CLA	C2D-C1D-ND	6.69	115.03	110.10
25	c	511	CLA	C2C-C1C-NC	6.69	116.24	109.97
25	C	509	CLA	C2D-C1D-ND	6.68	115.03	110.10
27	B	618	BCR	C20-C19-C18	6.68	145.17	126.42
25	b	604	CLA	C4A-NA-C1A	6.66	109.70	106.71
25	c	503	CLA	C2C-C1C-NC	6.66	116.21	109.97
25	c	509	CLA	C2D-C1D-ND	6.66	115.01	110.10
27	b	618	BCR	C20-C19-C18	6.66	145.13	126.42
25	c	502	CLA	C2C-C1C-NC	6.65	116.20	109.97
25	C	502	CLA	C2C-C1C-NC	6.64	116.20	109.97
25	b	609	CLA	C2D-C1D-ND	6.63	114.99	110.10
25	b	607	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	A	408	CLA	C2C-C1C-NC	6.62	116.17	109.97
25	b	606	CLA	C2D-C1D-ND	6.62	114.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	6.61	109.68	106.71
25	b	615	CLA	C2C-C1C-NC	6.60	116.15	109.97
25	B	606	CLA	C2D-C1D-ND	6.60	114.97	110.10
25	D	401	CLA	C2D-C1D-ND	6.60	114.97	110.10
25	C	508	CLA	C2C-C1C-NC	6.58	116.14	109.97
25	c	504	CLA	C2C-C1C-NC	6.58	116.13	109.97
25	B	615	CLA	C2C-C1C-NC	6.57	116.13	109.97
25	a	408	CLA	C2C-C1C-NC	6.57	116.13	109.97
25	B	609	CLA	C2D-C1D-ND	6.57	114.94	110.10
25	C	504	CLA	C2C-C1C-NC	6.55	116.11	109.97
25	C	512	CLA	CMD-C2D-C1D	6.55	136.25	124.71
25	c	512	CLA	CMD-C2D-C1D	6.55	136.25	124.71
25	b	602	CLA	C2D-C1D-ND	6.55	114.93	110.10
25	a	406	CLA	C2C-C1C-NC	6.54	116.10	109.97
25	d	401	CLA	C2D-C1D-ND	6.54	114.92	110.10
25	B	602	CLA	C2D-C1D-ND	6.54	114.92	110.10
25	c	508	CLA	C2C-C1C-NC	6.53	116.09	109.97
25	A	406	CLA	C2C-C1C-NC	6.53	116.09	109.97
27	C	522	BCR	C20-C19-C18	6.52	144.73	126.42
25	C	502	CLA	C2D-C1D-ND	6.51	114.90	110.10
27	c	522	BCR	C20-C19-C18	6.51	144.70	126.42
25	B	608	CLA	C2D-C1D-ND	6.51	114.90	110.10
25	B	607	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	b	608	CLA	C2D-C1D-ND	6.50	114.89	110.10
25	c	510	CLA	C2C-C1C-NC	6.50	116.06	109.97
25	B	614	CLA	C4A-NA-C1A	6.49	109.63	106.71
25	c	502	CLA	C2D-C1D-ND	6.49	114.89	110.10
25	C	510	CLA	C2C-C1C-NC	6.49	116.05	109.97
25	d	404	CLA	C2D-C1D-ND	6.48	114.88	110.10
25	B	604	CLA	C2D-C1D-ND	6.47	114.87	110.10
25	b	604	CLA	C2D-C1D-ND	6.47	114.87	110.10
25	D	404	CLA	C2D-C1D-ND	6.47	114.87	110.10
25	b	609	CLA	C2C-C1C-NC	6.45	116.01	109.97
25	c	501	CLA	C2C-C1C-NC	6.44	116.00	109.97
25	B	609	CLA	C2C-C1C-NC	6.43	116.00	109.97
25	C	501	CLA	C2C-C1C-NC	6.42	115.99	109.97
25	C	513	CLA	C2D-C1D-ND	6.41	114.83	110.10
25	C	508	CLA	C2D-C1D-ND	6.41	114.83	110.10
25	C	509	CLA	C2C-C1C-NC	6.39	115.96	109.97
25	c	513	CLA	C2D-C1D-ND	6.39	114.81	110.10
25	d	404	CLA	C2C-C1C-NC	6.38	115.95	109.97
25	b	612	CLA	C2C-C1C-NC	6.38	115.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	C2D-C1D-ND	6.37	114.80	110.10
25	B	612	CLA	C2C-C1C-NC	6.37	115.94	109.97
25	b	614	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	c	509	CLA	C2C-C1C-NC	6.34	115.91	109.97
25	B	616	CLA	C2C-C1C-NC	6.34	115.91	109.97
27	B	619	BCR	C20-C19-C18	6.33	144.19	126.42
27	b	619	BCR	C20-C19-C18	6.32	144.18	126.42
25	D	404	CLA	C2C-C1C-NC	6.31	115.88	109.97
25	b	616	CLA	C2C-C1C-NC	6.30	115.88	109.97
25	c	510	CLA	C2D-C1D-ND	6.27	114.73	110.10
25	C	510	CLA	C2D-C1D-ND	6.25	114.71	110.10
25	D	403	CLA	C2C-C1C-NC	6.25	115.82	109.97
25	b	611	CLA	C2C-C1C-NC	6.23	115.81	109.97
25	b	602	CLA	C2C-C1C-NC	6.22	115.80	109.97
25	B	601	CLA	C2C-C1C-NC	6.22	115.80	109.97
25	d	403	CLA	C2C-C1C-NC	6.21	115.79	109.97
25	B	606	CLA	C2C-C1C-NC	6.21	115.79	109.97
25	B	607	CLA	C2C-C1C-NC	6.21	115.79	109.97
25	b	601	CLA	C2C-C1C-NC	6.21	115.79	109.97
25	B	611	CLA	C2C-C1C-NC	6.21	115.79	109.97
25	B	602	CLA	C2C-C1C-NC	6.20	115.78	109.97
25	B	603	CLA	C2D-C1D-ND	6.19	114.67	110.10
25	b	603	CLA	C2D-C1D-ND	6.19	114.66	110.10
25	b	606	CLA	C2C-C1C-NC	6.18	115.77	109.97
25	b	607	CLA	C2C-C1C-NC	6.18	115.77	109.97
25	b	608	CLA	C2C-C1C-NC	6.15	115.73	109.97
25	B	608	CLA	C2C-C1C-NC	6.13	115.72	109.97
25	B	614	CLA	C2C-C1C-NC	6.10	115.69	109.97
25	C	501	CLA	C2D-C1D-ND	6.09	114.59	110.10
25	c	501	CLA	C2D-C1D-ND	6.07	114.58	110.10
25	b	614	CLA	C2C-C1C-NC	6.06	115.65	109.97
25	B	605	CLA	C2C-C1C-NC	6.05	115.64	109.97
25	b	605	CLA	C2C-C1C-NC	6.03	115.62	109.97
25	c	507	CLA	O2D-CGD-CBD	6.03	121.98	111.27
25	C	507	CLA	O2D-CGD-CBD	6.03	121.98	111.27
25	c	513	CLA	C2C-C1C-NC	6.01	115.60	109.97
25	B	612	CLA	C4A-NA-C1A	6.00	109.41	106.71
25	C	513	CLA	C2C-C1C-NC	6.00	115.59	109.97
25	b	612	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	c	505	CLA	O2D-CGD-CBD	5.95	121.84	111.27
25	C	505	CLA	O2D-CGD-CBD	5.94	121.82	111.27
25	c	506	CLA	C2D-C1D-ND	5.90	114.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	512	CLA	O2D-CGD-CBD	5.88	121.72	111.27
25	C	506	CLA	C2D-C1D-ND	5.87	114.43	110.10
25	c	512	CLA	O2D-CGD-CBD	5.87	121.70	111.27
25	b	603	CLA	C1C-C2C-C3C	-5.86	100.79	106.96
25	B	603	CLA	C1C-C2C-C3C	-5.86	100.80	106.96
25	B	613	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	D	404	CLA	O2D-CGD-CBD	5.85	121.66	111.27
25	d	404	CLA	O2D-CGD-CBD	5.84	121.65	111.27
25	b	613	CLA	C4A-NA-C1A	5.83	109.33	106.71
25	C	511	CLA	C4A-NA-C1A	5.82	109.32	106.71
25	c	511	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	c	502	CLA	O2D-CGD-CBD	5.80	121.57	111.27
25	C	502	CLA	O2D-CGD-CBD	5.77	121.53	111.27
25	c	507	CLA	C1C-C2C-C3C	-5.73	100.93	106.96
25	b	613	CLA	C1C-C2C-C3C	-5.73	100.93	106.96
25	B	613	CLA	C1C-C2C-C3C	-5.72	100.95	106.96
25	C	504	CLA	CHD-C1D-ND	-5.71	119.21	124.45
25	B	601	CLA	O2D-CGD-CBD	5.71	121.41	111.27
25	c	504	CLA	CHD-C1D-ND	-5.70	119.22	124.45
25	b	601	CLA	O2D-CGD-CBD	5.70	121.39	111.27
25	C	507	CLA	C1C-C2C-C3C	-5.69	100.97	106.96
25	d	404	CLA	CHD-C1D-ND	-5.66	119.25	124.45
25	c	505	CLA	C2D-C1D-ND	5.66	114.27	110.10
25	B	611	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	D	401	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	c	501	CLA	C1C-C2C-C3C	-5.64	101.02	106.96
25	b	605	CLA	C4A-NA-C1A	5.63	109.24	106.71
25	C	506	CLA	C1C-C2C-C3C	-5.63	101.04	106.96
25	A	405	CLA	C1D-ND-C4D	-5.62	102.34	106.33
25	B	605	CLA	C4A-NA-C1A	5.62	109.23	106.71
25	D	404	CLA	CHD-C1D-ND	-5.62	119.29	124.45
25	C	501	CLA	C1C-C2C-C3C	-5.62	101.05	106.96
25	a	405	CLA	C1D-ND-C4D	-5.62	102.35	106.33
25	C	505	CLA	C2D-C1D-ND	5.62	114.24	110.10
25	B	604	CLA	C1C-C2C-C3C	-5.61	101.05	106.96
25	B	603	CLA	O2A-CGA-O1A	-5.61	109.43	123.59
25	b	603	CLA	O2A-CGA-O1A	-5.61	109.44	123.59
25	b	616	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	D	403	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	c	503	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
25	c	501	CLA	CHD-C1D-ND	-5.59	119.32	124.45
25	b	604	CLA	C1C-C2C-C3C	-5.59	101.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
25	a	408	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
25	a	405	CLA	C3D-C2D-C1D	-5.58	98.21	105.83
25	A	406	CLA	C4A-NA-C1A	5.58	109.22	106.71
25	c	506	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
25	A	405	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
25	d	403	CLA	C4A-NA-C1A	5.58	109.21	106.71
25	D	403	CLA	C1C-C2C-C3C	-5.57	101.10	106.96
25	A	406	CLA	C1C-C2C-C3C	-5.57	101.10	106.96
25	a	406	CLA	C1C-C2C-C3C	-5.57	101.10	106.96
25	B	607	CLA	C3D-C2D-C1D	-5.57	98.24	105.83
25	C	503	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
25	d	401	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
25	b	611	CLA	C4A-NA-C1A	5.56	109.21	106.71
25	c	504	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
25	b	604	CLA	O2D-CGD-CBD	5.56	121.15	111.27
25	C	501	CLA	CHD-C1D-ND	-5.56	119.34	124.45
25	B	604	CLA	O2D-CGD-CBD	5.56	121.14	111.27
25	C	509	CLA	O2A-CGA-O1A	-5.56	109.57	123.59
25	c	509	CLA	O2A-CGA-O1A	-5.54	109.60	123.59
25	B	616	CLA	C4A-NA-C1A	5.54	109.20	106.71
25	d	403	CLA	C1C-C2C-C3C	-5.54	101.13	106.96
25	b	610	CLA	C4A-NA-C1A	5.54	109.20	106.71
25	a	406	CLA	C4A-NA-C1A	5.54	109.19	106.71
25	b	606	CLA	CHD-C1D-ND	-5.54	119.37	124.45
25	b	607	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
25	C	504	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
25	d	401	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	c	504	CLA	O2A-C1-C2	5.52	123.14	108.64
25	b	602	CLA	CHD-C1D-ND	-5.52	119.38	124.45
25	D	401	CLA	C1C-C2C-C3C	-5.52	101.16	106.96
25	c	510	CLA	C1C-C2C-C3C	-5.51	101.16	106.96
25	C	504	CLA	O2A-C1-C2	5.51	123.12	108.64
25	b	612	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
25	B	602	CLA	CHD-C1D-ND	-5.50	119.40	124.45
25	c	505	CLA	C1C-C2C-C3C	-5.50	101.18	106.96
25	B	610	CLA	C4A-NA-C1A	5.50	109.18	106.71
25	B	612	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
25	B	609	CLA	O2A-C1-C2	5.49	123.06	108.64
25	b	609	CLA	O2A-C1-C2	5.49	123.05	108.64
25	B	606	CLA	CHD-C1D-ND	-5.49	119.41	124.45
25	C	505	CLA	C1C-C2C-C3C	-5.49	101.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
25	B	614	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
25	b	614	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	a	408	CLA	C4A-NA-C1A	5.47	109.16	106.71
25	c	506	CLA	CHD-C1D-ND	-5.46	119.43	124.45
25	C	512	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
25	D	403	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
25	b	616	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
25	C	504	CLA	C4A-NA-C1A	5.43	109.14	106.71
25	c	512	CLA	C1C-C2C-C3C	-5.42	101.25	106.96
25	d	403	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
25	c	504	CLA	C4A-NA-C1A	5.42	109.14	106.71
25	d	403	CLA	CHD-C1D-ND	-5.42	119.47	124.45
25	b	604	CLA	C1-C2-C3	-5.42	116.67	126.04
25	A	408	CLA	C4A-NA-C1A	5.42	109.14	106.71
25	B	606	CLA	O2D-CGD-CBD	5.42	120.89	111.27
25	B	606	CLA	C1C-C2C-C3C	-5.41	101.26	106.96
25	b	601	CLA	CHD-C1D-ND	-5.41	119.48	124.45
25	C	506	CLA	CHD-C1D-ND	-5.41	119.48	124.45
25	C	502	CLA	O2A-C1-C2	5.41	122.85	108.64
25	b	606	CLA	O2D-CGD-CBD	5.40	120.87	111.27
25	b	610	CLA	O2D-CGD-CBD	5.40	120.87	111.27
25	B	616	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
25	D	403	CLA	CHD-C1D-ND	-5.40	119.49	124.45
25	c	502	CLA	O2A-C1-C2	5.40	122.83	108.64
25	b	606	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
25	B	610	CLA	O2D-CGD-CBD	5.39	120.85	111.27
25	B	601	CLA	CHD-C1D-ND	-5.39	119.50	124.45
25	B	604	CLA	C1-C2-C3	-5.39	116.71	126.04
25	c	507	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	B	601	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
25	c	506	CLA	O2A-C1-C2	5.39	122.80	108.64
25	C	506	CLA	O2A-C1-C2	5.39	122.80	108.64
25	b	601	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
25	c	503	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
25	c	507	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
25	d	404	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
25	C	503	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
25	C	507	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
25	a	408	CLA	CHD-C1D-ND	-5.37	119.52	124.45
25	B	605	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
25	B	613	CLA	C3D-C2D-C1D	-5.37	98.51	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	607	CLA	CHD-C1D-ND	-5.37	119.52	124.45
25	B	607	CLA	CHD-C1D-ND	-5.36	119.53	124.45
25	A	406	CLA	O2D-CGD-CBD	5.36	120.80	111.27
25	B	614	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
25	D	404	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
25	B	606	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	B	608	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	C	508	CLA	C1C-C2C-C3C	-5.35	101.34	106.96
25	C	502	CLA	C4A-NA-C1A	5.34	109.11	106.71
25	c	502	CLA	C4A-NA-C1A	5.34	109.11	106.71
25	b	605	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
25	C	505	CLA	C4A-NA-C1A	5.34	109.11	106.71
25	a	406	CLA	O2D-CGD-CBD	5.33	120.74	111.27
25	b	613	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
25	b	608	CLA	C4A-NA-C1A	5.33	109.10	106.71
25	B	609	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	b	614	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
25	B	603	CLA	O2D-CGD-CBD	5.32	120.72	111.27
25	B	609	CLA	C1C-C2C-C3C	-5.32	101.36	106.96
25	b	603	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	b	616	CLA	O2D-CGD-CBD	5.32	120.72	111.27
25	A	408	CLA	CHD-C1D-ND	-5.31	119.57	124.45
25	d	403	CLA	C1D-ND-C4D	-5.31	102.56	106.33
25	B	605	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
25	b	605	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
25	B	616	CLA	O2D-CGD-CBD	5.31	120.70	111.27
25	b	606	CLA	C4A-NA-C1A	5.31	109.09	106.71
25	A	405	CLA	C2C-C1C-NC	5.31	114.94	109.97
27	B	618	BCR	C24-C23-C22	-5.30	118.22	126.23
25	B	603	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	b	609	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
25	c	504	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
25	C	507	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	c	508	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
27	c	522	BCR	C7-C8-C9	-5.30	118.23	126.23
27	b	618	BCR	C24-C23-C22	-5.29	118.24	126.23
25	b	615	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
25	A	408	CLA	O2D-CGD-CBD	5.29	120.67	111.27
25	b	603	CLA	O2D-CGD-CBD	5.29	120.67	111.27
25	B	607	CLA	O2A-CGA-O1A	-5.29	110.25	123.59
25	b	609	CLA	C4A-NA-C1A	5.29	109.08	106.71
25	B	605	CLA	O2D-CGD-CBD	5.29	120.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	C1D-ND-C4D	-5.28	102.58	106.33
25	a	408	CLA	O2D-CGD-CBD	5.28	120.66	111.27
25	b	605	CLA	O2D-CGD-CBD	5.28	120.65	111.27
25	b	602	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
25	B	615	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
25	c	505	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	c	509	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	C	509	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
25	a	405	CLA	C2C-C1C-NC	5.28	114.92	109.97
25	C	504	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
25	a	406	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
25	b	610	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
25	A	406	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
25	b	615	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
25	B	602	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
25	b	607	CLA	O2A-CGA-O1A	-5.27	110.28	123.59
25	A	405	CLA	O2A-C1-C2	5.27	122.50	108.64
25	B	611	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
25	a	405	CLA	O2A-C1-C2	5.27	122.48	108.64
25	B	610	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
25	b	611	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
27	C	522	BCR	C7-C8-C9	-5.26	118.28	126.23
25	B	615	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
25	d	401	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
25	C	511	CLA	C1C-C2C-C3C	-5.25	101.43	106.96
25	c	509	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
25	D	401	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
25	c	511	CLA	O2A-CGA-O1A	-5.25	110.35	123.59
25	c	508	CLA	CHD-C1D-ND	-5.24	119.64	124.45
25	C	508	CLA	CHD-C1D-ND	-5.24	119.64	124.45
25	c	511	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
25	C	511	CLA	O2A-CGA-O1A	-5.23	110.39	123.59
25	b	611	CLA	CHD-C1D-ND	-5.22	119.65	124.45
32	A	418	BCT	O2-C-O1	5.22	133.09	119.55
25	C	504	CLA	O2D-CGD-CBD	5.22	120.54	111.27
25	c	504	CLA	O2D-CGD-CBD	5.22	120.54	111.27
25	c	509	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
25	B	611	CLA	CHD-C1D-ND	-5.21	119.66	124.45
25	C	509	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
25	B	610	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
25	b	610	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
32	a	418	BCT	O2-C-O1	5.20	133.03	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	C4A-NA-C1A	5.20	109.04	106.71
25	b	612	CLA	O2D-CGD-CBD	5.20	120.50	111.27
25	B	612	CLA	O2D-CGD-CBD	5.20	120.50	111.27
25	d	404	CLA	O2A-C1-C2	5.19	122.28	108.64
25	b	608	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
25	d	403	CLA	O2A-C1-C2	5.19	122.27	108.64
25	B	608	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
25	a	405	CLA	CHD-C1D-ND	-5.18	119.69	124.45
25	D	403	CLA	O2A-C1-C2	5.18	122.26	108.64
25	D	404	CLA	O2A-C1-C2	5.18	122.24	108.64
25	B	601	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
25	b	601	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
25	b	616	CLA	O2A-CGA-O1A	-5.17	110.55	123.59
25	A	406	CLA	CHD-C1D-ND	-5.17	119.71	124.45
25	a	406	CLA	CHD-C1D-ND	-5.17	119.71	124.45
25	B	607	CLA	C1C-C2C-C3C	-5.17	101.53	106.96
25	C	508	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
25	A	405	CLA	CHD-C1D-ND	-5.16	119.71	124.45
25	A	408	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
25	c	501	CLA	O2A-CGA-O1A	-5.16	110.57	123.59
25	d	401	CLA	O2D-CGD-CBD	5.16	120.43	111.27
27	d	405	BCR	C24-C23-C22	-5.16	118.44	126.23
25	b	602	CLA	C4A-NA-C1A	5.15	109.02	106.71
25	a	408	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	B	605	CLA	CHD-C1D-ND	-5.15	119.72	124.45
25	B	614	CLA	CHD-C1D-ND	-5.15	119.72	124.45
25	c	508	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	b	602	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
27	a	409	BCR	C24-C23-C22	-5.15	118.45	126.23
25	b	604	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
25	D	401	CLA	O2D-CGD-CBD	5.15	120.42	111.27
25	b	607	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
25	B	602	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
25	B	616	CLA	O2A-CGA-O1A	-5.14	110.61	123.59
25	b	606	CLA	O2A-CGA-O1A	-5.14	110.61	123.59
25	B	604	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
28	h	102	SQD	O9-S-C6	5.14	113.05	106.94
25	b	605	CLA	CHD-C1D-ND	-5.14	119.73	124.45
25	b	609	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
25	C	501	CLA	O2A-CGA-O1A	-5.14	110.62	123.59
27	D	405	BCR	C24-C23-C22	-5.14	118.47	126.23
25	B	615	CLA	O2D-CGD-CBD	5.14	120.40	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	CHD-C1D-ND	-5.14	119.73	124.45
25	B	606	CLA	O2A-CGA-O1A	-5.14	110.63	123.59
25	B	610	CLA	O2A-C1-C2	5.13	122.13	108.64
25	c	503	CLA	CHD-C1D-ND	-5.13	119.74	124.45
28	H	102	SQD	O9-S-C6	5.13	113.03	106.94
25	b	611	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
25	C	512	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	C	512	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	b	615	CLA	O2D-CGD-CBD	5.13	120.38	111.27
25	C	503	CLA	CHD-C1D-ND	-5.13	119.74	124.45
25	b	609	CLA	O2A-CGA-O1A	-5.12	110.66	123.59
25	c	512	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
25	b	610	CLA	O2A-C1-C2	5.12	122.09	108.64
27	A	409	BCR	C24-C23-C22	-5.12	118.50	126.23
25	b	609	CLA	CHD-C1D-ND	-5.12	119.75	124.45
25	B	609	CLA	O2A-CGA-O1A	-5.12	110.68	123.59
25	c	502	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
25	B	611	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
25	c	513	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
25	B	609	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
25	b	606	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
25	c	507	CLA	O2A-C1-C2	5.11	122.06	108.64
25	B	607	CLA	O2D-CGD-CBD	5.11	120.34	111.27
25	B	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	b	607	CLA	O2D-CGD-CBD	5.10	120.34	111.27
25	C	507	CLA	O2A-C1-C2	5.10	122.04	108.64
25	B	606	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	b	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27
25	C	502	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
25	C	510	CLA	O2D-CGD-CBD	5.10	120.32	111.27
25	c	510	CLA	O2D-CGD-CBD	5.09	120.32	111.27
25	B	609	CLA	CHD-C1D-ND	-5.09	119.77	124.45
25	b	611	CLA	O2A-CGA-O1A	-5.09	110.74	123.59
25	C	513	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
25	B	611	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
25	B	611	CLA	O2D-CGD-CBD	5.09	120.31	111.27
25	b	608	CLA	O2D-CGD-CBD	5.08	120.30	111.27
30	A	412	PL9	C7-C3-C4	5.08	121.00	116.88
25	B	605	CLA	C1D-ND-C4D	-5.08	102.73	106.33
25	d	404	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
30	a	412	PL9	C7-C3-C4	5.07	121.00	116.88
25	C	510	CLA	C3D-C2D-C1D	-5.07	98.92	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	O2A-C1-C2	5.06	121.94	108.64
25	D	404	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
25	B	608	CLA	O2D-CGD-CBD	5.06	120.26	111.27
25	c	510	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	B	612	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	C	511	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	b	612	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	c	511	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	b	605	CLA	C1D-ND-C4D	-5.05	102.74	106.33
25	B	615	CLA	O2A-C1-C2	5.05	121.92	108.64
25	C	513	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
25	c	508	CLA	C4A-NA-C1A	5.05	108.98	106.71
25	b	602	CLA	O2A-C1-C2	5.04	121.89	108.64
25	B	613	CLA	CHD-C1D-ND	-5.04	119.82	124.45
25	c	513	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
25	b	613	CLA	CHD-C1D-ND	-5.03	119.83	124.45
25	B	602	CLA	O2A-C1-C2	5.03	121.86	108.64
25	C	512	CLA	O2A-C1-C2	5.03	121.85	108.64
25	C	509	CLA	O2D-CGD-CBD	5.03	120.20	111.27
25	C	508	CLA	C4A-NA-C1A	5.03	108.97	106.71
25	c	503	CLA	O2D-CGD-CBD	5.03	120.20	111.27
25	B	612	CLA	C1D-ND-C4D	-5.03	102.76	106.33
25	C	510	CLA	O2A-CGA-O1A	-5.03	110.91	123.59
25	C	503	CLA	O2A-CGA-O1A	-5.02	110.91	123.59
25	C	513	CLA	CHD-C1D-ND	-5.02	119.84	124.45
25	c	509	CLA	O2D-CGD-CBD	5.02	120.19	111.27
25	c	510	CLA	O2A-CGA-O1A	-5.02	110.92	123.59
25	c	503	CLA	O2A-CGA-O1A	-5.02	110.92	123.59
25	b	603	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
25	C	503	CLA	O2D-CGD-CBD	5.02	120.18	111.27
25	B	603	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
25	c	511	CLA	O2D-CGD-CBD	5.01	120.18	111.27
25	C	506	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
25	c	512	CLA	O2A-C1-C2	5.01	121.80	108.64
25	C	511	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	c	502	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
25	c	513	CLA	CHD-C1D-ND	-5.00	119.86	124.45
25	a	406	CLA	C1D-ND-C4D	-5.00	102.78	106.33
25	c	512	CLA	C4A-NA-C1A	5.00	108.95	106.71
25	c	506	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
25	A	406	CLA	C1D-ND-C4D	-4.99	102.79	106.33
25	b	610	CLA	CHD-C1D-ND	-4.99	119.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	502	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	B	601	CLA	C4A-NA-C1A	4.98	108.94	106.71
25	b	612	CLA	C1D-ND-C4D	-4.98	102.80	106.33
25	C	513	CLA	O2A-C1-C2	4.97	121.70	108.64
25	A	405	CLA	O2A-CGA-O1A	-4.97	111.05	123.59
25	c	510	CLA	CHD-C1D-ND	-4.97	119.89	124.45
25	a	406	CLA	O2A-CGA-O1A	-4.97	111.06	123.59
25	c	513	CLA	O2A-C1-C2	4.97	121.69	108.64
25	A	406	CLA	O2A-CGA-O1A	-4.96	111.06	123.59
25	a	405	CLA	O2A-CGA-O1A	-4.96	111.07	123.59
25	B	602	CLA	O2D-CGD-CBD	4.96	120.08	111.27
25	C	501	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
25	c	501	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
25	b	602	CLA	O2D-CGD-CBD	4.95	120.06	111.27
25	B	604	CLA	O2A-C1-C2	4.95	121.63	108.64
25	B	610	CLA	CHD-C1D-ND	-4.95	119.91	124.45
25	C	510	CLA	CHD-C1D-ND	-4.94	119.91	124.45
25	B	612	CLA	O2A-CGA-O1A	-4.94	111.13	123.59
25	b	604	CLA	O2A-C1-C2	4.94	121.61	108.64
25	C	506	CLA	O2A-CGA-O1A	-4.94	111.13	123.59
27	b	619	BCR	C24-C23-C22	-4.93	118.78	126.23
25	C	508	CLA	O2A-CGA-O1A	-4.92	111.16	123.59
25	B	608	CLA	CHD-C1D-ND	-4.92	119.93	124.45
25	c	506	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
25	B	614	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
25	b	614	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
25	c	508	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
25	c	504	CLA	C1D-ND-C4D	-4.92	102.84	106.33
27	C	514	BCR	C24-C23-C22	-4.92	118.80	126.23
25	D	403	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
25	b	612	CLA	O2A-CGA-O1A	-4.92	111.19	123.59
25	B	613	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
25	b	608	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	B	619	BCR	C24-C23-C22	-4.91	118.81	126.23
25	b	613	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
25	b	612	CLA	CHD-C1D-ND	-4.91	119.94	124.45
25	c	501	CLA	O2D-CGD-CBD	4.91	119.99	111.27
25	b	616	CLA	C1D-ND-C4D	-4.91	102.85	106.33
27	Z	101	BCR	C24-C23-C22	-4.90	118.83	126.23
25	C	504	CLA	C1D-ND-C4D	-4.90	102.86	106.33
27	z	101	BCR	C24-C23-C22	-4.90	118.84	126.23
25	c	511	CLA	CHD-C1D-ND	-4.89	119.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	CLA	O2A-CGA-O1A	-4.89	111.24	123.59
25	B	616	CLA	C1D-ND-C4D	-4.89	102.86	106.33
25	b	601	CLA	C1D-ND-C4D	-4.89	102.86	106.33
28	A	414	SQD	O5-C5-C4	4.89	118.57	109.69
25	C	501	CLA	O2D-CGD-CBD	4.88	119.95	111.27
25	b	609	CLA	O2D-CGD-CBD	4.88	119.94	111.27
25	B	615	CLA	C4A-NA-C1A	4.88	108.90	106.71
28	a	414	SQD	O5-C5-C4	4.88	118.55	109.69
27	c	514	BCR	C24-C23-C22	-4.88	118.87	126.23
25	B	609	CLA	O2D-CGD-CBD	4.88	119.93	111.27
25	C	504	CLA	O2A-CGA-O1A	-4.88	111.29	123.59
25	c	504	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
25	B	601	CLA	C1D-ND-C4D	-4.87	102.87	106.33
25	B	608	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
25	b	601	CLA	C4A-NA-C1A	4.87	108.90	106.71
25	C	511	CLA	CHD-C1D-ND	-4.87	119.98	124.45
25	B	613	CLA	C1-C2-C3	-4.87	117.62	126.04
25	b	613	CLA	C1-C2-C3	-4.87	117.63	126.04
25	b	608	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
25	B	612	CLA	CHD-C1D-ND	-4.87	119.98	124.45
25	C	507	CLA	CHD-C1D-ND	-4.86	119.99	124.45
25	c	511	CLA	O2A-C1-C2	4.86	121.41	108.64
25	C	503	CLA	C4A-NA-C1A	4.85	108.89	106.71
25	C	511	CLA	O2A-C1-C2	4.85	121.39	108.64
25	c	510	CLA	O2A-C1-C2	4.85	121.39	108.64
25	b	615	CLA	C4A-NA-C1A	4.85	108.89	106.71
25	d	404	CLA	O2A-CGA-O1A	-4.85	111.36	123.59
25	D	404	CLA	O2A-CGA-O1A	-4.85	111.36	123.59
25	C	510	CLA	O2A-C1-C2	4.84	121.37	108.64
25	b	614	CLA	C1D-ND-C4D	-4.84	102.90	106.33
25	c	507	CLA	CHD-C1D-ND	-4.83	120.01	124.45
25	c	503	CLA	C4A-NA-C1A	4.83	108.88	106.71
25	C	502	CLA	CHD-C1D-ND	-4.83	120.01	124.45
25	B	614	CLA	C1D-ND-C4D	-4.83	102.91	106.33
25	b	610	CLA	C1D-ND-C4D	-4.82	102.91	106.33
25	D	401	CLA	O2A-CGA-O1A	-4.82	111.42	123.59
25	C	509	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	c	514	BCR	C38-C26-C25	-4.82	119.11	124.53
25	D	401	CLA	O2A-C1-C2	4.82	121.30	108.64
25	c	507	CLA	O2A-CGA-O1A	-4.82	111.43	123.59
25	c	513	CLA	O2A-CGA-O1A	-4.82	111.43	123.59
25	d	401	CLA	O2A-CGA-O1A	-4.81	111.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	O2A-C1-C2	4.81	121.28	108.64
25	c	502	CLA	CHD-C1D-ND	-4.81	120.03	124.45
25	C	507	CLA	O2A-CGA-O1A	-4.81	111.45	123.59
25	B	616	CLA	CHD-C1D-ND	-4.81	120.03	124.45
25	b	616	CLA	CHD-C1D-ND	-4.80	120.04	124.45
25	C	513	CLA	O2A-CGA-O1A	-4.80	111.48	123.59
25	B	601	CLA	O2A-CGA-O1A	-4.79	111.35	123.30
25	B	608	CLA	O2A-CGA-O1A	-4.79	111.49	123.59
25	c	509	CLA	CHD-C1D-ND	-4.79	120.05	124.45
25	b	608	CLA	C1D-ND-C4D	-4.79	102.93	106.33
25	b	608	CLA	O2A-C1-C2	4.79	121.23	108.64
25	C	512	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
25	B	608	CLA	O2A-C1-C2	4.79	121.22	108.64
25	B	610	CLA	C1D-ND-C4D	-4.79	102.93	106.33
25	b	601	CLA	O2A-CGA-O1A	-4.79	111.37	123.30
25	B	615	CLA	C1D-ND-C4D	-4.79	102.94	106.33
27	C	514	BCR	C38-C26-C25	-4.79	119.15	124.53
25	C	501	CLA	C4A-NA-C1A	4.78	108.86	106.71
25	b	608	CLA	O2A-CGA-O1A	-4.78	111.53	123.59
25	b	610	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
25	c	512	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
25	c	501	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	b	615	CLA	C1D-ND-C4D	-4.77	102.95	106.33
25	B	610	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
25	A	406	CLA	O2A-C1-C2	4.77	121.17	108.64
25	C	508	CLA	O2D-CGD-CBD	4.76	119.72	111.27
25	a	406	CLA	O2A-C1-C2	4.76	121.14	108.64
25	c	508	CLA	O2D-CGD-CBD	4.75	119.71	111.27
25	B	615	CLA	CHD-C1D-ND	-4.75	120.09	124.45
25	b	615	CLA	CHD-C1D-ND	-4.75	120.09	124.45
25	b	607	CLA	C1D-ND-C4D	-4.74	102.97	106.33
25	B	608	CLA	C1D-ND-C4D	-4.73	102.97	106.33
25	c	505	CLA	CHD-C1D-ND	-4.73	120.11	124.45
25	B	607	CLA	C1D-ND-C4D	-4.73	102.98	106.33
28	A	414	SQD	C1-O5-C5	4.72	122.94	113.69
25	d	404	CLA	C1D-ND-C4D	-4.72	102.98	106.33
25	c	513	CLA	O2D-CGD-CBD	4.71	119.64	111.27
25	C	513	CLA	O2D-CGD-CBD	4.71	119.63	111.27
28	F	101	SQD	O7-S-C6	4.71	112.53	106.94
25	b	614	CLA	O2A-C1-C2	4.70	120.99	108.64
28	a	414	SQD	C1-O5-C5	4.70	122.91	113.69
25	C	510	CLA	C4A-NA-C1A	4.69	108.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	C1D-ND-C4D	-4.69	103.00	106.33
25	B	614	CLA	O2A-C1-C2	4.69	120.97	108.64
28	f	101	SQD	O7-S-C6	4.69	112.51	106.94
25	c	510	CLA	C4A-NA-C1A	4.69	108.81	106.71
25	B	614	CLA	O2D-CGD-CBD	4.68	119.59	111.27
25	b	614	CLA	O2D-CGD-CBD	4.68	119.58	111.27
27	k	102	BCR	C24-C23-C22	-4.68	119.16	126.23
25	c	502	CLA	O2A-CGA-O1A	-4.67	111.80	123.59
25	C	505	CLA	CHD-C1D-ND	-4.67	120.16	124.45
27	K	102	BCR	C24-C23-C22	-4.67	119.18	126.23
28	a	413	SQD	O7-S-C6	4.67	112.49	106.94
25	C	502	CLA	O2A-CGA-O1A	-4.67	111.81	123.59
27	c	514	BCR	C7-C8-C9	-4.67	119.19	126.23
27	C	514	BCR	C7-C8-C9	-4.66	119.19	126.23
25	b	603	CLA	CHD-C1D-ND	-4.65	120.18	124.45
28	A	413	SQD	O7-S-C6	4.64	112.46	106.94
25	D	404	CLA	C4A-NA-C1A	4.63	108.79	106.71
25	b	605	CLA	O2A-CGA-O1A	-4.62	111.94	123.59
25	B	603	CLA	CHD-C1D-ND	-4.62	120.21	124.45
28	a	414	SQD	O7-S-C6	4.61	112.42	106.94
25	d	404	CLA	C4A-NA-C1A	4.60	108.78	106.71
25	D	401	CLA	CHD-C1D-ND	-4.60	120.22	124.45
25	B	605	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
25	B	613	CLA	O2A-C1-C2	4.60	120.73	108.64
28	A	414	SQD	O7-S-C6	4.60	112.40	106.94
25	a	408	CLA	O2A-CGA-O1A	-4.60	111.99	123.59
25	B	604	CLA	CHD-C1D-ND	-4.60	120.23	124.45
25	A	408	CLA	O2A-CGA-O1A	-4.59	112.01	123.59
25	b	604	CLA	O2A-CGA-O1A	-4.59	112.01	123.59
25	C	502	CLA	C1-C2-C3	-4.59	118.11	126.04
25	c	502	CLA	C1-C2-C3	-4.59	118.11	126.04
25	b	613	CLA	O2A-C1-C2	4.58	120.68	108.64
25	B	604	CLA	O2A-CGA-O1A	-4.58	112.03	123.59
25	b	604	CLA	CHD-C1D-ND	-4.56	120.26	124.45
33	A	419	LHG	O7-C7-C8	4.55	121.31	111.50
25	d	401	CLA	CHD-C1D-ND	-4.55	120.28	124.45
25	C	506	CLA	O2D-CGD-CBD	4.54	119.34	111.27
25	c	513	CLA	C4A-NA-C1A	4.54	108.75	106.71
25	D	403	CLA	O2D-CGD-CBD	4.53	119.32	111.27
25	c	506	CLA	O2D-CGD-CBD	4.53	119.32	111.27
33	a	419	LHG	O7-C7-C8	4.53	121.26	111.50
25	c	505	CLA	C1D-ND-C4D	-4.53	103.12	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	CLA	C1D-ND-C4D	-4.52	103.12	106.33
25	C	513	CLA	C4A-NA-C1A	4.52	108.74	106.71
27	K	102	BCR	C3-C4-C5	-4.52	106.02	114.08
25	b	609	CLA	C1D-ND-C4D	-4.51	103.13	106.33
27	A	409	BCR	C33-C5-C6	-4.51	119.46	124.53
25	c	512	CLA	CHD-C1D-ND	-4.50	120.31	124.45
25	A	405	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
25	C	512	CLA	CHD-C1D-ND	-4.50	120.32	124.45
25	B	607	CLA	O2A-C1-C2	4.50	120.47	108.64
25	b	607	CLA	O2A-C1-C2	4.50	120.47	108.64
25	d	403	CLA	O2D-CGD-CBD	4.50	119.26	111.27
25	B	602	CLA	O2A-CGA-O1A	-4.50	112.24	123.59
27	k	102	BCR	C3-C4-C5	-4.50	106.05	114.08
27	a	409	BCR	C33-C5-C6	-4.50	119.48	124.53
37	x	102	RRX	C30-C25-C26	-4.49	116.29	122.61
25	b	602	CLA	C1D-ND-C4D	-4.49	103.14	106.33
27	b	618	BCR	C7-C8-C9	-4.49	119.45	126.23
25	b	602	CLA	O2A-CGA-O1A	-4.49	112.26	123.59
25	C	505	CLA	C1D-ND-C4D	-4.49	103.14	106.33
27	b	619	BCR	C7-C8-C9	-4.49	119.45	126.23
25	b	611	CLA	O2A-C1-C2	4.49	120.42	108.64
25	c	505	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
25	B	616	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
25	B	611	CLA	O2A-C1-C2	4.48	120.41	108.64
25	C	505	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
25	B	613	CLA	C1D-ND-C4D	-4.48	103.16	106.33
25	b	606	CLA	C1D-ND-C4D	-4.48	103.16	106.33
25	a	405	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
37	X	102	RRX	C30-C25-C26	-4.47	116.31	122.61
25	B	609	CLA	C1D-ND-C4D	-4.47	103.16	106.33
25	B	606	CLA	C1D-ND-C4D	-4.47	103.16	106.33
25	A	408	CLA	C1D-ND-C4D	-4.47	103.16	106.33
27	B	619	BCR	C7-C8-C9	-4.47	119.48	126.23
25	B	615	CLA	O2A-CGA-O1A	-4.47	112.32	123.59
25	b	616	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
27	B	618	BCR	C7-C8-C9	-4.46	119.49	126.23
25	b	613	CLA	O2D-CGD-CBD	4.46	119.19	111.27
34	C	515	DGD	O2G-C1B-C2B	4.46	121.11	111.50
25	B	613	CLA	O2D-CGD-CBD	4.45	119.18	111.27
25	b	615	CLA	O2A-CGA-O1A	-4.45	112.35	123.59
34	c	515	DGD	O2G-C1B-C2B	4.45	121.10	111.50
25	b	613	CLA	C1D-ND-C4D	-4.45	103.17	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	z	102	LHG	O7-C7-C8	4.45	121.09	111.50
30	d	406	PL9	C7-C3-C4	4.45	120.49	116.88
25	c	509	CLA	C1D-ND-C4D	-4.44	103.18	106.33
33	Z	102	LHG	O7-C7-C8	4.44	121.07	111.50
25	C	509	CLA	C1D-ND-C4D	-4.43	103.19	106.33
25	d	401	CLA	C1D-ND-C4D	-4.43	103.19	106.33
25	C	502	CLA	C1D-ND-C4D	-4.43	103.19	106.33
30	D	406	PL9	C7-C3-C4	4.43	120.47	116.88
25	D	401	CLA	C1D-ND-C4D	-4.42	103.19	106.33
25	B	602	CLA	C1D-ND-C4D	-4.42	103.19	106.33
27	A	409	BCR	C38-C26-C25	-4.41	119.58	124.53
25	c	510	CLA	C1D-ND-C4D	-4.41	103.20	106.33
27	a	409	BCR	C38-C26-C25	-4.41	119.58	124.53
25	c	502	CLA	C1D-ND-C4D	-4.38	103.22	106.33
25	c	512	CLA	C1D-ND-C4D	-4.38	103.22	106.33
25	A	405	CLA	O2A-CGA-CBA	4.35	125.57	111.91
25	C	510	CLA	C1D-ND-C4D	-4.35	103.25	106.33
25	a	405	CLA	O2A-CGA-CBA	4.34	125.53	111.91
25	b	611	CLA	C1D-ND-C4D	-4.34	103.25	106.33
27	K	102	BCR	C7-C8-C9	-4.34	119.68	126.23
25	C	512	CLA	C1D-ND-C4D	-4.33	103.26	106.33
27	k	102	BCR	C7-C8-C9	-4.32	119.71	126.23
25	C	508	CLA	O2A-C1-C2	4.32	119.98	108.64
25	b	608	CLA	C1-C2-C3	-4.32	118.58	126.04
25	c	508	CLA	O2A-C1-C2	4.31	119.97	108.64
25	B	611	CLA	C1D-ND-C4D	-4.31	103.27	106.33
25	b	616	CLA	O2A-CGA-CBA	4.31	125.43	111.91
25	B	608	CLA	C1-C2-C3	-4.30	118.60	126.04
25	C	511	CLA	C1D-ND-C4D	-4.30	103.28	106.33
25	C	513	CLA	C1D-ND-C4D	-4.30	103.28	106.33
29	a	415	LMG	O7-C10-C11	4.30	120.77	111.50
29	A	415	LMG	O7-C10-C11	4.30	120.77	111.50
25	B	616	CLA	O2A-CGA-CBA	4.30	125.39	111.91
25	c	511	CLA	C1D-ND-C4D	-4.29	103.28	106.33
25	C	505	CLA	O2A-CGA-O1A	-4.28	112.79	123.59
25	c	501	CLA	O2A-C1-C2	4.28	119.88	108.64
25	c	505	CLA	O2A-CGA-O1A	-4.28	112.80	123.59
34	C	517	DGD	O2G-C1B-C2B	4.28	120.72	111.50
34	c	517	DGD	O2G-C1B-C2B	4.28	120.72	111.50
25	C	501	CLA	O2A-C1-C2	4.27	119.87	108.64
25	c	510	CLA	C1-C2-C3	-4.27	118.65	126.04
25	c	513	CLA	C1D-ND-C4D	-4.27	103.30	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	C1-C2-C3	-4.27	118.66	126.04
28	f	101	SQD	C1-O5-C5	4.27	122.07	113.69
25	C	509	CLA	O2A-C1-C2	4.27	119.86	108.64
25	c	509	CLA	O2A-C1-C2	4.25	119.81	108.64
25	B	610	CLA	O2A-CGA-CBA	4.25	125.25	111.91
25	b	610	CLA	O2A-CGA-CBA	4.25	125.24	111.91
27	a	409	BCR	C7-C8-C9	-4.25	119.82	126.23
28	F	101	SQD	C1-O5-C5	4.24	122.01	113.69
29	A	411	LMG	O7-C10-C11	4.23	120.63	111.50
25	b	616	CLA	O2A-C1-C2	4.23	119.75	108.64
29	a	411	LMG	O7-C10-C11	4.22	120.60	111.50
25	B	616	CLA	O2A-C1-C2	4.22	119.72	108.64
25	b	609	CLA	O2A-CGA-CBA	4.21	125.11	111.91
25	B	609	CLA	O2A-CGA-CBA	4.21	125.11	111.91
25	a	408	CLA	O2A-C1-C2	4.21	119.69	108.64
25	A	408	CLA	O2A-C1-C2	4.20	119.69	108.64
28	h	102	SQD	O47-C7-C8	4.20	120.55	111.50
27	D	405	BCR	C38-C26-C25	-4.20	119.81	124.53
27	A	409	BCR	C7-C8-C9	-4.19	119.90	126.23
34	C	516	DGD	O2G-C1B-C2B	4.19	120.53	111.50
27	Z	101	BCR	C38-C26-C25	-4.18	119.83	124.53
27	d	405	BCR	C38-C26-C25	-4.18	119.83	124.53
27	z	101	BCR	C38-C26-C25	-4.18	119.83	124.53
28	H	102	SQD	O47-C7-C8	4.18	120.50	111.50
34	c	516	DGD	O2G-C1B-C2B	4.17	120.48	111.50
25	c	503	CLA	C1D-ND-C4D	-4.15	103.39	106.33
28	f	101	SQD	C44-O6-C1	4.15	121.84	113.74
28	A	410	SQD	O6-C1-C2	4.15	114.78	108.30
25	d	401	CLA	C1-C2-C3	-4.14	118.88	126.04
25	b	604	CLA	C1D-ND-C4D	-4.14	103.39	106.33
33	D	407	LHG	O7-C7-C8	4.14	120.42	111.50
33	d	407	LHG	O7-C7-C8	4.14	120.42	111.50
25	C	503	CLA	C1D-ND-C4D	-4.14	103.40	106.33
28	F	101	SQD	C44-O6-C1	4.14	121.82	113.74
25	D	401	CLA	C1-C2-C3	-4.14	118.89	126.04
25	b	612	CLA	O2A-C1-C2	4.13	119.49	108.64
25	B	612	CLA	O2A-C1-C2	4.13	119.49	108.64
25	B	604	CLA	C1D-ND-C4D	-4.13	103.40	106.33
28	a	410	SQD	O6-C1-C2	4.12	114.73	108.30
37	X	102	RRX	C37-C22-C21	-4.12	117.16	122.92
25	b	603	CLA	O2A-CGA-CBA	4.12	124.83	111.91
37	x	102	RRX	C37-C22-C21	-4.11	117.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	O2A-CGA-CBA	4.11	124.81	111.91
28	F	101	SQD	O5-C5-C4	4.11	117.16	109.69
25	C	508	CLA	C1D-ND-C4D	-4.10	103.42	106.33
25	c	506	CLA	C4A-NA-C1A	4.10	108.55	106.71
28	f	101	SQD	O5-C5-C4	4.10	117.14	109.69
37	X	102	RRX	C34-C9-C10	-4.10	117.18	122.92
37	x	102	RRX	C34-C9-C10	-4.10	117.18	122.92
25	c	511	CLA	O2A-CGA-CBA	4.09	124.75	111.91
29	c	518	LMG	O7-C10-C11	4.09	120.31	111.50
25	c	507	CLA	C1D-ND-C4D	-4.09	103.43	106.33
25	C	511	CLA	O2A-CGA-CBA	4.08	124.73	111.91
29	C	518	LMG	O7-C10-C11	4.08	120.30	111.50
25	c	508	CLA	C1D-ND-C4D	-4.08	103.44	106.33
28	A	414	SQD	O9-S-C6	4.06	111.77	106.94
25	A	405	CLA	CMC-C2C-C1C	4.05	131.21	125.04
28	a	414	SQD	O9-S-C6	4.05	111.75	106.94
25	C	507	CLA	C1D-ND-C4D	-4.04	103.46	106.33
25	a	405	CLA	CMC-C2C-C1C	4.03	131.18	125.04
25	C	509	CLA	O2A-CGA-CBA	4.03	124.55	111.91
25	c	509	CLA	O2A-CGA-CBA	4.02	124.53	111.91
28	B	620	SQD	O9-S-C6	4.00	111.69	106.94
28	T	101	SQD	O9-S-C6	3.99	111.69	106.94
25	c	512	CLA	C1-C2-C3	-3.99	120.29	126.75
28	A	410	SQD	O7-S-C6	3.99	111.68	106.94
28	a	410	SQD	O7-S-C6	3.99	111.68	106.94
29	B	621	LMG	O7-C10-C11	3.99	120.09	111.50
29	b	620	LMG	O7-C10-C11	3.98	120.08	111.50
25	C	506	CLA	C4A-NA-C1A	3.97	108.49	106.71
25	C	512	CLA	C1-C2-C3	-3.97	120.32	126.75
27	k	102	BCR	C33-C5-C6	-3.97	120.07	124.53
31	A	416	LMT	C3'-C4'-C5'	-3.96	101.86	110.93
27	K	102	BCR	C33-C5-C6	-3.95	120.09	124.53
25	b	614	CLA	C1-C2-C3	-3.94	119.23	126.04
25	B	614	CLA	C1-C2-C3	-3.94	119.23	126.04
31	a	416	LMT	C3'-C4'-C5'	-3.94	101.90	110.93
25	C	510	CLA	O2A-CGA-CBA	3.93	124.25	111.91
25	a	406	CLA	C1-C2-C3	-3.93	119.25	126.04
25	c	510	CLA	O2A-CGA-CBA	3.93	124.24	111.91
25	A	406	CLA	C1-C2-C3	-3.93	119.25	126.04
29	C	523	LMG	O7-C10-C11	3.91	119.94	111.50
31	b	623	LMT	C3'-C4'-C5'	-3.91	103.26	110.24
29	c	523	LMG	O7-C10-C11	3.91	119.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMB-C2B-C3B	3.90	131.98	124.68
31	C	521	LMT	O5'-C5'-C4'	3.90	116.78	109.69
25	C	513	CLA	CMB-C2B-C3B	3.90	131.98	124.68
37	x	102	RRX	C15-C16-C17	3.90	131.47	123.47
31	B	624	LMT	C3'-C4'-C5'	-3.90	103.29	110.24
27	b	618	BCR	C38-C26-C25	-3.90	120.15	124.53
27	B	618	BCR	C38-C26-C25	-3.89	120.16	124.53
25	c	501	CLA	O2A-CGA-CBA	3.89	124.13	111.91
37	X	102	RRX	C15-C16-C17	3.89	131.44	123.47
31	c	521	LMT	O5'-C5'-C4'	3.88	116.75	109.69
25	B	612	CLA	O2A-CGA-CBA	3.88	124.09	111.91
25	C	501	CLA	O2A-CGA-CBA	3.88	124.09	111.91
25	b	612	CLA	O2A-CGA-CBA	3.88	124.07	111.91
25	B	607	CLA	O2A-CGA-CBA	3.88	124.07	111.91
25	C	501	CLA	C1D-ND-C4D	-3.87	103.59	106.33
25	b	607	CLA	O2A-CGA-CBA	3.87	124.05	111.91
25	c	501	CLA	C1D-ND-C4D	-3.87	103.59	106.33
27	C	522	BCR	C38-C26-C25	-3.86	120.19	124.53
27	c	522	BCR	C38-C26-C25	-3.86	120.19	124.53
25	c	506	CLA	C1D-ND-C4D	-3.86	103.59	106.33
25	d	404	CLA	C1-C2-C3	-3.86	119.37	126.04
31	d	412	LMT	O1'-C1'-C2'	3.84	114.31	108.30
25	D	403	CLA	O2A-CGA-CBA	3.84	123.96	111.91
25	D	404	CLA	C1-C2-C3	-3.84	119.41	126.04
31	D	412	LMT	O1'-C1'-C2'	3.84	114.29	108.30
29	d	409	LMG	O7-C10-C11	3.84	119.77	111.50
25	d	403	CLA	O2A-CGA-CBA	3.83	123.94	111.91
25	b	603	CLA	O2A-C1-C2	3.83	118.69	108.64
25	B	603	CLA	O2A-C1-C2	3.82	118.67	108.64
25	C	513	CLA	O2A-CGA-CBA	3.81	123.87	111.91
25	c	513	CLA	O2A-CGA-CBA	3.81	123.86	111.91
25	C	506	CLA	O2A-CGA-CBA	3.81	123.86	111.91
25	c	506	CLA	O2A-CGA-CBA	3.81	123.86	111.91
29	D	409	LMG	O7-C10-C11	3.81	119.71	111.50
25	C	506	CLA	C1D-ND-C4D	-3.80	103.63	106.33
27	B	618	BCR	C33-C5-C6	-3.80	120.26	124.53
25	a	405	CLA	O2D-CGD-CBD	3.80	118.02	111.27
27	c	522	BCR	C3-C4-C5	-3.79	107.31	114.08
25	A	405	CLA	O2D-CGD-CBD	3.79	117.99	111.27
27	C	522	BCR	C3-C4-C5	-3.78	107.32	114.08
25	A	408	CLA	CMB-C2B-C3B	3.78	131.75	124.68
27	b	618	BCR	C33-C5-C6	-3.78	120.29	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	505	CLA	C4-C3-C5	3.77	121.62	115.27
25	b	613	CLA	O2A-CGA-CBA	3.77	123.75	111.91
25	C	505	CLA	C4-C3-C5	3.77	121.62	115.27
25	B	608	CLA	CMB-C2B-C3B	3.77	131.74	124.68
25	B	613	CLA	O2A-CGA-CBA	3.77	123.74	111.91
25	c	503	CLA	O2A-C1-C2	3.77	118.54	108.64
25	b	608	CLA	CMB-C2B-C3B	3.77	131.73	124.68
25	C	503	CLA	O2A-C1-C2	3.76	118.53	108.64
25	a	408	CLA	CMB-C2B-C3B	3.76	131.72	124.68
31	a	416	LMT	O5B-C5B-C4B	3.76	116.52	109.69
28	h	102	SQD	O9-S-O7	-3.75	100.96	113.95
31	A	416	LMT	O5B-C5B-C4B	3.75	116.50	109.69
28	H	102	SQD	O9-S-O7	-3.74	101.00	113.95
28	a	414	SQD	O9-S-O7	-3.74	101.02	113.95
28	A	414	SQD	O9-S-O7	-3.74	101.02	113.95
25	c	512	CLA	O2A-CGA-CBA	3.73	123.63	111.91
25	C	512	CLA	O2A-CGA-CBA	3.73	123.63	111.91
27	B	617	BCR	C3-C4-C5	-3.73	107.42	114.08
33	b	621	LHG	O7-C7-C8	3.73	119.53	111.50
25	c	503	CLA	O2A-CGA-CBA	3.73	123.60	111.91
33	B	622	LHG	O7-C7-C8	3.72	119.53	111.50
25	C	503	CLA	O2A-CGA-CBA	3.72	123.57	111.91
27	b	617	BCR	C3-C4-C5	-3.72	107.44	114.08
25	b	609	CLA	C1-C2-C3	-3.70	119.64	126.04
25	B	614	CLA	O2A-CGA-CBA	3.70	123.52	111.91
25	b	614	CLA	O2A-CGA-CBA	3.70	123.51	111.91
34	h	103	DGD	O2G-C1B-C2B	3.69	119.45	111.50
25	b	611	CLA	O2A-CGA-CBA	3.69	123.49	111.91
28	a	413	SQD	O9-S-O7	-3.69	101.19	113.95
25	B	609	CLA	C1-C2-C3	-3.69	119.67	126.04
25	B	603	CLA	C1D-ND-C4D	-3.69	103.72	106.33
25	B	611	CLA	O2A-CGA-CBA	3.68	123.47	111.91
31	C	524	LMT	C3'-C4'-C5'	-3.68	102.48	110.93
31	c	524	LMT	C3'-C4'-C5'	-3.68	102.48	110.93
25	B	606	CLA	O2A-CGA-CBA	3.68	123.45	111.91
28	A	413	SQD	O9-S-O7	-3.67	101.23	113.95
31	Y	101	LMT	C3'-C4'-C5'	-3.67	103.69	110.24
34	H	103	DGD	O2G-C1B-C2B	3.67	119.42	111.50
25	b	606	CLA	O2A-CGA-CBA	3.67	123.44	111.91
28	B	620	SQD	O9-S-O7	-3.67	101.24	113.95
31	y	101	LMT	C3'-C4'-C5'	-3.67	103.69	110.24
25	C	508	CLA	CMB-C2B-C3B	3.67	131.54	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	PL9	C7-C3-C2	-3.67	118.48	123.30
28	T	101	SQD	O9-S-O7	-3.67	101.26	113.95
30	A	412	PL9	C7-C3-C2	-3.66	118.49	123.30
31	x	104	LMT	C1'-O5'-C5'	-3.66	107.38	113.67
25	c	508	CLA	CMB-C2B-C3B	3.66	131.53	124.68
33	d	408	LHG	O7-C7-C8	3.66	119.39	111.50
31	X	104	LMT	C1'-O5'-C5'	-3.66	107.38	113.67
25	C	511	CLA	C1-C2-C3	-3.64	119.74	126.04
25	b	603	CLA	C1D-ND-C4D	-3.64	103.75	106.33
33	D	408	LHG	O7-C7-C8	3.64	119.34	111.50
28	F	101	SQD	O9-S-O7	-3.63	101.39	113.95
33	e	102	LHG	O7-C7-C8	3.63	119.32	111.50
28	f	101	SQD	O9-S-O7	-3.63	101.40	113.95
25	B	606	CLA	O2A-C1-C2	3.62	118.16	108.64
25	b	606	CLA	O2A-C1-C2	3.62	118.15	108.64
33	E	102	LHG	O7-C7-C8	3.62	119.31	111.50
25	c	511	CLA	C1-C2-C3	-3.62	119.78	126.04
28	A	410	SQD	O9-S-O7	-3.61	101.45	113.95
28	a	410	SQD	O9-S-O7	-3.61	101.46	113.95
25	A	408	CLA	O2A-CGA-CBA	3.61	123.23	111.91
25	C	501	CLA	CMB-C2B-C3B	3.60	131.42	124.68
25	a	408	CLA	O2A-CGA-CBA	3.60	123.21	111.91
25	B	608	CLA	O2A-CGA-CBA	3.60	123.20	111.91
25	c	501	CLA	CMB-C2B-C3B	3.59	131.40	124.68
25	b	608	CLA	O2A-CGA-CBA	3.59	123.18	111.91
27	c	514	BCR	C3-C4-C5	-3.58	107.68	114.08
31	I	103	LMT	C1'-O5'-C5'	-3.58	106.67	113.69
31	i	103	LMT	C1'-O5'-C5'	-3.57	106.67	113.69
27	C	514	BCR	C3-C4-C5	-3.57	107.69	114.08
27	C	522	BCR	C33-C5-C6	-3.57	120.51	124.53
25	C	502	CLA	O2A-CGA-CBA	3.57	123.11	111.91
25	c	502	CLA	O2A-CGA-CBA	3.57	123.10	111.91
27	C	514	BCR	C33-C5-C6	-3.56	120.53	124.53
27	c	514	BCR	C33-C5-C6	-3.55	120.54	124.53
27	c	522	BCR	C33-C5-C6	-3.55	120.55	124.53
25	D	404	CLA	O2A-CGA-CBA	3.54	123.02	111.91
25	b	604	CLA	CMA-C3A-C4A	3.54	121.28	111.77
25	c	513	CLA	C1-C2-C3	-3.53	119.93	126.04
25	d	404	CLA	O2A-CGA-CBA	3.53	123.00	111.91
25	C	504	CLA	O2A-CGA-CBA	3.53	122.97	111.91
25	B	604	CLA	CMA-C3A-C4A	3.53	121.25	111.77
25	C	513	CLA	C1-C2-C3	-3.53	119.94	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	O2A-CGA-CBA	3.52	122.97	111.91
25	C	503	CLA	C1-C2-C3	-3.50	119.98	126.04
25	A	405	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	a	405	CLA	CMB-C2B-C3B	3.50	131.22	124.68
28	H	102	SQD	O7-S-C6	3.49	111.09	106.94
35	f	102	HEM	C4D-ND-C1D	3.49	108.68	105.07
25	b	604	CLA	O2A-CGA-CBA	3.49	122.86	111.91
25	c	504	CLA	C1-C2-C3	-3.49	120.01	126.04
25	C	504	CLA	C1-C2-C3	-3.49	120.01	126.04
28	h	102	SQD	O7-S-C6	3.49	111.08	106.94
25	b	606	CLA	CMB-C2B-C3B	3.49	131.20	124.68
25	B	604	CLA	O2A-CGA-CBA	3.48	122.84	111.91
25	B	605	CLA	CMB-C2B-C3B	3.48	131.19	124.68
28	f	101	SQD	O9-S-C6	3.48	111.08	106.94
28	a	413	SQD	O5-C1-C2	3.48	117.72	110.35
25	c	503	CLA	C1-C2-C3	-3.48	120.02	126.04
28	A	413	SQD	O5-C1-C2	3.48	117.71	110.35
25	b	605	CLA	CMB-C2B-C3B	3.47	131.18	124.68
25	B	605	CLA	C4-C3-C5	3.47	121.11	115.27
28	H	102	SQD	C44-O6-C1	3.47	120.51	113.74
28	h	102	SQD	C44-O6-C1	3.46	120.51	113.74
28	F	101	SQD	O9-S-C6	3.46	111.05	106.94
25	b	605	CLA	C4-C3-C5	3.45	121.08	115.27
25	B	602	CLA	CAA-C2A-C3A	-3.45	103.32	112.78
25	b	602	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
25	B	606	CLA	CMB-C2B-C3B	3.45	131.13	124.68
25	b	602	CLA	O2A-CGA-CBA	3.45	122.73	111.91
28	A	410	SQD	O9-S-C6	3.44	111.03	106.94
25	B	602	CLA	O2A-CGA-CBA	3.44	122.70	111.91
35	F	102	HEM	C4D-ND-C1D	3.43	108.62	105.07
37	x	102	RRX	C36-C18-C17	-3.43	118.12	122.92
28	a	410	SQD	O9-S-C6	3.42	111.01	106.94
27	c	522	BCR	C36-C18-C17	-3.42	118.13	122.92
25	B	603	CLA	C4-C3-C5	3.42	121.02	115.27
26	d	402	PHO	O1D-CGD-CBD	3.42	130.43	124.74
29	b	620	LMG	C8-O7-C10	-3.41	109.39	117.79
25	b	603	CLA	C4-C3-C5	3.41	121.01	115.27
29	B	621	LMG	C8-O7-C10	-3.41	109.39	117.79
25	D	403	CLA	CMC-C2C-C1C	3.41	130.23	125.04
37	X	102	RRX	C36-C18-C17	-3.41	118.15	122.92
28	B	620	SQD	O5-C5-C4	3.40	115.87	109.69
28	T	101	SQD	O5-C5-C4	3.40	115.87	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	CMB-C2B-C3B	3.40	131.04	124.68
31	a	417	LMT	C1'-C2'-C3'	3.40	117.08	110.00
26	D	402	PHO	O1D-CGD-CBD	3.40	130.40	124.74
27	C	522	BCR	C36-C18-C17	-3.40	118.16	122.92
25	A	406	CLA	CMB-C2B-C3B	3.40	131.03	124.68
31	t	701	LMT	C1'-O5'-C5'	-3.40	107.02	113.69
31	A	417	LMT	C1'-C2'-C3'	3.40	117.07	110.00
27	z	101	BCR	C7-C8-C9	-3.39	121.12	126.23
25	d	403	CLA	CMC-C2C-C1C	3.39	130.20	125.04
31	T	102	LMT	C1'-O5'-C5'	-3.39	107.04	113.69
25	C	508	CLA	O2A-CGA-CBA	3.38	122.53	111.91
35	F	102	HEM	CBD-CAD-C3D	-3.38	103.23	112.63
25	c	508	CLA	O2A-CGA-CBA	3.38	122.51	111.91
28	a	410	SQD	O47-C7-C8	3.38	118.78	111.50
28	A	410	SQD	O47-C7-C8	3.38	118.78	111.50
31	B	623	LMT	O1'-C1'-C2'	3.38	113.58	108.30
25	D	401	CLA	O2A-CGA-CBA	3.37	122.50	111.91
35	f	102	HEM	CBD-CAD-C3D	-3.37	103.25	112.63
31	b	622	LMT	O1'-C1'-C2'	3.37	113.56	108.30
27	Z	101	BCR	C7-C8-C9	-3.37	121.14	126.23
31	E	103	LMT	C3'-C4'-C5'	-3.37	103.21	110.93
25	d	401	CLA	O2A-CGA-CBA	3.37	122.47	111.91
31	e	103	LMT	C3'-C4'-C5'	-3.37	103.21	110.93
27	B	617	BCR	C37-C22-C21	-3.37	118.21	122.92
28	A	413	SQD	O9-S-C6	3.35	110.92	106.94
27	b	617	BCR	C37-C22-C21	-3.35	118.24	122.92
27	b	617	BCR	C24-C23-C22	-3.34	121.19	126.23
27	B	617	BCR	C24-C23-C22	-3.34	121.19	126.23
28	a	413	SQD	O9-S-C6	3.33	110.89	106.94
31	I	102	LMT	C3'-C4'-C5'	-3.32	104.31	110.24
28	a	413	SQD	O47-C7-C8	3.32	118.65	111.50
28	A	413	SQD	O47-C7-C8	3.32	118.65	111.50
25	B	610	CLA	C1-C2-C3	-3.31	120.31	126.04
27	Z	101	BCR	C15-C14-C13	-3.31	122.58	127.31
27	z	101	BCR	C15-C14-C13	-3.31	122.58	127.31
31	i	102	LMT	C3'-C4'-C5'	-3.31	104.33	110.24
25	b	610	CLA	C1-C2-C3	-3.29	120.34	126.04
25	C	501	CLA	C1-C2-C3	-3.29	120.36	126.04
25	c	510	CLA	CMB-C2B-C3B	3.29	130.83	124.68
26	d	402	PHO	O2D-CGD-O1D	-3.29	117.41	123.84
25	c	501	CLA	C1-C2-C3	-3.28	120.36	126.04
25	C	510	CLA	CMB-C2B-C3B	3.28	130.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	413	SQD	C44-O6-C1	3.28	120.14	113.74
27	b	619	BCR	C28-C27-C26	-3.28	108.23	114.08
25	b	612	CLA	CMC-C2C-C1C	3.28	130.03	125.04
25	B	601	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
27	b	618	BCR	C15-C14-C13	-3.27	122.64	127.31
28	a	413	SQD	C44-O6-C1	3.27	120.13	113.74
25	b	601	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
27	B	618	BCR	C15-C14-C13	-3.27	122.64	127.31
27	B	619	BCR	C28-C27-C26	-3.27	108.24	114.08
25	B	612	CLA	CMC-C2C-C1C	3.26	130.01	125.04
27	b	619	BCR	C33-C5-C6	-3.26	120.87	124.53
25	B	605	CLA	CMC-C2C-C1C	3.25	129.99	125.04
27	b	617	BCR	C19-C18-C17	3.25	123.93	118.94
28	K	101	SQD	O47-C7-C8	3.25	118.50	111.50
25	b	605	CLA	CMC-C2C-C1C	3.25	129.98	125.04
27	B	619	BCR	C33-C5-C6	-3.24	120.89	124.53
28	k	101	SQD	O47-C7-C8	3.24	118.49	111.50
25	B	612	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	d	405	BCR	C36-C18-C17	-3.24	118.39	122.92
25	C	511	CLA	CMA-C3A-C4A	3.24	120.48	111.77
25	c	511	CLA	CMA-C3A-C4A	3.24	120.48	111.77
27	D	405	BCR	C36-C18-C17	-3.24	118.39	122.92
26	D	402	PHO	O2D-CGD-O1D	-3.24	117.51	123.84
37	X	102	RRX	C35-C13-C14	-3.24	118.39	122.92
28	B	620	SQD	O8-S-C6	3.24	110.90	105.74
26	d	402	PHO	CMB-C2B-C3B	3.24	130.73	124.68
25	C	511	CLA	CMB-C2B-C3B	3.23	130.73	124.68
26	D	402	PHO	CMB-C2B-C3B	3.23	130.73	124.68
25	b	612	CLA	CMB-C2B-C3B	3.23	130.72	124.68
27	B	617	BCR	C19-C18-C17	3.23	123.90	118.94
28	f	101	SQD	O47-C7-C8	3.23	118.46	111.50
28	F	101	SQD	O47-C7-C8	3.23	118.45	111.50
25	b	601	CLA	O2A-CGA-CBA	3.22	124.39	114.03
25	c	511	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	T	101	SQD	O8-S-C6	3.22	110.87	105.74
25	B	601	CLA	O2A-CGA-CBA	3.22	124.36	114.03
37	x	102	RRX	C35-C13-C14	-3.22	118.42	122.92
25	b	614	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	a	406	CLA	O2A-CGA-CBA	3.21	121.99	111.91
25	c	509	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	B	611	CLA	C1-C2-C3	-3.21	120.49	126.04
25	B	614	CLA	CMB-C2B-C3B	3.21	130.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	CMB-C2B-C3B	3.20	130.67	124.68
25	A	406	CLA	O2A-CGA-CBA	3.20	121.96	111.91
25	b	611	CLA	C1-C2-C3	-3.20	120.51	126.04
37	x	102	RRX	C16-C15-C14	3.20	130.03	123.47
28	a	413	SQD	O8-S-C6	3.20	110.83	105.74
28	A	413	SQD	O8-S-C6	3.20	110.83	105.74
27	d	405	BCR	C19-C18-C17	3.19	123.84	118.94
27	c	522	BCR	C19-C18-C17	3.19	123.84	118.94
27	D	405	BCR	C19-C18-C17	3.19	123.83	118.94
37	X	102	RRX	C16-C15-C14	3.18	130.00	123.47
25	C	507	CLA	O2A-CGA-CBA	3.18	121.89	111.91
31	C	520	LMT	C3'-C4'-C5'	-3.18	104.57	110.24
31	c	520	LMT	C3'-C4'-C5'	-3.18	104.57	110.24
27	C	522	BCR	C19-C18-C17	3.17	123.81	118.94
29	a	411	LMG	C8-O7-C10	-3.17	109.99	117.79
25	c	503	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	c	507	CLA	O2A-CGA-CBA	3.17	121.84	111.91
29	A	411	LMG	C8-O7-C10	-3.16	110.00	117.79
25	C	505	CLA	CMD-C2D-C3D	-3.16	120.34	127.61
29	c	518	LMG	O8-C28-C29	3.16	121.83	111.91
25	c	503	CLA	CMA-C3A-C4A	3.16	120.27	111.77
25	C	503	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	c	505	CLA	CMD-C2D-C3D	-3.16	120.35	127.61
31	x	101	LMT	C3'-C4'-C5'	-3.16	104.61	110.24
27	K	102	BCR	C15-C14-C13	-3.16	122.80	127.31
25	B	607	CLA	CMB-C2B-C3B	3.16	130.58	124.68
29	C	518	LMG	O8-C28-C29	3.15	121.80	111.91
31	X	101	LMT	C3'-C4'-C5'	-3.15	104.62	110.24
25	b	607	CLA	CMB-C2B-C3B	3.15	130.57	124.68
31	E	101	LMT	C1'-O5'-C5'	-3.14	107.52	113.69
25	C	503	CLA	CMA-C3A-C4A	3.14	120.21	111.77
25	b	603	CLA	CMB-C2B-C3B	3.14	130.55	124.68
27	k	102	BCR	C15-C14-C13	-3.14	122.83	127.31
27	B	619	BCR	C19-C18-C17	3.13	123.75	118.94
25	c	504	CLA	CMB-C2B-C3B	3.13	130.54	124.68
27	b	617	BCR	C33-C5-C6	-3.13	121.01	124.53
27	b	619	BCR	C19-C18-C17	3.13	123.74	118.94
31	e	101	LMT	C1'-O5'-C5'	-3.13	107.55	113.69
25	C	504	CLA	CMB-C2B-C3B	3.12	130.52	124.68
27	b	619	BCR	C3-C4-C5	-3.12	108.50	114.08
25	B	603	CLA	CMB-C2B-C3B	3.12	130.52	124.68
30	d	406	PL9	C7-C3-C2	-3.12	119.19	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	406	PL9	C7-C3-C2	-3.11	119.21	123.30
25	D	403	CLA	C4-C3-C5	3.11	120.50	115.27
28	B	620	SQD	C4-C3-C2	3.11	116.25	110.82
25	B	615	CLA	CMC-C2C-C1C	3.10	129.77	125.04
27	B	617	BCR	C33-C5-C6	-3.10	121.05	124.53
25	b	609	CLA	CMB-C2B-C3B	3.10	130.48	124.68
28	T	101	SQD	C4-C3-C2	3.10	116.23	110.82
25	D	401	CLA	CAA-C2A-C3A	-3.10	104.29	112.78
27	a	409	BCR	C36-C18-C17	-3.10	118.58	122.92
25	B	615	CLA	O2A-CGA-CBA	3.10	121.63	111.91
25	b	615	CLA	O2A-CGA-CBA	3.10	121.63	111.91
25	B	609	CLA	CMB-C2B-C3B	3.10	130.47	124.68
27	B	619	BCR	C3-C4-C5	-3.09	108.55	114.08
27	b	619	BCR	C38-C26-C25	-3.09	121.06	124.53
25	d	401	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
25	c	507	CLA	CMC-C2C-C1C	3.09	129.75	125.04
25	b	615	CLA	CMC-C2C-C1C	3.09	129.74	125.04
27	b	617	BCR	C36-C18-C17	-3.09	118.60	122.92
37	X	102	RRX	C19-C18-C17	3.09	123.68	118.94
25	d	403	CLA	C4-C3-C5	3.09	120.46	115.27
25	B	612	CLA	C1-C2-C3	-3.09	120.71	126.04
27	B	617	BCR	C36-C18-C17	-3.08	118.60	122.92
27	B	619	BCR	C38-C26-C25	-3.08	121.06	124.53
25	c	502	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	C	505	CLA	C4D-C3D-CAD	3.08	111.72	108.10
33	l	101	LHG	O7-C7-C8	3.08	118.13	111.50
27	A	409	BCR	C36-C18-C17	-3.07	118.62	122.92
25	B	614	CLA	CMC-C2C-C1C	3.07	129.71	125.04
25	b	612	CLA	C1-C2-C3	-3.07	120.74	126.04
31	D	410	LMT	C3'-C4'-C5'	-3.07	104.77	110.24
37	x	102	RRX	C19-C18-C17	3.06	123.64	118.94
25	C	502	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
33	L	101	LHG	O7-C7-C8	3.06	118.10	111.50
25	C	507	CLA	CMC-C2C-C1C	3.06	129.70	125.04
25	b	604	CLA	CMC-C2C-C1C	3.06	129.70	125.04
25	c	502	CLA	CMB-C2B-C3B	3.06	130.40	124.68
28	a	414	SQD	C3-C4-C5	3.06	115.69	110.24
35	F	102	HEM	C4B-CHC-C1C	3.06	126.59	122.56
25	A	408	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
25	C	502	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	D	401	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	c	506	CLA	C1-C2-C3	-3.05	120.76	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	414	SQD	C3-C4-C5	3.05	115.68	110.24
28	A	410	SQD	O5-C5-C4	3.05	115.24	109.69
28	B	620	SQD	O7-S-C6	3.05	110.56	106.94
25	A	406	CLA	C3D-C4D-ND	3.05	115.17	110.24
28	a	410	SQD	O5-C5-C4	3.05	115.23	109.69
25	a	408	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
25	b	614	CLA	CMC-C2C-C1C	3.05	129.68	125.04
28	T	101	SQD	O7-S-C6	3.05	110.56	106.94
25	d	404	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
35	f	102	HEM	C4B-CHC-C1C	3.05	126.58	122.56
31	d	410	LMT	C3'-C4'-C5'	-3.05	104.80	110.24
