



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:53 AM UTC

PDB ID : 7O0W / pdb_00007o0w
EMDB ID : EMD-12681
Title : Cryo-EM structure of the RC-dLH complex (model_1b) from Gemmatimonas phototrophica at 2.47 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-27
Resolution : 2.47 Å (reported)
Based on initial models : 6ET5, 1LGH, 5Y5S

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

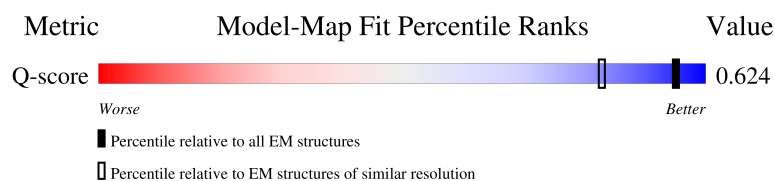
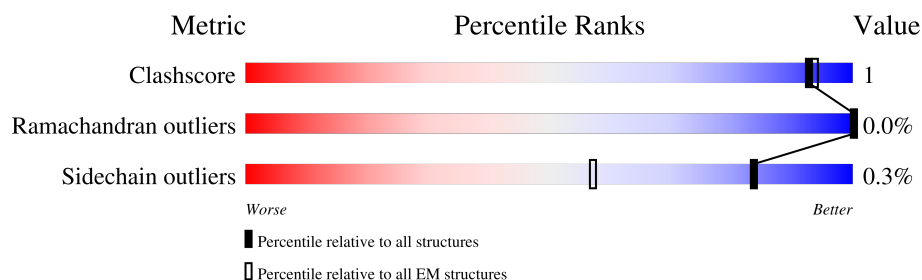
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6086 (1.98 - 2.97)

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

Mol	Chain	Length	Quality of chain
1	AA	54	
1	AB	54	
1	AC	54	
1	AD	54	

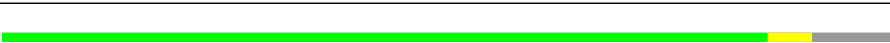
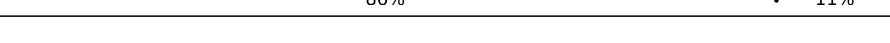
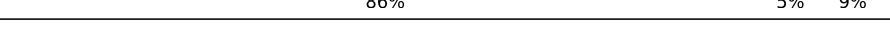
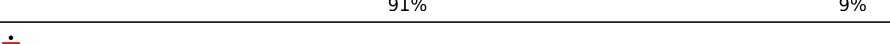
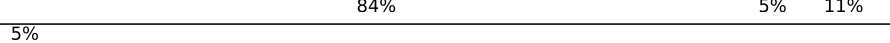
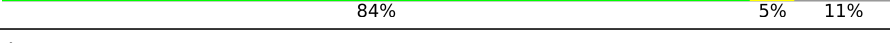
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	54	
1	AF	54	
1	AG	54	
1	AH	54	
1	AI	54	
1	AJ	54	
1	AK	54	
1	AL	54	
1	AM	54	
1	AN	54	
1	AO	54	
1	AP	54	
1	AQ	54	
1	AR	54	
1	AS	54	
1	AT	54	
1	AU	54	
1	AV	54	
1	AW	54	
1	AX	54	
2	BA	44	
2	BB	44	
2	BC	44	
2	BD	44	
2	BE	44	

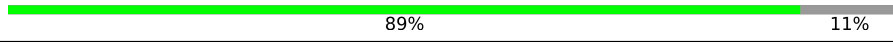
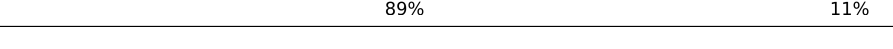
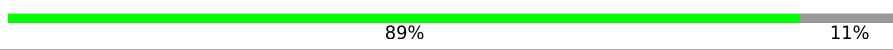
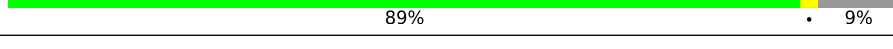
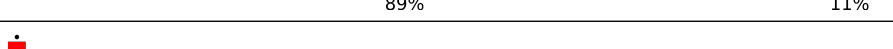
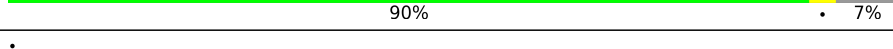
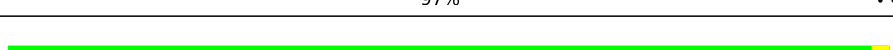
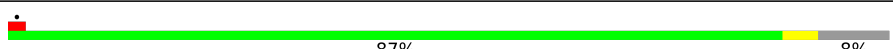
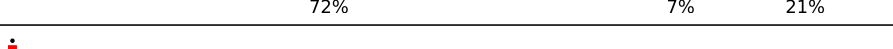
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BF	44	
2	BG	44	
2	BH	44	
2	BI	44	
2	BJ	44	
2	BK	44	
2	BL	44	
2	BM	44	
2	BN	44	
2	BO	44	
2	BP	44	
2	BQ	44	
2	BR	44	
2	BS	44	
2	BT	44	
2	BU	44	
2	BV	44	
2	BW	44	
2	BX	44	
2	ba	44	
2	bb	44	
2	bc	44	
2	bd	44	
2	be	44	
2	bf	44	

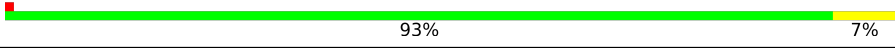
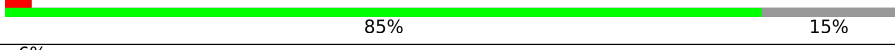
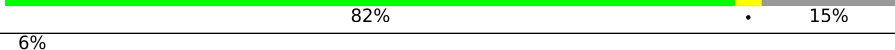
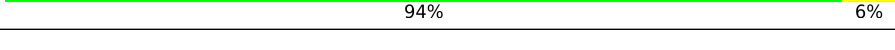
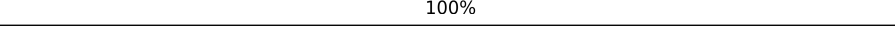
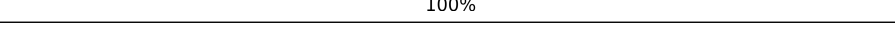
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	bg	44	
2	bh	44	
2	bi	44	
2	bj	44	
2	bk	44	
2	bl	44	
2	bm	44	
2	bn	44	
2	bo	44	
2	bp	44	
3	C	354	
4	C1	202	
5	C2	125	
6	H1	67	
7	H2	181	
8	L	274	
9	M	367	
10	aa	71	
11	ab	71	
11	ac	71	
11	ad	71	
11	ae	71	
11	af	71	
11	ag	71	
11	ah	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	ai	71	
11	aj	71	
11	ak	71	
11	al	71	
11	am	71	
11	an	71	
11	ao	71	
11	ap	71	
12	CG	2	
12	MG	2	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 56476 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 LHH-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AB	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AC	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
1	AD	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
1	AE	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AF	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AG	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AH	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AI	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AJ	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AK	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AL	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AM	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AN	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AO	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AP	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AQ	49	Total	C	N	O	S	0	0
			391	261	65	61	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AS	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AT	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AU	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AV	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AW	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AX	49	Total	C	N	O	S	0	0
			391	261	65	61	4		

- Molecule 2 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BB	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BC	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BD	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BE	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BF	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BG	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BH	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BI	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BJ	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BK	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BL	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BM	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BN	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BO	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BP	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BQ	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BR	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BS	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BT	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BU	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BV	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BW	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BX	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	ba	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bb	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bc	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bd	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	be	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bf	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bg	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bh	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bi	39	Total 323	C 213	N 55	O 53	S 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	bj	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bk	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bl	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bm	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bn	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	bo	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bp	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

- Molecule 3 is a protein called MULTIHEME_CYTC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	299	Total	C	N	O	S	0	0
			2325	1464	419	423	19		

- Molecule 4 is a protein called RC-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	103	Total	C	N	O	S	0	0
			806	506	151	145	4		

- Molecule 5 is a protein called RC-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C2	101	Total	C	N	O	S	0	0
			779	491	150	135	3		

- Molecule 6 is a protein called PRCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H1	62	Total	C	N	O	S	0	0
			522	343	89	88	2		

- Molecule 7 is a protein called RC-Hc.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H2	180	Total	C	N	O	S	0	0
			1404	894	239	267	4		

- Molecule 8 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	273	Total	C	N	O	S	0	0
			2165	1457	351	347	10		

- Molecule 9 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	336	Total	C	N	O	S	0	0
			2702	1795	443	454	10		

- Molecule 10 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aa	59	Total	C	N	O	S	0	0
			455	298	80	75	2		

- Molecule 11 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ab	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		
11	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ae	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	af	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ag	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		

Continued on next page...

Continued from previous page...

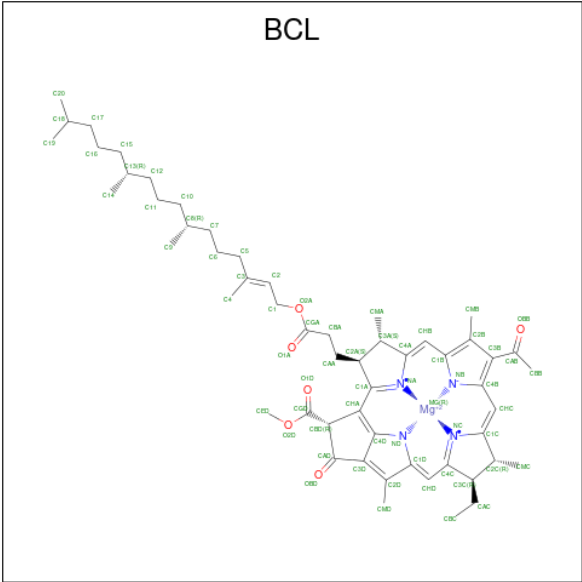
Mol	Chain	Residues	Atoms					AltConf	Trace
11	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	an	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ap	71	Total	C	N	O	S	0	0
			542	352	95	91	4		

- Molecule 12 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
12	CG	2	Total	C	O	0	0
			21	12	9		
12	MG	2	Total	C	O	0	0
			21	12	9		

- Molecule 13 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BR	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

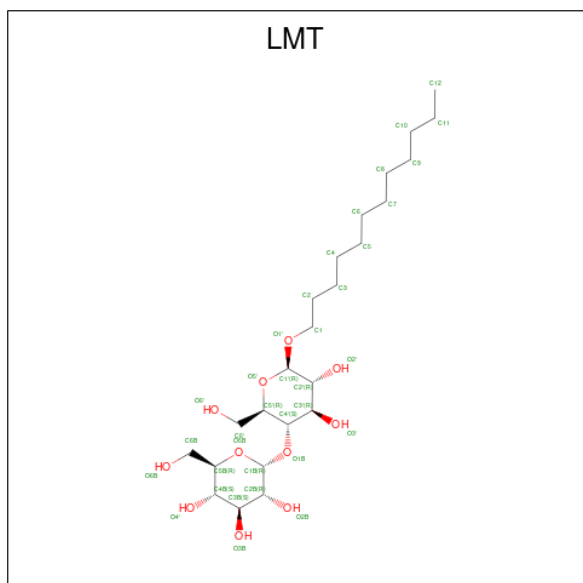
Mol	Chain	Residues	Atoms					AltConf
13	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	al	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	am	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	an	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ao	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ap	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bb	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bc	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	be	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bf	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	bg	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bh	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bi	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bj	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bk	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bl	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bm	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bn	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bo	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 14 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
14	AA	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	AB	1	Total	C	O	0
			35	24	11	
14	AC	1	Total	C	O	0
			35	24	11	
14	AD	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AG	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AL	1	Total	C	O	0
			35	24	11	
14	AM	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AP	1	Total	C	O	0
			35	24	11	
14	AQ	1	Total	C	O	0
			35	24	11	
14	AS	1	Total	C	O	0
			35	24	11	
14	AT	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	AT	1	Total	C	O	0
			35	24	11	
14	AU	1	Total	C	O	0
			35	24	11	
14	AV	1	Total	C	O	0
			35	24	11	
14	AV	1	Total	C	O	0
			35	24	11	
14	AX	1	Total	C	O	0
			35	24	11	
14	BA	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BF	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	BF	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BL	1	Total	C	O	0
			35	24	11	
14	BL	1	Total	C	O	0
			35	24	11	
14	BM	1	Total	C	O	0
			35	24	11	
14	BM	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	BM	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BQ	1	Total	C	O	0
			35	24	11	
14	BQ	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BT	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

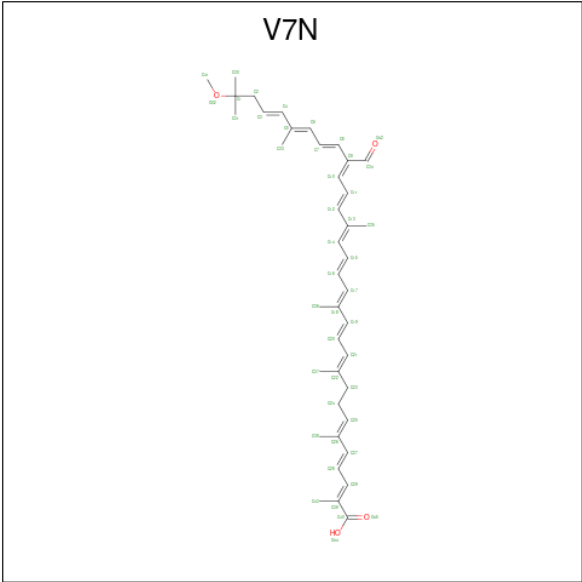
Mol	Chain	Residues	Atoms			AltConf
14	BT	1	Total	C	O	0
			35	24	11	
14	BT	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	C	1	Total	C	O	0
			35	24	11	
14	C2	1	Total	C	O	0
			35	24	11	
14	H2	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			35	24	11	
14	ac	1	Total	C	O	0
			35	24	11	
14	bc	1	Total	C	O	0
			35	24	11	
14	be	1	Total	C	O	0
			35	24	11	
14	be	1	Total	C	O	0
			35	24	11	
14	bf	1	Total	C	O	0
			35	24	11	
14	bg	1	Total	C	O	0
			35	24	11	
14	bh	1	Total	C	O	0
			35	24	11	
14	bi	1	Total	C	O	0
			35	24	11	
14	bj	1	Total	C	O	0
			35	24	11	
14	bk	1	Total	C	O	0
			35	24	11	
14	bl	1	Total	C	O	0
			35	24	11	
14	bm	1	Total	C	O	0
			35	24	11	
14	bn	1	Total	C	O	0
			35	24	11	
14	bo	1	Total	C	O	0
			35	24	11	
14	bp	1	Total	C	O	0
			35	24	11	
14	bp	1	Total	C	O	0
			35	24	11	

- Molecule 15 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriacont-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: C₄₁H₅₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	AA	1	Total	C	O	0
			45	41	4	
15	AD	1	Total	C	O	0
			45	41	4	
15	AM	1	Total	C	O	0
			45	41	4	
15	AS	1	Total	C	O	0
			45	41	4	
15	AW	1	Total	C	O	0
			45	41	4	
15	BA	1	Total	C	O	0
			45	41	4	
15	BD	1	Total	C	O	0
			45	41	4	
15	BE	1	Total	C	O	0
			45	41	4	
15	BF	1	Total	C	O	0
			45	41	4	
15	BG	1	Total	C	O	0
			45	41	4	
15	BH	1	Total	C	O	0
			45	41	4	
15	BI	1	Total	C	O	0
			45	41	4	
15	BJ	1	Total	C	O	0
			45	41	4	
15	BK	1	Total	C	O	0
			45	41	4	

Continued on next page...

Continued from previous page...

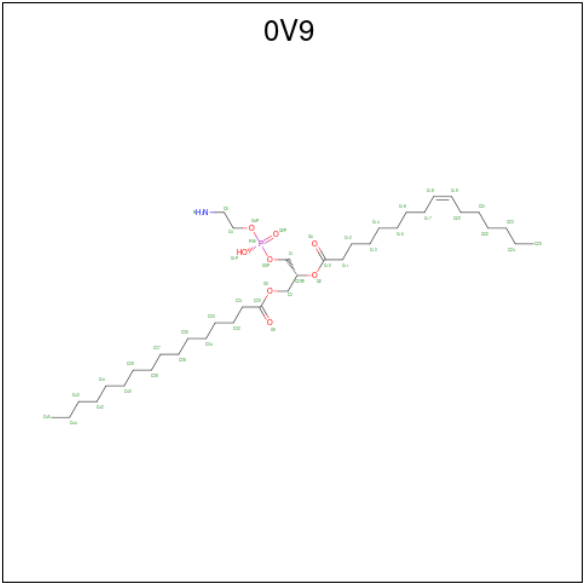
Mol	Chain	Residues	Atoms			AltConf
15	BM	1	Total	C	O	0
			45	41	4	
15	BN	1	Total	C	O	0
			45	41	4	
15	BO	1	Total	C	O	0
			45	41	4	
15	BP	1	Total	C	O	0
			45	41	4	
15	BQ	1	Total	C	O	0
			45	41	4	
15	BR	1	Total	C	O	0
			45	41	4	
15	BS	1	Total	C	O	0
			45	41	4	
15	BU	1	Total	C	O	0
			45	41	4	
15	BV	1	Total	C	O	0
			45	41	4	
15	BW	1	Total	C	O	0
			45	41	4	
15	ag	1	Total	C	O	0
			45	41	4	
15	ba	1	Total	C	O	0
			45	41	4	
15	bb	1	Total	C	O	0
			45	41	4	
15	bc	1	Total	C	O	0
			45	41	4	
15	bd	1	Total	C	O	0
			45	41	4	
15	be	1	Total	C	O	0
			45	41	4	
15	bg	1	Total	C	O	0
			45	41	4	
15	bh	1	Total	C	O	0
			45	41	4	
15	bi	1	Total	C	O	0
			45	41	4	
15	bj	1	Total	C	O	0
			45	41	4	
15	bk	1	Total	C	O	0
			45	41	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
15	bl	1	Total	C	O	0
			45	41	4	
15	bm	1	Total	C	O	0
			45	41	4	
15	bn	1	Total	C	O	0
			45	41	4	
15	bo	1	Total	C	O	0
			45	41	4	
15	bp	1	Total	C	O	0
			45	41	4	

- Molecule 16 is (19R,22S)-25-amino-22-hydroxy-22-oxido-16-oxo-17,21,23-trioxa-22lambda 5 -phosphapentacosan-19-yl (9Z)-hexadec-9-enoate (CCD ID: 0V9) (formula: C₃₇H₇₂NO₈P) (labeled as "Ligand of Interest" by depositor).



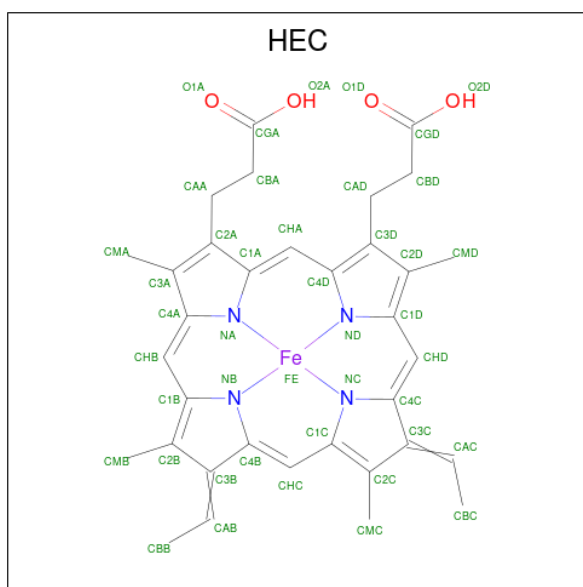
Mol	Chain	Residues	Atoms					AltConf
16	AQ	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	H1	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	ab	1	Total	C	N	O	P	0
			45	35	1	8	1	

Continued on next page...

Continued from previous page...

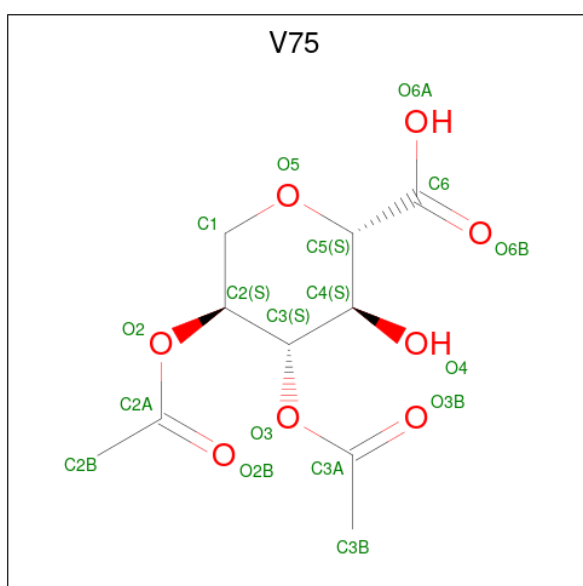
Mol	Chain	Residues	Atoms					AltConf
16	ad	1	Total 45	C 35	N 1	O 8	P 1	0
16	bb	1	Total 45	C 35	N 1	O 8	P 1	0
16	bd	1	Total 45	C 35	N 1	O 8	P 1	0
16	be	1	Total 45	C 35	N 1	O 8	P 1	0
16	bf	1	Total 45	C 35	N 1	O 8	P 1	0
16	bg	1	Total 45	C 35	N 1	O 8	P 1	0
16	bh	1	Total 45	C 35	N 1	O 8	P 1	0
16	bi	1	Total 45	C 35	N 1	O 8	P 1	0
16	bj	1	Total 45	C 35	N 1	O 8	P 1	0
16	bk	1	Total 45	C 35	N 1	O 8	P 1	0
16	bl	1	Total 45	C 35	N 1	O 8	P 1	0
16	bm	1	Total 45	C 35	N 1	O 8	P 1	0
16	bn	1	Total 45	C 35	N 1	O 8	P 1	0
16	bo	1	Total 45	C 35	N 1	O 8	P 1	0
16	bp	1	Total 45	C 35	N 1	O 8	P 1	0

- Molecule 17 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



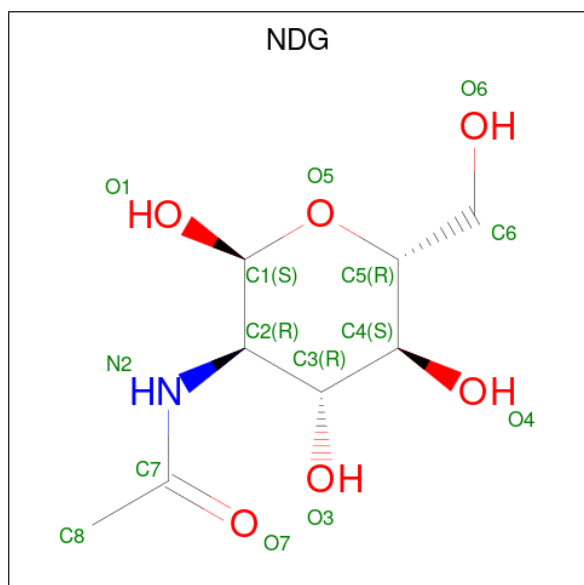
Mol	Chain	Residues	Atoms					AltConf
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 18 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (CCD ID: V75) (formula: C₁₀H₁₄O₈) (labeled as "Ligand of Interest" by depositor).



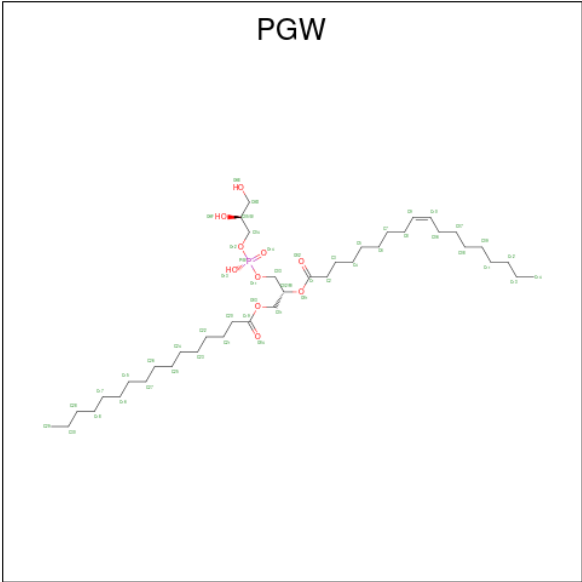
Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			18	10	8	
18	M	1	Total	C	O	0
			18	10	8	

- Molecule 19 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



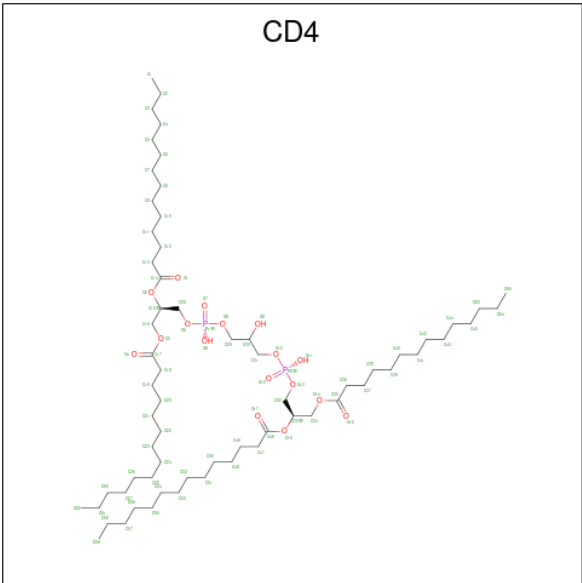
Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	N	O	0
			14	8	1	5	
19	C1	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 20 is (1R)-2-{-[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	H1	1	51	40	10	1	0

- Molecule 21 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



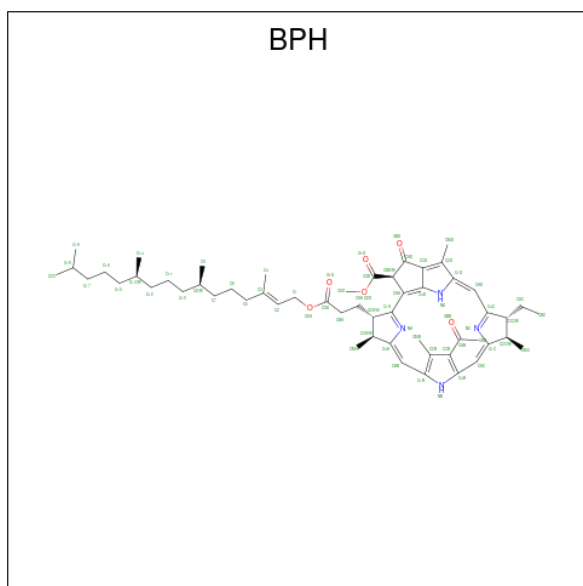
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	H1	1	84	65	17	2	0
21	M	1	84	65	17	2	0

Continued on next page...

Continued from previous page...

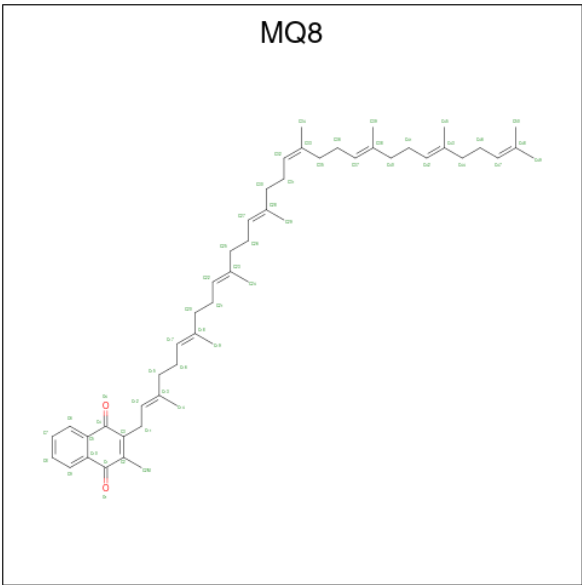
Mol	Chain	Residues	Atoms				AltConf
21	M	1	Total	C	O	P	0
			84	65	17	2	
21	ad	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 22 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	L	1	Total	C	N	O	0
			65	55	4	6	
22	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 23 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).

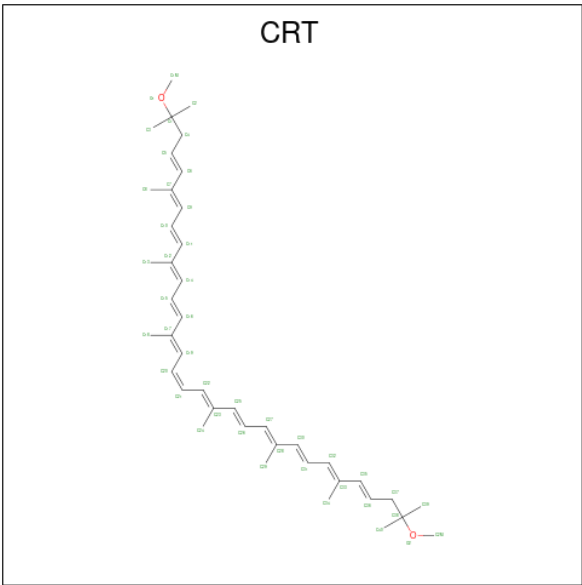


Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	ao	1	Total	C	O	0
			53	51	2	

- Molecule 24 is FE (III) ION (CCD ID: FE) (formula: Fe).

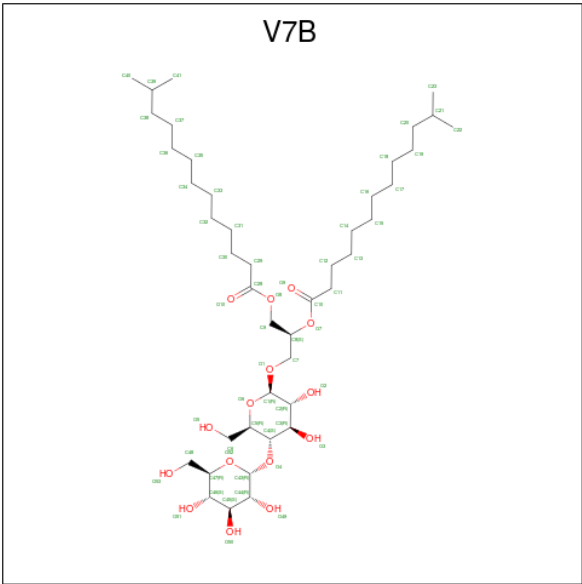
Mol	Chain	Residues	Atoms		AltConf
24	M	1	Total	Fe	0
			1	1	

- Molecule 25 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



Mol	Chain	Residues	Atoms			AltConf
25	M	1	Total	C	O	0
			44	42	2	

- Molecule 26 is [(2 {S})-3-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-2-(12-methyltridecanoyloxy)propyl] 12-methyltridecanoate (CCD ID: V7B) (formula: C₄₃H₈₀O₁₅) (labeled as "Ligand of Interest" by depositor).



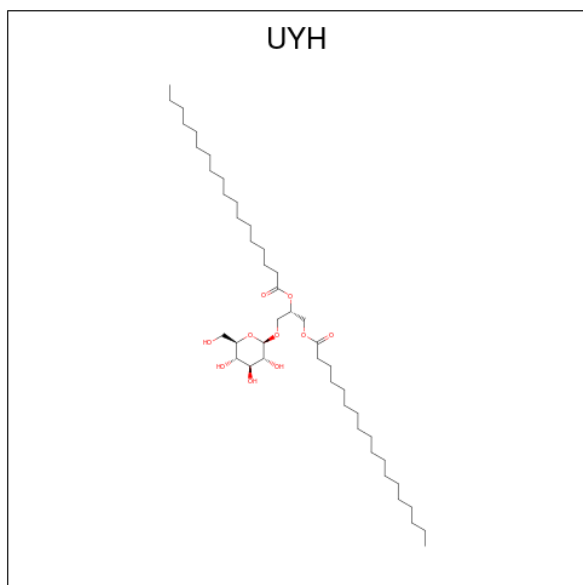
Mol	Chain	Residues	Atoms			AltConf
26	af	1	Total	C	O	0
			58	43	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
26	ag	1	Total	C	O	0
			58	43	15	

- Molecule 27 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (CCD ID: UYH) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	ai	1	Total	C	O	0
			55	45	10	

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	AA	2	Total	O	0
			2	2	
28	AC	1	Total	O	0
			1	1	
28	AD	2	Total	O	0
			2	2	
28	AE	2	Total	O	0
			2	2	
28	AG	3	Total	O	0
			3	3	
28	AH	2	Total	O	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
28	AI	1	Total 1	O 1	0
28	AJ	5	Total 5	O 5	0
28	AK	3	Total 3	O 3	0
28	AL	2	Total 2	O 2	0
28	AM	3	Total 3	O 3	0
28	AN	2	Total 2	O 2	0
28	AO	1	Total 1	O 1	0
28	AP	3	Total 3	O 3	0
28	AQ	5	Total 5	O 5	0
28	AR	3	Total 3	O 3	0
28	AS	4	Total 4	O 4	0
28	AT	4	Total 4	O 4	0
28	AV	2	Total 2	O 2	0
28	AW	3	Total 3	O 3	0
28	AX	1	Total 1	O 1	0
28	BJ	1	Total 1	O 1	0
28	C	67	Total 67	O 67	0
28	C1	36	Total 36	O 36	0
28	C2	1	Total 1	O 1	0
28	H1	4	Total 4	O 4	0
28	H2	27	Total 27	O 27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
28	L	48	Total 48	O 48	0
28	M	63	Total 63	O 63	0
28	aa	4	Total 4	O 4	0
28	ab	2	Total 2	O 2	0
28	ac	1	Total 1	O 1	0
28	ad	7	Total 7	O 7	0
28	ae	9	Total 9	O 9	0
28	af	14	Total 14	O 14	0
28	ag	4	Total 4	O 4	0
28	ah	3	Total 3	O 3	0
28	ai	3	Total 3	O 3	0
28	aj	2	Total 2	O 2	0
28	ak	6	Total 6	O 6	0
28	al	6	Total 6	O 6	0
28	am	5	Total 5	O 5	0
28	an	7	Total 7	O 7	0
28	ao	2	Total 2	O 2	0
28	ap	3	Total 3	O 3	0
28	bb	2	Total 2	O 2	0
28	bc	1	Total 1	O 1	0
28	bd	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

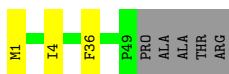
Mol	Chain	Residues	Atoms		AltConf
28	be	2	Total 2	O 2	0
28	bf	3	Total 3	O 3	0
28	bg	3	Total 3	O 3	0
28	bh	2	Total 2	O 2	0
28	bi	2	Total 2	O 2	0
28	bj	1	Total 1	O 1	0
28	bk	2	Total 2	O 2	0
28	bl	1	Total 1	O 1	0
28	bm	3	Total 3	O 3	0
28	bn	2	Total 2	O 2	0
28	bo	1	Total 1	O 1	0
28	bp	1	Total 1	O 1	0

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.

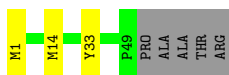
- Molecule 1: LHh-alpha

Chain AA: 



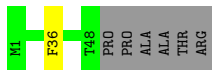
- Molecule 1: LHh-alpha

Chain AB: 



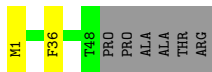
- Molecule 1: LHh-alpha

Chain AC: 



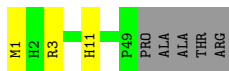
- Molecule 1: LHh-alpha

Chain AD: 



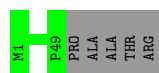
- Molecule 1: LHh-alpha

Chain AE: 



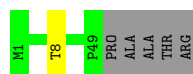
- Molecule 1: LHh-alpha

Chain AF:  91% 9%



• Molecule 1: LHh-alpha

Chain AG:  89% 9%



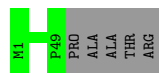
• Molecule 1: LHh-alpha

Chain AH:  81% 7% 9%



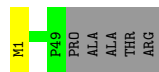
• Molecule 1: LHh-alpha

Chain AI:  91% 9%



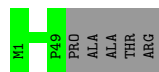
• Molecule 1: LHh-alpha

Chain AJ:  89% 9%



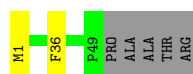
• Molecule 1: LHh-alpha

Chain AK:  91% 9%



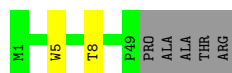
• Molecule 1: LHh-alpha

Chain AL:  87% 9%



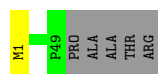
• Molecule 1: LHh-alpha

Chain AM:  87% 9%



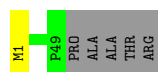
- Molecule 1: LHH-alpha

Chain AN:  89% 9%



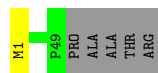
- Molecule 1: LHH-alpha

Chain AO:  89% 9%



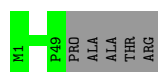
- Molecule 1: LHH-alpha

Chain AP:  89% 9%



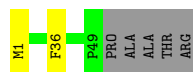
- Molecule 1: LHH-alpha

Chain AQ:  91% 9%



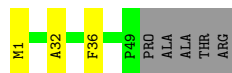
- Molecule 1: LHH-alpha

Chain AR:  87% 9%



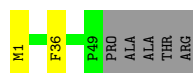
- Molecule 1: LHH-alpha

Chain AS:  85% 6% 9%



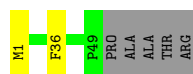
- Molecule 1: LHH-alpha

Chain AT:  87% 9%



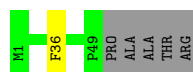
- Molecule 1: LHh-alpha

Chain AU:  87% 9%



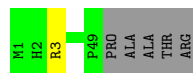
- Molecule 1: LHh-alpha

Chain AV:  89% 9%



- Molecule 1: LHh-alpha

Chain AW:  89% 9%



- Molecule 1: LHh-alpha

Chain AX:  83% 7% 9%



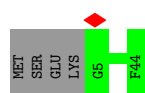
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BA:  86% 11%



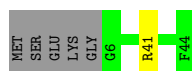
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  91% 9%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  86% • 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BD:  89% • 9%



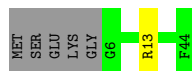
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BE:  89% • 9%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BF:  86% • 11%



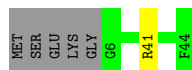
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  84% 5% 11%



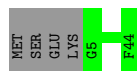
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BH:  86% • 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BI:  91% 9%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



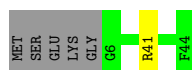
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  89% 11%



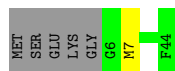
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BL:  86% 11%



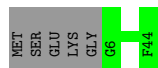
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BM:  86% 11%



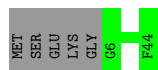
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  89% 11%



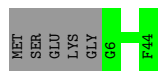
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  89% 11%



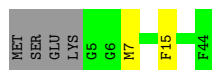
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BP:  89% 11%



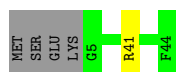
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BQ:  86% 5% 9%



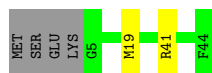
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BR:  89% 0% 9%



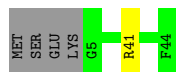
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BS:  86% 5% 9%



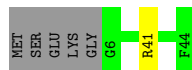
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  89% 0% 9%



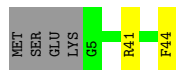
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  86% 0% 11%



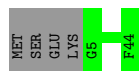
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BV:  86% 5% 9%

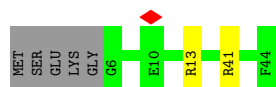
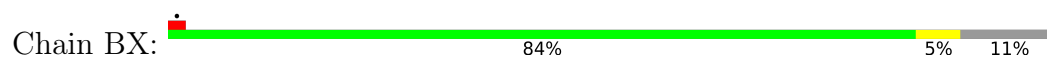


- Molecule 2: Light-harvesting protein B:885 subunit beta

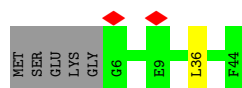
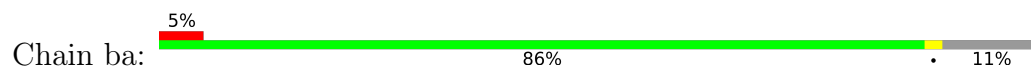
Chain BW:  91% 0% 9%



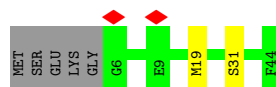
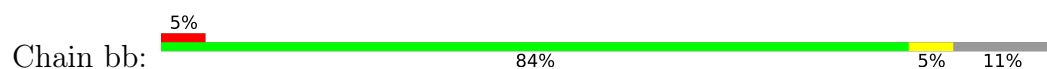
- Molecule 2: Light-harvesting protein B:885 subunit beta



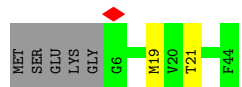
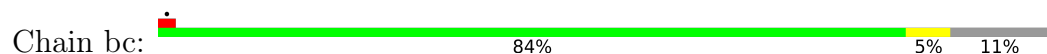
- Molecule 2: Light-harvesting protein B:885 subunit beta



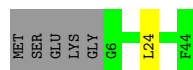
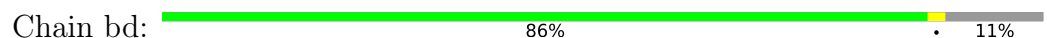
- Molecule 2: Light-harvesting protein B:885 subunit beta



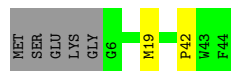
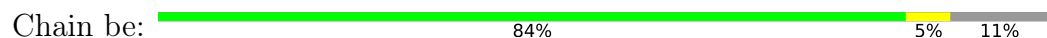
- Molecule 2: Light-harvesting protein B:885 subunit beta



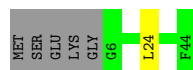
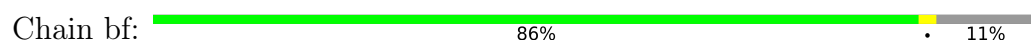
- Molecule 2: Light-harvesting protein B:885 subunit beta



- Molecule 2: Light-harvesting protein B:885 subunit beta

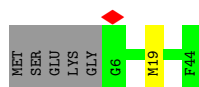


- Molecule 2: Light-harvesting protein B:885 subunit beta



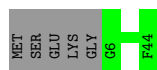
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bg:  86% 11%



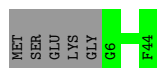
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bh:  89% 11%



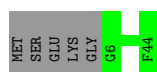
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bi:  89% 11%



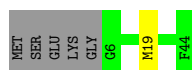
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bj:  89% 11%



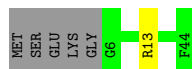
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bk:  86% 11%



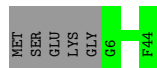
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bl:  86% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bm:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

MET
SER
GLU
LYS
G5
L24
F44

- Chain bo: 89% 11%

MET		
SER		
GLU		
LYS		
GLY		
G6		
F44		

- Chain bp: 84% 5% 11%

MET
 SER
 GLU
 LYS
 GLY
 G6
 E11
 M19
 P42
 W43
 F44

- Chain C:  82% 16%

[illegible]

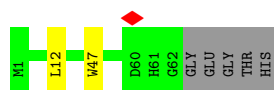
- Chain C1: 50% 49%

[illegible]

- Chain C2:  78% .. 19%

[illegible]

- Chain H1: 90% 7%



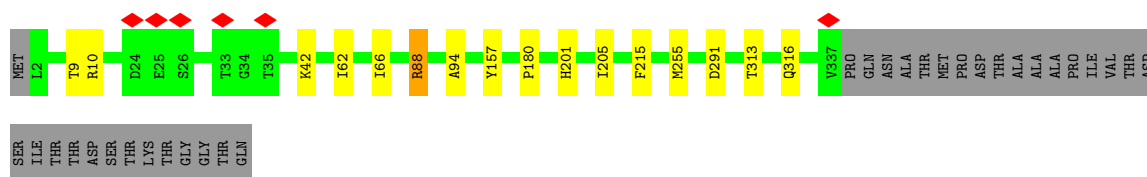
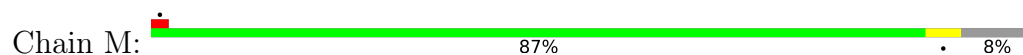
- Molecule 7: RC-Hc



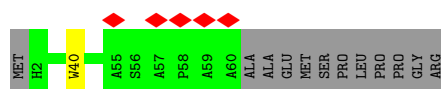
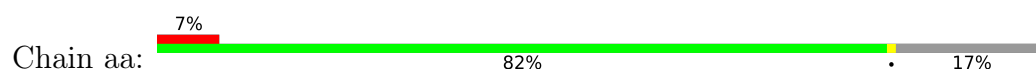
- Molecule 8: Photosynthetic reaction center L subunit



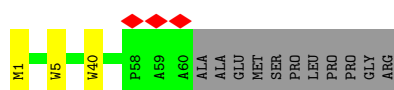
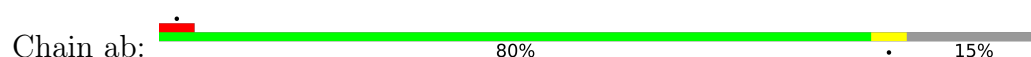
- Molecule 9: RC-M



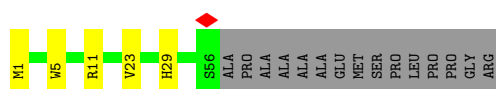
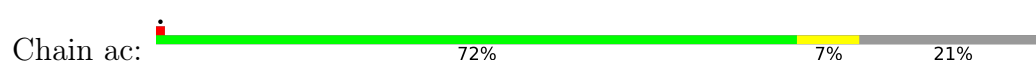
- Molecule 10: LHC domain-containing protein



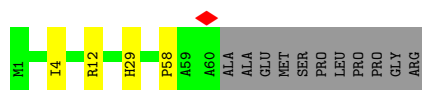
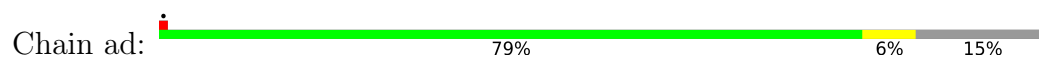
- Molecule 11: LHC domain-containing protein



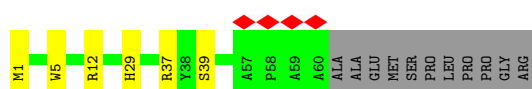
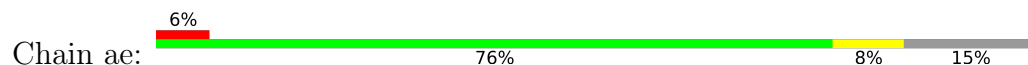
- Molecule 11: LHC domain-containing protein



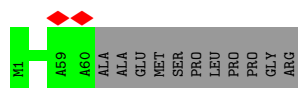
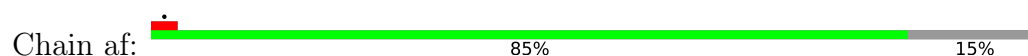
- Molecule 11: LHC domain-containing protein



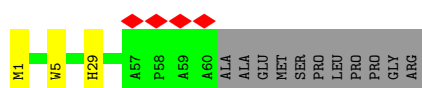
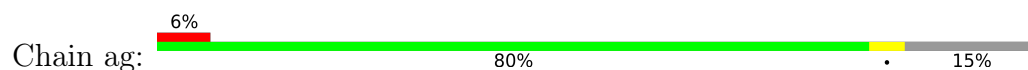
- Molecule 11: LHC domain-containing protein



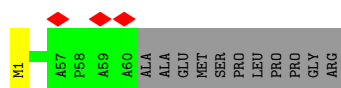
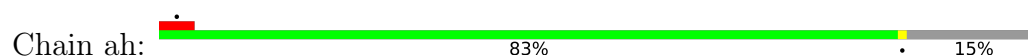
- Molecule 11: LHC domain-containing protein



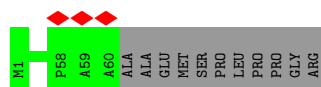
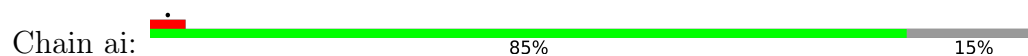
- Molecule 11: LHC domain-containing protein



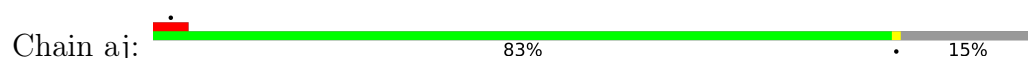
- Molecule 11: LHC domain-containing protein

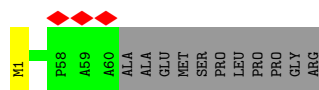


- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein

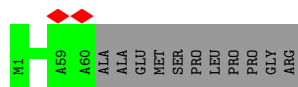
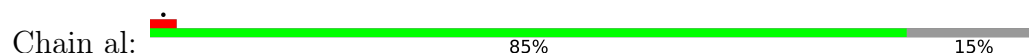




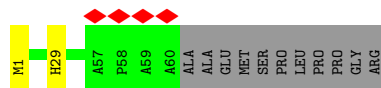
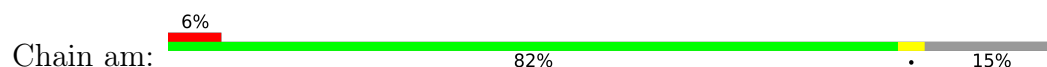
- Molecule 11: LHC domain-containing protein



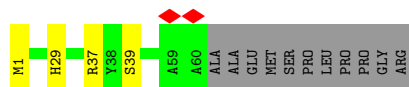
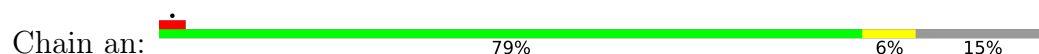
- Molecule 11: LHC domain-containing protein



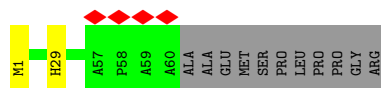
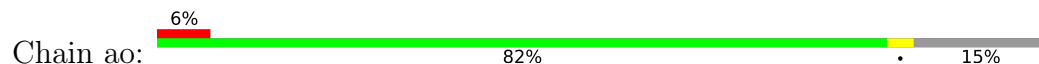
- Molecule 11: LHC domain-containing protein



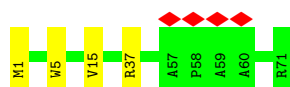
- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain CG:  100%

MAN1
MAN2

- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain MG:  100%

MAN1
MAN2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100616	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 ($e^-/\text{\AA}^2$)	24.8	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.199	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0233	Depositor
Map size (Å)	399.784, 399.784, 399.784	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99946, 0.99946, 0.99946	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: V7N, 0V9, RAM, MQ8, V75, NDG, FE, BPH, FME, CRT, BCL, PGW, V7B, HEC, CD4, UYH, LMT, MAN

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	AA	0.15	0/396	0.46	0/541
1	AB	0.16	0/396	0.45	0/541
1	AC	0.16	0/388	0.47	0/529
1	AD	0.16	0/388	0.48	0/529
1	AE	0.18	0/396	0.51	0/541
1	AF	0.16	0/396	0.47	0/541
1	AG	0.17	0/396	0.48	0/541
1	AH	0.18	0/396	0.46	0/541
1	AI	0.17	0/396	0.50	0/541
1	AJ	0.19	0/396	0.51	0/541
1	AK	0.18	0/396	0.50	0/541
1	AL	0.18	0/396	0.46	0/541
1	AM	0.16	0/396	0.47	0/541
1	AN	0.18	0/396	0.46	0/541
1	AO	0.16	0/396	0.49	0/541
1	AP	0.17	0/396	0.48	0/541
1	AQ	0.17	0/396	0.50	0/541
1	AR	0.17	0/396	0.44	0/541
1	AS	0.18	0/396	0.50	0/541
1	AT	0.17	0/396	0.48	0/541
1	AU	0.17	0/396	0.47	0/541
1	AV	0.18	0/396	0.47	0/541
1	AW	0.17	0/396	0.45	0/541
1	AX	0.17	0/396	0.51	0/541
2	BA	0.14	0/336	0.40	0/456
2	BB	0.14	0/340	0.43	0/461
2	BC	0.13	0/336	0.44	0/456
2	BD	0.14	0/340	0.42	0/461
2	BE	0.14	0/340	0.41	0/461
2	BF	0.14	0/336	0.46	0/456
2	BG	0.17	0/336	0.46	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.15	0/336	0.42	0/456
2	BI	0.14	0/340	0.43	0/461
2	BJ	0.16	0/336	0.45	0/456
2	BK	0.16	0/336	0.46	0/456
2	BL	0.15	0/336	0.42	0/456
2	BM	0.15	0/336	0.45	0/456
2	BN	0.16	0/336	0.45	0/456
2	BO	0.15	0/336	0.43	0/456
2	BP	0.17	0/336	0.45	0/456
2	BQ	0.15	0/340	0.45	0/461
2	BR	0.15	0/340	0.46	0/461
2	BS	0.14	0/340	0.41	0/461
2	BT	0.14	0/340	0.41	0/461
2	BU	0.16	0/336	0.43	0/456
2	BV	0.15	0/340	0.40	0/461
2	BW	0.14	0/340	0.45	0/461
2	BX	0.14	0/336	0.44	0/456
2	ba	0.16	0/336	0.42	0/456
2	bb	0.18	0/336	0.44	0/456
2	bc	0.15	0/336	0.42	0/456
2	bd	0.19	0/336	0.47	0/456
2	be	0.19	0/336	0.41	0/456
2	bf	0.19	0/336	0.41	0/456
2	bg	0.17	0/336	0.42	0/456
2	bh	0.19	0/336	0.50	0/456
2	bi	0.19	0/336	0.47	0/456
2	bj	0.20	0/336	0.46	0/456
2	bk	0.19	0/336	0.47	0/456
2	bl	0.22	0/336	0.52	0/456
2	bm	0.18	0/336	0.42	0/456
2	bn	0.20	0/340	0.51	0/461
2	bo	0.18	0/336	0.41	0/456
2	bp	0.18	0/336	0.45	0/456
3	C	0.22	0/2392	0.51	0/3263
4	C1	0.20	0/826	0.49	0/1128
5	C2	0.18	0/800	0.50	0/1094
6	H1	0.20	0/531	0.46	0/717
7	H2	0.19	0/1443	0.49	0/1970
8	L	0.21	0/2252	0.47	0/3081
9	M	0.23	0/2803	0.51	0/3835
10	aa	0.17	0/467	0.48	0/638
11	ab	0.17	0/467	0.49	0/638
11	ac	0.18	0/444	0.56	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	ad	0.20	0/467	0.49	0/638
11	ae	0.22	0/467	0.51	0/638
11	af	0.20	0/467	0.47	0/638
11	ag	0.20	0/467	0.46	0/638
11	ah	0.20	0/467	0.53	0/638
11	ai	0.18	0/467	0.48	0/638
11	aj	0.18	0/467	0.49	0/638
11	ak	0.21	0/547	0.51	0/748
11	al	0.19	0/467	0.53	0/638
11	am	0.20	0/467	0.48	0/638
11	an	0.20	0/467	0.46	0/638
11	ao	0.23	0/467	0.59	0/638
11	ap	0.19	0/547	0.46	0/748
All	All	0.18	0/41628	0.48	0/56738

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
1	AE	0	1
2	BF	0	1
2	bl	0	1
4	C1	0	1
5	C2	0	1
9	M	0	2
11	ac	0	1
11	ad	0	1
11	ak	0	1
11	an	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AE	3	ARG	Sidechain
2	BF	13	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	C1	166	ARG	Sidechain
5	C2	27	ARG	Sidechain
9	M	10	ARG	Sidechain
9	M	88	ARG	Sidechain
11	ac	11	ARG	Sidechain
11	ad	12	ARG	Sidechain
11	ak	11	ARG	Sidechain
11	an	37	ARG	Sidechain
2	bl	13	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	391	0	390	2	0
1	AB	391	0	390	2	0
1	AC	384	0	383	1	0
1	AD	384	0	383	1	0
1	AE	391	0	390	1	0
1	AF	391	0	390	0	0
1	AG	391	0	390	1	0
1	AH	391	0	390	3	0
1	AI	391	0	390	0	0
1	AJ	391	0	390	0	0
1	AK	391	0	390	0	0
1	AL	391	0	390	1	0
1	AM	391	0	390	2	0
1	AN	391	0	390	0	0
1	AO	391	0	390	0	0
1	AP	391	0	390	0	0
1	AQ	391	0	390	0	0
1	AR	391	0	390	1	0
1	AS	391	0	390	2	0
1	AT	391	0	390	1	0
1	AU	391	0	390	1	0
1	AV	391	0	390	1	0
1	AW	391	0	390	1	0
1	AX	391	0	390	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BA	323	0	300	1	0
2	BB	327	0	303	0	0
2	BC	323	0	300	1	0
2	BD	327	0	303	1	0
2	BE	327	0	303	0	0
2	BF	323	0	300	0	0
2	BG	323	0	300	1	0
2	BH	323	0	300	1	0
2	BI	327	0	303	0	0
2	BJ	323	0	300	0	0
2	BK	323	0	300	0	0
2	BL	323	0	300	1	0
2	BM	323	0	300	1	0
2	BN	323	0	300	0	0
2	BO	323	0	300	0	0
2	BP	323	0	300	0	0
2	BQ	327	0	303	1	0
2	BR	327	0	303	1	0
2	BS	327	0	303	2	0
2	BT	327	0	303	1	0
2	BU	323	0	300	1	0
2	BV	327	0	303	2	0
2	BW	327	0	303	0	0
2	BX	323	0	300	2	0
2	ba	323	0	300	1	0
2	bb	323	0	300	2	0
2	bc	323	0	300	2	0
2	bd	323	0	300	1	0
2	be	323	0	300	2	0
2	bf	323	0	300	1	0
2	bg	323	0	300	1	0
2	bh	323	0	300	0	0
2	bi	323	0	300	0	0
2	bj	323	0	300	0	0
2	bk	323	0	300	1	0
2	bl	323	0	300	0	0
2	bm	323	0	300	0	0
2	bn	327	0	303	1	0
2	bo	323	0	300	0	0
2	bp	323	0	300	2	0
3	C	2325	0	2245	5	0
4	C1	806	0	818	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C2	779	0	765	2	0
6	H1	522	0	503	2	0
7	H2	1404	0	1369	1	0
8	L	2165	0	2126	4	0
9	M	2702	0	2632	9	0
10	aa	455	0	464	1	0
11	ab	465	0	475	2	0
11	ac	443	0	453	4	0
11	ad	465	0	475	3	0
11	ae	465	0	475	6	0
11	af	465	0	475	0	0
11	ag	465	0	475	2	0
11	ah	465	0	475	0	0
11	ai	465	0	475	0	0
11	aj	465	0	475	0	0
11	ak	542	0	553	4	0
11	al	465	0	475	0	0
11	am	465	0	475	1	0
11	an	465	0	475	1	0
11	ao	465	0	475	1	0
11	ap	542	0	553	3	0
12	CG	21	0	18	0	0
12	MG	21	0	18	0	0
13	AA	132	0	148	3	0
13	AB	132	0	148	2	0
13	AC	132	0	148	4	0
13	AD	132	0	148	2	0
13	AE	198	0	222	2	0
13	AF	66	0	74	1	0
13	AG	132	0	148	1	0
13	AH	198	0	222	4	0
13	AI	66	0	74	3	0
13	AJ	132	0	148	1	0
13	AK	132	0	148	3	0
13	AL	132	0	148	1	0
13	AM	132	0	148	1	0
13	AN	132	0	148	3	0
13	AO	132	0	148	2	0
13	AP	132	0	148	1	0
13	AQ	198	0	222	2	0
13	AR	66	0	74	1	0
13	AS	132	0	148	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AT	132	0	148	5	0
13	AU	132	0	148	2	0
13	AV	132	0	148	1	0
13	AW	132	0	148	2	0
13	AX	132	0	148	2	0
13	BA	66	0	74	0	0
13	BB	66	0	74	0	0
13	BC	66	0	74	1	0
13	BD	66	0	74	0	0
13	BE	66	0	74	0	0
13	BF	66	0	74	0	0
13	BG	66	0	74	0	0
13	BH	66	0	74	1	0
13	BI	66	0	74	0	0
13	BJ	66	0	74	0	0
13	BK	66	0	74	0	0
13	BL	66	0	74	0	0
13	BM	66	0	74	0	0
13	BN	66	0	74	0	0
13	BO	66	0	74	0	0
13	BP	66	0	74	0	0
13	BQ	66	0	74	0	0
13	BR	66	0	74	0	0
13	BS	66	0	74	1	0
13	BT	66	0	74	0	0
13	BU	66	0	74	0	0
13	BV	66	0	74	0	0
13	BW	66	0	74	0	0
13	BX	66	0	74	0	0
13	L	132	0	148	2	0
13	M	132	0	148	4	0
13	aa	66	0	74	3	0
13	ab	66	0	74	3	0
13	ac	66	0	74	0	0
13	ad	66	0	74	1	0
13	ae	66	0	74	0	0
13	af	66	0	74	1	0
13	ag	66	0	74	0	0
13	ah	66	0	74	0	0
13	ai	66	0	74	0	0
13	aj	66	0	74	1	0
13	ak	66	0	74	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	al	66	0	74	0	0
13	am	66	0	74	1	0
13	an	66	0	74	0	0
13	ao	66	0	74	1	0
13	ap	66	0	74	1	0
13	ba	66	0	74	0	0
13	bb	66	0	74	0	0
13	bc	66	0	74	1	0
13	bd	66	0	74	2	0
13	be	66	0	74	1	0
13	bf	66	0	74	0	0
13	bg	66	0	74	1	0
13	bh	66	0	74	0	0
13	bi	66	0	74	0	0
13	bj	66	0	74	0	0
13	bk	66	0	74	1	0
13	bl	66	0	74	0	0
13	bm	66	0	74	2	0
13	bn	66	0	74	1	0
13	bo	66	0	74	1	0
13	bp	66	0	74	0	0
14	AA	35	0	44	0	0
14	AB	35	0	45	1	0
14	AC	35	0	46	0	0
14	AD	35	0	45	0	0
14	AE	105	0	135	1	0
14	AG	35	0	44	0	0
14	AH	70	0	91	1	0
14	AJ	70	0	89	0	0
14	AK	70	0	91	2	0
14	AL	35	0	46	0	0
14	AM	35	0	45	0	0
14	AN	70	0	90	1	0
14	AP	35	0	46	0	0
14	AQ	35	0	46	0	0
14	AS	35	0	44	0	0
14	AT	70	0	91	0	0
14	AU	35	0	45	1	0
14	AV	70	0	90	1	0
14	AX	35	0	45	0	0
14	BA	35	0	46	0	0
14	BB	140	0	182	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	BC	105	0	137	0	0
14	BD	140	0	182	0	0
14	BE	105	0	136	0	0
14	BF	70	0	91	0	0
14	BG	105	0	136	1	0
14	BH	105	0	135	0	0
14	BI	105	0	137	0	0
14	BJ	140	0	180	0	0
14	BK	105	0	136	0	0
14	BL	70	0	91	0	0
14	BM	105	0	137	0	0
14	BN	105	0	137	0	0
14	BO	105	0	137	0	0
14	BP	140	0	181	0	0
14	BQ	70	0	90	0	0
14	BR	140	0	181	0	0
14	BS	105	0	135	1	0
14	BT	105	0	137	0	0
14	BU	70	0	91	0	0
14	BV	105	0	138	0	0
14	BW	140	0	180	1	0
14	BX	105	0	135	0	0
14	C	35	0	45	0	0
14	C2	35	0	46	1	0
14	H2	35	0	46	0	0
14	L	175	0	226	1	0
14	ac	35	0	45	0	0
14	bc	35	0	45	1	0
14	be	70	0	89	0	0
14	bf	35	0	45	0	0
14	bg	35	0	45	0	0
14	bh	35	0	45	0	0
14	bi	35	0	45	0	0
14	bj	35	0	45	0	0
14	bk	35	0	45	0	0
14	bl	35	0	46	0	0
14	bm	35	0	44	0	0
14	bn	35	0	45	0	0
14	bo	35	0	45	0	0
14	bp	70	0	92	0	0
15	AA	45	0	0	1	0
15	AD	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AM	45	0	0	0	0
15	AS	45	0	0	0	0
15	AW	45	0	0	1	0
15	BA	45	0	0	0	0
15	BD	45	0	0	0	0
15	BE	45	0	0	0	0
15	BF	45	0	0	0	0
15	BG	45	0	0	0	0
15	BH	45	0	0	0	0
15	BI	45	0	0	0	0
15	BJ	45	0	0	0	0
15	BK	45	0	0	0	0
15	BM	45	0	0	0	0
15	BN	45	0	0	0	0
15	BO	45	0	0	0	0
15	BP	45	0	0	0	0
15	BQ	45	0	0	0	0
15	BR	45	0	0	0	0
15	BS	45	0	0	1	0
15	BU	45	0	0	0	0
15	BV	45	0	0	0	0
15	BW	45	0	0	0	0
15	ag	45	0	0	0	0
15	ba	45	0	0	0	0
15	bb	45	0	0	0	0
15	bc	45	0	0	0	0
15	bd	45	0	0	0	0
15	be	45	0	0	0	0
15	bg	45	0	0	0	0
15	bh	45	0	0	0	0
15	bi	45	0	0	0	0
15	bj	45	0	0	0	0
15	bk	45	0	0	0	0
15	bl	45	0	0	0	0
15	bm	45	0	0	0	0
15	bn	45	0	0	0	0
15	bo	45	0	0	0	0
15	bp	45	0	0	0	0
16	AQ	45	0	0	0	0
16	H1	45	0	0	0	0
16	L	45	0	0	0	0
16	M	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	ab	45	0	0	0	0
16	ad	45	0	0	0	0
16	bb	45	0	0	0	0
16	bd	45	0	0	0	0
16	be	45	0	0	0	0
16	bf	45	0	0	0	0
16	bg	45	0	0	0	0
16	bh	45	0	0	0	0
16	bi	45	0	0	0	0
16	bj	45	0	0	0	0
16	bk	45	0	0	0	0
16	bl	45	0	0	0	0
16	bm	45	0	0	1	0
16	bn	45	0	0	0	0
16	bo	45	0	0	0	0
16	bp	45	0	0	0	0
17	C	172	0	120	6	0
18	C	18	0	0	0	0
18	M	18	0	0	0	0
19	C	14	0	12	0	0
19	C1	14	0	12	0	0
20	H1	51	0	76	1	0
21	H1	84	0	124	1	0
21	M	168	0	248	0	0
21	ad	84	0	124	1	0
21	af	168	0	248	2	0
22	L	65	0	76	1	0
22	M	65	0	76	3	0
23	L	53	0	72	2	0
23	M	53	0	72	1	0
23	ao	53	0	72	0	0
24	M	1	0	0	0	0
25	M	44	0	60	4	0
26	af	58	0	0	0	0
26	ag	58	0	0	0	0
27	ai	55	0	0	1	0
28	AA	2	0	0	0	0
28	AC	1	0	0	0	0
28	AD	2	0	0	0	0
28	AE	2	0	0	0	0
28	AG	3	0	0	0	0
28	AH	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AI	1	0	0	0	0
28	AJ	5	0	0	0	0
28	AK	3	0	0	0	0
28	AL	2	0	0	0	0
28	AM	3	0	0	0	0
28	AN	2	0	0	0	0
28	AO	1	0	0	0	0
28	AP	3	0	0	0	0
28	AQ	5	0	0	0	0
28	AR	3	0	0	0	0
28	AS	4	0	0	0	0
28	AT	4	0	0	0	0
28	AV	2	0	0	0	0
28	AW	3	0	0	0	0
28	AX	1	0	0	0	0
28	BJ	1	0	0	0	0
28	C	67	0	0	0	0
28	C1	36	0	0	0	0
28	C2	1	0	0	0	0
28	H1	4	0	0	0	0
28	H2	27	0	0	0	0
28	L	48	0	0	0	0
28	M	63	0	0	0	0
28	aa	4	0	0	0	0
28	ab	2	0	0	0	0
28	ac	1	0	0	0	0
28	ad	7	0	0	0	0
28	ae	9	0	0	0	0
28	af	14	0	0	0	0
28	ag	4	0	0	0	0
28	ah	3	0	0	0	0
28	ai	3	0	0	0	0
28	aj	2	0	0	0	0
28	ak	6	0	0	0	0
28	al	6	0	0	0	0
28	am	5	0	0	0	0
28	an	7	0	0	0	0
28	ao	2	0	0	0	0
28	ap	3	0	0	0	0
28	bb	2	0	0	0	0
28	bc	1	0	0	0	0
28	bd	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	be	2	0	0	0	0
28	bf	3	0	0	0	0
28	bg	3	0	0	0	0
28	bh	2	0	0	0	0
28	bi	2	0	0	0	0
28	bj	1	0	0	0	0
28	bk	2	0	0	0	0
28	bl	1	0	0	0	0
28	bm	3	0	0	0	0
28	bn	2	0	0	0	0
28	bo	1	0	0	0	0
28	bp	1	0	0	0	0
All	All	56476	0	54550	157	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:407:BPH:HBB3	22:M:407:BPH:HHC	1.80	0.64
13:L:308:BCL:HBB2	13:L:308:BCL:HHC	1.85	0.59
16:bm:104:OV9:O1P	16:bm:104:OV9:N	2.36	0.58
13:AE:105:BCL:H41	2:bd:24:LEU:HD11	1.84	0.58
13:AU:103:BCL:H41	2:bn:24:LEU:HD21	1.86	0.57
23:L:303:MQ8:H142	11:ac:23:VAL:HB	1.87	0.57
9:M:66:ILE:HG13	11:ak:23:VAL:HG11	1.86	0.57
22:M:407:BPH:HHD	22:M:407:BPH:HBC3	1.86	0.57
13:M:406:BCL:HBB2	13:M:406:BCL:HHC	1.86	0.56
13:bm:102:BCL:H72	13:bm:102:BCL:H41	1.88	0.55
5:C2:3:ASP:CG	5:C2:27:ARG:HH22	2.15	0.55
14:C2:1001:LMT:H32	11:ap:15:VAL:HG13	1.89	0.55
2:BQ:7:MET:HE1	2:BQ:15:PHE:HB2	1.89	0.54
11:ap:37:ARG:NH1	2:bp:42:PRO:O	2.39	0.54
11:ae:12:ARG:HH21	21:af:102:CD4:H55	1.73	0.54
13:AN:103:BCL:HHC	13:AN:103:BCL:HBB3	1.91	0.51
17:C:1003:HEC:HBC3	17:C:1003:HEC:HMC1	1.91	0.51
13:BS:1004:BCL:H93	13:BS:1004:BCL:H51	1.93	0.51
13:AI:101:BCL:HMA2	13:BH:1005:BCL:H92	1.92	0.51
14:BS:1002:LMT:H4'	14:BS:1003:LMT:H2'	1.92	0.51
5:C2:86:ARG:HG3	5:C2:92:ALA:HB1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:ag:5:TRP:CZ2	2:bg:19:MET:HG2	2.46	0.50
17:C:1002:HEC:HBC3	17:C:1002:HEC:HMC1	1.94	0.50
21:ad:101:CD4:O13	11:ae:12:ARG:NH1	2.45	0.50
8:L:171:PRO:HB2	14:L:307:LMT:H71	1.94	0.50
13:AD:104:BCL:H3A	13:AD:104:BCL:CGA	2.43	0.49
1:AH:8:THR:HG21	1:AH:13:ILE:HD11	1.94	0.49
4:C1:101:TRP:CZ2	11:ad:58:PRO:HA	2.48	0.49
13:AS:102:BCL:HHC	13:AS:102:BCL:CBB	2.44	0.48
13:AW:101:BCL:HHC	13:AW:101:BCL:HBB3	1.96	0.48
1:AM:8:THR:HA	14:AN:101:LMT:H6E	1.96	0.48
1:AX:2:HIS:CD2	2:BX:13:ARG:HD2	2.49	0.48
13:AC:101:BCL:HBC3	13:AC:101:BCL:HHB	1.95	0.48
3:C:47:LEU:HB2	3:C:48:PRO:HD3	1.96	0.48
13:AQ:104:BCL:H41	13:AQ:104:BCL:H71	1.96	0.48
4:C1:180:ASP:CG	9:M:88:ARG:HH22	2.21	0.47
3:C:247:ASP:OD1	3:C:251:ASN:ND2	2.48	0.47
11:am:29:HIS:CE1	13:bm:102:BCL:HMD3	2.49	0.47
1:AW:3:ARG:HE	15:AW:103:V7N:C40	2.27	0.47
14:AK:101:LMT:H31	13:AK:102:BCL:HBB1	1.97	0.47
3:C:117:THR:HG23	17:C:1001:HEC:HMA3	1.96	0.47
11:ap:5:TRP:CZ2	2:bp:19:MET:HG3	2.50	0.47
13:AI:101:BCL:H61	13:AI:101:BCL:H41	1.81	0.46
13:AT:103:BCL:H141	2:BS:19:MET:HE2	1.96	0.46
9:M:94:ALA:HB2	9:M:180:PRO:HG2	1.96	0.46
13:aa:1001:BCL:HHC	13:aa:1001:BCL:HBB3	1.97	0.46
2:BV:44:PHE:CD2	14:BW:1002:LMT:H32	2.50	0.46
11:ab:5:TRP:CZ2	2:bb:19:MET:HG2	2.50	0.46
14:AK:101:LMT:C3	13:AK:102:BCL:HBB1	2.46	0.46
7:H2:9:ASP:OD1	7:H2:14:SER:OG	2.29	0.46
1:AH:20:PHE:HB2	13:AH:105:BCL:H42	1.97	0.45
11:ac:29:HIS:CE1	13:bc:103:BCL:HMD1	2.51	0.45
13:AA:1001:BCL:H191	2:ba:36:LEU:HD11	1.98	0.45
1:AR:36:PHE:O	2:BR:41:ARG:NH1	2.50	0.45
13:AV:101:BCL:HHC	13:AV:101:BCL:CBB	2.47	0.45
6:H1:47:TRP:CH2	21:H1:103:CD4:H109	2.52	0.45
11:an:29:HIS:CE1	13:bn:102:BCL:HMD3	2.52	0.45
13:AH:105:BCL:H41	2:bf:24:LEU:HD21	1.98	0.44
13:AC:102:BCL:H143	2:bb:31:SER:HB2	1.98	0.44
6:H1:12:LEU:HD23	20:H1:101:PGW:H01	1.99	0.44
22:L:301:BPH:CBB	22:L:301:BPH:HHC	2.48	0.44
1:AA:4:ILE:HD11	1:AB:14:MET:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AA:1002:BCL:H92	1:AX:13:ILE:HG23	1.99	0.44
13:AT:103:BCL:H141	13:AT:103:BCL:H162	1.82	0.44
11:ak:29:HIS:CE1	13:bk:103:BCL:HMD3	2.52	0.44
13:AB:1001:BCL:HHC	13:AB:1001:BCL:OBB	2.18	0.44
13:AU:101:BCL:HHC	13:AU:101:BCL:CBB	2.48	0.44
13:AN:103:BCL:HHC	13:AN:103:BCL:CBB	2.48	0.44
8:L:128:TYR:CD1	13:L:308:BCL:HBB1	2.53	0.44
11:ad:4:ILE:HG13	13:bd:102:BCL:H201	2.00	0.44
13:AQ:103:BCL:CBB	13:AQ:103:BCL:HHC	2.48	0.44
17:C:1004:HEC:HMC1	17:C:1004:HEC:HBC3	1.99	0.44
1:AA:36:PHE:O	2:BA:41:ARG:NH1	2.51	0.43
9:M:255:MET:CE	23:M:402:MQ8:H142	2.47	0.43
13:AO:102:BCL:HHC	13:AO:102:BCL:CBB	2.48	0.43
13:AX:102:BCL:HHC	13:AX:102:BCL:CBB	2.48	0.43
23:L:303:MQ8:H242	11:ac:23:VAL:HG13	1.99	0.43
1:AX:36:PHE:O	2:BX:41:ARG:NH1	2.52	0.43
11:ae:5:TRP:CZ2	2:be:19:MET:HG2	2.53	0.43
11:ag:29:HIS:CE1	13:bg:104:BCL:HMD3	2.53	0.43
25:M:404:CRT:H243	13:M:406:BCL:HBB2	2.01	0.43
13:AA:1001:BCL:CBB	13:AA:1001:BCL:HHC	2.48	0.43
1:AE:11:HIS:CG	14:AE:102:LMT:H6'2	2.54	0.43
13:AJ:104:BCL:HHC	13:AJ:104:BCL:CBB	2.49	0.43
14:AU:102:LMT:H6E	14:AU:102:LMT:H5B	2.01	0.43
13:AL:102:BCL:HHC	13:AL:102:BCL:CBB	2.48	0.43
3:C:53:PRO:O	3:C:80:ARG:NH1	2.47	0.43
11:ae:12:ARG:NH2	21:af:102:CD4:H55	2.33	0.43
13:AR:101:BCL:HHC	13:AR:101:BCL:CBB	2.49	0.42
1:AT:36:PHE:O	2:BT:41:ARG:NH1	2.51	0.42
8:L:231:ARG:HH22	9:M:9:THR:HG23	1.83	0.42
13:AE:104:BCL:HHC	13:AE:104:BCL:CBB	2.48	0.42
13:aj:101:BCL:OBB	13:aj:101:BCL:HHC	2.20	0.42
11:ak:5:TRP:CZ2	2:bk:19:MET:HG2	2.54	0.42
1:AS:36:PHE:O	2:BS:41:ARG:NH1	2.49	0.42
17:C:1001:HEC:HMC1	17:C:1001:HEC:HBC3	2.02	0.42
11:ab:40:TRP:HE1	13:ab:1001:BCL:HBB3	1.85	0.42
13:AP:102:BCL:HHC	13:AP:102:BCL:CBB	2.50	0.42
13:AT:101:BCL:HHC	13:AT:101:BCL:CBB	2.49	0.42
13:aa:1001:BCL:HHC	13:aa:1001:BCL:CBB	2.50	0.42
11:ae:37:ARG:NH1	2:be:42:PRO:O	2.52	0.42
14:AV:102:LMT:H5B	14:AV:102:LMT:H6E	2.01	0.42
11:ac:5:TRP:CZ2	2:bc:19:MET:HG2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AC:102:BCL:CBB	13:AC:102:BCL:HHC	2.50	0.42
13:AH:102:BCL:OBB	13:AH:102:BCL:HHC	2.20	0.42
13:AI:101:BCL:HHC	13:AI:101:BCL:CBB	2.49	0.42
1:AL:36:PHE:O	2:BL:41:ARG:NH1	2.53	0.42
13:AM:1004:BCL:HHC	13:AM:1004:BCL:CBB	2.49	0.42
13:ab:1001:BCL:HHC	13:ab:1001:BCL:CBB	2.49	0.42
13:AG:103:BCL:HHC	13:AG:103:BCL:CBB	2.50	0.42
13:ak:1001:BCL:OBB	13:ak:1001:BCL:HHC	2.19	0.42
13:AD:103:BCL:HHC	13:AD:103:BCL:OBB	2.19	0.41
1:AU:36:PHE:O	2:BU:41:ARG:NH1	2.52	0.41
9:M:313:THR:H	9:M:316:GLN:HE21	1.67	0.41
10:aa:40:TRP:HE1	13:aa:1001:BCL:HBB3	1.85	0.41
13:af:103:BCL:HHC	13:af:103:BCL:OBB	2.20	0.41
1:AB:33:TYR:HD2	14:AB:1003:LMT:H2'	1.84	0.41
13:M:406:BCL:HBB3	13:M:408:BCL:H62	2.01	0.41
11:ad:29:HIS:CE1	13:bd:102:BCL:HMD3	2.55	0.41
13:AH:103:BCL:CBB	13:AH:103:BCL:HHC	2.49	0.41
1:AS:32:ALA:HB1	13:AS:102:BCL:HBC1	2.01	0.41
27:ai:102:UYH:O2	27:ai:102:UYH:O9	2.38	0.41
11:ao:29:HIS:CE1	13:bo:102:BCL:HMD3	2.55	0.41
1:AC:36:PHE:O	2:BC:41:ARG:NH1	2.53	0.41
13:AT:101:BCL:HMB2	15:BS:1001:V7N:C4	2.51	0.41
13:AT:103:BCL:OBB	13:AT:103:BCL:HHC	2.20	0.41
1:AX:1:FME:SD	1:AX:1:FME:N	2.86	0.41
3:C:202:TYR:CD1	17:C:1003:HEC:HMB2	2.54	0.41
13:AX:102:BCL:H42	13:AX:103:BCL:HBA2	2.01	0.41
8:L:181:PHE:HB3	22:M:407:BPH:HBB2	2.02	0.41
25:M:404:CRT:H26	25:M:404:CRT:H241	1.83	0.41
13:am:1001:BCL:OBB	13:am:1001:BCL:HHC	2.20	0.41
13:AK:104:BCL:HHC	13:AK:104:BCL:CBB	2.50	0.41
13:AN:104:BCL:H143	13:AN:104:BCL:H161	1.94	0.41
9:M:201:HIS:CE1	9:M:205:ILE:HD11	2.55	0.41
13:ap:1001:BCL:OBB	13:ap:1001:BCL:HHC	2.20	0.41
13:BC:104:BCL:HHC	13:BC:104:BCL:OBB	2.20	0.41
2:BG:7:MET:HG3	2:BG:11:GLU:HB2	2.02	0.41
14:BG:1003:LMT:H4'	14:BG:1005:LMT:H2'	2.01	0.41
13:ab:1001:BCL:HBB3	13:ab:1001:BCL:HHC	2.01	0.41
11:ae:29:HIS:CE1	13:be:103:BCL:HMD3	2.55	0.41
1:AD:36:PHE:O	2:BD:41:ARG:NH1	2.53	0.41
1:AH:36:PHE:O	2:BH:41:ARG:NH1	2.52	0.41
9:M:62:ILE:HG22	11:ak:23:VAL:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:157:TYR:CZ	25:M:404:CRT:H293	2.56	0.41
13:AO:101:BCL:OBB	13:AO:101:BCL:HHC	2.21	0.40
13:ad:102:BCL:OBB	13:ad:102:BCL:HHC	2.22	0.40
15:AA:1004:V7N:C4	13:AC:102:BCL:HMB2	2.52	0.40
1:AG:8:THR:HA	14:AH:101:LMT:H4B	2.02	0.40
1:AV:36:PHE:O	2:BV:41:ARG:NH1	2.53	0.40
2:bc:21:THR:HG21	14:bc:102:LMT:H11	2.03	0.40
13:AW:101:BCL:HHC	13:AW:101:BCL:CBB	2.51	0.40
13:ao:102:BCL:H62	13:ao:102:BCL:H41	1.89	0.40
13:AB:1002:BCL:HHC	13:AB:1002:BCL:OBB	2.21	0.40
13:AF:1001:BCL:CBB	13:AF:1001:BCL:HHC	2.51	0.40
1:AM:5:TRP:HB3	2:BM:7:MET:HE3	2.03	0.40
25:M:404:CRT:H243	13:M:406:BCL:CBB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	47/54 (87%)	47 (100%)	0	0	100	100
1	AB	47/54 (87%)	47 (100%)	0	0	100	100
1	AC	46/54 (85%)	46 (100%)	0	0	100	100
1	AD	46/54 (85%)	46 (100%)	0	0	100	100
1	AE	47/54 (87%)	47 (100%)	0	0	100	100
1	AF	47/54 (87%)	47 (100%)	0	0	100	100
1	AG	47/54 (87%)	47 (100%)	0	0	100	100
1	AH	47/54 (87%)	47 (100%)	0	0	100	100
1	AI	47/54 (87%)	47 (100%)	0	0	100	100
1	AJ	47/54 (87%)	46 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	47/54 (87%)	47 (100%)	0	0	100	100
1	AL	47/54 (87%)	47 (100%)	0	0	100	100
1	AM	47/54 (87%)	47 (100%)	0	0	100	100
1	AN	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AO	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AP	47/54 (87%)	47 (100%)	0	0	100	100
1	AQ	47/54 (87%)	47 (100%)	0	0	100	100
1	AR	47/54 (87%)	47 (100%)	0	0	100	100
1	AS	47/54 (87%)	47 (100%)	0	0	100	100
1	AT	47/54 (87%)	47 (100%)	0	0	100	100
1	AU	47/54 (87%)	47 (100%)	0	0	100	100
1	AV	47/54 (87%)	47 (100%)	0	0	100	100
1	AW	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AX	47/54 (87%)	47 (100%)	0	0	100	100
2	BA	37/44 (84%)	37 (100%)	0	0	100	100
2	BB	38/44 (86%)	38 (100%)	0	0	100	100
2	BC	37/44 (84%)	37 (100%)	0	0	100	100
2	BD	38/44 (86%)	38 (100%)	0	0	100	100
2	BE	38/44 (86%)	38 (100%)	0	0	100	100
2	BF	37/44 (84%)	37 (100%)	0	0	100	100
2	BG	37/44 (84%)	37 (100%)	0	0	100	100
2	BH	37/44 (84%)	37 (100%)	0	0	100	100
2	BI	38/44 (86%)	38 (100%)	0	0	100	100
2	BJ	37/44 (84%)	37 (100%)	0	0	100	100
2	BK	37/44 (84%)	37 (100%)	0	0	100	100
2	BL	37/44 (84%)	37 (100%)	0	0	100	100
2	BM	37/44 (84%)	37 (100%)	0	0	100	100
2	BN	37/44 (84%)	37 (100%)	0	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	37/44 (84%)	37 (100%)	0	0	100	100
2	BQ	38/44 (86%)	38 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BR	38/44 (86%)	38 (100%)	0	0	100	100
2	BS	38/44 (86%)	38 (100%)	0	0	100	100
2	BT	38/44 (86%)	38 (100%)	0	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
2	BW	38/44 (86%)	38 (100%)	0	0	100	100
2	BX	37/44 (84%)	37 (100%)	0	0	100	100
2	ba	37/44 (84%)	37 (100%)	0	0	100	100
2	bb	37/44 (84%)	37 (100%)	0	0	100	100
2	bc	37/44 (84%)	37 (100%)	0	0	100	100
2	bd	37/44 (84%)	37 (100%)	0	0	100	100
2	be	37/44 (84%)	37 (100%)	0	0	100	100
2	bf	37/44 (84%)	37 (100%)	0	0	100	100
2	bg	37/44 (84%)	37 (100%)	0	0	100	100
2	bh	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bi	37/44 (84%)	37 (100%)	0	0	100	100
2	bj	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bk	37/44 (84%)	37 (100%)	0	0	100	100
2	bl	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bm	37/44 (84%)	37 (100%)	0	0	100	100
2	bn	38/44 (86%)	38 (100%)	0	0	100	100
2	bo	37/44 (84%)	37 (100%)	0	0	100	100
2	bp	37/44 (84%)	37 (100%)	0	0	100	100
3	C	297/354 (84%)	286 (96%)	11 (4%)	0	100	100
4	C1	101/202 (50%)	99 (98%)	2 (2%)	0	100	100
5	C2	99/125 (79%)	98 (99%)	1 (1%)	0	100	100
6	H1	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
7	H2	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
8	L	271/274 (99%)	264 (97%)	6 (2%)	1 (0%)	30	46
9	M	334/367 (91%)	325 (97%)	9 (3%)	0	100	100
10	aa	57/71 (80%)	56 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	ab	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ac	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
11	ad	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ae	58/71 (82%)	58 (100%)	0	0	100	100
11	af	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ag	58/71 (82%)	58 (100%)	0	0	100	100
11	ah	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	ai	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	aj	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	ak	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
11	al	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	an	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ap	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
All	All	4902/5762 (85%)	4834 (99%)	67 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	31	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	38/41 (93%)	38 (100%)	0	100	100
1	AB	38/41 (93%)	38 (100%)	0	100	100
1	AC	37/41 (90%)	37 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	37/41 (90%)	37 (100%)	0	100	100
1	AE	38/41 (93%)	38 (100%)	0	100	100
1	AF	38/41 (93%)	38 (100%)	0	100	100
1	AG	38/41 (93%)	38 (100%)	0	100	100
1	AH	38/41 (93%)	37 (97%)	1 (3%)	40	65
1	AI	38/41 (93%)	38 (100%)	0	100	100
1	AJ	38/41 (93%)	38 (100%)	0	100	100
1	AK	38/41 (93%)	38 (100%)	0	100	100
1	AL	38/41 (93%)	38 (100%)	0	100	100
1	AM	38/41 (93%)	38 (100%)	0	100	100
1	AN	38/41 (93%)	38 (100%)	0	100	100
1	AO	38/41 (93%)	38 (100%)	0	100	100
1	AP	38/41 (93%)	38 (100%)	0	100	100
1	AQ	38/41 (93%)	38 (100%)	0	100	100
1	AR	38/41 (93%)	38 (100%)	0	100	100
1	AS	38/41 (93%)	38 (100%)	0	100	100
1	AT	38/41 (93%)	38 (100%)	0	100	100
1	AU	38/41 (93%)	38 (100%)	0	100	100
1	AV	38/41 (93%)	38 (100%)	0	100	100
1	AW	38/41 (93%)	38 (100%)	0	100	100
1	AX	38/41 (93%)	38 (100%)	0	100	100
2	BA	31/35 (89%)	31 (100%)	0	100	100
2	BB	31/35 (89%)	31 (100%)	0	100	100
2	BC	31/35 (89%)	31 (100%)	0	100	100
2	BD	31/35 (89%)	31 (100%)	0	100	100
2	BE	31/35 (89%)	30 (97%)	1 (3%)	34	58
2	BF	31/35 (89%)	31 (100%)	0	100	100
2	BG	31/35 (89%)	31 (100%)	0	100	100
2	BH	31/35 (89%)	31 (100%)	0	100	100
2	BI	31/35 (89%)	31 (100%)	0	100	100
2	BJ	31/35 (89%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BK	31/35 (89%)	31 (100%)	0	100	100
2	BL	31/35 (89%)	31 (100%)	0	100	100
2	BM	31/35 (89%)	31 (100%)	0	100	100
2	BN	31/35 (89%)	31 (100%)	0	100	100
2	BO	31/35 (89%)	31 (100%)	0	100	100
2	BP	31/35 (89%)	31 (100%)	0	100	100
2	BQ	31/35 (89%)	31 (100%)	0	100	100
2	BR	31/35 (89%)	31 (100%)	0	100	100
2	BS	31/35 (89%)	31 (100%)	0	100	100
2	BT	31/35 (89%)	31 (100%)	0	100	100
2	BU	31/35 (89%)	31 (100%)	0	100	100
2	BV	31/35 (89%)	31 (100%)	0	100	100
2	BW	31/35 (89%)	31 (100%)	0	100	100
2	BX	31/35 (89%)	31 (100%)	0	100	100
2	ba	31/35 (89%)	31 (100%)	0	100	100
2	bb	31/35 (89%)	31 (100%)	0	100	100
2	bc	31/35 (89%)	31 (100%)	0	100	100
2	bd	31/35 (89%)	31 (100%)	0	100	100
2	be	31/35 (89%)	31 (100%)	0	100	100
2	bf	31/35 (89%)	31 (100%)	0	100	100
2	bg	31/35 (89%)	31 (100%)	0	100	100
2	bh	31/35 (89%)	31 (100%)	0	100	100
2	bi	31/35 (89%)	31 (100%)	0	100	100
2	bj	31/35 (89%)	31 (100%)	0	100	100
2	bk	31/35 (89%)	31 (100%)	0	100	100
2	bl	31/35 (89%)	31 (100%)	0	100	100
2	bm	31/35 (89%)	31 (100%)	0	100	100
2	bn	31/35 (89%)	31 (100%)	0	100	100
2	bo	31/35 (89%)	31 (100%)	0	100	100
2	bp	31/35 (89%)	31 (100%)	0	100	100
3	C	245/285 (86%)	244 (100%)	1 (0%)	84	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C1	88/156 (56%)	88 (100%)	0	100	100
5	C2	72/95 (76%)	72 (100%)	0	100	100
6	H1	50/53 (94%)	50 (100%)	0	100	100
7	H2	150/151 (99%)	148 (99%)	2 (1%)	61	80
8	L	215/216 (100%)	214 (100%)	1 (0%)	81	91
9	M	274/299 (92%)	271 (99%)	3 (1%)	65	83
10	aa	46/55 (84%)	46 (100%)	0	100	100
11	ab	46/54 (85%)	46 (100%)	0	100	100
11	ac	45/54 (83%)	45 (100%)	0	100	100
11	ad	46/54 (85%)	46 (100%)	0	100	100
11	ae	46/54 (85%)	45 (98%)	1 (2%)	45	70
11	af	46/54 (85%)	46 (100%)	0	100	100
11	ag	46/54 (85%)	46 (100%)	0	100	100
11	ah	46/54 (85%)	46 (100%)	0	100	100
11	ai	46/54 (85%)	46 (100%)	0	100	100
11	aj	46/54 (85%)	46 (100%)	0	100	100
11	ak	54/54 (100%)	54 (100%)	0	100	100
11	al	46/54 (85%)	46 (100%)	0	100	100
11	am	46/54 (85%)	46 (100%)	0	100	100
11	an	46/54 (85%)	45 (98%)	1 (2%)	45	70
11	ao	46/54 (85%)	46 (100%)	0	100	100
11	ap	54/54 (100%)	54 (100%)	0	100	100
All	All	3995/4504 (89%)	3984 (100%)	11 (0%)	84	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AH	8	THR
2	BE	11	GLU
3	C	164	SER
7	H2	159	ASP
7	H2	180	ILE
8	L	247	CYS
9	M	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	M	215	PHE
9	M	291	ASP
11	ae	39	SER
11	an	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	35	GLN
1	AE	11	HIS
1	AE	35	GLN
1	AE	37	ASN
1	AI	35	GLN
1	AK	35	GLN
1	AN	35	GLN
1	AR	29	HIS
1	AT	35	GLN
3	C	44	GLN
3	C	68	GLN
3	C	157	ASN
3	C	183	GLN
3	C	189	ASN
5	C2	24	HIS
8	L	104	GLN
8	L	213	ASN
9	M	110	ASN
9	M	311	GLN
9	M	316	GLN
11	ad	36	GLN
11	ai	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 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	$\# Z > 2$
11	FME	ac	1	11	8,9,10	0.94	0	8,9,11	0.97	1 (12%)
11	FME	ap	1	11	8,9,10	0.98	0	8,9,11	1.10	1 (12%)
1	FME	AW	1	1	8,9,10	0.99	0	8,9,11	0.87	0
1	FME	AC	1	1	8,9,10	0.98	0	8,9,11	0.87	0
1	FME	AR	1	1	8,9,10	0.98	0	8,9,11	0.95	1 (12%)
1	FME	AD	1	1	8,9,10	0.95	0	8,9,11	1.18	1 (12%)
11	FME	aj	1	11	8,9,10	0.96	0	8,9,11	0.92	1 (12%)
1	FME	AX	1	1	8,9,10	0.96	0	8,9,11	0.84	0
11	FME	ae	1	11	8,9,10	0.94	0	8,9,11	1.01	1 (12%)
1	FME	AJ	1	1	8,9,10	0.95	0	8,9,11	1.12	1 (12%)
1	FME	AB	1	1	8,9,10	0.93	0	8,9,11	1.30	1 (12%)
11	FME	an	1	11	8,9,10	0.94	0	8,9,11	1.13	1 (12%)
1	FME	AM	1	1	8,9,10	0.98	0	8,9,11	0.93	0
1	FME	AI	1	1	8,9,10	0.98	0	8,9,11	0.81	0
1	FME	AH	1	1	8,9,10	0.99	0	8,9,11	0.95	1 (12%)
11	FME	ad	1	11	8,9,10	0.97	0	8,9,11	0.87	0
11	FME	ab	1	11	8,9,10	0.91	0	8,9,11	1.65	1 (12%)
11	FME	ag	1	11	8,9,10	0.95	0	8,9,11	1.02	1 (12%)
1	FME	AL	1	1	8,9,10	0.96	0	8,9,11	1.03	1 (12%)
11	FME	al	1	11	8,9,10	0.98	0	8,9,11	0.82	0
1	FME	AA	1	1	8,9,10	0.96	0	8,9,11	0.97	1 (12%)
11	FME	ak	1	11	8,9,10	0.99	0	8,9,11	1.06	1 (12%)
1	FME	AF	1	1	8,9,10	0.97	0	8,9,11	0.90	0
6	FME	H1	1	6	8,9,10	0.99	0	8,9,11	1.02	0
1	FME	AE	1	1	8,9,10	0.94	0	8,9,11	1.03	1 (12%)
11	FME	ah	1	11	8,9,10	0.96	0	8,9,11	1.05	1 (12%)
1	FME	AG	1	1	8,9,10	0.96	0	8,9,11	1.00	0
1	FME	AO	1	1	8,9,10	0.95	0	8,9,11	1.15	2 (25%)
11	FME	ai	1	11	8,9,10	0.97	0	8,9,11	0.97	0
11	FME	af	1	11	8,9,10	1.00	0	8,9,11	0.76	0
1	FME	AP	1	1	8,9,10	0.93	0	8,9,11	1.25	1 (12%)
1	FME	AQ	1	1	8,9,10	0.95	0	8,9,11	0.86	0
1	FME	AV	1	1	8,9,10	1.00	0	8,9,11	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AT	1	1	8,9,10	0.97	0	8,9,11	0.99	1 (12%)
1	FME	AU	1	1	8,9,10	0.98	0	8,9,11	1.10	1 (12%)
11	FME	am	1	11	8,9,10	0.99	0	8,9,11	0.93	1 (12%)
11	FME	ao	1	11	8,9,10	0.88	0	8,9,11	2.04	2 (25%)
1	FME	AK	1	1	8,9,10	0.97	0	8,9,11	0.89	0
1	FME	AS	1	1	8,9,10	0.93	0	8,9,11	1.39	2 (25%)
1	FME	AN	1	1	8,9,10	0.96	0	8,9,11	1.10	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	ac	1	11	-	0/7/9/11	-
11	FME	ap	1	11	-	1/7/9/11	-
1	FME	AW	1	1	-	2/7/9/11	-
1	FME	AC	1	1	-	0/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
1	FME	AD	1	1	-	0/7/9/11	-
11	FME	aj	1	11	-	0/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-
11	FME	ae	1	11	-	2/7/9/11	-
1	FME	AJ	1	1	-	1/7/9/11	-
1	FME	AB	1	1	-	0/7/9/11	-
11	FME	an	1	11	-	0/7/9/11	-
1	FME	AM	1	1	-	2/7/9/11	-
1	FME	AI	1	1	-	1/7/9/11	-
1	FME	AH	1	1	-	1/7/9/11	-
11	FME	ad	1	11	-	1/7/9/11	-
11	FME	ab	1	11	-	1/7/9/11	-
11	FME	ag	1	11	-	0/7/9/11	-
1	FME	AL	1	1	-	0/7/9/11	-
11	FME	al	1	11	-	2/7/9/11	-
1	FME	AA	1	1	-	0/7/9/11	-
11	FME	ak	1	11	-	0/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
6	FME	H1	1	6	-	0/7/9/11	-
1	FME	AE	1	1	-	0/7/9/11	-
11	FME	ah	1	11	-	0/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AG	1	1	-	0/7/9/11	-
1	FME	AO	1	1	-	2/7/9/11	-
11	FME	ai	1	11	-	0/7/9/11	-
11	FME	af	1	11	-	2/7/9/11	-
1	FME	AP	1	1	-	2/7/9/11	-
1	FME	AQ	1	1	-	1/7/9/11	-
1	FME	AV	1	1	-	1/7/9/11	-
1	FME	AT	1	1	-	2/7/9/11	-
1	FME	AU	1	1	-	1/7/9/11	-
11	FME	am	1	11	-	0/7/9/11	-
11	FME	ao	1	11	-	2/7/9/11	-
1	FME	AK	1	1	-	2/7/9/11	-
1	FME	AS	1	1	-	2/7/9/11	-
1	FME	AN	1	1	-	0/7/9/11	-

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ao	1	FME	C-CA-N	4.29	117.78	109.50
11	ab	1	FME	CA-N-CN	4.25	129.36	122.82
11	ao	1	FME	CA-N-CN	3.63	128.40	122.82
1	AS	1	FME	C-CA-N	3.02	115.34	109.50
1	AB	1	FME	C-CA-N	2.71	114.72	109.50
1	AD	1	FME	C-CA-N	2.65	114.62	109.50
1	AP	1	FME	C-CA-N	2.65	114.61	109.50
1	AU	1	FME	C-CA-N	2.58	114.48	109.50
1	AJ	1	FME	C-CA-N	2.46	114.25	109.50
1	AN	1	FME	C-CA-N	2.39	114.11	109.50
11	ak	1	FME	C-CA-N	2.37	114.08	109.50
11	ah	1	FME	C-CA-N	2.36	114.05	109.50
1	AL	1	FME	C-CA-N	2.31	113.96	109.50
11	ap	1	FME	C-CA-N	2.31	113.95	109.50
11	ae	1	FME	C-CA-N	2.29	113.92	109.50
1	AE	1	FME	C-CA-N	2.25	113.85	109.50
11	ag	1	FME	C-CA-N	2.20	113.74	109.50
1	AA	1	FME	C-CA-N	2.16	113.66	109.50
1	AT	1	FME	C-CA-N	2.13	113.62	109.50
11	ac	1	FME	C-CA-N	2.13	113.61	109.50
11	an	1	FME	C-CA-N	2.12	113.58	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AH	1	FME	C-CA-N	2.11	113.57	109.50
1	AO	1	FME	CA-N-CN	2.09	126.04	122.82
1	AS	1	FME	CA-N-CN	2.07	126.00	122.82
11	am	1	FME	C-CA-N	2.07	113.49	109.50
1	AR	1	FME	C-CA-N	2.05	113.46	109.50
1	AO	1	FME	C-CA-N	2.04	113.44	109.50
11	aj	1	FME	C-CA-N	2.01	113.39	109.50

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	ab	1	FME	CB-CA-N-CN
11	ao	1	FME	C-CA-CB-CG
1	AF	1	FME	O-C-CA-CB
1	AH	1	FME	O-C-CA-CB
1	AI	1	FME	O-C-CA-CB
1	AK	1	FME	O-C-CA-CB
1	AP	1	FME	C-CA-CB-CG
1	AS	1	FME	C-CA-CB-CG
1	AT	1	FME	C-CA-CB-CG
1	AU	1	FME	O-C-CA-CB
1	AV	1	FME	O-C-CA-CB
1	AM	1	FME	CB-CG-SD-CE
11	al	1	FME	CB-CG-SD-CE
11	ad	1	FME	N-CA-CB-CG
1	AM	1	FME	N-CA-CB-CG
1	AT	1	FME	N-CA-CB-CG
11	ae	1	FME	CA-CB-CG-SD
1	AO	1	FME	C-CA-CB-CG
11	af	1	FME	CB-CA-N-CN
11	ae	1	FME	N-CA-CB-CG
1	AP	1	FME	N-CA-CB-CG
11	ao	1	FME	N-CA-CB-CG
1	AO	1	FME	N-CA-CB-CG
11	af	1	FME	N-CA-CB-CG
1	AJ	1	FME	N-CA-CB-CG
11	al	1	FME	CB-CA-N-CN
11	ap	1	FME	CB-CA-N-CN
1	AS	1	FME	CB-CA-N-CN
1	AW	1	FME	CB-CA-N-CN
1	AX	1	FME	CB-CA-N-CN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	AK	1	FME	CB-CG-SD-CE
1	AW	1	FME	CA-CB-CG-SD
1	AQ	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AX	1	FME	1	0

5.5 Carbohydrates [i](#)

4 monosaccharides 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	MAN	CG	1	12,3,18	11,11,12	0.92	1 (9%)	15,15,17	1.03	1 (6%)
12	RAM	CG	2	12	10,10,11	1.75	3 (30%)	14,14,16	0.85	1 (7%)
12	MAN	MG	1	12,18,9	11,11,12	0.78	1 (9%)	15,15,17	1.07	1 (6%)
12	RAM	MG	2	12	10,10,11	1.65	2 (20%)	14,14,16	1.98	3 (21%)

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	MAN	CG	1	12,3,18	-	1/2/19/22	0/1/1/1
12	RAM	CG	2	12	-	-	0/1/1/1
12	MAN	MG	1	12,18,9	-	0/2/19/22	0/1/1/1
12	RAM	MG	2	12	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	CG	2	RAM	O5-C1	4.17	1.50	1.43
12	MG	2	RAM	O5-C1	3.57	1.49	1.43
12	MG	2	RAM	C2-C3	-2.75	1.48	1.52
12	CG	1	MAN	O5-C1	-2.44	1.39	1.43
12	CG	2	RAM	C2-C3	-2.43	1.48	1.52
12	CG	2	RAM	O5-C5	2.14	1.47	1.43
12	MG	1	MAN	O5-C1	-2.03	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	MG	2	RAM	C6-C5-C4	-4.08	105.62	113.08
12	MG	2	RAM	C3-C4-C5	3.98	115.87	109.81
12	MG	2	RAM	O5-C5-C4	3.73	116.27	109.55
12	MG	1	MAN	C1-O5-C5	2.76	115.89	112.19
12	CG	1	MAN	C1-O5-C5	2.56	115.62	112.19
12	CG	2	RAM	C6-C5-C4	-2.12	109.21	113.08

There are no chirality outliers.

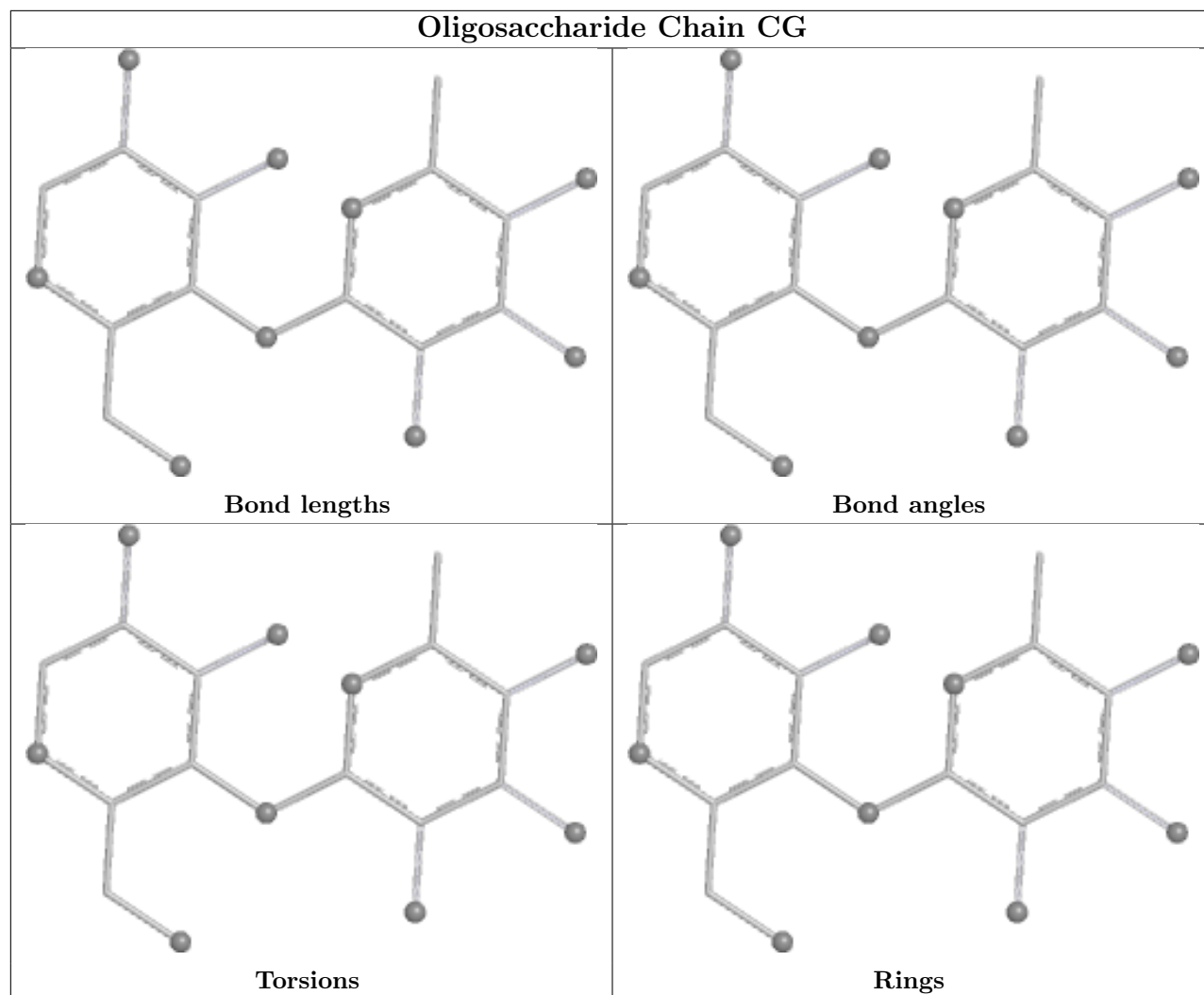
All (1) torsion outliers are listed below:

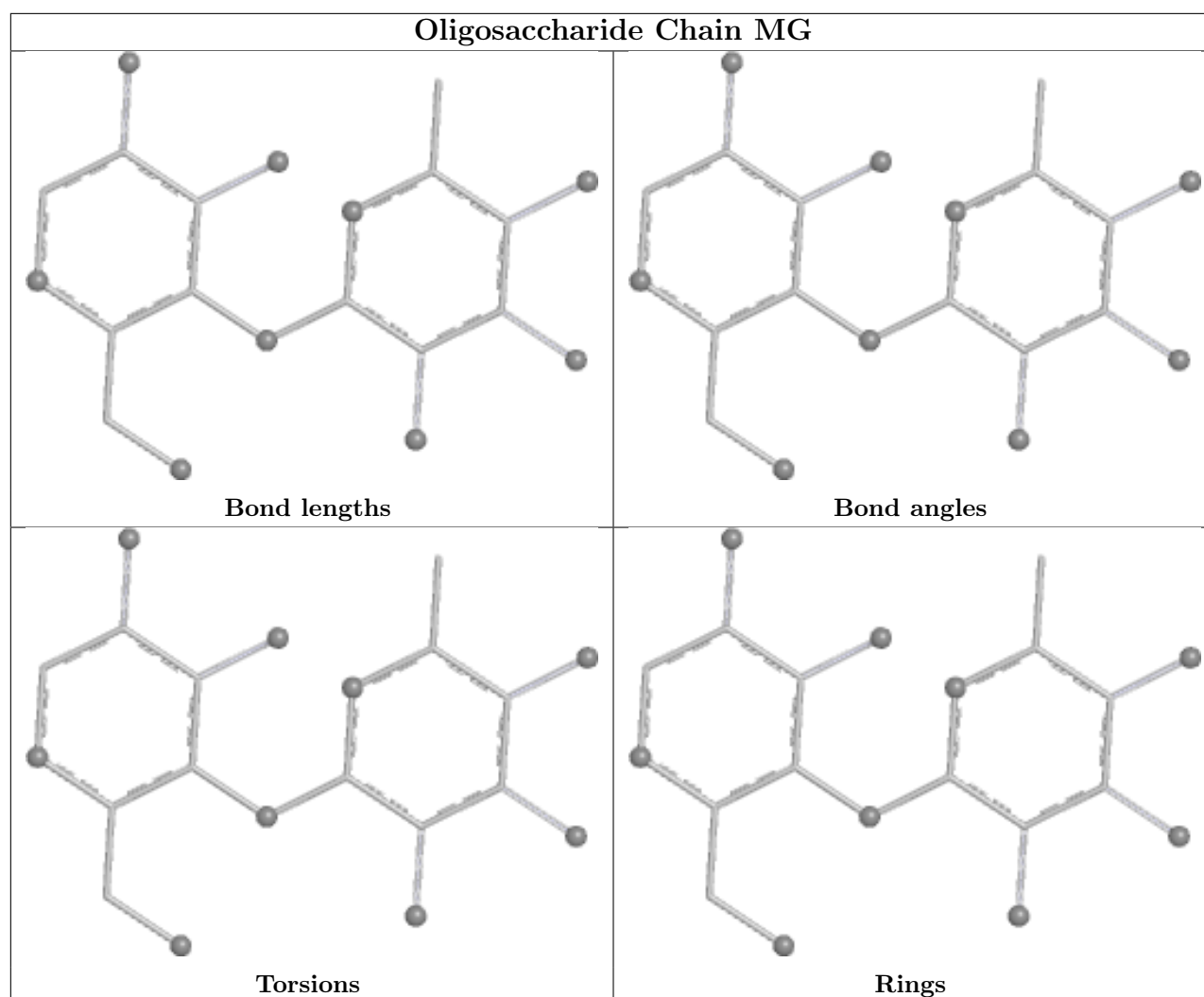
Mol	Chain	Res	Type	Atoms
12	CG	1	MAN	O5-C5-C6-O6

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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 1 is monoatomic - leaving 315 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	$\# Z > 2$
15	V7N	bc	101	-	44,44,44	1.70	9 (20%)	48,54,54	1.49	10 (20%)
16	0V9	bh	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.85	2 (4%)
13	BCL	BN	1005	-	69,74,74	1.11	6 (8%)	79,115,115	1.41	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CD4	M	409	-	83,83,83	0.47	0	89,95,95	1.05	5 (5%)
15	V7N	AW	103	-	44,44,44	1.67	7 (15%)	48,54,54	1.67	13 (27%)
14	LMT	BM	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.96	2 (4%)
15	V7N	BS	1001	-	44,44,44	1.64	7 (15%)	48,54,54	1.70	13 (27%)
14	LMT	AH	104	-	36,36,36	1.10	5 (13%)	47,47,47	0.94	2 (4%)
15	V7N	BR	1001	-	44,44,44	1.66	8 (18%)	48,54,54	1.58	11 (22%)
13	BCL	BS	1004	-	69,74,74	1.16	6 (8%)	79,115,115	1.41	12 (15%)
15	V7N	AA	1004	-	44,44,44	1.69	7 (15%)	48,54,54	1.65	9 (18%)
14	LMT	BE	105	-	36,36,36	1.07	4 (11%)	47,47,47	0.96	2 (4%)
16	0V9	L	310	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	2 (4%)
13	BCL	AD	103	-	69,74,74	1.12	6 (8%)	79,115,115	1.37	10 (12%)
16	0V9	bp	105	-	44,44,46	0.75	1 (2%)	47,49,51	0.93	2 (4%)
13	BCL	bo	102	-	69,74,74	1.11	5 (7%)	79,115,115	1.31	9 (11%)
13	BCL	BC	104	-	69,74,74	1.10	5 (7%)	79,115,115	1.32	9 (11%)
13	BCL	AE	103	28	69,74,74	1.14	5 (7%)	79,115,115	1.57	12 (15%)
13	BCL	BX	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.31	8 (10%)
16	0V9	H1	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.86	2 (4%)
14	LMT	AG	101	-	36,36,36	1.13	5 (13%)	47,47,47	1.03	2 (4%)
13	BCL	bm	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.31	10 (12%)
14	LMT	bm	103	-	36,36,36	1.10	4 (11%)	47,47,47	0.90	1 (2%)
13	BCL	AU	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.38	10 (12%)
13	BCL	AU	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.30	7 (8%)
13	BCL	BW	1005	-	69,74,74	1.12	5 (7%)	79,115,115	1.31	8 (10%)
13	BCL	AQ	102	28	69,74,74	1.15	6 (8%)	79,115,115	1.49	12 (15%)
14	LMT	BL	102	-	36,36,36	1.05	4 (11%)	47,47,47	1.00	1 (2%)
14	LMT	AN	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.96	1 (2%)
14	LMT	BT	104	-	36,36,36	1.05	3 (8%)	47,47,47	0.93	1 (2%)
13	BCL	ak	1001	-	69,74,74	1.13	6 (8%)	79,115,115	1.36	9 (11%)
13	BCL	bk	103	-	69,74,74	1.12	6 (8%)	79,115,115	1.40	10 (12%)
14	LMT	BR	1005	-	36,36,36	1.02	4 (11%)	47,47,47	1.04	2 (4%)
17	HEC	C	1002	3	46,50,50	1.85	4 (8%)	58,82,82	1.62	5 (8%)
14	LMT	BP	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.87	1 (2%)
13	BCL	M	406	-	69,74,74	1.16	6 (8%)	79,115,115	1.33	9 (11%)
14	LMT	BX	103	-	36,36,36	1.06	5 (13%)	47,47,47	0.89	1 (2%)
16	0V9	bm	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.89	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BC	102	-	36,36,36	1.04	3 (8%)	47,47,47	0.85	1 (2%)
15	V7N	BK	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.60	13 (27%)
14	LMT	bj	102	-	36,36,36	1.10	4 (11%)	47,47,47	0.94	2 (4%)
21	CD4	H1	103	-	83,83,83	0.46	0	89,95,95	0.99	5 (5%)
13	BCL	bf	102	-	69,74,74	1.11	6 (8%)	79,115,115	1.27	9 (11%)
14	LMT	BL	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	2 (4%)
14	LMT	AN	101	-	36,36,36	1.03	4 (11%)	47,47,47	0.99	4 (8%)
15	V7N	BE	101	-	44,44,44	1.65	7 (15%)	48,54,54	1.61	9 (18%)
13	BCL	al	1001	-	69,74,74	1.15	6 (8%)	79,115,115	1.34	9 (11%)
26	V7B	ag	103	-	59,59,59	0.87	4 (6%)	75,75,75	1.01	5 (6%)
14	LMT	BV	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.91	2 (4%)
15	V7N	BM	1001	-	44,44,44	1.64	8 (18%)	48,54,54	1.69	12 (25%)
14	LMT	BO	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.99	2 (4%)
13	BCL	BA	103	-	69,74,74	1.10	5 (7%)	79,115,115	1.30	9 (11%)
14	LMT	L	304	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	3 (6%)
13	BCL	ac	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.33	9 (11%)
13	BCL	AV	101	-	69,74,74	1.17	6 (8%)	79,115,115	1.28	8 (10%)
22	BPH	M	407	-	59,70,70	1.14	4 (6%)	59,101,101	1.86	9 (15%)
15	V7N	BN	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.99	13 (27%)
15	V7N	BP	1001	-	44,44,44	1.63	6 (13%)	48,54,54	1.73	12 (25%)
13	BCL	AE	104	-	69,74,74	1.14	5 (7%)	79,115,115	1.39	9 (11%)
14	LMT	BG	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.86	0
14	LMT	bl	103	-	36,36,36	1.06	4 (11%)	47,47,47	1.00	2 (4%)
13	BCL	BG	1004	-	69,74,74	1.10	6 (8%)	79,115,115	1.28	9 (11%)
14	LMT	AT	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.98	2 (4%)
14	LMT	BJ	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
13	BCL	bg	104	-	69,74,74	1.14	6 (8%)	79,115,115	1.26	8 (10%)
13	BCL	AA	1002	28	69,74,74	1.12	6 (8%)	79,115,115	1.37	10 (12%)
14	LMT	bh	102	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	3 (6%)
14	LMT	BB	103	-	36,36,36	1.04	4 (11%)	47,47,47	0.93	1 (2%)
21	CD4	ad	101	-	83,83,83	0.49	0	89,95,95	1.07	6 (6%)
14	LMT	AH	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.88	2 (4%)
14	LMT	AV	104	-	36,36,36	1.05	5 (13%)	47,47,47	1.06	2 (4%)
14	LMT	BD	105	-	36,36,36	1.10	4 (11%)	47,47,47	0.92	3 (6%)
14	LMT	BC	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	V7N	bo	101	-	44,44,44	1.66	8 (18%)	48,54,54	1.59	10 (20%)
13	BCL	bd	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.39	11 (13%)
14	LMT	BI	1005	-	36,36,36	1.08	4 (11%)	47,47,47	1.05	2 (4%)
14	LMT	AA	1003	-	36,36,36	1.11	4 (11%)	47,47,47	1.04	1 (2%)
23	MQ8	M	402	-	54,54,54	0.68	0	67,69,69	0.93	3 (4%)
14	LMT	BR	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.98	3 (6%)
13	BCL	BE	104	-	69,74,74	1.10	5 (7%)	79,115,115	1.32	8 (10%)
13	BCL	AL	103	-	69,74,74	1.19	5 (7%)	79,115,115	1.63	13 (16%)
14	LMT	BJ	1006	-	36,36,36	1.06	4 (11%)	47,47,47	0.89	1 (2%)
13	BCL	af	103	-	69,74,74	1.13	4 (5%)	79,115,115	1.32	9 (11%)
13	BCL	am	1001	-	69,74,74	1.15	6 (8%)	79,115,115	1.34	9 (11%)
14	LMT	be	104	-	36,36,36	1.10	4 (11%)	47,47,47	0.81	1 (2%)
13	BCL	AI	101	-	69,74,74	1.13	5 (7%)	79,115,115	1.34	8 (10%)
14	LMT	BR	1006	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	1 (2%)
16	0V9	bo	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.87	1 (2%)
16	0V9	bk	102	-	44,44,46	0.76	1 (2%)	47,49,51	0.97	3 (6%)
22	BPH	L	301	-	59,70,70	1.16	3 (5%)	59,101,101	1.85	9 (15%)
14	LMT	BS	1002	-	36,36,36	1.04	4 (11%)	47,47,47	0.96	2 (4%)
14	LMT	BB	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.92	2 (4%)
14	LMT	BH	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.95	2 (4%)
14	LMT	BA	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.93	1 (2%)
13	BCL	AM	1002	28	69,74,74	1.16	5 (7%)	79,115,115	1.53	11 (13%)
14	LMT	AB	1003	-	36,36,36	1.06	5 (13%)	47,47,47	0.99	2 (4%)
13	BCL	AJ	103	28	69,74,74	1.16	5 (7%)	79,115,115	1.43	12 (15%)
16	0V9	bg	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.83	2 (4%)
15	V7N	BF	101	-	44,44,44	1.69	5 (11%)	48,54,54	1.60	11 (22%)
15	V7N	BO	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.80	15 (31%)
15	V7N	be	102	-	44,44,44	1.66	7 (15%)	48,54,54	1.62	10 (20%)
13	BCL	AM	1004	-	69,74,74	1.12	6 (8%)	79,115,115	1.30	7 (8%)
13	BCL	AH	105	-	69,74,74	1.17	5 (7%)	79,115,115	1.47	12 (15%)
14	LMT	L	307	-	36,36,36	1.04	4 (11%)	47,47,47	0.90	2 (4%)
15	V7N	ag	101	-	44,44,44	1.64	5 (11%)	48,54,54	1.66	10 (20%)
16	0V9	bi	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.85	3 (6%)
14	LMT	AM	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	2 (4%)
14	LMT	BD	106	-	36,36,36	1.05	4 (11%)	47,47,47	1.02	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	AX	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	3 (6%)
15	V7N	BD	101	-	44,44,44	1.69	6 (13%)	48,54,54	1.48	7 (14%)
14	LMT	AV	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
15	V7N	BJ	1001	-	44,44,44	1.64	7 (15%)	48,54,54	1.64	12 (25%)
15	V7N	BQ	1001	-	44,44,44	1.66	6 (13%)	48,54,54	1.64	12 (25%)
14	LMT	BD	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.99	2 (4%)
16	0V9	bf	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	1 (2%)
25	CRT	M	404	-	43,43,43	0.59	0	48,54,54	0.77	0
14	LMT	AT	104	-	36,36,36	1.05	4 (11%)	47,47,47	1.03	2 (4%)
15	V7N	bk	101	-	44,44,44	1.68	7 (15%)	48,54,54	1.52	9 (18%)
13	BCL	AB	1002	-	69,74,74	1.15	5 (7%)	79,115,115	1.36	10 (12%)
13	BCL	ad	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.36	9 (11%)
14	LMT	bo	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.96	2 (4%)
13	BCL	ai	101	-	69,74,74	1.15	6 (8%)	79,115,115	1.34	9 (11%)
14	LMT	bp	103	-	36,36,36	1.06	4 (11%)	47,47,47	1.14	3 (6%)
16	0V9	M	403	-	44,44,46	0.76	1 (2%)	47,49,51	0.89	3 (6%)
13	BCL	ab	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.38	8 (10%)
13	BCL	M	408	-	69,74,74	1.16	7 (10%)	79,115,115	1.39	10 (12%)
14	LMT	BI	1003	-	36,36,36	1.05	3 (8%)	47,47,47	0.81	1 (2%)
18	V75	C	1006	12,19	18,18,18	1.60	5 (27%)	21,25,25	1.71	2 (9%)
14	LMT	BF	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.94	3 (6%)
15	V7N	BV	1001	-	44,44,44	1.65	8 (18%)	48,54,54	1.56	10 (20%)
13	BCL	BL	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
13	BCL	BU	1004	-	69,74,74	1.14	5 (7%)	79,115,115	1.29	9 (11%)
13	BCL	ap	1001	-	69,74,74	1.13	6 (8%)	79,115,115	1.44	11 (13%)
13	BCL	AQ	103	-	69,74,74	1.15	6 (8%)	79,115,115	1.37	8 (10%)
14	LMT	AP	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.97	2 (4%)
15	V7N	bi	101	-	44,44,44	1.68	6 (13%)	48,54,54	1.50	11 (22%)
13	BCL	an	1001	-	69,74,74	1.16	6 (8%)	79,115,115	1.37	10 (12%)
14	LMT	BG	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.94	2 (4%)
13	BCL	L	305	-	69,74,74	1.16	7 (10%)	79,115,115	1.31	8 (10%)
13	BCL	ba	102	-	69,74,74	1.12	4 (5%)	79,115,115	1.38	11 (13%)
13	BCL	BF	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.25	9 (11%)
14	LMT	BK	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.99	2 (4%)
14	LMT	AL	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.98	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BB	102	-	36,36,36	1.05	4 (11%)	47,47,47	1.01	3 (6%)
13	BCL	bi	102	-	69,74,74	1.14	6 (8%)	79,115,115	1.29	9 (11%)
16	0V9	be	105	-	44,44,46	0.76	1 (2%)	47,49,51	0.95	3 (6%)
13	BCL	BV	1005	-	69,74,74	1.12	6 (8%)	79,115,115	1.33	10 (12%)
16	0V9	bd	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.94	2 (4%)
13	BCL	AS	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.39	9 (11%)
16	0V9	AQ	105	-	44,44,46	0.76	1 (2%)	47,49,51	0.83	1 (2%)
13	BCL	AF	1001	-	69,74,74	1.14	6 (8%)	79,115,115	1.33	8 (10%)
13	BCL	AO	101	-	69,74,74	1.16	6 (8%)	79,115,115	1.31	10 (12%)
14	LMT	AE	102	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	2 (4%)
13	BCL	BD	104	-	69,74,74	1.16	6 (8%)	79,115,115	1.49	10 (12%)
14	LMT	BD	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	0
23	MQ8	ao	101	-	54,54,54	0.64	0	67,69,69	0.95	3 (4%)
15	V7N	bj	101	-	44,44,44	1.63	6 (13%)	48,54,54	1.59	10 (20%)
15	V7N	AM	1001	-	44,44,44	1.67	6 (13%)	48,54,54	1.58	9 (18%)
14	LMT	BW	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	2 (4%)
13	BCL	AG	102	28	69,74,74	1.14	6 (8%)	79,115,115	1.55	13 (16%)
14	LMT	BU	1002	-	36,36,36	1.04	4 (11%)	47,47,47	1.04	3 (6%)
13	BCL	AW	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	7 (8%)
13	BCL	AA	1001	-	69,74,74	1.13	5 (7%)	79,115,115	1.32	7 (8%)
15	V7N	BU	1001	-	44,44,44	1.68	6 (13%)	48,54,54	1.87	11 (22%)
14	LMT	BI	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.90	2 (4%)
14	LMT	C2	1001	-	36,36,36	1.06	5 (13%)	47,47,47	0.96	2 (4%)
14	LMT	AE	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.03	2 (4%)
15	V7N	bd	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.54	11 (22%)
14	LMT	be	101	-	36,36,36	1.06	4 (11%)	47,47,47	1.00	4 (8%)
21	CD4	af	102	-	83,83,83	0.48	0	89,95,95	1.18	7 (7%)
13	BCL	BM	1004	-	69,74,74	1.13	6 (8%)	79,115,115	1.39	11 (13%)
14	LMT	BX	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	1 (2%)
14	LMT	H2	201	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	2 (4%)
14	LMT	L	306	-	36,36,36	1.06	4 (11%)	47,47,47	0.90	1 (2%)
14	LMT	bg	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.86	1 (2%)
15	V7N	BI	1001	-	44,44,44	1.64	8 (18%)	48,54,54	1.74	14 (29%)
13	BCL	bh	103	-	69,74,74	1.12	6 (8%)	79,115,115	1.30	9 (11%)
14	LMT	BU	1003	-	36,36,36	1.04	4 (11%)	47,47,47	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BH	1002	-	36,36,36	1.07	5 (13%)	47,47,47	0.99	2 (4%)
14	LMT	BG	1003	-	36,36,36	1.05	4 (11%)	47,47,47	0.85	1 (2%)
15	V7N	bn	101	-	44,44,44	1.71	7 (15%)	48,54,54	1.79	15 (31%)
13	BCL	AO	102	-	69,74,74	1.15	6 (8%)	79,115,115	1.30	7 (8%)
16	0V9	ad	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.86	2 (4%)
13	BCL	BP	1003	-	69,74,74	1.26	7 (10%)	79,115,115	1.75	9 (11%)
14	LMT	BF	102	-	36,36,36	1.03	4 (11%)	47,47,47	0.96	1 (2%)
13	BCL	bp	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	9 (11%)
14	LMT	BB	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.82	0
13	BCL	bb	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.37	10 (12%)
14	LMT	BM	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	0
13	BCL	AK	102	28	69,74,74	1.19	7 (10%)	79,115,115	1.32	8 (10%)
13	BCL	BB	105	-	69,74,74	1.11	5 (7%)	79,115,115	1.33	10 (12%)
13	BCL	ao	102	-	69,74,74	1.16	6 (8%)	79,115,115	1.32	9 (11%)
14	LMT	L	309	-	36,36,36	1.07	4 (11%)	47,47,47	0.83	1 (2%)
21	CD4	af	104	-	83,83,83	0.47	0	89,95,95	1.04	4 (4%)
13	BCL	bj	104	-	69,74,74	1.13	5 (7%)	79,115,115	1.41	11 (13%)
15	V7N	AS	104	-	44,44,44	1.66	6 (13%)	48,54,54	1.53	10 (20%)
18	V75	M	410	12,19	18,18,18	1.65	5 (27%)	21,25,25	1.68	2 (9%)
13	BCL	bc	103	-	69,74,74	1.14	6 (8%)	79,115,115	1.42	12 (15%)
14	LMT	BQ	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	1 (2%)
14	LMT	BE	103	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	3 (6%)
13	BCL	AH	102	28	69,74,74	1.15	5 (7%)	79,115,115	1.48	15 (18%)
14	LMT	BW	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.87	1 (2%)
15	V7N	bg	101	-	44,44,44	1.66	6 (13%)	48,54,54	1.62	11 (22%)
13	BCL	ae	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	8 (10%)
14	LMT	BS	1005	-	36,36,36	1.04	4 (11%)	47,47,47	0.90	0
13	BCL	BQ	1004	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	10 (12%)
13	BCL	AH	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	7 (8%)
26	V7B	af	101	-	59,59,59	0.89	4 (6%)	75,75,75	1.10	5 (6%)
14	LMT	BP	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.89	1 (2%)
13	BCL	AN	104	28	69,74,74	1.13	5 (7%)	79,115,115	1.33	9 (11%)
13	BCL	L	308	-	69,74,74	1.11	7 (10%)	79,115,115	1.32	7 (8%)
15	V7N	BA	101	-	44,44,44	1.67	8 (18%)	48,54,54	1.68	12 (25%)
14	LMT	BE	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.22	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	bn	102	-	69,74,74	1.15	6 (8%)	79,115,115	1.30	9 (11%)
13	BCL	AB	1001	-	69,74,74	1.11	6 (8%)	79,115,115	1.41	11 (13%)
14	LMT	AC	103	-	36,36,36	1.04	3 (8%)	47,47,47	0.94	2 (4%)
13	BCL	AE	105	-	69,74,74	1.18	5 (7%)	79,115,115	1.38	10 (12%)
14	LMT	BC	103	-	36,36,36	1.03	4 (11%)	47,47,47	0.94	3 (6%)
14	LMT	bc	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.99	4 (8%)
13	BCL	AJ	104	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	7 (8%)
23	MQ8	L	303	-	54,54,54	0.68	0	67,69,69	1.09	5 (7%)
14	LMT	bk	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.95	2 (4%)
13	BCL	AV	103	28	69,74,74	1.11	5 (7%)	79,115,115	1.35	9 (11%)
16	0V9	bb	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.84	1 (2%)
19	NDG	C1	301	18	14,14,15	0.67	0	17,19,21	1.02	2 (11%)
14	LMT	BN	1004	-	36,36,36	1.09	4 (11%)	47,47,47	0.95	2 (4%)
19	NDG	C	1007	18	14,14,15	0.73	1 (7%)	17,19,21	0.84	0
14	LMT	BH	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.94	1 (2%)
13	BCL	AT	103	28	69,74,74	1.14	6 (8%)	79,115,115	1.40	10 (12%)
14	LMT	BW	1006	-	36,36,36	1.08	5 (13%)	47,47,47	0.91	2 (4%)
15	V7N	BH	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.70	14 (29%)
15	V7N	BG	1001	-	44,44,44	1.65	8 (18%)	48,54,54	1.70	12 (25%)
13	BCL	AP	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.36	9 (11%)
14	LMT	BN	1002	-	36,36,36	1.07	5 (13%)	47,47,47	0.78	0
13	BCL	BJ	1004	-	69,74,74	1.12	6 (8%)	79,115,115	1.27	8 (10%)
14	LMT	AQ	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.91	2 (4%)
14	LMT	BX	102	-	36,36,36	1.06	5 (13%)	47,47,47	0.99	2 (4%)
14	LMT	BQ	1002	-	36,36,36	1.09	4 (11%)	47,47,47	0.85	2 (4%)
13	BCL	BO	1003	-	69,74,74	1.12	6 (8%)	79,115,115	1.38	9 (11%)
13	BCL	AT	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.32	7 (8%)
14	LMT	BS	1003	-	36,36,36	1.04	3 (8%)	47,47,47	0.97	3 (6%)
14	LMT	AK	101	-	36,36,36	1.05	4 (11%)	47,47,47	1.07	2 (4%)
15	V7N	ba	101	-	44,44,44	1.68	7 (15%)	48,54,54	1.54	10 (20%)
16	0V9	bn	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.79	2 (4%)
16	0V9	bj	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.89	3 (6%)
17	HEC	C	1004	3	46,50,50	1.85	5 (10%)	58,82,82	1.61	5 (8%)
14	LMT	bi	104	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	2 (4%)
14	LMT	AJ	102	-	36,36,36	1.13	6 (16%)	47,47,47	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	bn	103	-	36,36,36	1.08	5 (13%)	47,47,47	1.02	2 (4%)
13	BCL	AK	104	-	69,74,74	1.15	6 (8%)	79,115,115	1.31	7 (8%)
14	LMT	ac	101	-	36,36,36	1.09	4 (11%)	47,47,47	0.87	1 (2%)
15	V7N	bb	101	-	44,44,44	1.70	8 (18%)	48,54,54	1.57	8 (16%)
14	LMT	L	302	-	36,36,36	1.07	4 (11%)	47,47,47	0.94	1 (2%)
14	LMT	BK	1004	-	36,36,36	1.07	4 (11%)	47,47,47	1.05	3 (6%)
13	BCL	be	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.28	9 (11%)
13	BCL	BT	103	-	69,74,74	1.13	6 (8%)	79,115,115	1.33	10 (12%)
14	LMT	AD	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.94	2 (4%)
27	UYH	ai	102	-	55,55,55	2.16	14 (25%)	63,63,63	0.98	1 (1%)
13	BCL	aj	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.32	10 (12%)
14	LMT	BO	1004	-	36,36,36	1.09	4 (11%)	47,47,47	0.88	0
15	V7N	BW	1001	-	44,44,44	1.65	8 (18%)	48,54,54	1.60	10 (20%)
14	LMT	BW	1004	-	36,36,36	1.07	5 (13%)	47,47,47	1.05	2 (4%)
14	LMT	bp	101	-	36,36,36	1.05	4 (11%)	47,47,47	1.03	3 (6%)
13	BCL	AC	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	7 (8%)
13	BCL	AP	103	28	69,74,74	1.15	5 (7%)	79,115,115	1.42	11 (13%)
13	BCL	AQ	104	-	69,74,74	1.21	5 (7%)	79,115,115	1.50	14 (17%)
20	PGW	H1	101	-	50,50,50	0.44	0	53,56,56	0.97	4 (7%)
13	BCL	AG	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)
14	LMT	AK	103	-	36,36,36	1.07	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	bl	104	-	69,74,74	1.15	5 (7%)	79,115,115	1.28	9 (11%)
17	HEC	C	1003	3	46,50,50	1.83	3 (6%)	58,82,82	1.66	6 (10%)
13	BCL	AL	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	7 (8%)
15	V7N	bl	101	-	44,44,44	1.65	7 (15%)	48,54,54	1.70	13 (27%)
13	BCL	AX	103	-	69,74,74	1.15	4 (5%)	79,115,115	1.41	11 (13%)
13	BCL	BK	1002	-	69,74,74	1.09	5 (7%)	79,115,115	1.39	11 (13%)
15	V7N	bm	101	-	44,44,44	1.64	7 (15%)	48,54,54	1.63	9 (18%)
17	HEC	C	1001	3	46,50,50	1.84	5 (10%)	58,82,82	1.66	7 (12%)
14	LMT	BJ	1005	-	36,36,36	1.08	4 (11%)	47,47,47	0.95	2 (4%)
13	BCL	AS	101	28	69,74,74	1.13	5 (7%)	79,115,115	1.41	9 (11%)
14	LMT	BP	1002	-	36,36,36	1.06	5 (13%)	47,47,47	0.96	3 (6%)
14	LMT	BO	1005	-	36,36,36	1.02	4 (11%)	47,47,47	0.87	2 (4%)
13	BCL	BI	1004	-	69,74,74	1.12	6 (8%)	79,115,115	1.37	10 (12%)
13	BCL	AD	104	28	69,74,74	1.13	5 (7%)	79,115,115	1.42	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	AU	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.85	1 (2%)
13	BCL	BH	1005	-	69,74,74	1.13	5 (7%)	79,115,115	1.34	9 (11%)
13	BCL	ah	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.35	9 (11%)
14	LMT	BN	1003	-	36,36,36	1.06	5 (13%)	47,47,47	1.04	2 (4%)
14	LMT	BK	1003	-	36,36,36	1.09	4 (11%)	47,47,47	0.96	2 (4%)
13	BCL	ag	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	9 (11%)
14	LMT	BP	1006	-	36,36,36	1.08	5 (13%)	47,47,47	0.94	3 (6%)
14	LMT	BR	1004	-	36,36,36	1.07	4 (11%)	47,47,47	0.91	1 (2%)
13	BCL	BR	1003	-	69,74,74	1.14	6 (8%)	79,115,115	1.31	9 (11%)
14	LMT	AJ	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.95	1 (2%)
13	BCL	AR	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
13	BCL	AN	103	-	69,74,74	1.12	6 (8%)	79,115,115	1.32	7 (8%)
14	LMT	BT	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.99	2 (4%)
13	BCL	aa	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.32	8 (10%)
15	V7N	bp	102	-	44,44,44	1.71	8 (18%)	48,54,54	1.71	12 (25%)
14	LMT	bf	101	-	36,36,36	1.04	3 (8%)	47,47,47	0.94	2 (4%)
14	LMT	BM	1002	-	36,36,36	1.07	4 (11%)	47,47,47	0.97	2 (4%)
16	0V9	ab	1002	-	44,44,46	0.76	1 (2%)	47,49,51	0.81	1 (2%)
13	BCL	AC	101	-	69,74,74	1.18	4 (5%)	79,115,115	1.37	9 (11%)
14	LMT	AE	106	-	36,36,36	1.03	4 (11%)	47,47,47	1.20	4 (8%)
14	LMT	BJ	1003	-	36,36,36	1.03	4 (11%)	47,47,47	0.95	1 (2%)
14	LMT	BV	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.94	2 (4%)
16	0V9	bl	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.90	1 (2%)
21	CD4	M	405	-	83,83,83	0.47	0	89,95,95	1.08	6 (6%)
14	LMT	BT	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.93	2 (4%)
13	BCL	AX	102	-	69,74,74	1.17	6 (8%)	79,115,115	1.32	8 (10%)
14	LMT	C	1005	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	2 (4%)
13	BCL	AW	102	28	69,74,74	1.13	6 (8%)	79,115,115	1.45	11 (13%)
15	V7N	AD	101	-	44,44,44	1.67	8 (18%)	48,54,54	1.65	11 (22%)
15	V7N	bh	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.59	12 (25%)
14	LMT	BV	1004	-	36,36,36	1.07	3 (8%)	47,47,47	0.94	2 (4%)
14	LMT	AS	103	-	36,36,36	1.12	5 (13%)	47,47,47	1.05	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	V7N	bc	101	-	-	7/53/53/53	-
16	0V9	bh	104	-	-	10/48/48/50	-
13	BCL	BN	1005	-	-	7/41/137/137	-
21	CD4	M	409	-	-	22/94/94/94	-
15	V7N	AW	103	-	-	5/53/53/53	-
14	LMT	BM	1005	-	-	5/21/61/61	0/2/2/2
15	V7N	BS	1001	-	-	4/53/53/53	-
14	LMT	AH	104	-	-	0/21/61/61	0/2/2/2
15	V7N	BR	1001	-	-	8/53/53/53	-
13	BCL	BS	1004	-	-	5/41/137/137	-
15	V7N	AA	1004	-	-	6/53/53/53	-
14	LMT	BE	105	-	-	4/21/61/61	0/2/2/2
16	0V9	L	310	-	-	8/48/48/50	-
13	BCL	AD	103	-	-	3/41/137/137	-
16	0V9	bp	105	-	-	12/48/48/50	-
13	BCL	bo	102	-	-	7/41/137/137	-
13	BCL	BC	104	-	-	6/41/137/137	-
13	BCL	AE	103	28	-	10/41/137/137	-
13	BCL	BX	101	-	-	5/41/137/137	-
16	0V9	H1	102	-	-	10/48/48/50	-
14	LMT	AG	101	-	-	8/21/61/61	0/2/2/2
13	BCL	bm	102	-	-	9/41/137/137	-
14	LMT	bm	103	-	-	8/21/61/61	0/2/2/2
13	BCL	AU	103	-	-	3/41/137/137	-
13	BCL	AU	101	-	-	2/41/137/137	-
13	BCL	BW	1005	-	-	3/41/137/137	-
13	BCL	AQ	102	28	-	5/41/137/137	-
14	LMT	BL	102	-	-	3/21/61/61	0/2/2/2
14	LMT	AN	102	-	-	6/21/61/61	0/2/2/2
14	LMT	BT	104	-	-	5/21/61/61	0/2/2/2
13	BCL	ak	1001	-	-	4/41/137/137	-
13	BCL	bk	103	-	-	6/41/137/137	-
14	LMT	BR	1005	-	-	10/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEC	C	1002	3	-	6/14/54/54	-
14	LMT	BP	1004	-	-	6/21/61/61	0/2/2/2
13	BCL	M	406	-	-	6/41/137/137	-
14	LMT	BX	103	-	-	5/21/61/61	0/2/2/2
16	0V9	bm	104	-	-	9/48/48/50	-
14	LMT	BC	102	-	-	4/21/61/61	0/2/2/2
15	V7N	BK	1001	-	-	5/53/53/53	-
14	LMT	bj	102	-	-	2/21/61/61	0/2/2/2
21	CD4	H1	103	-	-	18/94/94/94	-
13	BCL	bf	102	-	-	6/41/137/137	-
14	LMT	BL	101	-	-	6/21/61/61	0/2/2/2
14	LMT	AN	101	-	-	7/21/61/61	0/2/2/2
15	V7N	BE	101	-	-	5/53/53/53	-
13	BCL	al	1001	-	-	1/41/137/137	-
26	V7B	ag	103	-	-	11/48/88/88	0/2/2/2
14	LMT	BV	1003	-	-	2/21/61/61	0/2/2/2
15	V7N	BM	1001	-	-	6/53/53/53	-
14	LMT	BO	1002	-	-	6/21/61/61	0/2/2/2
13	BCL	BA	103	-	-	4/41/137/137	-
14	LMT	L	304	-	-	3/21/61/61	0/2/2/2
13	BCL	ac	102	-	-	4/41/137/137	-
13	BCL	AV	101	-	-	8/41/137/137	-
22	BPH	M	407	-	-	4/37/105/105	0/5/6/6
15	V7N	BN	1001	-	-	10/53/53/53	-
15	V7N	BP	1001	-	-	4/53/53/53	-
13	BCL	AE	104	-	-	3/41/137/137	-
14	LMT	BG	1005	-	-	3/21/61/61	0/2/2/2
14	LMT	bl	103	-	-	5/21/61/61	0/2/2/2
13	BCL	BG	1004	-	-	7/41/137/137	-
14	LMT	AT	102	-	-	8/21/61/61	0/2/2/2
14	LMT	BJ	1002	-	-	1/21/61/61	0/2/2/2
13	BCL	bg	104	-	-	8/41/137/137	-
13	BCL	AA	1002	28	-	6/41/137/137	-
14	LMT	bh	102	-	-	5/21/61/61	0/2/2/2
14	LMT	BB	103	-	-	1/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CD4	ad	101	-	-	15/94/94/94	-
14	LMT	AH	101	-	-	5/21/61/61	0/2/2/2
14	LMT	AV	104	-	-	6/21/61/61	0/2/2/2
14	LMT	BD	105	-	-	4/21/61/61	0/2/2/2
14	LMT	BC	101	-	-	6/21/61/61	0/2/2/2
15	V7N	bo	101	-	-	7/53/53/53	-
13	BCL	bd	102	-	-	8/41/137/137	-
14	LMT	BI	1005	-	-	6/21/61/61	0/2/2/2
14	LMT	AA	1003	-	-	7/21/61/61	0/2/2/2
23	MQ8	M	402	-	-	4/47/67/67	0/2/2/2
14	LMT	BR	1002	-	-	7/21/61/61	0/2/2/2
13	BCL	BE	104	-	-	5/41/137/137	-
13	BCL	AL	103	-	-	9/41/137/137	-
14	LMT	BJ	1006	-	-	3/21/61/61	0/2/2/2
13	BCL	af	103	-	-	7/41/137/137	-
13	BCL	am	1001	-	-	9/41/137/137	-
14	LMT	be	104	-	-	5/21/61/61	0/2/2/2
13	BCL	AI	101	-	-	8/41/137/137	-
14	LMT	BR	1006	-	-	4/21/61/61	0/2/2/2
16	0V9	bo	103	-	-	15/48/48/50	-
16	0V9	bk	102	-	-	12/48/48/50	-
22	BPH	L	301	-	-	2/37/105/105	0/5/6/6
14	LMT	BS	1002	-	-	4/21/61/61	0/2/2/2
14	LMT	BB	101	-	-	1/21/61/61	0/2/2/2
14	LMT	BH	1004	-	-	3/21/61/61	0/2/2/2
14	LMT	BA	102	-	-	5/21/61/61	0/2/2/2
13	BCL	AM	1002	28	-	6/41/137/137	-
14	LMT	AB	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	AJ	103	28	-	7/41/137/137	-
16	0V9	bg	103	-	-	10/48/48/50	-
15	V7N	BF	101	-	-	8/53/53/53	-
15	V7N	BO	1001	-	-	8/53/53/53	-
15	V7N	be	102	-	-	6/53/53/53	-
13	BCL	AM	1004	-	-	7/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	AH	105	-	-	8/41/137/137	-
14	LMT	L	307	-	-	5/21/61/61	0/2/2/2
15	V7N	ag	101	-	-	6/53/53/53	-
16	0V9	bi	103	-	-	16/48/48/50	-
14	LMT	AM	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	BD	106	-	-	7/21/61/61	0/2/2/2
14	LMT	AX	101	-	-	3/21/61/61	0/2/2/2
15	V7N	BD	101	-	-	5/53/53/53	-
14	LMT	AV	102	-	-	8/21/61/61	0/2/2/2
15	V7N	BJ	1001	-	-	4/53/53/53	-
15	V7N	BQ	1001	-	-	4/53/53/53	-
14	LMT	BD	102	-	-	4/21/61/61	0/2/2/2
16	0V9	bf	103	-	-	10/48/48/50	-
25	CRT	M	404	-	-	3/51/51/51	-
14	LMT	AT	104	-	-	6/21/61/61	0/2/2/2
15	V7N	bk	101	-	-	7/53/53/53	-
13	BCL	AB	1002	-	-	2/41/137/137	-
13	BCL	ad	102	-	-	3/41/137/137	-
14	LMT	bo	104	-	-	4/21/61/61	0/2/2/2
13	BCL	ai	101	-	-	2/41/137/137	-
14	LMT	bp	103	-	-	6/21/61/61	0/2/2/2
16	0V9	M	403	-	-	15/48/48/50	-
13	BCL	ab	1001	-	-	3/41/137/137	-
13	BCL	M	408	-	-	1/41/137/137	-
14	LMT	BI	1003	-	-	2/21/61/61	0/2/2/2
18	V75	C	1006	12,19	-	0/12/29/29	0/1/1/1
14	LMT	BF	104	-	-	7/21/61/61	0/2/2/2
15	V7N	BV	1001	-	-	6/53/53/53	-
13	BCL	BL	103	-	-	4/41/137/137	-
13	BCL	BU	1004	-	-	9/41/137/137	-
13	BCL	ap	1001	-	-	5/41/137/137	-
13	BCL	AQ	103	-	-	4/41/137/137	-
14	LMT	AP	101	-	-	10/21/61/61	0/2/2/2
15	V7N	bi	101	-	-	6/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	an	1001	-	-	5/41/137/137	-
14	LMT	BG	1002	-	-	3/21/61/61	0/2/2/2
13	BCL	L	305	-	-	0/41/137/137	-
13	BCL	ba	102	-	-	6/41/137/137	-
13	BCL	BF	103	-	-	6/41/137/137	-
14	LMT	BK	1005	-	-	6/21/61/61	0/2/2/2
14	LMT	AL	101	-	-	3/21/61/61	0/2/2/2
14	LMT	BB	102	-	-	0/21/61/61	0/2/2/2
13	BCL	bi	102	-	-	5/41/137/137	-
16	0V9	be	105	-	-	15/48/48/50	-
13	BCL	BV	1005	-	-	7/41/137/137	-
16	0V9	bd	103	-	-	9/48/48/50	-
13	BCL	AS	102	-	-	5/41/137/137	-
16	0V9	AQ	105	-	-	8/48/48/50	-
13	BCL	AF	1001	-	-	8/41/137/137	-
13	BCL	AO	101	-	-	6/41/137/137	-
14	LMT	AE	102	-	-	5/21/61/61	0/2/2/2
13	BCL	BD	104	-	-	5/41/137/137	-
14	LMT	BD	103	-	-	5/21/61/61	0/2/2/2
23	MQ8	ao	101	-	-	4/47/67/67	0/2/2/2
15	V7N	bj	101	-	-	4/53/53/53	-
15	V7N	AM	1001	-	-	4/53/53/53	-
14	LMT	BW	1002	-	-	3/21/61/61	0/2/2/2
13	BCL	AG	102	28	-	9/41/137/137	-
14	LMT	BU	1002	-	-	5/21/61/61	0/2/2/2
13	BCL	AW	101	-	-	1/41/137/137	-
13	BCL	AA	1001	-	-	3/41/137/137	-
15	V7N	BU	1001	-	-	8/53/53/53	-
14	LMT	BI	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	C2	1001	-	-	7/21/61/61	0/2/2/2
14	LMT	AE	101	-	-	5/21/61/61	0/2/2/2
15	V7N	bd	101	-	-	5/53/53/53	-
14	LMT	be	101	-	-	4/21/61/61	0/2/2/2
21	CD4	af	102	-	-	22/94/94/94	-
13	BCL	BM	1004	-	-	3/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BX	104	-	-	7/21/61/61	0/2/2/2
14	LMT	H2	201	-	-	7/21/61/61	0/2/2/2
14	LMT	L	306	-	-	7/21/61/61	0/2/2/2
14	LMT	bg	102	-	-	5/21/61/61	0/2/2/2
15	V7N	BI	1001	-	-	6/53/53/53	-
13	BCL	bh	103	-	-	6/41/137/137	-
14	LMT	BU	1003	-	-	10/21/61/61	0/2/2/2
14	LMT	BH	1002	-	-	7/21/61/61	0/2/2/2
14	LMT	BG	1003	-	-	2/21/61/61	0/2/2/2
15	V7N	bn	101	-	-	7/53/53/53	-
13	BCL	AO	102	-	-	2/41/137/137	-
16	0V9	ad	103	-	-	13/48/48/50	-
13	BCL	BP	1003	-	-	8/41/137/137	-
14	LMT	BF	102	-	-	10/21/61/61	0/2/2/2
13	BCL	bp	104	-	-	10/41/137/137	-
14	LMT	BB	104	-	-	4/21/61/61	0/2/2/2
13	BCL	bb	102	-	-	8/41/137/137	-
14	LMT	BM	1003	-	-	6/21/61/61	0/2/2/2
13	BCL	AK	102	28	-	6/41/137/137	-
13	BCL	BB	105	-	-	3/41/137/137	-
13	BCL	ao	102	-	-	4/41/137/137	-
14	LMT	L	309	-	-	1/21/61/61	0/2/2/2
21	CD4	af	104	-	-	20/94/94/94	-
13	BCL	bj	104	-	-	11/41/137/137	-
15	V7N	AS	104	-	-	6/53/53/53	-
18	V75	M	410	12,19	-	0/12/29/29	0/1/1/1
13	BCL	bc	103	-	-	6/41/137/137	-
14	LMT	BQ	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	BE	103	-	-	4/21/61/61	0/2/2/2
13	BCL	AH	102	28	-	11/41/137/137	-
14	LMT	BW	1003	-	-	7/21/61/61	0/2/2/2
15	V7N	bg	101	-	-	5/53/53/53	-
13	BCL	ae	1001	-	-	4/41/137/137	-
14	LMT	BS	1005	-	-	3/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BQ	1004	-	-	6/41/137/137	-
13	BCL	AH	103	-	-	2/41/137/137	-
26	V7B	af	101	-	-	11/48/88/88	0/2/2/2
14	LMT	BP	1005	-	-	3/21/61/61	0/2/2/2
13	BCL	AN	104	28	-	1/41/137/137	-
13	BCL	L	308	-	-	4/41/137/137	-
15	V7N	BA	101	-	-	4/53/53/53	-
14	LMT	BE	102	-	-	4/21/61/61	0/2/2/2
13	BCL	bn	102	-	-	8/41/137/137	-
13	BCL	AB	1001	-	-	1/41/137/137	-
14	LMT	AC	103	-	-	8/21/61/61	0/2/2/2
13	BCL	AE	105	-	-	5/41/137/137	-
14	LMT	BC	103	-	-	5/21/61/61	0/2/2/2
14	LMT	bc	102	-	-	5/21/61/61	0/2/2/2
13	BCL	AJ	104	-	-	6/41/137/137	-
23	MQ8	L	303	-	-	10/47/67/67	0/2/2/2
14	LMT	bk	104	-	-	5/21/61/61	0/2/2/2
13	BCL	AV	103	28	-	5/41/137/137	-
16	0V9	bb	103	-	-	8/48/48/50	-
19	NDG	C1	301	18	-	0/6/23/26	0/1/1/1
14	LMT	BN	1004	-	-	2/21/61/61	0/2/2/2
19	NDG	C	1007	18	-	0/6/23/26	0/1/1/1
14	LMT	BH	1003	-	-	1/21/61/61	0/2/2/2
13	BCL	AT	103	28	-	7/41/137/137	-
14	LMT	BW	1006	-	-	3/21/61/61	0/2/2/2
15	V7N	BH	1001	-	-	8/53/53/53	-
15	V7N	BG	1001	-	-	4/53/53/53	-
13	BCL	AP	102	-	-	6/41/137/137	-
14	LMT	BN	1002	-	-	2/21/61/61	0/2/2/2
13	BCL	BJ	1004	-	-	10/41/137/137	-
14	LMT	AQ	101	-	-	3/21/61/61	0/2/2/2
14	LMT	BX	102	-	-	9/21/61/61	0/2/2/2
14	LMT	BQ	1002	-	-	3/21/61/61	0/2/2/2
13	BCL	BO	1003	-	-	3/41/137/137	-
13	BCL	AT	101	-	-	1/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BS	1003	-	-	8/21/61/61	0/2/2/2
14	LMT	AK	101	-	-	6/21/61/61	0/2/2/2
15	V7N	ba	101	-	-	5/53/53/53	-
16	0V9	bn	104	-	-	9/48/48/50	-
16	0V9	bj	103	-	-	11/48/48/50	-
17	HEC	C	1004	3	-	6/14/54/54	-
14	LMT	bi	104	-	-	3/21/61/61	0/2/2/2
14	LMT	AJ	102	-	-	9/21/61/61	0/2/2/2
14	LMT	bn	103	-	-	7/21/61/61	0/2/2/2
13	BCL	AK	104	-	-	1/41/137/137	-
14	LMT	ac	101	-	-	2/21/61/61	0/2/2/2
15	V7N	bb	101	-	-	5/53/53/53	-
14	LMT	L	302	-	-	1/21/61/61	0/2/2/2
14	LMT	BK	1004	-	-	5/21/61/61	0/2/2/2
13	BCL	be	103	-	-	5/41/137/137	-
13	BCL	BT	103	-	-	4/41/137/137	-
14	LMT	AD	102	-	-	4/21/61/61	0/2/2/2
27	UYH	ai	102	-	-	11/50/70/70	0/1/1/1
13	BCL	aj	101	-	-	7/41/137/137	-
14	LMT	BO	1004	-	-	4/21/61/61	0/2/2/2
15	V7N	BW	1001	-	-	5/53/53/53	-
14	LMT	BW	1004	-	-	6/21/61/61	0/2/2/2
14	LMT	bp	101	-	-	4/21/61/61	0/2/2/2
13	BCL	AC	102	-	-	7/41/137/137	-
13	BCL	AP	103	28	-	8/41/137/137	-
13	BCL	AQ	104	-	-	8/41/137/137	-
20	PGW	H1	101	-	-	13/55/55/55	-
13	BCL	AG	103	-	-	5/41/137/137	-
14	LMT	AK	103	-	-	8/21/61/61	0/2/2/2
13	BCL	bl	104	-	-	7/41/137/137	-
17	HEC	C	1003	3	-	4/14/54/54	-
13	BCL	AL	102	-	-	4/41/137/137	-
15	V7N	bl	101	-	-	7/53/53/53	-
13	BCL	AX	103	-	-	7/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BK	1002	-	-	7/41/137/137	-
15	V7N	bm	101	-	-	5/53/53/53	-
17	HEC	C	1001	3	-	8/14/54/54	-
14	LMT	BJ	1005	-	-	4/21/61/61	0/2/2/2
13	BCL	AS	101	28	-	11/41/137/137	-
14	LMT	BP	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	BO	1005	-	-	4/21/61/61	0/2/2/2
13	BCL	BI	1004	-	-	5/41/137/137	-
13	BCL	AD	104	28	-	4/41/137/137	-
14	LMT	AU	102	-	-	3/21/61/61	0/2/2/2
13	BCL	BH	1005	-	-	7/41/137/137	-
13	BCL	ah	1001	-	-	3/41/137/137	-
14	LMT	BN	1003	-	-	5/21/61/61	0/2/2/2
14	LMT	BK	1003	-	-	3/21/61/61	0/2/2/2
13	BCL	ag	102	-	-	2/41/137/137	-
14	LMT	BP	1006	-	-	6/21/61/61	0/2/2/2
14	LMT	BR	1004	-	-	3/21/61/61	0/2/2/2
13	BCL	BR	1003	-	-	7/41/137/137	-
14	LMT	AJ	101	-	-	2/21/61/61	0/2/2/2
13	BCL	AR	101	-	-	1/41/137/137	-
13	BCL	AN	103	-	-	0/41/137/137	-
14	LMT	BT	101	-	-	7/21/61/61	0/2/2/2
13	BCL	aa	1001	-	-	3/41/137/137	-
15	V7N	bp	102	-	-	4/53/53/53	-
14	LMT	bf	101	-	-	6/21/61/61	0/2/2/2
14	LMT	BM	1002	-	-	6/21/61/61	0/2/2/2
16	0V9	ab	1002	-	-	13/48/48/50	-
13	BCL	AC	101	-	-	2/41/137/137	-
14	LMT	AE	106	-	-	5/21/61/61	0/2/2/2
14	LMT	BJ	1003	-	-	6/21/61/61	0/2/2/2
14	LMT	BV	1002	-	-	6/21/61/61	0/2/2/2
16	0V9	bl	102	-	-	11/48/48/50	-
21	CD4	M	405	-	-	17/94/94/94	-
14	LMT	BT	102	-	-	2/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	AX	102	-	-	4/41/137/137	-
14	LMT	C	1005	-	-	4/21/61/61	0/2/2/2
13	BCL	AW	102	28	-	7/41/137/137	-
15	V7N	AD	101	-	-	8/53/53/53	-
15	V7N	bh	101	-	-	4/53/53/53	-
14	LMT	BV	1004	-	-	6/21/61/61	0/2/2/2
14	LMT	AS	103	-	-	9/21/61/61	0/2/2/2

