



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:34 PM UTC

PDB ID : 7O0V / pdb_00007o0v
EMDB ID : EMD-12680
Title : Cryo-EM structure (model_2a) of the RC-dLH complex from Gemmatimonas phototrophica at 2.5 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-27
Resolution : 2.50 Å (reported)
Based on initial models : 1LGH, 6ET5, 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:

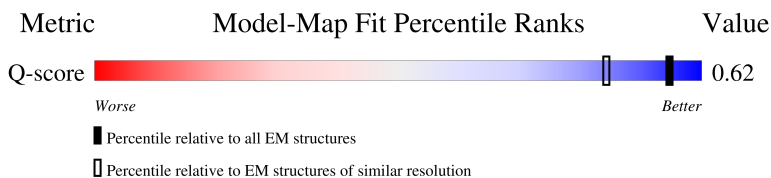
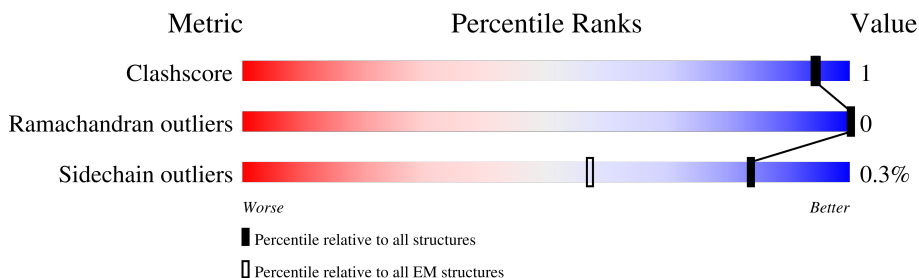
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.50 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	7115 (2.00 - 3.00)

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	AE	54	
1	AF	54	

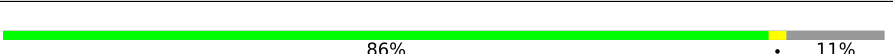
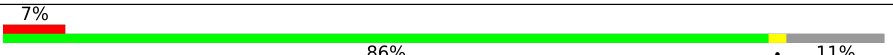
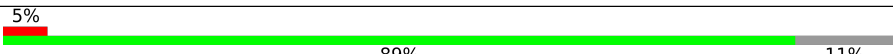
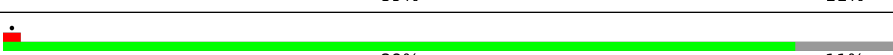
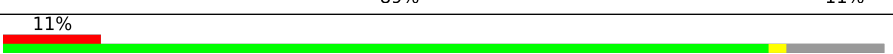
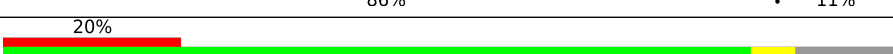
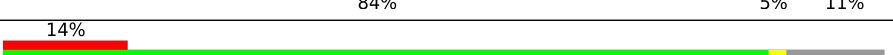
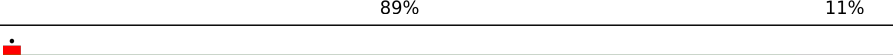
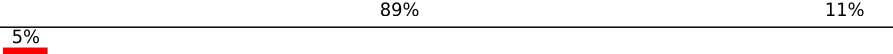
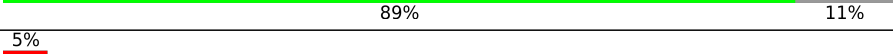
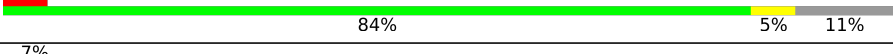
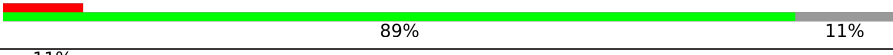
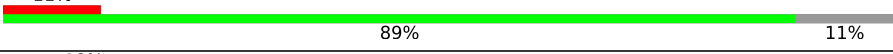
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Mol	Chain	Length	Quality of chain
1	AG	54	
1	AH	54	
1	AI	54	
1	AJ	54	
1	AK	54	
1	AL	54	
1	AM	54	
1	AN	54	
1	AO	54	
1	AP	54	
1	AQ	54	
1	AR	54	
1	AS	54	
1	AT	54	
1	AU	54	
1	AV	54	
1	AW	54	
1	AX	54	
2	AC	54	
2	AD	54	
3	BA	44	
3	BC	44	
3	BF	44	
3	BG	44	
3	BH	44	

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Mol	Chain	Length	Quality of chain
3	BJ	44	
3	BK	44	
3	BL	44	
3	BM	44	
3	BN	44	
3	BO	44	
3	BP	44	
3	BU	44	
3	BX	44	
3	ba	44	
3	bb	44	
3	bc	44	
3	bd	44	
3	be	44	
3	bf	44	
3	bg	44	
3	bh	44	
3	bi	44	
3	bj	44	
3	bk	44	
3	bl	44	
3	bm	44	
3	bo	44	
3	bp	44	
4	BB	43	

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Mol	Chain	Length	Quality of chain
4	BD	43	
4	BE	43	
4	BI	43	
4	BQ	43	
4	BR	43	
4	BS	43	
4	BT	43	
4	BV	43	
4	BW	43	
4	bn	43	
5	C	354	
6	C1	202	
7	H1	67	
8	H2	181	
9	L	274	
10	M	367	
11	aa	71	
12	ab	71	
12	ac	71	
12	ad	71	
12	ae	71	
12	af	71	
12	ag	71	
12	ah	71	
12	ai	71	

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

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 55475 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	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		
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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 LHH-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
2	AD	48	Total	C	N	O	S	0	0
			384	256	64	60	4		

- Molecule 3 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BC	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BF	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BG	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BH	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BJ	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BK	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BL	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BM	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BN	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BO	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BP	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BU	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BX	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	ba	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bb	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bc	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bd	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	be	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bf	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bg	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bh	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bi	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bj	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bk	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bl	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bm	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bo	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bp	39	Total 323	C 213	N 55	O 53	S 2	0	0

- Molecule 4 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BD	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BE	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BI	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BQ	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BR	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BS	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BT	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BV	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BW	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	bn	40	Total	C	N	O	S	0	0
			327	215	56	54	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	?	-	LYS	deletion	UNP A0A143BHS8
BD	?	-	LYS	deletion	UNP A0A143BHS8
BE	?	-	LYS	deletion	UNP A0A143BHS8
BI	?	-	LYS	deletion	UNP A0A143BHS8
BQ	?	-	LYS	deletion	UNP A0A143BHS8
BR	?	-	LYS	deletion	UNP A0A143BHS8
BS	?	-	LYS	deletion	UNP A0A143BHS8
BT	?	-	LYS	deletion	UNP A0A143BHS8
BV	?	-	LYS	deletion	UNP A0A143BHS8
BW	?	-	LYS	deletion	UNP A0A143BHS8
bn	?	-	LYS	deletion	UNP A0A143BHS8

- Molecule 5 is a protein called MULTHEME_CYTC domain-containing protein.

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

- Molecule 6 is a protein called RC-S.

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

- Molecule 7 is a protein called PRCH domain-containing protein.

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

- Molecule 8 is a protein called RC-Hc.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H2	174	Total	C	N	O	S	0	0
			1354	863	229	258	4		

- Molecule 9 is a protein called Photosynthetic reaction center L subunit.

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

- Molecule 10 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	315	Total	C	N	O	S	0	0
			2536	1691	417	418	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aa	55	Total	C	N	O	S	0	0
			433	284	76	71	2		

- Molecule 12 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	ab	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		

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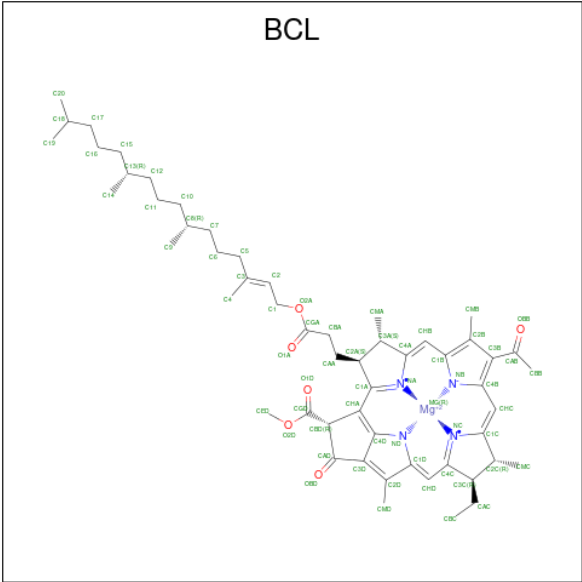
Mol	Chain	Residues	Atoms					AltConf	Trace
12	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ae	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	af	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ag	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
12	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	an	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
12	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ap	71	Total	C	N	O	S	0	0
			543	352	95	92	4		

- Molecule 13 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



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

- Molecule 14 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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

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

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

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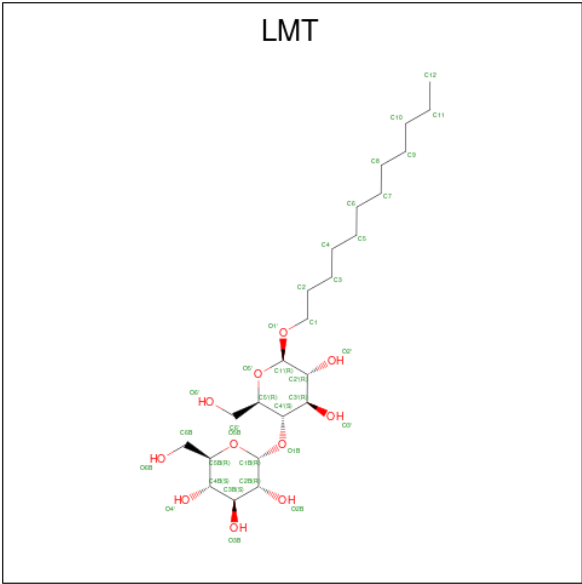
Mol	Chain	Residues	Atoms					AltConf
14	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ai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

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

- Molecule 15 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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Mol	Chain	Residues	Atoms			AltConf
15	AA	1	Total 35	C 24	O 11	0
15	AC	1	Total 35	C 24	O 11	0
15	AD	1	Total 35	C 24	O 11	0
15	AD	1	Total 35	C 24	O 11	0
15	AE	1	Total 35	C 24	O 11	0
15	AF	1	Total 35	C 24	O 11	0
15	AG	1	Total 35	C 24	O 11	0
15	AH	1	Total 35	C 24	O 11	0
15	AH	1	Total 35	C 24	O 11	0
15	AI	1	Total 35	C 24	O 11	0
15	AJ	1	Total 35	C 24	O 11	0
15	AJ	1	Total 35	C 24	O 11	0
15	AL	1	Total 35	C 24	O 11	0
15	AN	1	Total 35	C 24	O 11	0
15	AP	1	Total 35	C 24	O 11	0
15	AP	1	Total 35	C 24	O 11	0
15	AQ	1	Total 35	C 24	O 11	0
15	AS	1	Total 35	C 24	O 11	0
15	AT	1	Total 35	C 24	O 11	0
15	AU	1	Total 35	C 24	O 11	0
15	AX	1	Total 35	C 24	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
15	BA	1	Total 35	C 24	O 11	0
15	BA	1	Total 35	C 24	O 11	0
15	BA	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BE	1	Total 35	C 24	O 11	0
15	BE	1	Total 35	C 24	O 11	0
15	BF	1	Total 35	C 24	O 11	0
15	BF	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
15	BH	1	Total	C	O	0
			35	24	11	
15	BH	1	Total	C	O	0
			35	24	11	
15	BH	1	Total	C	O	0
			35	24	11	
15	BI	1	Total	C	O	0
			35	24	11	
15	BI	1	Total	C	O	0
			35	24	11	
15	BI	1	Total	C	O	0
			35	24	11	
15	BI	1	Total	C	O	0
			35	24	11	
15	BJ	1	Total	C	O	0
			35	24	11	
15	BJ	1	Total	C	O	0
			35	24	11	
15	BK	1	Total	C	O	0
			35	24	11	
15	BK	1	Total	C	O	0
			35	24	11	
15	BK	1	Total	C	O	0
			35	24	11	
15	BK	1	Total	C	O	0
			35	24	11	
15	BL	1	Total	C	O	0
			35	24	11	
15	BL	1	Total	C	O	0
			35	24	11	
15	BL	1	Total	C	O	0
			35	24	11	
15	BM	1	Total	C	O	0
			35	24	11	
15	BM	1	Total	C	O	0
			35	24	11	
15	BN	1	Total	C	O	0
			35	24	11	
15	BN	1	Total	C	O	0
			35	24	11	
15	BN	1	Total	C	O	0
			35	24	11	

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

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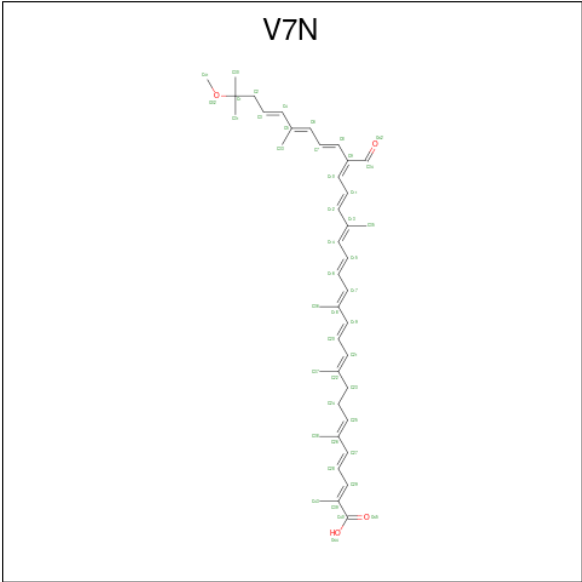
Mol	Chain	Residues	Atoms			AltConf
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BX	1	Total	C	O	0
			35	24	11	
15	BX	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	M	1	Total	C	O	0
			35	24	11	
15	ab	1	Total	C	O	0
			35	24	11	
15	bb	1	Total	C	O	0
			35	24	11	
15	bc	1	Total	C	O	0
			35	24	11	
15	bd	1	Total	C	O	0
			35	24	11	
15	be	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
15	bf	1	Total	C	O	0
			35	24	11	
15	bg	1	Total	C	O	0
			35	24	11	
15	bh	1	Total	C	O	0
			35	24	11	
15	bh	1	Total	C	O	0
			35	24	11	
15	bi	1	Total	C	O	0
			35	24	11	
15	bj	1	Total	C	O	0
			35	24	11	
15	bl	1	Total	C	O	0
			35	24	11	
15	bl	1	Total	C	O	0
			35	24	11	
15	bm	1	Total	C	O	0
			35	24	11	
15	bm	1	Total	C	O	0
			35	24	11	
15	bn	1	Total	C	O	0
			35	24	11	
15	bn	1	Total	C	O	0
			35	24	11	
15	bo	1	Total	C	O	0
			35	24	11	
15	bo	1	Total	C	O	0
			35	24	11	

- Molecule 16 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-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: C₄₁H₅₄O₄).



Mol	Chain	Residues	Atoms			AltConf
16	AE	1	Total	C	O	0
			45	41	4	
16	AO	1	Total	C	O	0
			45	41	4	
16	AS	1	Total	C	O	0
			45	41	4	
16	BA	1	Total	C	O	0
			45	41	4	
16	BB	1	Total	C	O	0
			45	41	4	
16	BC	1	Total	C	O	0
			45	41	4	
16	BD	1	Total	C	O	0
			45	41	4	
16	BE	1	Total	C	O	0
			45	41	4	
16	BG	1	Total	C	O	0
			45	41	4	
16	BH	1	Total	C	O	0
			45	41	4	
16	BI	1	Total	C	O	0
			45	41	4	
16	BJ	1	Total	C	O	0
			45	41	4	
16	BK	1	Total	C	O	0
			45	41	4	
16	BL	1	Total	C	O	0
			45	41	4	

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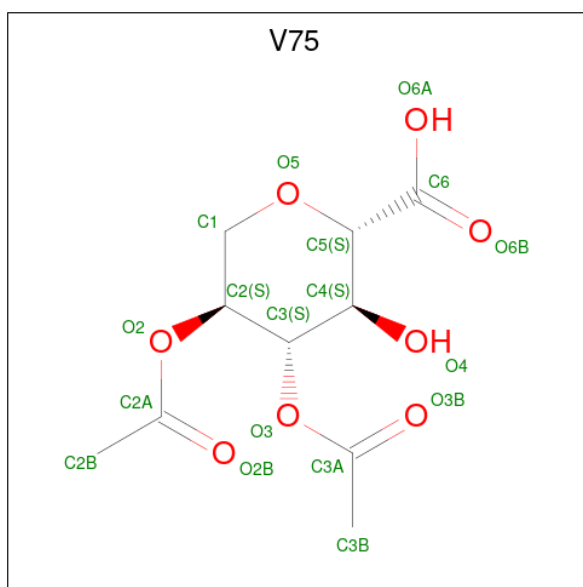
Mol	Chain	Residues	Atoms			AltConf
16	BM	1	Total	C	O	0
			45	41	4	
16	BO	1	Total	C	O	0
			45	41	4	
16	BP	1	Total	C	O	0
			45	41	4	
16	BQ	1	Total	C	O	0
			45	41	4	
16	BR	1	Total	C	O	0
			45	41	4	
16	BS	1	Total	C	O	0
			45	41	4	
16	BU	1	Total	C	O	0
			45	41	4	
16	BV	1	Total	C	O	0
			45	41	4	
16	BW	1	Total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

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

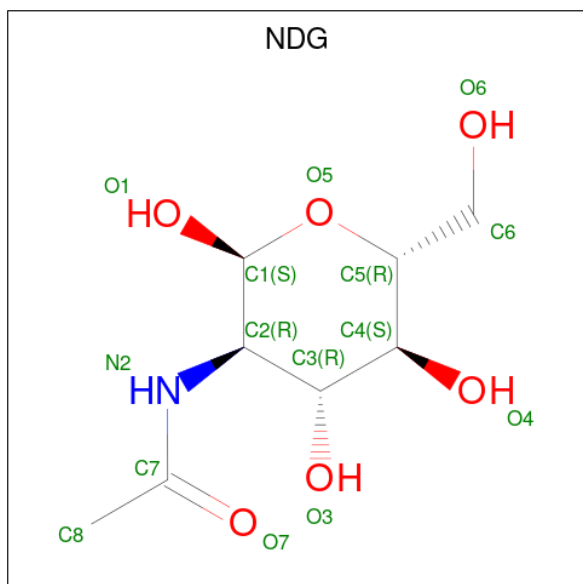
-
- The diagram illustrates the chemical structure of HEC (Hydroxyethylchlorin). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is highly substituted with various side chains and functional groups. Key features include:
- Central Core:** A central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. A central hydrogen bond (FE) is indicated between the iron atom and a nitrogen atom (NB).
 - Substituents:** The ring is substituted with various side chains, including:
 - Top Left:** A side chain with a carboxylic acid group (O1A, O1D) and a hydroxyl group (OH).
 - Top Right:** A side chain with a carboxylic acid group (O2A, O2D) and a hydroxyl group (OH).
 - Bottom Left:** A side chain with a carboxylic acid group (O1A, O1D) and a hydroxyl group (OH).
 - Bottom Right:** A side chain with a carboxylic acid group (O2A, O2D) and a hydroxyl group (OH).
 - Other Labels:** Numerous other labels (e.g., CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, C1A, C1B, C2A, C2B, C3C, C4C, C1D, C1E, C2D, C2E, C3D, C4D) are present, indicating specific atoms and bonds within the structure.

- 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).



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: $C_8H_{15}NO_6$).



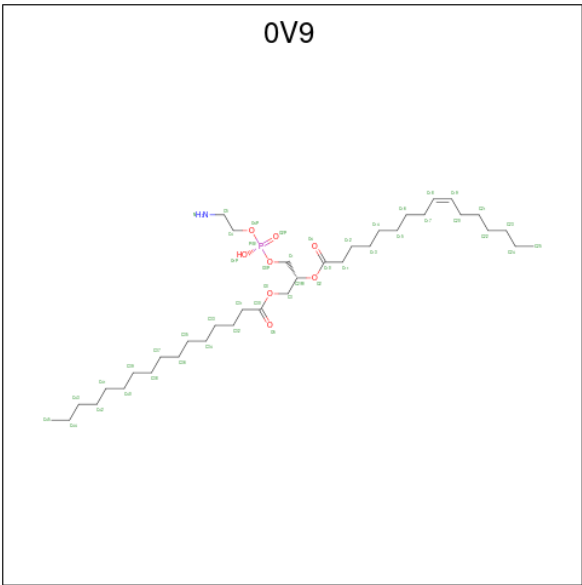
Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 20 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).



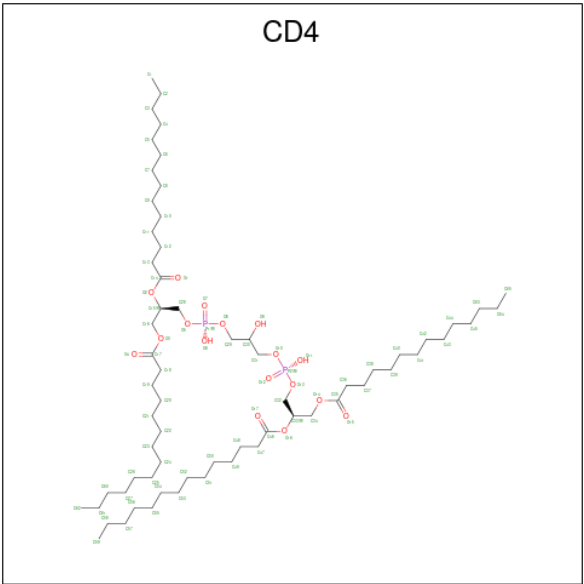
Mol	Chain	Residues	Atoms					AltConf
20	C1	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	H1	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	aj	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	ba	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bb	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bc	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	be	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	be	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bg	1	Total	C	N	O	P	0
			45	35	1	8	1	

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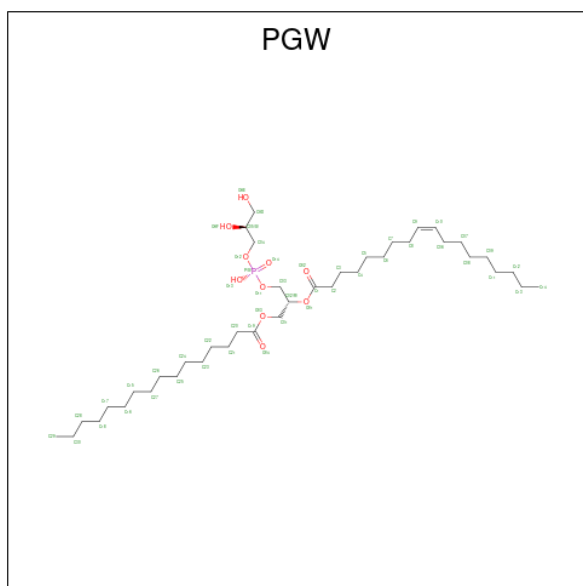
Mol	Chain	Residues	Atoms					AltConf
20	bg	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bh	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bi	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bj	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bk	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bk	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bl	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bm	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bn	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bo	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bp	1	Total	C	N	O	P	0
			45	35	1	8	1	

- 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).



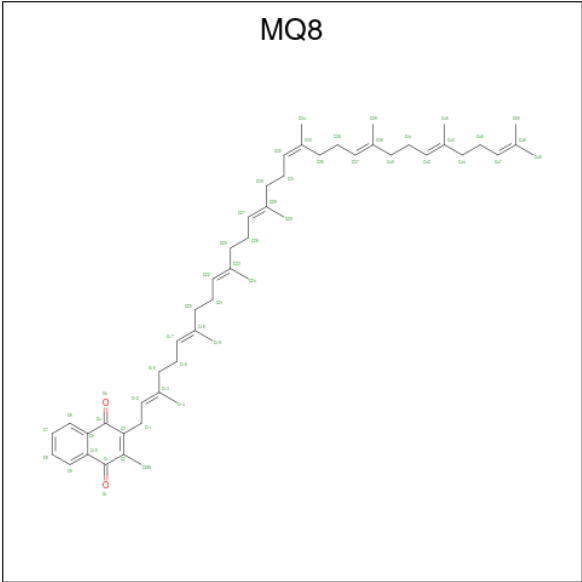
Mol	Chain	Residues	Atoms				AltConf
21	H1	1	Total	C	O	P	0
			84	65	17	2	
21	H1	1	Total	C	O	P	0
			84	65	17	2	
21	M	1	Total	C	O	P	0
			84	65	17	2	
21	ae	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	
21	aj	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 22 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



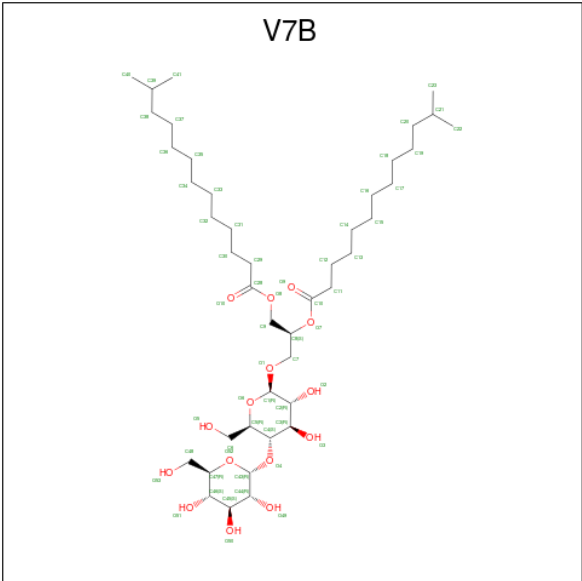
Mol	Chain	Residues	Atoms				AltConf
22	H1	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 23 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



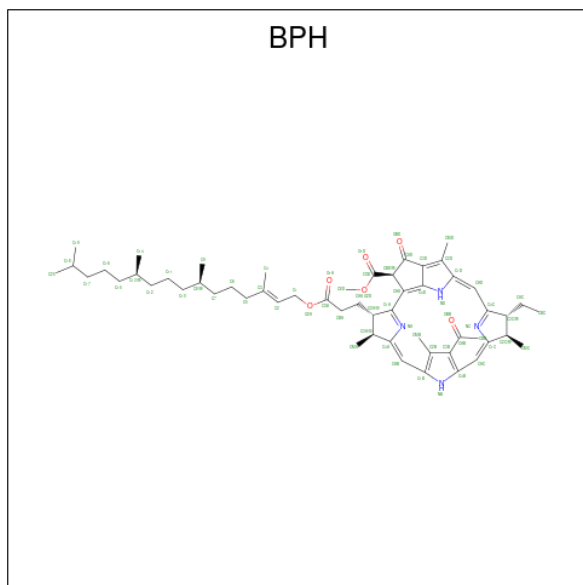
Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	ao	1	Total	C	O	0
			53	51	2	

- Molecule 24 is [(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).



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

- Molecule 25 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

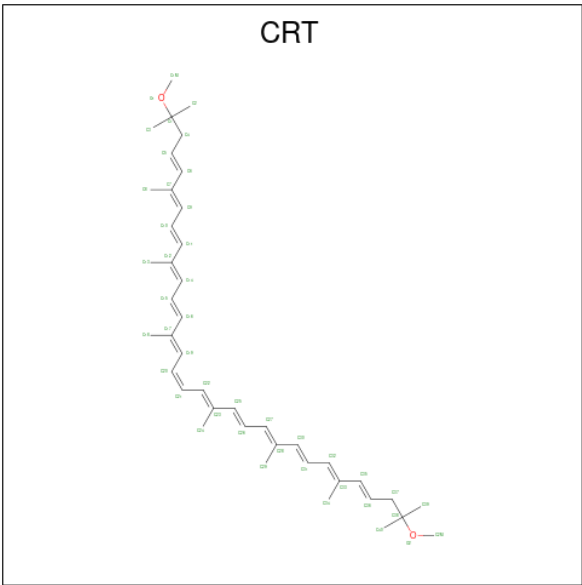


Mol	Chain	Residues	Atoms				AltConf
25	L	1	Total	C	N	O	0
			65	55	4	6	
25	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 26 is FE (III) ION (CCD ID: FE) (formula: Fe).

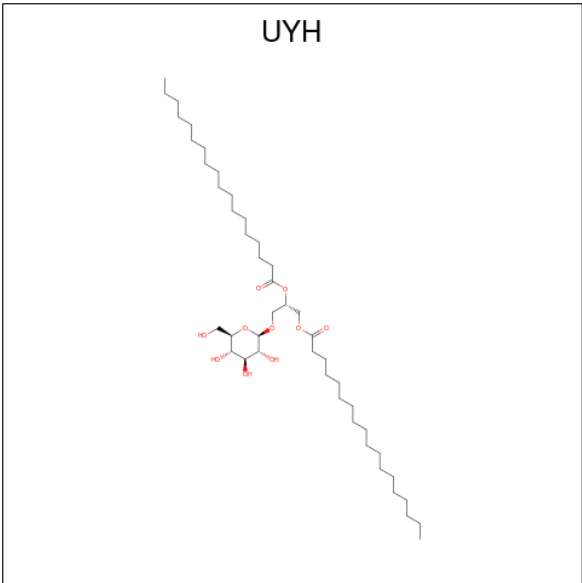
Mol	Chain	Residues	Atoms		AltConf
26	M	1	Total	Fe	0
			1	1	

- Molecule 27 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



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

- Molecule 28 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(o xidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (CCD ID: UYH) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	AltConf
29	AA	2	Total O 2 2	0
29	AB	3	Total O 3 3	0
29	AC	3	Total O 3 3	0
29	AD	1	Total O 1 1	0
29	AE	3	Total O 3 3	0
29	AF	2	Total O 2 2	0
29	AG	5	Total O 5 5	0
29	AH	1	Total O 1 1	0
29	AI	3	Total O 3 3	0
29	AJ	5	Total O 5 5	0
29	AK	4	Total O 4 4	0
29	AL	2	Total O 2 2	0
29	AM	6	Total O 6 6	0
29	AN	4	Total O 4 4	0
29	AO	4	Total O 4 4	0
29	AP	4	Total O 4 4	0
29	AQ	4	Total O 4 4	0
29	AS	6	Total O 6 6	0
29	AT	2	Total O 2 2	0
29	AU	1	Total O 1 1	0
29	AV	6	Total O 6 6	0
29	AW	2	Total O 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
29	AX	3	Total O 3 3	0
29	BB	1	Total O 1 1	0
29	BI	1	Total O 1 1	0
29	BJ	1	Total O 1 1	0
29	BO	1	Total O 1 1	0
29	BP	1	Total O 1 1	0
29	C	86	Total O 86 86	0
29	C1	42	Total O 42 42	0
29	H1	17	Total O 17 17	0
29	H2	9	Total O 9 9	0
29	L	51	Total O 51 51	0
29	M	58	Total O 58 58	0
29	aa	3	Total O 3 3	0
29	ab	3	Total O 3 3	0
29	ac	3	Total O 3 3	0
29	ad	6	Total O 6 6	0
29	ae	10	Total O 10 10	0
29	af	11	Total O 11 11	0
29	ag	7	Total O 7 7	0
29	ah	6	Total O 6 6	0
29	ai	5	Total O 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
29	aj	7	Total O 7 7	0
29	ak	13	Total O 13 13	0
29	al	5	Total O 5 5	0
29	am	5	Total O 5 5	0
29	an	9	Total O 9 9	0
29	ao	5	Total O 5 5	0
29	ap	11	Total O 11 11	0
29	ba	3	Total O 3 3	0
29	bb	4	Total O 4 4	0
29	bc	2	Total O 2 2	0
29	bd	3	Total O 3 3	0
29	be	4	Total O 4 4	0
29	bf	1	Total O 1 1	0
29	bg	2	Total O 2 2	0
29	bh	2	Total O 2 2	0
29	bi	2	Total O 2 2	0
29	bj	3	Total O 3 3	0
29	bk	3	Total O 3 3	0
29	bl	3	Total O 3 3	0
29	bm	2	Total O 2 2	0
29	bn	1	Total O 1 1	0

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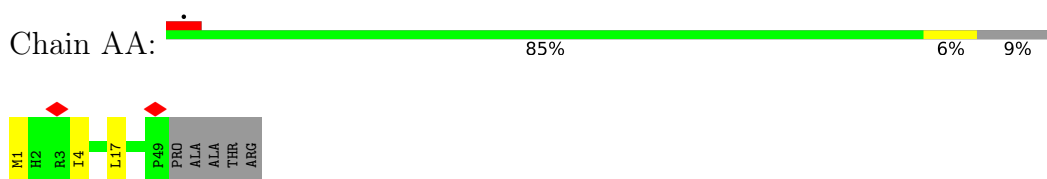
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Mol	Chain	Residues	Atoms		AltConf
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			1	1	

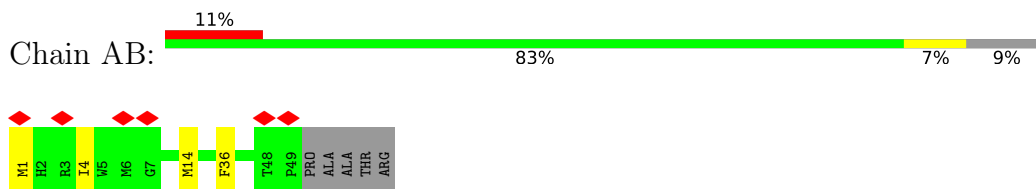
3 Residue-property plots [i](#)

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.

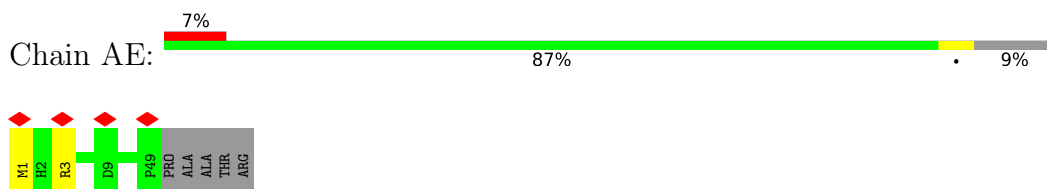
- Molecule 1: LHh-alpha



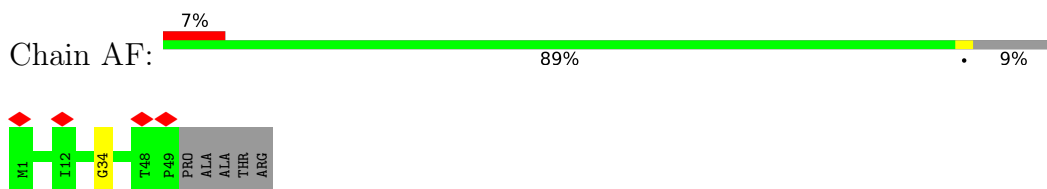
- Molecule 1: LHh-alpha



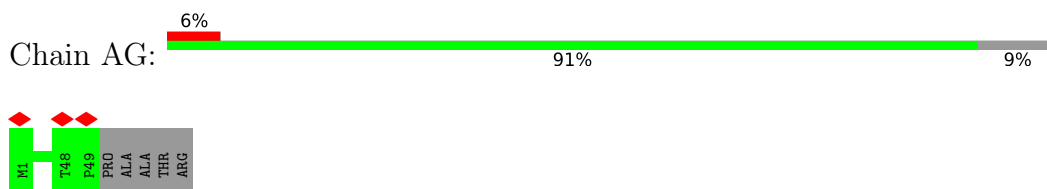
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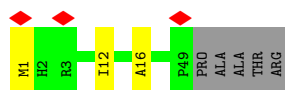
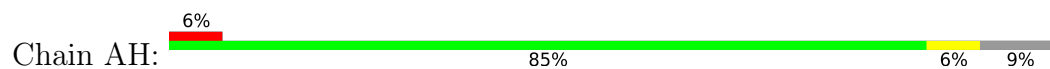
- Molecule 1: LHh-alpha



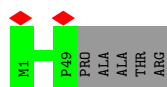
- Molecule 1: LHh-alpha



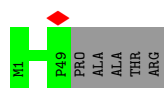
● Molecule 1: LHh-alpha



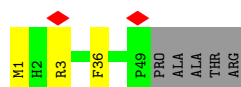
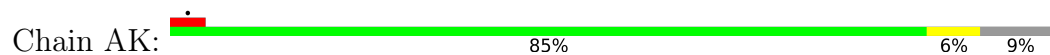
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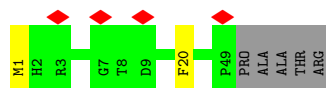
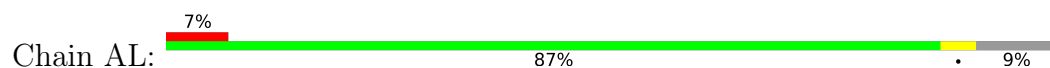
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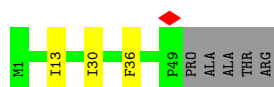
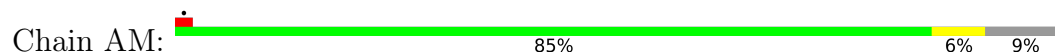
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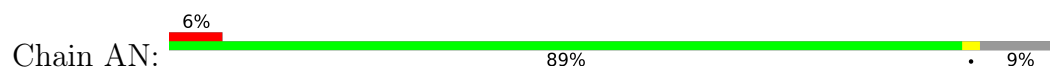
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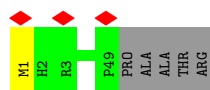


● Molecule 1: LHh-alpha

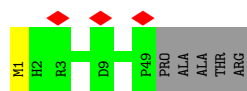
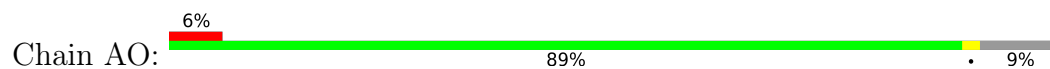


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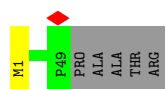




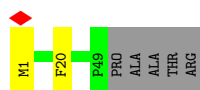
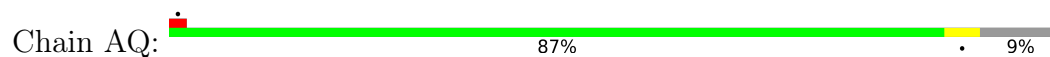
- Molecule 1: LHh-alpha



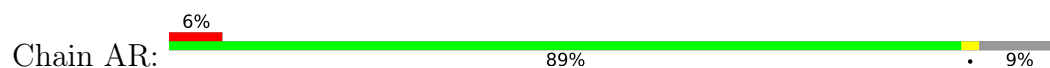
- Molecule 1: LHh-alpha



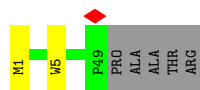
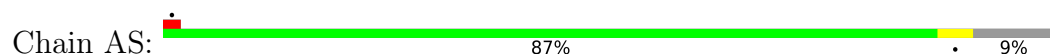
- Molecule 1: LHh-alpha



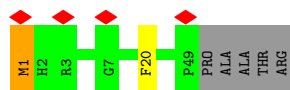
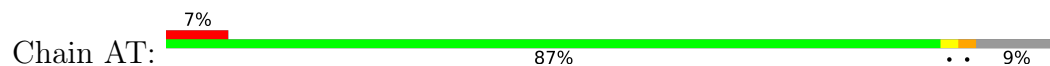
- Molecule 1: LHh-alpha



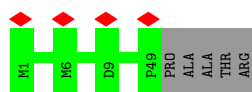
- Molecule 1: LHh-alpha



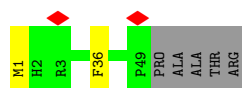
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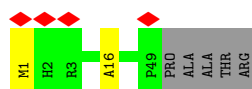
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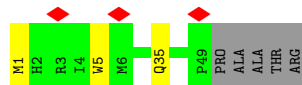
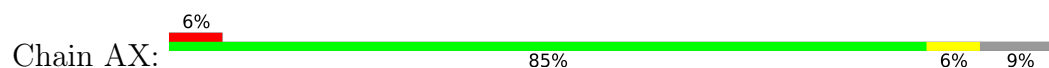
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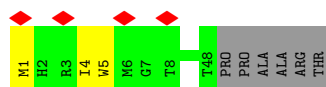
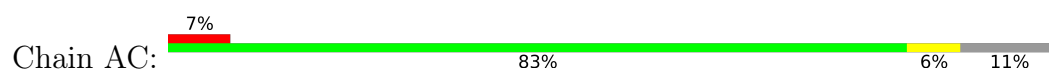
- Molecule 1: LHH-alpha



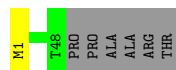
- Molecule 1: LHH-alpha



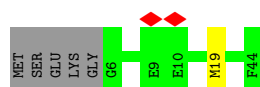
- Molecule 2: LHH-alpha



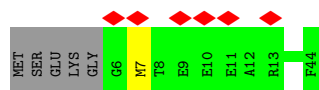
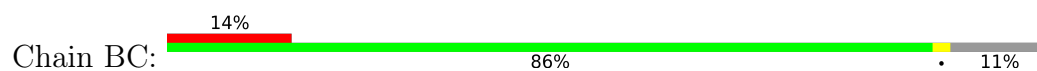
- Molecule 2: LHH-alpha



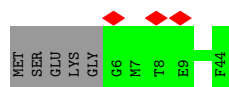
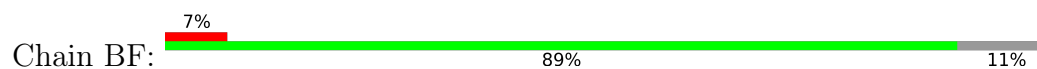
- Molecule 3: Light-harvesting protein B:885 subunit beta



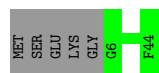
- Molecule 3: Light-harvesting protein B:885 subunit beta



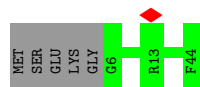
- Molecule 3: Light-harvesting protein B:885 subunit beta



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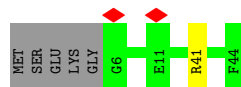
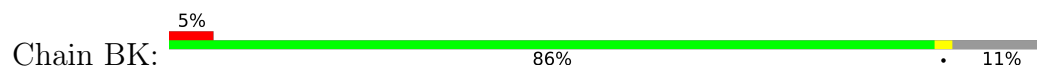
- Molecule 3: Light-harvesting protein B:885 subunit beta



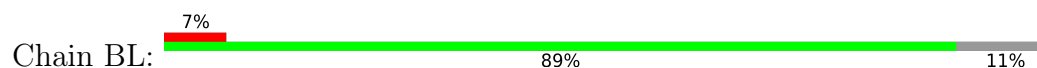
- Molecule 3: Light-harvesting protein B:885 subunit beta

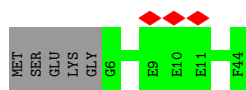


- Molecule 3: Light-harvesting protein B:885 subunit beta

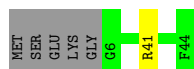
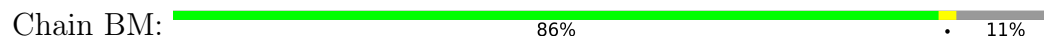


- Molecule 3: Light-harvesting protein B:885 subunit beta

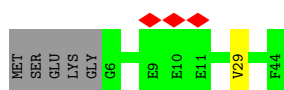
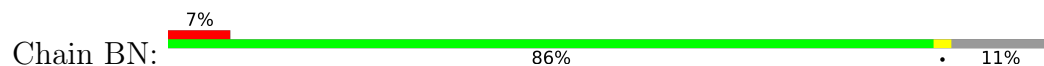




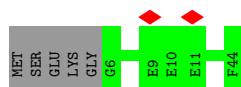
- Molecule 3: Light-harvesting protein B:885 subunit beta



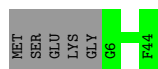
- Molecule 3: Light-harvesting protein B:885 subunit beta



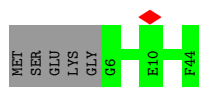
- Molecule 3: Light-harvesting protein B:885 subunit beta



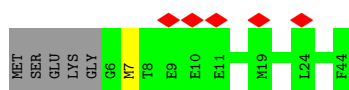
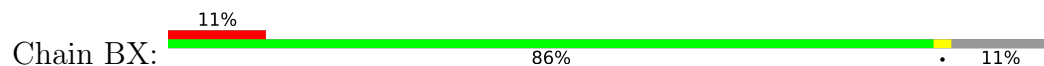
- Molecule 3: Light-harvesting protein B:885 subunit beta



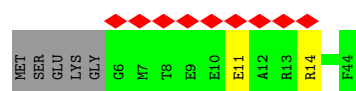
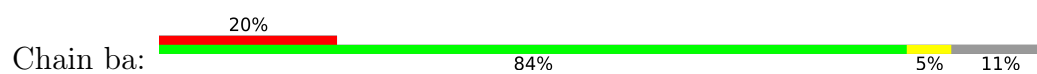
- Molecule 3: Light-harvesting protein B:885 subunit beta



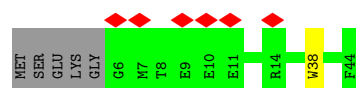
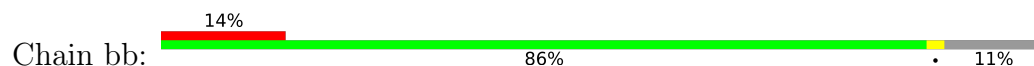
- Molecule 3: Light-harvesting protein B:885 subunit beta



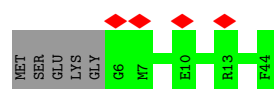
- Molecule 3: Light-harvesting protein B:885 subunit beta



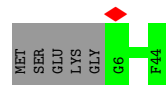
- Molecule 3: Light-harvesting protein B:885 subunit beta



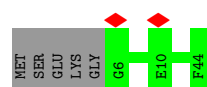
- Molecule 3: Light-harvesting protein B:885 subunit beta



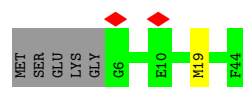
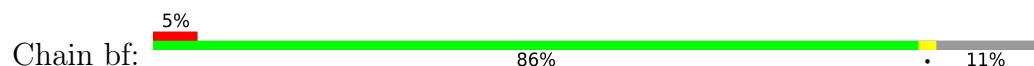
- Molecule 3: Light-harvesting protein B:885 subunit beta



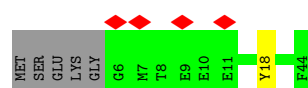
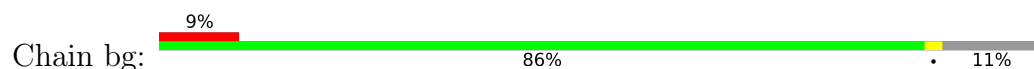
- Molecule 3: Light-harvesting protein B:885 subunit beta



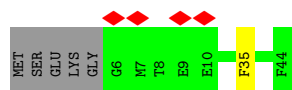
- Molecule 3: Light-harvesting protein B:885 subunit beta



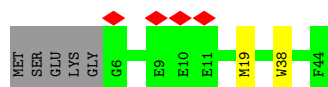
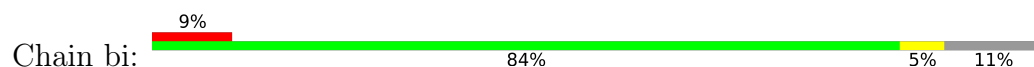
- Molecule 3: Light-harvesting protein B:885 subunit beta



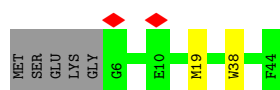
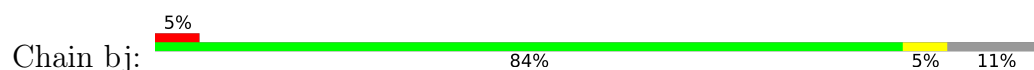
- Molecule 3: Light-harvesting protein B:885 subunit beta



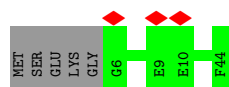
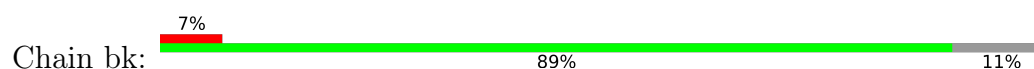
- Molecule 3: Light-harvesting protein B:885 subunit beta



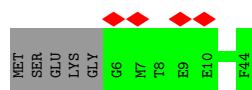
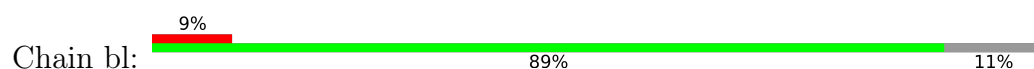
- Molecule 3: Light-harvesting protein B:885 subunit beta



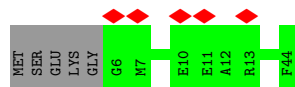
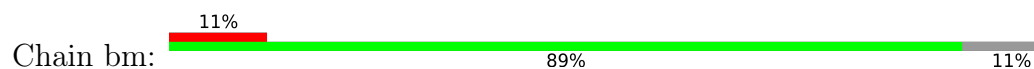
- Molecule 3: Light-harvesting protein B:885 subunit beta



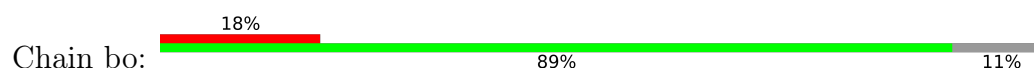
- Molecule 3: Light-harvesting protein B:885 subunit beta

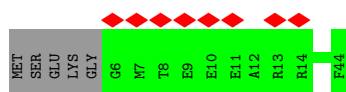


- Molecule 3: Light-harvesting protein B:885 subunit beta

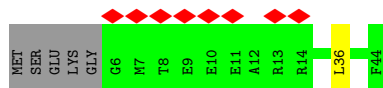
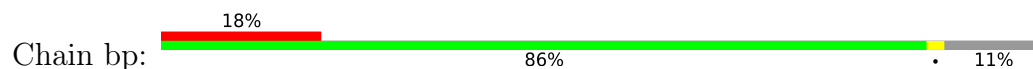


- Molecule 3: Light-harvesting protein B:885 subunit beta

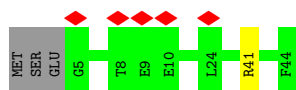




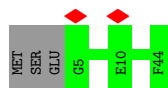
- Molecule 3: Light-harvesting protein B:885 subunit beta



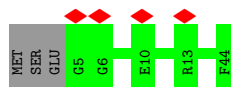
- Molecule 4: Light-harvesting protein B:885 subunit beta



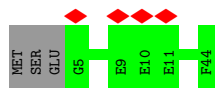
- Molecule 4: Light-harvesting protein B:885 subunit beta



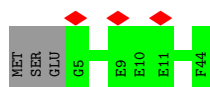
- Molecule 4: Light-harvesting protein B:885 subunit beta



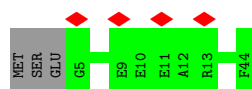
- Molecule 4: Light-harvesting protein B:885 subunit beta



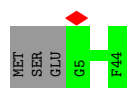
- Molecule 4: Light-harvesting protein B:885 subunit beta



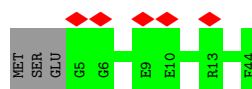
- Molecule 4: Light-harvesting protein B:885 subunit beta



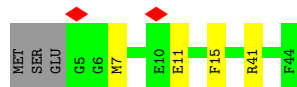
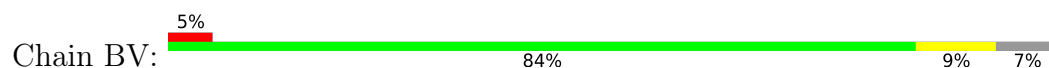
- Molecule 4: Light-harvesting protein B:885 subunit beta



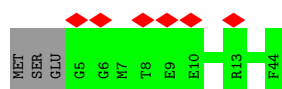
- Molecule 4: Light-harvesting protein B:885 subunit beta



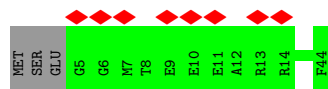
- Molecule 4: Light-harvesting protein B:885 subunit beta



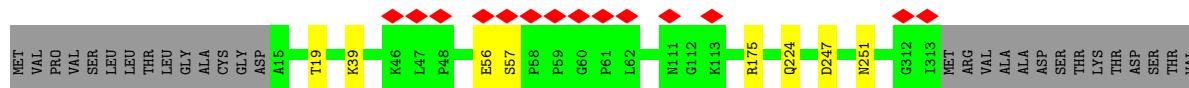
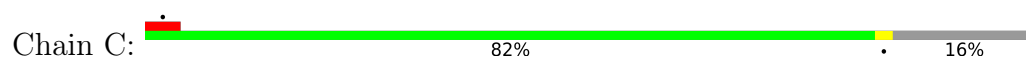
- Molecule 4: Light-harvesting protein B:885 subunit beta



- Molecule 4: Light-harvesting protein B:885 subunit beta



- Molecule 5: MULTHEME_CYTC domain-containing protein



VAL
ALA
ALA
PRO
ALA
ALA
ALA
PRO
ALA
ALA
GLN
ARG
THR
SER
ALA
ARG
PRO
GLY
SER
VAL
THR
THR
VAL
GLY
VAL
ASN

• Molecule 6: RC-S

Chain C1:  50% 49%

MET
PRO
ALA
SER
PRO
SER
PRO
LEU
PRO
ARG
SER
SER
GLY
VAL
ASP
ASN
ALA
SER
VAL
VAL
VAL
VAL
ALA
LEU
VAL
VAL
ALA
GLY
LEU
ALA
ALA
ARG
GLY
ASP
ALA
GLN
GLY
THR
GLN
PRO
PRO
VAL
ALA
PRO
PRO
ALA
ALA
THR
THR
ALA
ALA
PRO
ASP
LEU
VAL
GLN
ASP

SER
THR
LYS
ALA
ASP
SER
THR
ALA
VAL
ALA
ASP
THR
LEU
MET
LEU
LEU
MET
MET
VAL
MET
MET
ALA
GLU
GLU
ALA
ALA
ALA
ALA
THR
THR
THR
THR
ALA
PRO
VAL
VAL
ALA
ALA
P98
T99
A100
D104
P105
T106
T107
S154
D180
L200
GLY
GLN

• Molecule 7: PRCH domain-containing protein

Chain H1:  9% 91% 7%

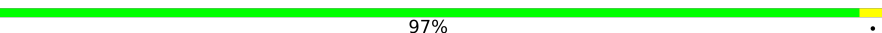
M1
Q9
H58
R59
D60
H61
G62
GLY
GLY
THR
THR
HIS

• Molecule 8: RC-Hc

Chain H2:  13% 96% 7%

MET
S1
D2
D57
A63
K64
G65
D66
K79
L104
A105
S106
G107
E108
R109
R110
M122
F123
G124
L125
W126
D129
D150
D159
E175
ARG
SER
GLN
PRO
ILE
ILE

• Molecule 9: Photosynthetic reaction center L subunit

Chain L:  97%

MET
A1
L77
L91
Y128
H144
F181
V197
C247
I248
V249
K273

• Molecule 10: RC-M

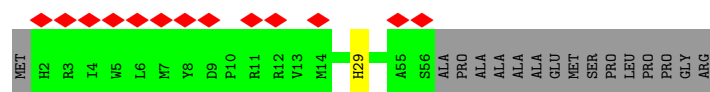
Chain M:  6% 83% 14%

MET
LEU
GLU
TYR
GLN
ASN
LEU
PHE
T9
R10
R14
T15
P16
E18
P19
G20
T21
PRO
ILE
ASP
GLU
SER
THR
GLY
THR
THR
ARG
TVR
GLY
THR
THR
THR
F36
S37
Y38
L39
A40
G41
K42
F43
G44
D45
A46
Q47
R88
E96
P97
M142
H201
T206
F215
A259

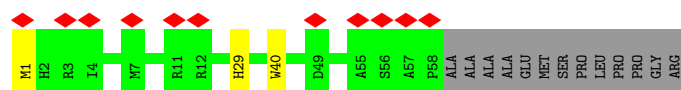
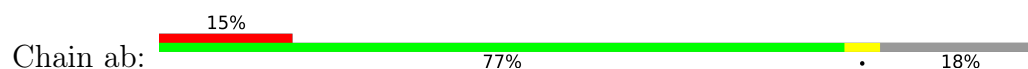
D291
V336
V337
PRO
GLN
ASN
ALA
THR
MET
PRO
ASP
THR
ALA
ALA
ALA
PRO
ILE
VAL
THR
ASP
SER
ILE
THR
THR
ASP
SER
THR
LYS
THR
GLY
GLY
THR
GLN

• Molecule 11: LHC domain-containing protein

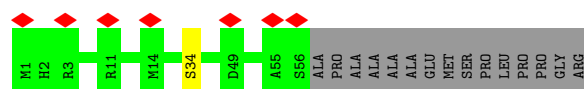
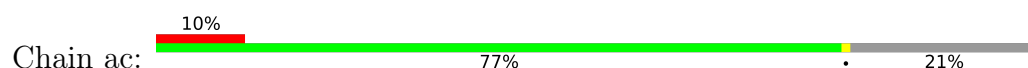
Chain aa:  18% 76% 23%



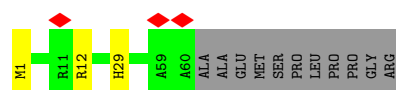
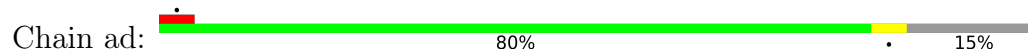
- Molecule 12: LHC domain-containing protein



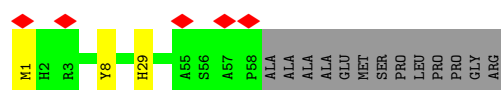
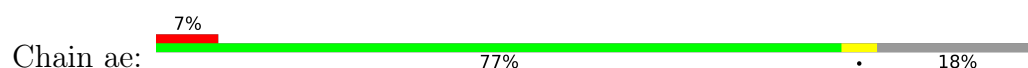
- Molecule 12: LHC domain-containing protein



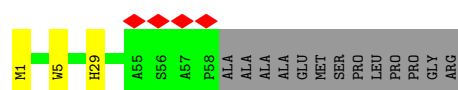
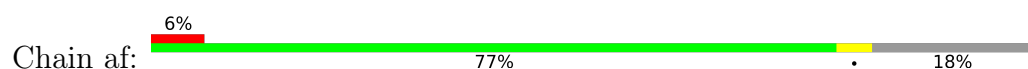
- Molecule 12: LHC domain-containing protein



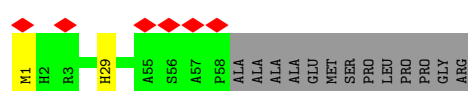
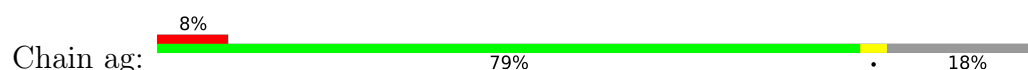
- Molecule 12: LHC domain-containing protein



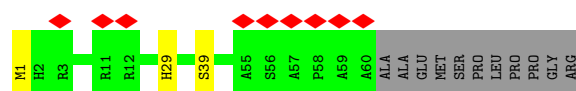
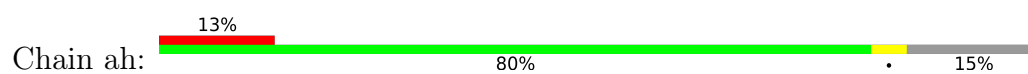
- Molecule 12: LHC domain-containing protein



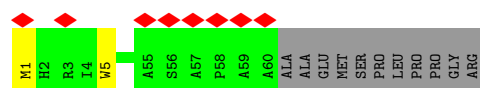
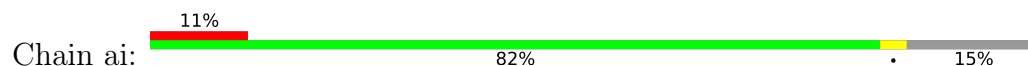
- Molecule 12: LHC domain-containing protein



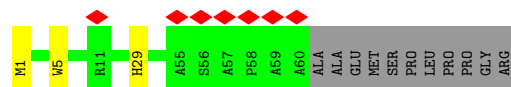
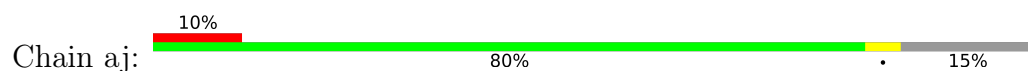
- Molecule 12: LHC domain-containing protein



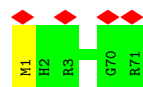
- Molecule 12: LHC domain-containing protein



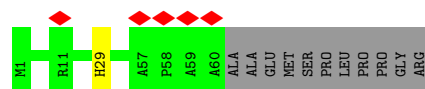
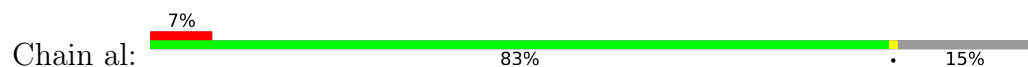
- Molecule 12: LHC domain-containing protein



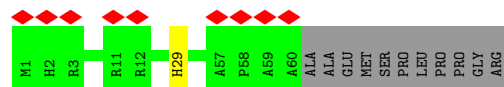
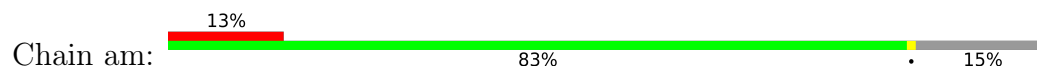
- Molecule 12: LHC domain-containing protein



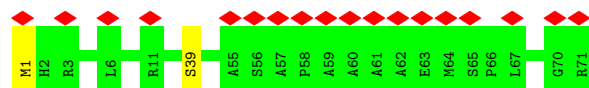
- Molecule 12: LHC domain-containing protein



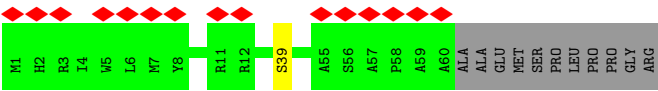
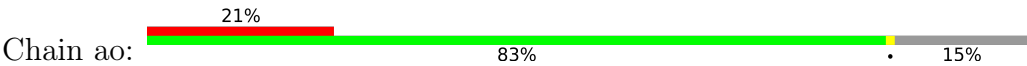
- Molecule 12: LHC domain-containing protein



- Molecule 12: LHC domain-containing protein



• Molecule 12: LHC domain-containing protein



• Molecule 12: LHC domain-containing protein



• Molecule 13: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose



• Molecule 13: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103156	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	0.192	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0348	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V75, FME, NDG, LMT, CRT, V7N, 0V9, V7B, PGW, MQ8, MAN, RAM, UYH, CD4, BPH, HEC, FE, BCL

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	0.14	0/396	0.47	0/541
1	AB	0.14	0/396	0.44	0/541
1	AE	0.14	0/396	0.45	0/541
1	AF	0.17	0/396	0.49	0/541
1	AG	0.14	0/396	0.45	0/541
1	AH	0.14	0/396	0.49	0/541
1	AI	0.14	0/396	0.46	0/541
1	AJ	0.14	0/396	0.47	0/541
1	AK	0.14	0/396	0.47	0/541
1	AL	0.14	0/396	0.44	0/541
1	AM	0.14	0/396	0.47	0/541
1	AN	0.14	0/396	0.45	0/541
1	AO	0.14	0/396	0.46	0/541
1	AP	0.15	0/396	0.49	0/541
1	AQ	0.13	0/396	0.43	0/541
1	AR	0.14	0/396	0.42	0/541
1	AS	0.14	0/396	0.45	0/541
1	AT	0.15	0/396	0.47	0/541
1	AU	0.14	0/396	0.44	0/541
1	AV	0.14	0/396	0.47	0/541
1	AW	0.14	0/396	0.43	0/541
1	AX	0.14	0/396	0.46	0/541
2	AC	0.13	0/388	0.44	0/529
2	AD	0.14	0/388	0.47	0/529
3	BA	0.11	0/336	0.37	0/456
3	BC	0.11	0/336	0.38	0/456
3	BF	0.12	0/336	0.43	0/456
3	BG	0.13	0/336	0.43	0/456
3	BH	0.12	0/336	0.40	0/456
3	BJ	0.12	0/336	0.39	0/456
3	BK	0.13	0/336	0.42	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BL	0.12	0/336	0.42	0/456
3	BM	0.13	0/336	0.43	0/456
3	BN	0.13	0/336	0.44	0/456
3	BO	0.11	0/336	0.41	0/456
3	BP	0.12	0/336	0.47	0/456
3	BU	0.11	0/336	0.40	0/456
3	BX	0.12	0/336	0.44	0/456
3	ba	0.13	0/336	0.40	0/456
3	bb	0.13	0/336	0.42	0/456
3	bc	0.15	0/336	0.45	0/456
3	bd	0.13	0/336	0.40	0/456
3	be	0.14	0/336	0.41	0/456
3	bf	0.13	0/336	0.38	0/456
3	bg	0.13	0/336	0.43	0/456
3	bh	0.12	0/336	0.37	0/456
3	bi	0.13	0/336	0.39	0/456
3	bj	0.13	0/336	0.46	0/456
3	bk	0.16	0/336	0.48	0/456
3	bl	0.13	0/336	0.43	0/456
3	bm	0.14	0/336	0.44	0/456
3	bo	0.13	0/336	0.45	0/456
3	bp	0.14	0/336	0.42	0/456
4	BB	0.12	0/340	0.47	0/461
4	BD	0.12	0/340	0.41	0/461
4	BE	0.11	0/340	0.37	0/461
4	BI	0.11	0/340	0.41	0/461
4	BQ	0.13	0/340	0.48	0/461
4	BR	0.12	0/340	0.40	0/461
4	BS	0.13	0/340	0.43	0/461
4	BT	0.14	0/340	0.46	0/461
4	BV	0.11	0/340	0.36	0/461
4	BW	0.13	0/340	0.44	0/461
4	bn	0.13	0/340	0.39	0/461
5	C	0.18	0/2392	0.49	0/3263
6	C1	0.16	0/826	0.44	0/1128
7	H1	0.16	0/531	0.44	0/717
8	H2	0.15	0/1392	0.45	0/1902
9	L	0.15	0/2252	0.46	0/3081
10	M	0.16	0/2632	0.48	0/3600
11	aa	0.15	0/444	0.46	0/605
12	ab	0.15	0/457	0.44	0/624
12	ac	0.14	0/444	0.46	0/605
12	ad	0.15	0/467	0.44	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	ae	0.17	0/457	0.47	0/624
12	af	0.15	0/457	0.44	0/624
12	ag	0.16	0/457	0.47	0/624
12	ah	0.16	0/467	0.46	0/638
12	ai	0.16	0/467	0.46	0/638
12	aj	0.15	0/467	0.47	0/638
12	ak	0.16	0/547	0.44	0/748
12	al	0.15	0/467	0.44	0/638
12	am	0.18	0/467	0.51	0/638
12	an	0.20	0/547	0.51	0/748
12	ao	0.16	0/467	0.47	0/638
12	ap	0.15	0/548	0.44	0/748
All	All	0.15	0/40624	0.45	0/55362

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
1	AK	0	1
10	M	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AE	3	ARG	Sidechain
1	AK	3	ARG	Sidechain
10	M	88	ARG	Sidechain

5.2 Too-close contacts

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	3	0
1	AE	391	0	390	0	0
1	AF	391	0	390	1	0
1	AG	391	0	390	0	0
1	AH	391	0	390	1	0
1	AI	391	0	390	0	0
1	AJ	391	0	390	0	0
1	AK	391	0	390	1	0
1	AL	391	0	390	1	0
1	AM	391	0	390	3	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	2	0
1	AR	391	0	390	1	0
1	AS	391	0	390	2	0
1	AT	391	0	390	2	0
1	AU	391	0	390	0	0
1	AV	391	0	390	1	0
1	AW	391	0	390	1	0
1	AX	391	0	390	1	0
2	AC	384	0	383	2	0
2	AD	384	0	383	0	0
3	BA	323	0	300	1	0
3	BC	323	0	300	1	0
3	BF	323	0	300	0	0
3	BG	323	0	300	0	0
3	BH	323	0	300	0	0
3	BJ	323	0	300	1	0
3	BK	323	0	300	1	0
3	BL	323	0	300	0	0
3	BM	323	0	300	1	0
3	BN	323	0	300	1	0
3	BO	323	0	300	0	0
3	BP	323	0	300	0	0
3	BU	323	0	300	0	0
3	BX	323	0	300	1	0
3	ba	323	0	300	1	0
3	bb	323	0	300	1	0
3	bc	323	0	300	0	0
3	bd	323	0	300	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	be	323	0	300	0	0
3	bf	323	0	300	1	0
3	bg	323	0	300	1	0
3	bh	323	0	300	1	0
3	bi	323	0	300	2	0
3	bj	323	0	300	2	0
3	bk	323	0	300	0	0
3	bl	323	0	300	0	0
3	bm	323	0	300	0	0
3	bo	323	0	300	0	0
3	bp	323	0	300	1	0
4	BB	327	0	303	1	0
4	BD	327	0	303	0	0
4	BE	327	0	303	0	0
4	BI	327	0	303	0	0
4	BQ	327	0	303	0	0
4	BR	327	0	303	0	0
4	BS	327	0	303	0	0
4	BT	327	0	303	0	0
4	BV	327	0	303	3	0
4	BW	327	0	303	0	0
4	bn	327	0	303	0	0
5	C	2325	0	2245	5	0
6	C1	806	0	818	1	0
7	H1	522	0	503	1	0
8	H2	1354	0	1314	0	0
9	L	2165	0	2126	6	0
10	M	2536	0	2479	7	0
11	aa	433	0	442	1	0
12	ab	455	0	465	2	0
12	ac	443	0	453	1	0
12	ad	465	0	475	2	0
12	ae	455	0	465	2	0
12	af	455	0	465	2	0
12	ag	455	0	465	1	0
12	ah	465	0	475	1	0
12	ai	465	0	475	1	0
12	aj	465	0	475	2	0
12	ak	542	0	553	0	0
12	al	465	0	475	1	0
12	am	465	0	475	1	0
12	an	542	0	553	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	ao	465	0	475	0	0
12	ap	543	0	553	1	0
13	CG	21	0	18	0	0
13	MG	21	0	18	1	0
14	AA	132	0	148	2	0
14	AB	132	0	148	2	0
14	AC	198	0	222	3	0
14	AD	66	0	74	0	0
14	AE	198	0	222	1	0
14	AF	66	0	74	2	0
14	AG	132	0	148	1	0
14	AH	132	0	148	2	0
14	AI	132	0	148	3	0
14	AJ	132	0	148	1	0
14	AK	132	0	148	1	0
14	AL	132	0	148	1	0
14	AM	132	0	148	2	0
14	AN	198	0	222	2	0
14	AO	66	0	74	1	0
14	AP	132	0	148	1	0
14	AQ	132	0	148	1	0
14	AR	132	0	148	3	0
14	AS	198	0	222	4	0
14	AT	66	0	74	1	0
14	AU	132	0	148	2	0
14	AV	198	0	222	2	0
14	AW	66	0	74	3	0
14	AX	132	0	148	3	0
14	BA	66	0	74	0	0
14	BB	66	0	74	0	0
14	BC	66	0	74	0	0
14	BD	66	0	74	0	0
14	BE	66	0	74	0	0
14	BF	66	0	73	0	0
14	BG	66	0	74	0	0
14	BH	66	0	74	0	0
14	BI	66	0	74	2	0
14	BJ	66	0	74	0	0
14	BK	66	0	74	0	0
14	BL	66	0	74	0	0
14	BM	66	0	74	1	0
14	BN	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	BO	66	0	74	0	0
14	BP	66	0	74	0	0
14	BQ	66	0	74	0	0
14	BR	66	0	74	0	0
14	BS	66	0	74	1	0
14	BT	66	0	74	0	0
14	BU	66	0	74	1	0
14	BV	66	0	74	0	0
14	BW	66	0	74	0	0
14	BX	66	0	74	0	0
14	L	132	0	148	2	0
14	M	132	0	148	2	0
14	aa	66	0	74	1	0
14	ab	66	0	74	2	0
14	ac	66	0	74	1	0
14	ad	66	0	74	0	0
14	ae	66	0	74	1	0
14	af	66	0	74	2	0
14	ag	66	0	74	1	0
14	ah	66	0	74	1	0
14	ai	66	0	74	1	0
14	aj	66	0	74	0	0
14	ak	66	0	74	0	0
14	al	66	0	74	0	0
14	am	66	0	74	1	0
14	an	66	0	74	0	0
14	ao	66	0	74	1	0
14	ap	66	0	74	0	0
14	ba	66	0	74	1	0
14	bb	66	0	74	1	0
14	bc	66	0	74	0	0
14	bd	66	0	74	1	0
14	be	66	0	74	1	0
14	bf	66	0	74	2	0
14	bg	66	0	74	1	0
14	bh	66	0	74	1	0
14	bi	66	0	74	0	0
14	bj	66	0	74	1	0
14	bk	66	0	74	0	0
14	bl	66	0	74	1	0
14	bm	66	0	74	1	0
14	bn	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bo	66	0	74	0	0
14	bp	66	0	74	1	0
15	AA	70	0	91	0	0
15	AC	35	0	46	0	0
15	AD	70	0	91	1	0
15	AE	35	0	45	0	0
15	AF	35	0	46	1	0
15	AG	35	0	46	0	0
15	AH	70	0	91	1	0
15	AI	35	0	45	0	0
15	AJ	70	0	91	0	0
15	AL	35	0	45	0	0
15	AN	35	0	46	0	0
15	AP	70	0	92	1	0
15	AQ	35	0	46	0	0
15	AS	35	0	45	0	0
15	AT	35	0	45	0	0
15	AU	35	0	45	0	0
15	AX	35	0	46	0	0
15	BA	105	0	136	1	0
15	BB	105	0	136	0	0
15	BC	140	0	184	0	0
15	BD	105	0	137	0	0
15	BE	70	0	92	0	0
15	BF	70	0	92	0	0
15	BG	140	0	183	1	0
15	BH	105	0	136	1	0
15	BI	140	0	182	0	0
15	BJ	70	0	91	0	0
15	BK	140	0	182	0	0
15	BL	105	0	137	0	0
15	BM	70	0	92	0	0
15	BN	140	0	183	0	0
15	BO	70	0	92	1	0
15	BP	105	0	137	0	0
15	BQ	105	0	136	0	0
15	BR	105	0	136	1	0
15	BS	140	0	182	0	0
15	BT	105	0	138	1	0
15	BU	70	0	91	0	0
15	BV	140	0	183	2	0
15	BW	105	0	134	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	BX	70	0	91	0	0
15	L	210	0	273	0	0
15	M	35	0	45	0	0
15	ab	35	0	46	0	0
15	bb	35	0	45	0	0
15	bc	35	0	45	1	0
15	bd	35	0	45	0	0
15	be	35	0	46	0	0
15	bf	35	0	45	0	0
15	bg	35	0	46	0	0
15	bh	70	0	90	0	0
15	bi	35	0	46	1	0
15	bj	35	0	45	0	0
15	bl	70	0	91	0	0
15	bm	70	0	92	0	0
15	bn	70	0	91	0	0
15	bo	70	0	91	1	0
16	AE	45	0	0	0	0
16	AO	45	0	0	0	0
16	AS	45	0	0	0	0
16	BA	45	0	0	0	0
16	BB	45	0	0	0	0
16	BC	45	0	0	0	0
16	BD	45	0	0	0	0
16	BE	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	0	0
16	BO	45	0	0	0	0
16	BP	45	0	0	0	0
16	BQ	45	0	0	0	0
16	BR	45	0	0	0	0
16	BS	45	0	0	0	0
16	BU	45	0	0	0	0
16	BV	45	0	0	1	0
16	BW	45	0	0	0	0
16	BX	45	0	0	0	0
16	ba	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	bb	45	0	0	0	0
16	bc	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	1	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	0	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	4	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	C1	45	0	0	0	0
20	H1	45	0	0	0	0
20	aj	45	0	0	0	0
20	ba	45	0	0	0	0
20	bb	45	0	0	0	0
20	bc	45	0	0	0	0
20	be	90	0	0	0	0
20	bg	90	0	0	0	0
20	bh	45	0	0	0	0
20	bi	45	0	0	0	0
20	bj	45	0	0	0	0
20	bk	90	0	0	0	0
20	bl	45	0	0	0	0
20	bm	45	0	0	1	0
20	bn	45	0	0	0	0
20	bo	45	0	0	0	0
20	bp	45	0	0	0	0
21	H1	168	0	248	0	0
21	M	84	0	124	0	0
21	ae	84	0	124	1	0
21	af	84	0	124	1	0
21	aj	84	0	124	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H1	51	0	76	1	0
23	L	53	0	72	1	0
23	M	53	0	72	2	0
23	ao	53	0	72	0	0
24	L	58	0	0	0	0
24	ag	58	0	0	0	0
25	L	65	0	76	2	0
25	M	65	0	76	3	0
26	M	1	0	0	0	0
27	M	44	0	60	2	0
28	ai	55	0	0	0	0
29	AA	2	0	0	0	0
29	AB	3	0	0	0	0
29	AC	3	0	0	0	0
29	AD	1	0	0	0	0
29	AE	3	0	0	0	0
29	AF	2	0	0	0	0
29	AG	5	0	0	0	0
29	AH	1	0	0	0	0
29	AI	3	0	0	0	0
29	AJ	5	0	0	0	0
29	AK	4	0	0	0	0
29	AL	2	0	0	0	0
29	AM	6	0	0	0	0
29	AN	4	0	0	0	0
29	AO	4	0	0	0	0
29	AP	4	0	0	0	0
29	AQ	4	0	0	0	0
29	AS	6	0	0	0	0
29	AT	2	0	0	0	0
29	AU	1	0	0	0	0
29	AV	6	0	0	0	0
29	AW	2	0	0	0	0
29	AX	3	0	0	0	0
29	BB	1	0	0	0	0
29	BI	1	0	0	0	0
29	BJ	1	0	0	0	0
29	BO	1	0	0	0	0
29	BP	1	0	0	0	0
29	C	86	0	0	0	0
29	C1	42	0	0	0	0
29	H1	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H2	9	0	0	0	0
29	L	51	0	0	0	0
29	M	58	0	0	0	0
29	aa	3	0	0	0	0
29	ab	3	0	0	0	0
29	ac	3	0	0	0	0
29	ad	6	0	0	0	0
29	ae	10	0	0	0	0
29	af	11	0	0	0	0
29	ag	7	0	0	0	0
29	ah	6	0	0	0	0
29	ai	5	0	0	0	0
29	aj	7	0	0	0	0
29	ak	13	0	0	0	0
29	al	5	0	0	0	0
29	am	5	0	0	0	0
29	an	9	0	0	0	0
29	ao	5	0	0	0	0
29	ap	11	0	0	0	0
29	ba	3	0	0	0	0
29	bb	4	0	0	0	0
29	bc	2	0	0	0	0
29	bd	3	0	0	0	0
29	be	4	0	0	0	0
29	bf	1	0	0	0	0
29	bg	2	0	0	0	0
29	bh	2	0	0	0	0
29	bi	2	0	0	0	0
29	bj	3	0	0	0	0
29	bk	3	0	0	0	0
29	bl	3	0	0	0	0
29	bm	2	0	0	0	0
29	bn	1	0	0	0	0
29	bo	1	0	0	0	0
All	All	55475	0	53489	135	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 (135) 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)
1:AS:5:TRP:HH2	14:AS:104:BCL:H143	1.51	0.76
14:BI:1003:BCL:H112	14:BI:1003:BCL:H41	1.75	0.68
14:AA:1001:BCL:H191	3:bp:36:LEU:HD11	1.77	0.67
12:ad:12:ARG:HG3	21:ae:101:CD4:H52	1.78	0.64
14:ag:1001:BCL:H143	14:bf:103:BCL:H41	1.83	0.60
14:BS:1003:BCL:H52	14:BS:1003:BCL:H92	1.83	0.60
25:M:406:BPH:HHC	25:M:406:BPH:HBB3	1.84	0.59
1:AS:5:TRP:CH2	14:AS:104:BCL:H143	2.37	0.57
15:BV:1003:LMT:H2'	15:BV:1006:LMT:H4'	1.88	0.56
14:L:1002:BCL:HBB2	14:L:1002:BCL:HHC	1.87	0.56
1:AT:1:FME:SD	1:AT:1:FME:N	2.78	0.56
14:M:408:BCL:HHC	14:M:408:BCL:HBB2	1.87	0.56
1:AF:34:GLY:HA3	15:AF:1002:LMT:H6D	1.90	0.54
23:M:407:MQ8:H371	23:M:407:MQ8:H453	1.91	0.53
12:af:5:TRP:CZ2	3:bf:19:MET:HG2	2.44	0.53
17:C:402:HEC:HMC1	17:C:402:HEC:HBC3	1.91	0.52
21:aj:102:CD4:H29	21:aj:102:CD4:H23	1.90	0.52
5:C:175:ARG:HA	13:MG:2:RAM:H62	1.92	0.51
5:C:224:GLN:HE21	5:C:224:GLN:HA	1.74	0.51
15:BT:101:LMT:H4'	15:BT:102:LMT:H2'	1.93	0.51
14:BM:1002:BCL:H13	3:BN:29:VAL:HG21	1.93	0.50
1:AL:20:PHE:CD2	14:AM:102:BCL:H12	2.47	0.50
17:C:401:HEC:HMC1	17:C:401:HEC:HBC3	1.94	0.49
12:aj:5:TRP:CZ2	3:bj:19:MET:HG2	2.48	0.49
15:BG:1005:LMT:H2'	15:BG:1006:LMT:H4'	1.94	0.49
25:M:406:BPH:HBC3	25:M:406:BPH:HHD	1.93	0.49
15:AP:101:LMT:H6E	3:bj:38:TRP:HE1	1.77	0.49
14:AW:101:BCL:H143	15:bo:101:LMT:H111	1.94	0.49
12:ap:29:HIS:CE1	14:bp:102:BCL:HMD3	2.49	0.48
14:AF:1001:BCL:H152	15:bc:104:LMT:H121	1.95	0.48
1:AR:16:ALA:HB3	14:AS:102:BCL:H92	1.96	0.48
17:C:404:HEC:HBC3	17:C:404:HEC:HMC1	1.96	0.47
3:bi:38:TRP:HE1	15:bi:102:LMT:H5'	1.78	0.47
1:AM:13:ILE:HG23	14:AN:101:BCL:H91	1.96	0.47
17:C:403:HEC:HBC3	17:C:403:HEC:HMC1	1.97	0.47
9:L:128:TYR:CD1	14:L:1002:BCL:HBB1	2.50	0.47
14:AH:101:BCL:HBB1	15:AH:104:LMT:H41	1.96	0.46
1:AH:16:ALA:HB1	14:AI:103:BCL:H41	1.97	0.46
12:ah:29:HIS:CE1	14:bh:105:BCL:HMD3	2.50	0.46
6:C1:180:ASP:CG	10:M:88:ARG:HH22	2.23	0.46
12:al:29:HIS:CE1	14:bl:104:BCL:HMD3	2.51	0.46
3:ba:11:GLU:CD	3:ba:14:ARG:HH22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AB:1001:BCL:HHC	14:AB:1001:BCL:OBB	2.16	0.45
4:BV:7:MET:HE1	4:BV:15:PHE:HB2	1.97	0.45
12:ae:29:HIS:CE1	14:be:105:BCL:HMD3	2.51	0.45
12:ae:8:TYR:CD1	21:af:102:CD4:H51	2.51	0.45
14:AP:102:BCL:HHC	14:AP:102:BCL:CBB	2.47	0.45
10:M:16:VAL:HB	10:M:17:PRO:HD3	1.98	0.45
10:M:96:GLU:CD	10:M:97:PRO:HD2	2.42	0.44
14:AR:101:BCL:HHC	14:AR:101:BCL:CBB	2.48	0.44
5:C:19:THR:HG21	9:L:144:HIS:HE1	1.82	0.44
25:L:1009:BPH:HHC	25:L:1009:BPH:CBB	2.48	0.44
27:M:404:CRT:H26	27:M:404:CRT:H241	1.84	0.44
14:AU:102:BCL:HHC	14:AU:102:BCL:CBB	2.48	0.44
12:ab:40:TRP:HE1	14:ab:102:BCL:HBB3	1.83	0.44
12:ad:29:HIS:CE1	14:bd:102:BCL:HMD3	2.52	0.44
14:AW:101:BCL:HHC	14:AW:101:BCL:CBB	2.48	0.43
14:AG:102:BCL:HHC	14:AG:102:BCL:CBB	2.48	0.43
14:AX:103:BCL:CBB	14:AX:103:BCL:HHC	2.48	0.43
1:AB:36:PHE:O	4:BB:41:ARG:NH1	2.51	0.43
12:am:29:HIS:CE1	14:bm:104:BCL:HMD1	2.53	0.43
14:AC:102:BCL:CBB	14:AC:102:BCL:HHC	2.49	0.43
2:AC:5:TRP:HB3	3:BC:7:MET:HE3	2.01	0.43
15:BH:1003:LMT:H2'	15:BH:1004:LMT:H2'	2.01	0.43
1:AA:17:LEU:HD22	3:BA:19:MET:HE1	2.01	0.43
14:AT:101:BCL:HHC	14:AT:101:BCL:CBB	2.49	0.43
14:AN:102:BCL:HHC	14:AN:102:BCL:CBB	2.49	0.43
14:AO:1002:BCL:HHC	14:AO:1002:BCL:CBB	2.49	0.43
1:AV:36:PHE:O	4:BV:41:ARG:NH1	2.52	0.43
1:AQ:20:PHE:CD1	14:AR:102:BCL:H42	2.53	0.43
3:bg:18:TYR:HB3	16:bg:101:V7N:C25	2.49	0.43
15:BO:1002:LMT:H11	15:BO:1003:LMT:H2'	2.00	0.42
14:AE:1001:BCL:HHC	14:AE:1001:BCL:HBB3	2.00	0.42
14:AQ:102:BCL:CBB	14:AQ:102:BCL:HHC	2.49	0.42
9:L:181:PHE:HB3	25:M:406:BPH:HBB2	2.01	0.42
2:AC:4:ILE:HD13	14:AC:103:BCL:HMD2	2.02	0.42
14:AS:103:BCL:HHC	14:AS:103:BCL:CBB	2.49	0.42
14:AV:103:BCL:OBB	14:AV:103:BCL:HHC	2.19	0.42
25:L:1009:BPH:HHC	25:L:1009:BPH:HBB3	2.02	0.42
14:AI:102:BCL:H62	14:AI:102:BCL:H41	1.84	0.42
14:ab:102:BCL:HBB3	14:ab:102:BCL:HHC	2.00	0.42
14:AL:103:BCL:HHC	14:AL:103:BCL:CBB	2.49	0.42
1:AT:20:PHE:HB2	14:AU:103:BCL:H42	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:247:ASP:OD1	5:C:251:ASN:ND2	2.46	0.42
14:af:101:BCL:H61	14:af:101:BCL:H41	1.88	0.42
14:ai:101:BCL:HHC	14:ai:101:BCL:OBB	2.20	0.42
12:aj:29:HIS:CE1	14:bj:103:BCL:HMD3	2.54	0.42
1:AX:5:TRP:HB3	3:BX:7:MET:HE3	2.01	0.42
14:AX:102:BCL:OBB	14:AX:102:BCL:HHC	2.20	0.42
14:AH:103:BCL:CBB	14:AH:103:BCL:HHC	2.50	0.42
1:AK:36:PHE:O	3:BK:41:ARG:NH1	2.51	0.42
14:AK:102:BCL:CBB	14:AK:102:BCL:HHC	2.49	0.42
1:AB:4:ILE:HD13	14:AC:101:BCL:HMD2	2.01	0.42
10:M:259:ALA:N	23:M:407:MQ8:H143	2.36	0.41
12:ab:29:HIS:CE1	14:bb:104:BCL:HMD1	2.54	0.41
1:AM:30:ILE:HD11	3:bh:35:PHE:HD2	1.84	0.41
10:M:201:HIS:CE1	10:M:205:ILE:HD11	2.55	0.41
14:AF:1001:BCL:HHC	14:AF:1001:BCL:CBB	2.50	0.41
14:AJ:101:BCL:HHC	14:AJ:101:BCL:CBB	2.50	0.41
1:AQ:20:PHE:CE1	14:AR:102:BCL:H42	2.55	0.41
14:BI:1003:BCL:H102	3:BJ:29:VAL:HG11	2.02	0.41
10:M:16:VAL:HB	10:M:17:PRO:CD	2.51	0.41
11:aa:29:HIS:CE1	14:ba:103:BCL:HMD3	2.56	0.41
1:AM:36:PHE:O	3:BM:41:ARG:NH1	2.54	0.41
1:AW:16:ALA:HB1	14:AX:102:BCL:H41	2.01	0.41
1:AA:4:ILE:HD11	1:AB:14:MET:HG3	2.02	0.41
14:AA:1001:BCL:CBB	14:AA:1001:BCL:HHC	2.50	0.41
14:AI:102:BCL:HHC	14:AI:102:BCL:CBB	2.50	0.41
14:AM:101:BCL:HHC	14:AM:101:BCL:CBB	2.50	0.41
14:BU:1004:BCL:H92	15:BV:1002:LMT:H122	2.02	0.41
5:C:56:GLU:HG2	5:C:57:SER:H	1.85	0.41
12:ag:29:HIS:CE1	14:bg:105:BCL:HMD3	2.56	0.41
20:bm:102:OV9:O1P	20:bm:102:OV9:N	2.54	0.41
14:AB:1002:BCL:OBB	14:AB:1002:BCL:HHC	2.21	0.41
4:BV:7:MET:HE2	4:BV:11:GLU:HB3	2.02	0.41
9:L:197:VAL:HG13	10:M:142:MET:HE3	2.02	0.41
14:af:101:BCL:OBB	14:af:101:BCL:HHC	2.21	0.41
14:ah:1001:BCL:OBB	14:ah:1001:BCL:HHC	2.21	0.41
15:BA:105:LMT:H5B	15:BA:105:LMT:H6D	2.01	0.41
7:H1:9:GLN:NE2	22:H1:103:PGW:O13	2.45	0.41
14:aa:1001:BCL:OBB	14:aa:1001:BCL:HHC	2.20	0.41
14:ae:102:BCL:OBB	14:ae:102:BCL:HHC	2.21	0.41
15:BR:1003:LMT:H2'	15:BR:1005:LMT:H4'	2.03	0.40
9:L:77:LEU:O	12:ac:34:SER:OG	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:ai:5:TRP:CZ2	3:bi:19:MET:HG2	2.55	0.40
15:AD:101:LMT:H6D	3:bb:38:TRP:HE1	1.86	0.40
14:AW:101:BCL:H43	16:BV:1001:V7N:C34	2.51	0.40
27:M:404:CRT:H31	27:M:404:CRT:H291	1.96	0.40
14:ac:1001:BCL:OBB	14:ac:1001:BCL:HHC	2.21	0.40
14:AV:102:BCL:CBB	14:AV:102:BCL:HHC	2.51	0.40
9:L:91:LEU:HD13	23:L:1001:MQ8:H243	2.04	0.40
14:M:408:BCL:HMA1	14:M:408:BCL:H142	2.04	0.40
12:af:29:HIS:CE1	14:bf:103:BCL:HMD1	2.56	0.40
14:ao:102:BCL:OBB	14:ao:102:BCL:HHC	2.21	0.40
14:am:1001:BCL:HHC	14:am:1001:BCL:OBB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	47/54 (87%)	47 (100%)	0	0	100	100
1	AB	47/54 (87%)	47 (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%)	47 (100%)	0	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	47/54 (87%)	47 (100%)	0	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%)	46 (98%)	1 (2%)	0	100	100
2	AC	46/54 (85%)	46 (100%)	0	0	100	100
2	AD	46/54 (85%)	46 (100%)	0	0	100	100
3	BA	37/44 (84%)	37 (100%)	0	0	100	100
3	BC	37/44 (84%)	37 (100%)	0	0	100	100
3	BF	37/44 (84%)	37 (100%)	0	0	100	100
3	BG	37/44 (84%)	37 (100%)	0	0	100	100
3	BH	37/44 (84%)	37 (100%)	0	0	100	100
3	BJ	37/44 (84%)	37 (100%)	0	0	100	100
3	BK	37/44 (84%)	37 (100%)	0	0	100	100
3	BL	37/44 (84%)	37 (100%)	0	0	100	100
3	BM	37/44 (84%)	37 (100%)	0	0	100	100
3	BN	37/44 (84%)	37 (100%)	0	0	100	100
3	BO	37/44 (84%)	37 (100%)	0	0	100	100
3	BP	37/44 (84%)	37 (100%)	0	0	100	100
3	BU	37/44 (84%)	37 (100%)	0	0	100	100
3	BX	37/44 (84%)	37 (100%)	0	0	100	100
3	ba	37/44 (84%)	37 (100%)	0	0	100	100
3	bb	37/44 (84%)	37 (100%)	0	0	100	100
3	bc	37/44 (84%)	37 (100%)	0	0	100	100
3	bd	37/44 (84%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	be	37/44 (84%)	37 (100%)	0	0	100	100
3	bf	37/44 (84%)	37 (100%)	0	0	100	100
3	bg	37/44 (84%)	37 (100%)	0	0	100	100
3	bh	37/44 (84%)	37 (100%)	0	0	100	100
3	bi	37/44 (84%)	37 (100%)	0	0	100	100
3	bj	37/44 (84%)	37 (100%)	0	0	100	100
3	bk	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
3	bl	37/44 (84%)	37 (100%)	0	0	100	100
3	bm	37/44 (84%)	37 (100%)	0	0	100	100
3	bo	37/44 (84%)	37 (100%)	0	0	100	100
3	bp	37/44 (84%)	37 (100%)	0	0	100	100
4	BB	38/43 (88%)	38 (100%)	0	0	100	100
4	BD	38/43 (88%)	38 (100%)	0	0	100	100
4	BE	38/43 (88%)	38 (100%)	0	0	100	100
4	BI	38/43 (88%)	38 (100%)	0	0	100	100
4	BQ	38/43 (88%)	38 (100%)	0	0	100	100
4	BR	38/43 (88%)	38 (100%)	0	0	100	100
4	BS	38/43 (88%)	38 (100%)	0	0	100	100
4	BT	38/43 (88%)	38 (100%)	0	0	100	100
4	BV	38/43 (88%)	38 (100%)	0	0	100	100
4	BW	38/43 (88%)	38 (100%)	0	0	100	100
4	bn	38/43 (88%)	38 (100%)	0	0	100	100
5	C	297/354 (84%)	285 (96%)	12 (4%)	0	100	100
6	C1	101/202 (50%)	100 (99%)	1 (1%)	0	100	100
7	H1	60/67 (90%)	60 (100%)	0	0	100	100
8	H2	172/181 (95%)	169 (98%)	3 (2%)	0	100	100
9	L	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
10	M	311/367 (85%)	298 (96%)	13 (4%)	0	100	100
11	aa	53/71 (75%)	53 (100%)	0	0	100	100
12	ab	56/71 (79%)	56 (100%)	0	0	100	100
12	ac	54/71 (76%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	ad	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
12	ae	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
12	af	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
12	ag	56/71 (79%)	56 (100%)	0	0	100	100
12	ah	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
12	ai	58/71 (82%)	58 (100%)	0	0	100	100
12	aj	58/71 (82%)	58 (100%)	0	0	100	100
12	ak	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
12	al	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
12	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
12	an	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
12	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
12	ap	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
All	All	4773/5626 (85%)	4717 (99%)	56 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	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	68
1	AI	38/41 (93%)	38 (100%)	0	100	100
1	AJ	38/41 (93%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	37 (97%)	1 (3%)	40	68
2	AC	37/41 (90%)	37 (100%)	0	100	100
2	AD	37/41 (90%)	37 (100%)	0	100	100
3	BA	31/35 (89%)	31 (100%)	0	100	100
3	BC	31/35 (89%)	31 (100%)	0	100	100
3	BF	31/35 (89%)	31 (100%)	0	100	100
3	BG	31/35 (89%)	31 (100%)	0	100	100
3	BH	31/35 (89%)	31 (100%)	0	100	100
3	BJ	31/35 (89%)	30 (97%)	1 (3%)	34	62
3	BK	31/35 (89%)	31 (100%)	0	100	100
3	BL	31/35 (89%)	31 (100%)	0	100	100
3	BM	31/35 (89%)	31 (100%)	0	100	100
3	BN	31/35 (89%)	31 (100%)	0	100	100
3	BO	31/35 (89%)	31 (100%)	0	100	100
3	BP	31/35 (89%)	31 (100%)	0	100	100
3	BU	31/35 (89%)	31 (100%)	0	100	100
3	BX	31/35 (89%)	31 (100%)	0	100	100
3	ba	31/35 (89%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	bb	31/35 (89%)	31 (100%)	0	100	100
3	bc	31/35 (89%)	31 (100%)	0	100	100
3	bd	31/35 (89%)	31 (100%)	0	100	100
3	be	31/35 (89%)	31 (100%)	0	100	100
3	bf	31/35 (89%)	31 (100%)	0	100	100
3	bg	31/35 (89%)	31 (100%)	0	100	100
3	bh	31/35 (89%)	31 (100%)	0	100	100
3	bi	31/35 (89%)	31 (100%)	0	100	100
3	bj	31/35 (89%)	31 (100%)	0	100	100
3	bk	31/35 (89%)	31 (100%)	0	100	100
3	bl	31/35 (89%)	31 (100%)	0	100	100
3	bm	31/35 (89%)	31 (100%)	0	100	100
3	bo	31/35 (89%)	31 (100%)	0	100	100
3	bp	31/35 (89%)	31 (100%)	0	100	100
4	BB	31/34 (91%)	31 (100%)	0	100	100
4	BD	31/34 (91%)	31 (100%)	0	100	100
4	BE	31/34 (91%)	31 (100%)	0	100	100
4	BI	31/34 (91%)	31 (100%)	0	100	100
4	BQ	31/34 (91%)	31 (100%)	0	100	100
4	BR	31/34 (91%)	31 (100%)	0	100	100
4	BS	31/34 (91%)	31 (100%)	0	100	100
4	BT	31/34 (91%)	31 (100%)	0	100	100
4	BV	31/34 (91%)	31 (100%)	0	100	100
4	BW	31/34 (91%)	31 (100%)	0	100	100
4	bn	31/34 (91%)	31 (100%)	0	100	100
5	C	245/285 (86%)	244 (100%)	1 (0%)	84	93
6	C1	88/156 (56%)	88 (100%)	0	100	100
7	H1	50/53 (94%)	50 (100%)	0	100	100
8	H2	144/151 (95%)	143 (99%)	1 (1%)	76	89
9	L	215/216 (100%)	213 (99%)	2 (1%)	70	87
10	M	256/299 (86%)	254 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	aa	45/55 (82%)	45 (100%)	0	100	100
12	ab	46/54 (85%)	46 (100%)	0	100	100
12	ac	45/54 (83%)	45 (100%)	0	100	100
12	ad	46/54 (85%)	46 (100%)	0	100	100
12	ae	46/54 (85%)	46 (100%)	0	100	100
12	af	46/54 (85%)	46 (100%)	0	100	100
12	ag	46/54 (85%)	46 (100%)	0	100	100
12	ah	46/54 (85%)	45 (98%)	1 (2%)	45	73
12	ai	46/54 (85%)	46 (100%)	0	100	100
12	aj	46/54 (85%)	46 (100%)	0	100	100
12	ak	54/54 (100%)	54 (100%)	0	100	100
12	al	46/54 (85%)	46 (100%)	0	100	100
12	am	46/54 (85%)	46 (100%)	0	100	100
12	an	54/54 (100%)	53 (98%)	1 (2%)	50	76
12	ao	46/54 (85%)	45 (98%)	1 (2%)	45	73
12	ap	54/54 (100%)	54 (100%)	0	100	100
All	All	3906/4398 (89%)	3894 (100%)	12 (0%)	84	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AH	12	ILE
1	AX	35	GLN
3	BJ	9	GLU
5	C	39	LYS
8	H2	159	ASP
9	L	247	CYS
9	L	249	VAL
10	M	215	PHE
10	M	291	ASP
12	ah	39	SER
12	an	39	SER
12	ao	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	35	GLN
1	AH	35	GLN
1	AI	35	GLN
1	AS	37	ASN
1	AT	35	GLN
5	C	32	ASN
5	C	157	ASN
5	C	183	GLN
5	C	189	ASN
6	C1	158	GLN
9	L	104	GLN
9	L	144	HIS
9	L	268	ASN
10	M	316	GLN
12	ae	36	GLN
12	af	50	GLN
12	ai	50	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	$\# Z > 2$
7	FME	H1	1	7	8,9,10	0.95	0	8,9,11	0.94	0
12	FME	ab	1	12	8,9,10	0.93	0	8,9,11	1.15	1 (12%)
12	FME	ae	1	12	8,9,10	0.96	0	8,9,11	1.07	1 (12%)
12	FME	ap	1	12	8,9,10	0.98	0	8,9,11	0.89	0
12	FME	ad	1	12	8,9,10	0.94	0	8,9,11	1.01	1 (12%)
12	FME	af	1	12	8,9,10	0.96	0	8,9,11	0.99	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AN	1	1	8,9,10	0.97	0	8,9,11	0.97	1 (12%)
1	FME	AF	1	1	8,9,10	0.97	0	8,9,11	0.85	0
1	FME	AG	1	1	8,9,10	0.96	0	8,9,11	0.94	0
2	FME	AC	1	2	8,9,10	0.98	0	8,9,11	1.03	1 (12%)
1	FME	AA	1	1	8,9,10	0.97	0	8,9,11	0.93	1 (12%)
12	FME	an	1	12	8,9,10	0.97	0	8,9,11	1.08	1 (12%)
1	FME	AQ	1	1	8,9,10	0.95	0	8,9,11	1.06	1 (12%)
1	FME	AS	1	1	8,9,10	0.96	0	8,9,11	1.04	1 (12%)
12	FME	ai	1	12	8,9,10	0.96	0	8,9,11	0.96	1 (12%)
12	FME	ac	1	12	8,9,10	0.94	0	8,9,11	0.83	0
12	FME	al	1	12	8,9,10	0.96	0	8,9,11	0.93	0
1	FME	AL	1	1	8,9,10	0.95	0	8,9,11	1.10	1 (12%)
1	FME	AE	1	1	8,9,10	0.93	0	8,9,11	0.96	1 (12%)
1	FME	AB	1	1	8,9,10	0.96	0	8,9,11	0.95	1 (12%)
1	FME	AI	1	1	8,9,10	0.98	0	8,9,11	0.88	0
1	FME	AJ	1	1	8,9,10	1.00	0	8,9,11	0.74	0
1	FME	AW	1	1	8,9,10	0.94	0	8,9,11	1.03	1 (12%)
1	FME	AX	1	1	8,9,10	0.94	0	8,9,11	1.17	1 (12%)
12	FME	ao	1	12	8,9,10	0.94	0	8,9,11	0.94	0
1	FME	AH	1	1	8,9,10	0.96	0	8,9,11	0.99	1 (12%)
12	FME	aj	1	12	8,9,10	0.97	0	8,9,11	0.99	1 (12%)
1	FME	AP	1	1	8,9,10	0.95	0	8,9,11	0.96	1 (12%)
1	FME	AR	1	1	8,9,10	0.96	0	8,9,11	0.90	0
12	FME	ah	1	12	8,9,10	0.97	0	8,9,11	1.03	1 (12%)
1	FME	AT	1	1	8,9,10	0.95	0	8,9,11	0.94	1 (12%)
1	FME	AU	1	1	8,9,10	0.95	0	8,9,11	0.93	0
1	FME	AK	1	1	8,9,10	0.95	0	8,9,11	1.02	1 (12%)
12	FME	am	1	12	8,9,10	0.94	0	8,9,11	0.91	0
12	FME	ak	1	12	8,9,10	0.98	0	8,9,11	1.06	1 (12%)
1	FME	AM	1	1	8,9,10	0.97	0	8,9,11	0.91	0
2	FME	AD	1	2	8,9,10	0.97	0	8,9,11	1.00	1 (12%)
1	FME	AO	1	1	8,9,10	0.95	0	8,9,11	0.95	1 (12%)
1	FME	AV	1	1	8,9,10	0.96	0	8,9,11	0.99	1 (12%)
12	FME	ag	1	12	8,9,10	0.95	0	8,9,11	0.96	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
7	FME	H1	1	7	-	0/7/9/11	-
12	FME	ab	1	12	-	1/7/9/11	-
12	FME	ae	1	12	-	1/7/9/11	-
12	FME	ap	1	12	-	1/7/9/11	-
12	FME	ad	1	12	-	0/7/9/11	-
12	FME	af	1	12	-	2/7/9/11	-
1	FME	AN	1	1	-	1/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
1	FME	AG	1	1	-	0/7/9/11	-
2	FME	AC	1	2	-	0/7/9/11	-
1	FME	AA	1	1	-	1/7/9/11	-
12	FME	an	1	12	-	1/7/9/11	-
1	FME	AQ	1	1	-	0/7/9/11	-
1	FME	AS	1	1	-	0/7/9/11	-
12	FME	ai	1	12	-	0/7/9/11	-
12	FME	ac	1	12	-	1/7/9/11	-
12	FME	al	1	12	-	2/7/9/11	-
1	FME	AL	1	1	-	1/7/9/11	-
1	FME	AE	1	1	-	1/7/9/11	-
1	FME	AB	1	1	-	1/7/9/11	-
1	FME	AI	1	1	-	1/7/9/11	-
1	FME	AJ	1	1	-	1/7/9/11	-
1	FME	AW	1	1	-	0/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-
12	FME	ao	1	12	-	1/7/9/11	-
1	FME	AH	1	1	-	0/7/9/11	-
12	FME	aj	1	12	-	1/7/9/11	-
1	FME	AP	1	1	-	1/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
12	FME	ah	1	12	-	0/7/9/11	-
1	FME	AT	1	1	-	0/7/9/11	-
1	FME	AU	1	1	-	1/7/9/11	-
1	FME	AK	1	1	-	0/7/9/11	-
12	FME	am	1	12	-	2/7/9/11	-
12	FME	ak	1	12	-	2/7/9/11	-
1	FME	AM	1	1	-	1/7/9/11	-
2	FME	AD	1	2	-	0/7/9/11	-
1	FME	AO	1	1	-	0/7/9/11	-
1	FME	AV	1	1	-	0/7/9/11	-
12	FME	ag	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AX	1	FME	C-CA-N	2.62	114.55	109.50
12	ab	1	FME	C-CA-N	2.56	114.44	109.50
1	AL	1	FME	C-CA-N	2.45	114.23	109.50
1	AQ	1	FME	C-CA-N	2.37	114.06	109.50
12	an	1	FME	C-CA-N	2.36	114.06	109.50
12	ak	1	FME	C-CA-N	2.33	113.99	109.50
1	AS	1	FME	C-CA-N	2.28	113.89	109.50
12	ah	1	FME	C-CA-N	2.25	113.85	109.50
12	ae	1	FME	C-CA-N	2.23	113.80	109.50
2	AC	1	FME	C-CA-N	2.21	113.76	109.50
12	af	1	FME	C-CA-N	2.20	113.75	109.50
1	AO	1	FME	C-CA-N	2.19	113.72	109.50
12	ad	1	FME	C-CA-N	2.18	113.71	109.50
1	AW	1	FME	C-CA-N	2.17	113.68	109.50
1	AK	1	FME	C-CA-N	2.15	113.64	109.50
2	AD	1	FME	C-CA-N	2.11	113.57	109.50
1	AH	1	FME	C-CA-N	2.10	113.55	109.50
1	AP	1	FME	C-CA-N	2.09	113.53	109.50
12	ai	1	FME	C-CA-N	2.09	113.52	109.50
1	AA	1	FME	C-CA-N	2.07	113.50	109.50
1	AN	1	FME	C-CA-N	2.07	113.49	109.50
12	aj	1	FME	C-CA-N	2.07	113.49	109.50
1	AE	1	FME	C-CA-N	2.07	113.49	109.50
1	AB	1	FME	C-CA-N	2.06	113.48	109.50
12	ag	1	FME	C-CA-N	2.06	113.48	109.50
1	AV	1	FME	C-CA-N	2.06	113.47	109.50
1	AT	1	FME	C-CA-N	2.02	113.40	109.50

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	ab	1	FME	O-C-CA-CB
12	ac	1	FME	O-C-CA-CB
12	af	1	FME	O-C-CA-CB
12	ak	1	FME	O-C-CA-CB
12	am	1	FME	CB-CA-N-CN
12	an	1	FME	O-C-CA-CB
1	AA	1	FME	O-C-CA-CB
1	AF	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	AI	1	FME	O-C-CA-CB
1	AJ	1	FME	O-C-CA-CB
1	AU	1	FME	O-C-CA-CB
12	ae	1	FME	CA-CB-CG-SD
12	af	1	FME	N-CA-CB-CG
12	am	1	FME	N-CA-CB-CG
1	AL	1	FME	N-CA-CB-CG
1	AM	1	FME	N-CA-CB-CG
1	AX	1	FME	N-CA-CB-CG
1	AN	1	FME	N-CA-CB-CG
12	ao	1	FME	N-CA-CB-CG
1	AB	1	FME	N-CA-CB-CG
1	AP	1	FME	CB-CG-SD-CE
1	AE	1	FME	CB-CG-SD-CE
12	al	1	FME	N-CA-CB-CG
12	aj	1	FME	C-CA-CB-CG
12	ak	1	FME	C-CA-CB-CG
12	ap	1	FME	CB-CA-N-CN
12	al	1	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AT	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	$\# Z > 2$
13	MAN	CG	1	5,13,18	11,11,12	0.79	1 (9%)	15,15,17	0.94	0
13	RAM	CG	2	13	10,10,11	1.67	3 (30%)	14,14,16	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	MG	1	13,18,10	11,11,12	0.70	0	15,15,17	0.99	1 (6%)
13	RAM	MG	2	13	10,10,11	1.45	1 (10%)	14,14,16	1.30	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
13	MAN	CG	1	5,13,18	-	1/2/19/22	0/1/1/1
13	RAM	CG	2	13	-	-	0/1/1/1
13	MAN	MG	1	13,18,10	-	0/2/19/22	0/1/1/1
13	RAM	MG	2	13	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	CG	2	RAM	O5-C1	4.00	1.50	1.43
13	MG	2	RAM	O5-C1	3.29	1.49	1.43
13	CG	2	RAM	C2-C3	-2.17	1.49	1.52
13	CG	2	RAM	O5-C5	2.12	1.47	1.43
13	CG	1	MAN	O5-C1	-2.05	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	MG	2	RAM	C6-C5-C4	-2.62	108.29	113.08
13	MG	1	MAN	C1-O5-C5	2.33	115.31	112.19
13	MG	2	RAM	C1-C2-C3	2.31	113.00	109.64
13	MG	2	RAM	C1-O5-C5	-2.20	107.77	112.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

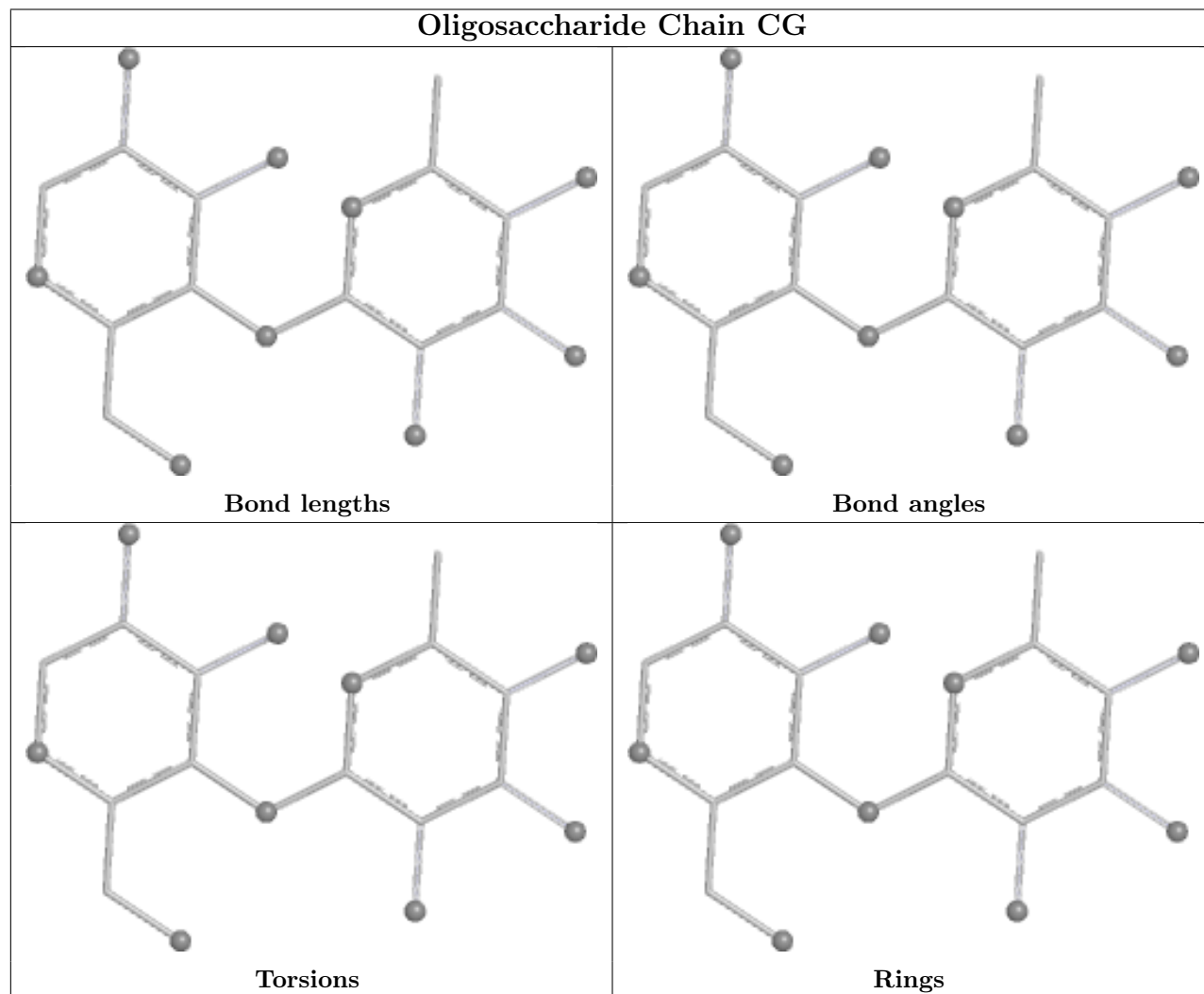
Mol	Chain	Res	Type	Atoms
13	CG	1	MAN	O5-C5-C6-O6

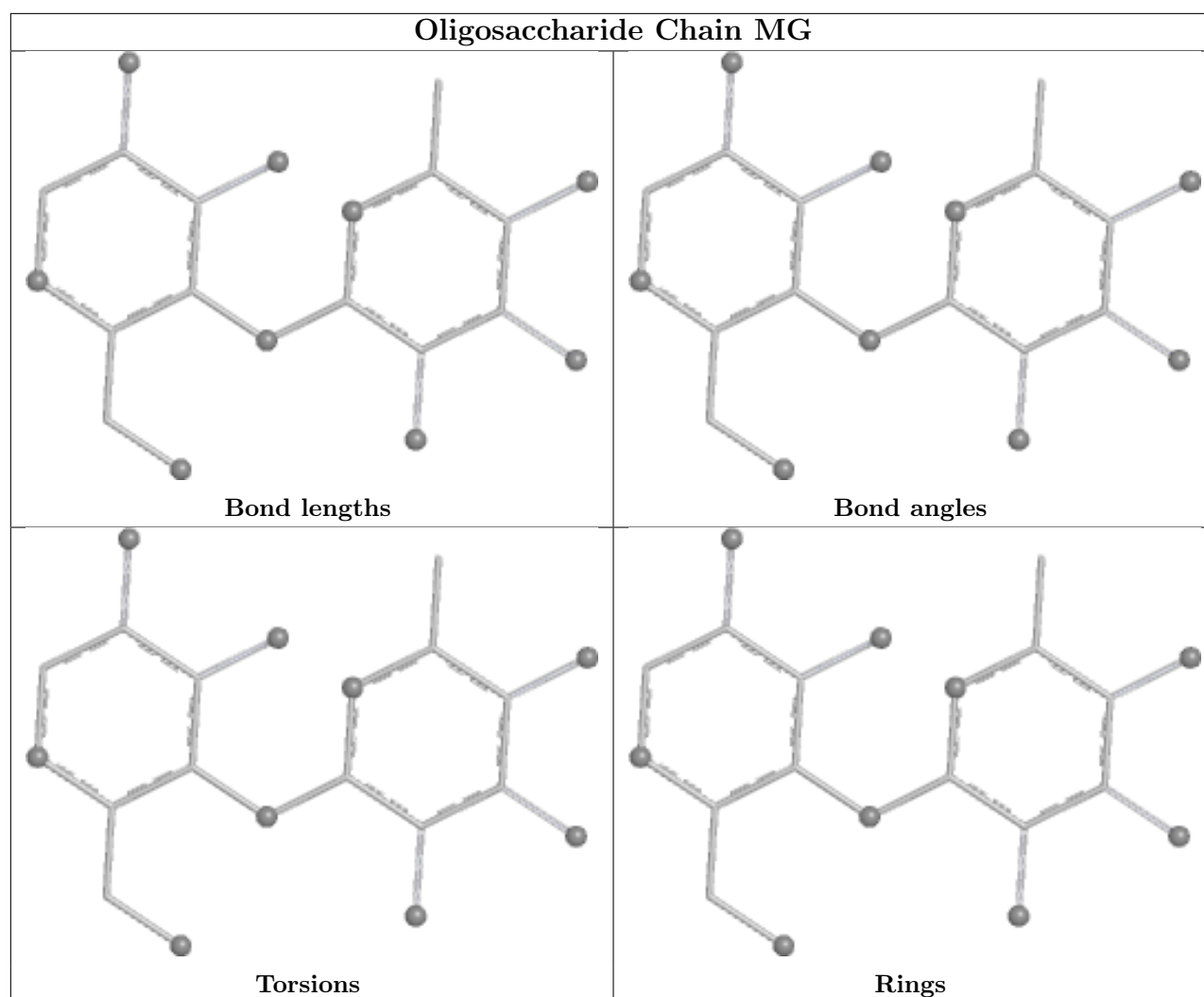
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	MG	2	RAM	1	0

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 313 ligands modelled in this entry, 1 is monoatomic - leaving 312 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	$\# Z > 2$
20	0V9	bl	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.91	3 (6%)
15	LMT	bc	104	-	36,36,36	1.07	4 (11%)	47,47,47	0.96	3 (6%)
16	V7N	BH	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.70	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PGW	H1	103	-	50,50,50	0.46	0	53,56,56	1.03	3 (5%)
20	0V9	aj	101	-	44,44,46	0.77	1 (2%)	47,49,51	0.83	2 (4%)
14	BCL	BI	1003	-	69,74,74	1.36	8 (11%)	79,115,115	1.81	13 (16%)
16	V7N	BW	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.56	10 (20%)
14	BCL	AL	101	-	69,74,74	1.19	5 (7%)	79,115,115	1.73	13 (16%)
20	0V9	bp	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.92	3 (6%)
21	CD4	H1	104	-	83,83,83	0.49	0	89,95,95	1.06	4 (4%)
15	LMT	ab	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.91	2 (4%)
15	LMT	BW	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.90	1 (2%)
14	BCL	AF	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.33	7 (8%)
20	0V9	bn	104	-	44,44,46	0.77	1 (2%)	47,49,51	0.89	2 (4%)
14	BCL	BH	1005	-	69,74,74	1.12	5 (7%)	79,115,115	1.35	10 (12%)
20	0V9	bb	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	1 (2%)
15	LMT	AA	1004	-	36,36,36	1.06	4 (11%)	47,47,47	0.95	2 (4%)
14	BCL	aa	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	9 (11%)
14	BCL	BL	1003	-	69,74,74	1.10	5 (7%)	79,115,115	1.35	10 (12%)
15	LMT	AP	101	-	36,36,36	1.05	4 (11%)	47,47,47	1.11	4 (8%)
15	LMT	AN	103	-	36,36,36	1.07	4 (11%)	47,47,47	0.95	2 (4%)
15	LMT	BG	1003	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	1 (2%)
14	BCL	AG	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.29	7 (8%)
15	LMT	BB	105	-	36,36,36	1.04	4 (11%)	47,47,47	0.93	2 (4%)
15	LMT	BK	1003	-	36,36,36	1.05	3 (8%)	47,47,47	1.13	4 (8%)
14	BCL	AS	104	29	69,74,74	1.19	5 (7%)	79,115,115	1.47	11 (13%)
16	V7N	bb	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.65	10 (20%)
14	BCL	al	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.37	10 (12%)
14	BCL	BV	1005	-	69,74,74	1.11	5 (7%)	79,115,115	1.29	9 (11%)
15	LMT	AL	102	-	36,36,36	1.06	4 (11%)	47,47,47	0.84	0
20	0V9	C1	1001	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	2 (4%)
14	BCL	BF	102	-	69,74,74	1.11	6 (8%)	79,115,115	2.01	12 (15%)
14	BCL	AI	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.33	7 (8%)
14	BCL	aj	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	9 (11%)
15	LMT	AD	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.98	2 (4%)
16	V7N	BD	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.55	11 (22%)
15	LMT	bo	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	2 (4%)
14	BCL	AE	1004	-	69,74,74	1.18	5 (7%)	79,115,115	1.37	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCL	ao	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	10 (12%)
14	BCL	bh	105	-	69,74,74	1.12	5 (7%)	79,115,115	1.34	11 (13%)
16	V7N	bg	101	-	44,44,44	1.69	8 (18%)	48,54,54	1.72	11 (22%)
15	LMT	BN	105	-	36,36,36	1.04	4 (11%)	47,47,47	0.90	1 (2%)
16	V7N	bo	102	-	44,44,44	1.69	9 (20%)	48,54,54	1.50	11 (22%)
14	BCL	BC	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.42	11 (13%)
15	LMT	BX	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	2 (4%)
15	LMT	BE	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.90	1 (2%)
14	BCL	bn	103	-	69,74,74	1.11	6 (8%)	79,115,115	1.27	9 (11%)
15	LMT	BH	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.96	2 (4%)
15	LMT	bh	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	1 (2%)
20	0V9	be	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.88	2 (4%)
15	LMT	BI	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.97	2 (4%)
16	V7N	BC	101	-	44,44,44	1.68	8 (18%)	48,54,54	1.56	12 (25%)
15	LMT	L	1011	-	36,36,36	1.05	4 (11%)	47,47,47	0.94	2 (4%)
14	BCL	AJ	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.31	7 (8%)
14	BCL	bl	104	-	69,74,74	1.13	6 (8%)	79,115,115	1.28	10 (12%)
16	V7N	BK	1001	-	44,44,44	1.69	8 (18%)	48,54,54	1.49	9 (18%)
14	BCL	AE	1003	29	69,74,74	1.13	5 (7%)	79,115,115	1.31	9 (11%)
15	LMT	BF	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	2 (4%)
14	BCL	AC	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.29	7 (8%)
24	V7B	L	1006	-	59,59,59	0.89	4 (6%)	75,75,75	1.05	5 (6%)
15	LMT	AC	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.97	2 (4%)
15	LMT	AJ	103	-	36,36,36	1.06	3 (8%)	47,47,47	1.23	5 (10%)
14	BCL	AK	101	29	69,74,74	1.16	6 (8%)	79,115,115	1.39	9 (11%)
15	LMT	BS	1005	-	36,36,36	1.05	4 (11%)	47,47,47	0.97	3 (6%)
14	BCL	BG	1004	-	69,74,74	1.12	5 (7%)	79,115,115	1.28	7 (8%)
15	LMT	AT	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.21	3 (6%)
15	LMT	BQ	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.88	1 (2%)
14	BCL	af	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.31	9 (11%)
14	BCL	M	408	-	69,74,74	1.13	5 (7%)	79,115,115	1.35	8 (10%)
15	LMT	bn	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.79	0
14	BCL	an	1001	-	69,74,74	1.13	5 (7%)	79,115,115	1.29	9 (11%)
16	V7N	bd	101	-	44,44,44	1.68	8 (18%)	48,54,54	1.58	11 (22%)
14	BCL	AJ	102	29	69,74,74	1.14	5 (7%)	79,115,115	1.41	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCL	L	1010	-	69,74,74	1.12	6 (8%)	79,115,115	1.25	9 (11%)
20	0V9	bi	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.86	2 (4%)
15	LMT	AE	1002	-	36,36,36	1.04	4 (11%)	47,47,47	1.05	4 (8%)
20	0V9	bc	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.95	3 (6%)
15	LMT	L	1005	-	36,36,36	1.02	4 (11%)	47,47,47	0.90	1 (2%)
14	BCL	be	105	-	69,74,74	1.14	5 (7%)	79,115,115	1.28	8 (10%)
15	LMT	BP	1003	-	36,36,36	1.03	4 (11%)	47,47,47	0.88	1 (2%)
15	LMT	BM	1003	-	36,36,36	1.05	3 (8%)	47,47,47	0.87	0
15	LMT	BW	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	1 (2%)
18	V75	C	405	13,19	18,18,18	1.59	4 (22%)	21,25,25	1.74	3 (14%)
14	BCL	am	1001	-	69,74,74	1.22	8 (11%)	79,115,115	1.76	11 (13%)
14	BCL	AX	103	-	69,74,74	1.16	5 (7%)	79,115,115	1.32	7 (8%)
18	V75	M	409	13,19	18,18,18	1.63	5 (27%)	21,25,25	1.72	2 (9%)
14	BCL	AE	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)
15	LMT	AJ	104	-	36,36,36	1.04	3 (8%)	47,47,47	0.96	3 (6%)
14	BCL	bm	104	-	69,74,74	1.10	6 (8%)	79,115,115	1.33	12 (15%)
14	BCL	AC	103	29	69,74,74	1.13	6 (8%)	79,115,115	1.32	10 (12%)
14	BCL	BJ	1002	-	69,74,74	1.10	5 (7%)	79,115,115	1.33	8 (10%)
20	0V9	bg	102	-	44,44,46	0.77	1 (2%)	47,49,51	1.09	3 (6%)
15	LMT	L	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.81	0
15	LMT	BS	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	2 (4%)
15	LMT	BU	1003	-	36,36,36	1.06	3 (8%)	47,47,47	0.81	1 (2%)
14	BCL	BD	105	-	69,74,74	1.12	5 (7%)	79,115,115	1.30	9 (11%)
15	LMT	BO	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.84	0
17	HEC	C	402	5	46,50,50	1.84	4 (8%)	58,82,82	1.63	6 (10%)
20	0V9	bm	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.84	1 (2%)
16	V7N	BP	1001	-	44,44,44	1.68	7 (15%)	48,54,54	1.52	9 (18%)
14	BCL	bg	105	-	69,74,74	1.11	5 (7%)	79,115,115	1.26	10 (12%)
15	LMT	AU	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.85	0
14	BCL	bd	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.27	10 (12%)
15	LMT	AG	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.87	2 (4%)
15	LMT	BR	1005	-	36,36,36	1.03	4 (11%)	47,47,47	0.87	0
15	LMT	BI	1004	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	3 (6%)
17	HEC	C	401	5	46,50,50	1.85	5 (10%)	58,82,82	1.61	6 (10%)
19	NDG	C1	1002	18	14,14,15	0.67	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	bm	103	-	36,36,36	1.02	4 (11%)	47,47,47	0.96	3 (6%)
15	LMT	BB	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.89	2 (4%)
15	LMT	BK	1002	-	36,36,36	1.07	5 (13%)	47,47,47	1.01	3 (6%)
21	CD4	M	402	-	83,83,83	0.48	0	89,95,95	1.08	5 (5%)
16	V7N	BX	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.67	13 (27%)
21	CD4	H1	102	-	83,83,83	0.46	0	89,95,95	1.02	5 (5%)
15	LMT	BK	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	2 (4%)
15	LMT	BO	1002	-	36,36,36	1.03	3 (8%)	47,47,47	0.91	1 (2%)
14	BCL	BP	1005	-	69,74,74	1.12	5 (7%)	79,115,115	1.29	9 (11%)
15	LMT	AH	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.00	3 (6%)
17	HEC	C	404	5	46,50,50	1.85	5 (10%)	58,82,82	1.64	6 (10%)
14	BCL	bp	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.35	10 (12%)
14	BCL	BW	1003	-	69,74,74	1.12	5 (7%)	79,115,115	1.36	11 (13%)
21	CD4	aj	102	-	83,83,83	0.50	0	89,95,95	1.22	8 (8%)
16	V7N	BA	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.55	10 (20%)
23	MQ8	L	1001	-	54,54,54	0.62	0	67,69,69	0.84	1 (1%)
14	BCL	BQ	1003	-	69,74,74	1.12	5 (7%)	79,115,115	1.30	9 (11%)
15	LMT	BC	105	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	1 (2%)
15	LMT	BP	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.90	0
14	BCL	AB	1002	29	69,74,74	1.13	4 (5%)	79,115,115	1.40	10 (12%)
14	BCL	ab	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.32	8 (10%)
14	BCL	bk	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.29	9 (11%)
15	LMT	BS	1006	-	36,36,36	1.03	4 (11%)	47,47,47	0.92	2 (4%)
15	LMT	bd	103	-	36,36,36	1.08	4 (11%)	47,47,47	0.88	2 (4%)
16	V7N	bp	101	-	44,44,44	1.69	8 (18%)	48,54,54	1.61	12 (25%)
15	LMT	BR	1003	-	36,36,36	1.05	4 (11%)	47,47,47	1.00	2 (4%)
16	V7N	AO	1001	-	44,44,44	1.66	8 (18%)	48,54,54	1.73	12 (25%)
15	LMT	AD	101	-	36,36,36	1.03	4 (11%)	47,47,47	1.02	3 (6%)
16	V7N	BR	1001	-	44,44,44	1.67	7 (15%)	48,54,54	1.70	13 (27%)
15	LMT	BV	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.96	1 (2%)
27	CRT	M	404	-	43,43,43	0.60	0	48,54,54	0.96	3 (6%)
14	BCL	BR	1004	-	69,74,74	1.11	5 (7%)	79,115,115	1.32	9 (11%)
24	V7B	ag	1002	-	59,59,59	0.88	4 (6%)	75,75,75	1.03	3 (4%)
15	LMT	BH	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.89	0
16	V7N	bk	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.51	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	BG	1006	-	36,36,36	1.05	4 (11%)	47,47,47	0.87	1 (2%)
16	V7N	bn	102	-	44,44,44	1.70	8 (18%)	48,54,54	1.61	11 (22%)
14	BCL	bj	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.31	10 (12%)
20	0V9	bh	103	-	44,44,46	0.77	1 (2%)	47,49,51	0.95	3 (6%)
16	V7N	BO	1001	-	44,44,44	1.67	6 (13%)	48,54,54	1.69	14 (29%)
15	LMT	L	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.98	1 (2%)
14	BCL	AV	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.26	7 (8%)
14	BCL	BN	103	-	69,74,74	1.30	7 (10%)	79,115,115	1.73	10 (12%)
15	LMT	BN	102	-	36,36,36	1.05	4 (11%)	47,47,47	1.00	2 (4%)
15	LMT	BL	1004	-	36,36,36	1.03	4 (11%)	47,47,47	0.94	3 (6%)
15	LMT	BP	1004	-	36,36,36	1.04	4 (11%)	47,47,47	0.96	2 (4%)
14	BCL	L	1002	-	69,74,74	1.11	5 (7%)	79,115,115	1.27	7 (8%)
15	LMT	BI	1005	-	36,36,36	1.05	4 (11%)	47,47,47	0.83	0
15	LMT	BC	102	-	36,36,36	1.06	4 (11%)	47,47,47	0.88	1 (2%)
15	LMT	BA	105	-	36,36,36	1.06	4 (11%)	47,47,47	0.88	1 (2%)
15	LMT	bo	105	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	3 (6%)
15	LMT	AS	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.97	2 (4%)
15	LMT	BT	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.87	2 (4%)
14	BCL	AR	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.46	14 (17%)
14	BCL	ae	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.36	10 (12%)
15	LMT	BF	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	1 (2%)
15	LMT	bj	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	2 (4%)
15	LMT	BD	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.91	2 (4%)
14	BCL	AH	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.43	13 (16%)
14	BCL	AI	103	-	69,74,74	1.15	4 (5%)	79,115,115	1.51	12 (15%)
15	LMT	bg	103	-	36,36,36	1.03	4 (11%)	47,47,47	0.92	2 (4%)
14	BCL	AD	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	9 (11%)
14	BCL	AP	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.34	8 (10%)
28	UYH	ai	102	-	55,55,55	2.15	14 (25%)	63,63,63	0.99	1 (1%)
14	BCL	AH	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.34	7 (8%)
15	LMT	bf	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.83	1 (2%)
14	BCL	AV	103	29	69,74,74	1.15	5 (7%)	79,115,115	1.36	9 (11%)
16	V7N	BI	1001	-	44,44,44	1.67	7 (15%)	48,54,54	1.57	11 (22%)
15	LMT	BL	1002	-	36,36,36	1.03	4 (11%)	47,47,47	1.01	2 (4%)
15	LMT	BS	1004	-	36,36,36	1.04	4 (11%)	47,47,47	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	V7N	BG	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.66	12 (25%)
16	V7N	BS	1001	-	44,44,44	1.66	5 (11%)	48,54,54	1.64	12 (25%)
16	V7N	ba	101	-	44,44,44	1.69	6 (13%)	48,54,54	2.03	16 (33%)
15	LMT	BM	1004	-	36,36,36	1.04	4 (11%)	47,47,47	0.88	2 (4%)
14	BCL	ai	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.49	10 (12%)
14	BCL	AC	101	-	69,74,74	1.19	6 (8%)	79,115,115	1.36	11 (13%)
20	0V9	ba	102	-	44,44,46	0.76	1 (2%)	47,49,51	0.80	1 (2%)
16	V7N	bi	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.58	13 (27%)
21	CD4	ae	101	-	83,83,83	0.47	0	89,95,95	1.07	3 (3%)
15	LMT	AA	1003	-	36,36,36	1.06	4 (11%)	47,47,47	1.05	2 (4%)
15	LMT	BC	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.86	1 (2%)
14	BCL	BB	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.36	9 (11%)
15	LMT	bl	101	-	36,36,36	1.05	4 (11%)	47,47,47	1.03	3 (6%)
14	BCL	AQ	101	29	69,74,74	1.15	4 (5%)	79,115,115	1.70	15 (18%)
16	V7N	bj	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.61	11 (22%)
15	LMT	bn	105	-	36,36,36	1.07	4 (11%)	47,47,47	0.99	2 (4%)
15	LMT	BU	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	1 (2%)
16	V7N	AE	1005	-	44,44,44	1.68	8 (18%)	48,54,54	1.65	9 (18%)
14	BCL	BE	104	-	69,74,74	1.13	5 (7%)	79,115,115	1.38	12 (15%)
14	BCL	AU	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.29	7 (8%)
15	LMT	BL	1005	-	36,36,36	1.05	4 (11%)	47,47,47	0.96	1 (2%)
14	BCL	BO	1004	-	69,74,74	1.12	5 (7%)	79,115,115	1.38	12 (15%)
15	LMT	L	1008	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	2 (4%)
15	LMT	AX	101	-	36,36,36	1.03	4 (11%)	47,47,47	0.97	3 (6%)
14	BCL	AP	103	29	69,74,74	1.15	5 (7%)	79,115,115	1.34	9 (11%)
14	BCL	bi	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.30	11 (13%)
15	LMT	BG	1002	-	36,36,36	1.02	4 (11%)	47,47,47	1.12	5 (10%)
25	BPH	L	1009	-	59,70,70	1.13	4 (6%)	59,101,101	1.78	9 (15%)
15	LMT	BD	104	-	36,36,36	1.07	4 (11%)	47,47,47	0.88	1 (2%)
17	HEC	C	403	5	46,50,50	1.84	5 (10%)	58,82,82	1.68	7 (12%)
14	BCL	bc	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.40	12 (15%)
15	LMT	BD	103	-	36,36,36	1.04	4 (11%)	47,47,47	1.08	3 (6%)
15	LMT	BB	102	-	36,36,36	1.06	4 (11%)	47,47,47	0.94	2 (4%)
14	BCL	bo	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.29	9 (11%)
14	BCL	AN	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	V7N	bl	102	-	44,44,44	1.67	7 (15%)	48,54,54	1.64	11 (22%)
16	V7N	BB	101	-	44,44,44	1.65	6 (13%)	48,54,54	1.66	12 (25%)
15	LMT	BG	1005	-	36,36,36	1.04	4 (11%)	47,47,47	0.86	0
14	BCL	AA	1002	29	69,74,74	1.13	5 (7%)	79,115,115	1.38	12 (15%)
14	BCL	BU	1004	-	69,74,74	1.11	5 (7%)	79,115,115	1.32	9 (11%)
16	V7N	bc	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.61	10 (20%)
15	LMT	be	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.95	2 (4%)
15	LMT	bm	105	-	36,36,36	1.04	4 (11%)	47,47,47	0.88	2 (4%)
15	LMT	BR	1002	-	36,36,36	1.05	4 (11%)	47,47,47	0.96	3 (6%)
16	V7N	BM	1001	-	44,44,44	1.66	8 (18%)	48,54,54	1.72	12 (25%)
14	BCL	bb	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.26	10 (12%)
19	NDG	C	406	18	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
14	BCL	AL	103	-	69,74,74	1.16	5 (7%)	79,115,115	1.31	7 (8%)
14	BCL	BT	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.38	11 (13%)
15	LMT	BT	102	-	36,36,36	1.02	3 (8%)	47,47,47	1.02	3 (6%)
15	LMT	BV	1003	-	36,36,36	1.05	4 (11%)	47,47,47	0.86	1 (2%)
14	BCL	AO	1002	-	69,74,74	1.14	5 (7%)	79,115,115	1.26	7 (8%)
14	BCL	AA	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.31	7 (8%)
15	LMT	BE	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.98	3 (6%)
20	0V9	H1	101	-	44,44,46	0.77	1 (2%)	47,49,51	0.80	3 (6%)
15	LMT	BK	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.99	2 (4%)
15	LMT	BA	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	2 (4%)
20	0V9	bk	103	-	44,44,46	0.77	1 (2%)	47,49,51	0.77	2 (4%)
15	LMT	BH	1002	-	36,36,36	1.07	4 (11%)	47,47,47	0.96	2 (4%)
16	V7N	be	101	-	44,44,44	1.68	8 (18%)	48,54,54	1.69	10 (20%)
16	V7N	bh	102	-	44,44,44	1.66	7 (15%)	48,54,54	1.63	9 (18%)
14	BCL	bf	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.31	11 (13%)
14	BCL	AR	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
15	LMT	BJ	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.89	1 (2%)
14	BCL	BS	1003	-	69,74,74	1.12	5 (7%)	79,115,115	1.40	9 (11%)
16	V7N	bf	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.66	13 (27%)
16	V7N	BU	1001	-	44,44,44	1.70	7 (15%)	48,54,54	1.69	10 (20%)
20	0V9	bj	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.92	3 (6%)
14	BCL	AW	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
14	BCL	ad	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	AF	1002	-	36,36,36	1.07	4 (11%)	47,47,47	0.86	1 (2%)
15	LMT	BN	101	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	1 (2%)
14	BCL	ah	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	10 (12%)
15	LMT	BN	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.83	0
14	BCL	AQ	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
16	V7N	BQ	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.59	13 (27%)
14	BCL	BA	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.54	11 (13%)
14	BCL	AS	102	29	69,74,74	1.13	5 (7%)	79,115,115	1.33	10 (12%)
16	V7N	BE	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.59	12 (25%)
15	LMT	M	403	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	2 (4%)
15	LMT	BV	1006	-	36,36,36	1.05	4 (11%)	47,47,47	0.82	0
25	BPH	M	406	-	59,70,70	1.11	3 (5%)	59,101,101	1.83	9 (15%)
14	BCL	AK	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.29	7 (8%)
15	LMT	BW	1005	-	36,36,36	1.09	4 (11%)	47,47,47	1.01	1 (2%)
20	0V9	bk	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	1 (2%)
15	LMT	bh	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	3 (6%)
14	BCL	ba	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.27	9 (11%)
16	V7N	AS	105	-	44,44,44	1.66	7 (15%)	48,54,54	1.76	10 (20%)
16	V7N	BV	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.64	12 (25%)
15	LMT	BQ	1002	-	36,36,36	1.07	4 (11%)	47,47,47	0.87	2 (4%)
15	LMT	BA	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.94	1 (2%)
14	BCL	AU	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.40	12 (15%)
14	BCL	AN	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	9 (11%)
21	CD4	af	102	-	83,83,83	0.47	0	89,95,95	1.15	6 (6%)
15	LMT	BV	1002	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	2 (4%)
20	0V9	bg	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.86	3 (6%)
14	BCL	AN	104	-	69,74,74	1.15	5 (7%)	79,115,115	1.39	11 (13%)
14	BCL	AS	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.31	7 (8%)
23	MQ8	M	407	-	54,54,54	0.66	0	67,69,69	0.92	4 (5%)
14	BCL	AV	101	29	69,74,74	1.12	5 (7%)	79,115,115	1.36	10 (12%)
15	LMT	AI	101	-	36,36,36	1.05	3 (8%)	47,47,47	1.14	3 (6%)
15	LMT	BX	1003	-	36,36,36	1.03	4 (11%)	47,47,47	0.97	2 (4%)
14	BCL	ac	1001	-	69,74,74	1.12	5 (7%)	79,115,115	1.33	9 (11%)
14	BCL	AX	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.46	14 (17%)
15	LMT	AP	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	BT	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	0
14	BCL	AB	1001	-	69,74,74	1.12	5 (7%)	79,115,115	1.38	11 (13%)
20	0V9	be	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.92	2 (4%)
23	MQ8	ao	101	-	54,54,54	0.62	0	67,69,69	1.04	2 (2%)
15	LMT	BQ	1004	-	36,36,36	1.07	4 (11%)	47,47,47	0.88	2 (4%)
16	V7N	bm	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.52	10 (20%)
20	0V9	bo	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.92	2 (4%)
15	LMT	bi	102	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	0
15	LMT	BJ	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.85	1 (2%)
14	BCL	ak	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.31	9 (11%)
16	V7N	BJ	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.66	14 (29%)
14	BCL	AM	102	29	69,74,74	1.16	6 (8%)	79,115,115	1.41	12 (15%)
14	BCL	ap	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.35	10 (12%)
15	LMT	BI	1006	-	36,36,36	1.04	4 (11%)	47,47,47	1.05	2 (4%)
14	BCL	ag	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	9 (11%)
15	LMT	AH	104	-	36,36,36	1.04	4 (11%)	47,47,47	1.09	3 (6%)
15	LMT	L	1007	-	36,36,36	1.07	4 (11%)	47,47,47	0.84	1 (2%)
15	LMT	BC	106	-	36,36,36	1.05	4 (11%)	47,47,47	0.82	1 (2%)
14	BCL	BM	1002	-	69,74,74	1.12	5 (7%)	79,115,115	1.28	8 (10%)
16	V7N	BL	1001	-	44,44,44	1.66	6 (13%)	48,54,54	1.65	13 (27%)
14	BCL	BK	1006	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	9 (11%)
15	LMT	bl	105	-	36,36,36	1.07	4 (11%)	47,47,47	0.84	2 (4%)
14	BCL	AT	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.30	7 (8%)
14	BCL	AG	101	29	69,74,74	1.13	6 (8%)	79,115,115	1.56	13 (16%)
14	BCL	BX	1002	-	69,74,74	1.11	5 (7%)	79,115,115	1.42	12 (15%)
15	LMT	bb	102	-	36,36,36	1.06	4 (11%)	47,47,47	1.13	4 (8%)
14	BCL	M	405	-	69,74,74	1.12	5 (7%)	79,115,115	1.36	9 (11%)
15	LMT	AQ	103	-	36,36,36	1.06	4 (11%)	47,47,47	1.02	3 (6%)
14	BCL	AM	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.30	7 (8%)

