



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2022 – 04:09 pm GMT

PDB ID : 7O0X  
EMDB ID : EMD-12682  
Title : Cryo-EM structure (model\_2b) of the RC-dLH complex from Gemmatimonas phototrophica at 2.44 Å  
Authors : Qian, P.; Koblizek, M.  
Deposited on : 2021-03-28  
Resolution : 2.44 Å (reported)  
Based on initial models : 6ET5, 5Y5S, 1LGH

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

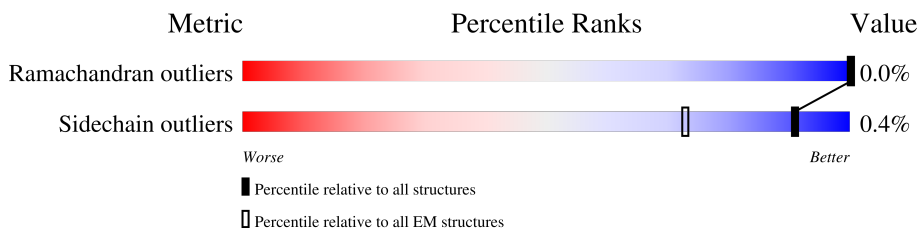
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 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 2.44 Å.

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













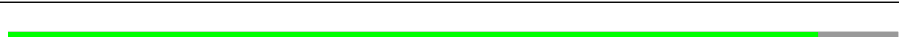


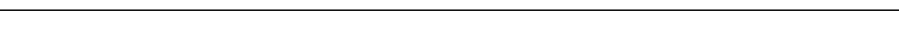
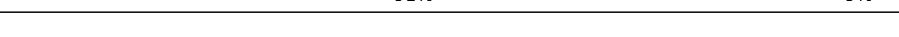
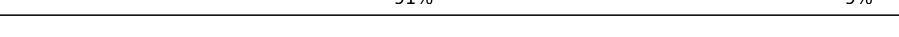

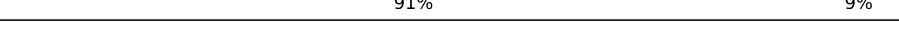

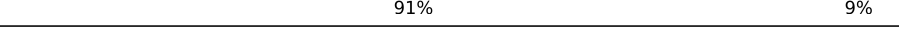
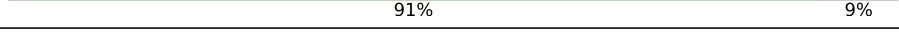




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AA	54	
1	AB	54	
1	AC	54	
1	AD	54	
1	AE	54	
1	AF	54	
1	AG	54	
1	AH	54	
1	AI	54	











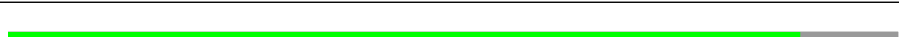


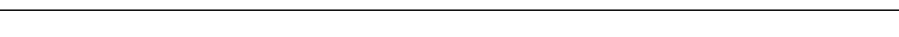
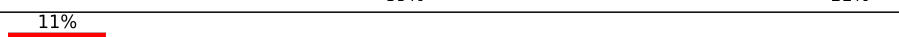
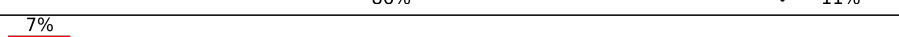



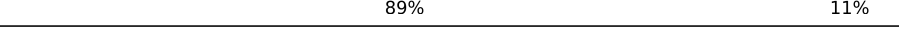





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Mol	Chain	Length	Quality of chain
1	AJ	54	 89% 9%
1	AK	54	 89% 9%
1	AL	54	 89% 9%
1	AM	54	 89% 9%
1	AN	54	 89% 9%
1	AO	54	 91% 9%
1	AP	54	 89% 9%
1	AQ	54	 89% 9%
1	AR	54	 89% 9%
1	AS	54	 89% 9%
1	AT	54	 91% 9%
1	AU	54	 91% 9%
1	AV	54	 89% 9%
1	AW	54	 91% 9%
1	AX	54	 91% 9%
2	BA	44	 89% 11%
2	BB	44	 91% 9%
2	BC	44	 89% 11%
2	BD	44	 91% 9%
2	BE	44	 91% 9%
2	BF	44	 89% 11%
2	BG	44	 89% 11%
2	BH	44	 86% 11%
2	BI	44	 91% 9%
2	BJ	44	 89% 11%

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Mol	Chain	Length	Quality of chain
2	BK	44	 86% 11%
2	BL	44	 89% 11%
2	BM	44	 89% 11%
2	BN	44	 89% 11%
2	BO	44	 89% 11%
2	BP	44	 89% 11%
2	BQ	44	 91% 9%
2	BR	44	 91% 9%
2	BS	44	 91% 9%
2	BT	44	 91% 9%
2	BU	44	 89% 11%
2	BV	44	 91% 9%
2	BW	44	 91% 9%
2	BX	44	 89% 11%
2	ba	44	 86% 11%
2	bb	44	 89% 11%
2	bc	44	 89% 11%
2	bd	44	 89% 11%
2	be	44	 89% 11%
2	bf	44	 89% 11%
2	bg	44	 89% 11%
2	bh	44	 89% 11%
2	bi	44	 89% 11%
2	bj	44	 89% 11%
2	bk	44	 89% 11%

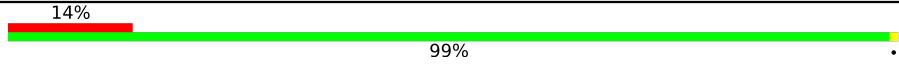

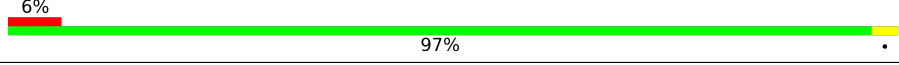
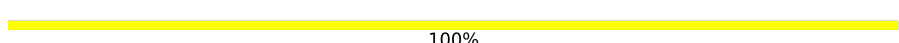
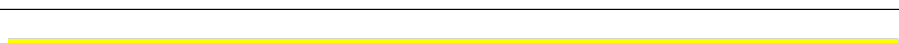
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Mol	Chain	Length	Quality of chain
2	bl	44	89% 11%
2	bm	44	89% 11%
2	bn	44	91% 9%
2	bo	44	86% 11%
2	bp	44	89% 11%
3	C	354	83% 16%
4	C1	202	51% 49%
5	C2	125	79% 21%
6	H1	67	90% 7%
7	H2	181	98%
8	L	274	98%
9	M	367	90% 9%
10	aa	71	76% 23%
11	ab	71	80% 18%
11	ac	71	79% 21%
11	ad	71	82% 15%
11	ae	71	79% 18%
11	af	71	80% 18%
11	ag	71	82% 18%
11	ah	71	83% 15%
11	ai	71	82% 15%
11	aj	71	83% 15%
11	ak	71	97%
11	al	71	83% 15%
11	am	71	85% 15%

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Mol	Chain	Length	Quality of chain
11	an	71	 14% 99%
11	ao	71	 6% 83% 15%
11	ap	71	 6% 97%
12	CG	2	 100%
12	MG	2	 100%

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 56446 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
			Total	C	N	O	S		
1	AA	49	391	261	65	61	4	0	0
1	AB	49	391	261	65	61	4	0	0
1	AC	48	384	256	64	60	4	0	0
1	AD	48	384	256	64	60	4	0	0
1	AE	49	391	261	65	61	4	0	0
1	AF	49	391	261	65	61	4	0	0
1	AG	49	391	261	65	61	4	0	0
1	AH	49	391	261	65	61	4	0	0
1	AI	49	391	261	65	61	4	0	0
1	AJ	49	391	261	65	61	4	0	0
1	AK	49	391	261	65	61	4	0	0
1	AL	49	391	261	65	61	4	0	0
1	AM	49	391	261	65	61	4	0	0
1	AN	49	391	261	65	61	4	0	0
1	AO	49	391	261	65	61	4	0	0
1	AP	49	391	261	65	61	4	0	0
1	AQ	49	391	261	65	61	4	0	0

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

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

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

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

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

- Molecule 3 is a protein called MULTIHEME\_CYTC domain-containing protein.

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

- Molecule 4 is a protein called RC-S.

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

- Molecule 5 is a protein called RC-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C2	99	Total	C	N	O	S	0	0
			766	483	148	132	3		

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

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

- Molecule 7 is a protein called RC-Hc.

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

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

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

- Molecule 9 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	335	Total	C	N	O	S	0	0
			2694	1789	442	453	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ab	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		
11	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ae	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	af	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ag	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		

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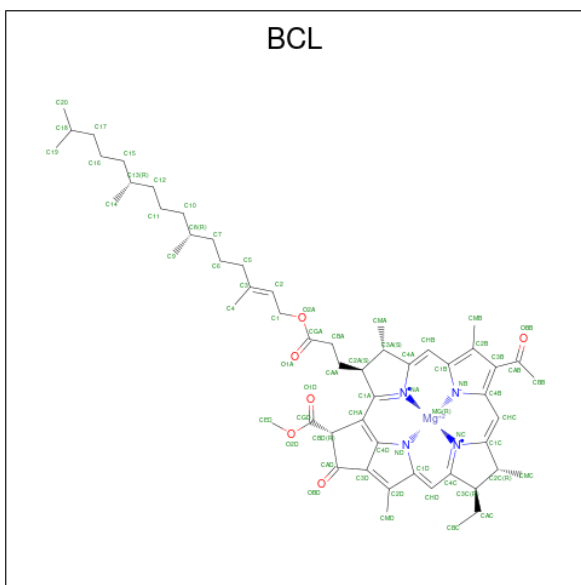
Mol	Chain	Residues	Atoms					AltConf	Trace
11	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	an	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ap	71	Total	C	N	O	S	0	0
			543	352	95	92	4		

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



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

- Molecule 13 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
13	AA	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AA	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AB	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AB	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AC	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AC	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AD	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AD	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AE	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AE	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AF	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AF	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AG	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
13	AG	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	AH	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AH	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AI	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AI	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AJ	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AJ	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AK	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AK	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AL	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AL	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AM	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AM	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AN	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AN	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AO	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AO	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AP	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AP	1	Total 132	C 110	Mg 2	N 8	O 12	0
13	AQ	1	Total 198	C 165	Mg 3	N 12	O 18	0
13	AQ	1	Total 198	C 165	Mg 3	N 12	O 18	0
13	AQ	1	Total 198	C 165	Mg 3	N 12	O 18	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	AR	1	66	55	1	4	6	0
13	AS	1	198	165	3	12	18	0
13	AS	1	198	165	3	12	18	0
13	AS	1	198	165	3	12	18	0
13	AT	1	66	55	1	4	6	0
13	AU	1	132	110	2	8	12	0
13	AU	1	132	110	2	8	12	0
13	AV	1	132	110	2	8	12	0
13	AV	1	132	110	2	8	12	0
13	AW	1	198	165	3	12	18	0
13	AW	1	198	165	3	12	18	0
13	AW	1	198	165	3	12	18	0
13	AX	1	66	55	1	4	6	0
13	BA	1	66	55	1	4	6	0
13	BB	1	66	55	1	4	6	0
13	BC	1	66	55	1	4	6	0
13	BD	1	66	55	1	4	6	0
13	BE	1	66	55	1	4	6	0
13	BF	1	66	55	1	4	6	0
13	BG	1	66	55	1	4	6	0
13	BH	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	BI	1	66	55	1	4	6	0
13	BJ	1	66	55	1	4	6	0
13	BK	1	66	55	1	4	6	0
13	BL	1	66	55	1	4	6	0
13	BM	1	66	55	1	4	6	0
13	BN	1	66	55	1	4	6	0
13	BO	1	66	55	1	4	6	0
13	BP	1	66	55	1	4	6	0
13	BQ	1	66	55	1	4	6	0
13	BR	1	66	55	1	4	6	0
13	BS	1	66	55	1	4	6	0
13	BT	1	66	55	1	4	6	0
13	BU	1	66	55	1	4	6	0
13	BV	1	66	55	1	4	6	0
13	BW	1	66	55	1	4	6	0
13	BX	1	66	55	1	4	6	0
13	L	1	132	110	2	8	12	0
13	L	1	132	110	2	8	12	0
13	M	1	132	110	2	8	12	0
13	M	1	132	110	2	8	12	0
13	aa	1	66	55	1	4	6	0

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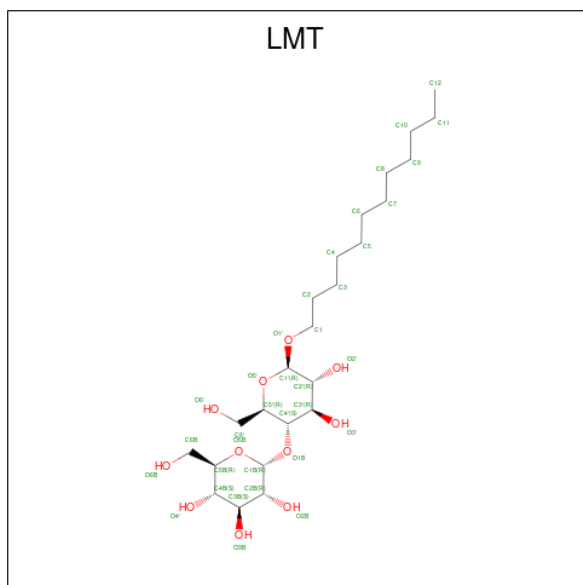
Mol	Chain	Residues	Atoms					AltConf
13	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ai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

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

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



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

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Mol	Chain	Residues	Atoms			AltConf
14	AB	1	Total	C	O	0
			70	48	22	
14	AB	1	Total	C	O	0
			70	48	22	
14	AD	1	Total	C	O	0
			70	48	22	
14	AD	1	Total	C	O	0
			70	48	22	
14	AF	1	Total	C	O	0
			35	24	11	
14	AG	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			105	72	33	
14	AH	1	Total	C	O	0
			105	72	33	
14	AH	1	Total	C	O	0
			105	72	33	
14	AI	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AL	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			70	48	22	
14	AN	1	Total	C	O	0
			70	48	22	
14	AO	1	Total	C	O	0
			35	24	11	
14	AP	1	Total	C	O	0
			35	24	11	
14	AR	1	Total	C	O	0
			35	24	11	
14	AS	1	Total	C	O	0
			35	24	11	
14	AT	1	Total	C	O	0
			35	24	11	
14	AU	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	AV	1	35	24	11	0
14	AW	1	35	24	11	0
14	BA	1	140	96	44	0
14	BA	1	140	96	44	0
14	BA	1	140	96	44	0
14	BA	1	140	96	44	0
14	BB	1	70	48	22	0
14	BB	1	70	48	22	0
14	BC	1	70	48	22	0
14	BC	1	70	48	22	0
14	BD	1	140	96	44	0
14	BD	1	140	96	44	0
14	BD	1	140	96	44	0
14	BD	1	140	96	44	0
14	BE	1	140	96	44	0
14	BE	1	140	96	44	0
14	BE	1	140	96	44	0
14	BE	1	140	96	44	0
14	BF	1	105	72	33	0
14	BF	1	105	72	33	0
14	BF	1	105	72	33	0

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Mol	Chain	Residues	Atoms			AltConf
14	BG	1	Total	C	O	0
			70	48	22	
14	BG	1	Total	C	O	0
			70	48	22	
14	BH	1	Total	C	O	0
			105	72	33	
14	BH	1	Total	C	O	0
			105	72	33	
14	BH	1	Total	C	O	0
			105	72	33	
14	BI	1	Total	C	O	0
			140	96	44	
14	BI	1	Total	C	O	0
			140	96	44	
14	BI	1	Total	C	O	0
			140	96	44	
14	BI	1	Total	C	O	0
			140	96	44	
14	BJ	1	Total	C	O	0
			70	48	22	
14	BJ	1	Total	C	O	0
			70	48	22	
14	BK	1	Total	C	O	0
			140	96	44	
14	BK	1	Total	C	O	0
			140	96	44	
14	BK	1	Total	C	O	0
			140	96	44	
14	BK	1	Total	C	O	0
			140	96	44	
14	BL	1	Total	C	O	0
			105	72	33	
14	BL	1	Total	C	O	0
			105	72	33	
14	BL	1	Total	C	O	0
			105	72	33	
14	BM	1	Total	C	O	0
			70	48	22	
14	BM	1	Total	C	O	0
			70	48	22	
14	BN	1	Total	C	O	0
			140	96	44	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	BN	1	140	96	44	0
14	BN	1	140	96	44	0
14	BN	1	140	96	44	0
14	BO	1	70	48	22	0
14	BO	1	70	48	22	0
14	BP	1	140	96	44	0
14	BP	1	140	96	44	0
14	BP	1	140	96	44	0
14	BP	1	140	96	44	0
14	BQ	1	70	48	22	0
14	BQ	1	70	48	22	0
14	BR	1	140	96	44	0
14	BR	1	140	96	44	0
14	BR	1	140	96	44	0
14	BR	1	140	96	44	0
14	BS	1	105	72	33	0
14	BS	1	105	72	33	0
14	BS	1	105	72	33	0
14	BT	1	105	72	33	0
14	BT	1	105	72	33	0
14	BT	1	105	72	33	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	BU	1	105	72	33	0
14	BU	1	105	72	33	0
14	BU	1	105	72	33	0
14	BV	1	70	48	22	0
14	BV	1	70	48	22	0
14	BW	1	140	96	44	0
14	BW	1	140	96	44	0
14	BW	1	140	96	44	0
14	BW	1	140	96	44	0
14	BW	1	140	96	44	0
14	BX	1	70	48	22	0
14	BX	1	70	48	22	0
14	L	1	175	120	55	0
14	L	1	175	120	55	0
14	L	1	175	120	55	0
14	L	1	175	120	55	0
14	L	1	175	120	55	0
14	M	1	35	24	11	0
14	ac	1	35	24	11	0
14	bb	1	35	24	11	0
14	bc	1	35	24	11	0
14	bd	1	35	24	11	0

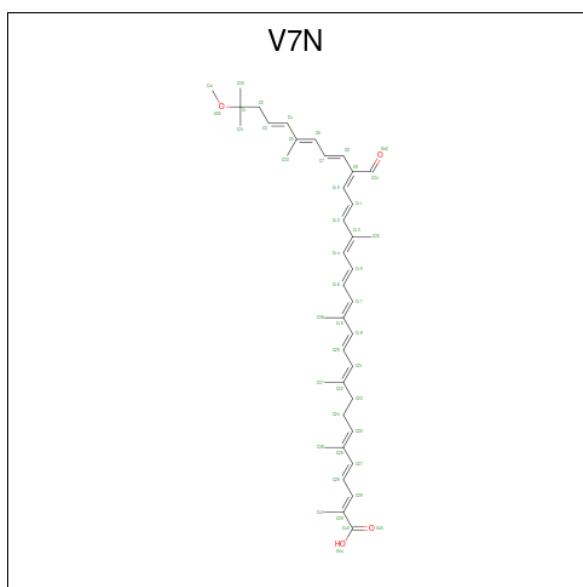
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	bf	1	70	48	22	0
14	bf	1	70	48	22	0
14	bg	1	35	24	11	0
14	bh	1	70	48	22	0
14	bh	1	70	48	22	0
14	bj	1	35	24	11	0
14	bk	1	35	24	11	0
14	bl	1	70	48	22	0
14	bl	1	70	48	22	0
14	bm	1	35	24	11	0
14	bn	1	35	24	11	0
14	bo	1	35	24	11	0
14	bp	1	35	24	11	0