25	a	406	CLA	C3D-C4D-ND	3.05	115.17	110.24
25	c	505	CLA	C4D-C3D-CAD	3.05	111.69	108.10
25	D	404	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
27	a	409	BCR	C37-C22-C21	-3.04	118.66	122.92
27	A	409	BCR	C37-C22-C21	-3.04	118.66	122.92
25	C	506	CLA	C1-C2-C3	-3.04	120.78	126.04
28	A	410	SQD	C4-C3-C2	3.04	116.13	110.82
25	b	605	CLA	O2A-C1-C2	3.04	116.62	108.64
25	b	616	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	c	506	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	B	604	CLA	CMC-C2C-C1C	3.04	129.66	125.04
25	B	603	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
25	B	612	CLA	C3C-C4C-NC	3.04	113.97	110.57
28	a	410	SQD	C4-C3-C2	3.03	116.12	110.82
25	b	603	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
25	C	507	CLA	C1-C2-C3	-3.03	120.80	126.04
25	d	401	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	C	506	CLA	CMB-C2B-C3B	3.03	130.35	124.68
33	Z	102	LHG	O8-C23-C24	3.03	121.41	111.91
25	B	605	CLA	O2A-C1-C2	3.03	116.59	108.64
25	c	507	CLA	C1-C2-C3	-3.03	120.81	126.04
25	B	616	CLA	CMB-C2B-C3B	3.03	130.34	124.68
27	a	409	BCR	C19-C18-C17	3.03	123.58	118.94
25	b	612	CLA	C3C-C4C-NC	3.02	113.96	110.57
33	z	102	LHG	O8-C23-C24	3.02	121.38	111.91
27	b	618	BCR	C36-C18-C17	-3.02	118.70	122.92
27	A	409	BCR	C19-C18-C17	3.02	123.57	118.94
28	B	620	SQD	C44-O6-C1	3.01	119.62	113.74
25	b	602	CLA	CMB-C2B-C3B	3.01	130.31	124.68
27	B	618	BCR	C36-C18-C17	-3.01	118.71	122.92
25	B	602	CLA	CMB-C2B-C3B	3.01	130.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	103	LMT	C1'-O5'-C5'	-3.00	107.80	113.69
28	T	101	SQD	C44-O6-C1	3.00	119.60	113.74
31	f	103	LMT	C1'-O5'-C5'	-3.00	107.81	113.69
25	b	615	CLA	CMB-C2B-C3B	2.99	130.28	124.68
31	B	626	LMT	C1'-O5'-C5'	-2.99	107.82	113.69
29	A	415	LMG	C8-O7-C10	-2.99	110.43	117.79
31	k	104	LMT	C1'-O5'-C5'	-2.99	107.82	113.69
27	z	101	BCR	C34-C9-C10	-2.98	118.74	122.92
28	F	101	SQD	O6-C1-C2	2.98	112.96	108.30
29	a	415	LMG	C8-O7-C10	-2.98	110.45	117.79
28	f	101	SQD	O6-C1-C2	2.98	112.96	108.30
25	A	405	CLA	CAC-C3C-C4C	2.98	128.68	124.81
28	H	102	SQD	C4-C3-C2	2.98	116.02	110.82
25	b	601	CLA	CMC-C2C-C1C	2.98	129.58	125.04
31	K	104	LMT	C1'-O5'-C5'	-2.98	107.84	113.69
28	h	102	SQD	C4-C3-C2	2.98	116.02	110.82
27	Z	101	BCR	C34-C9-C10	-2.98	118.75	122.92
31	b	625	LMT	C1'-O5'-C5'	-2.97	107.85	113.69
25	a	405	CLA	CAC-C3C-C4C	2.97	128.67	124.81
25	B	601	CLA	CMC-C2C-C1C	2.97	129.57	125.04
25	D	403	CLA	C1-C2-C3	-2.97	120.90	126.04
25	B	615	CLA	CMB-C2B-C3B	2.97	130.24	124.68
25	d	403	CLA	C1-C2-C3	-2.97	120.91	126.04
27	d	405	BCR	C7-C8-C9	-2.96	121.76	126.23
30	a	412	PL9	C7-C8-C9	-2.96	121.86	126.79
25	B	604	CLA	C3C-C4C-NC	2.96	113.89	110.57
28	f	101	SQD	O8-S-C6	2.96	110.45	105.74
25	B	615	CLA	C1-O2A-CGA	2.96	124.21	116.44
28	F	101	SQD	O8-S-C6	2.96	110.45	105.74
30	A	412	PL9	C7-C8-C9	-2.95	121.87	126.79
30	A	412	PL9	C40-C39-C41	2.95	120.24	115.27
25	C	512	CLA	CMB-C2B-C3B	2.95	130.20	124.68
25	c	511	CLA	C4-C3-C5	2.95	120.23	115.27
25	B	611	CLA	CMB-C2B-C3B	2.95	130.19	124.68
25	A	408	CLA	C4-C3-C5	2.94	120.22	115.27
25	C	511	CLA	C4-C3-C5	2.94	120.22	115.27
30	a	412	PL9	C40-C39-C41	2.94	120.22	115.27
25	b	611	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	b	615	CLA	C1-O2A-CGA	2.94	124.16	116.44
25	a	408	CLA	C4-C3-C5	2.94	120.22	115.27
25	C	512	CLA	C3C-C4C-NC	2.94	113.87	110.57
25	b	602	CLA	C1-C2-C3	-2.94	120.96	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	CMB-C2B-C3B	2.94	130.17	124.68
25	b	615	CLA	C1-C2-C3	-2.94	120.97	126.04
31	a	417	LMT	C3'-C4'-C5'	-2.94	105.00	110.24
31	A	417	LMT	C3'-C4'-C5'	-2.93	105.00	110.24
25	b	608	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	D	405	BCR	C7-C8-C9	-2.93	121.81	126.23
25	b	608	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
34	c	516	DGD	C2G-O2G-C1B	-2.93	110.59	117.79
28	a	413	SQD	C1-C2-C3	2.93	116.09	110.00
25	b	604	CLA	C3C-C4C-NC	2.92	113.85	110.57
28	A	413	SQD	C1-C2-C3	2.92	116.09	110.00
25	b	605	CLA	C3D-C4D-ND	2.92	114.96	110.24
25	B	602	CLA	C1-C2-C3	-2.92	120.99	126.04
27	z	101	BCR	C36-C18-C17	-2.92	118.84	122.92
25	c	512	CLA	C3C-C4C-NC	2.92	113.84	110.57
25	B	605	CLA	C3D-C4D-ND	2.92	114.96	110.24
25	B	615	CLA	C1-C2-C3	-2.92	121.00	126.04
25	d	404	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	Z	101	BCR	C36-C18-C17	-2.91	118.84	122.92
28	T	101	SQD	C1-O5-C5	2.91	119.41	113.69
25	c	509	CLA	C1-C2-C3	-2.91	121.01	126.04
25	C	507	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	c	507	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	C	511	CLA	C3C-C4C-NC	2.90	113.83	110.57
25	C	513	CLA	CMC-C2C-C1C	2.90	129.46	125.04
25	b	605	CLA	O2A-CGA-CBA	2.90	121.02	111.91
25	b	610	CLA	C3D-C4D-ND	2.90	114.93	110.24
25	a	405	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
25	D	404	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	B	618	BCR	C37-C22-C21	-2.90	118.86	122.92
25	B	608	CLA	C3D-C4D-ND	2.90	114.93	110.24
34	C	516	DGD	C2G-O2G-C1B	-2.90	110.65	117.79
25	A	405	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
25	B	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	c	513	CLA	CMC-C2C-C1C	2.90	129.45	125.04
25	B	605	CLA	O2A-CGA-CBA	2.90	121.00	111.91
25	c	511	CLA	C3C-C4C-NC	2.90	113.82	110.57
32	A	418	BCT	O3-C-O1	-2.89	112.04	119.55
28	B	620	SQD	C1-O5-C5	2.89	119.37	113.69
25	B	614	CLA	C4-C3-C5	2.89	120.14	115.27
25	B	610	CLA	C3D-C4D-ND	2.89	114.91	110.24
25	c	503	CLA	CMC-C2C-C1C	2.89	129.44	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	618	BCR	C37-C22-C21	-2.89	118.88	122.92
25	b	614	CLA	C4-C3-C5	2.88	120.12	115.27
25	B	613	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	a	405	CLA	CAA-C2A-C1A	-2.88	102.55	111.97
25	C	509	CLA	C1-C2-C3	-2.87	121.07	126.04
25	C	503	CLA	CMC-C2C-C1C	2.87	129.42	125.04
32	a	418	BCT	O3-C-O1	-2.87	112.09	119.55
25	A	405	CLA	CAA-C2A-C1A	-2.87	102.57	111.97
25	b	613	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	C	509	CLA	C4-C3-C5	2.87	120.09	115.27
25	c	509	CLA	C4-C3-C5	2.87	120.09	115.27
25	d	401	CLA	C3D-C4D-ND	2.86	114.87	110.24
31	M	102	LMT	O5B-C5B-C4B	2.86	114.90	109.69
25	A	408	CLA	CMC-C2C-C1C	2.86	129.40	125.04
25	B	610	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	B	606	CLA	C4-C3-C5	2.86	120.08	115.27
25	C	509	CLA	CMC-C2C-C1C	2.86	129.39	125.04
25	b	606	CLA	C4-C3-C5	2.86	120.07	115.27
29	A	411	LMG	O8-C28-C29	2.85	120.86	111.91
25	a	408	CLA	CMC-C2C-C1C	2.85	129.38	125.04
25	a	405	CLA	C4D-C3D-CAD	2.85	111.46	108.10
31	m	102	LMT	O5B-C5B-C4B	2.85	114.87	109.69
25	b	610	CLA	CMB-C2B-C3B	2.85	130.01	124.68
28	k	101	SQD	O6-C1-C2	2.85	112.75	108.30
29	a	411	LMG	O8-C28-C29	2.85	120.85	111.91
25	C	505	CLA	O2A-CGA-CBA	2.84	120.83	111.91
28	K	101	SQD	O6-C1-C2	2.84	112.74	108.30
25	A	406	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
25	b	615	CLA	C3C-C4C-NC	2.84	113.75	110.57
25	c	505	CLA	O2A-CGA-CBA	2.84	120.81	111.91
25	a	406	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
33	D	408	LHG	C5-O7-C7	-2.83	110.81	117.79
25	b	612	CLA	C4-C3-C5	2.83	120.04	115.27
25	d	403	CLA	C3D-C4D-ND	2.83	114.82	110.24
25	A	405	CLA	C4D-C3D-CAD	2.83	111.43	108.10
25	D	403	CLA	C3D-C4D-ND	2.83	114.82	110.24
25	a	408	CLA	C3D-C4D-ND	2.83	114.82	110.24
26	a	407	PHO	CMB-C2B-C3B	2.83	129.97	124.68
25	A	408	CLA	C3D-C4D-ND	2.83	114.81	110.24
25	C	504	CLA	C1-O2A-CGA	2.83	123.86	116.44
25	A	408	CLA	CMA-C3A-C4A	2.83	119.37	111.77
25	c	504	CLA	C3D-C4D-ND	2.83	114.81	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	CMC-C2C-C1C	2.82	129.34	125.04
25	a	405	CLA	C3D-C4D-ND	2.82	114.81	110.24
25	B	612	CLA	C4-C3-C5	2.82	120.02	115.27
25	b	613	CLA	C4-C3-C5	2.82	120.02	115.27
25	a	408	CLA	CMA-C3A-C4A	2.82	119.36	111.77
25	B	615	CLA	C3C-C4C-NC	2.82	113.73	110.57
25	D	401	CLA	C3D-C4D-ND	2.82	114.80	110.24
25	C	504	CLA	C3D-C4D-ND	2.82	114.80	110.24
33	d	408	LHG	C5-O7-C7	-2.82	110.86	117.79
25	c	504	CLA	C1-O2A-CGA	2.82	123.83	116.44
27	D	405	BCR	C38-C26-C27	2.81	119.02	113.62
26	A	407	PHO	CMB-C2B-C3B	2.81	129.94	124.68
25	C	502	CLA	C3D-C4D-ND	2.81	114.79	110.24
25	B	610	CLA	CMA-C3A-C4A	2.81	119.33	111.77
25	b	610	CLA	CMA-C3A-C4A	2.81	119.32	111.77
25	A	405	CLA	C3D-C4D-ND	2.81	114.78	110.24
31	a	417	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
25	b	616	CLA	C4-C3-C5	2.81	119.99	115.27
31	A	417	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
25	B	612	CLA	C3D-C4D-ND	2.80	114.77	110.24
25	c	502	CLA	C3D-C4D-ND	2.80	114.77	110.24
25	B	616	CLA	C4-C3-C5	2.80	119.98	115.27
25	B	614	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	B	613	CLA	C4-C3-C5	2.80	119.98	115.27
27	d	405	BCR	C38-C26-C27	2.80	118.99	113.62
25	b	614	CLA	C3C-C4C-NC	2.80	113.71	110.57
25	d	403	CLA	C3C-C4C-NC	2.79	113.70	110.57
25	c	501	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	a	408	CLA	C1-C2-C3	-2.79	121.22	126.04
25	C	501	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
25	b	614	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	A	408	CLA	C1-C2-C3	-2.78	121.23	126.04
25	B	610	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
25	b	612	CLA	C3D-C4D-ND	2.78	114.73	110.24
25	b	609	CLA	CMC-C2C-C1C	2.78	129.27	125.04
25	C	503	CLA	C4-C3-C5	2.77	119.94	115.27
25	b	610	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
25	D	403	CLA	CMB-C2B-C3B	2.77	129.86	124.68
33	Z	102	LHG	C5-O7-C7	-2.77	110.97	117.79
37	X	102	RRX	C12-C13-C14	2.77	123.19	118.94
25	b	602	CLA	C3D-C4D-ND	2.77	114.72	110.24
25	B	614	CLA	C3C-C4C-NC	2.76	113.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	C3C-C4C-NC	2.76	113.67	110.57
25	C	511	CLA	CMC-C2C-C1C	2.76	129.24	125.04
25	b	608	CLA	C3C-C4C-NC	2.76	113.67	110.57
25	B	609	CLA	CMC-C2C-C1C	2.76	129.24	125.04
25	c	503	CLA	C4-C3-C5	2.76	119.91	115.27
25	C	501	CLA	CMC-C2C-C1C	2.76	129.24	125.04
25	d	403	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	B	616	CLA	C3D-C4D-ND	2.76	114.70	110.24
25	B	610	CLA	C4-C3-C5	2.76	119.91	115.27
27	K	102	BCR	C34-C9-C10	-2.76	119.06	122.92
25	C	505	CLA	C3D-C4D-ND	2.76	114.70	110.24
33	z	102	LHG	C5-O7-C7	-2.76	111.01	117.79
25	c	511	CLA	CMC-C2C-C1C	2.75	129.23	125.04
25	c	505	CLA	C3D-C4D-ND	2.75	114.69	110.24
25	c	501	CLA	CMC-C2C-C1C	2.75	129.23	125.04
25	c	501	CLA	C4-C3-C5	2.75	119.90	115.27
25	B	608	CLA	C3C-C4C-NC	2.75	113.66	110.57
25	b	610	CLA	C4-C3-C5	2.75	119.90	115.27
25	d	404	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	b	613	CLA	CMC-C2C-C1C	2.75	129.22	125.04
25	A	406	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
31	b	622	LMT	O5'-C5'-C4'	2.75	114.68	109.69
25	b	616	CLA	C3D-C4D-ND	2.75	114.68	110.24
37	x	102	RRX	C12-C13-C14	2.75	123.15	118.94
25	B	613	CLA	CMC-C2C-C1C	2.75	129.22	125.04
27	B	619	BCR	C36-C18-C17	-2.74	119.08	122.92
28	T	101	SQD	O47-C7-C8	2.74	117.42	111.50
27	B	617	BCR	C29-C30-C25	2.74	114.70	110.48
27	b	617	BCR	C29-C30-C25	2.74	114.70	110.48
27	k	102	BCR	C34-C9-C10	-2.74	119.08	122.92
25	b	609	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	b	619	BCR	C36-C18-C17	-2.74	119.08	122.92
30	d	406	PL9	C22-C23-C24	-2.74	121.06	127.66
30	D	406	PL9	C22-C23-C24	-2.74	121.06	127.66
31	X	101	LMT	C1'-O5'-C5'	-2.74	108.31	113.69
25	B	602	CLA	C3D-C4D-ND	2.74	114.67	110.24
31	D	410	LMT	O5'-C5'-C4'	2.74	114.67	109.69
28	B	620	SQD	O47-C7-C8	2.74	117.40	111.50
25	D	404	CLA	CMB-C2B-C3B	2.74	129.80	124.68
25	B	609	CLA	C3D-C4D-ND	2.74	114.66	110.24
28	h	102	SQD	O8-S-C6	2.74	110.10	105.74
25	a	406	CLA	O2D-CGD-O1D	-2.74	118.49	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	412	LMT	O5'-C5'-C6'	2.73	113.23	106.44
25	b	608	CLA	CMC-C2C-C1C	2.73	129.20	125.04
25	C	508	CLA	C3D-C4D-ND	2.73	114.66	110.24
25	c	508	CLA	C3D-C4D-ND	2.73	114.66	110.24
27	d	405	BCR	C33-C5-C6	-2.73	121.46	124.53
25	C	508	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
27	C	522	BCR	C37-C22-C21	-2.73	119.10	122.92
31	d	412	LMT	O5'-C5'-C6'	2.73	113.23	106.44
25	d	401	CLA	C4-C3-C5	2.73	119.86	115.27
25	b	610	CLA	C3C-C4C-NC	2.73	113.63	110.57
25	c	508	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
31	x	101	LMT	C1'-O5'-C5'	-2.73	108.33	113.69
31	b	624	LMT	C1'-O5'-C5'	-2.73	108.34	113.69
25	C	509	CLA	C3C-C4C-NC	2.72	113.63	110.57
27	k	102	BCR	C33-C5-C4	2.72	118.85	113.62
25	B	608	CLA	CMC-C2C-C1C	2.72	129.19	125.04
25	c	512	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
25	B	610	CLA	C3C-C4C-NC	2.72	113.62	110.57
25	C	505	CLA	C3C-C4C-NC	2.72	113.62	110.57
31	B	625	LMT	C1'-O5'-C5'	-2.72	108.34	113.69
34	C	516	DGD	O1G-C1A-C2A	2.72	120.45	111.91
25	c	505	CLA	C3C-C4C-NC	2.72	113.62	110.57
31	d	410	LMT	O5'-C5'-C4'	2.72	114.64	109.69
33	l	101	LHG	O8-C23-C24	2.72	120.44	111.91
25	C	501	CLA	C4-C3-C5	2.72	119.84	115.27
31	i	104	LMT	C1'-O5'-C5'	-2.72	108.35	113.69
25	B	604	CLA	C6-C5-C3	-2.72	106.33	113.45
27	c	522	BCR	C37-C22-C21	-2.72	119.11	122.92
25	B	603	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	B	623	LMT	O5'-C5'-C4'	2.72	114.63	109.69
33	L	101	LHG	O8-C23-C24	2.71	120.42	111.91
25	C	503	CLA	C3C-C4C-NC	2.71	113.61	110.57
25	b	604	CLA	C6-C5-C3	-2.71	106.34	113.45
31	I	104	LMT	C1'-O5'-C5'	-2.71	108.36	113.69
25	B	601	CLA	CMA-C3A-C4A	2.71	119.06	111.77
25	C	512	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
34	c	516	DGD	O1G-C1A-C2A	2.71	120.41	111.91
27	K	102	BCR	C33-C5-C4	2.71	118.82	113.62
25	c	509	CLA	C3C-C4C-NC	2.71	113.61	110.57
25	b	603	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
25	b	601	CLA	C3D-C4D-ND	2.71	114.62	110.24
28	K	101	SQD	O5-C5-C4	2.71	114.38	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	102	SQD	O8-S-C6	2.70	110.05	105.74
25	D	401	CLA	C4-C3-C5	2.70	119.82	115.27
25	B	606	CLA	C3D-C4D-ND	2.70	114.61	110.24
28	k	101	SQD	O5-C5-C4	2.70	114.37	109.52
27	B	618	BCR	C19-C18-C17	2.70	123.08	118.94
25	c	503	CLA	C3C-C4C-NC	2.70	113.60	110.57
27	k	102	BCR	C30-C25-C26	-2.70	118.81	122.61
25	b	602	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	A	407	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
25	c	511	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
25	b	601	CLA	CMA-C3A-C4A	2.70	119.02	111.77
25	b	606	CLA	C3D-C4D-ND	2.69	114.60	110.24
27	D	405	BCR	C37-C22-C21	-2.69	119.15	122.92
26	a	407	PHO	O2D-CGD-O1D	-2.69	118.57	123.84
28	A	410	SQD	O8-S-C6	2.69	110.03	105.74
35	V	201	HEM	C4D-ND-C1D	2.69	107.85	105.07
27	K	102	BCR	C30-C25-C26	-2.69	118.82	122.61
25	C	511	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	B	602	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	b	618	BCR	C19-C18-C17	2.69	123.07	118.94
27	D	405	BCR	C33-C5-C6	-2.69	121.51	124.53
28	F	101	SQD	O48-C23-C24	2.69	120.34	111.91
25	c	505	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
28	f	101	SQD	O48-C23-C24	2.68	120.32	111.91
27	c	514	BCR	C33-C5-C4	2.68	118.77	113.62
27	C	514	BCR	C33-C5-C4	2.68	118.76	113.62
25	B	610	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	b	611	CLA	C3D-C4D-ND	2.68	114.57	110.24
25	b	610	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	B	601	CLA	C3D-C4D-ND	2.68	114.57	110.24
28	a	410	SQD	O8-S-C6	2.68	110.00	105.74
33	B	622	LHG	C5-O7-C7	-2.68	111.20	117.79
25	C	508	CLA	C4-C3-C5	2.68	119.77	115.27
33	b	621	LHG	C5-O7-C7	-2.67	111.21	117.79
27	c	514	BCR	C36-C18-C17	-2.67	119.18	122.92
25	C	505	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	C	514	BCR	C36-C18-C17	-2.67	119.18	122.92
25	B	611	CLA	C3D-C4D-ND	2.67	114.56	110.24
25	c	508	CLA	C1-C2-C3	-2.67	121.43	126.04
25	C	502	CLA	C3C-C4C-NC	2.67	113.56	110.57
25	c	508	CLA	C4-C3-C5	2.67	119.76	115.27
27	d	405	BCR	C37-C22-C21	-2.67	119.19	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C4D-C3D-CAD	2.67	111.24	108.10
31	x	103	LMT	C3'-C4'-C5'	-2.67	104.81	110.93
25	C	511	CLA	C3D-C4D-ND	2.66	114.55	110.24
25	c	502	CLA	C3C-C4C-NC	2.66	113.56	110.57
25	c	511	CLA	C3D-C4D-ND	2.66	114.54	110.24
25	c	510	CLA	C3D-C4D-ND	2.66	114.54	110.24
35	v	201	HEM	C4D-ND-C1D	2.66	107.82	105.07
34	C	517	DGD	O1G-C1A-C2A	2.66	120.25	111.91
25	C	512	CLA	CMC-C2C-C1C	2.66	129.09	125.04
31	X	103	LMT	C3'-C4'-C5'	-2.66	104.83	110.93
34	c	517	DGD	O1G-C1A-C2A	2.66	120.25	111.91
25	b	615	CLA	C3D-C4D-ND	2.65	114.53	110.24
25	C	507	CLA	C3C-C4C-NC	2.65	113.55	110.57
25	C	510	CLA	C3D-C4D-ND	2.65	114.53	110.24
25	c	513	CLA	C4-C3-C5	2.65	119.73	115.27
25	C	508	CLA	C1-C2-C3	-2.65	121.46	126.04
25	C	513	CLA	C4-C3-C5	2.65	119.73	115.27
25	c	507	CLA	CMB-C2B-C3B	2.65	129.63	124.68
25	C	507	CLA	CMB-C2B-C3B	2.65	129.63	124.68
25	c	507	CLA	CMA-C3A-C4A	2.65	118.89	111.77
27	K	102	BCR	C38-C26-C27	2.65	118.70	113.62
31	y	101	LMT	C1'-O5'-C5'	-2.65	108.49	113.69
25	B	608	CLA	C4-C3-C5	2.65	119.72	115.27
25	C	507	CLA	CMA-C3A-C4A	2.65	118.88	111.77
27	c	514	BCR	C37-C22-C21	-2.64	119.22	122.92
31	D	411	LMT	C1'-O5'-C5'	-2.64	108.50	113.69
31	Y	101	LMT	C1'-O5'-C5'	-2.64	108.50	113.69
29	b	620	LMG	O8-C28-C29	2.64	120.20	111.91
25	B	615	CLA	C3D-C4D-ND	2.64	114.51	110.24
25	b	611	CLA	CMC-C2C-C1C	2.64	129.06	125.04
31	d	411	LMT	C1'-O5'-C5'	-2.64	108.51	113.69
29	B	621	LMG	O8-C28-C29	2.64	120.19	111.91
25	B	601	CLA	C4D-C3D-CAD	2.64	111.20	108.10
27	k	102	BCR	C38-C26-C27	2.64	118.68	113.62
34	H	103	DGD	O1G-C1A-C2A	2.64	120.18	111.91
25	b	608	CLA	C4-C3-C5	2.63	119.70	115.27
25	C	506	CLA	CMC-C2C-C1C	2.63	129.05	125.04
25	d	404	CLA	CMC-C2C-C1C	2.63	129.05	125.04
35	V	201	HEM	C1B-NB-C4B	2.63	107.79	105.07
25	c	507	CLA	C3C-C4C-NC	2.63	113.52	110.57
34	h	103	DGD	O1G-C1A-C2A	2.63	120.17	111.91
25	c	506	CLA	C4-C3-C5	2.63	119.70	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	615	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
35	V	201	HEM	C4B-CHC-C1C	2.63	126.03	122.56
25	B	607	CLA	C3C-C4C-NC	2.63	113.52	110.57
30	d	406	PL9	C40-C39-C41	2.63	119.69	115.27
25	d	404	CLA	C4-C3-C5	2.63	119.69	115.27
30	D	406	PL9	C40-C39-C41	2.63	119.69	115.27
30	d	406	PL9	O1-C4-C3	-2.63	117.83	120.72
25	C	506	CLA	C4-C3-C5	2.63	119.69	115.27
27	C	514	BCR	C37-C22-C21	-2.62	119.25	122.92
25	c	513	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
25	b	608	CLA	C4D-C3D-CAD	2.62	111.19	108.10
25	C	507	CLA	C1-O2A-CGA	2.62	123.33	116.44
25	D	404	CLA	C4-C3-C5	2.62	119.68	115.27
25	B	608	CLA	CMA-C3A-C4A	2.62	118.82	111.77
35	v	201	HEM	C4B-CHC-C1C	2.62	126.02	122.56
35	v	201	HEM	C1B-NB-C4B	2.62	107.78	105.07
25	c	507	CLA	C1-O2A-CGA	2.62	123.32	116.44
25	b	608	CLA	CMA-C3A-C4A	2.62	118.81	111.77
25	B	611	CLA	CMC-C2C-C1C	2.62	129.03	125.04
25	c	512	CLA	CMC-C2C-C1C	2.62	129.02	125.04
25	b	607	CLA	C3C-C4C-NC	2.62	113.50	110.57
30	D	406	PL9	O1-C4-C3	-2.62	117.84	120.72
25	c	506	CLA	C3D-C4D-ND	2.61	114.47	110.24
25	B	608	CLA	C4D-C3D-CAD	2.61	111.18	108.10
27	b	619	BCR	C35-C13-C12	2.61	122.19	118.08
25	D	404	CLA	CMC-C2C-C1C	2.61	129.02	125.04
25	C	506	CLA	C3D-C4D-ND	2.61	114.46	110.24
27	B	617	BCR	C28-C27-C26	-2.61	109.42	114.08
25	B	616	CLA	C3C-C4C-NC	2.61	113.50	110.57
27	b	617	BCR	C28-C27-C26	-2.61	109.42	114.08
27	B	619	BCR	C35-C13-C12	2.61	122.19	118.08
25	b	607	CLA	C3D-C4D-ND	2.61	114.46	110.24
25	c	506	CLA	CMC-C2C-C1C	2.61	129.01	125.04
25	c	510	CLA	CMC-C2C-C1C	2.60	129.00	125.04
31	T	102	LMT	C3'-C4'-C5'	-2.60	105.60	110.24
25	C	513	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	b	615	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	a	408	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	t	701	LMT	C3'-C4'-C5'	-2.60	105.61	110.24
25	B	605	CLA	C3C-C4C-NC	2.60	113.48	110.57
25	A	408	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	B	613	CLA	C3C-C4C-NC	2.59	113.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
25	C	501	CLA	C3D-C4D-ND	2.59	114.43	110.24
25	b	614	CLA	C3D-C4D-ND	2.59	114.43	110.24
31	C	519	LMT	C3'-C4'-C5'	-2.59	104.98	110.93
31	c	519	LMT	C3'-C4'-C5'	-2.59	104.98	110.93
25	B	614	CLA	C3D-C4D-ND	2.59	114.43	110.24
25	d	404	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
25	C	510	CLA	CMC-C2C-C1C	2.59	128.98	125.04
25	C	505	CLA	C1-O2A-CGA	2.59	123.24	116.44
25	C	513	CLA	C3D-C4D-ND	2.59	114.42	110.24
25	b	605	CLA	C3C-C4C-NC	2.58	113.47	110.57
25	B	607	CLA	C3D-C4D-ND	2.58	114.42	110.24
33	D	408	LHG	O8-C23-C24	2.58	120.01	111.91
35	f	102	HEM	CBA-CAA-C2A	-2.58	108.22	112.62
27	K	102	BCR	C37-C22-C21	-2.58	119.31	122.92
25	c	513	CLA	C3D-C4D-ND	2.58	114.41	110.24
25	b	616	CLA	C3C-C4C-NC	2.58	113.46	110.57
25	B	601	CLA	C3C-C4C-NC	2.58	113.46	110.57
25	B	614	CLA	C1-O2A-CGA	2.58	123.21	116.44
25	c	505	CLA	C1-O2A-CGA	2.58	123.21	116.44
28	H	102	SQD	O48-C23-C24	2.58	119.99	111.91
33	d	408	LHG	O8-C23-C24	2.57	119.98	111.91
27	k	102	BCR	C37-C22-C21	-2.57	119.32	122.92
25	b	614	CLA	C1-O2A-CGA	2.57	123.20	116.44
25	B	616	CLA	CAC-C3C-C4C	2.57	128.15	124.81
25	B	603	CLA	C4D-C3D-CAD	2.57	111.13	108.10
31	i	103	LMT	C3'-C4'-C5'	-2.57	105.03	110.93
25	c	501	CLA	C3D-C4D-ND	2.57	114.39	110.24
25	C	504	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
28	h	102	SQD	O48-C23-C24	2.57	119.97	111.91
25	C	507	CLA	C4-C3-C5	2.57	119.59	115.27
31	I	103	LMT	C3'-C4'-C5'	-2.57	105.04	110.93
25	d	401	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
29	c	523	LMG	O8-C28-C29	2.56	119.96	111.91
25	b	603	CLA	C4D-C3D-CAD	2.56	111.12	108.10
31	i	104	LMT	C3'-C4'-C5'	-2.56	105.67	110.24
29	C	523	LMG	O8-C28-C29	2.56	119.95	111.91
25	A	406	CLA	CMC-C2C-C1C	2.56	128.94	125.04
25	b	613	CLA	C3C-C4C-NC	2.56	113.44	110.57
25	c	504	CLA	CMC-C2C-C1C	2.56	128.94	125.04
25	D	401	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
35	F	102	HEM	CBA-CAA-C2A	-2.56	108.25	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C3C-C4C-NC	2.56	113.44	110.57
31	I	104	LMT	C3'-C4'-C5'	-2.55	105.68	110.24
26	a	407	PHO	O1D-CGD-CBD	2.55	128.99	124.74
25	c	509	CLA	C3D-C4D-ND	2.55	114.37	110.24
27	B	617	BCR	C38-C26-C25	-2.55	121.66	124.53
25	a	406	CLA	CMC-C2C-C1C	2.55	128.92	125.04
30	d	406	PL9	C27-C28-C29	-2.55	121.52	127.66
25	C	504	CLA	CMC-C2C-C1C	2.55	128.92	125.04
25	c	507	CLA	C4-C3-C5	2.55	119.56	115.27
25	b	601	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
25	b	616	CLA	CAC-C3C-C4C	2.55	128.12	124.81
25	c	504	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	z	101	BCR	C37-C22-C21	-2.55	119.36	122.92
27	b	617	BCR	C38-C26-C25	-2.55	121.67	124.53
25	B	601	CLA	CMD-C2D-C3D	-2.55	121.76	127.61
25	B	602	CLA	C4-C3-C5	2.54	119.55	115.27
30	d	406	PL9	C7-C8-C9	-2.54	122.56	126.79
25	b	602	CLA	C4-C3-C5	2.54	119.55	115.27
25	D	403	CLA	C4D-C3D-CAD	2.54	111.09	108.10
26	A	407	PHO	O1D-CGD-CBD	2.54	128.97	124.74
25	C	509	CLA	C3D-C4D-ND	2.54	114.35	110.24
25	b	612	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
30	a	412	PL9	C27-C28-C29	-2.54	121.55	127.66
33	b	621	LHG	O8-C23-C24	2.54	119.87	111.91
31	M	103	LMT	C1'-O5'-C5'	-2.54	108.71	113.69
31	H	101	LMT	C3'-C4'-C5'	-2.54	105.71	110.24
30	D	406	PL9	C7-C8-C9	-2.54	122.57	126.79
30	A	412	PL9	C27-C28-C29	-2.54	121.56	127.66
27	b	619	BCR	C37-C22-C21	-2.53	119.37	122.92
33	B	622	LHG	O8-C23-C24	2.53	119.85	111.91
27	Z	101	BCR	C37-C22-C21	-2.53	119.38	122.92
25	B	604	CLA	C4-C3-C5	2.53	119.52	115.27
31	m	103	LMT	C1'-O5'-C5'	-2.53	108.73	113.69
25	B	612	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
25	d	403	CLA	C4D-C3D-CAD	2.52	111.07	108.10
31	h	101	LMT	C3'-C4'-C5'	-2.52	105.74	110.24
31	I	102	LMT	C1'-O5'-C5'	-2.52	108.73	113.69
25	b	613	CLA	C3D-C4D-ND	2.52	114.32	110.24
25	c	512	CLA	C3D-C4D-ND	2.52	114.32	110.24
25	B	613	CLA	C3D-C4D-ND	2.52	114.31	110.24
25	b	615	CLA	C4-C3-C5	2.52	119.51	115.27
31	c	524	LMT	C1'-C2'-C3'	2.52	115.25	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	PL9	C36-C34-C33	-2.52	116.02	121.12
25	b	604	CLA	C4-C3-C5	2.52	119.51	115.27
25	B	615	CLA	C4-C3-C5	2.52	119.51	115.27
30	D	406	PL9	C27-C28-C29	-2.52	121.59	127.66
31	C	524	LMT	C1'-C2'-C3'	2.52	115.24	110.00
30	A	412	PL9	C36-C34-C33	-2.52	116.02	121.12
31	i	102	LMT	C1'-O5'-C5'	-2.52	108.75	113.69
25	C	513	CLA	C3C-C4C-NC	2.52	113.39	110.57
25	B	607	CLA	C4-C3-C5	2.51	119.50	115.27
25	b	607	CLA	C4-C3-C5	2.51	119.50	115.27
29	A	415	LMG	O8-C28-C29	2.51	119.78	111.91
25	b	611	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
25	C	512	CLA	C3D-C4D-ND	2.51	114.29	110.24
28	B	620	SQD	O6-C1-C2	2.51	112.22	108.30
28	T	101	SQD	O6-C1-C2	2.51	112.22	108.30
25	c	510	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
27	c	522	BCR	C15-C14-C13	-2.50	123.74	127.31
25	B	611	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
29	a	415	LMG	O8-C28-C29	2.50	119.75	111.91
25	C	504	CLA	CAC-C3C-C4C	2.50	128.05	124.81
27	Z	101	BCR	C19-C18-C17	2.50	122.77	118.94
27	B	619	BCR	C37-C22-C21	-2.50	119.42	122.92
25	c	503	CLA	C6-C5-C3	-2.50	106.91	113.45
25	C	510	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	C	503	CLA	C6-C5-C3	-2.50	106.91	113.45
31	C	520	LMT	C1'-O5'-C5'	-2.50	108.79	113.69
27	z	101	BCR	C19-C18-C17	2.50	122.77	118.94
33	d	407	LHG	O8-C23-C24	2.49	119.74	111.91
28	a	414	SQD	O8-S-C6	2.49	109.72	105.74
31	A	417	LMT	C4'-C3'-C2'	2.49	115.18	110.82
25	c	513	CLA	C3C-C4C-NC	2.49	113.37	110.57
25	c	504	CLA	CAC-C3C-C4C	2.49	128.04	124.81
33	D	407	LHG	O8-C23-C24	2.49	119.73	111.91
25	c	505	CLA	CMC-C2C-C1C	2.49	128.83	125.04
31	a	417	LMT	C4'-C3'-C2'	2.49	115.17	110.82
30	d	406	PL9	C20-C19-C21	2.49	119.45	115.27
31	c	520	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
31	A	416	LMT	C1'-C2'-C3'	2.49	115.17	110.00
28	A	414	SQD	O8-S-C6	2.49	109.70	105.74
25	C	505	CLA	CMC-C2C-C1C	2.48	128.82	125.04
25	C	508	CLA	C3C-C4C-NC	2.48	113.35	110.57
31	b	623	LMT	C1'-O5'-C5'	-2.48	108.82	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	406	PL9	C20-C19-C21	2.48	119.44	115.27
27	b	619	BCR	C32-C1-C6	-2.48	106.28	110.30
25	B	609	CLA	C3C-C4C-NC	2.48	113.35	110.57
26	D	402	PHO	CMC-C2C-C3C	2.48	129.61	124.94
25	c	508	CLA	CMA-C3A-C4A	2.47	118.42	111.77
25	C	508	CLA	CMA-C3A-C4A	2.47	118.42	111.77
26	d	402	PHO	CMC-C2C-C3C	2.47	129.60	124.94
27	C	522	BCR	C15-C14-C13	-2.47	123.78	127.31
31	a	416	LMT	C1'-C2'-C3'	2.47	115.14	110.00
28	A	414	SQD	O47-C7-C8	2.47	116.82	111.50
25	b	603	CLA	CMC-C2C-C1C	2.47	128.80	125.04
27	B	619	BCR	C32-C1-C6	-2.47	106.30	110.30
31	M	103	LMT	C3'-C4'-C5'	-2.47	105.84	110.24
27	b	619	BCR	C34-C9-C10	-2.47	119.47	122.92
25	b	609	CLA	C3C-C4C-NC	2.46	113.33	110.57
25	a	406	CLA	CMA-C3A-C4A	2.46	118.39	111.77
31	B	624	LMT	C1'-O5'-C5'	-2.46	108.85	113.69
25	A	406	CLA	CMA-C3A-C4A	2.46	118.39	111.77
25	a	405	CLA	CAA-CBA-CGA	-2.46	106.06	113.25
28	K	101	SQD	C44-O6-C1	2.46	118.55	113.74
28	a	414	SQD	O47-C7-C8	2.46	116.80	111.50
28	H	102	SQD	C1-C2-C3	2.46	115.12	110.00
27	B	619	BCR	C34-C9-C10	-2.46	119.48	122.92
25	B	615	CLA	CMA-C3A-C4A	2.46	118.38	111.77
28	k	101	SQD	C44-O6-C1	2.46	118.54	113.74
28	h	102	SQD	C1-C2-C3	2.46	115.11	110.00
25	D	401	CLA	CMA-C3A-C4A	2.46	118.38	111.77
25	A	405	CLA	CAA-CBA-CGA	-2.46	106.08	113.25
25	a	406	CLA	C4-C3-C5	2.45	119.40	115.27
25	c	508	CLA	C3C-C4C-NC	2.45	113.32	110.57
25	b	615	CLA	CMA-C3A-C4A	2.45	118.36	111.77
25	c	509	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
25	B	611	CLA	CAC-C3C-C4C	2.45	127.99	124.81
25	A	406	CLA	C4-C3-C5	2.45	119.39	115.27
25	d	401	CLA	CMA-C3A-C4A	2.45	118.36	111.77
31	m	103	LMT	C3'-C4'-C5'	-2.45	105.87	110.24
25	B	603	CLA	CMC-C2C-C1C	2.45	128.77	125.04
31	d	411	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
27	c	514	BCR	C35-C13-C12	2.45	121.93	118.08
25	C	509	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
31	j	101	LMT	O5'-C5'-C6'	2.44	112.51	106.44
25	B	604	CLA	C4D-C3D-CAD	2.44	110.97	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	411	LMT	C3'-C4'-C5'	-2.44	105.33	110.93
27	C	522	BCR	C34-C9-C10	-2.44	119.51	122.92
25	c	506	CLA	CAC-C3C-C4C	2.44	127.97	124.81
28	H	102	SQD	O5-C1-C2	2.44	115.51	110.35
25	B	601	CLA	CMB-C2B-C3B	2.44	129.24	124.68
27	c	522	BCR	C34-C9-C10	-2.44	119.51	122.92
31	J	101	LMT	O5'-C5'-C6'	2.43	112.48	106.44
27	b	617	BCR	C8-C7-C6	-2.43	120.37	127.20
25	C	506	CLA	CAC-C3C-C4C	2.43	127.96	124.81
25	B	606	CLA	CMC-C2C-C1C	2.43	128.74	125.04
27	d	405	BCR	C34-C9-C10	-2.43	119.52	122.92
27	C	514	BCR	C35-C13-C12	2.43	121.90	118.08
28	K	101	SQD	C6-C5-C4	-2.43	108.59	113.07
25	C	502	CLA	CMA-C3A-C4A	2.43	118.29	111.77
28	h	102	SQD	O5-C1-C2	2.42	115.48	110.35
25	b	616	CLA	C1-C2-C3	-2.42	121.85	126.04
25	b	601	CLA	CMB-C2B-C3B	2.42	129.21	124.68
25	b	606	CLA	CMC-C2C-C1C	2.42	128.73	125.04
25	B	607	CLA	CAA-C2A-C1A	-2.42	104.04	111.97
27	D	405	BCR	C34-C9-C10	-2.42	119.53	122.92
25	b	604	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
25	C	506	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
27	B	617	BCR	C8-C7-C6	-2.42	120.41	127.20
25	B	604	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
25	B	602	CLA	C3C-C4C-NC	2.42	113.28	110.57
25	b	607	CLA	CAA-C2A-C1A	-2.42	104.06	111.97
25	c	506	CLA	C3C-C4C-NC	2.41	113.28	110.57
25	c	506	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
25	b	611	CLA	CAC-C3C-C4C	2.41	127.94	124.81
25	b	604	CLA	C4D-C3D-CAD	2.41	110.94	108.10
25	C	505	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
25	c	502	CLA	CMA-C3A-C4A	2.41	118.25	111.77
25	c	505	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
28	k	101	SQD	C6-C5-C4	-2.41	108.62	113.07
25	B	609	CLA	CED-O2D-CGD	2.41	121.38	115.94
25	C	510	CLA	C4-C3-C5	2.41	119.32	115.27
34	C	517	DGD	C2G-O2G-C1B	-2.41	111.86	117.79
25	b	610	CLA	CMC-C2C-C1C	2.41	128.70	125.04
35	F	102	HEM	C4C-CHD-C1D	2.40	125.73	122.56
25	b	615	CLA	C4D-C3D-CAD	2.40	110.92	108.10
25	c	510	CLA	C4-C3-C5	2.40	119.31	115.27
37	x	102	RRX	C23-C22-C21	2.40	122.62	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	C1-C2-C3	-2.40	121.90	126.04
34	c	517	DGD	C2G-O2G-C1B	-2.40	111.89	117.79
25	b	602	CLA	CAA-CBA-CGA	-2.40	106.25	113.25
25	C	508	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
25	a	405	CLA	CED-O2D-CGD	2.39	121.35	115.94
25	b	609	CLA	CED-O2D-CGD	2.39	121.35	115.94
28	a	414	SQD	O48-C23-C24	2.39	119.42	111.91
25	B	602	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
28	A	414	SQD	O48-C23-C24	2.39	119.41	111.91
25	B	610	CLA	CMC-C2C-C1C	2.39	128.68	125.04
25	b	602	CLA	C3C-C4C-NC	2.39	113.25	110.57
25	A	405	CLA	CED-O2D-CGD	2.39	121.34	115.94
37	X	102	RRX	C23-C22-C21	2.39	122.60	118.94
25	C	513	CLA	CMA-C3A-C4A	2.38	118.18	111.77
25	c	508	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
33	E	102	LHG	O8-C23-C24	2.38	119.38	111.91
27	C	522	BCR	C33-C5-C4	2.38	118.19	113.62
25	b	603	CLA	CMA-C3A-C4A	2.38	118.16	111.77
25	c	510	CLA	C4D-C3D-CAD	2.38	110.90	108.10
35	f	102	HEM	C4C-CHD-C1D	2.37	125.69	122.56
25	B	603	CLA	CMA-C3A-C4A	2.37	118.15	111.77
27	K	102	BCR	C27-C26-C25	-2.37	119.29	122.73
25	C	510	CLA	C4D-C3D-CAD	2.37	110.89	108.10
33	e	102	LHG	O8-C23-C24	2.37	119.34	111.91
25	C	510	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
25	b	610	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
25	c	513	CLA	CMA-C3A-C4A	2.37	118.13	111.77
35	V	201	HEM	CBA-CAA-C2A	-2.36	108.59	112.62
27	B	617	BCR	C33-C5-C4	2.36	118.16	113.62
25	C	506	CLA	C3C-C4C-NC	2.36	113.22	110.57
27	c	522	BCR	C33-C5-C4	2.36	118.15	113.62
25	c	510	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
27	b	617	BCR	C33-C5-C4	2.36	118.15	113.62
25	B	610	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
27	c	522	BCR	C28-C27-C26	-2.36	109.86	114.08
30	a	412	PL9	C22-C23-C24	-2.36	121.98	127.66
31	c	519	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
25	D	404	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
27	d	405	BCR	C3-C4-C5	-2.36	109.87	114.08
30	A	412	PL9	C22-C23-C24	-2.35	121.99	127.66
25	B	615	CLA	C4D-C3D-CAD	2.35	110.87	108.10
31	C	519	LMT	C1'-O5'-C5'	-2.35	109.07	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	BCR	C3-C4-C5	-2.35	109.88	114.08
27	k	102	BCR	C27-C26-C25	-2.35	119.32	122.73
35	v	201	HEM	CBA-CAA-C2A	-2.35	108.61	112.62
25	d	404	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
25	B	610	CLA	CAC-C3C-C4C	2.35	127.86	124.81
27	K	102	BCR	C2-C1-C6	2.35	114.09	110.48
35	V	201	HEM	CMC-C2C-C3C	2.34	129.06	124.68
25	b	604	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
27	C	522	BCR	C28-C27-C26	-2.34	109.90	114.08
25	b	606	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
27	Z	101	BCR	C38-C26-C27	2.34	118.11	113.62
25	B	604	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
25	B	604	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
25	b	606	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
25	C	501	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
25	b	604	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
29	B	621	LMG	O7-C10-O9	-2.33	118.07	123.70
31	e	103	LMT	O5B-C5B-C4B	2.33	113.93	109.69
28	a	414	SQD	O5-C1-C2	2.33	115.28	110.35
25	b	616	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
35	v	201	HEM	CMC-C2C-C3C	2.33	129.04	124.68
25	B	604	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
25	B	606	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	b	610	CLA	CAC-C3C-C4C	2.33	127.83	124.81
31	J	101	LMT	O5'-C5'-C4'	2.33	113.93	109.69
25	b	612	CLA	C4D-C3D-CAD	2.33	110.84	108.10
27	k	102	BCR	C2-C1-C6	2.33	114.07	110.48
29	b	620	LMG	O7-C10-O9	-2.33	118.08	123.70
25	b	604	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
25	B	606	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
27	z	101	BCR	C38-C26-C27	2.32	118.08	113.62
25	C	512	CLA	C5-C3-C4	2.32	119.73	114.60
25	c	512	CLA	C5-C3-C4	2.32	119.73	114.60
25	A	405	CLA	C3C-C4C-NC	2.32	113.18	110.57
30	a	412	PL9	O2-C1-C6	2.32	124.61	120.59
31	j	101	LMT	O5'-C5'-C4'	2.32	113.91	109.69
25	D	401	CLA	CHC-C1C-C2C	-2.32	120.30	126.72
28	A	414	SQD	O5-C1-C2	2.32	115.26	110.35
25	B	607	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
25	b	607	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
25	d	401	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
25	B	616	CLA	O2D-CGD-O1D	-2.32	119.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	412	PL9	O2-C1-C6	2.32	124.60	120.59
25	C	512	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
25	B	605	CLA	C1-C2-C3	-2.32	122.04	126.04
31	E	103	LMT	O5B-C5B-C4B	2.31	113.90	109.69
25	B	603	CLA	C3D-C4D-ND	2.31	113.98	110.24
25	C	510	CLA	C3C-C4C-NC	2.31	113.16	110.57
25	c	510	CLA	C3C-C4C-NC	2.31	113.16	110.57
25	c	501	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
25	b	604	CLA	CMB-C2B-C3B	2.31	129.00	124.68
25	D	403	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
25	B	611	CLA	C3C-C4C-NC	2.30	113.16	110.57
25	B	602	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
25	b	605	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	a	412	PL9	C32-C33-C34	-2.30	122.12	127.66
25	a	405	CLA	C3C-C4C-NC	2.30	113.15	110.57
25	d	404	CLA	C4D-C3D-CAD	2.30	110.80	108.10
25	A	406	CLA	CAC-C3C-C4C	2.30	127.79	124.81
25	c	507	CLA	C3D-C4D-ND	2.30	113.95	110.24
25	c	512	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
30	A	412	PL9	C32-C33-C34	-2.30	122.13	127.66
25	B	606	CLA	C6-C5-C3	-2.30	107.44	113.45
28	A	414	SQD	C44-O6-C1	2.30	118.22	113.74
25	B	604	CLA	CMB-C2B-C3B	2.30	128.97	124.68
25	C	507	CLA	C3D-C4D-ND	2.29	113.95	110.24
25	B	605	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
25	B	612	CLA	C4D-C3D-CAD	2.29	110.80	108.10
25	C	501	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
25	b	606	CLA	C6-C5-C3	-2.29	107.44	113.45
25	b	603	CLA	C3D-C4D-ND	2.29	113.94	110.24
26	A	407	PHO	CMC-C2C-C3C	2.29	129.26	124.94
25	D	404	CLA	C3C-C4C-NC	2.29	113.14	110.57
25	a	406	CLA	CAC-C3C-C4C	2.29	127.78	124.81
27	K	102	BCR	C36-C18-C17	-2.29	119.72	122.92
25	c	501	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
25	b	605	CLA	C1-C2-C3	-2.29	122.08	126.04
25	b	613	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
25	b	602	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
31	H	101	LMT	C1'-O5'-C5'	-2.28	109.20	113.69
25	c	503	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
31	h	101	LMT	C1'-O5'-C5'	-2.28	109.21	113.69
25	d	403	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
31	d	412	LMT	C1-O1'-C1'	2.28	117.62	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
26	d	402	PHO	C1-C2-C3	-2.28	122.10	126.04
25	C	507	CLA	C4D-C3D-CAD	2.28	110.78	108.10
28	a	414	SQD	C44-O6-C1	2.28	118.19	113.74
31	D	412	LMT	C1-O1'-C1'	2.28	117.61	113.84
25	c	506	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
25	d	404	CLA	C3C-C4C-NC	2.27	113.12	110.57
31	D	410	LMT	O1'-C1'-C2'	2.27	111.85	108.30
25	D	404	CLA	C4D-C3D-CAD	2.27	110.77	108.10
25	B	613	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	C	506	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
25	b	602	CLA	C4D-C3D-CAD	2.27	110.77	108.10
25	b	614	CLA	C4D-C3D-CAD	2.27	110.77	108.10
26	a	407	PHO	CMC-C2C-C3C	2.27	129.22	124.94
25	c	501	CLA	CMA-C3A-C4A	2.27	117.86	111.77
25	c	513	CLA	C4D-C3D-CAD	2.27	110.77	108.10
25	b	606	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
25	c	507	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
25	b	611	CLA	C3C-C4C-NC	2.26	113.11	110.57
25	B	614	CLA	C4D-C3D-CAD	2.26	110.76	108.10
30	D	406	PL9	C12-C13-C14	-2.26	122.21	127.66
28	T	101	SQD	O48-C23-C24	2.26	119.01	111.91
25	C	505	CLA	C6-C5-C3	-2.26	107.52	113.45
25	c	505	CLA	C6-C5-C3	-2.26	107.53	113.45
25	C	507	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
29	c	518	LMG	C8-O7-C10	-2.26	112.22	117.79
25	C	501	CLA	CMA-C3A-C4A	2.26	117.85	111.77
29	C	518	LMG	C8-O7-C10	-2.26	112.23	117.79
31	d	410	LMT	O1'-C1'-C2'	2.26	111.83	108.30
25	C	513	CLA	CAC-C3C-C4C	2.26	127.74	124.81
26	D	402	PHO	C1-C2-C3	-2.26	122.14	126.04
33	E	102	LHG	C5-O7-C7	-2.26	112.23	117.79
25	C	503	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
27	b	618	BCR	C34-C9-C10	-2.26	119.76	122.92
27	k	102	BCR	C36-C18-C17	-2.26	119.76	122.92
27	c	514	BCR	C38-C26-C27	2.26	117.95	113.62
25	B	602	CLA	C4D-C3D-CAD	2.26	110.75	108.10
27	B	618	BCR	C34-C9-C10	-2.26	119.76	122.92
27	Z	101	BCR	C3-C4-C5	-2.25	110.05	114.08
27	z	101	BCR	C3-C4-C5	-2.25	110.05	114.08
25	C	508	CLA	CMC-C2C-C1C	2.25	128.47	125.04
25	C	503	CLA	O2D-CGD-O1D	-2.25	119.43	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C3D-C4D-ND	2.25	113.88	110.24
25	c	504	CLA	C4D-C3D-CAD	2.25	110.75	108.10
27	k	102	BCR	C38-C26-C25	-2.25	122.00	124.53
27	a	409	BCR	C15-C14-C13	-2.25	124.10	127.31
28	B	620	SQD	O48-C23-C24	2.25	118.97	111.91
25	C	502	CLA	CAC-C3C-C4C	2.25	127.73	124.81
25	C	513	CLA	C4D-C3D-CAD	2.25	110.75	108.10
25	c	507	CLA	C4D-C3D-CAD	2.25	110.75	108.10
25	b	607	CLA	C4D-C3D-CAD	2.25	110.75	108.10
33	e	102	LHG	C5-O7-C7	-2.25	112.26	117.79
34	H	103	DGD	C2G-O2G-C1B	-2.25	112.26	117.79
27	A	409	BCR	C15-C14-C13	-2.25	124.11	127.31
27	C	514	BCR	C38-C26-C27	2.24	117.93	113.62
25	c	503	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
35	V	201	HEM	C3B-C2B-C1B	2.24	108.15	106.49
25	B	604	CLA	C3D-C4D-ND	2.24	113.87	110.24
27	K	102	BCR	C38-C26-C25	-2.24	122.01	124.53
25	B	611	CLA	C4-C3-C5	2.24	119.04	115.27
25	B	607	CLA	CMA-C3A-C4A	2.24	117.80	111.77
25	c	513	CLA	CAC-C3C-C4C	2.24	127.72	124.81
27	c	522	BCR	C31-C1-C6	-2.24	106.66	110.30
25	b	607	CLA	CMA-C3A-C4A	2.24	117.80	111.77
25	B	616	CLA	C4C-C3C-C2C	-2.24	103.63	106.90
27	C	522	BCR	C31-C1-C6	-2.24	106.67	110.30
25	C	503	CLA	C3D-C4D-ND	2.24	113.86	110.24
25	c	503	CLA	C3D-C4D-ND	2.24	113.86	110.24
35	v	201	HEM	C3B-C2B-C1B	2.23	108.14	106.49
30	a	412	PL9	C42-C43-C44	-2.23	122.28	127.66
25	B	607	CLA	C4D-C3D-CAD	2.23	110.73	108.10
34	h	103	DGD	C2G-O2G-C1B	-2.23	112.30	117.79
25	b	611	CLA	C4-C3-C5	2.23	119.02	115.27
25	c	509	CLA	C4D-C3D-CAD	2.23	110.72	108.10
30	d	406	PL9	C12-C13-C14	-2.23	122.30	127.66
25	B	608	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
29	D	409	LMG	C8-O7-C10	-2.22	112.32	117.79
25	C	509	CLA	C4D-C3D-CAD	2.22	110.72	108.10
30	A	412	PL9	C42-C43-C44	-2.22	122.31	127.66
25	c	512	CLA	CMA-C3A-C4A	2.22	117.75	111.77
25	C	512	CLA	CMA-C3A-C4A	2.22	117.74	111.77
25	b	616	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
25	c	502	CLA	CAC-C3C-C4C	2.22	127.69	124.81
25	b	609	CLA	O2D-CGD-O1D	-2.22	119.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	i	101	LMT	C1'-O5'-C5'	-2.22	109.34	113.69
25	b	605	CLA	CAA-C2A-C3A	-2.21	106.71	112.78
25	c	508	CLA	CMC-C2C-C1C	2.21	128.41	125.04
25	b	608	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
33	Z	102	LHG	O4-P-O5	2.21	119.34	110.68
25	C	504	CLA	C4D-C3D-CAD	2.21	110.70	108.10
25	B	609	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
33	z	102	LHG	O4-P-O5	2.21	119.33	110.68
31	I	101	LMT	C1'-O5'-C5'	-2.21	109.35	113.69
25	B	605	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
29	C	523	LMG	C8-O7-C10	-2.21	112.36	117.79
34	c	515	DGD	O1G-C1A-C2A	2.21	118.83	111.91
25	b	605	CLA	C1-O2A-CGA	2.21	122.23	116.44
25	b	606	CLA	C1-O2A-CGA	2.21	122.23	116.44
29	d	409	LMG	C8-O7-C10	-2.21	112.36	117.79
25	b	602	CLA	CMC-C2C-C1C	2.21	128.40	125.04
29	c	523	LMG	C8-O7-C10	-2.20	112.36	117.79
25	B	606	CLA	C1-O2A-CGA	2.20	122.23	116.44
25	B	616	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
25	b	606	CLA	C4D-C3D-CAD	2.20	110.69	108.10
33	a	419	LHG	O8-C23-C24	2.20	118.82	111.91
25	B	605	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
28	h	102	SQD	C1-O5-C5	2.20	118.00	113.69
25	B	606	CLA	C4D-C3D-CAD	2.20	110.69	108.10
28	H	102	SQD	C1-O5-C5	2.20	118.00	113.69
25	b	616	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
25	B	605	CLA	C1-O2A-CGA	2.20	122.21	116.44
27	C	514	BCR	C23-C24-C25	-2.20	121.04	127.20
25	B	615	CLA	CED-O2D-CGD	2.19	120.90	115.94
25	B	615	CLA	CAC-C3C-C4C	2.19	127.66	124.81
25	B	602	CLA	CMC-C2C-C1C	2.19	128.38	125.04
33	A	419	LHG	O8-C23-C24	2.19	118.79	111.91
28	a	413	SQD	O48-C23-O10	-2.19	118.06	123.59
27	C	522	BCR	C35-C13-C12	2.19	121.53	118.08
31	A	416	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
31	a	416	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
25	b	605	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
25	b	609	CLA	C4D-C3D-CAD	2.19	110.68	108.10
34	C	515	DGD	O1G-C1A-C2A	2.19	118.78	111.91
25	b	615	CLA	CED-O2D-CGD	2.19	120.89	115.94
33	D	407	LHG	C5-O7-C7	-2.19	112.40	117.79
25	C	506	CLA	O2D-CGD-O1D	-2.19	119.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
25	b	615	CLA	CAC-C3C-C4C	2.18	127.64	124.81
29	D	409	LMG	O8-C28-C29	2.18	118.76	111.91
30	d	406	PL9	C31-C32-C33	-2.18	104.70	111.88
27	b	617	BCR	C35-C13-C12	2.18	121.52	118.08
25	d	403	CLA	CAA-C2A-C1A	-2.18	104.82	111.97
25	C	504	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
33	d	407	LHG	C5-O7-C7	-2.18	112.42	117.79
29	d	409	LMG	O8-C28-C29	2.18	118.75	111.91
30	D	406	PL9	C31-C32-C33	-2.18	104.72	111.88
28	A	413	SQD	O48-C23-O10	-2.18	118.09	123.59
27	B	617	BCR	C35-C13-C12	2.18	121.51	118.08
27	c	522	BCR	C35-C13-C12	2.18	121.51	118.08
25	b	607	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
30	a	412	PL9	O2-C1-C2	-2.18	116.80	121.78
31	B	623	LMT	O5'-C5'-C6'	2.18	111.84	106.44
25	B	607	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
25	A	405	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
25	c	513	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
27	K	102	BCR	C19-C18-C17	2.17	122.28	118.94
27	c	514	BCR	C23-C24-C25	-2.17	121.10	127.20
25	B	609	CLA	C4D-C3D-CAD	2.17	110.66	108.10
31	j	101	LMT	O1'-C1'-C2'	2.17	111.69	108.30
25	B	606	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
30	A	412	PL9	O2-C1-C2	-2.17	116.80	121.78
25	C	507	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
25	c	507	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
31	b	622	LMT	O5'-C5'-C6'	2.17	111.83	106.44
25	D	401	CLA	C1-O2A-CGA	2.17	122.13	116.44
25	a	408	CLA	CAC-C3C-C4C	2.17	127.62	124.81
25	C	513	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
25	a	405	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
25	C	501	CLA	C4D-C3D-CAD	2.17	110.65	108.10
25	c	501	CLA	C4D-C3D-CAD	2.17	110.65	108.10
30	D	406	PL9	O2-C1-C6	2.17	124.34	120.59
25	c	504	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
27	d	405	BCR	C35-C13-C12	2.17	121.49	118.08
31	B	626	LMT	C3'-C4'-C5'	-2.17	106.38	110.24
25	c	506	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
31	D	410	LMT	C4'-C3'-C2'	-2.16	107.05	110.82
27	B	619	BCR	C33-C5-C4	2.16	117.77	113.62
25	b	606	CLA	CAA-C2A-C3A	-2.16	106.85	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	C1-O2A-CGA	2.16	122.12	116.44
30	d	406	PL9	O2-C1-C6	2.16	124.33	120.59
30	d	406	PL9	C32-C33-C34	-2.16	122.47	127.66
28	H	102	SQD	O5-C5-C4	2.16	113.61	109.69
25	B	613	CLA	C4D-C3D-CAD	2.16	110.64	108.10
28	h	102	SQD	O5-C5-C4	2.16	113.61	109.69
27	b	619	BCR	C33-C5-C4	2.15	117.75	113.62
30	D	406	PL9	C32-C33-C34	-2.15	122.48	127.66
25	b	613	CLA	C4D-C3D-CAD	2.15	110.63	108.10
25	d	401	CLA	C3C-C4C-NC	2.15	112.98	110.57
25	C	504	CLA	C4-C3-C5	2.15	118.89	115.27
31	b	625	LMT	C3'-C4'-C5'	-2.15	106.41	110.24
25	B	606	CLA	C3C-C4C-NC	2.15	112.98	110.57
31	d	410	LMT	C4'-C3'-C2'	-2.15	107.07	110.82
27	k	102	BCR	C19-C18-C17	2.15	122.23	118.94
27	D	405	BCR	C35-C13-C12	2.15	121.46	118.08
34	C	515	DGD	C2G-O2G-C1B	-2.14	112.51	117.79
25	A	408	CLA	CAC-C3C-C4C	2.14	127.59	124.81
25	b	606	CLA	C3C-C4C-NC	2.14	112.97	110.57
35	F	102	HEM	C1B-NB-C4B	2.14	107.28	105.07
31	e	103	LMT	O5'-C1'-C2'	2.14	114.88	110.35
31	J	101	LMT	O1'-C1'-C2'	2.14	111.64	108.30
25	B	611	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
34	c	515	DGD	C2G-O2G-C1B	-2.14	112.53	117.79
25	b	613	CLA	CED-O2D-CGD	2.14	120.77	115.94
30	a	412	PL9	C20-C19-C21	2.14	118.86	115.27
25	c	504	CLA	C4-C3-C5	2.14	118.86	115.27
25	b	611	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
28	T	101	SQD	O48-C23-O10	-2.13	118.21	123.59
30	D	406	PL9	C35-C34-C36	2.13	118.86	115.27
27	c	514	BCR	C19-C18-C17	2.13	122.21	118.94
30	A	412	PL9	C20-C19-C21	2.13	118.85	115.27
25	D	401	CLA	C3C-C4C-NC	2.13	112.96	110.57
30	d	406	PL9	C35-C34-C36	2.13	118.85	115.27
35	f	102	HEM	C1B-NB-C4B	2.13	107.27	105.07
28	B	620	SQD	O48-C23-O10	-2.12	118.23	123.59
25	B	613	CLA	CED-O2D-CGD	2.12	120.74	115.94
28	K	101	SQD	C1-O5-C5	2.12	117.32	113.67
25	B	606	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
25	C	505	CLA	CMB-C2B-C3B	2.12	128.64	124.68
25	A	408	CLA	C3C-C4C-NC	2.12	112.94	110.57
27	C	514	BCR	C19-C18-C17	2.11	122.19	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	CLA	C3C-C4C-NC	2.11	112.94	110.57
25	a	405	CLA	C4-C3-C5	2.11	118.82	115.27
31	E	103	LMT	O5'-C1'-C2'	2.11	114.81	110.35
27	c	522	BCR	C23-C22-C21	2.11	122.18	118.94
25	b	606	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
28	k	101	SQD	C1-O5-C5	2.11	117.29	113.67
27	C	522	BCR	C23-C22-C21	2.11	122.18	118.94
25	A	405	CLA	C4-C3-C5	2.11	118.82	115.27
25	b	603	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
31	a	416	LMT	C1B-O5B-C5B	2.11	117.82	113.69
25	B	602	CLA	C6-C5-C3	-2.11	107.93	113.45
25	B	603	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
25	c	505	CLA	CMB-C2B-C3B	2.10	128.61	124.68
25	C	503	CLA	CAC-C3C-C4C	2.10	127.54	124.81
25	b	602	CLA	C6-C5-C3	-2.10	107.94	113.45
35	f	102	HEM	C3D-C4D-ND	-2.10	107.83	110.17
29	A	411	LMG	O7-C10-O9	-2.10	118.63	123.70
25	b	607	CLA	CMC-C2C-C1C	2.10	128.24	125.04
31	A	416	LMT	C1B-O5B-C5B	2.10	117.81	113.69
33	z	102	LHG	O7-C7-O9	-2.10	118.64	123.70
25	d	404	CLA	CMA-C3A-C4A	2.10	117.41	111.77
25	c	502	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
35	v	201	HEM	CHC-C4B-NB	2.09	126.71	124.43
28	A	413	SQD	C1-O5-C5	2.09	117.79	113.69
35	F	102	HEM	C3D-C4D-ND	-2.09	107.84	110.17
25	B	607	CLA	CMC-C2C-C1C	2.09	128.22	125.04
29	a	411	LMG	O7-C10-O9	-2.09	118.65	123.70
28	a	413	SQD	C1-O5-C5	2.09	117.79	113.69
33	Z	102	LHG	O7-C7-O9	-2.09	118.66	123.70
25	b	605	CLA	CED-O2D-CGD	2.09	120.66	115.94
25	C	502	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
25	c	503	CLA	CAC-C3C-C4C	2.08	127.51	124.81
25	B	605	CLA	CED-O2D-CGD	2.08	120.65	115.94
25	B	609	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
25	b	609	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
25	D	404	CLA	CMA-C3A-C4A	2.08	117.36	111.77
35	V	201	HEM	CHC-C4B-NB	2.08	126.69	124.43
25	C	506	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
25	C	502	CLA	CMC-C2C-C1C	2.08	128.20	125.04
31	x	103	LMT	C1'-O5'-C5'	-2.07	109.62	113.69
25	c	506	CLA	CMA-C3A-C4A	2.07	117.33	111.77
25	c	506	CLA	CHC-C1C-C2C	-2.07	121.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	CAC-C3C-C4C	2.07	127.49	124.81
25	d	401	CLA	CAC-C3C-C4C	2.07	127.49	124.81
25	C	505	CLA	C5-C3-C2	-2.07	116.94	121.12
25	c	502	CLA	CMC-C2C-C1C	2.07	128.19	125.04
27	C	522	BCR	C38-C26-C27	2.07	117.58	113.62
30	a	412	PL9	C41-C39-C38	-2.06	116.94	121.12
31	K	104	LMT	C3'-C4'-C5'	-2.06	106.19	110.93
25	c	505	CLA	C5-C3-C2	-2.06	116.94	121.12
25	c	507	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
30	A	412	PL9	O1-C4-C3	-2.06	118.45	120.72
25	B	616	CLA	C4D-C3D-CAD	2.06	110.52	108.10
25	B	616	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
30	A	412	PL9	C41-C39-C38	-2.06	116.95	121.12
25	C	506	CLA	CMA-C3A-C4A	2.06	117.30	111.77
30	a	412	PL9	O1-C4-C3	-2.06	118.45	120.72
25	b	605	CLA	C4D-C3D-CAD	2.06	110.52	108.10
25	d	401	CLA	CMC-C2C-C3C	2.06	131.70	126.12
27	c	522	BCR	C38-C26-C27	2.05	117.56	113.62
30	d	406	PL9	O2-C1-C2	-2.05	117.08	121.78
25	A	406	CLA	C4D-C3D-CAD	2.05	110.52	108.10
31	k	104	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
25	C	502	CLA	C4-C3-C5	2.05	118.72	115.27
25	b	616	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
25	B	606	CLA	CED-O2D-CGD	2.05	120.58	115.94
35	V	201	HEM	C3D-C4D-ND	-2.05	107.88	110.17
25	B	610	CLA	C4D-C3D-CAD	2.05	110.51	108.10
25	C	507	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
25	C	509	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
25	D	401	CLA	CAC-C3C-C4C	2.05	127.47	124.81
28	K	101	SQD	C4-C3-C2	2.05	114.40	110.82
33	Z	102	LHG	O8-C23-O10	-2.05	118.43	123.59
25	c	502	CLA	C4-C3-C5	2.05	118.71	115.27
25	b	610	CLA	C4D-C3D-CAD	2.05	110.51	108.10
25	C	511	CLA	CAC-C3C-C4C	2.05	127.47	124.81
25	b	616	CLA	C4D-C3D-CAD	2.05	110.51	108.10
31	X	103	LMT	C1'-O5'-C5'	-2.04	109.67	113.69
27	C	514	BCR	C31-C1-C6	-2.04	106.98	110.30
25	a	406	CLA	C4D-C3D-CAD	2.04	110.50	108.10
25	B	611	CLA	C4D-C3D-CAD	2.04	110.50	108.10
33	z	102	LHG	O8-C23-O10	-2.04	118.44	123.59
30	D	406	PL9	O2-C1-C2	-2.04	117.11	121.78
25	b	606	CLA	CED-O2D-CGD	2.04	120.55	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401	CLA	C3B-C4B-NB	2.04	111.84	109.21
25	C	508	CLA	CED-O2D-CGD	2.04	120.55	115.94
33	L	101	LHG	C5-O7-C7	-2.04	112.78	117.79
25	c	509	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
25	c	508	CLA	CED-O2D-CGD	2.04	120.54	115.94
25	D	401	CLA	CMC-C2C-C3C	2.03	131.64	126.12
25	c	501	CLA	CAC-C3C-C4C	2.03	127.45	124.81
25	B	605	CLA	C4D-C3D-CAD	2.03	110.49	108.10
35	f	102	HEM	C2D-C1D-ND	-2.03	107.45	109.88
25	D	401	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
33	l	101	LHG	C5-O7-C7	-2.03	112.80	117.79
25	B	612	CLA	CHD-C4C-C3C	-2.03	121.86	124.84
25	c	501	CLA	C1-O2A-CGA	2.03	121.77	116.44
25	C	510	CLA	CED-O2D-CGD	2.03	120.52	115.94
27	b	617	BCR	C7-C8-C9	-2.03	123.17	126.23
31	m	101	LMT	C3'-C4'-C5'	-2.03	106.28	110.93
28	a	414	SQD	O47-C7-O49	-2.03	118.80	123.70
25	B	607	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
25	B	609	CLA	C4-C3-C5	2.03	118.68	115.27
25	b	609	CLA	C4-C3-C5	2.03	118.68	115.27
28	A	414	SQD	O47-C7-O49	-2.03	118.81	123.70
25	b	607	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
25	a	405	CLA	CMA-C3A-C4A	2.02	117.21	111.77
25	A	408	CLA	C1-O2A-CGA	2.02	121.75	116.44
35	v	201	HEM	C3D-C4D-ND	-2.02	107.91	110.17
25	a	408	CLA	C1-O2A-CGA	2.02	121.75	116.44
25	C	504	CLA	CED-O2D-CGD	2.02	120.51	115.94
25	A	405	CLA	CHD-C4C-C3C	-2.02	121.87	124.84
25	d	401	CLA	CED-O2D-CGD	2.02	120.51	115.94
25	b	604	CLA	C6-C7-C8	-2.02	109.38	115.92
25	b	612	CLA	CHD-C4C-C3C	-2.02	121.87	124.84
34	C	516	DGD	O2G-C1B-O1B	-2.02	118.82	123.70
27	c	514	BCR	C31-C1-C6	-2.02	107.02	110.30
25	d	401	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
29	C	518	LMG	O8-C28-O10	-2.02	118.49	123.59
25	c	504	CLA	CED-O2D-CGD	2.02	120.51	115.94
31	M	101	LMT	C3'-C4'-C5'	-2.02	106.30	110.93
25	B	604	CLA	C6-C7-C8	-2.02	109.39	115.92
25	C	501	CLA	C1-O2A-CGA	2.02	121.74	116.44
25	b	611	CLA	C4D-C3D-CAD	2.02	110.47	108.10
25	A	405	CLA	CMA-C3A-C4A	2.02	117.19	111.77
29	c	518	LMG	O8-C28-O10	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	CED-O2D-CGD	2.02	120.50	115.94
34	c	516	DGD	O2G-C1B-O1B	-2.02	118.83	123.70
25	A	406	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
28	A	410	SQD	O48-C23-C24	2.02	118.23	111.91
34	C	516	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
28	k	101	SQD	C4-C3-C2	2.02	114.34	110.82
25	D	403	CLA	CED-O2D-CGD	2.01	120.49	115.94
30	D	406	PL9	C42-C43-C44	-2.01	122.81	127.66
27	B	617	BCR	C7-C8-C9	-2.01	123.19	126.23
25	B	607	CLA	C1-O2A-CGA	2.01	121.72	116.44
25	d	401	CLA	C3B-C4B-NB	2.01	111.81	109.21
31	E	103	LMT	C3B-C4B-C5B	-2.01	106.66	110.24
25	a	406	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
25	b	616	CLA	CMA-C3A-C4A	2.01	117.17	111.77
25	C	513	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
31	e	103	LMT	C3B-C4B-C5B	-2.01	106.66	110.24
30	d	406	PL9	C42-C43-C44	-2.01	122.83	127.66
35	F	102	HEM	C2D-C1D-ND	-2.01	107.48	109.88
28	a	410	SQD	O48-C23-C24	2.01	118.20	111.91
27	B	618	BCR	C38-C26-C27	2.01	117.47	113.62
25	c	511	CLA	CAC-C3C-C4C	2.00	127.41	124.81
25	b	607	CLA	C1-O2A-CGA	2.00	121.70	116.44
25	D	401	CLA	CED-O2D-CGD	2.00	120.47	115.94
25	d	403	CLA	CED-O2D-CGD	2.00	120.47	115.94
25	c	513	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
27	z	101	BCR	C33-C5-C6	-2.00	122.28	124.53
25	d	403	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
27	Z	101	BCR	C33-C5-C6	-2.00	122.28	124.53
25	a	405	CLA	CHD-C4C-C3C	-2.00	121.90	124.84
25	C	503	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
27	b	618	BCR	C38-C26-C27	2.00	117.46	113.62
25	c	510	CLA	CHC-C1C-C2C	-2.00	121.19	126.72