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
20	0V9	bl	103	-	-	15/48/48/50	-
15	LMT	bc	104	-	-	6/21/61/61	0/2/2/2
16	V7N	BH	1001	-	-	6/53/53/53	-
22	PGW	H1	103	-	-	14/55/55/55	-
20	0V9	aj	101	-	-	13/48/48/50	-
14	BCL	BI	1003	-	-	9/41/137/137	-
16	V7N	BW	1001	-	-	4/53/53/53	-
14	BCL	AL	101	-	-	10/41/137/137	-
20	0V9	bp	103	-	-	14/48/48/50	-
21	CD4	H1	104	-	-	19/94/94/94	-
15	LMT	ab	101	-	-	3/21/61/61	0/2/2/2
15	LMT	BW	1004	-	-	4/21/61/61	0/2/2/2
14	BCL	AF	1001	-	-	3/41/137/137	-
20	0V9	bn	104	-	-	10/48/48/50	-
14	BCL	BH	1005	-	-	7/41/137/137	-
20	0V9	bb	103	-	-	11/48/48/50	-
15	LMT	AA	1004	-	-	3/21/61/61	0/2/2/2
14	BCL	aa	1001	-	-	6/41/137/137	-
14	BCL	BL	1003	-	-	2/41/137/137	-
15	LMT	AP	101	-	-	5/21/61/61	0/2/2/2
15	LMT	AN	103	-	-	2/21/61/61	0/2/2/2
15	LMT	BG	1003	-	-	2/21/61/61	0/2/2/2
14	BCL	AG	102	-	-	5/41/137/137	-
15	LMT	BB	105	-	-	5/21/61/61	0/2/2/2
15	LMT	BK	1003	-	-	8/21/61/61	0/2/2/2
14	BCL	AS	104	29	-	7/41/137/137	-
16	V7N	bb	101	-	-	12/53/53/53	-
14	BCL	al	1001	-	-	7/41/137/137	-
14	BCL	BV	1005	-	-	7/41/137/137	-
15	LMT	AL	102	-	-	1/21/61/61	0/2/2/2
20	0V9	C1	1001	-	-	12/48/48/50	-
14	BCL	BF	102	-	-	5/41/137/137	-
14	BCL	AI	102	-	-	8/41/137/137	-
14	BCL	aj	103	-	-	7/41/137/137	-
15	LMT	AD	103	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	V7N	BD	101	-	-	3/53/53/53	-
15	LMT	bo	101	-	-	0/21/61/61	0/2/2/2
14	BCL	AE	1004	-	-	5/41/137/137	-
14	BCL	ao	102	-	-	6/41/137/137	-
14	BCL	bh	105	-	-	5/41/137/137	-
16	V7N	bg	101	-	-	7/53/53/53	-
15	LMT	BN	105	-	-	2/21/61/61	0/2/2/2
16	V7N	bo	102	-	-	4/53/53/53	-
14	BCL	BC	104	-	-	7/41/137/137	-
15	LMT	BX	1004	-	-	5/21/61/61	0/2/2/2
15	LMT	BE	103	-	-	6/21/61/61	0/2/2/2
14	BCL	bn	103	-	-	7/41/137/137	-
15	LMT	BH	1003	-	-	8/21/61/61	0/2/2/2
15	LMT	bh	101	-	-	6/21/61/61	0/2/2/2
20	0V9	be	103	-	-	12/48/48/50	-
15	LMT	BI	1002	-	-	2/21/61/61	0/2/2/2
16	V7N	BC	101	-	-	3/53/53/53	-
15	LMT	L	1011	-	-	3/21/61/61	0/2/2/2
14	BCL	AJ	101	-	-	0/41/137/137	-
14	BCL	bl	104	-	-	11/41/137/137	-
16	V7N	BK	1001	-	-	3/53/53/53	-
14	BCL	AE	1003	29	-	10/41/137/137	-
15	LMT	BF	101	-	-	2/21/61/61	0/2/2/2
14	BCL	AC	102	-	-	5/41/137/137	-
24	V7B	L	1006	-	-	9/48/88/88	0/2/2/2
15	LMT	AC	104	-	-	4/21/61/61	0/2/2/2
15	LMT	AJ	103	-	-	10/21/61/61	0/2/2/2
14	BCL	AK	101	29	-	8/41/137/137	-
15	LMT	BS	1005	-	-	4/21/61/61	0/2/2/2
14	BCL	BG	1004	-	-	6/41/137/137	-
15	LMT	AT	102	-	-	3/21/61/61	0/2/2/2
15	LMT	BQ	1005	-	-	1/21/61/61	0/2/2/2
14	BCL	af	101	-	-	3/41/137/137	-
14	BCL	M	408	-	-	3/41/137/137	-
15	LMT	bn	101	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	an	1001	-	-	6/41/137/137	-
16	V7N	bd	101	-	-	4/53/53/53	-
14	BCL	AJ	102	29	-	9/41/137/137	-
14	BCL	L	1010	-	-	1/41/137/137	-
20	0V9	bi	103	-	-	10/48/48/50	-
15	LMT	AE	1002	-	-	4/21/61/61	0/2/2/2
20	0V9	bc	103	-	-	11/48/48/50	-
15	LMT	L	1005	-	-	1/21/61/61	0/2/2/2
14	BCL	be	105	-	-	6/41/137/137	-
15	LMT	BP	1003	-	-	3/21/61/61	0/2/2/2
15	LMT	BM	1003	-	-	7/21/61/61	0/2/2/2
15	LMT	BW	1002	-	-	3/21/61/61	0/2/2/2
18	V75	C	405	13,19	-	0/12/29/29	0/1/1/1
14	BCL	am	1001	-	-	4/41/137/137	-
14	BCL	AX	103	-	-	5/41/137/137	-
18	V75	M	409	13,19	-	0/12/29/29	0/1/1/1
14	BCL	AE	1001	-	-	1/41/137/137	-
15	LMT	AJ	104	-	-	7/21/61/61	0/2/2/2
14	BCL	bm	104	-	-	7/41/137/137	-
14	BCL	AC	103	29	-	4/41/137/137	-
14	BCL	BJ	1002	-	-	7/41/137/137	-
20	0V9	bg	102	-	-	17/48/48/50	-
15	LMT	L	1003	-	-	8/21/61/61	0/2/2/2
15	LMT	BS	1002	-	-	3/21/61/61	0/2/2/2
15	LMT	BU	1003	-	-	2/21/61/61	0/2/2/2
14	BCL	BD	105	-	-	3/41/137/137	-
15	LMT	BO	1003	-	-	1/21/61/61	0/2/2/2
17	HEC	C	402	5	-	4/14/54/54	-
20	0V9	bm	102	-	-	8/48/48/50	-
16	V7N	BP	1001	-	-	3/53/53/53	-
14	BCL	bg	105	-	-	5/41/137/137	-
15	LMT	AU	101	-	-	6/21/61/61	0/2/2/2
14	BCL	bd	102	-	-	4/41/137/137	-
15	LMT	AG	103	-	-	10/21/61/61	0/2/2/2
15	LMT	BR	1005	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	BI	1004	-	-	3/21/61/61	0/2/2/2
17	HEC	C	401	5	-	6/14/54/54	-
19	NDG	C1	1002	18	-	0/6/23/26	0/1/1/1
15	LMT	bm	103	-	-	8/21/61/61	0/2/2/2
15	LMT	BB	104	-	-	6/21/61/61	0/2/2/2
15	LMT	BK	1002	-	-	4/21/61/61	0/2/2/2
21	CD4	M	402	-	-	21/94/94/94	-
16	V7N	BX	1001	-	-	6/53/53/53	-
21	CD4	H1	102	-	-	21/94/94/94	-
15	LMT	BK	1004	-	-	5/21/61/61	0/2/2/2
15	LMT	BO	1002	-	-	3/21/61/61	0/2/2/2
14	BCL	BP	1005	-	-	6/41/137/137	-
15	LMT	AH	102	-	-	3/21/61/61	0/2/2/2
17	HEC	C	404	5	-	6/14/54/54	-
14	BCL	bp	102	-	-	11/41/137/137	-
14	BCL	BW	1003	-	-	7/41/137/137	-
21	CD4	aj	102	-	-	26/94/94/94	-
16	V7N	BA	101	-	-	4/53/53/53	-
23	MQ8	L	1001	-	-	8/47/67/67	0/2/2/2
14	BCL	BQ	1003	-	-	8/41/137/137	-
15	LMT	BC	105	-	-	4/21/61/61	0/2/2/2
15	LMT	BP	1002	-	-	6/21/61/61	0/2/2/2
14	BCL	AB	1002	29	-	5/41/137/137	-
14	BCL	ab	102	-	-	6/41/137/137	-
14	BCL	bk	102	-	-	9/41/137/137	-
15	LMT	BS	1006	-	-	3/21/61/61	0/2/2/2
15	LMT	bd	103	-	-	5/21/61/61	0/2/2/2
16	V7N	bp	101	-	-	5/53/53/53	-
15	LMT	BR	1003	-	-	8/21/61/61	0/2/2/2
16	V7N	AO	1001	-	-	7/53/53/53	-
15	LMT	AD	101	-	-	8/21/61/61	0/2/2/2
16	V7N	BR	1001	-	-	7/53/53/53	-
15	LMT	BV	1004	-	-	4/21/61/61	0/2/2/2
27	CRT	M	404	-	-	4/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	BR	1004	-	-	3/41/137/137	-
24	V7B	ag	1002	-	-	10/48/88/88	0/2/2/2
15	LMT	BH	1004	-	-	3/21/61/61	0/2/2/2
16	V7N	bk	101	-	-	3/53/53/53	-
15	LMT	BG	1006	-	-	1/21/61/61	0/2/2/2
16	V7N	bn	102	-	-	4/53/53/53	-
14	BCL	bj	103	-	-	6/41/137/137	-
20	0V9	bh	103	-	-	10/48/48/50	-
16	V7N	BO	1001	-	-	7/53/53/53	-
15	LMT	L	1004	-	-	4/21/61/61	0/2/2/2
14	BCL	AV	102	-	-	3/41/137/137	-
14	BCL	BN	103	-	-	8/41/137/137	-
15	LMT	BN	102	-	-	3/21/61/61	0/2/2/2
15	LMT	BL	1004	-	-	8/21/61/61	0/2/2/2
15	LMT	BP	1004	-	-	1/21/61/61	0/2/2/2
14	BCL	L	1002	-	-	5/41/137/137	-
15	LMT	BI	1005	-	-	1/21/61/61	0/2/2/2
15	LMT	BC	102	-	-	6/21/61/61	0/2/2/2
15	LMT	BA	105	-	-	6/21/61/61	0/2/2/2
15	LMT	bo	105	-	-	5/21/61/61	0/2/2/2
15	LMT	AS	101	-	-	9/21/61/61	0/2/2/2
15	LMT	BT	101	-	-	4/21/61/61	0/2/2/2
14	BCL	AR	102	-	-	9/41/137/137	-
14	BCL	ae	102	-	-	10/41/137/137	-
15	LMT	BF	103	-	-	4/21/61/61	0/2/2/2
15	LMT	bj	102	-	-	6/21/61/61	0/2/2/2
15	LMT	BD	102	-	-	6/21/61/61	0/2/2/2
14	BCL	AH	101	-	-	7/41/137/137	-
14	BCL	AI	103	-	-	8/41/137/137	-
15	LMT	bg	103	-	-	4/21/61/61	0/2/2/2
14	BCL	AD	102	-	-	1/41/137/137	-
14	BCL	AP	102	-	-	3/41/137/137	-
28	UYH	ai	102	-	-	7/50/70/70	0/1/1/1
14	BCL	AH	103	-	-	5/41/137/137	-
15	LMT	bf	102	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	AV	103	29	-	10/41/137/137	-
16	V7N	BI	1001	-	-	6/53/53/53	-
15	LMT	BL	1002	-	-	6/21/61/61	0/2/2/2
15	LMT	BS	1004	-	-	7/21/61/61	0/2/2/2
16	V7N	BG	1001	-	-	5/53/53/53	-
16	V7N	BS	1001	-	-	4/53/53/53	-
16	V7N	ba	101	-	-	8/53/53/53	-
15	LMT	BM	1004	-	-	1/21/61/61	0/2/2/2
14	BCL	ai	101	-	-	10/41/137/137	-
14	BCL	AC	101	-	-	8/41/137/137	-
20	0V9	ba	102	-	-	11/48/48/50	-
16	V7N	bi	101	-	-	10/53/53/53	-
21	CD4	ae	101	-	-	26/94/94/94	-
15	LMT	AA	1003	-	-	10/21/61/61	0/2/2/2
15	LMT	BC	103	-	-	3/21/61/61	0/2/2/2
14	BCL	BB	103	-	-	9/41/137/137	-
15	LMT	bl	101	-	-	8/21/61/61	0/2/2/2
14	BCL	AQ	101	29	-	10/41/137/137	-
16	V7N	bj	101	-	-	8/53/53/53	-
15	LMT	bn	105	-	-	5/21/61/61	0/2/2/2
15	LMT	BU	1002	-	-	8/21/61/61	0/2/2/2
16	V7N	AE	1005	-	-	5/53/53/53	-
14	BCL	BE	104	-	-	3/41/137/137	-
14	BCL	AU	102	-	-	2/41/137/137	-
15	LMT	BL	1005	-	-	2/21/61/61	0/2/2/2
14	BCL	BO	1004	-	-	7/41/137/137	-
15	LMT	L	1008	-	-	6/21/61/61	0/2/2/2
15	LMT	AX	101	-	-	10/21/61/61	0/2/2/2
14	BCL	AP	103	29	-	4/41/137/137	-
14	BCL	bi	104	-	-	6/41/137/137	-
15	LMT	BG	1002	-	-	7/21/61/61	0/2/2/2
25	BPH	L	1009	-	-	5/37/105/105	0/5/6/6
15	LMT	BD	104	-	-	3/21/61/61	0/2/2/2
17	HEC	C	403	5	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	bc	102	-	-	10/41/137/137	-
15	LMT	BD	103	-	-	6/21/61/61	0/2/2/2
15	LMT	BB	102	-	-	2/21/61/61	0/2/2/2
14	BCL	bo	103	-	-	5/41/137/137	-
14	BCL	AN	102	-	-	0/41/137/137	-
16	V7N	bl	102	-	-	5/53/53/53	-
16	V7N	BB	101	-	-	6/53/53/53	-
15	LMT	BG	1005	-	-	3/21/61/61	0/2/2/2
14	BCL	AA	1002	29	-	4/41/137/137	-
14	BCL	BU	1004	-	-	6/41/137/137	-
16	V7N	bc	101	-	-	5/53/53/53	-
15	LMT	be	104	-	-	9/21/61/61	0/2/2/2
15	LMT	bm	105	-	-	9/21/61/61	0/2/2/2
15	LMT	BR	1002	-	-	4/21/61/61	0/2/2/2
16	V7N	BM	1001	-	-	4/53/53/53	-
14	BCL	bb	104	-	-	8/41/137/137	-
19	NDG	C	406	18	-	0/6/23/26	0/1/1/1
14	BCL	AL	103	-	-	4/41/137/137	-
14	BCL	BT	103	-	-	5/41/137/137	-
15	LMT	BT	102	-	-	5/21/61/61	0/2/2/2
15	LMT	BV	1003	-	-	4/21/61/61	0/2/2/2
14	BCL	AO	1002	-	-	1/41/137/137	-
14	BCL	AA	1001	-	-	5/41/137/137	-
15	LMT	BE	102	-	-	3/21/61/61	0/2/2/2
20	0V9	H1	101	-	-	8/48/48/50	-
15	LMT	BK	1005	-	-	4/21/61/61	0/2/2/2
15	LMT	BA	104	-	-	7/21/61/61	0/2/2/2
20	0V9	bk	103	-	-	10/48/48/50	-
15	LMT	BH	1002	-	-	5/21/61/61	0/2/2/2
16	V7N	be	101	-	-	6/53/53/53	-
16	V7N	bh	102	-	-	6/53/53/53	-
14	BCL	bf	103	-	-	7/41/137/137	-
14	BCL	AR	101	-	-	3/41/137/137	-
15	LMT	BJ	1003	-	-	3/21/61/61	0/2/2/2
14	BCL	BS	1003	-	-	4/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	V7N	bf	101	-	-	6/53/53/53	-
16	V7N	BU	1001	-	-	8/53/53/53	-
20	0V9	bj	104	-	-	12/48/48/50	-
14	BCL	AW	101	-	-	1/41/137/137	-
14	BCL	ad	1001	-	-	8/41/137/137	-
15	LMT	AF	1002	-	-	6/21/61/61	0/2/2/2
15	LMT	BN	101	-	-	7/21/61/61	0/2/2/2
14	BCL	ah	1001	-	-	2/41/137/137	-
15	LMT	BN	104	-	-	5/21/61/61	0/2/2/2
14	BCL	AQ	102	-	-	0/41/137/137	-
16	V7N	BQ	1001	-	-	5/53/53/53	-
14	BCL	BA	103	-	-	7/41/137/137	-
14	BCL	AS	102	29	-	5/41/137/137	-
16	V7N	BE	101	-	-	4/53/53/53	-
15	LMT	M	403	-	-	5/21/61/61	0/2/2/2
15	LMT	BV	1006	-	-	2/21/61/61	0/2/2/2
25	BPH	M	406	-	-	5/37/105/105	0/5/6/6
14	BCL	AK	102	-	-	1/41/137/137	-
15	LMT	BW	1005	-	-	1/21/61/61	0/2/2/2
20	0V9	bk	104	-	-	13/48/48/50	-
15	LMT	bh	104	-	-	5/21/61/61	0/2/2/2
14	BCL	ba	103	-	-	3/41/137/137	-
16	V7N	AS	105	-	-	6/53/53/53	-
16	V7N	BV	1001	-	-	4/53/53/53	-
15	LMT	BQ	1002	-	-	3/21/61/61	0/2/2/2
15	LMT	BA	102	-	-	4/21/61/61	0/2/2/2
14	BCL	AU	103	-	-	3/41/137/137	-
14	BCL	AN	101	-	-	3/41/137/137	-
21	CD4	af	102	-	-	21/94/94/94	-
15	LMT	BV	1002	-	-	1/21/61/61	0/2/2/2
20	0V9	bg	104	-	-	8/48/48/50	-
14	BCL	AN	104	-	-	9/41/137/137	-
14	BCL	AS	103	-	-	2/41/137/137	-
23	MQ8	M	407	-	-	4/47/67/67	0/2/2/2
14	BCL	AV	101	29	-	3/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	AI	101	-	-	4/21/61/61	0/2/2/2
15	LMT	BX	1003	-	-	7/21/61/61	0/2/2/2
14	BCL	ac	1001	-	-	2/41/137/137	-
14	BCL	AX	102	-	-	9/41/137/137	-
15	LMT	AP	104	-	-	3/21/61/61	0/2/2/2
15	LMT	BT	104	-	-	6/21/61/61	0/2/2/2
14	BCL	AB	1001	-	-	3/41/137/137	-
20	0V9	be	102	-	-	10/48/48/50	-
23	MQ8	ao	101	-	-	10/47/67/67	0/2/2/2
15	LMT	BQ	1004	-	-	7/21/61/61	0/2/2/2
16	V7N	bm	101	-	-	8/53/53/53	-
20	0V9	bo	104	-	-	7/48/48/50	-
15	LMT	bi	102	-	-	3/21/61/61	0/2/2/2
15	LMT	BJ	1004	-	-	2/21/61/61	0/2/2/2
14	BCL	ak	1001	-	-	6/41/137/137	-
16	V7N	BJ	1001	-	-	5/53/53/53	-
14	BCL	AM	102	29	-	5/41/137/137	-
14	BCL	ap	1001	-	-	7/41/137/137	-
15	LMT	BI	1006	-	-	4/21/61/61	0/2/2/2
14	BCL	ag	1001	-	-	5/41/137/137	-
15	LMT	AH	104	-	-	6/21/61/61	0/2/2/2
15	LMT	L	1007	-	-	1/21/61/61	0/2/2/2
15	LMT	BC	106	-	-	3/21/61/61	0/2/2/2
14	BCL	BM	1002	-	-	14/41/137/137	-
16	V7N	BL	1001	-	-	6/53/53/53	-
14	BCL	BK	1006	-	-	5/41/137/137	-
15	LMT	bl	105	-	-	2/21/61/61	0/2/2/2
14	BCL	AT	101	-	-	0/41/137/137	-
14	BCL	AG	101	29	-	10/41/137/137	-
14	BCL	BX	1002	-	-	5/41/137/137	-
15	LMT	bb	102	-	-	9/21/61/61	0/2/2/2
14	BCL	M	405	-	-	1/41/137/137	-
15	LMT	AQ	103	-	-	7/21/61/61	0/2/2/2
14	BCL	AM	101	-	-	2/41/137/137	-

All (1395) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	bn	102	V7N	C28-C27	6.92	1.52	1.34
16	BI	1001	V7N	C28-C27	6.90	1.52	1.34
16	BC	101	V7N	C28-C27	6.89	1.52	1.34
16	BK	1001	V7N	C28-C27	6.87	1.52	1.34
16	BP	1001	V7N	C28-C27	6.87	1.52	1.34
16	be	101	V7N	C28-C27	6.86	1.52	1.34
16	bp	101	V7N	C28-C27	6.86	1.52	1.34
16	bg	101	V7N	C28-C27	6.82	1.52	1.34
16	BU	1001	V7N	C28-C27	6.81	1.52	1.34
16	BX	1001	V7N	C28-C27	6.81	1.52	1.34
16	BD	101	V7N	C28-C27	6.81	1.52	1.34
16	AE	1005	V7N	C28-C27	6.80	1.52	1.34
16	bo	102	V7N	C28-C27	6.80	1.52	1.34
16	BV	1001	V7N	C28-C27	6.79	1.52	1.34
16	BO	1001	V7N	C28-C27	6.79	1.52	1.34
16	BR	1001	V7N	C28-C27	6.79	1.52	1.34
16	BL	1001	V7N	C28-C27	6.78	1.52	1.34
16	bd	101	V7N	C28-C27	6.77	1.52	1.34
16	bb	101	V7N	C28-C27	6.77	1.52	1.34
16	ba	101	V7N	C28-C27	6.76	1.52	1.34
16	AO	1001	V7N	C28-C27	6.76	1.52	1.34
16	BE	101	V7N	C28-C27	6.76	1.52	1.34
16	BH	1001	V7N	C28-C27	6.75	1.52	1.34
16	BS	1001	V7N	C28-C27	6.75	1.52	1.34
16	BQ	1001	V7N	C28-C27	6.74	1.52	1.34
16	bi	101	V7N	C28-C27	6.74	1.52	1.34
16	bl	102	V7N	C28-C27	6.73	1.52	1.34
16	bm	101	V7N	C28-C27	6.73	1.52	1.34
16	bh	102	V7N	C28-C27	6.73	1.52	1.34
16	BJ	1001	V7N	C28-C27	6.73	1.52	1.34
16	bf	101	V7N	C28-C27	6.72	1.52	1.34
16	BM	1001	V7N	C28-C27	6.72	1.52	1.34
16	BW	1001	V7N	C28-C27	6.72	1.52	1.34
16	BA	101	V7N	C28-C27	6.71	1.52	1.34
16	BG	1001	V7N	C28-C27	6.69	1.52	1.34
16	AS	105	V7N	C28-C27	6.68	1.52	1.34
16	bj	101	V7N	C28-C27	6.67	1.52	1.34
16	BB	101	V7N	C28-C27	6.66	1.52	1.34
16	bk	101	V7N	C28-C27	6.66	1.52	1.34
16	bc	101	V7N	C28-C27	6.65	1.52	1.34
17	C	402	HEC	CAC-C3C	6.35	1.55	1.35
17	C	401	HEC	CAB-C3B	6.35	1.55	1.35
17	C	401	HEC	CAC-C3C	6.32	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	404	HEC	CAC-C3C	6.32	1.55	1.35
17	C	403	HEC	CAC-C3C	6.30	1.55	1.35
17	C	403	HEC	CAB-C3B	6.29	1.55	1.35
17	C	402	HEC	CAB-C3B	6.26	1.55	1.35
17	C	404	HEC	CAB-C3B	6.25	1.55	1.35
14	BI	1003	BCL	O2A-CGA	-5.64	1.16	1.33
17	C	404	HEC	C3D-C2D	5.54	1.53	1.38
17	C	402	HEC	C3D-C2D	5.48	1.53	1.38
17	C	403	HEC	C3D-C2D	5.48	1.53	1.38
17	C	401	HEC	C3D-C2D	5.44	1.53	1.38
14	AX	103	BCL	MG-NA	5.23	2.18	2.06
14	AE	1004	BCL	MG-NA	5.14	2.18	2.06
14	AN	101	BCL	MG-NA	5.13	2.18	2.06
14	AA	1001	BCL	MG-NA	5.12	2.18	2.06
14	AM	101	BCL	MG-NA	5.12	2.18	2.06
14	AR	102	BCL	MG-NA	5.12	2.18	2.06
14	AB	1001	BCL	MG-NA	5.10	2.18	2.06
14	AP	102	BCL	MG-NA	5.10	2.18	2.06
14	AD	102	BCL	MG-NA	5.09	2.18	2.06
14	AR	101	BCL	MG-NA	5.08	2.18	2.06
14	AV	102	BCL	MG-NA	5.08	2.18	2.06
14	AC	102	BCL	MG-NA	5.07	2.18	2.06
14	AL	103	BCL	MG-NA	5.06	2.18	2.06
14	AK	102	BCL	MG-NA	5.06	2.18	2.06
14	AC	101	BCL	MG-NA	5.06	2.18	2.06
14	AE	1001	BCL	MG-NA	5.06	2.18	2.06
14	AP	103	BCL	MG-NA	5.06	2.18	2.06
14	AH	103	BCL	MG-NA	5.04	2.18	2.06
14	AL	101	BCL	MG-NA	5.03	2.18	2.06
14	ah	1001	BCL	MG-NA	5.03	2.18	2.06
14	AG	102	BCL	MG-NA	5.03	2.18	2.06
14	AM	102	BCL	MG-NA	5.03	2.18	2.06
14	AT	101	BCL	MG-NA	5.03	2.18	2.06
14	AJ	101	BCL	MG-NA	5.02	2.18	2.06
14	AQ	102	BCL	MG-NA	5.01	2.18	2.06
14	AU	102	BCL	MG-NA	5.01	2.18	2.06
14	AJ	102	BCL	MG-NA	5.00	2.18	2.06
14	AW	101	BCL	MG-NA	4.99	2.18	2.06
14	AF	1001	BCL	MG-NA	4.99	2.18	2.06
14	AO	1002	BCL	MG-NA	4.97	2.18	2.06
14	aa	1001	BCL	MG-NA	4.97	2.18	2.06
14	al	1001	BCL	MG-NA	4.97	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ak	1001	BCL	MG-NA	4.96	2.18	2.06
14	AS	103	BCL	MG-NA	4.96	2.18	2.06
14	AS	104	BCL	MG-NA	4.95	2.18	2.06
14	AV	101	BCL	MG-NA	4.95	2.18	2.06
14	AI	102	BCL	MG-NA	4.94	2.18	2.06
14	bp	102	BCL	MG-NA	4.94	2.18	2.06
14	bh	105	BCL	MG-NA	4.94	2.18	2.06
14	ab	102	BCL	MG-NA	4.91	2.17	2.06
14	ad	1001	BCL	MG-NA	4.90	2.17	2.06
14	af	101	BCL	MG-NA	4.89	2.17	2.06
14	ao	102	BCL	MG-NA	4.89	2.17	2.06
14	ap	1001	BCL	MG-NA	4.89	2.17	2.06
14	AN	102	BCL	MG-NA	4.89	2.17	2.06
14	AV	103	BCL	MG-NA	4.89	2.17	2.06
14	AX	102	BCL	MG-NA	4.88	2.17	2.06
14	ae	102	BCL	MG-NA	4.88	2.17	2.06
14	bi	104	BCL	MG-NA	4.88	2.17	2.06
14	ac	1001	BCL	MG-NA	4.88	2.17	2.06
14	AQ	101	BCL	MG-NA	4.86	2.17	2.06
14	BX	1002	BCL	MG-NA	4.85	2.17	2.06
14	AU	103	BCL	MG-NA	4.85	2.17	2.06
14	ag	1001	BCL	MG-NA	4.85	2.17	2.06
14	AS	102	BCL	MG-NA	4.84	2.17	2.06
14	BA	103	BCL	MG-NA	4.84	2.17	2.06
14	AH	101	BCL	MG-NA	4.84	2.17	2.06
14	AK	101	BCL	MG-NA	4.83	2.17	2.06
14	ba	103	BCL	MG-NA	4.83	2.17	2.06
14	bn	103	BCL	MG-NA	4.83	2.17	2.06
14	am	1001	BCL	MG-NA	4.82	2.17	2.06
14	BN	103	BCL	O2A-CGA	-4.82	1.19	1.33
14	ai	101	BCL	MG-NA	4.82	2.17	2.06
14	BO	1004	BCL	MG-NA	4.81	2.17	2.06
14	AI	103	BCL	MG-NA	4.81	2.17	2.06
14	BD	105	BCL	MG-NA	4.81	2.17	2.06
14	BK	1006	BCL	MG-NA	4.81	2.17	2.06
14	BE	104	BCL	MG-NA	4.81	2.17	2.06
14	BL	1003	BCL	MG-NA	4.81	2.17	2.06
14	BH	1005	BCL	MG-NA	4.80	2.17	2.06
14	BV	1005	BCL	MG-NA	4.80	2.17	2.06
14	bc	102	BCL	MG-NA	4.80	2.17	2.06
14	M	405	BCL	MG-NA	4.79	2.17	2.06
14	an	1001	BCL	MG-NA	4.79	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BI	1003	BCL	MG-NA	4.78	2.17	2.06
14	BC	104	BCL	MG-NA	4.78	2.17	2.06
14	BW	1003	BCL	MG-NA	4.78	2.17	2.06
14	BT	103	BCL	MG-NA	4.77	2.17	2.06
14	bd	102	BCL	MG-NA	4.76	2.17	2.06
14	BJ	1002	BCL	MG-NA	4.76	2.17	2.06
14	aj	103	BCL	MG-NA	4.76	2.17	2.06
14	AE	1003	BCL	MG-NA	4.75	2.17	2.06
14	bl	104	BCL	MG-NA	4.74	2.17	2.06
14	BN	103	BCL	MG-NA	4.74	2.17	2.06
14	be	105	BCL	MG-NA	4.74	2.17	2.06
14	bf	103	BCL	MG-NA	4.74	2.17	2.06
14	BB	103	BCL	MG-NA	4.73	2.17	2.06
14	bb	104	BCL	MG-NA	4.73	2.17	2.06
14	bk	102	BCL	MG-NA	4.73	2.17	2.06
14	BM	1002	BCL	MG-NA	4.72	2.17	2.06
14	BS	1003	BCL	MG-NA	4.72	2.17	2.06
14	BF	102	BCL	MG-NA	4.72	2.17	2.06
14	BQ	1003	BCL	MG-NA	4.69	2.17	2.06
14	AA	1002	BCL	MG-NA	4.69	2.17	2.06
14	AG	101	BCL	MG-NA	4.69	2.17	2.06
14	bg	105	BCL	MG-NA	4.69	2.17	2.06
14	L	1010	BCL	MG-NA	4.68	2.17	2.06
14	L	1002	BCL	MG-NA	4.68	2.17	2.06
14	AC	103	BCL	MG-NA	4.68	2.17	2.06
14	AN	104	BCL	MG-NA	4.67	2.17	2.06
28	ai	102	UYH	O8-C28	4.67	1.46	1.33
14	bo	103	BCL	MG-NA	4.66	2.17	2.06
14	bm	104	BCL	MG-NA	4.65	2.17	2.06
14	BG	1004	BCL	MG-NA	4.65	2.17	2.06
14	bj	103	BCL	MG-NA	4.64	2.17	2.06
14	M	408	BCL	MG-NA	4.64	2.17	2.06
14	BP	1005	BCL	MG-NA	4.63	2.17	2.06
14	BR	1004	BCL	MG-NA	4.60	2.17	2.06
14	BU	1004	BCL	MG-NA	4.58	2.17	2.06
28	ai	102	UYH	O7-C10	4.51	1.47	1.34
14	AB	1002	BCL	MG-NA	4.37	2.16	2.06
25	M	406	BPH	CBD-CGD	-4.18	1.47	1.52
25	L	1009	BPH	CBD-CGD	-4.14	1.47	1.52
14	AC	101	BCL	MG-NC	3.87	2.15	2.06
20	H1	101	0V9	P-O2P	-3.83	1.37	1.50
20	bb	103	0V9	P-O2P	-3.81	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	bk	103	OV9	P-O2P	-3.79	1.37	1.50
20	bn	104	OV9	P-O2P	-3.79	1.37	1.50
20	bc	103	OV9	P-O2P	-3.79	1.37	1.50
14	AE	1004	BCL	MG-NC	3.78	2.15	2.06
20	C1	1001	OV9	P-O2P	-3.77	1.37	1.50
20	bh	103	OV9	P-O2P	-3.77	1.37	1.50
20	bo	104	OV9	P-O2P	-3.76	1.37	1.50
20	bj	104	OV9	P-O2P	-3.76	1.37	1.50
20	aj	101	OV9	P-O2P	-3.75	1.37	1.50
20	bg	104	OV9	P-O2P	-3.75	1.37	1.50
20	bi	103	OV9	P-O2P	-3.75	1.37	1.50
20	bm	102	OV9	P-O2P	-3.74	1.37	1.50
20	ba	102	OV9	P-O2P	-3.74	1.37	1.50
20	bk	104	OV9	P-O2P	-3.74	1.37	1.50
20	bl	103	OV9	P-O2P	-3.73	1.37	1.50
20	be	102	OV9	P-O2P	-3.73	1.37	1.50
20	bp	103	OV9	P-O2P	-3.72	1.37	1.50
20	be	103	OV9	P-O2P	-3.72	1.37	1.50
20	bg	102	OV9	P-O2P	-3.71	1.38	1.50
28	ai	102	UYH	C4-C5	3.69	1.60	1.53
25	L	1009	BPH	C3B-C4B	3.62	1.47	1.41
14	AV	103	BCL	MG-NC	3.61	2.14	2.06
14	AL	101	BCL	MG-NC	3.59	2.14	2.06
14	AR	102	BCL	MG-NC	3.58	2.14	2.06
14	AX	103	BCL	MG-NC	3.55	2.14	2.06
14	AB	1001	BCL	MG-NC	3.55	2.14	2.06
14	AA	1001	BCL	MG-NC	3.54	2.14	2.06
14	AI	103	BCL	MG-NC	3.54	2.14	2.06
18	M	409	V75	O2-C2	-3.54	1.40	1.46
14	AM	101	BCL	MG-NC	3.53	2.14	2.06
14	AD	102	BCL	MG-NC	3.53	2.14	2.06
14	bn	103	BCL	MG-NC	3.52	2.14	2.06
14	AG	102	BCL	MG-NC	3.52	2.14	2.06
14	bp	102	BCL	MG-NC	3.52	2.14	2.06
14	AV	102	BCL	MG-NC	3.51	2.14	2.06
14	AJ	101	BCL	MG-NC	3.51	2.14	2.06
14	AN	101	BCL	MG-NC	3.51	2.14	2.06
14	AN	104	BCL	MG-NC	3.50	2.14	2.06
14	AJ	102	BCL	MG-NC	3.50	2.14	2.06
14	AC	102	BCL	MG-NC	3.49	2.14	2.06
14	AX	102	BCL	MG-NC	3.49	2.14	2.06
14	AH	101	BCL	MG-NC	3.49	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AP	102	BCL	MG-NC	3.49	2.14	2.06
14	ad	1001	BCL	MG-NC	3.46	2.14	2.06
14	AM	102	BCL	MG-NC	3.45	2.14	2.06
14	AG	101	BCL	MG-NC	3.45	2.14	2.06
14	AE	1001	BCL	MG-NC	3.45	2.14	2.06
14	bh	105	BCL	MG-NC	3.45	2.14	2.06
14	AW	101	BCL	MG-NC	3.44	2.14	2.06
14	AU	102	BCL	MG-NC	3.44	2.14	2.06
14	AQ	102	BCL	MG-NC	3.43	2.14	2.06
14	AS	103	BCL	MG-NC	3.43	2.14	2.06
14	bl	104	BCL	MG-NC	3.42	2.14	2.06
14	AQ	101	BCL	MG-NC	3.42	2.14	2.06
14	al	1001	BCL	MG-NC	3.42	2.14	2.06
14	AK	102	BCL	MG-NC	3.42	2.14	2.06
14	AE	1003	BCL	MG-NC	3.41	2.14	2.06
14	AL	103	BCL	MG-NC	3.41	2.14	2.06
14	ba	103	BCL	MG-NC	3.41	2.14	2.06
14	ah	1001	BCL	MG-NC	3.41	2.14	2.06
14	AS	104	BCL	MG-NC	3.40	2.14	2.06
14	ab	102	BCL	MG-NC	3.40	2.14	2.06
14	L	1010	BCL	MG-NC	3.40	2.14	2.06
14	AT	101	BCL	MG-NC	3.39	2.14	2.06
14	AK	101	BCL	MG-NC	3.39	2.14	2.06
14	bd	102	BCL	MG-NC	3.39	2.14	2.06
14	AF	1001	BCL	MG-NC	3.39	2.14	2.06
14	AP	103	BCL	MG-NC	3.38	2.14	2.06
14	bk	102	BCL	MG-NC	3.38	2.14	2.06
14	be	105	BCL	MG-NC	3.38	2.14	2.06
14	bc	102	BCL	MG-NC	3.38	2.14	2.06
14	BE	104	BCL	MG-NC	3.37	2.14	2.06
14	ak	1001	BCL	MG-NC	3.37	2.14	2.06
14	bb	104	BCL	MG-NC	3.37	2.14	2.06
14	aa	1001	BCL	MG-NC	3.37	2.14	2.06
14	BW	1003	BCL	MG-NC	3.37	2.14	2.06
14	bf	103	BCL	MG-NC	3.37	2.14	2.06
14	bi	104	BCL	MG-NC	3.36	2.14	2.06
14	AN	102	BCL	MG-NC	3.36	2.14	2.06
14	bj	103	BCL	MG-NC	3.36	2.14	2.06
14	AV	101	BCL	MG-NC	3.35	2.14	2.06
14	af	101	BCL	MG-NC	3.35	2.14	2.06
14	AA	1002	BCL	MG-NC	3.35	2.14	2.06
14	AI	102	BCL	MG-NC	3.34	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ae	102	BCL	MG-NC	3.34	2.14	2.06
14	ao	102	BCL	MG-NC	3.34	2.14	2.06
14	AH	103	BCL	MG-NC	3.33	2.14	2.06
14	BT	103	BCL	MG-NC	3.33	2.14	2.06
14	BL	1003	BCL	MG-NC	3.33	2.14	2.06
18	C	405	V75	O2-C2	-3.33	1.40	1.46
28	ai	102	UYH	O1-C1	3.32	1.45	1.40
14	BA	103	BCL	MG-NC	3.32	2.14	2.06
14	AR	101	BCL	MG-NC	3.31	2.14	2.06
14	BK	1006	BCL	MG-NC	3.31	2.14	2.06
14	ap	1001	BCL	MG-NC	3.31	2.14	2.06
14	bm	104	BCL	MG-NC	3.30	2.14	2.06
14	bg	105	BCL	MG-NC	3.30	2.14	2.06
14	am	1001	BCL	MG-NC	3.30	2.14	2.06
14	BV	1005	BCL	MG-NC	3.30	2.14	2.06
14	BI	1003	BCL	MG-NC	3.30	2.14	2.06
14	AO	1002	BCL	MG-NC	3.30	2.14	2.06
14	BD	105	BCL	MG-NC	3.30	2.14	2.06
14	BC	104	BCL	MG-NC	3.30	2.14	2.06
14	BB	103	BCL	MG-NC	3.29	2.14	2.06
14	BX	1002	BCL	MG-NC	3.29	2.14	2.06
14	AV	102	BCL	C3B-C4B	3.29	1.47	1.41
14	AA	1001	BCL	C3B-C4B	3.29	1.47	1.41
14	BG	1004	BCL	MG-NC	3.29	2.14	2.06
14	AC	103	BCL	MG-NC	3.29	2.14	2.06
14	M	408	BCL	MG-NC	3.28	2.14	2.06
14	AS	102	BCL	MG-NC	3.28	2.14	2.06
14	an	1001	BCL	MG-NC	3.28	2.14	2.06
14	ac	1001	BCL	MG-NC	3.28	2.14	2.06
14	BQ	1003	BCL	MG-NC	3.28	2.14	2.06
14	BU	1004	BCL	MG-NC	3.27	2.14	2.06
14	ai	101	BCL	MG-NC	3.27	2.14	2.06
25	M	406	BPH	C3D-CAD	-3.26	1.41	1.47
14	AF	1001	BCL	C3B-C4B	3.26	1.47	1.41
14	AI	102	BCL	C3B-C4B	3.25	1.47	1.41
14	bo	103	BCL	MG-NC	3.25	2.14	2.06
14	BO	1004	BCL	MG-NC	3.25	2.14	2.06
14	BH	1005	BCL	MG-NC	3.25	2.14	2.06
14	BJ	1002	BCL	MG-NC	3.25	2.14	2.06
14	AQ	102	BCL	C3B-C4B	3.24	1.47	1.41
14	BM	1002	BCL	MG-NC	3.24	2.14	2.06
14	aj	103	BCL	MG-NC	3.24	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ag	1001	BCL	MG-NC	3.23	2.14	2.06
28	ai	102	UYH	C3-C4	3.23	1.60	1.52
14	AU	103	BCL	MG-NC	3.23	2.13	2.06
28	ai	102	UYH	C29-C28	3.22	1.60	1.50
14	AW	101	BCL	C3B-C4B	3.22	1.47	1.41
14	AH	103	BCL	C3B-C4B	3.22	1.47	1.41
14	AB	1002	BCL	MG-NC	3.22	2.13	2.06
14	AJ	101	BCL	C3B-C4B	3.22	1.47	1.41
14	AT	101	BCL	C3B-C4B	3.22	1.47	1.41
14	AL	103	BCL	C3B-C4B	3.22	1.47	1.41
14	BN	103	BCL	MG-NC	3.22	2.13	2.06
14	AU	102	BCL	C3B-C4B	3.22	1.47	1.41
14	BS	1003	BCL	MG-NC	3.22	2.13	2.06
14	ab	102	BCL	C3B-C4B	3.22	1.47	1.41
14	AO	1002	BCL	C3B-C4B	3.21	1.47	1.41
14	BP	1005	BCL	MG-NC	3.20	2.13	2.06
14	AX	103	BCL	C3B-C4B	3.20	1.47	1.41
14	BF	102	BCL	MG-NC	3.19	2.13	2.06
14	AC	102	BCL	C3B-C4B	3.19	1.47	1.41
14	AN	102	BCL	C3B-C4B	3.18	1.47	1.41
14	BR	1004	BCL	MG-NC	3.17	2.13	2.06
14	L	1002	BCL	MG-NC	3.17	2.13	2.06
14	AS	103	BCL	C3B-C4B	3.16	1.47	1.41
28	ai	102	UYH	C11-C10	3.16	1.59	1.50
14	AE	1001	BCL	C3B-C4B	3.15	1.47	1.41
14	AK	102	BCL	C3B-C4B	3.14	1.47	1.41
18	M	409	V75	O3-C3	-3.14	1.40	1.44
14	AG	102	BCL	C3B-C4B	3.11	1.47	1.41
14	AR	101	BCL	C3B-C4B	3.11	1.47	1.41
18	C	405	V75	O3-C3	-3.10	1.40	1.44
14	AP	102	BCL	C3B-C4B	3.08	1.47	1.41
25	L	1009	BPH	C3D-CAD	-3.08	1.41	1.47
14	AM	101	BCL	C3B-C4B	3.07	1.47	1.41
14	M	405	BCL	MG-NC	3.04	2.13	2.06
14	AI	103	BCL	C3B-C4B	3.03	1.47	1.41
28	ai	102	UYH	C3-C2	2.99	1.60	1.52
14	aj	103	BCL	C3B-C4B	2.96	1.47	1.41
14	AR	102	BCL	C3B-C4B	2.95	1.46	1.41
14	AX	102	BCL	C3B-C4B	2.94	1.46	1.41
28	ai	102	UYH	C9-C8	2.94	1.60	1.50
14	ag	1001	BCL	C3B-C4B	2.92	1.46	1.41
14	M	408	BCL	C3B-C4B	2.90	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ap	1001	BCL	C3B-C4B	2.90	1.46	1.41
14	AS	104	BCL	C3B-C4B	2.90	1.46	1.41
16	bm	101	V7N	C14-C13	2.90	1.42	1.35
14	AN	104	BCL	C3B-C4B	2.90	1.46	1.41
25	M	406	BPH	C3B-C4B	2.90	1.46	1.41
16	bo	102	V7N	C14-C13	2.89	1.42	1.35
14	am	1001	BCL	C3B-C4B	2.89	1.46	1.41
14	AQ	101	BCL	C3B-C4B	2.88	1.46	1.41
16	BU	1001	V7N	C14-C13	2.88	1.42	1.35
14	af	101	BCL	C3B-C4B	2.88	1.46	1.41
14	AM	102	BCL	C3B-C4B	2.87	1.46	1.41
14	ai	101	BCL	C3B-C4B	2.87	1.46	1.41
14	ak	1001	BCL	C3B-C4B	2.86	1.46	1.41
14	ac	1001	BCL	C3B-C4B	2.86	1.46	1.41
14	aa	1001	BCL	C3B-C4B	2.86	1.46	1.41
16	ba	101	V7N	C14-C13	2.85	1.42	1.35
16	bn	102	V7N	C14-C13	2.85	1.42	1.35
14	al	1001	BCL	C3B-C4B	2.85	1.46	1.41
14	ae	102	BCL	C3B-C4B	2.84	1.46	1.41
14	ao	102	BCL	C3B-C4B	2.84	1.46	1.41
16	BC	101	V7N	C14-C13	2.83	1.42	1.35
16	bi	101	V7N	C14-C13	2.83	1.42	1.35
16	BO	1001	V7N	C14-C13	2.82	1.42	1.35
16	bk	101	V7N	C14-C13	2.82	1.42	1.35
14	ah	1001	BCL	C3B-C4B	2.82	1.46	1.41
16	bp	101	V7N	C14-C13	2.82	1.42	1.35
14	AB	1002	BCL	C3B-C4B	2.82	1.46	1.41
16	bb	101	V7N	C14-C13	2.80	1.42	1.35
14	AB	1002	BCL	CHD-C1D	2.80	1.43	1.38
16	bl	102	V7N	C14-C13	2.79	1.42	1.35
14	ad	1001	BCL	C3B-C4B	2.78	1.46	1.41
16	AE	1005	V7N	C14-C13	2.78	1.42	1.35
16	bc	101	V7N	C14-C13	2.78	1.42	1.35
16	bf	101	V7N	C14-C13	2.77	1.42	1.35
16	BA	101	V7N	C14-C13	2.77	1.42	1.35
16	BE	101	V7N	C14-C13	2.77	1.42	1.35
16	BQ	1001	V7N	C14-C13	2.77	1.42	1.35
16	bd	101	V7N	C14-C13	2.77	1.42	1.35
16	bj	101	V7N	C14-C13	2.76	1.42	1.35
16	BR	1001	V7N	C14-C13	2.76	1.42	1.35
16	bg	101	V7N	C14-C13	2.76	1.42	1.35
14	AL	101	BCL	C3B-C4B	2.75	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AP	103	BCL	C3B-C4B	2.75	1.46	1.41
14	an	1001	BCL	C3B-C4B	2.75	1.46	1.41
16	bp	101	V7N	C17-C18	2.74	1.42	1.35
28	ai	102	UYH	C7-C8	2.74	1.59	1.50
14	AC	101	BCL	C3B-C4B	2.73	1.46	1.41
14	M	405	BCL	C3B-C4B	2.73	1.46	1.41
16	bm	101	V7N	C17-C18	2.73	1.42	1.35
16	bh	102	V7N	C14-C13	2.72	1.42	1.35
16	BH	1001	V7N	C14-C13	2.72	1.42	1.35
14	bk	102	BCL	C3B-C4B	2.72	1.46	1.41
16	bo	102	V7N	C17-C18	2.72	1.42	1.35
16	BU	1001	V7N	C17-C18	2.71	1.42	1.35
16	bn	102	V7N	C17-C18	2.71	1.42	1.35
16	BS	1001	V7N	C14-C13	2.71	1.42	1.35
14	ba	103	BCL	C3B-C4B	2.70	1.46	1.41
16	BW	1001	V7N	C14-C13	2.70	1.42	1.35
14	AA	1002	BCL	C3B-C4B	2.70	1.46	1.41
14	AU	103	BCL	C3B-C4B	2.69	1.46	1.41
16	BO	1001	V7N	C17-C18	2.69	1.42	1.35
14	L	1010	BCL	C3B-C4B	2.69	1.46	1.41
16	bd	101	V7N	C17-C18	2.69	1.42	1.35
16	BK	1001	V7N	C14-C13	2.68	1.42	1.35
16	AS	105	V7N	C14-C13	2.68	1.42	1.35
16	BB	101	V7N	C14-C13	2.68	1.42	1.35
16	BI	1001	V7N	C14-C13	2.68	1.42	1.35
14	be	105	BCL	C3B-C4B	2.68	1.46	1.41
16	ba	101	V7N	C17-C18	2.67	1.42	1.35
14	bc	102	BCL	C3B-C4B	2.67	1.46	1.41
14	AN	104	BCL	CHD-C1D	2.67	1.43	1.38
16	BV	1001	V7N	C14-C13	2.67	1.42	1.35
16	BC	101	V7N	C17-C18	2.66	1.42	1.35
16	bf	101	V7N	C17-C18	2.66	1.41	1.35
16	BD	101	V7N	C14-C13	2.66	1.41	1.35
14	AN	101	BCL	C3B-C4B	2.65	1.46	1.41
14	AC	101	BCL	CHD-C1D	2.65	1.43	1.38
16	bb	101	V7N	C17-C18	2.64	1.41	1.35
16	bi	101	V7N	C17-C18	2.64	1.41	1.35
14	AG	101	BCL	CHD-C1D	2.64	1.43	1.38
14	AC	103	BCL	CHD-C1D	2.64	1.43	1.38
14	L	1002	BCL	C3B-C4B	2.64	1.46	1.41
14	AE	1004	BCL	C3B-C4B	2.64	1.46	1.41
16	AO	1001	V7N	C14-C13	2.64	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	bl	102	V7N	C17-C18	2.64	1.41	1.35
14	bf	103	BCL	C3B-C4B	2.63	1.46	1.41
28	ai	102	UYH	C6-C5	2.63	1.60	1.51
16	BM	1001	V7N	C14-C13	2.63	1.41	1.35
14	BH	1005	BCL	C3B-C4B	2.63	1.46	1.41
16	BP	1001	V7N	C14-C13	2.63	1.41	1.35
16	BA	101	V7N	C17-C18	2.63	1.41	1.35
14	bg	105	BCL	C3B-C4B	2.63	1.46	1.41
16	BJ	1001	V7N	C14-C13	2.62	1.41	1.35
16	BL	1001	V7N	C14-C13	2.62	1.41	1.35
16	bc	101	V7N	C17-C18	2.62	1.41	1.35
16	bk	101	V7N	C17-C18	2.62	1.41	1.35
14	bj	103	BCL	C3B-C4B	2.61	1.46	1.41
16	BH	1001	V7N	C17-C18	2.61	1.41	1.35
14	AS	102	BCL	C3B-C4B	2.61	1.46	1.41
14	bd	102	BCL	C3B-C4B	2.61	1.46	1.41
14	AU	103	BCL	CHD-C1D	2.61	1.43	1.38
16	BG	1001	V7N	C14-C13	2.60	1.41	1.35
14	AV	103	BCL	C3B-C4B	2.60	1.46	1.41
16	BE	101	V7N	C17-C18	2.60	1.41	1.35
16	BR	1001	V7N	C17-C18	2.59	1.41	1.35
16	bh	102	V7N	C17-C18	2.59	1.41	1.35
16	BX	1001	V7N	C14-C13	2.59	1.41	1.35
14	bp	102	BCL	C3B-C4B	2.59	1.46	1.41
14	AC	103	BCL	C3B-C4B	2.59	1.46	1.41
16	AS	105	V7N	C17-C18	2.59	1.41	1.35
24	ag	1002	V7B	O7-C8	-2.59	1.40	1.46
16	BQ	1001	V7N	C17-C18	2.58	1.41	1.35
16	bg	101	V7N	C17-C18	2.58	1.41	1.35
16	be	101	V7N	C14-C13	2.58	1.41	1.35
15	AE	1002	LMT	O3'-C3'	-2.58	1.36	1.43
14	AG	101	BCL	C3B-C4B	2.57	1.46	1.41
14	BN	103	BCL	O2A-C1	-2.57	1.39	1.46
16	BS	1001	V7N	C17-C18	2.57	1.41	1.35
14	am	1001	BCL	O1A-CGA	-2.57	1.14	1.22
15	AJ	104	LMT	O3'-C3'	-2.57	1.36	1.43
14	BT	103	BCL	C3B-C4B	2.57	1.46	1.41
14	AE	1003	BCL	C3B-C4B	2.57	1.46	1.41
14	AJ	102	BCL	C3B-C4B	2.57	1.46	1.41
16	bj	101	V7N	C17-C18	2.56	1.41	1.35
15	bb	102	LMT	O3'-C3'	-2.56	1.36	1.43
15	BX	1004	LMT	O3'-C3'	-2.55	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	BW	1001	V7N	C17-C18	2.55	1.41	1.35
15	BH	1002	LMT	O3'-C3'	-2.55	1.36	1.43
14	AP	103	BCL	CHD-C1D	2.55	1.43	1.38
14	AK	101	BCL	C3B-C4B	2.54	1.46	1.41
16	BU	1001	V7N	C6-C5	2.54	1.41	1.35
15	BA	104	LMT	O3'-C3'	-2.54	1.36	1.43
15	BN	101	LMT	O3'-C3'	-2.54	1.36	1.43
15	M	403	LMT	O3'-C3'	-2.54	1.36	1.43
14	AH	101	BCL	C3B-C4B	2.54	1.46	1.41
14	BQ	1003	BCL	C3B-C4B	2.54	1.46	1.41
14	AS	102	BCL	CHD-C1D	2.54	1.43	1.38
15	bf	102	LMT	O3'-C3'	-2.53	1.36	1.43
15	BU	1003	LMT	O3'-C3'	-2.53	1.36	1.43
14	BK	1006	BCL	C3B-C4B	2.53	1.46	1.41
14	bl	104	BCL	C3B-C4B	2.53	1.46	1.41
15	AA	1003	LMT	O3'-C3'	-2.53	1.36	1.43
15	AT	102	LMT	O3'-C3'	-2.53	1.36	1.43
14	AI	103	BCL	CHD-C1D	2.53	1.43	1.38
15	BK	1005	LMT	O3'-C3'	-2.53	1.36	1.43
15	BH	1003	LMT	O3'-C3'	-2.52	1.36	1.43
15	BW	1005	LMT	O3'-C3'	-2.52	1.36	1.43
14	AN	101	BCL	CHD-C1D	2.52	1.43	1.38
16	BI	1001	V7N	C17-C18	2.52	1.41	1.35
14	bo	103	BCL	C3B-C4B	2.52	1.46	1.41
15	bj	102	LMT	O3'-C3'	-2.52	1.36	1.43
16	AE	1005	V7N	C17-C18	2.52	1.41	1.35
14	M	408	BCL	CHD-C1D	2.52	1.43	1.38
14	AV	101	BCL	C3B-C4B	2.52	1.46	1.41
15	bd	103	LMT	O3'-C3'	-2.51	1.36	1.43
16	BB	101	V7N	C17-C18	2.51	1.41	1.35
15	BA	105	LMT	O3'-C3'	-2.51	1.36	1.43
15	BB	104	LMT	O3'-C3'	-2.51	1.36	1.43
15	AH	104	LMT	O3'-C3'	-2.51	1.36	1.43
15	BQ	1004	LMT	O3'-C3'	-2.51	1.36	1.43
14	BP	1005	BCL	C3B-C4B	2.51	1.46	1.41
14	AH	101	BCL	CHD-C1D	2.51	1.43	1.38
16	BV	1001	V7N	C17-C18	2.51	1.41	1.35
16	BK	1001	V7N	C17-C18	2.51	1.41	1.35
14	bh	105	BCL	C3B-C4B	2.50	1.46	1.41
14	AE	1003	BCL	CHD-C1D	2.50	1.43	1.38
15	BI	1005	LMT	O3'-C3'	-2.50	1.36	1.43
15	BB	102	LMT	O3'-C3'	-2.50	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BI	1002	LMT	O3'-C3'	-2.50	1.36	1.43
15	bn	101	LMT	O3'-C3'	-2.50	1.36	1.43
15	BK	1002	LMT	O3'-C3'	-2.50	1.36	1.43
15	bc	104	LMT	O3'-C3'	-2.50	1.36	1.43
16	BP	1001	V7N	C17-C18	2.50	1.41	1.35
15	BR	1002	LMT	O3'-C3'	-2.50	1.36	1.43
15	BV	1002	LMT	O3'-C3'	-2.49	1.36	1.43
15	BD	103	LMT	O3'-C3'	-2.49	1.36	1.43
15	BS	1005	LMT	O3'-C3'	-2.49	1.36	1.43
16	BG	1001	V7N	C17-C18	2.49	1.41	1.35
15	AD	103	LMT	O3'-C3'	-2.49	1.36	1.43
15	L	1005	LMT	O3'-C3'	-2.49	1.36	1.43
15	BJ	1003	LMT	O3'-C3'	-2.49	1.36	1.43
14	BG	1004	BCL	C3B-C4B	2.49	1.46	1.41
15	bl	105	LMT	O3'-C3'	-2.49	1.36	1.43
15	BP	1004	LMT	O3'-C3'	-2.49	1.36	1.43
15	BS	1002	LMT	O3'-C3'	-2.49	1.36	1.43
15	AU	101	LMT	O3'-C3'	-2.49	1.36	1.43
15	AL	102	LMT	O3'-C3'	-2.49	1.36	1.43
15	BG	1003	LMT	O3'-C3'	-2.48	1.36	1.43
16	BX	1001	V7N	C17-C18	2.48	1.41	1.35
14	BN	103	BCL	C3B-C4B	2.48	1.46	1.41
15	L	1008	LMT	O3'-C3'	-2.48	1.36	1.43
14	AX	102	BCL	CHD-C1D	2.48	1.43	1.38
15	BR	1005	LMT	O3'-C3'	-2.48	1.36	1.43
16	BD	101	V7N	C17-C18	2.48	1.41	1.35
15	L	1007	LMT	O3'-C3'	-2.48	1.36	1.43
14	BM	1002	BCL	C3B-C4B	2.48	1.46	1.41
15	AI	101	LMT	O3'-C3'	-2.47	1.36	1.43
16	ba	101	V7N	C11-C12	2.47	1.41	1.34
15	AS	101	LMT	O3'-C3'	-2.47	1.36	1.43
15	bo	105	LMT	O3'-C3'	-2.47	1.36	1.43
15	bh	104	LMT	O3'-C3'	-2.47	1.36	1.43
16	BU	1001	V7N	C11-C12	2.47	1.41	1.34
15	BL	1005	LMT	O3'-C3'	-2.47	1.36	1.43
15	BW	1002	LMT	O3'-C3'	-2.47	1.36	1.43
15	BJ	1004	LMT	O3'-C3'	-2.47	1.36	1.43
14	BR	1004	BCL	C3B-C4B	2.47	1.46	1.41
15	L	1003	LMT	O3'-C3'	-2.47	1.36	1.43
14	BE	104	BCL	C3B-C4B	2.47	1.46	1.41
15	BN	105	LMT	O3'-C3'	-2.47	1.36	1.43
15	BV	1004	LMT	O3'-C3'	-2.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BN	102	LMT	O3'-C3'	-2.47	1.36	1.43
15	BT	101	LMT	O3'-C3'	-2.47	1.36	1.43
15	ab	101	LMT	O3'-C3'	-2.47	1.36	1.43
28	ai	102	UYH	C1-C2	2.47	1.59	1.52
15	BB	105	LMT	O3'-C3'	-2.47	1.36	1.43
15	BC	103	LMT	O3'-C3'	-2.47	1.36	1.43
15	AH	102	LMT	O3'-C3'	-2.46	1.36	1.43
15	BT	104	LMT	O3'-C3'	-2.46	1.36	1.43
14	BB	103	BCL	C3B-C4B	2.46	1.46	1.41
15	BI	1004	LMT	O3'-C3'	-2.46	1.36	1.43
15	BP	1002	LMT	O3'-C3'	-2.46	1.36	1.43
15	AJ	103	LMT	O3'-C3'	-2.46	1.36	1.43
15	BD	104	LMT	O3'-C3'	-2.46	1.36	1.43
14	bi	104	BCL	C3B-C4B	2.46	1.46	1.41
15	bn	105	LMT	O3'-C3'	-2.46	1.36	1.43
15	BS	1004	LMT	O3'-C3'	-2.46	1.36	1.43
16	BL	1001	V7N	C17-C18	2.46	1.41	1.35
15	AP	101	LMT	O3'-C3'	-2.46	1.36	1.43
15	BT	102	LMT	O3'-C3'	-2.46	1.36	1.43
15	AP	104	LMT	O3'-C3'	-2.46	1.36	1.43
14	BD	105	BCL	C3B-C4B	2.46	1.46	1.41
15	BL	1002	LMT	O3'-C3'	-2.46	1.36	1.43
15	BO	1003	LMT	O3'-C3'	-2.46	1.36	1.43
15	BC	106	LMT	O3'-C3'	-2.46	1.36	1.43
24	L	1006	V7B	O7-C8	-2.46	1.40	1.46
15	BC	102	LMT	O3'-C3'	-2.46	1.36	1.43
14	AD	102	BCL	C3B-C4B	2.45	1.46	1.41
15	BU	1002	LMT	O3'-C3'	-2.45	1.36	1.43
16	bm	101	V7N	C11-C12	2.45	1.41	1.34
15	BD	102	LMT	O3'-C3'	-2.45	1.36	1.43
16	AO	1001	V7N	C17-C18	2.45	1.41	1.35
14	AW	101	BCL	CHD-C1D	2.45	1.43	1.38
15	BQ	1005	LMT	O3'-C3'	-2.45	1.36	1.43
15	bi	102	LMT	O3'-C3'	-2.45	1.36	1.43
14	L	1002	BCL	CHD-C1D	2.45	1.43	1.38
16	be	101	V7N	C17-C18	2.45	1.41	1.35
15	BG	1005	LMT	O3'-C3'	-2.45	1.36	1.43
15	L	1004	LMT	O3'-C3'	-2.45	1.36	1.43
15	BQ	1002	LMT	O3'-C3'	-2.45	1.36	1.43
15	L	1011	LMT	O3'-C3'	-2.44	1.36	1.43
15	bh	101	LMT	O3'-C3'	-2.44	1.36	1.43
15	BG	1002	LMT	O3'-C3'	-2.44	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BK	1004	LMT	O3'-C3'	-2.44	1.36	1.43
15	bg	103	LMT	O3'-C3'	-2.44	1.36	1.43
15	bo	101	LMT	O3'-C3'	-2.44	1.36	1.43
14	AS	104	BCL	CHD-C1D	2.44	1.43	1.38
14	AB	1001	BCL	C3B-C4B	2.44	1.45	1.41
24	ag	1002	V7B	O8-C28	2.44	1.40	1.33
16	BM	1001	V7N	C17-C18	2.44	1.41	1.35
15	BH	1004	LMT	O3'-C3'	-2.43	1.36	1.43
14	AL	101	BCL	CHD-C1D	2.43	1.43	1.38
15	bm	105	LMT	O3'-C3'	-2.43	1.36	1.43
15	AN	103	LMT	O3'-C3'	-2.43	1.36	1.43
24	L	1006	V7B	O8-C28	2.43	1.40	1.33
15	AQ	103	LMT	O3'-C3'	-2.43	1.36	1.43
15	bm	103	LMT	O3'-C3'	-2.43	1.36	1.43
15	AA	1004	LMT	O3'-C3'	-2.43	1.36	1.43
15	AF	1002	LMT	O3'-C3'	-2.43	1.36	1.43
15	BV	1006	LMT	O3'-C3'	-2.43	1.36	1.43
14	AR	102	BCL	CHD-C1D	2.43	1.43	1.38
16	bo	102	V7N	C11-C12	2.43	1.41	1.34
14	AA	1002	BCL	CHD-C1D	2.42	1.43	1.38
15	AD	101	LMT	O3'-C3'	-2.42	1.37	1.43
15	BW	1004	LMT	O3'-C3'	-2.42	1.37	1.43
14	BS	1003	BCL	C3B-C4B	2.42	1.45	1.41
14	bb	104	BCL	C3B-C4B	2.42	1.45	1.41
15	AC	104	LMT	O3'-C3'	-2.42	1.37	1.43
16	BJ	1001	V7N	C17-C18	2.42	1.41	1.35
15	BG	1006	LMT	O3'-C3'	-2.42	1.37	1.43
14	BF	102	BCL	C3B-C4B	2.41	1.45	1.41
15	BF	103	LMT	O3'-C3'	-2.41	1.37	1.43
15	BM	1004	LMT	O3'-C3'	-2.41	1.37	1.43
15	BX	1003	LMT	O3'-C3'	-2.41	1.37	1.43
15	BI	1006	LMT	O3'-C3'	-2.41	1.37	1.43
15	BF	101	LMT	O3'-C3'	-2.41	1.37	1.43
15	BL	1004	LMT	O3'-C3'	-2.41	1.37	1.43
15	BM	1003	LMT	O3'-C3'	-2.41	1.37	1.43
15	BV	1003	LMT	O3'-C3'	-2.41	1.37	1.43
14	AK	101	BCL	CHD-C1D	2.41	1.43	1.38
15	BP	1003	LMT	O3'-C3'	-2.40	1.37	1.43
15	BE	103	LMT	O3'-C3'	-2.40	1.37	1.43
14	BS	1003	BCL	CHD-C1D	2.39	1.43	1.38
15	BO	1002	LMT	O3'-C3'	-2.39	1.37	1.43
14	BN	103	BCL	CHD-C1D	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	102	LMT	O3'-C3'	-2.39	1.37	1.43
14	AO	1002	BCL	CHD-C1D	2.39	1.43	1.38
16	BO	1001	V7N	C11-C12	2.39	1.40	1.34
14	BW	1003	BCL	CHD-C1D	2.39	1.43	1.38
14	BJ	1002	BCL	C3B-C4B	2.39	1.45	1.41
24	L	1006	V7B	O7-C10	2.39	1.41	1.34
15	BK	1003	LMT	O3'-C3'	-2.39	1.37	1.43
14	AJ	102	BCL	CHD-C1D	2.39	1.43	1.38
18	C	405	V75	O2-C2A	2.39	1.40	1.35
14	AI	102	BCL	CHD-C1D	2.38	1.43	1.38
14	AE	1004	BCL	CHD-C1D	2.38	1.43	1.38
14	AX	103	BCL	CHD-C1D	2.38	1.43	1.38
15	AX	101	LMT	O3'-C3'	-2.38	1.37	1.43
14	BO	1004	BCL	CHD-C1D	2.38	1.43	1.38
14	AV	101	BCL	CHD-C1D	2.38	1.43	1.38
15	BC	105	LMT	O3'-C3'	-2.38	1.37	1.43
14	AU	102	BCL	CHD-C1D	2.38	1.43	1.38
14	AC	102	BCL	CHD-C1D	2.38	1.43	1.38
15	BA	102	LMT	O3'-C3'	-2.38	1.37	1.43
16	bn	102	V7N	C11-C12	2.37	1.40	1.34
14	BW	1003	BCL	C3B-C4B	2.37	1.45	1.41
14	BC	104	BCL	CHD-C1D	2.37	1.43	1.38
16	bd	101	V7N	C11-C12	2.37	1.40	1.34
14	AQ	101	BCL	CHD-C1D	2.37	1.43	1.38
16	bf	101	V7N	C11-C12	2.37	1.40	1.34
16	bm	101	V7N	C7-C8	2.37	1.40	1.34
14	BB	103	BCL	CHD-C1D	2.37	1.43	1.38
14	BI	1003	BCL	O2A-C1	-2.37	1.39	1.46
14	ao	102	BCL	CHD-C1D	2.37	1.43	1.38
14	BV	1005	BCL	C3B-C4B	2.36	1.45	1.41
15	AU	101	LMT	O2'-C2'	-2.36	1.37	1.43
14	AT	101	BCL	CHD-C1D	2.36	1.43	1.38
16	BK	1001	V7N	C12-C13	-2.36	1.40	1.46
15	BN	104	LMT	O3'-C3'	-2.36	1.37	1.43
15	be	104	LMT	O3'-C3'	-2.36	1.37	1.43
14	BK	1006	BCL	CHD-C1D	2.36	1.43	1.38
14	BA	103	BCL	CHD-C1D	2.35	1.43	1.38
14	BG	1004	BCL	CHD-C1D	2.35	1.43	1.38
16	bi	101	V7N	C11-C12	2.35	1.40	1.34
14	BX	1002	BCL	CHD-C1D	2.35	1.43	1.38
16	bm	101	V7N	C6-C5	2.35	1.41	1.35
15	BS	1006	LMT	O3'-C3'	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BO	1004	BCL	C3B-C4B	2.35	1.45	1.41
14	AN	102	BCL	CHD-C1D	2.35	1.43	1.38
14	AM	102	BCL	CHD-C1D	2.35	1.43	1.38
16	be	101	V7N	C12-C13	-2.35	1.40	1.46
15	bl	101	LMT	O3'-C3'	-2.35	1.37	1.43
14	BR	1004	BCL	CHD-C1D	2.35	1.43	1.38
16	bp	101	V7N	C11-C12	2.35	1.40	1.34
15	BR	1003	LMT	O3'-C3'	-2.34	1.37	1.43
14	BE	104	BCL	CHD-C1D	2.34	1.43	1.38
15	BN	101	LMT	O2'-C2'	-2.34	1.37	1.43
14	BP	1005	BCL	CHD-C1D	2.34	1.43	1.38
16	bk	101	V7N	C11-C12	2.34	1.40	1.34
16	bj	101	V7N	C11-C12	2.34	1.40	1.34
16	bb	101	V7N	C11-C12	2.33	1.40	1.34
14	AE	1001	BCL	CHD-C1D	2.33	1.42	1.38
16	BV	1001	V7N	C12-C13	-2.33	1.41	1.46
14	BM	1002	BCL	CHD-C1D	2.33	1.42	1.38
15	BK	1002	LMT	O2'-C2'	-2.33	1.37	1.43
14	AD	102	BCL	CHD-C1D	2.33	1.42	1.38
15	BD	103	LMT	O2'-C2'	-2.33	1.37	1.43
14	BD	105	BCL	CHD-C1D	2.33	1.42	1.38
16	BL	1001	V7N	C12-C13	-2.32	1.41	1.46
16	BP	1001	V7N	C12-C13	-2.32	1.41	1.46
14	AH	103	BCL	CHD-C1D	2.32	1.42	1.38
14	ap	1001	BCL	CHD-C1D	2.32	1.42	1.38
14	bm	104	BCL	C3B-C4B	2.32	1.45	1.41
14	AR	101	BCL	CHD-C1D	2.32	1.42	1.38
15	AG	103	LMT	O2'-C2'	-2.32	1.37	1.43
16	bl	102	V7N	C11-C12	2.32	1.40	1.34
16	BC	101	V7N	C11-C12	2.32	1.40	1.34
14	BJ	1002	BCL	CHD-C1D	2.32	1.42	1.38
15	AG	103	LMT	O3'-C3'	-2.32	1.37	1.43
15	BH	1003	LMT	O2'-C2'	-2.32	1.37	1.43
16	BM	1001	V7N	C12-C13	-2.32	1.41	1.46
14	BA	103	BCL	C3B-C4B	2.32	1.45	1.41
16	bc	101	V7N	C11-C12	2.32	1.40	1.34
14	BI	1003	BCL	CHD-C1D	2.31	1.42	1.38
16	BA	101	V7N	C11-C12	2.31	1.40	1.34
16	BE	101	V7N	C11-C12	2.31	1.40	1.34
14	BH	1005	BCL	CHD-C1D	2.31	1.42	1.38
15	bn	105	LMT	O2'-C2'	-2.31	1.37	1.43
14	BU	1004	BCL	CHD-C1D	2.31	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bl	101	LMT	O2B-C2B	-2.31	1.37	1.43
14	AL	103	BCL	CHD-C1D	2.31	1.42	1.38
16	BB	101	V7N	C12-C13	-2.31	1.41	1.46
16	BD	101	V7N	C12-C13	-2.30	1.41	1.46
14	an	1001	BCL	CHD-C1D	2.30	1.42	1.38
14	BC	104	BCL	C3B-C4B	2.30	1.45	1.41
14	BV	1005	BCL	CHD-C1D	2.30	1.42	1.38
14	BL	1003	BCL	CHD-C1D	2.30	1.42	1.38
14	al	1001	BCL	CHD-C1D	2.30	1.42	1.38
15	AH	104	LMT	O3B-C3B	-2.29	1.37	1.43
16	AE	1005	V7N	C11-C12	2.29	1.40	1.34
14	AJ	101	BCL	CHD-C1D	2.29	1.42	1.38
14	AP	102	BCL	CHD-C1D	2.29	1.42	1.38
16	bh	102	V7N	C11-C12	2.29	1.40	1.34
14	BT	103	BCL	CHD-C1D	2.29	1.42	1.38
14	BF	102	BCL	CHD-C1D	2.29	1.42	1.38
14	AS	103	BCL	CHD-C1D	2.29	1.42	1.38
16	bg	101	V7N	C11-C12	2.28	1.40	1.34
16	BX	1001	V7N	C12-C13	-2.28	1.41	1.46
14	AF	1001	BCL	CHD-C1D	2.28	1.42	1.38
16	AS	105	V7N	C12-C13	-2.28	1.41	1.46
16	BW	1001	V7N	C11-C12	2.28	1.40	1.34
14	aj	103	BCL	CHD-C1D	2.27	1.42	1.38
14	bn	103	BCL	C3B-C4B	2.27	1.45	1.41
14	ak	1001	BCL	CHD-C1D	2.27	1.42	1.38
15	BI	1004	LMT	O2'-C2'	-2.27	1.37	1.43
15	bc	104	LMT	O2'-C2'	-2.27	1.37	1.43
15	AC	104	LMT	O2'-C2'	-2.27	1.37	1.43
14	BU	1004	BCL	C3B-C4B	2.27	1.45	1.41
14	BL	1003	BCL	C3B-C4B	2.27	1.45	1.41
14	AA	1001	BCL	CHD-C1D	2.27	1.42	1.38
16	BR	1001	V7N	C11-C12	2.27	1.40	1.34
14	BI	1003	BCL	C3B-C4B	2.27	1.45	1.41
15	AA	1004	LMT	O2'-C2'	-2.27	1.37	1.43
15	AJ	104	LMT	O3B-C3B	-2.26	1.37	1.43
14	AB	1001	BCL	CHD-C1D	2.26	1.42	1.38
15	BI	1002	LMT	O2'-C2'	-2.26	1.37	1.43
16	BH	1001	V7N	C11-C12	2.26	1.40	1.34
16	BQ	1001	V7N	C11-C12	2.26	1.40	1.34
14	AV	103	BCL	CHD-C1D	2.26	1.42	1.38
14	M	405	BCL	CHD-C1D	2.26	1.42	1.38
14	AQ	102	BCL	CHD-C1D	2.26	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	405	V75	O3-C3A	2.26	1.40	1.35
16	AS	105	V7N	C11-C12	2.26	1.40	1.34
14	BX	1002	BCL	C3B-C4B	2.26	1.45	1.41
14	BI	1003	BCL	C2-C3	-2.26	1.27	1.33
15	BG	1003	LMT	O2'-C2'	-2.26	1.37	1.43
14	ah	1001	BCL	CHD-C1D	2.25	1.42	1.38
15	L	1005	LMT	O2'-C2'	-2.25	1.37	1.43
15	be	104	LMT	O2B-C2B	-2.25	1.37	1.43
14	BQ	1003	BCL	CHD-C1D	2.25	1.42	1.38
15	AP	104	LMT	O2'-C2'	-2.25	1.37	1.43
24	ag	1002	V7B	O7-C10	2.25	1.40	1.34
16	BG	1001	V7N	C12-C13	-2.25	1.41	1.46
14	aa	1001	BCL	CHD-C1D	2.25	1.42	1.38
14	bm	104	BCL	C3D-C4D	-2.25	1.39	1.44
14	AK	102	BCL	CHD-C1D	2.24	1.42	1.38
18	M	409	V75	O3-C3A	2.24	1.40	1.35
18	M	409	V75	O2-C2A	2.24	1.40	1.35
16	BI	1001	V7N	C12-C13	-2.24	1.41	1.46
16	AO	1001	V7N	C11-C12	2.24	1.40	1.34
16	be	101	V7N	C19-C18	-2.24	1.41	1.46
14	AV	102	BCL	CHD-C1D	2.24	1.42	1.38
15	BD	104	LMT	O2'-C2'	-2.24	1.37	1.43
14	am	1001	BCL	CHD-C1D	2.24	1.42	1.38
16	BS	1001	V7N	C11-C12	2.24	1.40	1.34
14	ad	1001	BCL	CHD-C1D	2.24	1.42	1.38
14	ai	101	BCL	CHD-C1D	2.24	1.42	1.38
16	ba	101	V7N	C7-C8	2.24	1.40	1.34
15	AE	1002	LMT	O2'-C2'	-2.23	1.37	1.43
16	be	101	V7N	C11-C12	2.23	1.40	1.34
15	BK	1003	LMT	O3B-C3B	-2.23	1.37	1.43
15	bb	102	LMT	O2B-C2B	-2.23	1.37	1.43
15	BA	105	LMT	O2'-C2'	-2.23	1.37	1.43
16	BJ	1001	V7N	C12-C13	-2.23	1.41	1.46
16	bo	102	V7N	C7-C8	2.23	1.40	1.34
16	BV	1001	V7N	C11-C12	2.23	1.40	1.34
16	BK	1001	V7N	C11-C12	2.23	1.40	1.34
15	BN	105	LMT	O2'-C2'	-2.23	1.37	1.43
15	AP	101	LMT	O2'-C2'	-2.22	1.37	1.43
15	BC	102	LMT	O3B-C3B	-2.22	1.37	1.43
15	AI	101	LMT	O3B-C3B	-2.22	1.37	1.43
14	bc	102	BCL	CHD-C1D	2.22	1.42	1.38
16	BS	1001	V7N	C12-C13	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	AE	1005	V7N	C12-C13	-2.22	1.41	1.46
16	ba	101	V7N	C6-C5	2.22	1.40	1.35
14	ac	1001	BCL	CHD-C1D	2.22	1.42	1.38
16	bo	102	V7N	C6-C5	2.22	1.40	1.35
15	BG	1006	LMT	O2'-C2'	-2.22	1.37	1.43
16	bk	101	V7N	C7-C8	2.22	1.40	1.34
15	bn	101	LMT	O3B-C3B	-2.22	1.37	1.43
16	BW	1001	V7N	C12-C13	-2.22	1.41	1.46
14	ab	102	BCL	CHD-C1D	2.22	1.42	1.38
15	BT	101	LMT	O2'-C2'	-2.22	1.37	1.43
16	BM	1001	V7N	C11-C12	2.22	1.40	1.34
15	BC	102	LMT	O2'-C2'	-2.22	1.37	1.43
15	M	403	LMT	O2'-C2'	-2.21	1.37	1.43
14	AM	101	BCL	CHD-C1D	2.21	1.42	1.38
15	BS	1006	LMT	O3B-C3B	-2.21	1.37	1.43
16	BG	1001	V7N	C11-C12	2.21	1.40	1.34
15	BC	103	LMT	O2'-C2'	-2.21	1.37	1.43
15	BK	1003	LMT	O2'-C2'	-2.21	1.37	1.43
14	ae	102	BCL	CHD-C1D	2.21	1.42	1.38
15	AJ	103	LMT	O2'-C2'	-2.21	1.37	1.43
15	BF	103	LMT	O2'-C2'	-2.21	1.37	1.43
15	BX	1004	LMT	O2'-C2'	-2.21	1.37	1.43
16	bg	101	V7N	C12-C13	-2.21	1.41	1.46
15	AE	1002	LMT	O2B-C2B	-2.21	1.37	1.43
16	bb	101	V7N	C7-C8	2.21	1.40	1.34
16	bn	102	V7N	C6-C5	2.21	1.40	1.35
25	L	1009	BPH	C1D-C2D	2.21	1.42	1.39
16	BU	1001	V7N	C7-C8	2.21	1.40	1.34
15	BA	104	LMT	O2'-C2'	-2.21	1.37	1.43
15	AH	102	LMT	O2'-C2'	-2.21	1.37	1.43
15	BR	1002	LMT	O2'-C2'	-2.20	1.37	1.43
15	BV	1002	LMT	O2'-C2'	-2.20	1.37	1.43
15	BH	1002	LMT	O2'-C2'	-2.20	1.37	1.43
14	AG	102	BCL	CHD-C1D	2.20	1.42	1.38
14	bk	102	BCL	CHD-C1D	2.20	1.42	1.38
16	BP	1001	V7N	C11-C12	2.20	1.40	1.34
15	AJ	103	LMT	O3B-C3B	-2.20	1.37	1.43
16	bn	102	V7N	C7-C8	2.20	1.40	1.34
15	BV	1002	LMT	O3B-C3B	-2.20	1.37	1.43
15	BB	104	LMT	O3B-C3B	-2.20	1.37	1.43
15	bl	105	LMT	O2'-C2'	-2.20	1.37	1.43
15	BJ	1004	LMT	O3B-C3B	-2.20	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bh	104	LMT	O2B-C2B	-2.20	1.37	1.43
16	BB	101	V7N	C11-C12	2.20	1.40	1.34
15	L	1007	LMT	O3B-C3B	-2.19	1.37	1.43
16	bi	101	V7N	C7-C8	2.19	1.40	1.34
15	AP	101	LMT	O2B-C2B	-2.19	1.37	1.43
14	M	405	BCL	C3D-C4D	-2.19	1.39	1.44
15	AF	1002	LMT	O2'-C2'	-2.19	1.37	1.43
15	BT	104	LMT	O2'-C2'	-2.19	1.37	1.43
14	bg	105	BCL	CHD-C1D	2.19	1.42	1.38
14	bl	104	BCL	C3D-C4D	-2.19	1.39	1.44
16	BI	1001	V7N	C11-C12	2.19	1.40	1.34
16	BL	1001	V7N	C11-C12	2.19	1.40	1.34
16	BO	1001	V7N	C7-C8	2.19	1.40	1.34
15	bm	103	LMT	O3B-C3B	-2.19	1.37	1.43
15	BV	1004	LMT	O2'-C2'	-2.19	1.37	1.43
16	BD	101	V7N	C11-C12	2.19	1.40	1.34
16	bf	101	V7N	C7-C8	2.19	1.40	1.34
15	BV	1004	LMT	O3B-C3B	-2.19	1.37	1.43
15	bn	105	LMT	O2B-C2B	-2.19	1.37	1.43
14	bg	105	BCL	C3D-C4D	-2.19	1.39	1.44
16	BJ	1001	V7N	C11-C12	2.19	1.40	1.34
14	be	105	BCL	CHD-C1D	2.19	1.42	1.38
15	bi	102	LMT	O2'-C2'	-2.19	1.37	1.43
15	BP	1004	LMT	O2'-C2'	-2.19	1.37	1.43
16	bj	101	V7N	C6-C5	2.19	1.40	1.35
15	AL	102	LMT	O2'-C2'	-2.19	1.37	1.43
14	BT	103	BCL	C3D-C4D	-2.19	1.39	1.44
15	AD	103	LMT	O3B-C3B	-2.19	1.37	1.43
15	BS	1002	LMT	O3B-C3B	-2.19	1.37	1.43
14	BB	103	BCL	C3D-C4D	-2.18	1.39	1.44
16	bd	101	V7N	C7-C8	2.18	1.40	1.34
14	bo	103	BCL	CHD-C1D	2.18	1.42	1.38
16	AO	1001	V7N	C12-C13	-2.18	1.41	1.46
14	bm	104	BCL	CHD-C1D	2.18	1.42	1.38
16	bl	102	V7N	C12-C13	-2.18	1.41	1.46
15	ab	101	LMT	O2'-C2'	-2.18	1.37	1.43
15	BR	1003	LMT	O3B-C3B	-2.18	1.37	1.43
15	BS	1005	LMT	O2'-C2'	-2.18	1.37	1.43
16	BQ	1001	V7N	C12-C13	-2.18	1.41	1.46
14	bb	104	BCL	CHD-C1D	2.18	1.42	1.38
15	BG	1005	LMT	O2'-C2'	-2.18	1.37	1.43
15	BB	102	LMT	O3B-C3B	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	1003	LMT	O2'-C2'	-2.18	1.37	1.43
15	BO	1002	LMT	O3B-C3B	-2.18	1.37	1.43
15	BI	1004	LMT	O3B-C3B	-2.18	1.37	1.43
15	BS	1002	LMT	O2'-C2'	-2.18	1.37	1.43
15	BW	1005	LMT	O3B-C3B	-2.18	1.37	1.43
15	AT	102	LMT	O2B-C2B	-2.18	1.37	1.43
15	bo	105	LMT	O3B-C3B	-2.18	1.37	1.43
14	ag	1001	BCL	CHD-C1D	2.18	1.42	1.38
15	AT	102	LMT	O3B-C3B	-2.18	1.37	1.43
15	L	1008	LMT	O2B-C2B	-2.18	1.37	1.43
16	bp	101	V7N	C7-C8	2.18	1.40	1.34
16	BO	1001	V7N	C6-C5	2.18	1.40	1.35
15	BP	1002	LMT	O2'-C2'	-2.18	1.37	1.43
15	BM	1003	LMT	O3B-C3B	-2.18	1.37	1.43
15	AH	102	LMT	O2B-C2B	-2.18	1.37	1.43
15	AP	101	LMT	O3B-C3B	-2.18	1.37	1.43
15	AS	101	LMT	O2'-C2'	-2.18	1.37	1.43
15	BL	1004	LMT	O2'-C2'	-2.18	1.37	1.43
14	BI	1003	BCL	C3D-C4D	-2.17	1.39	1.44
15	AL	102	LMT	O2B-C2B	-2.17	1.37	1.43
15	bh	101	LMT	O2'-C2'	-2.17	1.37	1.43
15	be	104	LMT	O2'-C2'	-2.17	1.37	1.43
15	bj	102	LMT	O2'-C2'	-2.17	1.37	1.43
15	BT	104	LMT	O3B-C3B	-2.17	1.37	1.43
15	AA	1004	LMT	O3B-C3B	-2.17	1.37	1.43
15	BD	103	LMT	O3B-C3B	-2.17	1.37	1.43
15	BV	1004	LMT	O2B-C2B	-2.17	1.37	1.43
14	BM	1002	BCL	C3D-C4D	-2.17	1.39	1.44
14	bj	103	BCL	C3D-C4D	-2.17	1.39	1.44
15	AG	103	LMT	O3B-C3B	-2.17	1.37	1.43
15	L	1005	LMT	O3B-C3B	-2.17	1.37	1.43
15	BP	1002	LMT	O3B-C3B	-2.17	1.37	1.43
14	AL	101	BCL	C1D-ND	2.17	1.40	1.37
16	bj	101	V7N	C7-C8	2.17	1.40	1.34
28	ai	102	UYH	C30-C29	2.17	1.60	1.52
15	BB	102	LMT	O2'-C2'	-2.17	1.37	1.43
14	BK	1006	BCL	C3D-C4D	-2.17	1.39	1.44
15	BH	1004	LMT	O3B-C3B	-2.17	1.37	1.43
15	BQ	1004	LMT	O2'-C2'	-2.17	1.37	1.43
14	L	1010	BCL	CHD-C1D	2.17	1.42	1.38
15	AL	102	LMT	O3B-C3B	-2.17	1.37	1.43
15	BT	101	LMT	O3B-C3B	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bm	103	LMT	O2B-C2B	-2.17	1.37	1.43
14	an	1001	BCL	C3D-C4D	-2.17	1.39	1.44
14	AM	102	BCL	O1A-CGA	-2.17	1.16	1.22
15	bn	105	LMT	O3B-C3B	-2.17	1.37	1.43
15	bf	102	LMT	O2B-C2B	-2.17	1.37	1.43
16	BA	101	V7N	C12-C13	-2.17	1.41	1.46
16	BE	101	V7N	C12-C13	-2.16	1.41	1.46
15	BC	103	LMT	O3B-C3B	-2.16	1.37	1.43
15	BM	1003	LMT	O2'-C2'	-2.16	1.37	1.43
14	bb	104	BCL	C3D-C4D	-2.16	1.39	1.44
15	BE	103	LMT	O2B-C2B	-2.16	1.37	1.43
15	AH	104	LMT	O2'-C2'	-2.16	1.37	1.43
15	bi	102	LMT	O3B-C3B	-2.16	1.37	1.43
14	BP	1005	BCL	C3D-C4D	-2.16	1.39	1.44
15	BU	1003	LMT	O3B-C3B	-2.16	1.37	1.43
15	BM	1004	LMT	O2B-C2B	-2.16	1.37	1.43
14	BR	1004	BCL	C3D-C4D	-2.16	1.39	1.44
15	BL	1005	LMT	O3B-C3B	-2.16	1.37	1.43
15	BP	1003	LMT	O2'-C2'	-2.16	1.37	1.43
14	AU	103	BCL	C1D-ND	2.16	1.40	1.37
15	BX	1004	LMT	O3B-C3B	-2.16	1.37	1.43
15	bl	101	LMT	O3B-C3B	-2.16	1.37	1.43
15	BW	1004	LMT	O2'-C2'	-2.16	1.37	1.43
15	L	1007	LMT	O2B-C2B	-2.16	1.37	1.43
16	bh	102	V7N	C12-C13	-2.16	1.41	1.46
15	BS	1006	LMT	O2'-C2'	-2.16	1.37	1.43
16	BX	1001	V7N	C11-C12	2.16	1.40	1.34
15	BQ	1004	LMT	O3B-C3B	-2.16	1.37	1.43
15	L	1004	LMT	O3B-C3B	-2.16	1.37	1.43
15	AS	101	LMT	O3B-C3B	-2.16	1.37	1.43
15	BP	1004	LMT	O2B-C2B	-2.16	1.37	1.43
15	L	1003	LMT	O3B-C3B	-2.16	1.37	1.43
15	BB	105	LMT	O3B-C3B	-2.16	1.37	1.43
15	bh	101	LMT	O2B-C2B	-2.16	1.37	1.43
16	bd	101	V7N	C6-C5	2.16	1.40	1.35
15	BH	1002	LMT	O3B-C3B	-2.16	1.37	1.43
16	bg	101	V7N	C7-C8	2.16	1.40	1.34
18	M	409	V75	O5-C1	-2.16	1.40	1.43
15	AA	1003	LMT	O3B-C3B	-2.15	1.37	1.43
15	AU	101	LMT	O3B-C3B	-2.15	1.37	1.43
15	BF	101	LMT	O2'-C2'	-2.15	1.37	1.43
15	M	403	LMT	O3B-C3B	-2.15	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ak	1001	BCL	C3D-C4D	-2.15	1.39	1.44
16	bi	101	V7N	C6-C5	2.15	1.40	1.35
14	BX	1002	BCL	C3D-C4D	-2.15	1.39	1.44
15	bj	102	LMT	O3B-C3B	-2.15	1.37	1.43
15	BR	1002	LMT	O3B-C3B	-2.15	1.37	1.43
14	AT	101	BCL	C3D-C4D	-2.15	1.39	1.44
14	BU	1004	BCL	C3D-C4D	-2.15	1.39	1.44
14	BQ	1003	BCL	C3D-C4D	-2.15	1.39	1.44
15	AC	104	LMT	O2B-C2B	-2.15	1.37	1.43
15	be	104	LMT	O3B-C3B	-2.15	1.37	1.43
15	bl	105	LMT	O3B-C3B	-2.15	1.37	1.43
15	BS	1002	LMT	O2B-C2B	-2.15	1.37	1.43
15	BS	1005	LMT	O2B-C2B	-2.15	1.37	1.43
14	AN	102	BCL	C3D-C4D	-2.15	1.39	1.44
14	af	101	BCL	CHD-C1D	2.15	1.42	1.38
15	BS	1004	LMT	O3B-C3B	-2.15	1.37	1.43
14	bn	103	BCL	C3D-C4D	-2.15	1.39	1.44
15	BA	105	LMT	O3B-C3B	-2.15	1.37	1.43
15	bg	103	LMT	O3B-C3B	-2.15	1.37	1.43
15	BO	1003	LMT	O2'-C2'	-2.15	1.37	1.43
15	BX	1003	LMT	O3B-C3B	-2.15	1.37	1.43
15	bl	105	LMT	O2B-C2B	-2.15	1.37	1.43
15	AQ	103	LMT	O2'-C2'	-2.15	1.37	1.43
15	BK	1004	LMT	O2B-C2B	-2.15	1.37	1.43
15	BH	1003	LMT	O3B-C3B	-2.15	1.37	1.43
15	BR	1003	LMT	O2'-C2'	-2.15	1.37	1.43
15	BT	102	LMT	O3B-C3B	-2.15	1.37	1.43
15	AA	1003	LMT	O2B-C2B	-2.15	1.37	1.43
15	AE	1002	LMT	O3B-C3B	-2.15	1.37	1.43
15	BE	102	LMT	O3B-C3B	-2.15	1.37	1.43
15	bd	103	LMT	O2B-C2B	-2.15	1.37	1.43
15	BU	1002	LMT	O2B-C2B	-2.15	1.37	1.43
15	BN	101	LMT	O2B-C2B	-2.15	1.37	1.43
15	BP	1004	LMT	O3B-C3B	-2.15	1.37	1.43
15	BW	1004	LMT	O3B-C3B	-2.15	1.37	1.43
15	bh	101	LMT	O3B-C3B	-2.15	1.37	1.43
14	bi	104	BCL	CHD-C1D	2.15	1.42	1.38
15	BV	1006	LMT	O2'-C2'	-2.15	1.37	1.43
14	AE	1003	BCL	C1D-ND	2.15	1.40	1.37
15	AN	103	LMT	O3B-C3B	-2.15	1.37	1.43
15	AP	104	LMT	O3B-C3B	-2.15	1.37	1.43
15	AD	101	LMT	O3B-C3B	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bj	102	LMT	O2B-C2B	-2.14	1.37	1.43
15	AA	1003	LMT	O2'-C2'	-2.14	1.37	1.43
15	AQ	103	LMT	O2B-C2B	-2.14	1.37	1.43
15	bd	103	LMT	O3B-C3B	-2.14	1.37	1.43
15	BP	1003	LMT	O3B-C3B	-2.14	1.37	1.43
15	bg	103	LMT	O2'-C2'	-2.14	1.37	1.43
15	bm	105	LMT	O2'-C2'	-2.14	1.37	1.43
15	BH	1004	LMT	O2B-C2B	-2.14	1.37	1.43
15	BV	1003	LMT	O3B-C3B	-2.14	1.37	1.43
15	AD	103	LMT	O2B-C2B	-2.14	1.37	1.43
15	BV	1003	LMT	O2'-C2'	-2.14	1.37	1.43
15	bh	104	LMT	O3B-C3B	-2.14	1.37	1.43
16	BE	101	V7N	C6-C5	2.14	1.40	1.35
14	be	105	BCL	C3D-C4D	-2.14	1.39	1.44
16	BC	101	V7N	C12-C13	-2.14	1.41	1.46
15	L	1004	LMT	O2'-C2'	-2.14	1.37	1.43
15	L	1005	LMT	O2B-C2B	-2.14	1.37	1.43
16	bf	101	V7N	C6-C5	2.14	1.40	1.35
15	BK	1004	LMT	O2'-C2'	-2.14	1.37	1.43
15	bo	101	LMT	O3B-C3B	-2.14	1.37	1.43
15	BK	1004	LMT	O3B-C3B	-2.14	1.37	1.43
16	bj	101	V7N	C12-C13	-2.14	1.41	1.46
15	L	1008	LMT	O3B-C3B	-2.14	1.37	1.43
14	BA	103	BCL	C3D-C4D	-2.14	1.39	1.44
14	bd	102	BCL	C3D-C4D	-2.14	1.39	1.44
15	BG	1005	LMT	O3B-C3B	-2.14	1.37	1.43
16	bb	101	V7N	C12-C13	-2.14	1.41	1.46
15	AH	102	LMT	O3B-C3B	-2.14	1.37	1.43
16	bb	101	V7N	C6-C5	2.14	1.40	1.35
16	BR	1001	V7N	C7-C8	2.14	1.40	1.34
15	bc	104	LMT	O3B-C3B	-2.14	1.37	1.43
15	AD	103	LMT	O2'-C2'	-2.14	1.37	1.43
15	BC	103	LMT	O2B-C2B	-2.14	1.37	1.43
15	AN	103	LMT	O2B-C2B	-2.14	1.37	1.43
17	C	402	HEC	CMC-C2C	2.14	1.55	1.50
15	BN	101	LMT	O3B-C3B	-2.14	1.37	1.43
15	BC	105	LMT	O3B-C3B	-2.14	1.37	1.43
15	BN	105	LMT	O3B-C3B	-2.14	1.37	1.43
15	bo	101	LMT	O2'-C2'	-2.14	1.37	1.43
15	bf	102	LMT	O3B-C3B	-2.13	1.37	1.43
14	ab	102	BCL	C3D-C4D	-2.13	1.39	1.44
15	BA	104	LMT	O3B-C3B	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BL	1002	LMT	O3B-C3B	-2.13	1.37	1.43
15	AD	101	LMT	O2'-C2'	-2.13	1.37	1.43
15	BI	1006	LMT	O3B-C3B	-2.13	1.37	1.43
14	bn	103	BCL	CHD-C1D	2.13	1.42	1.38
15	BN	104	LMT	O3B-C3B	-2.13	1.37	1.43
15	bd	103	LMT	O2'-C2'	-2.13	1.37	1.43
15	bm	103	LMT	O2'-C2'	-2.13	1.37	1.43
16	BK	1001	V7N	C7-C8	2.13	1.40	1.34
16	bh	102	V7N	C7-C8	2.13	1.40	1.34
15	BI	1002	LMT	O3B-C3B	-2.13	1.37	1.43
15	bn	101	LMT	O2'-C2'	-2.13	1.37	1.43
15	BB	102	LMT	O2B-C2B	-2.13	1.37	1.43
15	BK	1005	LMT	O3B-C3B	-2.13	1.37	1.43
15	BW	1002	LMT	O3B-C3B	-2.13	1.37	1.43
15	BD	102	LMT	O2'-C2'	-2.13	1.37	1.43
15	BW	1004	LMT	O2B-C2B	-2.13	1.37	1.43
15	bg	103	LMT	O2B-C2B	-2.13	1.37	1.43
16	BH	1001	V7N	C12-C13	-2.13	1.41	1.46
14	bi	104	BCL	C3D-C4D	-2.13	1.39	1.44
14	ba	103	BCL	C3D-C4D	-2.13	1.39	1.44
15	BO	1002	LMT	O2'-C2'	-2.13	1.37	1.43
14	BW	1003	BCL	C3D-C4D	-2.13	1.39	1.44
14	AC	102	BCL	C3D-C4D	-2.13	1.39	1.44
16	bl	102	V7N	C7-C8	2.13	1.40	1.34
14	bd	102	BCL	CHD-C1D	2.13	1.42	1.38
14	bk	102	BCL	C3D-C4D	-2.13	1.39	1.44
15	BD	102	LMT	O3B-C3B	-2.13	1.37	1.43
15	BL	1004	LMT	O3B-C3B	-2.13	1.37	1.43
16	bp	101	V7N	C6-C5	2.12	1.40	1.35
15	BA	102	LMT	O2B-C2B	-2.12	1.37	1.43
16	bn	102	V7N	C20-C19	2.12	1.40	1.34
15	BV	1006	LMT	O3B-C3B	-2.12	1.37	1.43
15	BL	1004	LMT	O2B-C2B	-2.12	1.37	1.43
16	AE	1005	V7N	C7-C8	2.12	1.40	1.34
15	BF	103	LMT	O3B-C3B	-2.12	1.37	1.43
15	BG	1002	LMT	O2B-C2B	-2.12	1.37	1.43
15	BE	102	LMT	O2'-C2'	-2.12	1.37	1.43
15	BI	1006	LMT	O2B-C2B	-2.12	1.37	1.43
15	BJ	1003	LMT	O2B-C2B	-2.12	1.37	1.43
15	BG	1006	LMT	O3B-C3B	-2.12	1.37	1.43
16	BR	1001	V7N	C6-C5	2.12	1.40	1.35
15	BA	102	LMT	O2'-C2'	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bb	102	LMT	O3B-C3B	-2.12	1.37	1.43
15	BG	1003	LMT	O2B-C2B	-2.12	1.37	1.43
14	AS	103	BCL	C3D-C4D	-2.12	1.39	1.44
15	BA	105	LMT	O2B-C2B	-2.12	1.37	1.43
15	ab	101	LMT	O3B-C3B	-2.12	1.37	1.43
15	bf	102	LMT	O2'-C2'	-2.12	1.37	1.43
17	C	403	HEC	CMC-C2C	2.12	1.55	1.50
14	bc	102	BCL	C3D-C4D	-2.12	1.39	1.44
15	AG	103	LMT	O2B-C2B	-2.12	1.37	1.43
15	BG	1005	LMT	O2B-C2B	-2.12	1.37	1.43
14	AP	102	BCL	C3D-C4D	-2.12	1.39	1.44
15	AF	1002	LMT	O3B-C3B	-2.12	1.37	1.43
16	BW	1001	V7N	C7-C8	2.12	1.40	1.34
14	AN	101	BCL	C1D-ND	2.12	1.40	1.37
17	C	401	HEC	CMC-C2C	2.12	1.55	1.50
14	BN	103	BCL	C3D-C4D	-2.12	1.39	1.44
15	BG	1002	LMT	O3B-C3B	-2.12	1.37	1.43
17	C	404	HEC	CMB-C2B	2.12	1.55	1.50
15	BB	105	LMT	O2'-C2'	-2.12	1.37	1.43
16	bk	101	V7N	C12-C13	-2.12	1.41	1.46
15	L	1011	LMT	O2'-C2'	-2.12	1.37	1.43
14	bf	103	BCL	C3D-C4D	-2.12	1.39	1.44
15	BC	102	LMT	O2B-C2B	-2.12	1.37	1.43
16	bf	101	V7N	C12-C13	-2.12	1.41	1.46
15	AJ	104	LMT	O2'-C2'	-2.12	1.37	1.43
15	BP	1002	LMT	O2B-C2B	-2.12	1.37	1.43
15	bn	101	LMT	O2B-C2B	-2.11	1.37	1.43
14	AI	102	BCL	C3D-C4D	-2.11	1.39	1.44
15	BQ	1004	LMT	O2B-C2B	-2.11	1.37	1.43
16	be	101	V7N	C7-C8	2.11	1.40	1.34
16	BC	101	V7N	C7-C8	2.11	1.40	1.34
15	BE	102	LMT	O2B-C2B	-2.11	1.37	1.43
16	BD	101	V7N	C7-C8	2.11	1.40	1.34
16	BE	101	V7N	C7-C8	2.11	1.40	1.34
15	BI	1005	LMT	O3B-C3B	-2.11	1.37	1.43
14	BV	1005	BCL	C3D-C4D	-2.11	1.39	1.44
15	AF	1002	LMT	O2B-C2B	-2.11	1.37	1.43
15	BB	104	LMT	O2'-C2'	-2.11	1.37	1.43
14	ba	103	BCL	CHD-C1D	2.11	1.42	1.38
15	BM	1004	LMT	O3B-C3B	-2.11	1.37	1.43
15	BS	1004	LMT	O2B-C2B	-2.11	1.37	1.43
15	BH	1002	LMT	O2B-C2B	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BH	1004	LMT	O2'-C2'	-2.11	1.37	1.43
15	AS	101	LMT	O2B-C2B	-2.11	1.37	1.43
15	BC	105	LMT	O2B-C2B	-2.11	1.37	1.43
15	BU	1002	LMT	O3B-C3B	-2.11	1.37	1.43
17	C	403	HEC	CMB-C2B	2.11	1.55	1.50
15	BG	1003	LMT	O3B-C3B	-2.11	1.37	1.43
15	L	1011	LMT	O3B-C3B	-2.11	1.37	1.43
14	BH	1005	BCL	C3D-C4D	-2.11	1.39	1.44
15	AH	104	LMT	O2B-C2B	-2.11	1.37	1.43
15	BA	102	LMT	O3B-C3B	-2.11	1.37	1.43
15	AC	104	LMT	O3B-C3B	-2.11	1.37	1.43
15	BV	1003	LMT	O2B-C2B	-2.11	1.37	1.43
14	AL	103	BCL	C3D-C4D	-2.11	1.39	1.44
15	BW	1005	LMT	O2B-C2B	-2.11	1.37	1.43
14	bl	104	BCL	CHD-C1D	2.11	1.42	1.38
14	M	408	BCL	C3D-C4D	-2.11	1.39	1.44
15	BR	1002	LMT	O2B-C2B	-2.11	1.37	1.43
15	BT	104	LMT	O2B-C2B	-2.11	1.37	1.43
14	bh	105	BCL	CHD-C1D	2.11	1.42	1.38
15	BV	1002	LMT	O2B-C2B	-2.10	1.37	1.43
15	BK	1005	LMT	O2'-C2'	-2.10	1.37	1.43
15	BQ	1002	LMT	O2B-C2B	-2.10	1.37	1.43
16	BM	1001	V7N	C7-C8	2.10	1.40	1.34
15	AA	1004	LMT	O2B-C2B	-2.10	1.37	1.43
15	AX	101	LMT	O2B-C2B	-2.10	1.37	1.43
15	BE	103	LMT	O3B-C3B	-2.10	1.37	1.43
15	BQ	1002	LMT	O3B-C3B	-2.10	1.37	1.43
15	BR	1005	LMT	O2B-C2B	-2.10	1.37	1.43
14	bo	103	BCL	C3D-C4D	-2.10	1.39	1.44
16	BR	1001	V7N	C12-C13	-2.10	1.41	1.46
15	BF	103	LMT	O2B-C2B	-2.10	1.37	1.43
15	L	1004	LMT	O2B-C2B	-2.10	1.37	1.43
15	BC	105	LMT	O2'-C2'	-2.10	1.37	1.43
15	BK	1002	LMT	O2B-C2B	-2.10	1.37	1.43
15	BN	104	LMT	O2B-C2B	-2.10	1.37	1.43
15	BO	1003	LMT	O3B-C3B	-2.10	1.37	1.43
15	BQ	1005	LMT	O3B-C3B	-2.10	1.37	1.43
24	ag	1002	V7B	O8-C9	-2.10	1.40	1.45
15	BD	104	LMT	O3B-C3B	-2.10	1.37	1.43
28	ai	102	UYH	C12-C11	2.10	1.59	1.52
15	AX	101	LMT	O3B-C3B	-2.10	1.37	1.43
15	BN	102	LMT	O2B-C2B	-2.10	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BV	1006	LMT	O2B-C2B	-2.10	1.37	1.43
16	bk	101	V7N	C6-C5	2.10	1.40	1.35
14	am	1001	BCL	C2-C3	-2.10	1.28	1.33
16	bc	101	V7N	C12-C13	-2.10	1.41	1.46
14	AV	102	BCL	C3D-C4D	-2.10	1.39	1.44
15	BL	1005	LMT	O2B-C2B	-2.10	1.37	1.43
15	BO	1003	LMT	O2B-C2B	-2.10	1.37	1.43
14	AH	101	BCL	C1D-ND	2.10	1.40	1.37
15	bo	101	LMT	O2B-C2B	-2.10	1.37	1.43
16	BC	101	V7N	C6-C5	2.10	1.40	1.35
14	AC	103	BCL	C1D-ND	2.10	1.40	1.37
15	BK	1002	LMT	O3B-C3B	-2.10	1.37	1.43
14	AE	1004	BCL	C1D-ND	2.10	1.40	1.37
16	bp	101	V7N	C12-C13	-2.10	1.41	1.46
15	BR	1005	LMT	O3B-C3B	-2.10	1.37	1.43
15	BS	1005	LMT	O3B-C3B	-2.10	1.37	1.43
15	bm	105	LMT	O3B-C3B	-2.10	1.37	1.43
14	L	1002	BCL	C3D-C4D	-2.10	1.39	1.44
16	BA	101	V7N	C6-C5	2.10	1.40	1.35
15	BB	105	LMT	O2B-C2B	-2.10	1.37	1.43
14	BL	1003	BCL	C3D-C4D	-2.10	1.39	1.44
15	BN	102	LMT	O3B-C3B	-2.10	1.37	1.43
15	L	1007	LMT	O2'-C2'	-2.10	1.37	1.43
16	bo	102	V7N	C20-C19	2.10	1.40	1.34
16	bd	101	V7N	C12-C13	-2.10	1.41	1.46
15	BJ	1004	LMT	O2B-C2B	-2.10	1.37	1.43
14	ap	1001	BCL	C3D-C4D	-2.10	1.39	1.44
14	AO	1002	BCL	C3D-C4D	-2.10	1.39	1.44
15	BC	106	LMT	O3B-C3B	-2.09	1.37	1.43
15	BM	1004	LMT	O2'-C2'	-2.09	1.37	1.43
15	BI	1004	LMT	O2B-C2B	-2.09	1.37	1.43
15	BR	1005	LMT	O2'-C2'	-2.09	1.37	1.43
15	BS	1004	LMT	O2'-C2'	-2.09	1.37	1.43
15	L	1003	LMT	O2B-C2B	-2.09	1.37	1.43
15	BF	101	LMT	O3B-C3B	-2.09	1.37	1.43
15	BB	104	LMT	O2B-C2B	-2.09	1.37	1.43
15	BI	1005	LMT	O2B-C2B	-2.09	1.37	1.43
15	AT	102	LMT	O2'-C2'	-2.09	1.37	1.43
15	BL	1005	LMT	O2'-C2'	-2.09	1.37	1.43
15	BU	1003	LMT	O2B-C2B	-2.09	1.37	1.43
15	BT	102	LMT	O2B-C2B	-2.09	1.37	1.43
14	BE	104	BCL	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BG	1004	BCL	C3D-C4D	-2.09	1.39	1.44
15	BE	103	LMT	O2'-C2'	-2.09	1.37	1.43
15	bo	105	LMT	O2B-C2B	-2.09	1.37	1.43
15	BJ	1003	LMT	O3B-C3B	-2.09	1.37	1.43
15	bm	105	LMT	O2B-C2B	-2.09	1.37	1.43
16	bn	102	V7N	C12-C13	-2.09	1.41	1.46
14	bl	104	BCL	C1D-C2D	-2.09	1.41	1.45
16	BH	1001	V7N	C6-C5	2.09	1.40	1.35
17	C	404	HEC	CMC-C2C	2.09	1.55	1.50
14	aj	103	BCL	C3D-C4D	-2.09	1.39	1.44
15	BP	1003	LMT	O2B-C2B	-2.09	1.37	1.43
15	BR	1003	LMT	O2B-C2B	-2.09	1.37	1.43
14	BD	105	BCL	C3D-C4D	-2.09	1.39	1.44
15	AU	101	LMT	O2B-C2B	-2.09	1.37	1.43
15	AQ	103	LMT	O3B-C3B	-2.08	1.37	1.43
15	M	403	LMT	O2B-C2B	-2.08	1.37	1.43
14	BF	102	BCL	C3D-C4D	-2.08	1.39	1.44
15	BC	106	LMT	O2B-C2B	-2.08	1.37	1.43
15	BW	1002	LMT	O2'-C2'	-2.08	1.37	1.43
14	bf	103	BCL	CHD-C1D	2.08	1.42	1.38
14	AK	102	BCL	C3D-C4D	-2.08	1.39	1.44
14	ag	1001	BCL	C3D-C4D	-2.08	1.39	1.44
14	al	1001	BCL	C3D-C4D	-2.08	1.39	1.44
15	BC	106	LMT	O2'-C2'	-2.08	1.37	1.43
16	BH	1001	V7N	C7-C8	2.08	1.40	1.34
15	BU	1002	LMT	O2'-C2'	-2.08	1.37	1.43
16	AS	105	V7N	C7-C8	2.08	1.40	1.34
14	BO	1004	BCL	C3D-C4D	-2.08	1.39	1.44
14	L	1010	BCL	C3D-C4D	-2.08	1.39	1.44
15	BF	101	LMT	O2B-C2B	-2.08	1.37	1.43
15	BQ	1005	LMT	O2B-C2B	-2.08	1.37	1.43
15	BK	1005	LMT	O2B-C2B	-2.08	1.37	1.43
16	BM	1001	V7N	C6-C5	2.08	1.40	1.35
14	BJ	1002	BCL	C3D-C4D	-2.08	1.39	1.44
17	C	401	HEC	CMB-C2B	2.08	1.55	1.50
16	bc	101	V7N	C7-C8	2.08	1.40	1.34
14	bh	105	BCL	C3D-C4D	-2.08	1.39	1.44
16	BW	1001	V7N	C6-C5	2.08	1.40	1.35
16	BX	1001	V7N	C7-C8	2.08	1.40	1.34
14	AV	101	BCL	C1D-ND	2.08	1.40	1.37
15	BI	1005	LMT	O2'-C2'	-2.08	1.37	1.43
14	AP	103	BCL	C1D-ND	2.08	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	ad	1001	BCL	C3D-C4D	-2.07	1.39	1.44
15	BD	102	LMT	O2B-C2B	-2.07	1.37	1.43
15	BD	103	LMT	O2B-C2B	-2.07	1.37	1.43
15	ab	101	LMT	O2B-C2B	-2.07	1.37	1.43
14	AQ	102	BCL	C3D-C4D	-2.07	1.39	1.44
14	aa	1001	BCL	C3D-C4D	-2.07	1.39	1.44
16	BA	101	V7N	C7-C8	2.07	1.40	1.34
16	AS	105	V7N	C6-C5	2.07	1.40	1.35
16	BK	1001	V7N	C6-C5	2.07	1.40	1.35
14	AU	102	BCL	C3D-C4D	-2.07	1.39	1.44
15	AD	101	LMT	O2B-C2B	-2.07	1.37	1.43
15	bl	101	LMT	O2'-C2'	-2.07	1.37	1.43
14	BS	1003	BCL	C3D-C4D	-2.07	1.39	1.44
14	bp	102	BCL	C3D-C4D	-2.07	1.39	1.44
15	BD	104	LMT	O2B-C2B	-2.07	1.37	1.43
16	BQ	1001	V7N	C6-C5	2.07	1.40	1.35
16	bg	101	V7N	C6-C5	2.07	1.40	1.35
15	BT	104	LMT	O1'-C1'	-2.07	1.36	1.40
14	AC	103	BCL	C3D-C4D	-2.07	1.39	1.44
16	BQ	1001	V7N	C7-C8	2.07	1.40	1.34
15	BN	104	LMT	O2'-C2'	-2.07	1.37	1.43
14	AR	101	BCL	C3D-C4D	-2.07	1.39	1.44
14	ac	1001	BCL	C3D-C4D	-2.07	1.39	1.44
14	ao	102	BCL	C3D-C4D	-2.07	1.39	1.44
16	BJ	1001	V7N	C7-C8	2.07	1.40	1.34
14	AF	1001	BCL	C3D-C4D	-2.07	1.39	1.44
15	bi	102	LMT	O2B-C2B	-2.07	1.37	1.43
15	BW	1002	LMT	O2B-C2B	-2.07	1.37	1.43
15	L	1011	LMT	O2B-C2B	-2.07	1.37	1.43
15	BL	1002	LMT	O2B-C2B	-2.06	1.37	1.43
16	BD	101	V7N	C6-C5	2.06	1.40	1.35
14	AS	104	BCL	C1D-ND	2.06	1.40	1.37
14	BC	104	BCL	C3D-C4D	-2.06	1.39	1.44
15	BJ	1004	LMT	O2'-C2'	-2.06	1.37	1.43
15	BX	1003	LMT	O2'-C2'	-2.06	1.37	1.43
15	BT	101	LMT	O2B-C2B	-2.06	1.37	1.43
14	bj	103	BCL	CHD-C1D	2.06	1.42	1.38
14	AX	102	BCL	C1D-ND	2.06	1.40	1.37
15	BH	1003	LMT	O2B-C2B	-2.06	1.37	1.43
14	AG	102	BCL	C3D-C4D	-2.06	1.39	1.44
15	BN	105	LMT	O2B-C2B	-2.06	1.37	1.43
16	BK	1001	V7N	C19-C18	-2.06	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	AN	103	LMT	O2'-C2'	-2.06	1.37	1.43
15	BI	1002	LMT	O2B-C2B	-2.06	1.37	1.43
15	BI	1006	LMT	O2'-C2'	-2.06	1.37	1.43
15	BQ	1002	LMT	O2'-C2'	-2.06	1.37	1.43
14	ah	1001	BCL	C3D-C4D	-2.06	1.39	1.44
14	am	1001	BCL	O2A-CGA	-2.06	1.27	1.33
14	bp	102	BCL	C1D-C2D	-2.06	1.41	1.45
14	AM	101	BCL	C3D-C4D	-2.05	1.39	1.44
15	BQ	1005	LMT	O2'-C2'	-2.05	1.37	1.43
16	AE	1005	V7N	C6-C5	2.05	1.40	1.35
14	am	1001	BCL	C3D-C4D	-2.05	1.39	1.44
16	bl	102	V7N	C6-C5	2.05	1.40	1.35
14	AH	103	BCL	C3D-C4D	-2.05	1.39	1.44
16	bm	101	V7N	C20-C19	2.05	1.40	1.34
15	BL	1002	LMT	O2'-C2'	-2.05	1.37	1.43
16	bp	101	V7N	C20-C19	2.05	1.40	1.34
19	C	406	NDG	C1-C2	2.05	1.55	1.52
14	AC	101	BCL	C1D-ND	2.05	1.40	1.37
14	AJ	101	BCL	C3D-C4D	-2.05	1.39	1.44
14	AA	1001	BCL	C3D-C4D	-2.05	1.39	1.44
15	AI	101	LMT	O2'-C2'	-2.05	1.37	1.43
15	BN	102	LMT	O2'-C2'	-2.04	1.37	1.43
15	BG	1006	LMT	O2B-C2B	-2.04	1.37	1.43
15	L	1008	LMT	O2'-C2'	-2.04	1.37	1.43
16	bc	101	V7N	C6-C5	2.04	1.40	1.35
14	AD	102	BCL	C3D-C4D	-2.04	1.39	1.44
14	AW	101	BCL	C3D-C4D	-2.04	1.39	1.44
16	AO	1001	V7N	C19-C18	-2.04	1.41	1.46
14	AK	101	BCL	C3D-C4D	-2.04	1.39	1.44
15	BJ	1003	LMT	O2'-C2'	-2.04	1.37	1.43
14	AS	102	BCL	C1D-ND	2.04	1.40	1.37
16	BX	1001	V7N	C6-C5	2.04	1.40	1.35
14	AE	1001	BCL	C3D-C4D	-2.04	1.39	1.44
14	AM	102	BCL	C1D-ND	2.04	1.40	1.37
14	ai	101	BCL	C3D-C4D	-2.04	1.39	1.44
15	BA	104	LMT	O2B-C2B	-2.04	1.37	1.43
16	AO	1001	V7N	C7-C8	2.04	1.40	1.34
16	bi	101	V7N	C12-C13	-2.04	1.41	1.46
16	BP	1001	V7N	C6-C5	2.04	1.40	1.35
16	bg	101	V7N	C19-C18	-2.04	1.41	1.46
16	AE	1005	V7N	C19-C18	-2.03	1.41	1.46
15	bc	104	LMT	O2B-C2B	-2.03	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AC	101	BCL	C3D-C4D	-2.03	1.39	1.44
15	BS	1006	LMT	O2B-C2B	-2.03	1.37	1.43
14	BF	102	BCL	C2-C3	-2.03	1.28	1.33
14	AB	1001	BCL	C3D-C4D	-2.03	1.39	1.44
14	ae	102	BCL	C3D-C4D	-2.03	1.39	1.44
16	BB	101	V7N	C7-C8	2.03	1.40	1.34
14	AN	104	BCL	C1D-ND	2.03	1.40	1.37
15	BK	1002	LMT	O4'-C4B	-2.03	1.37	1.43
16	be	101	V7N	C6-C5	2.03	1.40	1.35
14	AR	102	BCL	C3D-C4D	-2.03	1.39	1.44
14	AA	1002	BCL	C3D-C4D	-2.03	1.39	1.44
16	bo	102	V7N	C27-C26	2.02	1.50	1.46
14	AK	101	BCL	C1D-ND	2.02	1.40	1.37
15	bh	104	LMT	O2'-C2'	-2.02	1.37	1.43
15	BG	1002	LMT	O2'-C2'	-2.02	1.37	1.43
16	BI	1001	V7N	C6-C5	2.02	1.40	1.35
16	BC	101	V7N	C20-C19	2.02	1.40	1.34
14	AX	103	BCL	C3D-C4D	-2.02	1.39	1.44
15	BW	1005	LMT	O4'-C4B	-2.02	1.37	1.43
14	AG	101	BCL	C3D-C4D	-2.02	1.39	1.44
16	BU	1001	V7N	C20-C19	2.02	1.40	1.34
14	AV	103	BCL	C3D-C4D	-2.02	1.39	1.44
15	BX	1003	LMT	O2B-C2B	-2.02	1.38	1.43
14	bp	102	BCL	CHD-C1D	2.02	1.42	1.38
16	BL	1001	V7N	C7-C8	2.02	1.39	1.34
16	AO	1001	V7N	C6-C5	2.02	1.40	1.35
16	BG	1001	V7N	C19-C18	-2.02	1.41	1.46
15	bo	105	LMT	O2'-C2'	-2.02	1.38	1.43
15	BX	1004	LMT	O2B-C2B	-2.02	1.38	1.43
14	af	101	BCL	C3D-C4D	-2.02	1.39	1.44
14	AG	101	BCL	C1D-ND	2.01	1.40	1.37
15	bb	102	LMT	O2'-C2'	-2.01	1.38	1.43
14	bm	104	BCL	C1D-C2D	-2.01	1.41	1.45
16	BJ	1001	V7N	C6-C5	2.01	1.40	1.35
24	L	1006	V7B	O8-C9	-2.01	1.40	1.45
14	bn	103	BCL	C1D-C2D	-2.01	1.41	1.45
15	AP	104	LMT	O2B-C2B	-2.01	1.38	1.43
16	bh	102	V7N	C6-C5	2.01	1.40	1.35
14	AH	101	BCL	C3D-C4D	-2.01	1.39	1.44
16	BI	1001	V7N	C7-C8	2.01	1.39	1.34
14	AJ	102	BCL	C3D-C4D	-2.01	1.39	1.44
15	AX	101	LMT	O2'-C2'	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	1010	BCL	C1D-C2D	-2.01	1.41	1.45
16	BV	1001	V7N	C6-C5	2.00	1.40	1.35
16	BM	1001	V7N	C19-C18	-2.00	1.41	1.46
16	BG	1001	V7N	C7-C8	2.00	1.39	1.34
16	bd	101	V7N	C20-C19	2.00	1.39	1.34
16	bo	102	V7N	C12-C13	-2.00	1.41	1.46
16	BP	1001	V7N	C19-C18	-2.00	1.41	1.46
16	BV	1001	V7N	C7-C8	2.00	1.39	1.34