- Molecule 15 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (three-letter code: V7N) (formula: C<sub>41</sub>H<sub>54</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
15	AE	1	Total	C	O	0
			45	41	4	
15	AH	1	Total	C	O	0
			45	41	4	
15	AT	1	Total	C	O	0
			45	41	4	
15	BA	1	Total	C	O	0
			45	41	4	
15	BB	1	Total	C	O	0
			45	41	4	
15	BC	1	Total	C	O	0
			45	41	4	
15	BD	1	Total	C	O	0
			45	41	4	
15	BE	1	Total	C	O	0
			45	41	4	
15	BG	1	Total	C	O	0
			45	41	4	
15	BH	1	Total	C	O	0
			45	41	4	
15	BJ	1	Total	C	O	0
			45	41	4	
15	BK	1	Total	C	O	0
			45	41	4	
15	BL	1	Total	C	O	0
			45	41	4	
15	BM	1	Total	C	O	0
			45	41	4	

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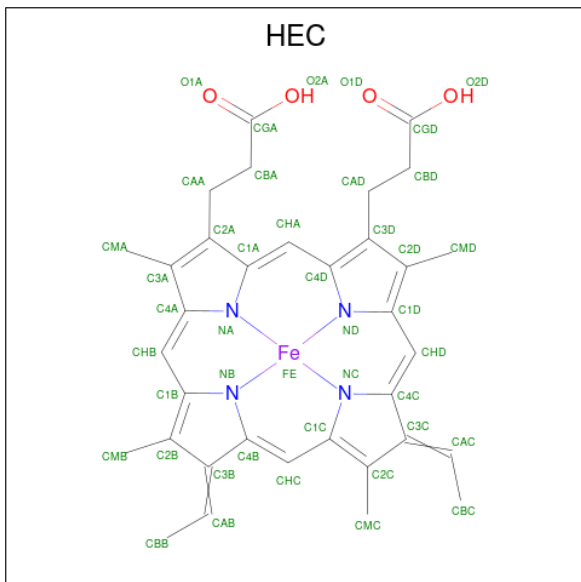
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	BN	1	45	41	4	0
15	BO	1	45	41	4	0
15	BP	1	45	41	4	0
15	BQ	1	45	41	4	0
15	BR	1	45	41	4	0
15	BS	1	45	41	4	0
15	BT	1	45	41	4	0
15	BV	1	45	41	4	0
15	BW	1	45	41	4	0
15	BX	1	45	41	4	0
15	ba	1	45	41	4	0
15	bb	1	45	41	4	0
15	bc	1	45	41	4	0
15	bd	1	45	41	4	0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

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

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



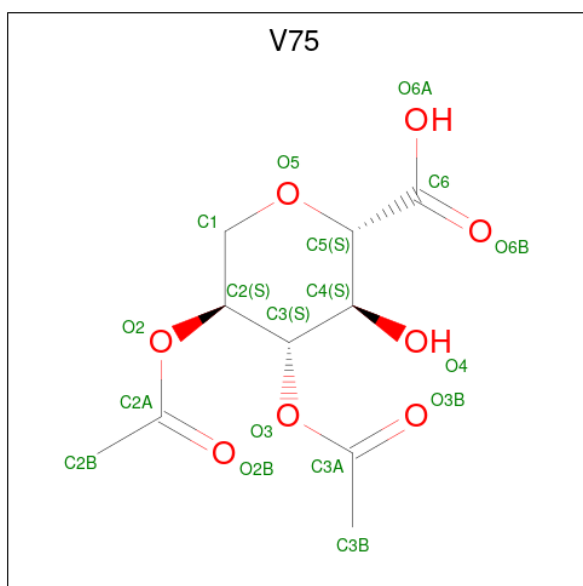
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
16	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
16	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
16	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	

- Molecule 17 is 2-acetamido-2-deoxy- $\alpha$ -D-glucopyranose (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 18 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (three-letter code: V75) (formula:  $C_{10}H_{14}O_8$ ) (labeled as "Ligand of Interest" by depositor).



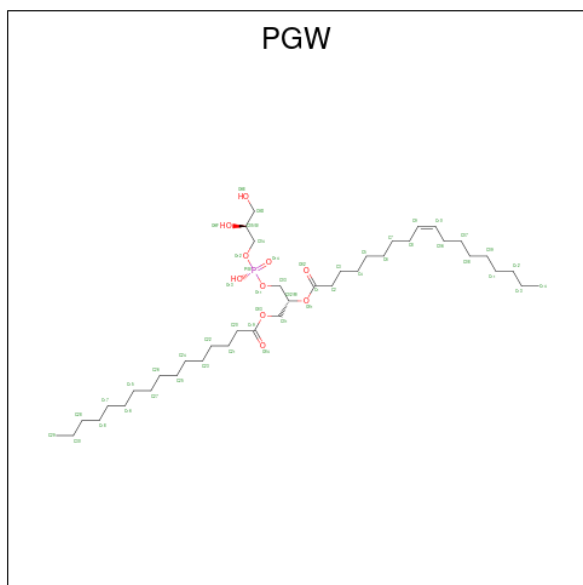
Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			18	10	8	

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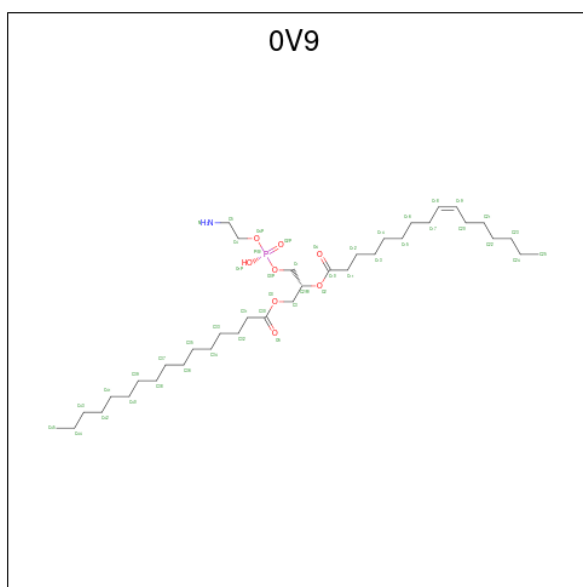
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	M	1	18	10	8	0

- Molecule 19 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



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

- Molecule 20 is (19R,22S)-25-amino-22-hydroxy-22-oxido-16-oxo-17,21,23-trioxa-22lambda da 5 -phosphapentacosan-19-yl (9Z)-hexadec-9-enoate (three-letter code: OV9) (formula: C<sub>37</sub>H<sub>72</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



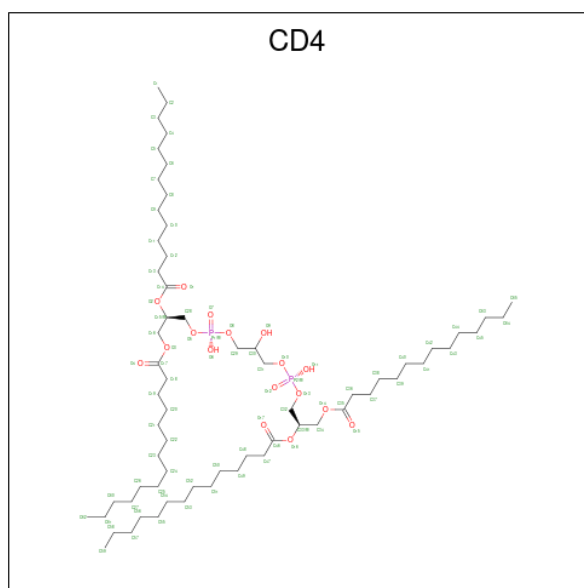
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	H1	1	45	35	1	8	1	0
20	L	1	45	35	1	8	1	0
20	aj	1	45	35	1	8	1	0
20	ba	1	90	70	2	16	2	0
20	ba	1	90	70	2	16	2	0
20	bb	1	45	35	1	8	1	0
20	bc	1	45	35	1	8	1	0
20	be	1	90	70	2	16	2	0
20	be	1	90	70	2	16	2	0
20	bf	1	45	35	1	8	1	0
20	bg	1	45	35	1	8	1	0
20	bh	1	45	35	1	8	1	0
20	bi	1	45	35	1	8	1	0
20	bj	1	45	35	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	bk	1	Total 90	C 70	N 2	O 16	P 2	0
20	bk	1	Total 90	C 70	N 2	O 16	P 2	0
20	bl	1	Total 45	C 35	N 1	O 8	P 1	0
20	bm	1	Total 45	C 35	N 1	O 8	P 1	0
20	bn	1	Total 45	C 35	N 1	O 8	P 1	0
20	bo	1	Total 45	C 35	N 1	O 8	P 1	0

- Molecule 21 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula:  $C_{65}H_{126}O_{17}P_2$ ).



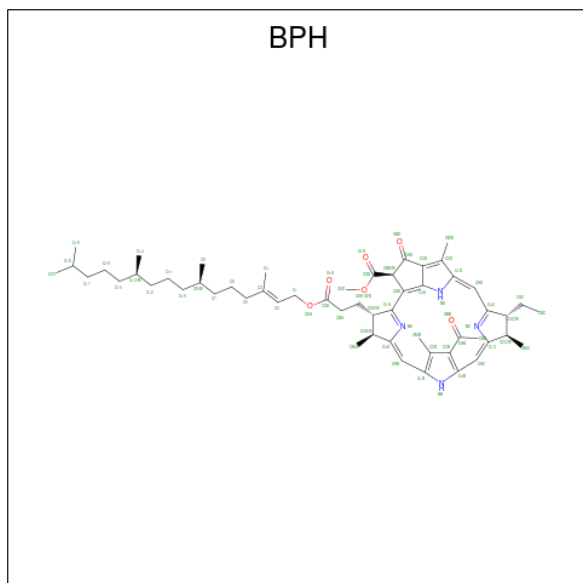
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	H1	1	Total 84	C 65	O 17	P 2	0
21	M	1	Total 84	C 65	O 17	P 2	0
21	ad	1	Total 84	C 65	O 17	P 2	0
21	af	1	Total 168	C 130	O 34	P 4	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	af	1	168	130	34	4	0
21	ai	1	84	65	17	2	0

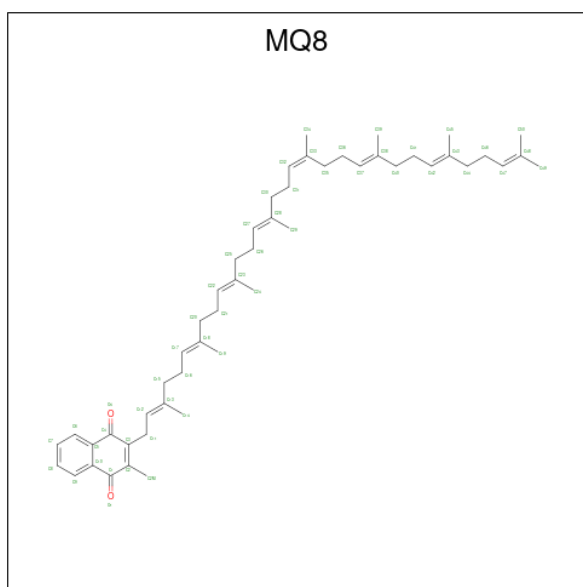
- Molecule 22 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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



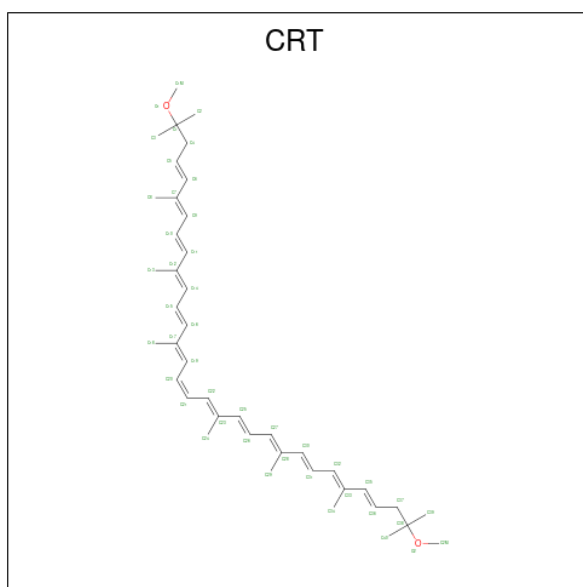


Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	an	1	Total	C	O	0
			53	51	2	

- Molecule 24 is FE (III) ION (three-letter code: FE) (formula: Fe).

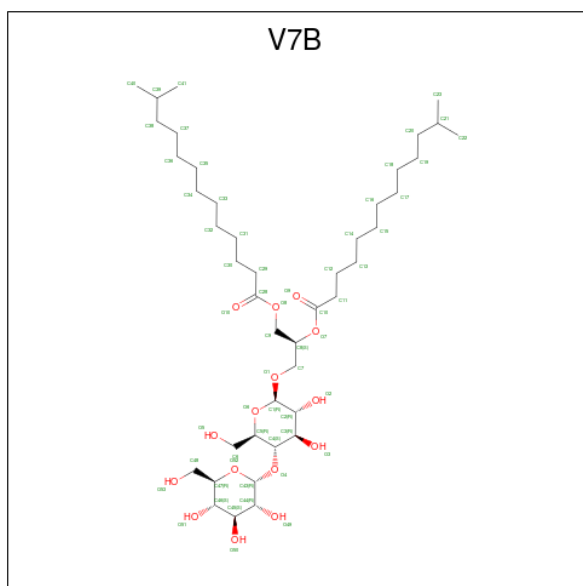
Mol	Chain	Residues	Atoms		AltConf
24	M	1	Total	Fe	0
			1	1	

- Molecule 25 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



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

- Molecule 26 is [(2 {S})-3-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-2-(12-methyltridecanoyloxy)propyl] 12-methyltridecanoate (three-letter code: V7B) (formula: C<sub>43</sub>H<sub>80</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



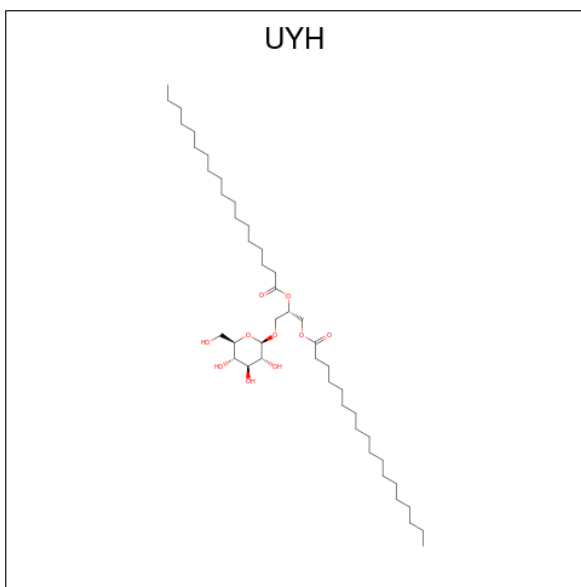
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	af	1	58	43	15	0

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

- Molecule 27 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (three-letter code: UYH) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	AA	3	Total	O	0
			3	3	
28	AB	3	Total	O	0
			3	3	
28	AC	2	Total	O	0
			2	2	
28	AD	5	Total	O	0
			5	5	
28	AG	2	Total	O	0
			2	2	
28	AH	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
28	AI	3	Total 3	O 3	0
28	AJ	6	Total 6	O 6	0
28	AK	3	Total 3	O 3	0
28	AL	3	Total 3	O 3	0
28	AM	4	Total 4	O 4	0
28	AN	3	Total 3	O 3	0
28	AO	2	Total 2	O 2	0
28	AP	3	Total 3	O 3	0
28	AQ	5	Total 5	O 5	0
28	AR	2	Total 2	O 2	0
28	AS	5	Total 5	O 5	0
28	AT	7	Total 7	O 7	0
28	AV	6	Total 6	O 6	0
28	AW	6	Total 6	O 6	0
28	AX	5	Total 5	O 5	0
28	BD	1	Total 1	O 1	0
28	BE	1	Total 1	O 1	0
28	BF	1	Total 1	O 1	0
28	BO	1	Total 1	O 1	0
28	BW	1	Total 1	O 1	0
28	C	98	Total 98	O 98	0

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Mol	Chain	Residues	Atoms		AltConf
28	C1	48	Total 48	O 48	0
28	C2	3	Total 3	O 3	0
28	H1	9	Total 9	O 9	0
28	H2	35	Total 35	O 35	0
28	L	53	Total 53	O 53	0
28	M	59	Total 59	O 59	0
28	aa	3	Total 3	O 3	0
28	ab	3	Total 3	O 3	0
28	ac	4	Total 4	O 4	0
28	ad	9	Total 9	O 9	0
28	ae	7	Total 7	O 7	0
28	af	7	Total 7	O 7	0
28	ag	7	Total 7	O 7	0
28	ah	6	Total 6	O 6	0
28	ai	3	Total 3	O 3	0
28	aj	6	Total 6	O 6	0
28	ak	14	Total 14	O 14	0
28	al	8	Total 8	O 8	0
28	am	8	Total 8	O 8	0
28	an	5	Total 5	O 5	0
28	ao	2	Total 2	O 2	0

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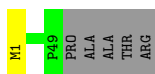
Mol	Chain	Residues	Atoms		AltConf
28	ap	8	Total 8	O 8	0
28	bb	2	Total 2	O 2	0
28	bc	2	Total 2	O 2	0
28	bd	1	Total 1	O 1	0
28	be	1	Total 1	O 1	0
28	bf	1	Total 1	O 1	0
28	bg	1	Total 1	O 1	0
28	bh	2	Total 2	O 2	0
28	bi	3	Total 3	O 3	0
28	bk	4	Total 4	O 4	0
28	bl	3	Total 3	O 3	0
28	bm	4	Total 4	O 4	0
28	bn	3	Total 3	O 3	0
28	bo	2	Total 2	O 2	0
28	bp	1	Total 1	O 1	0

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

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

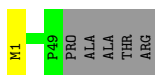
- Molecule 1: LHh-alpha

Chain AA:  89% 9%




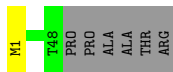
- Molecule 1: LHh-alpha

Chain AB:  89% 9%




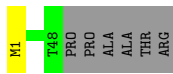
- Molecule 1: LHh-alpha

Chain AC:  87% 11%



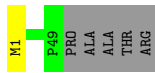
- Molecule 1: LHh-alpha

Chain AD:  87% 11%

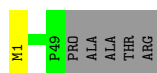
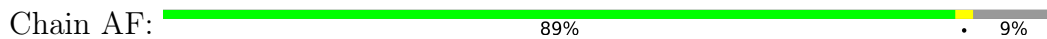


- Molecule 1: LHh-alpha

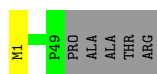
Chain AE:  89% 9%



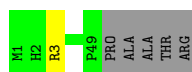
- Molecule 1: LHh-alpha



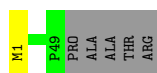
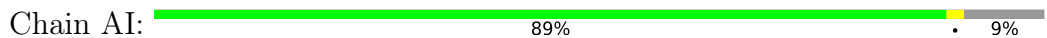
● Molecule 1: Lhh-alpha