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	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	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

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Mol	Chain	Res	Type	Atom
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	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	d	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND

All (2529) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	405	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	C11-C10-C8-C9
25	B	605	CLA	C2-C3-C5-C6
25	B	605	CLA	C4-C3-C5-C6
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C3A-C2A-CAA-CBA
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	C2-C1-O2A-CGA
25	C	509	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	401	CLA	CHA-CBD-CGD-O1D
25	D	401	CLA	CHA-CBD-CGD-O2D
25	D	404	CLA	C4-C3-C5-C6
25	a	405	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	604	CLA	C11-C10-C8-C9
25	b	605	CLA	C2-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C3A-C2A-CAA-CBA
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O1D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C2-C1-O2A-CGA
25	c	509	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	CBD-CGD-O2D-CED
25	d	401	CLA	CHA-CBD-CGD-O1D
25	d	401	CLA	CHA-CBD-CGD-O2D
25	d	404	CLA	C4-C3-C5-C6
27	A	409	BCR	C7-C8-C9-C10
27	A	409	BCR	C7-C8-C9-C34
27	A	409	BCR	C11-C10-C9-C8
27	A	409	BCR	C11-C10-C9-C34
27	B	617	BCR	C17-C18-C19-C20
27	B	617	BCR	C36-C18-C19-C20
27	B	618	BCR	C7-C8-C9-C10
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C10-C9-C8
27	B	618	BCR	C11-C10-C9-C34
27	B	618	BCR	C10-C11-C12-C13
27	B	618	BCR	C11-C12-C13-C14
27	B	618	BCR	C11-C12-C13-C35
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C7-C8-C9-C10
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C10-C9-C8
27	B	619	BCR	C11-C10-C9-C34
27	C	514	BCR	C23-C24-C25-C30
27	C	522	BCR	C11-C10-C9-C8
27	C	522	BCR	C11-C10-C9-C34
27	C	522	BCR	C10-C11-C12-C13
27	C	522	BCR	C17-C18-C19-C20
27	C	522	BCR	C36-C18-C19-C20
27	D	405	BCR	C11-C10-C9-C8
27	D	405	BCR	C11-C10-C9-C34
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	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
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	Z	101	BCR	C7-C8-C9-C10
27	Z	101	BCR	C7-C8-C9-C34
27	a	409	BCR	C7-C8-C9-C10
27	a	409	BCR	C7-C8-C9-C34
27	a	409	BCR	C11-C10-C9-C8
27	a	409	BCR	C11-C10-C9-C34
27	b	617	BCR	C17-C18-C19-C20
27	b	617	BCR	C36-C18-C19-C20
27	b	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C10-C11-C12-C13
27	b	618	BCR	C11-C12-C13-C14
27	b	618	BCR	C11-C12-C13-C35
27	b	619	BCR	C1-C6-C7-C8
27	b	619	BCR	C7-C8-C9-C10
27	b	619	BCR	C7-C8-C9-C34
27	b	619	BCR	C11-C10-C9-C8
27	b	619	BCR	C11-C10-C9-C34
27	c	514	BCR	C23-C24-C25-C30
27	c	522	BCR	C11-C10-C9-C8
27	c	522	BCR	C11-C10-C9-C34
27	c	522	BCR	C10-C11-C12-C13
27	c	522	BCR	C17-C18-C19-C20
27	c	522	BCR	C36-C18-C19-C20
27	d	405	BCR	C11-C10-C9-C8
27	d	405	BCR	C11-C10-C9-C34
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	C7-C8-C9-C34
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	z	101	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C34
28	A	410	SQD	C5-C6-S-O7
28	A	410	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
28	A	410	SQD	C5-C6-S-O9
28	A	413	SQD	O49-C7-O47-C45
28	A	413	SQD	C8-C7-O47-C45
28	A	413	SQD	C24-C23-O48-C46
28	A	413	SQD	C5-C6-S-O8
28	A	413	SQD	C5-C6-S-O9
28	A	414	SQD	C2-C1-O6-C44
28	B	620	SQD	O5-C5-C6-S
28	F	101	SQD	C45-C44-O6-C1
28	F	101	SQD	C2-C1-O6-C44
28	F	101	SQD	O5-C1-O6-C44
28	H	102	SQD	O6-C44-C45-O47
28	H	102	SQD	O49-C7-O47-C45
28	H	102	SQD	C8-C7-O47-C45
28	H	102	SQD	C5-C6-S-O7
28	H	102	SQD	C5-C6-S-O8
28	H	102	SQD	C5-C6-S-O9
28	K	101	SQD	O5-C1-O6-C44
28	T	101	SQD	O5-C5-C6-S
28	a	410	SQD	C5-C6-S-O7
28	a	410	SQD	C5-C6-S-O8
28	a	410	SQD	C5-C6-S-O9
28	a	413	SQD	O49-C7-O47-C45
28	a	413	SQD	C8-C7-O47-C45
28	a	413	SQD	C24-C23-O48-C46
28	a	413	SQD	C5-C6-S-O8
28	a	413	SQD	C5-C6-S-O9
28	a	414	SQD	C2-C1-O6-C44
28	f	101	SQD	C45-C44-O6-C1
28	f	101	SQD	C2-C1-O6-C44
28	f	101	SQD	O5-C1-O6-C44
28	h	102	SQD	O6-C44-C45-O47
28	h	102	SQD	O49-C7-O47-C45
28	h	102	SQD	C8-C7-O47-C45
28	h	102	SQD	C5-C6-S-O7
28	h	102	SQD	C5-C6-S-O8
28	h	102	SQD	C5-C6-S-O9
28	k	101	SQD	O5-C1-O6-C44
29	C	523	LMG	C2-C1-O1-C7
29	C	523	LMG	O6-C1-O1-C7
29	c	523	LMG	C2-C1-O1-C7
29	c	523	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
30	A	412	PL9	C17-C18-C19-C20
30	A	412	PL9	C17-C18-C19-C21
30	A	412	PL9	C22-C23-C24-C25
30	A	412	PL9	C22-C23-C24-C26
30	A	412	PL9	C24-C26-C27-C28
30	A	412	PL9	C27-C28-C29-C30
30	A	412	PL9	C34-C36-C37-C38
30	A	412	PL9	C37-C38-C39-C40
30	A	412	PL9	C37-C38-C39-C41
30	A	412	PL9	C38-C39-C41-C42
30	A	412	PL9	C39-C41-C42-C43
30	A	412	PL9	C42-C43-C44-C46
30	D	406	PL9	C42-C43-C44-C45
30	D	406	PL9	C42-C43-C44-C46
30	a	412	PL9	C17-C18-C19-C20
30	a	412	PL9	C17-C18-C19-C21
30	a	412	PL9	C22-C23-C24-C25
30	a	412	PL9	C22-C23-C24-C26
30	a	412	PL9	C24-C26-C27-C28
30	a	412	PL9	C27-C28-C29-C30
30	a	412	PL9	C34-C36-C37-C38
30	a	412	PL9	C37-C38-C39-C40
30	a	412	PL9	C37-C38-C39-C41
30	a	412	PL9	C38-C39-C41-C42
30	a	412	PL9	C39-C41-C42-C43
30	a	412	PL9	C42-C43-C44-C46
30	d	406	PL9	C42-C43-C44-C45
30	d	406	PL9	C42-C43-C44-C46
31	A	416	LMT	C2'-C1'-O1'-C1
31	A	416	LMT	C2-C1-O1'-C1'
31	A	417	LMT	C2-C1-O1'-C1'
31	B	623	LMT	C2-C1-O1'-C1'
31	B	624	LMT	O5'-C1'-O1'-C1
31	B	626	LMT	C2-C1-O1'-C1'
31	C	521	LMT	C2'-C1'-O1'-C1
31	C	521	LMT	O5'-C1'-O1'-C1
31	C	521	LMT	C2-C1-O1'-C1'
31	C	524	LMT	C2'-C1'-O1'-C1
31	C	524	LMT	O5'-C1'-O1'-C1
31	D	410	LMT	C2'-C1'-O1'-C1
31	D	410	LMT	O5'-C1'-O1'-C1
31	D	412	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	D	412	LMT	O5'-C1'-O1'-C1
31	E	101	LMT	O5'-C1'-O1'-C1
31	E	103	LMT	C2-C1-O1'-C1'
31	F	103	LMT	C2'-C1'-O1'-C1
31	F	103	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	102	LMT	C2'-C1'-O1'-C1
31	I	102	LMT	O5'-C1'-O1'-C1
31	I	102	LMT	C2-C1-O1'-C1'
31	J	101	LMT	C2-C1-O1'-C1'
31	M	101	LMT	O5'-C1'-O1'-C1
31	M	103	LMT	C2'-C1'-O1'-C1
31	M	103	LMT	O5'-C1'-O1'-C1
31	M	103	LMT	C2-C1-O1'-C1'
31	T	102	LMT	C2-C1-O1'-C1'
31	X	101	LMT	C2'-C1'-O1'-C1
31	X	101	LMT	O5'-C1'-O1'-C1
31	X	104	LMT	C2'-C1'-O1'-C1
31	X	104	LMT	O5'-C1'-O1'-C1
31	a	416	LMT	C2'-C1'-O1'-C1
31	a	416	LMT	C2-C1-O1'-C1'
31	a	417	LMT	C2-C1-O1'-C1'
31	b	622	LMT	C2-C1-O1'-C1'
31	b	623	LMT	O5'-C1'-O1'-C1
31	b	625	LMT	C2-C1-O1'-C1'
31	c	521	LMT	C2'-C1'-O1'-C1
31	c	521	LMT	O5'-C1'-O1'-C1
31	c	521	LMT	C2-C1-O1'-C1'
31	c	524	LMT	C2'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	d	410	LMT	C2'-C1'-O1'-C1
31	d	410	LMT	O5'-C1'-O1'-C1
31	d	412	LMT	C2'-C1'-O1'-C1
31	d	412	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	e	103	LMT	C2-C1-O1'-C1'
31	f	103	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
31	h	101	LMT	C2'-C1'-O1'-C1
31	h	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	i	101	LMT	C2-C1-O1'-C1'
31	i	102	LMT	C2'-C1'-O1'-C1
31	i	102	LMT	O5'-C1'-O1'-C1
31	i	102	LMT	C2-C1-O1'-C1'
31	j	101	LMT	C2-C1-O1'-C1'
31	m	101	LMT	O5'-C1'-O1'-C1
31	m	103	LMT	C2'-C1'-O1'-C1
31	m	103	LMT	O5'-C1'-O1'-C1
31	m	103	LMT	C2-C1-O1'-C1'
31	t	701	LMT	C2-C1-O1'-C1'
31	x	101	LMT	C2'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
31	x	104	LMT	C2'-C1'-O1'-C1
31	x	104	LMT	O5'-C1'-O1'-C1
33	A	419	LHG	C4-O6-P-O4
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	D	407	LHG	C1-C2-C3-O3
33	D	407	LHG	C3-O3-P-O6
33	D	408	LHG	O1-C1-C2-C3
33	E	102	LHG	O1-C1-C2-O2
33	E	102	LHG	O1-C1-C2-C3
33	E	102	LHG	C4-O6-P-O4
33	E	102	LHG	C4-O6-P-O5
33	E	102	LHG	C8-C7-O7-C5
33	L	101	LHG	C4-O6-P-O5
33	Z	102	LHG	C4-O6-P-O3
33	a	419	LHG	C4-O6-P-O4
33	b	621	LHG	O1-C1-C2-C3
33	b	621	LHG	C2-C3-O3-P
33	b	621	LHG	C3-O3-P-O5
33	d	407	LHG	C1-C2-C3-O3
33	d	407	LHG	C3-O3-P-O6
33	d	408	LHG	O1-C1-C2-C3
33	e	102	LHG	O1-C1-C2-O2
33	e	102	LHG	O1-C1-C2-C3
33	e	102	LHG	C4-O6-P-O4
33	e	102	LHG	C4-O6-P-O5
33	e	102	LHG	C8-C7-O7-C5
33	l	101	LHG	C4-O6-P-O5
33	z	102	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
34	C	515	DGD	C2A-C1A-O1G-C1G
34	c	515	DGD	C2A-C1A-O1G-C1G
37	X	102	RRX	C23-C24-C25-C26
37	x	102	RRX	C23-C24-C25-C26
31	M	102	LMT	C3'-C4'-O1B-C1B
31	m	102	LMT	C3'-C4'-O1B-C1B
25	C	509	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
28	B	620	SQD	O10-C23-O48-C46
28	H	102	SQD	O10-C23-O48-C46
28	T	101	SQD	O10-C23-O48-C46
28	h	102	SQD	O10-C23-O48-C46
29	A	411	LMG	O10-C28-O8-C9
29	a	411	LMG	O10-C28-O8-C9
34	C	515	DGD	O1A-C1A-O1G-C1G
34	c	515	DGD	O1A-C1A-O1G-C1G
31	B	625	LMT	C3'-C4'-O1B-C1B
31	b	624	LMT	C3'-C4'-O1B-C1B
25	A	405	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
28	H	102	SQD	C24-C23-O48-C46
28	h	102	SQD	C24-C23-O48-C46
29	A	411	LMG	C29-C28-O8-C9
29	a	411	LMG	C29-C28-O8-C9
25	A	408	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	a	408	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
28	A	413	SQD	O10-C23-O48-C46
28	F	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	a	413	SQD	O10-C23-O48-C46
28	f	101	SQD	O10-C23-O48-C46
29	A	415	LMG	O10-C28-O8-C9
29	C	523	LMG	O10-C28-O8-C9
29	a	415	LMG	O10-C28-O8-C9
29	c	523	LMG	O10-C28-O8-C9
25	C	509	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
25	C	513	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
31	K	104	LMT	O5B-C1B-O1B-C4'
31	k	104	LMT	O5B-C1B-O1B-C4'
25	C	510	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
28	F	101	SQD	O49-C7-O47-C45
28	f	101	SQD	O49-C7-O47-C45
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
25	D	404	CLA	C3-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
28	F	101	SQD	C24-C23-O48-C46
28	f	101	SQD	C24-C23-O48-C46
29	A	415	LMG	C29-C28-O8-C9
29	a	415	LMG	C29-C28-O8-C9
25	B	602	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
31	B	624	LMT	C4'-C5'-C6'-O6'
31	b	623	LMT	C4'-C5'-C6'-O6'
31	J	101	LMT	O5'-C5'-C6'-O6'
31	j	101	LMT	O5'-C5'-C6'-O6'
25	D	403	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
29	A	411	LMG	C17-C18-C19-C20
29	A	411	LMG	C20-C21-C22-C23
29	C	518	LMG	C17-C18-C19-C20
29	C	518	LMG	C20-C21-C22-C23
29	C	518	LMG	C38-C39-C40-C41
29	C	523	LMG	C17-C18-C19-C20
29	C	523	LMG	C38-C39-C40-C41
29	a	411	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	a	411	LMG	C20-C21-C22-C23
29	c	518	LMG	C17-C18-C19-C20
29	c	518	LMG	C20-C21-C22-C23
29	c	518	LMG	C38-C39-C40-C41
29	c	523	LMG	C17-C18-C19-C20
29	c	523	LMG	C38-C39-C40-C41
34	C	516	DGD	C8B-C9B-CAB-CBB
34	C	516	DGD	CBB-CCB-CDB-CEB
34	C	517	DGD	C8A-C9A-CAA-CBA
34	C	517	DGD	C8B-C9B-CAB-CBB
34	H	103	DGD	CBB-CCB-CDB-CEB
34	c	516	DGD	C8B-C9B-CAB-CBB
34	c	516	DGD	CBB-CCB-CDB-CEB
34	c	517	DGD	C8A-C9A-CAA-CBA
34	c	517	DGD	C8B-C9B-CAB-CBB
34	h	103	DGD	CBB-CCB-CDB-CEB
29	C	523	LMG	C29-C28-O8-C9
29	c	523	LMG	C29-C28-O8-C9
31	K	104	LMT	O5B-C5B-C6B-O6B
31	k	104	LMT	O5B-C5B-C6B-O6B
31	H	101	LMT	C4'-C5'-C6'-O6'
31	h	101	LMT	C4'-C5'-C6'-O6'
30	A	412	PL9	C12-C13-C14-C15
30	a	412	PL9	C12-C13-C14-C15
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
30	A	412	PL9	C12-C13-C14-C16
30	A	412	PL9	C27-C28-C29-C31
30	a	412	PL9	C12-C13-C14-C16
30	a	412	PL9	C27-C28-C29-C31
31	A	417	LMT	C4'-C5'-C6'-O6'
31	a	417	LMT	C4'-C5'-C6'-O6'
25	B	604	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	O1A-CGA-O2A-C1
25	b	604	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O10-C23-O8-C6
33	l	101	LHG	O10-C23-O8-C6
25	B	616	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
33	L	101	LHG	C5-C6-O8-C23
33	l	101	LHG	C5-C6-O8-C23
31	H	101	LMT	O5'-C5'-C6'-O6'
31	I	103	LMT	O5'-C5'-C6'-O6'
31	X	103	LMT	O5B-C5B-C6B-O6B
31	h	101	LMT	O5'-C5'-C6'-O6'
31	i	103	LMT	O5'-C5'-C6'-O6'
31	x	103	LMT	O5B-C5B-C6B-O6B
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
33	D	407	LHG	O2-C2-C3-O3
33	d	407	LHG	O2-C2-C3-O3
25	C	509	CLA	CBA-CGA-O2A-C1
25	D	404	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
28	B	620	SQD	C24-C23-O48-C46
28	T	101	SQD	C24-C23-O48-C46
33	L	101	LHG	C24-C23-O8-C6
33	l	101	LHG	C24-C23-O8-C6
31	C	521	LMT	O5'-C5'-C6'-O6'
31	c	521	LMT	O5'-C5'-C6'-O6'
25	B	613	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
31	E	103	LMT	O5B-C5B-C6B-O6B
31	M	102	LMT	O5'-C5'-C6'-O6'
31	M	103	LMT	O5'-C5'-C6'-O6'
31	e	103	LMT	O5B-C5B-C6B-O6B
31	m	102	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	O5'-C5'-C6'-O6'
33	B	622	LHG	C11-C10-C9-C8
33	b	621	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	B	623	LMT	O5'-C5'-C6'-O6'
31	I	101	LMT	O5'-C5'-C6'-O6'
31	b	622	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
25	B	606	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	CBA-CGA-O2A-C1
25	b	604	CLA	CBA-CGA-O2A-C1
31	B	626	LMT	O5'-C5'-C6'-O6'
31	C	520	LMT	O5'-C5'-C6'-O6'
31	b	625	LMT	O5'-C5'-C6'-O6'
31	c	520	LMT	O5'-C5'-C6'-O6'
31	E	103	LMT	C4'-C5'-C6'-O6'
31	X	103	LMT	C4B-C5B-C6B-O6B
31	e	103	LMT	C4'-C5'-C6'-O6'
31	x	103	LMT	C4B-C5B-C6B-O6B
33	D	407	LHG	C26-C27-C28-C29
33	d	407	LHG	C26-C27-C28-C29
31	A	417	LMT	O5'-C5'-C6'-O6'
31	B	624	LMT	O5'-C5'-C6'-O6'
31	D	412	LMT	O5'-C5'-C6'-O6'
31	a	417	LMT	O5'-C5'-C6'-O6'
31	b	623	LMT	O5'-C5'-C6'-O6'
31	d	412	LMT	O5'-C5'-C6'-O6'
25	B	614	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
30	A	412	PL9	C40-C39-C41-C42
30	a	412	PL9	C40-C39-C41-C42
31	A	416	LMT	C4B-C5B-C6B-O6B
31	K	104	LMT	C4B-C5B-C6B-O6B
31	a	416	LMT	C4B-C5B-C6B-O6B
31	k	104	LMT	C4B-C5B-C6B-O6B
25	B	614	CLA	C2-C3-C5-C6
25	D	404	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
25	d	404	CLA	C2-C3-C5-C6
31	C	524	LMT	O5B-C5B-C6B-O6B
31	F	103	LMT	O5'-C5'-C6'-O6'
31	K	104	LMT	O5'-C5'-C6'-O6'
31	Y	101	LMT	O5'-C5'-C6'-O6'
31	c	524	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	k	104	LMT	O5'-C5'-C6'-O6'
31	y	101	LMT	O5'-C5'-C6'-O6'
28	B	620	SQD	O5-C1-O6-C44
28	T	101	SQD	O5-C1-O6-C44
31	Y	101	LMT	O5'-C1'-O1'-C1
31	y	101	LMT	O5'-C1'-O1'-C1
30	A	412	PL9	C9-C11-C12-C13
30	D	406	PL9	C39-C41-C42-C43
30	a	412	PL9	C9-C11-C12-C13
30	d	406	PL9	C39-C41-C42-C43
25	C	508	CLA	CBA-CGA-O2A-C1
25	c	508	CLA	CBA-CGA-O2A-C1
33	E	102	LHG	C16-C17-C18-C19
33	e	102	LHG	C16-C17-C18-C19
28	k	101	SQD	O10-C23-O48-C46
28	F	101	SQD	C8-C7-O47-C45
28	f	101	SQD	C8-C7-O47-C45
31	K	104	LMT	C4'-C5'-C6'-O6'
31	k	104	LMT	C4'-C5'-C6'-O6'
31	M	102	LMT	O5B-C5B-C6B-O6B
31	m	102	LMT	O5B-C5B-C6B-O6B
33	B	622	LHG	C1-C2-C3-O3
33	b	621	LHG	C1-C2-C3-O3
31	B	623	LMT	C4'-C5'-C6'-O6'
31	C	524	LMT	C4B-C5B-C6B-O6B
31	Y	101	LMT	C4'-C5'-C6'-O6'
31	c	524	LMT	C4B-C5B-C6B-O6B
31	y	101	LMT	C4'-C5'-C6'-O6'
28	K	101	SQD	O10-C23-O48-C46
25	C	506	CLA	C3-C5-C6-C7
25	c	506	CLA	C3-C5-C6-C7
25	B	609	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	b	609	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
31	B	626	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	M	102	LMT	C4'-C5'-C6'-O6'
31	b	622	LMT	C4'-C5'-C6'-O6'
31	b	625	LMT	C4'-C5'-C6'-O6'
31	m	102	LMT	C4'-C5'-C6'-O6'
30	A	412	PL9	C47-C48-C49-C50
30	a	412	PL9	C47-C48-C49-C50
33	Z	102	LHG	C11-C10-C9-C8
33	z	102	LHG	C11-C10-C9-C8
31	M	101	LMT	O5'-C5'-C6'-O6'
31	m	101	LMT	O5'-C5'-C6'-O6'
28	A	413	SQD	C2-C1-O6-C44
28	H	102	SQD	C2-C1-O6-C44
28	a	413	SQD	C2-C1-O6-C44
28	h	102	SQD	C2-C1-O6-C44
25	B	616	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
31	E	101	LMT	O5'-C5'-C6'-O6'
31	e	101	LMT	O5'-C5'-C6'-O6'
25	B	609	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C10-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C10-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	b	616	CLA	C6-C7-C8-C9
25	c	501	CLA	C14-C13-C15-C16
25	c	502	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9
25	c	513	CLA	C6-C7-C8-C9
25	D	401	CLA	CBD-CGD-O2D-CED
25	d	401	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	C5-C6-C7-C8
25	b	615	CLA	C5-C6-C7-C8
25	D	404	CLA	O1D-CGD-O2D-CED
31	J	101	LMT	C4'-C5'-C6'-O6'
31	j	101	LMT	C4'-C5'-C6'-O6'
29	C	518	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	c	518	LMG	C28-C29-C30-C31
25	C	504	CLA	C15-C16-C17-C18
25	c	504	CLA	C15-C16-C17-C18
25	c	506	CLA	C8-C10-C11-C12
25	d	404	CLA	O1D-CGD-O2D-CED
31	I	102	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	C8-C10-C11-C12
25	B	614	CLA	C13-C15-C16-C17
25	B	614	CLA	C15-C16-C17-C18
25	C	506	CLA	C8-C10-C11-C12
25	a	406	CLA	C8-C10-C11-C12
25	b	614	CLA	C13-C15-C16-C17
25	b	614	CLA	C15-C16-C17-C18
25	c	505	CLA	C5-C6-C7-C8
31	E	103	LMT	O5'-C5'-C6'-O6'
31	e	103	LMT	O5'-C5'-C6'-O6'
33	L	101	LHG	C11-C10-C9-C8
33	l	101	LHG	C11-C10-C9-C8
28	A	410	SQD	C7-C8-C9-C10
28	F	101	SQD	C7-C8-C9-C10
28	a	410	SQD	C7-C8-C9-C10
28	f	101	SQD	C7-C8-C9-C10
33	Z	102	LHG	C23-C24-C25-C26
33	z	102	LHG	C23-C24-C25-C26
25	C	511	CLA	O1D-CGD-O2D-CED
31	F	103	LMT	C4'-C5'-C6'-O6'
31	f	103	LMT	C4'-C5'-C6'-O6'
29	A	415	LMG	O6-C5-C6-O5
29	a	415	LMG	O6-C5-C6-O5
25	B	604	CLA	C8-C10-C11-C12
25	B	608	CLA	C15-C16-C17-C18
25	B	613	CLA	C10-C11-C12-C13
25	C	503	CLA	C15-C16-C17-C18
25	C	505	CLA	C5-C6-C7-C8
25	b	604	CLA	C8-C10-C11-C12
25	b	608	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
25	c	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	609	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
30	A	412	PL9	C42-C43-C44-C45
30	a	412	PL9	C42-C43-C44-C45
28	A	414	SQD	C23-C24-C25-C26
28	a	414	SQD	C23-C24-C25-C26
29	A	411	LMG	C10-C11-C12-C13
29	C	523	LMG	C10-C11-C12-C13
29	a	411	LMG	C10-C11-C12-C13
29	c	523	LMG	C10-C11-C12-C13
33	E	102	LHG	C23-C24-C25-C26
33	e	102	LHG	C23-C24-C25-C26
31	T	102	LMT	O1'-C1-C2-C3
31	t	701	LMT	O1'-C1-C2-C3
31	E	103	LMT	C4B-C5B-C6B-O6B
31	e	103	LMT	C4B-C5B-C6B-O6B
25	B	614	CLA	C8-C10-C11-C12
25	b	614	CLA	C8-C10-C11-C12
31	f	103	LMT	C3-C4-C5-C6
28	A	414	SQD	O49-C7-O47-C45
28	B	620	SQD	O49-C7-O47-C45
28	T	101	SQD	O49-C7-O47-C45
28	a	414	SQD	O49-C7-O47-C45
25	B	612	CLA	C2-C1-O2A-CGA
25	b	612	CLA	C2-C1-O2A-CGA
31	E	103	LMT	O1'-C1-C2-C3
31	F	103	LMT	C3-C4-C5-C6
31	e	103	LMT	O1'-C1-C2-C3
25	A	408	CLA	C10-C11-C12-C13
25	B	607	CLA	C15-C16-C17-C18
25	b	607	CLA	C15-C16-C17-C18
33	Z	102	LHG	C7-C8-C9-C10
33	z	102	LHG	C7-C8-C9-C10
33	D	407	LHG	C17-C18-C19-C20
33	d	407	LHG	C17-C18-C19-C20
31	K	104	LMT	C5'-C4'-O1B-C1B
31	k	104	LMT	C5'-C4'-O1B-C1B
25	C	506	CLA	C15-C16-C17-C18
25	C	510	CLA	C8-C10-C11-C12
25	a	408	CLA	C10-C11-C12-C13
25	c	506	CLA	C15-C16-C17-C18
25	c	510	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C11-C12-C13-C15
25	B	609	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
33	B	622	LHG	C23-C24-C25-C26
33	b	621	LHG	C23-C24-C25-C26
25	B	605	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
25	C	506	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	C2A-CAA-CBA-CGA
25	A	408	CLA	O1D-CGD-O2D-CED
25	a	408	CLA	O1D-CGD-O2D-CED
28	A	414	SQD	O5-C1-O6-C44
28	a	414	SQD	O5-C1-O6-C44
31	A	416	LMT	O5'-C1'-O1'-C1
31	a	416	LMT	O5'-C1'-O1'-C1
25	C	507	CLA	C13-C15-C16-C17
25	c	507	CLA	C13-C15-C16-C17
25	B	602	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	O1D-CGD-O2D-CED
30	A	412	PL9	C44-C46-C47-C48
30	D	406	PL9	C44-C46-C47-C48
30	a	412	PL9	C44-C46-C47-C48
30	d	406	PL9	C44-C46-C47-C48
31	B	625	LMT	O1'-C1-C2-C3
31	b	624	LMT	O1'-C1-C2-C3
31	i	103	LMT	O1'-C1-C2-C3
27	A	409	BCR	C10-C11-C12-C13
27	C	514	BCR	C10-C11-C12-C13
27	D	405	BCR	C10-C11-C12-C13
27	a	409	BCR	C10-C11-C12-C13
27	c	514	BCR	C10-C11-C12-C13
27	d	405	BCR	C10-C11-C12-C13
31	I	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	X	104	LMT	O1'-C1-C2-C3
31	x	104	LMT	O1'-C1-C2-C3
34	C	516	DGD	CAA-CBA-CCA-CDA
34	c	516	DGD	CAA-CBA-CCA-CDA
33	B	622	LHG	O2-C2-C3-O3
33	b	621	LHG	O2-C2-C3-O3
25	C	509	CLA	C3-C5-C6-C7
25	c	509	CLA	C3-C5-C6-C7
25	B	609	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
25	b	613	CLA	C5-C6-C7-C8
31	D	412	LMT	C4'-C5'-C6'-O6'
31	F	103	LMT	C4B-C5B-C6B-O6B
31	d	412	LMT	C4'-C5'-C6'-O6'
31	f	103	LMT	C4B-C5B-C6B-O6B
25	A	406	CLA	C15-C16-C17-C18
25	B	616	CLA	C8-C10-C11-C12
25	a	406	CLA	C15-C16-C17-C18
25	b	616	CLA	C8-C10-C11-C12
31	C	524	LMT	O1'-C1-C2-C3
31	c	524	LMT	O1'-C1-C2-C3
31	I	103	LMT	C4'-C5'-C6'-O6'
31	i	103	LMT	C4'-C5'-C6'-O6'
25	C	508	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
33	L	101	LHG	C8-C7-O7-C5
33	l	101	LHG	C8-C7-O7-C5
25	B	604	CLA	C5-C6-C7-C8
25	B	611	CLA	C13-C15-C16-C17
25	B	611	CLA	C15-C16-C17-C18
25	B	613	CLA	C5-C6-C7-C8
25	B	614	CLA	C10-C11-C12-C13
25	B	616	CLA	C10-C11-C12-C13
25	C	509	CLA	C13-C15-C16-C17
25	b	604	CLA	C5-C6-C7-C8
25	b	611	CLA	C13-C15-C16-C17
25	b	611	CLA	C15-C16-C17-C18
25	b	614	CLA	C10-C11-C12-C13
25	b	616	CLA	C10-C11-C12-C13
25	c	509	CLA	C13-C15-C16-C17
33	D	408	LHG	C4-O6-P-O3
33	E	102	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C4-O6-P-O3
33	d	408	LHG	C4-O6-P-O3
33	e	102	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
28	K	101	SQD	C23-C24-C25-C26
28	k	101	SQD	C23-C24-C25-C26
25	C	506	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
31	M	103	LMT	C4'-C5'-C6'-O6'
33	L	101	LHG	O9-C7-O7-C5
33	l	101	LHG	O9-C7-O7-C5
31	m	103	LMT	C4'-C5'-C6'-O6'
31	M	101	LMT	O1'-C1-C2-C3
31	m	101	LMT	O1'-C1-C2-C3
25	C	508	CLA	C16-C17-C18-C20
25	b	616	CLA	C11-C12-C13-C15
25	c	508	CLA	C16-C17-C18-C20
29	d	409	LMG	C18-C19-C20-C21
31	D	410	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5'-C5'-C6'-O6'
33	A	419	LHG	C23-C24-C25-C26
33	a	419	LHG	C23-C24-C25-C26
28	A	410	SQD	C26-C27-C28-C29
29	D	409	LMG	C18-C19-C20-C21
33	D	407	LHG	C25-C26-C27-C28
33	a	419	LHG	C16-C17-C18-C19
33	d	407	LHG	C25-C26-C27-C28
25	D	403	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
29	C	518	LMG	C11-C10-O7-C8
29	c	518	LMG	C11-C10-O7-C8
27	C	514	BCR	C11-C10-C9-C34
27	Z	101	BCR	C11-C10-C9-C34
27	c	514	BCR	C11-C10-C9-C34
27	z	101	BCR	C11-C10-C9-C34
31	F	103	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5B-C5B-C6B-O6B
28	A	413	SQD	C11-C10-C9-C8
28	H	102	SQD	C14-C15-C16-C17
28	a	410	SQD	C26-C27-C28-C29
28	a	413	SQD	C11-C10-C9-C8
28	h	102	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	C	523	LMG	C14-C15-C16-C17
29	D	409	LMG	C33-C34-C35-C36
29	c	523	LMG	C14-C15-C16-C17
29	d	409	LMG	C33-C34-C35-C36
31	J	101	LMT	C5-C6-C7-C8
31	j	101	LMT	C5-C6-C7-C8
33	A	419	LHG	C16-C17-C18-C19
25	B	613	CLA	C16-C17-C18-C20
25	B	616	CLA	C11-C12-C13-C15
25	b	613	CLA	C16-C17-C18-C20
28	B	620	SQD	C34-C35-C36-C37
28	F	101	SQD	C11-C10-C9-C8
28	H	102	SQD	C31-C32-C33-C34
28	T	101	SQD	C34-C35-C36-C37
28	f	101	SQD	C11-C10-C9-C8
28	h	102	SQD	C31-C32-C33-C34
29	B	621	LMG	C13-C14-C15-C16
29	b	620	LMG	C13-C14-C15-C16
31	D	410	LMT	C7-C8-C9-C10
31	F	103	LMT	C6-C7-C8-C9
31	I	101	LMT	C6-C7-C8-C9
31	d	410	LMT	C7-C8-C9-C10
31	f	103	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
34	C	517	DGD	C7B-C8B-C9B-CAB
28	A	413	SQD	C44-C45-O47-C7
28	A	414	SQD	C44-C45-O47-C7
28	F	101	SQD	C44-C45-O47-C7
28	a	413	SQD	C44-C45-O47-C7
28	a	414	SQD	C44-C45-O47-C7
28	f	101	SQD	C44-C45-O47-C7
25	C	503	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
29	C	518	LMG	O9-C10-O7-C8
29	c	518	LMG	O9-C10-O7-C8
28	A	410	SQD	C11-C12-C13-C14
28	a	410	SQD	C11-C12-C13-C14
29	D	409	LMG	C32-C33-C34-C35
29	c	518	LMG	C11-C12-C13-C14
29	d	409	LMG	C32-C33-C34-C35
31	T	102	LMT	C3-C4-C5-C6
31	x	104	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C15-C16-C17-C18
34	C	517	DGD	C4B-C5B-C6B-C7B
34	c	517	DGD	C4B-C5B-C6B-C7B
34	c	517	DGD	C7B-C8B-C9B-CAB
25	c	502	CLA	O1D-CGD-O2D-CED
28	K	101	SQD	C10-C11-C12-C13
29	C	518	LMG	C11-C12-C13-C14
31	D	411	LMT	C2-C3-C4-C5
31	J	101	LMT	C7-C8-C9-C10
31	X	104	LMT	C6-C7-C8-C9
31	d	411	LMT	C2-C3-C4-C5
31	j	101	LMT	C7-C8-C9-C10
31	t	701	LMT	C3-C4-C5-C6
33	l	101	LHG	C15-C16-C17-C18
25	C	502	CLA	O1D-CGD-O2D-CED
28	A	413	SQD	C27-C28-C29-C30
28	a	413	SQD	C27-C28-C29-C30
28	k	101	SQD	C10-C11-C12-C13
31	D	410	LMT	C5-C6-C7-C8
31	X	101	LMT	C6-C7-C8-C9
31	x	101	LMT	C6-C7-C8-C9
33	B	622	LHG	C24-C25-C26-C27
33	b	621	LHG	C24-C25-C26-C27
33	d	408	LHG	C26-C27-C28-C29
34	c	517	DGD	C1A-C2A-C3A-C4A
25	B	610	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
27	C	514	BCR	C11-C10-C9-C8
27	Z	101	BCR	C11-C10-C9-C8
27	c	514	BCR	C11-C10-C9-C8
27	z	101	BCR	C11-C10-C9-C8
28	K	101	SQD	C2-C1-O6-C44
28	k	101	SQD	C2-C1-O6-C44
31	J	101	LMT	C2'-C1'-O1'-C1
31	j	101	LMT	C2'-C1'-O1'-C1
28	A	413	SQD	C32-C33-C34-C35
28	a	413	SQD	C32-C33-C34-C35
31	K	104	LMT	C3'-C4'-O1B-C1B
31	d	410	LMT	C5-C6-C7-C8
33	D	408	LHG	C26-C27-C28-C29
33	L	101	LHG	C12-C13-C14-C15
33	l	101	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	C15-C16-C17-C18
25	d	404	CLA	C15-C16-C17-C18
25	B	605	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
25	B	611	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
30	A	412	PL9	C45-C44-C46-C47
30	a	412	PL9	C45-C44-C46-C47
28	B	620	SQD	C26-C27-C28-C29
28	H	102	SQD	C12-C13-C14-C15
28	T	101	SQD	C26-C27-C28-C29
31	B	623	LMT	C11-C10-C9-C8
31	I	102	LMT	C6-C7-C8-C9
31	I	103	LMT	C6-C7-C8-C9
31	b	622	LMT	C11-C10-C9-C8
31	i	102	LMT	C6-C7-C8-C9
31	i	103	LMT	C6-C7-C8-C9
31	k	104	LMT	C3'-C4'-O1B-C1B
31	t	701	LMT	C4-C5-C6-C7
34	H	103	DGD	C6A-C7A-C8A-C9A
34	h	103	DGD	C6A-C7A-C8A-C9A
25	B	604	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	b	604	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C12-C13-C14
34	C	517	DGD	C1A-C2A-C3A-C4A
28	A	410	SQD	C27-C28-C29-C30
28	K	101	SQD	C25-C26-C27-C28
28	a	410	SQD	C27-C28-C29-C30
28	h	102	SQD	C12-C13-C14-C15
28	k	101	SQD	C25-C26-C27-C28
29	A	411	LMG	C39-C40-C41-C42
31	I	103	LMT	C7-C8-C9-C10
31	T	102	LMT	C4-C5-C6-C7
31	i	103	LMT	C7-C8-C9-C10
33	B	622	LHG	C11-C12-C13-C14
33	Z	102	LHG	C28-C29-C30-C31
33	e	102	LHG	C11-C12-C13-C14
33	z	102	LHG	C28-C29-C30-C31
29	A	411	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	C18-C19-C20-C21
29	a	411	LMG	C14-C15-C16-C17
29	a	411	LMG	C39-C40-C41-C42
29	c	518	LMG	C18-C19-C20-C21
33	E	102	LHG	C11-C12-C13-C14
33	b	621	LHG	C11-C12-C13-C14
33	d	408	LHG	C28-C29-C30-C31
29	B	621	LMG	C12-C13-C14-C15
29	b	620	LMG	C12-C13-C14-C15
31	A	417	LMT	C5-C6-C7-C8
31	a	417	LMT	C5-C6-C7-C8
33	A	419	LHG	C9-C10-C11-C12
33	D	408	LHG	C28-C29-C30-C31
33	a	419	LHG	C9-C10-C11-C12
33	D	408	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
28	A	410	SQD	C12-C13-C14-C15
28	A	414	SQD	C11-C12-C13-C14
28	A	414	SQD	C12-C13-C14-C15
28	a	410	SQD	C12-C13-C14-C15
28	a	414	SQD	C11-C12-C13-C14
28	a	414	SQD	C12-C13-C14-C15
31	D	411	LMT	C3-C4-C5-C6
31	M	102	LMT	C3-C4-C5-C6
31	d	411	LMT	C3-C4-C5-C6
31	m	102	LMT	C3-C4-C5-C6
33	D	407	LHG	C34-C35-C36-C37
33	d	407	LHG	C34-C35-C36-C37
33	l	101	LHG	C11-C12-C13-C14
31	M	102	LMT	C1-C2-C3-C4
31	m	102	LMT	C1-C2-C3-C4
25	B	611	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C14
25	C	508	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C19
25	b	616	CLA	C11-C12-C13-C14
25	c	508	CLA	C16-C17-C18-C19
31	J	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	j	101	LMT	O5'-C1'-O1'-C1
25	C	512	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
28	A	414	SQD	C26-C27-C28-C29
28	A	414	SQD	C28-C29-C30-C31
28	K	101	SQD	C9-C10-C11-C12
28	a	414	SQD	C26-C27-C28-C29
28	a	414	SQD	C28-C29-C30-C31
28	k	101	SQD	C9-C10-C11-C12
31	B	624	LMT	C3-C4-C5-C6
31	b	623	LMT	C3-C4-C5-C6
33	L	101	LHG	C11-C12-C13-C14
33	Z	102	LHG	C33-C34-C35-C36
33	z	102	LHG	C33-C34-C35-C36
26	D	402	PHO	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
28	A	413	SQD	C12-C13-C14-C15
28	a	413	SQD	C12-C13-C14-C15
31	A	416	LMT	C6-C7-C8-C9
31	C	524	LMT	C2-C3-C4-C5
31	D	411	LMT	C6-C7-C8-C9
31	D	412	LMT	C11-C10-C9-C8
31	a	416	LMT	C6-C7-C8-C9
31	c	524	LMT	C2-C3-C4-C5
31	d	411	LMT	C6-C7-C8-C9
31	d	412	LMT	C11-C10-C9-C8
33	L	101	LHG	C16-C17-C18-C19
33	l	101	LHG	C16-C17-C18-C19
34	C	515	DGD	CAA-CBA-CCA-CDA
34	c	515	DGD	CAA-CBA-CCA-CDA
28	K	101	SQD	C7-C8-C9-C10
28	k	101	SQD	C7-C8-C9-C10
25	B	616	CLA	C5-C6-C7-C8
25	C	511	CLA	C13-C15-C16-C17
25	a	408	CLA	C8-C10-C11-C12
25	b	616	CLA	C5-C6-C7-C8
25	c	511	CLA	C13-C15-C16-C17
25	C	506	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
29	C	523	LMG	C32-C33-C34-C35
29	c	523	LMG	C32-C33-C34-C35
31	M	101	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	m	101	LMT	C11-C10-C9-C8
33	L	101	LHG	C24-C25-C26-C27
33	l	101	LHG	C24-C25-C26-C27
29	D	409	LMG	C19-C20-C21-C22
29	d	409	LMG	C19-C20-C21-C22
31	E	103	LMT	C7-C8-C9-C10
31	e	103	LMT	C7-C8-C9-C10
25	A	408	CLA	C8-C10-C11-C12
25	B	605	CLA	C8-C10-C11-C12
25	b	605	CLA	C8-C10-C11-C12
31	B	625	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C2-C1-O1'-C1'
31	E	103	LMT	C4-C5-C6-C7
31	F	103	LMT	O1'-C1-C2-C3
31	e	103	LMT	C4-C5-C6-C7
31	f	103	LMT	O1'-C1-C2-C3
33	D	407	LHG	C13-C14-C15-C16
33	d	407	LHG	C13-C14-C15-C16
25	B	613	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
28	K	101	SQD	C12-C13-C14-C15
28	k	101	SQD	C12-C13-C14-C15
25	C	504	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
28	A	413	SQD	C26-C27-C28-C29
28	B	620	SQD	C27-C28-C29-C30
28	T	101	SQD	C27-C28-C29-C30
28	a	413	SQD	C26-C27-C28-C29
31	C	520	LMT	C11-C10-C9-C8
31	c	520	LMT	C11-C10-C9-C8
25	B	602	CLA	O2A-C1-C2-C3
25	b	602	CLA	O2A-C1-C2-C3
25	B	613	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
31	D	412	LMT	C3-C4-C5-C6
31	d	412	LMT	C3-C4-C5-C6
34	c	517	DGD	C9A-CAA-CBA-CCA
30	D	406	PL9	C15-C14-C16-C17
30	d	406	PL9	C15-C14-C16-C17
33	D	408	LHG	C34-C35-C36-C37
33	d	408	LHG	C34-C35-C36-C37
34	C	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
31	A	416	LMT	O5B-C5B-C6B-O6B
33	B	622	LHG	O1-C1-C2-O2
33	b	621	LHG	O1-C1-C2-O2
28	A	410	SQD	C17-C18-C19-C20
28	a	410	SQD	C17-C18-C19-C20
34	C	517	DGD	CCA-CDA-CEA-CFA
34	c	517	DGD	CCA-CDA-CEA-CFA
31	a	416	LMT	O5B-C5B-C6B-O6B
25	c	513	CLA	C15-C16-C17-C18
25	b	608	CLA	CBD-CGD-O2D-CED
31	B	624	LMT	C2-C3-C4-C5
31	b	623	LMT	C2-C3-C4-C5
34	C	517	DGD	C5A-C6A-C7A-C8A
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	b	610	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
25	c	507	CLA	C2-C1-O2A-CGA
31	C	519	LMT	C4'-C5'-C6'-O6'
31	I	101	LMT	C4'-C5'-C6'-O6'
31	c	519	LMT	C4'-C5'-C6'-O6'
31	i	101	LMT	C4'-C5'-C6'-O6'
28	A	413	SQD	C28-C29-C30-C31
28	a	413	SQD	C28-C29-C30-C31
31	C	520	LMT	O1'-C1-C2-C3
31	D	410	LMT	C3-C4-C5-C6
31	M	101	LMT	C4-C5-C6-C7
31	c	520	LMT	O1'-C1-C2-C3
31	d	410	LMT	C3-C4-C5-C6
31	m	101	LMT	C4-C5-C6-C7
34	c	517	DGD	C5A-C6A-C7A-C8A
25	B	602	CLA	C10-C11-C12-C13
25	C	513	CLA	C15-C16-C17-C18
25	b	602	CLA	C10-C11-C12-C13
31	C	521	LMT	C4'-C5'-C6'-O6'
31	c	521	LMT	C4'-C5'-C6'-O6'
29	C	523	LMG	C12-C13-C14-C15
29	c	523	LMG	C12-C13-C14-C15
34	C	515	DGD	C4B-C5B-C6B-C7B
34	c	515	DGD	C4B-C5B-C6B-C7B
27	B	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	B	617	BCR	C5-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C26
27	D	405	BCR	C23-C24-C25-C26
27	D	405	BCR	C23-C24-C25-C30
27	b	617	BCR	C1-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	b	619	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	d	405	BCR	C23-C24-C25-C26
27	d	405	BCR	C23-C24-C25-C30
37	X	102	RRX	C23-C24-C25-C30
37	X	102	RRX	C5-C6-C7-C8
37	x	102	RRX	C23-C24-C25-C30
37	x	102	RRX	C5-C6-C7-C8
31	I	104	LMT	O5'-C5'-C6'-O6'
31	i	104	LMT	O5'-C5'-C6'-O6'
31	t	701	LMT	O5'-C5'-C6'-O6'
28	a	410	SQD	C24-C25-C26-C27
31	D	411	LMT	C5-C6-C7-C8
31	d	411	LMT	C5-C6-C7-C8
34	C	517	DGD	C6B-C7B-C8B-C9B
28	A	410	SQD	C24-C25-C26-C27
33	A	419	LHG	C26-C27-C28-C29
33	a	419	LHG	C26-C27-C28-C29
34	c	517	DGD	C6B-C7B-C8B-C9B
31	T	102	LMT	O5'-C5'-C6'-O6'
25	B	608	CLA	CBD-CGD-O2D-CED
31	E	103	LMT	C1-C2-C3-C4
31	e	103	LMT	C1-C2-C3-C4
25	d	401	CLA	C2C-C3C-CAC-CBC
25	B	604	CLA	C6-C7-C8-C10
25	B	610	CLA	C11-C10-C8-C7
25	C	501	CLA	C12-C13-C15-C16
25	C	508	CLA	C11-C12-C13-C15
25	C	510	CLA	C2-C3-C5-C6
25	C	513	CLA	C6-C7-C8-C10
25	b	604	CLA	C6-C7-C8-C10
25	b	610	CLA	C11-C10-C8-C7
25	c	501	CLA	C12-C13-C15-C16
25	c	508	CLA	C11-C12-C13-C15
25	c	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C6-C7-C8-C10
25	D	401	CLA	C2C-C3C-CAC-CBC
33	A	419	LHG	C14-C15-C16-C17
25	D	403	CLA	C15-C16-C17-C18
25	d	403	CLA	C15-C16-C17-C18
25	A	405	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
29	A	411	LMG	O9-C10-O7-C8
29	a	411	LMG	O9-C10-O7-C8
28	K	101	SQD	C24-C23-O48-C46
28	k	101	SQD	C24-C23-O48-C46
33	a	419	LHG	C14-C15-C16-C17
31	T	102	LMT	C1-C2-C3-C4
31	t	701	LMT	C1-C2-C3-C4
25	C	501	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	O1D-CGD-O2D-CED
25	D	401	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C8-C10-C11-C12
31	I	101	LMT	C5-C6-C7-C8
31	f	103	LMT	C11-C10-C9-C8
25	d	401	CLA	O1D-CGD-O2D-CED
31	F	103	LMT	C11-C10-C9-C8
31	i	101	LMT	C5-C6-C7-C8
33	D	407	LHG	C29-C30-C31-C32
33	d	407	LHG	C29-C30-C31-C32
33	L	101	LHG	C13-C14-C15-C16
33	l	101	LHG	C13-C14-C15-C16
31	M	102	LMT	O5'-C1'-O1'-C1
31	m	102	LMT	O5'-C1'-O1'-C1
25	B	602	CLA	C15-C16-C17-C18
25	b	602	CLA	C15-C16-C17-C18
31	B	624	LMT	C4-C5-C6-C7
31	b	623	LMT	C4-C5-C6-C7
33	D	407	LHG	C11-C10-C9-C8
33	Z	102	LHG	C34-C35-C36-C37
33	z	102	LHG	C34-C35-C36-C37
28	K	101	SQD	C8-C7-O47-C45
28	k	101	SQD	C8-C7-O47-C45
29	A	411	LMG	C11-C10-O7-C8
29	a	411	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	d	407	LHG	C11-C10-C9-C8
25	B	607	CLA	C13-C15-C16-C17
25	b	607	CLA	C13-C15-C16-C17
25	B	602	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
33	E	102	LHG	O7-C5-C6-O8
33	Z	102	LHG	O7-C5-C6-O8
33	e	102	LHG	O7-C5-C6-O8
33	z	102	LHG	O7-C5-C6-O8
25	B	615	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
28	A	410	SQD	C9-C10-C11-C12
33	D	407	LHG	C31-C32-C33-C34
33	d	407	LHG	C31-C32-C33-C34
34	C	515	DGD	O6E-C5E-C6E-O5E
34	c	515	DGD	O6E-C5E-C6E-O5E
25	B	604	CLA	C4-C3-C5-C6
25	C	510	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
28	a	410	SQD	C9-C10-C11-C12
25	A	406	CLA	C6-C7-C8-C9
25	a	406	CLA	C6-C7-C8-C9
25	C	507	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
33	D	407	LHG	C24-C25-C26-C27
33	d	407	LHG	C24-C25-C26-C27
27	D	405	BCR	C36-C18-C19-C20
27	d	405	BCR	C36-C18-C19-C20
28	B	620	SQD	C9-C10-C11-C12
28	T	101	SQD	C9-C10-C11-C12
31	D	410	LMT	C6-C7-C8-C9
31	d	410	LMT	C6-C7-C8-C9
25	A	408	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	a	408	CLA	C1A-C2A-CAA-CBA
25	b	604	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
28	A	410	SQD	O49-C7-O47-C45
33	b	621	LHG	C8-C7-O7-C5
28	A	413	SQD	C14-C15-C16-C17
28	a	413	SQD	C14-C15-C16-C17
29	C	518	LMG	C34-C35-C36-C37
29	c	518	LMG	C34-C35-C36-C37
31	X	104	LMT	C3-C4-C5-C6
31	x	104	LMT	C3-C4-C5-C6
33	D	408	LHG	C13-C14-C15-C16
33	d	408	LHG	C13-C14-C15-C16
31	C	520	LMT	C4'-C5'-C6'-O6'
31	c	520	LMT	C4'-C5'-C6'-O6'
25	B	610	CLA	C13-C15-C16-C17
25	C	506	CLA	C13-C15-C16-C17
25	b	610	CLA	C13-C15-C16-C17
25	c	506	CLA	C13-C15-C16-C17
31	X	104	LMT	C1-C2-C3-C4
31	x	104	LMT	C1-C2-C3-C4
33	B	622	LHG	C3-O3-P-O6
33	b	621	LHG	C3-O3-P-O6
33	Z	102	LHG	C25-C26-C27-C28
33	z	102	LHG	C25-C26-C27-C28
33	D	408	LHG	O6-C4-C5-C6
33	d	408	LHG	O6-C4-C5-C6
31	M	102	LMT	C11-C10-C9-C8
31	m	102	LMT	C11-C10-C9-C8
29	c	518	LMG	C10-C11-C12-C13
31	C	520	LMT	C6-C7-C8-C9
31	c	520	LMT	C6-C7-C8-C9
33	D	407	LHG	C28-C29-C30-C31
33	D	408	LHG	C31-C32-C33-C34
33	d	407	LHG	C28-C29-C30-C31
33	d	408	LHG	C31-C32-C33-C34
25	B	609	CLA	C5-C6-C7-C8
25	b	609	CLA	C5-C6-C7-C8
31	I	103	LMT	C4B-C5B-C6B-O6B
31	i	103	LMT	C4B-C5B-C6B-O6B
33	B	622	LHG	C12-C13-C14-C15
31	i	102	LMT	C2-C3-C4-C5
33	b	621	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	C10-C11-C12-C13
31	I	102	LMT	C2-C3-C4-C5
25	B	611	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
28	a	410	SQD	O49-C7-O47-C45
30	D	406	PL9	C30-C29-C31-C32
30	d	406	PL9	C30-C29-C31-C32
28	A	414	SQD	C9-C10-C11-C12
28	a	414	SQD	C9-C10-C11-C12
31	I	101	LMT	C3-C4-C5-C6
31	i	101	LMT	C3-C4-C5-C6
31	i	102	LMT	C7-C8-C9-C10
29	C	518	LMG	C19-C20-C21-C22
29	c	518	LMG	C19-C20-C21-C22
31	C	521	LMT	C4-C5-C6-C7
31	I	102	LMT	C7-C8-C9-C10
31	c	521	LMT	C4-C5-C6-C7
33	B	622	LHG	C31-C32-C33-C34
33	D	408	LHG	C27-C28-C29-C30
33	L	101	LHG	C31-C32-C33-C34
33	b	621	LHG	C31-C32-C33-C34
33	d	408	LHG	C27-C28-C29-C30
33	l	101	LHG	C31-C32-C33-C34
33	B	622	LHG	C8-C7-O7-C5
28	H	102	SQD	C11-C10-C9-C8
28	f	101	SQD	C24-C25-C26-C27
28	h	102	SQD	C11-C10-C9-C8
31	D	410	LMT	C4-C5-C6-C7
31	d	410	LMT	C4-C5-C6-C7
33	E	102	LHG	C4-C5-C6-O8
33	Z	102	LHG	C4-C5-C6-O8
33	e	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C11-C12-C13-C14
28	F	101	SQD	C24-C25-C26-C27
33	Z	102	LHG	C11-C12-C13-C14
34	C	516	DGD	C2G-C3G-O3G-C1D
34	c	516	DGD	C2G-C3G-O3G-C1D
28	H	102	SQD	C26-C27-C28-C29
28	h	102	SQD	C26-C27-C28-C29
25	B	604	CLA	C16-C17-C18-C19
25	b	604	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	C	523	LMG	C13-C14-C15-C16
29	c	523	LMG	C13-C14-C15-C16
33	D	408	LHG	C29-C30-C31-C32
33	D	408	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
28	A	410	SQD	C45-C46-O48-C23
28	a	410	SQD	C45-C46-O48-C23
33	Z	102	LHG	C24-C25-C26-C27
33	d	408	LHG	C29-C30-C31-C32
33	z	102	LHG	C24-C25-C26-C27
34	C	517	DGD	C2A-C3A-C4A-C5A
34	c	517	DGD	C2A-C3A-C4A-C5A
28	A	410	SQD	C29-C30-C31-C32
28	a	410	SQD	C29-C30-C31-C32
29	C	523	LMG	O6-C5-C6-O5
29	D	409	LMG	O6-C5-C6-O5
29	c	523	LMG	O6-C5-C6-O5
29	d	409	LMG	O6-C5-C6-O5
25	b	604	CLA	C3-C5-C6-C7
28	A	414	SQD	C14-C15-C16-C17
28	a	414	SQD	C14-C15-C16-C17
33	D	408	LHG	C35-C36-C37-C38
25	B	604	CLA	C13-C15-C16-C17
25	b	604	CLA	C13-C15-C16-C17
33	B	622	LHG	C13-C14-C15-C16
33	b	621	LHG	C13-C14-C15-C16
33	d	408	LHG	C35-C36-C37-C38
28	B	620	SQD	C46-C45-O47-C7
28	T	101	SQD	C46-C45-O47-C7
25	C	513	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
25	d	404	CLA	C2-C1-O2A-CGA
25	B	604	CLA	C3-C5-C6-C7
28	A	410	SQD	C16-C17-C18-C19
31	F	103	LMT	C4-C5-C6-C7
33	Z	102	LHG	C4-O6-P-O5
33	z	102	LHG	C4-O6-P-O5
28	a	410	SQD	C16-C17-C18-C19
31	f	103	LMT	C4-C5-C6-C7
33	L	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C14-C15-C16-C17
33	E	102	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C24-C23-O8-C6
28	T	101	SQD	C24-C25-C26-C27
33	D	407	LHG	C19-C20-C21-C22
33	d	407	LHG	C19-C20-C21-C22
25	A	406	CLA	C13-C15-C16-C17
25	D	404	CLA	C5-C6-C7-C8
25	a	406	CLA	C13-C15-C16-C17
25	d	404	CLA	C5-C6-C7-C8
28	B	620	SQD	C24-C25-C26-C27
28	B	620	SQD	C13-C14-C15-C16
28	T	101	SQD	C13-C14-C15-C16
31	K	104	LMT	C2-C3-C4-C5
31	k	104	LMT	C2-C3-C4-C5
33	B	622	LHG	C25-C26-C27-C28
33	B	622	LHG	C32-C33-C34-C35
33	D	407	LHG	C14-C15-C16-C17
33	b	621	LHG	C25-C26-C27-C28
33	b	621	LHG	C32-C33-C34-C35
33	d	407	LHG	C14-C15-C16-C17
29	A	411	LMG	C11-C12-C13-C14
29	a	411	LMG	C11-C12-C13-C14
31	M	101	LMT	C4'-C5'-C6'-O6'
31	m	101	LMT	C4'-C5'-C6'-O6'
31	C	520	LMT	C1-C2-C3-C4
31	c	520	LMT	C1-C2-C3-C4
28	K	101	SQD	O47-C45-C46-O48
28	k	101	SQD	O47-C45-C46-O48
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
26	d	402	PHO	CHA-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
28	A	414	SQD	C32-C33-C34-C35
28	a	414	SQD	C32-C33-C34-C35
25	A	406	CLA	C6-C7-C8-C10
25	B	602	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C10-C8-C7
25	B	605	CLA	C11-C10-C8-C7
25	B	605	CLA	C12-C13-C15-C16
25	B	606	CLA	C11-C10-C8-C7
25	B	608	CLA	C11-C12-C13-C15
25	C	502	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	a	406	CLA	C6-C7-C8-C10
25	b	602	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C10-C8-C7
25	b	605	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	c	502	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C10-C8-C7
29	C	518	LMG	C29-C30-C31-C32
29	c	518	LMG	C29-C30-C31-C32
31	X	104	LMT	C7-C8-C9-C10
31	x	104	LMT	C7-C8-C9-C10
25	B	605	CLA	C11-C10-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	B	606	CLA	C11-C10-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C9
25	D	403	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C9
25	b	608	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C9
25	d	403	CLA	C6-C7-C8-C9
31	D	410	LMT	C1-C2-C3-C4
31	d	410	LMT	C1-C2-C3-C4
31	C	524	LMT	C3-C4-C5-C6
31	c	524	LMT	C3-C4-C5-C6
33	A	419	LHG	C24-C23-O8-C6
33	a	419	LHG	C24-C23-O8-C6
25	B	611	CLA	C8-C10-C11-C12
25	b	611	CLA	C8-C10-C11-C12
25	A	408	CLA	C2A-CAA-CBA-CGA
25	a	408	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
27	Z	101	BCR	C11-C12-C13-C35
25	C	508	CLA	C13-C15-C16-C17
34	C	515	DGD	C2B-C1B-O2G-C2G
34	c	515	DGD	C2B-C1B-O2G-C2G
31	E	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	C4'-C5'-C6'-O6'
33	D	407	LHG	C11-C12-C13-C14
33	d	407	LHG	C11-C12-C13-C14
25	c	508	CLA	C13-C15-C16-C17
29	B	621	LMG	C30-C31-C32-C33
29	b	620	LMG	C30-C31-C32-C33
34	C	517	DGD	CAA-CBA-CCA-CDA
34	c	517	DGD	CAA-CBA-CCA-CDA
28	H	102	SQD	C13-C14-C15-C16
28	h	102	SQD	C13-C14-C15-C16
31	B	624	LMT	C7-C8-C9-C10
31	C	521	LMT	C7-C8-C9-C10
31	b	623	LMT	C7-C8-C9-C10
31	c	521	LMT	C7-C8-C9-C10
25	A	405	CLA	C15-C16-C17-C18
25	a	405	CLA	C15-C16-C17-C18
29	B	621	LMG	C10-C11-C12-C13
29	b	620	LMG	C10-C11-C12-C13
25	c	513	CLA	C13-C15-C16-C17
30	A	412	PL9	C43-C44-C46-C47
30	a	412	PL9	C43-C44-C46-C47
28	F	101	SQD	C23-C24-C25-C26
28	a	414	SQD	C7-C8-C9-C10
28	f	101	SQD	C23-C24-C25-C26
29	C	523	LMG	C11-C12-C13-C14
29	c	523	LMG	C11-C12-C13-C14
34	C	517	DGD	C6A-C7A-C8A-C9A
34	c	517	DGD	C6A-C7A-C8A-C9A
25	B	603	CLA	C16-C17-C18-C20
25	b	603	CLA	C16-C17-C18-C20
31	A	416	LMT	C7-C8-C9-C10
31	a	416	LMT	C7-C8-C9-C10
25	C	513	CLA	C13-C15-C16-C17
28	A	414	SQD	C7-C8-C9-C10
25	B	608	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
33	A	419	LHG	C28-C29-C30-C31
31	C	520	LMT	C2-C1-O1'-C1'
31	C	524	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2-C1-O1'-C1'
31	K	104	LMT	C2-C1-O1'-C1'
31	c	520	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	c	524	LMT	C2-C1-O1'-C1'
31	d	410	LMT	C2-C1-O1'-C1'
31	k	104	LMT	C2-C1-O1'-C1'
31	B	625	LMT	C7-C8-C9-C10
31	b	624	LMT	C7-C8-C9-C10
33	a	419	LHG	C28-C29-C30-C31
34	C	516	DGD	C2A-C3A-C4A-C5A
34	c	516	DGD	C2A-C3A-C4A-C5A
31	D	412	LMT	O1'-C1-C2-C3
25	C	504	CLA	CBA-CGA-O2A-C1
25	D	401	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
25	d	401	CLA	CBA-CGA-O2A-C1
31	d	412	LMT	O1'-C1-C2-C3
28	A	413	SQD	O6-C44-C45-C46
28	K	101	SQD	C44-C45-C46-O48
28	a	413	SQD	O6-C44-C45-C46
28	k	101	SQD	C44-C45-C46-O48
29	A	411	LMG	C7-C8-C9-O8
29	a	411	LMG	C7-C8-C9-O8
33	L	101	LHG	C4-C5-C6-O8
33	l	101	LHG	C4-C5-C6-O8
33	B	622	LHG	O9-C7-O7-C5
33	b	621	LHG	O9-C7-O7-C5
33	B	622	LHG	C27-C28-C29-C30
33	E	102	LHG	C12-C13-C14-C15
33	b	621	LHG	C27-C28-C29-C30
33	e	102	LHG	C12-C13-C14-C15
29	D	409	LMG	C39-C40-C41-C42
29	d	409	LMG	C39-C40-C41-C42
33	A	419	LHG	C15-C16-C17-C18
25	A	405	CLA	C16-C17-C18-C19
25	B	603	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C20
30	A	412	PL9	C33-C34-C36-C37
30	a	412	PL9	C33-C34-C36-C37
29	A	415	LMG	C33-C34-C35-C36
29	a	415	LMG	C33-C34-C35-C36
33	a	419	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	D	412	LMT	C4-C5-C6-C7
31	d	412	LMT	C4-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
33	B	622	LHG	O6-C4-C5-O7
33	b	621	LHG	O6-C4-C5-O7
25	B	613	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
28	A	413	SQD	C7-C8-C9-C10
28	a	413	SQD	C7-C8-C9-C10
33	L	101	LHG	O2-C2-C3-O3
33	l	101	LHG	O2-C2-C3-O3
28	A	410	SQD	C14-C15-C16-C17
28	a	410	SQD	C14-C15-C16-C17
33	L	101	LHG	C25-C26-C27-C28
33	L	101	LHG	C28-C29-C30-C31
33	l	101	LHG	C25-C26-C27-C28
33	l	101	LHG	C28-C29-C30-C31
34	C	516	DGD	CCA-CDA-CEA-CFA
34	c	516	DGD	CCA-CDA-CEA-CFA
28	A	410	SQD	O47-C45-C46-O48
28	a	410	SQD	O47-C45-C46-O48
29	A	411	LMG	O7-C8-C9-O8
29	a	411	LMG	O7-C8-C9-O8
25	B	612	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
33	D	407	LHG	C35-C36-C37-C38
33	E	102	LHG	C26-C27-C28-C29
33	d	407	LHG	C35-C36-C37-C38
33	e	102	LHG	C26-C27-C28-C29
28	B	620	SQD	C8-C7-O47-C45
28	T	101	SQD	C8-C7-O47-C45
25	B	609	CLA	C16-C17-C18-C19
25	b	609	CLA	C16-C17-C18-C19
34	C	516	DGD	O6E-C1E-O5D-C6D
34	c	516	DGD	O6E-C1E-O5D-C6D
33	L	101	LHG	C1-C2-C3-O3
33	l	101	LHG	C1-C2-C3-O3
25	B	602	CLA	C2-C1-O2A-CGA
25	C	501	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C2-C1-O2A-CGA
25	b	602	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	c	501	CLA	C2-C1-O2A-CGA
25	B	602	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14
25	C	507	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	b	602	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C10-C8-C9
25	d	404	CLA	C11-C12-C13-C14
34	c	515	DGD	C5B-C6B-C7B-C8B
25	C	504	CLA	C10-C11-C12-C13
25	c	504	CLA	C10-C11-C12-C13
33	A	419	LHG	C2-C3-O3-P
33	a	419	LHG	C2-C3-O3-P
31	I	102	LMT	C1-C2-C3-C4
31	i	102	LMT	C1-C2-C3-C4
29	D	409	LMG	C22-C23-C24-C25
29	d	409	LMG	C22-C23-C24-C25
34	C	515	DGD	C5B-C6B-C7B-C8B
25	B	614	CLA	C16-C17-C18-C20
25	C	503	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
27	A	409	BCR	C5-C6-C7-C8
27	A	409	BCR	C23-C24-C25-C26
27	A	409	BCR	C23-C24-C25-C30
27	B	618	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	D	405	BCR	C1-C6-C7-C8
27	D	405	BCR	C5-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C30
27	Z	101	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C30
27	a	409	BCR	C5-C6-C7-C8
27	a	409	BCR	C23-C24-C25-C26
27	a	409	BCR	C23-C24-C25-C30
27	b	618	BCR	C5-C6-C7-C8
27	b	619	BCR	C23-C24-C25-C26
27	d	405	BCR	C1-C6-C7-C8
27	d	405	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	k	102	BCR	C23-C24-C25-C30
27	z	101	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C30
37	X	102	RRX	C1-C6-C7-C8
37	x	102	RRX	C1-C6-C7-C8
25	B	614	CLA	C5-C6-C7-C8
25	b	614	CLA	C5-C6-C7-C8
27	z	101	BCR	C11-C12-C13-C35
28	A	410	SQD	C30-C31-C32-C33
28	a	410	SQD	C30-C31-C32-C33
31	a	416	LMT	C5-C6-C7-C8
26	D	402	PHO	O1D-CGD-O2D-CED
26	d	402	PHO	O1D-CGD-O2D-CED
31	A	416	LMT	C5-C6-C7-C8
34	C	515	DGD	O1B-C1B-O2G-C2G
34	c	515	DGD	O1B-C1B-O2G-C2G
28	A	414	SQD	C8-C7-O47-C45
28	a	414	SQD	C8-C7-O47-C45
28	A	410	SQD	C19-C20-C21-C22
28	a	410	SQD	C19-C20-C21-C22
25	C	502	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C19
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	D	403	CLA	C13-C15-C16-C17
25	d	403	CLA	C13-C15-C16-C17
31	C	520	LMT	C2-C3-C4-C5
34	C	516	DGD	C3A-C4A-C5A-C6A
34	c	516	DGD	C3A-C4A-C5A-C6A
25	D	401	CLA	O1A-CGA-O2A-C1
25	d	401	CLA	O1A-CGA-O2A-C1
29	c	518	LMG	C15-C16-C17-C18
31	c	520	LMT	C2-C3-C4-C5
33	B	622	LHG	O6-C4-C5-C6
33	E	102	LHG	O6-C4-C5-C6
33	b	621	LHG	O6-C4-C5-C6
33	e	102	LHG	O6-C4-C5-C6
29	C	518	LMG	C15-C16-C17-C18
25	B	604	CLA	C11-C10-C8-C7
25	B	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C10-C8-C7
25	b	608	CLA	C12-C13-C15-C16
25	b	611	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C10-C8-C7
25	c	507	CLA	C11-C10-C8-C7
25	d	404	CLA	C11-C12-C13-C15
31	K	104	LMT	C4-C5-C6-C7
31	k	104	LMT	C4-C5-C6-C7
34	H	103	DGD	CCB-CDB-CEB-CFB
34	h	103	DGD	CCB-CDB-CEB-CFB
25	C	503	CLA	C8-C10-C11-C12
25	C	507	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	507	CLA	C5-C6-C7-C8
27	B	618	BCR	C9-C10-C11-C12
27	K	102	BCR	C9-C10-C11-C12
27	b	618	BCR	C9-C10-C11-C12
27	k	102	BCR	C9-C10-C11-C12
31	m	101	LMT	C7-C8-C9-C10
25	b	608	CLA	O1D-CGD-O2D-CED
33	E	102	LHG	O10-C23-O8-C6
33	e	102	LHG	O10-C23-O8-C6
25	C	503	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
31	C	520	LMT	C5-C6-C7-C8
31	M	101	LMT	C7-C8-C9-C10
31	c	520	LMT	C5-C6-C7-C8
31	M	103	LMT	C1-C2-C3-C4
33	Z	102	LHG	C4-O6-P-O4
33	z	102	LHG	C4-O6-P-O4
28	A	410	SQD	C23-C24-C25-C26
28	a	410	SQD	C23-C24-C25-C26
31	m	103	LMT	C1-C2-C3-C4
25	B	608	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
25	c	501	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	608	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
31	D	412	LMT	C2-C3-C4-C5
31	X	101	LMT	C5-C6-C7-C8
31	x	101	LMT	C5-C6-C7-C8
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
26	A	407	PHO	CAD-CBD-CGD-O2D
26	a	407	PHO	CAD-CBD-CGD-O2D
28	K	101	SQD	C27-C28-C29-C30
28	k	101	SQD	C27-C28-C29-C30
31	d	412	LMT	C2-C3-C4-C5
33	D	407	LHG	C9-C10-C11-C12
33	d	407	LHG	C9-C10-C11-C12
25	C	501	CLA	CBA-CGA-O2A-C1
31	J	101	LMT	C4-C5-C6-C7
31	j	101	LMT	C4-C5-C6-C7
31	C	520	LMT	O5'-C1'-O1'-C1
28	A	410	SQD	C44-C45-C46-O48
28	B	620	SQD	C44-C45-C46-O48
28	H	102	SQD	O6-C44-C45-C46
28	T	101	SQD	C44-C45-C46-O48
28	a	410	SQD	C44-C45-C46-O48
28	h	102	SQD	O6-C44-C45-C46
31	I	102	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4'-C5'-C6'-O6'
33	Z	102	LHG	O6-C4-C5-O7
33	z	102	LHG	O6-C4-C5-O7
34	H	103	DGD	O2G-C1B-C2B-C3B
34	h	103	DGD	O2G-C1B-C2B-C3B
31	M	101	LMT	C6-C7-C8-C9
31	m	101	LMT	C6-C7-C8-C9
25	B	607	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
25	C	506	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	A	406	CLA	CHA-CBD-CGD-O1D
25	A	406	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	a	406	CLA	CHA-CBD-CGD-O1D
25	a	406	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	C	506	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	O1A-CGA-O2A-C1
28	H	102	SQD	C11-C12-C13-C14
33	d	408	LHG	C16-C17-C18-C19
31	E	101	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
28	h	102	SQD	C11-C12-C13-C14
31	e	103	LMT	C11-C10-C9-C8
33	D	408	LHG	C16-C17-C18-C19
28	B	620	SQD	O6-C44-C45-O47
28	H	102	SQD	O47-C45-C46-O48
28	T	101	SQD	O6-C44-C45-O47
28	f	101	SQD	O6-C44-C45-O47
28	h	102	SQD	O47-C45-C46-O48
33	B	622	LHG	O7-C5-C6-O8
33	L	101	LHG	O7-C5-C6-O8
33	b	621	LHG	O7-C5-C6-O8
33	l	101	LHG	O7-C5-C6-O8
31	E	103	LMT	C11-C10-C9-C8
33	A	419	LHG	O10-C23-O8-C6
33	a	419	LHG	O10-C23-O8-C6
31	C	521	LMT	C2-C3-C4-C5
31	c	521	LMT	C2-C3-C4-C5
33	D	407	LHG	C33-C34-C35-C36
33	d	407	LHG	C33-C34-C35-C36
25	A	406	CLA	C3-C5-C6-C7
25	a	406	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	A	419	LHG	C10-C11-C12-C13
33	a	419	LHG	C10-C11-C12-C13
25	B	613	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
30	D	406	PL9	C13-C14-C16-C17
30	d	406	PL9	C13-C14-C16-C17
25	B	602	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBA-CGA-O2A-C1
25	A	408	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	a	408	CLA	C11-C10-C8-C9
25	b	616	CLA	C11-C10-C8-C9
25	c	506	CLA	C14-C13-C15-C16
28	A	413	SQD	C23-C24-C25-C26
28	a	413	SQD	C23-C24-C25-C26
29	c	518	LMG	C33-C34-C35-C36
29	C	518	LMG	C33-C34-C35-C36
31	C	521	LMT	C1-C2-C3-C4
33	L	101	LHG	C30-C31-C32-C33
31	c	521	LMT	C1-C2-C3-C4
33	l	101	LHG	C30-C31-C32-C33
27	D	405	BCR	C17-C18-C19-C20
27	d	405	BCR	C17-C18-C19-C20
25	B	605	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C1A-C2A-CAA-CBA
31	d	411	LMT	C4-C5-C6-C7
25	A	406	CLA	C2-C1-O2A-CGA
25	a	406	CLA	C2-C1-O2A-CGA
31	D	411	LMT	C4-C5-C6-C7
33	A	419	LHG	C4-O6-P-O3
33	a	419	LHG	C4-O6-P-O3
29	B	621	LMG	C40-C41-C42-C43
29	D	409	LMG	C14-C15-C16-C17
29	d	409	LMG	C14-C15-C16-C17
31	X	103	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
33	E	102	LHG	C2-C3-O3-P
33	e	102	LHG	C2-C3-O3-P
28	B	620	SQD	C12-C13-C14-C15
31	x	103	LMT	C6-C7-C8-C9
33	Z	102	LHG	C29-C30-C31-C32
33	A	419	LHG	C4-O6-P-O5
33	B	622	LHG	C3-O3-P-O4
33	D	407	LHG	C3-O3-P-O4
33	D	408	LHG	C4-O6-P-O5
33	a	419	LHG	C4-O6-P-O5
33	b	621	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O4
33	d	408	LHG	C4-O6-P-O5
28	T	101	SQD	C12-C13-C14-C15
29	b	620	LMG	C40-C41-C42-C43
33	z	102	LHG	C29-C30-C31-C32
31	c	520	LMT	O5'-C1'-O1'-C1
31	D	412	LMT	C5'-C4'-O1B-C1B
31	d	412	LMT	C5'-C4'-O1B-C1B
30	A	412	PL9	C36-C37-C38-C39
30	a	412	PL9	C36-C37-C38-C39
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CAD-CBD-CGD-O1D
28	A	413	SQD	C5-C6-S-O7
28	A	414	SQD	C5-C6-S-O9
28	a	413	SQD	C5-C6-S-O7
28	a	414	SQD	C5-C6-S-O9
29	A	415	LMG	C30-C31-C32-C33
29	a	415	LMG	C30-C31-C32-C33
28	A	413	SQD	C25-C26-C27-C28
25	A	408	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	C	501	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	a	408	CLA	C11-C10-C8-C7
25	b	616	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	506	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
33	D	408	LHG	O6-C4-C5-O7
33	d	408	LHG	O6-C4-C5-O7
28	a	413	SQD	C25-C26-C27-C28
33	B	622	LHG	C30-C31-C32-C33
33	b	621	LHG	C30-C31-C32-C33
31	I	103	LMT	C2-C1-O1'-C1'
31	i	103	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C4B-C5B-C6B-O6B
33	A	419	LHG	C30-C31-C32-C33
33	a	419	LHG	C30-C31-C32-C33
25	D	401	CLA	C4C-C3C-CAC-CBC
31	E	103	LMT	C5'-C4'-O1B-C1B
31	e	103	LMT	C5'-C4'-O1B-C1B
33	L	101	LHG	C35-C36-C37-C38
33	l	101	LHG	C35-C36-C37-C38
31	B	625	LMT	C4B-C5B-C6B-O6B
25	d	401	CLA	C4C-C3C-CAC-CBC
28	B	620	SQD	O6-C44-C45-C46
28	T	101	SQD	O6-C44-C45-C46
31	C	519	LMT	O1'-C1-C2-C3
31	c	519	LMT	O1'-C1-C2-C3
34	C	516	DGD	C2E-C1E-O5D-C6D
34	c	516	DGD	C2E-C1E-O5D-C6D
28	B	620	SQD	O47-C45-C46-O48
28	F	101	SQD	O6-C44-C45-O47
28	T	101	SQD	O47-C45-C46-O48
25	c	510	CLA	C15-C16-C17-C18
31	H	101	LMT	C9-C10-C11-C12
31	d	410	LMT	C2-C3-C4-C5
31	h	101	LMT	C9-C10-C11-C12
31	D	410	LMT	C2-C3-C4-C5
33	D	407	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	C	519	LMT	O5'-C5'-C6'-O6'
31	c	519	LMT	O5'-C5'-C6'-O6'
34	C	516	DGD	C5D-C6D-O5D-C1E
34	c	516	DGD	C5D-C6D-O5D-C1E
25	B	606	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C12-C13-C15
25	C	510	CLA	C15-C16-C17-C18
33	d	407	LHG	C16-C17-C18-C19
31	I	103	LMT	C2-C3-C4-C5
31	i	103	LMT	C2-C3-C4-C5
31	m	101	LMT	C5-C6-C7-C8
31	x	101	LMT	O1'-C1-C2-C3
25	B	608	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C12-C13-C14
25	C	511	CLA	C11-C12-C13-C14
25	b	608	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C12-C13-C14
34	C	515	DGD	C1B-C2B-C3B-C4B
34	c	515	DGD	C1B-C2B-C3B-C4B
31	M	101	LMT	C5-C6-C7-C8
31	X	101	LMT	O1'-C1-C2-C3
31	T	102	LMT	O5'-C1'-O1'-C1
31	t	701	LMT	O5'-C1'-O1'-C1
25	B	602	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
27	K	102	BCR	C18-C19-C20-C21
27	k	102	BCR	C18-C19-C20-C21
25	B	614	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
29	C	523	LMG	C30-C31-C32-C33
29	a	411	LMG	C21-C22-C23-C24
29	c	523	LMG	C30-C31-C32-C33
33	B	622	LHG	C9-C10-C11-C12
33	b	621	LHG	C9-C10-C11-C12
29	A	411	LMG	C21-C22-C23-C24
29	A	415	LMG	C4-C5-C6-O5
33	D	408	LHG	C30-C31-C32-C33
29	a	415	LMG	C4-C5-C6-O5
28	A	413	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	a	413	SQD	C35-C36-C37-C38
31	I	101	LMT	C4-C5-C6-C7
31	i	101	LMT	C4-C5-C6-C7
33	E	102	LHG	C25-C26-C27-C28
33	d	408	LHG	C30-C31-C32-C33
33	e	102	LHG	C25-C26-C27-C28
28	A	410	SQD	C44-C45-O47-C7
28	a	410	SQD	C44-C45-O47-C7
33	Z	102	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
25	A	405	CLA	C2A-CAA-CBA-CGA
25	a	405	CLA	C2A-CAA-CBA-CGA
29	C	518	LMG	C40-C41-C42-C43
29	c	518	LMG	C40-C41-C42-C43
31	E	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	O1'-C1-C2-C3
25	A	408	CLA	C2-C1-O2A-CGA
25	D	401	CLA	C2-C1-O2A-CGA
25	a	408	CLA	C2-C1-O2A-CGA
25	d	401	CLA	C2-C1-O2A-CGA
25	C	510	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C19
31	H	101	LMT	C3-C4-C5-C6
31	h	101	LMT	C3-C4-C5-C6
28	H	102	SQD	C10-C11-C12-C13
28	h	102	SQD	C10-C11-C12-C13
25	C	507	CLA	C16-C17-C18-C19
25	C	511	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
29	A	411	LMG	C33-C34-C35-C36
25	A	408	CLA	C3-C5-C6-C7
25	a	408	CLA	C3-C5-C6-C7
27	A	409	BCR	C1-C6-C7-C8
27	B	618	BCR	C1-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C30
27	K	102	BCR	C23-C24-C25-C26
27	a	409	BCR	C1-C6-C7-C8
27	b	618	BCR	C1-C6-C7-C8
27	b	619	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C26
29	a	411	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
34	H	103	DGD	C9A-CAA-CBA-CCA
34	h	103	DGD	C9A-CAA-CBA-CCA
25	B	609	CLA	C16-C17-C18-C20
25	C	503	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
34	C	515	DGD	O6D-C5D-C6D-O5D
34	c	515	DGD	O6D-C5D-C6D-O5D
31	B	626	LMT	O5'-C1'-O1'-C1
31	K	104	LMT	O5'-C1'-O1'-C1
31	X	103	LMT	O5'-C1'-O1'-C1
31	b	625	LMT	O5'-C1'-O1'-C1
31	k	104	LMT	O5'-C1'-O1'-C1
31	x	103	LMT	O5'-C1'-O1'-C1
29	b	620	LMG	C33-C34-C35-C36
31	C	520	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	c	520	LMT	C2'-C1'-O1'-C1
31	m	102	LMT	C2'-C1'-O1'-C1
29	B	621	LMG	C33-C34-C35-C36
29	A	415	LMG	O7-C8-C9-O8
29	a	415	LMG	O7-C8-C9-O8
28	T	101	SQD	C28-C29-C30-C31
31	Y	101	LMT	C5-C6-C7-C8
31	y	101	LMT	C5-C6-C7-C8
34	H	103	DGD	C2A-C3A-C4A-C5A
34	h	103	DGD	C2A-C3A-C4A-C5A
33	B	622	LHG	C4-O6-P-O3
33	D	408	LHG	C3-O3-P-O6
33	E	102	LHG	C3-O3-P-O6
33	L	101	LHG	C3-O3-P-O6
33	b	621	LHG	C4-O6-P-O3
33	d	408	LHG	C3-O3-P-O6
33	e	102	LHG	C3-O3-P-O6
33	l	101	LHG	C3-O3-P-O6
28	B	620	SQD	C28-C29-C30-C31
34	h	103	DGD	CCA-CDA-CEA-CFA
34	H	103	DGD	CCA-CDA-CEA-CFA
25	B	615	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
34	c	515	DGD	C5A-C6A-C7A-C8A
34	C	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
30	D	406	PL9	C40-C39-C41-C42
30	d	406	PL9	C40-C39-C41-C42
25	C	511	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	c	511	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C12-C13-C15
31	B	626	LMT	C2-C3-C4-C5
31	b	625	LMT	C2-C3-C4-C5
25	B	602	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	c	509	CLA	C11-C10-C8-C9
27	D	405	BCR	C19-C20-C21-C22
27	d	405	BCR	C13-C14-C15-C16
25	B	612	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C20
25	b	612	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C20
31	I	102	LMT	C3-C4-C5-C6
31	b	622	LMT	C9-C10-C11-C12
31	B	623	LMT	C9-C10-C11-C12
31	i	102	LMT	C3-C4-C5-C6
27	Z	101	BCR	C11-C12-C13-C14
27	z	101	BCR	C11-C12-C13-C14
33	D	408	LHG	C17-C18-C19-C20
33	d	408	LHG	C17-C18-C19-C20
25	B	607	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
31	I	104	LMT	O1'-C1-C2-C3
25	B	615	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
31	i	104	LMT	O1'-C1-C2-C3
33	E	102	LHG	C9-C10-C11-C12
33	e	102	LHG	C9-C10-C11-C12
31	I	103	LMT	O5'-C1'-O1'-C1
31	i	103	LMT	O5'-C1'-O1'-C1
27	C	522	BCR	C9-C10-C11-C12
27	D	405	BCR	C13-C14-C15-C16
27	Z	101	BCR	C19-C20-C21-C22
27	c	522	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	d	405	BCR	C19-C20-C21-C22
27	z	101	BCR	C19-C20-C21-C22
31	B	625	LMT	C1-C2-C3-C4
31	b	624	LMT	C1-C2-C3-C4
28	F	101	SQD	C10-C11-C12-C13
28	f	101	SQD	C10-C11-C12-C13
28	K	101	SQD	C34-C35-C36-C37
34	C	515	DGD	C4D-C5D-C6D-O5D
34	c	515	DGD	C4D-C5D-C6D-O5D
28	k	101	SQD	C34-C35-C36-C37
30	D	406	PL9	C28-C29-C31-C32
30	d	406	PL9	C28-C29-C31-C32
25	B	607	CLA	C2-C1-O2A-CGA
25	C	511	CLA	C2-C1-O2A-CGA
25	b	607	CLA	C2-C1-O2A-CGA
25	c	511	CLA	C2-C1-O2A-CGA
29	c	523	LMG	C19-C20-C21-C22
29	C	523	LMG	C19-C20-C21-C22
25	b	607	CLA	C10-C11-C12-C13
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
28	A	414	SQD	O47-C45-C46-O48
28	a	414	SQD	O47-C45-C46-O48
28	B	620	SQD	C25-C26-C27-C28
28	T	101	SQD	C25-C26-C27-C28
29	C	523	LMG	O9-C10-O7-C8
29	c	523	LMG	O9-C10-O7-C8
25	B	607	CLA	C10-C11-C12-C13
31	a	417	LMT	C4-C5-C6-C7
34	C	515	DGD	C2A-C3A-C4A-C5A
34	c	515	DGD	C2A-C3A-C4A-C5A
31	A	417	LMT	C4-C5-C6-C7
31	b	622	LMT	C3-C4-C5-C6
31	B	623	LMT	C3-C4-C5-C6
33	A	419	LHG	C13-C14-C15-C16
33	a	419	LHG	C13-C14-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	b	605	CLA	C6-C7-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C12-C13-C14
25	b	606	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	V	201	HEM	CAD-CBD-CGD-O1D
35	v	201	HEM	CAD-CBD-CGD-O1D
29	a	411	LMG	C30-C31-C32-C33
31	M	102	LMT	C4-C5-C6-C7
31	m	102	LMT	C4-C5-C6-C7
27	K	102	BCR	C20-C21-C22-C37
27	k	102	BCR	C20-C21-C22-C37
29	B	621	LMG	C7-C8-C9-O8
29	b	620	LMG	C7-C8-C9-O8
33	B	622	LHG	C4-C5-C6-O8
33	b	621	LHG	C4-C5-C6-O8
29	A	411	LMG	C30-C31-C32-C33
31	A	416	LMT	C4-C5-C6-C7
31	X	101	LMT	C2-C3-C4-C5
31	a	416	LMT	C4-C5-C6-C7
31	x	101	LMT	C2-C3-C4-C5
25	C	511	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C19
31	I	101	LMT	O5'-C1'-O1'-C1
31	i	101	LMT	O5'-C1'-O1'-C1
34	C	515	DGD	O6E-C1E-O5D-C6D
34	c	515	DGD	O6E-C1E-O5D-C6D
34	C	515	DGD	C6B-C7B-C8B-C9B
34	c	515	DGD	C6B-C7B-C8B-C9B
28	K	101	SQD	C30-C31-C32-C33
28	k	101	SQD	C30-C31-C32-C33
33	Z	102	LHG	C35-C36-C37-C38
33	z	102	LHG	C35-C36-C37-C38
33	L	101	LHG	C6-C5-O7-C7
33	l	101	LHG	C6-C5-O7-C7
25	A	406	CLA	C1A-C2A-CAA-CBA
25	B	608	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C20
25	d	404	CLA	C16-C17-C18-C20
25	B	613	CLA	C6-C7-C8-C10
25	B	615	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	b	613	CLA	C6-C7-C8-C10
25	b	615	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C11-C10-C8-C7
28	B	620	SQD	C35-C36-C37-C38
28	T	101	SQD	C35-C36-C37-C38
31	B	624	LMT	C11-C10-C9-C8
31	b	623	LMT	C11-C10-C9-C8
31	E	103	LMT	C3-C4-C5-C6
31	e	103	LMT	C3-C4-C5-C6
33	D	408	LHG	C11-C12-C13-C14
33	d	408	LHG	C11-C12-C13-C14
25	D	404	CLA	C16-C17-C18-C20
31	x	104	LMT	C2-C3-C4-C5
28	A	414	SQD	O47-C7-C8-C9
28	a	414	SQD	O47-C7-C8-C9
31	X	104	LMT	C2-C3-C4-C5
34	C	516	DGD	C9A-CAA-CBA-CCA
34	c	516	DGD	C9A-CAA-CBA-CCA
31	J	101	LMT	C6-C7-C8-C9
31	j	101	LMT	C6-C7-C8-C9
25	B	601	CLA	CAA-CBA-CGA-O2A
25	b	601	CLA	CAA-CBA-CGA-O2A
27	K	102	BCR	C20-C21-C22-C23
27	k	102	BCR	C20-C21-C22-C23
28	A	410	SQD	C34-C35-C36-C37
28	a	410	SQD	C34-C35-C36-C37
31	a	416	LMT	O1'-C1-C2-C3
31	A	416	LMT	O1'-C1-C2-C3
34	C	516	DGD	O1A-C1A-O1G-C1G
34	c	516	DGD	O1A-C1A-O1G-C1G
33	A	419	LHG	C1-C2-C3-O3
33	a	419	LHG	C1-C2-C3-O3
31	d	412	LMT	C3'-C4'-O1B-C1B
26	A	407	PHO	C14-C13-C15-C16
26	a	407	PHO	C14-C13-C15-C16
31	D	412	LMT	C3'-C4'-O1B-C1B
25	B	614	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
31	B	623	LMT	C2-C3-C4-C5
31	b	622	LMT	C2-C3-C4-C5
25	B	601	CLA	CAA-CBA-CGA-O1A
25	b	601	CLA	CAA-CBA-CGA-O1A
25	B	607	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	B	618	BCR	C23-C24-C25-C30
27	C	522	BCR	C1-C6-C7-C8
27	C	522	BCR	C5-C6-C7-C8
27	b	618	BCR	C23-C24-C25-C26
27	b	618	BCR	C23-C24-C25-C30
27	c	522	BCR	C1-C6-C7-C8
27	c	522	BCR	C5-C6-C7-C8
34	C	515	DGD	O2G-C1B-C2B-C3B
34	c	515	DGD	O2G-C1B-C2B-C3B
31	C	524	LMT	C9-C10-C11-C12
31	c	524	LMT	C9-C10-C11-C12
25	B	603	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
29	C	523	LMG	C8-C7-O1-C1
29	c	523	LMG	C8-C7-O1-C1
34	C	515	DGD	C5D-C6D-O5D-C1E
34	c	515	DGD	C5D-C6D-O5D-C1E
28	A	410	SQD	C33-C34-C35-C36
28	a	410	SQD	C33-C34-C35-C36
25	C	501	CLA	C16-C17-C18-C20
25	c	501	CLA	C16-C17-C18-C20
28	H	102	SQD	C24-C25-C26-C27
31	M	103	LMT	C3-C4-C5-C6
33	E	102	LHG	O6-C4-C5-O7
33	e	102	LHG	O6-C4-C5-O7
28	h	102	SQD	C24-C25-C26-C27
31	m	103	LMT	C3-C4-C5-C6
25	B	601	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	O1A-CGA-O2A-C1
26	A	407	PHO	C3-C5-C6-C7
26	a	407	PHO	C3-C5-C6-C7
35	F	102	HEM	CAD-CBD-CGD-O1D
35	f	102	HEM	CAD-CBD-CGD-O1D
25	B	603	CLA	O1A-CGA-O2A-C1
28	T	101	SQD	C11-C12-C13-C14
25	B	609	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
28	B	620	SQD	C11-C12-C13-C14
29	C	523	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	c	523	LMG	O8-C28-C29-C30
34	C	517	DGD	O1G-C1A-C2A-C3A
34	c	517	DGD	O1G-C1A-C2A-C3A
28	A	410	SQD	C2-C1-O6-C44
28	a	410	SQD	C2-C1-O6-C44
31	K	104	LMT	C2'-C1'-O1'-C1
31	X	103	LMT	C2'-C1'-O1'-C1
31	k	104	LMT	C2'-C1'-O1'-C1
31	x	103	LMT	C2'-C1'-O1'-C1
33	D	408	LHG	C1-C2-C3-O3
33	d	408	LHG	C1-C2-C3-O3
28	A	413	SQD	O47-C45-C46-O48
28	a	413	SQD	O47-C45-C46-O48
29	C	518	LMG	O7-C10-C11-C12
29	c	518	LMG	O7-C10-C11-C12
31	i	101	LMT	C2-C3-C4-C5
31	I	101	LMT	C2-C3-C4-C5
34	C	516	DGD	C2A-C1A-O1G-C1G
34	c	516	DGD	C2A-C1A-O1G-C1G
25	C	508	CLA	C8-C10-C11-C12
25	c	508	CLA	C8-C10-C11-C12
34	C	516	DGD	C2B-C3B-C4B-C5B
34	c	516	DGD	C2B-C3B-C4B-C5B
25	B	613	CLA	C6-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	501	CLA	C11-C12-C13-C14
25	b	613	CLA	C6-C7-C8-C9
25	b	615	CLA	C14-C13-C15-C16
25	c	501	CLA	C11-C12-C13-C14
31	C	521	LMT	C9-C10-C11-C12
31	c	521	LMT	C9-C10-C11-C12
26	D	402	PHO	C3A-C2A-CAA-CBA
26	d	402	PHO	C3A-C2A-CAA-CBA
28	A	410	SQD	C25-C26-C27-C28
28	a	410	SQD	C25-C26-C27-C28
25	A	405	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
34	C	517	DGD	O6D-C5D-C6D-O5D
34	c	517	DGD	O6D-C5D-C6D-O5D
35	V	201	HEM	CAD-CBD-CGD-O2D
35	v	201	HEM	CAD-CBD-CGD-O2D
25	B	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	612	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	C	512	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
25	B	612	CLA	C10-C11-C12-C13
25	b	612	CLA	C10-C11-C12-C13
33	D	407	LHG	O9-C7-O7-C5
33	d	407	LHG	O9-C7-O7-C5
25	C	513	CLA	C8-C10-C11-C12
25	c	513	CLA	C8-C10-C11-C12
25	B	609	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
30	D	406	PL9	C38-C39-C41-C42
30	d	406	PL9	C38-C39-C41-C42
25	b	612	CLA	CAA-CBA-CGA-O2A
28	K	101	SQD	O47-C7-C8-C9
28	k	101	SQD	O47-C7-C8-C9
29	C	523	LMG	O7-C10-C11-C12
29	c	523	LMG	O7-C10-C11-C12
31	X	104	LMT	C11-C10-C9-C8
31	x	104	LMT	C11-C10-C9-C8
28	F	101	SQD	O6-C44-C45-C46
28	f	101	SQD	O6-C44-C45-C46
34	C	515	DGD	C1G-C2G-C3G-O3G
34	c	515	DGD	C1G-C2G-C3G-O3G
25	B	612	CLA	CAA-CBA-CGA-O2A
29	c	523	LMG	C28-C29-C30-C31
28	A	410	SQD	C28-C29-C30-C31
28	a	410	SQD	C28-C29-C30-C31
26	A	407	PHO	O2A-C1-C2-C3
26	a	407	PHO	O2A-C1-C2-C3
25	B	603	CLA	CBA-CGA-O2A-C1
25	b	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	m	102	LMT	C4B-C5B-C6B-O6B
28	H	102	SQD	C23-C24-C25-C26
28	h	102	SQD	C23-C24-C25-C26
29	D	409	LMG	O7-C10-C11-C12
29	d	409	LMG	O7-C10-C11-C12
31	X	103	LMT	O1'-C1-C2-C3
31	x	103	LMT	O1'-C1-C2-C3
25	D	404	CLA	C16-C17-C18-C19
25	d	404	CLA	C16-C17-C18-C19
28	A	414	SQD	C27-C28-C29-C30
28	a	414	SQD	C27-C28-C29-C30
29	C	523	LMG	C28-C29-C30-C31
29	B	621	LMG	C31-C32-C33-C34
31	k	104	LMT	C3-C4-C5-C6
25	B	604	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	b	604	CLA	CHA-CBD-CGD-O2D
25	b	609	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	C	513	CLA	CAA-CBA-CGA-O2A
25	c	513	CLA	CAA-CBA-CGA-O2A
28	B	620	SQD	O47-C7-C8-C9
28	T	101	SQD	O47-C7-C8-C9
29	A	415	LMG	O8-C28-C29-C30
29	a	415	LMG	O8-C28-C29-C30
31	K	104	LMT	C3-C4-C5-C6
29	D	409	LMG	C37-C38-C39-C40
29	b	620	LMG	C31-C32-C33-C34
31	M	102	LMT	C4B-C5B-C6B-O6B
29	d	409	LMG	C37-C38-C39-C40
34	C	515	DGD	O2G-C2G-C3G-O3G
34	c	515	DGD	O2G-C2G-C3G-O3G
33	E	102	LHG	C11-C10-C9-C8
33	e	102	LHG	C11-C10-C9-C8
25	B	613	CLA	CAA-CBA-CGA-O2A
25	b	613	CLA	CAA-CBA-CGA-O2A
25	C	511	CLA	C2A-CAA-CBA-CGA
25	c	511	CLA	C2A-CAA-CBA-CGA
29	C	523	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	c	523	LMG	C11-C10-O7-C8
33	B	622	LHG	O8-C23-C24-C25
33	b	621	LHG	O8-C23-C24-C25
25	B	602	CLA	C12-C13-C15-C16
25	B	611	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C10-C8-C7
25	B	614	CLA	C12-C13-C15-C16
25	b	602	CLA	C12-C13-C15-C16
25	b	611	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C10-C8-C7
25	b	614	CLA	C12-C13-C15-C16
25	B	614	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
25	B	602	CLA	C14-C13-C15-C16
25	B	611	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	C	513	CLA	C14-C13-C15-C16
25	b	602	CLA	C14-C13-C15-C16
25	b	611	CLA	C6-C7-C8-C9
25	c	513	CLA	C11-C12-C13-C14
25	c	513	CLA	C14-C13-C15-C16
34	c	515	DGD	C3B-C4B-C5B-C6B
34	C	515	DGD	C3B-C4B-C5B-C6B
28	A	413	SQD	C4-C5-C6-S
28	A	414	SQD	C4-C5-C6-S
28	A	414	SQD	C5-C6-S-O8
28	a	413	SQD	C4-C5-C6-S
28	a	414	SQD	C4-C5-C6-S
28	a	414	SQD	C5-C6-S-O8
33	D	407	LHG	C8-C7-O7-C5
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
29	d	409	LMG	C13-C14-C15-C16
25	A	405	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
33	e	102	LHG	C24-C25-C26-C27
25	B	603	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	D	409	LMG	C13-C14-C15-C16
33	E	102	LHG	C24-C25-C26-C27
33	d	407	LHG	C8-C7-O7-C5
28	A	413	SQD	O49-C7-C8-C9
28	a	413	SQD	O49-C7-C8-C9
29	a	415	LMG	O10-C28-C29-C30
29	c	523	LMG	C31-C32-C33-C34
31	a	416	LMT	C11-C10-C9-C8
35	F	102	HEM	CAD-CBD-CGD-O2D
35	f	102	HEM	CAD-CBD-CGD-O2D
28	H	102	SQD	C44-C45-C46-O48
28	h	102	SQD	C44-C45-C46-O48
29	C	523	LMG	C31-C32-C33-C34
25	B	610	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
31	A	416	LMT	C11-C10-C9-C8
25	C	513	CLA	CAA-CBA-CGA-O1A
25	c	513	CLA	CAA-CBA-CGA-O1A
29	A	415	LMG	O10-C28-C29-C30
29	C	523	LMG	O9-C10-C11-C12
29	c	523	LMG	O9-C10-C11-C12
31	B	626	LMT	C2'-C1'-O1'-C1
31	b	625	LMT	C2'-C1'-O1'-C1
25	b	606	CLA	C10-C11-C12-C13
33	D	408	LHG	C3-O3-P-O5
33	E	102	LHG	C3-O3-P-O5
33	d	408	LHG	C3-O3-P-O5
33	e	102	LHG	C3-O3-P-O5
25	B	613	CLA	CAA-CBA-CGA-O1A
25	b	613	CLA	CAA-CBA-CGA-O1A
29	C	523	LMG	O10-C28-C29-C30
29	c	523	LMG	O10-C28-C29-C30
25	B	606	CLA	C10-C11-C12-C13
27	B	618	BCR	C23-C24-C25-C26
27	C	522	BCR	C23-C24-C25-C26
27	C	522	BCR	C23-C24-C25-C30
27	c	522	BCR	C23-C24-C25-C26
27	c	522	BCR	C23-C24-C25-C30
29	D	409	LMG	O9-C10-C11-C12
29	d	409	LMG	O9-C10-C11-C12
25	B	608	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	i	102	LMT	C4-C5-C6-C7
31	I	102	LMT	C4-C5-C6-C7
34	C	516	DGD	CCB-CDB-CEB-CFB
34	c	516	DGD	CCB-CDB-CEB-CFB
33	b	621	LHG	O10-C23-C24-C25
25	B	607	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
28	A	413	SQD	O5-C5-C6-S
28	A	414	SQD	O5-C5-C6-S
28	H	102	SQD	O5-C5-C6-S
28	a	413	SQD	O5-C5-C6-S
28	a	414	SQD	O5-C5-C6-S
28	h	102	SQD	O5-C5-C6-S
33	L	101	LHG	C4-C5-O7-C7
33	l	101	LHG	C4-C5-O7-C7
25	D	403	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
33	B	622	LHG	O10-C23-C24-C25
25	C	506	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C10-C8-C9
29	A	415	LMG	C11-C12-C13-C14
29	a	415	LMG	C11-C12-C13-C14
25	C	504	CLA	C16-C17-C18-C19
25	c	504	CLA	C16-C17-C18-C19
28	k	101	SQD	C13-C14-C15-C16
31	J	101	LMT	C3-C4-C5-C6
31	j	101	LMT	C3-C4-C5-C6
28	K	101	SQD	C13-C14-C15-C16
31	A	417	LMT	C2-C3-C4-C5
31	a	417	LMT	C2-C3-C4-C5
25	C	510	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
29	A	411	LMG	O7-C10-C11-C12
29	a	411	LMG	O7-C10-C11-C12
33	B	622	LHG	O7-C7-C8-C9
33	E	102	LHG	O8-C23-C24-C25
33	b	621	LHG	O7-C7-C8-C9
33	e	102	LHG	O8-C23-C24-C25
25	B	614	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	B	609	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
30	A	412	PL9	C12-C11-C9-C10
30	a	412	PL9	C12-C11-C9-C10
31	B	623	LMT	C6-C7-C8-C9
31	b	622	LMT	C6-C7-C8-C9
25	C	506	CLA	C11-C10-C8-C7
25	D	403	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C10-C8-C7
25	d	403	CLA	C12-C13-C15-C16
34	H	103	DGD	O1B-C1B-C2B-C3B
34	h	103	DGD	O1B-C1B-C2B-C3B
27	C	514	BCR	C7-C8-C9-C10
27	c	514	BCR	C7-C8-C9-C10
37	X	102	RRX	C7-C8-C9-C10
37	x	102	RRX	C7-C8-C9-C10
28	H	102	SQD	O49-C7-C8-C9
28	f	101	SQD	O49-C7-C8-C9
28	h	102	SQD	O49-C7-C8-C9
25	A	408	CLA	CAA-CBA-CGA-O2A
25	a	408	CLA	CAA-CBA-CGA-O2A
25	A	406	CLA	O1A-CGA-O2A-C1
25	a	406	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
28	F	101	SQD	O49-C7-C8-C9
28	A	410	SQD	O47-C7-C8-C9
28	a	410	SQD	O47-C7-C8-C9
25	B	607	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
35	F	102	HEM	CAA-CBA-CGA-O2A
35	f	102	HEM	CAA-CBA-CGA-O2A
33	l	101	LHG	C7-C8-C9-C10
33	Z	102	LHG	O8-C23-C24-C25
33	z	102	LHG	O8-C23-C24-C25

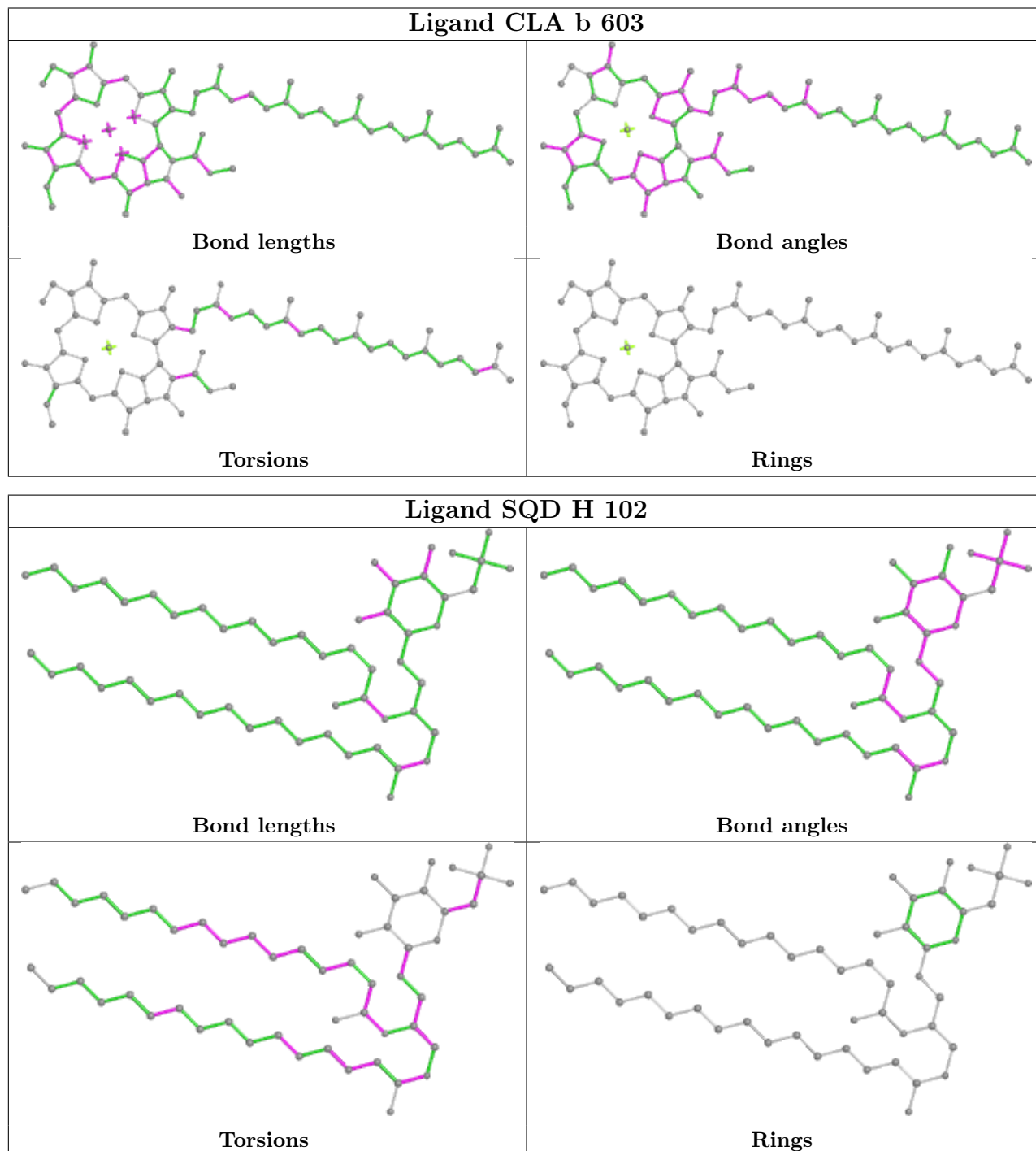
There are no ring outliers.

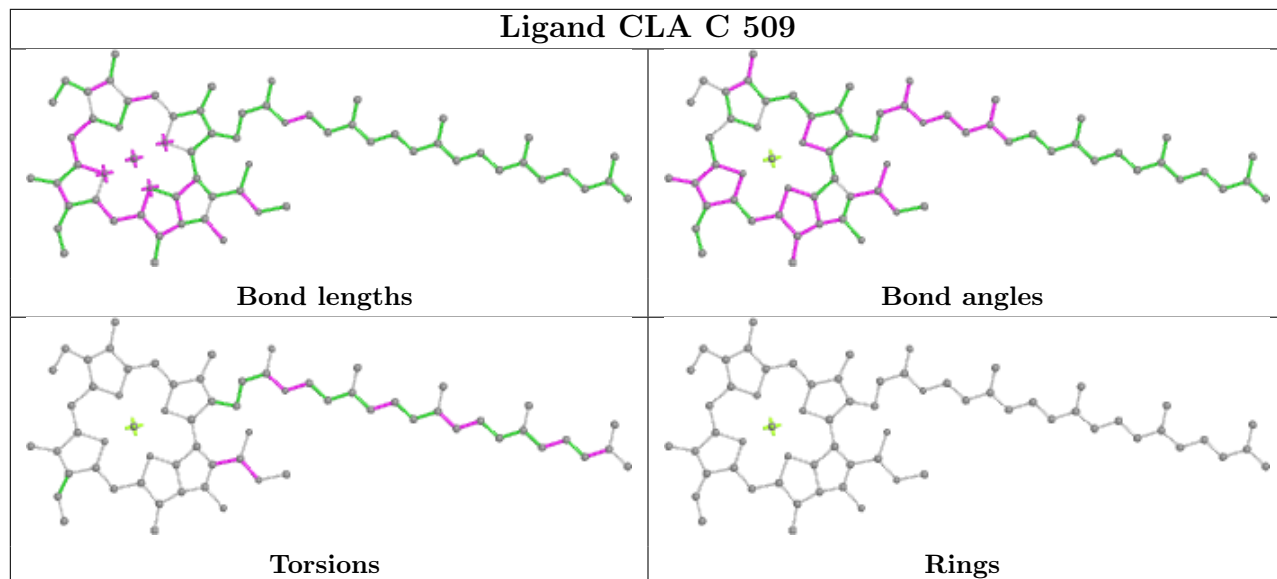
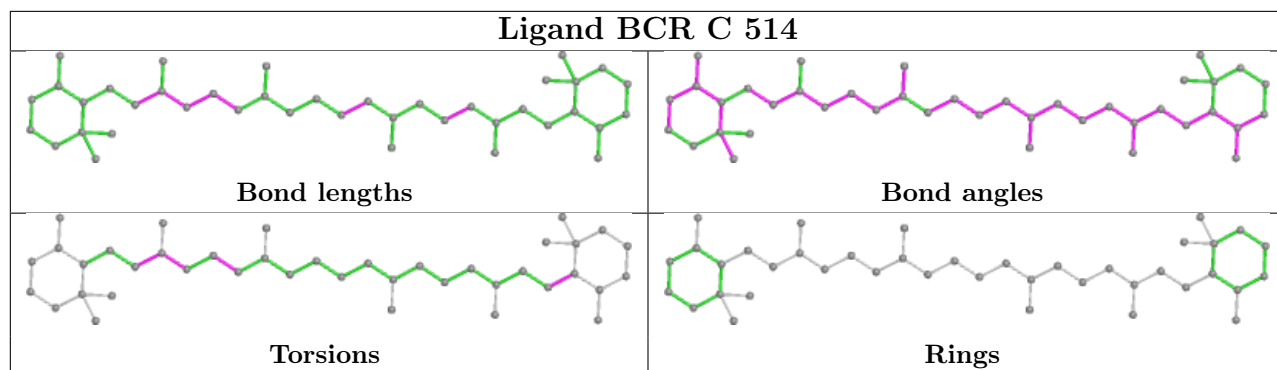
No monomer is involved in short contacts.