All (1846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BF	102	BCL	C1-C2-C3	12.90	147.32	126.20
25	M	406	BPH	C4D-CHA-CBD	-10.01	103.65	108.45
14	BI	1003	BCL	C1-O2A-CGA	9.89	140.59	116.65
14	am	1001	BCL	C1-C2-C3	9.47	141.72	126.20
25	L	1009	BPH	C4D-CHA-CBD	-9.24	104.02	108.45
14	BN	103	BCL	C1-O2A-CGA	9.21	138.95	116.65
14	AL	101	BCL	C1-O2A-CGA	7.91	135.80	116.65
16	AS	105	V7N	C28-C27-C26	-7.47	105.88	126.36
16	bg	101	V7N	C28-C27-C26	-7.01	107.13	126.36
16	BU	1001	V7N	C28-C27-C26	-6.99	107.21	126.36
14	AQ	101	BCL	C1-O2A-CGA	6.90	133.37	116.65
17	C	403	HEC	CBC-CAC-C3C	-6.56	114.33	127.43
17	C	404	HEC	CBC-CAC-C3C	-6.50	114.45	127.43
14	AG	101	BCL	C1-C2-C3	6.42	136.72	126.20
14	BA	103	BCL	C1-C2-C3	6.40	136.69	126.20
17	C	402	HEC	CBB-CAB-C3B	-6.21	115.02	127.43
17	C	401	HEC	CBC-CAC-C3C	-6.15	115.14	127.43
14	ai	101	BCL	C1-C2-C3	6.13	136.24	126.20
16	be	101	V7N	C28-C27-C26	-6.01	109.89	126.36
17	C	404	HEC	CBB-CAB-C3B	-5.99	115.45	127.43
17	C	403	HEC	CBB-CAB-C3B	-5.99	115.47	127.43
16	BX	1001	V7N	C28-C27-C26	-5.88	110.24	126.36
21	af	102	CD4	O2-C14-C13	5.70	123.81	111.48
14	AC	103	BCL	C4D-CHA-C1A	5.66	128.00	121.24
14	AP	103	BCL	C4D-CHA-C1A	5.66	128.00	121.24
14	AV	101	BCL	C4D-CHA-C1A	5.65	127.98	121.24
14	AJ	102	BCL	C4D-CHA-C1A	5.62	127.94	121.24
21	aj	102	CD4	O2-C14-C13	5.60	123.59	111.48
21	H1	104	CD4	O2-C14-C13	5.60	123.59	111.48
14	AC	101	BCL	C4D-CHA-C1A	5.56	127.88	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AN	101	BCL	C4D-CHA-C1A	5.55	127.86	121.24
14	BP	1005	BCL	C4D-CHA-C1A	5.53	127.84	121.24
14	AL	101	BCL	C4D-CHA-C1A	5.52	127.83	121.24
14	AH	101	BCL	C4D-CHA-C1A	5.52	127.83	121.24
14	AX	102	BCL	C4D-CHA-C1A	5.50	127.81	121.24
23	ao	101	MQ8	C11-C3-C4	-5.50	112.79	118.58
14	AN	104	BCL	C4D-CHA-C1A	5.50	127.80	121.24
16	bj	101	V7N	C29-C28-C27	-5.48	107.32	123.20
14	BC	104	BCL	C4D-CHA-C1A	5.47	127.77	121.24
14	BN	103	BCL	C4D-CHA-C1A	5.47	127.77	121.24
14	BU	1004	BCL	C4D-CHA-C1A	5.47	127.76	121.24
14	an	1001	BCL	C4D-CHA-C1A	5.46	127.75	121.24
16	bp	101	V7N	C28-C27-C26	-5.45	111.41	126.36
14	AM	102	BCL	C4D-CHA-C1A	5.45	127.75	121.24
17	C	402	HEC	CBC-CAC-C3C	-5.45	116.55	127.43
14	bi	104	BCL	C4D-CHA-C1A	5.44	127.73	121.24
14	BO	1004	BCL	C4D-CHA-C1A	5.44	127.73	121.24
14	M	405	BCL	C4D-CHA-C1A	5.43	127.72	121.24
14	ao	102	BCL	C4D-CHA-C1A	5.43	127.72	121.24
14	AA	1002	BCL	C4D-CHA-C1A	5.43	127.72	121.24
14	BD	105	BCL	C4D-CHA-C1A	5.43	127.72	121.24
14	bk	102	BCL	C4D-CHA-C1A	5.42	127.71	121.24
14	ae	102	BCL	C4D-CHA-C1A	5.42	127.71	121.24
14	AX	103	BCL	C4D-CHA-C1A	5.41	127.70	121.24
14	BM	1002	BCL	C4D-CHA-C1A	5.41	127.70	121.24
14	ag	1001	BCL	C4D-CHA-C1A	5.41	127.70	121.24
14	BF	102	BCL	C4D-CHA-C1A	5.40	127.69	121.24
16	AE	1005	V7N	C28-C27-C26	-5.40	111.55	126.36
14	BV	1005	BCL	C4D-CHA-C1A	5.40	127.69	121.24
14	BX	1002	BCL	C4D-CHA-C1A	5.40	127.68	121.24
14	be	105	BCL	C4D-CHA-C1A	5.40	127.68	121.24
14	BW	1003	BCL	C4D-CHA-C1A	5.39	127.68	121.24
14	BR	1004	BCL	C4D-CHA-C1A	5.39	127.68	121.24
14	BI	1003	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	aa	1001	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	al	1001	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	AS	102	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	BB	103	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	BT	103	BCL	C4D-CHA-C1A	5.39	127.67	121.24
14	BG	1004	BCL	C4D-CHA-C1A	5.38	127.66	121.24
14	AQ	101	BCL	C4D-CHA-C1A	5.38	127.66	121.24
14	BS	1003	BCL	C4D-CHA-C1A	5.37	127.66	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AW	101	BCL	C4D-CHA-C1A	5.37	127.65	121.24
14	BJ	1002	BCL	C4D-CHA-C1A	5.37	127.65	121.24
14	BA	103	BCL	C4D-CHA-C1A	5.37	127.64	121.24
14	AG	101	BCL	C4D-CHA-C1A	5.36	127.64	121.24
14	BK	1006	BCL	C4D-CHA-C1A	5.36	127.63	121.24
14	bm	104	BCL	C4D-CHA-C1A	5.35	127.62	121.24
14	bl	104	BCL	C4D-CHA-C1A	5.35	127.62	121.24
14	bc	102	BCL	C4D-CHA-C1A	5.35	127.62	121.24
14	am	1001	BCL	C4D-CHA-C1A	5.34	127.61	121.24
14	af	101	BCL	C4D-CHA-C1A	5.33	127.61	121.24
14	ai	101	BCL	C4D-CHA-C1A	5.33	127.60	121.24
14	bj	103	BCL	C4D-CHA-C1A	5.33	127.60	121.24
14	BL	1003	BCL	C4D-CHA-C1A	5.33	127.60	121.24
14	bo	103	BCL	C4D-CHA-C1A	5.32	127.59	121.24
14	L	1002	BCL	C4D-CHA-C1A	5.32	127.58	121.24
14	AN	102	BCL	C4D-CHA-C1A	5.31	127.58	121.24
14	ad	1001	BCL	C4D-CHA-C1A	5.31	127.58	121.24
14	aj	103	BCL	C4D-CHA-C1A	5.31	127.58	121.24
14	BQ	1003	BCL	C4D-CHA-C1A	5.31	127.58	121.24
14	ab	102	BCL	C4D-CHA-C1A	5.31	127.57	121.24
14	bg	105	BCL	C4D-CHA-C1A	5.31	127.57	121.24
14	AB	1001	BCL	C4D-CHA-C1A	5.30	127.57	121.24
14	BH	1005	BCL	C4D-CHA-C1A	5.30	127.57	121.24
14	ah	1001	BCL	C4D-CHA-C1A	5.30	127.56	121.24
14	bh	105	BCL	C4D-CHA-C1A	5.30	127.56	121.24
14	AF	1001	BCL	C4D-CHA-C1A	5.29	127.55	121.24
14	bp	102	BCL	C4D-CHA-C1A	5.29	127.55	121.24
14	AQ	102	BCL	C4D-CHA-C1A	5.28	127.55	121.24
14	ap	1001	BCL	C4D-CHA-C1A	5.28	127.54	121.24
14	bf	103	BCL	C4D-CHA-C1A	5.28	127.54	121.24
14	bn	103	BCL	C4D-CHA-C1A	5.27	127.53	121.24
14	AE	1001	BCL	C4D-CHA-C1A	5.26	127.52	121.24
14	AI	103	BCL	C4D-CHA-C1A	5.26	127.52	121.24
14	AR	101	BCL	C4D-CHA-C1A	5.26	127.51	121.24
14	ak	1001	BCL	C4D-CHA-C1A	5.26	127.51	121.24
16	BW	1001	V7N	C29-C28-C27	-5.24	108.01	123.20
14	bb	104	BCL	C4D-CHA-C1A	5.24	127.50	121.24
14	AH	103	BCL	C4D-CHA-C1A	5.24	127.49	121.24
17	C	401	HEC	CBB-CAB-C3B	-5.23	116.98	127.43
14	ba	103	BCL	C4D-CHA-C1A	5.23	127.48	121.24
14	AL	103	BCL	C4D-CHA-C1A	5.20	127.45	121.24
14	AS	104	BCL	C4D-CHA-C1A	5.19	127.43	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AD	102	BCL	C4D-CHA-C1A	5.18	127.42	121.24
14	bd	102	BCL	C4D-CHA-C1A	5.17	127.41	121.24
14	AI	102	BCL	C4D-CHA-C1A	5.17	127.41	121.24
14	AU	102	BCL	C4D-CHA-C1A	5.16	127.40	121.24
14	AJ	101	BCL	C4D-CHA-C1A	5.16	127.39	121.24
14	BE	104	BCL	C4D-CHA-C1A	5.15	127.39	121.24
14	M	408	BCL	C4D-CHA-C1A	5.15	127.38	121.24
14	AK	101	BCL	C4D-CHA-C1A	5.15	127.38	121.24
14	AT	101	BCL	C4D-CHA-C1A	5.15	127.38	121.24
14	ac	1001	BCL	C4D-CHA-C1A	5.14	127.38	121.24
14	AO	1002	BCL	C4D-CHA-C1A	5.13	127.36	121.24
14	AP	102	BCL	C4D-CHA-C1A	5.11	127.33	121.24
14	AS	103	BCL	C4D-CHA-C1A	5.11	127.33	121.24
14	AC	102	BCL	C4D-CHA-C1A	5.09	127.32	121.24
14	AM	101	BCL	C4D-CHA-C1A	5.09	127.32	121.24
16	BC	101	V7N	C28-C27-C26	-5.07	112.46	126.36
16	bd	101	V7N	C29-C28-C27	-5.04	108.59	123.20
14	AK	102	BCL	C4D-CHA-C1A	5.03	127.24	121.24
14	AR	102	BCL	C4D-CHA-C1A	5.01	127.22	121.24
16	ba	101	V7N	C28-C27-C26	-5.00	112.65	126.36
16	bo	102	V7N	C28-C27-C26	-5.00	112.66	126.36
14	AE	1004	BCL	C4D-CHA-C1A	4.98	127.18	121.24
14	AV	102	BCL	C4D-CHA-C1A	4.97	127.17	121.24
14	AG	102	BCL	C4D-CHA-C1A	4.96	127.17	121.24
14	AV	103	BCL	C4D-CHA-C1A	4.93	127.12	121.24
16	bk	101	V7N	C29-C28-C27	-4.89	109.05	123.20
14	AU	103	BCL	C4D-CHA-C1A	4.88	127.07	121.24
14	AA	1001	BCL	C4D-CHA-C1A	4.86	127.04	121.24
14	L	1010	BCL	C4D-CHA-C1A	4.85	127.02	121.24
16	bi	101	V7N	C29-C28-C27	-4.83	109.19	123.20
16	BM	1001	V7N	C28-C27-C26	-4.83	113.12	126.36
16	BE	101	V7N	C29-C28-C27	-4.83	109.21	123.20
16	bl	102	V7N	C29-C28-C27	-4.82	109.23	123.20
14	AE	1003	BCL	C4D-CHA-C1A	4.82	126.99	121.24
16	BP	1001	V7N	C28-C27-C26	-4.79	113.23	126.36
15	AT	102	LMT	C1-O1'-C1'	4.78	121.84	113.68
16	bc	101	V7N	C29-C28-C27	-4.78	109.36	123.20
14	AB	1002	BCL	C4D-CHA-C1A	4.77	126.94	121.24
16	bf	101	V7N	C28-C27-C26	-4.76	113.31	126.36
14	AI	103	BCL	C1-O2A-CGA	4.75	128.16	116.65
14	AS	104	BCL	C1-O2A-CGA	4.74	128.14	116.65
21	M	402	CD4	O2-C14-C13	4.73	121.72	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BJ	1001	V7N	C28-C27-C26	-4.69	113.51	126.36
16	BO	1001	V7N	C29-C28-C27	-4.67	109.66	123.20
16	BR	1001	V7N	C28-C27-C26	-4.66	113.60	126.36
18	C	405	V75	O3-C3A-C3B	4.62	119.32	111.09
16	bn	102	V7N	C29-C28-C27	-4.59	109.89	123.20
16	BA	101	V7N	C29-C28-C27	-4.59	109.91	123.20
16	BB	101	V7N	C29-C28-C27	-4.58	109.94	123.20
16	BK	1001	V7N	C28-C27-C26	-4.55	113.88	126.36
20	bg	102	0V9	C2-O2-C10	4.54	128.67	117.80
18	M	409	V75	O3-C3A-C3B	4.53	119.17	111.09
16	BH	1001	V7N	C28-C27-C26	-4.52	113.96	126.36
16	BG	1001	V7N	C28-C27-C26	-4.52	113.96	126.36
16	BQ	1001	V7N	C29-C28-C27	-4.51	110.12	123.20
18	C	405	V75	O2-C2A-C2B	4.48	119.08	111.09
21	ae	101	CD4	O2-C14-C13	4.47	121.16	111.48
16	BL	1001	V7N	C28-C27-C26	-4.47	114.10	126.36
16	BD	101	V7N	C28-C27-C26	-4.45	114.15	126.36
16	bm	101	V7N	C29-C28-C27	-4.44	110.34	123.20
16	bh	102	V7N	C29-C28-C27	-4.43	110.36	123.20
16	BV	1001	V7N	C29-C28-C27	-4.43	110.37	123.20
16	BV	1001	V7N	C28-C27-C26	-4.42	114.23	126.36
16	ba	101	V7N	C2-C3-C4	-4.41	118.71	124.91
16	bh	102	V7N	C28-C27-C26	-4.38	114.36	126.36
16	BS	1001	V7N	C28-C27-C26	-4.36	114.41	126.36
14	AL	101	BCL	C1-C2-C3	-4.34	119.09	126.20
16	AO	1001	V7N	C28-C27-C26	-4.33	114.49	126.36
16	BI	1001	V7N	C28-C27-C26	-4.30	114.57	126.36
18	M	409	V75	O2-C2A-C2B	4.30	118.75	111.09
16	BM	1001	V7N	C29-C28-C27	-4.29	110.76	123.20
16	BD	101	V7N	C29-C28-C27	-4.29	110.78	123.20
16	BG	1001	V7N	C29-C28-C27	-4.27	110.83	123.20
16	BJ	1001	V7N	C29-C28-C27	-4.25	110.88	123.20
16	AO	1001	V7N	C29-C28-C27	-4.20	111.03	123.20
16	BB	101	V7N	C28-C27-C26	-4.15	114.99	126.36
16	BS	1001	V7N	C29-C28-C27	-4.12	111.26	123.20
16	bb	101	V7N	C28-C27-C26	-4.12	115.07	126.36
25	M	406	BPH	C4D-ND-C1D	-4.12	103.94	108.87
16	BQ	1001	V7N	C28-C27-C26	-4.11	115.09	126.36
15	AI	101	LMT	C3'-C4'-C5'	-4.07	101.90	110.93
16	BO	1001	V7N	C28-C27-C26	-4.07	115.21	126.36
16	BH	1001	V7N	C29-C28-C27	-4.06	111.43	123.20
25	L	1009	BPH	C4D-ND-C1D	-4.05	104.01	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	bn	102	V7N	C28-C27-C26	-4.05	115.26	126.36
16	BR	1001	V7N	C7-C6-C5	-4.04	121.62	127.28
16	bl	102	V7N	C28-C27-C26	-4.02	115.33	126.36
16	ba	101	V7N	C29-C28-C27	-3.98	111.68	123.20
16	AO	1001	V7N	C7-C6-C5	-3.97	121.71	127.28
14	AN	104	BCL	CHD-C1D-ND	-3.97	119.21	124.80
14	AB	1002	BCL	CHD-C1D-ND	-3.96	119.22	124.80
14	ac	1001	BCL	C4A-NA-C1A	3.94	108.48	106.68
16	ba	101	V7N	C27-C26-C25	3.94	123.97	118.49
14	M	408	BCL	CHD-C1D-ND	-3.89	119.33	124.80
16	BL	1001	V7N	C29-C28-C27	-3.87	111.98	123.20
14	M	405	BCL	C4A-NA-C1A	3.86	108.44	106.68
14	AQ	101	BCL	C1-C2-C3	-3.85	119.89	126.20
14	AV	103	BCL	CHD-C1D-ND	-3.85	119.38	124.80
16	ba	101	V7N	C38-C26-C27	-3.84	112.22	118.09
14	L	1002	BCL	C1D-ND-C4D	-3.84	103.62	106.31
21	ae	101	CD4	O3-C16-C15	3.83	119.44	108.40
16	bm	101	V7N	C28-C27-C26	-3.82	115.88	126.36
16	AE	1005	V7N	C15-C14-C13	-3.82	121.92	127.28
14	AG	101	BCL	CHD-C1D-ND	-3.81	119.44	124.80
23	ao	101	MQ8	C12-C11-C3	3.81	121.47	112.08
16	BU	1001	V7N	C7-C6-C5	3.81	132.62	127.28
16	BA	101	V7N	C28-C27-C26	-3.81	115.93	126.36
14	AB	1002	BCL	C1D-ND-C4D	-3.79	103.65	106.31
16	BR	1001	V7N	C29-C28-C27	-3.77	112.28	123.20
14	L	1002	BCL	CHD-C1D-ND	-3.75	119.52	124.80
14	AE	1004	BCL	CHD-C1D-ND	-3.73	119.55	124.80
15	BI	1006	LMT	C1-O1'-C1'	3.72	120.04	113.68
14	AX	102	BCL	CHD-C1D-ND	-3.72	119.57	124.80
14	AP	103	BCL	C4A-NA-C1A	3.71	108.37	106.68
14	AR	101	BCL	C4A-NA-C1A	3.71	108.37	106.68
14	ae	102	BCL	C4A-NA-C1A	3.71	108.37	106.68
15	BW	1005	LMT	C3'-C4'-C5'	-3.69	102.74	110.93
14	M	408	BCL	C1D-ND-C4D	-3.69	103.72	106.31
14	AI	103	BCL	CHD-C1D-ND	-3.68	119.62	124.80
14	bp	102	BCL	C4A-NA-C1A	3.67	108.35	106.68
16	BI	1001	V7N	C29-C28-C27	-3.67	112.58	123.20
14	BH	1005	BCL	C4A-NA-C1A	3.66	108.35	106.68
14	aj	103	BCL	C4A-NA-C1A	3.66	108.35	106.68
14	ah	1001	BCL	C4A-NA-C1A	3.66	108.35	106.68
14	BL	1003	BCL	C4A-NA-C1A	3.65	108.34	106.68
14	AH	103	BCL	C4A-NA-C1A	3.64	108.34	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AH	101	BCL	CHD-C1D-ND	-3.64	119.69	124.80
14	AA	1002	BCL	CHD-C1D-ND	-3.63	119.69	124.80
14	AX	102	BCL	C4A-NA-C1A	3.63	108.33	106.68
14	aa	1001	BCL	C4A-NA-C1A	3.60	108.32	106.68
14	BG	1004	BCL	CHD-C1D-ND	-3.60	119.74	124.80
14	ai	101	BCL	C4A-NA-C1A	3.59	108.32	106.68
25	L	1009	BPH	C3D-C4D-ND	3.59	112.30	107.71
14	AH	101	BCL	C1D-ND-C4D	-3.59	103.80	106.31
14	AU	103	BCL	C4A-NA-C1A	3.58	108.31	106.68
14	AK	101	BCL	CHD-C1D-ND	-3.58	119.76	124.80
14	BR	1004	BCL	CHD-C1D-ND	-3.58	119.76	124.80
14	AL	103	BCL	C4A-NA-C1A	3.58	108.31	106.68
14	AV	101	BCL	C4A-NA-C1A	3.58	108.31	106.68
16	BC	101	V7N	C29-C28-C27	-3.58	112.84	123.20
14	AA	1001	BCL	C4A-NA-C1A	3.57	108.31	106.68
14	BN	103	BCL	CHD-C1D-ND	-3.57	119.78	124.80
14	AI	103	BCL	C1D-ND-C4D	-3.56	103.81	106.31
14	BC	104	BCL	CHD-C1D-ND	-3.56	119.80	124.80
15	AA	1003	LMT	C3'-C4'-C5'	-3.56	103.05	110.93
15	BN	102	LMT	C1-O1'-C1'	3.55	119.75	113.68
14	BJ	1002	BCL	C4A-NA-C1A	3.55	108.30	106.68
16	bc	101	V7N	C28-C27-C26	-3.55	116.62	126.36
14	AC	101	BCL	CHD-C1D-ND	-3.55	119.81	124.80
14	al	1001	BCL	C4A-NA-C1A	3.55	108.30	106.68
14	BJ	1002	BCL	CHD-C1D-ND	-3.55	119.81	124.80
14	AL	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
14	AG	102	BCL	C4A-NA-C1A	3.53	108.29	106.68
14	BQ	1003	BCL	CHD-C1D-ND	-3.53	119.83	124.80
16	bj	101	V7N	C28-C27-C26	-3.52	116.70	126.36
14	AS	102	BCL	CHD-C1D-ND	-3.52	119.84	124.80
14	AC	103	BCL	CHD-C1D-ND	-3.52	119.84	124.80
14	ad	1001	BCL	C4A-NA-C1A	3.52	108.29	106.68
14	AQ	101	BCL	CHD-C1D-ND	-3.52	119.85	124.80
14	BP	1005	BCL	CHD-C1D-ND	-3.52	119.85	124.80
14	aj	103	BCL	C1D-ND-C4D	-3.52	103.84	106.31
14	AQ	101	BCL	CAA-CBA-CGA	3.51	123.19	113.21
14	BC	104	BCL	C4A-NA-C1A	3.51	108.28	106.68
14	BU	1004	BCL	CHD-C1D-ND	-3.51	119.86	124.80
14	L	1010	BCL	CHD-C1D-ND	-3.51	119.87	124.80
14	BF	102	BCL	CHD-C1D-ND	-3.51	119.87	124.80
14	BM	1002	BCL	CHD-C1D-ND	-3.51	119.87	124.80
14	AN	101	BCL	C4A-NA-C1A	3.50	108.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BW	1001	V7N	C28-C27-C26	-3.50	116.76	126.36
14	bc	102	BCL	C4A-NA-C1A	3.50	108.28	106.68
14	BS	1003	BCL	CHD-C1D-ND	-3.50	119.88	124.80
15	AP	101	LMT	O1'-C1'-C2'	3.50	113.59	108.27
14	am	1001	BCL	C4A-NA-C1A	3.50	108.27	106.68
16	BX	1001	V7N	C15-C14-C13	-3.49	122.38	127.28
14	AX	103	BCL	CHA-C1A-NA	-3.49	118.48	126.39
14	BN	103	BCL	C1D-ND-C4D	-3.49	103.86	106.31
16	BH	1001	V7N	C7-C6-C5	-3.49	122.38	127.28
14	AS	104	BCL	CHD-C1D-ND	-3.49	119.89	124.80
14	BH	1005	BCL	CHD-C1D-ND	-3.49	119.89	124.80
14	AU	103	BCL	CHD-C1D-ND	-3.49	119.89	124.80
14	AI	103	BCL	C1-C2-C3	-3.49	120.48	126.20
14	ak	1001	BCL	C4A-NA-C1A	3.49	108.27	106.68
14	AD	102	BCL	C4A-NA-C1A	3.49	108.27	106.68
14	AJ	102	BCL	CHD-C1D-ND	-3.48	119.90	124.80
14	AS	104	BCL	C1D-ND-C4D	-3.48	103.87	106.31
14	AP	103	BCL	CHD-C1D-ND	-3.48	119.90	124.80
14	AE	1004	BCL	C4A-NA-C1A	3.48	108.27	106.68
14	AK	101	BCL	C1D-ND-C4D	-3.48	103.87	106.31
14	M	405	BCL	CHD-C1D-ND	-3.47	119.91	124.80
14	aj	103	BCL	CHD-C1D-ND	-3.47	119.92	124.80
21	aj	102	CD4	O16-C46-C47	3.47	118.99	111.48
14	AH	101	BCL	C4A-NA-C1A	3.47	108.26	106.68
14	BK	1006	BCL	CHD-C1D-ND	-3.47	119.92	124.80
14	ai	101	BCL	CHD-C1D-ND	-3.47	119.92	124.80
14	ag	1001	BCL	C4A-NA-C1A	3.47	108.26	106.68
14	BI	1003	BCL	CHD-C1D-ND	-3.46	119.93	124.80
14	BO	1004	BCL	CHD-C1D-ND	-3.46	119.93	124.80
14	BR	1004	BCL	C1D-ND-C4D	-3.46	103.88	106.31
14	BC	104	BCL	C1D-ND-C4D	-3.46	103.89	106.31
14	BB	103	BCL	CHD-C1D-ND	-3.46	119.94	124.80
14	AR	102	BCL	CHD-C1D-ND	-3.46	119.94	124.80
14	ab	102	BCL	C4A-NA-C1A	3.46	108.26	106.68
14	be	105	BCL	CHD-C1D-ND	-3.46	119.94	124.80
14	BE	104	BCL	C4A-NA-C1A	3.45	108.25	106.68
14	AF	1001	BCL	C4A-NA-C1A	3.45	108.25	106.68
17	C	402	HEC	C4D-ND-C1D	3.45	111.44	105.82
14	BW	1003	BCL	CHD-C1D-ND	-3.45	119.95	124.80
14	BG	1004	BCL	C1D-ND-C4D	-3.44	103.89	106.31
14	ad	1001	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	ap	1001	BCL	C4A-NA-C1A	3.44	108.25	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AN	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	am	1001	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	ap	1001	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	AJ	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
14	AK	102	BCL	C4A-NA-C1A	3.44	108.25	106.68
14	AU	102	BCL	C4A-NA-C1A	3.44	108.25	106.68
21	ae	101	CD4	O16-C46-C47	3.44	118.92	111.48
15	BD	103	LMT	C1-O1'-C1'	3.43	119.55	113.68
14	AR	102	BCL	C4A-NA-C1A	3.43	108.25	106.68
14	AX	102	BCL	C1D-ND-C4D	-3.43	103.90	106.31
14	ag	1001	BCL	CHD-C1D-ND	-3.43	119.97	124.80
14	af	101	BCL	C4A-NA-C1A	3.43	108.24	106.68
16	BB	101	V7N	C15-C14-C13	-3.43	122.47	127.28
14	BL	1003	BCL	CHD-C1D-ND	-3.43	119.98	124.80
14	bc	102	BCL	CHD-C1D-ND	-3.42	119.98	124.80
14	AJ	102	BCL	C1-O2A-CGA	3.42	124.94	116.65
21	H1	102	CD4	C15-O2-C14	3.42	125.99	117.80
14	al	1001	BCL	CHD-C1D-ND	-3.42	119.99	124.80
14	AL	101	BCL	C1D-ND-C4D	-3.42	103.91	106.31
14	AI	102	BCL	C4A-NA-C1A	3.42	108.24	106.68
14	BT	103	BCL	CHD-C1D-ND	-3.42	119.99	124.80
14	bj	103	BCL	CHD-C1D-ND	-3.42	119.99	124.80
15	bb	102	LMT	C3'-C4'-C5'	-3.42	103.35	110.93
14	AT	101	BCL	C4A-NA-C1A	3.42	108.24	106.68
14	an	1001	BCL	CHD-C1D-ND	-3.42	120.00	124.80
16	AE	1005	V7N	C29-C28-C27	-3.41	113.31	123.20
14	AM	102	BCL	CHD-C1D-ND	-3.41	120.00	124.80
16	BM	1001	V7N	C38-C26-C27	-3.41	112.87	118.09
14	BA	103	BCL	CHD-C1D-ND	-3.41	120.00	124.80
15	AC	104	LMT	C1-O1'-C1'	3.41	119.51	113.68
14	BD	105	BCL	CHD-C1D-ND	-3.41	120.01	124.80
14	AM	102	BCL	C1D-ND-C4D	-3.41	103.92	106.31
14	AM	101	BCL	C4A-NA-C1A	3.41	108.23	106.68
14	BX	1002	BCL	C4A-NA-C1A	3.41	108.23	106.68
14	BN	103	BCL	C4A-NA-C1A	3.40	108.23	106.68
16	BE	101	V7N	C28-C27-C26	-3.40	117.03	126.36
14	AV	101	BCL	CHD-C1D-ND	-3.40	120.01	124.80
14	ae	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
14	ao	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
14	AQ	101	BCL	C1D-ND-C4D	-3.40	103.93	106.31
15	L	1004	LMT	C1-O1'-C1'	3.40	119.48	113.68
14	BS	1003	BCL	C1-C2-C3	-3.40	120.63	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	aa	1001	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	ac	1001	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	af	101	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	BF	102	BCL	C1D-ND-C4D	-3.39	103.93	106.31
14	AO	1002	BCL	C4A-NA-C1A	3.39	108.23	106.68
14	BX	1002	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	bk	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	BI	1003	BCL	C4A-NA-C1A	3.39	108.23	106.68
14	ah	1001	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	BT	103	BCL	C4A-NA-C1A	3.39	108.22	106.68
14	AD	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80
14	aa	1001	BCL	C1D-ND-C4D	-3.39	103.94	106.31
17	C	401	HEC	C4D-ND-C1D	3.38	111.34	105.82
14	BV	1005	BCL	CHD-C1D-ND	-3.38	120.04	124.80
14	ad	1001	BCL	C1D-ND-C4D	-3.38	103.94	106.31
14	bg	105	BCL	CHD-C1D-ND	-3.38	120.05	124.80
14	ac	1001	BCL	C1D-ND-C4D	-3.37	103.95	106.31
14	AE	1003	BCL	CHD-C1D-ND	-3.37	120.06	124.80
14	bn	103	BCL	CHD-C1D-ND	-3.37	120.06	124.80
14	AA	1002	BCL	C1D-ND-C4D	-3.37	103.95	106.31
14	BQ	1003	BCL	C1D-ND-C4D	-3.37	103.95	106.31
14	ao	102	BCL	C1D-ND-C4D	-3.37	103.95	106.31
14	bf	103	BCL	CHD-C1D-ND	-3.37	120.06	124.80
14	bo	103	BCL	CHD-C1D-ND	-3.37	120.06	124.80
14	AG	101	BCL	C1D-ND-C4D	-3.36	103.95	106.31
14	M	405	BCL	C1D-ND-C4D	-3.36	103.95	106.31
14	bb	104	BCL	CHD-C1D-ND	-3.36	120.07	124.80
14	AQ	102	BCL	C4A-NA-C1A	3.36	108.21	106.68
14	ak	1001	BCL	C1D-ND-C4D	-3.36	103.95	106.31
14	ab	102	BCL	CHD-C1D-ND	-3.36	120.07	124.80
14	AN	101	BCL	C1D-ND-C4D	-3.36	103.95	106.31
14	AW	101	BCL	CHD-C1D-ND	-3.36	120.08	124.80
16	BM	1001	V7N	C27-C26-C25	3.36	123.17	118.49
14	bh	105	BCL	CHD-C1D-ND	-3.35	120.08	124.80
16	AS	105	V7N	C20-C21-C22	-3.35	122.97	127.69
14	BE	104	BCL	CHD-C1D-ND	-3.35	120.08	124.80
14	ap	1001	BCL	C1D-ND-C4D	-3.35	103.96	106.31
14	BI	1003	BCL	C1D-ND-C4D	-3.35	103.96	106.31
14	bd	102	BCL	CHD-C1D-ND	-3.35	120.09	124.80
14	AS	104	BCL	C4A-NA-C1A	3.35	108.21	106.68
14	an	1001	BCL	C1D-ND-C4D	-3.35	103.96	106.31
14	BJ	1002	BCL	C1D-ND-C4D	-3.35	103.97	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	ab	102	BCL	C1D-ND-C4D	-3.35	103.97	106.31
14	BM	1002	BCL	C1D-ND-C4D	-3.34	103.97	106.31
16	ba	101	V7N	C3-C4-C5	3.34	130.94	125.89
14	bp	102	BCL	CHD-C1D-ND	-3.34	120.11	124.80
14	am	1001	BCL	C1D-ND-C4D	-3.34	103.97	106.31
14	AU	103	BCL	C1D-ND-C4D	-3.34	103.97	106.31
14	BH	1005	BCL	C1D-ND-C4D	-3.33	103.97	106.31
14	ag	1001	BCL	C1D-ND-C4D	-3.33	103.97	106.31
14	AF	1001	BCL	CHD-C1D-ND	-3.33	120.11	124.80
14	bl	104	BCL	CHD-C1D-ND	-3.33	120.11	124.80
14	ak	1001	BCL	CHD-C1D-ND	-3.33	120.12	124.80
14	bi	104	BCL	CHD-C1D-ND	-3.33	120.12	124.80
14	af	101	BCL	C1D-ND-C4D	-3.33	103.98	106.31
14	bj	103	BCL	C1D-ND-C4D	-3.32	103.98	106.31
14	ai	101	BCL	C1D-ND-C4D	-3.32	103.98	106.31
14	ba	103	BCL	CHD-C1D-ND	-3.32	120.13	124.80
17	C	403	HEC	C4D-ND-C1D	3.32	111.23	105.82
14	BP	1005	BCL	C1D-ND-C4D	-3.32	103.98	106.31
14	bc	102	BCL	C1D-ND-C4D	-3.32	103.98	106.31
14	AS	103	BCL	C4A-NA-C1A	3.32	108.19	106.68
16	bk	101	V7N	C28-C27-C26	-3.31	117.28	126.36
17	C	403	HEC	CMC-C2C-C1C	-3.31	120.37	125.42
16	BM	1001	V7N	C15-C14-C13	-3.31	122.63	127.28
14	ah	1001	BCL	C1D-ND-C4D	-3.31	103.99	106.31
16	bd	101	V7N	O44-C40-O45	-3.31	116.02	123.90
14	AH	103	BCL	CHD-C1D-ND	-3.31	120.15	124.80
14	al	1001	BCL	C1D-ND-C4D	-3.31	103.99	106.31
15	BG	1002	LMT	C1-O1'-C1'	3.31	119.33	113.68
14	AE	1004	BCL	C1D-ND-C4D	-3.31	103.99	106.31
14	BS	1003	BCL	C1D-ND-C4D	-3.30	103.99	106.31
14	AC	102	BCL	C4A-NA-C1A	3.30	108.19	106.68
14	AJ	101	BCL	C4A-NA-C1A	3.30	108.19	106.68
14	ae	102	BCL	C1D-ND-C4D	-3.30	104.00	106.31
14	BD	105	BCL	C1D-ND-C4D	-3.30	104.00	106.31
14	AM	101	BCL	CHD-C1D-ND	-3.30	120.16	124.80
14	AS	103	BCL	CHD-C1D-ND	-3.30	120.16	124.80
14	AI	102	BCL	CHD-C1D-ND	-3.29	120.17	124.80
14	AE	1001	BCL	C4A-NA-C1A	3.29	108.18	106.68
14	AW	101	BCL	C4A-NA-C1A	3.29	108.18	106.68
14	BU	1004	BCL	C1D-ND-C4D	-3.29	104.00	106.31
16	ba	101	V7N	O44-C40-O45	-3.29	116.06	123.90
14	AA	1001	BCL	CHD-C1D-ND	-3.29	120.17	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	401	HEC	CMC-C2C-C1C	-3.29	120.41	125.42
14	AN	102	BCL	CHD-C1D-ND	-3.29	120.18	124.80
14	M	405	BCL	CHA-C1A-NA	-3.28	118.95	126.39
14	BT	103	BCL	C1D-ND-C4D	-3.28	104.01	106.31
14	AT	101	BCL	CHD-C1D-ND	-3.28	120.18	124.80
14	BL	1003	BCL	C1D-ND-C4D	-3.28	104.01	106.31
14	BO	1004	BCL	C4A-NA-C1A	3.28	108.18	106.68
14	bi	104	BCL	C4A-NA-C1A	3.28	108.18	106.68
15	BK	1005	LMT	C1-O1'-C1'	3.28	119.28	113.68
14	AU	102	BCL	CHD-C1D-ND	-3.28	120.19	124.80
16	BO	1001	V7N	C7-C6-C5	-3.28	122.68	127.28
14	AG	102	BCL	CHD-C1D-ND	-3.28	120.19	124.80
16	bd	101	V7N	C28-C27-C26	-3.28	117.38	126.36
16	bn	102	V7N	O44-C40-O45	-3.27	116.10	123.90
14	AB	1001	BCL	CHD-C1D-ND	-3.27	120.19	124.80
25	M	406	BPH	C3D-C4D-ND	3.27	111.90	107.71
15	AT	102	LMT	C3'-C4'-C5'	-3.27	103.68	110.93
14	bc	102	BCL	C1-O2A-CGA	3.27	124.57	116.65
14	AC	102	BCL	CHD-C1D-ND	-3.27	120.20	124.80
14	AO	1002	BCL	CHD-C1D-ND	-3.27	120.20	124.80
14	AR	101	BCL	CHD-C1D-ND	-3.27	120.20	124.80
14	bm	104	BCL	CHD-C1D-ND	-3.27	120.20	124.80
14	AP	103	BCL	C1D-ND-C4D	-3.27	104.02	106.31
14	BK	1006	BCL	C1D-ND-C4D	-3.26	104.02	106.31
14	L	1010	BCL	C1D-ND-C4D	-3.26	104.02	106.31
14	BW	1003	BCL	C4A-NA-C1A	3.26	108.17	106.68
14	AE	1001	BCL	CHD-C1D-ND	-3.26	120.22	124.80
14	bl	104	BCL	C1D-ND-C4D	-3.26	104.03	106.31
14	bp	102	BCL	C1D-ND-C4D	-3.26	104.03	106.31
14	BF	102	BCL	C4A-NA-C1A	3.25	108.16	106.68
14	AQ	102	BCL	CHD-C1D-ND	-3.25	120.22	124.80
14	AQ	102	BCL	CHA-C1A-NA	-3.25	119.03	126.39
16	BE	101	V7N	O44-C40-O45	-3.25	116.16	123.90
14	AB	1001	BCL	C4A-NA-C1A	3.25	108.16	106.68
14	AL	101	BCL	C4A-NA-C1A	3.25	108.16	106.68
21	M	402	CD4	O16-C46-C47	3.25	118.51	111.48
17	C	404	HEC	C4D-ND-C1D	3.25	111.12	105.82
17	C	402	HEC	CMC-C2C-C1C	-3.25	120.47	125.42
14	be	105	BCL	C1D-ND-C4D	-3.25	104.03	106.31
14	BS	1003	BCL	C4A-NA-C1A	3.25	108.16	106.68
14	AV	102	BCL	CHD-C1D-ND	-3.24	120.24	124.80
21	aj	102	CD4	C28-C15-C16	-3.24	104.23	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AK	102	BCL	CHD-C1D-ND	-3.24	120.24	124.80
14	AJ	101	BCL	C1D-ND-C4D	-3.24	104.04	106.31
16	bo	102	V7N	O44-C40-O45	-3.24	116.20	123.90
16	bp	101	V7N	O44-C40-O45	-3.23	116.20	123.90
14	BB	103	BCL	C1D-ND-C4D	-3.23	104.04	106.31
14	BW	1003	BCL	C1D-ND-C4D	-3.23	104.04	106.31
16	BH	1001	V7N	O44-C40-O45	-3.23	116.20	123.90
14	AX	103	BCL	CHD-C1D-ND	-3.23	120.25	124.80
24	L	1006	V7B	O7-C10-C11	3.23	118.47	111.48
14	AL	103	BCL	CHD-C1D-ND	-3.23	120.26	124.80
16	bi	101	V7N	O44-C40-O45	-3.23	116.21	123.90
16	bb	101	V7N	C16-C17-C18	-3.23	122.75	127.28
16	bc	101	V7N	O44-C40-O45	-3.23	116.21	123.90
16	AO	1001	V7N	O44-C40-O45	-3.23	116.22	123.90
16	bm	101	V7N	O44-C40-O45	-3.23	116.22	123.90
22	H1	103	PGW	C02-O01-C1	3.23	125.52	117.80
16	BL	1001	V7N	O44-C40-O45	-3.23	116.22	123.90
14	BX	1002	BCL	C1D-ND-C4D	-3.22	104.05	106.31
14	AV	103	BCL	C1D-ND-C4D	-3.22	104.05	106.31
16	BL	1001	V7N	C15-C14-C13	-3.22	122.76	127.28
16	AE	1005	V7N	O44-C40-O45	-3.22	116.23	123.90
14	AP	102	BCL	CHA-C1A-NA	-3.22	119.10	126.39
16	bb	101	V7N	O44-C40-O45	-3.22	116.23	123.90
16	bi	101	V7N	C28-C27-C26	-3.22	117.54	126.36
16	BA	101	V7N	O44-C40-O45	-3.22	116.24	123.90
14	AK	102	BCL	CHA-C1A-NA	-3.22	119.10	126.39
14	BO	1004	BCL	C1D-ND-C4D	-3.22	104.06	106.31
14	bf	103	BCL	C1D-ND-C4D	-3.21	104.06	106.31
14	AR	102	BCL	C1D-ND-C4D	-3.21	104.06	106.31
14	bh	105	BCL	CHA-C1A-NA	-3.21	119.12	126.39
14	ao	102	BCL	C4A-NA-C1A	3.21	108.14	106.68
14	bi	104	BCL	C1D-ND-C4D	-3.21	104.06	106.31
14	AJ	102	BCL	C4A-NA-C1A	3.21	108.14	106.68
16	BM	1001	V7N	O44-C40-O45	-3.21	116.27	123.90
14	AM	101	BCL	C1D-ND-C4D	-3.21	104.06	106.31
16	BS	1001	V7N	O44-C40-O45	-3.20	116.27	123.90
16	bg	101	V7N	O44-C40-O45	-3.20	116.27	123.90
14	AN	104	BCL	C1D-ND-C4D	-3.20	104.06	106.31
16	BQ	1001	V7N	O44-C40-O45	-3.20	116.28	123.90
14	AJ	102	BCL	C1D-ND-C4D	-3.20	104.07	106.31
14	AE	1001	BCL	CHA-C1A-NA	-3.20	119.14	126.39
16	BK	1001	V7N	O44-C40-O45	-3.20	116.29	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AK	101	BCL	C4A-NA-C1A	3.20	108.14	106.68
14	AB	1001	BCL	CHA-C1A-NA	-3.19	119.16	126.39
14	BQ	1003	BCL	CHA-C1A-NA	-3.19	119.16	126.39
16	BK	1001	V7N	C15-C14-C13	-3.19	122.80	127.28
21	af	102	CD4	C15-O2-C14	-3.19	110.16	117.80
16	BE	101	V7N	C15-C14-C13	-3.19	122.81	127.28
25	L	1009	BPH	OBD-CAD-CBD	-3.19	121.14	125.82
15	BG	1002	LMT	O1'-C1'-C2'	3.19	113.12	108.27
16	BW	1001	V7N	O44-C40-O45	-3.19	116.31	123.90
14	AK	101	BCL	C1-O2A-CGA	3.19	124.37	116.65
14	AQ	101	BCL	C4A-NA-C1A	3.18	108.13	106.68
14	AL	103	BCL	CHA-C1A-NA	-3.18	119.18	126.39
14	BA	103	BCL	CHA-C1A-NA	-3.18	119.18	126.39
16	BV	1001	V7N	O44-C40-O45	-3.18	116.32	123.90
14	AS	102	BCL	C1D-ND-C4D	-3.18	104.08	106.31
14	bd	102	BCL	C1D-ND-C4D	-3.18	104.08	106.31
16	bb	101	V7N	C29-C28-C27	-3.18	113.98	123.20
14	AP	102	BCL	CHD-C1D-ND	-3.18	120.33	124.80
14	AA	1001	BCL	C1D-ND-C4D	-3.18	104.08	106.31
14	BA	103	BCL	C1D-ND-C4D	-3.18	104.08	106.31
16	bf	101	V7N	O44-C40-O45	-3.18	116.33	123.90
16	BJ	1001	V7N	O44-C40-O45	-3.18	116.33	123.90
14	AE	1003	BCL	C1D-ND-C4D	-3.18	104.08	106.31
16	BB	101	V7N	O44-C40-O45	-3.18	116.34	123.90
24	L	1006	V7B	C1-O6-C5	3.18	119.92	113.72
14	AB	1001	BCL	C1D-ND-C4D	-3.18	104.08	106.31
14	ba	103	BCL	C1D-ND-C4D	-3.18	104.08	106.31
14	bb	104	BCL	C1D-ND-C4D	-3.18	104.08	106.31
14	AV	101	BCL	CHA-C1A-NA	-3.18	119.20	126.39
16	BC	101	V7N	O44-C40-O45	-3.17	116.34	123.90
14	AH	103	BCL	CHA-C1A-NA	-3.17	119.21	126.39
16	be	101	V7N	O44-C40-O45	-3.17	116.35	123.90
16	bk	101	V7N	O44-C40-O45	-3.17	116.35	123.90
14	BB	103	BCL	CHA-C1A-NA	-3.17	119.22	126.39
16	BO	1001	V7N	O44-C40-O45	-3.17	116.36	123.90
25	M	406	BPH	OBD-CAD-CBD	-3.17	121.18	125.82
21	aj	102	CD4	O3-C16-C15	-3.16	99.27	108.40
14	AD	102	BCL	C1D-ND-C4D	-3.16	104.09	106.31
14	AU	102	BCL	CHA-C1A-NA	-3.16	119.23	126.39
14	AM	101	BCL	CHA-C1A-NA	-3.16	119.23	126.39
14	AP	102	BCL	C4A-NA-C1A	3.16	108.12	106.68
14	am	1001	BCL	CHA-C1A-NA	-3.16	119.24	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AR	101	BCL	CHA-C1A-NA	-3.16	119.24	126.39
15	BK	1002	LMT	O1'-C1'-C2'	3.16	113.07	108.27
14	AF	1001	BCL	C1D-ND-C4D	-3.16	104.10	106.31
14	AI	102	BCL	CHA-C1A-NA	-3.16	119.24	126.39
14	AN	102	BCL	C4A-NA-C1A	3.16	108.12	106.68
14	AN	102	BCL	CHA-C1A-NA	-3.16	119.25	126.39
16	BP	1001	V7N	O44-C40-O45	-3.16	116.39	123.90
14	AC	102	BCL	CHA-C1A-NA	-3.15	119.25	126.39
16	BI	1001	V7N	O44-C40-O45	-3.15	116.39	123.90
14	AT	101	BCL	CHA-C1A-NA	-3.15	119.25	126.39
14	BV	1005	BCL	CHA-C1A-NA	-3.15	119.26	126.39
16	BG	1001	V7N	O44-C40-O45	-3.15	116.40	123.90
14	bg	105	BCL	C1D-ND-C4D	-3.15	104.10	106.31
14	BV	1005	BCL	C4A-NA-C1A	3.15	108.12	106.68
16	bh	102	V7N	O44-C40-O45	-3.15	116.40	123.90
16	bj	101	V7N	O44-C40-O45	-3.15	116.40	123.90
14	AD	102	BCL	CHA-C1A-NA	-3.15	119.27	126.39
14	AV	101	BCL	C1D-ND-C4D	-3.15	104.11	106.31
14	AW	101	BCL	C1D-ND-C4D	-3.15	104.11	106.31
14	bk	102	BCL	C1D-ND-C4D	-3.15	104.11	106.31
14	AC	102	BCL	C1D-ND-C4D	-3.14	104.11	106.31
14	AA	1001	BCL	CHA-C1A-NA	-3.14	119.27	126.39
14	AM	102	BCL	CHA-C1A-NA	-3.14	119.27	126.39
14	BV	1005	BCL	C1D-ND-C4D	-3.14	104.11	106.31
14	BK	1006	BCL	C4A-NA-C1A	3.14	108.11	106.68
14	bh	105	BCL	C1D-ND-C4D	-3.14	104.11	106.31
14	BU	1004	BCL	CHA-C1A-NA	-3.14	119.28	126.39
14	AC	101	BCL	C1D-ND-C4D	-3.14	104.11	106.31
14	AR	102	BCL	CHA-C1A-NA	-3.14	119.29	126.39
14	BC	104	BCL	CHA-C1A-NA	-3.14	119.29	126.39
14	BI	1003	BCL	C11-C10-C8	3.14	126.39	115.97
16	BR	1001	V7N	O44-C40-O45	-3.14	116.43	123.90
14	AU	103	BCL	CHA-C1A-NA	-3.13	119.29	126.39
14	BE	104	BCL	C1D-ND-C4D	-3.13	104.11	106.31
14	bm	104	BCL	C1D-ND-C4D	-3.13	104.11	106.31
14	bn	103	BCL	C1D-ND-C4D	-3.13	104.11	106.31
16	BU	1001	V7N	O44-C40-O45	-3.13	116.45	123.90
14	AV	103	BCL	C4A-NA-C1A	3.13	108.11	106.68
14	BR	1004	BCL	CHA-C1A-NA	-3.13	119.31	126.39
14	AL	103	BCL	C1D-ND-C4D	-3.13	104.12	106.31
14	AO	1002	BCL	CHA-C1A-NA	-3.13	119.31	126.39
14	AG	102	BCL	C1D-ND-C4D	-3.13	104.12	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AS	103	BCL	CHA-C1A-NA	-3.13	119.31	126.39
14	AW	101	BCL	CHA-C1A-NA	-3.12	119.31	126.39
14	BL	1003	BCL	CHA-C1A-NA	-3.12	119.31	126.39
14	AV	102	BCL	CHA-C1A-NA	-3.12	119.32	126.39
14	AC	103	BCL	C1D-ND-C4D	-3.12	104.12	106.31
14	AK	102	BCL	C1D-ND-C4D	-3.12	104.12	106.31
14	BD	105	BCL	CHA-C1A-NA	-3.12	119.33	126.39
24	ag	1002	V7B	C1-O6-C5	3.12	119.81	113.72
14	BW	1003	BCL	CHA-C1A-NA	-3.12	119.33	126.39
14	AF	1001	BCL	CHA-C1A-NA	-3.12	119.33	126.39
14	AJ	101	BCL	CHA-C1A-NA	-3.11	119.34	126.39
14	BK	1006	BCL	CHA-C1A-NA	-3.11	119.34	126.39
14	AT	101	BCL	C1D-ND-C4D	-3.11	104.13	106.31
14	AN	101	BCL	CHA-C1A-NA	-3.11	119.34	126.39
16	AS	105	V7N	C15-C14-C13	-3.11	122.91	127.28
14	AG	102	BCL	CHA-C1A-NA	-3.11	119.34	126.39
14	AV	102	BCL	C1D-ND-C4D	-3.11	104.13	106.31
14	bo	103	BCL	C1D-ND-C4D	-3.11	104.13	106.31
16	bl	102	V7N	O44-C40-O45	-3.11	116.50	123.90
16	BK	1001	V7N	C29-C28-C27	-3.11	114.19	123.20
14	BQ	1003	BCL	C4A-NA-C1A	3.11	108.10	106.68
14	BT	103	BCL	CHA-C1A-NA	-3.11	119.36	126.39
14	AE	1004	BCL	C1-C2-C3	-3.11	121.11	126.20
16	BX	1001	V7N	O44-C40-O45	-3.11	116.51	123.90
16	bf	101	V7N	C29-C28-C27	-3.11	114.20	123.20
14	AR	101	BCL	C1D-ND-C4D	-3.10	104.14	106.31
14	BE	104	BCL	CHA-C1A-NA	-3.10	119.36	126.39
16	BP	1001	V7N	C29-C28-C27	-3.10	114.21	123.20
14	AQ	102	BCL	C1D-ND-C4D	-3.10	104.14	106.31
14	BF	102	BCL	CHA-C1A-NA	-3.10	119.37	126.39
14	AS	103	BCL	C1D-ND-C4D	-3.10	104.14	106.31
14	AU	102	BCL	C1D-ND-C4D	-3.10	104.14	106.31
22	H1	103	PGW	O03-C01-C02	3.10	117.33	108.40
16	BD	101	V7N	O44-C40-O45	-3.10	116.52	123.90
15	BP	1004	LMT	C3'-C4'-C5'	-3.09	104.07	110.93
14	BO	1004	BCL	CHA-C1A-NA	-3.09	119.38	126.39
14	AC	103	BCL	CHA-C1A-NA	-3.09	119.39	126.39
15	AJ	103	LMT	C1B-O1B-C4'	3.09	125.31	117.98
14	BA	103	BCL	C4A-NA-C1A	3.09	108.09	106.68
14	BB	103	BCL	C4A-NA-C1A	3.09	108.09	106.68
14	ba	103	BCL	CHA-C1A-NA	-3.09	119.40	126.39
14	AB	1002	BCL	C1C-NC-C4C	3.09	108.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BX	1002	BCL	CHA-C1A-NA	-3.09	119.40	126.39
14	AX	103	BCL	C4A-NA-C1A	3.08	108.09	106.68
24	ag	1002	V7B	O7-C10-C11	3.08	118.14	111.48
14	BG	1004	BCL	CHA-C1A-NA	-3.08	119.42	126.39
14	AN	102	BCL	C1D-ND-C4D	-3.08	104.15	106.31
14	bn	103	BCL	CHA-C1A-NA	-3.07	119.43	126.39
14	BI	1003	BCL	CHA-C1A-NA	-3.07	119.43	126.39
14	AS	102	BCL	CHA-C1A-NA	-3.07	119.44	126.39
14	BN	103	BCL	CHA-C1A-NA	-3.07	119.44	126.39
14	ao	102	BCL	CHA-C1A-NA	-3.07	119.44	126.39
14	AX	103	BCL	C1D-ND-C4D	-3.06	104.16	106.31
14	AM	102	BCL	C4A-NA-C1A	3.06	108.08	106.68
14	AH	103	BCL	C1D-ND-C4D	-3.06	104.17	106.31
14	BS	1003	BCL	CHA-C1A-NA	-3.06	119.47	126.39
14	AE	1001	BCL	C1D-ND-C4D	-3.06	104.17	106.31
14	AS	104	BCL	CHA-C1A-NA	-3.05	119.47	126.39
14	AO	1002	BCL	C1D-ND-C4D	-3.05	104.17	106.31
14	an	1001	BCL	CHA-C1A-NA	-3.05	119.48	126.39
14	AJ	102	BCL	CHA-C1A-NA	-3.05	119.48	126.39
14	AR	102	BCL	C1-O2A-CGA	3.05	124.04	116.65
14	AK	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
14	BH	1005	BCL	CHA-C1A-NA	-3.05	119.49	126.39
14	BM	1002	BCL	CHA-C1A-NA	-3.05	119.49	126.39
20	bo	104	0V9	C2-O2-C10	3.05	125.09	117.80
14	AP	103	BCL	CHA-C1A-NA	-3.05	119.49	126.39
16	ba	101	V7N	C33-C5-C4	3.04	122.74	118.09
14	AI	102	BCL	C1D-ND-C4D	-3.04	104.18	106.31
14	BI	1003	BCL	O2A-CGA-O1A	-3.04	116.02	123.63
14	BC	104	BCL	C1-O2A-CGA	3.04	124.01	116.65
14	bi	104	BCL	CHA-C1A-NA	-3.04	119.51	126.39
16	be	101	V7N	C35-C13-C12	3.04	122.73	118.09
14	AC	101	BCL	CHA-C1A-NA	-3.04	119.52	126.39
14	AL	101	BCL	CHA-C1A-NA	-3.03	119.53	126.39
16	AS	105	V7N	O44-C40-O45	-3.03	116.70	123.90
14	BJ	1002	BCL	CHA-C1A-NA	-3.02	119.55	126.39
14	BP	1005	BCL	CHA-C1A-NA	-3.01	119.57	126.39
15	AJ	103	LMT	O1B-C1B-C2B	3.01	115.50	108.09
14	bm	104	BCL	CHA-C1A-NA	-3.01	119.58	126.39
14	AP	102	BCL	C1D-ND-C4D	-3.01	104.20	106.31
15	AP	104	LMT	C3'-C4'-C5'	-3.00	104.27	110.93
16	BS	1001	V7N	C15-C14-C13	-3.00	123.07	127.28
14	bl	104	BCL	CHA-C1A-NA	-3.00	119.59	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	bb	104	BCL	CHA-C1A-NA	-3.00	119.60	126.39
15	AT	102	LMT	O5'-C1'-O1'	-3.00	102.96	110.04
14	ai	101	BCL	CHA-C1A-NA	-2.99	119.61	126.39
14	ac	1001	BCL	CHA-C1A-NA	-2.99	119.62	126.39
16	bh	102	V7N	C33-C5-C4	2.99	122.65	118.09
14	AA	1002	BCL	CHA-C1A-NA	-2.98	119.63	126.39
14	bg	105	BCL	CHA-C1A-NA	-2.98	119.64	126.39
14	af	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
14	ak	1001	BCL	CHA-C1A-NA	-2.98	119.65	126.39
14	bf	103	BCL	CHA-C1A-NA	-2.98	119.65	126.39
14	AV	102	BCL	C4A-NA-C1A	2.97	108.04	106.68
14	al	1001	BCL	CHA-C1A-NA	-2.97	119.66	126.39
14	AG	101	BCL	C1-O2A-CGA	2.97	123.85	116.65
16	BM	1001	V7N	C36-C18-C19	2.97	122.62	118.09
16	bj	101	V7N	C35-C13-C12	2.96	122.62	118.09
14	AB	1002	BCL	CAA-CBA-CGA	2.96	121.63	113.21
14	AB	1001	BCL	C1-C2-C3	2.96	131.05	126.20
16	bh	102	V7N	C35-C13-C12	2.96	122.61	118.09
16	bl	102	V7N	C35-C13-C12	2.95	122.60	118.09
14	AQ	102	BCL	C2A-C1A-CHA	2.95	128.99	123.87
14	ae	102	BCL	CHA-C1A-NA	-2.95	119.70	126.39
14	bp	102	BCL	CHA-C1A-NA	-2.95	119.70	126.39
16	BP	1001	V7N	C36-C18-C19	2.95	122.60	118.09
14	ab	102	BCL	CHA-C1A-NA	-2.95	119.71	126.39
14	bk	102	BCL	CHA-C1A-NA	-2.95	119.71	126.39
14	bd	102	BCL	CHA-C1A-NA	-2.95	119.72	126.39
14	bj	103	BCL	CHA-C1A-NA	-2.95	119.72	126.39
14	AK	102	BCL	C2A-C1A-CHA	2.94	128.97	123.87
14	L	1002	BCL	CHA-C1A-NA	-2.94	119.74	126.39
14	bo	103	BCL	CHA-C1A-NA	-2.94	119.74	126.39
15	BS	1005	LMT	O1'-C1'-C2'	2.93	112.73	108.27
14	aa	1001	BCL	CHA-C1A-NA	-2.93	119.75	126.39
15	AQ	103	LMT	C1-O1'-C1'	2.93	118.69	113.68
16	bl	102	V7N	C33-C5-C4	2.93	122.56	118.09
16	bd	101	V7N	C35-C13-C12	2.93	122.56	118.09
14	BR	1004	BCL	C4A-NA-C1A	2.93	108.02	106.68
16	bf	101	V7N	C33-C5-C4	2.93	122.56	118.09
16	bf	101	V7N	C27-C26-C25	2.93	122.56	118.49
14	AG	101	BCL	CHA-C1A-NA	-2.92	119.77	126.39
14	BP	1005	BCL	C4A-NA-C1A	2.92	108.01	106.68
14	M	408	BCL	C4A-NA-C1A	2.92	108.01	106.68
16	bb	101	V7N	C33-C5-C4	2.92	122.55	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AX	102	BCL	C1-C2-C3	-2.92	121.42	126.20
14	BM	1002	BCL	C4A-NA-C1A	2.92	108.01	106.68
15	AH	102	LMT	C1-O1'-C1'	2.92	118.66	113.68
14	AN	104	BCL	C1C-NC-C4C	2.92	108.01	106.68
16	BL	1001	V7N	C36-C18-C19	2.91	122.54	118.09
15	BX	1003	LMT	C1-O1'-C1'	2.91	118.66	113.68
14	AE	1001	BCL	C2A-C1A-CHA	2.91	128.92	123.87
15	BK	1003	LMT	C1B-O1B-C4'	2.91	124.88	117.98
14	ap	1001	BCL	CHA-C1A-NA	-2.91	119.79	126.39
16	AE	1005	V7N	C35-C13-C14	-2.91	118.10	122.82
14	AQ	101	BCL	CHA-C1A-NA	-2.91	119.80	126.39
14	M	408	BCL	C1-O2A-CGA	2.91	123.69	116.65
14	ag	1001	BCL	CHA-C1A-NA	-2.90	119.81	126.39
14	bb	104	BCL	C4A-NA-C1A	2.90	108.00	106.68
14	ad	1001	BCL	CHA-C1A-NA	-2.90	119.83	126.39
14	AH	101	BCL	CHA-C1A-NA	-2.90	119.83	126.39
14	ah	1001	BCL	CHA-C1A-NA	-2.89	119.84	126.39
14	BC	104	BCL	CBA-CAA-C2A	2.89	122.40	113.79
14	BG	1004	BCL	C4A-NA-C1A	2.89	108.00	106.68
14	AH	103	BCL	C2A-C1A-CHA	2.89	128.89	123.87
14	AA	1002	BCL	C1-C2-C3	2.89	130.94	126.20
14	L	1010	BCL	CHA-C1A-NA	-2.89	119.84	126.39
14	AD	102	BCL	C2A-C1A-CHA	2.89	128.88	123.87
14	AI	103	BCL	C4A-NA-C1A	2.89	108.00	106.68
15	BD	102	LMT	C1-O1'-C1'	2.89	118.61	113.68
14	aj	103	BCL	CHA-C1A-NA	-2.89	119.85	126.39
14	AN	104	BCL	CHA-C1A-NA	-2.89	119.86	126.39
14	AE	1003	BCL	CHA-C1A-NA	-2.88	119.86	126.39
14	be	105	BCL	CHA-C1A-NA	-2.88	119.87	126.39
15	bo	105	LMT	C3'-C4'-C5'	-2.88	104.55	110.93
14	bk	102	BCL	C4A-NA-C1A	2.88	107.99	106.68
16	be	101	V7N	C16-C17-C18	-2.87	123.25	127.28
14	bf	103	BCL	C4A-NA-C1A	2.87	107.99	106.68
16	bo	102	V7N	C29-C28-C27	-2.87	114.88	123.20
14	M	405	BCL	C2A-C1A-CHA	2.87	128.85	123.87
14	AE	1004	BCL	CHA-C1A-NA	-2.87	119.90	126.39
14	BD	105	BCL	C4A-NA-C1A	2.87	107.99	106.68
14	bd	102	BCL	C4A-NA-C1A	2.87	107.99	106.68
15	BK	1005	LMT	C3'-C4'-C5'	-2.87	104.58	110.93
14	M	408	BCL	CHA-C1A-NA	-2.86	119.91	126.39
14	AI	102	BCL	C2A-C1A-CHA	2.86	128.83	123.87
14	bc	102	BCL	CHA-C1A-NA	-2.86	119.92	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AN	102	BCL	C2A-C1A-CHA	2.86	128.83	123.87
14	AF	1001	BCL	C2A-C1A-CHA	2.85	128.82	123.87
16	BG	1001	V7N	C36-C18-C19	2.85	122.44	118.09
14	bl	104	BCL	C4A-NA-C1A	2.85	107.98	106.68
16	BI	1001	V7N	C15-C14-C13	-2.85	123.28	127.28
14	AT	101	BCL	C2A-C1A-CHA	2.85	128.81	123.87
14	BF	102	BCL	CAA-CBA-CGA	2.85	121.29	113.21
14	AC	102	BCL	C2A-C1A-CHA	2.85	128.81	123.87
14	AX	102	BCL	CHA-C1A-NA	-2.85	119.95	126.39
14	AI	103	BCL	CHA-C1A-NA	-2.85	119.95	126.39
14	AW	101	BCL	C2A-C1A-CHA	2.84	128.80	123.87
16	BQ	1001	V7N	C20-C21-C22	-2.84	123.69	127.69
15	BL	1005	LMT	C3'-C4'-C5'	-2.84	104.63	110.93
20	bc	103	OV9	O2-C10-O4	-2.84	117.06	123.70
14	BX	1002	BCL	O2A-CGA-O1A	-2.84	116.53	123.63
16	bc	101	V7N	C33-C5-C4	2.84	122.42	118.09
14	AJ	101	BCL	C2A-C1A-CHA	2.84	128.79	123.87
16	bk	101	V7N	C35-C13-C12	2.84	122.42	118.09
15	BB	102	LMT	O1'-C1'-C2'	2.84	112.58	108.27
16	BV	1001	V7N	C15-C14-C13	-2.84	123.30	127.28
15	BI	1002	LMT	C1-O1'-C1'	2.83	118.52	113.68
14	AU	102	BCL	C2A-C1A-CHA	2.83	128.78	123.87
14	AX	102	BCL	C1-O2A-CGA	2.83	123.49	116.65
14	AS	104	BCL	O2A-CGA-O1A	-2.83	116.56	123.63
14	AR	101	BCL	C2A-C1A-CHA	2.83	128.77	123.87
14	AV	103	BCL	CHA-C1A-NA	-2.82	120.00	126.39
14	an	1001	BCL	C4A-NA-C1A	2.82	107.97	106.68
16	BJ	1001	V7N	C38-C26-C27	-2.82	113.78	118.09
16	BL	1001	V7N	C27-C26-C25	2.82	122.42	118.49
15	BC	105	LMT	C1-O1'-C1'	2.82	118.50	113.68
14	AL	103	BCL	C2A-C1A-CHA	2.82	128.75	123.87
16	bn	102	V7N	C36-C18-C17	-2.82	118.25	122.82
16	ba	101	V7N	C11-C10-C9	2.81	130.91	127.28
16	bb	101	V7N	C36-C18-C17	-2.81	118.26	122.82
14	AM	101	BCL	C2A-C1A-CHA	2.81	128.75	123.87
16	BV	1001	V7N	C20-C21-C22	-2.81	123.74	127.69
14	AS	103	BCL	C2A-C1A-CHA	2.81	128.74	123.87
14	AS	104	BCL	C2A-C1A-CHA	2.81	128.74	123.87
15	BI	1002	LMT	C3'-C4'-C5'	-2.81	104.71	110.93
14	AA	1002	BCL	C2A-C1A-CHA	2.80	128.73	123.87
14	bh	105	BCL	C2A-C1A-CHA	2.80	128.73	123.87
14	L	1002	BCL	C4A-NA-C1A	2.80	107.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BJ	1003	LMT	C3'-C4'-C5'	-2.80	104.73	110.93
14	AR	102	BCL	C2A-C1A-CHA	2.80	128.72	123.87
14	AA	1001	BCL	C2A-C1A-CHA	2.79	128.72	123.87
15	AD	103	LMT	C1-O1'-C1'	2.79	118.45	113.68
16	ba	101	V7N	C35-C13-C12	2.79	122.35	118.09
15	L	1008	LMT	C3'-C4'-C5'	-2.79	104.74	110.93
15	BT	102	LMT	C3'-C4'-C5'	-2.79	104.75	110.93
21	af	102	CD4	O16-C46-C47	2.79	117.51	111.48
14	L	1010	BCL	C2A-C1A-CHA	2.79	128.71	123.87
14	AO	1002	BCL	C2A-C1A-CHA	2.79	128.70	123.87
14	AB	1002	BCL	CMB-C2B-C1B	-2.78	121.18	125.42
16	BD	101	V7N	C20-C21-C22	-2.78	123.78	127.69
14	AA	1002	BCL	C4A-NA-C1A	2.77	107.94	106.68
14	be	105	BCL	C4A-NA-C1A	2.77	107.94	106.68
15	AD	103	LMT	C3'-C4'-C5'	-2.77	104.79	110.93
14	BA	103	BCL	C2A-C1A-CHA	2.77	128.67	123.87
14	bo	103	BCL	C4A-NA-C1A	2.77	107.94	106.68
16	bg	101	V7N	C20-C21-C22	-2.77	123.80	127.69
14	AB	1002	BCL	CHA-C1A-NA	-2.77	120.13	126.39
16	bc	101	V7N	C10-C9-C34	2.77	122.58	116.43
14	BE	104	BCL	C2A-C1A-CHA	2.76	128.66	123.87
14	AB	1002	BCL	C2A-C1A-CHA	2.76	128.66	123.87
14	AG	102	BCL	C2A-C1A-CHA	2.76	128.66	123.87
21	M	402	CD4	O3-C16-C15	-2.76	100.45	108.40
23	L	1001	MQ8	C11-C3-C4	-2.75	115.68	118.58
16	bn	102	V7N	C35-C13-C12	2.75	122.29	118.09
14	AV	101	BCL	C2A-C1A-CHA	2.75	128.64	123.87
14	BF	102	BCL	C1-O2A-CGA	2.75	123.31	116.65
15	AD	101	LMT	O1'-C1'-C2'	2.75	112.44	108.27
15	BK	1004	LMT	O1'-C1'-C2'	2.74	112.44	108.27
14	ap	1001	BCL	C1-O2A-CGA	2.74	123.29	116.65
14	bj	103	BCL	C4A-NA-C1A	2.74	107.93	106.68
14	AV	102	BCL	C2A-C1A-CHA	2.74	128.62	123.87
16	AO	1001	V7N	C36-C18-C19	2.74	122.27	118.09
16	bp	101	V7N	C33-C5-C4	2.74	122.27	118.09
14	AL	101	BCL	CAA-CBA-CGA	2.74	120.97	113.21
17	C	402	HEC	CBD-CAD-C3D	-2.74	104.97	112.53
15	M	403	LMT	C1-O1'-C1'	2.73	118.35	113.68
15	AH	102	LMT	C3'-C4'-C5'	-2.73	104.88	110.93
14	AJ	102	BCL	C1-C2-C3	-2.73	121.73	126.20
16	BJ	1001	V7N	C36-C18-C19	2.72	122.25	118.09
14	AK	101	BCL	CBA-CAA-C2A	2.72	121.89	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AE	1003	BCL	C4A-NA-C1A	2.71	107.92	106.68
19	C	406	NDG	C1-O5-C5	2.71	115.82	112.19
15	bc	104	LMT	C1-O1'-C1'	2.71	118.31	113.68
16	BR	1001	V7N	C20-C21-C22	-2.71	123.89	127.69
15	BH	1002	LMT	C3'-C4'-C5'	-2.70	104.93	110.93
15	BP	1004	LMT	C1-O1'-C1'	2.70	118.30	113.68
14	BK	1006	BCL	C2A-C1A-CHA	2.70	128.56	123.87
16	BS	1001	V7N	C10-C9-C34	2.70	122.44	116.43
16	BO	1001	V7N	C27-C26-C25	2.70	122.25	118.49
15	AS	101	LMT	C3'-C4'-C5'	-2.70	104.95	110.93
15	BL	1004	LMT	C1'-O5'-C5'	-2.70	108.46	113.72
14	am	1001	BCL	C2A-C1A-CHA	2.69	128.54	123.87
16	BI	1001	V7N	C20-C21-C22	-2.69	123.90	127.69
14	AR	102	BCL	O2D-CGD-CBD	2.69	115.94	111.23
16	be	101	V7N	C33-C5-C4	2.69	122.20	118.09
16	BS	1001	V7N	C20-C21-C22	-2.69	123.91	127.69
14	AM	102	BCL	C2A-C1A-CHA	2.69	128.53	123.87
16	BG	1001	V7N	C38-C26-C27	-2.69	113.98	118.09
15	L	1011	LMT	C3'-C4'-C5'	-2.69	104.98	110.93
16	BU	1001	V7N	C35-C13-C14	-2.68	118.47	122.82
15	BU	1002	LMT	C1-O1'-C1'	2.68	118.26	113.68
16	BV	1001	V7N	C36-C18-C19	2.68	122.18	118.09
14	AS	102	BCL	C4A-NA-C1A	2.68	107.90	106.68
15	bo	101	LMT	C3'-C4'-C5'	-2.67	105.00	110.93
17	C	404	HEC	CMC-C2C-C1C	-2.67	121.35	125.42
16	BB	101	V7N	C36-C18-C19	2.67	122.16	118.09
16	BV	1001	V7N	C10-C9-C34	2.67	122.36	116.43
14	BX	1002	BCL	C1-O2A-CGA	2.67	123.10	116.65
14	AS	102	BCL	C2A-C1A-CHA	2.66	128.49	123.87
14	AI	103	BCL	CAA-CBA-CGA	2.66	120.77	113.21
27	M	404	CRT	C31-C32-C33	-2.66	123.54	127.28
16	BI	1001	V7N	C10-C9-C34	2.66	122.35	116.43
16	bh	102	V7N	C10-C9-C34	2.66	122.35	116.43
14	AQ	101	BCL	CBA-CAA-C2A	2.66	121.71	113.79
16	bf	101	V7N	C35-C13-C12	2.66	122.15	118.09
16	AS	105	V7N	C35-C13-C14	-2.66	118.51	122.82
14	BB	103	BCL	C2A-C1A-CHA	2.66	128.48	123.87
16	BE	101	V7N	C35-C13-C14	-2.65	118.52	122.82
16	BG	1001	V7N	C33-C5-C4	2.65	122.14	118.09
14	BW	1003	BCL	CAA-CBA-CGA	2.65	120.74	113.21
14	AP	102	BCL	C2A-C1A-CHA	2.65	128.46	123.87
14	al	1001	BCL	C1-O2A-CGA	2.65	123.06	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	BCL	C2A-C1A-CHA	2.65	128.46	123.87
14	AE	1003	BCL	C2A-C1A-CHA	2.64	128.46	123.87
15	BA	102	LMT	C3'-C4'-C5'	-2.64	105.07	110.93
14	BW	1003	BCL	C2A-C1A-CHA	2.64	128.45	123.87
14	AJ	102	BCL	CBA-CAA-C2A	2.64	121.66	113.79
15	BB	105	LMT	C3'-C4'-C5'	-2.64	105.09	110.93
14	AE	1003	BCL	CAA-CBA-CGA	2.64	120.69	113.21
16	BE	101	V7N	C10-C9-C34	2.63	122.29	116.43
15	L	1008	LMT	O5'-C1'-O1'	-2.63	103.82	110.04
16	BP	1001	V7N	C10-C9-C34	2.63	122.28	116.43
15	BK	1003	LMT	O1B-C1B-C2B	2.63	114.57	108.09
16	BJ	1001	V7N	C27-C26-C25	2.63	122.16	118.49
15	BE	102	LMT	C1'-O5'-C5'	-2.63	108.58	113.72
16	bp	101	V7N	C1-C2-C3	2.63	119.81	112.98
21	aj	102	CD4	O2-C14-O1	-2.63	117.56	123.70
14	BE	104	BCL	C1-O2A-CGA	2.63	123.01	116.65
16	AO	1001	V7N	C33-C5-C6	-2.63	118.56	122.82
15	AH	104	LMT	C3'-C4'-C5'	-2.62	105.11	110.93
14	bc	102	BCL	CBA-CAA-C2A	2.62	121.60	113.79
15	bc	104	LMT	C3'-C4'-C5'	-2.62	105.11	110.93
16	BG	1001	V7N	C10-C9-C34	2.62	122.26	116.43
16	BR	1001	V7N	C33-C5-C6	-2.62	118.57	122.82
20	bh	103	OV9	O3P-P-O2P	2.62	119.32	108.94
14	L	1002	BCL	C2A-C1A-CHA	2.62	128.41	123.87
14	AR	102	BCL	C1-C2-C3	2.62	130.49	126.20
15	bh	104	LMT	C3'-C4'-C5'	-2.62	105.13	110.93
15	bl	101	LMT	C1'-O5'-C5'	-2.62	108.61	113.72
16	bm	101	V7N	C35-C13-C14	-2.62	118.58	122.82
15	bg	103	LMT	O1'-C1'-C2'	2.61	112.24	108.27
21	H1	102	CD4	O2-C14-C13	2.61	117.13	111.48
16	BX	1001	V7N	C20-C21-C22	-2.61	124.02	127.69
16	BB	101	V7N	C10-C9-C34	2.61	122.23	116.43
16	AO	1001	V7N	C15-C14-C13	-2.61	123.62	127.28
15	BL	1004	LMT	C3'-C4'-C5'	-2.61	105.15	110.93
16	BS	1001	V7N	C33-C5-C4	2.61	122.07	118.09
15	AJ	104	LMT	C3'-C4'-C5'	-2.61	105.15	110.93
15	BW	1002	LMT	C3'-C4'-C5'	-2.61	105.16	110.93
16	BX	1001	V7N	C35-C13-C14	-2.60	118.60	122.82
16	BJ	1001	V7N	C35-C13-C12	2.60	122.07	118.09
14	AP	103	BCL	C2A-C1A-CHA	2.60	128.38	123.87
14	bg	105	BCL	C4A-NA-C1A	2.60	107.87	106.68
14	AU	103	BCL	C2A-C1A-CHA	2.60	128.38	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BR	1001	V7N	C2-C3-C4	-2.60	121.26	124.91
16	BK	1001	V7N	C36-C18-C19	2.60	122.06	118.09
14	AE	1004	BCL	C2A-C1A-CHA	2.60	128.37	123.87
16	bg	101	V7N	C36-C18-C17	-2.59	118.62	122.82
16	bp	101	V7N	C29-C28-C27	-2.59	115.69	123.20
16	BX	1001	V7N	C29-C28-C27	-2.59	115.69	123.20
16	bl	102	V7N	C10-C9-C34	2.59	122.19	116.43
16	BQ	1001	V7N	C10-C9-C34	2.59	122.19	116.43
16	bn	102	V7N	C36-C18-C19	2.59	122.05	118.09
16	bj	101	V7N	C33-C5-C4	2.59	122.04	118.09
14	bn	103	BCL	C4A-NA-C1A	2.59	107.86	106.68
15	BJ	1004	LMT	C3'-C4'-C5'	-2.58	105.20	110.93
16	BS	1001	V7N	C35-C13-C14	-2.58	118.63	122.82
14	AB	1001	BCL	C2A-C1A-CHA	2.58	128.35	123.87
16	ba	101	V7N	C10-C9-C34	2.58	122.17	116.43
16	BA	101	V7N	C10-C9-C34	2.58	122.17	116.43
16	bg	101	V7N	C10-C9-C34	2.58	122.17	116.43
14	AL	101	BCL	CBA-CAA-C2A	2.58	121.47	113.79
21	H1	102	CD4	O3-C17-C18	2.58	119.70	111.83
16	bi	101	V7N	C35-C13-C12	2.58	122.03	118.09
16	BG	1001	V7N	C27-C26-C25	2.58	122.08	118.49
15	BG	1003	LMT	C3'-C4'-C5'	-2.58	105.21	110.93
16	BJ	1001	V7N	C10-C9-C34	2.58	122.16	116.43
14	BE	104	BCL	CAA-CBA-CGA	2.58	120.53	113.21
16	BD	101	V7N	C36-C18-C19	2.58	122.03	118.09
16	BH	1001	V7N	C33-C5-C6	-2.58	118.64	122.82
14	AN	104	BCL	C2A-C1A-CHA	2.58	128.34	123.87
14	AG	101	BCL	C1C-NC-C4C	2.58	107.85	106.68
14	ba	103	BCL	C4A-NA-C1A	2.58	107.85	106.68
15	AD	101	LMT	C1'-O5'-C5'	-2.58	108.69	113.72
14	AK	101	BCL	C2A-C1A-CHA	2.57	128.33	123.87
16	bg	101	V7N	C33-C5-C4	2.57	122.02	118.09
16	BC	101	V7N	C10-C9-C34	2.57	122.14	116.43
14	AH	101	BCL	CBA-CAA-C2A	2.57	121.43	113.79
16	BR	1001	V7N	C3-C4-C5	2.57	129.77	125.89
16	BD	101	V7N	C33-C5-C4	2.56	122.01	118.09
16	BW	1001	V7N	C10-C9-C34	2.56	122.13	116.43
16	BX	1001	V7N	C10-C9-C34	2.56	122.13	116.43
16	BI	1001	V7N	C36-C18-C19	2.56	122.00	118.09
16	bl	102	V7N	C36-C18-C19	2.56	122.00	118.09
16	BX	1001	V7N	C33-C5-C4	2.56	122.00	118.09
16	be	101	V7N	C36-C18-C17	-2.56	118.67	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AC	101	BCL	CBA-CAA-C2A	2.56	121.41	113.79
16	BO	1001	V7N	C35-C13-C12	2.56	122.00	118.09
14	BE	104	BCL	C1-C2-C3	-2.56	122.01	126.20
16	BL	1001	V7N	C10-C9-C34	2.56	122.11	116.43
16	BH	1001	V7N	C36-C18-C19	2.55	121.99	118.09
16	bn	102	V7N	C10-C9-C34	2.55	122.11	116.43
16	BL	1001	V7N	C35-C13-C12	2.55	121.99	118.09
21	af	102	CD4	C48-C47-C46	-2.55	104.34	113.69
15	BF	103	LMT	C1-O1'-C1'	2.55	118.04	113.68
14	bh	105	BCL	C4A-NA-C1A	2.55	107.84	106.68
14	BF	102	BCL	C2A-C1A-CHA	2.55	128.29	123.87
14	AG	101	BCL	C2A-C1A-CHA	2.55	128.29	123.87
16	AO	1001	V7N	C35-C13-C12	2.55	121.98	118.09
16	bf	101	V7N	C10-C9-C34	2.54	122.08	116.43
21	af	102	CD4	O2-C14-O1	-2.54	117.76	123.70
16	BG	1001	V7N	C15-C14-C13	-2.54	123.71	127.28
16	BA	101	V7N	C20-C21-C22	-2.54	124.12	127.69
14	AX	103	BCL	C2A-C1A-CHA	2.54	128.28	123.87
14	AG	101	BCL	C4A-NA-C1A	2.54	107.84	106.68
16	BS	1001	V7N	C36-C18-C19	2.54	121.96	118.09
14	BV	1005	BCL	C2A-C1A-CHA	2.54	128.27	123.87
25	L	1009	BPH	OBB-CAB-CBB	-2.54	114.79	120.19
16	bj	101	V7N	C10-C9-C34	2.53	122.06	116.43
23	M	407	MQ8	C12-C11-C3	2.53	118.32	112.08
16	BK	1001	V7N	C35-C13-C14	-2.53	118.71	122.82
14	BC	104	BCL	C2A-C1A-CHA	2.53	128.26	123.87
14	AI	103	BCL	C1C-NC-C4C	2.53	107.83	106.68
16	be	101	V7N	C10-C9-C34	2.53	122.06	116.43
16	BV	1001	V7N	C33-C5-C4	2.53	121.95	118.09
16	bk	101	V7N	C33-C5-C4	2.53	121.95	118.09
14	BD	105	BCL	C2A-C1A-CHA	2.53	128.25	123.87
15	M	403	LMT	C3'-C4'-C5'	-2.53	105.33	110.93
16	BG	1001	V7N	C35-C13-C12	2.53	121.95	118.09
14	bp	102	BCL	CBA-CAA-C2A	2.53	121.31	113.79
14	ac	1001	BCL	C2A-C1A-CHA	2.52	128.25	123.87
16	bc	101	V7N	C35-C13-C12	2.52	121.94	118.09
14	AX	102	BCL	CBA-CAA-C2A	2.52	121.30	113.79
14	ai	101	BCL	C2A-C1A-CHA	2.52	128.24	123.87
16	bp	101	V7N	C10-C9-C34	2.52	122.03	116.43
15	BI	1006	LMT	C3'-C4'-C5'	-2.52	105.34	110.93
14	af	101	BCL	C2A-C1A-CHA	2.52	128.24	123.87
16	AE	1005	V7N	C10-C9-C34	2.52	122.03	116.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BH	1003	LMT	C3'-C4'-C5'	-2.52	105.35	110.93
15	bn	105	LMT	C1'-O5'-C5'	-2.52	108.80	113.72
14	AN	101	BCL	C2A-C1A-CHA	2.52	128.23	123.87
14	AS	102	BCL	C1-C2-C3	2.52	130.32	126.20
16	bo	102	V7N	C33-C5-C4	2.52	121.93	118.09
16	BL	1001	V7N	C33-C5-C4	2.51	121.93	118.09
21	H1	102	CD4	O16-C46-C47	2.51	116.92	111.48
16	bb	101	V7N	C35-C13-C12	2.51	121.92	118.09
16	bd	101	V7N	C10-C9-C34	2.51	122.01	116.43
14	AV	103	BCL	C2A-C1A-CHA	2.51	128.22	123.87
14	BJ	1002	BCL	C2A-C1A-CHA	2.51	128.22	123.87
15	AC	104	LMT	C3'-C4'-C5'	-2.51	105.37	110.93
14	ao	102	BCL	C2A-C1A-CHA	2.51	128.22	123.87
14	AN	104	BCL	CBA-CAA-C2A	2.50	121.25	113.79
22	H1	103	PGW	O01-C1-C2	2.50	116.89	111.48
16	BO	1001	V7N	C38-C26-C27	-2.50	114.27	118.09
15	BR	1002	LMT	C3'-C4'-C5'	-2.50	105.39	110.93
20	be	102	OV9	O3-C30-O5	-2.50	117.37	123.63
15	bm	103	LMT	O5B-C5B-C4B	2.50	114.20	109.70
16	BL	1001	V7N	C35-C13-C14	-2.50	118.77	122.82
16	bm	101	V7N	C35-C13-C12	2.50	121.91	118.09
14	ae	102	BCL	C2A-C1A-CHA	2.50	128.20	123.87
16	bi	101	V7N	C1-C2-C3	2.50	119.47	112.98
14	BT	103	BCL	C2A-C1A-CHA	2.50	128.20	123.87
14	BX	1002	BCL	C1-C2-C3	-2.50	122.11	126.20
16	BO	1001	V7N	C2-C3-C4	-2.50	121.41	124.91
16	BH	1001	V7N	C35-C13-C12	2.49	121.90	118.09
14	ag	1001	BCL	CMB-C2B-C1B	-2.49	121.62	125.42
16	BB	101	V7N	C35-C13-C14	-2.49	118.78	122.82
15	BG	1002	LMT	C3'-C4'-C5'	-2.49	105.41	110.93
16	BQ	1001	V7N	C35-C13-C14	-2.49	118.78	122.82
16	AO	1001	V7N	C10-C9-C34	2.49	121.97	116.43
14	AL	101	BCL	C2A-C1A-CHA	2.49	128.19	123.87
14	AQ	101	BCL	C2A-C1A-CHA	2.49	128.19	123.87
16	BB	101	V7N	C38-C26-C27	-2.49	114.29	118.09
16	BC	101	V7N	C36-C18-C19	2.49	121.89	118.09
14	AC	103	BCL	C2A-C1A-CHA	2.49	128.18	123.87
16	BP	1001	V7N	C35-C13-C12	2.49	121.89	118.09
16	BM	1001	V7N	C35-C13-C14	-2.49	118.79	122.82
16	bn	102	V7N	C33-C5-C4	2.48	121.88	118.09
16	BX	1001	V7N	C36-C18-C19	2.48	121.88	118.09
14	AI	103	BCL	C2A-C1A-CHA	2.48	128.18	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	ak	1001	BCL	C2A-C1A-CHA	2.48	128.18	123.87
16	BQ	1001	V7N	C33-C5-C4	2.48	121.88	118.09
16	BB	101	V7N	C27-C26-C25	2.48	121.95	118.49
15	BH	1003	LMT	C1-O1'-C1'	2.48	117.92	113.68
16	bi	101	V7N	C10-C9-C34	2.48	121.94	116.43
15	BV	1004	LMT	C3'-C4'-C5'	-2.48	105.43	110.93
16	bn	102	V7N	C27-C26-C25	2.48	121.94	118.49
16	BJ	1001	V7N	C33-C5-C4	2.48	121.88	118.09
16	BP	1001	V7N	C33-C5-C4	2.48	121.88	118.09
25	M	406	BPH	C2D-C1D-ND	2.48	111.22	109.43
16	BV	1001	V7N	C35-C13-C12	2.48	121.87	118.09
16	bo	102	V7N	C35-C13-C14	-2.48	118.80	122.82
14	AV	103	BCL	CAB-C3B-C2B	2.47	132.88	127.74
15	AA	1003	LMT	O1'-C1'-C2'	2.47	112.03	108.27
15	AX	101	LMT	O5'-C1'-C2'	-2.47	105.29	110.37
16	AS	105	V7N	C10-C9-C34	2.47	121.93	116.43
14	BU	1004	BCL	C2A-C1A-CHA	2.47	128.16	123.87
16	BA	101	V7N	C35-C13-C12	2.47	121.86	118.09
16	AS	105	V7N	C36-C18-C17	-2.47	118.81	122.82
14	an	1001	BCL	C2A-C1A-CHA	2.47	128.15	123.87
16	BO	1001	V7N	C3-C4-C5	2.47	129.62	125.89
16	bb	101	V7N	C10-C9-C34	2.47	121.92	116.43
14	ab	102	BCL	C2A-C1A-CHA	2.47	128.15	123.87
16	bd	101	V7N	C36-C18-C19	2.46	121.85	118.09
14	AI	102	BCL	OBB-CAB-CBB	-2.46	114.25	119.77
16	BO	1001	V7N	C35-C13-C14	-2.46	118.82	122.82
16	bi	101	V7N	C35-C13-C14	-2.46	118.83	122.82
16	ba	101	V7N	C35-C13-C14	-2.46	118.83	122.82
19	C1	1002	NDG	C1-O5-C5	2.46	115.48	112.19
15	BT	102	LMT	O5B-C5B-C4B	2.46	114.13	109.70
15	BQ	1005	LMT	C3'-C4'-C5'	-2.46	105.48	110.93
16	BH	1001	V7N	C35-C13-C14	-2.46	118.83	122.82
27	M	404	CRT	C35-C33-C32	2.46	122.88	119.01
15	BE	103	LMT	C1'-O5'-C5'	-2.46	108.92	113.72
21	M	402	CD4	O14-C35-C36	2.46	119.32	111.83
14	AK	102	BCL	OBB-CAB-CBB	-2.45	114.27	119.77
14	BR	1004	BCL	C2A-C1A-CHA	2.45	128.12	123.87
16	bd	101	V7N	C33-C5-C4	2.45	121.83	118.09
15	AX	101	LMT	O1'-C1'-C2'	2.45	112.00	108.27
16	AO	1001	V7N	C35-C13-C14	-2.45	118.85	122.82
16	BB	101	V7N	C33-C5-C4	2.45	121.83	118.09
14	ak	1001	BCL	CMB-C2B-C1B	-2.45	121.69	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	404	CRT	C36-C35-C33	2.45	129.59	125.89
14	BO	1004	BCL	C2A-C1A-CHA	2.44	128.11	123.87
14	AU	102	BCL	OBB-CAB-CBB	-2.44	114.30	119.77
14	AQ	102	BCL	OBB-CAB-CBB	-2.44	114.30	119.77
15	BS	1005	LMT	C3'-C4'-C5'	-2.44	105.51	110.93
14	ap	1001	BCL	C2A-C1A-CHA	2.44	128.10	123.87
16	BW	1001	V7N	C36-C18-C19	2.44	121.82	118.09
14	AA	1002	BCL	C1C-NC-C4C	2.44	107.79	106.68
14	BM	1002	BCL	C2A-C1A-CHA	2.44	128.10	123.87
16	BH	1001	V7N	C10-C9-C34	2.44	121.84	116.43
14	AP	102	BCL	OBB-CAB-CBB	-2.44	114.31	119.77
14	AN	104	BCL	C4A-NA-C1A	2.44	107.79	106.68
14	AM	101	BCL	OBB-CAB-CBB	-2.44	114.32	119.77
15	bn	105	LMT	O1'-C1'-C2'	2.44	111.97	108.27
15	BF	101	LMT	O1'-C1'-C2'	2.43	111.97	108.27
20	aj	101	0V9	C2-O2-C10	2.43	123.61	117.80
14	AB	1001	BCL	CAB-C3B-C2B	2.43	132.79	127.74
14	AR	102	BCL	C6-C5-C3	2.43	119.39	113.47
14	AL	103	BCL	OBB-CAB-CBB	-2.43	114.33	119.77
16	bo	102	V7N	C10-C9-C34	2.43	121.83	116.43
16	BQ	1001	V7N	C15-C14-C13	-2.43	123.87	127.28
16	BI	1001	V7N	C35-C13-C14	-2.43	118.89	122.82
16	AO	1001	V7N	C2-C3-C4	-2.43	121.51	124.91
15	BQ	1002	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
15	AE	1002	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
16	BA	101	V7N	C36-C18-C19	2.42	121.79	118.09
20	bi	103	0V9	O2-C10-O4	-2.42	118.04	123.70
14	AV	102	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
14	AJ	101	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
16	BW	1001	V7N	C15-C14-C13	-2.42	123.88	127.28
14	ad	1001	BCL	C2A-C1A-CHA	2.42	128.07	123.87
14	AR	101	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
14	AT	101	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
14	AJ	102	BCL	C2A-C1A-CHA	2.42	128.06	123.87
16	BO	1001	V7N	C10-C9-C34	2.42	121.80	116.43
14	AC	101	BCL	C2A-C1A-CHA	2.41	128.06	123.87
16	bg	101	V7N	C16-C17-C18	-2.41	123.89	127.28
16	BQ	1001	V7N	C35-C13-C12	2.41	121.77	118.09
15	AA	1004	LMT	C3'-C4'-C5'	-2.41	105.58	110.93
14	AC	101	BCL	CAC-C3C-C4C	2.41	117.94	112.58
14	AA	1001	BCL	OBB-CAB-CBB	-2.41	114.37	119.77
14	AH	101	BCL	C2A-C1A-CHA	2.41	128.05	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H1	104	CD4	O2-C14-O1	-2.41	118.08	123.70
14	AX	103	BCL	OBB-CAB-CBB	-2.41	114.38	119.77
14	aj	103	BCL	C2A-C1A-CHA	2.41	128.04	123.87
16	BC	101	V7N	C35-C13-C14	-2.41	118.92	122.82
14	AX	102	BCL	C2A-C1A-CHA	2.41	128.04	123.87
14	AN	102	BCL	OBB-CAB-CBB	-2.41	114.38	119.77
20	bb	103	0V9	O2-C10-O4	-2.41	118.08	123.70
14	AO	1002	BCL	OBB-CAB-CBB	-2.41	114.38	119.77
14	BH	1005	BCL	C2A-C1A-CHA	2.40	128.04	123.87
15	AE	1002	LMT	O1'-C1'-C2'	2.40	111.92	108.27
14	AH	103	BCL	OBB-CAB-CBB	-2.40	114.39	119.77
15	BC	103	LMT	C3'-C4'-C5'	-2.40	105.60	110.93
15	BQ	1002	LMT	O5'-C1'-O1'	-2.40	104.37	110.04
16	BP	1001	V7N	C15-C14-C13	-2.40	123.91	127.28
16	BI	1001	V7N	C35-C13-C12	2.40	121.76	118.09
16	BW	1001	V7N	C35-C13-C12	2.40	121.76	118.09
16	bh	102	V7N	C36-C18-C19	2.40	121.76	118.09
16	BU	1001	V7N	C36-C18-C17	-2.40	118.93	122.82
14	AS	103	BCL	OBB-CAB-CBB	-2.40	114.39	119.77
16	BE	101	V7N	C11-C10-C9	2.40	130.37	127.28
21	aj	102	CD4	O2-C15-C28	2.40	116.95	108.34
15	BX	1004	LMT	C1-O1'-C1'	2.40	117.78	113.68
14	AF	1001	BCL	OBB-CAB-CBB	-2.40	114.40	119.77
16	BA	101	V7N	C33-C5-C4	2.40	121.75	118.09
25	L	1009	BPH	C2D-C1D-ND	2.39	111.16	109.43
15	BN	105	LMT	C3'-C4'-C5'	-2.39	105.62	110.93
15	bb	102	LMT	O5'-C1'-O1'	-2.39	104.39	110.04
16	BE	101	V7N	C36-C18-C19	2.39	121.75	118.09
14	al	1001	BCL	C2A-C1A-CHA	2.39	128.02	123.87
14	aj	103	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
14	ba	103	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
14	AM	102	BCL	C6-C5-C3	2.39	119.30	113.47
16	bo	102	V7N	C36-C18-C17	-2.39	118.94	122.82
16	BH	1001	V7N	C3-C4-C5	2.39	129.50	125.89
14	AW	101	BCL	OBB-CAB-CBB	-2.39	114.42	119.77
16	BO	1001	V7N	C36-C18-C19	2.39	121.74	118.09
14	BX	1002	BCL	C2A-C1A-CHA	2.39	128.01	123.87
14	AB	1001	BCL	OBB-CAB-CBB	-2.39	114.42	119.77
16	bj	101	V7N	C1-C2-C3	2.39	119.18	112.98
16	bc	101	V7N	C35-C13-C14	-2.39	118.95	122.82
14	ac	1001	BCL	CMB-C2B-C1B	-2.39	121.79	125.42
15	AN	103	LMT	C3'-C4'-C5'	-2.38	105.65	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	ba	103	BCL	C2A-C1A-CHA	2.38	128.00	123.87
16	BH	1001	V7N	C2-C3-C4	-2.38	121.57	124.91
25	L	1009	BPH	CMB-C2B-C3B	2.38	129.44	124.68
16	BM	1001	V7N	C33-C5-C4	2.38	121.73	118.09
14	bp	102	BCL	C2A-C1A-CHA	2.38	128.00	123.87
14	BU	1004	BCL	C4A-NA-C1A	2.38	107.76	106.68
16	BQ	1001	V7N	C36-C18-C19	2.38	121.72	118.09
14	M	405	BCL	CMB-C2B-C1B	-2.38	121.80	125.42
14	AM	102	BCL	CMB-C2B-C1B	-2.37	121.80	125.42
14	bm	104	BCL	C4A-NA-C1A	2.37	107.76	106.68
16	ba	101	V7N	C7-C6-C5	2.37	130.60	127.28
14	AC	102	BCL	OBB-CAB-CBB	-2.37	114.46	119.77
15	bm	105	LMT	C3'-C4'-C5'	-2.37	105.67	110.93
14	ap	1001	BCL	CMB-C2B-C1B	-2.37	121.81	125.42
16	bc	101	V7N	C36-C18-C19	2.37	121.71	118.09
21	H1	104	CD4	O16-C46-C47	2.37	116.60	111.48
16	BD	101	V7N	C35-C13-C12	2.37	121.70	118.09
14	AG	102	BCL	OBB-CAB-CBB	-2.37	114.47	119.77
14	AD	102	BCL	CAB-C3B-C2B	2.36	132.66	127.74
14	ae	102	BCL	CMB-C2B-C1B	-2.36	121.82	125.42
14	BC	104	BCL	CAB-C3B-C2B	2.36	132.65	127.74
14	am	1001	BCL	CMB-C2B-C1B	-2.36	121.82	125.42
15	BG	1006	LMT	C1'-O5'-C5'	-2.36	109.11	113.72
17	C	402	HEC	C2A-C1A-NA	-2.36	108.04	110.32
15	AH	104	LMT	O5B-C5B-C4B	2.36	113.95	109.70
14	bd	102	BCL	C2A-C1A-CHA	2.36	127.96	123.87
14	AH	101	BCL	C1-O2A-CGA	2.36	122.36	116.65
16	BO	1001	V7N	C33-C5-C6	-2.36	119.00	122.82
14	BL	1003	BCL	CAB-C3B-C2B	2.36	132.64	127.74
16	BR	1001	V7N	C10-C9-C34	2.36	121.67	116.43
16	BR	1001	V7N	C35-C13-C12	2.36	121.69	118.09
16	bi	101	V7N	C33-C5-C4	2.36	121.69	118.09
14	ao	102	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
16	BG	1001	V7N	C35-C13-C14	-2.35	119.01	122.82
15	L	1007	LMT	C3'-C4'-C5'	-2.35	105.72	110.93
15	BV	1002	LMT	O1'-C1'-C2'	2.35	111.84	108.27
14	BQ	1003	BCL	C2A-C1A-CHA	2.35	127.94	123.87
16	AO	1001	V7N	C27-C26-C25	2.35	121.76	118.49
14	aa	1001	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
15	BK	1003	LMT	O5'-C1'-C2'	-2.35	105.55	110.37
16	BM	1001	V7N	C35-C13-C12	2.35	121.67	118.09
16	bf	101	V7N	C11-C10-C9	2.35	130.31	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	401	HEC	C2A-C1A-NA	-2.35	108.06	110.32
14	am	1001	BCL	OBB-CAB-CBB	-2.35	114.52	119.77
16	bg	101	V7N	C35-C13-C12	2.35	121.67	118.09
14	BN	103	BCL	C2A-C1A-CHA	2.35	127.94	123.87
15	BK	1002	LMT	C1'-O5'-C5'	-2.34	109.14	113.72
14	al	1001	BCL	CMB-C2B-C1B	-2.34	121.85	125.42
20	bg	104	OV9	O3-C30-O5	-2.34	117.76	123.63
14	AX	102	BCL	CMB-C2B-C1B	-2.34	121.85	125.42
16	bg	101	V7N	C35-C13-C14	-2.34	119.02	122.82
14	BO	1004	BCL	O2A-CGA-CBA	2.34	118.98	111.83
16	BC	101	V7N	C27-C26-C25	2.34	121.75	118.49
14	AS	104	BCL	CMB-C2B-C1B	-2.34	121.86	125.42
15	BX	1004	LMT	C3'-C4'-C5'	-2.34	105.74	110.93
14	ae	102	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
14	ag	1001	BCL	C2A-C1A-CHA	2.34	127.93	123.87
14	ai	101	BCL	CMB-C2B-C1B	-2.34	121.86	125.42
14	AX	102	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
16	BW	1001	V7N	C35-C13-C14	-2.34	119.03	122.82
14	BG	1004	BCL	C2A-C1A-CHA	2.34	127.92	123.87
15	BA	104	LMT	C1'-O5'-C5'	-2.33	109.16	113.72
14	aa	1001	BCL	OBB-CAB-CBB	-2.33	114.54	119.77
15	BP	1003	LMT	C1'-O5'-C5'	-2.33	109.16	113.72
24	L	1006	V7B	C43-O4-C4	-2.33	112.45	117.98
14	bg	105	BCL	C1C-NC-C4C	2.33	107.74	106.68
15	BR	1002	LMT	O5B-C5B-C4B	2.33	113.90	109.70
15	BN	102	LMT	C3'-C4'-C5'	-2.33	105.77	110.93
14	ab	102	BCL	OBB-CAB-CBB	-2.33	114.56	119.77
16	bd	101	V7N	C35-C13-C14	-2.33	119.04	122.82
14	bh	105	BCL	O2D-CGD-CBD	2.33	115.30	111.23
15	AE	1002	LMT	O1B-C4'-C3'	2.33	113.15	107.23
14	al	1001	BCL	OBB-CAB-CBB	-2.33	114.56	119.77
14	BS	1003	BCL	C2A-C1A-CHA	2.33	127.91	123.87
21	H1	104	CD4	O3-C17-C18	2.32	118.92	111.83
14	BP	1005	BCL	C2A-C1A-CHA	2.32	127.90	123.87
15	BF	101	LMT	C1'-O5'-C5'	-2.32	109.18	113.72
15	BX	1003	LMT	C3'-C4'-C5'	-2.32	105.78	110.93
14	BL	1003	BCL	C2A-C1A-CHA	2.32	127.90	123.87
14	M	408	BCL	C1C-NC-C4C	2.32	107.74	106.68
20	bi	103	OV9	O3P-P-O2P	2.32	118.13	108.94
15	AN	103	LMT	C1-O1'-C1'	2.32	117.64	113.68
14	AV	101	BCL	C1C-NC-C4C	2.32	107.74	106.68
16	BW	1001	V7N	C33-C5-C4	2.32	121.63	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BA	101	V7N	C35-C13-C14	-2.32	119.06	122.82
14	L	1010	BCL	C4A-NA-C1A	2.32	107.74	106.68
14	BN	103	BCL	CAB-C3B-C2B	2.32	132.56	127.74
14	AI	103	BCL	CMB-C2B-C1B	-2.31	121.89	125.42
14	AQ	101	BCL	CMB-C2B-C1B	-2.31	121.89	125.42
15	BH	1002	LMT	C1-O1'-C1'	2.31	117.63	113.68
14	aj	103	BCL	OBB-CAB-CBB	-2.31	114.59	119.77
17	C	403	HEC	CBD-CAD-C3D	-2.31	106.14	112.53
14	ad	1001	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
15	bm	103	LMT	O5'-C1'-C2'	-2.31	105.62	110.37
15	BL	1002	LMT	C3'-C4'-C5'	-2.31	105.81	110.93
16	ba	101	V7N	C4-C5-C6	-2.31	115.38	119.01
14	be	105	BCL	C1C-NC-C4C	2.31	107.73	106.68
15	BR	1002	LMT	O1'-C1'-C2'	2.31	111.78	108.27
16	bb	101	V7N	C2-C3-C4	-2.31	121.67	124.91
20	bg	102	OV9	O3P-P-O2P	2.31	118.08	108.94
14	AP	103	BCL	CMB-C2B-C1B	-2.31	121.91	125.42
14	AE	1001	BCL	OBB-CAB-CBB	-2.31	114.61	119.77
14	ab	102	BCL	C1-O2A-CGA	2.31	122.23	116.65
14	bi	104	BCL	CBA-CAA-C2A	2.31	120.65	113.79
16	BU	1001	V7N	C27-C26-C25	2.30	121.70	118.49
15	BR	1003	LMT	O5'-C1'-C2'	-2.30	105.64	110.37
14	ag	1001	BCL	OBB-CAB-CBB	-2.30	114.61	119.77
15	BI	1004	LMT	O1'-C1'-C2'	2.30	111.77	108.27
16	bk	101	V7N	C36-C18-C19	2.30	121.60	118.09
14	an	1001	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
14	ah	1001	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
15	bb	102	LMT	C1-O1'-C1'	2.30	117.61	113.68
14	ap	1001	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
15	BC	102	LMT	C3'-C4'-C5'	-2.30	105.84	110.93
15	BS	1004	LMT	C3'-C4'-C5'	-2.30	105.84	110.93
15	AP	101	LMT	O5'-C1'-C2'	-2.30	105.65	110.37
16	bl	102	V7N	C2-C3-C4	-2.30	121.69	124.91
14	AV	103	BCL	OBB-CAB-CBB	-2.29	114.63	119.77
14	bm	104	BCL	C2A-C1A-CHA	2.29	127.85	123.87
14	AH	101	BCL	CAA-CBA-CGA	2.29	119.72	113.21
15	BD	102	LMT	C3'-C4'-C5'	-2.29	105.85	110.93
20	bl	103	OV9	O3P-P-O2P	2.29	118.02	108.94
14	bm	104	BCL	CAB-C3B-C2B	2.29	132.50	127.74
14	ai	101	BCL	OBB-CAB-CBB	-2.29	114.64	119.77
16	BR	1001	V7N	C35-C13-C14	-2.29	119.10	122.82
16	bc	101	V7N	C15-C14-C13	-2.29	124.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	ac	1001	BCL	OBB-CAB-CBB	-2.29	114.64	119.77
14	ak	1001	BCL	OBB-CAB-CBB	-2.29	114.64	119.77
17	C	403	HEC	C2A-C1A-NA	-2.29	108.11	110.32
16	bp	101	V7N	C35-C13-C14	-2.29	119.11	122.82
15	be	104	LMT	O5B-C5B-C4B	2.29	113.82	109.70
14	BR	1004	BCL	CAB-C3B-C2B	2.29	132.50	127.74
16	BI	1001	V7N	C33-C5-C4	2.29	121.58	118.09
15	bo	105	LMT	C1-O1'-C1'	2.29	117.59	113.68
14	BU	1004	BCL	CAB-C3B-C2B	2.29	132.50	127.74
16	BC	101	V7N	C35-C13-C12	2.29	121.58	118.09
14	L	1002	BCL	C1-O2A-CGA	2.29	122.18	116.65
20	bg	104	OV9	O2-C10-O4	-2.29	118.36	123.70
16	bj	101	V7N	C36-C18-C19	2.28	121.58	118.09
14	AV	101	BCL	CMB-C2B-C1B	-2.28	121.94	125.42
16	bj	101	V7N	C35-C13-C14	-2.28	119.12	122.82
14	AB	1002	BCL	OBB-CAB-CBB	-2.28	114.66	119.77
14	aa	1001	BCL	C2A-C1A-CHA	2.28	127.83	123.87
14	af	101	BCL	OBB-CAB-CBB	-2.28	114.66	119.77
16	BH	1001	V7N	C15-C14-C13	-2.28	124.08	127.28
16	BS	1001	V7N	C35-C13-C12	2.28	121.57	118.09
14	BW	1003	BCL	C1-O2A-CGA	2.28	122.16	116.65
14	BN	103	BCL	O2A-C1-C2	-2.28	99.35	108.11
14	AR	102	BCL	CMB-C2B-C1B	-2.27	121.95	125.42
14	bn	103	BCL	C2A-C1A-CHA	2.27	127.81	123.87
14	M	405	BCL	OBB-CAB-CBB	-2.27	114.67	119.77
15	AH	102	LMT	O5'-C1'-O1'	-2.27	104.67	110.04
14	af	101	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
16	bd	101	V7N	C1-C2-C3	2.27	118.89	112.98
16	BV	1001	V7N	C35-C13-C14	-2.27	119.13	122.82
14	BR	1004	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
16	bi	101	V7N	C36-C18-C17	-2.27	119.13	122.82
20	be	103	OV9	O2-C10-O4	-2.27	118.40	123.70
16	bb	101	V7N	C35-C13-C14	-2.27	119.14	122.82
16	ba	101	V7N	C36-C18-C17	-2.27	119.14	122.82
14	BT	103	BCL	CBA-CAA-C2A	2.27	120.54	113.79
14	ah	1001	BCL	CMB-C2B-C1B	-2.27	121.97	125.42
14	AQ	101	BCL	C6-C5-C3	2.27	118.99	113.47
16	BE	101	V7N	C35-C13-C12	2.27	121.55	118.09
16	bf	101	V7N	C35-C13-C14	-2.27	119.14	122.82
15	BK	1003	LMT	O5'-C5'-C4'	2.27	114.41	109.72
14	bk	102	BCL	C1C-NC-C4C	2.26	107.71	106.68
15	AQ	103	LMT	C3B-C4B-C5B	-2.26	106.13	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	af	102	CD4	O14-C35-C36	2.26	118.74	111.83
14	AU	103	BCL	CAC-C3C-C4C	2.26	117.61	112.58
20	C1	1001	0V9	O3-C30-O5	-2.26	117.97	123.63
14	bh	105	BCL	CMB-C2B-C1B	-2.26	121.97	125.42
16	bm	101	V7N	C36-C18-C19	2.26	121.54	118.09
16	BL	1001	V7N	C38-C26-C27	-2.26	114.63	118.09
17	C	404	HEC	C2A-C1A-NA	-2.26	108.14	110.32
21	H1	102	CD4	O3-C16-C15	-2.26	101.89	108.40
14	bb	104	BCL	C2A-C1A-CHA	2.26	127.79	123.87
15	AE	1002	LMT	O5B-C5B-C4B	2.26	113.76	109.70
14	BX	1002	BCL	CAB-C3B-C2B	2.26	132.43	127.74
21	M	402	CD4	O2-C14-O1	-2.25	118.44	123.70
16	BU	1001	V7N	C10-C9-C34	2.25	121.44	116.43
16	BP	1001	V7N	C35-C13-C14	-2.25	119.17	122.82
14	bk	102	BCL	CMB-C2B-C1B	-2.25	121.99	125.42
16	BU	1001	V7N	C35-C13-C12	2.25	121.53	118.09
25	M	406	BPH	OBB-CAB-C3B	2.25	123.75	119.99
14	bi	104	BCL	C2A-C1A-CHA	2.25	127.78	123.87
14	an	1001	BCL	CMB-C2B-C1B	-2.25	121.99	125.42
14	BO	1004	BCL	O2A-CGA-O1A	-2.25	118.00	123.63
14	bg	105	BCL	C2A-C1A-CHA	2.25	127.77	123.87
14	AD	102	BCL	OBB-CAB-CBB	-2.25	114.73	119.77
14	BH	1005	BCL	CMB-C2B-C1B	-2.25	122.00	125.42
20	bk	104	0V9	O3P-P-O2P	2.25	117.83	108.94
14	ao	102	BCL	OBB-CAB-CBB	-2.24	114.74	119.77
16	bf	101	V7N	C2-C3-C4	-2.24	121.76	124.91
14	AI	103	BCL	OBB-CAB-CBB	-2.24	114.75	119.77
16	AE	1005	V7N	C33-C5-C4	2.24	121.51	118.09
14	bd	102	BCL	C1C-NC-C4C	2.24	107.70	106.68
14	AQ	101	BCL	OBB-CAB-CBB	-2.24	114.75	119.77
23	M	407	MQ8	C14-C13-C15	-2.24	111.34	115.23
14	BO	1004	BCL	CMB-C2B-C1B	-2.24	122.01	125.42
15	BR	1003	LMT	C1-O1'-C1'	2.24	117.50	113.68
14	AM	102	BCL	OBB-CAB-CBB	-2.24	114.76	119.77
16	be	101	V7N	C29-C28-C27	-2.24	116.72	123.20
21	aj	102	CD4	O14-C35-C36	2.24	118.66	111.83
14	BH	1005	BCL	CBA-CAA-C2A	2.24	120.44	113.79
16	BW	1001	V7N	C20-C21-C22	-2.23	124.55	127.69
14	AM	102	BCL	C1-O2A-CGA	2.23	122.06	116.65
14	BA	103	BCL	CAB-C3B-C2B	2.23	132.38	127.74
16	BC	101	V7N	C33-C5-C4	2.23	121.50	118.09
16	AS	105	V7N	C33-C5-C4	2.23	121.50	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AA	1002	BCL	C6-C5-C3	2.23	118.91	113.47
15	BD	103	LMT	C3'-C4'-C5'	-2.23	105.98	110.93
15	bg	103	LMT	C3'-C4'-C5'	-2.23	105.98	110.93
14	bg	105	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
14	ao	102	BCL	C6-C5-C3	2.23	118.90	113.47
16	bf	101	V7N	C20-C21-C22	-2.23	124.56	127.69
14	AX	102	BCL	CAB-C3B-C2B	2.23	132.37	127.74
16	BJ	1001	V7N	C20-C21-C22	-2.23	124.56	127.69
14	BQ	1003	BCL	CMB-C2B-C1B	-2.23	122.03	125.42
20	bn	104	OV9	O3-C30-O5	-2.23	118.06	123.63
20	H1	101	OV9	O2-C10-O4	-2.23	118.50	123.70
24	L	1006	V7B	O8-C28-C29	2.23	118.62	111.83
14	ah	1001	BCL	C1-O2A-CGA	2.23	122.04	116.65
16	BK	1001	V7N	C33-C5-C4	2.23	121.49	118.09
20	be	102	OV9	O3P-P-O2P	2.22	117.75	108.94
15	bm	103	LMT	C1-O1'-C1'	2.22	117.48	113.68
15	BS	1006	LMT	O1'-C1'-C2'	2.22	111.65	108.27
14	AA	1002	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
14	ad	1001	BCL	OBB-CAB-CBB	-2.22	114.80	119.77
14	AC	103	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
14	bj	103	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
14	AC	101	BCL	C4A-NA-C1A	2.22	107.69	106.68
16	bi	101	V7N	C36-C18-C19	2.21	121.47	118.09
14	BP	1005	BCL	CAB-C3B-C2B	2.21	132.34	127.74
16	bf	101	V7N	C36-C18-C17	-2.21	119.23	122.82
14	bl	104	BCL	C2A-C1A-CHA	2.21	127.71	123.87
16	bp	101	V7N	C20-C21-C22	-2.21	124.58	127.69
14	BI	1003	BCL	CAB-C3B-C2B	2.21	132.33	127.74
15	BS	1002	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
16	BX	1001	V7N	C27-C26-C25	2.21	121.57	118.49
15	AQ	103	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
16	BJ	1001	V7N	C35-C13-C14	-2.21	119.24	122.82
14	BD	105	BCL	CAB-C3B-C2B	2.21	132.33	127.74
14	bj	103	BCL	C1C-NC-C4C	2.21	107.69	106.68
15	BE	102	LMT	O5'-C1'-C2'	-2.21	105.84	110.37
14	AS	104	BCL	OBB-CAB-CBB	-2.21	114.83	119.77
15	AP	101	LMT	C1'-O5'-C5'	-2.21	109.41	113.72
14	BR	1004	BCL	OBB-CAB-CBB	-2.20	114.83	119.77
14	AR	102	BCL	CED-O2D-CGD	2.20	120.91	115.92
15	BD	104	LMT	C1'-O5'-C5'	-2.20	109.42	113.72
16	bk	101	V7N	C35-C13-C14	-2.20	119.25	122.82
15	BG	1002	LMT	O5'-C1'-O1'	-2.20	104.84	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BB	104	LMT	C1-O1'-C1'	2.20	117.44	113.68
15	AJ	104	LMT	O5B-C5B-C4B	2.20	113.66	109.70
14	bb	104	BCL	CMB-C2B-C1B	-2.20	122.07	125.42
14	AP	102	BCL	C6-C5-C3	2.20	118.82	113.47
14	BI	1003	BCL	C2A-C1A-CHA	2.20	127.68	123.87
14	aa	1001	BCL	CAB-C3B-C2B	2.19	132.30	127.74
14	BK	1006	BCL	CBA-CAA-C2A	2.19	120.32	113.79
16	BD	101	V7N	C27-C26-C25	2.19	121.54	118.49
15	BA	104	LMT	C3'-C4'-C5'	-2.19	106.07	110.93
17	C	404	HEC	CAD-CBD-CGD	-2.19	107.85	113.67
14	bm	104	BCL	CMB-C2B-C1B	-2.19	122.08	125.42
14	BI	1003	BCL	O2A-C1-C2	-2.19	99.68	108.11
20	bc	103	OV9	O3P-P-O2P	2.19	117.62	108.94
14	bj	103	BCL	OBB-CAB-CBB	-2.19	114.86	119.77
14	ah	1001	BCL	C2A-C1A-CHA	2.19	127.67	123.87
15	BB	102	LMT	C1'-O5'-C5'	-2.19	109.45	113.72
15	bl	101	LMT	O5B-C5B-C4B	2.19	113.64	109.70
20	bg	104	OV9	O3P-P-O2P	2.19	117.61	108.94
14	BJ	1002	BCL	CAB-C3B-C2B	2.19	132.29	127.74
14	BS	1003	BCL	CAB-C3B-C2B	2.19	132.28	127.74
16	bp	101	V7N	C35-C13-C12	2.19	121.43	118.09
16	bn	102	V7N	C35-C13-C14	-2.19	119.28	122.82
14	BT	103	BCL	CAB-C3B-C2B	2.19	132.28	127.74
18	C	405	V75	C3-O3-C3A	-2.19	114.32	117.72
14	L	1010	BCL	OBB-CAB-CBB	-2.18	114.88	119.77
14	AL	101	BCL	CMB-C2B-C1B	-2.18	122.09	125.42
16	BX	1001	V7N	C36-C18-C17	-2.18	119.28	122.82
14	BN	103	BCL	OBB-CAB-CBB	-2.18	114.88	119.77
14	AJ	102	BCL	CMB-C2B-C1B	-2.18	122.10	125.42
20	be	103	OV9	O3P-P-O2P	2.18	117.58	108.94
14	AQ	101	BCL	C1C-NC-C4C	2.18	107.67	106.68
15	bo	105	LMT	O5'-C1'-O1'	-2.18	104.89	110.04
15	BL	1002	LMT	C3B-C4B-C5B	-2.18	106.28	110.23
15	BN	101	LMT	C3'-C4'-C5'	-2.18	106.10	110.93
14	bf	103	BCL	C1C-NC-C4C	2.18	107.67	106.68
20	bg	102	OV9	O1P-P-O4P	-2.18	97.69	107.57
14	BP	1005	BCL	CMB-C2B-C1B	-2.18	122.10	125.42
23	M	407	MQ8	C15-C13-C12	2.18	126.06	121.17
14	AP	103	BCL	OBB-CAB-CBB	-2.18	114.89	119.77
15	bd	103	LMT	C3'-C4'-C5'	-2.18	106.11	110.93
25	M	406	BPH	C1-C2-C3	2.18	129.76	126.20
15	BS	1004	LMT	O1'-C1'-C2'	2.18	111.58	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	ag	1002	V7B	O8-C9-C8	2.18	114.67	108.40
14	BQ	1003	BCL	CAB-C3B-C2B	2.17	132.26	127.74
14	am	1001	BCL	C6-C5-C3	-2.17	108.17	113.47
14	AD	102	BCL	CMB-C2B-C1B	-2.17	122.11	125.42
16	bp	101	V7N	C36-C18-C19	2.17	121.41	118.09
14	AC	101	BCL	CAB-C3B-C2B	2.17	132.26	127.74
20	bm	102	OV9	O2-C10-O4	-2.17	118.62	123.70
16	bh	102	V7N	C20-C21-C22	-2.17	124.64	127.69
14	ae	102	BCL	C6-C5-C3	2.17	118.76	113.47
16	BR	1001	V7N	C36-C18-C19	2.17	121.41	118.09
16	bp	101	V7N	C27-C26-C25	2.17	121.52	118.49
14	AM	102	BCL	C1-C2-C3	2.17	129.75	126.20
16	bh	102	V7N	C36-C18-C17	-2.17	119.30	122.82
16	BE	101	V7N	C20-C21-C22	-2.17	124.64	127.69
16	bk	101	V7N	C2-C3-C4	-2.17	121.87	124.91
14	BW	1003	BCL	CAB-C3B-C2B	2.17	132.25	127.74
14	AU	103	BCL	C1-C2-C3	2.17	129.75	126.20
14	bl	104	BCL	CMB-C2B-C1B	-2.17	122.12	125.42
14	BE	104	BCL	CAB-C3B-C2B	2.17	132.25	127.74
15	AP	101	LMT	O5'-C5'-C4'	2.17	114.20	109.72
14	bn	103	BCL	CAB-C3B-C2B	2.17	132.24	127.74
25	M	406	BPH	O2D-CGD-CBD	2.17	113.33	110.95
14	AC	101	BCL	CMB-C2B-C1B	-2.17	122.12	125.42
15	BE	102	LMT	O5'-C5'-C4'	2.16	114.20	109.72
14	ai	101	BCL	CAB-C3B-C2B	2.16	132.24	127.74
14	AG	101	BCL	CMB-C2B-C1B	-2.16	122.12	125.42
16	bf	101	V7N	C36-C18-C19	2.16	121.39	118.09
14	BV	1005	BCL	CAB-C3B-C2B	2.16	132.23	127.74
15	bl	101	LMT	O1'-C1'-C2'	2.16	111.56	108.27
15	AI	101	LMT	O1B-C1B-C2B	2.16	113.41	108.09
16	bm	101	V7N	C36-C18-C17	-2.16	119.31	122.82
15	BV	1002	LMT	C3'-C4'-C5'	-2.16	106.14	110.93
20	H1	101	OV9	O3-C30-O5	-2.16	118.22	123.63
20	bp	103	OV9	O3-C30-O5	-2.16	118.22	123.63
14	bf	103	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
16	BO	1001	V7N	C36-C18-C17	-2.16	119.32	122.82
16	bl	102	V7N	C1-C2-C3	2.16	118.59	112.98
16	BC	101	V7N	C15-C14-C13	-2.16	124.25	127.28
14	ba	103	BCL	C1C-NC-C4C	2.16	107.66	106.68
14	bj	103	BCL	CAB-C3B-C2B	2.16	132.22	127.74
16	BU	1001	V7N	C20-C21-C22	-2.16	124.66	127.69
17	C	403	HEC	CHC-C4B-NB	2.15	126.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AE	1003	BCL	CAB-C3B-C2B	2.15	132.22	127.74
14	AB	1001	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
14	AK	101	BCL	C1-C2-C3	-2.15	122.67	126.20
14	AE	1004	BCL	C1-O2A-CGA	2.15	121.86	116.65
15	bj	102	LMT	C1-O1'-C1'	2.15	117.36	113.68
14	AL	101	BCL	C1C-NC-C4C	2.15	107.66	106.68
14	AN	104	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
20	ba	102	0V9	O3-C30-O5	-2.15	118.25	123.63
14	BQ	1003	BCL	OBb-CAB-CBB	-2.15	114.95	119.77
14	BB	103	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
14	bd	102	BCL	CMB-C2B-C1B	-2.15	122.14	125.42
15	AJ	103	LMT	C1-O1'-C1'	2.15	117.36	113.68
16	bp	101	V7N	C36-C18-C17	-2.15	119.33	122.82
14	BO	1004	BCL	CAB-C3B-C2B	2.15	132.21	127.74
14	ah	1001	BCL	CAB-C3B-C2B	2.15	132.20	127.74
15	bc	104	LMT	C3B-C4B-C5B	-2.14	106.34	110.23
14	bl	104	BCL	C1C-NC-C4C	2.14	107.66	106.68
14	BF	102	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
14	AC	103	BCL	CAB-C3B-C2B	2.14	132.19	127.74
14	M	405	BCL	CAB-C3B-C2B	2.14	132.19	127.74
14	AV	101	BCL	CAB-C3B-C2B	2.14	132.19	127.74
23	M	407	MQ8	C21-C20-C18	2.14	120.28	113.19
14	bo	103	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
14	AV	103	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
20	C1	1001	0V9	O3P-P-O2P	2.14	117.42	108.94
14	BP	1005	BCL	OBb-CAB-CBB	-2.14	114.98	119.77
14	AG	101	BCL	CAB-C3B-C2B	2.14	132.19	127.74
24	L	1006	V7B	C43-O52-C47	2.14	117.89	113.72
15	BL	1004	LMT	O5B-C5B-C4B	2.14	113.55	109.70
20	bl	103	0V9	O3-C30-O5	-2.14	118.28	123.63
15	BM	1004	LMT	O1'-C1'-C2'	2.14	111.52	108.27
15	AJ	103	LMT	C1'-O5'-C5'	-2.14	109.55	113.72
14	AQ	101	BCL	CAB-C3B-C2B	2.14	132.18	127.74
14	ao	102	BCL	CAB-C3B-C2B	2.14	132.18	127.74
15	bm	105	LMT	O1'-C1'-C2'	2.13	111.52	108.27
14	AS	102	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
14	bp	102	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
14	BF	102	BCL	CAB-C3B-C2B	2.13	132.18	127.74
16	bd	101	V7N	C27-C26-C25	2.13	121.46	118.49
16	AS	105	V7N	C16-C17-C18	-2.13	124.29	127.28
14	AC	101	BCL	OBb-CAB-CBB	-2.13	114.99	119.77
14	bm	104	BCL	C1C-NC-C4C	2.13	107.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	bj	104	OV9	O3P-P-O2P	2.13	117.39	108.94
14	bf	103	BCL	C11-C10-C8	2.13	123.05	115.97
14	bf	103	BCL	OBB-CAB-CBB	-2.13	114.99	119.77
15	bl	105	LMT	C1'-O5'-C5'	-2.13	109.56	113.72
16	bc	101	V7N	C36-C18-C17	-2.13	119.36	122.82
14	BD	105	BCL	OBB-CAB-CBB	-2.13	115.00	119.77
14	AN	101	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
15	AG	103	LMT	O5B-C5B-C4B	2.13	113.54	109.70
20	bo	104	OV9	O3-C30-O5	-2.13	118.30	123.63
15	BU	1003	LMT	C3'-C4'-C5'	-2.13	106.21	110.93
14	AJ	102	BCL	C1C-NC-C4C	2.13	107.65	106.68
14	AR	102	BCL	OBB-CAB-CBB	-2.13	115.00	119.77
14	BK	1006	BCL	CMB-C2B-C1B	-2.12	122.18	125.42
15	BQ	1004	LMT	C3'-C4'-C5'	-2.12	106.22	110.93
16	AE	1005	V7N	C36-C18-C19	2.12	121.33	118.09
15	bj	102	LMT	C1'-O5'-C5'	-2.12	109.57	113.72
14	BD	105	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
16	bo	102	V7N	C15-C14-C13	-2.12	124.30	127.28
14	af	101	BCL	CAB-C3B-C2B	2.12	132.15	127.74
14	AC	103	BCL	C4A-NA-C1A	2.12	107.65	106.68
14	bc	102	BCL	C1C-NC-C4C	2.12	107.64	106.68
16	BB	101	V7N	C35-C13-C12	2.12	121.32	118.09
14	AP	103	BCL	CAB-C3B-C2B	2.12	132.14	127.74
14	bd	102	BCL	CAB-C3B-C2B	2.12	132.14	127.74
16	bo	102	V7N	C35-C13-C12	2.11	121.32	118.09
16	BV	1001	V7N	C27-C26-C25	2.11	121.43	118.49
14	BC	104	BCL	OBB-CAB-CBB	-2.11	115.04	119.77
25	L	1009	BPH	C1-O2A-CGA	2.11	121.76	116.65
14	BM	1002	BCL	CAB-C3B-C2B	2.11	132.13	127.74
14	bl	104	BCL	CAB-C3B-C2B	2.11	132.13	127.74
14	AN	104	BCL	OBB-CAB-CBB	-2.11	115.04	119.77
16	BE	101	V7N	C33-C5-C4	2.11	121.31	118.09
14	ap	1001	BCL	CAB-C3B-C2B	2.11	132.13	127.74
15	AA	1004	LMT	O1'-C1'-C2'	2.11	111.48	108.27
25	M	406	BPH	CMD-C2D-C3D	2.11	128.90	124.68
14	BW	1003	BCL	CMB-C2B-C1B	-2.11	122.21	125.42
14	AE	1004	BCL	CAB-C3B-C2B	2.11	132.12	127.74
14	L	1010	BCL	CMB-C2B-C1B	-2.11	122.21	125.42
14	BU	1004	BCL	C9-C8-C10	-2.11	103.76	111.27
14	bb	104	BCL	CAB-C3B-C2B	2.11	132.12	127.74
15	AJ	103	LMT	C2'-C3'-C4'	2.11	114.46	109.68
15	BI	1004	LMT	C3'-C4'-C5'	-2.11	106.26	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AE	1005	V7N	C36-C18-C17	-2.11	119.40	122.82
15	bh	101	LMT	O1'-C1'-C2'	2.11	111.47	108.27
14	AS	102	BCL	CAB-C3B-C2B	2.11	132.12	127.74
16	bm	101	V7N	C33-C5-C6	-2.11	119.41	122.82
14	BG	1004	BCL	CAB-C3B-C2B	2.11	132.12	127.74
15	bh	104	LMT	C1-O1'-C1'	2.11	117.28	113.68
14	AU	103	BCL	CMB-C2B-C1B	-2.10	122.21	125.42
14	BE	104	BCL	CMB-C2B-C1B	-2.10	122.21	125.42
14	an	1001	BCL	CAB-C3B-C2B	2.10	132.12	127.74
14	be	105	BCL	CMB-C2B-C1B	-2.10	122.22	125.42
15	bb	102	LMT	O5B-C5B-C4B	2.10	113.48	109.70
20	bj	104	0V9	C2-O2-C10	2.10	122.82	117.80
21	aj	102	CD4	C15-O2-C14	2.10	122.82	117.80
14	bd	102	BCL	OBB-CAB-CBB	-2.10	115.07	119.77
15	BC	106	LMT	C3'-C4'-C5'	-2.10	106.28	110.93
15	BM	1004	LMT	C3'-C4'-C5'	-2.10	106.28	110.93
14	BB	103	BCL	CAB-C3B-C2B	2.10	132.10	127.74
14	bm	104	BCL	C1-C2-C3	2.10	129.63	126.20
15	BK	1004	LMT	C1'-O5'-C5'	-2.10	109.63	113.72
17	C	401	HEC	CMB-C2B-C1B	-2.10	122.23	125.42
16	bo	102	V7N	C36-C18-C19	2.10	121.29	118.09
16	bg	101	V7N	C15-C14-C13	-2.09	124.34	127.28
16	be	101	V7N	C20-C21-C22	-2.09	124.74	127.69
16	BH	1001	V7N	C27-C26-C25	2.09	121.41	118.49
14	AB	1002	BCL	CAB-C3B-C2B	2.09	132.09	127.74
15	AS	101	LMT	O5B-C5B-C4B	2.09	113.47	109.70
16	BD	101	V7N	O45-C40-C39	2.09	127.49	122.09
16	BD	101	V7N	C35-C13-C14	-2.09	119.43	122.82
16	BC	101	V7N	C36-C18-C17	-2.09	119.43	122.82
16	BS	1001	V7N	C36-C18-C17	-2.09	119.43	122.82
14	BH	1005	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
20	bh	103	0V9	O2-C10-O4	-2.09	118.82	123.70
15	AD	101	LMT	C3'-C4'-C5'	-2.09	106.30	110.93
14	BF	102	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
14	bh	105	BCL	CAB-C3B-C2B	2.09	132.08	127.74
14	ba	103	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
16	BK	1001	V7N	C35-C13-C12	2.09	121.28	118.09
14	BE	104	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
14	AH	101	BCL	C6-C5-C3	2.09	118.55	113.47
15	BA	105	LMT	C1'-O5'-C5'	-2.09	109.64	113.72
14	AX	102	BCL	C1C-NC-C4C	2.09	107.63	106.68
16	bl	102	V7N	C3-C4-C5	2.09	129.04	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	bd	101	V7N	C36-C18-C17	-2.09	119.44	122.82
15	BO	1002	LMT	C1'-O5'-C5'	-2.09	109.65	113.72
15	be	104	LMT	C1'-O5'-C5'	-2.09	109.65	113.72
14	AN	104	BCL	C1-C2-C3	-2.09	122.78	126.20
14	AC	103	BCL	OBB-CAB-CBB	-2.09	115.10	119.77
14	BM	1002	BCL	CMB-C2B-C1B	-2.09	122.24	125.42
16	BK	1001	V7N	C36-C18-C17	-2.08	119.44	122.82
14	bh	105	BCL	OBB-CAB-CBB	-2.08	115.11	119.77
25	L	1009	BPH	CMD-C2D-C3D	2.08	128.84	124.68
14	BV	1005	BCL	CMB-C2B-C1B	-2.08	122.25	125.42
14	BX	1002	BCL	CMB-C2B-C1B	-2.08	122.25	125.42
14	AN	101	BCL	OBB-CAB-CBB	-2.08	115.11	119.77
16	BX	1001	V7N	C35-C13-C12	2.08	121.27	118.09
14	ak	1001	BCL	CAB-C3B-C2B	2.08	132.07	127.74
15	BT	101	LMT	O5'-C1'-C2'	-2.08	106.09	110.37
15	AX	101	LMT	O5'-C5'-C4'	2.08	114.03	109.72
14	BC	104	BCL	CMB-C2B-C1B	-2.08	122.25	125.42
14	BL	1003	BCL	CMB-C2B-C1B	-2.08	122.25	125.42
15	bl	105	LMT	C3'-C4'-C5'	-2.08	106.32	110.93
14	ac	1001	BCL	CAB-C3B-C2B	2.08	132.06	127.74
16	BQ	1001	V7N	C27-C26-C25	2.08	121.39	118.49
14	AM	102	BCL	CAB-C3B-C2B	2.08	132.06	127.74
28	ai	102	UYH	O7-C10-C11	2.08	115.98	111.48
14	bo	103	BCL	C1C-NC-C4C	2.08	107.63	106.68
14	AV	101	BCL	OBB-CAB-CBB	-2.08	115.12	119.77
14	bj	103	BCL	C2A-C1A-CHA	2.08	127.47	123.87
20	bp	103	OV9	O2-C10-O4	-2.08	118.85	123.70
14	bl	104	BCL	OBB-CAB-CBB	-2.08	115.12	119.77
15	BT	101	LMT	C1-O1'-C1'	2.08	117.23	113.68
14	BL	1003	BCL	CBA-CAA-C2A	2.07	119.97	113.79
14	bk	102	BCL	OBB-CAB-CBB	-2.07	115.13	119.77
15	L	1011	LMT	C1-O1'-C1'	2.07	117.22	113.68
14	AG	101	BCL	CBA-CAA-C2A	2.07	119.96	113.79
16	BA	101	V7N	C36-C18-C17	-2.07	119.46	122.82
14	BA	103	BCL	C7-C6-C5	2.07	118.78	113.26
14	AH	101	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
15	AJ	104	LMT	C1'-O5'-C5'	-2.07	109.68	113.72
15	BS	1005	LMT	C1'-O5'-C5'	-2.07	109.68	113.72
14	AB	1001	BCL	C6-C5-C3	2.07	118.50	113.47
14	bp	102	BCL	OBB-CAB-CBB	-2.07	115.14	119.77
16	BR	1001	V7N	C36-C18-C17	-2.07	119.47	122.82
14	bm	104	BCL	OBB-CAB-CBB	-2.06	115.14	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	ab	101	LMT	C1'-O5'-C5'	-2.06	109.69	113.72
14	BX	1002	BCL	OBB-CAB-CBB	-2.06	115.15	119.77
16	BS	1001	V7N	C27-C26-C25	2.06	121.36	118.49
14	AA	1002	BCL	OBB-CAB-CBB	-2.06	115.15	119.77
14	bp	102	BCL	CAB-C3B-C2B	2.06	132.03	127.74
14	bo	103	BCL	C2A-C1A-CHA	2.06	127.45	123.87
14	AJ	102	BCL	OBB-CAB-CBB	-2.06	115.15	119.77
16	bm	101	V7N	C27-C26-C25	2.06	121.36	118.49
15	AI	101	LMT	O5'-C1'-O1'	-2.06	105.17	110.04
16	bm	101	V7N	C3-C4-C5	2.06	129.01	125.89
16	BM	1001	V7N	O45-C40-C39	2.06	127.41	122.09
14	ae	102	BCL	CAB-C3B-C2B	2.06	132.03	127.74
14	aj	103	BCL	CAB-C3B-C2B	2.06	132.02	127.74
14	al	1001	BCL	CAB-C3B-C2B	2.06	132.02	127.74
14	bg	105	BCL	OBB-CAB-CBB	-2.06	115.16	119.77
14	ad	1001	BCL	CAB-C3B-C2B	2.06	132.02	127.74
16	BC	101	V7N	C11-C10-C9	2.06	129.94	127.28
14	BA	103	BCL	CMB-C2B-C1B	-2.06	122.28	125.42
20	bp	103	0V9	O3P-P-O2P	2.06	117.09	108.94
15	BT	102	LMT	O5'-C1'-O1'	-2.06	105.18	110.04
14	AE	1003	BCL	C6-C5-C3	2.06	118.48	113.47
14	bc	102	BCL	CMB-C2B-C1B	-2.06	122.29	125.42
20	bj	104	0V9	O3-C30-O5	-2.05	118.49	123.63
16	BB	101	V7N	C11-C10-C9	2.05	129.93	127.28
20	bk	103	0V9	O3-C30-O5	-2.05	118.49	123.63
15	BW	1004	LMT	C1'-O5'-C5'	-2.05	109.71	113.72
14	AR	102	BCL	O2D-CGD-O1D	-2.05	119.85	123.85
14	AS	102	BCL	OBB-CAB-CBB	-2.05	115.17	119.77
14	BT	103	BCL	CMB-C2B-C1B	-2.05	122.30	125.42
14	be	105	BCL	OBB-CAB-CBB	-2.05	115.18	119.77
15	L	1005	LMT	O5'-C1'-C2'	-2.05	106.16	110.37
14	BL	1003	BCL	OBB-CAB-CBB	-2.05	115.18	119.77
14	AU	103	BCL	OBB-CAB-CBB	-2.05	115.18	119.77
16	BJ	1001	V7N	C36-C18-C17	-2.05	119.50	122.82
14	BJ	1002	BCL	OBB-CAB-CBB	-2.05	115.18	119.77
16	bj	101	V7N	C11-C10-C9	2.05	129.92	127.28
15	AG	103	LMT	C3'-C4'-C5'	-2.05	106.39	110.93
14	BI	1003	BCL	CMB-C2B-C1B	-2.05	122.30	125.42
16	BX	1001	V7N	O45-C40-C39	2.05	127.37	122.09
14	AL	101	BCL	OBB-CAB-CBB	-2.05	115.19	119.77
14	AE	1004	BCL	C6-C5-C3	2.05	118.45	113.47
14	bg	105	BCL	CAB-C3B-C2B	2.04	131.99	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BW	1003	BCL	OBB-CAB-CBB	-2.04	115.19	119.77
14	BO	1004	BCL	C1-O2A-CGA	2.04	121.60	116.65
16	BD	101	V7N	C36-C18-C17	-2.04	119.50	122.82
15	ab	101	LMT	C3'-C4'-C5'	-2.04	106.40	110.93
20	bn	104	0V9	O3P-P-O2P	2.04	117.03	108.94
16	BI	1001	V7N	C36-C18-C17	-2.04	119.51	122.82
16	bk	101	V7N	C36-C18-C17	-2.04	119.51	122.82
16	bl	102	V7N	C35-C13-C14	-2.04	119.51	122.82
20	bk	103	0V9	O3P-P-O2P	2.04	117.03	108.94
14	BH	1005	BCL	CAB-C3B-C2B	2.04	131.99	127.74
20	bh	103	0V9	O1P-P-O4P	-2.04	98.31	107.57
16	BQ	1001	V7N	C36-C18-C17	-2.04	119.51	122.82
16	BV	1001	V7N	C36-C18-C17	-2.04	119.51	122.82
20	bl	103	0V9	O1P-P-O4P	-2.04	98.32	107.57
14	L	1010	BCL	C1C-NC-C4C	2.04	107.61	106.68
16	BQ	1001	V7N	O45-C40-C39	2.04	127.35	122.09
14	bi	104	BCL	CMB-C2B-C1B	-2.04	122.32	125.42
14	AA	1002	BCL	CAB-C3B-C2B	2.04	131.98	127.74
14	am	1001	BCL	CAB-C3B-C2B	2.04	131.97	127.74
14	bc	102	BCL	CAB-C3B-C2B	2.04	131.97	127.74
16	bn	102	V7N	O45-C40-C39	2.04	127.34	122.09
14	bn	103	BCL	CMB-C2B-C1B	-2.04	122.32	125.42
14	bc	102	BCL	C2A-C1A-CHA	2.04	127.40	123.87
16	BJ	1001	V7N	C15-C14-C13	-2.04	124.42	127.28
16	BL	1001	V7N	C20-C21-C22	-2.04	124.83	127.69
16	bj	101	V7N	O45-C40-C39	2.04	127.34	122.09
14	AH	101	BCL	CAB-C3B-C2B	2.04	131.97	127.74
16	ba	101	V7N	C16-C17-C18	-2.03	124.42	127.28
15	bd	103	LMT	C1'-O5'-C5'	-2.03	109.75	113.72
14	BS	1003	BCL	CMB-C2B-C1B	-2.03	122.33	125.42
14	AG	101	BCL	OBB-CAB-CBB	-2.03	115.22	119.77
14	BT	103	BCL	C1-C2-C3	-2.03	122.87	126.20
14	AU	103	BCL	CAA-CBA-CGA	2.03	118.97	113.21
14	BT	103	BCL	OBB-CAB-CBB	-2.03	115.22	119.77
15	BQ	1004	LMT	O1'-C1'-C2'	2.03	111.36	108.27
15	BS	1002	LMT	C1'-O5'-C5'	-2.03	109.76	113.72
15	BG	1002	LMT	O5B-C5B-C4B	2.03	113.36	109.70
15	BS	1006	LMT	C1'-O5'-C5'	-2.03	109.76	113.72
14	AU	103	BCL	CAB-C3B-C2B	2.03	131.96	127.74
14	BU	1004	BCL	CMB-C2B-C1B	-2.03	122.33	125.42
15	BB	105	LMT	C1-O1'-C1'	2.03	117.14	113.68
14	AX	102	BCL	CAA-CBA-CGA	2.03	118.96	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	bf	103	BCL	C2A-C1A-CHA	2.03	127.39	123.87
14	bm	104	BCL	C4-C3-C5	-2.03	111.71	115.23
14	BV	1005	BCL	OBB-CAB-CBB	-2.03	115.23	119.77
16	BH	1001	V7N	O45-C40-C39	2.03	127.32	122.09
16	BJ	1001	V7N	O45-C40-C39	2.03	127.32	122.09
14	BK	1006	BCL	OBB-CAB-CBB	-2.03	115.23	119.77
15	BK	1002	LMT	C3B-C4B-C5B	-2.02	106.56	110.23
20	bc	103	0V9	O1P-P-O4P	-2.02	98.39	107.57
14	AH	101	BCL	C1C-NC-C4C	2.02	107.60	106.68
16	bo	102	V7N	O45-C40-C39	2.02	127.31	122.09
14	BO	1004	BCL	OBB-CAB-CBB	-2.02	115.25	119.77
16	BL	1001	V7N	O45-C40-C39	2.02	127.30	122.09
14	AJ	102	BCL	CAB-C3B-C2B	2.02	131.94	127.74
14	bb	104	BCL	OBB-CAB-CBB	-2.02	115.25	119.77
16	bi	101	V7N	C15-C14-C13	-2.02	124.45	127.28
16	be	101	V7N	C38-C26-C27	-2.02	115.01	118.09
16	BG	1001	V7N	O45-C40-C39	2.01	127.29	122.09
14	bh	105	BCL	C1C-NC-C4C	2.01	107.60	106.68
15	BD	103	LMT	O5'-C1'-C2'	-2.01	106.23	110.37
16	bg	101	V7N	C27-C26-C25	2.01	121.30	118.49
14	bo	103	BCL	OBB-CAB-CBB	-2.01	115.26	119.77
16	AS	105	V7N	C35-C13-C12	2.01	121.16	118.09
15	AH	104	LMT	C1B-O5B-C5B	2.01	117.65	113.72
15	BI	1004	LMT	C1'-O5'-C5'	-2.01	109.79	113.72
14	bc	102	BCL	OBB-CAB-CBB	-2.01	115.27	119.77
14	ag	1001	BCL	CAB-C3B-C2B	2.01	131.92	127.74
20	H1	101	0V9	O3P-P-O2P	2.01	116.90	108.94
16	BU	1001	V7N	O45-C40-C39	2.01	127.27	122.09
16	BE	101	V7N	C36-C18-C17	-2.01	119.56	122.82
14	AN	101	BCL	CAB-C3B-C2B	2.01	131.91	127.74
14	bk	102	BCL	C2A-C1A-CHA	2.01	127.35	123.87
14	BA	103	BCL	OBB-CAB-CBB	-2.01	115.27	119.77
15	AF	1002	LMT	C1'-O5'-C5'	-2.01	109.80	113.72
14	bb	104	BCL	C1C-NC-C4C	2.01	107.59	106.68
14	bi	104	BCL	C1C-NC-C4C	2.01	107.59	106.68
14	BI	1003	BCL	OBB-CAB-CBB	-2.01	115.27	119.77
14	bi	104	BCL	OBB-CAB-CBB	-2.01	115.27	119.77
15	BB	104	LMT	C1'-O5'-C5'	-2.01	109.80	113.72
14	AC	103	BCL	CAC-C3C-C4C	2.01	117.04	112.58
16	bi	101	V7N	O45-C40-C39	2.01	127.27	122.09
14	BB	103	BCL	OBB-CAB-CBB	-2.01	115.28	119.77
14	bf	103	BCL	CAB-C3B-C2B	2.01	131.91	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BV	1003	LMT	O1'-C1'-C2'	2.01	111.32	108.27
15	bh	104	LMT	O5B-C5B-C4B	2.01	113.31	109.70
15	bf	102	LMT	C1'-O5'-C5'	-2.01	109.80	113.72
20	aj	101	OV9	O3P-P-O2P	2.00	116.88	108.94
16	BM	1001	V7N	C36-C18-C17	-2.00	119.57	122.82
14	bi	104	BCL	CAB-C3B-C2B	2.00	131.90	127.74
16	bi	101	V7N	C11-C10-C9	2.00	129.86	127.28
14	bn	103	BCL	OBb-CAB-CBB	-2.00	115.29	119.77
15	bo	101	LMT	C1'-O5'-C5'	-2.00	109.81	113.72
14	AS	104	BCL	CAB-C3B-C2B	2.00	131.90	127.74

There are no chirality outliers.

All (1824) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	AB	1002	BCL	C1A-C2A-CAA-CBA
14	AB	1002	BCL	C3A-C2A-CAA-CBA
14	AC	101	BCL	C1A-C2A-CAA-CBA
14	AC	101	BCL	C3A-C2A-CAA-CBA
14	AC	103	BCL	C3A-C2A-CAA-CBA
14	AE	1003	BCL	C1A-C2A-CAA-CBA
14	AG	101	BCL	C2C-C3C-CAC-CBC
14	AG	101	BCL	C4C-C3C-CAC-CBC
14	AH	101	BCL	C1A-C2A-CAA-CBA
14	AH	101	BCL	C3A-C2A-CAA-CBA
14	AJ	102	BCL	C1A-C2A-CAA-CBA
14	AJ	102	BCL	C3A-C2A-CAA-CBA
14	AK	101	BCL	C1A-C2A-CAA-CBA
14	AK	101	BCL	C3A-C2A-CAA-CBA
14	AL	101	BCL	C1A-C2A-CAA-CBA
14	AN	104	BCL	C1A-C2A-CAA-CBA
14	AN	104	BCL	C3A-C2A-CAA-CBA
14	AQ	101	BCL	C1A-C2A-CAA-CBA
14	AQ	101	BCL	C3A-C2A-CAA-CBA
14	AR	102	BCL	C1A-C2A-CAA-CBA
14	AR	102	BCL	CBD-CGD-O2D-CED
14	AS	104	BCL	CBA-CGA-O2A-C1
14	AS	104	BCL	O1A-CGA-O2A-C1
14	AV	103	BCL	C1A-C2A-CAA-CBA
14	AV	103	BCL	C3A-C2A-CAA-CBA
14	AX	102	BCL	C1A-C2A-CAA-CBA
14	AX	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	BG	1004	BCL	C1A-C2A-CAA-CBA
14	BG	1004	BCL	C3A-C2A-CAA-CBA
14	BO	1004	BCL	CBA-CGA-O2A-C1
14	BO	1004	BCL	O1A-CGA-O2A-C1
14	BP	1005	BCL	C1A-C2A-CAA-CBA
14	BP	1005	BCL	C3A-C2A-CAA-CBA
14	BQ	1003	BCL	C1A-C2A-CAA-CBA
14	BR	1004	BCL	C1A-C2A-CAA-CBA
14	BU	1004	BCL	C1A-C2A-CAA-CBA
14	BX	1002	BCL	CBA-CGA-O2A-C1
14	BX	1002	BCL	O1A-CGA-O2A-C1
14	ao	102	BCL	C4-C3-C5-C6
14	bc	102	BCL	C3A-C2A-CAA-CBA
14	be	105	BCL	C1A-C2A-CAA-CBA
14	be	105	BCL	C3A-C2A-CAA-CBA
14	bf	103	BCL	C1A-C2A-CAA-CBA
14	bf	103	BCL	C3A-C2A-CAA-CBA
14	bj	103	BCL	C1A-C2A-CAA-CBA
14	bj	103	BCL	C3A-C2A-CAA-CBA
14	bm	104	BCL	C1A-C2A-CAA-CBA
14	bm	104	BCL	C3A-C2A-CAA-CBA
14	bo	103	BCL	C1A-C2A-CAA-CBA
14	bo	103	BCL	C3A-C2A-CAA-CBA
15	AA	1003	LMT	C2'-C1'-O1'-C1
15	AA	1003	LMT	O5'-C1'-O1'-C1
15	AA	1004	LMT	C2'-C1'-O1'-C1
15	AA	1004	LMT	O5'-C1'-O1'-C1
15	AH	102	LMT	C2'-C1'-O1'-C1
15	AP	101	LMT	C2'-C1'-O1'-C1
15	AP	101	LMT	O5'-C1'-O1'-C1
15	AQ	103	LMT	C2'-C1'-O1'-C1
15	AQ	103	LMT	O5'-C1'-O1'-C1
15	AT	102	LMT	O5'-C1'-O1'-C1
15	AX	101	LMT	O5'-C1'-O1'-C1
15	BG	1002	LMT	O5'-C1'-O1'-C1
15	BG	1002	LMT	C2-C1-O1'-C1'
15	BK	1003	LMT	C2'-C1'-O1'-C1
15	BP	1004	LMT	C2-C1-O1'-C1'
15	BT	102	LMT	O5'-C1'-O1'-C1
15	BU	1002	LMT	O5'-C1'-O1'-C1
15	BV	1004	LMT	O5'-C1'-O1'-C1
15	L	1003	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
15	L	1008	LMT	C2-C1-O1'-C1'
15	bb	102	LMT	O5'-C1'-O1'-C1
15	bg	103	LMT	C2'-C1'-O1'-C1
15	bg	103	LMT	O5'-C1'-O1'-C1
15	bm	105	LMT	C2'-C1'-O1'-C1
15	bm	105	LMT	O5'-C1'-O1'-C1
15	bo	105	LMT	O5'-C1'-O1'-C1
16	AS	105	V7N	C25-C26-C27-C28
16	AS	105	V7N	C38-C26-C27-C28
16	BA	101	V7N	C25-C26-C27-C28
16	BA	101	V7N	C38-C26-C27-C28
16	BG	1001	V7N	C25-C26-C27-C28
16	BI	1001	V7N	C25-C26-C27-C28
16	BI	1001	V7N	C38-C26-C27-C28
16	BI	1001	V7N	C27-C28-C29-C39
16	BK	1001	V7N	C27-C28-C29-C39
16	BM	1001	V7N	C25-C26-C27-C28
16	BP	1001	V7N	C27-C28-C29-C39
16	BQ	1001	V7N	O42-C34-C9-C10
16	BU	1001	V7N	O42-C34-C9-C10
16	BW	1001	V7N	C25-C26-C27-C28
16	BX	1001	V7N	C27-C28-C29-C39
16	ba	101	V7N	C1-C2-C3-C4
16	ba	101	V7N	C23-C24-C25-C26
16	ba	101	V7N	C26-C27-C28-C29
16	bb	101	V7N	C25-C26-C27-C28
16	bb	101	V7N	C38-C26-C27-C28
16	bb	101	V7N	C26-C27-C28-C29
16	bc	101	V7N	C25-C26-C27-C28
16	bd	101	V7N	C27-C28-C29-C39
16	be	101	V7N	C26-C27-C28-C29
16	be	101	V7N	C27-C28-C29-C39
16	bg	101	V7N	C38-C26-C27-C28
16	bh	102	V7N	C25-C26-C27-C28
16	bh	102	V7N	C38-C26-C27-C28
16	bj	101	V7N	C2-C1-O32-C41
16	bm	101	V7N	C30-C1-C2-C3
16	bm	101	V7N	C31-C1-C2-C3
16	bm	101	V7N	O32-C1-C2-C3
16	bm	101	V7N	C25-C26-C27-C28
16	bm	101	V7N	C38-C26-C27-C28
16	bo	102	V7N	O42-C34-C9-C10

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Mol	Chain	Res	Type	Atoms
16	bp	101	V7N	C27-C28-C29-C39
17	C	401	HEC	C2B-C3B-CAB-CBB
17	C	401	HEC	C4B-C3B-CAB-CBB
17	C	401	HEC	C2C-C3C-CAC-CBC
17	C	401	HEC	C4C-C3C-CAC-CBC
17	C	402	HEC	C2B-C3B-CAB-CBB
17	C	402	HEC	C4B-C3B-CAB-CBB
17	C	402	HEC	C2C-C3C-CAC-CBC
17	C	402	HEC	C4C-C3C-CAC-CBC
17	C	403	HEC	C2B-C3B-CAB-CBB
17	C	403	HEC	C4B-C3B-CAB-CBB
17	C	403	HEC	C2C-C3C-CAC-CBC
17	C	403	HEC	C4C-C3C-CAC-CBC
17	C	404	HEC	C2B-C3B-CAB-CBB
17	C	404	HEC	C4B-C3B-CAB-CBB
17	C	404	HEC	C2C-C3C-CAC-CBC
17	C	404	HEC	C4C-C3C-CAC-CBC
20	C1	1001	0V9	C1-O3P-P-O2P
20	C1	1001	0V9	C1-O3P-P-O4P
20	C1	1001	0V9	C4-O4P-P-O2P
20	C1	1001	0V9	C4-O4P-P-O3P
20	aj	101	0V9	C1-O3P-P-O1P
20	ba	102	0V9	C2-C1-O3P-P
20	ba	102	0V9	C5-C4-O4P-P
20	ba	102	0V9	C4-O4P-P-O1P
20	bb	103	0V9	C2-C1-O3P-P
20	bc	103	0V9	C2-C1-O3P-P
20	bc	103	0V9	C1-O3P-P-O4P
20	bc	103	0V9	C4-O4P-P-O3P
20	be	102	0V9	C1-O3P-P-O1P
20	bg	102	0V9	C5-C4-O4P-P
20	bg	102	0V9	C1-O3P-P-O1P
20	bg	102	0V9	C1-O3P-P-O2P
20	bg	102	0V9	C1-O3P-P-O4P
20	bh	103	0V9	C2-C1-O3P-P
20	bh	103	0V9	C1-O3P-P-O1P
20	bi	103	0V9	C2-C1-O3P-P
20	bi	103	0V9	C5-C4-O4P-P
20	bi	103	0V9	C1-O3P-P-O2P
20	bi	103	0V9	C1-O3P-P-O4P
20	bj	104	0V9	C2-C1-O3P-P
20	bj	104	0V9	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
20	bj	104	0V9	C1-O3P-P-O2P
20	bj	104	0V9	C1-O3P-P-O4P
20	bk	103	0V9	C1-O3P-P-O2P
20	bk	103	0V9	C1-O3P-P-O4P
20	bk	104	0V9	C5-C4-O4P-P
20	bk	104	0V9	C1-O3P-P-O1P
20	bk	104	0V9	C4-O4P-P-O3P
20	bl	103	0V9	C2-C1-O3P-P
20	bl	103	0V9	C5-C4-O4P-P
20	bl	103	0V9	C1-O3P-P-O2P
20	bl	103	0V9	C1-O3P-P-O4P
20	bm	102	0V9	C2-C1-O3P-P
20	bn	104	0V9	C2-C1-O3P-P
20	bn	104	0V9	C1-O3P-P-O2P
20	bn	104	0V9	C1-O3P-P-O4P
20	bo	104	0V9	C2-C1-O3P-P
20	bo	104	0V9	C5-C4-O4P-P
20	bp	103	0V9	C2-C1-O3P-P
20	bp	103	0V9	C5-C4-O4P-P
20	bp	103	0V9	C1-O3P-P-O4P
21	H1	102	CD4	C28-O5-P1-O7
21	H1	104	CD4	C13-C14-O2-C15
21	H1	104	CD4	C31-O10-P2-O11
21	H1	104	CD4	C31-O10-P2-O12
21	H1	104	CD4	C31-O10-P2-O13
21	M	402	CD4	C13-C14-O2-C15
21	M	402	CD4	C29-C30-C31-O10
21	M	402	CD4	O9-C30-C31-O10
21	M	402	CD4	C32-O13-P2-O10
21	M	402	CD4	C32-O13-P2-O11
21	M	402	CD4	C32-O13-P2-O12
21	ae	101	CD4	O1-C14-O2-C15
21	ae	101	CD4	C15-C28-O5-P1
21	ae	101	CD4	C29-O8-P1-O5
21	ae	101	CD4	C29-O8-P1-O6
21	af	102	CD4	C15-C28-O5-P1
21	aj	102	CD4	C13-C14-O2-C15
21	aj	102	CD4	C15-C28-O5-P1
21	aj	102	CD4	C29-O8-P1-O5
21	aj	102	CD4	C29-O8-P1-O7
22	H1	103	PGW	C04-O12-P-O14
27	M	404	CRT	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
15	AJ	103	LMT	O5B-C1B-O1B-C4'
15	BK	1003	LMT	O5B-C1B-O1B-C4'
15	AJ	103	LMT	C2B-C1B-O1B-C4'
15	AH	104	LMT	O5B-C1B-O1B-C4'
15	BK	1003	LMT	C2B-C1B-O1B-C4'
15	AJ	104	LMT	O5B-C1B-O1B-C4'
15	BL	1002	LMT	O5B-C1B-O1B-C4'
14	AR	102	BCL	O1D-CGD-O2D-CED
14	BI	1003	BCL	O1A-CGA-O2A-C1
15	BT	102	LMT	O5B-C1B-O1B-C4'
15	AJ	104	LMT	C2B-C1B-O1B-C4'
21	H1	104	CD4	O1-C14-O2-C15
21	M	402	CD4	O1-C14-O2-C15
21	aj	102	CD4	O1-C14-O2-C15
14	AK	101	BCL	C3-C5-C6-C7
14	AS	104	BCL	C3-C5-C6-C7
14	AV	103	BCL	C3-C5-C6-C7
14	BN	103	BCL	C3-C5-C6-C7
14	bj	103	BCL	C3-C5-C6-C7
21	ae	101	CD4	C18-C17-O3-C16
15	bb	102	LMT	O5'-C5'-C6'-O6'
15	AE	1002	LMT	C3'-C4'-O1B-C1B
21	ae	101	CD4	C13-C14-O2-C15
14	ao	102	BCL	C2-C3-C5-C6
14	BC	104	BCL	C2A-CAA-CBA-CGA
16	AS	105	V7N	C27-C28-C29-C39
16	BL	1001	V7N	C27-C28-C29-C39
16	BO	1001	V7N	C27-C28-C29-C39
16	bb	101	V7N	C27-C28-C29-C39
16	bg	101	V7N	C27-C28-C29-C39
16	bi	101	V7N	C27-C28-C29-C39
16	bo	102	V7N	C27-C28-C29-C39
15	be	104	LMT	C4'-C5'-C6'-O6'
14	AC	101	BCL	C3-C5-C6-C7
14	AU	102	BCL	C3-C5-C6-C7
15	BX	1003	LMT	O5B-C1B-O1B-C4'
15	BO	1002	LMT	C2B-C1B-O1B-C4'
21	H1	102	CD4	O9-C30-C31-O10
15	BA	105	LMT	O5'-C5'-C6'-O6'
15	BH	1003	LMT	O5'-C5'-C6'-O6'
15	BR	1003	LMT	C3'-C4'-O1B-C1B
15	BO	1002	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
15	BX	1004	LMT	O5B-C1B-O1B-C4'
15	BM	1003	LMT	C2B-C1B-O1B-C4'
15	BF	103	LMT	O5'-C5'-C6'-O6'
15	BW	1004	LMT	O5'-C5'-C6'-O6'
15	BM	1003	LMT	O5B-C1B-O1B-C4'
14	BI	1003	BCL	CBA-CGA-O2A-C1
14	BN	103	BCL	O1A-CGA-O2A-C1
15	M	403	LMT	O5'-C5'-C6'-O6'
28	ai	102	UYH	O6-C5-C6-O5
23	L	1001	MQ8	C33-C35-C36-C37
15	bb	102	LMT	C4'-C5'-C6'-O6'
15	bo	105	LMT	C4'-C5'-C6'-O6'
15	AP	104	LMT	C2B-C1B-O1B-C4'
15	AP	104	LMT	O5B-C1B-O1B-C4'
15	AH	102	LMT	O5'-C1'-O1'-C1
15	AJ	103	LMT	O5'-C1'-O1'-C1
15	BA	104	LMT	O5'-C1'-O1'-C1
15	BC	103	LMT	O5'-C1'-O1'-C1
15	BD	103	LMT	O5'-C1'-O1'-C1
15	BH	1003	LMT	O5'-C1'-O1'-C1
15	BK	1003	LMT	O5'-C1'-O1'-C1
15	BL	1002	LMT	O5'-C1'-O1'-C1
15	L	1003	LMT	O5'-C1'-O1'-C1
15	be	104	LMT	O5'-C5'-C6'-O6'
15	bm	105	LMT	O5'-C5'-C6'-O6'
15	bo	105	LMT	O5'-C5'-C6'-O6'
15	AI	101	LMT	C2B-C1B-O1B-C4'
15	AF	1002	LMT	O5'-C5'-C6'-O6'
15	be	104	LMT	O5B-C1B-O1B-C4'
15	BS	1004	LMT	O5B-C1B-O1B-C4'
15	AF	1002	LMT	O5B-C5B-C6B-O6B
15	bh	101	LMT	O5'-C5'-C6'-O6'
20	bb	103	0V9	C11-C10-O2-C2
15	BS	1006	LMT	O5B-C1B-O1B-C4'
15	BA	105	LMT	C4'-C5'-C6'-O6'
15	BC	106	LMT	C4'-C5'-C6'-O6'
15	BS	1006	LMT	C2B-C1B-O1B-C4'
14	BM	1002	BCL	C3-C5-C6-C7
14	AE	1003	BCL	C11-C12-C13-C14
14	AN	104	BCL	C6-C7-C8-C9
14	BA	103	BCL	C6-C7-C8-C9
14	BS	1003	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	BX	1002	BCL	C6-C7-C8-C9
14	ab	102	BCL	C6-C7-C8-C9
14	an	1001	BCL	C11-C10-C8-C9
15	AG	103	LMT	O5B-C5B-C6B-O6B
15	AX	101	LMT	C2'-C1'-O1'-C1
15	BA	104	LMT	C2'-C1'-O1'-C1
15	BD	103	LMT	C2'-C1'-O1'-C1
15	BH	1003	LMT	C2'-C1'-O1'-C1
15	BL	1002	LMT	C2'-C1'-O1'-C1
15	BU	1002	LMT	C2'-C1'-O1'-C1
21	ae	101	CD4	O9-C30-C31-O10
15	BD	102	LMT	O5'-C5'-C6'-O6'
15	BM	1003	LMT	O5'-C5'-C6'-O6'
15	BQ	1004	LMT	O5'-C5'-C6'-O6'
21	ae	101	CD4	O4-C17-O3-C16
15	bh	101	LMT	C4'-C5'-C6'-O6'
16	AE	1005	V7N	C38-C26-C27-C28
16	AO	1001	V7N	C3-C4-C5-C33
16	BB	101	V7N	C38-C26-C27-C28
16	BC	101	V7N	C38-C26-C27-C28
16	BD	101	V7N	C38-C26-C27-C28
16	BG	1001	V7N	C38-C26-C27-C28
16	BH	1001	V7N	C3-C4-C5-C33
16	BJ	1001	V7N	C38-C26-C27-C28
16	BL	1001	V7N	C38-C26-C27-C28
16	BL	1001	V7N	C3-C4-C5-C33
16	BM	1001	V7N	C38-C26-C27-C28
16	BQ	1001	V7N	C38-C26-C27-C28
16	BR	1001	V7N	C3-C4-C5-C33
16	BS	1001	V7N	C38-C26-C27-C28
16	BW	1001	V7N	C38-C26-C27-C28
16	ba	101	V7N	C38-C26-C27-C28
16	bb	101	V7N	C3-C4-C5-C33
16	bc	101	V7N	C38-C26-C27-C28
16	bd	101	V7N	C38-C26-C27-C28
16	be	101	V7N	C38-C26-C27-C28
16	bf	101	V7N	C38-C26-C27-C28
16	bf	101	V7N	C3-C4-C5-C33
16	bh	102	V7N	C3-C4-C5-C33
16	bj	101	V7N	C38-C26-C27-C28
16	bk	101	V7N	C38-C26-C27-C28
16	bn	102	V7N	C38-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
16	AE	1005	V7N	C25-C26-C27-C28
16	AO	1001	V7N	C3-C4-C5-C6
16	BB	101	V7N	C25-C26-C27-C28
16	BD	101	V7N	C25-C26-C27-C28
16	BE	101	V7N	C25-C26-C27-C28
16	BH	1001	V7N	C3-C4-C5-C6
16	BJ	1001	V7N	C25-C26-C27-C28
16	BL	1001	V7N	C25-C26-C27-C28
16	BO	1001	V7N	C3-C4-C5-C6
16	BQ	1001	V7N	C25-C26-C27-C28
16	BR	1001	V7N	C3-C4-C5-C6
16	BS	1001	V7N	C25-C26-C27-C28
16	BU	1001	V7N	C25-C26-C27-C28
16	bd	101	V7N	C25-C26-C27-C28
16	bf	101	V7N	C25-C26-C27-C28
16	bg	101	V7N	C25-C26-C27-C28
16	bj	101	V7N	C25-C26-C27-C28
16	bk	101	V7N	C25-C26-C27-C28
16	bl	102	V7N	C25-C26-C27-C28
16	bn	102	V7N	C25-C26-C27-C28
27	M	404	CRT	C32-C33-C35-C36
14	an	1001	BCL	C2A-CAA-CBA-CGA
15	AD	103	LMT	O5'-C5'-C6'-O6'
15	AF	1002	LMT	C4B-C5B-C6B-O6B
20	bh	103	0V9	O2-C2-C3-O3
14	AA	1001	BCL	C10-C11-C12-C13
15	AJ	103	LMT	C4'-C5'-C6'-O6'
21	H1	104	CD4	C42-C43-C44-C45
15	bb	102	LMT	C3'-C4'-O1B-C1B
15	be	104	LMT	C3'-C4'-O1B-C1B
14	AI	102	BCL	C10-C11-C12-C13
15	AI	101	LMT	O5B-C1B-O1B-C4'
15	BK	1002	LMT	O5B-C1B-O1B-C4'
15	BR	1003	LMT	O5B-C1B-O1B-C4'
15	AQ	103	LMT	O5'-C5'-C6'-O6'
15	BH	1003	LMT	C4'-C5'-C6'-O6'
14	AO	1002	BCL	C10-C11-C12-C13
15	bc	104	LMT	O5'-C5'-C6'-O6'
15	bn	101	LMT	O5'-C5'-C6'-O6'
21	af	102	CD4	C53-C54-C55-C56
15	AJ	104	LMT	O5'-C5'-C6'-O6'
15	bi	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
16	BU	1001	V7N	C27-C28-C29-C39
16	ba	101	V7N	C27-C28-C29-C39
16	bf	101	V7N	C27-C28-C29-C39
15	BV	1003	LMT	O5'-C5'-C6'-O6'
15	ab	101	LMT	O5'-C5'-C6'-O6'
23	ao	101	MQ8	C33-C35-C36-C37
15	M	403	LMT	O1'-C1-C2-C3
14	AC	102	BCL	C3-C5-C6-C7
15	AC	104	LMT	O5B-C5B-C6B-O6B
15	BW	1004	LMT	C4'-C5'-C6'-O6'
21	af	102	CD4	C11-C12-C13-C14
15	BB	105	LMT	O5B-C1B-O1B-C4'
14	BQ	1003	BCL	C5-C6-C7-C8
14	ad	1001	BCL	C10-C11-C12-C13
14	bk	102	BCL	C15-C16-C17-C18
15	BH	1004	LMT	O5'-C5'-C6'-O6'
20	bc	103	0V9	C10-C11-C12-C13
14	BT	103	BCL	C3-C5-C6-C7
15	BM	1003	LMT	O5'-C1'-O1'-C1
15	BQ	1004	LMT	O5'-C1'-O1'-C1
24	ag	1002	V7B	O6-C1-O1-C7
14	AE	1004	BCL	C15-C16-C17-C18
14	AS	103	BCL	C8-C10-C11-C12
14	ap	1001	BCL	C8-C10-C11-C12
21	aj	102	CD4	O9-C30-C31-O10
15	BR	1005	LMT	C3'-C4'-O1B-C1B
15	AU	101	LMT	O5'-C5'-C6'-O6'
14	AV	102	BCL	C13-C15-C16-C17
14	an	1001	BCL	C10-C11-C12-C13
15	BC	106	LMT	O5'-C5'-C6'-O6'
15	BH	1002	LMT	O5B-C1B-O1B-C4'
15	BQ	1002	LMT	O1'-C1-C2-C3
15	bm	103	LMT	O5B-C5B-C6B-O6B
14	BN	103	BCL	CBA-CGA-O2A-C1
15	BK	1004	LMT	O5'-C5'-C6'-O6'
15	AD	101	LMT	O5B-C1B-O1B-C4'
15	BC	102	LMT	O5B-C1B-O1B-C4'
16	bj	101	V7N	C27-C28-C29-C39
16	bn	102	V7N	C27-C28-C29-C39
14	AE	1001	BCL	C13-C15-C16-C17
21	H1	104	CD4	C46-C47-C48-C49
20	bb	103	0V9	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
15	bb	102	LMT	C5'-C4'-O1B-C1B
21	aj	102	CD4	C29-C30-C31-O10
14	BF	102	BCL	C10-C11-C12-C13
14	BJ	1002	BCL	C10-C11-C12-C13
14	ae	102	BCL	C5-C6-C7-C8
14	bb	104	BCL	C15-C16-C17-C18
15	BL	1002	LMT	C5'-C4'-O1B-C1B
15	be	104	LMT	C5'-C4'-O1B-C1B
15	bl	101	LMT	C5'-C4'-O1B-C1B
14	AI	103	BCL	C13-C15-C16-C17
14	AU	102	BCL	C10-C11-C12-C13
14	bd	102	BCL	C8-C10-C11-C12
15	AL	102	LMT	O5'-C5'-C6'-O6'
15	BU	1002	LMT	O5'-C5'-C6'-O6'
15	BR	1005	LMT	C5'-C4'-O1B-C1B
14	AR	101	BCL	C5-C6-C7-C8
14	AS	102	BCL	C5-C6-C7-C8
14	AS	103	BCL	C10-C11-C12-C13
14	ac	1001	BCL	C10-C11-C12-C13
15	BA	104	LMT	O5B-C1B-O1B-C4'
14	ap	1001	BCL	C13-C15-C16-C17
14	AI	102	BCL	C3-C5-C6-C7
14	AR	101	BCL	C3-C5-C6-C7
20	bc	103	0V9	C11-C10-O2-C2
15	BO	1003	LMT	O5'-C5'-C6'-O6'
15	AJ	103	LMT	C2'-C1'-O1'-C1
15	BM	1003	LMT	C2'-C1'-O1'-C1
15	BQ	1004	LMT	C2'-C1'-O1'-C1
15	BT	102	LMT	C2'-C1'-O1'-C1
15	BX	1004	LMT	C2'-C1'-O1'-C1
15	bo	105	LMT	C2'-C1'-O1'-C1
24	ag	1002	V7B	C2-C1-O1-C7
14	an	1001	BCL	C13-C15-C16-C17
15	M	403	LMT	C4'-C5'-C6'-O6'
16	AO	1001	V7N	C38-C26-C27-C28
16	BE	101	V7N	C38-C26-C27-C28
16	BH	1001	V7N	C38-C26-C27-C28
16	BI	1001	V7N	C3-C4-C5-C33
16	BO	1001	V7N	C38-C26-C27-C28
16	BO	1001	V7N	C3-C4-C5-C33
16	BQ	1001	V7N	C3-C4-C5-C33
16	BU	1001	V7N	C38-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
16	BV	1001	V7N	C38-C26-C27-C28
16	BX	1001	V7N	C38-C26-C27-C28
16	BX	1001	V7N	C3-C4-C5-C33
16	bb	101	V7N	C36-C18-C19-C20
16	bi	101	V7N	C38-C26-C27-C28
16	bl	102	V7N	C38-C26-C27-C28
16	bp	101	V7N	C38-C26-C27-C28
20	aj	101	0V9	C2-C1-O3P-P
20	be	103	0V9	C2-C1-O3P-P
20	bg	102	0V9	C2-C1-O3P-P
27	M	404	CRT	C34-C33-C35-C36
15	BB	104	LMT	O1'-C1-C2-C3
16	AO	1001	V7N	C25-C26-C27-C28
16	BC	101	V7N	C25-C26-C27-C28
16	BH	1001	V7N	C25-C26-C27-C28
16	BO	1001	V7N	C25-C26-C27-C28
16	BV	1001	V7N	C25-C26-C27-C28
16	BX	1001	V7N	C25-C26-C27-C28
16	ba	101	V7N	C25-C26-C27-C28
16	be	101	V7N	C25-C26-C27-C28
16	bf	101	V7N	C3-C4-C5-C6
16	bi	101	V7N	C25-C26-C27-C28
16	bm	101	V7N	C3-C4-C5-C6
16	bp	101	V7N	C25-C26-C27-C28
28	ai	102	UYH	C4-C5-C6-O5
14	BL	1003	BCL	C2A-CAA-CBA-CGA
14	BU	1004	BCL	C2A-CAA-CBA-CGA
14	bk	102	BCL	C16-C17-C18-C19
14	bk	102	BCL	C16-C17-C18-C20
20	be	103	0V9	C12-C13-C14-C15
15	L	1004	LMT	O1'-C1-C2-C3
14	AJ	102	BCL	C13-C15-C16-C17
15	BX	1004	LMT	O5'-C1'-O1'-C1
14	bm	104	BCL	C8-C10-C11-C12
14	bp	102	BCL	C8-C10-C11-C12
15	AJ	103	LMT	O5B-C5B-C6B-O6B
15	BG	1005	LMT	O5'-C5'-C6'-O6'
15	BK	1003	LMT	O5'-C5'-C6'-O6'
15	bn	105	LMT	O5'-C5'-C6'-O6'
21	aj	102	CD4	O16-C33-C34-O14
15	BT	101	LMT	O1'-C1-C2-C3
14	AG	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	AJ	102	BCL	C2-C1-O2A-CGA
14	AK	101	BCL	C2-C1-O2A-CGA
14	BF	102	BCL	C2-C1-O2A-CGA
14	ai	101	BCL	C2-C1-O2A-CGA
14	AM	102	BCL	C16-C17-C18-C19
14	AM	102	BCL	C16-C17-C18-C20
14	AV	103	BCL	C16-C17-C18-C20
14	AM	101	BCL	C15-C16-C17-C18
21	H1	102	CD4	C47-C48-C49-C50
15	BF	103	LMT	C4'-C5'-C6'-O6'
15	BT	104	LMT	O5B-C1B-O1B-C4'
15	bl	101	LMT	O5B-C1B-O1B-C4'
15	AA	1004	LMT	C2-C1-O1'-C1'
15	BN	101	LMT	C2-C1-O1'-C1'
15	BQ	1002	LMT	C2-C1-O1'-C1'
15	AP	101	LMT	C5-C6-C7-C8
14	ae	102	BCL	C8-C10-C11-C12
15	BT	102	LMT	O1'-C1-C2-C3
15	BU	1003	LMT	C6-C7-C8-C9
14	AV	103	BCL	C16-C17-C18-C19
14	AN	104	BCL	C10-C11-C12-C13
14	M	408	BCL	C5-C6-C7-C8
14	bl	104	BCL	C12-C13-C15-C16
15	bo	105	LMT	C6-C7-C8-C9
14	AK	101	BCL	C8-C10-C11-C12
14	af	101	BCL	C13-C15-C16-C17
15	bh	104	LMT	O5'-C5'-C6'-O6'
15	bd	103	LMT	C6-C7-C8-C9
14	BM	1002	BCL	C3A-C2A-CAA-CBA
14	BQ	1003	BCL	C3A-C2A-CAA-CBA
14	BR	1004	BCL	C3A-C2A-CAA-CBA
14	BU	1004	BCL	C3A-C2A-CAA-CBA
14	bi	104	BCL	C3A-C2A-CAA-CBA
14	bk	102	BCL	C3A-C2A-CAA-CBA
14	bn	103	BCL	C3A-C2A-CAA-CBA
20	bb	103	0V9	C32-C33-C34-C35
20	bp	103	0V9	C34-C35-C36-C37
14	BJ	1002	BCL	C15-C16-C17-C18
14	bc	102	BCL	C8-C10-C11-C12
14	bc	102	BCL	C15-C16-C17-C18
21	aj	102	CD4	C46-C47-C48-C49
15	bm	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	AX	101	LMT	O5'-C5'-C6'-O6'
15	BN	102	LMT	O5'-C5'-C6'-O6'
15	L	1011	LMT	C3-C4-C5-C6
15	AA	1003	LMT	C6-C7-C8-C9
21	M	402	CD4	C32-C33-C34-O14
15	bf	102	LMT	C5-C6-C7-C8
14	bl	104	BCL	C3-C5-C6-C7
20	C1	1001	0V9	C10-C11-C12-C13
15	L	1008	LMT	C4B-C5B-C6B-O6B
15	AG	103	LMT	C6-C7-C8-C9
14	AM	101	BCL	C10-C11-C12-C13
15	bj	102	LMT	C5-C6-C7-C8
14	aa	1001	BCL	C16-C17-C18-C20
20	H1	101	0V9	C10-C11-C12-C13
21	ae	101	CD4	C35-C36-C37-C38
21	aj	102	CD4	C51-C52-C53-C54
14	BI	1003	BCL	C15-C16-C17-C18
14	bc	102	BCL	C10-C11-C12-C13
21	H1	102	CD4	C33-C32-O13-P2
15	BS	1004	LMT	C3-C4-C5-C6
21	af	102	CD4	C24-C25-C26-C27
15	bj	102	LMT	O5'-C5'-C6'-O6'
20	bc	103	0V9	O4-C10-O2-C2
14	BG	1004	BCL	C4-C3-C5-C6
14	BO	1004	BCL	C4-C3-C5-C6
16	bg	101	V7N	C26-C27-C28-C29
14	AN	101	BCL	C10-C11-C12-C13
20	bm	102	0V9	C13-C14-C15-C16
21	af	102	CD4	C43-C44-C45-C63
21	af	102	CD4	C46-C47-C48-C49
14	BI	1003	BCL	C11-C10-C8-C9
15	BM	1004	LMT	O5B-C5B-C6B-O6B
15	AU	101	LMT	O5'-C1'-O1'-C1
15	BC	105	LMT	O5B-C5B-C6B-O6B
15	BJ	1003	LMT	O5'-C5'-C6'-O6'
15	L	1007	LMT	O5'-C5'-C6'-O6'
15	BE	102	LMT	C2'-C1'-O1'-C1
15	BG	1002	LMT	C2'-C1'-O1'-C1
15	bb	102	LMT	C2'-C1'-O1'-C1
15	bn	105	LMT	C2'-C1'-O1'-C1
15	AD	101	LMT	C4-C5-C6-C7
15	AA	1003	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
20	bj	104	0V9	C11-C10-O2-C2
20	bl	103	0V9	C11-C10-O2-C2
21	H1	102	CD4	C13-C14-O2-C15
23	ao	101	MQ8	C3-C11-C12-C13
15	AF	1002	LMT	C4'-C5'-C6'-O6'
15	AG	103	LMT	O1'-C1-C2-C3
15	AX	101	LMT	C5-C6-C7-C8
20	be	103	0V9	C2-C3-O3-C30
20	bj	104	0V9	O4-C10-O2-C2
15	AH	104	LMT	C2-C3-C4-C5
20	bm	102	0V9	C31-C32-C33-C34
16	bm	101	V7N	C3-C4-C5-C33
14	BA	103	BCL	C3-C5-C6-C7
16	bb	101	V7N	C3-C4-C5-C6
16	bh	102	V7N	C3-C4-C5-C6
14	BB	103	BCL	C16-C17-C18-C19
14	aa	1001	BCL	C16-C17-C18-C19
14	AB	1002	BCL	C4-C3-C5-C6
14	bi	104	BCL	C4-C3-C5-C6
16	AS	105	V7N	C37-C22-C23-C24
20	bg	104	0V9	C10-C11-C12-C13
15	BU	1002	LMT	O1'-C1-C2-C3
14	ak	1001	BCL	C3-C5-C6-C7
14	ag	1001	BCL	C5-C6-C7-C8
14	be	105	BCL	C5-C6-C7-C8
15	L	1003	LMT	C7-C8-C9-C10
21	aj	102	CD4	O2-C15-C28-O5
15	AH	104	LMT	C5'-C4'-O1B-C1B
22	H1	103	PGW	C16-C17-C18-C28
21	af	102	CD4	C13-C14-O2-C15
14	AC	102	BCL	C10-C11-C12-C13
14	BQ	1003	BCL	C15-C16-C17-C18
15	AX	101	LMT	O1'-C1-C2-C3
20	bo	104	0V9	C11-C12-C13-C14
15	BD	103	LMT	C5'-C4'-O1B-C1B
15	BK	1003	LMT	C3'-C4'-O1B-C1B
15	AI	101	LMT	O5B-C5B-C6B-O6B
24	L	1006	V7B	C16-C17-C18-C19
15	BG	1005	LMT	C1-C2-C3-C4
14	BL	1003	BCL	C13-C15-C16-C17
14	BO	1004	BCL	C5-C6-C7-C8
15	BC	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
15	BJ	1004	LMT	O5B-C5B-C6B-O6B
15	BQ	1002	LMT	O5'-C5'-C6'-O6'
14	BP	1005	BCL	C3-C5-C6-C7
20	be	102	0V9	O2-C2-C3-O3
20	bp	103	0V9	O2-C2-C3-O3
21	M	402	CD4	O16-C33-C34-O14
15	BR	1003	LMT	O5'-C5'-C6'-O6'
15	BA	104	LMT	C5'-C4'-O1B-C1B
15	BR	1003	LMT	C5'-C4'-O1B-C1B
14	BE	104	BCL	C2-C1-O2A-CGA
15	BW	1002	LMT	O5'-C5'-C6'-O6'
20	bg	104	0V9	C2-C1-O3P-P
21	af	102	CD4	C30-C29-O8-P1
21	aj	102	CD4	C30-C31-O10-P2
15	bm	103	LMT	O5'-C5'-C6'-O6'
14	ai	101	BCL	C4-C3-C5-C6
14	BO	1004	BCL	C2-C3-C5-C6
14	ab	102	BCL	C2-C3-C5-C6
14	be	105	BCL	C2-C3-C5-C6
14	bh	105	BCL	C2-C3-C5-C6
16	AS	105	V7N	C21-C22-C23-C24
21	H1	102	CD4	O1-C14-O2-C15
21	M	402	CD4	C51-C52-C53-C54
14	AB	1002	BCL	C2A-CAA-CBA-CGA
15	BN	104	LMT	O5'-C5'-C6'-O6'
15	bd	103	LMT	O5'-C5'-C6'-O6'
15	BA	102	LMT	C3-C4-C5-C6
24	L	1006	V7B	C17-C18-C19-C20
20	bl	103	0V9	C13-C14-C15-C16
15	BL	1002	LMT	C3'-C4'-O1B-C1B
21	ae	101	CD4	C22-C23-C24-C25
24	L	1006	V7B	O52-C47-C48-O53
14	AA	1002	BCL	C3-C5-C6-C7
14	AC	103	BCL	C1A-C2A-CAA-CBA
14	AE	1004	BCL	C1A-C2A-CAA-CBA
14	AG	101	BCL	C1A-C2A-CAA-CBA
14	AS	102	BCL	C1A-C2A-CAA-CBA
14	BM	1002	BCL	C1A-C2A-CAA-CBA
14	bc	102	BCL	C1A-C2A-CAA-CBA
14	bk	102	BCL	C1A-C2A-CAA-CBA
14	bn	103	BCL	C1A-C2A-CAA-CBA
15	bl	101	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
15	BB	104	LMT	C5-C6-C7-C8
14	BH	1005	BCL	C10-C11-C12-C13
25	M	406	BPH	C13-C15-C16-C17
20	be	102	0V9	O3P-C1-C2-C3
20	bk	103	0V9	O3P-C1-C2-C3
15	BI	1005	LMT	O5'-C5'-C6'-O6'
20	bl	103	0V9	O4-C10-O2-C2
14	AA	1001	BCL	C12-C13-C15-C16
14	AG	101	BCL	C6-C7-C8-C10
14	AI	102	BCL	C6-C7-C8-C10
14	AQ	101	BCL	C12-C13-C15-C16
14	ae	102	BCL	C11-C12-C13-C15
14	ak	1001	BCL	C12-C13-C15-C16
14	bn	103	BCL	C11-C10-C8-C7
14	BB	103	BCL	C16-C17-C18-C20
14	bm	104	BCL	C13-C15-C16-C17
22	H1	103	PGW	C02-C01-O03-C19
15	BS	1005	LMT	O5'-C5'-C6'-O6'
15	bn	101	LMT	C2B-C1B-O1B-C4'
14	AU	103	BCL	C4-C3-C5-C6
14	AA	1002	BCL	C2-C3-C5-C6
14	AB	1002	BCL	C2-C3-C5-C6
14	AU	103	BCL	C2-C3-C5-C6
24	ag	1002	V7B	C12-C13-C14-C15
14	AH	101	BCL	C8-C10-C11-C12
14	AA	1001	BCL	C11-C10-C8-C9
14	AI	102	BCL	C6-C7-C8-C9
14	AK	101	BCL	C6-C7-C8-C9
14	AQ	101	BCL	C14-C13-C15-C16
14	BI	1003	BCL	C11-C12-C13-C14
14	bk	102	BCL	C11-C10-C8-C9
14	bl	104	BCL	C11-C10-C8-C9
14	bn	103	BCL	C11-C10-C8-C9
14	bp	102	BCL	C14-C13-C15-C16
21	H1	102	CD4	C54-C55-C56-C57
21	H1	104	CD4	C11-C10-C9-C8
21	aj	102	CD4	C26-C27-C60-C61
15	AG	103	LMT	O5'-C5'-C6'-O6'
15	AJ	104	LMT	C7-C8-C9-C10
14	bb	104	BCL	C10-C11-C12-C13
15	BC	103	LMT	O5'-C5'-C6'-O6'
15	bf	102	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	bn	101	LMT	O5B-C1B-O1B-C4'
15	AT	102	LMT	C2'-C1'-O1'-C1
15	BL	1004	LMT	C2'-C1'-O1'-C1
15	bl	101	LMT	C2'-C1'-O1'-C1
15	BL	1004	LMT	O5B-C5B-C6B-O6B
15	BT	104	LMT	O5'-C5'-C6'-O6'
20	be	102	0V9	C10-C11-C12-C13
20	bo	104	0V9	C1-C2-C3-O3
15	AD	103	LMT	C4'-C5'-C6'-O6'
15	AD	103	LMT	O5B-C5B-C6B-O6B
15	AN	103	LMT	O5'-C5'-C6'-O6'
16	bi	101	V7N	C2-C1-O32-C41
20	H1	101	0V9	C35-C36-C37-C38
15	BW	1002	LMT	C4-C5-C6-C7
15	bd	103	LMT	C3-C4-C5-C6
24	L	1006	V7B	C33-C34-C35-C36
15	BD	102	LMT	O1'-C1-C2-C3
14	AX	102	BCL	C13-C15-C16-C17
14	ah	1001	BCL	C10-C11-C12-C13
14	bi	104	BCL	C3-C5-C6-C7
15	BV	1006	LMT	O5'-C5'-C6'-O6'
15	AU	101	LMT	C2B-C1B-O1B-C4'
14	ab	102	BCL	C4-C3-C5-C6
14	bh	105	BCL	C4-C3-C5-C6
23	ao	101	MQ8	C34-C33-C35-C36
14	AR	102	BCL	C2-C3-C5-C6
14	BG	1004	BCL	C2-C3-C5-C6
14	ai	101	BCL	C2-C3-C5-C6
14	bi	104	BCL	C2-C3-C5-C6
14	bg	105	BCL	C8-C10-C11-C12
15	BK	1004	LMT	O1'-C1-C2-C3
15	AG	103	LMT	C4B-C5B-C6B-O6B
15	bn	101	LMT	C1-C2-C3-C4
15	AD	101	LMT	O5'-C5'-C6'-O6'
15	AH	104	LMT	O5'-C5'-C6'-O6'
15	AS	101	LMT	O5B-C5B-C6B-O6B
15	AS	101	LMT	O5'-C5'-C6'-O6'
15	BO	1002	LMT	O5B-C5B-C6B-O6B
16	BL	1001	V7N	C3-C4-C5-C6
14	BM	1002	BCL	C13-C15-C16-C17
14	BS	1003	BCL	C2A-CAA-CBA-CGA
15	AI	101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
15	AJ	103	LMT	O5'-C5'-C6'-O6'
15	BX	1003	LMT	O5'-C5'-C6'-O6'
14	BA	103	BCL	O2A-C1-C2-C3
14	BB	103	BCL	O2A-C1-C2-C3
14	BC	104	BCL	O2A-C1-C2-C3
14	aa	1001	BCL	O2A-C1-C2-C3
21	aj	102	CD4	C16-C15-O2-C14
16	BS	1001	V7N	C26-C27-C28-C29
14	am	1001	BCL	C15-C16-C17-C18
14	an	1001	BCL	C8-C10-C11-C12
21	af	102	CD4	C48-C49-C50-C51
15	BK	1003	LMT	C5'-C4'-O1B-C1B
20	bk	103	0V9	C39-C40-C41-C42
20	aj	101	0V9	O3P-C1-C2-O2
14	AI	102	BCL	C8-C10-C11-C12
15	bl	105	LMT	C4-C5-C6-C7
14	AL	101	BCL	CBA-CGA-O2A-C1
15	bg	103	LMT	C9-C10-C11-C12
14	AV	101	BCL	C10-C11-C12-C13
14	AN	104	BCL	C4-C3-C5-C6
14	ad	1001	BCL	C4-C3-C5-C6
14	AN	104	BCL	C2-C3-C5-C6
14	ad	1001	BCL	C2-C3-C5-C6
14	ag	1001	BCL	C2-C3-C5-C6
23	M	407	MQ8	C12-C13-C15-C16
23	ao	101	MQ8	C32-C33-C35-C36
15	BA	105	LMT	O5B-C1B-O1B-C4'
15	BI	1004	LMT	O5B-C1B-O1B-C4'
21	M	402	CD4	C20-C21-C22-C23
15	BP	1003	LMT	C11-C10-C9-C8
21	aj	102	CD4	C24-C25-C26-C27
20	ba	102	0V9	O2-C2-C3-O3
20	bg	102	0V9	O2-C2-C3-O3
20	bo	104	0V9	O2-C2-C3-O3
15	BI	1006	LMT	O1'-C1-C2-C3
15	BD	102	LMT	C4'-C5'-C6'-O6'
15	bl	105	LMT	C3-C4-C5-C6
14	AP	103	BCL	C3-C5-C6-C7
14	ab	102	BCL	C3-C5-C6-C7
15	BP	1002	LMT	O5B-C1B-O1B-C4'
14	BJ	1002	BCL	C8-C10-C11-C12
23	L	1001	MQ8	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
15	BJ	1003	LMT	C7-C8-C9-C10
15	BK	1005	LMT	O1'-C1-C2-C3
15	BA	104	LMT	O5B-C5B-C6B-O6B
15	AU	101	LMT	O5B-C1B-O1B-C4'
15	AS	101	LMT	C4-C5-C6-C7
16	bi	101	V7N	C30-C1-O32-C41
16	bi	101	V7N	C31-C1-O32-C41
16	bj	101	V7N	C30-C1-O32-C41
15	AG	103	LMT	C5'-C4'-O1B-C1B
15	bb	102	LMT	C4-C5-C6-C7
21	ae	101	CD4	C4-C5-C6-C7
15	BX	1003	LMT	O5B-C5B-C6B-O6B
16	BU	1001	V7N	C5-C6-C7-C8
20	bp	103	0V9	C37-C38-C39-C40
14	AI	103	BCL	C4-C3-C5-C6
14	BN	103	BCL	C4-C3-C5-C6
14	BQ	1003	BCL	C4-C3-C5-C6
14	be	105	BCL	C4-C3-C5-C6
14	bf	103	BCL	C4-C3-C5-C6
15	bj	102	LMT	C9-C10-C11-C12
23	L	1001	MQ8	C17-C18-C20-C21
20	bk	104	0V9	C11-C12-C13-C14
14	BM	1002	BCL	C5-C6-C7-C8
14	L	1002	BCL	C15-C16-C17-C18
20	bm	102	0V9	C12-C13-C14-C15
15	AC	104	LMT	C2-C1-O1'-C1'
15	AG	103	LMT	C2-C1-O1'-C1'
15	AQ	103	LMT	C2-C1-O1'-C1'
15	AT	102	LMT	C2-C1-O1'-C1'
15	AX	101	LMT	C2-C1-O1'-C1'
15	BC	105	LMT	C2-C1-O1'-C1'
15	BD	103	LMT	C2-C1-O1'-C1'
15	BE	103	LMT	C2-C1-O1'-C1'
15	BF	103	LMT	C2-C1-O1'-C1'
15	BH	1002	LMT	C2-C1-O1'-C1'
15	BH	1003	LMT	C2-C1-O1'-C1'
15	BI	1002	LMT	C2-C1-O1'-C1'
15	BI	1006	LMT	C2-C1-O1'-C1'
15	BK	1004	LMT	C2-C1-O1'-C1'
15	BK	1005	LMT	C2-C1-O1'-C1'
15	BN	102	LMT	C2-C1-O1'-C1'
15	BT	101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
15	BU	1002	LMT	C2-C1-O1'-C1'
15	L	1003	LMT	C2-C1-O1'-C1'
15	bc	104	LMT	C2-C1-O1'-C1'
15	bm	103	LMT	C2-C1-O1'-C1'
14	AA	1001	BCL	C14-C13-C15-C16
14	AF	1001	BCL	C11-C12-C13-C14
14	AH	103	BCL	C11-C12-C13-C14
14	aj	103	BCL	C14-C13-C15-C16
14	ak	1001	BCL	C14-C13-C15-C16
14	bj	103	BCL	C6-C7-C8-C9
14	bl	104	BCL	C14-C13-C15-C16
15	AA	1003	LMT	C7-C8-C9-C10
20	be	102	0V9	C2-C1-O3P-P
20	bk	104	0V9	C2-C1-O3P-P
15	L	1011	LMT	C6-C7-C8-C9
21	ae	101	CD4	C43-C44-C45-C63
14	AF	1001	BCL	C10-C11-C12-C13
14	BO	1004	BCL	C2A-CAA-CBA-CGA
14	bp	102	BCL	C2A-CAA-CBA-CGA
15	bn	105	LMT	C3-C4-C5-C6
15	AE	1002	LMT	C2'-C1'-O1'-C1
14	BW	1003	BCL	C5-C6-C7-C8
24	L	1006	V7B	C13-C14-C15-C16
15	AA	1003	LMT	C9-C10-C11-C12
20	aj	101	0V9	O3P-C1-C2-C3
20	ba	102	0V9	O3P-C1-C2-C3
20	bb	103	0V9	O3P-C1-C2-C3
20	bg	102	0V9	O3P-C1-C2-C3
20	bl	103	0V9	O3P-C1-C2-C3
20	bp	103	0V9	O3P-C1-C2-C3
21	H1	102	CD4	O13-C32-C33-C34
15	AE	1002	LMT	C5'-C4'-O1B-C1B
14	AA	1001	BCL	C11-C10-C8-C7
14	AF	1001	BCL	C11-C12-C13-C15
14	AG	102	BCL	C6-C7-C8-C10
14	AK	101	BCL	C6-C7-C8-C10
14	BI	1003	BCL	C11-C12-C13-C15
14	aj	103	BCL	C12-C13-C15-C16
14	bc	102	BCL	C12-C13-C15-C16
14	bk	102	BCL	C11-C10-C8-C7
14	bl	104	BCL	C11-C10-C8-C7
14	bp	102	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	BS	1004	LMT	C2-C3-C4-C5
20	bb	103	0V9	C35-C36-C37-C38
16	BU	1001	V7N	O42-C34-C9-C8
15	BN	104	LMT	C4-C5-C6-C7
14	AA	1002	BCL	C4-C3-C5-C6
14	AE	1003	BCL	C3A-C2A-CAA-CBA
14	AH	101	BCL	C4-C3-C5-C6
14	AL	101	BCL	C3A-C2A-CAA-CBA
14	BK	1006	BCL	C3A-C2A-CAA-CBA
14	ag	1001	BCL	C4-C3-C5-C6
14	bp	102	BCL	C3A-C2A-CAA-CBA
23	M	407	MQ8	C14-C13-C15-C16
14	BN	103	BCL	C5-C6-C7-C8
15	BG	1002	LMT	C3-C4-C5-C6
14	AI	103	BCL	C2-C3-C5-C6
14	ae	102	BCL	C2-C3-C5-C6
15	BG	1003	LMT	O5'-C1'-O1'-C1
14	AL	101	BCL	O1A-CGA-O2A-C1
16	BE	101	V7N	C27-C28-C29-C39
16	BW	1001	V7N	C27-C28-C29-C39
16	bm	101	V7N	C27-C28-C29-C39
15	BC	105	LMT	O1'-C1-C2-C3
15	BN	104	LMT	C7-C8-C9-C10
15	BE	103	LMT	O5'-C5'-C6'-O6'
14	AX	103	BCL	C13-C15-C16-C17
20	bi	103	0V9	C14-C15-C16-C17
14	BV	1005	BCL	C10-C11-C12-C13
20	be	103	0V9	C1-C2-C3-O3
20	bg	102	0V9	C1-C2-C3-O3
20	bh	103	0V9	C1-C2-C3-O3
21	H1	104	CD4	C28-C15-C16-O3
21	M	402	CD4	C28-C15-C16-O3
21	aj	102	CD4	C32-C33-C34-O14
14	BQ	1003	BCL	C3-C5-C6-C7
15	BI	1006	LMT	O5'-C5'-C6'-O6'
14	BK	1006	BCL	C10-C11-C12-C13
14	AG	101	BCL	C4-C3-C5-C6
14	AL	101	BCL	C4-C3-C5-C6
14	AR	102	BCL	C4-C3-C5-C6
14	AV	103	BCL	C4-C3-C5-C6
23	L	1001	MQ8	C19-C18-C20-C21
21	H1	104	CD4	C49-C50-C51-C52