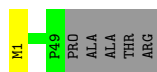
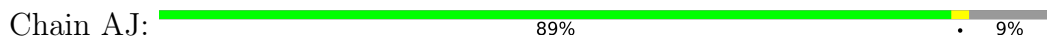
● Molecule 1: Lhh-alpha



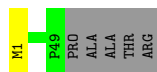
● Molecule 1: Lhh-alpha



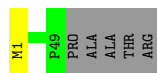
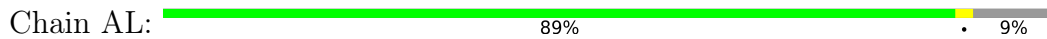
● Molecule 1: Lhh-alpha



● Molecule 1: Lhh-alpha



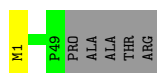
● Molecule 1: Lhh-alpha



● Molecule 1: Lhh-alpha

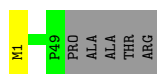


Chain AM:  89% 9%



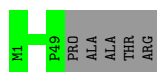
● Molecule 1: Lhh-alpha

Chain AN:  89% 9%



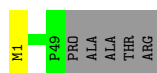
● Molecule 1: Lhh-alpha

Chain AO:  91% 9%



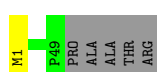
● Molecule 1: Lhh-alpha

Chain AP:  89% 9%



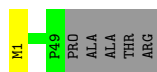
● Molecule 1: Lhh-alpha

Chain AQ:  89% 9%




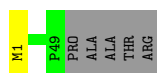
● Molecule 1: Lhh-alpha

Chain AR:  89% 9%



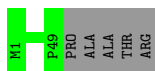
● Molecule 1: Lhh-alpha

Chain AS:  89% 9%



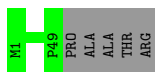
● Molecule 1: Lhh-alpha

Chain AT:  91% 9%



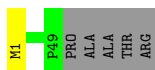
- Molecule 1: Lhh-alpha

Chain AU:  91% 9%



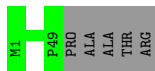
- Molecule 1: Lhh-alpha

Chain AV:  89% 9%



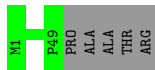
- Molecule 1: Lhh-alpha

Chain AW:  91% 9%



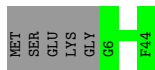
- Molecule 1: Lhh-alpha

Chain AX:  91% 9%



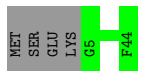
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BA:  89% 11%




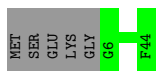
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  91% 9%



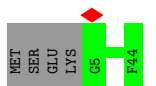
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  89% 11%



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

Chain BD:  91% 9%



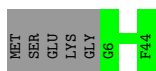
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BE:  91% 9%



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

Chain BF:  89% 11%




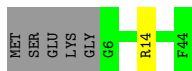
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  89% 11%



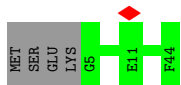
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BH:  86% 11%




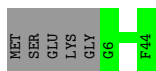
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BI:  91% 9%




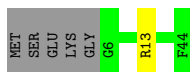
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



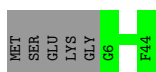
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  86% 11%



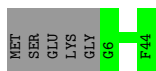
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BL:  89% 11%



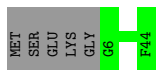
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BM:  89% 11%



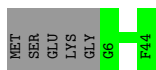
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  89% 11%



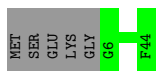
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  89% 11%



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

Chain BP:  89% 11%



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

Chain BQ:  91% 9%



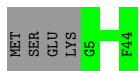
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BR:  91% 9%



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

Chain BS:  91% 9%



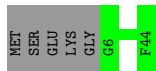
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  91% 9%



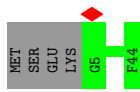
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  89% 11%



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

Chain BV:  91% 9%

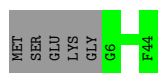


- Molecule 2: Light-harvesting protein B:885 subunit beta

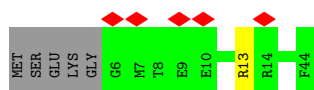
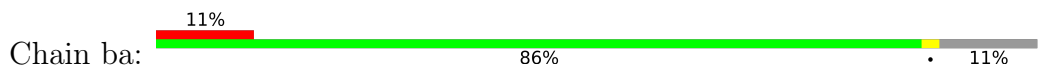
Chain BW:  91% 9%



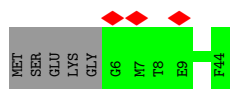
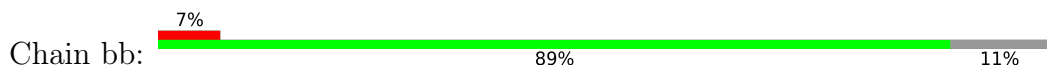
- Molecule 2: Light-harvesting protein B:885 subunit beta



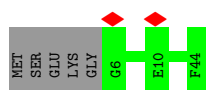
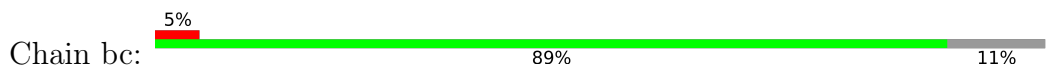
- Molecule 2: Light-harvesting protein B:885 subunit beta



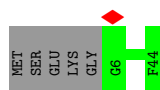
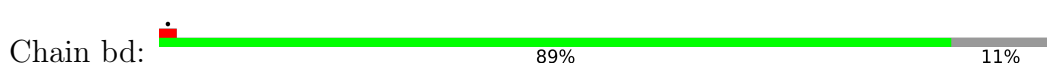
- Molecule 2: Light-harvesting protein B:885 subunit beta



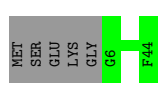
- Molecule 2: Light-harvesting protein B:885 subunit beta



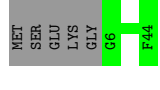
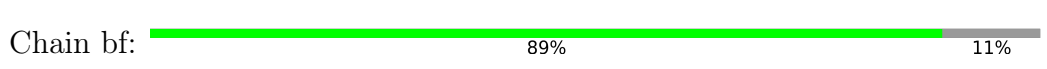
- Molecule 2: Light-harvesting protein B:885 subunit beta




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

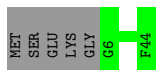


- Molecule 2: Light-harvesting protein B:885 subunit beta



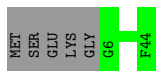
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bg:  89% 11%




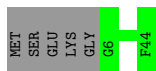
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bh:  89% 11%




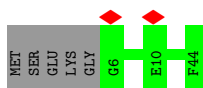
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bi:  89% 11%




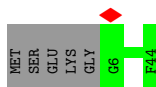
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bj:  5% 89% 11%




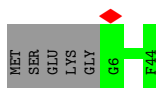
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bk:  5% 89% 11%



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

Chain bl:  5% 89% 11%



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

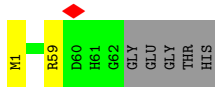
Chain bm:  89% 11%



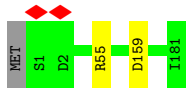
- Molecule 2: Light-harvesting protein B:885 subunit beta







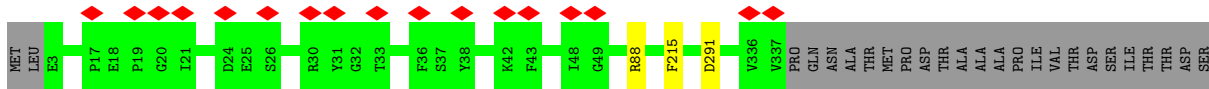
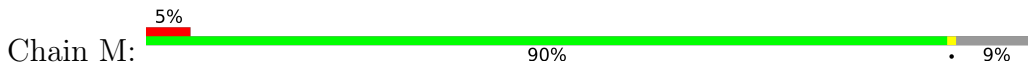
• Molecule 7: RC-Hc



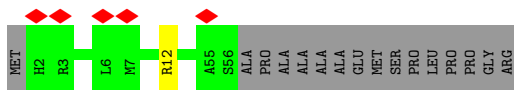
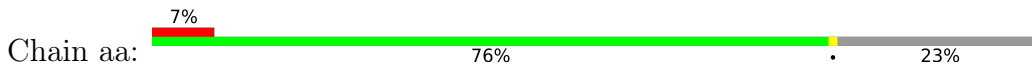
• Molecule 8: Photosynthetic reaction center L subunit



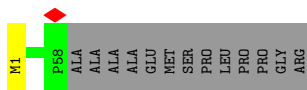
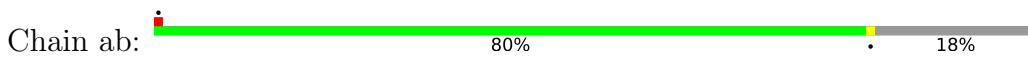
• Molecule 9: RC-M



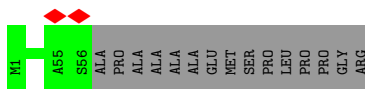
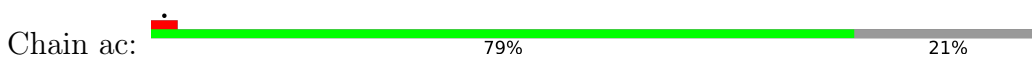
• Molecule 10: LHC domain-containing protein



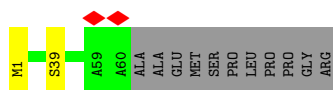
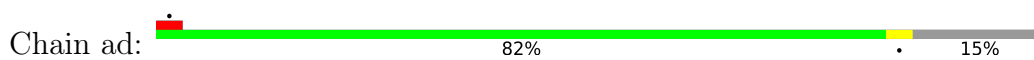
• Molecule 11: LHC domain-containing protein



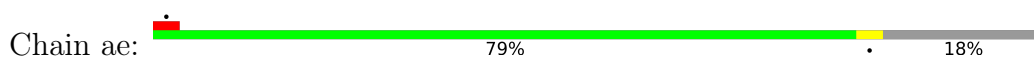
• Molecule 11: LHC domain-containing protein



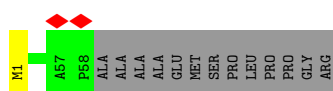
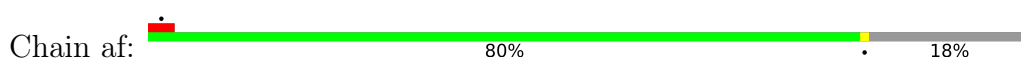
• Molecule 11: LHC domain-containing protein



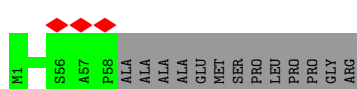
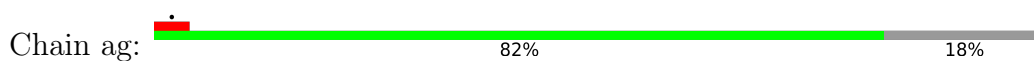
• Molecule 11: LHC domain-containing protein



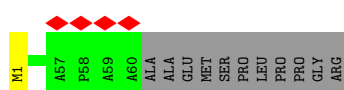
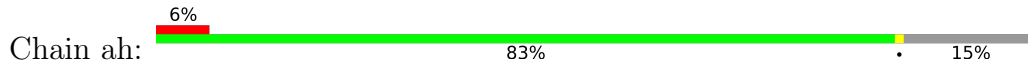
• Molecule 11: LHC domain-containing protein



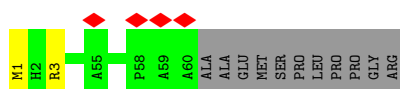
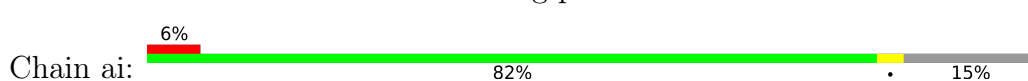
• Molecule 11: LHC domain-containing protein



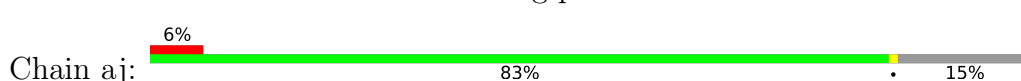
• Molecule 11: LHC domain-containing protein

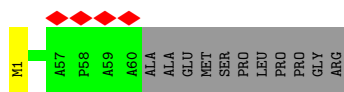


• Molecule 11: LHC domain-containing protein

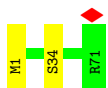


• Molecule 11: LHC domain-containing protein

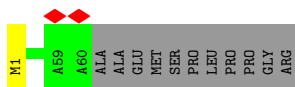
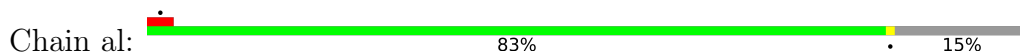




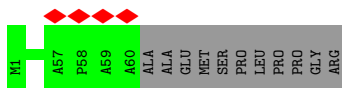
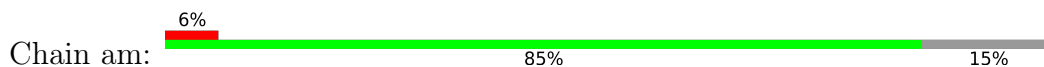
- Molecule 11: LHC domain-containing protein



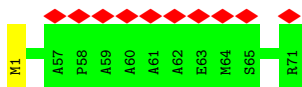
- Molecule 11: LHC domain-containing protein



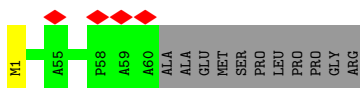
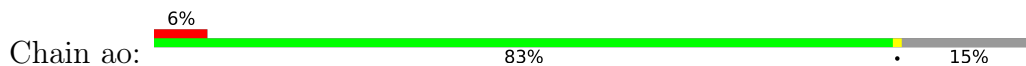
- Molecule 11: LHC domain-containing protein



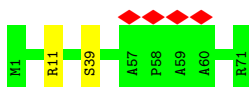
- Molecule 11: LHC domain-containing protein




- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



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

Chain MG:  100%

MAN1  
RAM2

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

Chain CG:  100%

MAN1  
RAM2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73853	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	0.204	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0292	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: HEC, CRT, V7B, NDG, UYH, RAM, LMT, MAN, FE, 0V9, BCL, FME, BPH, CD4, PGW, V75, MQ8, V7N

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	0.24	0/396	0.49	0/541
1	AB	0.24	0/396	0.50	0/541
1	AC	0.25	0/388	0.53	0/529
1	AD	0.25	0/388	0.52	0/529
1	AE	0.24	0/396	0.52	0/541
1	AF	0.24	0/396	0.50	0/541
1	AG	0.25	0/396	0.50	0/541
1	AH	0.24	0/396	0.51	0/541
1	AI	0.24	0/396	0.50	0/541
1	AJ	0.24	0/396	0.52	0/541
1	AK	0.25	0/396	0.51	0/541
1	AL	0.24	0/396	0.52	0/541
1	AM	0.24	0/396	0.48	0/541
1	AN	0.24	0/396	0.53	0/541
1	AO	0.23	0/396	0.50	0/541
1	AP	0.24	0/396	0.49	0/541
1	AQ	0.24	0/396	0.51	0/541
1	AR	0.24	0/396	0.50	0/541
1	AS	0.24	0/396	0.53	0/541
1	AT	0.24	0/396	0.52	0/541
1	AU	0.24	0/396	0.50	0/541
1	AV	0.24	0/396	0.51	0/541
1	AW	0.24	0/396	0.53	0/541
1	AX	0.24	0/396	0.51	0/541
2	BA	0.24	0/336	0.50	0/456
2	BB	0.25	0/340	0.49	0/461
2	BC	0.24	0/336	0.49	0/456
2	BD	0.25	0/340	0.50	0/461
2	BE	0.25	0/340	0.49	0/461
2	BF	0.24	0/336	0.50	0/456
2	BG	0.24	0/336	0.49	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	BH	0.24	0/336	0.48	0/456
2	BI	0.25	0/340	0.49	0/461
2	BJ	0.24	0/336	0.49	0/456
2	BK	0.24	0/336	0.50	0/456
2	BL	0.25	0/336	0.54	0/456
2	BM	0.25	0/336	0.51	0/456
2	BN	0.25	0/336	0.51	0/456
2	BO	0.24	0/336	0.51	0/456
2	BP	0.24	0/336	0.51	0/456
2	BQ	0.24	0/340	0.50	0/461
2	BR	0.26	0/340	0.52	0/461
2	BS	0.24	0/340	0.49	0/461
2	BT	0.24	0/340	0.52	0/461
2	BU	0.24	0/336	0.50	0/456
2	BV	0.24	0/340	0.50	0/461
2	BW	0.24	0/340	0.49	0/461
2	BX	0.24	0/336	0.48	0/456
2	ba	0.25	0/336	0.53	0/456
2	bb	0.24	0/336	0.49	0/456
2	bc	0.25	0/336	0.51	0/456
2	bd	0.26	0/336	0.49	0/456
2	be	0.26	0/336	0.53	0/456
2	bf	0.24	0/336	0.48	0/456
2	bg	0.26	0/336	0.51	0/456
2	bh	0.24	0/336	0.49	0/456
2	bi	0.27	0/336	0.51	0/456
2	bj	0.27	0/336	0.52	0/456
2	bk	0.26	0/336	0.52	0/456
2	bl	0.25	0/336	0.49	0/456
2	bm	0.26	0/336	0.50	0/456
2	bn	0.25	0/340	0.50	0/461
2	bo	0.25	0/336	0.49	0/456
2	bp	0.25	0/336	0.49	0/456
3	C	0.27	0/2392	0.55	0/3263
4	C1	0.24	0/826	0.58	0/1128
5	C2	0.24	0/787	0.56	0/1075
6	H1	0.27	0/531	0.52	0/717
7	H2	0.25	0/1443	0.55	0/1970
8	L	0.25	0/2252	0.51	0/3081
9	M	0.26	0/2795	0.54	0/3824
10	aa	0.24	0/444	0.54	0/605
11	ab	0.25	0/457	0.51	0/624
11	ac	0.26	0/444	0.55	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	ad	0.25	0/467	0.54	0/638
11	ae	0.26	0/457	0.53	0/624
11	af	0.25	0/457	0.52	0/624
11	ag	0.25	0/457	0.56	0/624
11	ah	0.26	0/467	0.54	0/638
11	ai	0.25	0/467	0.53	0/638
11	aj	0.25	0/467	0.55	0/638
11	ak	0.27	0/547	0.53	0/748
11	al	0.26	0/467	0.54	0/638
11	am	0.26	0/467	0.53	0/638
11	an	0.26	0/547	0.55	0/748
11	ao	0.26	0/467	0.55	0/638
11	ap	0.25	0/548	0.55	0/748
All	All	0.25	0/41625	0.52	0/56729