All (1458) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bc	101	V7N	C28-C27	7.00	1.53	1.34
15	BD	101	V7N	C28-C27	6.90	1.52	1.34
15	BF	101	V7N	C28-C27	6.85	1.52	1.34
15	bi	101	V7N	C28-C27	6.84	1.52	1.34
15	BU	1001	V7N	C28-C27	6.84	1.52	1.34
15	bn	101	V7N	C28-C27	6.83	1.52	1.34
15	bk	101	V7N	C28-C27	6.82	1.52	1.34
15	AM	1001	V7N	C28-C27	6.81	1.52	1.34
15	bp	102	V7N	C28-C27	6.81	1.52	1.34
15	bb	101	V7N	C28-C27	6.79	1.52	1.34
15	AD	101	V7N	C28-C27	6.78	1.52	1.34
15	ba	101	V7N	C28-C27	6.78	1.52	1.34
15	AA	1004	V7N	C28-C27	6.77	1.52	1.34
15	BK	1001	V7N	C28-C27	6.76	1.52	1.34
15	bg	101	V7N	C28-C27	6.74	1.52	1.34
15	BE	101	V7N	C28-C27	6.73	1.52	1.34
15	AW	103	V7N	C28-C27	6.72	1.52	1.34
15	BA	101	V7N	C28-C27	6.70	1.52	1.34
15	BW	1001	V7N	C28-C27	6.70	1.52	1.34
15	BQ	1001	V7N	C28-C27	6.70	1.52	1.34
15	bh	101	V7N	C28-C27	6.70	1.52	1.34
15	BR	1001	V7N	C28-C27	6.69	1.52	1.34
15	BN	1001	V7N	C28-C27	6.69	1.52	1.34
15	AS	104	V7N	C28-C27	6.69	1.52	1.34
15	be	102	V7N	C28-C27	6.68	1.52	1.34
15	bd	101	V7N	C28-C27	6.68	1.52	1.34
15	BG	1001	V7N	C28-C27	6.67	1.52	1.34
15	BO	1001	V7N	C28-C27	6.65	1.52	1.34
15	bo	101	V7N	C28-C27	6.64	1.52	1.34
15	BS	1001	V7N	C28-C27	6.63	1.52	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BJ	1001	V7N	C28-C27	6.63	1.52	1.34
15	BV	1001	V7N	C28-C27	6.63	1.52	1.34
15	BM	1001	V7N	C28-C27	6.63	1.52	1.34
15	BI	1001	V7N	C28-C27	6.63	1.52	1.34
15	BH	1001	V7N	C28-C27	6.61	1.51	1.34
15	ag	101	V7N	C28-C27	6.61	1.51	1.34
15	BP	1001	V7N	C28-C27	6.56	1.51	1.34
15	bl	101	V7N	C28-C27	6.54	1.51	1.34
15	bm	101	V7N	C28-C27	6.51	1.51	1.34
15	bj	101	V7N	C28-C27	6.49	1.51	1.34
17	C	1004	HEC	CAC-C3C	6.39	1.55	1.35
17	C	1001	HEC	CAC-C3C	6.31	1.55	1.35
17	C	1002	HEC	CAB-C3B	6.31	1.55	1.35
17	C	1002	HEC	CAC-C3C	6.29	1.55	1.35
17	C	1003	HEC	CAC-C3C	6.28	1.55	1.35
17	C	1003	HEC	CAB-C3B	6.27	1.55	1.35
17	C	1001	HEC	CAB-C3B	6.21	1.55	1.35
17	C	1004	HEC	CAB-C3B	6.18	1.55	1.35
17	C	1002	HEC	C3D-C2D	5.48	1.53	1.38
17	C	1004	HEC	C3D-C2D	5.45	1.53	1.38
17	C	1003	HEC	C3D-C2D	5.43	1.53	1.38
17	C	1001	HEC	C3D-C2D	5.39	1.53	1.38
13	AX	102	BCL	MG-NA	5.23	2.18	2.06
13	AQ	104	BCL	MG-NA	5.22	2.18	2.06
13	AS	102	BCL	MG-NA	5.18	2.18	2.06
13	AC	101	BCL	MG-NA	5.11	2.18	2.06
13	AB	1001	BCL	MG-NA	5.11	2.18	2.06
13	AH	105	BCL	MG-NA	5.08	2.18	2.06
13	an	1001	BCL	MG-NA	5.08	2.18	2.06
13	AE	105	BCL	MG-NA	5.08	2.18	2.06
13	AL	103	BCL	MG-NA	5.07	2.18	2.06
13	AR	101	BCL	MG-NA	5.07	2.18	2.06
13	AW	101	BCL	MG-NA	5.06	2.18	2.06
13	AV	101	BCL	MG-NA	5.05	2.18	2.06
13	AD	103	BCL	MG-NA	5.05	2.18	2.06
13	AE	104	BCL	MG-NA	5.05	2.18	2.06
13	AL	102	BCL	MG-NA	5.04	2.18	2.06
13	AT	103	BCL	MG-NA	5.03	2.18	2.06
13	AO	102	BCL	MG-NA	5.03	2.18	2.06
13	AG	103	BCL	MG-NA	5.02	2.18	2.06
13	AK	102	BCL	MG-NA	5.02	2.18	2.06
13	AP	102	BCL	MG-NA	5.02	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AF	1001	BCL	MG-NA	5.01	2.18	2.06
13	AB	1002	BCL	MG-NA	5.01	2.18	2.06
13	AJ	104	BCL	MG-NA	5.01	2.18	2.06
13	AK	104	BCL	MG-NA	5.01	2.18	2.06
13	ap	1001	BCL	MG-NA	5.00	2.18	2.06
13	ak	1001	BCL	MG-NA	4.99	2.18	2.06
13	AQ	103	BCL	MG-NA	4.99	2.18	2.06
13	AC	102	BCL	MG-NA	4.97	2.18	2.06
13	AT	101	BCL	MG-NA	4.97	2.18	2.06
13	ai	101	BCL	MG-NA	4.96	2.18	2.06
13	AP	103	BCL	MG-NA	4.96	2.18	2.06
13	ah	1001	BCL	MG-NA	4.96	2.18	2.06
13	AH	103	BCL	MG-NA	4.96	2.18	2.06
13	AX	103	BCL	MG-NA	4.95	2.18	2.06
13	aa	1001	BCL	MG-NA	4.95	2.18	2.06
13	ad	102	BCL	MG-NA	4.94	2.18	2.06
13	AN	104	BCL	MG-NA	4.94	2.18	2.06
13	AU	101	BCL	MG-NA	4.94	2.18	2.06
13	AS	101	BCL	MG-NA	4.93	2.18	2.06
13	AQ	102	BCL	MG-NA	4.93	2.18	2.06
13	am	1001	BCL	MG-NA	4.93	2.18	2.06
13	AN	103	BCL	MG-NA	4.92	2.18	2.06
13	AM	1002	BCL	MG-NA	4.91	2.17	2.06
13	bc	103	BCL	MG-NA	4.90	2.17	2.06
13	AA	1001	BCL	MG-NA	4.90	2.17	2.06
13	AV	103	BCL	MG-NA	4.90	2.17	2.06
13	AW	102	BCL	MG-NA	4.89	2.17	2.06
13	ao	102	BCL	MG-NA	4.89	2.17	2.06
13	AI	101	BCL	MG-NA	4.88	2.17	2.06
13	bk	103	BCL	MG-NA	4.88	2.17	2.06
13	ae	1001	BCL	MG-NA	4.88	2.17	2.06
13	M	408	BCL	MG-NA	4.88	2.17	2.06
13	ab	1001	BCL	MG-NA	4.87	2.17	2.06
13	AM	1004	BCL	MG-NA	4.86	2.17	2.06
13	AU	103	BCL	MG-NA	4.85	2.17	2.06
13	ag	102	BCL	MG-NA	4.84	2.17	2.06
13	bj	104	BCL	MG-NA	4.84	2.17	2.06
13	AJ	103	BCL	MG-NA	4.84	2.17	2.06
13	ba	102	BCL	MG-NA	4.83	2.17	2.06
13	AH	102	BCL	MG-NA	4.83	2.17	2.06
13	AA	1002	BCL	MG-NA	4.82	2.17	2.06
13	bi	102	BCL	MG-NA	4.78	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bg	104	BCL	MG-NA	4.77	2.17	2.06
13	BE	104	BCL	MG-NA	4.77	2.17	2.06
13	BN	1005	BCL	MG-NA	4.76	2.17	2.06
13	ac	102	BCL	MG-NA	4.76	2.17	2.06
13	AG	102	BCL	MG-NA	4.75	2.17	2.06
13	BO	1003	BCL	MG-NA	4.75	2.17	2.06
13	af	103	BCL	MG-NA	4.75	2.17	2.06
13	bd	102	BCL	MG-NA	4.74	2.17	2.06
13	BW	1005	BCL	MG-NA	4.74	2.17	2.06
13	L	308	BCL	MG-NA	4.74	2.17	2.06
13	bh	103	BCL	MG-NA	4.74	2.17	2.06
13	BK	1002	BCL	MG-NA	4.74	2.17	2.06
13	BQ	1004	BCL	MG-NA	4.73	2.17	2.06
13	bl	104	BCL	MG-NA	4.73	2.17	2.06
13	al	1001	BCL	MG-NA	4.72	2.17	2.06
13	AO	101	BCL	MG-NA	4.72	2.17	2.06
13	BD	104	BCL	MG-NA	4.72	2.17	2.06
13	AE	103	BCL	MG-NA	4.71	2.17	2.06
13	BV	1005	BCL	MG-NA	4.70	2.17	2.06
13	aj	101	BCL	MG-NA	4.70	2.17	2.06
13	bb	102	BCL	MG-NA	4.70	2.17	2.06
13	be	103	BCL	MG-NA	4.70	2.17	2.06
13	BM	1004	BCL	MG-NA	4.70	2.17	2.06
13	BL	103	BCL	MG-NA	4.69	2.17	2.06
13	BS	1004	BCL	MG-NA	4.68	2.17	2.06
13	BT	103	BCL	MG-NA	4.68	2.17	2.06
13	bn	102	BCL	MG-NA	4.68	2.17	2.06
27	ai	102	UYH	O8-C28	4.67	1.47	1.33
13	BP	1003	BCL	MG-NA	4.67	2.17	2.06
13	BI	1004	BCL	MG-NA	4.66	2.17	2.06
13	bo	102	BCL	MG-NA	4.65	2.17	2.06
13	L	305	BCL	MG-NA	4.65	2.17	2.06
13	bp	104	BCL	MG-NA	4.65	2.17	2.06
22	M	407	BPH	CBD-CGD	-4.64	1.46	1.52
13	bm	102	BCL	MG-NA	4.64	2.17	2.06
13	BB	105	BCL	MG-NA	4.64	2.17	2.06
13	bf	102	BCL	MG-NA	4.63	2.17	2.06
13	BR	1003	BCL	MG-NA	4.62	2.17	2.06
13	BG	1004	BCL	MG-NA	4.62	2.17	2.06
13	BX	101	BCL	MG-NA	4.62	2.17	2.06
13	BJ	1004	BCL	MG-NA	4.61	2.17	2.06
13	M	406	BCL	MG-NA	4.61	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BC	104	BCL	MG-NA	4.60	2.17	2.06
13	BH	1005	BCL	MG-NA	4.59	2.17	2.06
13	BA	103	BCL	MG-NA	4.59	2.17	2.06
13	BF	103	BCL	MG-NA	4.54	2.17	2.06
13	AD	104	BCL	MG-NA	4.54	2.17	2.06
13	BU	1004	BCL	MG-NA	4.51	2.17	2.06
27	ai	102	UYH	O7-C10	4.47	1.46	1.34
22	L	301	BPH	CBD-CGD	-4.43	1.46	1.52
13	BP	1003	BCL	O2A-CGA	-4.27	1.20	1.33
16	H1	102	0V9	P-O2P	-3.85	1.37	1.50
16	bp	105	0V9	P-O2P	-3.80	1.37	1.50
16	ad	103	0V9	P-O2P	-3.79	1.37	1.50
16	bi	103	0V9	P-O2P	-3.78	1.37	1.50
16	bm	104	0V9	P-O2P	-3.78	1.37	1.50
16	bj	103	0V9	P-O2P	-3.78	1.37	1.50
16	AQ	105	0V9	P-O2P	-3.77	1.37	1.50
16	bb	103	0V9	P-O2P	-3.77	1.37	1.50
16	M	403	0V9	P-O2P	-3.77	1.37	1.50
16	bl	102	0V9	P-O2P	-3.76	1.37	1.50
16	L	310	0V9	P-O2P	-3.76	1.37	1.50
16	bn	104	0V9	P-O2P	-3.76	1.37	1.50
16	ab	1002	0V9	P-O2P	-3.76	1.37	1.50
16	bg	103	0V9	P-O2P	-3.76	1.37	1.50
16	be	105	0V9	P-O2P	-3.76	1.37	1.50
16	bd	103	0V9	P-O2P	-3.76	1.37	1.50
27	ai	102	UYH	O1-C1	3.75	1.46	1.40
16	bo	103	0V9	P-O2P	-3.74	1.37	1.50
16	bk	102	0V9	P-O2P	-3.73	1.37	1.50
13	AQ	104	BCL	MG-NC	3.72	2.15	2.06
16	bf	103	0V9	P-O2P	-3.71	1.37	1.50
13	AC	101	BCL	MG-NC	3.71	2.15	2.06
16	bh	104	0V9	P-O2P	-3.71	1.38	1.50
22	L	301	BPH	C3B-C4B	3.69	1.47	1.41
13	AR	101	BCL	MG-NC	3.64	2.14	2.06
13	AK	102	BCL	MG-NC	3.61	2.14	2.06
13	AS	102	BCL	MG-NC	3.61	2.14	2.06
13	AE	105	BCL	MG-NC	3.56	2.14	2.06
18	M	410	V75	O2-C2	-3.54	1.40	1.46
13	AH	105	BCL	MG-NC	3.54	2.14	2.06
13	AV	101	BCL	MG-NC	3.52	2.14	2.06
13	AO	102	BCL	MG-NC	3.51	2.14	2.06
13	L	305	BCL	MG-NC	3.49	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AL	103	BCL	MG-NC	3.49	2.14	2.06
13	bk	103	BCL	MG-NC	3.49	2.14	2.06
13	AG	103	BCL	MG-NC	3.49	2.14	2.06
13	AO	101	BCL	MG-NC	3.48	2.14	2.06
13	bc	103	BCL	MG-NC	3.48	2.14	2.06
13	AM	1002	BCL	MG-NC	3.47	2.14	2.06
13	AX	102	BCL	MG-NC	3.46	2.14	2.06
13	AN	104	BCL	MG-NC	3.46	2.14	2.06
13	bl	104	BCL	MG-NC	3.46	2.14	2.06
13	an	1001	BCL	MG-NC	3.45	2.14	2.06
13	ad	102	BCL	MG-NC	3.45	2.14	2.06
13	bf	102	BCL	MG-NC	3.45	2.14	2.06
13	bn	102	BCL	MG-NC	3.43	2.14	2.06
13	AT	103	BCL	MG-NC	3.43	2.14	2.06
13	ah	1001	BCL	MG-NC	3.43	2.14	2.06
27	ai	102	UYH	C4-C5	3.43	1.60	1.53
13	AD	103	BCL	MG-NC	3.43	2.14	2.06
13	am	1001	BCL	MG-NC	3.42	2.14	2.06
13	bh	103	BCL	MG-NC	3.42	2.14	2.06
13	AL	102	BCL	MG-NC	3.41	2.14	2.06
13	AQ	102	BCL	MG-NC	3.41	2.14	2.06
13	AX	103	BCL	MG-NC	3.41	2.14	2.06
13	AW	101	BCL	MG-NC	3.41	2.14	2.06
13	AU	103	BCL	MG-NC	3.40	2.14	2.06
13	AE	104	BCL	MG-NC	3.40	2.14	2.06
13	ba	102	BCL	MG-NC	3.39	2.14	2.06
13	ak	1001	BCL	MG-NC	3.39	2.14	2.06
22	M	407	BPH	C3D-CAD	-3.38	1.41	1.47
13	AH	102	BCL	MG-NC	3.38	2.14	2.06
13	bg	104	BCL	MG-NC	3.38	2.14	2.06
13	AA	1001	BCL	MG-NC	3.38	2.14	2.06
13	AP	103	BCL	MG-NC	3.38	2.14	2.06
13	AF	1001	BCL	MG-NC	3.38	2.14	2.06
13	be	103	BCL	MG-NC	3.38	2.14	2.06
13	M	406	BCL	MG-NC	3.37	2.14	2.06
13	AD	104	BCL	MG-NC	3.37	2.14	2.06
13	AS	101	BCL	MG-NC	3.37	2.14	2.06
13	ai	101	BCL	MG-NC	3.37	2.14	2.06
13	bj	104	BCL	MG-NC	3.37	2.14	2.06
13	AB	1002	BCL	MG-NC	3.37	2.14	2.06
27	ai	102	UYH	C29-C28	3.37	1.60	1.50
13	bm	102	BCL	MG-NC	3.36	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AU	101	BCL	MG-NC	3.36	2.14	2.06
22	L	301	BPH	C3D-CAD	-3.36	1.41	1.47
13	AP	102	BCL	MG-NC	3.36	2.14	2.06
13	AB	1001	BCL	MG-NC	3.36	2.14	2.06
13	AE	103	BCL	MG-NC	3.35	2.14	2.06
18	C	1006	V75	O2-C2	-3.35	1.40	1.46
13	AH	103	BCL	MG-NC	3.35	2.14	2.06
13	aa	1001	BCL	MG-NC	3.34	2.14	2.06
13	BN	1005	BCL	MG-NC	3.34	2.14	2.06
13	AJ	103	BCL	MG-NC	3.33	2.14	2.06
18	M	410	V75	O3-C3	-3.33	1.39	1.44
13	AM	1004	BCL	MG-NC	3.32	2.14	2.06
13	ap	1001	BCL	MG-NC	3.32	2.14	2.06
13	bo	102	BCL	MG-NC	3.32	2.14	2.06
13	AC	102	BCL	MG-NC	3.31	2.14	2.06
13	ab	1001	BCL	MG-NC	3.31	2.14	2.06
13	bb	102	BCL	MG-NC	3.30	2.14	2.06
13	AW	102	BCL	MG-NC	3.30	2.14	2.06
13	AQ	103	BCL	MG-NC	3.30	2.14	2.06
13	AT	101	BCL	MG-NC	3.29	2.14	2.06
13	AK	104	BCL	MG-NC	3.29	2.14	2.06
13	AJ	104	BCL	MG-NC	3.29	2.14	2.06
13	BP	1003	BCL	MG-NC	3.29	2.14	2.06
13	ae	1001	BCL	MG-NC	3.28	2.14	2.06
13	AN	103	BCL	MG-NC	3.28	2.14	2.06
13	AA	1002	BCL	MG-NC	3.26	2.14	2.06
13	BO	1003	BCL	MG-NC	3.25	2.14	2.06
13	BE	104	BCL	MG-NC	3.25	2.14	2.06
13	af	103	BCL	MG-NC	3.25	2.14	2.06
13	AI	101	BCL	MG-NC	3.24	2.14	2.06
13	BJ	1004	BCL	MG-NC	3.24	2.14	2.06
13	al	1001	BCL	MG-NC	3.24	2.14	2.06
13	BL	103	BCL	MG-NC	3.23	2.13	2.06
13	BW	1005	BCL	MG-NC	3.23	2.13	2.06
13	BT	103	BCL	MG-NC	3.22	2.13	2.06
13	ac	102	BCL	MG-NC	3.21	2.13	2.06
13	AG	102	BCL	MG-NC	3.21	2.13	2.06
13	AV	103	BCL	MG-NC	3.21	2.13	2.06
13	BQ	1004	BCL	MG-NC	3.21	2.13	2.06
13	ag	102	BCL	MG-NC	3.21	2.13	2.06
13	BI	1004	BCL	MG-NC	3.20	2.13	2.06
13	BV	1005	BCL	MG-NC	3.20	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bp	104	BCL	MG-NC	3.20	2.13	2.06
13	BH	1005	BCL	MG-NC	3.19	2.13	2.06
13	bi	102	BCL	MG-NC	3.19	2.13	2.06
13	BU	1004	BCL	MG-NC	3.18	2.13	2.06
13	BG	1004	BCL	MG-NC	3.17	2.13	2.06
13	ao	102	BCL	MG-NC	3.17	2.13	2.06
13	bd	102	BCL	MG-NC	3.17	2.13	2.06
13	BD	104	BCL	MG-NC	3.16	2.13	2.06
13	BC	104	BCL	MG-NC	3.16	2.13	2.06
13	aj	101	BCL	MG-NC	3.15	2.13	2.06
13	BS	1004	BCL	MG-NC	3.15	2.13	2.06
13	BA	103	BCL	MG-NC	3.14	2.13	2.06
27	ai	102	UYH	C3-C2	3.13	1.60	1.52
13	AX	102	BCL	C3B-C4B	3.13	1.47	1.41
13	BK	1002	BCL	MG-NC	3.13	2.13	2.06
13	BB	105	BCL	MG-NC	3.13	2.13	2.06
13	BX	101	BCL	MG-NC	3.12	2.13	2.06
13	BM	1004	BCL	MG-NC	3.12	2.13	2.06
13	AK	104	BCL	C3B-C4B	3.12	1.47	1.41
13	BF	103	BCL	MG-NC	3.11	2.13	2.06
13	ab	1001	BCL	C3B-C4B	3.10	1.47	1.41
13	AV	101	BCL	C3B-C4B	3.10	1.47	1.41
27	ai	102	UYH	C3-C4	3.10	1.60	1.52
13	AI	101	BCL	C3B-C4B	3.10	1.47	1.41
13	BR	1003	BCL	MG-NC	3.09	2.13	2.06
13	M	408	BCL	MG-NC	3.09	2.13	2.06
27	ai	102	UYH	C11-C10	3.09	1.59	1.50
13	AF	1001	BCL	C3B-C4B	3.08	1.47	1.41
13	AC	102	BCL	C3B-C4B	3.08	1.47	1.41
13	AU	103	BCL	C3B-C4B	3.08	1.47	1.41
13	AT	101	BCL	C3B-C4B	3.08	1.47	1.41
13	AH	103	BCL	C3B-C4B	3.07	1.47	1.41
13	AP	102	BCL	C3B-C4B	3.07	1.47	1.41
13	AO	102	BCL	C3B-C4B	3.06	1.47	1.41
18	C	1006	V75	O3-C3	-3.06	1.40	1.44
13	AM	1004	BCL	C3B-C4B	3.05	1.47	1.41
15	bp	102	V7N	C14-C13	3.03	1.42	1.35
13	AL	102	BCL	C3B-C4B	3.03	1.47	1.41
13	AQ	103	BCL	C3B-C4B	3.02	1.47	1.41
13	AA	1001	BCL	C3B-C4B	3.02	1.47	1.41
13	AX	103	BCL	C3B-C4B	3.01	1.47	1.41
13	ag	102	BCL	C3B-C4B	2.99	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AE	105	BCL	C3B-C4B	2.99	1.47	1.41
13	AL	103	BCL	C3B-C4B	2.99	1.47	1.41
13	AU	101	BCL	C3B-C4B	2.99	1.47	1.41
13	AR	101	BCL	C3B-C4B	2.98	1.47	1.41
13	ae	1001	BCL	C3B-C4B	2.98	1.47	1.41
13	L	305	BCL	O1A-CGA	-2.98	1.13	1.22
13	AG	103	BCL	C3B-C4B	2.97	1.47	1.41
15	bb	101	V7N	C14-C13	2.97	1.42	1.35
13	AJ	104	BCL	C3B-C4B	2.97	1.47	1.41
13	L	308	BCL	MG-NC	2.94	2.13	2.06
27	ai	102	UYH	C9-C8	2.93	1.60	1.50
13	AQ	104	BCL	C3B-C4B	2.93	1.46	1.41
13	aa	1001	BCL	C3B-C4B	2.90	1.46	1.41
13	AE	104	BCL	C3B-C4B	2.90	1.46	1.41
15	bn	101	V7N	C14-C13	2.90	1.42	1.35
13	AW	101	BCL	C3B-C4B	2.88	1.46	1.41
13	AO	101	BCL	C3B-C4B	2.87	1.46	1.41
15	bp	102	V7N	C17-C18	2.86	1.42	1.35
13	M	408	BCL	C3B-C4B	2.86	1.46	1.41
15	BU	1001	V7N	C14-C13	2.85	1.42	1.35
13	AM	1002	BCL	C3B-C4B	2.84	1.46	1.41
13	al	1001	BCL	C3B-C4B	2.84	1.46	1.41
15	AA	1004	V7N	C14-C13	2.83	1.42	1.35
14	AA	1003	LMT	O2'-C2'	-2.82	1.36	1.43
27	ai	102	UYH	C7-C8	2.82	1.59	1.50
15	BH	1001	V7N	C14-C13	2.82	1.42	1.35
13	AH	102	BCL	C3B-C4B	2.82	1.46	1.41
13	AB	1002	BCL	C3B-C4B	2.82	1.46	1.41
13	AE	103	BCL	C3B-C4B	2.81	1.46	1.41
15	bk	101	V7N	C14-C13	2.81	1.42	1.35
13	AH	105	BCL	C3B-C4B	2.80	1.46	1.41
15	BA	101	V7N	C14-C13	2.80	1.42	1.35
15	AW	103	V7N	C14-C13	2.79	1.42	1.35
15	bm	101	V7N	C14-C13	2.78	1.42	1.35
13	ao	102	BCL	C3B-C4B	2.78	1.46	1.41
14	AK	101	LMT	O3'-C3'	-2.78	1.36	1.43
15	ba	101	V7N	C14-C13	2.78	1.42	1.35
13	AW	102	BCL	C3B-C4B	2.77	1.46	1.41
13	AU	103	BCL	CHD-C1D	2.77	1.43	1.38
13	AP	103	BCL	C3B-C4B	2.76	1.46	1.41
13	ad	102	BCL	C3B-C4B	2.76	1.46	1.41
15	BD	101	V7N	C14-C13	2.76	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bi	101	V7N	C14-C13	2.76	1.42	1.35
15	bb	101	V7N	C17-C18	2.76	1.42	1.35
15	bl	101	V7N	C14-C13	2.75	1.42	1.35
15	bc	101	V7N	C14-C13	2.74	1.42	1.35
13	AG	102	BCL	CHD-C1D	2.74	1.43	1.38
15	bo	101	V7N	C14-C13	2.73	1.42	1.35
13	AN	103	BCL	C3B-C4B	2.73	1.46	1.41
15	bg	101	V7N	C14-C13	2.73	1.42	1.35
13	AQ	102	BCL	C3B-C4B	2.72	1.46	1.41
15	bk	101	V7N	C17-C18	2.72	1.42	1.35
13	an	1001	BCL	C3B-C4B	2.72	1.46	1.41
13	AJ	103	BCL	C3B-C4B	2.72	1.46	1.41
15	bh	101	V7N	C14-C13	2.71	1.42	1.35
15	be	102	V7N	C14-C13	2.70	1.42	1.35
15	BU	1001	V7N	C17-C18	2.70	1.42	1.35
15	BO	1001	V7N	C14-C13	2.70	1.42	1.35
14	bc	102	LMT	O3'-C3'	-2.70	1.36	1.43
13	ah	1001	BCL	C3B-C4B	2.69	1.46	1.41
13	AB	1002	BCL	CHD-C1D	2.69	1.43	1.38
13	AS	101	BCL	C3B-C4B	2.69	1.46	1.41
26	af	101	V7B	O7-C8	-2.69	1.40	1.46
15	AW	103	V7N	C17-C18	2.69	1.42	1.35
13	ac	102	BCL	C3B-C4B	2.69	1.46	1.41
14	bj	102	LMT	O3'-C3'	-2.68	1.36	1.43
13	AS	102	BCL	C3B-C4B	2.68	1.46	1.41
14	bo	104	LMT	O3'-C3'	-2.68	1.36	1.43
14	bm	103	LMT	O3'-C3'	-2.68	1.36	1.43
15	bd	101	V7N	C14-C13	2.68	1.42	1.35
15	bn	101	V7N	C17-C18	2.68	1.42	1.35
13	bp	104	BCL	C3B-C4B	2.68	1.46	1.41
15	BF	101	V7N	C14-C13	2.67	1.42	1.35
13	AG	102	BCL	C3B-C4B	2.67	1.46	1.41
15	AD	101	V7N	C14-C13	2.67	1.42	1.35
15	BI	1001	V7N	C14-C13	2.67	1.42	1.35
15	ag	101	V7N	C14-C13	2.67	1.42	1.35
14	L	306	LMT	O3'-C3'	-2.66	1.36	1.43
15	bc	101	V7N	C17-C18	2.66	1.41	1.35
13	AS	102	BCL	CHD-C1D	2.66	1.43	1.38
27	ai	102	UYH	C1-C2	2.65	1.60	1.52
15	BW	1001	V7N	C14-C13	2.64	1.41	1.35
15	bo	101	V7N	C17-C18	2.64	1.41	1.35
15	ba	101	V7N	C17-C18	2.64	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BK	1001	V7N	C14-C13	2.64	1.41	1.35
13	ai	101	BCL	C3B-C4B	2.64	1.46	1.41
15	BN	1001	V7N	C14-C13	2.64	1.41	1.35
14	BR	1004	LMT	O3'-C3'	-2.64	1.36	1.43
13	AH	105	BCL	CHD-C1D	2.64	1.43	1.38
15	BR	1001	V7N	C14-C13	2.63	1.41	1.35
15	BS	1001	V7N	C14-C13	2.63	1.41	1.35
13	M	406	BCL	C3B-C4B	2.63	1.46	1.41
15	BJ	1001	V7N	C14-C13	2.63	1.41	1.35
14	AS	103	LMT	O2B-C2B	-2.63	1.36	1.43
15	bd	101	V7N	C17-C18	2.63	1.41	1.35
15	BH	1001	V7N	C17-C18	2.63	1.41	1.35
15	BV	1001	V7N	C14-C13	2.63	1.41	1.35
14	BJ	1005	LMT	O3'-C3'	-2.62	1.36	1.43
15	AA	1004	V7N	C17-C18	2.62	1.41	1.35
15	bi	101	V7N	C17-C18	2.62	1.41	1.35
13	AN	104	BCL	C3B-C4B	2.62	1.46	1.41
14	BW	1002	LMT	O3'-C3'	-2.61	1.36	1.43
14	BX	102	LMT	O3'-C3'	-2.61	1.36	1.43
14	bh	102	LMT	O3'-C3'	-2.61	1.36	1.43
15	BQ	1001	V7N	C14-C13	2.61	1.41	1.35
13	aj	101	BCL	C3B-C4B	2.61	1.46	1.41
13	bl	104	BCL	C3B-C4B	2.61	1.46	1.41
13	AT	103	BCL	C3B-C4B	2.60	1.46	1.41
15	AS	104	V7N	C14-C13	2.60	1.41	1.35
13	AL	103	BCL	CHD-C1D	2.60	1.43	1.38
27	ai	102	UYH	C6-C5	2.60	1.60	1.51
14	AA	1003	LMT	O3'-C3'	-2.60	1.36	1.43
14	C	1005	LMT	O3'-C3'	-2.59	1.36	1.43
14	BM	1002	LMT	O3'-C3'	-2.59	1.36	1.43
15	bh	101	V7N	C17-C18	2.59	1.41	1.35
14	BI	1002	LMT	O3'-C3'	-2.59	1.36	1.43
14	ac	101	LMT	O3'-C3'	-2.59	1.36	1.43
15	bl	101	V7N	C17-C18	2.59	1.41	1.35
14	BN	1004	LMT	O3'-C3'	-2.59	1.36	1.43
15	bj	101	V7N	C14-C13	2.59	1.41	1.35
26	ag	103	V7B	O7-C8	-2.58	1.40	1.46
14	AM	1003	LMT	O3'-C3'	-2.58	1.36	1.43
15	BA	101	V7N	C17-C18	2.58	1.41	1.35
15	bj	101	V7N	C17-C18	2.58	1.41	1.35
13	bd	102	BCL	C3B-C4B	2.58	1.46	1.41
15	BD	101	V7N	C17-C18	2.58	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BW	1005	BCL	C3B-C4B	2.57	1.46	1.41
13	AD	104	BCL	C3B-C4B	2.57	1.46	1.41
14	be	104	LMT	O3'-C3'	-2.57	1.36	1.43
13	M	406	BCL	CHD-C1D	2.57	1.43	1.38
15	BG	1001	V7N	C14-C13	2.57	1.41	1.35
14	AV	102	LMT	O3'-C3'	-2.57	1.36	1.43
15	BO	1001	V7N	C17-C18	2.57	1.41	1.35
13	AE	105	BCL	CHD-C1D	2.56	1.43	1.38
14	bk	104	LMT	O3'-C3'	-2.56	1.36	1.43
14	BB	101	LMT	O3'-C3'	-2.56	1.36	1.43
14	bg	102	LMT	O3'-C3'	-2.56	1.36	1.43
13	ap	1001	BCL	C3B-C4B	2.56	1.46	1.41
14	AH	104	LMT	O3'-C3'	-2.56	1.36	1.43
14	BJ	1003	LMT	O3'-C3'	-2.56	1.36	1.43
15	BE	101	V7N	C14-C13	2.56	1.41	1.35
13	AK	102	BCL	CHD-C1D	2.56	1.43	1.38
13	ak	1001	BCL	C3B-C4B	2.55	1.46	1.41
15	AD	101	V7N	C17-C18	2.55	1.41	1.35
14	L	309	LMT	O3'-C3'	-2.55	1.36	1.43
14	AG	101	LMT	O3'-C3'	-2.55	1.36	1.43
15	AM	1001	V7N	C14-C13	2.55	1.41	1.35
13	am	1001	BCL	C3B-C4B	2.55	1.46	1.41
14	AT	102	LMT	O3'-C3'	-2.55	1.36	1.43
13	bi	102	BCL	C3B-C4B	2.55	1.46	1.41
13	BR	1003	BCL	C3B-C4B	2.55	1.46	1.41
13	AC	101	BCL	CHD-C1D	2.55	1.43	1.38
14	BW	1003	LMT	O3'-C3'	-2.55	1.36	1.43
14	BB	102	LMT	O3'-C3'	-2.54	1.36	1.43
14	BG	1002	LMT	O3'-C3'	-2.54	1.36	1.43
13	AC	101	BCL	C3B-C4B	2.54	1.46	1.41
15	bm	101	V7N	C17-C18	2.54	1.41	1.35
14	bi	104	LMT	O3'-C3'	-2.54	1.36	1.43
14	bn	103	LMT	O3'-C3'	-2.54	1.36	1.43
14	BE	103	LMT	O3'-C3'	-2.54	1.36	1.43
14	BW	1004	LMT	O3'-C3'	-2.54	1.36	1.43
14	AJ	102	LMT	O3'-C3'	-2.54	1.36	1.43
14	AS	103	LMT	O3'-C3'	-2.54	1.36	1.43
15	bg	101	V7N	C17-C18	2.54	1.41	1.35
13	AW	102	BCL	CHD-C1D	2.53	1.43	1.38
14	BO	1004	LMT	O3'-C3'	-2.53	1.36	1.43
13	af	103	BCL	C3B-C4B	2.53	1.46	1.41
13	be	103	BCL	C3B-C4B	2.53	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BM	1001	V7N	C14-C13	2.53	1.41	1.35
14	BJ	1002	LMT	O3'-C3'	-2.53	1.36	1.43
14	AB	1003	LMT	O3'-C3'	-2.52	1.36	1.43
14	AN	101	LMT	O3'-C3'	-2.52	1.36	1.43
14	bf	101	LMT	O3'-C3'	-2.52	1.36	1.43
14	BG	1005	LMT	O3'-C3'	-2.52	1.36	1.43
15	BF	101	V7N	C17-C18	2.52	1.41	1.35
14	AE	106	LMT	O3'-C3'	-2.52	1.36	1.43
14	BS	1003	LMT	O3'-C3'	-2.52	1.36	1.43
14	BP	1006	LMT	O3'-C3'	-2.52	1.36	1.43
14	BK	1005	LMT	O3'-C3'	-2.51	1.36	1.43
13	bb	102	BCL	C3B-C4B	2.51	1.46	1.41
14	AD	102	LMT	O3'-C3'	-2.51	1.36	1.43
15	BP	1001	V7N	C14-C13	2.51	1.41	1.35
14	BT	102	LMT	O3'-C3'	-2.51	1.36	1.43
13	AQ	102	BCL	CHD-C1D	2.51	1.43	1.38
14	AN	102	LMT	O3'-C3'	-2.51	1.36	1.43
14	BL	101	LMT	O3'-C3'	-2.51	1.36	1.43
14	BD	105	LMT	O3'-C3'	-2.51	1.36	1.43
13	AE	103	BCL	CHD-C1D	2.50	1.43	1.38
13	AH	102	BCL	CHD-C1D	2.50	1.43	1.38
14	BH	1002	LMT	O3'-C3'	-2.50	1.36	1.43
14	BH	1003	LMT	O3'-C3'	-2.50	1.36	1.43
15	BR	1001	V7N	C17-C18	2.50	1.41	1.35
14	BC	103	LMT	O3'-C3'	-2.50	1.36	1.43
15	be	102	V7N	C17-C18	2.50	1.41	1.35
14	BP	1004	LMT	O3'-C3'	-2.49	1.36	1.43
14	BQ	1002	LMT	O3'-C3'	-2.49	1.36	1.43
14	BP	1002	LMT	O3'-C3'	-2.49	1.36	1.43
13	AX	103	BCL	CHD-C1D	2.49	1.43	1.38
14	L	304	LMT	O3'-C3'	-2.49	1.36	1.43
14	BR	1002	LMT	O3'-C3'	-2.49	1.36	1.43
15	BK	1001	V7N	C17-C18	2.49	1.41	1.35
15	BU	1001	V7N	C6-C5	2.48	1.41	1.35
15	bp	102	V7N	C11-C12	2.48	1.41	1.34
14	BE	105	LMT	O2'-C2'	-2.48	1.36	1.43
14	BX	104	LMT	O3'-C3'	-2.48	1.36	1.43
13	AN	104	BCL	CHD-C1D	2.48	1.43	1.38
14	BD	102	LMT	O3'-C3'	-2.48	1.36	1.43
14	AJ	101	LMT	O3'-C3'	-2.48	1.36	1.43
14	BR	1006	LMT	O3'-C3'	-2.48	1.36	1.43
14	BJ	1006	LMT	O3'-C3'	-2.48	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BX	103	LMT	O3'-C3'	-2.48	1.36	1.43
13	bo	102	BCL	C3B-C4B	2.47	1.46	1.41
14	BF	104	LMT	O3'-C3'	-2.47	1.36	1.43
14	BK	1003	LMT	O3'-C3'	-2.47	1.36	1.43
13	bg	104	BCL	C3B-C4B	2.47	1.46	1.41
14	BS	1002	LMT	O3'-C3'	-2.47	1.36	1.43
14	AE	101	LMT	O3'-C3'	-2.47	1.36	1.43
14	be	104	LMT	O2'-C2'	-2.47	1.36	1.43
14	BW	1006	LMT	O3'-C3'	-2.47	1.36	1.43
14	BU	1002	LMT	O3'-C3'	-2.47	1.36	1.43
13	M	408	BCL	C3D-C4D	-2.47	1.38	1.44
15	AS	104	V7N	C17-C18	2.47	1.41	1.35
13	bm	102	BCL	C3B-C4B	2.47	1.46	1.41
14	AH	101	LMT	O3'-C3'	-2.47	1.36	1.43
14	BV	1003	LMT	O3'-C3'	-2.47	1.36	1.43
14	BU	1003	LMT	O3'-C3'	-2.46	1.36	1.43
14	AV	104	LMT	O3'-C3'	-2.46	1.36	1.43
14	bp	101	LMT	O3'-C3'	-2.46	1.36	1.43
14	BN	1002	LMT	O3'-C3'	-2.46	1.36	1.43
14	bl	103	LMT	O3'-C3'	-2.46	1.36	1.43
14	BV	1002	LMT	O3'-C3'	-2.46	1.36	1.43
14	BT	101	LMT	O3'-C3'	-2.46	1.36	1.43
14	AP	101	LMT	O3'-C3'	-2.46	1.36	1.43
14	BF	102	LMT	O3'-C3'	-2.46	1.36	1.43
14	BV	1004	LMT	O3'-C3'	-2.46	1.36	1.43
15	bb	101	V7N	C11-C12	2.46	1.41	1.34
14	BI	1003	LMT	O3'-C3'	-2.46	1.36	1.43
14	H2	201	LMT	O3'-C3'	-2.45	1.36	1.43
15	BQ	1001	V7N	C17-C18	2.45	1.41	1.35
15	BN	1001	V7N	C17-C18	2.45	1.41	1.35
13	BD	104	BCL	O2A-CGA	-2.45	1.26	1.33
15	ag	101	V7N	C17-C18	2.45	1.41	1.35
14	BB	103	LMT	O3'-C3'	-2.45	1.36	1.43
14	bp	103	LMT	O3'-C3'	-2.45	1.36	1.43
13	bc	103	BCL	C3B-C4B	2.45	1.45	1.41
15	AM	1001	V7N	C17-C18	2.44	1.41	1.35
14	AQ	101	LMT	O3'-C3'	-2.44	1.36	1.43
14	BE	105	LMT	O3'-C3'	-2.44	1.36	1.43
15	BW	1001	V7N	C17-C18	2.44	1.41	1.35
13	AS	101	BCL	CHD-C1D	2.44	1.43	1.38
14	AK	103	LMT	O3'-C3'	-2.44	1.36	1.43
14	BO	1002	LMT	O3'-C3'	-2.44	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	302	LMT	O3'-C3'	-2.44	1.36	1.43
14	BG	1003	LMT	O3'-C3'	-2.44	1.36	1.43
14	BP	1005	LMT	O3'-C3'	-2.44	1.36	1.43
14	BO	1005	LMT	O3'-C3'	-2.44	1.36	1.43
13	BT	103	BCL	C3B-C4B	2.44	1.45	1.41
14	BQ	1003	LMT	O3'-C3'	-2.44	1.36	1.43
14	BB	104	LMT	O3'-C3'	-2.44	1.36	1.43
14	BN	1003	LMT	O3'-C3'	-2.44	1.36	1.43
13	ba	102	BCL	C3B-C4B	2.44	1.45	1.41
14	AC	103	LMT	O3'-C3'	-2.43	1.36	1.43
14	BK	1005	LMT	O2'-C2'	-2.43	1.36	1.43
14	bh	102	LMT	O2'-C2'	-2.43	1.36	1.43
14	BI	1005	LMT	O3'-C3'	-2.43	1.36	1.43
14	AX	101	LMT	O3'-C3'	-2.43	1.36	1.43
13	L	308	BCL	C3B-C4B	2.43	1.45	1.41
14	AE	102	LMT	O3'-C3'	-2.43	1.36	1.43
14	BL	102	LMT	O3'-C3'	-2.43	1.36	1.43
13	AM	1002	BCL	CHD-C1D	2.43	1.43	1.38
15	BV	1001	V7N	C12-C13	-2.43	1.40	1.46
14	AE	101	LMT	O2'-C2'	-2.42	1.37	1.43
14	BR	1002	LMT	O2'-C2'	-2.42	1.37	1.43
15	BU	1001	V7N	C11-C12	2.42	1.41	1.34
15	BI	1001	V7N	C17-C18	2.42	1.41	1.35
13	AT	103	BCL	CHD-C1D	2.42	1.43	1.38
14	BT	104	LMT	O3'-C3'	-2.42	1.37	1.43
14	BD	102	LMT	O2'-C2'	-2.42	1.37	1.43
15	bn	101	V7N	C11-C12	2.42	1.41	1.34
13	BV	1005	BCL	C3B-C4B	2.42	1.45	1.41
13	bl	104	BCL	C1D-C2D	-2.41	1.40	1.45
13	BH	1005	BCL	CHD-C1D	2.41	1.43	1.38
14	AU	102	LMT	O3'-C3'	-2.41	1.37	1.43
14	BV	1002	LMT	O2'-C2'	-2.41	1.37	1.43
13	L	305	BCL	C3B-C4B	2.41	1.45	1.41
13	bm	102	BCL	C3D-C4D	-2.41	1.38	1.44
13	bk	103	BCL	C3B-C4B	2.41	1.45	1.41
14	BC	102	LMT	O3'-C3'	-2.41	1.37	1.43
13	M	406	BCL	C3D-C4D	-2.40	1.38	1.44
13	AJ	103	BCL	CHD-C1D	2.40	1.43	1.38
13	BK	1002	BCL	C3B-C4B	2.40	1.45	1.41
13	M	406	BCL	O1A-CGA	-2.40	1.15	1.22
14	C2	1001	LMT	O3'-C3'	-2.40	1.37	1.43
15	BE	101	V7N	C17-C18	2.40	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AQ	101	LMT	O2'-C2'	-2.40	1.37	1.43
13	AA	1002	BCL	CHD-C1D	2.39	1.43	1.38
13	bl	104	BCL	C3D-C4D	-2.39	1.38	1.44
13	BO	1003	BCL	C3D-C4D	-2.39	1.38	1.44
14	BW	1002	LMT	O2'-C2'	-2.39	1.37	1.43
15	BS	1001	V7N	C17-C18	2.38	1.41	1.35
14	bn	103	LMT	O2'-C2'	-2.38	1.37	1.43
14	BS	1005	LMT	O3'-C3'	-2.38	1.37	1.43
15	ba	101	V7N	C11-C12	2.38	1.40	1.34
14	BA	102	LMT	O3'-C3'	-2.38	1.37	1.43
13	bc	103	BCL	C1D-C2D	-2.38	1.40	1.45
15	BG	1001	V7N	C17-C18	2.38	1.41	1.35
15	bl	101	V7N	C11-C12	2.38	1.40	1.34
13	BM	1004	BCL	C3B-C4B	2.38	1.45	1.41
13	AC	102	BCL	CHD-C1D	2.38	1.43	1.38
14	L	306	LMT	O2'-C2'	-2.38	1.37	1.43
15	BJ	1001	V7N	C17-C18	2.38	1.41	1.35
13	AD	104	BCL	CHD-C1D	2.38	1.43	1.38
14	L	307	LMT	O3'-C3'	-2.38	1.37	1.43
14	BC	101	LMT	O3'-C3'	-2.37	1.37	1.43
14	BM	1005	LMT	O3'-C3'	-2.37	1.37	1.43
13	bj	104	BCL	CHD-C1D	2.37	1.43	1.38
14	BO	1002	LMT	O2'-C2'	-2.37	1.37	1.43
13	AQ	104	BCL	CHD-C1D	2.37	1.43	1.38
15	AW	103	V7N	C11-C12	2.37	1.40	1.34
13	BS	1004	BCL	C3B-C4B	2.37	1.45	1.41
14	BE	103	LMT	O2'-C2'	-2.37	1.37	1.43
14	BD	106	LMT	O3'-C3'	-2.37	1.37	1.43
14	BJ	1002	LMT	O2'-C2'	-2.36	1.37	1.43
14	BR	1005	LMT	O3'-C3'	-2.36	1.37	1.43
13	AW	101	BCL	CHD-C1D	2.36	1.43	1.38
15	AA	1004	V7N	C11-C12	2.36	1.40	1.34
14	AL	101	LMT	O3'-C3'	-2.36	1.37	1.43
13	M	408	BCL	CHD-C1D	2.36	1.43	1.38
13	bg	104	BCL	C3D-C4D	-2.36	1.38	1.44
13	BA	103	BCL	C3B-C4B	2.36	1.45	1.41
15	bk	101	V7N	C11-C12	2.36	1.40	1.34
13	bk	103	BCL	C3D-C4D	-2.36	1.38	1.44
13	AA	1002	BCL	C3B-C4B	2.35	1.45	1.41
13	L	308	BCL	CHD-C1D	2.35	1.43	1.38
14	AT	104	LMT	O3'-C3'	-2.35	1.37	1.43
13	BD	104	BCL	C3B-C4B	2.35	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	M	407	BPH	C3B-C4B	2.35	1.45	1.41
13	bd	102	BCL	C3D-C4D	-2.35	1.38	1.44
13	AU	101	BCL	CHD-C1D	2.35	1.43	1.38
14	bg	102	LMT	O2'-C2'	-2.35	1.37	1.43
13	BP	1003	BCL	O2A-C1	-2.35	1.39	1.46
13	BI	1004	BCL	C3D-C4D	-2.35	1.38	1.44
13	aj	101	BCL	C3D-C4D	-2.35	1.38	1.44
15	BP	1001	V7N	C12-C13	-2.35	1.40	1.46
26	af	101	V7B	O8-C9	-2.34	1.39	1.45
14	AL	101	LMT	O2'-C2'	-2.34	1.37	1.43
14	BM	1003	LMT	O3'-C3'	-2.34	1.37	1.43
13	am	1001	BCL	C3D-C4D	-2.34	1.38	1.44
15	AM	1001	V7N	C12-C13	-2.34	1.40	1.46
13	bh	103	BCL	C3B-C4B	2.34	1.45	1.41
15	BV	1001	V7N	C17-C18	2.34	1.41	1.35
14	be	101	LMT	O3'-C3'	-2.34	1.37	1.43
14	bo	104	LMT	O2'-C2'	-2.34	1.37	1.43
14	BX	103	LMT	O2'-C2'	-2.33	1.37	1.43
13	bo	102	BCL	C3D-C4D	-2.33	1.38	1.44
18	C	1006	V75	O2-C2A	2.33	1.40	1.35
14	BD	103	LMT	O3'-C3'	-2.33	1.37	1.43
14	bp	101	LMT	O2'-C2'	-2.33	1.37	1.43
13	AO	101	BCL	CHD-C1D	2.33	1.42	1.38
15	BH	1001	V7N	C11-C12	2.33	1.40	1.34
14	BH	1002	LMT	O2'-C2'	-2.33	1.37	1.43
26	ag	103	V7B	O8-C28	2.33	1.40	1.33
15	BM	1001	V7N	C12-C13	-2.33	1.41	1.46
13	BQ	1004	BCL	C3D-C4D	-2.33	1.39	1.44
13	AN	103	BCL	CHD-C1D	2.33	1.42	1.38
13	al	1001	BCL	C3D-C4D	-2.33	1.39	1.44
13	BL	103	BCL	C3D-C4D	-2.33	1.39	1.44
14	be	101	LMT	O2'-C2'	-2.33	1.37	1.43
13	bj	104	BCL	C3D-C4D	-2.32	1.39	1.44
13	BG	1004	BCL	C3D-C4D	-2.32	1.39	1.44
13	bj	104	BCL	C3B-C4B	2.32	1.45	1.41
13	BN	1005	BCL	C3D-C4D	-2.32	1.39	1.44
15	BD	101	V7N	C11-C12	2.32	1.40	1.34
13	BE	104	BCL	CHD-C1D	2.32	1.42	1.38
13	AS	102	BCL	C3D-C4D	-2.32	1.39	1.44
13	AP	103	BCL	CHD-C1D	2.32	1.42	1.38
14	AX	101	LMT	O2'-C2'	-2.32	1.37	1.43
14	bj	102	LMT	O2'-C2'	-2.32	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BB	105	BCL	CHD-C1D	2.32	1.42	1.38
13	BU	1004	BCL	C3D-C4D	-2.32	1.39	1.44
15	BO	1001	V7N	C11-C12	2.32	1.40	1.34
13	AV	103	BCL	CHD-C1D	2.32	1.42	1.38
13	BB	105	BCL	C3B-C4B	2.32	1.45	1.41
13	ag	102	BCL	C3D-C4D	-2.32	1.39	1.44
15	bb	101	V7N	C7-C8	2.32	1.40	1.34
13	BC	104	BCL	C3B-C4B	2.31	1.45	1.41
14	AG	101	LMT	O2'-C2'	-2.31	1.37	1.43
15	BP	1001	V7N	C17-C18	2.31	1.41	1.35
15	BE	101	V7N	C12-C13	-2.31	1.41	1.46
13	ao	102	BCL	C3D-C4D	-2.31	1.39	1.44
13	BE	104	BCL	C3B-C4B	2.31	1.45	1.41
13	ah	1001	BCL	C3D-C4D	-2.31	1.39	1.44
14	BH	1004	LMT	O3'-C3'	-2.31	1.37	1.43
13	bi	102	BCL	C3D-C4D	-2.31	1.39	1.44
15	BK	1001	V7N	C11-C12	2.31	1.40	1.34
14	be	101	LMT	O3B-C3B	-2.31	1.37	1.43
14	BE	102	LMT	O3'-C3'	-2.31	1.37	1.43
13	AI	101	BCL	CHD-C1D	2.31	1.42	1.38
15	bk	101	V7N	C7-C8	2.31	1.40	1.34
13	bn	102	BCL	C3D-C4D	-2.31	1.39	1.44
13	AK	102	BCL	C3B-C4B	2.31	1.45	1.41
13	bn	102	BCL	C3B-C4B	2.31	1.45	1.41
13	be	103	BCL	C3D-C4D	-2.31	1.39	1.44
13	BJ	1004	BCL	C3D-C4D	-2.30	1.39	1.44
14	bf	101	LMT	O2'-C2'	-2.30	1.37	1.43
13	L	308	BCL	C3D-C4D	-2.30	1.39	1.44
13	BR	1003	BCL	C3D-C4D	-2.30	1.39	1.44
14	AJ	101	LMT	O2'-C2'	-2.30	1.37	1.43
14	BP	1006	LMT	O2'-C2'	-2.30	1.37	1.43
13	bm	102	BCL	C1D-C2D	-2.30	1.40	1.45
13	BL	103	BCL	CHD-C1D	2.30	1.42	1.38
15	BM	1001	V7N	C17-C18	2.30	1.41	1.35
14	L	302	LMT	O2'-C2'	-2.30	1.37	1.43
14	BJ	1005	LMT	O2'-C2'	-2.30	1.37	1.43
14	L	304	LMT	O3B-C3B	-2.30	1.37	1.43
14	BV	1004	LMT	O2'-C2'	-2.30	1.37	1.43
13	bc	103	BCL	C3D-C4D	-2.30	1.39	1.44
15	bd	101	V7N	C11-C12	2.29	1.40	1.34
13	BM	1004	BCL	C3D-C4D	-2.29	1.39	1.44
14	bo	104	LMT	O2B-C2B	-2.29	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BI	1002	LMT	O2'-C2'	-2.29	1.37	1.43
14	BK	1004	LMT	O3'-C3'	-2.29	1.37	1.43
14	AH	101	LMT	O3B-C3B	-2.29	1.37	1.43
13	al	1001	BCL	CHD-C1D	2.29	1.42	1.38
15	bm	101	V7N	C11-C12	2.29	1.40	1.34
13	BM	1004	BCL	CHD-C1D	2.29	1.42	1.38
13	AL	102	BCL	CHD-C1D	2.29	1.42	1.38
13	AP	102	BCL	C3D-C4D	-2.29	1.39	1.44
14	BD	105	LMT	O2'-C2'	-2.29	1.37	1.43
14	BG	1002	LMT	O2'-C2'	-2.29	1.37	1.43
15	bh	101	V7N	C11-C12	2.29	1.40	1.34
14	AE	101	LMT	O2B-C2B	-2.29	1.37	1.43
14	BW	1004	LMT	O2'-C2'	-2.28	1.37	1.43
15	bp	102	V7N	C7-C8	2.28	1.40	1.34
13	AG	103	BCL	C3D-C4D	-2.28	1.39	1.44
13	bb	102	BCL	C3D-C4D	-2.28	1.39	1.44
26	ag	103	V7B	O7-C10	2.28	1.40	1.34
14	AJ	102	LMT	O2B-C2B	-2.28	1.37	1.43
14	BP	1002	LMT	O2'-C2'	-2.28	1.37	1.43
15	BA	101	V7N	C11-C12	2.28	1.40	1.34
15	bg	101	V7N	C11-C12	2.28	1.40	1.34
14	AS	103	LMT	O2'-C2'	-2.28	1.37	1.43
13	BB	105	BCL	C3D-C4D	-2.28	1.39	1.44
14	BM	1002	LMT	O2'-C2'	-2.28	1.37	1.43
13	BS	1004	BCL	C3D-C4D	-2.28	1.39	1.44
15	BR	1001	V7N	C11-C12	2.28	1.40	1.34
27	ai	102	UYH	C12-C11	2.28	1.60	1.52
14	bi	104	LMT	O3B-C3B	-2.28	1.37	1.43
13	AV	103	BCL	C3B-C4B	2.28	1.45	1.41
13	AU	101	BCL	C3D-C4D	-2.28	1.39	1.44
13	BG	1004	BCL	CHD-C1D	2.28	1.42	1.38
13	AV	101	BCL	C3D-C4D	-2.28	1.39	1.44
15	bo	101	V7N	C11-C12	2.28	1.40	1.34
27	ai	102	UYH	C30-C29	2.28	1.60	1.52
13	BX	101	BCL	C3D-C4D	-2.28	1.39	1.44
13	BF	103	BCL	C3D-C4D	-2.28	1.39	1.44
14	BR	1004	LMT	O2'-C2'	-2.27	1.37	1.43
13	BH	1005	BCL	C3B-C4B	2.27	1.45	1.41
15	BW	1001	V7N	C12-C13	-2.27	1.41	1.46
13	ae	1001	BCL	C3D-C4D	-2.27	1.39	1.44
13	AN	103	BCL	C3D-C4D	-2.27	1.39	1.44
15	AA	1004	V7N	C7-C8	2.27	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BQ	1004	BCL	C3B-C4B	2.27	1.45	1.41
14	bo	104	LMT	O3B-C3B	-2.27	1.37	1.43
13	BA	103	BCL	C3D-C4D	-2.27	1.39	1.44
14	AT	102	LMT	O2'-C2'	-2.27	1.37	1.43
14	bn	103	LMT	O3B-C3B	-2.27	1.37	1.43
13	BP	1003	BCL	C3D-C4D	-2.27	1.39	1.44
15	BG	1001	V7N	C12-C13	-2.27	1.41	1.46
13	AB	1001	BCL	C3B-C4B	2.27	1.45	1.41
13	AJ	104	BCL	C3D-C4D	-2.27	1.39	1.44
13	BU	1004	BCL	CHD-C1D	2.27	1.42	1.38
13	ai	101	BCL	C3D-C4D	-2.27	1.39	1.44
13	bh	103	BCL	C3D-C4D	-2.27	1.39	1.44
14	C	1005	LMT	O2'-C2'	-2.27	1.37	1.43
14	bk	104	LMT	O2'-C2'	-2.27	1.37	1.43
15	be	102	V7N	C12-C13	-2.27	1.41	1.46
18	M	410	V75	O3-C3A	2.26	1.40	1.35
13	AD	103	BCL	C3D-C4D	-2.26	1.39	1.44
15	BQ	1001	V7N	C12-C13	-2.26	1.41	1.46
13	AT	101	BCL	C3D-C4D	-2.26	1.39	1.44
13	BA	103	BCL	CHD-C1D	2.26	1.42	1.38
13	L	305	BCL	C3D-C4D	-2.26	1.39	1.44
14	AT	104	LMT	O2'-C2'	-2.26	1.37	1.43
13	AA	1001	BCL	C3D-C4D	-2.26	1.39	1.44
14	BC	101	LMT	O3B-C3B	-2.26	1.37	1.43
14	AE	106	LMT	O2'-C2'	-2.26	1.37	1.43
14	BW	1006	LMT	O2'-C2'	-2.26	1.37	1.43
13	bf	102	BCL	C3D-C4D	-2.26	1.39	1.44
14	AK	103	LMT	O3B-C3B	-2.26	1.37	1.43
14	AQ	101	LMT	O2B-C2B	-2.26	1.37	1.43
15	bo	101	V7N	C7-C8	2.26	1.40	1.34
14	AU	102	LMT	O2B-C2B	-2.26	1.37	1.43
14	AE	102	LMT	O2'-C2'	-2.25	1.37	1.43
13	BP	1003	BCL	C3B-C4B	2.25	1.45	1.41
13	AK	104	BCL	C3D-C4D	-2.25	1.39	1.44
14	AG	101	LMT	O2B-C2B	-2.25	1.37	1.43
15	AS	104	V7N	C11-C12	2.25	1.40	1.34
14	ac	101	LMT	O2'-C2'	-2.25	1.37	1.43
15	AD	101	V7N	C11-C12	2.25	1.40	1.34
14	L	306	LMT	O2B-C2B	-2.25	1.37	1.43
14	AH	104	LMT	O3B-C3B	-2.25	1.37	1.43
14	bc	102	LMT	O3B-C3B	-2.25	1.37	1.43
14	AN	102	LMT	O2B-C2B	-2.25	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bm	103	LMT	O3B-C3B	-2.25	1.37	1.43
18	C	1006	V75	O3-C3A	2.25	1.40	1.35
14	L	304	LMT	O2'-C2'	-2.25	1.37	1.43
13	BT	103	BCL	CHD-C1D	2.25	1.42	1.38
15	bi	101	V7N	C11-C12	2.25	1.40	1.34
13	AA	1001	BCL	CHD-C1D	2.25	1.42	1.38
15	bj	101	V7N	C11-C12	2.25	1.40	1.34
14	BP	1004	LMT	O2'-C2'	-2.25	1.37	1.43
15	bp	102	V7N	C6-C5	2.25	1.41	1.35
13	AM	1004	BCL	CHD-C1D	2.24	1.42	1.38
13	an	1001	BCL	C3D-C4D	-2.24	1.39	1.44
14	AB	1003	LMT	O2'-C2'	-2.24	1.37	1.43
15	BN	1001	V7N	C12-C13	-2.24	1.41	1.46
15	BR	1001	V7N	C12-C13	-2.24	1.41	1.46
14	AV	102	LMT	O3B-C3B	-2.24	1.37	1.43
13	AK	104	BCL	CHD-C1D	2.24	1.42	1.38
13	bp	104	BCL	C3D-C4D	-2.24	1.39	1.44
13	AQ	103	BCL	CHD-C1D	2.24	1.42	1.38
14	AV	104	LMT	O3B-C3B	-2.24	1.37	1.43
14	AE	101	LMT	O3B-C3B	-2.24	1.37	1.43
14	BX	104	LMT	O3B-C3B	-2.24	1.37	1.43
15	AS	104	V7N	C12-C13	-2.24	1.41	1.46
13	ab	1001	BCL	CHD-C1D	2.24	1.42	1.38
15	BF	101	V7N	C12-C13	-2.24	1.41	1.46
13	aa	1001	BCL	CHD-C1D	2.24	1.42	1.38
13	AF	1001	BCL	C3D-C4D	-2.24	1.39	1.44
14	AJ	102	LMT	O4'-C4B	-2.24	1.37	1.43
14	BM	1005	LMT	O3B-C3B	-2.24	1.37	1.43
13	BT	103	BCL	C3D-C4D	-2.24	1.39	1.44
13	aa	1001	BCL	C3D-C4D	-2.24	1.39	1.44
15	BJ	1001	V7N	C12-C13	-2.23	1.41	1.46
15	bc	101	V7N	C11-C12	2.23	1.40	1.34
15	AA	1004	V7N	C6-C5	2.23	1.41	1.35
15	bm	101	V7N	C12-C13	-2.23	1.41	1.46
14	BT	101	LMT	O3B-C3B	-2.23	1.37	1.43
14	BO	1004	LMT	O2'-C2'	-2.23	1.37	1.43
14	L	304	LMT	O2B-C2B	-2.23	1.37	1.43
14	L	307	LMT	O3B-C3B	-2.23	1.37	1.43
13	BD	104	BCL	CHD-C1D	2.23	1.42	1.38
13	BK	1002	BCL	C3D-C4D	-2.23	1.39	1.44
15	BS	1001	V7N	C12-C13	-2.23	1.41	1.46
14	be	104	LMT	O3B-C3B	-2.23	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bg	104	BCL	C1D-C2D	-2.23	1.40	1.45
14	AJ	101	LMT	O3B-C3B	-2.23	1.37	1.43
15	ag	101	V7N	C12-C13	-2.23	1.41	1.46
13	AD	103	BCL	CHD-C1D	2.23	1.42	1.38
13	bf	102	BCL	C3B-C4B	2.23	1.45	1.41
13	am	1001	BCL	C1D-C2D	-2.23	1.40	1.45
15	bn	101	V7N	C7-C8	2.23	1.40	1.34
14	AX	101	LMT	O3B-C3B	-2.23	1.37	1.43
19	C	1007	NDG	C1-C2	2.23	1.55	1.52
15	BQ	1001	V7N	C11-C12	2.23	1.40	1.34
14	BV	1003	LMT	O2'-C2'	-2.23	1.37	1.43
13	BW	1005	BCL	C3D-C4D	-2.23	1.39	1.44
15	BS	1001	V7N	C11-C12	2.23	1.40	1.34
14	BS	1002	LMT	O2B-C2B	-2.23	1.37	1.43
15	AM	1001	V7N	C11-C12	2.23	1.40	1.34
13	AE	104	BCL	CHD-C1D	2.23	1.42	1.38
13	AC	102	BCL	C3D-C4D	-2.23	1.39	1.44
14	BD	105	LMT	O2B-C2B	-2.22	1.37	1.43
13	BQ	1004	BCL	CHD-C1D	2.22	1.42	1.38
15	AA	1004	V7N	C12-C13	-2.22	1.41	1.46
14	BF	104	LMT	O2'-C2'	-2.22	1.37	1.43
14	BX	102	LMT	O2'-C2'	-2.22	1.37	1.43
14	AK	103	LMT	O2'-C2'	-2.22	1.37	1.43
13	AM	1004	BCL	C3D-C4D	-2.22	1.39	1.44
13	AQ	103	BCL	C3D-C4D	-2.22	1.39	1.44
15	bj	101	V7N	C12-C13	-2.22	1.41	1.46
14	BG	1005	LMT	O2B-C2B	-2.22	1.37	1.43
13	AB	1002	BCL	C1D-ND	2.22	1.40	1.37
13	BJ	1004	BCL	C3B-C4B	2.22	1.45	1.41
14	BQ	1003	LMT	O2'-C2'	-2.22	1.37	1.43
14	BR	1002	LMT	O2B-C2B	-2.22	1.37	1.43
14	C2	1001	LMT	O3B-C3B	-2.22	1.37	1.43
13	BE	104	BCL	C3D-C4D	-2.22	1.39	1.44
13	AO	102	BCL	C3D-C4D	-2.22	1.39	1.44
14	BO	1002	LMT	O3B-C3B	-2.22	1.37	1.43
14	bg	102	LMT	O2B-C2B	-2.22	1.37	1.43
15	BF	101	V7N	C11-C12	2.22	1.40	1.34
14	BR	1002	LMT	O3B-C3B	-2.22	1.37	1.43
13	BD	104	BCL	C3D-C4D	-2.22	1.39	1.44
13	BS	1004	BCL	CHD-C1D	2.22	1.42	1.38
13	ao	102	BCL	CHD-C1D	2.22	1.42	1.38
13	AB	1001	BCL	CHD-C1D	2.22	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BX	101	BCL	CHD-C1D	2.22	1.42	1.38
14	BN	1003	LMT	O3B-C3B	-2.22	1.37	1.43
14	bp	103	LMT	O2'-C2'	-2.22	1.37	1.43
14	AB	1003	LMT	O3B-C3B	-2.22	1.37	1.43
13	bn	102	BCL	C1D-C2D	-2.21	1.41	1.45
13	AW	101	BCL	C3D-C4D	-2.21	1.39	1.44
14	AE	106	LMT	O3B-C3B	-2.21	1.37	1.43
14	AG	101	LMT	O3B-C3B	-2.21	1.37	1.43
14	AH	104	LMT	O2'-C2'	-2.21	1.37	1.43
15	BM	1001	V7N	C11-C12	2.21	1.40	1.34
14	BF	104	LMT	O3B-C3B	-2.21	1.37	1.43
13	BG	1004	BCL	C3B-C4B	2.21	1.45	1.41
15	bp	102	V7N	C20-C19	2.21	1.40	1.34
14	AN	102	LMT	O3B-C3B	-2.21	1.37	1.43
15	BE	101	V7N	C11-C12	2.21	1.40	1.34
15	AD	101	V7N	C12-C13	-2.21	1.41	1.46
14	BA	102	LMT	O3B-C3B	-2.21	1.37	1.43
14	BQ	1003	LMT	O3B-C3B	-2.21	1.37	1.43
14	AJ	102	LMT	O3B-C3B	-2.21	1.37	1.43
14	BG	1002	LMT	O2B-C2B	-2.21	1.37	1.43
15	BI	1001	V7N	C11-C12	2.21	1.40	1.34
13	AH	103	BCL	C3D-C4D	-2.21	1.39	1.44
13	BH	1005	BCL	C3D-C4D	-2.21	1.39	1.44
14	BF	102	LMT	O2'-C2'	-2.21	1.37	1.43
15	ba	101	V7N	C7-C8	2.21	1.40	1.34
15	BA	101	V7N	C12-C13	-2.21	1.41	1.46
15	bb	101	V7N	C20-C19	2.21	1.40	1.34
14	BE	102	LMT	O2'-C2'	-2.21	1.37	1.43
13	ac	102	BCL	C3D-C4D	-2.21	1.39	1.44
14	BI	1005	LMT	O2'-C2'	-2.21	1.37	1.43
14	bk	104	LMT	O2B-C2B	-2.20	1.37	1.43
14	AN	102	LMT	O2'-C2'	-2.20	1.37	1.43
13	BF	103	BCL	CHD-C1D	2.20	1.42	1.38
13	AT	101	BCL	CHD-C1D	2.20	1.42	1.38
15	BI	1001	V7N	C12-C13	-2.20	1.41	1.46
13	AL	102	BCL	C3D-C4D	-2.20	1.39	1.44
13	BP	1003	BCL	CHD-C1D	2.20	1.42	1.38
14	AG	101	LMT	O4'-C4B	-2.20	1.37	1.43
14	BT	102	LMT	O3B-C3B	-2.20	1.37	1.43
14	bh	102	LMT	O2B-C2B	-2.20	1.37	1.43
14	AH	101	LMT	O2'-C2'	-2.20	1.37	1.43
13	AB	1001	BCL	C3D-C4D	-2.20	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BG	1002	LMT	O3B-C3B	-2.20	1.37	1.43
14	BW	1006	LMT	O2B-C2B	-2.20	1.37	1.43
14	bm	103	LMT	O2'-C2'	-2.20	1.37	1.43
18	M	410	V75	O2-C2A	2.20	1.40	1.35
15	be	102	V7N	C11-C12	2.20	1.40	1.34
14	AN	101	LMT	O2B-C2B	-2.20	1.37	1.43
14	BC	101	LMT	O2'-C2'	-2.20	1.37	1.43
14	BH	1003	LMT	O2'-C2'	-2.20	1.37	1.43
13	AN	103	BCL	C1D-C2D	-2.20	1.41	1.45
13	BC	104	BCL	CHD-C1D	2.20	1.42	1.38
14	L	302	LMT	O3B-C3B	-2.20	1.37	1.43
13	bf	102	BCL	C1D-C2D	-2.20	1.41	1.45
13	AX	102	BCL	CHD-C1D	2.20	1.42	1.38
15	bk	101	V7N	C6-C5	2.20	1.40	1.35
14	BB	104	LMT	O3B-C3B	-2.20	1.37	1.43
15	bl	101	V7N	C7-C8	2.20	1.40	1.34
14	H2	201	LMT	O2'-C2'	-2.19	1.37	1.43
13	ac	102	BCL	CHD-C1D	2.19	1.42	1.38
14	BG	1003	LMT	O2'-C2'	-2.19	1.37	1.43
14	AM	1003	LMT	O2B-C2B	-2.19	1.37	1.43
14	BJ	1005	LMT	O2B-C2B	-2.19	1.37	1.43
14	BM	1005	LMT	O2'-C2'	-2.19	1.37	1.43
13	AR	101	BCL	C3D-C4D	-2.19	1.39	1.44
14	AB	1003	LMT	O2B-C2B	-2.19	1.37	1.43
15	BN	1001	V7N	C11-C12	2.19	1.40	1.34
13	ab	1001	BCL	C3D-C4D	-2.19	1.39	1.44
14	BR	1005	LMT	O3B-C3B	-2.19	1.37	1.43
15	BD	101	V7N	C12-C13	-2.19	1.41	1.46
14	BG	1005	LMT	O2'-C2'	-2.19	1.37	1.43
14	BX	103	LMT	O3B-C3B	-2.19	1.37	1.43
14	AU	102	LMT	O2'-C2'	-2.19	1.37	1.43
15	BJ	1001	V7N	C11-C12	2.19	1.40	1.34
13	BF	103	BCL	C3B-C4B	2.19	1.45	1.41
14	BL	101	LMT	O2B-C2B	-2.19	1.37	1.43
14	bl	103	LMT	O3B-C3B	-2.19	1.37	1.43
14	bf	101	LMT	O3B-C3B	-2.19	1.37	1.43
13	BI	1004	BCL	C3B-C4B	2.19	1.45	1.41
14	AE	102	LMT	O3B-C3B	-2.19	1.37	1.43
15	BI	1001	V7N	C7-C8	2.18	1.40	1.34
14	BU	1002	LMT	O3B-C3B	-2.18	1.37	1.43
18	M	410	V75	O5-C1	-2.18	1.40	1.43
13	AK	102	BCL	C1D-ND	2.18	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	ag	101	V7N	C11-C12	2.18	1.40	1.34
15	bl	101	V7N	C6-C5	2.18	1.40	1.35
14	AP	101	LMT	O3B-C3B	-2.18	1.37	1.43
14	BV	1002	LMT	O3B-C3B	-2.18	1.37	1.43
14	bg	102	LMT	O3B-C3B	-2.18	1.37	1.43
13	BJ	1004	BCL	CHD-C1D	2.18	1.42	1.38
14	AP	101	LMT	O2B-C2B	-2.18	1.37	1.43
14	bm	103	LMT	O2B-C2B	-2.18	1.37	1.43
14	AV	104	LMT	O2B-C2B	-2.18	1.37	1.43
14	BR	1004	LMT	O3B-C3B	-2.18	1.37	1.43
14	BV	1003	LMT	O2B-C2B	-2.18	1.37	1.43
26	ag	103	V7B	O8-C9	-2.18	1.40	1.45
13	AV	101	BCL	CHD-C1D	2.18	1.42	1.38
14	AS	103	LMT	O3B-C3B	-2.18	1.37	1.43
14	BN	1004	LMT	O2'-C2'	-2.18	1.37	1.43
13	ad	102	BCL	C3D-C4D	-2.18	1.39	1.44
14	BM	1003	LMT	O2B-C2B	-2.18	1.37	1.43
13	BI	1004	BCL	CHD-C1D	2.18	1.42	1.38
13	BK	1002	BCL	CHD-C1D	2.18	1.42	1.38
13	ba	102	BCL	C3D-C4D	-2.18	1.39	1.44
14	AC	103	LMT	O3B-C3B	-2.18	1.37	1.43
14	AM	1003	LMT	O3B-C3B	-2.18	1.37	1.43
14	BB	104	LMT	O2'-C2'	-2.18	1.37	1.43
14	BK	1004	LMT	O2'-C2'	-2.18	1.37	1.43
14	AK	101	LMT	O2B-C2B	-2.18	1.37	1.43
13	ag	102	BCL	CHD-C1D	2.18	1.42	1.38
15	bi	101	V7N	C12-C13	-2.18	1.41	1.46
14	BK	1004	LMT	O3B-C3B	-2.18	1.37	1.43
13	BI	1004	BCL	C1D-C2D	-2.18	1.41	1.45
14	BS	1003	LMT	O3B-C3B	-2.18	1.37	1.43
14	BB	103	LMT	O3B-C3B	-2.18	1.37	1.43
14	BS	1005	LMT	O3B-C3B	-2.18	1.37	1.43
13	an	1001	BCL	C1D-C2D	-2.18	1.41	1.45
13	AO	102	BCL	CHD-C1D	2.18	1.42	1.38
14	BJ	1002	LMT	O2B-C2B	-2.18	1.37	1.43
14	BC	102	LMT	O3B-C3B	-2.17	1.37	1.43
14	BO	1005	LMT	O2'-C2'	-2.17	1.37	1.43
15	bg	101	V7N	C12-C13	-2.17	1.41	1.46
13	AI	101	BCL	C3D-C4D	-2.17	1.39	1.44
14	BJ	1005	LMT	O3B-C3B	-2.17	1.37	1.43
14	BU	1003	LMT	O2B-C2B	-2.17	1.37	1.43
13	bm	102	BCL	CHD-C1D	2.17	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BP	1005	LMT	O2'-C2'	-2.17	1.37	1.43
15	AW	103	V7N	C7-C8	2.17	1.40	1.34
13	AX	102	BCL	C3D-C4D	-2.17	1.39	1.44
14	AV	102	LMT	O2B-C2B	-2.17	1.37	1.43
13	af	103	BCL	C3D-C4D	-2.17	1.39	1.44
15	BK	1001	V7N	C12-C13	-2.17	1.41	1.46
13	AR	101	BCL	CHD-C1D	2.17	1.42	1.38
14	BW	1006	LMT	O3B-C3B	-2.17	1.37	1.43
13	L	305	BCL	C1D-C2D	-2.17	1.41	1.45
13	BV	1005	BCL	CHD-C1D	2.17	1.42	1.38
14	bl	103	LMT	O2'-C2'	-2.17	1.37	1.43
13	BR	1003	BCL	CHD-C1D	2.17	1.42	1.38
14	BP	1005	LMT	O3B-C3B	-2.16	1.37	1.43
15	BJ	1001	V7N	C7-C8	2.16	1.40	1.34
14	AJ	102	LMT	O2'-C2'	-2.16	1.37	1.43
13	bb	102	BCL	CHD-C1D	2.16	1.42	1.38
14	BB	101	LMT	O2'-C2'	-2.16	1.37	1.43
14	bp	103	LMT	O2B-C2B	-2.16	1.37	1.43
13	BX	101	BCL	C3B-C4B	2.16	1.45	1.41
13	AL	103	BCL	C1D-ND	2.16	1.40	1.37
14	BD	102	LMT	O2B-C2B	-2.16	1.37	1.43
14	BT	104	LMT	O3B-C3B	-2.16	1.37	1.43
14	BF	102	LMT	O3B-C3B	-2.16	1.37	1.43
14	BQ	1002	LMT	O2'-C2'	-2.16	1.37	1.43
14	BT	104	LMT	O2'-C2'	-2.16	1.37	1.43
13	AF	1001	BCL	CHD-C1D	2.16	1.42	1.38
13	AJ	104	BCL	CHD-C1D	2.16	1.42	1.38
13	ak	1001	BCL	CHD-C1D	2.16	1.42	1.38
13	ap	1001	BCL	C3D-C4D	-2.16	1.39	1.44
14	BK	1003	LMT	O3B-C3B	-2.16	1.37	1.43
14	AT	102	LMT	O2B-C2B	-2.16	1.37	1.43
14	AT	102	LMT	O3B-C3B	-2.16	1.37	1.43
15	BG	1001	V7N	C11-C12	2.16	1.40	1.34
14	ac	101	LMT	O3B-C3B	-2.16	1.37	1.43
14	BE	103	LMT	O3B-C3B	-2.16	1.37	1.43
14	BI	1003	LMT	O3B-C3B	-2.16	1.37	1.43
14	BA	102	LMT	O2B-C2B	-2.16	1.37	1.43
14	BM	1003	LMT	O3B-C3B	-2.16	1.37	1.43
15	bb	101	V7N	C6-C5	2.15	1.40	1.35
14	L	307	LMT	O2B-C2B	-2.15	1.37	1.43
14	AD	102	LMT	O2B-C2B	-2.15	1.37	1.43
14	BV	1004	LMT	O3B-C3B	-2.15	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AL	101	LMT	O3B-C3B	-2.15	1.37	1.43
14	bj	102	LMT	O3B-C3B	-2.15	1.37	1.43
13	L	308	BCL	O1A-CGA	-2.15	1.16	1.22
15	BV	1001	V7N	C19-C18	-2.15	1.41	1.46
15	BA	101	V7N	C6-C5	2.15	1.40	1.35
15	BA	101	V7N	C7-C8	2.15	1.40	1.34
14	AT	104	LMT	O2B-C2B	-2.15	1.37	1.43
14	BU	1002	LMT	O2'-C2'	-2.15	1.37	1.43
13	AO	101	BCL	C3D-C4D	-2.15	1.39	1.44
15	BV	1001	V7N	C11-C12	2.15	1.40	1.34
13	AH	103	BCL	CHD-C1D	2.15	1.42	1.38
14	C2	1001	LMT	O2B-C2B	-2.15	1.37	1.43
13	BW	1005	BCL	CHD-C1D	2.15	1.42	1.38
14	BI	1002	LMT	O3B-C3B	-2.15	1.37	1.43
15	bm	101	V7N	C7-C8	2.15	1.40	1.34
14	AN	101	LMT	O3B-C3B	-2.15	1.37	1.43
14	BQ	1002	LMT	O3B-C3B	-2.15	1.37	1.43
14	bc	102	LMT	O2'-C2'	-2.15	1.37	1.43
13	BC	104	BCL	C3D-C4D	-2.15	1.39	1.44
13	AD	103	BCL	C3B-C4B	2.15	1.45	1.41
14	AH	104	LMT	O4'-C4B	-2.15	1.37	1.43
13	BO	1003	BCL	C1D-C2D	-2.14	1.41	1.45
14	BH	1002	LMT	O3B-C3B	-2.14	1.37	1.43
14	BJ	1002	LMT	O3B-C3B	-2.14	1.37	1.43
13	AP	102	BCL	CHD-C1D	2.14	1.42	1.38
13	AJ	103	BCL	C3D-C4D	-2.14	1.39	1.44
14	BH	1004	LMT	O3B-C3B	-2.14	1.37	1.43
22	M	407	BPH	O1A-CGA	-2.14	1.16	1.22
15	BI	1001	V7N	C6-C5	2.14	1.40	1.35
13	aj	101	BCL	CHD-C1D	2.14	1.42	1.38
14	AT	104	LMT	O3B-C3B	-2.14	1.37	1.43
14	BP	1006	LMT	O3B-C3B	-2.14	1.37	1.43
15	bn	101	V7N	C6-C5	2.14	1.40	1.35
13	AG	103	BCL	CHD-C1D	2.14	1.42	1.38
14	BX	102	LMT	O3B-C3B	-2.14	1.37	1.43
14	AD	102	LMT	O3B-C3B	-2.14	1.37	1.43
13	bd	102	BCL	CHD-C1D	2.14	1.42	1.38
13	AH	105	BCL	C1D-ND	2.14	1.40	1.37
14	AL	101	LMT	O2B-C2B	-2.14	1.37	1.43
14	AX	101	LMT	O2B-C2B	-2.14	1.37	1.43
14	AQ	101	LMT	O3B-C3B	-2.14	1.37	1.43
14	BB	102	LMT	O3B-C3B	-2.14	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BH	1003	LMT	O3B-C3B	-2.14	1.37	1.43
14	BR	1004	LMT	O2B-C2B	-2.14	1.37	1.43
15	AW	103	V7N	C6-C5	2.14	1.40	1.35
15	BW	1001	V7N	C11-C12	2.14	1.40	1.34
14	AM	1003	LMT	O2'-C2'	-2.14	1.37	1.43
14	BO	1004	LMT	O3B-C3B	-2.14	1.37	1.43
13	an	1001	BCL	CHD-C1D	2.14	1.42	1.38
14	BK	1005	LMT	O3B-C3B	-2.14	1.37	1.43
13	AE	104	BCL	C3D-C4D	-2.14	1.39	1.44
13	M	408	BCL	O1A-CGA	-2.13	1.16	1.22
14	BP	1006	LMT	O2B-C2B	-2.13	1.37	1.43
15	bc	101	V7N	C12-C13	-2.13	1.41	1.46
14	BL	101	LMT	O3B-C3B	-2.13	1.37	1.43
14	BS	1002	LMT	O2'-C2'	-2.13	1.37	1.43
13	BV	1005	BCL	C3D-C4D	-2.13	1.39	1.44
14	BK	1004	LMT	O2B-C2B	-2.13	1.37	1.43
13	ad	102	BCL	CHD-C1D	2.13	1.42	1.38
15	bh	101	V7N	C7-C8	2.13	1.40	1.34
14	BE	103	LMT	O2B-C2B	-2.13	1.37	1.43
14	BJ	1003	LMT	O3B-C3B	-2.13	1.37	1.43
14	BO	1005	LMT	O3B-C3B	-2.13	1.37	1.43
14	BP	1002	LMT	O2B-C2B	-2.13	1.37	1.43
14	BW	1003	LMT	O2'-C2'	-2.13	1.37	1.43
14	L	307	LMT	O2'-C2'	-2.13	1.37	1.43
13	AG	102	BCL	C1D-ND	2.13	1.40	1.37
14	BB	101	LMT	O3B-C3B	-2.13	1.37	1.43
14	BL	102	LMT	O2B-C2B	-2.13	1.37	1.43
14	BP	1002	LMT	O3B-C3B	-2.13	1.37	1.43
14	BQ	1003	LMT	O2B-C2B	-2.13	1.37	1.43
15	BM	1001	V7N	C19-C18	-2.13	1.41	1.46
14	BD	106	LMT	O2'-C2'	-2.13	1.37	1.43
14	BS	1005	LMT	O2B-C2B	-2.13	1.37	1.43
14	BQ	1002	LMT	O2B-C2B	-2.13	1.37	1.43
14	C2	1001	LMT	O2'-C2'	-2.13	1.37	1.43
14	BJ	1006	LMT	O2'-C2'	-2.13	1.37	1.43
15	BV	1001	V7N	C7-C8	2.13	1.40	1.34
14	BX	103	LMT	O2B-C2B	-2.13	1.37	1.43
14	AP	101	LMT	O2'-C2'	-2.13	1.37	1.43
14	BC	103	LMT	O2'-C2'	-2.13	1.37	1.43
14	BL	102	LMT	O3B-C3B	-2.13	1.37	1.43
14	BB	104	LMT	O2B-C2B	-2.12	1.37	1.43
14	BN	1004	LMT	O2B-C2B	-2.12	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AV	104	LMT	O2'-C2'	-2.12	1.37	1.43
14	bc	102	LMT	O2B-C2B	-2.12	1.37	1.43
14	BC	103	LMT	O3B-C3B	-2.12	1.37	1.43
14	BD	103	LMT	O3B-C3B	-2.12	1.37	1.43
14	BT	101	LMT	O2B-C2B	-2.12	1.37	1.43
14	bl	103	LMT	O2B-C2B	-2.12	1.37	1.43
13	bk	103	BCL	CHD-C1D	2.12	1.42	1.38
14	BN	1004	LMT	O3B-C3B	-2.12	1.37	1.43
14	BX	104	LMT	O2'-C2'	-2.12	1.37	1.43
13	BO	1003	BCL	CHD-C1D	2.12	1.42	1.38
14	BO	1002	LMT	O2B-C2B	-2.12	1.37	1.43
14	BW	1004	LMT	O2B-C2B	-2.12	1.37	1.43
14	BI	1005	LMT	O3B-C3B	-2.12	1.37	1.43
14	bj	102	LMT	O2B-C2B	-2.12	1.37	1.43
14	BU	1003	LMT	O3B-C3B	-2.12	1.37	1.43
15	BO	1001	V7N	C12-C13	-2.12	1.41	1.46
15	BS	1001	V7N	C19-C18	-2.12	1.41	1.46
15	bh	101	V7N	C12-C13	-2.12	1.41	1.46
14	C	1005	LMT	O3B-C3B	-2.12	1.37	1.43
14	L	309	LMT	O2'-C2'	-2.12	1.37	1.43
13	bi	102	BCL	CHD-C1D	2.12	1.42	1.38
14	BS	1005	LMT	O2'-C2'	-2.12	1.37	1.43
15	BG	1001	V7N	C7-C8	2.12	1.40	1.34
14	BR	1006	LMT	O2B-C2B	-2.12	1.37	1.43
14	bp	103	LMT	O3B-C3B	-2.12	1.37	1.43
15	BH	1001	V7N	C12-C13	-2.12	1.41	1.46
14	bi	104	LMT	O2'-C2'	-2.11	1.37	1.43
14	AH	104	LMT	O2B-C2B	-2.11	1.37	1.43
14	BC	101	LMT	O2B-C2B	-2.11	1.37	1.43
14	BE	102	LMT	O3B-C3B	-2.11	1.37	1.43
15	BJ	1001	V7N	C6-C5	2.11	1.40	1.35
15	BK	1001	V7N	C6-C5	2.11	1.40	1.35
13	L	305	BCL	CHD-C1D	2.11	1.42	1.38
14	BN	1002	LMT	O2'-C2'	-2.11	1.37	1.43
14	BV	1002	LMT	O2B-C2B	-2.11	1.37	1.43
13	BU	1004	BCL	C3B-C4B	2.11	1.45	1.41
14	BD	103	LMT	O2'-C2'	-2.11	1.37	1.43
13	bo	102	BCL	C1D-C2D	-2.11	1.41	1.45
14	BJ	1006	LMT	O2B-C2B	-2.11	1.37	1.43
15	bo	101	V7N	C12-C13	-2.11	1.41	1.46
15	bc	101	V7N	C7-C8	2.11	1.40	1.34
14	bn	103	LMT	O2B-C2B	-2.11	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	ak	1001	BCL	C3D-C4D	-2.11	1.39	1.44
14	C	1005	LMT	O2B-C2B	-2.11	1.37	1.43
14	C2	1001	LMT	O4'-C4B	-2.11	1.37	1.43
13	AK	102	BCL	C5-C3	2.11	1.55	1.51
14	BH	1004	LMT	O2'-C2'	-2.11	1.37	1.43
14	L	309	LMT	O2B-C2B	-2.11	1.37	1.43
14	BI	1005	LMT	O2B-C2B	-2.11	1.37	1.43
14	BC	103	LMT	O2B-C2B	-2.11	1.37	1.43
13	ai	101	BCL	CHD-C1D	2.11	1.42	1.38
13	BR	1003	BCL	CBD-CGD	-2.11	1.46	1.52
15	bn	101	V7N	C12-C13	-2.11	1.41	1.46
14	BD	102	LMT	O3B-C3B	-2.11	1.37	1.43
14	BM	1002	LMT	O3B-C3B	-2.11	1.37	1.43
14	BT	102	LMT	O2'-C2'	-2.11	1.37	1.43
14	BV	1003	LMT	O3B-C3B	-2.11	1.37	1.43
15	BR	1001	V7N	C19-C18	-2.11	1.41	1.46
14	AS	103	LMT	O4'-C4B	-2.10	1.37	1.43
14	BS	1002	LMT	O3B-C3B	-2.10	1.37	1.43
13	AV	103	BCL	C3D-C4D	-2.10	1.39	1.44
14	bk	104	LMT	O4'-C4B	-2.10	1.37	1.43
15	BK	1001	V7N	C7-C8	2.10	1.40	1.34
15	bd	101	V7N	C6-C5	2.10	1.40	1.35
14	BG	1005	LMT	O3B-C3B	-2.10	1.37	1.43
13	bp	104	BCL	CHD-C1D	2.10	1.42	1.38
13	BN	1005	BCL	C3B-C4B	2.10	1.45	1.41
14	AC	103	LMT	O2'-C2'	-2.10	1.37	1.43
15	ba	101	V7N	C6-C5	2.10	1.40	1.35
14	H2	201	LMT	O3B-C3B	-2.10	1.37	1.43
14	AE	102	LMT	O2B-C2B	-2.10	1.37	1.43
14	BA	102	LMT	O2'-C2'	-2.10	1.37	1.43
14	BN	1002	LMT	O2B-C2B	-2.10	1.37	1.43
15	BP	1001	V7N	C19-C18	-2.10	1.41	1.46
13	be	103	BCL	C1D-C2D	-2.10	1.41	1.45
13	AT	103	BCL	C3D-C4D	-2.10	1.39	1.44
15	BP	1001	V7N	C11-C12	2.10	1.40	1.34
14	AV	102	LMT	O2'-C2'	-2.10	1.37	1.43
14	H2	201	LMT	O2B-C2B	-2.10	1.37	1.43
15	bd	101	V7N	C7-C8	2.10	1.40	1.34
14	bp	101	LMT	O2B-C2B	-2.10	1.37	1.43
14	BT	101	LMT	O2'-C2'	-2.10	1.37	1.43
14	BR	1006	LMT	O3B-C3B	-2.10	1.37	1.43
13	AW	102	BCL	C1D-ND	2.10	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bk	104	LMT	O3B-C3B	-2.09	1.37	1.43
17	C	1001	HEC	CMB-C2B	2.09	1.55	1.50
13	AD	103	BCL	C1D-C2D	-2.09	1.41	1.45
15	BM	1001	V7N	C7-C8	2.09	1.40	1.34
14	BP	1005	LMT	O2B-C2B	-2.09	1.37	1.43
14	BW	1003	LMT	O3B-C3B	-2.09	1.37	1.43
14	BJ	1003	LMT	O2'-C2'	-2.09	1.37	1.43
13	AU	101	BCL	C1D-C2D	-2.09	1.41	1.45
13	ae	1001	BCL	C1D-C2D	-2.09	1.41	1.45
14	BE	105	LMT	O3B-C3B	-2.09	1.37	1.43
14	BL	102	LMT	O2'-C2'	-2.09	1.37	1.43
14	BN	1002	LMT	O3B-C3B	-2.09	1.37	1.43
14	be	101	LMT	O2B-C2B	-2.09	1.37	1.43
14	AU	102	LMT	O3B-C3B	-2.09	1.37	1.43
15	BH	1001	V7N	C7-C8	2.09	1.40	1.34
15	AW	103	V7N	C12-C13	-2.09	1.41	1.46
14	BJ	1006	LMT	O3B-C3B	-2.09	1.37	1.43
15	bo	101	V7N	C6-C5	2.09	1.40	1.35
14	BG	1003	LMT	O3B-C3B	-2.09	1.37	1.43
14	BR	1005	LMT	O2B-C2B	-2.09	1.37	1.43
14	BW	1002	LMT	O2B-C2B	-2.09	1.37	1.43
14	BM	1002	LMT	O2B-C2B	-2.08	1.37	1.43
13	bk	103	BCL	C1D-C2D	-2.08	1.41	1.45
15	bh	101	V7N	C6-C5	2.08	1.40	1.35
14	BP	1004	LMT	O3B-C3B	-2.08	1.37	1.43
14	BE	102	LMT	O2B-C2B	-2.08	1.37	1.43
13	BN	1005	BCL	CHD-C1D	2.08	1.42	1.38
13	L	308	BCL	C1D-C2D	-2.08	1.41	1.45
13	ah	1001	BCL	CHD-C1D	2.08	1.42	1.38
15	BG	1001	V7N	C6-C5	2.08	1.40	1.35
15	bp	102	V7N	C16-C15	2.08	1.41	1.36
14	BK	1003	LMT	O2'-C2'	-2.08	1.37	1.43
15	AS	104	V7N	C19-C18	-2.08	1.41	1.46
13	AT	103	BCL	C1D-ND	2.08	1.40	1.37
14	BU	1002	LMT	O2B-C2B	-2.08	1.37	1.43
14	BB	103	LMT	O2B-C2B	-2.08	1.37	1.43
14	BD	105	LMT	O3B-C3B	-2.08	1.37	1.43
13	AX	102	BCL	C1D-C2D	-2.08	1.41	1.45
15	BR	1001	V7N	C7-C8	2.08	1.40	1.34
14	BW	1002	LMT	O3B-C3B	-2.08	1.37	1.43
14	BB	103	LMT	O2'-C2'	-2.08	1.37	1.43
14	BH	1004	LMT	O2B-C2B	-2.08	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BW	1004	LMT	O3B-C3B	-2.08	1.37	1.43
15	bj	101	V7N	C7-C8	2.08	1.40	1.34
14	AA	1003	LMT	O3B-C3B	-2.08	1.37	1.43
15	BW	1001	V7N	C7-C8	2.08	1.40	1.34
14	BK	1003	LMT	O2B-C2B	-2.08	1.37	1.43
14	BW	1004	LMT	O4'-C4B	-2.08	1.37	1.43
14	L	309	LMT	O3B-C3B	-2.08	1.37	1.43
14	BD	106	LMT	O2B-C2B	-2.07	1.37	1.43
13	al	1001	BCL	C1D-C2D	-2.07	1.41	1.45
14	AK	103	LMT	O2B-C2B	-2.07	1.37	1.43
14	L	306	LMT	O3B-C3B	-2.07	1.37	1.43
15	BR	1001	V7N	C6-C5	2.07	1.40	1.35
14	be	104	LMT	O2B-C2B	-2.07	1.37	1.43
15	BD	101	V7N	C7-C8	2.07	1.40	1.34
14	BC	102	LMT	O2B-C2B	-2.07	1.37	1.43
14	BW	1003	LMT	O2B-C2B	-2.07	1.37	1.43
15	BI	1001	V7N	C19-C18	-2.07	1.41	1.46
13	BN	1005	BCL	C1D-C2D	-2.07	1.41	1.45
14	BD	103	LMT	O2B-C2B	-2.07	1.37	1.43
13	AP	103	BCL	C3D-C4D	-2.07	1.39	1.44
17	C	1004	HEC	CMC-C2C	2.07	1.55	1.50
17	C	1002	HEC	CMC-C2C	2.06	1.55	1.50
13	AU	103	BCL	C1D-ND	2.06	1.40	1.37
15	BO	1001	V7N	C6-C5	2.06	1.40	1.35
13	am	1001	BCL	CHD-C1D	2.06	1.42	1.38
13	M	408	BCL	CBD-CGD	-2.06	1.46	1.52
14	BN	1002	LMT	O4'-C4B	-2.06	1.37	1.43
14	BF	104	LMT	O2B-C2B	-2.06	1.37	1.43
14	BX	102	LMT	O2B-C2B	-2.06	1.37	1.43
15	ba	101	V7N	C12-C13	-2.06	1.41	1.46
14	BE	105	LMT	O2B-C2B	-2.06	1.37	1.43
14	BH	1003	LMT	O2B-C2B	-2.06	1.37	1.43
26	af	101	V7B	O8-C28	2.06	1.39	1.33
14	BB	101	LMT	O2B-C2B	-2.06	1.37	1.43
15	BU	1001	V7N	C7-C8	2.06	1.40	1.34
15	bm	101	V7N	C6-C5	2.06	1.40	1.35
14	BI	1003	LMT	O2B-C2B	-2.06	1.37	1.43
15	BH	1001	V7N	C6-C5	2.06	1.40	1.35
15	BM	1001	V7N	C6-C5	2.05	1.40	1.35
14	BM	1005	LMT	O2B-C2B	-2.05	1.37	1.43
13	AT	101	BCL	C1D-C2D	-2.05	1.41	1.45
14	bp	101	LMT	O3B-C3B	-2.05	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BO	1004	LMT	O2B-C2B	-2.05	1.37	1.43
14	L	302	LMT	O2B-C2B	-2.05	1.37	1.43
13	bf	102	BCL	CHD-C1D	2.05	1.42	1.38
14	BD	106	LMT	O3B-C3B	-2.05	1.37	1.43
13	bn	102	BCL	CHD-C1D	2.05	1.42	1.38
14	BS	1003	LMT	O2'-C2'	-2.05	1.37	1.43
18	C	1006	V75	O5-C1	-2.05	1.40	1.43
13	bh	103	BCL	C1D-C2D	-2.05	1.41	1.45
14	AE	106	LMT	O2B-C2B	-2.05	1.37	1.43
13	BL	103	BCL	C3B-C4B	2.05	1.45	1.41
13	AF	1001	BCL	C1D-C2D	-2.05	1.41	1.45
13	bd	102	BCL	C1D-C2D	-2.05	1.41	1.45
14	AK	101	LMT	O2'-C2'	-2.05	1.37	1.43
13	AG	102	BCL	C3D-C4D	-2.05	1.39	1.44
15	BG	1001	V7N	C19-C18	-2.05	1.41	1.46
14	BN	1003	LMT	O2B-C2B	-2.05	1.37	1.43
15	BO	1001	V7N	C7-C8	2.05	1.40	1.34
13	AA	1002	BCL	C3D-C4D	-2.05	1.39	1.44
14	AD	102	LMT	O2'-C2'	-2.05	1.37	1.43
13	ai	101	BCL	C1D-C2D	-2.05	1.41	1.45
13	AE	103	BCL	C3D-C4D	-2.05	1.39	1.44
14	BJ	1003	LMT	O2B-C2B	-2.05	1.37	1.43
13	AB	1001	BCL	C1D-C2D	-2.05	1.41	1.45
14	BN	1003	LMT	O2'-C2'	-2.05	1.37	1.43
13	AH	102	BCL	C1D-ND	2.05	1.40	1.37
14	BR	1005	LMT	O2'-C2'	-2.05	1.37	1.43
13	bi	102	BCL	C1D-C2D	-2.05	1.41	1.45
14	BG	1003	LMT	O2B-C2B	-2.05	1.37	1.43
14	BR	1006	LMT	O2'-C2'	-2.05	1.37	1.43
14	AV	102	LMT	O4'-C4B	-2.05	1.37	1.43
15	BV	1001	V7N	C6-C5	2.05	1.40	1.35
14	BI	1002	LMT	O2B-C2B	-2.05	1.37	1.43
13	AV	101	BCL	C1D-C2D	-2.05	1.41	1.45
14	AA	1003	LMT	O2B-C2B	-2.04	1.37	1.43
13	ap	1001	BCL	C1D-C2D	-2.04	1.41	1.45
13	ao	102	BCL	C1D-C2D	-2.04	1.41	1.45
14	bi	104	LMT	O2B-C2B	-2.04	1.37	1.43
14	BX	104	LMT	O2B-C2B	-2.04	1.37	1.43
13	aj	101	BCL	C1D-C2D	-2.04	1.41	1.45
15	bc	101	V7N	C6-C5	2.04	1.40	1.35
14	BL	101	LMT	O2'-C2'	-2.04	1.37	1.43
15	bg	101	V7N	C7-C8	2.04	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AQ	103	BCL	C1D-C2D	-2.04	1.41	1.45
14	BX	102	LMT	O4'-C4B	-2.04	1.37	1.43
13	AM	1002	BCL	C3D-C4D	-2.04	1.39	1.44
14	AK	101	LMT	O3B-C3B	-2.04	1.37	1.43
15	AD	101	V7N	C19-C18	-2.04	1.41	1.46
14	BH	1002	LMT	O2B-C2B	-2.04	1.37	1.43
14	BO	1005	LMT	O2B-C2B	-2.04	1.37	1.43
14	bh	102	LMT	O3B-C3B	-2.04	1.37	1.43
14	bn	103	LMT	O4'-C4B	-2.04	1.37	1.43
13	ap	1001	BCL	CHD-C1D	2.04	1.42	1.38
14	BM	1003	LMT	O2'-C2'	-2.04	1.37	1.43
13	ak	1001	BCL	C1D-C2D	-2.03	1.41	1.45
13	AW	102	BCL	C3D-C4D	-2.03	1.39	1.44
14	AV	104	LMT	O4'-C4B	-2.03	1.37	1.43
14	AN	101	LMT	O2'-C2'	-2.03	1.37	1.43
14	AH	101	LMT	O2B-C2B	-2.03	1.37	1.43
14	BB	102	LMT	O2'-C2'	-2.03	1.37	1.43
15	bd	101	V7N	C12-C13	-2.03	1.41	1.46
13	BS	1004	BCL	C1D-C2D	-2.03	1.41	1.45
13	BG	1004	BCL	C1D-C2D	-2.03	1.41	1.45
17	C	1004	HEC	CMB-C2B	2.03	1.54	1.50
15	BN	1001	V7N	C19-C18	-2.03	1.41	1.46
15	be	102	V7N	C19-C18	-2.03	1.41	1.46
13	BO	1003	BCL	C3B-C4B	2.03	1.45	1.41
13	AQ	104	BCL	C3D-C4D	-2.03	1.39	1.44
14	BB	102	LMT	O2B-C2B	-2.03	1.37	1.43
13	AK	102	BCL	C3D-C4D	-2.03	1.39	1.44
15	BE	101	V7N	C7-C8	2.03	1.40	1.34
15	BN	1001	V7N	C7-C8	2.03	1.40	1.34
15	AD	101	V7N	C7-C8	2.03	1.40	1.34
13	AE	105	BCL	C1D-ND	2.03	1.40	1.37
13	AO	102	BCL	C1D-C2D	-2.02	1.41	1.45
13	AA	1002	BCL	C1D-ND	2.02	1.40	1.37
13	AQ	102	BCL	C3D-C4D	-2.02	1.39	1.44
13	AN	104	BCL	C3D-C4D	-2.02	1.39	1.44
14	BF	102	LMT	O2B-C2B	-2.02	1.38	1.43
14	BN	1003	LMT	O4'-C4B	-2.02	1.38	1.43
15	bk	101	V7N	C12-C13	-2.02	1.41	1.46
14	ac	101	LMT	O2B-C2B	-2.02	1.38	1.43
14	BH	1002	LMT	O4'-C4B	-2.02	1.38	1.43
13	bc	103	BCL	CHD-C1D	2.02	1.42	1.38
13	BJ	1004	BCL	C1D-C2D	-2.02	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BP	1004	LMT	O2B-C2B	-2.02	1.38	1.43
15	bi	101	V7N	C7-C8	2.02	1.39	1.34
15	AM	1001	V7N	C7-C8	2.02	1.39	1.34
13	BT	103	BCL	C1D-C2D	-2.02	1.41	1.45
15	BW	1001	V7N	C6-C5	2.02	1.40	1.35
14	BP	1002	LMT	O4'-C4B	-2.02	1.38	1.43
15	be	102	V7N	C7-C8	2.02	1.39	1.34
15	BQ	1001	V7N	C7-C8	2.02	1.39	1.34
15	BW	1001	V7N	C19-C18	-2.02	1.41	1.46
17	C	1001	HEC	CMC-C2C	2.01	1.54	1.50
14	BP	1006	LMT	O4'-C4B	-2.01	1.38	1.43
14	BX	103	LMT	O4'-C4B	-2.01	1.38	1.43
13	AD	104	BCL	C3D-C4D	-2.01	1.39	1.44
14	BK	1005	LMT	O2B-C2B	-2.01	1.38	1.43
13	AM	1004	BCL	C1D-C2D	-2.01	1.41	1.45
14	AK	103	LMT	O4'-C4B	-2.01	1.38	1.43
14	BW	1006	LMT	O4'-C4B	-2.01	1.38	1.43
15	bl	101	V7N	C12-C13	-2.01	1.41	1.46
14	AE	101	LMT	O4'-C4B	-2.01	1.38	1.43
15	AD	101	V7N	C6-C5	2.01	1.40	1.35
13	BV	1005	BCL	C1D-C2D	-2.01	1.41	1.45
13	BM	1004	BCL	C1D-C2D	-2.01	1.41	1.45
14	AB	1003	LMT	O4'-C4B	-2.01	1.38	1.43
15	BA	101	V7N	C20-C19	2.01	1.39	1.34
15	bc	101	V7N	C20-C19	2.01	1.39	1.34
15	bb	101	V7N	C12-C13	-2.01	1.41	1.46
13	bh	103	BCL	CHD-C1D	2.01	1.42	1.38
15	BE	101	V7N	C19-C18	-2.01	1.41	1.46
14	BU	1003	LMT	O2'-C2'	-2.01	1.38	1.43
13	bg	104	BCL	CHD-C1D	2.01	1.42	1.38
15	bo	101	V7N	C19-C18	-2.01	1.41	1.46
15	bc	101	V7N	C28-C29	2.00	1.49	1.43
14	BH	1004	LMT	O4'-C4B	-2.00	1.38	1.43
13	AS	101	BCL	C3D-C4D	-2.00	1.39	1.44
14	BT	102	LMT	O2B-C2B	-2.00	1.38	1.43
14	AJ	102	LMT	O1'-C1'	-2.00	1.36	1.40
13	AO	101	BCL	C1D-C2D	-2.00	1.41	1.45
14	AJ	101	LMT	O2B-C2B	-2.00	1.38	1.43
13	AK	104	BCL	C1D-C2D	-2.00	1.41	1.45
15	BS	1001	V7N	C7-C8	2.00	1.39	1.34
13	AQ	102	BCL	C1D-ND	2.00	1.40	1.37
26	af	101	V7B	O7-C10	2.00	1.39	1.34