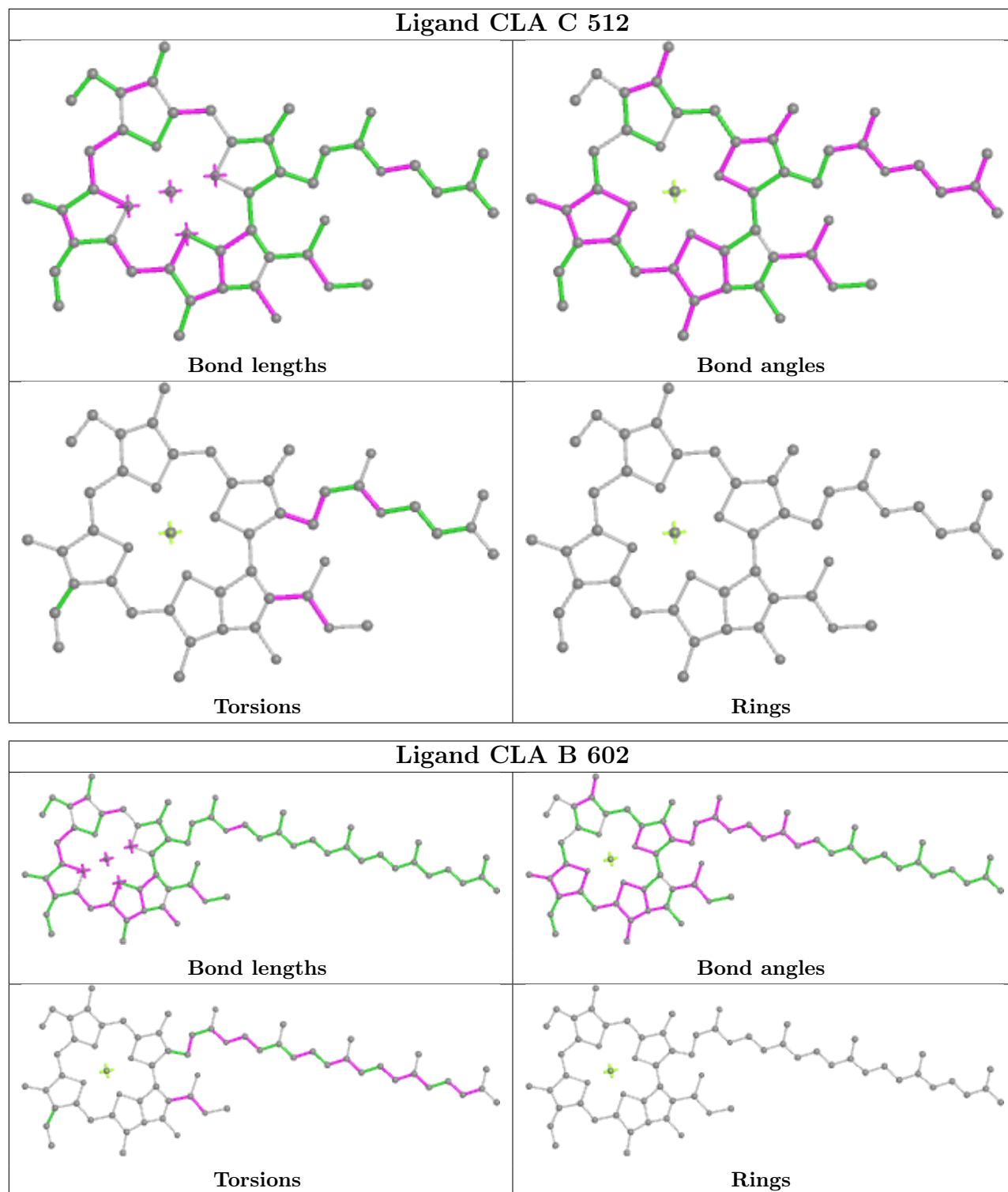
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

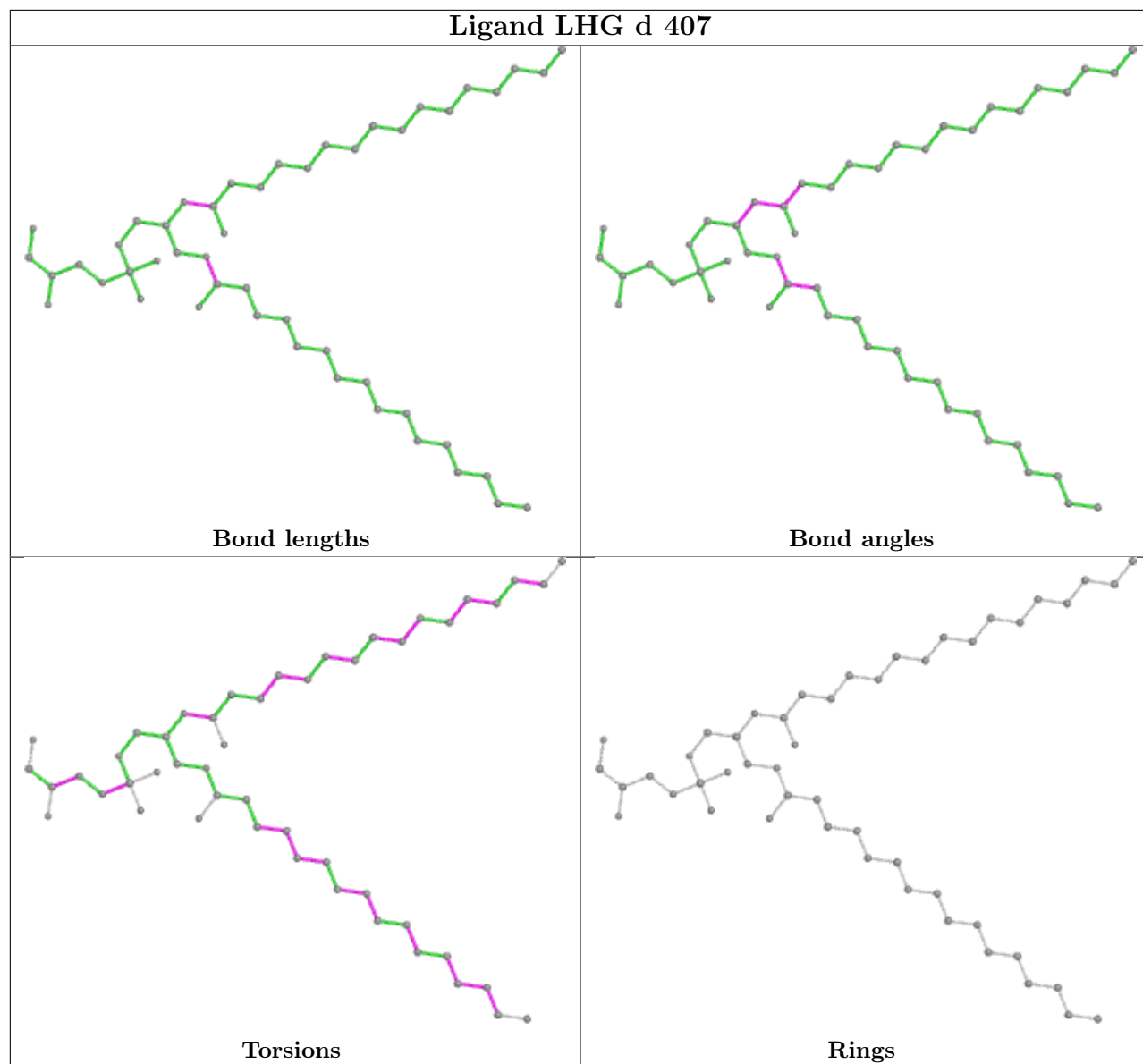


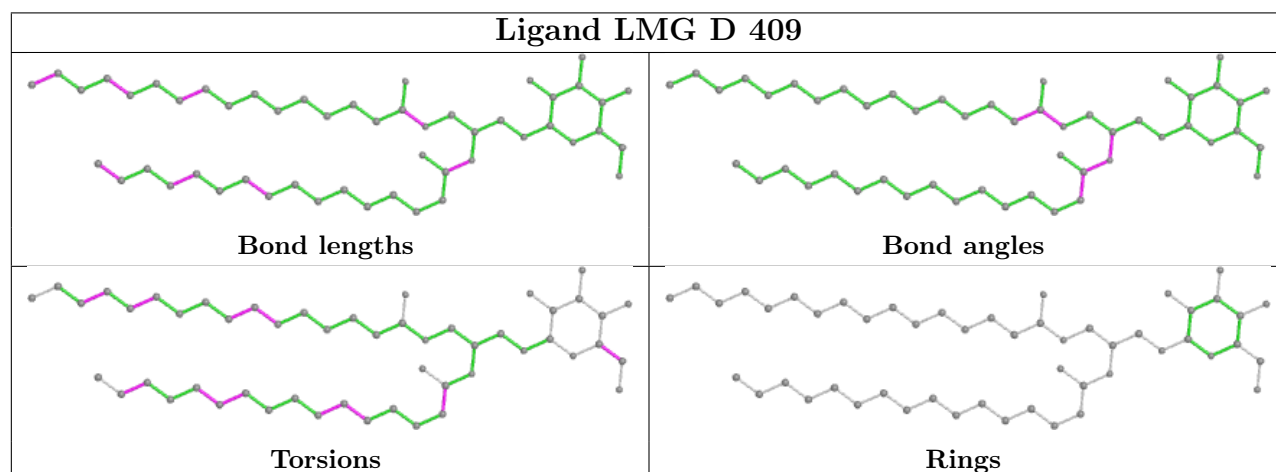
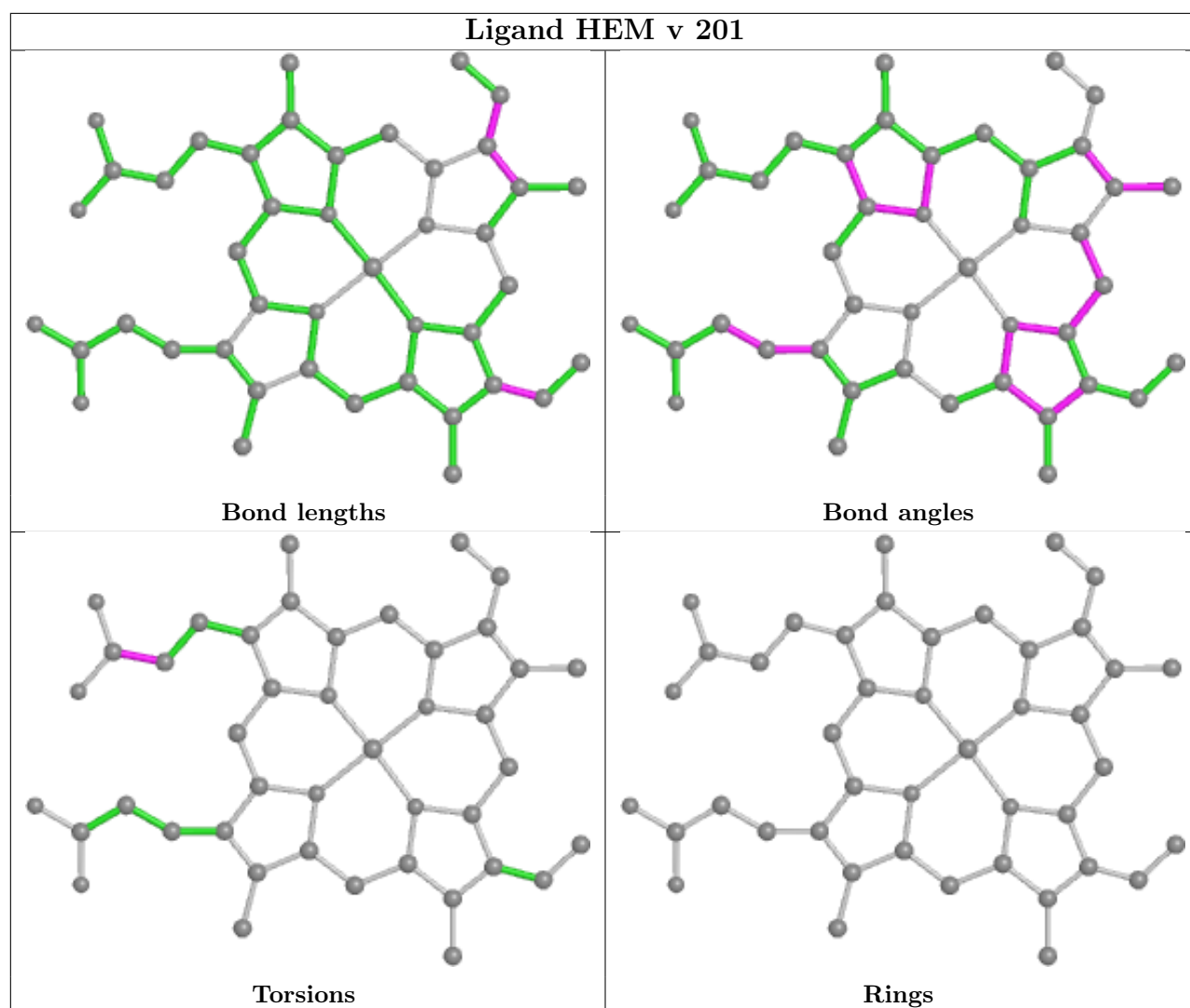
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

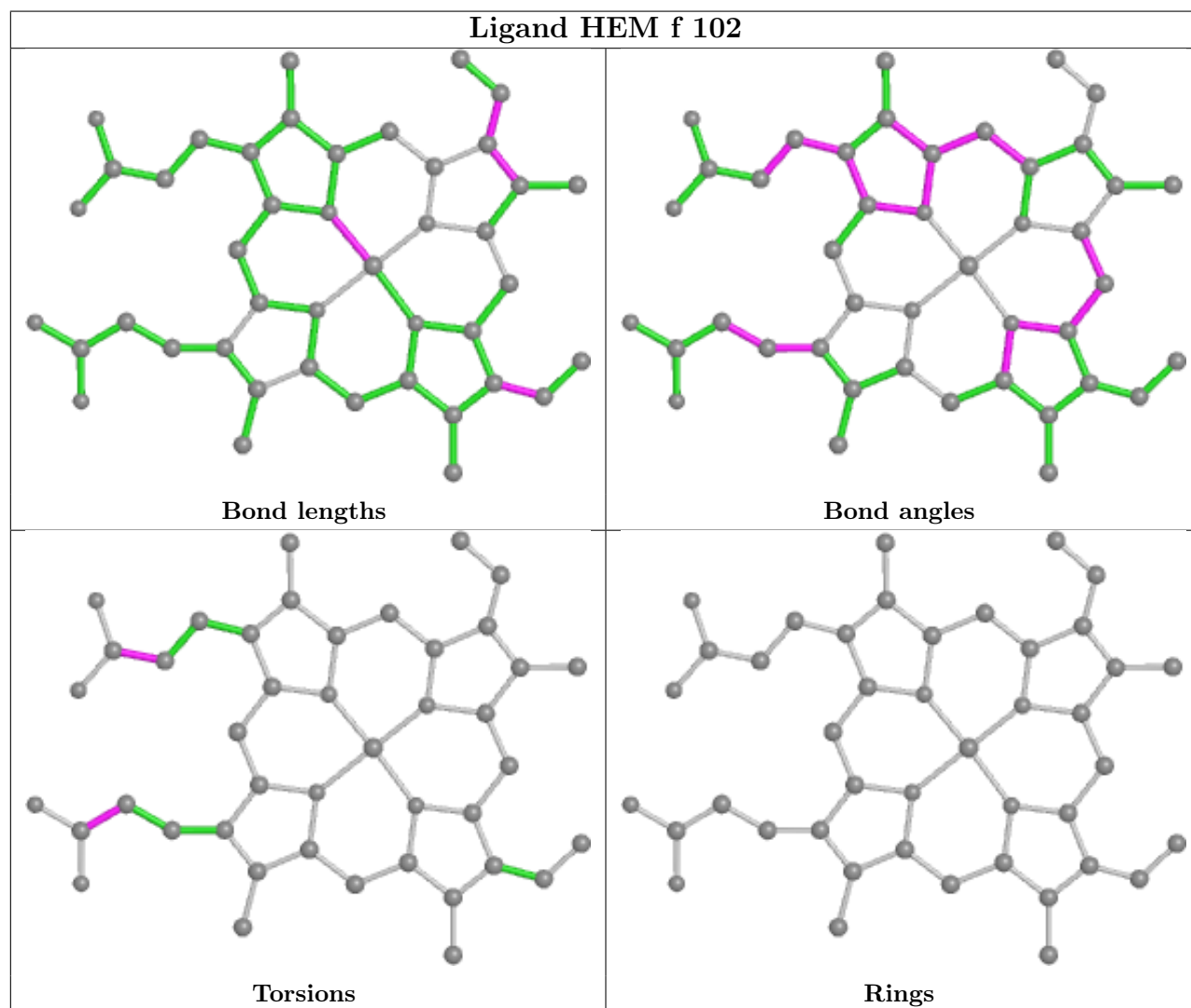
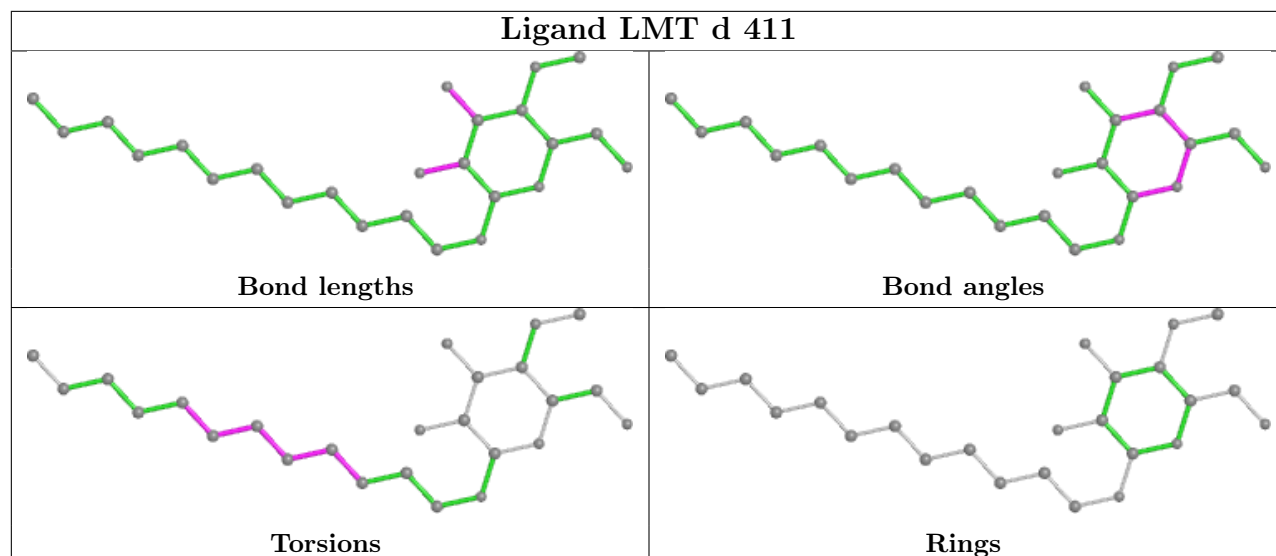


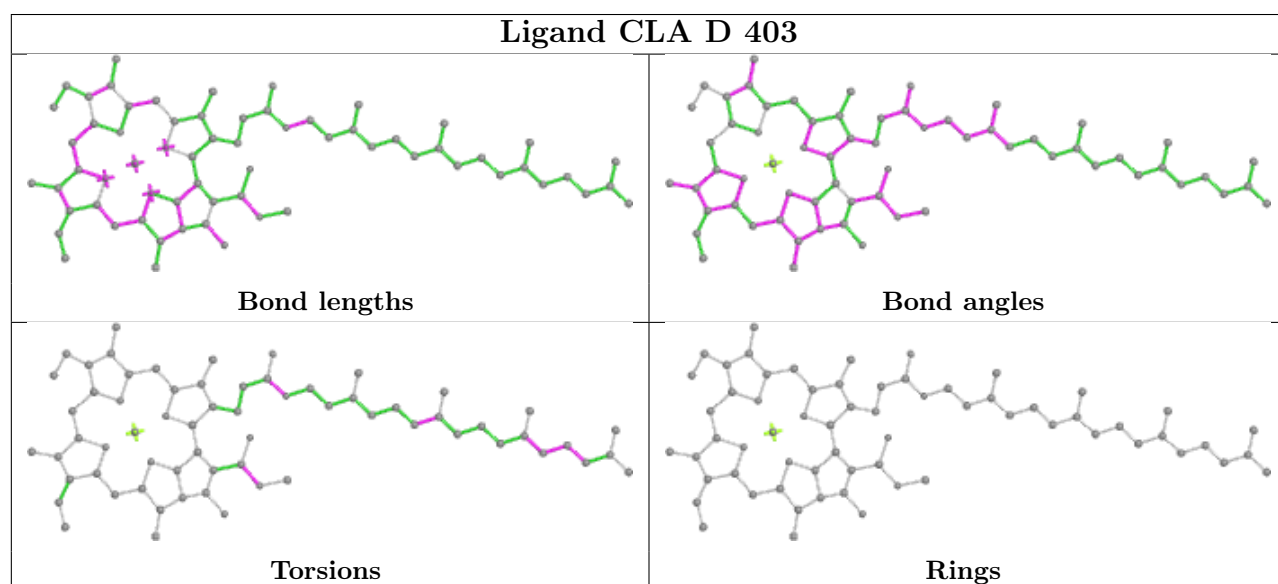
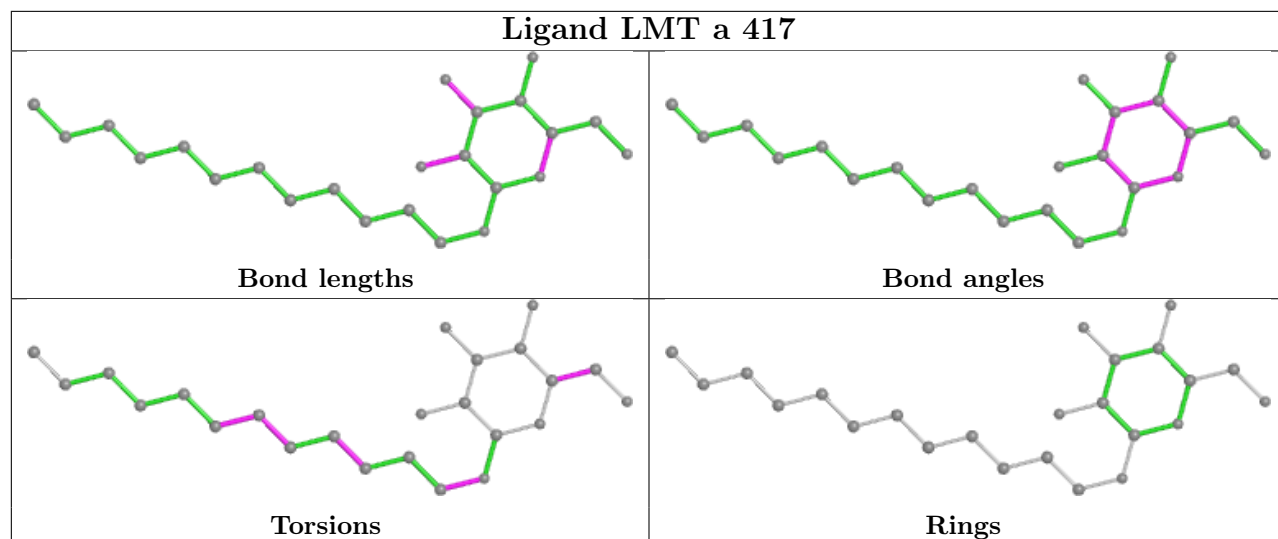


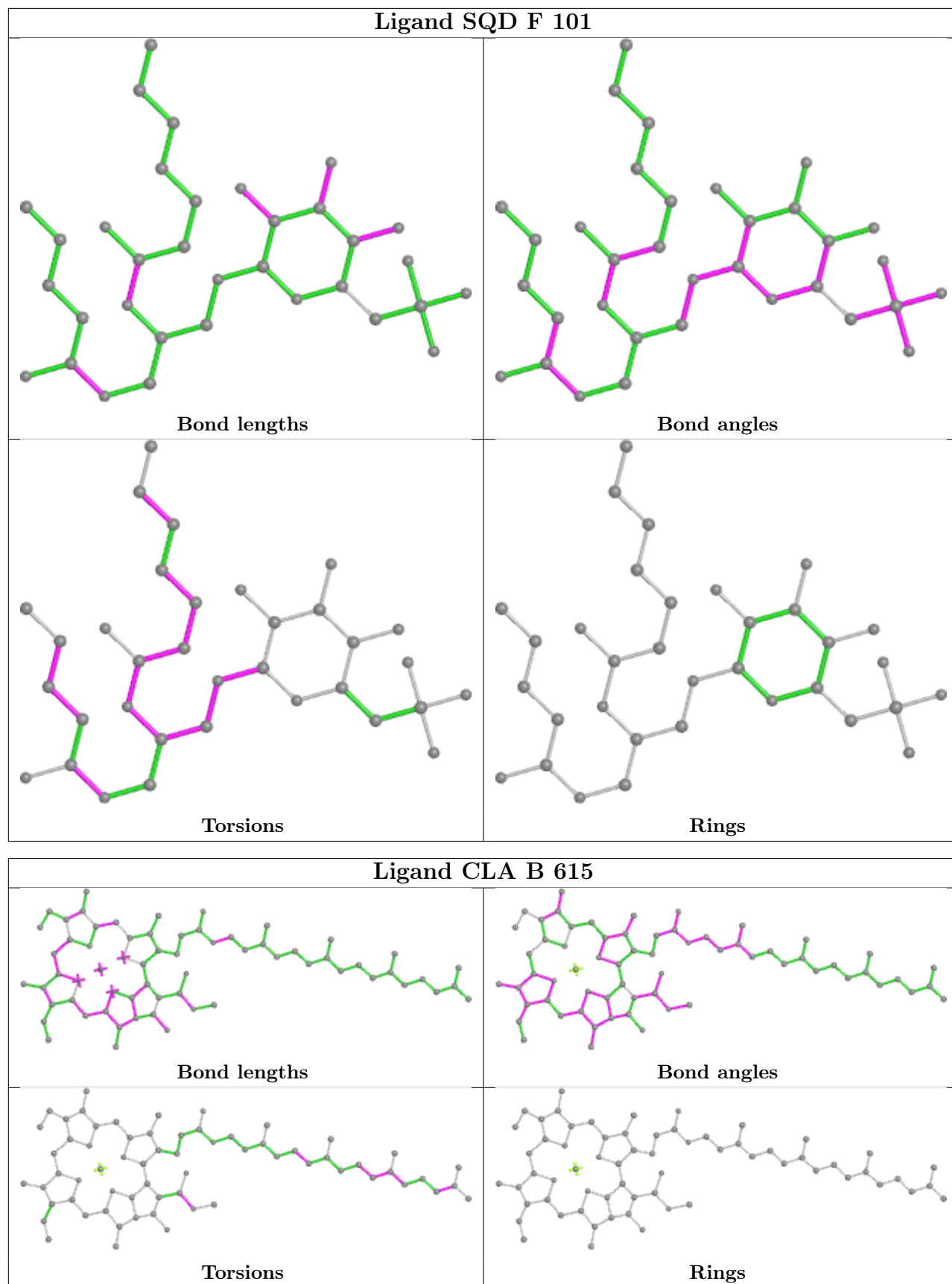




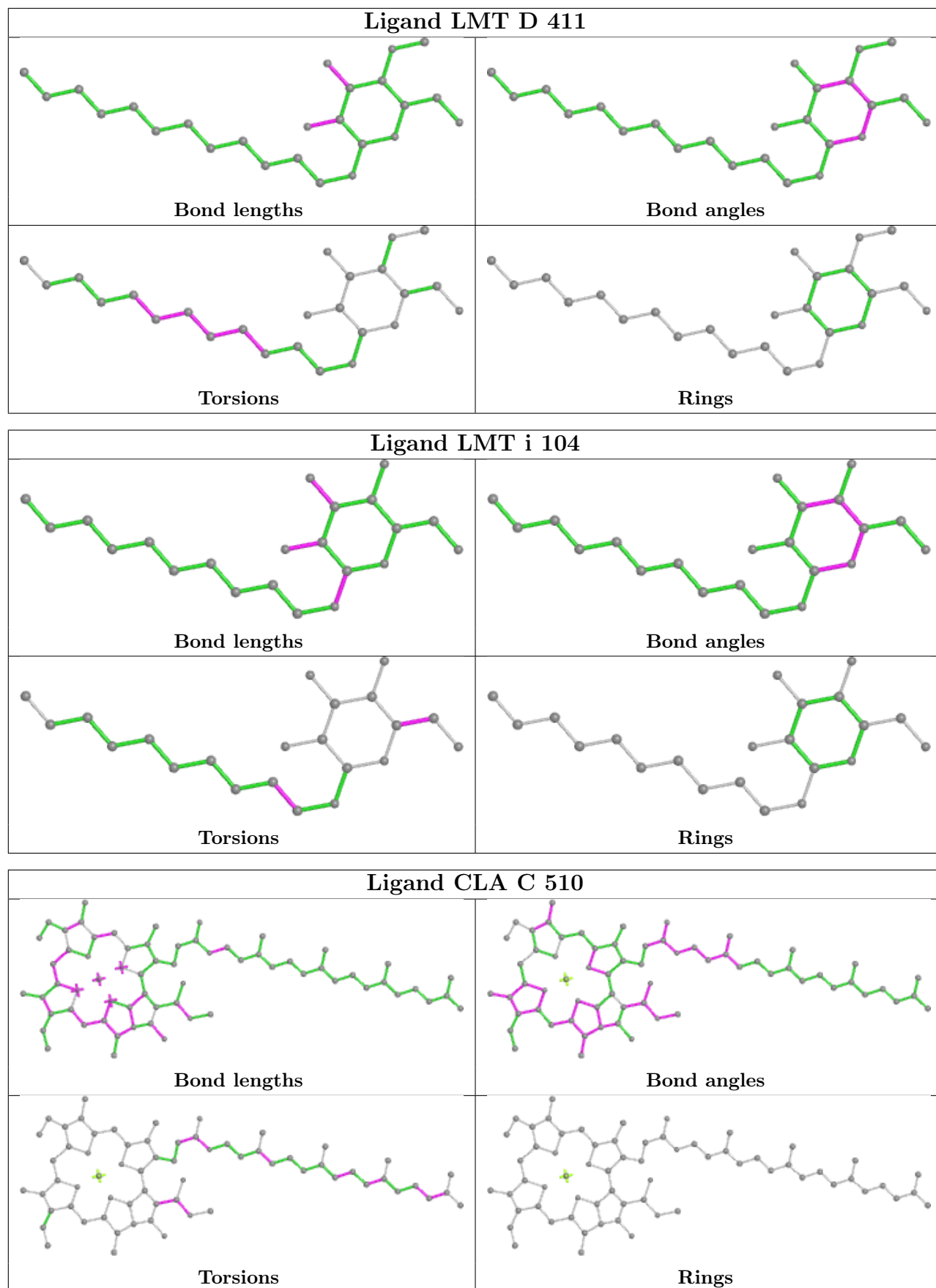


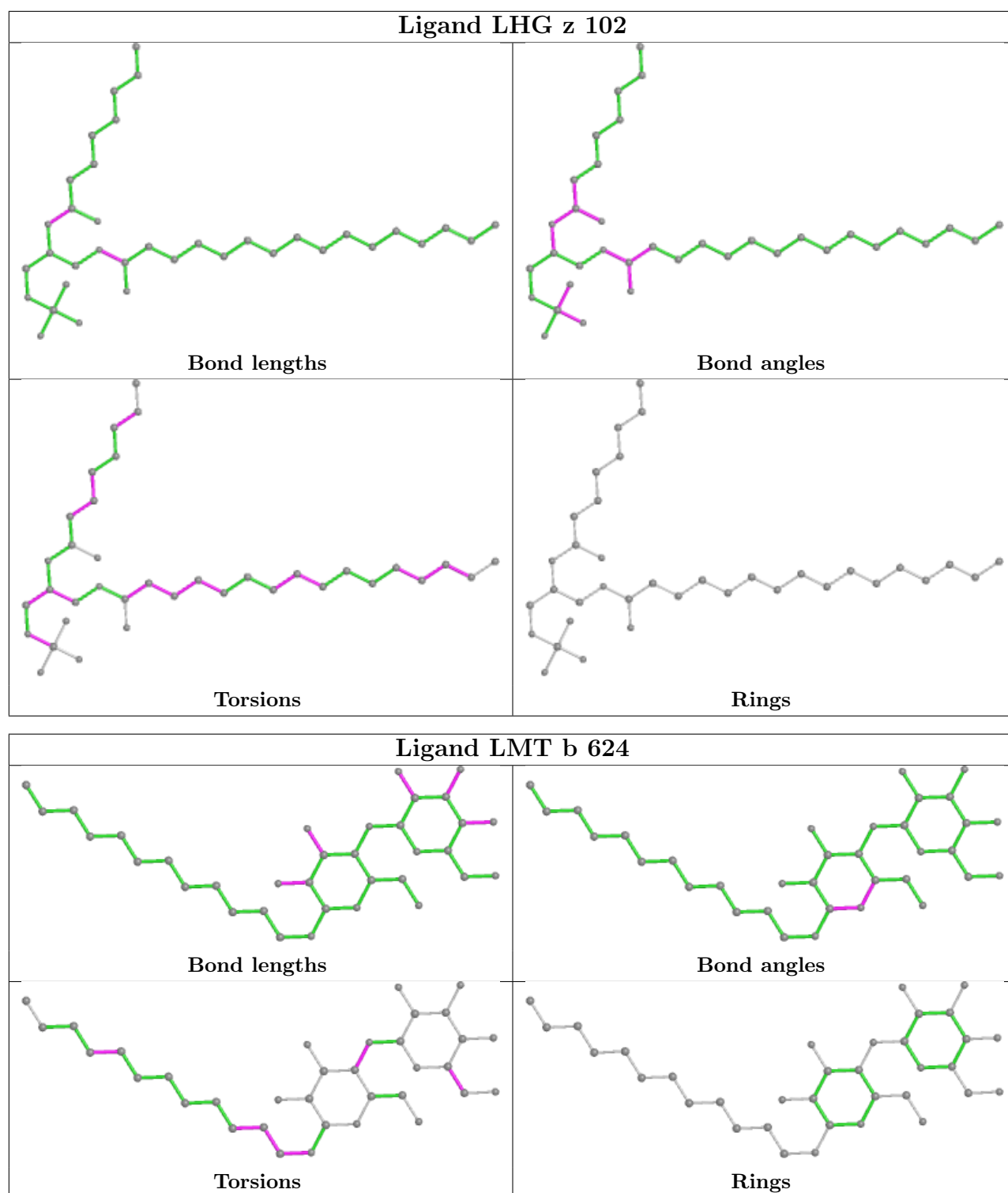


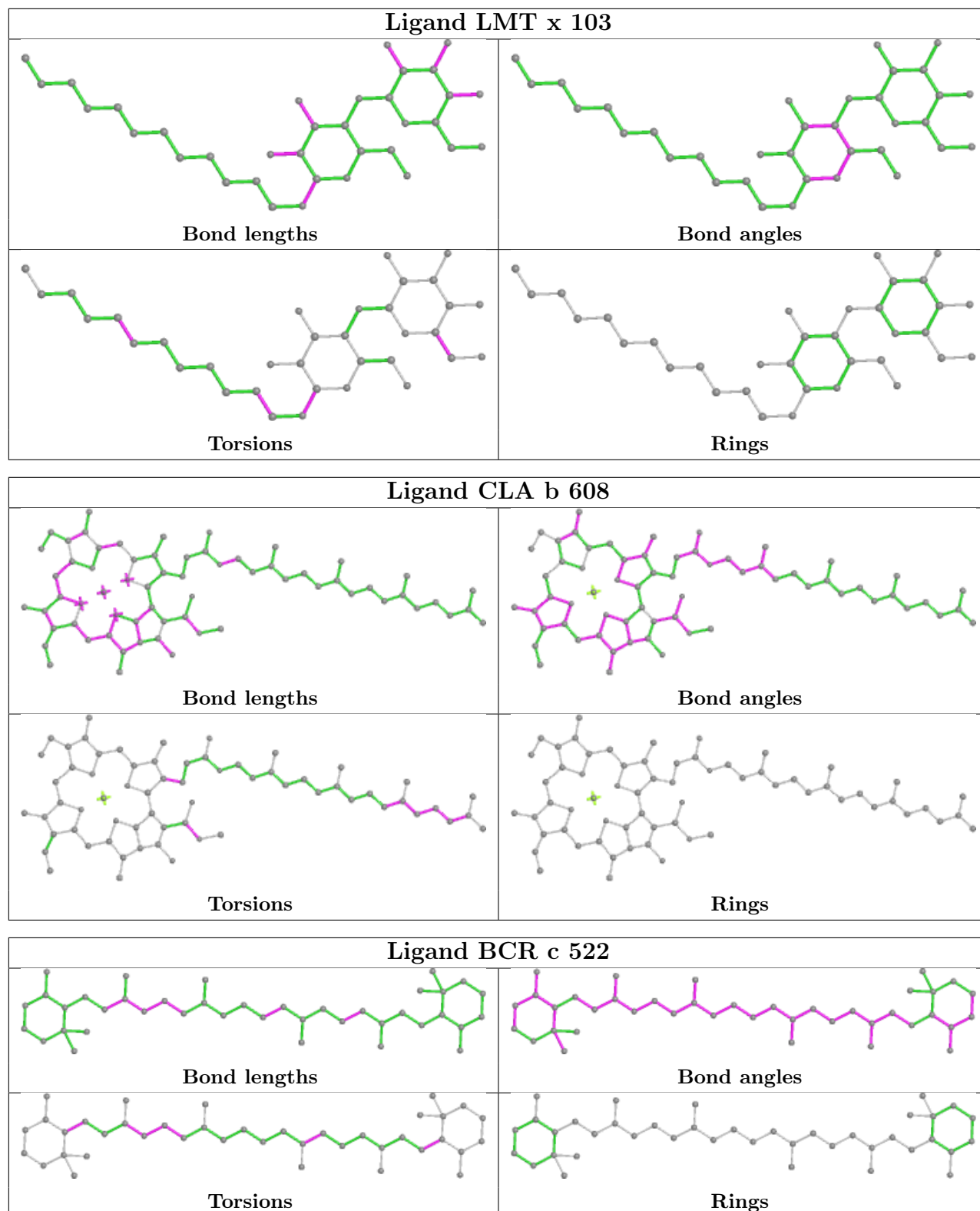


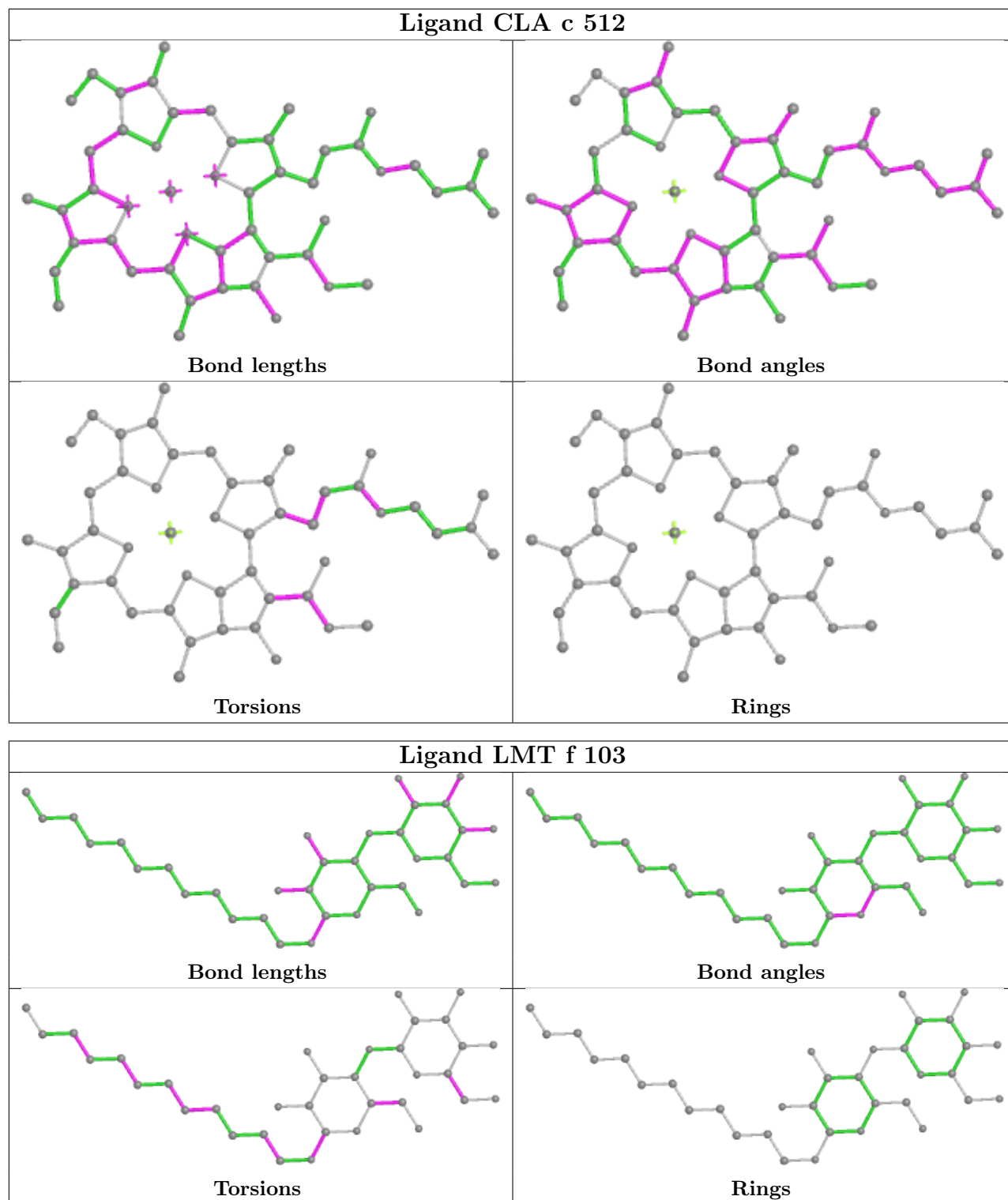


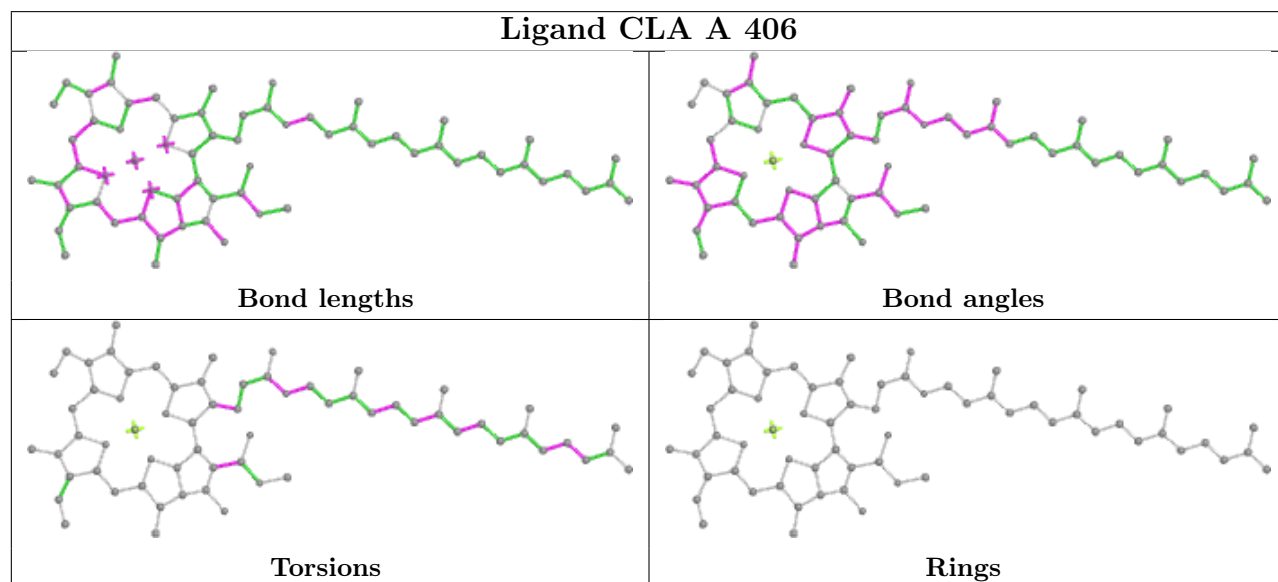
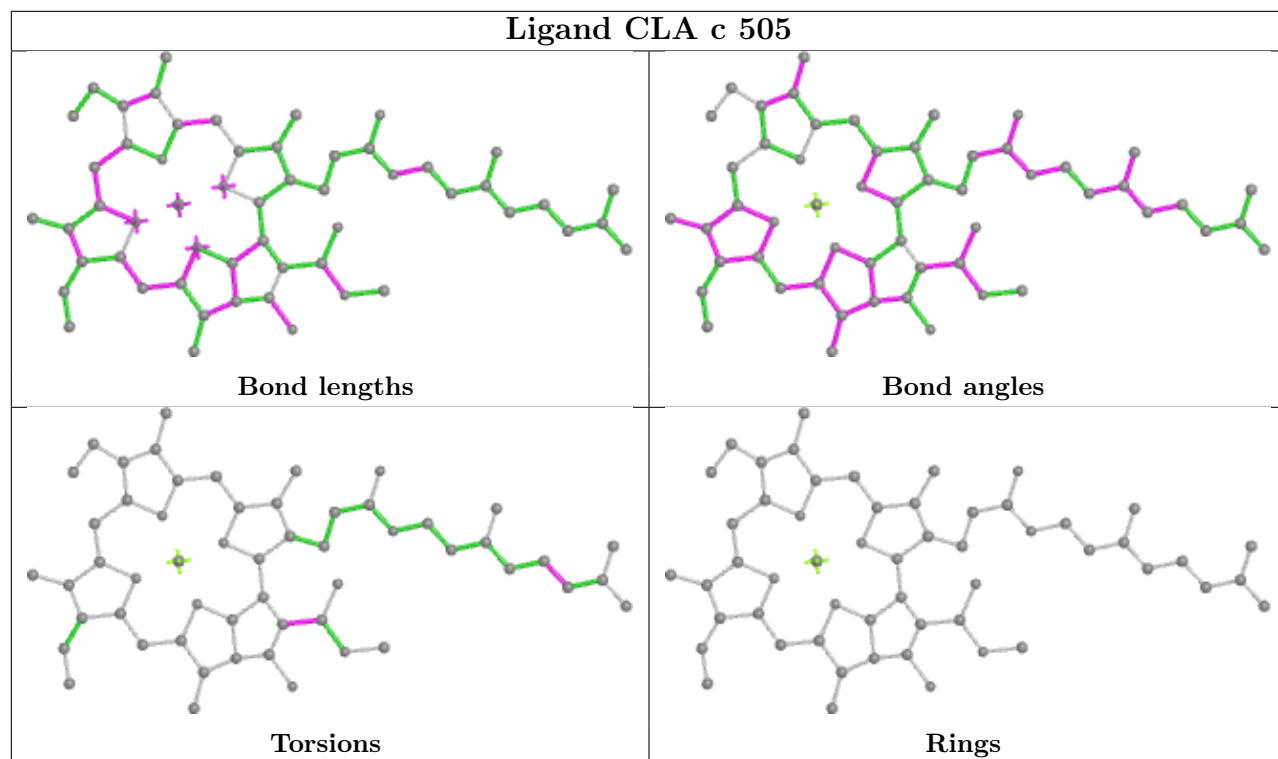


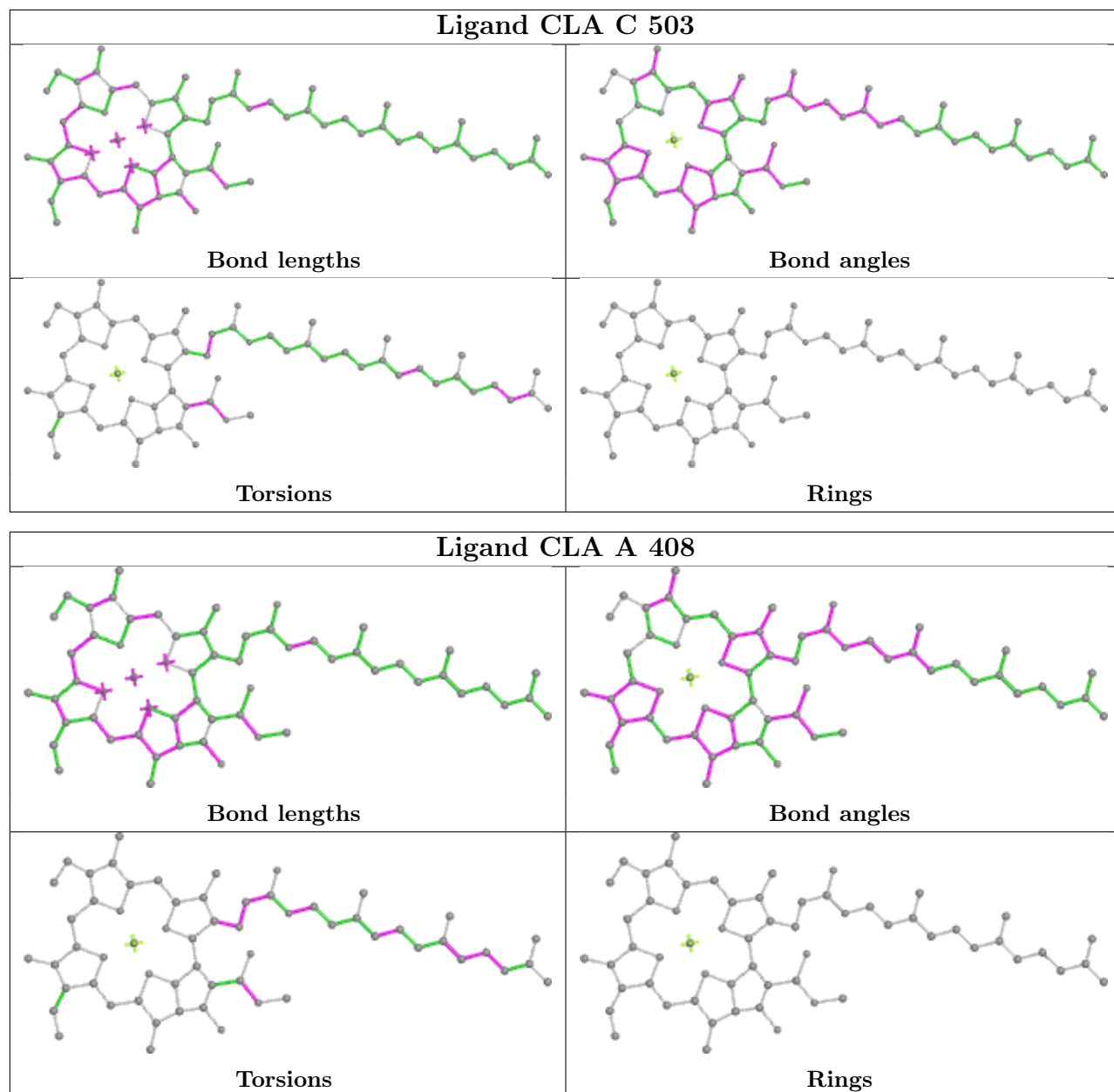


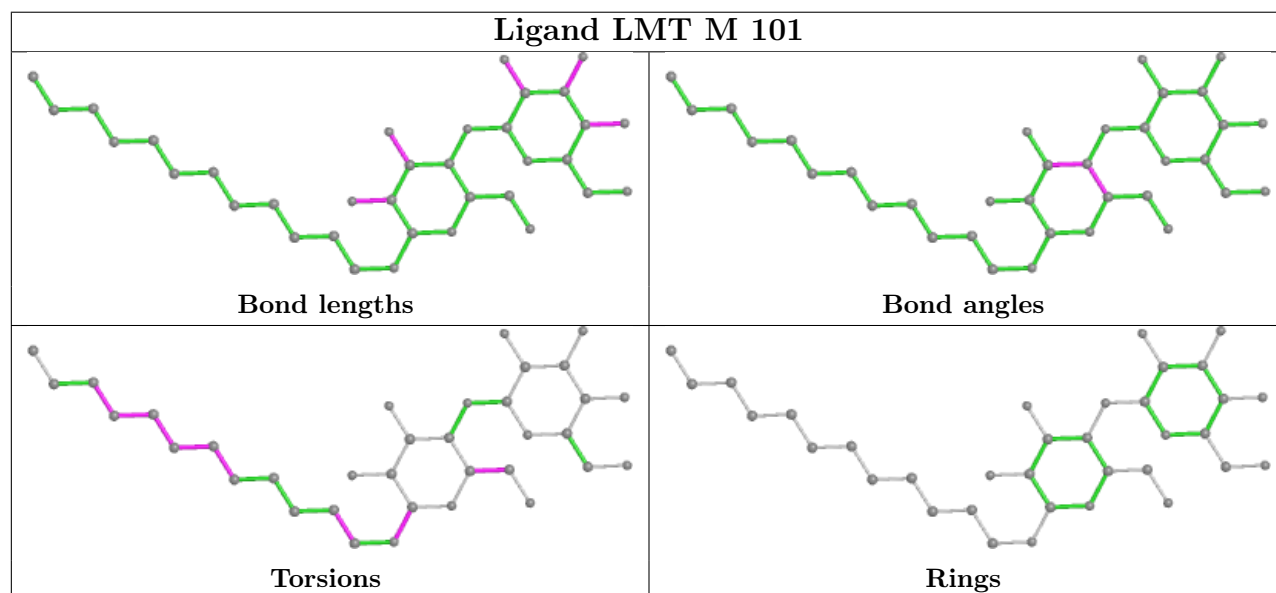
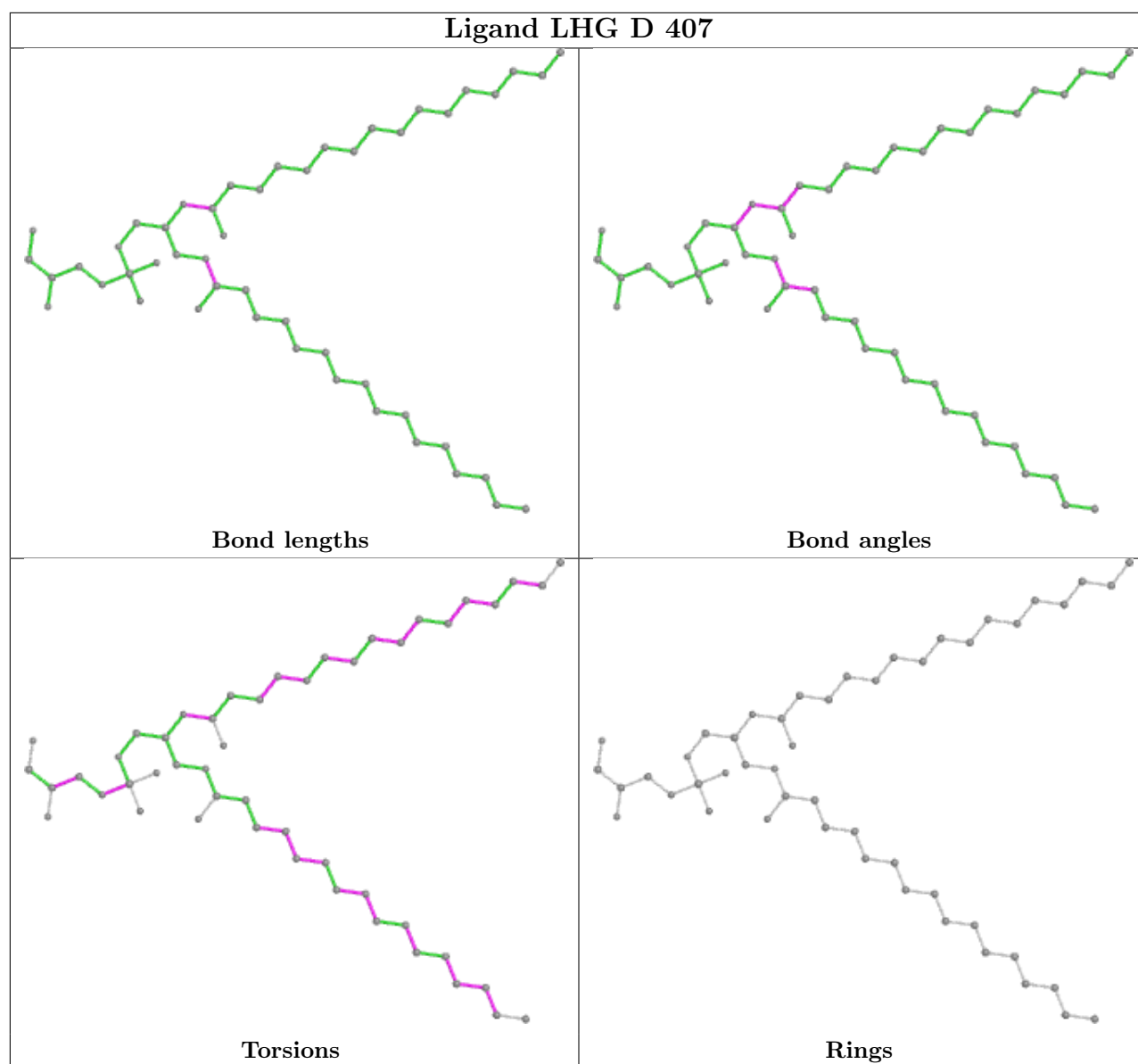


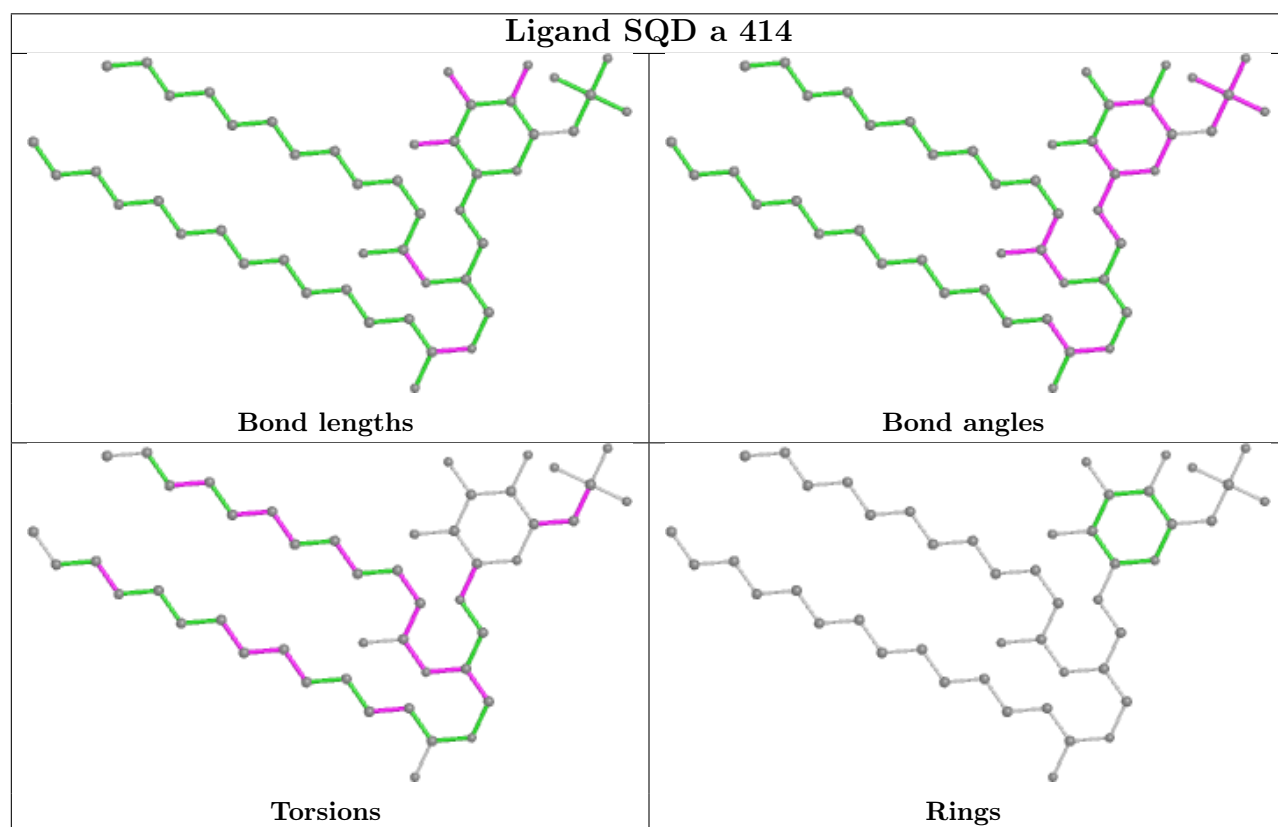
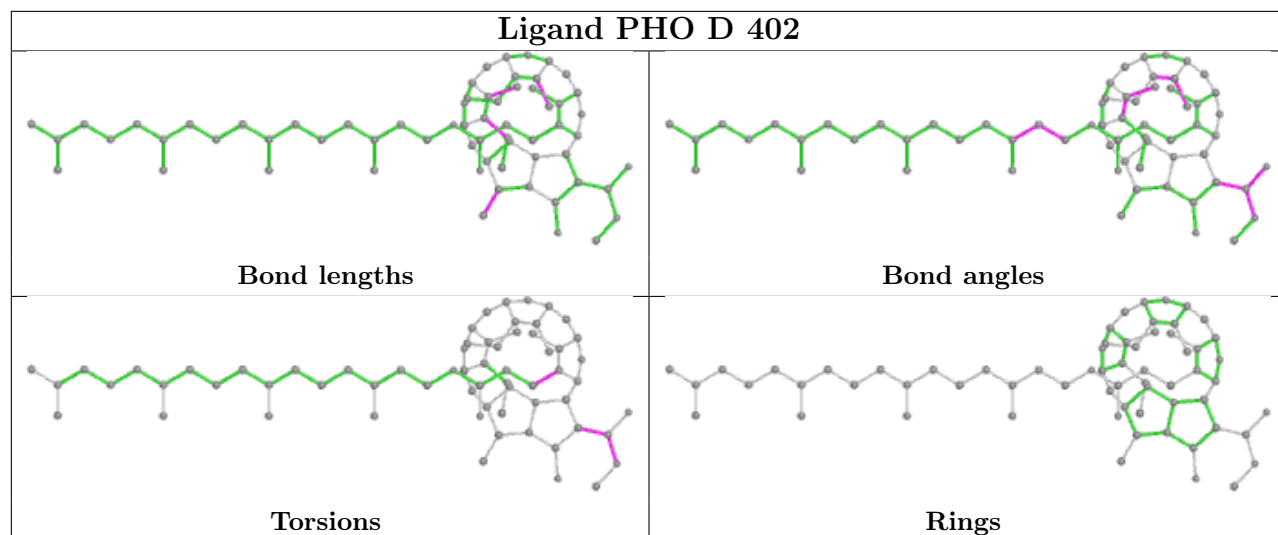




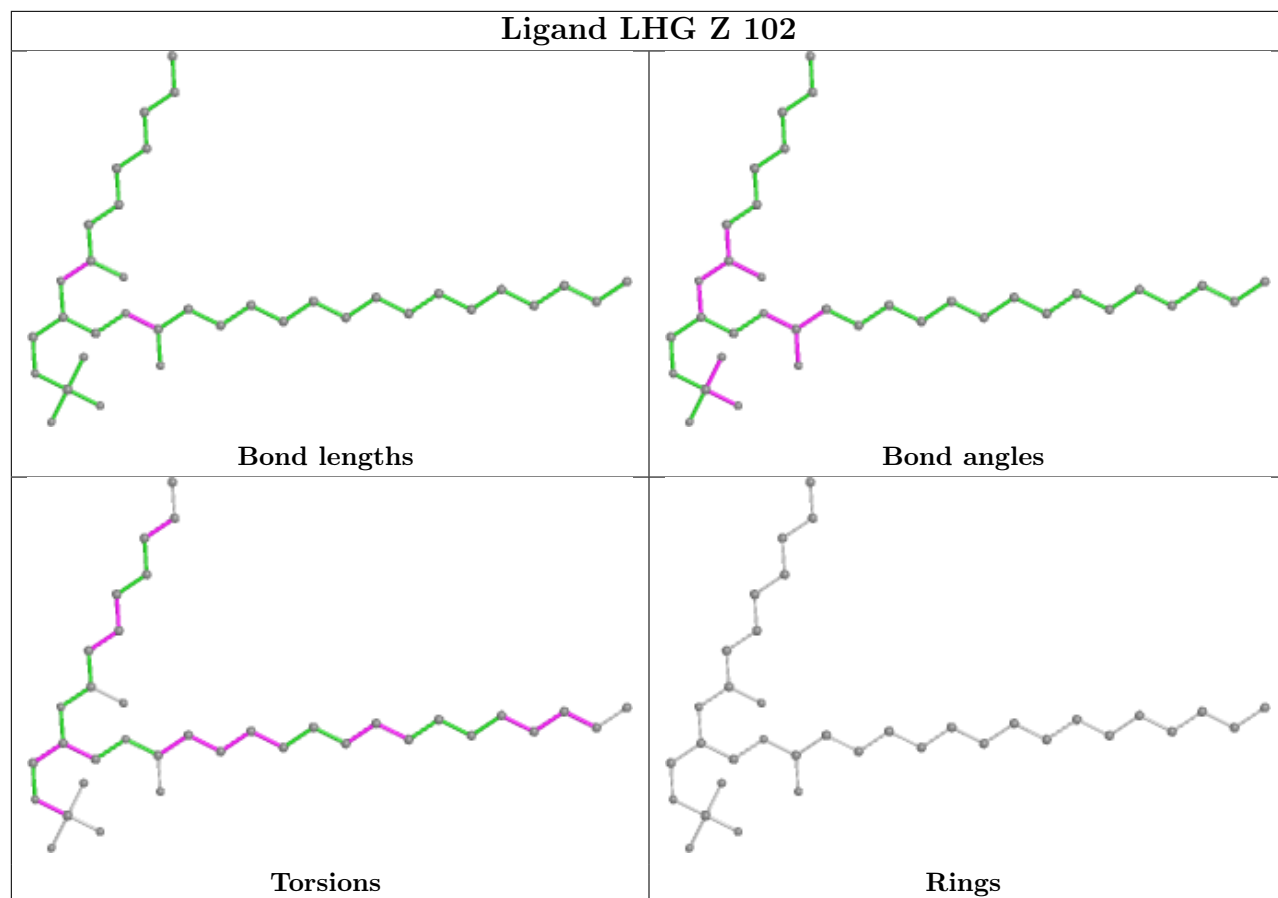


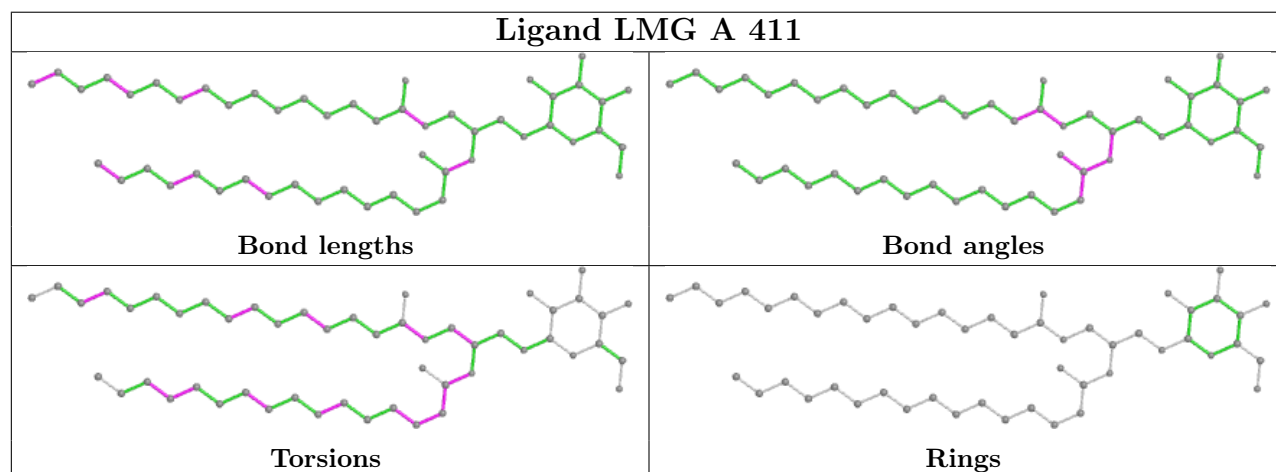
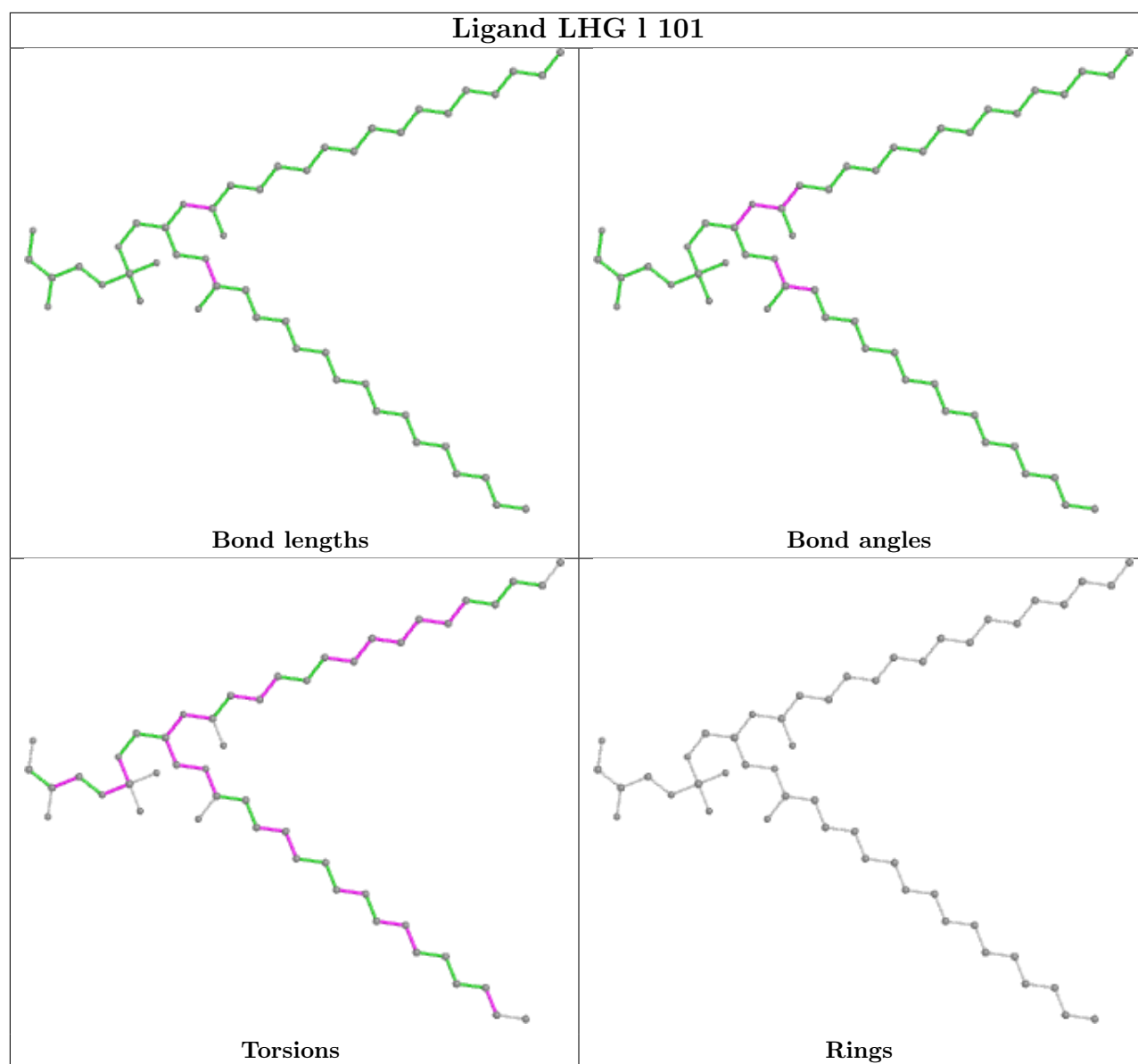


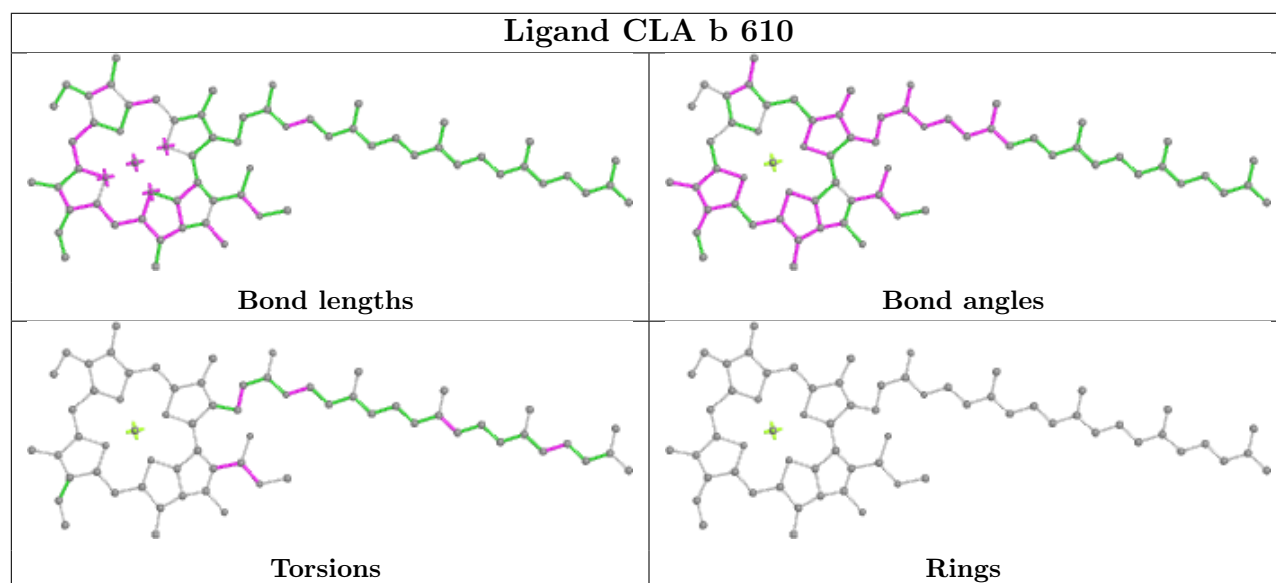
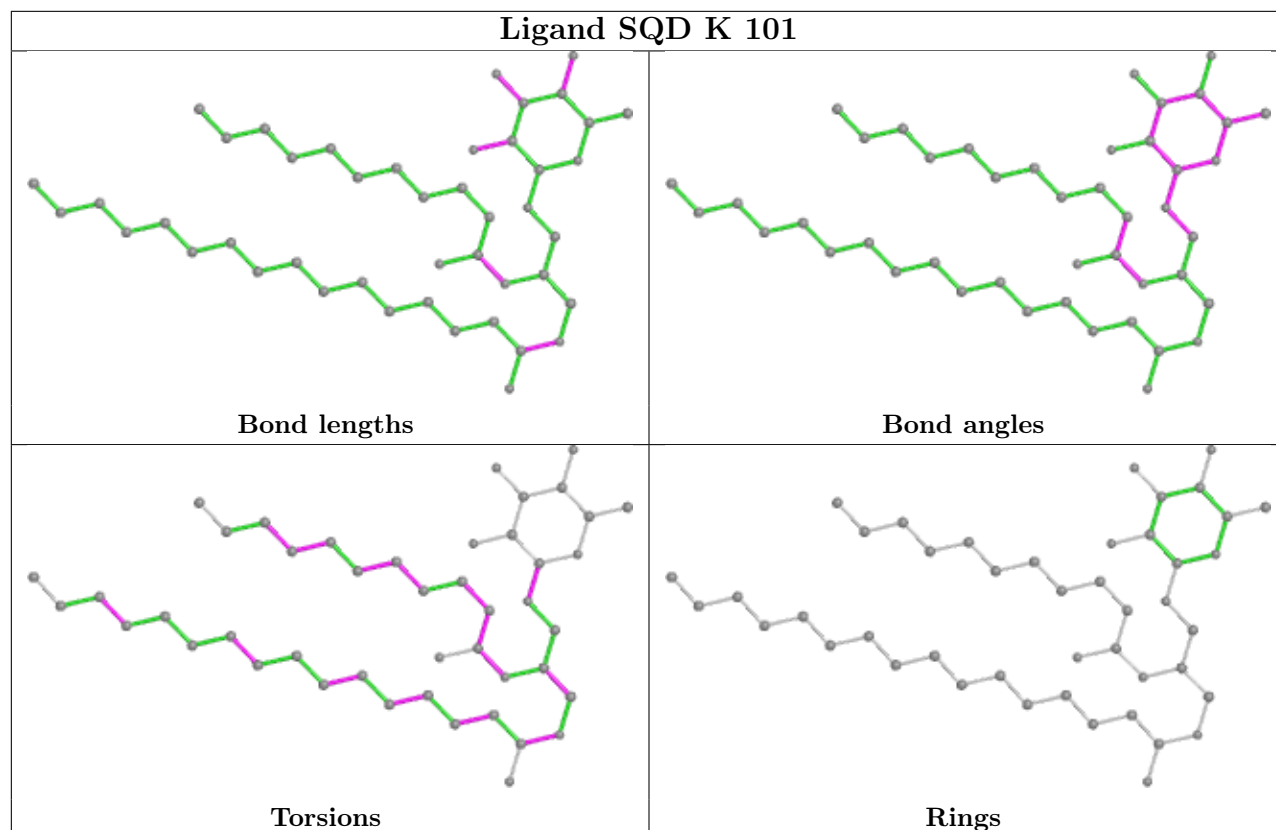
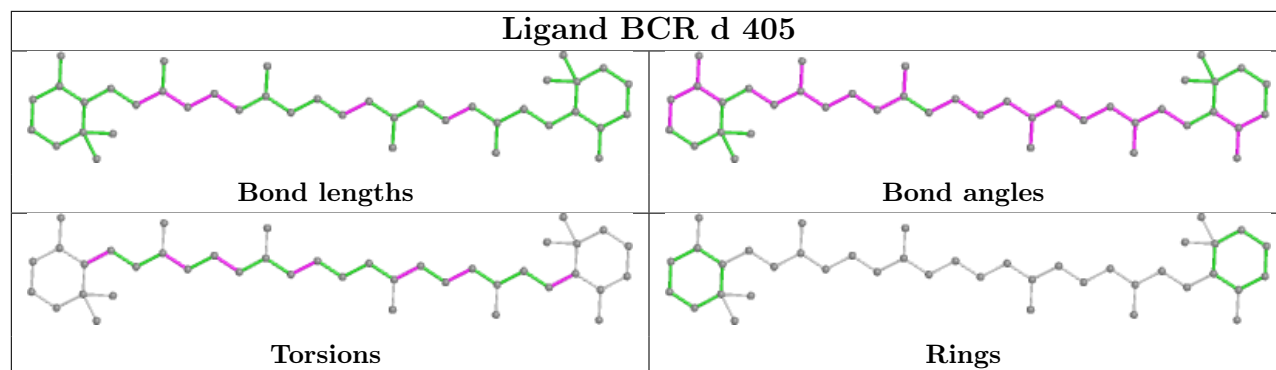


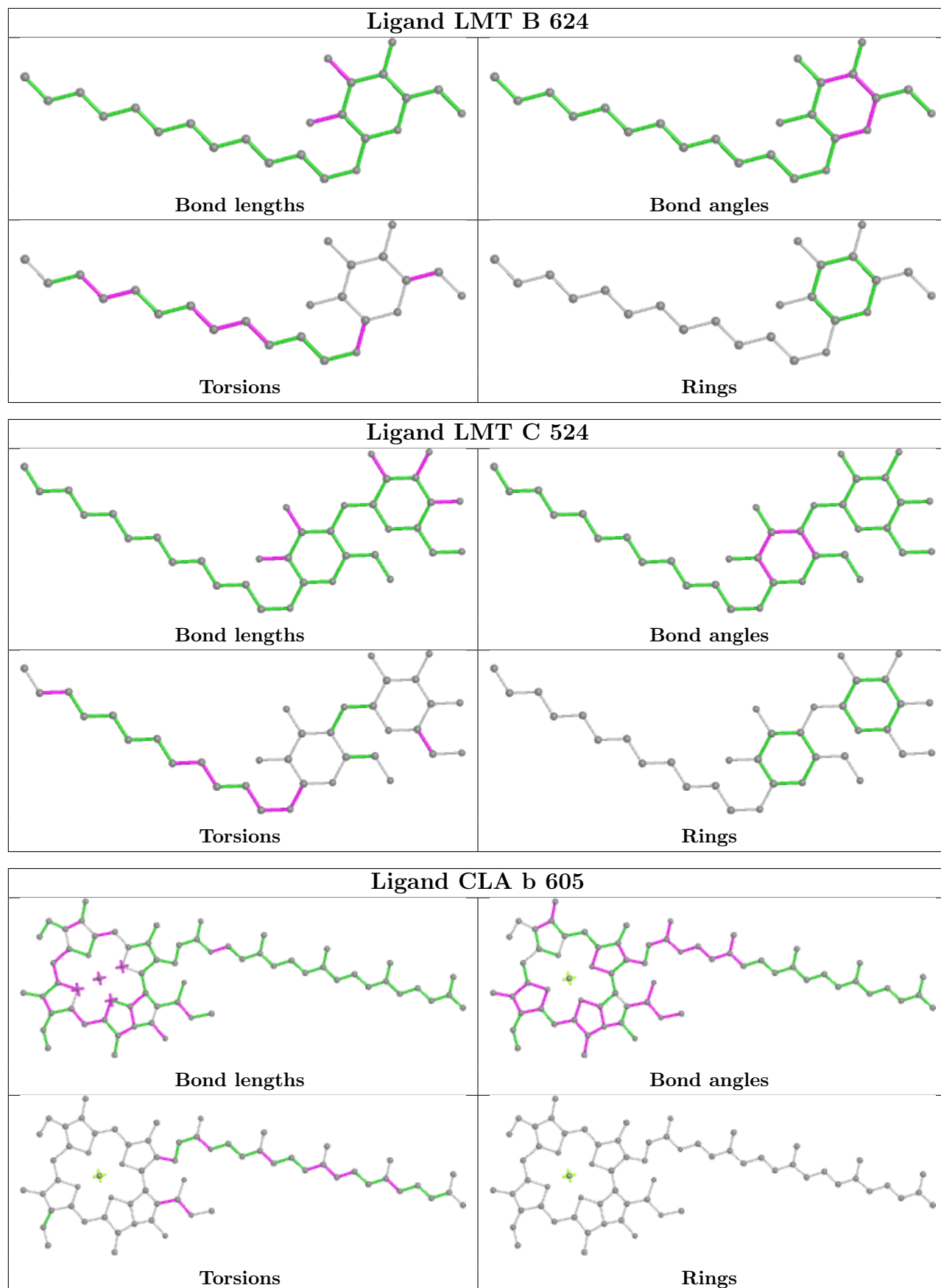


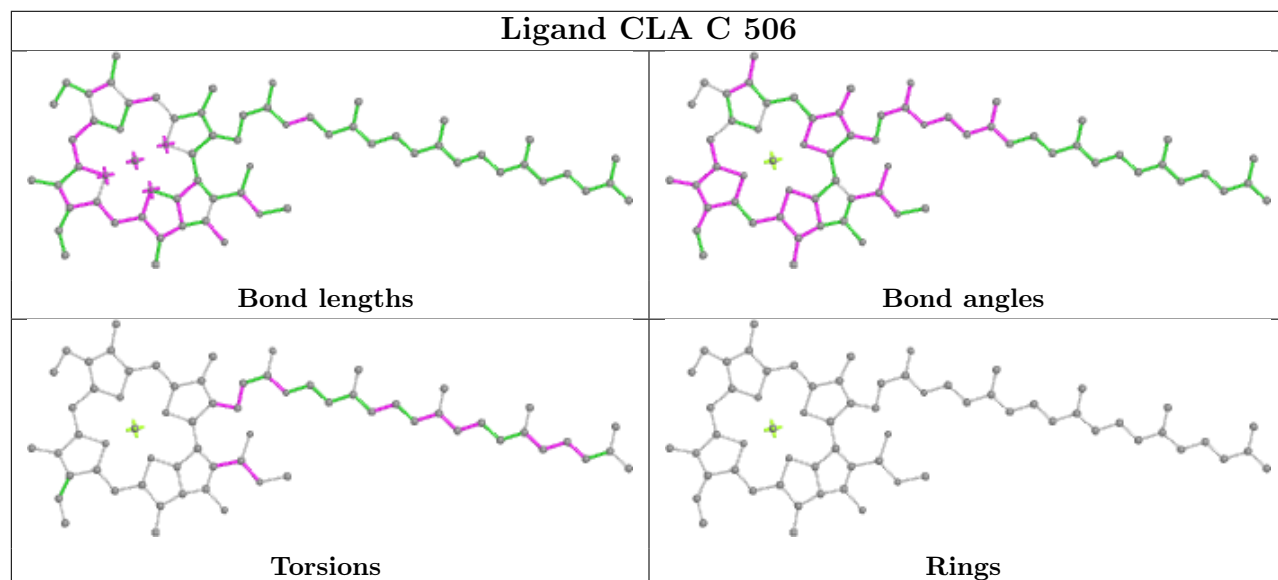
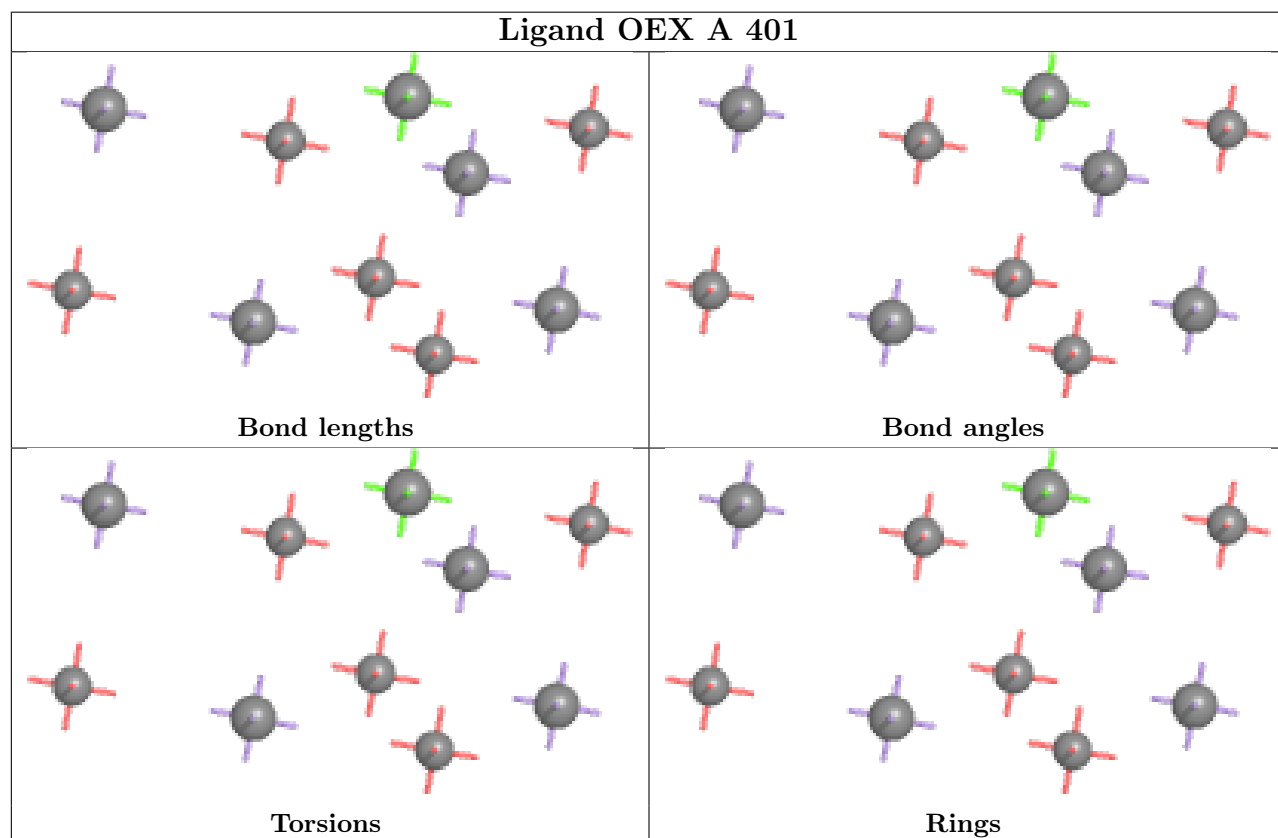
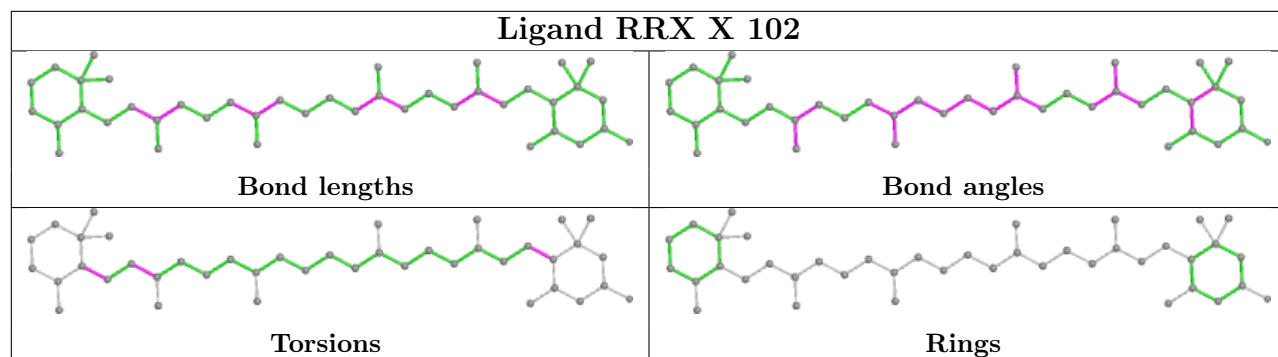


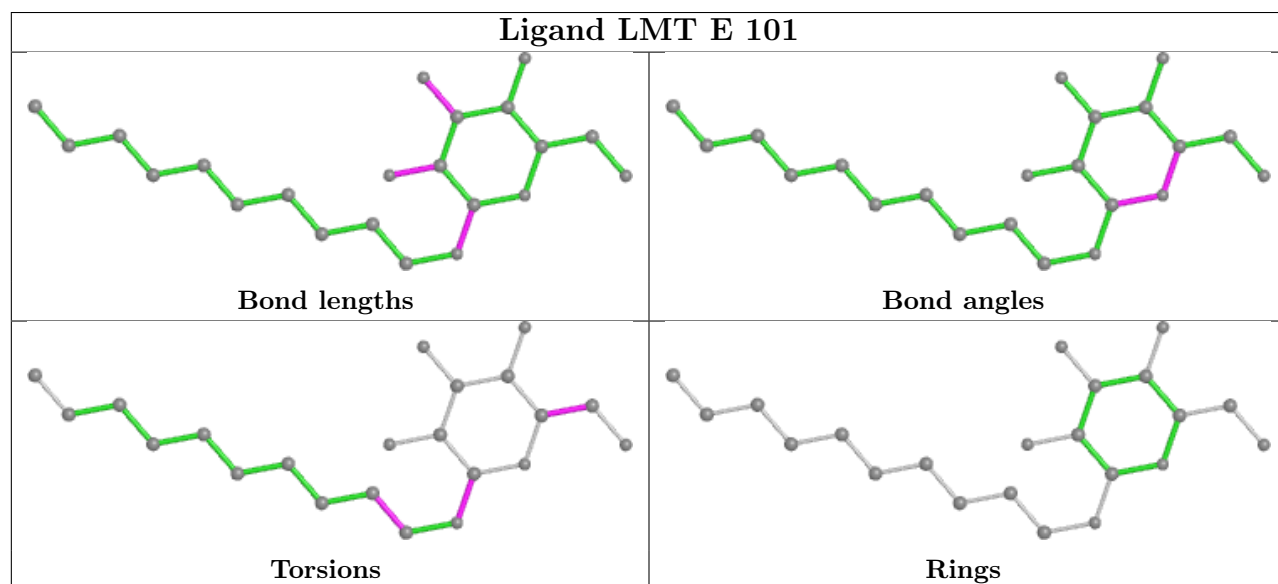
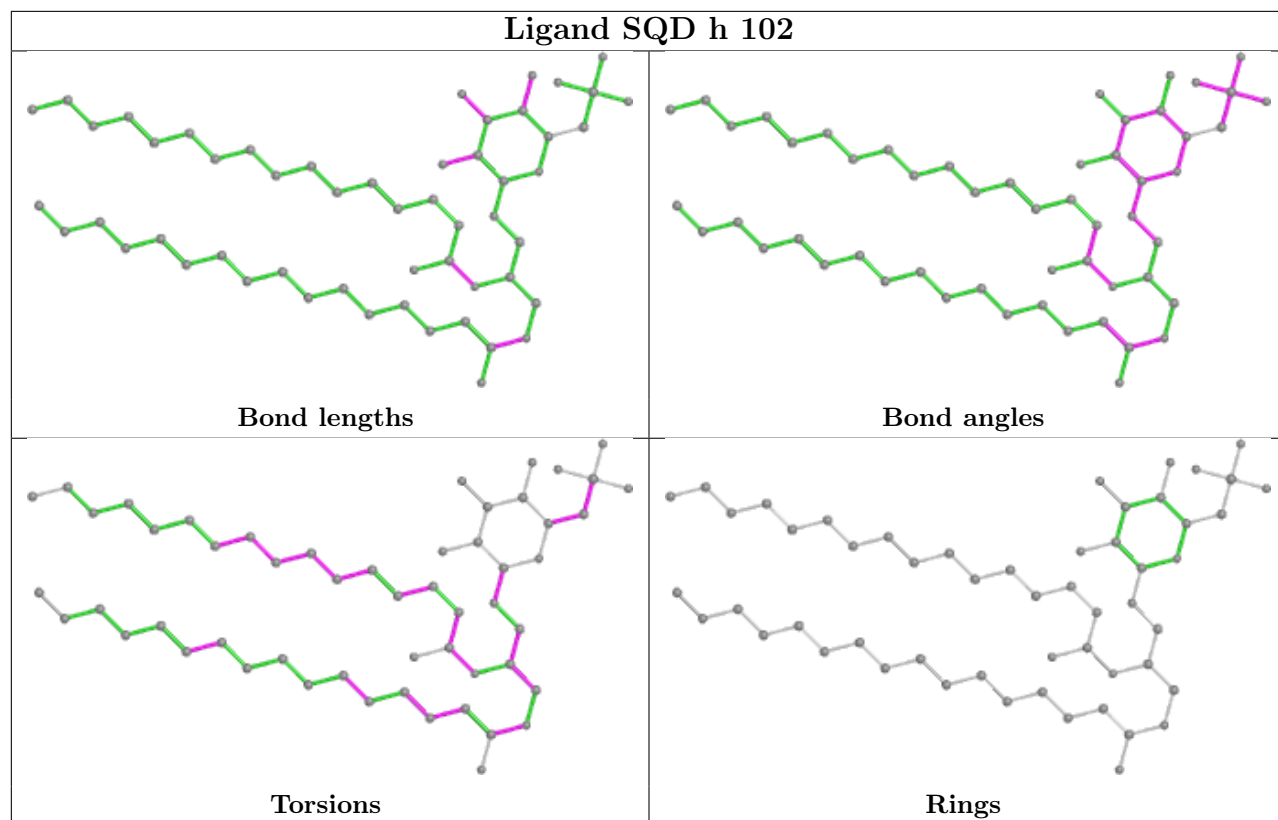