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	AH	0	1
2	BH	0	1
2	bo	0	1
3	C	0	1
6	H1	0	1
7	H2	0	1
8	L	0	1
9	M	0	1
11	ae	0	1
11	ai	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AH	3	ARG	Sidechain
2	BH	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	170	ARG	Sidechain
6	H1	59	ARG	Sidechain
7	H2	55	ARG	Sidechain
8	L	12	ARG	Sidechain
9	M	88	ARG	Sidechain
11	ae	3	ARG	Sidechain
11	ai	3	ARG	Sidechain
2	bo	13	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AM	47/54 (87%)	47 (100%)	0	0	100	100
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%)	47 (100%)	0	0	100	100
2	BA	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	BB	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
2	BC	37/44 (84%)	37 (100%)	0	0	100	100
2	BD	38/44 (86%)	38 (100%)	0	0	100	100
2	BE	38/44 (86%)	38 (100%)	0	0	100	100
2	BF	37/44 (84%)	37 (100%)	0	0	100	100
2	BG	37/44 (84%)	37 (100%)	0	0	100	100
2	BH	37/44 (84%)	37 (100%)	0	0	100	100
2	BI	38/44 (86%)	38 (100%)	0	0	100	100
2	BJ	37/44 (84%)	37 (100%)	0	0	100	100
2	BK	37/44 (84%)	37 (100%)	0	0	100	100
2	BL	37/44 (84%)	37 (100%)	0	0	100	100
2	BM	37/44 (84%)	37 (100%)	0	0	100	100
2	BN	37/44 (84%)	37 (100%)	0	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	37/44 (84%)	37 (100%)	0	0	100	100
2	BQ	38/44 (86%)	38 (100%)	0	0	100	100
2	BR	38/44 (86%)	38 (100%)	0	0	100	100
2	BS	38/44 (86%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BT	38/44 (86%)	38 (100%)	0	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	38/44 (86%)	38 (100%)	0	0	100	100
2	BW	38/44 (86%)	38 (100%)	0	0	100	100
2	BX	37/44 (84%)	37 (100%)	0	0	100	100
2	ba	37/44 (84%)	37 (100%)	0	0	100	100
2	bb	37/44 (84%)	37 (100%)	0	0	100	100
2	bc	37/44 (84%)	37 (100%)	0	0	100	100
2	bd	37/44 (84%)	37 (100%)	0	0	100	100
2	be	37/44 (84%)	37 (100%)	0	0	100	100
2	bf	37/44 (84%)	37 (100%)	0	0	100	100
2	bg	37/44 (84%)	37 (100%)	0	0	100	100
2	bh	37/44 (84%)	37 (100%)	0	0	100	100
2	bi	37/44 (84%)	37 (100%)	0	0	100	100
2	bj	37/44 (84%)	37 (100%)	0	0	100	100
2	bk	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bl	37/44 (84%)	37 (100%)	0	0	100	100
2	bm	37/44 (84%)	37 (100%)	0	0	100	100
2	bn	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
2	bo	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bp	37/44 (84%)	37 (100%)	0	0	100	100
3	C	297/354 (84%)	283 (95%)	13 (4%)	1 (0%)	41	49
4	C1	101/202 (50%)	97 (96%)	4 (4%)	0	100	100
5	C2	97/125 (78%)	96 (99%)	1 (1%)	0	100	100
6	H1	60/67 (90%)	60 (100%)	0	0	100	100
7	H2	178/181 (98%)	173 (97%)	5 (3%)	0	100	100
8	L	271/274 (99%)	263 (97%)	8 (3%)	0	100	100
9	M	333/367 (91%)	324 (97%)	9 (3%)	0	100	100
10	aa	53/71 (75%)	53 (100%)	0	0	100	100
11	ab	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ac	54/71 (76%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	ad	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ae	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	af	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ag	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ah	58/71 (82%)	58 (100%)	0	0	100	100
11	ai	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	aj	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ak	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
11	al	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	an	69/71 (97%)	64 (93%)	5 (7%)	0	100	100
11	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ap	69/71 (97%)	69 (100%)	0	0	100	100
All	All	4898/5762 (85%)	4828 (99%)	69 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ARG

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

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	38 (100%)	0	100	100
1	AI	38/41 (93%)	38 (100%)	0	100	100
1	AJ	38/41 (93%)	38 (100%)	0	100	100
1	AK	38/41 (93%)	38 (100%)	0	100	100
1	AL	38/41 (93%)	38 (100%)	0	100	100
1	AM	38/41 (93%)	38 (100%)	0	100	100
1	AN	38/41 (93%)	38 (100%)	0	100	100
1	AO	38/41 (93%)	38 (100%)	0	100	100
1	AP	38/41 (93%)	38 (100%)	0	100	100
1	AQ	38/41 (93%)	38 (100%)	0	100	100
1	AR	38/41 (93%)	38 (100%)	0	100	100
1	AS	38/41 (93%)	38 (100%)	0	100	100
1	AT	38/41 (93%)	38 (100%)	0	100	100
1	AU	38/41 (93%)	38 (100%)	0	100	100
1	AV	38/41 (93%)	38 (100%)	0	100	100
1	AW	38/41 (93%)	38 (100%)	0	100	100
1	AX	38/41 (93%)	38 (100%)	0	100	100
2	BA	31/35 (89%)	31 (100%)	0	100	100
2	BB	31/35 (89%)	31 (100%)	0	100	100
2	BC	31/35 (89%)	31 (100%)	0	100	100
2	BD	31/35 (89%)	31 (100%)	0	100	100
2	BE	31/35 (89%)	31 (100%)	0	100	100
2	BF	31/35 (89%)	31 (100%)	0	100	100
2	BG	31/35 (89%)	31 (100%)	0	100	100
2	BH	31/35 (89%)	31 (100%)	0	100	100
2	BI	31/35 (89%)	31 (100%)	0	100	100
2	BJ	31/35 (89%)	31 (100%)	0	100	100
2	BK	31/35 (89%)	30 (97%)	1 (3%)	39	50
2	BL	31/35 (89%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BM	31/35 (89%)	31 (100%)	0	100	100
2	BN	31/35 (89%)	31 (100%)	0	100	100
2	BO	31/35 (89%)	31 (100%)	0	100	100
2	BP	31/35 (89%)	31 (100%)	0	100	100
2	BQ	31/35 (89%)	31 (100%)	0	100	100
2	BR	31/35 (89%)	31 (100%)	0	100	100
2	BS	31/35 (89%)	31 (100%)	0	100	100
2	BT	31/35 (89%)	31 (100%)	0	100	100
2	BU	31/35 (89%)	31 (100%)	0	100	100
2	BV	31/35 (89%)	31 (100%)	0	100	100
2	BW	31/35 (89%)	31 (100%)	0	100	100
2	BX	31/35 (89%)	31 (100%)	0	100	100
2	ba	31/35 (89%)	30 (97%)	1 (3%)	39	50
2	bb	31/35 (89%)	31 (100%)	0	100	100
2	bc	31/35 (89%)	31 (100%)	0	100	100
2	bd	31/35 (89%)	31 (100%)	0	100	100
2	be	31/35 (89%)	31 (100%)	0	100	100
2	bf	31/35 (89%)	31 (100%)	0	100	100
2	bg	31/35 (89%)	31 (100%)	0	100	100
2	bh	31/35 (89%)	31 (100%)	0	100	100
2	bi	31/35 (89%)	31 (100%)	0	100	100
2	bj	31/35 (89%)	31 (100%)	0	100	100
2	bk	31/35 (89%)	31 (100%)	0	100	100
2	bl	31/35 (89%)	31 (100%)	0	100	100
2	bm	31/35 (89%)	31 (100%)	0	100	100
2	bn	31/35 (89%)	31 (100%)	0	100	100
2	bo	31/35 (89%)	31 (100%)	0	100	100
2	bp	31/35 (89%)	31 (100%)	0	100	100
3	C	245/285 (86%)	242 (99%)	3 (1%)	71	81
4	C1	88/156 (56%)	88 (100%)	0	100	100
5	C2	70/95 (74%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H1	50/53 (94%)	50 (100%)	0	100	100
7	H2	150/151 (99%)	149 (99%)	1 (1%)	84	90
8	L	215/216 (100%)	212 (99%)	3 (1%)	67	78
9	M	273/299 (91%)	271 (99%)	2 (1%)	84	90
10	aa	45/55 (82%)	44 (98%)	1 (2%)	52	64
11	ab	46/54 (85%)	46 (100%)	0	100	100
11	ac	45/54 (83%)	45 (100%)	0	100	100
11	ad	46/54 (85%)	45 (98%)	1 (2%)	52	64
11	ae	46/54 (85%)	45 (98%)	1 (2%)	52	64
11	af	46/54 (85%)	46 (100%)	0	100	100
11	ag	46/54 (85%)	46 (100%)	0	100	100
11	ah	46/54 (85%)	46 (100%)	0	100	100
11	ai	46/54 (85%)	46 (100%)	0	100	100
11	aj	46/54 (85%)	46 (100%)	0	100	100
11	ak	54/54 (100%)	53 (98%)	1 (2%)	57	69
11	al	46/54 (85%)	46 (100%)	0	100	100
11	am	46/54 (85%)	46 (100%)	0	100	100
11	an	54/54 (100%)	54 (100%)	0	100	100
11	ao	46/54 (85%)	46 (100%)	0	100	100
11	ap	54/54 (100%)	52 (96%)	2 (4%)	34	45
All	All	3999/4504 (89%)	3982 (100%)	17 (0%)	91	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BK	13	ARG
3	C	116	TYR
3	C	202	TYR
3	C	277	VAL
7	H2	159	ASP
8	L	247	CYS
8	L	249	VAL
8	L	272	TRP
9	M	215	PHE
9	M	291	ASP

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Mol	Chain	Res	Type
10	aa	12	ARG
11	ad	39	SER
11	ae	39	SER
11	ak	34	SER
11	ap	11	ARG
11	ap	39	SER
2	ba	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	AG	35	GLN
1	AJ	35	GLN
4	C1	158	GLN
5	C2	24	HIS
7	H2	12	ASN
7	H2	119	GLN
8	L	104	GLN
8	L	116	HIS
9	M	110	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	FME	ad	1	11	8,9,10	0.90	0	7,9,11	1.31	1 (14%)
1	FME	AW	1	1	8,9,10	0.89	0	7,9,11	0.96	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	AG	1	1	8,9,10	0.89	0	7,9,11	1.22	1 (14%)
11	FME	ae	1	11	8,9,10	0.92	0	7,9,11	0.91	0
1	FME	AH	1	1	8,9,10	0.93	0	7,9,11	0.97	0
1	FME	AR	1	1	8,9,10	0.94	0	7,9,11	0.96	1 (14%)
1	FME	AK	1	1	8,9,10	0.92	0	7,9,11	1.10	1 (14%)
11	FME	ab	1	11	8,9,10	0.91	0	7,9,11	1.30	1 (14%)
1	FME	AM	1	1	8,9,10	0.93	0	7,9,11	1.01	1 (14%)
1	FME	AD	1	1	8,9,10	0.92	0	7,9,11	1.12	1 (14%)
11	FME	ag	1	11	8,9,10	0.90	0	7,9,11	1.01	0
11	FME	ah	1	11	8,9,10	0.92	0	7,9,11	1.21	1 (14%)
1	FME	AV	1	1	8,9,10	0.96	0	7,9,11	0.95	1 (14%)
11	FME	an	1	11	8,9,10	0.96	0	7,9,11	1.03	1 (14%)
1	FME	AO	1	1	8,9,10	0.94	0	7,9,11	0.95	0
11	FME	aj	1	11	8,9,10	0.92	0	7,9,11	1.14	1 (14%)
11	FME	ap	1	11	8,9,10	0.92	0	7,9,11	0.99	0
1	FME	AU	1	1	8,9,10	0.96	0	7,9,11	0.95	0
1	FME	AX	1	1	8,9,10	0.97	0	7,9,11	0.90	0
1	FME	AI	1	1	8,9,10	0.95	0	7,9,11	0.98	1 (14%)
1	FME	AB	1	1	8,9,10	0.91	0	7,9,11	1.08	1 (14%)
11	FME	ao	1	11	8,9,10	0.94	0	7,9,11	1.06	1 (14%)
11	FME	ai	1	11	8,9,10	0.95	0	7,9,11	1.17	1 (14%)
11	FME	ak	1	11	8,9,10	0.94	0	7,9,11	1.02	1 (14%)
1	FME	AL	1	1	8,9,10	0.93	0	7,9,11	1.09	1 (14%)
1	FME	AN	1	1	8,9,10	0.91	0	7,9,11	1.10	1 (14%)
1	FME	AP	1	1	8,9,10	0.91	0	7,9,11	1.04	1 (14%)
1	FME	AS	1	1	8,9,10	0.93	0	7,9,11	1.15	1 (14%)
11	FME	am	1	11	8,9,10	0.93	0	7,9,11	0.70	0
1	FME	AF	1	1	8,9,10	0.91	0	7,9,11	1.36	2 (28%)
1	FME	AT	1	1	8,9,10	0.94	0	7,9,11	0.90	0
1	FME	AC	1	1	8,9,10	0.91	0	7,9,11	1.37	2 (28%)
6	FME	H1	1	6	8,9,10	0.92	0	7,9,11	1.13	1 (14%)
1	FME	AE	1	1	8,9,10	0.93	0	7,9,11	1.08	1 (14%)
1	FME	AQ	1	1	8,9,10	0.91	0	7,9,11	1.21	1 (14%)
11	FME	ac	1	11	8,9,10	0.96	0	7,9,11	1.02	0
11	FME	al	1	11	8,9,10	0.94	0	7,9,11	1.14	1 (14%)
1	FME	AJ	1	1	8,9,10	0.93	0	7,9,11	1.04	1 (14%)
1	FME	AA	1	1	8,9,10	0.93	0	7,9,11	1.08	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	FME	af	1	11	8,9,10	0.91	0	7,9,11	1.29	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	ad	1	11	-	2/7/9/11	-
1	FME	AW	1	1	-	3/7/9/11	-
1	FME	AG	1	1	-	1/7/9/11	-
11	FME	ae	1	11	-	0/7/9/11	-
1	FME	AH	1	1	-	0/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
1	FME	AK	1	1	-	1/7/9/11	-
11	FME	ab	1	11	-	0/7/9/11	-
1	FME	AM	1	1	-	2/7/9/11	-
1	FME	AD	1	1	-	1/7/9/11	-
11	FME	ag	1	11	-	1/7/9/11	-
11	FME	ah	1	11	-	1/7/9/11	-
1	FME	AV	1	1	-	0/7/9/11	-
11	FME	an	1	11	-	0/7/9/11	-
1	FME	AO	1	1	-	0/7/9/11	-
11	FME	aj	1	11	-	0/7/9/11	-
11	FME	ap	1	11	-	1/7/9/11	-
1	FME	AU	1	1	-	0/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-
1	FME	AI	1	1	-	0/7/9/11	-
1	FME	AB	1	1	-	2/7/9/11	-
11	FME	ao	1	11	-	0/7/9/11	-
11	FME	ai	1	11	-	0/7/9/11	-
11	FME	ak	1	11	-	1/7/9/11	-
1	FME	AL	1	1	-	0/7/9/11	-
1	FME	AN	1	1	-	2/7/9/11	-
1	FME	AP	1	1	-	1/7/9/11	-
1	FME	AS	1	1	-	1/7/9/11	-
11	FME	am	1	11	-	1/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
1	FME	AT	1	1	-	1/7/9/11	-
1	FME	AC	1	1	-	0/7/9/11	-
6	FME	H1	1	6	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AE	1	1	-	0/7/9/11	-
1	FME	AQ	1	1	-	1/7/9/11	-
11	FME	ac	1	11	-	1/7/9/11	-
11	FME	al	1	11	-	0/7/9/11	-
1	FME	AJ	1	1	-	0/7/9/11	-
1	FME	AA	1	1	-	1/7/9/11	-
11	FME	af	1	11	-	0/7/9/11	-

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ad	1	FME	C-CA-N	2.85	114.88	109.73
11	af	1	FME	C-CA-N	2.85	114.87	109.73
11	ab	1	FME	C-CA-N	2.77	114.72	109.73
11	ah	1	FME	C-CA-N	2.64	114.49	109.73
1	AC	1	FME	C-CA-N	2.58	114.39	109.73
1	AG	1	FME	C-CA-N	2.49	114.23	109.73
1	AQ	1	FME	C-CA-N	2.47	114.20	109.73
11	ai	1	FME	C-CA-N	2.46	114.16	109.73
11	al	1	FME	C-CA-N	2.44	114.14	109.73
1	AS	1	FME	C-CA-N	2.44	114.13	109.73
11	aj	1	FME	C-CA-N	2.43	114.11	109.73
1	AD	1	FME	C-CA-N	2.33	113.93	109.73
1	AA	1	FME	C-CA-N	2.33	113.93	109.73
1	AN	1	FME	C-CA-N	2.29	113.87	109.73
1	AK	1	FME	C-CA-N	2.29	113.87	109.73
1	AE	1	FME	C-CA-N	2.29	113.86	109.73
1	AF	1	FME	C-CA-N	2.29	113.86	109.73
1	AB	1	FME	C-CA-N	2.27	113.83	109.73
1	AP	1	FME	C-CA-N	2.19	113.68	109.73
11	an	1	FME	C-CA-N	2.19	113.68	109.73
1	AF	1	FME	CA-N-CN	2.18	126.17	122.82
11	ao	1	FME	C-CA-N	2.16	113.62	109.73
1	AL	1	FME	C-CA-N	2.15	113.62	109.73
1	AJ	1	FME	C-CA-N	2.15	113.61	109.73
1	AM	1	FME	C-CA-N	2.12	113.56	109.73
6	H1	1	FME	CA-N-CN	2.11	126.06	122.82
1	AC	1	FME	CA-N-CN	2.09	126.04	122.82
11	ak	1	FME	C-CA-N	2.07	113.47	109.73
1	AR	1	FME	C-CA-N	2.06	113.45	109.73
1	AI	1	FME	C-CA-N	2.05	113.43	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AV	1	FME	C-CA-N	2.02	113.38	109.73

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	ah	1	FME	O-C-CA-CB
1	AB	1	FME	O-C-CA-CB
1	AK	1	FME	O-C-CA-CB
1	AM	1	FME	O-C-CA-CB
1	AN	1	FME	O-C-CA-CB
1	AQ	1	FME	C-CA-CB-CG
1	AS	1	FME	O-C-CA-CB
1	AT	1	FME	O-C-CA-CB
1	AW	1	FME	N-CA-CB-CG
1	AW	1	FME	CA-CB-CG-SD
11	ac	1	FME	N-CA-CB-CG
11	ak	1	FME	N-CA-CB-CG
1	AA	1	FME	N-CA-CB-CG
1	AN	1	FME	N-CA-CB-CG
1	AX	1	FME	CB-CG-SD-CE
11	ap	1	FME	N-CA-CB-CG
6	H1	1	FME	N-CA-CB-CG
11	ad	1	FME	N-CA-CB-CG
1	AB	1	FME	N-CA-CB-CG
1	AP	1	FME	N-CA-CB-CG
6	H1	1	FME	CB-CG-SD-CE
1	AM	1	FME	N-CA-CB-CG
11	ad	1	FME	CA-CB-CG-SD
1	AF	1	FME	N-CA-CB-CG
1	AG	1	FME	C-CA-CB-CG
11	am	1	FME	CB-CG-SD-CE
1	AD	1	FME	CA-CB-CG-SD
11	ag	1	FME	CB-CA-N-CN
1	AW	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	MAN	CG	1	3,18,12	11,11,12	0.81	1 (9%)	15,15,17	1.06	1 (6%)
12	RAM	CG	2	12	10,10,11	1.76	2 (20%)	14,14,16	0.81	0
12	MAN	MG	1	9,18,12	11,11,12	0.92	0	15,15,17	1.15	1 (6%)
12	RAM	MG	2	12	10,10,11	1.85	3 (30%)	14,14,16	2.17	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	CG	1	3,18,12	-	2/2/19/22	0/1/1/1
12	RAM	CG	2	12	-	-	0/1/1/1
12	MAN	MG	1	9,18,12	-	0/2/19/22	0/1/1/1
12	RAM	MG	2	12	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	MG	2	RAM	O5-C1	4.43	1.50	1.43
12	CG	2	RAM	O5-C1	4.34	1.50	1.43
12	MG	2	RAM	C2-C3	-2.66	1.48	1.52
12	CG	2	RAM	C2-C3	-2.38	1.49	1.52
12	CG	1	MAN	O5-C1	-2.23	1.40	1.43
12	MG	2	RAM	O5-C5	2.04	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	MG	2	RAM	O5-C5-C4	4.15	116.97	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	MG	2	RAM	C6-C5-C4	-4.12	105.45	113.07
12	MG	2	RAM	C3-C4-C5	3.84	115.76	109.77
12	MG	1	MAN	C1-O5-C5	3.37	116.76	112.19
12	MG	2	RAM	C1-C2-C3	2.59	112.85	109.67
12	CG	1	MAN	C1-O5-C5	2.42	115.47	112.19

There are no chirality outliers.