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Mol	Chain	Res	Type	Atoms
14	AG	101	BCL	C2-C3-C5-C6
14	AL	101	BCL	C2-C3-C5-C6
14	AV	103	BCL	C2-C3-C5-C6
14	BN	103	BCL	C2-C3-C5-C6
14	BQ	1003	BCL	C2-C3-C5-C6
20	bb	103	0V9	O3P-C1-C2-O2
21	H1	102	CD4	O13-C32-C33-O16
21	M	402	CD4	O2-C15-C28-O5
15	AS	101	LMT	C2-C3-C4-C5
15	BL	1004	LMT	C4-C5-C6-C7
15	BA	104	LMT	C3'-C4'-O1B-C1B
15	BG	1003	LMT	O1'-C1-C2-C3
21	ae	101	CD4	C7-C8-C9-C10
14	bm	104	BCL	C15-C16-C17-C18
20	aj	101	0V9	O2-C2-C3-O3
20	bl	103	0V9	O2-C2-C3-O3
15	AD	101	LMT	C1-C2-C3-C4
14	AC	103	BCL	C4-C3-C5-C6
14	AE	1003	BCL	C4-C3-C5-C6
23	L	1001	MQ8	C45-C43-C44-C46
23	ao	101	MQ8	C45-C43-C44-C46
16	BV	1001	V7N	C26-C27-C28-C29
14	AH	103	BCL	C15-C16-C17-C18
14	aa	1001	BCL	C10-C11-C12-C13
23	L	1001	MQ8	C42-C43-C44-C46
15	BR	1005	LMT	O5'-C5'-C6'-O6'
21	aj	102	CD4	C41-C42-C43-C44
14	AG	102	BCL	C6-C7-C8-C9
14	AG	102	BCL	C11-C12-C13-C14
14	bc	102	BCL	C14-C13-C15-C16
15	BD	103	LMT	C3'-C4'-O1B-C1B
15	bm	105	LMT	C4'-C5'-C6'-O6'
15	bf	102	LMT	O1'-C1-C2-C3
21	H1	102	CD4	C6-C7-C8-C9
21	ae	101	CD4	C5-C6-C7-C8
16	bb	101	V7N	C22-C23-C24-C25
23	ao	101	MQ8	C43-C44-C46-C47
14	AW	101	BCL	C8-C10-C11-C12
15	AH	104	LMT	C3'-C4'-O1B-C1B
15	AQ	103	LMT	C4-C5-C6-C7
21	ae	101	CD4	C42-C43-C44-C45
14	AU	103	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	bl	103	0V9	C31-C30-O3-C3
14	AX	102	BCL	C4-C3-C5-C6
16	BJ	1001	V7N	C27-C28-C29-C39
14	AE	1003	BCL	C2-C3-C5-C6
14	AH	101	BCL	C2-C3-C5-C6
14	bf	103	BCL	C2-C3-C5-C6
15	BV	1004	LMT	O1'-C1-C2-C3
15	BE	102	LMT	C5-C6-C7-C8
15	AD	101	LMT	C5'-C4'-O1B-C1B
14	AG	102	BCL	C13-C15-C16-C17
15	BX	1003	LMT	C5'-C4'-O1B-C1B
21	H1	102	CD4	C29-C30-C31-O10
21	ae	101	CD4	C29-C30-C31-O10
15	AC	104	LMT	C3-C4-C5-C6
14	AR	102	BCL	C3-C5-C6-C7
15	BT	101	LMT	C4-C5-C6-C7
20	H1	101	0V9	O3P-C1-C2-C3
20	bn	104	0V9	O3P-C1-C2-C3
21	aj	102	CD4	C16-C15-C28-O5
22	H1	103	PGW	C07-C06-C10-C9
16	BJ	1001	V7N	C23-C24-C25-C26
14	ao	102	BCL	C8-C10-C11-C12
14	AG	102	BCL	C11-C12-C13-C15
14	AV	102	BCL	C6-C7-C8-C10
14	AX	102	BCL	C11-C10-C8-C7
14	BK	1006	BCL	C11-C12-C13-C15
14	BP	1005	BCL	C11-C12-C13-C15
15	BB	104	LMT	C1-C2-C3-C4
20	aj	101	0V9	C10-C11-C12-C13
15	AF	1002	LMT	C7-C8-C9-C10
14	bk	102	BCL	C10-C11-C12-C13
16	BI	1001	V7N	C3-C4-C5-C6
16	BQ	1001	V7N	C3-C4-C5-C6
16	BX	1001	V7N	C3-C4-C5-C6
23	ao	101	MQ8	C12-C11-C3-C2
24	ag	1002	V7B	C8-C7-O1-C1
14	BM	1002	BCL	C8-C10-C11-C12
14	AX	103	BCL	C2A-CAA-CBA-CGA
15	BR	1003	LMT	C5-C6-C7-C8
28	ai	102	UYH	C15-C16-C17-C18
14	af	101	BCL	C4-C3-C5-C6
14	AX	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	bn	103	BCL	C2-C3-C5-C6
23	ao	101	MQ8	C42-C43-C44-C46
15	BD	104	LMT	C4-C5-C6-C7
14	AR	102	BCL	O2A-C1-C2-C3
14	BH	1005	BCL	O2A-C1-C2-C3
14	bi	104	BCL	O2A-C1-C2-C3
16	BU	1001	V7N	C7-C8-C9-C10
20	bj	104	0V9	C3-C2-O2-C10
15	BP	1002	LMT	O5B-C5B-C6B-O6B
15	bh	104	LMT	O5B-C5B-C6B-O6B
21	ae	101	CD4	C44-C45-C63-C64
20	C1	1001	0V9	C19-C20-C21-C22
16	BA	101	V7N	C27-C28-C29-C39
15	AA	1003	LMT	C5'-C4'-O1B-C1B
15	AP	101	LMT	C1-C2-C3-C4
20	H1	101	0V9	O3P-C1-C2-O2
20	ba	102	0V9	O3P-C1-C2-O2
20	be	102	0V9	O3P-C1-C2-O2
20	bk	103	0V9	O3P-C1-C2-O2
20	bl	103	0V9	O3P-C1-C2-O2
21	ae	101	CD4	O13-C32-C33-O16
21	af	102	CD4	O13-C32-C33-O16
20	bc	103	0V9	C38-C39-C40-C41
15	BE	102	LMT	O5'-C1'-O1'-C1
15	L	1004	LMT	O5'-C1'-O1'-C1
15	BR	1005	LMT	O1'-C1-C2-C3
20	be	102	0V9	C1-C2-C3-O3
23	ao	101	MQ8	C28-C30-C31-C32
14	BE	104	BCL	C13-C15-C16-C17
15	bn	105	LMT	C7-C8-C9-C10
14	ae	102	BCL	C4-C3-C5-C6
14	bn	103	BCL	C4-C3-C5-C6
16	BK	1001	V7N	C37-C22-C23-C24
15	BN	101	LMT	C5'-C4'-O1B-C1B
16	AE	1005	V7N	O42-C34-C9-C10
16	AO	1001	V7N	O42-C34-C9-C10
16	AS	105	V7N	O42-C34-C9-C10
16	BA	101	V7N	O42-C34-C9-C10
16	BB	101	V7N	O42-C34-C9-C10
16	BC	101	V7N	O42-C34-C9-C10
16	BE	101	V7N	O42-C34-C9-C10
16	BG	1001	V7N	O42-C34-C9-C10

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Mol	Chain	Res	Type	Atoms
16	BH	1001	V7N	O42-C34-C9-C10
16	BI	1001	V7N	O42-C34-C9-C10
16	BJ	1001	V7N	O42-C34-C9-C10
16	BL	1001	V7N	O42-C34-C9-C10
16	BO	1001	V7N	O42-C34-C9-C10
16	BP	1001	V7N	O42-C34-C9-C10
16	BR	1001	V7N	O42-C34-C9-C10
16	BS	1001	V7N	O42-C34-C9-C10
16	BV	1001	V7N	O42-C34-C9-C10
16	BW	1001	V7N	O42-C34-C9-C10
16	BX	1001	V7N	O42-C34-C9-C10
16	ba	101	V7N	O42-C34-C9-C10
16	bb	101	V7N	O42-C34-C9-C10
16	bc	101	V7N	O42-C34-C9-C10
16	bd	101	V7N	O42-C34-C9-C10
16	be	101	V7N	O42-C34-C9-C10
16	bf	101	V7N	O42-C34-C9-C10
16	bg	101	V7N	O42-C34-C9-C10
16	bh	102	V7N	O42-C34-C9-C10
16	bi	101	V7N	O42-C34-C9-C10
16	bj	101	V7N	O42-C34-C9-C10
16	bl	102	V7N	O42-C34-C9-C10
16	bn	102	V7N	O42-C34-C9-C10
16	bp	101	V7N	O42-C34-C9-C10
20	C1	1001	0V9	C5-C4-O4P-P
20	H1	101	0V9	C5-C4-O4P-P
20	aj	101	0V9	C5-C4-O4P-P
20	bc	103	0V9	C5-C4-O4P-P
20	be	103	0V9	C5-C4-O4P-P
20	bh	103	0V9	C5-C4-O4P-P
20	bk	103	0V9	C5-C4-O4P-P
23	ao	101	MQ8	C12-C11-C3-C4
14	BI	1003	BCL	C13-C15-C16-C17
20	bk	104	0V9	O2-C2-C3-O3
21	M	402	CD4	O2-C15-C16-O3
14	BG	1004	BCL	C5-C6-C7-C8
14	AE	1004	BCL	C6-C7-C8-C9
14	AM	102	BCL	C14-C13-C15-C16
14	AV	102	BCL	C6-C7-C8-C9
14	BK	1006	BCL	C11-C12-C13-C14
14	BP	1005	BCL	C11-C12-C13-C14
14	bj	103	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	bf	102	LMT	C1-C2-C3-C4
20	bh	103	0V9	C14-C15-C16-C17
20	bn	104	0V9	C34-C35-C36-C37
20	bk	104	0V9	C36-C37-C38-C39
16	bl	102	V7N	O32-C1-C2-C3
16	bp	101	V7N	O32-C1-C2-C3
27	M	404	CRT	C36-C37-C38-O2
15	BR	1005	LMT	C2-C3-C4-C5
15	BS	1005	LMT	C4-C5-C6-C7
15	BL	1004	LMT	O5B-C1B-O1B-C4'
20	bb	103	0V9	C33-C34-C35-C36
14	BW	1003	BCL	C2-C1-O2A-CGA
15	AU	101	LMT	C2'-C1'-O1'-C1
16	BM	1001	V7N	C23-C24-C25-C26
15	M	403	LMT	C1-C2-C3-C4
15	BQ	1005	LMT	O5'-C5'-C6'-O6'
20	be	102	0V9	C30-C31-C32-C33
15	BA	105	LMT	C4-C5-C6-C7
14	AG	101	BCL	C3-C5-C6-C7
15	BQ	1004	LMT	C4'-C5'-C6'-O6'
15	BS	1005	LMT	O5B-C1B-O1B-C4'
15	bl	101	LMT	O1'-C1-C2-C3
15	AH	102	LMT	C2-C1-O1'-C1'
15	AH	104	LMT	C2-C1-O1'-C1'
15	BD	102	LMT	C2-C1-O1'-C1'
15	BX	1003	LMT	C2-C1-O1'-C1'
15	BX	1004	LMT	C2-C1-O1'-C1'
15	L	1004	LMT	C2-C1-O1'-C1'
15	L	1011	LMT	C2-C1-O1'-C1'
14	am	1001	BCL	C3-C5-C6-C7
15	L	1008	LMT	O5B-C5B-C6B-O6B
28	ai	102	UYH	C17-C18-C19-C20
14	AI	103	BCL	C1A-C2A-CAA-CBA
14	AV	101	BCL	C1A-C2A-CAA-CBA
14	bi	104	BCL	C1A-C2A-CAA-CBA
14	bp	102	BCL	C1A-C2A-CAA-CBA
14	AQ	101	BCL	CBA-CGA-O2A-C1
15	BP	1002	LMT	C4-C5-C6-C7
14	BM	1002	BCL	C4-C3-C5-C6
14	al	1001	BCL	C4-C3-C5-C6
14	aj	103	BCL	C8-C10-C11-C12
15	BE	103	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	bi	103	0V9	C35-C36-C37-C38
21	M	402	CD4	C36-C37-C38-C39
20	be	103	0V9	O3P-C1-C2-C3
21	H1	102	CD4	C16-C15-C28-O5
21	M	402	CD4	C16-C15-C28-O5
21	af	102	CD4	O13-C32-C33-C34
15	AX	101	LMT	O5B-C1B-O1B-C4'
21	af	102	CD4	O1-C14-O2-C15
15	bm	105	LMT	O1'-C1-C2-C3
14	AH	103	BCL	C12-C13-C15-C16
14	AN	104	BCL	C6-C7-C8-C10
14	BM	1002	BCL	C6-C7-C8-C10
14	BS	1003	BCL	C6-C7-C8-C10
14	BW	1003	BCL	C12-C13-C15-C16
14	ag	1001	BCL	C11-C12-C13-C15
14	al	1001	BCL	C12-C13-C15-C16
15	bh	104	LMT	C11-C10-C9-C8
20	bm	102	0V9	C37-C38-C39-C40
15	AG	103	LMT	C3'-C4'-O1B-C1B
14	BH	1005	BCL	C13-C15-C16-C17
21	H1	102	CD4	C30-C29-O8-P1
20	bn	104	0V9	C32-C33-C34-C35
14	BV	1005	BCL	C3A-C2A-CAA-CBA
14	AE	1003	BCL	C16-C17-C18-C20
15	BN	101	LMT	C9-C10-C11-C12
15	BG	1006	LMT	O5'-C5'-C6'-O6'
14	AI	102	BCL	C2-C3-C5-C6
20	be	103	0V9	O3P-C1-C2-O2
20	bg	102	0V9	O3P-C1-C2-O2
20	bp	103	0V9	O3P-C1-C2-O2
20	aj	101	0V9	C35-C36-C37-C38
20	bb	103	0V9	C15-C16-C17-C18
15	bh	101	LMT	C11-C10-C9-C8
21	aj	102	CD4	C23-C24-C25-C26
14	AH	103	BCL	C14-C13-C15-C16
14	AX	102	BCL	C11-C10-C8-C9
15	be	104	LMT	C7-C8-C9-C10
16	BG	1001	V7N	C27-C28-C29-C39
16	bc	101	V7N	C27-C28-C29-C39
21	H1	102	CD4	C42-C43-C44-C45
15	BS	1002	LMT	C4-C5-C6-C7
15	bc	104	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	be	103	0V9	O2-C2-C3-O3
21	H1	104	CD4	O2-C15-C16-O3
21	ae	101	CD4	O2-C15-C16-O3
24	L	1006	V7B	O1-C7-C8-O7
24	ag	1002	V7B	O1-C7-C8-O7
15	BC	102	LMT	C4-C5-C6-C7
14	ae	102	BCL	C13-C15-C16-C17
15	BM	1003	LMT	C5-C6-C7-C8
15	AG	103	LMT	C4-C5-C6-C7
20	H1	101	0V9	C1-C2-C3-O3
20	aj	101	0V9	C1-C2-C3-O3
20	bk	104	0V9	C1-C2-C3-O3
21	af	102	CD4	C28-C15-C16-O3
24	L	1006	V7B	O1-C7-C8-C9
15	AP	101	LMT	C3-C4-C5-C6
14	BM	1002	BCL	C2-C3-C5-C6
14	af	101	BCL	C2-C3-C5-C6
14	bh	105	BCL	CAD-CBD-CGD-O2D
14	BE	104	BCL	C5-C6-C7-C8
15	BN	101	LMT	O5B-C1B-O1B-C4'
15	bn	101	LMT	O5'-C1'-O1'-C1
15	BL	1004	LMT	C5'-C4'-O1B-C1B
14	BH	1005	BCL	C2A-CAA-CBA-CGA
14	bd	102	BCL	C2A-CAA-CBA-CGA
15	BU	1002	LMT	O5B-C5B-C6B-O6B
15	AS	101	LMT	O1'-C1-C2-C3
15	AX	101	LMT	C6-C7-C8-C9
15	BQ	1004	LMT	C3-C4-C5-C6
15	BG	1002	LMT	O5B-C5B-C6B-O6B
14	bh	105	BCL	CAD-CBD-CGD-O1D
16	bk	101	V7N	C27-C28-C29-C39
20	C1	1001	0V9	C1-O3P-P-O1P
20	C1	1001	0V9	C4-O4P-P-O1P
20	aj	101	0V9	O4P-C4-C5-N
20	aj	101	0V9	C4-O4P-P-O2P
20	ba	102	0V9	C1-O3P-P-O2P
20	ba	102	0V9	C4-O4P-P-O2P
20	bb	103	0V9	C1-O3P-P-O2P
20	bc	103	0V9	C1-O3P-P-O2P
20	bg	102	0V9	C4-O4P-P-O2P
20	bi	103	0V9	C4-O4P-P-O3P
20	bk	103	0V9	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
20	bk	103	0V9	C4-O4P-P-O2P
20	bl	103	0V9	C4-O4P-P-O3P
20	bm	102	0V9	C4-O4P-P-O2P
20	bn	104	0V9	C1-O3P-P-O1P
20	bp	103	0V9	C1-O3P-P-O2P
21	ae	101	CD4	C29-O8-P1-O7
21	af	102	CD4	C32-O13-P2-O12
21	aj	102	CD4	C29-O8-P1-O6
22	H1	103	PGW	C03-O11-P-O14
22	H1	103	PGW	C04-O12-P-O11
22	H1	103	PGW	C04-O12-P-O13
14	BU	1004	BCL	C16-C17-C18-C19
21	H1	104	CD4	C37-C38-C39-C40
14	AE	1003	BCL	C5-C6-C7-C8
14	BV	1005	BCL	C4-C3-C5-C6
16	bb	101	V7N	C37-C22-C23-C24
16	BK	1001	V7N	C21-C22-C23-C24
15	BR	1005	LMT	C7-C8-C9-C10
20	C1	1001	0V9	C2-C1-O3P-P
20	bk	103	0V9	C2-C1-O3P-P
22	H1	103	PGW	C02-C03-O11-P
15	AQ	103	LMT	C4'-C5'-C6'-O6'
15	bn	101	LMT	C4-C5-C6-C7
14	ad	1001	BCL	C8-C10-C11-C12
15	BC	105	LMT	O5'-C5'-C6'-O6'
15	BB	102	LMT	C4-C5-C6-C7
24	L	1006	V7B	C10-C11-C12-C13
15	BN	101	LMT	O1'-C1-C2-C3
15	BA	105	LMT	C2B-C1B-O1B-C4'
14	ak	1001	BCL	C8-C10-C11-C12
14	AB	1001	BCL	C8-C10-C11-C12
20	bg	102	0V9	C1-C2-O2-C10
15	bc	104	LMT	C4'-C5'-C6'-O6'
15	BS	1006	LMT	O1'-C1-C2-C3
16	bh	102	V7N	C27-C28-C29-C39
14	AE	1003	BCL	C16-C17-C18-C19
21	ae	101	CD4	O13-C32-C33-C34
15	AS	101	LMT	C1-C2-C3-C4
15	BP	1003	LMT	C5'-C4'-O1B-C1B
15	AX	101	LMT	C2B-C1B-O1B-C4'
15	BP	1002	LMT	C2B-C1B-O1B-C4'
14	AC	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	AL	103	BCL	C11-C10-C8-C9
14	AV	103	BCL	C11-C10-C8-C9
14	BW	1003	BCL	C14-C13-C15-C16
14	AL	103	BCL	C11-C10-C8-C7
14	al	1001	BCL	C6-C7-C8-C10
20	bn	104	0V9	O3P-C1-C2-O2
15	BV	1006	LMT	C5-C6-C7-C8
15	BC	102	LMT	C5'-C4'-O1B-C1B
14	AJ	102	BCL	C10-C11-C12-C13
15	BM	1003	LMT	C4'-C5'-C6'-O6'
15	BC	103	LMT	O1'-C1-C2-C3
15	BR	1002	LMT	O5B-C1B-O1B-C4'
14	BU	1004	BCL	C16-C17-C18-C20
14	AC	102	BCL	C8-C10-C11-C12
15	BD	102	LMT	C2-C3-C4-C5
15	BF	101	LMT	C4-C5-C6-C7
20	bc	103	0V9	C37-C38-C39-C40
15	BV	1004	LMT	O5B-C1B-O1B-C4'
21	H1	104	CD4	C15-C28-O5-P1
15	bc	104	LMT	C2B-C1B-O1B-C4'
15	BP	1002	LMT	C5'-C4'-O1B-C1B
20	H1	101	0V9	O2-C2-C3-O3
15	AE	1002	LMT	C3-C4-C5-C6
14	AH	103	BCL	C8-C10-C11-C12
15	BI	1004	LMT	C2B-C1B-O1B-C4'
15	be	104	LMT	C5-C6-C7-C8
20	bp	103	0V9	C10-C11-C12-C13
20	bn	104	0V9	C38-C39-C40-C41
21	H1	104	CD4	C39-C40-C41-C42
14	BC	104	BCL	C15-C16-C17-C18
15	BV	1003	LMT	O5B-C5B-C6B-O6B
15	BS	1004	LMT	C5'-C4'-O1B-C1B
20	bj	104	0V9	C35-C36-C37-C38
14	aj	103	BCL	C2-C1-O2A-CGA
14	an	1001	BCL	C2-C1-O2A-CGA
20	bg	104	0V9	C15-C16-C17-C18
15	AD	101	LMT	C7-C8-C9-C10
20	bp	103	0V9	C1-C2-C3-O3
21	ae	101	CD4	C28-C15-C16-O3
15	AJ	103	LMT	C7-C8-C9-C10
15	bn	101	LMT	C5-C6-C7-C8
20	bn	104	0V9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
21	H1	104	CD4	C21-C22-C23-C24
16	bj	101	V7N	C31-C1-O32-C41
15	AS	101	LMT	C5'-C4'-O1B-C1B
15	L	1003	LMT	C1-C2-C3-C4
15	bh	104	LMT	O5B-C1B-O1B-C4'
15	BS	1002	LMT	C5'-C4'-O1B-C1B
16	BG	1001	V7N	C23-C24-C25-C26
15	BL	1005	LMT	C4-C5-C6-C7
22	H1	103	PGW	C15-C16-C17-C18
14	AG	101	BCL	C2A-CAA-CBA-CGA
16	AE	1005	V7N	C27-C28-C29-C39
15	BF	103	LMT	O1'-C1-C2-C3
15	AF	1002	LMT	O5'-C1'-O1'-C1
15	bn	105	LMT	O5'-C1'-O1'-C1
20	bi	103	OV9	C15-C16-C17-C18
21	H1	104	CD4	C36-C37-C38-C39
22	H1	103	PGW	C06-C07-C08-C09
14	bp	102	BCL	C4-C3-C5-C6
23	L	1001	MQ8	C34-C33-C35-C36
23	M	407	MQ8	C19-C18-C20-C21
15	BT	104	LMT	C2B-C1B-O1B-C4'
23	M	407	MQ8	C17-C18-C20-C21
15	BK	1005	LMT	O5B-C1B-O1B-C4'
15	BR	1002	LMT	C4-C5-C6-C7
15	AP	104	LMT	C2-C1-O1'-C1'
15	BB	102	LMT	C2-C1-O1'-C1'
15	BB	104	LMT	C2-C1-O1'-C1'
15	BQ	1004	LMT	C2-C1-O1'-C1'
15	BR	1003	LMT	C2-C1-O1'-C1'
15	BT	104	LMT	C2-C1-O1'-C1'
15	M	403	LMT	C2-C1-O1'-C1'
15	BI	1002	LMT	O5B-C1B-O1B-C4'
14	AX	103	BCL	C11-C10-C8-C9
14	BM	1002	BCL	C6-C7-C8-C9
14	al	1001	BCL	C6-C7-C8-C9
14	bf	103	BCL	C6-C7-C8-C9
15	BK	1004	LMT	O5B-C5B-C6B-O6B
15	be	104	LMT	C3-C4-C5-C6
15	AJ	103	LMT	C3'-C4'-O1B-C1B
15	AA	1003	LMT	O5B-C5B-C6B-O6B
14	AN	101	BCL	C15-C16-C17-C18
14	BF	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	be	104	LMT	C2-C3-C4-C5
20	be	103	0V9	C31-C30-O3-C3
15	AS	101	LMT	O5B-C1B-O1B-C4'
28	ai	102	UYH	C22-C23-C24-C25
14	AS	104	BCL	C4-C3-C5-C6
16	bg	101	V7N	C37-C22-C23-C24
15	BT	102	LMT	C5'-C4'-O1B-C1B
14	bp	102	BCL	C2-C3-C5-C6
16	bb	101	V7N	C21-C22-C23-C24
20	bj	104	0V9	C18-C19-C20-C21
15	L	1004	LMT	C2-C3-C4-C5
15	AQ	103	LMT	C3-C4-C5-C6
20	bk	104	0V9	O5-C30-O3-C3
15	bl	101	LMT	C2B-C1B-O1B-C4'
15	bm	103	LMT	C4B-C5B-C6B-O6B
15	BA	104	LMT	C2B-C1B-O1B-C4'
15	BL	1004	LMT	C2B-C1B-O1B-C4'
20	bh	103	0V9	C33-C34-C35-C36
14	BA	103	BCL	C6-C7-C8-C10
14	BI	1003	BCL	C6-C7-C8-C10
14	BN	103	BCL	C11-C12-C13-C15
20	aj	101	0V9	C33-C34-C35-C36
15	BH	1004	LMT	C4'-C5'-C6'-O6'
15	BI	1004	LMT	C4-C5-C6-C7
21	H1	104	CD4	C15-C16-O3-C17
14	bb	104	BCL	C16-C17-C18-C20
14	bp	102	BCL	C5-C6-C7-C8
14	AQ	101	BCL	O1A-CGA-O2A-C1
14	AR	102	BCL	C3A-C2A-CAA-CBA
14	BA	103	BCL	C3A-C2A-CAA-CBA
14	BB	103	BCL	C3A-C2A-CAA-CBA
14	BH	1005	BCL	C3A-C2A-CAA-CBA
14	BT	103	BCL	C3A-C2A-CAA-CBA
16	BR	1001	V7N	C37-C22-C23-C24
25	L	1009	BPH	C4-C3-C5-C6
15	bm	103	LMT	C5-C6-C7-C8
20	bi	103	0V9	C32-C33-C34-C35
15	bn	101	LMT	C4'-C5'-C6'-O6'
14	AJ	102	BCL	C5-C6-C7-C8
14	bb	104	BCL	C16-C17-C18-C19
15	BR	1003	LMT	C6-C7-C8-C9
15	bj	102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	BT	104	LMT	C4-C5-C6-C7
16	BB	101	V7N	C27-C28-C29-C39
16	BD	101	V7N	C9-C10-C11-C12
16	BM	1001	V7N	C27-C28-C29-C39
15	BV	1004	LMT	C5'-C4'-O1B-C1B
16	bo	102	V7N	C38-C26-C27-C28
20	C1	1001	0V9	C20-C21-C22-C23
15	BX	1003	LMT	C3'-C4'-O1B-C1B
14	ai	101	BCL	C10-C11-C12-C13
14	BV	1005	BCL	C2-C3-C5-C6
20	bg	102	0V9	C35-C36-C37-C38
20	ba	102	0V9	C1-C2-C3-O3
20	be	103	0V9	C16-C17-C18-C19
14	ap	1001	BCL	C3-C5-C6-C7
14	AC	101	BCL	C11-C12-C13-C14
14	AR	102	BCL	C14-C13-C15-C16
14	AS	104	BCL	C11-C12-C13-C14
14	BS	1003	BCL	C11-C10-C8-C9
14	ae	102	BCL	C11-C10-C8-C9
14	bo	103	BCL	C14-C13-C15-C16
15	bh	104	LMT	C2B-C1B-O1B-C4'
14	L	1002	BCL	C2B-C3B-CAB-OB
20	bl	103	0V9	C1-C2-O2-C10
20	bl	103	0V9	C3-C2-O2-C10
20	bo	104	0V9	C3-C2-O2-C10
22	H1	103	PGW	C03-C02-O01-C1
21	aj	102	CD4	C9-C10-C11-C12
15	AD	101	LMT	C3'-C4'-O1B-C1B
14	AI	102	BCL	C4-C3-C5-C6
20	bg	102	0V9	C10-C11-C12-C13
16	bg	101	V7N	C21-C22-C23-C24
15	BV	1002	LMT	C4-C5-C6-C7
15	BH	1002	LMT	C2B-C1B-O1B-C4'
17	C	404	HEC	CAD-CBD-CGD-O1D
14	BX	1002	BCL	C2A-CAA-CBA-CGA
15	BS	1004	LMT	O5B-C5B-C6B-O6B
14	AM	102	BCL	C1A-C2A-CAA-CBA
14	BF	102	BCL	C1A-C2A-CAA-CBA
14	BW	1003	BCL	C1A-C2A-CAA-CBA
14	ba	103	BCL	C1A-C2A-CAA-CBA
14	bb	104	BCL	C1A-C2A-CAA-CBA
14	bg	105	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	bl	104	BCL	C1A-C2A-CAA-CBA
15	BD	104	LMT	O5B-C1B-O1B-C4'
17	C	404	HEC	CAD-CBD-CGD-O2D
15	BN	105	LMT	O5'-C1'-O1'-C1
15	BB	105	LMT	C5-C6-C7-C8
15	AN	103	LMT	C7-C8-C9-C10
21	M	402	CD4	C40-C41-C42-C43
15	bi	102	LMT	C4'-C5'-C6'-O6'
20	bm	102	0V9	C31-C30-O3-C3
20	bj	104	0V9	C13-C14-C15-C16
14	BF	102	BCL	C4-C3-C5-C6
14	BB	103	BCL	C2-C3-C5-C6
14	BJ	1002	BCL	C2-C3-C5-C6
15	bi	102	LMT	C6-C7-C8-C9
20	bg	104	0V9	C35-C36-C37-C38
16	BB	101	V7N	C23-C24-C25-C26
15	BD	103	LMT	O5B-C1B-O1B-C4'
15	AJ	104	LMT	O5B-C5B-C6B-O6B
15	L	1008	LMT	C6-C7-C8-C9
14	AC	102	BCL	C11-C10-C8-C7
14	AX	103	BCL	C11-C10-C8-C7
14	BM	1002	BCL	C11-C12-C13-C15
14	ap	1001	BCL	C11-C12-C13-C15
14	bb	104	BCL	C12-C13-C15-C16
15	BH	1002	LMT	C4-C5-C6-C7
15	BL	1005	LMT	C2-C3-C4-C5
20	bh	103	0V9	C34-C35-C36-C37
14	AE	1004	BCL	C2A-CAA-CBA-CGA
15	bj	102	LMT	C3-C4-C5-C6
14	AK	102	BCL	C8-C10-C11-C12
14	AX	103	BCL	C8-C10-C11-C12
20	bk	103	0V9	C18-C19-C20-C21
21	ae	101	CD4	O16-C33-C34-O14
24	L	1006	V7B	O7-C8-C9-O8
15	BH	1003	LMT	C3-C4-C5-C6
16	bi	101	V7N	C31-C1-C2-C3
20	be	102	0V9	C31-C30-O3-C3
20	be	102	0V9	C20-C21-C22-C23
15	BC	106	LMT	O5B-C5B-C6B-O6B
20	bc	103	0V9	C35-C36-C37-C38
25	M	406	BPH	C8-C10-C11-C12
16	BR	1001	V7N	C38-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
15	BA	105	LMT	C5'-C4'-O1B-C1B
14	BJ	1002	BCL	C4-C3-C5-C6
14	ap	1001	BCL	C4-C3-C5-C6
16	AE	1005	V7N	C37-C22-C23-C24
16	AO	1001	V7N	C37-C22-C23-C24
15	AA	1003	LMT	C3-C4-C5-C6
20	bk	104	0V9	O2-C10-C11-C12
14	AS	104	BCL	C2-C3-C5-C6
14	ap	1001	BCL	C2-C3-C5-C6
16	BR	1001	V7N	C21-C22-C23-C24
15	bg	103	LMT	O5'-C5'-C6'-O6'
15	BN	101	LMT	C3'-C4'-O1B-C1B
15	AX	101	LMT	C4-C5-C6-C7
21	aj	102	CD4	C6-C7-C8-C9
14	AE	1003	BCL	C15-C16-C17-C18
14	AP	102	BCL	C15-C16-C17-C18
14	bc	102	BCL	C5-C6-C7-C8
14	bm	104	BCL	C5-C6-C7-C8
25	M	406	BPH	C10-C11-C12-C13
17	C	403	HEC	CAD-CBD-CGD-O2D
15	bm	105	LMT	C3-C4-C5-C6
15	ab	101	LMT	C6-C7-C8-C9
14	AL	101	BCL	C15-C16-C17-C18
21	H1	104	CD4	C24-C25-C26-C27
14	al	1001	BCL	C3-C5-C6-C7
15	BW	1004	LMT	O5B-C1B-O1B-C4'
14	BM	1002	BCL	C11-C10-C8-C9
15	BD	104	LMT	C5'-C4'-O1B-C1B
14	ah	1001	BCL	C13-C15-C16-C17
15	BS	1005	LMT	C2B-C1B-O1B-C4'
15	BB	104	LMT	O5B-C5B-C6B-O6B
15	bl	101	LMT	C4B-C5B-C6B-O6B
14	BB	103	BCL	C4-C3-C5-C6
16	BH	1001	V7N	C37-C22-C23-C24
16	BU	1001	V7N	C37-C22-C23-C24
15	BS	1002	LMT	O5B-C5B-C6B-O6B
15	BH	1003	LMT	C2-C3-C4-C5
21	af	102	CD4	C37-C38-C39-C40
20	bg	104	0V9	O4-C10-O2-C2
14	AC	101	BCL	C15-C16-C17-C18
15	BK	1004	LMT	C6-C7-C8-C9
14	BO	1004	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	bb	102	LMT	C11-C10-C9-C8
20	be	103	0V9	C36-C37-C38-C39
15	L	1003	LMT	O5'-C5'-C6'-O6'
14	BB	103	BCL	C2A-CAA-CBA-CGA
14	BJ	1002	BCL	C2A-CAA-CBA-CGA
14	bl	104	BCL	C2A-CAA-CBA-CGA
20	be	103	0V9	C15-C16-C17-C18
15	AD	101	LMT	C2B-C1B-O1B-C4'
15	BX	1004	LMT	C5'-C4'-O1B-C1B
15	AJ	104	LMT	C4'-C5'-C6'-O6'
14	aa	1001	BCL	C8-C10-C11-C12
15	BW	1004	LMT	C4-C5-C6-C7
16	BB	101	V7N	C37-C22-C23-C24
16	AO	1001	V7N	C27-C28-C29-C39
15	BC	102	LMT	C2B-C1B-O1B-C4'
15	L	1008	LMT	C4-C5-C6-C7
15	bd	103	LMT	C4-C5-C6-C7
15	BR	1002	LMT	C5'-C4'-O1B-C1B
15	BB	105	LMT	C2B-C1B-O1B-C4'
15	bc	104	LMT	C2-C3-C4-C5
20	bm	102	0V9	O5-C30-O3-C3
15	BS	1004	LMT	C9-C10-C11-C12
15	BV	1003	LMT	C4'-C5'-C6'-O6'
14	M	405	BCL	CAA-CBA-CGA-O2A
21	H1	102	CD4	C10-C11-C12-C13
17	C	403	HEC	CAD-CBD-CGD-O1D
15	bj	102	LMT	C5'-C4'-O1B-C1B
14	AC	101	BCL	C16-C17-C18-C19
24	ag	1002	V7B	C30-C31-C32-C33
25	L	1009	BPH	CHA-CBD-CGD-O1D
15	bb	102	LMT	C1-C2-C3-C4
14	AC	101	BCL	C16-C17-C18-C20
20	bj	104	0V9	C31-C32-C33-C34
15	bm	103	LMT	C11-C10-C9-C8
21	M	402	CD4	C52-C53-C54-C55
14	AL	103	BCL	C13-C15-C16-C17
14	BD	105	BCL	C11-C10-C8-C9
14	ag	1001	BCL	C11-C12-C13-C14
14	ai	101	BCL	C11-C10-C8-C9
14	ai	101	BCL	C14-C13-C15-C16
14	ao	102	BCL	C11-C12-C13-C14
14	bg	105	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	bl	104	BCL	C6-C7-C8-C9
20	ba	102	0V9	C15-C16-C17-C18
20	bg	104	0V9	C36-C37-C38-C39
14	BW	1003	BCL	CAA-CBA-CGA-O2A
14	AP	102	BCL	C8-C10-C11-C12
20	aj	101	0V9	C16-C17-C18-C19
14	BV	1005	BCL	C2A-CAA-CBA-CGA
14	L	1010	BCL	C2-C1-O2A-CGA
14	AI	103	BCL	C3A-C2A-CAA-CBA
14	AM	102	BCL	C3A-C2A-CAA-CBA
14	bg	105	BCL	C3A-C2A-CAA-CBA
14	bl	104	BCL	C3A-C2A-CAA-CBA
14	AC	103	BCL	C2-C3-C5-C6
14	AS	104	BCL	O2A-C1-C2-C3
14	L	1002	BCL	C2B-C3B-CAB-CBB
14	M	408	BCL	C2B-C3B-CAB-OB
14	bp	102	BCL	O2A-C1-C2-C3
20	bo	104	0V9	C1-C2-O2-C10
25	L	1009	BPH	O2A-C1-C2-C3
20	bh	103	0V9	C16-C17-C18-C19
20	bk	104	0V9	C19-C20-C21-C22
15	BN	104	LMT	C5'-C4'-O1B-C1B
15	BT	101	LMT	C1-C2-C3-C4
15	BA	102	LMT	O5B-C1B-O1B-C4'
15	BU	1003	LMT	O5B-C5B-C6B-O6B
14	BN	103	BCL	C2A-CAA-CBA-CGA
14	BR	1004	BCL	C2A-CAA-CBA-CGA
15	BT	104	LMT	C5'-C4'-O1B-C1B
15	BL	1002	LMT	C6-C7-C8-C9
21	H1	104	CD4	C2-C3-C4-C5
15	BG	1002	LMT	C5'-C4'-O1B-C1B
15	AC	104	LMT	O5B-C1B-O1B-C4'
14	AS	102	BCL	C8-C10-C11-C12
15	AG	103	LMT	C7-C8-C9-C10
15	bh	101	LMT	C5-C6-C7-C8
15	BL	1004	LMT	O1'-C1-C2-C3
20	bl	103	0V9	C1-C2-C3-O3
24	ag	1002	V7B	O1-C7-C8-C9
15	BQ	1004	LMT	C7-C8-C9-C10
15	bm	103	LMT	C5'-C4'-O1B-C1B
14	bf	103	BCL	C10-C11-C12-C13
21	M	402	CD4	C48-C49-C50-C51

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Mol	Chain	Res	Type	Atoms
14	AC	101	BCL	C4-C3-C5-C6
16	bc	101	V7N	C37-C22-C23-C24
16	bl	102	V7N	C37-C22-C23-C24
15	BB	105	LMT	C5'-C4'-O1B-C1B
23	L	1001	MQ8	C32-C33-C35-C36
15	BJ	1003	LMT	C1-C2-C3-C4
15	L	1008	LMT	C1-C2-C3-C4
15	BE	103	LMT	C3-C4-C5-C6
21	aj	102	CD4	C36-C37-C38-C39
15	BN	101	LMT	C2B-C1B-O1B-C4'
15	BK	1002	LMT	O1'-C1-C2-C3
14	AQ	101	BCL	CAA-CBA-CGA-O2A
14	L	1002	BCL	C4B-C3B-CAB-CBB
21	af	102	CD4	O2-C15-C16-O3
15	BN	104	LMT	C3-C4-C5-C6
17	C	401	HEC	CAA-CBA-CGA-O1A
14	AA	1002	BCL	C11-C10-C8-C9
14	AI	102	BCL	C14-C13-C15-C16
17	C	401	HEC	CAA-CBA-CGA-O2A
16	BR	1001	V7N	C25-C26-C27-C28
15	BW	1002	LMT	C9-C10-C11-C12
14	bl	104	BCL	C5-C6-C7-C8
14	AP	103	BCL	C4-C3-C5-C6
16	bi	101	V7N	O32-C1-C2-C3
20	bk	104	OV9	C14-C15-C16-C17
14	AE	1003	BCL	C11-C12-C13-C15
14	BC	104	BCL	C11-C10-C8-C7
14	BD	105	BCL	C11-C10-C8-C7
14	BI	1003	BCL	C11-C10-C8-C7
14	BM	1002	BCL	C11-C10-C8-C7
14	BQ	1003	BCL	C11-C10-C8-C7
14	BX	1002	BCL	C6-C7-C8-C10
14	ab	102	BCL	C6-C7-C8-C10
14	ae	102	BCL	C11-C10-C8-C7
14	ai	101	BCL	C12-C13-C15-C16
14	am	1001	BCL	C6-C7-C8-C10
14	ao	102	BCL	C11-C12-C13-C15
14	bg	105	BCL	C6-C7-C8-C10
14	bk	102	BCL	C12-C13-C15-C16
14	bl	104	BCL	C6-C7-C8-C10
14	bn	103	BCL	C11-C12-C13-C15
14	bo	103	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	M	406	BPH	C11-C12-C13-C15
21	aj	102	CD4	C1-C2-C3-C4
15	BN	102	LMT	O5B-C5B-C6B-O6B
20	H1	101	0V9	C34-C35-C36-C37
15	BK	1002	LMT	C5'-C4'-O1B-C1B
15	BU	1002	LMT	C9-C10-C11-C12
14	ad	1001	BCL	CAA-CBA-CGA-O2A
14	AG	101	BCL	C2-C1-O2A-CGA
14	AI	103	BCL	C2-C1-O2A-CGA
14	AQ	101	BCL	C2-C1-O2A-CGA
15	bm	105	LMT	C2B-C1B-O1B-C4'
20	bg	102	0V9	O2-C10-C11-C12
28	ai	102	UYH	C16-C17-C18-C19
14	ao	102	BCL	C15-C16-C17-C18
14	bm	104	BCL	C4-C3-C5-C6
14	AV	101	BCL	C2-C3-C5-C6
14	al	1001	BCL	C2-C3-C5-C6
15	BP	1003	LMT	C3'-C4'-O1B-C1B
15	L	1005	LMT	C2B-C1B-O1B-C4'
21	H1	102	CD4	C47-C46-O16-C33
15	BF	101	LMT	C5'-C4'-O1B-C1B
15	BD	102	LMT	C9-C10-C11-C12
15	BA	102	LMT	C2-C3-C4-C5
15	bm	105	LMT	C6-C7-C8-C9
21	ae	101	CD4	C6-C7-C8-C9
16	be	101	V7N	C23-C24-C25-C26
20	bp	103	0V9	C35-C36-C37-C38
15	BR	1002	LMT	C2B-C1B-O1B-C4'
15	ab	101	LMT	C4'-C5'-C6'-O6'
15	AU	101	LMT	C5-C6-C7-C8
21	af	102	CD4	O2-C15-C28-O5
15	BK	1005	LMT	C5'-C4'-O1B-C1B
15	BU	1002	LMT	C6-C7-C8-C9
14	aj	103	BCL	CAA-CBA-CGA-O2A
16	BP	1001	V7N	C23-C24-C25-C26
14	AX	102	BCL	CAA-CBA-CGA-O2A
14	BC	104	BCL	CAA-CBA-CGA-O2A
14	bc	102	BCL	CBA-CGA-O2A-C1
14	AJ	102	BCL	CBD-CGD-O2D-CED
14	AB	1001	BCL	C6-C7-C8-C9
14	AP	103	BCL	C6-C7-C8-C9
14	BT	103	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	ba	103	BCL	C15-C16-C17-C18
24	ag	1002	V7B	C10-C11-C12-C13
14	AL	101	BCL	CAA-CBA-CGA-O2A
21	H1	102	CD4	C12-C13-C14-O2
14	ak	1001	BCL	C13-C15-C16-C17
14	AN	101	BCL	C1A-C2A-CAA-CBA
14	BA	103	BCL	C1A-C2A-CAA-CBA
14	BB	103	BCL	C1A-C2A-CAA-CBA
14	BH	1005	BCL	C1A-C2A-CAA-CBA
14	BK	1006	BCL	C1A-C2A-CAA-CBA
14	BT	103	BCL	C1A-C2A-CAA-CBA
14	BV	1005	BCL	C1A-C2A-CAA-CBA
14	aa	1001	BCL	C1A-C2A-CAA-CBA
14	ab	102	BCL	C1A-C2A-CAA-CBA
14	ad	1001	BCL	C1A-C2A-CAA-CBA
14	bd	102	BCL	C1A-C2A-CAA-CBA
14	bh	105	BCL	C1A-C2A-CAA-CBA
20	bh	103	0V9	C31-C30-O3-C3
14	aj	103	BCL	C4-C3-C5-C6
14	AV	103	BCL	CAA-CBA-CGA-O2A
14	ai	101	BCL	CAA-CBA-CGA-O2A
21	ae	101	CD4	O3-C17-C18-C19
20	bg	104	0V9	O2-C2-C3-O3
20	bj	104	0V9	O2-C2-C3-O3
15	BG	1002	LMT	C6-C7-C8-C9
15	AS	101	LMT	C2B-C1B-O1B-C4'
14	BH	1005	BCL	C8-C10-C11-C12
14	BJ	1002	BCL	CAA-CBA-CGA-O2A
22	H1	103	PGW	O01-C1-C2-C3
15	AJ	103	LMT	C5'-C4'-O1B-C1B
14	AL	101	BCL	C2A-CAA-CBA-CGA
14	BG	1004	BCL	C2A-CAA-CBA-CGA
14	BT	103	BCL	C2A-CAA-CBA-CGA
21	H1	102	CD4	C45-C63-C64-C65
15	BX	1003	LMT	C5-C6-C7-C8
20	bk	104	0V9	C30-C31-C32-C33
15	bh	101	LMT	C9-C10-C11-C12
20	bi	103	0V9	O2-C10-C11-C12
15	BE	103	LMT	C1-C2-C3-C4
20	bp	103	0V9	C36-C37-C38-C39
14	AB	1001	BCL	C6-C7-C8-C10
14	AQ	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	AS	102	BCL	C12-C13-C15-C16
14	ai	101	BCL	C11-C10-C8-C7
14	bp	102	BCL	C11-C10-C8-C7
15	BN	105	LMT	C2-C3-C4-C5
15	BK	1003	LMT	C4-C5-C6-C7
14	M	408	BCL	C2B-C3B-CAB-CBB
21	H1	102	CD4	C28-C15-O2-C14
22	H1	103	PGW	C01-C02-O01-C1
15	bd	103	LMT	O5B-C5B-C6B-O6B
15	BR	1003	LMT	C2B-C1B-O1B-C4'
15	BB	105	LMT	C3-C4-C5-C6
14	bc	102	BCL	O1A-CGA-O2A-C1
14	AK	101	BCL	CAA-CBA-CGA-O2A
14	AP	103	BCL	C8-C10-C11-C12
25	L	1009	BPH	C8-C10-C11-C12
15	BI	1006	LMT	C4B-C5B-C6B-O6B
15	BB	104	LMT	O5'-C5'-C6'-O6'
14	AV	103	BCL	C2A-CAA-CBA-CGA
14	ac	1001	BCL	C16-C17-C18-C20
20	bg	104	0V9	C33-C34-C35-C36
14	BV	1005	BCL	C5-C6-C7-C8
15	BH	1002	LMT	C5'-C4'-O1B-C1B
15	BJ	1004	LMT	C5'-C4'-O1B-C1B
15	BL	1004	LMT	C3'-C4'-O1B-C1B
15	AJ	104	LMT	C11-C10-C9-C8
15	BC	102	LMT	C3'-C4'-O1B-C1B
14	AE	1004	BCL	C3A-C2A-CAA-CBA
14	AS	102	BCL	C3A-C2A-CAA-CBA
14	BW	1003	BCL	C3A-C2A-CAA-CBA
14	ba	103	BCL	C3A-C2A-CAA-CBA
14	bb	104	BCL	C3A-C2A-CAA-CBA
14	bd	102	BCL	C3A-C2A-CAA-CBA
21	aj	102	CD4	C11-C10-C9-C8
20	bb	103	0V9	C13-C14-C15-C16
20	bg	102	0V9	O4-C10-C11-C12
15	BW	1005	LMT	C6-C7-C8-C9
15	BP	1002	LMT	C3'-C4'-O1B-C1B
21	af	102	CD4	C17-C18-C19-C20
24	ag	1002	V7B	C28-C29-C30-C31
20	bg	102	0V9	C18-C19-C20-C21
14	L	1002	BCL	C4B-C3B-CAB-OB
15	bl	101	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	BK	1002	LMT	C2B-C1B-O1B-C4'
14	BB	103	BCL	C15-C16-C17-C18
14	AI	103	BCL	CBA-CGA-O2A-C1
14	AP	102	BCL	C6-C7-C8-C9
14	BM	1002	BCL	C11-C12-C13-C14
14	al	1001	BCL	C14-C13-C15-C16
14	ap	1001	BCL	C11-C12-C13-C14
14	bb	104	BCL	C14-C13-C15-C16
25	M	406	BPH	C11-C12-C13-C14
14	BC	104	BCL	CAA-CBA-CGA-O1A
24	ag	1002	V7B	C32-C33-C34-C35
15	AA	1003	LMT	C3'-C4'-O1B-C1B
14	be	105	BCL	C8-C10-C11-C12
15	bm	105	LMT	C2-C3-C4-C5
14	AJ	102	BCL	O1D-CGD-O2D-CED
14	ak	1001	BCL	C5-C6-C7-C8
25	L	1009	BPH	C2-C3-C5-C6
14	bf	103	BCL	C8-C10-C11-C12
16	bi	101	V7N	C1-C2-C3-C4
16	bj	101	V7N	C1-C2-C3-C4
14	AQ	101	BCL	CAA-CBA-CGA-O1A
14	AJ	102	BCL	C15-C16-C17-C18
21	af	102	CD4	C51-C52-C53-C54
21	M	402	CD4	O16-C46-C47-C48
16	bb	101	V7N	C17-C18-C19-C20
16	bo	102	V7N	C25-C26-C27-C28
14	ae	102	BCL	CAA-CBA-CGA-O1A
21	ae	101	CD4	C1-C2-C3-C4
14	AD	102	BCL	C10-C11-C12-C13
14	BC	104	BCL	C5-C6-C7-C8
21	aj	102	CD4	O2-C15-C16-O3
15	BA	102	LMT	C5'-C4'-O1B-C1B
14	ad	1001	BCL	CAA-CBA-CGA-O1A
14	ai	101	BCL	CAA-CBA-CGA-O1A
14	BU	1004	BCL	CAA-CBA-CGA-O2A
14	BP	1005	BCL	C5-C6-C7-C8
14	BA	103	BCL	C2A-CAA-CBA-CGA
14	BD	105	BCL	C2A-CAA-CBA-CGA
16	ba	101	V7N	C22-C23-C24-C25
15	BV	1003	LMT	C5-C6-C7-C8
21	af	102	CD4	C12-C13-C14-O1
14	bo	103	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	BO	1001	V7N	C23-C24-C25-C26
14	AL	103	BCL	C5-C6-C7-C8
15	BG	1005	LMT	C9-C10-C11-C12
21	H1	102	CD4	C39-C40-C41-C42
14	AR	101	BCL	C10-C11-C12-C13
14	AL	101	BCL	CAA-CBA-CGA-O1A
14	AX	102	BCL	CAA-CBA-CGA-O1A
14	aj	103	BCL	CAA-CBA-CGA-O1A
15	BS	1004	LMT	C3'-C4'-O1B-C1B
20	C1	1001	0V9	O3-C30-C31-C32
20	bg	102	0V9	O3-C30-C31-C32
21	af	102	CD4	C12-C13-C14-O2
21	H1	102	CD4	C12-C13-C14-O1
15	BH	1003	LMT	C5'-C4'-O1B-C1B
15	BH	1004	LMT	C3-C4-C5-C6
28	ai	102	UYH	C21-C22-C23-C24
14	ad	1001	BCL	C2-C1-O2A-CGA
20	bp	103	0V9	C13-C14-C15-C16
22	H1	103	PGW	O02-C1-C2-C3
14	am	1001	BCL	C1-C2-C3-C4
14	AN	104	BCL	C16-C17-C18-C19
14	AN	104	BCL	C16-C17-C18-C20
15	L	1003	LMT	O5B-C1B-O1B-C4'
15	L	1003	LMT	C2B-C1B-O1B-C4'
15	bh	101	LMT	C1-C2-C3-C4
14	bj	103	BCL	C5-C6-C7-C8
15	BE	103	LMT	O5B-C5B-C6B-O6B
14	AH	101	BCL	CAA-CBA-CGA-O2A
14	ae	102	BCL	CAA-CBA-CGA-O2A
14	AH	101	BCL	CAA-CBA-CGA-O1A
20	ba	102	0V9	C16-C17-C18-C19
21	M	402	CD4	O14-C35-C36-C37
14	AI	103	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

100 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bc	104	LMT	1	0
22	H1	103	PGW	1	0
14	BI	1003	BCL	2	0
14	AF	1001	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aa	1001	BCL	1	0
15	AP	101	LMT	1	0
14	AG	102	BCL	1	0
14	AS	104	BCL	2	0
14	AI	102	BCL	2	0
15	bo	101	LMT	1	0
14	ao	102	BCL	1	0
14	bh	105	BCL	1	0
16	bg	101	V7N	1	0
15	BH	1003	LMT	1	0
14	AJ	101	BCL	1	0
14	bl	104	BCL	1	0
14	AC	102	BCL	1	0
14	af	101	BCL	2	0
14	M	408	BCL	2	0
14	be	105	BCL	1	0
14	am	1001	BCL	1	0
14	AX	103	BCL	1	0
14	AE	1001	BCL	1	0
14	bm	104	BCL	1	0
14	AC	103	BCL	1	0
15	BO	1003	LMT	1	0
17	C	402	HEC	1	0
20	bm	102	0V9	1	0
14	bg	105	BCL	1	0
14	bd	102	BCL	1	0
15	BR	1005	LMT	1	0
17	C	401	HEC	1	0
15	BO	1002	LMT	1	0
17	C	404	HEC	1	0
14	bp	102	BCL	1	0
21	aj	102	CD4	1	0
23	L	1001	MQ8	1	0
14	AB	1002	BCL	1	0
14	ab	102	BCL	2	0
15	BR	1003	LMT	1	0
15	AD	101	LMT	1	0
27	M	404	CRT	2	0
15	BH	1004	LMT	1	0
15	BG	1006	LMT	1	0
14	bj	103	BCL	1	0
14	AV	102	BCL	1	0

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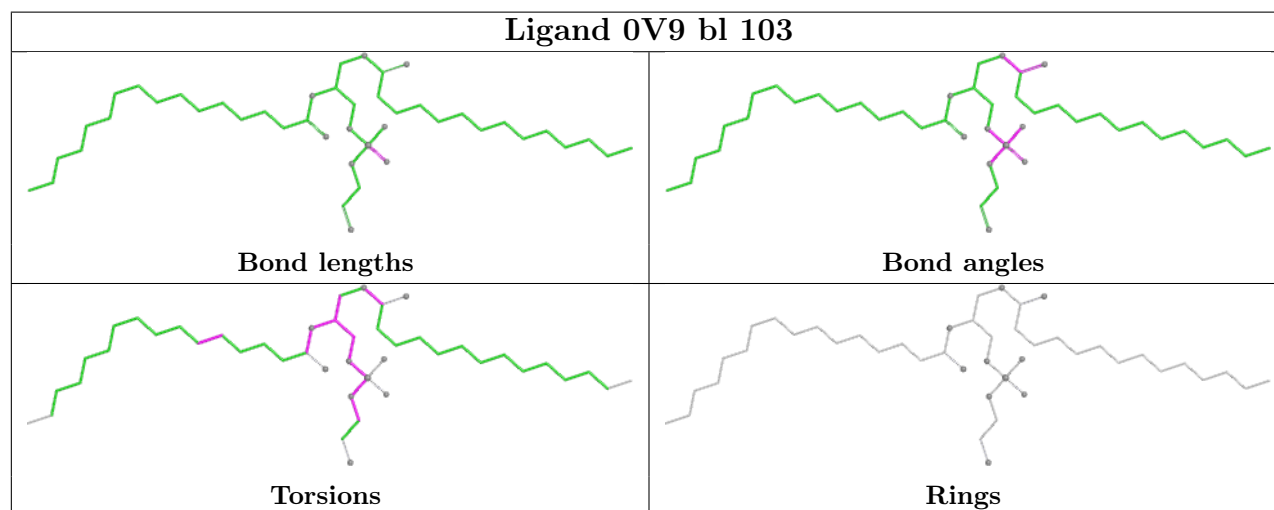
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	1002	BCL	2	0
15	BA	105	LMT	1	0
15	BT	101	LMT	1	0
14	AR	102	BCL	2	0
14	ae	102	BCL	1	0
14	AH	101	BCL	1	0
14	AI	103	BCL	1	0
14	AP	102	BCL	1	0
14	AH	103	BCL	1	0
14	AV	103	BCL	1	0
14	ai	101	BCL	1	0
14	AC	101	BCL	1	0
21	ae	101	CD4	1	0
14	AU	102	BCL	1	0
25	L	1009	BPH	2	0
17	C	403	HEC	1	0
14	AN	102	BCL	1	0
15	BG	1005	LMT	1	0
14	BU	1004	BCL	1	0
14	bb	104	BCL	1	0
14	AL	103	BCL	1	0
15	BT	102	LMT	1	0
15	BV	1003	LMT	1	0
14	AO	1002	BCL	1	0
14	AA	1001	BCL	2	0
14	bf	103	BCL	2	0
14	AR	101	BCL	1	0
14	BS	1003	BCL	1	0
14	AW	101	BCL	3	0
15	AF	1002	LMT	1	0
14	ah	1001	BCL	1	0
14	AQ	102	BCL	1	0
14	AS	102	BCL	1	0
15	BV	1006	LMT	1	0
25	M	406	BPH	3	0
14	AK	102	BCL	1	0
14	ba	103	BCL	1	0
16	BV	1001	V7N	1	0
14	AU	103	BCL	1	0
14	AN	101	BCL	1	0
21	af	102	CD4	1	0
15	BV	1002	LMT	1	0

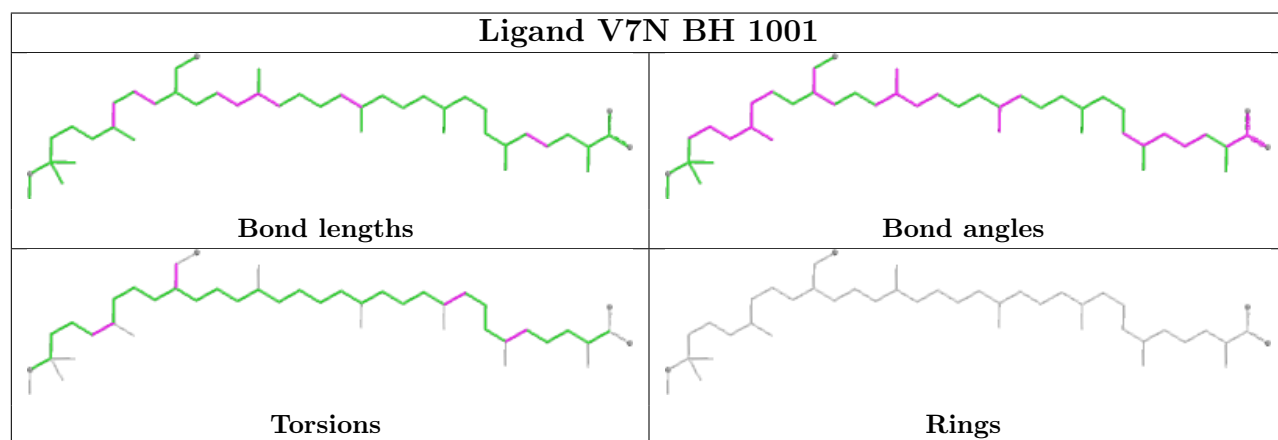
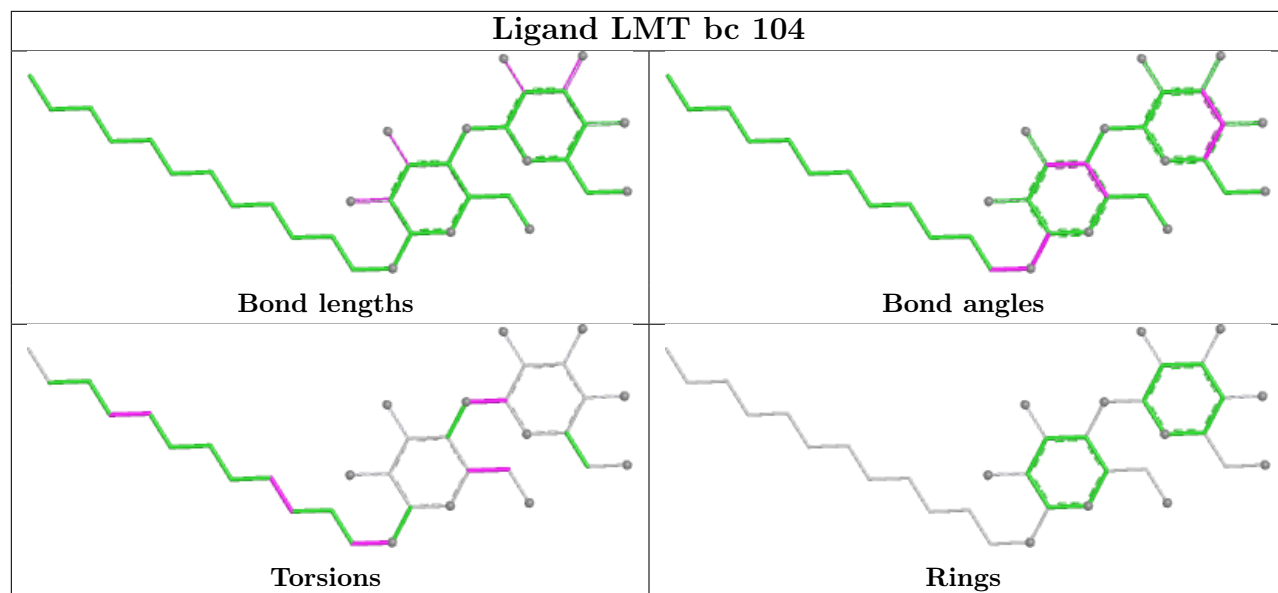
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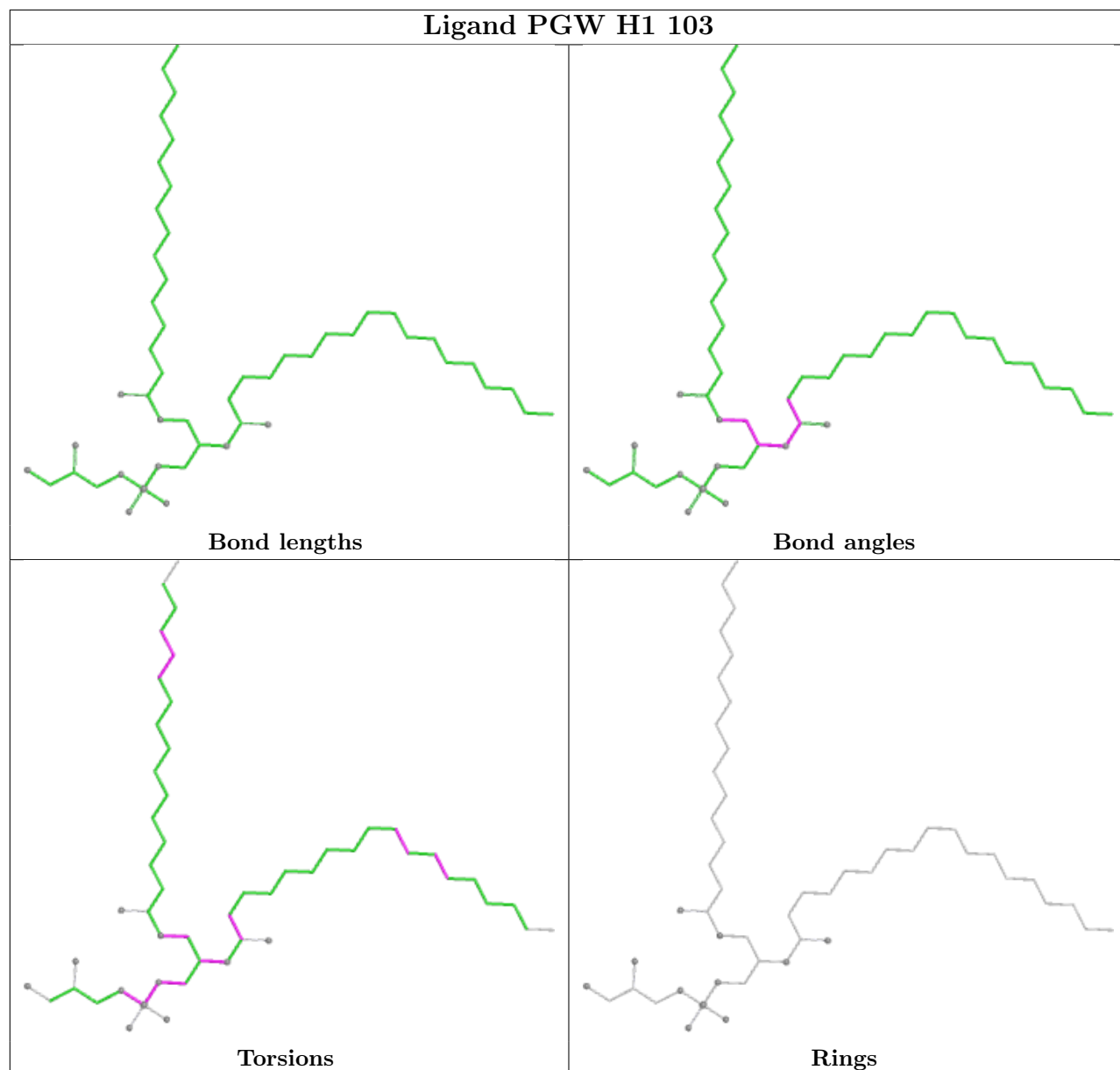
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AS	103	BCL	1	0
23	M	407	MQ8	2	0
14	ac	1001	BCL	1	0
14	AX	102	BCL	2	0
14	AB	1001	BCL	1	0
15	bi	102	LMT	1	0
14	AM	102	BCL	1	0
14	ag	1001	BCL	1	0
15	AH	104	LMT	1	0
14	BM	1002	BCL	1	0
14	AT	101	BCL	1	0
14	AM	101	BCL	1	0

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.

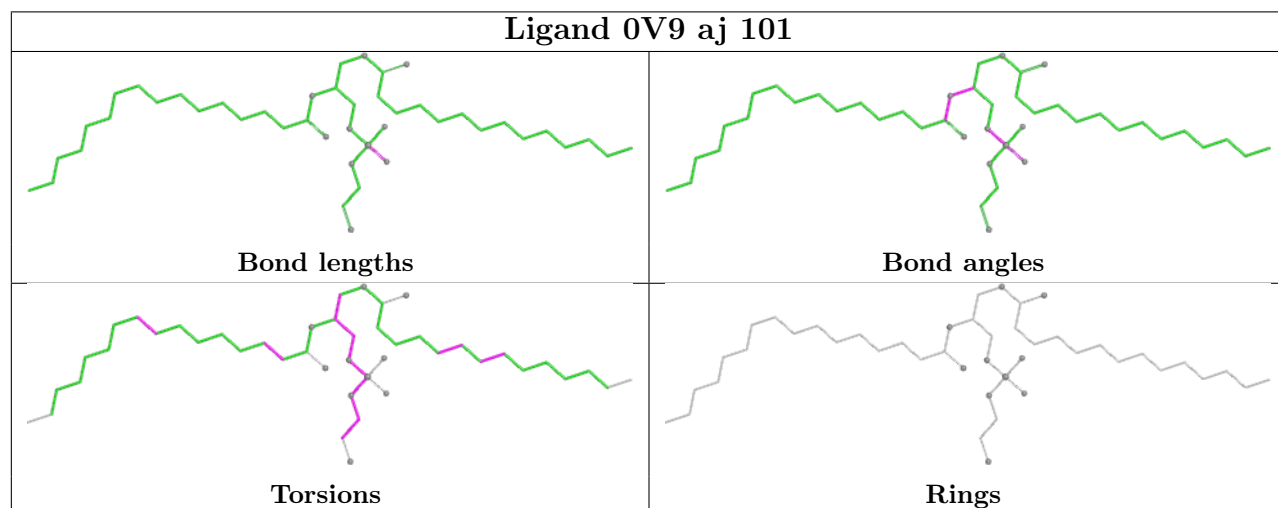


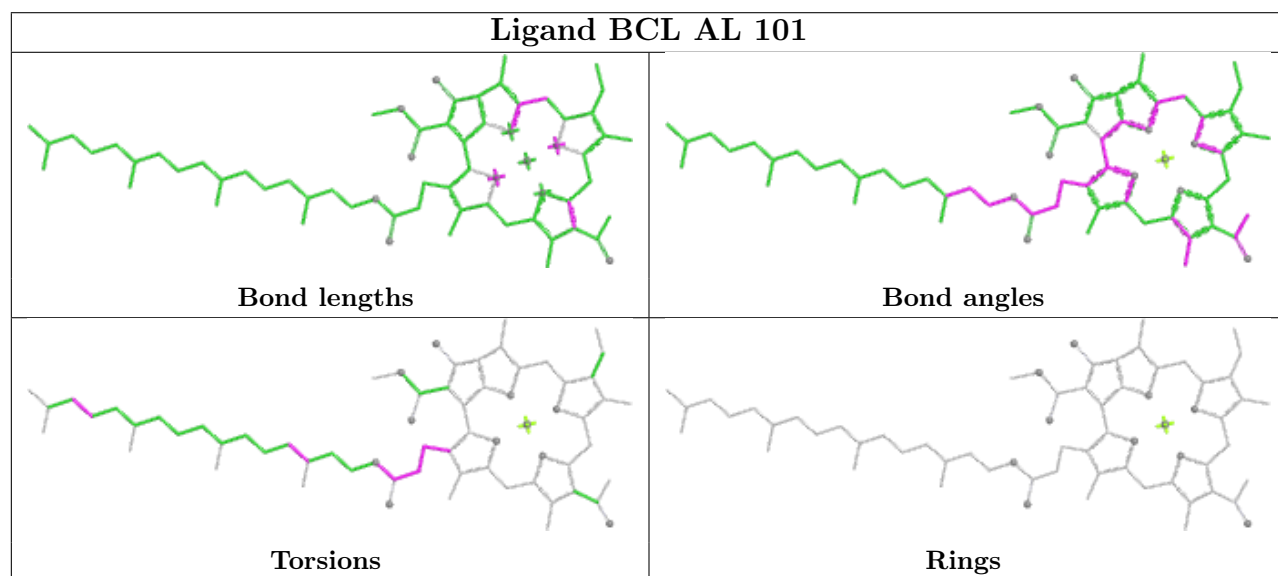
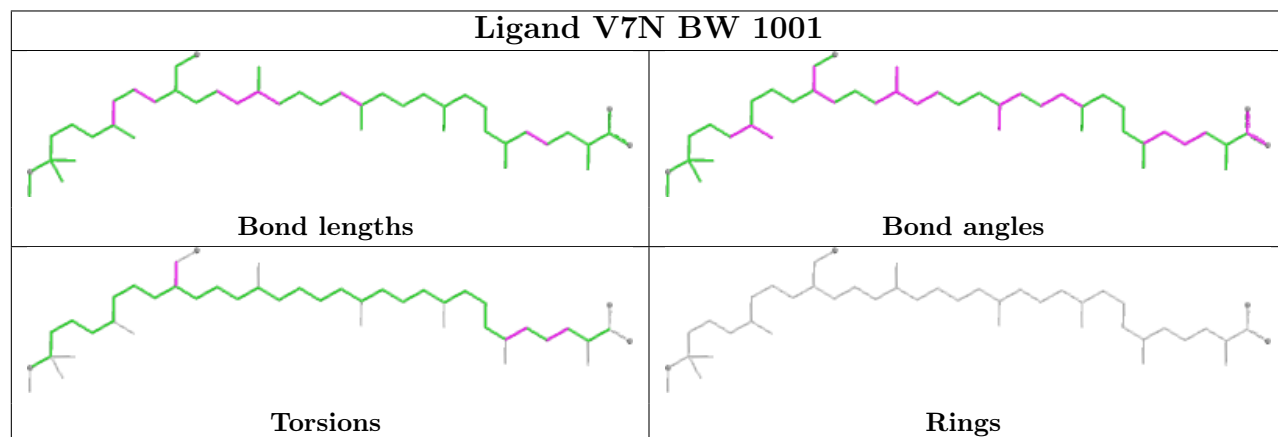
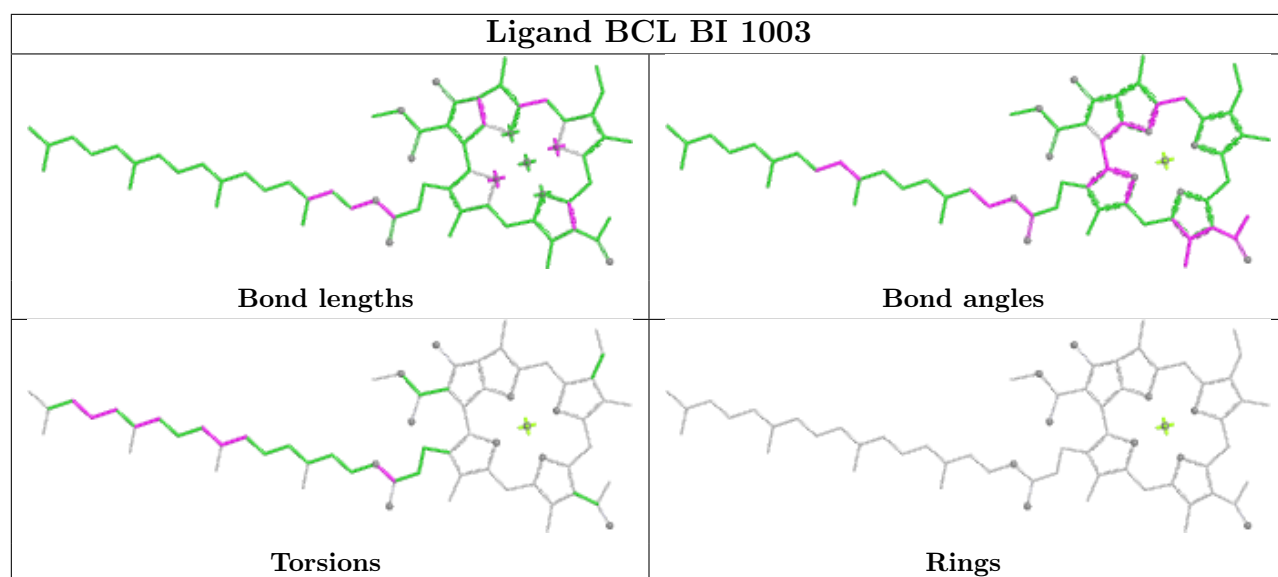


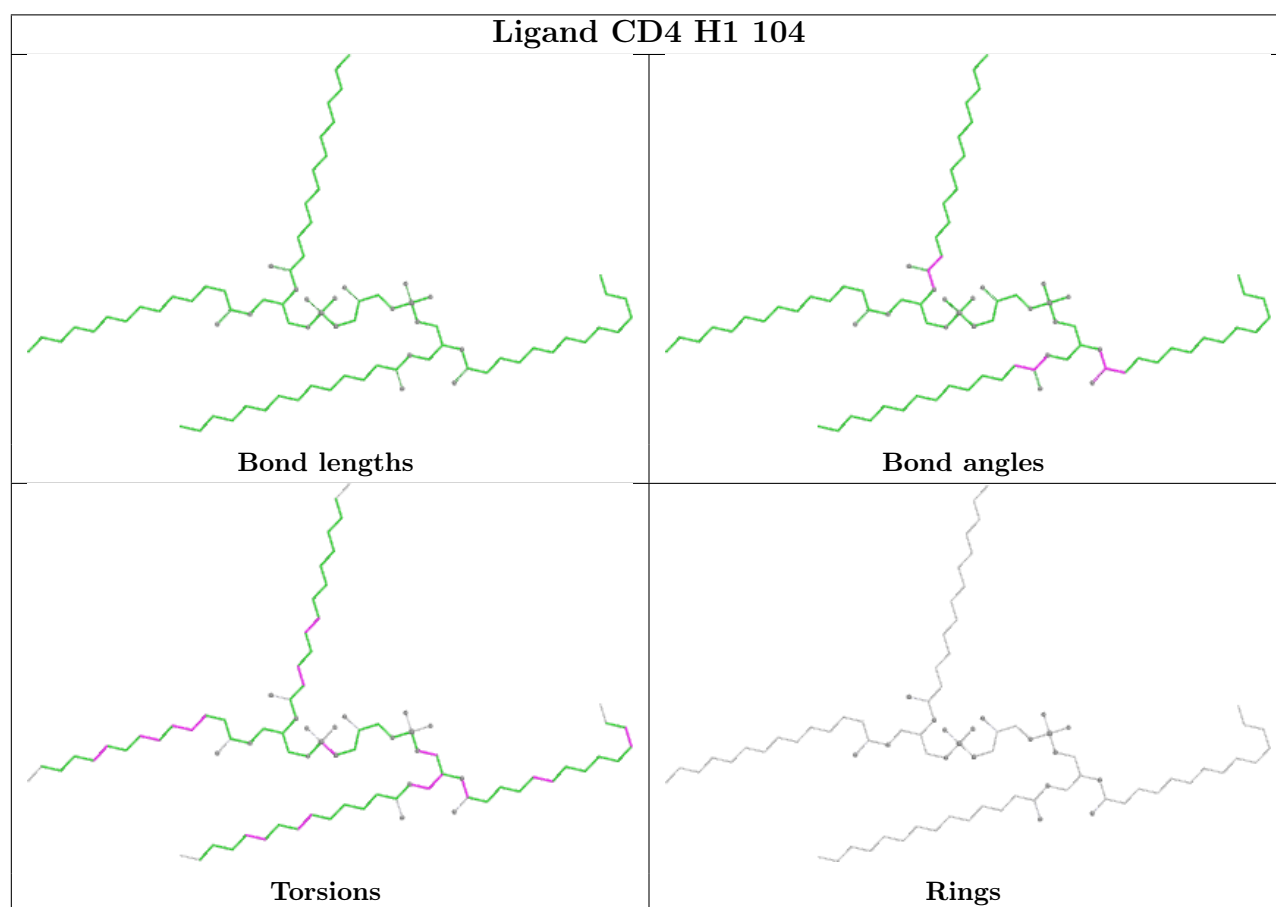
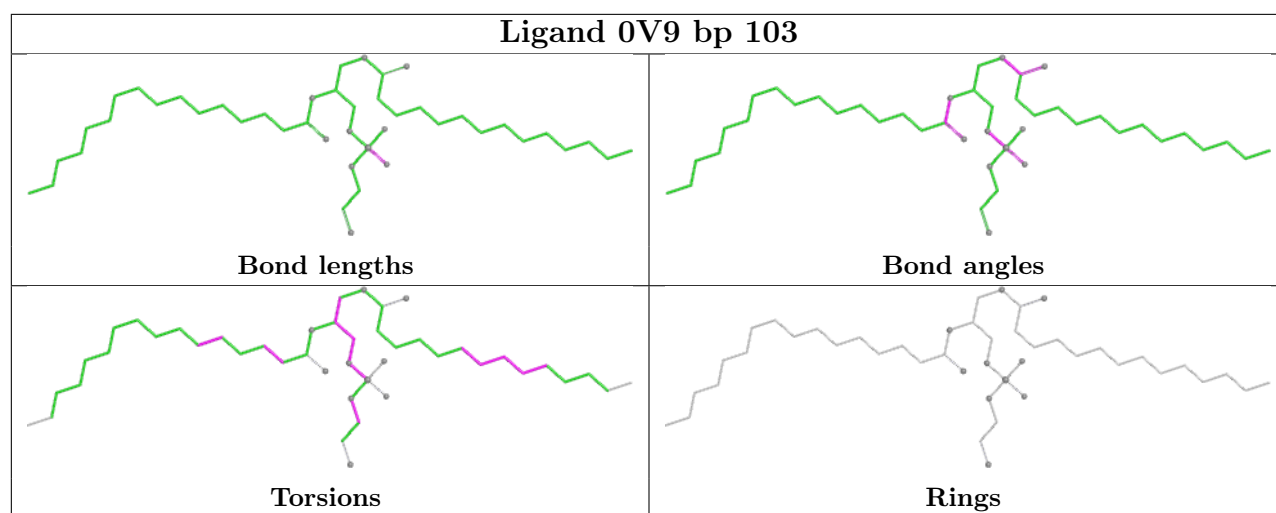
Ligand PGW H1 103

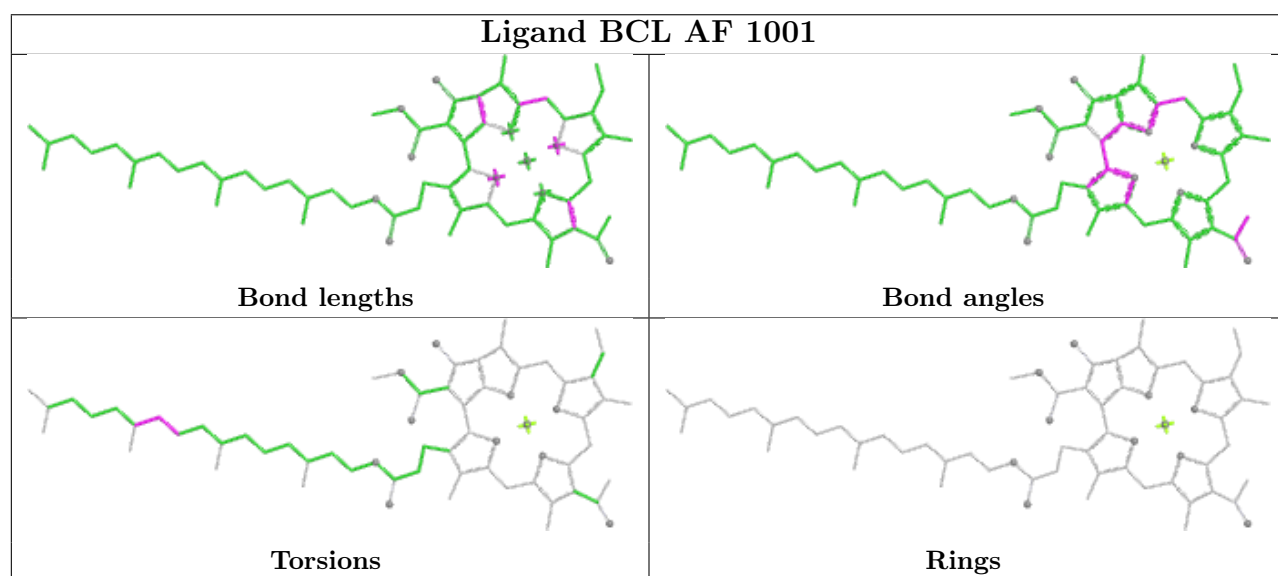
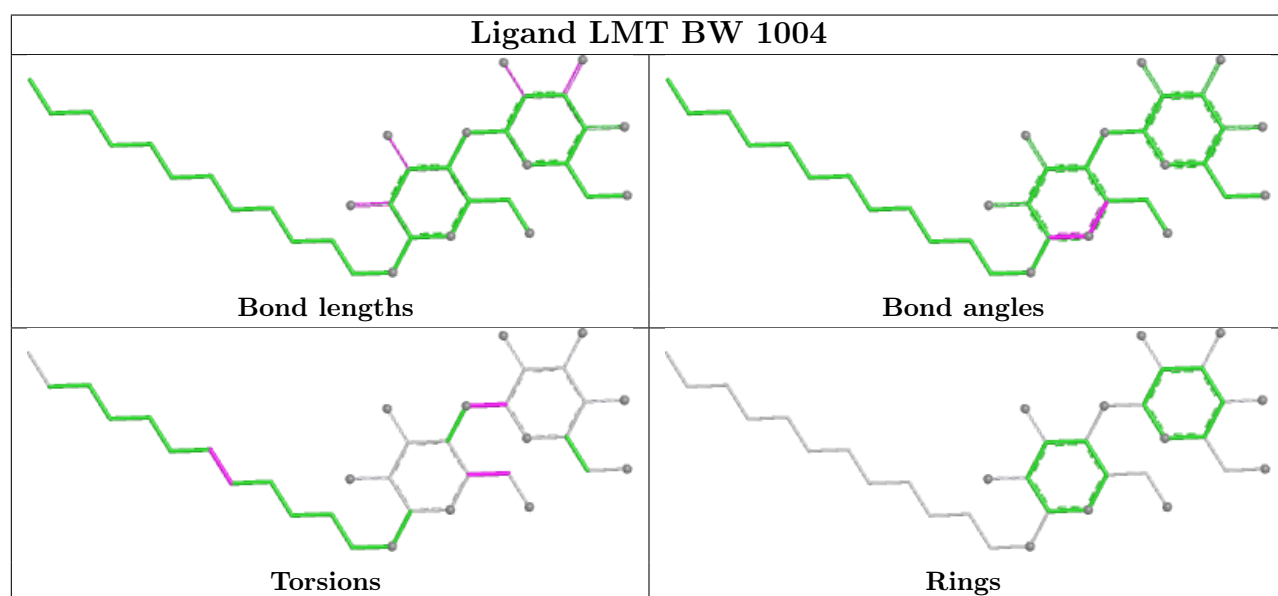
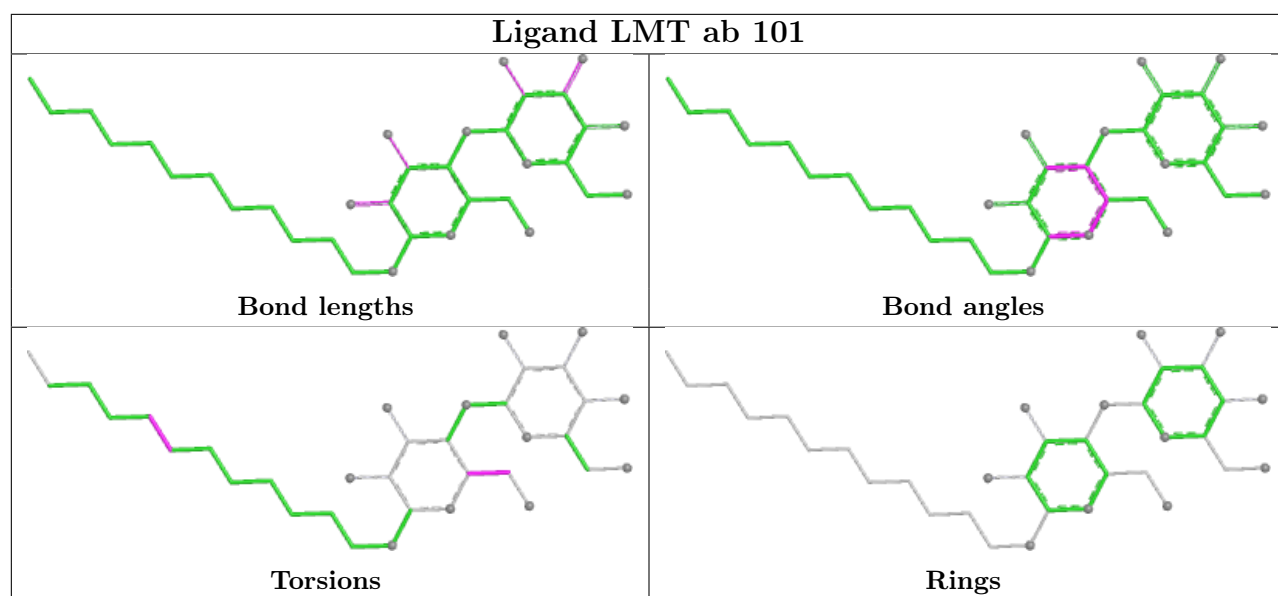


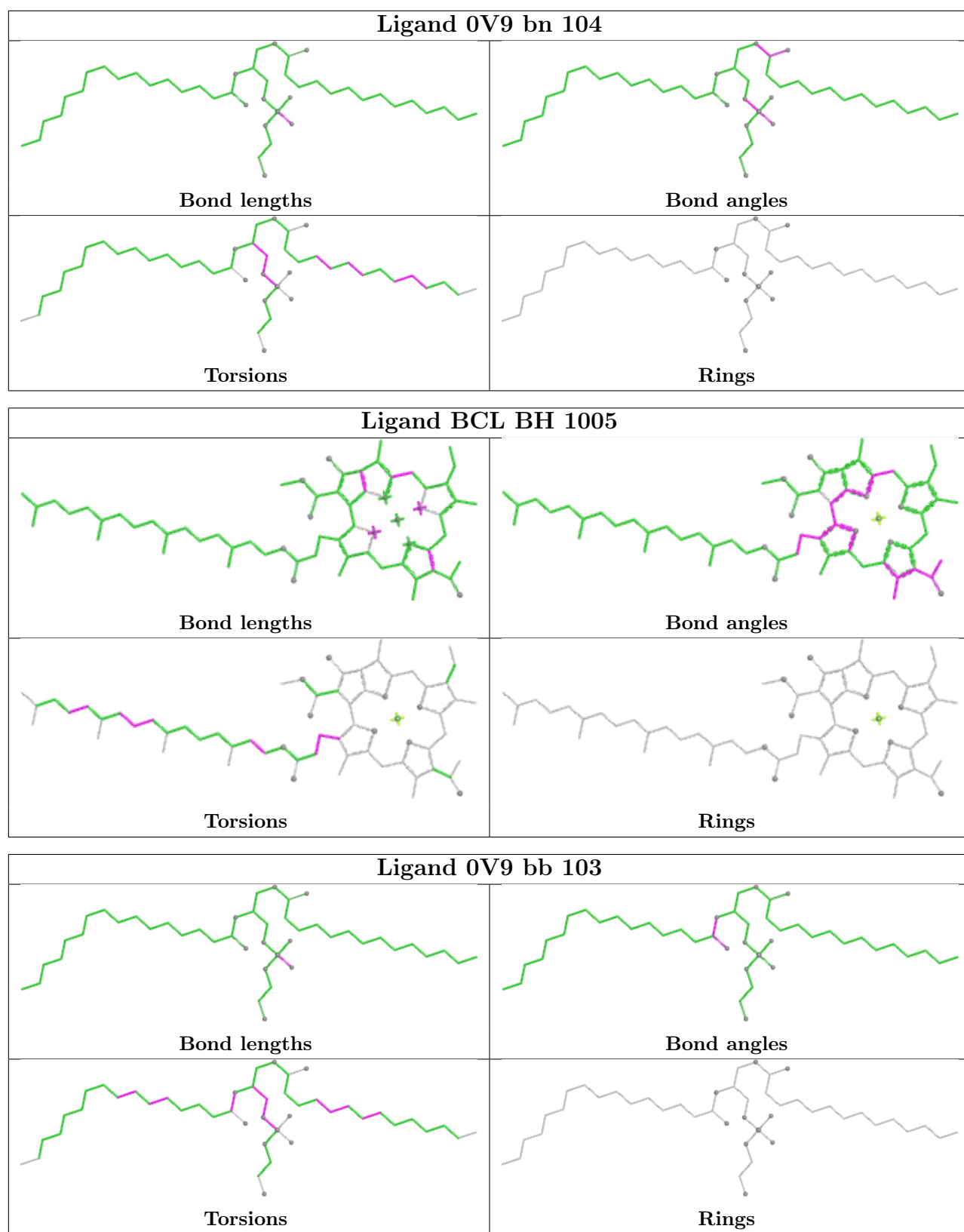
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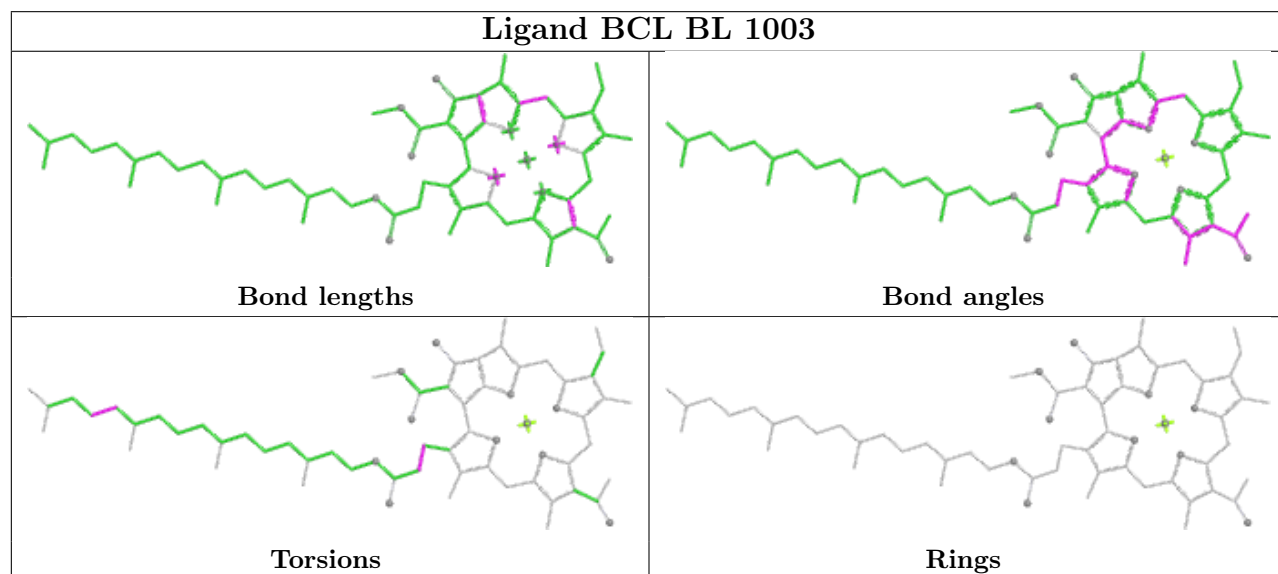
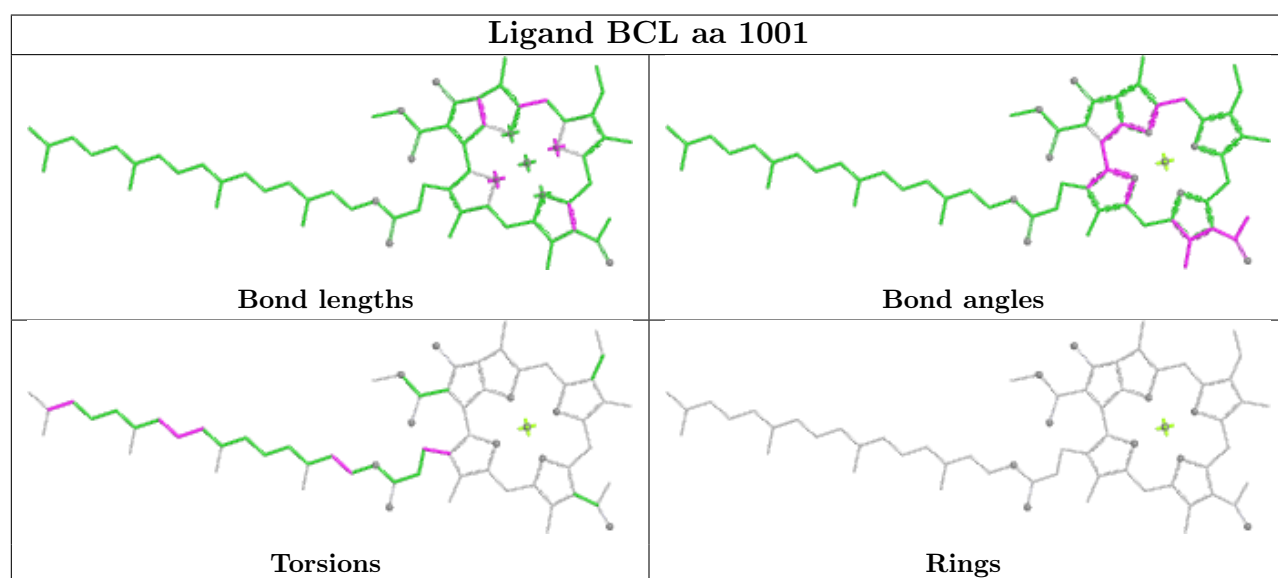
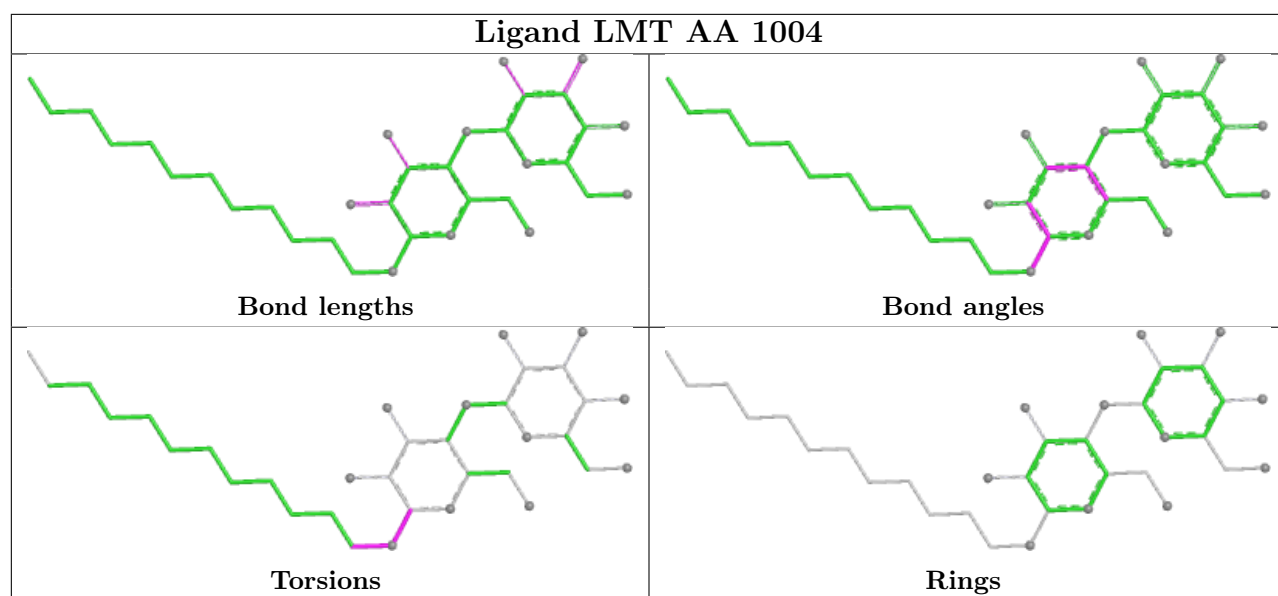


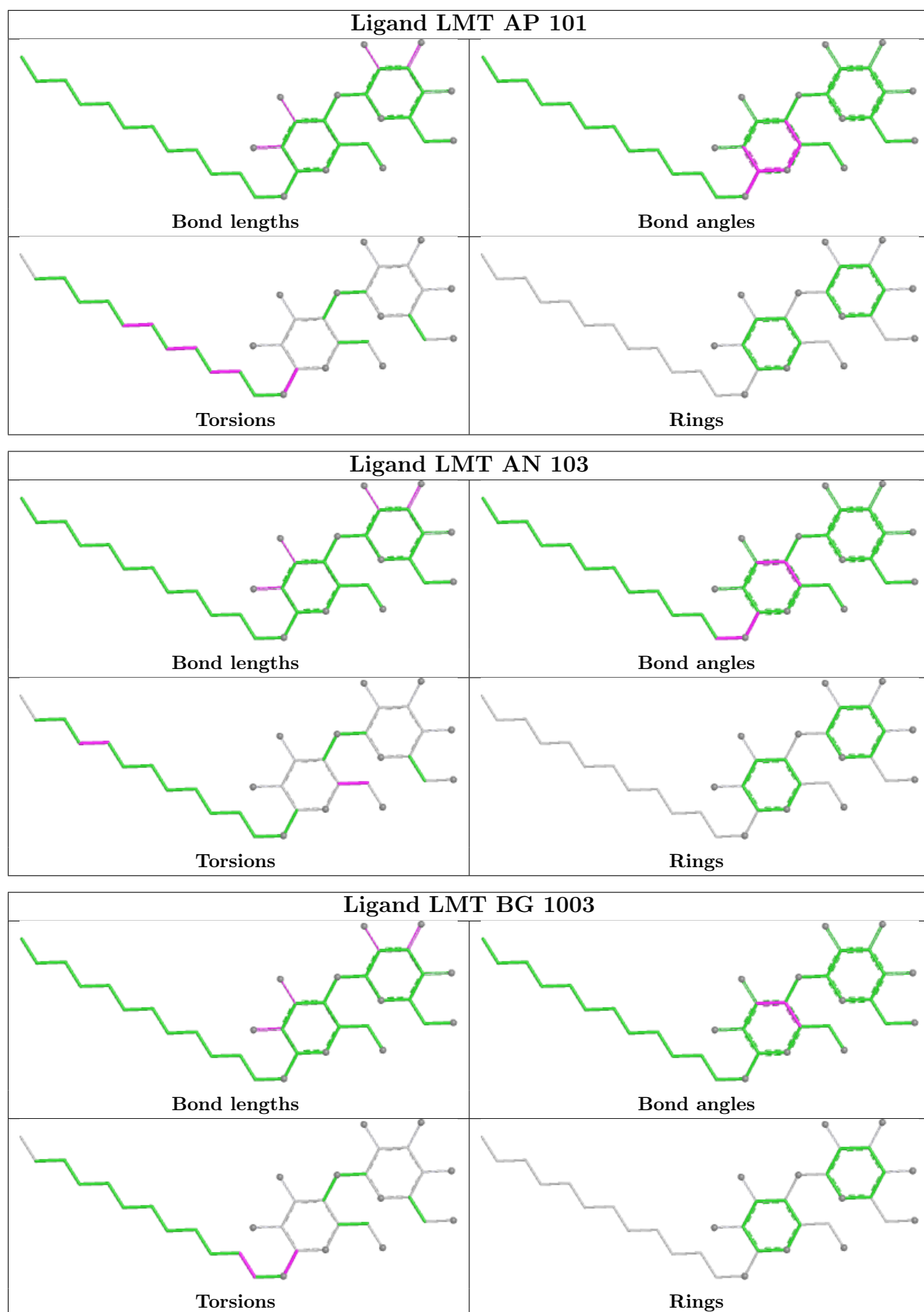


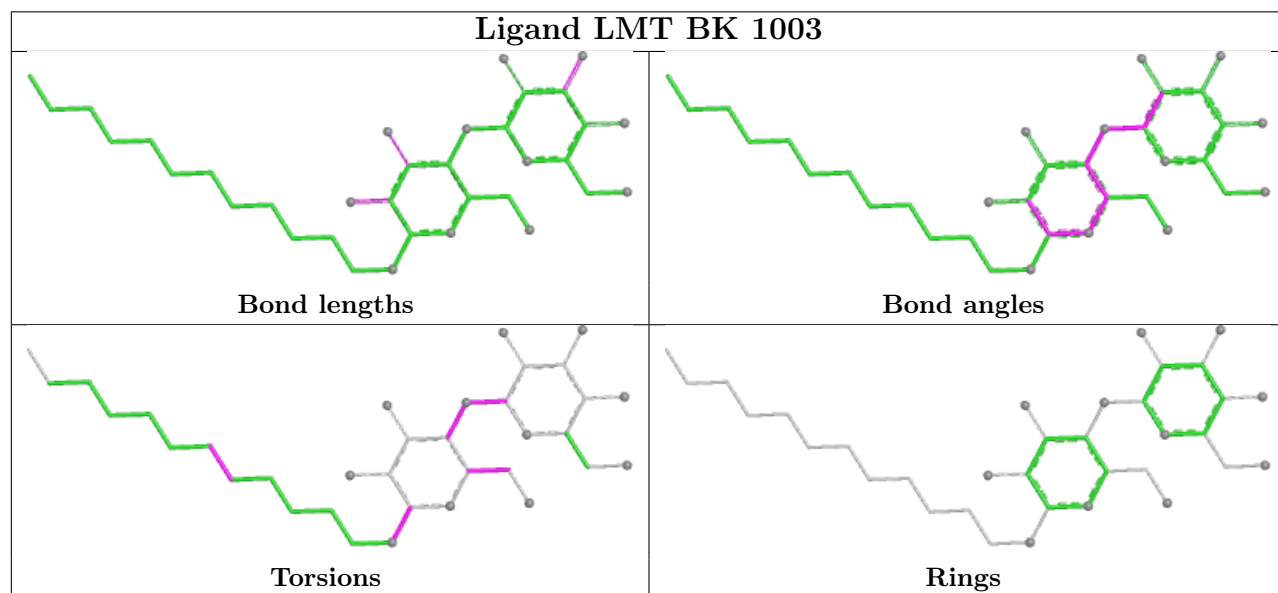
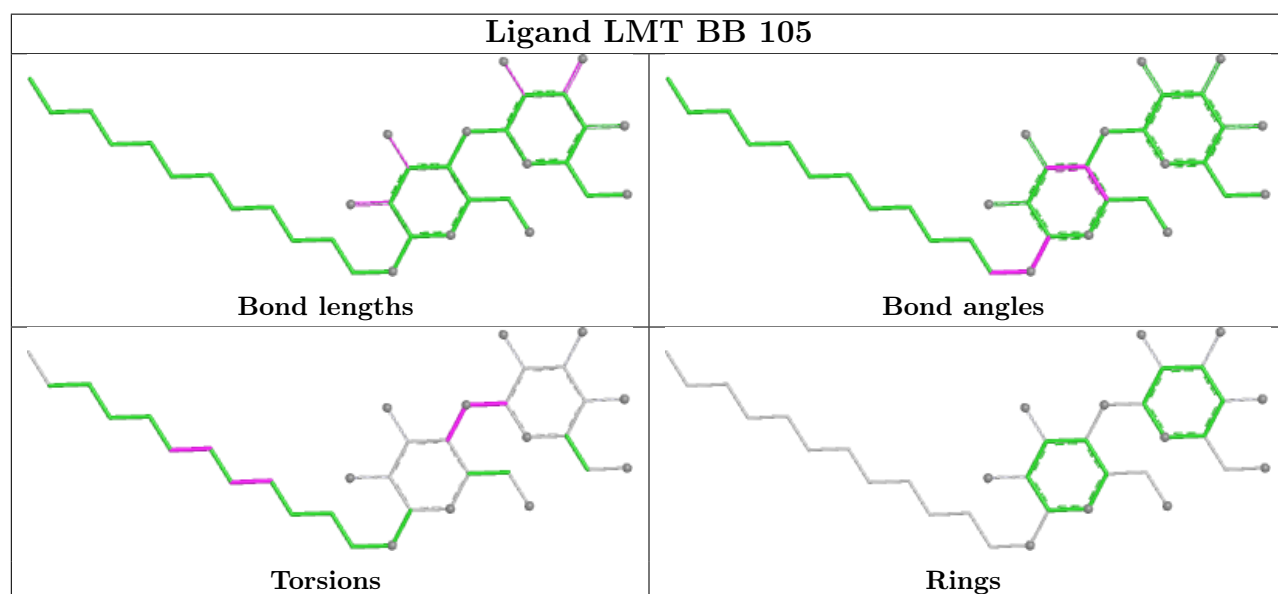
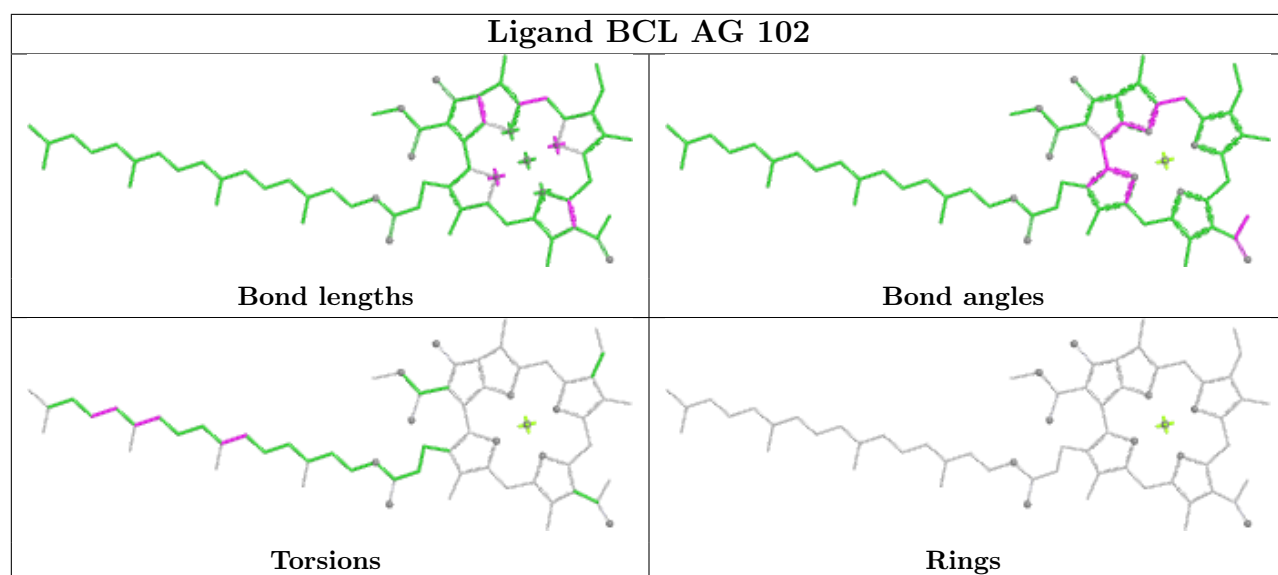


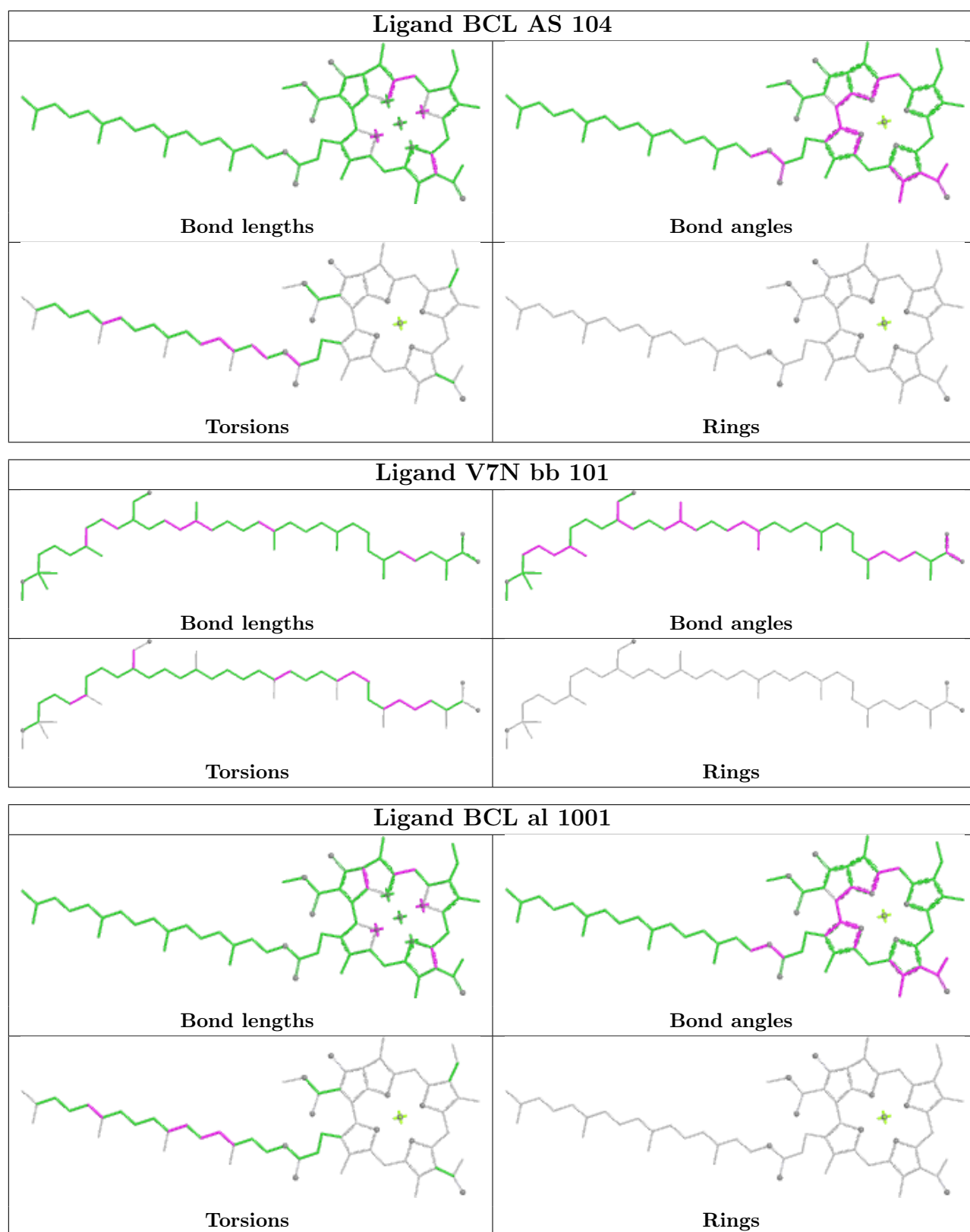


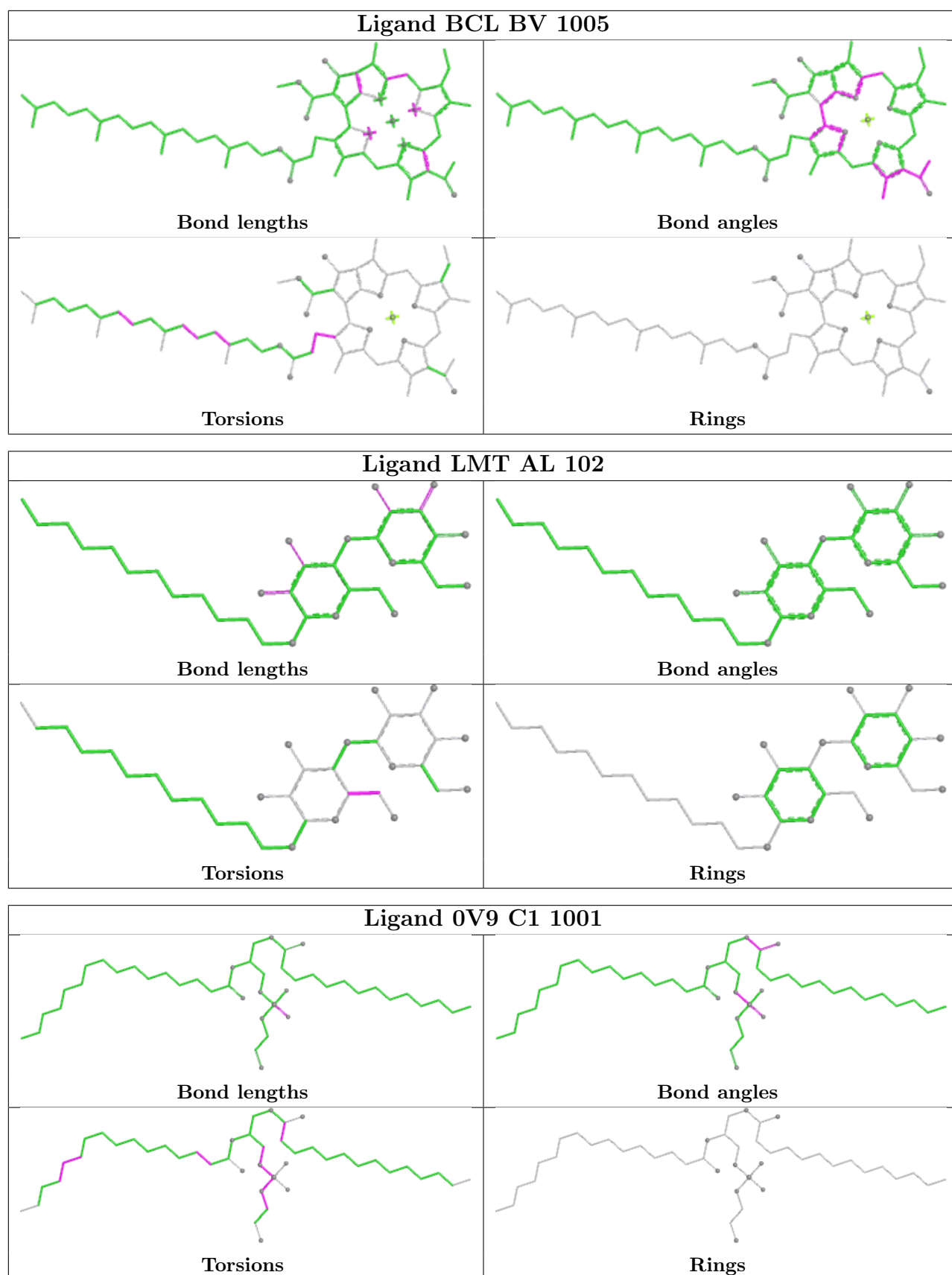


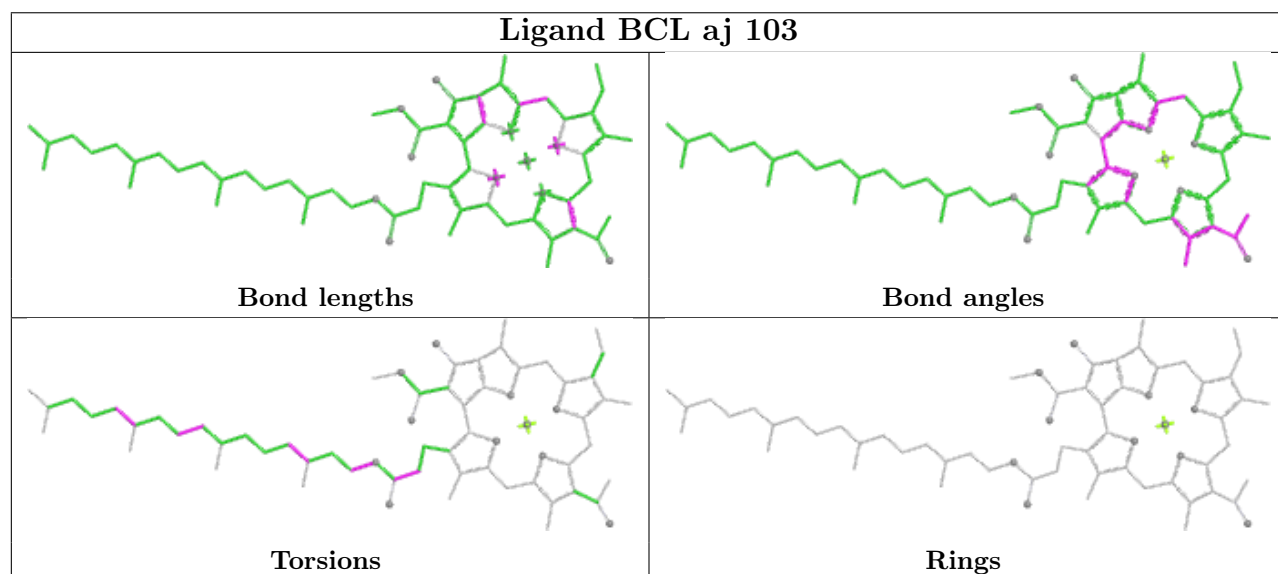
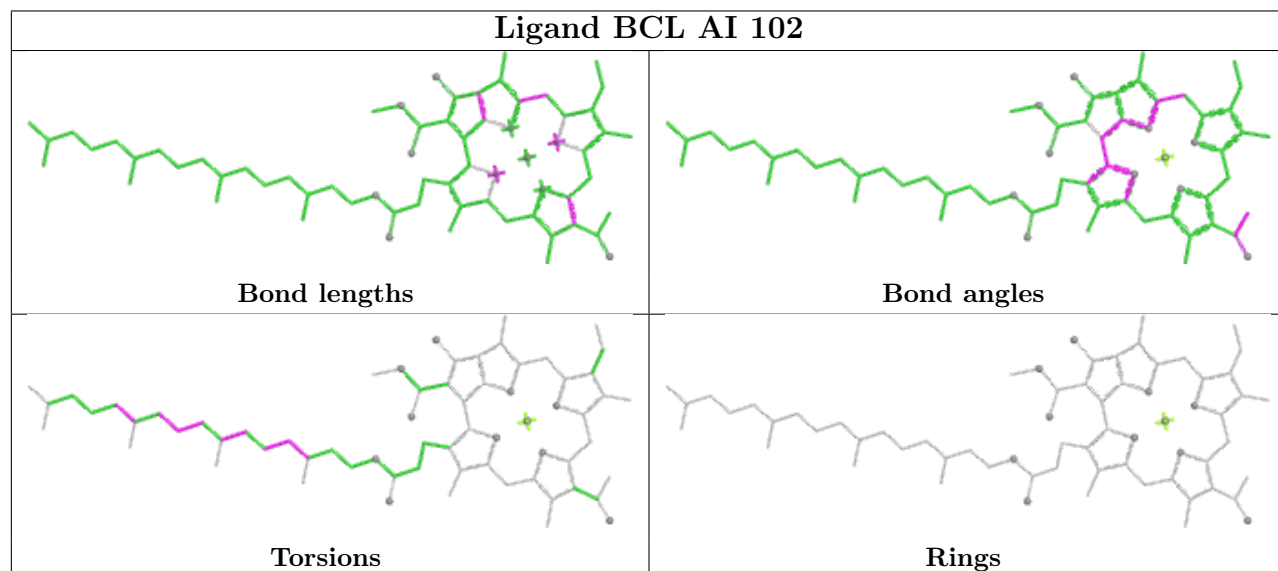
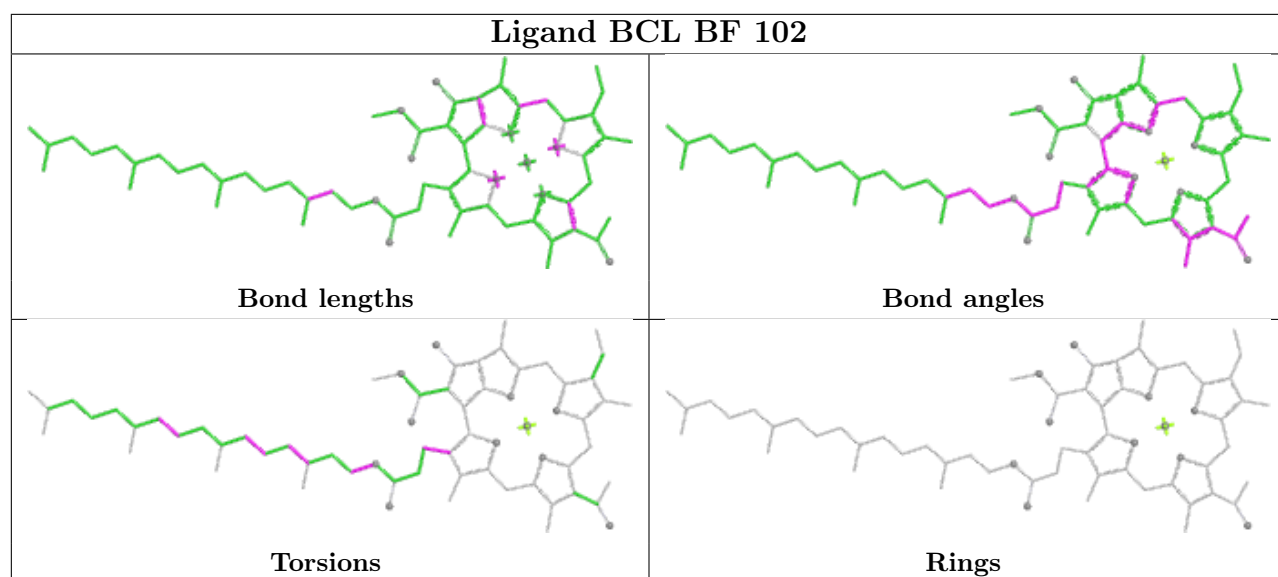


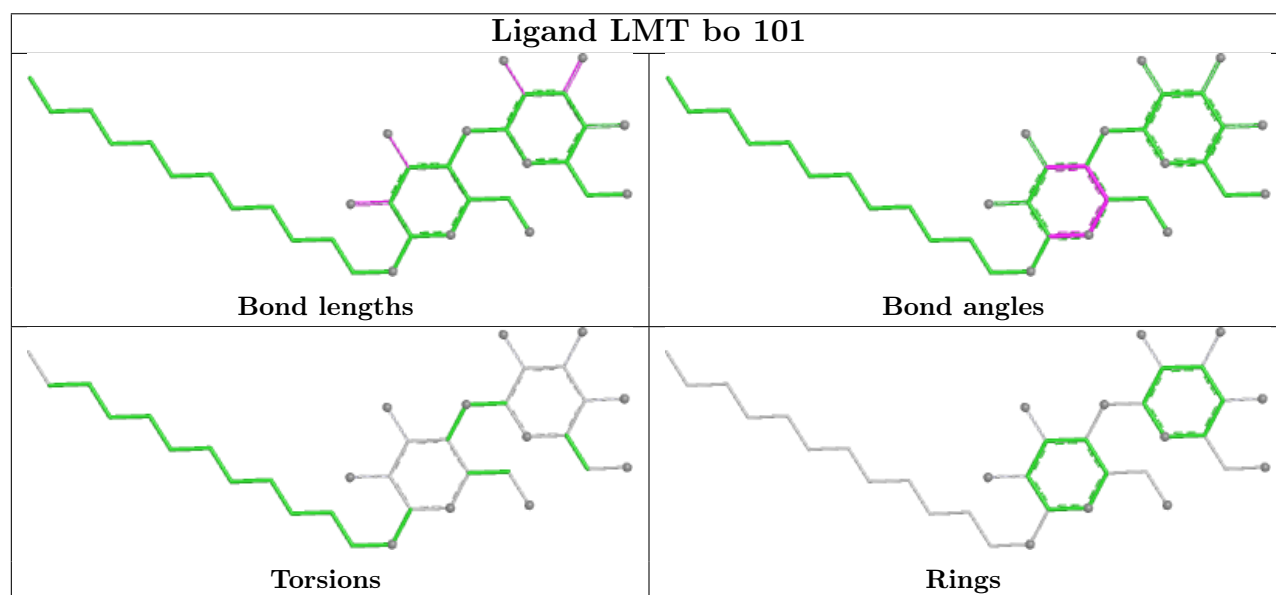
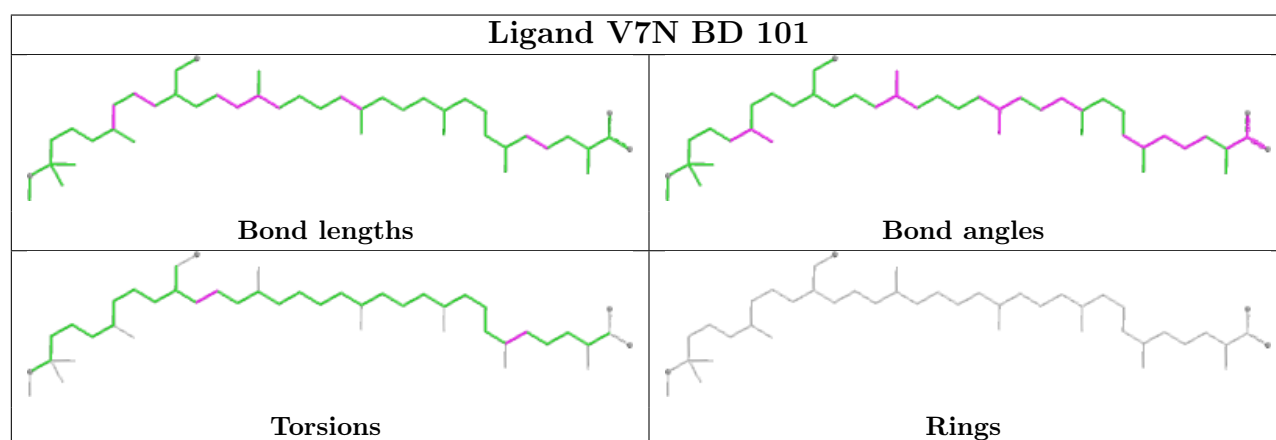
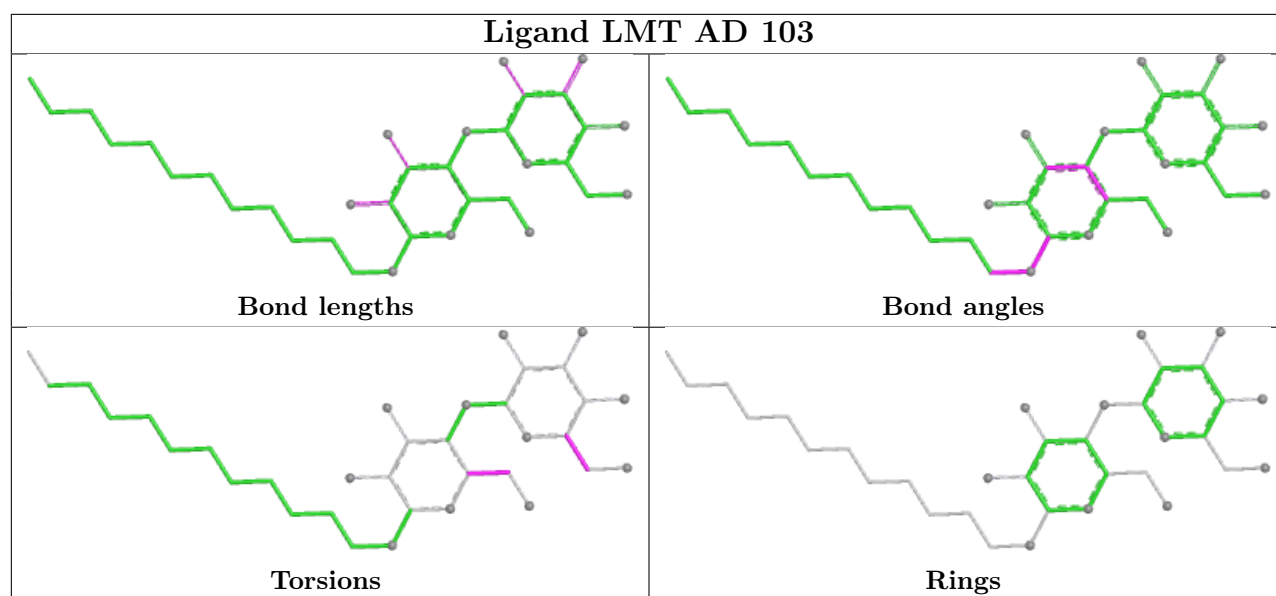