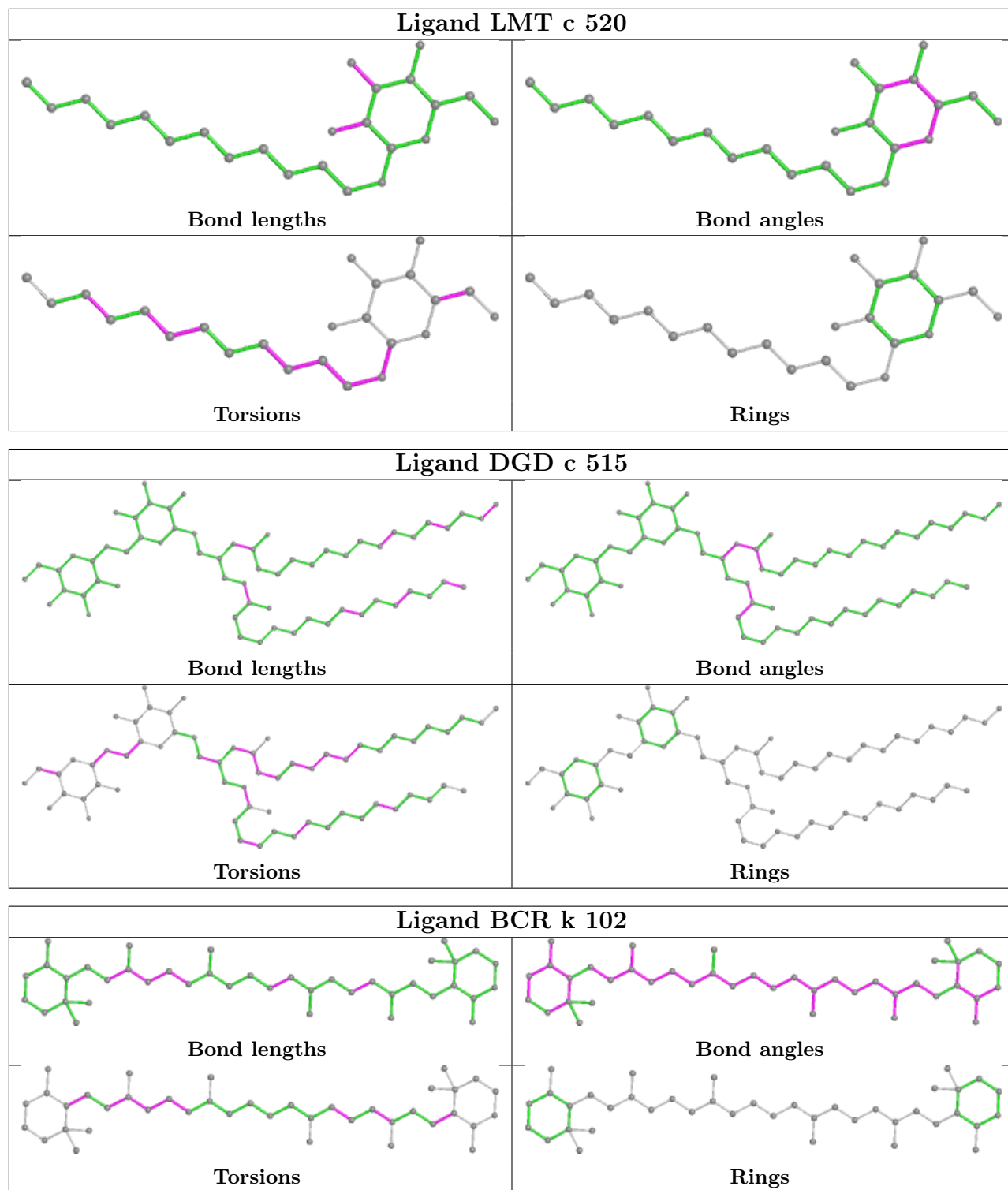


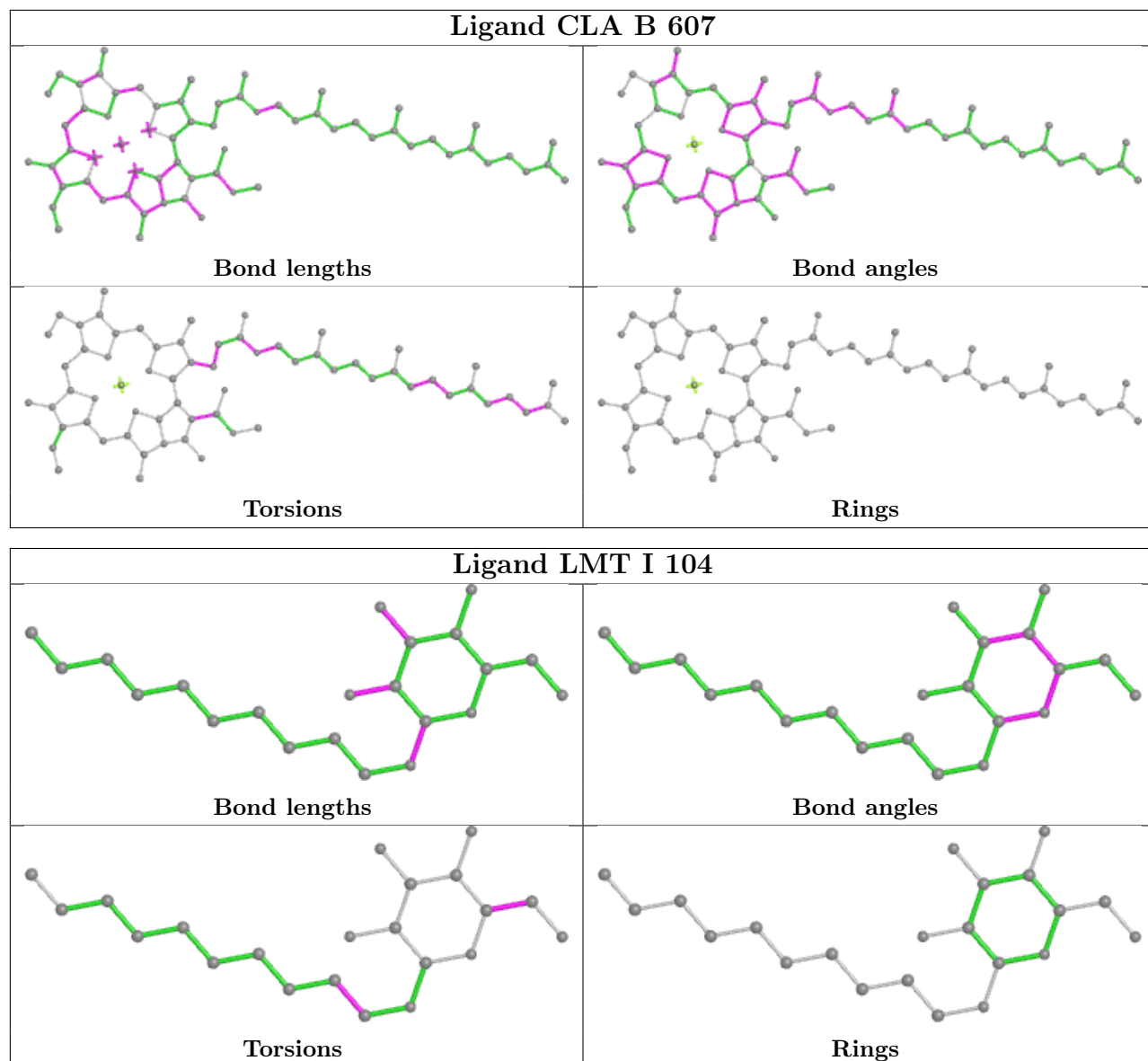




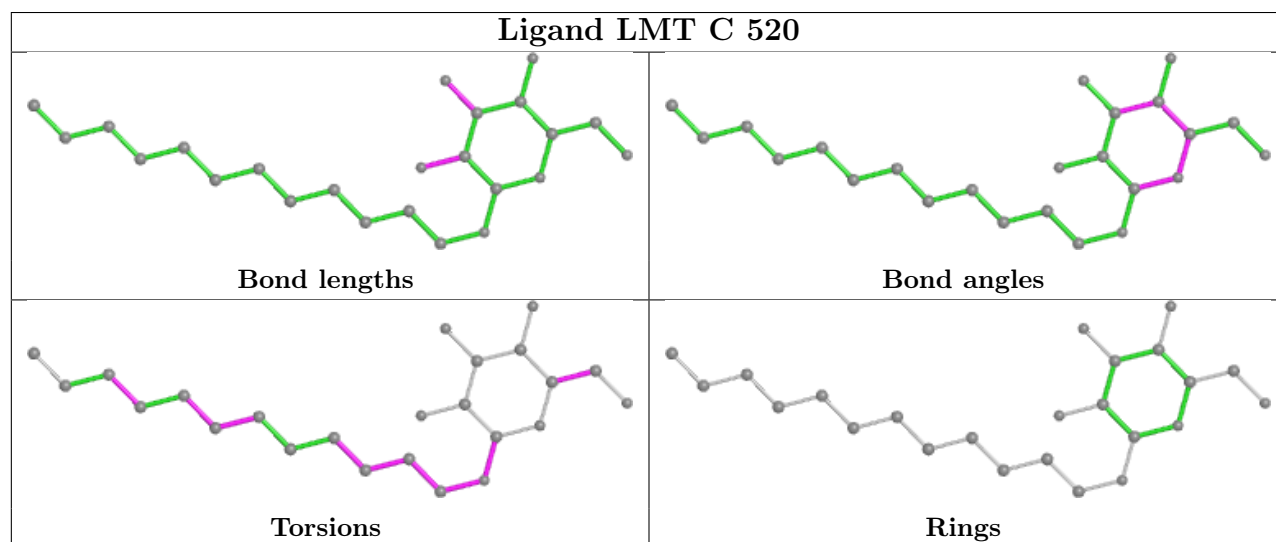
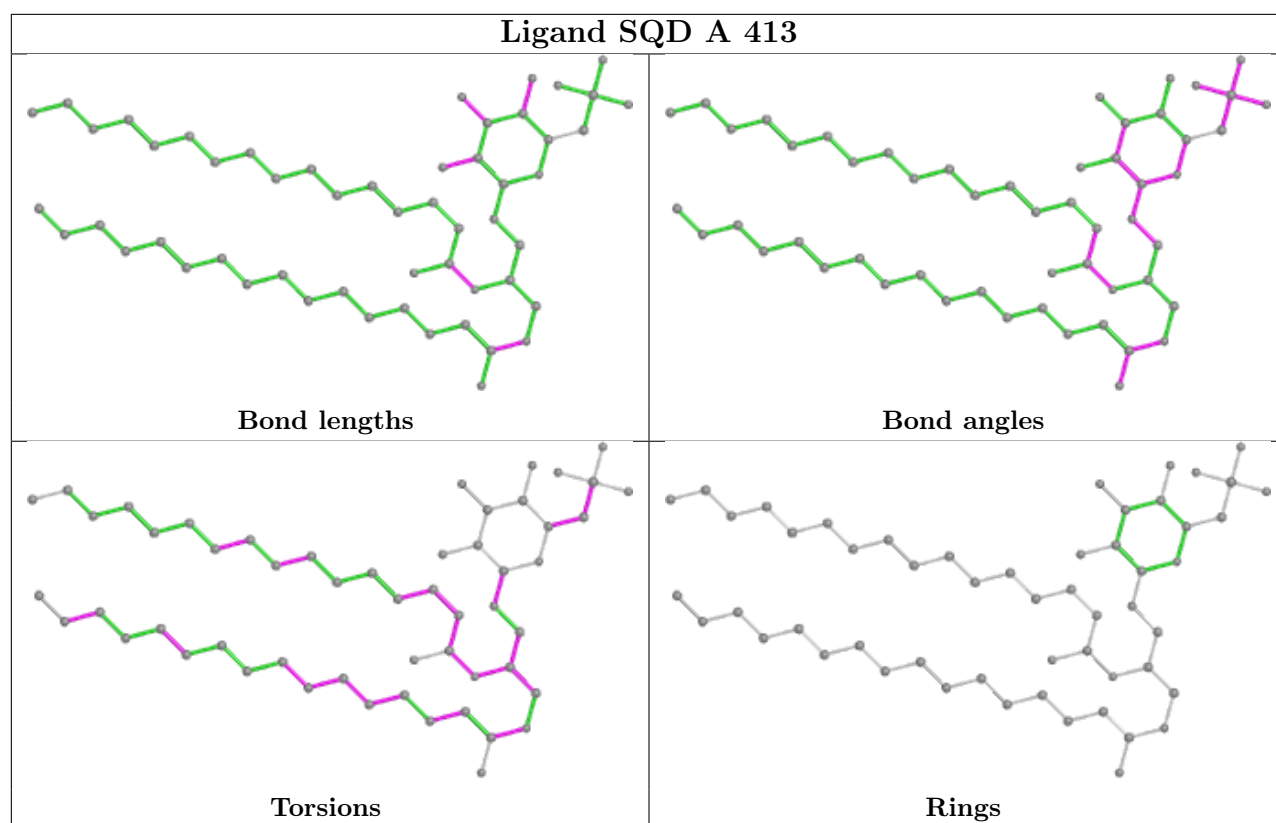


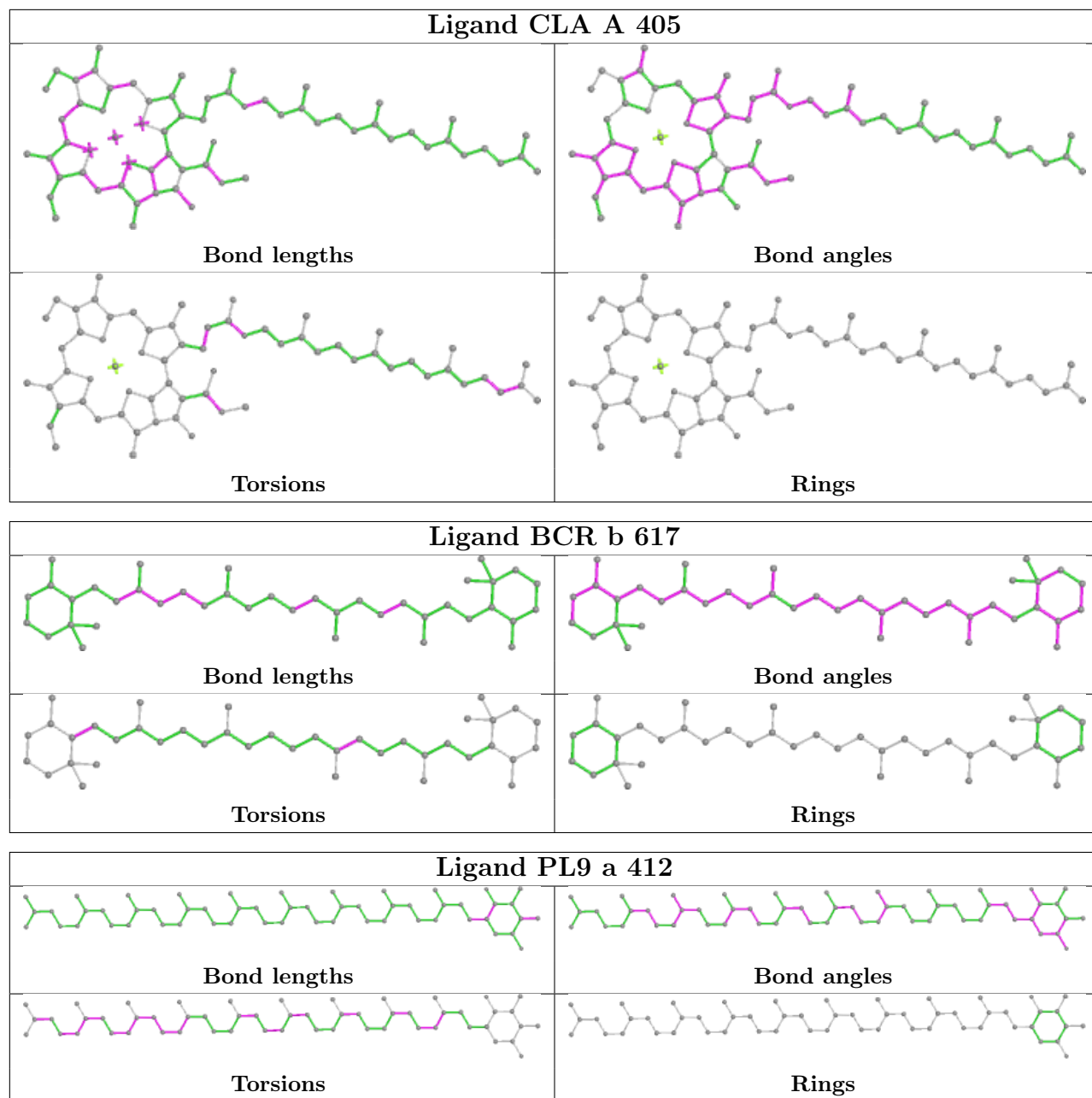


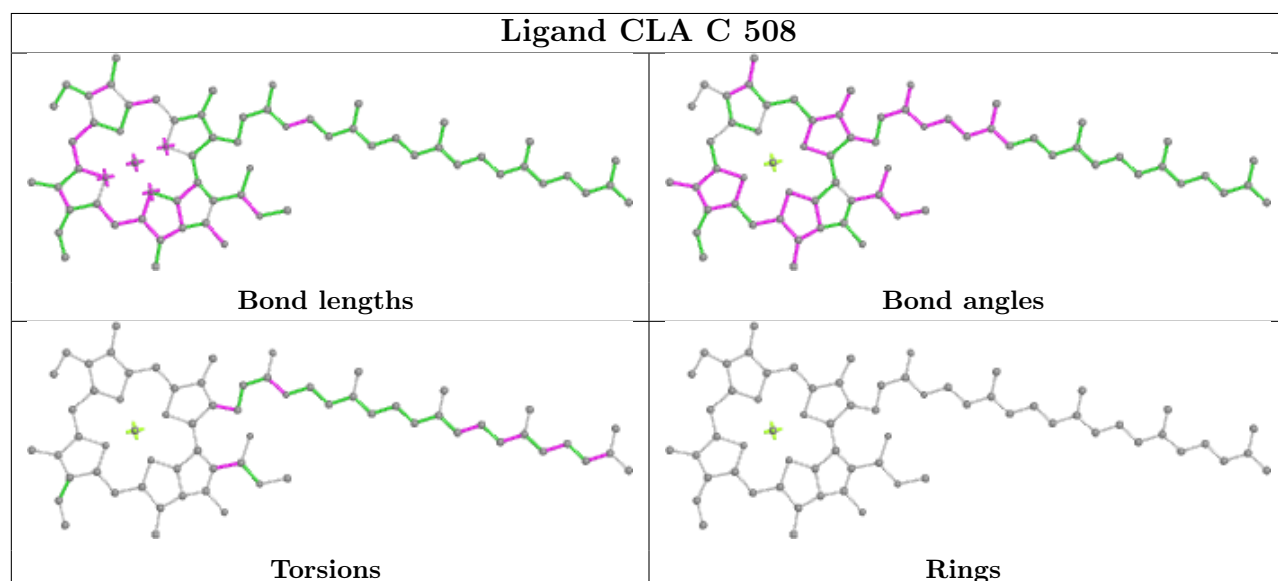
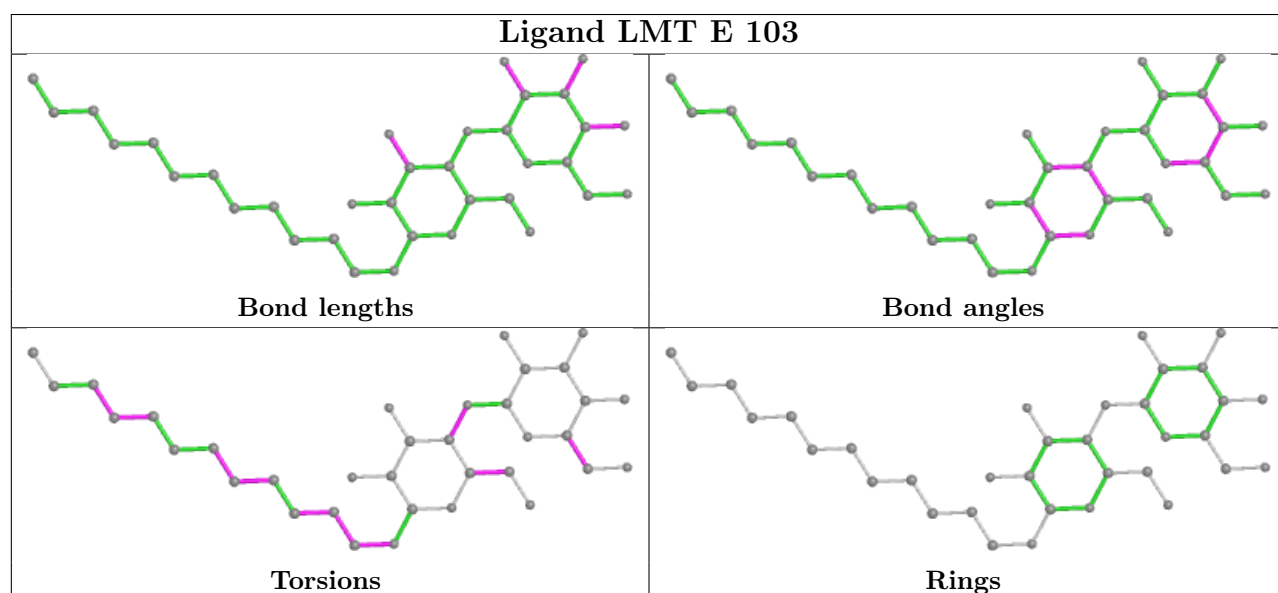
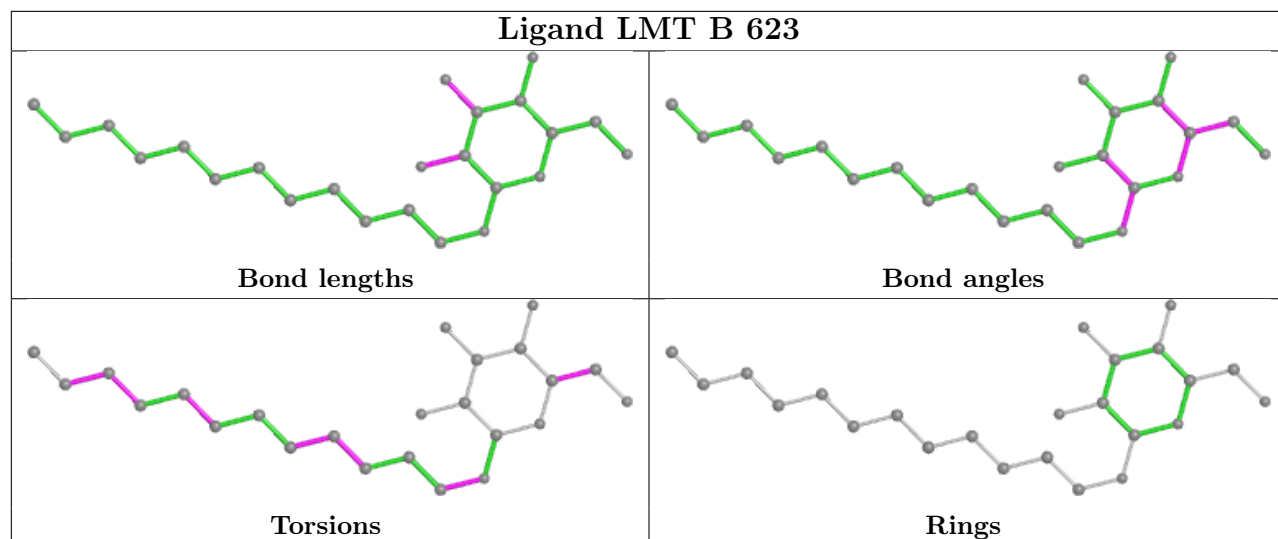


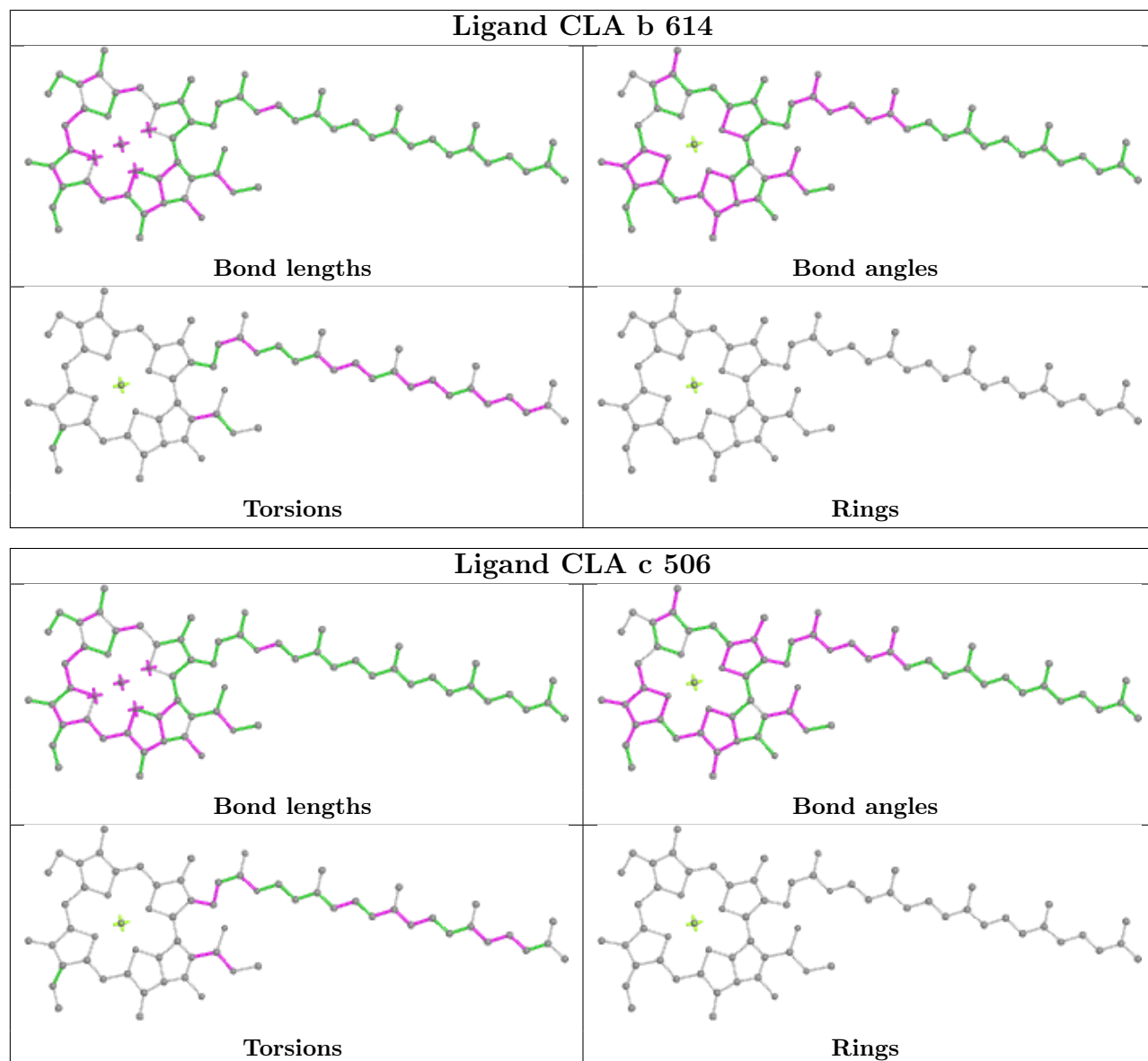


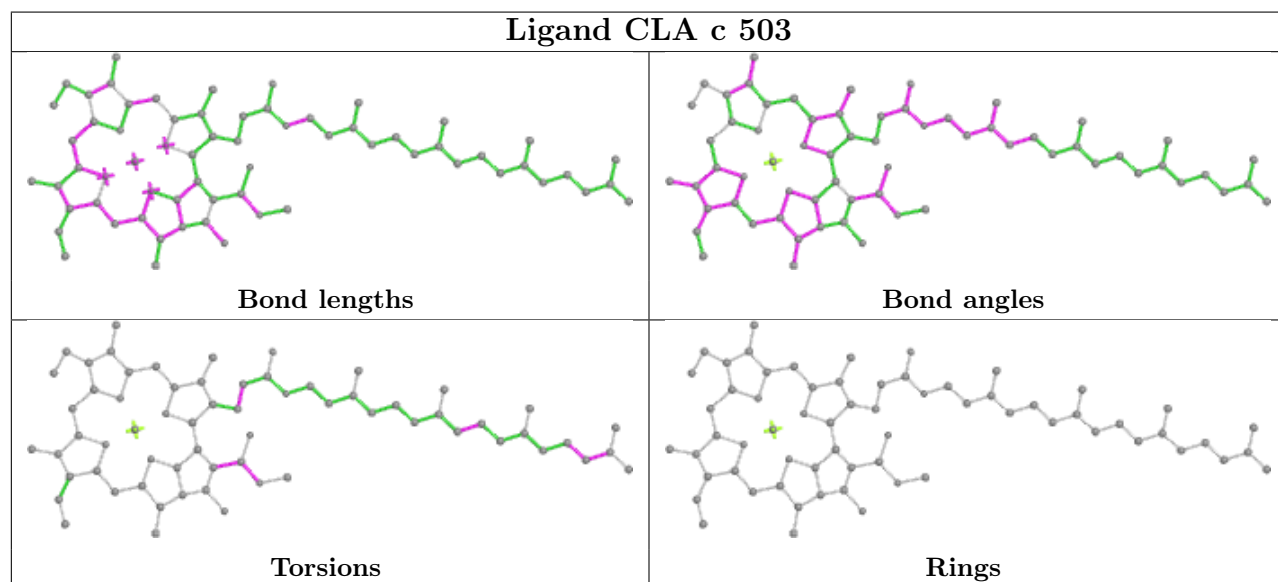
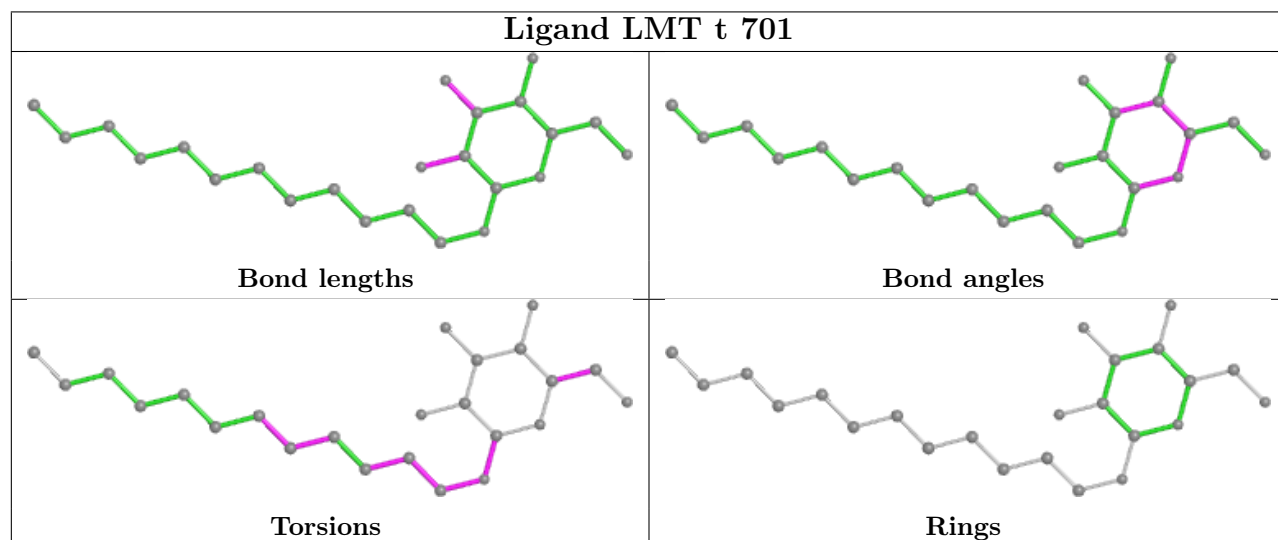
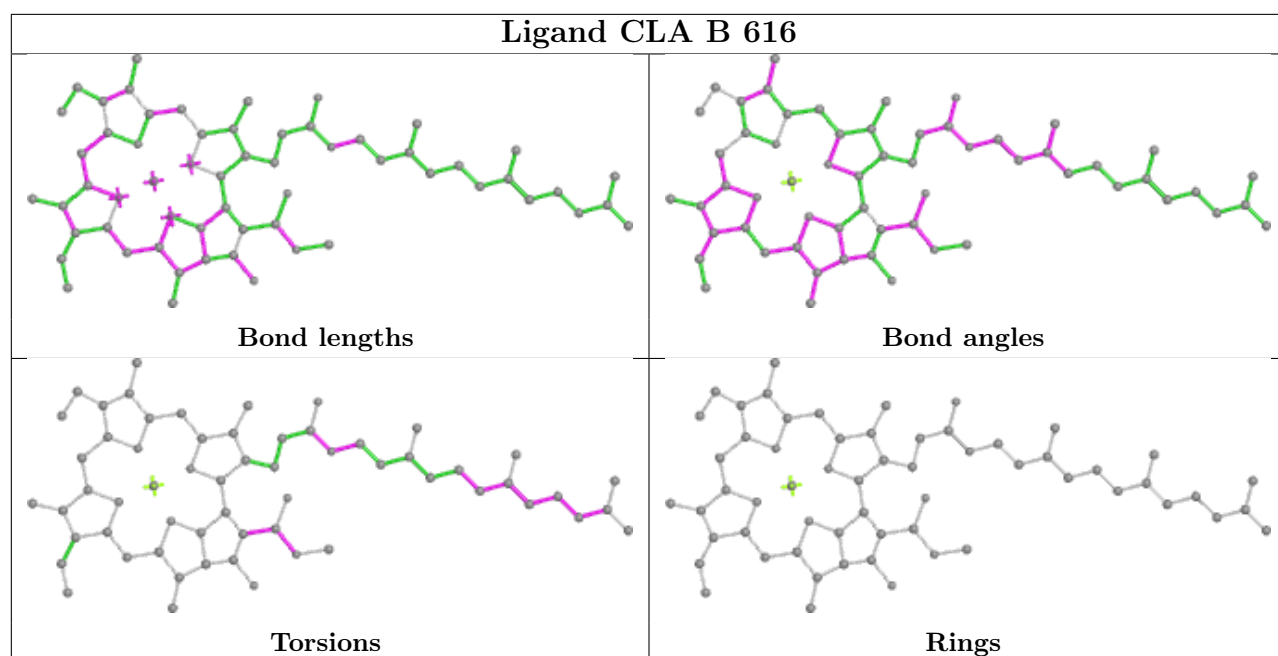


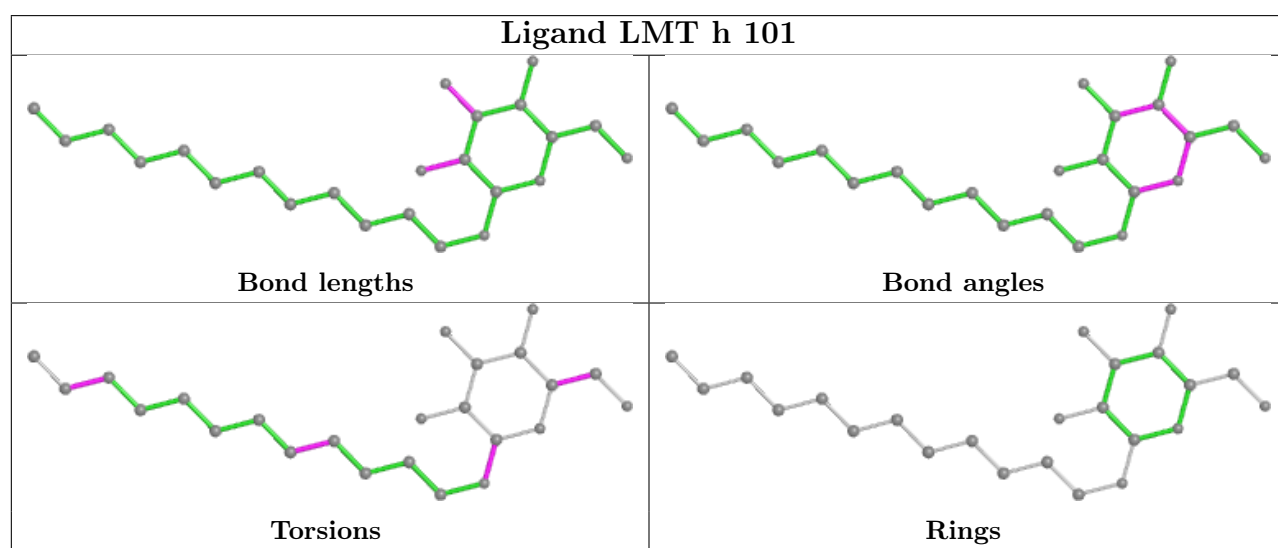
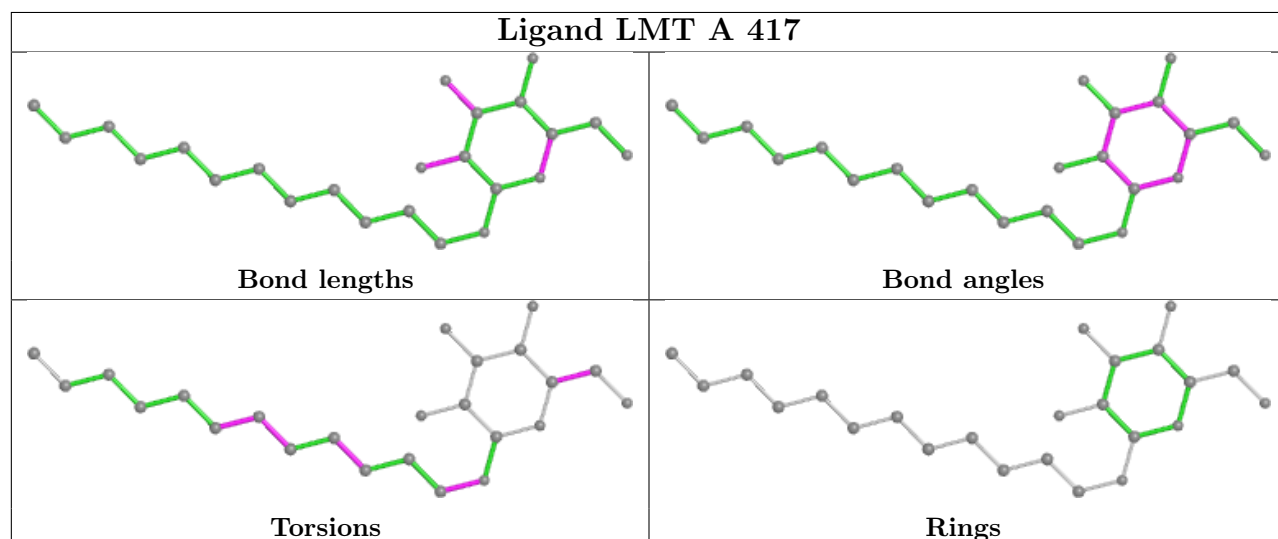
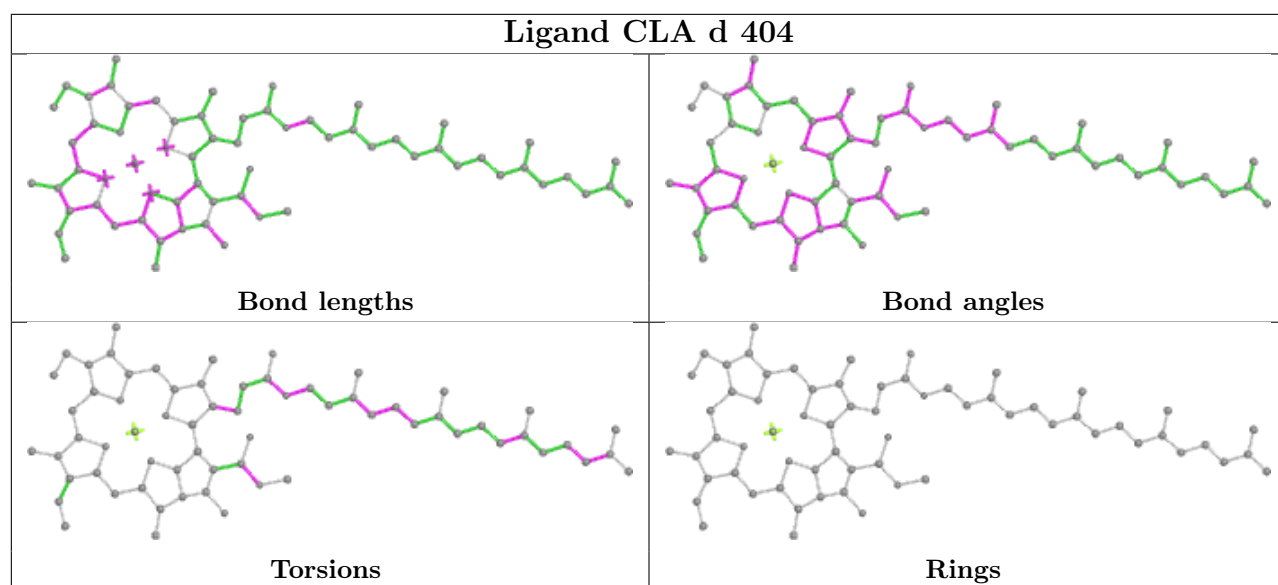


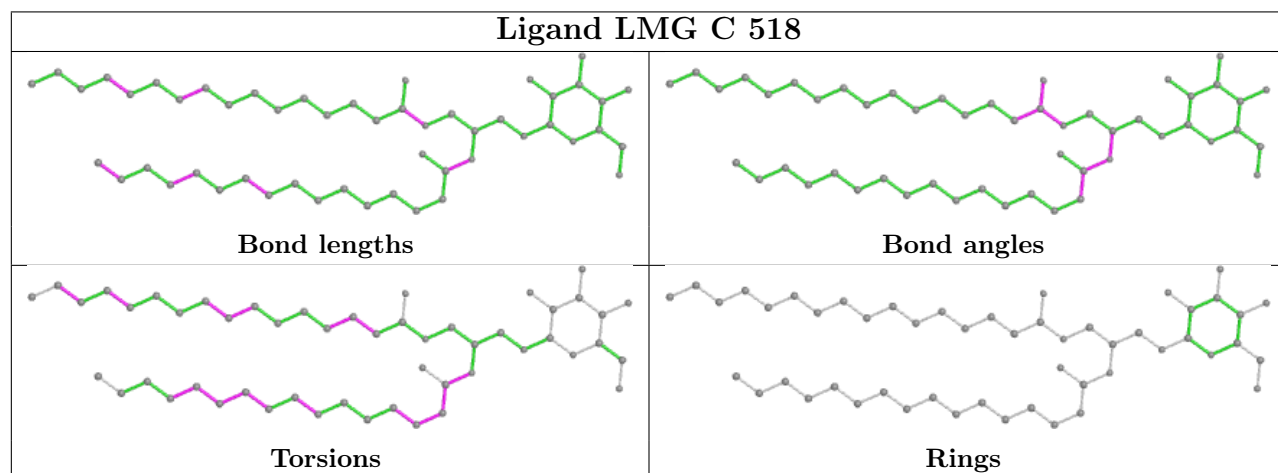
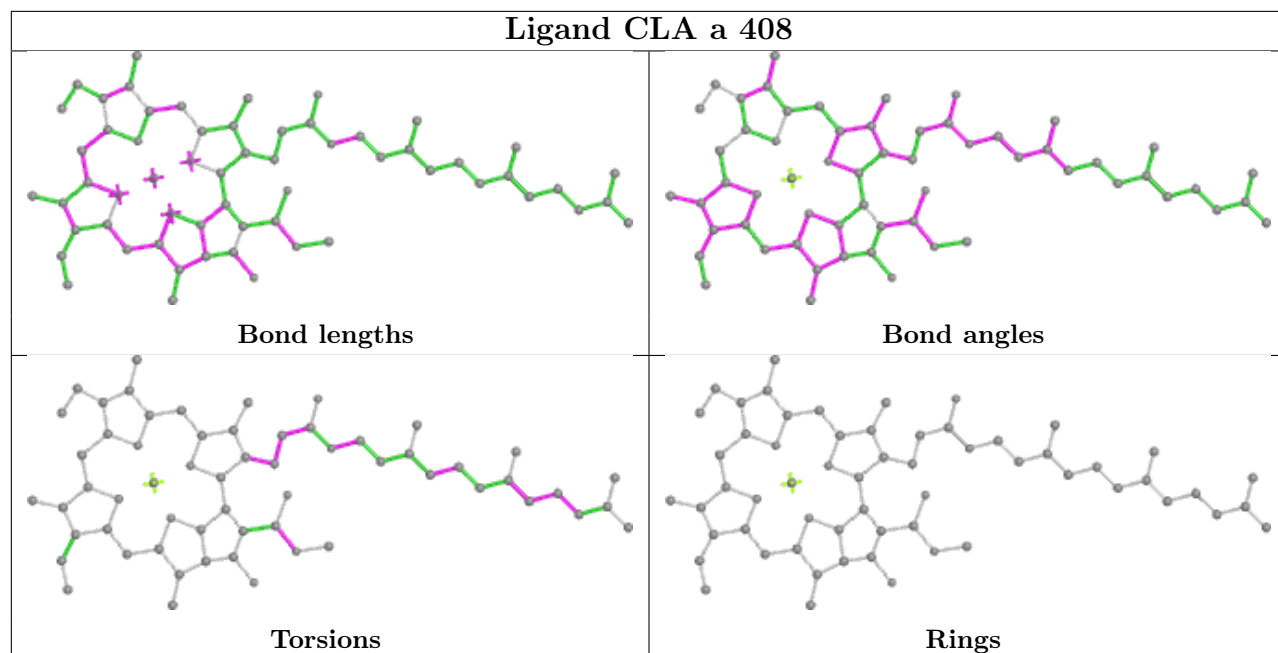


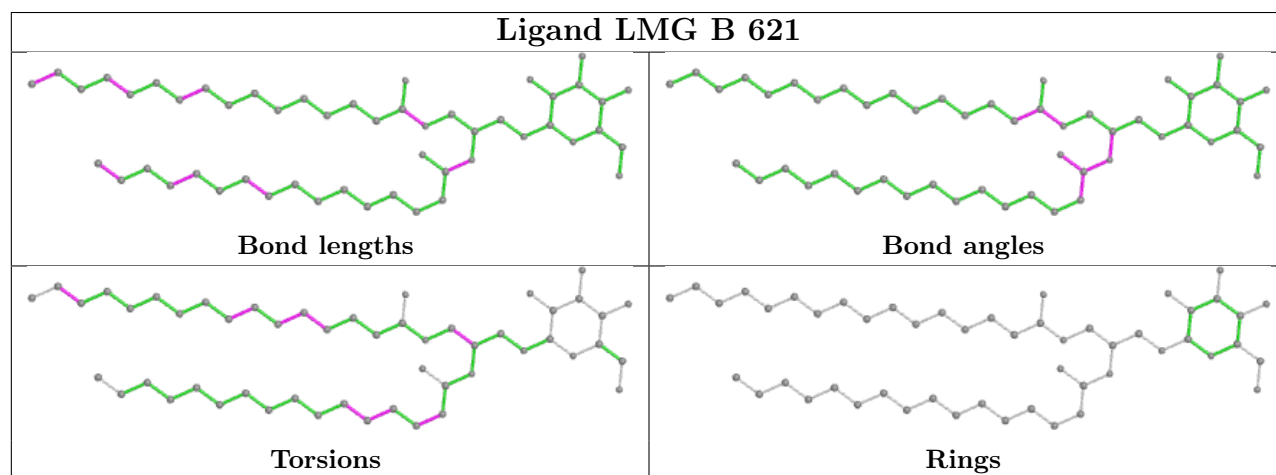
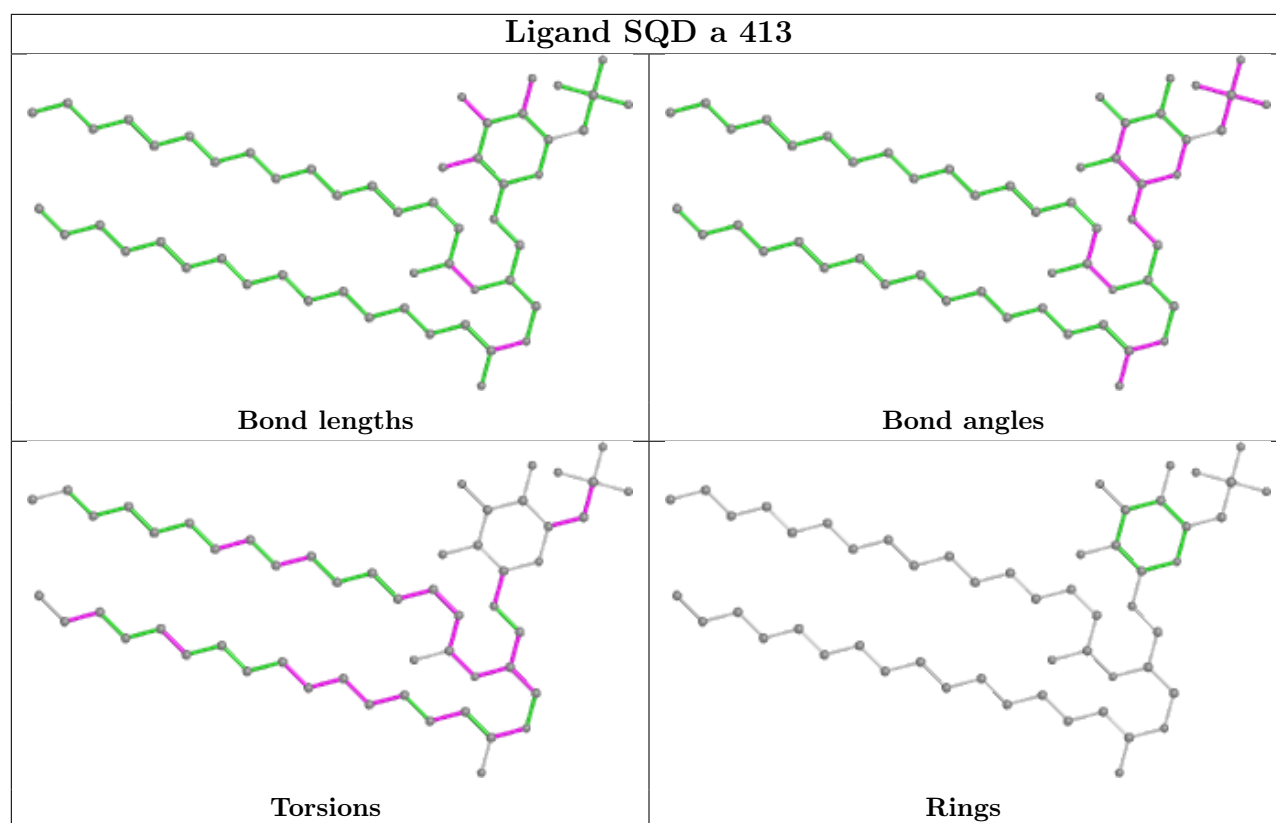




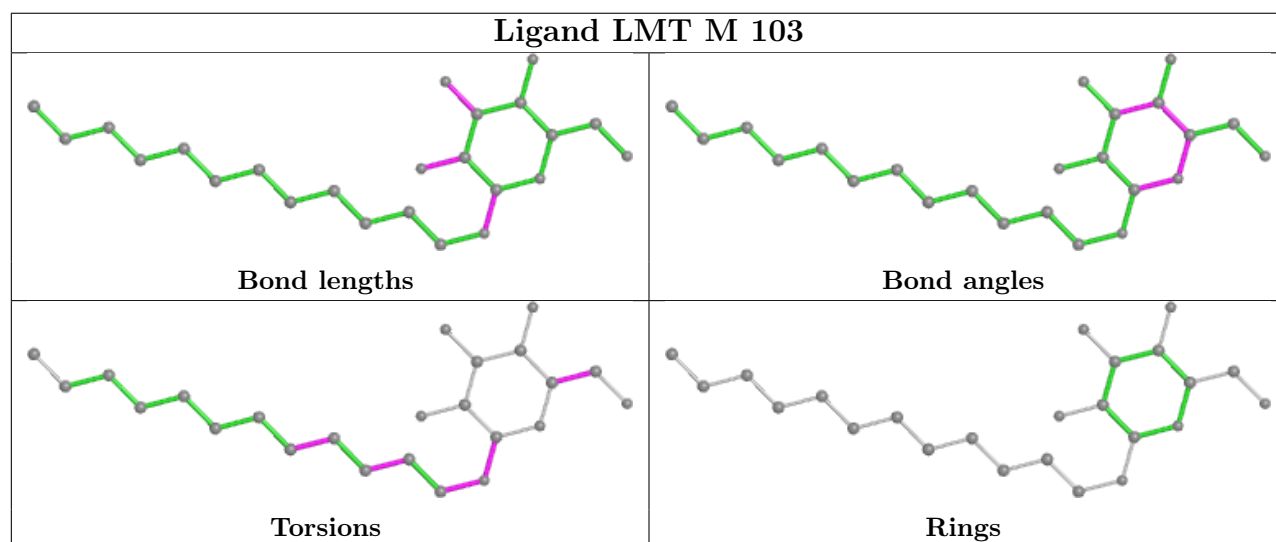
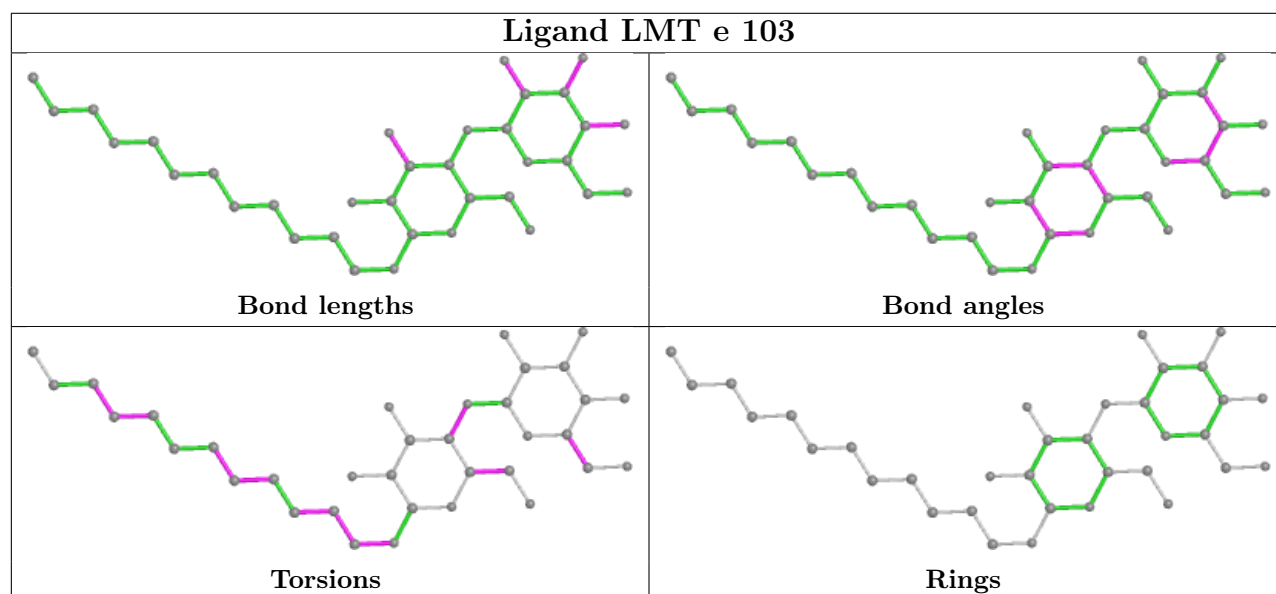
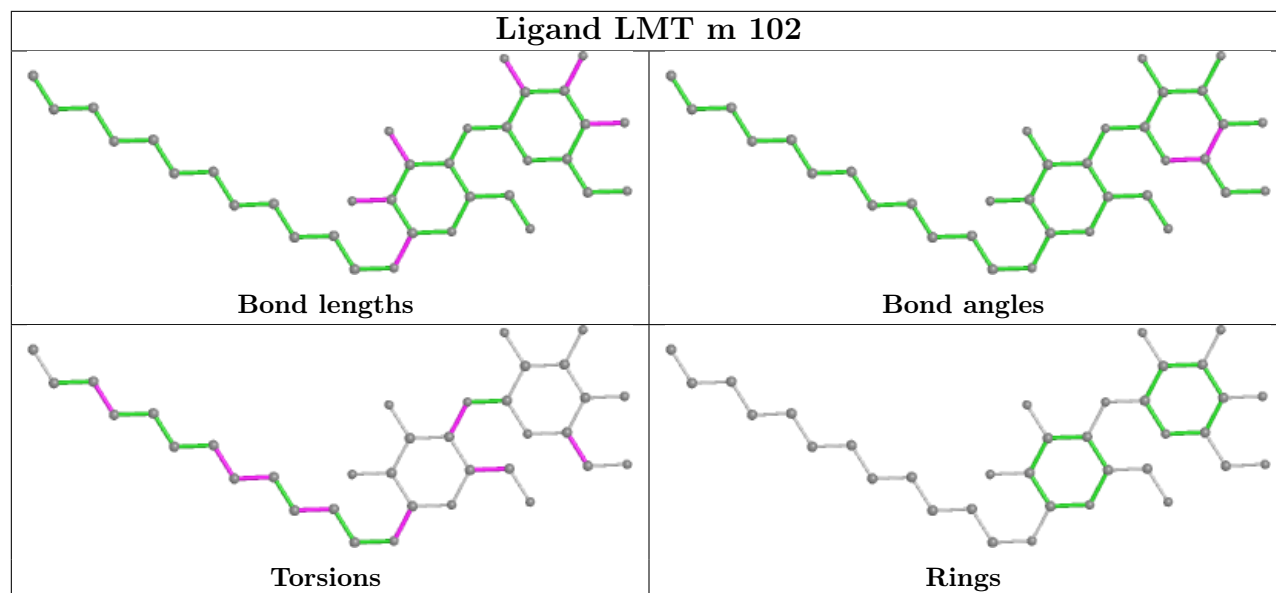


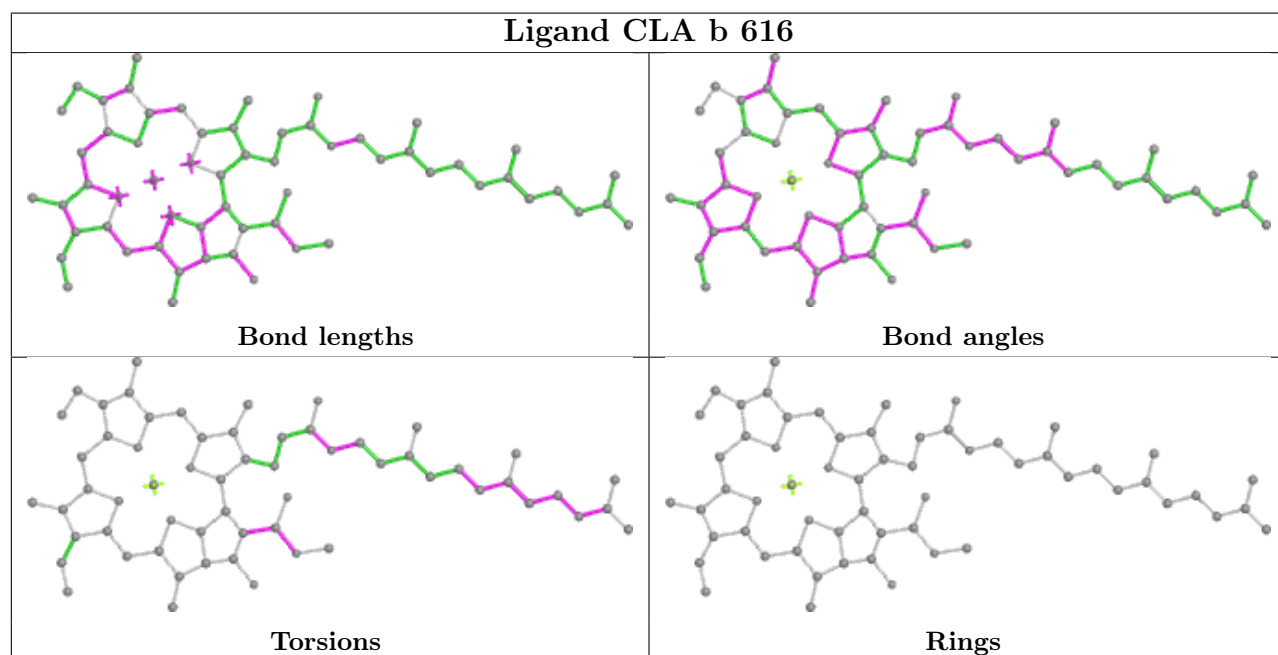
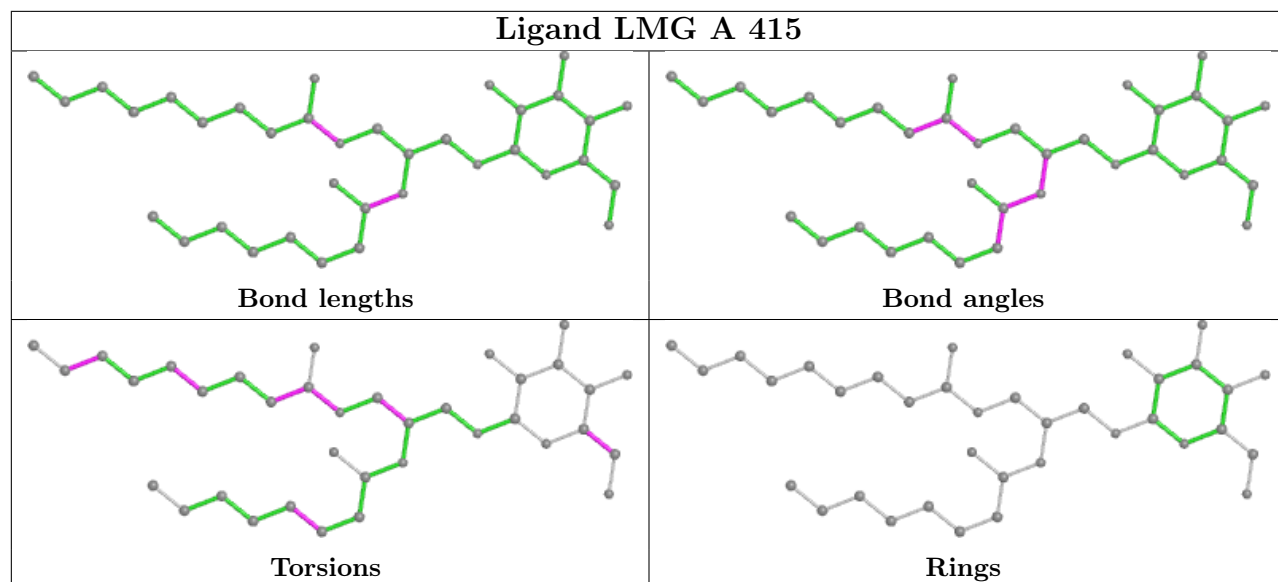


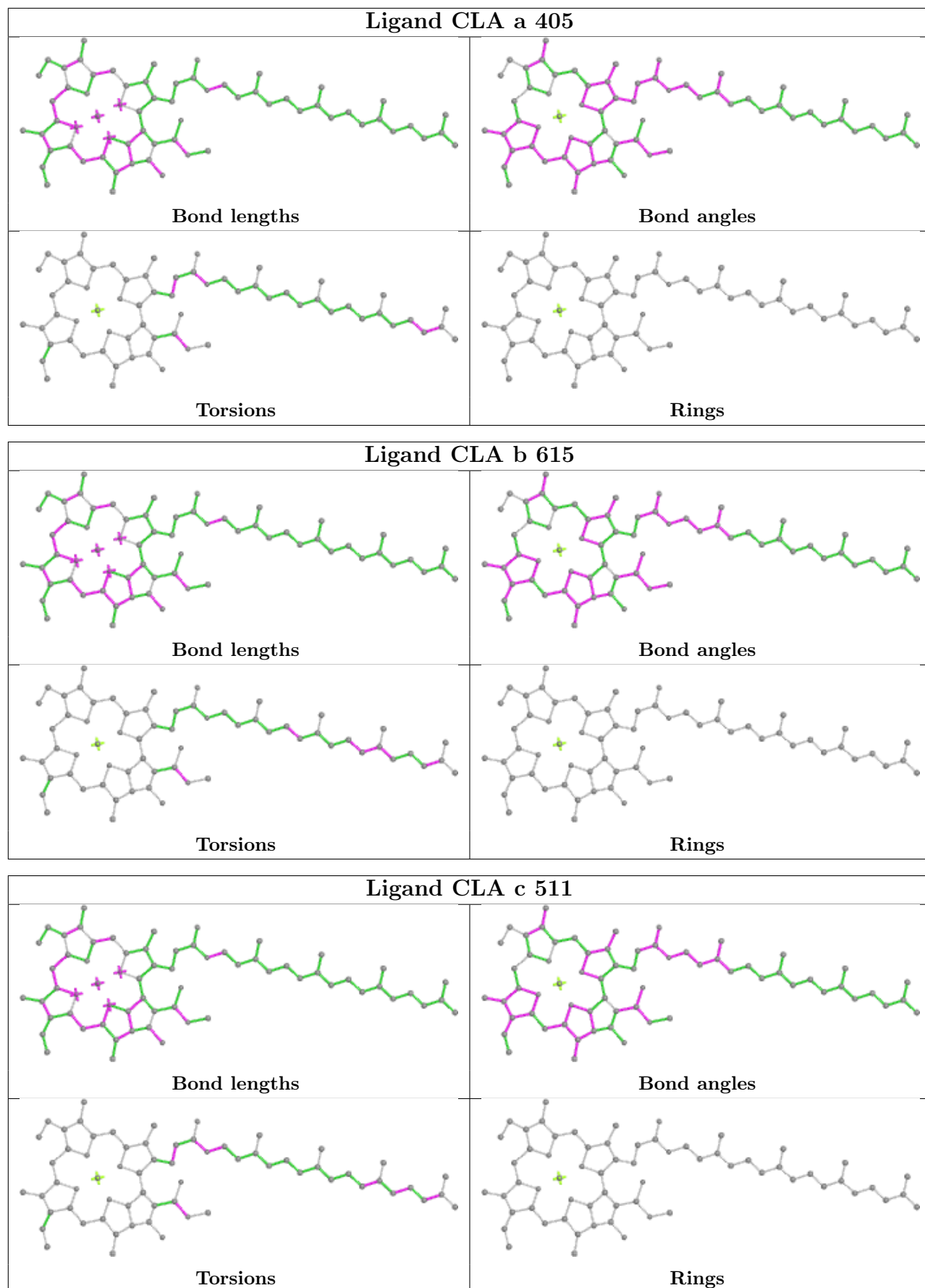


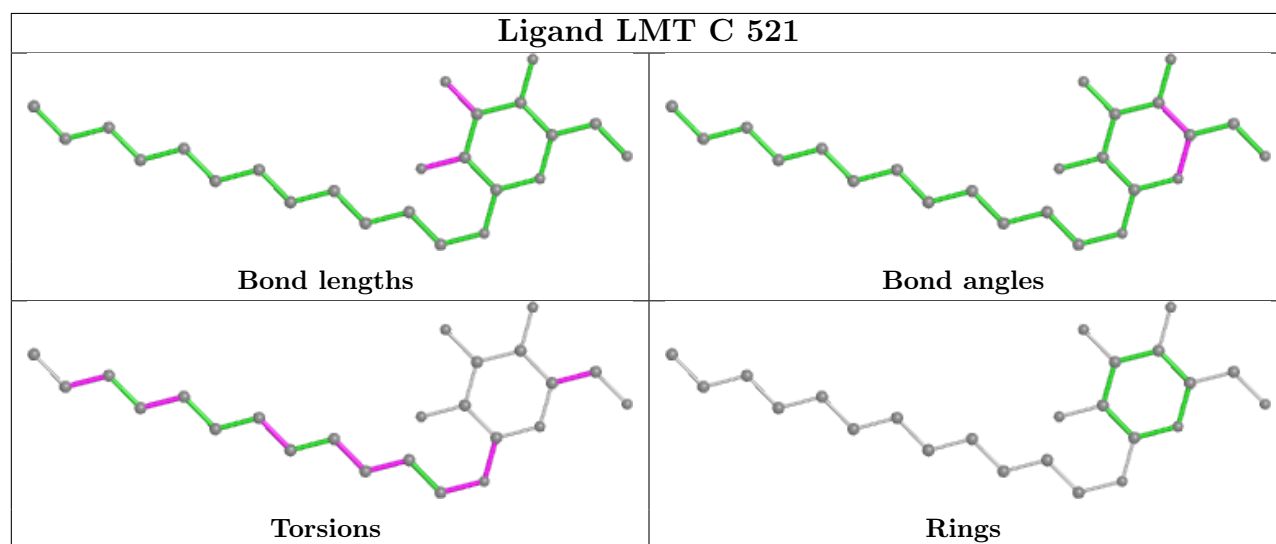
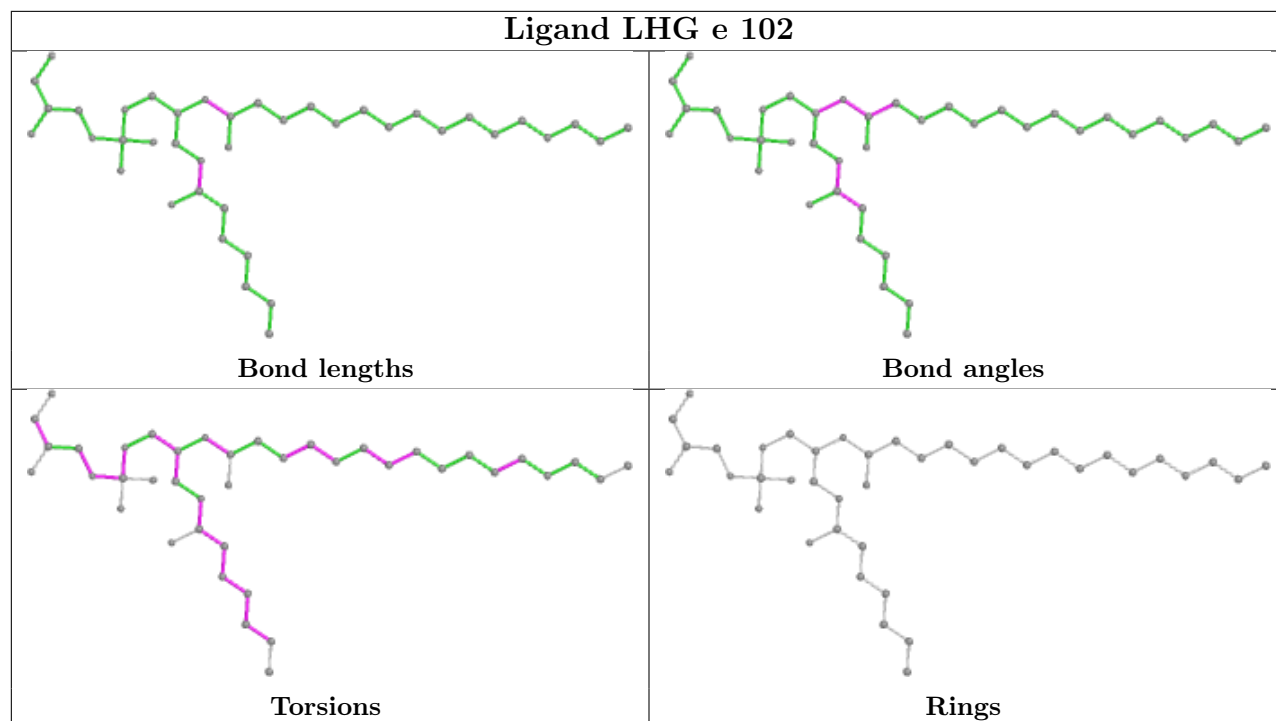


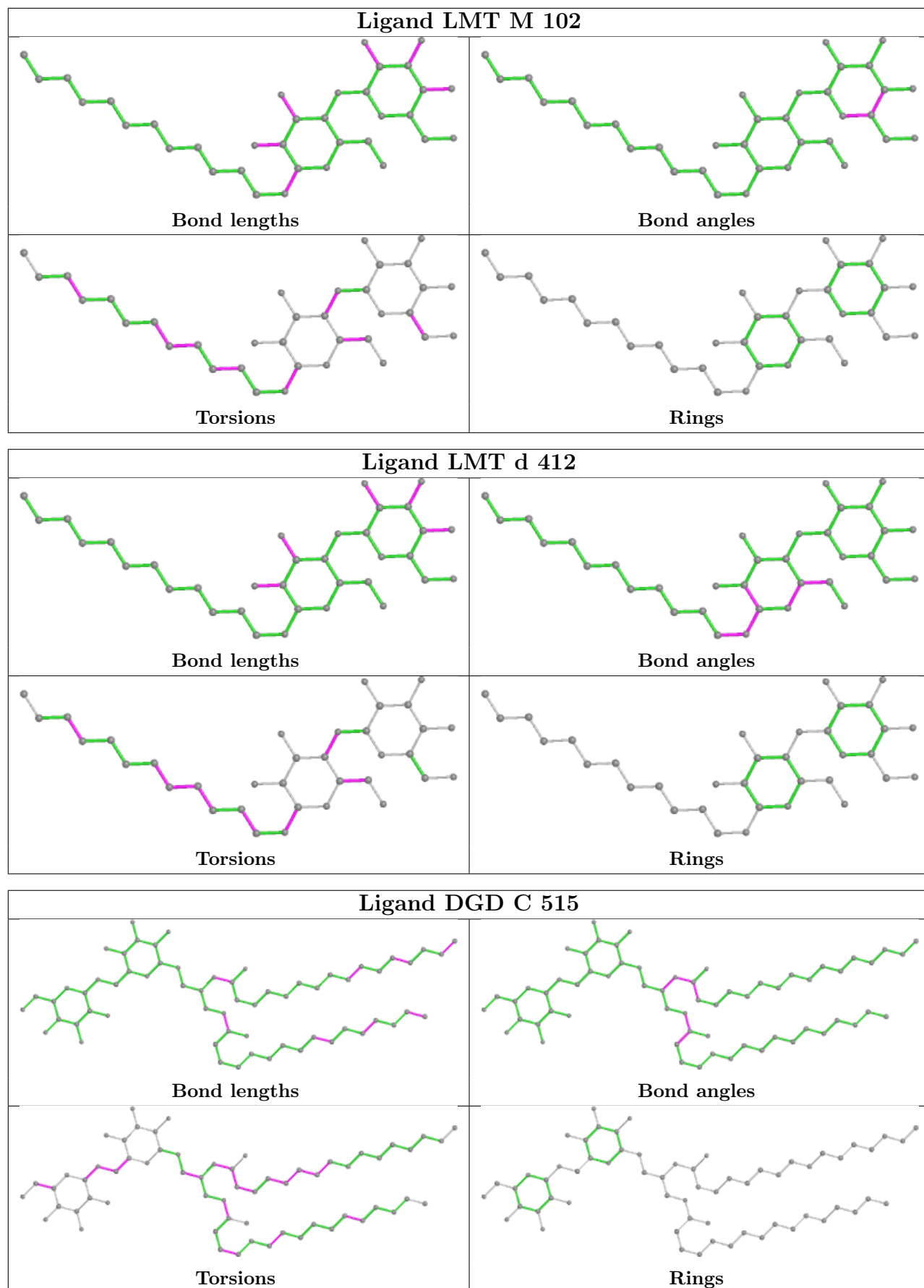


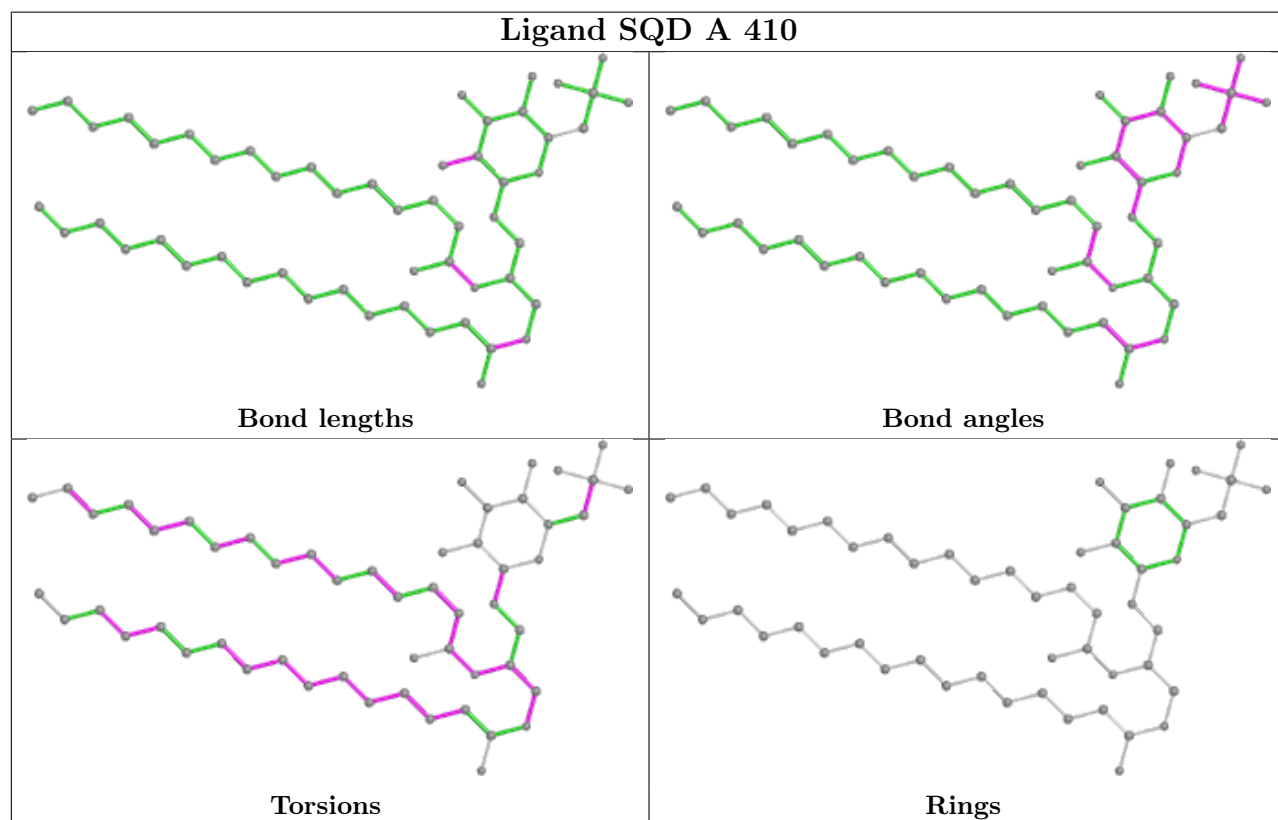
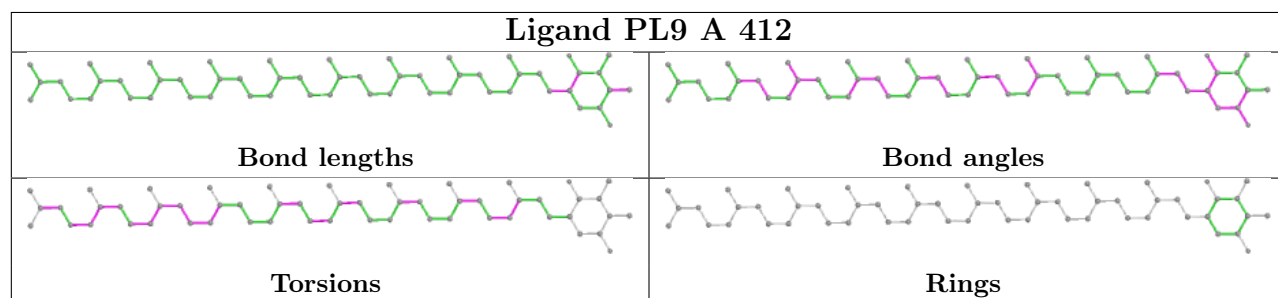
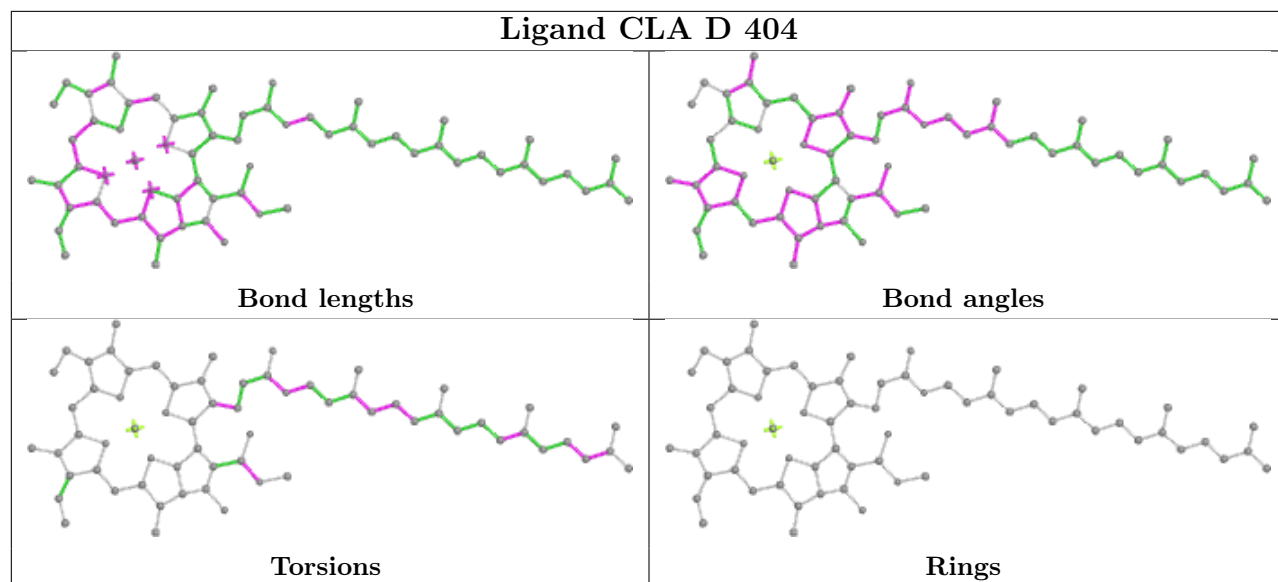