All (1826) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	407	BPH	C4D-CHA-CBD	-10.31	103.51	108.45
22	L	301	BPH	C4D-CHA-CBD	-9.94	103.69	108.45
13	BP	1003	BCL	C1-O2A-CGA	9.31	139.18	116.65
15	BU	1001	V7N	C28-C27-C26	-7.45	105.93	126.36
15	AA	1004	V7N	C28-C27-C26	-6.99	107.20	126.36
17	C	1001	HEC	CBC-CAC-C3C	-6.50	114.45	127.43
17	C	1003	HEC	CBB-CAB-C3B	-6.46	114.53	127.43
13	AE	103	BCL	C1-O2A-CGA	6.46	132.28	116.65
13	AL	103	BCL	C1-O2A-CGA	6.43	132.22	116.65
17	C	1004	HEC	CBC-CAC-C3C	-6.41	114.61	127.43
17	C	1002	HEC	CBC-CAC-C3C	-6.19	115.06	127.43
15	bb	101	V7N	C28-C27-C26	-5.96	110.03	126.36
17	C	1004	HEC	CBB-CAB-C3B	-5.95	115.54	127.43
13	AM	1002	BCL	C1-O2A-CGA	5.85	130.81	116.65
15	BN	1001	V7N	C28-C27-C26	-5.82	110.40	126.36
17	C	1001	HEC	CBB-CAB-C3B	-5.81	115.81	127.43
15	BQ	1001	V7N	C28-C27-C26	-5.77	110.54	126.36
15	AM	1001	V7N	C28-C27-C26	-5.77	110.54	126.36
13	BD	104	BCL	C1-O2A-CGA	5.74	130.54	116.65
21	af	102	CD4	O2-C14-C13	5.69	123.79	111.48
13	M	408	BCL	C4D-CHA-C1A	5.67	128.01	121.24
13	AS	101	BCL	C4D-CHA-C1A	5.66	128.00	121.24
17	C	1002	HEC	CBB-CAB-C3B	-5.62	116.20	127.43
15	bl	101	V7N	C29-C28-C27	-5.62	106.93	123.20
13	AK	102	BCL	C4D-CHA-C1A	5.61	127.93	121.24
13	AV	103	BCL	C4D-CHA-C1A	5.58	127.90	121.24
13	AQ	102	BCL	C4D-CHA-C1A	5.58	127.90	121.24
15	BR	1001	V7N	C28-C27-C26	-5.57	111.08	126.36
15	BN	1001	V7N	C7-C6-C5	-5.57	119.47	127.28
13	AG	102	BCL	C4D-CHA-C1A	5.56	127.87	121.24
13	AP	103	BCL	C4D-CHA-C1A	5.56	127.87	121.24
13	AE	105	BCL	C4D-CHA-C1A	5.56	127.87	121.24
13	AG	102	BCL	C1-C2-C3	5.55	135.29	126.20
13	AJ	103	BCL	C4D-CHA-C1A	5.55	127.86	121.24
13	AL	103	BCL	C4D-CHA-C1A	5.54	127.86	121.24
13	AE	103	BCL	C4D-CHA-C1A	5.54	127.85	121.24
13	AD	104	BCL	C4D-CHA-C1A	5.54	127.85	121.24
13	bi	102	BCL	C4D-CHA-C1A	5.51	127.82	121.24
13	BW	1005	BCL	C4D-CHA-C1A	5.51	127.82	121.24
13	al	1001	BCL	C4D-CHA-C1A	5.51	127.81	121.24
13	am	1001	BCL	C4D-CHA-C1A	5.50	127.81	121.24
13	ap	1001	BCL	C4D-CHA-C1A	5.50	127.81	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AT	103	BCL	C4D-CHA-C1A	5.50	127.80	121.24
13	bd	102	BCL	C4D-CHA-C1A	5.49	127.79	121.24
15	bm	101	V7N	C29-C28-C27	-5.49	107.30	123.20
13	AH	105	BCL	C4D-CHA-C1A	5.48	127.78	121.24
13	BP	1003	BCL	C4D-CHA-C1A	5.48	127.78	121.24
17	C	1003	HEC	CBC-CAC-C3C	-5.48	116.48	127.43
13	AM	1002	BCL	C4D-CHA-C1A	5.48	127.78	121.24
13	AN	104	BCL	C4D-CHA-C1A	5.48	127.78	121.24
13	AL	102	BCL	C4D-CHA-C1A	5.47	127.77	121.24
13	BF	103	BCL	C4D-CHA-C1A	5.47	127.77	121.24
13	aa	1001	BCL	C4D-CHA-C1A	5.47	127.77	121.24
13	BV	1005	BCL	C4D-CHA-C1A	5.47	127.77	121.24
13	aj	101	BCL	C4D-CHA-C1A	5.46	127.76	121.24
13	BH	1005	BCL	C4D-CHA-C1A	5.46	127.75	121.24
13	ak	1001	BCL	C4D-CHA-C1A	5.46	127.75	121.24
13	ab	1001	BCL	C4D-CHA-C1A	5.46	127.75	121.24
13	AB	1001	BCL	C4D-CHA-C1A	5.45	127.74	121.24
13	BB	105	BCL	C4D-CHA-C1A	5.45	127.74	121.24
13	AN	103	BCL	C4D-CHA-C1A	5.44	127.73	121.24
13	AT	101	BCL	C4D-CHA-C1A	5.44	127.73	121.24
13	BT	103	BCL	C4D-CHA-C1A	5.44	127.73	121.24
13	bl	104	BCL	C4D-CHA-C1A	5.43	127.73	121.24
13	BJ	1004	BCL	C4D-CHA-C1A	5.43	127.72	121.24
13	BI	1004	BCL	C4D-CHA-C1A	5.42	127.71	121.24
13	BL	103	BCL	C4D-CHA-C1A	5.42	127.70	121.24
13	AE	104	BCL	C4D-CHA-C1A	5.41	127.70	121.24
13	BN	1005	BCL	C4D-CHA-C1A	5.40	127.69	121.24
13	BD	104	BCL	C4D-CHA-C1A	5.40	127.68	121.24
13	BX	101	BCL	C4D-CHA-C1A	5.40	127.68	121.24
13	ae	1001	BCL	C4D-CHA-C1A	5.40	127.68	121.24
13	BM	1004	BCL	C4D-CHA-C1A	5.39	127.67	121.24
13	BE	104	BCL	C4D-CHA-C1A	5.38	127.67	121.24
13	AF	1001	BCL	C4D-CHA-C1A	5.38	127.66	121.24
13	AQ	103	BCL	C4D-CHA-C1A	5.38	127.66	121.24
13	BG	1004	BCL	C4D-CHA-C1A	5.38	127.66	121.24
13	ac	102	BCL	C4D-CHA-C1A	5.38	127.66	121.24
13	BC	104	BCL	C4D-CHA-C1A	5.37	127.65	121.24
13	AI	101	BCL	C4D-CHA-C1A	5.37	127.65	121.24
13	AH	103	BCL	C4D-CHA-C1A	5.37	127.65	121.24
13	AB	1002	BCL	C4D-CHA-C1A	5.36	127.64	121.24
13	AD	103	BCL	C4D-CHA-C1A	5.36	127.64	121.24
13	L	308	BCL	C4D-CHA-C1A	5.36	127.64	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AW	101	BCL	C4D-CHA-C1A	5.36	127.63	121.24
13	BS	1004	BCL	C4D-CHA-C1A	5.36	127.63	121.24
13	AS	102	BCL	C4D-CHA-C1A	5.36	127.63	121.24
13	AW	102	BCL	C4D-CHA-C1A	5.35	127.63	121.24
13	BK	1002	BCL	C4D-CHA-C1A	5.35	127.63	121.24
13	bo	102	BCL	C4D-CHA-C1A	5.35	127.63	121.24
13	AP	102	BCL	C4D-CHA-C1A	5.35	127.62	121.24
13	AX	103	BCL	C4D-CHA-C1A	5.34	127.61	121.24
13	bb	102	BCL	C4D-CHA-C1A	5.34	127.61	121.24
13	AA	1002	BCL	C4D-CHA-C1A	5.34	127.61	121.24
13	ba	102	BCL	C4D-CHA-C1A	5.33	127.61	121.24
13	an	1001	BCL	C4D-CHA-C1A	5.33	127.61	121.24
13	bj	104	BCL	C4D-CHA-C1A	5.33	127.61	121.24
21	ad	101	CD4	C15-O2-C14	5.32	130.54	117.80
13	be	103	BCL	C4D-CHA-C1A	5.32	127.59	121.24
13	AC	101	BCL	C4D-CHA-C1A	5.32	127.59	121.24
13	bf	102	BCL	C4D-CHA-C1A	5.32	127.58	121.24
13	ad	102	BCL	C4D-CHA-C1A	5.31	127.58	121.24
13	ag	102	BCL	C4D-CHA-C1A	5.31	127.58	121.24
13	bk	103	BCL	C4D-CHA-C1A	5.31	127.58	121.24
13	bp	104	BCL	C4D-CHA-C1A	5.31	127.58	121.24
13	BU	1004	BCL	C4D-CHA-C1A	5.31	127.57	121.24
13	BR	1003	BCL	C4D-CHA-C1A	5.30	127.56	121.24
13	bc	103	BCL	C4D-CHA-C1A	5.29	127.55	121.24
13	bg	104	BCL	C4D-CHA-C1A	5.28	127.54	121.24
13	AH	102	BCL	C4D-CHA-C1A	5.26	127.52	121.24
13	bn	102	BCL	C4D-CHA-C1A	5.25	127.51	121.24
13	BQ	1004	BCL	C4D-CHA-C1A	5.24	127.50	121.24
13	BA	103	BCL	C4D-CHA-C1A	5.23	127.48	121.24
13	AU	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24
13	AK	104	BCL	C4D-CHA-C1A	5.21	127.46	121.24
13	ao	102	BCL	C4D-CHA-C1A	5.20	127.45	121.24
13	bh	103	BCL	C4D-CHA-C1A	5.20	127.45	121.24
13	ai	101	BCL	C4D-CHA-C1A	5.19	127.44	121.24
13	AC	102	BCL	C4D-CHA-C1A	5.18	127.42	121.24
13	AG	103	BCL	C4D-CHA-C1A	5.18	127.42	121.24
13	M	406	BCL	C4D-CHA-C1A	5.15	127.39	121.24
13	af	103	BCL	C4D-CHA-C1A	5.15	127.39	121.24
13	bm	102	BCL	C4D-CHA-C1A	5.15	127.39	121.24
13	AU	103	BCL	C4D-CHA-C1A	5.14	127.37	121.24
15	bj	101	V7N	C29-C28-C27	-5.14	108.31	123.20
13	AR	101	BCL	C4D-CHA-C1A	5.13	127.36	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BO	1003	BCL	C4D-CHA-C1A	5.12	127.35	121.24
13	ah	1001	BCL	C4D-CHA-C1A	5.12	127.34	121.24
15	bg	101	V7N	C29-C28-C27	-5.11	108.39	123.20
13	AJ	104	BCL	C4D-CHA-C1A	5.10	127.33	121.24
15	ag	101	V7N	C29-C28-C27	-5.10	108.42	123.20
13	AA	1001	BCL	C4D-CHA-C1A	5.10	127.33	121.24
13	AO	102	BCL	C4D-CHA-C1A	5.09	127.32	121.24
13	AM	1004	BCL	C4D-CHA-C1A	5.09	127.31	121.24
15	bp	102	V7N	C27-C26-C25	5.07	125.55	118.49
13	AX	102	BCL	C4D-CHA-C1A	5.04	127.25	121.24
13	L	305	BCL	C4D-CHA-C1A	4.99	127.20	121.24
15	BG	1001	V7N	C28-C27-C26	-4.90	112.94	126.36
15	bp	102	V7N	C29-C28-C27	-4.88	109.06	123.20
13	AQ	104	BCL	C4D-CHA-C1A	4.88	127.06	121.24
15	be	102	V7N	C29-C28-C27	-4.87	109.10	123.20
13	AV	101	BCL	C4D-CHA-C1A	4.83	127.01	121.24
15	BI	1001	V7N	C29-C28-C27	-4.83	109.20	123.20
15	bo	101	V7N	C29-C28-C27	-4.82	109.24	123.20
15	bh	101	V7N	C29-C28-C27	-4.79	109.32	123.20
15	BM	1001	V7N	C29-C28-C27	-4.78	109.34	123.20
15	BJ	1001	V7N	C28-C27-C26	-4.78	113.25	126.36
21	af	104	CD4	O2-C14-C13	4.76	121.77	111.48
15	BM	1001	V7N	C28-C27-C26	-4.75	113.34	126.36
15	BS	1001	V7N	C29-C28-C27	-4.74	109.47	123.20
15	BA	101	V7N	C29-C28-C27	-4.72	109.51	123.20
15	BP	1001	V7N	C29-C28-C27	-4.72	109.52	123.20
15	BU	1001	V7N	C7-C6-C5	4.70	133.87	127.28
13	BO	1003	BCL	C1-C2-C3	4.68	133.86	126.20
15	BW	1001	V7N	C29-C28-C27	-4.62	109.80	123.20
21	M	405	CD4	O2-C14-C13	4.62	121.48	111.48
15	BE	101	V7N	C29-C28-C27	-4.61	109.84	123.20
18	C	1006	V75	O3-C3A-C3B	4.61	119.31	111.09
15	AD	101	V7N	C29-C28-C27	-4.58	109.94	123.20
15	BD	101	V7N	C28-C27-C26	-4.58	113.81	126.36
15	BO	1001	V7N	C29-C28-C27	-4.53	110.07	123.20
18	C	1006	V75	O2-C2A-C2B	4.51	119.13	111.09
15	BH	1001	V7N	C29-C28-C27	-4.50	110.16	123.20
15	BK	1001	V7N	C29-C28-C27	-4.46	110.28	123.20
15	BN	1001	V7N	C1-C2-C3	4.45	124.55	112.98
13	AO	101	BCL	C4D-CHA-C1A	4.45	126.55	121.24
15	BJ	1001	V7N	C29-C28-C27	-4.44	110.34	123.20
15	AW	103	V7N	C29-C28-C27	-4.40	110.45	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BH	1001	V7N	C28-C27-C26	-4.38	114.34	126.36
18	M	410	V75	O2-C2A-C2B	4.37	118.87	111.09
18	M	410	V75	O3-C3A-C3B	4.34	118.83	111.09
13	AQ	104	BCL	C1-O2A-CGA	4.33	127.14	116.65
15	bn	101	V7N	C28-C27-C26	-4.29	114.60	126.36
15	BV	1001	V7N	C29-C28-C27	-4.24	110.91	123.20
15	bd	101	V7N	C29-C28-C27	-4.24	110.92	123.20
15	BF	101	V7N	C28-C27-C26	-4.22	114.79	126.36
13	AW	102	BCL	C4A-NA-C1A	4.21	108.60	106.68
13	AQ	102	BCL	C1-C2-C3	-4.20	119.31	126.20
21	M	409	CD4	O2-C14-C13	4.20	120.56	111.48
15	bc	101	V7N	C28-C27-C26	-4.15	114.97	126.36
26	af	101	V7B	C1-O6-C5	4.12	121.77	113.72
15	BI	1001	V7N	C28-C27-C26	-4.11	115.09	126.36
22	M	407	BPH	C4D-ND-C1D	-4.11	103.95	108.87
15	ba	101	V7N	C29-C28-C27	-4.10	111.31	123.20
15	BV	1001	V7N	C28-C27-C26	-4.10	115.12	126.36
15	BW	1001	V7N	C28-C27-C26	-4.10	115.13	126.36
15	BS	1001	V7N	C28-C27-C26	-4.09	115.15	126.36
15	BG	1001	V7N	C29-C28-C27	-4.08	111.36	123.20
13	AD	104	BCL	CHD-C1D-ND	-4.07	119.07	124.80
15	BP	1001	V7N	C28-C27-C26	-4.07	115.20	126.36
15	bk	101	V7N	C28-C27-C26	-4.04	115.27	126.36
13	AD	104	BCL	C1-C2-C3	4.04	132.81	126.20
13	AH	105	BCL	C1-C2-C3	-4.03	119.59	126.20
14	AK	101	LMT	C3'-C4'-C5'	-4.01	102.03	110.93
15	bi	101	V7N	C28-C27-C26	-4.01	115.37	126.36
15	AW	103	V7N	C28-C27-C26	-4.00	115.38	126.36
22	L	301	BPH	C4D-ND-C1D	-4.00	104.08	108.87
15	BE	101	V7N	C28-C27-C26	-3.99	115.43	126.36
13	ao	102	BCL	C4A-NA-C1A	3.98	108.50	106.68
15	AS	104	V7N	C28-C27-C26	-3.97	115.47	126.36
14	BN	1003	LMT	C1-O1'-C1'	3.97	120.45	113.68
15	BO	1001	V7N	C28-C27-C26	-3.95	115.53	126.36
15	ba	101	V7N	C28-C27-C26	-3.94	115.55	126.36
13	ak	1001	BCL	C4A-NA-C1A	3.94	108.48	106.68
13	L	308	BCL	C1D-ND-C4D	-3.92	103.56	106.31
13	ap	1001	BCL	C1-O2A-CGA	3.91	126.12	116.65
15	bd	101	V7N	C28-C27-C26	-3.91	115.64	126.36
15	bk	101	V7N	C29-C28-C27	-3.90	111.91	123.20
13	M	408	BCL	C4A-NA-C1A	3.90	108.46	106.68
13	ad	102	BCL	C4A-NA-C1A	3.89	108.45	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AH	102	BCL	C1-C2-C3	-3.88	119.84	126.20
15	bn	101	V7N	C27-C26-C25	3.88	123.89	118.49
13	AP	103	BCL	C4A-NA-C1A	3.85	108.44	106.68
15	bh	101	V7N	C28-C27-C26	-3.83	115.86	126.36
13	L	308	BCL	CHD-C1D-ND	-3.83	119.41	124.80
13	AX	103	BCL	CHD-C1D-ND	-3.83	119.41	124.80
15	ag	101	V7N	C28-C27-C26	-3.82	115.88	126.36
13	AO	101	BCL	CHD-C1D-ND	-3.82	119.42	124.80
15	BK	1001	V7N	C27-C26-C25	3.81	123.79	118.49
15	AW	103	V7N	C15-C14-C13	-3.80	121.95	127.28
15	bn	101	V7N	C29-C28-C27	-3.80	112.19	123.20
13	AJ	103	BCL	C1-C2-C3	-3.80	119.97	126.20
13	AE	105	BCL	CHD-C1D-ND	-3.80	119.46	124.80
15	bo	101	V7N	C28-C27-C26	-3.79	115.96	126.36
13	M	406	BCL	CHD-C1D-ND	-3.79	119.46	124.80
13	ah	1001	BCL	C4A-NA-C1A	3.74	108.39	106.68
15	bg	101	V7N	C28-C27-C26	-3.74	116.11	126.36
13	AS	101	BCL	C1D-ND-C4D	-3.74	103.69	106.31
14	AA	1003	LMT	C3'-C4'-C5'	-3.74	102.64	110.93
17	C	1002	HEC	CMC-C2C-C1C	-3.73	119.74	125.42
13	AW	102	BCL	C1D-ND-C4D	-3.72	103.70	106.31
13	ai	101	BCL	C4A-NA-C1A	3.72	108.38	106.68
13	BN	1005	BCL	C4A-NA-C1A	3.72	108.37	106.68
13	AH	105	BCL	CHD-C1D-ND	-3.71	119.58	124.80
13	AU	103	BCL	CHD-C1D-ND	-3.71	119.58	124.80
13	an	1001	BCL	C4A-NA-C1A	3.70	108.37	106.68
13	L	305	BCL	CHD-C1D-ND	-3.70	119.59	124.80
14	BI	1005	LMT	C1-O1'-C1'	3.70	119.99	113.68
21	af	102	CD4	O16-C46-C47	3.68	119.44	111.48
13	AJ	104	BCL	C4A-NA-C1A	3.68	108.36	106.68
13	AG	102	BCL	CHD-C1D-ND	-3.68	119.63	124.80
13	bb	102	BCL	C1-C2-C3	-3.67	120.18	126.20
14	AS	103	LMT	C3'-C4'-C5'	-3.67	102.79	110.93
13	AC	101	BCL	CHD-C1D-ND	-3.67	119.63	124.80
13	AS	101	BCL	C4A-NA-C1A	3.67	108.35	106.68
13	af	103	BCL	C4A-NA-C1A	3.67	108.35	106.68
13	AS	101	BCL	CHD-C1D-ND	-3.67	119.64	124.80
13	AT	103	BCL	C4A-NA-C1A	3.66	108.35	106.68
13	AJ	103	BCL	CHD-C1D-ND	-3.66	119.65	124.80
13	AL	103	BCL	C1-C2-C3	-3.66	120.20	126.20
13	AQ	102	BCL	C1-O2A-CGA	3.66	125.51	116.65
13	BP	1003	BCL	C4A-NA-C1A	3.65	108.35	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BW	1004	LMT	O1'-C1'-C2'	3.65	113.81	108.27
21	H1	103	CD4	C15-O2-C14	3.64	126.50	117.80
13	AL	103	BCL	CHD-C1D-ND	-3.63	119.69	124.80
13	AW	101	BCL	C4A-NA-C1A	3.63	108.33	106.68
13	AQ	102	BCL	CHD-C1D-ND	-3.62	119.70	124.80
13	AK	102	BCL	CHD-C1D-ND	-3.62	119.71	124.80
13	bk	103	BCL	C4A-NA-C1A	3.62	108.33	106.68
13	BK	1002	BCL	C1-C2-C3	3.62	132.12	126.20
13	AX	102	BCL	C4A-NA-C1A	3.60	108.32	106.68
13	AW	102	BCL	CHD-C1D-ND	-3.59	119.75	124.80
13	BU	1004	BCL	CHD-C1D-ND	-3.59	119.75	124.80
13	AP	103	BCL	CHD-C1D-ND	-3.59	119.75	124.80
14	BR	1005	LMT	C1-O1'-C1'	3.58	119.80	113.68
13	bd	102	BCL	C1-C2-C3	3.58	132.06	126.20
13	ap	1001	BCL	C4A-NA-C1A	3.57	108.31	106.68
13	BH	1005	BCL	CHD-C1D-ND	-3.57	119.78	124.80
13	AH	103	BCL	C4A-NA-C1A	3.57	108.31	106.68
13	BD	104	BCL	C4A-NA-C1A	3.56	108.30	106.68
13	AE	103	BCL	CHD-C1D-ND	-3.56	119.79	124.80
13	bj	104	BCL	C4A-NA-C1A	3.56	108.30	106.68
20	H1	101	PGW	C02-O01-C1	3.56	126.31	117.80
14	AE	101	LMT	C1-O1'-C1'	3.56	119.75	113.68
13	BI	1004	BCL	CHD-C1D-ND	-3.56	119.80	124.80
13	AN	103	BCL	C4A-NA-C1A	3.55	108.30	106.68
13	AM	1002	BCL	CHD-C1D-ND	-3.55	119.81	124.80
13	AV	103	BCL	C4A-NA-C1A	3.55	108.30	106.68
15	be	102	V7N	C28-C27-C26	-3.55	116.63	126.36
13	ab	1001	BCL	C4A-NA-C1A	3.54	108.30	106.68
15	AD	101	V7N	C28-C27-C26	-3.54	116.64	126.36
15	BA	101	V7N	C27-C26-C25	3.54	123.42	118.49
13	AQ	102	BCL	C1D-ND-C4D	-3.54	103.83	106.31
13	AB	1001	BCL	C4A-NA-C1A	3.54	108.29	106.68
15	AD	101	V7N	C27-C26-C25	3.54	123.42	118.49
13	BC	104	BCL	CHD-C1D-ND	-3.54	119.83	124.80
13	BX	101	BCL	CHD-C1D-ND	-3.54	119.83	124.80
13	AU	103	BCL	C1D-ND-C4D	-3.53	103.83	106.31
13	AM	1002	BCL	C4A-NA-C1A	3.53	108.29	106.68
13	AT	103	BCL	CHD-C1D-ND	-3.53	119.83	124.80
17	C	1001	HEC	CMC-C2C-C1C	-3.53	120.05	125.42
13	BR	1003	BCL	C4A-NA-C1A	3.52	108.29	106.68
13	AN	104	BCL	CHD-C1D-ND	-3.52	119.85	124.80
13	bk	103	BCL	CHD-C1D-ND	-3.52	119.85	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ac	102	BCL	C4A-NA-C1A	3.52	108.28	106.68
13	BW	1005	BCL	CHD-C1D-ND	-3.51	119.86	124.80
13	BD	104	BCL	CHD-C1D-ND	-3.51	119.86	124.80
15	BW	1001	V7N	C20-C21-C22	-3.51	122.75	127.69
13	bg	104	BCL	CHD-C1D-ND	-3.51	119.86	124.80
14	AV	104	LMT	C1-O1'-C1'	3.50	119.66	113.68
14	BK	1005	LMT	C1-O1'-C1'	3.50	119.66	113.68
14	BT	101	LMT	C1-O1'-C1'	3.50	119.66	113.68
13	AK	104	BCL	C4A-NA-C1A	3.50	108.28	106.68
17	C	1003	HEC	C4D-ND-C1D	3.49	111.52	105.82
17	C	1003	HEC	CMC-C2C-C1C	-3.49	120.11	125.42
13	ac	102	BCL	CHD-C1D-ND	-3.49	119.89	124.80
13	AF	1001	BCL	C4A-NA-C1A	3.49	108.27	106.68
13	BM	1004	BCL	CHD-C1D-ND	-3.49	119.89	124.80
13	BP	1003	BCL	C11-C10-C8	3.49	127.56	115.97
15	BD	101	V7N	C29-C28-C27	-3.48	113.11	123.20
13	BJ	1004	BCL	CHD-C1D-ND	-3.48	119.90	124.80
13	AX	103	BCL	C4A-NA-C1A	3.48	108.27	106.68
13	BW	1005	BCL	C1D-ND-C4D	-3.48	103.87	106.31
13	BG	1004	BCL	CHD-C1D-ND	-3.47	119.92	124.80
13	BC	104	BCL	C1D-ND-C4D	-3.47	103.88	106.31
13	ag	102	BCL	CHD-C1D-ND	-3.47	119.92	124.80
13	BU	1004	BCL	C1D-ND-C4D	-3.47	103.88	106.31
13	AB	1002	BCL	CHD-C1D-ND	-3.47	119.92	124.80
13	BB	105	BCL	CHD-C1D-ND	-3.47	119.92	124.80
13	AV	103	BCL	CHD-C1D-ND	-3.46	119.93	124.80
14	AT	102	LMT	C1-O1'-C1'	3.46	119.59	113.68
13	ba	102	BCL	CHD-C1D-ND	-3.46	119.94	124.80
13	al	1001	BCL	CHD-C1D-ND	-3.46	119.94	124.80
13	BE	104	BCL	CHD-C1D-ND	-3.46	119.94	124.80
13	ap	1001	BCL	CHD-C1D-ND	-3.46	119.94	124.80
13	ak	1001	BCL	CHD-C1D-ND	-3.45	119.94	124.80
13	AX	102	BCL	CHA-C1A-NA	-3.45	118.57	126.39
13	BL	103	BCL	CHD-C1D-ND	-3.45	119.94	124.80
13	BA	103	BCL	CHD-C1D-ND	-3.45	119.95	124.80
13	BP	1003	BCL	C1D-ND-C4D	-3.45	103.89	106.31
13	M	406	BCL	C1D-ND-C4D	-3.45	103.89	106.31
13	AS	102	BCL	C1-C2-C3	-3.44	120.56	126.20
13	AT	103	BCL	C1D-ND-C4D	-3.44	103.90	106.31
13	AA	1002	BCL	CHD-C1D-ND	-3.44	119.96	124.80
13	BF	103	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	AB	1003	LMT	C1-O1'-C1'	3.44	119.55	113.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AH	102	BCL	CHD-C1D-ND	-3.44	119.96	124.80
13	bi	102	BCL	CHD-C1D-ND	-3.44	119.96	124.80
13	BE	104	BCL	C1D-ND-C4D	-3.43	103.90	106.31
13	AG	102	BCL	C1-O2A-CGA	3.43	124.96	116.65
13	am	1001	BCL	CHD-C1D-ND	-3.43	119.98	124.80
13	bh	103	BCL	CHD-C1D-ND	-3.43	119.98	124.80
13	BR	1003	BCL	CHD-C1D-ND	-3.43	119.98	124.80
13	bj	104	BCL	CHD-C1D-ND	-3.42	119.98	124.80
13	AP	103	BCL	C1D-ND-C4D	-3.42	103.91	106.31
13	bo	102	BCL	C1D-ND-C4D	-3.42	103.91	106.31
13	BP	1003	BCL	CHD-C1D-ND	-3.42	119.99	124.80
13	be	103	BCL	CHD-C1D-ND	-3.42	119.99	124.80
13	AG	103	BCL	C4A-NA-C1A	3.41	108.24	106.68
13	ac	102	BCL	C1D-ND-C4D	-3.41	103.92	106.31
13	ad	102	BCL	CHD-C1D-ND	-3.41	120.00	124.80
13	BS	1004	BCL	CHD-C1D-ND	-3.41	120.00	124.80
13	bm	102	BCL	CHD-C1D-ND	-3.41	120.00	124.80
13	AD	103	BCL	C1-C2-C3	3.41	131.78	126.20
13	bc	103	BCL	C4A-NA-C1A	3.41	108.23	106.68
13	ab	1001	BCL	C1-O2A-CGA	3.41	124.90	116.65
17	C	1002	HEC	C4D-ND-C1D	3.40	111.37	105.82
13	AD	104	BCL	C1D-ND-C4D	-3.40	103.93	106.31
13	ao	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
13	an	1001	BCL	CHD-C1D-ND	-3.40	120.02	124.80
13	bd	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
13	BG	1004	BCL	C1D-ND-C4D	-3.40	103.93	106.31
13	bl	104	BCL	CHD-C1D-ND	-3.40	120.02	124.80
13	BL	103	BCL	C4A-NA-C1A	3.40	108.23	106.68
13	M	408	BCL	CHD-C1D-ND	-3.40	120.02	124.80
13	BT	103	BCL	CHD-C1D-ND	-3.39	120.03	124.80
15	bj	101	V7N	C28-C27-C26	-3.39	117.06	126.36
15	BA	101	V7N	C28-C27-C26	-3.39	117.06	126.36
13	AO	102	BCL	C4A-NA-C1A	3.39	108.23	106.68
15	BP	1001	V7N	C36-C18-C19	3.39	123.26	118.09
13	AN	104	BCL	C1D-ND-C4D	-3.39	103.94	106.31
13	aa	1001	BCL	CHD-C1D-ND	-3.38	120.04	124.80
13	BV	1005	BCL	C4A-NA-C1A	3.38	108.22	106.68
13	AJ	103	BCL	C1D-ND-C4D	-3.38	103.94	106.31
13	bb	102	BCL	CHD-C1D-ND	-3.38	120.05	124.80
13	BJ	1004	BCL	C1D-ND-C4D	-3.38	103.94	106.31
15	BG	1001	V7N	C27-C26-C25	3.38	123.19	118.49
13	BI	1004	BCL	C1D-ND-C4D	-3.37	103.94	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	af	103	BCL	C1D-ND-C4D	-3.37	103.95	106.31
13	ae	1001	BCL	CHD-C1D-ND	-3.37	120.06	124.80
13	AR	101	BCL	C4A-NA-C1A	3.37	108.22	106.68
15	BK	1001	V7N	C28-C27-C26	-3.37	117.13	126.36
13	bf	102	BCL	CHD-C1D-ND	-3.37	120.06	124.80
14	bh	102	LMT	C3'-C4'-C5'	-3.37	103.47	110.93
13	ba	102	BCL	C4A-NA-C1A	3.37	108.22	106.68
13	BH	1005	BCL	C1D-ND-C4D	-3.37	103.95	106.31
13	ao	102	BCL	C1D-ND-C4D	-3.36	103.95	106.31
13	AQ	104	BCL	CHD-C1D-ND	-3.36	120.07	124.80
13	ae	1001	BCL	C1D-ND-C4D	-3.36	103.95	106.31
14	BE	102	LMT	O1'-C1'-C2'	3.36	113.38	108.27
13	bo	102	BCL	CHD-C1D-ND	-3.36	120.07	124.80
13	al	1001	BCL	C4A-NA-C1A	3.36	108.21	106.68
22	M	407	BPH	C3D-C4D-ND	3.36	112.02	107.71
14	BU	1002	LMT	C1-O1'-C1'	3.36	119.42	113.68
13	ag	102	BCL	C1D-ND-C4D	-3.36	103.96	106.31
13	AE	104	BCL	C1-C2-C3	3.36	131.70	126.20
13	AV	101	BCL	CHD-C1D-ND	-3.36	120.08	124.80
13	aj	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
13	AR	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
13	ai	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
13	AL	103	BCL	C4A-NA-C1A	3.35	108.21	106.68
22	L	301	BPH	C3D-C4D-ND	3.35	112.00	107.71
13	BO	1003	BCL	CHD-C1D-ND	-3.35	120.09	124.80
13	AM	1004	BCL	CHD-C1D-ND	-3.35	120.09	124.80
13	ab	1001	BCL	CHD-C1D-ND	-3.35	120.09	124.80
13	AM	1002	BCL	C1D-ND-C4D	-3.35	103.97	106.31
13	AC	102	BCL	C4A-NA-C1A	3.34	108.20	106.68
13	am	1001	BCL	C1D-ND-C4D	-3.34	103.97	106.31
13	AA	1002	BCL	C1D-ND-C4D	-3.34	103.97	106.31
13	af	103	BCL	CHD-C1D-ND	-3.34	120.10	124.80
13	BV	1005	BCL	CHD-C1D-ND	-3.34	120.10	124.80
13	BN	1005	BCL	C1D-ND-C4D	-3.34	103.97	106.31
13	AW	101	BCL	CHD-C1D-ND	-3.34	120.10	124.80
13	BS	1004	BCL	C1D-ND-C4D	-3.34	103.97	106.31
15	BF	101	V7N	C29-C28-C27	-3.34	113.53	123.20
15	bp	102	V7N	C38-C26-C27	-3.33	113.00	118.09
13	ap	1001	BCL	C1D-ND-C4D	-3.33	103.97	106.31
13	BN	1005	BCL	CHD-C1D-ND	-3.33	120.11	124.80
15	BN	1001	V7N	C3-C4-C5	3.33	130.93	125.89
13	BA	103	BCL	C1D-ND-C4D	-3.33	103.97	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BM	1004	BCL	C1D-ND-C4D	-3.33	103.97	106.31
13	AO	102	BCL	CHD-C1D-ND	-3.33	120.11	124.80
15	BI	1001	V7N	C7-C6-C5	-3.33	122.61	127.28
13	M	408	BCL	CHA-C1A-NA	-3.33	118.85	126.39
13	AX	103	BCL	C1D-ND-C4D	-3.33	103.97	106.31
13	bk	103	BCL	C1D-ND-C4D	-3.33	103.98	106.31
13	BK	1002	BCL	CHD-C1D-ND	-3.33	120.12	124.80
17	C	1001	HEC	C4D-ND-C1D	3.33	111.25	105.82
15	BO	1001	V7N	C27-C26-C25	3.33	123.13	118.49
15	BF	101	V7N	O44-C40-O45	-3.32	115.99	123.90
15	BF	101	V7N	C15-C14-C13	-3.32	122.62	127.28
13	be	103	BCL	C1D-ND-C4D	-3.32	103.98	106.31
13	AC	101	BCL	C4A-NA-C1A	3.32	108.19	106.68
23	L	303	MQ8	O4-C4-C5	-3.32	116.26	121.57
13	bh	103	BCL	C1D-ND-C4D	-3.32	103.98	106.31
13	AQ	103	BCL	CHA-C1A-NA	-3.32	118.88	126.39
13	AD	103	BCL	C4A-NA-C1A	3.32	108.19	106.68
13	bp	104	BCL	CHD-C1D-ND	-3.32	120.14	124.80
13	ba	102	BCL	C1D-ND-C4D	-3.32	103.99	106.31
13	BL	103	BCL	C1D-ND-C4D	-3.31	103.99	106.31
15	bb	101	V7N	O44-C40-O45	-3.31	116.01	123.90
13	bg	104	BCL	C1D-ND-C4D	-3.31	103.99	106.31
13	BK	1002	BCL	C4A-NA-C1A	3.31	108.19	106.68
13	AG	102	BCL	C1D-ND-C4D	-3.31	103.99	106.31
13	BQ	1004	BCL	CHD-C1D-ND	-3.31	120.15	124.80
15	BU	1001	V7N	C35-C13-C14	-3.31	117.46	122.82
13	AV	103	BCL	C1D-ND-C4D	-3.31	103.99	106.31
13	AE	105	BCL	C4A-NA-C1A	3.31	108.19	106.68
13	ai	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
14	BE	102	LMT	C1'-O5'-C5'	-3.31	107.26	113.72
15	BN	1001	V7N	C4-C5-C6	3.31	124.21	119.01
13	bn	102	BCL	CHD-C1D-ND	-3.31	120.15	124.80
13	AC	102	BCL	CHD-C1D-ND	-3.30	120.15	124.80
13	AU	101	BCL	CHD-C1D-ND	-3.30	120.15	124.80
13	AI	101	BCL	CHD-C1D-ND	-3.30	120.15	124.80
13	an	1001	BCL	C1D-ND-C4D	-3.30	104.00	106.31
13	AH	103	BCL	CHD-C1D-ND	-3.30	120.16	124.80
13	BX	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31
13	AO	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31
13	BM	1004	BCL	C1-O2A-CGA	3.29	124.62	116.65
13	AE	103	BCL	C1D-ND-C4D	-3.29	104.00	106.31
13	AL	103	BCL	C1D-ND-C4D	-3.29	104.00	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bp	102	V7N	O44-C40-O45	-3.29	116.06	123.90
14	BB	103	LMT	C3'-C4'-C5'	-3.29	103.64	110.93
13	AS	102	BCL	CHD-C1D-ND	-3.29	120.17	124.80
13	ab	1001	BCL	C1D-ND-C4D	-3.29	104.00	106.31
13	bc	103	BCL	C1D-ND-C4D	-3.29	104.00	106.31
13	AU	101	BCL	C4A-NA-C1A	3.29	108.18	106.68
13	BM	1004	BCL	C4A-NA-C1A	3.29	108.18	106.68
13	AT	101	BCL	CHD-C1D-ND	-3.29	120.18	124.80
13	ag	102	BCL	C4A-NA-C1A	3.29	108.18	106.68
13	am	1001	BCL	C4A-NA-C1A	3.29	108.18	106.68
15	bc	101	V7N	C29-C28-C27	-3.28	113.70	123.20
13	BO	1003	BCL	C1D-ND-C4D	-3.28	104.01	106.31
13	bm	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
13	bp	104	BCL	C1D-ND-C4D	-3.28	104.01	106.31
13	BB	105	BCL	C4A-NA-C1A	3.28	108.17	106.68
22	M	407	BPH	OBD-CAD-CBD	-3.27	121.02	125.82
13	AV	101	BCL	C1D-ND-C4D	-3.27	104.02	106.31
13	BI	1004	BCL	C4A-NA-C1A	3.27	108.17	106.68
13	BO	1003	BCL	C4A-NA-C1A	3.27	108.17	106.68
13	AA	1001	BCL	CHD-C1D-ND	-3.27	120.20	124.80
13	AL	102	BCL	CHD-C1D-ND	-3.27	120.20	124.80
13	BA	103	BCL	C4A-NA-C1A	3.27	108.17	106.68
13	bj	104	BCL	CBA-CAA-C2A	3.27	123.52	113.79
15	AS	104	V7N	C29-C28-C27	-3.27	113.73	123.20
13	AS	102	BCL	CHA-C1A-NA	-3.27	118.99	126.39
13	ae	1001	BCL	C4A-NA-C1A	3.27	108.17	106.68
13	AP	102	BCL	CHD-C1D-ND	-3.27	120.20	124.80
13	AE	105	BCL	C1D-ND-C4D	-3.27	104.02	106.31
13	bd	102	BCL	C1D-ND-C4D	-3.27	104.02	106.31
13	AK	102	BCL	C1D-ND-C4D	-3.26	104.02	106.31
13	BD	104	BCL	C1D-ND-C4D	-3.26	104.02	106.31
14	BO	1002	LMT	C3'-C4'-C5'	-3.26	103.70	110.93
13	AE	103	BCL	CAA-CBA-CGA	3.26	122.47	113.21
13	AG	103	BCL	CHD-C1D-ND	-3.26	120.21	124.80
13	AN	103	BCL	CHD-C1D-ND	-3.26	120.21	124.80
13	AF	1001	BCL	CHD-C1D-ND	-3.26	120.21	124.80
13	BB	105	BCL	C1D-ND-C4D	-3.26	104.02	106.31
15	bc	101	V7N	O44-C40-O45	-3.26	116.14	123.90
13	BS	1004	BCL	C4A-NA-C1A	3.26	108.17	106.68
13	AH	105	BCL	C1-O2A-CGA	3.26	124.53	116.65
13	ad	102	BCL	C1D-ND-C4D	-3.25	104.03	106.31
13	BQ	1004	BCL	C4A-NA-C1A	3.25	108.16	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1004	HEC	C4D-ND-C1D	3.25	111.12	105.82
15	AD	101	V7N	O44-C40-O45	-3.25	116.16	123.90
13	AL	102	BCL	CHA-C1A-NA	-3.25	119.03	126.39
21	ad	101	CD4	O16-C46-C47	3.25	118.51	111.48
15	AW	103	V7N	O44-C40-O45	-3.24	116.18	123.90
13	AQ	104	BCL	C1D-ND-C4D	-3.24	104.04	106.31
13	bi	102	BCL	C1D-ND-C4D	-3.24	104.04	106.31
15	AA	1004	V7N	C20-C21-C22	-3.24	123.13	127.69
15	BO	1001	V7N	C7-C6-C5	-3.24	122.73	127.28
13	AT	101	BCL	CHA-C1A-NA	-3.24	119.05	126.39
14	BD	102	LMT	O1'-C1'-C2'	3.24	113.19	108.27
14	BO	1002	LMT	C1-O1'-C1'	3.24	119.21	113.68
13	AB	1002	BCL	C1D-ND-C4D	-3.24	104.04	106.31
13	AE	104	BCL	CHD-C1D-ND	-3.24	120.25	124.80
13	ah	1001	BCL	CHD-C1D-ND	-3.24	120.25	124.80
13	bc	103	BCL	CHD-C1D-ND	-3.23	120.25	124.80
13	BT	103	BCL	C4A-NA-C1A	3.23	108.15	106.68
13	AE	104	BCL	CHA-C1A-NA	-3.23	119.08	126.39
13	AJ	104	BCL	CHA-C1A-NA	-3.23	119.08	126.39
13	ah	1001	BCL	C1D-ND-C4D	-3.23	104.05	106.31
13	AB	1001	BCL	CHA-C1A-NA	-3.22	119.09	126.39
13	AP	102	BCL	CHA-C1A-NA	-3.22	119.09	126.39
13	ak	1001	BCL	C1D-ND-C4D	-3.22	104.05	106.31
13	AB	1001	BCL	CHD-C1D-ND	-3.22	120.27	124.80
15	BM	1001	V7N	C38-C26-C27	-3.22	113.17	118.09
13	AK	104	BCL	CHA-C1A-NA	-3.22	119.11	126.39
15	bk	101	V7N	O44-C40-O45	-3.22	116.24	123.90
13	AF	1001	BCL	CHA-C1A-NA	-3.22	119.11	126.39
15	bn	101	V7N	O44-C40-O45	-3.22	116.24	123.90
13	AD	103	BCL	CHA-C1A-NA	-3.22	119.11	126.39
13	BR	1003	BCL	CHA-C1A-NA	-3.21	119.11	126.39
13	BF	103	BCL	C1D-ND-C4D	-3.21	104.06	106.31
13	AK	104	BCL	CHD-C1D-ND	-3.21	120.28	124.80
15	BS	1001	V7N	O44-C40-O45	-3.21	116.26	123.90
13	AQ	103	BCL	CHD-C1D-ND	-3.21	120.29	124.80
14	bc	102	LMT	C3'-C4'-C5'	-3.21	103.83	110.93
13	AU	101	BCL	CHA-C1A-NA	-3.20	119.13	126.39
13	BX	101	BCL	C4A-NA-C1A	3.20	108.14	106.68
13	AW	101	BCL	CHA-C1A-NA	-3.20	119.14	126.39
13	AJ	104	BCL	CHD-C1D-ND	-3.20	120.30	124.80
13	AW	101	BCL	C1D-ND-C4D	-3.20	104.07	106.31
13	aj	101	BCL	C1D-ND-C4D	-3.20	104.07	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BU	1001	V7N	O44-C40-O45	-3.20	116.28	123.90
13	AH	102	BCL	C1D-ND-C4D	-3.20	104.07	106.31
13	AU	103	BCL	C4A-NA-C1A	3.20	108.14	106.68
13	BO	1003	BCL	CHA-C1A-NA	-3.20	119.16	126.39
13	AO	102	BCL	C1D-ND-C4D	-3.20	104.07	106.31
23	ao	101	MQ8	C12-C11-C3	3.20	119.95	112.08
13	AF	1001	BCL	C1D-ND-C4D	-3.19	104.07	106.31
15	BK	1001	V7N	O44-C40-O45	-3.19	116.30	123.90
13	BE	104	BCL	C4A-NA-C1A	3.19	108.13	106.68
15	BE	101	V7N	O44-C40-O45	-3.19	116.31	123.90
13	AM	1004	BCL	C1D-ND-C4D	-3.19	104.08	106.31
26	af	101	V7B	C43-O4-C4	-3.19	110.42	117.98
13	AH	105	BCL	C4A-NA-C1A	3.19	108.13	106.68
13	L	305	BCL	C1D-ND-C4D	-3.19	104.08	106.31
13	BG	1004	BCL	CHA-C1A-NA	-3.19	119.18	126.39
15	bh	101	V7N	O44-C40-O45	-3.18	116.32	123.90
13	BV	1005	BCL	C1D-ND-C4D	-3.18	104.08	106.31
15	AA	1004	V7N	O44-C40-O45	-3.18	116.32	123.90
13	AX	102	BCL	CHD-C1D-ND	-3.18	120.32	124.80
14	BC	103	LMT	C1-O1'-C1'	3.18	119.11	113.68
15	bj	101	V7N	O44-C40-O45	-3.18	116.33	123.90
13	AR	101	BCL	CHA-C1A-NA	-3.18	119.19	126.39
13	BT	103	BCL	CHA-C1A-NA	-3.18	119.19	126.39
15	BW	1001	V7N	O44-C40-O45	-3.18	116.34	123.90
13	AA	1001	BCL	CHA-C1A-NA	-3.18	119.20	126.39
13	AO	102	BCL	CHA-C1A-NA	-3.18	119.20	126.39
13	BT	103	BCL	C1D-ND-C4D	-3.18	104.08	106.31
15	BD	101	V7N	O44-C40-O45	-3.18	116.34	123.90
15	BU	1001	V7N	C15-C14-C13	-3.18	122.83	127.28
13	AR	101	BCL	C1D-ND-C4D	-3.17	104.08	106.31
15	bg	101	V7N	O44-C40-O45	-3.17	116.34	123.90
13	AD	103	BCL	CHD-C1D-ND	-3.17	120.34	124.80
13	BJ	1004	BCL	CHA-C1A-NA	-3.17	119.22	126.39
13	aa	1001	BCL	C1D-ND-C4D	-3.17	104.09	106.31
13	AV	103	BCL	CHA-C1A-NA	-3.17	119.22	126.39
26	ag	103	V7B	C1-O6-C5	3.17	119.90	113.72
13	M	408	BCL	C1D-ND-C4D	-3.16	104.09	106.31
15	BO	1001	V7N	O44-C40-O45	-3.16	116.37	123.90
13	BK	1002	BCL	CHA-C1A-NA	-3.16	119.23	126.39
13	AU	101	BCL	C1D-ND-C4D	-3.16	104.09	106.31
13	BX	101	BCL	CHA-C1A-NA	-3.16	119.24	126.39
15	BG	1001	V7N	C38-C26-C27	-3.16	113.26	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BR	1001	V7N	C29-C28-C27	-3.16	114.05	123.20
15	BJ	1001	V7N	O44-C40-O45	-3.16	116.38	123.90
13	AB	1001	BCL	C1D-ND-C4D	-3.16	104.10	106.31
15	BA	101	V7N	O44-C40-O45	-3.16	116.39	123.90
13	BH	1005	BCL	CHA-C1A-NA	-3.16	119.25	126.39
15	BG	1001	V7N	O44-C40-O45	-3.16	116.39	123.90
13	AC	102	BCL	CHA-C1A-NA	-3.15	119.25	126.39
13	AI	101	BCL	CHA-C1A-NA	-3.15	119.25	126.39
15	ag	101	V7N	C33-C5-C4	3.15	122.91	118.09
15	ba	101	V7N	O44-C40-O45	-3.15	116.39	123.90
13	bh	103	BCL	C4A-NA-C1A	3.15	108.12	106.68
13	AO	101	BCL	C2A-C1A-CHA	3.15	129.34	123.87
13	AA	1002	BCL	CHA-C1A-NA	-3.15	119.25	126.39
13	AA	1001	BCL	C4A-NA-C1A	3.15	108.12	106.68
13	L	308	BCL	C4A-NA-C1A	3.15	108.12	106.68
14	bp	101	LMT	C1-O1'-C1'	3.15	119.06	113.68
13	AG	103	BCL	CHA-C1A-NA	-3.15	119.27	126.39
13	AH	103	BCL	CHA-C1A-NA	-3.15	119.27	126.39
15	bl	101	V7N	O44-C40-O45	-3.15	116.41	123.90
15	BQ	1001	V7N	O44-C40-O45	-3.14	116.41	123.90
15	bd	101	V7N	O44-C40-O45	-3.14	116.41	123.90
13	bl	104	BCL	C1D-ND-C4D	-3.14	104.11	106.31
13	BW	1005	BCL	CHA-C1A-NA	-3.14	119.27	126.39
13	al	1001	BCL	C1D-ND-C4D	-3.14	104.11	106.31
13	AP	102	BCL	C4A-NA-C1A	3.14	108.11	106.68
15	be	102	V7N	O44-C40-O45	-3.14	116.42	123.90
13	bj	104	BCL	C1D-ND-C4D	-3.14	104.11	106.31
13	BQ	1004	BCL	CHA-C1A-NA	-3.14	119.29	126.39
13	AT	101	BCL	C4A-NA-C1A	3.14	108.11	106.68
13	bp	104	BCL	C4A-NA-C1A	3.14	108.11	106.68
13	AM	1004	BCL	CHA-C1A-NA	-3.13	119.30	126.39
13	bn	102	BCL	C1D-ND-C4D	-3.13	104.11	106.31
15	bm	101	V7N	O44-C40-O45	-3.13	116.45	123.90
13	BR	1003	BCL	C1D-ND-C4D	-3.13	104.12	106.31
15	BV	1001	V7N	O44-C40-O45	-3.13	116.45	123.90
13	AN	103	BCL	CHA-C1A-NA	-3.13	119.31	126.39
15	BN	1001	V7N	O44-C40-O45	-3.12	116.46	123.90
13	AA	1002	BCL	C4A-NA-C1A	3.12	108.10	106.68
15	BI	1001	V7N	O44-C40-O45	-3.12	116.47	123.90
15	BG	1001	V7N	C36-C18-C19	3.12	122.86	118.09
13	AP	102	BCL	C1D-ND-C4D	-3.12	104.12	106.31
14	BH	1002	LMT	C1-O1'-C1'	3.12	119.01	113.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AV	101	BCL	CHA-C1A-NA	-3.11	119.34	126.39
15	bo	101	V7N	O44-C40-O45	-3.11	116.49	123.90
13	ap	1001	BCL	C1-C2-C3	3.11	131.29	126.20
13	bb	102	BCL	C1D-ND-C4D	-3.11	104.13	106.31
14	BD	106	LMT	C1-O1'-C1'	3.11	118.99	113.68
14	AV	102	LMT	C3'-C4'-C5'	-3.11	104.04	110.93
15	bi	101	V7N	C29-C28-C27	-3.11	114.19	123.20
13	AG	103	BCL	C1D-ND-C4D	-3.11	104.13	106.31
13	AC	102	BCL	C1D-ND-C4D	-3.11	104.13	106.31
15	ag	101	V7N	O44-C40-O45	-3.11	116.50	123.90
13	AQ	104	BCL	CHA-C1A-NA	-3.11	119.36	126.39
13	aa	1001	BCL	C4A-NA-C1A	3.11	108.10	106.68
13	BB	105	BCL	CHA-C1A-NA	-3.10	119.36	126.39
13	BC	104	BCL	CHA-C1A-NA	-3.10	119.36	126.39
13	AV	101	BCL	C4A-NA-C1A	3.10	108.09	106.68
13	AN	103	BCL	C1D-ND-C4D	-3.10	104.14	106.31
15	AM	1001	V7N	O44-C40-O45	-3.10	116.52	123.90
15	BP	1001	V7N	O44-C40-O45	-3.10	116.52	123.90
13	aj	101	BCL	CHA-C1A-NA	-3.10	119.38	126.39
13	AI	101	BCL	C4A-NA-C1A	3.09	108.09	106.68
13	BU	1004	BCL	CHA-C1A-NA	-3.09	119.39	126.39
13	AM	1002	BCL	CHA-C1A-NA	-3.09	119.39	126.39
13	BF	103	BCL	CHA-C1A-NA	-3.09	119.39	126.39
15	bi	101	V7N	O44-C40-O45	-3.09	116.54	123.90
13	AC	101	BCL	C1D-ND-C4D	-3.09	104.15	106.31
13	AQ	103	BCL	C4A-NA-C1A	3.09	108.09	106.68
13	AA	1001	BCL	C1D-ND-C4D	-3.09	104.15	106.31
13	AX	102	BCL	C1D-ND-C4D	-3.08	104.15	106.31
13	BS	1004	BCL	CHA-C1A-NA	-3.08	119.41	126.39
23	L	303	MQ8	O4-C4-C3	3.08	125.62	120.67
15	BM	1001	V7N	O44-C40-O45	-3.08	116.57	123.90
15	BI	1001	V7N	C15-C14-C13	-3.07	122.97	127.28
13	AB	1002	BCL	C4A-NA-C1A	3.07	108.08	106.68
13	AQ	103	BCL	C1D-ND-C4D	-3.07	104.16	106.31
13	am	1001	BCL	CHA-C1A-NA	-3.07	119.44	126.39
13	AK	102	BCL	CHA-C1A-NA	-3.07	119.45	126.39
13	AQ	104	BCL	C4A-NA-C1A	3.06	108.08	106.68
13	BH	1005	BCL	C4A-NA-C1A	3.06	108.08	106.68
13	AE	104	BCL	C1D-ND-C4D	-3.06	104.16	106.31
13	bf	102	BCL	C1D-ND-C4D	-3.06	104.16	106.31
22	L	301	BPH	OBD-CAD-CBD	-3.06	121.33	125.82
15	bn	101	V7N	C15-C14-C13	-3.06	122.99	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AS	104	V7N	O44-C40-O45	-3.06	116.62	123.90
13	AT	103	BCL	CHA-C1A-NA	-3.06	119.47	126.39
13	BD	104	BCL	CHA-C1A-NA	-3.06	119.47	126.39
13	bo	102	BCL	CHA-C1A-NA	-3.06	119.47	126.39
13	BE	104	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	BL	103	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	AD	103	BCL	C1D-ND-C4D	-3.05	104.17	106.31
13	BV	1005	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	BP	1003	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	AE	103	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	bn	102	BCL	CHA-C1A-NA	-3.05	119.48	126.39
13	AQ	102	BCL	CHA-C1A-NA	-3.05	119.49	126.39
13	BA	103	BCL	CHA-C1A-NA	-3.05	119.49	126.39
13	AT	101	BCL	C1D-ND-C4D	-3.05	104.17	106.31
13	bc	103	BCL	CHA-C1A-NA	-3.04	119.50	126.39
15	BH	1001	V7N	O44-C40-O45	-3.04	116.65	123.90
13	AB	1002	BCL	CHA-C1A-NA	-3.04	119.50	126.39
13	bm	102	BCL	C4A-NA-C1A	3.04	108.07	106.68
13	AC	101	BCL	CHA-C1A-NA	-3.04	119.51	126.39
15	bm	101	V7N	C28-C27-C26	-3.04	118.03	126.36
13	AH	105	BCL	CHA-C1A-NA	-3.04	119.51	126.39
13	AL	103	BCL	CHA-C1A-NA	-3.04	119.51	126.39
14	BJ	1003	LMT	C1-O1'-C1'	3.04	118.87	113.68
13	ah	1001	BCL	CHA-C1A-NA	-3.04	119.52	126.39
15	BI	1001	V7N	C3-C4-C5	3.04	130.48	125.89
13	BI	1004	BCL	CHA-C1A-NA	-3.04	119.52	126.39
13	AI	101	BCL	C1D-ND-C4D	-3.03	104.18	106.31
13	L	308	BCL	CHA-C1A-NA	-3.03	119.52	126.39
13	bl	104	BCL	CHA-C1A-NA	-3.03	119.52	126.39
13	AW	102	BCL	CHA-C1A-NA	-3.03	119.53	126.39
14	AC	103	LMT	C1-O1'-C1'	3.03	118.86	113.68
15	BM	1001	V7N	C36-C18-C19	3.03	122.71	118.09
15	bl	101	V7N	C33-C5-C4	3.03	122.71	118.09
13	AJ	104	BCL	C1D-ND-C4D	-3.03	104.19	106.31
13	BC	104	BCL	C4A-NA-C1A	3.03	108.06	106.68
15	BR	1001	V7N	O44-C40-O45	-3.03	116.70	123.90
13	bd	102	BCL	CHA-C1A-NA	-3.03	119.54	126.39
13	BM	1004	BCL	CHA-C1A-NA	-3.02	119.54	126.39
13	ba	102	BCL	CHA-C1A-NA	-3.02	119.54	126.39
13	AH	105	BCL	C1D-ND-C4D	-3.02	104.19	106.31
13	AL	102	BCL	C1D-ND-C4D	-3.02	104.19	106.31
15	BO	1001	V7N	C3-C4-C5	3.02	130.46	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AD	104	BCL	CHA-C1A-NA	-3.02	119.55	126.39
13	AH	103	BCL	C1D-ND-C4D	-3.02	104.19	106.31
23	L	303	MQ8	C11-C3-C2	-3.02	119.72	124.89
13	aa	1001	BCL	CHA-C1A-NA	-3.02	119.56	126.39
14	BB	102	LMT	C3'-C4'-C5'	-3.01	104.25	110.93
13	AL	102	BCL	C4A-NA-C1A	3.01	108.05	106.68
13	bf	102	BCL	CHA-C1A-NA	-3.01	119.57	126.39
13	ab	1001	BCL	CHA-C1A-NA	-3.01	119.57	126.39
14	AJ	102	LMT	C3'-C4'-C5'	-3.01	104.26	110.93
15	BH	1001	V7N	C7-C6-C5	-3.01	123.06	127.28
13	AP	103	BCL	C1-C2-C3	-3.01	121.27	126.20
13	ae	1001	BCL	CHA-C1A-NA	-3.01	119.58	126.39
15	BE	101	V7N	C35-C13-C12	3.01	122.68	118.09
14	AT	104	LMT	C1-O1'-C1'	3.01	118.82	113.68
15	BO	1001	V7N	C38-C26-C27	-3.01	113.49	118.09
13	AS	102	BCL	C1D-ND-C4D	-3.01	104.20	106.31
15	BS	1001	V7N	C36-C18-C19	3.01	122.68	118.09
13	AS	102	BCL	C2A-C1A-CHA	3.00	129.08	123.87
13	an	1001	BCL	CHA-C1A-NA	-3.00	119.59	126.39
13	AS	101	BCL	CHA-C1A-NA	-3.00	119.59	126.39
13	AE	104	BCL	C4A-NA-C1A	3.00	108.05	106.68
13	ak	1001	BCL	CHA-C1A-NA	-3.00	119.60	126.39
15	bm	101	V7N	C2-C3-C4	-3.00	120.70	124.91
13	AU	101	BCL	C2A-C1A-CHA	3.00	129.07	123.87
13	bn	102	BCL	C4A-NA-C1A	3.00	108.05	106.68
13	AN	104	BCL	CHA-C1A-NA	-3.00	119.60	126.39
13	bi	102	BCL	CHA-C1A-NA	-3.00	119.61	126.39
13	AE	105	BCL	CHA-C1A-NA	-3.00	119.61	126.39
13	bb	102	BCL	CHA-C1A-NA	-3.00	119.61	126.39
23	M	402	MQ8	C14-C13-C15	-3.00	110.03	115.23
13	bg	104	BCL	C4A-NA-C1A	2.99	108.04	106.68
13	af	103	BCL	CHA-C1A-NA	-2.99	119.62	126.39
13	BS	1004	BCL	C11-C10-C8	2.99	125.90	115.97
13	BN	1005	BCL	CHA-C1A-NA	-2.99	119.62	126.39
13	AO	102	BCL	C2A-C1A-CHA	2.99	129.05	123.87
21	M	409	CD4	O16-C46-C47	2.99	117.94	111.48
13	AK	104	BCL	C1D-ND-C4D	-2.99	104.22	106.31
13	AG	102	BCL	CHA-C1A-NA	-2.99	119.63	126.39
15	BJ	1001	V7N	C38-C26-C27	-2.98	113.53	118.09
15	BP	1001	V7N	C15-C14-C13	-2.98	123.09	127.28
13	ad	102	BCL	CHA-C1A-NA	-2.98	119.64	126.39
13	ai	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AT	102	LMT	C3'-C4'-C5'	-2.98	104.33	110.93
13	AG	102	BCL	C4A-NA-C1A	2.98	108.04	106.68
14	BH	1002	LMT	C3'-C4'-C5'	-2.98	104.33	110.93
15	BJ	1001	V7N	C27-C26-C25	2.98	122.63	118.49
13	AQ	103	BCL	C2A-C1A-CHA	2.97	129.03	123.87
15	BP	1001	V7N	C27-C26-C25	2.97	122.63	118.49
15	BW	1001	V7N	C15-C14-C13	-2.97	123.11	127.28
13	al	1001	BCL	CHA-C1A-NA	-2.97	119.67	126.39
13	bk	103	BCL	CHA-C1A-NA	-2.97	119.67	126.39
14	BU	1002	LMT	C3'-C4'-C5'	-2.96	104.36	110.93
15	BA	101	V7N	C38-C26-C27	-2.96	113.56	118.09
13	BU	1004	BCL	C4A-NA-C1A	2.96	108.03	106.68
13	bh	103	BCL	CHA-C1A-NA	-2.96	119.69	126.39
14	AE	106	LMT	O5B-C5B-C4B	2.96	115.03	109.70
13	be	103	BCL	CHA-C1A-NA	-2.96	119.69	126.39
15	bh	101	V7N	C35-C13-C12	2.96	122.61	118.09
13	AW	101	BCL	C2A-C1A-CHA	2.95	129.00	123.87
21	H1	103	CD4	O16-C46-C47	2.95	117.87	111.48
13	AX	102	BCL	C2A-C1A-CHA	2.95	128.99	123.87
15	BJ	1001	V7N	C36-C18-C19	2.95	122.60	118.09
13	AJ	103	BCL	CHA-C1A-NA	-2.95	119.71	126.39
15	BG	1001	V7N	C15-C14-C13	-2.95	123.14	127.28
15	bl	101	V7N	C28-C27-C26	-2.95	118.28	126.36
13	bp	104	BCL	CHA-C1A-NA	-2.95	119.72	126.39
21	af	102	CD4	O2-C14-O1	-2.94	116.82	123.70
13	ap	1001	BCL	CHA-C1A-NA	-2.94	119.73	126.39
15	AM	1001	V7N	C36-C18-C19	2.94	122.58	118.09
13	bj	104	BCL	CHA-C1A-NA	-2.94	119.73	126.39
13	BJ	1004	BCL	C4A-NA-C1A	2.94	108.02	106.68
13	AQ	104	BCL	CED-O2D-CGD	2.94	122.58	115.92
13	ag	102	BCL	CHA-C1A-NA	-2.94	119.74	126.39
13	AQ	104	BCL	O2D-CGD-CBD	2.94	116.36	111.23
13	bk	103	BCL	CBA-CAA-C2A	2.94	122.53	113.79
13	AU	103	BCL	CHA-C1A-NA	-2.93	119.75	126.39
13	AN	104	BCL	C4A-NA-C1A	2.93	108.02	106.68
13	BK	1002	BCL	C1D-ND-C4D	-2.93	104.26	106.31
13	AH	102	BCL	CHA-C1A-NA	-2.93	119.76	126.39
15	bm	101	V7N	C33-C5-C4	2.93	122.56	118.09
13	ao	102	BCL	CHA-C1A-NA	-2.92	119.77	126.39
13	AP	103	BCL	CHA-C1A-NA	-2.92	119.77	126.39
26	ag	103	V7B	O7-C10-C11	2.92	117.80	111.48
14	AJ	101	LMT	O1'-C1'-C2'	2.92	112.71	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AL	101	LMT	O1'-C1'-C2'	2.92	112.71	108.27
13	AO	101	BCL	CHA-C1A-NA	-2.92	119.79	126.39
21	M	405	CD4	O16-C46-C47	2.92	117.79	111.48
13	bm	102	BCL	CHA-C1A-NA	-2.92	119.79	126.39
13	BQ	1004	BCL	C1D-ND-C4D	-2.91	104.27	106.31
15	bb	101	V7N	C27-C26-C25	2.91	122.55	118.49
15	BV	1001	V7N	C15-C14-C13	-2.91	123.19	127.28
13	AM	1004	BCL	C2A-C1A-CHA	2.91	128.92	123.87
13	bg	104	BCL	CHA-C1A-NA	-2.91	119.80	126.39
14	AE	101	LMT	C3'-C4'-C5'	-2.91	104.48	110.93
14	BK	1003	LMT	C1-O1'-C1'	2.91	118.64	113.68
13	AQ	102	BCL	C4A-NA-C1A	2.91	108.00	106.68
13	ac	102	BCL	CHA-C1A-NA	-2.91	119.81	126.39
14	BQ	1003	LMT	C3'-C4'-C5'	-2.91	104.49	110.93
13	AX	103	BCL	CHA-C1A-NA	-2.90	119.81	126.39
13	bc	103	BCL	C1-O2A-CGA	2.90	123.68	116.65
15	BD	101	V7N	C36-C18-C19	2.90	122.52	118.09
15	bl	101	V7N	C35-C13-C12	2.90	122.52	118.09
14	BW	1004	LMT	C1-O1'-C1'	2.90	118.63	113.68
13	M	408	BCL	C2A-C1A-CHA	2.90	128.89	123.87
13	AJ	103	BCL	C4A-NA-C1A	2.89	108.00	106.68
14	be	101	LMT	O5'-C1'-C2'	-2.89	104.43	110.37
13	bi	102	BCL	C4A-NA-C1A	2.89	108.00	106.68
26	af	101	V7B	O7-C10-C11	2.89	117.73	111.48
13	AT	101	BCL	C2A-C1A-CHA	2.89	128.88	123.87
15	bc	101	V7N	C35-C13-C12	2.88	122.49	118.09
13	AQ	102	BCL	CBA-CAA-C2A	2.88	122.36	113.79
14	BK	1004	LMT	O5'-C5'-C6'	2.88	113.57	106.44
13	AV	101	BCL	C2A-C1A-CHA	2.88	128.86	123.87
14	AP	101	LMT	C1-O1'-C1'	2.87	118.59	113.68
14	AQ	101	LMT	C3'-C4'-C5'	-2.87	104.56	110.93
19	C1	301	NDG	C1-O5-C5	2.87	116.03	112.19
15	be	102	V7N	C35-C13-C12	2.87	122.47	118.09
15	AD	101	V7N	C38-C26-C27	-2.87	113.71	118.09
15	BQ	1001	V7N	C36-C18-C19	2.86	122.46	118.09
15	bl	101	V7N	C1-C2-C3	2.86	120.42	112.98
13	AK	104	BCL	C2A-C1A-CHA	2.86	128.83	123.87
13	M	406	BCL	CHA-C1A-NA	-2.86	119.92	126.39
13	bd	102	BCL	C4A-NA-C1A	2.86	107.98	106.68
13	bc	103	BCL	CBA-CAA-C2A	2.86	122.29	113.79
14	BE	102	LMT	C2'-C3'-C4'	2.85	116.14	109.68
13	AH	102	BCL	C4A-NA-C1A	2.85	107.98	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	305	BCL	CHA-C1A-NA	-2.85	119.94	126.39
13	AA	1002	BCL	C2A-C1A-CHA	2.85	128.81	123.87
13	AF	1001	BCL	C2A-C1A-CHA	2.85	128.81	123.87
13	AD	103	BCL	C2A-C1A-CHA	2.85	128.81	123.87
13	AC	102	BCL	C2A-C1A-CHA	2.84	128.80	123.87
15	AD	101	V7N	C15-C14-C13	-2.84	123.29	127.28
15	bd	101	V7N	C35-C13-C12	2.84	122.43	118.09
13	be	103	BCL	C4A-NA-C1A	2.84	107.97	106.68
15	BS	1001	V7N	C10-C9-C34	2.83	122.73	116.43
15	AS	104	V7N	C10-C9-C34	2.83	122.73	116.43
13	AR	101	BCL	C2A-C1A-CHA	2.83	128.78	123.87
13	AA	1001	BCL	C2A-C1A-CHA	2.83	128.78	123.87
13	BF	103	BCL	C4A-NA-C1A	2.83	107.97	106.68
13	bo	102	BCL	C4A-NA-C1A	2.83	107.97	106.68
17	C	1004	HEC	CMC-C2C-C1C	-2.82	121.12	125.42
15	bj	101	V7N	C35-C13-C12	2.82	122.40	118.09
15	bo	101	V7N	C1-C2-C3	2.82	120.31	112.98
15	BN	1001	V7N	C33-C5-C6	-2.82	118.25	122.82
15	BR	1001	V7N	C35-C13-C12	2.82	122.39	118.09
13	AD	104	BCL	C1C-NC-C4C	2.81	107.96	106.68
15	AW	103	V7N	C27-C26-C25	2.81	122.41	118.49
13	bl	104	BCL	C4A-NA-C1A	2.81	107.96	106.68
13	ba	102	BCL	CBA-CAA-C2A	2.81	122.16	113.79
13	AB	1001	BCL	C2A-C1A-CHA	2.81	128.74	123.87
14	BB	101	LMT	C3'-C4'-C5'	-2.81	104.71	110.93
15	BH	1001	V7N	C3-C4-C5	2.81	130.13	125.89
15	bm	101	V7N	C35-C13-C12	2.81	122.37	118.09
14	BX	102	LMT	C3'-C4'-C5'	-2.80	104.71	110.93
15	AW	103	V7N	C35-C13-C14	-2.80	118.28	122.82
15	BA	101	V7N	C15-C14-C13	-2.80	123.35	127.28
14	BN	1004	LMT	C3'-C4'-C5'	-2.80	104.73	110.93
13	AI	101	BCL	C2A-C1A-CHA	2.80	128.72	123.87
14	AB	1003	LMT	C3'-C4'-C5'	-2.80	104.73	110.93
13	AL	102	BCL	C2A-C1A-CHA	2.79	128.72	123.87
13	AE	103	BCL	CBA-CAA-C2A	2.79	122.10	113.79
23	L	303	MQ8	C31-C30-C28	-2.79	103.94	113.19
15	ag	101	V7N	C35-C13-C12	2.79	122.35	118.09
13	AP	102	BCL	C2A-C1A-CHA	2.79	128.70	123.87
14	AG	101	LMT	O1'-C1'-C2'	2.78	112.50	108.27
13	AE	103	BCL	C1-C2-C3	-2.78	121.64	126.20
13	BW	1005	BCL	C4A-NA-C1A	2.78	107.95	106.68
14	AT	104	LMT	O1'-C1'-C2'	2.78	112.50	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BE	105	LMT	C3'-C4'-C5'	-2.78	104.76	110.93
15	bn	101	V7N	C38-C26-C27	-2.78	113.84	118.09
13	L	308	BCL	C2A-C1A-CHA	2.78	128.69	123.87
14	BM	1002	LMT	C1-O1'-C1'	2.78	118.43	113.68
13	L	305	BCL	C2A-C1A-CHA	2.78	128.69	123.87
13	BN	1005	BCL	CBA-CAA-C2A	2.78	122.05	113.79
15	ba	101	V7N	C35-C13-C14	-2.77	118.32	122.82
14	BG	1002	LMT	C3'-C4'-C5'	-2.77	104.79	110.93
13	AM	1004	BCL	C4A-NA-C1A	2.77	107.94	106.68
14	BB	102	LMT	C1-O1'-C1'	2.77	118.41	113.68
13	AK	102	BCL	C2A-C1A-CHA	2.77	128.67	123.87
14	BP	1005	LMT	C3'-C4'-C5'	-2.77	104.80	110.93
13	AV	103	BCL	C2A-C1A-CHA	2.77	128.67	123.87
15	BS	1001	V7N	C35-C13-C12	2.77	122.31	118.09
13	BI	1004	BCL	C1-O2A-CGA	2.77	123.35	116.65
15	bn	101	V7N	C1-C2-C3	2.76	120.15	112.98
13	M	406	BCL	C4A-NA-C1A	2.76	107.94	106.68
15	BM	1001	V7N	C27-C26-C25	2.76	122.33	118.49
13	AG	103	BCL	C2A-C1A-CHA	2.75	128.65	123.87
13	BG	1004	BCL	C2A-C1A-CHA	2.75	128.64	123.87
15	BK	1001	V7N	C20-C21-C22	-2.75	123.82	127.69
13	BG	1004	BCL	C4A-NA-C1A	2.75	107.93	106.68
14	AE	102	LMT	O1'-C1'-C2'	2.75	112.45	108.27
14	BR	1002	LMT	O1'-C1'-C2'	2.75	112.44	108.27
13	AH	103	BCL	C2A-C1A-CHA	2.75	128.63	123.87
15	bn	101	V7N	C35-C13-C14	-2.74	118.38	122.82
13	AN	103	BCL	C2A-C1A-CHA	2.74	128.62	123.87
13	AE	104	BCL	C2A-C1A-CHA	2.74	128.62	123.87
14	BA	102	LMT	C1-O1'-C1'	2.73	118.35	113.68
15	BV	1001	V7N	C36-C18-C17	-2.73	118.39	122.82
13	AS	102	BCL	C4A-NA-C1A	2.73	107.92	106.68
15	BO	1001	V7N	C2-C3-C4	-2.73	121.09	124.91
21	af	104	CD4	C15-O2-C14	2.72	124.31	117.80
14	BN	1003	LMT	C3'-C4'-C5'	-2.72	104.91	110.93
14	AQ	101	LMT	C1-O1'-C1'	2.72	118.32	113.68
15	AM	1001	V7N	C35-C13-C12	2.72	122.24	118.09
13	AH	105	BCL	CBA-CAA-C2A	2.72	121.87	113.79
14	AM	1003	LMT	C3'-C4'-C5'	-2.71	104.91	110.93
13	M	406	BCL	C1C-NC-C4C	2.71	107.92	106.68
13	AP	102	BCL	C1-C2-C3	2.71	130.64	126.20
13	bb	102	BCL	C4A-NA-C1A	2.71	107.92	106.68
16	bk	102	OV9	C2-O2-C10	2.71	124.28	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BF	101	V7N	C36-C18-C19	2.71	122.22	118.09
15	AM	1001	V7N	C1-C2-C3	2.71	120.01	112.98
14	C	1005	LMT	C1-O1'-C1'	2.70	118.30	113.68
15	BP	1001	V7N	C38-C26-C27	-2.70	113.96	118.09
15	bg	101	V7N	C10-C9-C34	2.70	122.44	116.43
13	AJ	104	BCL	C2A-C1A-CHA	2.70	128.56	123.87
14	bk	104	LMT	C3'-C4'-C5'	-2.70	104.94	110.93
15	BF	101	V7N	C35-C13-C14	-2.70	118.44	122.82
14	bp	103	LMT	O1'-C1'-C2'	2.70	112.37	108.27
15	bg	101	V7N	C33-C5-C4	2.70	122.21	118.09
13	AN	104	BCL	C2A-C1A-CHA	2.69	128.54	123.87
13	AX	103	BCL	C1-O2A-CGA	2.69	123.17	116.65
13	AQ	104	BCL	C2A-C1A-CHA	2.69	128.53	123.87
15	BJ	1001	V7N	C15-C14-C13	-2.69	123.51	127.28
14	AE	106	LMT	C1B-O5B-C5B	2.68	118.96	113.72
17	C	1003	HEC	CBD-CAD-C3D	-2.68	105.11	112.53
15	BA	101	V7N	C35-C13-C14	-2.68	118.47	122.82
14	bp	103	LMT	O5B-C5B-C4B	2.68	114.53	109.70
15	BV	1001	V7N	C16-C17-C18	-2.68	123.52	127.28
14	C	1005	LMT	C3'-C4'-C5'	-2.68	104.99	110.93
15	BN	1001	V7N	C20-C21-C22	-2.68	123.92	127.69
21	M	405	CD4	O3-C16-C15	-2.68	100.68	108.40
14	AP	101	LMT	C3'-C4'-C5'	-2.68	105.00	110.93
15	BS	1001	V7N	C33-C5-C4	2.68	122.17	118.09
14	BM	1002	LMT	C3'-C4'-C5'	-2.67	105.00	110.93
15	BP	1001	V7N	C10-C9-C34	2.67	122.37	116.43
15	bh	101	V7N	C33-C5-C4	2.67	122.17	118.09
15	BE	101	V7N	C33-C5-C4	2.66	122.16	118.09
13	BH	1005	BCL	C2A-C1A-CHA	2.66	128.49	123.87
14	BT	104	LMT	C3'-C4'-C5'	-2.66	105.04	110.93
14	AK	103	LMT	C3'-C4'-C5'	-2.66	105.04	110.93
13	bm	102	BCL	C1-C2-C3	-2.66	121.84	126.20
15	bd	101	V7N	C20-C21-C22	-2.66	123.96	127.69
15	BI	1001	V7N	C36-C18-C19	2.65	122.14	118.09
15	bi	101	V7N	C10-C9-C34	2.65	122.33	116.43
14	BW	1002	LMT	C1-O1'-C1'	2.65	118.20	113.68
15	bp	102	V7N	C28-C27-C26	-2.65	119.11	126.36
15	bj	101	V7N	C33-C5-C4	2.64	122.13	118.09
13	bk	103	BCL	CMB-C2B-C1B	-2.64	121.39	125.42
15	BE	101	V7N	C36-C18-C19	2.64	122.12	118.09
15	BN	1001	V7N	C35-C13-C12	2.64	122.12	118.09
13	BE	104	BCL	C2A-C1A-CHA	2.64	128.45	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BI	1001	V7N	C35-C13-C14	-2.64	118.54	122.82
14	L	307	LMT	C3'-C4'-C5'	-2.64	105.08	110.93
15	bi	101	V7N	C33-C5-C4	2.63	122.11	118.09
13	L	308	BCL	C1-O2A-CGA	2.63	123.02	116.65
27	ai	102	UYH	C12-C11-C10	-2.63	104.05	113.69
14	AD	102	LMT	C3'-C4'-C5'	-2.63	105.09	110.93
15	be	102	V7N	C1-C2-C3	2.63	119.80	112.98
15	BR	1001	V7N	C20-C21-C22	-2.63	124.00	127.69
13	BQ	1004	BCL	C2A-C1A-CHA	2.63	128.42	123.87
15	bc	101	V7N	C36-C18-C19	2.63	122.10	118.09
15	AS	104	V7N	C35-C13-C12	2.62	122.10	118.09
15	BQ	1001	V7N	C35-C13-C12	2.62	122.09	118.09
15	AD	101	V7N	C36-C18-C19	2.62	122.09	118.09
15	BU	1001	V7N	C20-C21-C22	-2.62	124.01	127.69
15	BH	1001	V7N	C2-C3-C4	-2.62	121.24	124.91
22	L	301	BPH	OBB-CAB-CBB	-2.62	114.61	120.19
14	BR	1004	LMT	C3'-C4'-C5'	-2.62	105.13	110.93
15	be	102	V7N	C33-C5-C4	2.62	122.08	118.09
13	AA	1002	BCL	C11-C10-C8	2.61	124.65	115.97
13	AW	102	BCL	C2A-C1A-CHA	2.61	128.40	123.87
13	AI	101	BCL	OBB-CAB-CBB	-2.61	113.92	119.77
15	BO	1001	V7N	C35-C13-C12	2.61	122.07	118.09
13	AM	1002	BCL	C2A-C1A-CHA	2.61	128.39	123.87
16	be	105	OV9	O3-C30-O5	-2.61	117.11	123.63
13	AT	103	BCL	C1-C2-C3	-2.60	121.93	126.20
13	AH	105	BCL	C2A-C1A-CHA	2.60	128.39	123.87
15	bk	101	V7N	C35-C13-C12	2.60	122.07	118.09
15	BD	101	V7N	C10-C9-C34	2.60	122.22	116.43
21	af	104	CD4	O16-C46-C47	2.60	117.11	111.48
14	BH	1003	LMT	C3'-C4'-C5'	-2.60	105.17	110.93
13	AE	105	BCL	C2A-C1A-CHA	2.60	128.38	123.87
13	BS	1004	BCL	C9-C8-C10	2.60	120.54	111.27
13	aa	1001	BCL	C1-O2A-CGA	2.60	122.94	116.65
15	BH	1001	V7N	C35-C13-C12	2.59	122.05	118.09
15	bj	101	V7N	C10-C9-C34	2.59	122.20	116.43
15	BQ	1001	V7N	C10-C9-C34	2.59	122.19	116.43
14	be	101	LMT	O1'-C1'-C2'	2.59	112.20	108.27
13	bo	102	BCL	C2A-C1A-CHA	2.58	128.35	123.87
14	BQ	1002	LMT	O5'-C1'-O1'	-2.58	103.95	110.04
15	BQ	1001	V7N	C33-C5-C4	2.58	122.03	118.09
22	L	301	BPH	C2D-C1D-ND	2.58	111.29	109.43
14	AH	101	LMT	C1'-O5'-C5'	-2.58	108.69	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BE	102	LMT	C1-O1'-C1'	2.58	118.08	113.68
15	BI	1001	V7N	C38-C26-C27	-2.58	114.15	118.09
21	M	409	CD4	O14-C35-C36	2.57	119.69	111.83
15	ag	101	V7N	C10-C9-C34	2.57	122.15	116.43
15	BU	1001	V7N	C27-C26-C25	2.57	122.07	118.49
15	be	102	V7N	C10-C9-C34	2.57	122.14	116.43
15	bl	101	V7N	C2-C3-C4	-2.57	121.31	124.91
15	bd	101	V7N	C10-C9-C34	2.57	122.14	116.43
14	BJ	1002	LMT	C3'-C4'-C5'	-2.57	105.24	110.93
15	ba	101	V7N	C10-C9-C34	2.57	122.14	116.43
15	bn	101	V7N	C16-C17-C18	-2.57	123.68	127.28
21	H1	103	CD4	O2-C14-C13	2.57	117.03	111.48
15	AD	101	V7N	C35-C13-C14	-2.56	118.66	122.82
13	AJ	103	BCL	CMB-C2B-C1B	-2.56	121.52	125.42
15	AW	103	V7N	C36-C18-C19	2.56	122.00	118.09
13	AD	104	BCL	C2A-C1A-CHA	2.56	128.31	123.87
15	AW	103	V7N	C10-C9-C34	2.56	122.12	116.43
15	BK	1001	V7N	C38-C26-C27	-2.56	114.18	118.09
13	BC	104	BCL	C2A-C1A-CHA	2.56	128.30	123.87
15	bb	101	V7N	C35-C13-C12	2.55	121.99	118.09
15	bk	101	V7N	C35-C13-C14	-2.55	118.68	122.82
15	BR	1001	V7N	C10-C9-C34	2.55	122.10	116.43
14	BJ	1006	LMT	C1'-O5'-C5'	-2.55	108.74	113.72
23	ao	101	MQ8	C11-C3-C4	-2.55	115.89	118.58
26	ag	103	V7B	C43-O4-C4	-2.55	111.94	117.98
14	BE	102	LMT	O5'-C1'-C2'	-2.55	105.14	110.37
15	BP	1001	V7N	C35-C13-C12	2.55	121.98	118.09
15	bo	101	V7N	C35-C13-C12	2.55	121.98	118.09
15	BI	1001	V7N	C35-C13-C12	2.54	121.97	118.09
15	bk	101	V7N	C7-C6-C5	-2.54	123.72	127.28
13	BK	1002	BCL	C1-O2A-CGA	-2.54	110.51	116.65
15	BM	1001	V7N	C15-C14-C13	-2.54	123.72	127.28
13	BB	105	BCL	C2A-C1A-CHA	2.54	128.27	123.87
15	BW	1001	V7N	C36-C18-C19	2.54	121.96	118.09
15	bi	101	V7N	C35-C13-C12	2.54	121.96	118.09
15	BR	1001	V7N	C36-C18-C19	2.53	121.96	118.09
14	BO	1005	LMT	C3'-C4'-C5'	-2.53	105.32	110.93
14	BQ	1002	LMT	C3'-C4'-C5'	-2.53	105.32	110.93
15	BF	101	V7N	C10-C9-C34	2.53	122.05	116.43
13	AL	103	BCL	C2A-C1A-CHA	2.53	128.25	123.87
21	H1	103	CD4	O14-C35-C36	2.53	119.54	111.83
13	AM	1004	BCL	OBB-CAB-CBB	-2.53	114.11	119.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ai	101	BCL	CMB-C2B-C1B	-2.52	121.58	125.42
13	AL	103	BCL	CAA-CBA-CGA	2.52	120.37	113.21
13	AC	101	BCL	CAC-C3C-C4C	2.52	118.19	112.58
13	AH	102	BCL	C6-C5-C3	2.52	119.61	113.47
13	AG	103	BCL	OBB-CAB-CBB	-2.52	114.12	119.77
13	BA	103	BCL	C2A-C1A-CHA	2.52	128.25	123.87
13	AH	103	BCL	OBB-CAB-CBB	-2.52	114.12	119.77
15	bh	101	V7N	C10-C9-C34	2.52	122.02	116.43
14	BE	103	LMT	C3'-C4'-C5'	-2.52	105.35	110.93
15	BA	101	V7N	C10-C9-C34	2.52	122.02	116.43
15	bn	101	V7N	C36-C18-C17	-2.52	118.74	122.82
15	ba	101	V7N	C35-C13-C12	2.52	121.93	118.09
14	AK	103	LMT	C1-O1'-C1'	2.51	117.97	113.68
15	BH	1001	V7N	C36-C18-C19	2.51	121.93	118.09
15	BD	101	V7N	C33-C5-C4	2.51	121.92	118.09
15	BK	1001	V7N	C36-C18-C19	2.51	121.92	118.09
13	AS	101	BCL	C2A-C1A-CHA	2.51	128.22	123.87
13	BT	103	BCL	C2A-C1A-CHA	2.51	128.22	123.87
15	AA	1004	V7N	C27-C26-C25	2.51	121.99	118.49
13	ab	1001	BCL	C2A-C1A-CHA	2.51	128.22	123.87
13	AD	103	BCL	CAB-C3B-C2B	2.51	132.96	127.74
14	C2	1001	LMT	C3'-C4'-C5'	-2.51	105.37	110.93
13	al	1001	BCL	C2A-C1A-CHA	2.51	128.22	123.87
14	AE	102	LMT	O5'-C1'-C2'	-2.51	105.22	110.37
13	ba	102	BCL	C1-C2-C3	-2.51	122.09	126.20
13	ah	1001	BCL	OBB-CAB-CBB	-2.51	114.16	119.77
15	AS	104	V7N	C33-C5-C4	2.51	121.92	118.09
16	bk	102	OV9	O3P-P-O2P	2.51	118.87	108.94
23	M	402	MQ8	C15-C13-C12	2.51	126.79	121.17
13	AK	104	BCL	OBB-CAB-CBB	-2.51	114.16	119.77
13	AE	105	BCL	C1-C2-C3	-2.51	122.09	126.20
13	AV	101	BCL	OBB-CAB-CBB	-2.50	114.16	119.77
15	be	102	V7N	C2-C3-C4	-2.50	121.40	124.91
15	bo	101	V7N	C33-C5-C4	2.50	121.91	118.09
13	AG	102	BCL	C2A-C1A-CHA	2.50	128.21	123.87
13	AH	102	BCL	CBA-CAA-C2A	2.50	121.24	113.79
13	BV	1005	BCL	C2A-C1A-CHA	2.50	128.21	123.87
13	ao	102	BCL	C2A-C1A-CHA	2.50	128.21	123.87
15	bl	101	V7N	C10-C9-C34	2.50	121.98	116.43
15	bp	102	V7N	C35-C13-C14	-2.50	118.77	122.82
14	bf	101	LMT	C3'-C4'-C5'	-2.50	105.39	110.93
15	ba	101	V7N	C33-C5-C4	2.50	121.90	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AQ	103	BCL	OBB-CAB-CBB	-2.50	114.18	119.77
15	AD	101	V7N	C10-C9-C34	2.49	121.97	116.43
15	bp	102	V7N	C33-C5-C4	2.49	121.89	118.09
13	M	406	BCL	C2A-C1A-CHA	2.49	128.19	123.87
13	AS	102	BCL	OBB-CAB-CBB	-2.49	114.20	119.77
13	ae	1001	BCL	C2A-C1A-CHA	2.49	128.19	123.87
13	ae	1001	BCL	OBB-CAB-CBB	-2.49	114.20	119.77
14	AG	101	LMT	C3'-C4'-C5'	-2.49	105.42	110.93
15	BE	101	V7N	C10-C9-C34	2.49	121.96	116.43
23	ao	101	MQ8	C16-C17-C18	-2.49	121.93	127.62
13	BC	104	BCL	CAB-C3B-C2B	2.49	132.91	127.74
13	AT	103	BCL	C2A-C1A-CHA	2.49	128.18	123.87
13	AP	103	BCL	C2A-C1A-CHA	2.48	128.18	123.87
13	bf	102	BCL	C4A-NA-C1A	2.48	107.81	106.68
15	bk	101	V7N	C33-C5-C6	-2.48	118.80	122.82
15	BS	1001	V7N	C38-C26-C27	-2.48	114.30	118.09
14	BK	1004	LMT	C1-O1'-C1'	2.48	117.91	113.68
14	AX	101	LMT	O5'-C1'-C2'	-2.48	105.28	110.37
14	bn	103	LMT	O5B-C5B-C4B	2.48	114.16	109.70
15	BW	1001	V7N	C33-C5-C4	2.47	121.87	118.09
14	BR	1006	LMT	C3'-C4'-C5'	-2.47	105.45	110.93
13	M	408	BCL	CMB-C2B-C1B	-2.47	121.65	125.42
22	M	407	BPH	C6-C5-C3	2.47	119.48	113.47
14	bg	102	LMT	C1'-O5'-C5'	-2.47	108.90	113.72
15	bo	101	V7N	C10-C9-C34	2.47	121.92	116.43
15	bb	101	V7N	C36-C18-C17	-2.47	118.82	122.82
13	ag	102	BCL	CMB-C2B-C1B	-2.47	121.66	125.42
15	bh	101	V7N	C11-C10-C9	2.47	130.46	127.28
14	AH	104	LMT	C3'-C4'-C5'	-2.47	105.46	110.93
14	bl	103	LMT	C3'-C4'-C5'	-2.47	105.47	110.93
15	ag	101	V7N	C36-C18-C19	2.47	121.85	118.09
13	bk	103	BCL	C2A-C1A-CHA	2.46	128.14	123.87
13	AC	101	BCL	C2A-C1A-CHA	2.46	128.14	123.87
13	bf	102	BCL	C2A-C1A-CHA	2.46	128.14	123.87
13	BN	1005	BCL	C1-C2-C3	2.46	130.23	126.20
13	AJ	104	BCL	OBB-CAB-CBB	-2.46	114.26	119.77
13	BM	1004	BCL	C2A-C1A-CHA	2.46	128.14	123.87
15	BO	1001	V7N	C35-C13-C14	-2.46	118.83	122.82
13	AQ	104	BCL	CMB-C2B-C1B	-2.46	121.67	125.42
13	BK	1002	BCL	C2A-C1A-CHA	2.46	128.13	123.87
13	BL	103	BCL	CAB-C3B-C2B	2.46	132.85	127.74
15	BN	1001	V7N	C36-C18-C19	2.46	121.84	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BS	1001	V7N	C11-C10-C9	2.46	130.45	127.28
15	bg	101	V7N	C20-C21-C22	-2.46	124.24	127.69
13	ad	102	BCL	OBB-CAB-CBB	-2.45	114.27	119.77
13	an	1001	BCL	C2A-C1A-CHA	2.45	128.13	123.87
13	AU	101	BCL	OBB-CAB-CBB	-2.45	114.27	119.77
15	BH	1001	V7N	C27-C26-C25	2.45	121.91	118.49
15	AM	1001	V7N	C38-C26-C27	-2.45	114.34	118.09
13	bd	102	BCL	CMB-C2B-C1B	-2.45	121.69	125.42
21	M	409	CD4	C15-O2-C14	2.45	123.66	117.80
13	AL	102	BCL	OBB-CAB-CBB	-2.45	114.28	119.77
13	AP	102	BCL	OBB-CAB-CBB	-2.45	114.29	119.77
14	BX	104	LMT	C1-O1'-C1'	2.45	117.86	113.68
13	AR	101	BCL	OBB-CAB-CBB	-2.45	114.29	119.77
13	aj	101	BCL	C4A-NA-C1A	2.45	107.80	106.68
14	BP	1006	LMT	C3'-C4'-C5'	-2.44	105.51	110.93
13	BW	1005	BCL	C2A-C1A-CHA	2.44	128.11	123.87
13	AF	1001	BCL	OBB-CAB-CBB	-2.44	114.30	119.77
14	BF	104	LMT	C1-O1'-C1'	2.44	117.85	113.68
13	AA	1001	BCL	OBB-CAB-CBB	-2.44	114.30	119.77
16	bb	103	OV9	O3-C30-O5	-2.44	117.52	123.63
15	bp	102	V7N	C10-C9-C34	2.44	121.86	116.43
13	BL	103	BCL	C2A-C1A-CHA	2.44	128.10	123.87
13	AO	102	BCL	OBB-CAB-CBB	-2.44	114.30	119.77
15	BV	1001	V7N	C35-C13-C14	-2.44	118.86	122.82
15	AD	101	V7N	C35-C13-C12	2.44	121.81	118.09
15	bi	101	V7N	C20-C21-C22	-2.44	124.26	127.69
15	AW	103	V7N	C11-C10-C9	2.44	130.42	127.28
15	BV	1001	V7N	C33-C5-C4	2.44	121.81	118.09
13	am	1001	BCL	C2A-C1A-CHA	2.44	128.09	123.87
13	AX	102	BCL	OBB-CAB-CBB	-2.43	114.32	119.77
13	BN	1005	BCL	C2A-C1A-CHA	2.43	128.09	123.87
13	AI	101	BCL	C6-C5-C3	2.43	119.39	113.47
13	BU	1004	BCL	C2A-C1A-CHA	2.43	128.09	123.87
14	BH	1004	LMT	O1'-C1'-C2'	2.43	111.97	108.27
13	AE	104	BCL	OBB-CAB-CBB	-2.43	114.33	119.77
13	AQ	103	BCL	C1-C2-C3	-2.43	122.22	126.20
16	L	310	OV9	O3-C30-O5	-2.43	117.55	123.63
13	al	1001	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
15	BQ	1001	V7N	C27-C26-C25	2.43	121.87	118.49
14	be	101	LMT	O5'-C5'-C4'	2.43	114.74	109.72
15	bj	101	V7N	C36-C18-C19	2.43	121.80	118.09
13	bc	103	BCL	C2A-C1A-CHA	2.43	128.08	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ad	102	BCL	C2A-C1A-CHA	2.42	128.07	123.87
15	bn	101	V7N	C33-C5-C4	2.42	121.79	118.09
16	bd	103	0V9	C2-O2-C10	2.42	123.59	117.80
15	AS	104	V7N	C36-C18-C19	2.42	121.79	118.09
14	bp	101	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
13	an	1001	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
13	af	103	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
15	BK	1001	V7N	C35-C13-C14	-2.42	118.90	122.82
13	ae	1001	BCL	CMB-C2B-C1B	-2.42	121.74	125.42
15	bc	101	V7N	C10-C9-C34	2.42	121.81	116.43
13	ah	1001	BCL	CMB-C2B-C1B	-2.42	121.74	125.42
15	BF	101	V7N	C1-C2-C3	2.42	119.26	112.98
14	BR	1005	LMT	C3'-C4'-C5'	-2.42	105.58	110.93
13	AT	101	BCL	OBB-CAB-CBB	-2.41	114.36	119.77
22	M	407	BPH	C2D-C1D-ND	2.41	111.17	109.43
15	BA	101	V7N	C36-C18-C19	2.41	121.77	118.09
13	ap	1001	BCL	OBB-CAB-CBB	-2.41	114.37	119.77
13	ag	102	BCL	OBB-CAB-CBB	-2.41	114.38	119.77
22	M	407	BPH	OBB-CAB-C3B	2.41	124.02	119.99
13	AQ	102	BCL	CMB-C2B-C1B	-2.41	121.75	125.42
15	bc	101	V7N	C1-C2-C3	2.41	119.23	112.98
17	C	1003	HEC	C2A-C1A-NA	-2.41	108.00	110.32
15	bn	101	V7N	C10-C9-C34	2.41	121.78	116.43
13	ak	1001	BCL	C2A-C1A-CHA	2.41	128.04	123.87
13	AM	1002	BCL	CMB-C2B-C1B	-2.41	121.76	125.42
14	ac	101	LMT	C3'-C4'-C5'	-2.40	105.60	110.93
15	BA	101	V7N	C33-C5-C4	2.40	121.76	118.09
15	BO	1001	V7N	C36-C18-C19	2.40	121.76	118.09
15	AM	1001	V7N	C33-C5-C4	2.40	121.76	118.09
23	M	402	MQ8	C21-C20-C18	2.40	121.14	113.19
13	AH	102	BCL	C2A-C1A-CHA	2.40	128.03	123.87
15	BU	1001	V7N	C36-C18-C17	-2.40	118.93	122.82
13	bp	104	BCL	C1C-NC-C4C	2.40	107.77	106.68
13	BS	1004	BCL	C6-C5-C3	2.39	119.30	113.47
15	BM	1001	V7N	C35-C13-C14	-2.39	118.94	122.82
13	an	1001	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
13	AC	102	BCL	OBB-CAB-CBB	-2.39	114.41	119.77
15	bd	101	V7N	C35-C13-C14	-2.39	118.94	122.82
14	BP	1002	LMT	C1'-O5'-C5'	-2.39	109.05	113.72
13	AB	1001	BCL	C6-C5-C3	2.39	119.29	113.47
15	BG	1001	V7N	C35-C13-C12	2.39	121.74	118.09
13	bb	102	BCL	C1C-NC-C4C	2.39	107.77	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ah	1001	BCL	C2A-C1A-CHA	2.39	128.01	123.87
14	bh	102	LMT	O5'-C1'-O1'	-2.39	104.41	110.04
13	ac	102	BCL	C2A-C1A-CHA	2.38	128.01	123.87
15	AW	103	V7N	C38-C26-C27	-2.38	114.45	118.09
15	BQ	1001	V7N	C20-C21-C22	-2.38	124.34	127.69
15	bm	101	V7N	C3-C4-C5	2.38	129.49	125.89
15	BR	1001	V7N	C35-C13-C14	-2.38	118.96	122.82
15	BK	1001	V7N	C15-C14-C13	-2.38	123.94	127.28
13	BI	1004	BCL	C2A-C1A-CHA	2.38	128.00	123.87
13	aa	1001	BCL	C2A-C1A-CHA	2.38	128.00	123.87
15	BS	1001	V7N	C27-C26-C25	2.38	121.80	118.49
15	BI	1001	V7N	C33-C5-C6	-2.38	118.96	122.82
15	bb	101	V7N	C33-C5-C4	2.38	121.72	118.09
13	AO	101	BCL	CMB-C2B-C1B	-2.38	121.80	125.42
14	AX	101	LMT	O1'-C1'-C2'	2.38	111.88	108.27
13	BX	101	BCL	C2A-C1A-CHA	2.37	127.98	123.87
13	AB	1002	BCL	CMB-C2B-C1B	-2.37	121.81	125.42
13	AJ	103	BCL	C1C-NC-C4C	2.37	107.76	106.68
14	be	104	LMT	C3'-C4'-C5'	-2.37	105.68	110.93
13	AB	1002	BCL	C2A-C1A-CHA	2.37	127.98	123.87
13	bi	102	BCL	C2A-C1A-CHA	2.37	127.98	123.87
13	AJ	103	BCL	CBA-CAA-C2A	2.37	120.83	113.79
13	AL	103	BCL	CMB-C2B-C1B	-2.36	121.82	125.42
15	BG	1001	V7N	C35-C13-C14	-2.36	118.99	122.82
14	AU	102	LMT	O1'-C1'-C2'	2.36	111.86	108.27
13	ab	1001	BCL	OBB-CAB-CBB	-2.36	114.48	119.77
15	BG	1001	V7N	C33-C5-C4	2.36	121.69	118.09
14	BX	102	LMT	C1-O1'-C1'	2.36	117.71	113.68
22	L	301	BPH	CMB-C2B-C3B	2.36	129.40	124.68
15	BM	1001	V7N	C35-C13-C12	2.36	121.69	118.09
15	BW	1001	V7N	C35-C13-C14	-2.36	119.00	122.82
13	AB	1001	BCL	OBB-CAB-CBB	-2.36	114.49	119.77
13	bo	102	BCL	CMB-C2B-C1B	-2.36	121.83	125.42
14	BL	101	LMT	C3'-C4'-C5'	-2.35	105.71	110.93
21	af	102	CD4	C20-C19-C18	-2.35	104.48	113.13
14	BC	102	LMT	C3'-C4'-C5'	-2.35	105.72	110.93
13	AW	102	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
14	bn	103	LMT	C3'-C4'-C5'	-2.35	105.73	110.93
15	bc	101	V7N	C33-C5-C4	2.35	121.67	118.09
14	BV	1003	LMT	O1'-C1'-C2'	2.35	111.84	108.27
13	AB	1001	BCL	CAB-C3B-C2B	2.35	132.62	127.74
23	L	303	MQ8	C41-C40-C38	-2.35	105.41	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bo	102	BCL	C1C-NC-C4C	2.35	107.75	106.68
16	bk	102	0V9	O3-C30-O5	-2.35	117.76	123.63
15	BN	1001	V7N	C10-C9-C34	2.35	121.64	116.43
13	BR	1003	BCL	C2A-C1A-CHA	2.34	127.94	123.87
14	BN	1004	LMT	C1-O1'-C1'	2.34	117.68	113.68
14	H2	201	LMT	C1-O1'-C1'	2.34	117.68	113.68
13	AU	103	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
15	BO	1001	V7N	C10-C9-C34	2.34	121.63	116.43
13	bm	102	BCL	C1C-NC-C4C	2.34	107.75	106.68
15	BH	1001	V7N	C35-C13-C14	-2.34	119.03	122.82
13	ao	102	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
15	BN	1001	V7N	C35-C13-C14	-2.34	119.03	122.82
13	aj	101	BCL	CMB-C2B-C1B	-2.34	121.86	125.42
15	BI	1001	V7N	C2-C3-C4	-2.33	121.64	124.91
15	BP	1001	V7N	C35-C13-C14	-2.33	119.03	122.82
13	L	305	BCL	C1C-NC-C4C	2.33	107.74	106.68
14	bc	102	LMT	O1B-C4'-C3'	2.33	113.16	107.23
14	BS	1002	LMT	O1'-C1'-C2'	2.33	111.82	108.27
16	bm	104	0V9	O2-C10-O4	-2.33	118.25	123.70
14	BT	102	LMT	C3'-C4'-C5'	-2.33	105.77	110.93
13	AU	103	BCL	C2A-C1A-CHA	2.33	127.91	123.87
14	AN	102	LMT	C3'-C4'-C5'	-2.33	105.77	110.93
14	BS	1002	LMT	C1'-O5'-C5'	-2.33	109.18	113.72
14	AD	102	LMT	O1'-C1'-C2'	2.33	111.81	108.27
16	bd	103	0V9	O3P-P-O2P	2.33	118.16	108.94
15	bh	101	V7N	C36-C18-C19	2.33	121.64	118.09
14	BT	101	LMT	C3'-C4'-C5'	-2.33	105.78	110.93
13	AQ	102	BCL	C2A-C1A-CHA	2.32	127.90	123.87
13	bm	102	BCL	C2A-C1A-CHA	2.32	127.90	123.87
15	bg	101	V7N	C35-C13-C14	-2.32	119.05	122.82
13	BU	1004	BCL	CAB-C3B-C2B	2.32	132.57	127.74
13	AN	103	BCL	OBB-CAB-CBB	-2.32	114.57	119.77
17	C	1001	HEC	CBD-CAD-C3D	-2.32	106.12	112.53
13	AA	1002	BCL	CAB-C3B-C2B	2.32	132.56	127.74
14	AE	106	LMT	O5B-C1B-C2B	2.32	115.14	110.37
13	al	1001	BCL	OBB-CAB-CBB	-2.32	114.58	119.77
21	H1	103	CD4	O3-C17-C18	2.32	118.90	111.83
15	BM	1001	V7N	C33-C5-C4	2.32	121.63	118.09
13	BS	1004	BCL	C2A-C1A-CHA	2.32	127.89	123.87
13	af	103	BCL	CMB-C2B-C1B	-2.32	121.89	125.42
13	ad	102	BCL	CMB-C2B-C1B	-2.31	121.89	125.42
13	aa	1001	BCL	OBB-CAB-CBB	-2.31	114.59	119.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	ad	103	OV9	O3-C30-O5	-2.31	117.84	123.63
13	AV	103	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
14	L	306	LMT	C1-O1'-C1'	2.31	117.63	113.68
15	BH	1001	V7N	C33-C5-C6	-2.31	119.07	122.82
13	ak	1001	BCL	CAB-C3B-C2B	2.31	132.54	127.74
13	bg	104	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
13	BP	1003	BCL	C2A-C1A-CHA	2.31	127.88	123.87
13	AJ	103	BCL	CAA-CBA-CGA	2.31	119.77	113.21
13	AU	103	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
13	bb	102	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
15	BR	1001	V7N	C11-C10-C9	2.31	130.26	127.28
13	AH	102	BCL	OBB-CAB-CBB	-2.31	114.60	119.77
15	BD	101	V7N	C35-C13-C12	2.31	121.61	118.09
13	ag	102	BCL	C2A-C1A-CHA	2.31	127.87	123.87
15	BA	101	V7N	C36-C18-C17	-2.31	119.08	122.82
21	ad	101	CD4	C31-C30-C29	-2.31	106.01	112.65
14	BH	1004	LMT	O5'-C1'-C2'	-2.31	105.63	110.37
13	af	103	BCL	C2A-C1A-CHA	2.30	127.87	123.87
15	AA	1004	V7N	C35-C13-C14	-2.30	119.08	122.82
13	bb	102	BCL	C2A-C1A-CHA	2.30	127.86	123.87
15	bg	101	V7N	C35-C13-C12	2.30	121.61	118.09
13	AQ	102	BCL	OBB-CAB-CBB	-2.30	114.61	119.77
15	BQ	1001	V7N	C11-C10-C9	2.30	130.25	127.28
21	af	102	CD4	O3-C17-C18	2.30	118.85	111.83
13	ap	1001	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
14	bl	103	LMT	O5B-C5B-C4B	2.30	113.84	109.70
14	BG	1003	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
13	AQ	104	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
13	AV	103	BCL	CAB-C3B-C2B	2.30	132.52	127.74
14	L	304	LMT	O5'-C1'-C2'	-2.30	105.65	110.37
15	AS	104	V7N	C35-C13-C14	-2.30	119.09	122.82
13	AJ	103	BCL	C2A-C1A-CHA	2.30	127.86	123.87
13	bh	103	BCL	C2A-C1A-CHA	2.30	127.85	123.87
13	aj	101	BCL	OBB-CAB-CBB	-2.30	114.63	119.77
14	AV	102	LMT	C1'-O5'-C5'	-2.30	109.24	113.72
14	BI	1002	LMT	C1-O1'-C1'	2.30	117.60	113.68
13	AH	102	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
21	M	405	CD4	C28-C15-C16	-2.29	106.44	111.78
13	AO	101	BCL	OBB-CAB-CBB	-2.29	114.64	119.77
13	bp	104	BCL	C2A-C1A-CHA	2.29	127.84	123.87
16	be	105	OV9	O3P-P-O2P	2.29	118.02	108.94
13	bp	104	BCL	CMB-C2B-C1B	-2.29	121.93	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BH	1001	V7N	C10-C9-C34	2.29	121.52	116.43
13	bl	104	BCL	C1C-NC-C4C	2.29	107.72	106.68
13	bn	102	BCL	CAB-C3B-C2B	2.29	132.50	127.74
13	BD	104	BCL	C2A-C1A-CHA	2.29	127.84	123.87
15	BR	1001	V7N	C33-C5-C4	2.29	121.58	118.09
13	bc	103	BCL	C6-C5-C3	2.29	119.04	113.47
13	M	408	BCL	OBB-CAB-CBB	-2.29	114.65	119.77
13	AD	103	BCL	OBB-CAB-CBB	-2.29	114.65	119.77
13	AE	105	BCL	CMB-C2B-C1B	-2.29	121.94	125.42
13	AX	103	BCL	C2A-C1A-CHA	2.29	127.83	123.87
15	BF	101	V7N	C33-C5-C4	2.28	121.58	118.09
14	BC	103	LMT	C3'-C4'-C5'	-2.28	105.87	110.93
13	ai	101	BCL	OBB-CAB-CBB	-2.28	114.65	119.77
13	AW	101	BCL	OBB-CAB-CBB	-2.28	114.66	119.77
13	AP	103	BCL	CMB-C2B-C1B	-2.28	121.94	125.42
15	bk	101	V7N	C3-C4-C5	2.28	129.34	125.89
13	am	1001	BCL	OBB-CAB-CBB	-2.28	114.66	119.77
14	BU	1002	LMT	O5'-C1'-O1'	-2.28	104.66	110.04
13	bj	104	BCL	C2A-C1A-CHA	2.28	127.82	123.87
13	BS	1004	BCL	CAB-C3B-C2B	2.28	132.47	127.74
14	H2	201	LMT	C3'-C4'-C5'	-2.28	105.88	110.93
13	L	305	BCL	CMB-C2B-C1B	-2.28	121.95	125.42
13	bi	102	BCL	CMB-C2B-C1B	-2.28	121.95	125.42
13	aj	101	BCL	C1-O2A-CGA	2.28	122.16	116.65
14	BI	1003	LMT	C3'-C4'-C5'	-2.28	105.89	110.93
13	bn	102	BCL	CMB-C2B-C1B	-2.27	121.95	125.42
15	BJ	1001	V7N	C33-C5-C4	2.27	121.56	118.09
13	BC	104	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
13	BN	1005	BCL	CAB-C3B-C2B	2.27	132.46	127.74
13	ac	102	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
13	AE	105	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
16	ab	1002	OV9	O3P-P-O2P	2.27	117.93	108.94
13	BK	1002	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
13	AT	103	BCL	CAB-C3B-C2B	2.27	132.45	127.74
13	ap	1001	BCL	C2A-C1A-CHA	2.27	127.80	123.87
13	AG	102	BCL	CMB-C2B-C1B	-2.27	121.97	125.42
14	BL	102	LMT	C3'-C4'-C5'	-2.27	105.91	110.93
13	BM	1004	BCL	OBB-CAB-CBB	-2.27	114.70	119.77
14	BU	1003	LMT	O5B-C5B-C4B	2.27	113.78	109.70
14	AV	104	LMT	C3'-C4'-C5'	-2.27	105.91	110.93
14	bo	104	LMT	C1-O1'-C1'	2.26	117.55	113.68
13	AD	104	BCL	C4A-NA-C1A	2.26	107.71	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AP	103	BCL	C1C-NC-C4C	2.26	107.71	106.68
15	bg	101	V7N	C36-C18-C17	-2.26	119.15	122.82
15	AA	1004	V7N	C36-C18-C17	-2.26	119.16	122.82
14	BP	1002	LMT	C3'-C4'-C5'	-2.26	105.92	110.93
15	BJ	1001	V7N	C35-C13-C14	-2.26	119.16	122.82
14	BV	1004	LMT	O5'-C1'-C2'	-2.26	105.73	110.37
15	bd	101	V7N	C27-C26-C25	2.26	121.63	118.49
14	BP	1006	LMT	O1'-C1'-C2'	2.26	111.70	108.27
22	M	407	BPH	O2D-CGD-CBD	2.26	113.42	110.95
13	ai	101	BCL	C2A-C1A-CHA	2.26	127.78	123.87
15	BW	1001	V7N	C36-C18-C17	-2.25	119.16	122.82
13	bi	102	BCL	OBB-CAB-CBB	-2.25	114.72	119.77
14	bp	101	LMT	C3B-C4B-C5B	-2.25	106.15	110.23
13	AE	103	BCL	C2A-C1A-CHA	2.25	127.78	123.87
14	BW	1006	LMT	C1'-O5'-C5'	-2.25	109.32	113.72
14	BM	1005	LMT	O5'-C1'-C2'	-2.25	105.74	110.37
13	bf	102	BCL	C1C-NC-C4C	2.25	107.71	106.68
15	BO	1001	V7N	C33-C5-C6	-2.25	119.17	122.82
13	AD	104	BCL	CAB-C3B-C2B	2.25	132.42	127.74
13	AK	102	BCL	CMB-C2B-C1B	-2.25	121.99	125.42
14	AC	103	LMT	C3'-C4'-C5'	-2.25	105.94	110.93
13	BS	1004	BCL	OBB-CAB-CBB	-2.25	114.73	119.77
15	BU	1001	V7N	C4-C5-C6	-2.25	115.47	119.01
13	bk	103	BCL	OBB-CAB-CBB	-2.25	114.74	119.77
13	AB	1002	BCL	OBB-CAB-CBB	-2.25	114.74	119.77
15	BS	1001	V7N	C35-C13-C14	-2.24	119.18	122.82
13	bm	102	BCL	CMB-C2B-C1B	-2.24	122.00	125.42
15	bc	101	V7N	C35-C13-C14	-2.24	119.19	122.82
15	bi	101	V7N	C35-C13-C14	-2.24	119.19	122.82
15	AD	101	V7N	C33-C5-C4	2.24	121.51	118.09
13	BF	103	BCL	C2A-C1A-CHA	2.24	127.75	123.87
14	BF	104	LMT	C3'-C4'-C5'	-2.24	105.97	110.93
13	AG	102	BCL	CBA-CAA-C2A	2.24	120.45	113.79
15	BM	1001	V7N	C36-C18-C17	-2.24	119.19	122.82
16	M	403	OV9	O3P-P-O2P	2.23	117.79	108.94
14	BD	105	LMT	C3'-C4'-C5'	-2.23	105.98	110.93
13	ak	1001	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
13	BJ	1004	BCL	C2A-C1A-CHA	2.23	127.74	123.87
14	BW	1006	LMT	O1'-C1'-C2'	2.23	111.66	108.27
14	BB	102	LMT	C1'-O5'-C5'	-2.23	109.36	113.72
13	AE	103	BCL	OBB-CAB-CBB	-2.23	114.77	119.77
15	AA	1004	V7N	C35-C13-C12	2.23	121.50	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AH	102	BCL	CAB-C3B-C2B	2.23	132.38	127.74
13	AK	102	BCL	C1C-NC-C4C	2.23	107.70	106.68
16	bh	104	0V9	O3P-P-O2P	2.23	117.77	108.94
13	BT	103	BCL	CMB-C2B-C1B	-2.23	122.03	125.42
13	BH	1005	BCL	CAB-C3B-C2B	2.23	132.37	127.74
13	AN	104	BCL	CMB-C2B-C1B	-2.23	122.03	125.42
16	bl	102	0V9	O2-C10-O4	-2.23	118.50	123.70
13	AQ	104	BCL	C1-C2-C3	-2.23	122.55	126.20
13	AP	103	BCL	OBB-CAB-CBB	-2.23	114.79	119.77
13	AX	103	BCL	CMB-C2B-C1B	-2.22	122.03	125.42
13	ao	102	BCL	CMB-C2B-C1B	-2.22	122.03	125.42
13	AS	101	BCL	OBB-CAB-CBB	-2.22	114.79	119.77
13	AX	103	BCL	OBB-CAB-CBB	-2.22	114.79	119.77
13	AL	103	BCL	OBB-CAB-CBB	-2.22	114.79	119.77
15	bg	101	V7N	C1-C2-C3	2.22	118.75	112.98
13	AM	1002	BCL	OBB-CAB-CBB	-2.22	114.79	119.77
13	be	103	BCL	C2A-C1A-CHA	2.22	127.72	123.87
13	ak	1001	BCL	OBB-CAB-CBB	-2.22	114.80	119.77
13	be	103	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
15	bn	101	V7N	C11-C10-C9	2.22	130.14	127.28
15	bo	101	V7N	C36-C18-C19	2.22	121.48	118.09
13	BV	1005	BCL	CBA-CAA-C2A	2.22	120.39	113.79
15	bi	101	V7N	C36-C18-C19	2.22	121.48	118.09
16	bj	103	0V9	O3P-P-O2P	2.22	117.72	108.94
21	af	102	CD4	C12-C13-C14	-2.22	105.57	113.69
13	BV	1005	BCL	CAB-C3B-C2B	2.21	132.34	127.74
13	AE	103	BCL	CMB-C2B-C1B	-2.21	122.05	125.42
13	BW	1005	BCL	CMB-C2B-C1B	-2.21	122.05	125.42
15	bk	101	V7N	C10-C9-C34	2.21	121.35	116.43
21	af	104	CD4	O2-C14-O1	-2.21	118.53	123.70
15	bp	102	V7N	C11-C10-C9	2.21	130.13	127.28
13	be	103	BCL	C1C-NC-C4C	2.21	107.69	106.68
13	bi	102	BCL	C1C-NC-C4C	2.21	107.69	106.68
14	BI	1005	LMT	O5'-C1'-C2'	-2.21	105.83	110.37
15	BQ	1001	V7N	C15-C14-C13	-2.21	124.18	127.28
14	bj	102	LMT	C3B-C4B-C5B	-2.21	106.22	110.23
13	AG	102	BCL	CAC-C3C-C4C	2.21	117.49	112.58
15	AM	1001	V7N	C27-C26-C25	2.21	121.57	118.49
14	BW	1003	LMT	C1-O1'-C1'	2.21	117.45	113.68
14	C2	1001	LMT	C1-O1'-C1'	2.21	117.45	113.68
16	bg	103	0V9	O3P-P-O2P	2.21	117.69	108.94
15	bl	101	V7N	C3-C4-C5	2.21	129.23	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AP	102	BCL	C6-C5-C3	2.21	118.84	113.47
14	BX	103	LMT	C1'-O5'-C5'	-2.21	109.41	113.72
14	L	304	LMT	O1'-C1'-C2'	2.21	111.62	108.27
15	BH	1001	V7N	C38-C26-C27	-2.21	114.72	118.09
13	BB	105	BCL	CAB-C3B-C2B	2.20	132.32	127.74
13	ba	102	BCL	OBB-CAB-CBB	-2.20	114.83	119.77
13	BT	103	BCL	CAB-C3B-C2B	2.20	132.32	127.74
13	AE	104	BCL	C6-C5-C3	2.20	118.84	113.47
13	bg	104	BCL	C2A-C1A-CHA	2.20	127.69	123.87
13	AB	1002	BCL	CAB-C3B-C2B	2.20	132.31	127.74
13	ai	101	BCL	C1-O2A-CGA	2.20	121.98	116.65
13	ba	102	BCL	CAB-C3B-C2B	2.20	132.31	127.74
16	bp	105	OV9	O2-C10-O4	-2.20	118.56	123.70
13	AX	102	BCL	C1-O2A-CGA	2.20	121.97	116.65
21	M	409	CD4	C33-O16-C46	2.20	123.06	117.80
15	bm	101	V7N	C36-C18-C19	2.20	121.44	118.09
21	ad	101	CD4	O3-C17-C18	2.20	118.53	111.83
13	ag	102	BCL	C1C-NC-C4C	2.20	107.68	106.68
13	bp	104	BCL	OBB-CAB-CBB	-2.20	114.85	119.77
15	AS	104	V7N	C11-C10-C9	2.20	130.11	127.28
17	C	1002	HEC	C2A-C1A-NA	-2.20	108.20	110.32
14	AK	101	LMT	C1-O1'-C1'	2.19	117.43	113.68
14	bm	103	LMT	O1'-C1'-C2'	2.19	111.60	108.27
16	bo	103	OV9	O3P-P-O2P	2.19	117.61	108.94
21	af	102	CD4	O14-C35-C36	2.19	118.51	111.83
13	BM	1004	BCL	CMB-C2B-C1B	-2.19	122.08	125.42
15	AW	103	V7N	C33-C5-C4	2.19	121.43	118.09
13	BA	103	BCL	CAB-C3B-C2B	2.19	132.29	127.74
13	BE	104	BCL	CMB-C2B-C1B	-2.19	122.09	125.42
26	ag	103	V7B	C7-O1-C1	2.19	118.49	113.80
13	L	305	BCL	C4A-NA-C1A	2.19	107.68	106.68
15	BQ	1001	V7N	C35-C13-C14	-2.19	119.27	122.82
15	BE	101	V7N	C35-C13-C14	-2.19	119.27	122.82
13	BR	1003	BCL	CMB-C2B-C1B	-2.19	122.09	125.42
13	AH	102	BCL	CAA-CBA-CGA	2.19	119.42	113.21
15	BQ	1001	V7N	C29-C28-C27	-2.19	116.87	123.20
13	AO	101	BCL	C4A-NA-C1A	2.19	107.68	106.68
14	AN	101	LMT	O5B-C5B-C4B	2.18	113.64	109.70
13	BD	104	BCL	OBB-CAB-CBB	-2.18	114.88	119.77
15	bl	101	V7N	C35-C13-C14	-2.18	119.28	122.82
15	BM	1001	V7N	O45-C40-C39	2.18	127.71	122.09
13	ac	102	BCL	CMB-C2B-C1B	-2.18	122.10	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BL	103	BCL	OBB-CAB-CBB	-2.18	114.89	119.77
15	bd	101	V7N	C36-C18-C19	2.18	121.42	118.09
14	L	304	LMT	O5'-C5'-C4'	2.18	114.22	109.72
13	BO	1003	BCL	C2A-C1A-CHA	2.17	127.64	123.87
15	AW	103	V7N	C36-C18-C17	-2.17	119.29	122.82
14	L	309	LMT	C3'-C4'-C5'	-2.17	106.11	110.93
14	BC	101	LMT	C1'-O5'-C5'	-2.17	109.48	113.72
13	al	1001	BCL	C1-O2A-CGA	2.17	121.91	116.65
15	be	102	V7N	C36-C18-C19	2.17	121.40	118.09
13	AG	102	BCL	C6-C7-C8	-2.17	108.75	115.97
13	AE	103	BCL	CAB-C3B-C2B	2.17	132.25	127.74
13	AB	1001	BCL	C9-C8-C10	-2.17	103.55	111.27
13	BS	1004	BCL	CMB-C2B-C1B	-2.17	122.12	125.42
14	BF	102	LMT	O1'-C1'-C2'	2.17	111.56	108.27
13	bd	102	BCL	OBB-CAB-CBB	-2.16	114.92	119.77
13	BF	103	BCL	CAB-C3B-C2B	2.16	132.24	127.74
13	AE	105	BCL	CAB-C3B-C2B	2.16	132.24	127.74
13	aj	101	BCL	C2A-C1A-CHA	2.16	127.62	123.87
15	BU	1001	V7N	C10-C9-C34	2.16	121.23	116.43
13	AS	101	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
15	BJ	1001	V7N	C20-C21-C22	-2.16	124.65	127.69
13	BB	105	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
15	BW	1001	V7N	C35-C13-C12	2.16	121.39	118.09
14	BS	1003	LMT	C1'-O5'-C5'	-2.16	109.50	113.72
13	bh	103	BCL	CAB-C3B-C2B	2.16	132.23	127.74
14	BT	102	LMT	C1-O1'-C1'	2.16	117.37	113.68
13	AB	1001	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
13	AA	1002	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
13	AH	102	BCL	C11-C10-C8	2.16	123.14	115.97
15	ag	101	V7N	C35-C13-C14	-2.15	119.33	122.82
15	bj	101	V7N	C35-C13-C14	-2.15	119.33	122.82
14	BB	101	LMT	O1'-C1'-C2'	2.15	111.54	108.27
13	BF	103	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
15	bo	101	V7N	C35-C13-C14	-2.15	119.33	122.82
14	BS	1003	LMT	C3B-C4B-C5B	-2.15	106.33	110.23
13	AX	103	BCL	CAB-C3B-C2B	2.15	132.21	127.74
14	bi	104	LMT	C3'-C4'-C5'	-2.15	106.16	110.93
14	bf	101	LMT	O1B-C1B-C2B	2.15	113.38	108.09
15	BJ	1001	V7N	C35-C13-C12	2.15	121.37	118.09
13	AT	103	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
13	bj	104	BCL	C1-O2A-CGA	2.15	121.86	116.65
16	H1	102	OV9	O3-C30-O5	-2.15	118.25	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BK	1002	BCL	OBB-CAB-CBB	-2.15	114.96	119.77
15	BK	1001	V7N	C33-C5-C4	2.15	121.37	118.09
15	BO	1001	V7N	C15-C14-C13	-2.15	124.27	127.28
13	BG	1004	BCL	CMB-C2B-C1B	-2.15	122.15	125.42
13	BN	1005	BCL	OBB-CAB-CBB	-2.15	114.96	119.77
14	BD	105	LMT	C3B-C4B-C5B	-2.14	106.34	110.23
13	AJ	103	BCL	OBB-CAB-CBB	-2.14	114.97	119.77
15	BK	1001	V7N	C36-C18-C17	-2.14	119.34	122.82
21	M	405	CD4	O14-C35-C36	2.14	118.37	111.83
14	BV	1002	LMT	C3'-C4'-C5'	-2.14	106.18	110.93
13	BB	105	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
14	BI	1002	LMT	C3'-C4'-C5'	-2.14	106.19	110.93
13	bm	102	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
13	bf	102	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
14	bi	104	LMT	C1-O1'-C1'	2.14	117.33	113.68
14	BK	1005	LMT	C3'-C4'-C5'	-2.14	106.19	110.93
16	M	403	OV9	O2-C10-O4	-2.14	118.71	123.70
16	AQ	105	OV9	O3P-P-O2P	2.14	117.41	108.94
13	BK	1002	BCL	CAB-C3B-C2B	2.14	132.18	127.74
14	L	307	LMT	C1-O1'-C1'	2.14	117.33	113.68
13	bo	102	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
13	bk	103	BCL	C1C-NC-C4C	2.14	107.65	106.68
13	AV	103	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
22	L	301	BPH	C1-O2A-CGA	2.14	121.82	116.65
13	AQ	102	BCL	CAB-C3B-C2B	2.14	132.18	127.74
16	bf	103	OV9	O3P-P-O2P	2.13	117.40	108.94
16	M	403	OV9	O1P-P-O4P	-2.13	97.90	107.57
13	aj	101	BCL	CAB-C3B-C2B	2.13	132.17	127.74
13	an	1001	BCL	C1-O2A-CGA	2.13	121.81	116.65
13	BI	1004	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
13	BR	1003	BCL	OBB-CAB-CBB	-2.13	114.99	119.77
16	bj	103	OV9	O2-C10-O4	-2.13	118.72	123.70
14	BO	1005	LMT	O5B-C5B-C4B	2.13	113.54	109.70
13	BD	104	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
13	bc	103	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
13	bl	104	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
13	AS	102	BCL	CAC-C3C-C4C	2.13	117.31	112.58
13	BJ	1004	BCL	CAB-C3B-C2B	2.13	132.17	127.74
17	C	1001	HEC	CHC-C4B-NB	2.13	126.77	124.45
13	bf	102	BCL	OBB-CAB-CBB	-2.13	115.00	119.77
13	BW	1005	BCL	OBB-CAB-CBB	-2.13	115.00	119.77
14	BR	1002	LMT	C1'-O5'-C5'	-2.13	109.56	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AT	103	BCL	OBB-CAB-CBB	-2.13	115.00	119.77
13	AK	102	BCL	C4A-NA-C1A	2.13	107.65	106.68
13	BM	1004	BCL	CAB-C3B-C2B	2.13	132.16	127.74
13	bd	102	BCL	C6-C5-C3	2.13	118.65	113.47
13	bj	104	BCL	CAB-C3B-C2B	2.13	132.16	127.74
15	bc	101	V7N	C36-C18-C17	-2.13	119.37	122.82
15	bo	101	V7N	C27-C26-C25	2.12	121.45	118.49
13	BM	1004	BCL	CBA-CAA-C2A	2.12	120.11	113.79
13	am	1001	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
13	M	408	BCL	C11-C12-C13	-2.12	108.91	115.97
13	AN	104	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
16	bn	104	0V9	O3-C30-O5	-2.12	118.32	123.63
13	AN	104	BCL	C1C-NC-C4C	2.12	107.65	106.68
13	BO	1003	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
13	AV	101	BCL	C1-C2-C3	2.12	129.67	126.20
13	BH	1005	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
13	bj	104	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
15	BP	1001	V7N	C1-C2-C3	2.12	118.49	112.98
15	ag	101	V7N	C2-C3-C4	-2.12	121.94	124.91
13	BQ	1004	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
13	BU	1004	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
14	BJ	1002	LMT	O1'-C1'-C2'	2.12	111.49	108.27
13	bc	103	BCL	CAB-C3B-C2B	2.12	132.14	127.74
22	M	407	BPH	CMD-C2D-C3D	2.12	128.92	124.68
14	BD	102	LMT	C3'-C4'-C5'	-2.12	106.24	110.93
13	AD	103	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
13	BC	104	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
20	H1	101	PGW	O03-C19-C20	2.12	118.29	111.83
15	BN	1001	V7N	C27-C26-C25	2.12	121.44	118.49
15	BE	101	V7N	C36-C18-C17	-2.12	119.39	122.82
14	BS	1003	LMT	C3'-C4'-C5'	-2.12	106.24	110.93
13	BO	1003	BCL	CAB-C3B-C2B	2.12	132.14	127.74
13	AP	103	BCL	C1-O2A-CGA	2.11	121.77	116.65
15	BU	1001	V7N	O45-C40-C39	2.11	127.54	122.09
13	BQ	1004	BCL	CMB-C2B-C1B	-2.11	122.20	125.42
14	AJ	102	LMT	C1'-O5'-C5'	-2.11	109.59	113.72
13	AH	102	BCL	C1-O2A-CGA	2.11	121.76	116.65
14	AN	101	LMT	O5'-C1'-C2'	-2.11	106.03	110.37
15	bl	101	V7N	C36-C18-C19	2.11	121.31	118.09
15	bh	101	V7N	C1-C2-C3	2.11	118.47	112.98
15	BS	1001	V7N	C15-C14-C13	-2.11	124.32	127.28
16	bh	104	0V9	O3-C30-O5	-2.11	118.35	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BV	1001	V7N	C20-C21-C22	-2.11	124.72	127.69
13	be	103	BCL	OBB-CAB-CBB	-2.11	115.05	119.77
13	BD	104	BCL	CAB-C3B-C2B	2.11	132.12	127.74
15	bh	101	V7N	O45-C40-C39	2.11	127.53	122.09
13	am	1001	BCL	CAB-C3B-C2B	2.11	132.12	127.74
14	BK	1003	LMT	C2'-C3'-C4'	2.11	114.46	109.68
13	AW	102	BCL	OBB-CAB-CBB	-2.11	115.05	119.77
15	BH	1001	V7N	C36-C18-C17	-2.11	119.41	122.82
14	BE	103	LMT	O1'-C1'-C2'	2.10	111.47	108.27
13	AU	103	BCL	CAB-C3B-C2B	2.10	132.11	127.74
13	BH	1005	BCL	CMB-C2B-C1B	-2.10	122.22	125.42
13	BT	103	BCL	CBA-CAA-C2A	2.10	120.05	113.79
13	af	103	BCL	CAB-C3B-C2B	2.10	132.11	127.74
13	AM	1002	BCL	CAA-CBA-CGA	2.10	119.18	113.21
15	bp	102	V7N	C36-C18-C17	-2.10	119.41	122.82
14	AL	101	LMT	O5B-C5B-C4B	2.10	113.49	109.70
13	BV	1005	BCL	CMB-C2B-C1B	-2.10	122.22	125.42
13	AC	101	BCL	C6-C5-C3	2.10	118.58	113.47
14	BW	1002	LMT	C3'-C4'-C5'	-2.10	106.28	110.93
17	C	1004	HEC	CAD-CBD-CGD	-2.10	108.10	113.67
14	AH	104	LMT	C1'-O5'-C5'	-2.10	109.62	113.72
13	BG	1004	BCL	CAB-C3B-C2B	2.10	132.10	127.74
15	bd	101	V7N	C36-C18-C17	-2.10	119.42	122.82
14	BE	102	LMT	O5'-C5'-C4'	2.10	114.06	109.72
15	BI	1001	V7N	O45-C40-C39	2.10	127.50	122.09
15	ba	101	V7N	C36-C18-C19	2.09	121.29	118.09
13	bh	103	BCL	OBB-CAB-CBB	-2.09	115.08	119.77
26	af	101	V7B	O7-C8-C9	-2.09	100.83	108.34
14	BV	1003	LMT	O5'-C1'-C2'	-2.09	106.07	110.37
13	AG	102	BCL	OBB-CAB-CBB	-2.09	115.08	119.77
13	AW	102	BCL	C4-C3-C5	-2.09	111.60	115.23
16	L	310	OV9	O3P-P-O2P	2.09	117.22	108.94
15	AM	1001	V7N	C35-C13-C14	-2.09	119.43	122.82
22	L	301	BPH	CMD-C2D-C3D	2.09	128.86	124.68
13	bl	104	BCL	C2A-C1A-CHA	2.09	127.49	123.87
13	AH	105	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
13	AL	103	BCL	CAB-C3B-C2B	2.09	132.08	127.74
14	BU	1003	LMT	O5'-C1'-C2'	-2.09	106.08	110.37
13	AQ	104	BCL	CAB-C3B-C2B	2.09	132.08	127.74
14	AN	101	LMT	C2'-C3'-C4'	2.09	114.42	109.68
13	bn	102	BCL	C2A-C1A-CHA	2.09	127.49	123.87
13	an	1001	BCL	C6-C5-C3	2.09	118.55	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ap	1001	BCL	CAB-C3B-C2B	2.09	132.07	127.74
14	BJ	1005	LMT	C3B-C4B-C5B	-2.08	106.45	110.23
14	AL	101	LMT	O5'-C1'-C2'	-2.08	106.09	110.37
15	bg	101	V7N	C36-C18-C19	2.08	121.27	118.09
16	bj	103	0V9	O3-C30-O5	-2.08	118.42	123.63
14	bp	103	LMT	C1'-O5'-C5'	-2.08	109.65	113.72
14	BF	104	LMT	C3B-C4B-C5B	-2.08	106.46	110.23
13	bg	104	BCL	OBB-CAB-CBB	-2.08	115.11	119.77
14	AE	106	LMT	O5'-C1'-C2'	-2.08	106.10	110.37
14	bj	102	LMT	C1-O1'-C1'	2.08	117.23	113.68
13	AA	1002	BCL	OBB-CAB-CBB	-2.08	115.11	119.77
13	ba	102	BCL	C2A-C1A-CHA	2.08	127.47	123.87
13	AX	103	BCL	CAA-CBA-CGA	2.08	119.11	113.21
21	ad	101	CD4	O14-C35-C36	2.08	118.17	111.83
13	BA	103	BCL	CMB-C2B-C1B	-2.08	122.26	125.42
13	AO	101	BCL	CAB-C3B-C2B	2.08	132.06	127.74
15	bp	102	V7N	C1-C2-C3	2.08	118.38	112.98
13	AD	104	BCL	OBB-CAB-CBB	-2.08	115.12	119.77
13	bj	104	BCL	CMB-C2B-C1B	-2.08	122.26	125.42
13	BR	1003	BCL	CAB-C3B-C2B	2.08	132.05	127.74
16	bg	103	0V9	O3-C30-O5	-2.08	118.44	123.63
15	BO	1001	V7N	C7-C8-C9	-2.08	123.78	127.30
15	AA	1004	V7N	C36-C18-C19	2.08	121.26	118.09
15	BI	1001	V7N	C27-C26-C25	2.07	121.38	118.49
20	H1	101	PGW	O03-C01-C02	2.07	114.38	108.40
14	AM	1003	LMT	C1'-O5'-C5'	-2.07	109.67	113.72
20	H1	101	PGW	O01-C1-C2	2.07	115.97	111.48
14	L	302	LMT	O1'-C1'-C2'	2.07	111.42	108.27
13	BF	103	BCL	OBB-CAB-CBB	-2.07	115.13	119.77
14	BG	1002	LMT	C1-O1'-C1'	2.07	117.22	113.68
14	BP	1004	LMT	C1-O1'-C1'	2.07	117.22	113.68
15	bl	101	V7N	C36-C18-C17	-2.07	119.46	122.82
13	BT	103	BCL	OBB-CAB-CBB	-2.07	115.14	119.77
13	BQ	1004	BCL	CAB-C3B-C2B	2.07	132.04	127.74
13	BJ	1004	BCL	OBB-CAB-CBB	-2.07	115.14	119.77
13	AH	105	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
14	BR	1002	LMT	C3'-C4'-C5'	-2.07	106.34	110.93
13	BI	1004	BCL	OBB-CAB-CBB	-2.07	115.14	119.77
15	bd	101	V7N	C33-C5-C4	2.07	121.25	118.09
15	BS	1001	V7N	O45-C40-C39	2.07	127.42	122.09
15	bm	101	V7N	O45-C40-C39	2.07	127.42	122.09
13	BI	1004	BCL	CAB-C3B-C2B	2.07	132.03	127.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ad	102	BCL	CAB-C3B-C2B	2.07	132.03	127.74
13	AL	103	BCL	CAC-C3C-C4C	2.07	117.17	112.58
15	AS	104	V7N	C15-C14-C13	-2.07	124.38	127.28
15	bh	101	V7N	C20-C21-C22	-2.07	124.78	127.69
15	bb	101	V7N	C36-C18-C19	2.07	121.24	118.09
21	M	405	CD4	C19-C18-C17	-2.06	106.13	113.69
15	BP	1001	V7N	C33-C5-C4	2.06	121.24	118.09
13	BX	101	BCL	CMB-C2B-C1B	-2.06	122.28	125.42
15	ag	101	V7N	C36-C18-C17	-2.06	119.47	122.82
13	AS	101	BCL	CAB-C3B-C2B	2.06	132.03	127.74
14	BC	101	LMT	O1'-C1'-C2'	2.06	111.41	108.27
13	BX	101	BCL	CAB-C3B-C2B	2.06	132.02	127.74
13	BP	1003	BCL	OBb-CAB-CBB	-2.06	115.15	119.77
15	ba	101	V7N	C15-C14-C13	-2.06	124.39	127.28
13	AO	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
16	bn	104	0V9	O2-C10-O4	-2.06	118.89	123.70
21	ad	101	CD4	O2-C15-C28	2.06	115.73	108.34
13	ba	102	BCL	CMB-C2B-C1B	-2.06	122.28	125.42
13	AW	102	BCL	O2A-CGA-O1A	-2.06	118.48	123.63
15	bl	101	V7N	C11-C10-C9	2.06	129.93	127.28
15	BV	1001	V7N	C36-C18-C19	2.06	121.23	118.09
14	bc	102	LMT	C1B-O1B-C4'	2.06	122.85	117.98
15	bp	102	V7N	C20-C21-C22	-2.05	124.80	127.69
15	be	102	V7N	C35-C13-C14	-2.05	119.49	122.82
16	ad	103	0V9	O3P-P-O2P	2.05	117.07	108.94
13	BB	105	BCL	CBA-CAA-C2A	2.05	119.90	113.79
14	bk	104	LMT	O5'-C1'-O1'	-2.05	105.20	110.04
13	BV	1005	BCL	OBb-CAB-CBB	-2.05	115.18	119.77
13	AH	105	BCL	CAB-C3B-C2B	2.05	132.00	127.74
17	C	1001	HEC	C2A-C1A-NA	-2.05	108.35	110.32
16	H1	102	0V9	O2-C10-O4	-2.05	118.92	123.70
13	BE	104	BCL	OBb-CAB-CBB	-2.05	115.19	119.77
15	BJ	1001	V7N	O45-C40-C39	2.05	127.37	122.09
15	AW	103	V7N	O45-C40-C39	2.05	127.37	122.09
13	bl	104	BCL	OBb-CAB-CBB	-2.05	115.19	119.77
16	bi	103	0V9	O3P-P-O2P	2.05	117.04	108.94
15	bi	101	V7N	C36-C18-C17	-2.04	119.50	122.82
14	BP	1006	LMT	C1'-O5'-C5'	-2.04	109.73	113.72
13	AB	1002	BCL	CAA-CBA-CGA	2.04	119.01	113.21
14	BK	1004	LMT	C2'-C3'-C4'	2.04	114.31	109.68
16	be	105	0V9	O2-C10-O4	-2.04	118.93	123.70
13	AC	101	BCL	CMB-C2B-C1B	-2.04	122.31	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BG	1001	V7N	O45-C40-C39	2.04	127.35	122.09
14	BJ	1005	LMT	C1'-O5'-C5'	-2.04	109.74	113.72
13	bh	103	BCL	C1-O2A-CGA	2.04	121.59	116.65
15	bn	101	V7N	C2-C3-C4	-2.04	122.05	124.91
13	AF	1001	BCL	CMB-C2B-C1B	-2.04	122.31	125.42
13	BG	1004	BCL	OBB-CAB-CBB	-2.04	115.20	119.77
15	bj	101	V7N	O45-C40-C39	2.04	127.35	122.09
13	AU	103	BCL	CAC-C3C-C4C	2.04	117.11	112.58
13	bd	102	BCL	C1C-NC-C4C	2.04	107.61	106.68
13	bb	102	BCL	OBB-CAB-CBB	-2.04	115.21	119.77
15	BR	1001	V7N	C36-C18-C17	-2.04	119.52	122.82
13	BQ	1004	BCL	C1-C2-C3	2.04	129.53	126.20
14	AX	101	LMT	O5B-C5B-C6B	2.04	111.48	106.44
15	ba	101	V7N	C36-C18-C17	-2.04	119.52	122.82
14	AN	101	LMT	O5'-C5'-C4'	2.04	113.93	109.72
15	BG	1001	V7N	C20-C21-C22	-2.04	124.83	127.69
15	bi	101	V7N	O45-C40-C39	2.03	127.34	122.09
13	AM	1002	BCL	CAB-C3B-C2B	2.03	131.97	127.74
26	ag	103	V7B	O8-C28-C29	2.03	118.04	111.83
14	BV	1002	LMT	C1'-O5'-C5'	-2.03	109.75	113.72
15	AA	1004	V7N	C33-C5-C4	2.03	121.19	118.09
15	bb	101	V7N	C29-C28-C27	-2.03	117.31	123.20
13	AQ	104	BCL	O2D-CGD-O1D	-2.03	119.89	123.85
13	BU	1004	BCL	CMB-C2B-C1B	-2.03	122.33	125.42
13	AW	102	BCL	C6-C5-C3	2.03	118.41	113.47
15	BK	1001	V7N	C35-C13-C12	2.03	121.19	118.09
13	bc	103	BCL	OBB-CAB-CBB	-2.03	115.23	119.77
19	C1	301	NDG	O4-C4-C3	-2.03	105.59	110.38
13	ac	102	BCL	CAB-C3B-C2B	2.03	131.96	127.74
15	bn	101	V7N	C35-C13-C12	2.03	121.18	118.09
14	bo	104	LMT	C3'-C4'-C5'	-2.03	106.44	110.93
13	BA	103	BCL	OBB-CAB-CBB	-2.03	115.23	119.77
15	bh	101	V7N	C35-C13-C14	-2.03	119.53	122.82
15	BF	101	V7N	O45-C40-C39	2.02	127.31	122.09
13	M	408	BCL	CAB-C3B-C2B	2.02	131.94	127.74
15	BA	101	V7N	C11-C10-C9	2.02	129.89	127.28
16	bi	103	OV9	O2-C10-O4	-2.02	118.98	123.70
14	BM	1005	LMT	C1'-O5'-C5'	-2.02	109.77	113.72
14	BP	1002	LMT	O5B-C5B-C4B	2.02	113.34	109.70
16	bp	105	OV9	O3P-P-O2P	2.02	116.92	108.94
13	BN	1005	BCL	CMB-C2B-C1B	-2.01	122.35	125.42
15	BF	101	V7N	C35-C13-C12	2.01	121.17	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	406	BCL	C11-C10-C8	-2.01	109.27	115.97
14	BE	103	LMT	C1'-O5'-C5'	-2.01	109.79	113.72
14	bh	102	LMT	C1-O1'-C1'	2.01	117.12	113.68
14	BC	103	LMT	O5B-C5B-C4B	2.01	113.33	109.70
14	BD	105	LMT	C1'-O5'-C5'	-2.01	109.79	113.72
14	BE	105	LMT	C1'-O5'-C5'	-2.01	109.79	113.72
14	bc	102	LMT	O5B-C5B-C4B	2.01	113.32	109.70
13	ah	1001	BCL	CAB-C3B-C2B	2.01	131.92	127.74
13	ao	102	BCL	CAB-C3B-C2B	2.01	131.91	127.74
14	BV	1004	LMT	O5B-C5B-C4B	2.01	113.31	109.70
14	be	101	LMT	C2'-C3'-C4'	2.01	114.23	109.68
26	af	101	V7B	C3-C4-C5	-2.00	106.49	110.93
16	bi	103	OV9	O3-C30-O5	-2.00	118.61	123.63
14	BL	101	LMT	C1'-O5'-C5'	-2.00	109.81	113.72
13	bn	102	BCL	OBB-CAB-CBB	-2.00	115.28	119.77
15	bj	101	V7N	C20-C21-C22	-2.00	124.87	127.69
15	BK	1001	V7N	O45-C40-C39	2.00	127.25	122.09
13	M	406	BCL	OBB-CAB-CBB	-2.00	115.29	119.77
14	AH	101	LMT	O1'-C1'-C2'	2.00	111.31	108.27
13	bd	102	BCL	C1-O2A-CGA	-2.00	111.81	116.65

There are no chirality outliers.

All (1836) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	AE	103	BCL	C3A-C2A-CAA-CBA
13	AE	105	BCL	C1A-C2A-CAA-CBA
13	AH	102	BCL	C1A-C2A-CAA-CBA
13	AH	102	BCL	C3A-C2A-CAA-CBA
13	AH	105	BCL	C1A-C2A-CAA-CBA
13	AH	105	BCL	C3A-C2A-CAA-CBA
13	AJ	103	BCL	C1A-C2A-CAA-CBA
13	AJ	103	BCL	C3A-C2A-CAA-CBA
13	AJ	103	BCL	C4C-C3C-CAC-CBC
13	AO	101	BCL	C1A-C2A-CAA-CBA
13	AO	101	BCL	C3A-C2A-CAA-CBA
13	AP	103	BCL	C1A-C2A-CAA-CBA
13	AQ	102	BCL	C1A-C2A-CAA-CBA
13	AQ	102	BCL	C3A-C2A-CAA-CBA
13	AQ	104	BCL	CBD-CGD-O2D-CED
13	AW	102	BCL	C1A-C2A-CAA-CBA
13	AW	102	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AX	103	BCL	C1A-C2A-CAA-CBA
13	BA	103	BCL	C1A-C2A-CAA-CBA
13	BF	103	BCL	C1A-C2A-CAA-CBA
13	BF	103	BCL	C3A-C2A-CAA-CBA
13	BG	1004	BCL	C1A-C2A-CAA-CBA
13	BG	1004	BCL	C3A-C2A-CAA-CBA
13	BJ	1004	BCL	C1A-C2A-CAA-CBA
13	BJ	1004	BCL	C3A-C2A-CAA-CBA
13	BO	1003	BCL	C1A-C2A-CAA-CBA
13	BS	1004	BCL	C1A-C2A-CAA-CBA
13	BU	1004	BCL	C1A-C2A-CAA-CBA
13	BU	1004	BCL	C3A-C2A-CAA-CBA
13	BW	1005	BCL	C1A-C2A-CAA-CBA
13	bc	103	BCL	C1A-C2A-CAA-CBA
13	bc	103	BCL	C3A-C2A-CAA-CBA
13	bj	104	BCL	C3A-C2A-CAA-CBA
13	bk	103	BCL	C1A-C2A-CAA-CBA
13	bk	103	BCL	C3A-C2A-CAA-CBA
13	bm	102	BCL	C1A-C2A-CAA-CBA
13	bn	102	BCL	C1A-C2A-CAA-CBA
13	bn	102	BCL	C3A-C2A-CAA-CBA
14	AH	101	LMT	C2'-C1'-O1'-C1
14	AK	101	LMT	O5'-C1'-O1'-C1
14	AP	101	LMT	C2'-C1'-O1'-C1
14	AS	103	LMT	O5'-C1'-O1'-C1
14	AT	104	LMT	C2'-C1'-O1'-C1
14	AT	104	LMT	O5'-C1'-O1'-C1
14	AT	104	LMT	C2-C1-O1'-C1'
14	AV	104	LMT	O5'-C1'-O1'-C1
14	AV	104	LMT	C2-C1-O1'-C1'
14	BA	102	LMT	C2-C1-O1'-C1'
14	BF	102	LMT	C2'-C1'-O1'-C1
14	BF	102	LMT	O5'-C1'-O1'-C1
14	BF	102	LMT	C2-C1-O1'-C1'
14	BI	1002	LMT	C2-C1-O1'-C1'
14	BS	1003	LMT	C2-C1-O1'-C1'
14	BT	104	LMT	C2-C1-O1'-C1'
14	BU	1003	LMT	C2'-C1'-O1'-C1
14	BU	1003	LMT	O5'-C1'-O1'-C1
14	bh	102	LMT	C2-C1-O1'-C1'
14	bm	103	LMT	C2'-C1'-O1'-C1
14	bm	103	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bp	103	LMT	C2'-C1'-O1'-C1
14	bp	103	LMT	O5'-C1'-O1'-C1
15	AA	1004	V7N	C25-C26-C27-C28
15	AD	101	V7N	O42-C34-C9-C10
15	AM	1001	V7N	C27-C28-C29-C39
15	AS	104	V7N	C25-C26-C27-C28
15	AS	104	V7N	C38-C26-C27-C28
15	AS	104	V7N	C27-C28-C29-C39
15	AW	103	V7N	C25-C26-C27-C28
15	AW	103	V7N	C38-C26-C27-C28
15	BE	101	V7N	C25-C26-C27-C28
15	BF	101	V7N	C31-C1-O32-C41
15	BF	101	V7N	C21-C22-C23-C24
15	BF	101	V7N	C37-C22-C23-C24
15	BF	101	V7N	C25-C26-C27-C28
15	BF	101	V7N	C38-C26-C27-C28
15	BF	101	V7N	C27-C28-C29-C39
15	BG	1001	V7N	C25-C26-C27-C28
15	BH	1001	V7N	C25-C26-C27-C28
15	BH	1001	V7N	O42-C34-C9-C10
15	BI	1001	V7N	C25-C26-C27-C28
15	BJ	1001	V7N	C25-C26-C27-C28
15	BK	1001	V7N	C27-C28-C29-C39
15	BN	1001	V7N	C1-C2-C3-C4
15	BN	1001	V7N	C25-C26-C27-C28
15	BN	1001	V7N	C38-C26-C27-C28
15	BN	1001	V7N	C27-C28-C29-C39
15	BQ	1001	V7N	C27-C28-C29-C39
15	BR	1001	V7N	C27-C28-C29-C39
15	BS	1001	V7N	C25-C26-C27-C28
15	BU	1001	V7N	O42-C34-C9-C10
15	BV	1001	V7N	C25-C26-C27-C28
15	BV	1001	V7N	C38-C26-C27-C28
15	BV	1001	V7N	C26-C27-C28-C29
15	BV	1001	V7N	C27-C28-C29-C39
15	ag	101	V7N	C25-C26-C27-C28
15	ag	101	V7N	C38-C26-C27-C28
15	ba	101	V7N	C27-C28-C29-C39
15	bb	101	V7N	C25-C26-C27-C28
15	bb	101	V7N	C38-C26-C27-C28
15	bb	101	V7N	C27-C28-C29-C39
15	bc	101	V7N	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bc	101	V7N	C27-C28-C29-C39
15	bd	101	V7N	C26-C27-C28-C29
15	be	102	V7N	O42-C34-C9-C10
15	bh	101	V7N	C25-C26-C27-C28
15	bh	101	V7N	C38-C26-C27-C28
15	bi	101	V7N	C26-C27-C28-C29
15	bj	101	V7N	C25-C26-C27-C28
15	bj	101	V7N	C38-C26-C27-C28
15	bk	101	V7N	C27-C28-C29-C39
15	bl	101	V7N	C25-C26-C27-C28
15	bm	101	V7N	C25-C26-C27-C28
15	bm	101	V7N	C38-C26-C27-C28
15	bn	101	V7N	C27-C28-C29-C39
15	bo	101	V7N	O32-C1-C2-C3
16	AQ	105	0V9	C1-O3P-P-O1P
16	AQ	105	0V9	C1-O3P-P-O2P
16	AQ	105	0V9	C1-O3P-P-O4P
16	L	310	0V9	C5-C4-O4P-P
16	L	310	0V9	C1-O3P-P-O4P
16	M	403	0V9	C2-C1-O3P-P
16	M	403	0V9	C1-O3P-P-O2P
16	M	403	0V9	C1-O3P-P-O4P
16	bb	103	0V9	C2-C1-O3P-P
16	bb	103	0V9	C5-C4-O4P-P
16	be	105	0V9	C5-C4-O4P-P
16	bf	103	0V9	C2-C1-O3P-P
16	bf	103	0V9	C1-O3P-P-O4P
16	bh	104	0V9	C2-C1-O3P-P
16	bh	104	0V9	C1-O3P-P-O1P
16	bi	103	0V9	O2-C2-C3-O3
16	bi	103	0V9	C4-O4P-P-O2P
16	bi	103	0V9	C4-O4P-P-O3P
16	bj	103	0V9	C2-C1-O3P-P
16	bj	103	0V9	C5-C4-O4P-P
16	bj	103	0V9	C1-O3P-P-O1P
16	bj	103	0V9	C4-O4P-P-O3P
16	bk	102	0V9	C2-C1-O3P-P
16	bk	102	0V9	C1-O3P-P-O1P
16	bl	102	0V9	O2-C2-C3-O3
16	bl	102	0V9	C2-C1-O3P-P
16	bl	102	0V9	C5-C4-O4P-P
16	bl	102	0V9	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	bm	104	0V9	O2-C2-C3-O3
16	bm	104	0V9	C2-C1-O3P-P
16	bn	104	0V9	C2-C1-O3P-P
16	bn	104	0V9	C5-C4-O4P-P
16	bn	104	0V9	C4-O4P-P-O1P
16	bn	104	0V9	C4-O4P-P-O3P
16	bo	103	0V9	O2-C2-C3-O3
16	bo	103	0V9	C5-C4-O4P-P
16	bo	103	0V9	C4-O4P-P-O2P
16	bo	103	0V9	C4-O4P-P-O3P
17	C	1001	HEC	C2B-C3B-CAB-CBB
17	C	1001	HEC	C4B-C3B-CAB-CBB
17	C	1001	HEC	C2C-C3C-CAC-CBC
17	C	1001	HEC	C4C-C3C-CAC-CBC
17	C	1002	HEC	C2B-C3B-CAB-CBB
17	C	1002	HEC	C4B-C3B-CAB-CBB
17	C	1002	HEC	C2C-C3C-CAC-CBC
17	C	1002	HEC	C4C-C3C-CAC-CBC
17	C	1003	HEC	C2B-C3B-CAB-CBB
17	C	1003	HEC	C4B-C3B-CAB-CBB
17	C	1003	HEC	C2C-C3C-CAC-CBC
17	C	1003	HEC	C4C-C3C-CAC-CBC
17	C	1004	HEC	C2B-C3B-CAB-CBB
17	C	1004	HEC	C4B-C3B-CAB-CBB
17	C	1004	HEC	C2C-C3C-CAC-CBC
17	C	1004	HEC	C4C-C3C-CAC-CBC
20	H1	101	PGW	C03-O11-P-O14
21	H1	103	CD4	C29-O8-P1-O5
21	H1	103	CD4	C29-O8-P1-O6
21	H1	103	CD4	C29-O8-P1-O7
21	H1	103	CD4	C29-C30-C31-O10
21	H1	103	CD4	O9-C30-C31-O10
21	M	405	CD4	C13-C14-O2-C15
21	M	405	CD4	C16-C15-O2-C14
21	M	405	CD4	C30-C31-O10-P2
21	M	409	CD4	C13-C14-O2-C15
21	ad	101	CD4	C29-O8-P1-O7
21	ad	101	CD4	C31-O10-P2-O12
21	ad	101	CD4	C31-O10-P2-O13
21	af	102	CD4	O1-C14-O2-C15
21	af	102	CD4	O2-C15-C28-O5
21	af	102	CD4	C30-C29-O8-P1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	af	102	CD4	C31-O10-P2-O12
21	af	102	CD4	O16-C33-C34-O14
21	af	104	CD4	C13-C14-O2-C15
21	af	104	CD4	C31-O10-P2-O11
21	af	104	CD4	C31-O10-P2-O12
21	af	104	CD4	C31-O10-P2-O13
23	L	303	MQ8	C12-C11-C3-C2
23	L	303	MQ8	C12-C11-C3-C4
25	M	404	CRT	C36-C37-C38-O2
26	af	101	V7B	O6-C1-O1-C7
13	AQ	104	BCL	O1D-CGD-O2D-CED
14	BL	102	LMT	O5B-C1B-O1B-C4'
14	bl	103	LMT	O5B-C1B-O1B-C4'
14	bn	103	LMT	O5B-C1B-O1B-C4'
14	bp	103	LMT	O5B-C1B-O1B-C4'
14	BP	1002	LMT	O5B-C1B-O1B-C4'
21	M	409	CD4	O1-C14-O2-C15
21	af	104	CD4	O1-C14-O2-C15
13	AE	103	BCL	C3-C5-C6-C7
13	AK	102	BCL	C3-C5-C6-C7
13	bp	104	BCL	C3-C5-C6-C7
21	af	102	CD4	C13-C14-O2-C15
14	AK	103	LMT	O5B-C1B-O1B-C4'
14	BX	102	LMT	O5B-C1B-O1B-C4'
14	bf	101	LMT	O5B-C1B-O1B-C4'
14	AG	101	LMT	O5B-C1B-O1B-C4'
14	bf	101	LMT	C2B-C1B-O1B-C4'
13	BJ	1004	BCL	C3-C5-C6-C7
14	AK	103	LMT	C2B-C1B-O1B-C4'
15	BD	101	V7N	C27-C28-C29-C39
15	BU	1001	V7N	C27-C28-C29-C39
21	M	405	CD4	O1-C14-O2-C15
13	bd	102	BCL	C3-C5-C6-C7
21	M	409	CD4	O9-C30-C31-O10
14	BW	1003	LMT	O5'-C5'-C6'-O6'
14	AE	102	LMT	O5'-C5'-C6'-O6'
14	AH	101	LMT	O5'-C5'-C6'-O6'
14	AV	102	LMT	C4'-C5'-C6'-O6'
14	BJ	1005	LMT	O5B-C1B-O1B-C4'
14	C2	1001	LMT	O5B-C1B-O1B-C4'
13	AV	101	BCL	C3-C5-C6-C7
14	AK	103	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	AN	101	LMT	O5B-C5B-C6B-O6B
14	AN	102	LMT	O5'-C5'-C6'-O6'
14	AV	102	LMT	O5'-C5'-C6'-O6'
14	BJ	1003	LMT	O5'-C5'-C6'-O6'
14	BP	1004	LMT	O5'-C5'-C6'-O6'
14	BQ	1002	LMT	O5'-C5'-C6'-O6'
15	BV	1001	V7N	C22-C23-C24-C25
23	L	303	MQ8	C18-C20-C21-C22
23	ao	101	MQ8	C13-C15-C16-C17
14	BM	1003	LMT	C4'-C5'-C6'-O6'
14	BO	1005	LMT	C2B-C1B-O1B-C4'
16	bp	105	0V9	C2-C1-O3P-P
14	BL	101	LMT	O5'-C5'-C6'-O6'
26	af	101	V7B	O52-C47-C48-O53
14	BM	1005	LMT	O5B-C1B-O1B-C4'
14	BO	1005	LMT	O5B-C1B-O1B-C4'
16	bi	103	0V9	C11-C12-C13-C14
14	AG	101	LMT	O5'-C1'-O1'-C1
14	AH	101	LMT	O5'-C1'-O1'-C1
14	AP	101	LMT	O5'-C1'-O1'-C1
14	BJ	1005	LMT	O5'-C1'-O1'-C1
14	BL	101	LMT	O5'-C1'-O1'-C1
14	BM	1003	LMT	O5'-C1'-O1'-C1
14	BU	1002	LMT	O5'-C1'-O1'-C1
14	BX	102	LMT	O5'-C1'-O1'-C1
14	be	104	LMT	O5'-C1'-O1'-C1
14	bh	102	LMT	O5'-C1'-O1'-C1
14	bl	103	LMT	O5'-C1'-O1'-C1
26	ag	103	V7B	O6-C1-O1-C7
14	BA	102	LMT	O5'-C5'-C6'-O6'
14	BF	102	LMT	O5'-C5'-C6'-O6'
14	BW	1004	LMT	O5'-C5'-C6'-O6'
26	ag	103	V7B	O52-C47-C48-O53
14	BW	1003	LMT	C4'-C5'-C6'-O6'
14	AE	106	LMT	O5B-C1B-O1B-C4'
14	BS	1003	LMT	O5B-C1B-O1B-C4'
15	AA	1004	V7N	C27-C28-C29-C39
15	BA	101	V7N	C27-C28-C29-C39
14	bc	102	LMT	C3'-C4'-O1B-C1B
14	BD	102	LMT	O5B-C1B-O1B-C4'
16	bk	102	0V9	C11-C12-C13-C14
14	AN	102	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AI	101	BCL	C4-C3-C5-C6
13	AI	101	BCL	C2-C3-C5-C6
13	AH	105	BCL	C6-C7-C8-C9
13	AS	101	BCL	C14-C13-C15-C16
13	BJ	1004	BCL	C11-C12-C13-C14
13	BS	1004	BCL	C11-C10-C8-C9
13	BU	1004	BCL	C6-C7-C8-C9
13	BU	1004	BCL	C11-C10-C8-C9
13	ad	102	BCL	C6-C7-C8-C9
13	ag	102	BCL	C11-C10-C8-C9
13	aj	101	BCL	C6-C7-C8-C9
13	an	1001	BCL	C11-C10-C8-C9
13	bf	102	BCL	C11-C12-C13-C14
14	AA	1003	LMT	C2'-C1'-O1'-C1
14	AG	101	LMT	C2'-C1'-O1'-C1
14	AS	103	LMT	C2'-C1'-O1'-C1
14	AV	104	LMT	C2'-C1'-O1'-C1
14	BL	101	LMT	C2'-C1'-O1'-C1
14	BU	1002	LMT	C2'-C1'-O1'-C1
14	BW	1004	LMT	C2'-C1'-O1'-C1
14	be	104	LMT	C2'-C1'-O1'-C1
14	bh	102	LMT	C2'-C1'-O1'-C1
14	bl	103	LMT	C2'-C1'-O1'-C1
14	bc	102	LMT	O5'-C5'-C6'-O6'
14	BW	1004	LMT	C4'-C5'-C6'-O6'
14	BX	103	LMT	O5B-C1B-O1B-C4'
15	AA	1004	V7N	C38-C26-C27-C28
15	AD	101	V7N	C38-C26-C27-C28
15	AM	1001	V7N	C38-C26-C27-C28
15	BE	101	V7N	C38-C26-C27-C28
15	BG	1001	V7N	C38-C26-C27-C28
15	BH	1001	V7N	C38-C26-C27-C28
15	BH	1001	V7N	C3-C4-C5-C33
15	BI	1001	V7N	C38-C26-C27-C28
15	BI	1001	V7N	C3-C4-C5-C33
15	BJ	1001	V7N	C38-C26-C27-C28
15	BK	1001	V7N	C38-C26-C27-C28
15	BM	1001	V7N	C38-C26-C27-C28
15	BO	1001	V7N	C38-C26-C27-C28
15	BO	1001	V7N	C3-C4-C5-C33
15	BP	1001	V7N	C38-C26-C27-C28
15	BR	1001	V7N	C38-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	BS	1001	V7N	C38-C26-C27-C28
15	BU	1001	V7N	C38-C26-C27-C28
15	ba	101	V7N	C38-C26-C27-C28
15	bc	101	V7N	C38-C26-C27-C28
15	bg	101	V7N	C38-C26-C27-C28
15	bi	101	V7N	C38-C26-C27-C28
15	bl	101	V7N	C38-C26-C27-C28
15	bo	101	V7N	C38-C26-C27-C28
15	bp	102	V7N	C38-C26-C27-C28
14	BI	1005	LMT	O5'-C5'-C6'-O6'
14	H2	201	LMT	O5'-C5'-C6'-O6'
15	AD	101	V7N	C25-C26-C27-C28
15	AM	1001	V7N	C25-C26-C27-C28
15	BH	1001	V7N	C3-C4-C5-C6
15	BI	1001	V7N	C3-C4-C5-C6
15	BK	1001	V7N	C25-C26-C27-C28
15	BM	1001	V7N	C25-C26-C27-C28
15	BN	1001	V7N	C3-C4-C5-C6
15	BO	1001	V7N	C25-C26-C27-C28
15	BO	1001	V7N	C3-C4-C5-C6
15	BP	1001	V7N	C25-C26-C27-C28
15	BR	1001	V7N	C25-C26-C27-C28
15	BU	1001	V7N	C25-C26-C27-C28
15	ba	101	V7N	C25-C26-C27-C28
15	bd	101	V7N	C25-C26-C27-C28
15	bg	101	V7N	C25-C26-C27-C28
15	bi	101	V7N	C25-C26-C27-C28
15	bo	101	V7N	C25-C26-C27-C28
15	bp	102	V7N	C25-C26-C27-C28
13	BP	1003	BCL	O1A-CGA-O2A-C1
13	AF	1001	BCL	C3-C5-C6-C7
14	AN	101	LMT	O5'-C5'-C6'-O6'
14	BM	1003	LMT	O5'-C5'-C6'-O6'
14	bf	101	LMT	O5'-C5'-C6'-O6'
14	bg	102	LMT	O5'-C5'-C6'-O6'
14	bp	103	LMT	C3'-C4'-O1B-C1B
14	AE	101	LMT	O5B-C5B-C6B-O6B
14	AT	102	LMT	O5B-C5B-C6B-O6B
14	BG	1003	LMT	O5'-C5'-C6'-O6'
14	BX	103	LMT	O5'-C5'-C6'-O6'
16	ab	1002	0V9	O2-C2-C3-O3
16	bk	102	0V9	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	ai	102	UYH	O7-C8-C9-O8
14	BM	1005	LMT	C2B-C1B-O1B-C4'
14	AJ	101	LMT	C4'-C5'-C6'-O6'
14	AN	102	LMT	C4'-C5'-C6'-O6'
13	AI	101	BCL	C10-C11-C12-C13
13	AC	102	BCL	C3-C5-C6-C7
13	ae	1001	BCL	C3-C5-C6-C7
14	AE	106	LMT	C2B-C1B-O1B-C4'
13	ak	1001	BCL	C10-C11-C12-C13
14	BL	102	LMT	C5'-C4'-O1B-C1B
14	BN	1003	LMT	O5'-C5'-C6'-O6'
14	AJ	101	LMT	O5'-C5'-C6'-O6'
14	BX	102	LMT	O5'-C5'-C6'-O6'
26	ag	103	V7B	C29-C30-C31-C32
13	aj	101	BCL	C8-C10-C11-C12
15	bg	101	V7N	C27-C28-C29-C39
15	bi	101	V7N	C22-C23-C24-C25
26	ag	103	V7B	C46-C47-C48-O53
14	BD	103	LMT	O5'-C5'-C6'-O6'
14	BS	1002	LMT	O5B-C5B-C6B-O6B
14	bm	103	LMT	O5B-C5B-C6B-O6B
14	bm	103	LMT	C4B-C5B-C6B-O6B
13	BM	1004	BCL	C8-C10-C11-C12
16	AQ	105	0V9	C2-C1-O3P-P
14	AE	102	LMT	O5B-C5B-C6B-O6B
14	AJ	102	LMT	O5'-C5'-C6'-O6'
14	BO	1004	LMT	O5'-C5'-C6'-O6'
14	BD	106	LMT	C5'-C4'-O1B-C1B
13	AF	1001	BCL	C13-C15-C16-C17
14	AA	1003	LMT	O5'-C1'-O1'-C1
14	BW	1004	LMT	O5'-C1'-O1'-C1
14	H2	201	LMT	O5'-C1'-O1'-C1
14	bk	104	LMT	O5'-C5'-C6'-O6'
13	AT	103	BCL	C8-C10-C11-C12
14	AM	1003	LMT	O5B-C1B-O1B-C4'
14	BE	103	LMT	O5B-C1B-O1B-C4'
13	AJ	103	BCL	C13-C15-C16-C17
14	BF	104	LMT	O5'-C5'-C6'-O6'
14	BP	1002	LMT	O5B-C5B-C6B-O6B
14	BD	103	LMT	O1'-C1-C2-C3
14	AE	102	LMT	C4'-C5'-C6'-O6'
14	BM	1002	LMT	O1'-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	AC	103	LMT	O5B-C5B-C6B-O6B
16	bg	103	0V9	C10-C11-C12-C13
14	AP	101	LMT	O5B-C1B-O1B-C4'
15	AD	101	V7N	C27-C28-C29-C39
15	BO	1001	V7N	C27-C28-C29-C39
13	bc	103	BCL	C5-C6-C7-C8
13	AQ	104	BCL	C2A-CAA-CBA-CGA
13	AF	1001	BCL	C10-C11-C12-C13
13	AQ	103	BCL	C15-C16-C17-C18
13	AS	102	BCL	C8-C10-C11-C12
13	AS	102	BCL	C10-C11-C12-C13
13	AU	101	BCL	C10-C11-C12-C13
13	BD	104	BCL	C5-C6-C7-C8
13	ae	1001	BCL	C13-C15-C16-C17
13	ae	1001	BCL	C15-C16-C17-C18
13	be	103	BCL	C15-C16-C17-C18
14	BV	1004	LMT	O1'-C1-C2-C3
13	AQ	104	BCL	C15-C16-C17-C18
13	BG	1004	BCL	C10-C11-C12-C13
14	AK	103	LMT	O5B-C5B-C6B-O6B
14	AU	102	LMT	O5B-C5B-C6B-O6B
14	BH	1002	LMT	O1'-C1-C2-C3
13	AA	1001	BCL	C13-C15-C16-C17
13	BG	1004	BCL	C13-C15-C16-C17
13	aa	1001	BCL	C8-C10-C11-C12
14	BE	105	LMT	O5B-C1B-O1B-C4'
13	AP	103	BCL	C3-C5-C6-C7
13	AT	103	BCL	C11-C12-C13-C14
14	L	309	LMT	O5'-C5'-C6'-O6'
14	BM	1003	LMT	C2'-C1'-O1'-C1
14	BX	102	LMT	C2'-C1'-O1'-C1
14	H2	201	LMT	C2'-C1'-O1'-C1
13	AJ	104	BCL	C10-C11-C12-C13
14	AS	103	LMT	O1'-C1-C2-C3
15	BA	101	V7N	C38-C26-C27-C28
15	BD	101	V7N	C38-C26-C27-C28
15	BN	1001	V7N	C3-C4-C5-C33
15	BQ	1001	V7N	C38-C26-C27-C28
15	BW	1001	V7N	C38-C26-C27-C28
15	BW	1001	V7N	C3-C4-C5-C33
15	ag	101	V7N	C3-C4-C5-C33
15	bd	101	V7N	C38-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bk	101	V7N	C3-C4-C5-C33
15	bn	101	V7N	C38-C26-C27-C28
14	AM	1003	LMT	O5'-C5'-C6'-O6'
14	BK	1003	LMT	O5'-C5'-C6'-O6'
15	BA	101	V7N	C25-C26-C27-C28
15	BQ	1001	V7N	C25-C26-C27-C28
15	BW	1001	V7N	C25-C26-C27-C28
15	bk	101	V7N	C3-C4-C5-C6
15	bn	101	V7N	C25-C26-C27-C28
13	BB	105	BCL	C2A-CAA-CBA-CGA
13	BW	1005	BCL	C2A-CAA-CBA-CGA
13	bd	102	BCL	C2A-CAA-CBA-CGA
13	AO	102	BCL	C10-C11-C12-C13
14	AB	1003	LMT	O5'-C1'-O1'-C1
14	BD	106	LMT	O5'-C1'-O1'-C1
14	BG	1002	LMT	O5'-C1'-O1'-C1
14	bc	102	LMT	C5'-C4'-O1B-C1B
14	bp	103	LMT	C5'-C4'-O1B-C1B
13	BP	1003	BCL	CBA-CGA-O2A-C1
14	AN	102	LMT	C5'-C4'-O1B-C1B
13	ad	102	BCL	C15-C16-C17-C18
13	bg	104	BCL	C15-C16-C17-C18
14	BU	1002	LMT	O1'-C1-C2-C3
13	AH	102	BCL	C3-C5-C6-C7
14	BD	105	LMT	O5B-C1B-O1B-C4'
13	BL	103	BCL	C2-C1-O2A-CGA
13	bh	103	BCL	C2-C1-O2A-CGA
14	BX	104	LMT	O5'-C5'-C6'-O6'
14	BT	104	LMT	C1-C2-C3-C4
14	BI	1003	LMT	O5'-C5'-C6'-O6'
14	AN	101	LMT	C4B-C5B-C6B-O6B
14	AJ	102	LMT	C6-C7-C8-C9
14	AP	101	LMT	C5-C6-C7-C8
14	BJ	1003	LMT	C2-C3-C4-C5
14	BS	1002	LMT	C7-C8-C9-C10
14	L	306	LMT	C3-C4-C5-C6
16	bb	103	OV9	C39-C40-C41-C42
14	BU	1002	LMT	O5'-C5'-C6'-O6'
14	BK	1003	LMT	C2-C1-O1'-C1'
14	BK	1005	LMT	C2-C1-O1'-C1'
14	BN	1004	LMT	C2-C1-O1'-C1'
14	BO	1004	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BP	1005	LMT	C2-C1-O1'-C1'
14	BW	1002	LMT	C2-C1-O1'-C1'
14	BX	102	LMT	C2-C1-O1'-C1'
14	C2	1001	LMT	C2-C1-O1'-C1'
14	L	307	LMT	C2-C1-O1'-C1'
14	ac	101	LMT	C2-C1-O1'-C1'
14	BL	101	LMT	C5-C6-C7-C8
21	af	102	CD4	C50-C51-C52-C53
14	BU	1003	LMT	O1'-C1-C2-C3
14	bn	103	LMT	O5B-C5B-C6B-O6B
16	bb	103	OV9	C15-C16-C17-C18
14	L	304	LMT	C6-C7-C8-C9
13	AG	102	BCL	C13-C15-C16-C17
13	AR	101	BCL	C15-C16-C17-C18
13	bg	104	BCL	C11-C12-C13-C15
16	M	403	OV9	C14-C15-C16-C17
13	al	1001	BCL	C13-C15-C16-C17
26	af	101	V7B	C46-C47-C48-O53
13	AE	105	BCL	C3A-C2A-CAA-CBA
13	AX	103	BCL	C3A-C2A-CAA-CBA
13	BA	103	BCL	C3A-C2A-CAA-CBA
13	BO	1003	BCL	C3A-C2A-CAA-CBA
13	BS	1004	BCL	C3A-C2A-CAA-CBA
13	BW	1005	BCL	C3A-C2A-CAA-CBA
13	BX	101	BCL	C3A-C2A-CAA-CBA
13	bd	102	BCL	C3A-C2A-CAA-CBA
13	bg	104	BCL	C3A-C2A-CAA-CBA
13	bm	102	BCL	C3A-C2A-CAA-CBA
14	AL	101	LMT	O5'-C5'-C6'-O6'
13	AD	104	BCL	C8-C10-C11-C12
13	ab	1001	BCL	C8-C10-C11-C12
14	BJ	1003	LMT	C4'-C5'-C6'-O6'
15	BI	1001	V7N	C27-C28-C29-C39
13	bb	102	BCL	C16-C17-C18-C20
14	BE	102	LMT	C5'-C4'-O1B-C1B
14	BA	102	LMT	C1-C2-C3-C4
14	BC	103	LMT	C5-C6-C7-C8
21	ad	101	CD4	C3-C4-C5-C6
14	BP	1006	LMT	O5B-C1B-O1B-C4'
13	ah	1001	BCL	C13-C15-C16-C17
14	bm	103	LMT	C4-C5-C6-C7
21	M	409	CD4	C29-C30-C31-O10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BK	1005	LMT	C4-C5-C6-C7
14	bk	104	LMT	C4-C5-C6-C7
13	AA	1002	BCL	C3-C5-C6-C7
13	AB	1001	BCL	C8-C10-C11-C12
13	BK	1002	BCL	C5-C6-C7-C8
13	bk	103	BCL	C15-C16-C17-C18
14	AD	102	LMT	C4-C5-C6-C7
14	bc	102	LMT	C11-C10-C9-C8
14	bk	104	LMT	O1'-C1-C2-C3
14	AH	101	LMT	C4'-C5'-C6'-O6'
14	BL	102	LMT	C3'-C4'-O1B-C1B
14	BQ	1003	LMT	C6-C7-C8-C9
21	af	102	CD4	C25-C26-C27-C60
13	am	1001	BCL	C16-C17-C18-C19
14	BO	1002	LMT	O1'-C1-C2-C3
14	AV	104	LMT	C5'-C4'-O1B-C1B
14	AG	101	LMT	C4-C5-C6-C7
16	bf	103	OV9	C19-C20-C21-C22
20	H1	101	PGW	C10-C06-C07-C08
13	BN	1005	BCL	C15-C16-C17-C18
13	BG	1004	BCL	C3-C5-C6-C7
13	ba	102	BCL	C3-C5-C6-C7
21	H1	103	CD4	C25-C26-C27-C60
13	ap	1001	BCL	C10-C11-C12-C13
14	L	306	LMT	O5'-C5'-C6'-O6'
14	BI	1002	LMT	O5B-C1B-O1B-C4'
14	BF	102	LMT	C4-C5-C6-C7
15	BM	1001	V7N	C26-C27-C28-C29
15	BW	1001	V7N	C26-C27-C28-C29
15	be	102	V7N	C26-C27-C28-C29
15	bn	101	V7N	C26-C27-C28-C29
13	be	103	BCL	C10-C11-C12-C13
21	M	409	CD4	C46-C47-C48-C49
13	AE	103	BCL	C11-C12-C13-C14
13	AO	101	BCL	C6-C7-C8-C9
14	bl	103	LMT	C5'-C4'-O1B-C1B
14	BO	1004	LMT	C2-C3-C4-C5
13	bi	102	BCL	C8-C10-C11-C12
26	af	101	V7B	C29-C30-C31-C32
14	BP	1004	LMT	O5'-C1'-O1'-C1
21	ad	101	CD4	C11-C10-C9-C8
14	BM	1005	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	af	101	V7B	C2-C1-O1-C7
13	M	406	BCL	C5-C6-C7-C8
14	BT	102	LMT	C3-C4-C5-C6
14	AA	1003	LMT	C7-C8-C9-C10
13	BA	103	BCL	C15-C16-C17-C18
14	BG	1005	LMT	O5'-C5'-C6'-O6'
14	BU	1003	LMT	O5B-C5B-C6B-O6B
13	bb	102	BCL	C16-C17-C18-C19
14	AS	103	LMT	C2-C3-C4-C5
14	BD	106	LMT	C3'-C4'-O1B-C1B
14	AN	101	LMT	C1-C2-C3-C4
14	BK	1004	LMT	C1-C2-C3-C4
14	C	1005	LMT	O5'-C5'-C6'-O6'
14	AP	101	LMT	O1'-C1-C2-C3
14	BC	102	LMT	C4'-C5'-C6'-O6'
14	BQ	1002	LMT	C4'-C5'-C6'-O6'
14	BE	102	LMT	C3'-C4'-O1B-C1B
14	be	101	LMT	O5'-C5'-C6'-O6'
15	AW	103	V7N	C3-C4-C5-C33
26	ag	103	V7B	C8-C7-O1-C1
13	bh	103	BCL	C8-C10-C11-C12
14	BV	1002	LMT	O5B-C1B-O1B-C4'
13	AL	103	BCL	C4-C3-C5-C6
23	M	402	MQ8	C14-C13-C15-C16
13	AE	105	BCL	C2-C3-C5-C6
13	AU	101	BCL	C8-C10-C11-C12
14	bc	102	LMT	C4'-C5'-C6'-O6'
14	BQ	1003	LMT	C4-C5-C6-C7
13	AQ	104	BCL	C3-C5-C6-C7
13	bm	102	BCL	C3-C5-C6-C7
14	AG	101	LMT	O5'-C5'-C6'-O6'
14	L	304	LMT	O5B-C5B-C6B-O6B
14	BB	104	LMT	O5'-C5'-C6'-O6'
21	af	102	CD4	C54-C55-C56-C57
14	BP	1004	LMT	C4'-C5'-C6'-O6'
14	AD	102	LMT	O5'-C5'-C6'-O6'
16	bi	103	0V9	C21-C22-C23-C24
14	BV	1003	LMT	O5'-C5'-C6'-O6'
14	C2	1001	LMT	O5'-C5'-C6'-O6'
14	bm	103	LMT	O5'-C5'-C6'-O6'
16	be	105	0V9	O2-C2-C3-O3
16	bf	103	0V9	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BA	102	LMT	C4'-C5'-C6'-O6'
15	BU	1001	V7N	C5-C6-C7-C8
13	am	1001	BCL	C16-C17-C18-C20
16	ad	103	0V9	C2-C1-O3P-P
14	BC	103	LMT	O5B-C5B-C6B-O6B
14	BF	104	LMT	O5B-C1B-O1B-C4'
13	AE	105	BCL	C4-C3-C5-C6
13	AL	103	BCL	C2-C3-C5-C6
13	BT	103	BCL	C2A-CAA-CBA-CGA
13	bh	103	BCL	C2A-CAA-CBA-CGA
14	BD	106	LMT	O5'-C5'-C6'-O6'
14	BO	1005	LMT	O5B-C5B-C6B-O6B
14	BR	1002	LMT	O5B-C5B-C6B-O6B
16	bd	103	0V9	C2-C3-O3-C30
16	bm	104	0V9	C2-C3-O3-C30
13	AK	104	BCL	C10-C11-C12-C13
13	AV	103	BCL	C15-C16-C17-C18
13	bp	104	BCL	C13-C15-C16-C17
14	AJ	102	LMT	O5B-C5B-C6B-O6B
21	af	104	CD4	C10-C11-C12-C13
14	BR	1002	LMT	O1'-C1-C2-C3
14	BP	1006	LMT	C4-C5-C6-C7
21	M	409	CD4	C43-C44-C45-C63
21	af	104	CD4	C47-C48-C49-C50
14	BT	101	LMT	O5'-C5'-C6'-O6'
14	BJ	1003	LMT	C3-C4-C5-C6
14	BP	1004	LMT	C1-C2-C3-C4
13	AE	103	BCL	C1A-C2A-CAA-CBA
13	AG	102	BCL	C1A-C2A-CAA-CBA
13	AK	102	BCL	C1A-C2A-CAA-CBA
13	AL	103	BCL	C1A-C2A-CAA-CBA
13	AM	1002	BCL	C1A-C2A-CAA-CBA
13	AQ	104	BCL	C1A-C2A-CAA-CBA
13	AS	101	BCL	C1A-C2A-CAA-CBA
13	AT	103	BCL	C1A-C2A-CAA-CBA
13	BX	101	BCL	C1A-C2A-CAA-CBA
13	bd	102	BCL	C1A-C2A-CAA-CBA
13	bg	104	BCL	C1A-C2A-CAA-CBA
13	bj	104	BCL	C1A-C2A-CAA-CBA
14	BT	104	LMT	O5'-C5'-C6'-O6'
21	M	409	CD4	C24-C25-C26-C27
21	H1	103	CD4	C49-C50-C51-C52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	AQ	105	0V9	O3P-C1-C2-C3
16	H1	102	0V9	O3P-C1-C2-C3
21	af	102	CD4	C16-C15-C28-O5
13	AC	102	BCL	C11-C10-C8-C7
13	AL	102	BCL	C11-C10-C8-C7
13	AX	102	BCL	C11-C10-C8-C7
13	BJ	1004	BCL	C6-C7-C8-C10
13	aj	101	BCL	C6-C7-C8-C10
13	bf	102	BCL	C11-C12-C13-C15
13	AJ	103	BCL	C2C-C3C-CAC-CBC
25	M	404	CRT	C36-C37-C38-C39
25	M	404	CRT	C36-C37-C38-C40
14	AV	102	LMT	O5B-C1B-O1B-C4'
14	BR	1006	LMT	O5B-C1B-O1B-C4'
14	BF	102	LMT	C4'-C5'-C6'-O6'
23	M	402	MQ8	C12-C13-C15-C16
14	BD	102	LMT	O5'-C5'-C6'-O6'
14	BS	1002	LMT	C3-C4-C5-C6
13	AH	102	BCL	C15-C16-C17-C18
13	AI	101	BCL	C5-C6-C7-C8
13	BS	1004	BCL	C5-C6-C7-C8
14	BV	1002	LMT	O1'-C1-C2-C3
13	AD	103	BCL	C3-C5-C6-C7
16	M	403	0V9	C11-C10-O2-C2
13	AW	102	BCL	C2A-CAA-CBA-CGA
13	bc	103	BCL	C2A-CAA-CBA-CGA
13	AC	102	BCL	C11-C10-C8-C9
13	AJ	104	BCL	C11-C10-C8-C9
13	AJ	104	BCL	C14-C13-C15-C16
13	AL	102	BCL	C11-C10-C8-C9
14	BH	1003	LMT	O5'-C5'-C6'-O6'
14	BV	1003	LMT	C3-C4-C5-C6
21	ad	101	CD4	C18-C19-C20-C21
14	be	101	LMT	C2B-C1B-O1B-C4'
21	M	409	CD4	C51-C52-C53-C54
14	AS	103	LMT	O5B-C5B-C6B-O6B
16	M	403	0V9	C1-C2-C3-O3
16	ab	1002	0V9	C1-C2-C3-O3
16	be	105	0V9	C1-C2-C3-O3
16	bl	102	0V9	C1-C2-C3-O3
16	bm	104	0V9	C1-C2-C3-O3
16	bo	103	0V9	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	M	405	CD4	C28-C15-C16-O3
14	BH	1002	LMT	O5B-C1B-O1B-C4'
14	AN	102	LMT	O5B-C5B-C6B-O6B
14	AX	101	LMT	O5'-C5'-C6'-O6'
14	BN	1002	LMT	O5'-C5'-C6'-O6'
14	BE	105	LMT	C1-C2-C3-C4
14	bo	104	LMT	C7-C8-C9-C10
14	L	306	LMT	O5B-C5B-C6B-O6B
14	BP	1006	LMT	C5-C6-C7-C8
14	L	307	LMT	C1-C2-C3-C4
14	BD	106	LMT	C4-C5-C6-C7
14	BK	1004	LMT	C5'-C4'-O1B-C1B
13	AU	103	BCL	C5-C6-C7-C8
14	BP	1005	LMT	O1'-C1-C2-C3
13	AQ	102	BCL	C2-C3-C5-C6
13	AU	103	BCL	C2-C3-C5-C6
13	bn	102	BCL	C2-C3-C5-C6
13	bj	104	BCL	C8-C10-C11-C12
15	be	102	V7N	C38-C26-C27-C28
16	ab	1002	0V9	C38-C39-C40-C41
14	AC	103	LMT	O5'-C5'-C6'-O6'
14	AP	101	LMT	O5'-C5'-C6'-O6'
14	AS	103	LMT	O5'-C5'-C6'-O6'
14	BH	1004	LMT	O5'-C5'-C6'-O6'
14	BR	1005	LMT	O5'-C5'-C6'-O6'
13	bh	103	BCL	C10-C11-C12-C13
14	AK	103	LMT	C4'-C5'-C6'-O6'
13	an	1001	BCL	C10-C11-C12-C13
14	BT	104	LMT	O5B-C1B-O1B-C4'
13	BH	1005	BCL	O2A-C1-C2-C3
13	BK	1002	BCL	O2A-C1-C2-C3
13	BN	1005	BCL	O2A-C1-C2-C3
13	BQ	1004	BCL	O2A-C1-C2-C3
13	aa	1001	BCL	O2A-C1-C2-C3
21	ad	101	CD4	C28-C15-O2-C14
21	af	104	CD4	C16-C15-O2-C14
14	bh	102	LMT	C11-C10-C9-C8
21	M	409	CD4	C22-C23-C24-C25
16	bb	103	0V9	C19-C20-C21-C22
16	bg	103	0V9	C15-C16-C17-C18
15	BM	1001	V7N	C27-C28-C29-C39
15	bi	101	V7N	C27-C28-C29-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	bj	103	0V9	O3P-C1-C2-O2
14	AT	102	LMT	O5'-C1'-O1'-C1
16	ad	103	0V9	C31-C30-O3-C3
14	bn	103	LMT	C5'-C4'-O1B-C1B
14	BS	1003	LMT	O1'-C1-C2-C3
16	bm	104	0V9	C35-C36-C37-C38
21	H1	103	CD4	C37-C38-C39-C40
13	bn	102	BCL	C4-C3-C5-C6
14	AT	104	LMT	C5-C6-C7-C8
16	bd	103	0V9	C10-C11-C12-C13
16	M	403	0V9	O2-C2-C3-O3
16	ad	103	0V9	O2-C2-C3-O3
14	BR	1005	LMT	C6-C7-C8-C9
13	AC	101	BCL	C10-C11-C12-C13
16	bp	105	0V9	C10-C11-C12-C13
15	BF	101	V7N	C30-C1-O32-C41
27	ai	102	UYH	C11-C10-O7-C8
14	be	101	LMT	O5B-C1B-O1B-C4'
14	AE	101	LMT	C4B-C5B-C6B-O6B
13	AK	102	BCL	C5-C6-C7-C8
13	AQ	102	BCL	C4-C3-C5-C6
13	AU	103	BCL	C4-C3-C5-C6
13	BJ	1004	BCL	C4-C3-C5-C6
13	bd	102	BCL	C4-C3-C5-C6
23	L	303	MQ8	C19-C18-C20-C21
23	ao	101	MQ8	C34-C33-C35-C36
26	ag	103	V7B	C31-C32-C33-C34
14	AV	104	LMT	C3'-C4'-O1B-C1B
16	bp	105	0V9	C31-C30-O3-C3
14	BH	1004	LMT	C3-C4-C5-C6
14	BK	1004	LMT	C3'-C4'-O1B-C1B
14	bi	104	LMT	O5'-C5'-C6'-O6'
14	be	104	LMT	C7-C8-C9-C10
14	BC	103	LMT	C2-C1-O1'-C1'
14	BD	106	LMT	C2-C1-O1'-C1'
14	BF	104	LMT	C2-C1-O1'-C1'
14	BH	1002	LMT	C2-C1-O1'-C1'
14	BI	1005	LMT	C2-C1-O1'-C1'
14	BJ	1003	LMT	C2-C1-O1'-C1'
14	BK	1004	LMT	C2-C1-O1'-C1'
14	BN	1003	LMT	C2-C1-O1'-C1'
14	BO	1002	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BP	1004	LMT	C2-C1-O1'-C1'
14	BQ	1002	LMT	C2-C1-O1'-C1'
14	BR	1005	LMT	C2-C1-O1'-C1'
14	BT	101	LMT	C2-C1-O1'-C1'
14	BT	102	LMT	C2-C1-O1'-C1'
14	BU	1003	LMT	C2-C1-O1'-C1'
14	BW	1003	LMT	C2-C1-O1'-C1'
14	BX	104	LMT	C2-C1-O1'-C1'
14	H2	201	LMT	C2-C1-O1'-C1'
14	L	306	LMT	C2-C1-O1'-C1'
14	bk	104	LMT	C2-C1-O1'-C1'
14	bn	103	LMT	C2-C1-O1'-C1'
14	bp	101	LMT	C2-C1-O1'-C1'
13	AF	1001	BCL	C14-C13-C15-C16
13	AX	102	BCL	C11-C10-C8-C9
13	am	1001	BCL	C11-C12-C13-C14
13	bj	104	BCL	C11-C12-C13-C14
14	bl	103	LMT	C3'-C4'-O1B-C1B
13	ah	1001	BCL	C5-C6-C7-C8
16	bi	103	OV9	C2-C1-O3P-P
21	H1	103	CD4	C15-C28-O5-P1
21	af	102	CD4	C33-C32-O13-P2
14	BL	101	LMT	C4'-C5'-C6'-O6'
13	AH	102	BCL	C13-C15-C16-C17
13	ba	102	BCL	C5-C6-C7-C8
14	AB	1003	LMT	C2'-C1'-O1'-C1
14	AK	101	LMT	C2'-C1'-O1'-C1
13	bn	102	BCL	C3-C5-C6-C7
16	bh	104	OV9	O3P-C1-C2-C3
21	af	102	CD4	O13-C32-C33-C34
14	AS	103	LMT	C1-C2-C3-C4
13	AF	1001	BCL	C12-C13-C15-C16
13	AJ	104	BCL	C11-C10-C8-C7
13	AJ	104	BCL	C12-C13-C15-C16
13	am	1001	BCL	C11-C12-C13-C15
13	bj	104	BCL	C11-C12-C13-C15
22	M	407	BPH	C6-C7-C8-C10
15	BH	1001	V7N	O42-C34-C9-C8
15	BU	1001	V7N	O42-C34-C9-C8
15	be	102	V7N	O42-C34-C9-C8
13	AE	103	BCL	C4-C3-C5-C6
13	BH	1005	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	BN	1005	BCL	C3A-C2A-CAA-CBA
13	BQ	1004	BCL	C3A-C2A-CAA-CBA
13	BT	103	BCL	C3A-C2A-CAA-CBA
13	BV	1005	BCL	C3A-C2A-CAA-CBA
13	ba	102	BCL	C3A-C2A-CAA-CBA
13	bb	102	BCL	C3A-C2A-CAA-CBA
13	bl	104	BCL	C3A-C2A-CAA-CBA
14	bp	101	LMT	O5'-C1'-O1'-C1
13	AV	103	BCL	C5-C6-C7-C8
16	bj	103	0V9	C35-C36-C37-C38
14	BS	1003	LMT	C1-C2-C3-C4
15	BJ	1001	V7N	C27-C28-C29-C39
15	bb	101	V7N	C19-C20-C21-C22
15	bl	101	V7N	C27-C28-C29-C39
15	bm	101	V7N	C27-C28-C29-C39
13	AM	1004	BCL	C8-C10-C11-C12
14	BO	1002	LMT	C9-C10-C11-C12
16	bf	103	0V9	C1-C2-C3-O3
16	bg	103	0V9	C1-C2-C3-O3
16	bk	102	0V9	C1-C2-C3-O3
21	af	102	CD4	C32-C33-C34-O14
21	af	104	CD4	C28-C15-C16-O3
26	ag	103	V7B	O1-C7-C8-C9
27	ai	102	UYH	C7-C8-C9-O8
13	BH	1005	BCL	C5-C6-C7-C8
14	BX	102	LMT	C1-C2-C3-C4
13	aj	101	BCL	C4-C3-C5-C6
13	BH	1005	BCL	C2-C3-C5-C6
13	BJ	1004	BCL	C2-C3-C5-C6
13	bd	102	BCL	C2-C3-C5-C6
13	BD	104	BCL	O1A-CGA-O2A-C1
16	bd	103	0V9	O3P-C1-C2-O2
16	be	105	0V9	O3P-C1-C2-O2
16	bh	104	0V9	O3P-C1-C2-O2
21	H1	103	CD4	O2-C15-C28-O5
21	M	405	CD4	O2-C15-C28-O5
21	af	104	CD4	O2-C15-C28-O5
16	L	310	0V9	C36-C37-C38-C39
16	ab	1002	0V9	C2-C1-O3P-P
13	AM	1004	BCL	C15-C16-C17-C18
13	BT	103	BCL	C5-C6-C7-C8
14	BI	1005	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bf	101	LMT	C4'-C5'-C6'-O6'
14	L	307	LMT	C4-C5-C6-C7
16	bm	104	0V9	O2-C10-C11-C12
13	BP	1003	BCL	C10-C11-C12-C13
16	bg	103	0V9	O2-C2-C3-O3
21	M	405	CD4	O2-C15-C16-O3
21	M	409	CD4	O2-C15-C16-O3
21	af	104	CD4	O2-C15-C16-O3
26	ag	103	V7B	O1-C7-C8-O7
14	BC	101	LMT	C5'-C4'-O1B-C1B
13	BO	1003	BCL	C8-C10-C11-C12
14	BG	1003	LMT	C4'-C5'-C6'-O6'
16	bp	105	0V9	C40-C41-C42-C43
27	ai	102	UYH	C32-C33-C34-C35
20	H1	101	PGW	C1-C2-C3-C4
21	af	102	CD4	C45-C63-C64-C65
13	ak	1001	BCL	C4-C3-C5-C6
13	AH	102	BCL	C2-C3-C5-C6
13	aj	101	BCL	C2-C3-C5-C6
23	ao	101	MQ8	C32-C33-C35-C36
14	AJ	102	LMT	C9-C10-C11-C12
16	ad	103	0V9	C31-C32-C33-C34
21	M	405	CD4	C49-C50-C51-C52
14	BR	1005	LMT	C5'-C4'-O1B-C1B
14	BG	1002	LMT	O1'-C1-C2-C3
14	BX	104	LMT	O5B-C1B-O1B-C4'
13	AB	1002	BCL	C14-C13-C15-C16
13	AM	1004	BCL	C6-C7-C8-C9
13	AP	102	BCL	C6-C7-C8-C9
13	BI	1004	BCL	C11-C10-C8-C9
13	BJ	1004	BCL	C6-C7-C8-C9
16	bg	103	0V9	O3-C30-C31-C32
14	BG	1005	LMT	C3-C4-C5-C6
14	BK	1005	LMT	O5B-C1B-O1B-C4'
14	AN	102	LMT	O5'-C1'-O1'-C1
14	BV	1004	LMT	O5'-C1'-O1'-C1
13	AM	1004	BCL	C10-C11-C12-C13
14	BT	101	LMT	O1'-C1-C2-C3
14	BE	102	LMT	C2'-C1'-O1'-C1
14	C	1005	LMT	C2-C3-C4-C5
13	AD	104	BCL	C4C-C3C-CAC-CBC
13	AQ	104	BCL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AS	102	BCL	C4C-C3C-CAC-CBC
14	BS	1005	LMT	O5B-C1B-O1B-C4'
14	BP	1006	LMT	C3-C4-C5-C6
14	H2	201	LMT	C4'-C5'-C6'-O6'
21	af	104	CD4	C35-C36-C37-C38
21	M	409	CD4	C21-C22-C23-C24
14	BK	1004	LMT	O1'-C1-C2-C3
13	am	1001	BCL	C3-C5-C6-C7
13	AL	103	BCL	CBA-CGA-O2A-C1
14	bg	102	LMT	C4'-C5'-C6'-O6'
13	AE	103	BCL	C2-C3-C5-C6
13	ak	1001	BCL	C2-C3-C5-C6
23	L	303	MQ8	C17-C18-C20-C21
23	M	402	MQ8	C37-C38-C40-C41
14	BX	103	LMT	C4'-C5'-C6'-O6'
16	L	310	0V9	C20-C21-C22-C23
20	H1	101	PGW	C3-C4-C5-C6
13	BS	1004	BCL	C3-C5-C6-C7
16	bn	104	0V9	C31-C30-O3-C3
14	AA	1003	LMT	C4-C5-C6-C7
16	ab	1002	0V9	C31-C32-C33-C34
16	bd	103	0V9	O3P-C1-C2-C3
16	be	105	0V9	O3P-C1-C2-C3
16	bj	103	0V9	O3P-C1-C2-C3
14	AT	104	LMT	O1'-C1-C2-C3
13	AG	102	BCL	C15-C16-C17-C18
13	AC	102	BCL	C6-C7-C8-C10
13	AM	1004	BCL	C6-C7-C8-C10
13	AP	102	BCL	C6-C7-C8-C10
13	bp	104	BCL	C11-C10-C8-C7
14	BX	104	LMT	C1-C2-C3-C4
16	bo	103	0V9	C2-C3-O3-C30
14	AN	101	LMT	C5'-C4'-O1B-C1B
13	AP	103	BCL	C13-C15-C16-C17
15	BD	101	V7N	C25-C26-C27-C28
15	BW	1001	V7N	C3-C4-C5-C6
15	ag	101	V7N	C3-C4-C5-C6
15	be	102	V7N	C25-C26-C27-C28
13	AH	103	BCL	C8-C10-C11-C12
14	BW	1006	LMT	O5B-C1B-O1B-C4'
14	BV	1002	LMT	C9-C10-C11-C12
14	BP	1002	LMT	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	ai	102	UYH	C36-C37-C38-C39
13	ap	1001	BCL	C8-C10-C11-C12
13	BC	104	BCL	O2A-C1-C2-C3
13	ak	1001	BCL	O2A-C1-C2-C3
13	bj	104	BCL	O2A-C1-C2-C3
15	BU	1001	V7N	C7-C8-C9-C10
14	AV	104	LMT	C6-C7-C8-C9
21	af	104	CD4	C9-C10-C11-C12
14	be	101	LMT	C9-C10-C11-C12
13	bb	102	BCL	C3-C5-C6-C7
21	M	409	CD4	C50-C51-C52-C53
27	ai	102	UYH	O9-C10-O7-C8
16	H1	102	0V9	O3P-C1-C2-O2
16	bk	102	0V9	O3P-C1-C2-O2
16	bo	103	0V9	O3P-C1-C2-O2
21	M	409	CD4	O2-C15-C28-O5
21	ad	101	CD4	O2-C15-C28-O5
14	AX	101	LMT	C2B-C1B-O1B-C4'
14	BQ	1003	LMT	C11-C10-C9-C8
16	be	105	0V9	C31-C32-C33-C34
16	bn	104	0V9	C38-C39-C40-C41
21	H1	103	CD4	C48-C49-C50-C51
15	BM	1001	V7N	C22-C23-C24-C25
16	bi	103	0V9	C1-C2-C3-O3
16	ab	1002	0V9	C2-C3-O3-C30
13	AO	102	BCL	C13-C15-C16-C17
14	BO	1002	LMT	C4'-C5'-C6'-O6'
13	BI	1004	BCL	C3-C5-C6-C7
14	BO	1005	LMT	C4'-C5'-C6'-O6'
13	AG	102	BCL	C4-C3-C5-C6
14	BJ	1003	LMT	C4-C5-C6-C7
15	AS	104	V7N	O42-C34-C9-C10
15	AW	103	V7N	O42-C34-C9-C10
15	BA	101	V7N	O42-C34-C9-C10
15	BD	101	V7N	O42-C34-C9-C10
15	BE	101	V7N	O42-C34-C9-C10
15	BF	101	V7N	O42-C34-C9-C10
15	BN	1001	V7N	O42-C34-C9-C10
15	BO	1001	V7N	O42-C34-C9-C10
15	BP	1001	V7N	O42-C34-C9-C10
15	BQ	1001	V7N	O42-C34-C9-C10
15	BR	1001	V7N	O42-C34-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	BS	1001	V7N	O42-C34-C9-C10
15	ag	101	V7N	O42-C34-C9-C10
15	ba	101	V7N	O42-C34-C9-C10
15	bc	101	V7N	O42-C34-C9-C10
15	bd	101	V7N	O42-C34-C9-C10
15	bg	101	V7N	O42-C34-C9-C10
15	bh	101	V7N	O42-C34-C9-C10
15	bi	101	V7N	O42-C34-C9-C10
15	bj	101	V7N	O42-C34-C9-C10
15	bk	101	V7N	O42-C34-C9-C10
15	bl	101	V7N	O42-C34-C9-C10
15	bn	101	V7N	O42-C34-C9-C10
15	bo	101	V7N	O42-C34-C9-C10
15	bp	102	V7N	O42-C34-C9-C10
16	AQ	105	0V9	C5-C4-O4P-P
16	H1	102	0V9	C5-C4-O4P-P
16	M	403	0V9	C5-C4-O4P-P
16	ab	1002	0V9	C5-C4-O4P-P
16	ad	103	0V9	C5-C4-O4P-P
16	bd	103	0V9	C5-C4-O4P-P
16	bf	103	0V9	C5-C4-O4P-P
16	bh	104	0V9	C5-C4-O4P-P
16	bi	103	0V9	C5-C4-O4P-P
23	ao	101	MQ8	C12-C11-C3-C4
14	L	302	LMT	C1-C2-C3-C4
16	ad	103	0V9	O5-C30-O3-C3
14	AS	103	LMT	C3-C4-C5-C6
13	BV	1005	BCL	C3-C5-C6-C7
13	ap	1001	BCL	C3-C5-C6-C7
26	af	101	V7B	O1-C7-C8-O7
22	M	407	BPH	C6-C7-C8-C9
16	bf	103	0V9	C36-C37-C38-C39
21	af	104	CD4	C41-C42-C43-C44
14	BM	1005	LMT	O5B-C5B-C6B-O6B
14	BF	102	LMT	C3-C4-C5-C6
16	bl	102	0V9	C11-C12-C13-C14
13	AW	101	BCL	C8-C10-C11-C12
15	bg	101	V7N	O32-C1-C2-C3
15	bl	101	V7N	O32-C1-C2-C3
15	bn	101	V7N	O32-C1-C2-C3
13	AT	103	BCL	C5-C6-C7-C8
14	BR	1005	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AQ	102	BCL	C2-C1-O2A-CGA
21	ad	101	CD4	C30-C31-O10-P2
14	AE	106	LMT	C7-C8-C9-C10
14	BO	1002	LMT	C5-C6-C7-C8
13	AA	1002	BCL	C4-C3-C5-C6
23	M	402	MQ8	C39-C38-C40-C41
13	AA	1002	BCL	C2-C3-C5-C6
14	BU	1003	LMT	C1-C2-C3-C4
14	BX	102	LMT	C5'-C4'-O1B-C1B
27	ai	102	UYH	C34-C35-C36-C37
13	AG	103	BCL	C16-C17-C18-C19
13	AS	101	BCL	C13-C15-C16-C17
14	AE	101	LMT	C6-C7-C8-C9
14	AV	102	LMT	C2B-C1B-O1B-C4'
14	AN	101	LMT	C4'-C5'-C6'-O6'
14	AB	1003	LMT	C2-C1-O1'-C1'
14	AC	103	LMT	C2-C1-O1'-C1'
14	AQ	101	LMT	C2-C1-O1'-C1'
14	BM	1002	LMT	C2-C1-O1'-C1'
14	BV	1004	LMT	C2-C1-O1'-C1'
14	C	1005	LMT	C2-C1-O1'-C1'
14	AC	103	LMT	C7-C8-C9-C10
15	AD	101	V7N	C3-C4-C5-C33
15	BR	1001	V7N	C3-C4-C5-C33
13	BC	104	BCL	C1A-C2A-CAA-CBA
13	BR	1003	BCL	C1A-C2A-CAA-CBA
13	bb	102	BCL	C1A-C2A-CAA-CBA
13	BD	104	BCL	CBA-CGA-O2A-C1
16	bk	102	0V9	C33-C34-C35-C36
13	AK	102	BCL	C4-C3-C5-C6
14	BE	102	LMT	C2-C3-C4-C5
15	AW	103	V7N	C3-C4-C5-C6
14	BR	1002	LMT	O5B-C1B-O1B-C4'
16	H1	102	0V9	C32-C33-C34-C35
13	bn	102	BCL	C16-C17-C18-C20
14	BK	1005	LMT	C5-C6-C7-C8
14	AD	102	LMT	O5B-C1B-O1B-C4'
14	BT	101	LMT	O5B-C1B-O1B-C4'
14	bn	103	LMT	C3'-C4'-O1B-C1B
21	M	405	CD4	C36-C37-C38-C39
14	AH	101	LMT	O5B-C5B-C6B-O6B
16	bk	102	0V9	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	bo	103	0V9	O3P-C1-C2-C3
14	BV	1002	LMT	C2B-C1B-O1B-C4'
14	AJ	102	LMT	O5B-C1B-O1B-C4'
14	BR	1004	LMT	C5-C6-C7-C8
15	BM	1001	V7N	C23-C24-C25-C26
14	L	307	LMT	C4B-C5B-C6B-O6B
13	AE	104	BCL	C6-C7-C8-C10
13	af	103	BCL	C12-C13-C15-C16
13	bl	104	BCL	C6-C7-C8-C10
13	bm	102	BCL	C11-C12-C13-C15
13	bn	102	BCL	C16-C17-C18-C19
16	bb	103	0V9	C12-C13-C14-C15
14	BF	102	LMT	C5'-C4'-O1B-C1B
15	bk	101	V7N	C31-C1-C2-C3
14	BC	101	LMT	O5B-C1B-O1B-C4'
14	BS	1005	LMT	C4-C5-C6-C7
14	BI	1002	LMT	C2B-C1B-O1B-C4'
14	AK	101	LMT	C2-C3-C4-C5
13	AL	103	BCL	O1A-CGA-O2A-C1
20	H1	101	PGW	C02-C03-O11-P
14	BX	103	LMT	C4-C5-C6-C7
14	BM	1002	LMT	O5B-C1B-O1B-C4'
13	AK	102	BCL	C3A-C2A-CAA-CBA
13	AP	103	BCL	C3A-C2A-CAA-CBA
13	BF	103	BCL	C4-C3-C5-C6
14	AS	103	LMT	C6-C7-C8-C9
21	M	405	CD4	O13-C32-C33-O16
21	af	102	CD4	O13-C32-C33-O16
21	M	405	CD4	C17-C18-C19-C20
14	BX	104	LMT	C5'-C4'-O1B-C1B
13	BC	104	BCL	C2A-CAA-CBA-CGA
13	BV	1005	BCL	C2A-CAA-CBA-CGA
13	bj	104	BCL	C2A-CAA-CBA-CGA
13	AC	102	BCL	C6-C7-C8-C9
13	af	103	BCL	C14-C13-C15-C16
13	ba	102	BCL	C11-C12-C13-C14
13	bl	104	BCL	C6-C7-C8-C9
13	bm	102	BCL	C11-C12-C13-C14
13	bp	104	BCL	C11-C10-C8-C9
26	af	101	V7B	O7-C10-C11-C12
13	BX	101	BCL	C5-C6-C7-C8
16	bl	102	0V9	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BJ	1002	LMT	C4-C5-C6-C7
14	bj	102	LMT	O1'-C1-C2-C3
13	bd	102	BCL	C5-C6-C7-C8
14	BG	1005	LMT	O5B-C5B-C6B-O6B
16	bn	104	0V9	O5-C30-O3-C3
13	AN	104	BCL	C13-C15-C16-C17
13	af	103	BCL	C10-C11-C12-C13
14	AT	104	LMT	O5B-C5B-C6B-O6B
16	H1	102	0V9	C1-C2-C3-O3
21	M	409	CD4	C28-C15-C16-O3
13	AH	102	BCL	C4-C3-C5-C6
14	C2	1001	LMT	O1'-C1-C2-C3
14	BT	101	LMT	C5'-C4'-O1B-C1B
14	BD	105	LMT	C4-C5-C6-C7
16	H1	102	0V9	C34-C35-C36-C37
14	AK	101	LMT	C9-C10-C11-C12
16	bp	105	0V9	C16-C17-C18-C19
13	AP	102	BCL	C8-C10-C11-C12
13	af	103	BCL	C5-C6-C7-C8
13	AH	105	BCL	CBD-CGD-O2D-CED
14	BB	103	LMT	C5'-C4'-O1B-C1B
13	AM	1002	BCL	C2A-CAA-CBA-CGA
13	BA	103	BCL	C2A-CAA-CBA-CGA
13	BE	104	BCL	C2A-CAA-CBA-CGA
13	bk	103	BCL	C2A-CAA-CBA-CGA
14	AK	103	LMT	C5-C6-C7-C8
14	BI	1005	LMT	C3'-C4'-O1B-C1B
16	ad	103	0V9	O4-C10-O2-C2
15	BG	1001	V7N	C27-C28-C29-C39
15	bj	101	V7N	C27-C28-C29-C39
16	bf	103	0V9	C1-O3P-P-O2P
16	bg	103	0V9	O4P-C4-C5-N
16	bg	103	0V9	C1-O3P-P-O4P
16	bh	104	0V9	C1-O3P-P-O2P
16	bh	104	0V9	C1-O3P-P-O4P
16	bi	103	0V9	O4P-C4-C5-N
16	bl	102	0V9	C1-O3P-P-O2P
16	bl	102	0V9	C4-O4P-P-O3P
16	bo	103	0V9	C1-O3P-P-O2P
20	H1	101	PGW	C04-O12-P-O11
20	H1	101	PGW	C04-O12-P-O13
21	ad	101	CD4	C29-O8-P1-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AW	102	BCL	C3-C5-C6-C7
16	L	310	0V9	C10-C11-C12-C13
14	AN	101	LMT	C3'-C4'-O1B-C1B
13	AS	101	BCL	C4-C3-C5-C6
13	BQ	1004	BCL	C4-C3-C5-C6
14	bg	102	LMT	C6-C7-C8-C9
13	AP	103	BCL	C15-C16-C17-C18
16	be	105	0V9	C2-C1-O3P-P
16	bo	103	0V9	C2-C1-O3P-P
21	H1	103	CD4	C33-C32-O13-P2
21	M	409	CD4	C30-C31-O10-P2
21	ad	101	CD4	C33-C32-O13-P2
21	af	104	CD4	C30-C29-O8-P1
21	af	104	CD4	C30-C31-O10-P2
21	af	104	CD4	C43-C44-C45-C63
14	BP	1006	LMT	C2B-C1B-O1B-C4'
14	be	104	LMT	O5B-C5B-C6B-O6B
14	BR	1002	LMT	C5'-C4'-O1B-C1B
16	bp	105	0V9	C20-C21-C22-C23
15	BG	1001	V7N	C23-C24-C25-C26
15	BI	1001	V7N	C23-C24-C25-C26
14	BW	1006	LMT	C4-C5-C6-C7
14	BT	104	LMT	C2B-C1B-O1B-C4'
21	ad	101	CD4	C45-C63-C64-C65
16	be	105	0V9	C16-C17-C18-C19
14	BJ	1005	LMT	O1'-C1-C2-C3
27	ai	102	UYH	O6-C5-C6-O5
14	AX	101	LMT	O5B-C1B-O1B-C4'
13	AJ	104	BCL	C8-C10-C11-C12
21	af	102	CD4	C40-C41-C42-C43
21	M	409	CD4	C28-C15-O2-C14
13	AC	102	BCL	C5-C6-C7-C8
13	am	1001	BCL	C8-C10-C11-C12
13	AG	102	BCL	C2-C3-C5-C6
14	BN	1003	LMT	C4'-C5'-C6'-O6'
14	BP	1002	LMT	C5'-C4'-O1B-C1B
13	AA	1001	BCL	C16-C17-C18-C19
13	AG	103	BCL	C16-C17-C18-C20
21	M	405	CD4	O13-C32-C33-C34
21	M	409	CD4	C16-C15-C28-O5
13	AE	103	BCL	CBA-CGA-O2A-C1
15	BJ	1001	V7N	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AE	104	BCL	C6-C7-C8-C9
13	bb	102	BCL	C11-C12-C13-C14
14	BH	1002	LMT	C2B-C1B-O1B-C4'
13	AH	105	BCL	C6-C7-C8-C10
13	AS	101	BCL	C12-C13-C15-C16
13	ag	102	BCL	C11-C10-C8-C7
21	M	409	CD4	C35-C36-C37-C38
16	AQ	105	0V9	O3P-C1-C2-O2
14	AT	102	LMT	C4B-C5B-C6B-O6B
14	BD	106	LMT	C2'-C1'-O1'-C1
13	bp	104	BCL	C4-C3-C5-C6
15	AA	1004	V7N	C37-C22-C23-C24
14	BD	105	LMT	C2B-C1B-O1B-C4'
14	BH	1002	LMT	C5-C6-C7-C8
16	ad	103	0V9	C11-C12-C13-C14
14	BR	1006	LMT	C3-C4-C5-C6
13	AP	102	BCL	C16-C17-C18-C19
15	AM	1001	V7N	C23-C24-C25-C26
14	AV	102	LMT	C5'-C4'-O1B-C1B
14	BF	104	LMT	C2B-C1B-O1B-C4'
14	AK	101	LMT	C4-C5-C6-C7
14	AC	103	LMT	C5-C6-C7-C8
13	AM	1002	BCL	CBA-CGA-O2A-C1
14	BB	101	LMT	C4-C5-C6-C7
16	bj	103	0V9	C31-C32-C33-C34
13	AH	102	BCL	C8-C10-C11-C12
14	BI	1005	LMT	C4'-C5'-C6'-O6'
13	am	1001	BCL	C13-C15-C16-C17
15	BS	1001	V7N	C23-C24-C25-C26
13	AX	103	BCL	C4-C3-C5-C6
13	BP	1003	BCL	C4-C3-C5-C6
13	af	103	BCL	C4-C3-C5-C6
16	bj	103	0V9	C19-C20-C21-C22
16	bk	102	0V9	C2-C3-O3-C30
21	M	409	CD4	C6-C7-C8-C9
15	BK	1001	V7N	C3-C4-C5-C33
14	BB	104	LMT	C4-C5-C6-C7
14	AJ	102	LMT	C1-C2-C3-C4
14	BD	102	LMT	O1'-C1-C2-C3
16	bn	104	0V9	C16-C17-C18-C19
14	bk	104	LMT	C4'-C5'-C6'-O6'
13	BL	103	BCL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BC	101	LMT	C3'-C4'-O1B-C1B
16	bm	104	0V9	C19-C20-C21-C22
13	an	1001	BCL	C3-C5-C6-C7
16	bg	103	0V9	C36-C37-C38-C39
13	BU	1004	BCL	C4-C3-C5-C6
13	BF	103	BCL	C2-C3-C5-C6
14	BC	101	LMT	C4-C5-C6-C7
14	bn	103	LMT	C4-C5-C6-C7
14	AE	101	LMT	C5'-C4'-O1B-C1B
14	BS	1003	LMT	O5'-C5'-C6'-O6'
14	BR	1006	LMT	C2B-C1B-O1B-C4'
26	ag	103	V7B	C15-C16-C17-C18
14	AB	1003	LMT	O5B-C5B-C6B-O6B
14	AA	1003	LMT	C2-C1-O1'-C1'
14	AE	101	LMT	C2-C1-O1'-C1'
14	AE	102	LMT	C2-C1-O1'-C1'
14	AK	103	LMT	C2-C1-O1'-C1'
14	AP	101	LMT	C2-C1-O1'-C1'
14	AT	102	LMT	C2-C1-O1'-C1'
14	BD	103	LMT	C2-C1-O1'-C1'
14	BU	1002	LMT	C2-C1-O1'-C1'
14	BW	1004	LMT	C2-C1-O1'-C1'
14	bj	102	LMT	C2-C1-O1'-C1'
13	AP	102	BCL	C16-C17-C18-C20
16	H1	102	0V9	C10-C11-C12-C13
16	be	105	0V9	C31-C30-O3-C3
16	bp	105	0V9	C37-C38-C39-C40
14	H2	201	LMT	C11-C10-C9-C8
14	BD	103	LMT	C9-C10-C11-C12
14	BR	1005	LMT	O5B-C5B-C6B-O6B
14	BU	1003	LMT	C7-C8-C9-C10
14	L	307	LMT	C9-C10-C11-C12
14	BK	1005	LMT	C5'-C4'-O1B-C1B
14	BW	1004	LMT	C2-C3-C4-C5
26	af	101	V7B	C29-C28-O8-C9
14	BC	101	LMT	C4'-C5'-C6'-O6'
13	AL	103	BCL	C15-C16-C17-C18
13	BE	104	BCL	C4-C3-C5-C6
13	BN	1005	BCL	C4-C3-C5-C6
13	BX	101	BCL	C4-C3-C5-C6
13	ab	1001	BCL	C4-C3-C5-C6
15	BR	1001	V7N	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bo	104	LMT	C9-C10-C11-C12
13	AK	102	BCL	C2-C3-C5-C6
13	AX	103	BCL	C2-C3-C5-C6
13	BU	1004	BCL	C2-C3-C5-C6
13	bc	103	BCL	C2-C3-C5-C6
13	bp	104	BCL	C2-C3-C5-C6
14	AT	102	LMT	C2'-C1'-O1'-C1
14	bo	104	LMT	O5'-C5'-C6'-O6'
21	af	102	CD4	C47-C48-C49-C50
14	bp	101	LMT	C5'-C4'-O1B-C1B
15	BH	1001	V7N	C27-C28-C29-C39
14	BJ	1006	LMT	O5'-C5'-C6'-O6'
16	H1	102	0V9	C12-C13-C14-C15
13	AL	102	BCL	C12-C13-C15-C16
13	AS	101	BCL	C11-C10-C8-C7
13	BR	1003	BCL	C11-C10-C8-C7
13	ai	101	BCL	C11-C12-C13-C15
13	an	1001	BCL	C11-C10-C8-C7
14	BR	1005	LMT	O5B-C1B-O1B-C4'
14	BV	1004	LMT	O5B-C5B-C6B-O6B
14	BX	104	LMT	C2B-C1B-O1B-C4'
16	bk	102	0V9	O4-C10-O2-C2
14	BU	1003	LMT	C5'-C4'-O1B-C1B
16	ab	1002	0V9	C18-C19-C20-C21
16	be	105	0V9	C30-C31-C32-C33
14	BM	1005	LMT	C6-C7-C8-C9
13	AA	1002	BCL	C10-C11-C12-C13
13	AD	104	BCL	C3-C5-C6-C7
21	H1	103	CD4	O2-C15-C16-O3
13	AL	103	BCL	C3A-C2A-CAA-CBA
13	AP	103	BCL	C4-C3-C5-C6
13	BC	104	BCL	C3A-C2A-CAA-CBA
13	BH	1005	BCL	C3A-C2A-CAA-CBA
13	BR	1003	BCL	C3A-C2A-CAA-CBA
13	bb	102	BCL	C4-C3-C5-C6
14	BW	1006	LMT	C2B-C1B-O1B-C4'
13	BE	104	BCL	C2-C3-C5-C6
13	BQ	1004	BCL	C2-C3-C5-C6
13	af	103	BCL	C2-C3-C5-C6
13	AX	102	BCL	C2A-CAA-CBA-CGA
13	BH	1005	BCL	C2A-CAA-CBA-CGA
13	ba	102	BCL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	AT	102	LMT	C11-C10-C9-C8
14	BC	102	LMT	O5'-C5'-C6'-O6'
14	BV	1002	LMT	O5'-C1'-O1'-C1
14	BS	1003	LMT	C5'-C4'-O1B-C1B
14	BA	102	LMT	C6-C7-C8-C9
14	bf	101	LMT	C7-C8-C9-C10
13	AJ	103	BCL	C2-C1-O2A-CGA
15	ba	101	V7N	C13-C14-C15-C16
14	BE	103	LMT	C4-C5-C6-C7
16	bd	103	0V9	C20-C21-C22-C23
13	AD	103	BCL	C10-C11-C12-C13
14	BF	102	LMT	O5B-C5B-C6B-O6B
13	AH	103	BCL	C13-C15-C16-C17
15	BR	1001	V7N	C3-C4-C5-C6
13	ap	1001	BCL	C4-C3-C5-C6
13	bi	102	BCL	C4-C3-C5-C6
15	bc	101	V7N	C37-C22-C23-C24
13	BN	1005	BCL	C2-C3-C5-C6
14	BX	102	LMT	C4'-C5'-C6'-O6'
14	BM	1003	LMT	C3'-C4'-O1B-C1B
14	BR	1005	LMT	C3'-C4'-O1B-C1B
13	BP	1003	BCL	C8-C10-C11-C12
14	BS	1005	LMT	C2B-C1B-O1B-C4'
16	M	403	0V9	C33-C34-C35-C36
13	aj	101	BCL	C2A-CAA-CBA-CGA
16	bm	104	0V9	O4-C10-C11-C12
14	BK	1003	LMT	C4-C5-C6-C7
13	AD	104	BCL	C14-C13-C15-C16
13	AM	1004	BCL	C11-C12-C13-C14
13	AO	101	BCL	C11-C12-C13-C14
13	AQ	103	BCL	C6-C7-C8-C9
13	AS	101	BCL	C11-C10-C8-C9
13	BK	1002	BCL	C11-C12-C13-C14
13	BQ	1004	BCL	C11-C12-C13-C14
13	BR	1003	BCL	C11-C10-C8-C9
13	BV	1005	BCL	C14-C13-C15-C16
13	M	406	BCL	C14-C13-C15-C16
13	ae	1001	BCL	C11-C10-C8-C9
13	ai	101	BCL	C11-C12-C13-C14
13	bn	102	BCL	C6-C7-C8-C9
14	BJ	1006	LMT	C9-C10-C11-C12
13	AA	1001	BCL	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	af	102	CD4	C43-C44-C45-C63
13	L	308	BCL	C2B-C3B-CAB-OBB
13	L	308	BCL	C2B-C3B-CAB-CBB
13	M	406	BCL	C2B-C3B-CAB-OBB
13	M	406	BCL	C2B-C3B-CAB-CBB
16	M	403	OV9	C1-C2-O2-C10
16	bd	103	OV9	C3-C2-O2-C10
20	H1	101	PGW	C03-C02-O01-C1
21	H1	103	CD4	C28-C15-O2-C14
13	AX	103	BCL	C8-C10-C11-C12
14	BU	1003	LMT	O5'-C5'-C6'-O6'
13	AH	105	BCL	O1D-CGD-O2D-CED
15	bn	101	V7N	C37-C22-C23-C24
23	L	303	MQ8	C45-C43-C44-C46
21	ad	101	CD4	C5-C6-C7-C8
13	BP	1003	BCL	C2-C3-C5-C6
13	bb	102	BCL	C2-C3-C5-C6
15	bc	101	V7N	C21-C22-C23-C24
14	AE	102	LMT	O5B-C1B-O1B-C4'
14	AT	102	LMT	O5'-C5'-C6'-O6'
14	bi	104	LMT	C4-C5-C6-C7
13	AB	1002	BCL	C1A-C2A-CAA-CBA
13	AV	103	BCL	C1A-C2A-CAA-CBA
13	BN	1005	BCL	C1A-C2A-CAA-CBA
13	BQ	1004	BCL	C1A-C2A-CAA-CBA
13	BV	1005	BCL	C1A-C2A-CAA-CBA
13	ba	102	BCL	C1A-C2A-CAA-CBA
13	be	103	BCL	C1A-C2A-CAA-CBA
13	bf	102	BCL	C1A-C2A-CAA-CBA
13	bi	102	BCL	C1A-C2A-CAA-CBA
13	bl	104	BCL	C1A-C2A-CAA-CBA
13	bo	102	BCL	C1A-C2A-CAA-CBA
14	BR	1004	LMT	O5B-C1B-O1B-C4'
14	BW	1003	LMT	O1'-C1-C2-C3
16	M	403	OV9	C20-C21-C22-C23
14	AV	102	LMT	C1-C2-C3-C4
17	C	1004	HEC	CAD-CBD-CGD-O2D
13	AM	1002	BCL	C8-C10-C11-C12
21	M	405	CD4	C33-C32-O13-P2
14	bg	102	LMT	C7-C8-C9-C10
17	C	1004	HEC	CAD-CBD-CGD-O1D
14	AQ	101	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	AG	101	LMT	C6-C7-C8-C9
14	BU	1003	LMT	C2-C3-C4-C5
21	af	104	CD4	C16-C15-C28-O5
13	ab	1001	BCL	C2-C3-C5-C6
15	AA	1004	V7N	C21-C22-C23-C24
15	BR	1001	V7N	C21-C22-C23-C24
15	BP	1001	V7N	C23-C24-C25-C26
14	BB	104	LMT	C5'-C4'-O1B-C1B
14	BI	1002	LMT	O1'-C1-C2-C3
14	BW	1002	LMT	O5B-C1B-O1B-C4'
13	AC	101	BCL	C12-C13-C15-C16
13	AG	103	BCL	C6-C7-C8-C10
13	AM	1004	BCL	C11-C12-C13-C15
13	BU	1004	BCL	C6-C7-C8-C10
16	bi	103	0V9	C31-C32-C33-C34
13	AS	101	BCL	C2A-CAA-CBA-CGA
16	AQ	105	0V9	C16-C17-C18-C19
16	H1	102	0V9	O2-C2-C3-O3
15	BN	1001	V7N	C30-C1-C2-C3
15	bl	101	V7N	C30-C1-C2-C3
15	bo	101	V7N	C30-C1-C2-C3
15	bo	101	V7N	C31-C1-C2-C3
16	bk	102	0V9	C19-C20-C21-C22
16	bn	104	0V9	C19-C20-C21-C22
14	BN	1002	LMT	C5-C6-C7-C8
15	AS	104	V7N	C37-C22-C23-C24
15	BE	101	V7N	C37-C22-C23-C24
15	BU	1001	V7N	C37-C22-C23-C24
15	BV	1001	V7N	C37-C22-C23-C24
23	L	303	MQ8	C34-C33-C35-C36
14	L	306	LMT	O1'-C1-C2-C3
14	AC	103	LMT	C4B-C5B-C6B-O6B
13	AP	103	BCL	C2-C3-C5-C6
13	BX	101	BCL	C2-C3-C5-C6
13	ap	1001	BCL	C2-C3-C5-C6
23	L	303	MQ8	C32-C33-C35-C36
14	BE	105	LMT	C2B-C1B-O1B-C4'
14	L	306	LMT	C11-C10-C9-C8
16	be	105	0V9	C33-C34-C35-C36
21	af	104	CD4	C7-C8-C9-C10
13	BI	1004	BCL	C15-C16-C17-C18
21	M	405	CD4	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	308	BCL	C4B-C3B-CAB-OBB
13	L	308	BCL	C4B-C3B-CAB-CBB
14	BH	1002	LMT	C5'-C4'-O1B-C1B
16	ad	103	0V9	C11-C10-O2-C2
14	bp	103	LMT	C11-C10-C9-C8
13	BN	1005	BCL	C2A-CAA-CBA-CGA
13	BP	1003	BCL	C2A-CAA-CBA-CGA
13	AV	101	BCL	C6-C7-C8-C9
13	bf	102	BCL	C14-C13-C15-C16
14	BW	1003	LMT	C5'-C4'-O1B-C1B
14	AU	102	LMT	C5-C6-C7-C8
14	AJ	102	LMT	C2B-C1B-O1B-C4'
14	BX	103	LMT	C5'-C4'-O1B-C1B
14	BN	1003	LMT	O1'-C1-C2-C3
13	AP	102	BCL	C4-C3-C5-C6
13	ao	102	BCL	C4-C3-C5-C6
15	be	102	V7N	C37-C22-C23-C24
15	bo	101	V7N	C37-C22-C23-C24
13	AQ	103	BCL	C8-C10-C11-C12
13	AT	103	BCL	C15-C16-C17-C18
13	ao	102	BCL	C2-C3-C5-C6
16	bi	103	0V9	C36-C37-C38-C39
13	AE	103	BCL	O1A-CGA-O2A-C1
14	bf	101	LMT	C9-C10-C11-C12
14	BP	1004	LMT	C2'-C1'-O1'-C1
14	L	304	LMT	C2B-C1B-O1B-C4'
14	AU	102	LMT	C4-C5-C6-C7
14	BS	1002	LMT	C4B-C5B-C6B-O6B
14	BR	1002	LMT	C11-C10-C9-C8
16	ad	103	0V9	C1-C2-C3-O3
26	af	101	V7B	O1-C7-C8-C9
20	H1	101	PGW	C4-C5-C6-C7
26	af	101	V7B	C34-C35-C36-C37
14	BX	102	LMT	C3'-C4'-O1B-C1B
14	BM	1002	LMT	C9-C10-C11-C12
13	AO	101	BCL	C4C-C3C-CAC-CBC
13	BB	105	BCL	C4C-C3C-CAC-CBC
13	BL	103	BCL	C4C-C3C-CAC-CBC
13	BM	1004	BCL	C4C-C3C-CAC-CBC
14	BV	1004	LMT	O5'-C5'-C6'-O6'
13	M	408	BCL	CAA-CBA-CGA-O2A
14	BV	1002	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BC	103	LMT	C1-C2-C3-C4
14	BH	1002	LMT	C4'-C5'-C6'-O6'
14	AG	101	LMT	C5'-C4'-O1B-C1B
14	BW	1002	LMT	C5'-C4'-O1B-C1B
13	bo	102	BCL	C4-C3-C5-C6
15	AD	101	V7N	C37-C22-C23-C24
15	bm	101	V7N	C37-C22-C23-C24
13	AE	105	BCL	CAA-CBA-CGA-O2A
13	AV	101	BCL	C13-C15-C16-C17
16	bb	103	0V9	C18-C19-C20-C21
17	C	1001	HEC	CAD-CBD-CGD-O2D
14	BJ	1005	LMT	C5'-C4'-O1B-C1B
16	H1	102	0V9	C19-C20-C21-C22
13	bl	104	BCL	C10-C11-C12-C13
13	bl	104	BCL	C2A-CAA-CBA-CGA
13	bi	102	BCL	C2-C3-C5-C6
15	AS	104	V7N	C21-C22-C23-C24
16	ab	1002	0V9	C16-C17-C18-C19
16	bm	104	0V9	C16-C17-C18-C19
14	BB	104	LMT	O5'-C1'-O1'-C1
21	M	409	CD4	C33-C32-O13-P2
13	AV	101	BCL	C6-C7-C8-C10
16	bg	103	0V9	C2-C3-O3-C30
14	AE	106	LMT	C2-C3-C4-C5
15	ag	101	V7N	C27-C28-C29-C39
14	BX	104	LMT	C3'-C4'-O1B-C1B
14	bi	104	LMT	C11-C10-C9-C8
14	bn	103	LMT	C7-C8-C9-C10
16	M	403	0V9	C35-C36-C37-C38
15	AD	101	V7N	C3-C4-C5-C6
13	bg	104	BCL	C11-C10-C8-C9
13	bk	103	BCL	C11-C12-C13-C14
13	bo	102	BCL	C6-C7-C8-C9
14	AP	101	LMT	C2-C3-C4-C5
16	be	105	0V9	C36-C37-C38-C39
16	ad	103	0V9	C18-C19-C20-C21
13	AT	103	BCL	C2A-CAA-CBA-CGA
13	AG	102	BCL	C2-C1-O2A-CGA
13	AQ	104	BCL	C2-C1-O2A-CGA
14	BD	102	LMT	C9-C10-C11-C12
13	AM	1002	BCL	C3A-C2A-CAA-CBA
13	BB	105	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	BI	1004	BCL	C3A-C2A-CAA-CBA
13	BK	1002	BCL	C3A-C2A-CAA-CBA
13	be	103	BCL	C3A-C2A-CAA-CBA
13	bf	102	BCL	C3A-C2A-CAA-CBA
13	bh	103	BCL	C4-C3-C5-C6
13	bo	102	BCL	C3A-C2A-CAA-CBA
17	C	1001	HEC	CAD-CBD-CGD-O1D
16	bi	103	0V9	C2-C3-O3-C30
16	ab	1002	0V9	C33-C34-C35-C36
14	bp	101	LMT	C2'-C1'-O1'-C1
13	ah	1001	BCL	C10-C11-C12-C13
13	BV	1005	BCL	O2A-C1-C2-C3
22	L	301	BPH	O2A-C1-C2-C3
16	bd	103	0V9	C16-C17-C18-C19
14	AJ	102	LMT	C5'-C4'-O1B-C1B
26	ag	103	V7B	C16-C17-C18-C19
17	C	1002	HEC	CAA-CBA-CGA-O2A
14	BN	1004	LMT	C4-C5-C6-C7
13	BR	1003	BCL	C8-C10-C11-C12
13	AL	103	BCL	C2A-CAA-CBA-CGA
13	BD	104	BCL	C2A-CAA-CBA-CGA
13	bo	102	BCL	C2A-CAA-CBA-CGA
14	ac	101	LMT	C6-C7-C8-C9
14	BR	1006	LMT	C5'-C4'-O1B-C1B
14	BE	103	LMT	C2B-C1B-O1B-C4'
14	BR	1002	LMT	C2B-C1B-O1B-C4'
14	BF	102	LMT	C3'-C4'-O1B-C1B
13	bg	104	BCL	C13-C15-C16-C17
16	bh	104	0V9	C18-C19-C20-C21
16	bo	103	0V9	C18-C19-C20-C21
17	C	1002	HEC	CAA-CBA-CGA-O1A
14	AM	1003	LMT	C2B-C1B-O1B-C4'
14	BK	1005	LMT	C2B-C1B-O1B-C4'
21	H1	103	CD4	C30-C31-O10-P2
15	BD	101	V7N	C23-C24-C25-C26
15	BO	1001	V7N	C23-C24-C25-C26
15	bl	101	V7N	C23-C24-C25-C26
14	AD	102	LMT	C2B-C1B-O1B-C4'
14	bo	104	LMT	C3-C4-C5-C6
14	AE	106	LMT	C4-C5-C6-C7
13	BE	104	BCL	C5-C6-C7-C8
14	AK	101	LMT	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BD	105	LMT	C5'-C4'-O1B-C1B
21	af	104	CD4	C44-C45-C63-C64
16	bj	103	0V9	C33-C34-C35-C36
26	af	101	V7B	C35-C36-C37-C38
13	AG	103	BCL	C15-C16-C17-C18
13	BC	104	BCL	C5-C6-C7-C8
14	BR	1005	LMT	C2-C3-C4-C5
13	M	406	BCL	C4B-C3B-CAB-CBB
13	BL	103	BCL	C3-C5-C6-C7
22	L	301	BPH	C8-C10-C11-C12
13	ao	102	BCL	C11-C12-C13-C14
13	bg	104	BCL	C11-C12-C13-C14
13	bj	104	BCL	C16-C17-C18-C19
14	BI	1002	LMT	C5'-C4'-O1B-C1B
14	BO	1002	LMT	C5'-C4'-O1B-C1B
14	AJ	102	LMT	C2-C3-C4-C5
16	be	105	0V9	C18-C19-C20-C21
16	bo	103	0V9	C16-C17-C18-C19
13	ac	102	BCL	CAA-CBA-CGA-O2A
16	L	310	0V9	O3-C30-C31-C32
16	bp	105	0V9	O3-C30-C31-C32
20	H1	101	PGW	O01-C1-C2-C3
21	af	102	CD4	O3-C17-C18-C19
16	M	403	0V9	O4-C10-O2-C2
21	H1	103	CD4	C26-C27-C60-C61
14	AP	101	LMT	C2B-C1B-O1B-C4'
14	C2	1001	LMT	C5'-C4'-O1B-C1B
21	H1	103	CD4	C16-C15-C28-O5
13	BR	1003	BCL	C4-C3-C5-C6
15	BN	1001	V7N	O32-C1-C2-C3
15	bk	101	V7N	O32-C1-C2-C3
21	M	405	CD4	C21-C22-C23-C24
13	bm	102	BCL	C15-C16-C17-C18
13	BG	1004	BCL	CAA-CBA-CGA-O2A
14	AA	1003	LMT	C5-C6-C7-C8
14	AL	101	LMT	C9-C10-C11-C12
13	AI	101	BCL	C12-C13-C15-C16
13	AO	101	BCL	C12-C13-C15-C16
13	AS	102	BCL	C11-C12-C13-C15
13	AV	103	BCL	C11-C10-C8-C7
13	BJ	1004	BCL	C11-C12-C13-C15
13	BV	1005	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	ad	102	BCL	C6-C7-C8-C10
13	af	103	BCL	C11-C10-C8-C7
13	bf	102	BCL	C12-C13-C15-C16
13	bk	103	BCL	C11-C12-C13-C15
13	bo	102	BCL	C6-C7-C8-C10
13	AS	101	BCL	C3-C5-C6-C7
14	BT	101	LMT	C3'-C4'-O1B-C1B
13	bp	104	BCL	CAA-CBA-CGA-O2A
16	bd	103	OV9	O4-C10-O2-C2
14	bg	102	LMT	C5-C6-C7-C8
13	bj	104	BCL	C2-C1-O2A-CGA
13	AL	102	BCL	C10-C11-C12-C13
14	BC	101	LMT	C2B-C1B-O1B-C4'
14	BR	1005	LMT	C3-C4-C5-C6
21	ad	101	CD4	O3-C17-C18-C19
13	am	1001	BCL	C5-C6-C7-C8
14	AC	103	LMT	C5'-C4'-O1B-C1B
13	bj	104	BCL	C15-C16-C17-C18
16	ab	1002	OV9	O2-C10-C11-C12
16	bf	103	OV9	O3-C30-C31-C32
13	AS	101	BCL	C2-C3-C5-C6
14	BL	101	LMT	C4-C5-C6-C7
14	bm	103	LMT	C3-C4-C5-C6
16	bh	104	OV9	O3-C30-C31-C32
21	M	409	CD4	O3-C17-C18-C19
14	BW	1003	LMT	O5B-C1B-O1B-C4'
14	BD	103	LMT	C4'-C5'-C6'-O6'
20	H1	101	PGW	C20-C19-O03-C01
16	bp	105	OV9	O2-C10-C11-C12
16	bj	103	OV9	C30-C31-C32-C33
14	BR	1004	LMT	C1-C2-C3-C4
14	C2	1001	LMT	C11-C10-C9-C8
13	AV	101	BCL	C4-C3-C5-C6
13	BK	1002	BCL	C4-C3-C5-C6
13	AE	103	BCL	CAA-CBA-CGA-O2A
13	AH	102	BCL	CAA-CBA-CGA-O2A
13	bm	102	BCL	CAA-CBA-CGA-O2A
16	bo	103	OV9	O2-C10-C11-C12
16	M	403	OV9	C36-C37-C38-C39
20	H1	101	PGW	C25-C26-C27-C15
27	ai	102	UYH	C15-C16-C17-C18
14	BC	102	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	BE	101	V7N	C23-C24-C25-C26
15	bm	101	V7N	C23-C24-C25-C26
14	BS	1003	LMT	C2B-C1B-O1B-C4'
17	C	1001	HEC	CAA-CBA-CGA-O1A
13	AT	101	BCL	C15-C16-C17-C18
14	BF	104	LMT	C5'-C4'-O1B-C1B
14	C2	1001	LMT	C3-C4-C5-C6
13	AP	103	BCL	C8-C10-C11-C12
14	AT	102	LMT	C3-C4-C5-C6
13	AG	103	BCL	C6-C7-C8-C9
13	ac	102	BCL	C11-C12-C13-C14
14	BE	105	LMT	C5'-C4'-O1B-C1B
14	BP	1002	LMT	C3'-C4'-O1B-C1B
14	BV	1004	LMT	C5'-C4'-O1B-C1B
13	AA	1002	BCL	C1A-C2A-CAA-CBA
13	BH	1005	BCL	C1A-C2A-CAA-CBA
13	BI	1004	BCL	C1A-C2A-CAA-CBA
13	BK	1002	BCL	C1A-C2A-CAA-CBA
13	BT	103	BCL	C1A-C2A-CAA-CBA
13	aa	1001	BCL	C1A-C2A-CAA-CBA
13	bp	104	BCL	C1A-C2A-CAA-CBA
21	M	405	CD4	C9-C10-C11-C12
14	AV	102	LMT	O5'-C1'-O1'-C1
14	BO	1004	LMT	O5'-C1'-O1'-C1
17	C	1001	HEC	CAA-CBA-CGA-O2A
14	BI	1005	LMT	O5B-C5B-C6B-O6B
14	BJ	1006	LMT	C5-C6-C7-C8
14	BT	101	LMT	C2B-C1B-O1B-C4'
15	AA	1004	V7N	C3-C4-C5-C6
15	BK	1001	V7N	C3-C4-C5-C6
15	bd	101	V7N	C27-C28-C29-C39
13	AM	1002	BCL	O1A-CGA-O2A-C1
16	bl	102	0V9	C16-C17-C18-C19
14	L	306	LMT	C5'-C4'-O1B-C1B
16	bi	103	0V9	C20-C21-C22-C23
27	ai	102	UYH	C20-C21-C22-C23
13	BE	104	BCL	CAA-CBA-CGA-O2A
14	BR	1002	LMT	C3'-C4'-O1B-C1B
13	AG	102	BCL	C2A-CAA-CBA-CGA
13	BF	103	BCL	C2A-CAA-CBA-CGA
13	BK	1002	BCL	C2A-CAA-CBA-CGA
13	BM	1004	BCL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	BG	1002	LMT	C5'-C4'-O1B-C1B
13	AH	105	BCL	CAA-CBA-CGA-O2A
14	AM	1003	LMT	C5-C6-C7-C8
13	bd	102	BCL	C8-C10-C11-C12
13	bm	102	BCL	C10-C11-C12-C13
21	af	102	CD4	C18-C19-C20-C21
15	BH	1001	V7N	C23-C24-C25-C26
13	AV	101	BCL	C5-C6-C7-C8
14	BF	104	LMT	C4'-C5'-C6'-O6'
13	AW	102	BCL	C4-C3-C5-C6
13	aj	101	BCL	C2-C1-O2A-CGA
13	AI	101	BCL	CAA-CBA-CGA-O2A
13	AH	102	BCL	C11-C12-C13-C15
13	BR	1003	BCL	C6-C7-C8-C10
13	BU	1004	BCL	C11-C10-C8-C7
13	ac	102	BCL	C11-C12-C13-C15
13	bg	104	BCL	C11-C10-C8-C7
13	bp	104	BCL	C11-C12-C13-C15
14	BW	1003	LMT	C2-C3-C4-C5
14	H2	201	LMT	C5'-C4'-O1B-C1B
16	ab	1002	0V9	C1-C2-O2-C10
16	bb	103	0V9	C3-C2-O2-C10
16	bg	103	0V9	O5-C30-C31-C32
13	AF	1001	BCL	C5-C6-C7-C8
13	AX	102	BCL	C5-C6-C7-C8
13	an	1001	BCL	C13-C15-C16-C17
13	AS	102	BCL	C2C-C3C-CAC-CBC
15	BN	1001	V7N	C31-C1-C2-C3
15	bk	101	V7N	C30-C1-C2-C3
16	bi	103	0V9	O4-C10-O2-C2
16	be	105	0V9	O2-C10-C11-C12
16	ad	103	0V9	C32-C33-C34-C35
21	H1	103	CD4	C50-C51-C52-C53
13	AG	102	BCL	C3A-C2A-CAA-CBA
13	AS	101	BCL	C3A-C2A-CAA-CBA
13	AT	103	BCL	C3A-C2A-CAA-CBA
13	bi	102	BCL	C3A-C2A-CAA-CBA
15	bb	101	V7N	C37-C22-C23-C24
23	L	303	MQ8	C39-C38-C40-C41
21	M	409	CD4	O4-C17-C18-C19
13	AA	1002	BCL	C15-C16-C17-C18
16	bk	102	0V9	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	AJ	103	BCL	C15-C16-C17-C18
14	BM	1002	LMT	C4-C5-C6-C7
13	AH	102	BCL	CAA-CBA-CGA-O1A
16	bh	104	0V9	O5-C30-C31-C32
14	BP	1006	LMT	C5'-C4'-O1B-C1B
13	AV	101	BCL	CAA-CBA-CGA-O2A
16	bi	103	0V9	O2-C10-C11-C12
14	AP	101	LMT	C5'-C4'-O1B-C1B
23	L	303	MQ8	C40-C41-C42-C43
13	bm	102	BCL	CAA-CBA-CGA-O1A
16	ab	1002	0V9	O4-C10-C11-C12
16	bf	103	0V9	O5-C30-C31-C32
16	bp	105	0V9	O4-C10-C11-C12
21	ad	101	CD4	O4-C17-C18-C19
13	M	406	BCL	C4B-C3B-CAB-OBB
13	AI	101	BCL	C14-C13-C15-C16
13	AV	103	BCL	C11-C10-C8-C9
22	M	407	BPH	C14-C13-C15-C16
13	AH	105	BCL	CAA-CBA-CGA-O1A
16	L	310	0V9	C32-C33-C34-C35
16	bl	102	0V9	C35-C36-C37-C38
14	BQ	1003	LMT	C9-C10-C11-C12
13	AI	101	BCL	C3-C5-C6-C7
13	BD	104	BCL	C10-C11-C12-C13
13	AW	102	BCL	CAA-CBA-CGA-O2A
13	AV	101	BCL	C2-C3-C5-C6
13	bo	102	BCL	C2-C3-C5-C6
22	M	407	BPH	C13-C15-C16-C17
15	BO	1001	V7N	C1-C2-C3-C4
15	bc	101	V7N	C1-C2-C3-C4
15	bh	101	V7N	C1-C2-C3-C4
15	bp	102	V7N	C1-C2-C3-C4
13	AE	103	BCL	CAA-CBA-CGA-O1A
13	AX	103	BCL	CAA-CBA-CGA-O1A
14	C	1005	LMT	C5-C6-C7-C8
14	BC	103	LMT	C5'-C4'-O1B-C1B
13	BJ	1004	BCL	C13-C15-C16-C17
26	ag	103	V7B	C33-C34-C35-C36
21	M	405	CD4	C7-C8-C9-C10
13	AF	1001	BCL	CAA-CBA-CGA-O2A
13	AW	102	BCL	C15-C16-C17-C18
13	bl	104	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	bp	104	BCL	CAA-CBA-CGA-O1A
20	H1	101	PGW	O02-C1-C2-C3
14	AG	101	LMT	C5-C6-C7-C8
14	be	104	LMT	C5-C6-C7-C8
13	ac	102	BCL	CAA-CBA-CGA-O1A
13	AQ	103	BCL	C13-C15-C16-C17
13	am	1001	BCL	C10-C11-C12-C13
14	BS	1003	LMT	C3'-C4'-O1B-C1B
13	be	103	BCL	C2A-CAA-CBA-CGA
14	BN	1003	LMT	O5B-C5B-C6B-O6B
16	L	310	0V9	O5-C30-C31-C32
15	AD	101	V7N	C23-C24-C25-C26
14	BF	104	LMT	C1-C2-C3-C4
14	BH	1004	LMT	C1-C2-C3-C4
13	BP	1003	BCL	C5-C6-C7-C8
14	AL	101	LMT	C5'-C4'-O1B-C1B
13	BG	1004	BCL	CAA-CBA-CGA-O1A
16	bo	103	0V9	C10-C11-C12-C13
16	ad	103	0V9	C35-C36-C37-C38
14	AA	1003	LMT	C1-C2-C3-C4
14	BP	1005	LMT	C5-C6-C7-C8
16	M	403	0V9	C2-C3-O3-C30
16	bo	103	0V9	O4-C10-C11-C12
16	bp	105	0V9	O5-C30-C31-C32
14	BC	102	LMT	C5'-C4'-O1B-C1B
13	AF	1001	BCL	C15-C16-C17-C18
16	bp	105	0V9	O5-C30-O3-C3
14	BI	1003	LMT	C5-C6-C7-C8
14	bh	102	LMT	C4'-C5'-C6'-O6'
13	BF	103	BCL	C5-C6-C7-C8
14	AQ	101	LMT	C7-C8-C9-C10
21	af	102	CD4	O4-C17-C18-C19
13	AC	102	BCL	CAA-CBA-CGA-O2A
13	AG	102	BCL	CAA-CBA-CGA-O2A
13	AL	103	BCL	CAA-CBA-CGA-O2A
14	BM	1002	LMT	C2B-C1B-O1B-C4'
27	ai	102	UYH	O7-C10-C11-C12
13	bj	104	BCL	C16-C17-C18-C20
21	af	102	CD4	C49-C50-C51-C52
13	ao	102	BCL	C8-C10-C11-C12
13	BU	1004	BCL	C2A-CAA-CBA-CGA
14	BE	103	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	AK	103	LMT	C6-C7-C8-C9
14	AV	102	LMT	C6-C7-C8-C9
14	bm	103	LMT	C6-C7-C8-C9
13	bc	103	BCL	C4-C3-C5-C6
13	BC	104	BCL	C11-C12-C13-C15
13	AX	103	BCL	CAA-CBA-CGA-O2A
14	AC	103	LMT	C9-C10-C11-C12
13	AE	104	BCL	C8-C10-C11-C12
16	bi	103	OV9	C11-C10-O2-C2
16	be	105	OV9	O4-C10-C11-C12
13	AD	103	BCL	CAA-CBA-CGA-O2A
13	bh	103	BCL	CAA-CBA-CGA-O2A
14	BM	1003	LMT	C5'-C4'-O1B-C1B