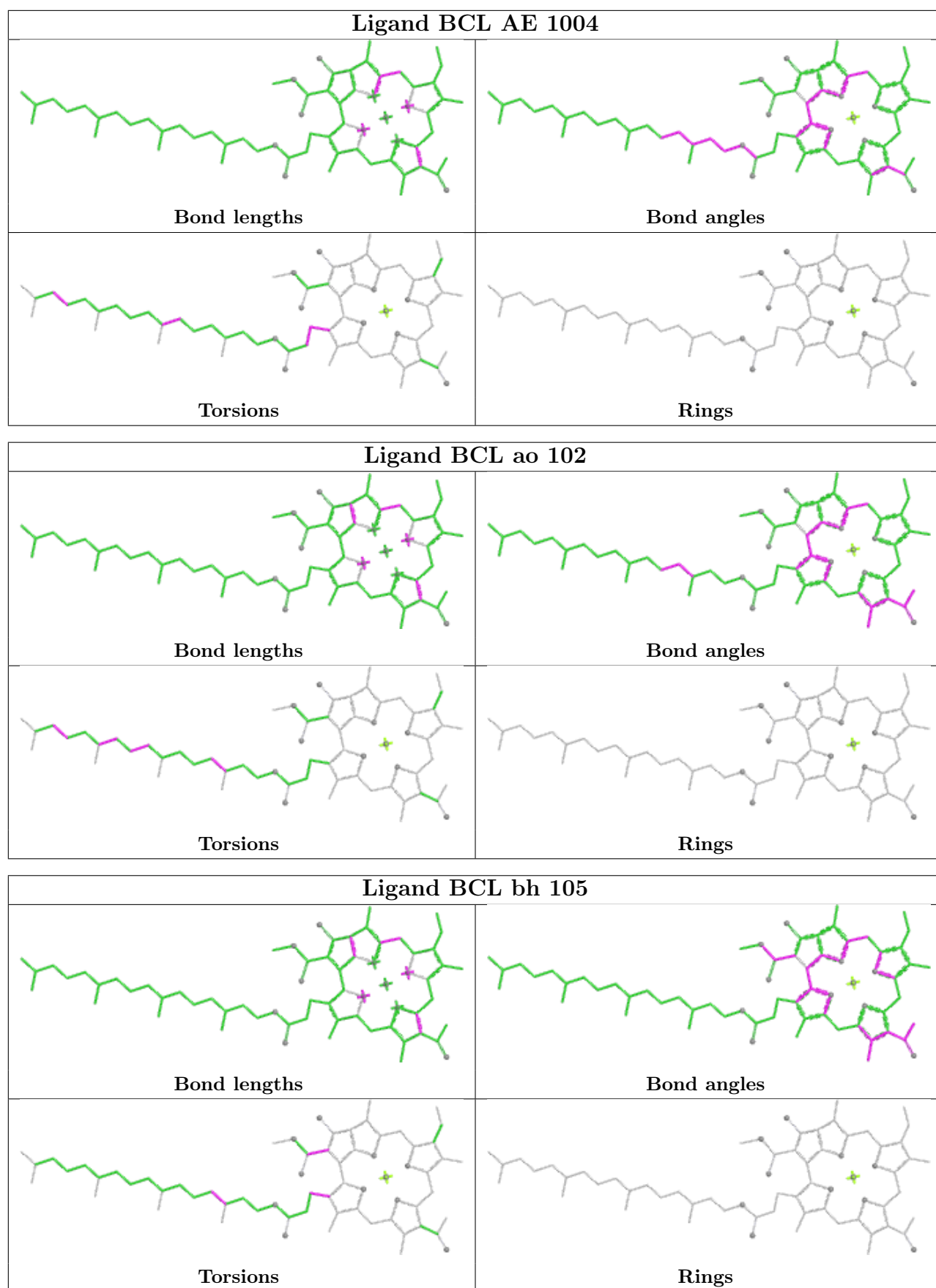


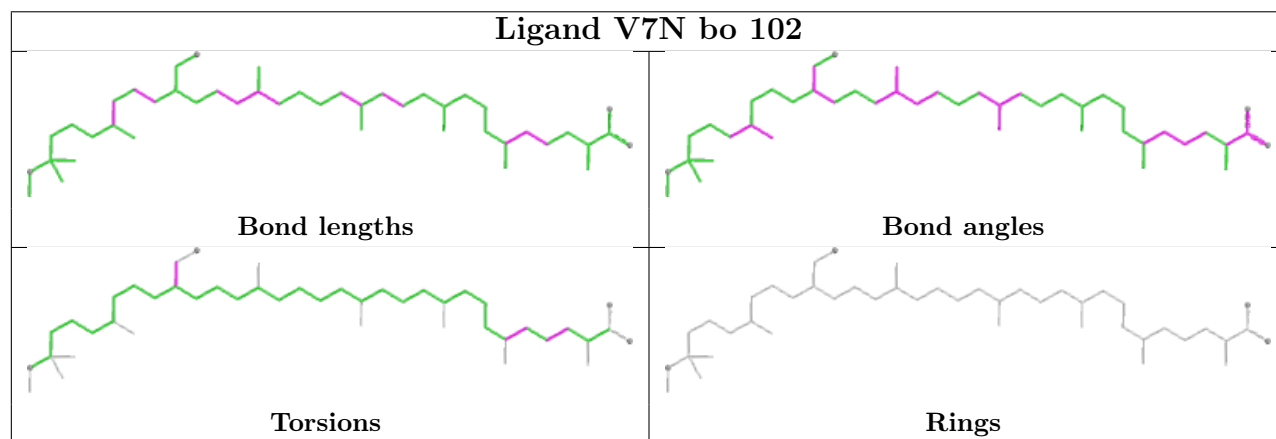
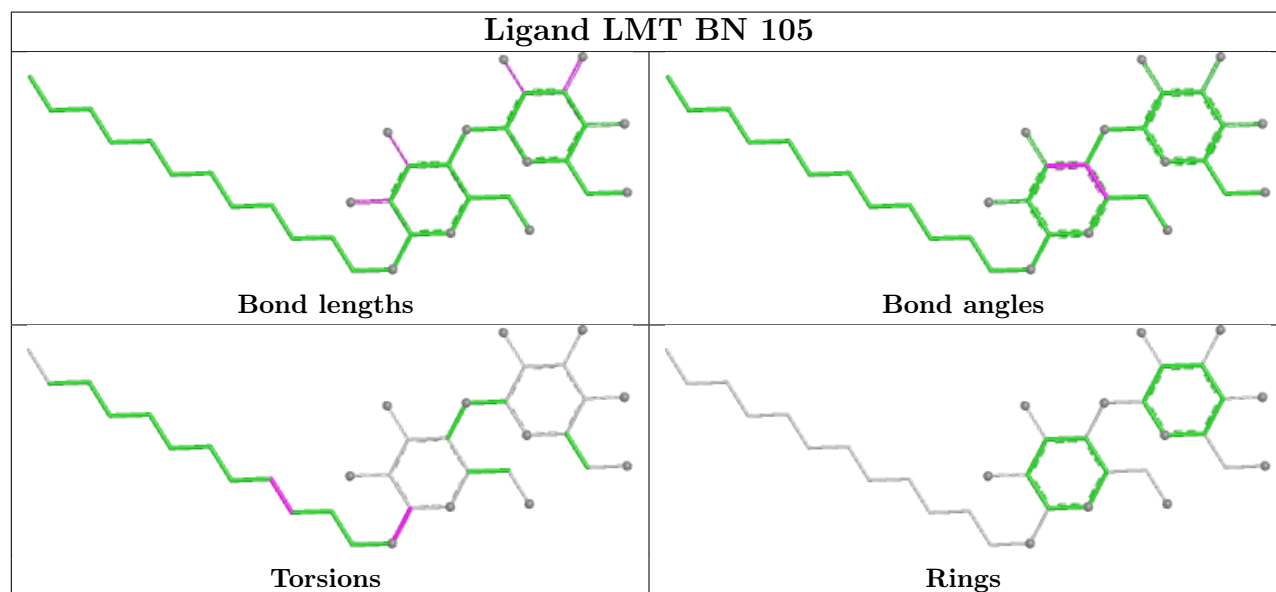
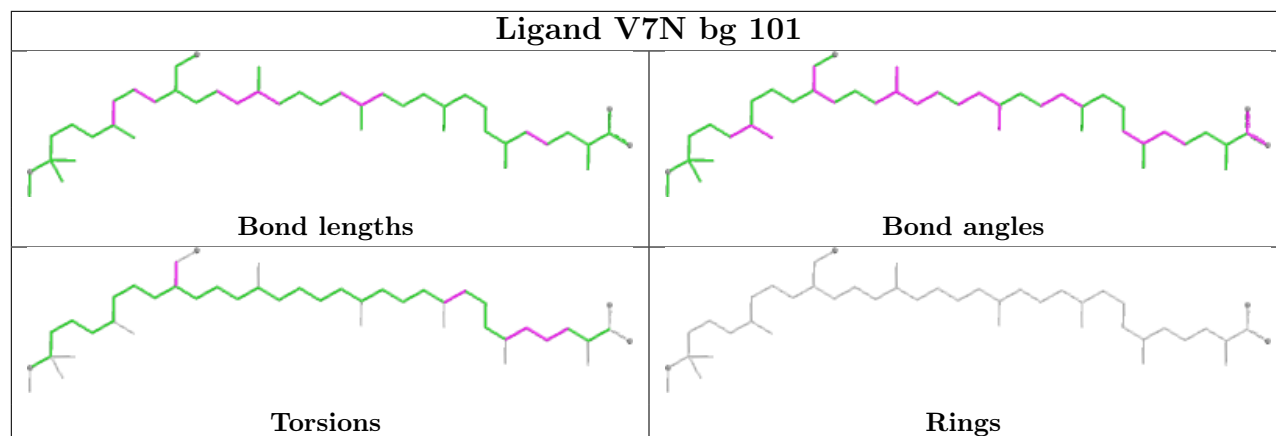


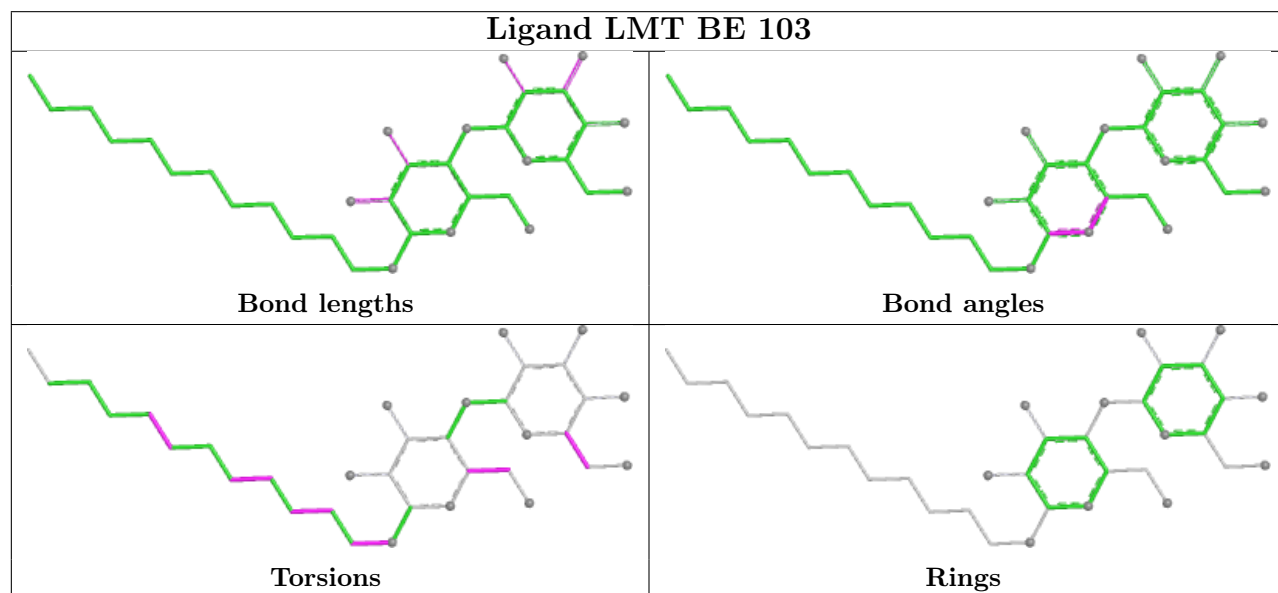
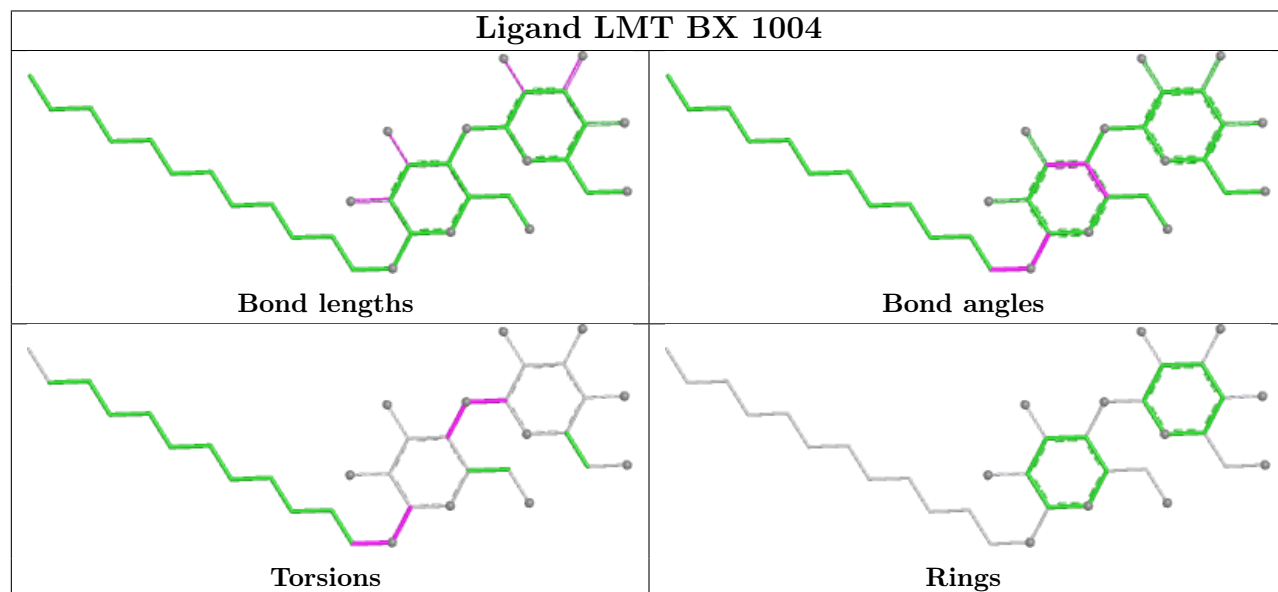
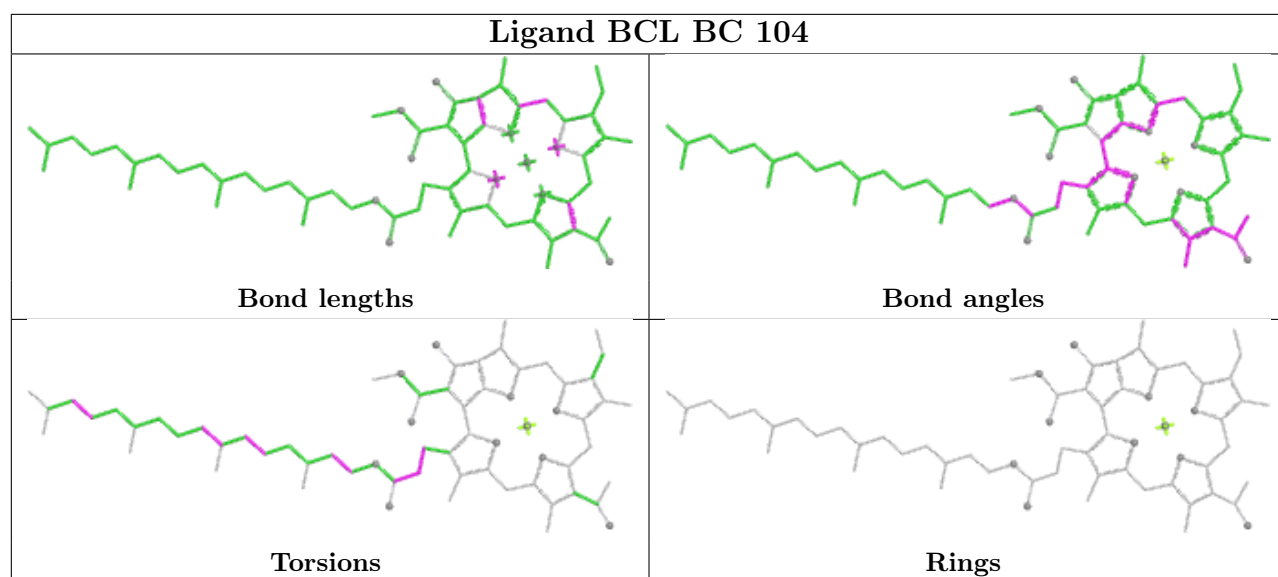


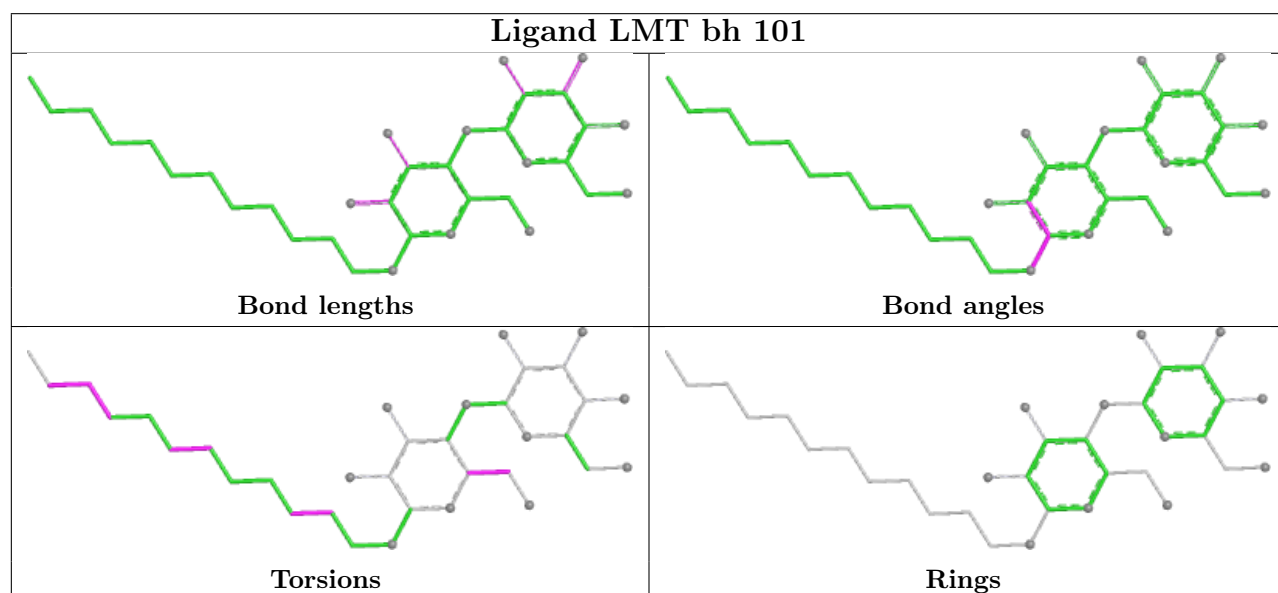
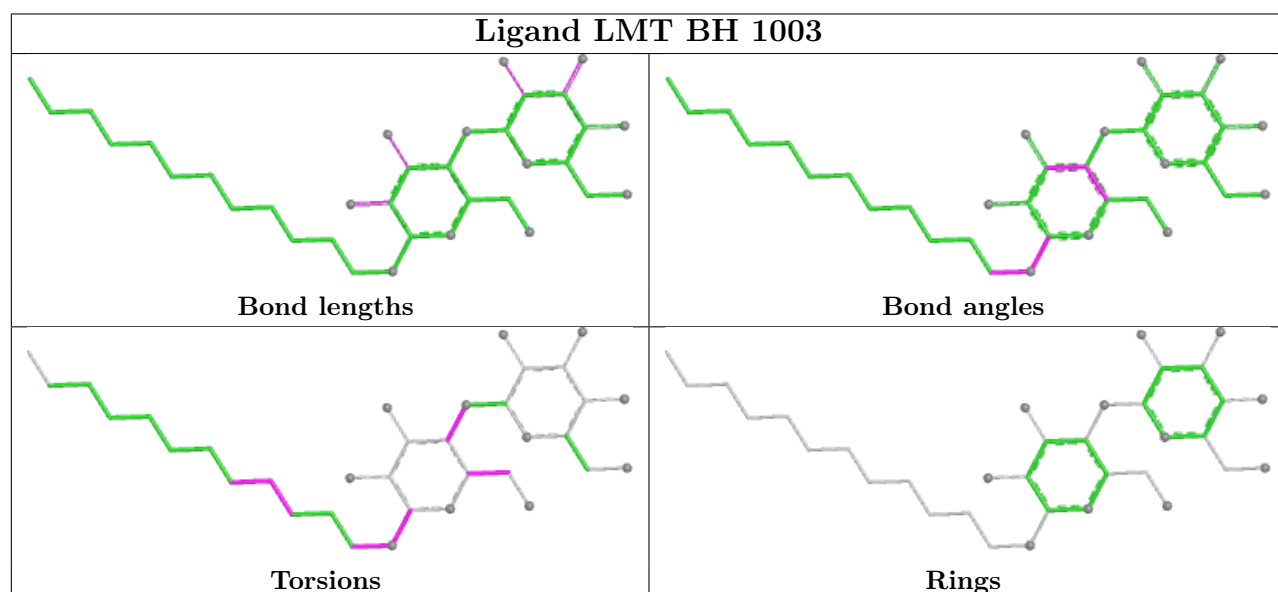
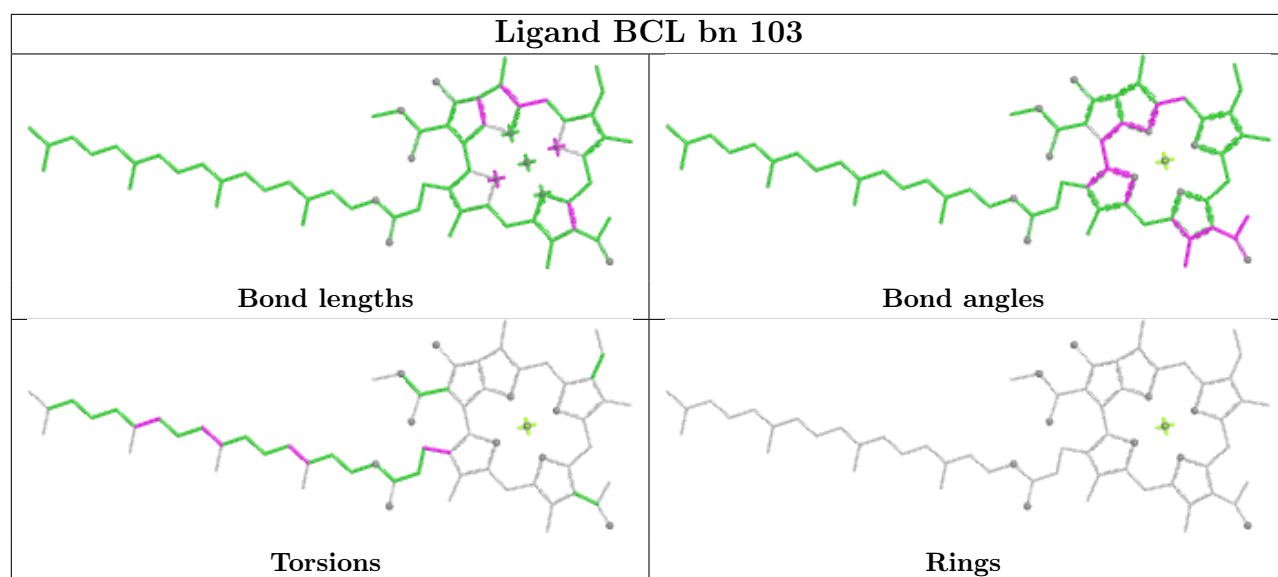


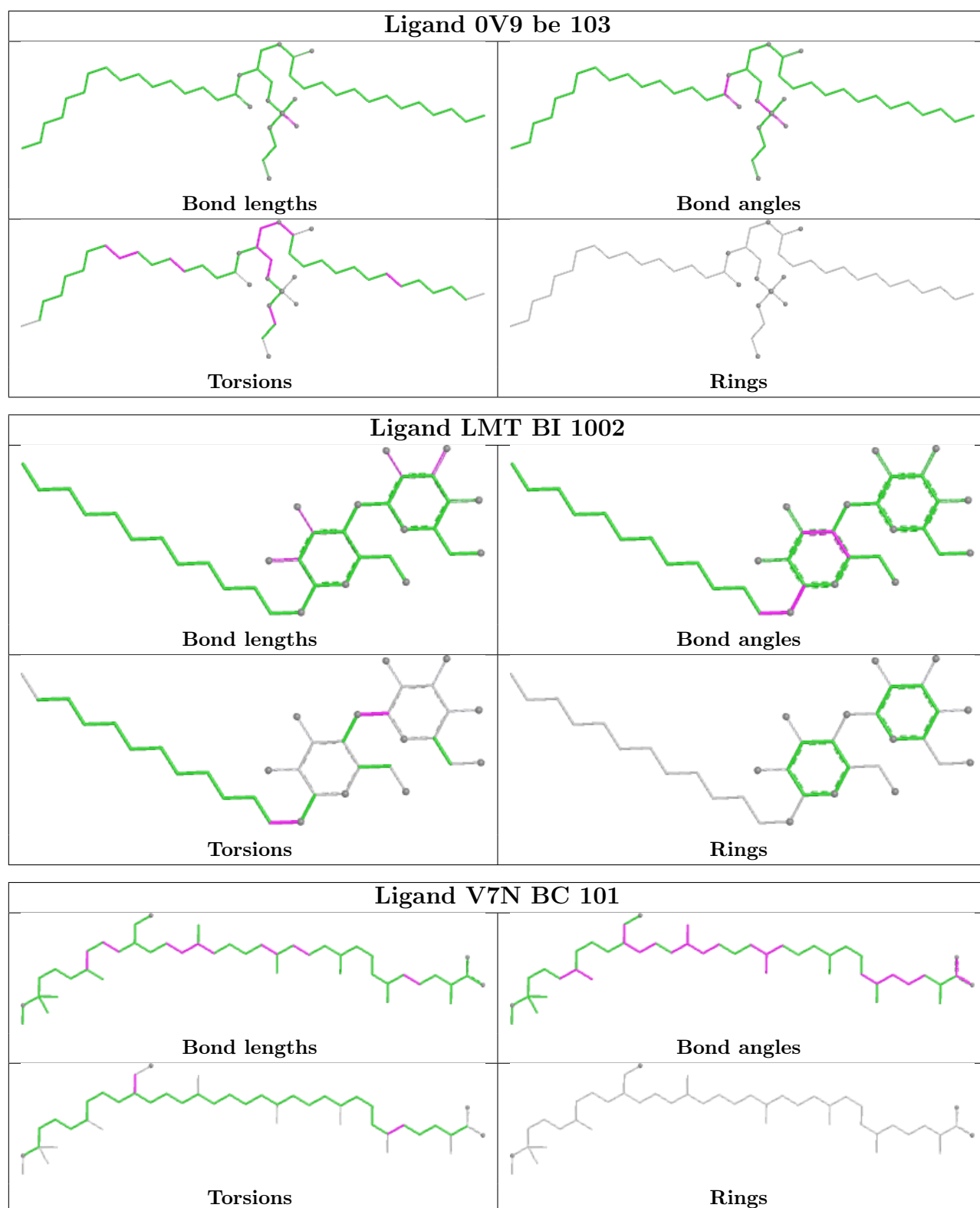


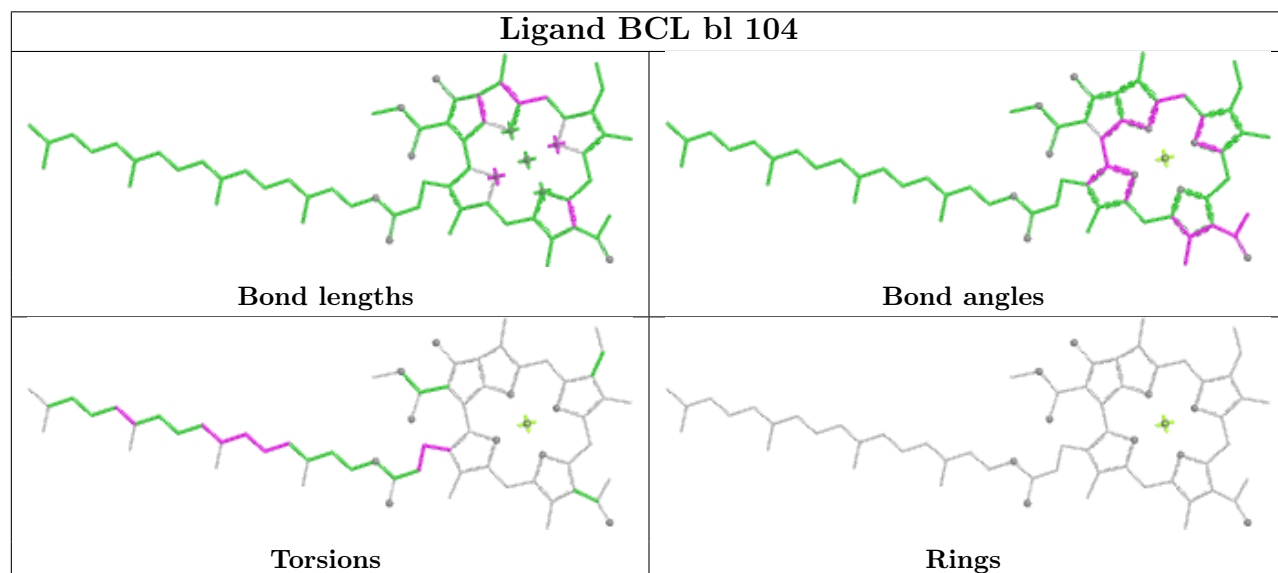
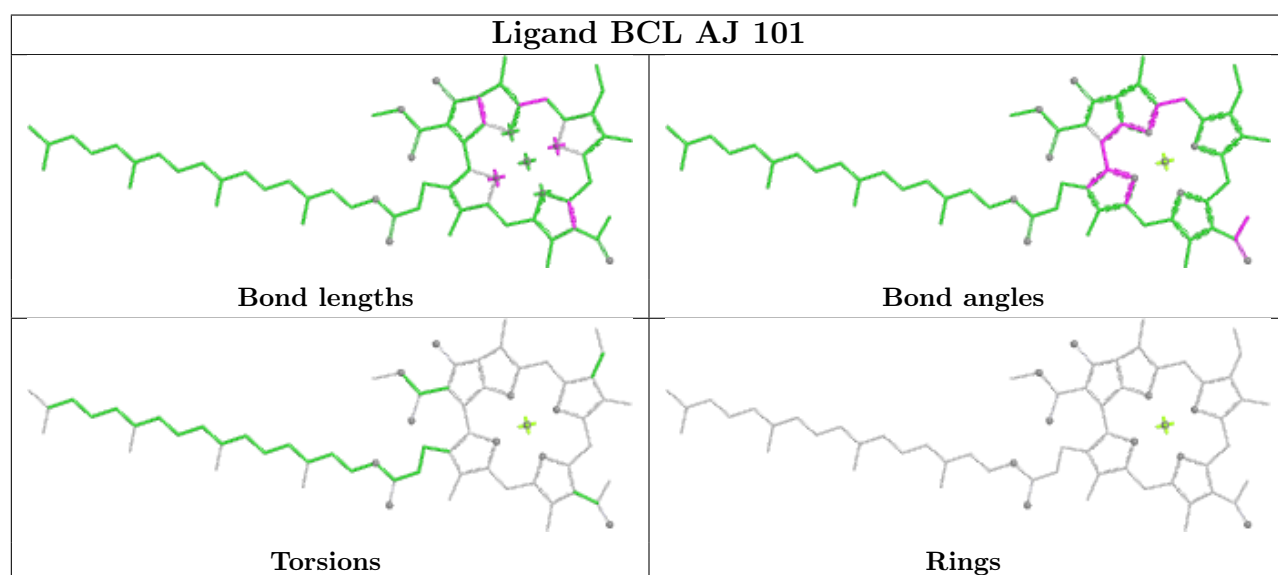
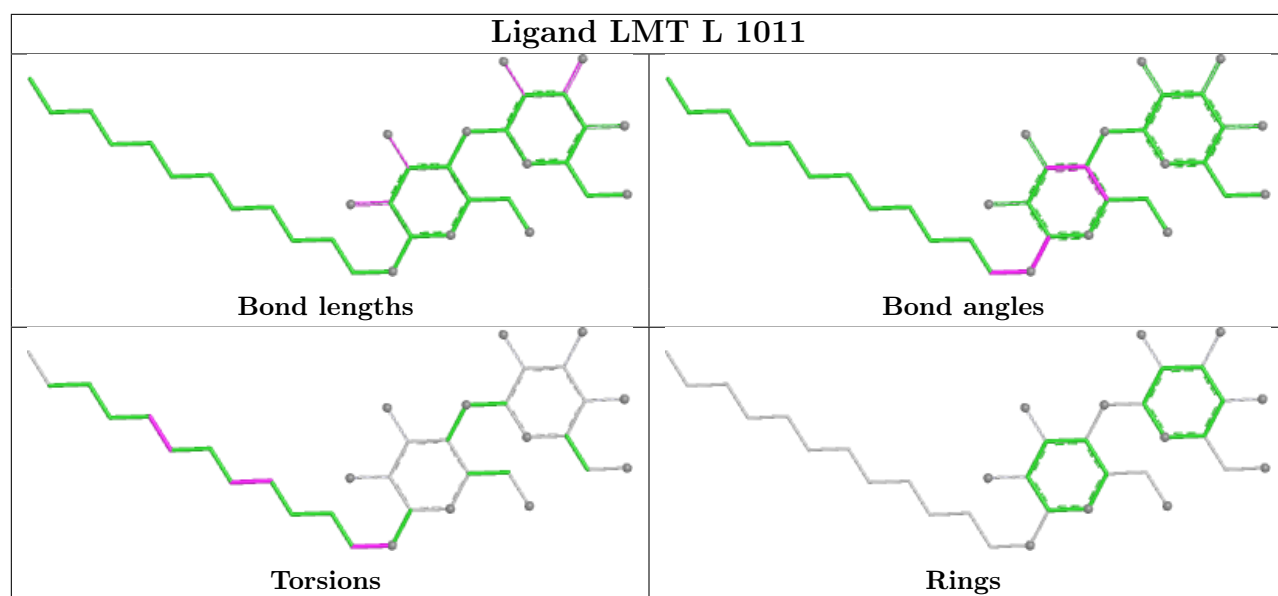


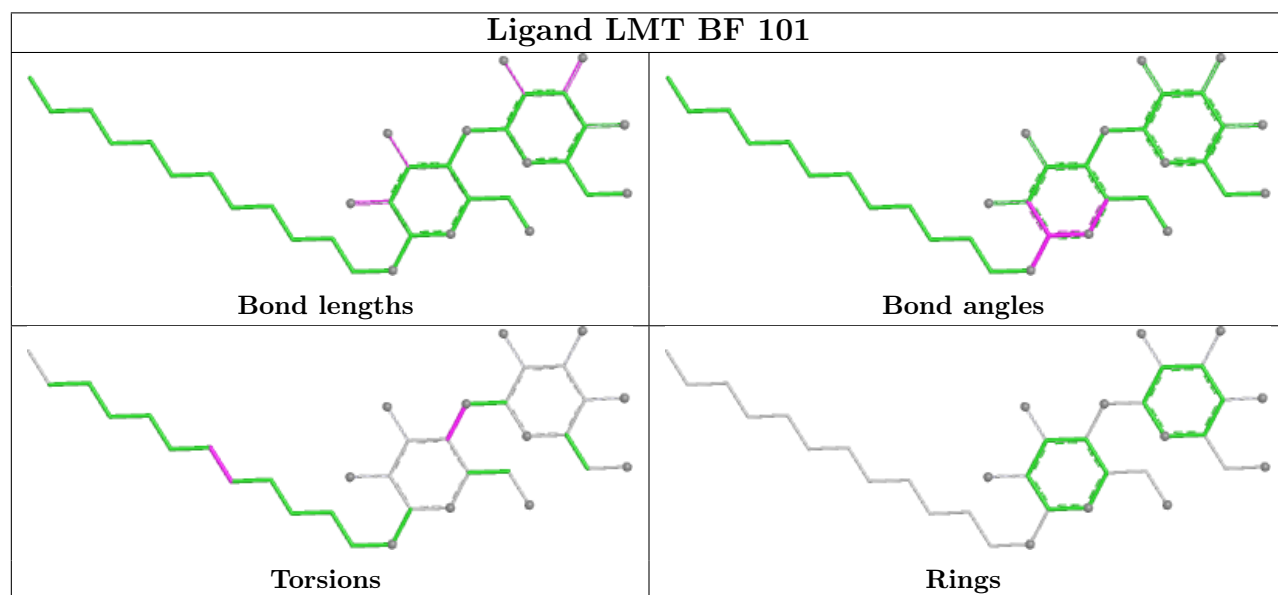
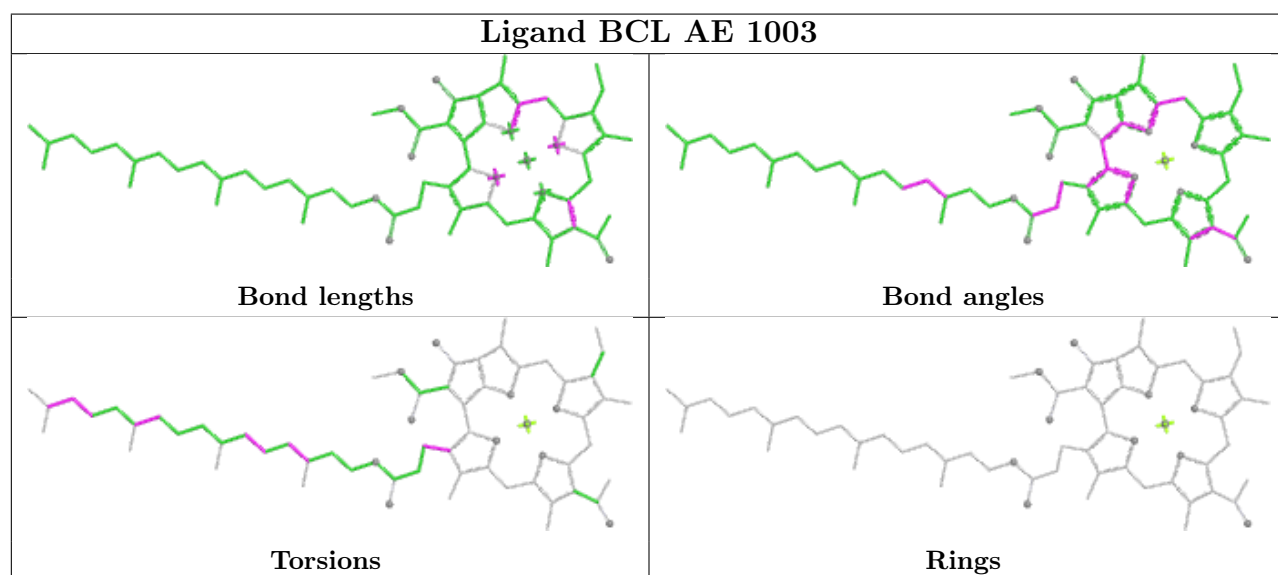
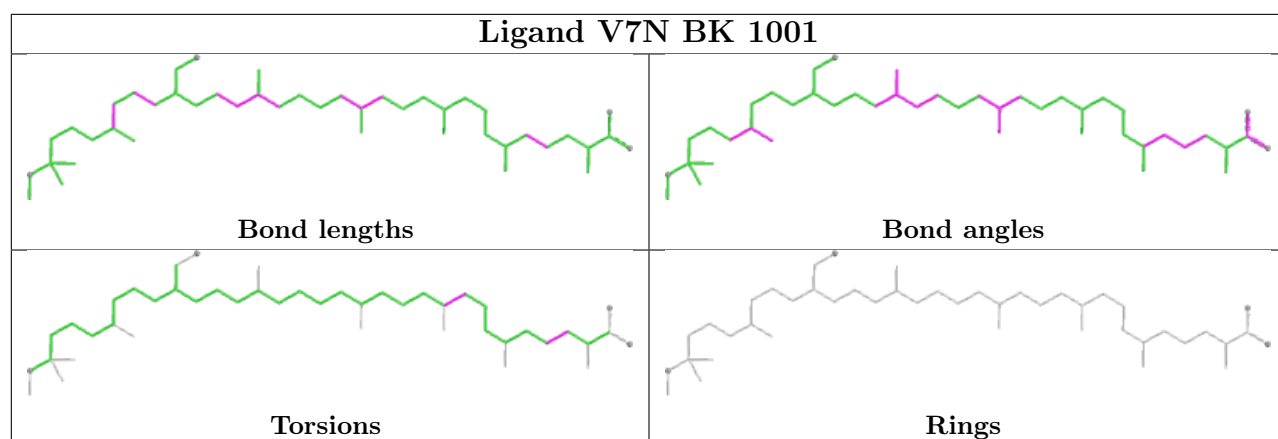


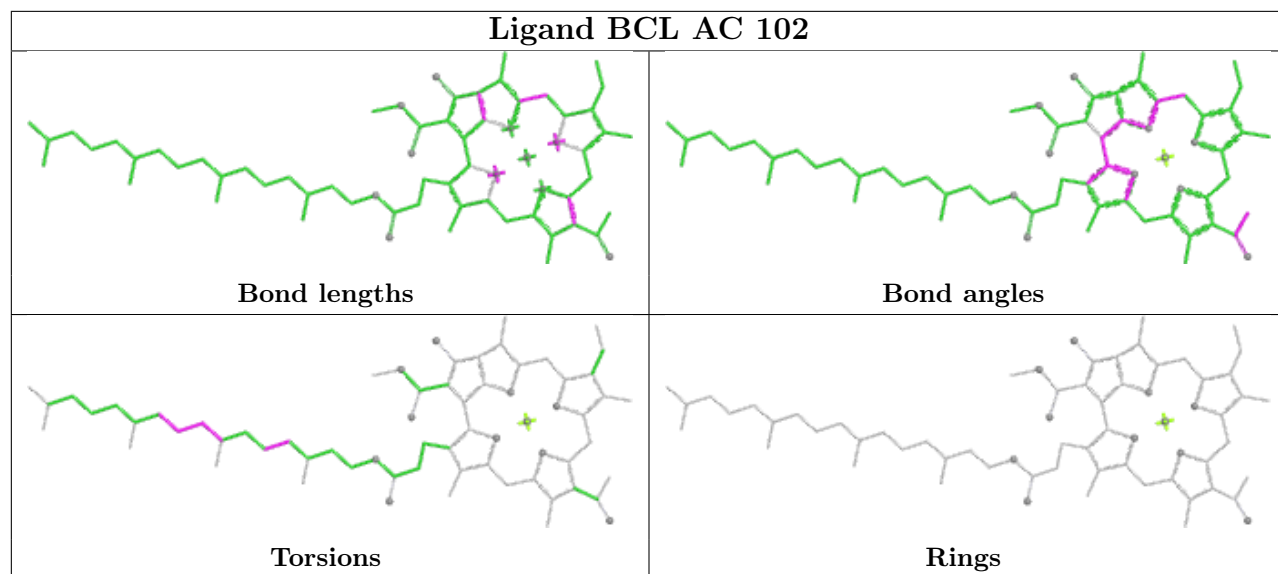


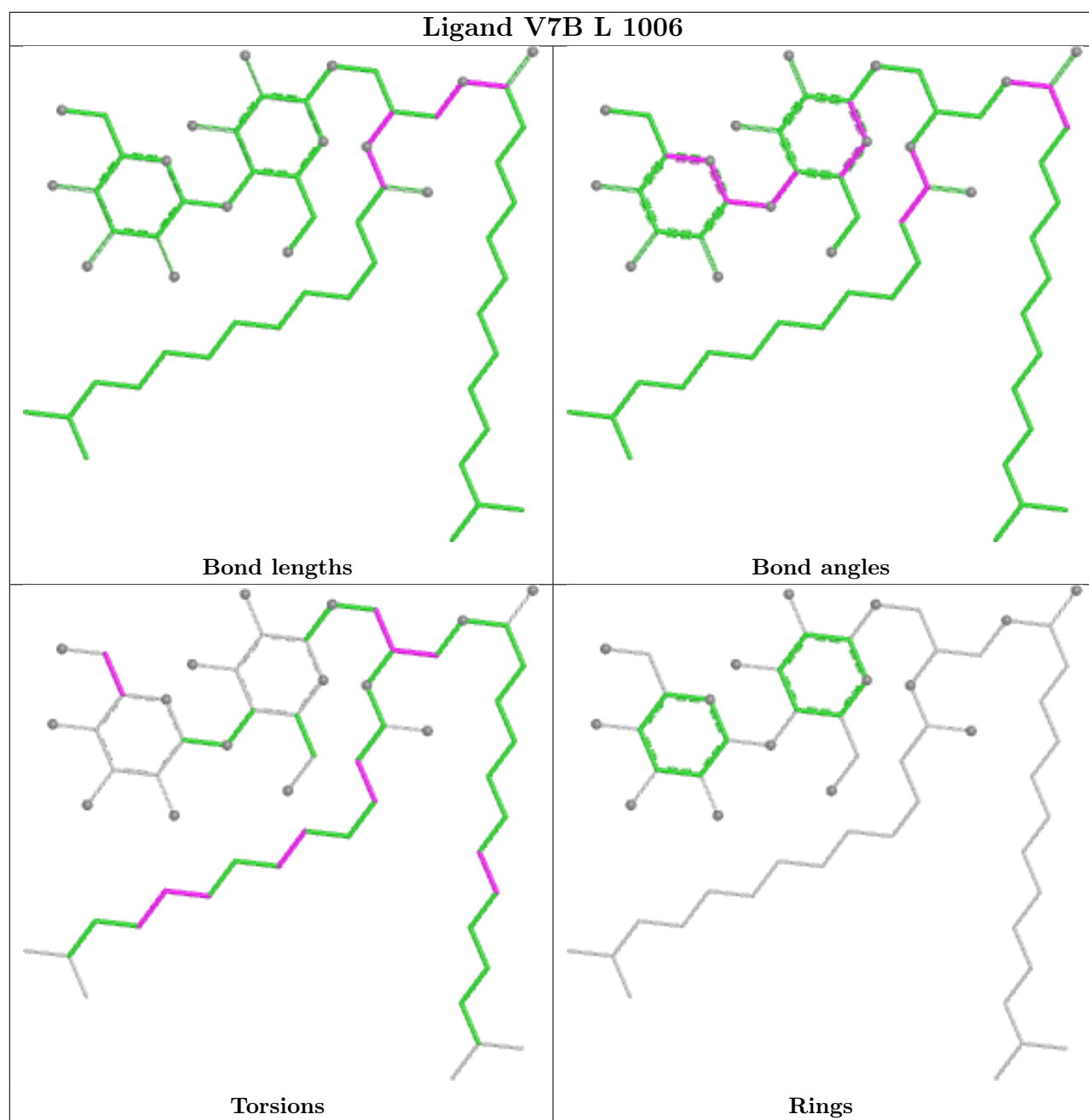


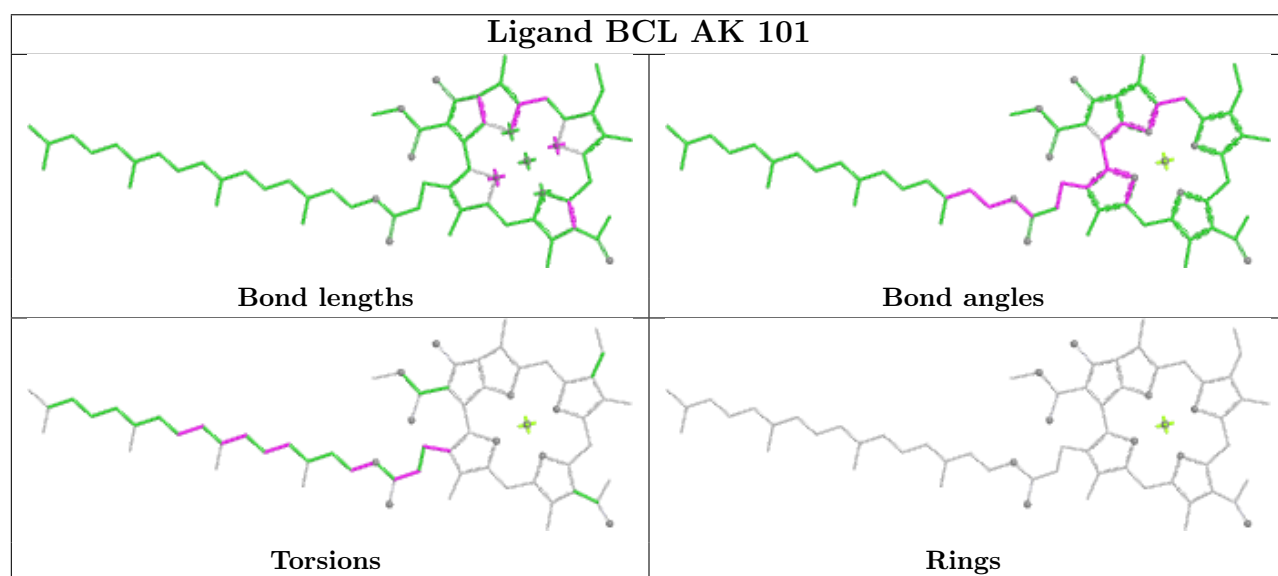
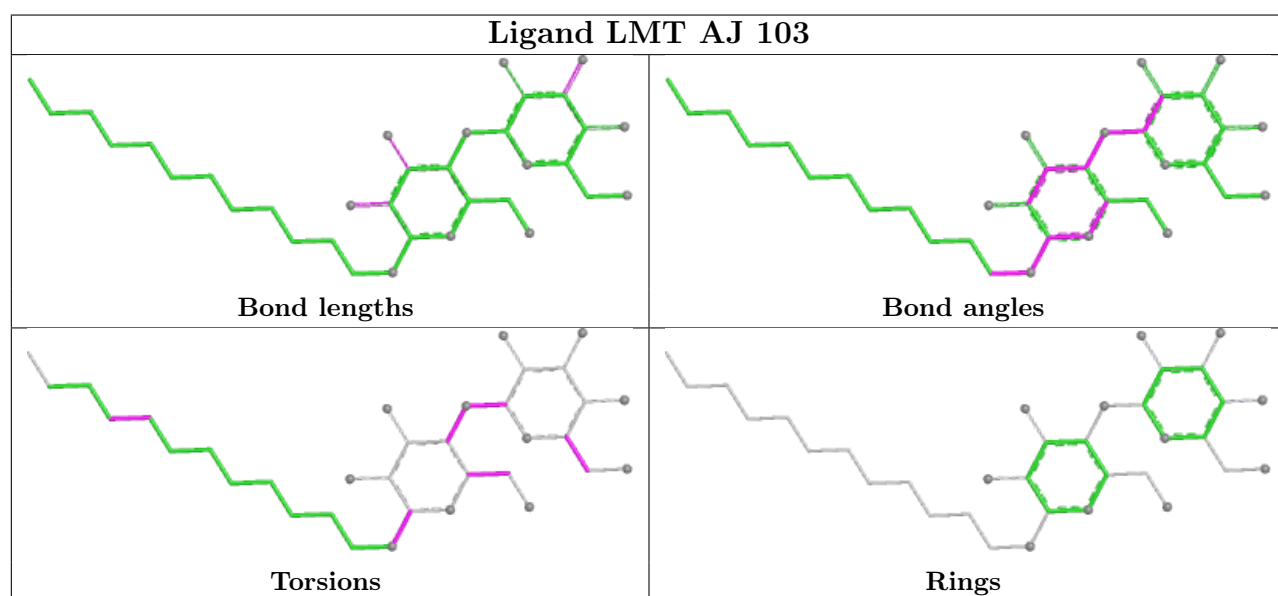
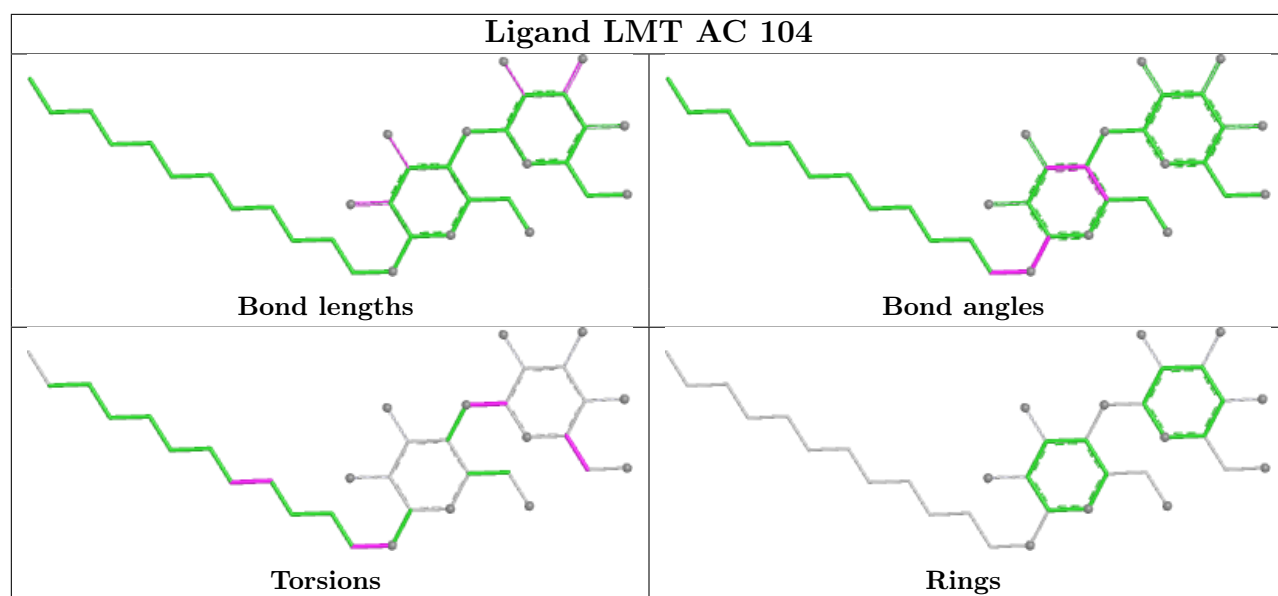


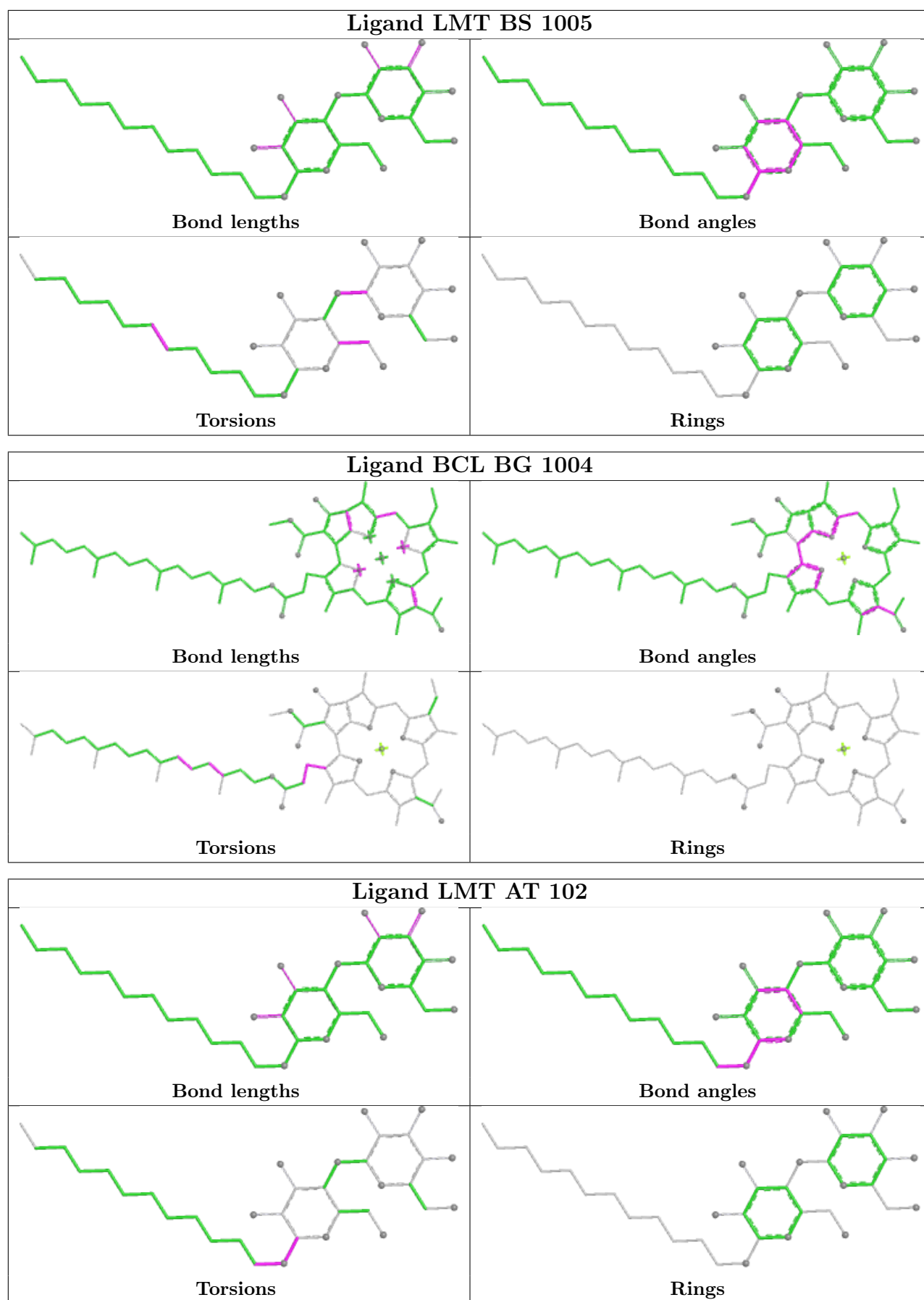


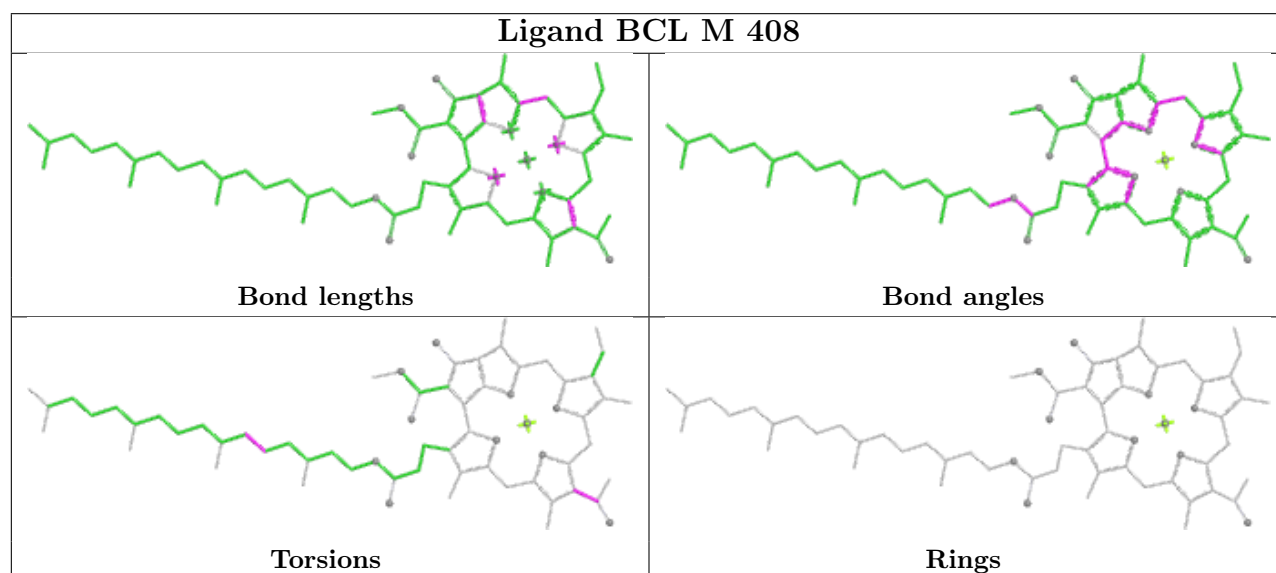
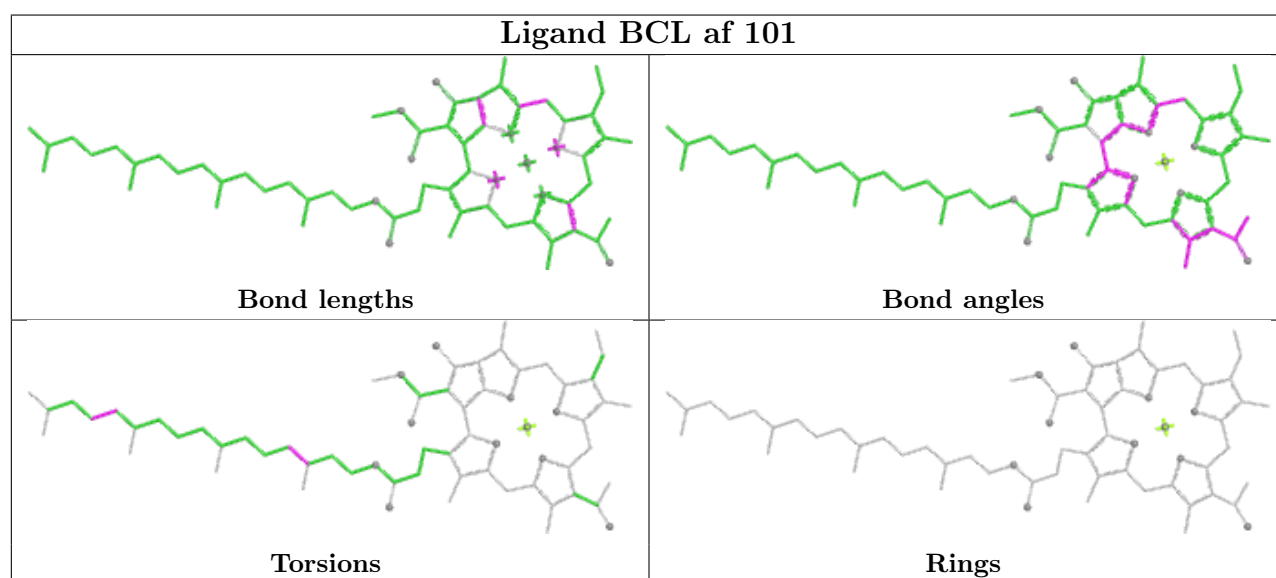
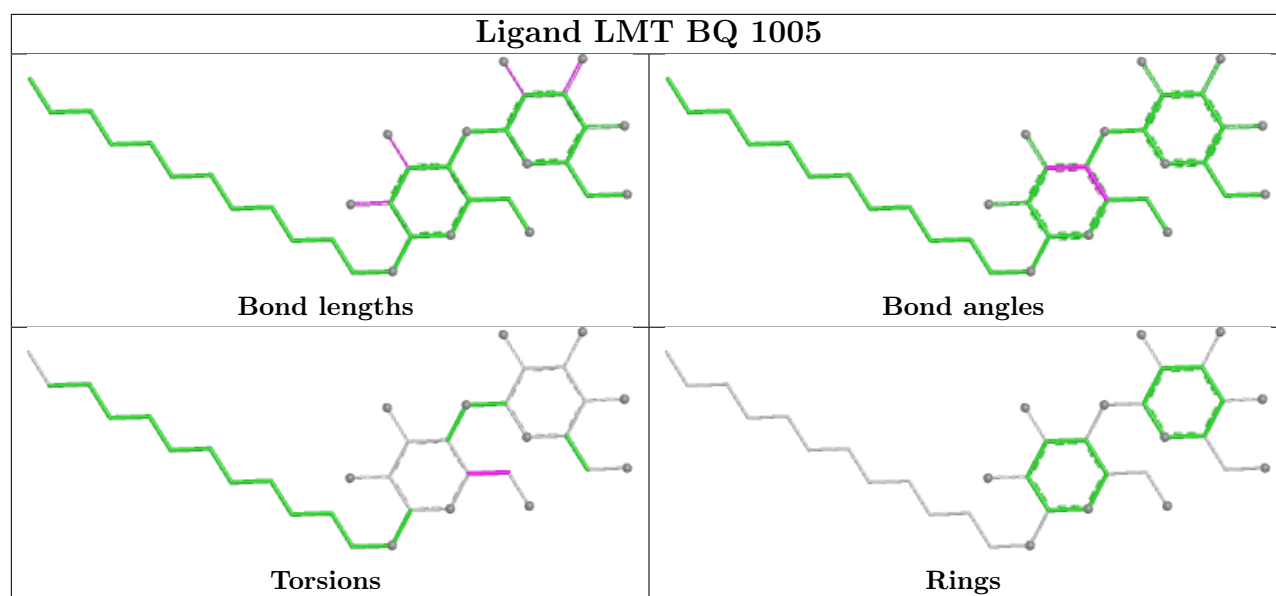


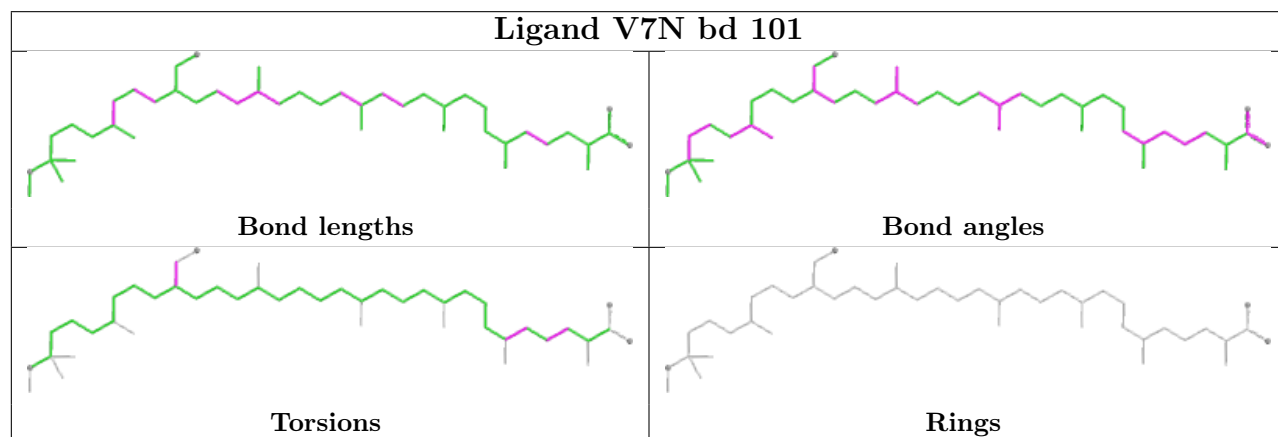
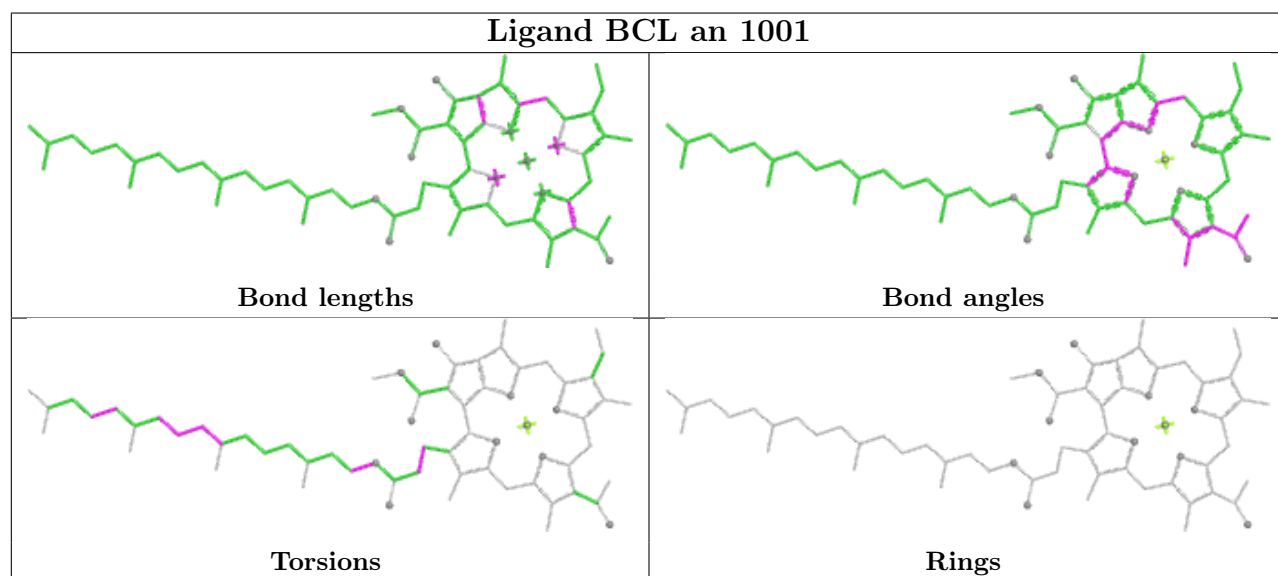
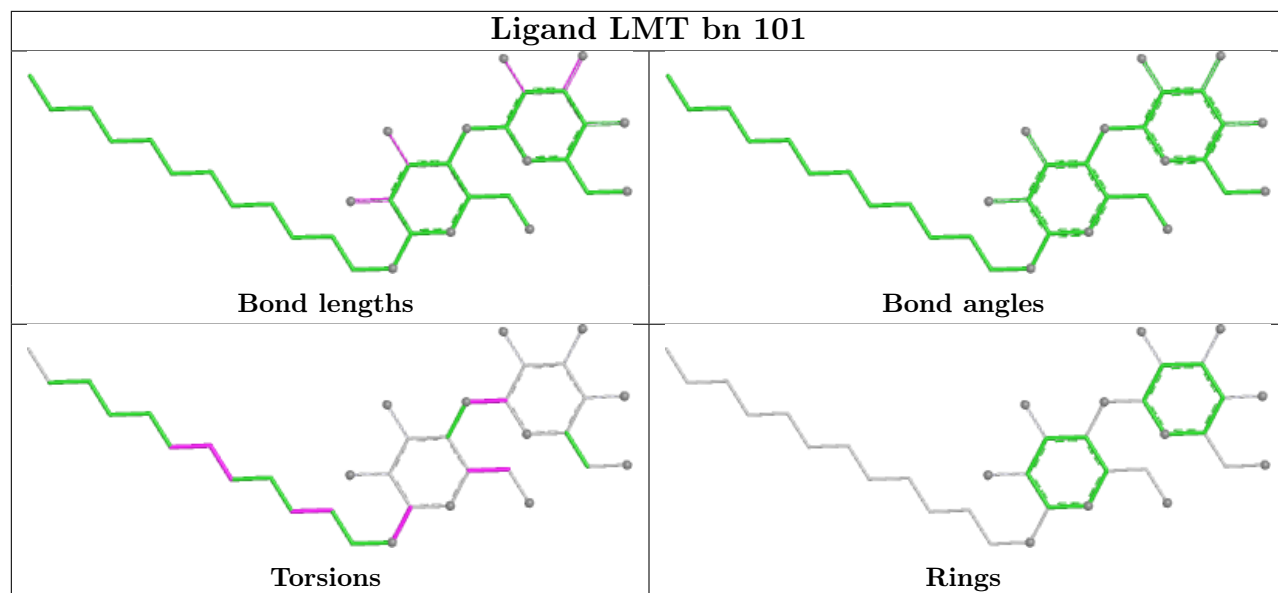


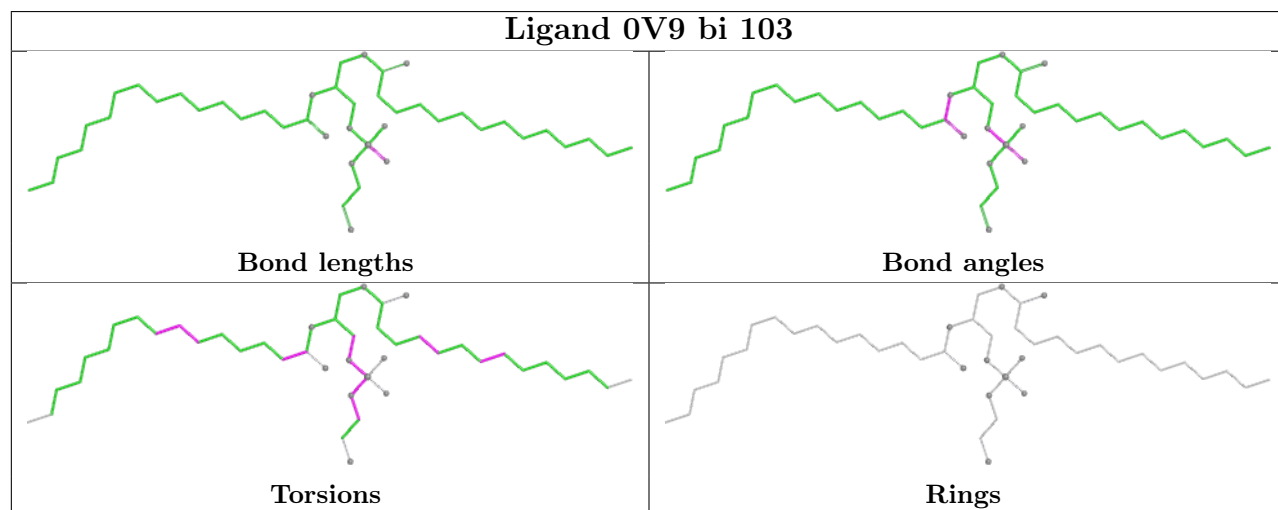
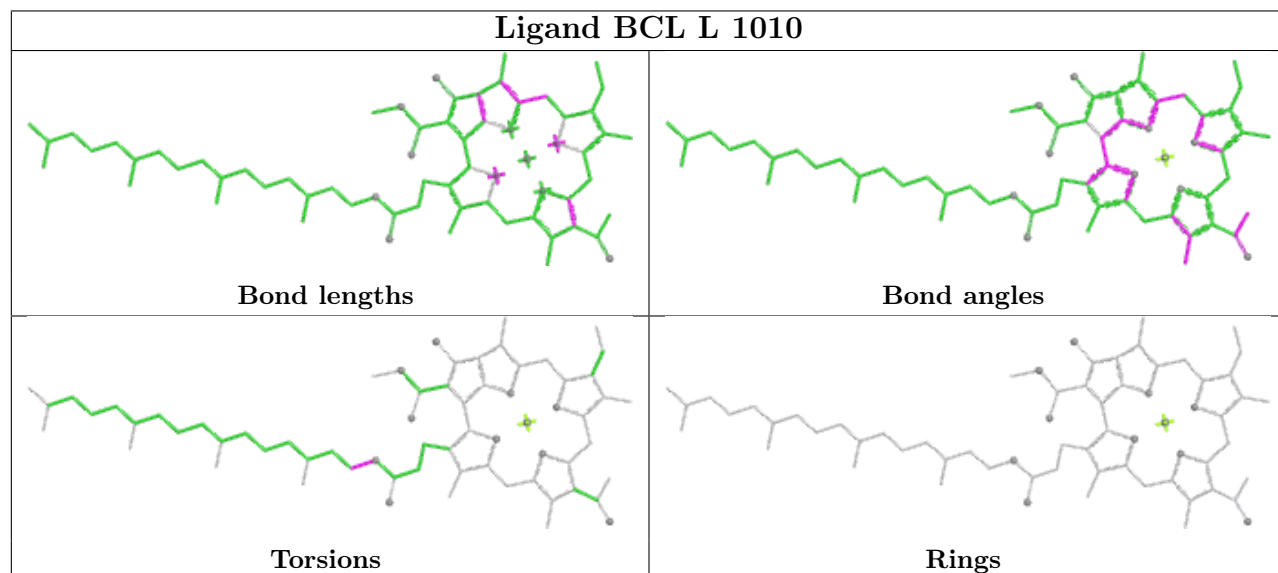
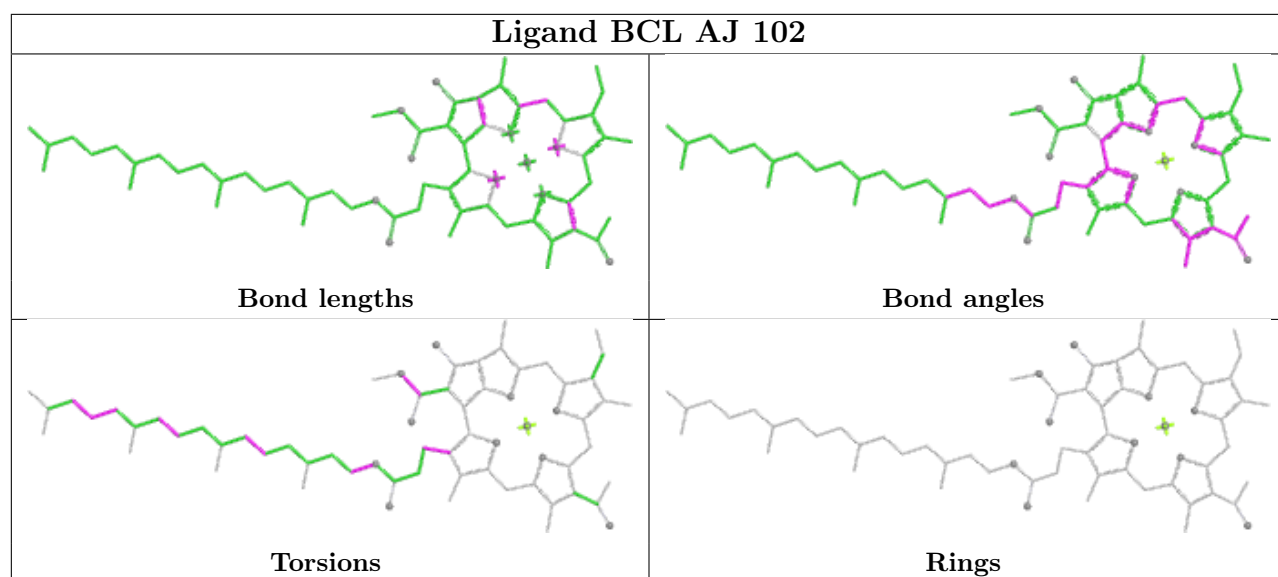


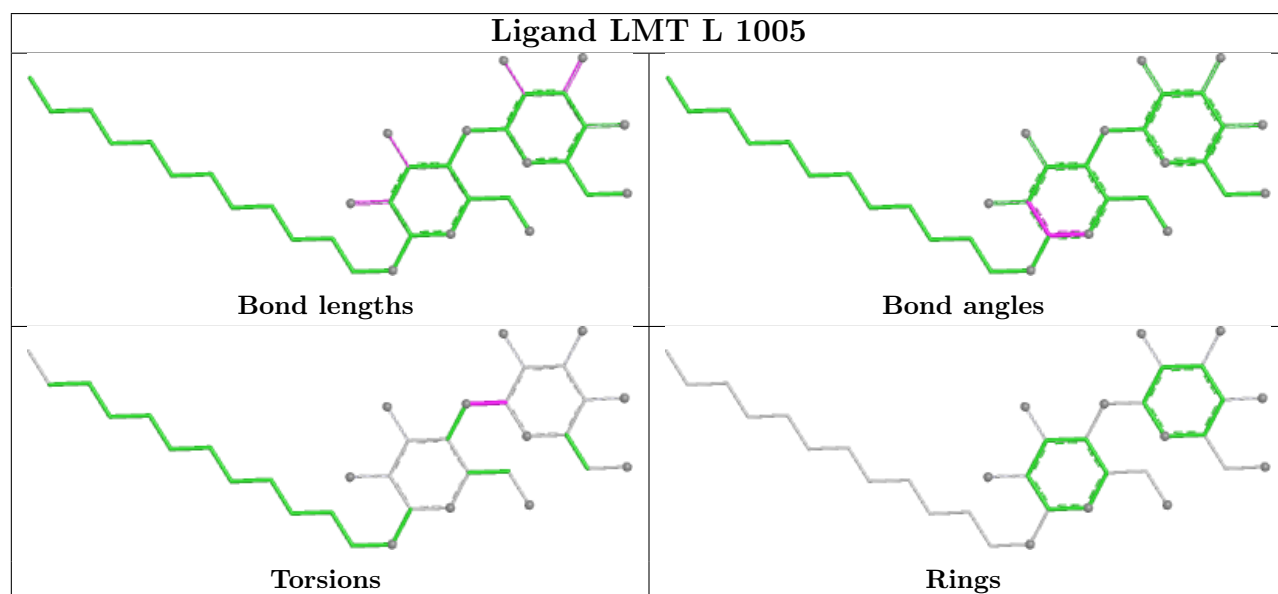
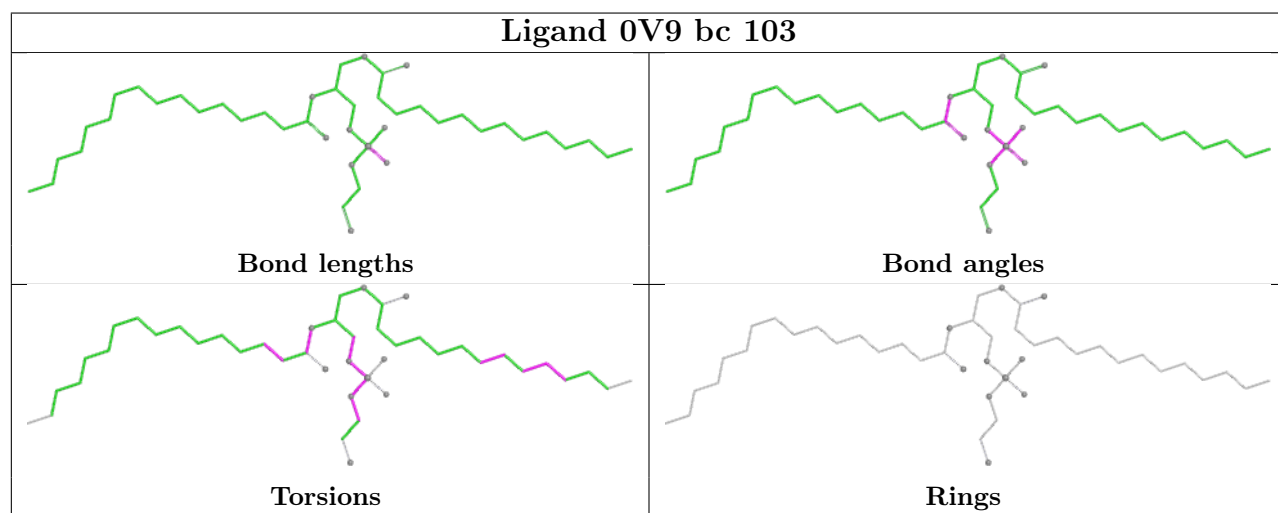
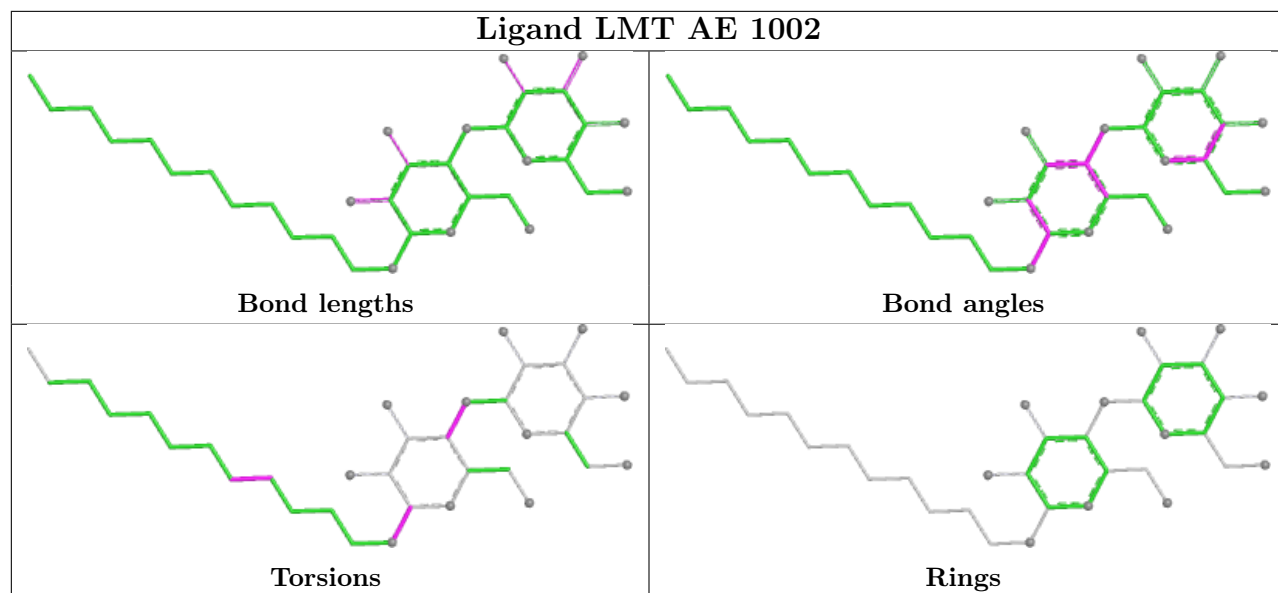


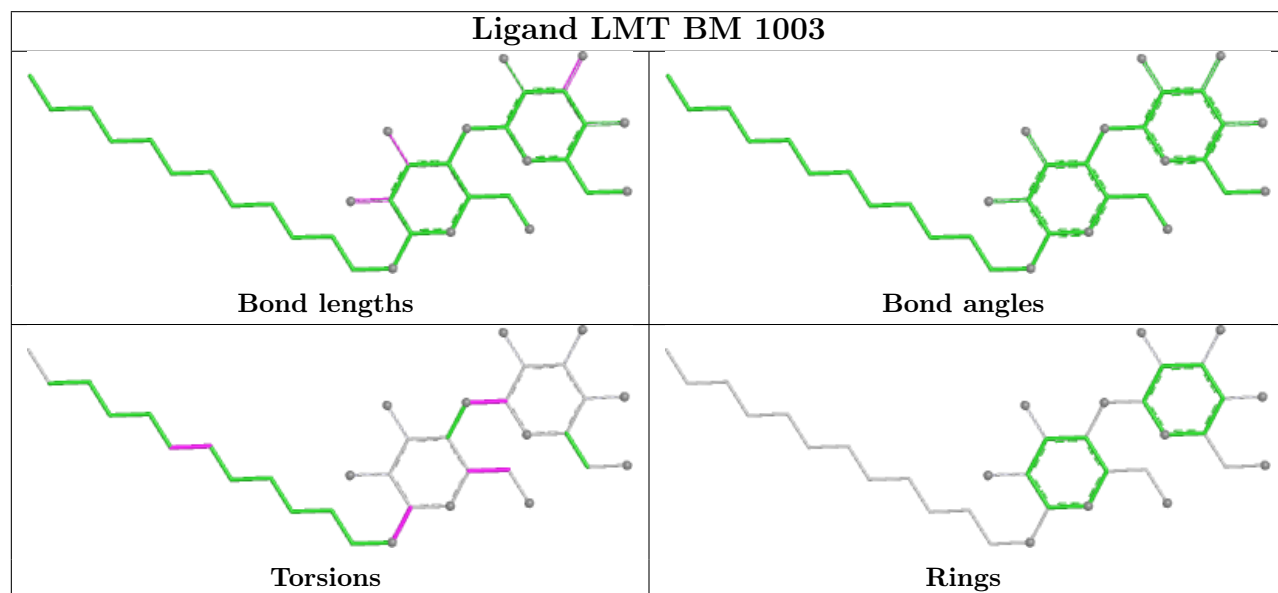
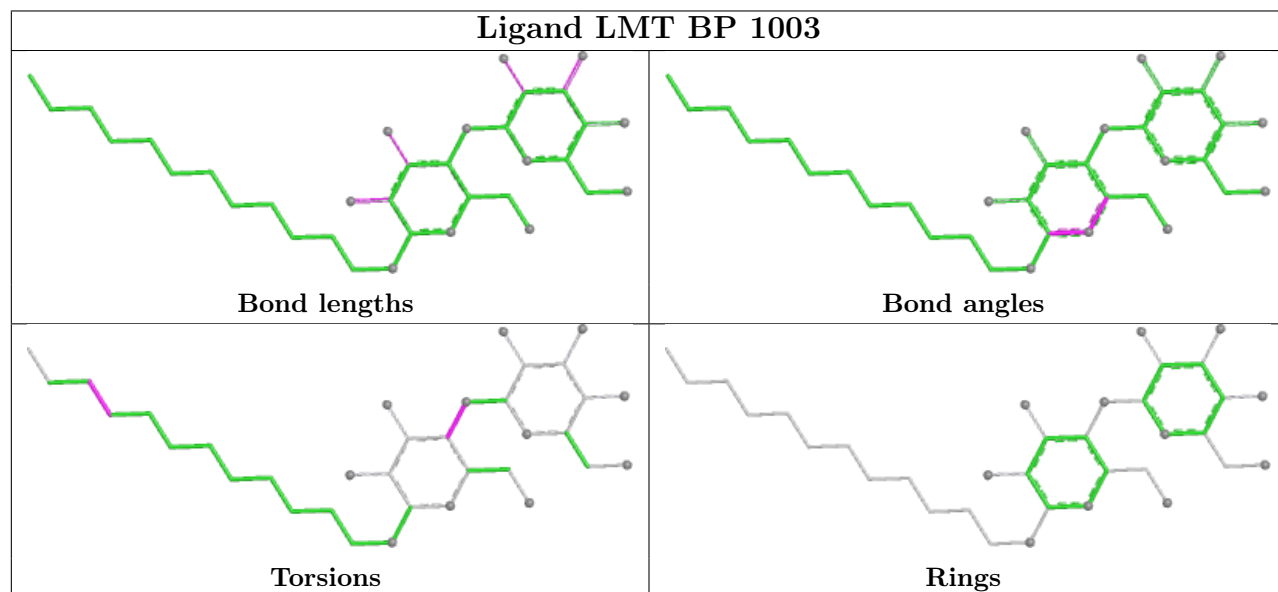
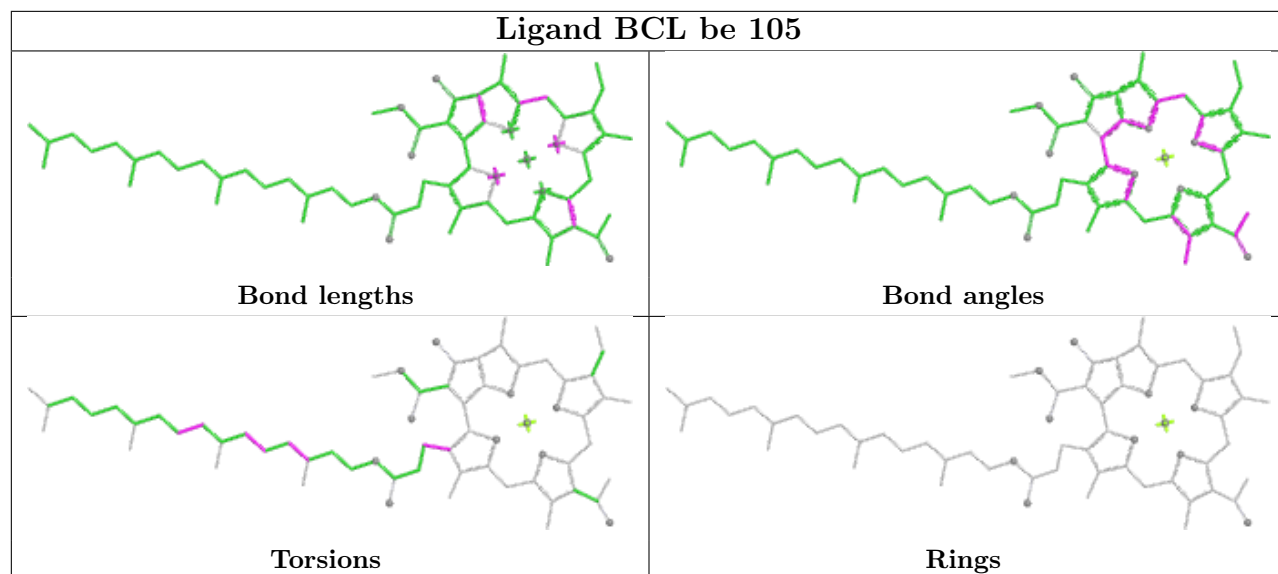


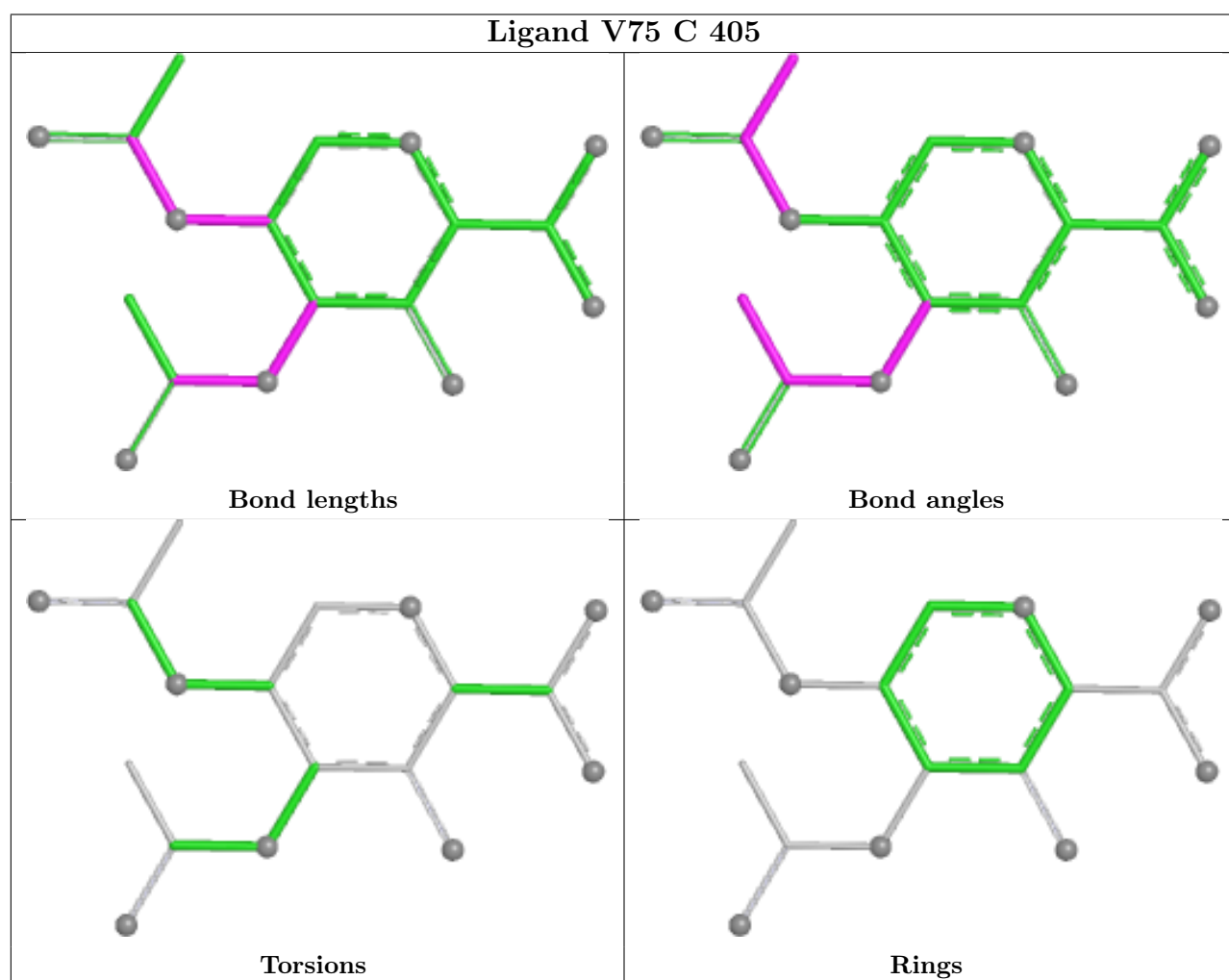
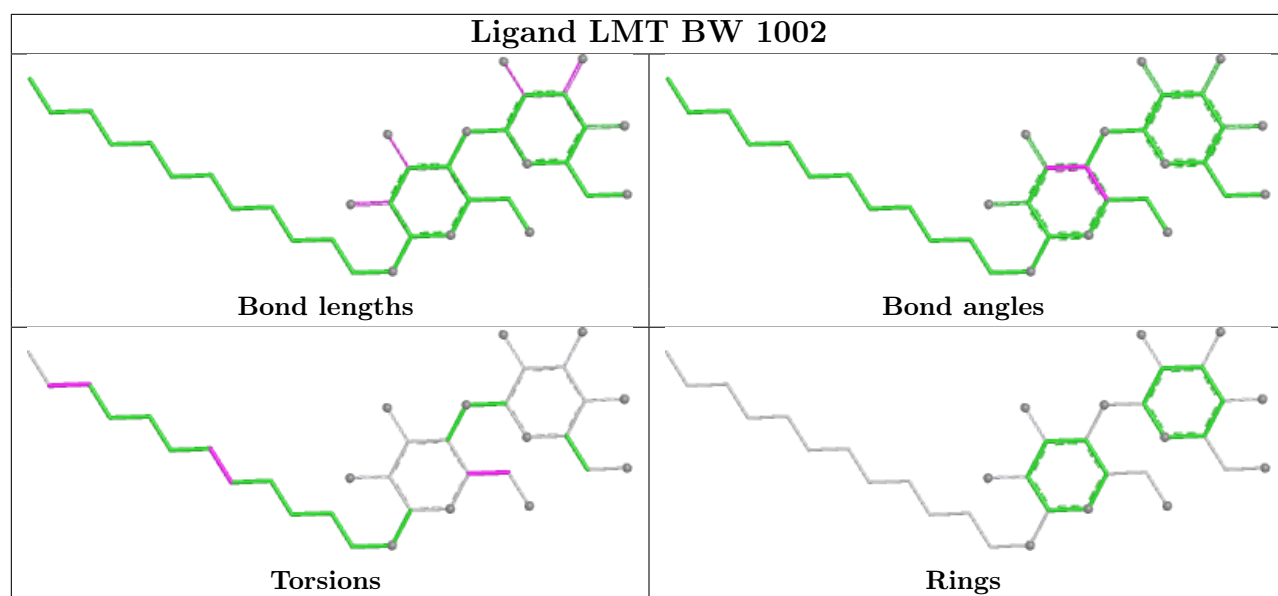


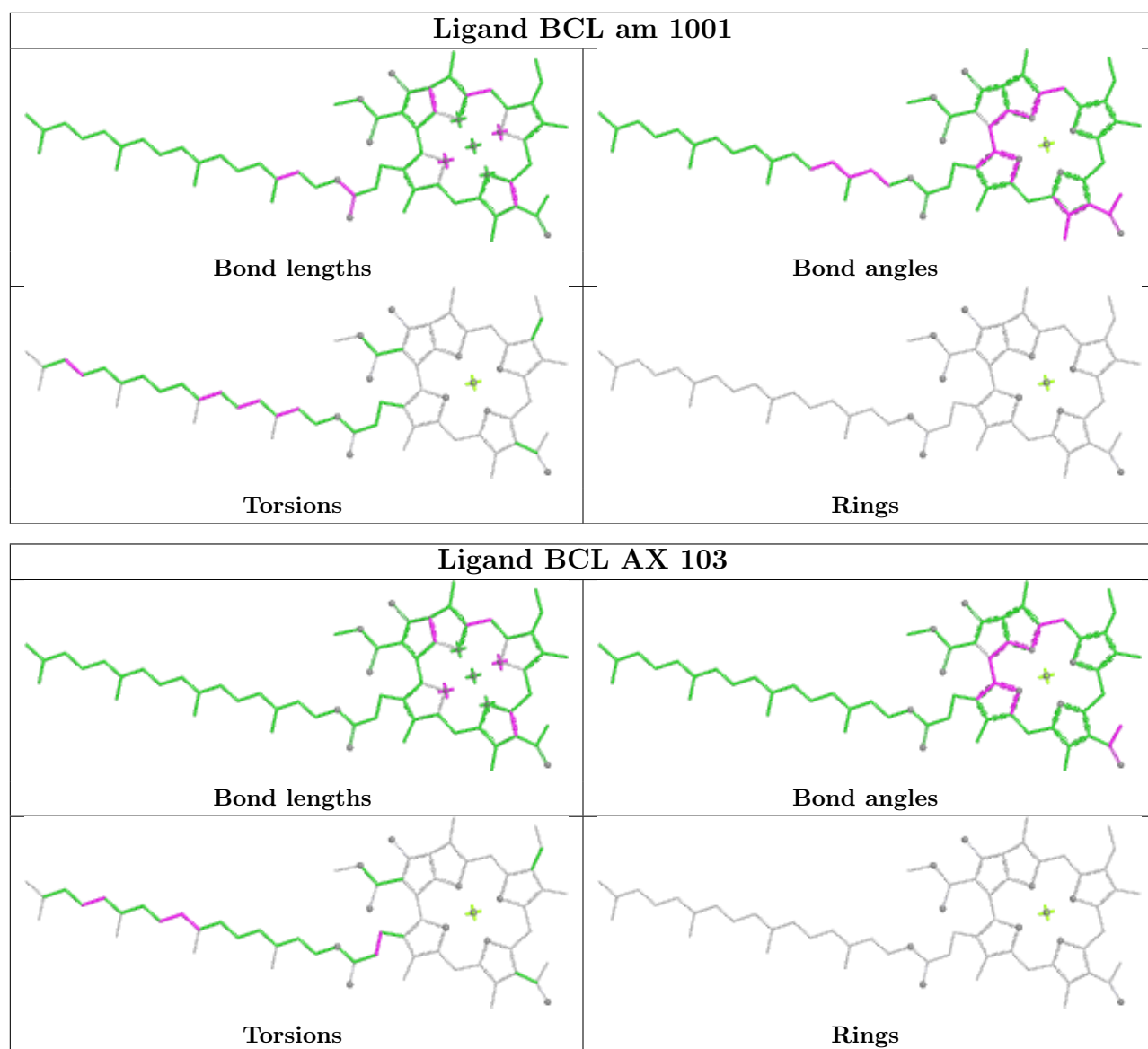




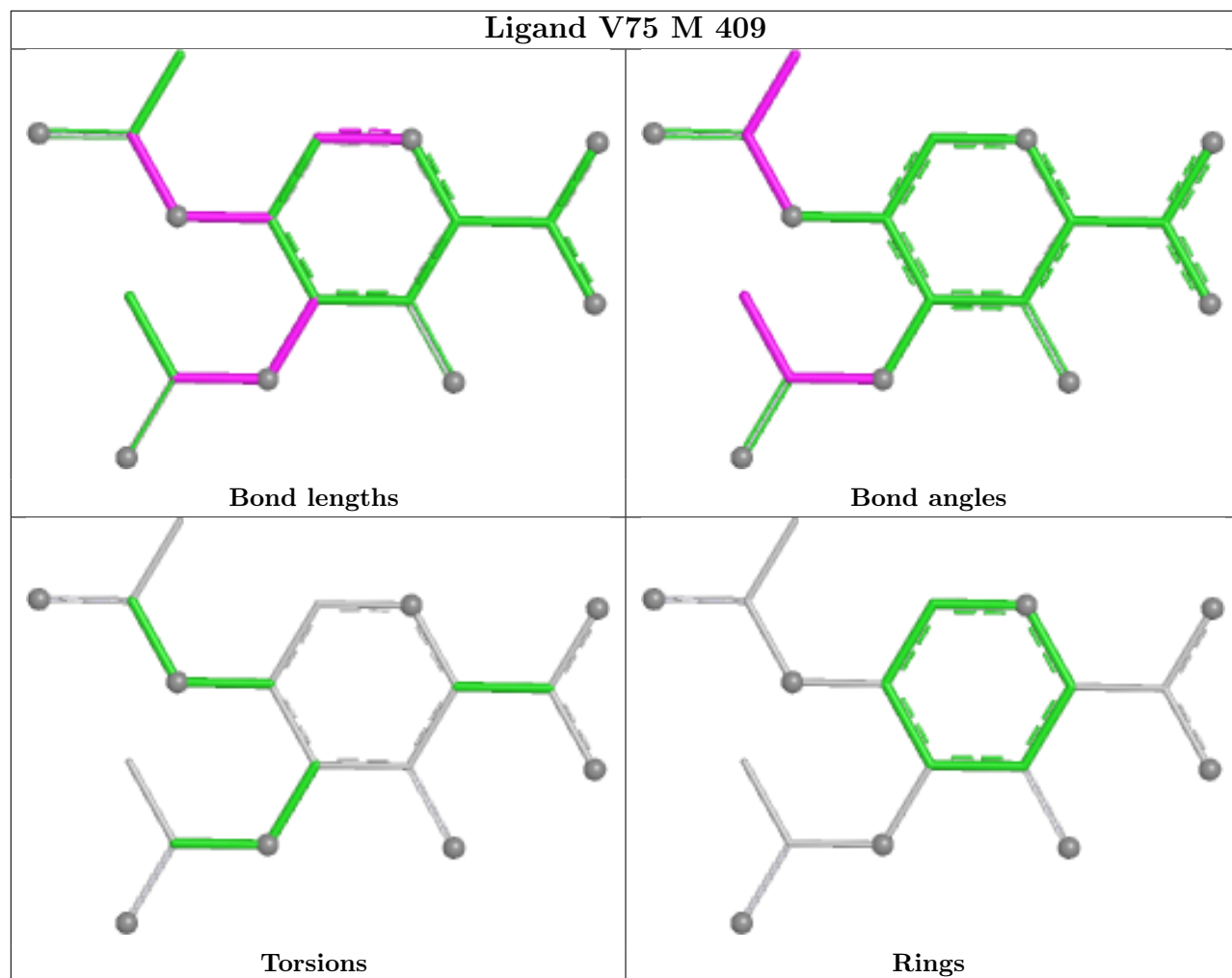




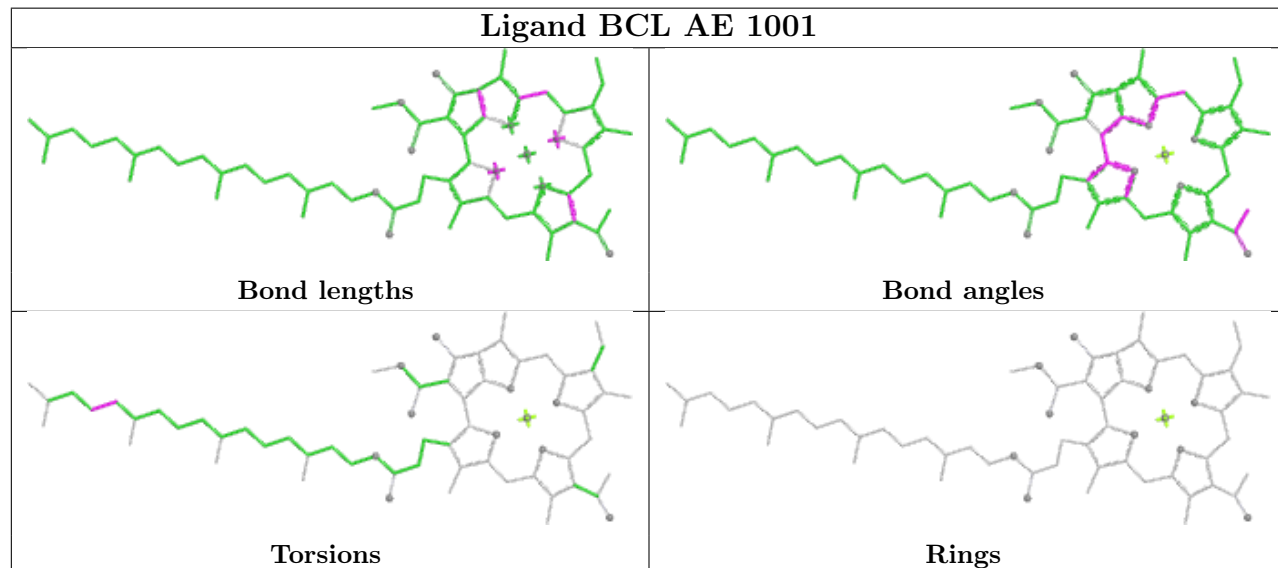


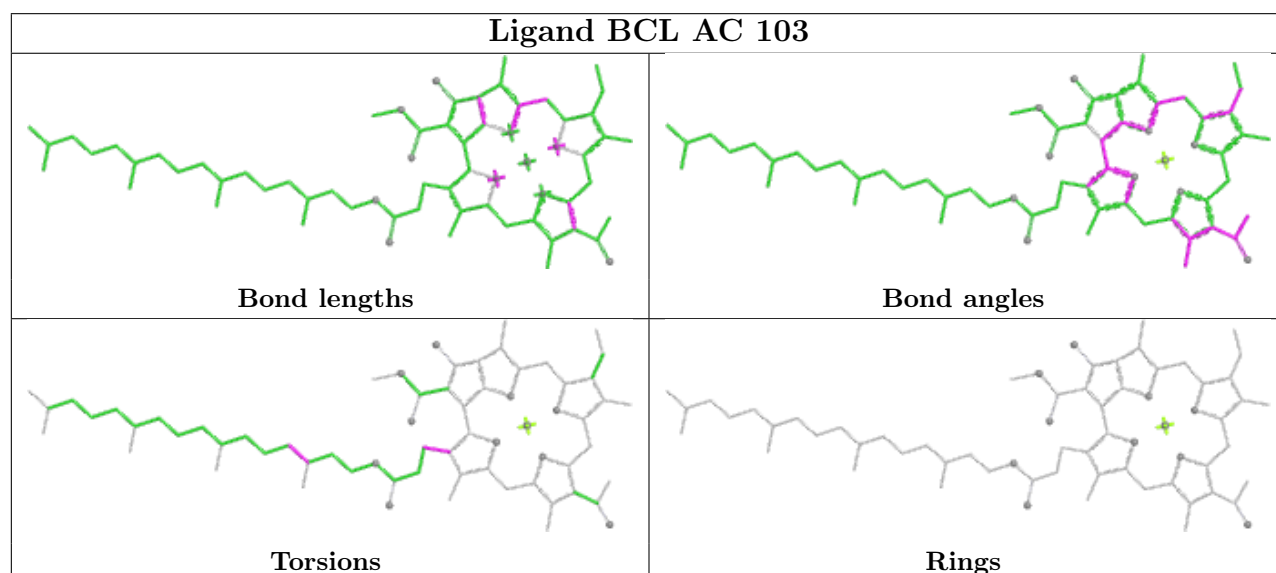
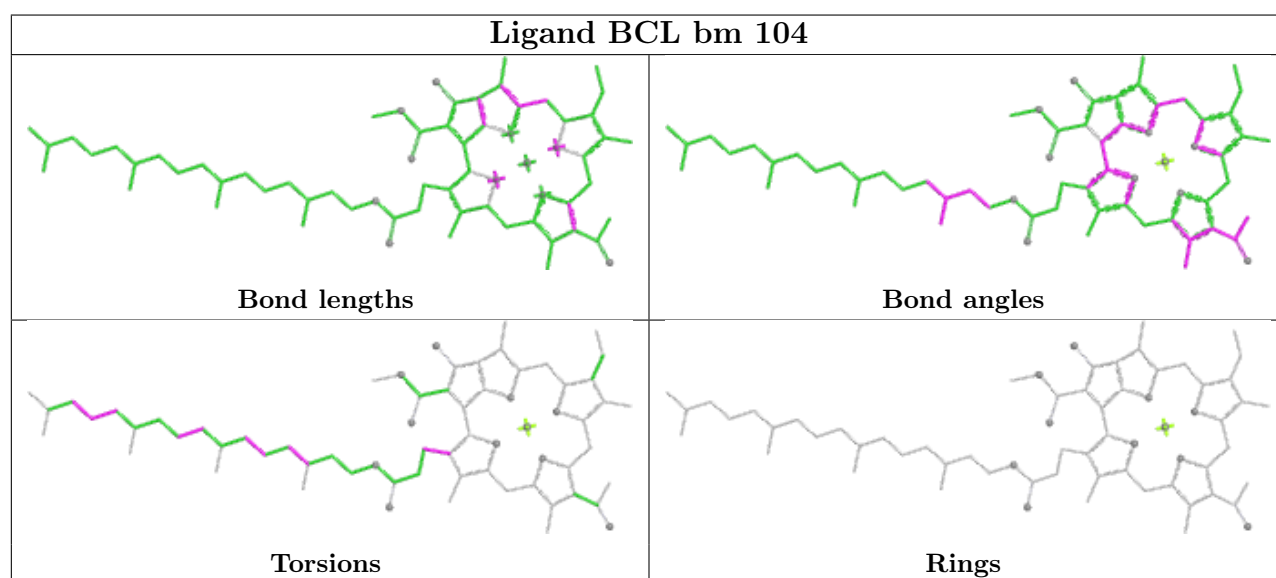
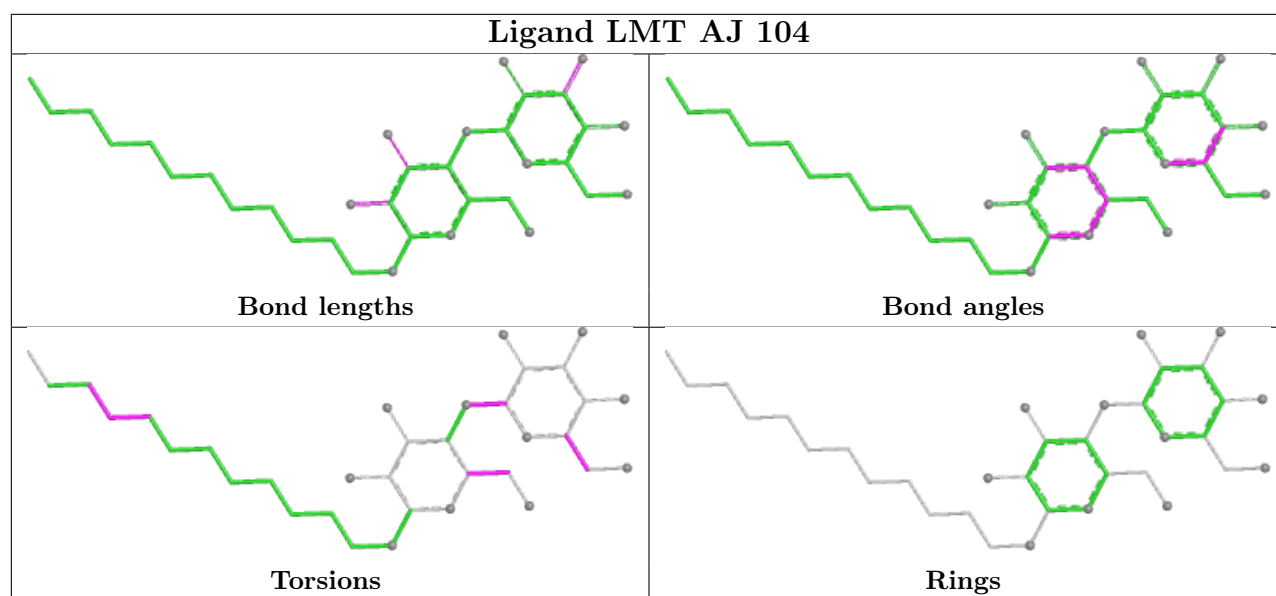


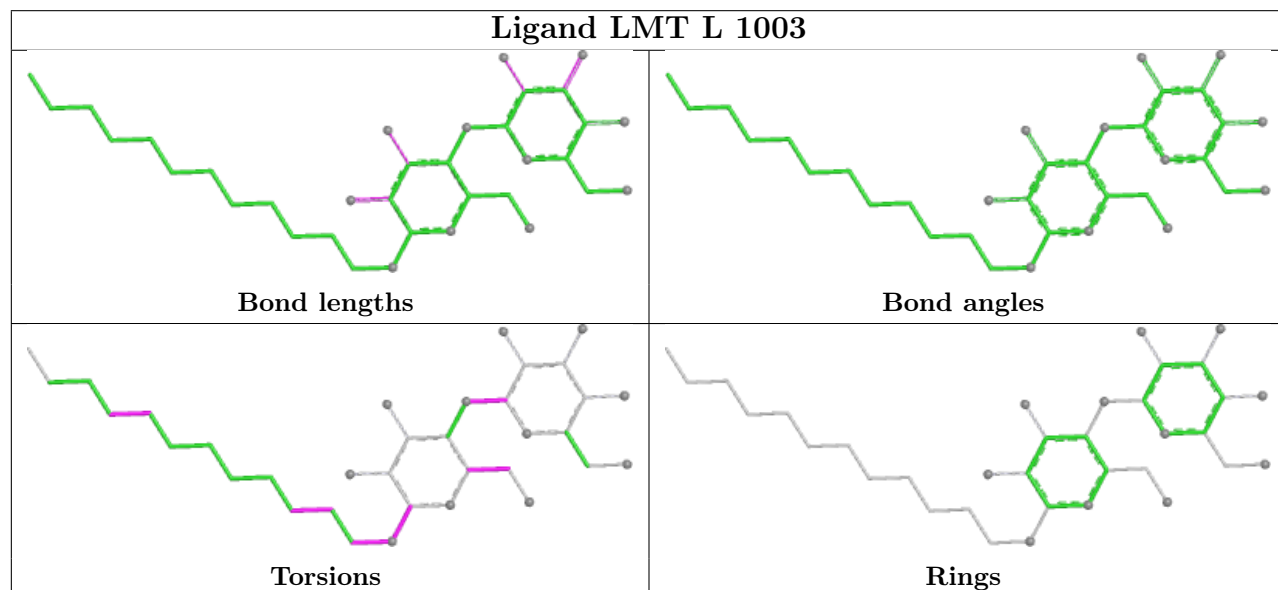
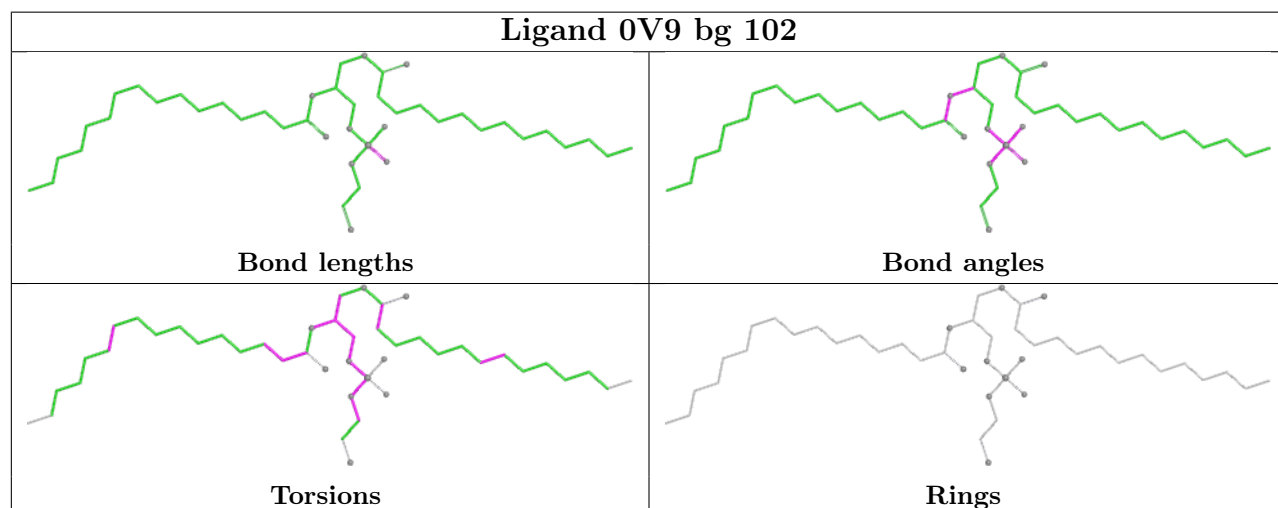
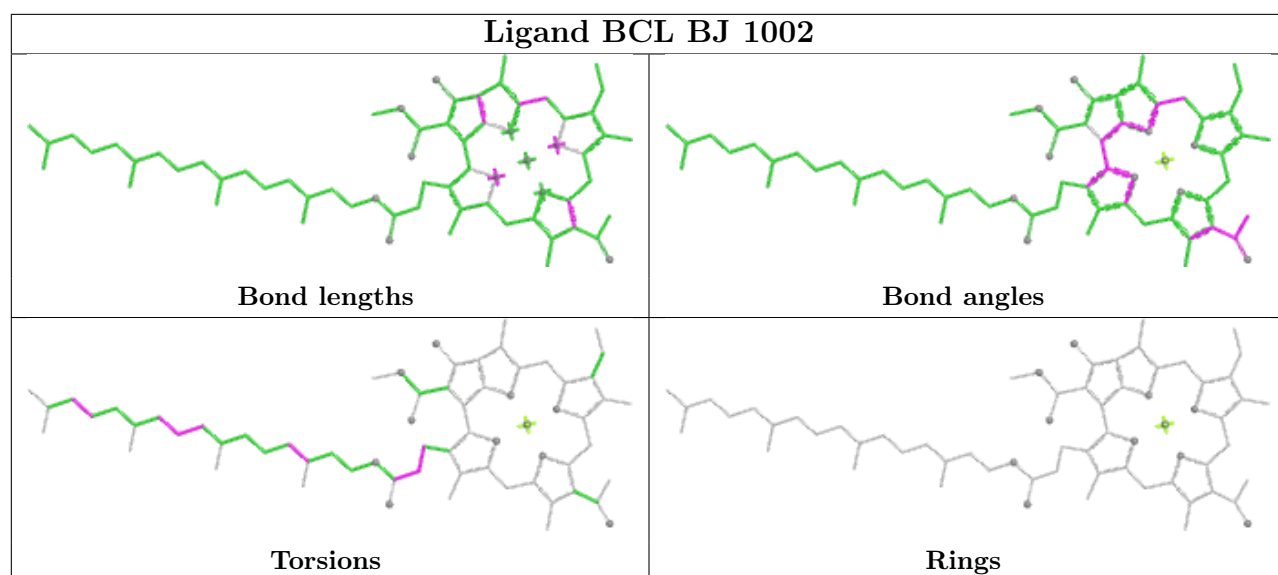
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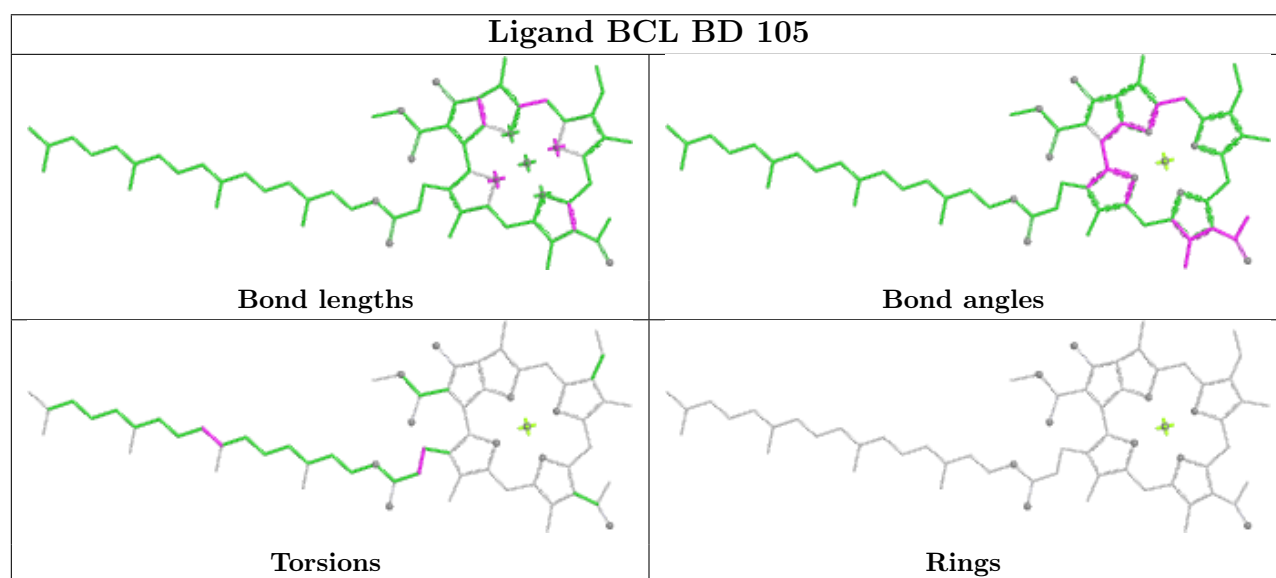
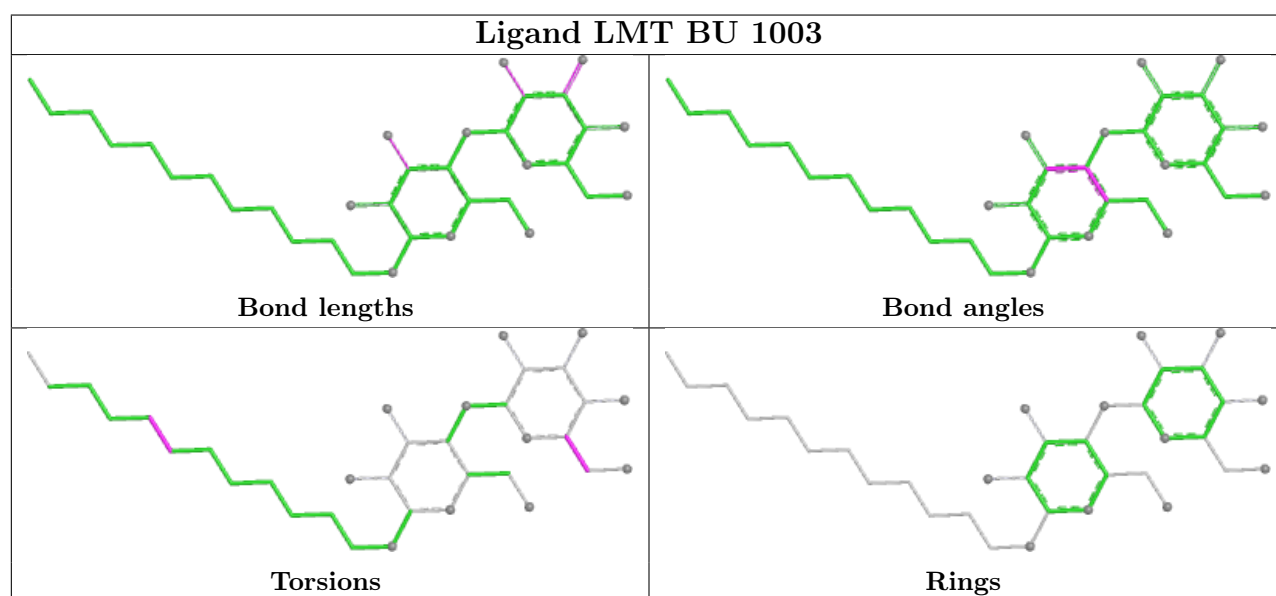
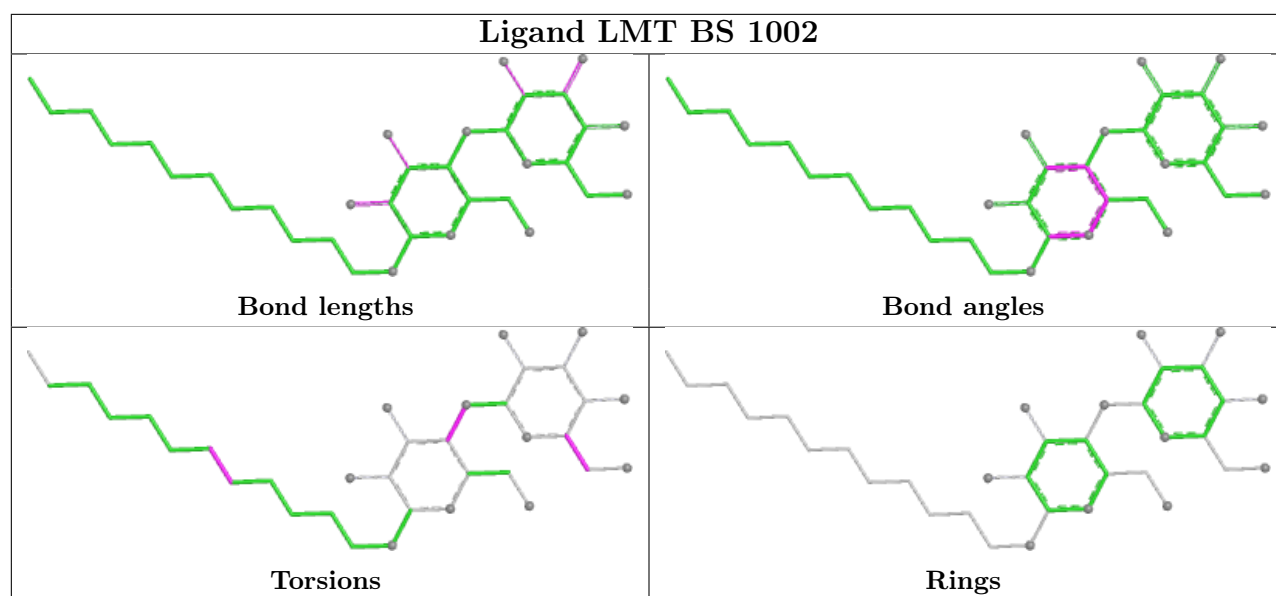


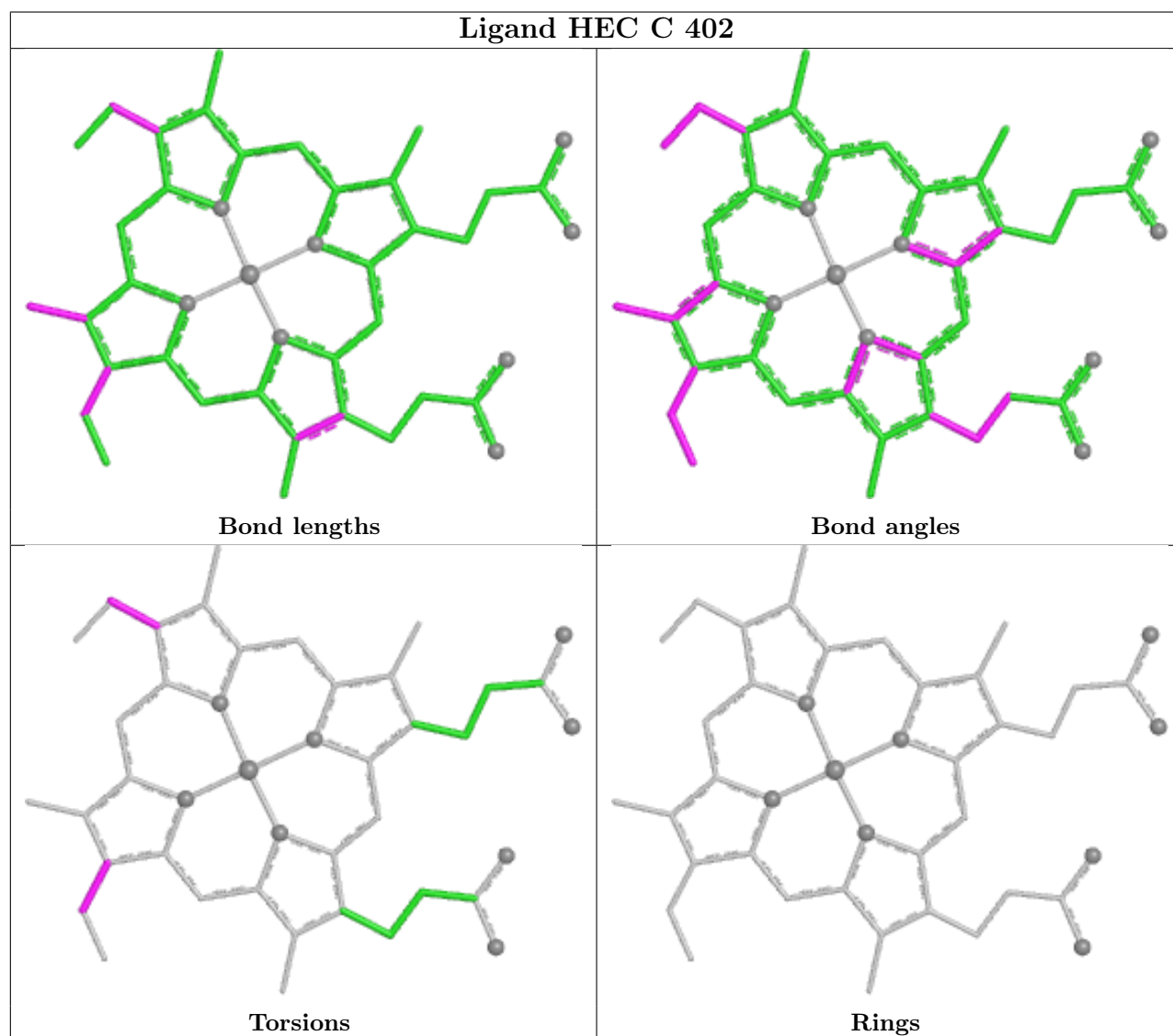
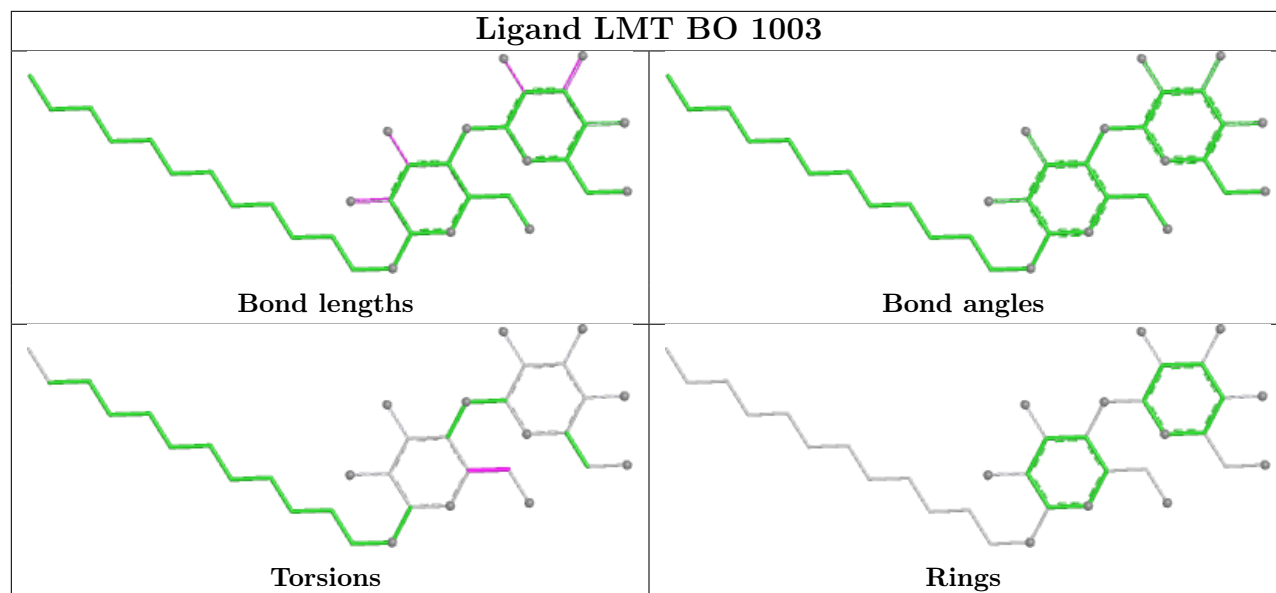
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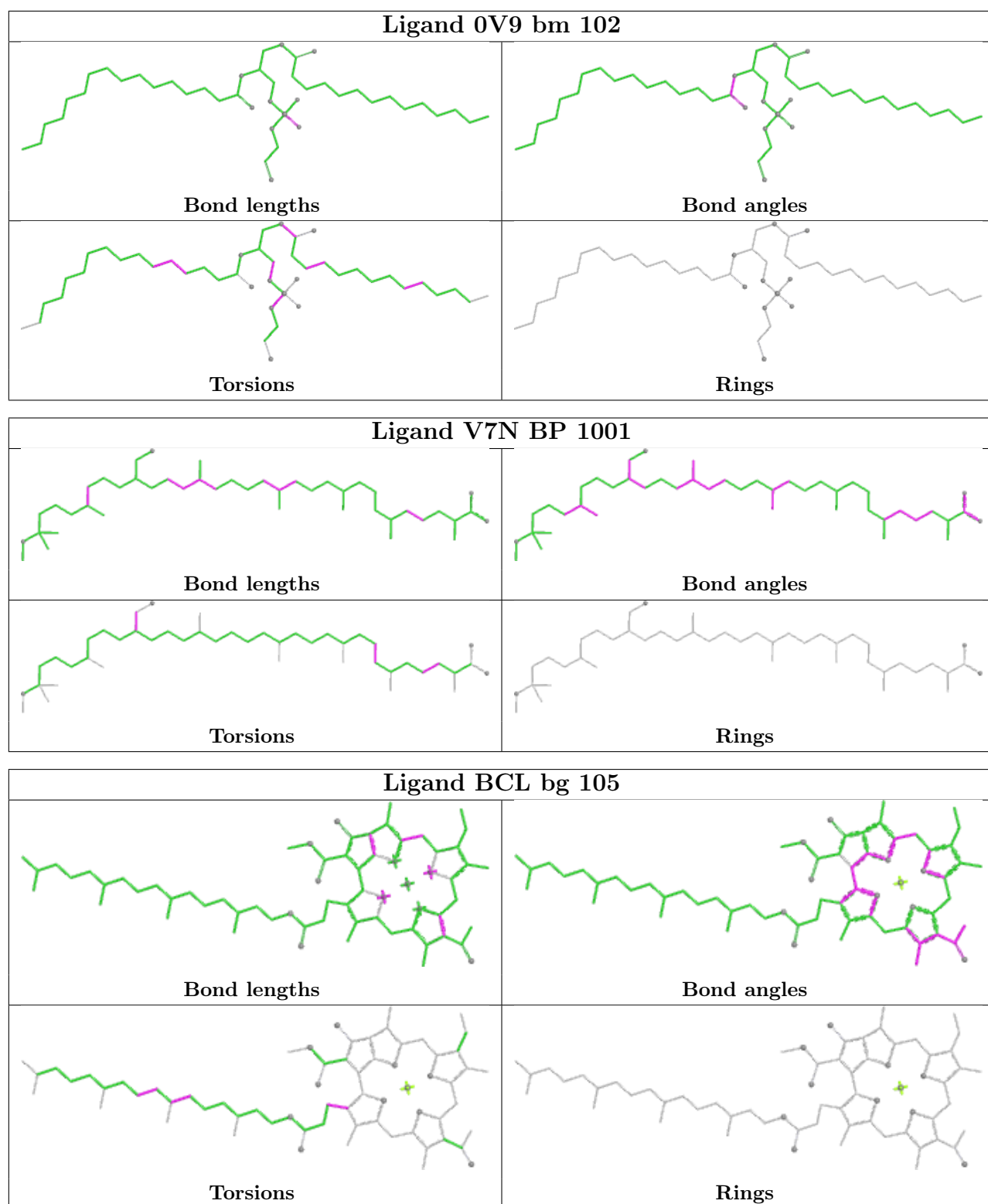


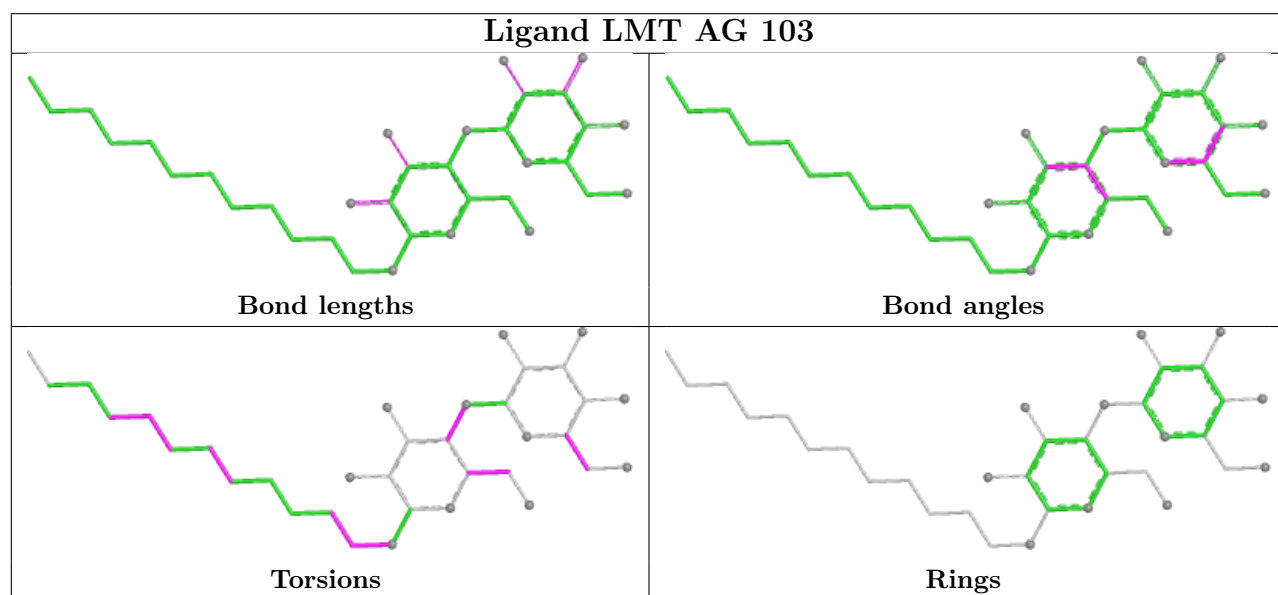
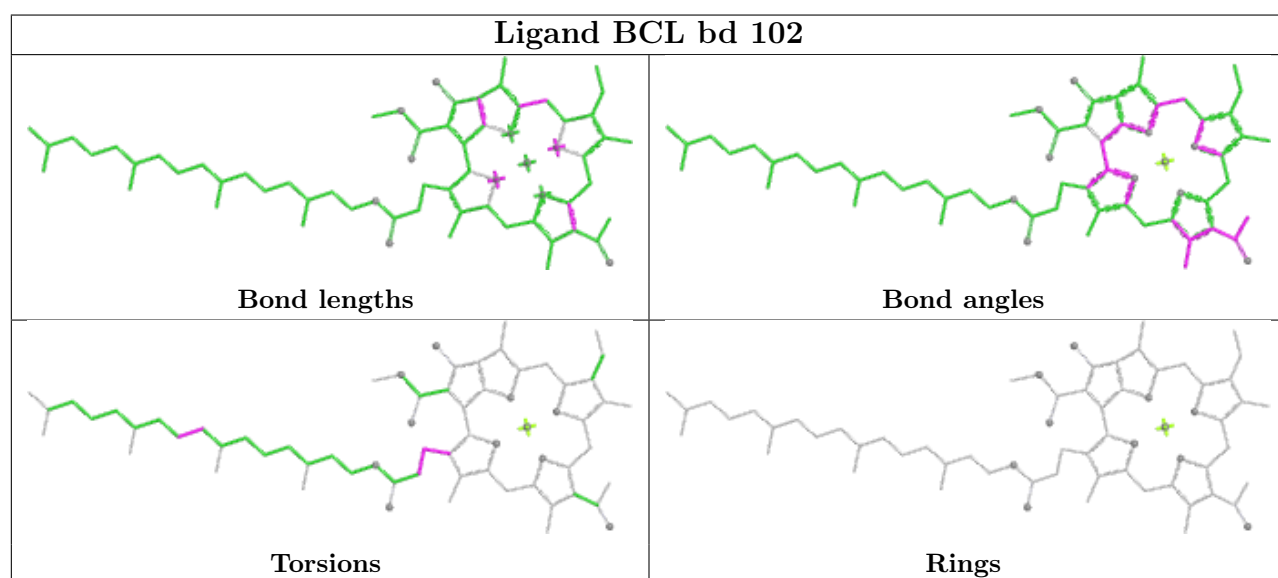
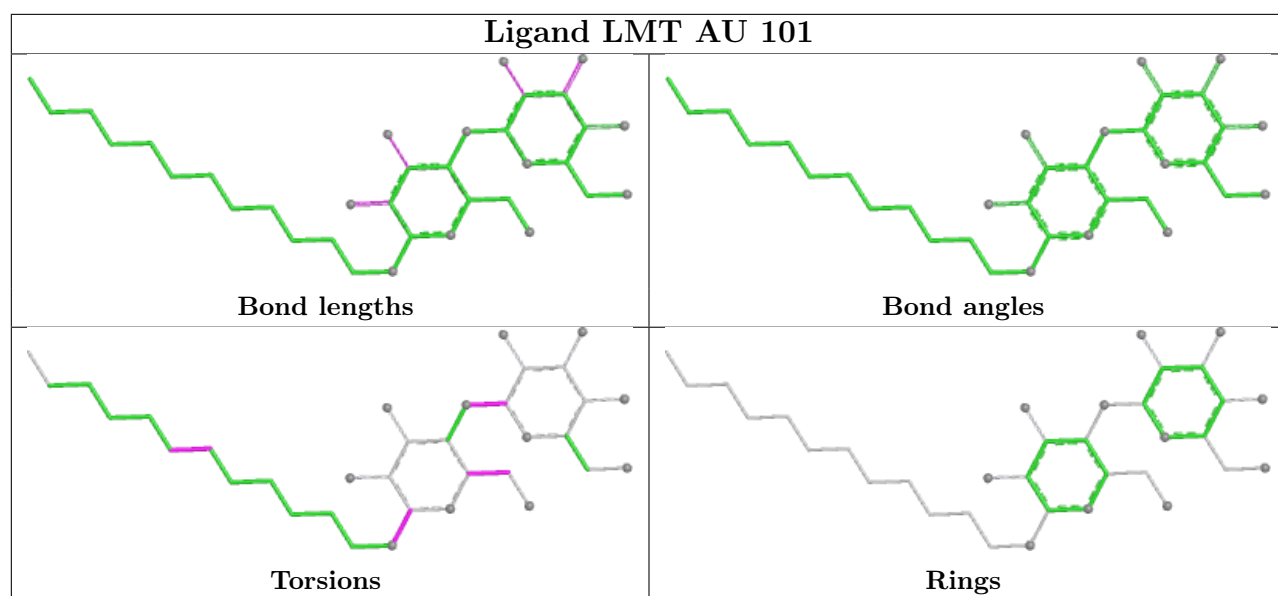


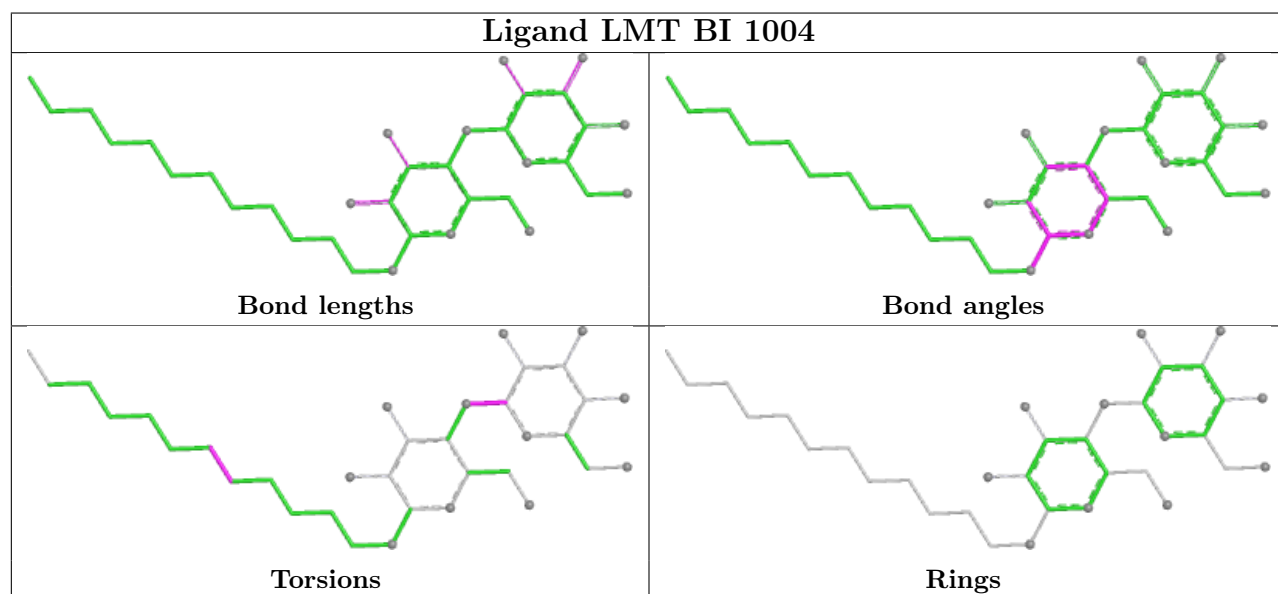
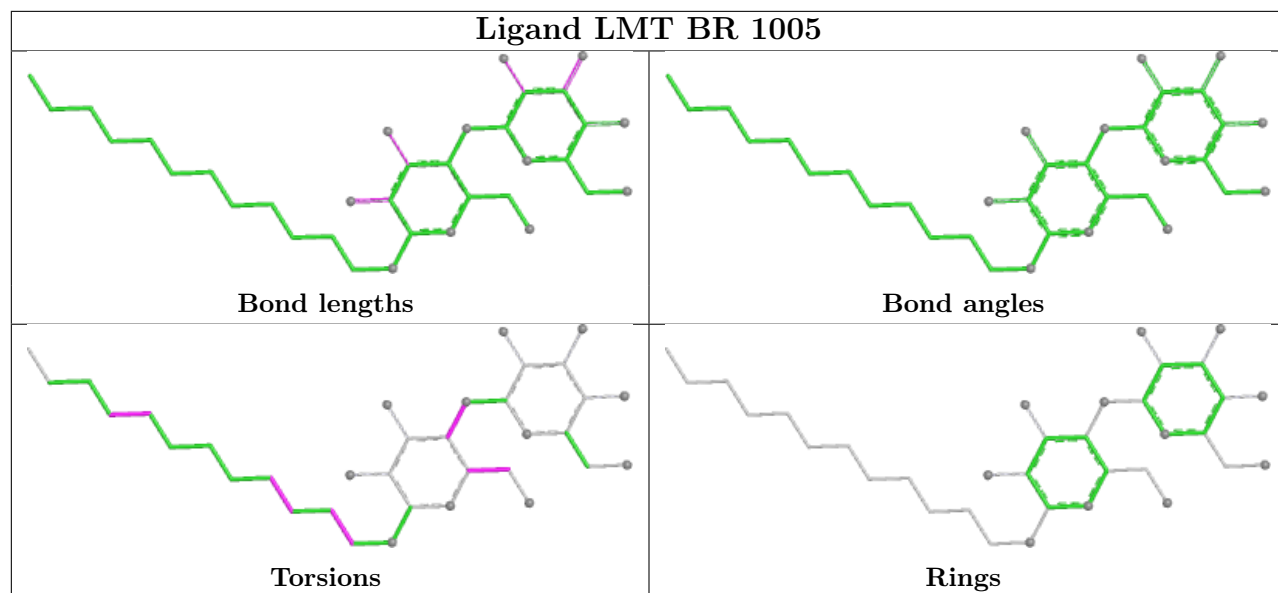