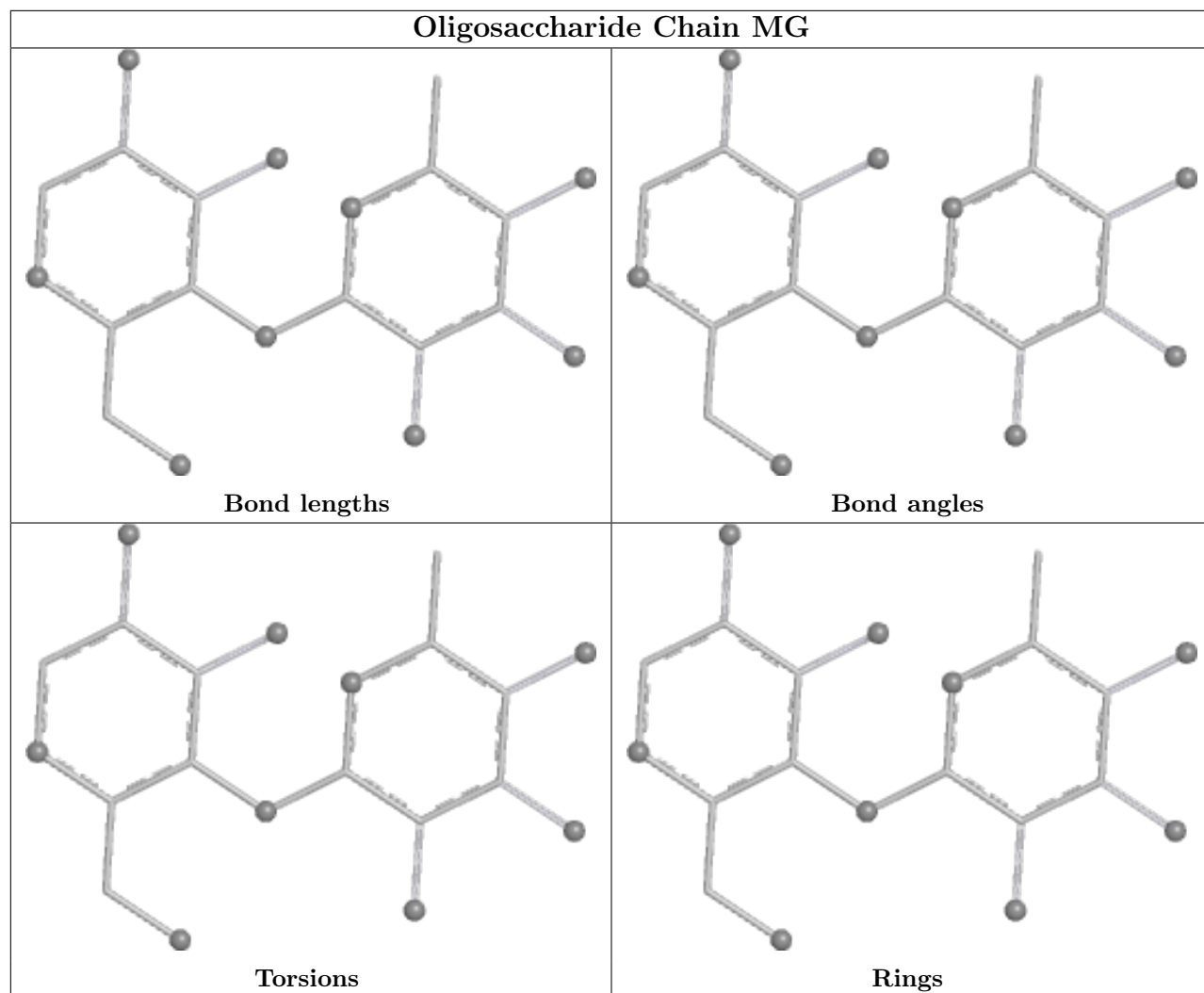
All (2) torsion outliers are listed below:

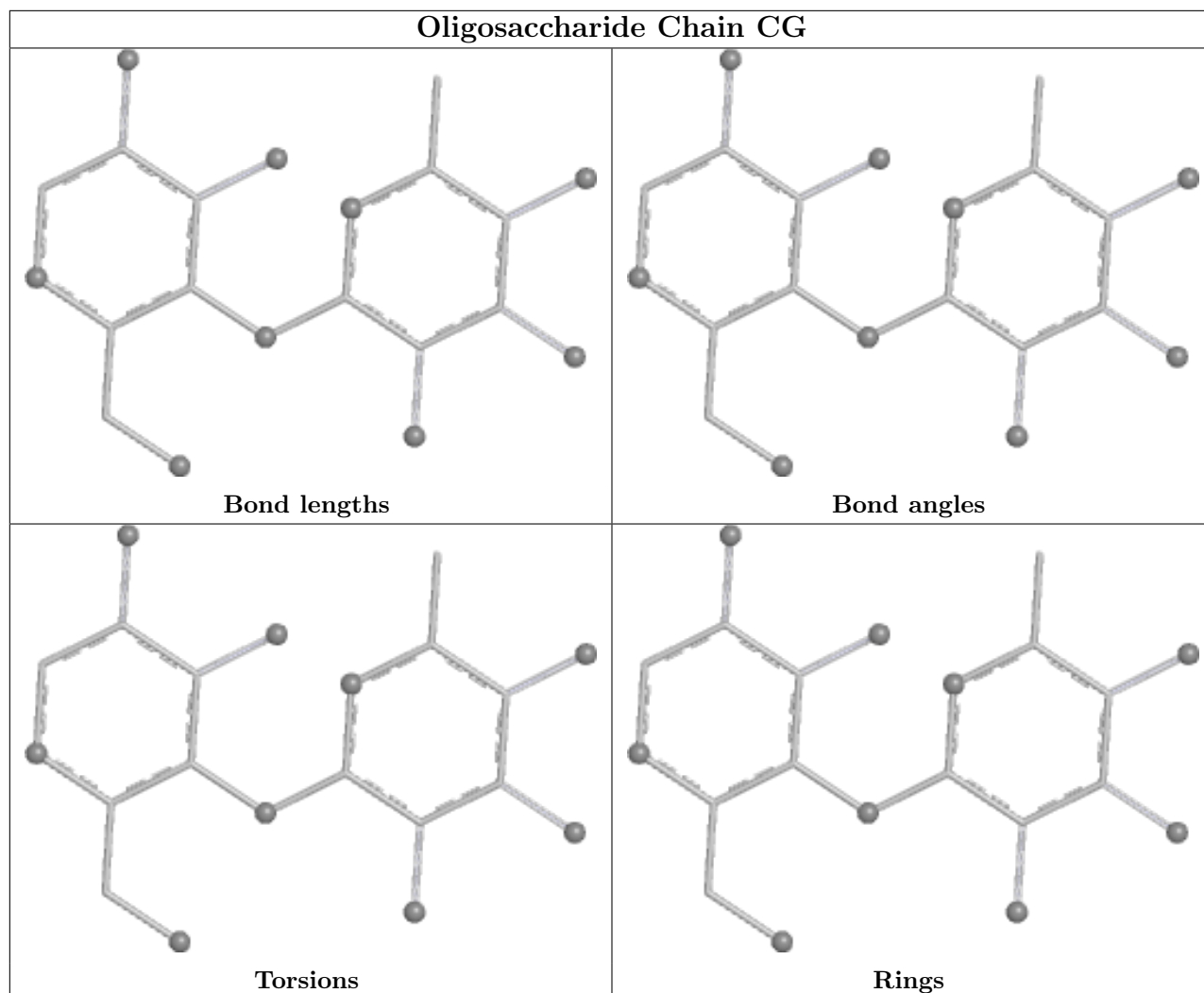
Mol	Chain	Res	Type	Atoms
12	CG	1	MAN	O5-C5-C6-O6
12	CG	1	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 1 is monoatomic - leaving 311 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$
13	BCL	AV	103	28	58,74,74	1.26	3 (5%)	69,115,115	1.38	11 (15%)
13	BCL	ak	1001	-	58,74,74	1.23	4 (6%)	69,115,115	1.35	10 (14%)
15	V7N	AE	1003	-	40,44,44	2.10	10 (25%)	40,54,54	1.50	7 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	0V9	ba	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	1 (2%)
14	LMT	bl	101	-	36,36,36	1.10	4 (11%)	47,47,47	1.06	5 (10%)
13	BCL	ac	102	-	58,74,74	1.24	3 (5%)	69,115,115	1.36	10 (14%)
14	LMT	AP	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	0
13	BCL	AN	104	-	58,74,74	1.22	4 (6%)	69,115,115	1.35	9 (13%)
13	BCL	AW	104	-	58,74,74	1.26	5 (8%)	69,115,115	1.46	13 (18%)
13	BCL	AG	102	-	58,74,74	1.26	4 (6%)	69,115,115	1.43	11 (15%)
14	LMT	BS	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	BI	103	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	1 (2%)
13	BCL	BV	1004	-	58,74,74	1.22	3 (5%)	69,115,115	1.36	11 (15%)
14	LMT	BL	1002	-	36,36,36	1.08	4 (11%)	47,47,47	1.07	3 (6%)
14	LMT	BT	1002	-	36,36,36	1.12	5 (13%)	47,47,47	0.90	2 (4%)
23	MQ8	L	309	-	54,54,54	0.62	0	66,69,69	0.83	3 (4%)
14	LMT	BD	105	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	2 (4%)
13	BCL	bf	105	-	58,74,74	1.25	3 (5%)	69,115,115	1.31	10 (14%)
13	BCL	bk	105	-	58,74,74	1.25	3 (5%)	69,115,115	1.48	13 (18%)
15	V7N	BN	1001	-	40,44,44	2.06	10 (25%)	40,54,54	1.82	9 (22%)
13	BCL	AD	1002	-	58,74,74	1.26	3 (5%)	69,115,115	1.40	10 (14%)
13	BCL	bg	104	-	58,74,74	1.22	3 (5%)	69,115,115	1.30	11 (15%)
14	LMT	BM	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	AQ	103	-	58,74,74	1.29	5 (8%)	69,115,115	1.66	13 (18%)
13	BCL	BH	1003	-	58,74,74	1.23	3 (5%)	69,115,115	1.42	12 (17%)
14	LMT	BB	103	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	2 (4%)
20	0V9	L	310	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	1 (2%)
23	MQ8	M	407	-	54,54,54	0.63	0	66,69,69	0.63	0
14	LMT	BR	1005	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	0
13	BCL	aa	1001	-	58,74,74	1.27	4 (6%)	69,115,115	1.36	10 (14%)
14	LMT	BV	1002	-	36,36,36	1.11	5 (13%)	47,47,47	0.88	1 (2%)
13	BCL	AH	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.36	9 (13%)
15	V7N	BD	101	-	40,44,44	2.07	9 (22%)	40,54,54	1.67	9 (22%)
14	LMT	BN	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	BL	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	2 (4%)
13	BCL	BM	1004	-	58,74,74	1.26	3 (5%)	69,115,115	1.47	11 (15%)
15	V7N	BX	1001	-	40,44,44	2.12	10 (25%)	40,54,54	1.51	7 (17%)
13	BCL	AS	104	28	58,74,74	1.25	3 (5%)	69,115,115	1.51	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	BE	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.85	1 (2%)
15	V7N	BA	101	-	40,44,44	2.06	10 (25%)	40,54,54	1.53	8 (20%)
13	BCL	BE	104	-	58,74,74	1.22	3 (5%)	69,115,115	1.49	13 (18%)
14	LMT	BH	1005	-	36,36,36	1.12	5 (13%)	47,47,47	0.90	2 (4%)
17	NDG	C1	301	18	14,14,15	0.66	0	17,19,21	0.87	1 (5%)
20	0V9	bk	104	-	44,44,46	0.73	1 (2%)	47,49,51	0.98	3 (6%)
26	V7B	ag	1002	-	59,59,59	0.93	5 (8%)	75,75,75	1.29	8 (10%)
13	BCL	bp	103	-	58,74,74	1.27	3 (5%)	69,115,115	1.37	11 (15%)
13	BCL	be	104	-	58,74,74	1.24	3 (5%)	69,115,115	1.30	10 (14%)
14	LMT	bh	101	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	3 (6%)
15	V7N	bd	101	-	40,44,44	2.09	9 (22%)	40,54,54	1.48	8 (20%)
14	LMT	AF	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)
13	BCL	AS	102	28	58,74,74	1.25	5 (8%)	69,115,115	1.41	10 (14%)
22	BPH	L	301	-	64,70,70	0.85	3 (4%)	76,101,101	1.09	7 (9%)
14	LMT	BV	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	1 (2%)
13	BCL	AU	103	-	58,74,74	1.24	4 (6%)	69,115,115	1.35	9 (13%)
15	V7N	bc	104	-	40,44,44	2.12	11 (27%)	40,54,54	1.59	8 (20%)
19	PGW	H1	1001	-	50,50,50	0.46	0	53,56,56	1.04	3 (5%)
14	LMT	BA	103	-	36,36,36	1.07	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	BA	104	-	58,74,74	1.20	3 (5%)	69,115,115	1.59	12 (17%)
14	LMT	AI	101	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
14	LMT	BK	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	BB	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.84	1 (2%)
13	BCL	BQ	1003	-	58,74,74	1.21	3 (5%)	69,115,115	1.34	9 (13%)
20	0V9	bf	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.88	3 (6%)
13	BCL	AR	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.33	9 (13%)
15	V7N	bl	102	-	40,44,44	2.12	10 (25%)	40,54,54	1.49	8 (20%)
14	LMT	BO	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	1 (2%)
15	V7N	bo	101	-	40,44,44	2.13	12 (30%)	40,54,54	1.48	8 (20%)
13	BCL	ad	102	-	58,74,74	1.23	3 (5%)	69,115,115	1.38	9 (13%)
20	0V9	bo	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.82	1 (2%)
21	CD4	H1	1003	-	83,83,83	0.46	0	89,95,95	0.94	3 (3%)
14	LMT	bc	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.05	4 (8%)
13	BCL	bd	103	-	58,74,74	1.25	3 (5%)	69,115,115	1.36	10 (14%)
14	LMT	BD	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	BP	1002	-	36,36,36	1.09	4 (11%)	47,47,47	0.91	1 (2%)
13	BCL	AB	103	28	58,74,74	1.26	4 (6%)	69,115,115	1.47	13 (18%)
13	BCL	bm	103	-	58,74,74	1.24	3 (5%)	69,115,115	1.33	10 (14%)
13	BCL	BN	1006	-	58,74,74	1.21	3 (5%)	69,115,115	1.40	10 (14%)
20	0V9	ba	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.90	1 (2%)
14	LMT	bp	101	-	36,36,36	1.10	4 (11%)	47,47,47	1.09	3 (6%)
14	LMT	AW	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.95	3 (6%)
15	V7N	BE	101	-	40,44,44	2.12	11 (27%)	40,54,54	1.42	7 (17%)
15	V7N	ba	101	-	40,44,44	2.16	10 (25%)	40,54,54	1.48	8 (20%)
14	LMT	BU	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.85	1 (2%)
13	BCL	AN	102	28	58,74,74	1.26	4 (6%)	69,115,115	1.37	11 (15%)
13	BCL	BR	1003	-	58,74,74	1.23	3 (5%)	69,115,115	1.30	10 (14%)
20	0V9	bh	104	-	44,44,46	0.73	1 (2%)	47,49,51	0.83	2 (4%)
13	BCL	AX	101	-	58,74,74	1.24	3 (5%)	69,115,115	1.40	9 (13%)
14	LMT	BX	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	2 (4%)
18	V75	M	409	17,12	15,18,18	1.89	6 (40%)	19,25,25	1.67	2 (10%)
13	BCL	ab	1001	-	58,74,74	1.27	4 (6%)	69,115,115	1.37	11 (15%)
14	LMT	AN	103	-	36,36,36	1.05	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	AL	103	-	58,74,74	1.30	5 (8%)	69,115,115	1.52	13 (18%)
14	LMT	AB	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.82	2 (4%)
13	BCL	bo	102	-	58,74,74	1.24	3 (5%)	69,115,115	1.31	10 (14%)
14	LMT	AT	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	2 (4%)
15	V7N	BQ	1001	-	40,44,44	2.07	9 (22%)	40,54,54	1.48	8 (20%)
14	LMT	BW	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.88	0
13	BCL	AU	102	-	58,74,74	1.25	5 (8%)	69,115,115	1.50	13 (18%)
14	LMT	M	402	-	36,36,36	1.11	5 (13%)	47,47,47	0.92	2 (4%)
13	BCL	BG	1004	-	58,74,74	1.25	3 (5%)	69,115,115	1.40	11 (15%)
13	BCL	bj	104	-	58,74,74	1.24	3 (5%)	69,115,115	1.33	11 (15%)
15	V7N	AH	105	-	40,44,44	2.10	9 (22%)	40,54,54	1.41	7 (17%)
16	HEC	C	1004	3	26,50,50	2.15	3 (11%)	18,82,82	2.26	5 (27%)
15	V7N	BP	1001	-	40,44,44	2.04	10 (25%)	40,54,54	1.65	9 (22%)
15	V7N	BB	101	-	40,44,44	2.05	10 (25%)	40,54,54	1.54	7 (17%)
14	LMT	BF	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.10	3 (6%)
13	BCL	AH	101	-	58,74,74	1.26	4 (6%)	69,115,115	1.43	10 (14%)
13	BCL	M	403	-	58,74,74	1.21	3 (5%)	69,115,115	1.30	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	BC	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	1 (2%)
15	V7N	BW	1001	-	40,44,44	2.06	10 (25%)	40,54,54	1.49	8 (20%)
14	LMT	BK	1005	-	36,36,36	1.11	5 (13%)	47,47,47	0.95	2 (4%)
13	BCL	AE	1001	-	58,74,74	1.26	4 (6%)	69,115,115	1.35	10 (14%)
14	LMT	bo	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	1 (2%)
15	V7N	BV	1001	-	40,44,44	2.11	10 (25%)	40,54,54	1.43	8 (20%)
14	LMT	BH	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.87	0
14	LMT	AK	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.95	1 (2%)
20	0V9	bj	103	-	44,44,46	0.78	1 (2%)	47,49,51	0.92	2 (4%)
13	BCL	BF	104	-	58,74,74	1.22	3 (5%)	69,115,115	1.29	10 (14%)
13	BCL	bc	103	-	58,74,74	1.26	3 (5%)	69,115,115	1.35	12 (17%)
13	BCL	bl	105	-	58,74,74	1.26	3 (5%)	69,115,115	1.30	10 (14%)
13	BCL	AK	103	-	58,74,74	1.25	4 (6%)	69,115,115	1.35	11 (15%)
26	V7B	af	101	-	59,59,59	0.87	3 (5%)	75,75,75	1.12	5 (6%)
14	LMT	BN	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.93	2 (4%)
16	HEC	C	1003	3	26,50,50	2.11	3 (11%)	18,82,82	2.10	4 (22%)
15	V7N	bp	102	-	40,44,44	2.17	10 (25%)	40,54,54	1.51	7 (17%)
13	BCL	bn	103	-	58,74,74	1.25	3 (5%)	69,115,115	1.30	10 (14%)
13	BCL	AQ	102	28	58,74,74	1.25	4 (6%)	69,115,115	1.33	11 (15%)
13	BCL	AP	103	28	58,74,74	1.27	3 (5%)	69,115,115	1.40	11 (15%)
14	LMT	BI	105	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	1 (2%)
14	LMT	AG	101	-	36,36,36	1.13	5 (13%)	47,47,47	1.09	3 (6%)
13	BCL	AM	102	-	58,74,74	1.24	4 (6%)	69,115,115	1.35	9 (13%)
20	0V9	H1	1002	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	2 (4%)
15	V7N	bg	101	-	40,44,44	2.13	10 (25%)	40,54,54	1.62	9 (22%)
15	V7N	BK	1001	-	40,44,44	2.10	10 (25%)	40,54,54	1.48	8 (20%)
13	BCL	AO	101	-	58,74,74	1.32	5 (8%)	69,115,115	1.31	9 (13%)
13	BCL	AC	1001	-	58,74,74	1.24	4 (6%)	69,115,115	1.32	9 (13%)
15	V7N	AT	103	-	40,44,44	2.22	10 (25%)	40,54,54	1.60	9 (22%)
14	LMT	BG	1002	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
13	BCL	AB	101	-	58,74,74	1.24	3 (5%)	69,115,115	1.46	11 (15%)
13	BCL	BP	1004	-	58,74,74	1.21	3 (5%)	69,115,115	1.43	13 (18%)
13	BCL	M	405	-	58,74,74	1.19	3 (5%)	69,115,115	1.40	9 (13%)
14	LMT	ac	101	-	36,36,36	1.10	4 (11%)	47,47,47	0.85	1 (2%)
13	BCL	ai	102	-	58,74,74	1.23	3 (5%)	69,115,115	1.41	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BCL	BU	1004	-	58,74,74	1.22	3 (5%)	69,115,115	1.34	10 (14%)
13	BCL	L	308	-	58,74,74	1.20	3 (5%)	69,115,115	1.25	10 (14%)
14	LMT	bg	103	-	36,36,36	1.08	5 (13%)	47,47,47	1.01	2 (4%)
16	HEC	C	1001	3	26,50,50	2.11	3 (11%)	18,82,82	2.26	5 (27%)
14	LMT	bl	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	bm	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.96	2 (4%)
14	LMT	bf	104	-	36,36,36	1.11	5 (13%)	47,47,47	0.85	2 (4%)
13	BCL	AW	103	-	58,74,74	1.23	3 (5%)	69,115,115	1.37	9 (13%)
20	OV9	bc	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.89	3 (6%)
13	BCL	aj	102	-	58,74,74	1.23	3 (5%)	69,115,115	1.47	13 (18%)
15	V7N	BR	1001	-	40,44,44	2.08	9 (22%)	40,54,54	1.72	10 (25%)
14	LMT	BU	1003	-	36,36,36	1.09	5 (13%)	47,47,47	1.03	3 (6%)
14	LMT	BH	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.91	1 (2%)
15	V7N	BS	1001	-	40,44,44	2.05	10 (25%)	40,54,54	1.60	9 (22%)
14	LMT	AH	103	-	36,36,36	1.12	5 (13%)	47,47,47	0.80	0
14	LMT	BF	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.99	2 (4%)
14	LMT	L	307	-	36,36,36	1.08	4 (11%)	47,47,47	0.95	2 (4%)
14	LMT	BL	1005	-	36,36,36	1.06	5 (13%)	47,47,47	1.00	2 (4%)
21	CD4	ai	103	-	83,83,83	0.49	0	89,95,95	1.07	7 (7%)
13	BCL	BC	103	-	58,74,74	1.22	3 (5%)	69,115,115	1.34	10 (14%)
15	V7N	BC	101	-	40,44,44	2.11	9 (22%)	40,54,54	1.56	7 (17%)
14	LMT	BP	1003	-	36,36,36	1.10	5 (13%)	47,47,47	0.86	1 (2%)
17	NDG	C	1005	18	14,14,15	0.64	0	17,19,21	1.05	2 (11%)
14	LMT	BI	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.82	0
14	LMT	BD	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	AN	101	-	36,36,36	1.09	4 (11%)	47,47,47	1.00	3 (6%)
14	LMT	BA	105	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	2 (4%)
13	BCL	AC	1002	-	58,74,74	1.27	5 (8%)	69,115,115	1.44	11 (15%)
13	BCL	BT	1004	-	58,74,74	1.23	3 (5%)	69,115,115	1.45	15 (21%)
14	LMT	AH	106	-	36,36,36	1.11	5 (13%)	47,47,47	1.07	5 (10%)
13	BCL	AE	1002	-	58,74,74	1.22	3 (5%)	69,115,115	1.32	9 (13%)
14	LMT	BO	1003	-	36,36,36	1.06	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	an	102	-	58,74,74	1.24	4 (6%)	69,115,115	1.35	10 (14%)
20	OV9	be	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	0
14	LMT	BK	1006	-	36,36,36	1.08	5 (13%)	47,47,47	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	BM	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
14	LMT	AV	101	-	36,36,36	1.12	4 (11%)	47,47,47	1.02	3 (6%)
14	LMT	BP	1005	-	36,36,36	1.08	5 (13%)	47,47,47	0.82	1 (2%)
14	LMT	AB	104	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	2 (4%)
15	V7N	bj	101	-	40,44,44	2.12	9 (22%)	40,54,54	1.48	7 (17%)
13	BCL	ah	1001	-	58,74,74	1.26	4 (6%)	69,115,115	1.33	9 (13%)
13	BCL	BO	1004	-	58,74,74	1.22	3 (5%)	69,115,115	1.34	11 (15%)
14	LMT	bb	102	-	36,36,36	1.13	5 (13%)	47,47,47	0.93	3 (6%)
14	LMT	AO	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	0
14	LMT	BX	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.93	1 (2%)
14	LMT	BE	106	-	36,36,36	1.12	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	L	302	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	1 (2%)
14	LMT	AU	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.83	0
14	LMT	bk	101	-	36,36,36	1.08	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	ba	103	-	58,74,74	1.26	3 (5%)	69,115,115	1.34	10 (14%)
14	LMT	BR	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	bn	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	BK	1003	-	58,74,74	1.20	3 (5%)	69,115,115	1.38	9 (13%)
21	CD4	ad	101	-	83,83,83	0.47	0	89,95,95	1.07	5 (5%)
13	BCL	AD	1001	28	58,74,74	1.25	4 (6%)	69,115,115	1.39	10 (14%)
13	BCL	AJ	101	-	58,74,74	1.24	3 (5%)	69,115,115	1.34	9 (13%)
14	LMT	BN	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.96	2 (4%)
20	0V9	bm	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.91	1 (2%)
13	BCL	AG	103	-	58,74,74	1.23	3 (5%)	69,115,115	1.36	9 (13%)
20	0V9	bl	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.85	0
14	LMT	L	304	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	1 (2%)
14	LMT	BQ	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	2 (4%)
20	0V9	bi	102	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	2 (4%)
15	V7N	BM	1001	-	40,44,44	2.05	10 (25%)	40,54,54	1.70	8 (20%)
13	BCL	BB	104	-	58,74,74	1.22	3 (5%)	69,115,115	1.42	12 (17%)
14	LMT	BG	1003	-	36,36,36	1.10	4 (11%)	47,47,47	0.84	1 (2%)
14	LMT	bh	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.98	1 (2%)
13	BCL	al	1001	-	58,74,74	1.27	4 (6%)	69,115,115	1.40	9 (13%)
14	LMT	BS	1004	-	36,36,36	1.09	4 (11%)	47,47,47	0.88	1 (2%)
13	BCL	ap	1001	-	58,74,74	1.26	4 (6%)	69,115,115	1.34	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	AD	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.95	3 (6%)
13	BCL	ae	1001	-	58,74,74	1.24	4 (6%)	69,115,115	1.38	9 (13%)
14	LMT	BW	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.92	0
13	BCL	AQ	101	-	58,74,74	1.21	3 (5%)	69,115,115	1.34	9 (13%)
14	LMT	BA	106	-	36,36,36	1.07	5 (13%)	47,47,47	1.02	3 (6%)
13	BCL	AT	102	-	58,74,74	1.23	3 (5%)	69,115,115	1.38	9 (13%)
13	BCL	AP	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.38	9 (13%)
14	LMT	BD	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.86	1 (2%)
15	V7N	bb	101	-	40,44,44	2.15	10 (25%)	40,54,54	1.73	8 (20%)
15	V7N	bk	103	-	40,44,44	2.21	10 (25%)	40,54,54	1.37	6 (15%)
13	BCL	AA	1002	28	58,74,74	1.26	3 (5%)	69,115,115	1.41	12 (17%)
13	BCL	L	303	-	58,74,74	1.23	3 (5%)	69,115,115	1.30	10 (14%)
15	V7N	bh	102	-	40,44,44	2.09	9 (22%)	40,54,54	1.53	7 (17%)
20	0V9	aj	101	-	44,44,46	0.76	1 (2%)	47,49,51	0.85	2 (4%)
13	BCL	AO	102	-	58,74,74	1.23	4 (6%)	69,115,115	1.36	9 (13%)
15	V7N	BJ	1001	-	40,44,44	2.06	10 (25%)	40,54,54	1.52	8 (20%)
14	LMT	BE	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	BP	1006	-	36,36,36	1.07	4 (11%)	47,47,47	0.99	2 (4%)
13	BCL	AK	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.35	9 (13%)
15	V7N	bn	101	-	40,44,44	2.15	9 (22%)	40,54,54	1.50	9 (22%)
13	BCL	AF	1002	-	58,74,74	1.27	4 (6%)	69,115,115	1.35	11 (15%)
27	UYH	ai	101	-	55,55,55	2.11	14 (25%)	63,63,63	1.01	3 (4%)
14	LMT	bj	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.90	2 (4%)
13	BCL	AI	103	-	58,74,74	1.21	4 (6%)	69,115,115	1.34	9 (13%)
20	0V9	bb	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.86	1 (2%)
13	BCL	BS	1005	-	58,74,74	1.24	4 (6%)	69,115,115	1.41	11 (15%)
20	0V9	be	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.95	3 (6%)