There are no ring outliers.

94 monomers are involved in 117 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	AW	103	V7N	1	0
15	BS	1001	V7N	1	0
13	BS	1004	BCL	1	0
15	AA	1004	V7N	1	0
13	AD	103	BCL	1	0
13	bo	102	BCL	1	0
13	BC	104	BCL	1	0
13	bm	102	BCL	2	0
13	AU	103	BCL	1	0
13	AU	101	BCL	1	0
13	ak	1001	BCL	1	0
13	bk	103	BCL	1	0
17	C	1002	HEC	1	0
13	M	406	BCL	4	0
16	bm	104	OV9	1	0
21	H1	103	CD4	1	0
14	AN	101	LMT	1	0
13	AV	101	BCL	1	0
22	M	407	BPH	3	0
13	AE	104	BCL	1	0
14	BG	1005	LMT	1	0
13	bg	104	BCL	1	0
13	AA	1002	BCL	1	0
21	ad	101	CD4	1	0

Continued on next page...

Continued from previous page...

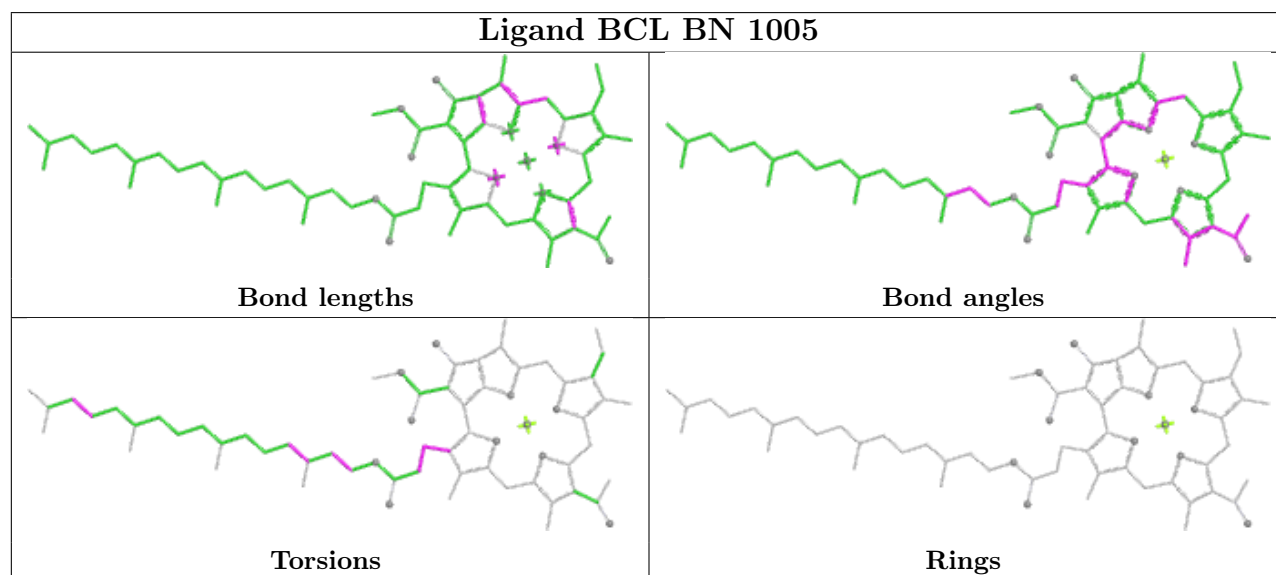
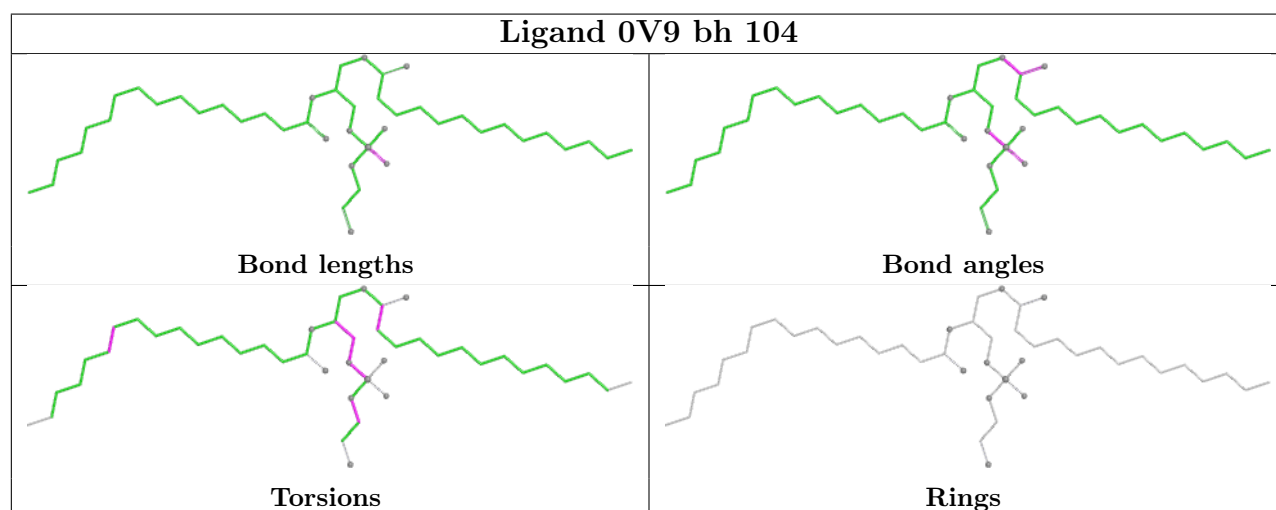
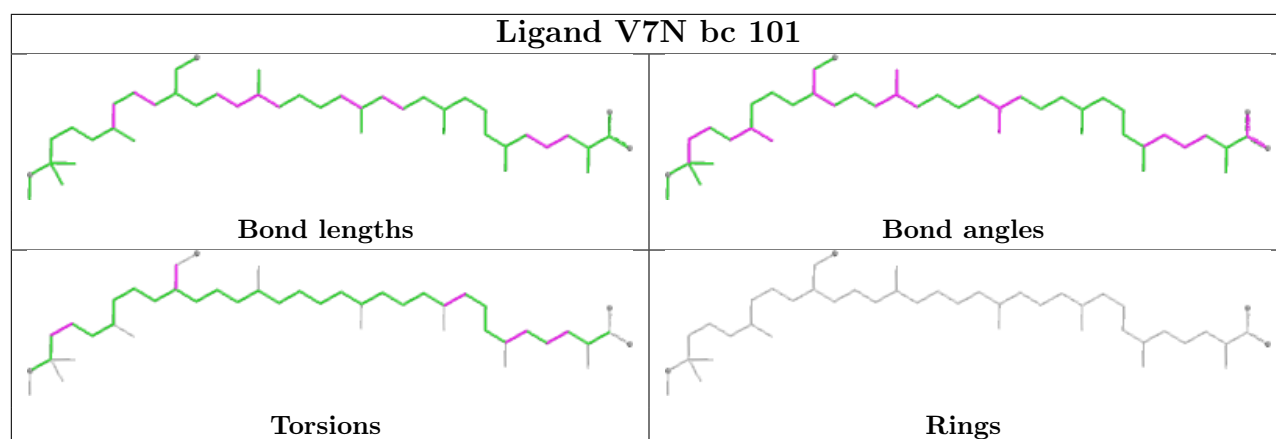
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AH	101	LMT	1	0
13	bd	102	BCL	2	0
23	M	402	MQ8	1	0
13	af	103	BCL	1	0
13	am	1001	BCL	1	0
13	AI	101	BCL	3	0
22	L	301	BPH	1	0
14	BS	1002	LMT	1	0
14	AB	1003	LMT	1	0
13	AM	1004	BCL	1	0
13	AH	105	BCL	2	0
14	L	307	LMT	1	0
14	AV	102	LMT	1	0
25	M	404	CRT	4	0
13	AB	1002	BCL	1	0
13	ad	102	BCL	1	0
13	ab	1001	BCL	3	0
13	M	408	BCL	1	0
13	ap	1001	BCL	1	0
13	AQ	103	BCL	1	0
13	AS	102	BCL	2	0
13	AF	1001	BCL	1	0
13	AO	101	BCL	1	0
14	AE	102	LMT	1	0
14	BW	1002	LMT	1	0
13	AW	101	BCL	2	0
13	AA	1001	BCL	2	0
14	C2	1001	LMT	1	0
21	af	102	CD4	2	0
14	BG	1003	LMT	1	0
13	AO	102	BCL	1	0
13	AK	102	BCL	2	0
13	ao	102	BCL	1	0
13	bc	103	BCL	1	0
13	AH	102	BCL	1	0
13	AH	103	BCL	1	0
13	AN	104	BCL	1	0
13	L	308	BCL	2	0
13	bn	102	BCL	1	0
13	AB	1001	BCL	1	0
13	AE	105	BCL	1	0
14	bc	102	LMT	1	0

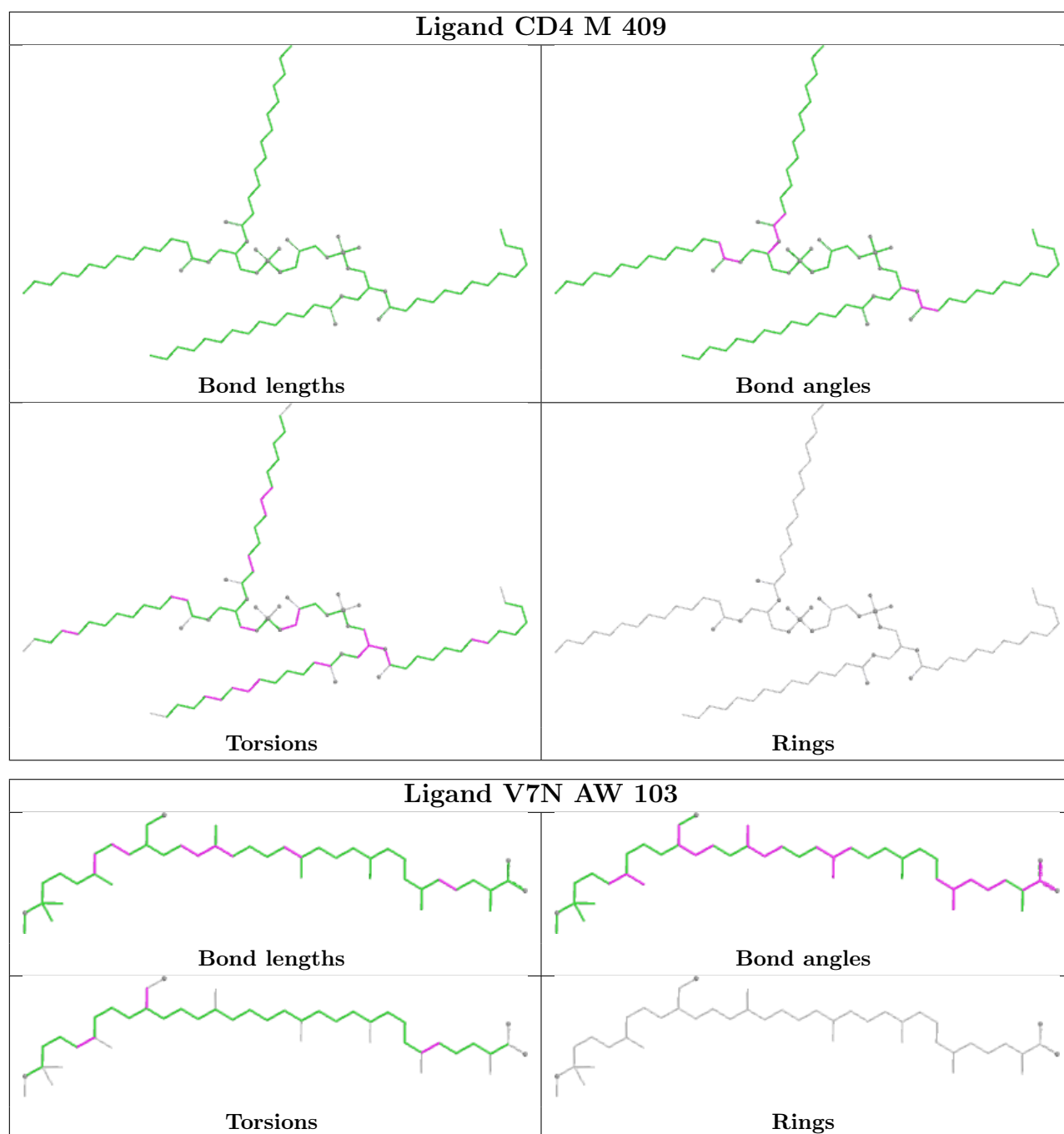
Continued on next page...

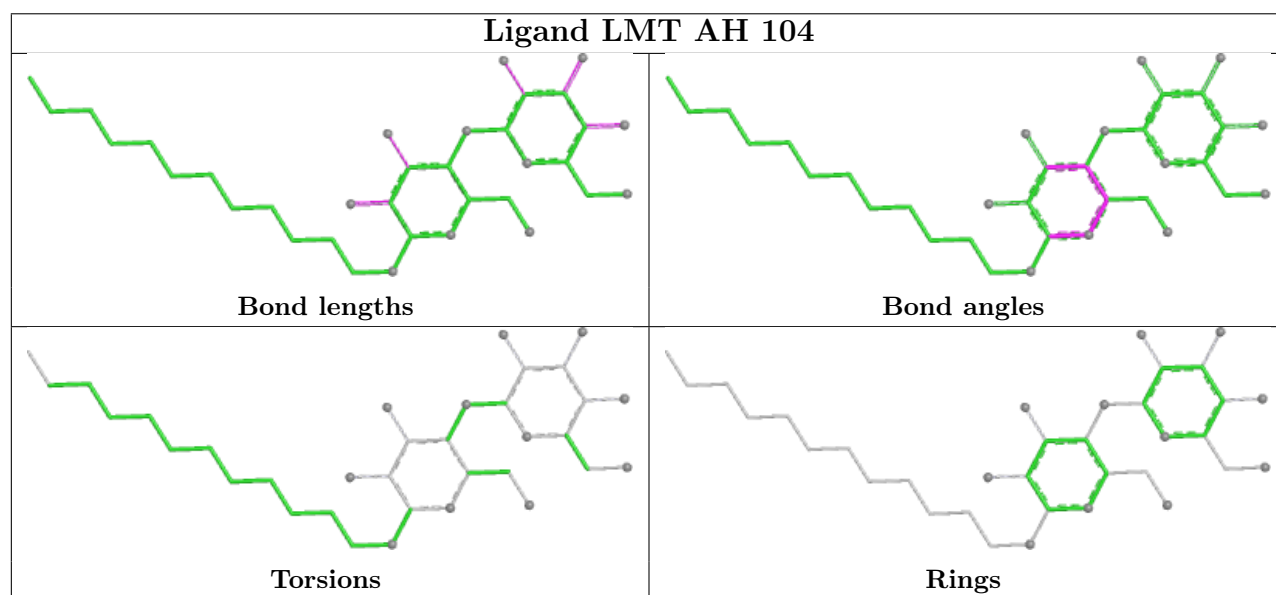
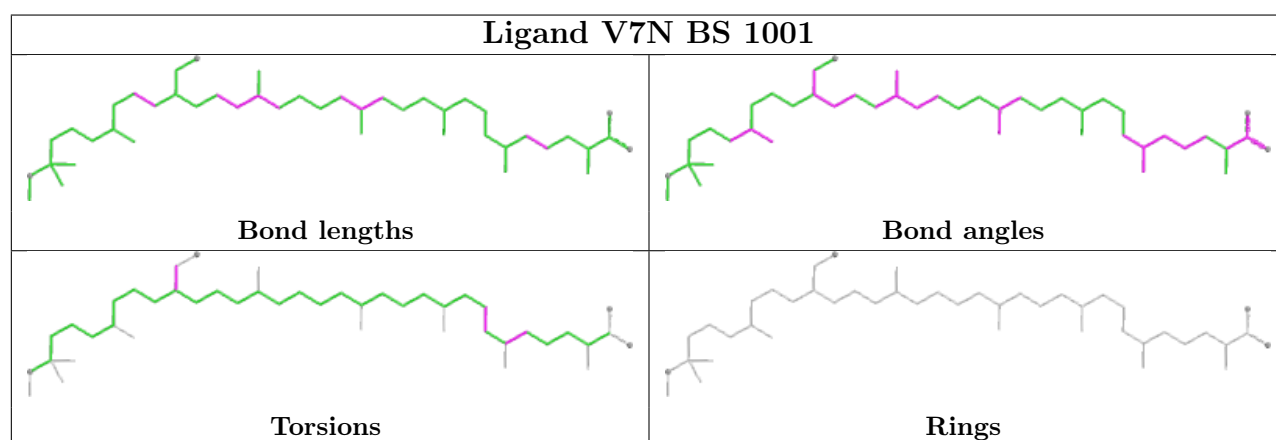
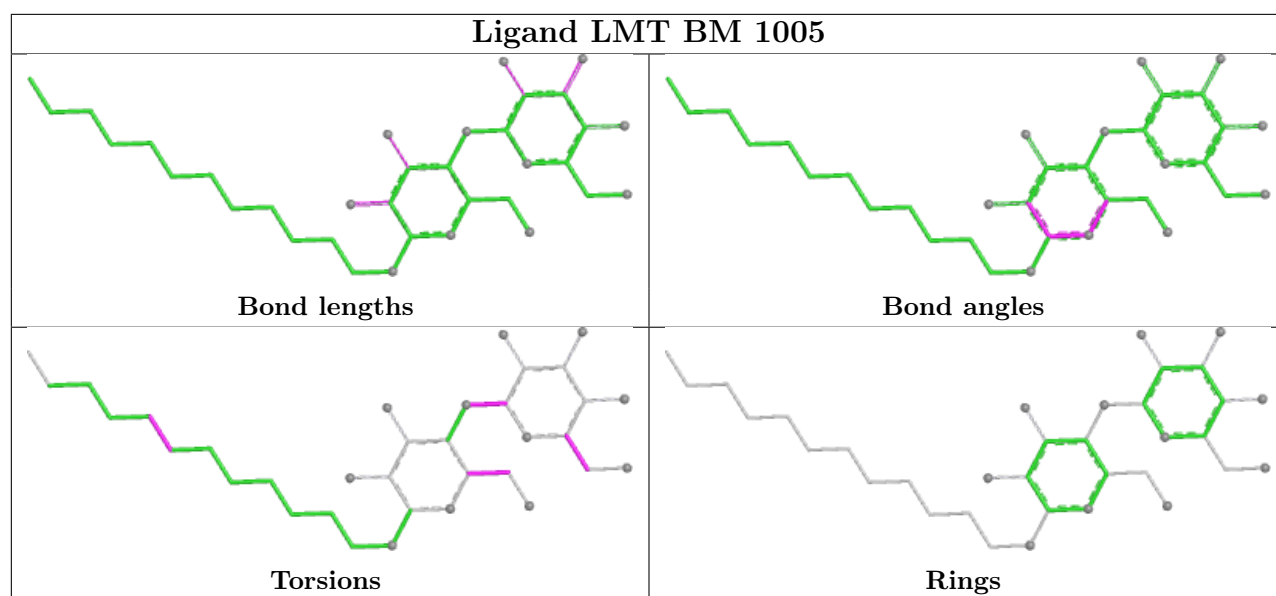
Continued from previous page...

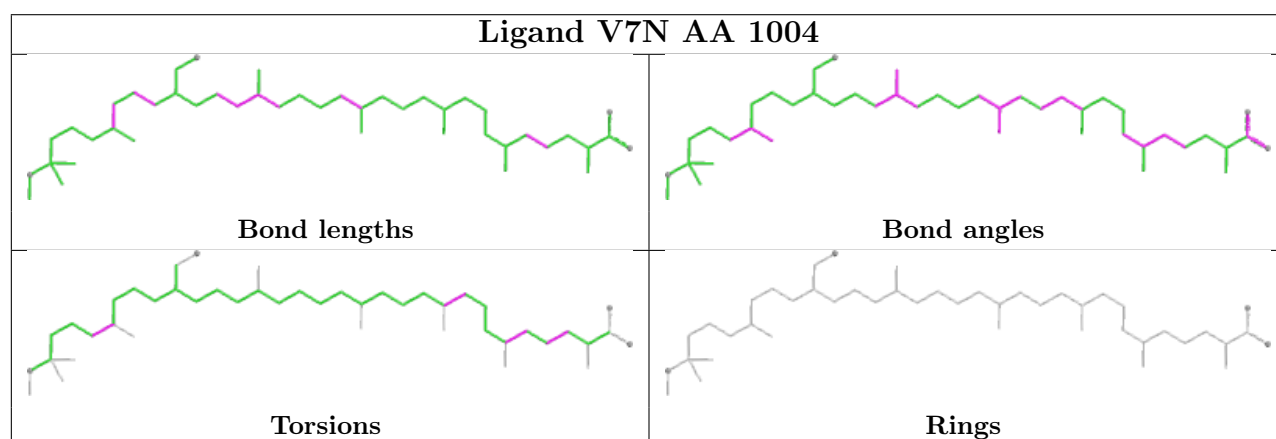
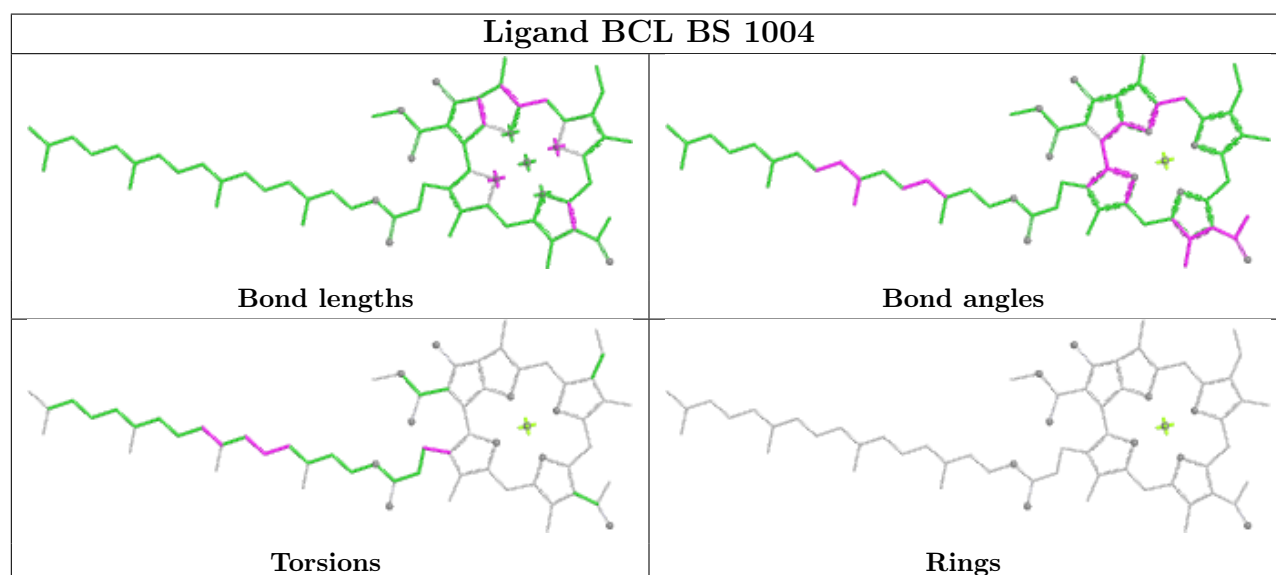
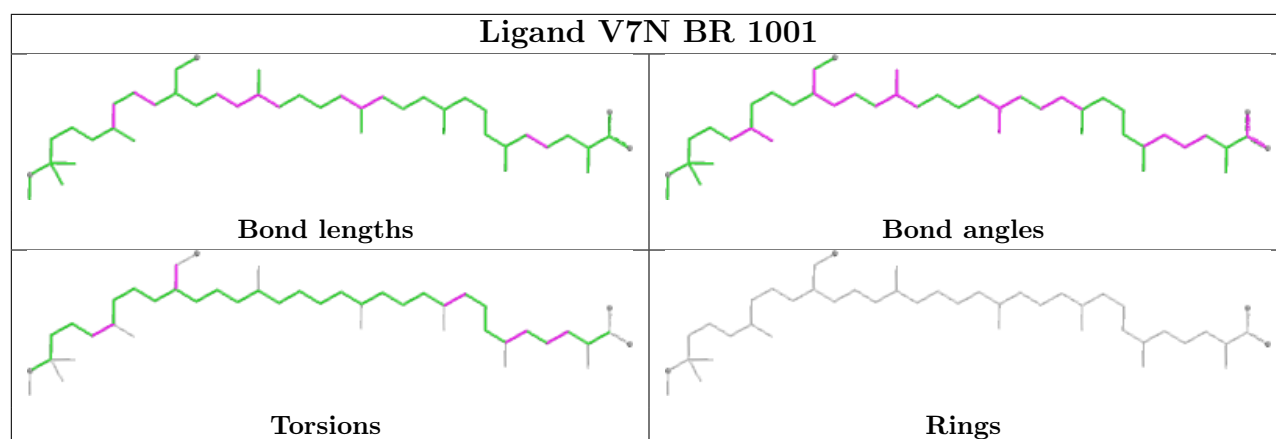
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	AJ	104	BCL	1	0
23	L	303	MQ8	2	0
13	AT	103	BCL	3	0
13	AP	102	BCL	1	0
13	AT	101	BCL	2	0
14	BS	1003	LMT	1	0
14	AK	101	LMT	2	0
17	C	1004	HEC	1	0
13	AK	104	BCL	1	0
13	be	103	BCL	1	0
27	ai	102	UYH	1	0
13	aj	101	BCL	1	0
13	AC	102	BCL	3	0
13	AQ	104	BCL	1	0
20	H1	101	PGW	1	0
13	AG	103	BCL	1	0
17	C	1003	HEC	2	0
13	AL	102	BCL	1	0
13	AX	103	BCL	1	0
17	C	1001	HEC	2	0
13	AD	104	BCL	1	0
14	AU	102	LMT	1	0
13	BH	1005	BCL	1	0
13	AR	101	BCL	1	0
13	AN	103	BCL	2	0
13	aa	1001	BCL	3	0
13	AC	101	BCL	1	0
13	AX	102	BCL	2	0

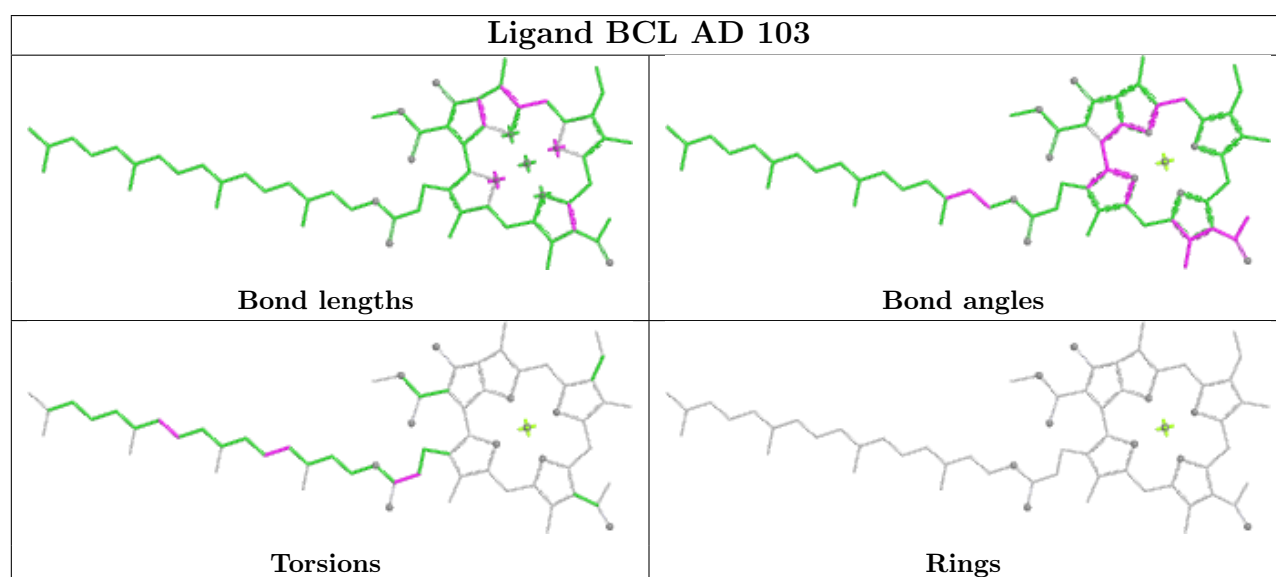
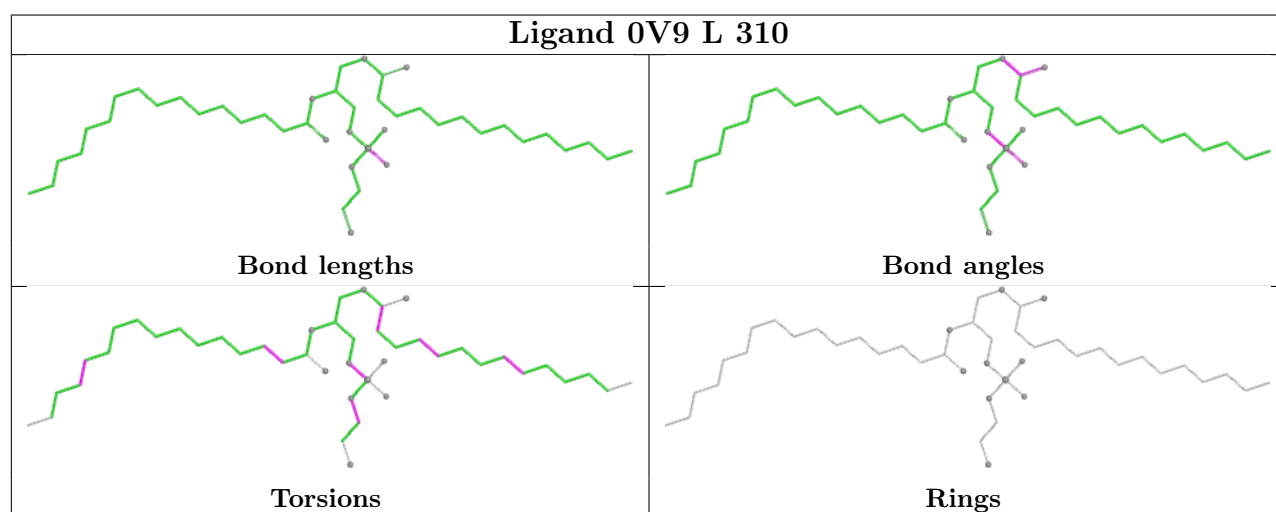
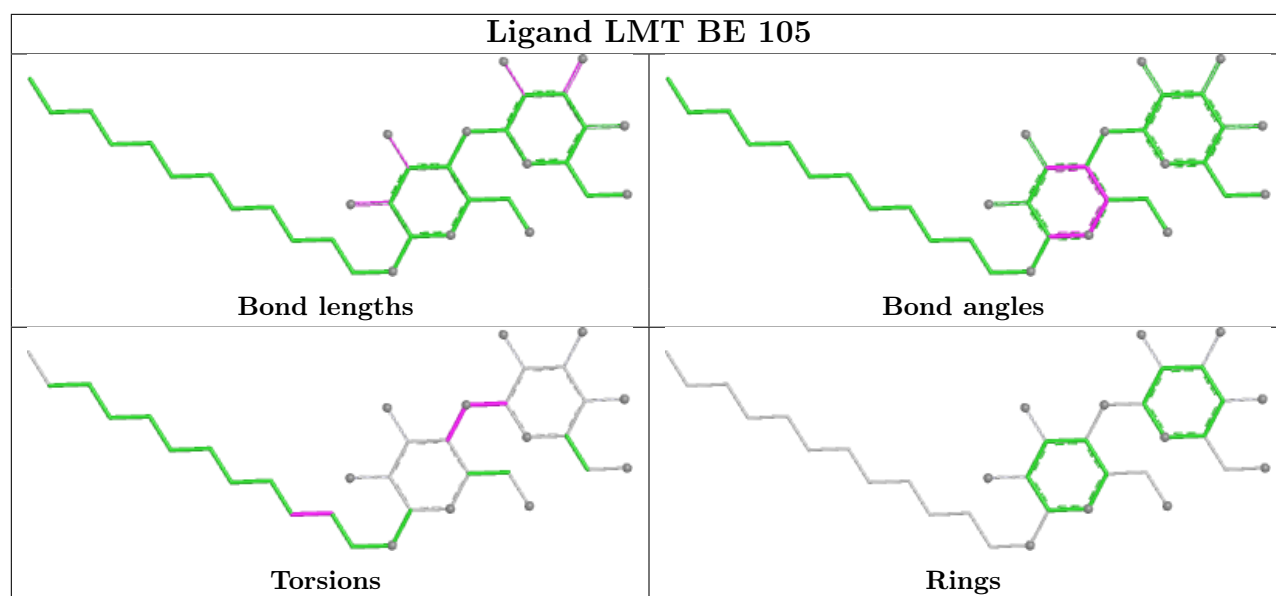
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

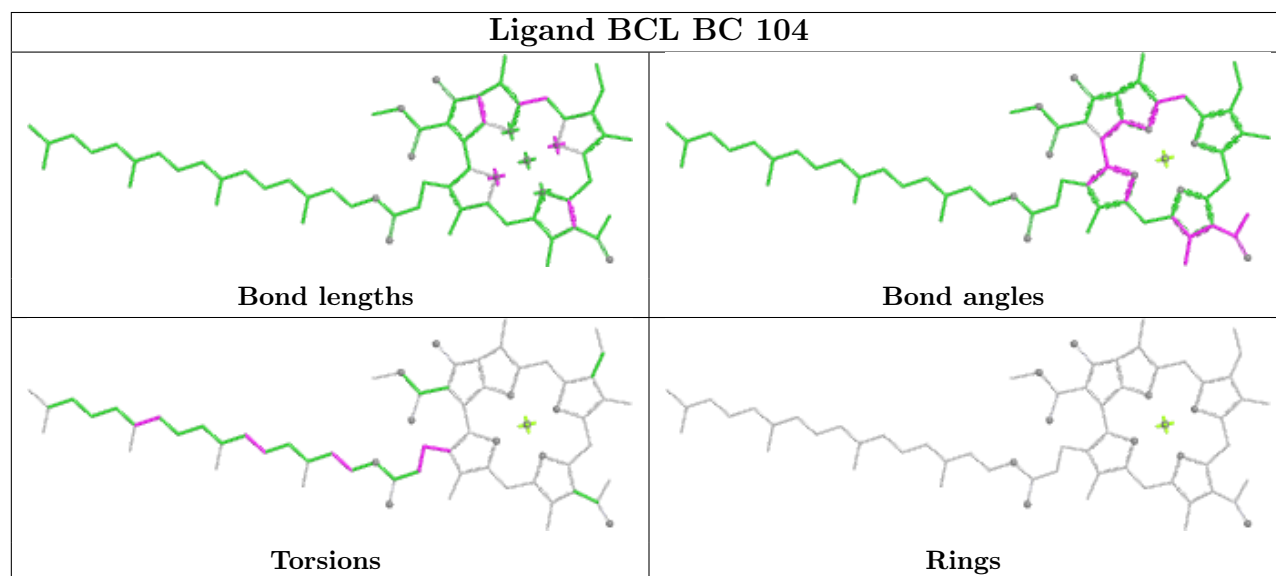
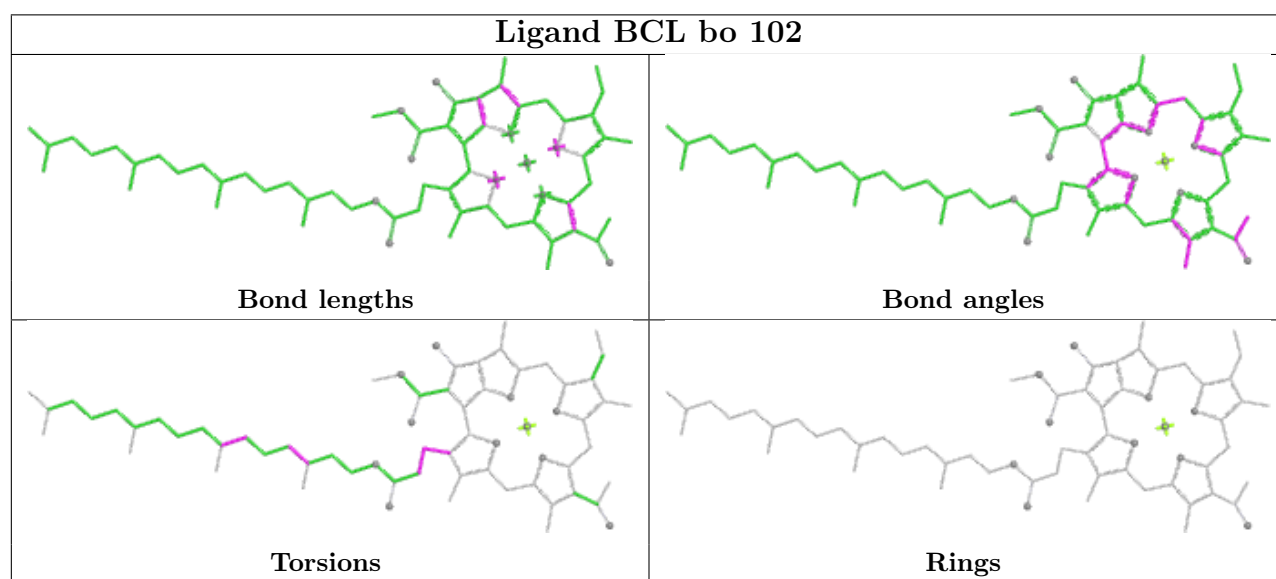
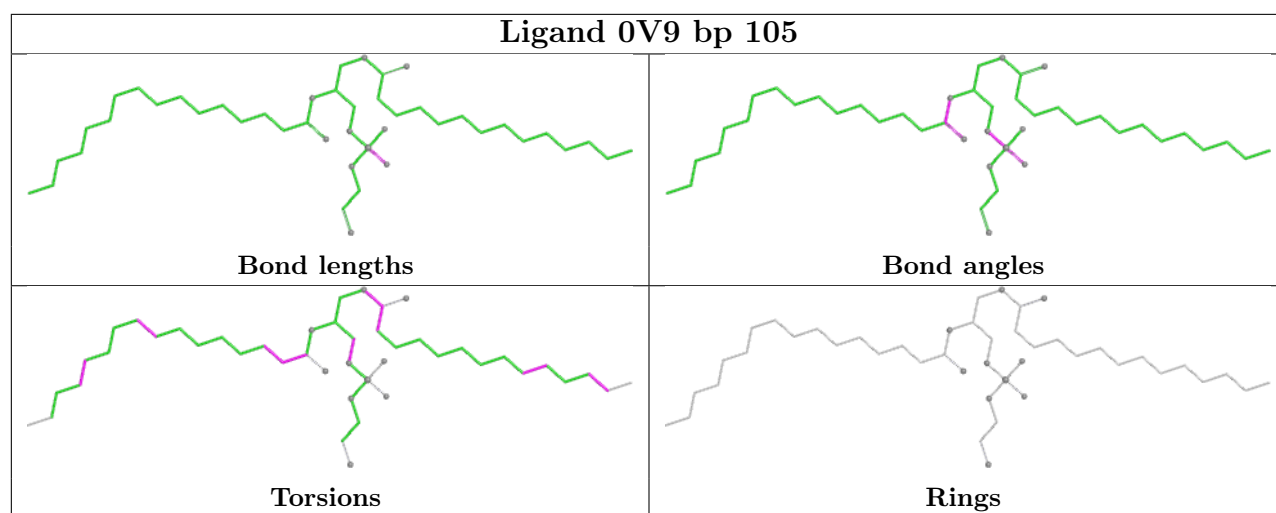


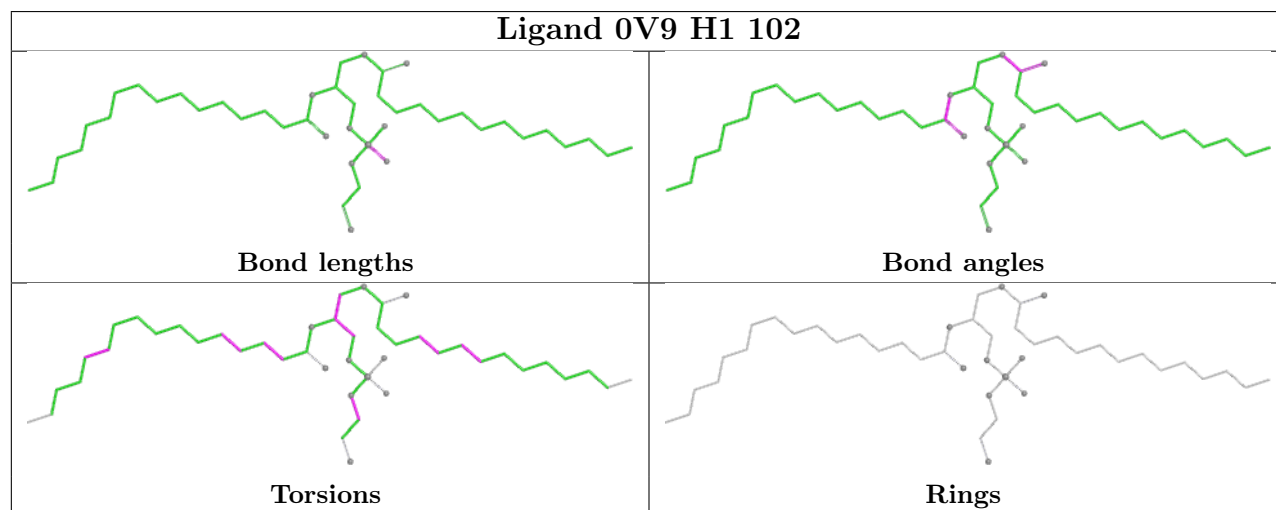
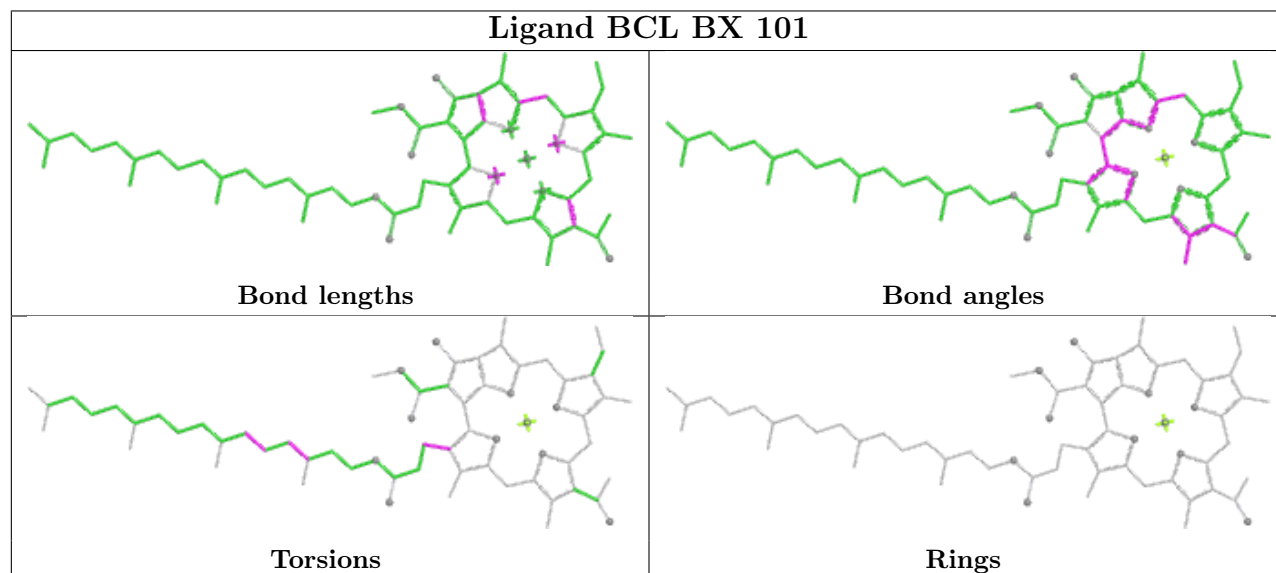
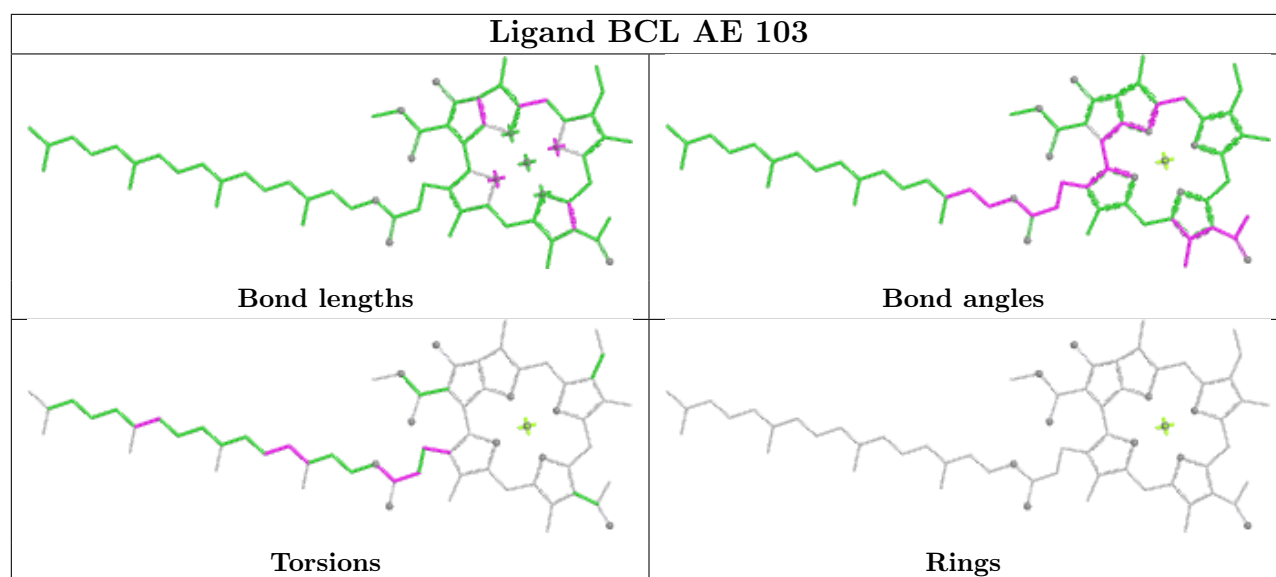


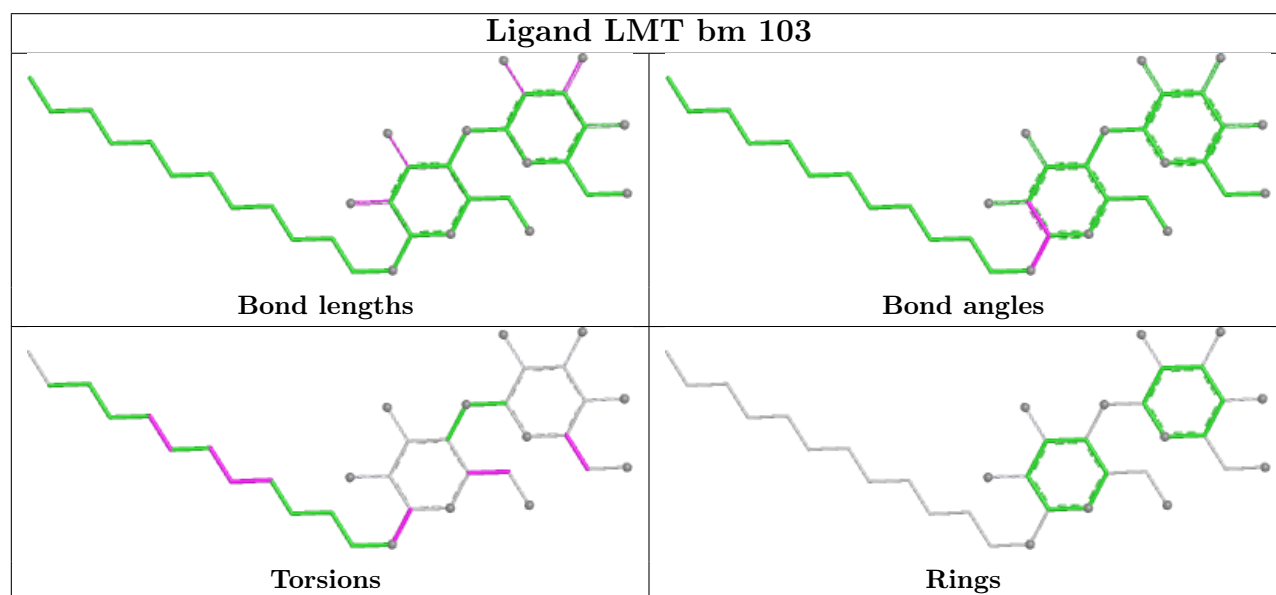
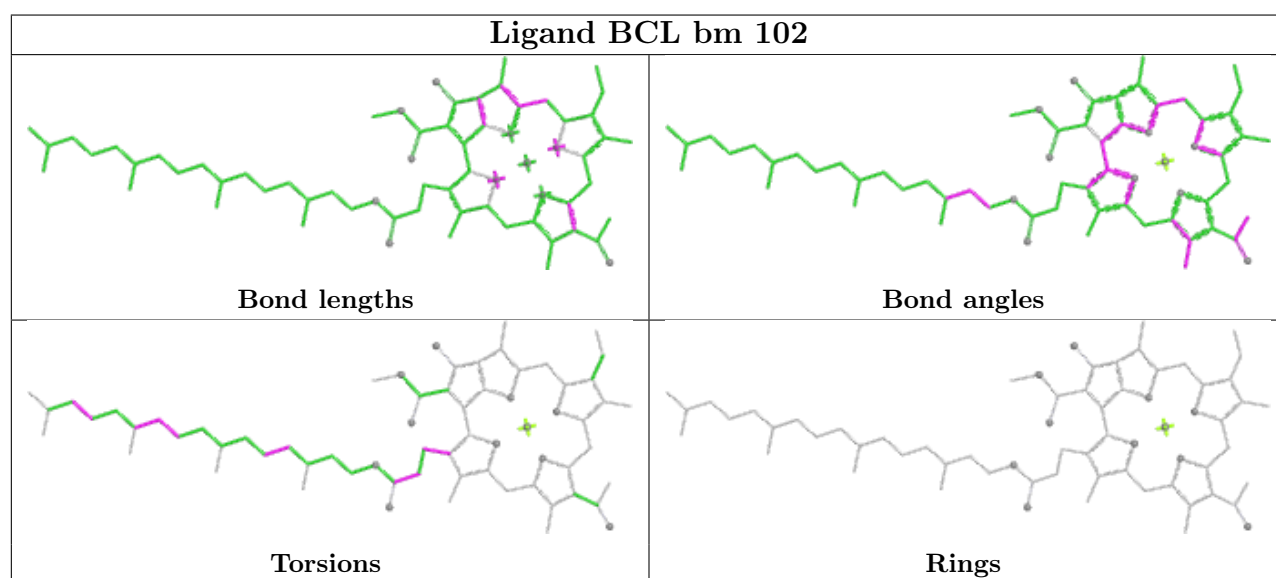
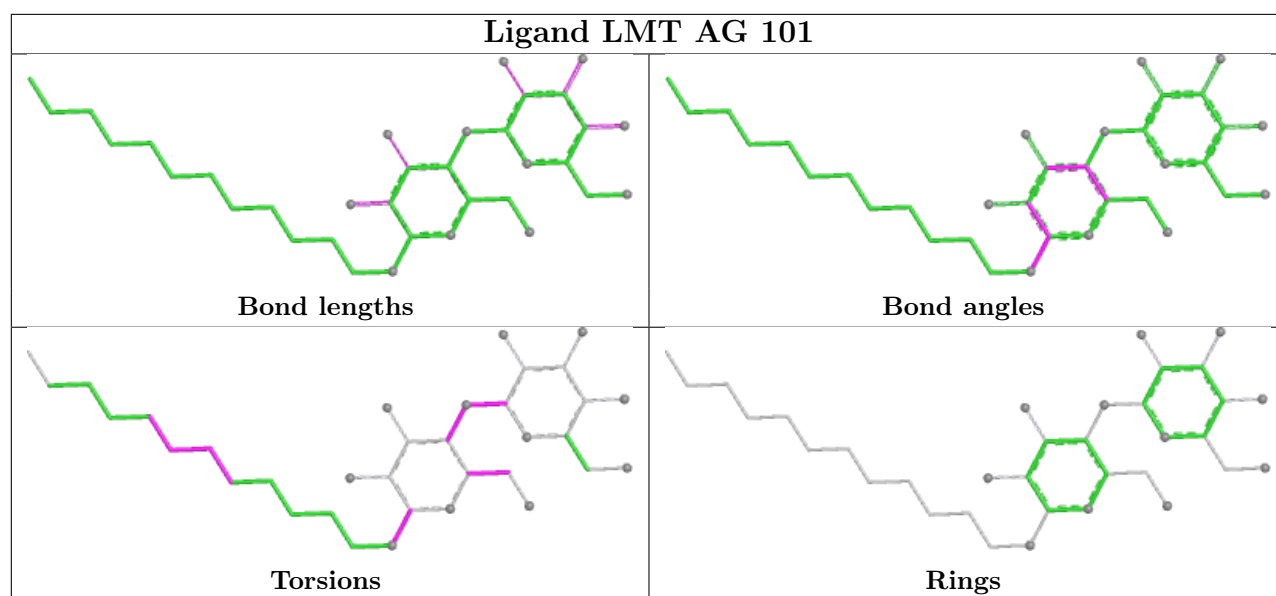


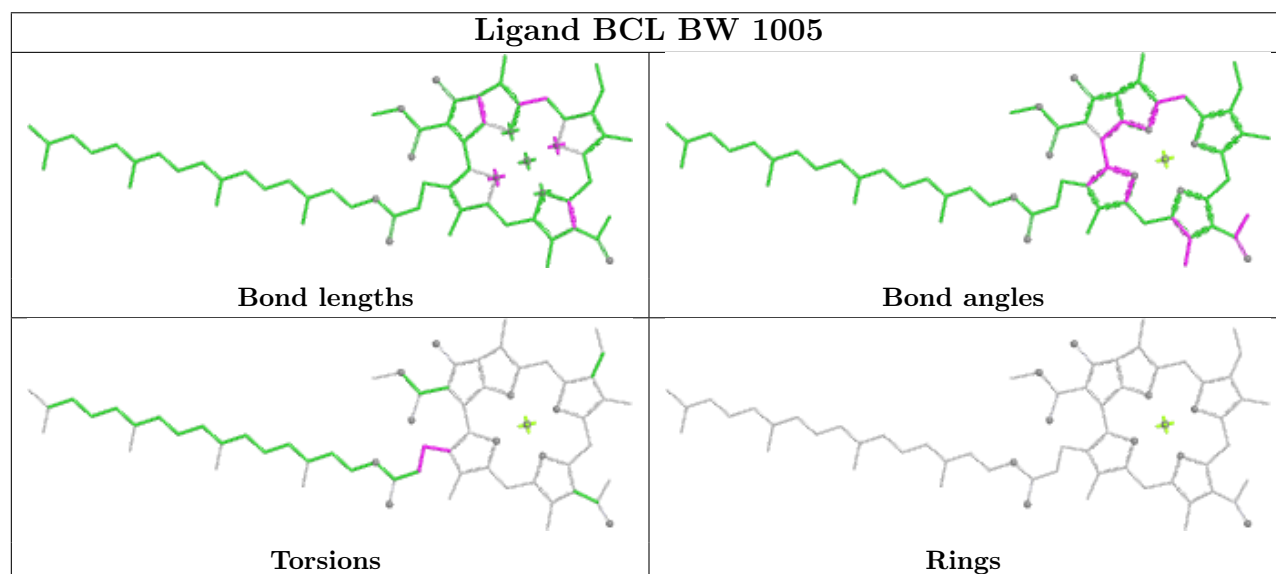
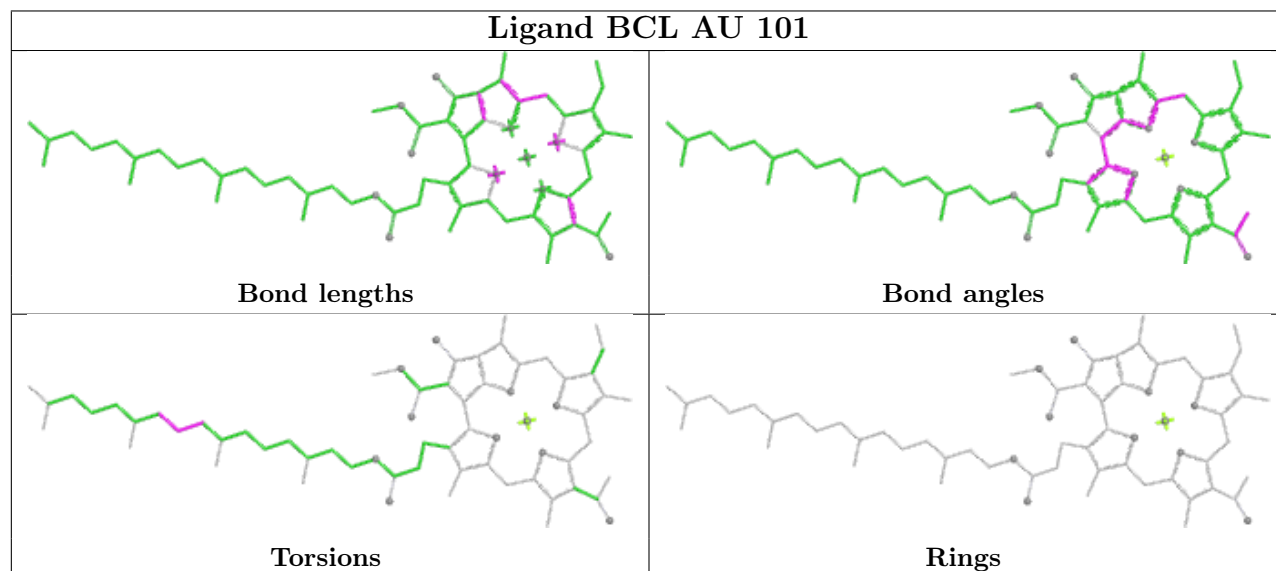
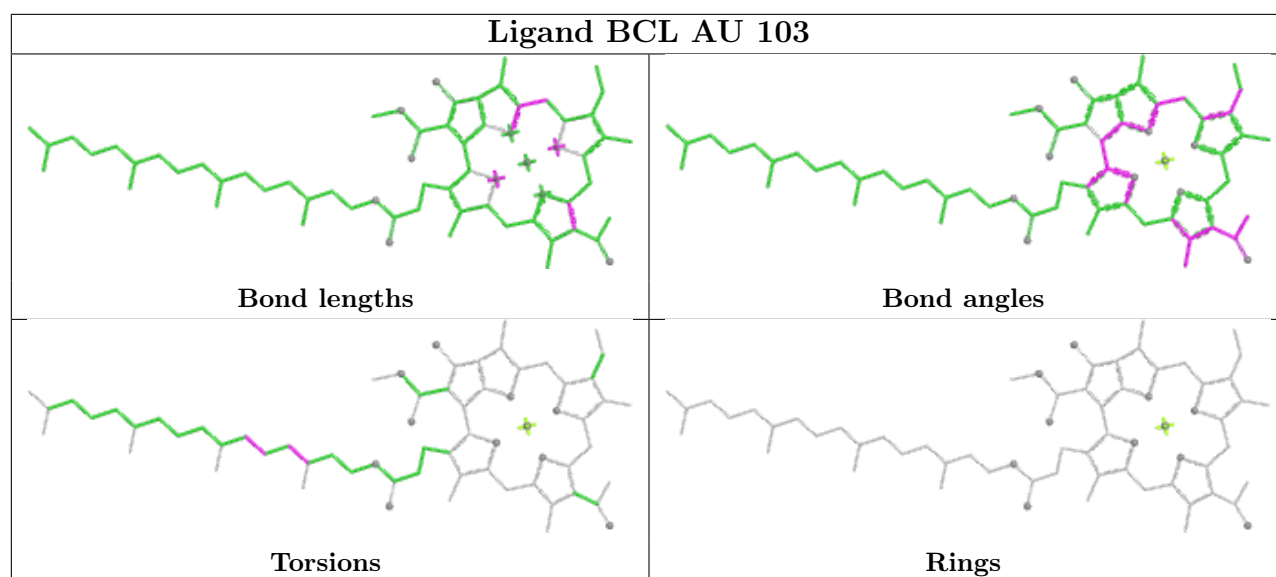


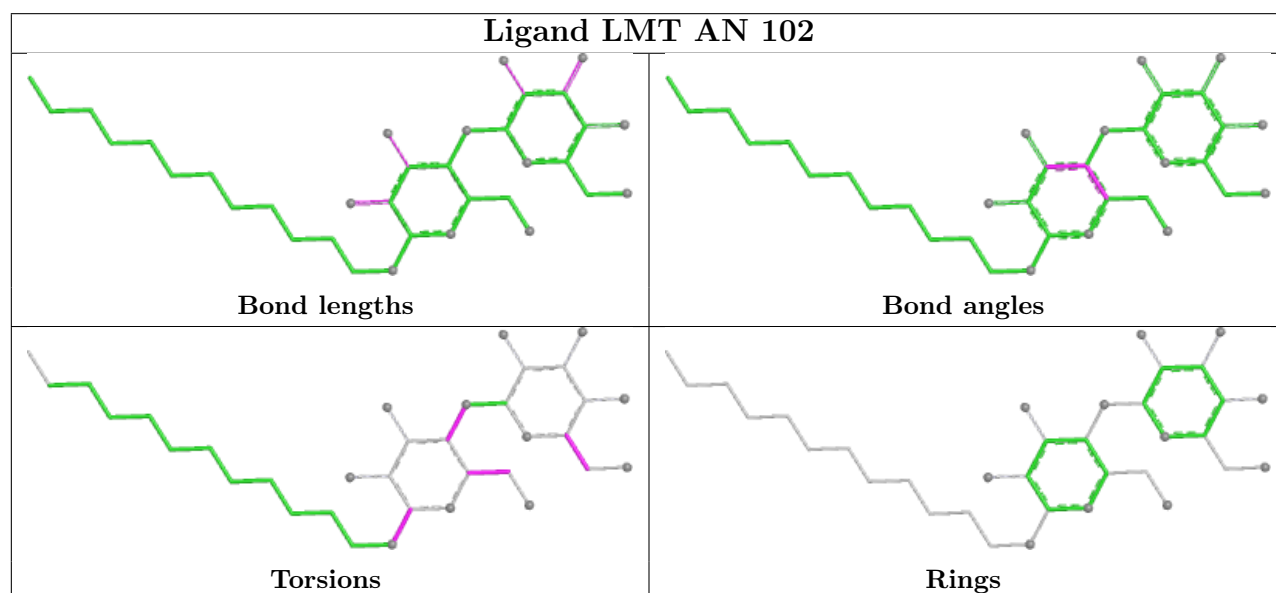
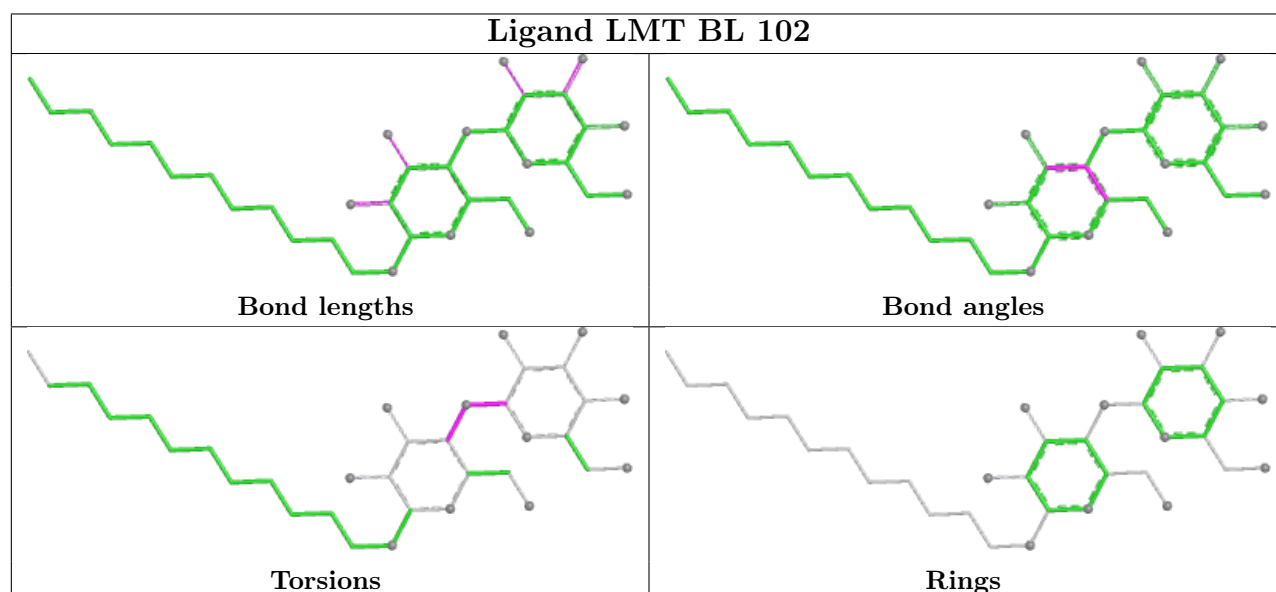
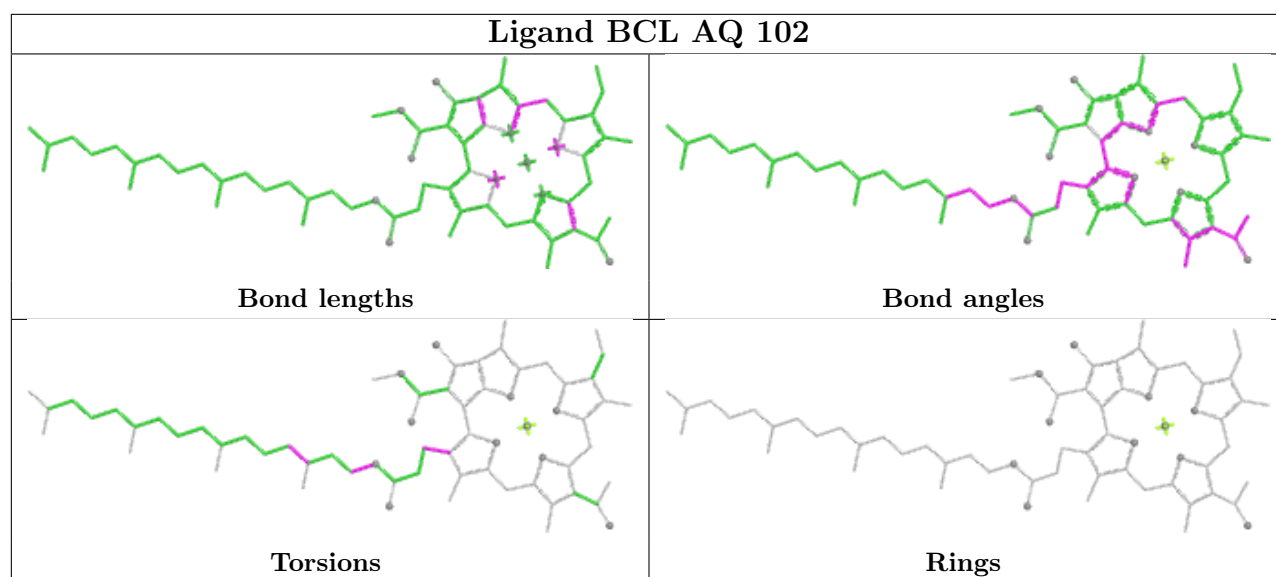


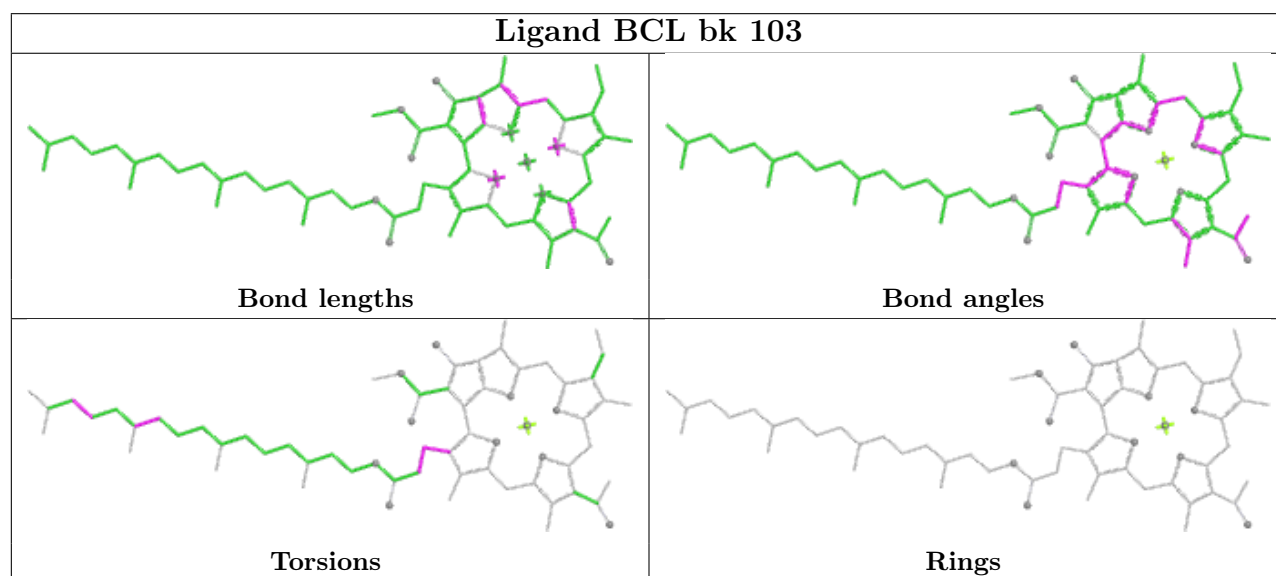
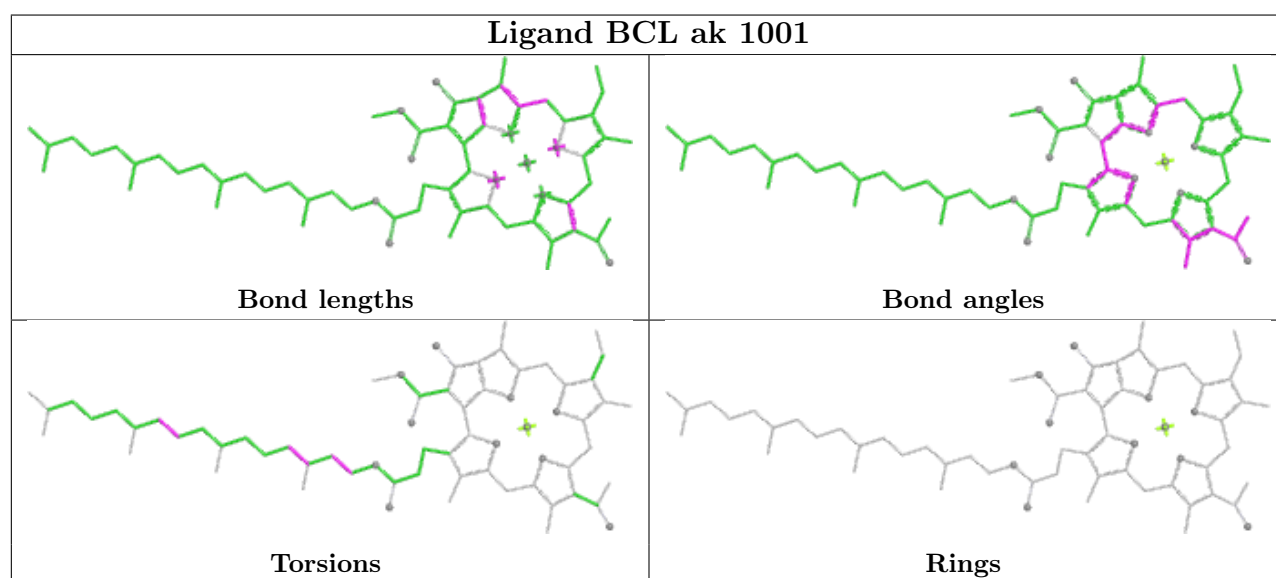
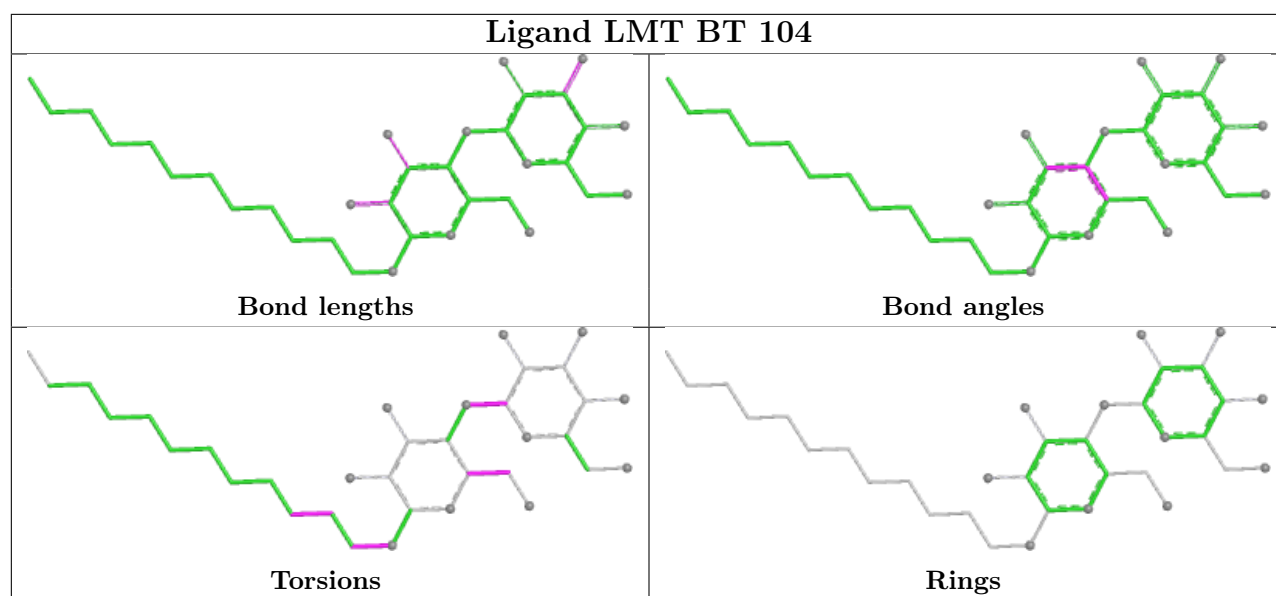


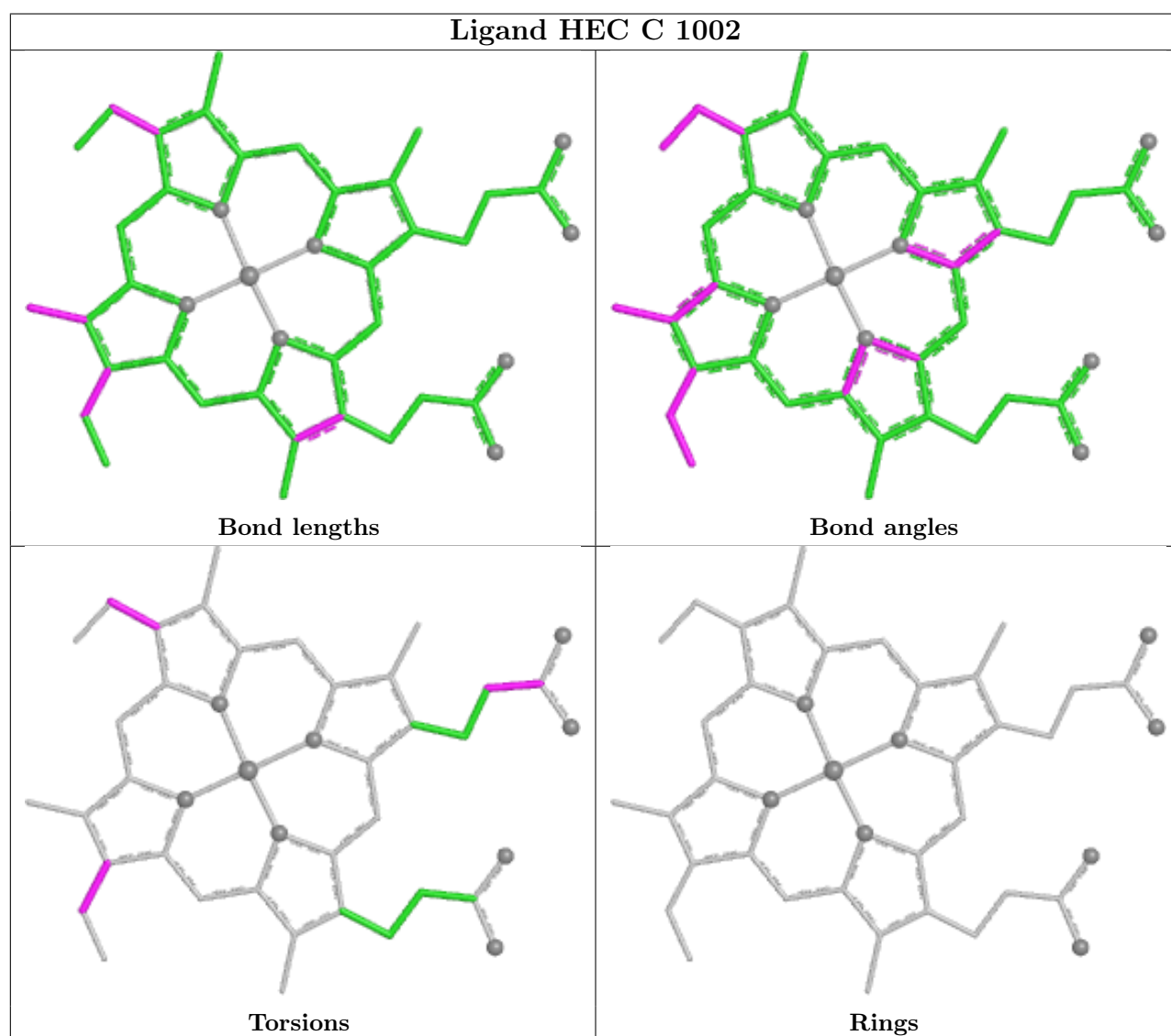
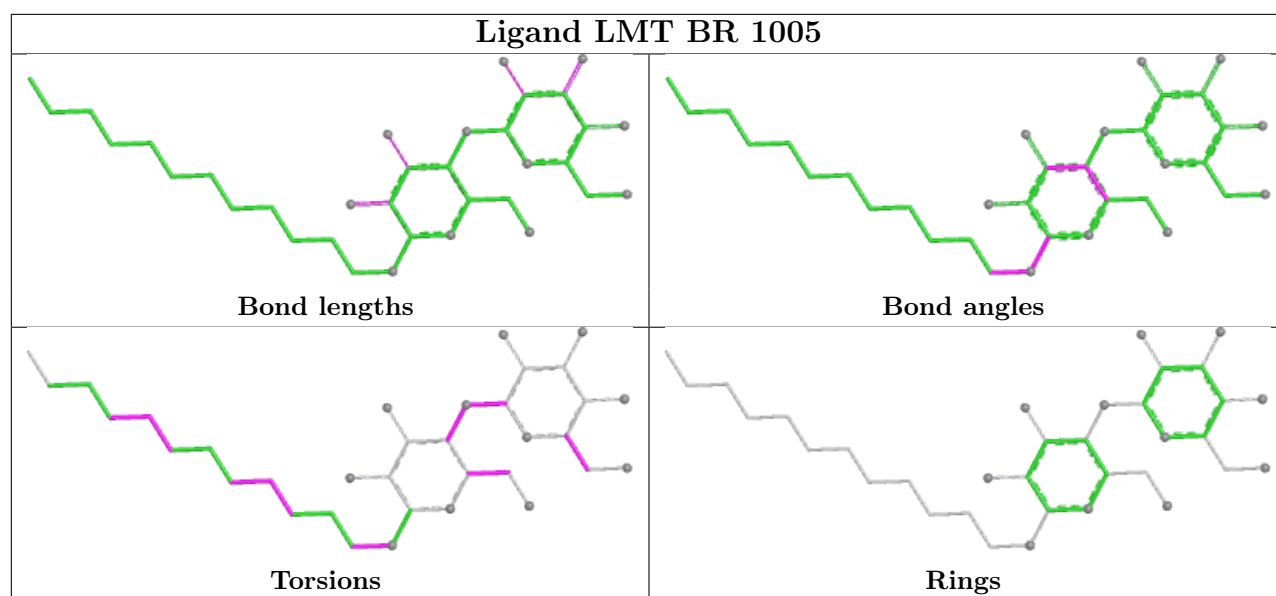


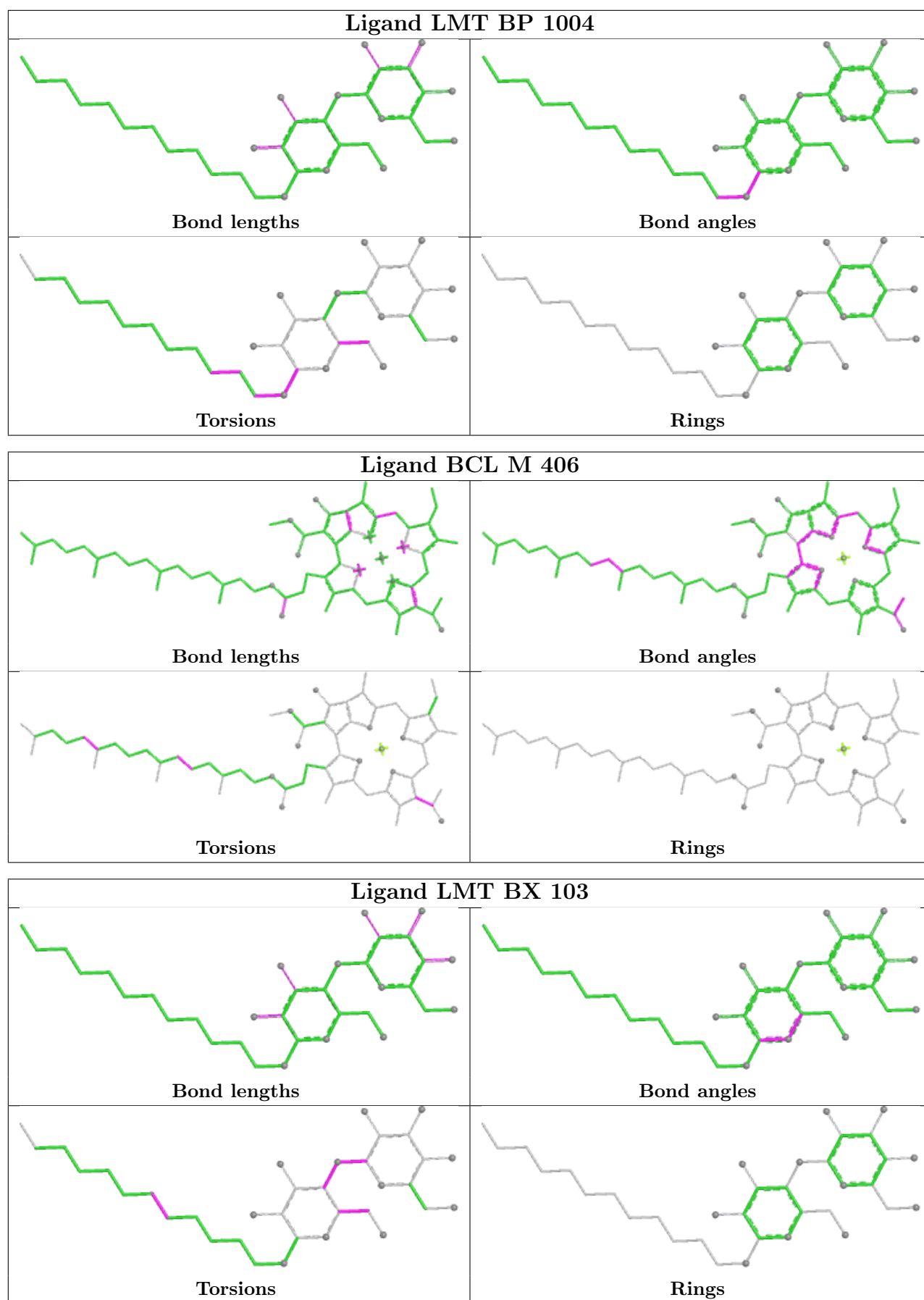


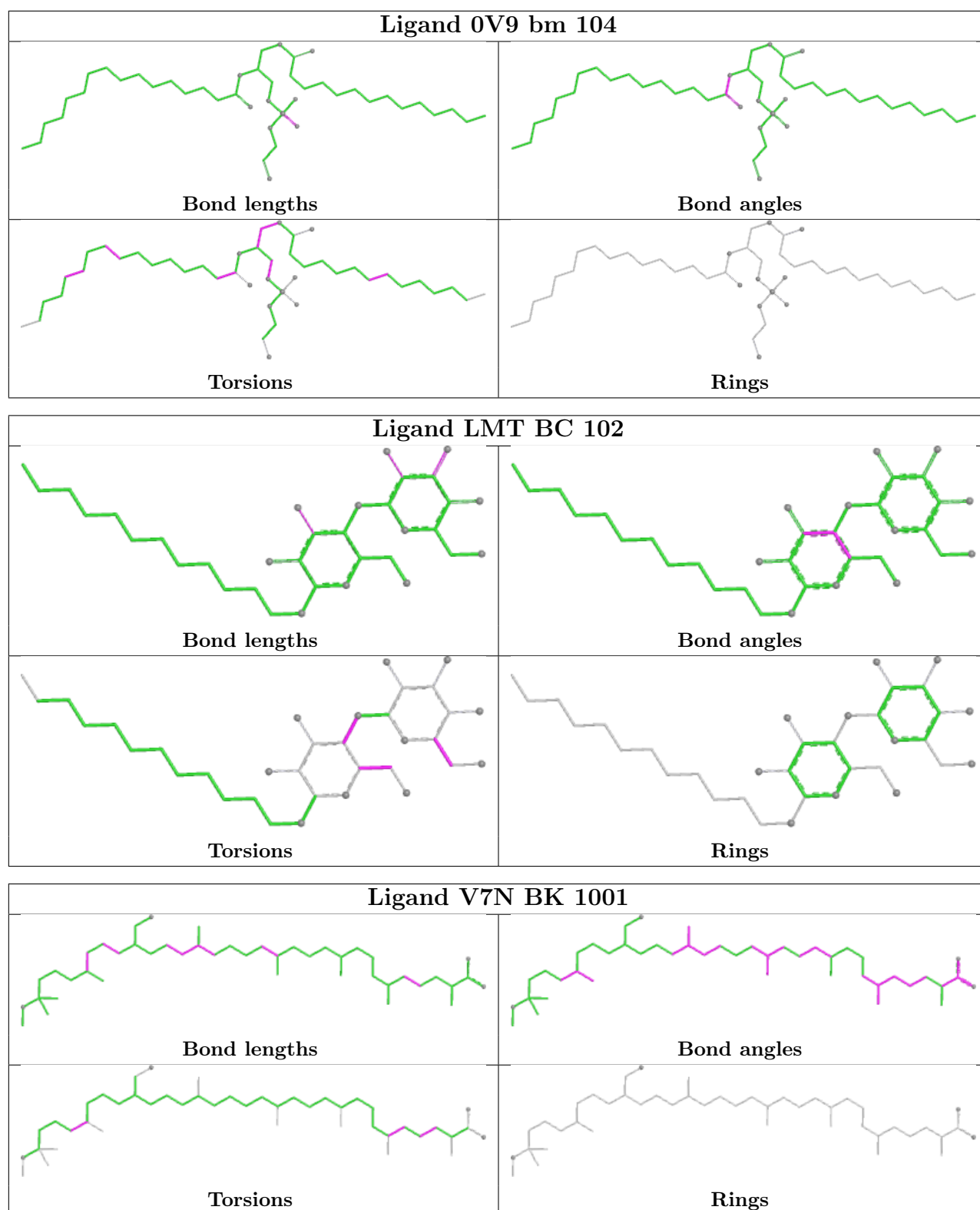


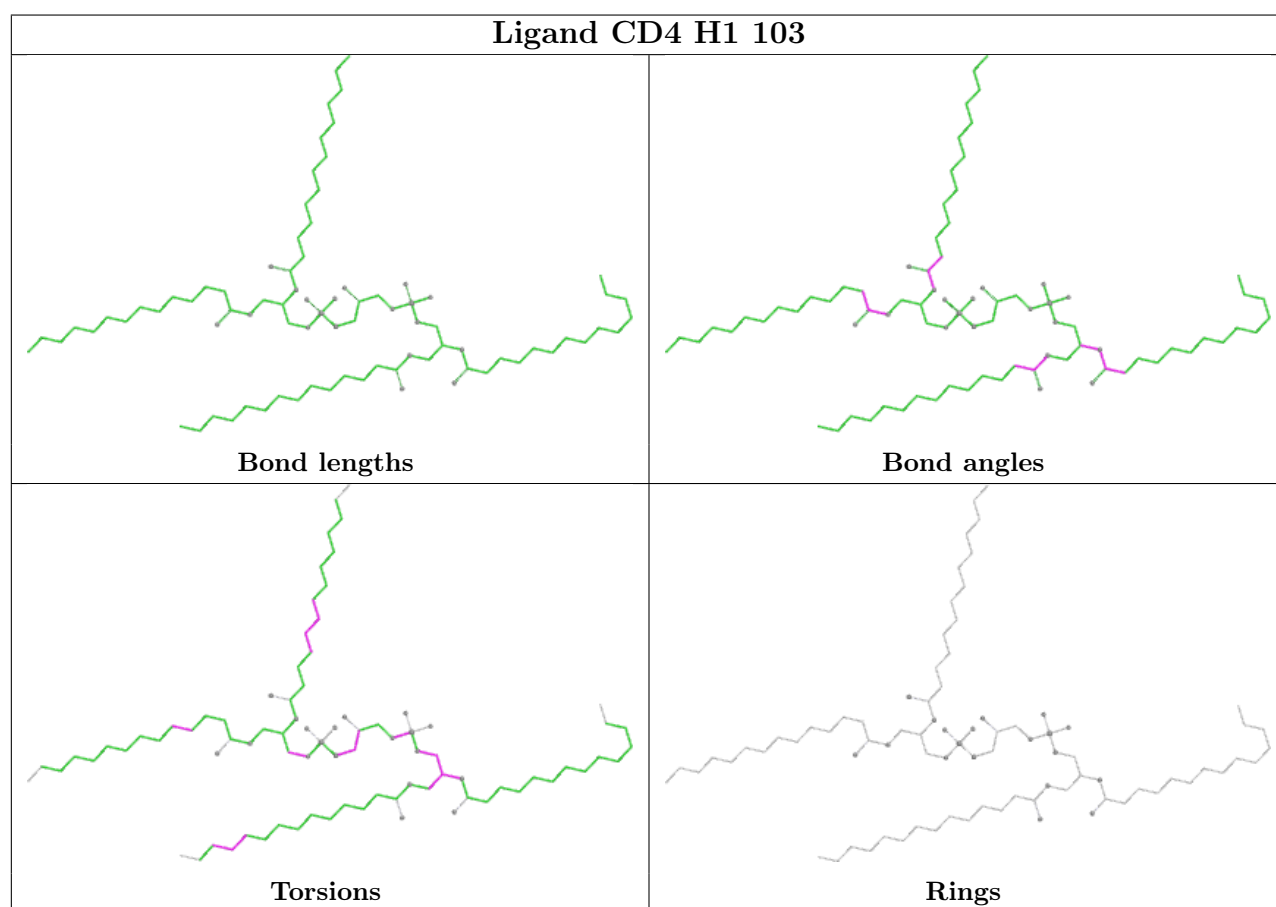
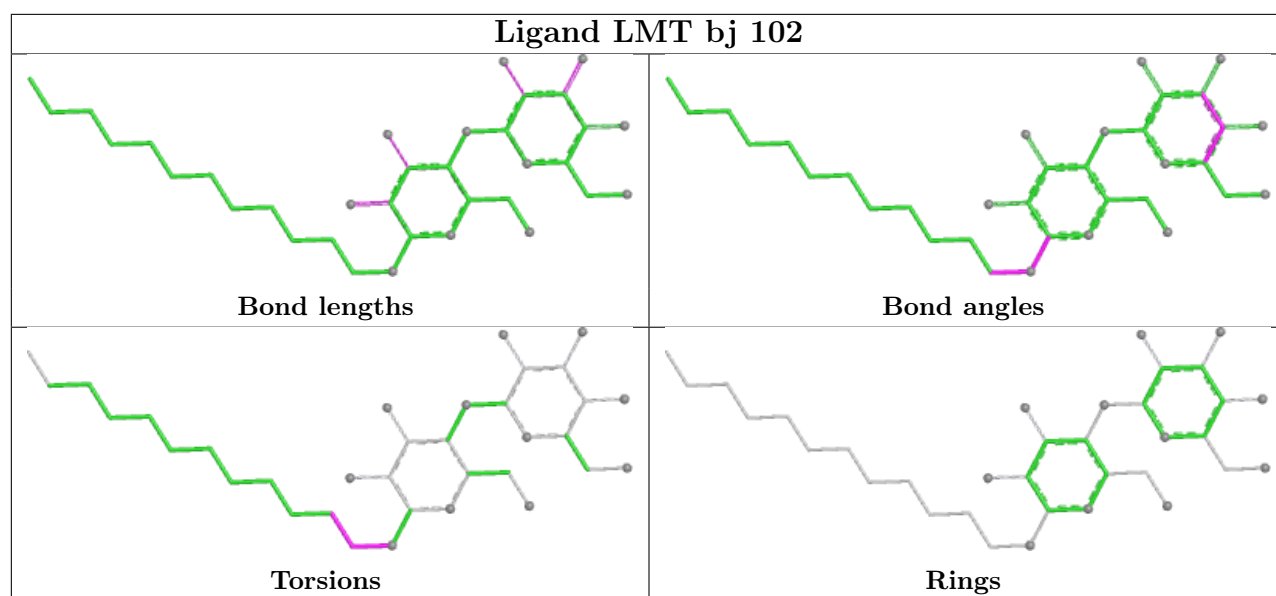


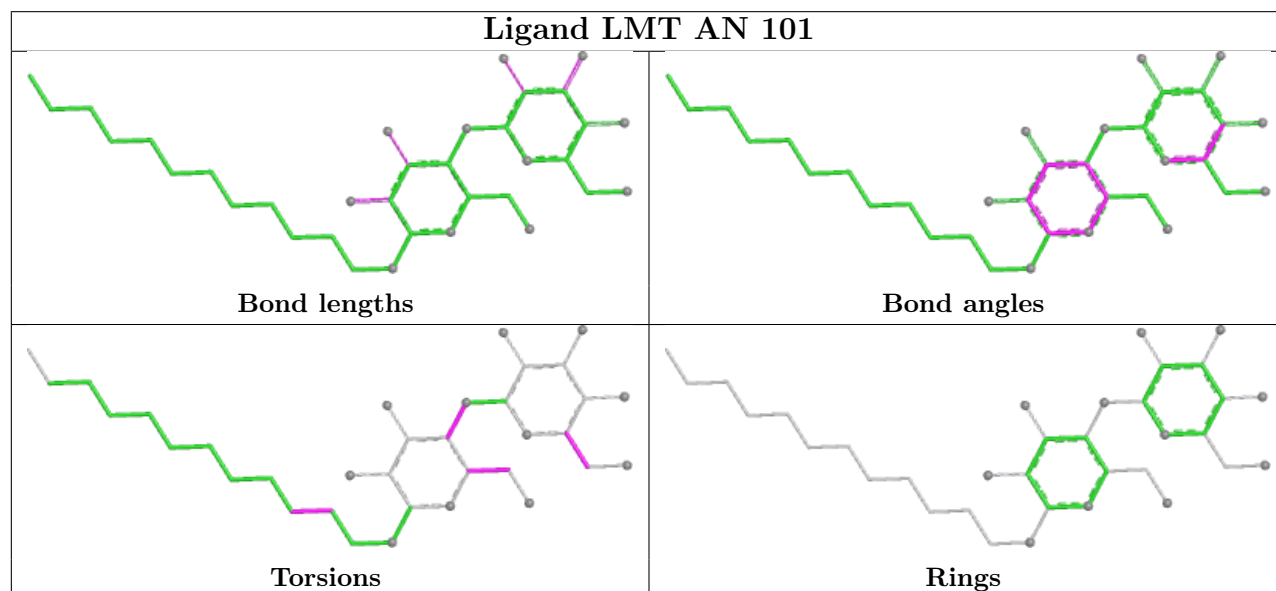
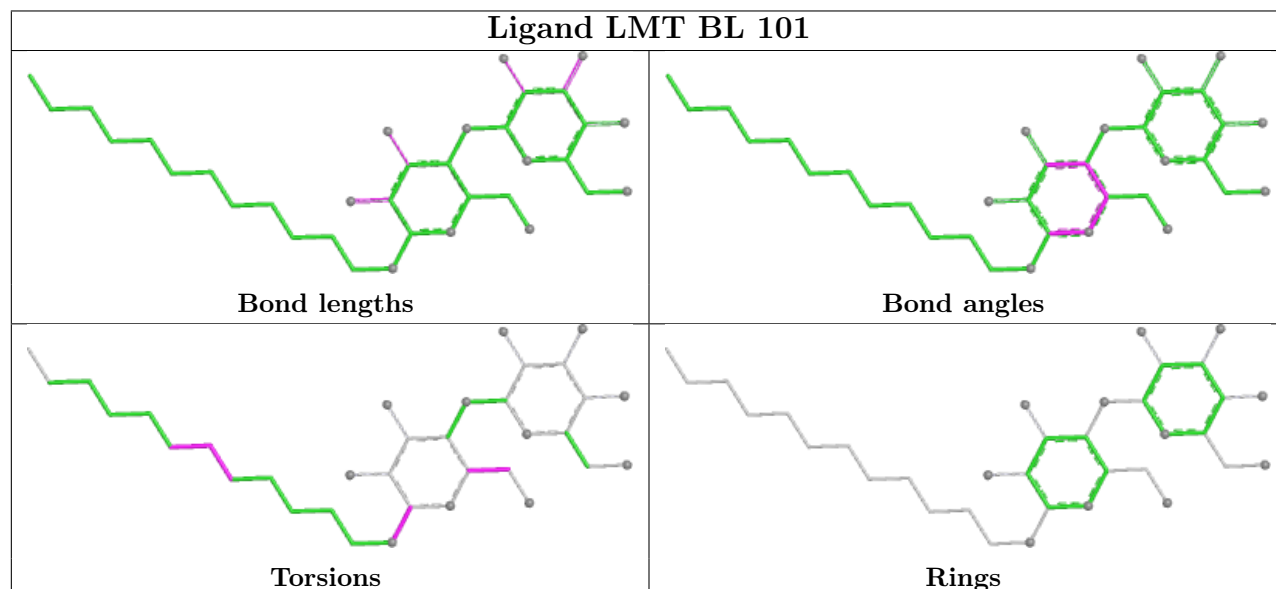
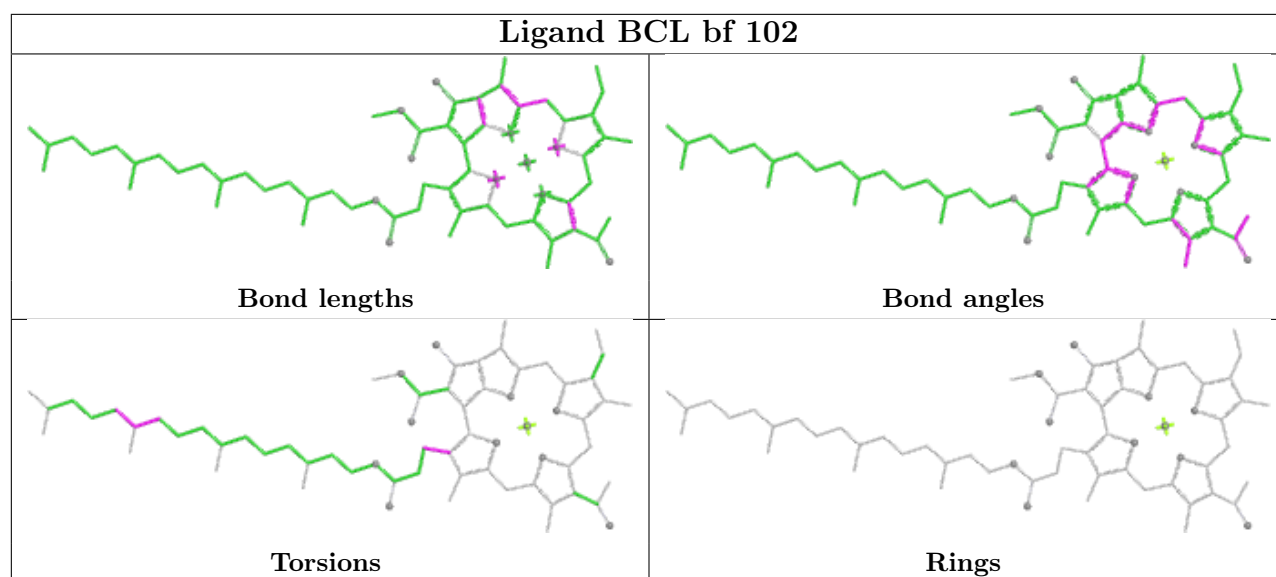


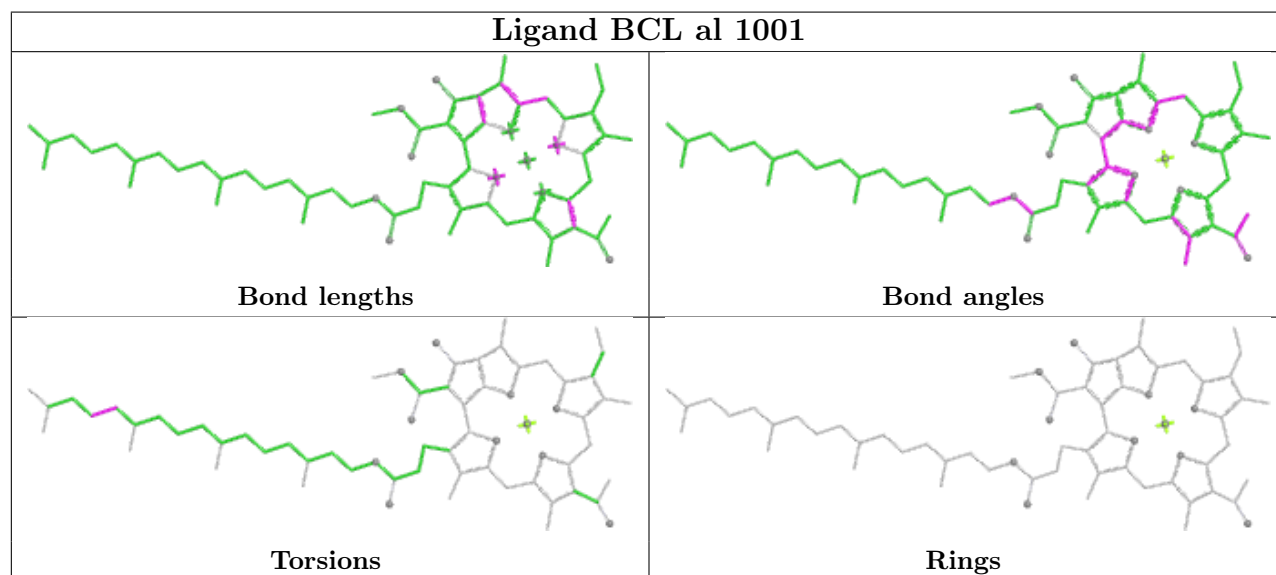
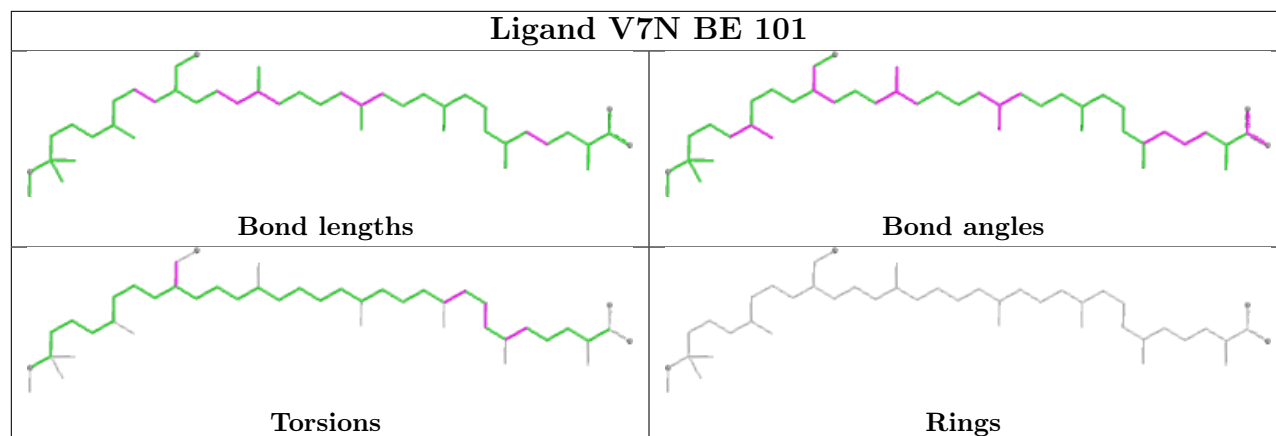