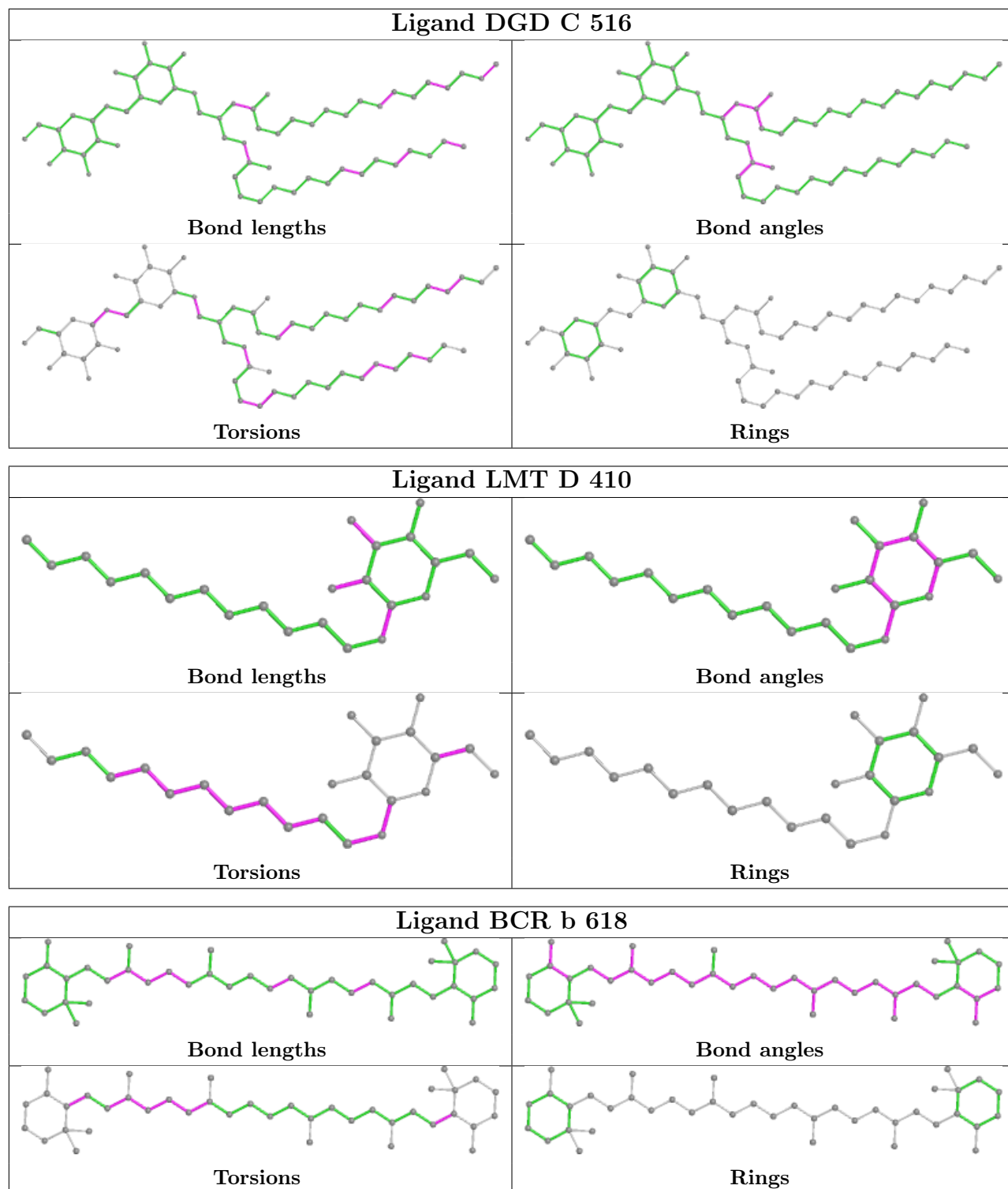


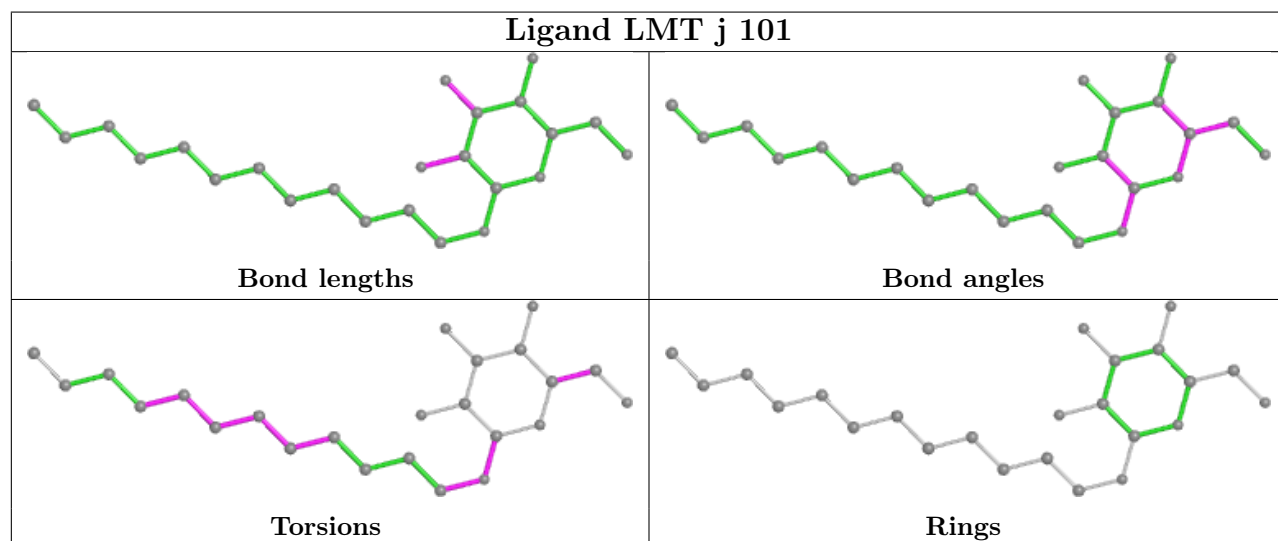
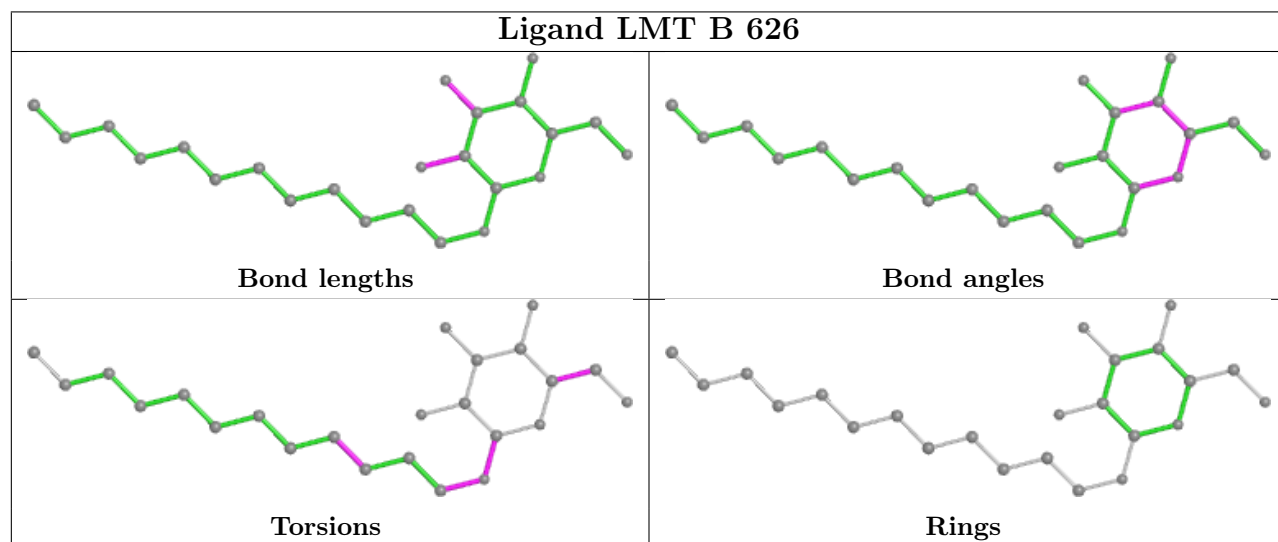
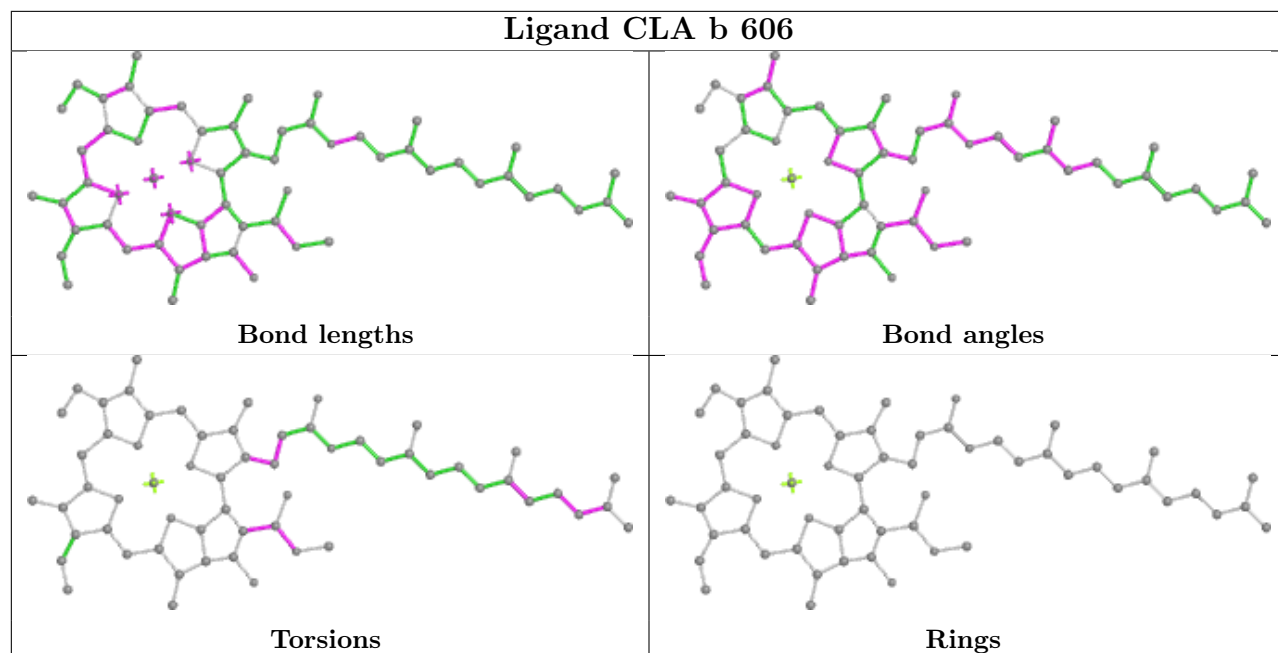




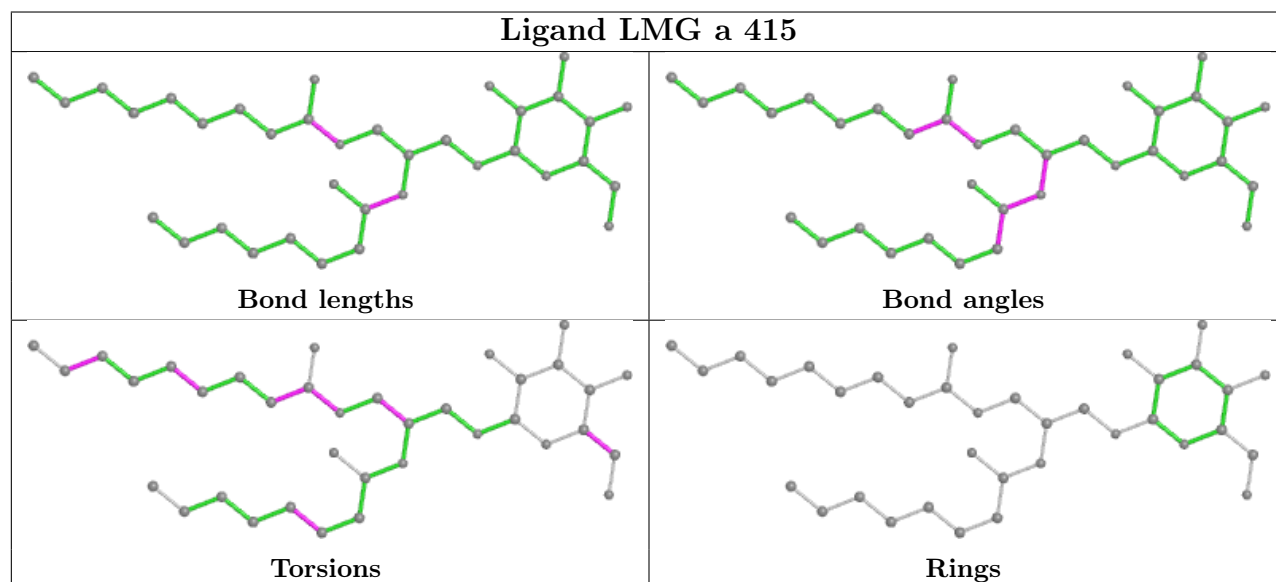
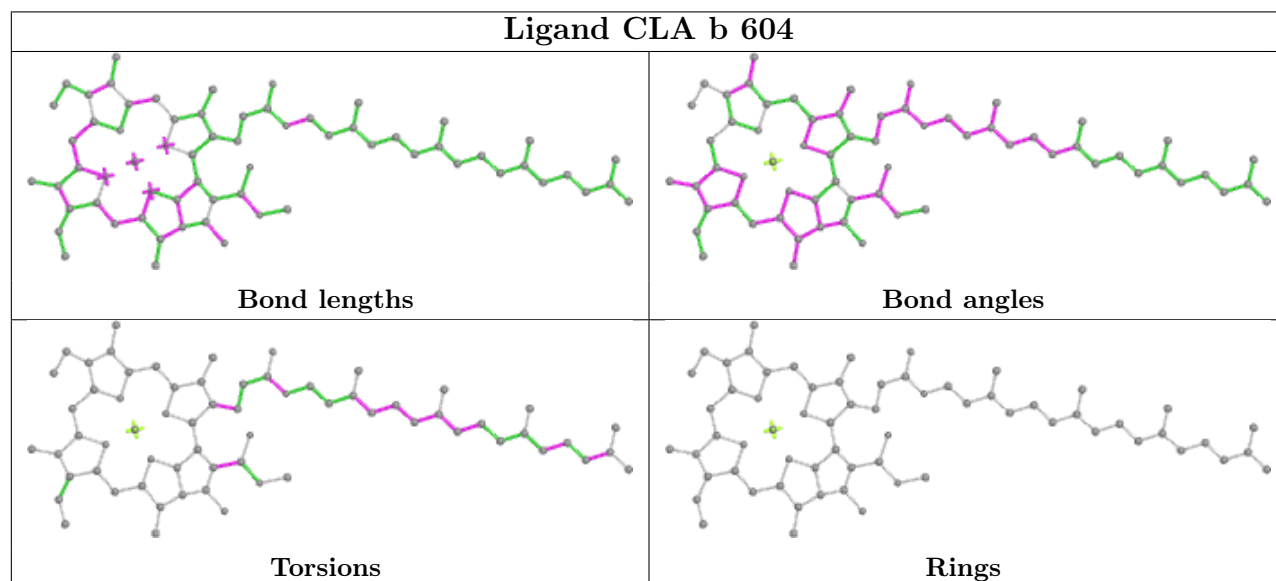
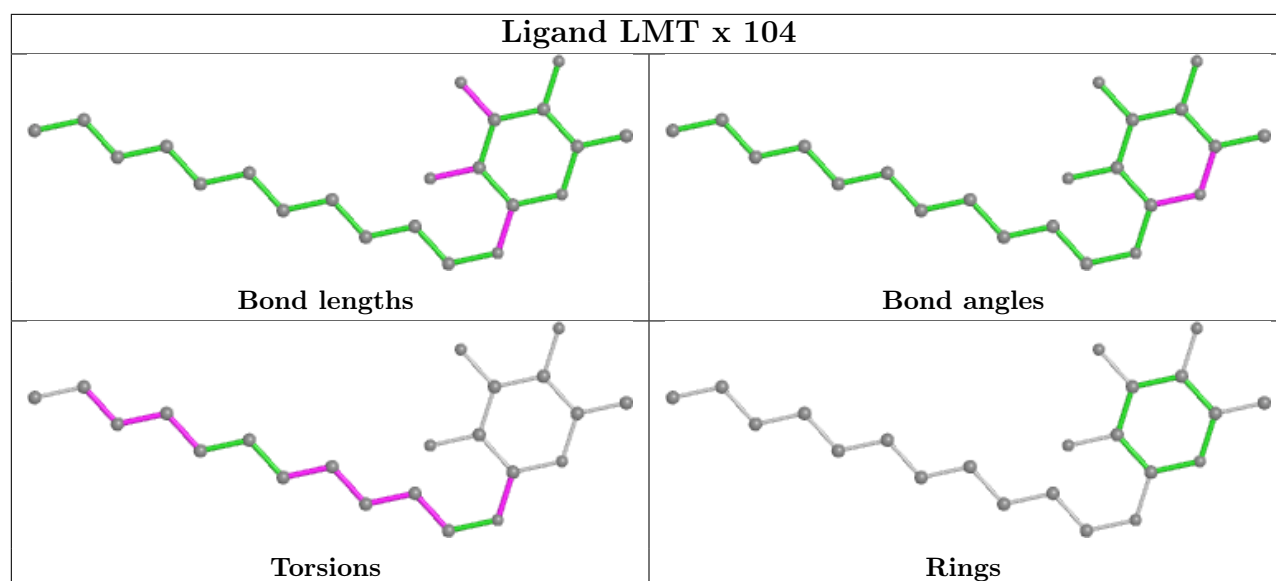


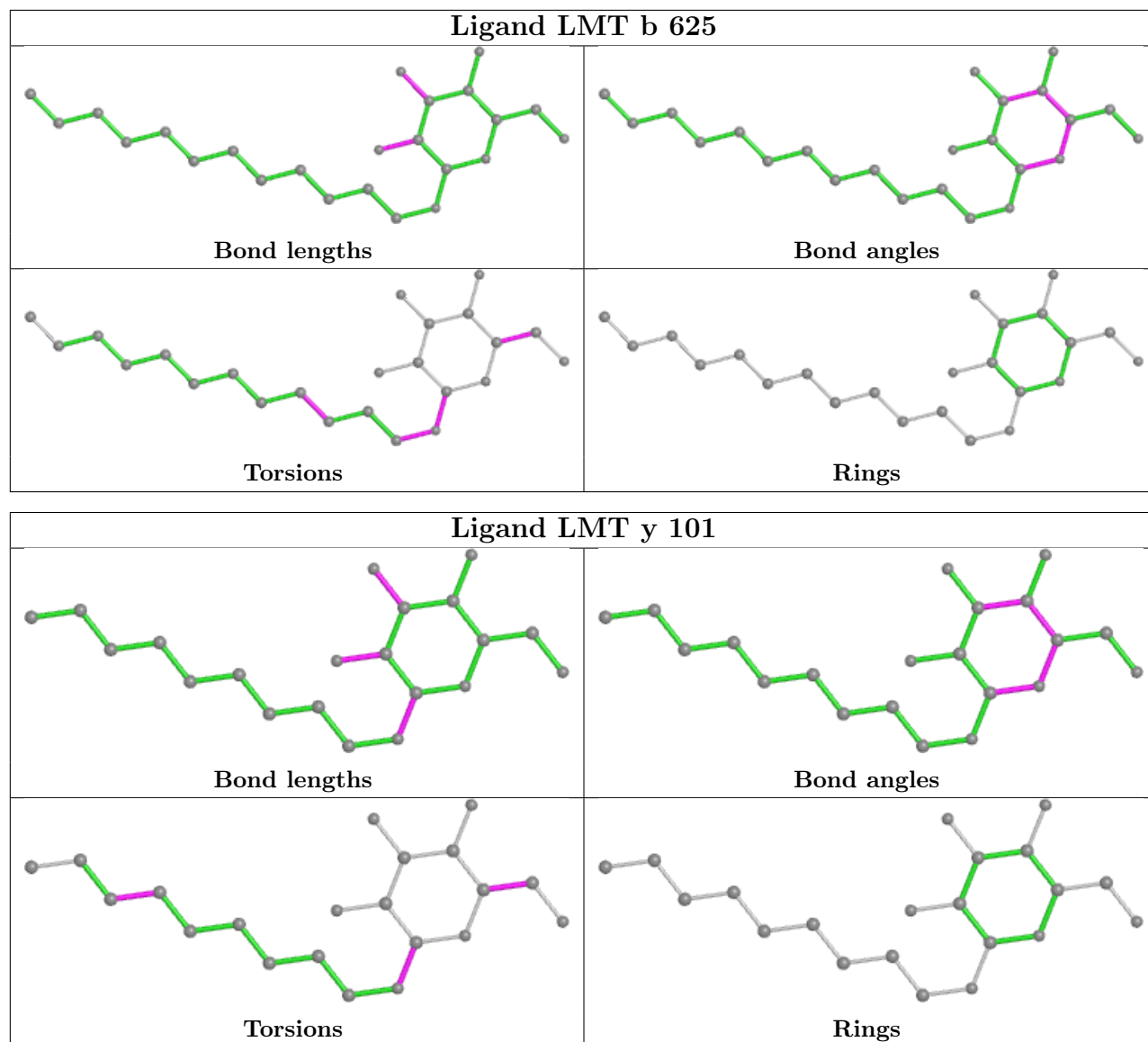


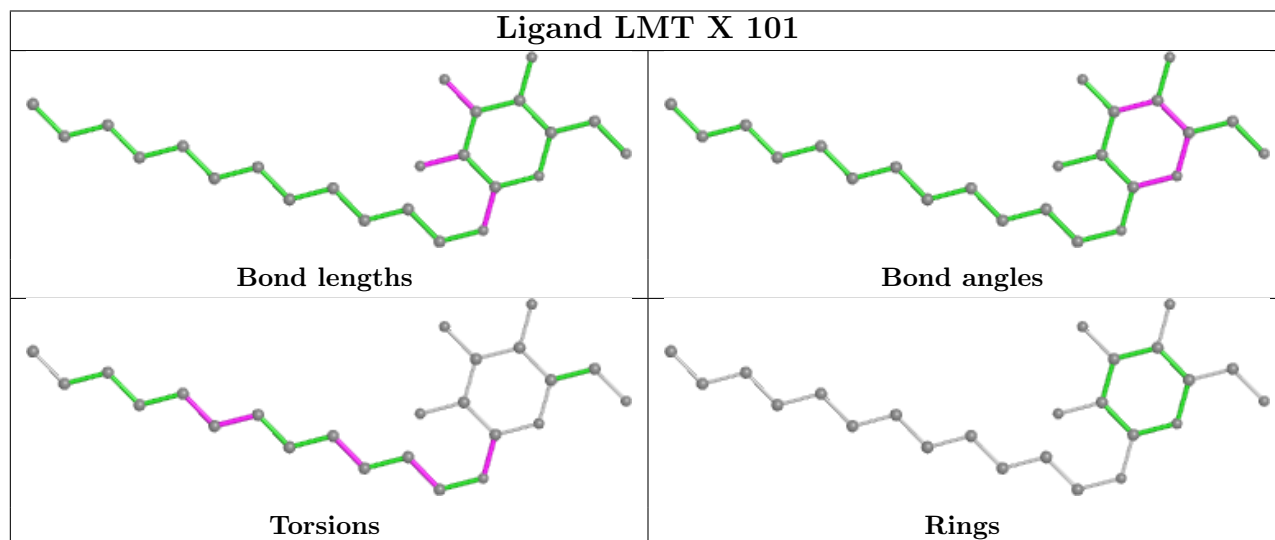
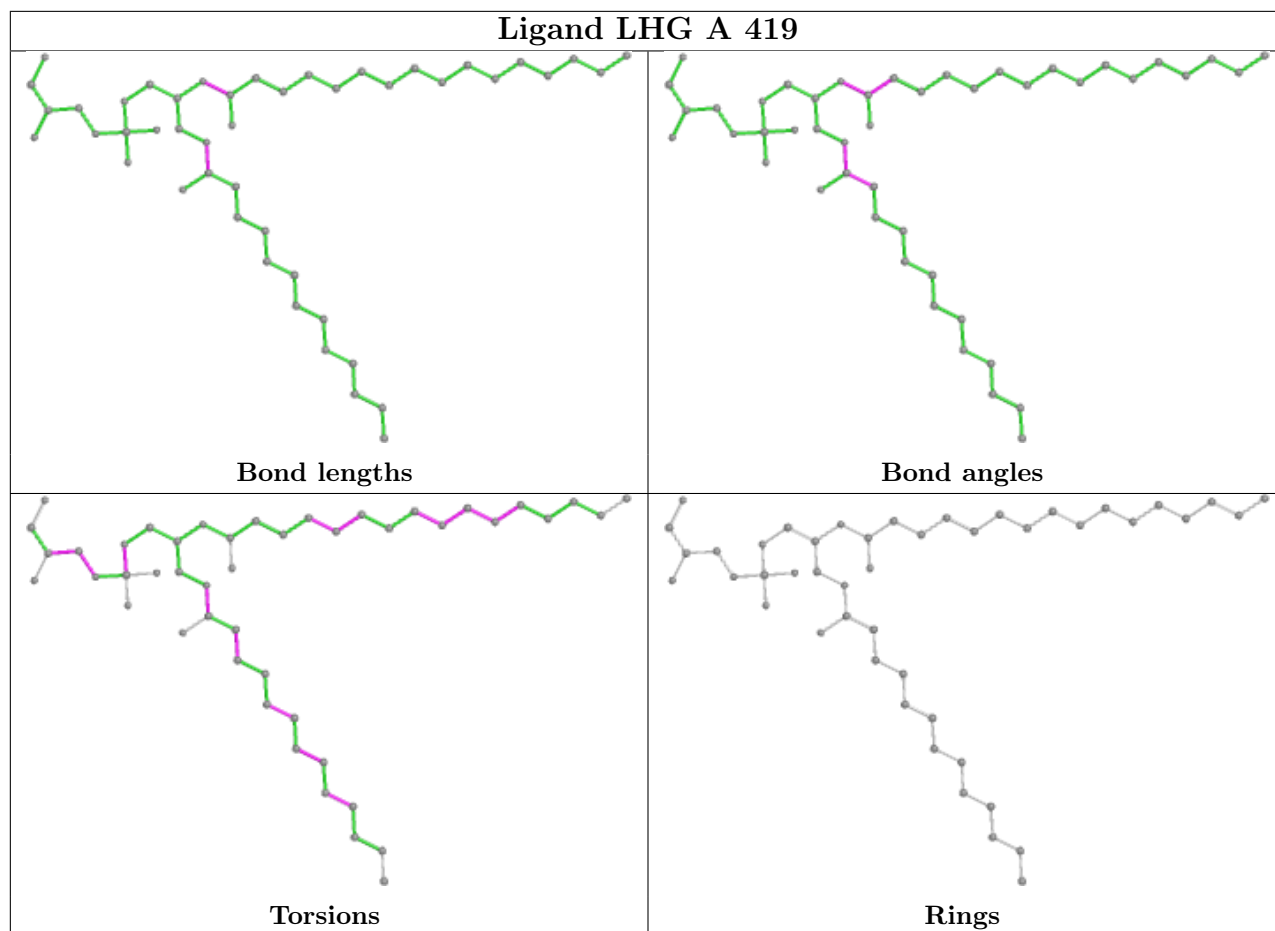


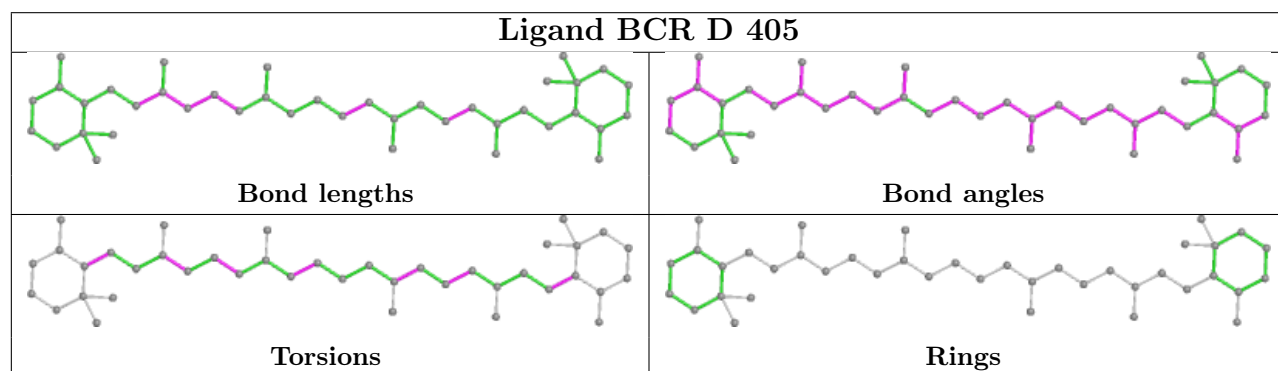
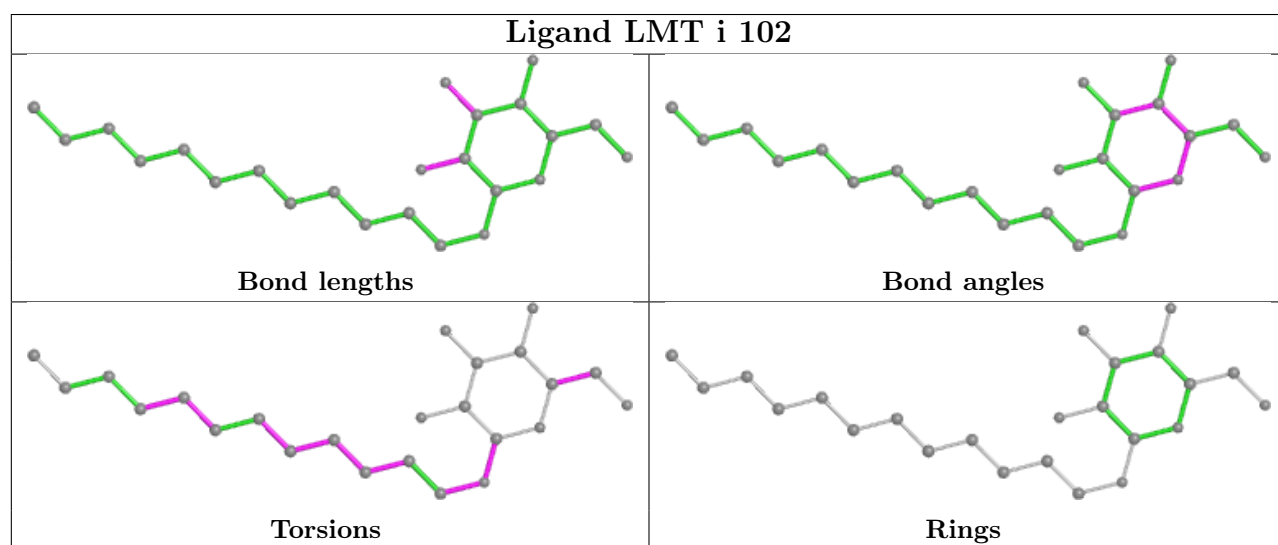
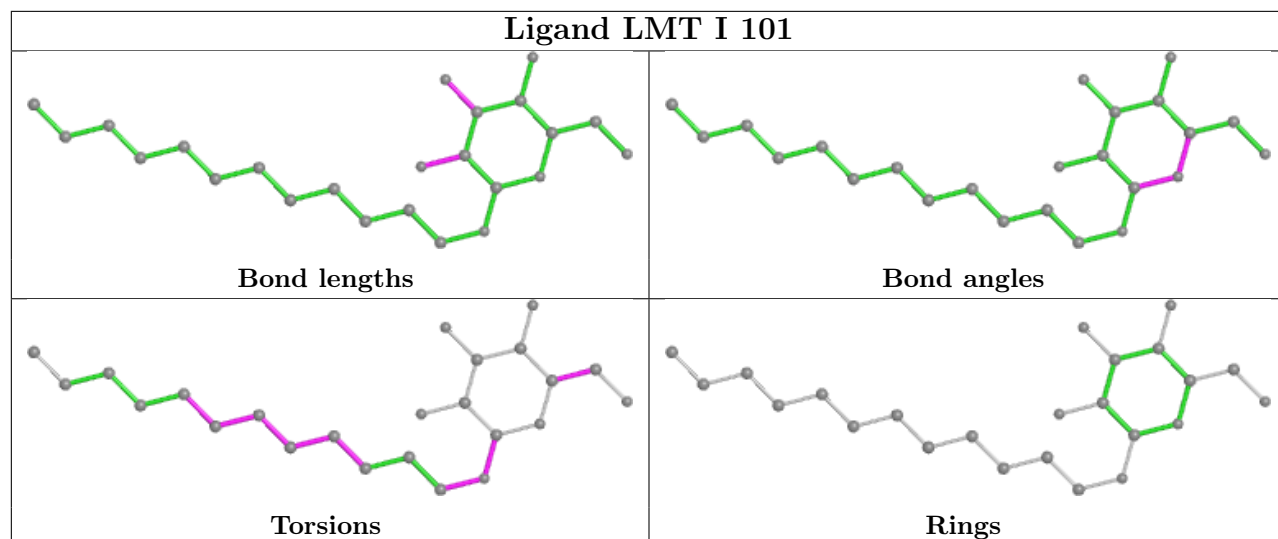


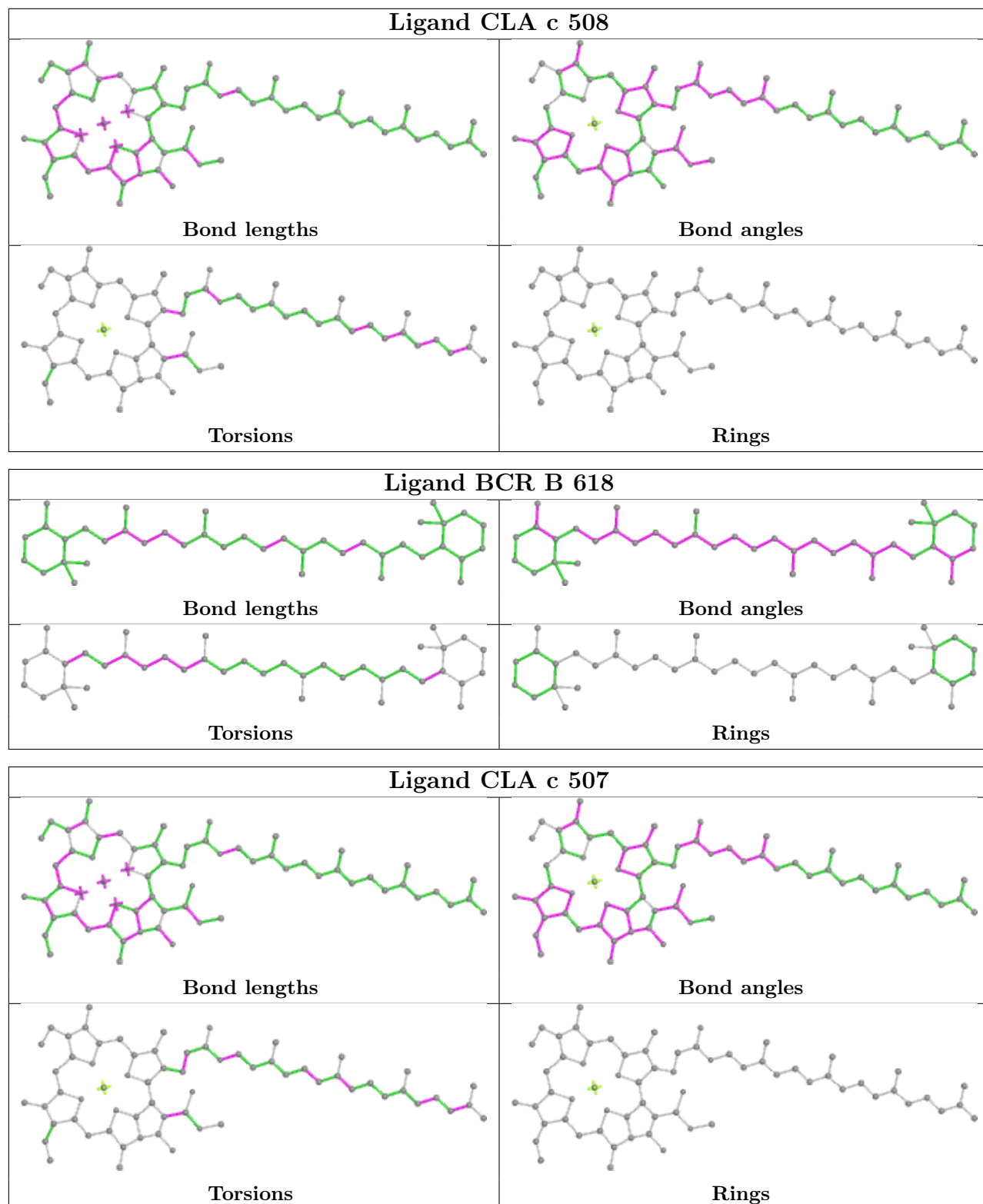


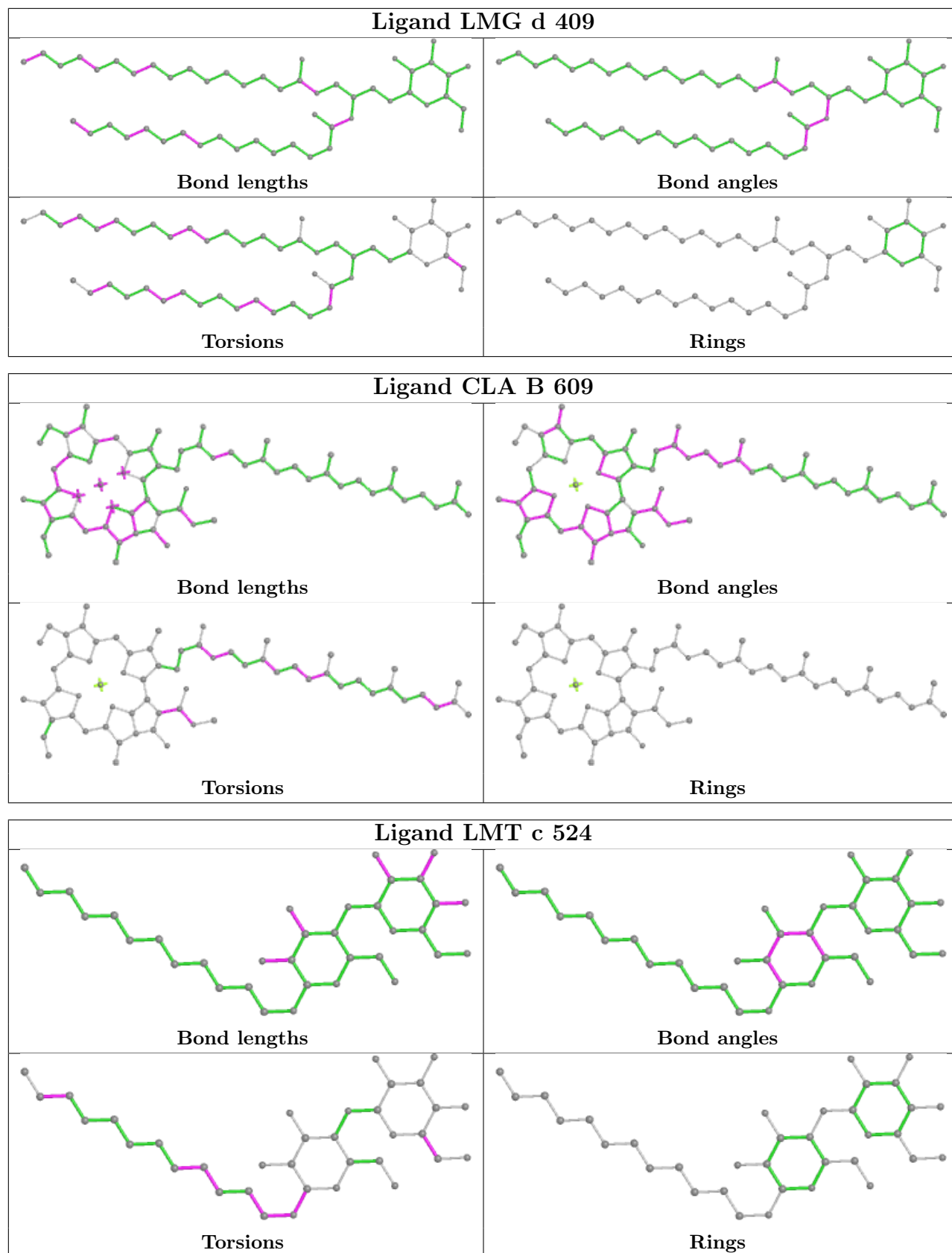


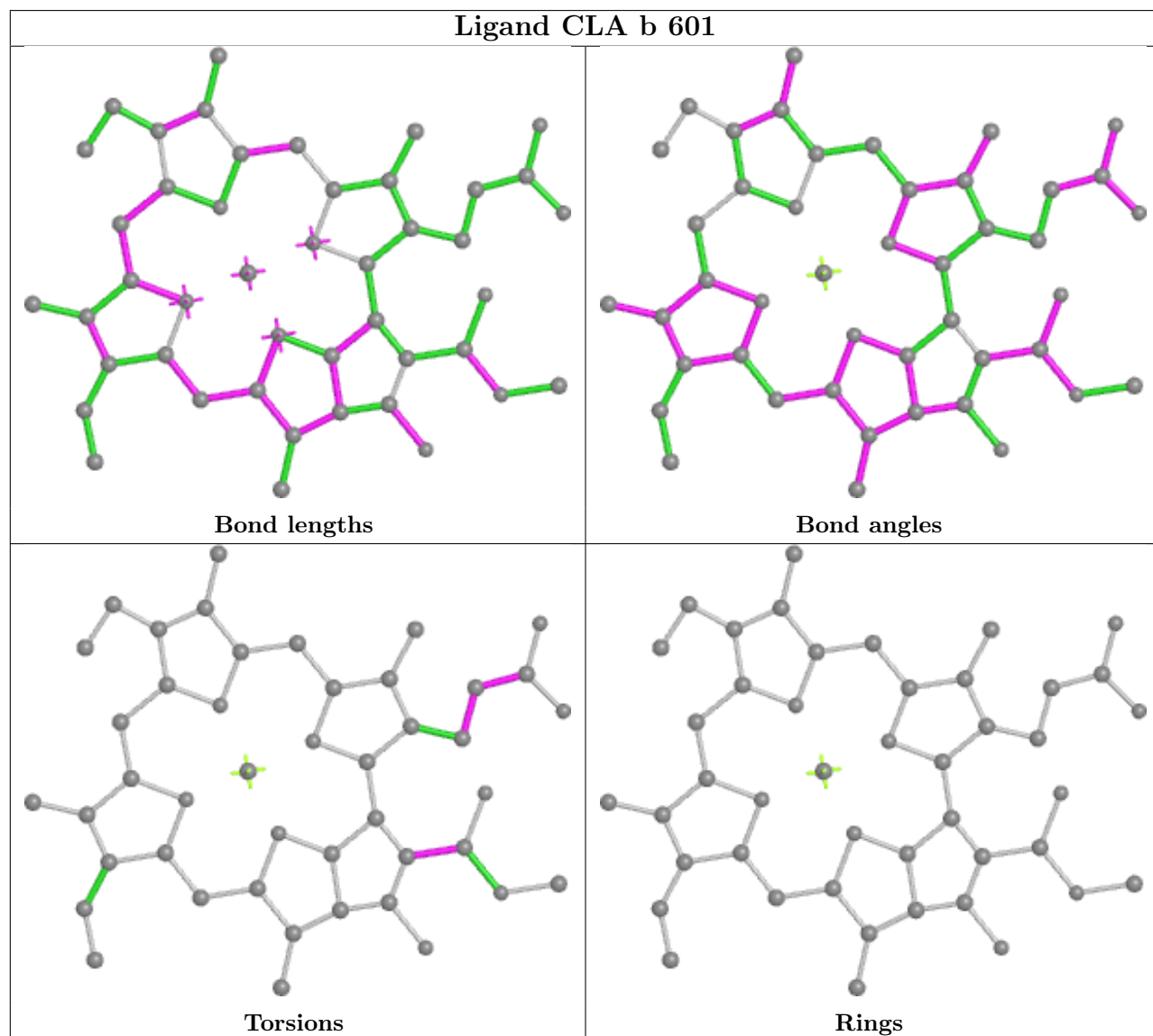
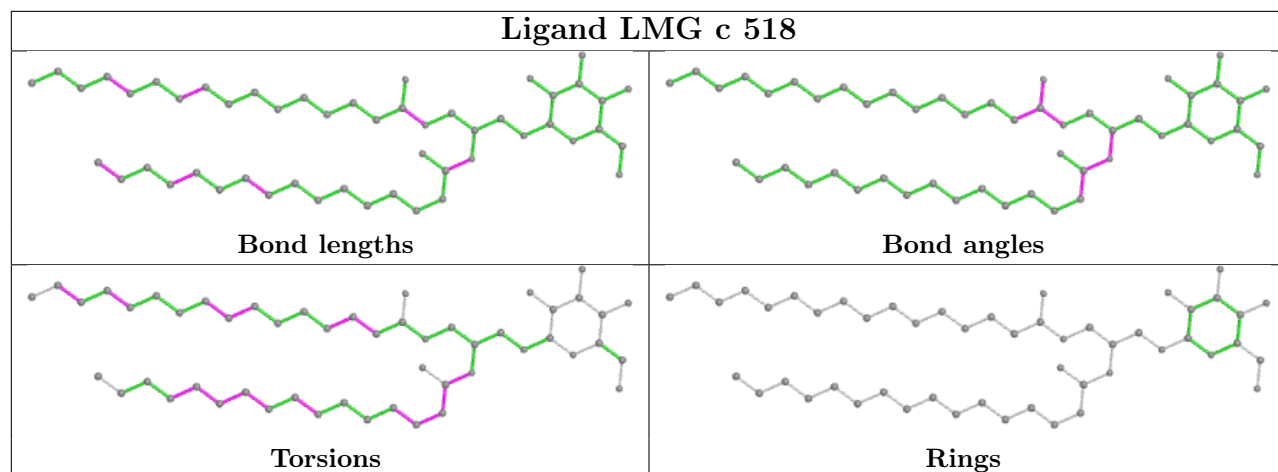


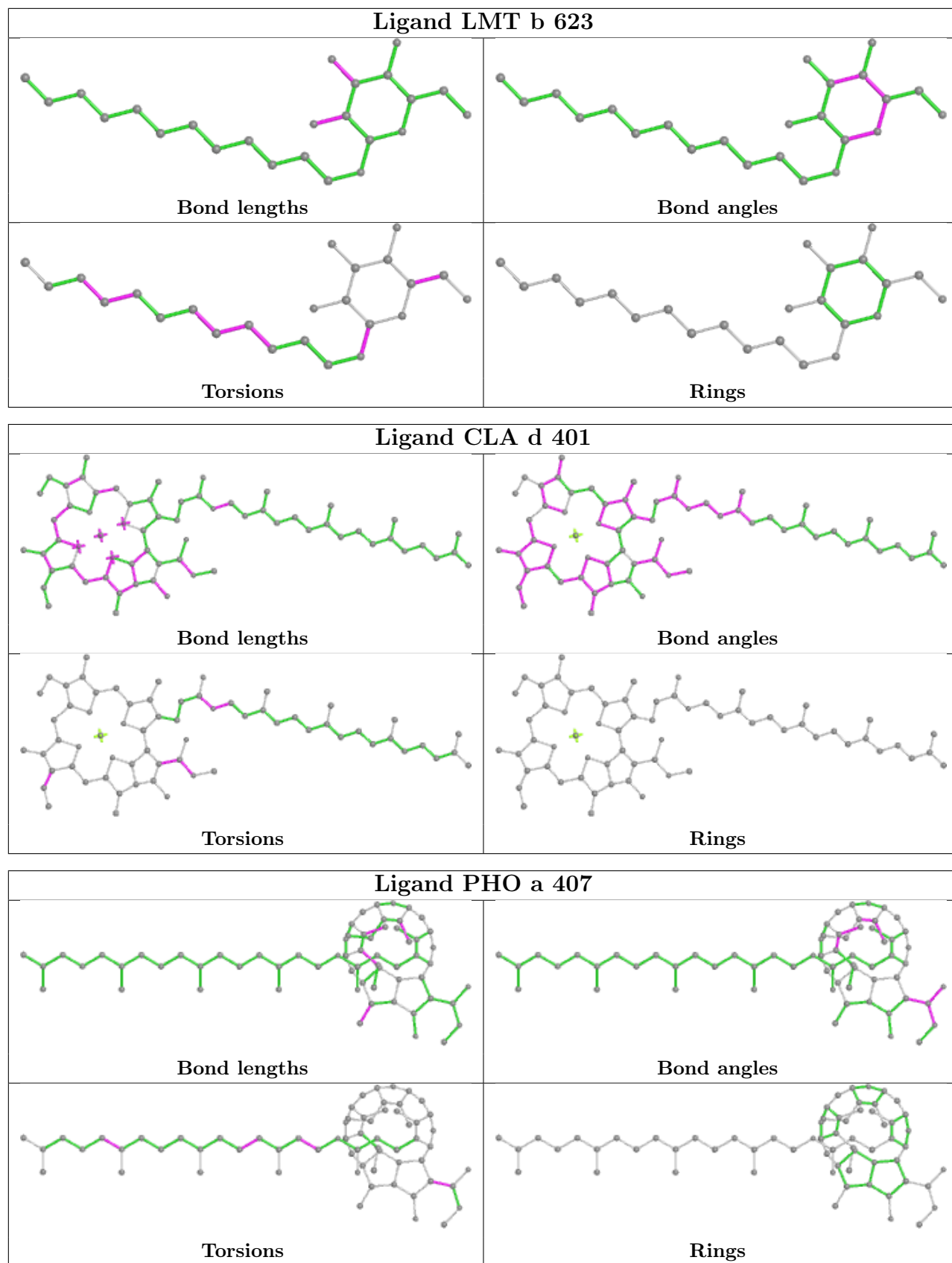




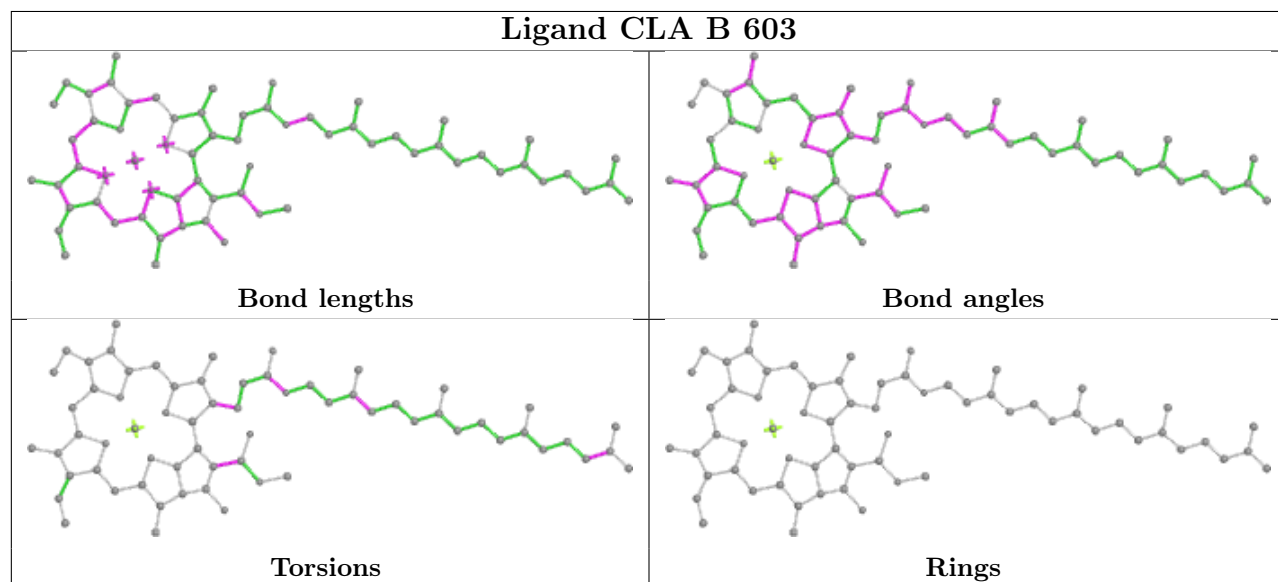
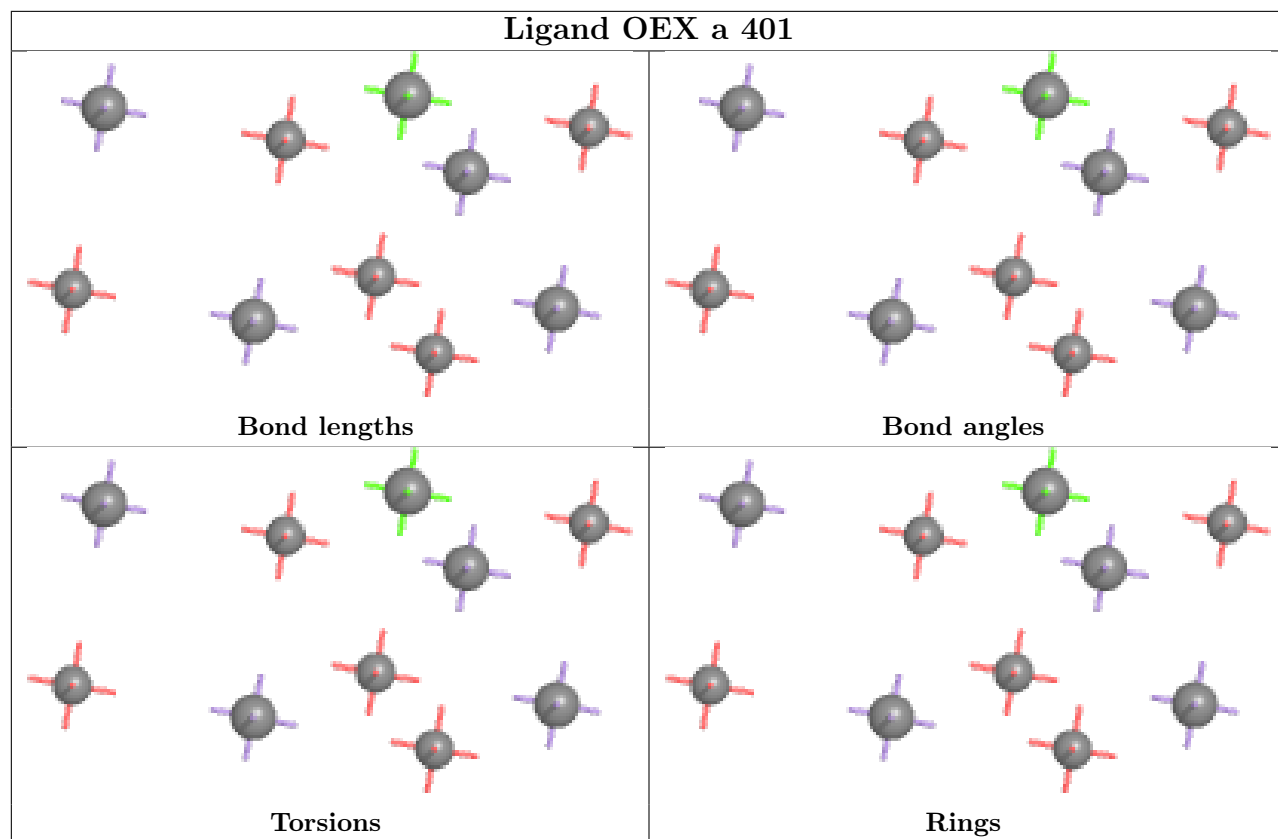


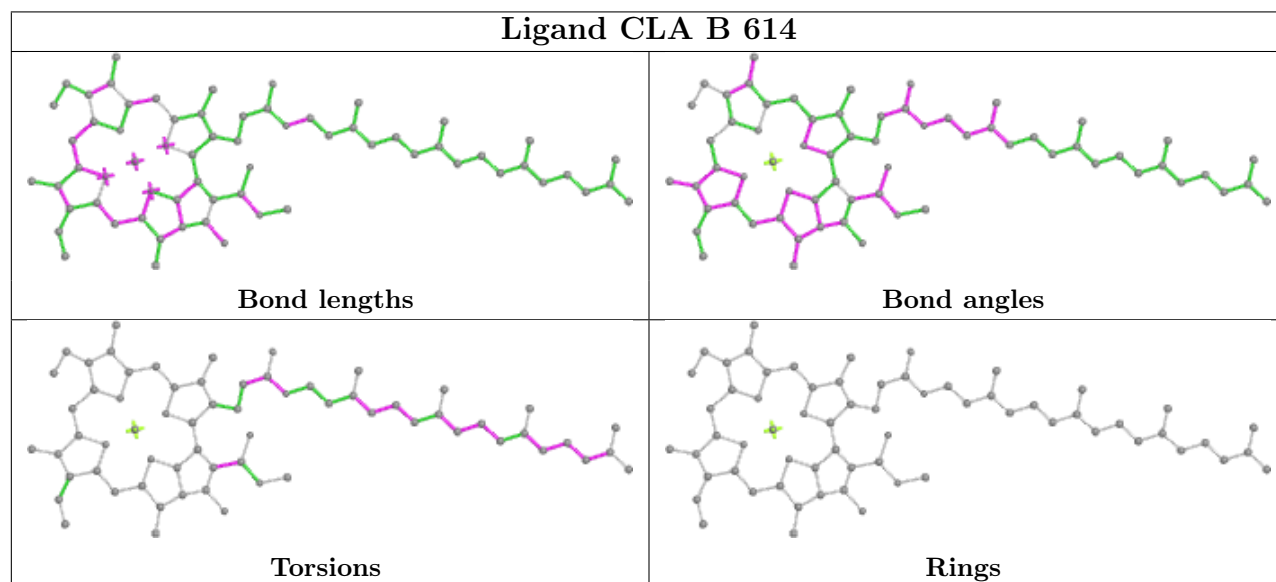
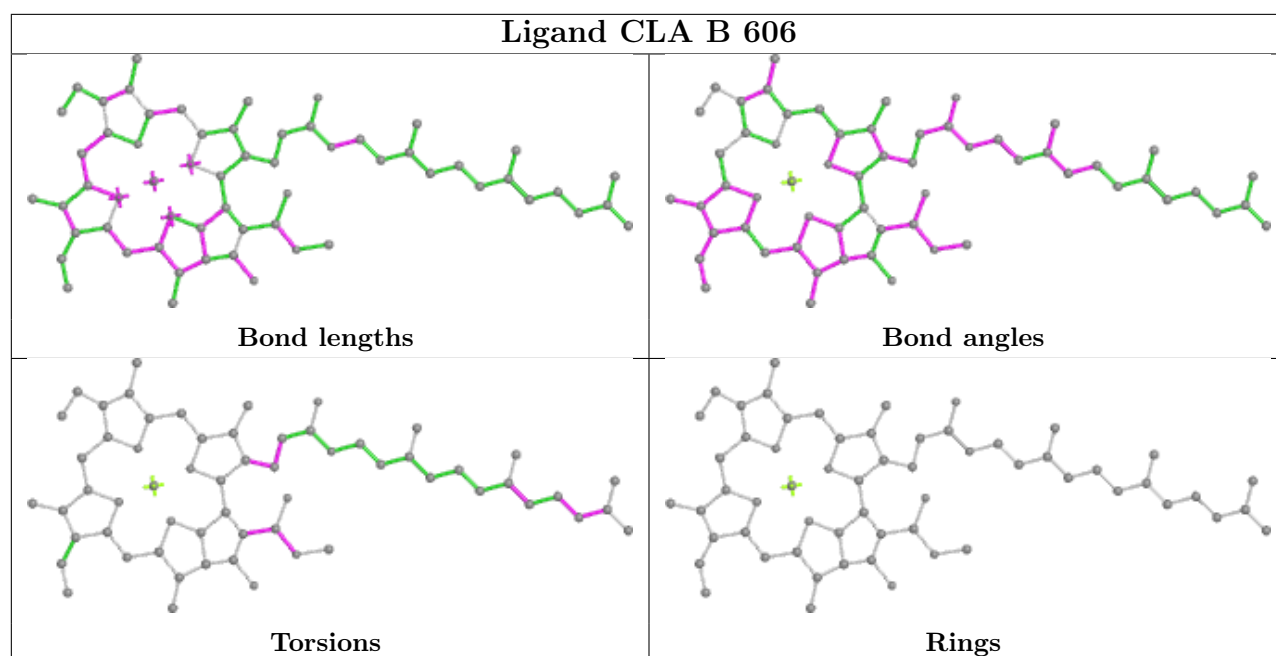


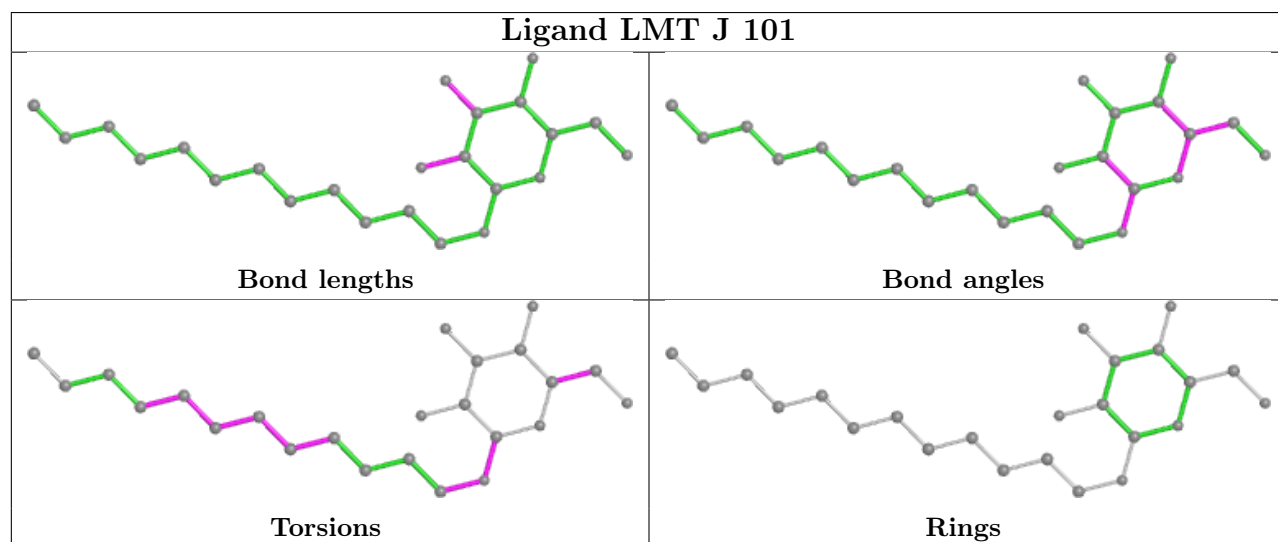
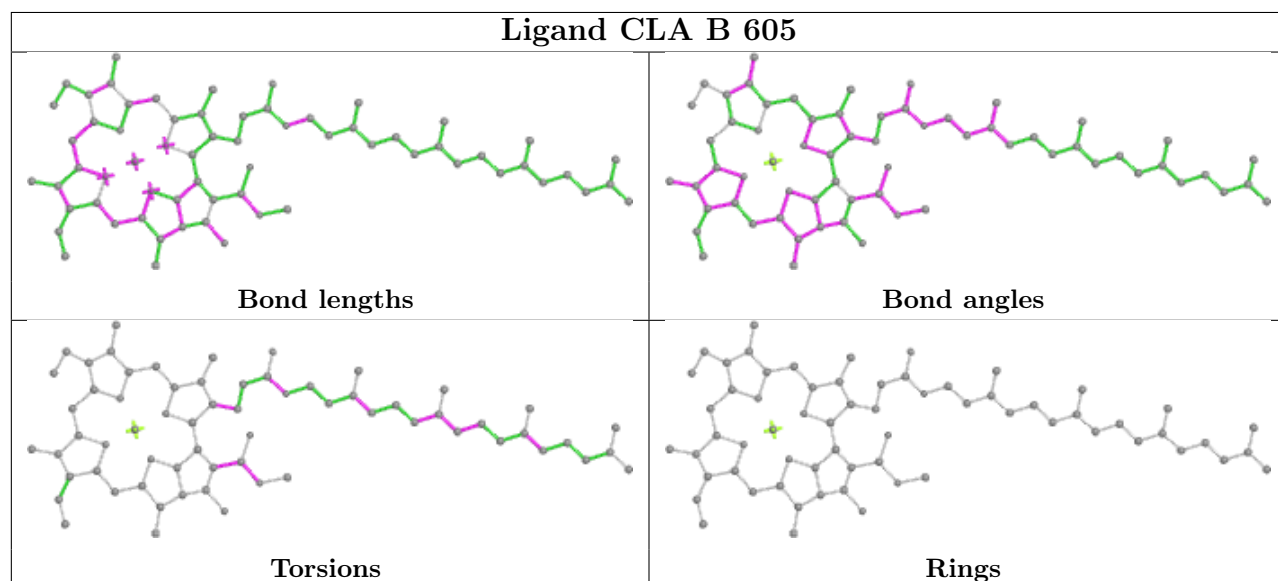
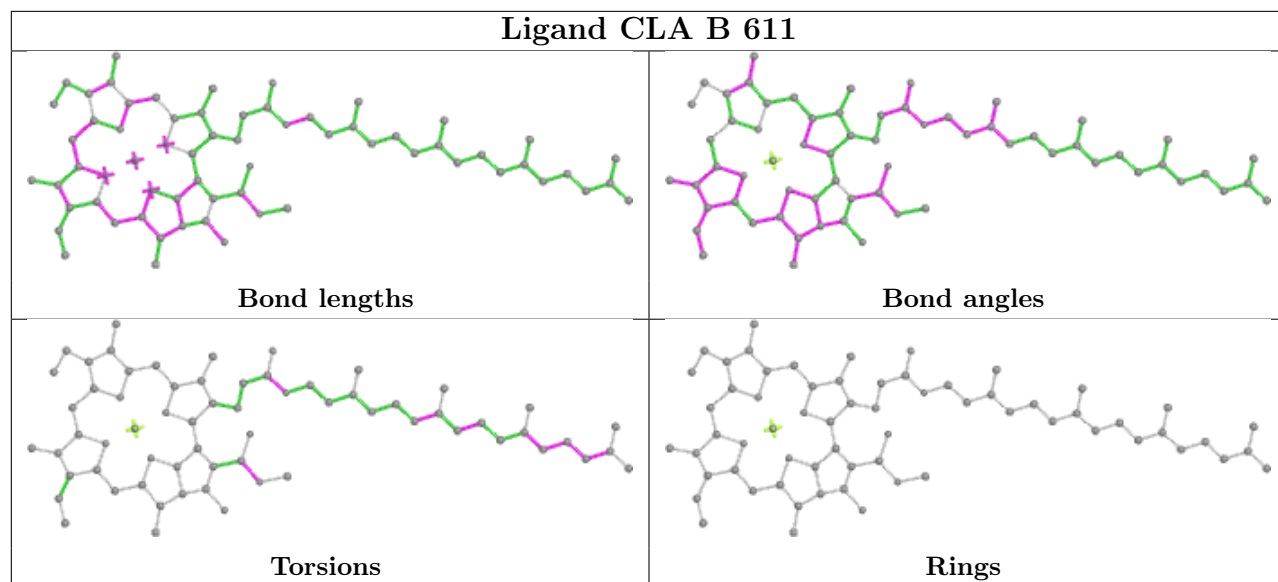


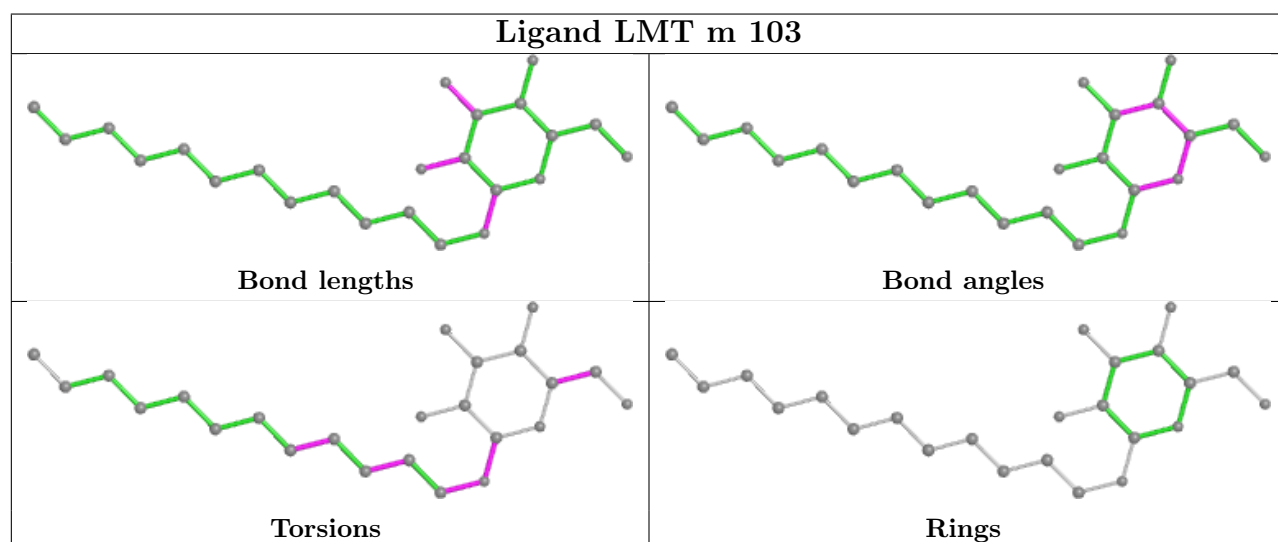
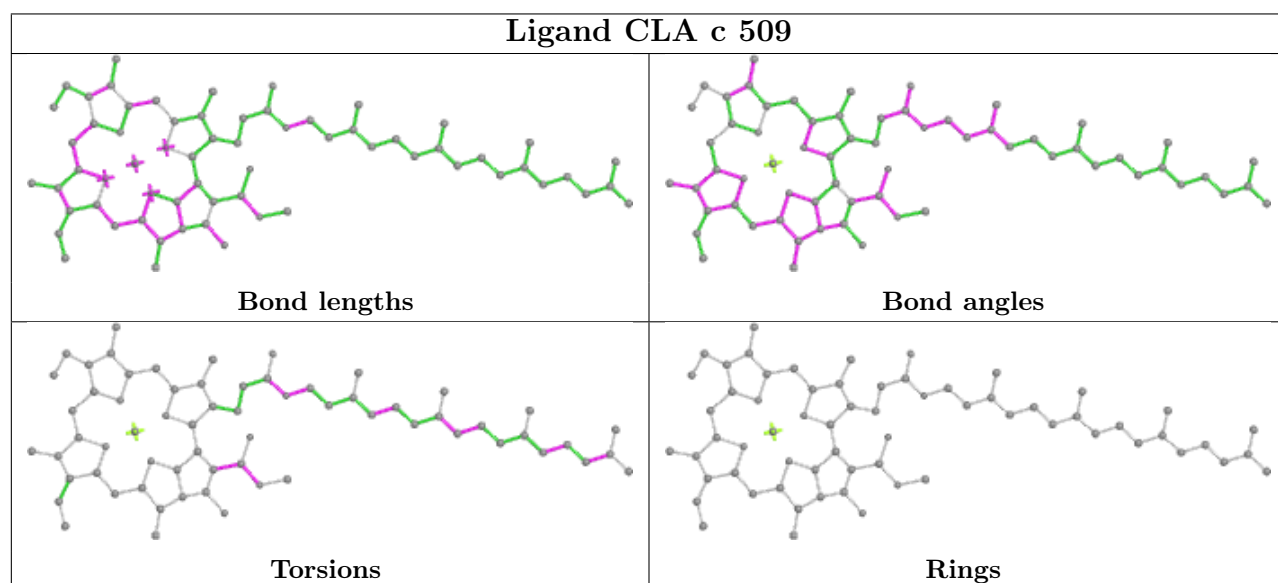
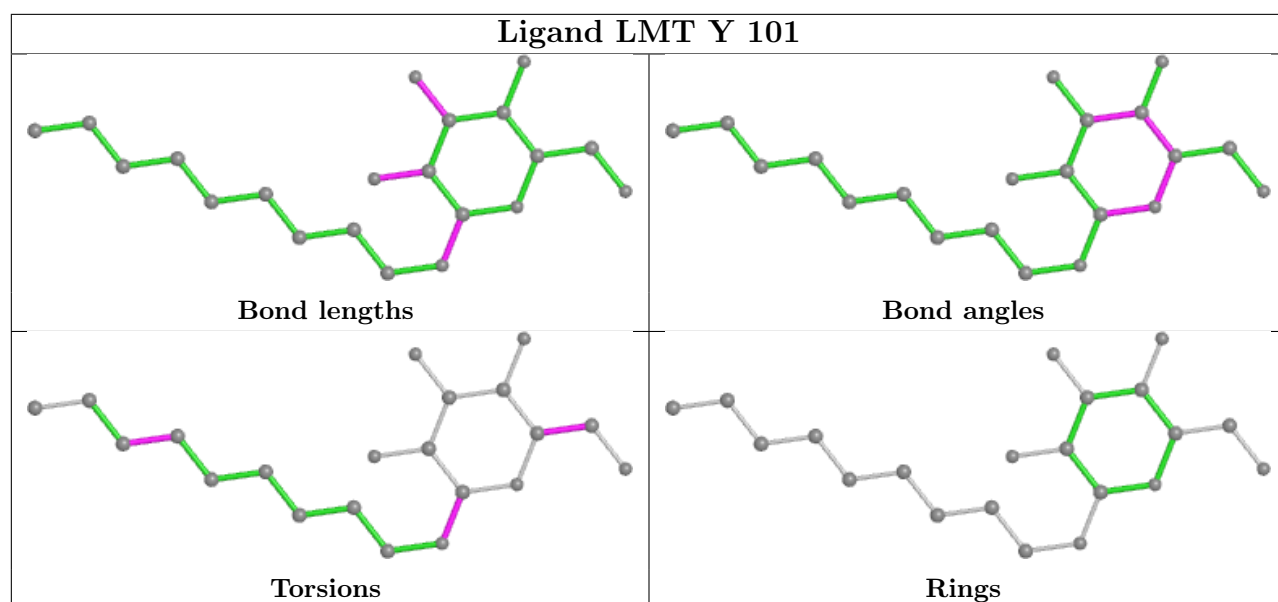


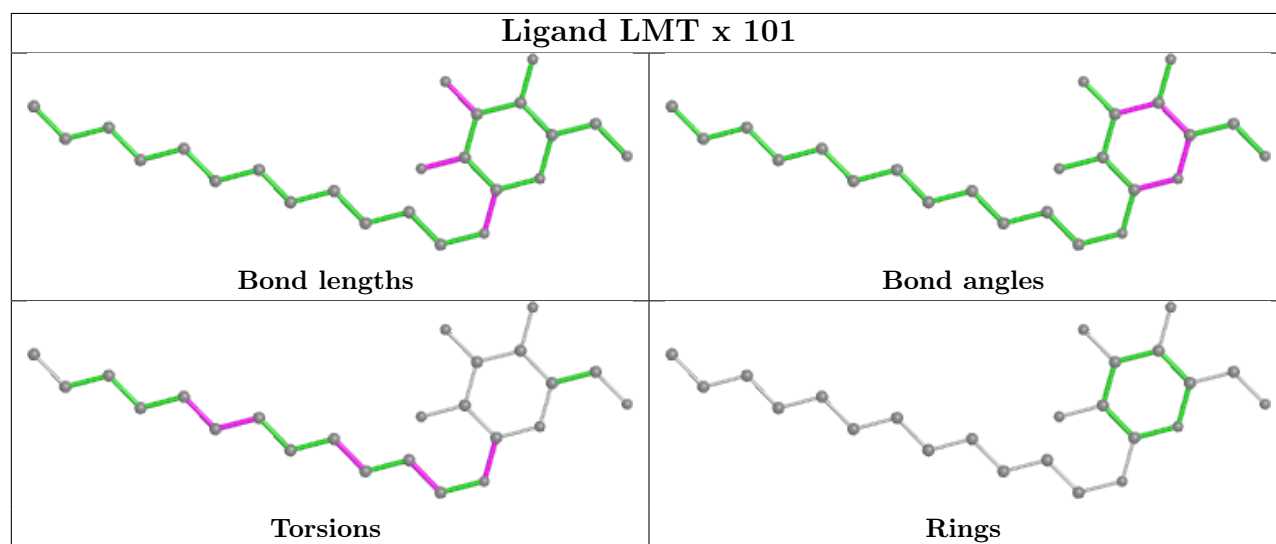
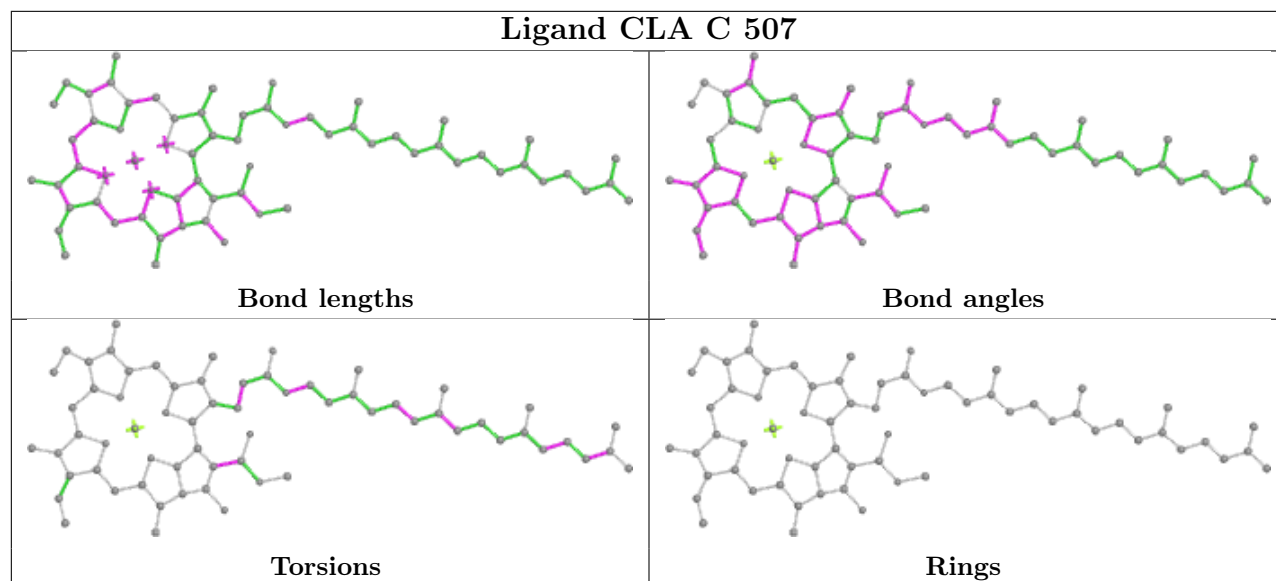
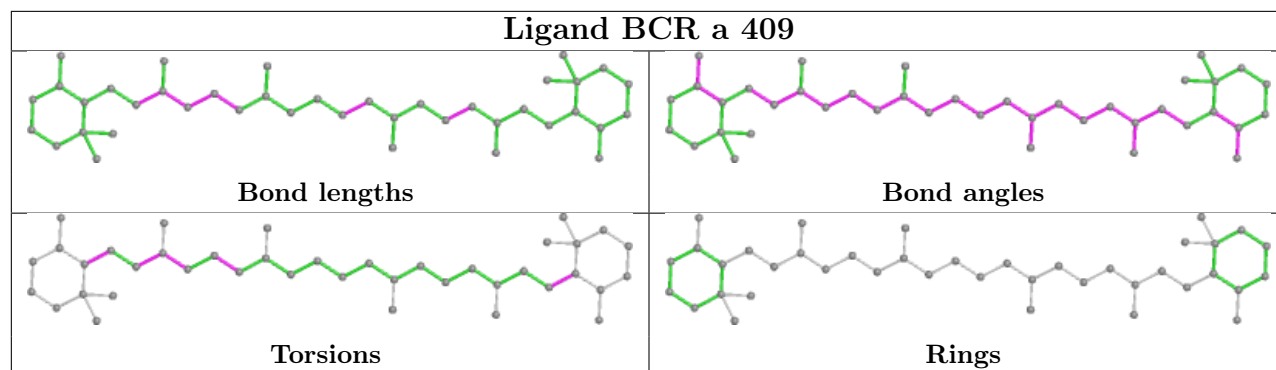


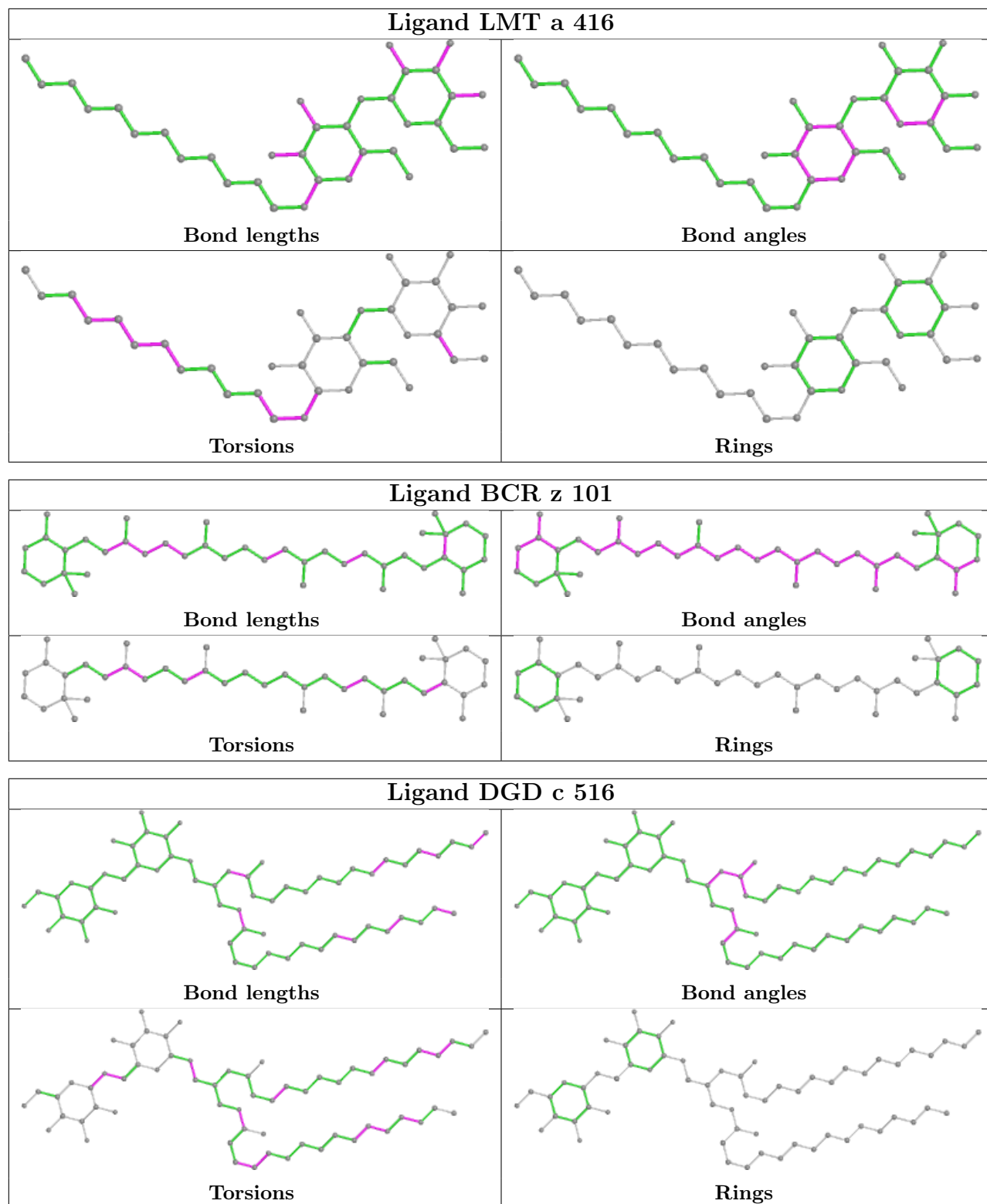


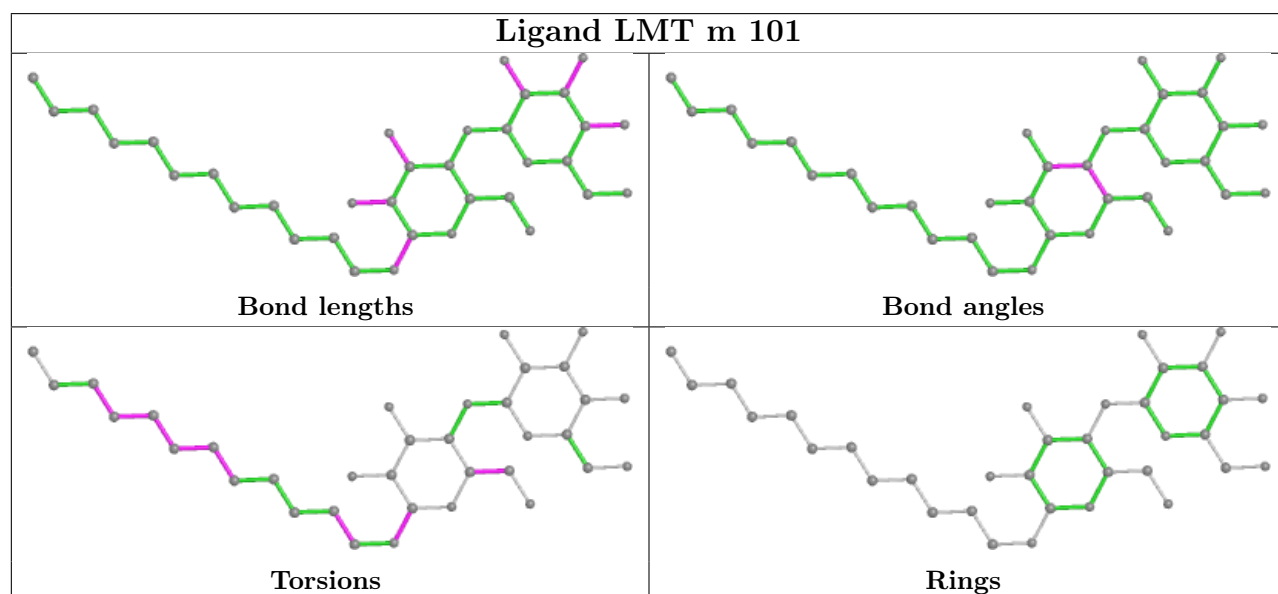
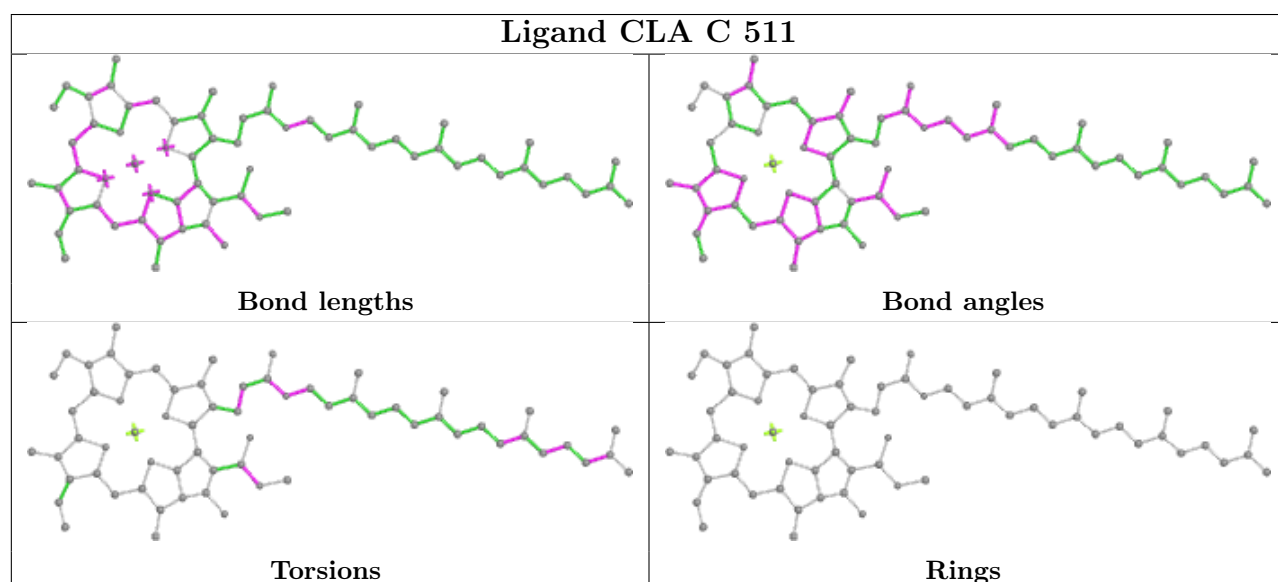
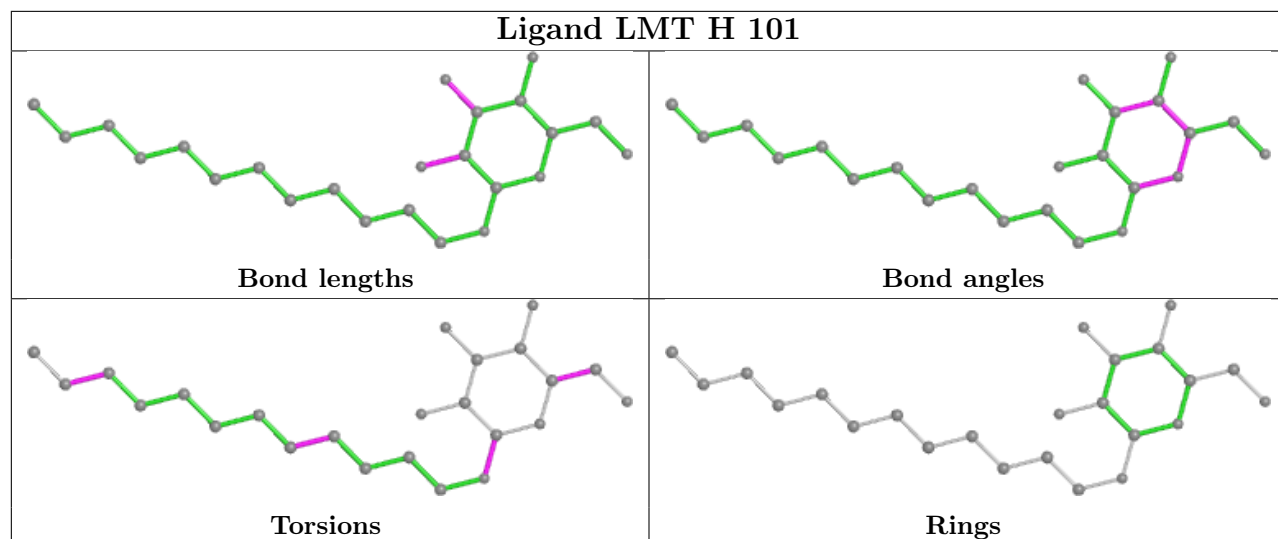