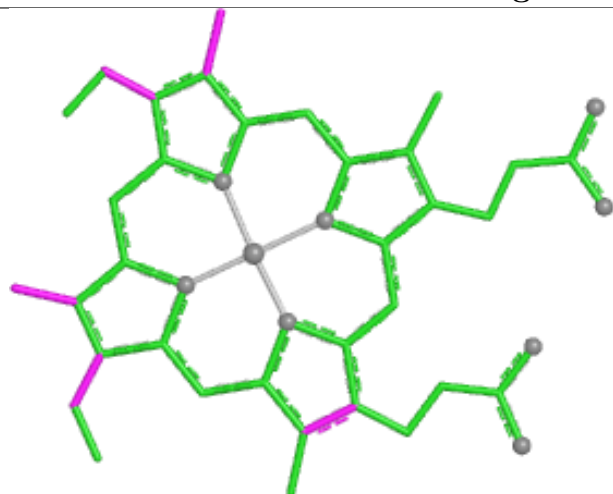




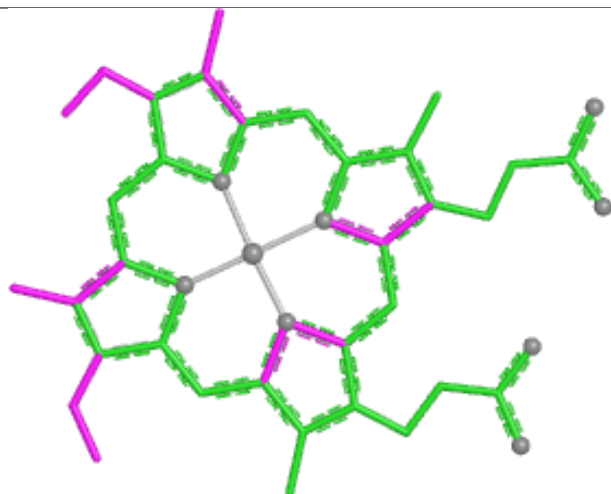




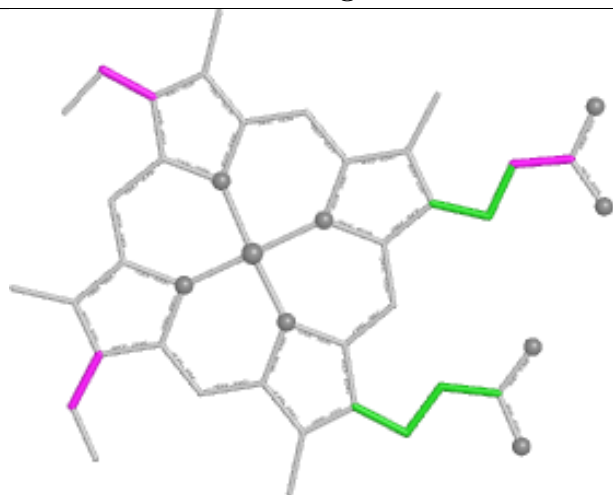
Ligand HEC C 401



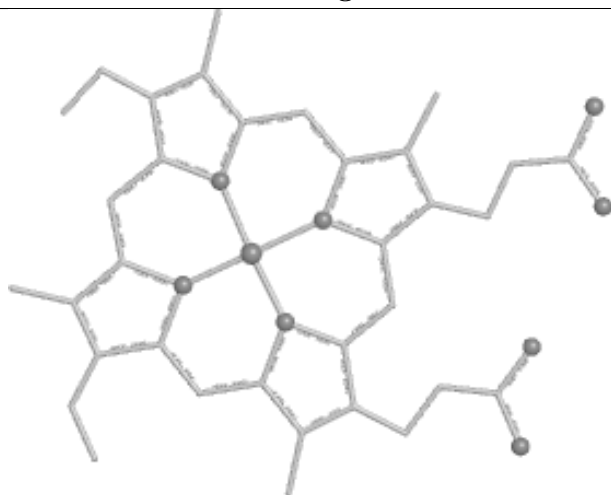
Bond lengths



Bond angles

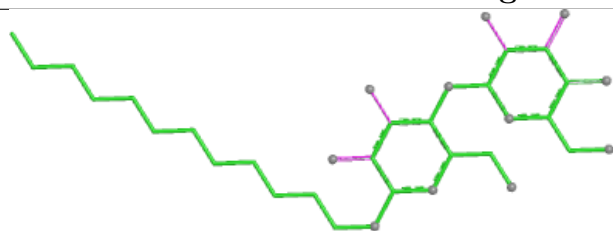


Torsions

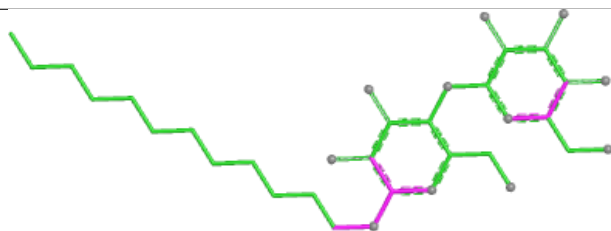


Rings

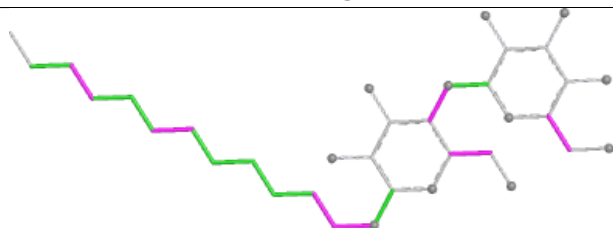
Ligand LMT bm 103



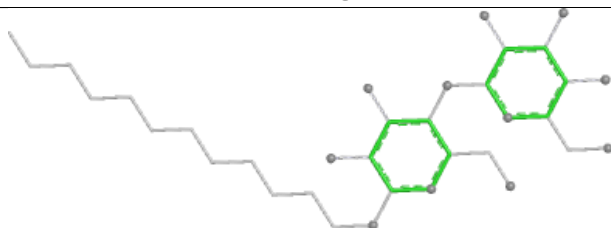
Bond lengths



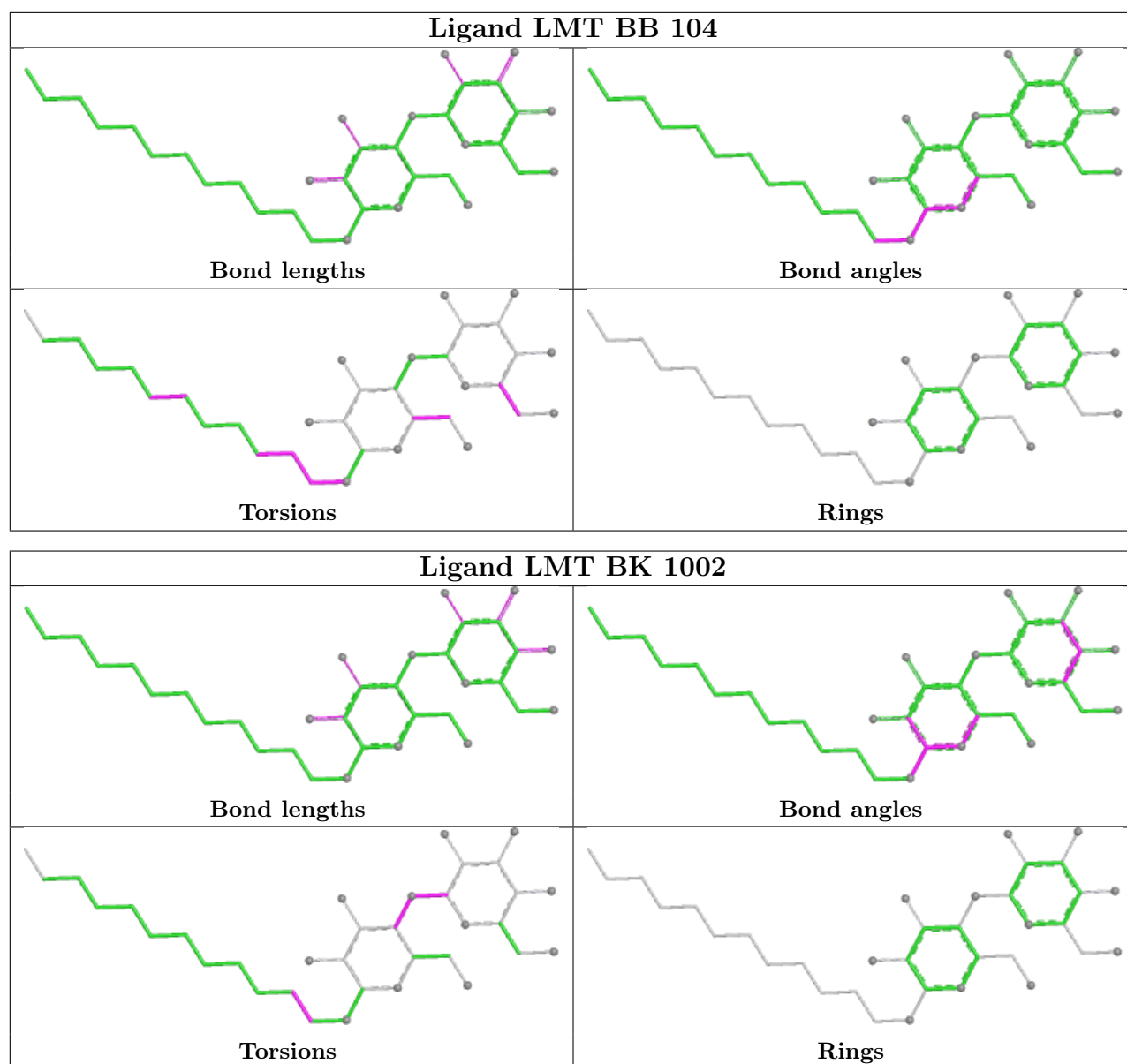
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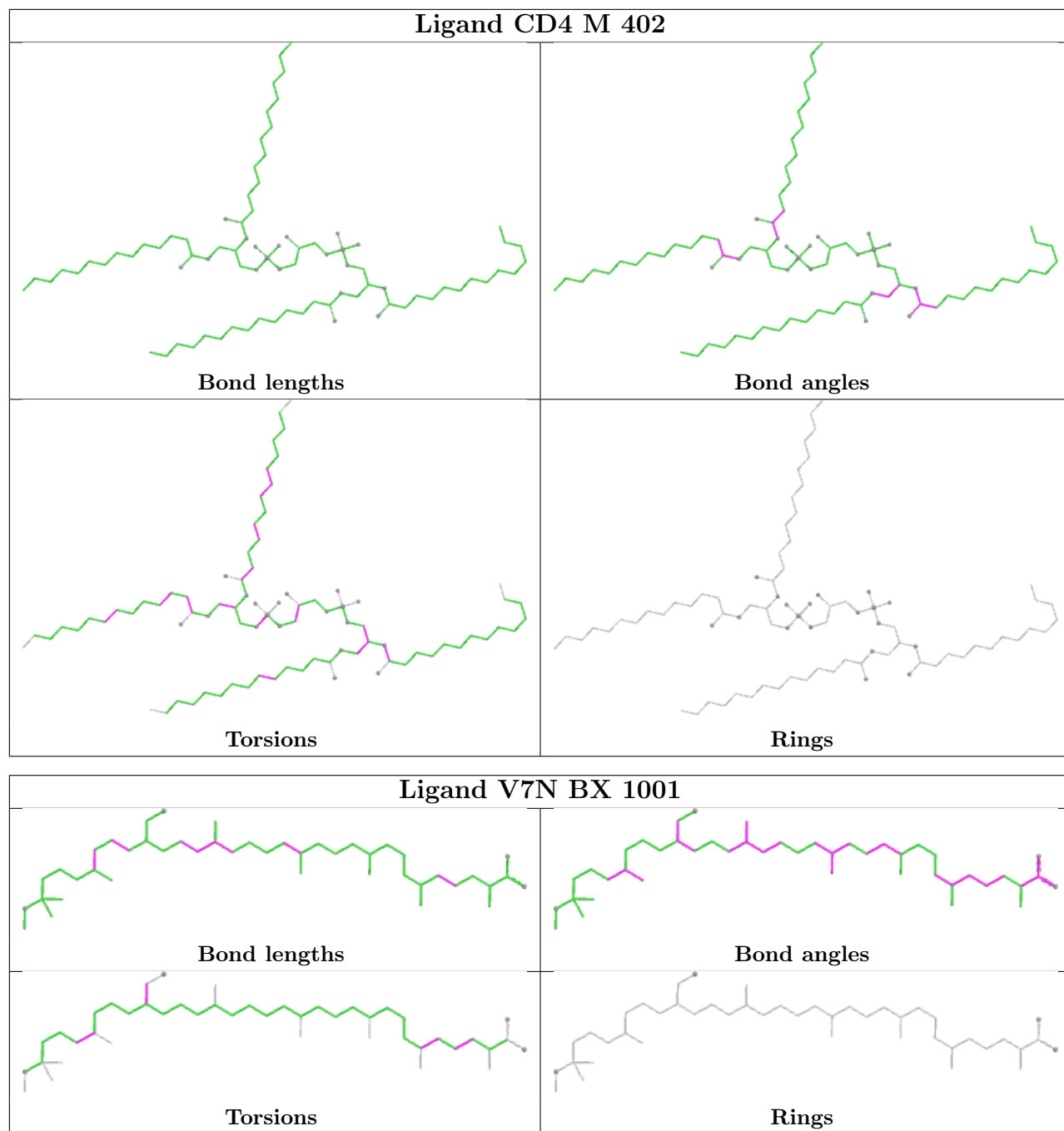


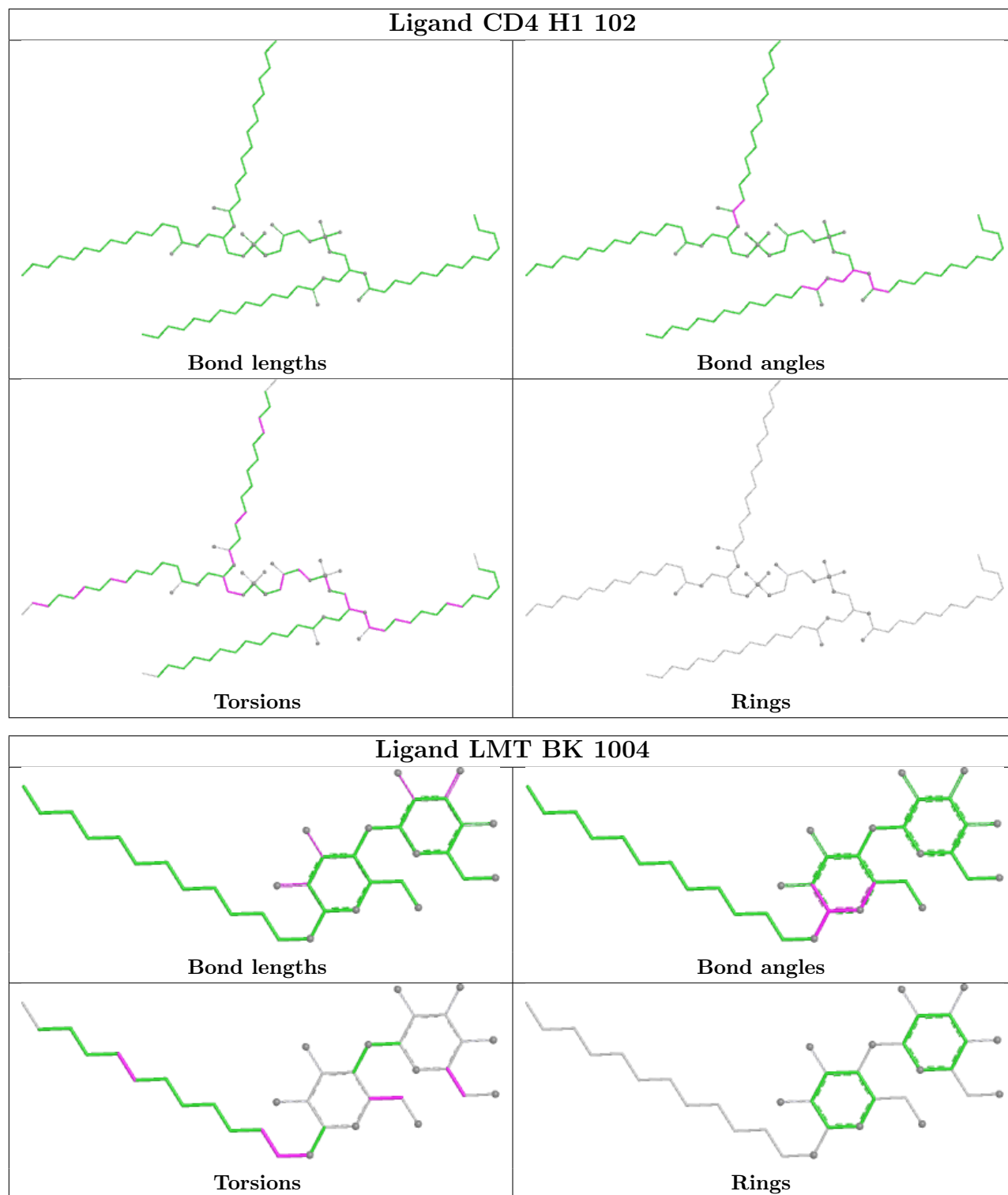
Torsions

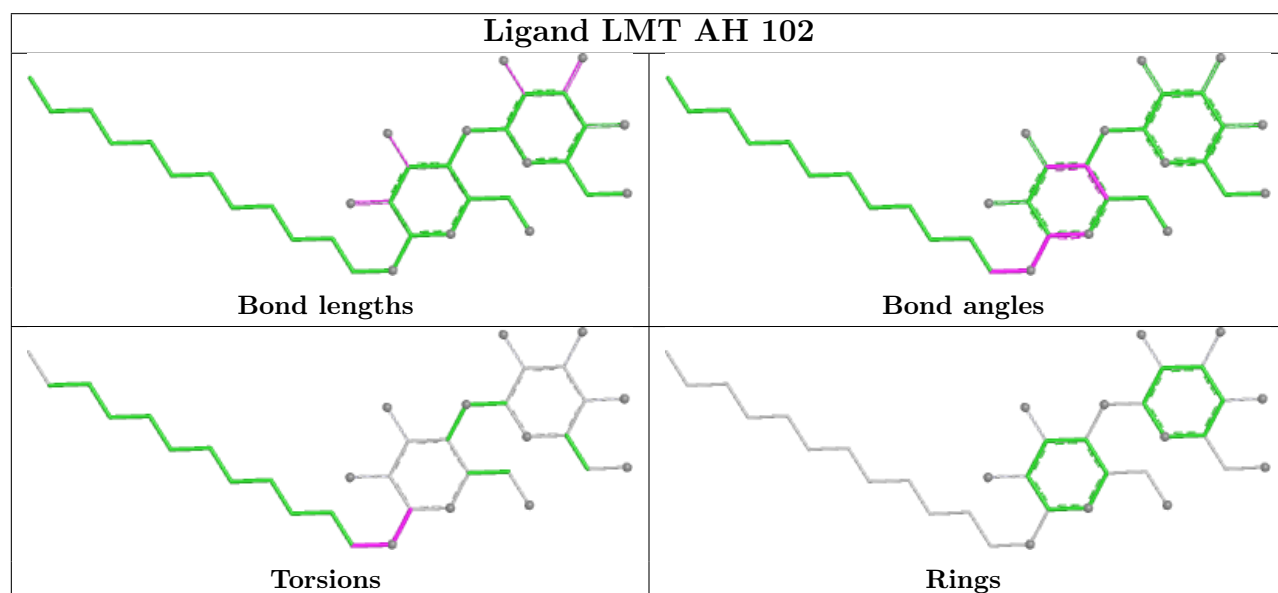
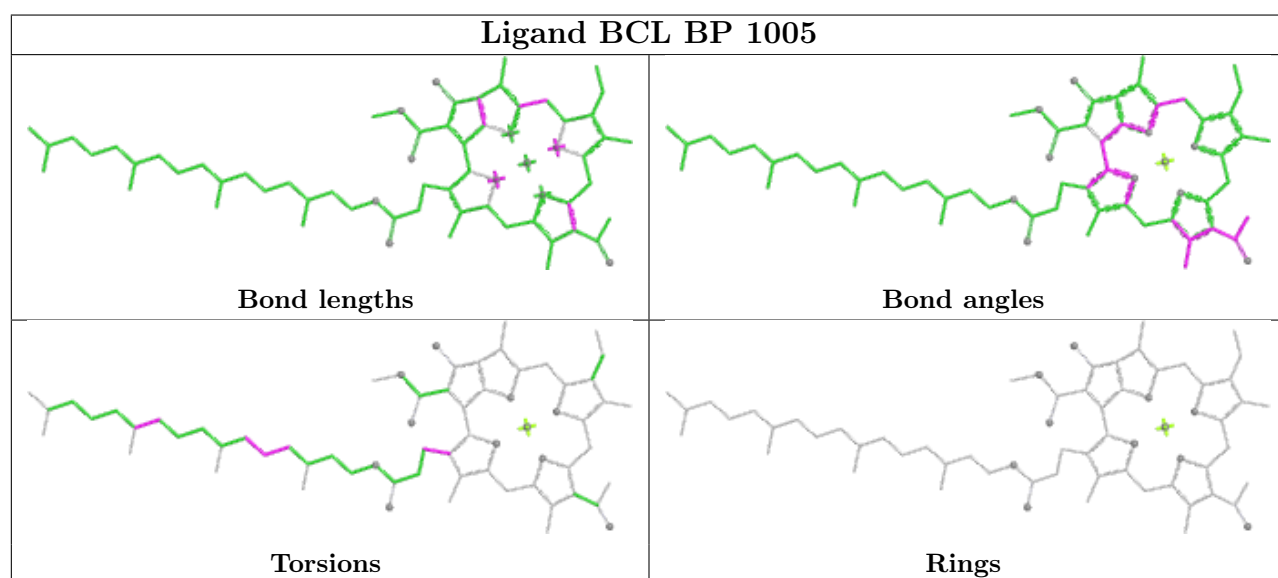
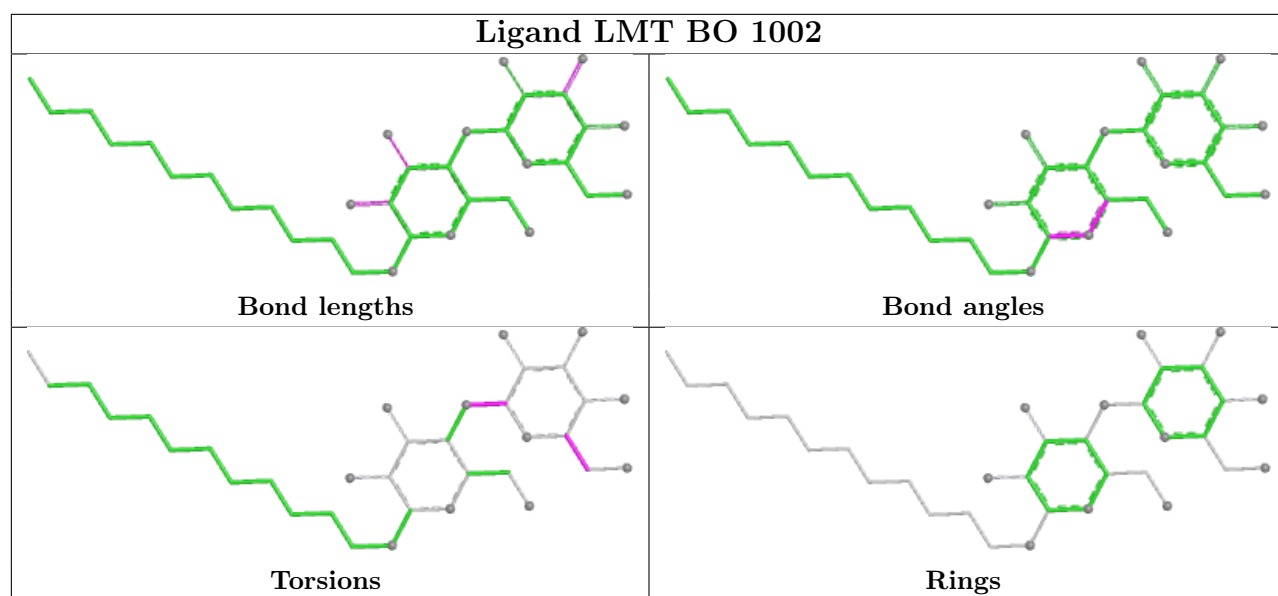


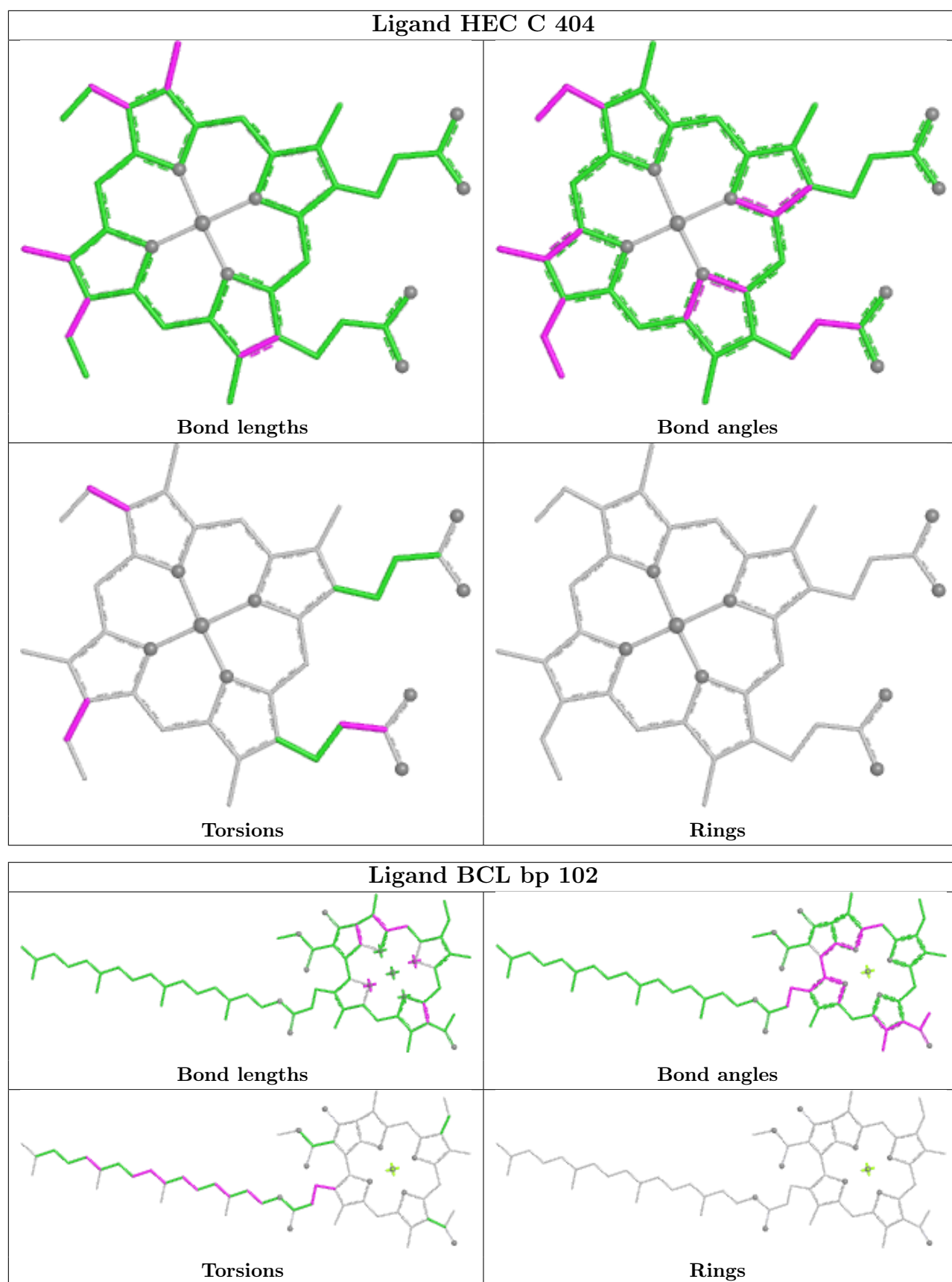
Rings

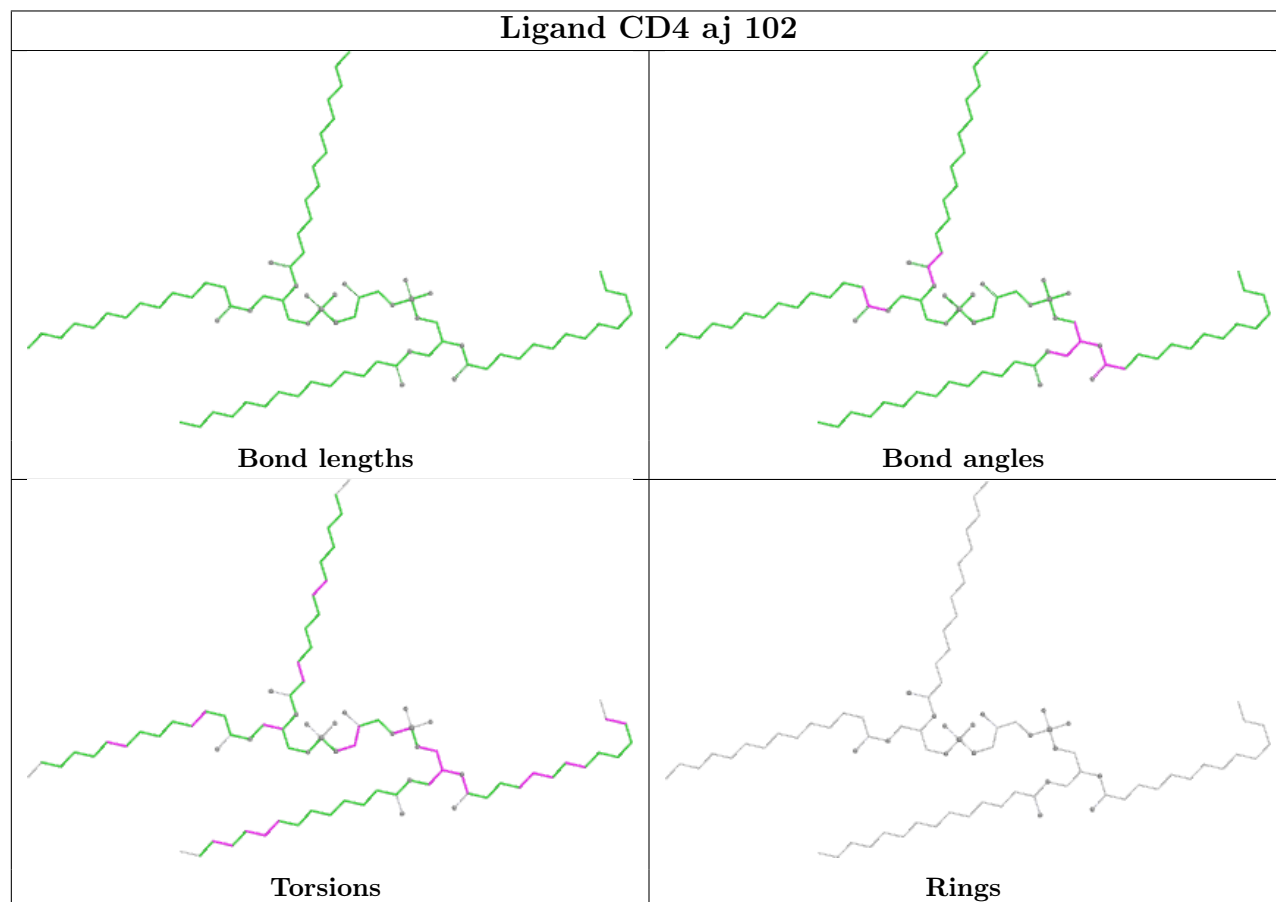
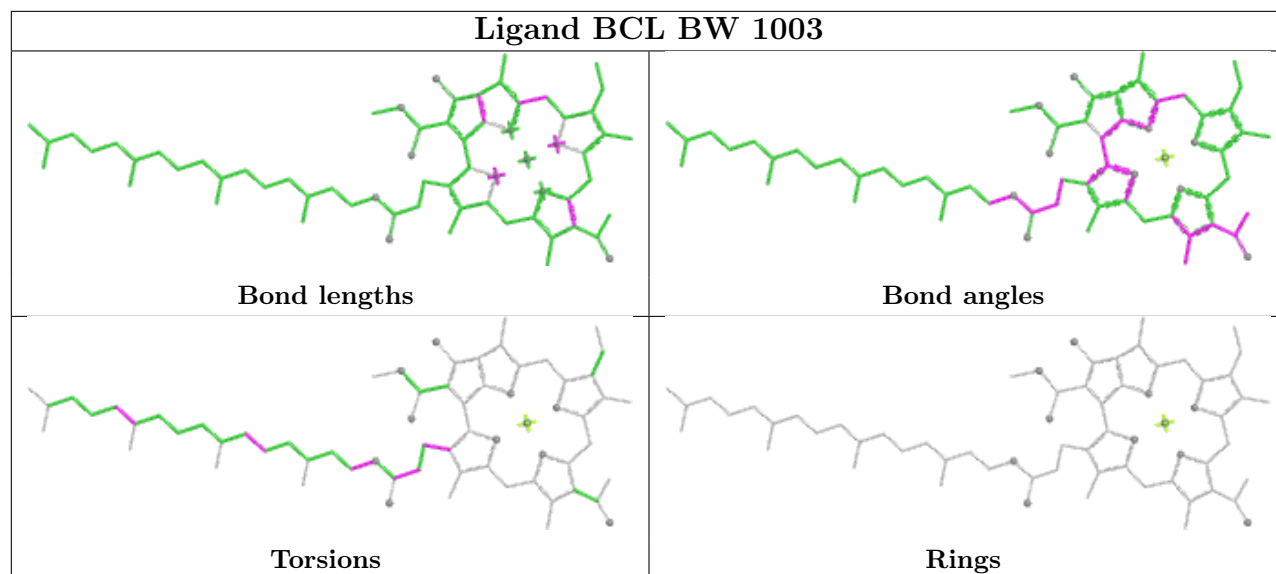


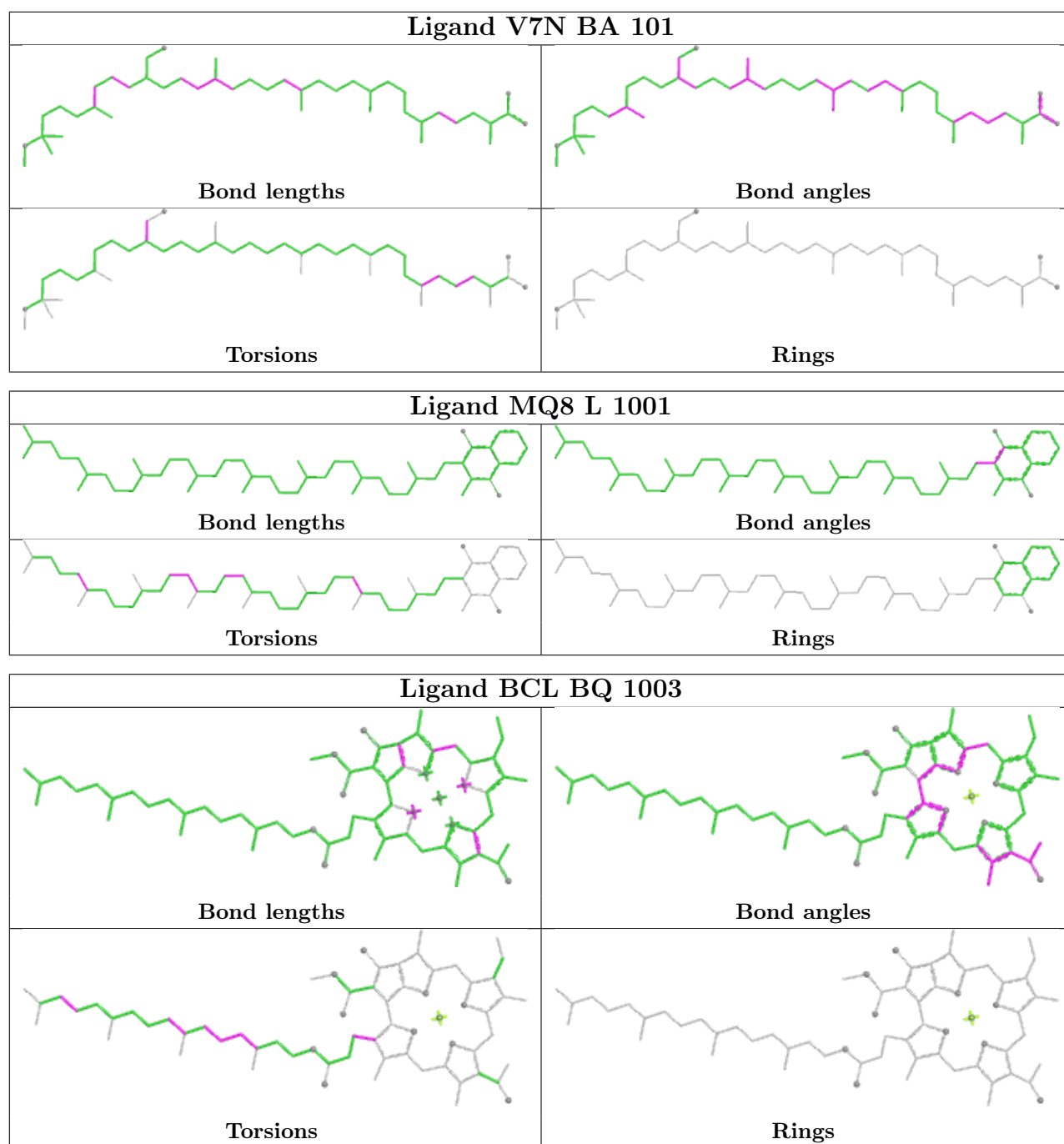


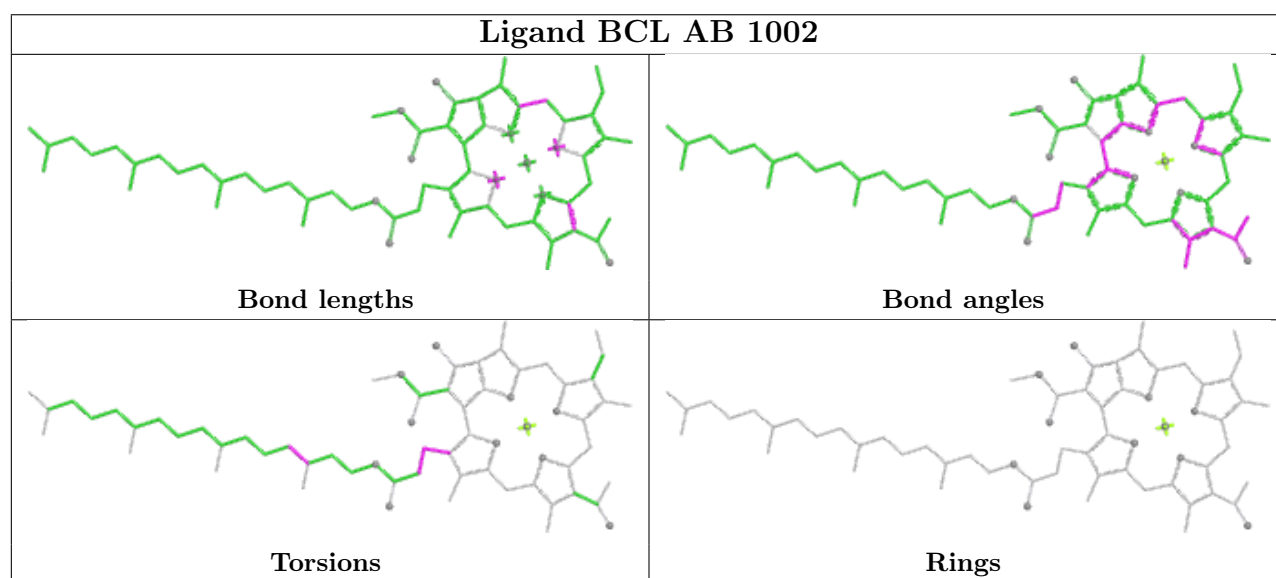
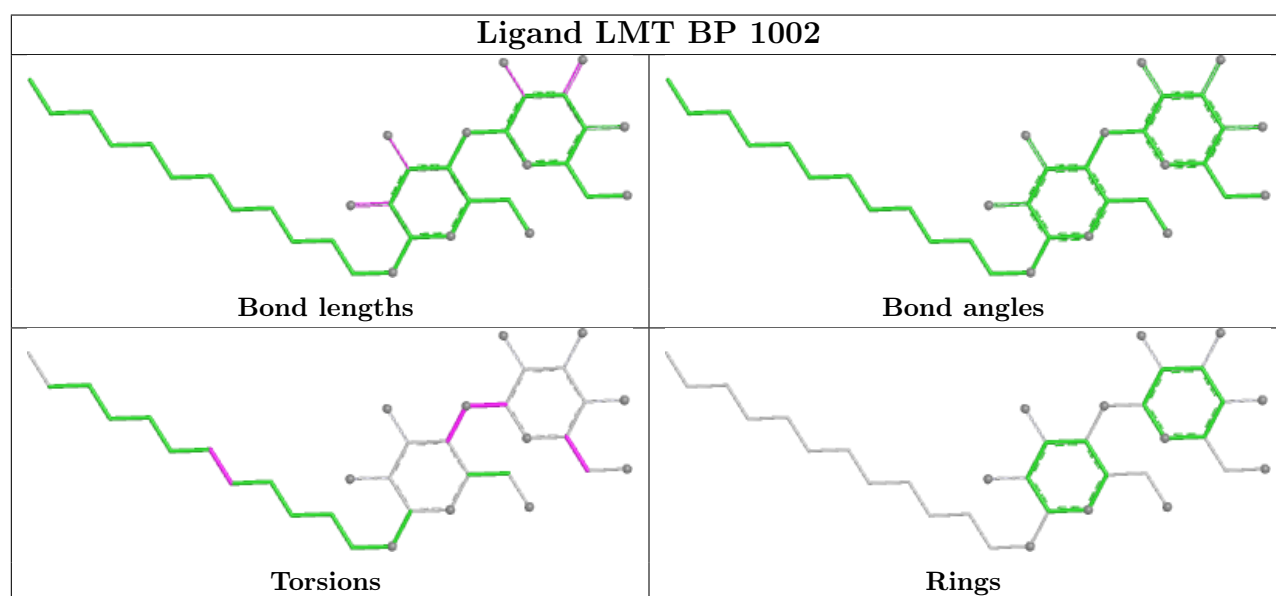
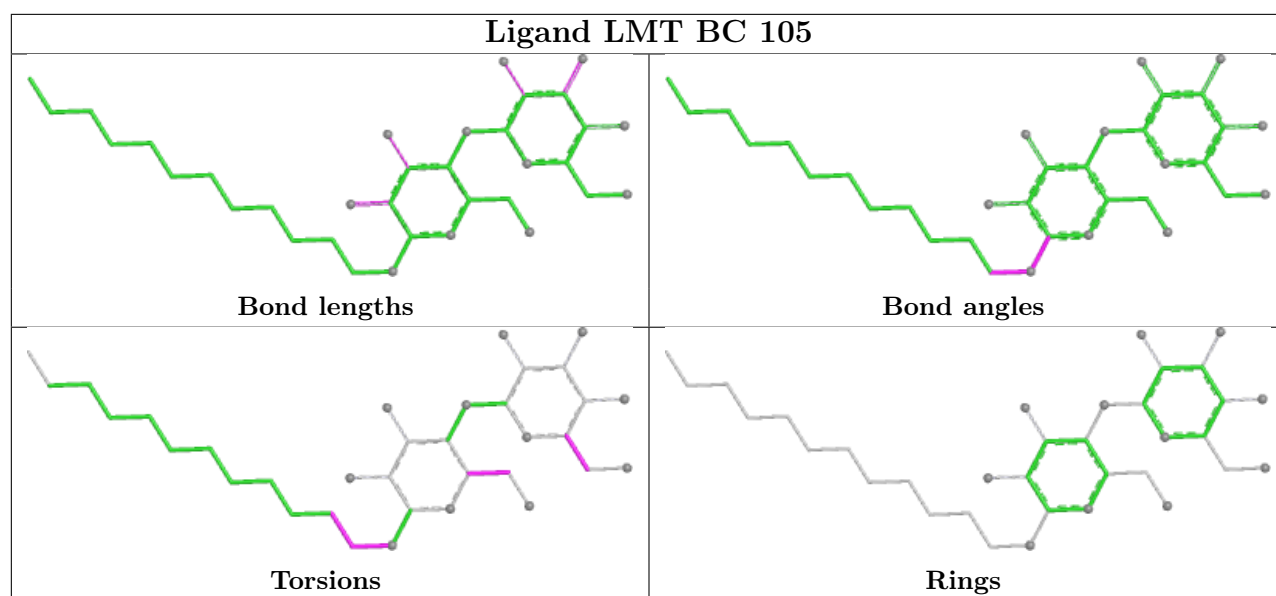


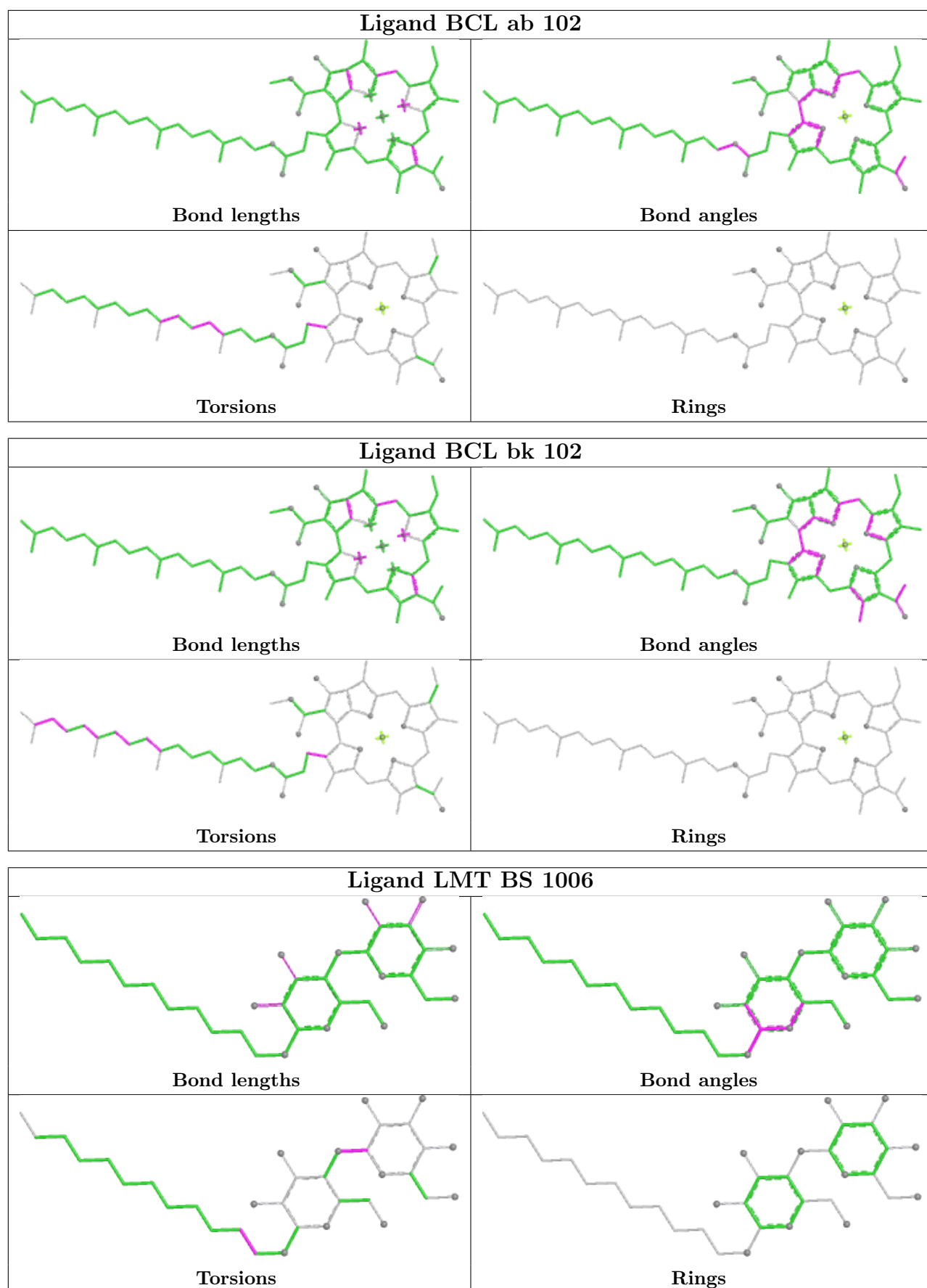


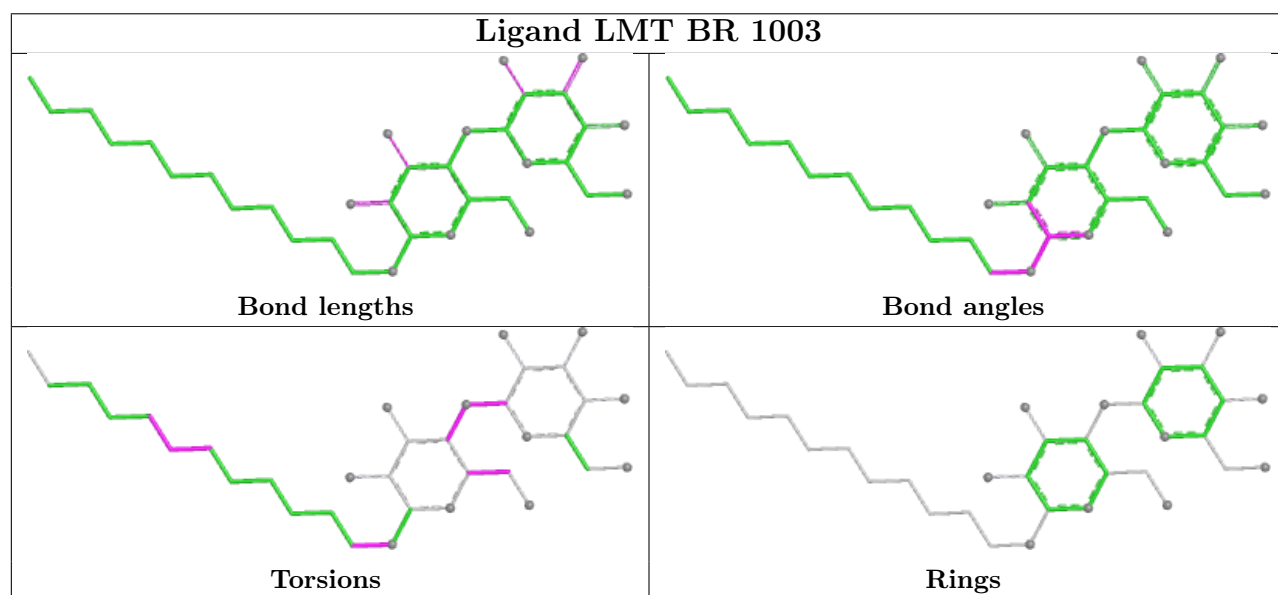
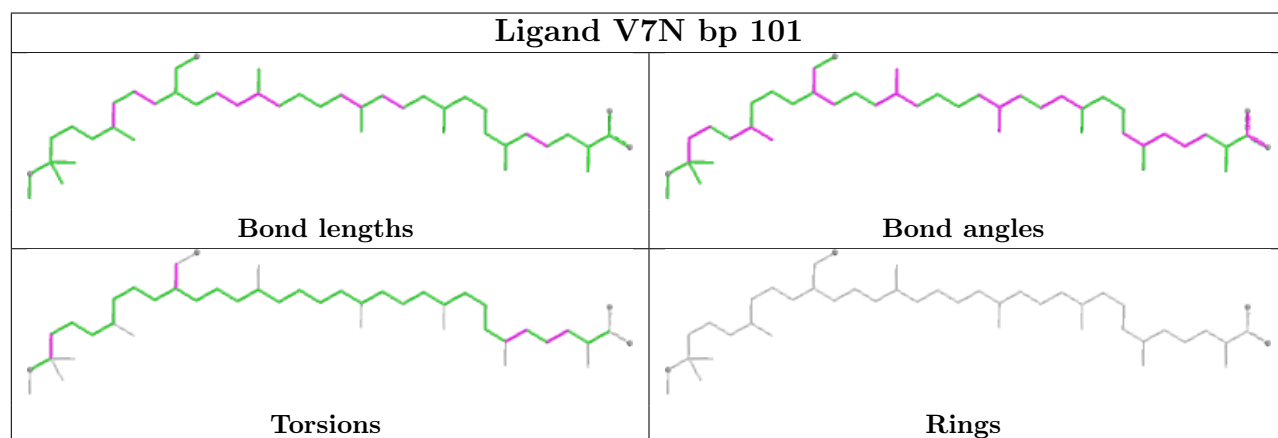
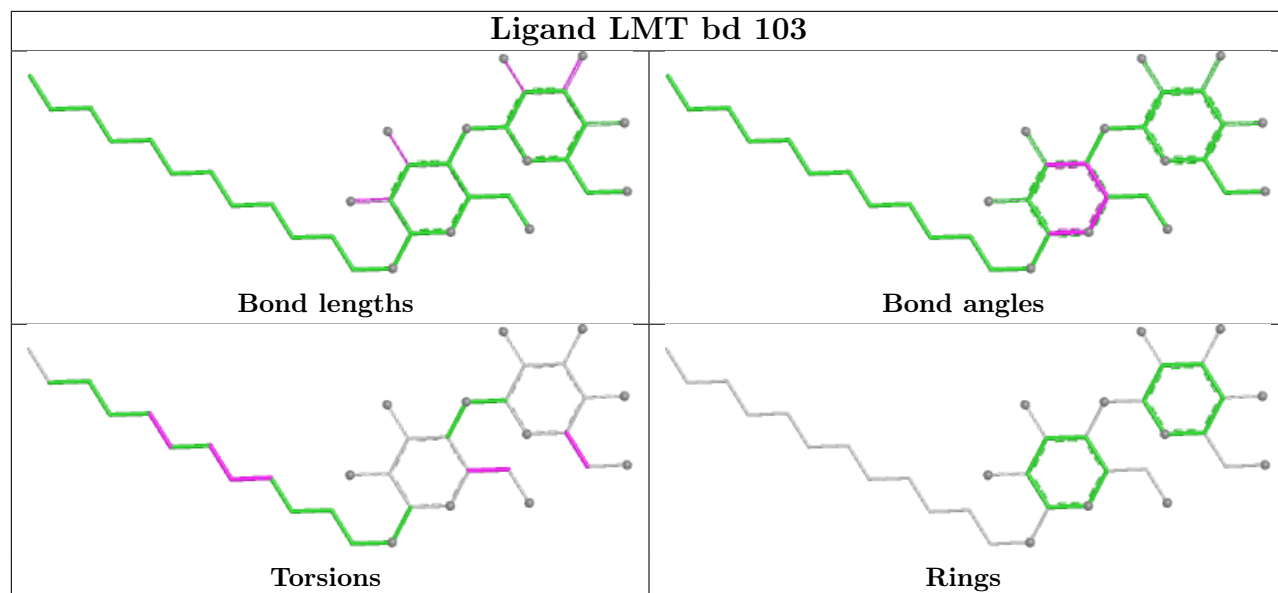


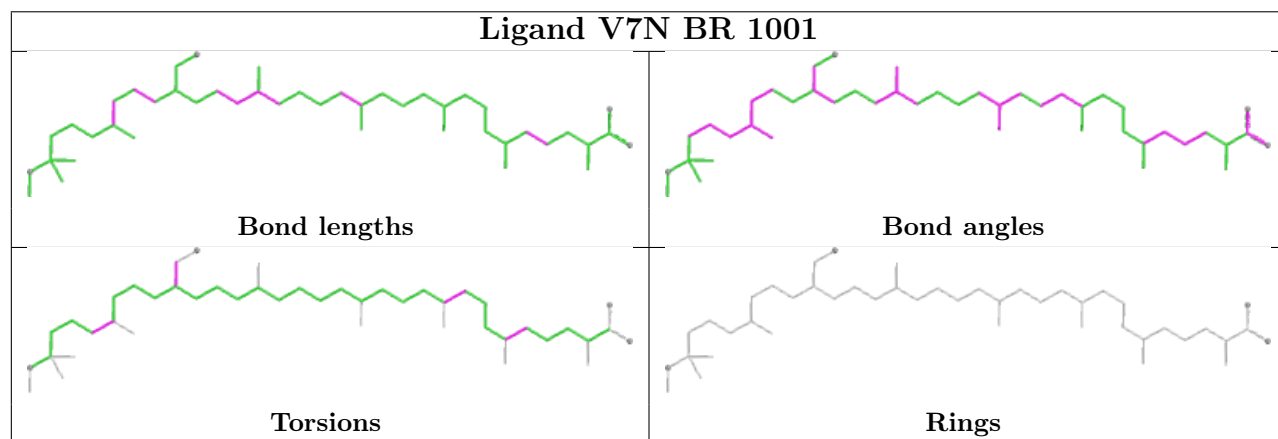
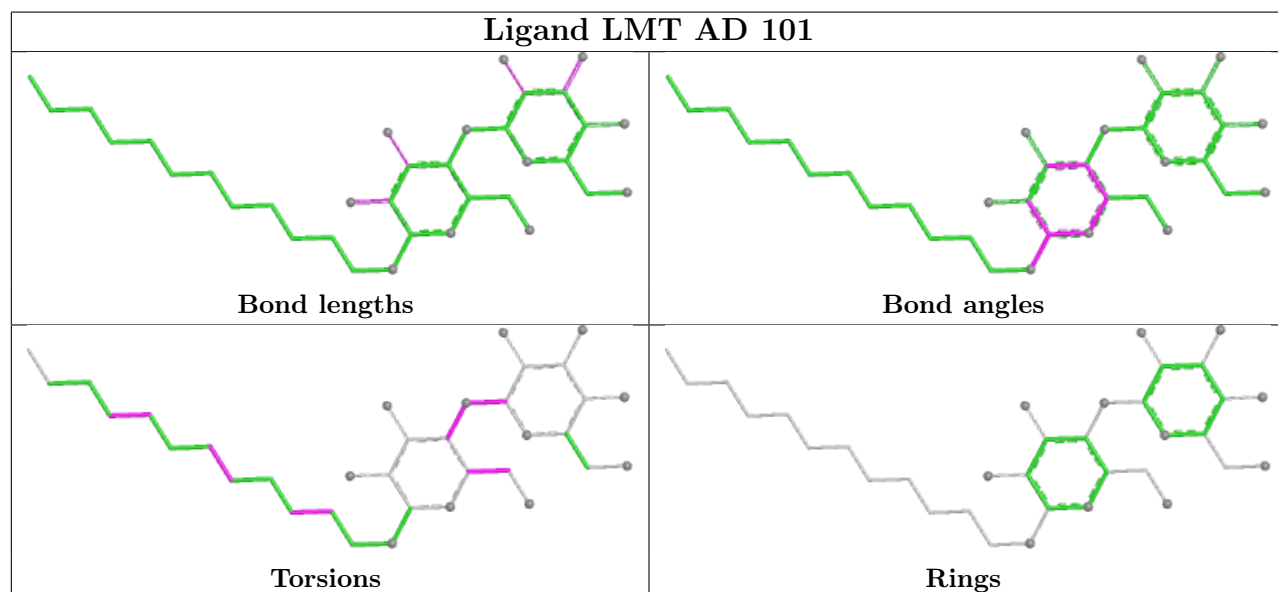
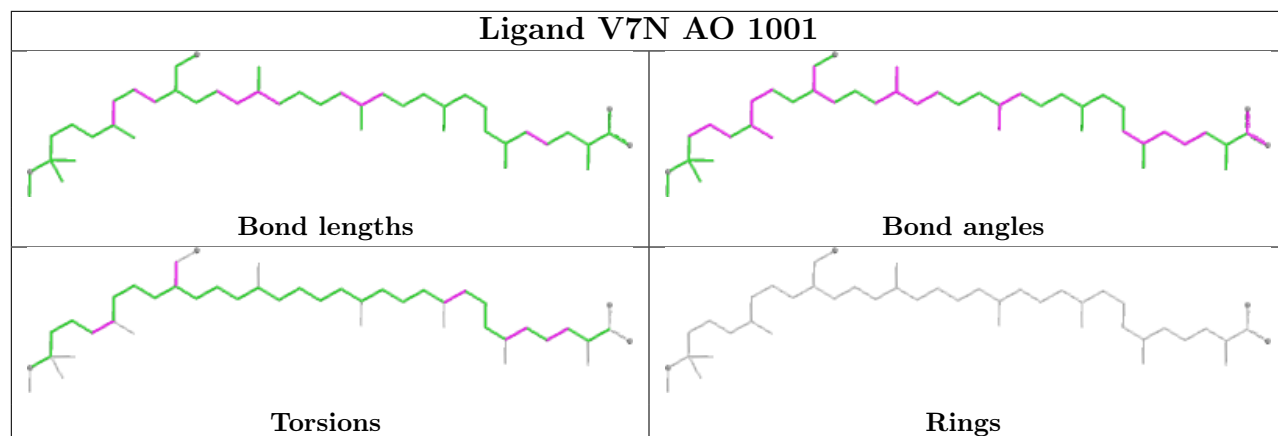


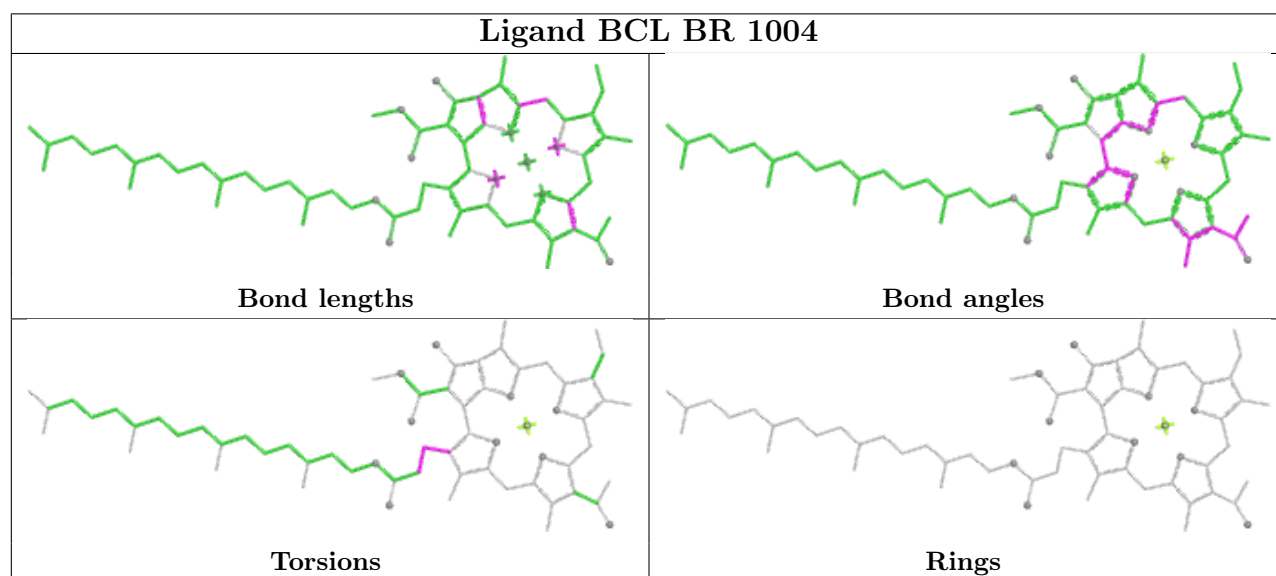
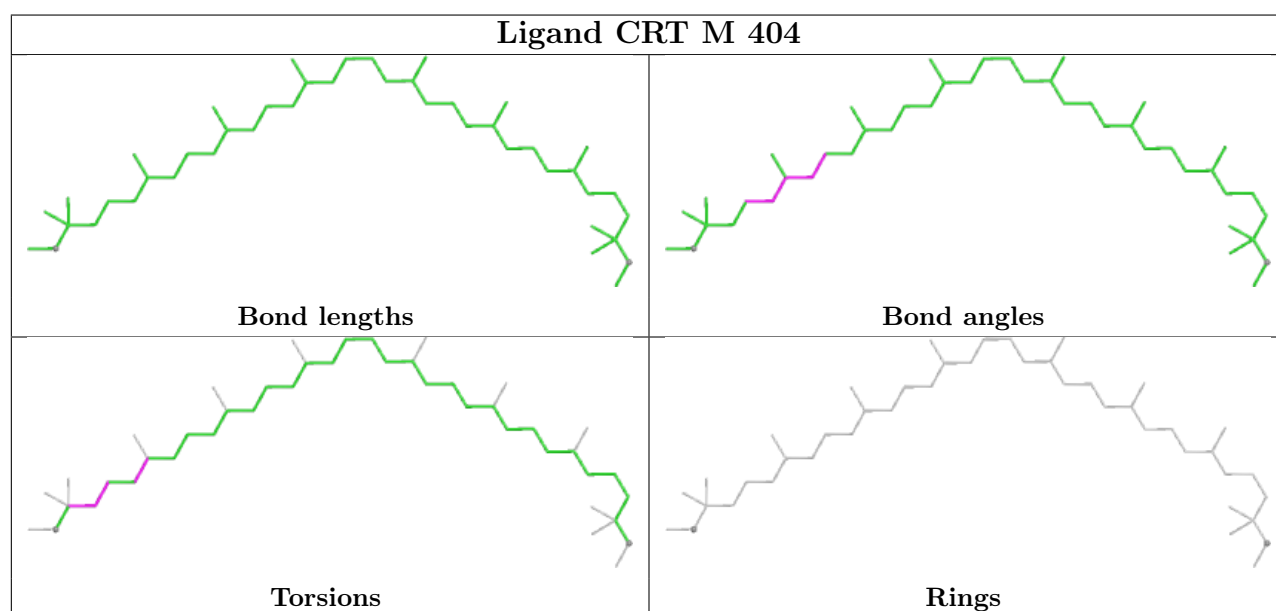
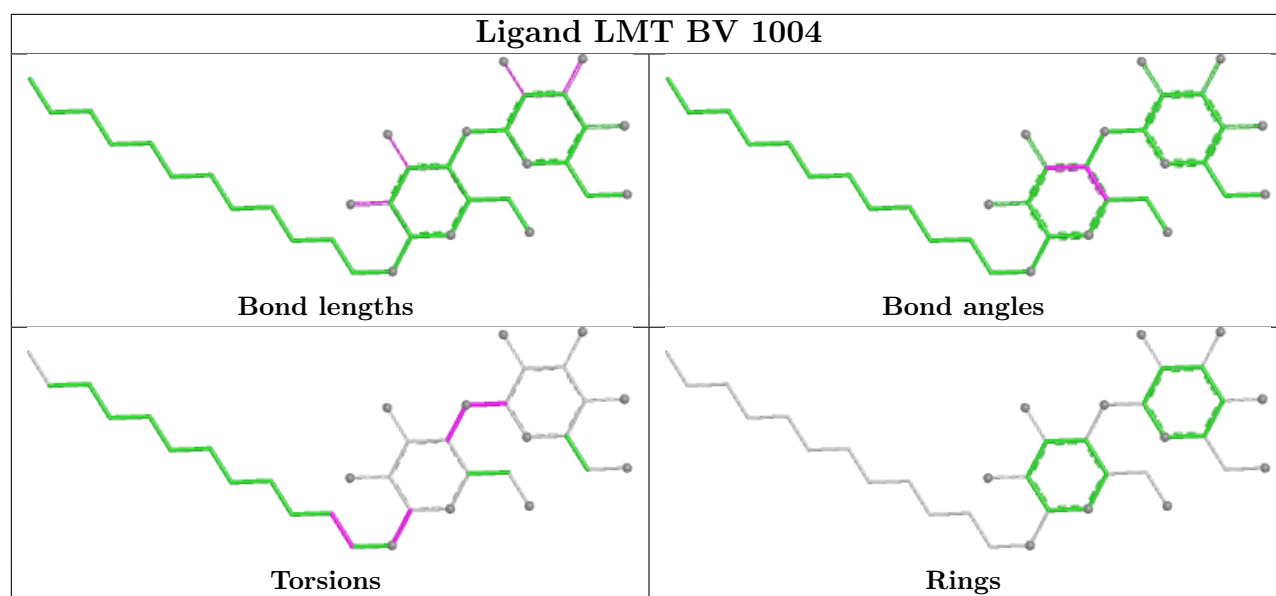


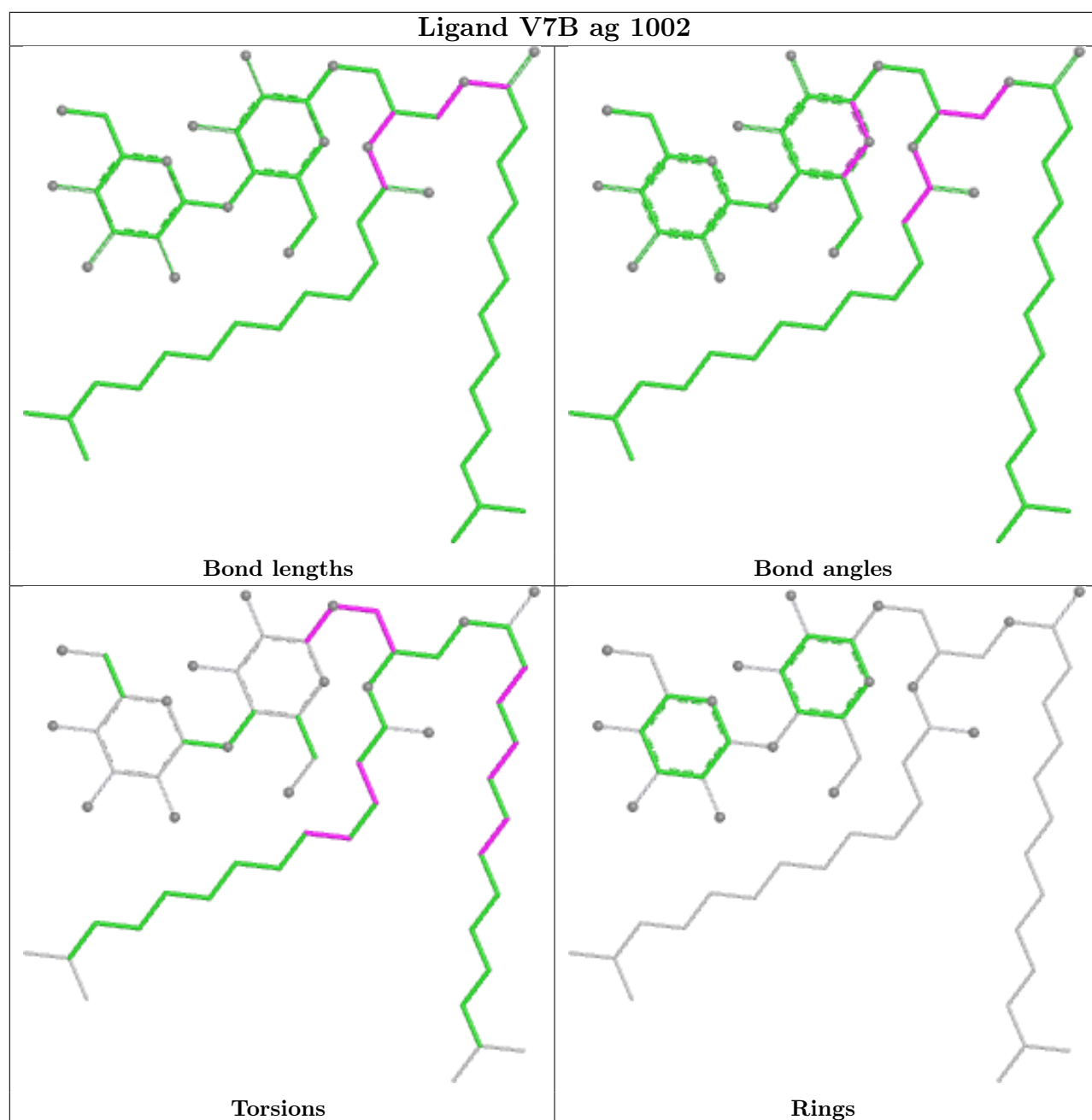


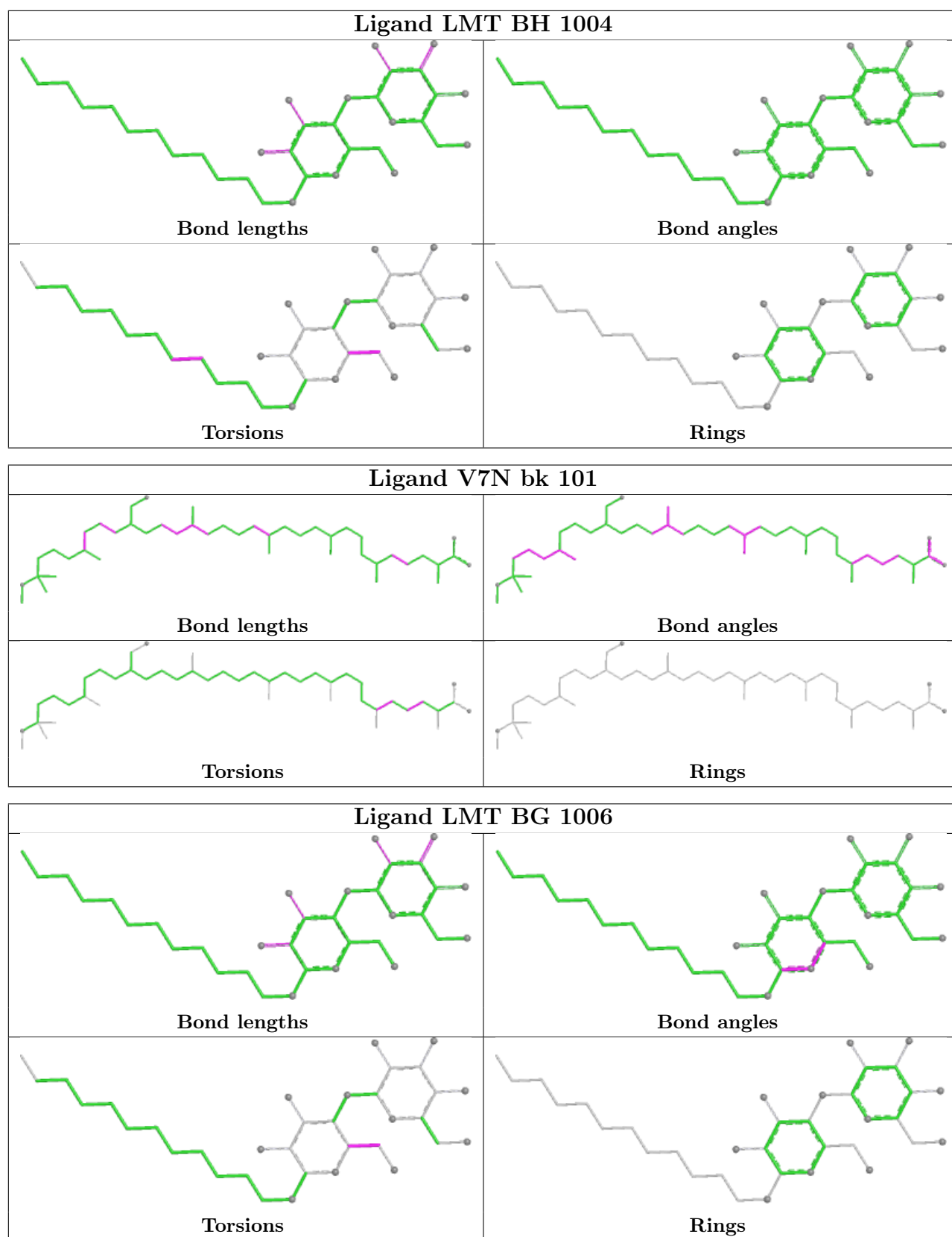


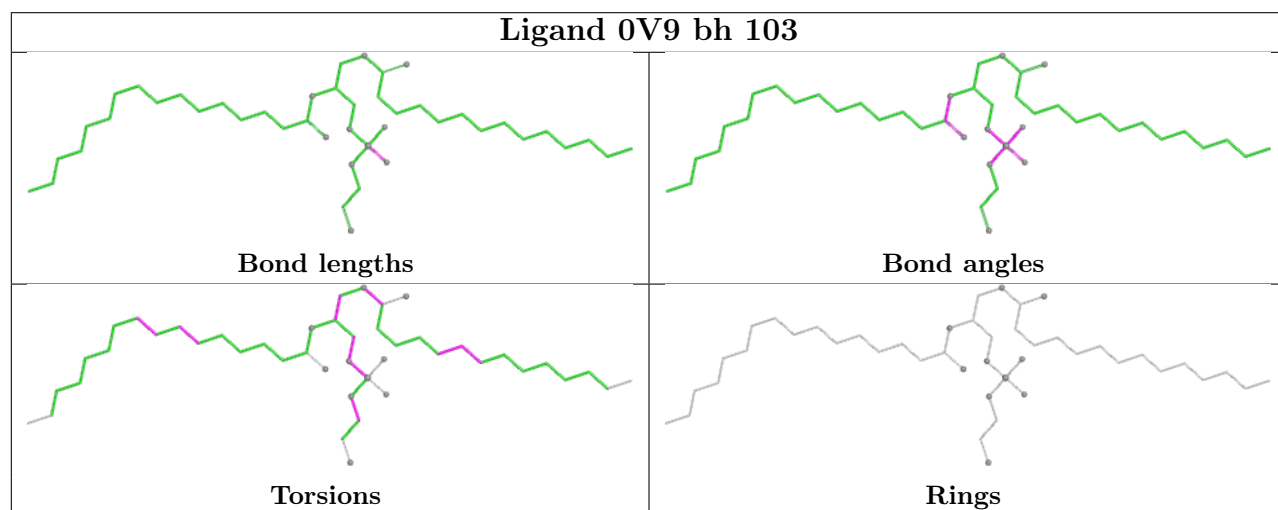
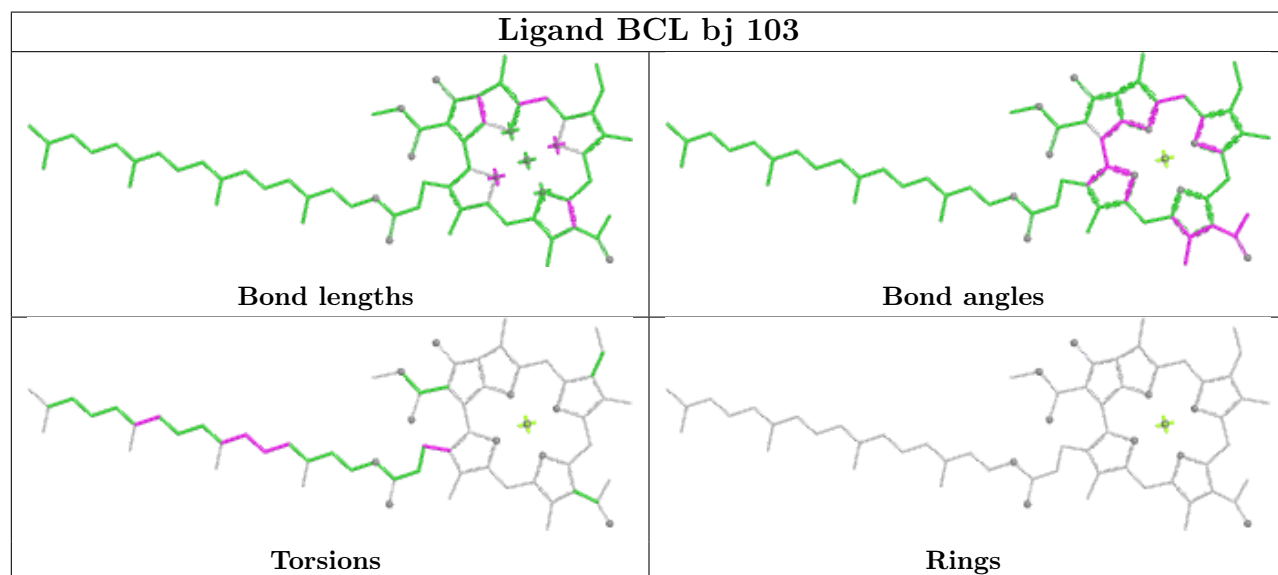
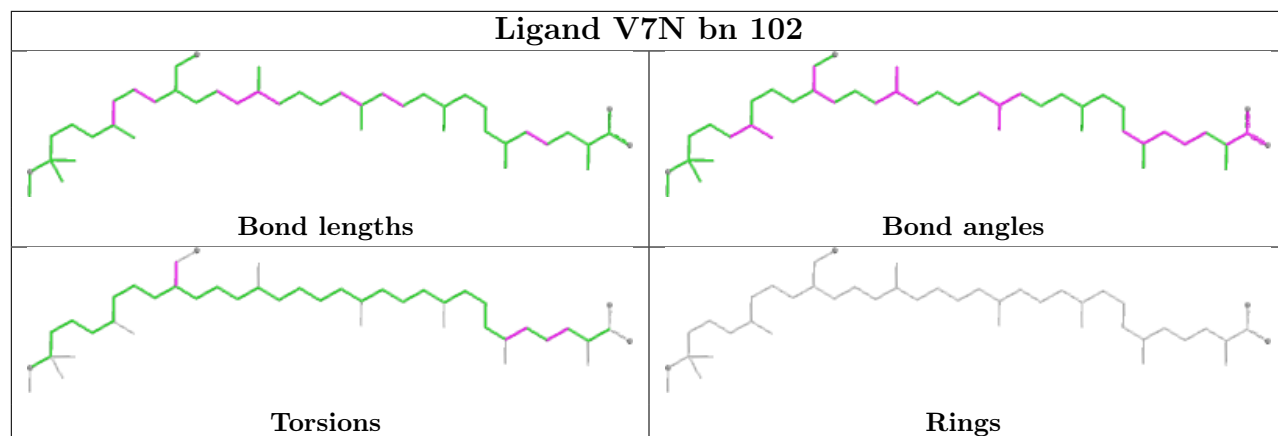


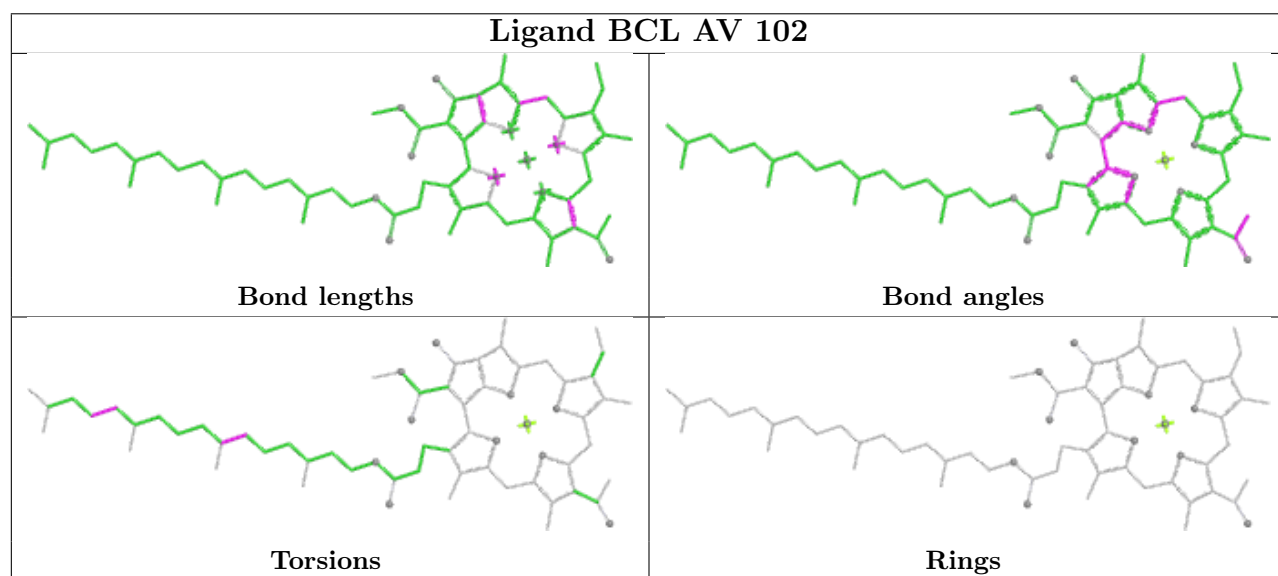
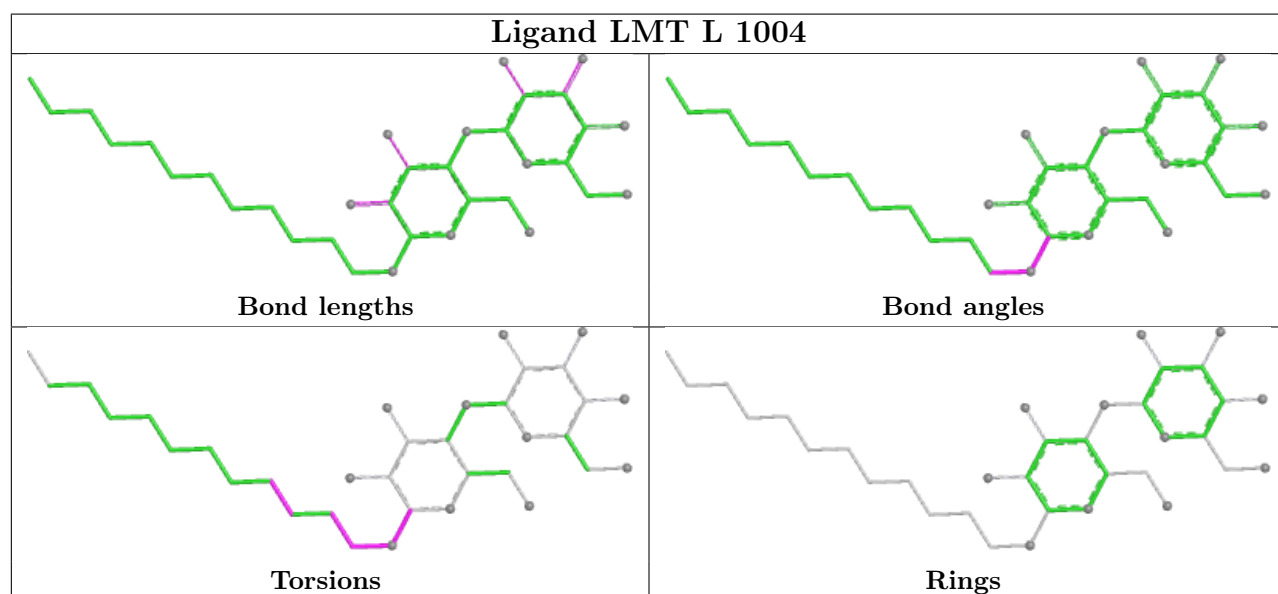
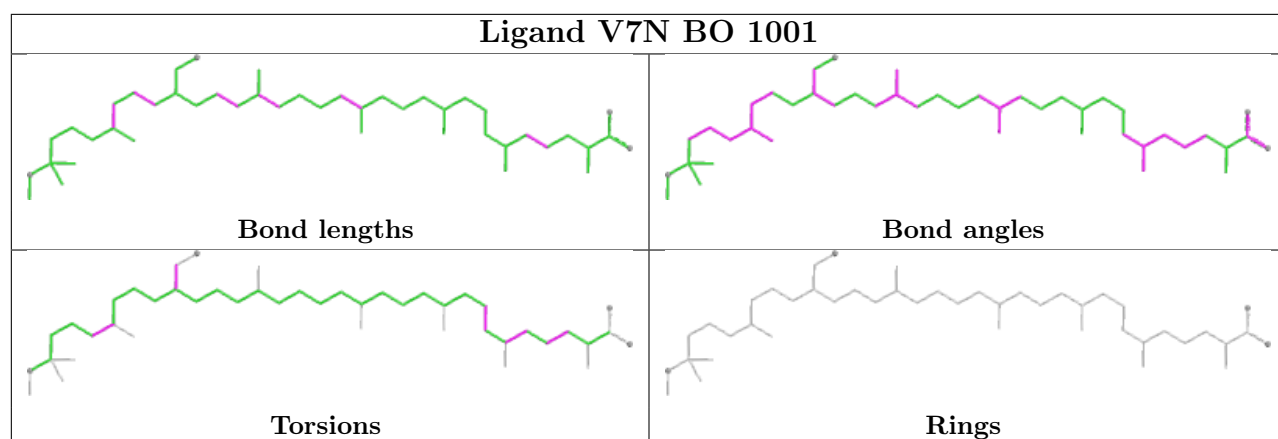


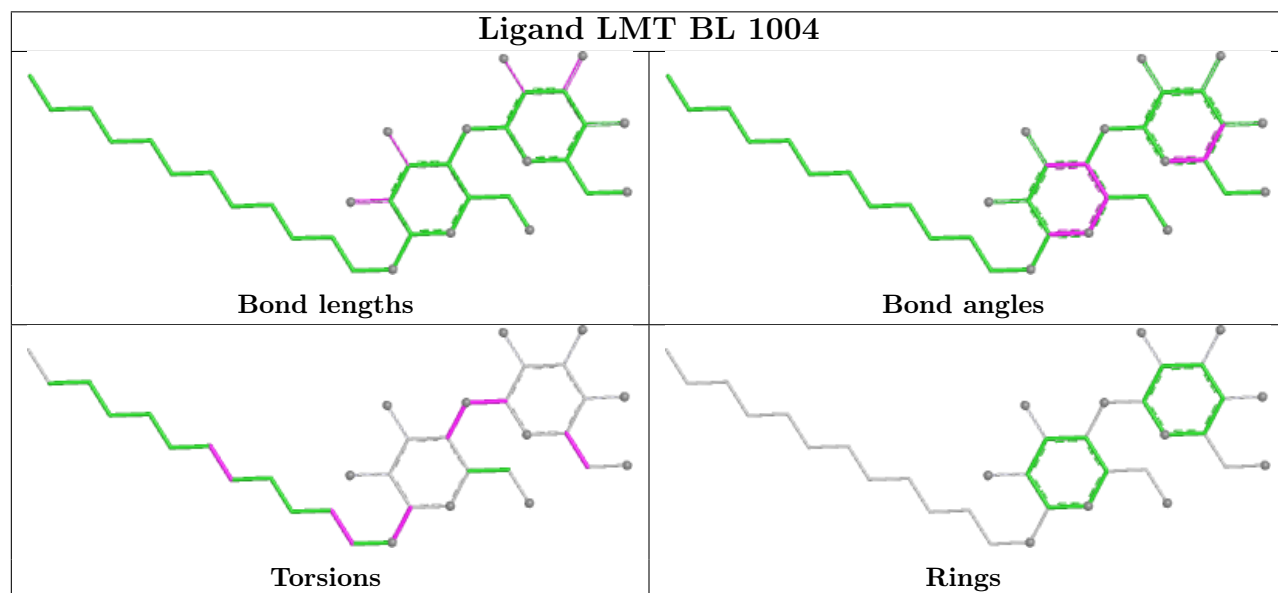
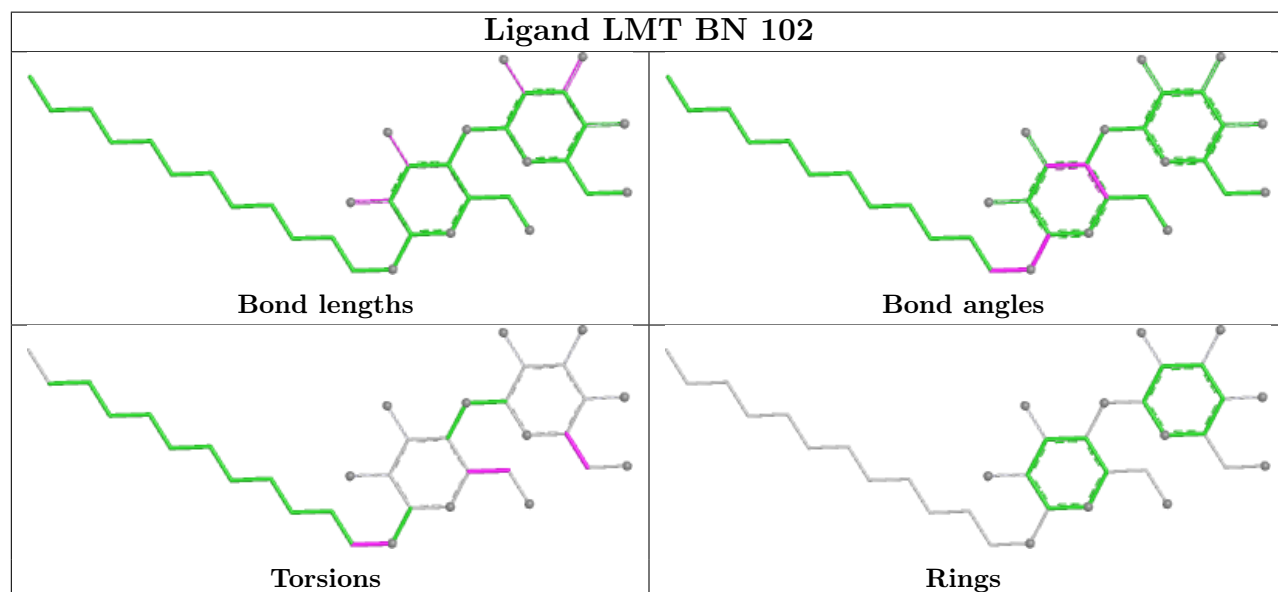
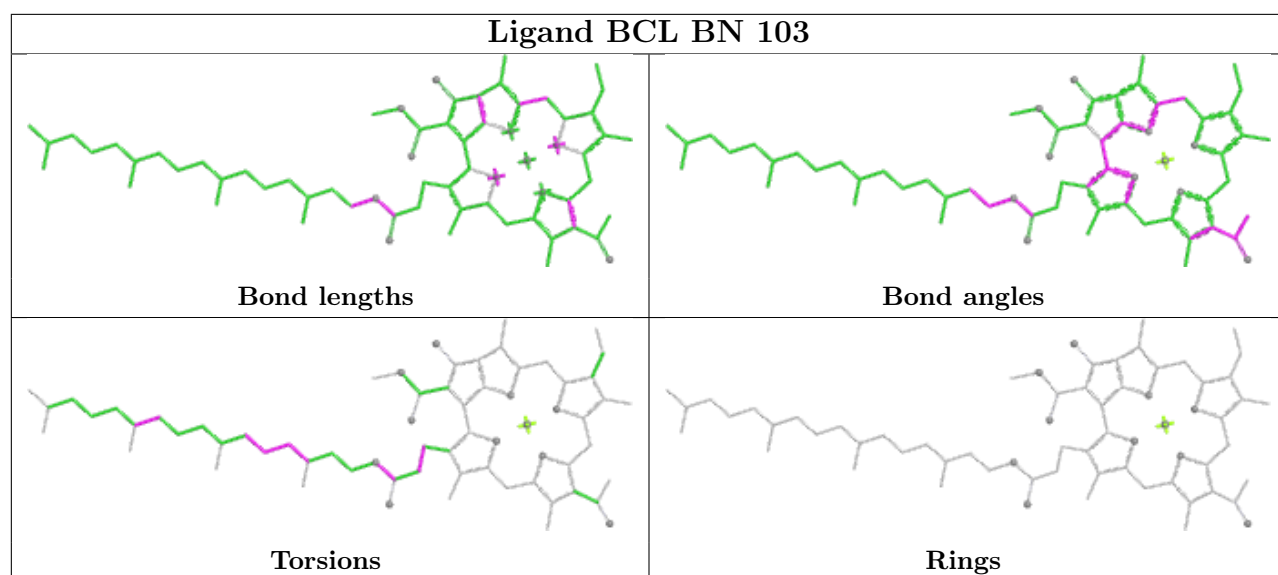


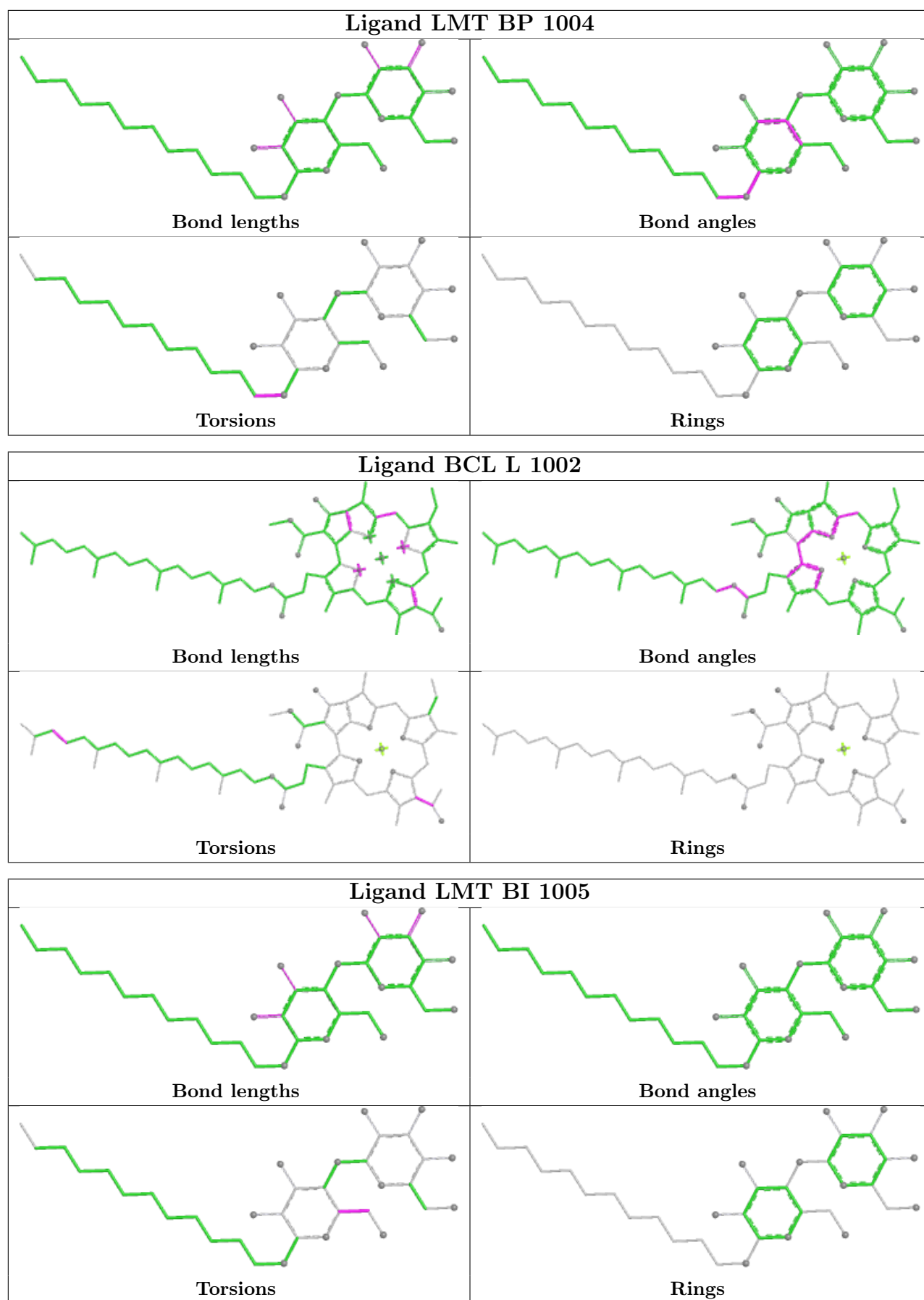


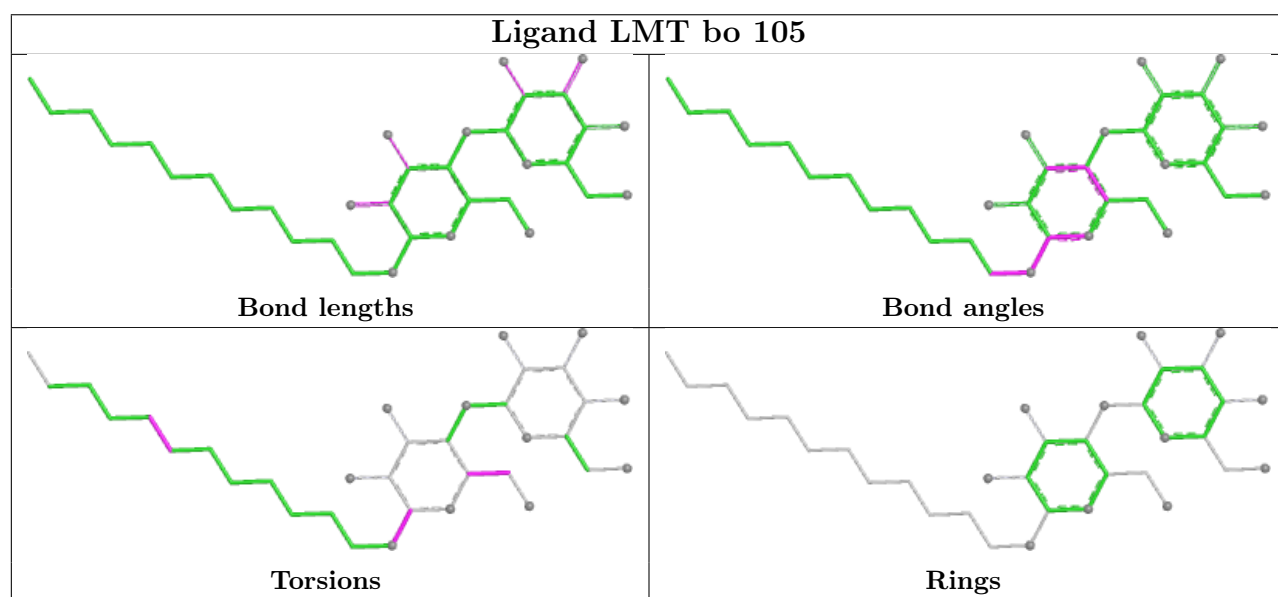
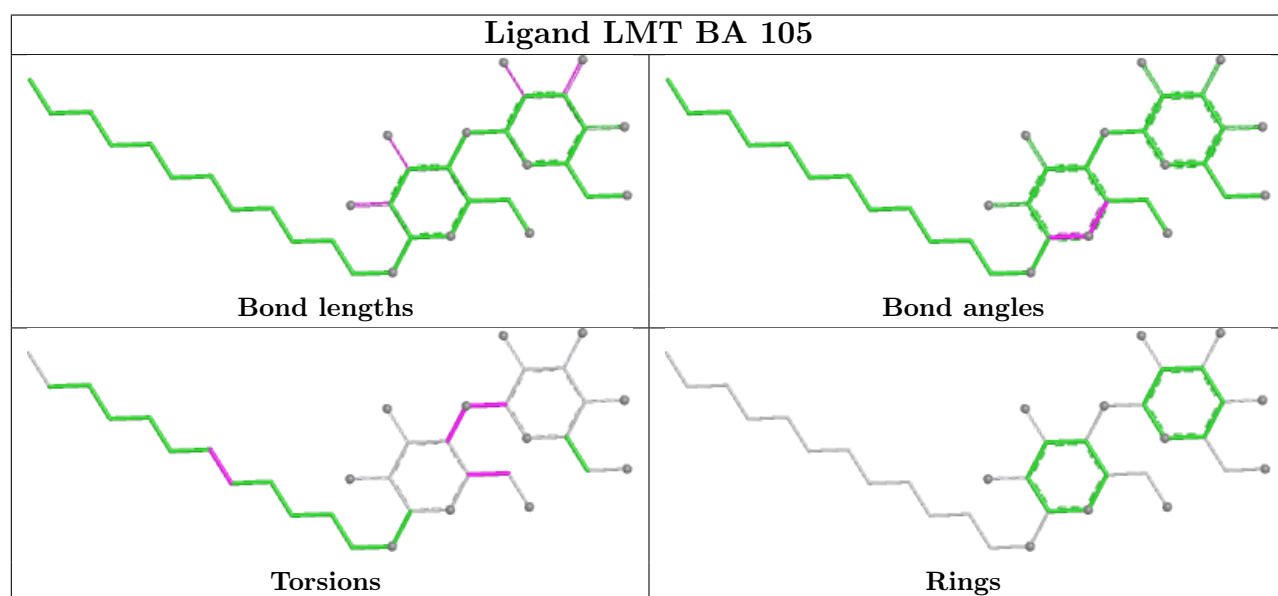
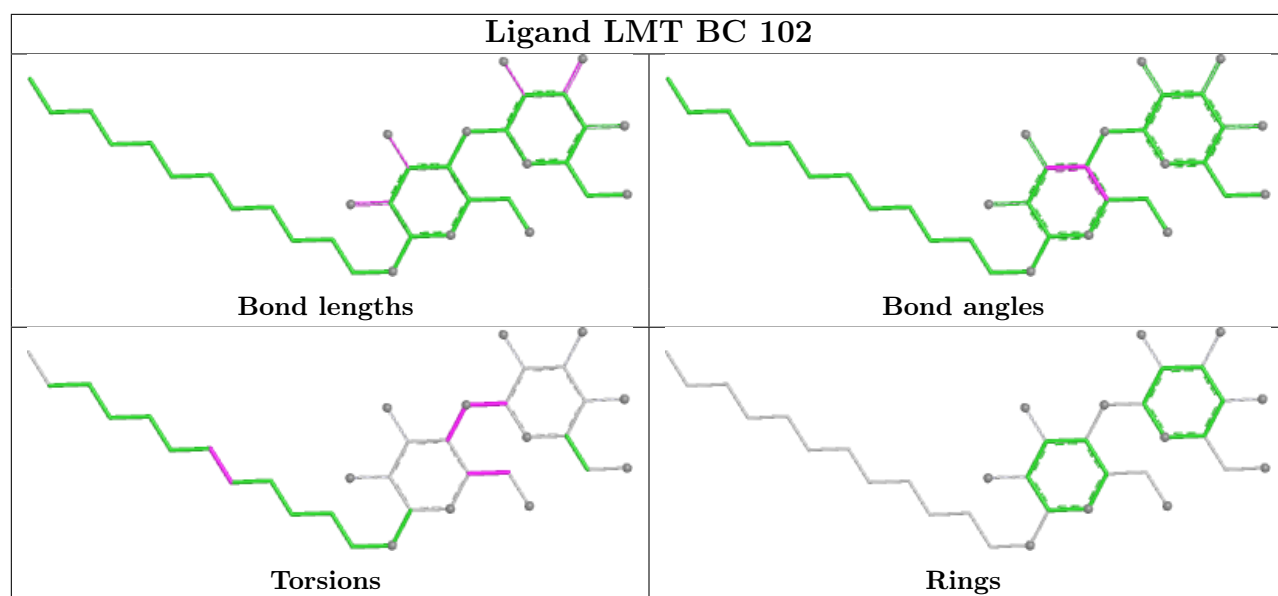


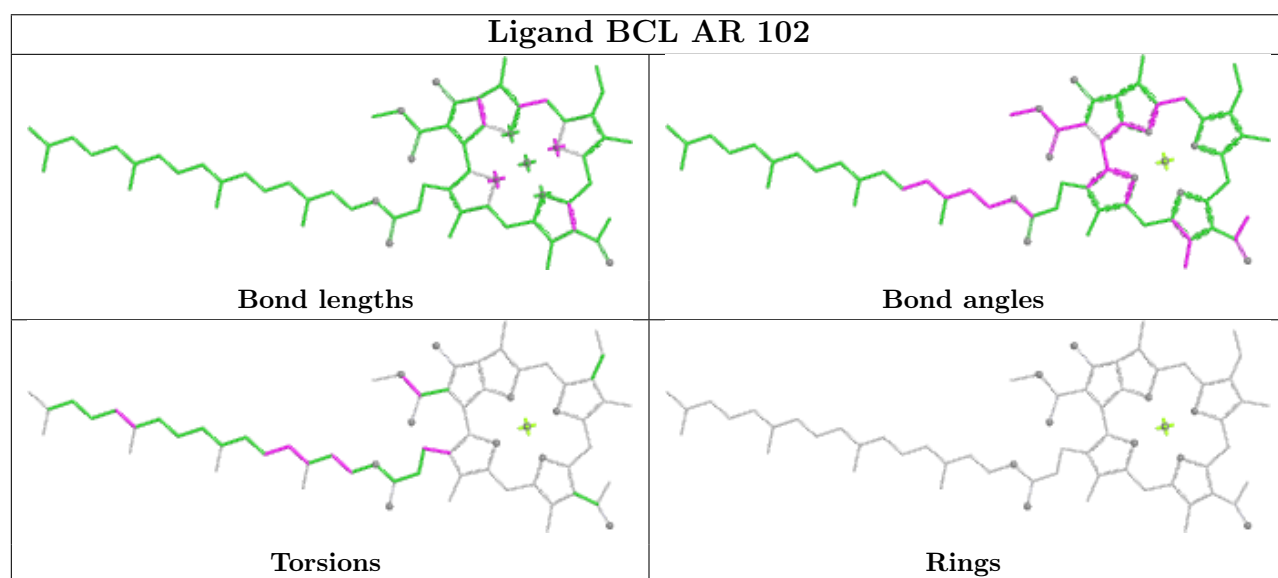
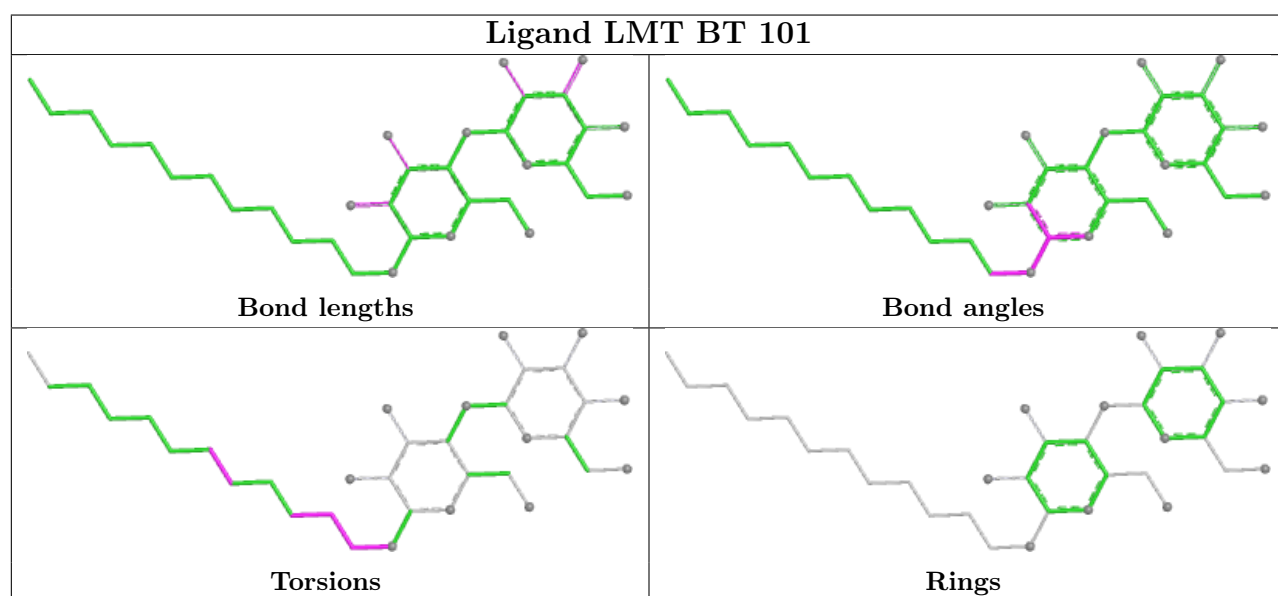
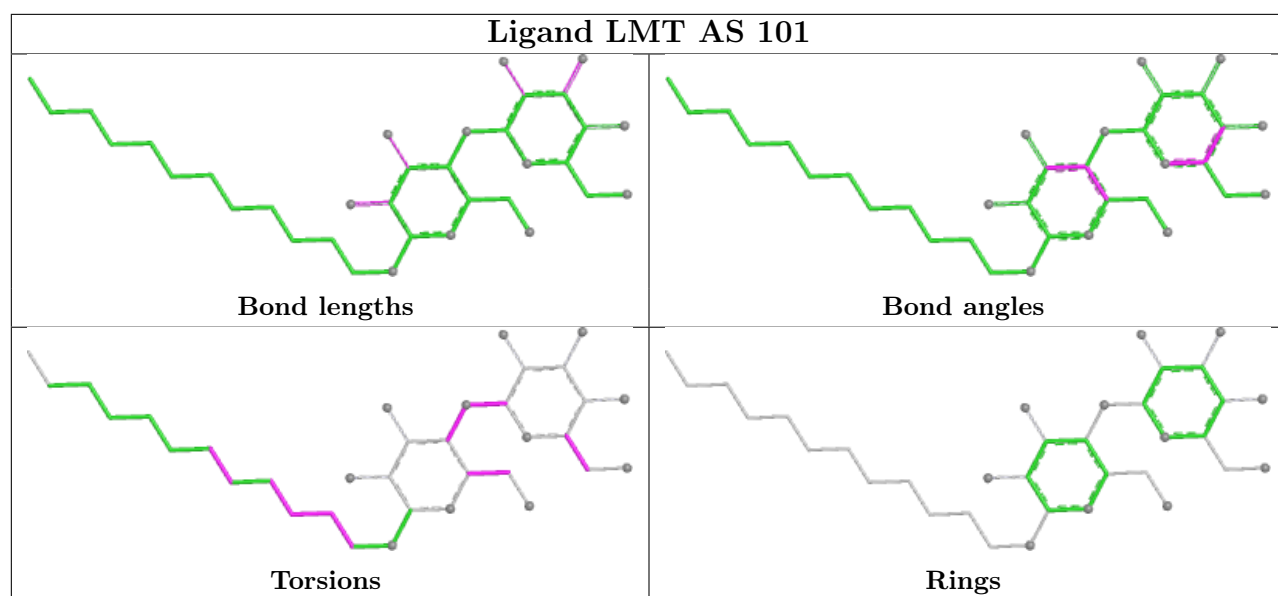


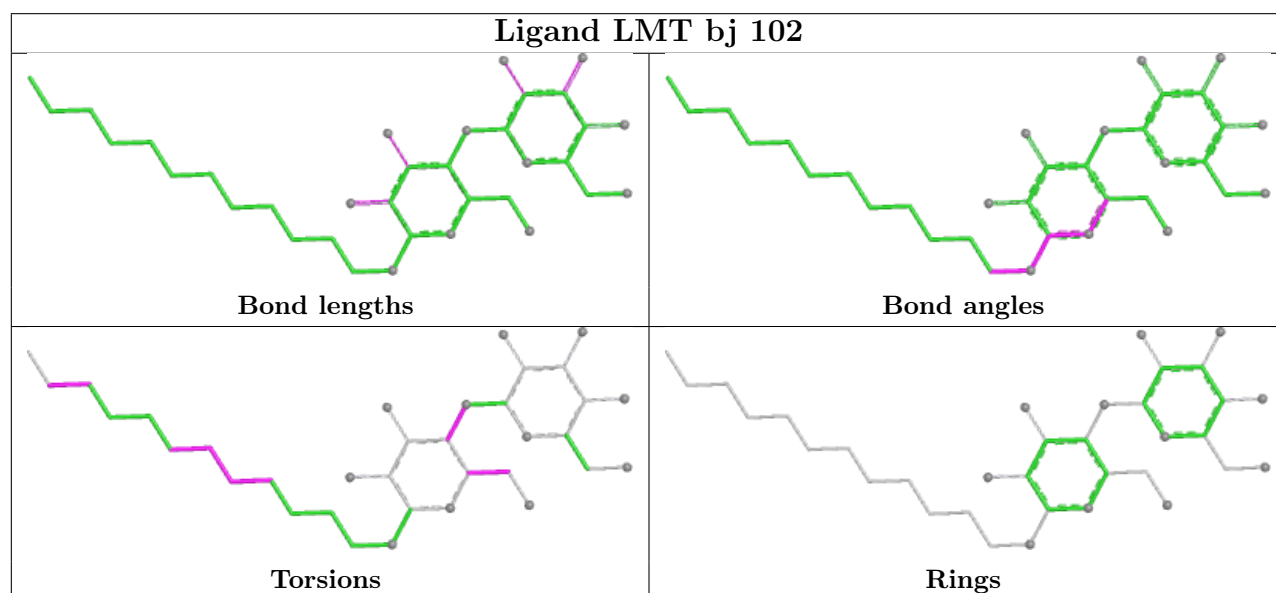
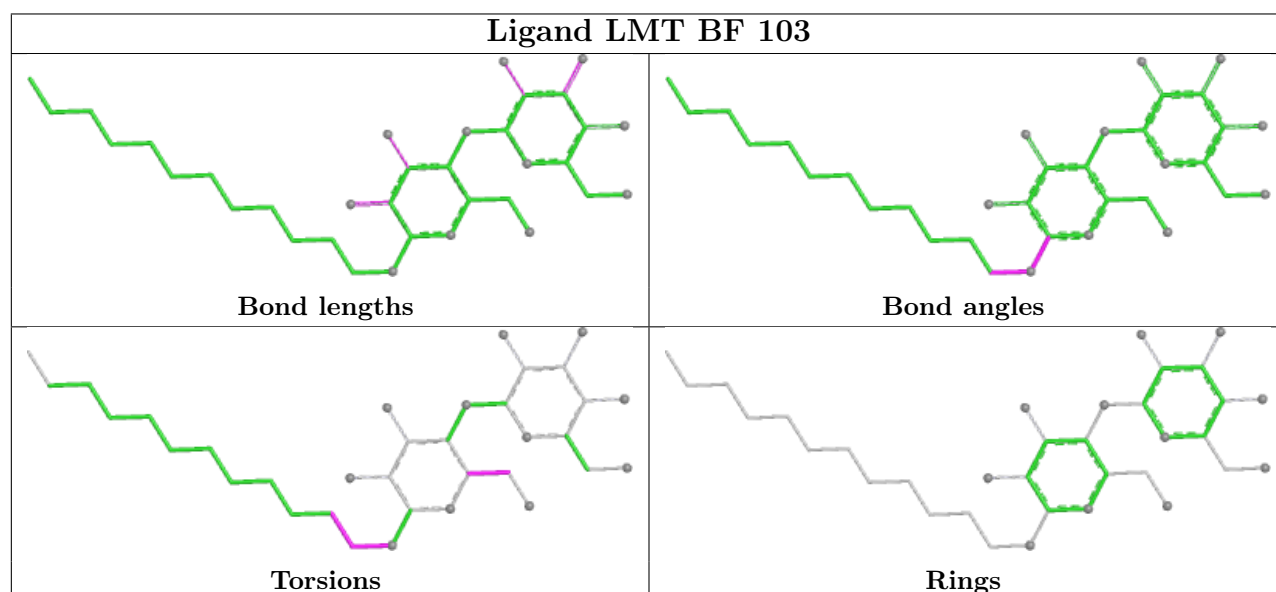
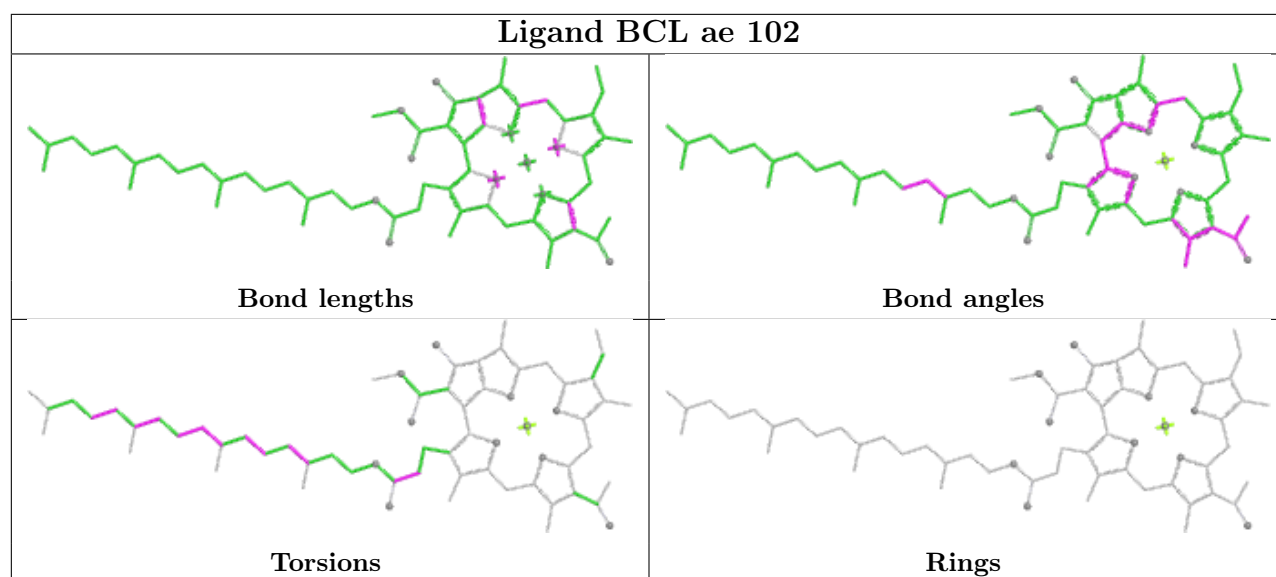


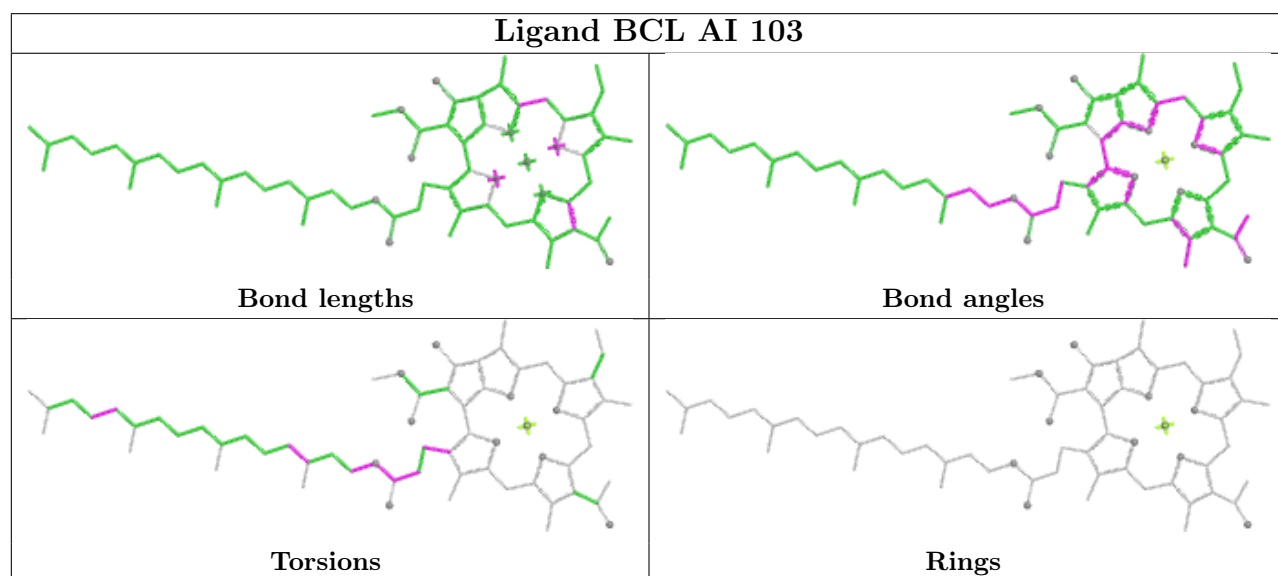
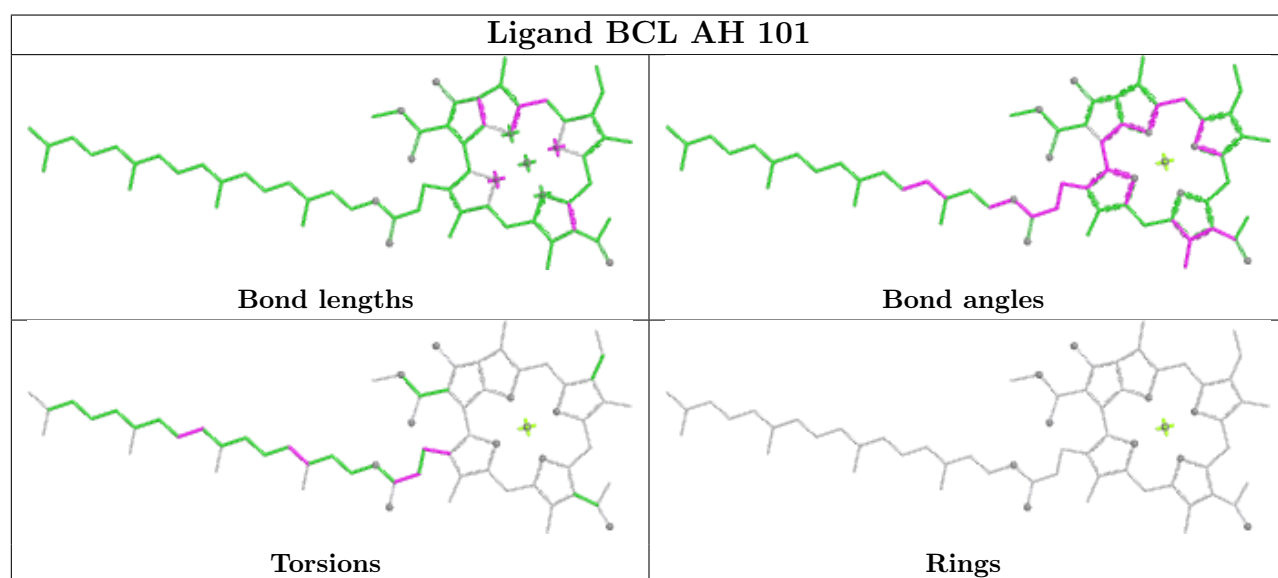
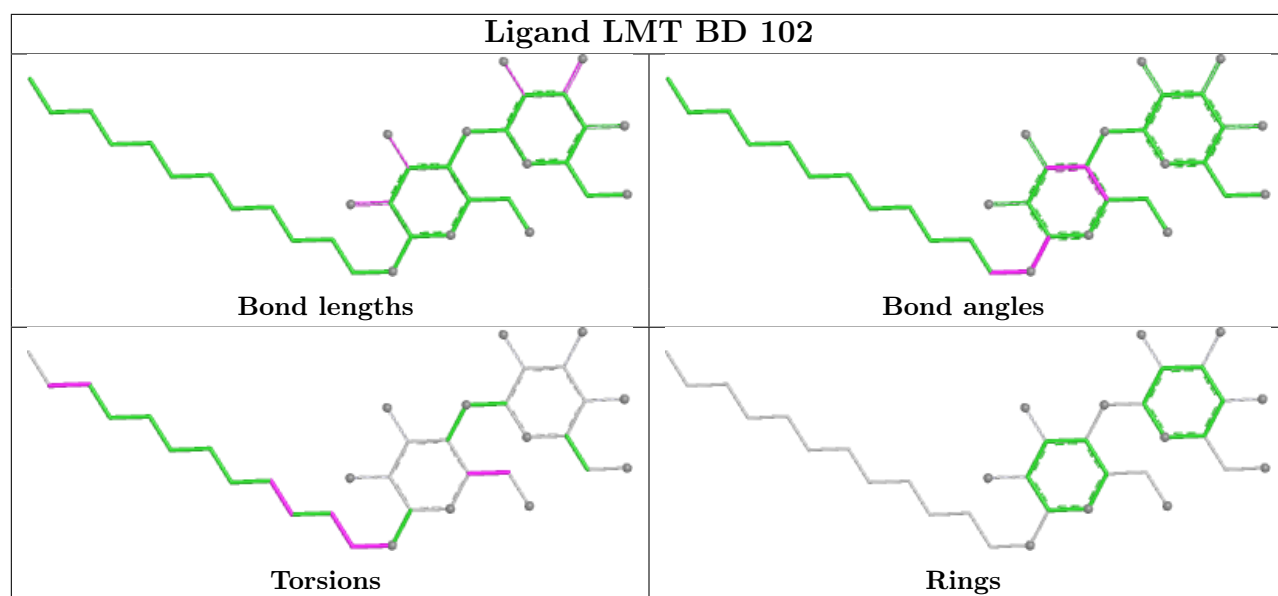


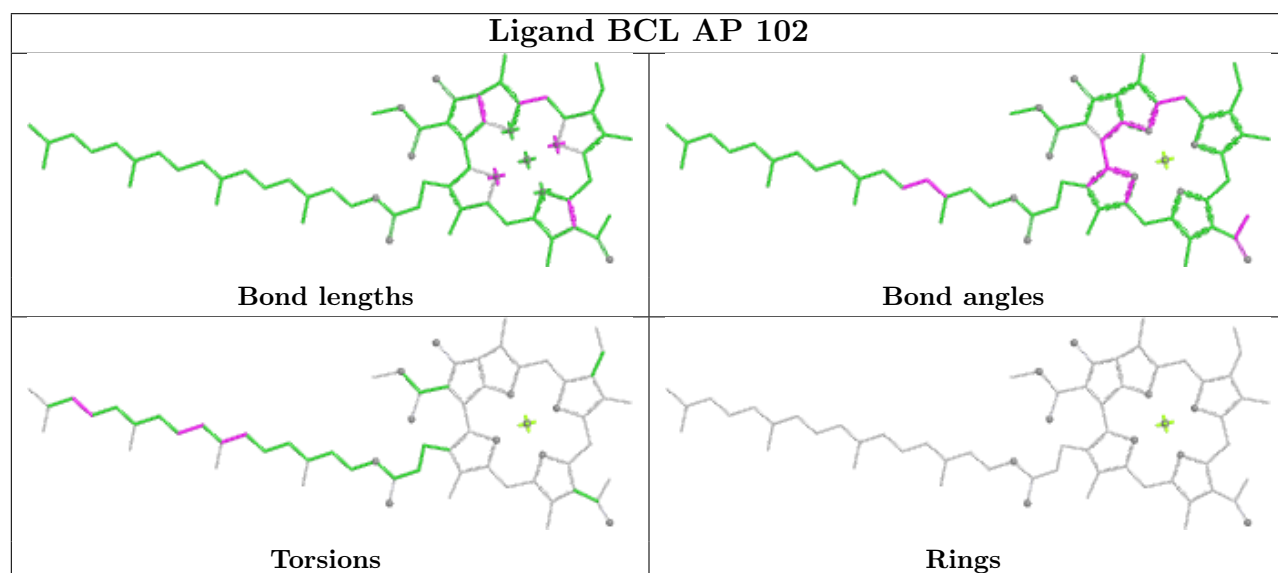
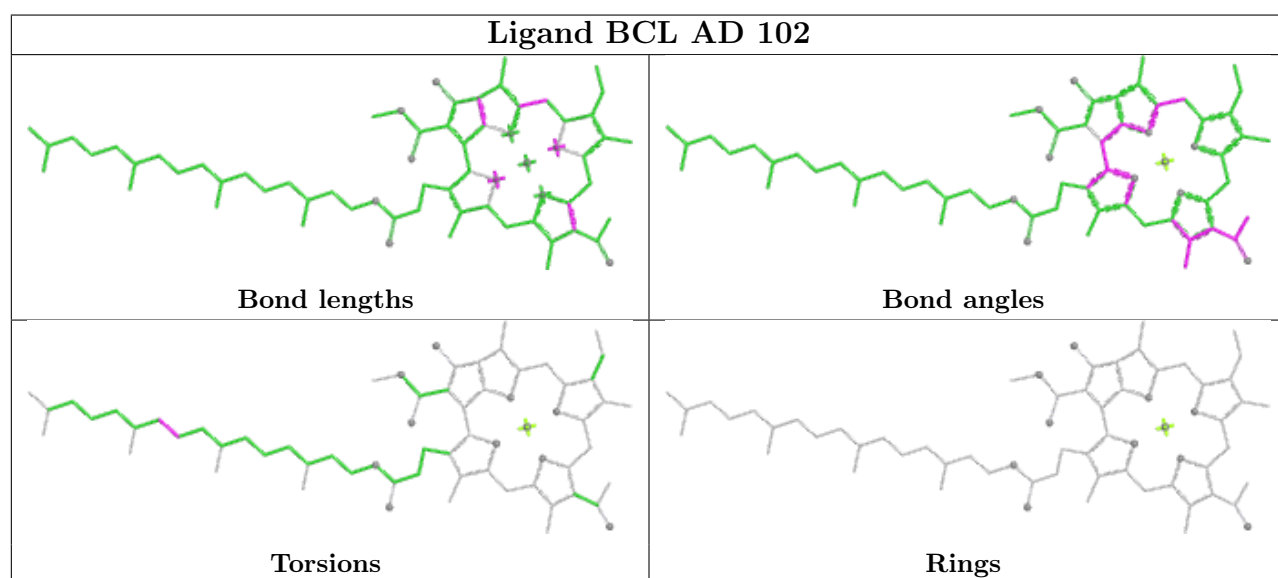
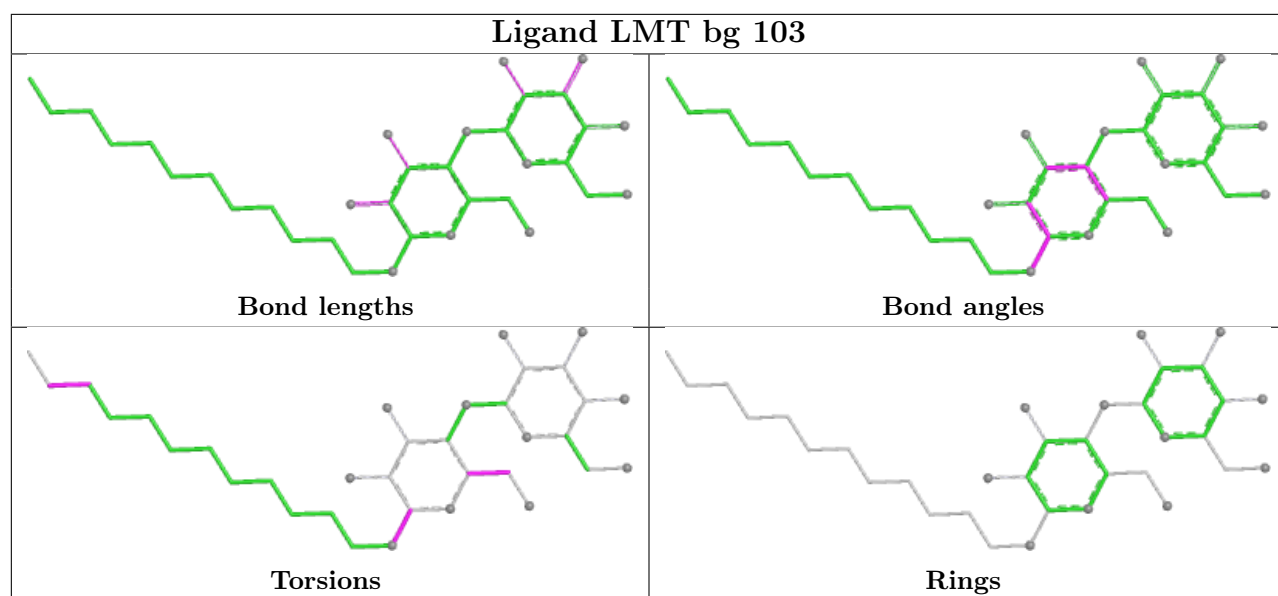


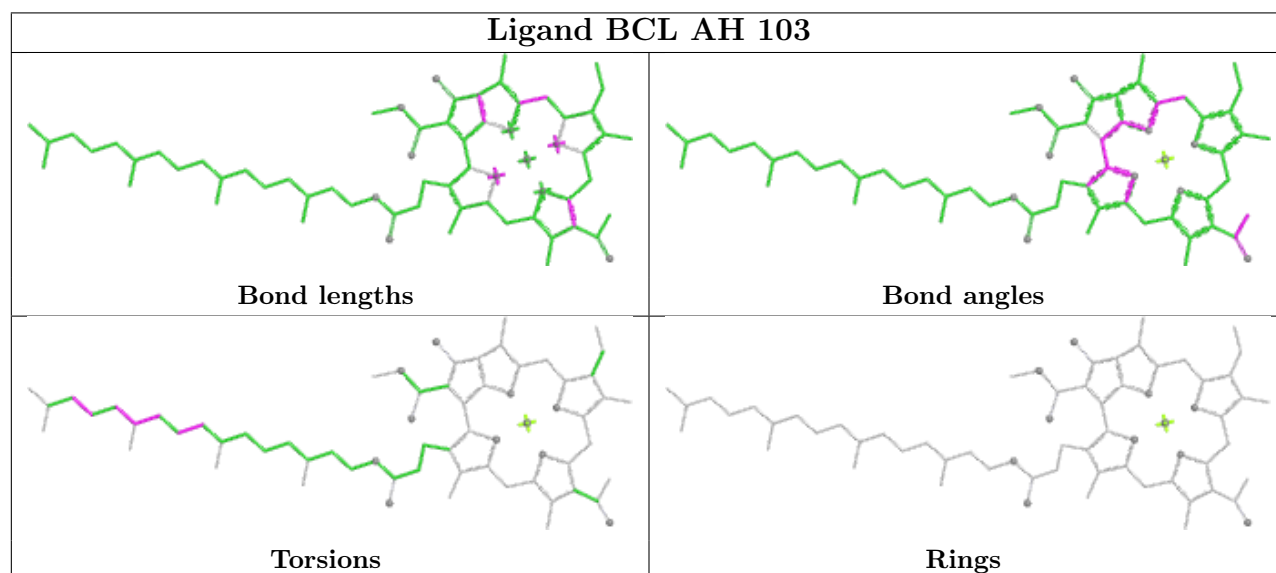
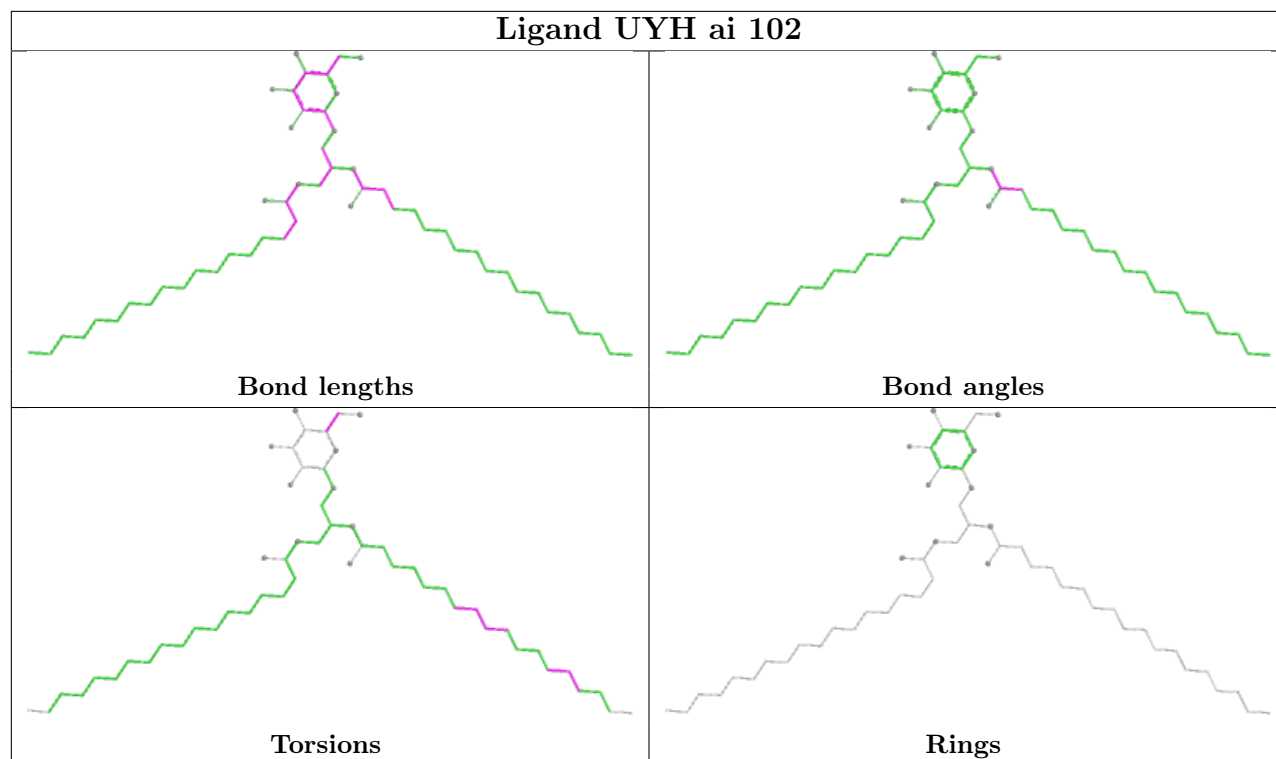


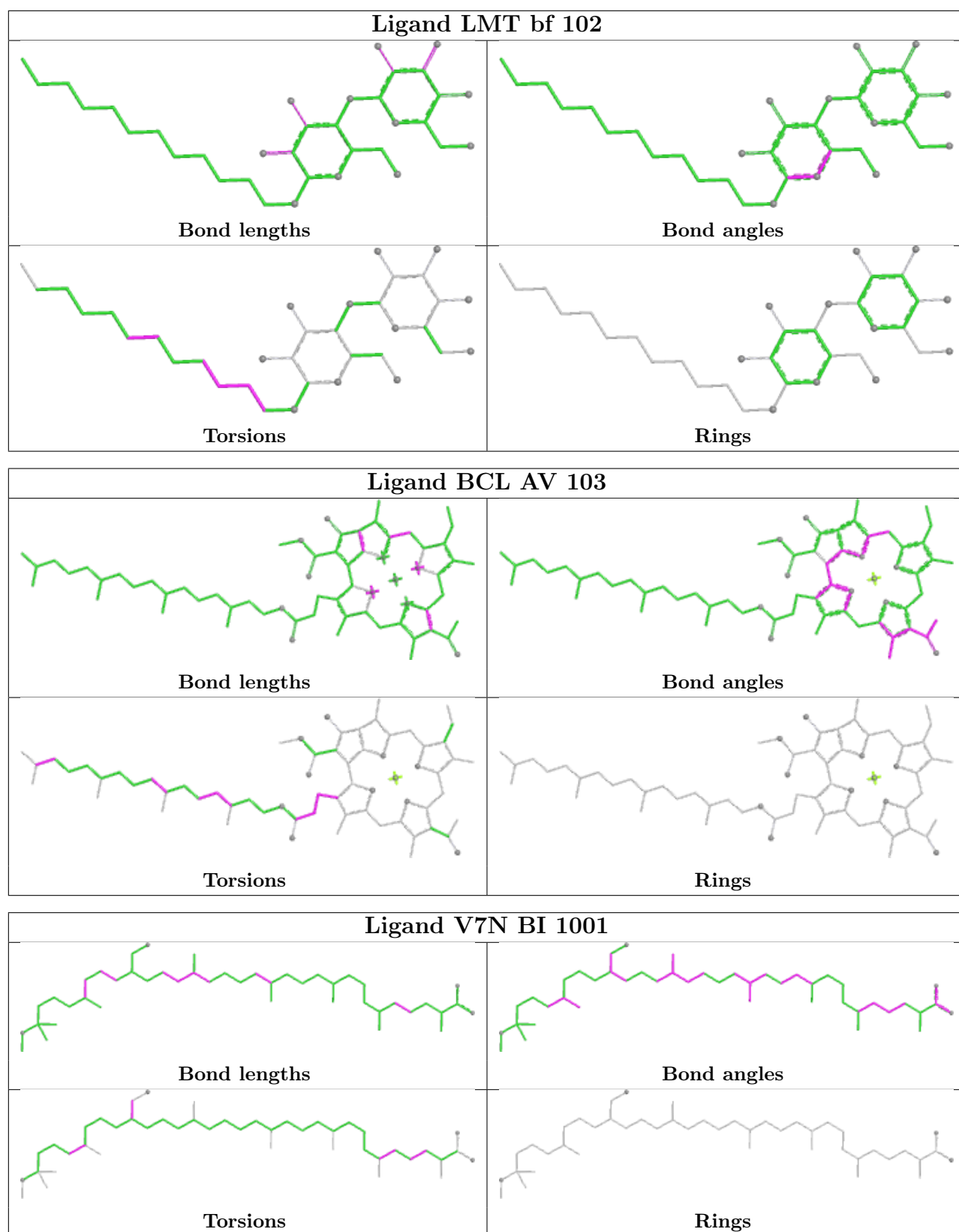


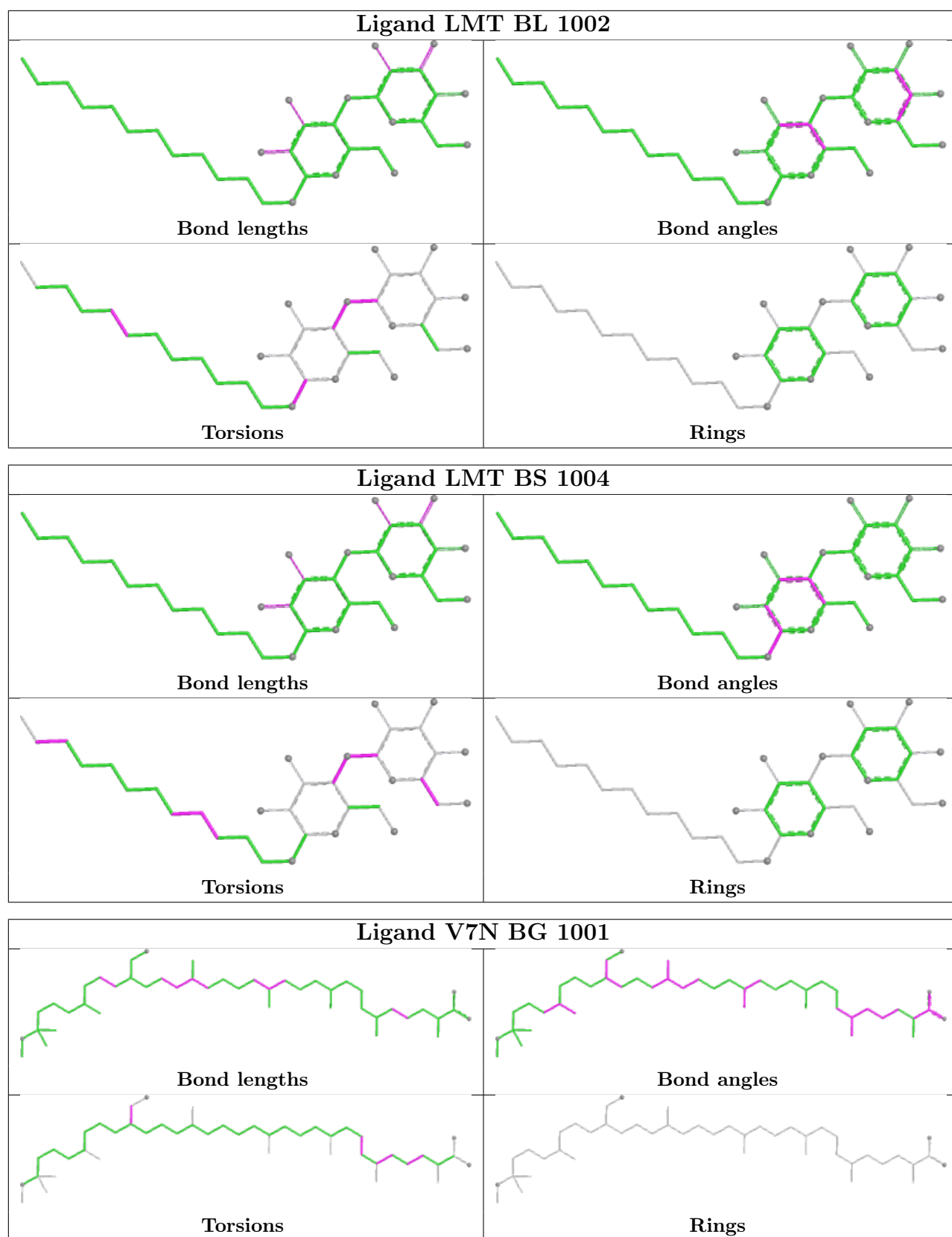


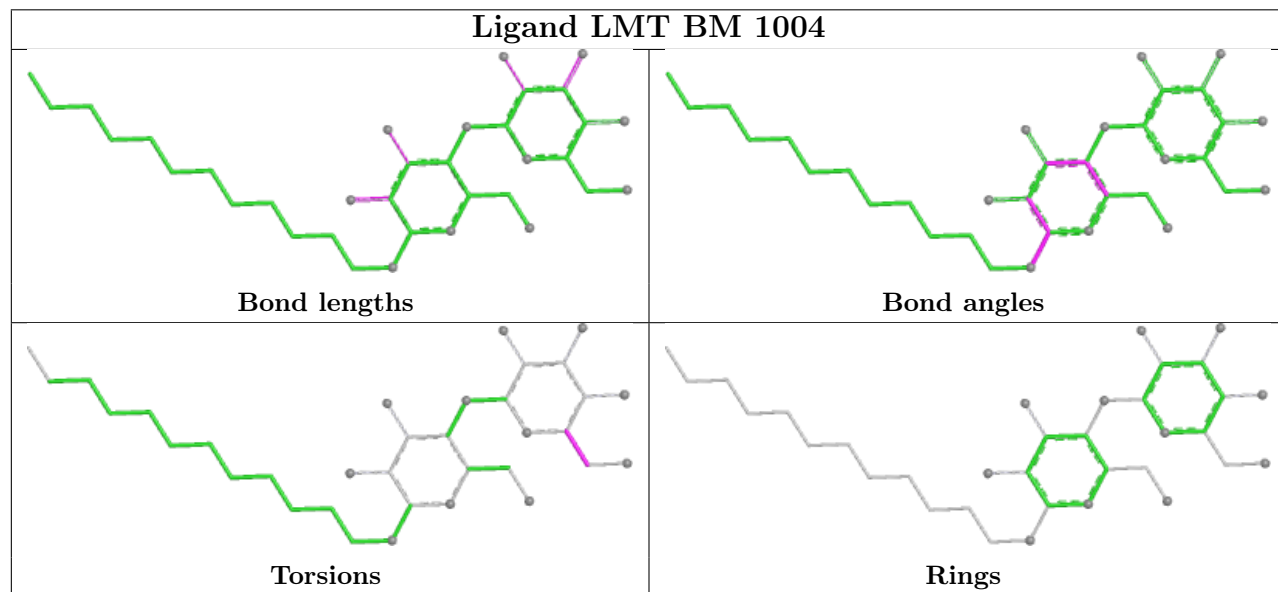
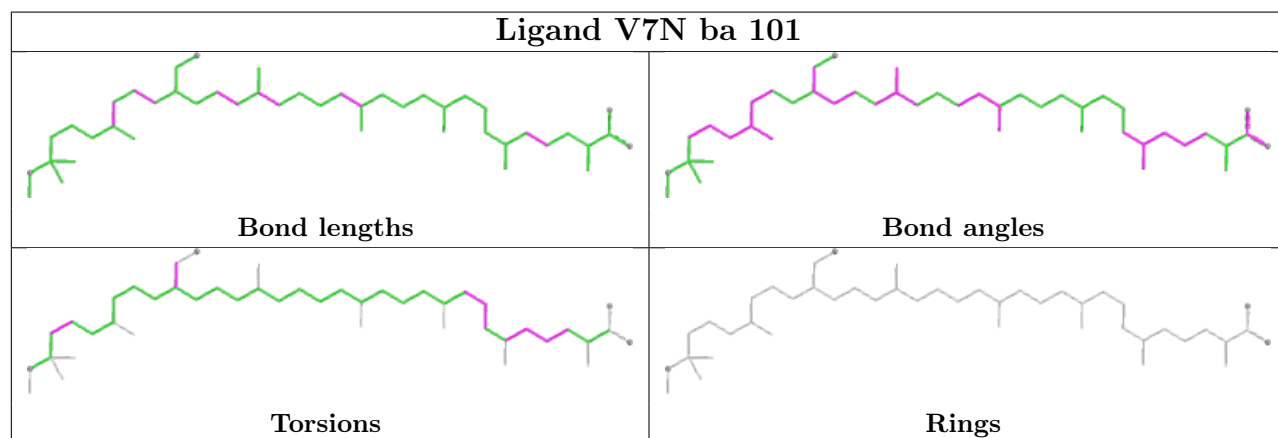
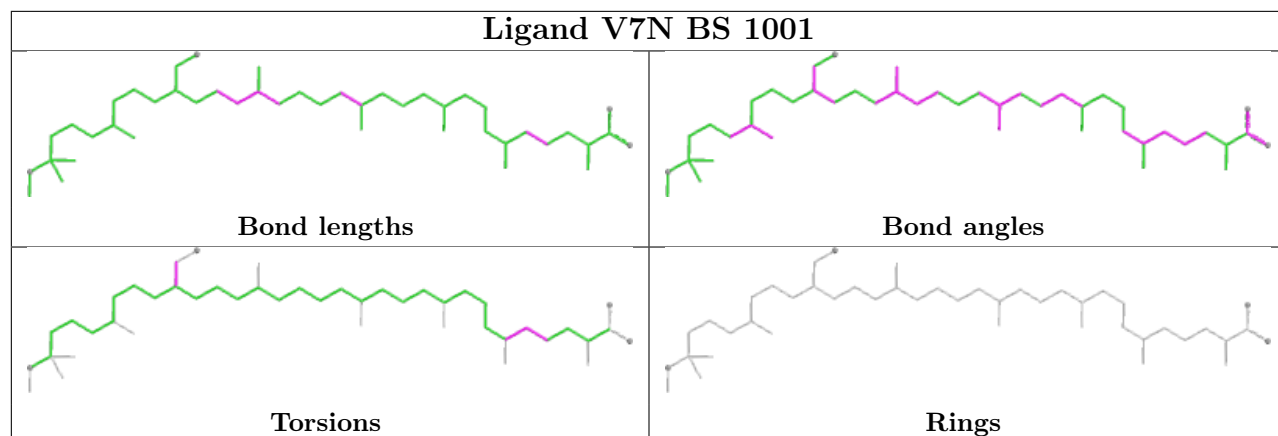