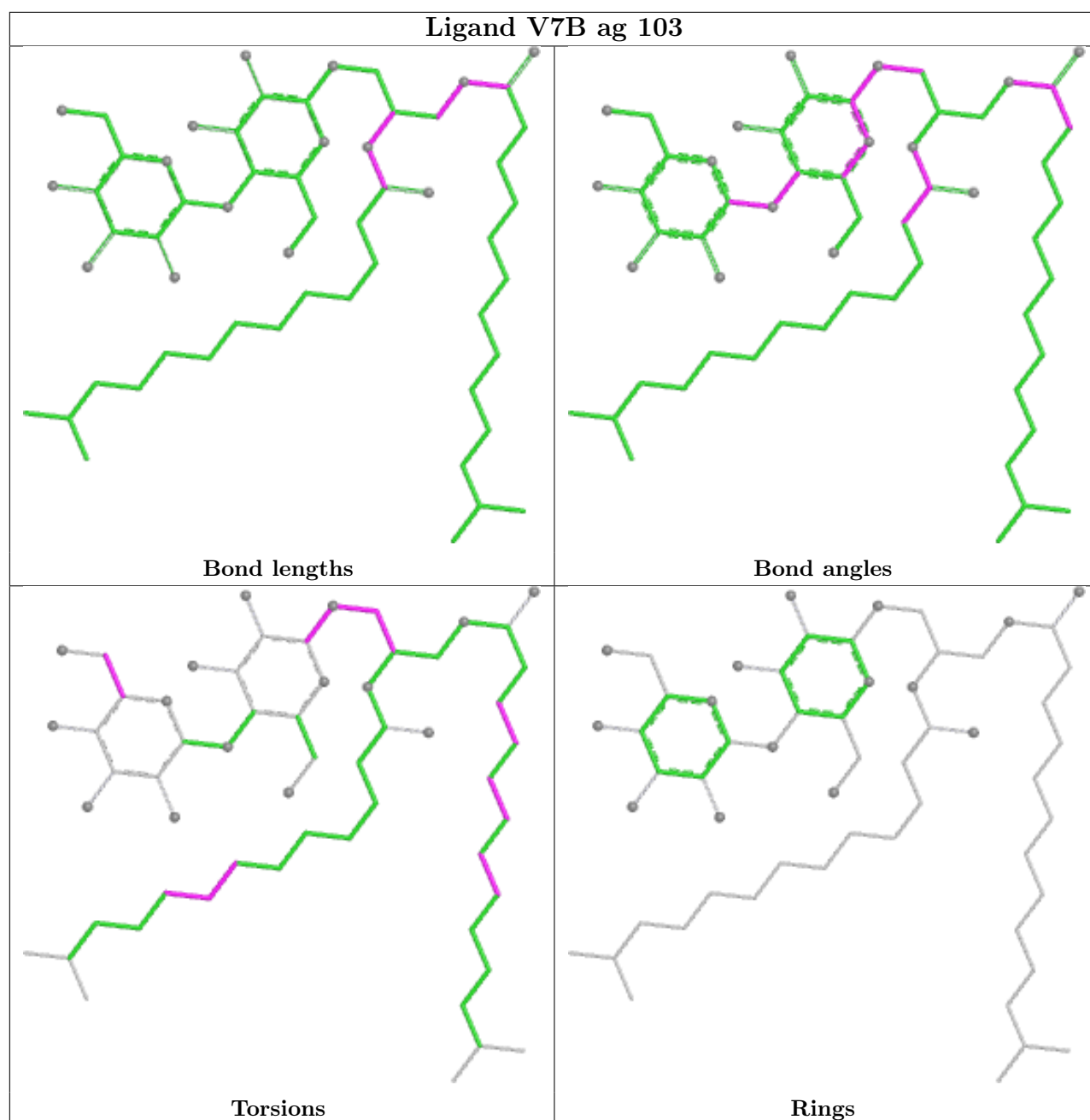


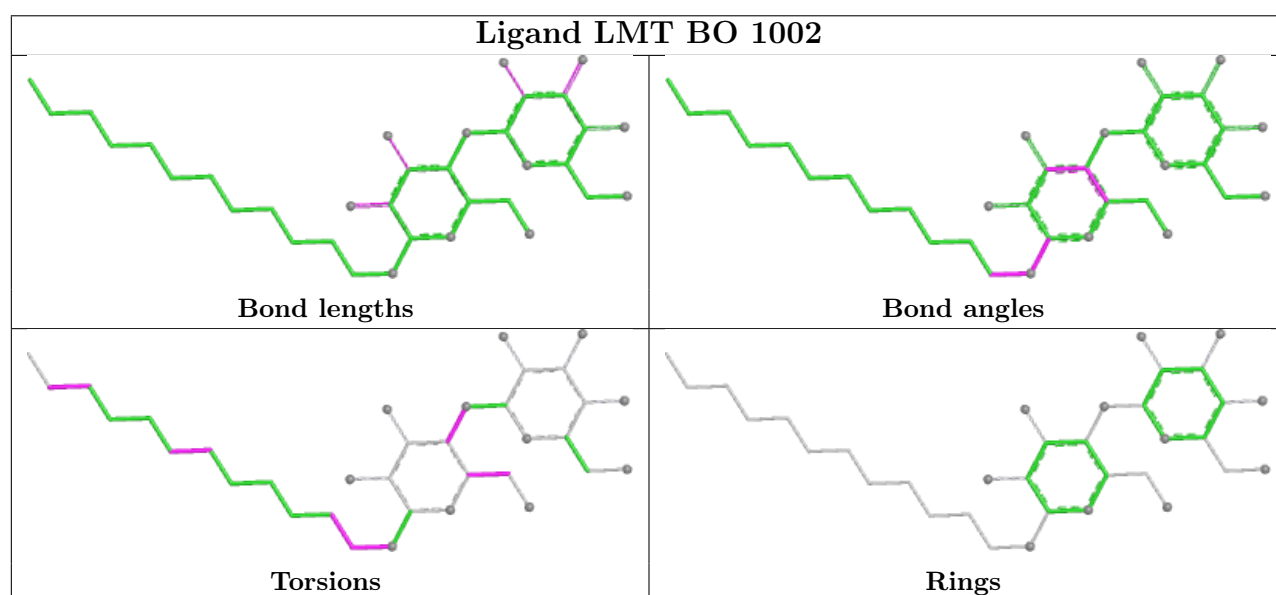
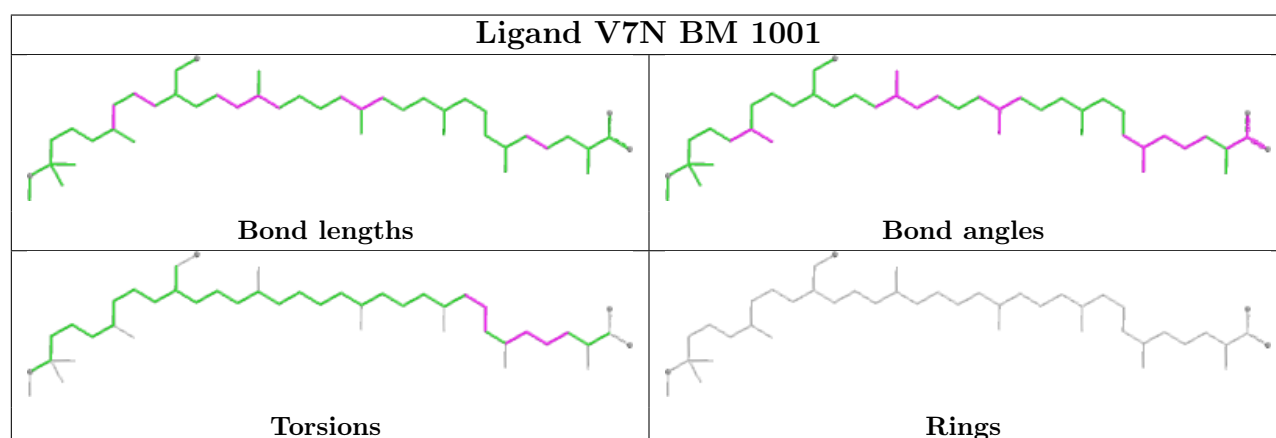
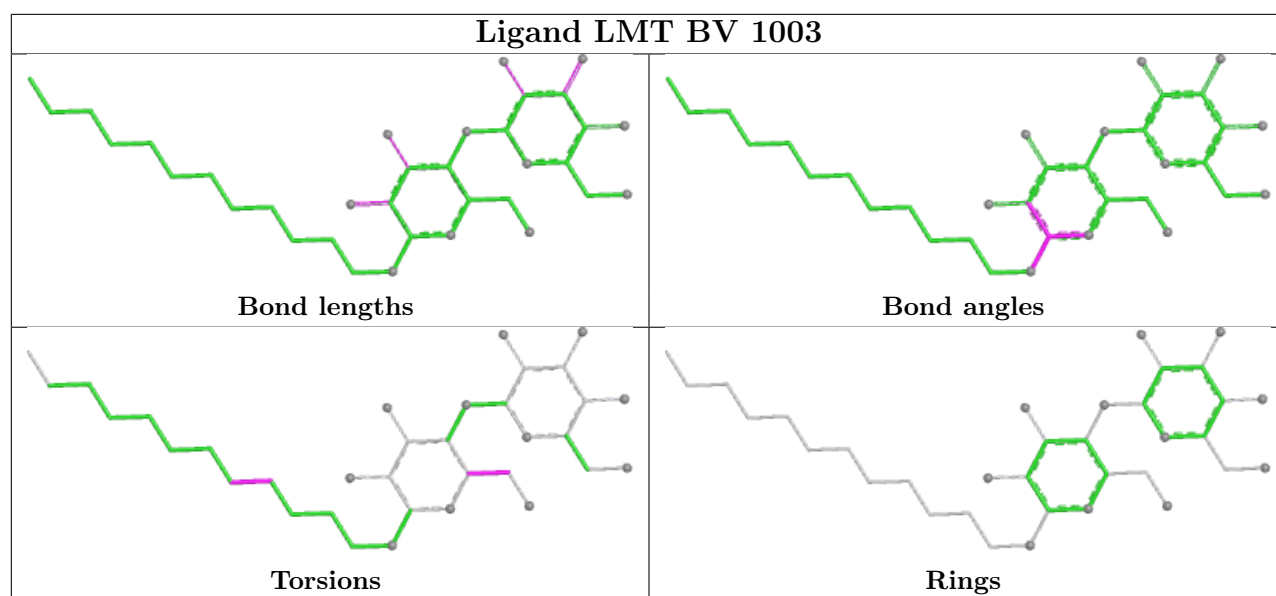


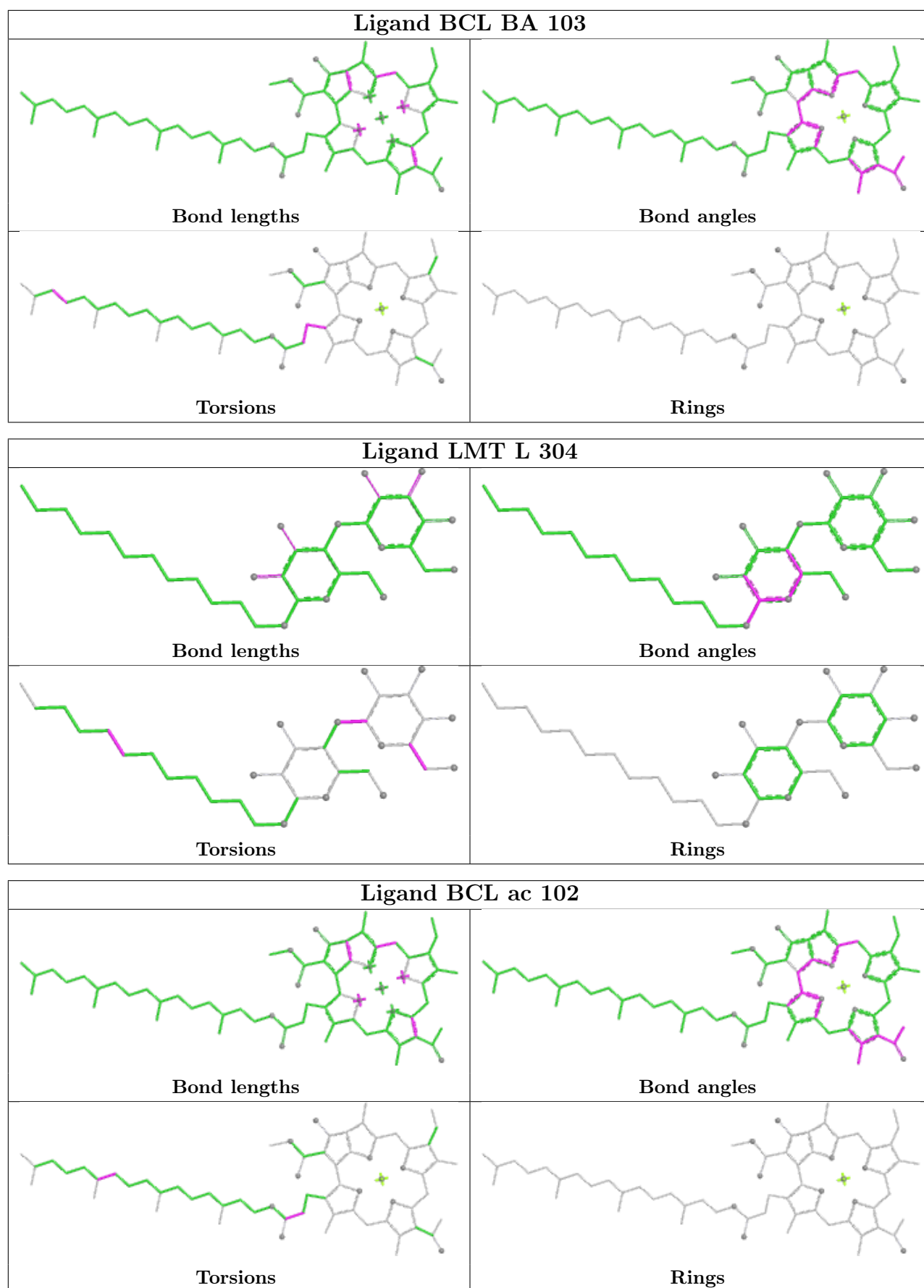


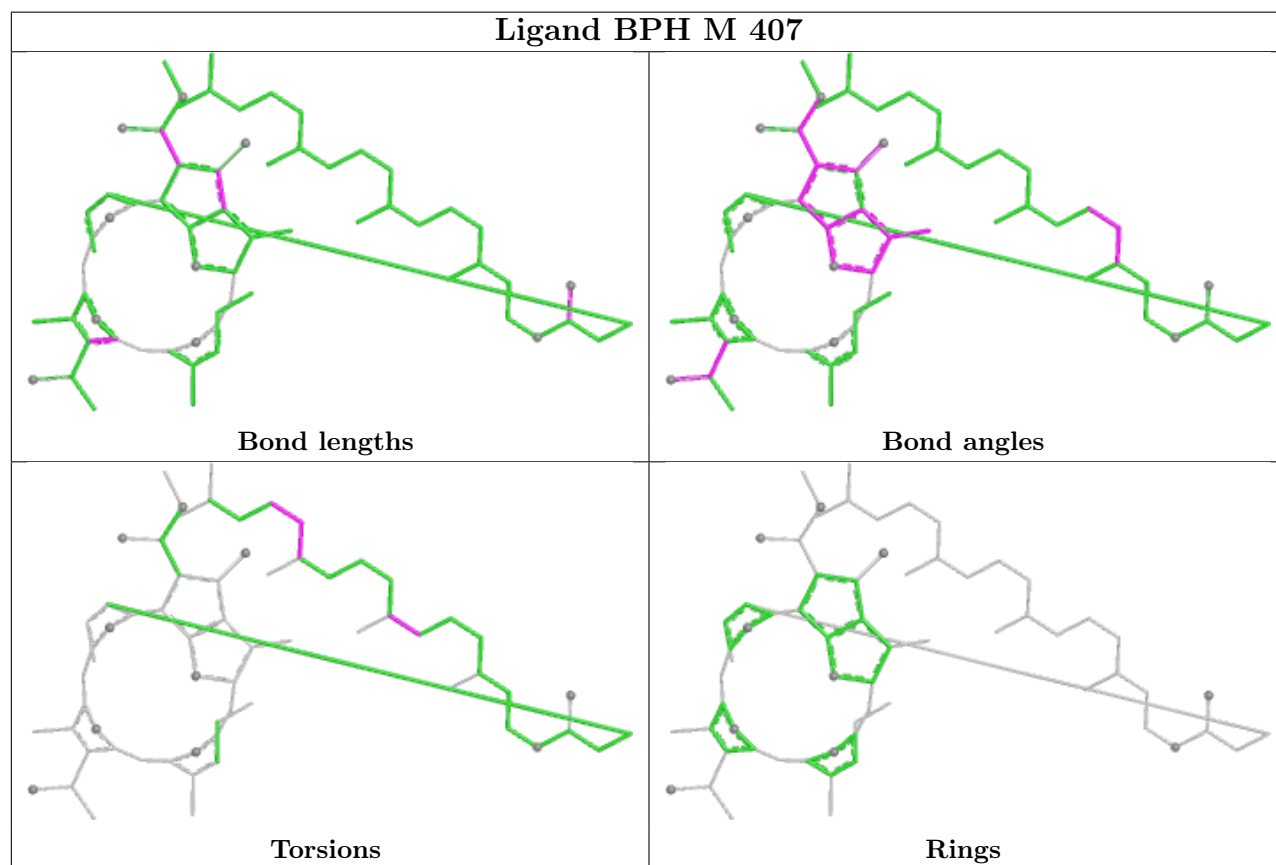
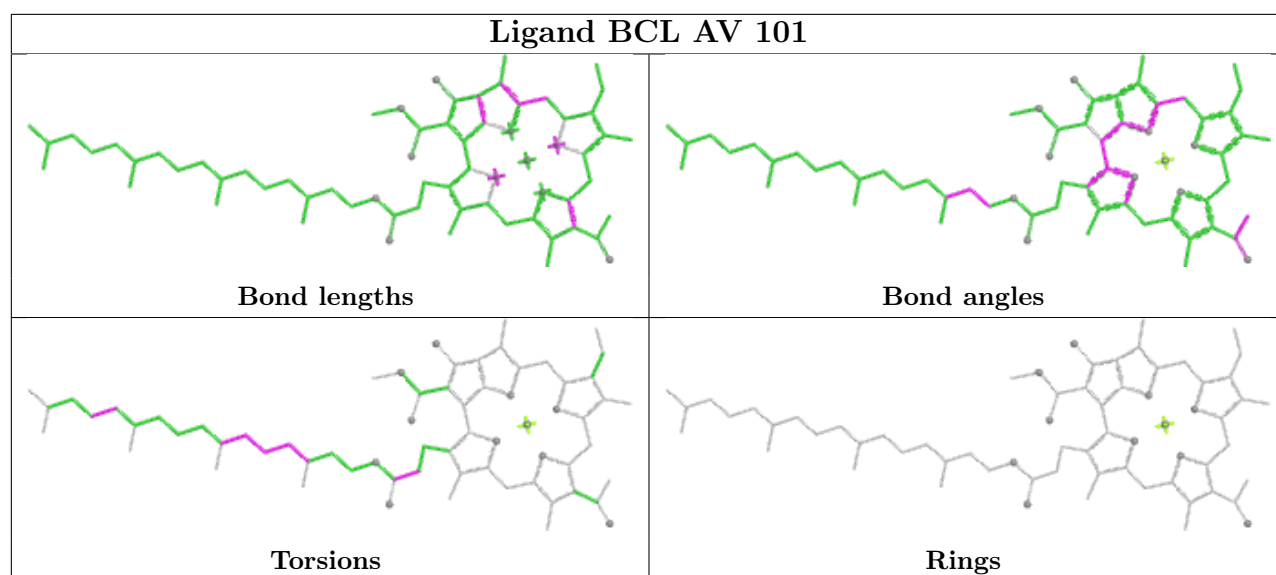


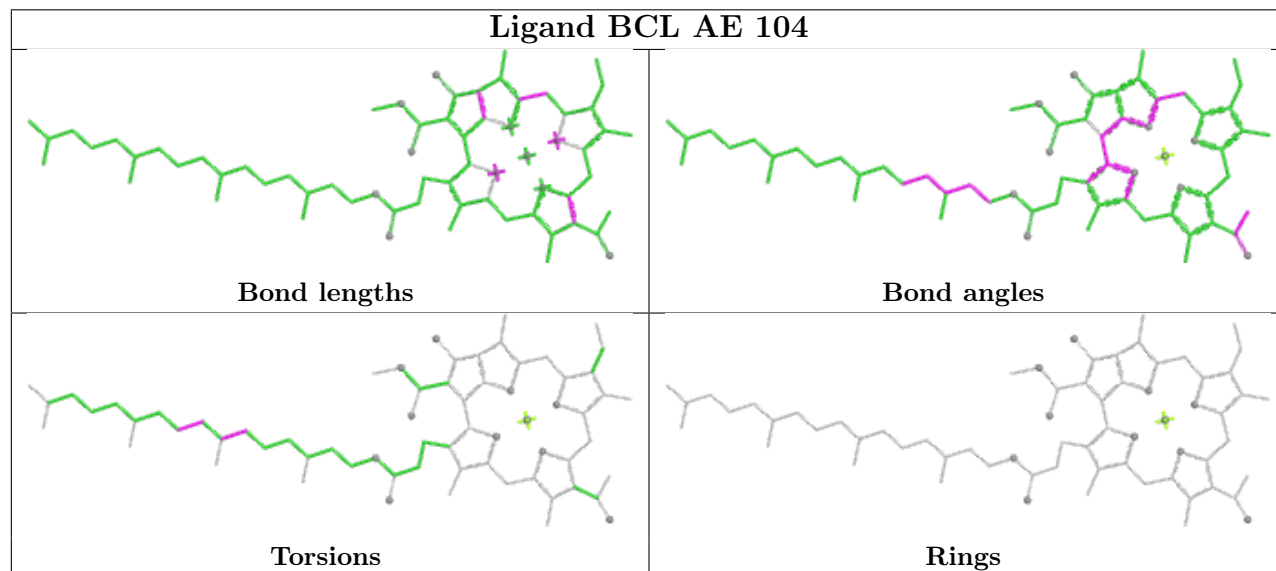
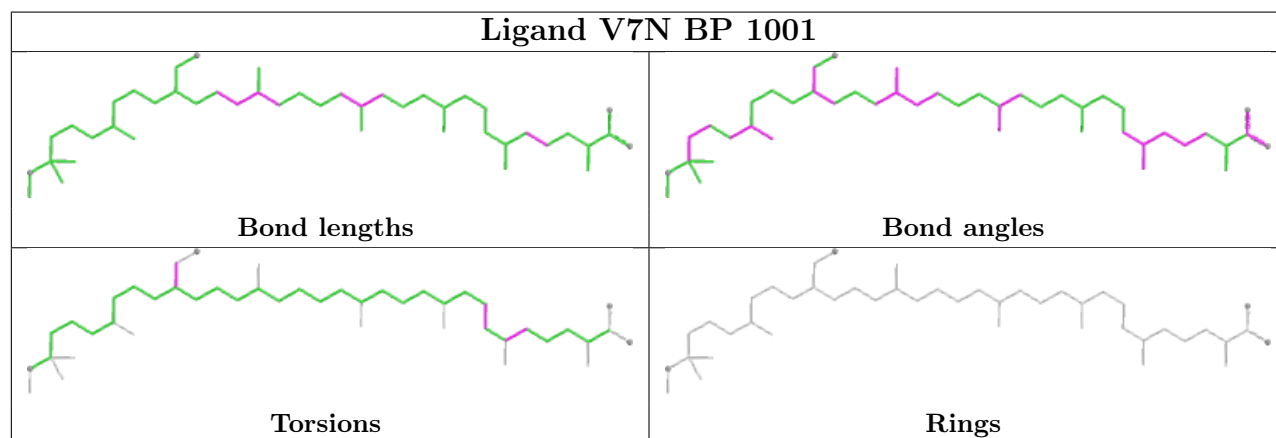
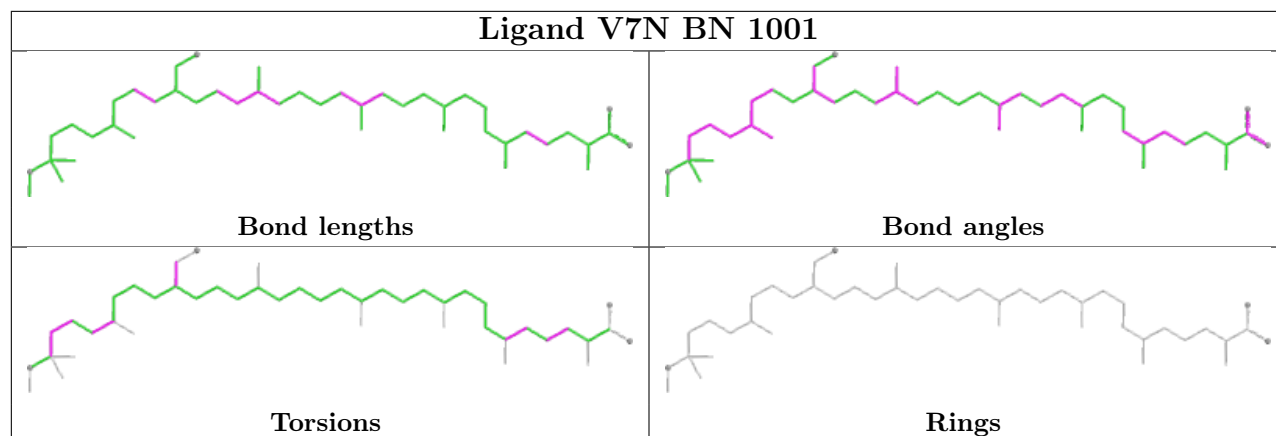


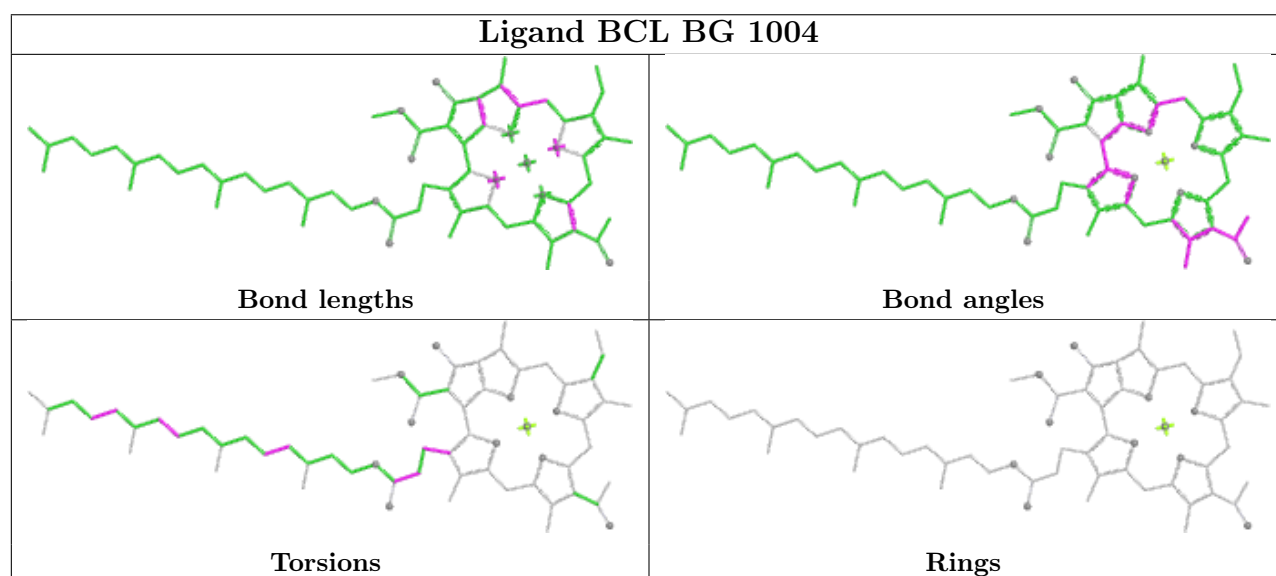
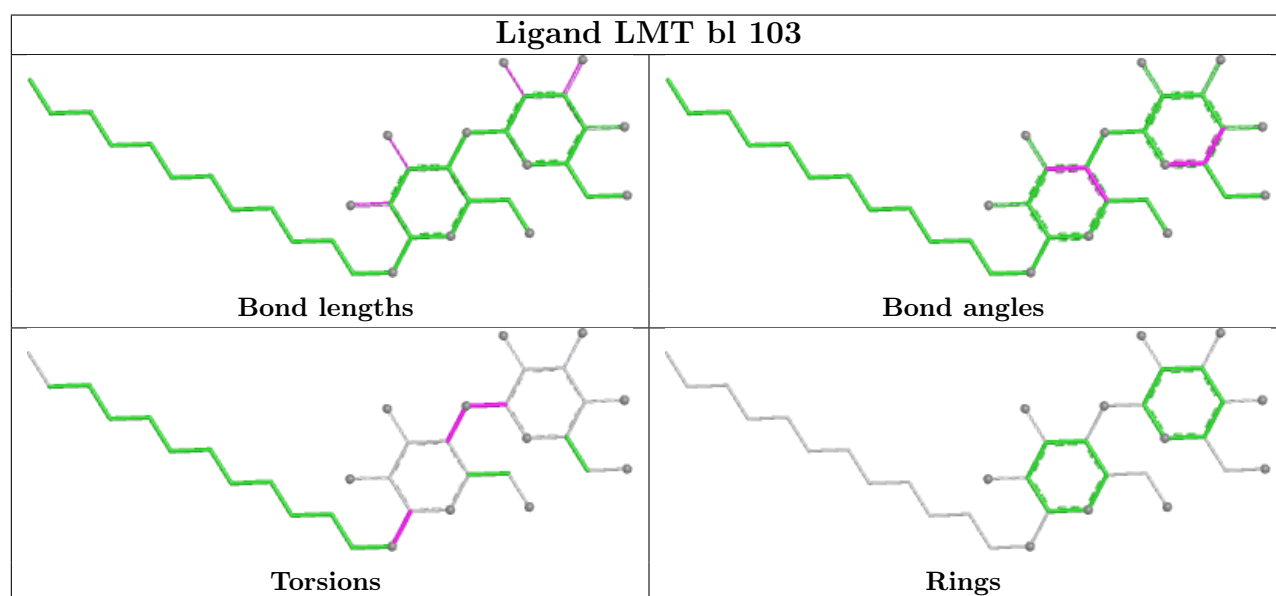
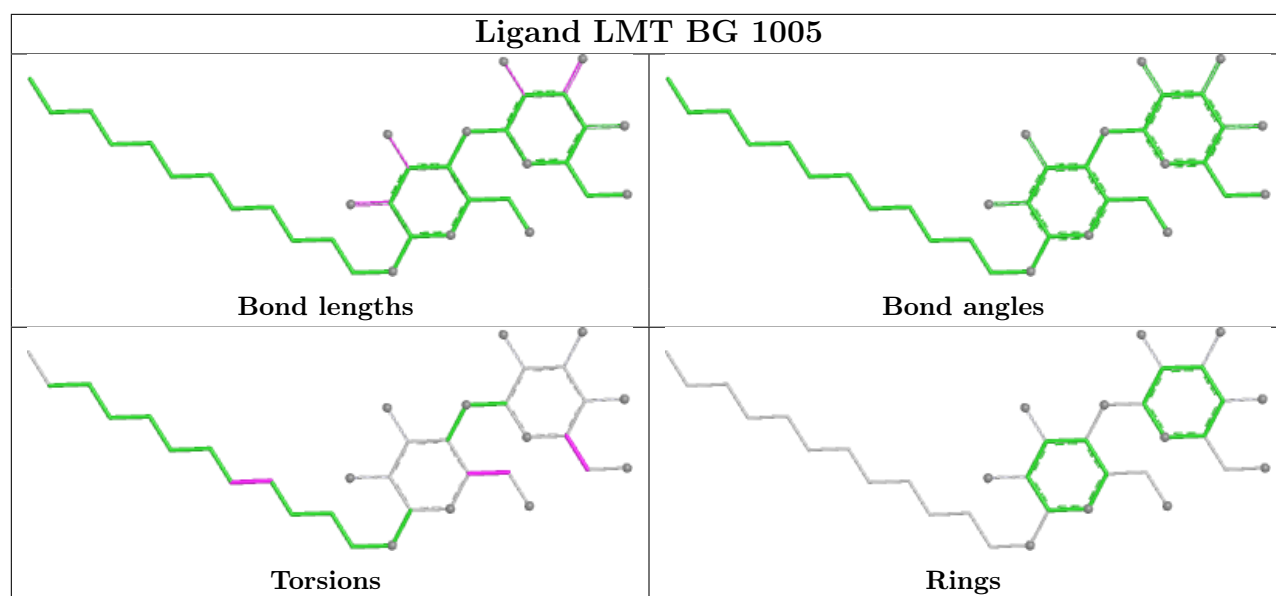


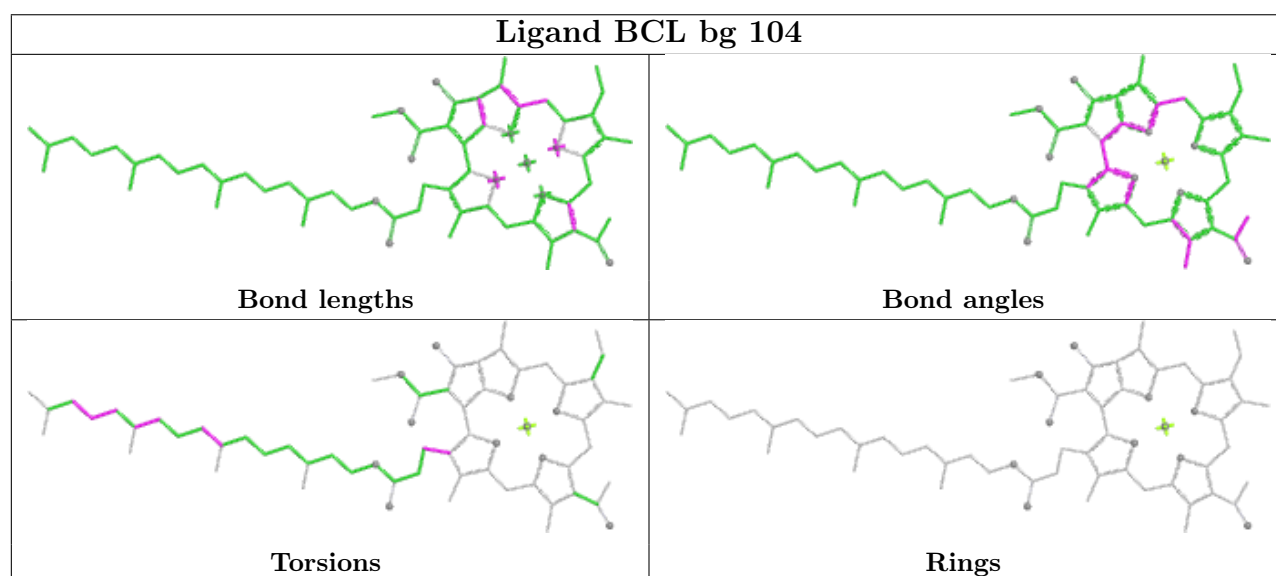
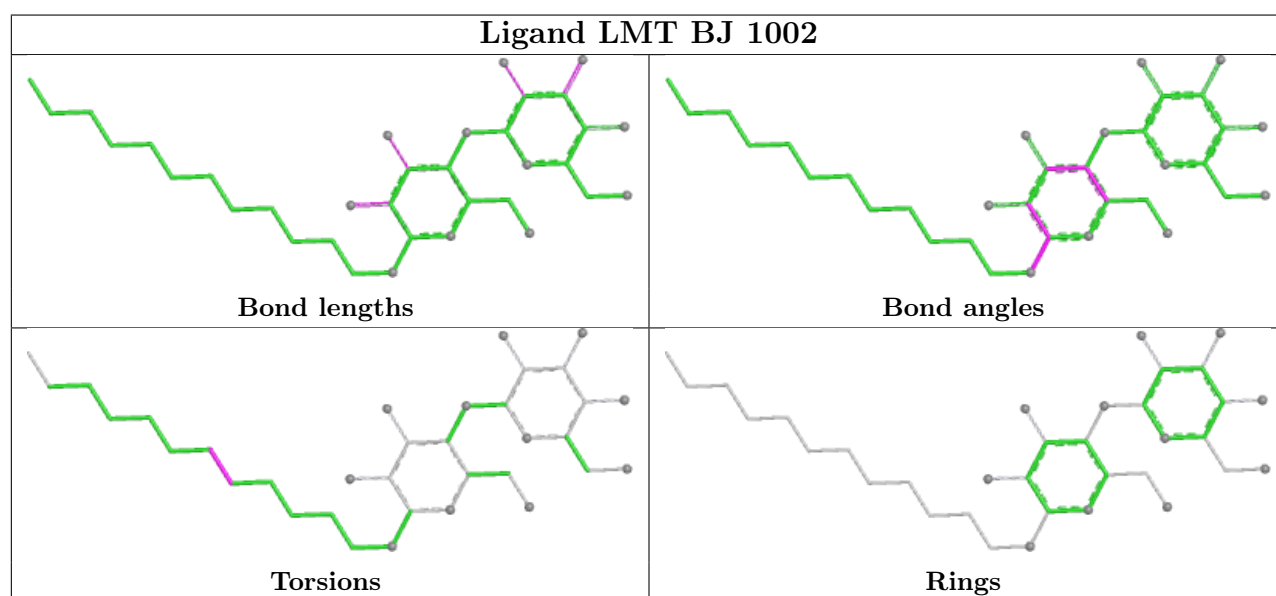
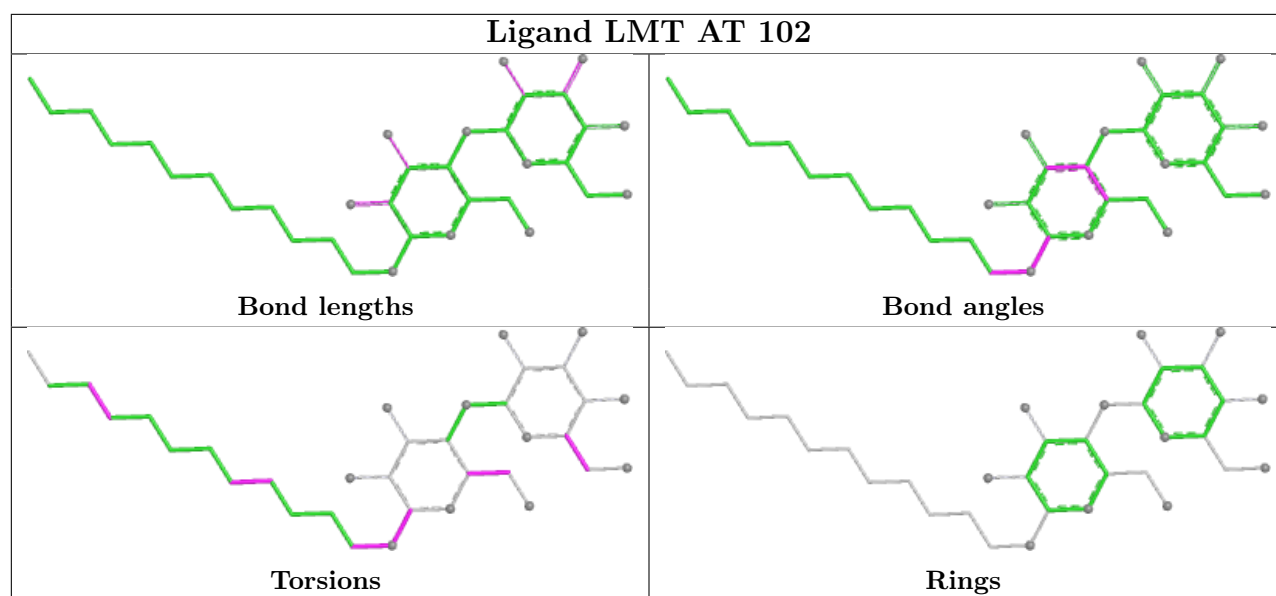


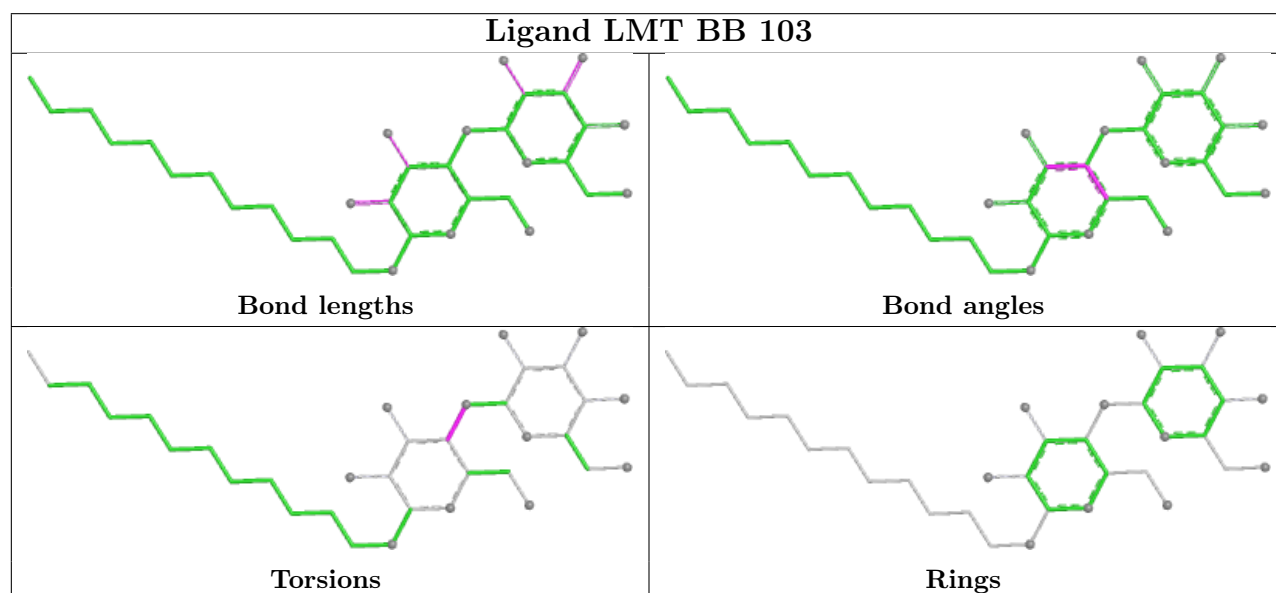
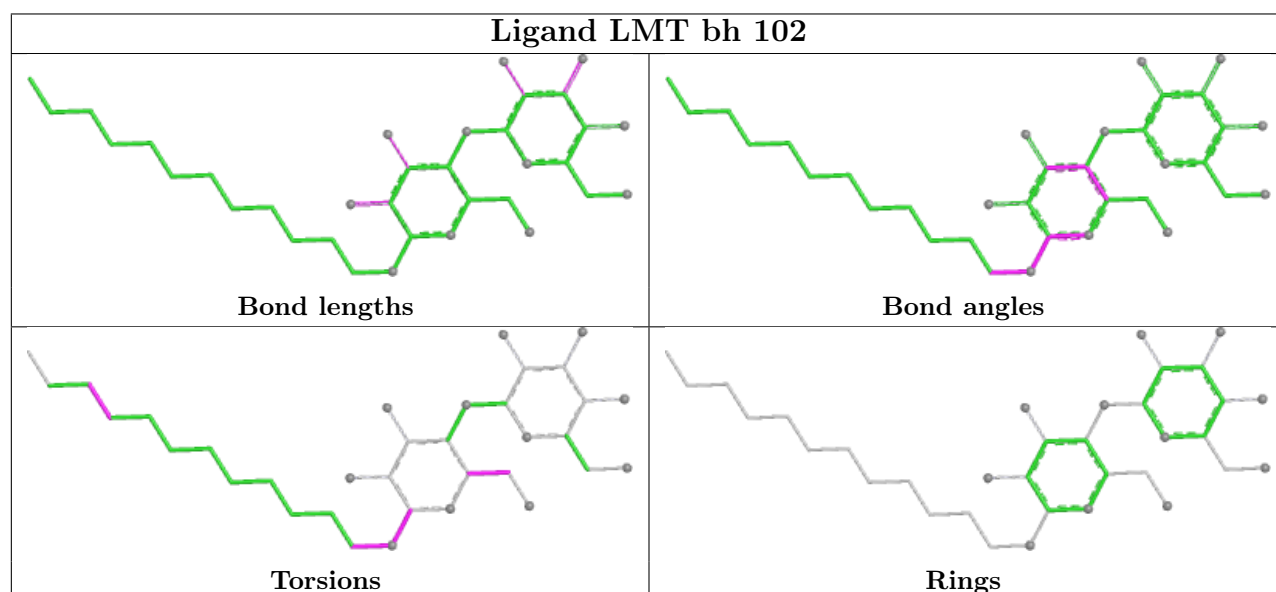
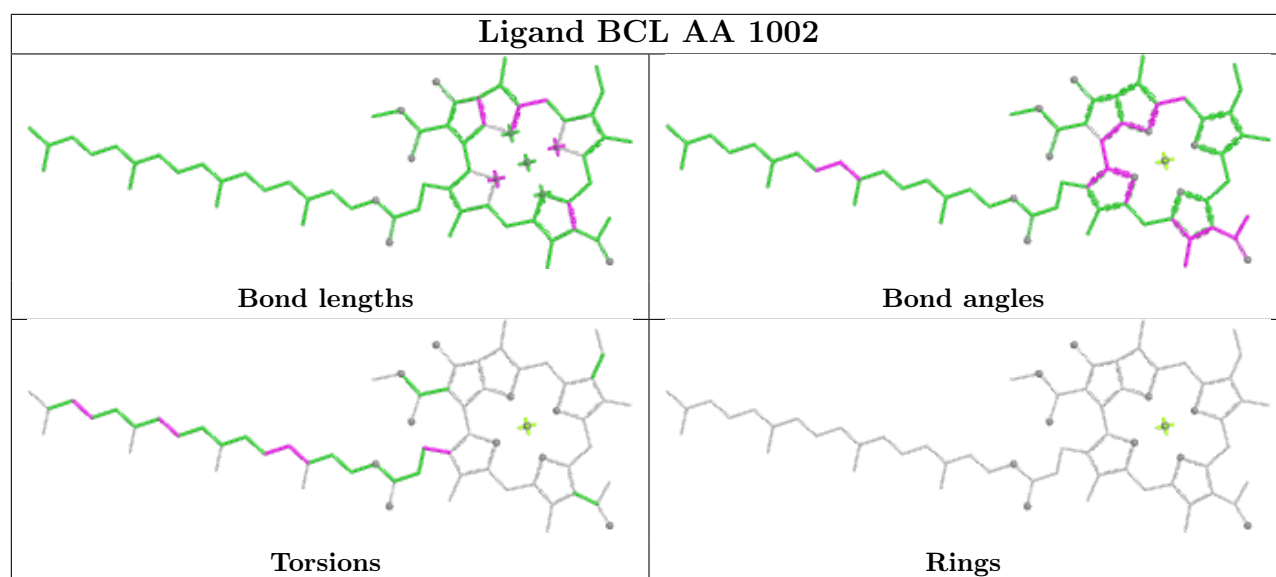


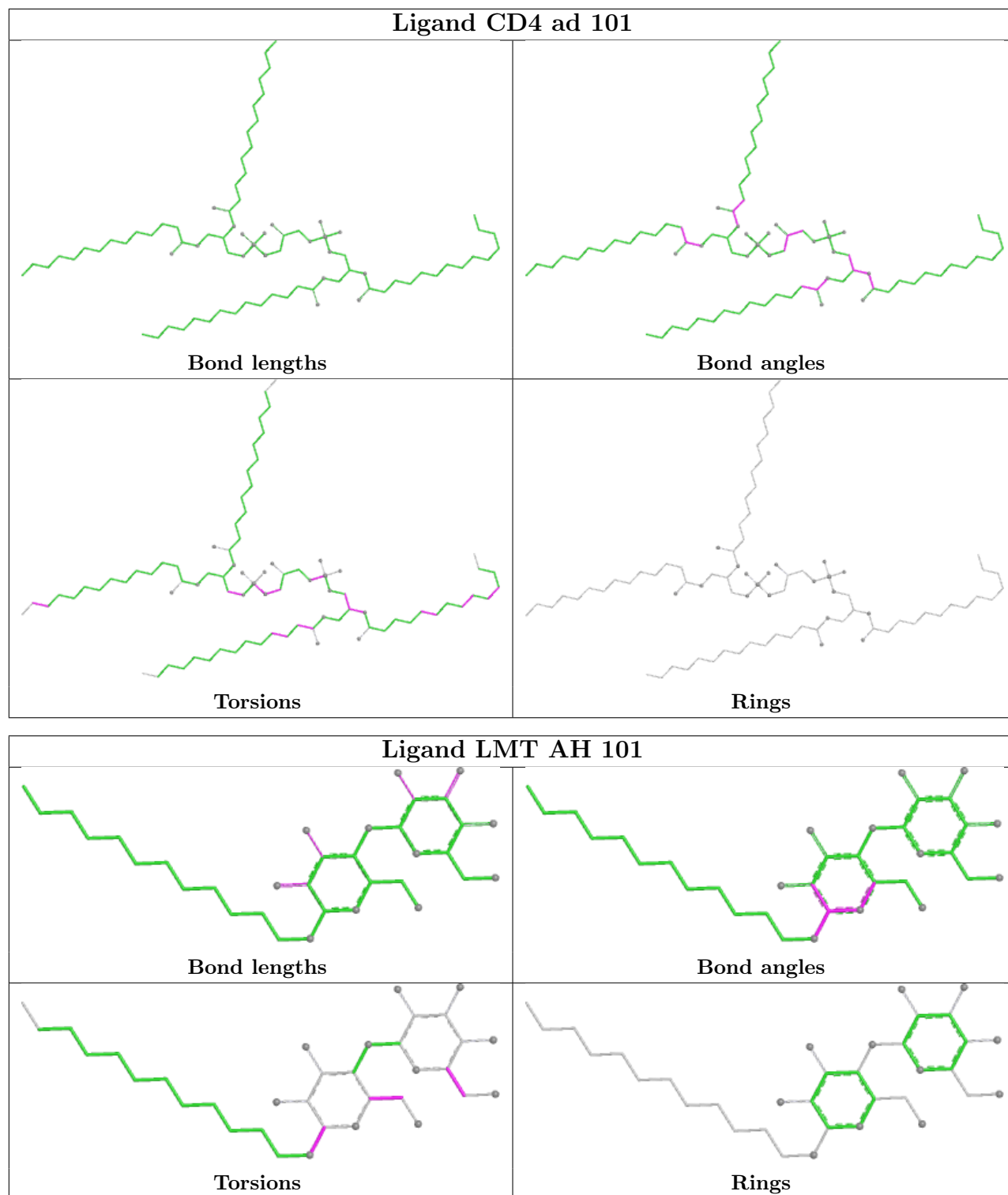


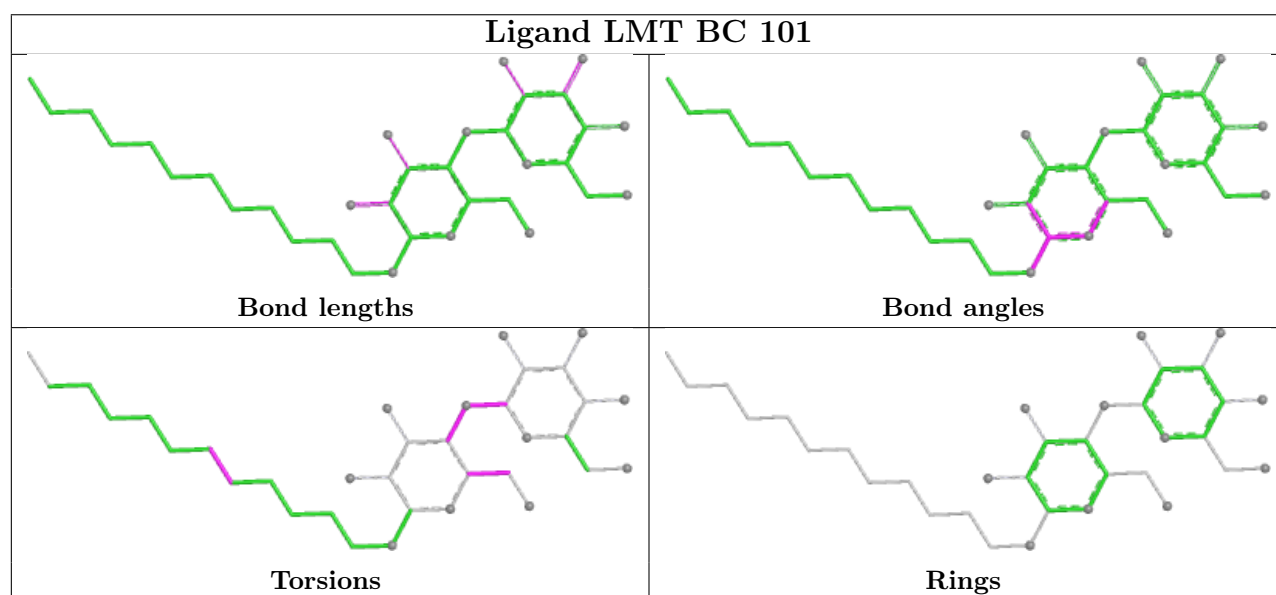
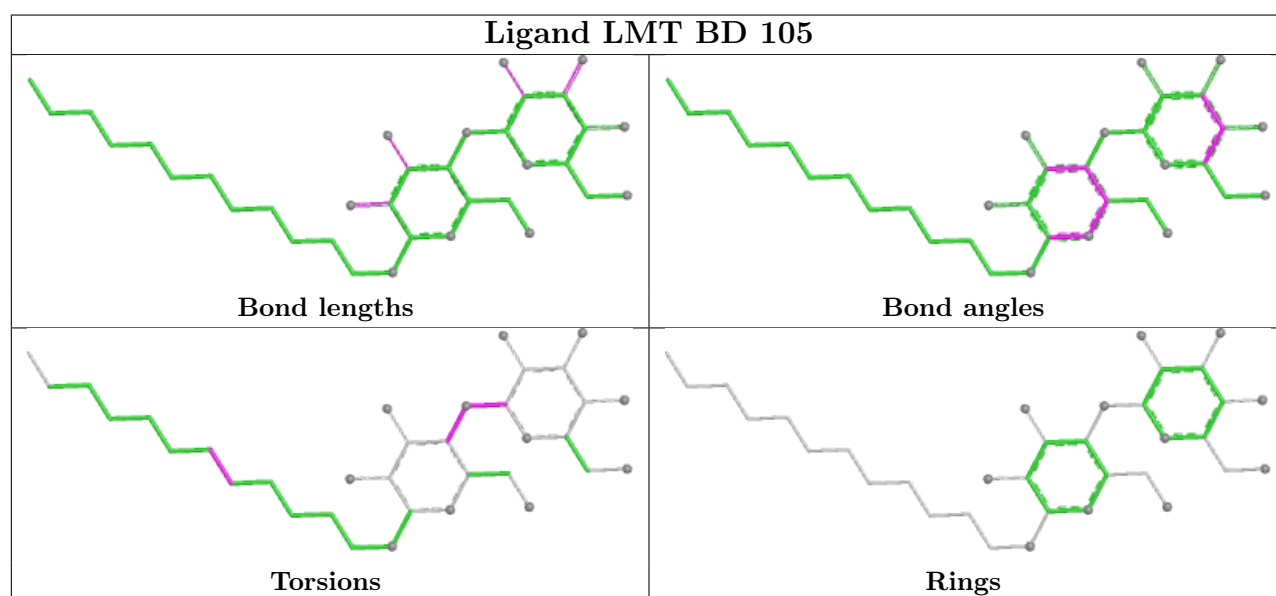
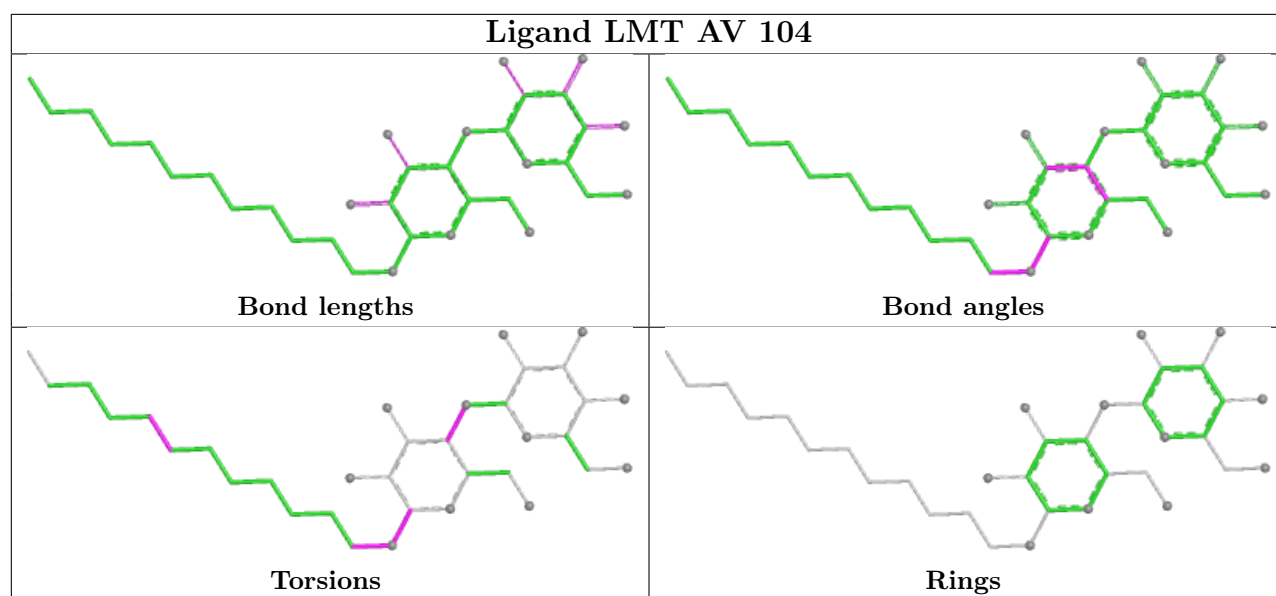


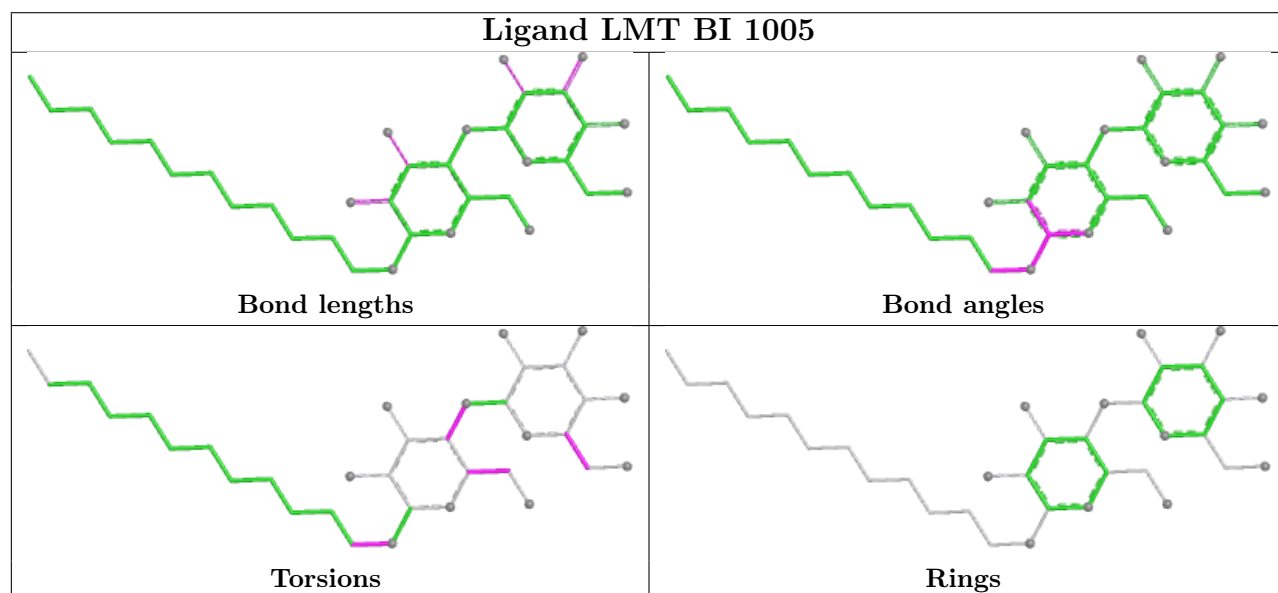
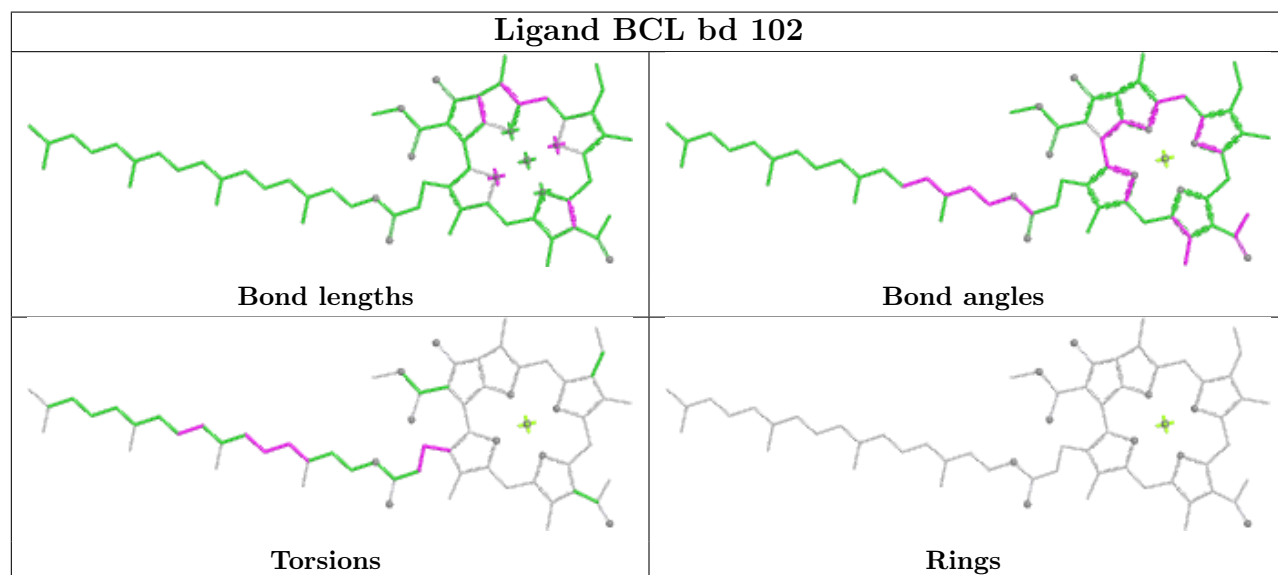
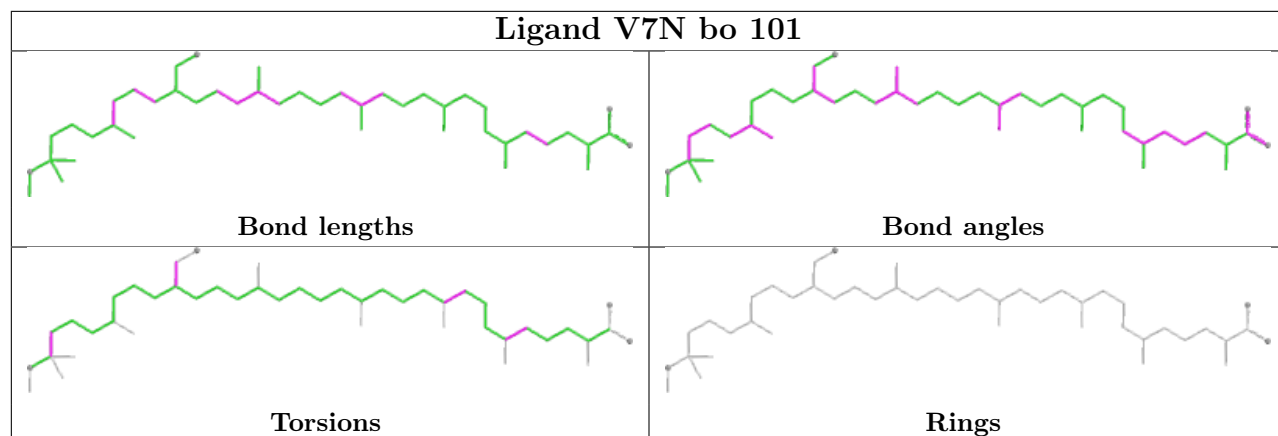


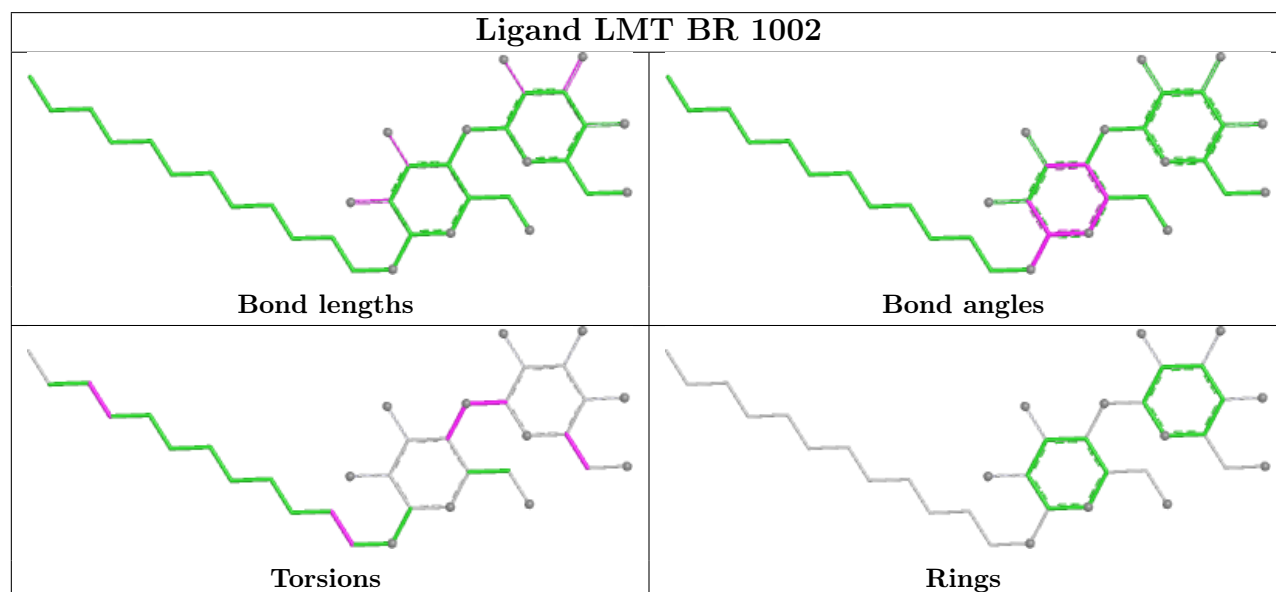
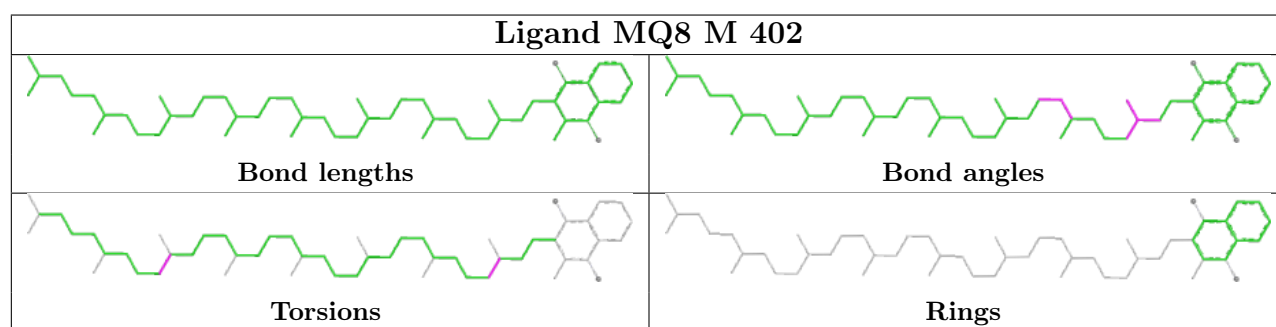
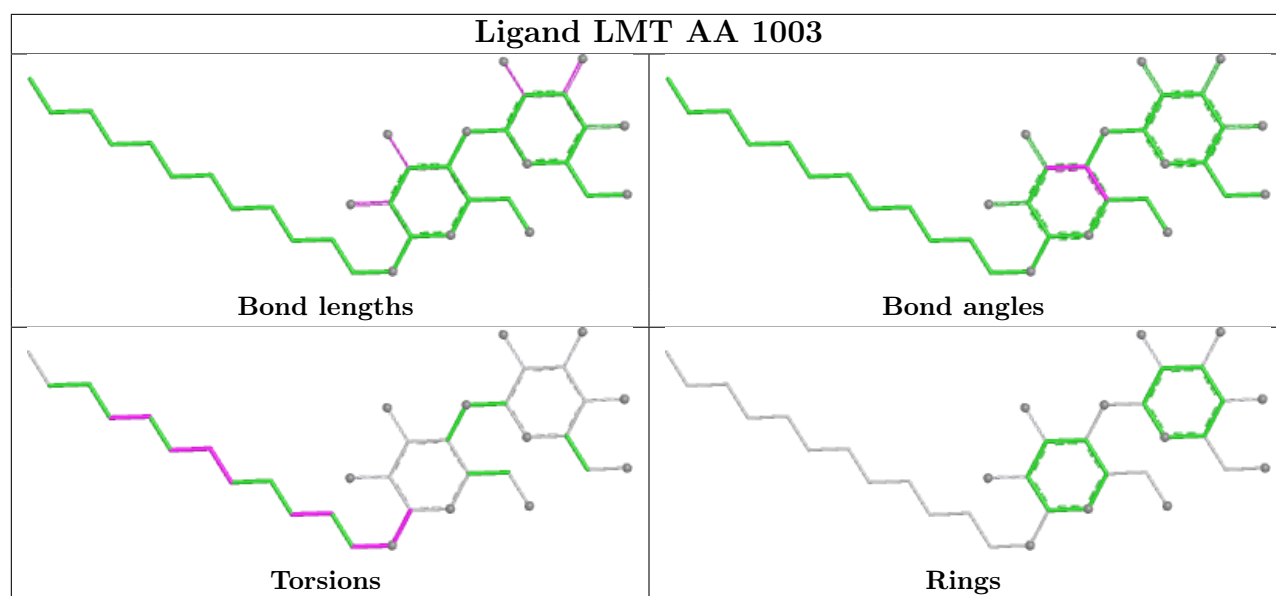


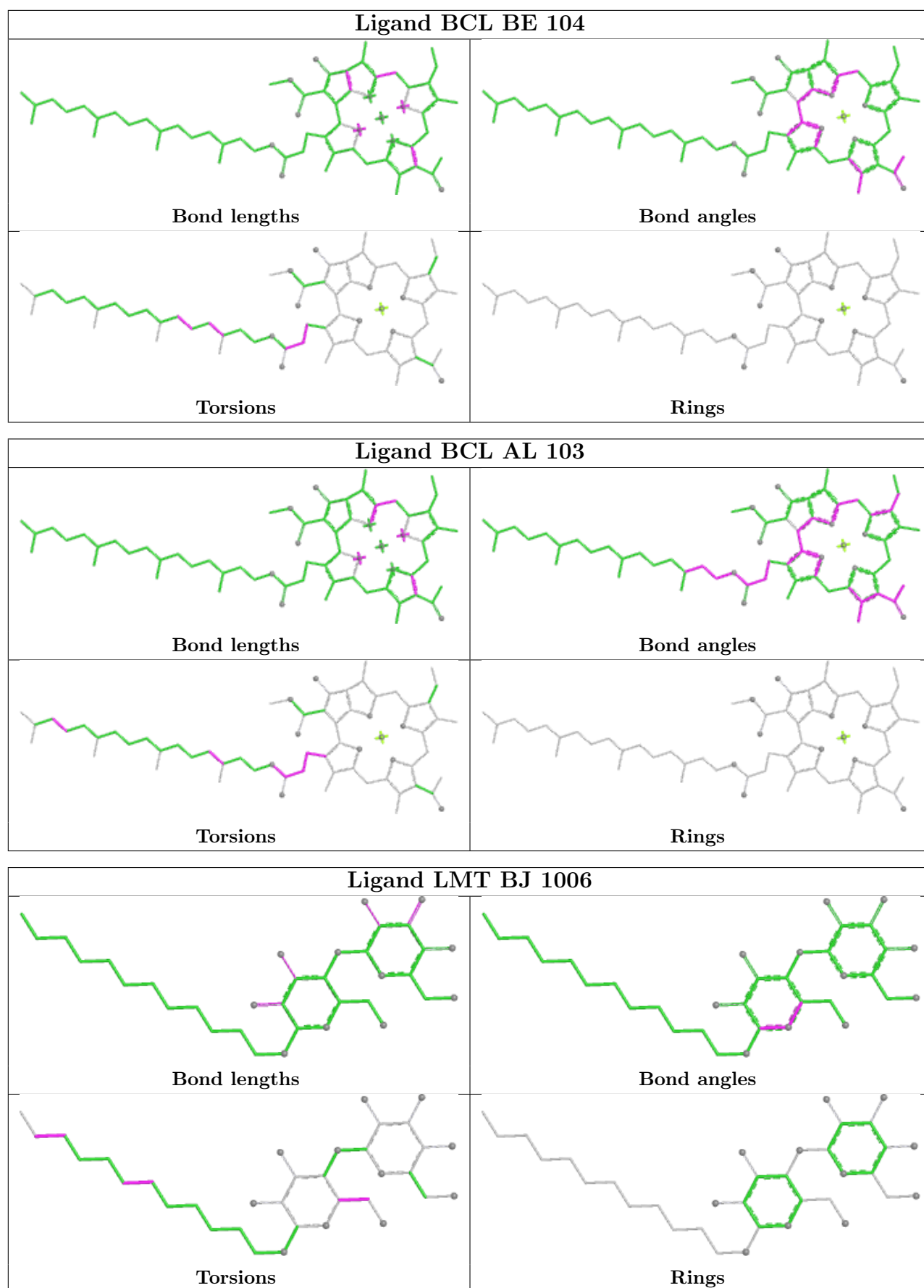


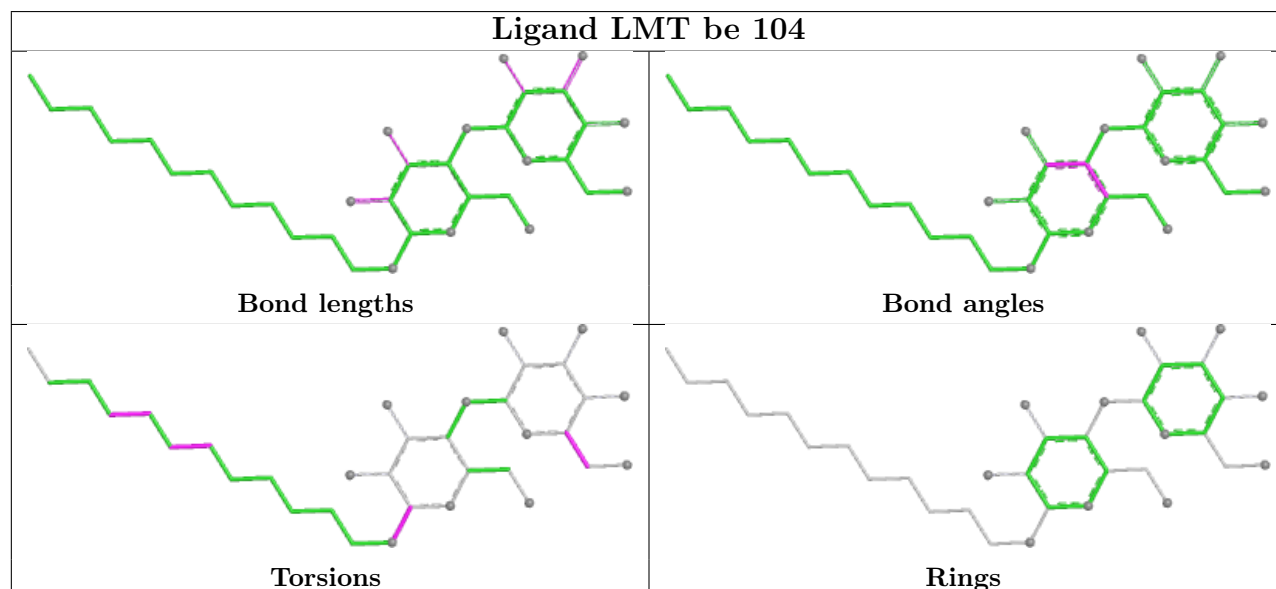
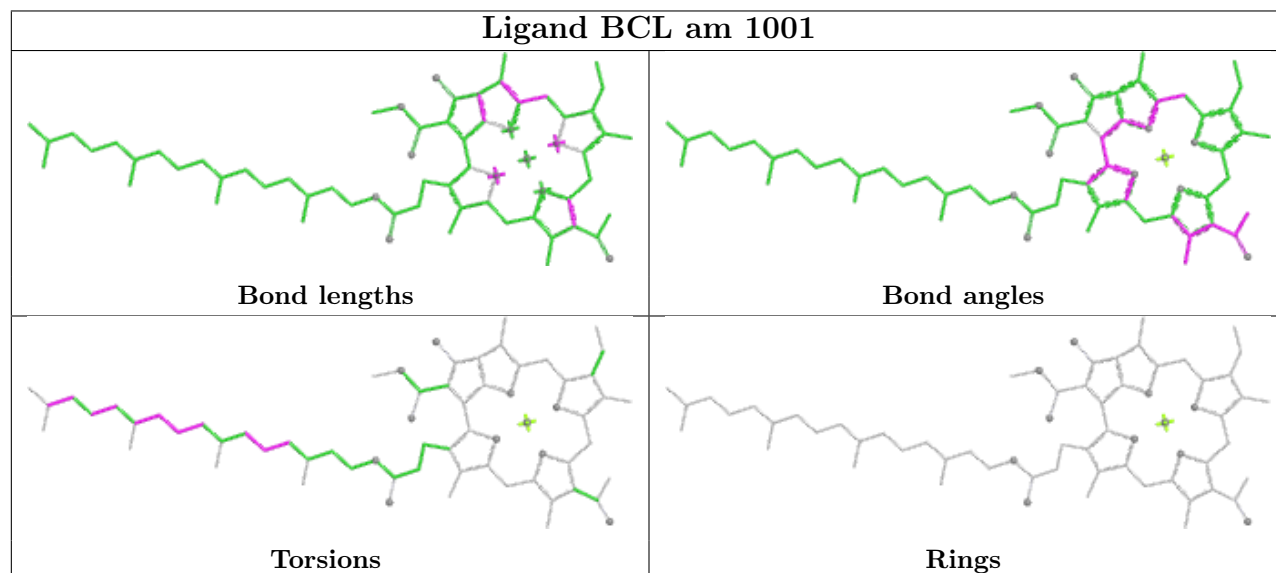
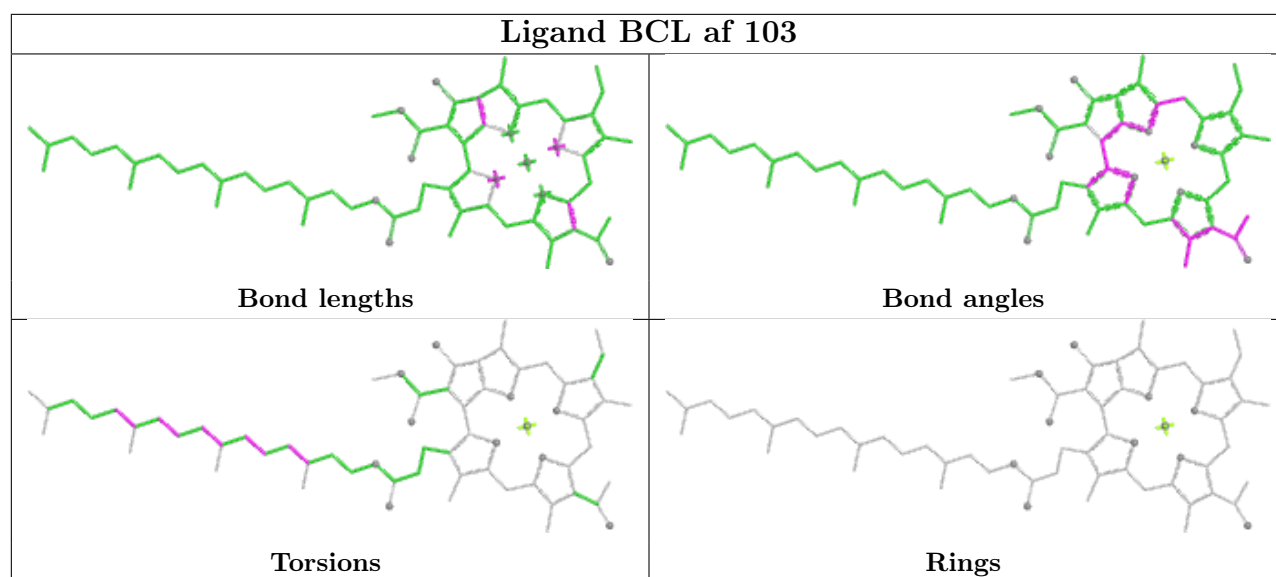


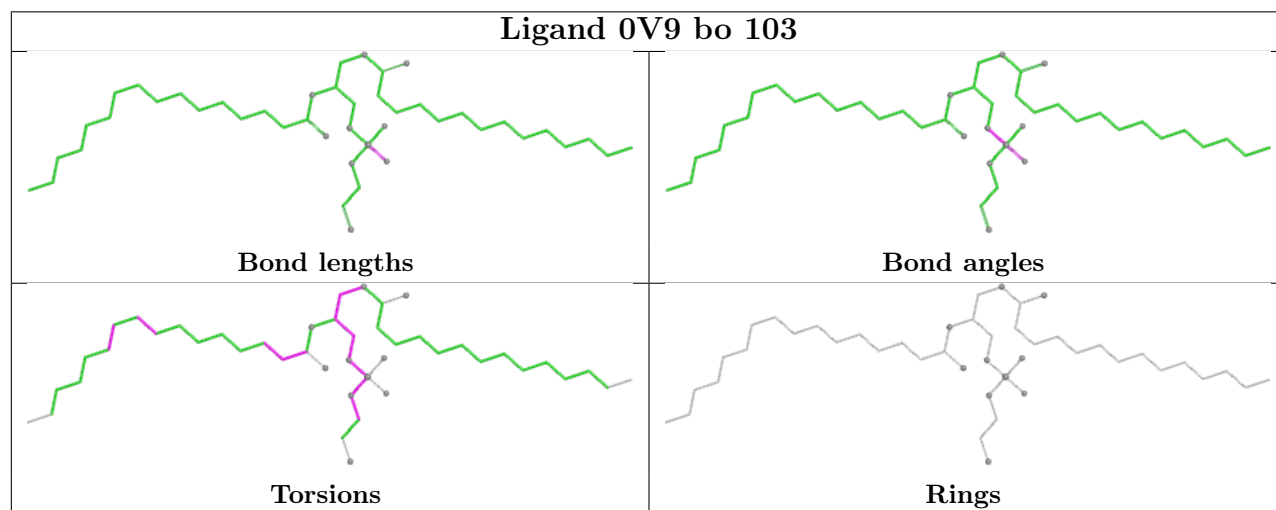
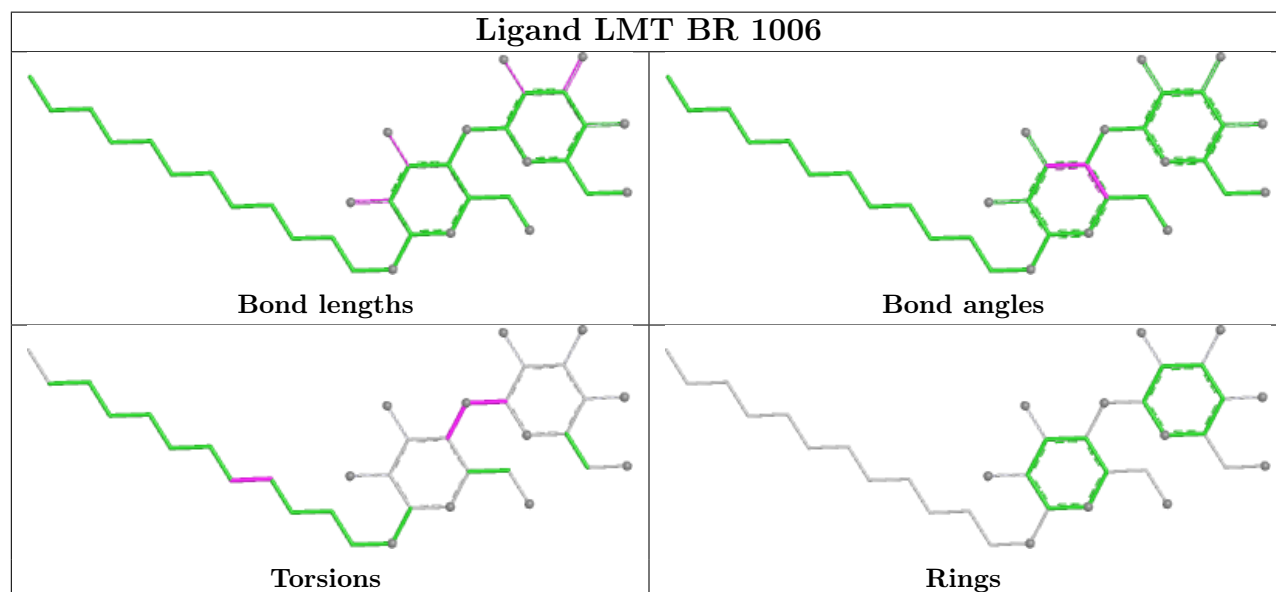
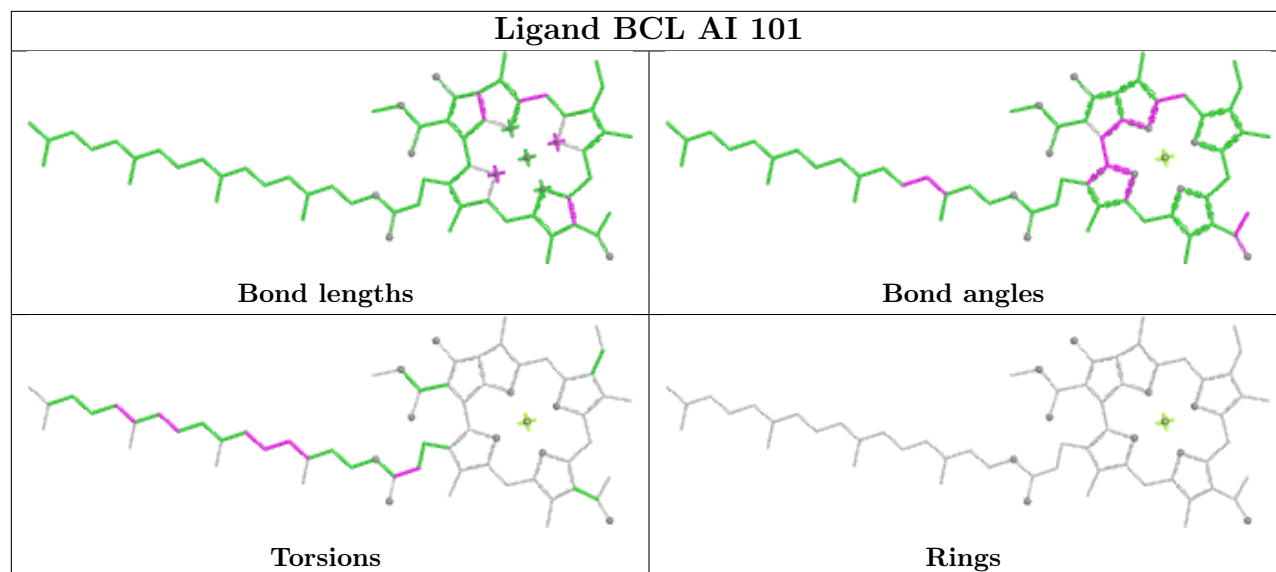


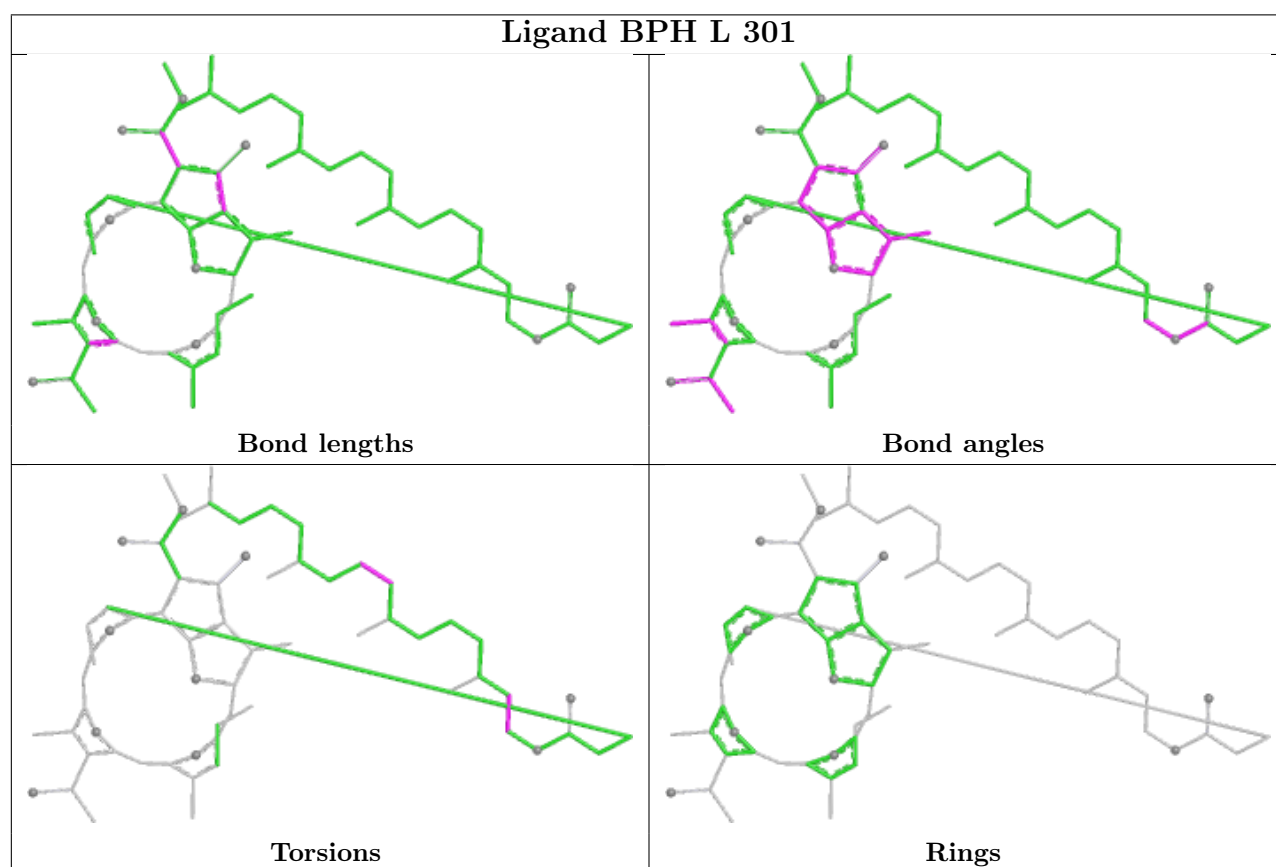
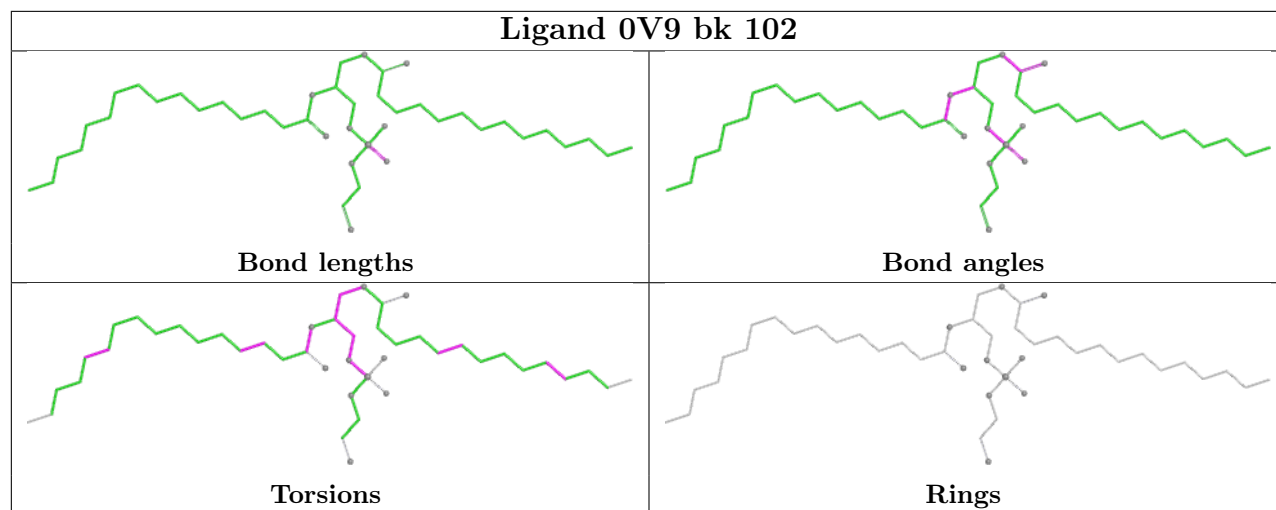


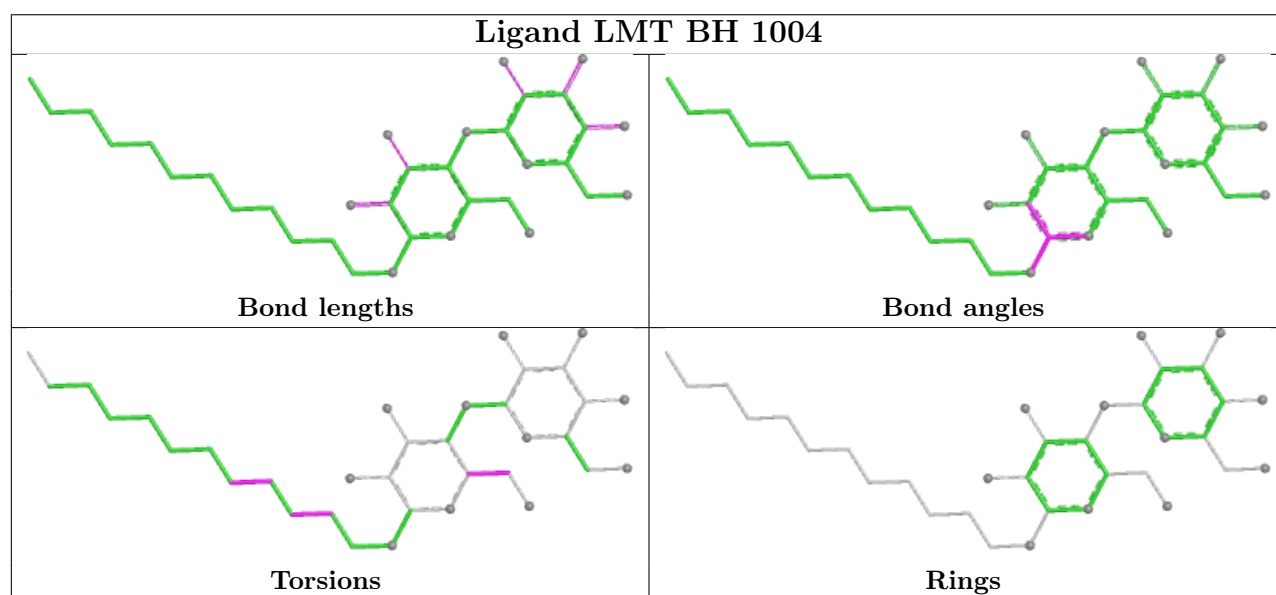
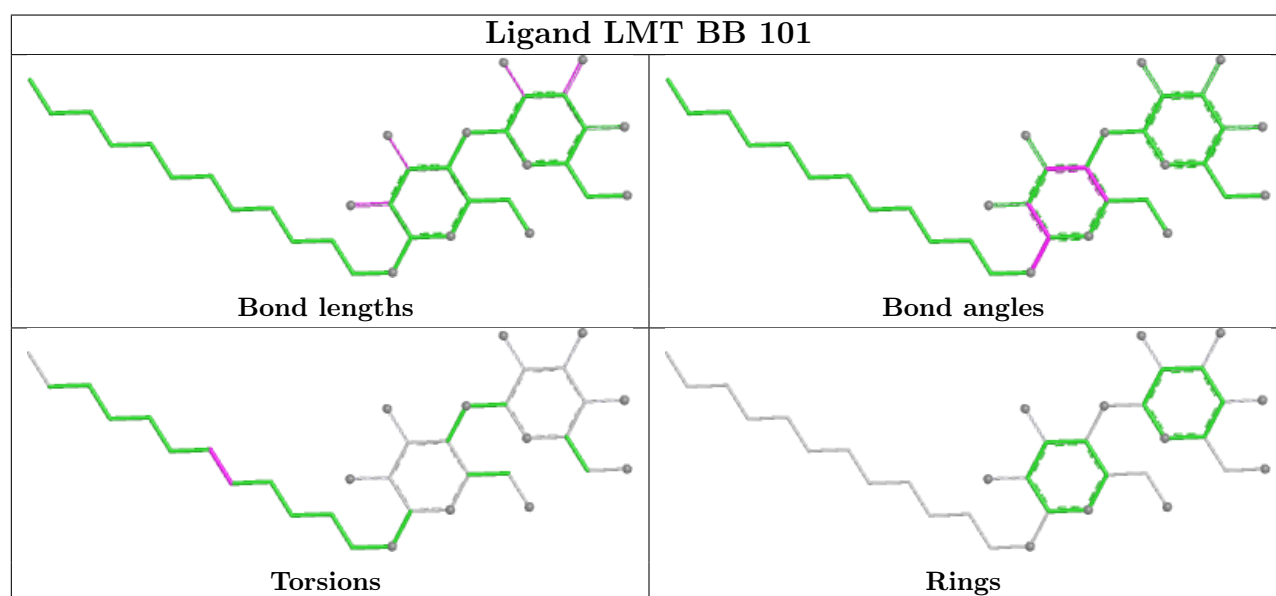
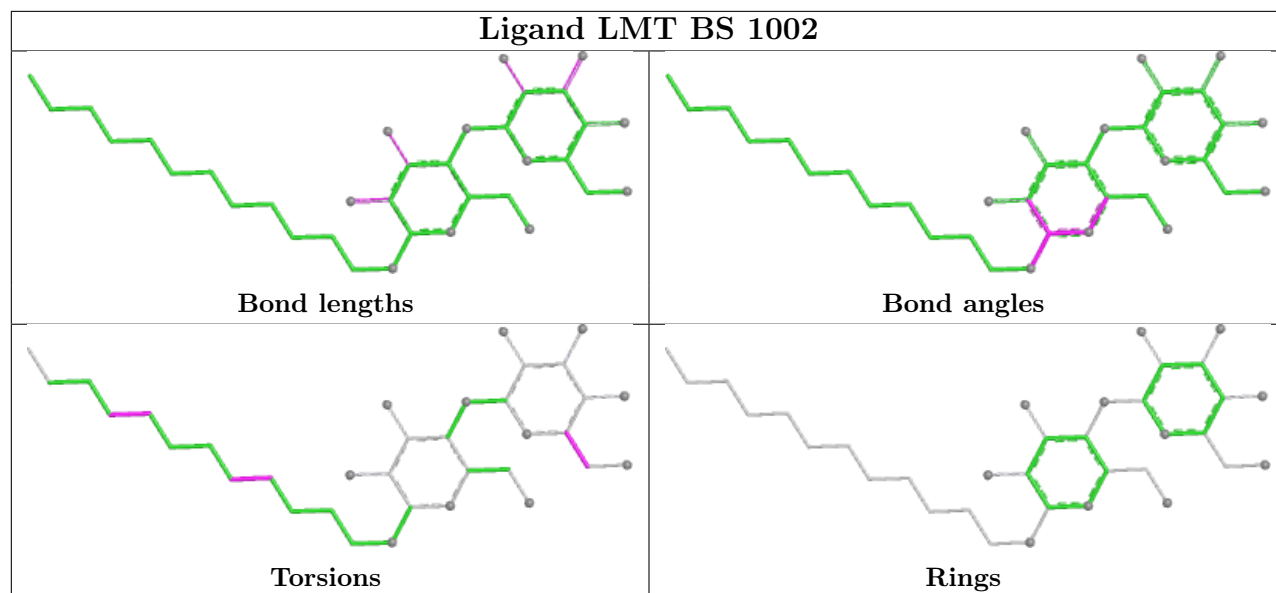


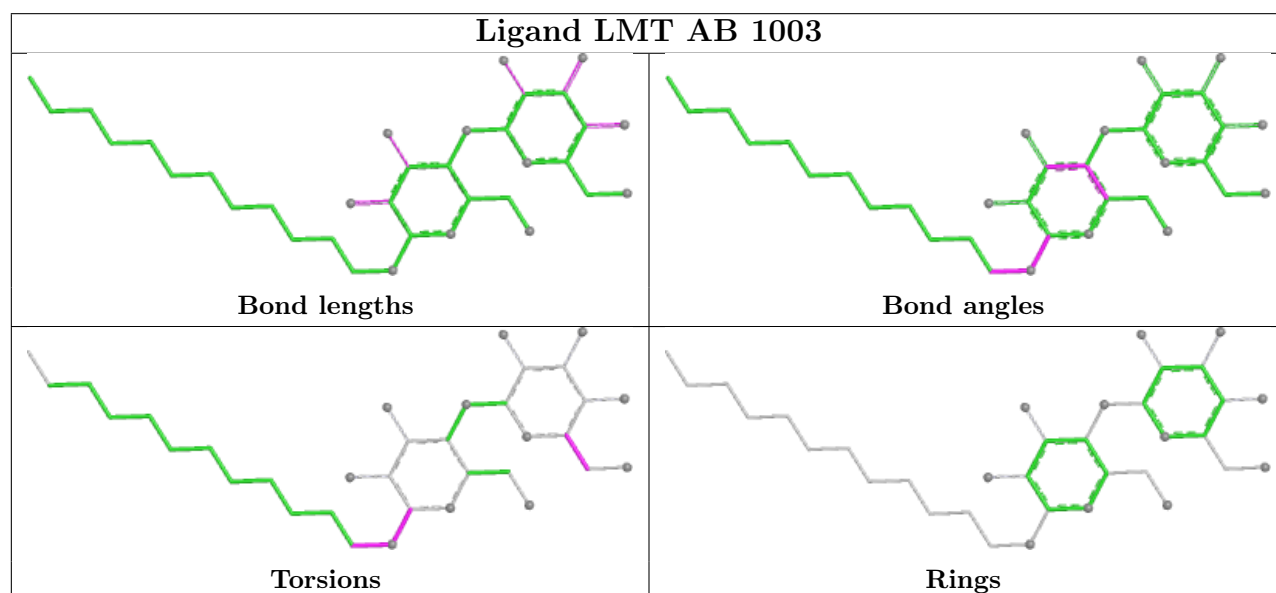
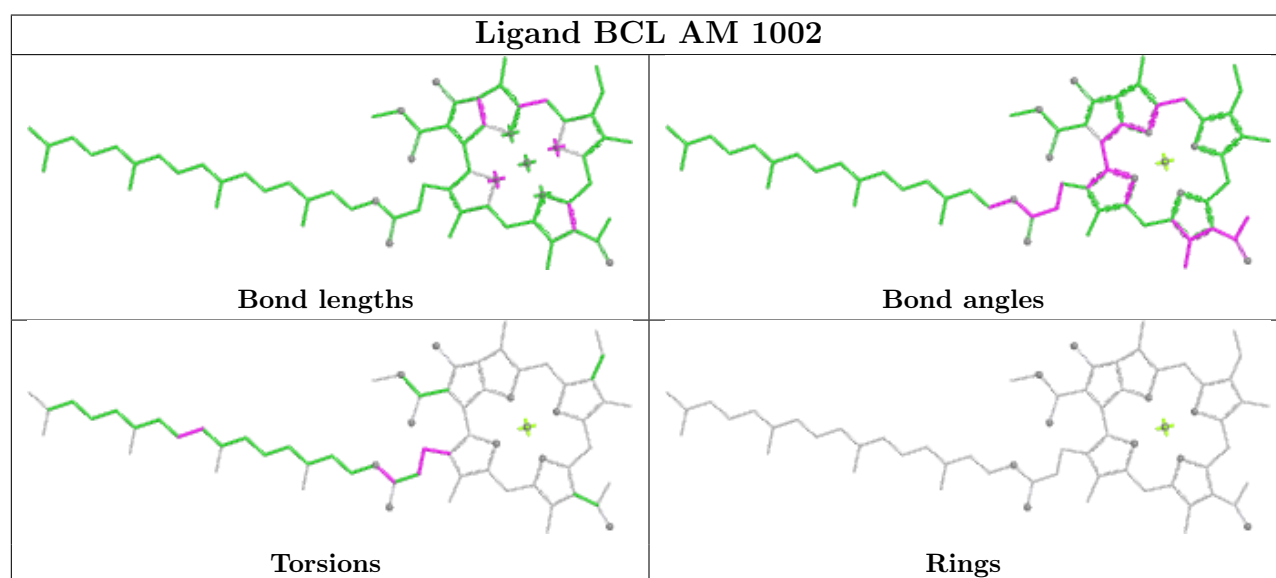
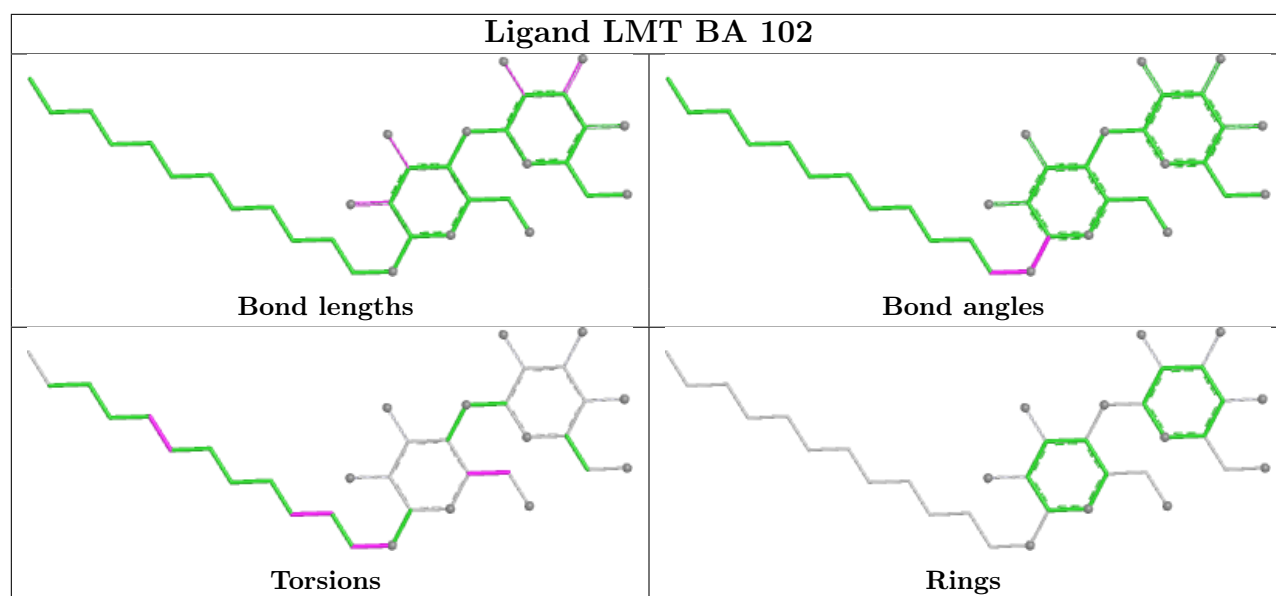


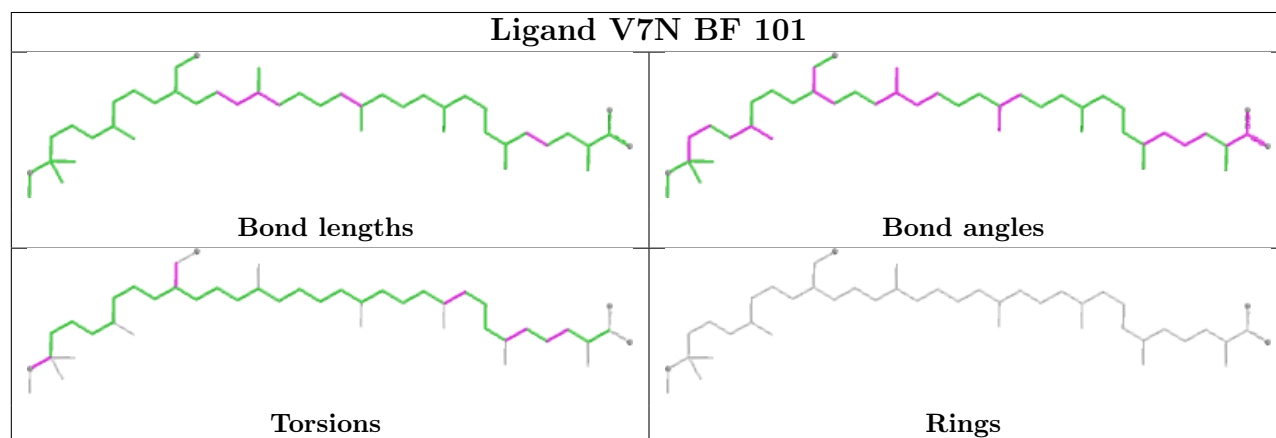
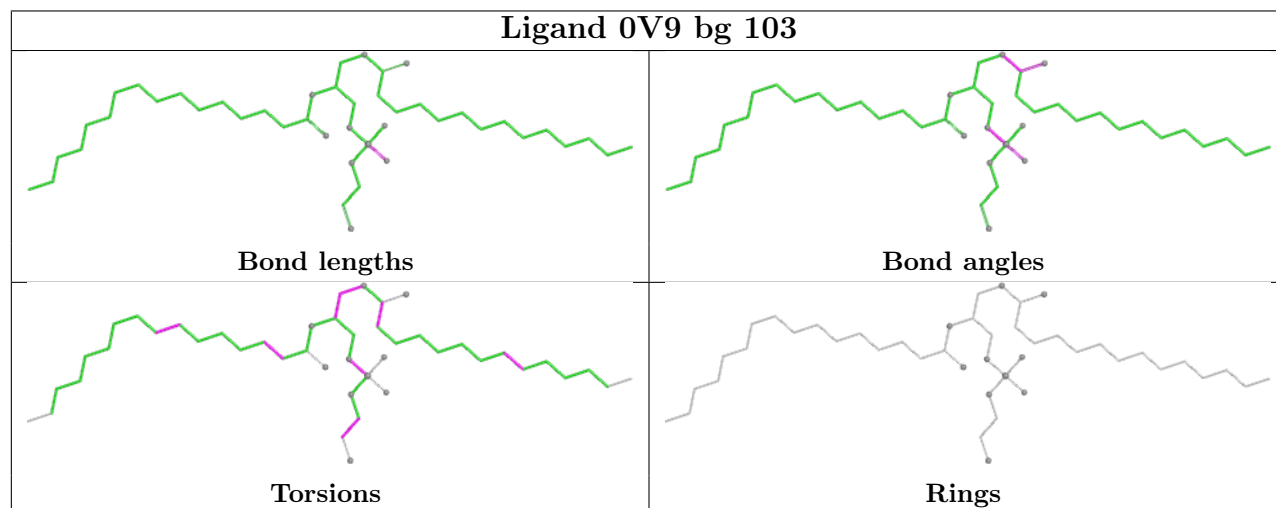
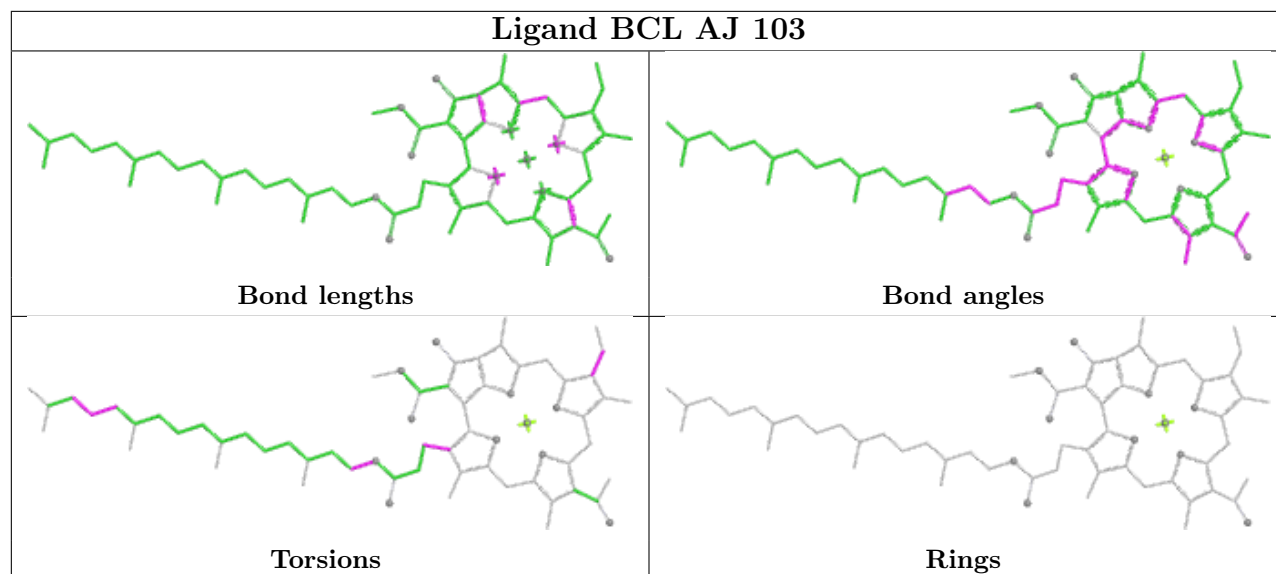


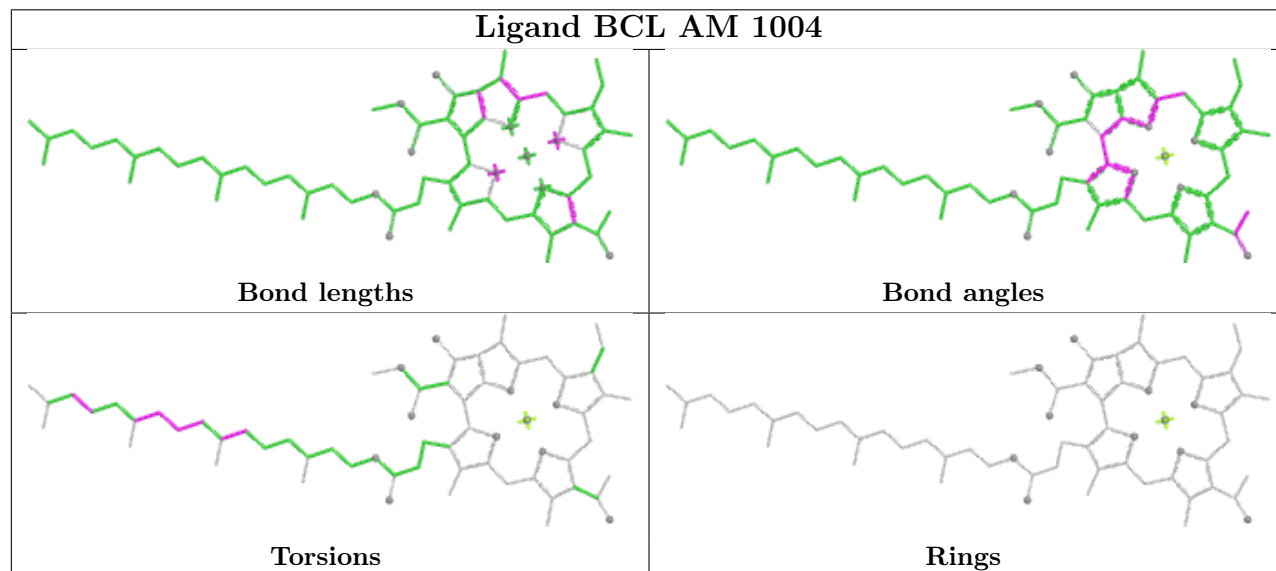
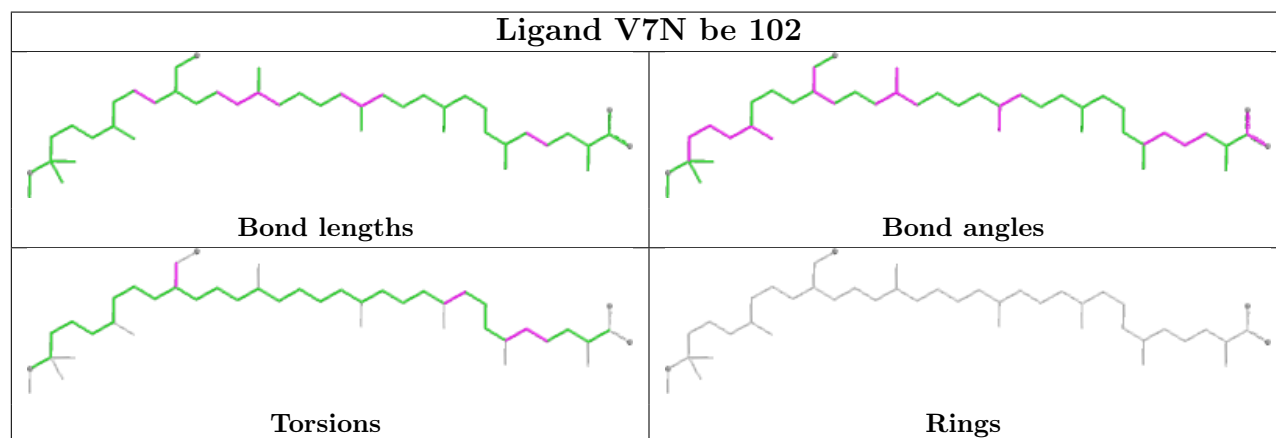
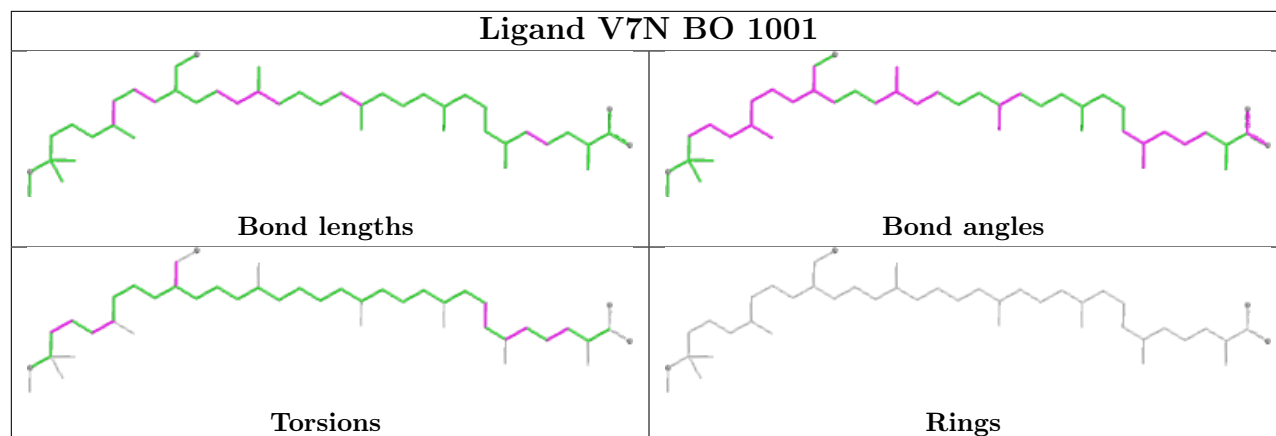


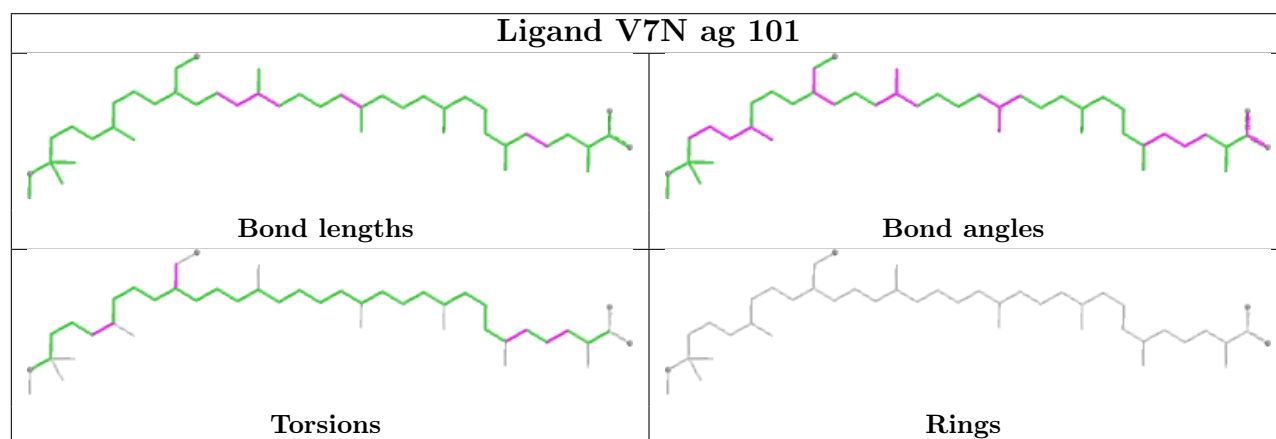
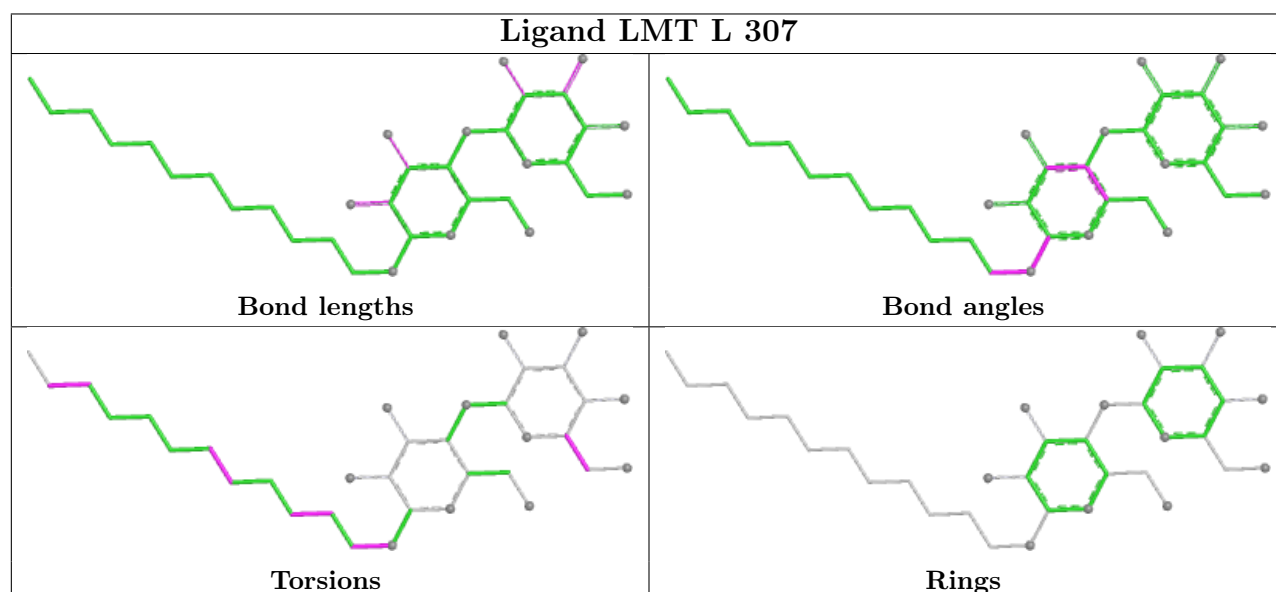
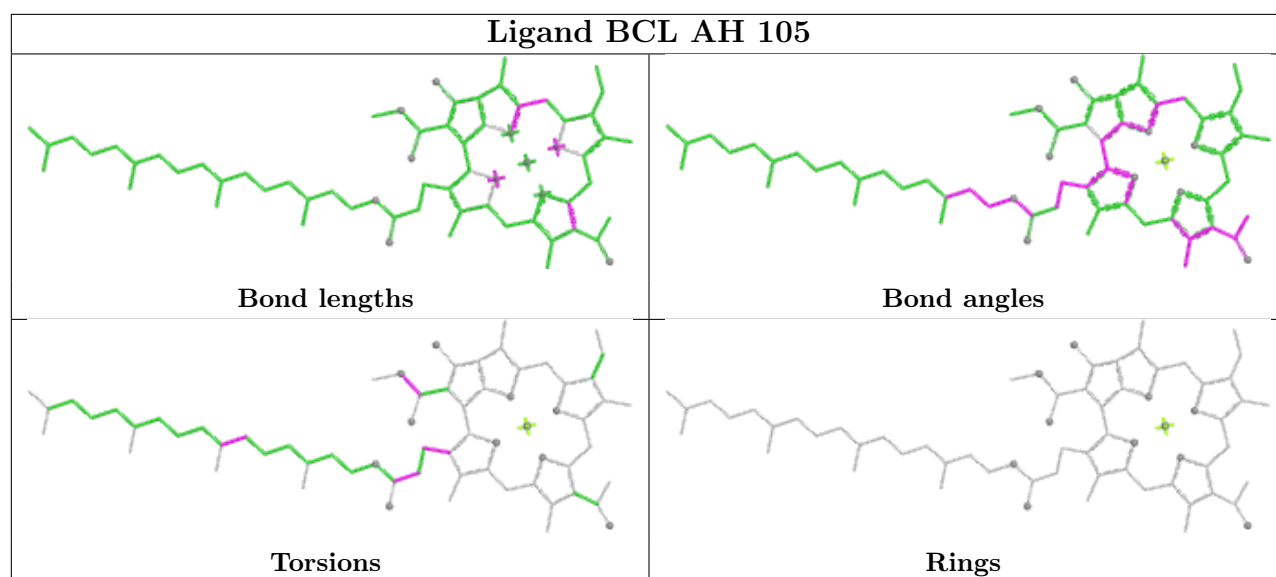


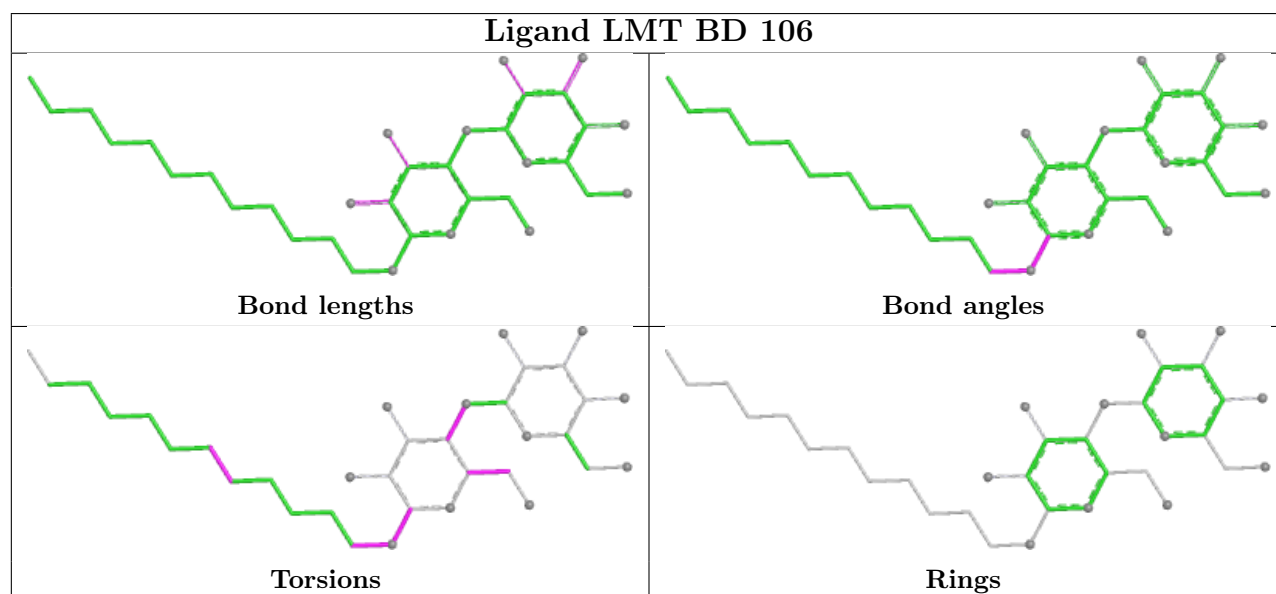
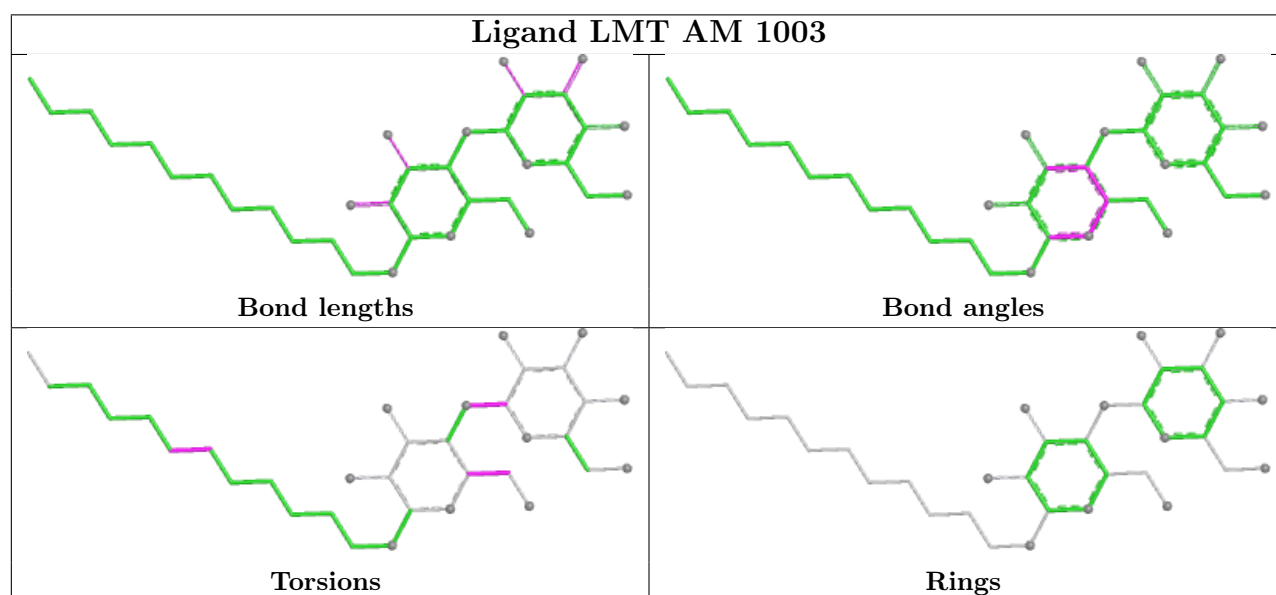
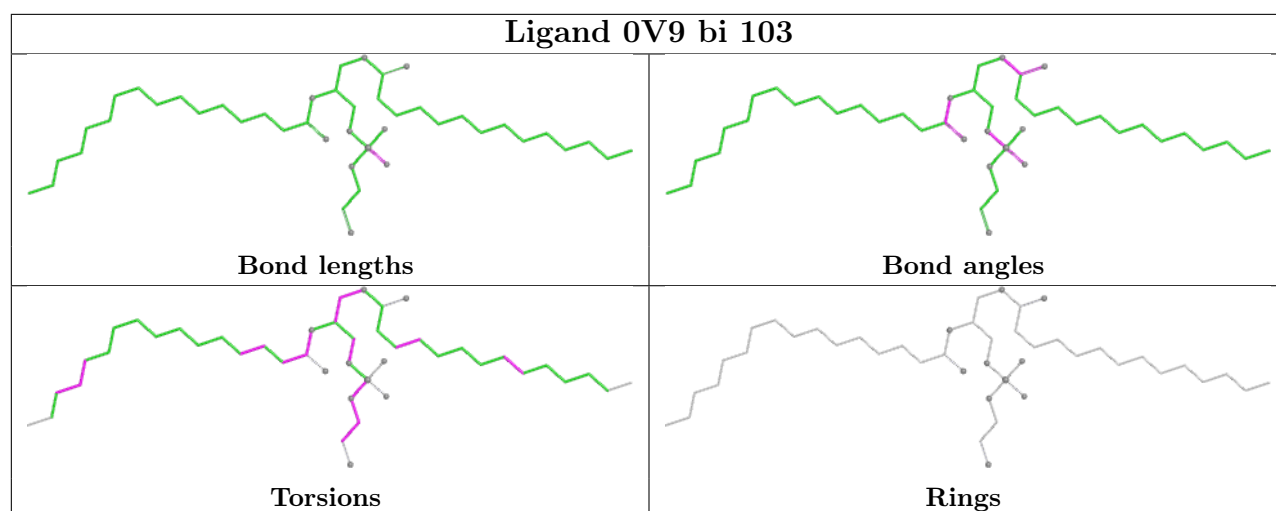


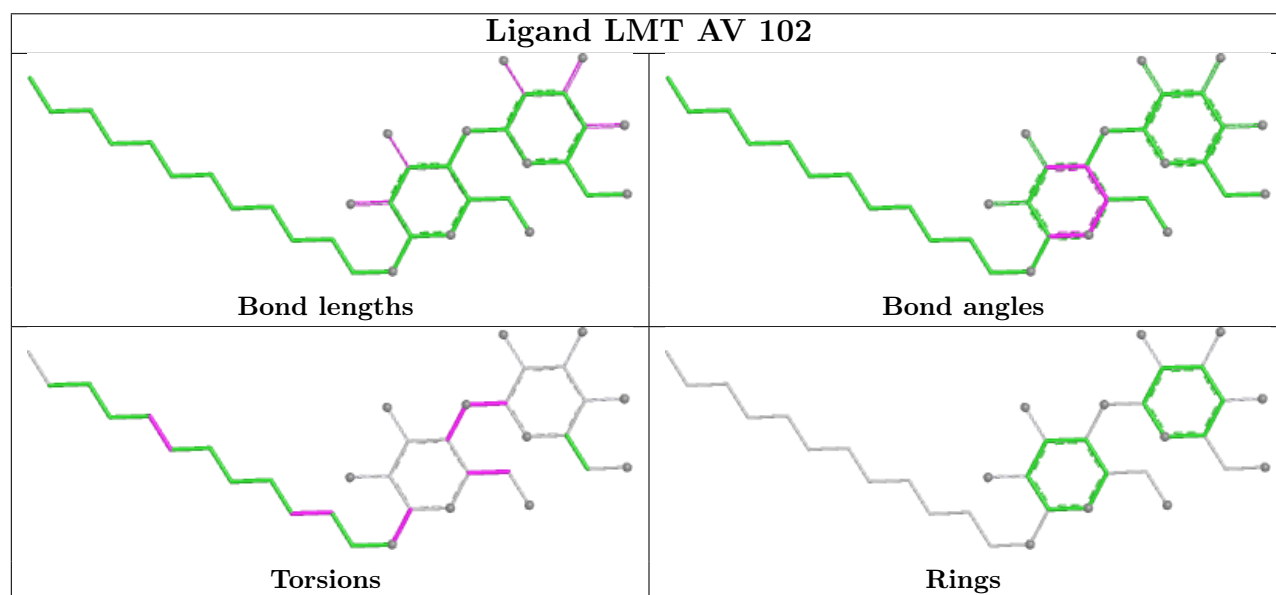
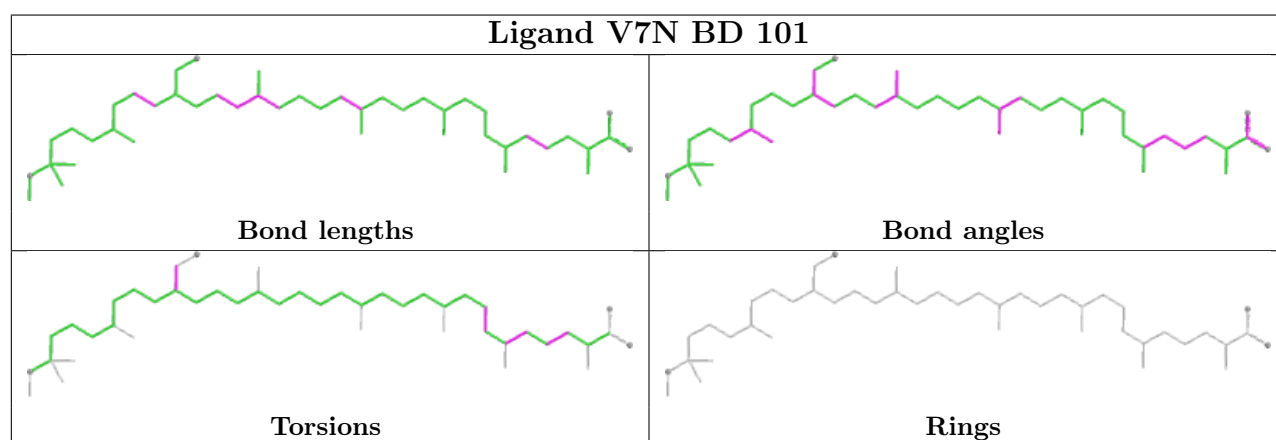
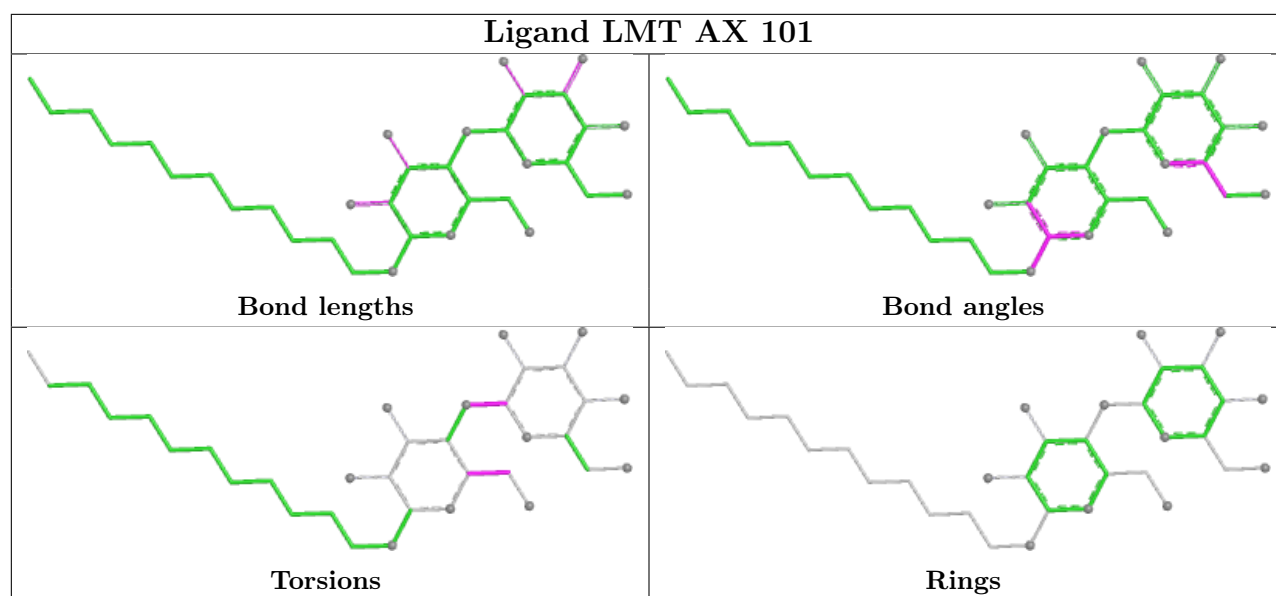


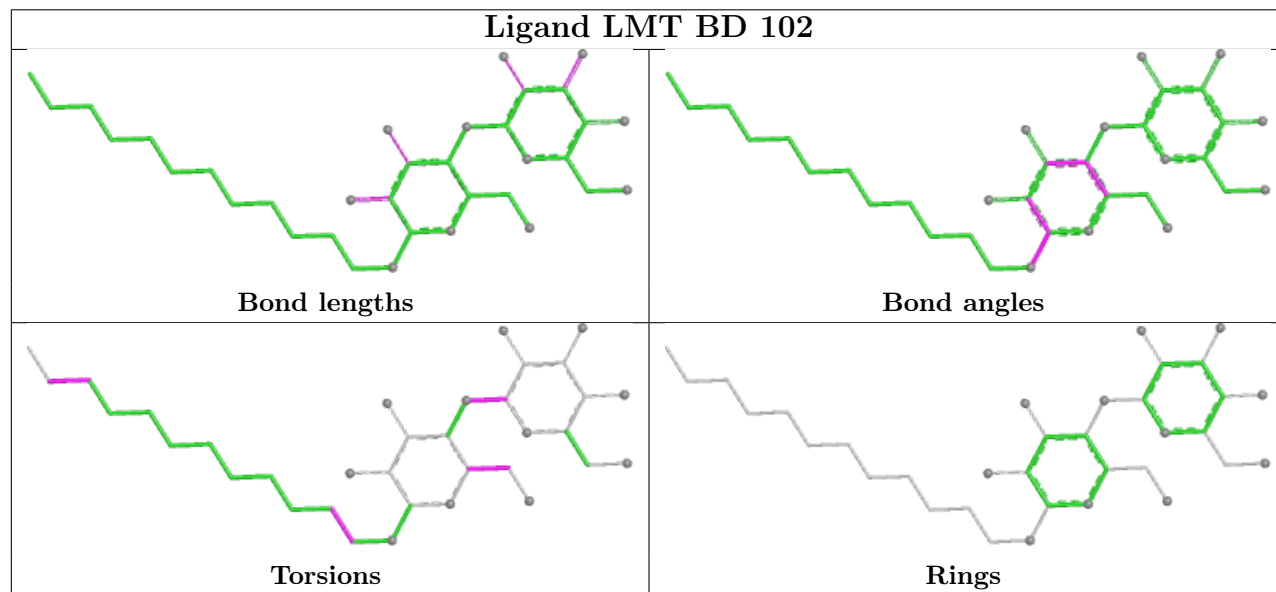
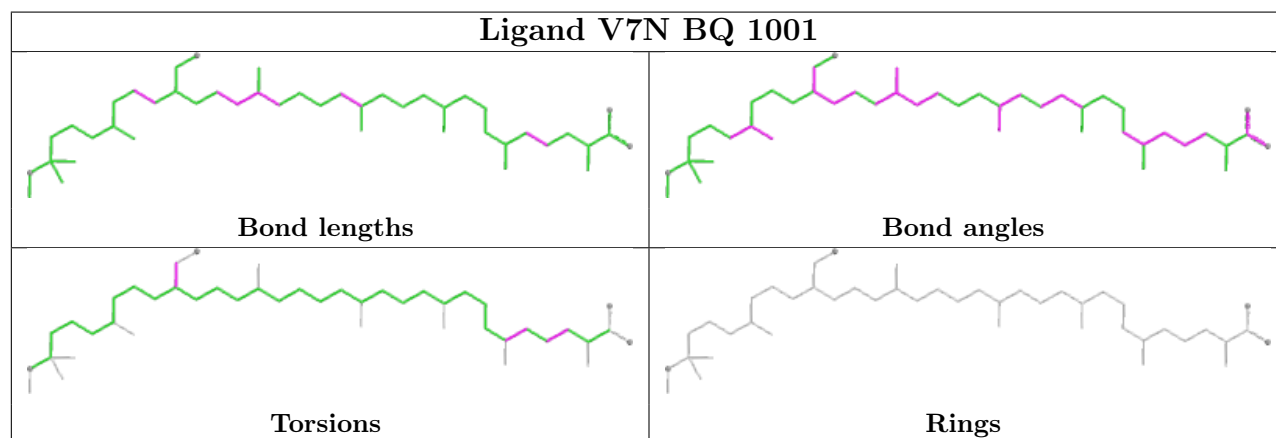
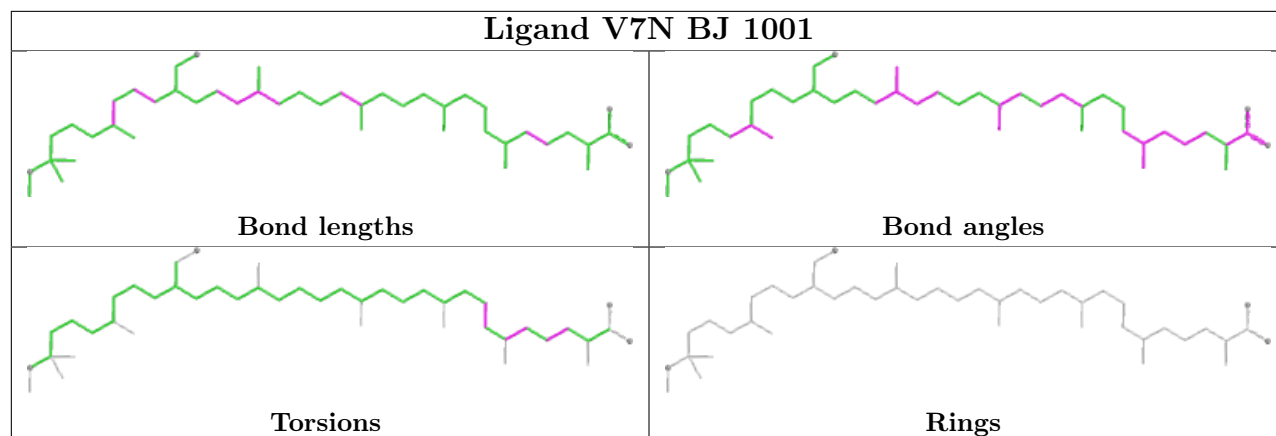


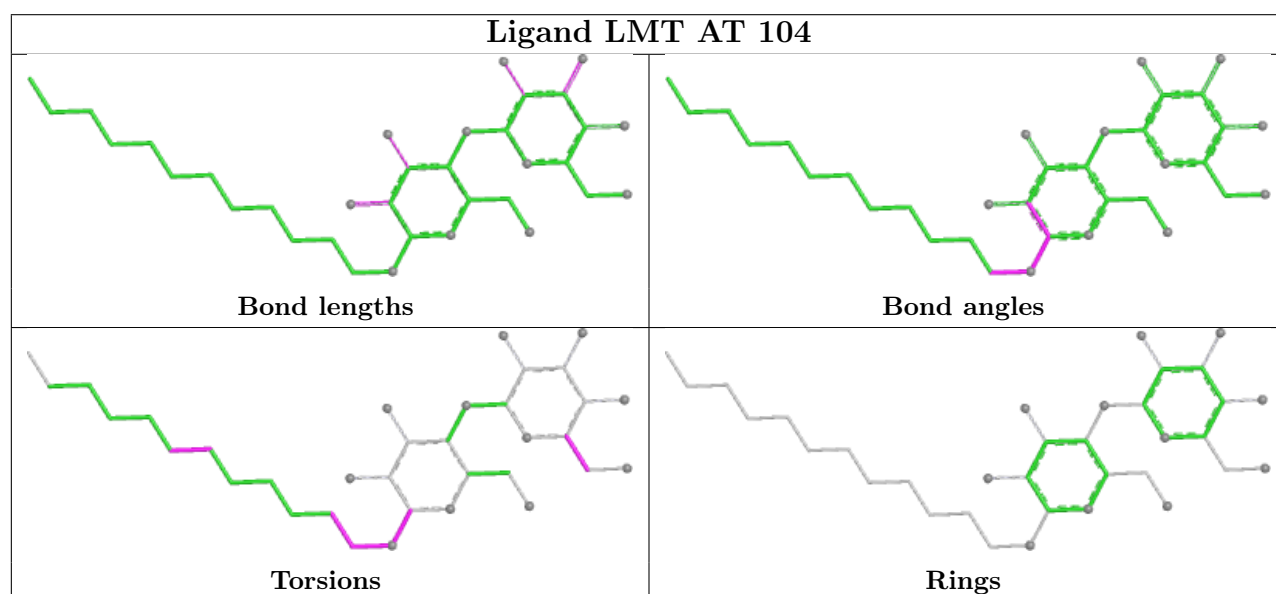
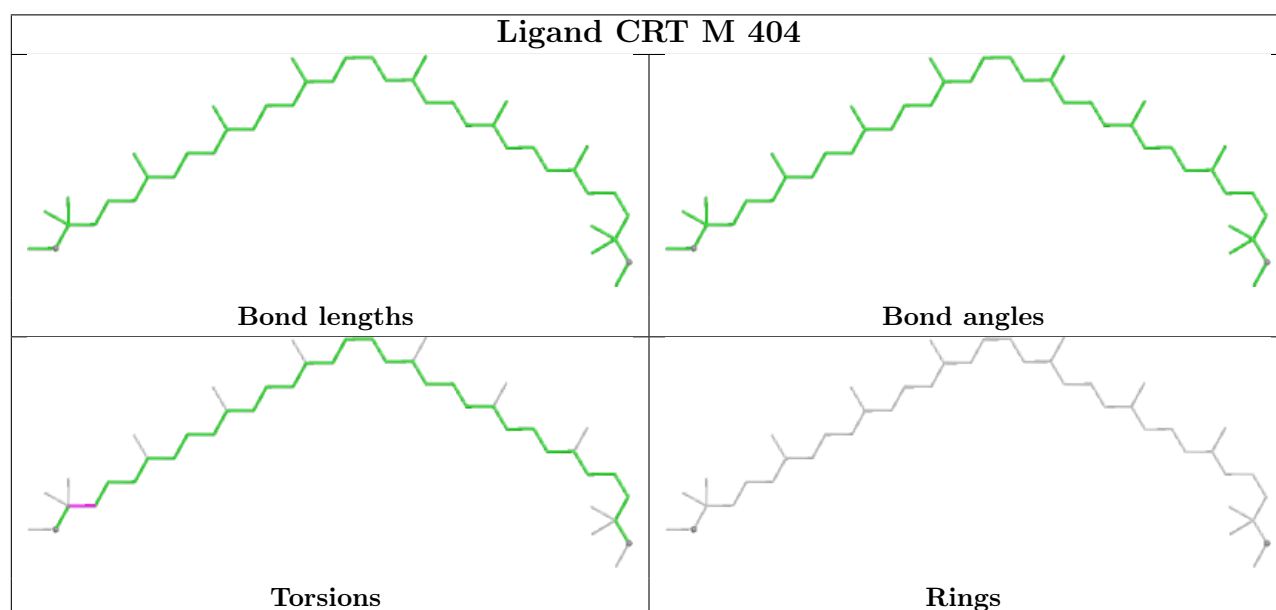
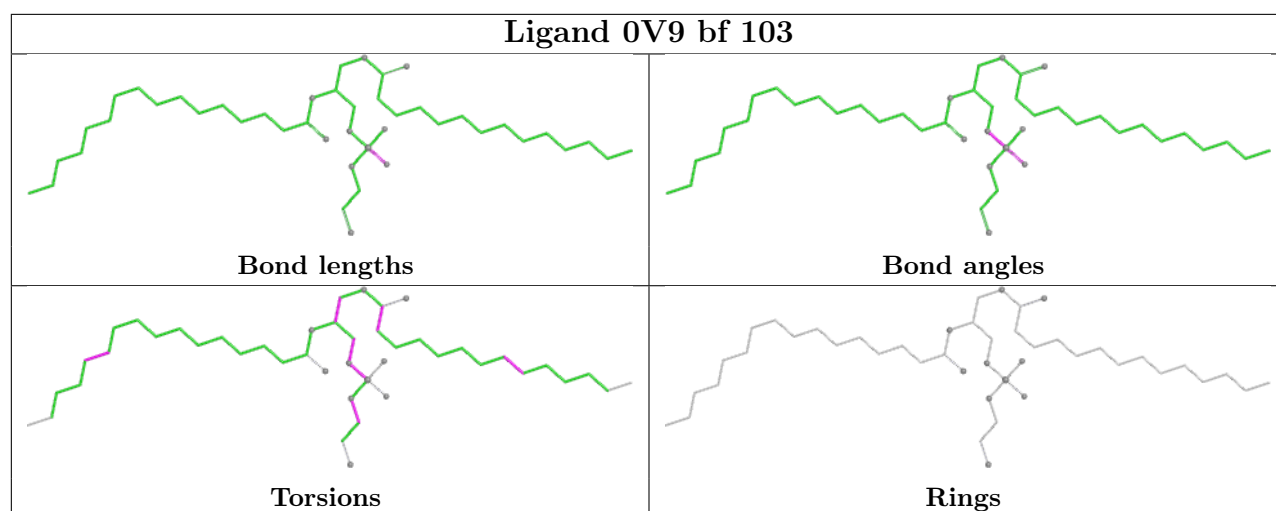


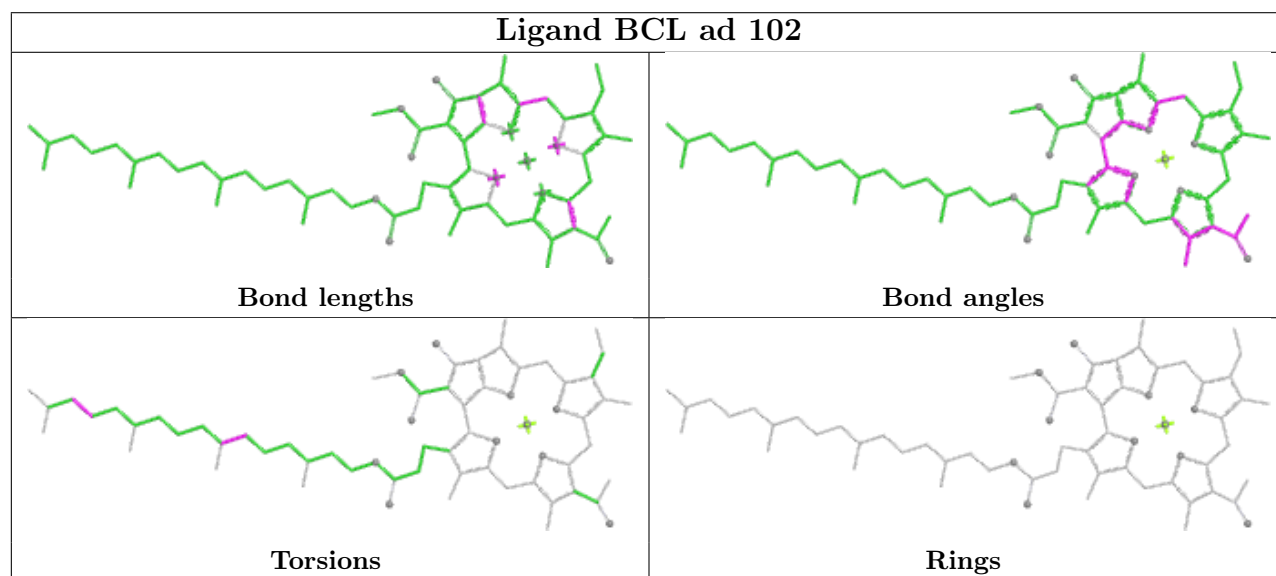
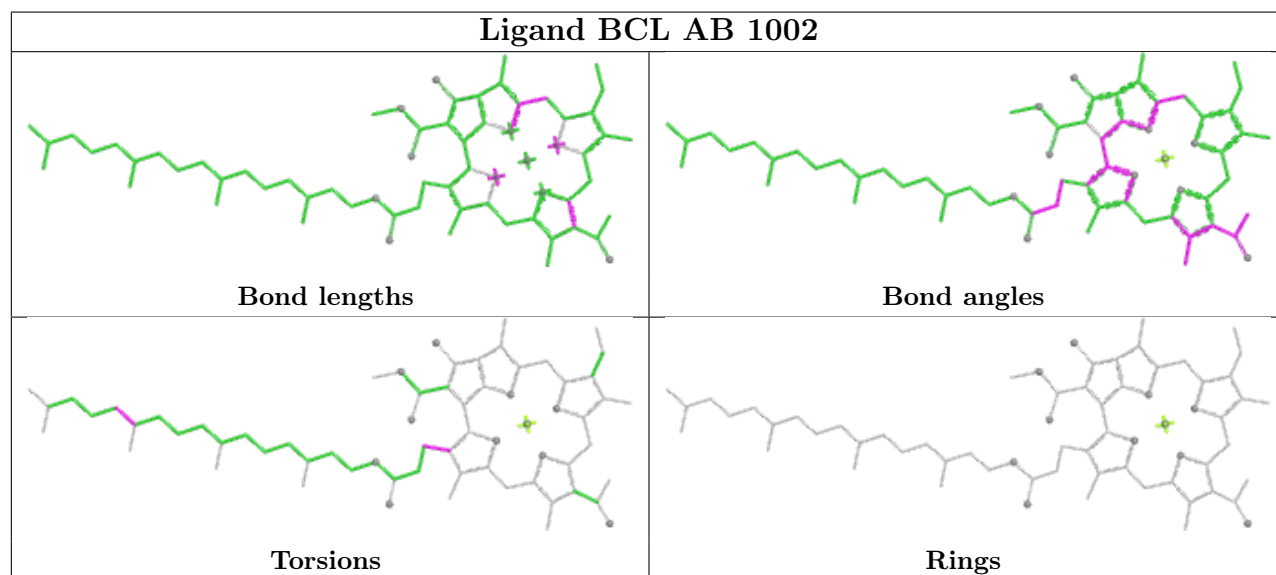
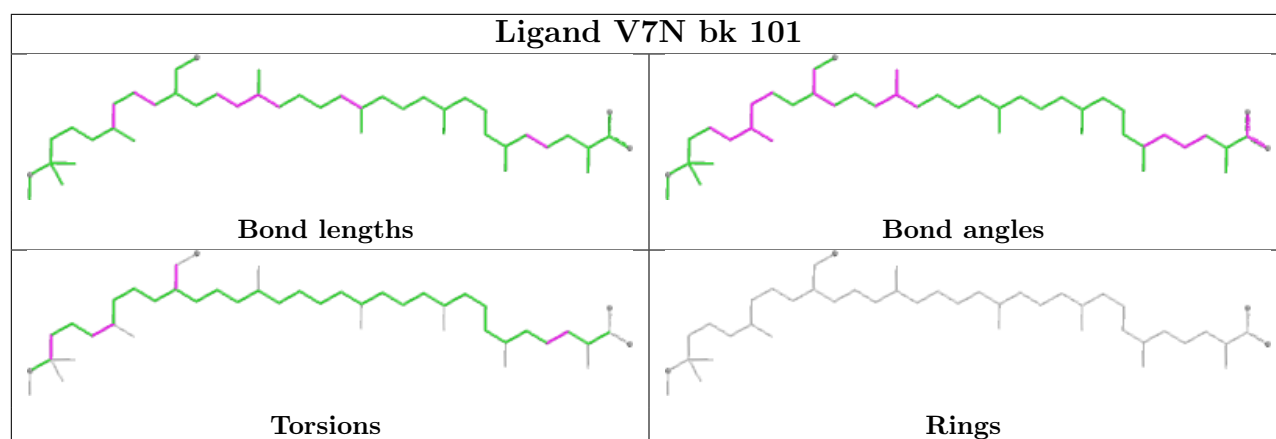