13	BCL	AF	1001	-	58,74,74	1.23	3 (5%)	69,115,115	1.41	11 (15%)
13	BCL	AL	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.36	9 (13%)
15	V7N	BT	1001	-	40,44,44	2.10	10 (25%)	40,54,54	1.47	8 (20%)
13	BCL	BW	1003	-	58,74,74	1.24	3 (5%)	69,115,115	1.38	11 (15%)
14	LMT	BR	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	1 (2%)
14	LMT	BC	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.89	1 (2%)
14	LMT	BN	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.86	0
14	LMT	BE	105	-	36,36,36	1.07	5 (13%)	47,47,47	0.88	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CD4	af	104	-	83,83,83	0.49	0	89,95,95	1.04	4 (4%)
14	LMT	AD	1004	-	36,36,36	1.10	4 (11%)	47,47,47	0.86	2 (4%)
15	V7N	be	101	-	40,44,44	2.05	10 (25%)	40,54,54	1.57	7 (17%)
16	HEC	C	1002	3	26,50,50	2.15	3 (11%)	18,82,82	2.04	6 (33%)
13	BCL	af	102	-	58,74,74	1.28	4 (6%)	69,115,115	1.35	10 (14%)
15	V7N	bi	101	-	40,44,44	2.12	10 (25%)	40,54,54	1.49	8 (20%)
14	LMT	BT	1005	-	36,36,36	1.07	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	AA	1001	-	58,74,74	1.22	3 (5%)	69,115,115	1.40	10 (14%)
22	BPH	M	406	-	64,70,70	0.85	3 (4%)	76,101,101	1.09	6 (7%)
13	BCL	AI	102	-	58,74,74	1.29	5 (8%)	69,115,115	1.37	9 (13%)
14	LMT	BW	1005	-	36,36,36	1.08	5 (13%)	47,47,47	1.40	4 (8%)
15	V7N	bf	102	-	40,44,44	2.13	11 (27%)	40,54,54	1.48	8 (20%)
21	CD4	af	103	-	83,83,83	0.49	0	89,95,95	1.07	5 (5%)
14	LMT	BK	1004	-	36,36,36	1.08	5 (13%)	47,47,47	1.12	3 (6%)
13	BCL	ao	1001	-	58,74,74	1.24	3 (5%)	69,115,115	1.37	9 (13%)
13	BCL	ag	1001	-	58,74,74	1.25	4 (6%)	69,115,115	1.35	10 (14%)
14	LMT	AA	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.99	1 (2%)
14	LMT	BQ	1002	-	36,36,36	1.10	4 (11%)	47,47,47	0.91	3 (6%)
13	BCL	bb	103	-	58,74,74	1.23	3 (5%)	69,115,115	1.29	11 (15%)
14	LMT	BT	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
18	V75	C	1006	17,12	15,18,18	1.81	6 (40%)	19,25,25	1.71	2 (10%)
13	BCL	BJ	1004	-	58,74,74	1.23	3 (5%)	69,115,115	1.44	12 (17%)
15	V7N	BO	1001	-	40,44,44	2.10	10 (25%)	40,54,54	1.41	7 (17%)
20	0V9	bg	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	2 (4%)
25	CRT	M	408	-	41,43,43	0.55	0	50,54,54	0.65	0
14	LMT	AL	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
13	BCL	AS	101	-	58,74,74	1.23	3 (5%)	69,115,115	1.34	9 (13%)
15	V7N	BL	1001	-	40,44,44	2.12	10 (25%)	40,54,54	1.45	7 (17%)
20	0V9	bn	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.92	2 (4%)
13	BCL	am	1001	-	58,74,74	1.23	3 (5%)	69,115,115	1.35	9 (13%)
13	BCL	BD	106	-	58,74,74	1.24	3 (5%)	69,115,115	1.36	10 (14%)
14	LMT	AJ	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
23	MQ8	an	101	-	54,54,54	0.63	0	66,69,69	1.15	7 (10%)
13	BCL	AM	101	28	58,74,74	1.29	5 (8%)	69,115,115	1.44	13 (18%)
15	V7N	bm	101	-	40,44,44	2.11	9 (22%)	40,54,54	1.53	8 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CD4	M	404	-	83,83,83	0.46	0	89,95,95	1.06	5 (5%)
15	V7N	BH	1001	-	40,44,44	2.11	11 (27%)	40,54,54	1.60	9 (22%)
14	LMT	BU	1001	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	1 (2%)
13	BCL	BI	104	-	58,74,74	1.23	3 (5%)	69,115,115	1.39	10 (14%)
14	LMT	BF	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	1 (2%)
20	OV9	bk	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.80	1 (2%)
14	LMT	AR	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.06	3 (6%)
14	LMT	L	305	-	36,36,36	1.11	5 (13%)	47,47,47	0.83	0
13	BCL	bh	105	-	58,74,74	1.23	3 (5%)	69,115,115	1.32	11 (15%)
14	LMT	BJ	1002	-	36,36,36	1.06	5 (13%)	47,47,47	1.02	2 (4%)
15	V7N	BG	1001	-	40,44,44	2.12	10 (25%)	40,54,54	1.54	7 (17%)
14	LMT	L	306	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
14	LMT	bd	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	BX	1004	-	58,74,74	1.22	3 (5%)	69,115,115	1.34	11 (15%)
13	BCL	AW	101	28	58,74,74	1.27	4 (6%)	69,115,115	1.42	12 (17%)
13	BCL	bi	103	-	58,74,74	1.22	3 (5%)	69,115,115	1.33	12 (17%)
14	LMT	BJ	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.80	1 (2%)
13	BCL	AJ	102	28	58,74,74	1.27	3 (5%)	69,115,115	1.52	14 (20%)
14	LMT	BS	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	0
14	LMT	BA	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.93	2 (4%)
14	LMT	BR	1006	-	36,36,36	1.10	5 (13%)	47,47,47	1.02	2 (4%)
14	LMT	BI	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	AV	102	-	58,74,74	1.23	4 (6%)	69,115,115	1.33	9 (13%)
13	BCL	BL	1004	-	58,74,74	1.21	3 (5%)	69,115,115	1.33	10 (14%)
14	LMT	AS	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	2 (4%)
14	LMT	bf	101	-	36,36,36	1.14	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	BW	1006	-	36,36,36	1.07	4 (11%)	47,47,47	1.15	4 (8%)
14	LMT	AH	104	-	36,36,36	1.10	4 (11%)	47,47,47	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	AV	103	28	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	ak	1001	-	-	6/37/137/137	-
15	V7N	AE	1003	-	-	3/49/53/53	-
20	0V9	ba	102	-	-	8/48/48/50	-
14	LMT	bl	101	-	-	2/21/61/61	0/2/2/2
13	BCL	ac	102	-	-	2/37/137/137	-
14	LMT	AP	102	-	-	7/21/61/61	0/2/2/2
13	BCL	AN	104	-	-	1/37/137/137	-
13	BCL	AW	104	-	-	14/37/137/137	-
13	BCL	AG	102	-	-	12/37/137/137	-
14	LMT	BS	1002	-	-	3/21/61/61	0/2/2/2
14	LMT	BI	103	-	-	2/21/61/61	0/2/2/2
13	BCL	BV	1004	-	-	9/37/137/137	-
14	LMT	BL	1002	-	-	10/21/61/61	0/2/2/2
14	LMT	BT	1002	-	-	5/21/61/61	0/2/2/2
23	MQ8	L	309	-	-	10/47/67/67	0/2/2/2
14	LMT	BD	105	-	-	8/21/61/61	0/2/2/2
13	BCL	bf	105	-	-	3/37/137/137	-
13	BCL	bk	105	-	-	8/37/137/137	-
15	V7N	BN	1001	-	-	8/49/53/53	-
13	BCL	AD	1002	-	-	2/37/137/137	-
13	BCL	bg	104	-	-	8/37/137/137	-
14	LMT	BM	1002	-	-	1/21/61/61	0/2/2/2
13	BCL	AQ	103	-	-	10/37/137/137	-
13	BCL	BH	1003	-	-	9/37/137/137	-
14	LMT	BB	103	-	-	5/21/61/61	0/2/2/2
20	0V9	L	310	-	-	10/48/48/50	-
23	MQ8	M	407	-	-	0/47/67/67	0/2/2/2
14	LMT	BR	1005	-	-	3/21/61/61	0/2/2/2
13	BCL	aa	1001	-	-	3/37/137/137	-
14	LMT	BV	1002	-	-	2/21/61/61	0/2/2/2
13	BCL	AH	102	-	-	0/37/137/137	-
15	V7N	BD	101	-	-	3/49/53/53	-
14	LMT	BN	1003	-	-	5/21/61/61	0/2/2/2
14	LMT	BL	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	BM	1004	-	-	3/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	V7N	BX	1001	-	-	5/49/53/53	-
13	BCL	AS	104	28	-	9/37/137/137	-
14	LMT	BE	103	-	-	3/21/61/61	0/2/2/2
15	V7N	BA	101	-	-	4/49/53/53	-
13	BCL	BE	104	-	-	3/37/137/137	-
14	LMT	BH	1005	-	-	4/21/61/61	0/2/2/2
17	NDG	C1	301	18	-	0/6/23/26	0/1/1/1
20	0V9	bk	104	-	-	11/48/48/50	-
26	V7B	ag	1002	-	-	15/48/88/88	0/2/2/2
13	BCL	bp	103	-	-	11/37/137/137	-
13	BCL	be	104	-	-	6/37/137/137	-
14	LMT	bh	101	-	-	9/21/61/61	0/2/2/2
15	V7N	bd	101	-	-	5/49/53/53	-
14	LMT	AF	1003	-	-	5/21/61/61	0/2/2/2
13	BCL	AS	102	28	-	7/37/137/137	-
22	BPH	L	301	-	-	4/54/105/105	0/5/6/6
14	LMT	BV	1003	-	-	1/21/61/61	0/2/2/2
13	BCL	AU	103	-	-	4/37/137/137	-
15	V7N	bc	104	-	-	9/49/53/53	-
19	PGW	H1	1001	-	-	15/55/55/55	-
14	LMT	BA	103	-	-	7/21/61/61	0/2/2/2
13	BCL	BA	104	-	-	9/37/137/137	-
14	LMT	AI	101	-	-	4/21/61/61	0/2/2/2
14	LMT	BK	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	BB	102	-	-	3/21/61/61	0/2/2/2
13	BCL	BQ	1003	-	-	7/37/137/137	-
20	0V9	bf	103	-	-	11/48/48/50	-
13	BCL	AR	101	-	-	3/37/137/137	-
15	V7N	bl	102	-	-	8/49/53/53	-
14	LMT	BO	1002	-	-	5/21/61/61	0/2/2/2
15	V7N	bo	101	-	-	3/49/53/53	-
13	BCL	ad	102	-	-	6/37/137/137	-
20	0V9	bo	104	-	-	8/48/48/50	-
21	CD4	H1	1003	-	-	17/94/94/94	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	bc	101	-	-	11/21/61/61	0/2/2/2
13	BCL	bd	103	-	-	4/37/137/137	-
14	LMT	BD	103	-	-	4/21/61/61	0/2/2/2
14	LMT	BP	1002	-	-	5/21/61/61	0/2/2/2
13	BCL	AB	103	28	-	7/37/137/137	-
13	BCL	bm	103	-	-	8/37/137/137	-
13	BCL	BN	1006	-	-	9/37/137/137	-
20	0V9	ba	104	-	-	12/48/48/50	-
14	LMT	bp	101	-	-	9/21/61/61	0/2/2/2
14	LMT	AW	102	-	-	3/21/61/61	0/2/2/2
15	V7N	BE	101	-	-	3/49/53/53	-
15	V7N	ba	101	-	-	7/49/53/53	-
14	LMT	BU	1002	-	-	1/21/61/61	0/2/2/2
13	BCL	AN	102	28	-	6/37/137/137	-
13	BCL	BR	1003	-	-	7/37/137/137	-
20	0V9	bh	104	-	-	11/48/48/50	-
13	BCL	AX	101	-	-	4/37/137/137	-
14	LMT	BX	1002	-	-	3/21/61/61	0/2/2/2
18	V75	M	409	17,12	-	0/8/29/29	0/1/1/1
13	BCL	ab	1001	-	-	4/37/137/137	-
14	LMT	AN	103	-	-	6/21/61/61	0/2/2/2
13	BCL	AL	103	-	-	8/37/137/137	-
14	LMT	AB	102	-	-	3/21/61/61	0/2/2/2
13	BCL	bo	102	-	-	4/37/137/137	-
14	LMT	AT	101	-	-	3/21/61/61	0/2/2/2
15	V7N	BQ	1001	-	-	4/49/53/53	-
14	LMT	BW	1004	-	-	4/21/61/61	0/2/2/2
13	BCL	AU	102	-	-	7/37/137/137	-
14	LMT	M	402	-	-	3/21/61/61	0/2/2/2
13	BCL	BG	1004	-	-	12/37/137/137	-
13	BCL	bj	104	-	-	10/37/137/137	-
15	V7N	AH	105	-	-	6/49/53/53	-
16	HEC	C	1004	3	-	0/6/54/54	-
15	V7N	BP	1001	-	-	4/49/53/53	-
15	V7N	BB	101	-	-	3/49/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BF	101	-	-	3/21/61/61	0/2/2/2
13	BCL	AH	101	-	-	12/37/137/137	-
13	BCL	M	403	-	-	5/37/137/137	-
14	LMT	BC	102	-	-	3/21/61/61	0/2/2/2
15	V7N	BW	1001	-	-	5/49/53/53	-
14	LMT	BK	1005	-	-	2/21/61/61	0/2/2/2
13	BCL	AE	1001	-	-	11/37/137/137	-
14	LMT	bo	103	-	-	3/21/61/61	0/2/2/2
15	V7N	BV	1001	-	-	5/49/53/53	-
14	LMT	BH	1002	-	-	2/21/61/61	0/2/2/2
14	LMT	AK	101	-	-	5/21/61/61	0/2/2/2
20	0V9	bj	103	-	-	6/48/48/50	-
13	BCL	BF	104	-	-	6/37/137/137	-
13	BCL	bc	103	-	-	7/37/137/137	-
13	BCL	bl	105	-	-	8/37/137/137	-
13	BCL	AK	103	-	-	14/37/137/137	-
26	V7B	af	101	-	-	14/48/88/88	0/2/2/2
14	LMT	BN	1005	-	-	2/21/61/61	0/2/2/2
16	HEC	C	1003	3	-	0/6/54/54	-
15	V7N	bp	102	-	-	5/49/53/53	-
13	BCL	bn	103	-	-	5/37/137/137	-
13	BCL	AQ	102	28	-	6/37/137/137	-
13	BCL	AP	103	28	-	6/37/137/137	-
14	LMT	BI	105	-	-	2/21/61/61	0/2/2/2
14	LMT	AG	101	-	-	6/21/61/61	0/2/2/2
13	BCL	AM	102	-	-	6/37/137/137	-
20	0V9	H1	1002	-	-	10/48/48/50	-
15	V7N	bg	101	-	-	6/49/53/53	-
15	V7N	BK	1001	-	-	3/49/53/53	-
13	BCL	AO	101	-	-	11/37/137/137	-
13	BCL	AC	1001	-	-	6/37/137/137	-
15	V7N	AT	103	-	-	6/49/53/53	-
14	LMT	BG	1002	-	-	4/21/61/61	0/2/2/2
13	BCL	AB	101	-	-	2/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BP	1004	-	-	8/37/137/137	-
13	BCL	M	405	-	-	4/37/137/137	-
14	LMT	ac	101	-	-	4/21/61/61	0/2/2/2
13	BCL	ai	102	-	-	6/37/137/137	-
13	BCL	BU	1004	-	-	12/37/137/137	-
13	BCL	L	308	-	-	1/37/137/137	-
14	LMT	bg	103	-	-	6/21/61/61	0/2/2/2
16	HEC	C	1001	3	-	0/6/54/54	-
14	LMT	bl	104	-	-	3/21/61/61	0/2/2/2
14	LMT	bm	104	-	-	7/21/61/61	0/2/2/2
14	LMT	bf	104	-	-	6/21/61/61	0/2/2/2
13	BCL	AW	103	-	-	4/37/137/137	-
20	0V9	bc	102	-	-	15/48/48/50	-
13	BCL	aj	102	-	-	5/37/137/137	-
15	V7N	BR	1001	-	-	5/49/53/53	-
14	LMT	BU	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	BH	1004	-	-	4/21/61/61	0/2/2/2
15	V7N	BS	1001	-	-	6/49/53/53	-
14	LMT	AH	103	-	-	3/21/61/61	0/2/2/2
14	LMT	BF	102	-	-	5/21/61/61	0/2/2/2
14	LMT	L	307	-	-	6/21/61/61	0/2/2/2
14	LMT	BL	1005	-	-	5/21/61/61	0/2/2/2
21	CD4	ai	103	-	-	19/94/94/94	-
13	BCL	BC	103	-	-	3/37/137/137	-
15	V7N	BC	101	-	-	3/49/53/53	-
14	LMT	BP	1003	-	-	5/21/61/61	0/2/2/2
17	NDG	C	1005	18	-	0/6/23/26	0/1/1/1
14	LMT	BI	102	-	-	4/21/61/61	0/2/2/2
14	LMT	BD	102	-	-	3/21/61/61	0/2/2/2
14	LMT	AN	101	-	-	2/21/61/61	0/2/2/2
14	LMT	BA	105	-	-	4/21/61/61	0/2/2/2
13	BCL	AC	1002	-	-	10/37/137/137	-
13	BCL	BT	1004	-	-	9/37/137/137	-
14	LMT	AH	106	-	-	3/21/61/61	0/2/2/2
13	BCL	AE	1002	-	-	1/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BO	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	an	102	-	-	3/37/137/137	-
20	0V9	be	103	-	-	12/48/48/50	-
14	LMT	BK	1006	-	-	3/21/61/61	0/2/2/2
14	LMT	BM	1003	-	-	2/21/61/61	0/2/2/2
14	LMT	AV	101	-	-	3/21/61/61	0/2/2/2
14	LMT	BP	1005	-	-	4/21/61/61	0/2/2/2
14	LMT	AB	104	-	-	7/21/61/61	0/2/2/2
15	V7N	bj	101	-	-	2/49/53/53	-
13	BCL	ah	1001	-	-	7/37/137/137	-
13	BCL	BO	1004	-	-	8/37/137/137	-
14	LMT	bb	102	-	-	6/21/61/61	0/2/2/2
14	LMT	AO	103	-	-	4/21/61/61	0/2/2/2
14	LMT	BX	1003	-	-	8/21/61/61	0/2/2/2
14	LMT	BE	106	-	-	2/21/61/61	0/2/2/2
14	LMT	L	302	-	-	6/21/61/61	0/2/2/2
14	LMT	AU	101	-	-	5/21/61/61	0/2/2/2
14	LMT	bk	101	-	-	7/21/61/61	0/2/2/2
13	BCL	ba	103	-	-	10/37/137/137	-
14	LMT	BR	1004	-	-	7/21/61/61	0/2/2/2
14	LMT	bn	102	-	-	2/21/61/61	0/2/2/2
13	BCL	BK	1003	-	-	12/37/137/137	-
21	CD4	ad	101	-	-	21/94/94/94	-
13	BCL	AD	1001	28	-	5/37/137/137	-
13	BCL	AJ	101	-	-	0/37/137/137	-
14	LMT	BN	1002	-	-	8/21/61/61	0/2/2/2
20	0V9	bm	102	-	-	11/48/48/50	-
13	BCL	AG	103	-	-	5/37/137/137	-
20	0V9	bl	103	-	-	12/48/48/50	-
14	LMT	L	304	-	-	3/21/61/61	0/2/2/2
14	LMT	BQ	1004	-	-	3/21/61/61	0/2/2/2
20	0V9	bi	102	-	-	7/48/48/50	-
15	V7N	BM	1001	-	-	7/49/53/53	-
13	BCL	BB	104	-	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BG	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	bh	103	-	-	1/21/61/61	0/2/2/2
13	BCL	al	1001	-	-	6/37/137/137	-
14	LMT	BS	1004	-	-	3/21/61/61	0/2/2/2
13	BCL	ap	1001	-	-	11/37/137/137	-
14	LMT	AD	1003	-	-	6/21/61/61	0/2/2/2
13	BCL	ae	1001	-	-	9/37/137/137	-
14	LMT	BW	1002	-	-	3/21/61/61	0/2/2/2
13	BCL	AQ	101	-	-	3/37/137/137	-
14	LMT	BA	106	-	-	7/21/61/61	0/2/2/2
13	BCL	AT	102	-	-	1/37/137/137	-
13	BCL	AP	101	-	-	5/37/137/137	-
14	LMT	BD	104	-	-	2/21/61/61	0/2/2/2
15	V7N	bb	101	-	-	17/49/53/53	-
15	V7N	bk	103	-	-	8/49/53/53	-
13	BCL	AA	1002	28	-	9/37/137/137	-
13	BCL	L	303	-	-	4/37/137/137	-
15	V7N	bh	102	-	-	5/49/53/53	-
20	0V9	aj	101	-	-	16/48/48/50	-
13	BCL	AO	102	-	-	3/37/137/137	-
15	V7N	BJ	1001	-	-	4/49/53/53	-
14	LMT	BE	102	-	-	5/21/61/61	0/2/2/2
14	LMT	BP	1006	-	-	3/21/61/61	0/2/2/2
13	BCL	AK	102	-	-	1/37/137/137	-
15	V7N	bn	101	-	-	5/49/53/53	-
13	BCL	AF	1002	-	-	10/37/137/137	-
27	UYH	ai	101	-	-	9/50/70/70	0/1/1/1
14	LMT	bj	102	-	-	5/21/61/61	0/2/2/2
13	BCL	AI	103	-	-	6/37/137/137	-
20	0V9	bb	104	-	-	10/48/48/50	-
13	BCL	BS	1005	-	-	8/37/137/137	-
20	0V9	be	102	-	-	16/48/48/50	-
13	BCL	AF	1001	-	-	7/37/137/137	-
13	BCL	AL	101	-	-	1/37/137/137	-
15	V7N	BT	1001	-	-	3/49/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BW	1003	-	-	5/37/137/137	-
14	LMT	BR	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	BC	104	-	-	6/21/61/61	0/2/2/2
14	LMT	BN	1004	-	-	4/21/61/61	0/2/2/2
14	LMT	BE	105	-	-	2/21/61/61	0/2/2/2
21	CD4	af	104	-	-	20/94/94/94	-
14	LMT	AD	1004	-	-	1/21/61/61	0/2/2/2
15	V7N	be	101	-	-	6/49/53/53	-
16	HEC	C	1002	3	-	0/6/54/54	-
13	BCL	af	102	-	-	3/37/137/137	-
15	V7N	bi	101	-	-	3/49/53/53	-
14	LMT	BT	1005	-	-	6/21/61/61	0/2/2/2
13	BCL	AA	1001	-	-	3/37/137/137	-
22	BPH	M	406	-	-	6/54/105/105	0/5/6/6
13	BCL	AI	102	-	-	8/37/137/137	-
14	LMT	BW	1005	-	-	6/21/61/61	0/2/2/2
15	V7N	bf	102	-	-	3/49/53/53	-
21	CD4	af	103	-	-	30/94/94/94	-
14	LMT	BK	1004	-	-	7/21/61/61	0/2/2/2
13	BCL	ao	1001	-	-	7/37/137/137	-
13	BCL	ag	1001	-	-	5/37/137/137	-
14	LMT	AA	1003	-	-	7/21/61/61	0/2/2/2
14	LMT	BQ	1002	-	-	1/21/61/61	0/2/2/2
13	BCL	bb	103	-	-	5/37/137/137	-
14	LMT	BT	1003	-	-	4/21/61/61	0/2/2/2
18	V75	C	1006	17,12	-	0/8/29/29	0/1/1/1
13	BCL	BJ	1004	-	-	8/37/137/137	-
15	V7N	BO	1001	-	-	6/49/53/53	-
20	0V9	bg	102	-	-	15/48/48/50	-
25	CRT	M	408	-	-	3/51/51/51	-
14	LMT	AL	102	-	-	5/21/61/61	0/2/2/2
13	BCL	AS	101	-	-	7/37/137/137	-
15	V7N	BL	1001	-	-	7/49/53/53	-
20	0V9	bn	104	-	-	12/48/48/50	-
13	BCL	am	1001	-	-	2/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BD	106	-	-	6/37/137/137	-
14	LMT	AJ	103	-	-	2/21/61/61	0/2/2/2
23	MQ8	an	101	-	-	4/47/67/67	0/2/2/2
13	BCL	AM	101	28	-	10/37/137/137	-
15	V7N	bm	101	-	-	4/49/53/53	-
21	CD4	M	404	-	-	21/94/94/94	-
15	V7N	BH	1001	-	-	4/49/53/53	-
14	LMT	BU	1001	-	-	5/21/61/61	0/2/2/2
13	BCL	BI	104	-	-	12/37/137/137	-
14	LMT	BF	103	-	-	1/21/61/61	0/2/2/2
20	0V9	bk	102	-	-	12/48/48/50	-
14	LMT	AR	102	-	-	11/21/61/61	0/2/2/2
14	LMT	L	305	-	-	7/21/61/61	0/2/2/2
13	BCL	bh	105	-	-	6/37/137/137	-
14	LMT	BJ	1002	-	-	6/21/61/61	0/2/2/2
15	V7N	BG	1001	-	-	5/49/53/53	-
14	LMT	L	306	-	-	3/21/61/61	0/2/2/2
14	LMT	bd	102	-	-	8/21/61/61	0/2/2/2
13	BCL	BX	1004	-	-	6/37/137/137	-
13	BCL	AW	101	28	-	8/37/137/137	-
13	BCL	bi	103	-	-	6/37/137/137	-
14	LMT	BJ	1003	-	-	2/21/61/61	0/2/2/2
13	BCL	AJ	102	28	-	11/37/137/137	-
14	LMT	BS	1003	-	-	6/21/61/61	0/2/2/2
14	LMT	BA	102	-	-	2/21/61/61	0/2/2/2
14	LMT	BR	1006	-	-	2/21/61/61	0/2/2/2
14	LMT	BI	101	-	-	2/21/61/61	0/2/2/2
13	BCL	AV	102	-	-	3/37/137/137	-
13	BCL	BL	1004	-	-	6/37/137/137	-
14	LMT	AS	103	-	-	8/21/61/61	0/2/2/2
14	LMT	bf	101	-	-	7/21/61/61	0/2/2/2
14	LMT	BW	1006	-	-	9/21/61/61	0/2/2/2
14	LMT	AH	104	-	-	2/21/61/61	0/2/2/2