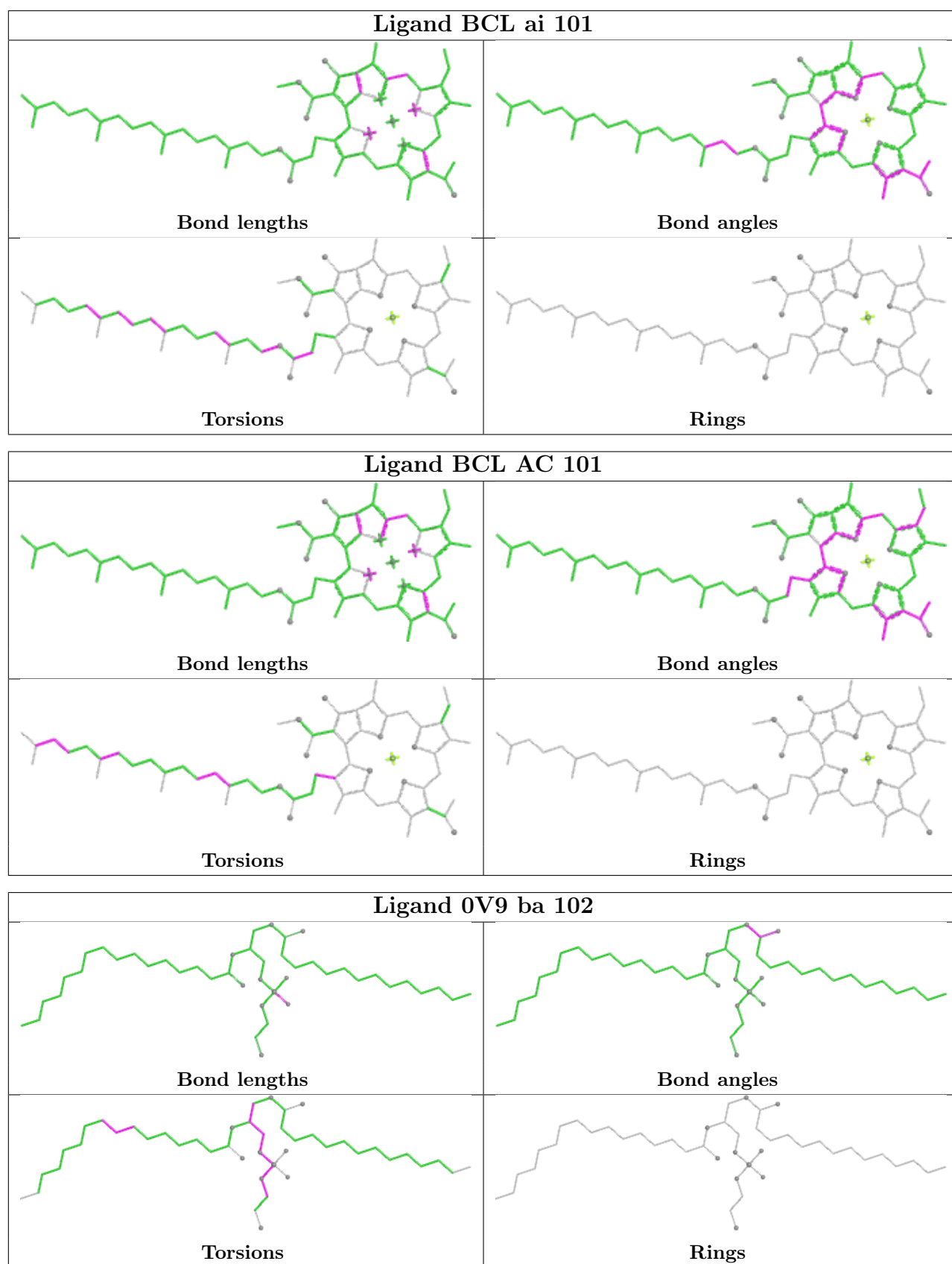


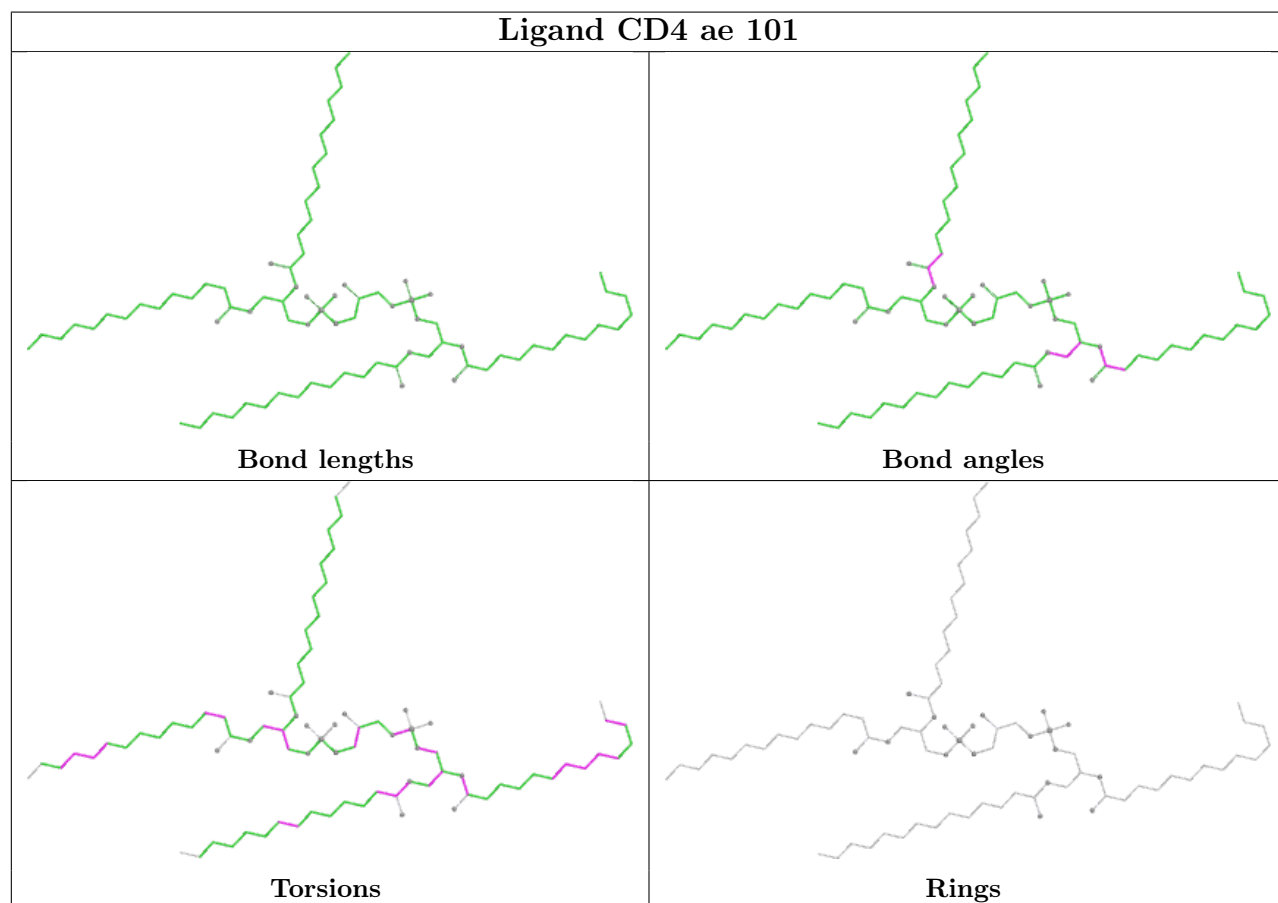
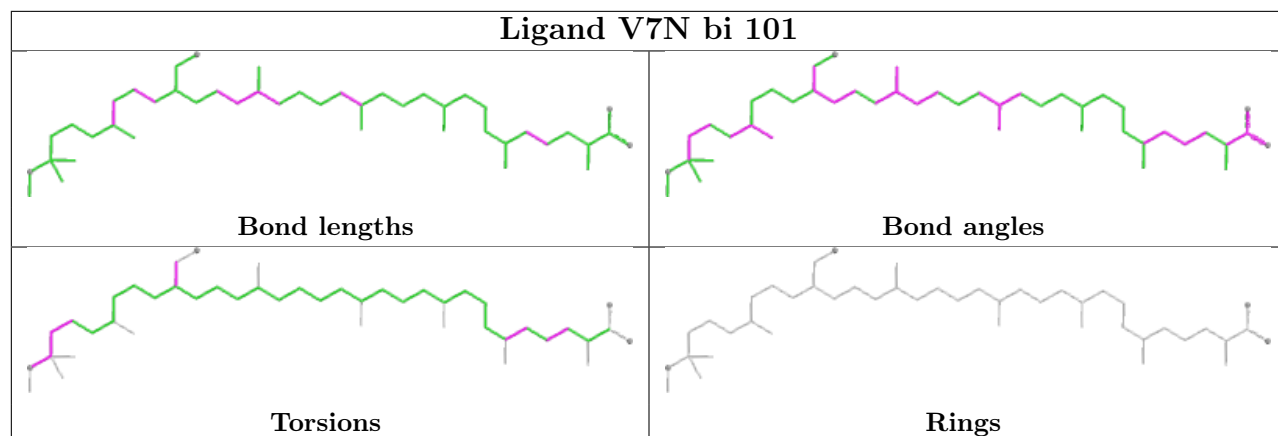


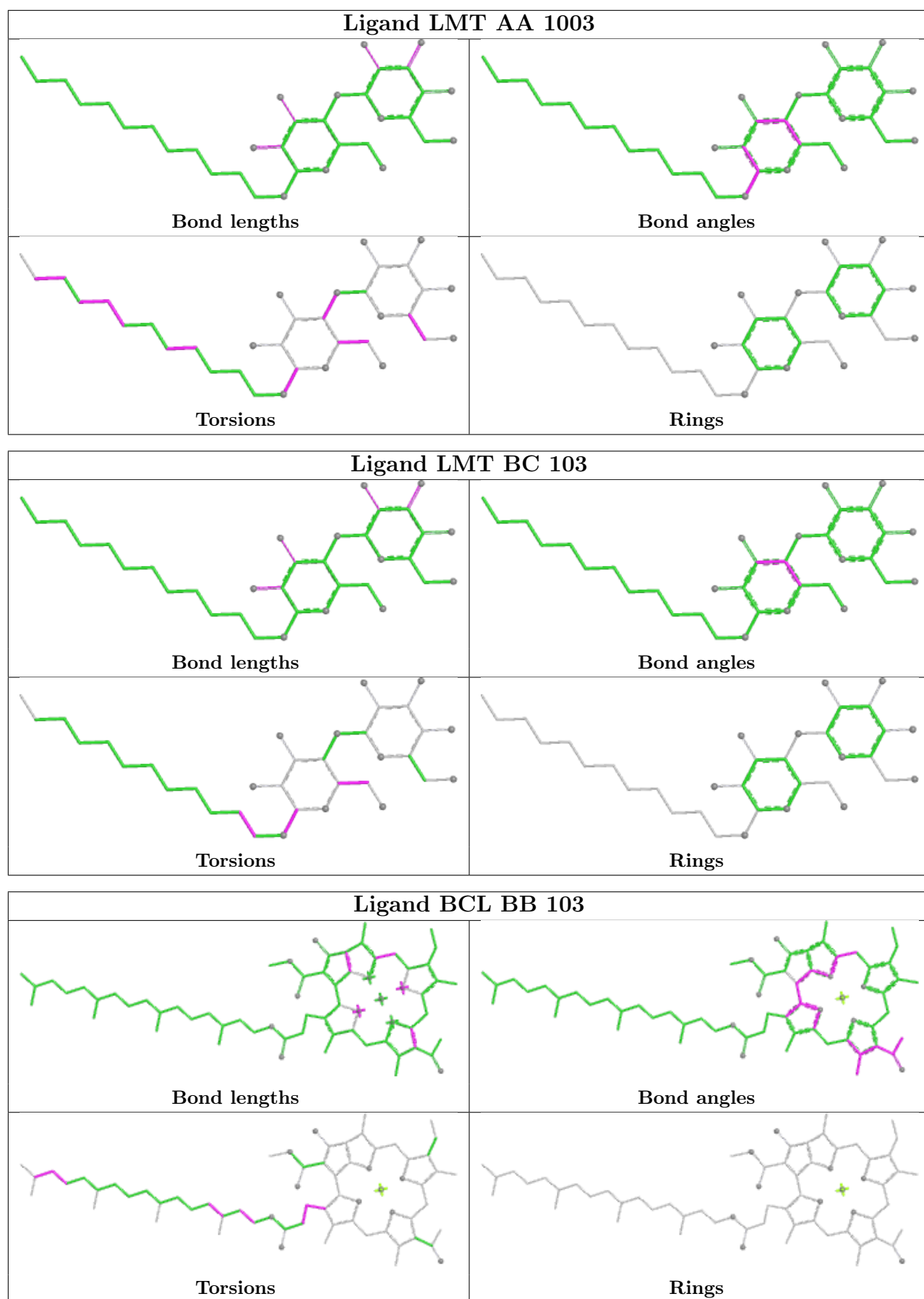


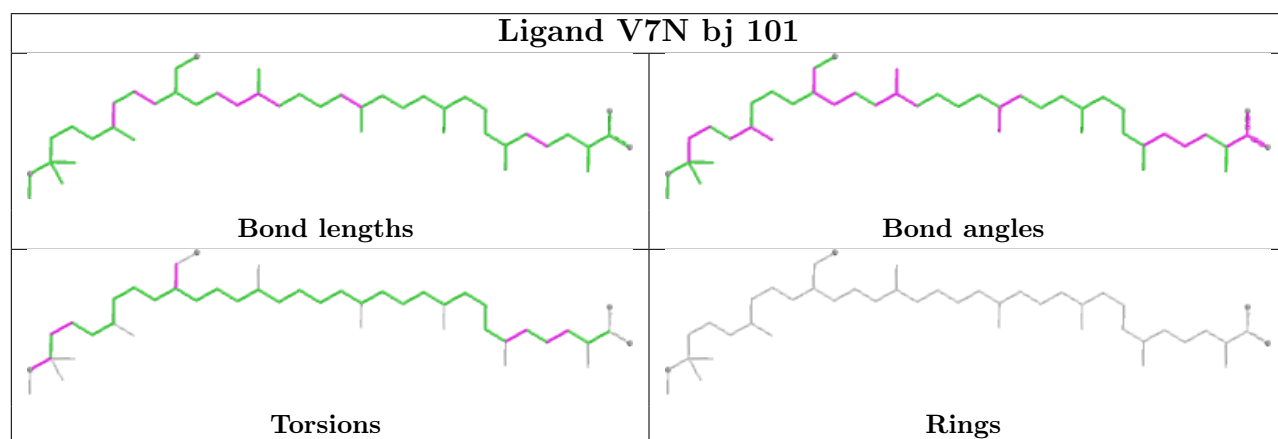
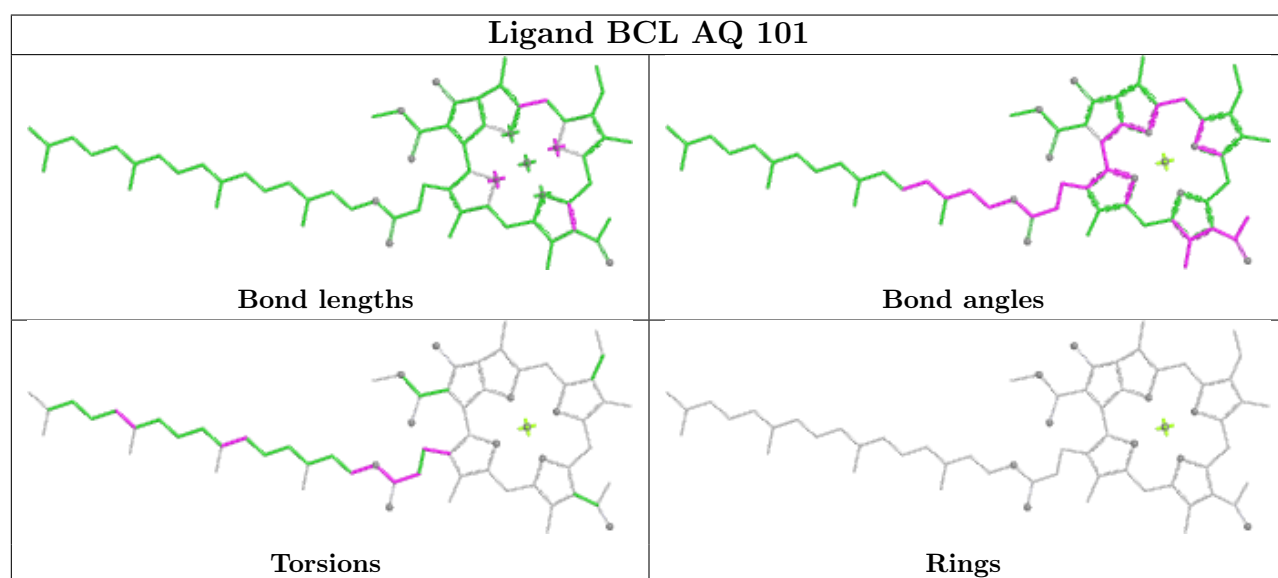
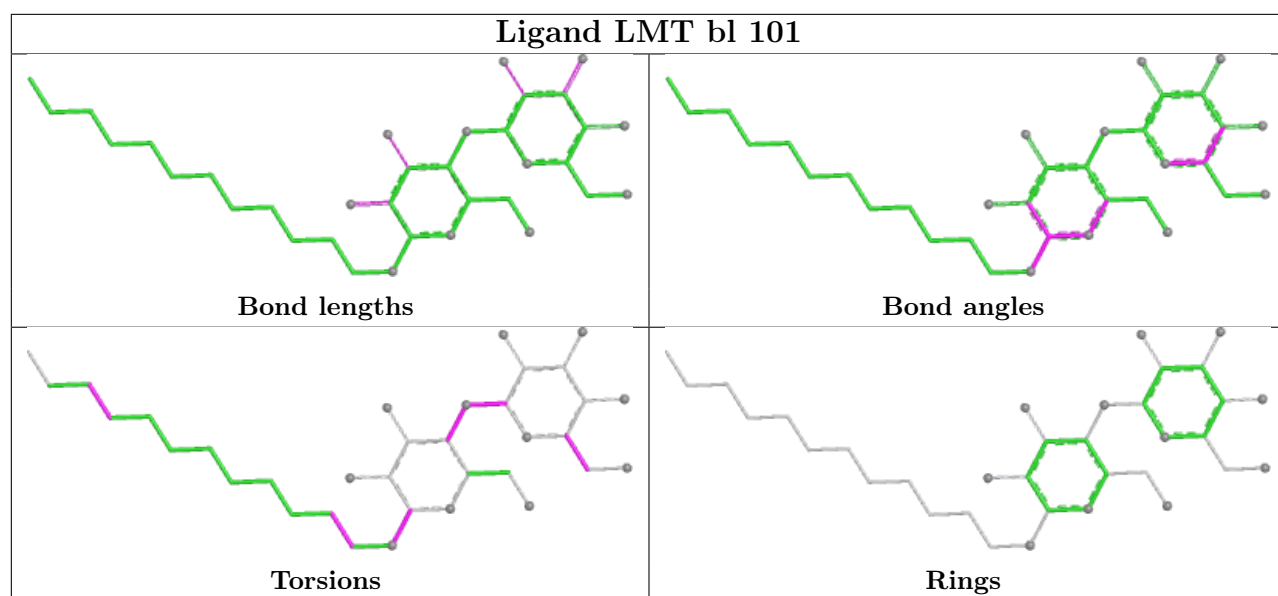


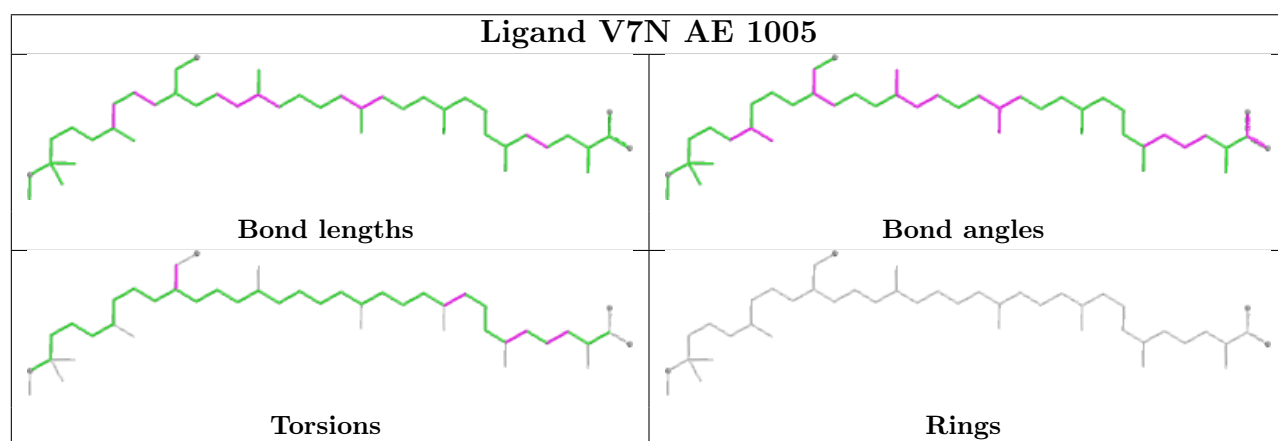
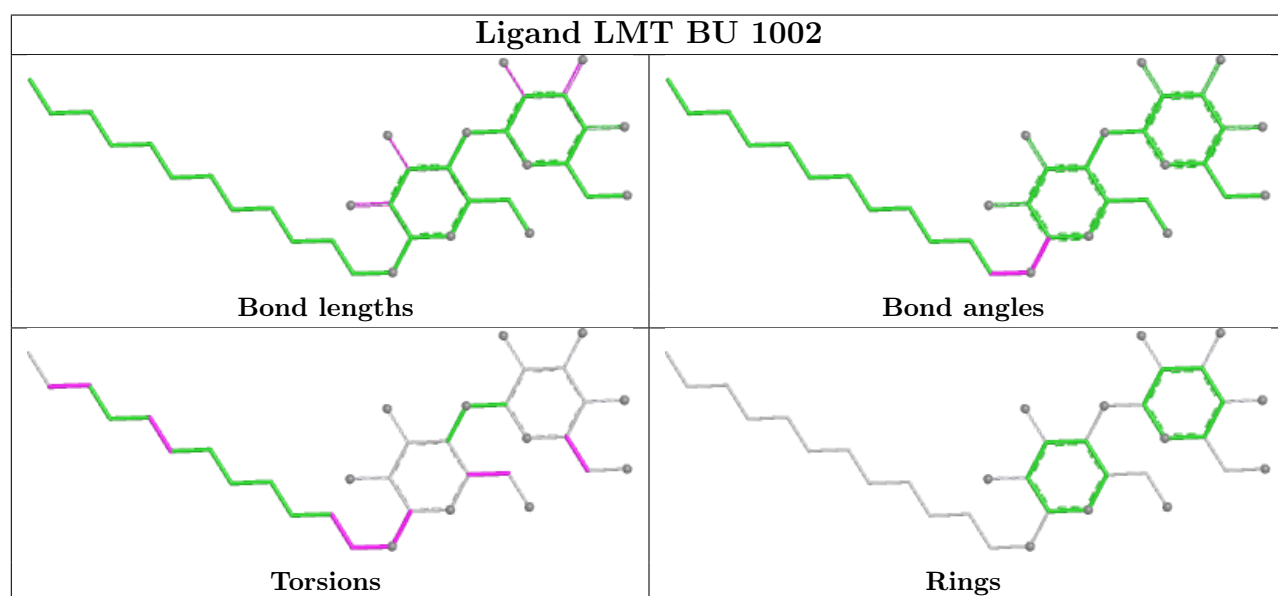
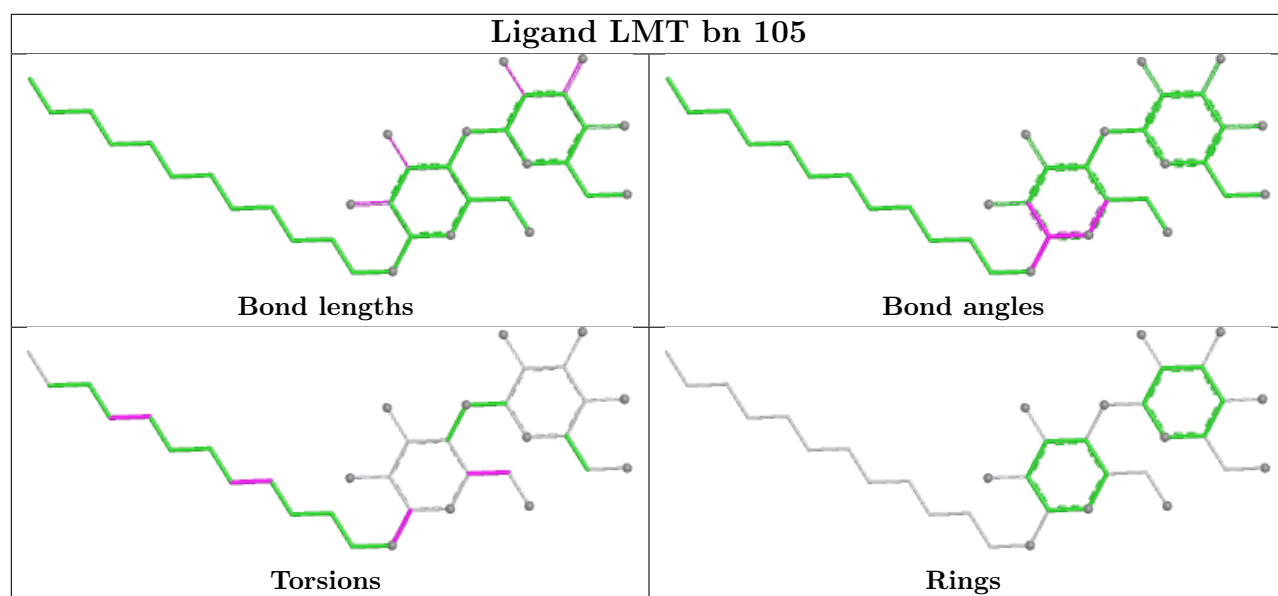


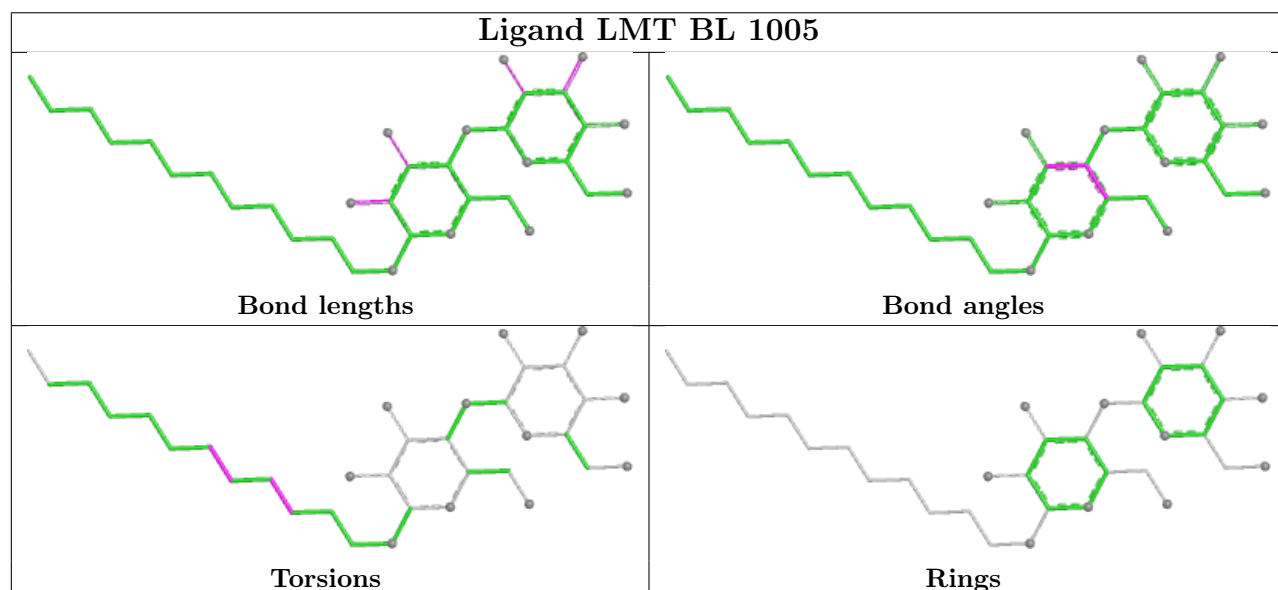
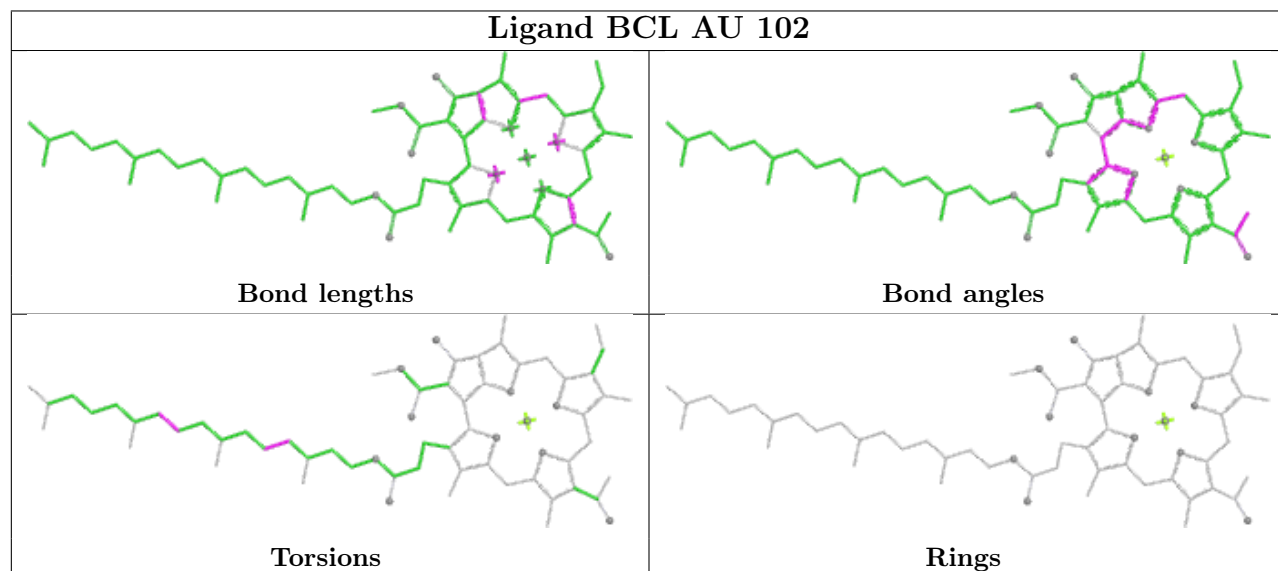
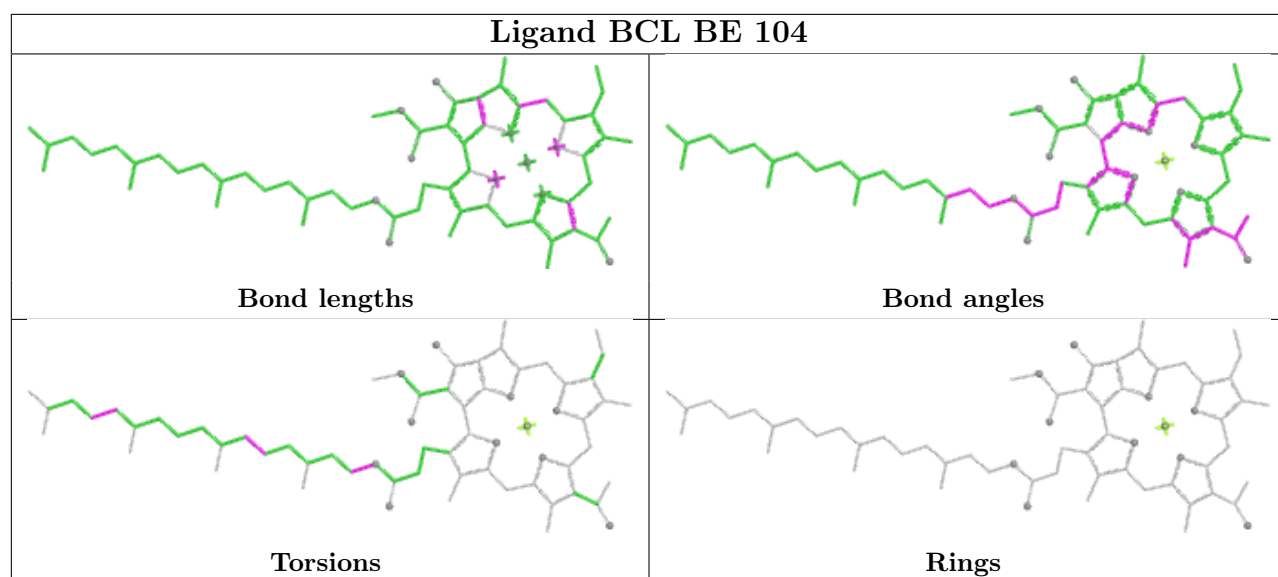


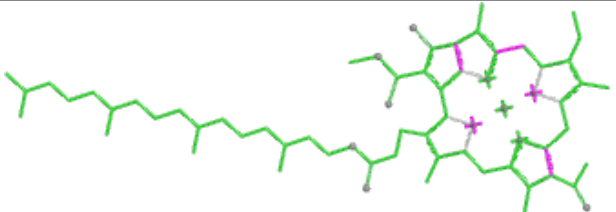
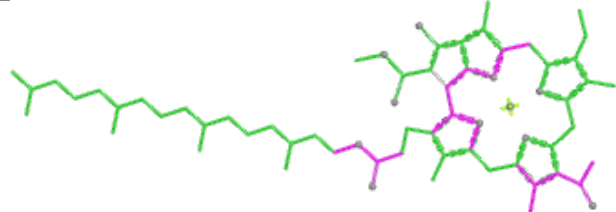
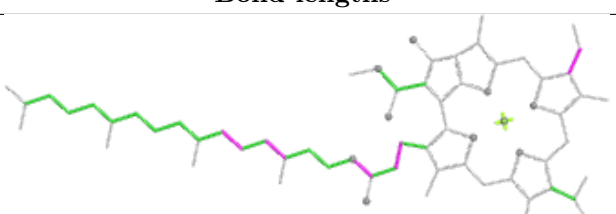
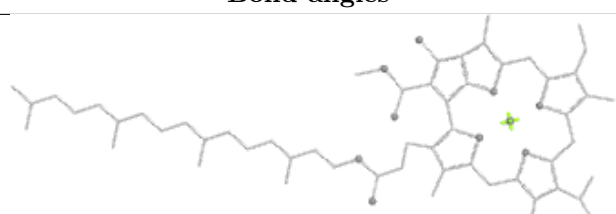


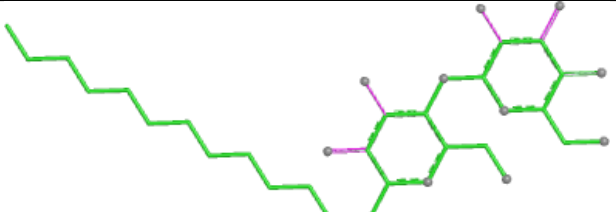
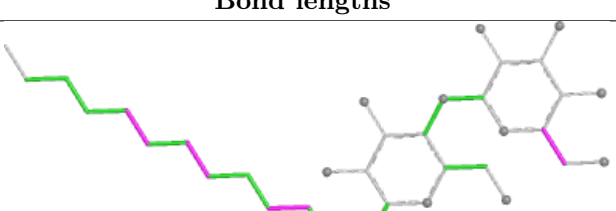
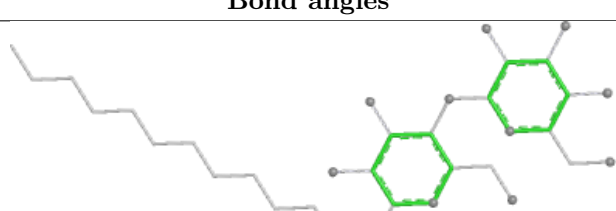


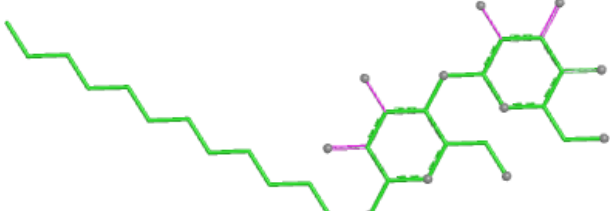
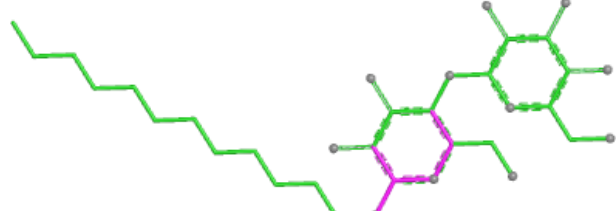
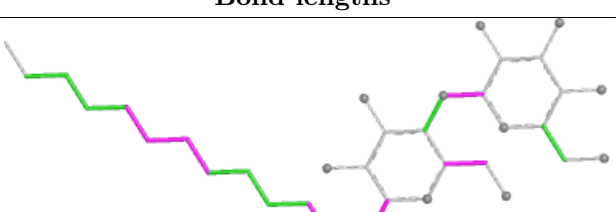
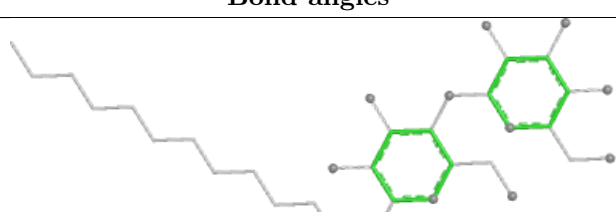


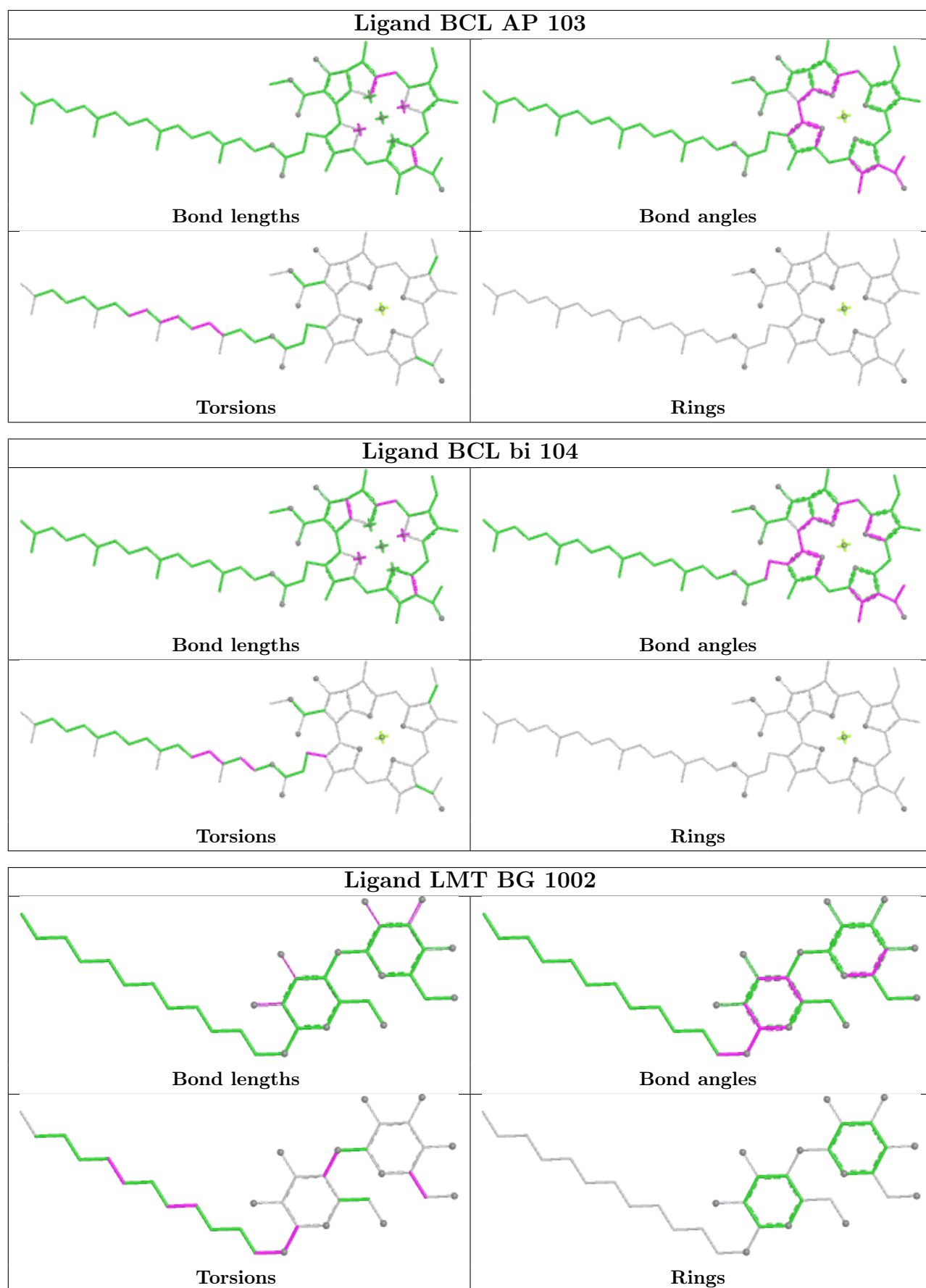


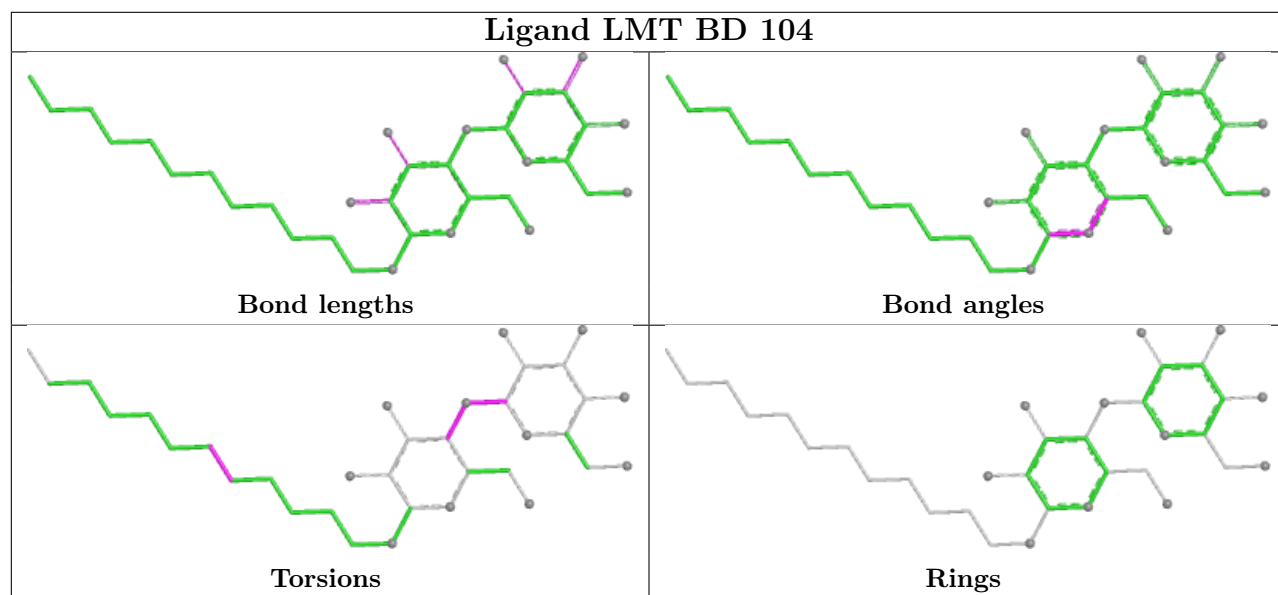
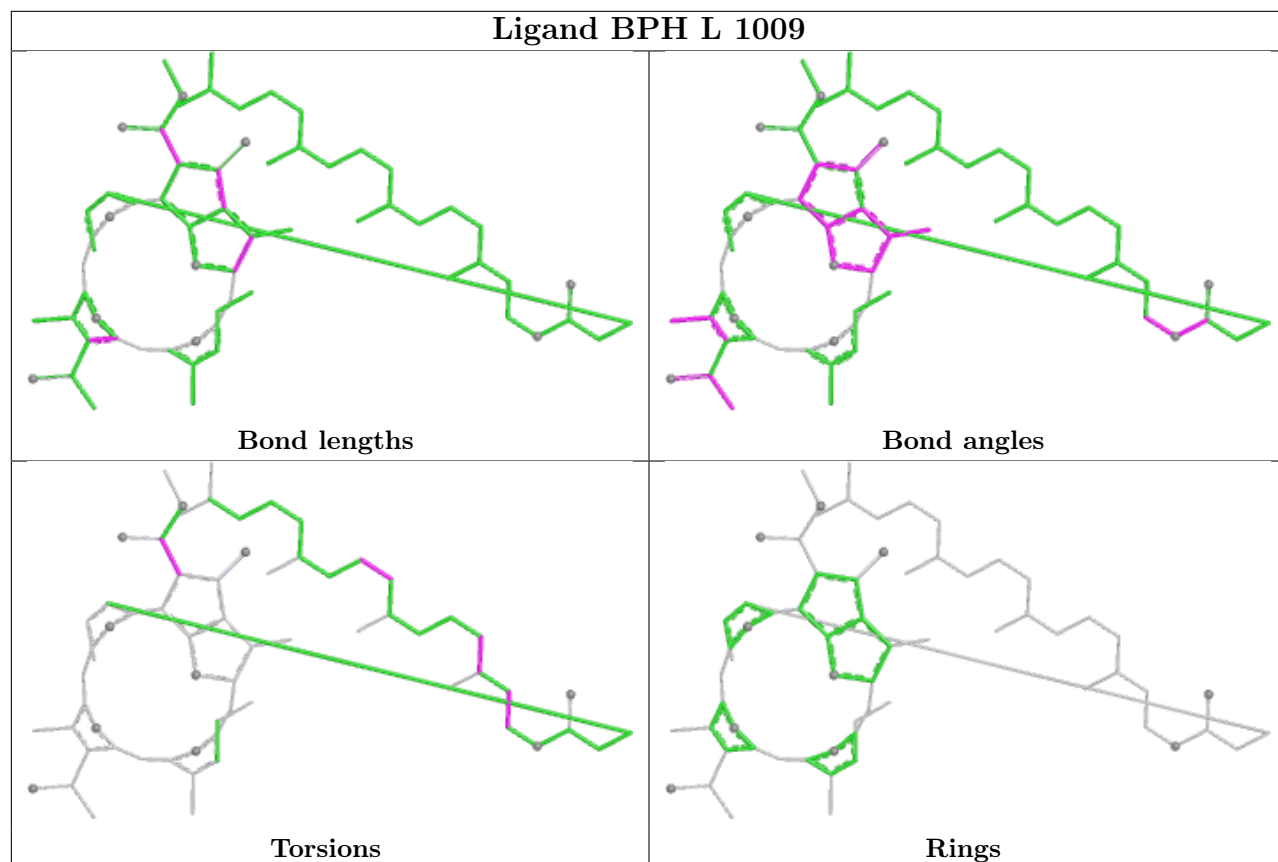


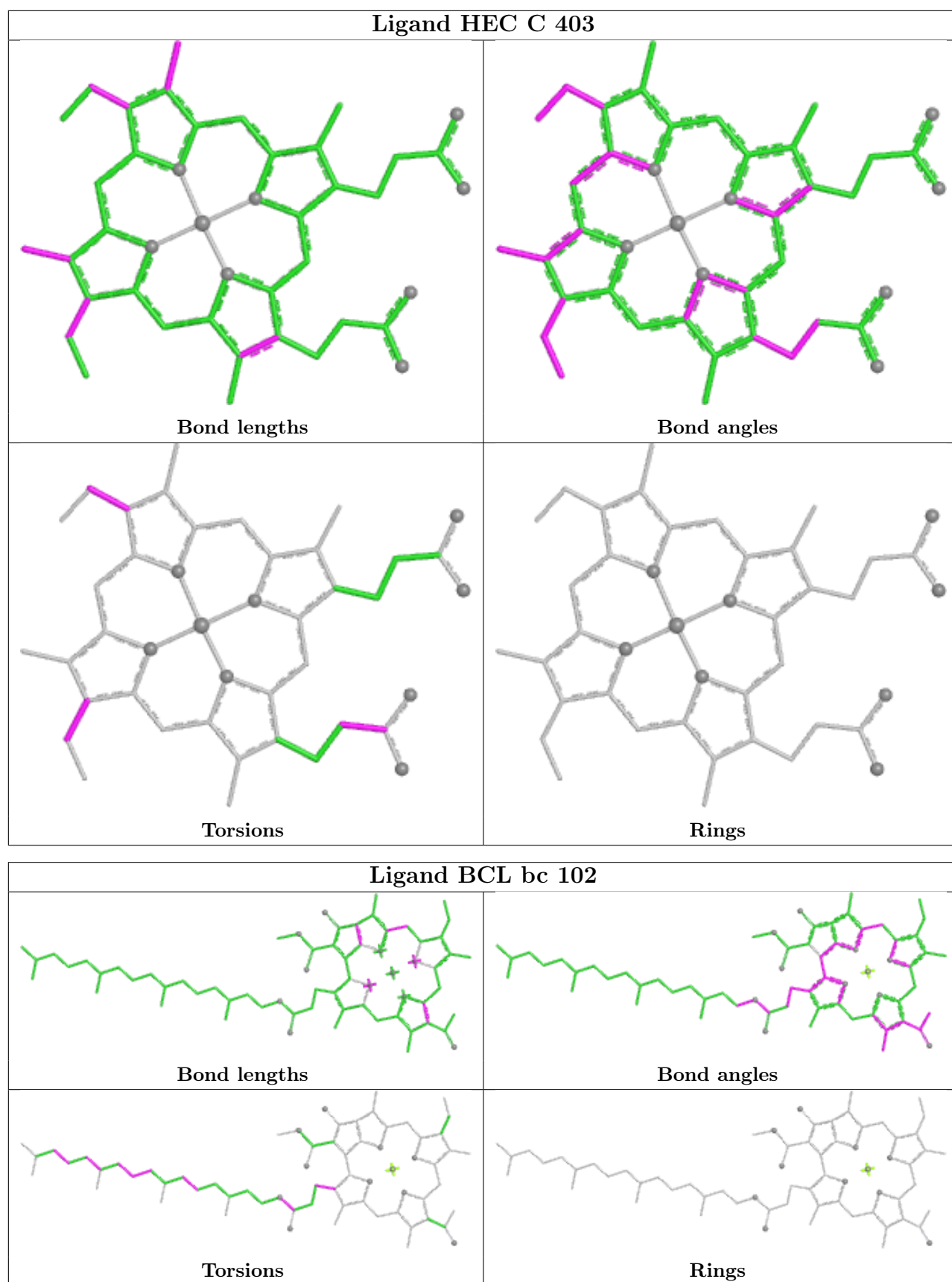
Ligand BCL BO 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

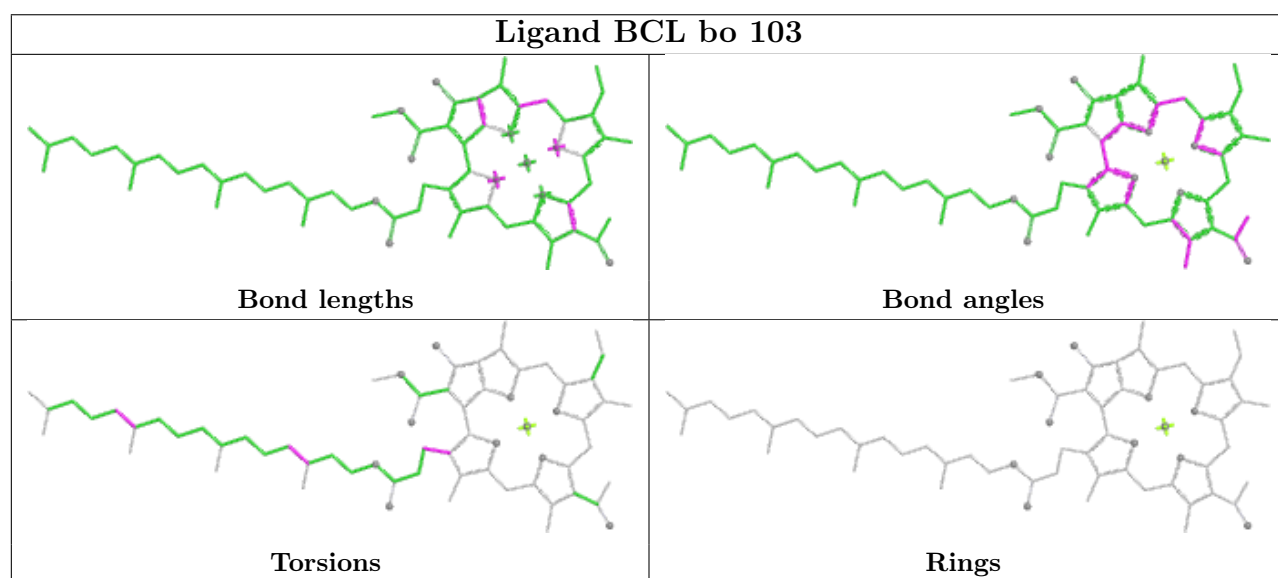
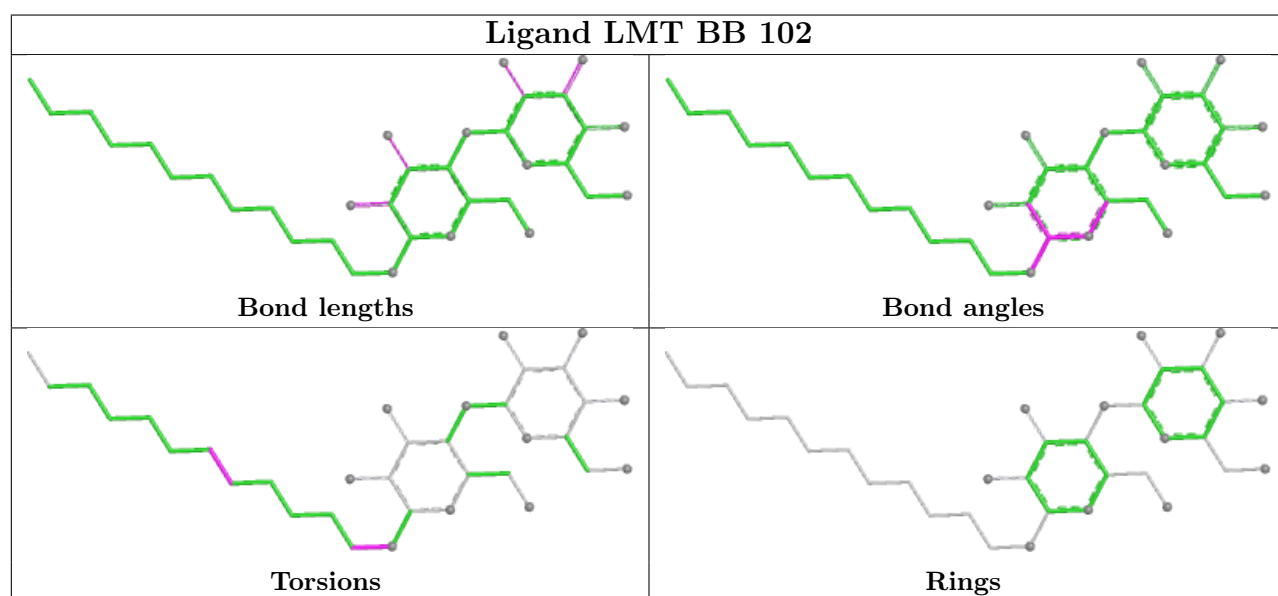
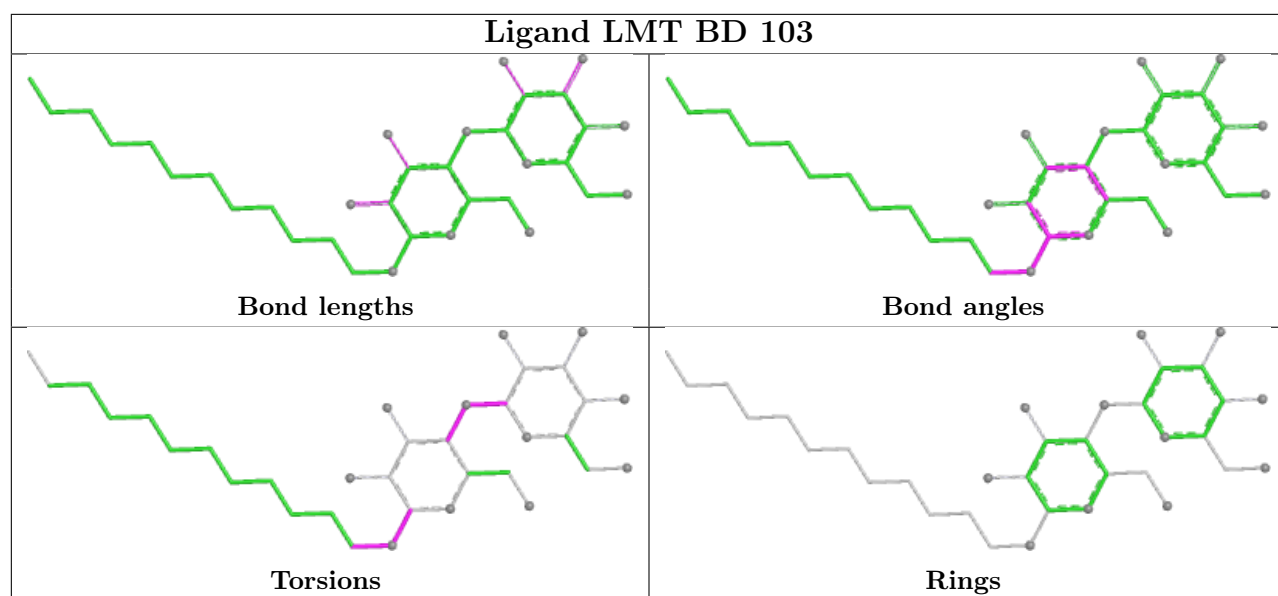
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Bond lengths	Bond angles
	
Torsions	Rings

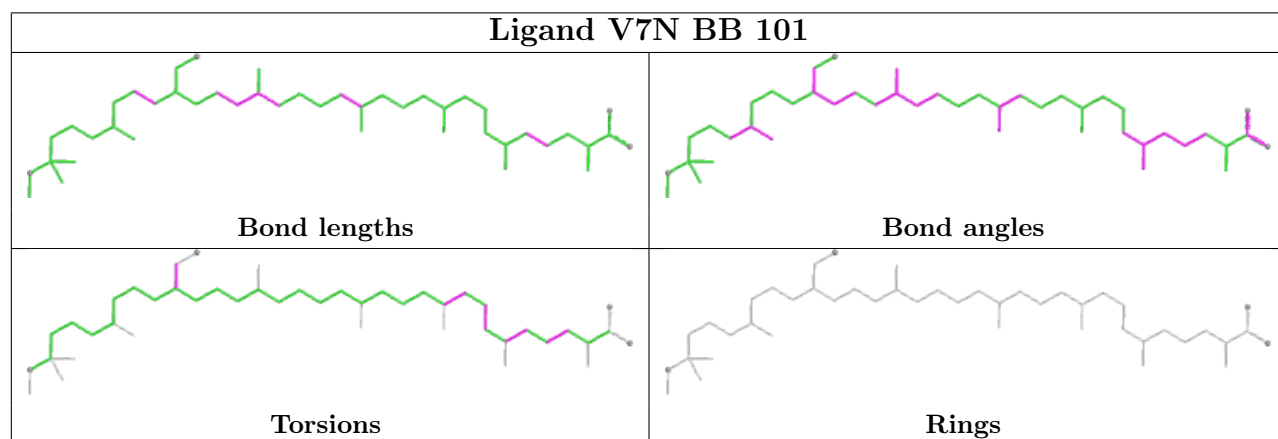
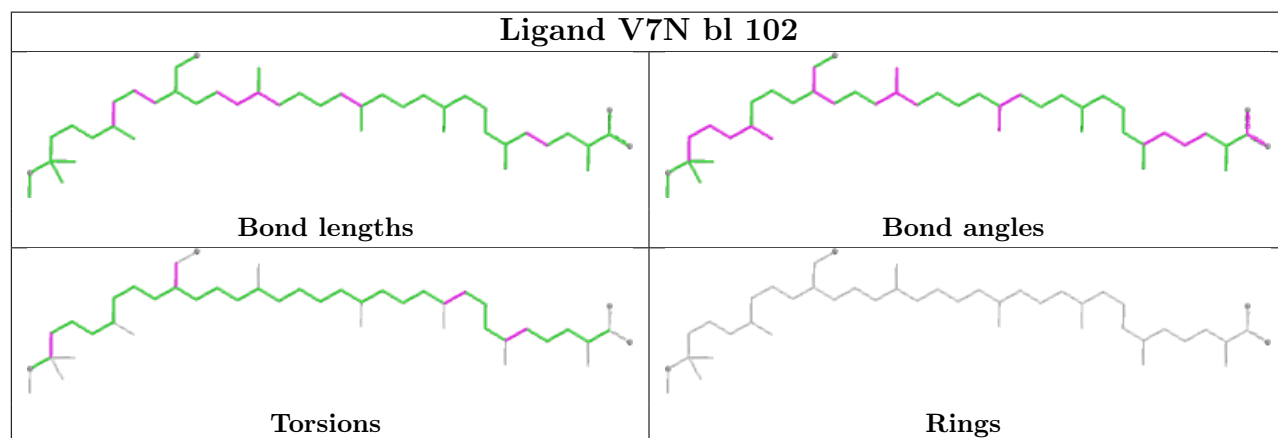
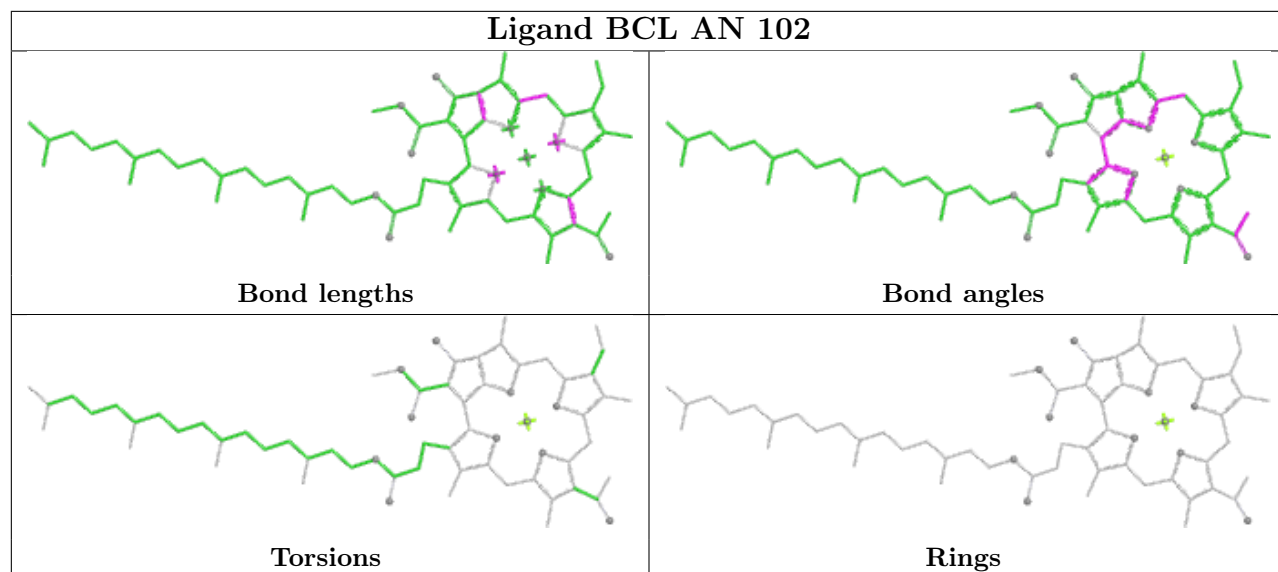
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Bond lengths	Bond angles
	
Torsions	Rings

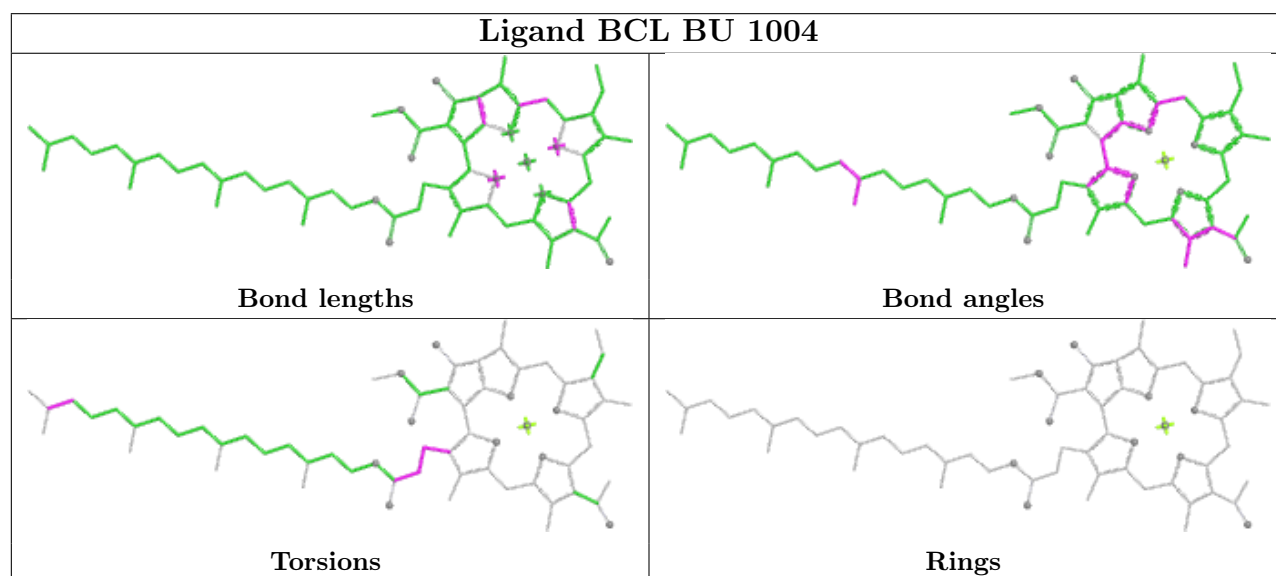
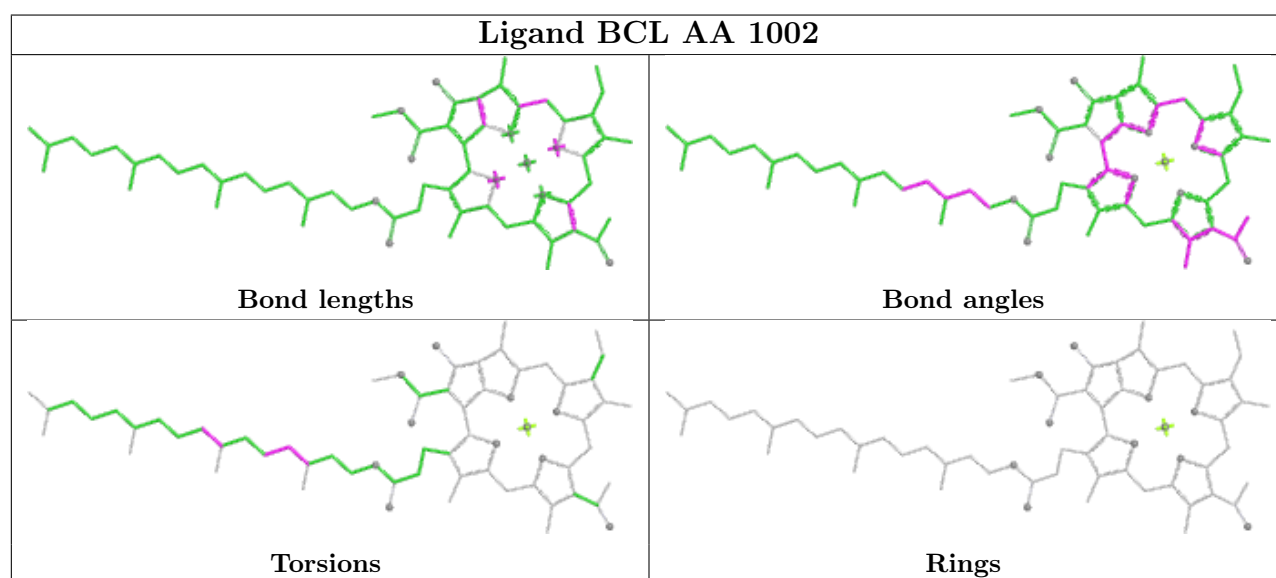
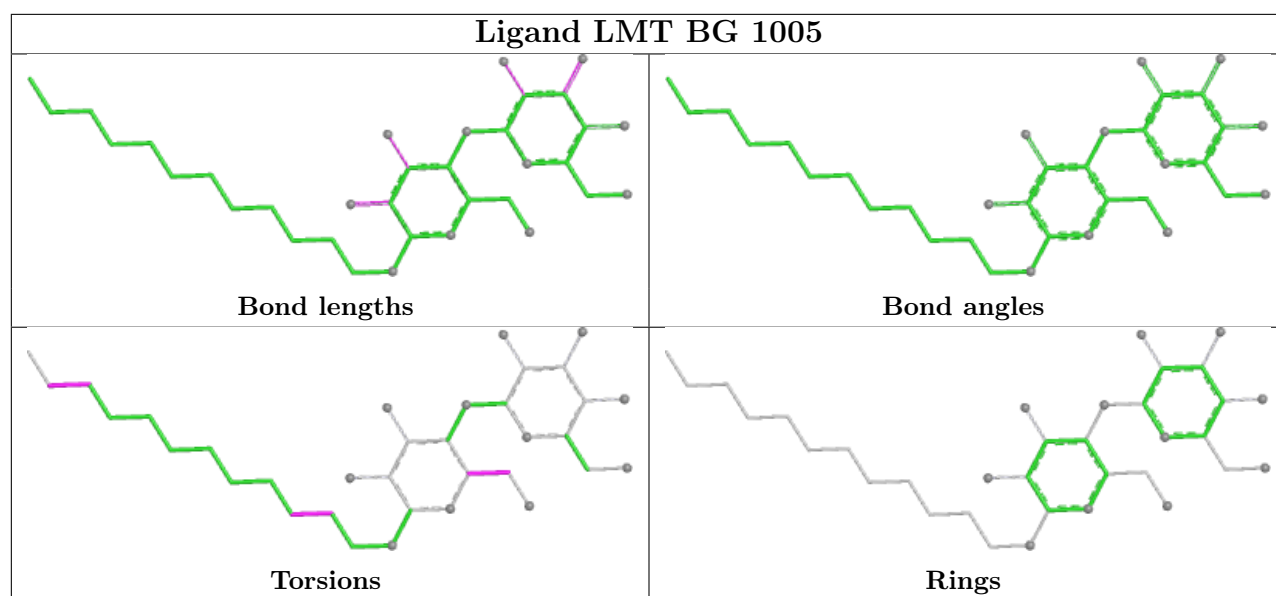


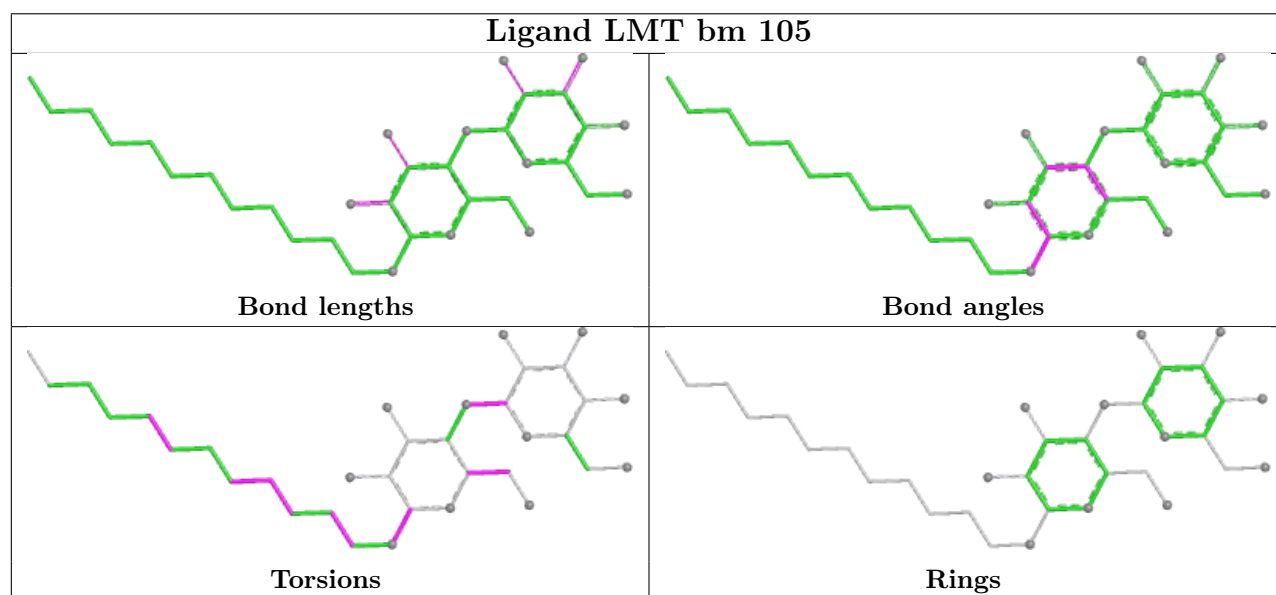
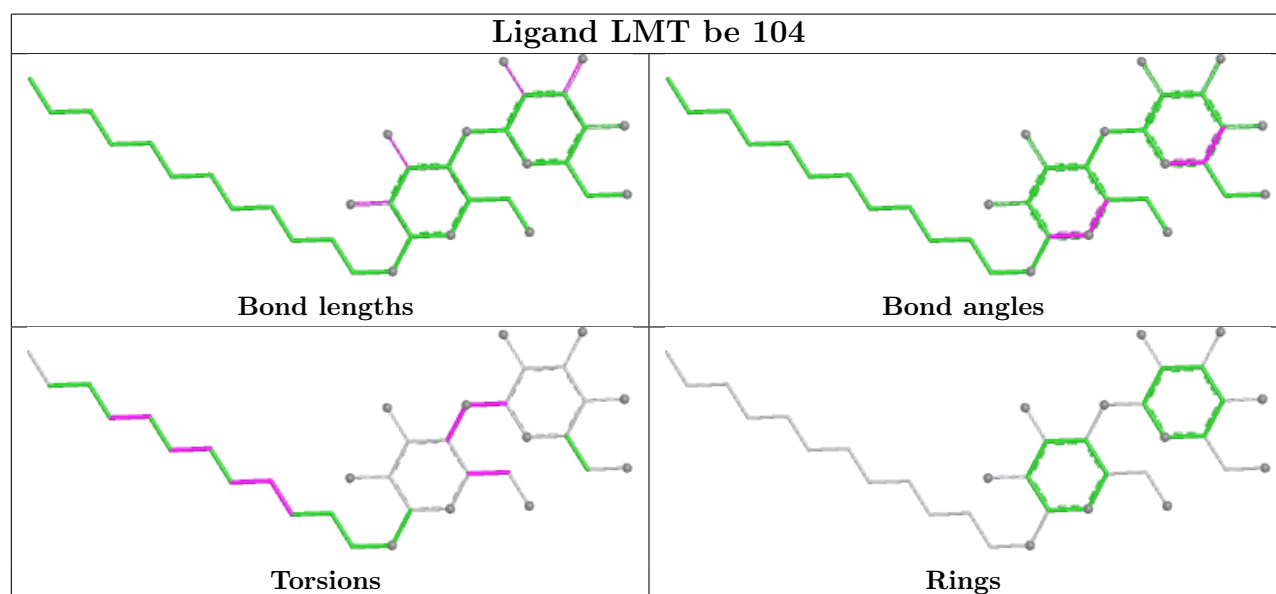
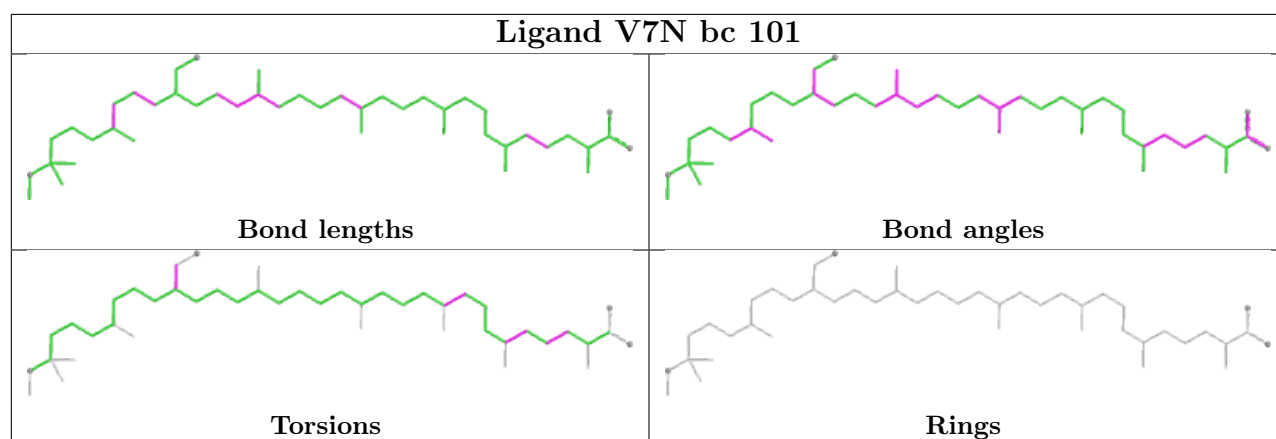


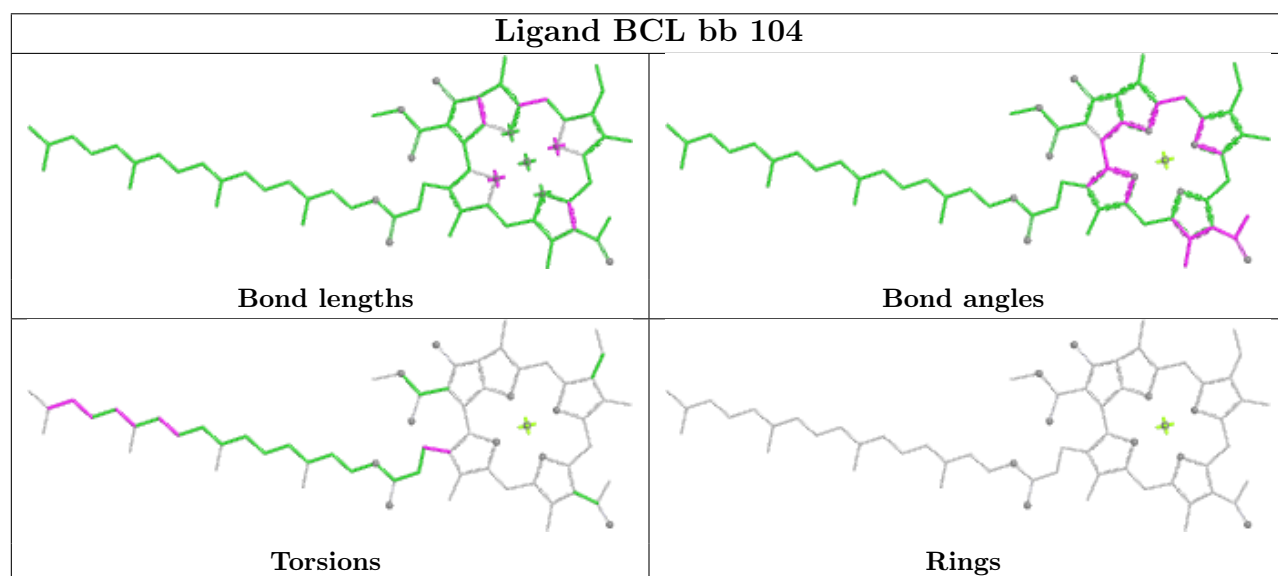
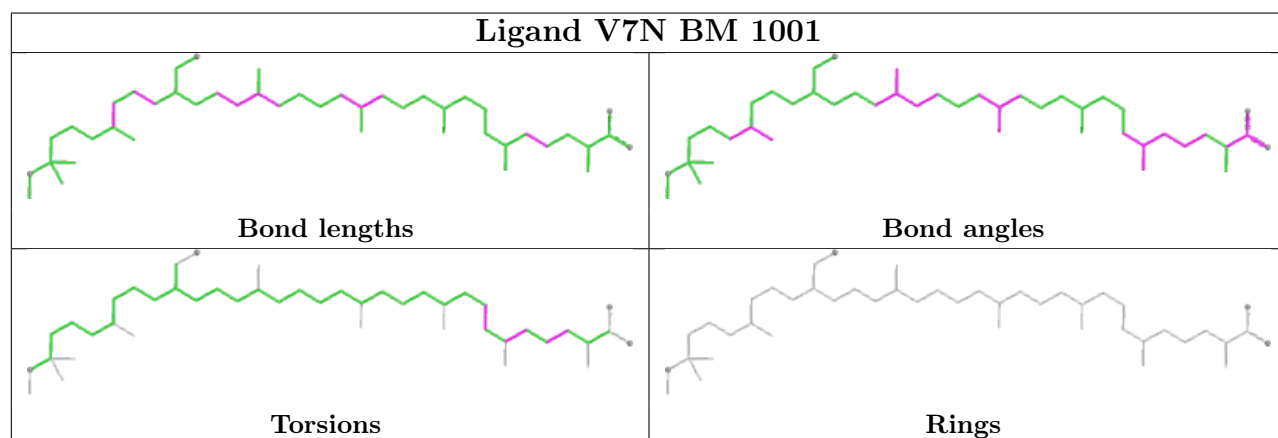
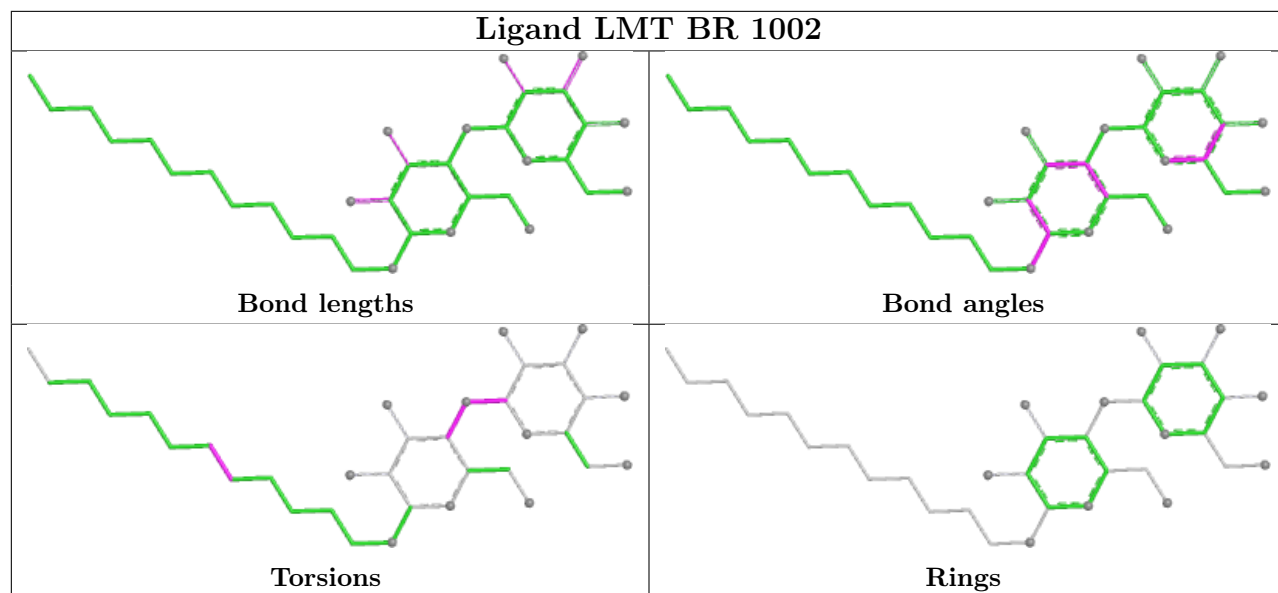


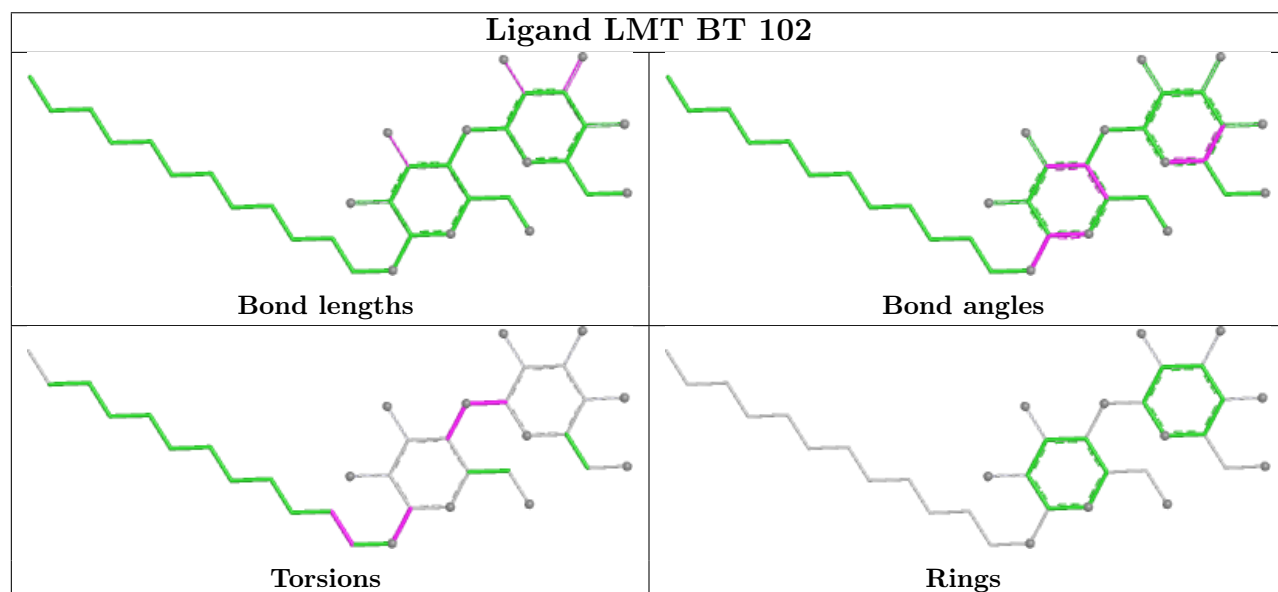
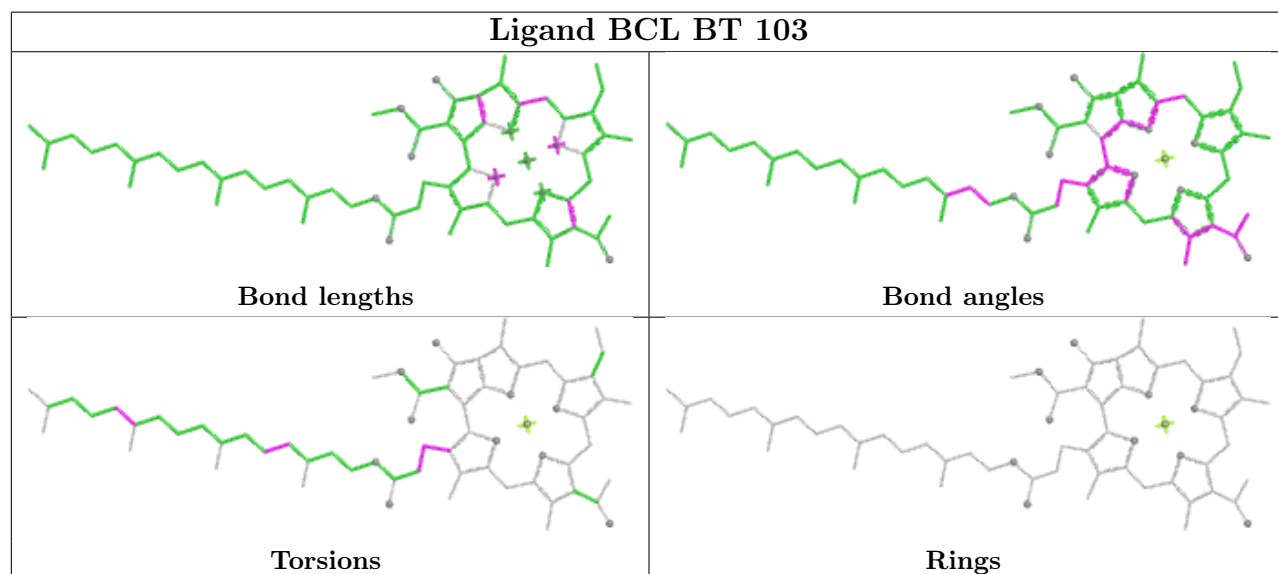
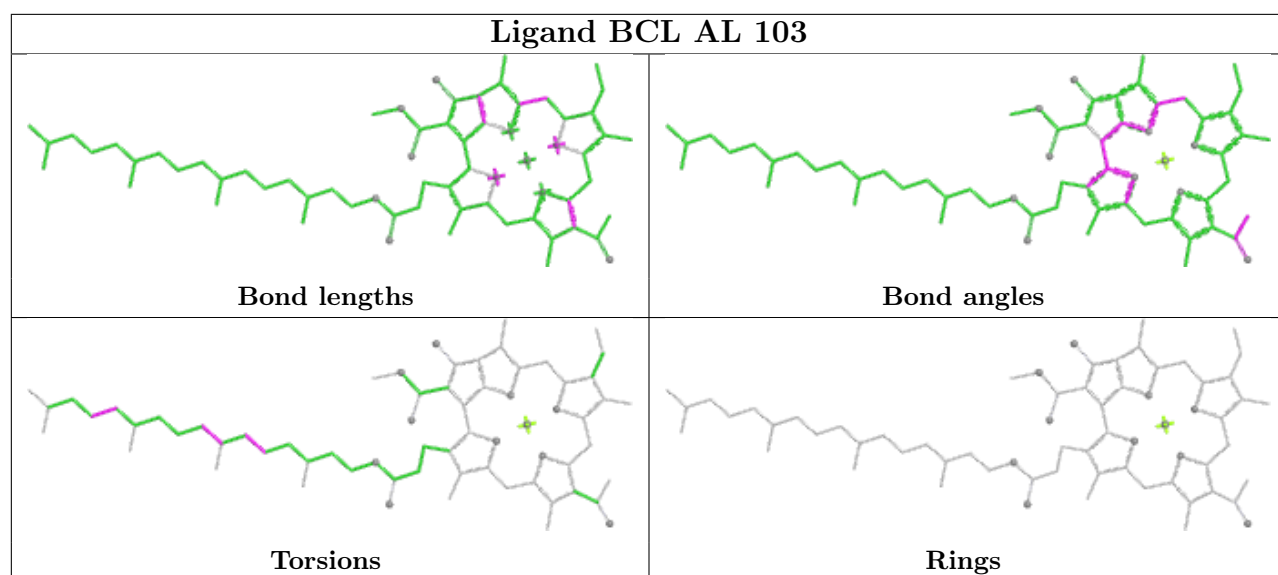


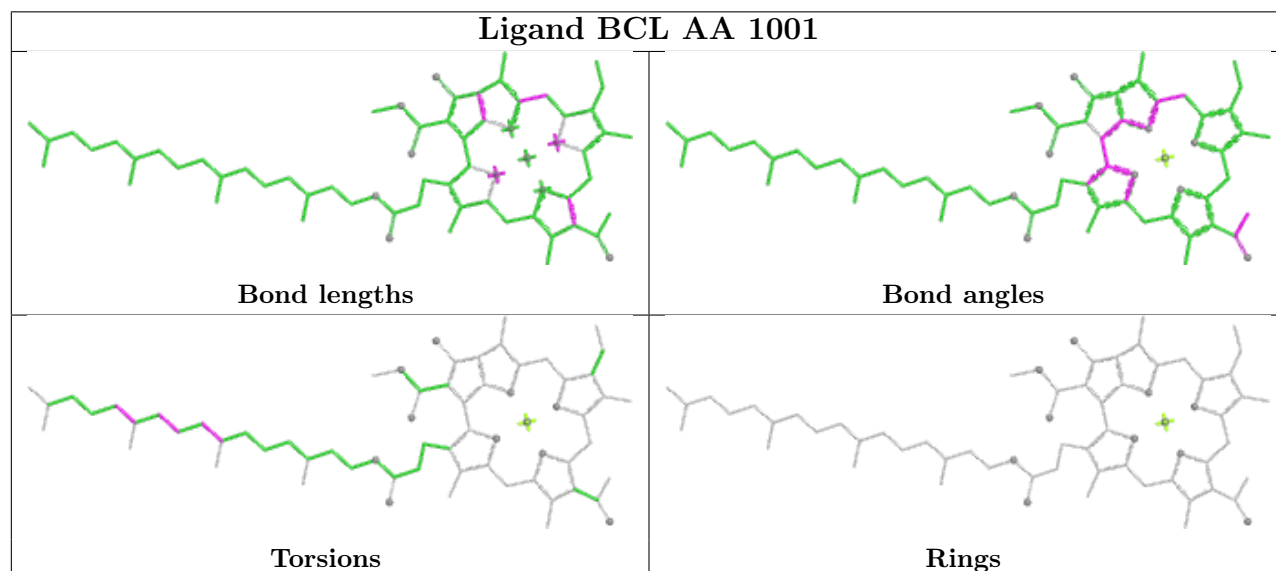
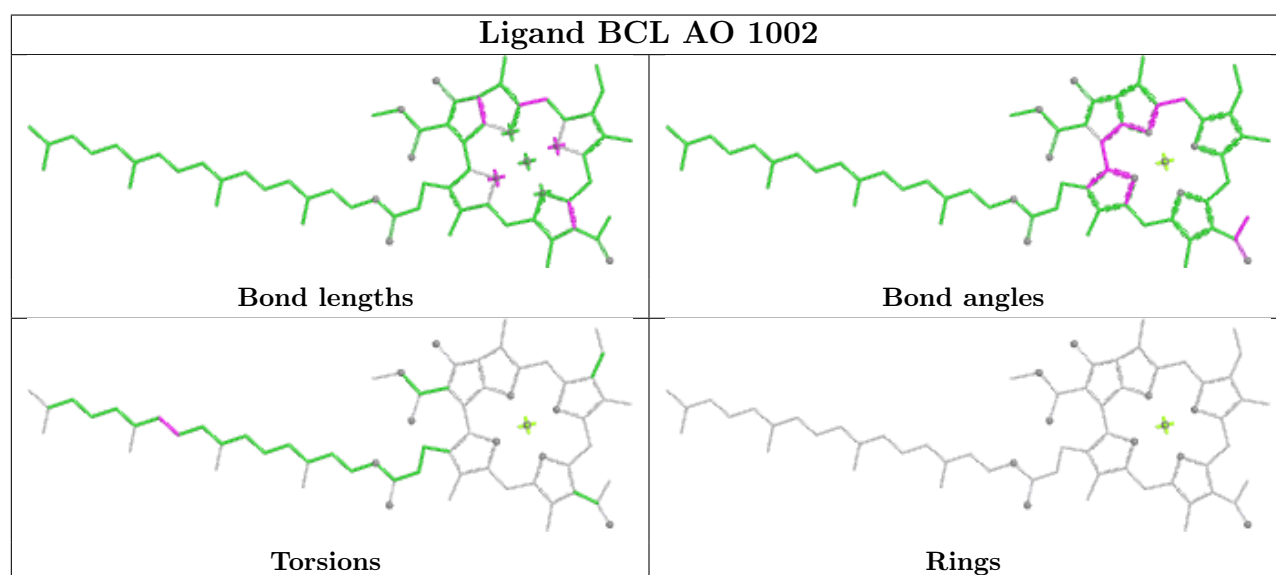
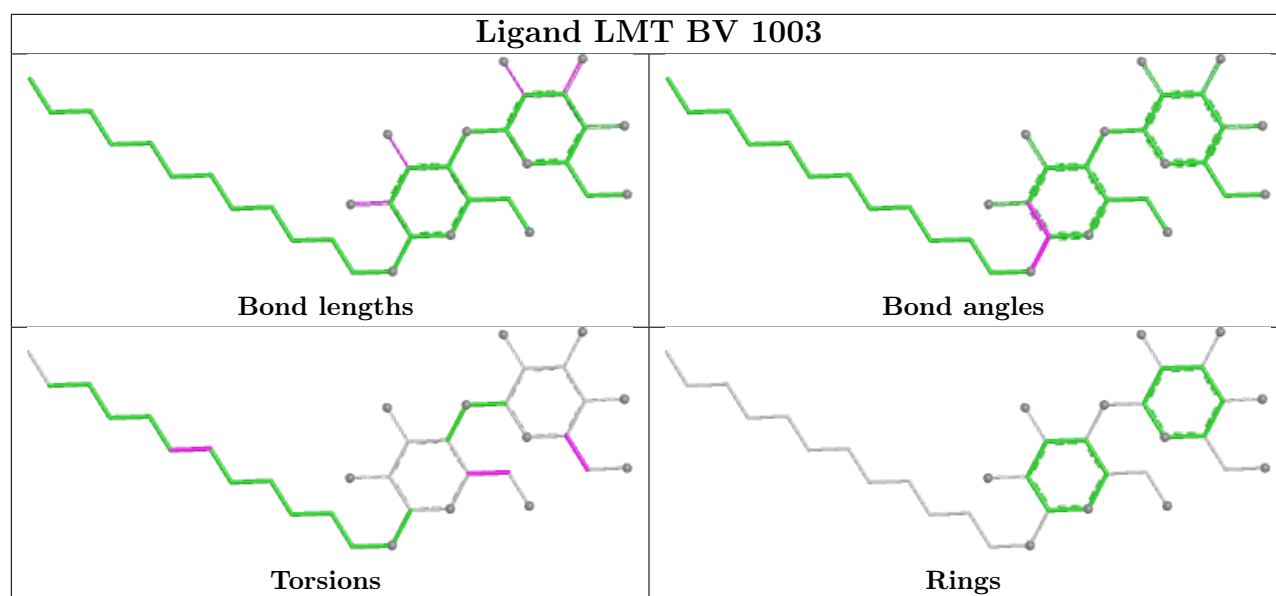


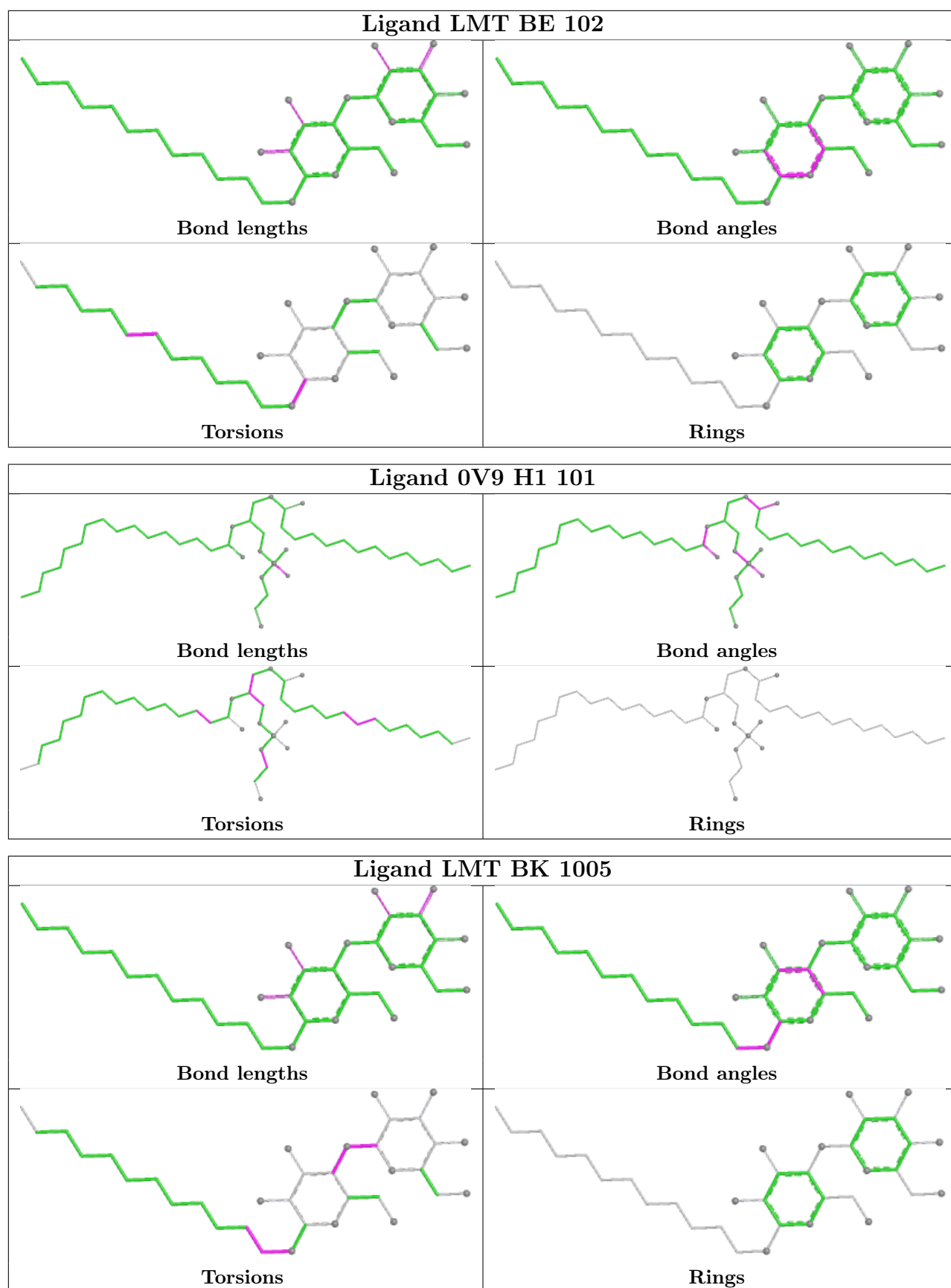


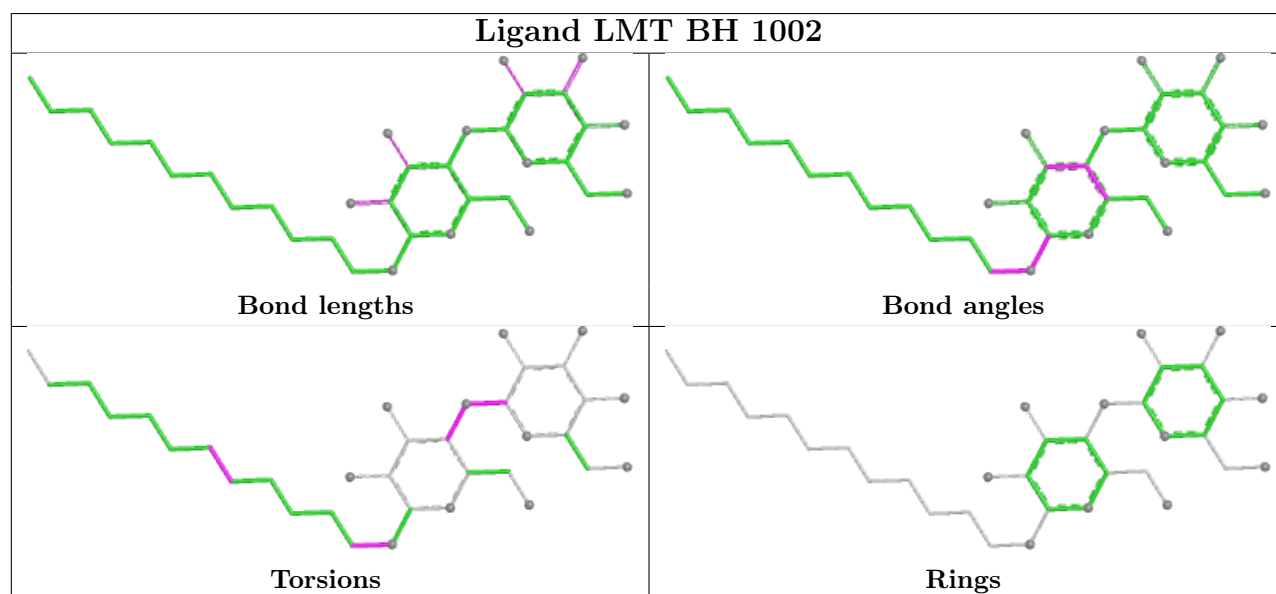
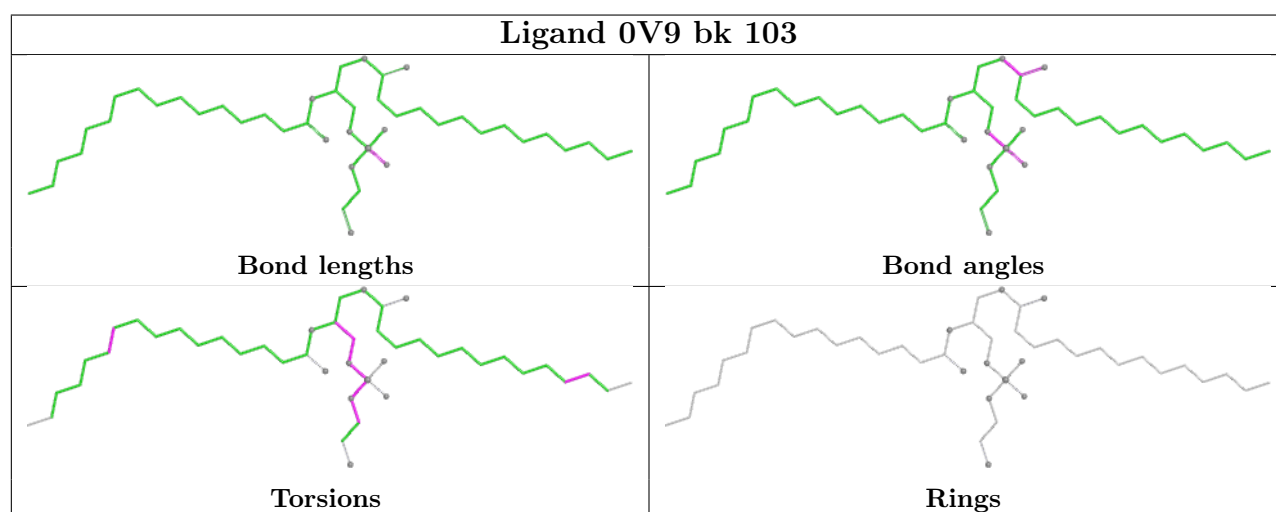
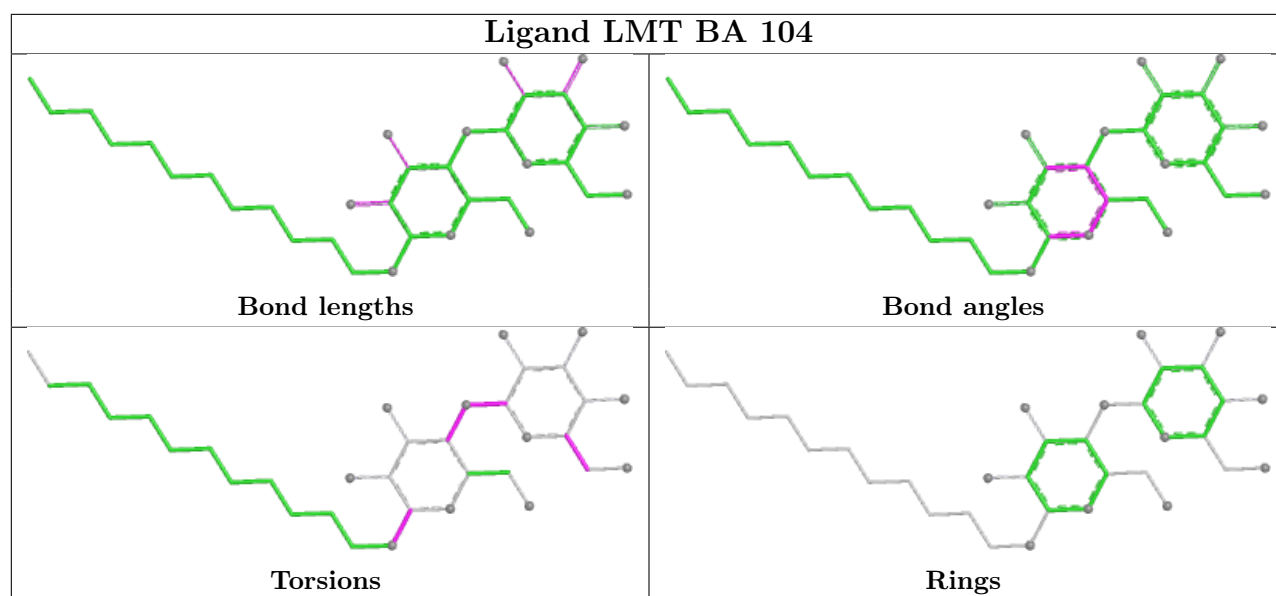


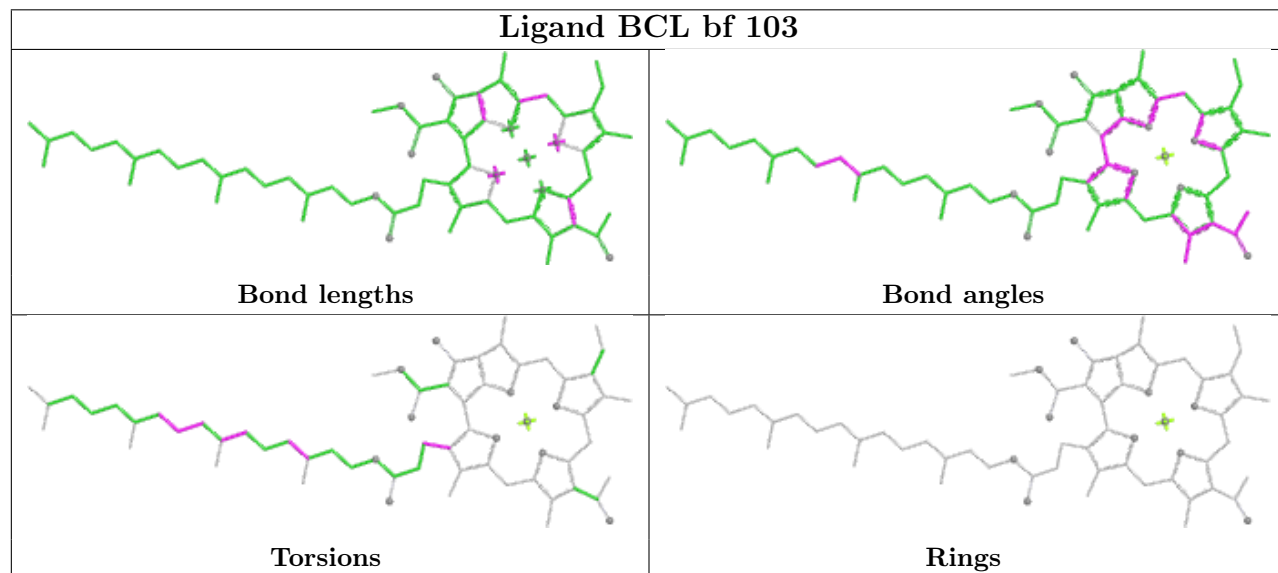
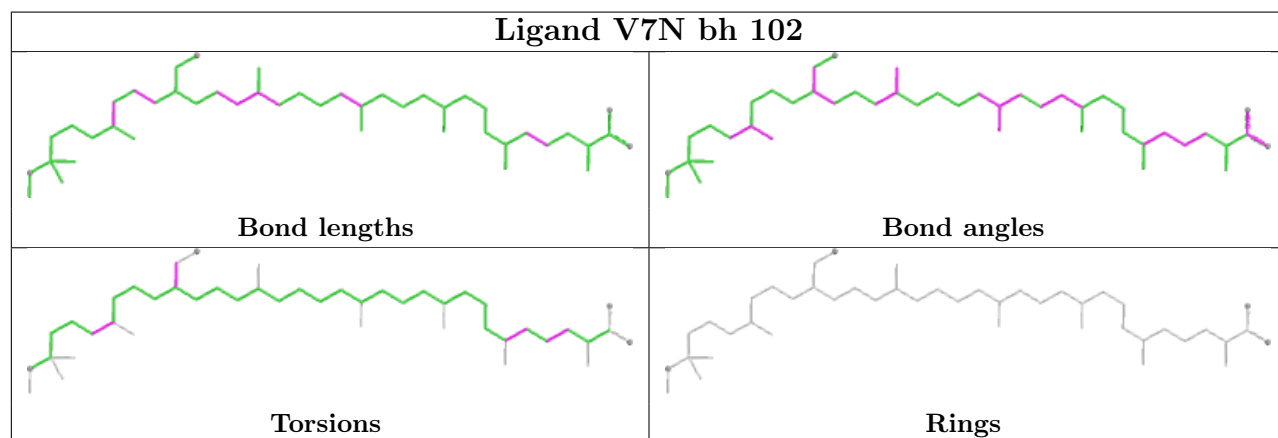
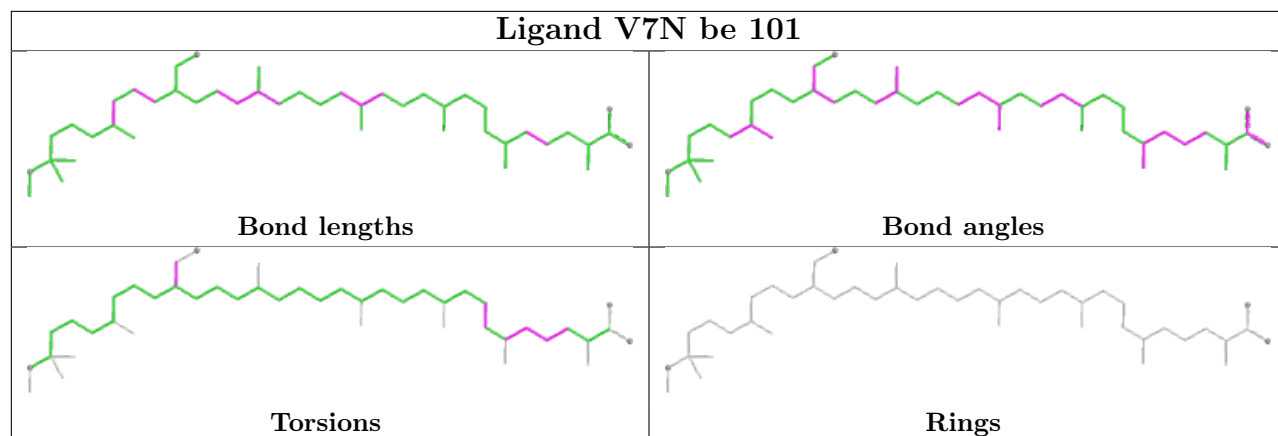


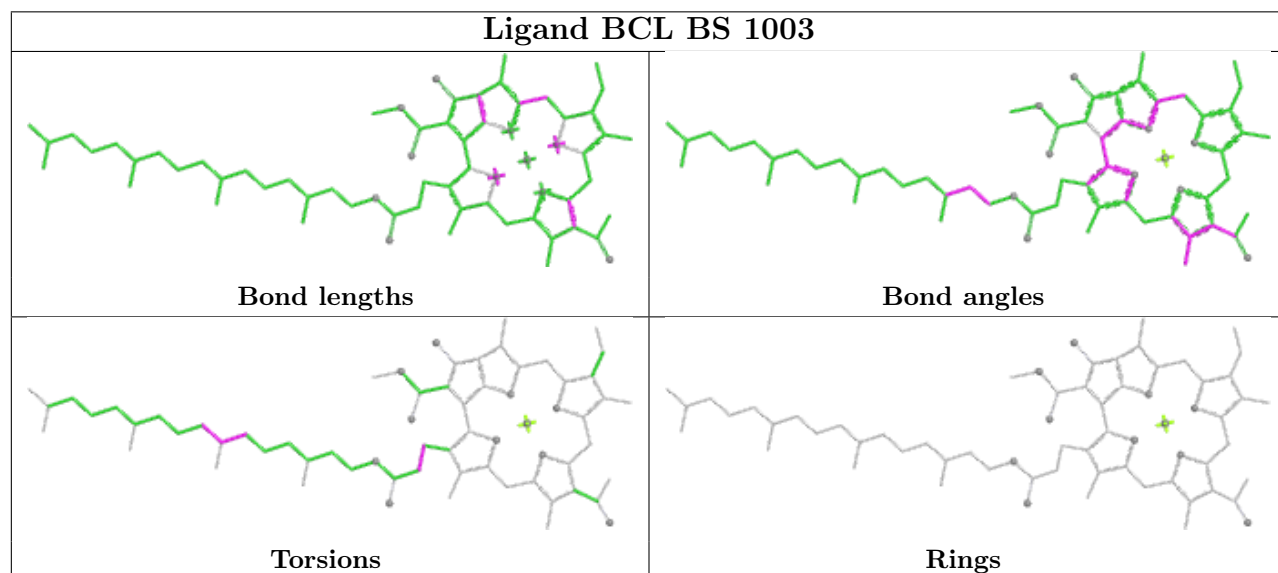
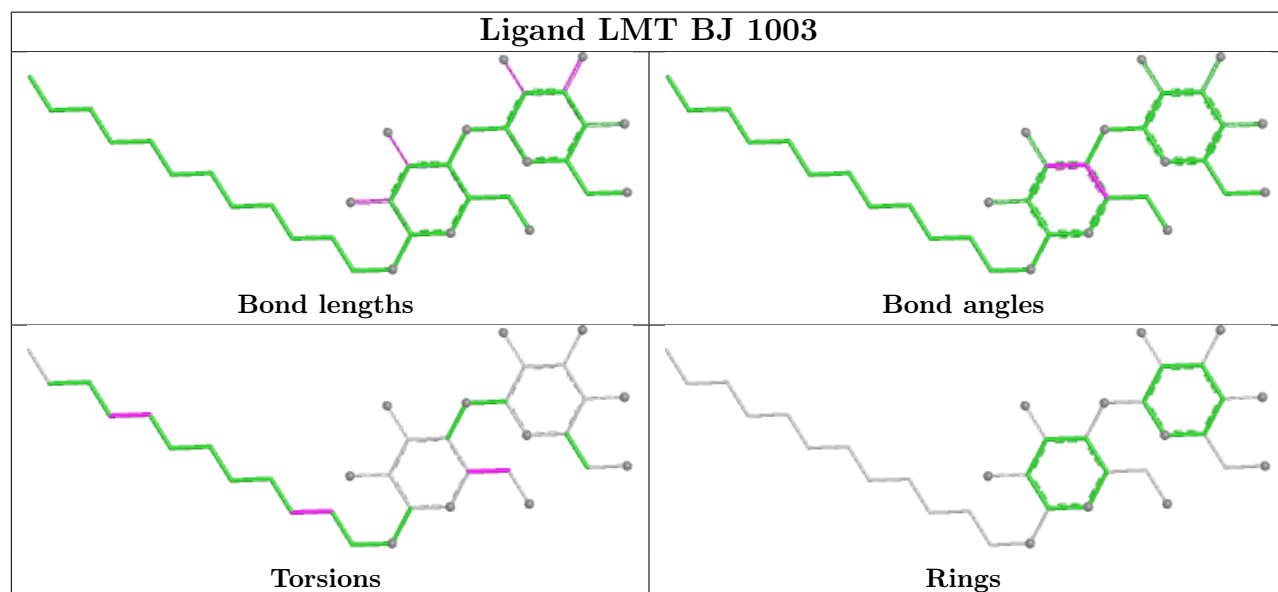
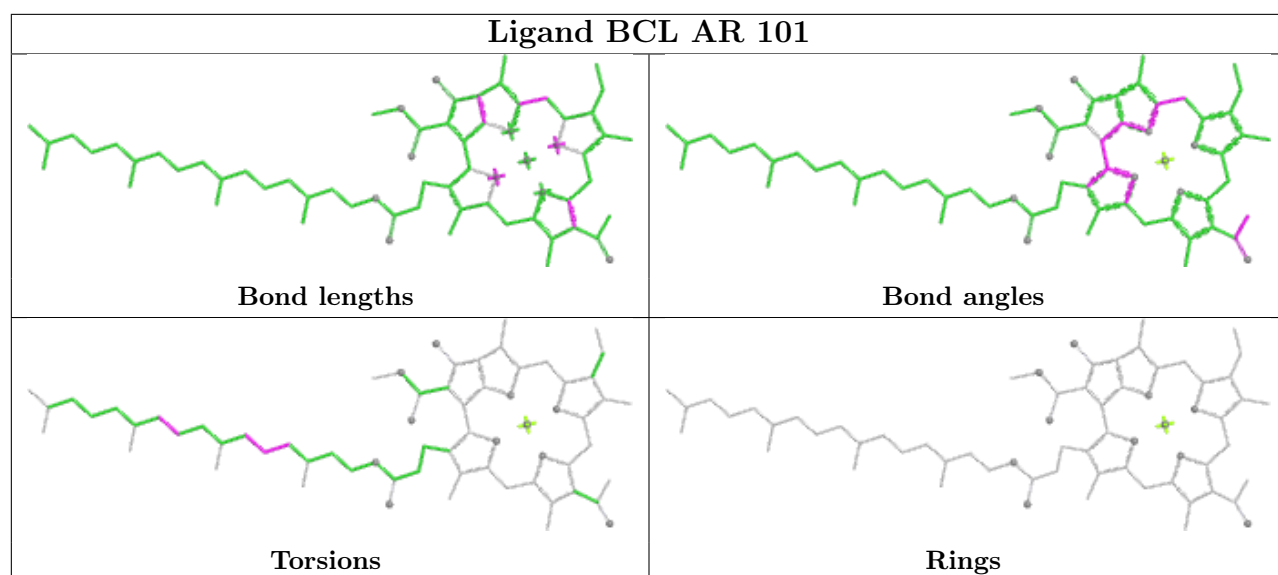


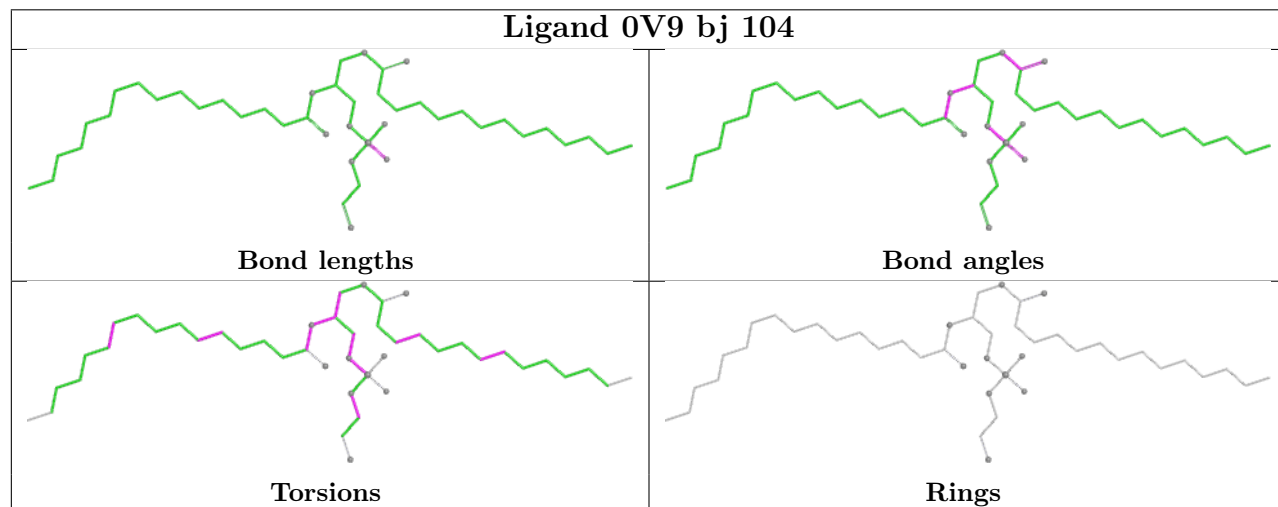
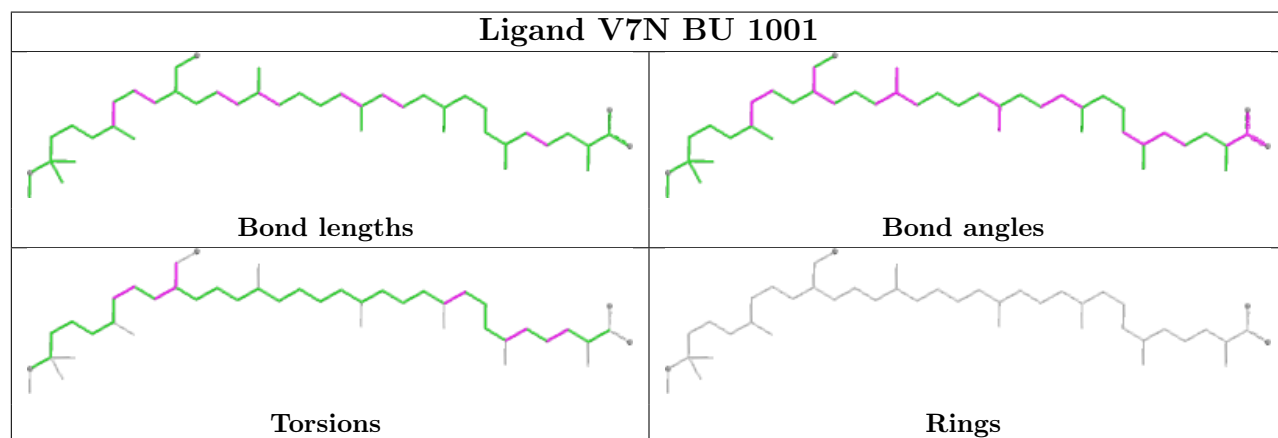
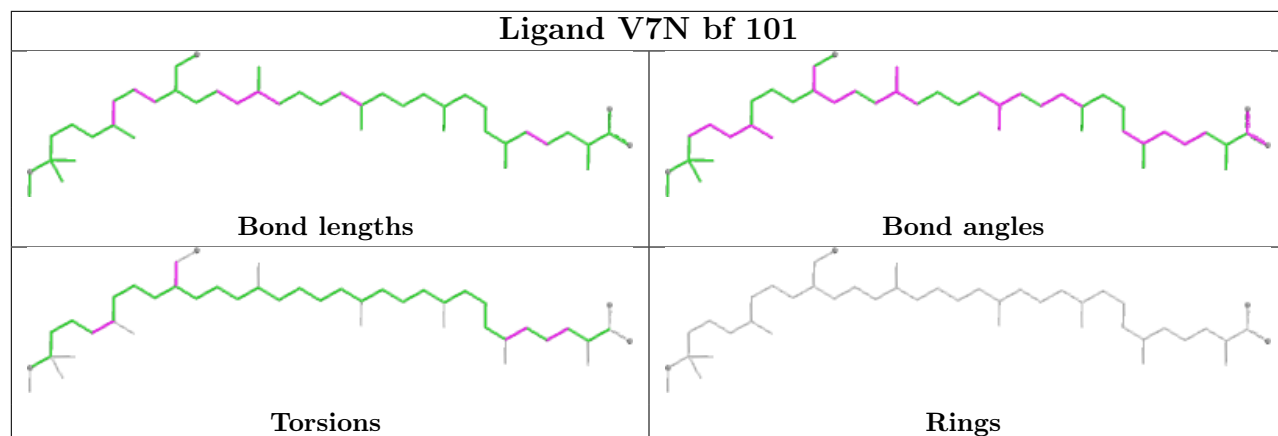


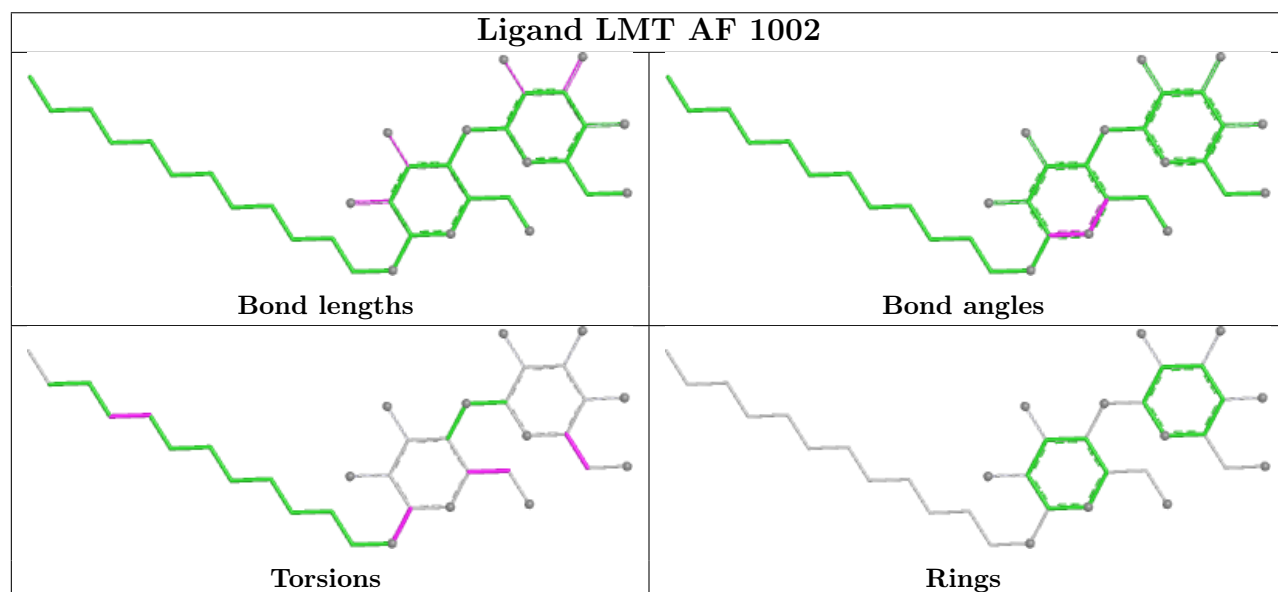
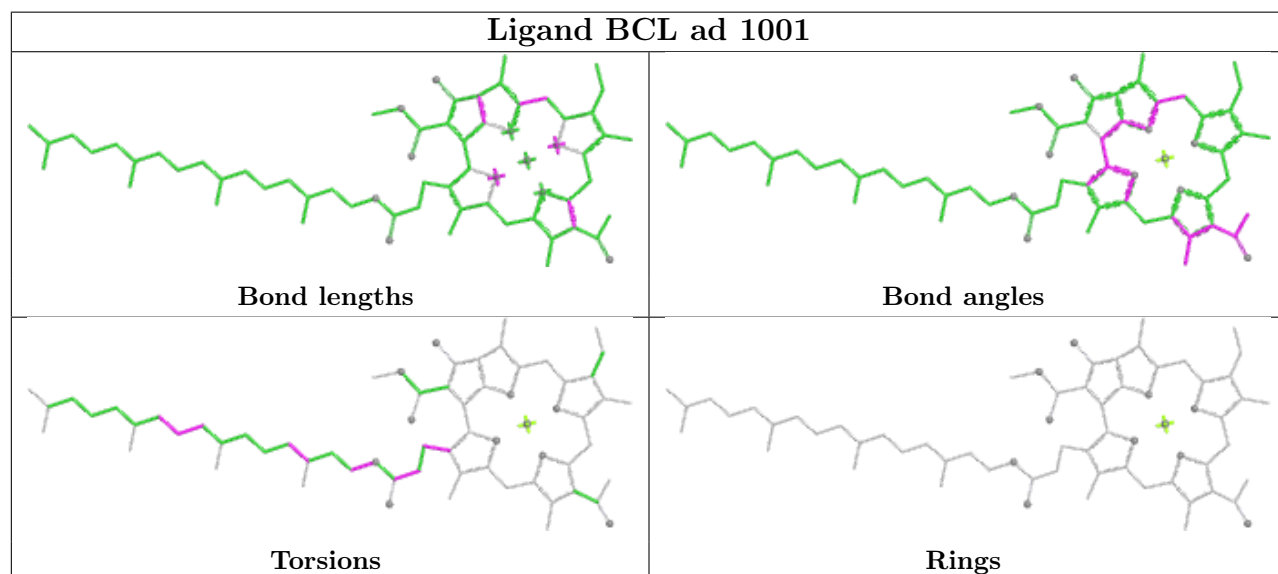
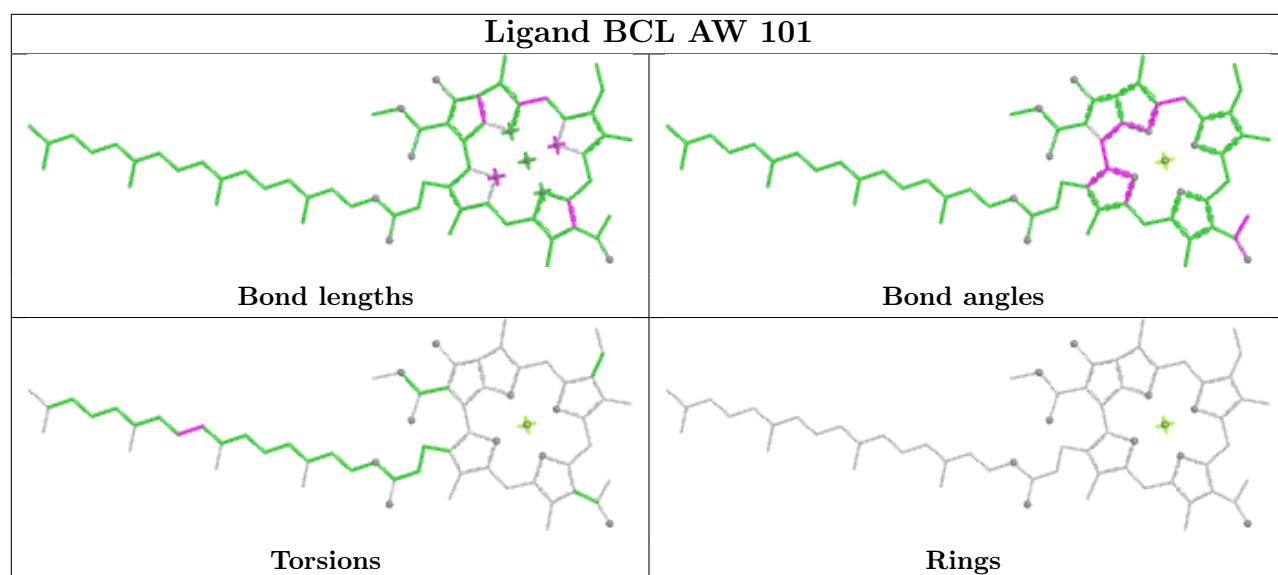


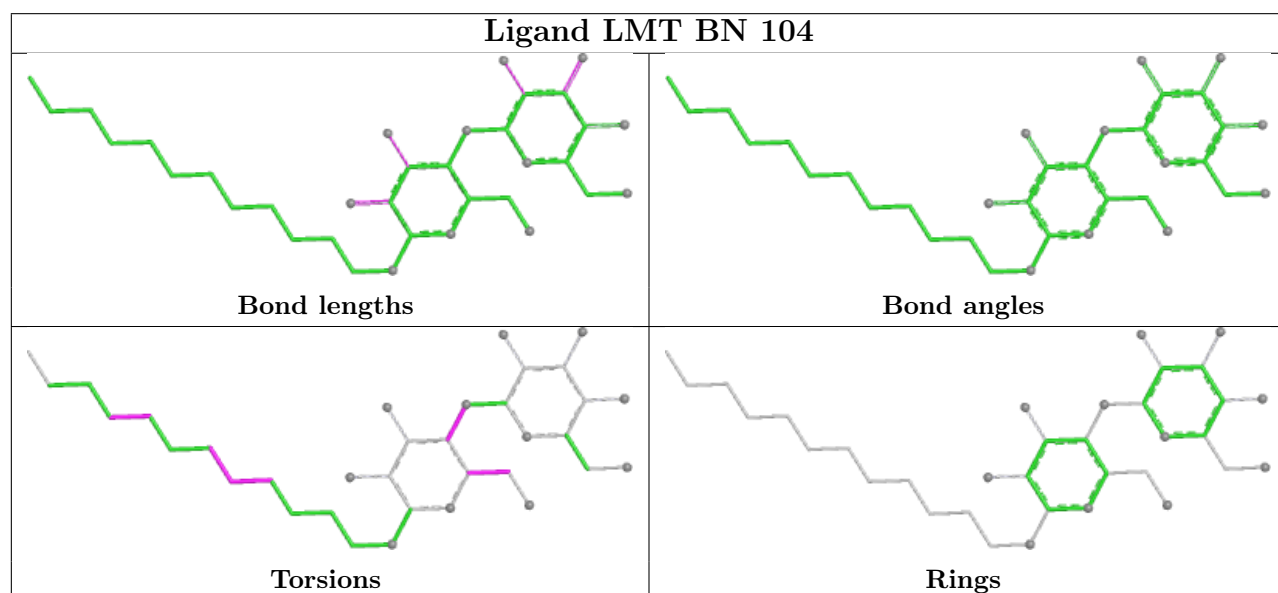
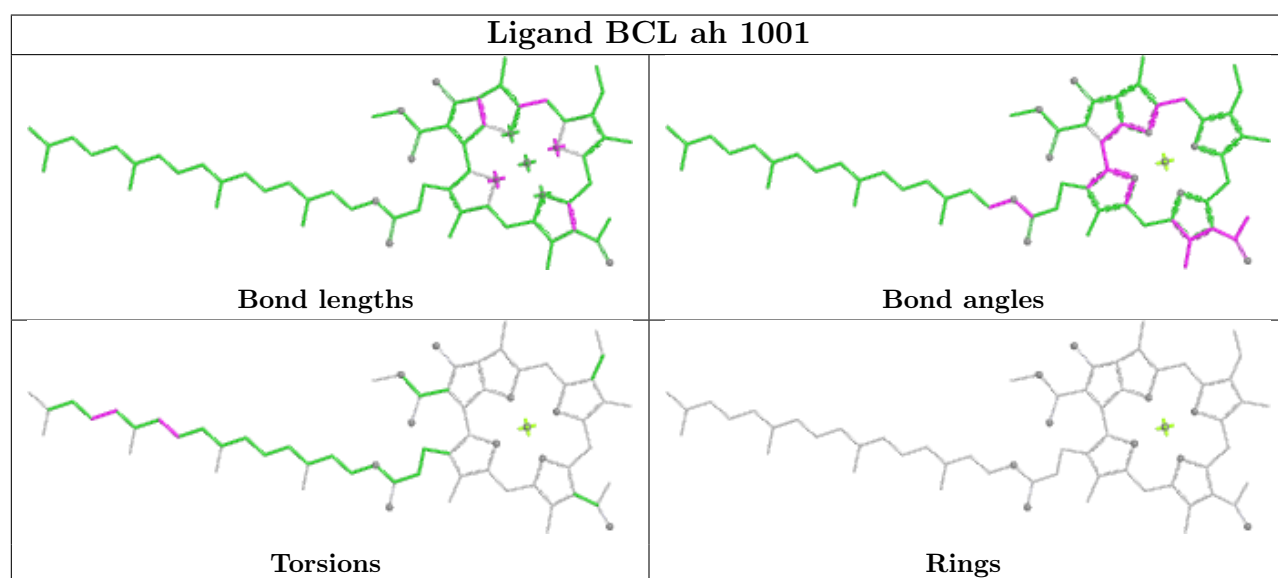
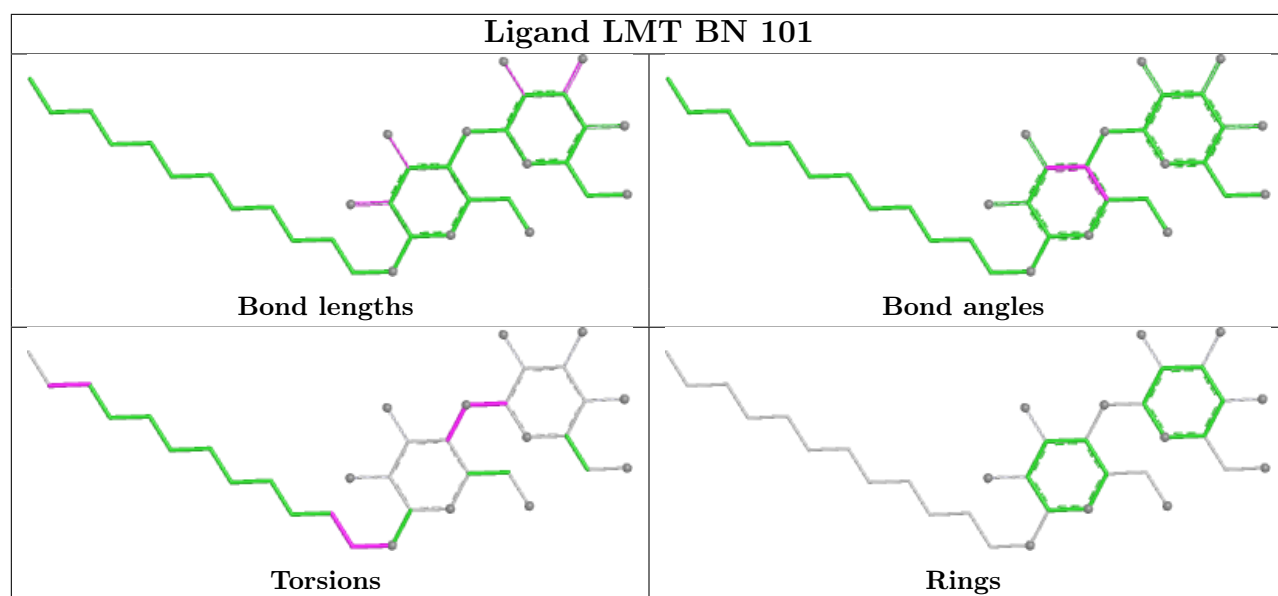