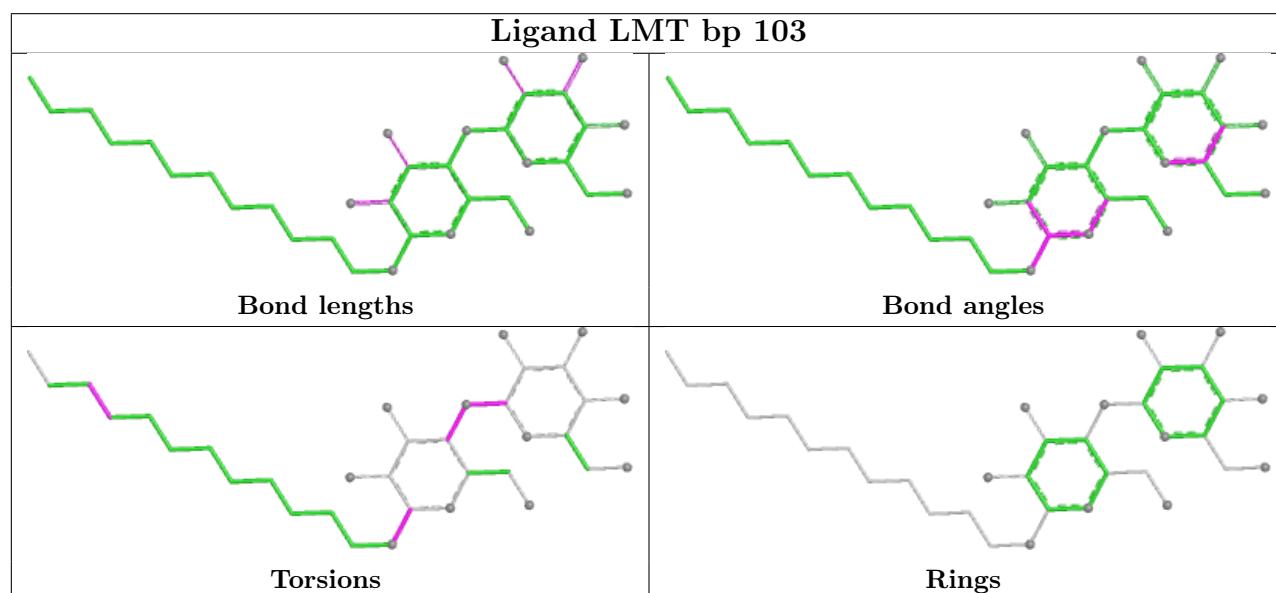
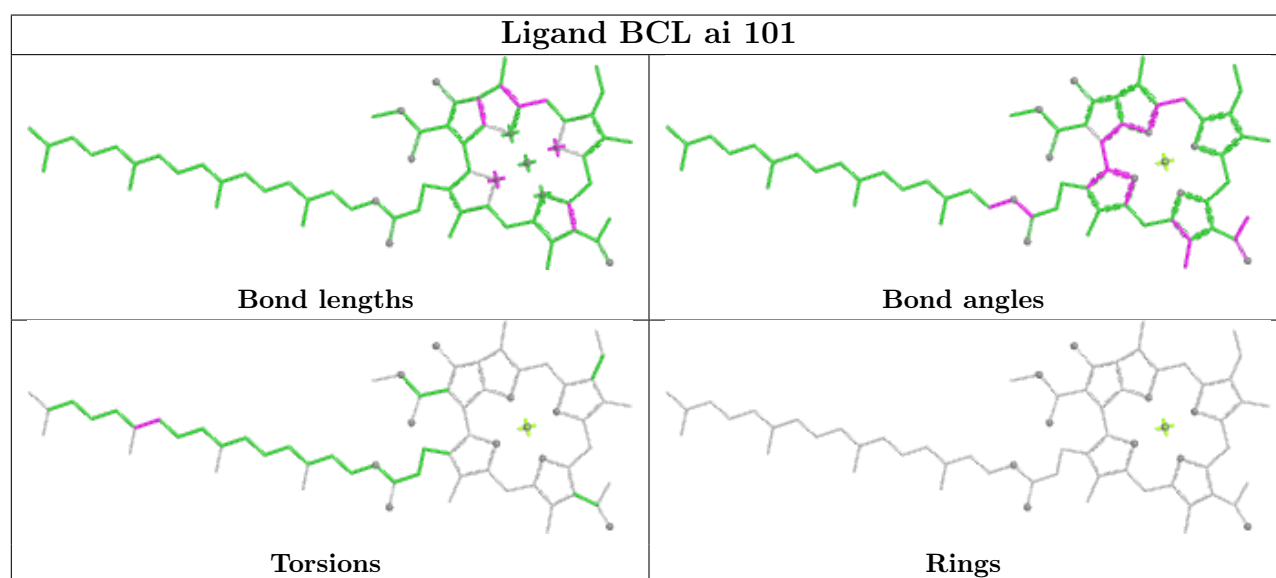
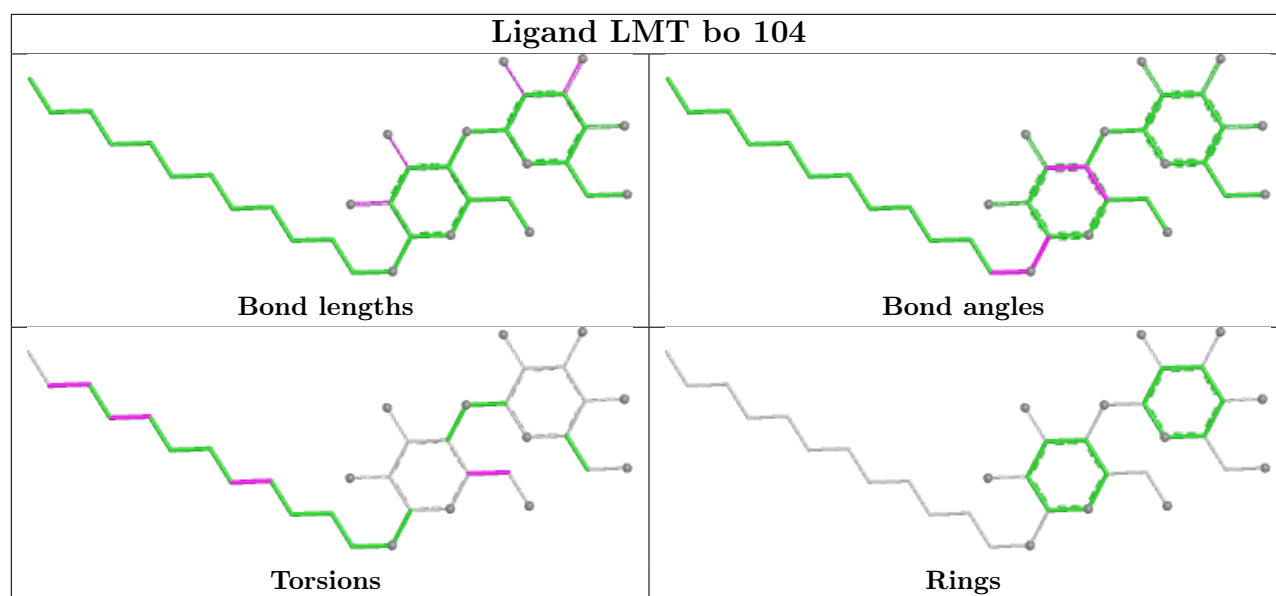


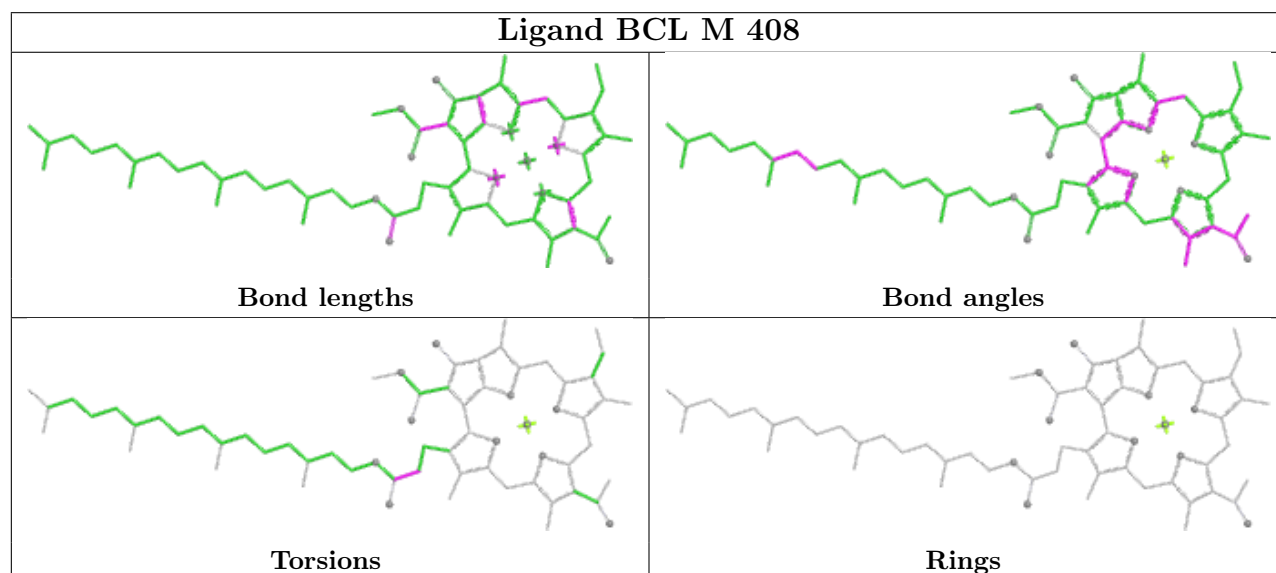
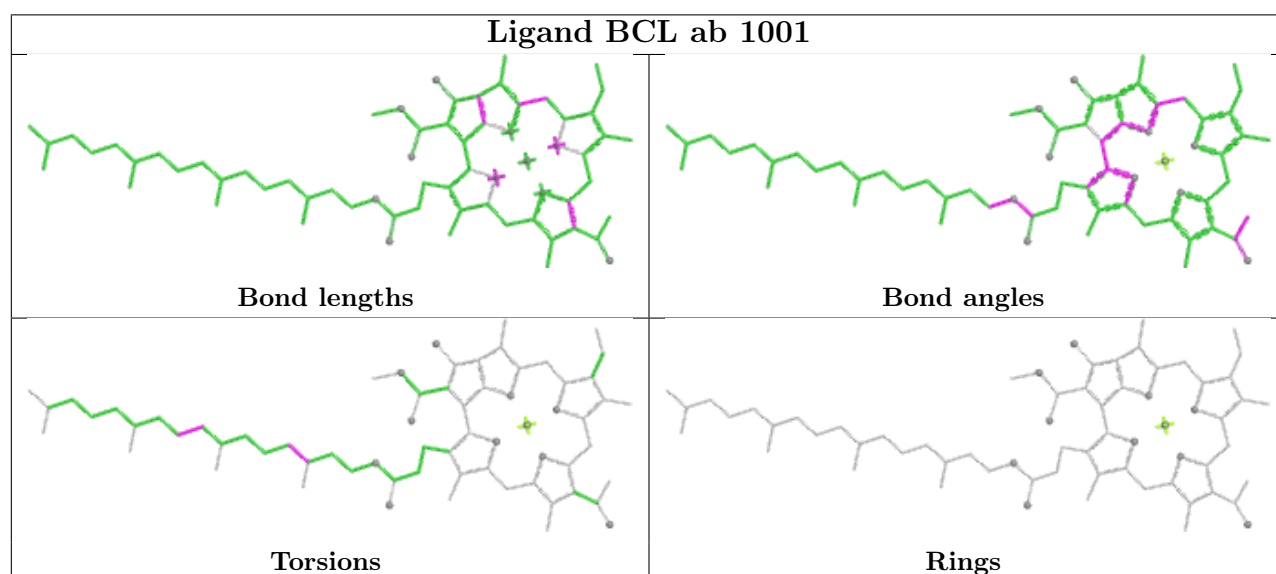
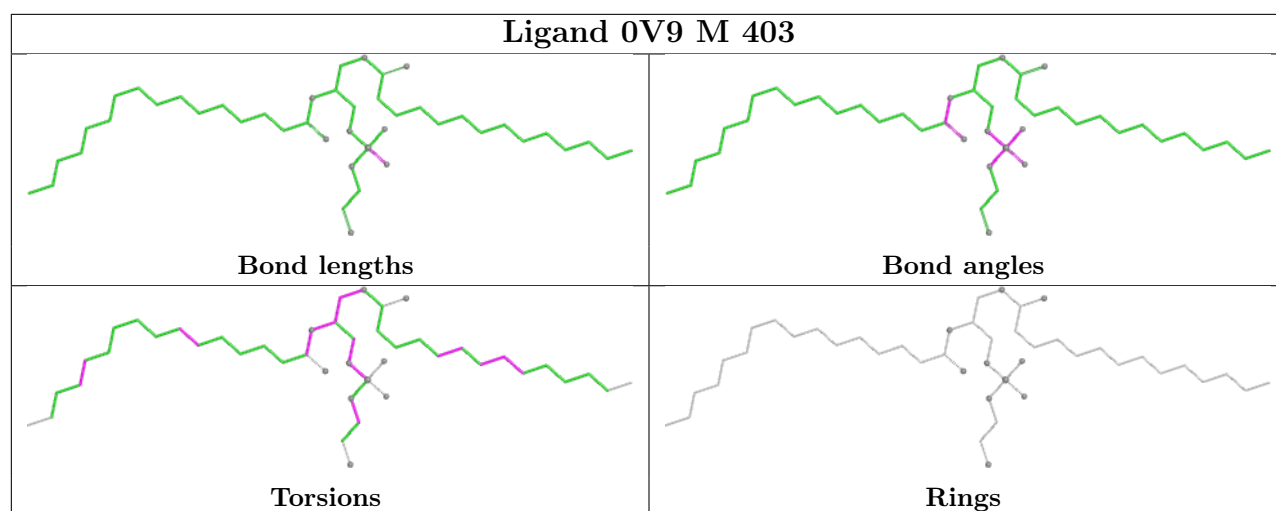


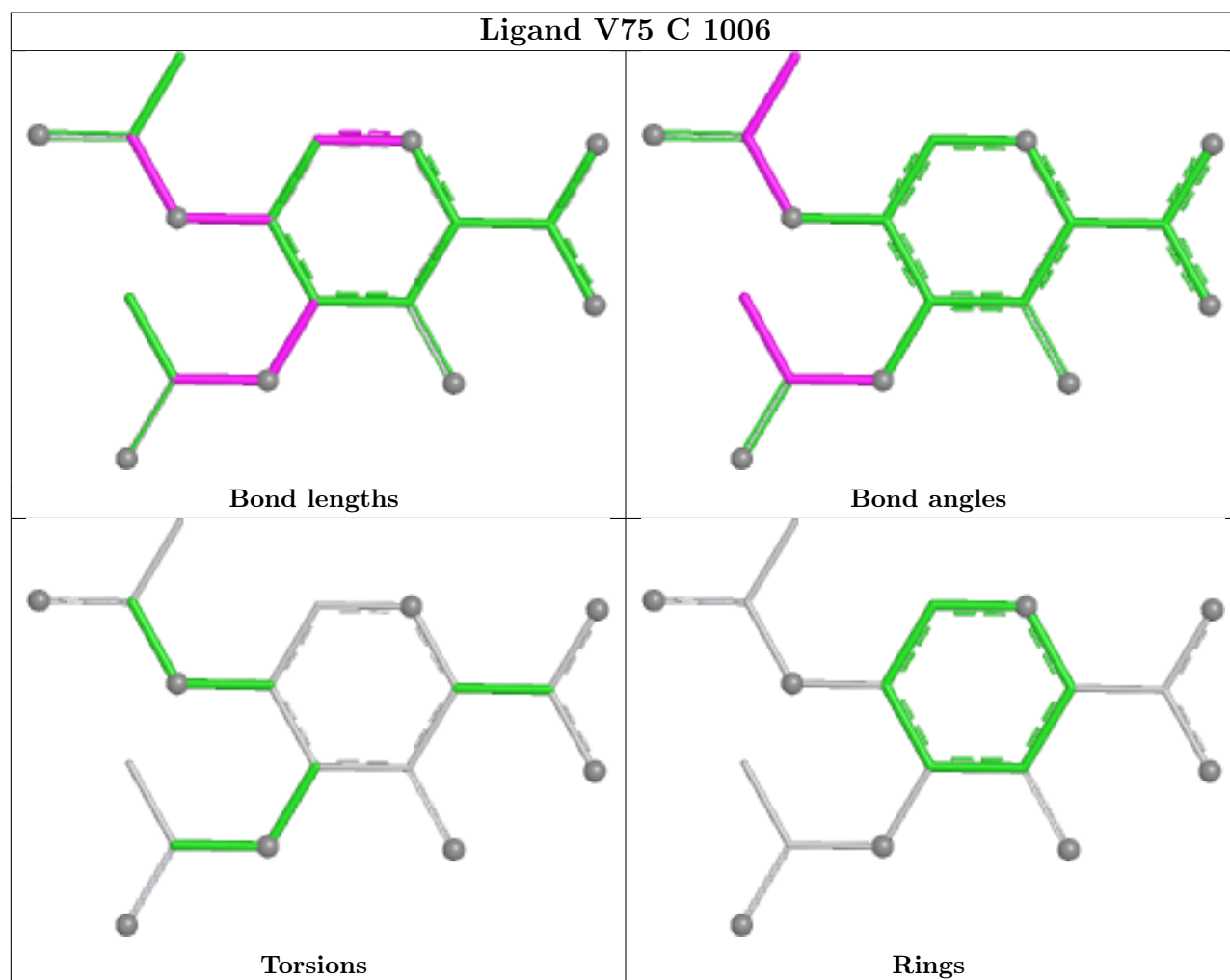
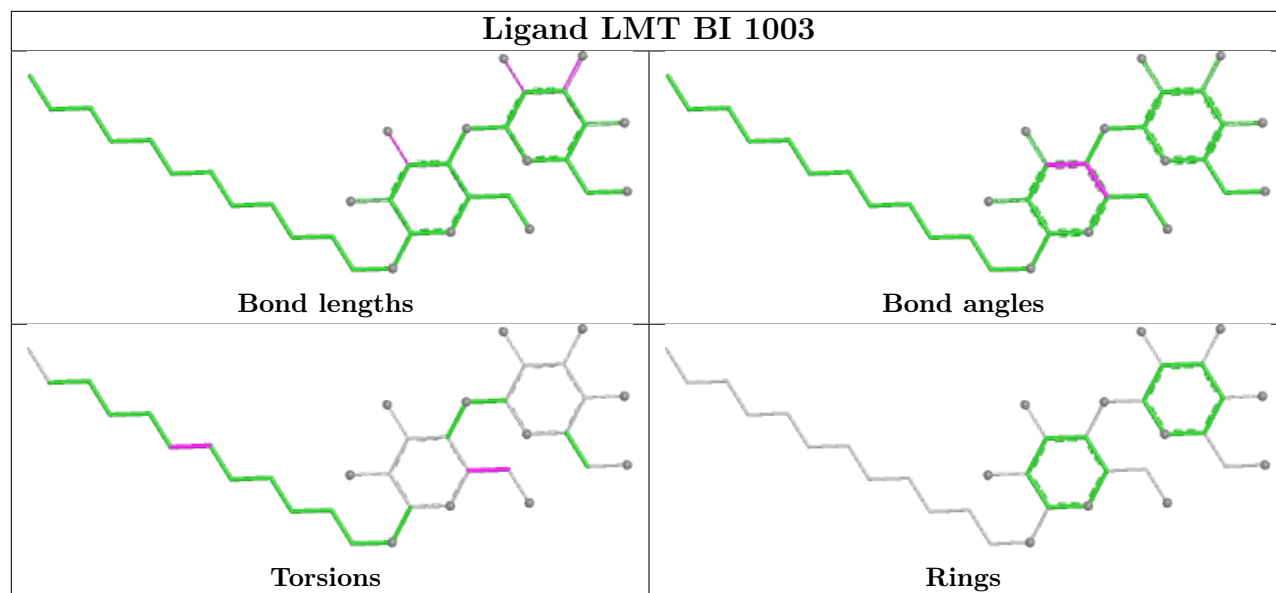


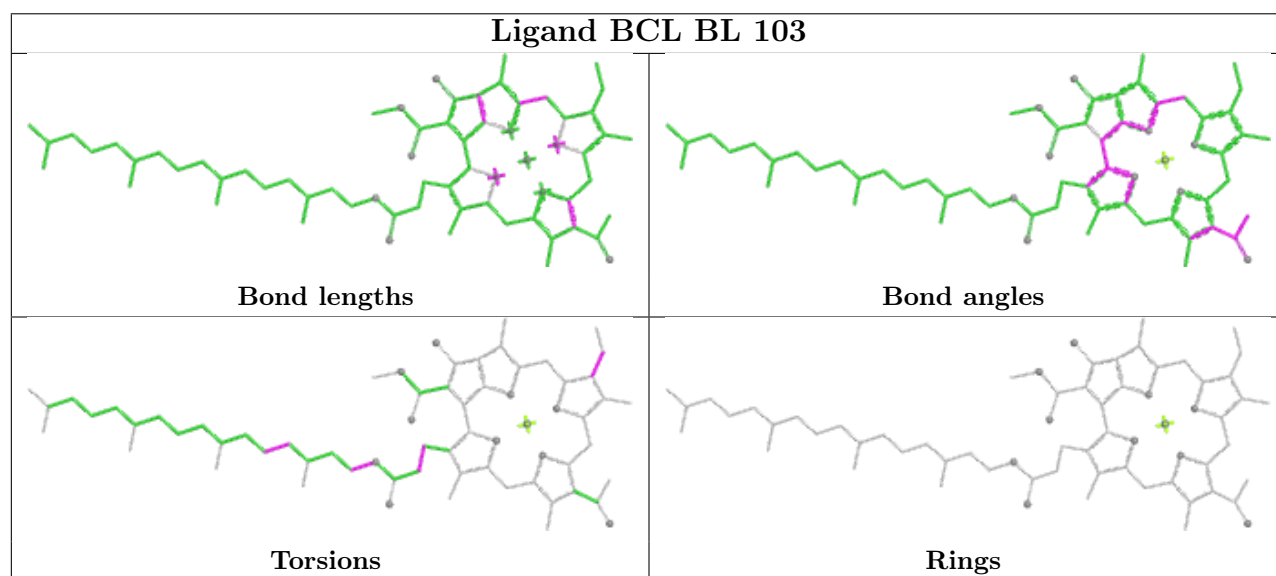
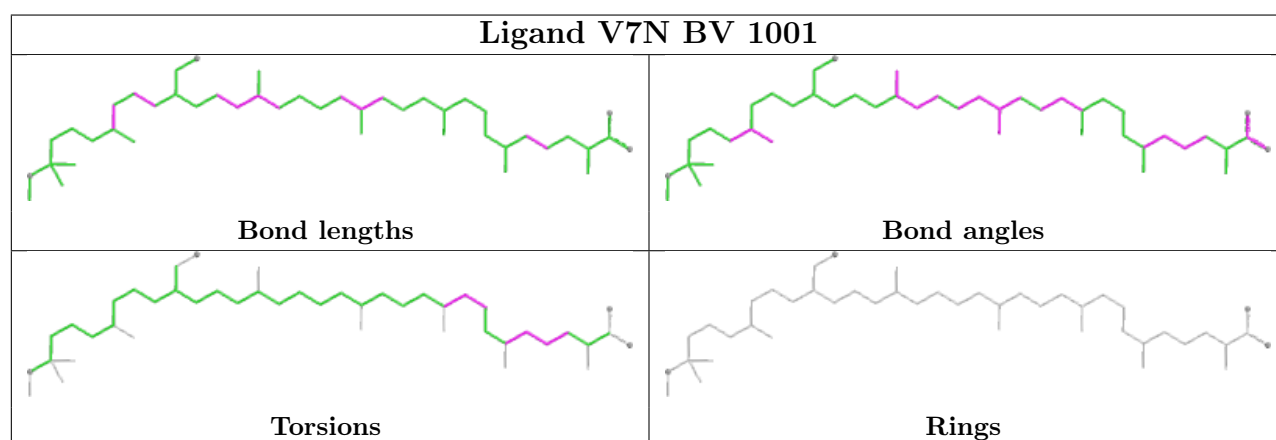
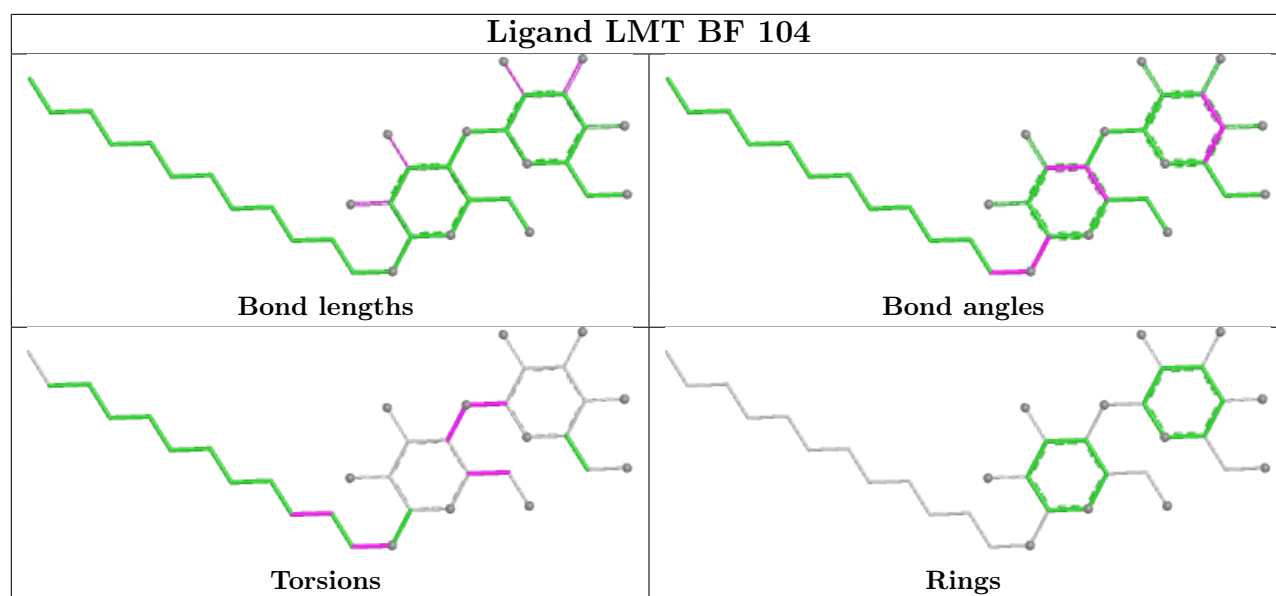


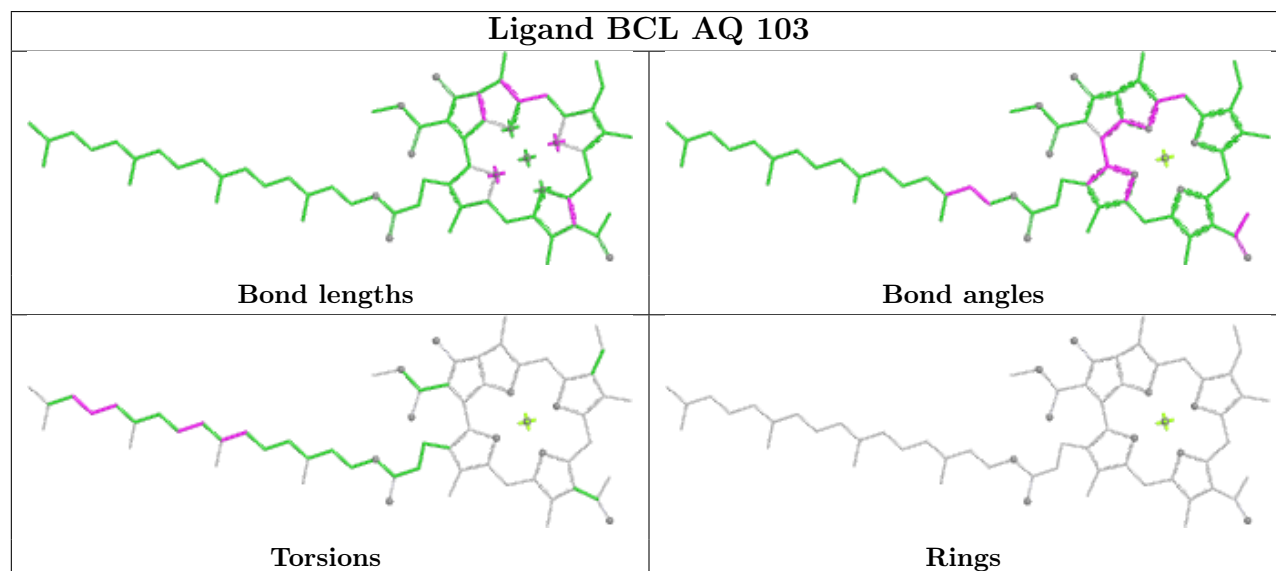
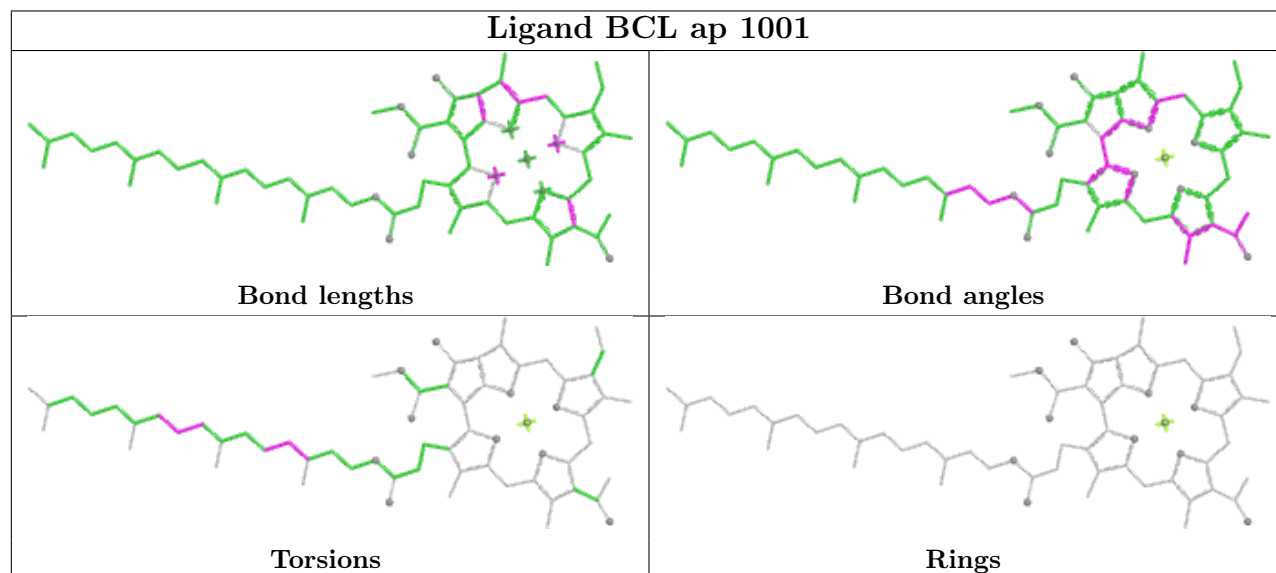
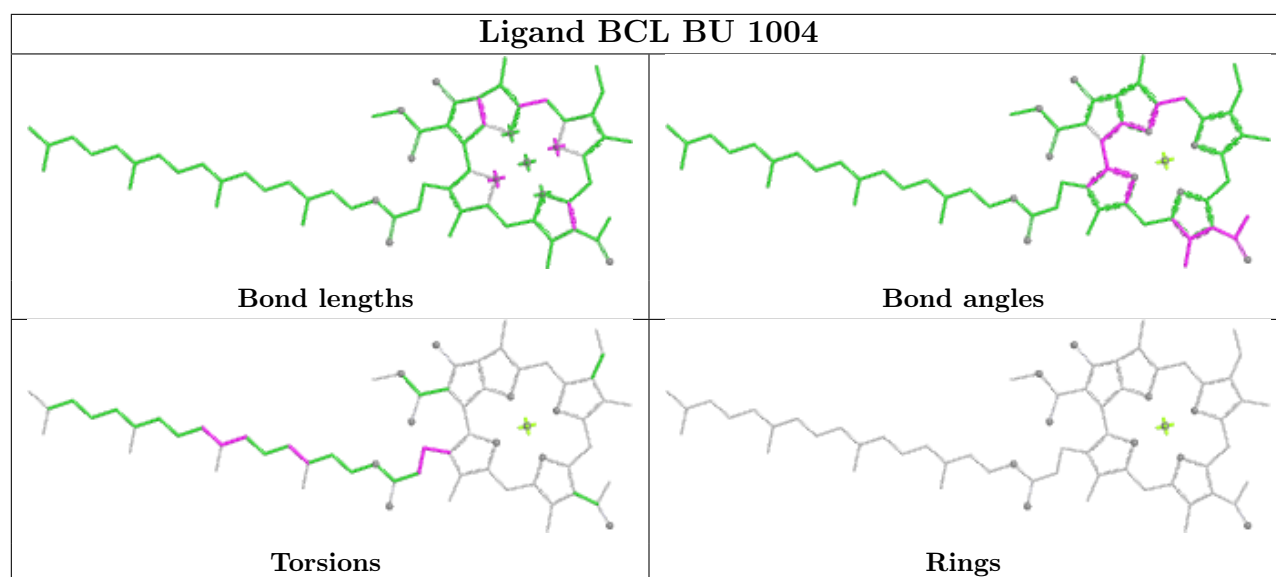


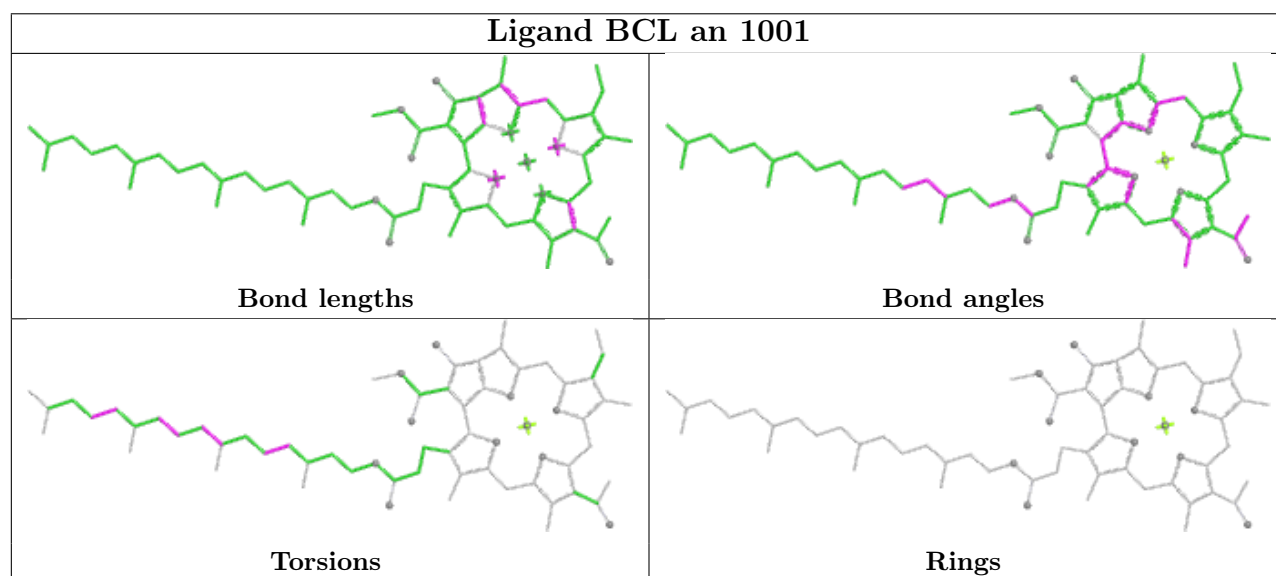
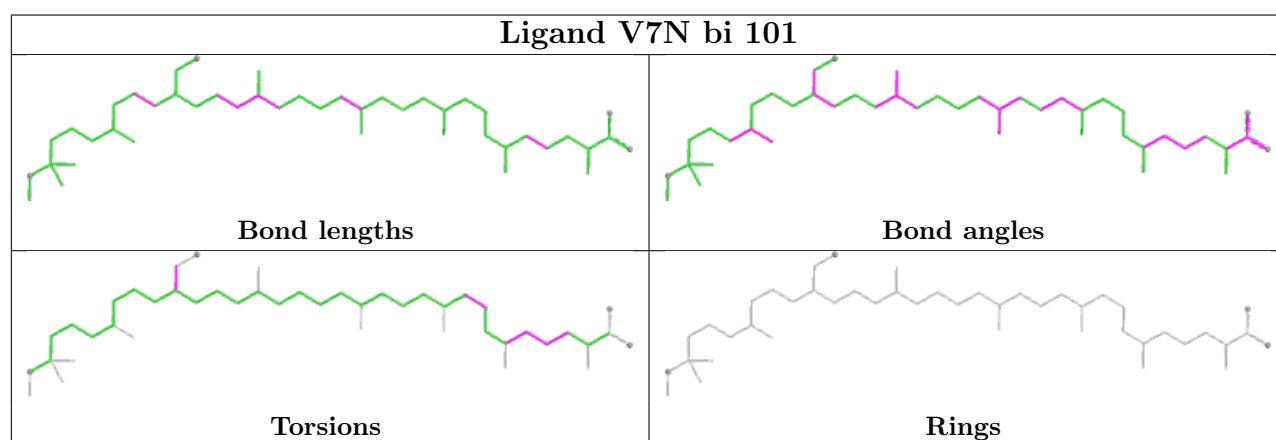
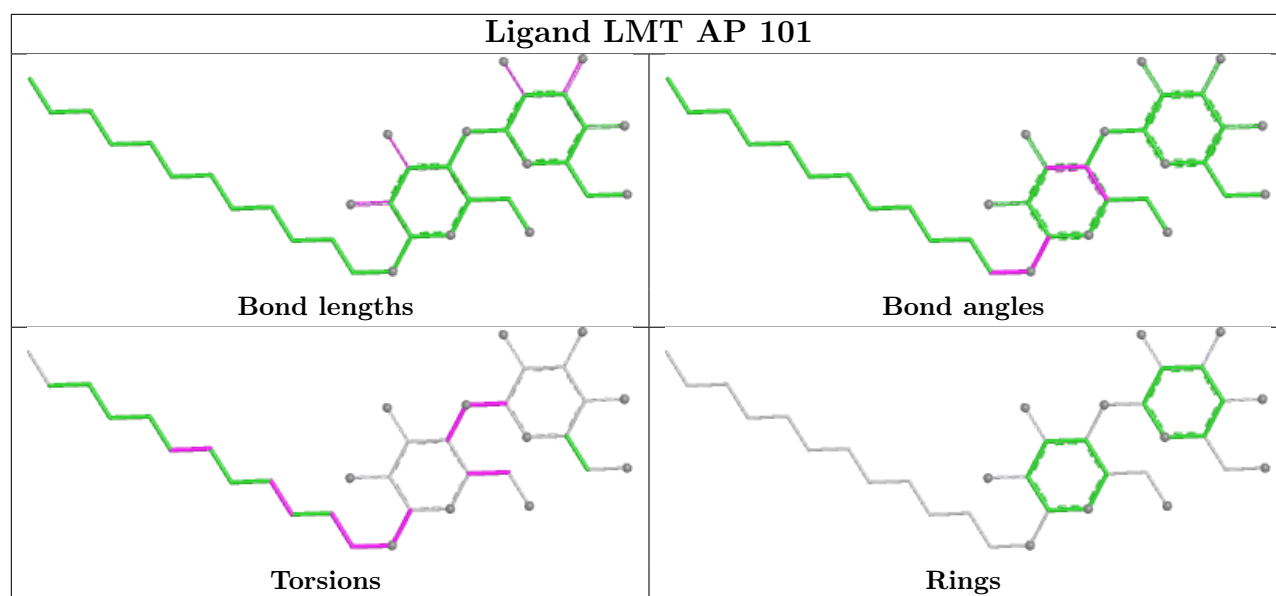


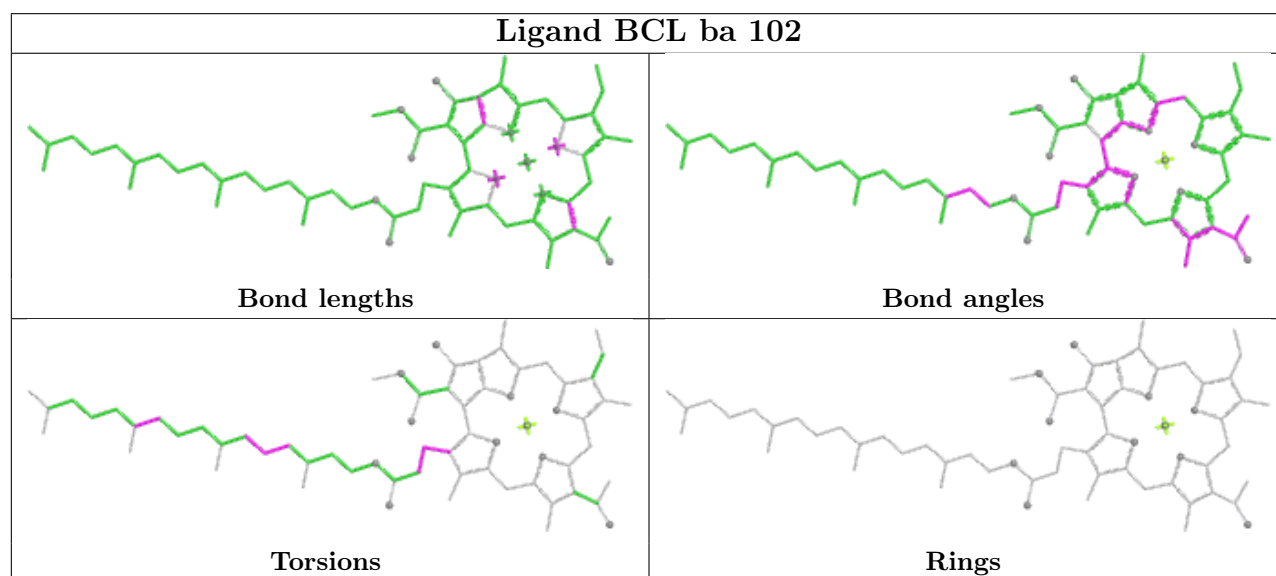
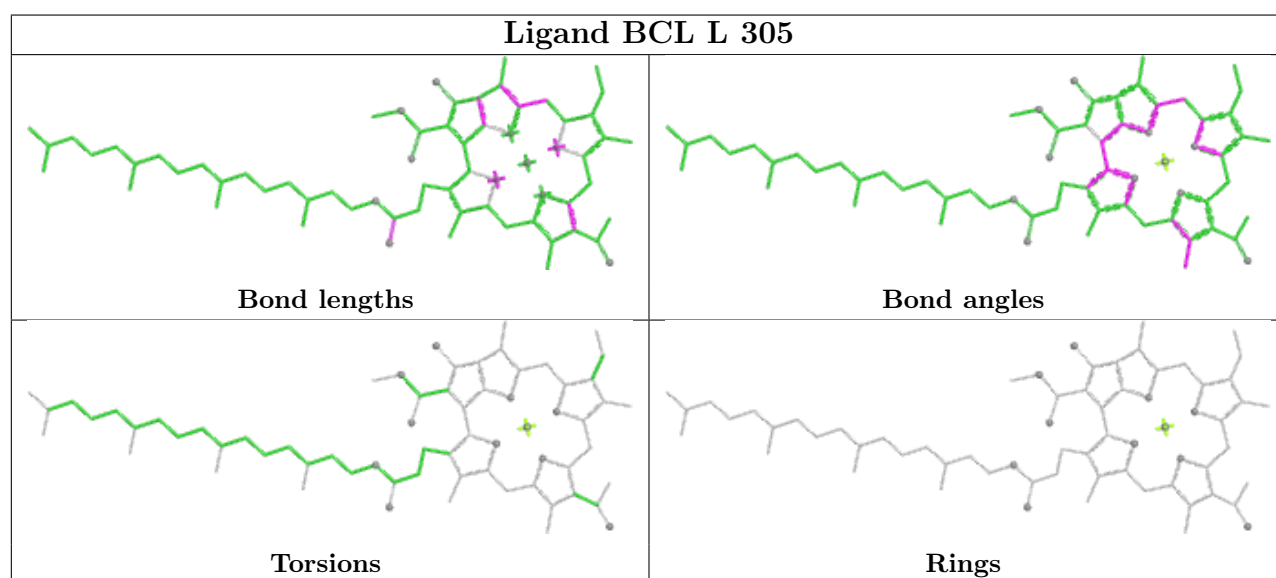
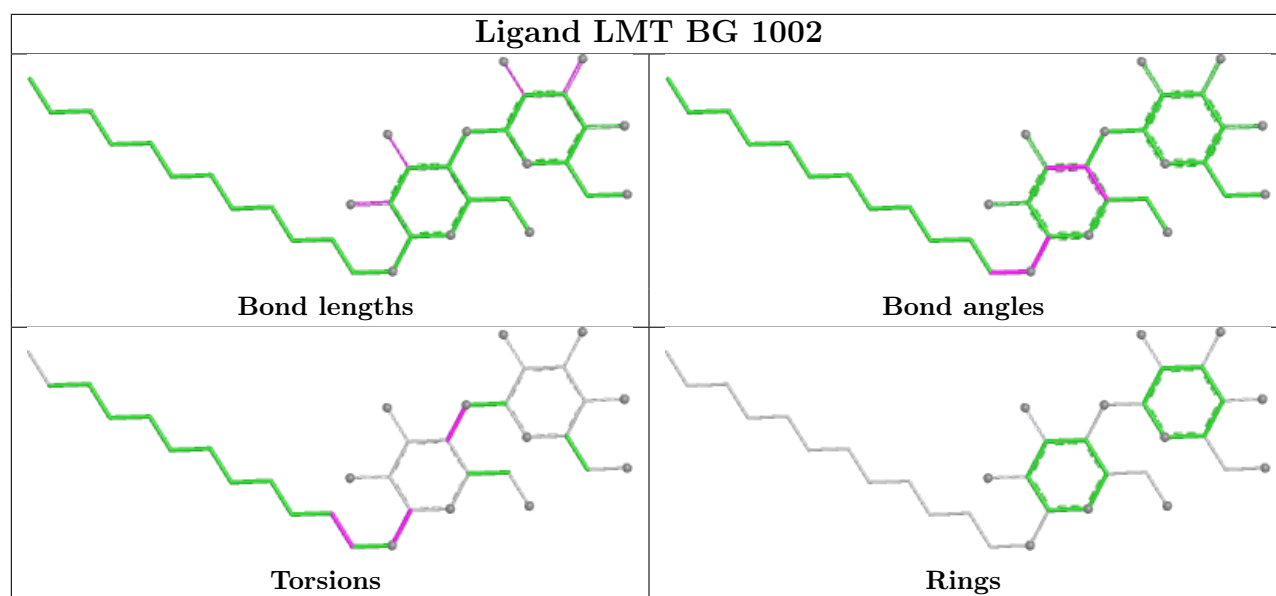


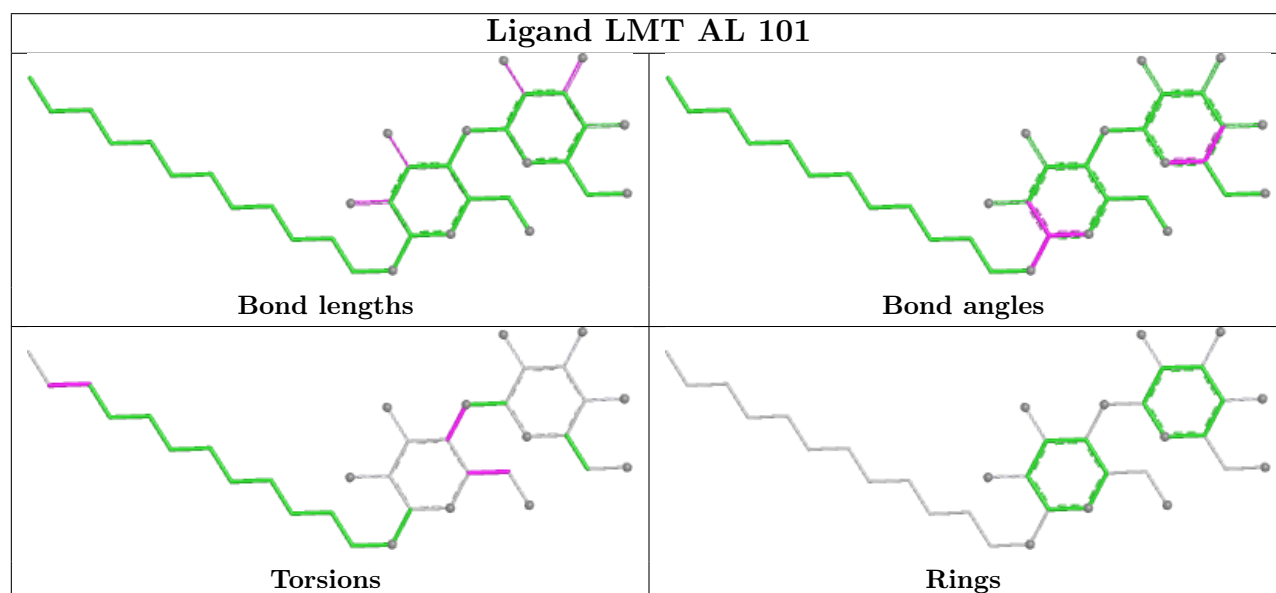
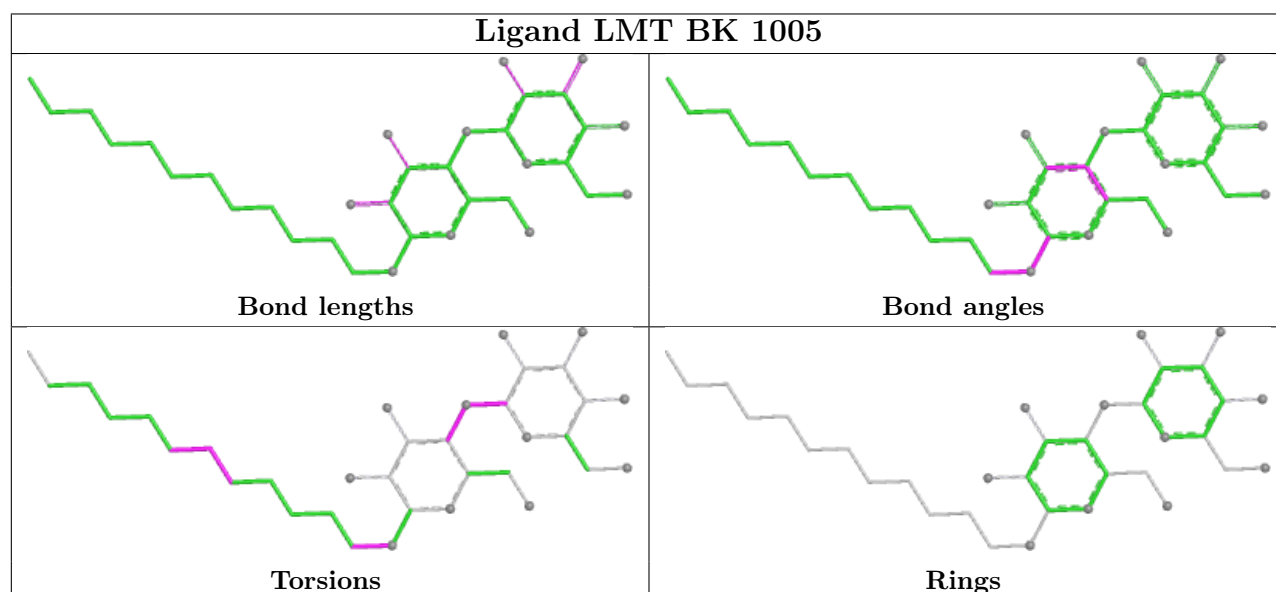
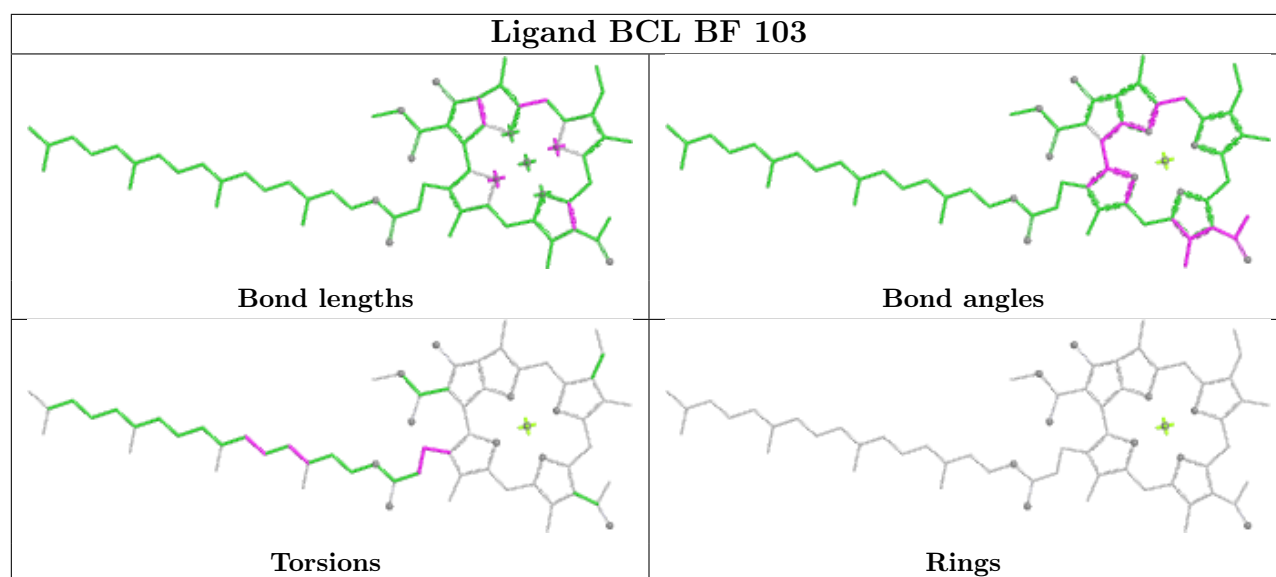


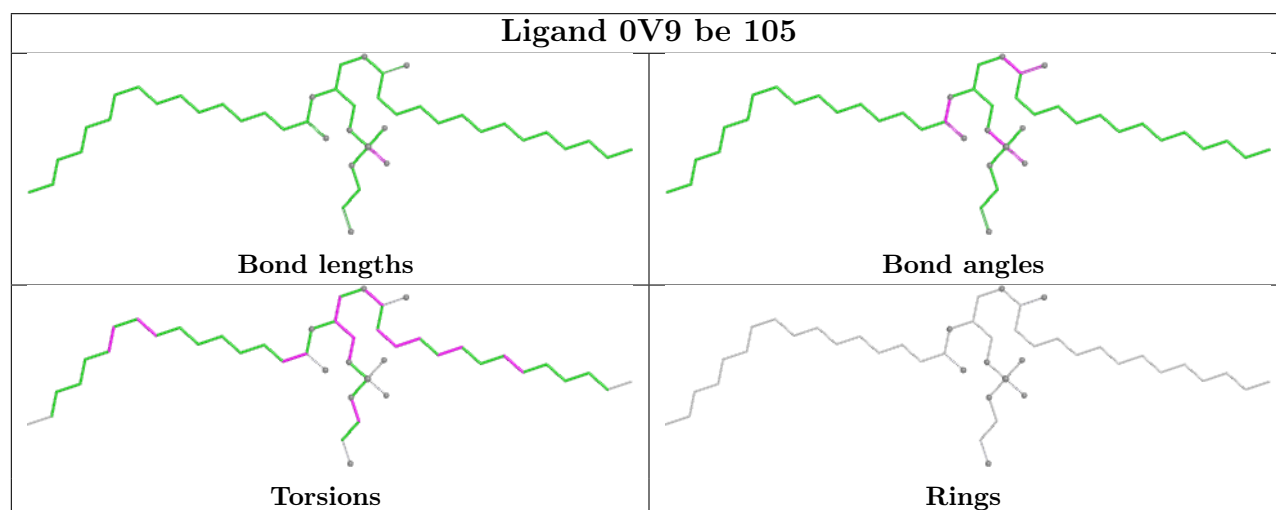
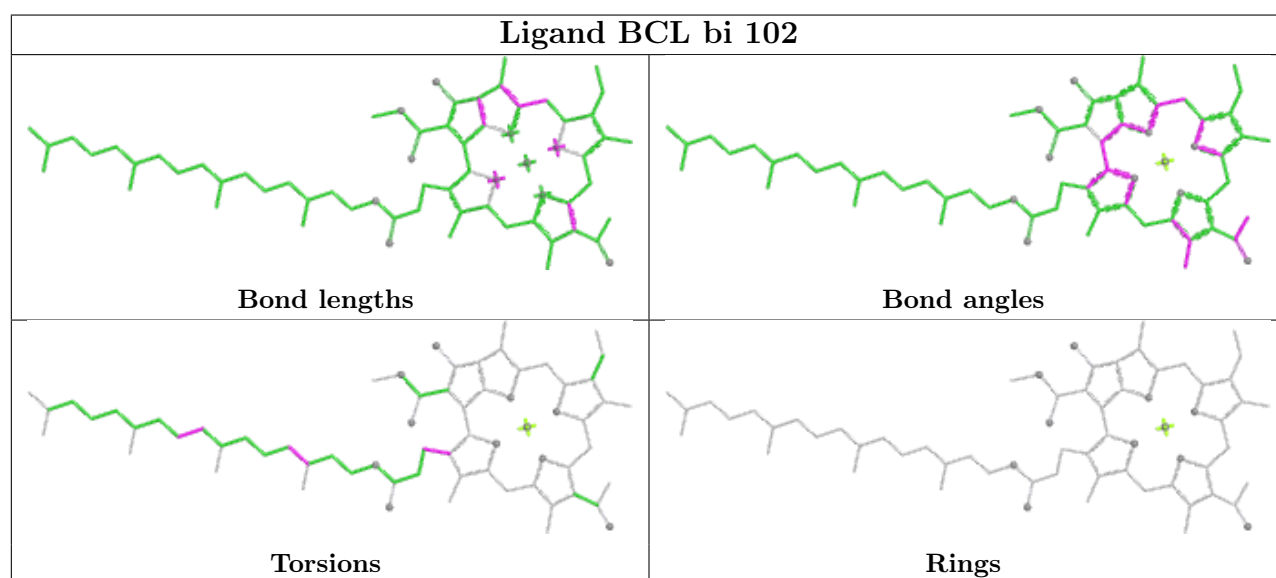
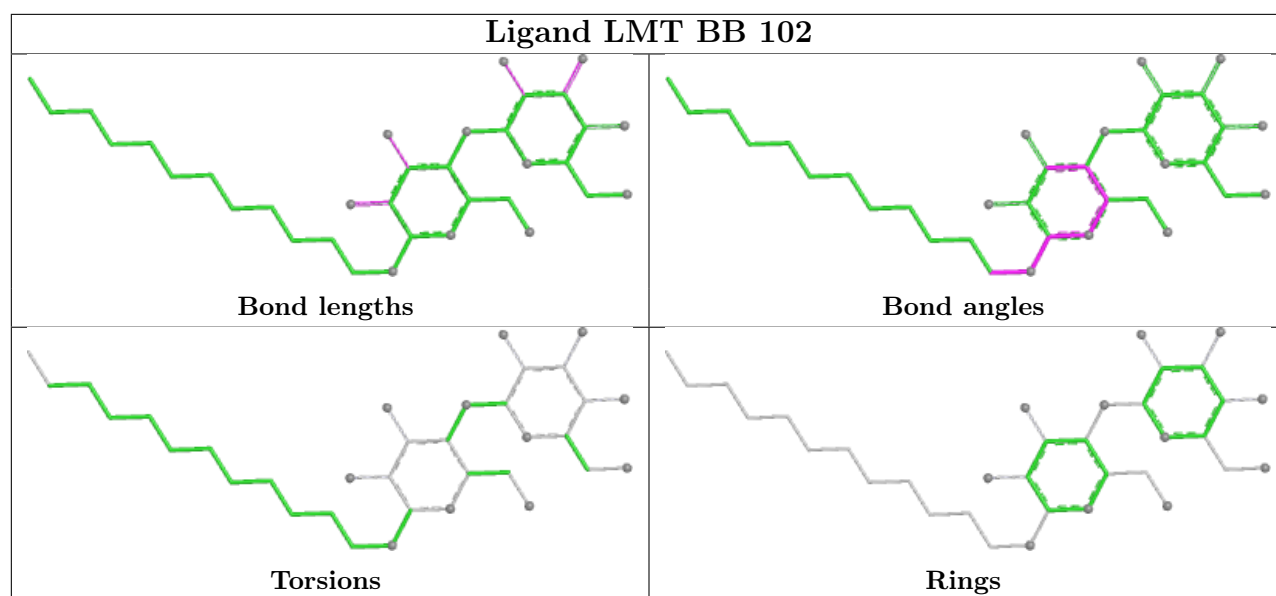


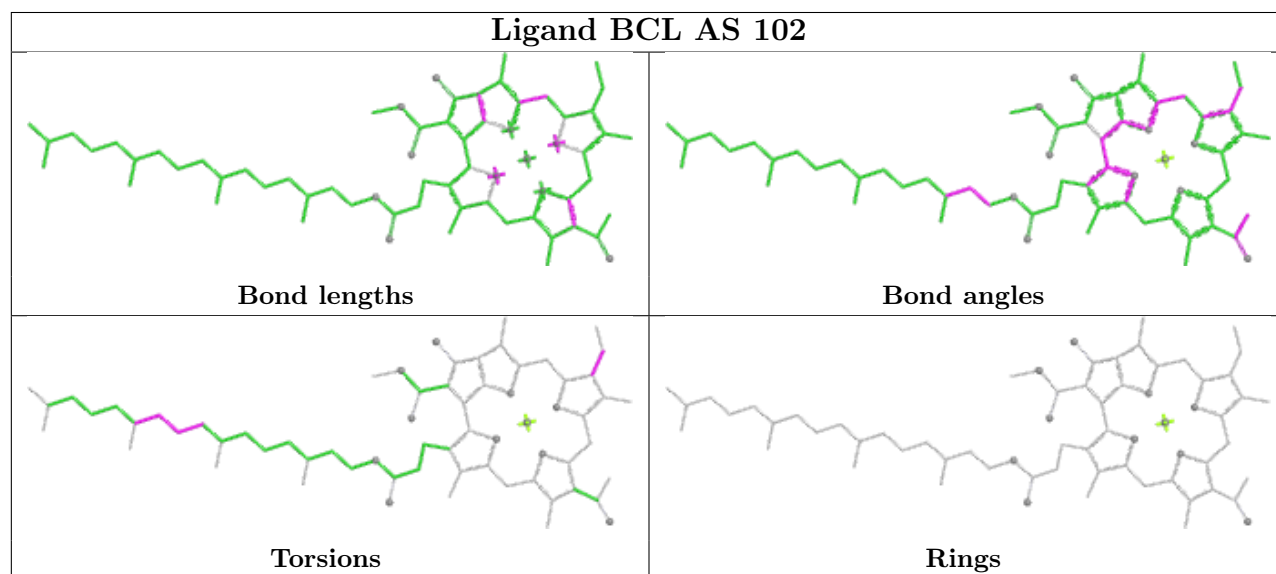
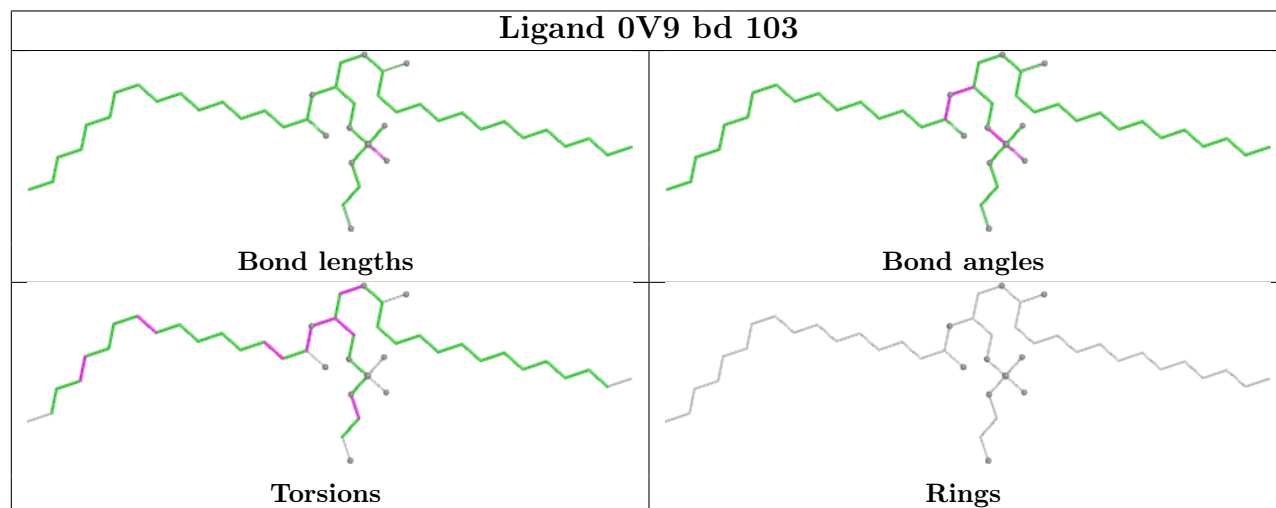
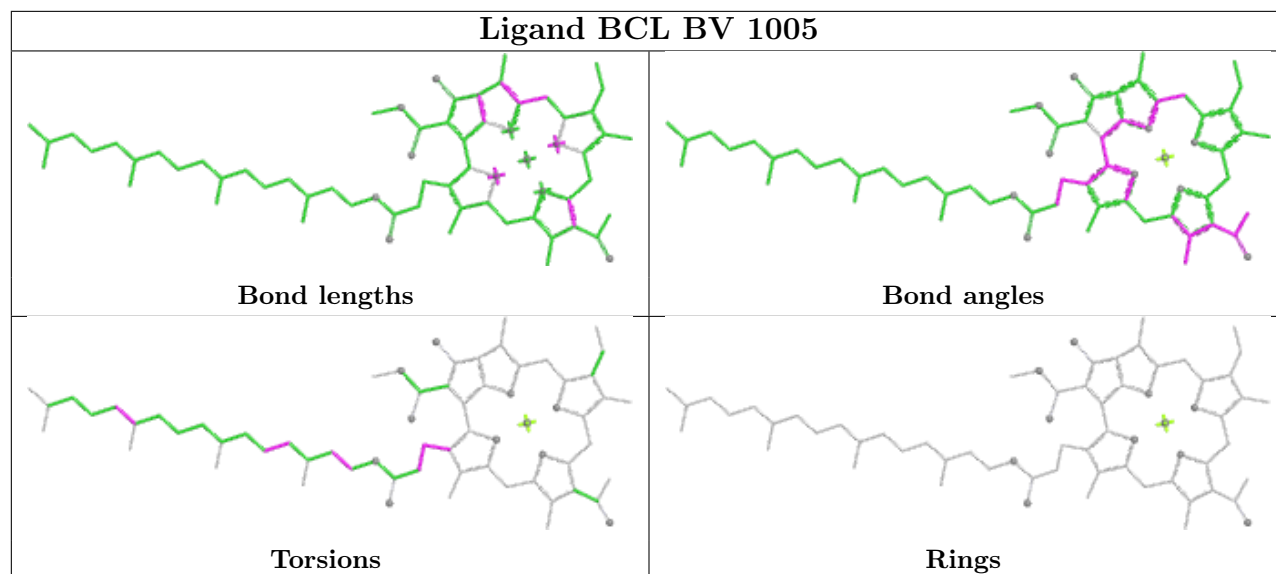


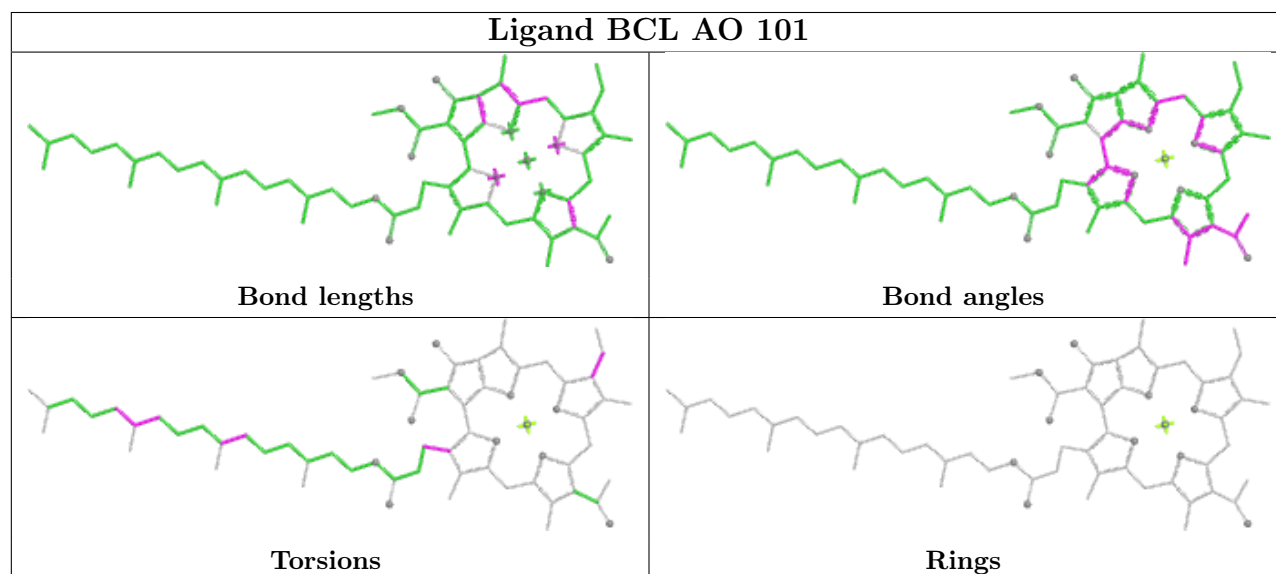
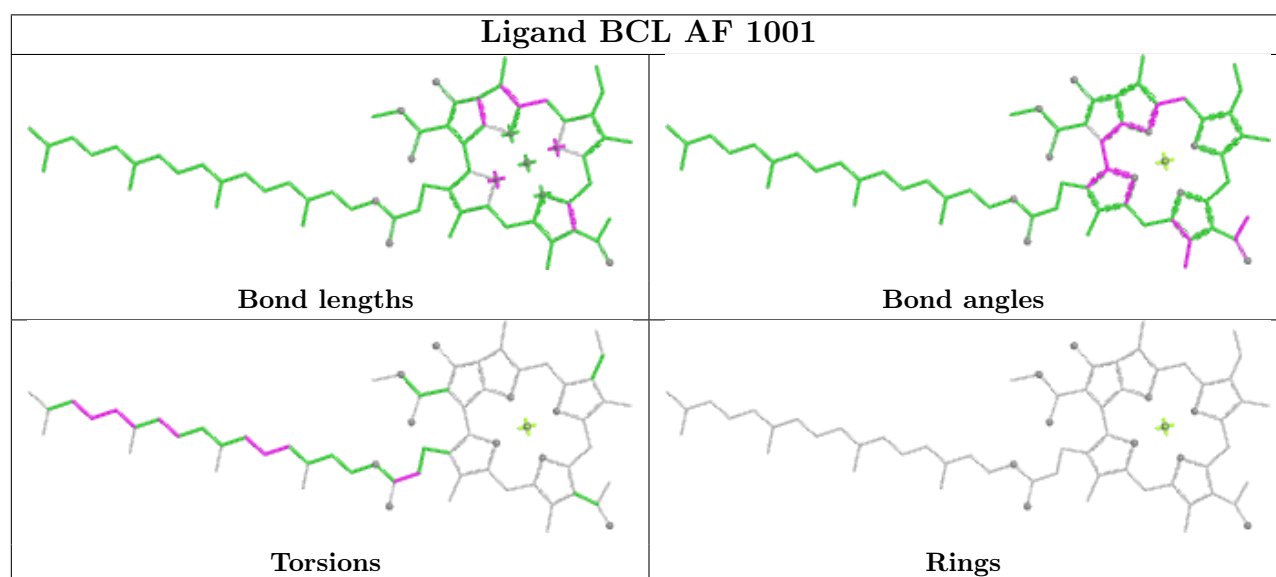
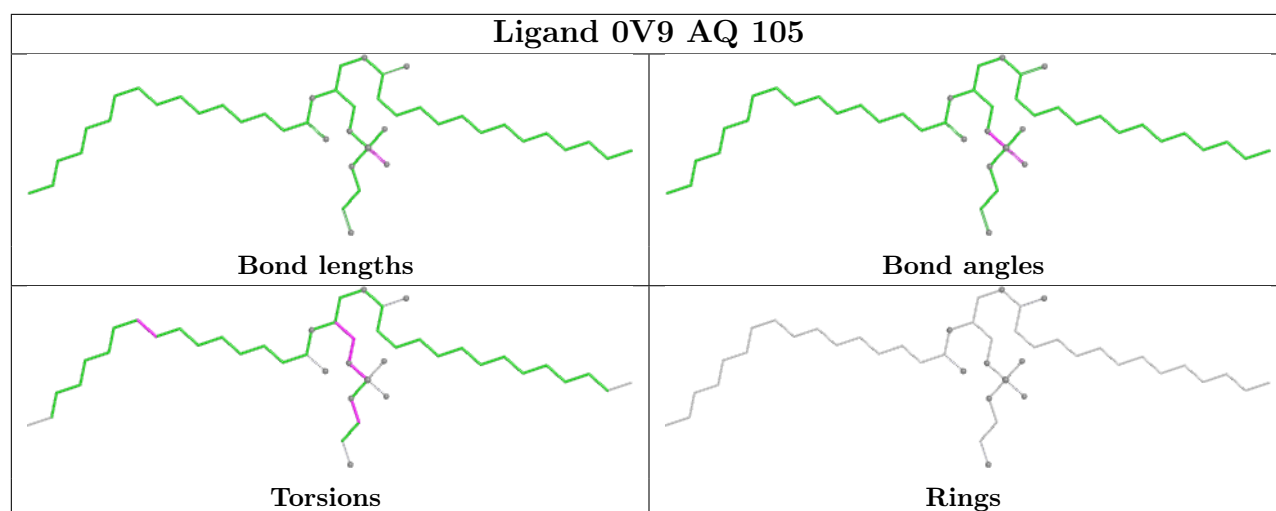


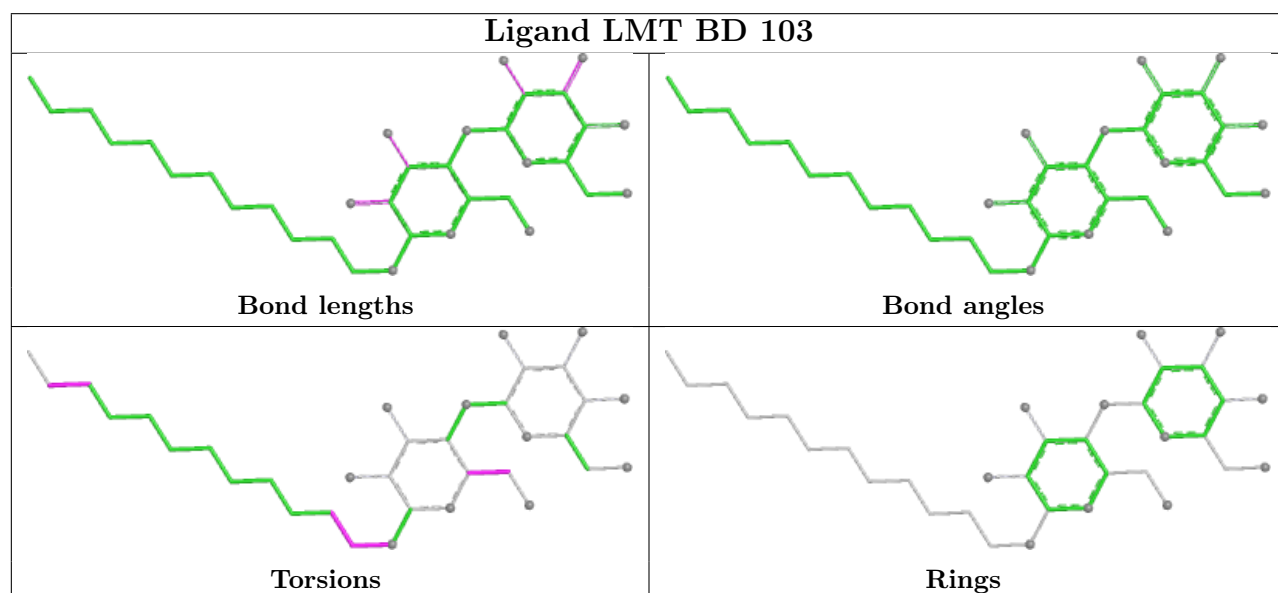
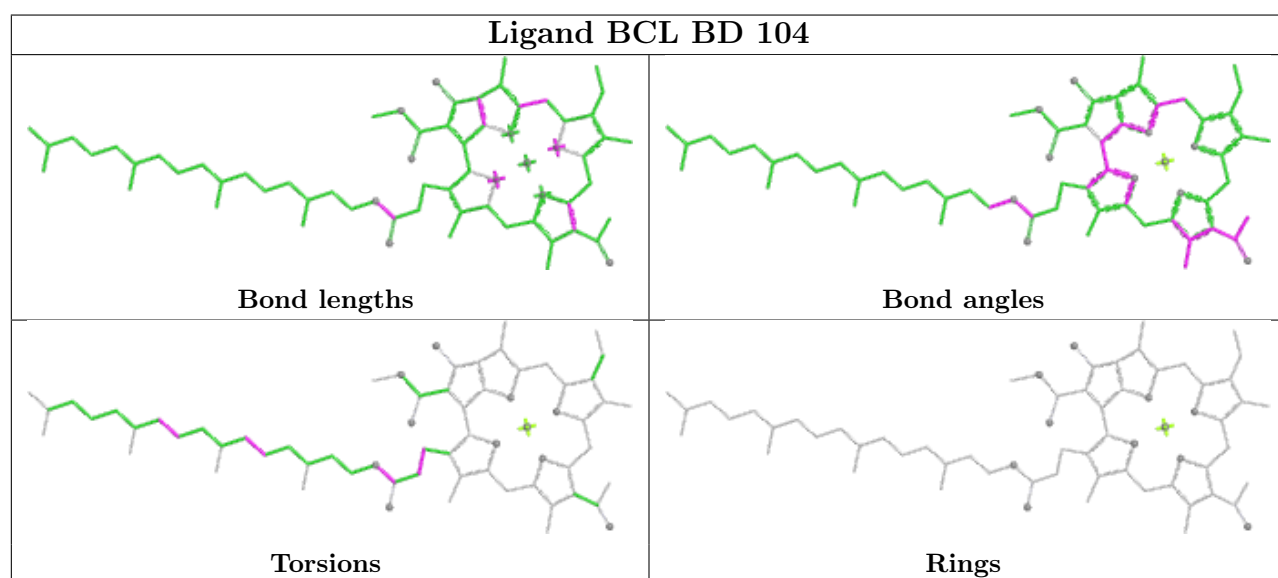
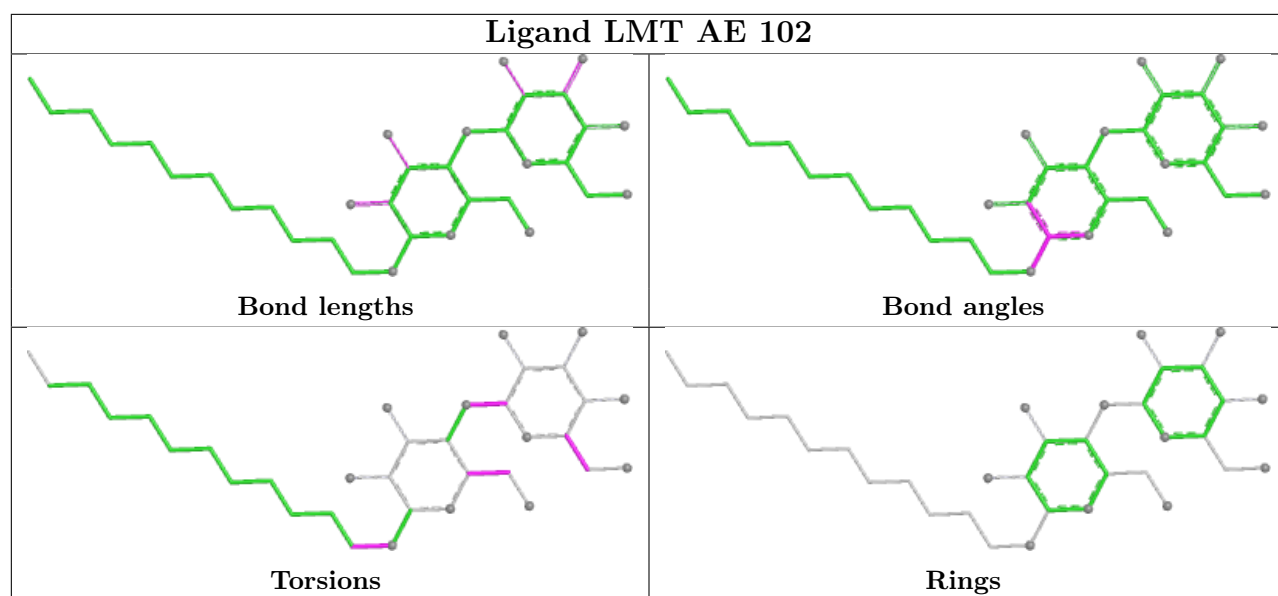


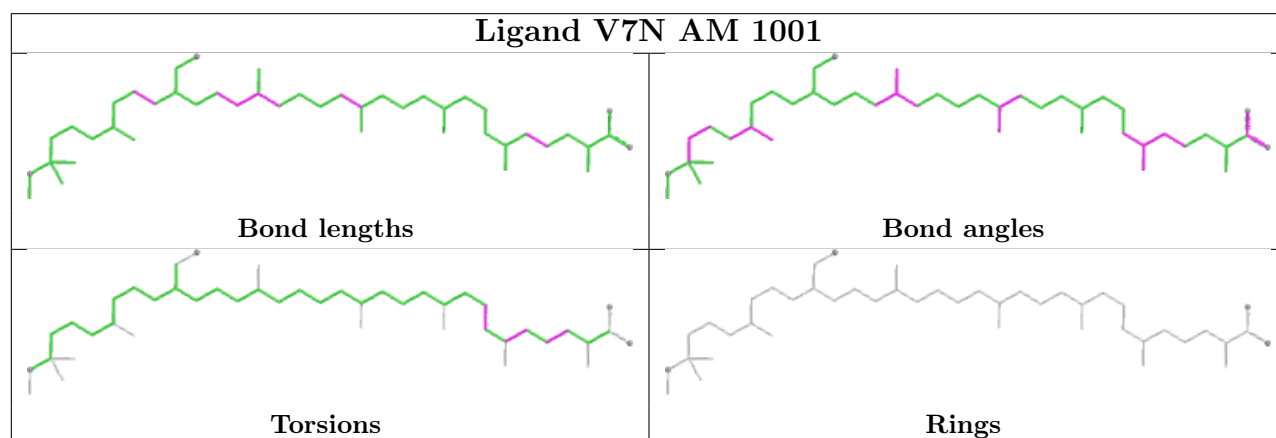
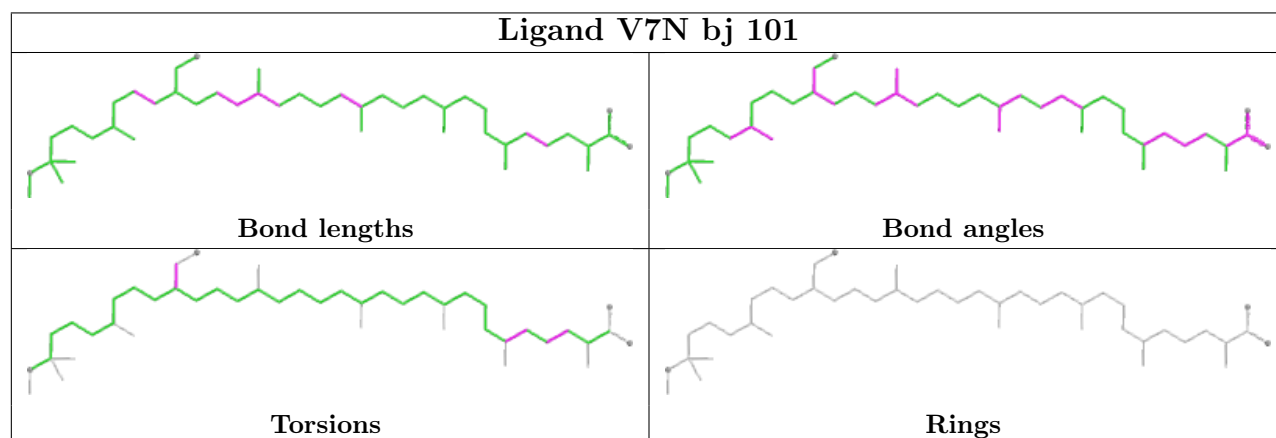
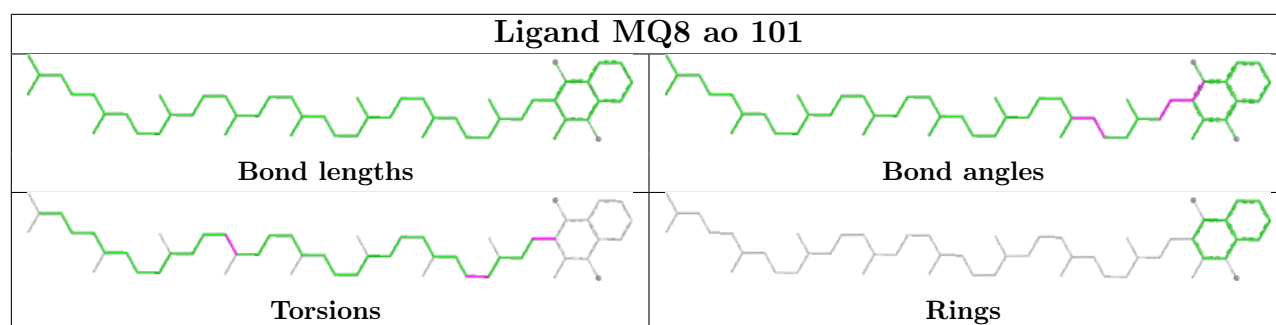


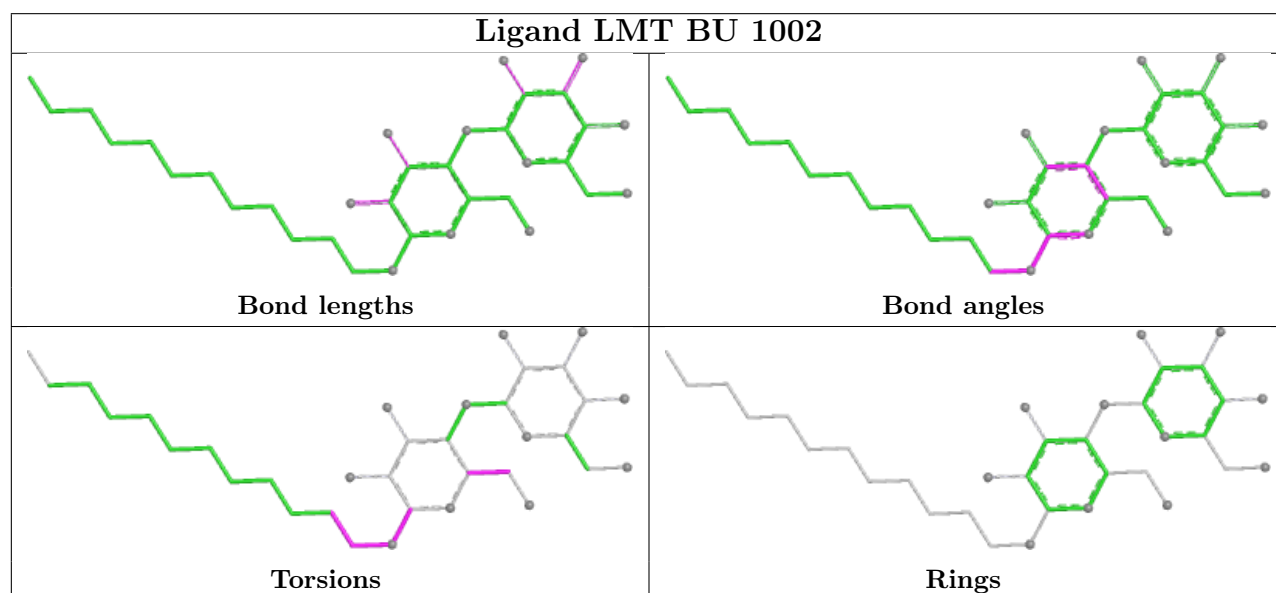
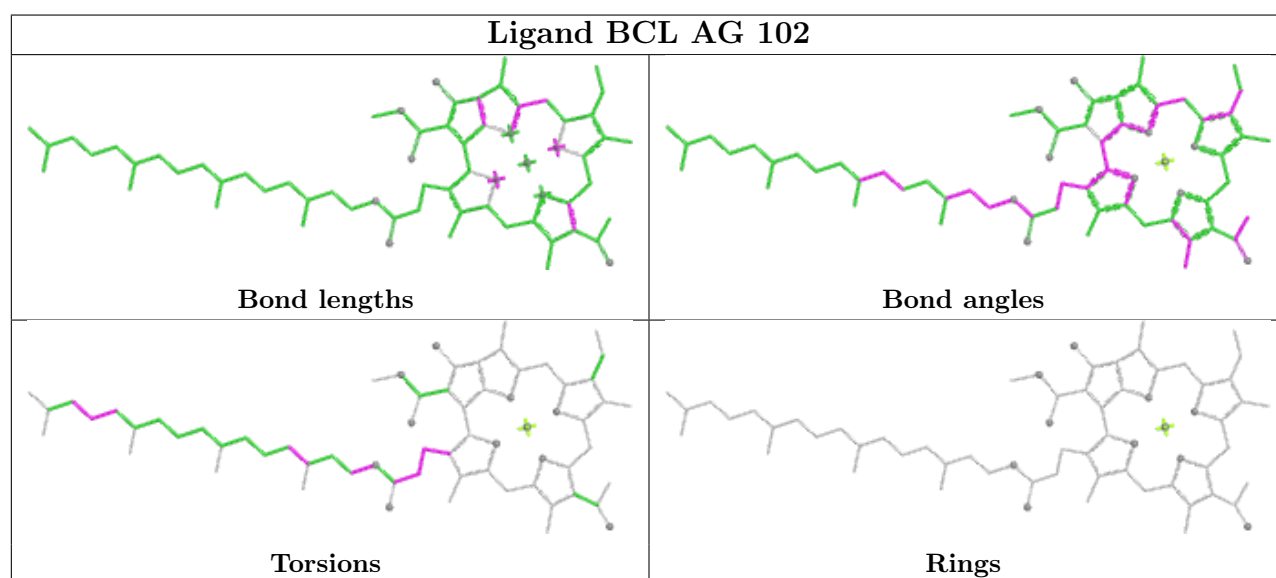
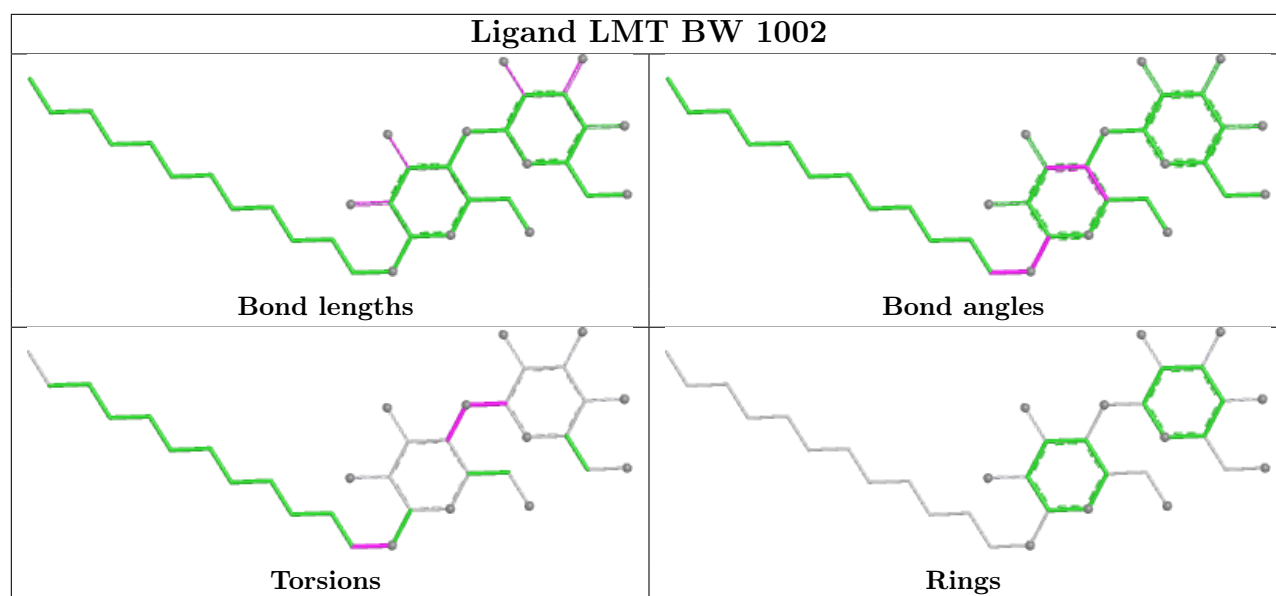


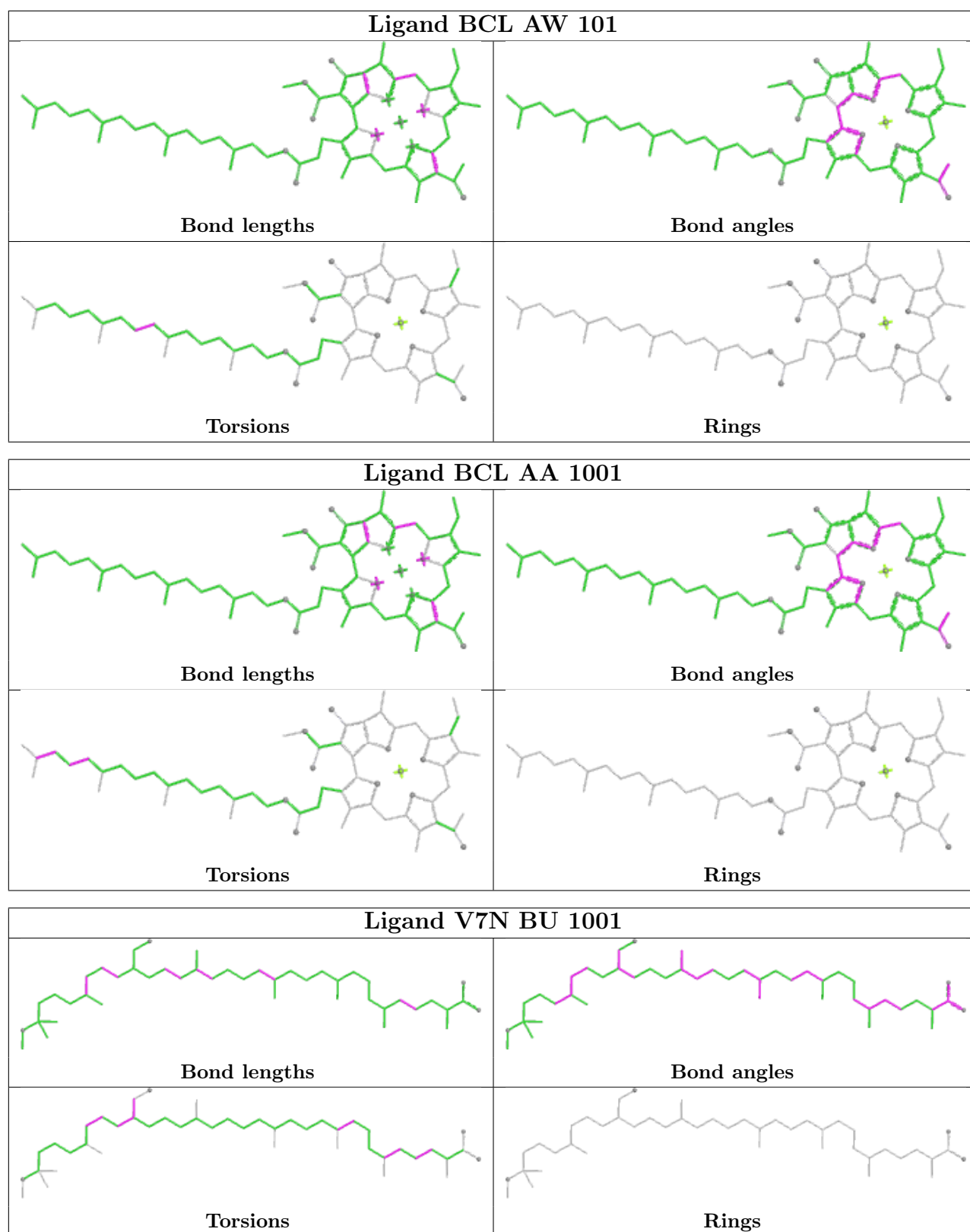


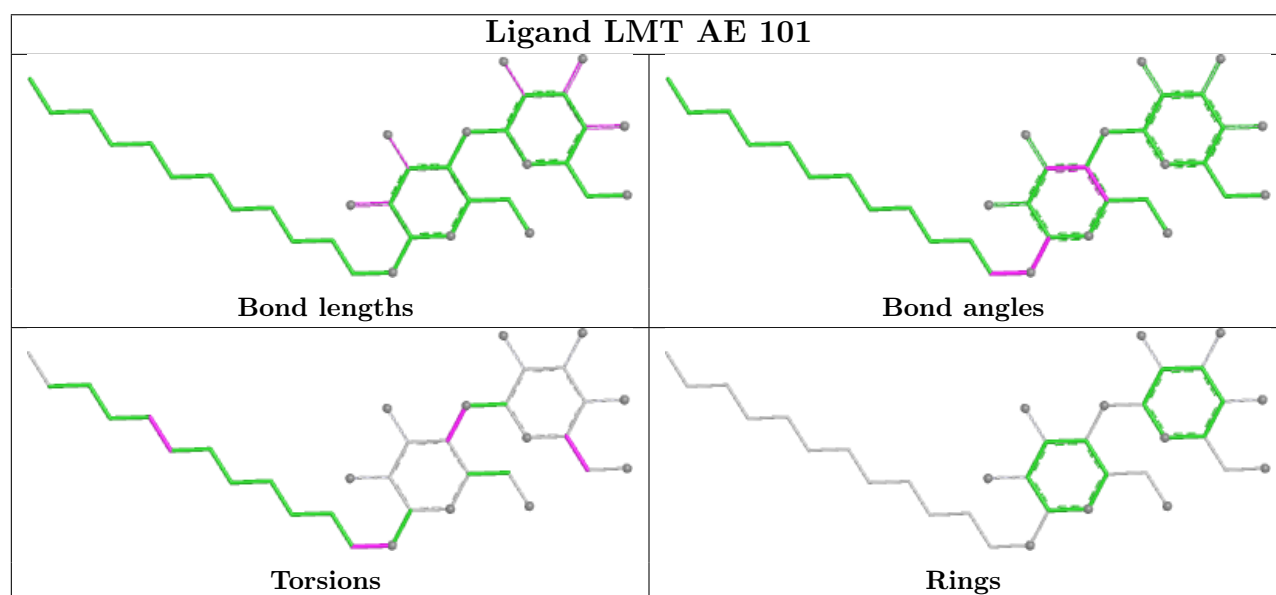
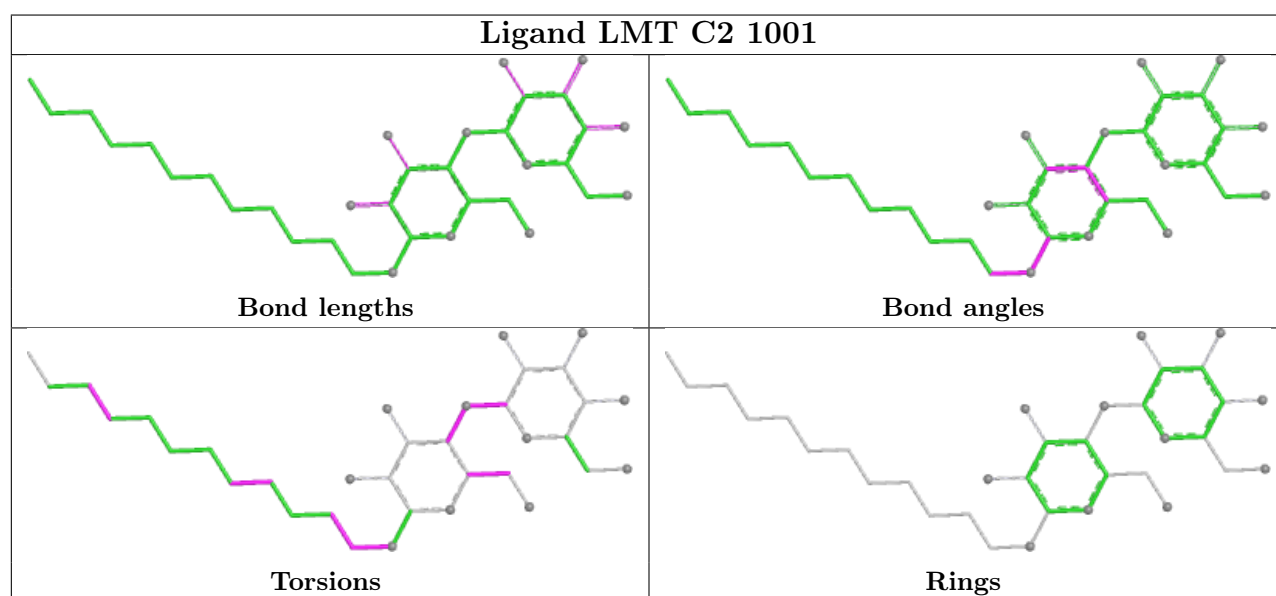
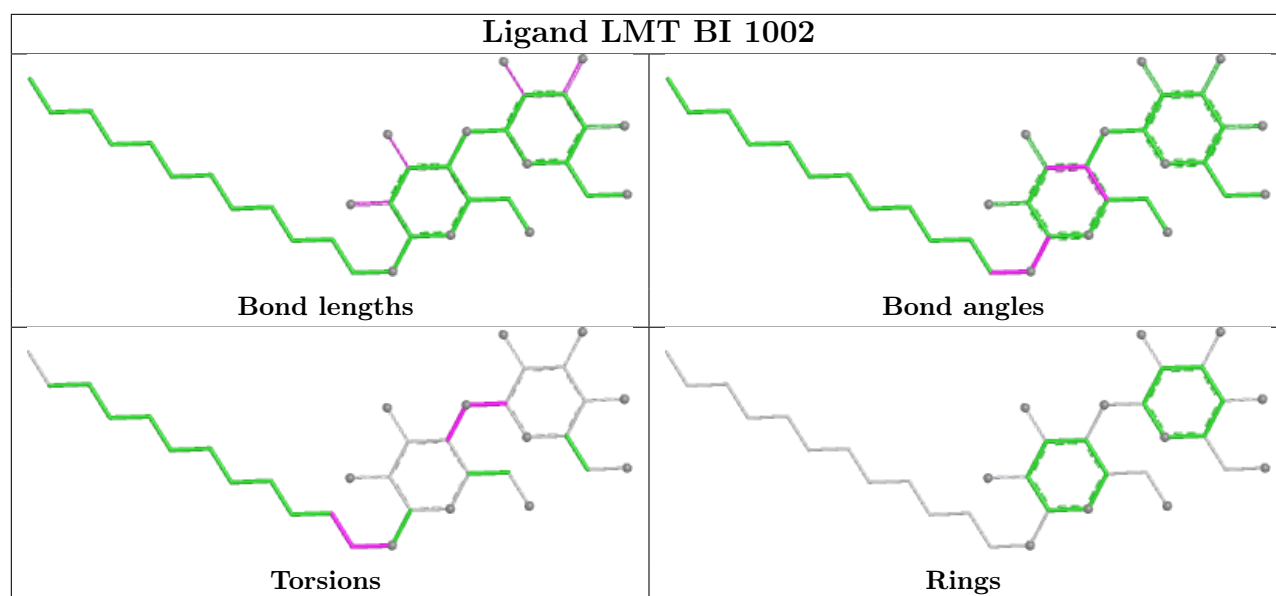


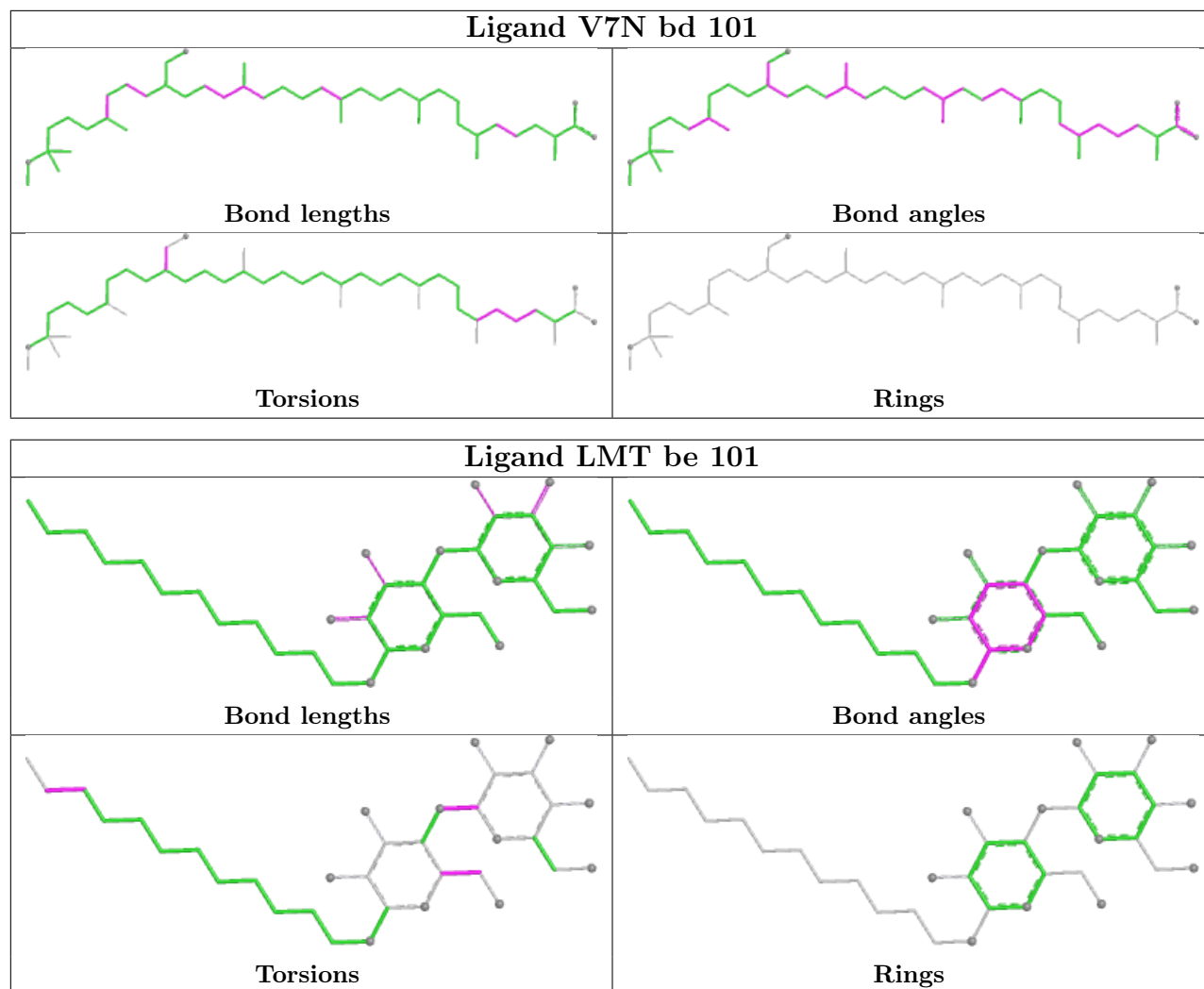


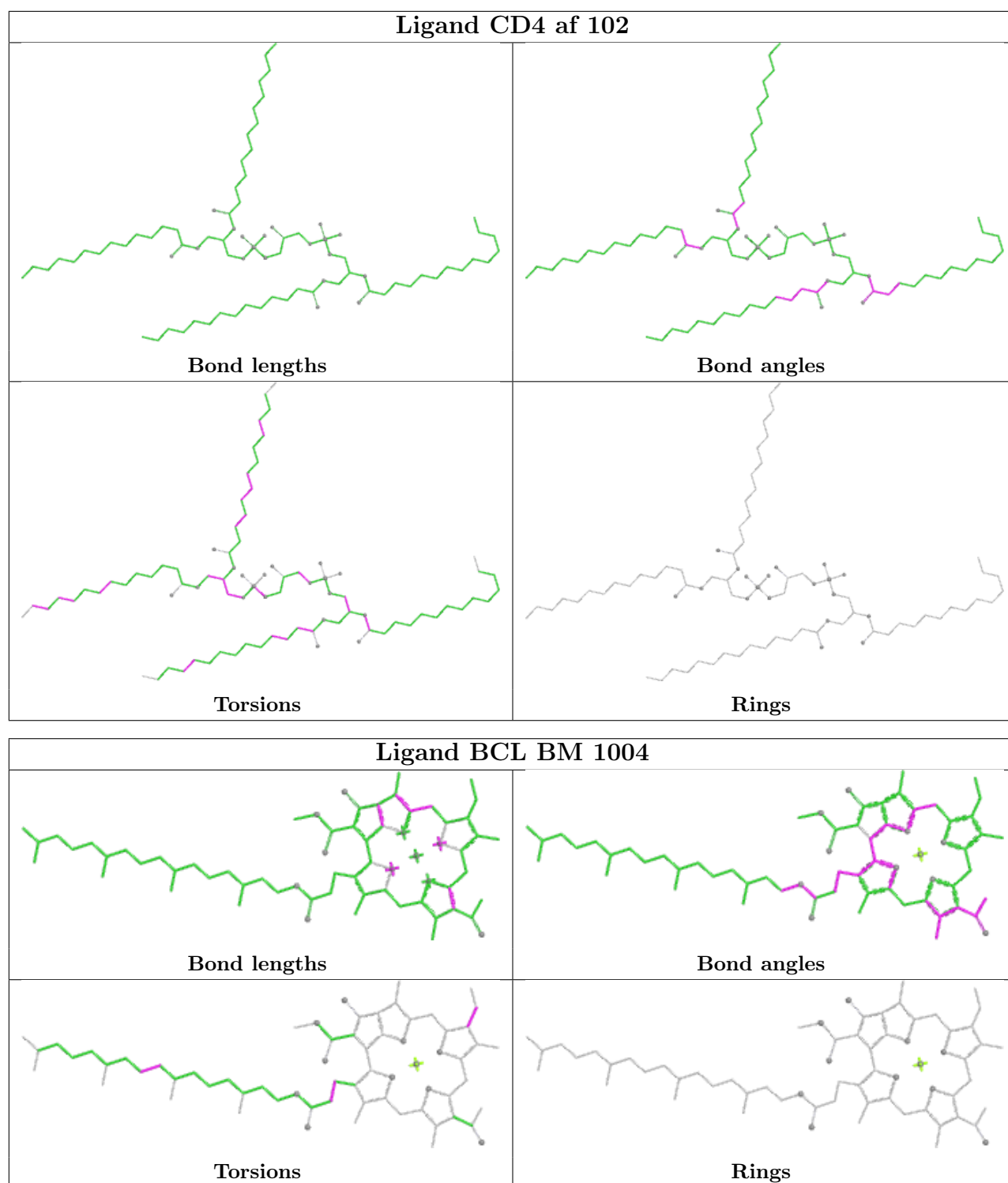


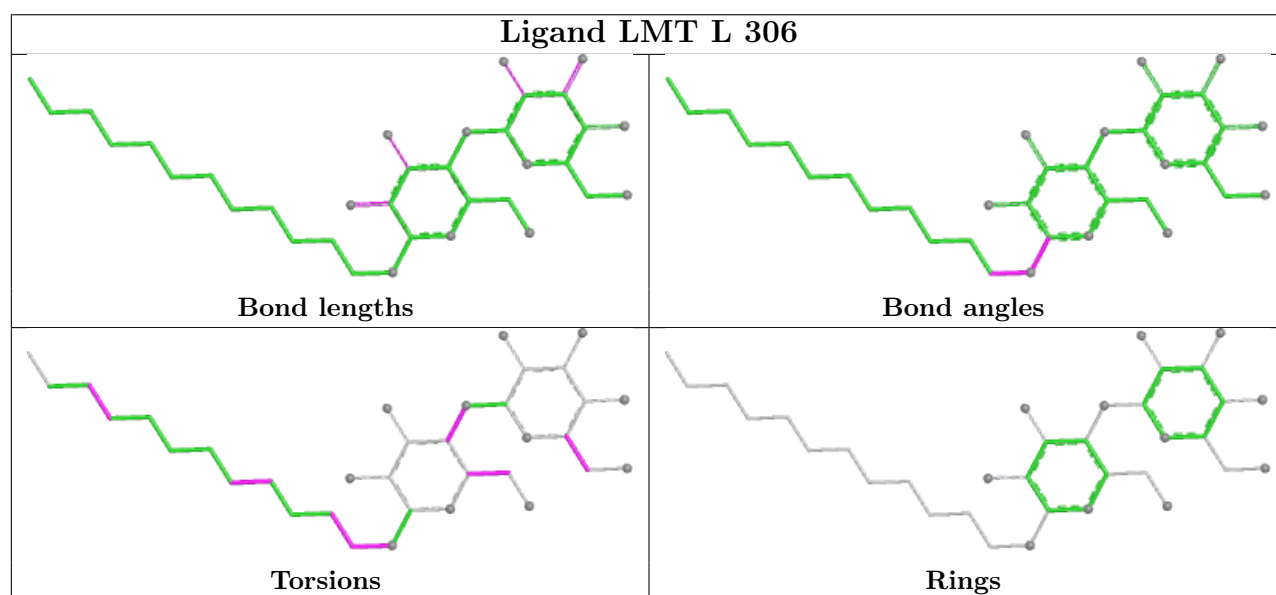
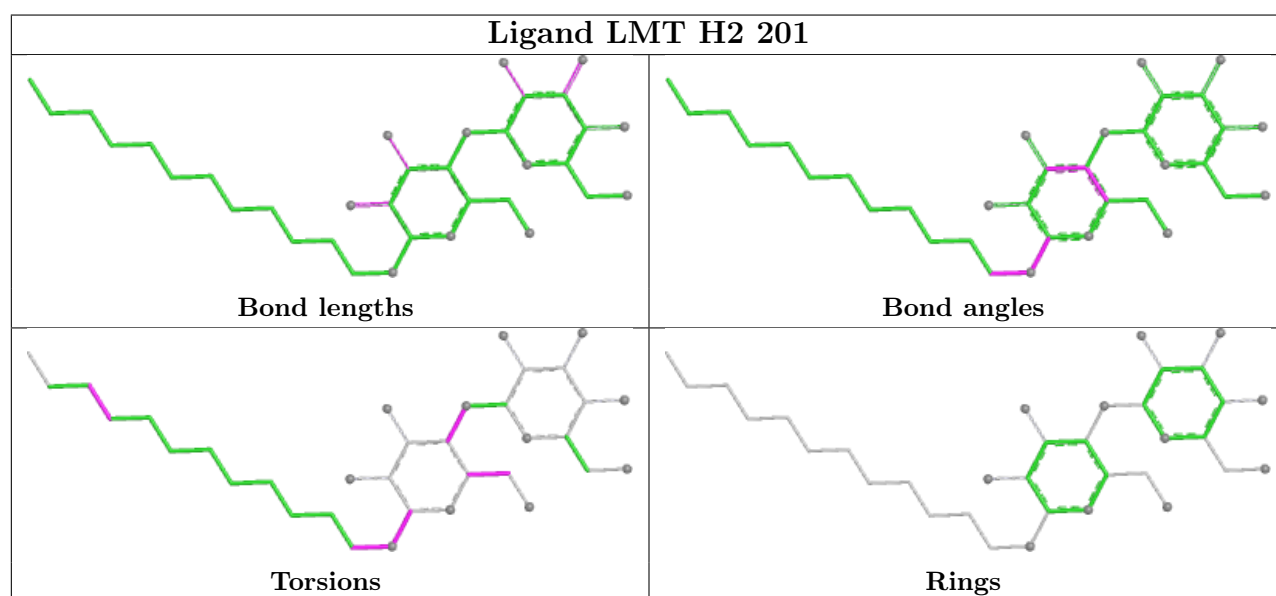
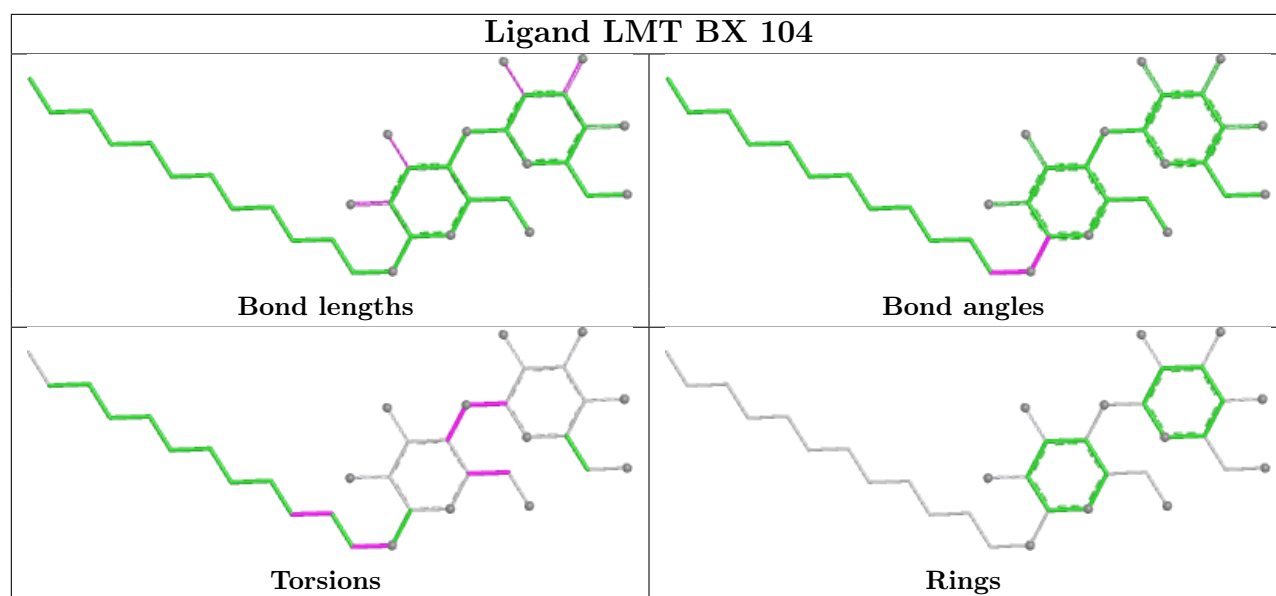


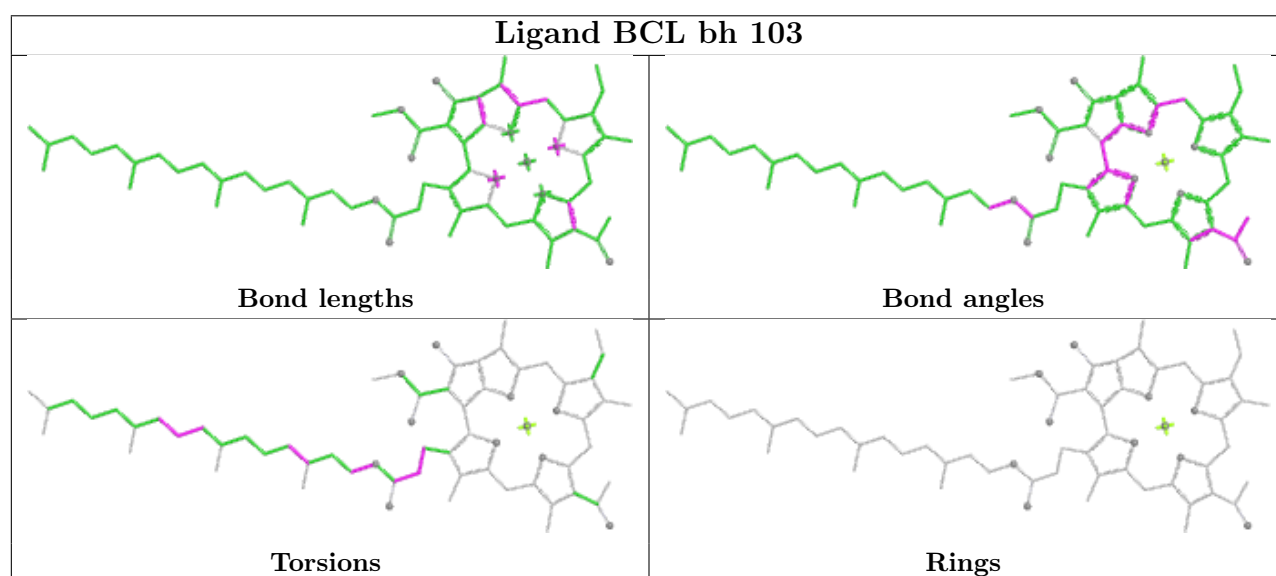
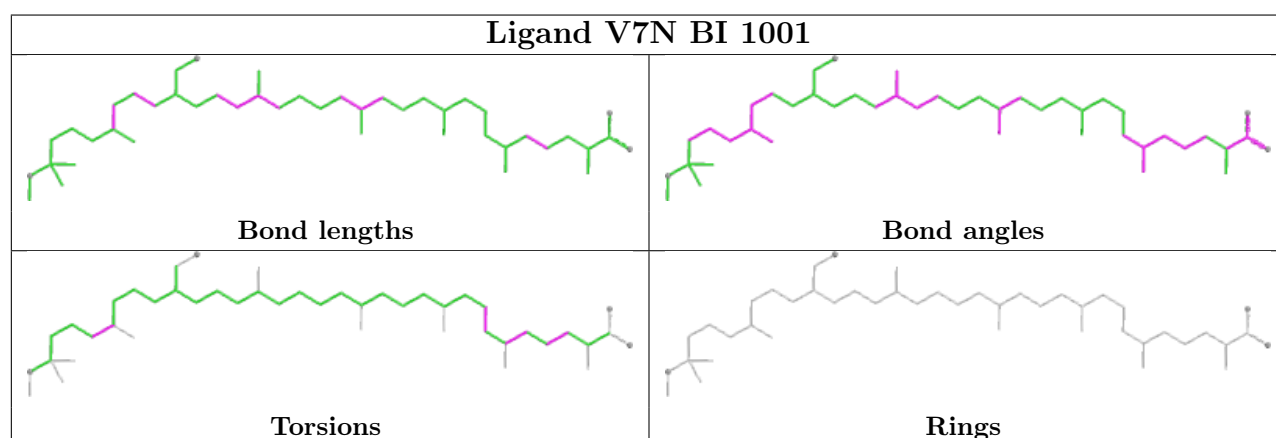
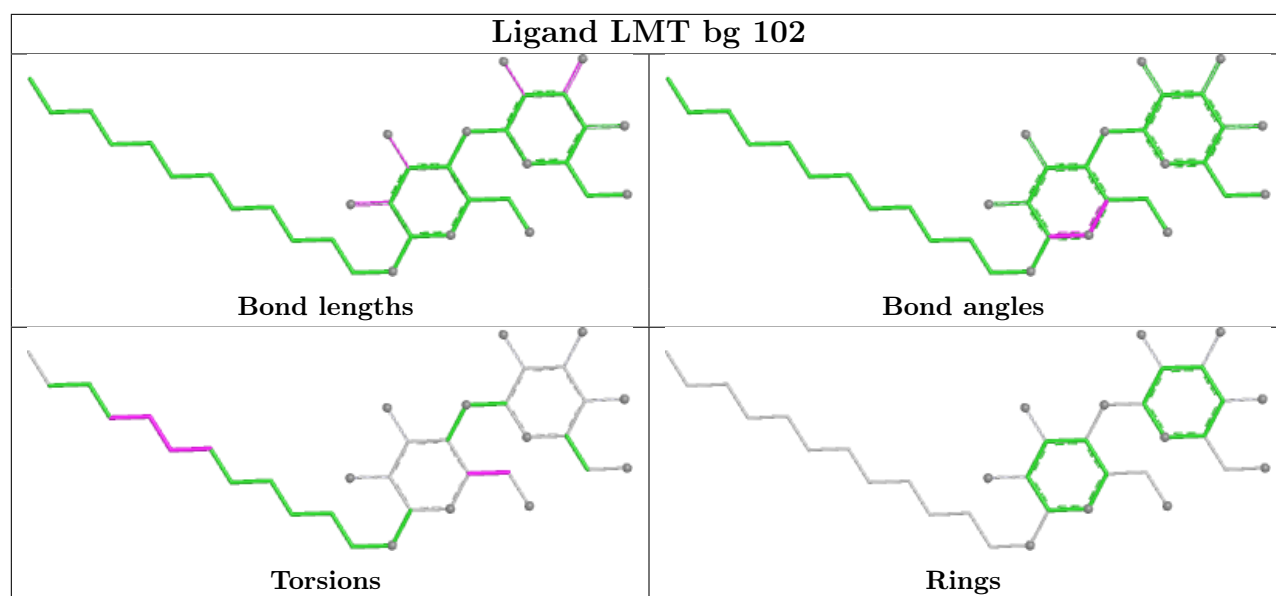


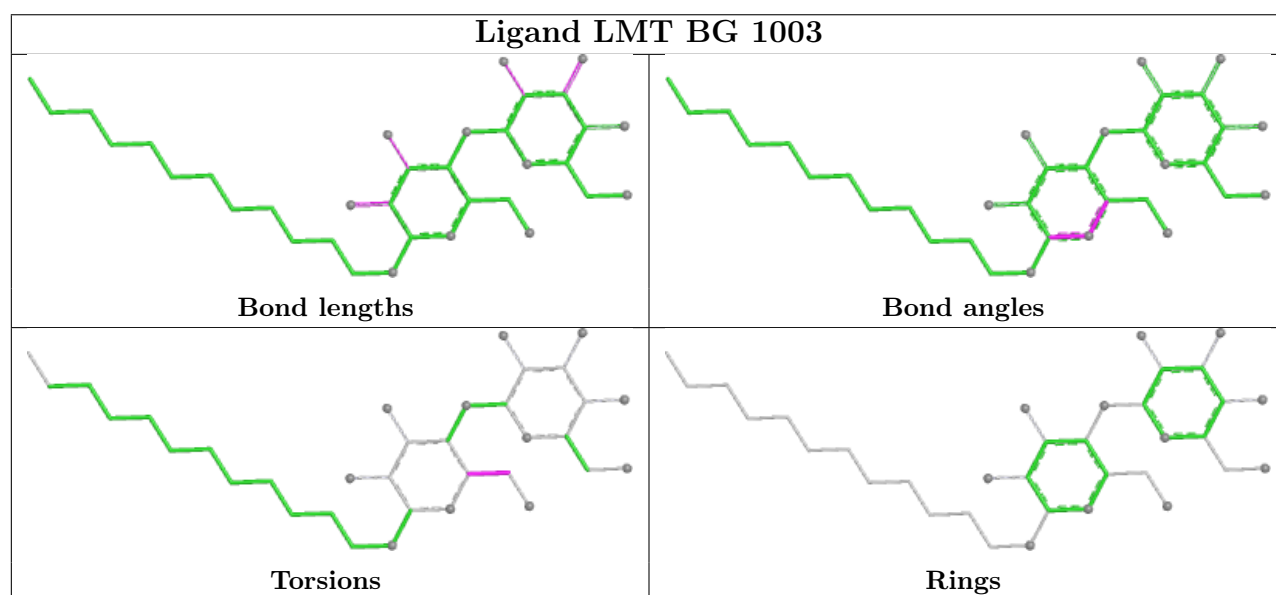
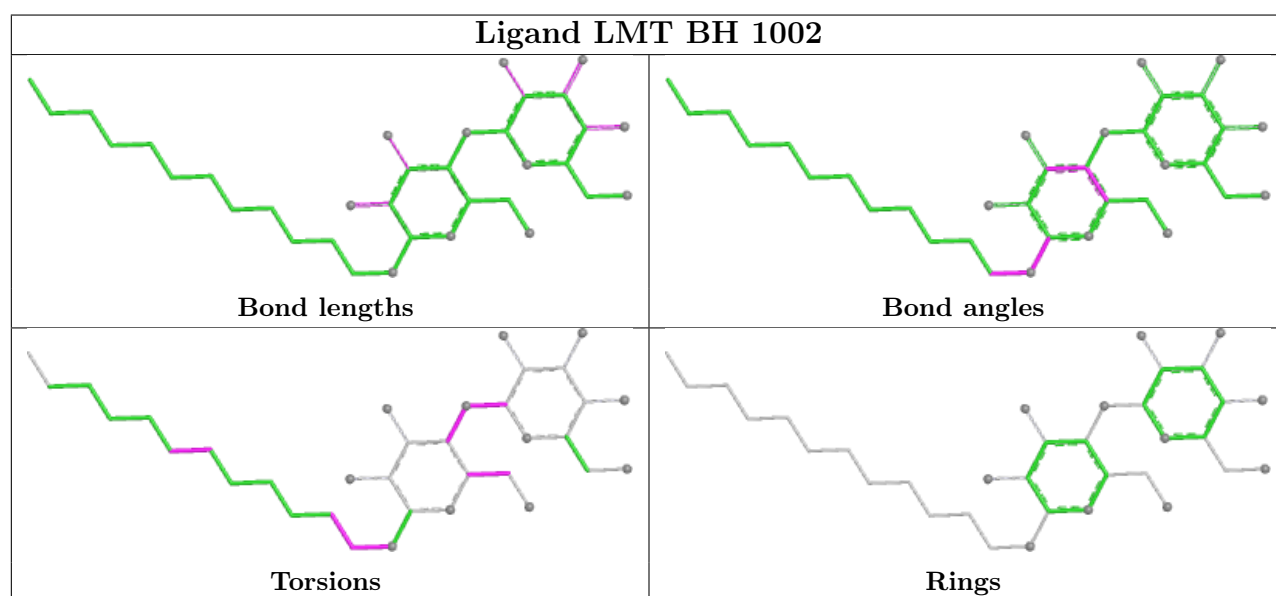
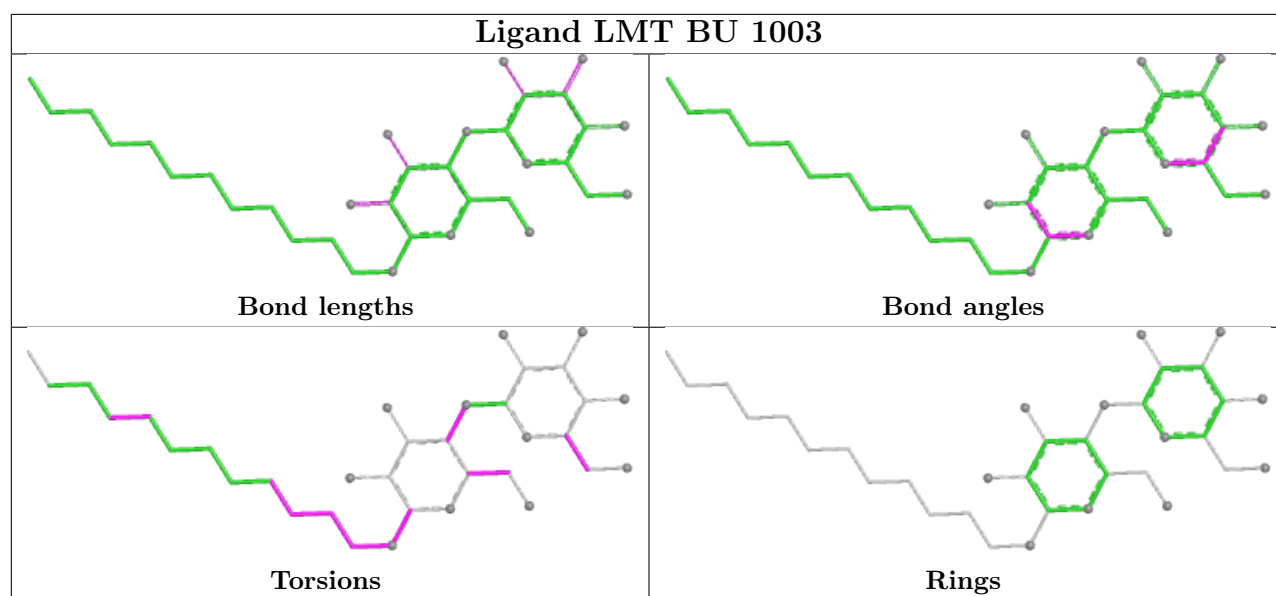


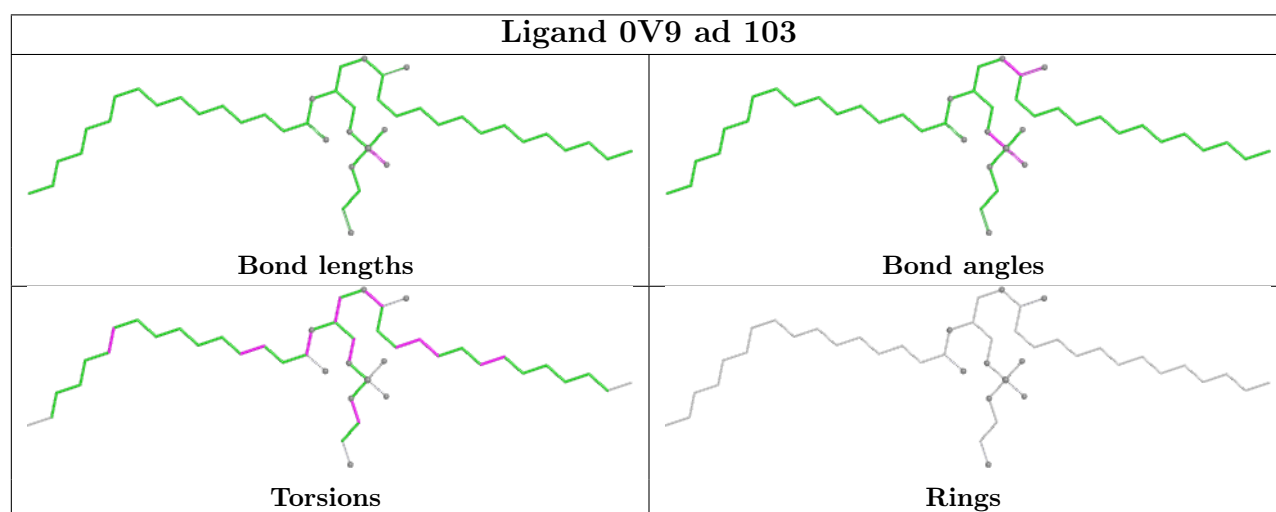
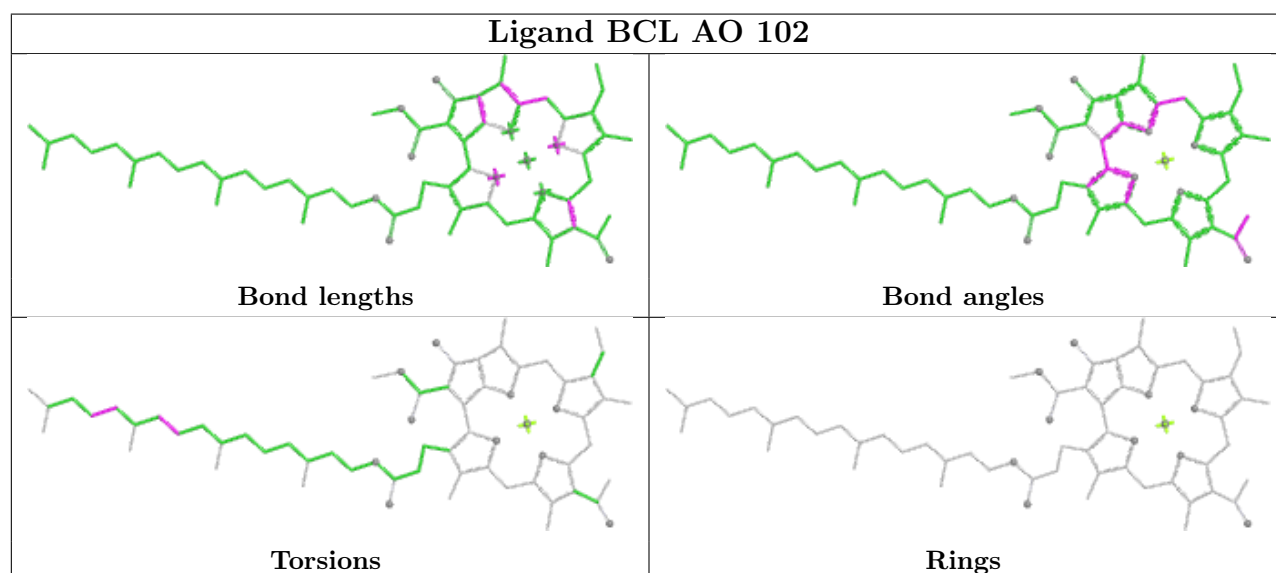
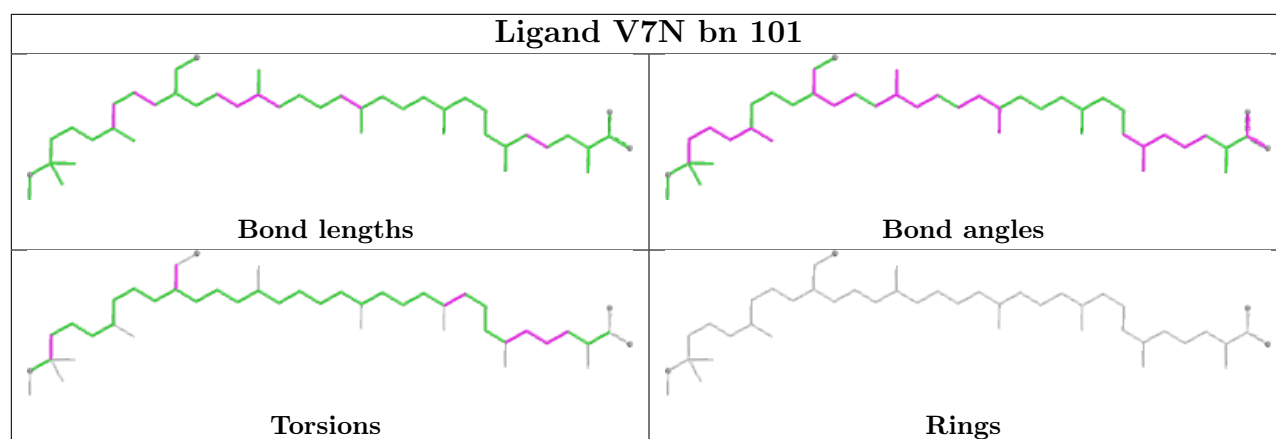


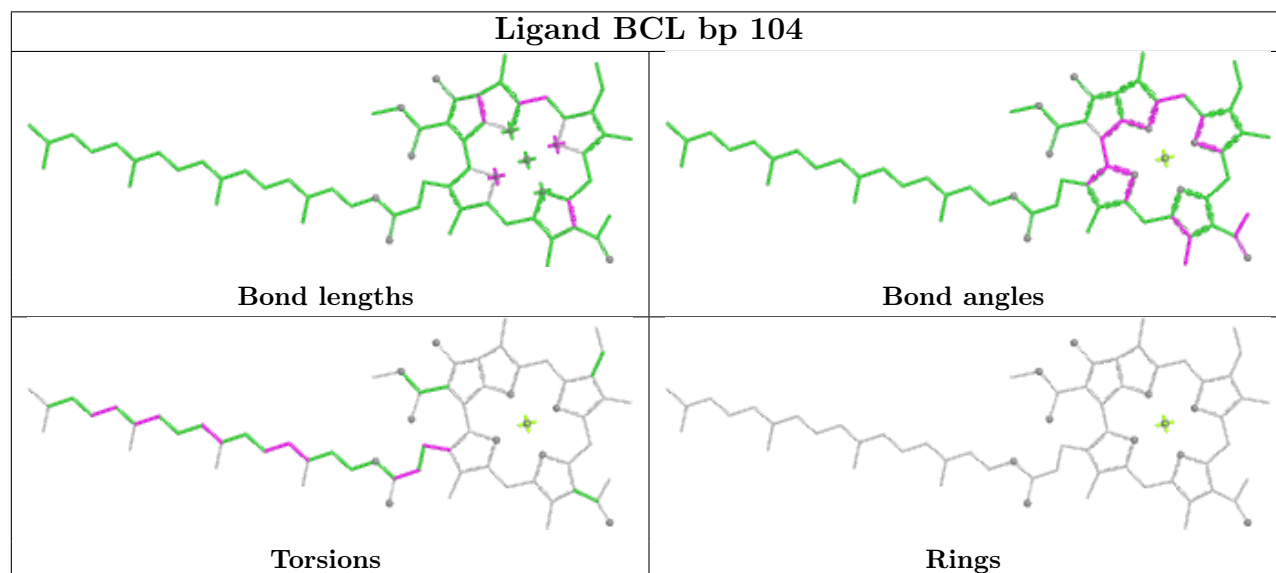
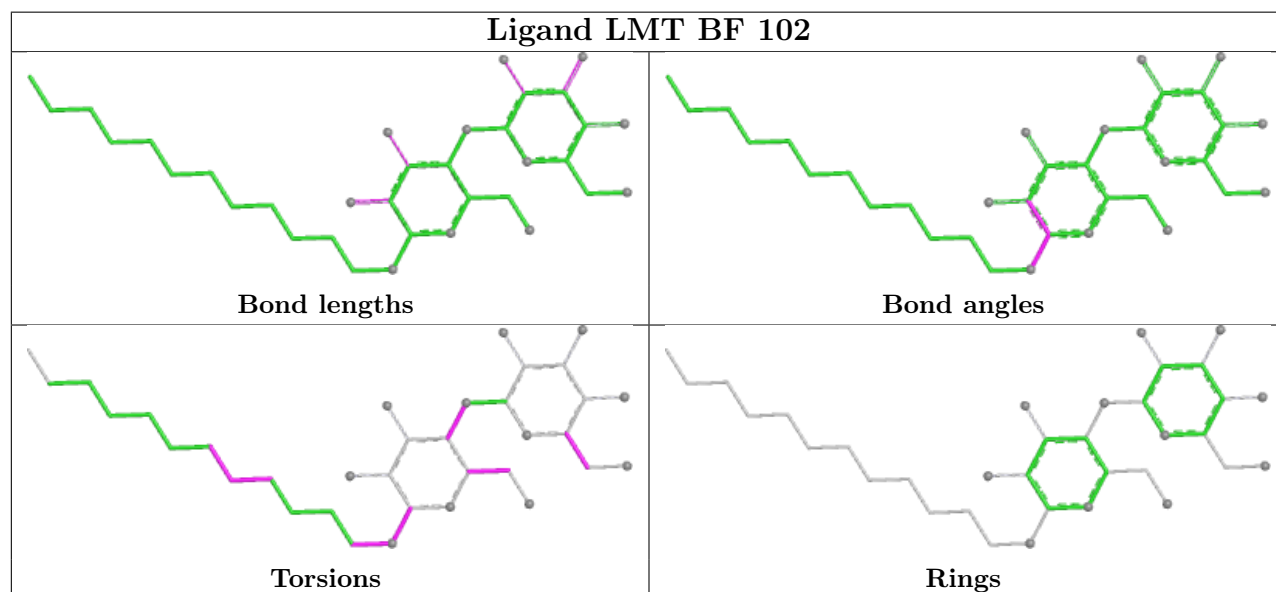
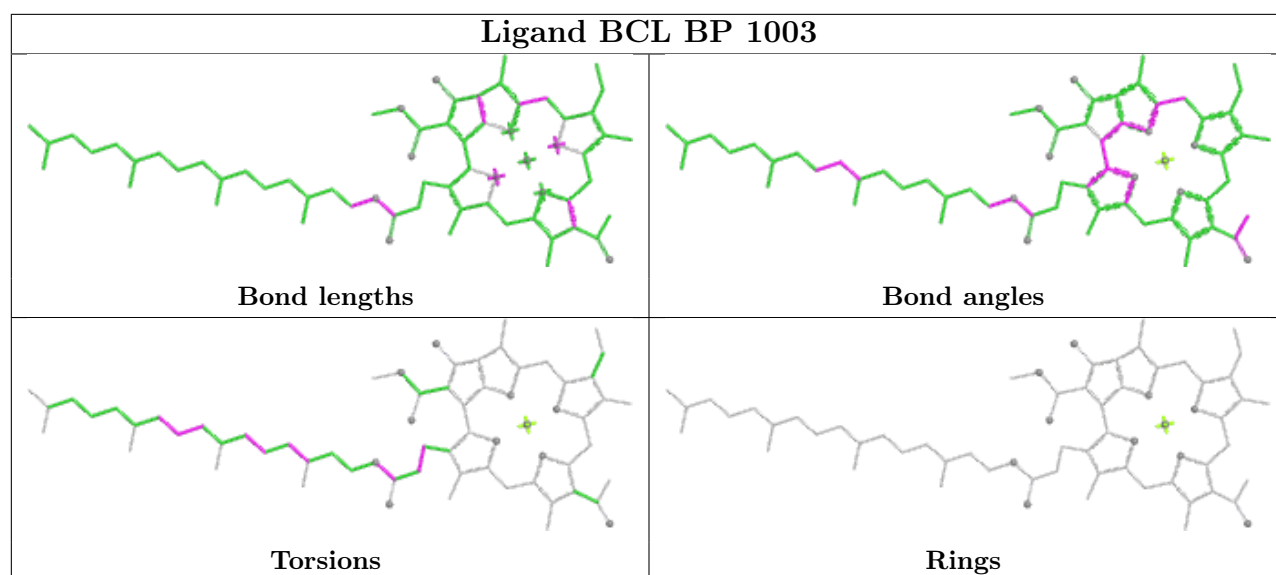


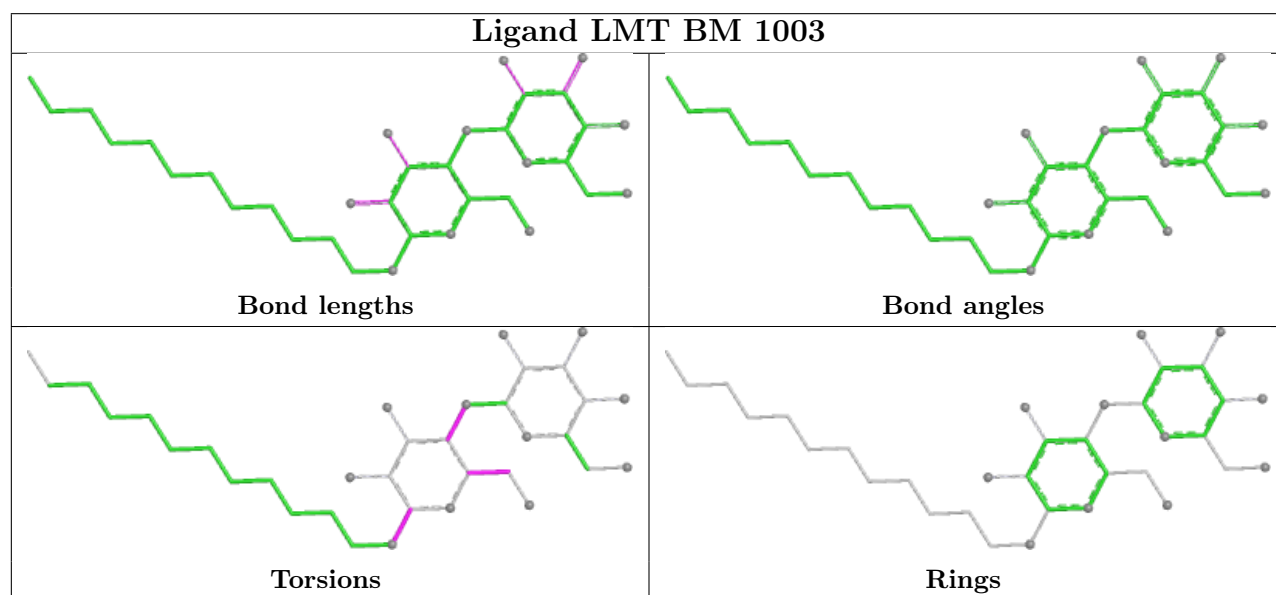
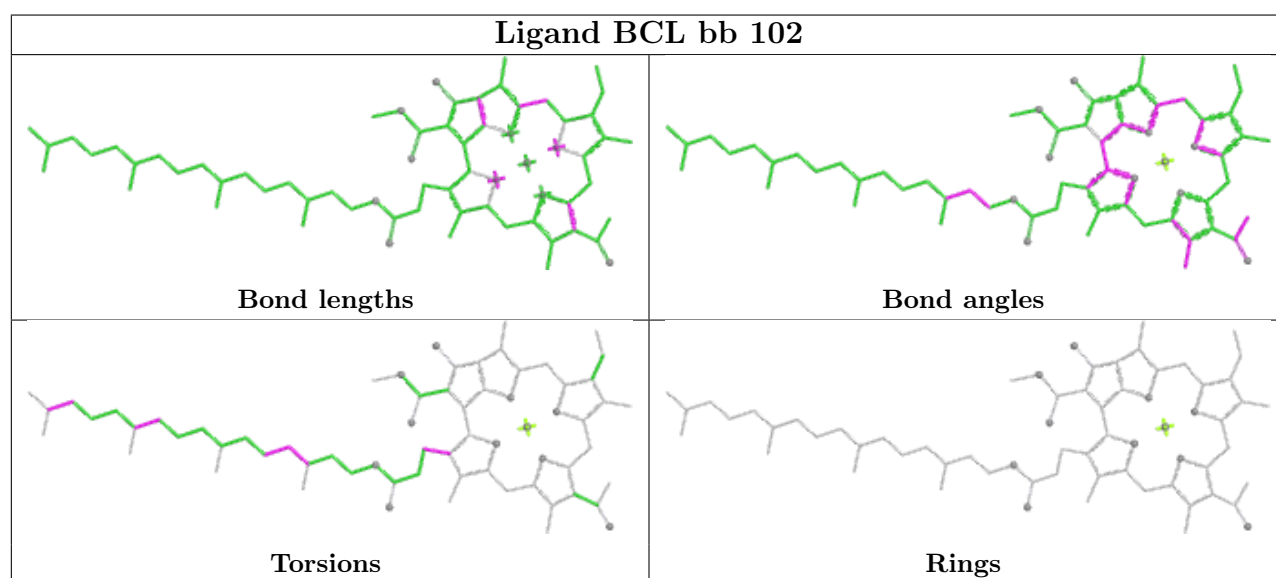
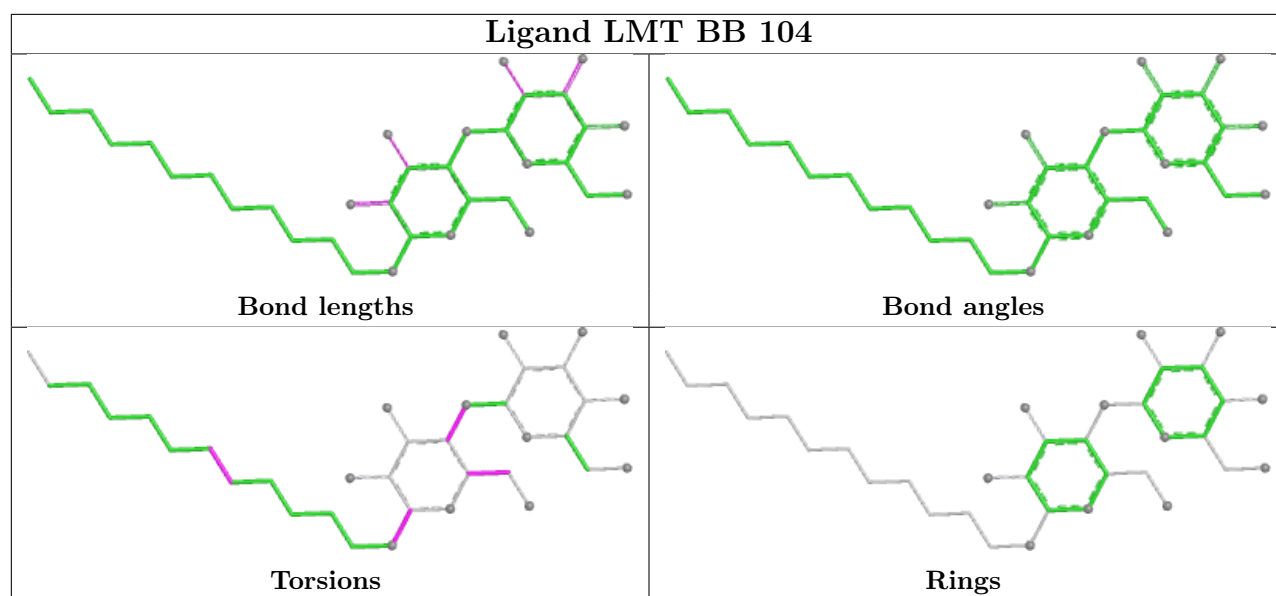


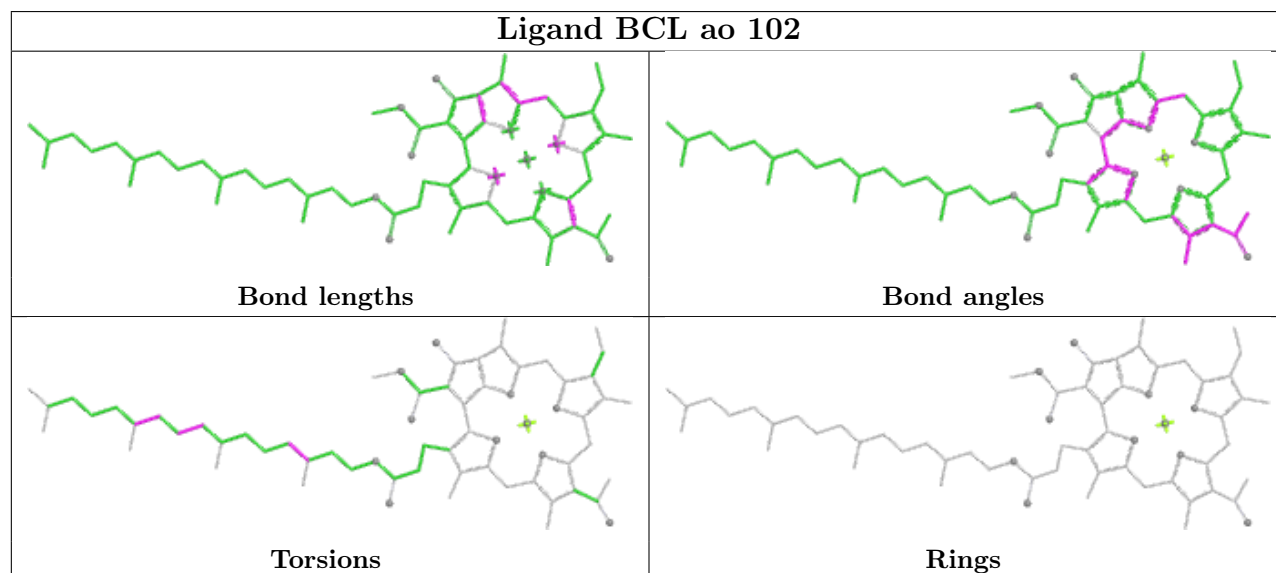
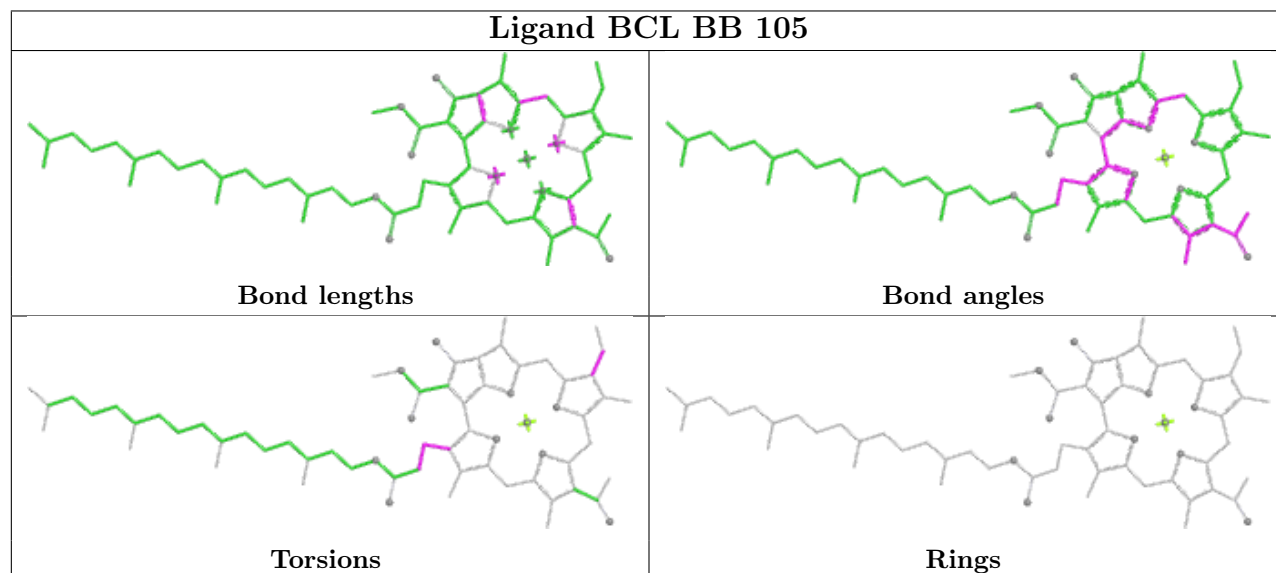
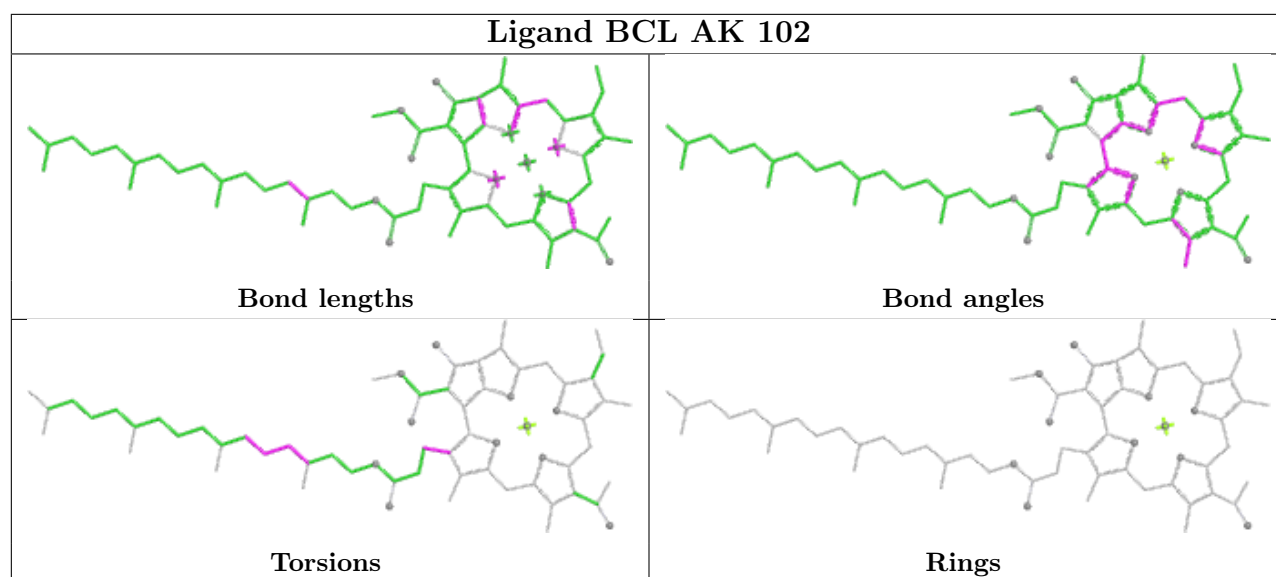