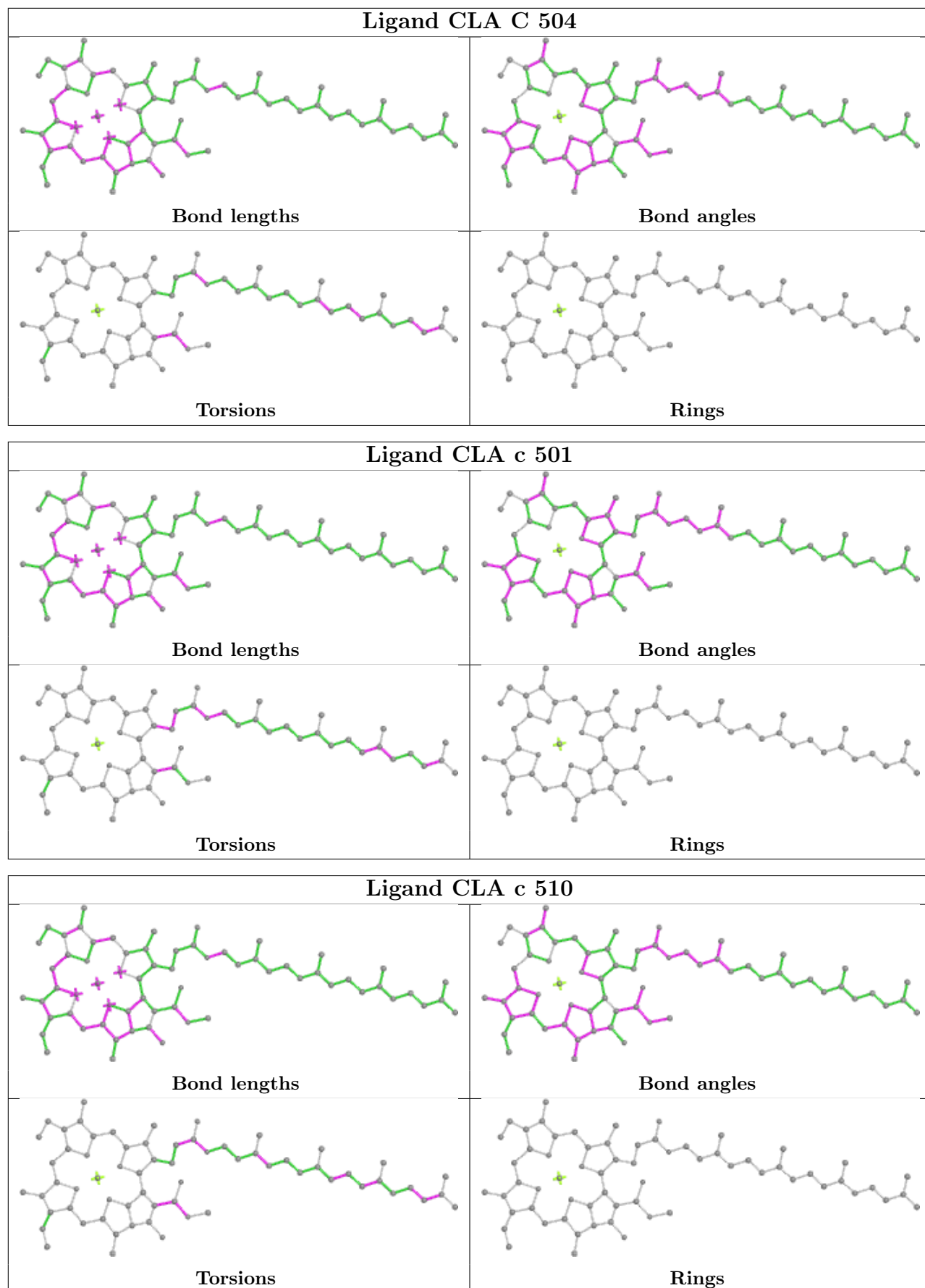




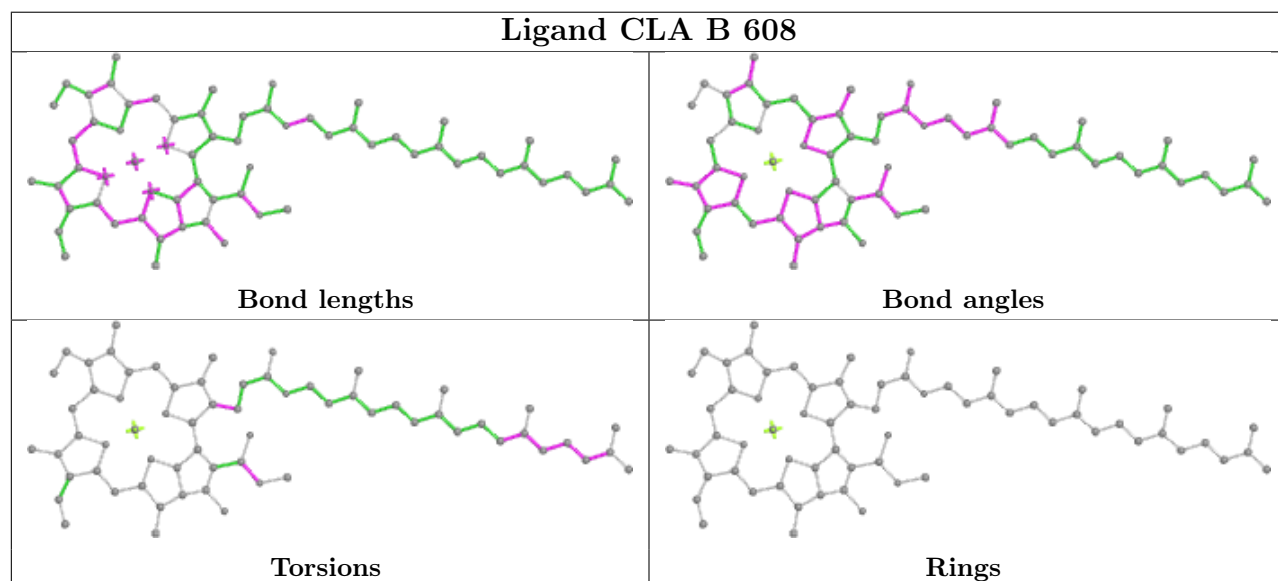
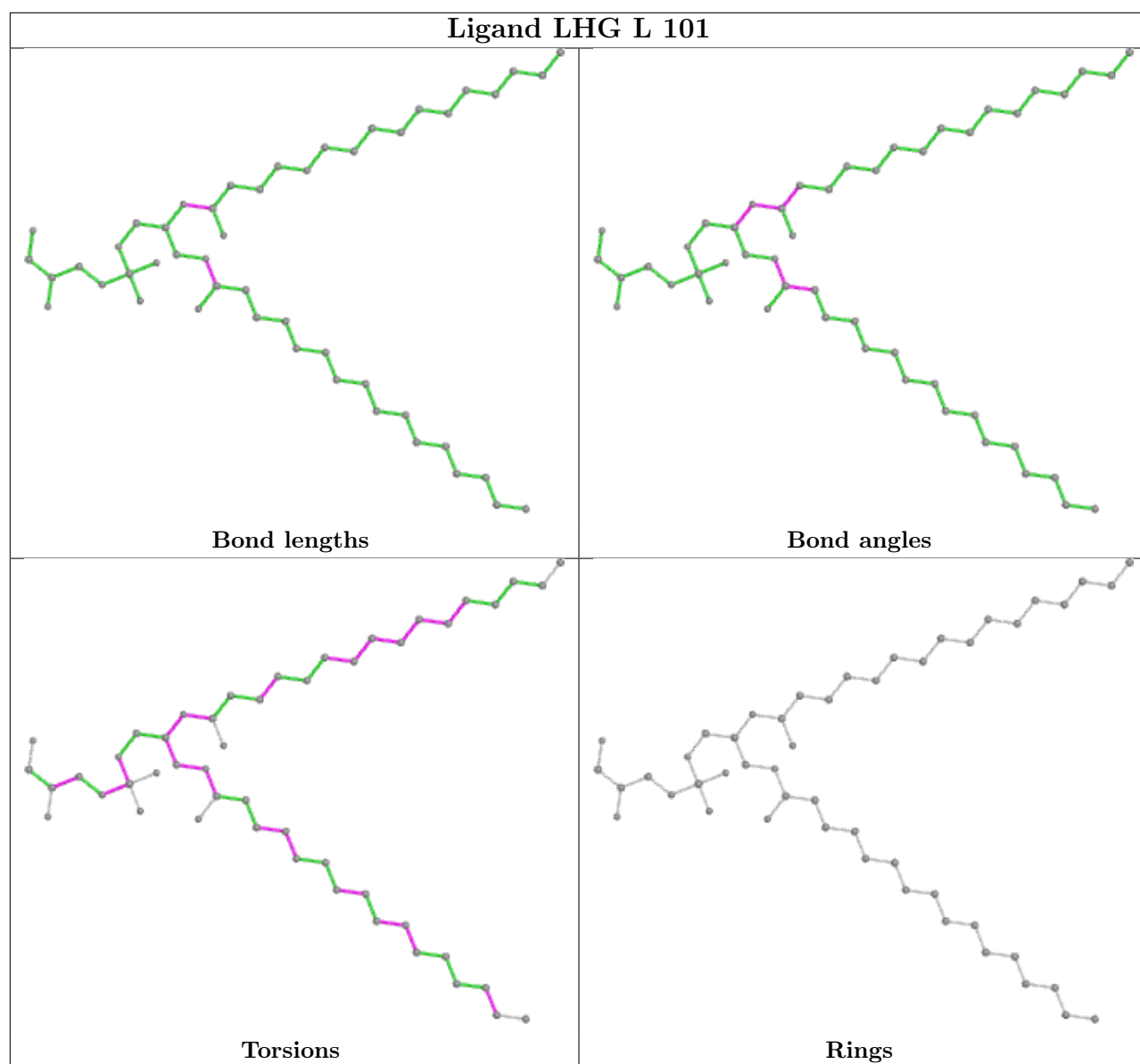


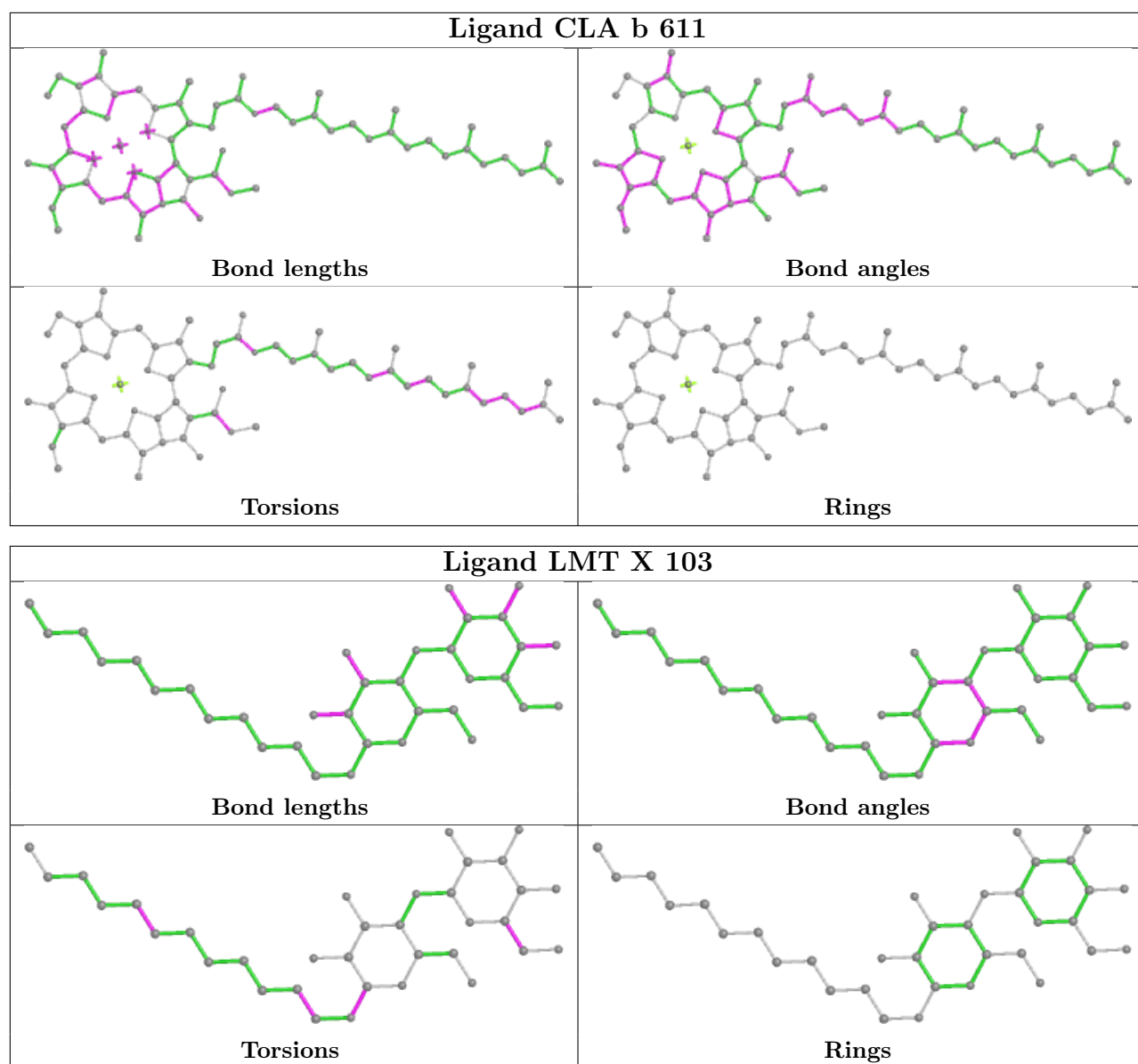


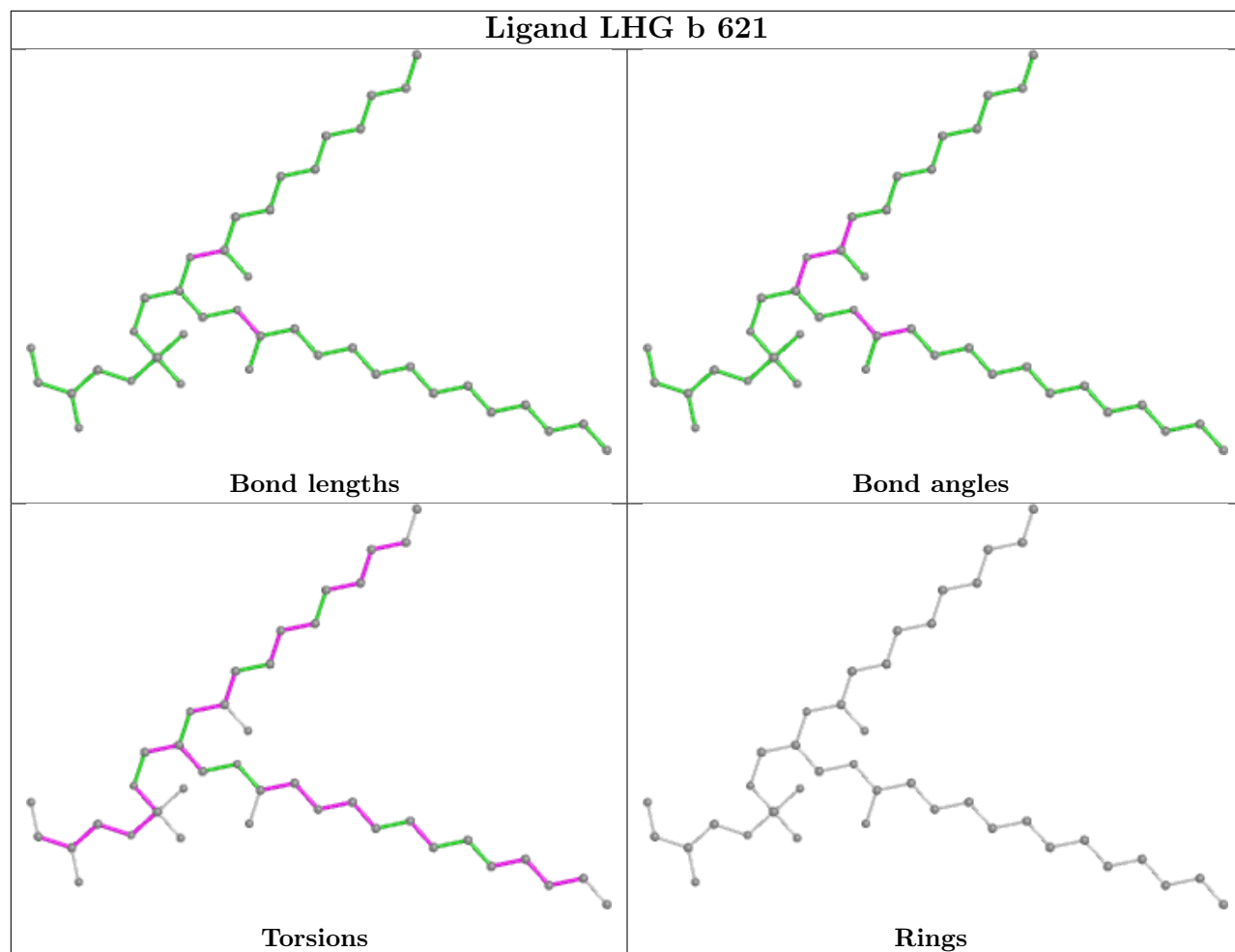


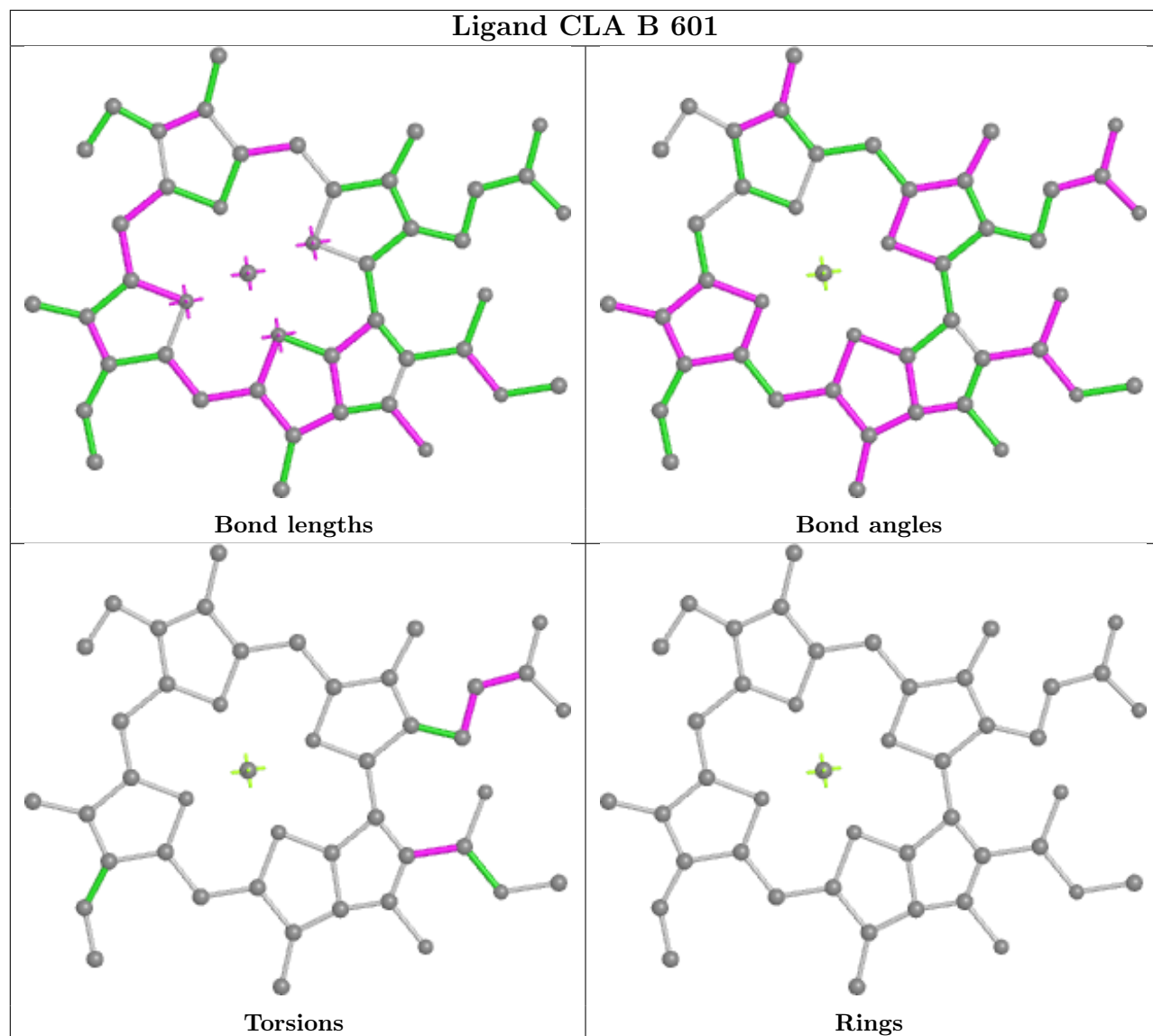


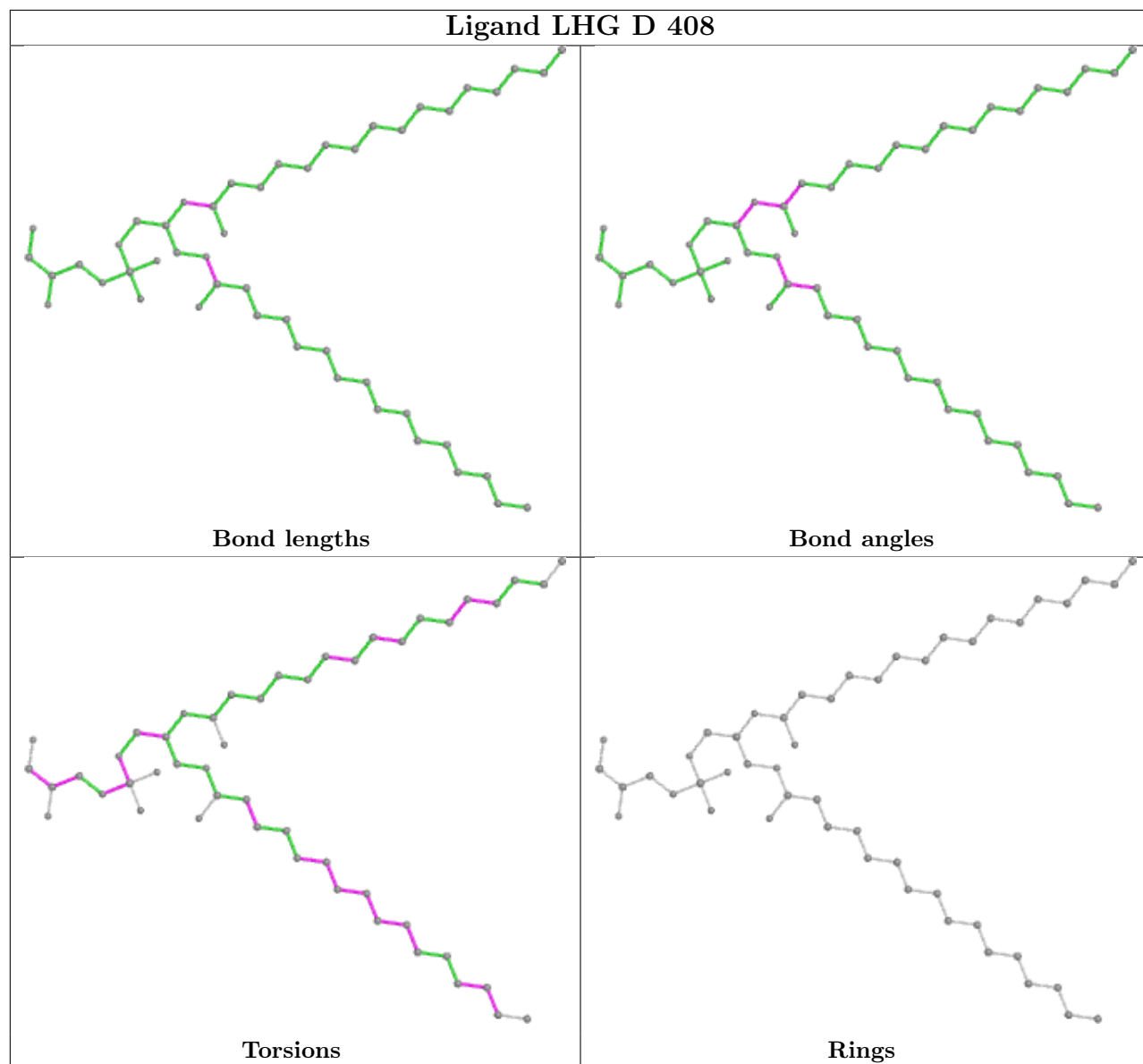


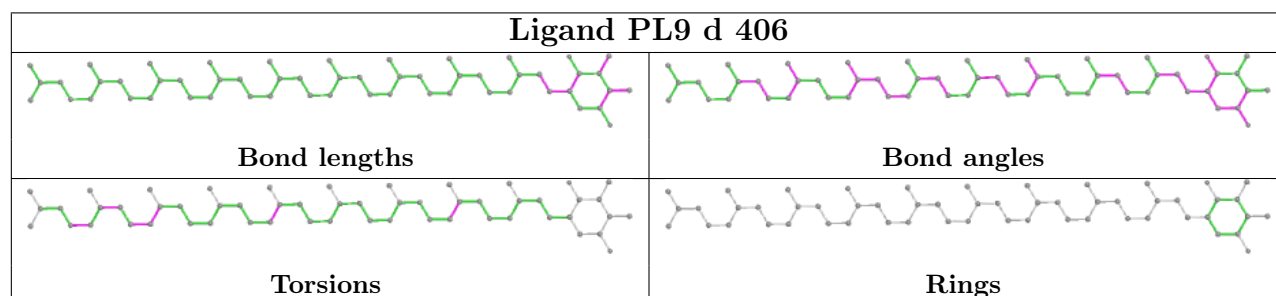
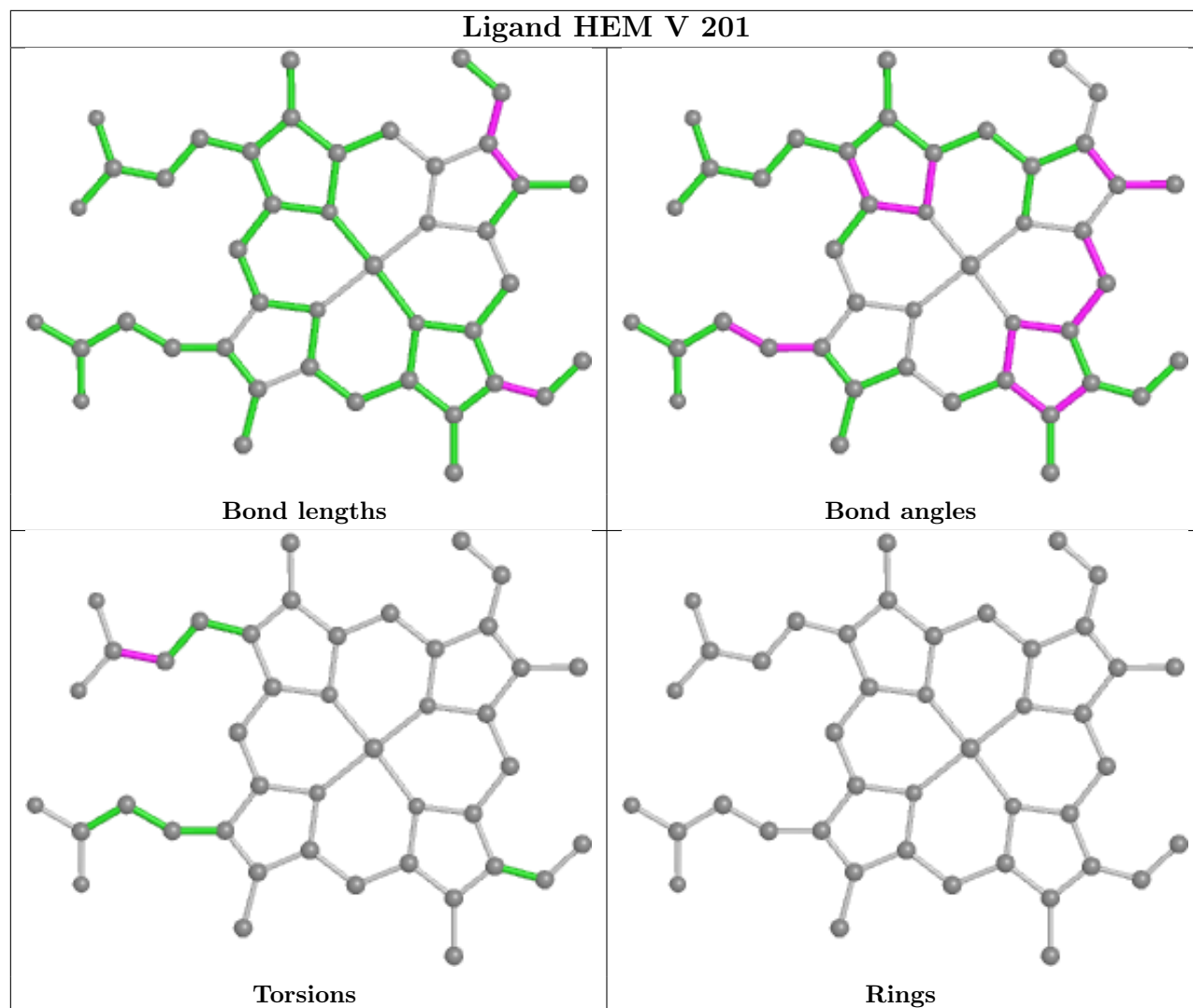


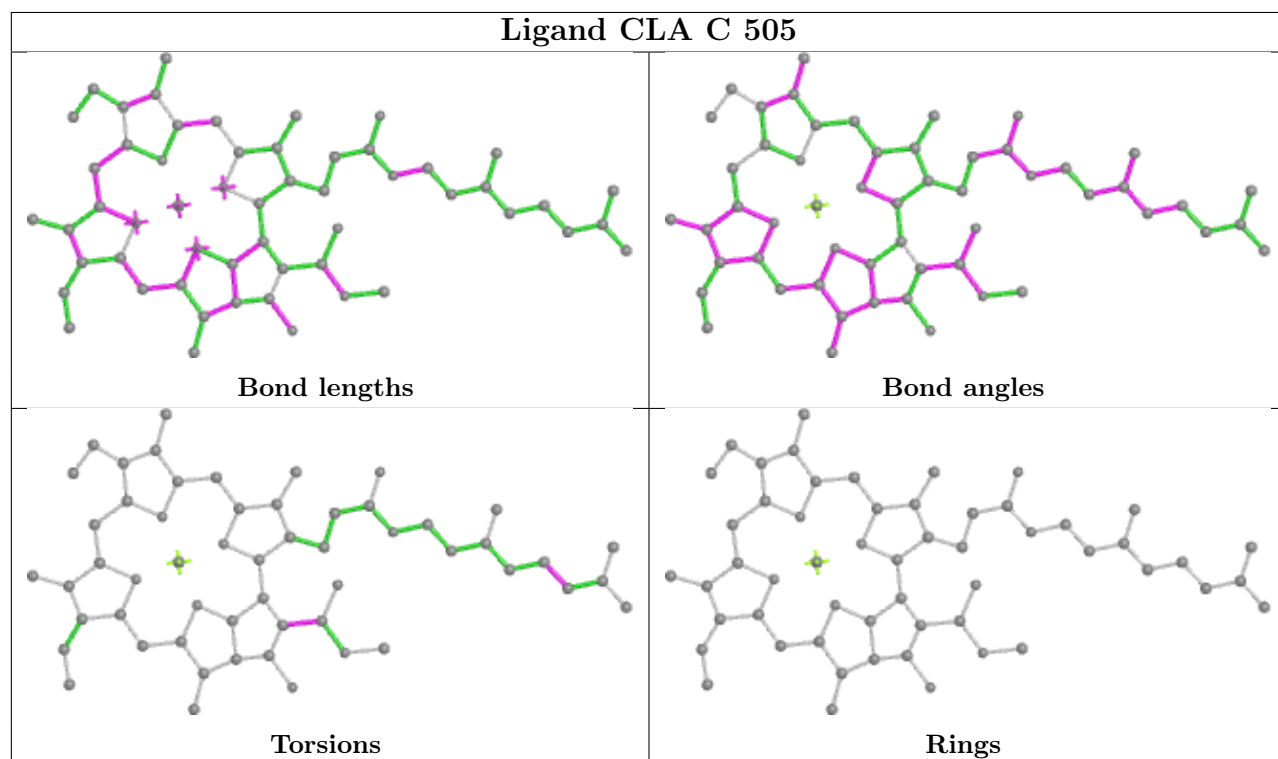
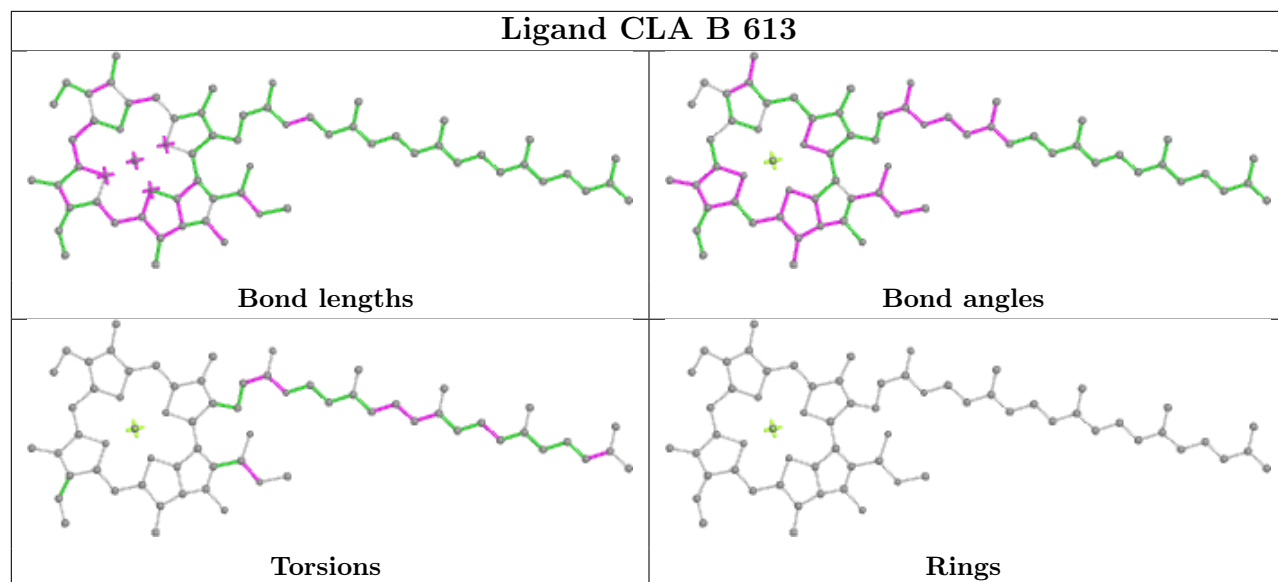


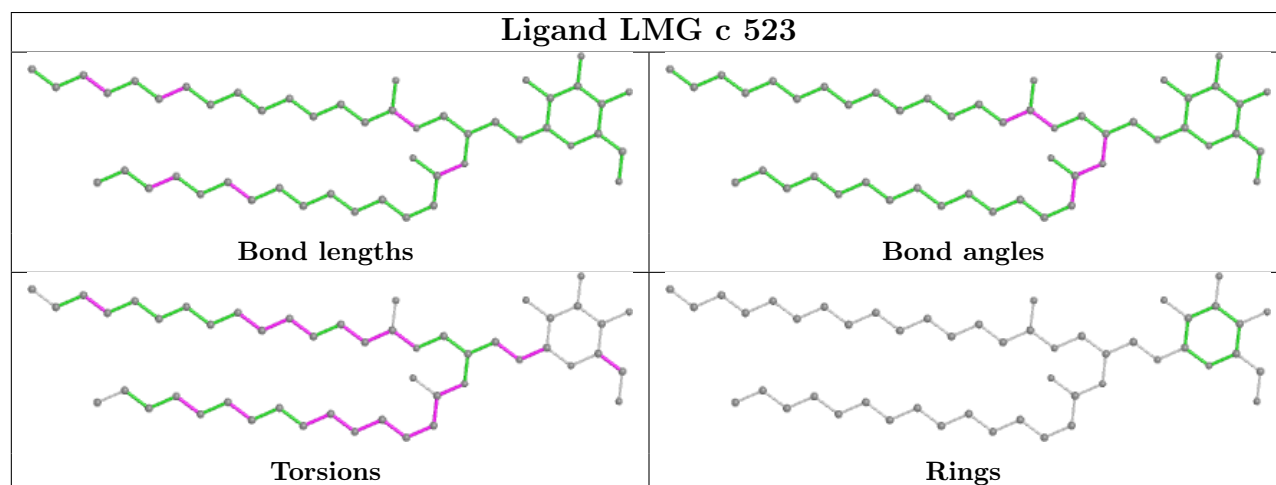
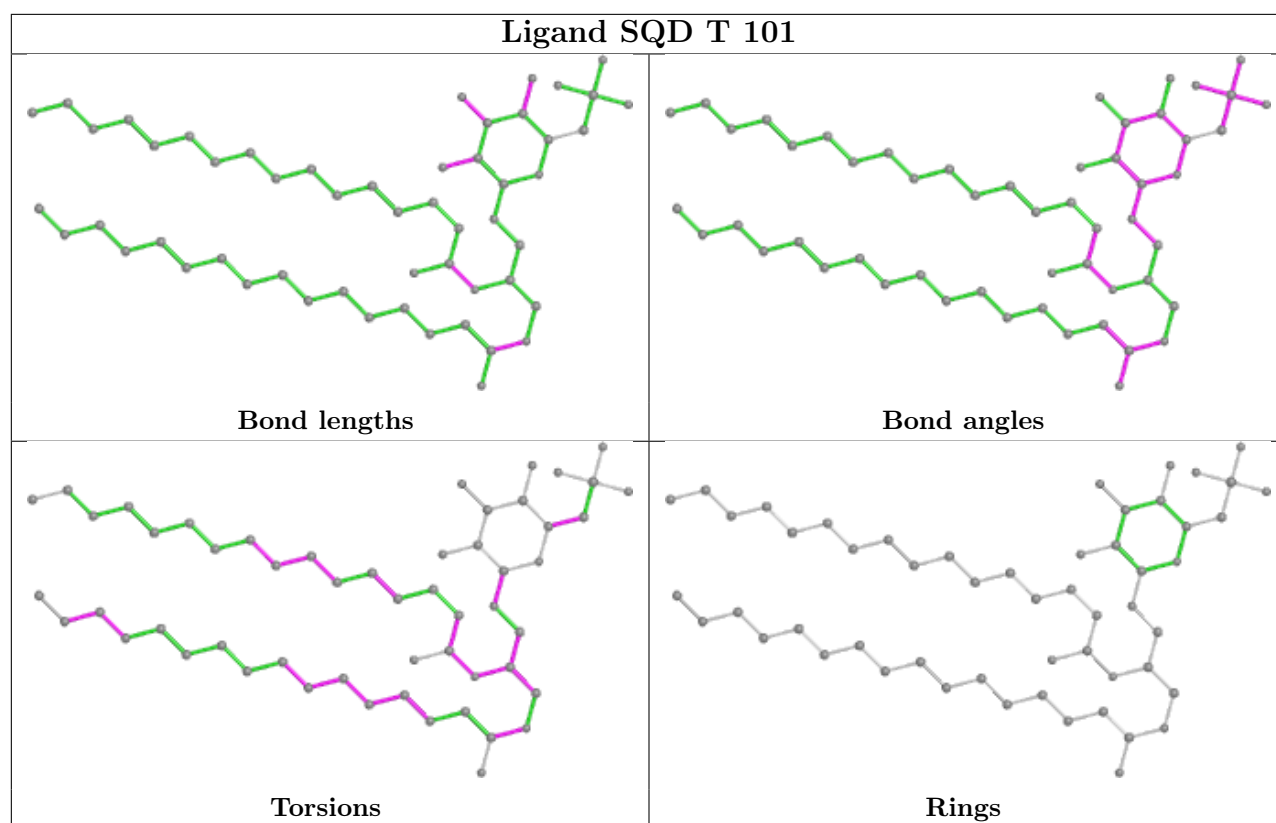




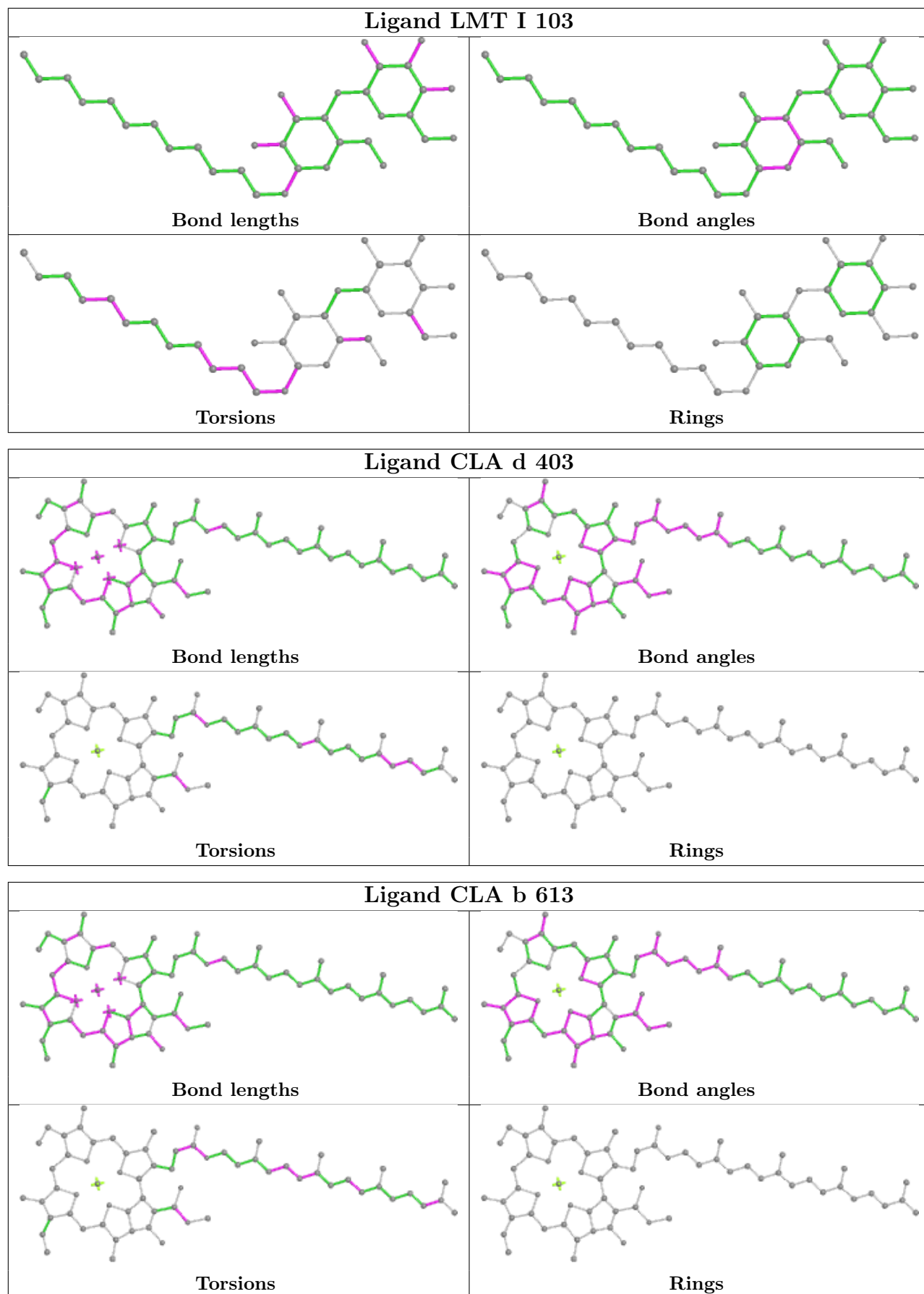


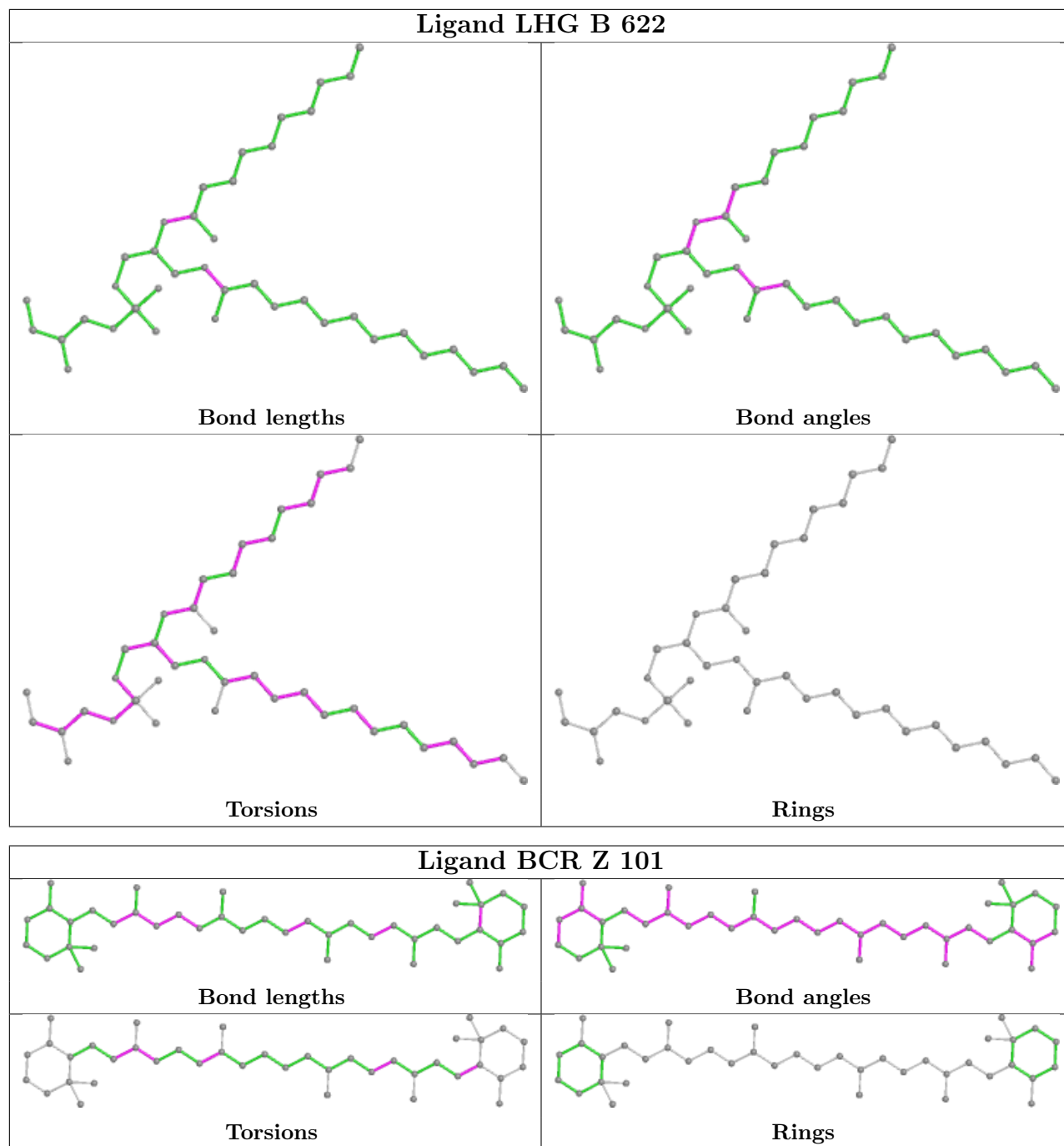


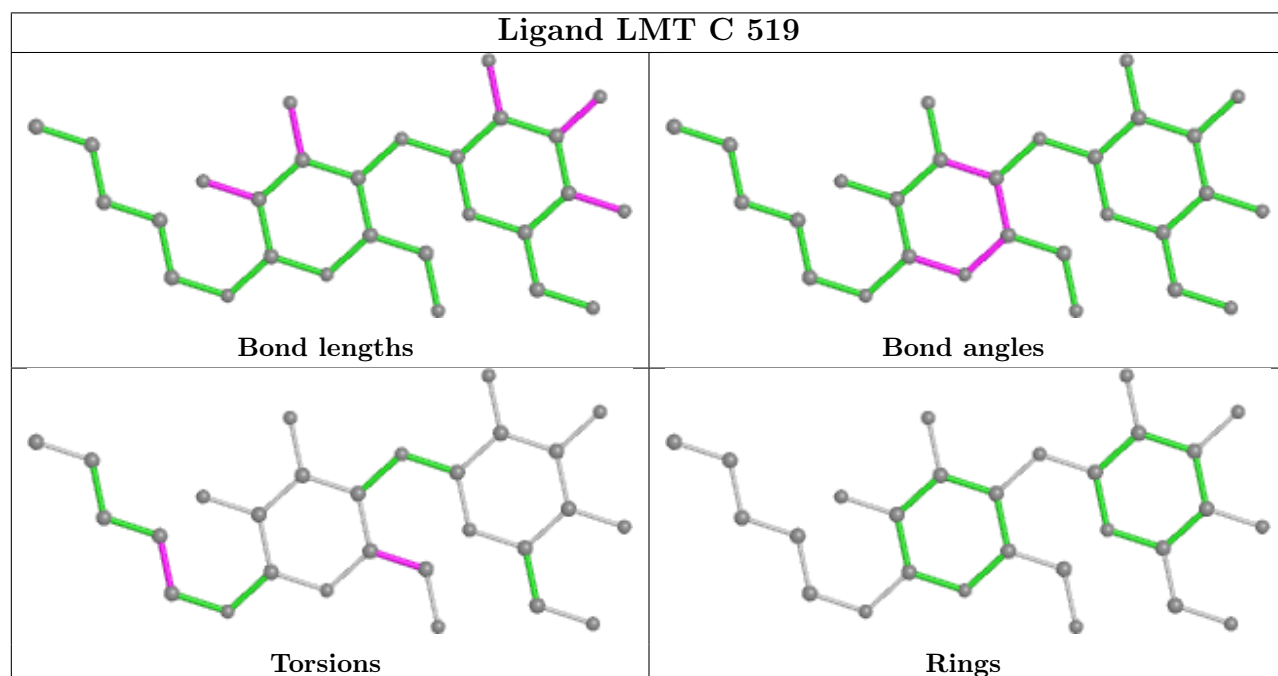
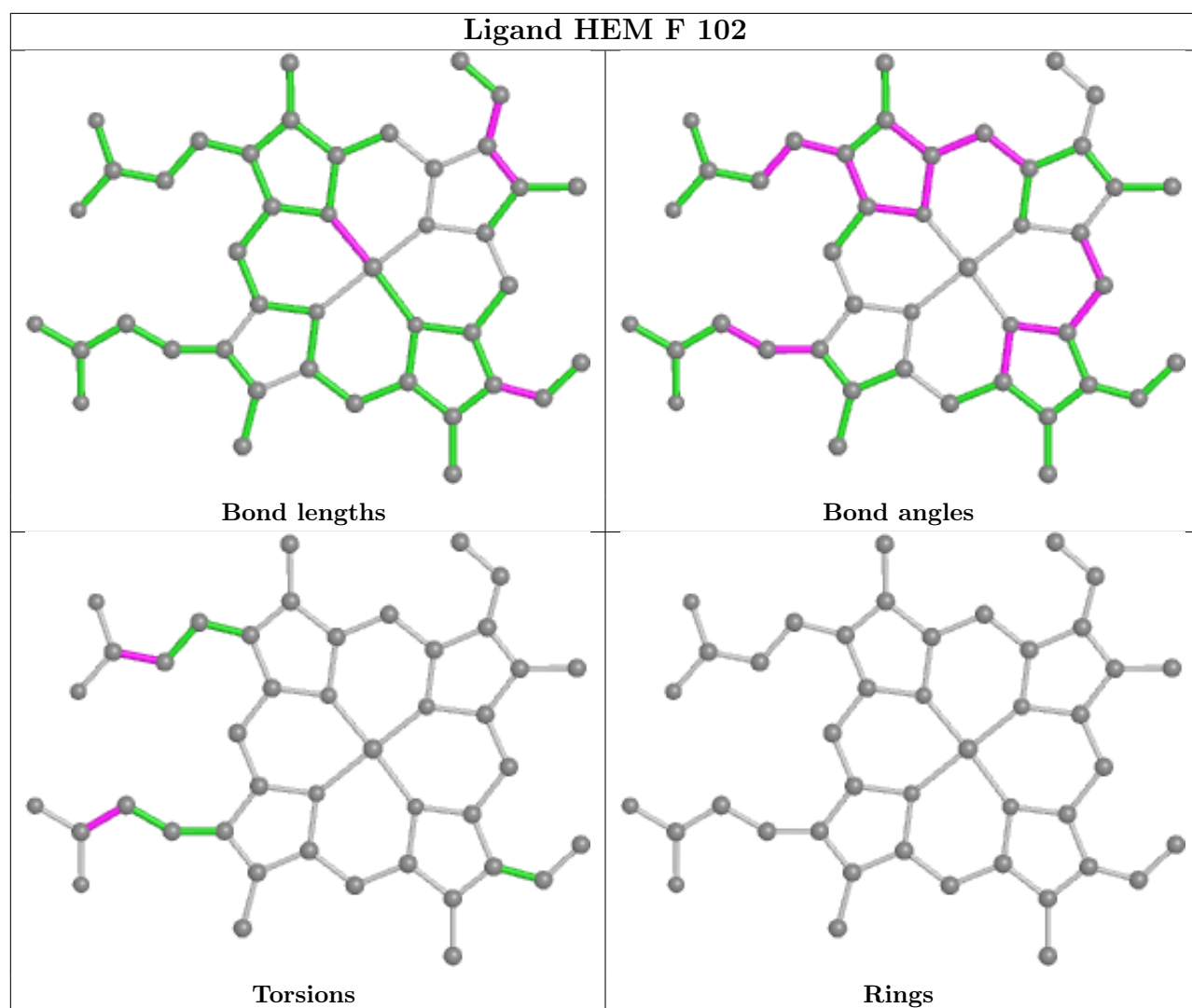


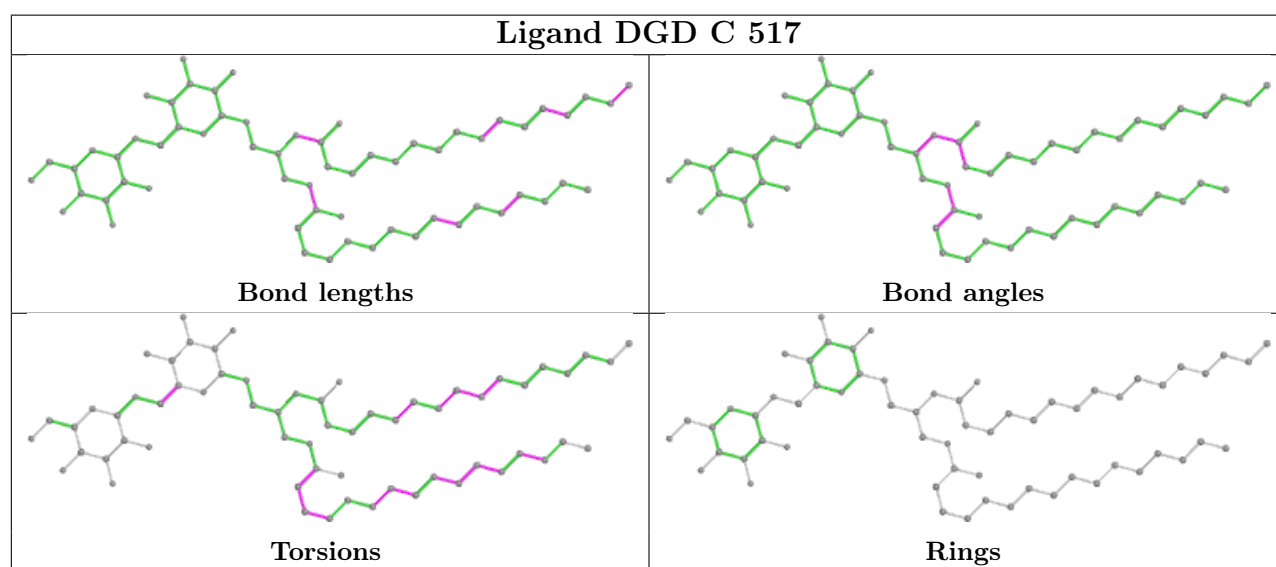
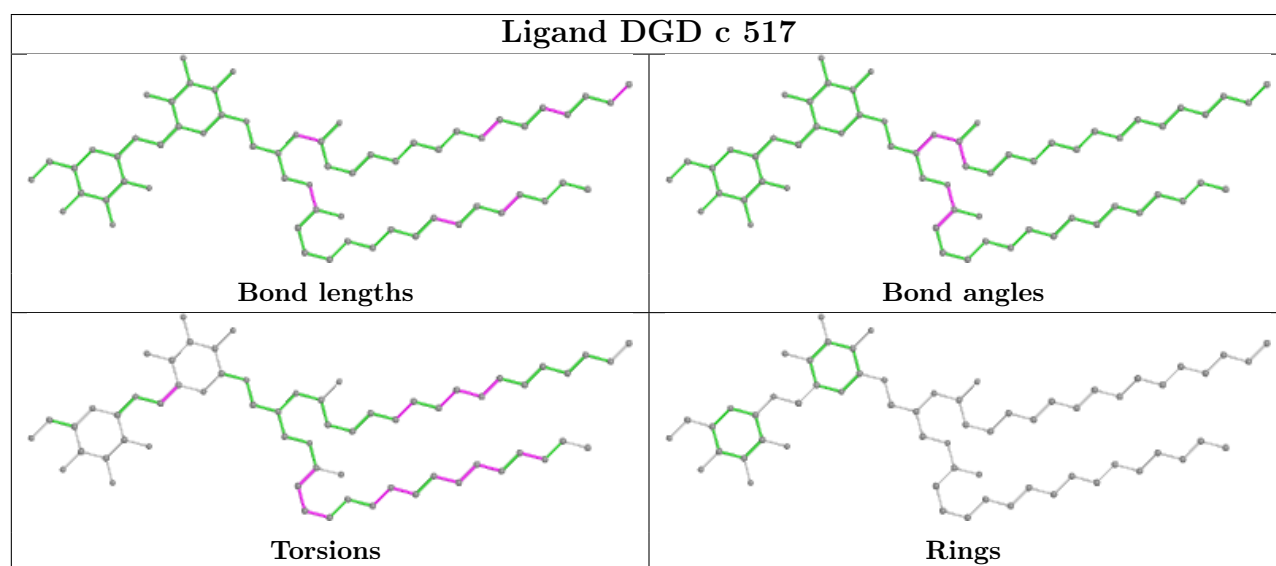
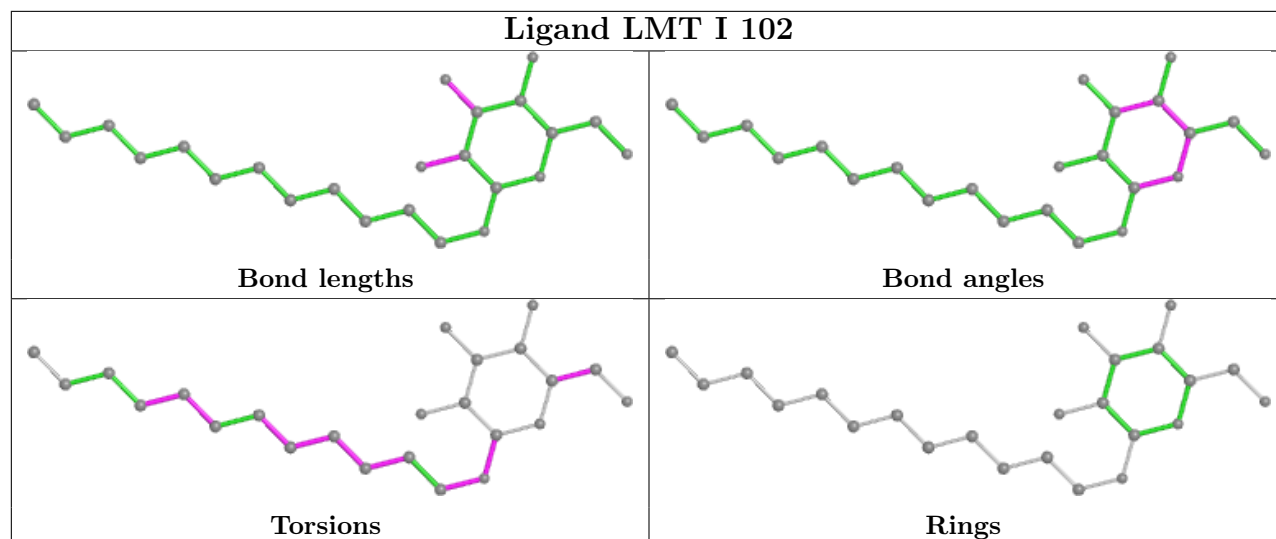


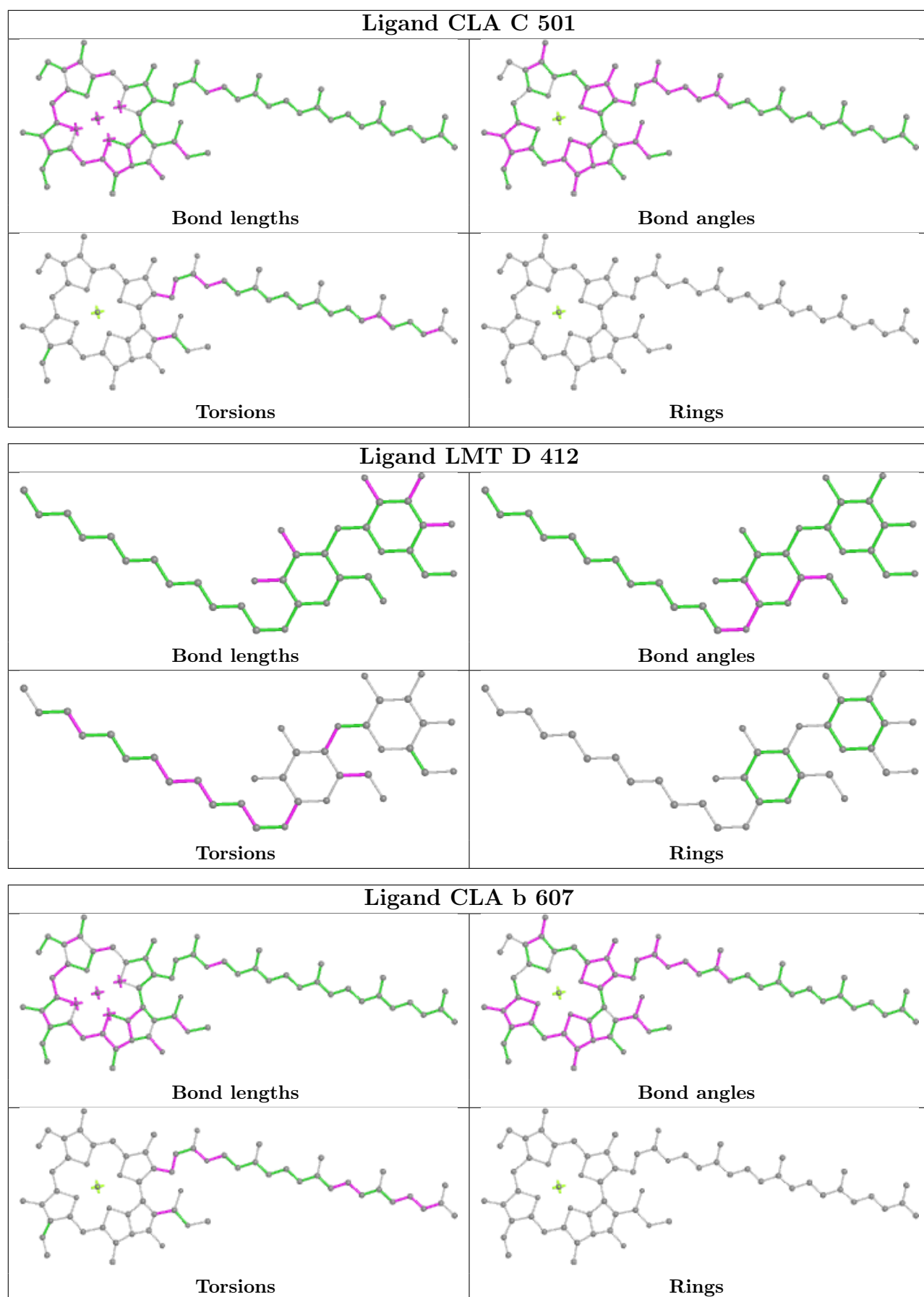


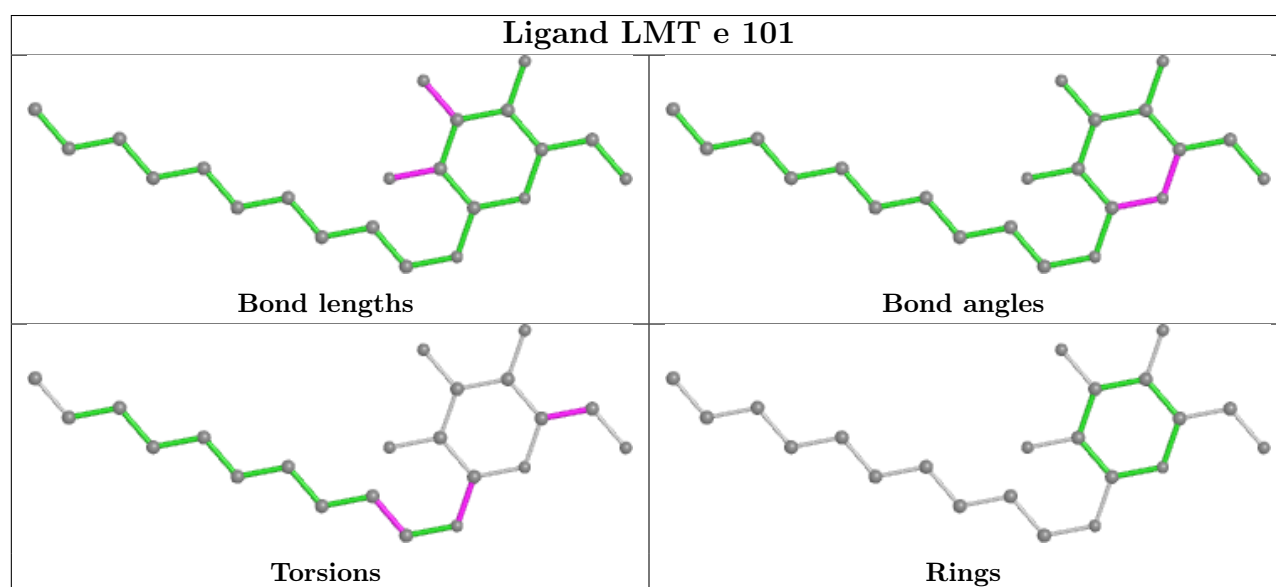
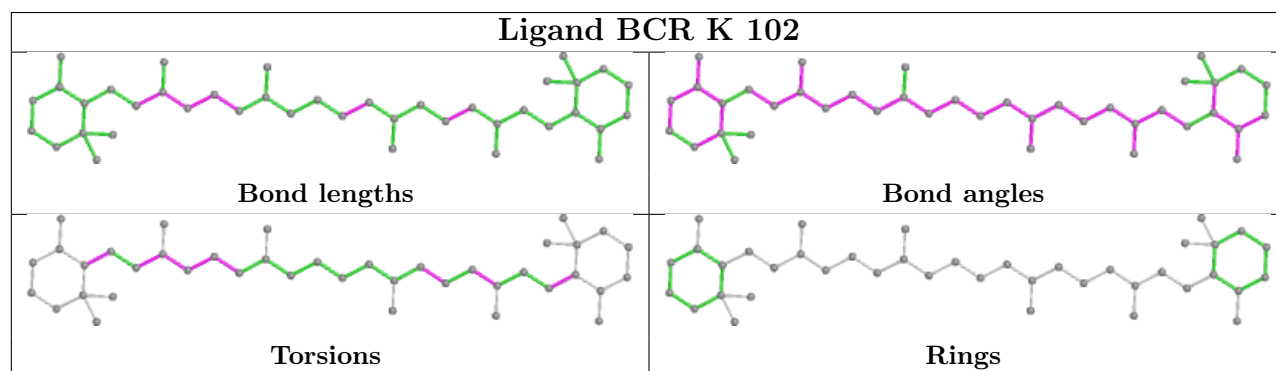
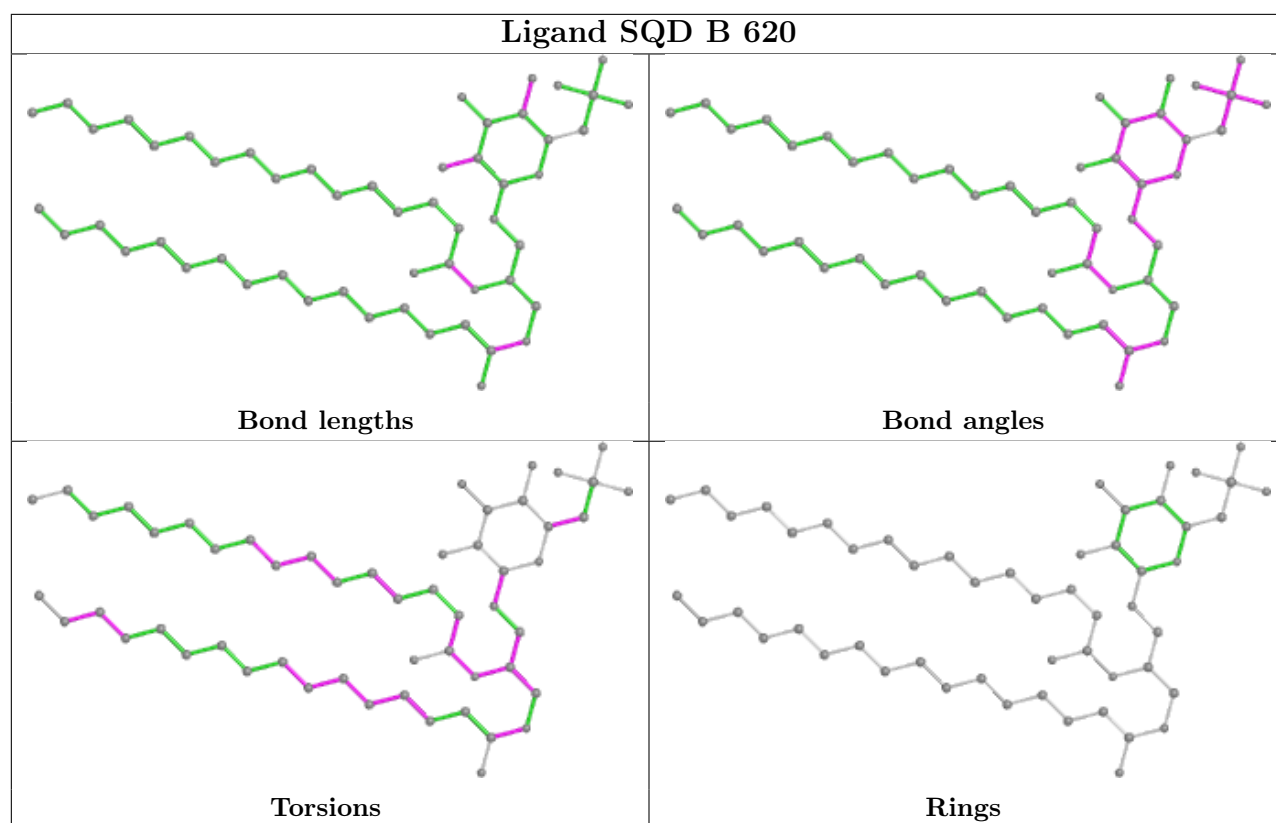


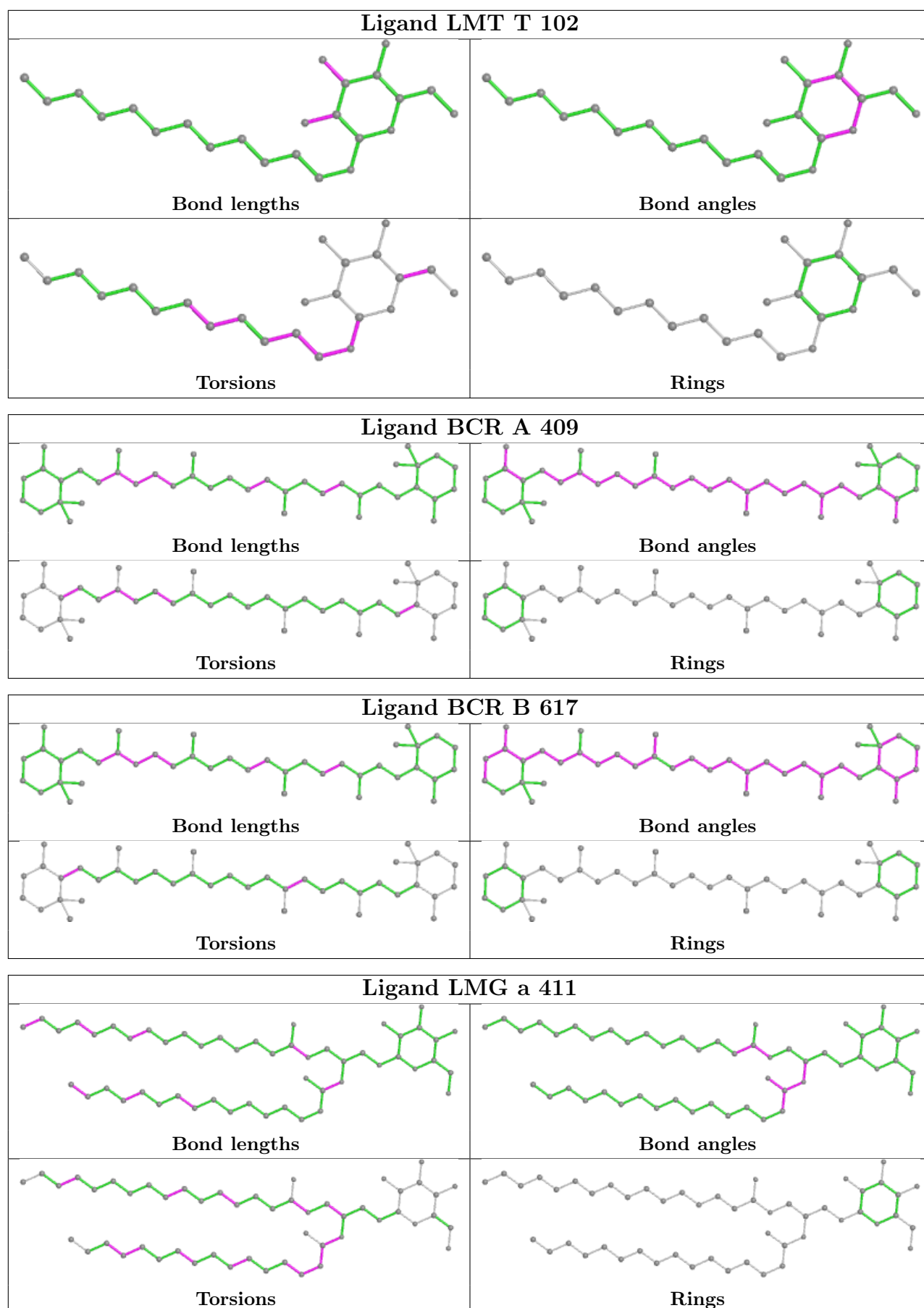


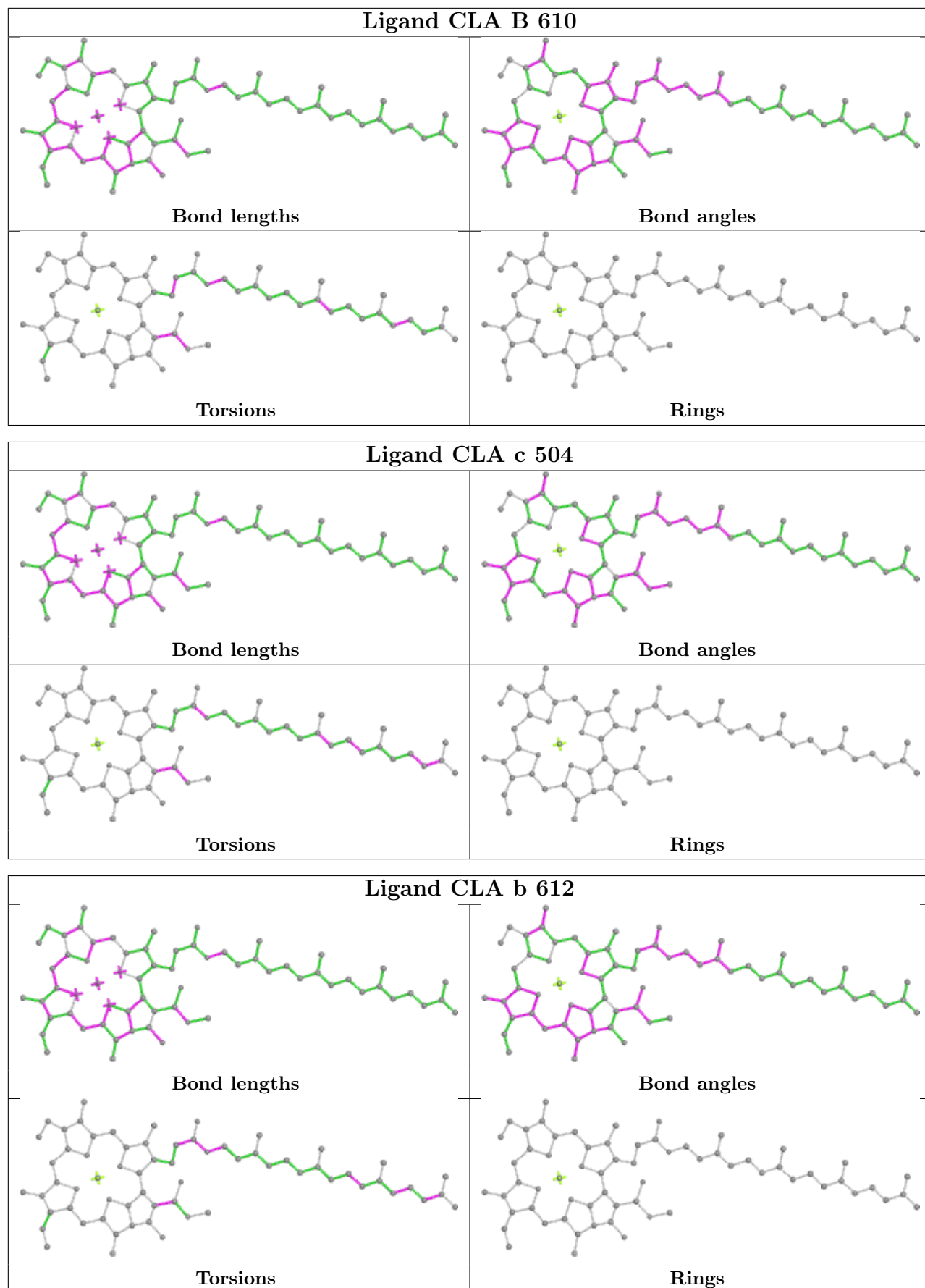




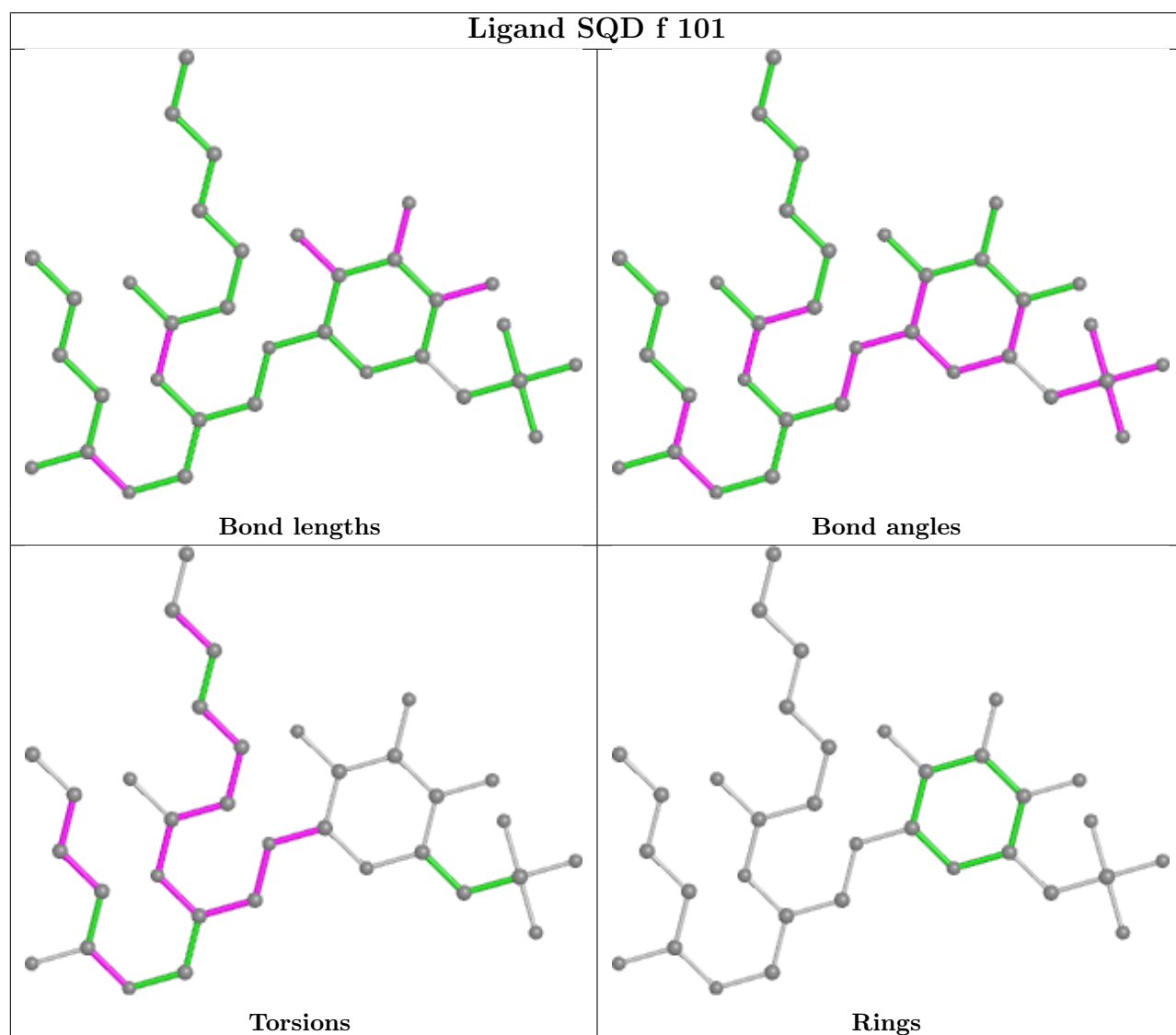
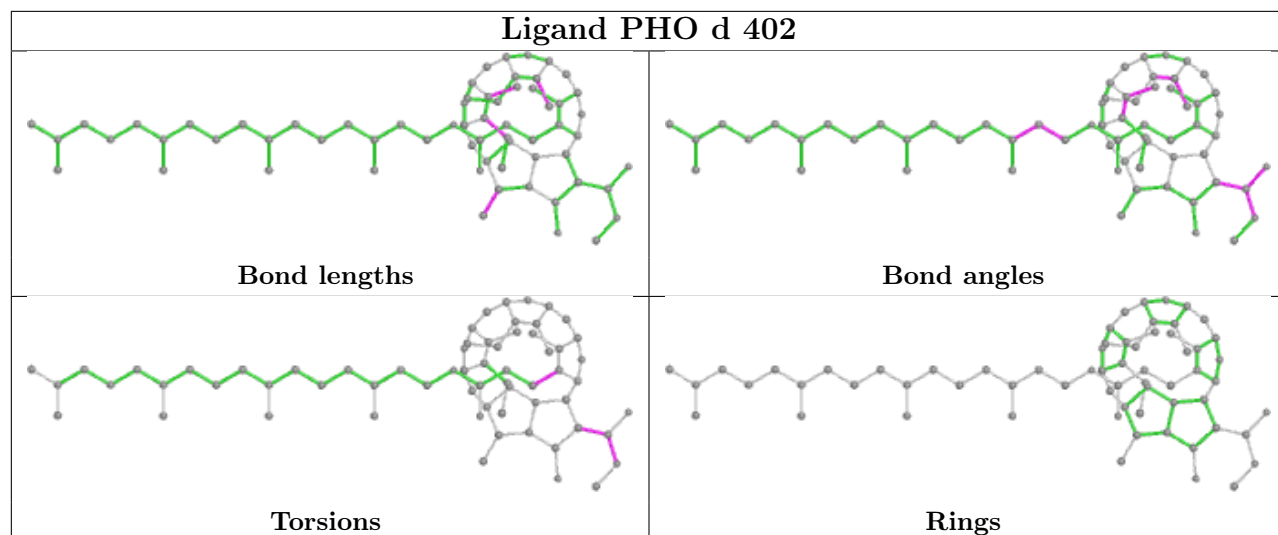


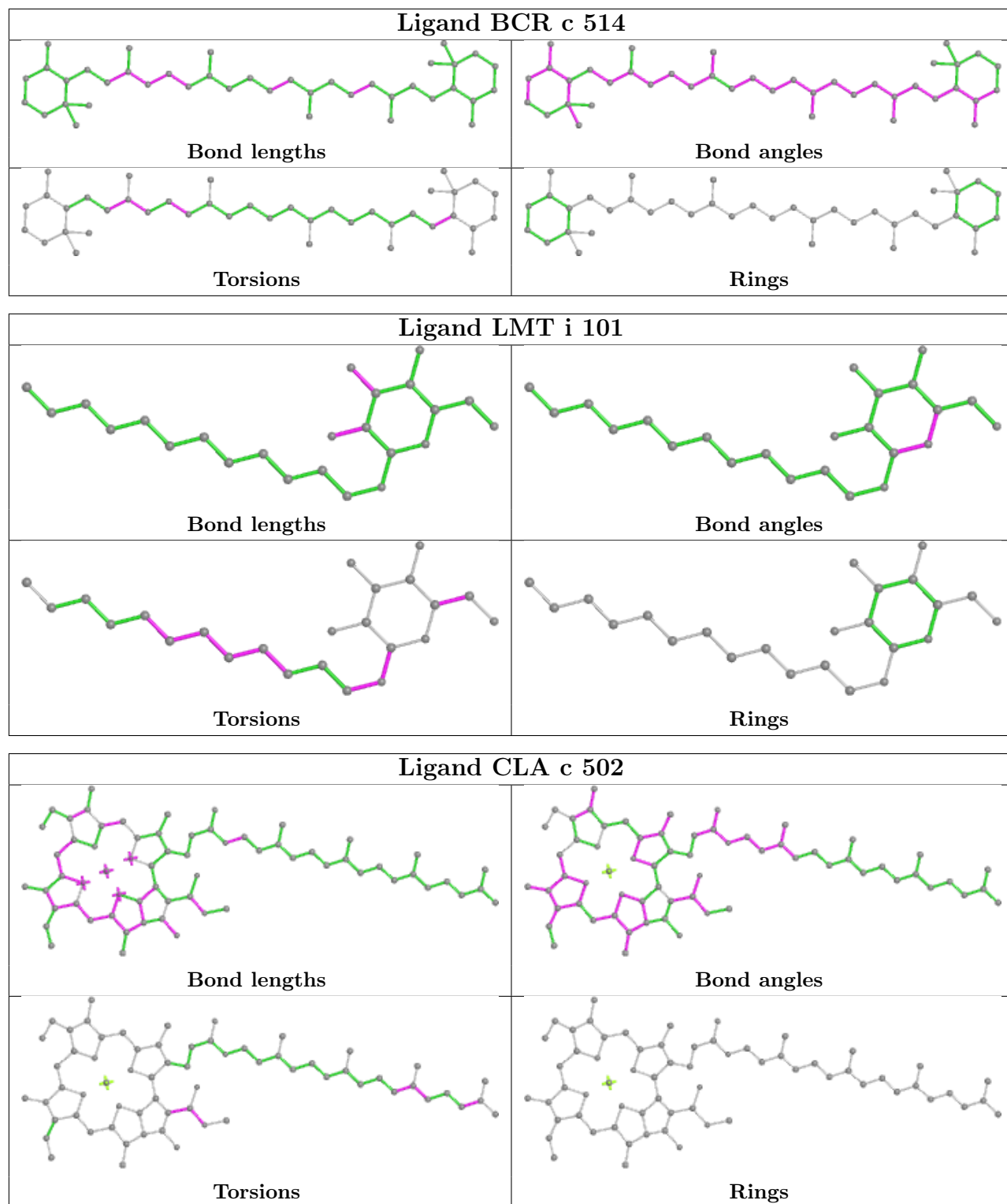


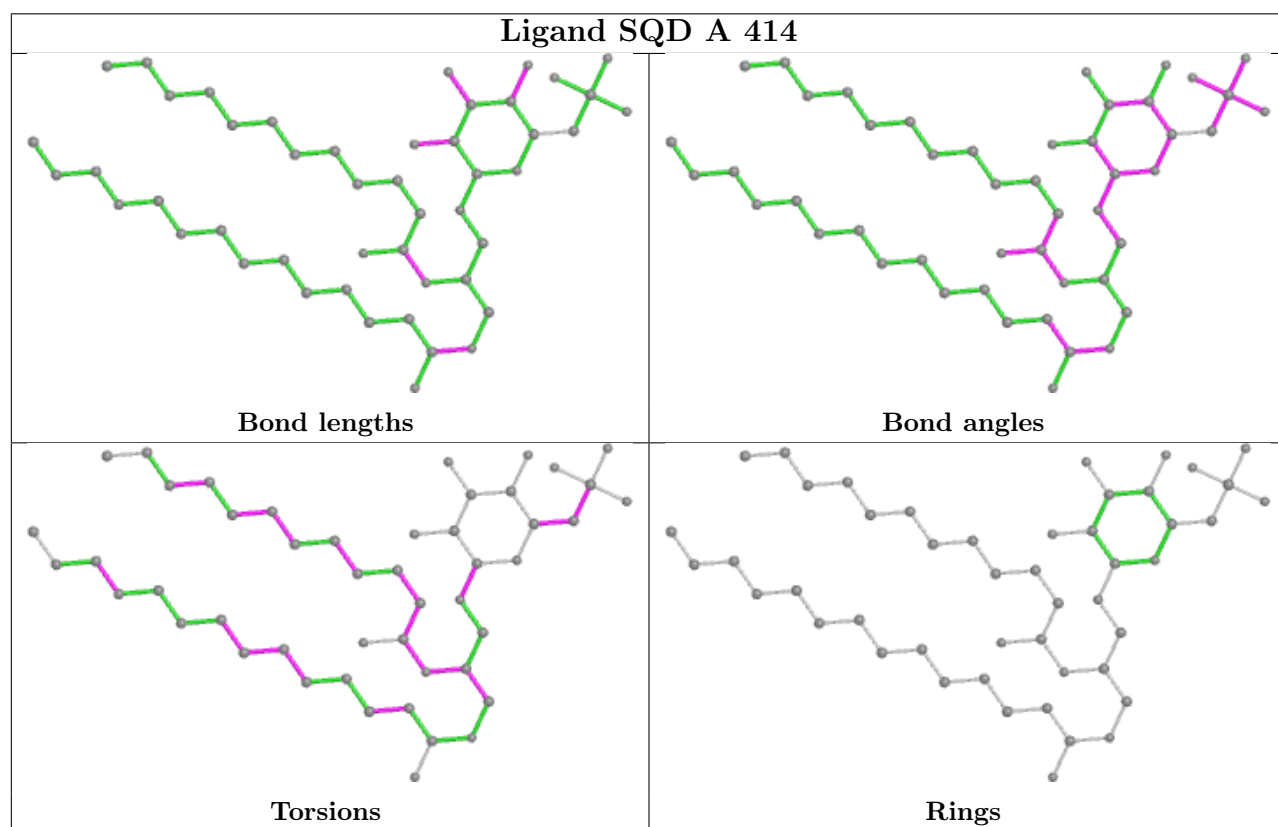
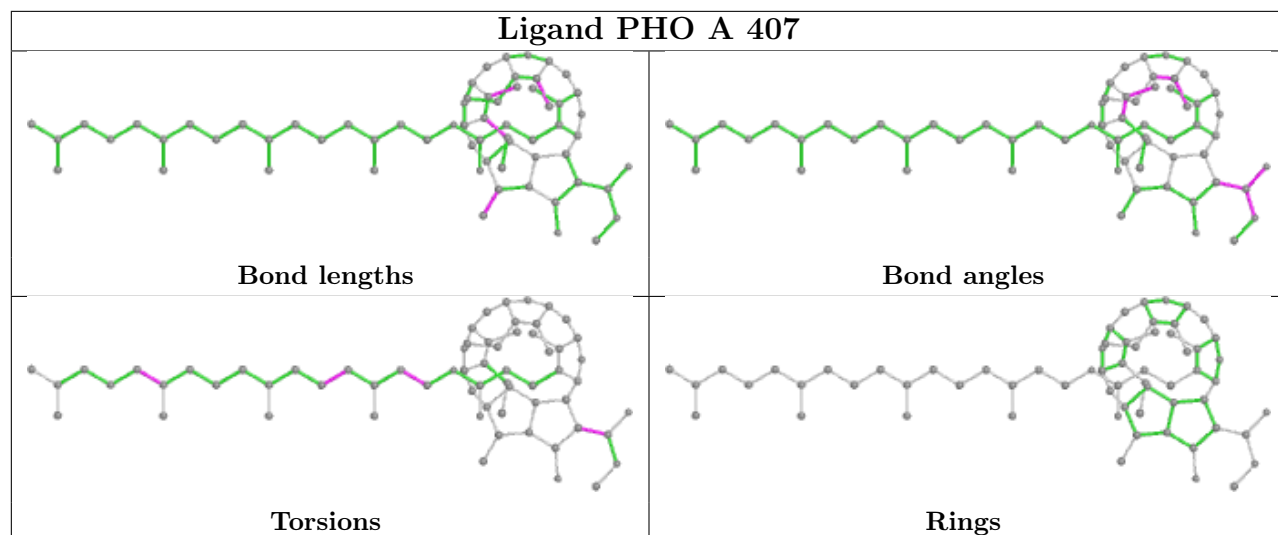