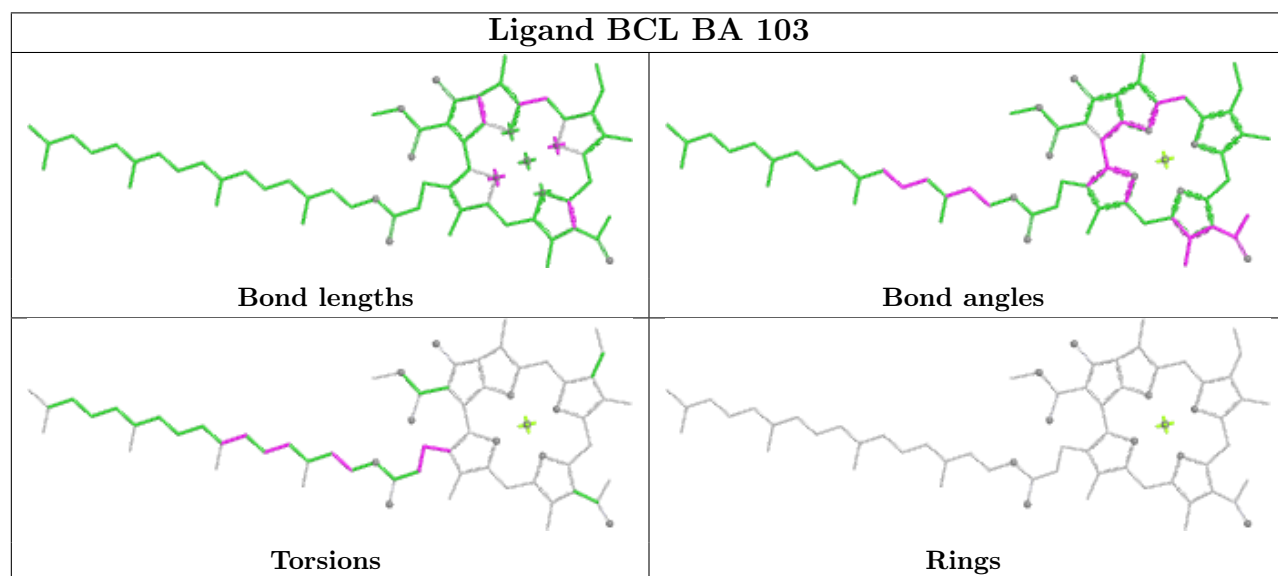
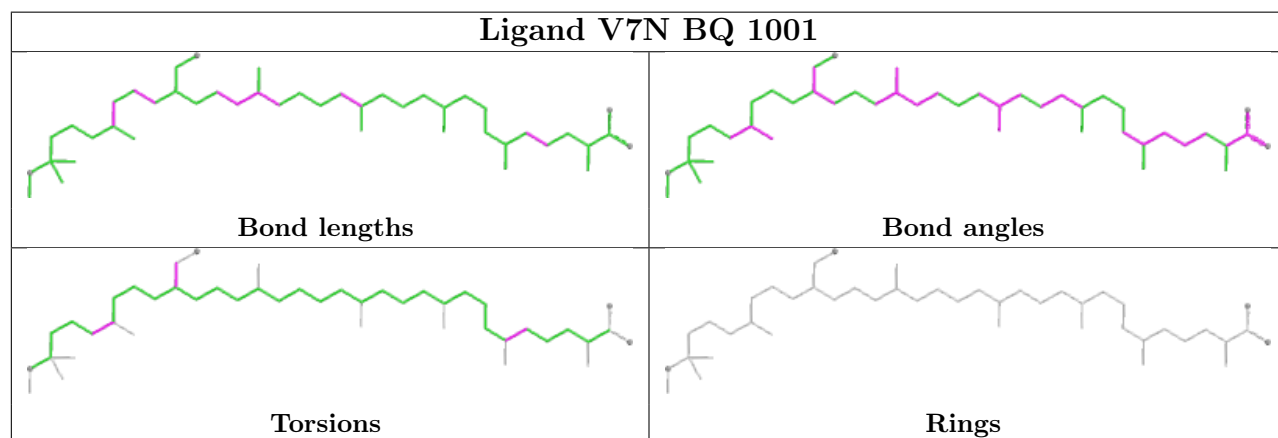
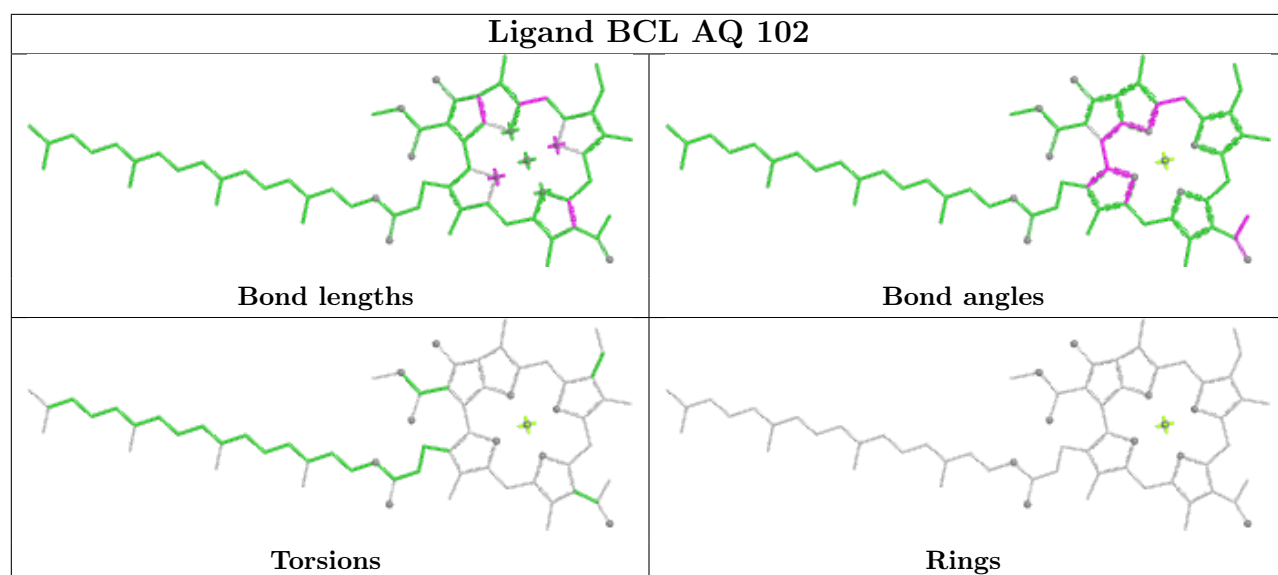


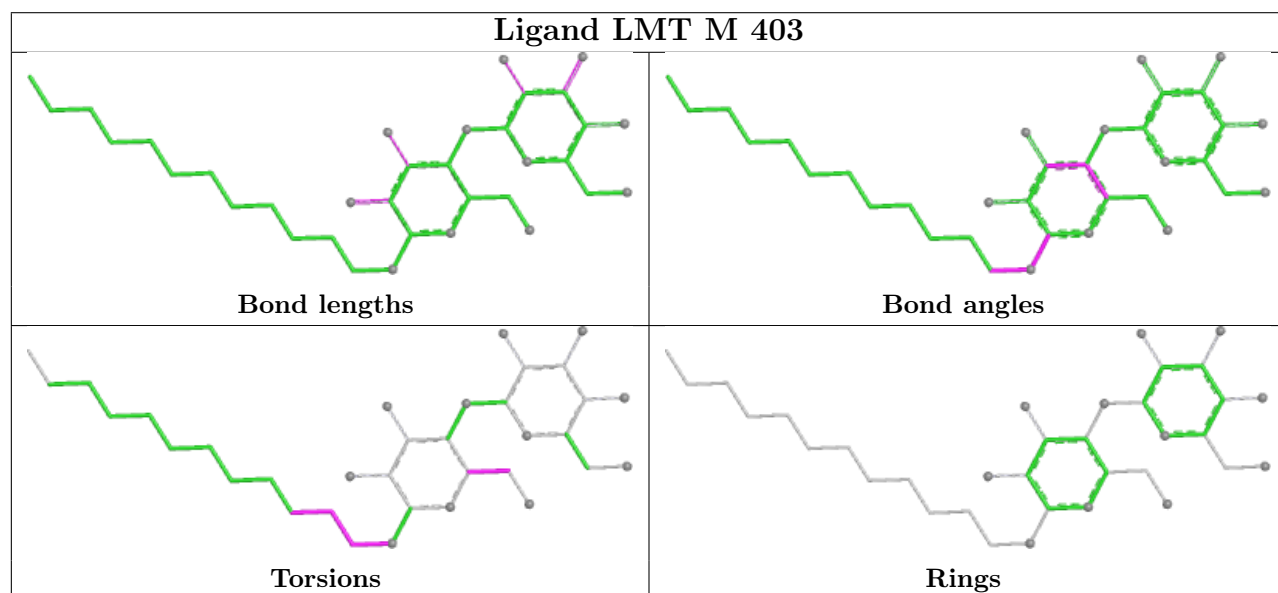
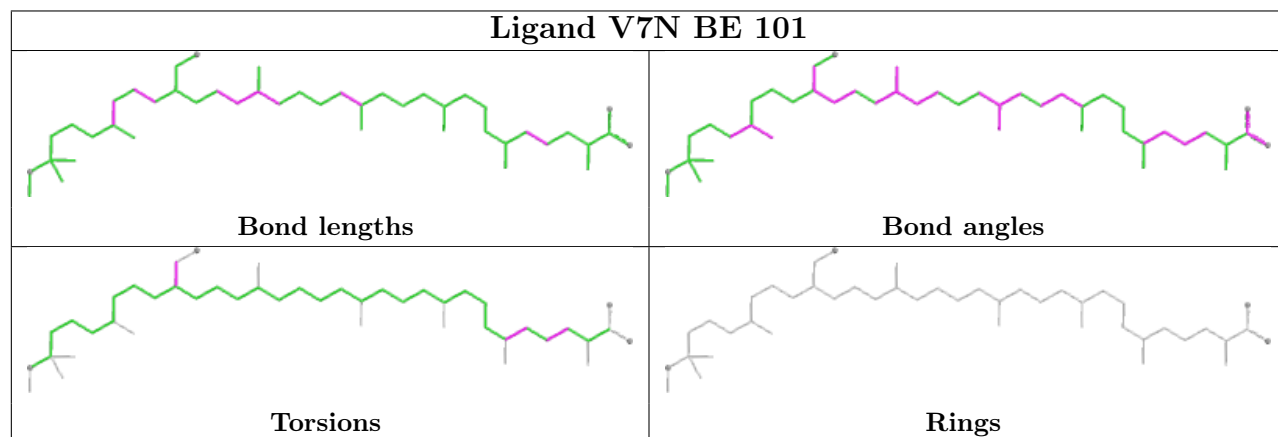
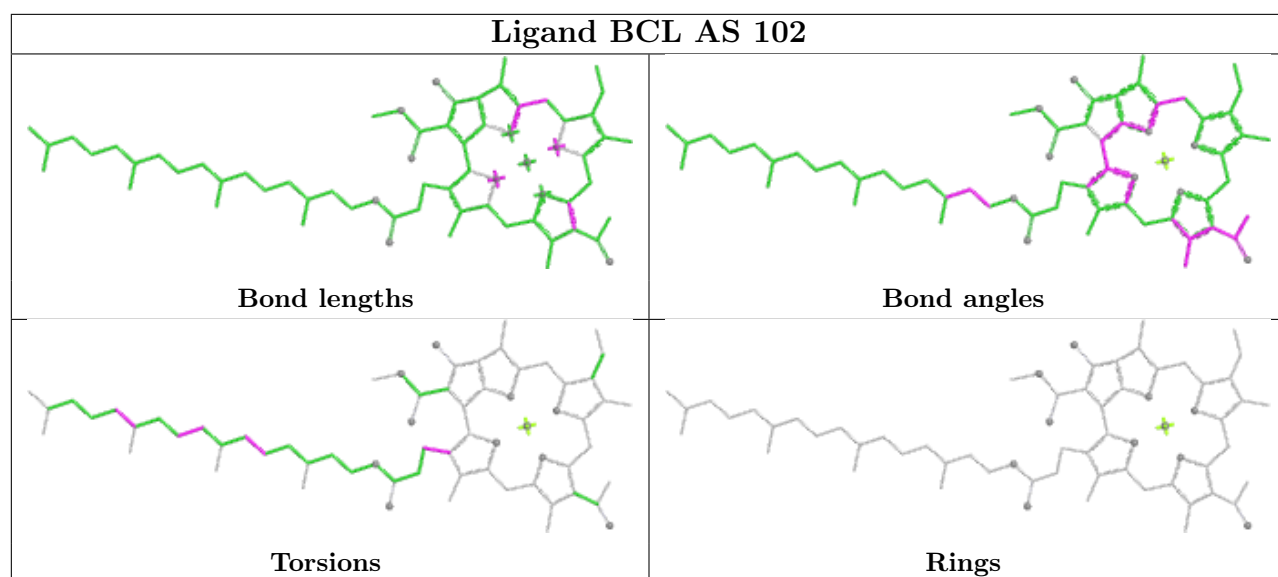


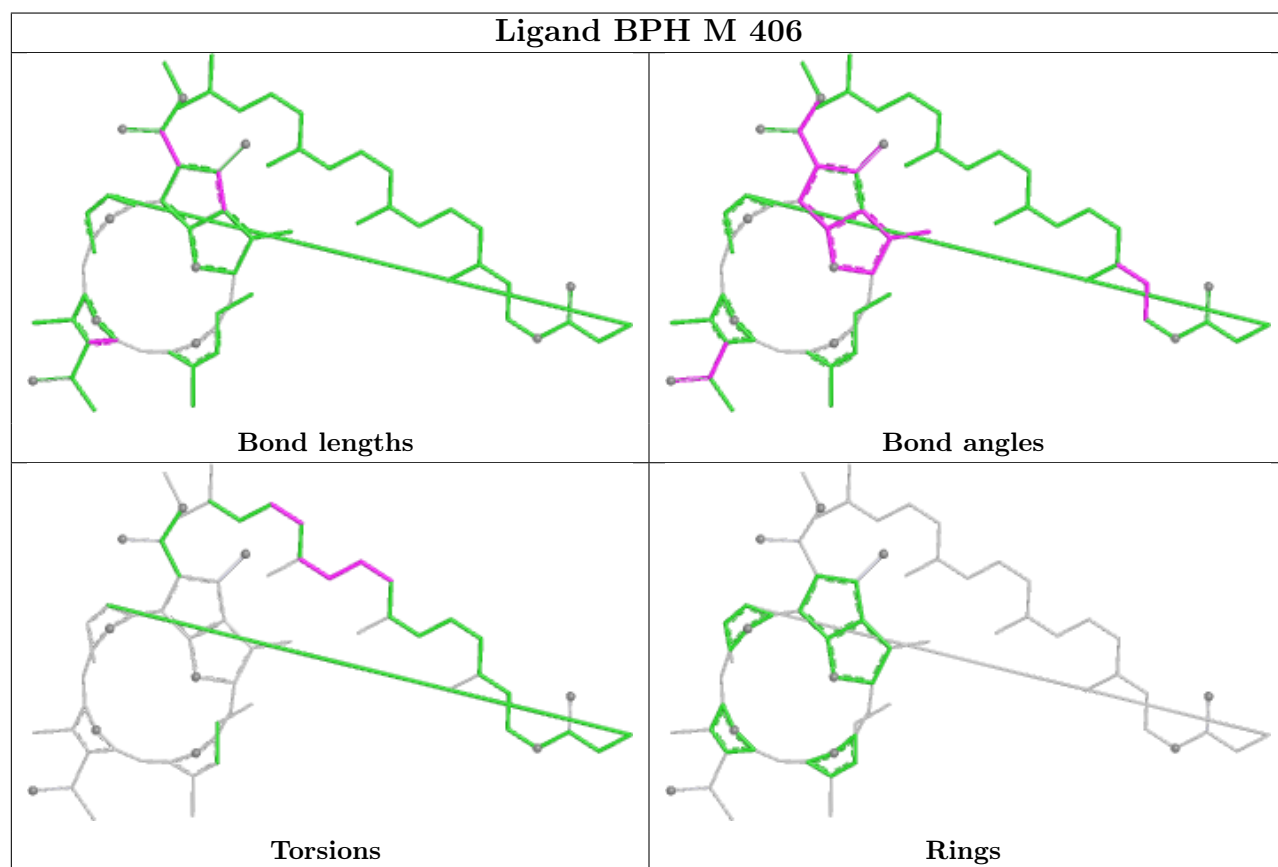
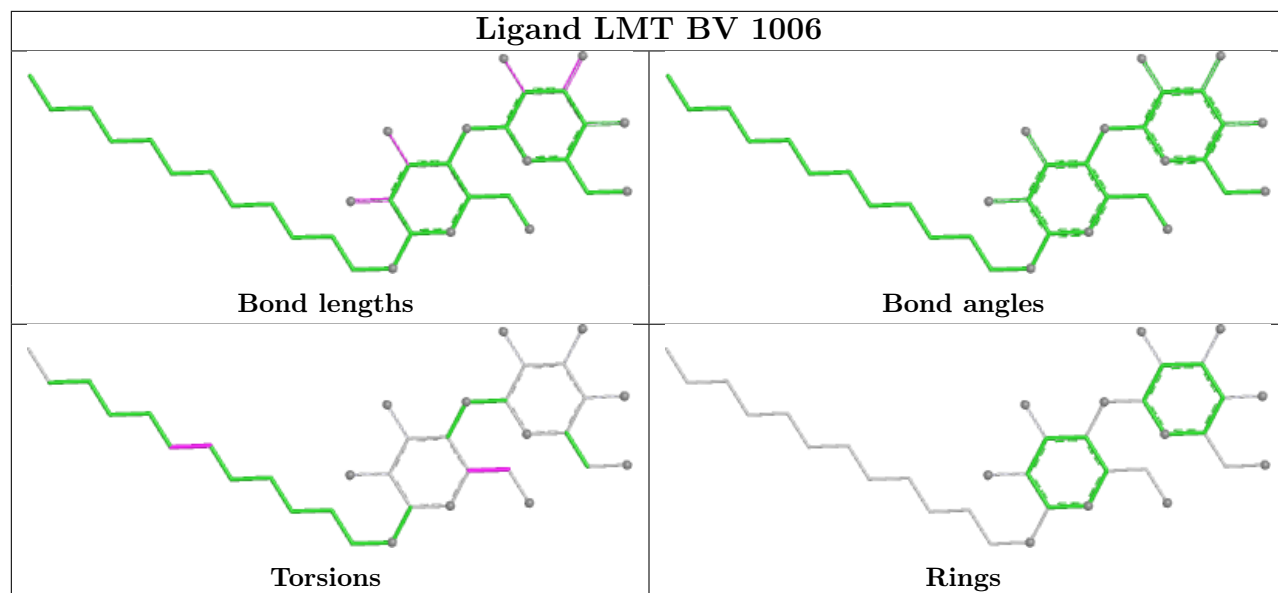


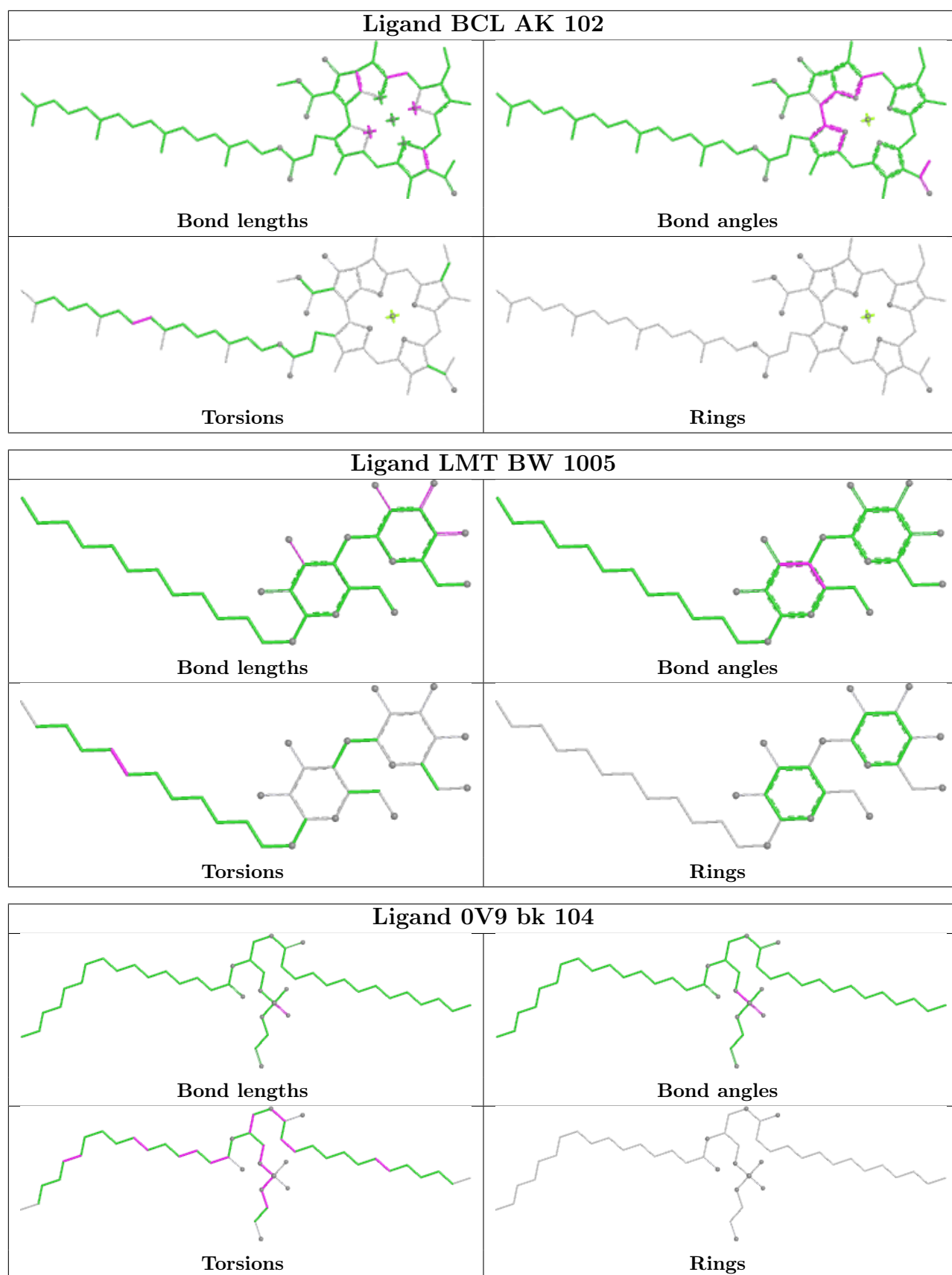


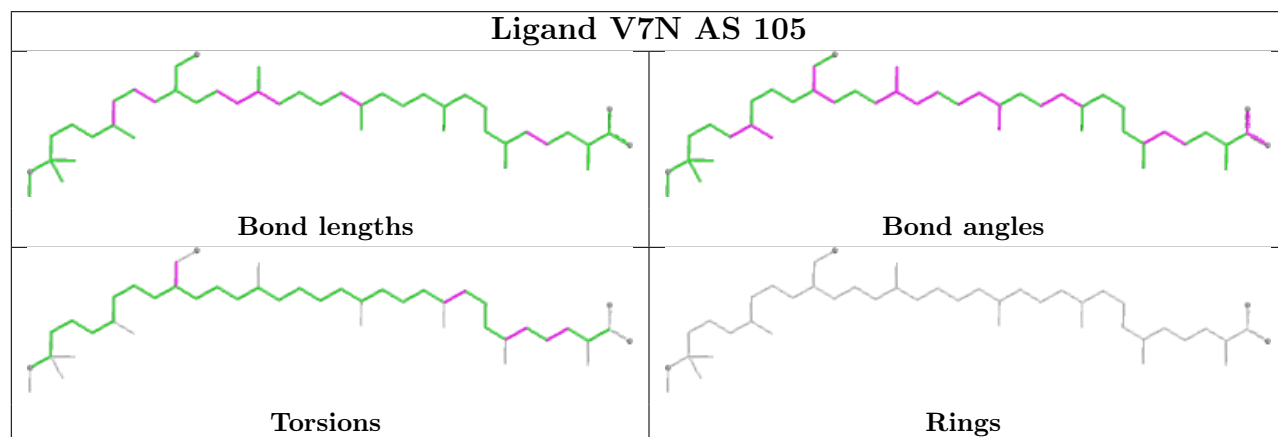
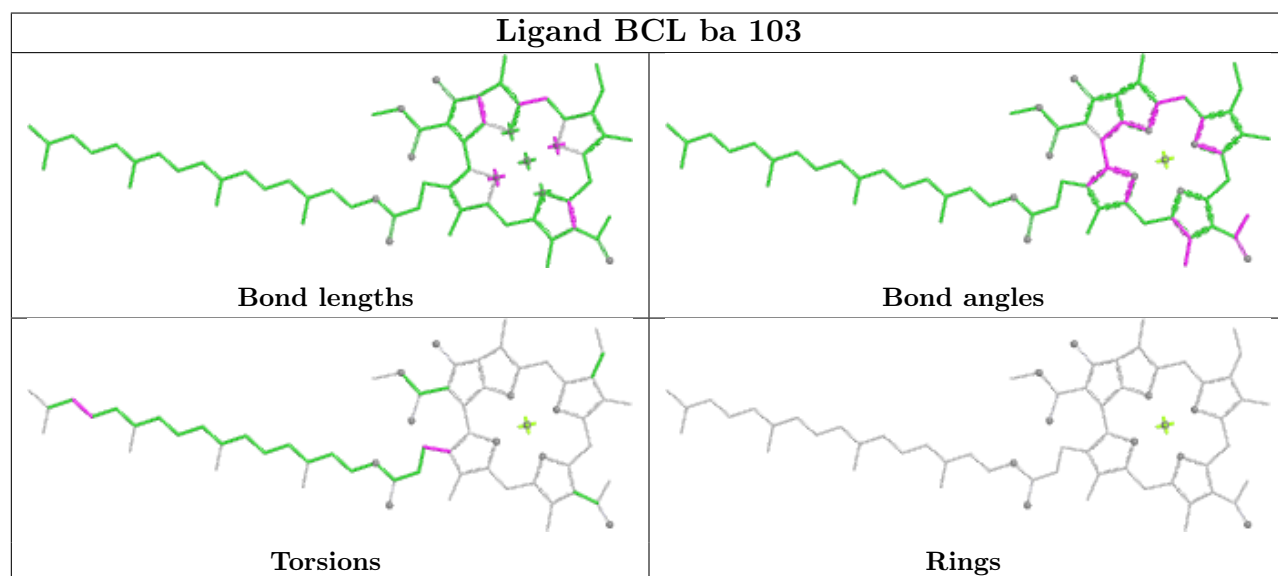
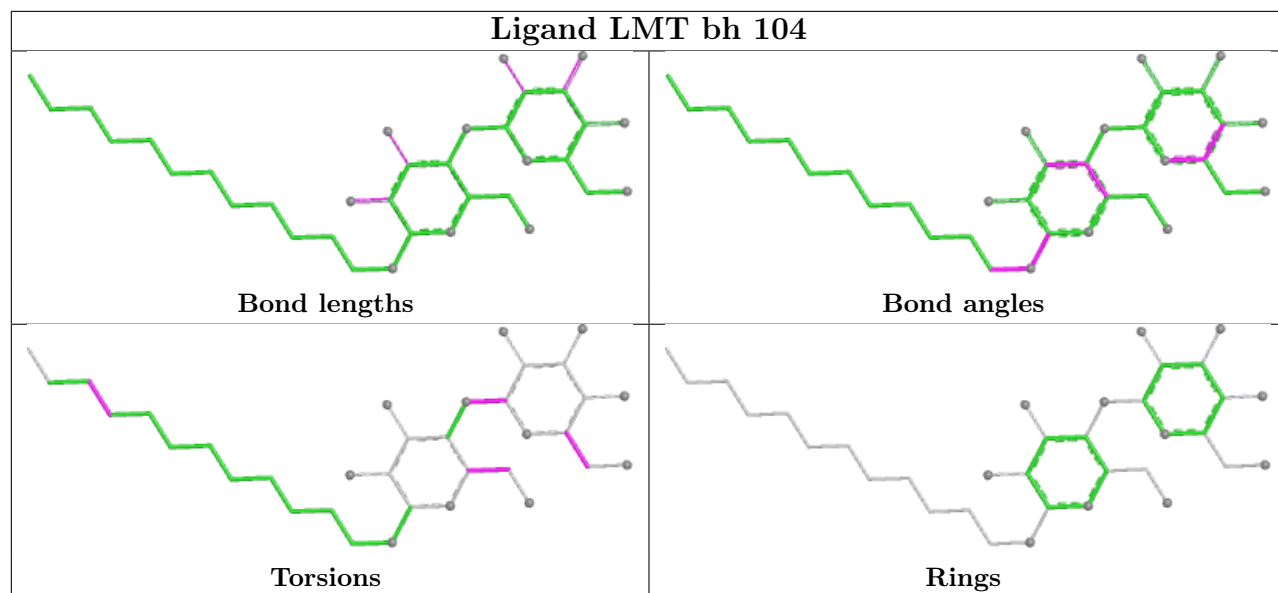


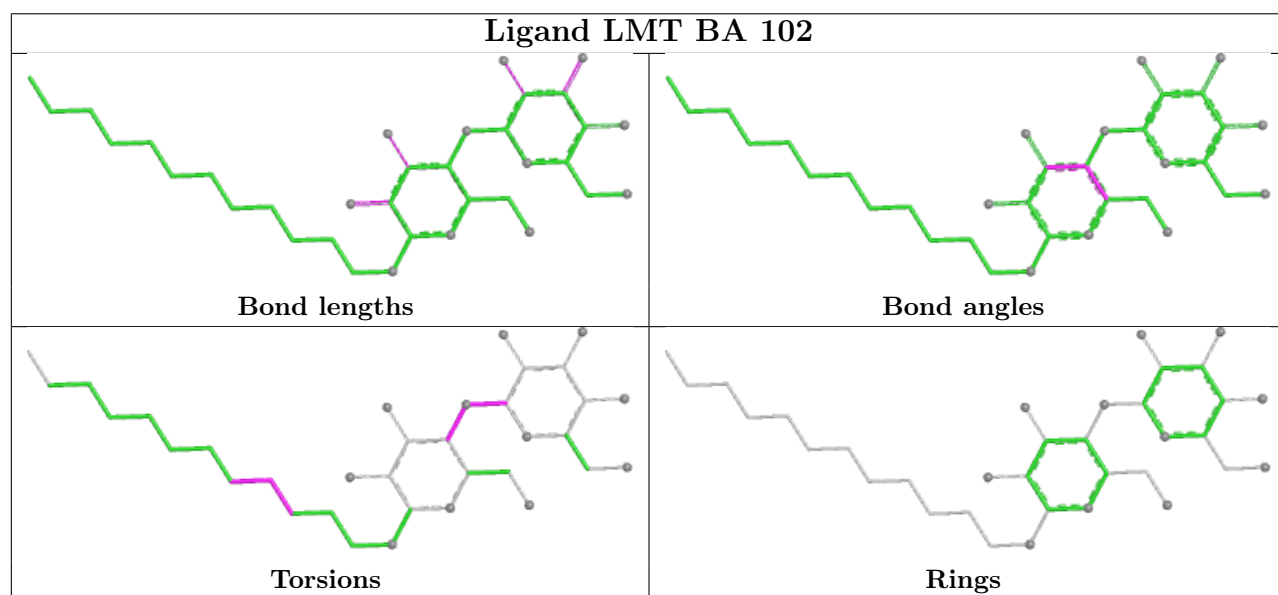
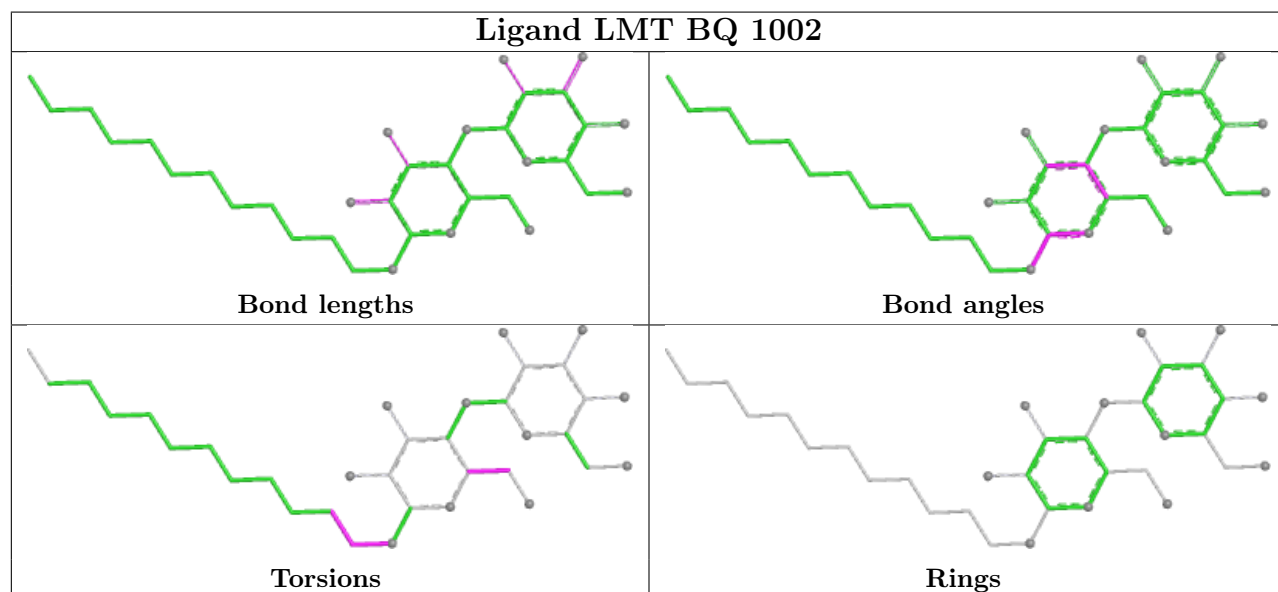
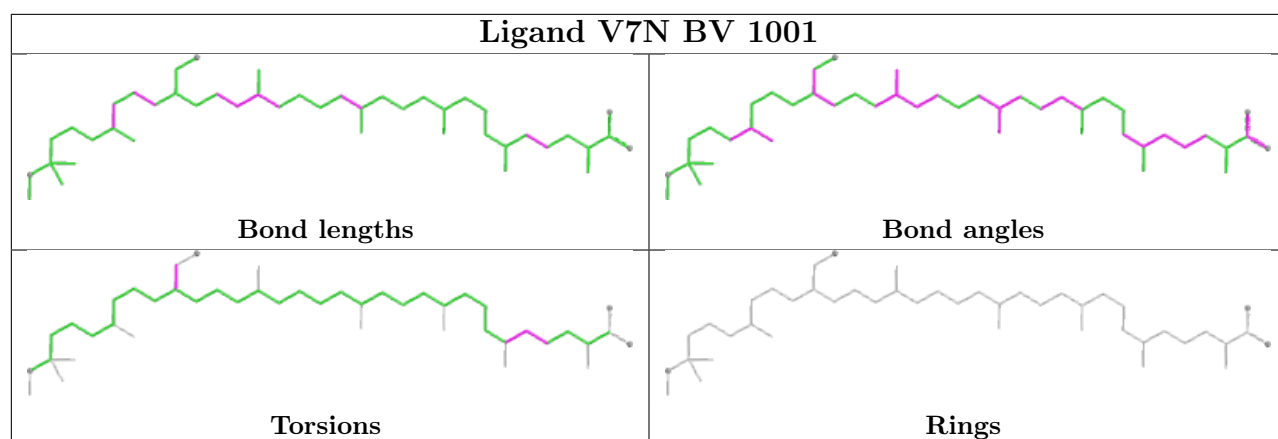


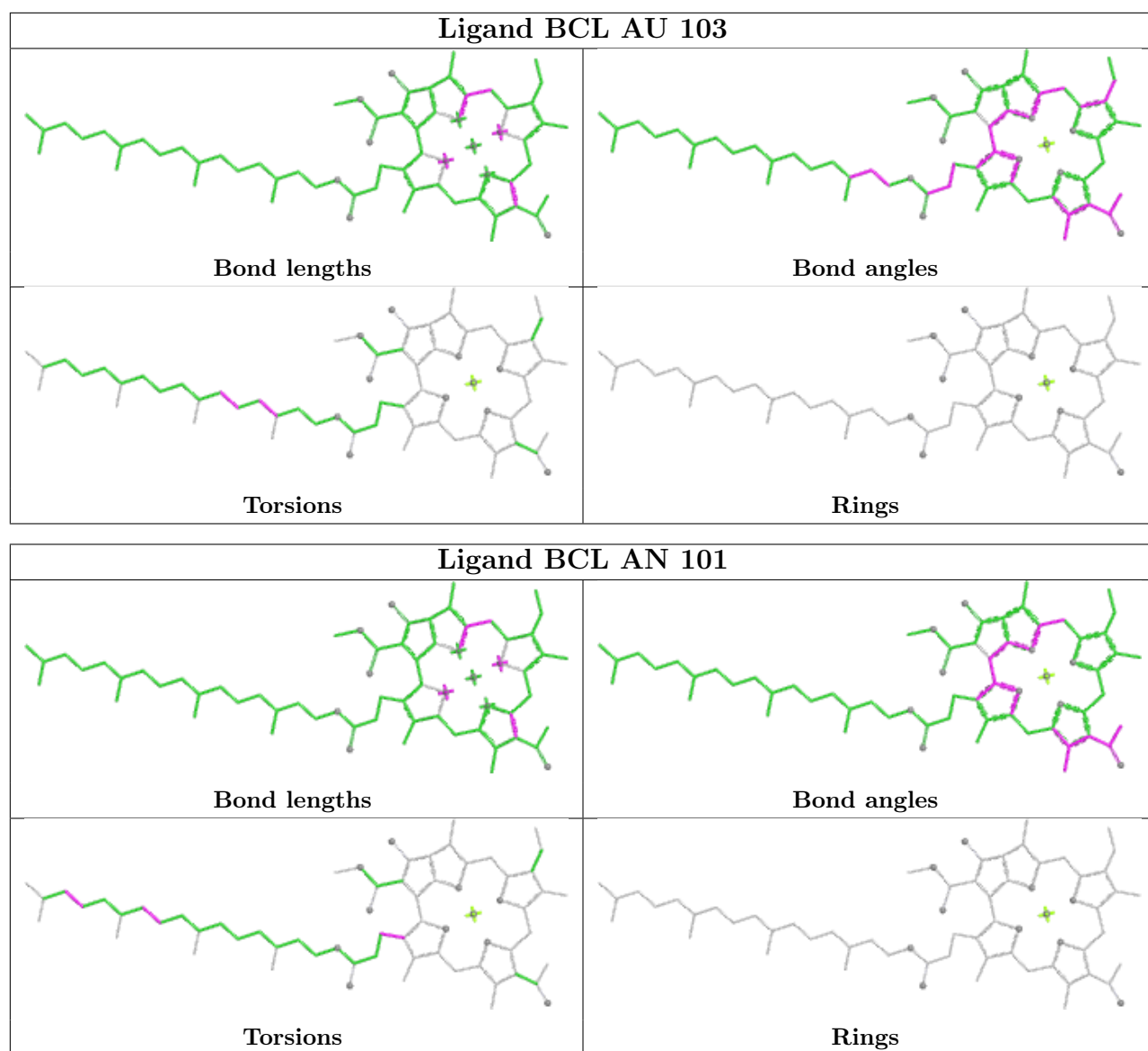


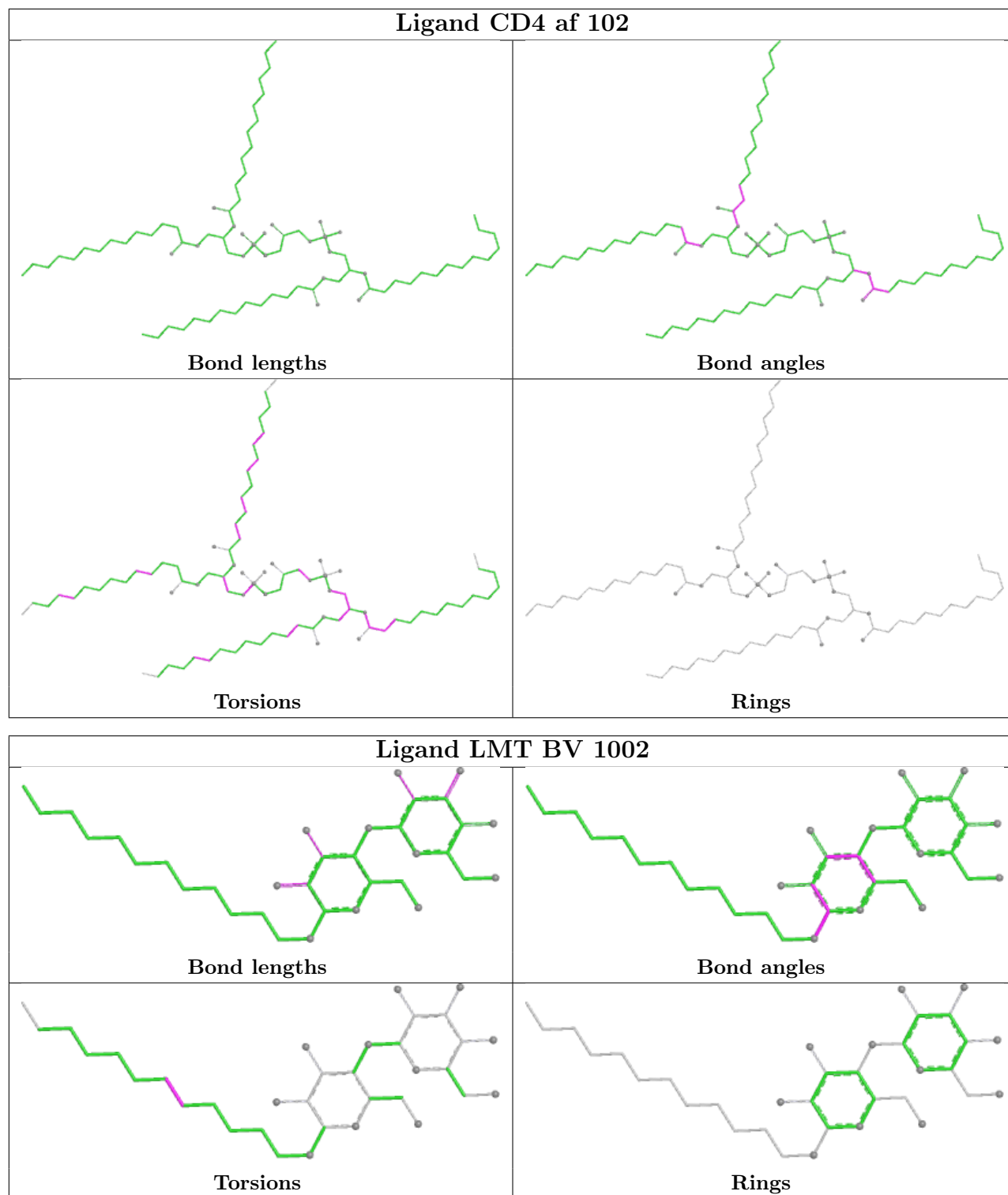


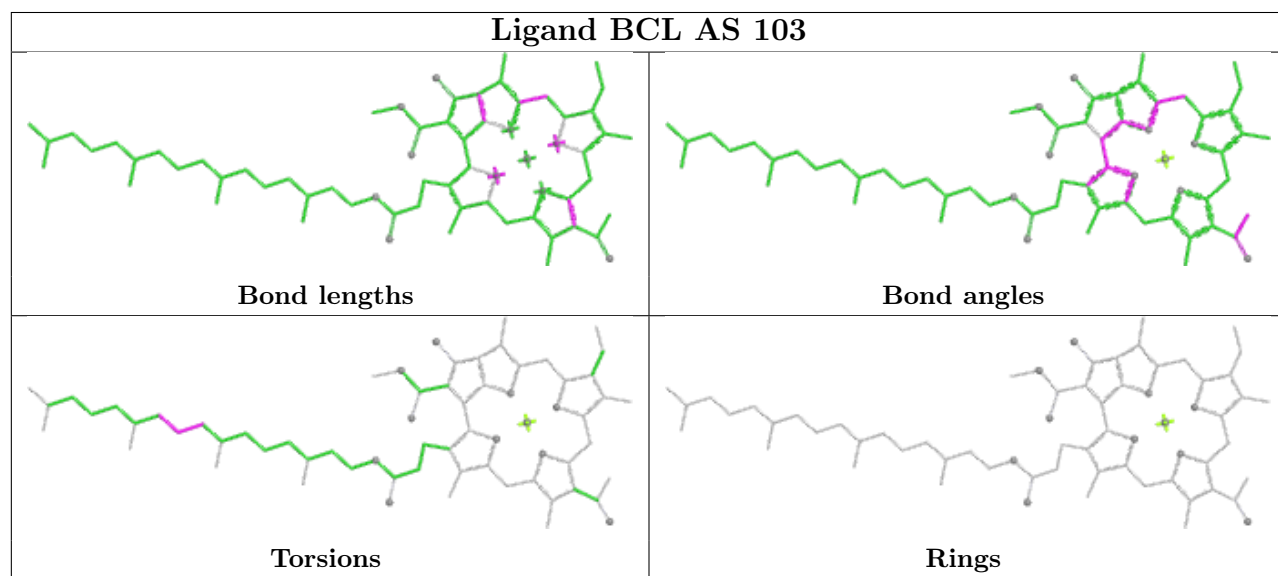
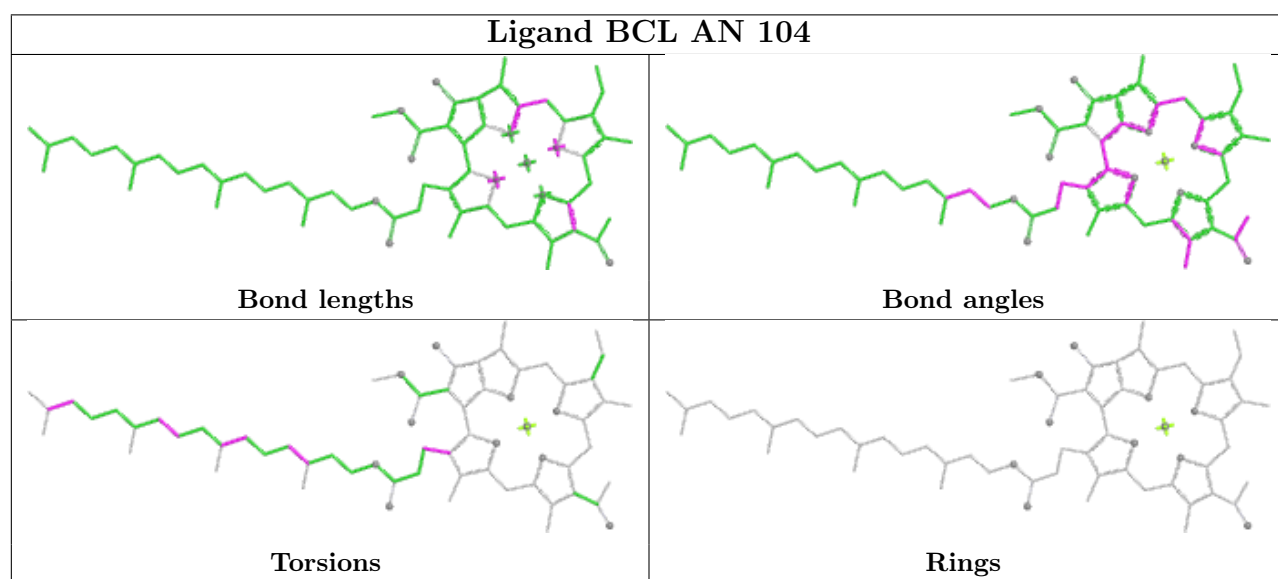
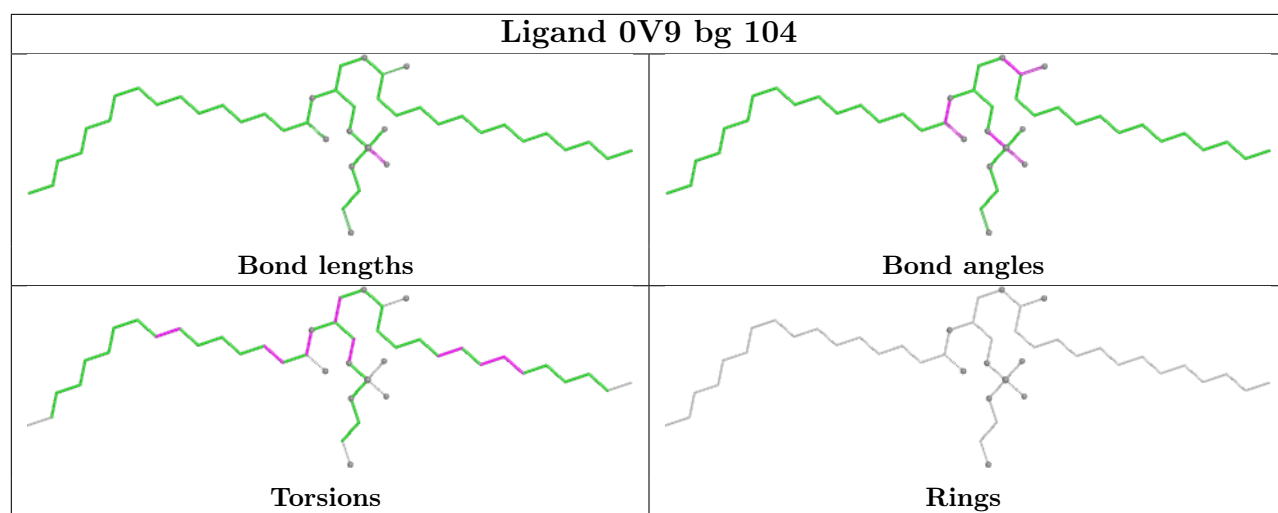


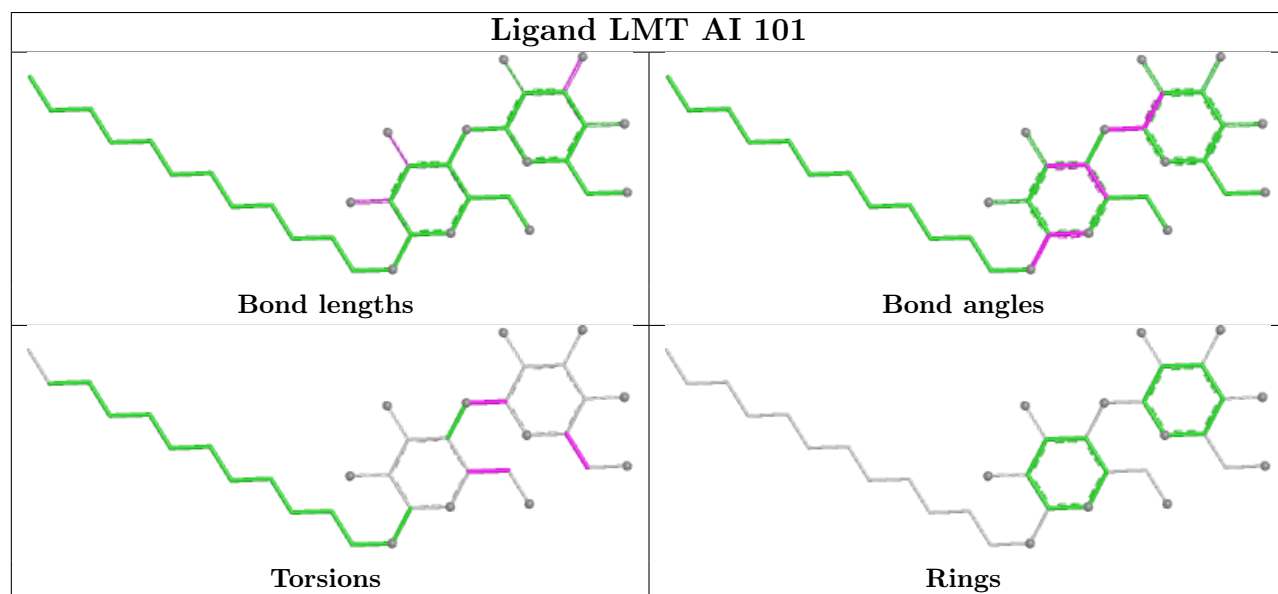
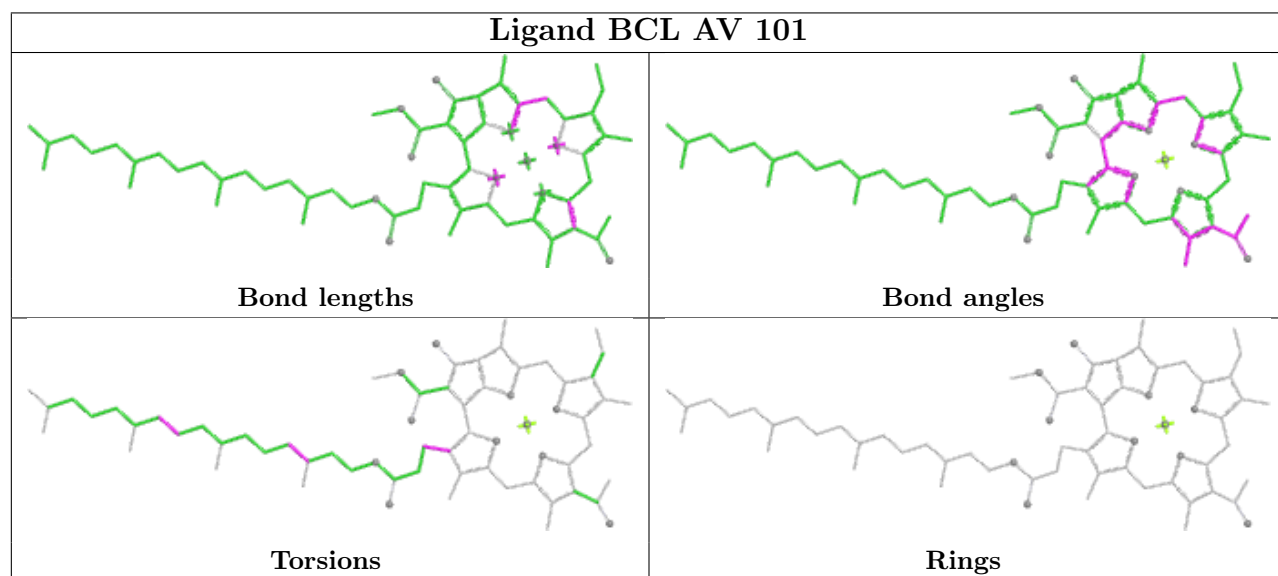
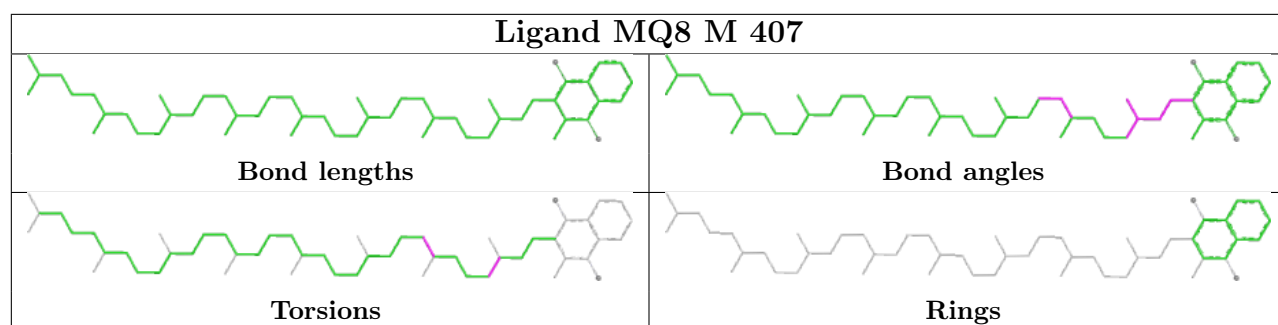


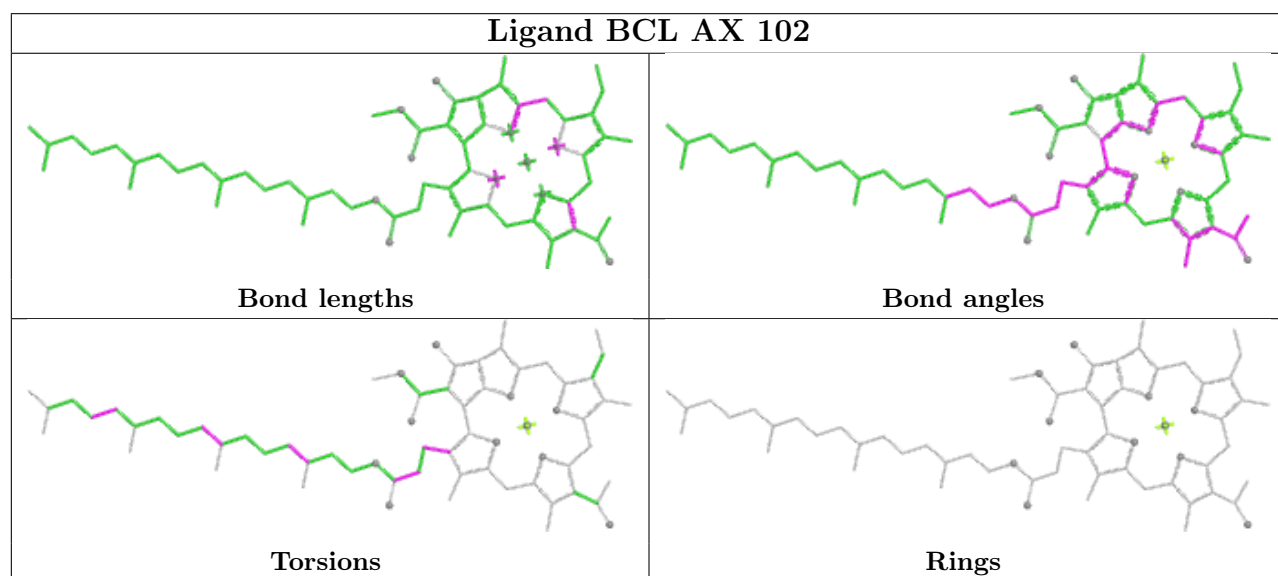
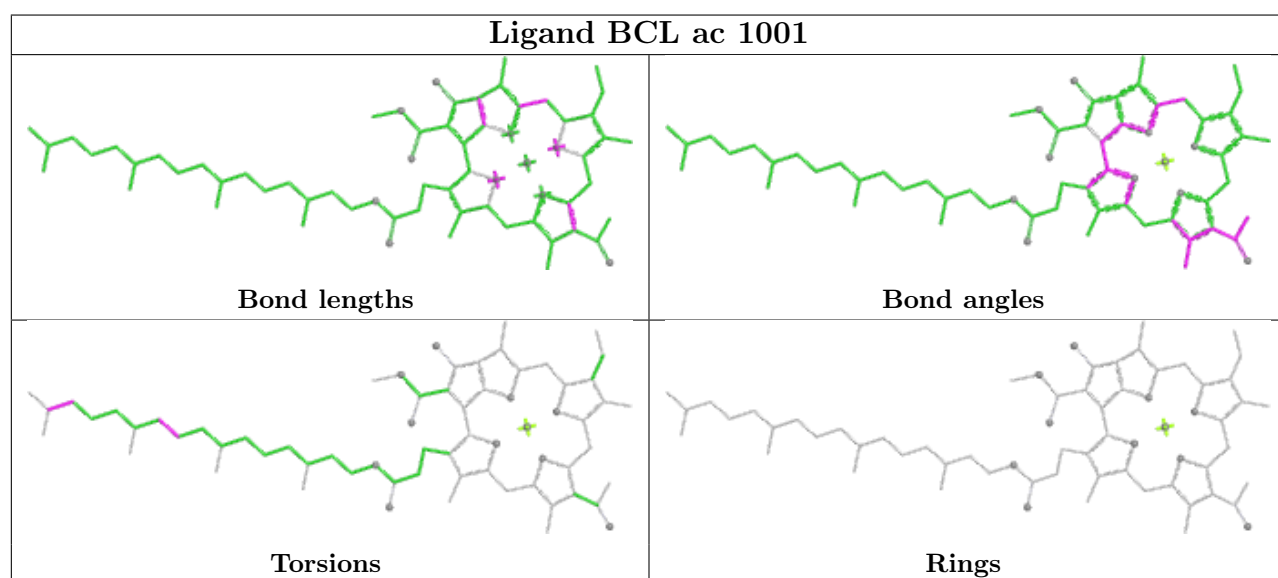
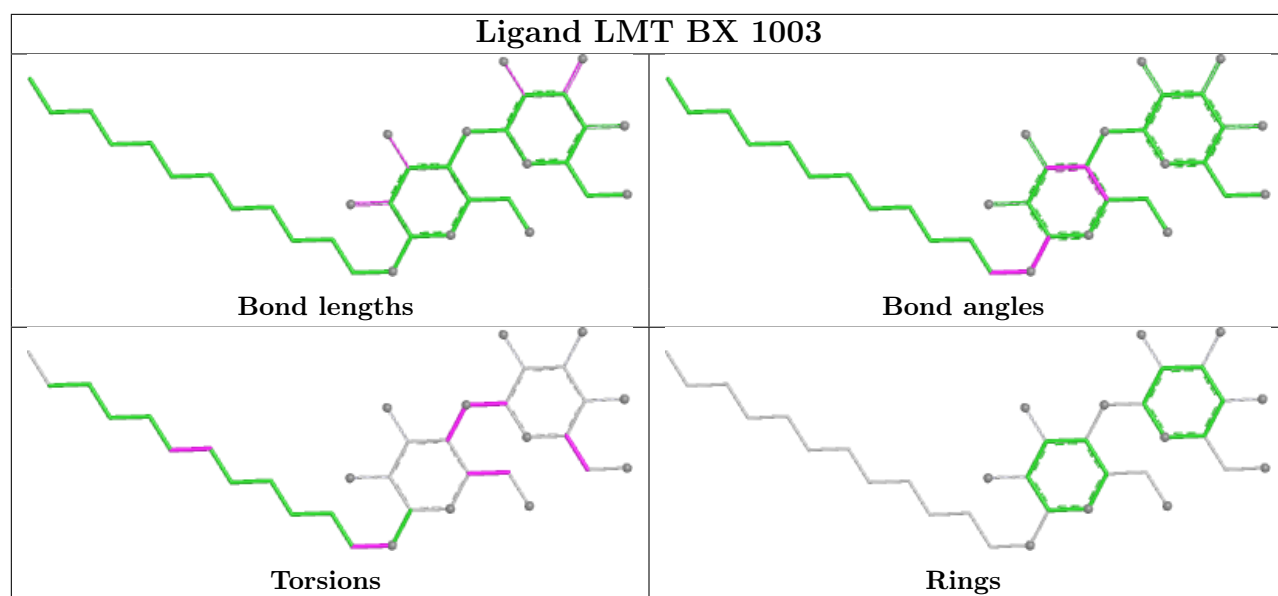


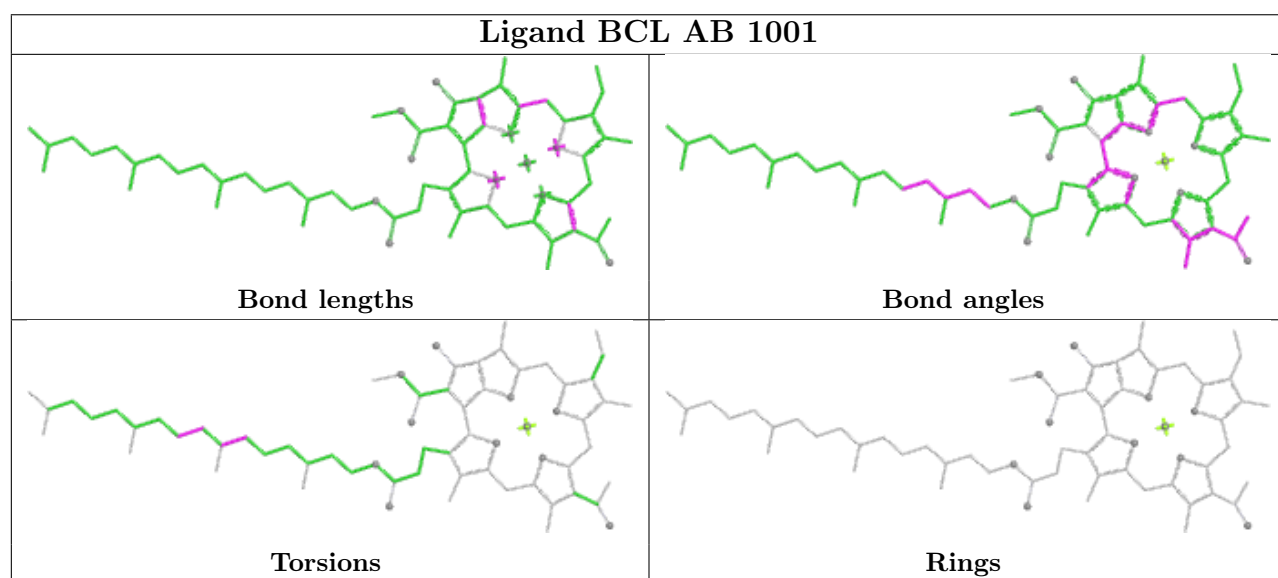
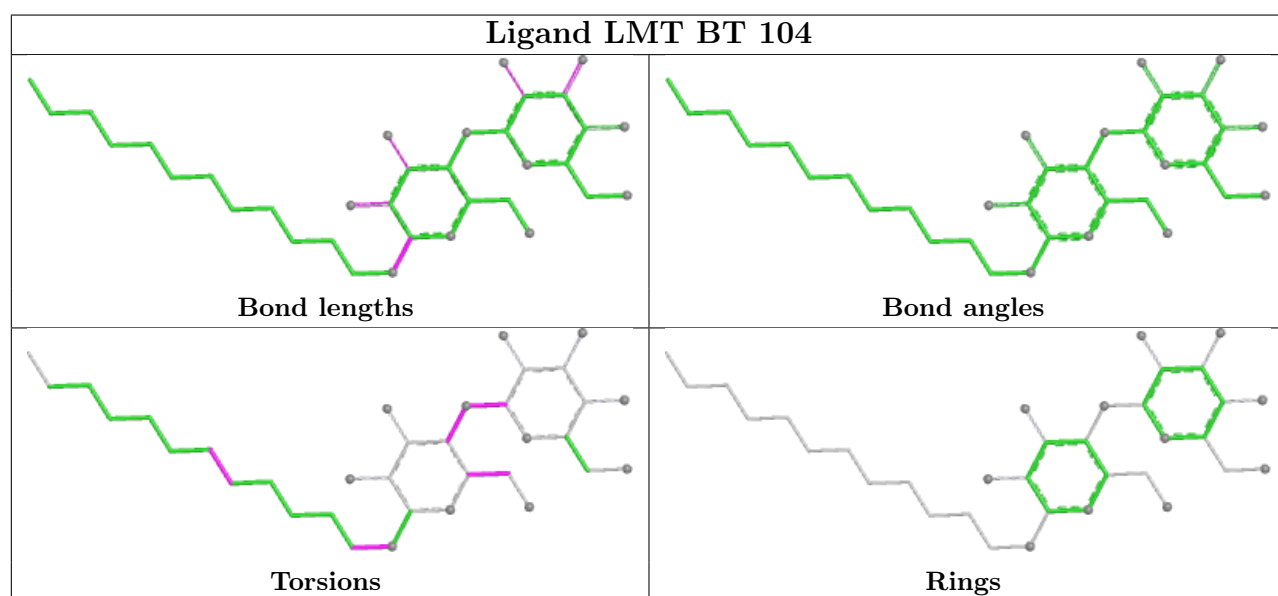
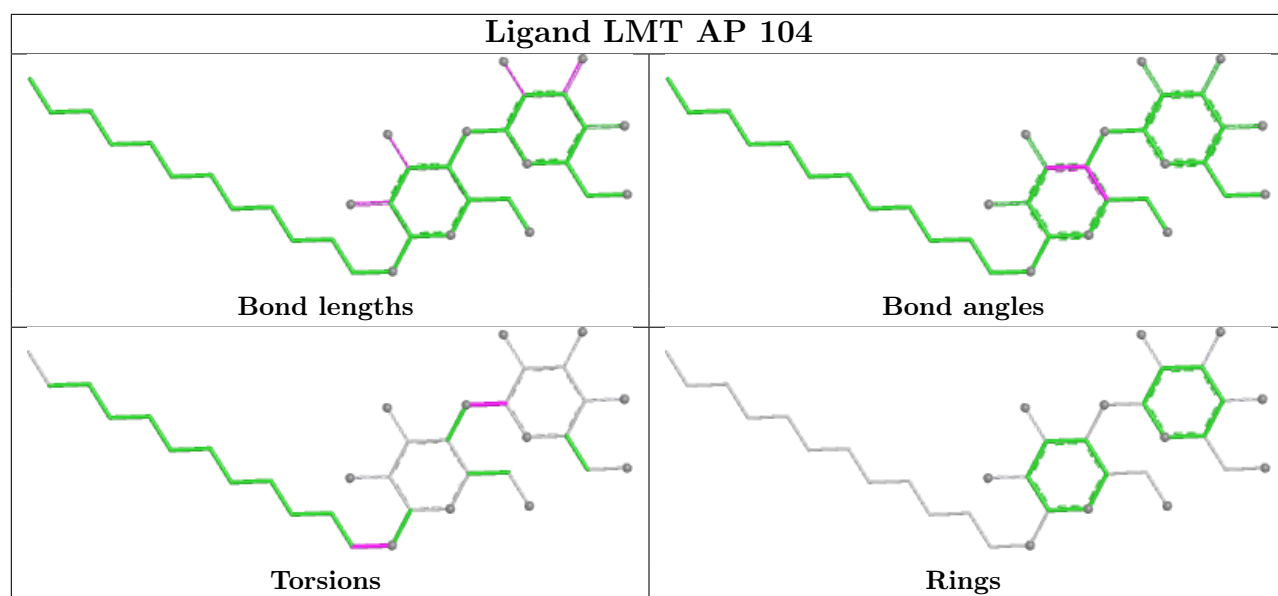


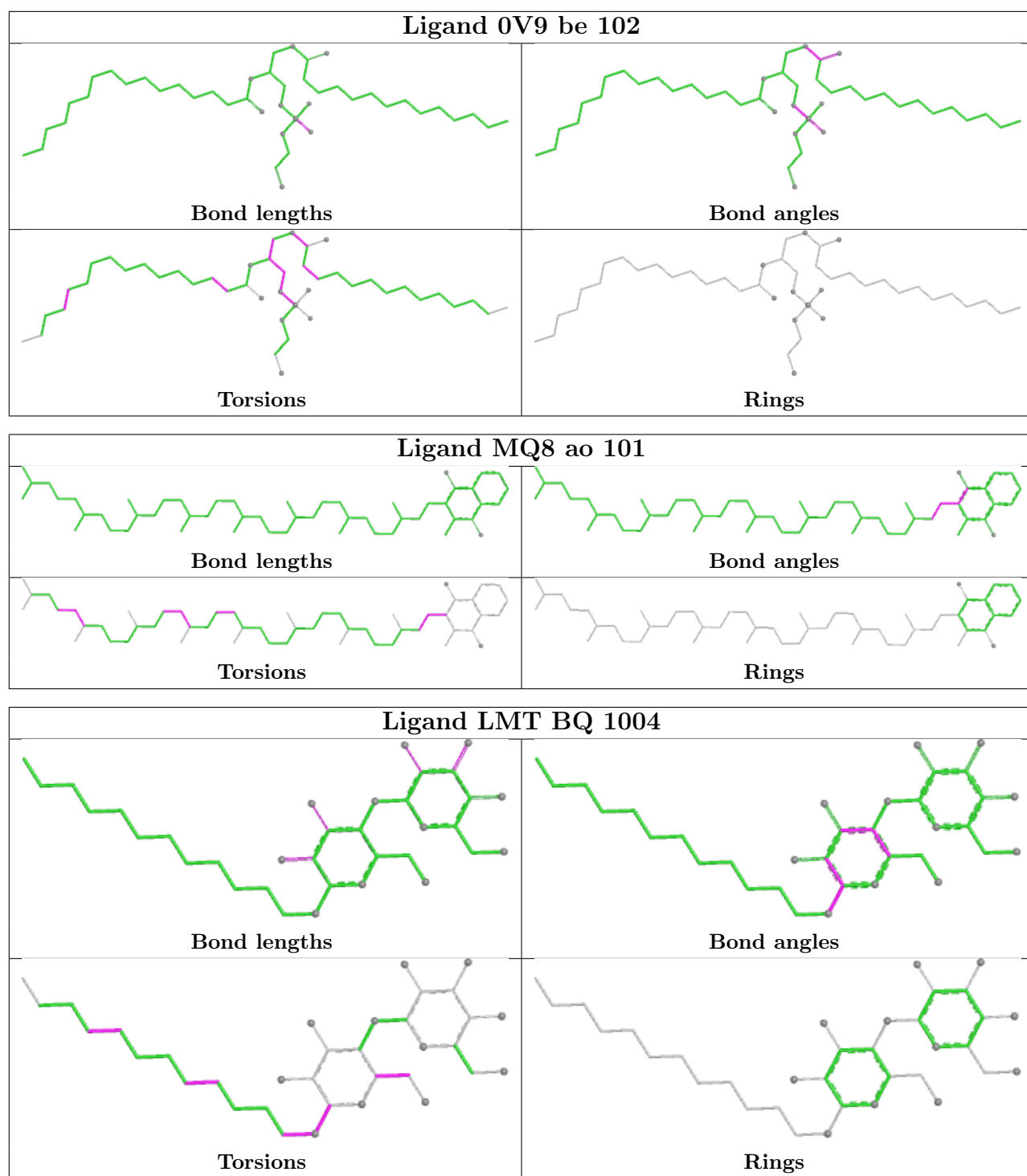


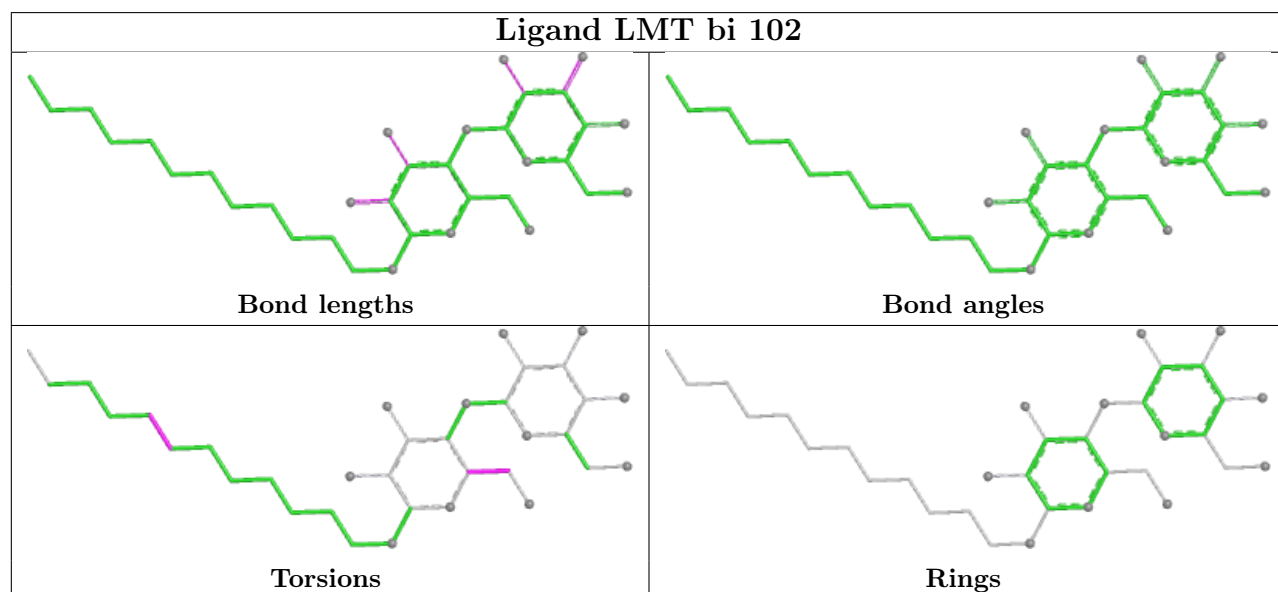
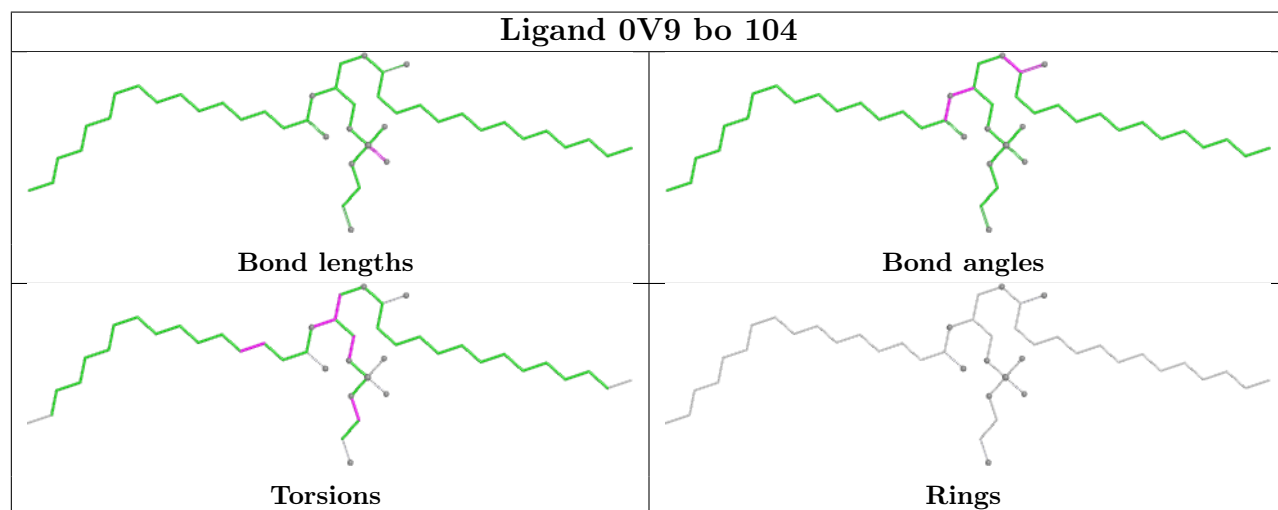
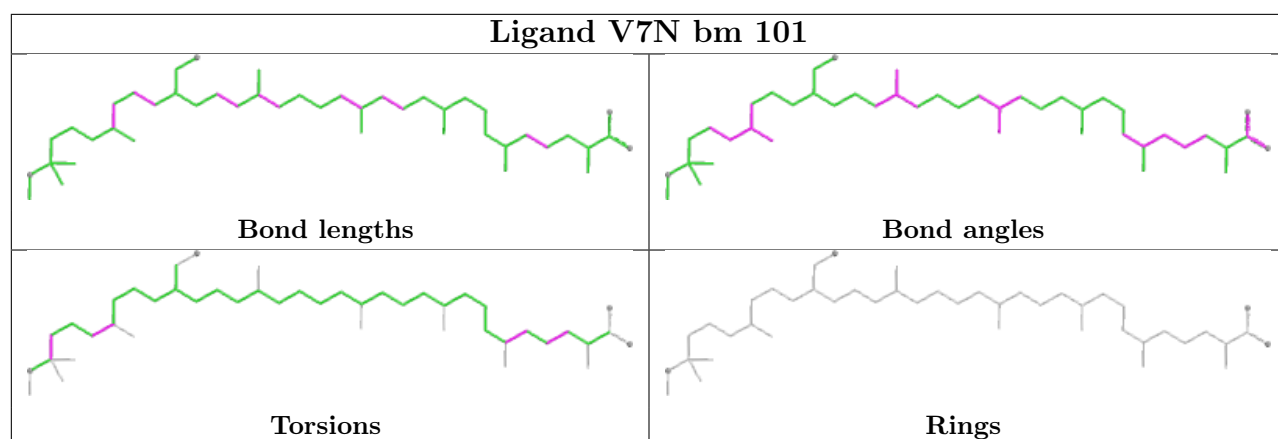


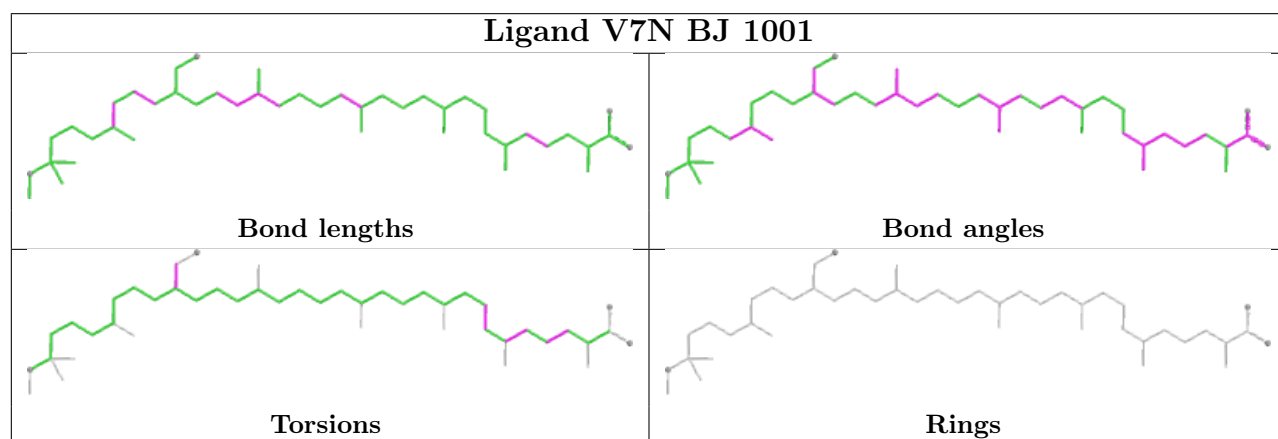
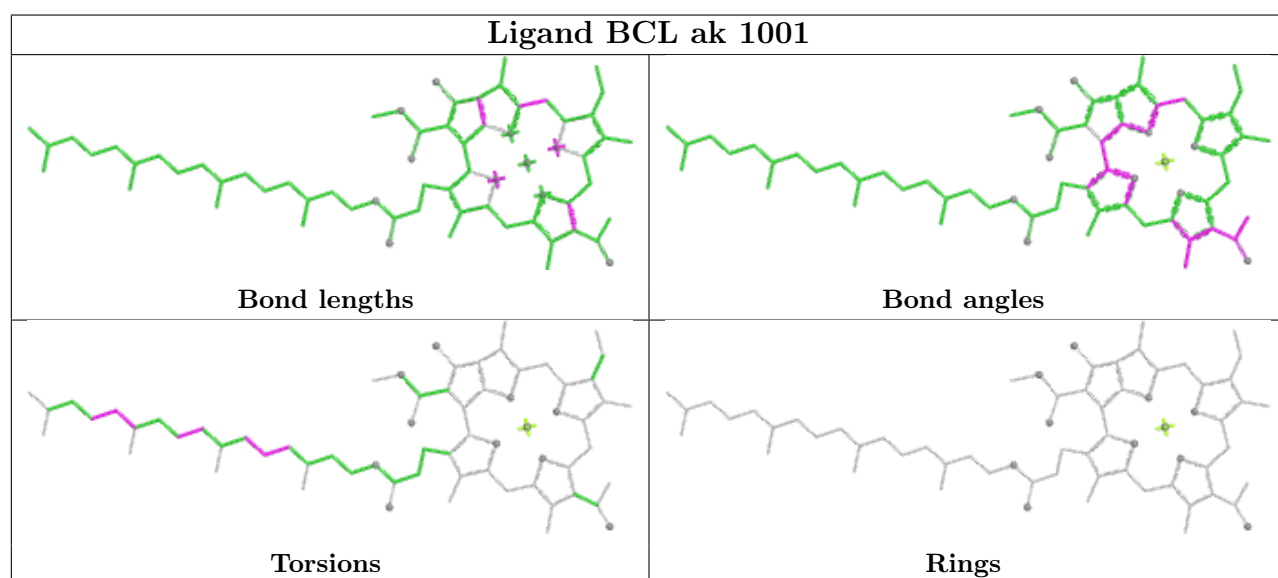
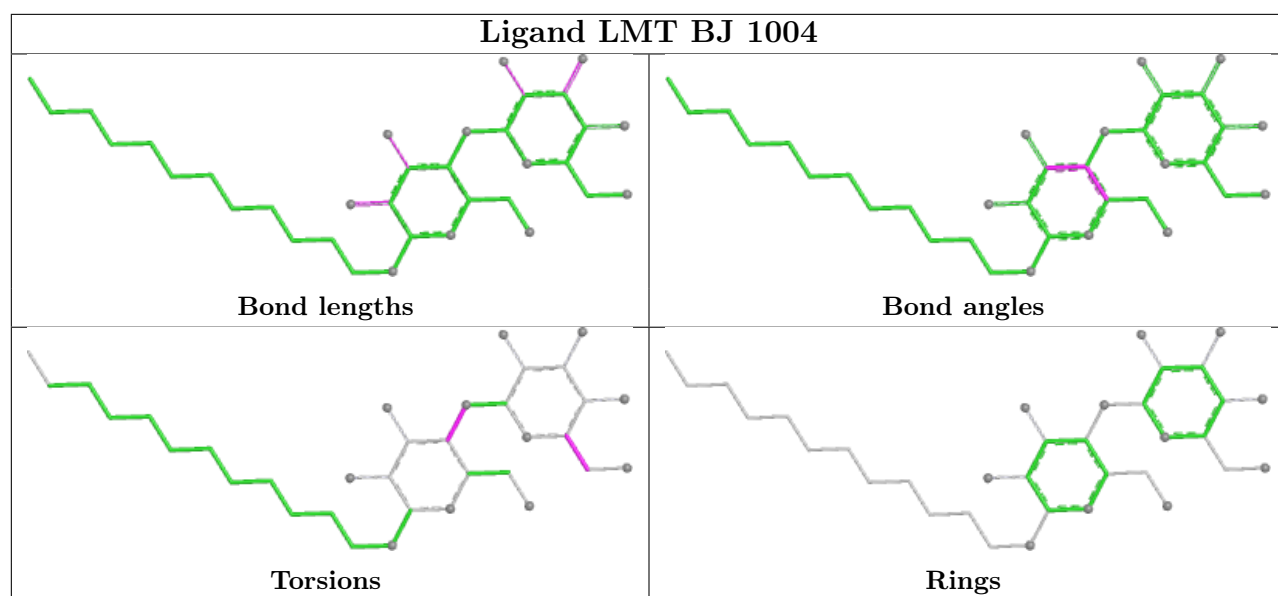


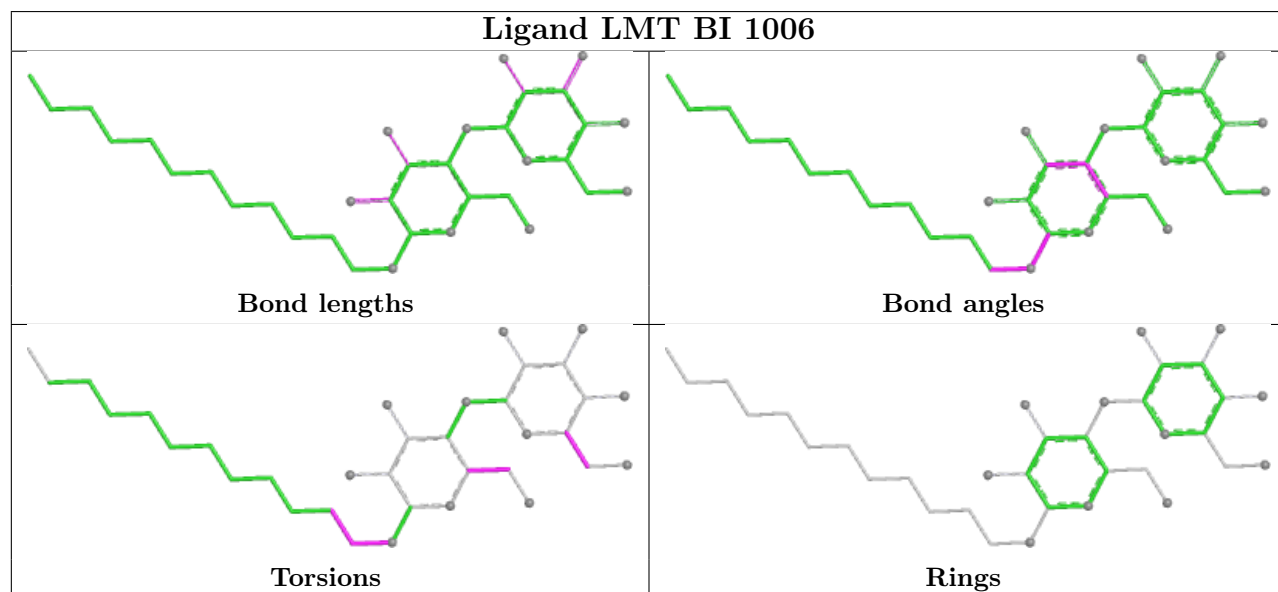
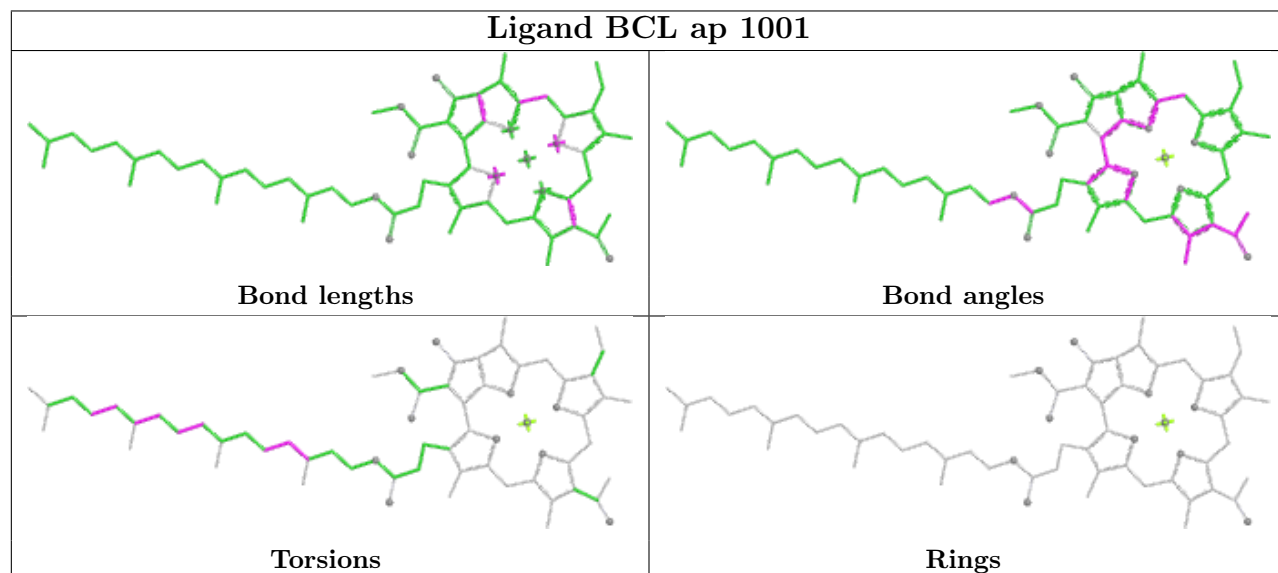
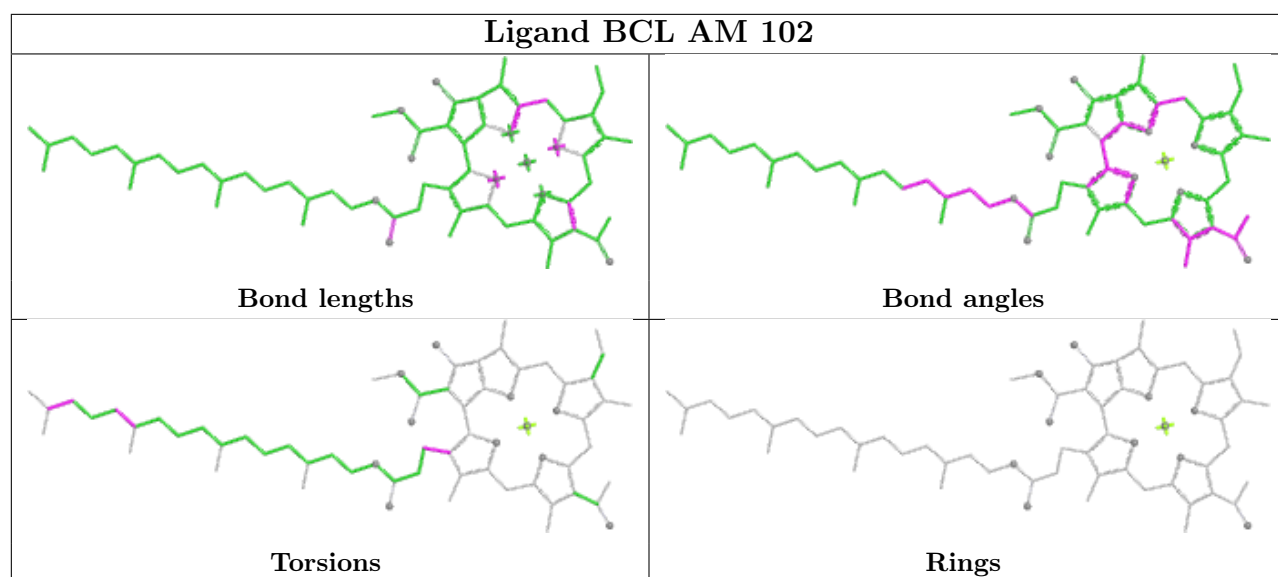


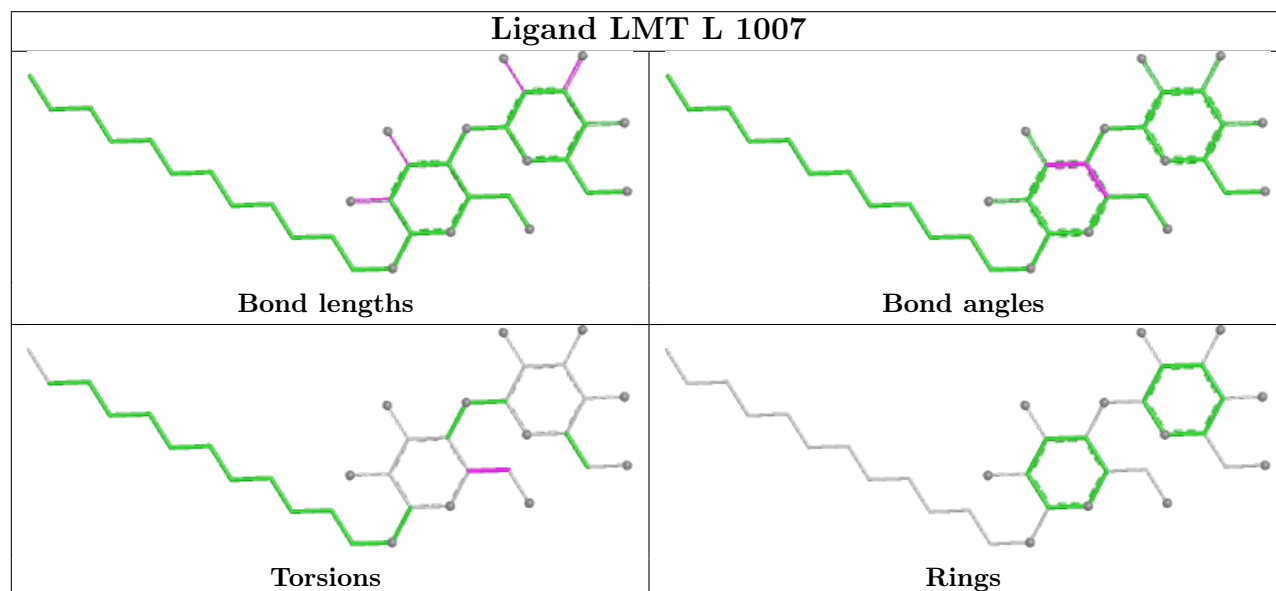
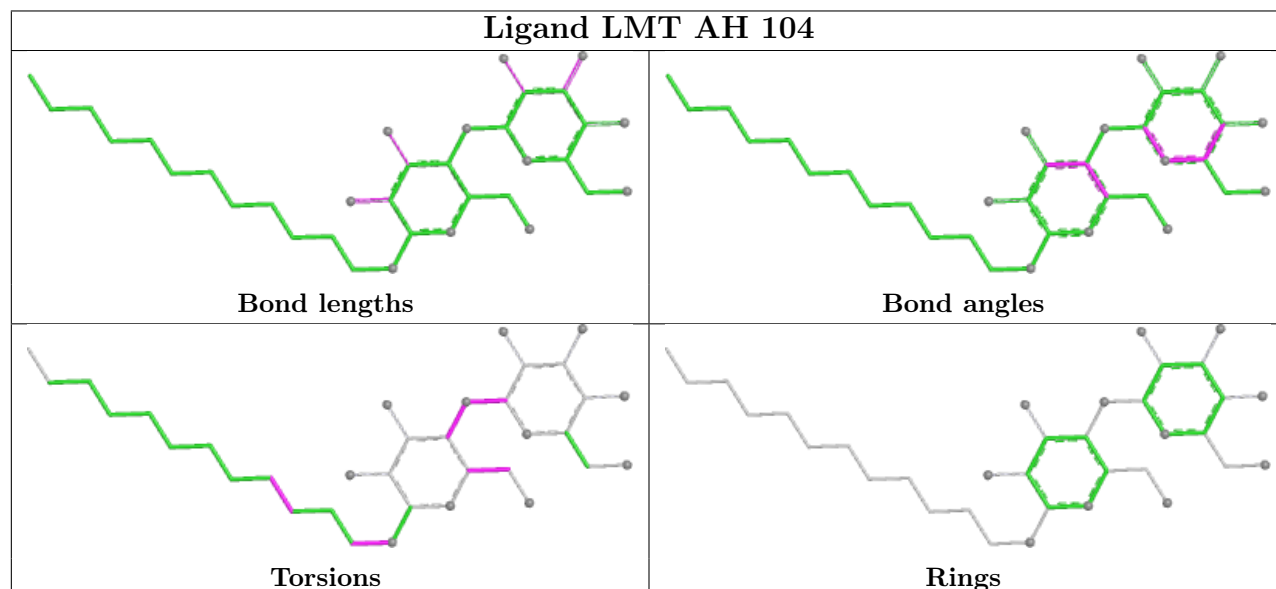
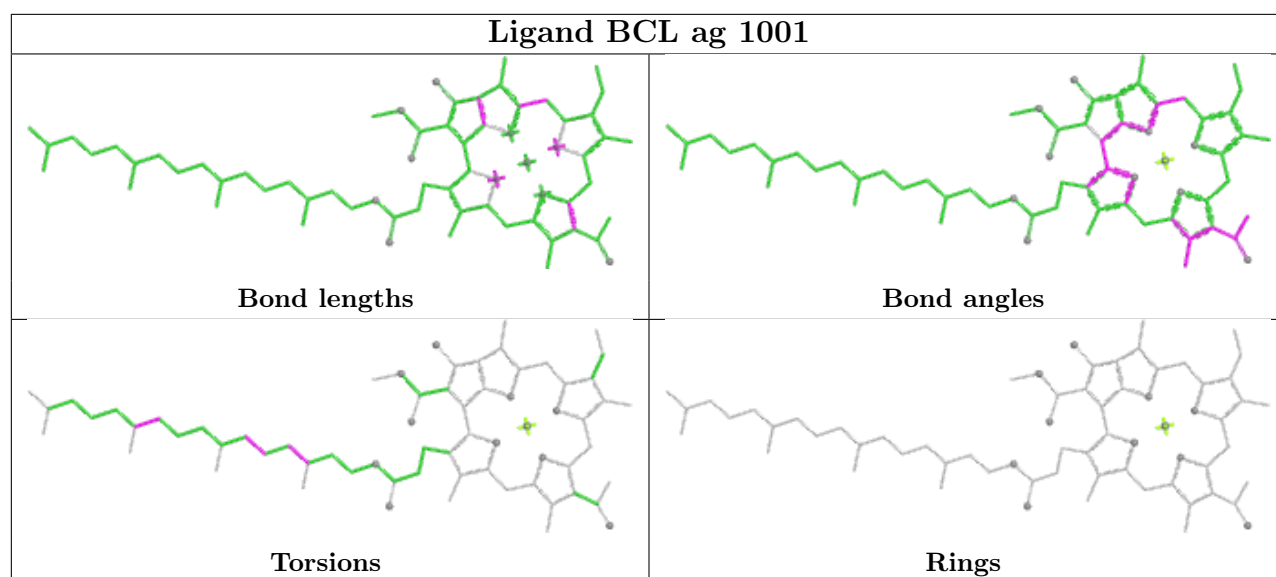


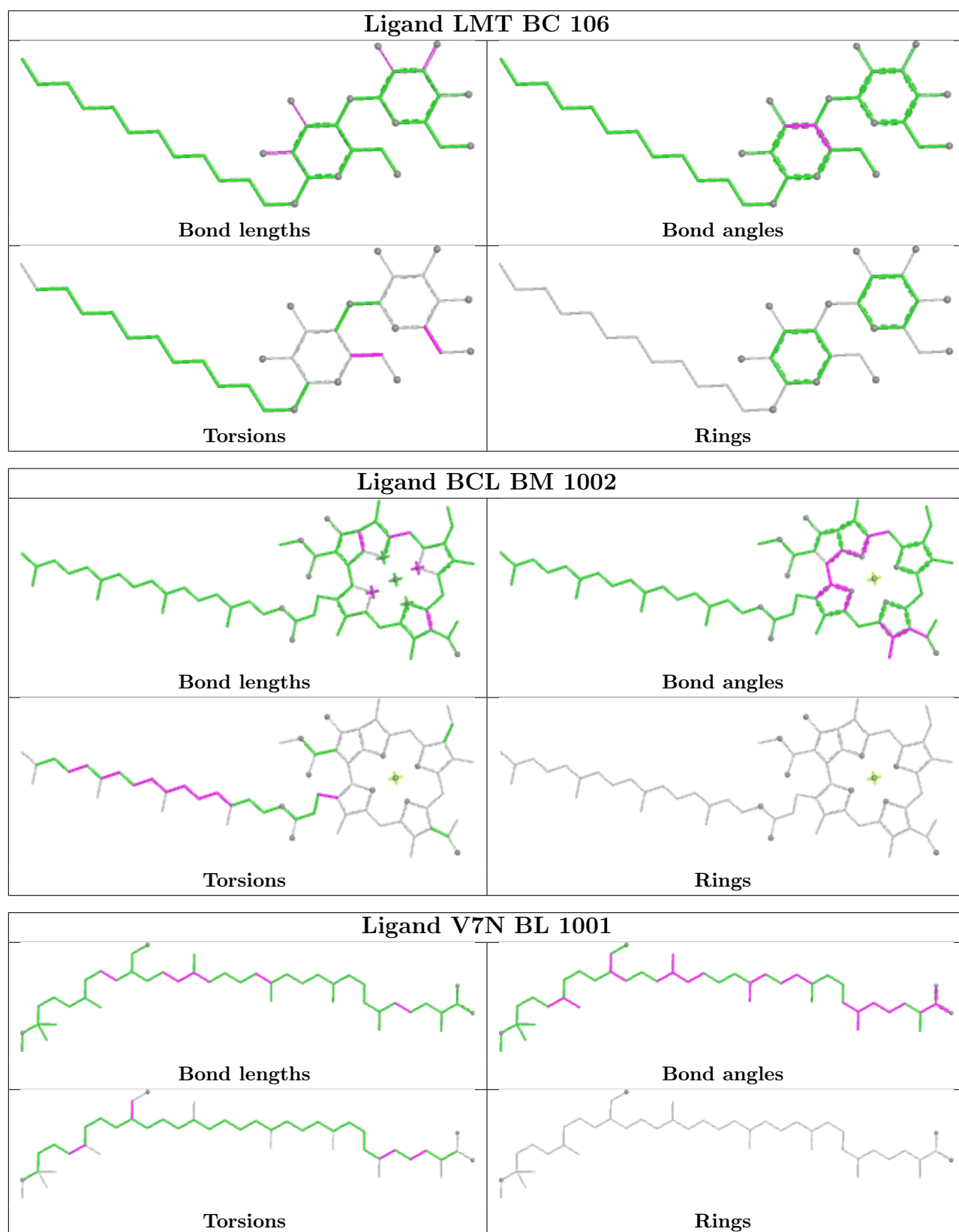


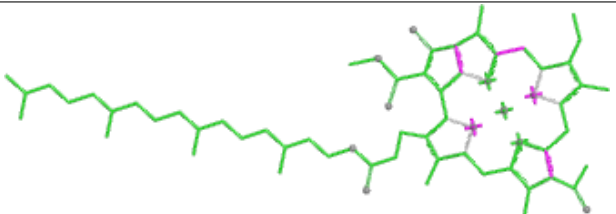
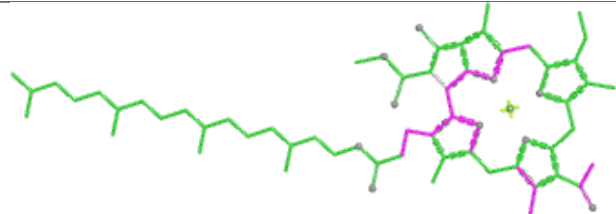
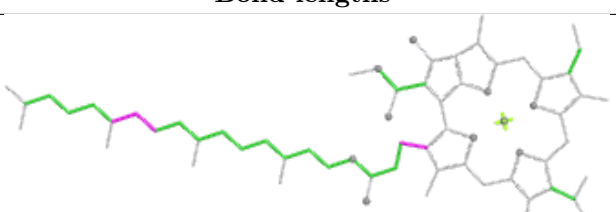
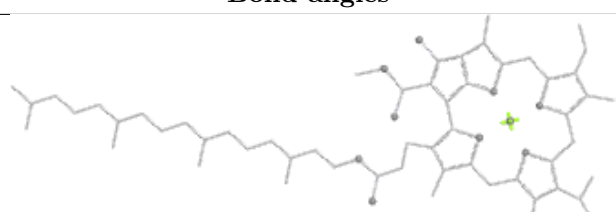


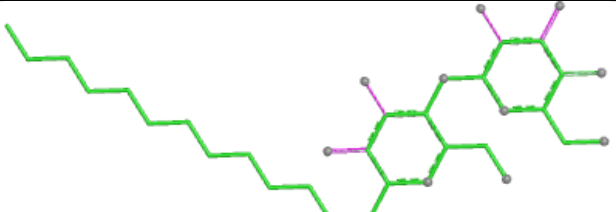
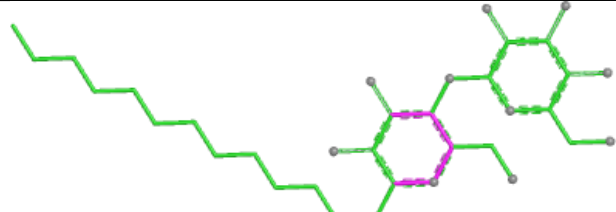
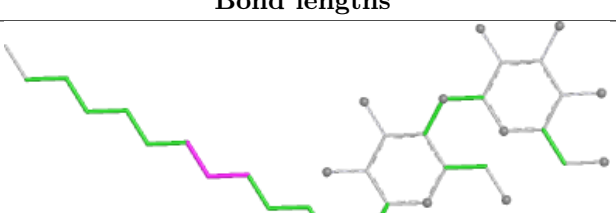
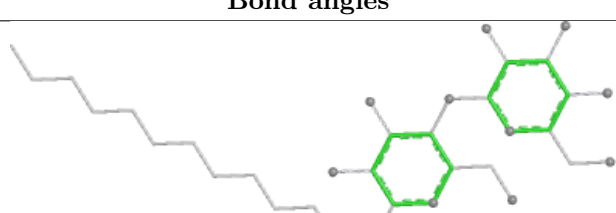


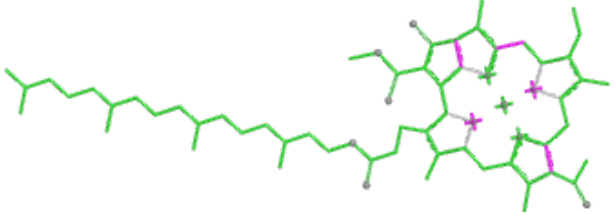
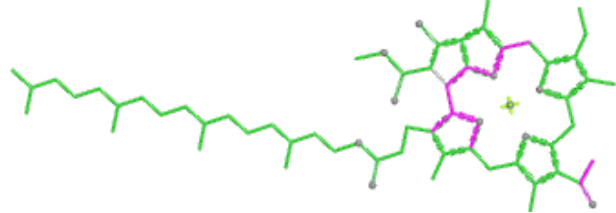
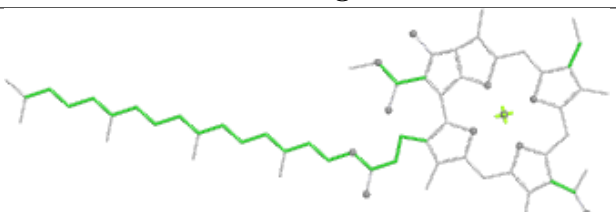
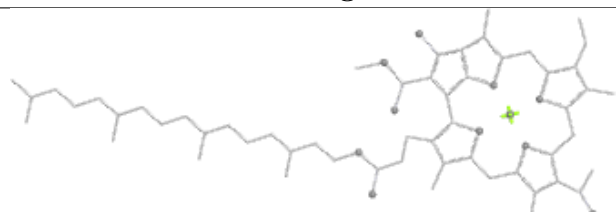


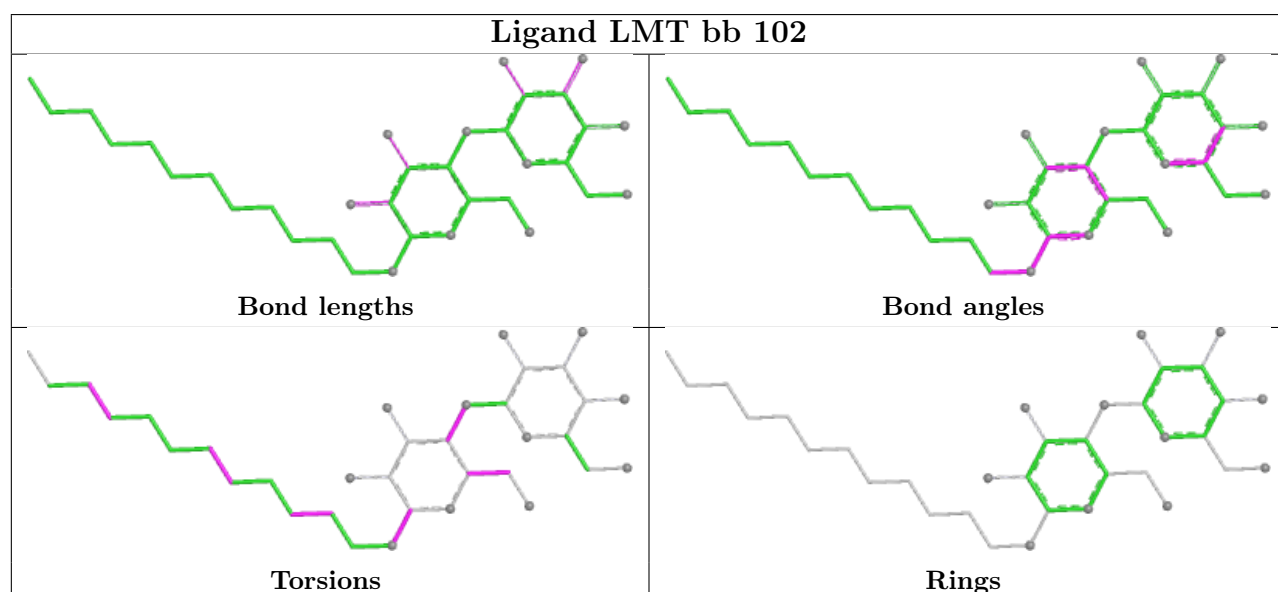
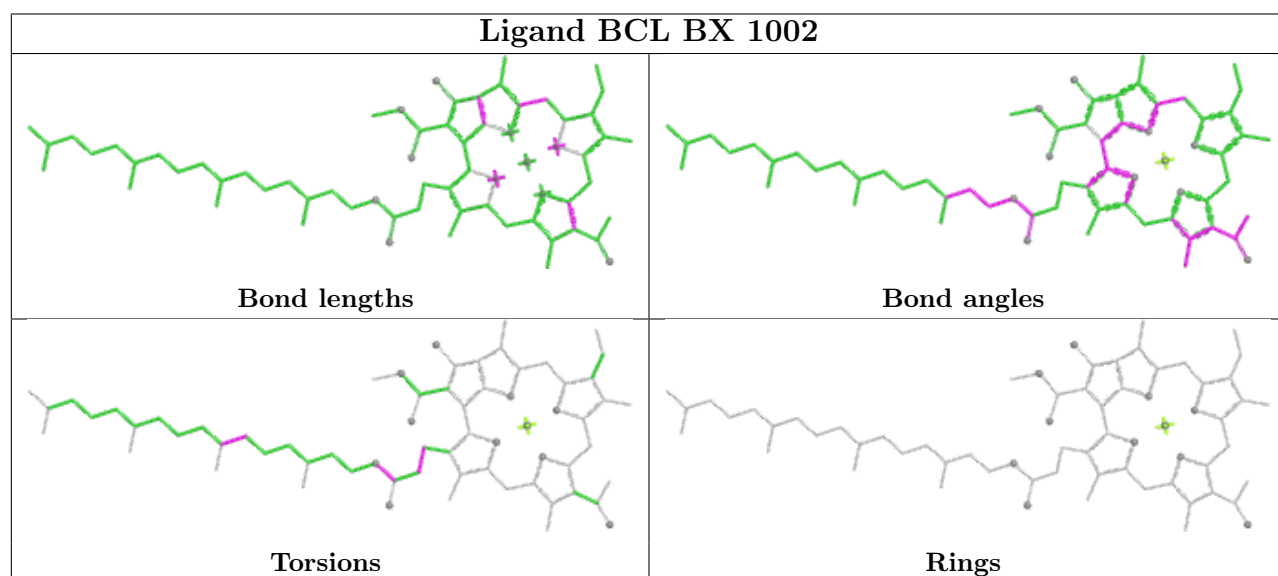
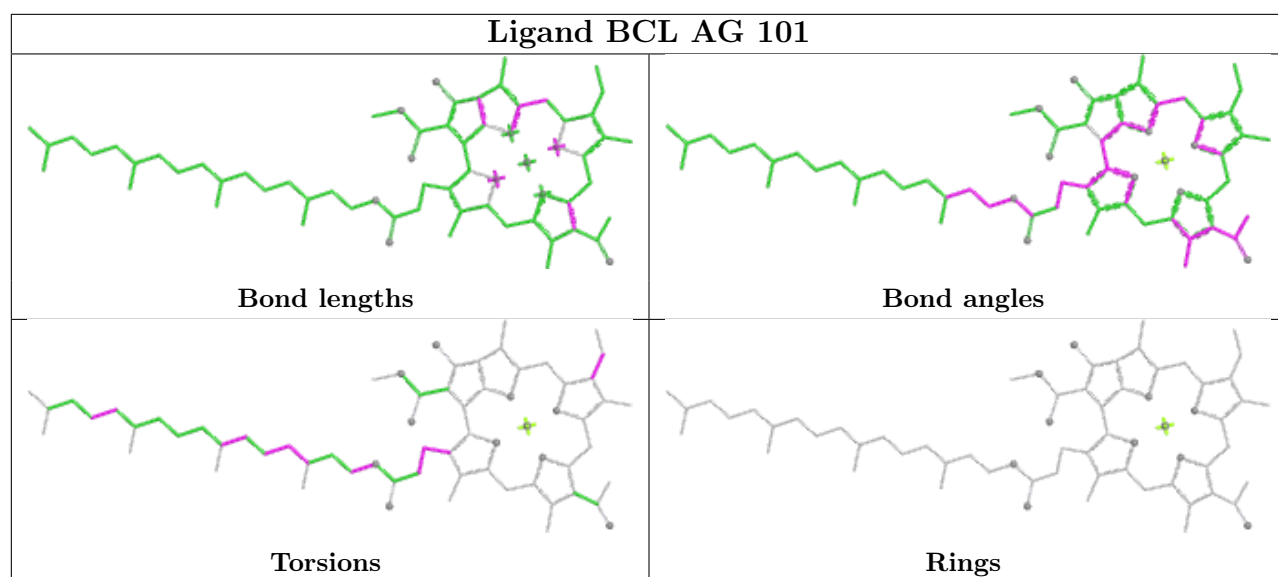


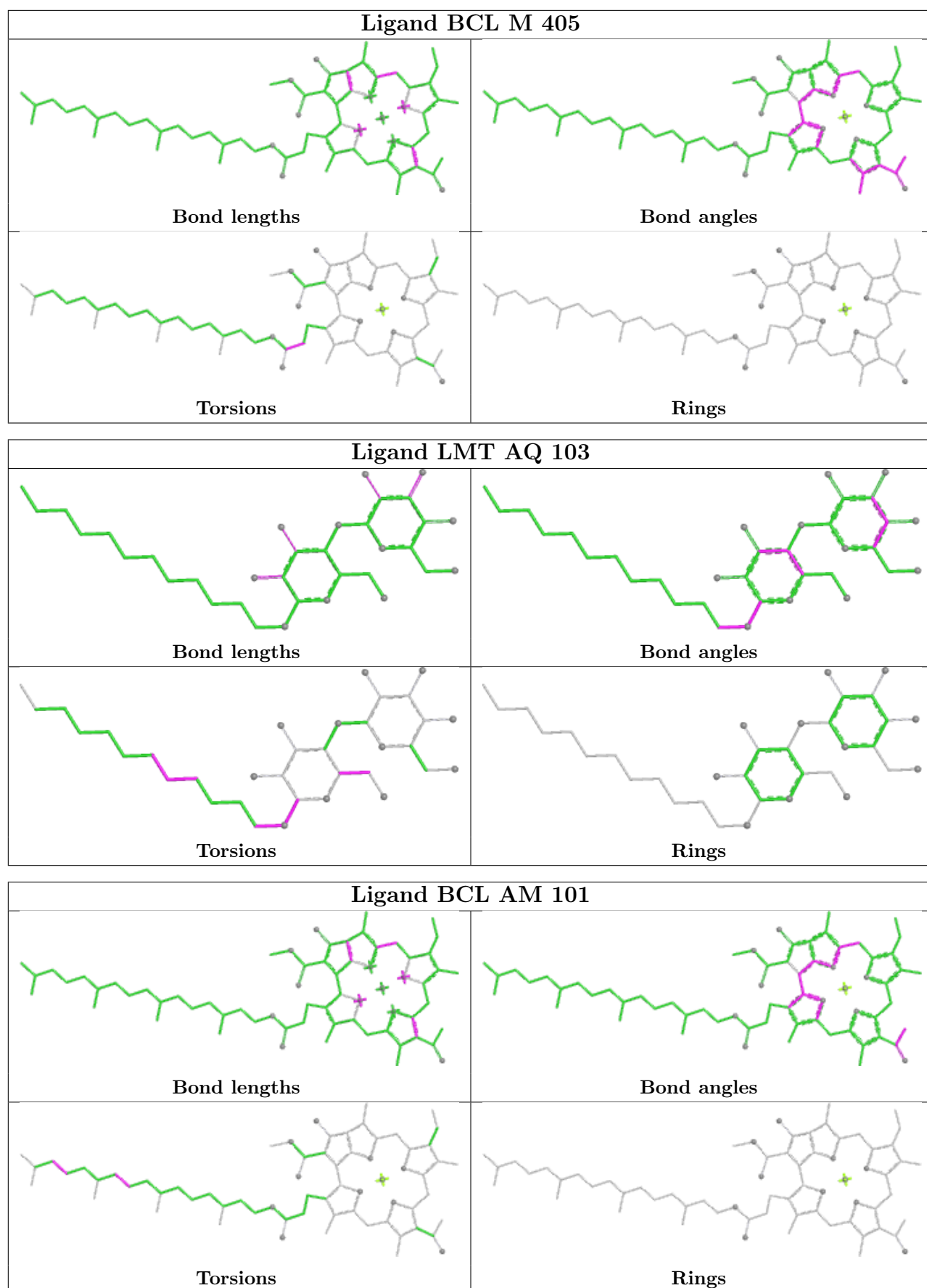


Ligand BCL BK 1006	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT bl 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL AT 101	
	
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.

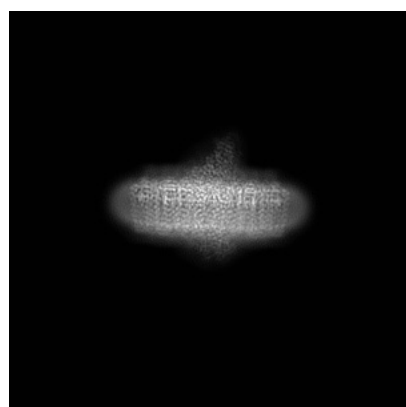
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12680. These allow visual inspection of the internal detail of the map and identification of artifacts.

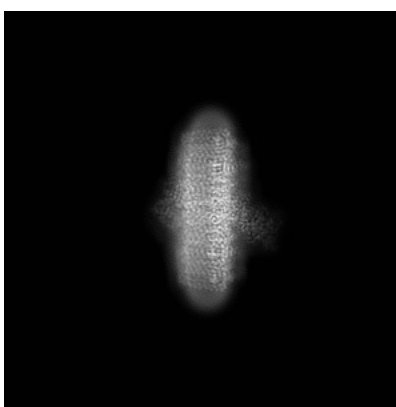
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

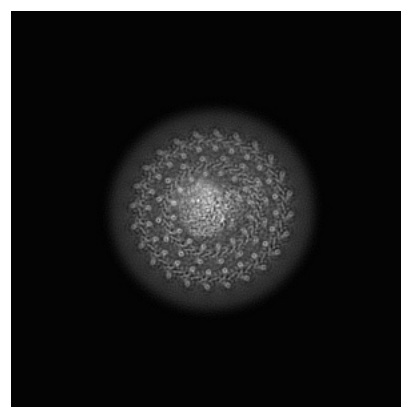
6.1.1 Primary map



X



Y

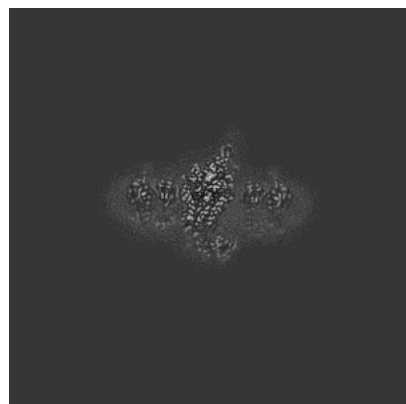


Z

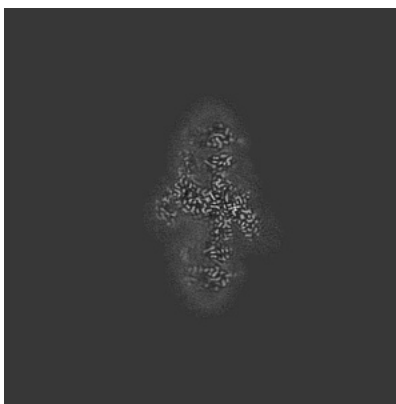
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

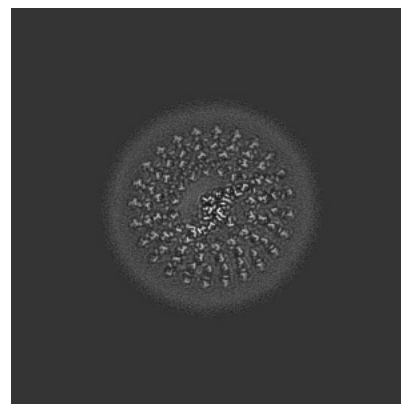
6.2.1 Primary map



X Index: 200



Y Index: 200

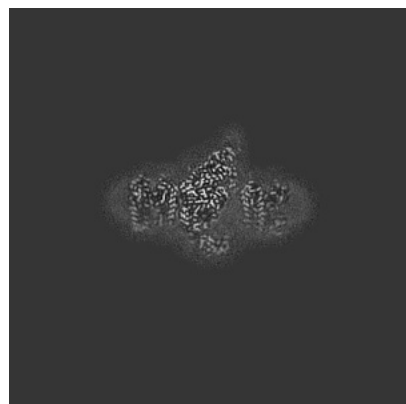


Z Index: 200

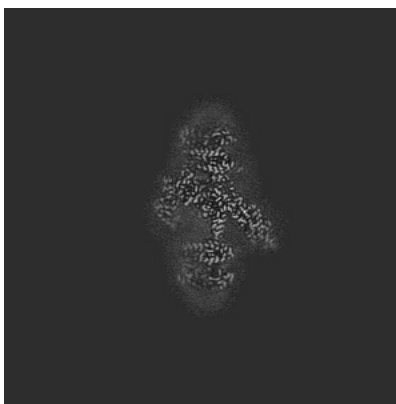
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

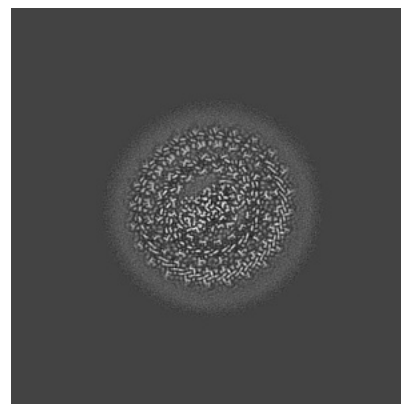
6.3.1 Primary map



X Index: 193



Y Index: 209

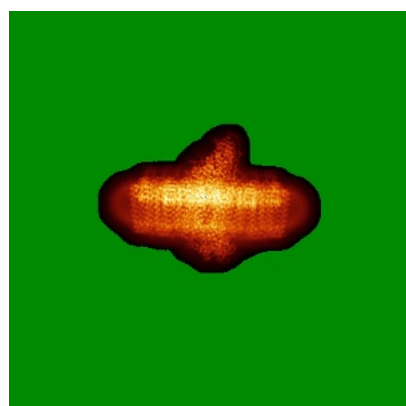


Z Index: 214

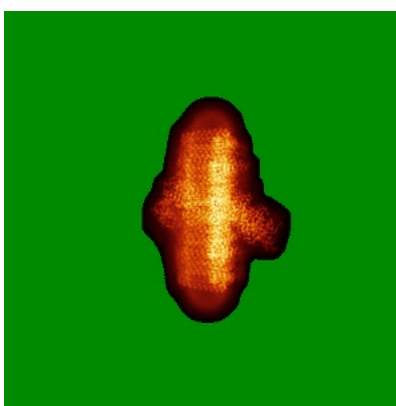
The images above show the largest variance slices of the map in three orthogonal directions.

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

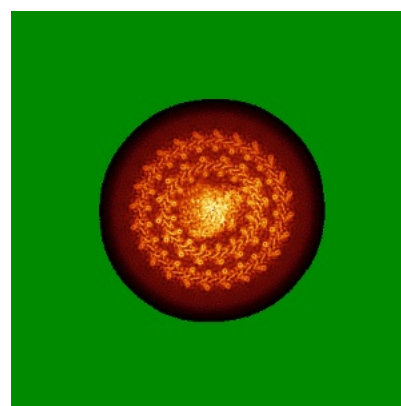
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

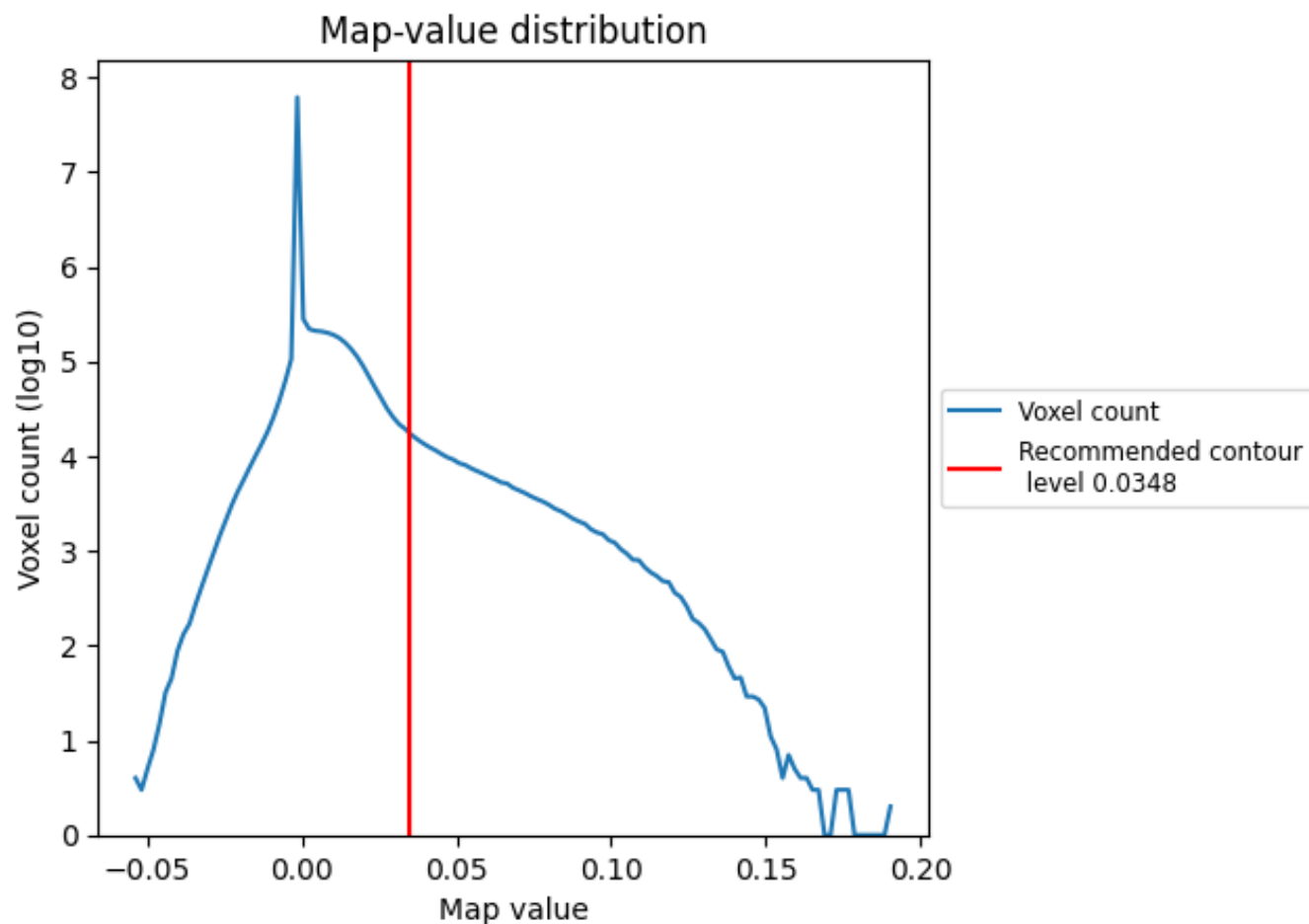
6.6 Mask visualisation

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

7 Map analysis [i](#)

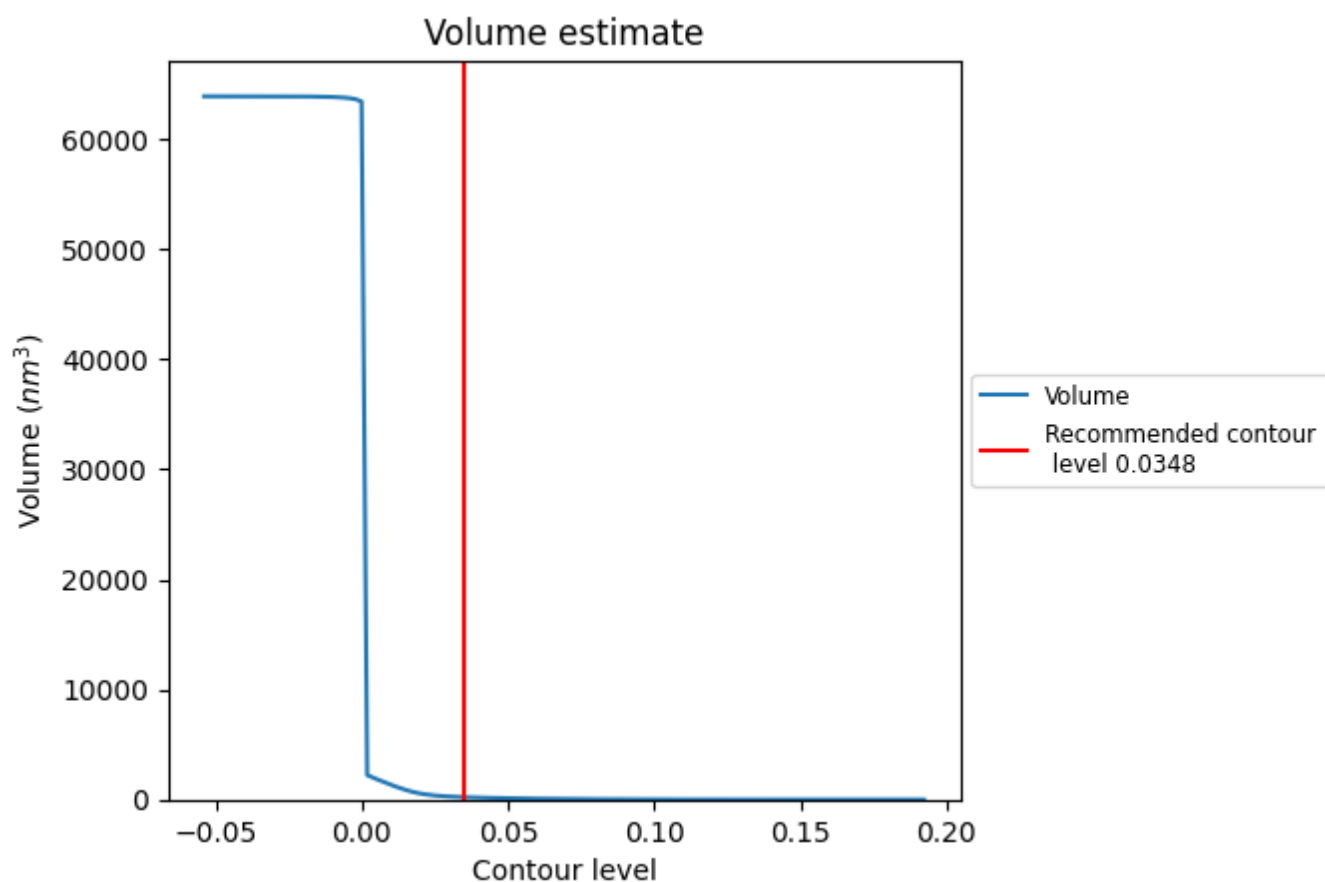
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

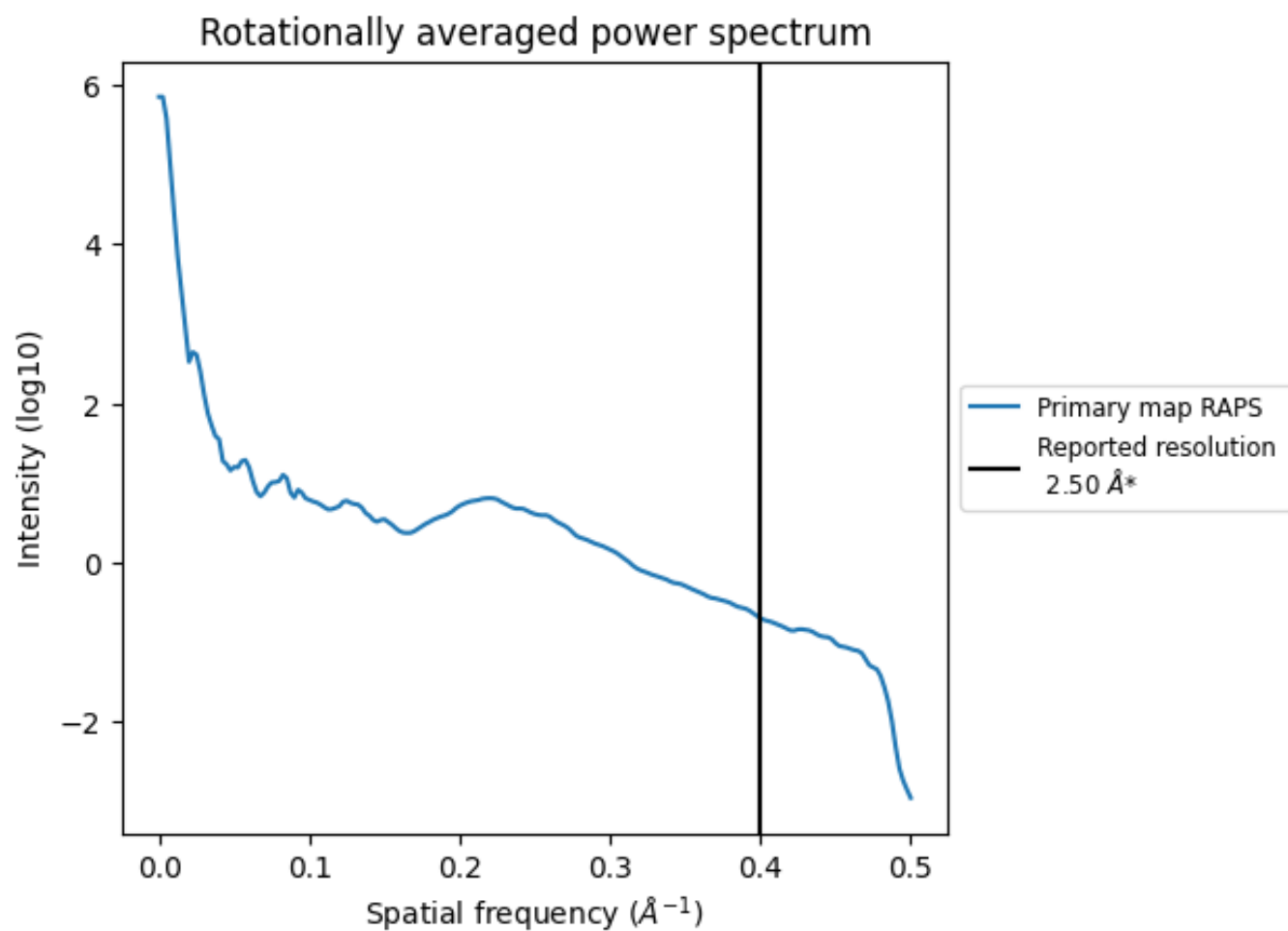
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 ⓘ

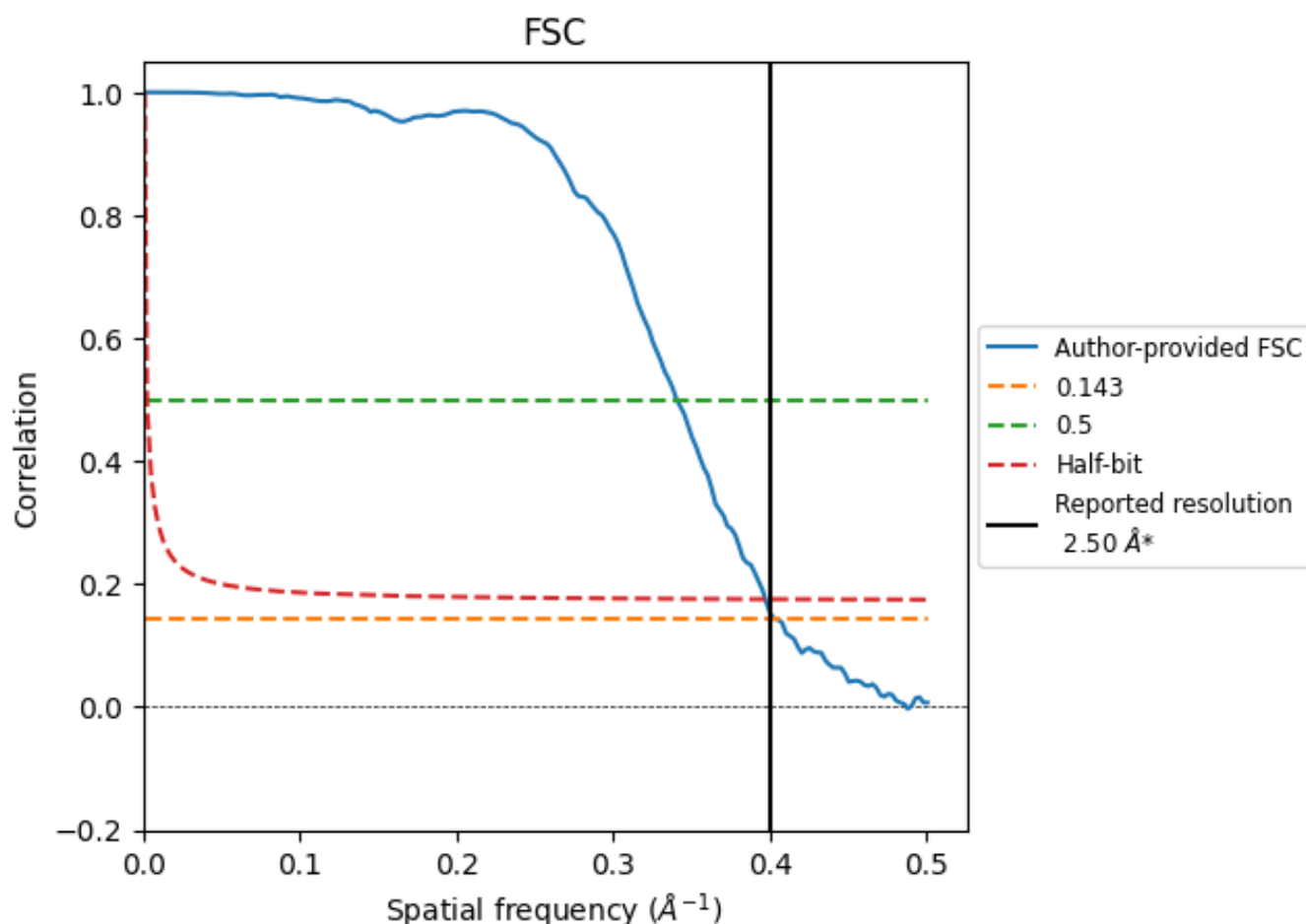


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

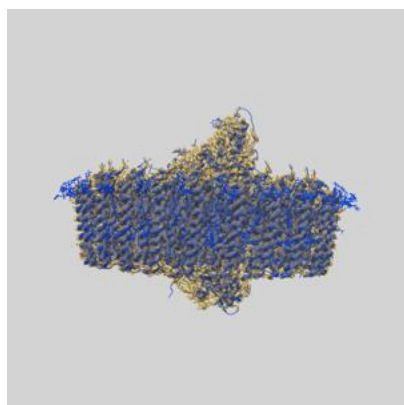
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.94	2.52
Unmasked-calculated*	-	-	-

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

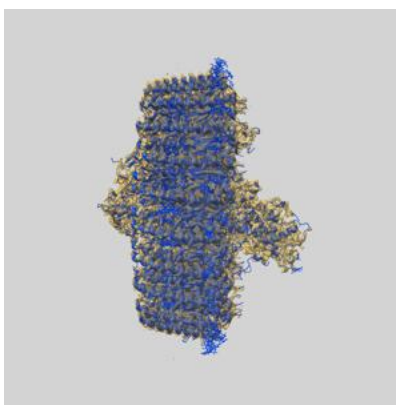
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12680 and PDB model 7O0V. Per-residue inclusion information can be found in [section 3](#) on [page 39](#).

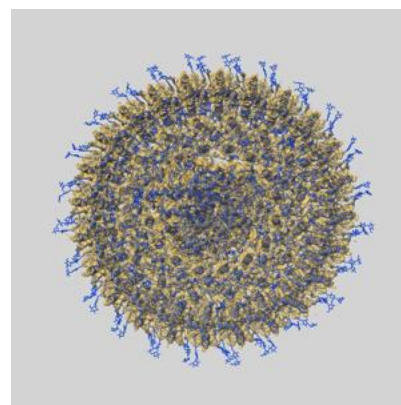
9.1 Map-model overlay [i](#)



X



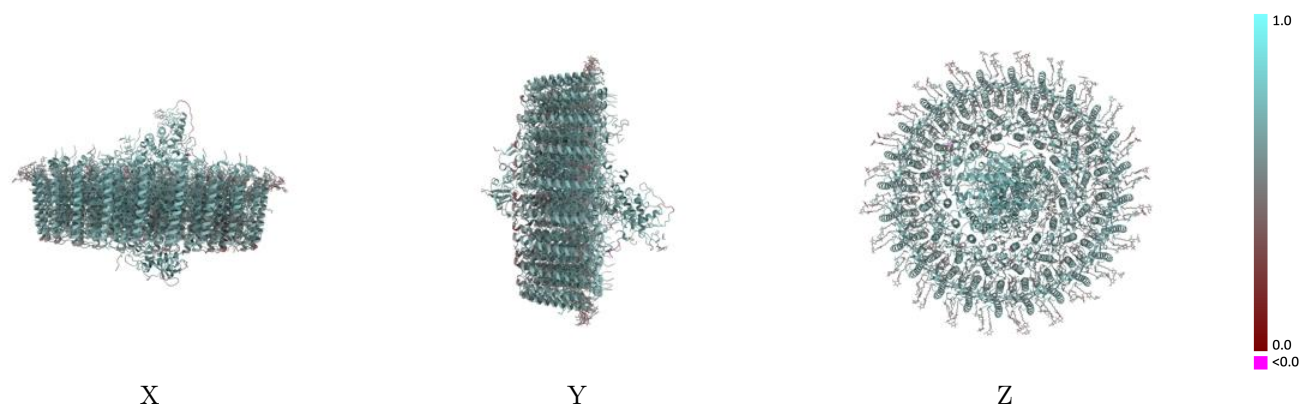
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0348 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](#)

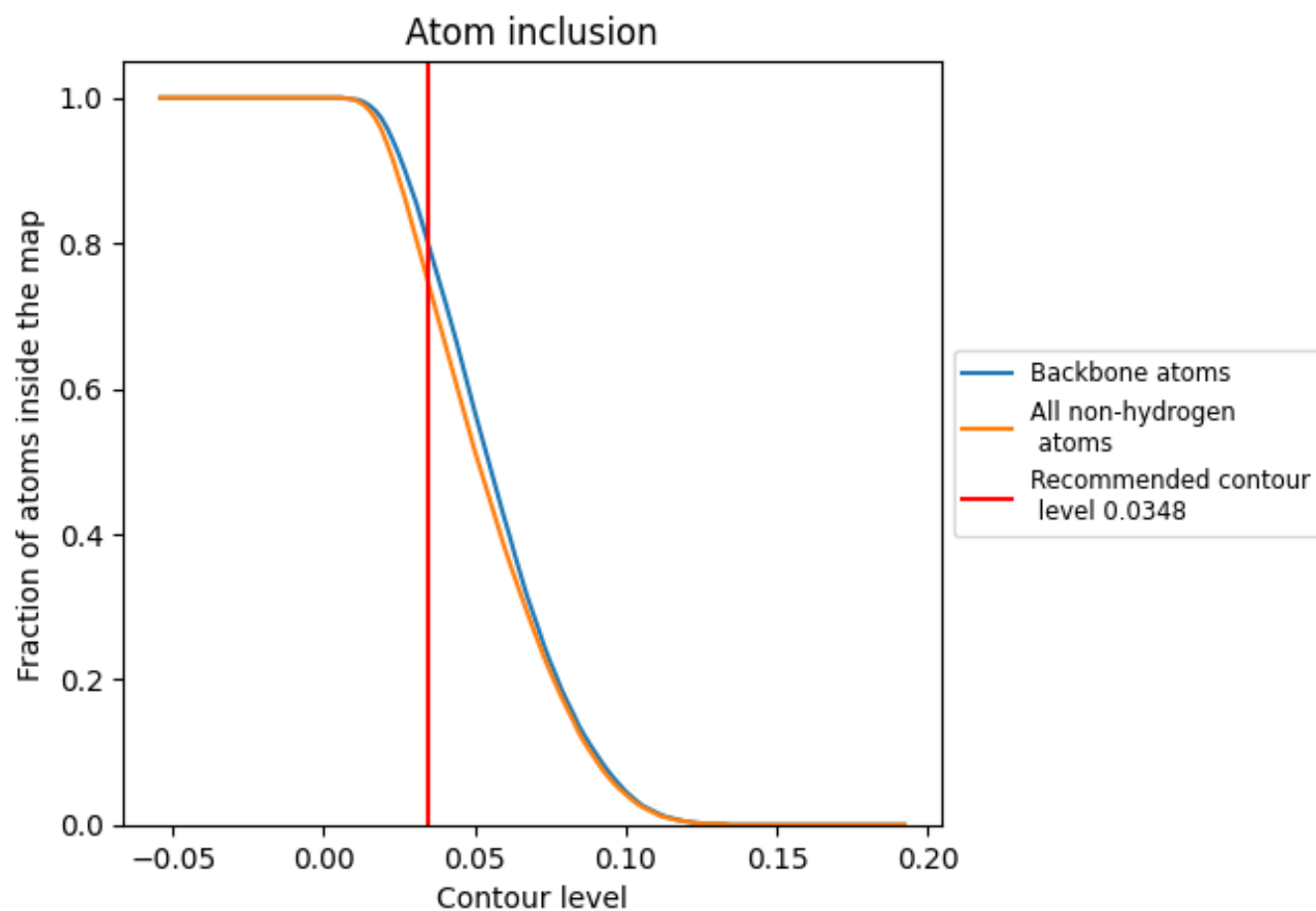


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0348) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.6200
AA	 0.7230	 0.6150
AB	 0.7170	 0.6040
AC	 0.5990	 0.5800
AD	 0.7860	 0.6170
AE	 0.6220	 0.5890
AF	 0.7400	 0.6050
AG	 0.7640	 0.6210
AH	 0.7390	 0.6200
AI	 0.7180	 0.6030
AJ	 0.8150	 0.6380
AK	 0.8010	 0.6360
AL	 0.6780	 0.5990
AM	 0.8230	 0.6430
AN	 0.6830	 0.6060
AO	 0.8090	 0.6280
AP	 0.7820	 0.6280
AQ	 0.7570	 0.6270
AR	 0.7300	 0.6120
AS	 0.7340	 0.6230
AT	 0.8230	 0.6390
AU	 0.7020	 0.6020
AV	 0.7300	 0.6250
AW	 0.7940	 0.6240
AX	 0.6650	 0.5980
BA	 0.6340	 0.5780
BB	 0.6040	 0.5650
BC	 0.5730	 0.5530
BD	 0.6160	 0.5740
BE	 0.6370	 0.5800
BF	 0.6580	 0.5810
BG	 0.6600	 0.5800
BH	 0.6700	 0.5930
BI	 0.6500	 0.5940
BJ	 0.7220	 0.6150



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Chain	Atom inclusion	Q-score
BK	 0.6920	 0.6040
BL	 0.6450	 0.5830
BM	 0.6930	 0.6030
BN	 0.6500	 0.5700
BO	 0.6690	 0.6010
BP	 0.7140	 0.6000
BQ	 0.6610	 0.5810
BR	 0.6510	 0.5920
BS	 0.6680	 0.6050
BT	 0.6460	 0.5780
BU	 0.6500	 0.5840
BV	 0.6480	 0.5810
BW	 0.6310	 0.5720
BX	 0.6140	 0.5720
C	 0.8820	 0.6630
C1	 0.8260	 0.6580
CG	 0.3810	 0.5410
H1	 0.7240	 0.6280
H2	 0.7200	 0.6080
L	 0.9010	 0.6790
M	 0.8970	 0.6830
MG	 0.9520	 0.6170
aa	 0.6690	 0.6100
ab	 0.7090	 0.6210
ac	 0.7750	 0.6250
ad	 0.8850	 0.6710
ae	 0.8320	 0.6540
af	 0.8030	 0.6490
ag	 0.7480	 0.6240
ah	 0.7960	 0.6400
ai	 0.7250	 0.6220
aj	 0.7580	 0.6230
ak	 0.8610	 0.6680
al	 0.8160	 0.6570
am	 0.7500	 0.6230
an	 0.6590	 0.5980
ao	 0.6430	 0.5970
ap	 0.6820	 0.6010
ba	 0.6570	 0.5920
bb	 0.6870	 0.6050
bc	 0.7130	 0.6110
bd	 0.8190	 0.6430

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Chain	Atom inclusion	Q-score
be	 0.7810	 0.6270
bf	 0.8240	 0.6480
bg	 0.7550	 0.6200
bh	 0.7470	 0.6210
bi	 0.7510	 0.6130
bj	 0.8060	 0.6370
bk	 0.7620	 0.6300
bl	 0.7150	 0.6170
bm	 0.7080	 0.6000
bn	 0.6730	 0.6000
bo	 0.6440	 0.5970
bp	 0.7050	 0.6030