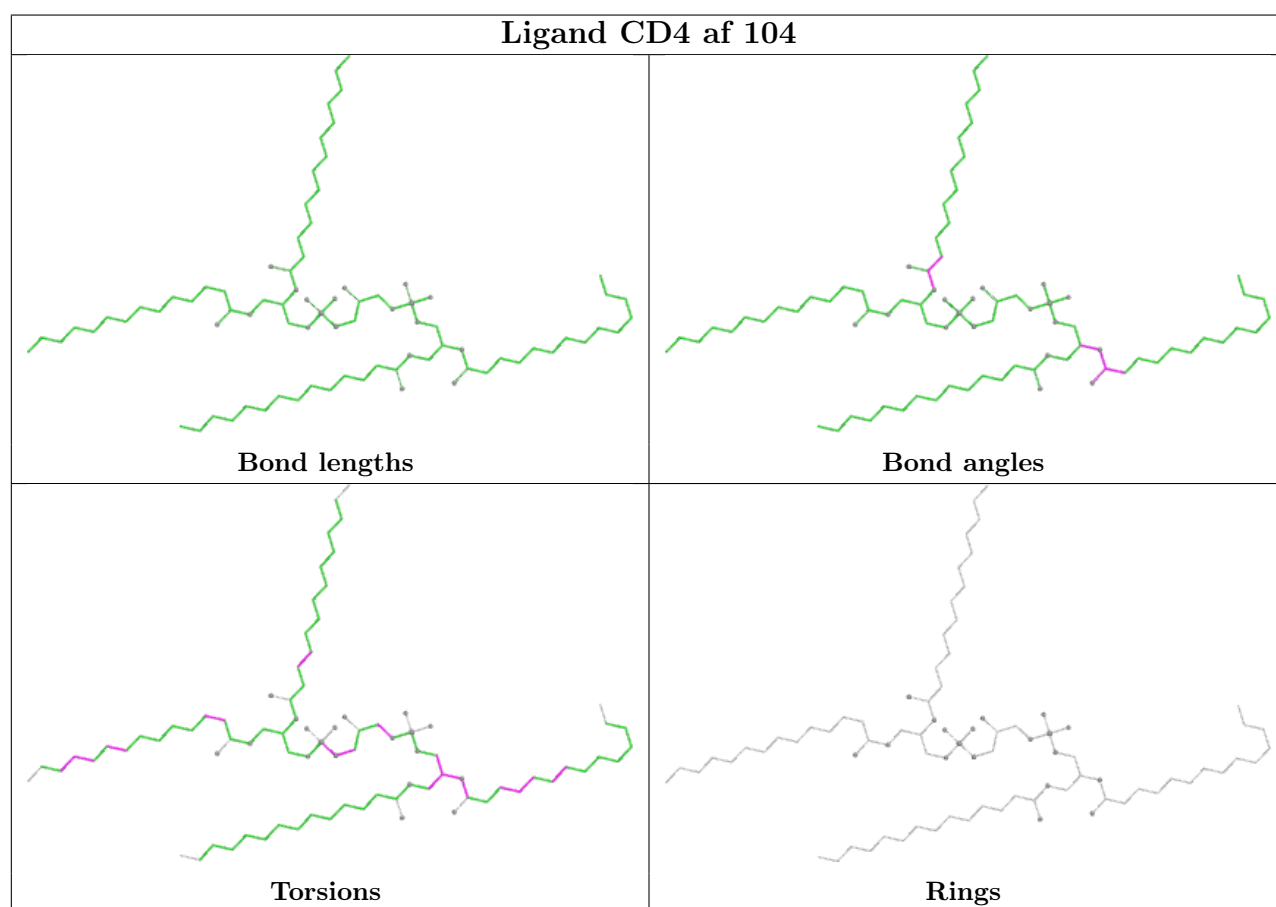
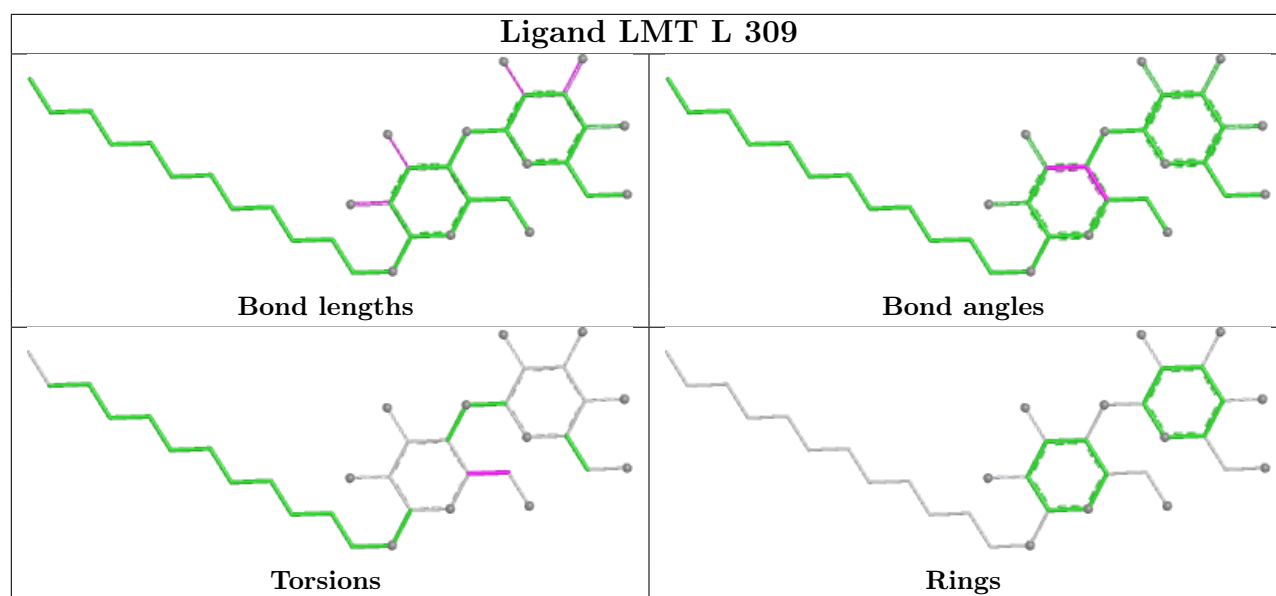


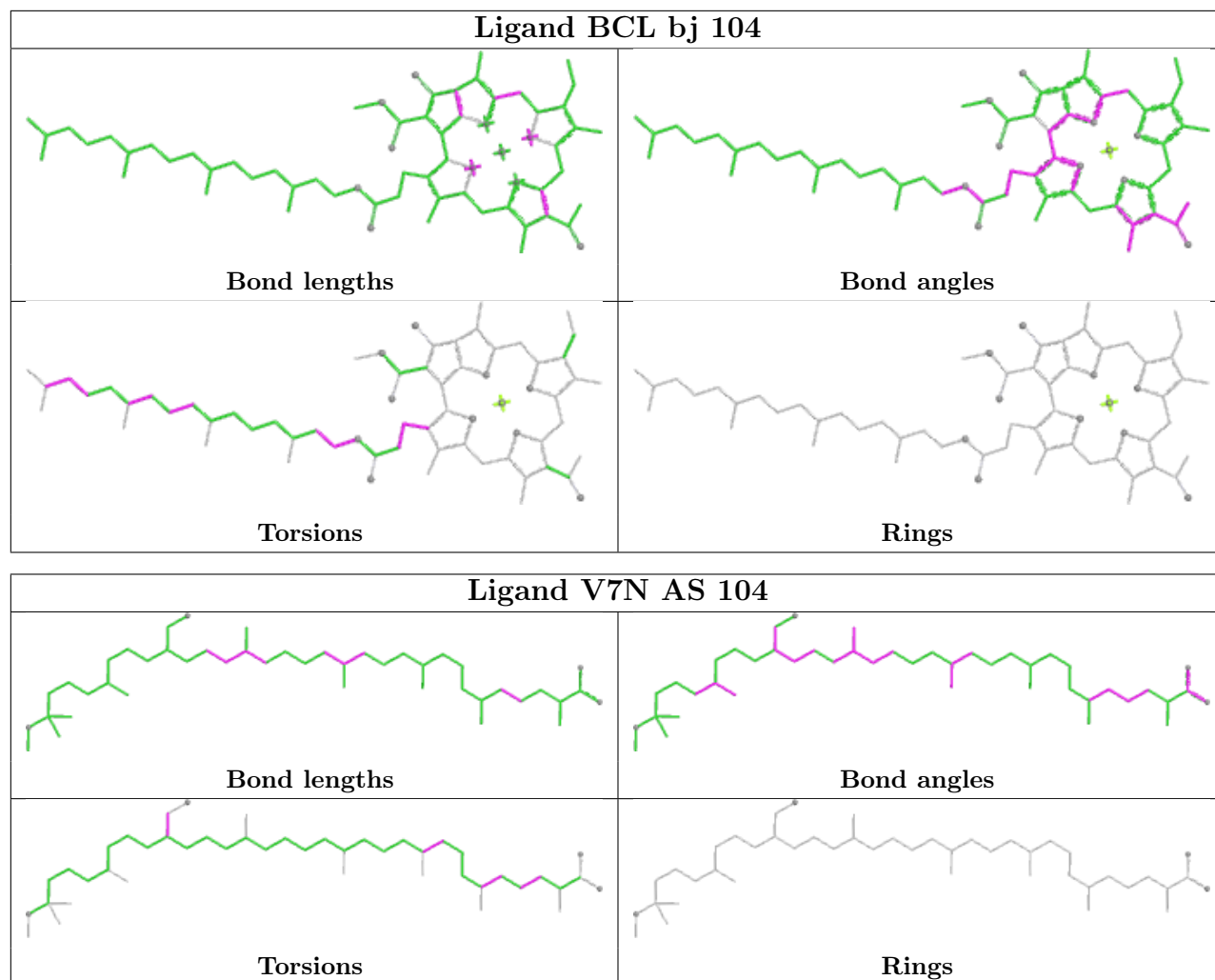




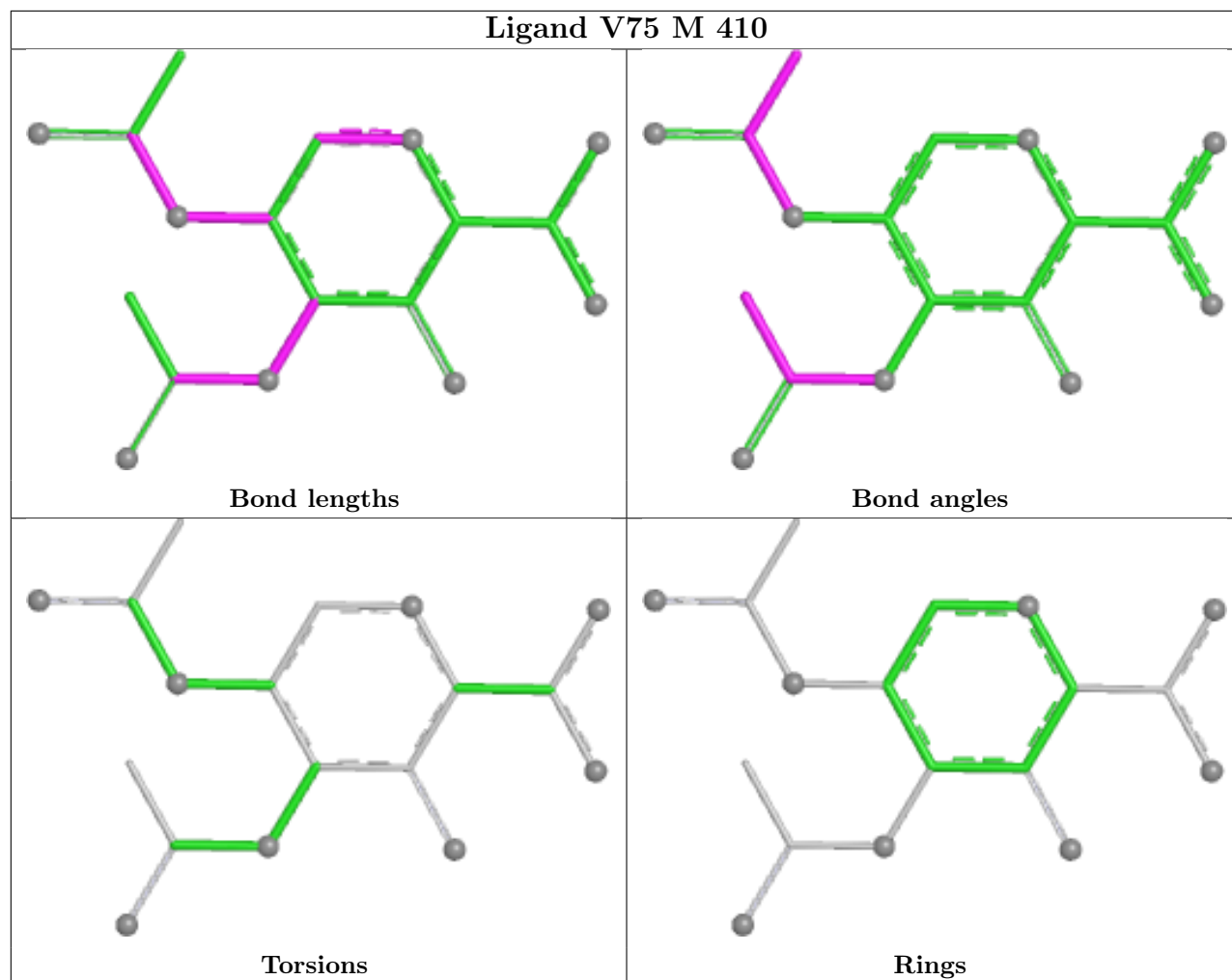




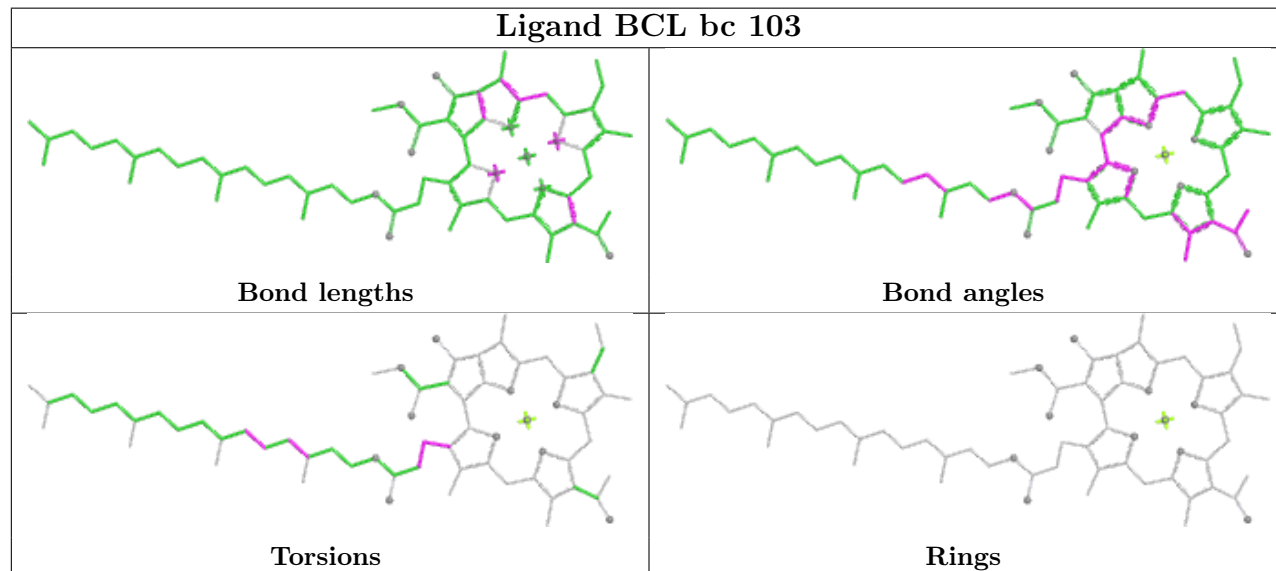


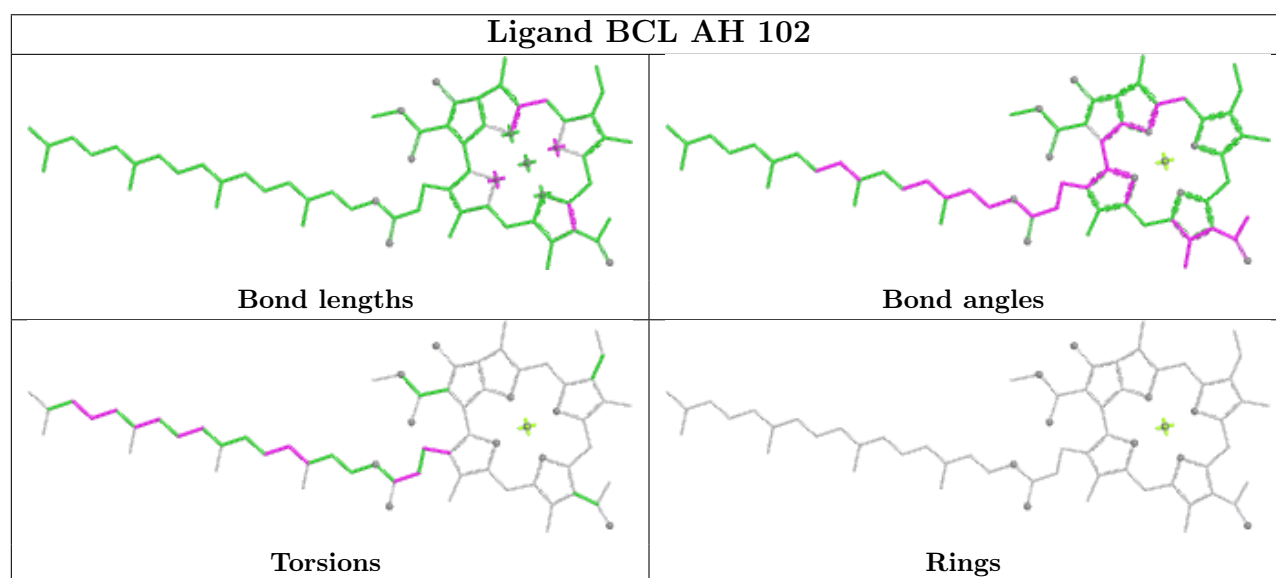
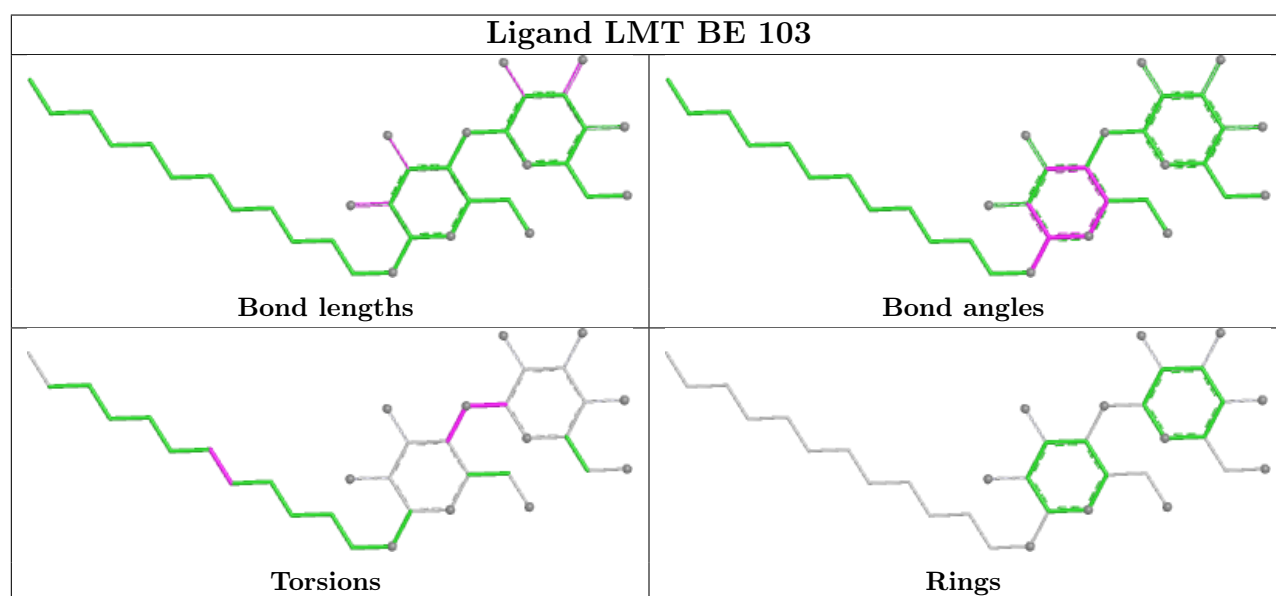
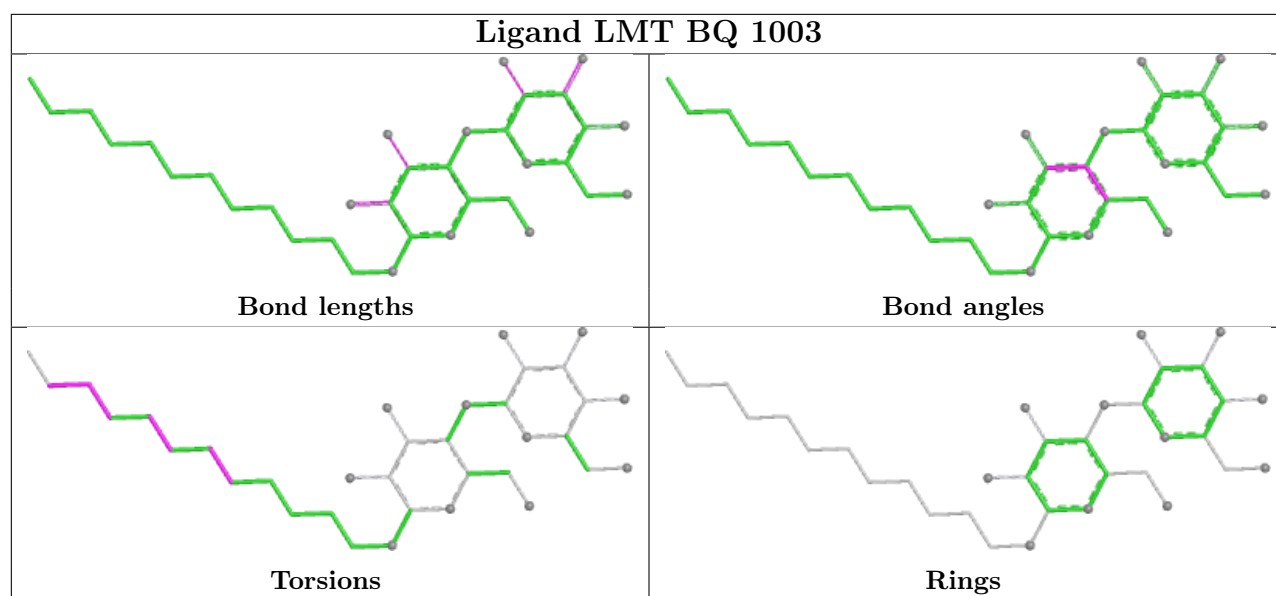


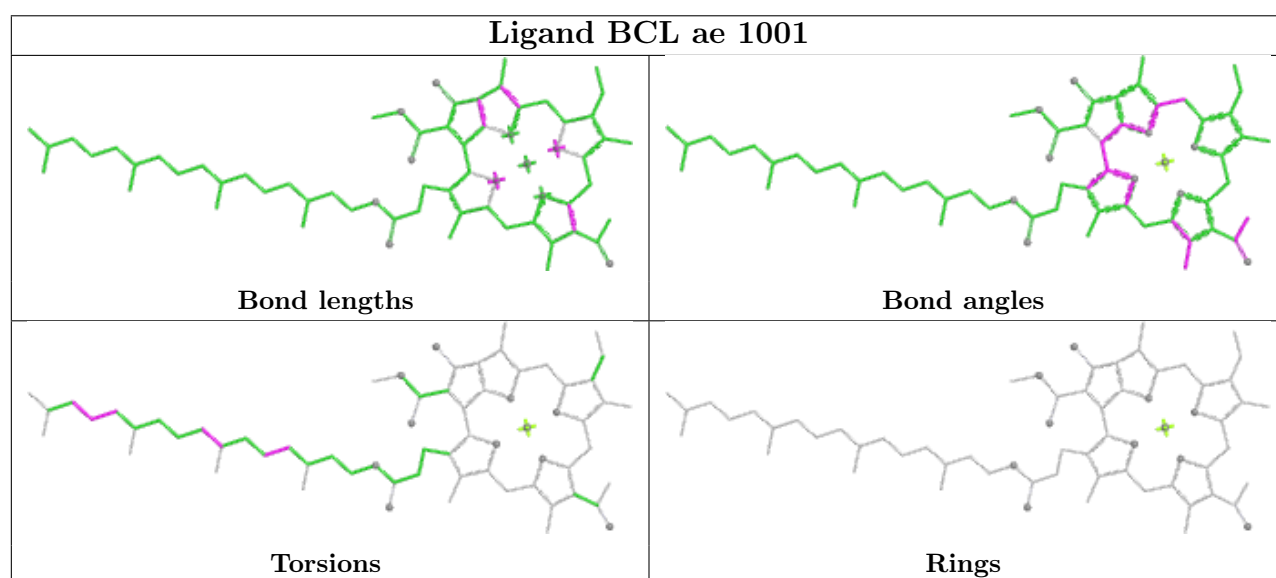
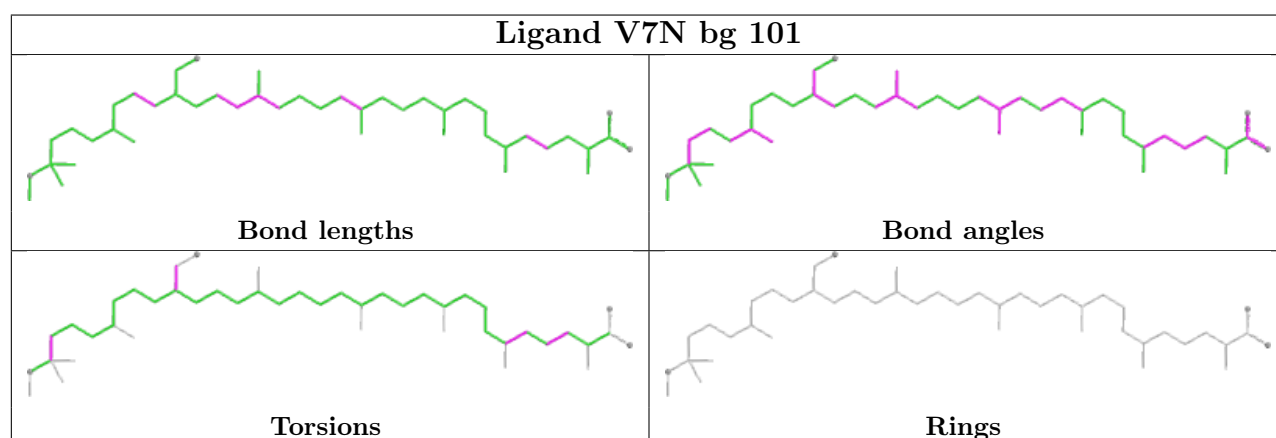
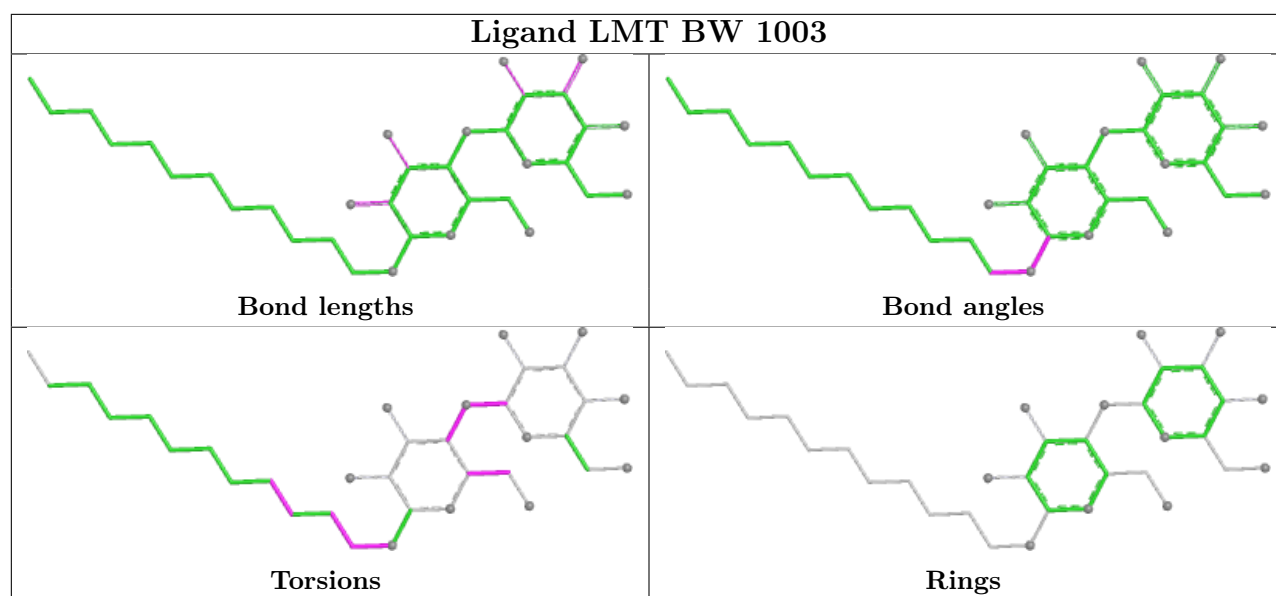
Ligand V75 M 410

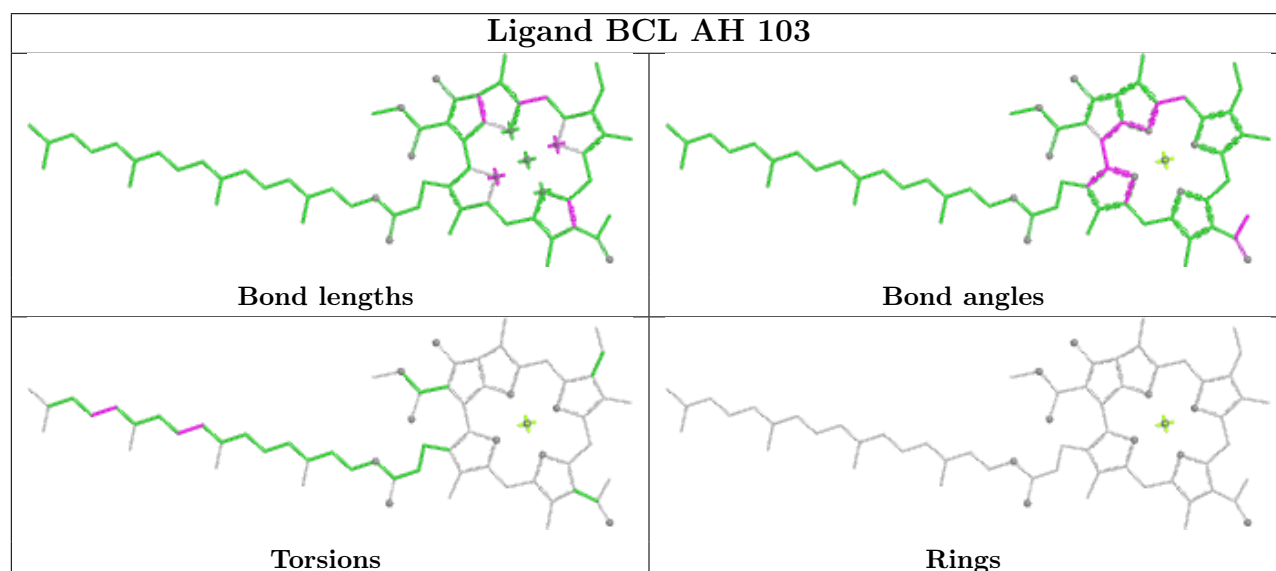
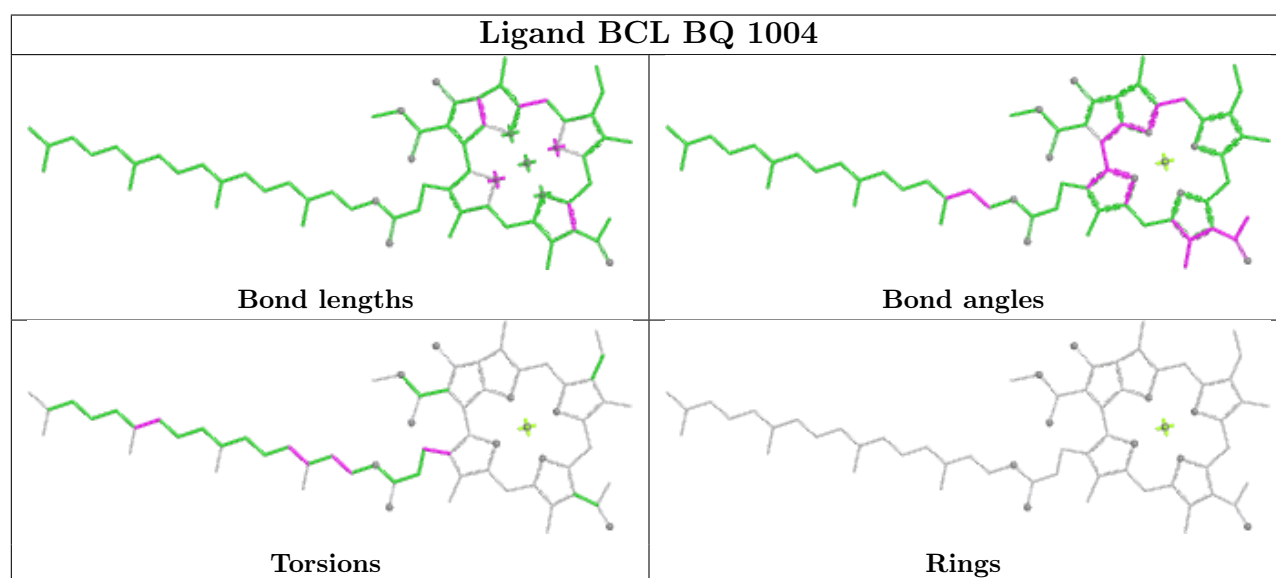
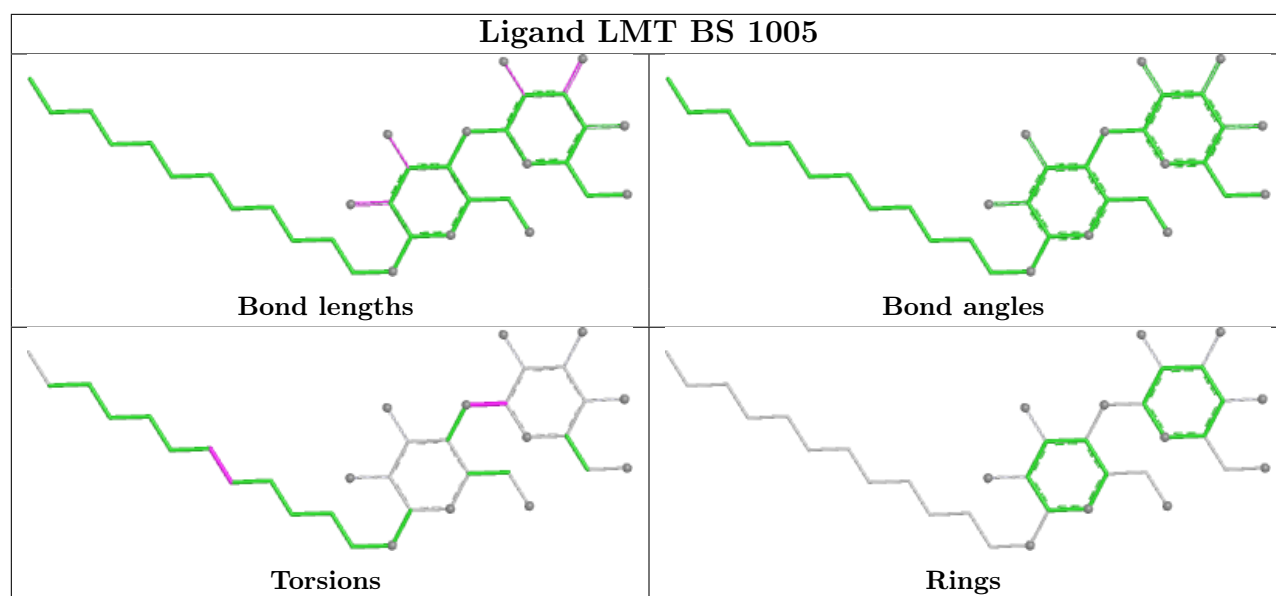


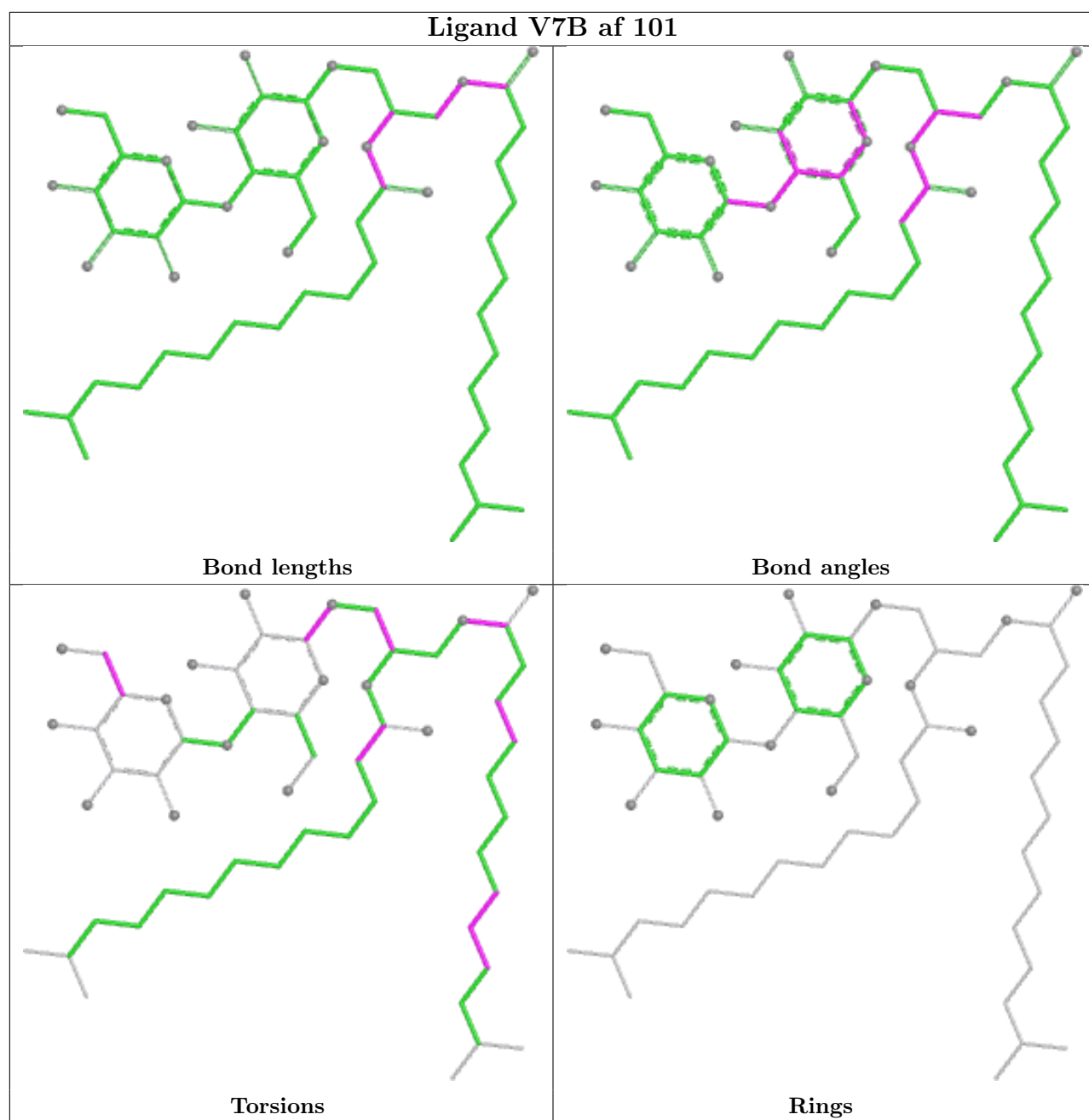
Ligand BCL bc 103

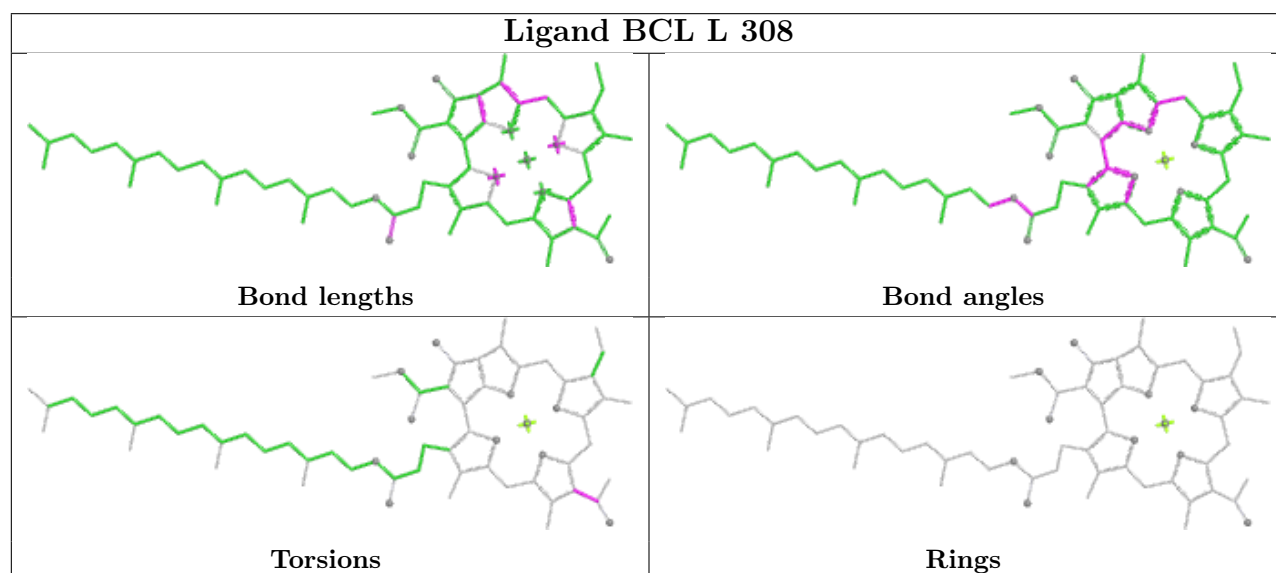
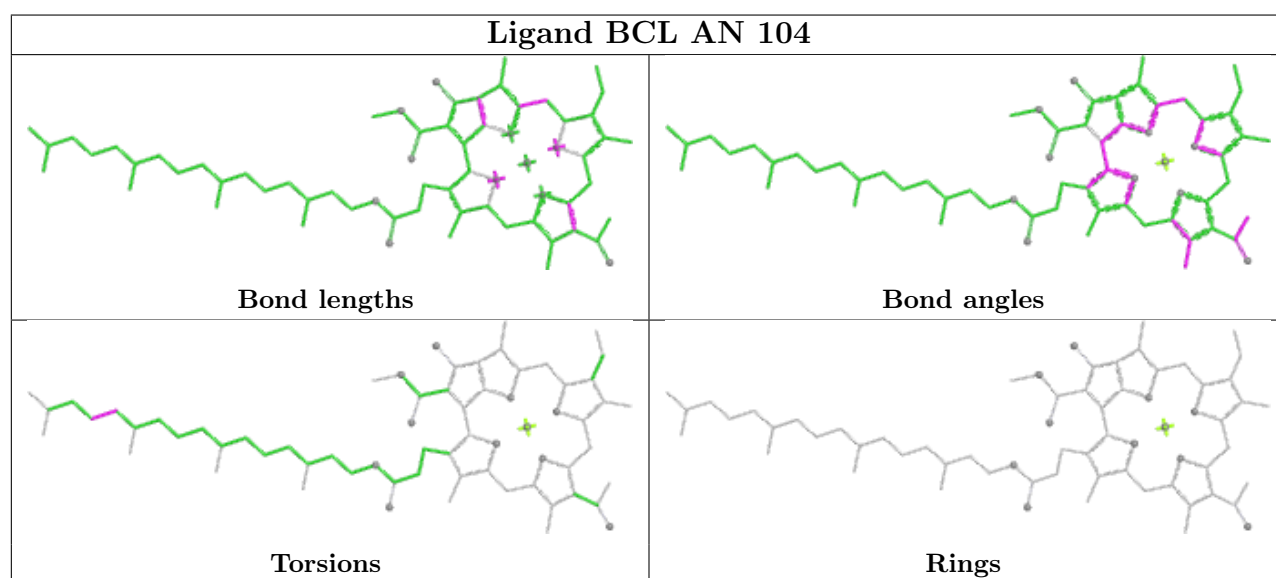
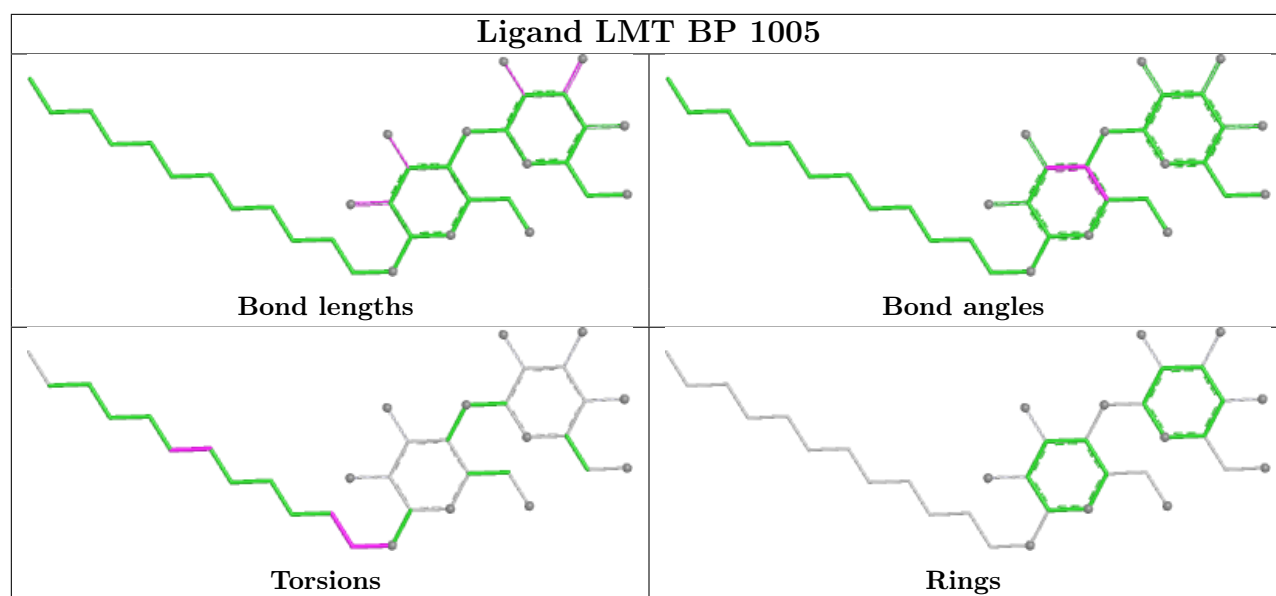


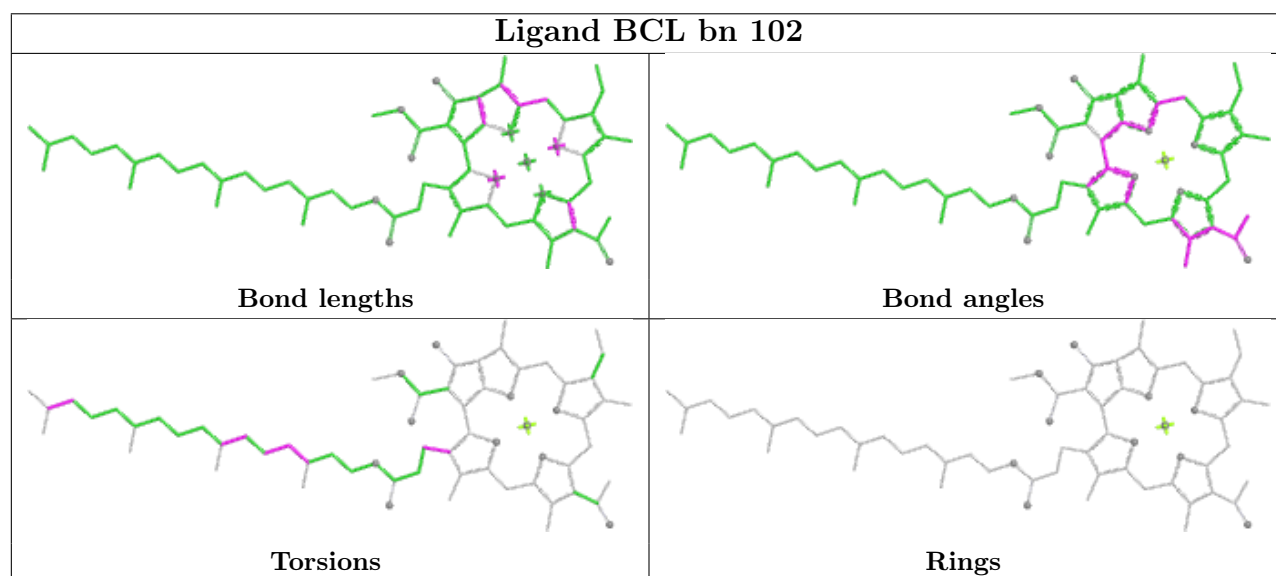
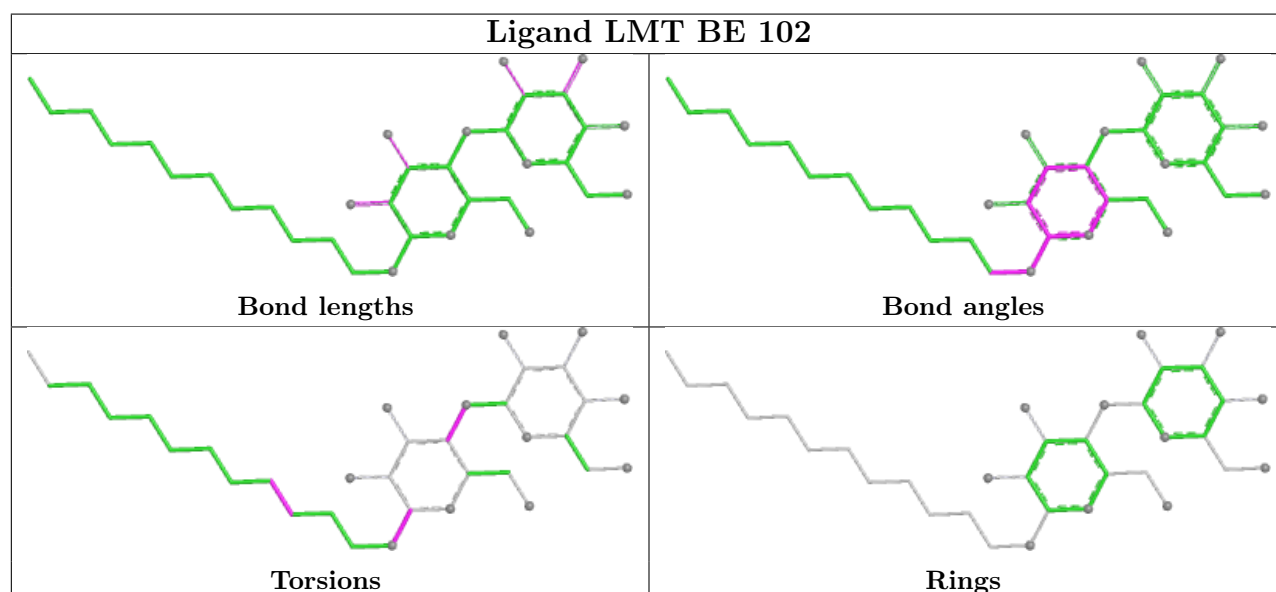
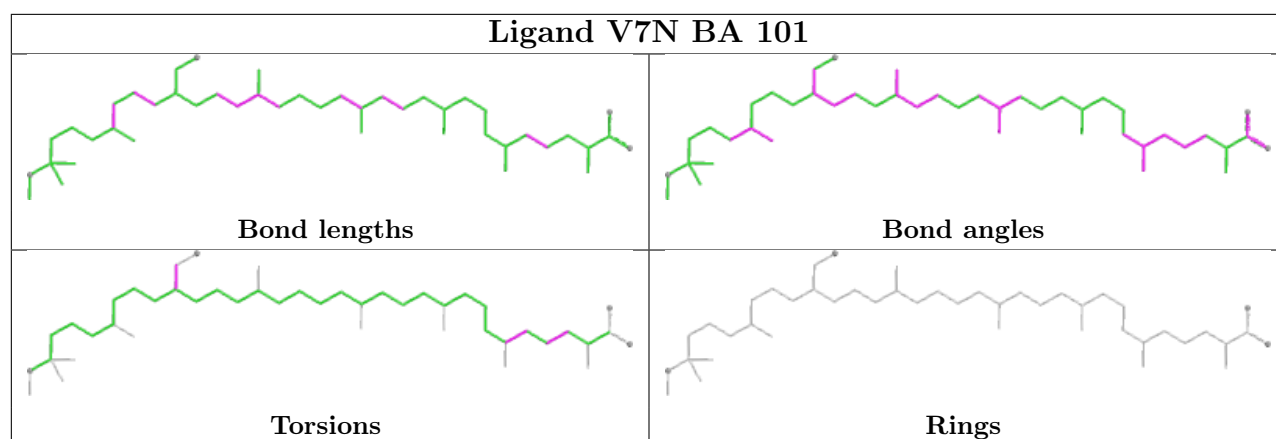


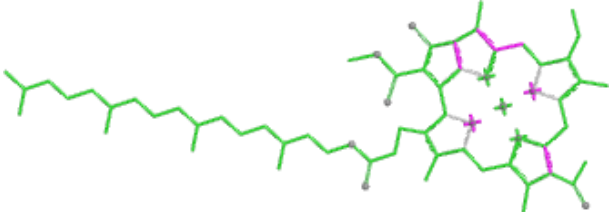
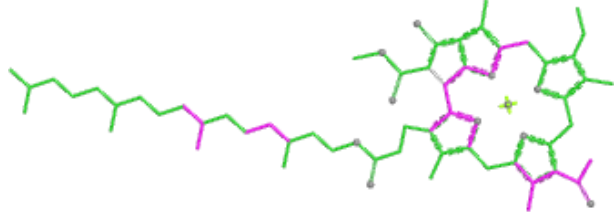
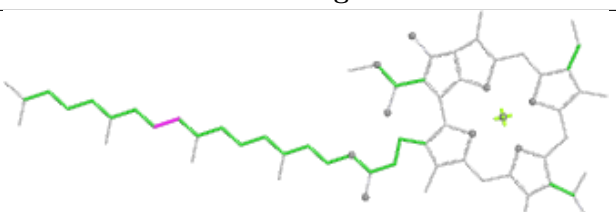
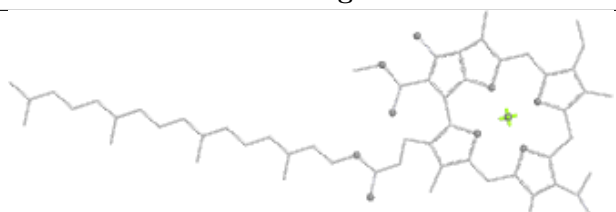
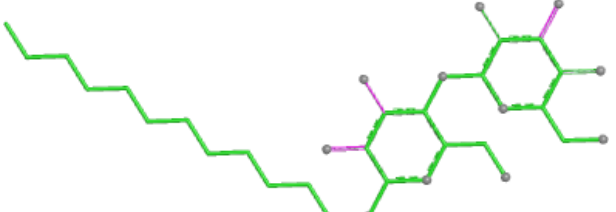
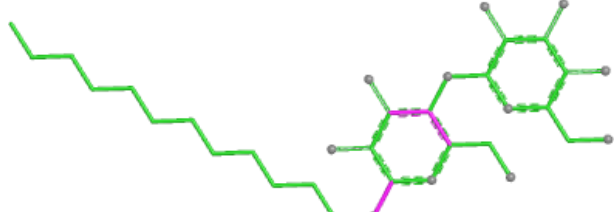
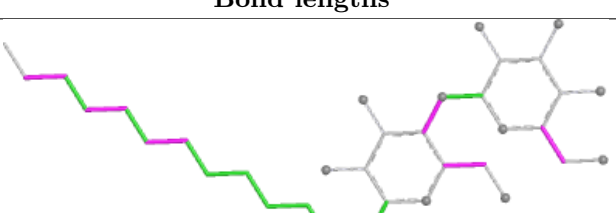
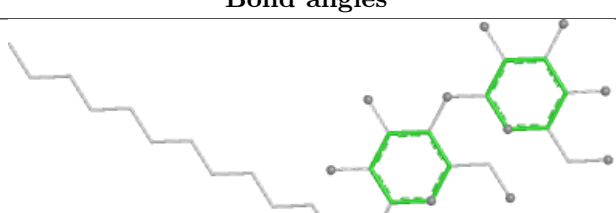
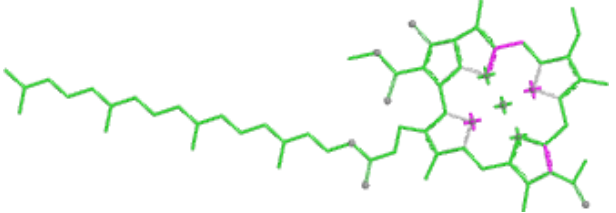
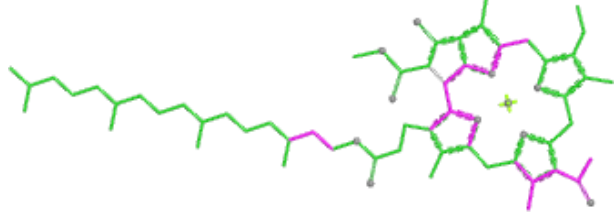
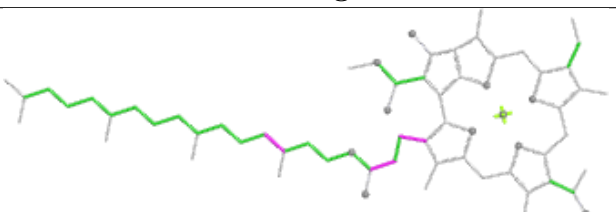
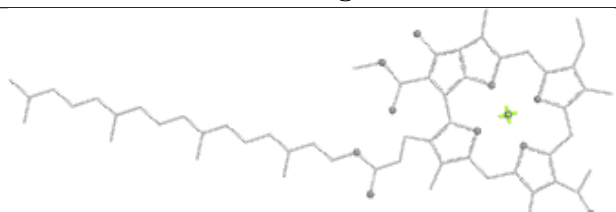


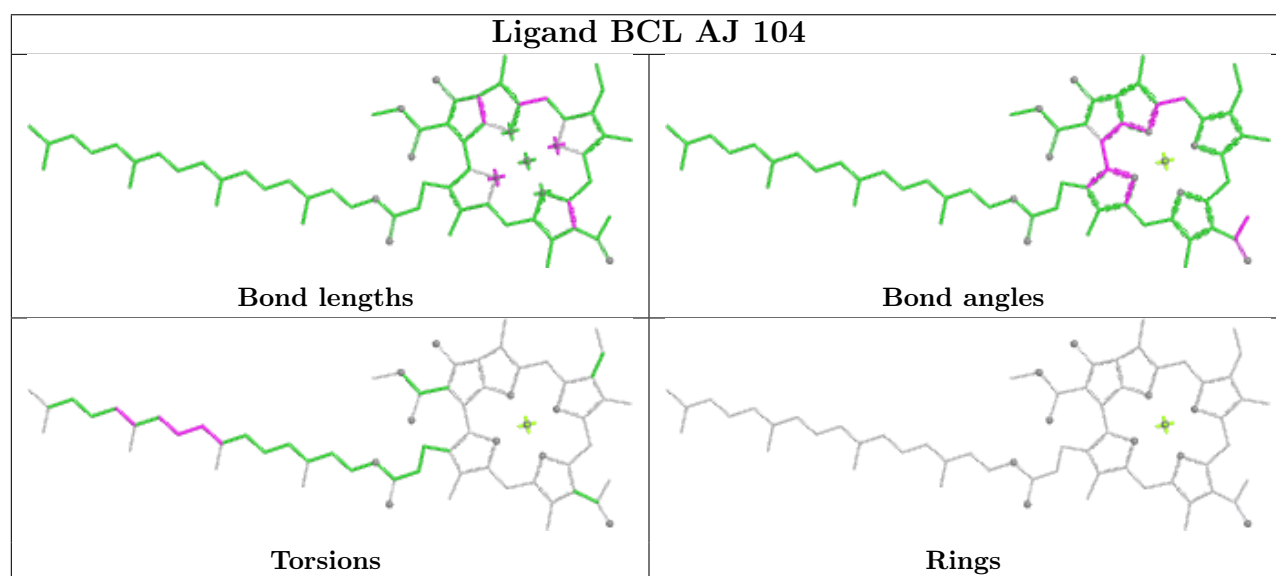
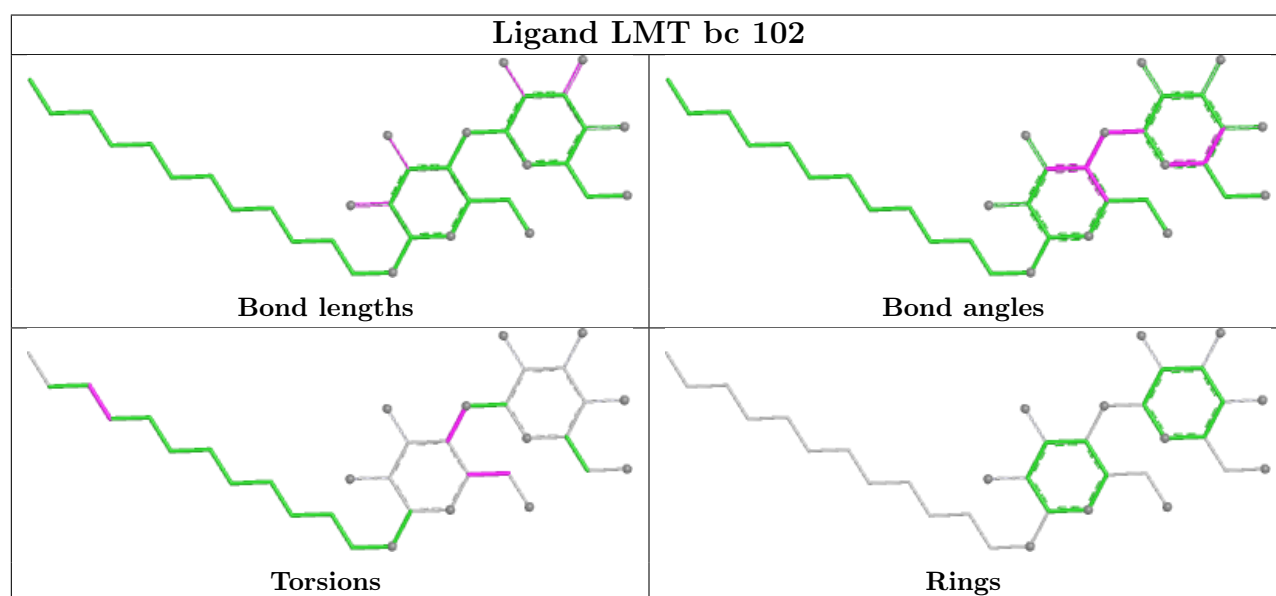
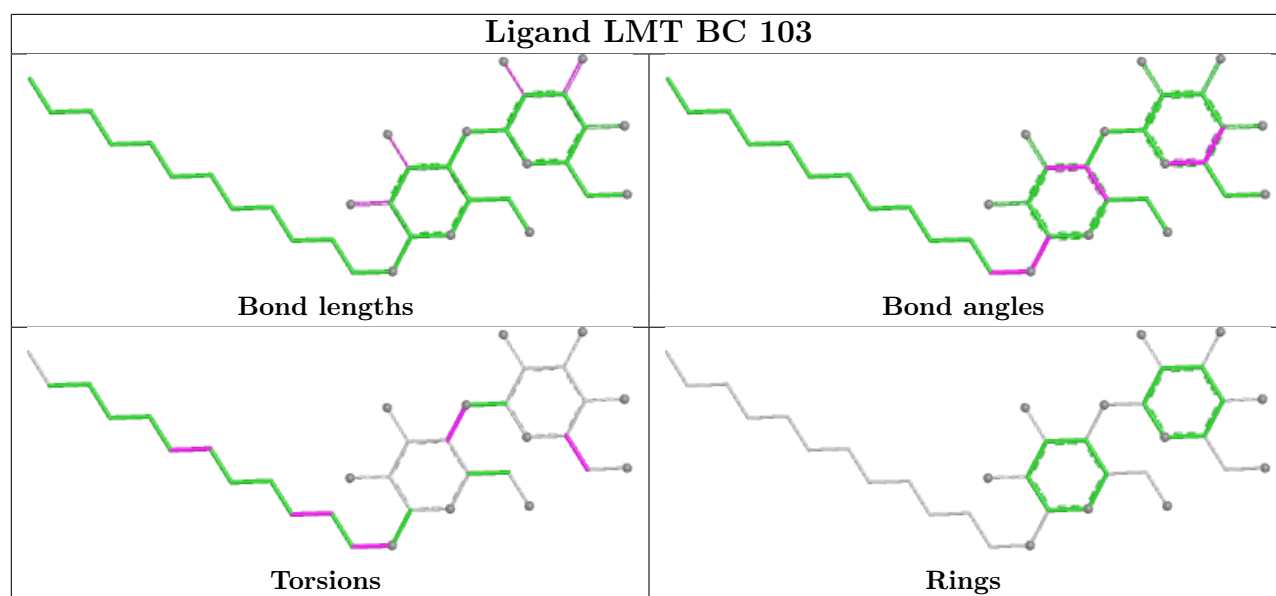


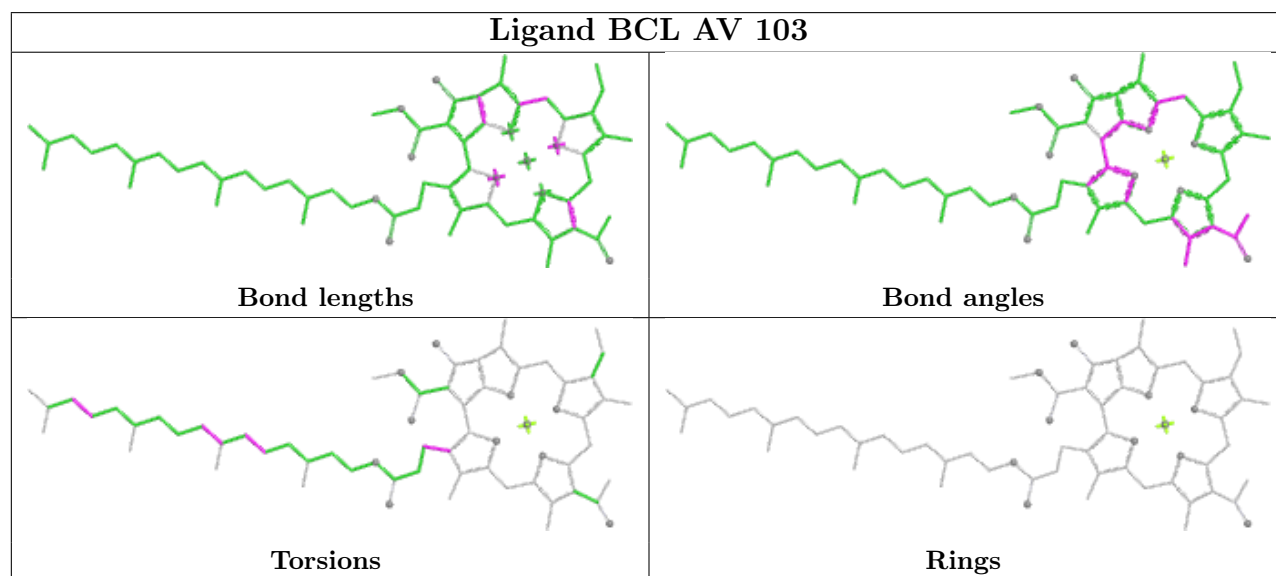
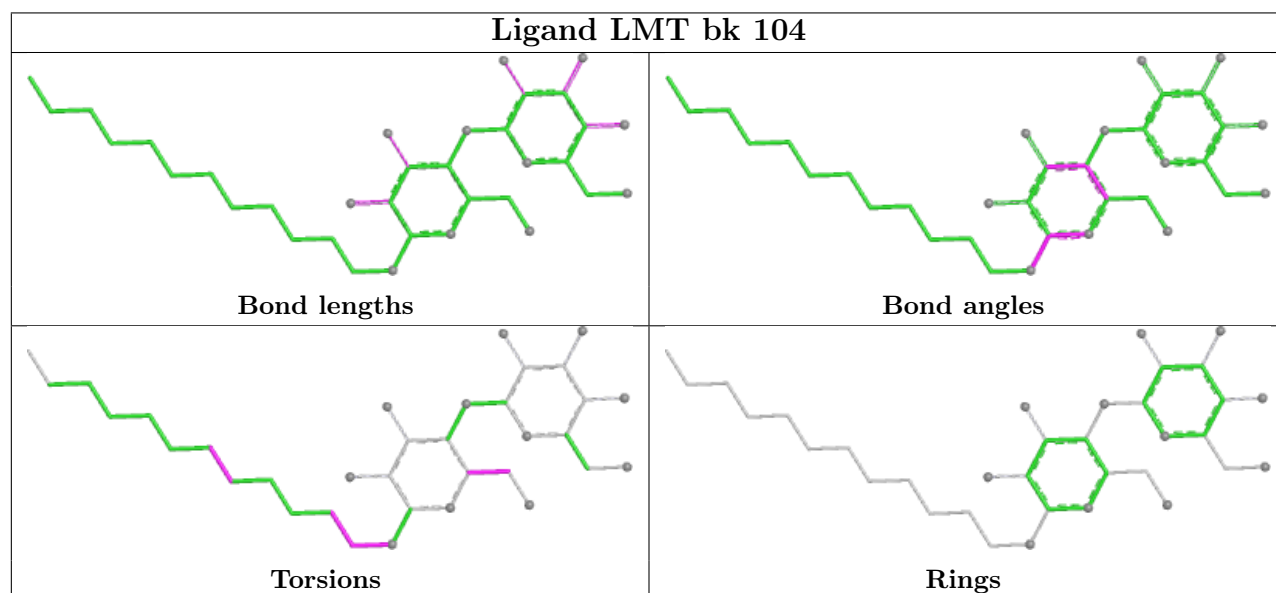
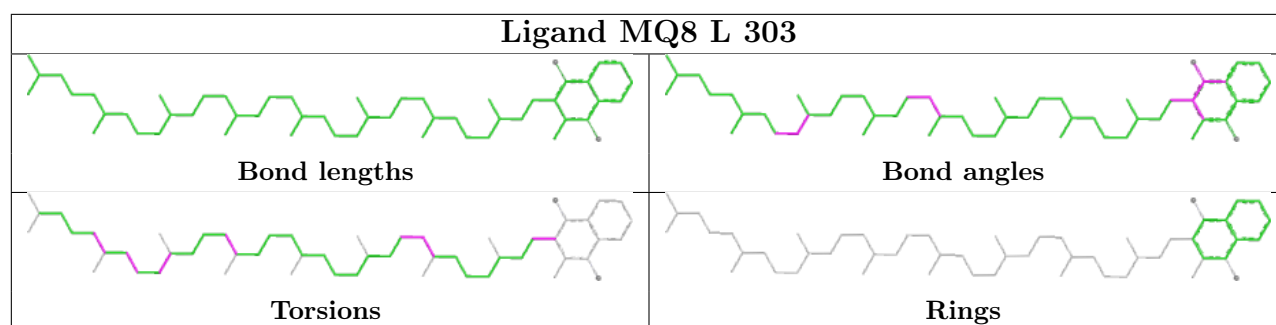


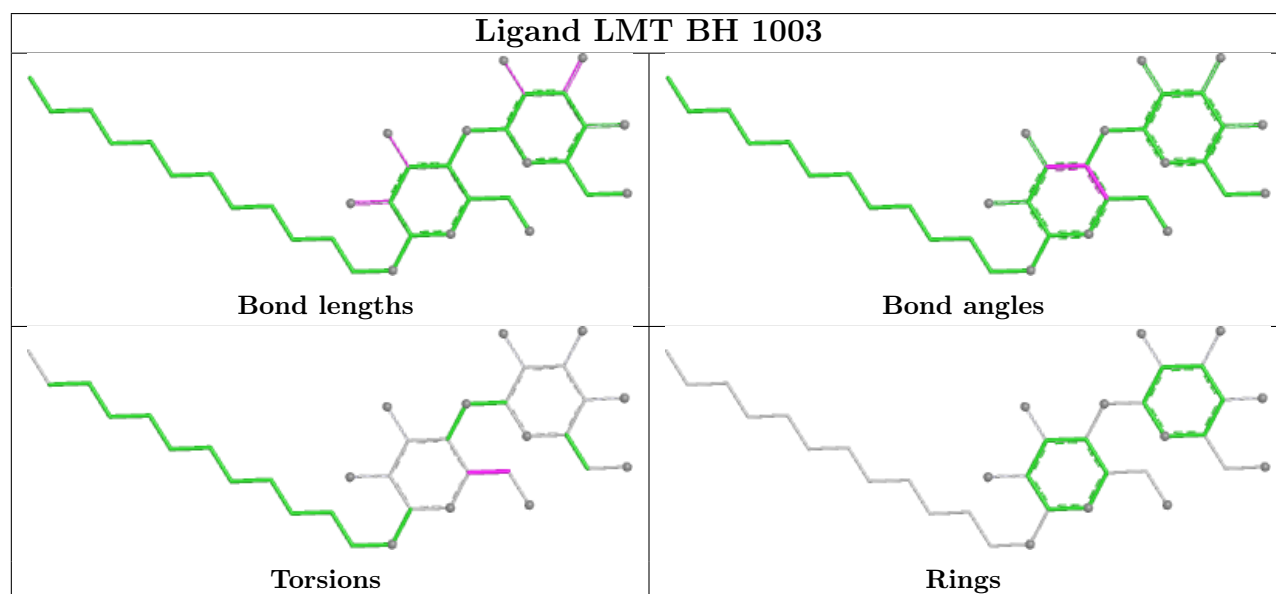
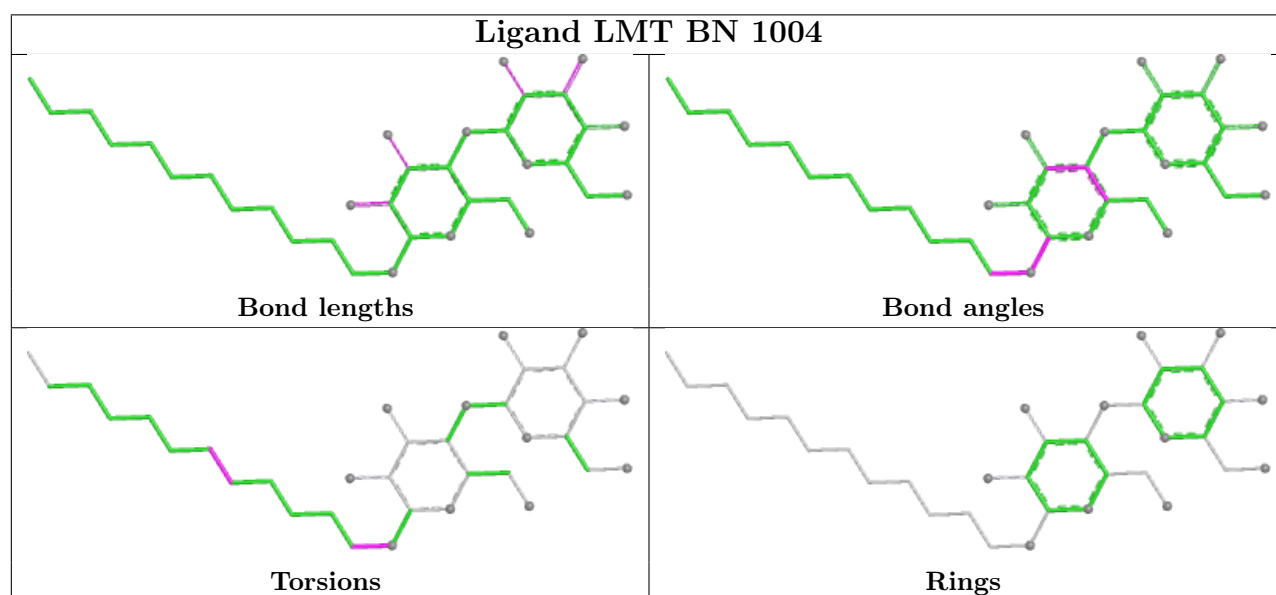
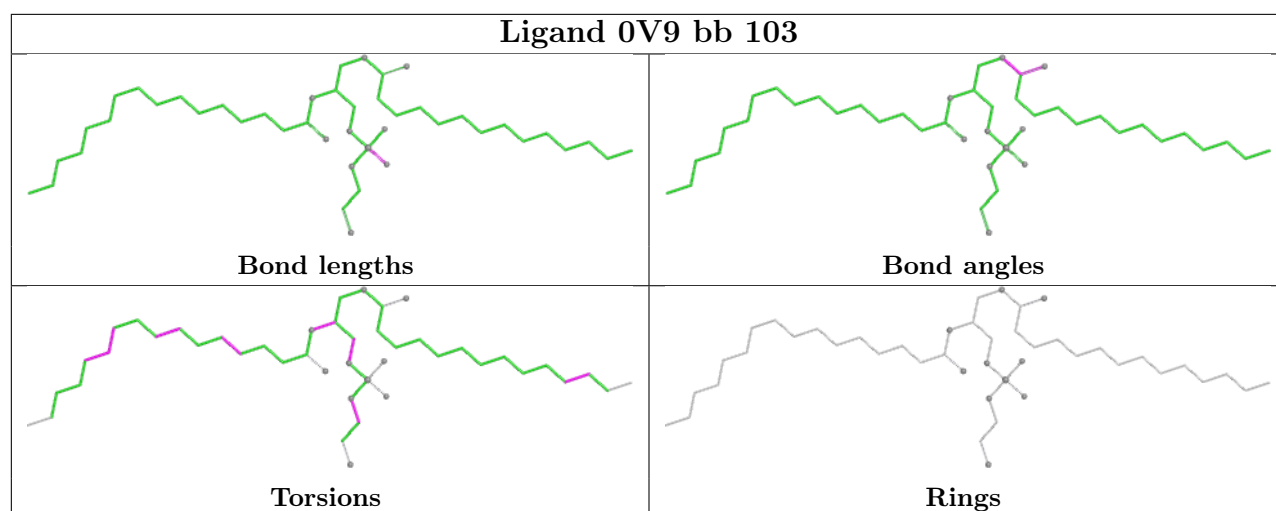


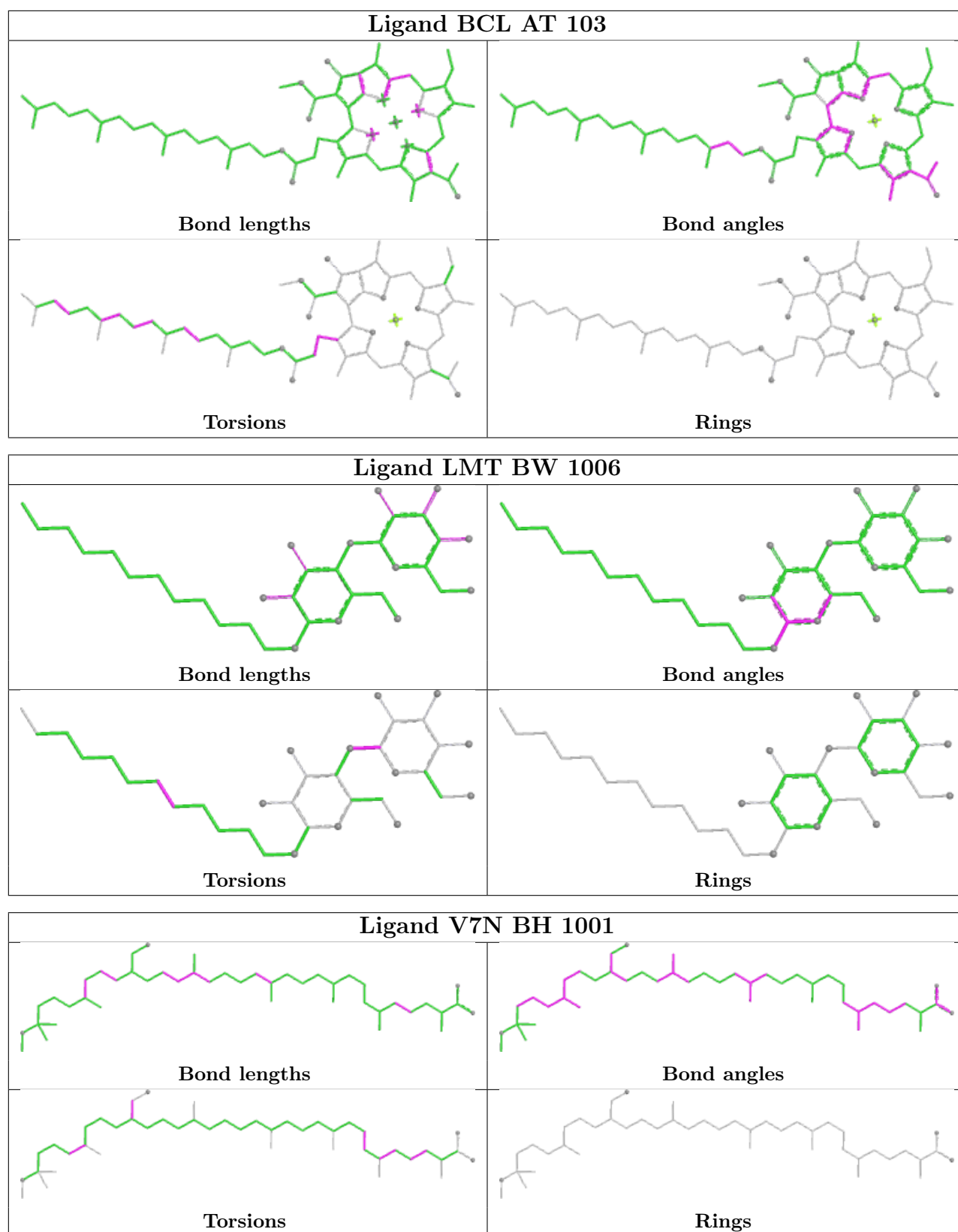


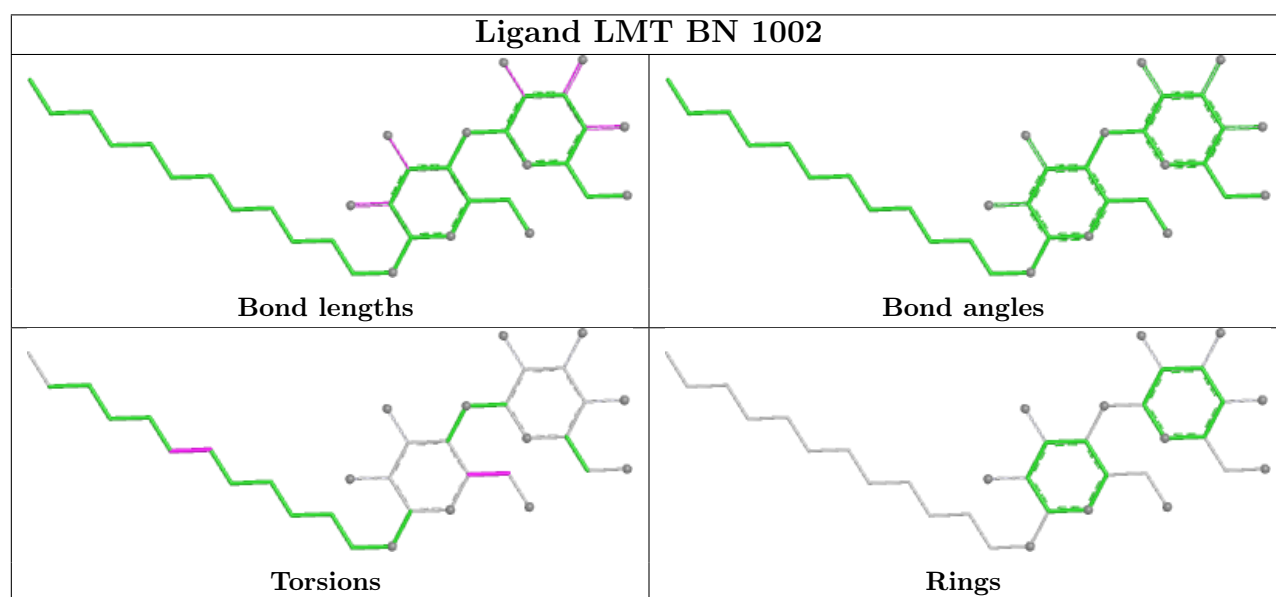
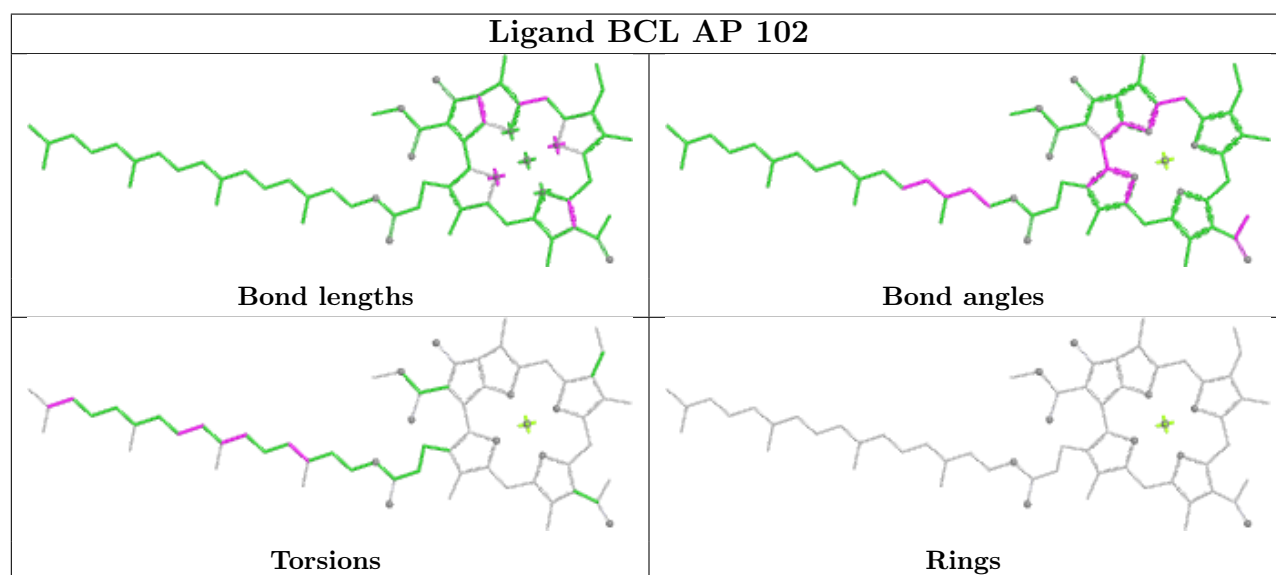
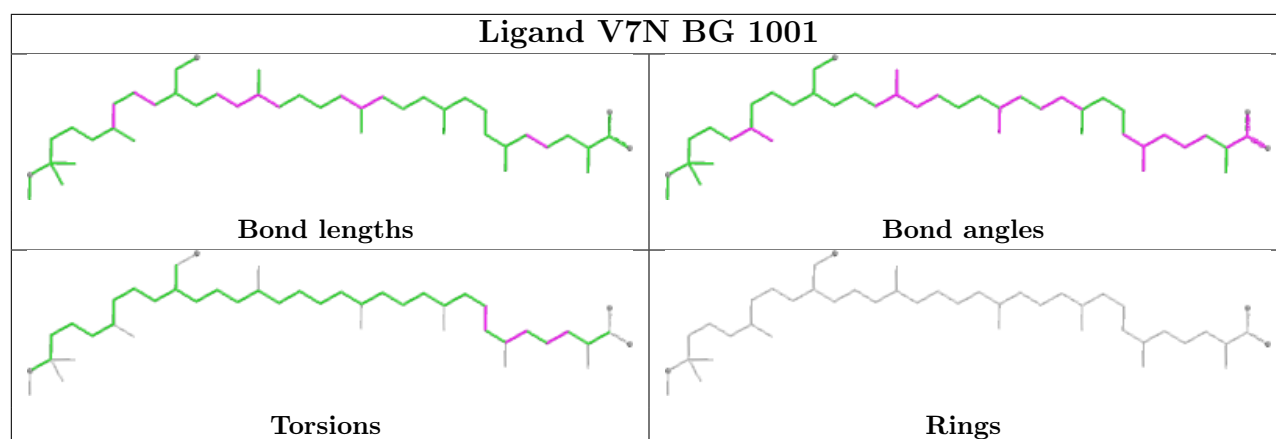
Ligand BCL AB 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT AC 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL AE 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

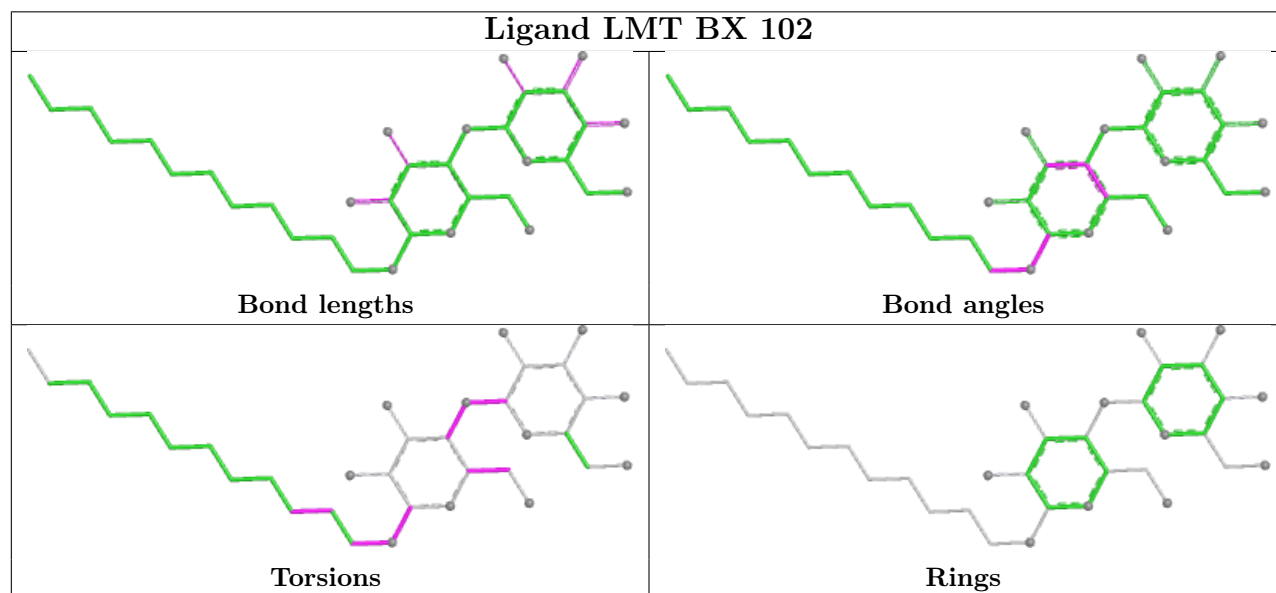
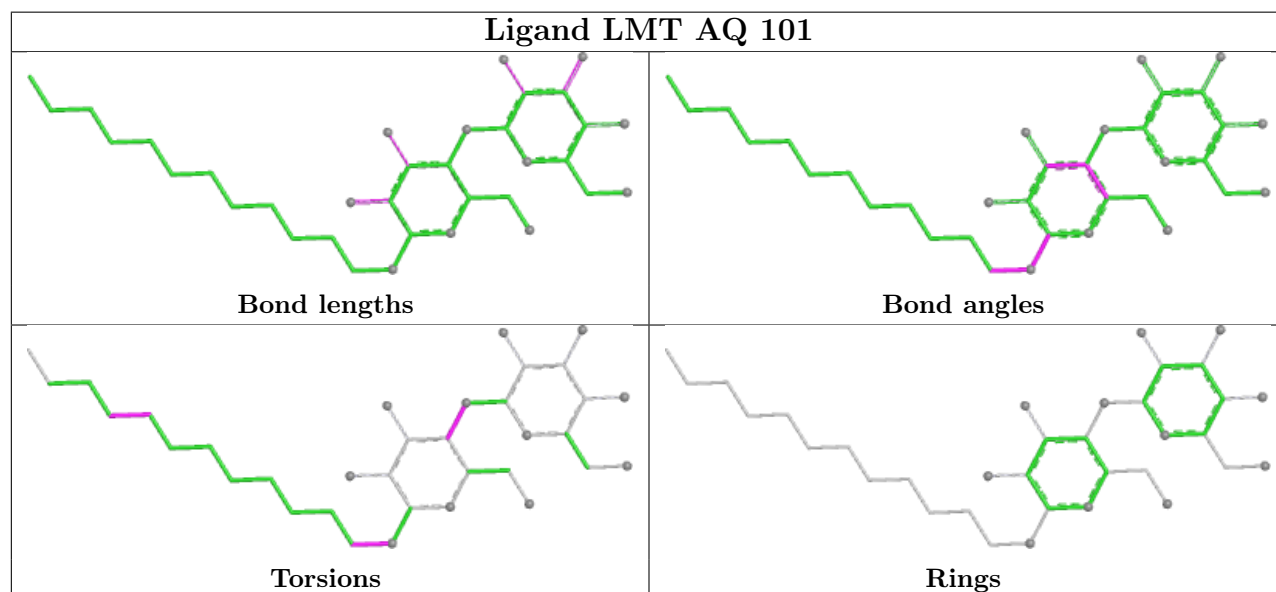
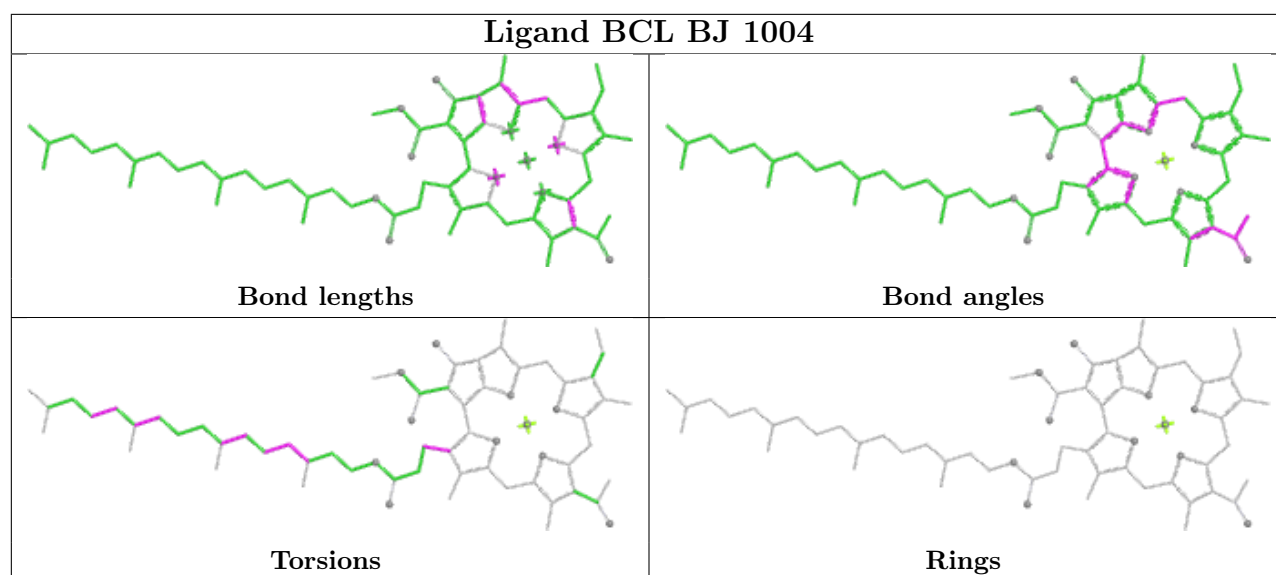


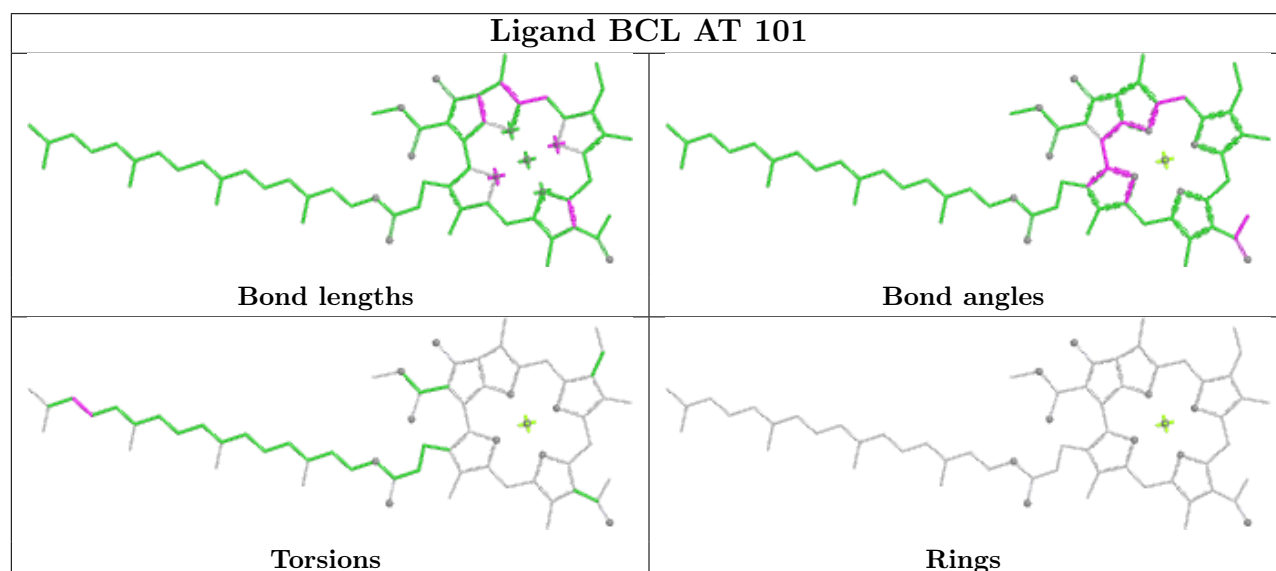
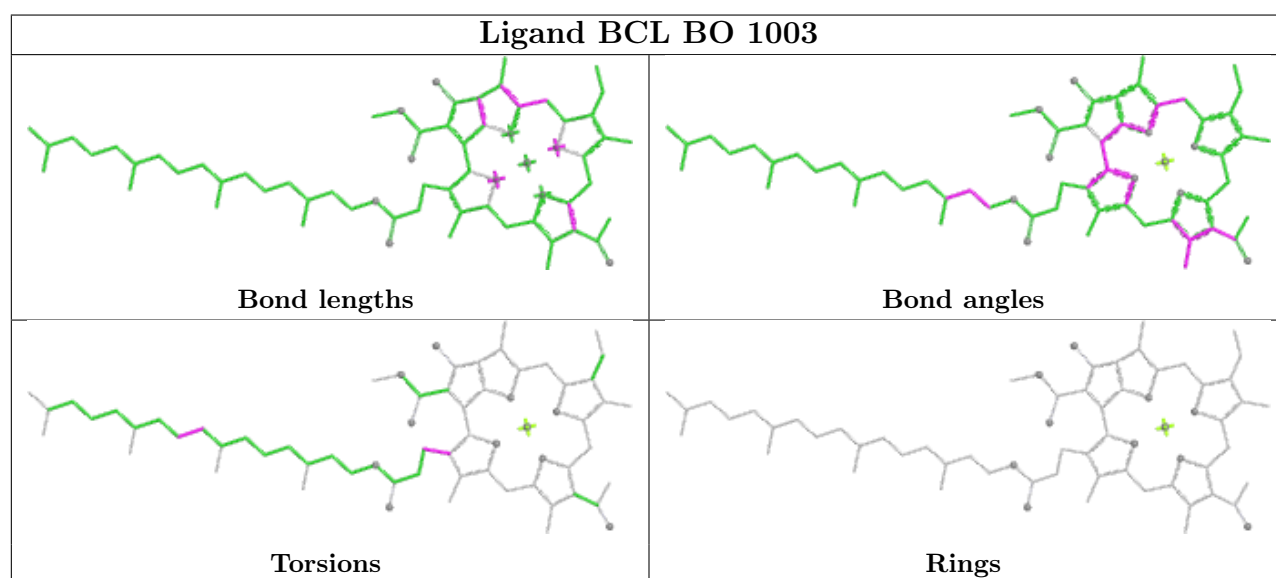
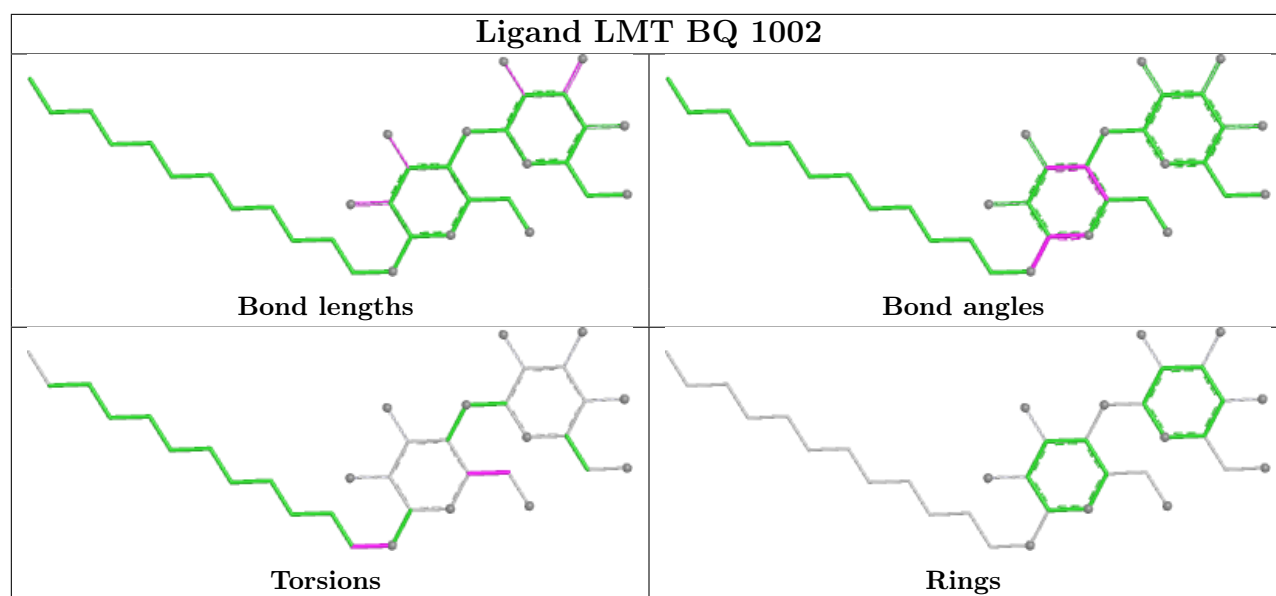


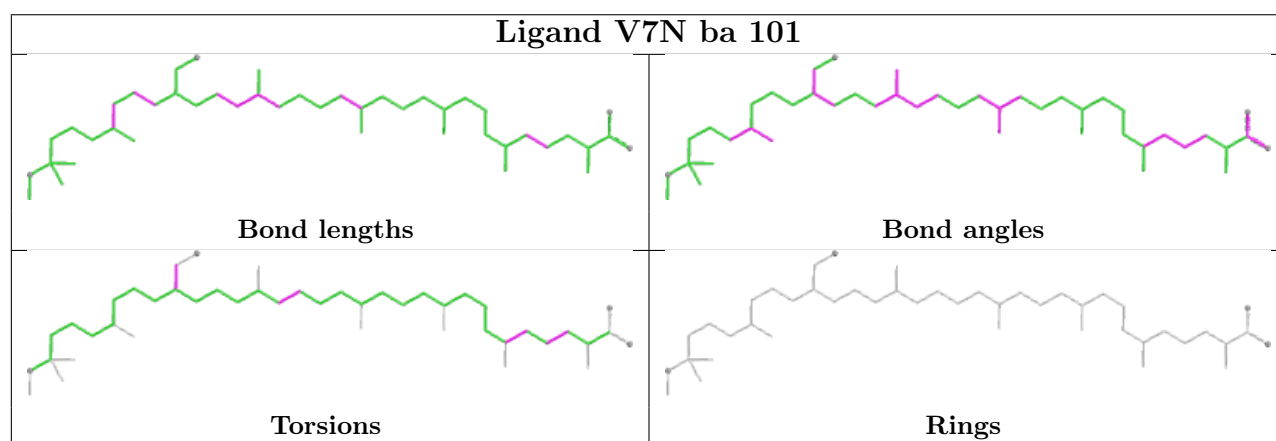
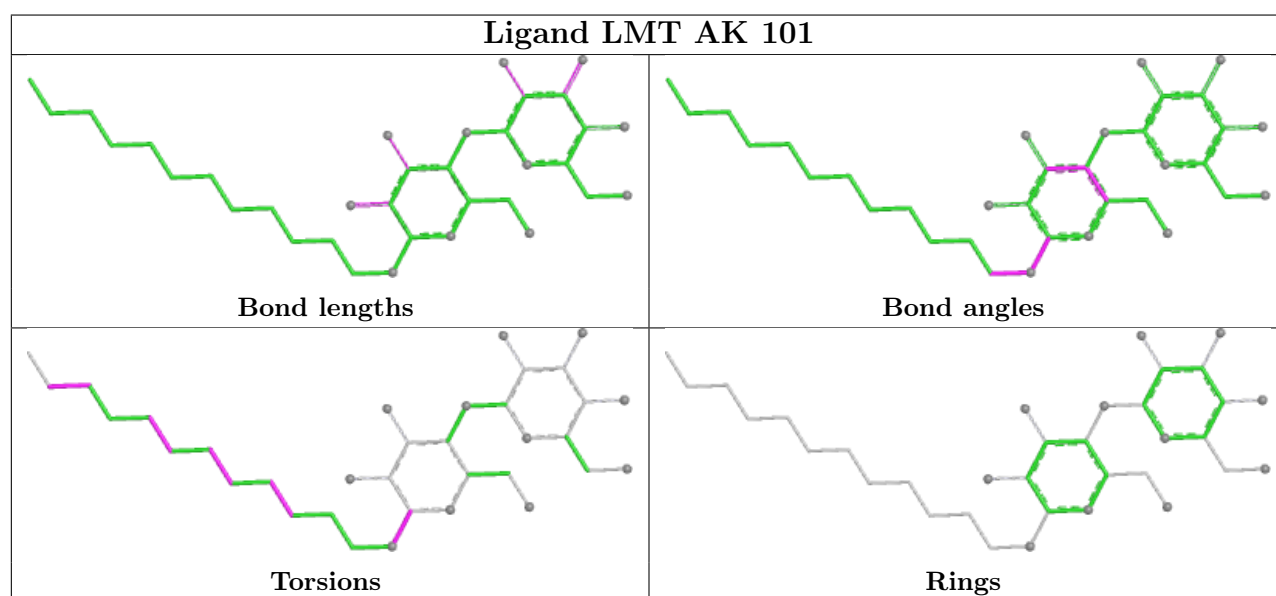
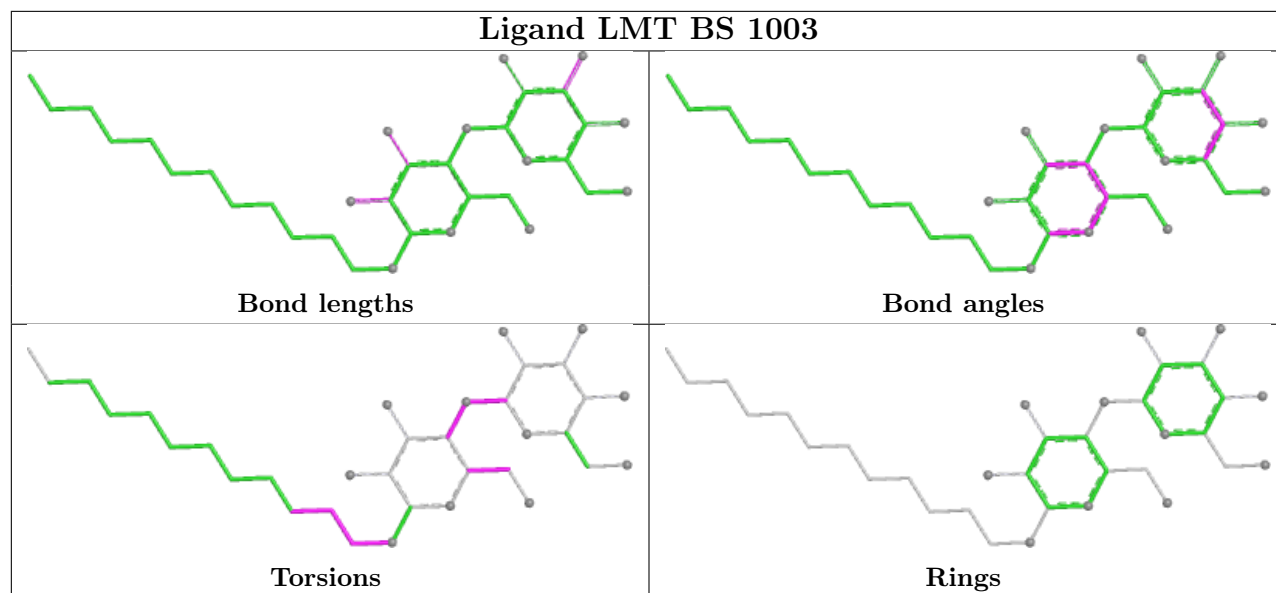


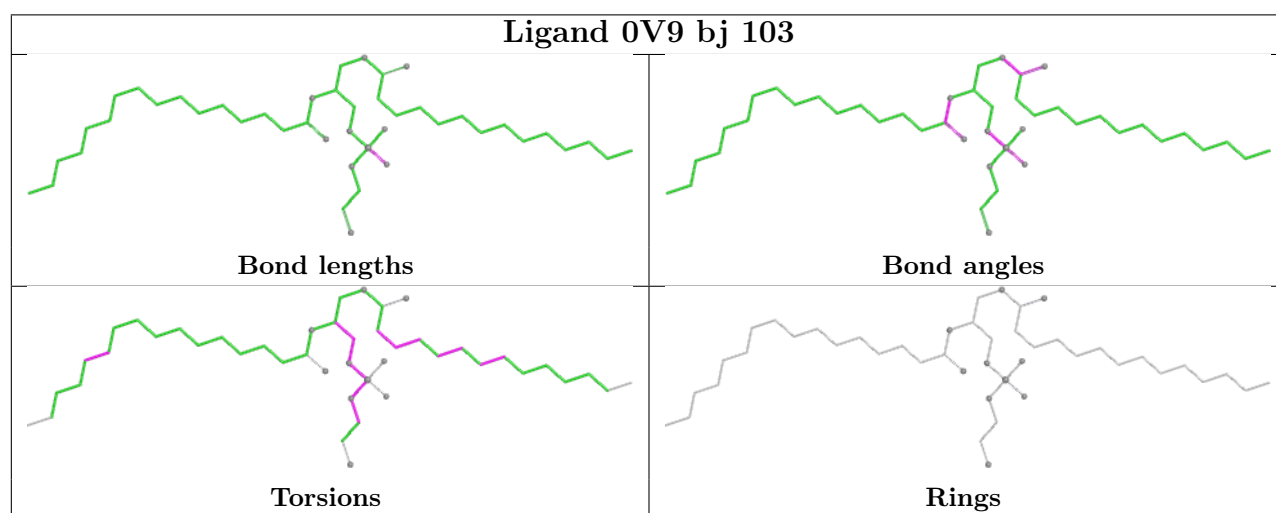
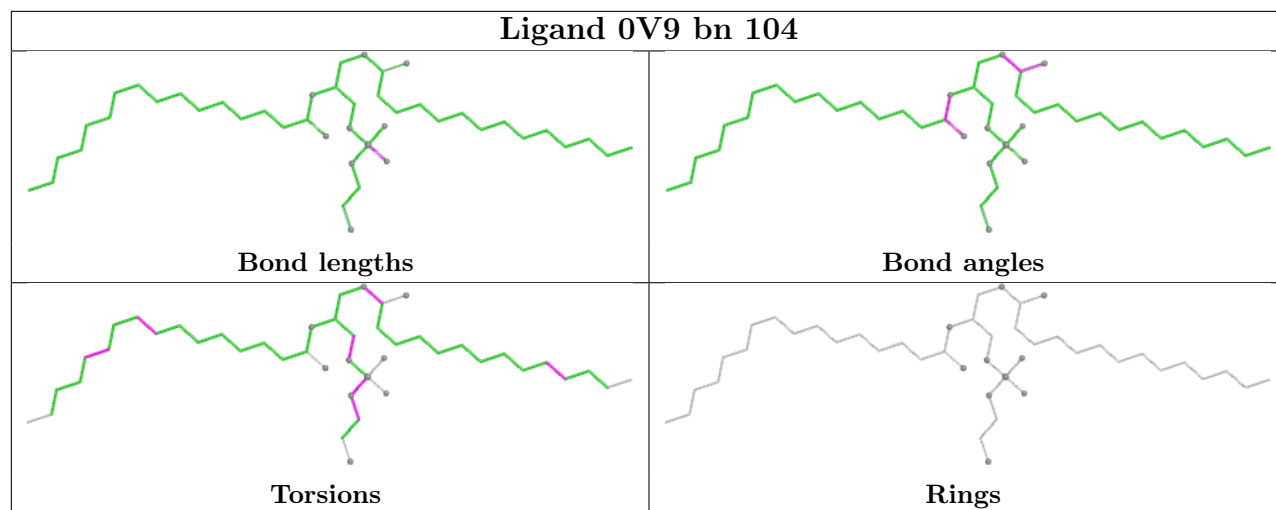




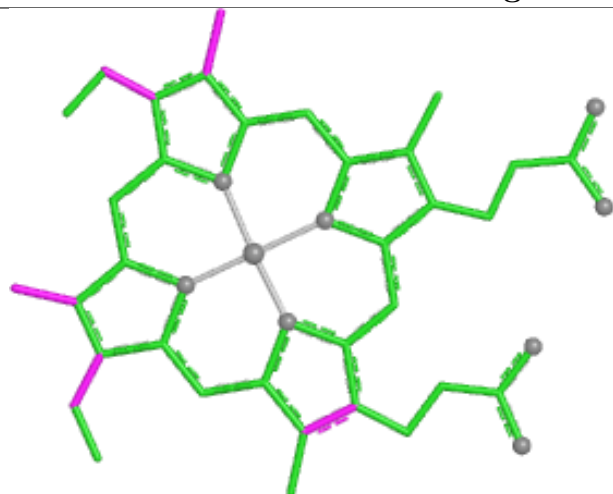




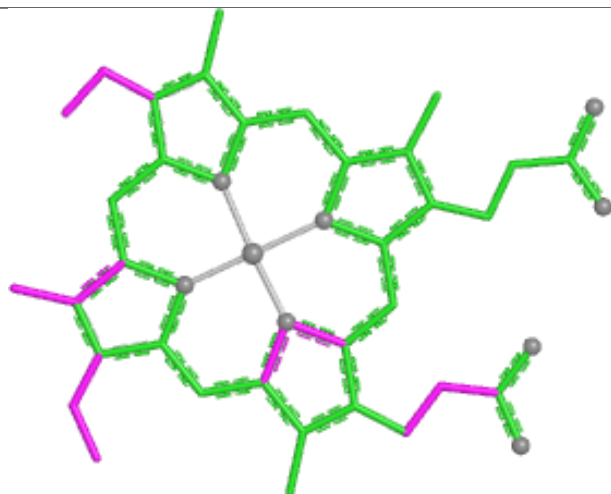




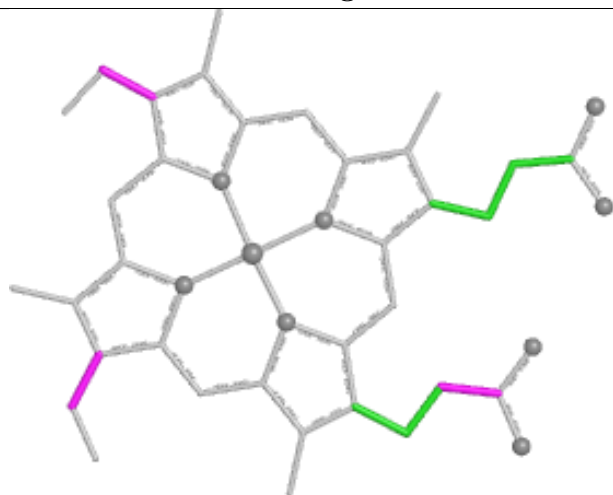
Ligand HEC C 1004



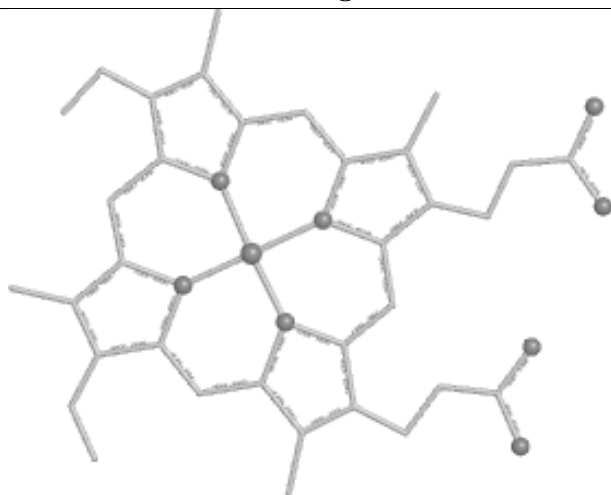
Bond lengths



Bond angles

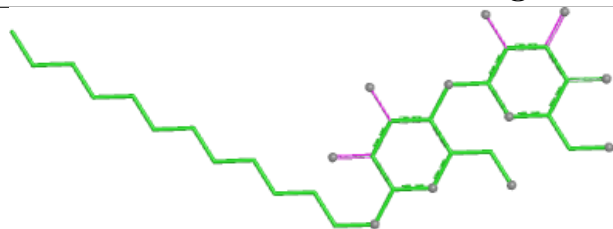


Torsions

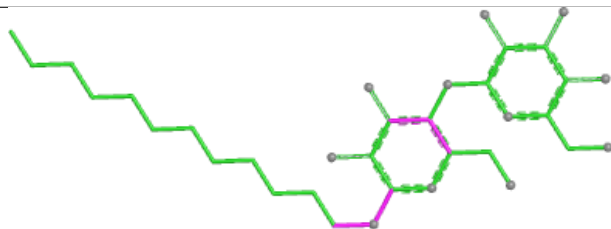


Rings

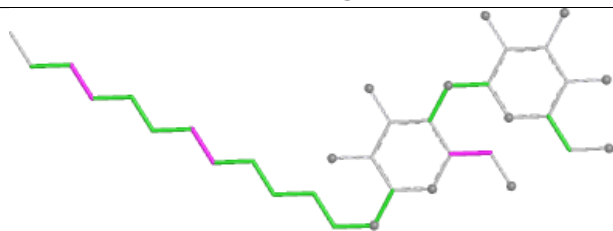
Ligand LMT bi 104



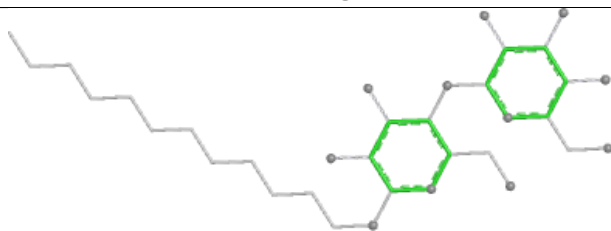
Bond lengths



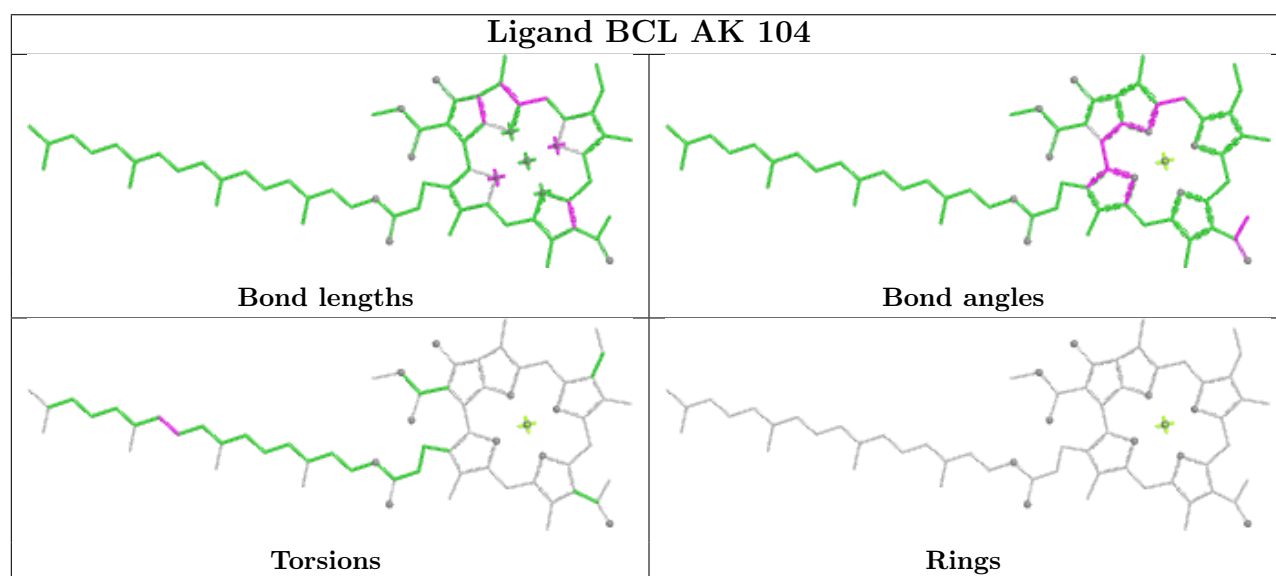
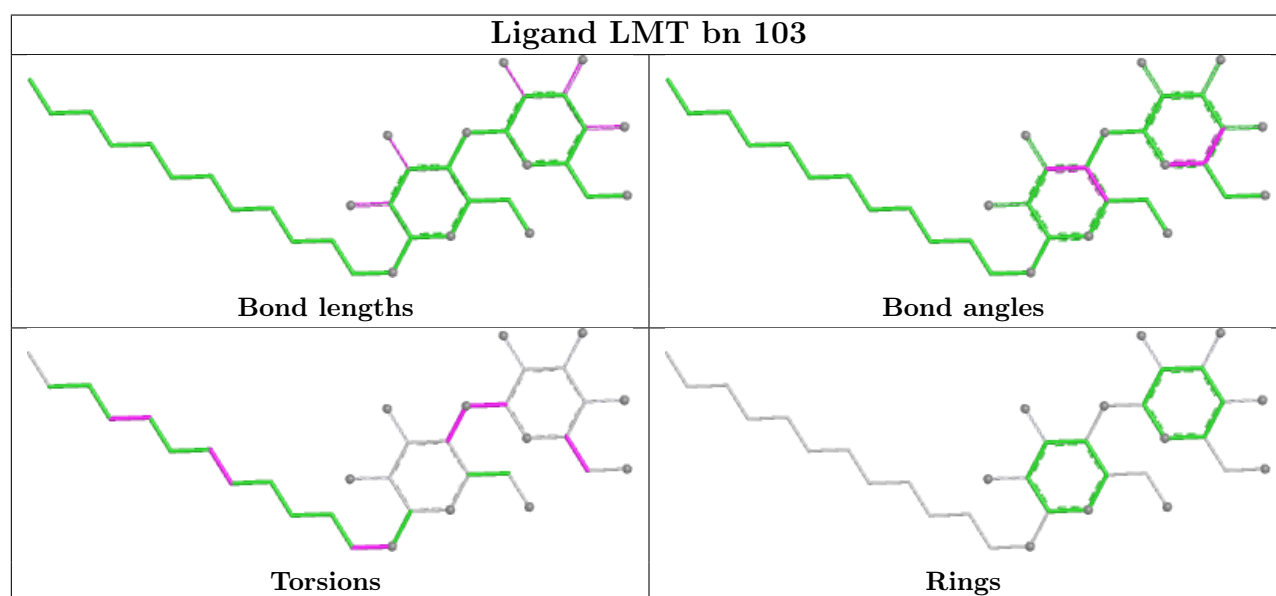
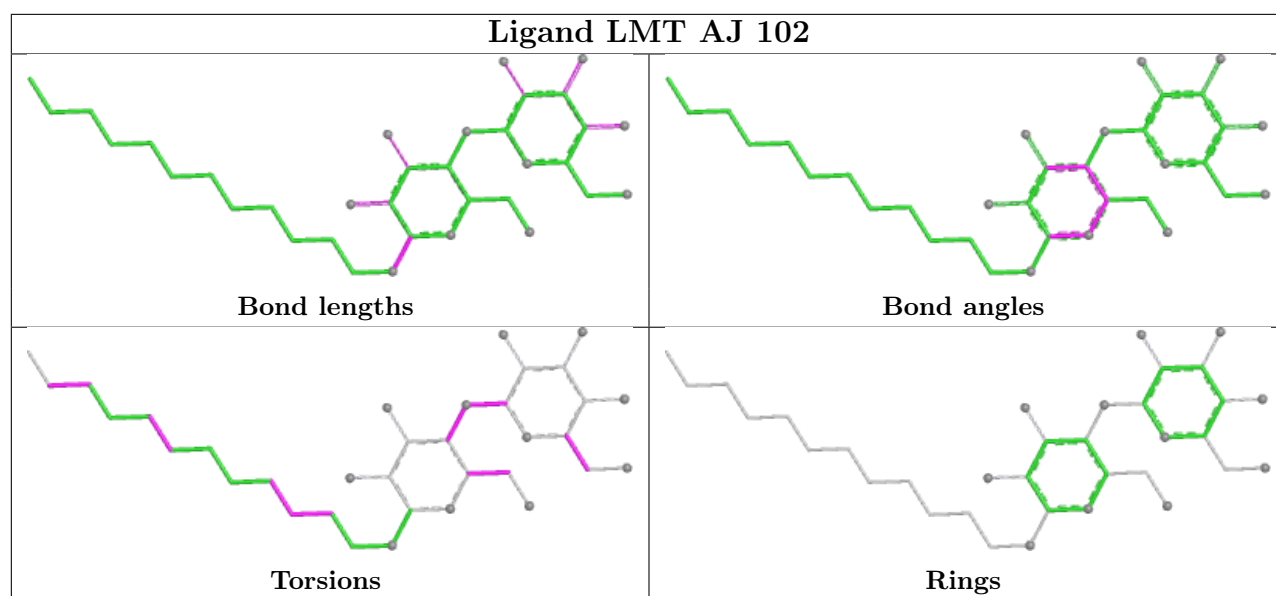
Bond angles

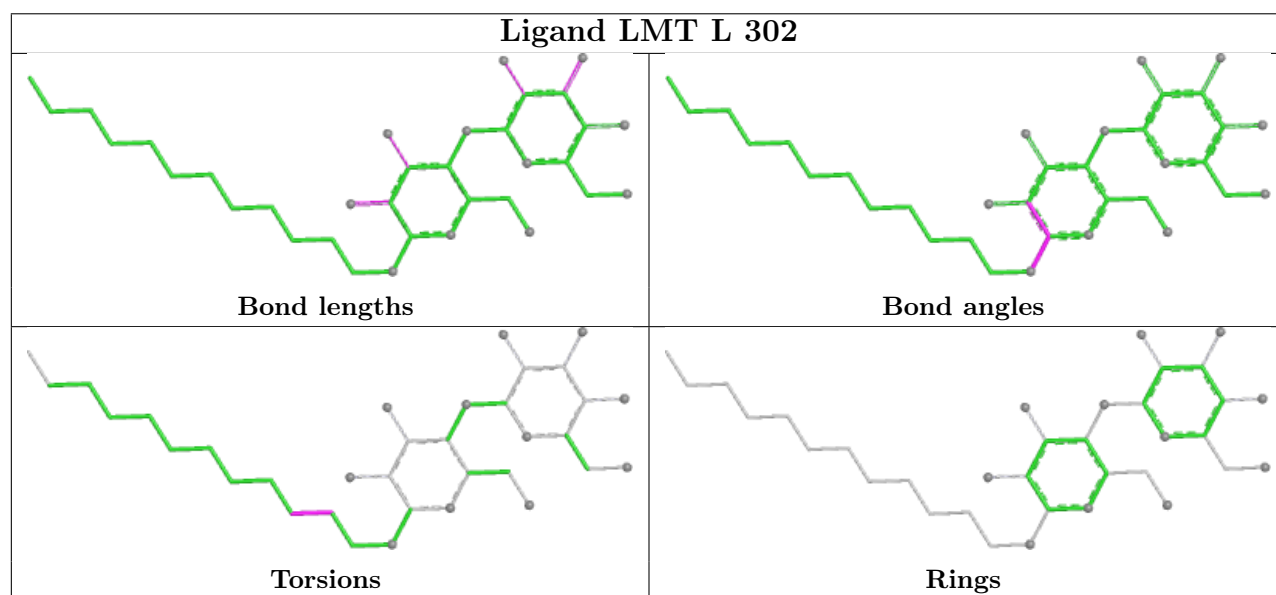
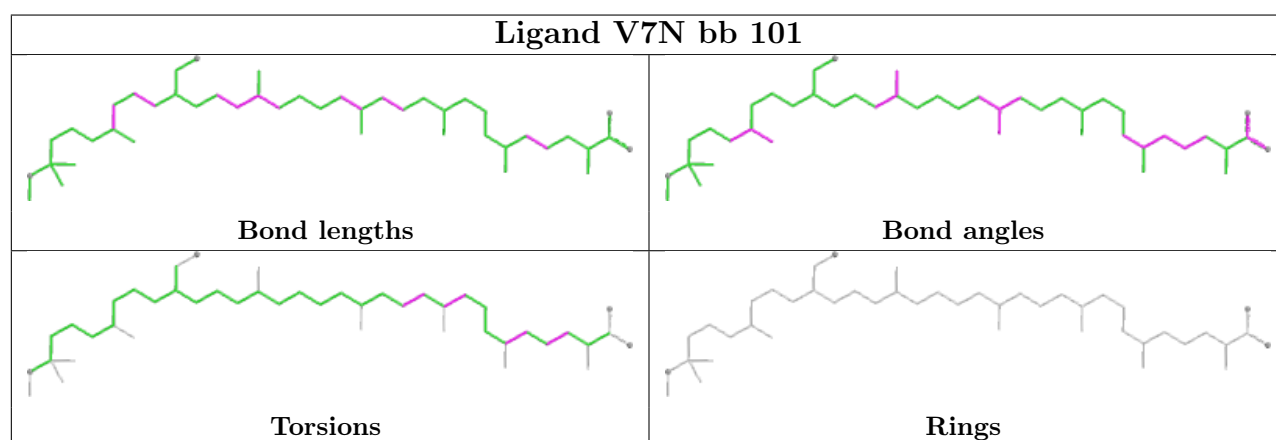
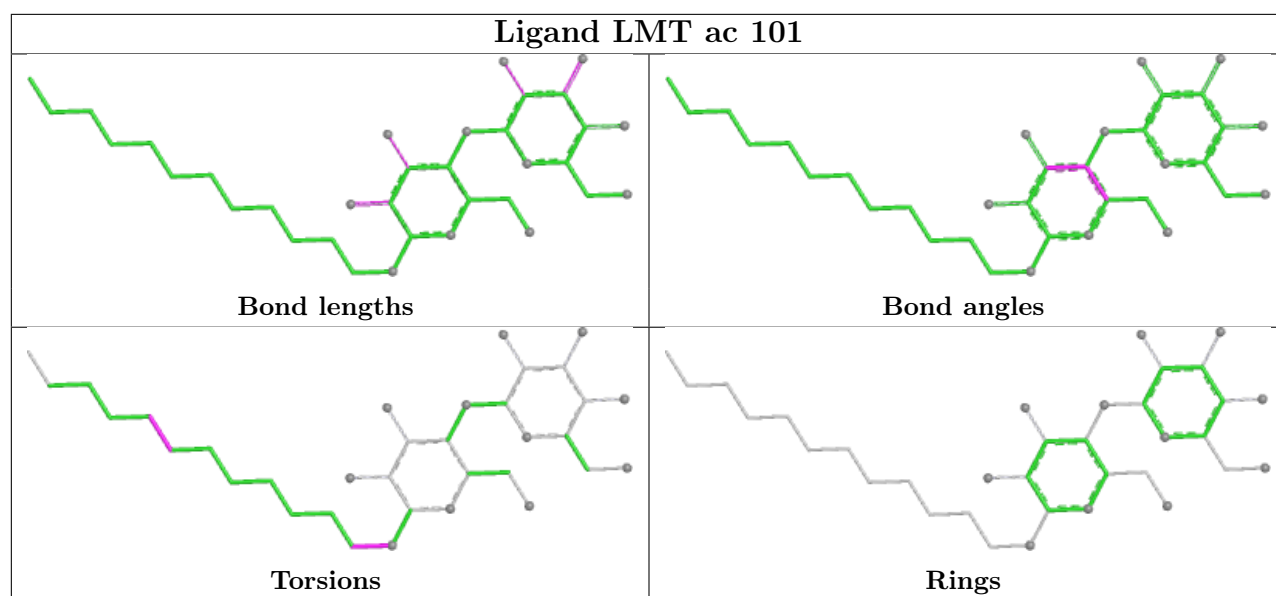


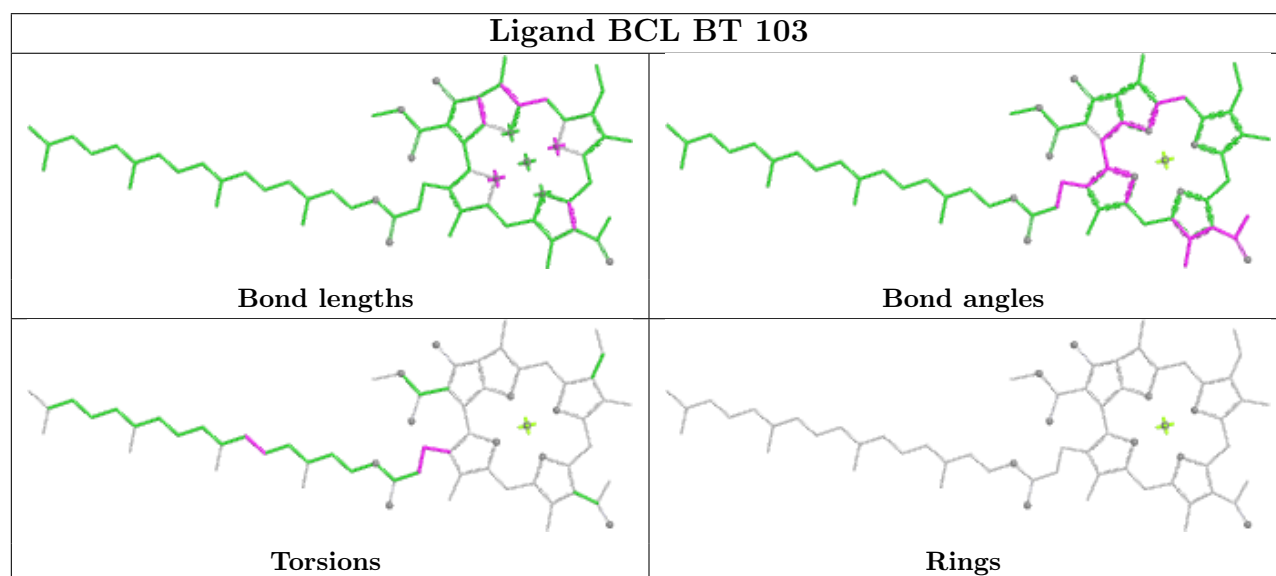
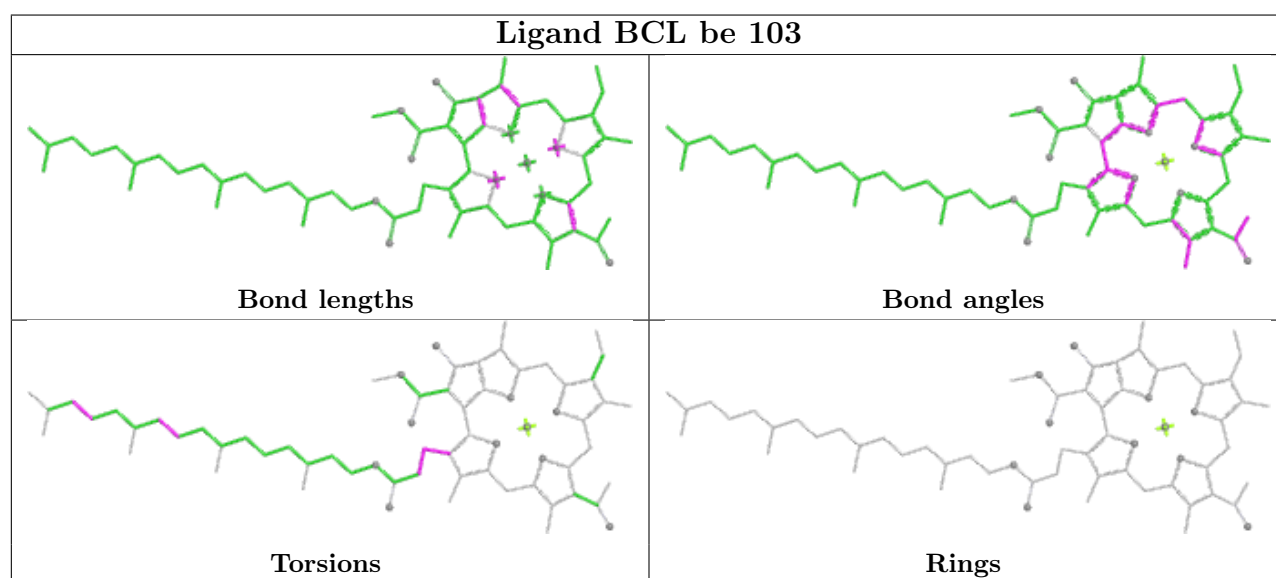
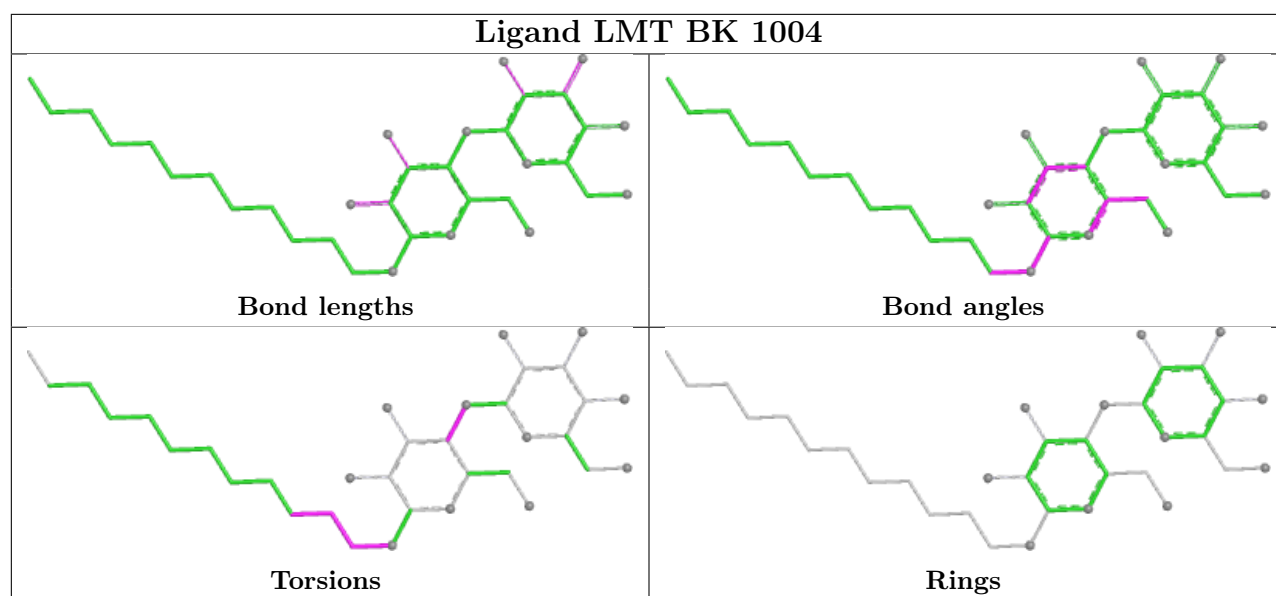
Torsions

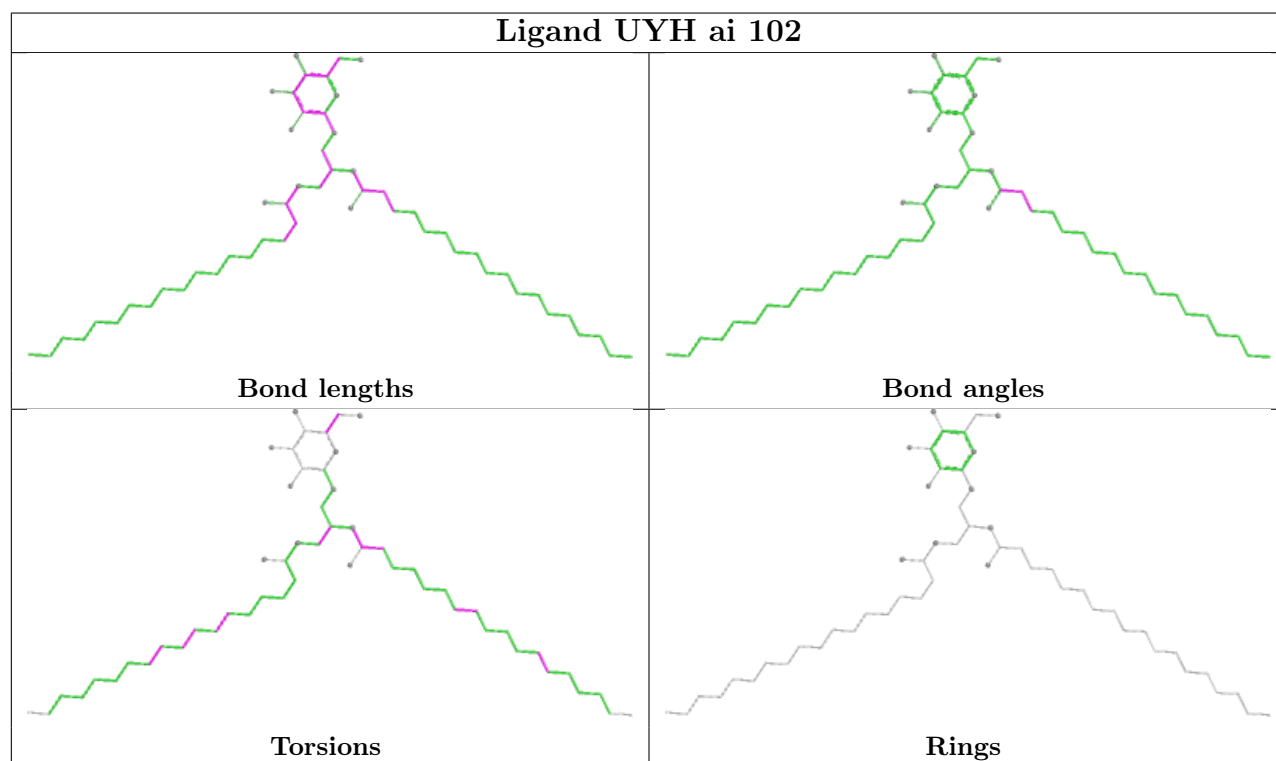
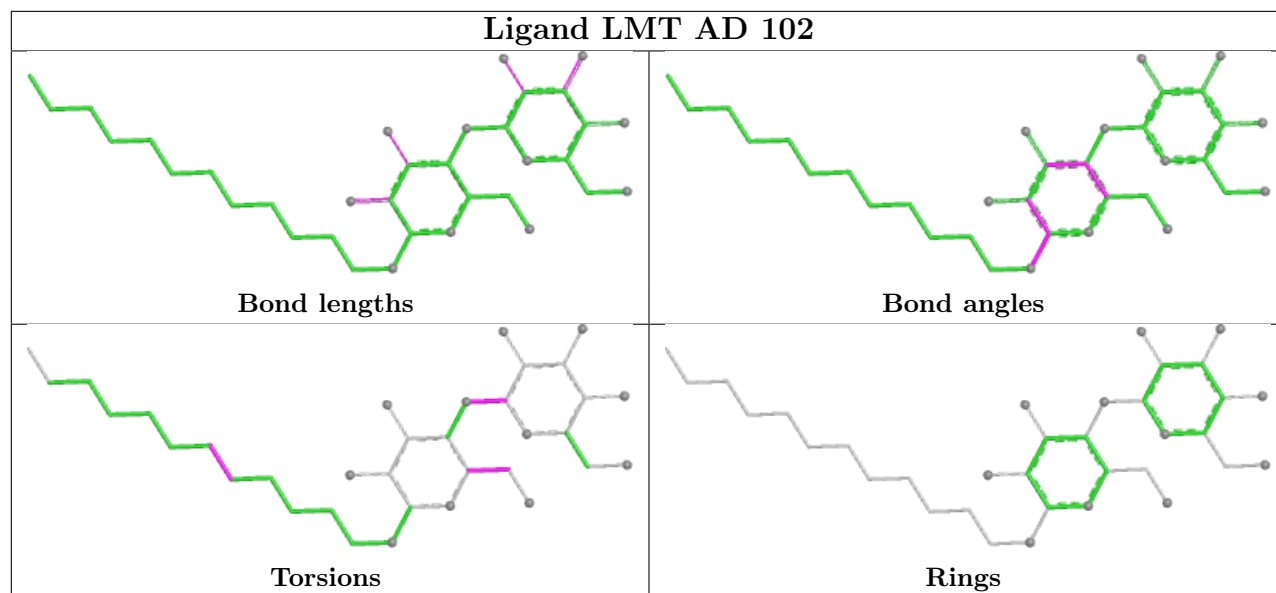


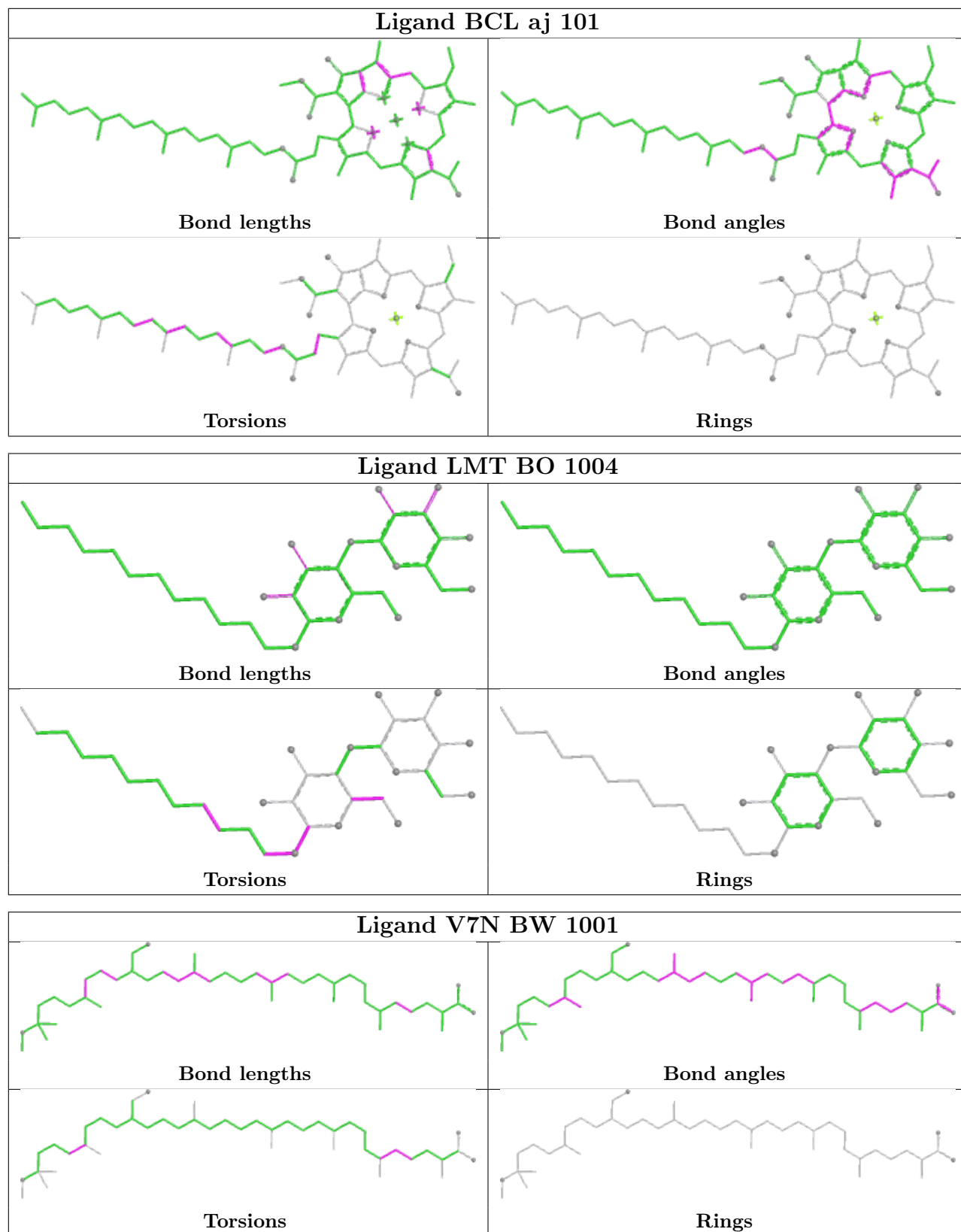
Rings

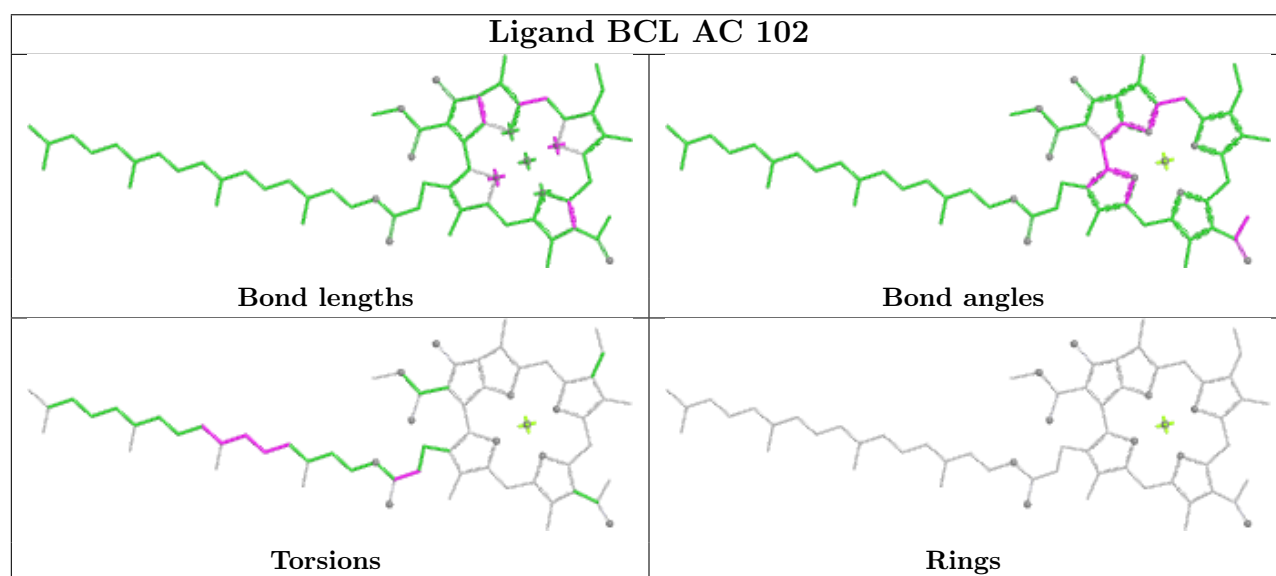
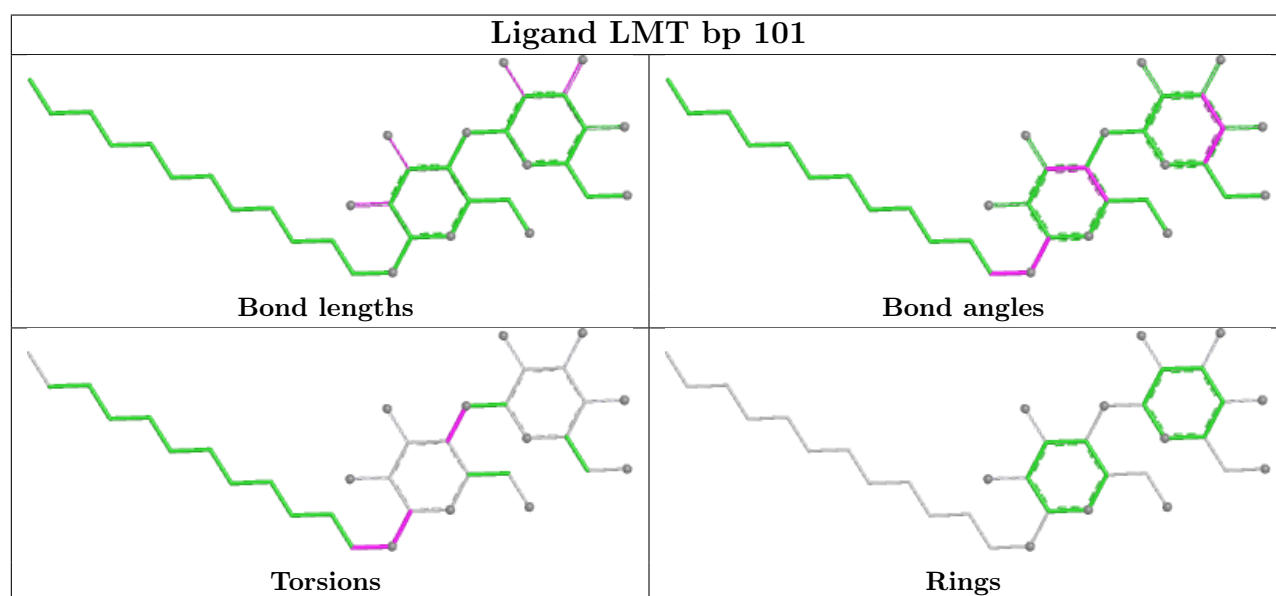
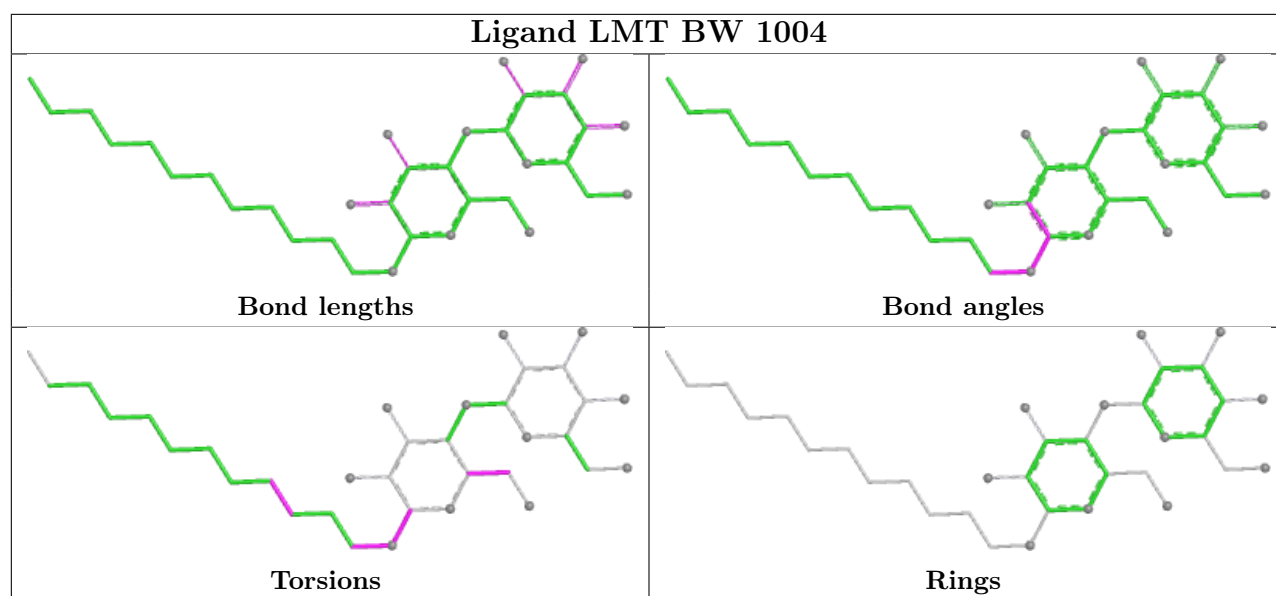