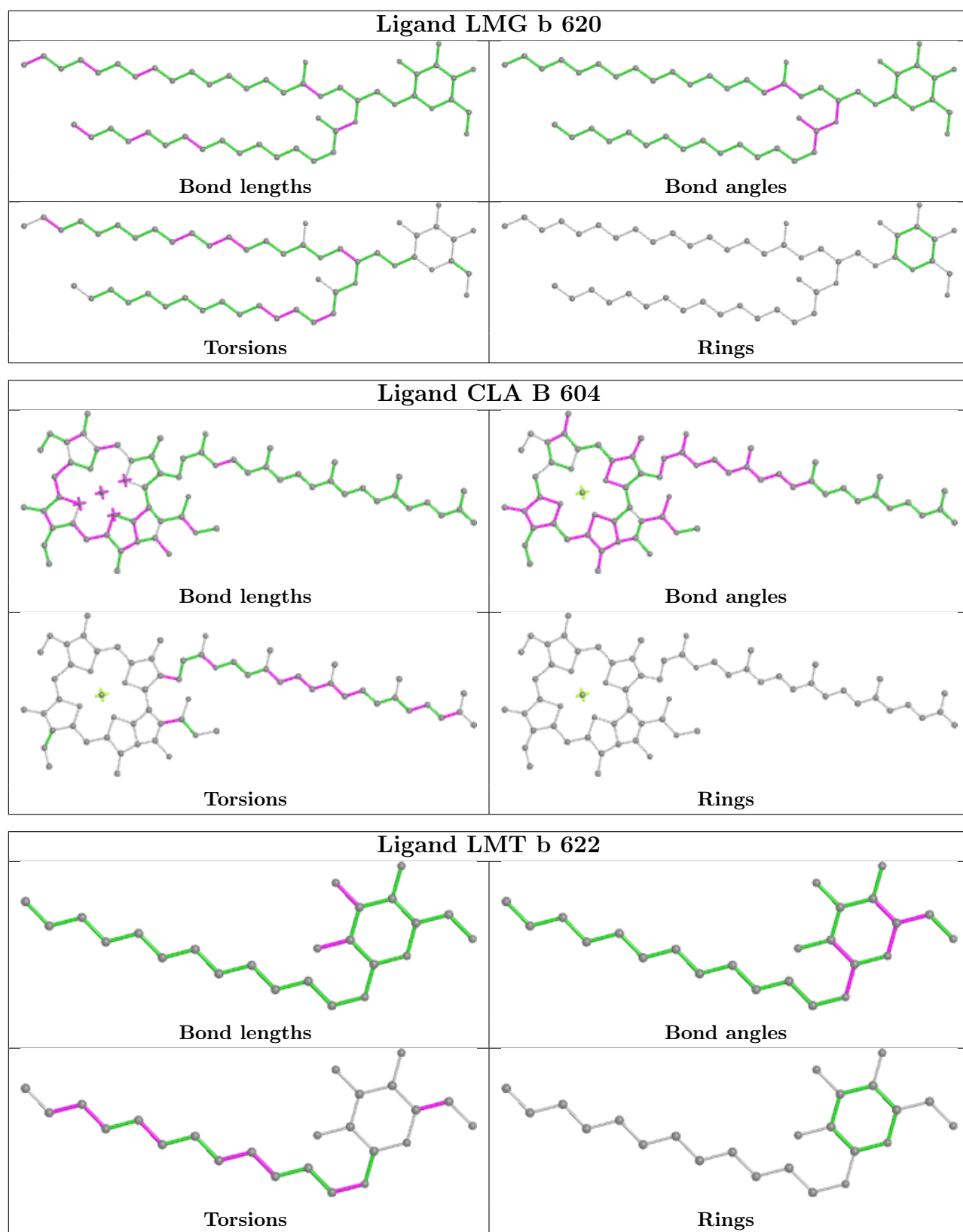


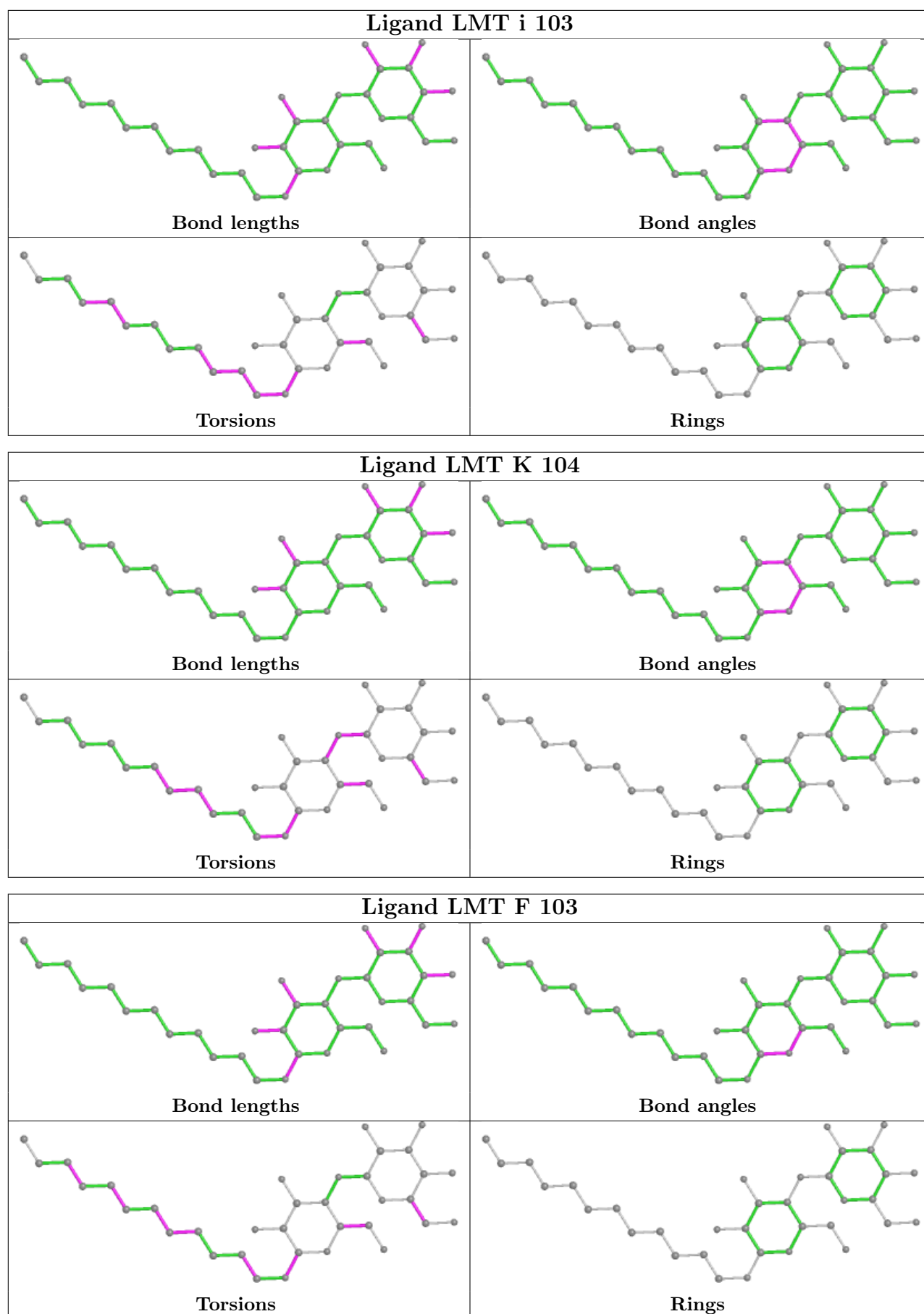


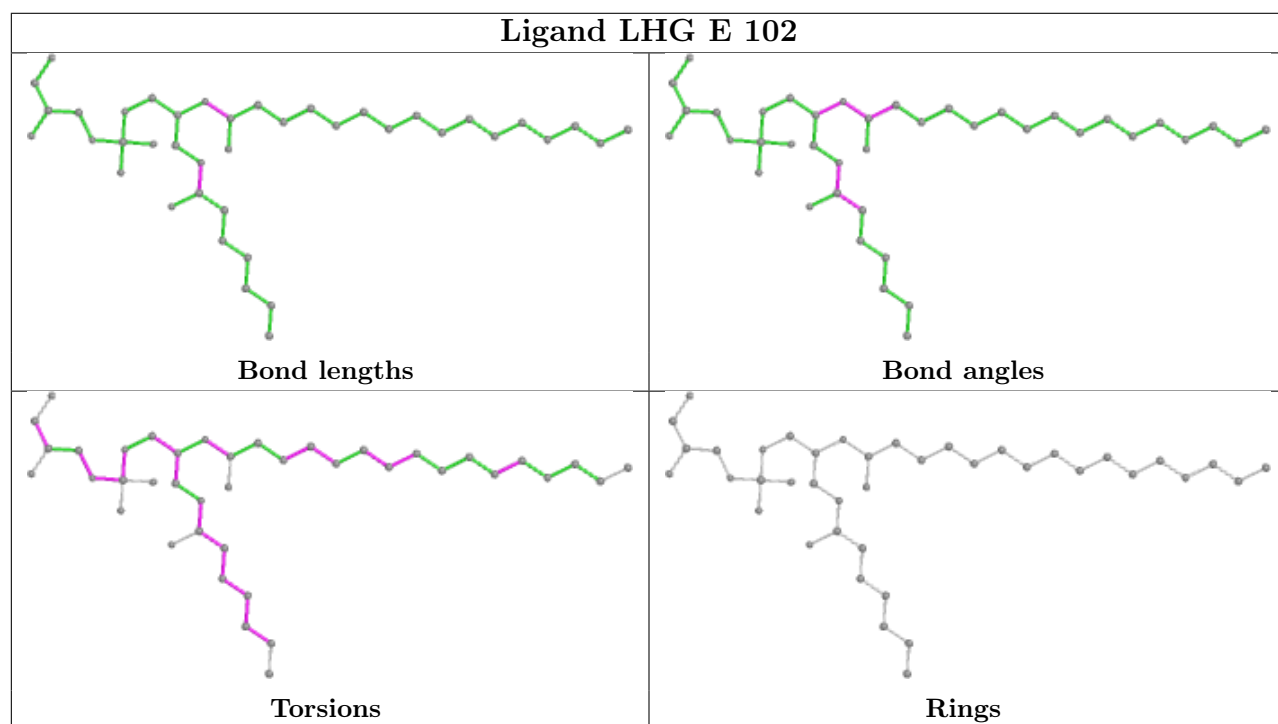
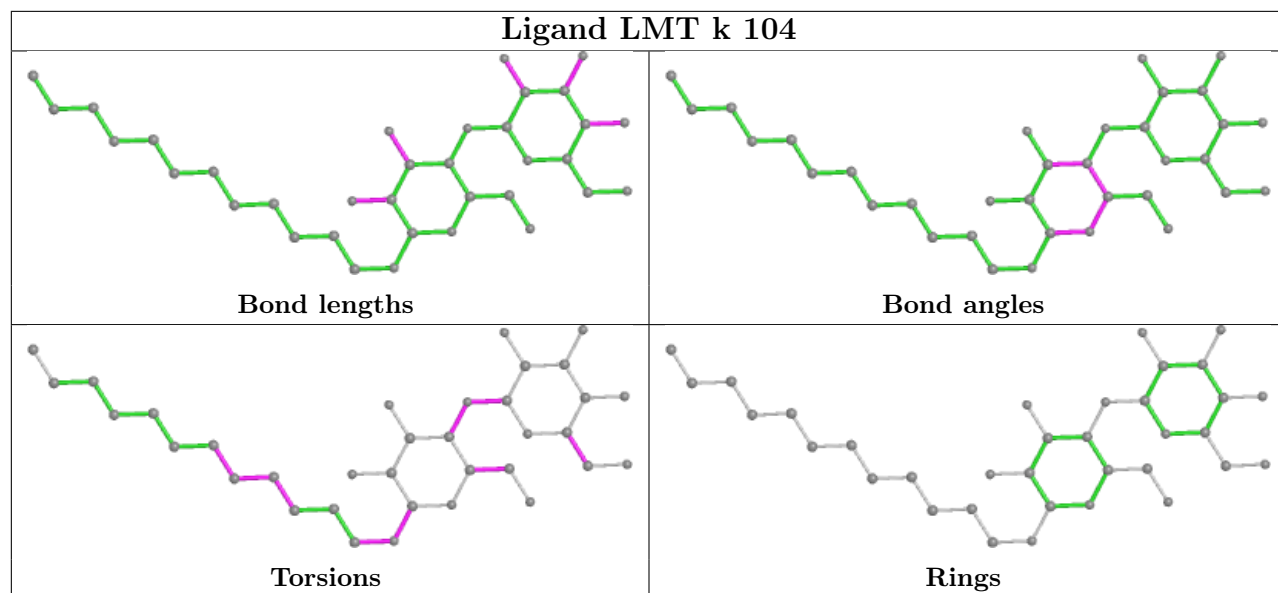


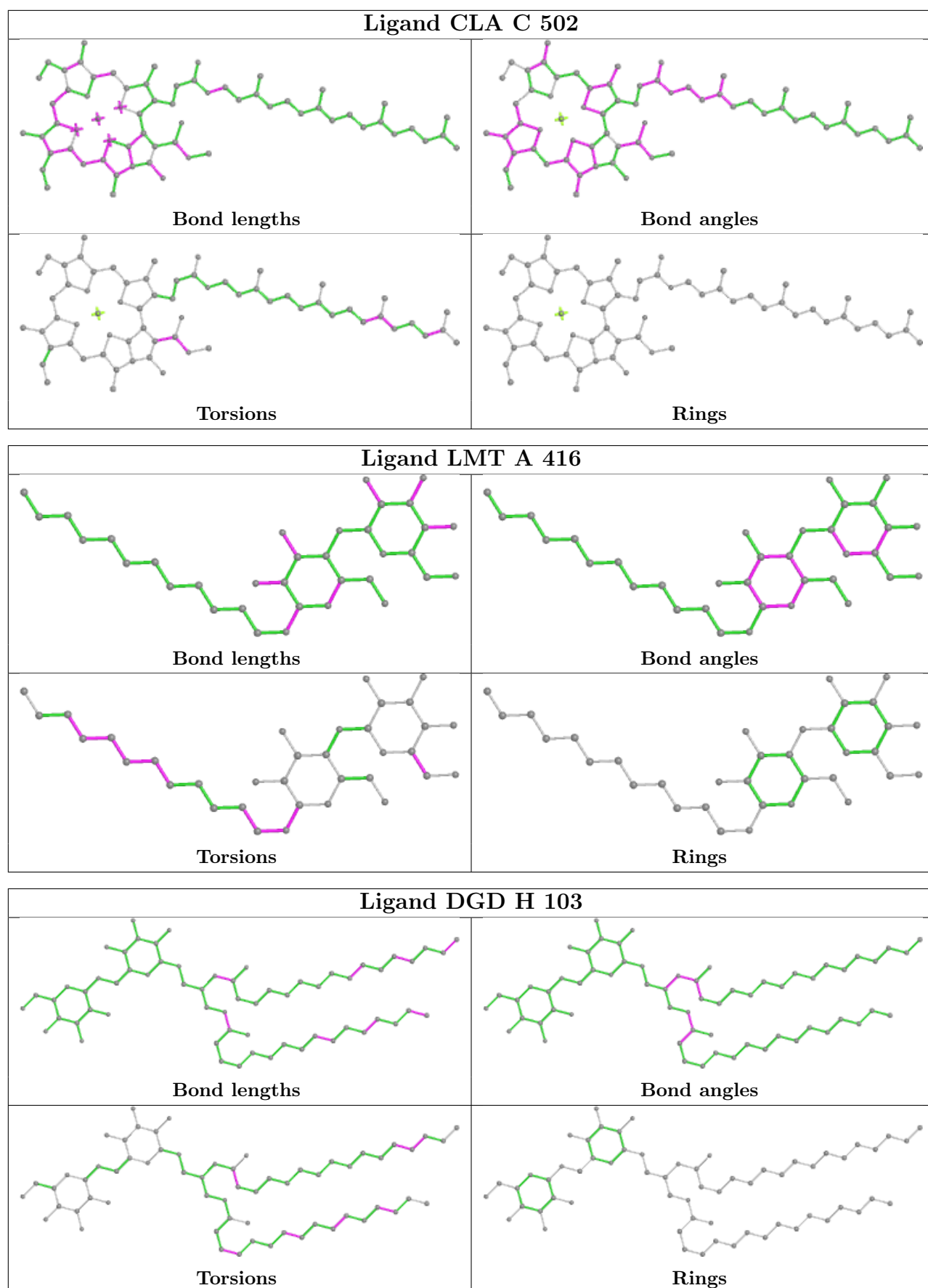


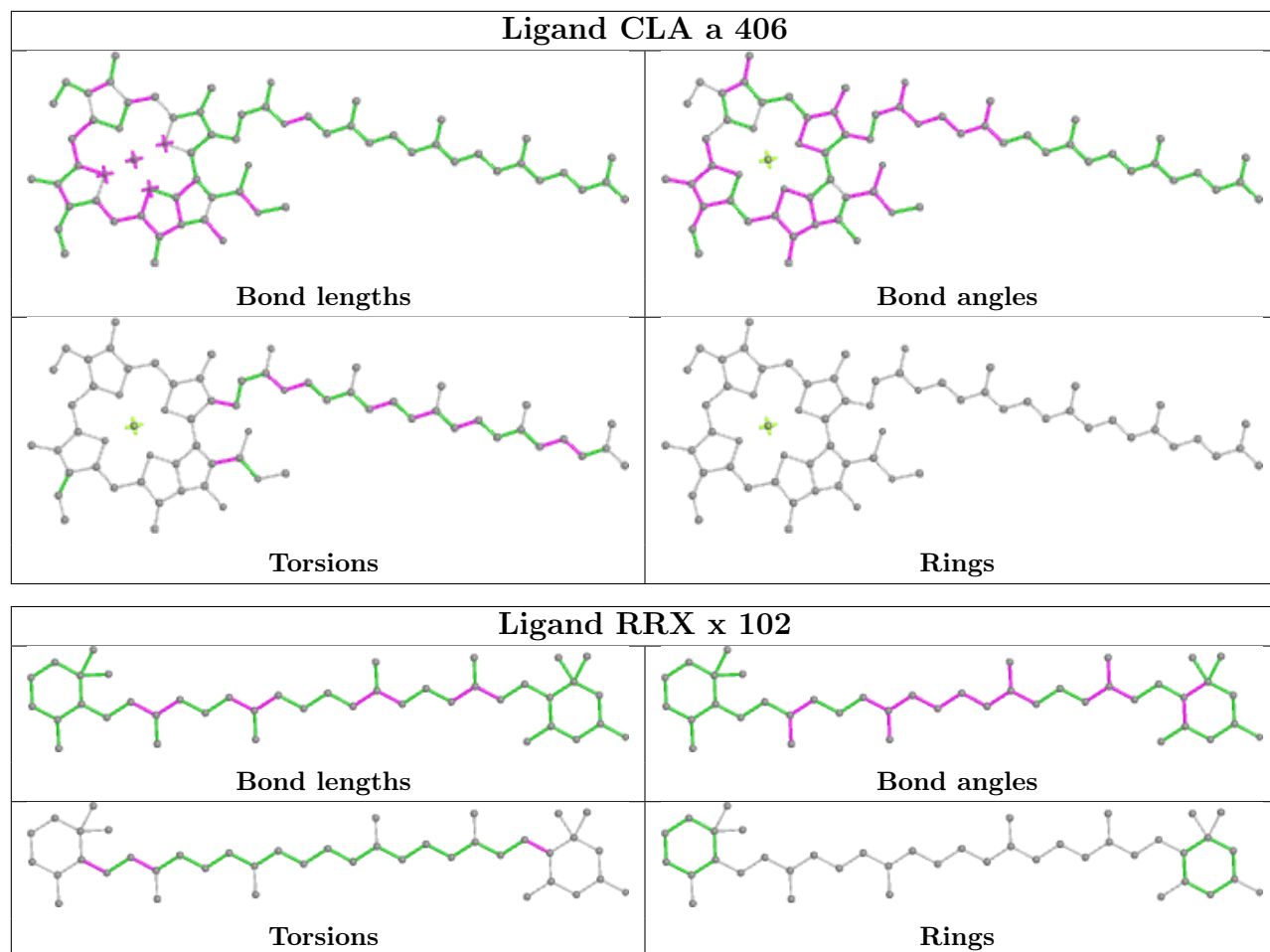




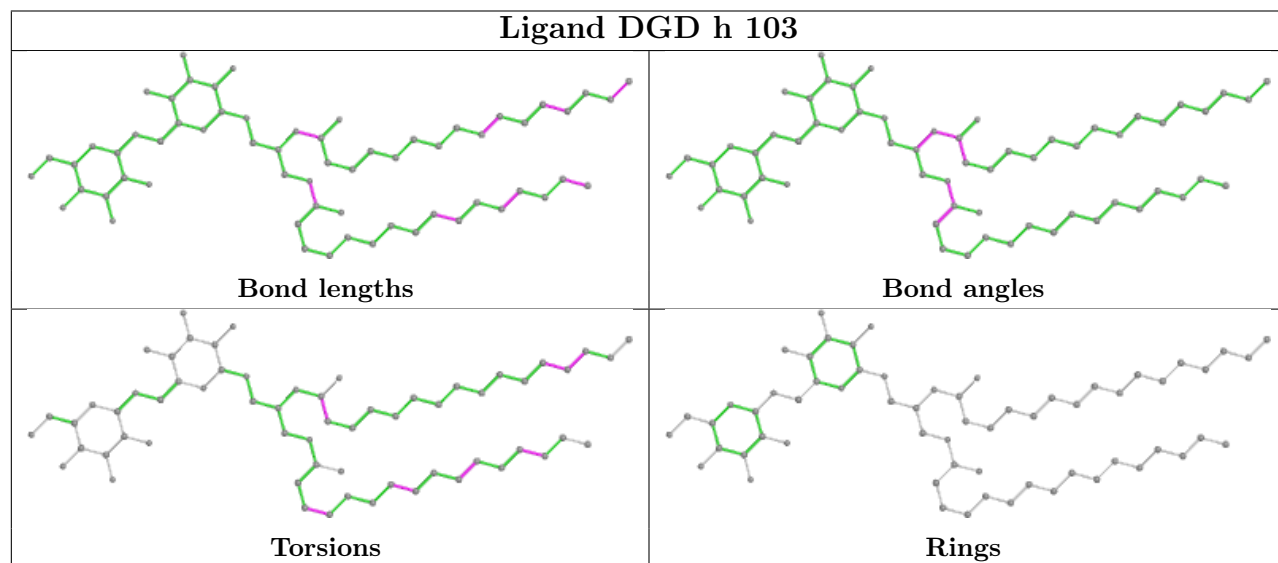
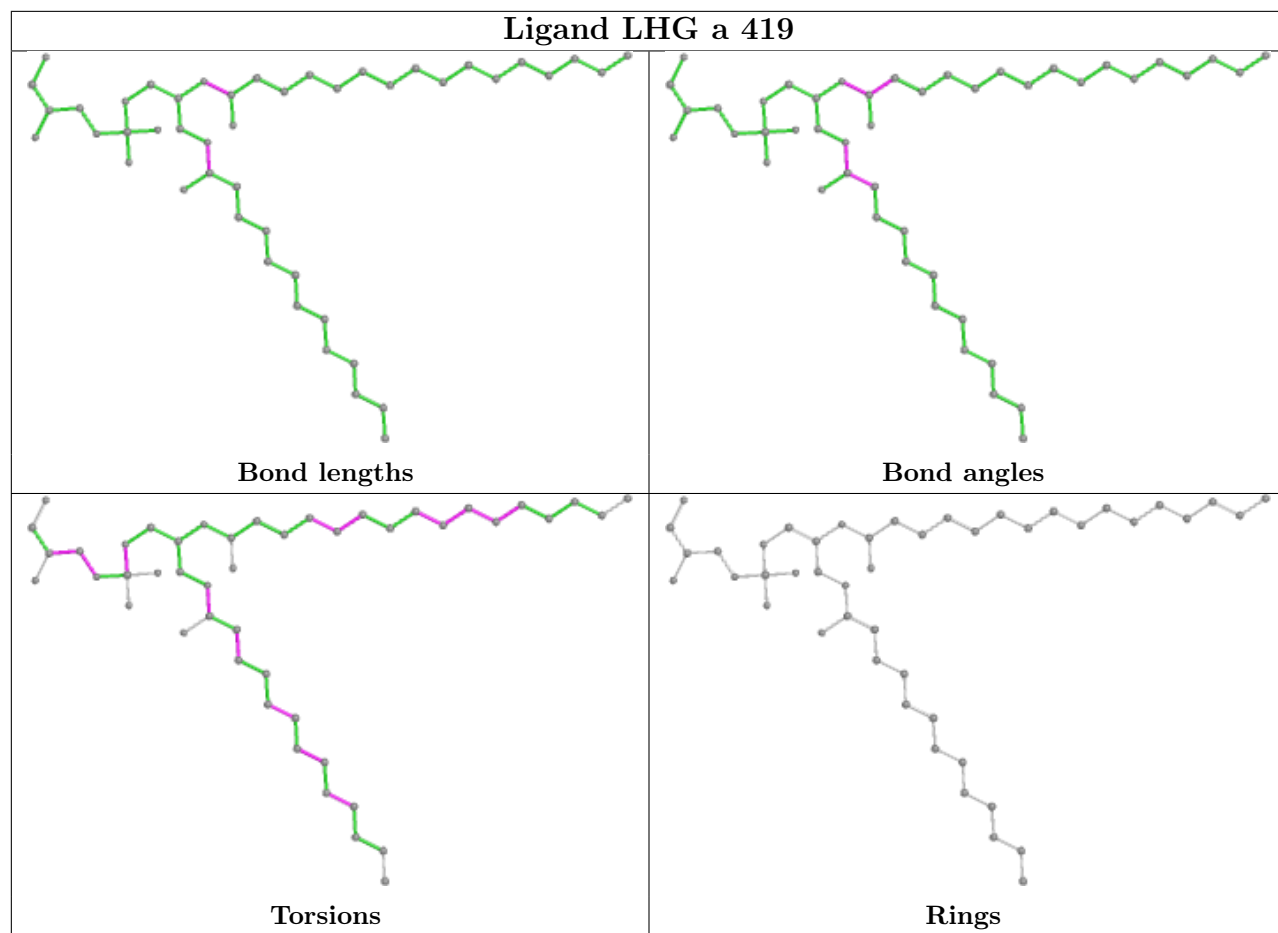


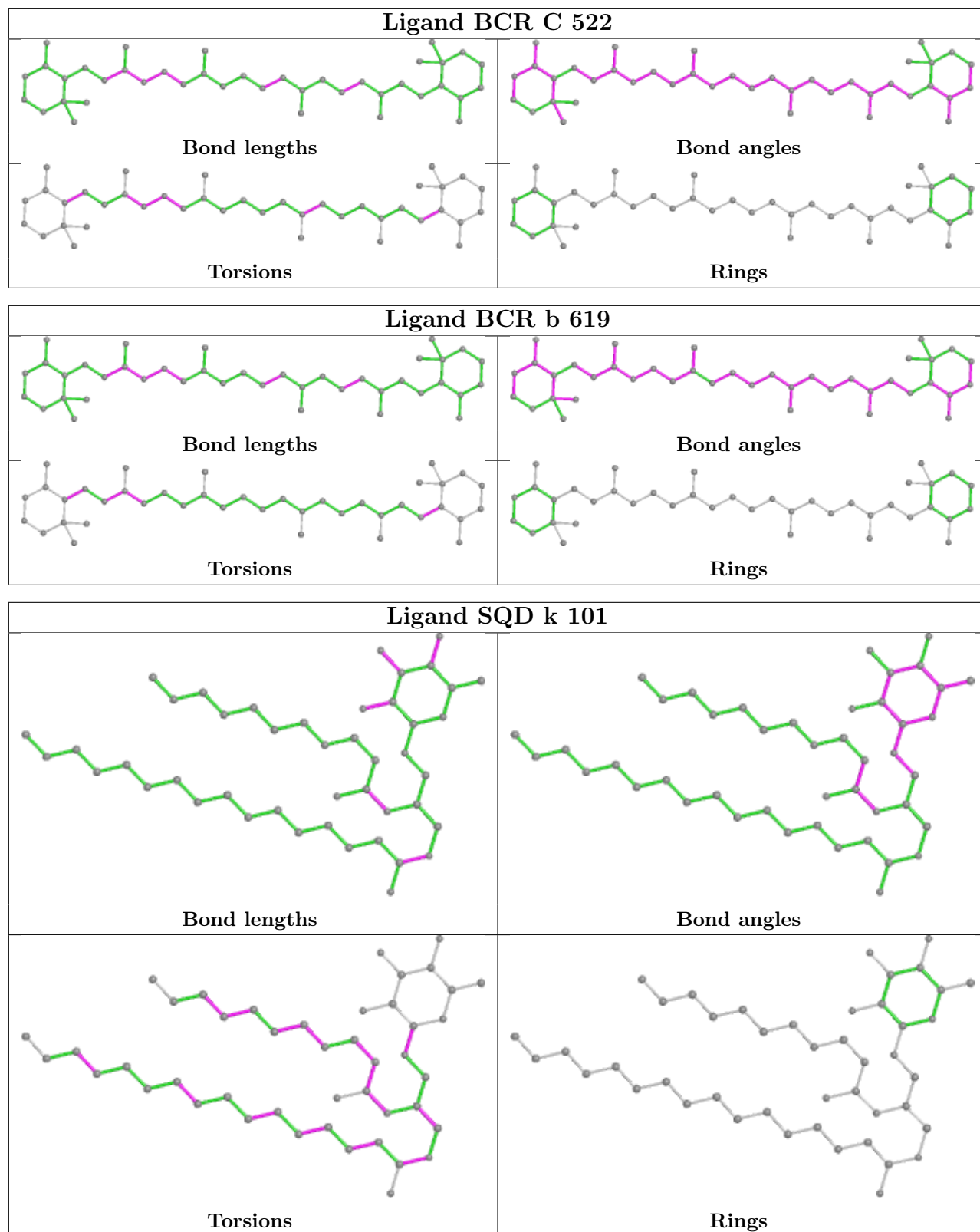


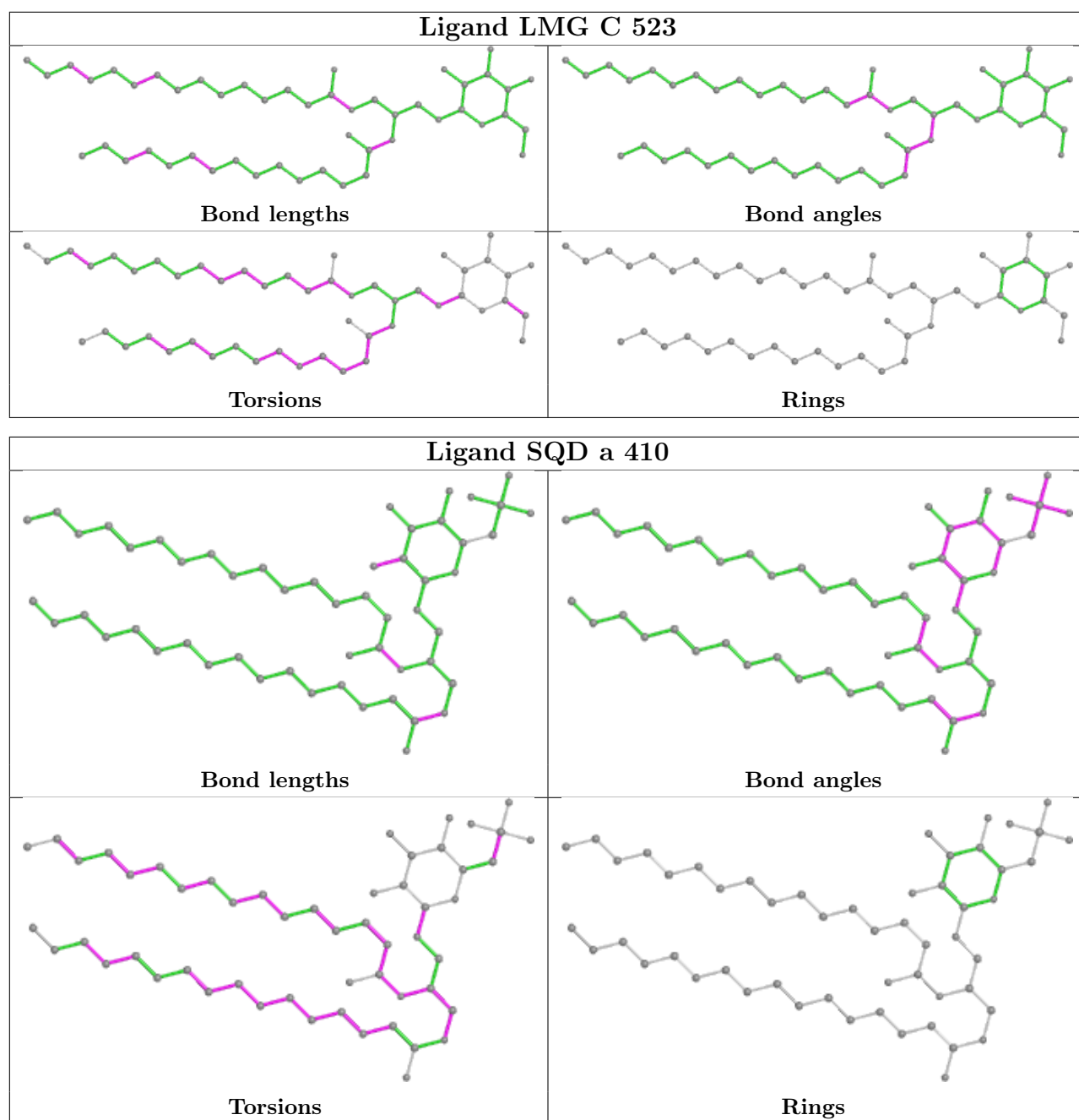


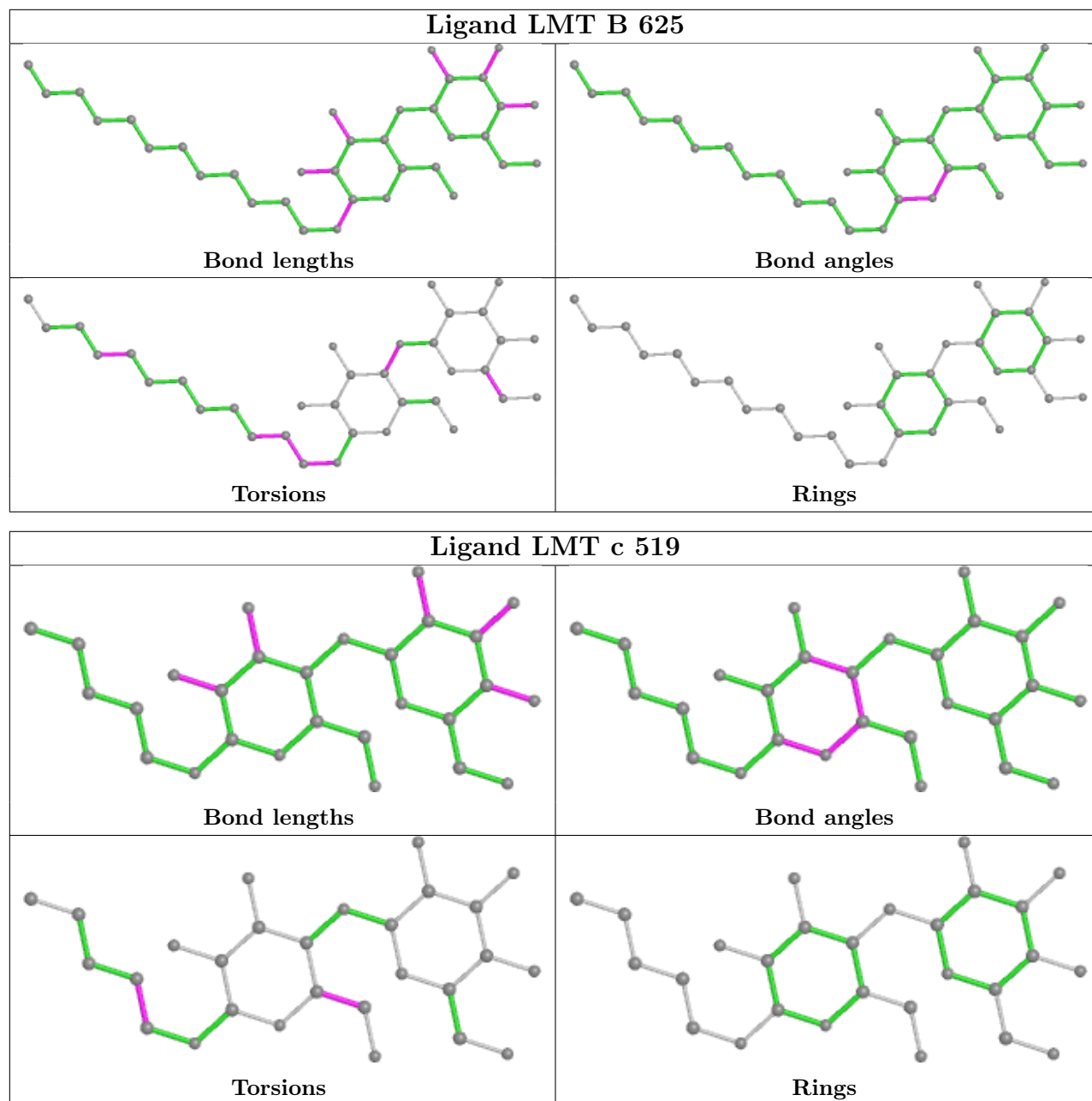


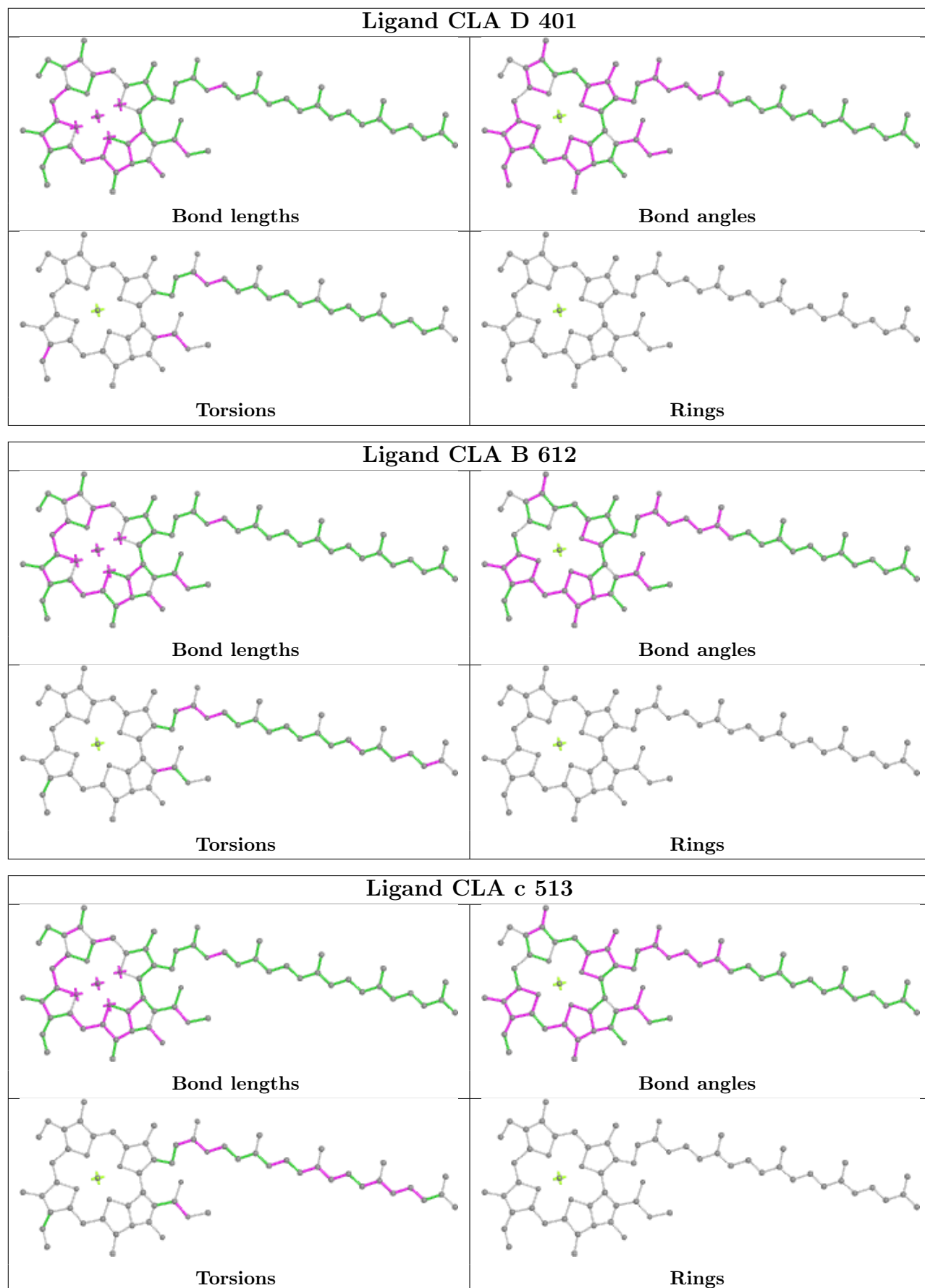


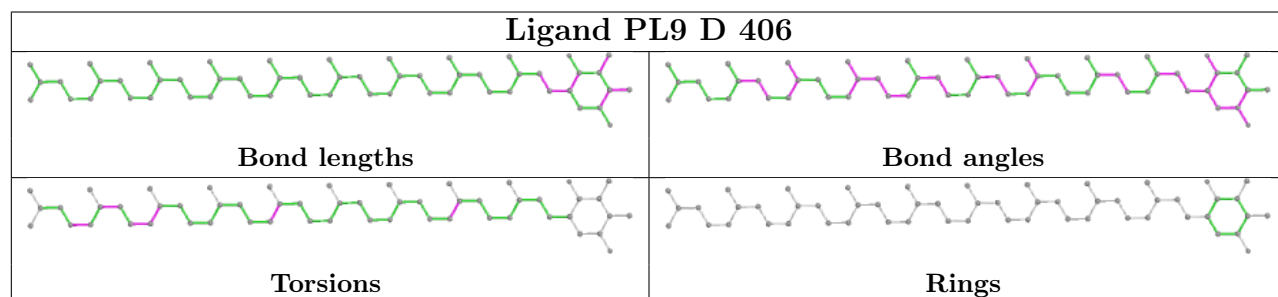
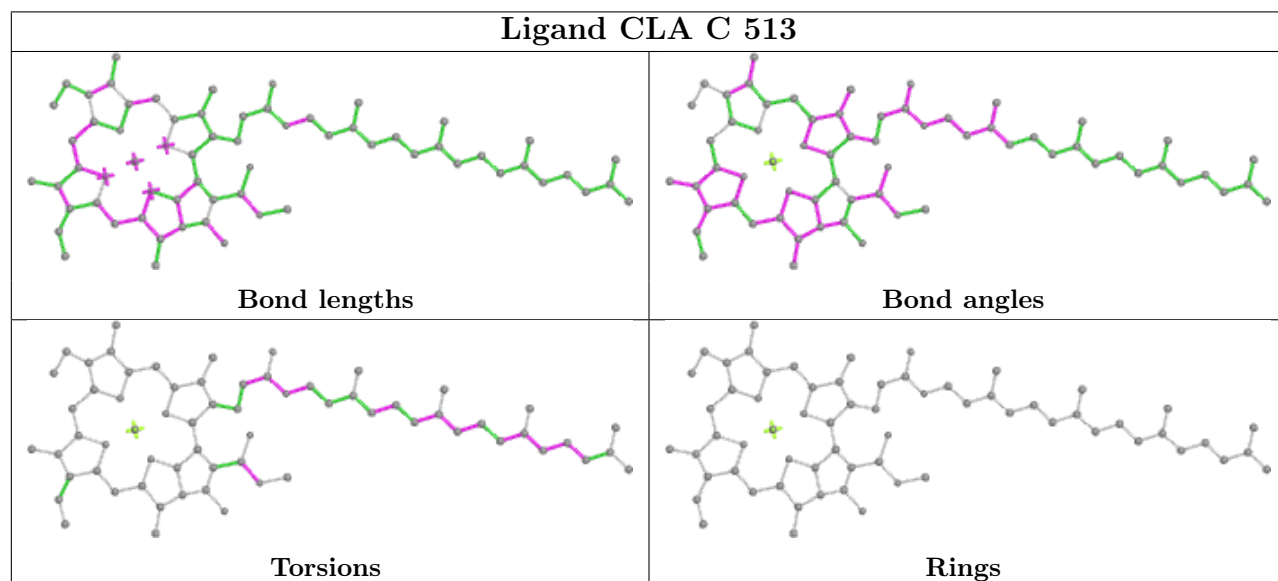
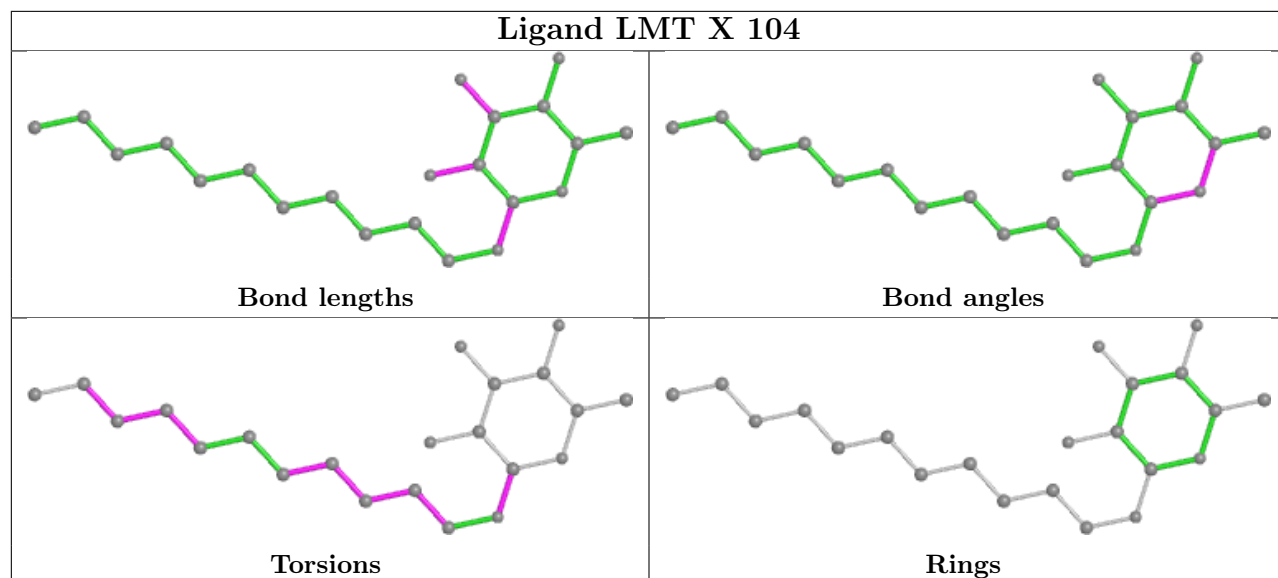


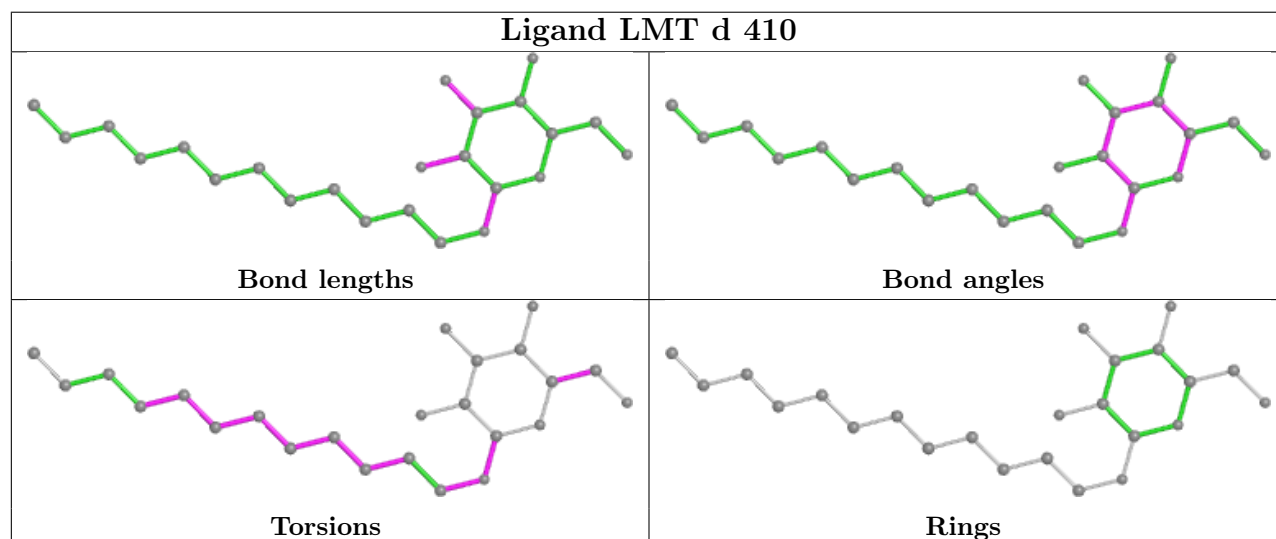
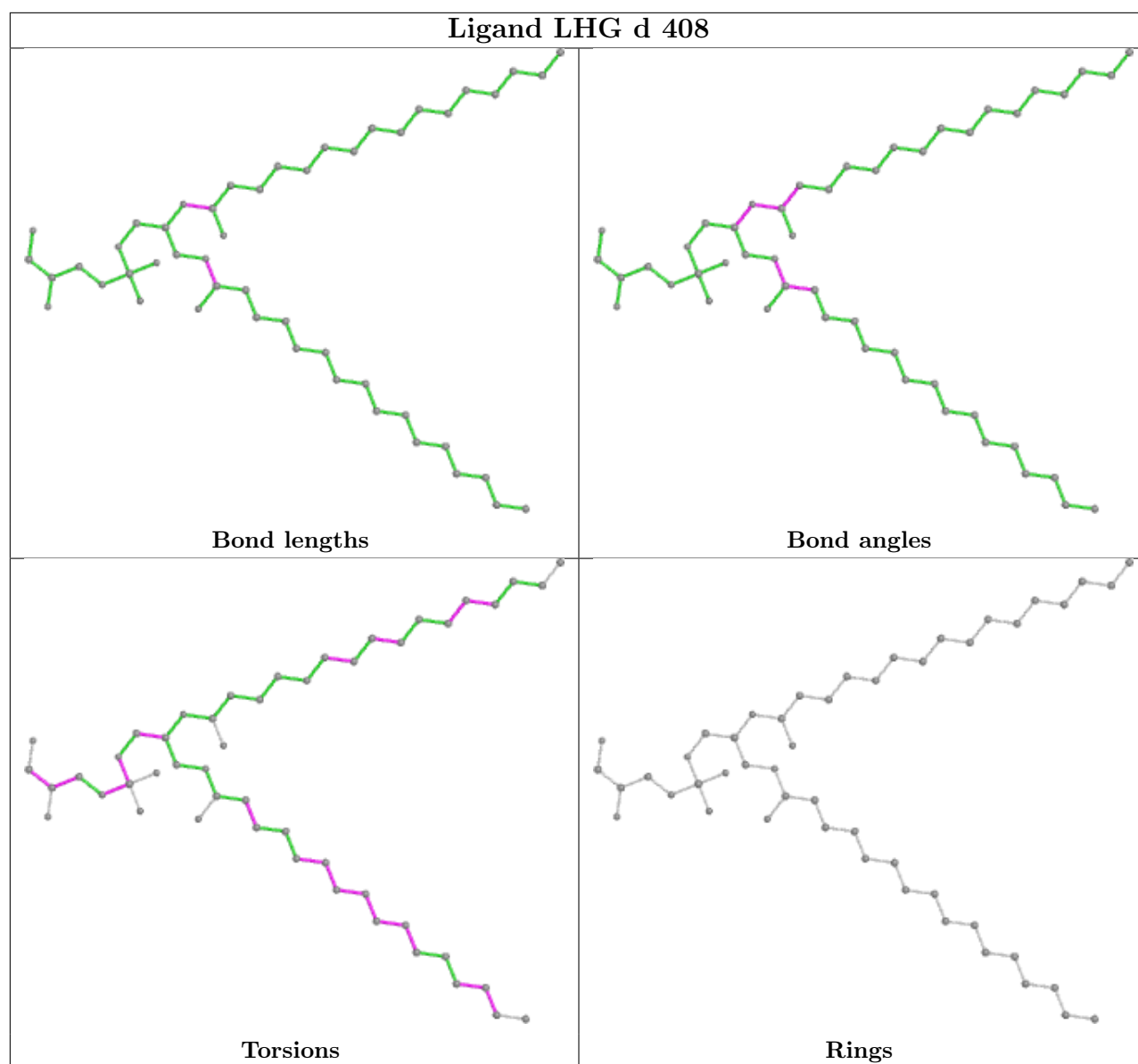


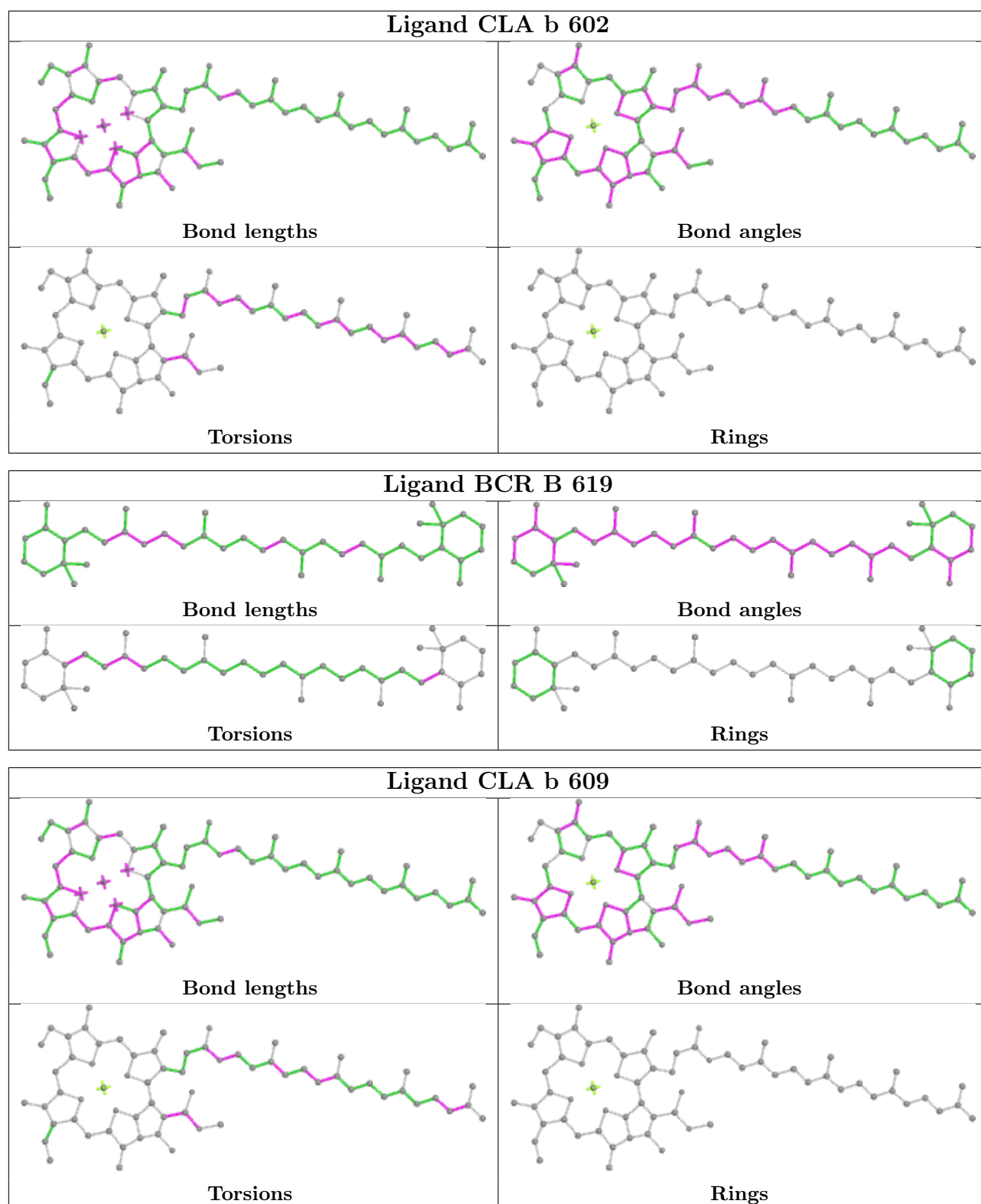




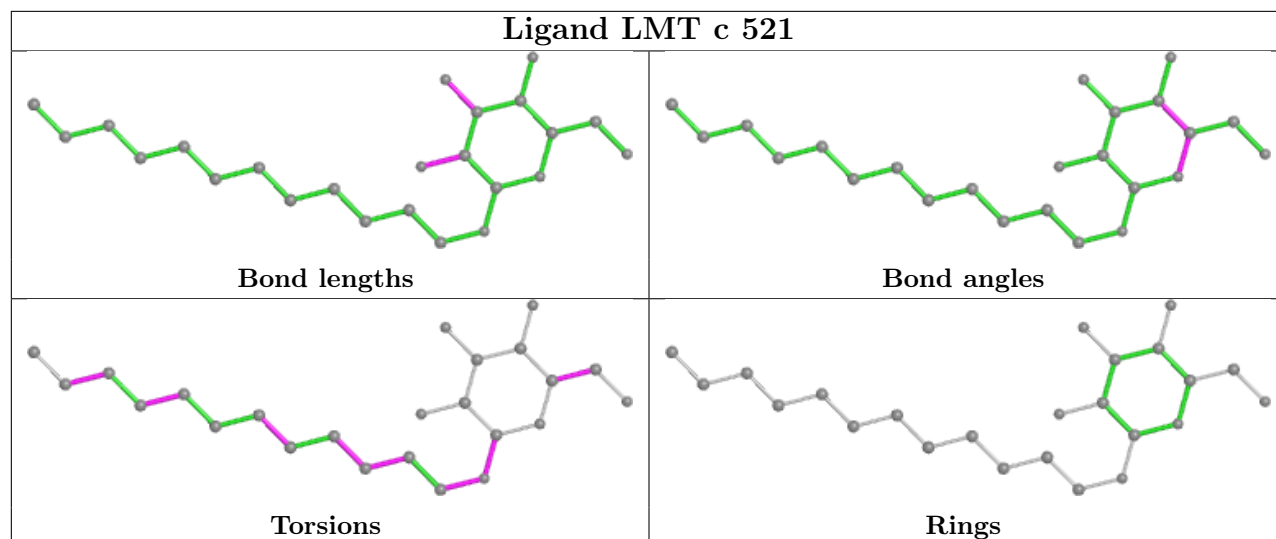












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

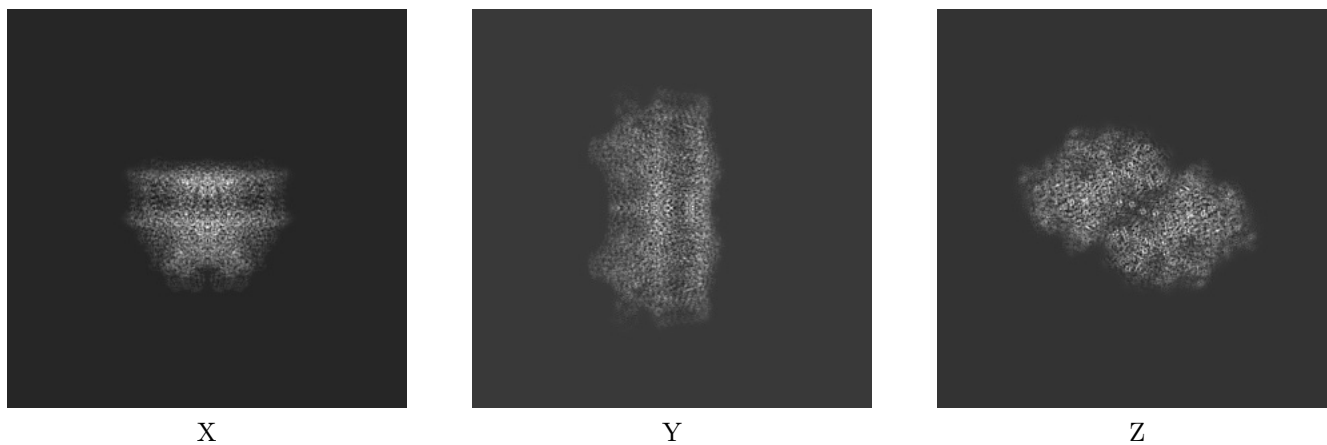
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24407. 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](#)

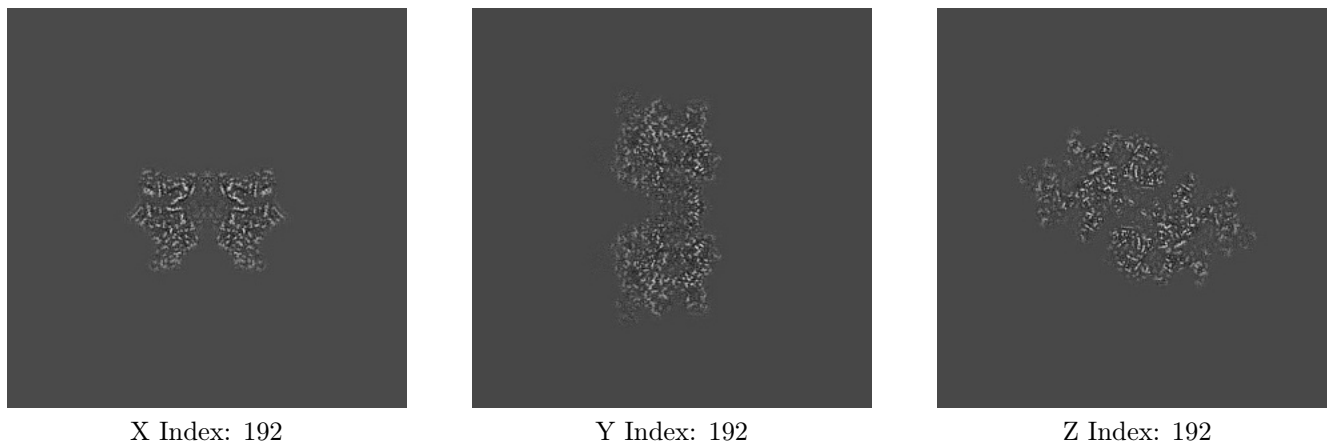
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



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

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

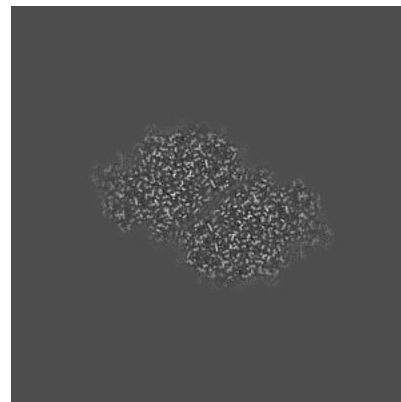
### 6.3.1 Primary map



X Index: 194



Y Index: 187



Z Index: 179

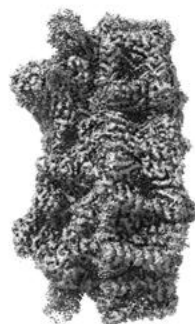
The images above show the largest variance slices of the map in three orthogonal directions.

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

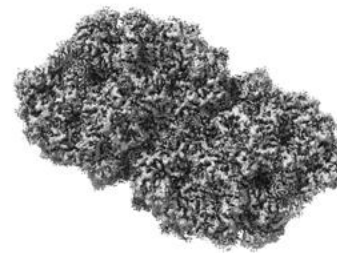
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

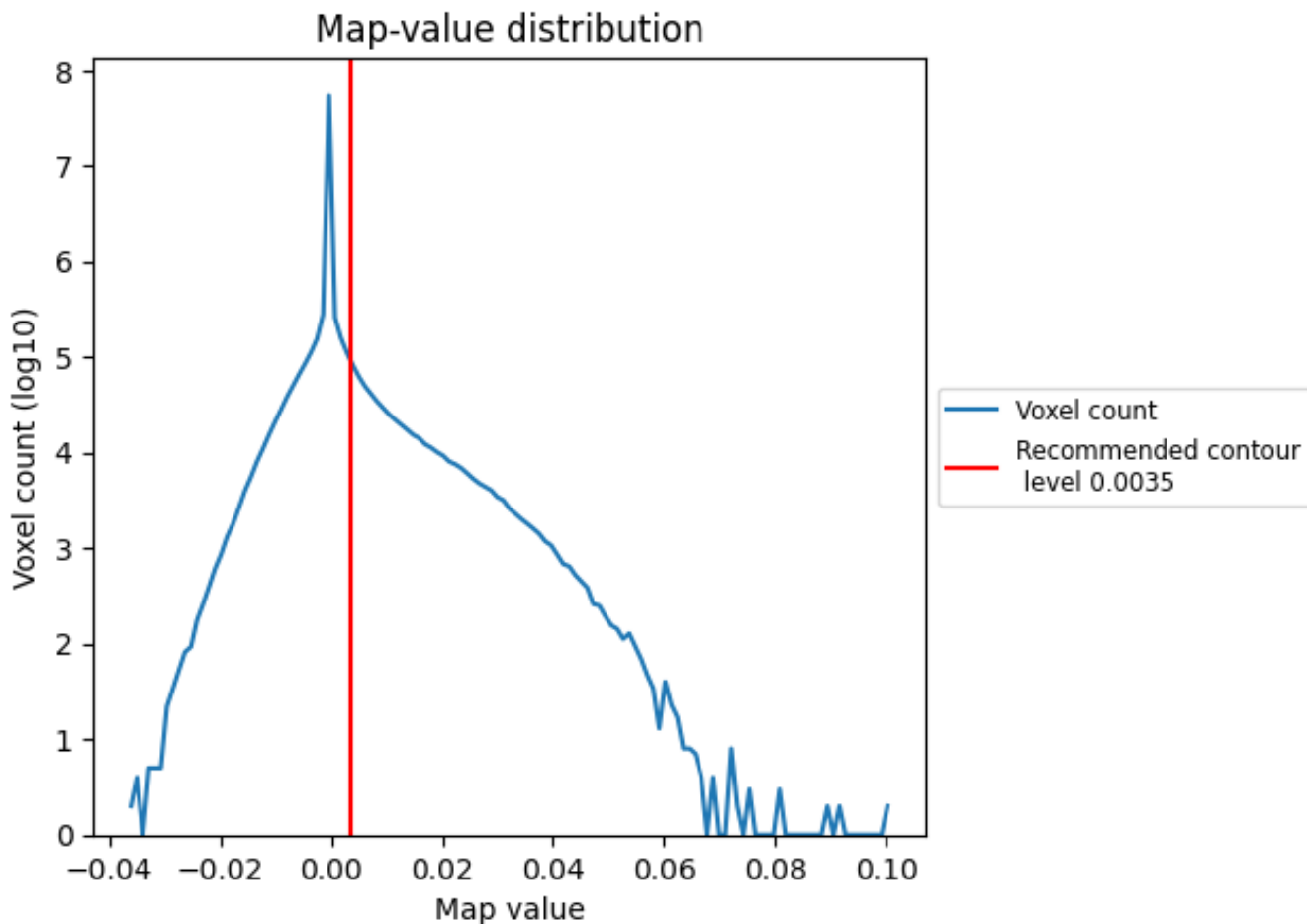
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

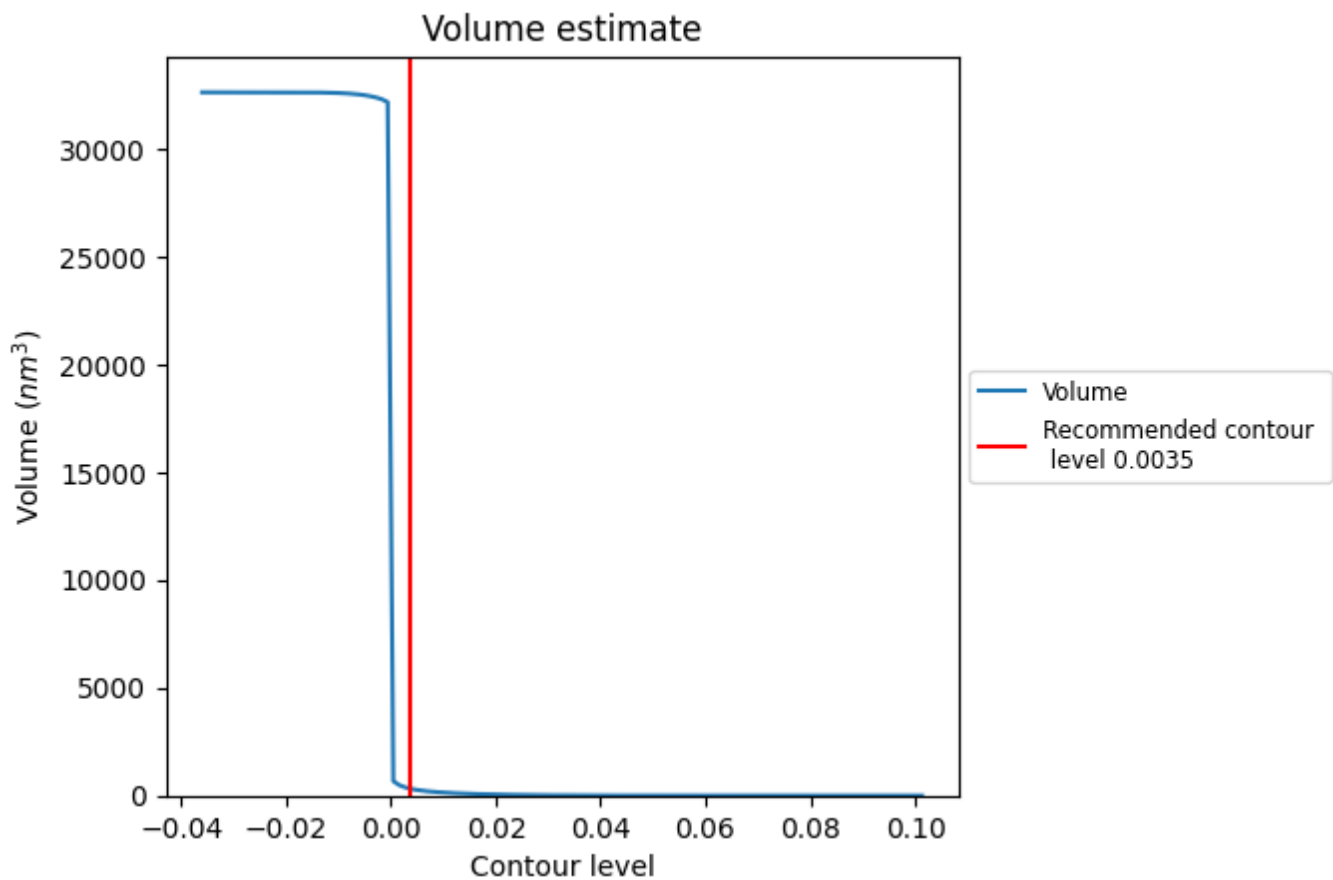
This section contains the results of statistical analysis of the map.

### 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.

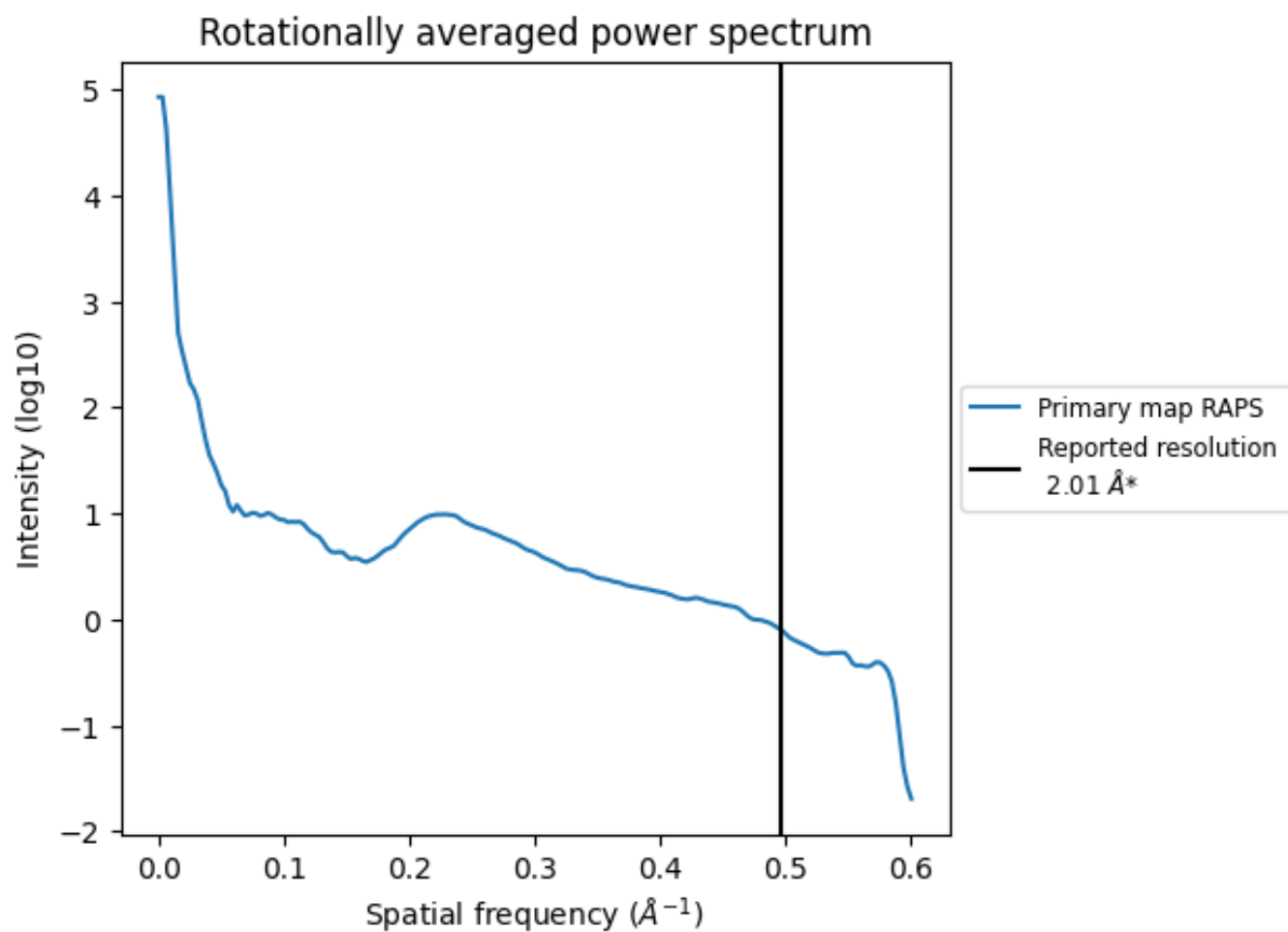
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 331 nm<sup>3</sup>; this corresponds to an approximate mass of 299 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 i

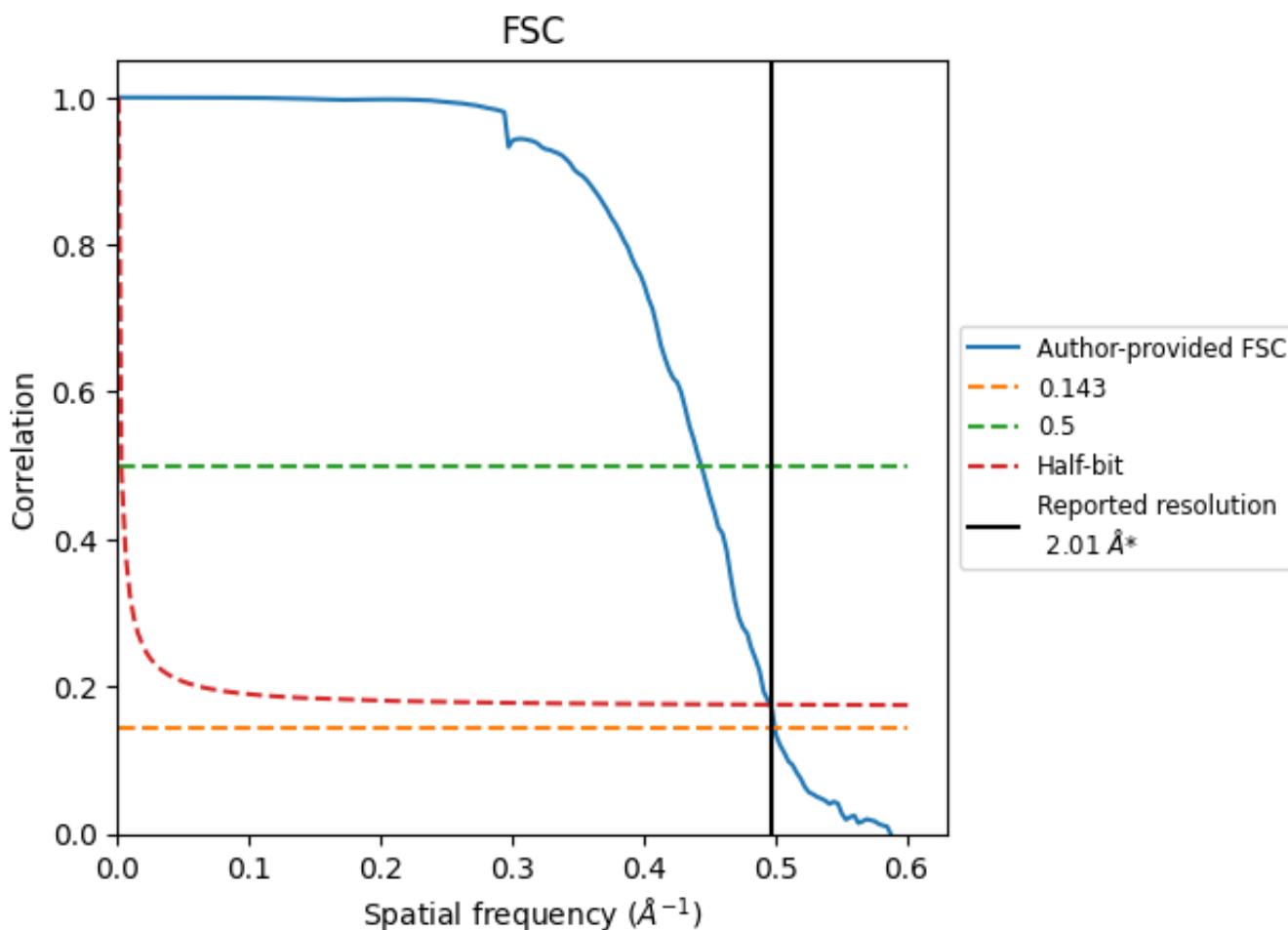


\*Reported resolution corresponds to spatial frequency of 0.498 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.498 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

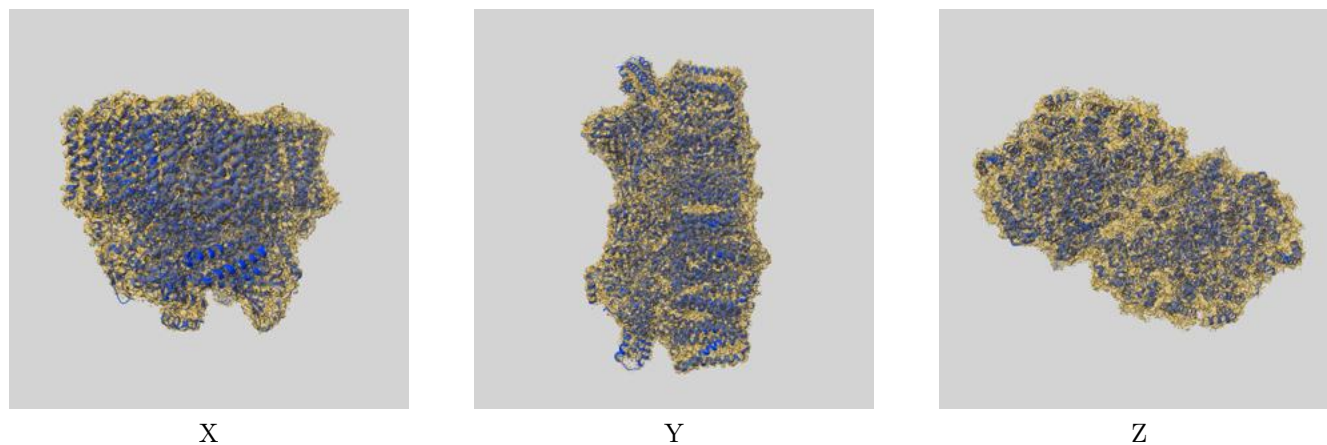
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.00	2.25	2.02
Unmasked-calculated*	-	-	-

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

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

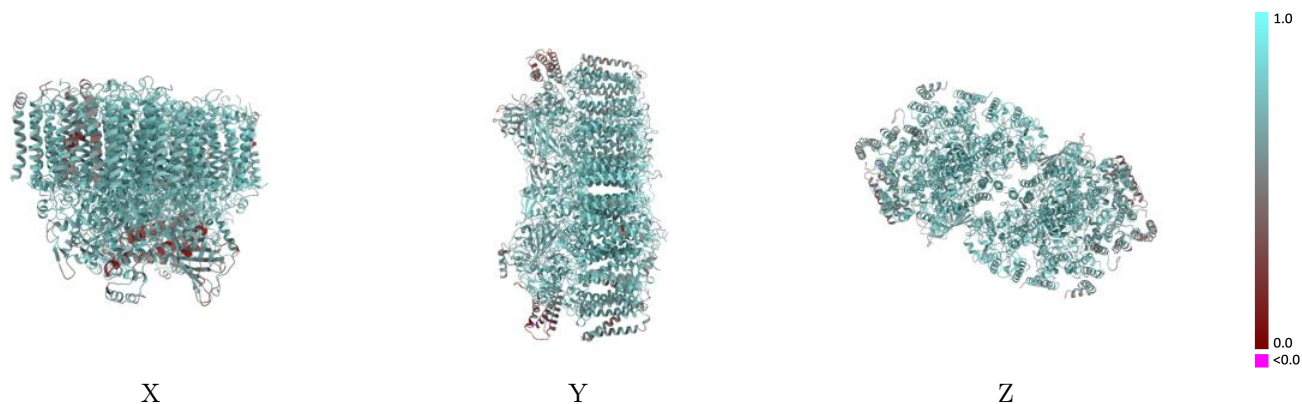
This section contains information regarding the fit between EMDB map EMD-24407 and PDB model 7RCV. Per-residue inclusion information can be found in section 3 on page 31.

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



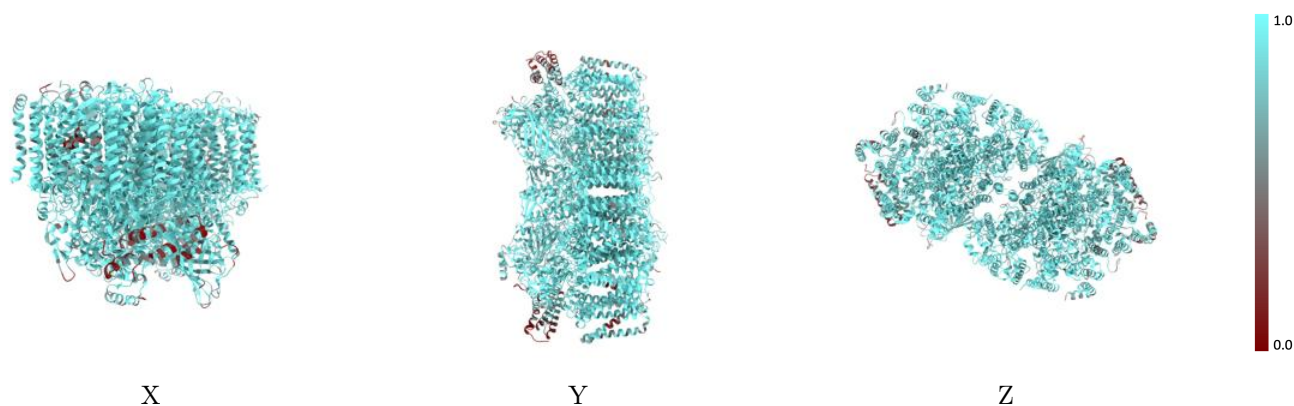
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



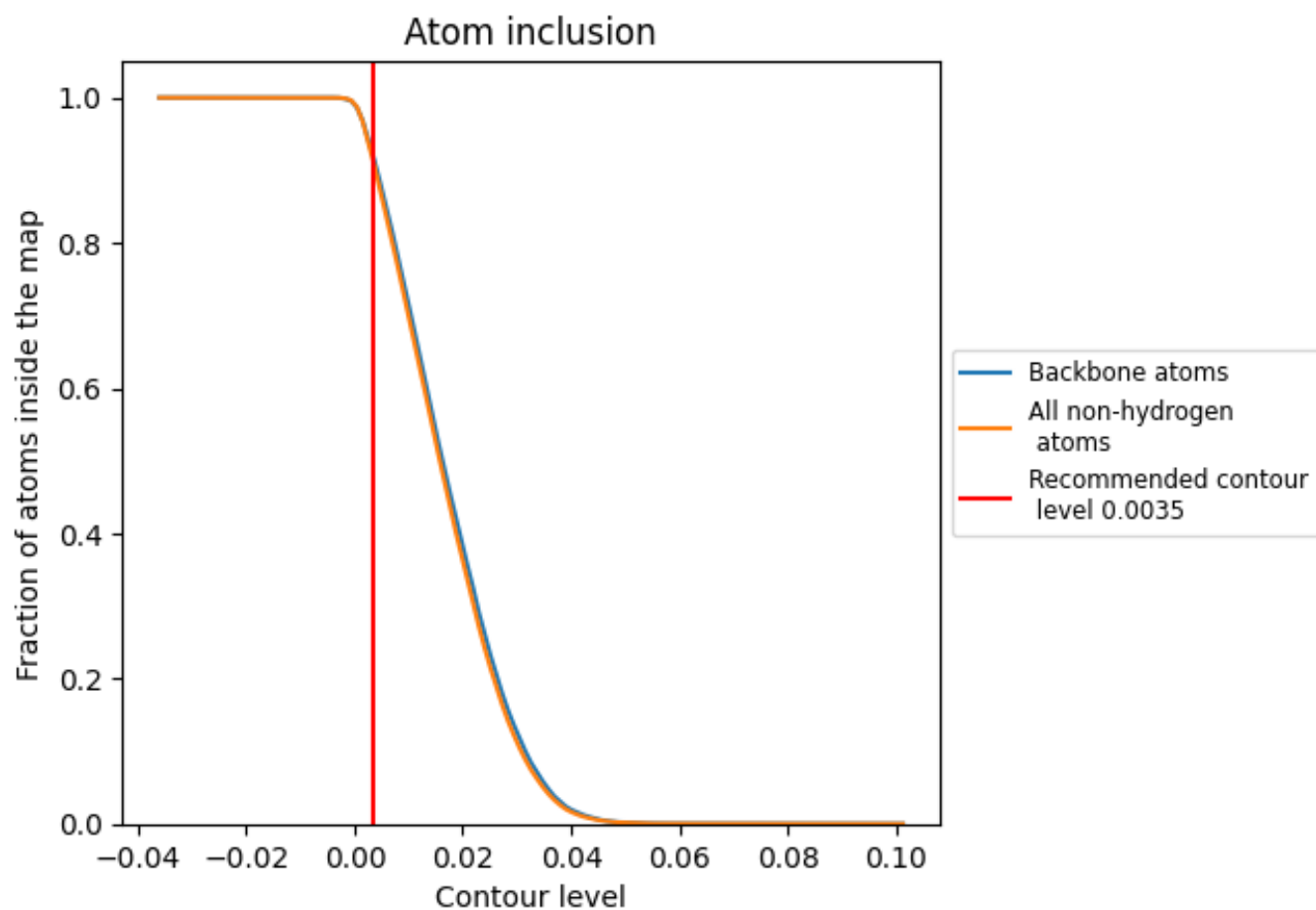
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9118	 0.6990
A	 0.9521	 0.7560
B	 0.9502	 0.7430
C	 0.9510	 0.7290
D	 0.9717	 0.7680
E	 0.9242	 0.6910
F	 0.9003	 0.6800
H	 0.9103	 0.7050
I	 0.8886	 0.6920
J	 0.8188	 0.6180
K	 0.8756	 0.6430
L	 0.9636	 0.7470
M	 0.9204	 0.6790
O	 0.8752	 0.6390
Q	 0.5178	 0.4520
R	 0.8294	 0.5760
T	 0.8726	 0.6710
U	 0.8805	 0.6600
V	 0.9013	 0.6800
X	 0.8796	 0.6450
Y	 0.7893	 0.5820
Z	 0.7283	 0.5440
a	 0.9533	 0.7560
b	 0.9514	 0.7380
c	 0.9445	 0.7050
d	 0.9713	 0.7600
e	 0.9160	 0.6730
f	 0.9055	 0.6680
h	 0.9135	 0.6980
i	 0.8653	 0.6620
j	 0.8121	 0.6110
k	 0.8780	 0.6260
l	 0.9692	 0.7460
m	 0.9027	 0.6760
o	 0.8627	 0.6060



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
q	 0.5100	 0.4320
r	 0.8214	 0.5700
t	 0.8885	 0.6880
u	 0.8736	 0.6560
v	 0.9077	 0.6730
x	 0.8698	 0.6330
y	 0.7663	 0.5490
z	 0.6906	 0.4910