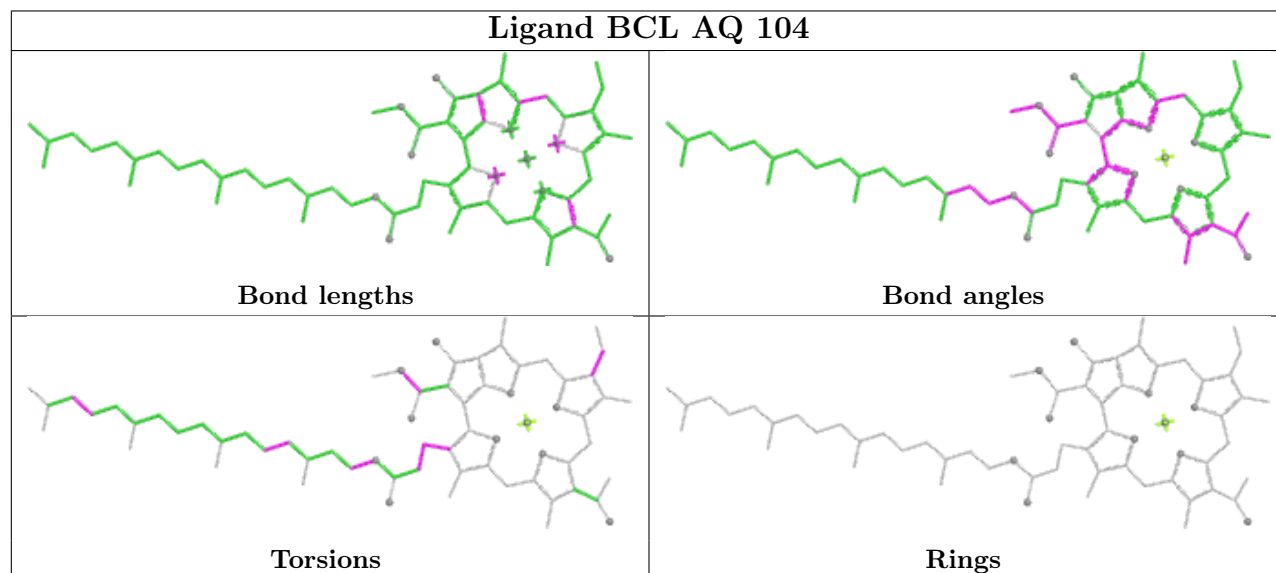
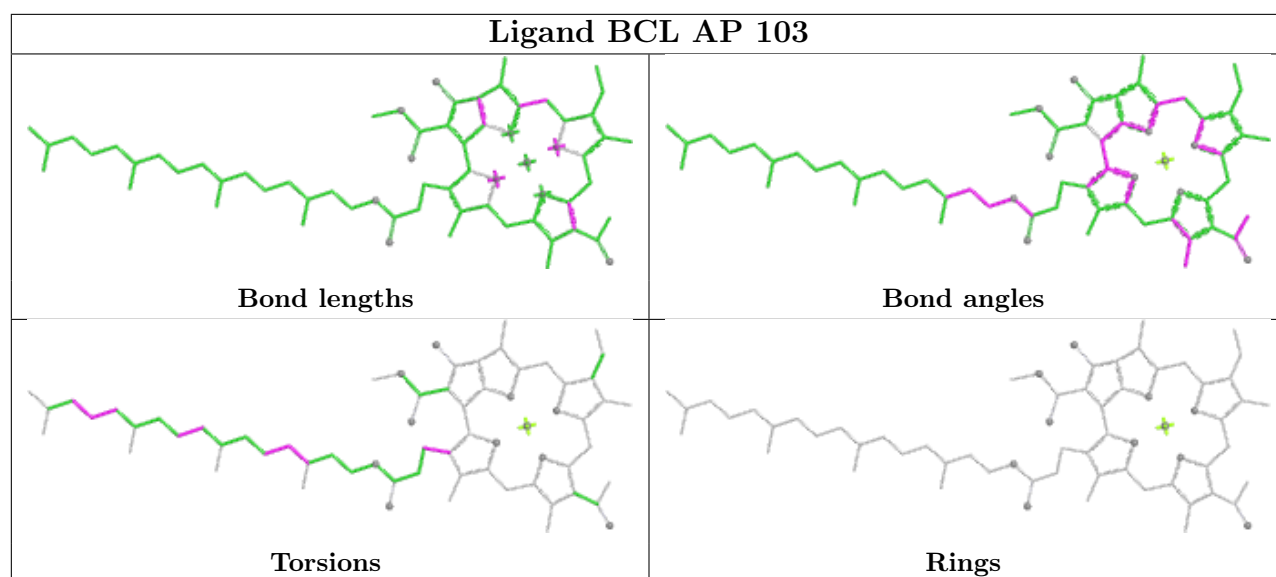




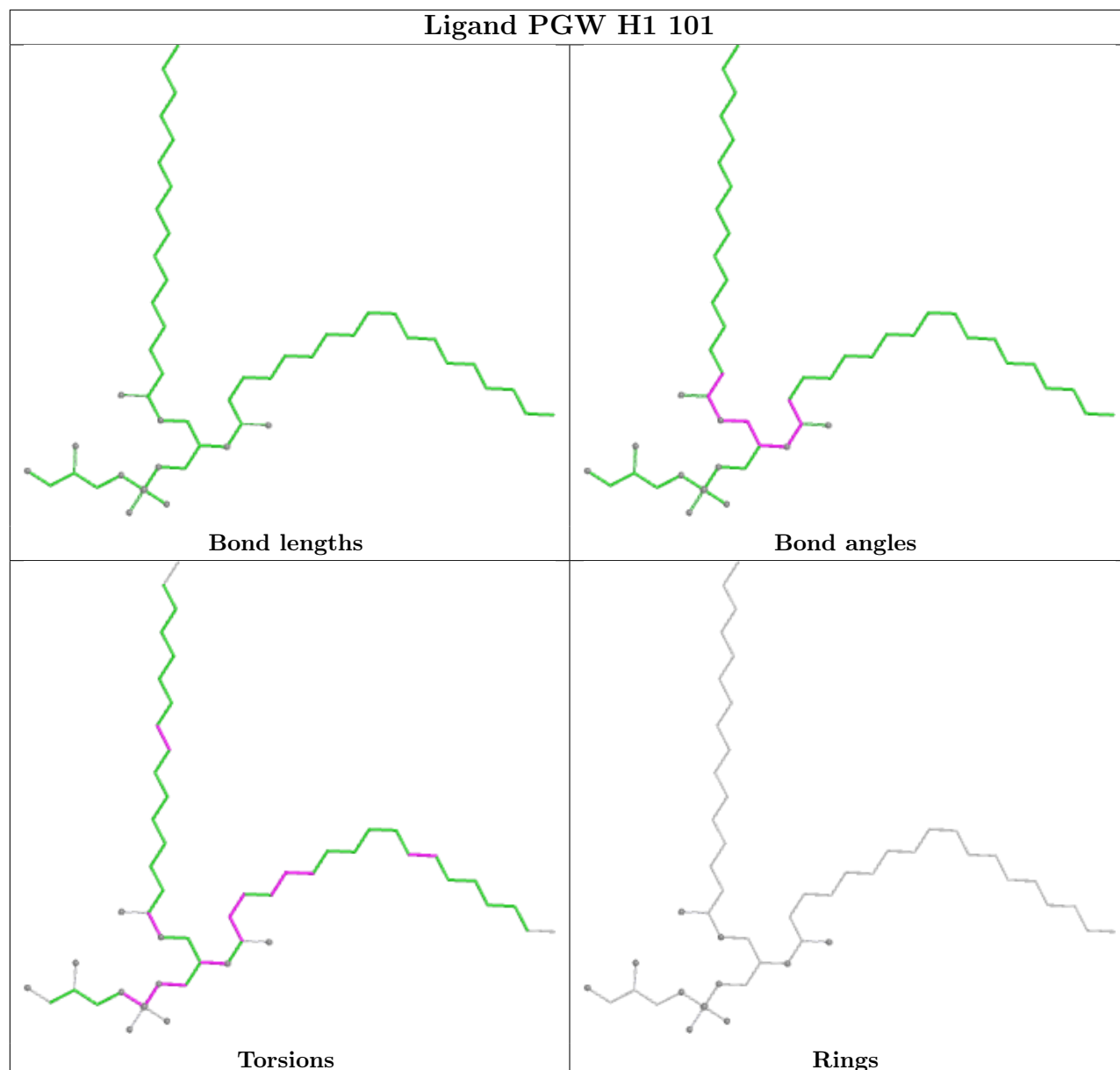




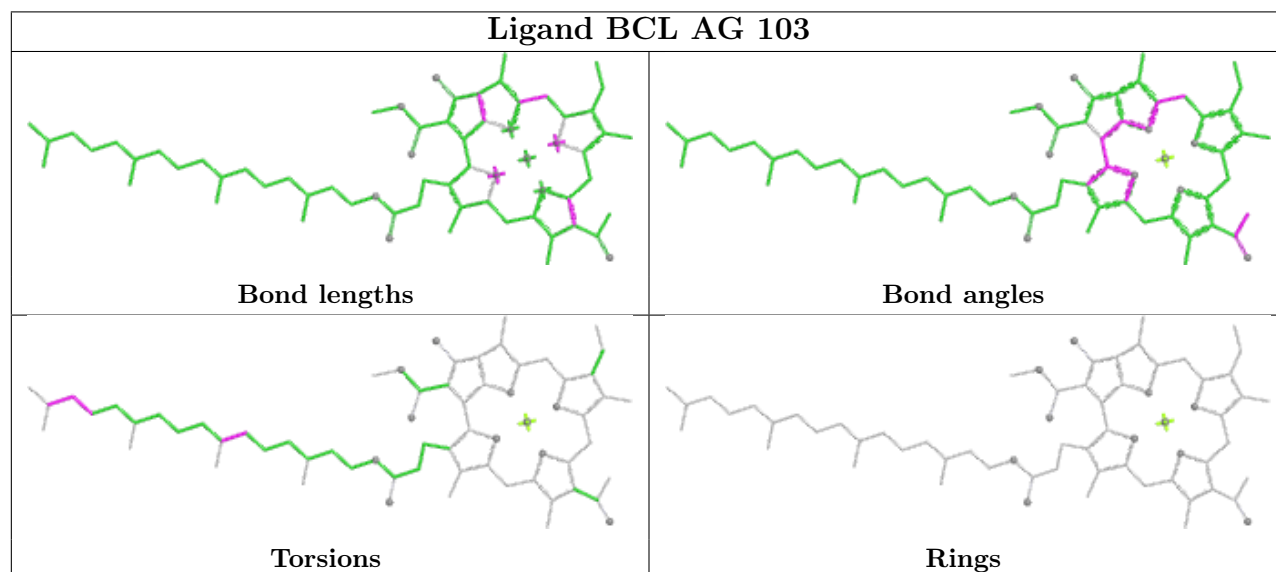


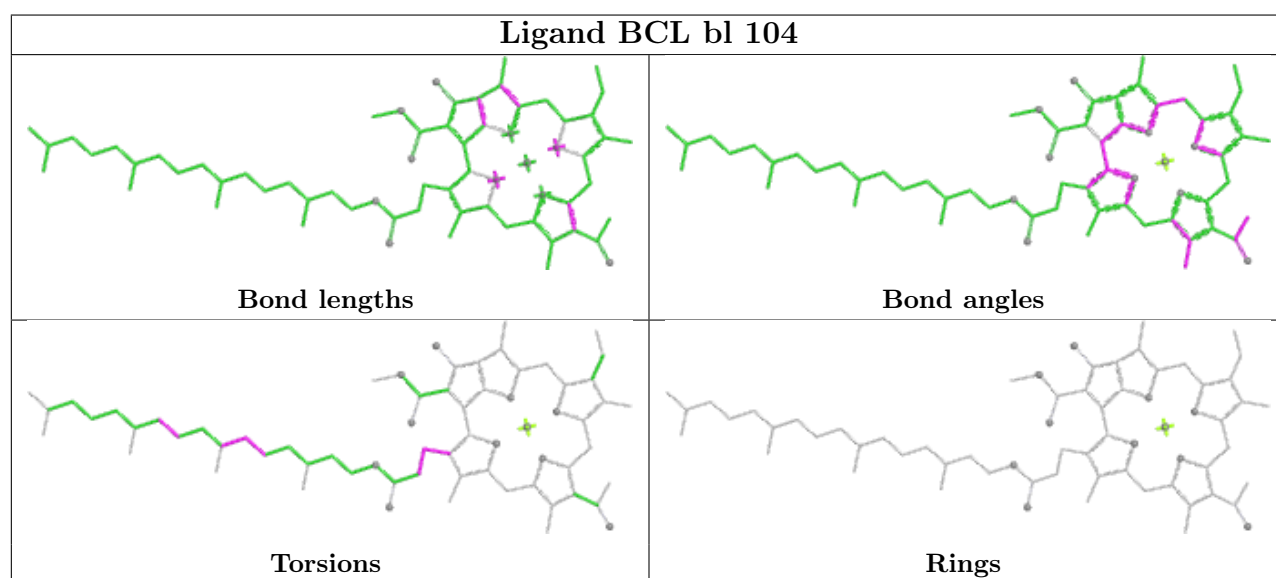
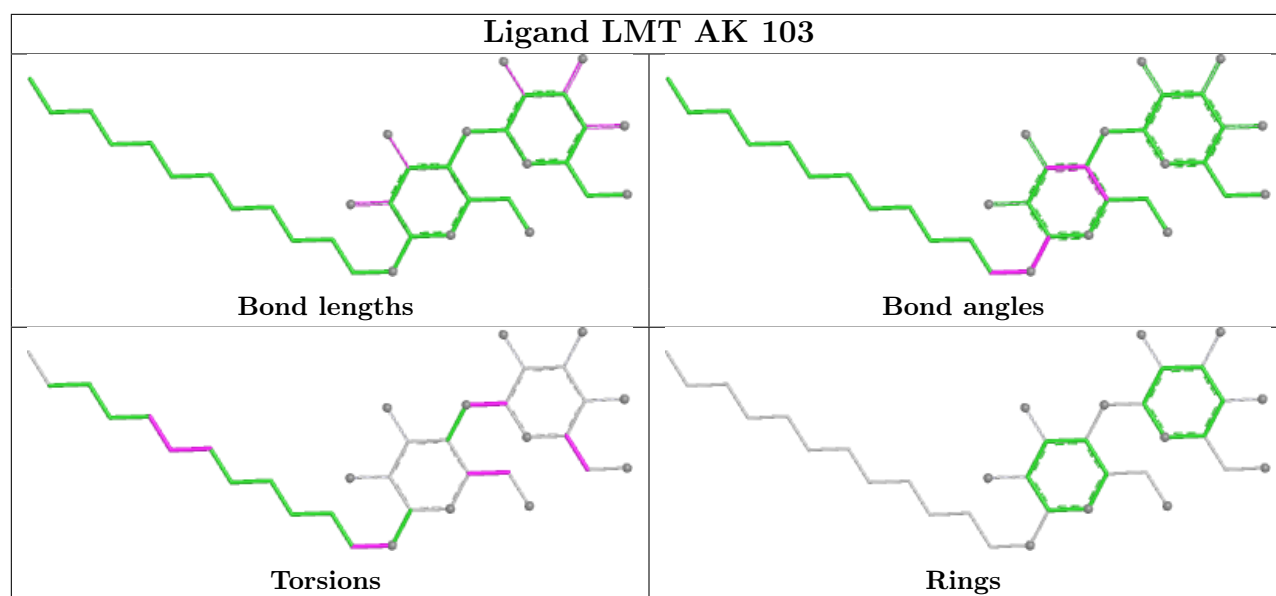


Ligand PGW H1 101

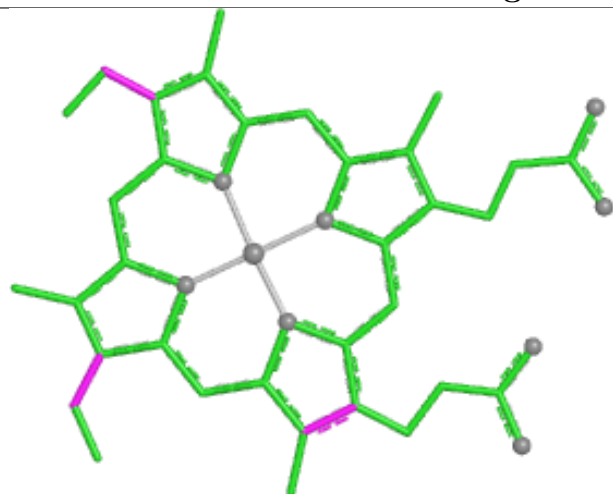


Ligand BCL AG 103

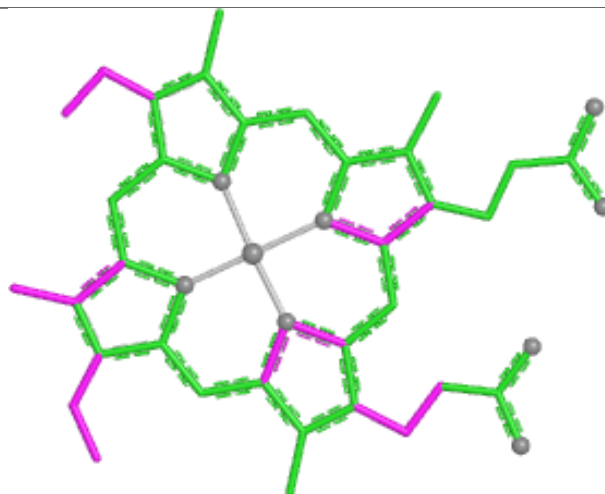




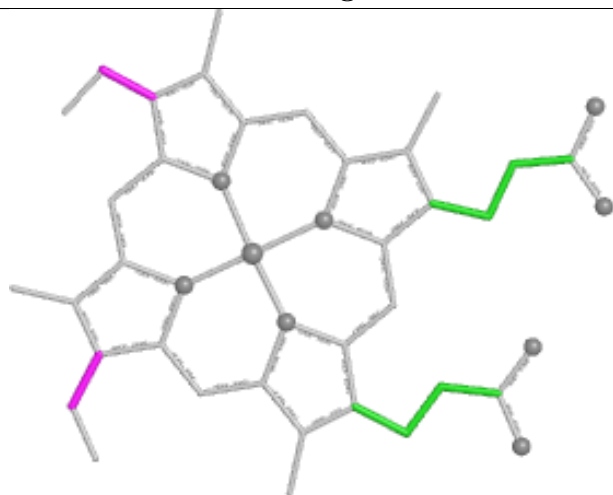
Ligand HEC C 1003



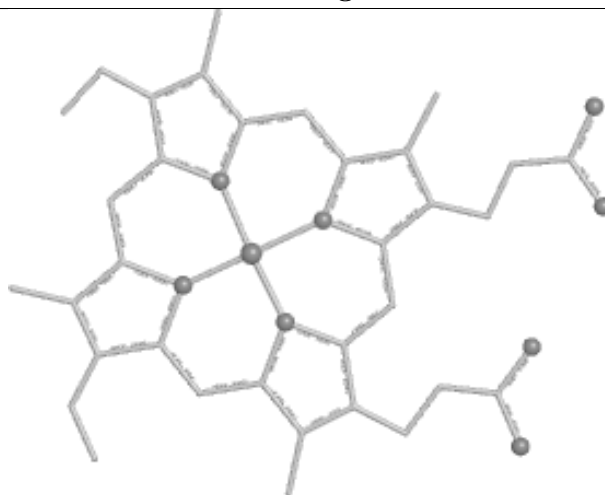
Bond lengths



Bond angles

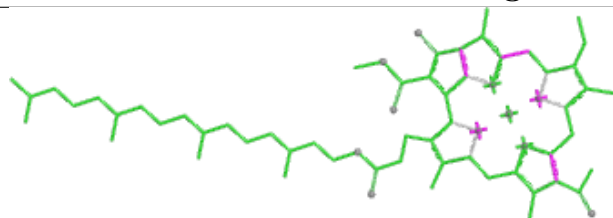


Torsions

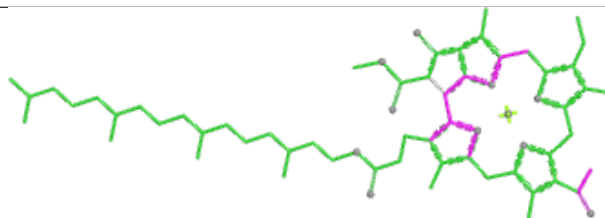


Rings

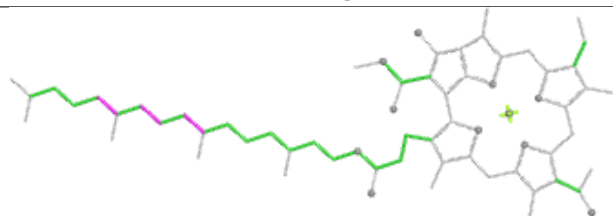
Ligand BCL AL 102



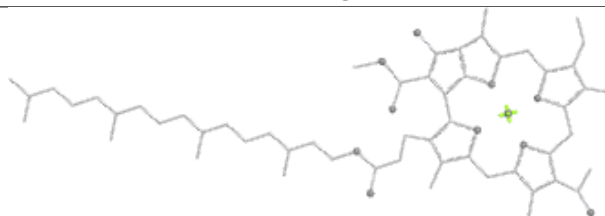
Bond lengths



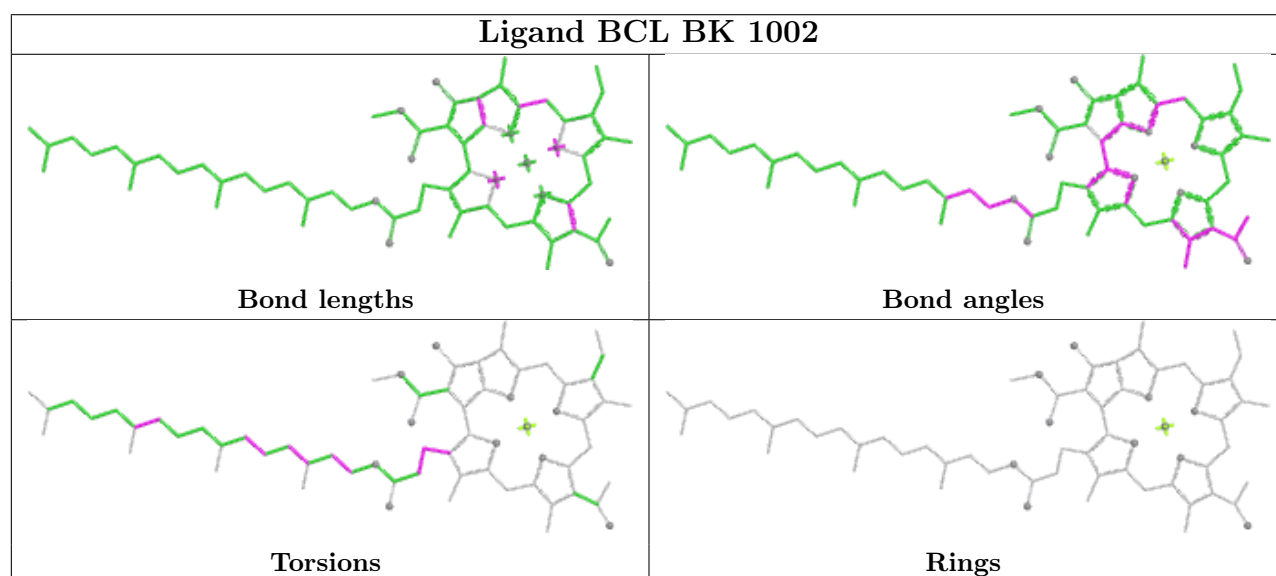
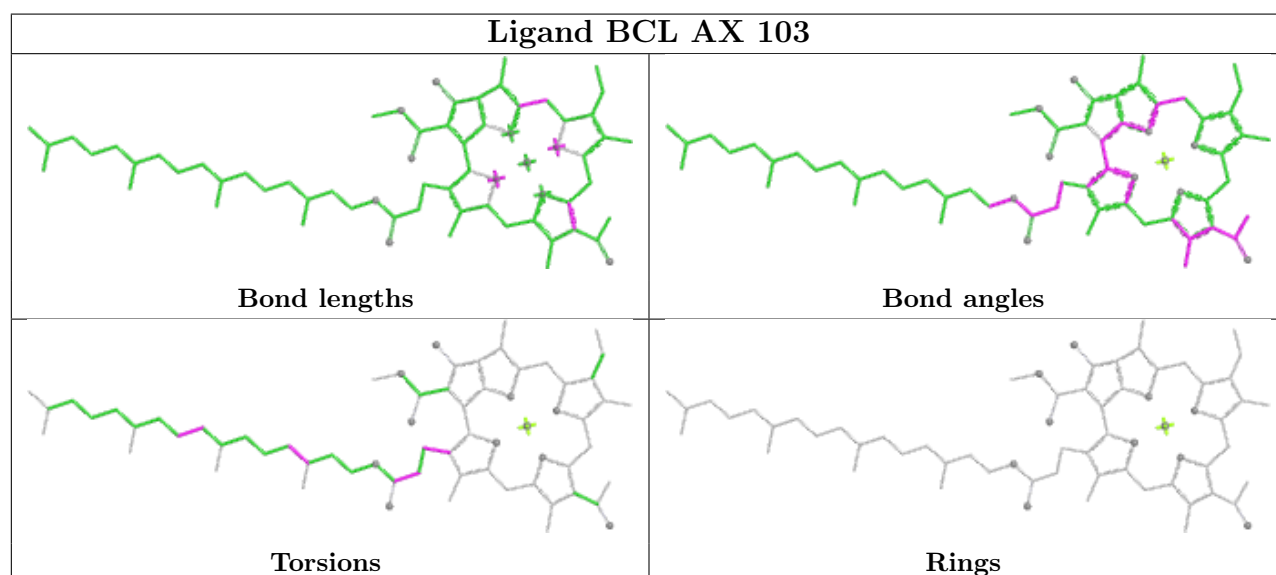
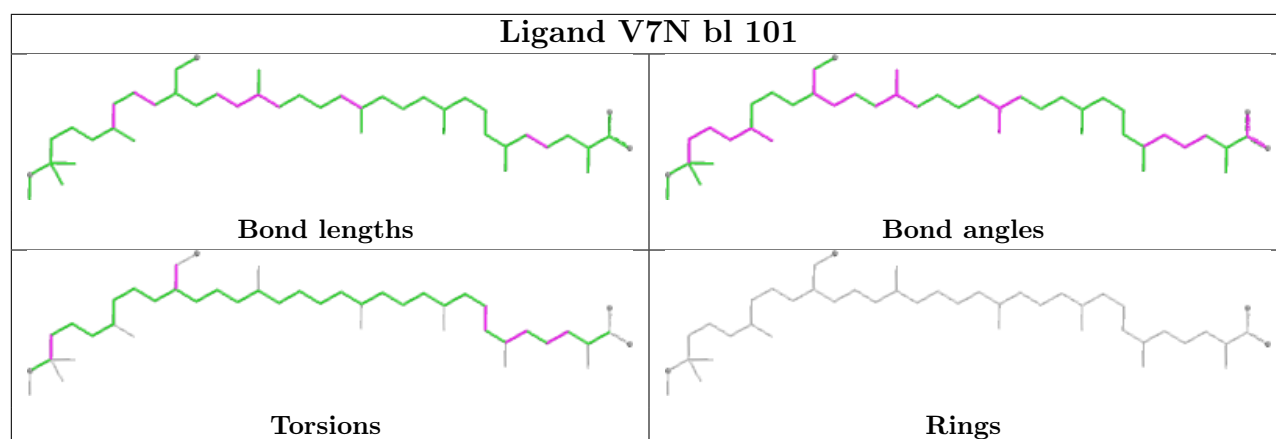
Bond angles

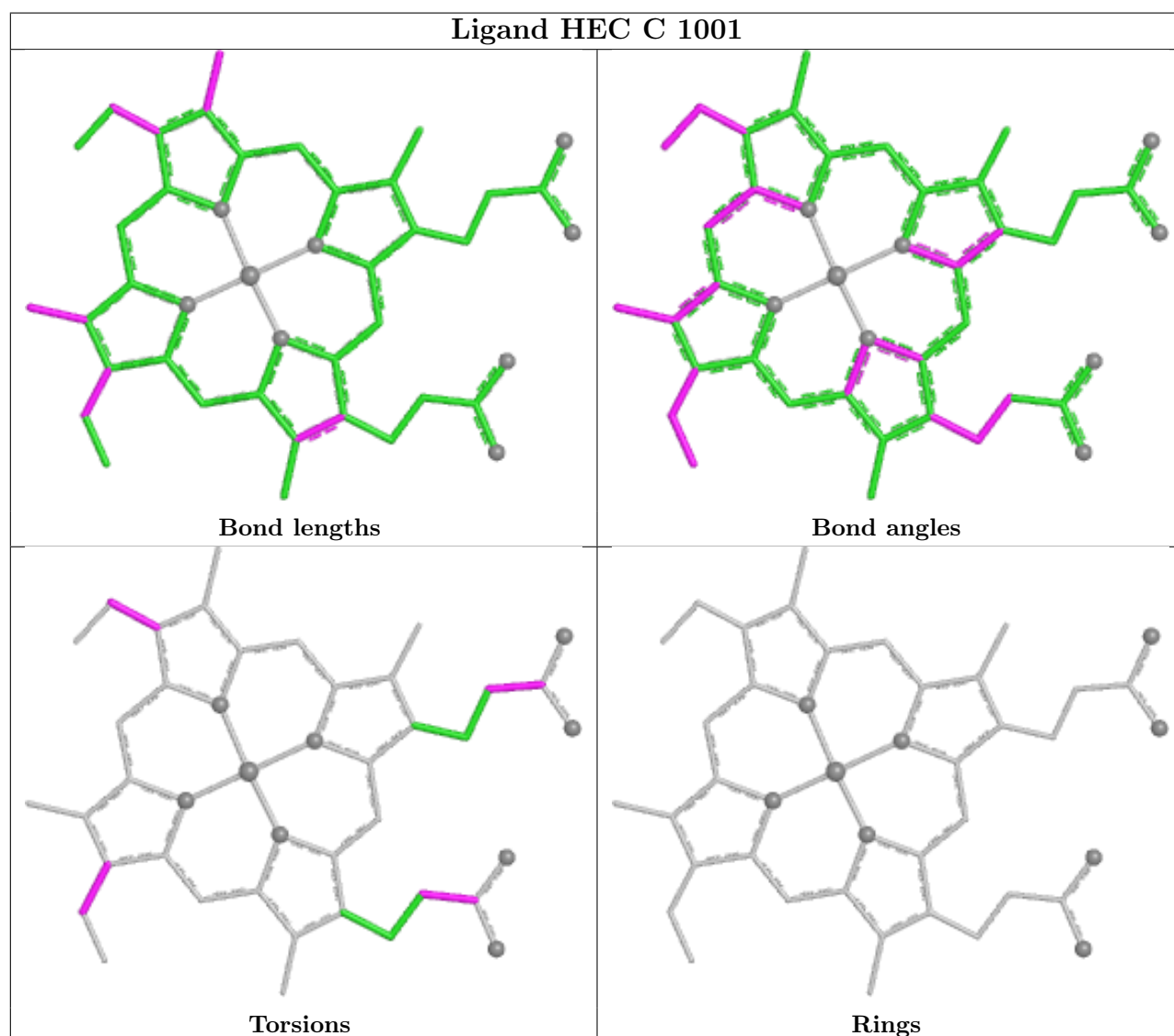
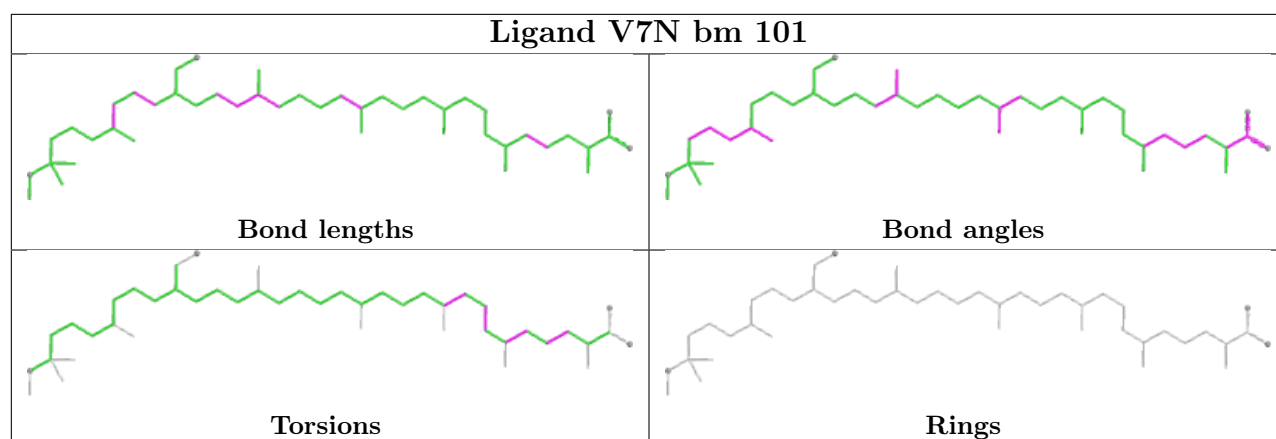


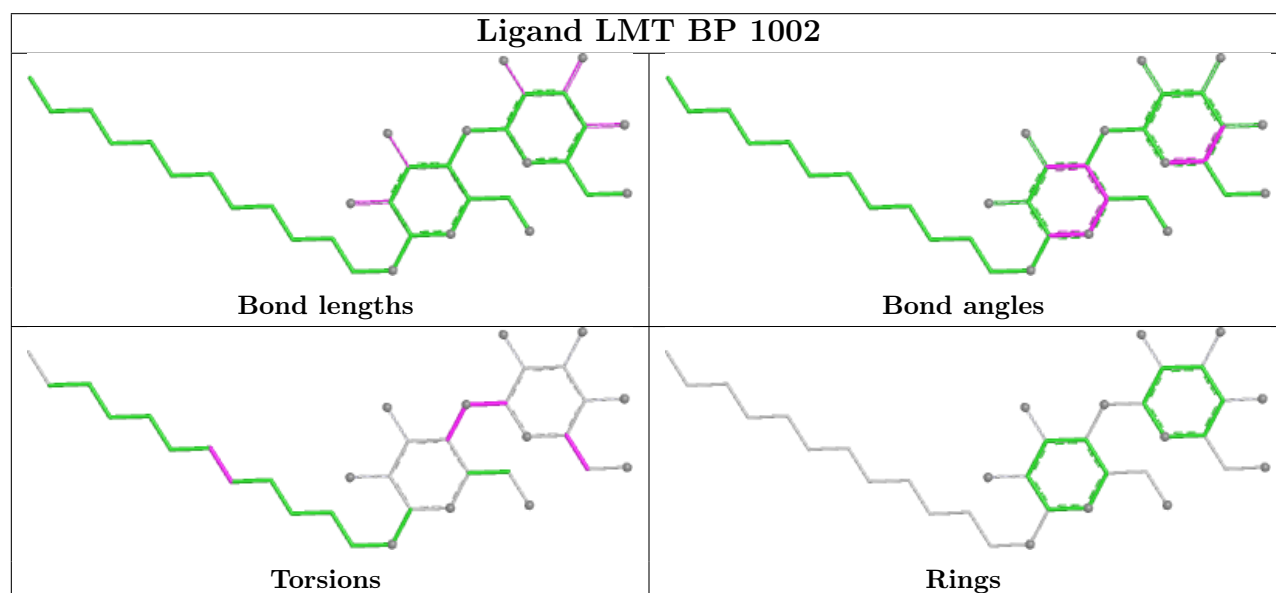
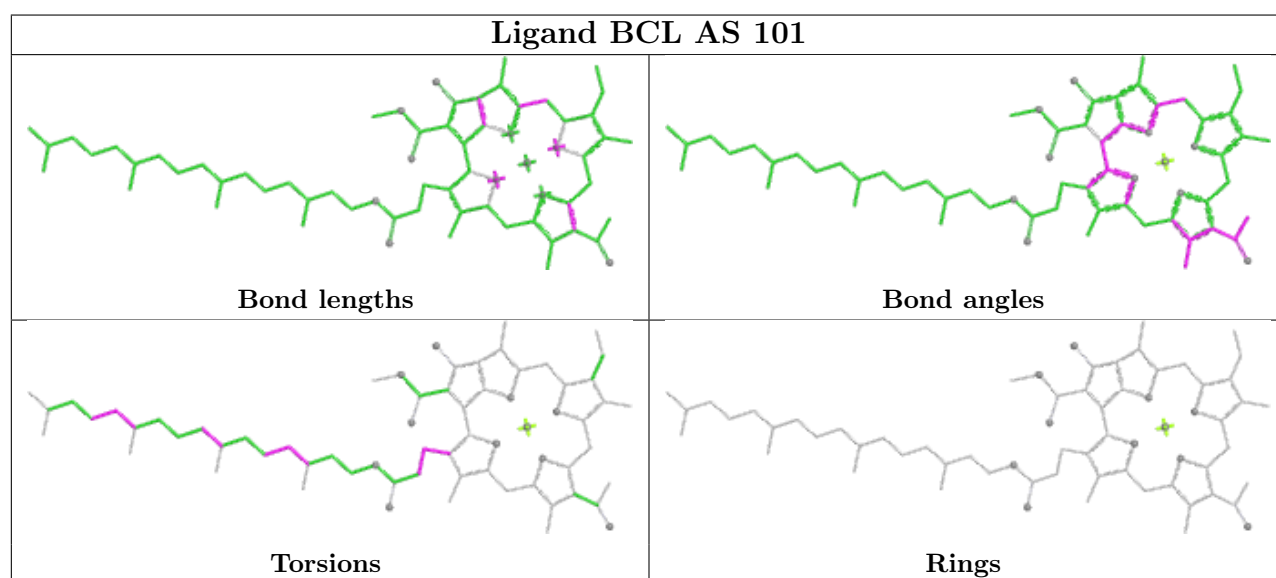
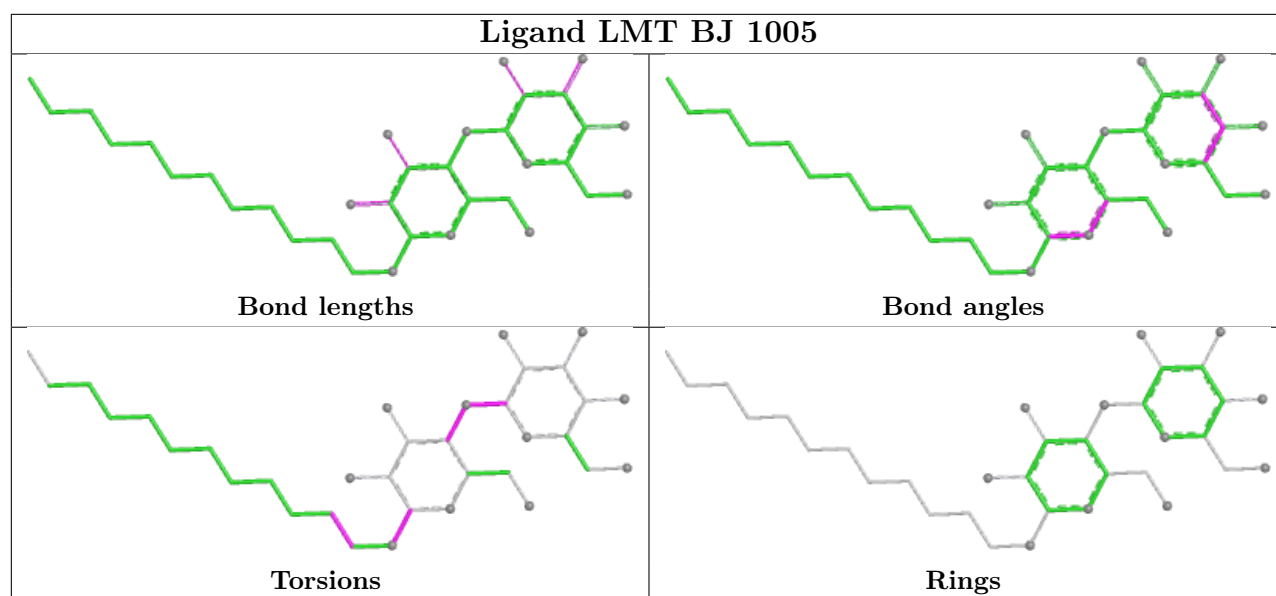
Torsions

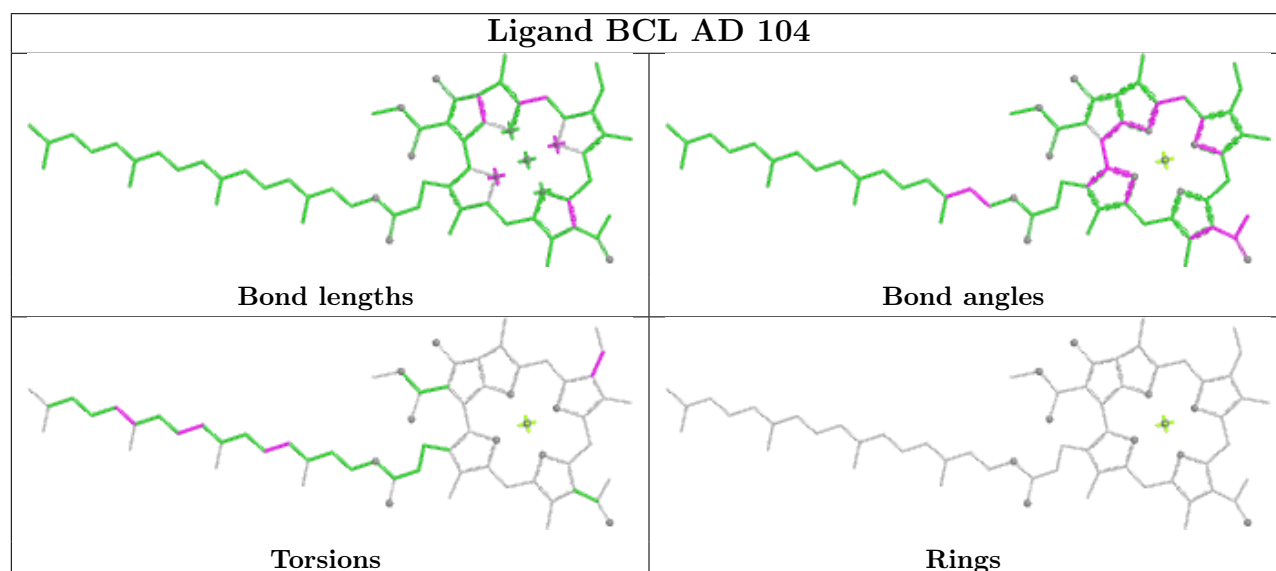
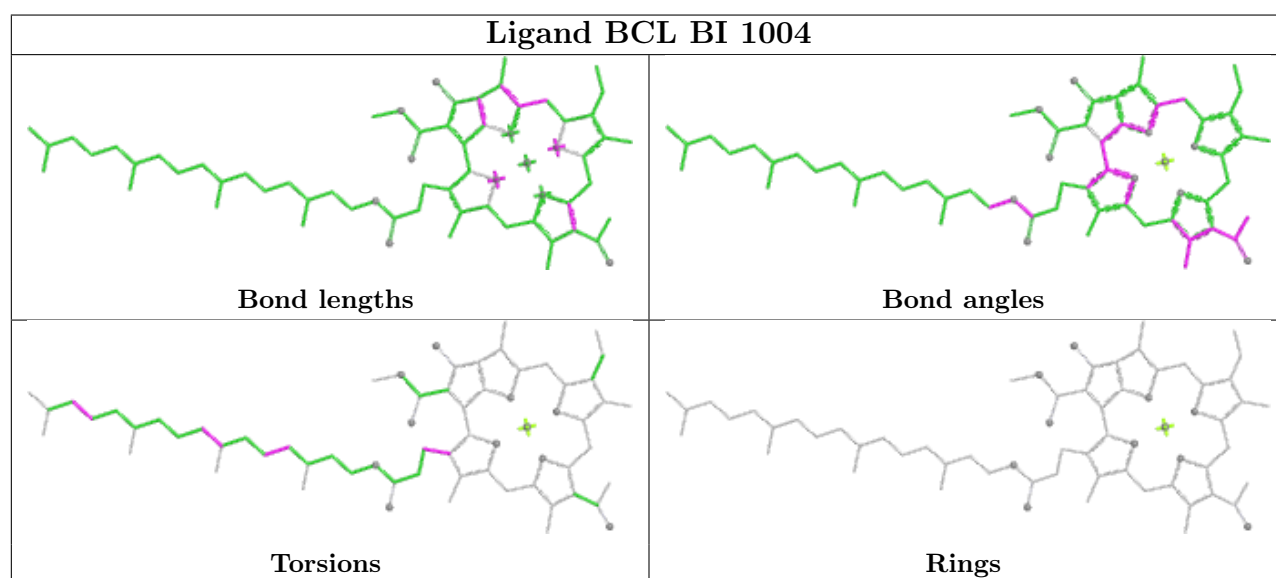
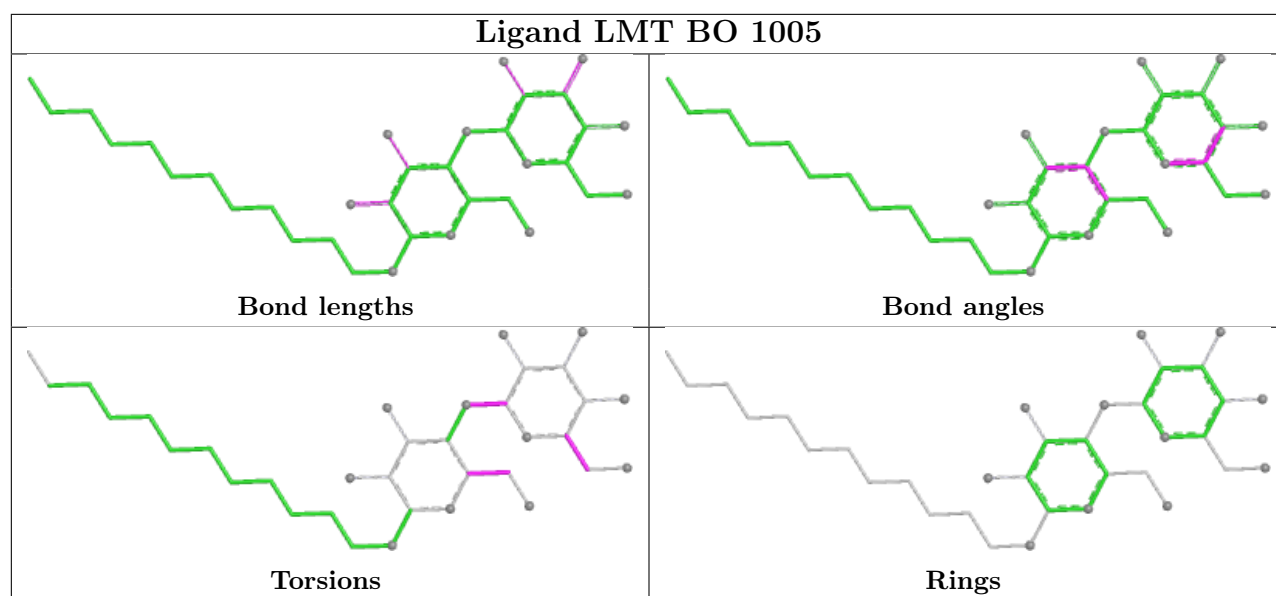


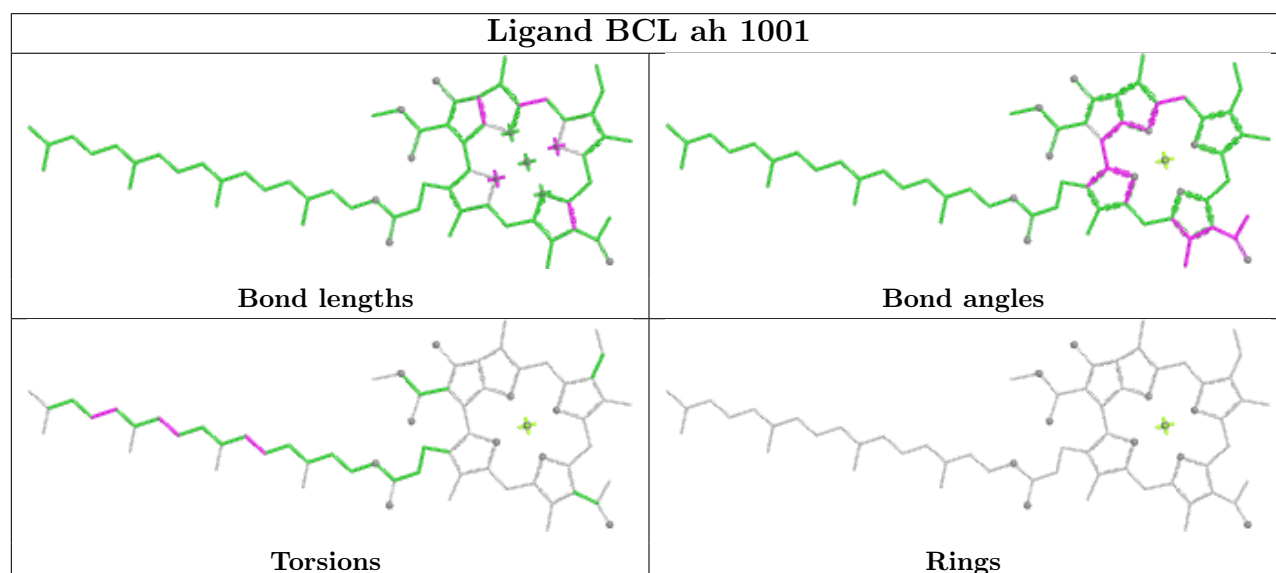
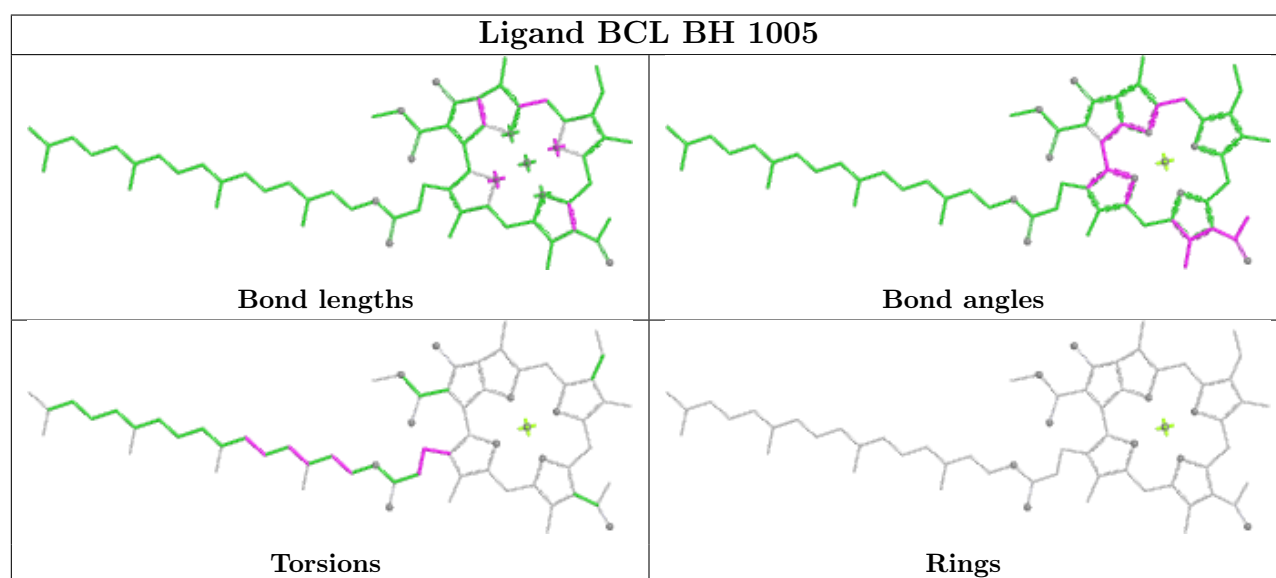
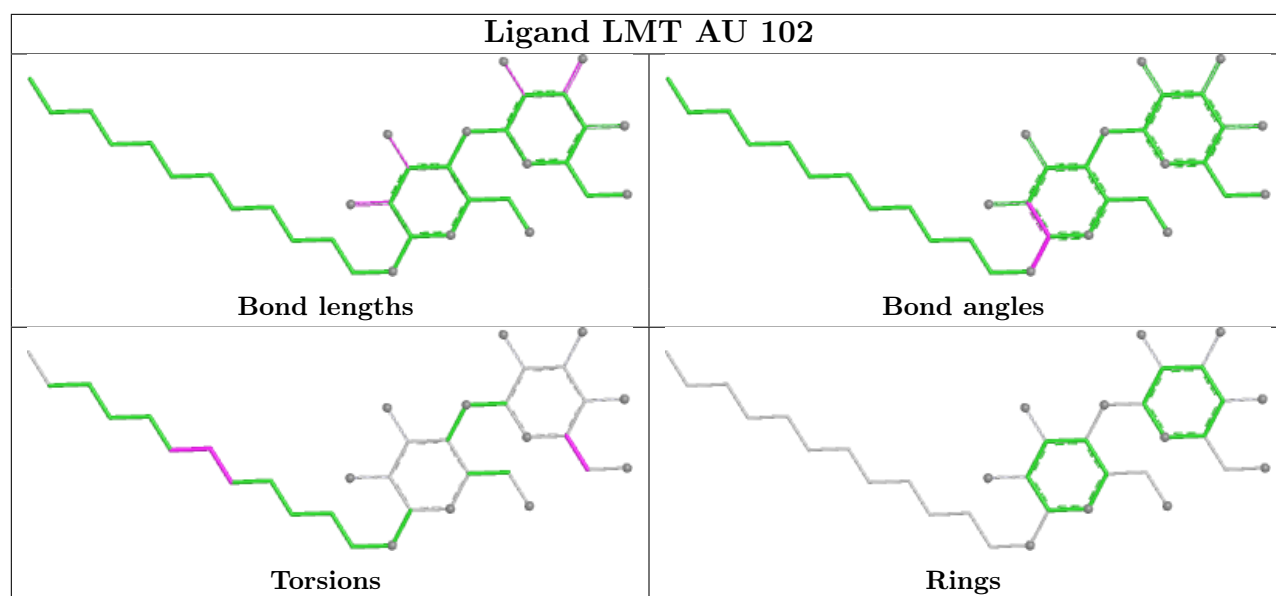
Rings

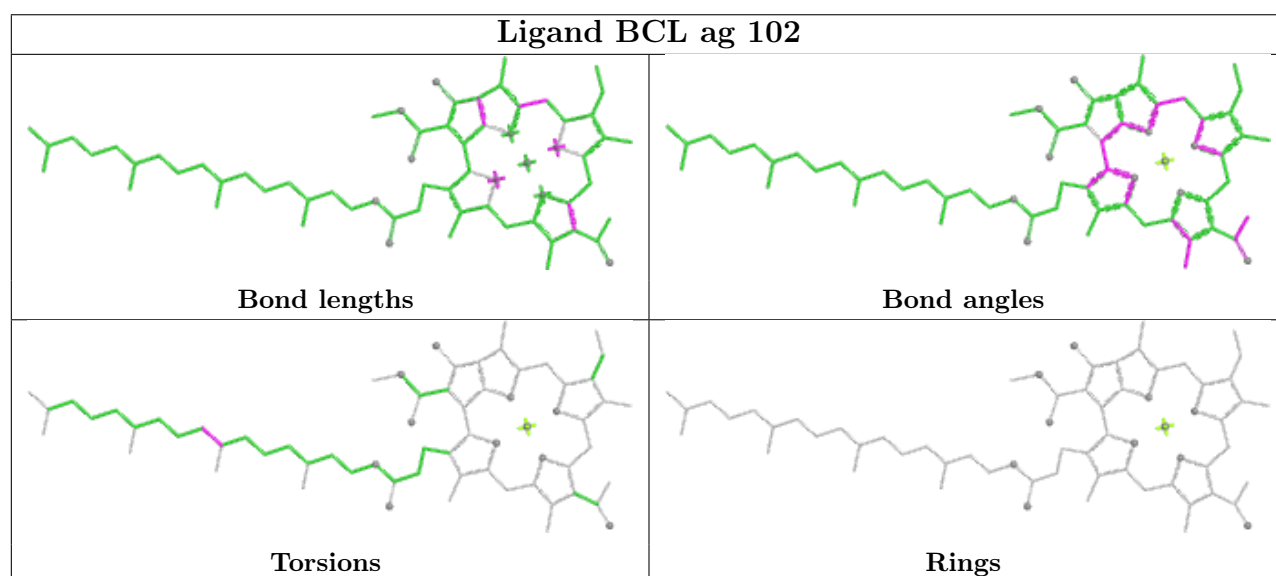
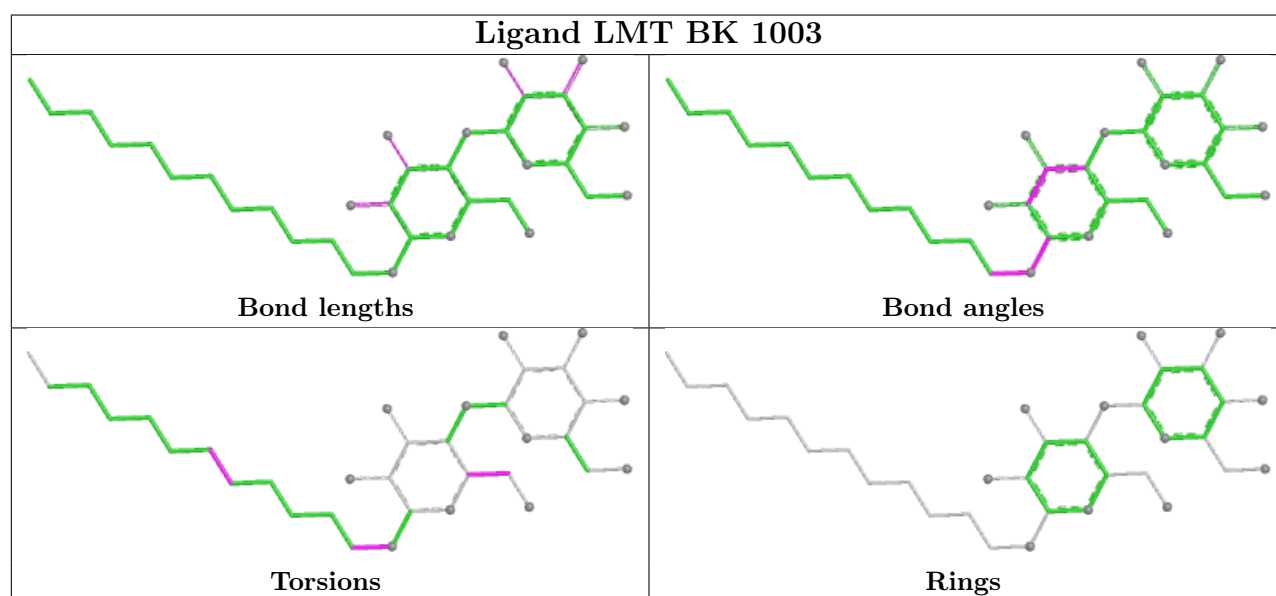
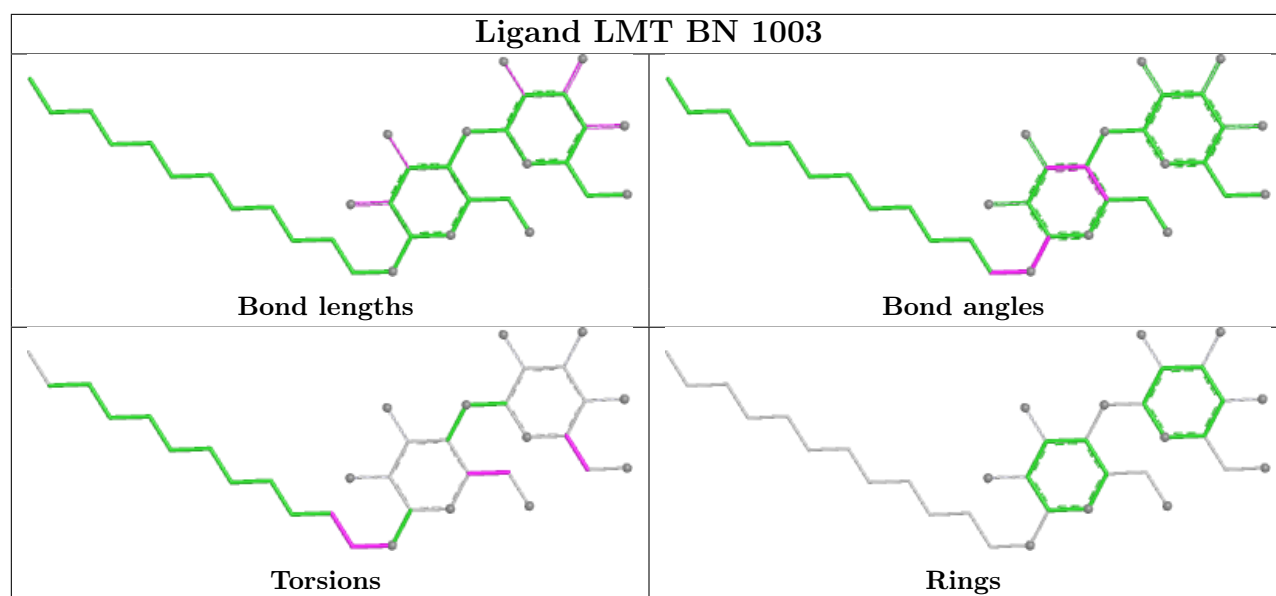


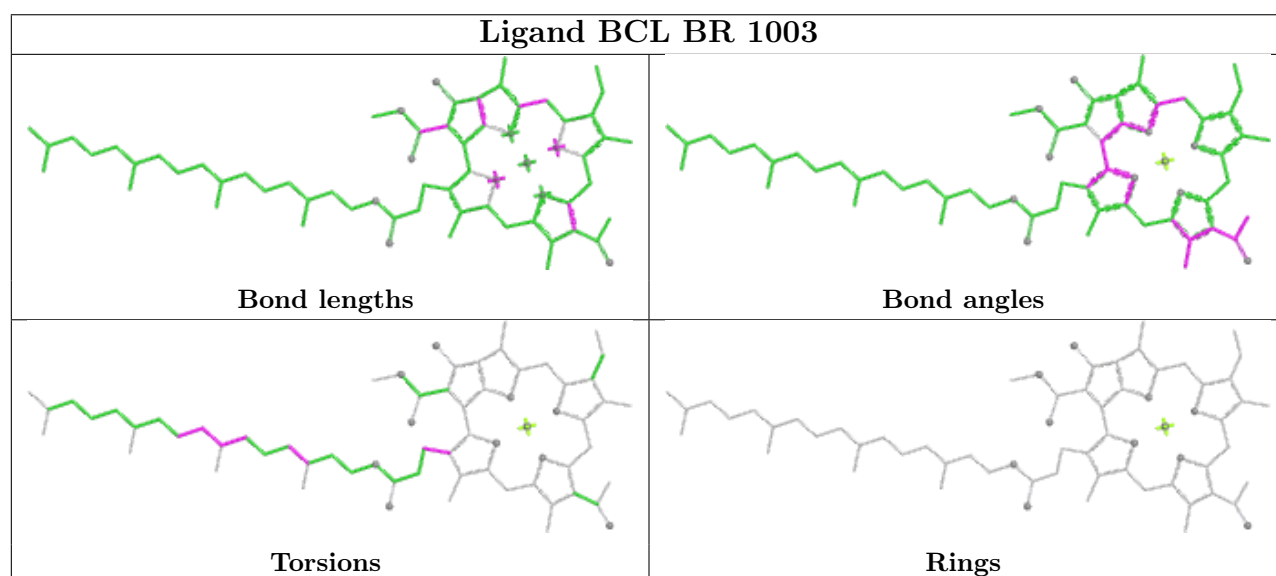
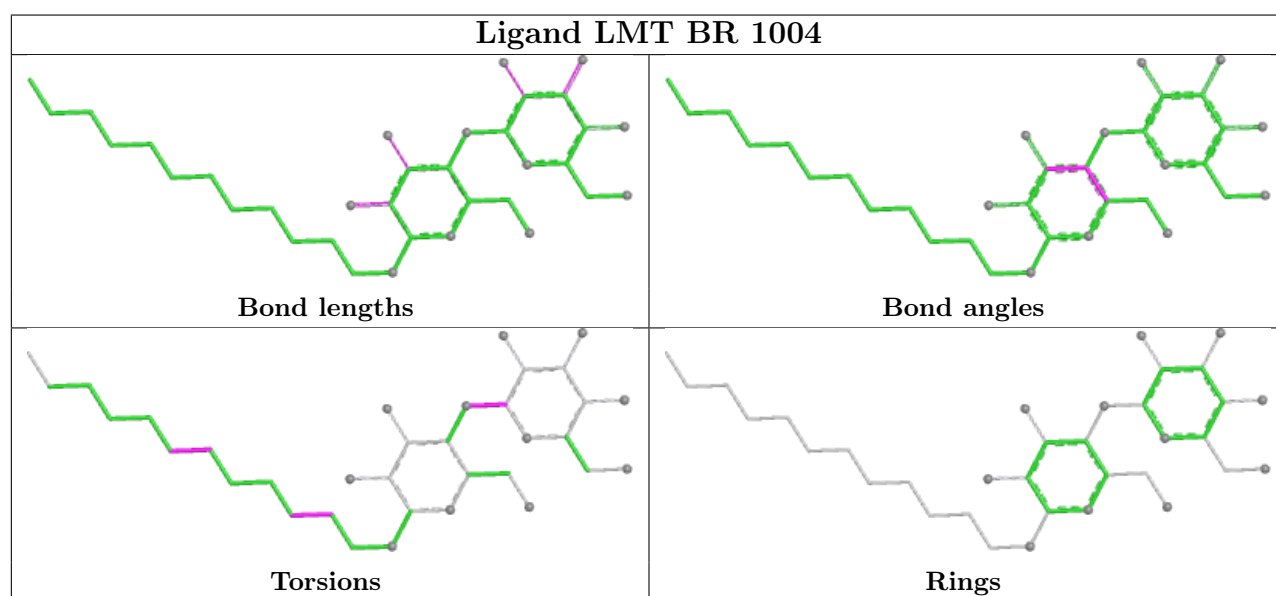
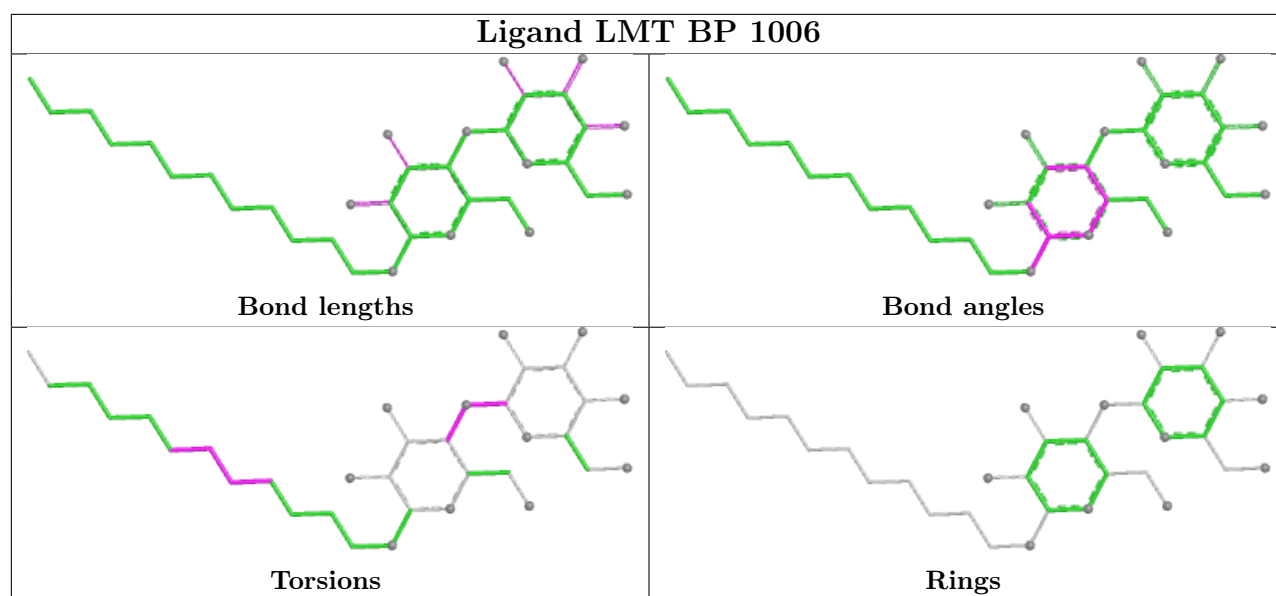


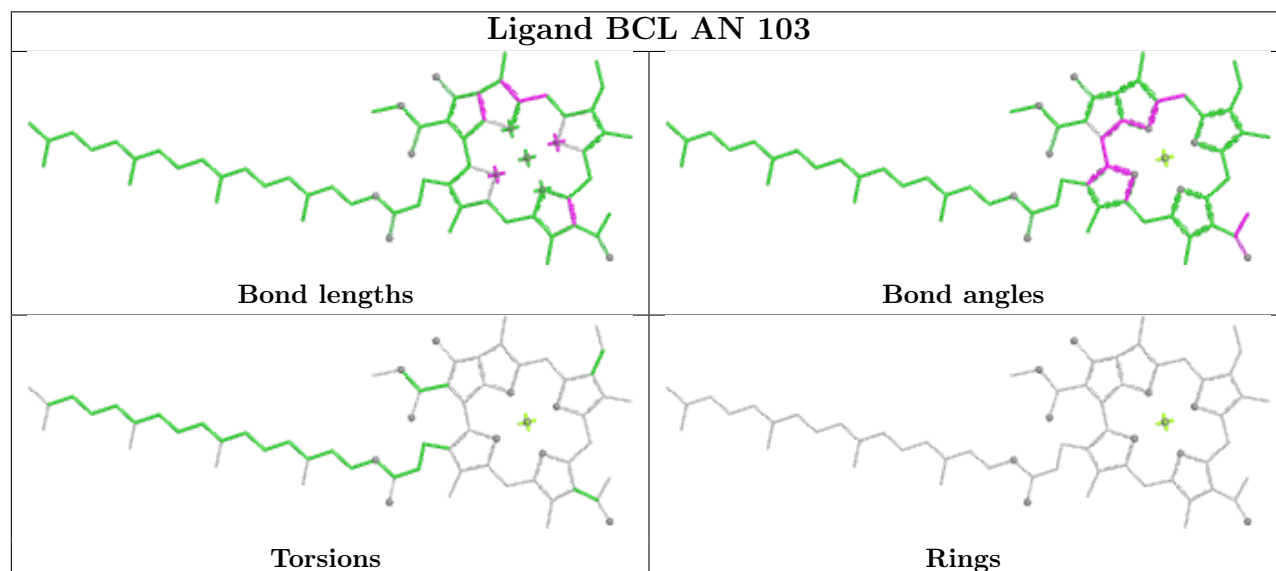
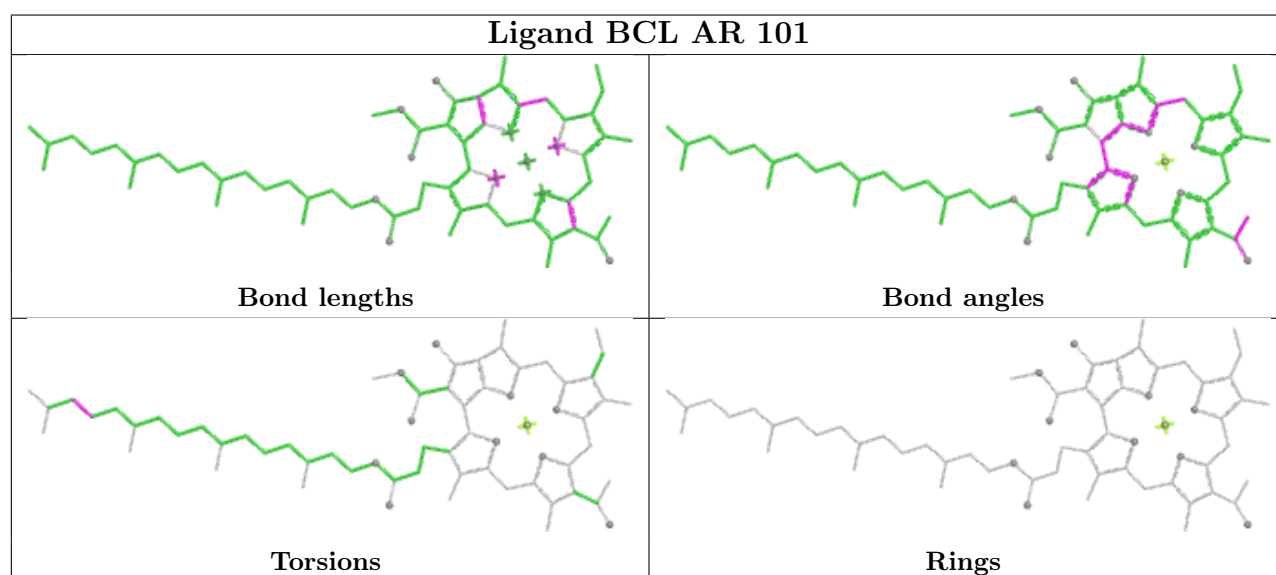
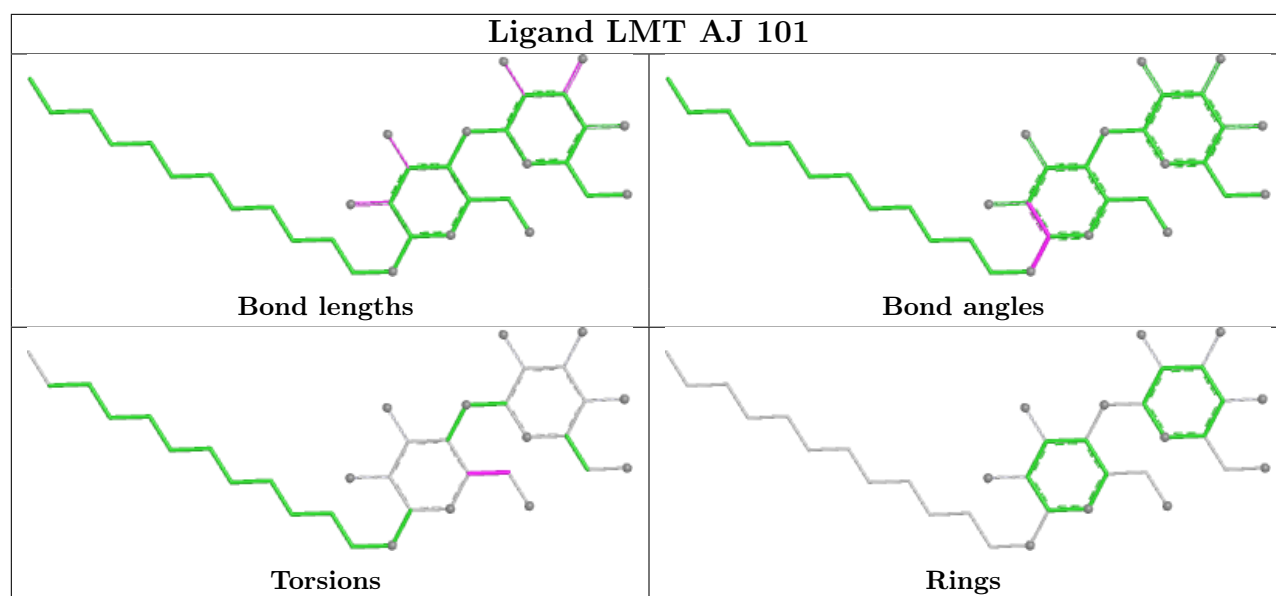


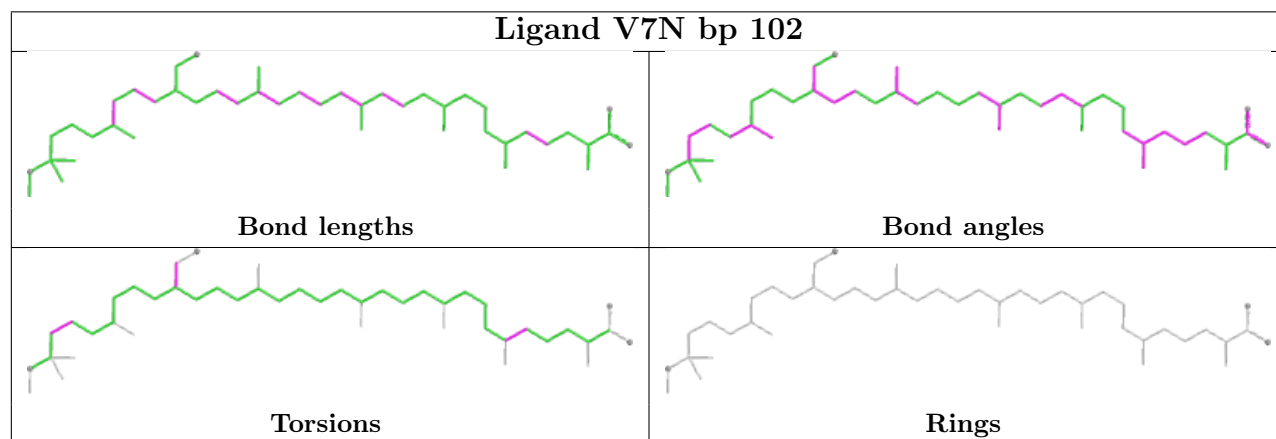
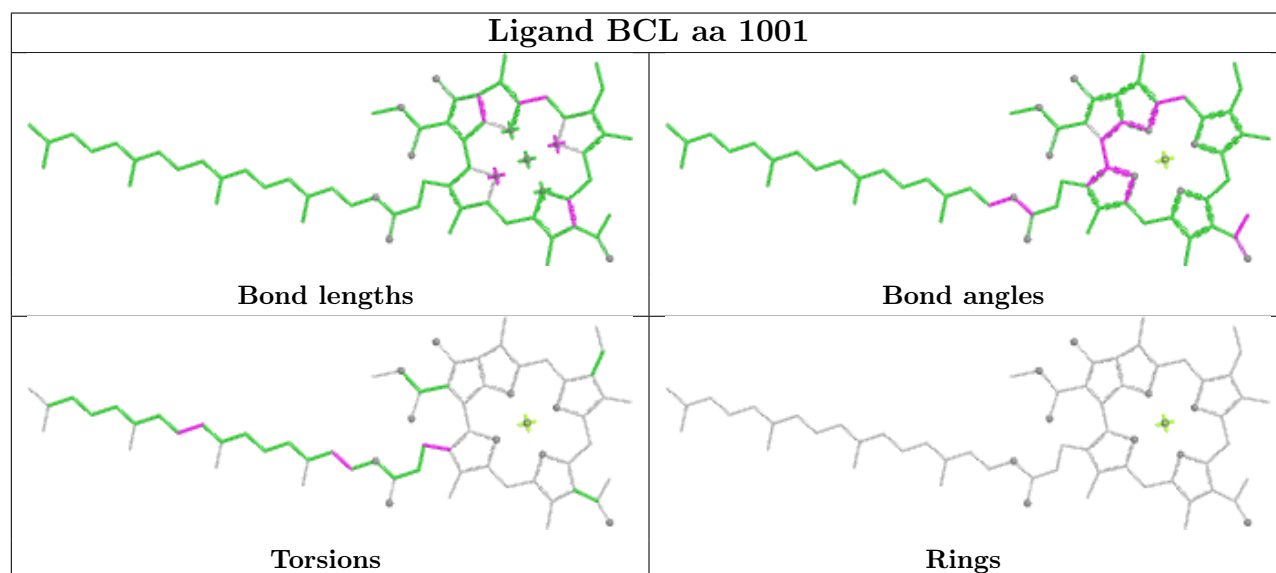
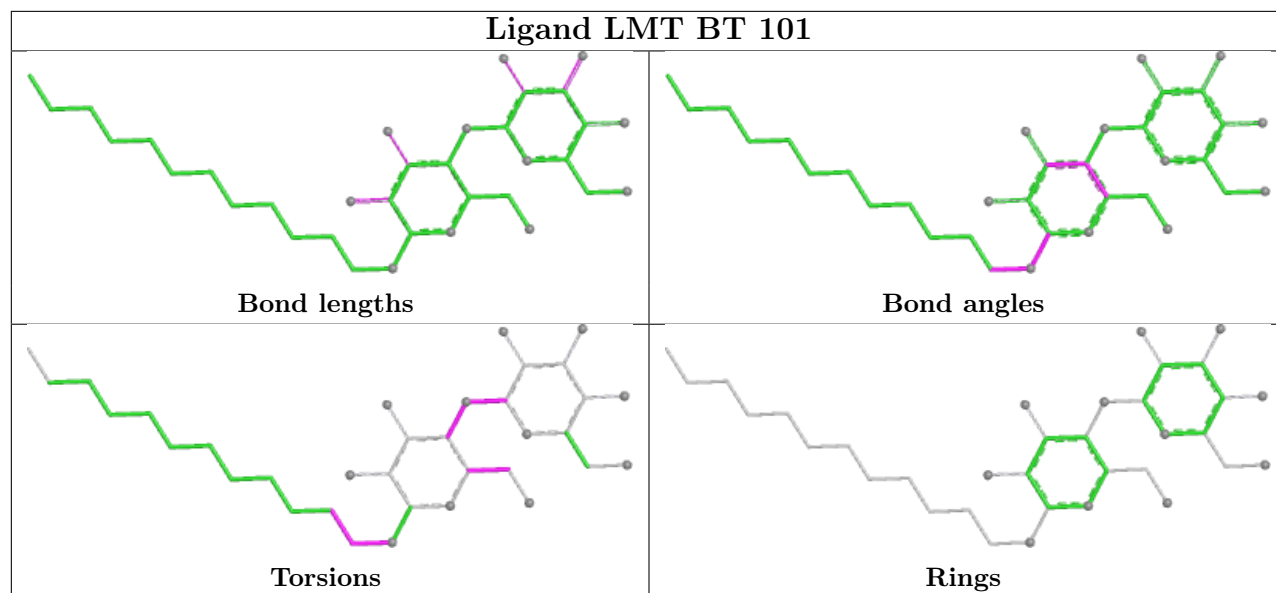


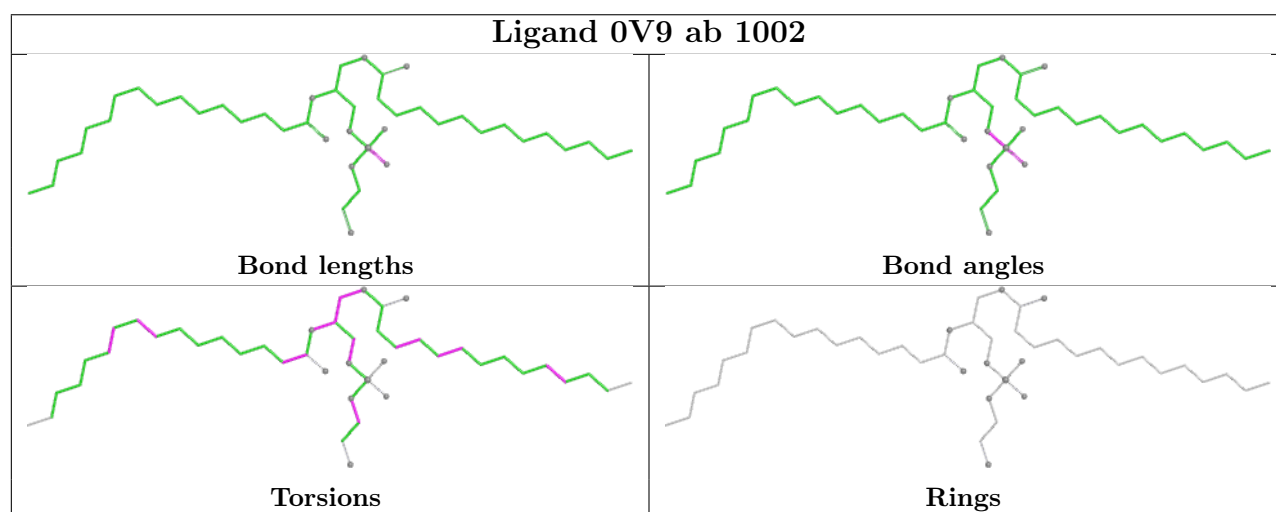
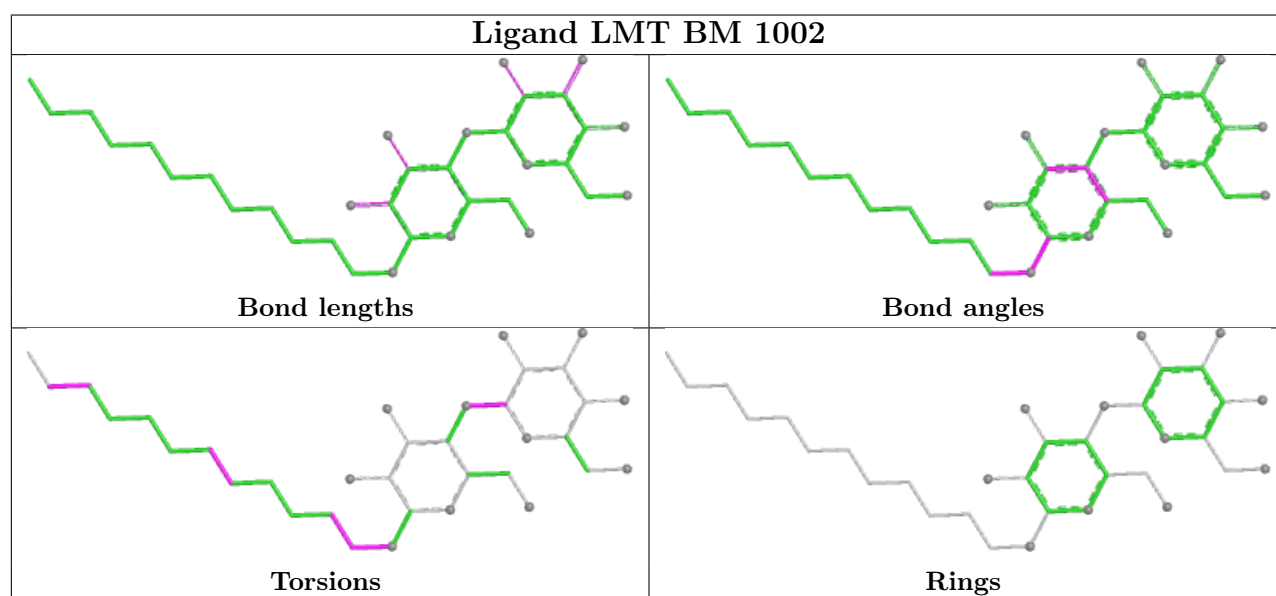
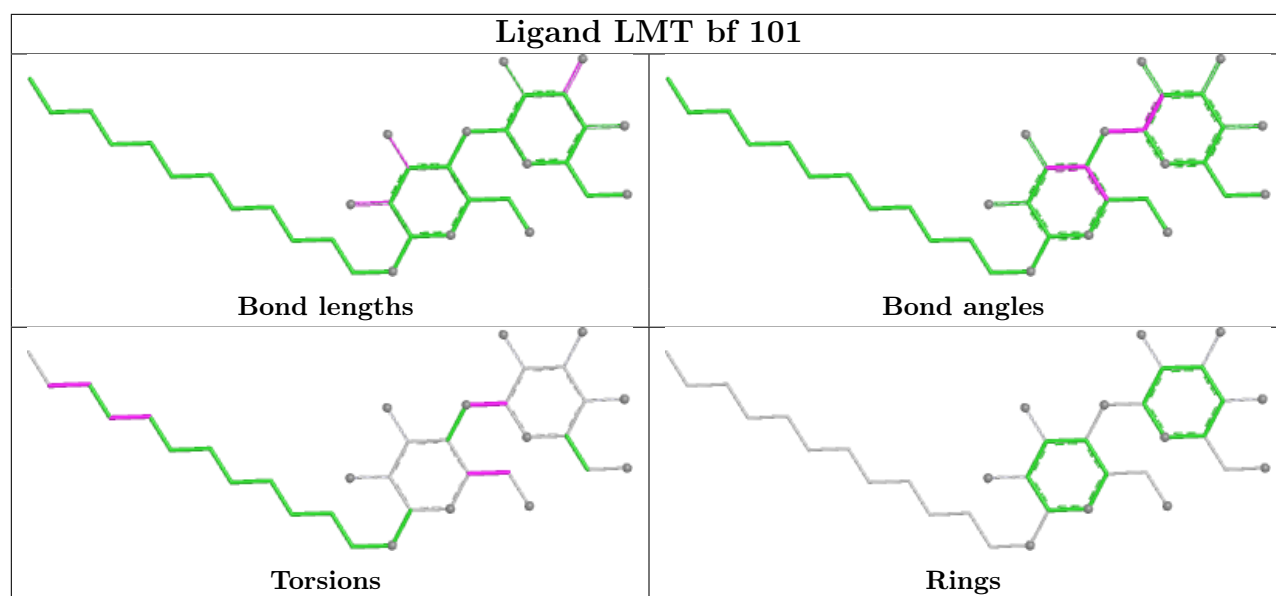


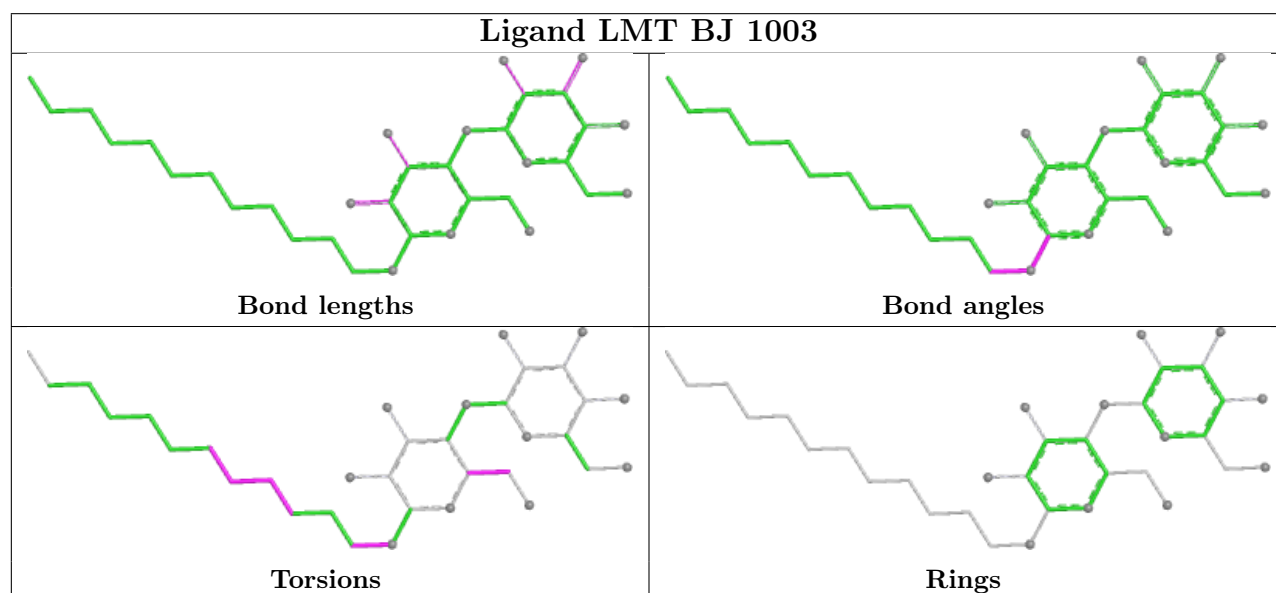
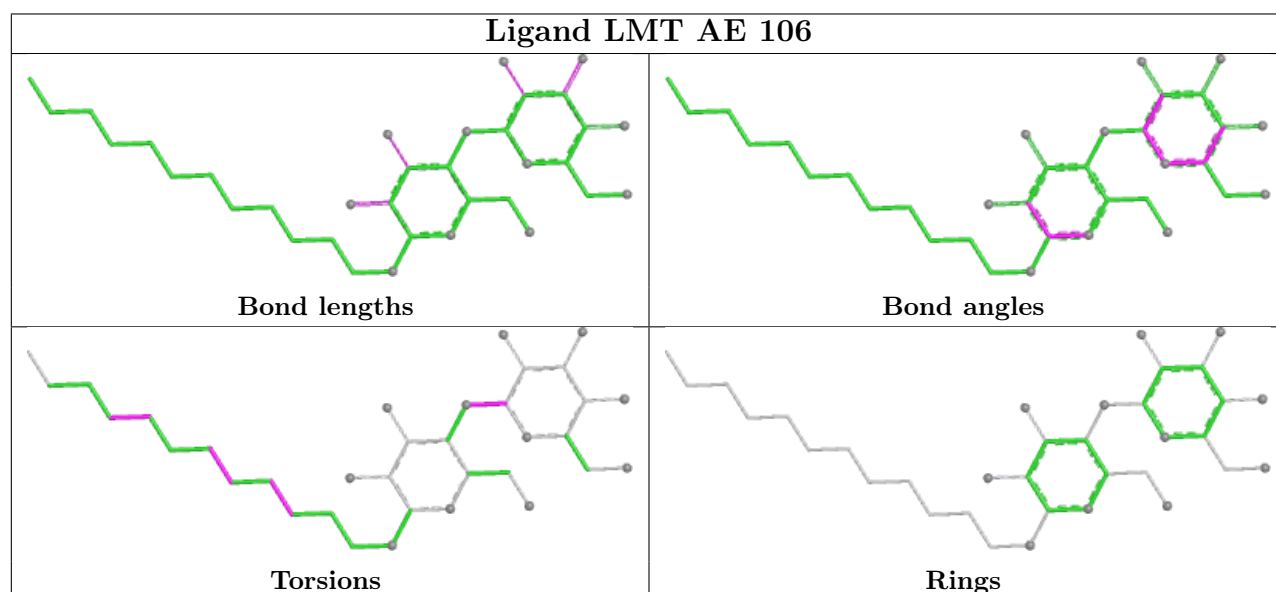
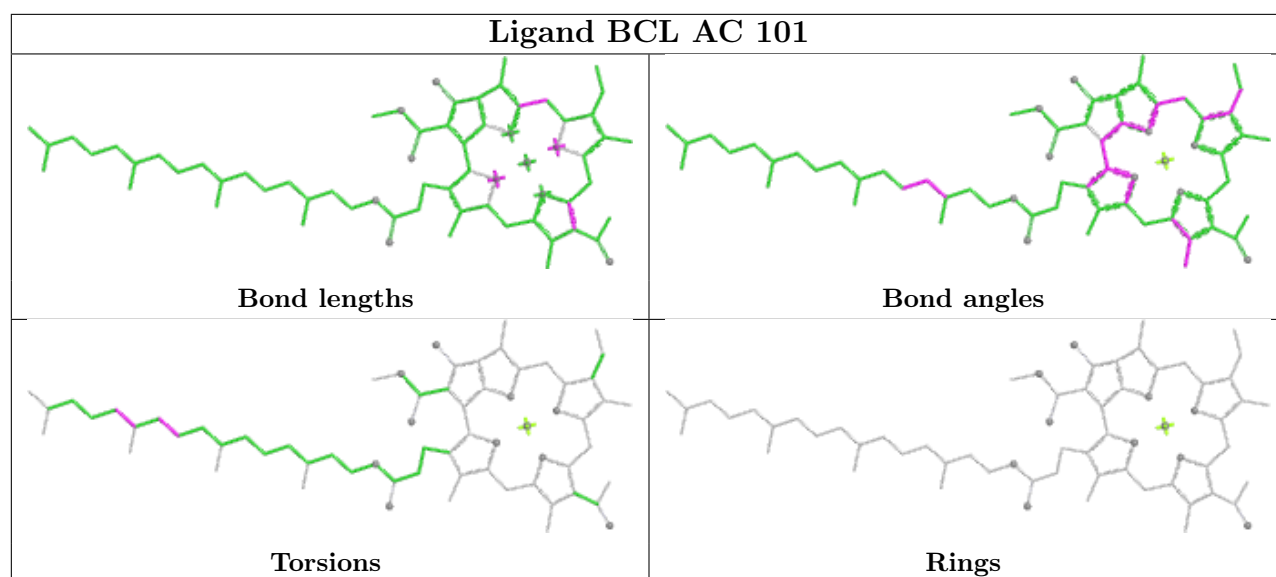


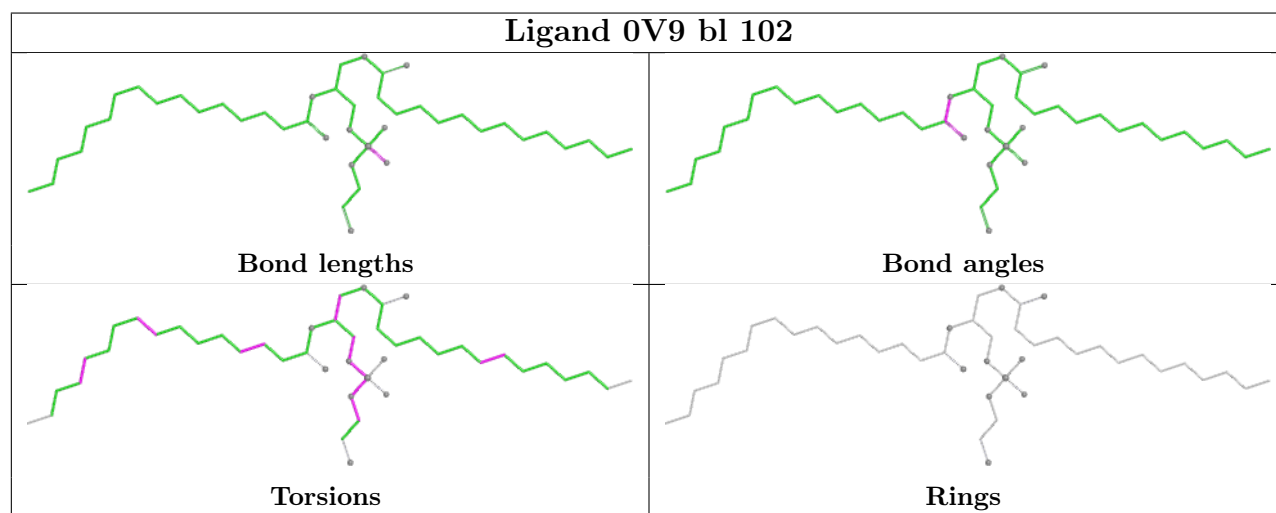
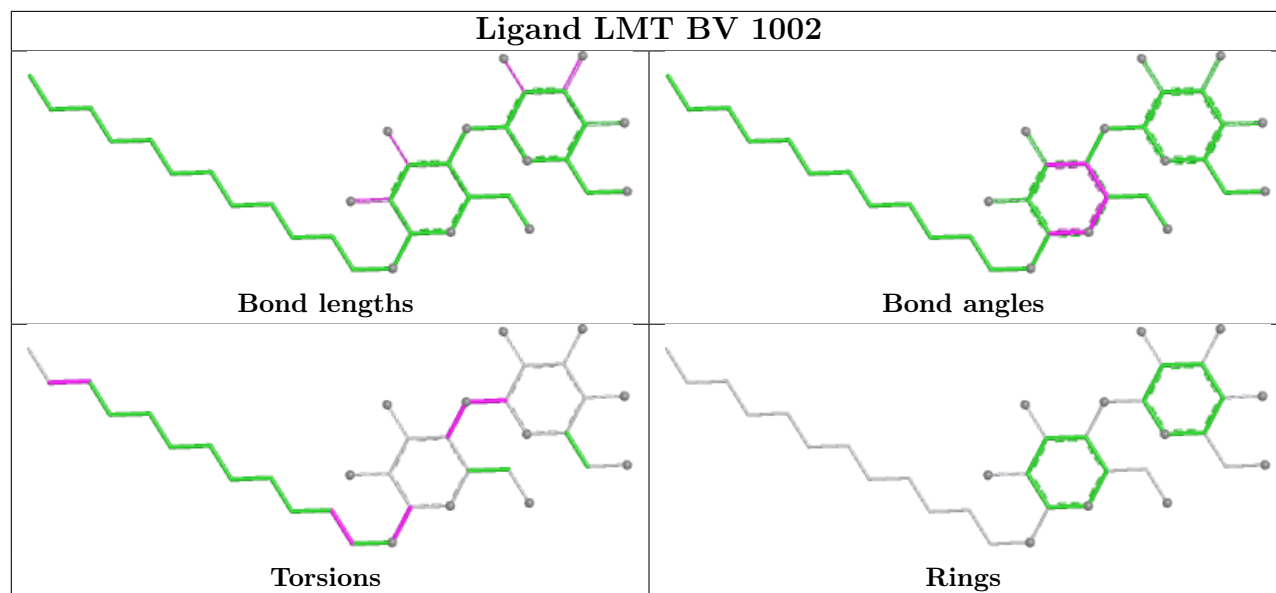


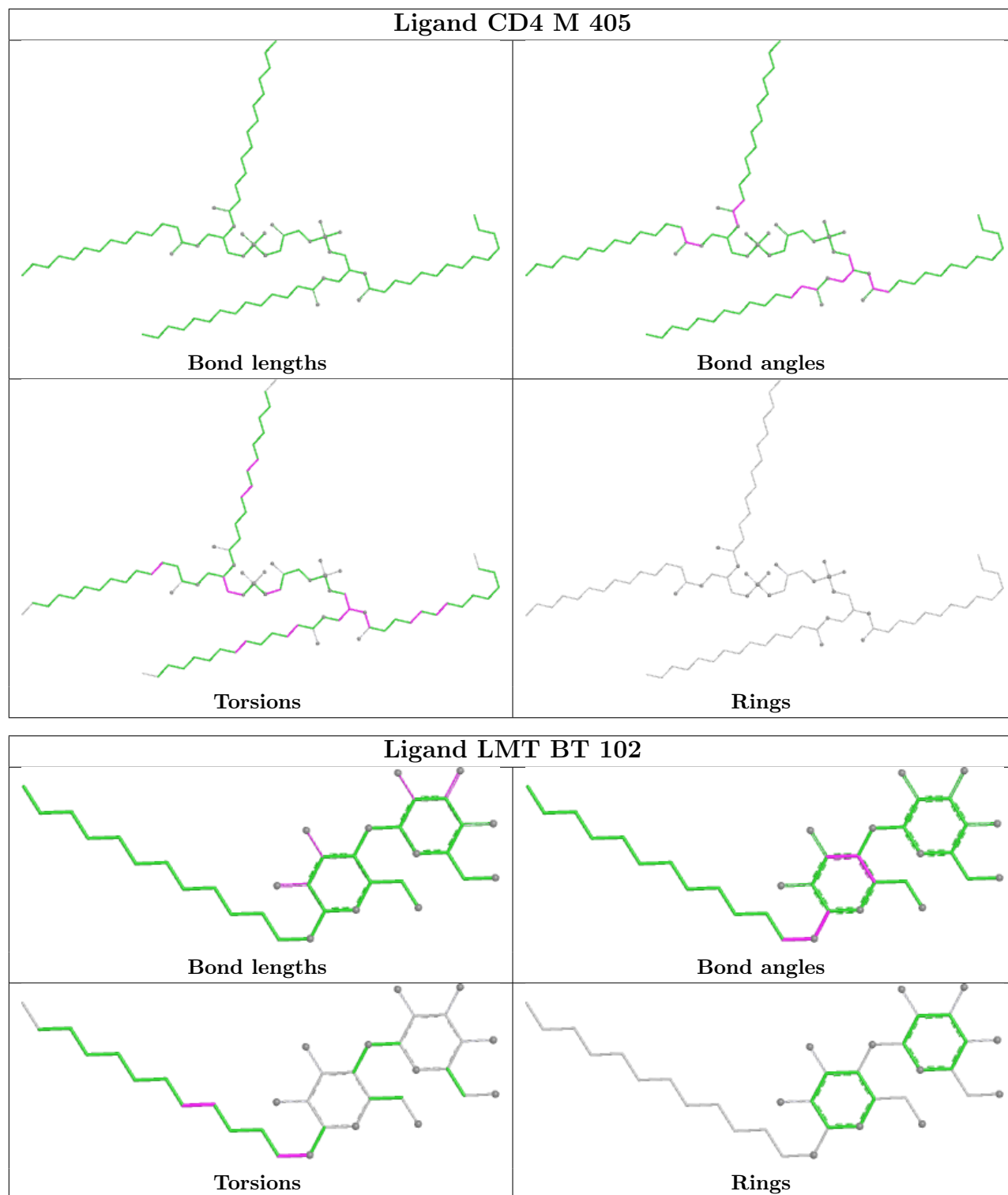


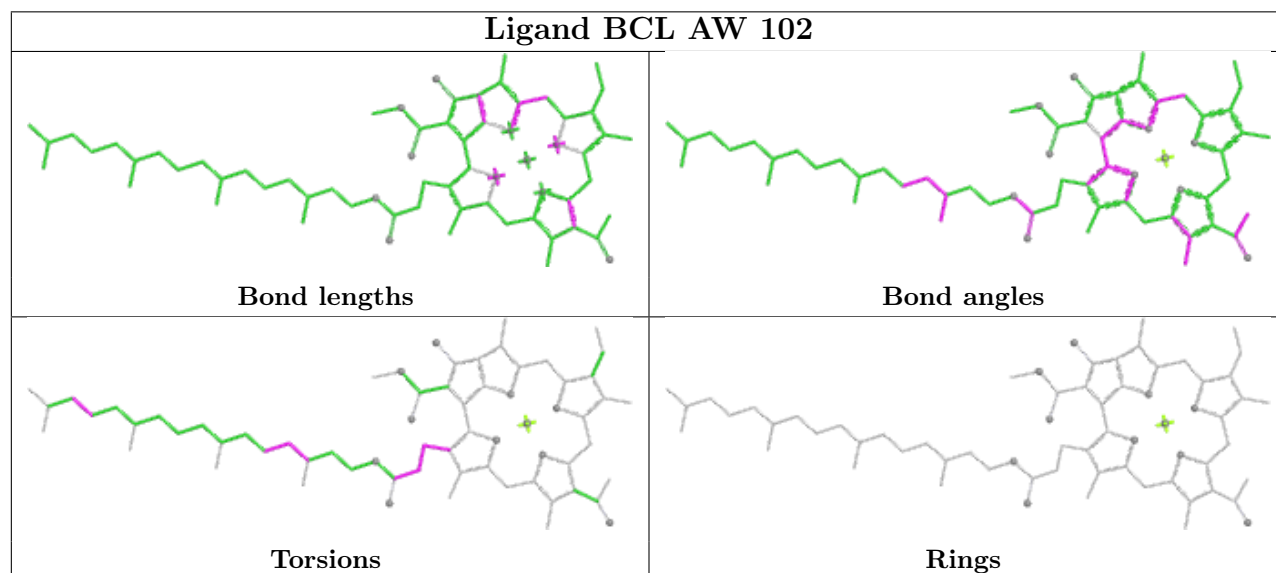
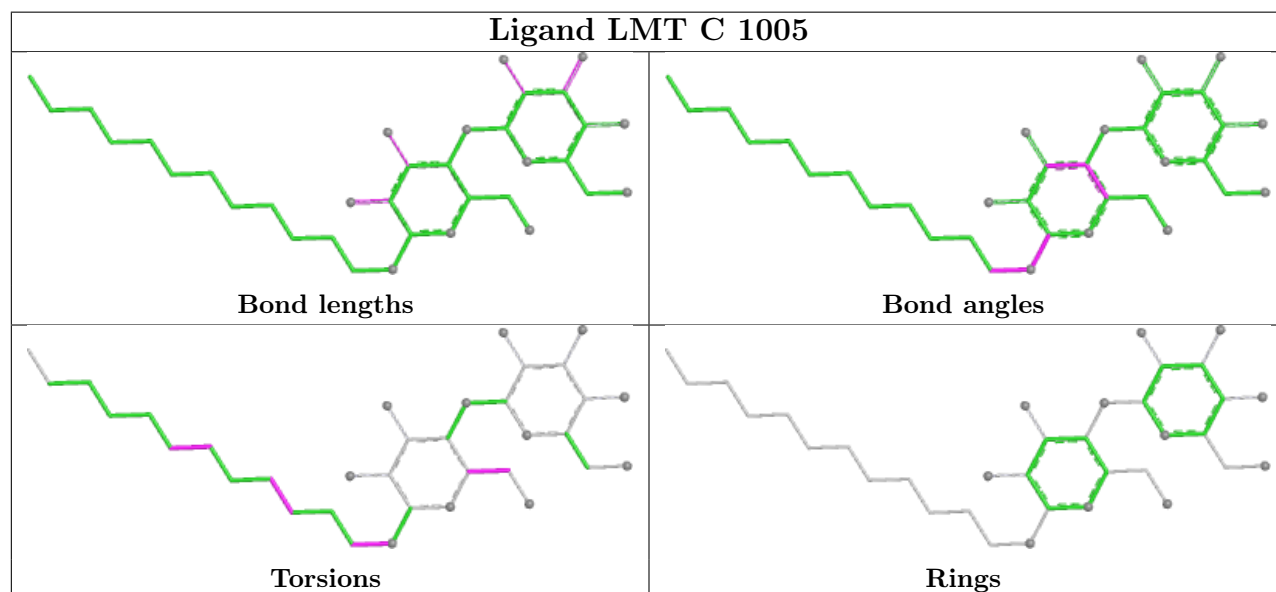
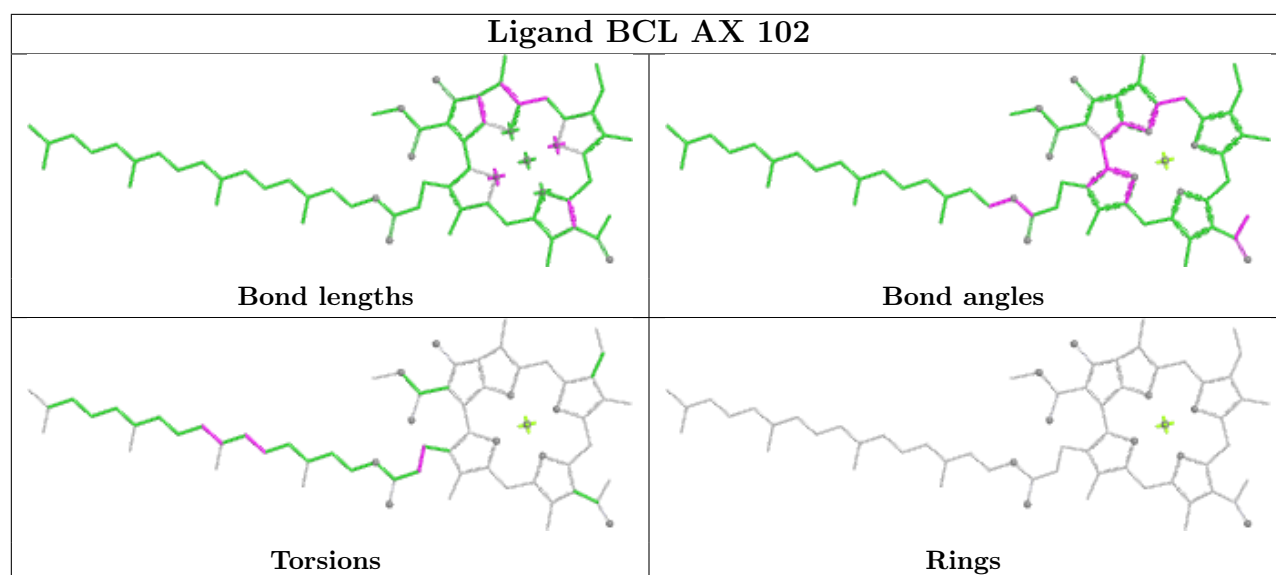


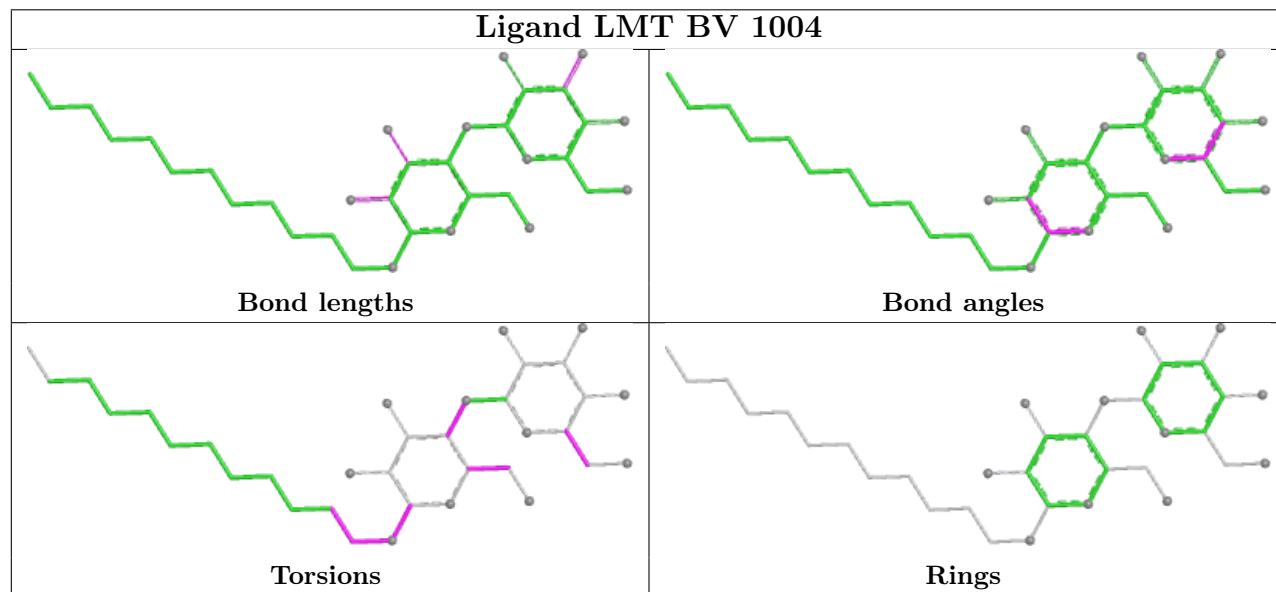
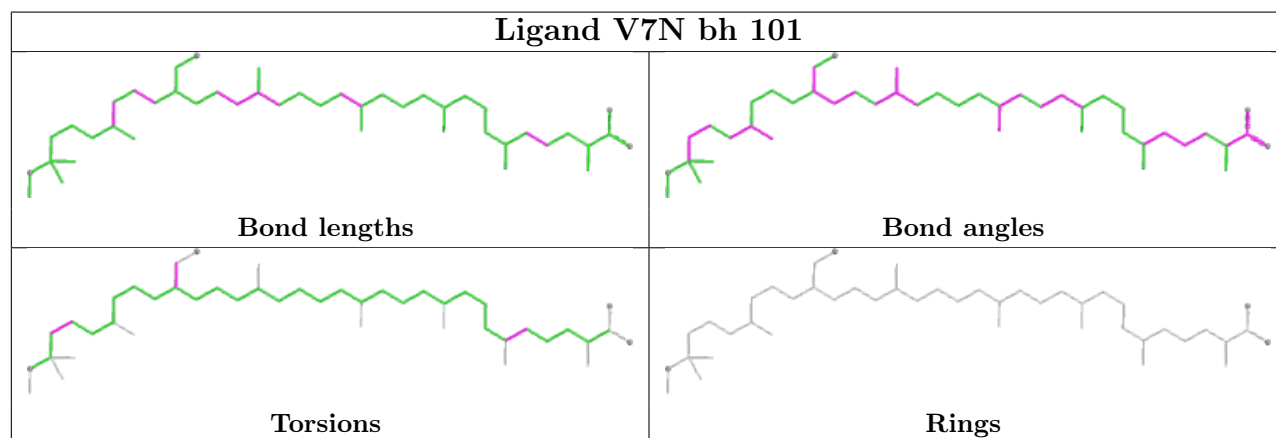
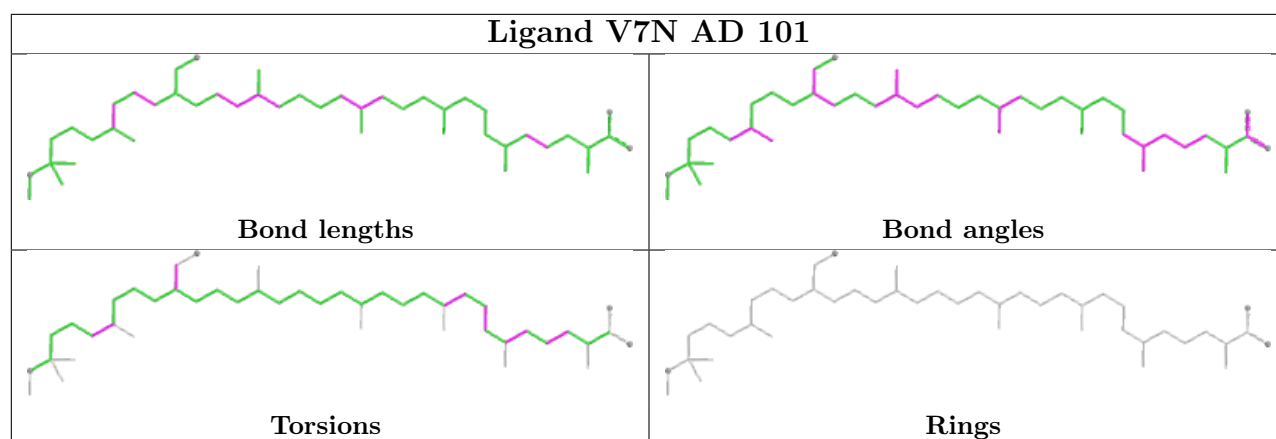


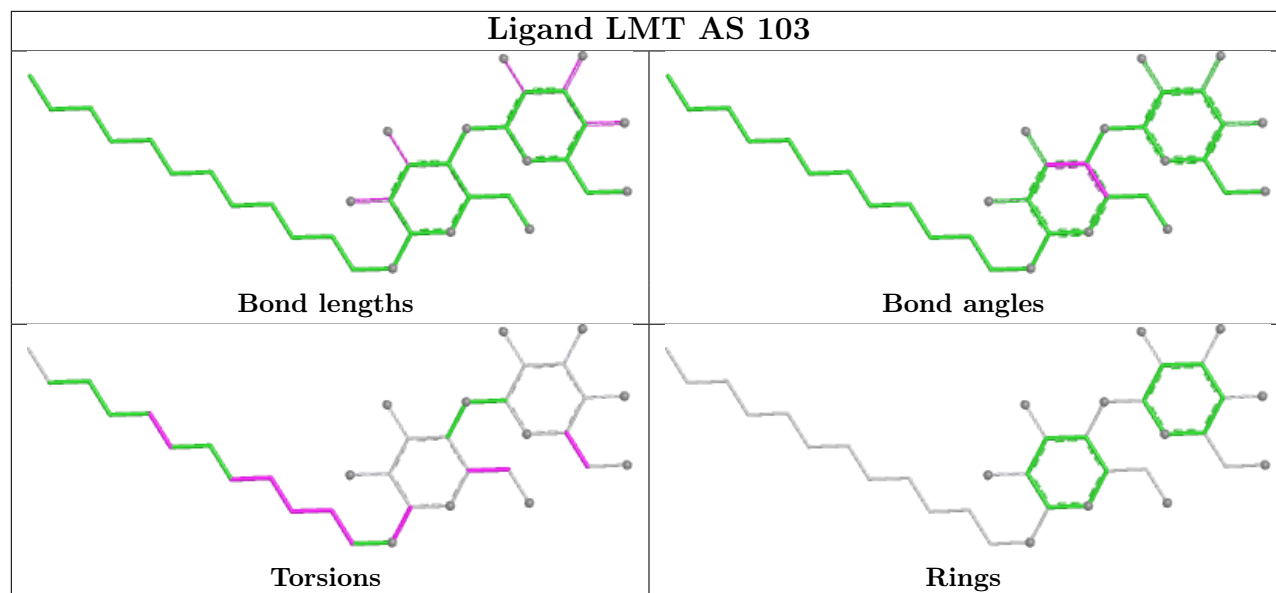












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

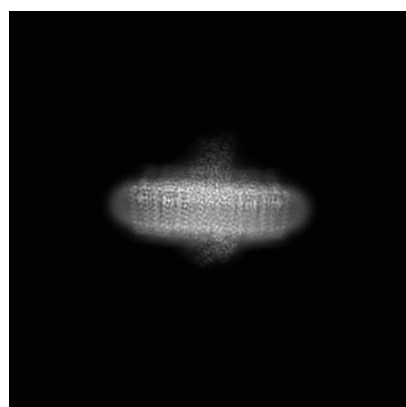
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12681. These allow visual inspection of the internal detail of the map and identification of artifacts.

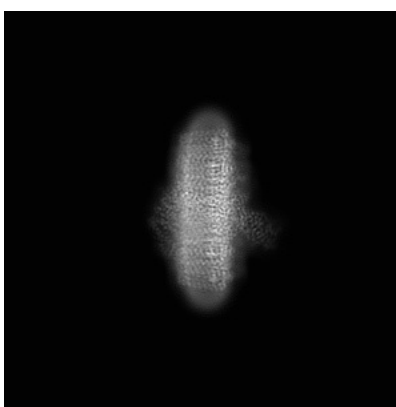
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

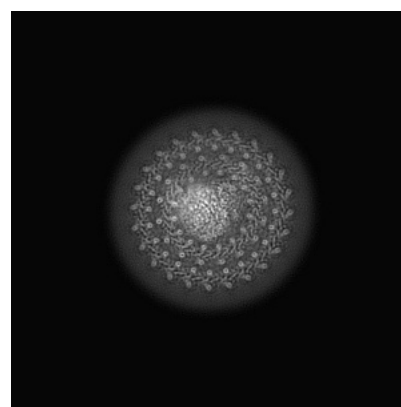
6.1.1 Primary map



X



Y

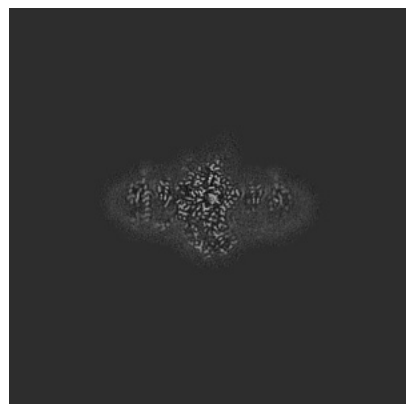


Z

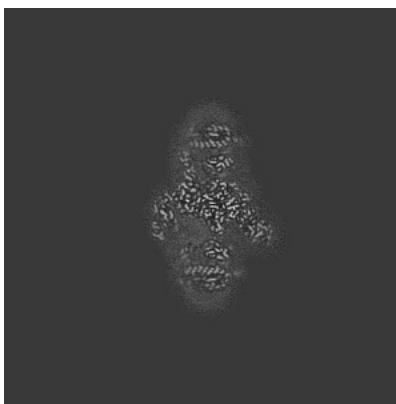
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

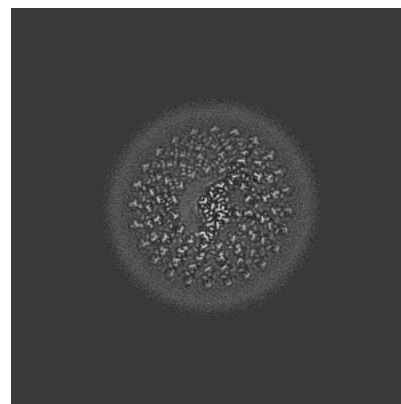
6.2.1 Primary map



X Index: 200



Y Index: 200

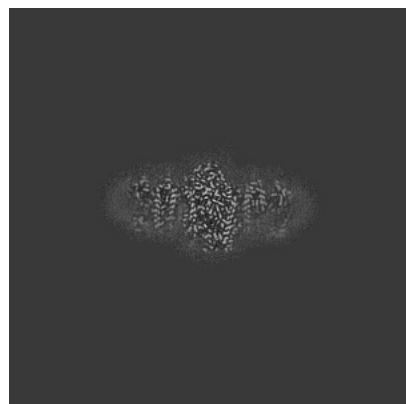


Z Index: 200

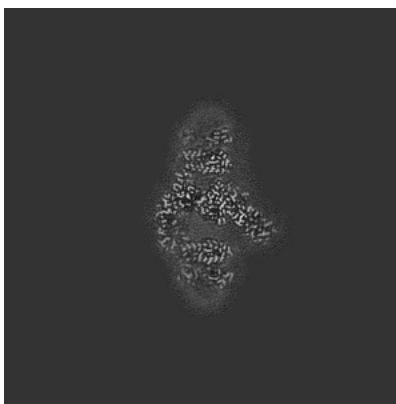
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

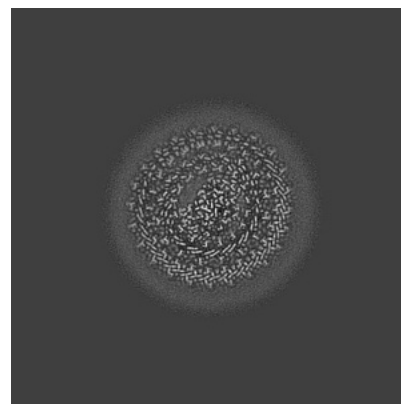
6.3.1 Primary map



X Index: 209



Y Index: 208

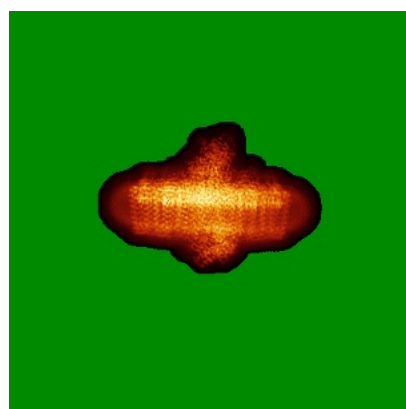


Z Index: 212

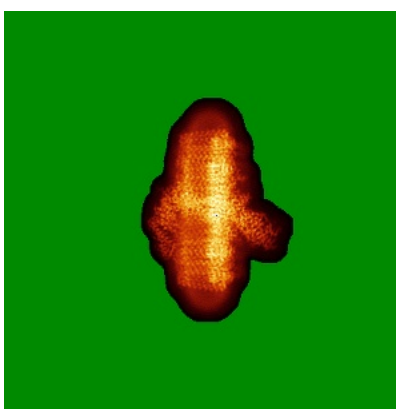
The images above show the largest variance slices of the map in three orthogonal directions.

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

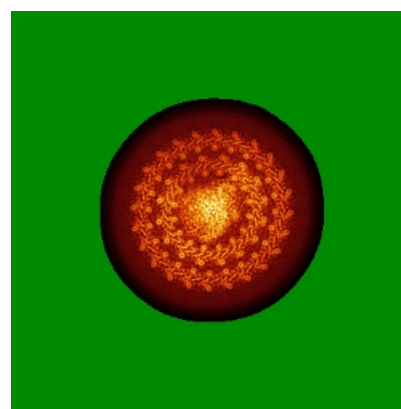
6.4.1 Primary map



X



Y

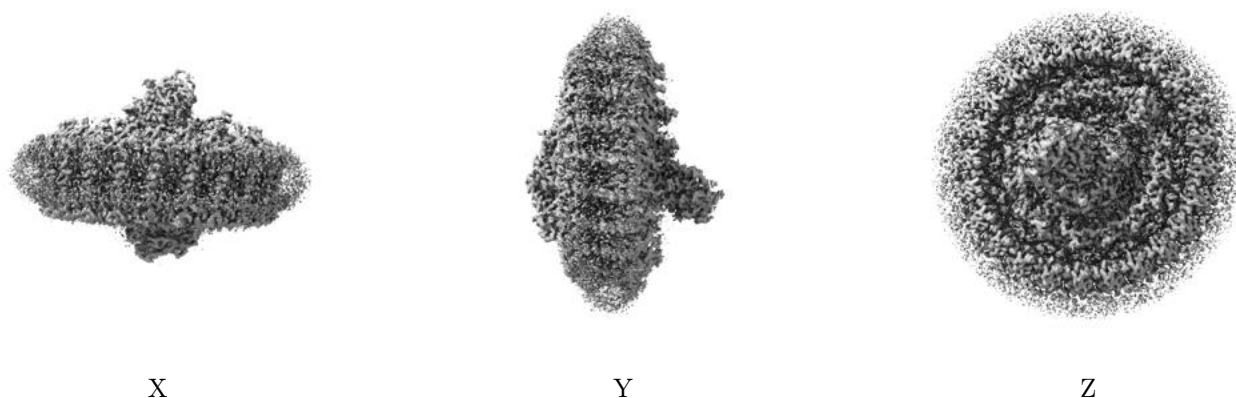


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0233. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

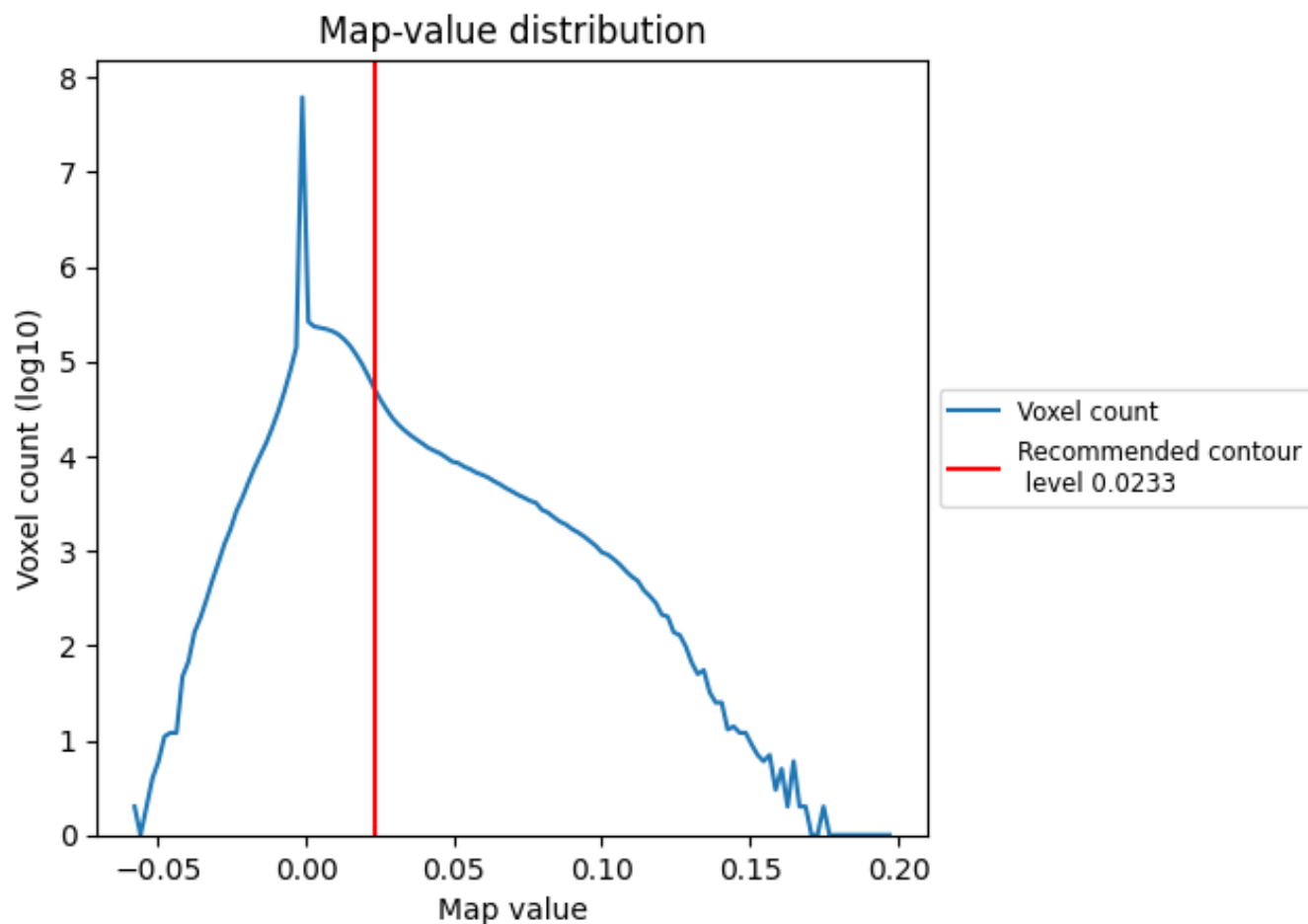
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

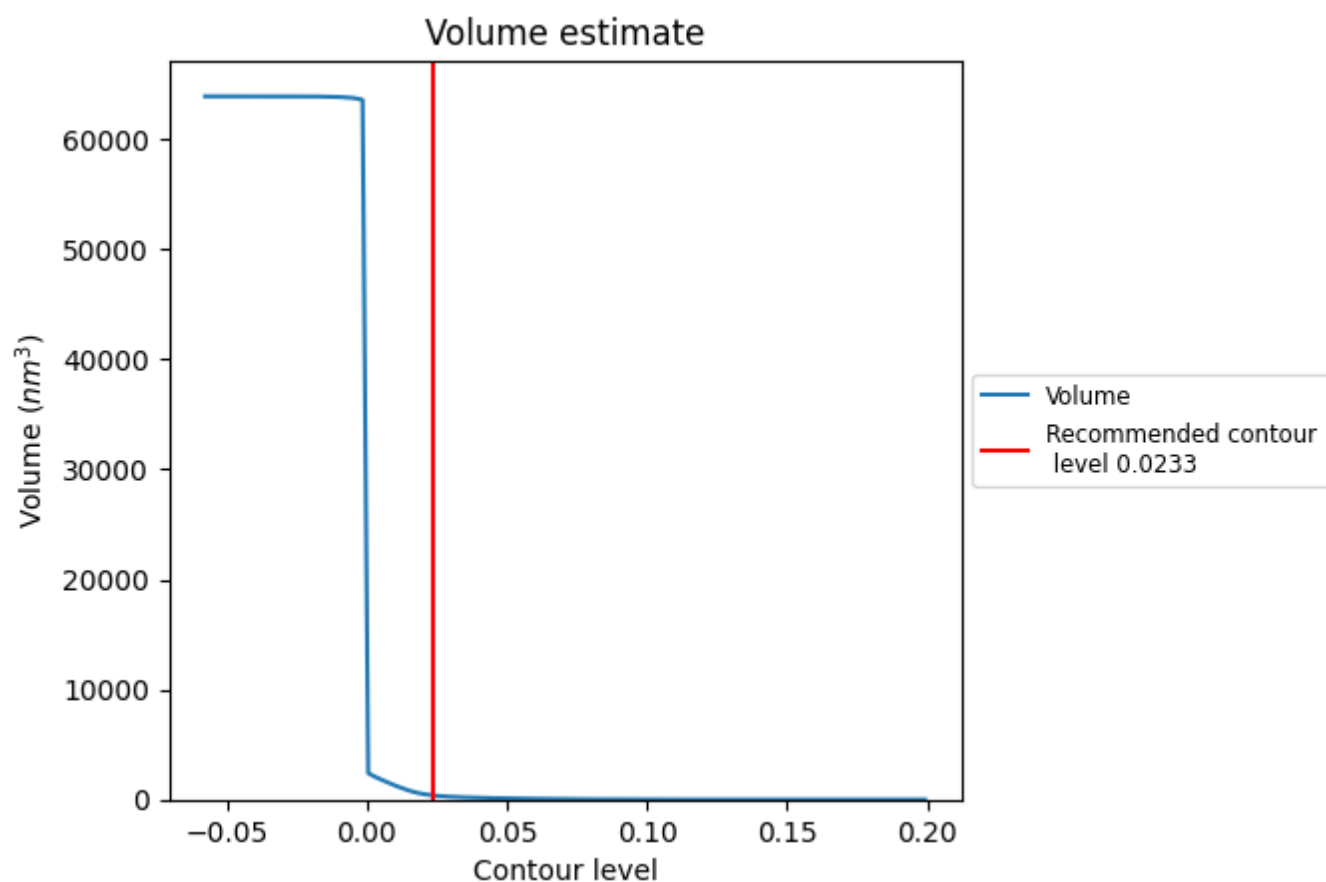
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

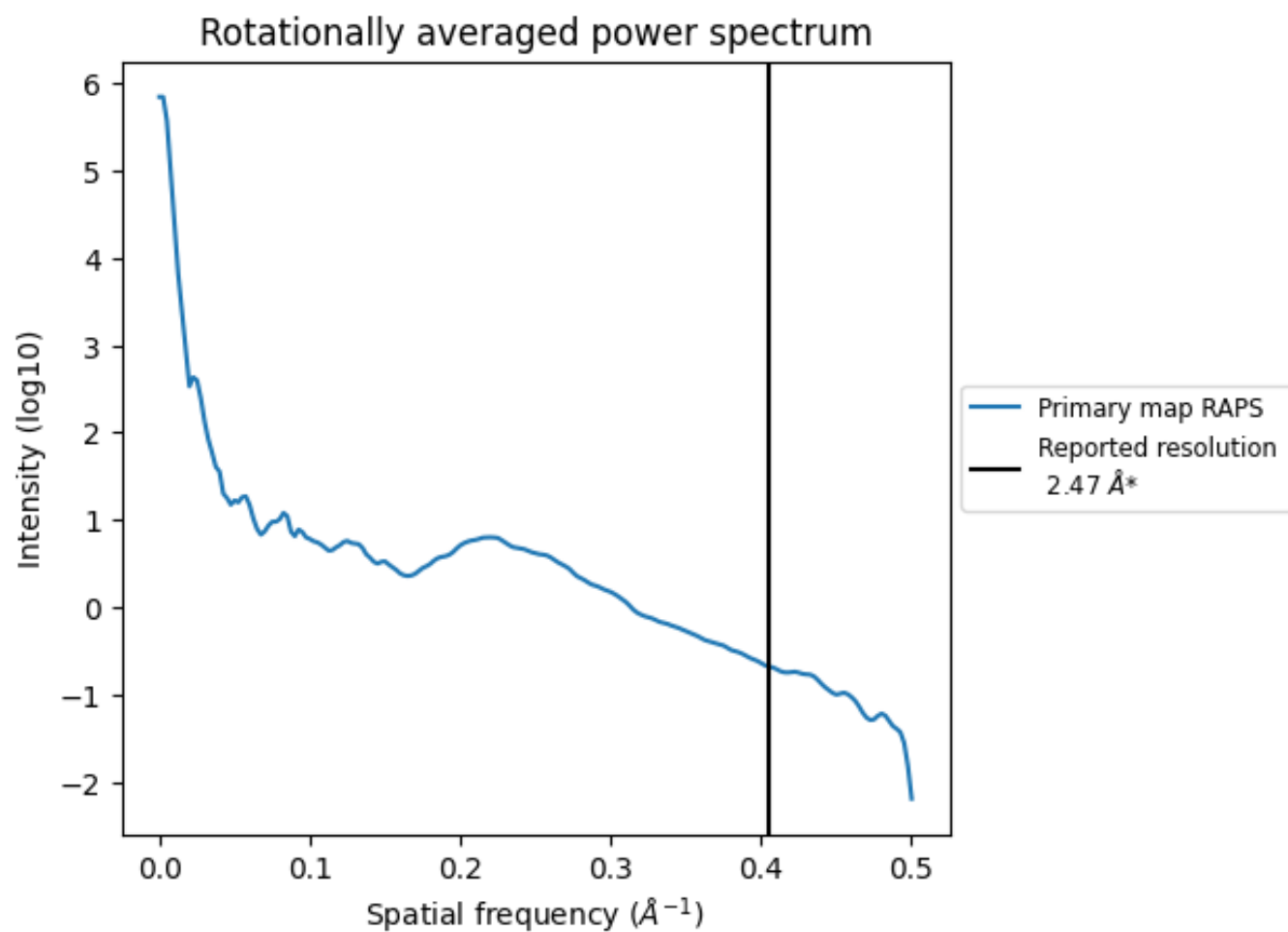
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm^3 ; this corresponds to an approximate mass of 348 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

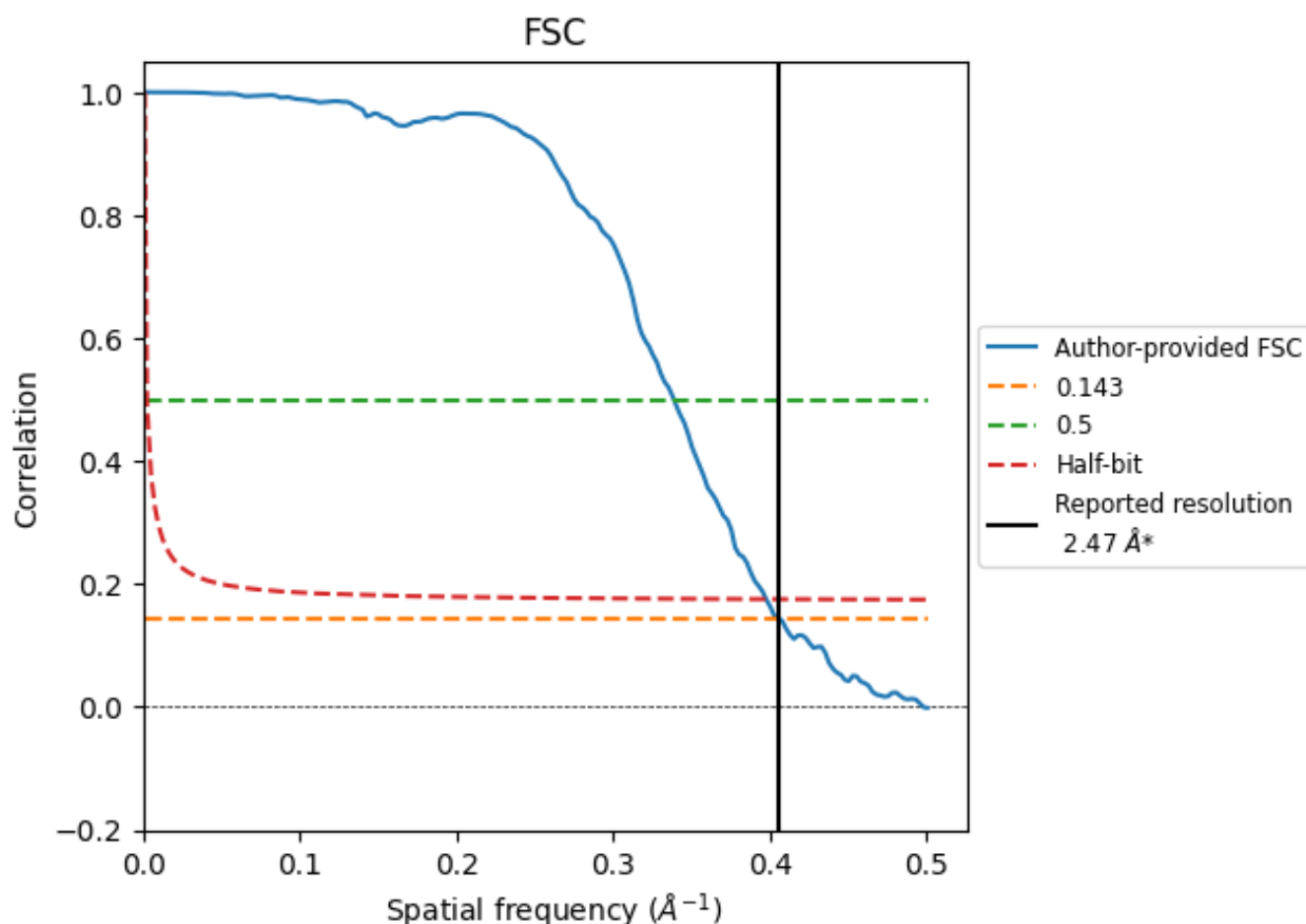


*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8.2 Resolution estimates [i](#)

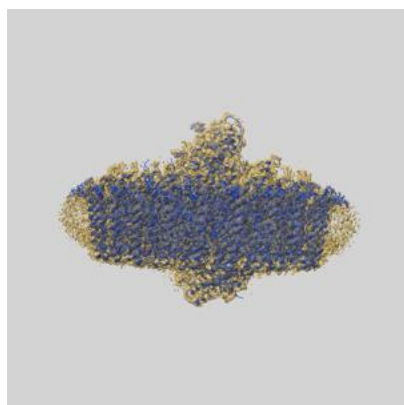
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.46	2.95	2.52
Unmasked-calculated*	-	-	-

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

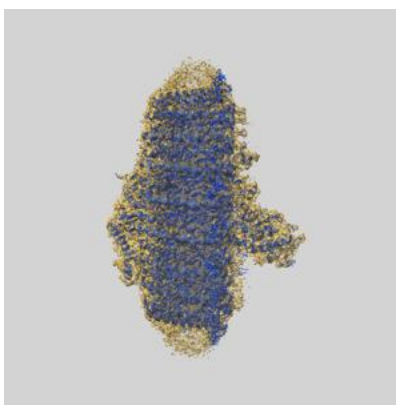
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12681 and PDB model 7O0W. Per-residue inclusion information can be found in section [3](#) on page [39](#).

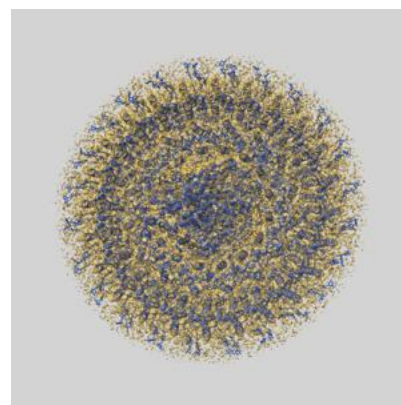
9.1 Map-model overlay [i](#)



X



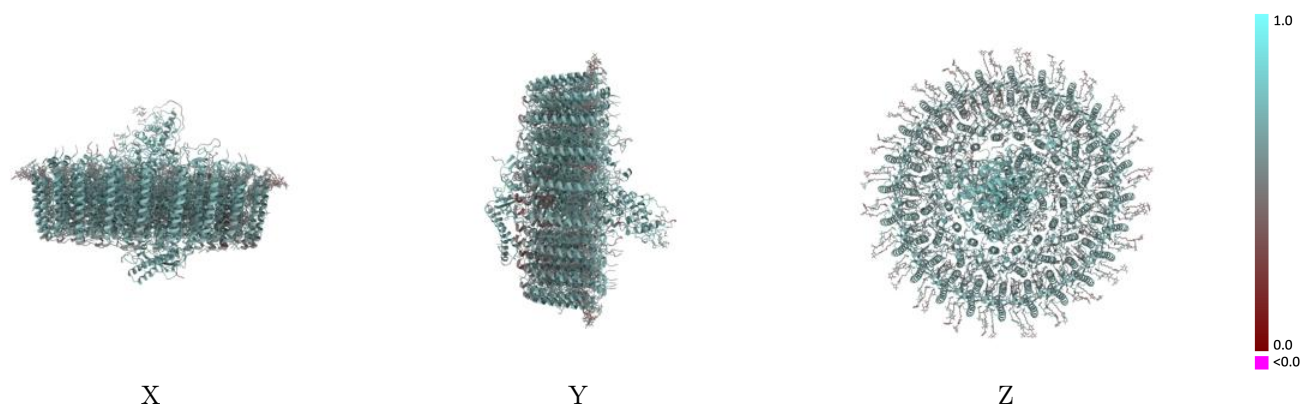
Y



Z

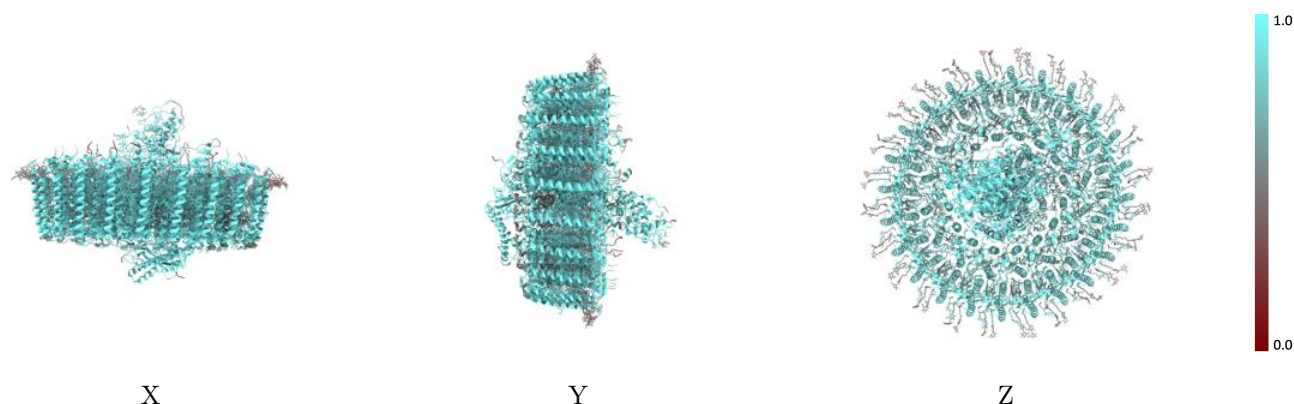
The images above show the 3D surface view of the map at the recommended contour level 0.0233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



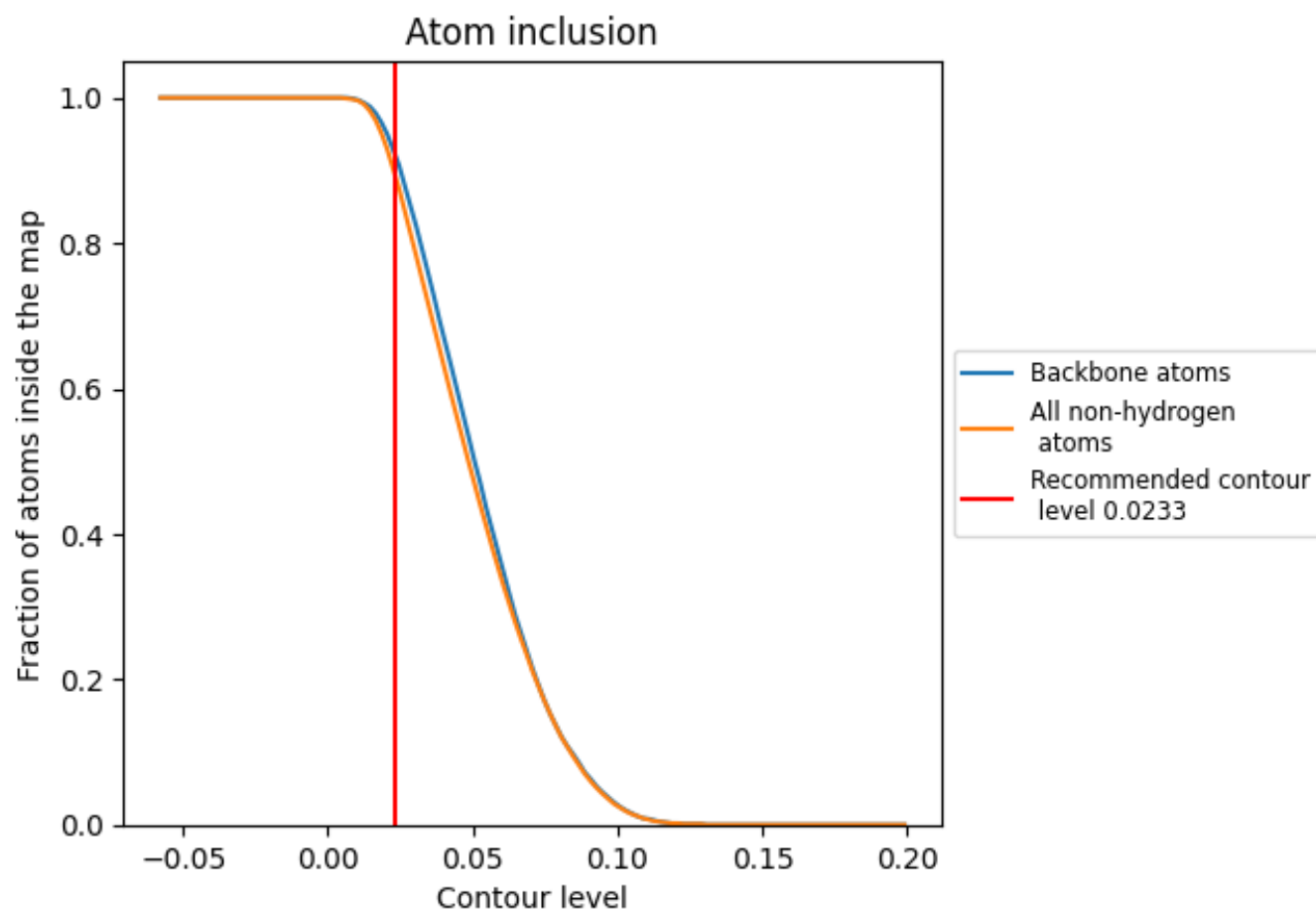
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0233).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.6240
AA	 0.8590	 0.5870
AB	 0.8510	 0.5800
AC	 0.8190	 0.5610
AD	 0.8930	 0.6190
AE	 0.8120	 0.5800
AF	 0.9480	 0.6370
AG	 0.9480	 0.6470
AH	 0.8420	 0.5970
AI	 0.9640	 0.6460
AJ	 0.9310	 0.6380
AK	 0.8930	 0.6160
AL	 0.8730	 0.6060
AM	 0.9460	 0.6460
AN	 0.9070	 0.6210
AO	 0.8760	 0.6080
AP	 0.9500	 0.6410
AQ	 0.8630	 0.6060
AR	 0.9690	 0.6490
AS	 0.9520	 0.6440
AT	 0.9240	 0.6290
AU	 0.9020	 0.6180
AV	 0.9240	 0.6210
AW	 0.9040	 0.6150
AX	 0.8010	 0.5580
BA	 0.8110	 0.5650
BB	 0.7300	 0.5280
BC	 0.7500	 0.5360
BD	 0.7940	 0.5800
BE	 0.8300	 0.5780
BF	 0.8430	 0.5850
BG	 0.8590	 0.6100
BH	 0.8470	 0.5960
BI	 0.8240	 0.5800
BJ	 0.8320	 0.5970



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BK	 0.8510	 0.6060
BL	 0.7970	 0.5640
BM	 0.8320	 0.5950
BN	 0.8320	 0.5890
BO	 0.8380	 0.5820
BP	 0.8350	 0.6010
BQ	 0.8500	 0.6070
BR	 0.8150	 0.5920
BS	 0.8330	 0.6020
BT	 0.8070	 0.5840
BU	 0.8410	 0.5990
BV	 0.8310	 0.5890
BW	 0.7990	 0.5780
BX	 0.7740	 0.5410
C	 0.9440	 0.6660
C1	 0.9470	 0.6680
C2	 0.9200	 0.6080
CG	 0.7620	 0.5370
H1	 0.9080	 0.6510
H2	 0.9400	 0.6490
L	 0.9740	 0.6910
M	 0.9430	 0.6760
MG	 1.0000	 0.6310
aa	 0.8320	 0.5920
ab	 0.8520	 0.5940
ac	 0.9070	 0.6260
ad	 0.9270	 0.6420
ae	 0.9340	 0.6700
af	 0.8780	 0.6230
ag	 0.9010	 0.6380
ah	 0.9030	 0.6230
ai	 0.9100	 0.6400
aj	 0.9220	 0.6500
ak	 0.9630	 0.6660
al	 0.9220	 0.6500
am	 0.9180	 0.6510
an	 0.9440	 0.6490
ao	 0.9010	 0.6270
ap	 0.8950	 0.6050
ba	 0.8640	 0.6070
bb	 0.8530	 0.5940
bc	 0.8810	 0.6240

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
bd	 0.9090	 0.6420
be	 0.9040	 0.6300
bf	 0.9250	 0.6360
bg	 0.9300	 0.6400
bh	 0.9040	 0.6190
bi	 0.9160	 0.6280
bj	 0.9200	 0.6350
bk	 0.9320	 0.6480
bl	 0.9200	 0.6290
bm	 0.9400	 0.6410
bn	 0.9100	 0.6220
bo	 0.9400	 0.6400
bp	 0.8650	 0.5860