All (1406) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	ba	101	V7N	C28-C27	7.01	1.52	1.34
15	BV	1001	V7N	C28-C27	7.01	1.52	1.34
15	bp	102	V7N	C28-C27	7.00	1.52	1.34
15	bl	102	V7N	C28-C27	6.99	1.52	1.34
15	bg	101	V7N	C28-C27	6.99	1.52	1.34
15	AT	103	V7N	C28-C27	6.98	1.52	1.34
15	BN	1001	V7N	C28-C27	6.97	1.52	1.34
15	BA	101	V7N	C28-C27	6.96	1.52	1.34
15	BG	1001	V7N	C28-C27	6.94	1.52	1.34
15	BL	1001	V7N	C28-C27	6.94	1.52	1.34
15	bb	101	V7N	C28-C27	6.93	1.52	1.34
15	AE	1003	V7N	C28-C27	6.92	1.52	1.34
15	bf	102	V7N	C28-C27	6.92	1.52	1.34
15	BC	101	V7N	C28-C27	6.91	1.52	1.34
15	bk	103	V7N	C28-C27	6.90	1.52	1.34
15	BX	1001	V7N	C28-C27	6.90	1.52	1.34
15	AH	105	V7N	C28-C27	6.90	1.52	1.34
15	bj	101	V7N	C28-C27	6.89	1.52	1.34
15	bn	101	V7N	C28-C27	6.89	1.52	1.34
15	bi	101	V7N	C28-C27	6.87	1.52	1.34
15	BE	101	V7N	C28-C27	6.86	1.52	1.34
15	BQ	1001	V7N	C28-C27	6.84	1.52	1.34
15	BT	1001	V7N	C28-C27	6.84	1.52	1.34
15	BJ	1001	V7N	C28-C27	6.84	1.52	1.34
15	bc	104	V7N	C28-C27	6.84	1.52	1.34
15	BR	1001	V7N	C28-C27	6.84	1.52	1.34
15	bd	101	V7N	C28-C27	6.84	1.52	1.34
15	BO	1001	V7N	C28-C27	6.83	1.52	1.34
15	BK	1001	V7N	C28-C27	6.83	1.52	1.34
15	BM	1001	V7N	C28-C27	6.83	1.52	1.34
15	BH	1001	V7N	C28-C27	6.82	1.52	1.34
15	bo	101	V7N	C28-C27	6.82	1.52	1.34
15	BS	1001	V7N	C28-C27	6.82	1.52	1.34
15	bh	102	V7N	C28-C27	6.81	1.52	1.34
15	bm	101	V7N	C28-C27	6.81	1.52	1.34
15	BB	101	V7N	C28-C27	6.79	1.52	1.34
15	BD	101	V7N	C28-C27	6.78	1.52	1.34
15	BW	1001	V7N	C28-C27	6.78	1.52	1.34
15	BP	1001	V7N	C28-C27	6.75	1.52	1.34
15	be	101	V7N	C28-C27	6.74	1.51	1.34
16	C	1001	HEC	C3C-C2C	-5.44	1.35	1.40
16	C	1004	HEC	C2B-C3B	-5.42	1.35	1.40
16	C	1004	HEC	C3C-C2C	-5.40	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1003	HEC	C3C-C2C	-5.37	1.35	1.40
16	C	1002	HEC	C3C-C2C	-5.35	1.35	1.40
16	C	1002	HEC	C2B-C3B	-5.35	1.35	1.40
16	C	1002	HEC	C3D-C2D	5.33	1.53	1.37
16	C	1001	HEC	C3D-C2D	5.28	1.53	1.37
16	C	1004	HEC	C3D-C2D	5.26	1.53	1.37
16	C	1003	HEC	C3D-C2D	5.26	1.53	1.37
15	bk	103	V7N	C14-C13	5.23	1.42	1.35
13	AX	101	BCL	MG-NA	5.23	2.18	2.06
13	AW	101	BCL	C1B-NB	5.22	1.39	1.35
13	AV	102	BCL	MG-NA	5.16	2.18	2.06
13	AB	101	BCL	MG-NA	5.15	2.18	2.06
13	AQ	103	BCL	MG-NA	5.14	2.18	2.06
13	AJ	101	BCL	MG-NA	5.14	2.18	2.06
15	AT	103	V7N	C14-C13	5.13	1.42	1.35
13	AO	102	BCL	MG-NA	5.12	2.18	2.06
13	al	1001	BCL	MG-NA	5.12	2.18	2.06
13	AD	1002	BCL	MG-NA	5.11	2.18	2.06
13	AE	1001	BCL	C1B-NB	5.10	1.39	1.35
13	AD	1001	BCL	C1B-NB	5.09	1.39	1.35
13	AU	103	BCL	MG-NA	5.09	2.18	2.06
13	AP	101	BCL	MG-NA	5.09	2.18	2.06
13	AN	104	BCL	MG-NA	5.09	2.18	2.06
13	AI	102	BCL	MG-NA	5.08	2.18	2.06
13	AR	101	BCL	MG-NA	5.08	2.18	2.06
13	AL	103	BCL	C1B-NB	5.08	1.39	1.35
13	AM	102	BCL	MG-NA	5.08	2.18	2.06
13	an	102	BCL	MG-NA	5.07	2.18	2.06
13	AS	101	BCL	MG-NA	5.07	2.18	2.06
13	AS	104	BCL	C1B-NB	5.07	1.39	1.35
13	AN	102	BCL	MG-NA	5.06	2.18	2.06
13	AO	101	BCL	MG-NA	5.06	2.18	2.06
13	AL	101	BCL	MG-NA	5.06	2.18	2.06
16	C	1001	HEC	C2B-C3B	-5.06	1.35	1.40
13	AK	102	BCL	MG-NA	5.05	2.18	2.06
13	AI	102	BCL	C1B-NB	5.05	1.39	1.35
13	AL	103	BCL	MG-NA	5.05	2.18	2.06
13	AF	1001	BCL	MG-NA	5.04	2.18	2.06
13	AA	1001	BCL	MG-NA	5.04	2.18	2.06
13	af	102	BCL	MG-NA	5.04	2.18	2.06
13	AG	103	BCL	MG-NA	5.04	2.18	2.06
13	AP	103	BCL	C1B-NB	5.03	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	1001	BCL	MG-NA	5.03	2.18	2.06
13	ap	1001	BCL	MG-NA	5.03	2.18	2.06
15	bp	102	V7N	C14-C13	5.03	1.42	1.35
13	AT	102	BCL	MG-NA	5.02	2.18	2.06
13	AA	1002	BCL	C1B-NB	5.02	1.39	1.35
13	AU	102	BCL	MG-NA	5.01	2.18	2.06
13	AH	101	BCL	C1B-NB	5.01	1.39	1.35
13	AV	103	BCL	MG-NA	5.01	2.18	2.06
13	AM	101	BCL	C1B-NB	5.01	1.39	1.35
13	AJ	102	BCL	C1B-NB	5.01	1.39	1.35
13	AW	103	BCL	MG-NA	5.01	2.18	2.06
13	AS	102	BCL	MG-NA	5.00	2.18	2.06
13	aa	1001	BCL	MG-NA	5.00	2.18	2.06
13	AH	102	BCL	MG-NA	4.99	2.18	2.06
13	AI	103	BCL	MG-NA	4.99	2.18	2.06
13	AO	101	BCL	C1B-NB	4.99	1.39	1.35
13	AE	1002	BCL	MG-NA	4.98	2.18	2.06
13	AJ	102	BCL	MG-NA	4.98	2.18	2.06
13	AB	103	BCL	C1B-NB	4.98	1.39	1.35
13	AF	1002	BCL	C1B-NB	4.98	1.39	1.35
13	am	1001	BCL	MG-NA	4.98	2.18	2.06
13	AG	102	BCL	MG-NA	4.98	2.18	2.06
15	bb	101	V7N	C14-C13	4.98	1.42	1.35
13	AQ	102	BCL	MG-NA	4.98	2.18	2.06
16	C	1003	HEC	C2B-C3B	-4.97	1.35	1.40
13	bc	103	BCL	MG-NA	4.97	2.18	2.06
13	AP	103	BCL	MG-NA	4.97	2.18	2.06
15	bn	101	V7N	C14-C13	4.97	1.42	1.35
13	ap	1001	BCL	C1B-NB	4.97	1.39	1.35
13	BM	1004	BCL	MG-NA	4.96	2.18	2.06
13	BB	104	BCL	MG-NA	4.96	2.18	2.06
13	M	403	BCL	C1B-NB	4.96	1.39	1.35
15	bo	101	V7N	C14-C13	4.96	1.42	1.35
15	bk	103	V7N	C17-C18	4.96	1.42	1.35
13	ah	1001	BCL	MG-NA	4.96	2.18	2.06
13	AW	104	BCL	C1B-NB	4.95	1.39	1.35
13	aa	1001	BCL	C1B-NB	4.95	1.39	1.35
15	AT	103	V7N	C17-C18	4.95	1.42	1.35
13	bl	105	BCL	C1B-NB	4.95	1.39	1.35
13	ah	1001	BCL	C1B-NB	4.94	1.39	1.35
13	ab	1001	BCL	MG-NA	4.94	2.18	2.06
13	AQ	102	BCL	C1B-NB	4.94	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	ab	1001	BCL	C1B-NB	4.94	1.39	1.35
13	AG	102	BCL	C1B-NB	4.94	1.39	1.35
13	AK	103	BCL	MG-NA	4.94	2.18	2.06
13	AC	1002	BCL	MG-NA	4.93	2.18	2.06
13	ae	1001	BCL	MG-NA	4.93	2.18	2.06
13	AC	1001	BCL	C1B-NB	4.93	1.39	1.35
15	BE	101	V7N	C14-C13	4.93	1.42	1.35
13	aj	102	BCL	C1B-NB	4.93	1.39	1.35
13	ac	102	BCL	MG-NA	4.92	2.18	2.06
13	af	102	BCL	C1B-NB	4.92	1.39	1.35
13	AQ	101	BCL	MG-NA	4.92	2.18	2.06
13	BG	1004	BCL	MG-NA	4.91	2.17	2.06
13	BW	1003	BCL	MG-NA	4.91	2.17	2.06
13	AB	101	BCL	C1B-NB	4.91	1.39	1.35
13	AF	1002	BCL	MG-NA	4.91	2.17	2.06
13	AV	103	BCL	C1B-NB	4.90	1.39	1.35
13	ai	102	BCL	C1B-NB	4.90	1.39	1.35
13	AN	102	BCL	C1B-NB	4.89	1.39	1.35
15	bp	102	V7N	C17-C18	4.89	1.42	1.35
13	ak	1001	BCL	MG-NA	4.89	2.17	2.06
15	bf	102	V7N	C14-C13	4.89	1.42	1.35
15	bi	101	V7N	C14-C13	4.89	1.42	1.35
13	AW	104	BCL	MG-NA	4.89	2.17	2.06
13	AD	1002	BCL	C1B-NB	4.88	1.39	1.35
13	ag	1001	BCL	C1B-NB	4.88	1.39	1.35
13	be	104	BCL	C1B-NB	4.88	1.39	1.35
15	bn	101	V7N	C17-C18	4.88	1.42	1.35
13	bd	103	BCL	MG-NA	4.88	2.17	2.06
13	al	1001	BCL	C1B-NB	4.88	1.39	1.35
13	ba	103	BCL	C1B-NB	4.88	1.39	1.35
13	L	308	BCL	C1B-NB	4.88	1.39	1.35
13	bp	103	BCL	MG-NA	4.88	2.17	2.06
13	bp	103	BCL	C1B-NB	4.88	1.39	1.35
13	ai	102	BCL	MG-NA	4.87	2.17	2.06
13	ad	102	BCL	MG-NA	4.87	2.17	2.06
15	BH	1001	V7N	C14-C13	4.87	1.42	1.35
13	AC	1002	BCL	C1B-NB	4.87	1.39	1.35
13	BD	106	BCL	MG-NA	4.87	2.17	2.06
13	bb	103	BCL	C1B-NB	4.86	1.39	1.35
13	BV	1004	BCL	MG-NA	4.86	2.17	2.06
13	bk	105	BCL	MG-NA	4.86	2.17	2.06
13	bn	103	BCL	C1B-NB	4.86	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BD	106	BCL	C1B-NB	4.85	1.39	1.35
13	AF	1001	BCL	C1B-NB	4.85	1.39	1.35
13	AT	102	BCL	C1B-NB	4.85	1.39	1.35
13	ao	1001	BCL	MG-NA	4.85	2.17	2.06
13	M	405	BCL	MG-NA	4.85	2.17	2.06
13	aj	102	BCL	MG-NA	4.85	2.17	2.06
15	bc	104	V7N	C14-C13	4.85	1.42	1.35
13	ag	1001	BCL	MG-NA	4.85	2.17	2.06
13	AM	101	BCL	MG-NA	4.84	2.17	2.06
13	bm	103	BCL	MG-NA	4.84	2.17	2.06
15	bg	101	V7N	C14-C13	4.84	1.42	1.35
13	AD	1001	BCL	MG-NA	4.84	2.17	2.06
13	AB	103	BCL	MG-NA	4.84	2.17	2.06
13	AU	102	BCL	C1B-NB	4.84	1.39	1.35
13	AK	103	BCL	C1B-NB	4.83	1.39	1.35
13	BI	104	BCL	MG-NA	4.83	2.17	2.06
13	AA	1002	BCL	MG-NA	4.83	2.17	2.06
15	bj	101	V7N	C14-C13	4.83	1.42	1.35
15	BX	1001	V7N	C14-C13	4.83	1.42	1.35
13	ad	102	BCL	C1B-NB	4.83	1.39	1.35
13	AQ	103	BCL	C1B-NB	4.83	1.39	1.35
15	ba	101	V7N	C14-C13	4.83	1.42	1.35
13	AE	1001	BCL	MG-NA	4.82	2.17	2.06
13	bj	104	BCL	MG-NA	4.82	2.17	2.06
15	AE	1003	V7N	C14-C13	4.82	1.42	1.35
13	AU	103	BCL	C1B-NB	4.81	1.39	1.35
13	AL	101	BCL	C1B-NB	4.81	1.39	1.35
13	AJ	101	BCL	C1B-NB	4.81	1.39	1.35
13	AE	1002	BCL	C1B-NB	4.81	1.39	1.35
13	BJ	1004	BCL	MG-NA	4.80	2.17	2.06
13	BS	1005	BCL	MG-NA	4.80	2.17	2.06
13	AP	101	BCL	C1B-NB	4.80	1.39	1.35
13	BE	104	BCL	MG-NA	4.80	2.17	2.06
13	bo	102	BCL	MG-NA	4.80	2.17	2.06
13	bn	103	BCL	MG-NA	4.79	2.17	2.06
15	BL	1001	V7N	C14-C13	4.79	1.42	1.35
13	BT	1004	BCL	MG-NA	4.79	2.17	2.06
15	BG	1001	V7N	C14-C13	4.79	1.42	1.35
13	AH	101	BCL	MG-NA	4.79	2.17	2.06
13	ae	1001	BCL	C1B-NB	4.79	1.39	1.35
13	AM	102	BCL	C1B-NB	4.78	1.39	1.35
13	BF	104	BCL	C1B-NB	4.78	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BT	1001	V7N	C14-C13	4.78	1.42	1.35
13	ba	103	BCL	MG-NA	4.78	2.17	2.06
13	AG	103	BCL	C1B-NB	4.78	1.39	1.35
13	BH	1003	BCL	MG-NA	4.78	2.17	2.06
13	BP	1004	BCL	MG-NA	4.77	2.17	2.06
13	AQ	101	BCL	C1B-NB	4.77	1.39	1.35
15	bb	101	V7N	C17-C18	4.77	1.42	1.35
13	BQ	1003	BCL	MG-NA	4.77	2.17	2.06
15	AH	105	V7N	C14-C13	4.77	1.42	1.35
13	BA	104	BCL	MG-NA	4.77	2.17	2.06
13	ao	1001	BCL	C1B-NB	4.77	1.39	1.35
13	BO	1004	BCL	MG-NA	4.77	2.17	2.06
13	bm	103	BCL	C1B-NB	4.77	1.39	1.35
13	L	303	BCL	C1B-NB	4.76	1.39	1.35
13	bd	103	BCL	C1B-NB	4.76	1.39	1.35
15	bm	101	V7N	C14-C13	4.76	1.42	1.35
13	AA	1001	BCL	C1B-NB	4.76	1.39	1.35
13	AS	102	BCL	C1B-NB	4.76	1.39	1.35
13	bf	105	BCL	MG-NA	4.76	2.17	2.06
13	bf	105	BCL	C1B-NB	4.76	1.39	1.35
15	bh	102	V7N	C14-C13	4.75	1.42	1.35
13	BL	1004	BCL	C1B-NB	4.75	1.39	1.35
13	BK	1003	BCL	MG-NA	4.75	2.17	2.06
13	bh	105	BCL	MG-NA	4.75	2.17	2.06
13	AH	102	BCL	C1B-NB	4.75	1.39	1.35
15	bd	101	V7N	C14-C13	4.75	1.42	1.35
13	AW	103	BCL	C1B-NB	4.75	1.39	1.35
13	bg	104	BCL	MG-NA	4.74	2.17	2.06
13	bl	105	BCL	MG-NA	4.74	2.17	2.06
13	AO	102	BCL	C1B-NB	4.74	1.39	1.35
13	BH	1003	BCL	C1B-NB	4.74	1.39	1.35
13	ac	102	BCL	C1B-NB	4.74	1.39	1.35
15	bl	102	V7N	C14-C13	4.74	1.42	1.35
13	BR	1003	BCL	C1B-NB	4.74	1.39	1.35
15	BC	101	V7N	C14-C13	4.73	1.42	1.35
13	BC	103	BCL	C1B-NB	4.73	1.39	1.35
13	BS	1005	BCL	C1B-NB	4.73	1.39	1.35
13	ak	1001	BCL	C1B-NB	4.73	1.39	1.35
13	be	104	BCL	MG-NA	4.73	2.17	2.06
13	bb	103	BCL	MG-NA	4.73	2.17	2.06
13	AX	101	BCL	C1B-NB	4.73	1.39	1.35
13	BU	1004	BCL	C1B-NB	4.72	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BK	1001	V7N	C14-C13	4.72	1.42	1.35
13	BX	1004	BCL	MG-NA	4.72	2.17	2.06
13	BU	1004	BCL	MG-NA	4.72	2.17	2.06
13	bo	102	BCL	C1B-NB	4.72	1.39	1.35
15	BR	1001	V7N	C14-C13	4.72	1.42	1.35
15	BO	1001	V7N	C14-C13	4.72	1.42	1.35
13	BN	1006	BCL	C1B-NB	4.72	1.39	1.35
13	bh	105	BCL	C1B-NB	4.72	1.39	1.35
13	BA	104	BCL	C1B-NB	4.72	1.39	1.35
13	bc	103	BCL	C1B-NB	4.71	1.39	1.35
13	BO	1004	BCL	C1B-NB	4.71	1.39	1.35
13	BG	1004	BCL	C1B-NB	4.71	1.39	1.35
13	BW	1003	BCL	C1B-NB	4.71	1.39	1.35
13	BM	1004	BCL	C1B-NB	4.71	1.39	1.35
13	BT	1004	BCL	C1B-NB	4.71	1.39	1.35
15	ba	101	V7N	C17-C18	4.71	1.42	1.35
13	AS	101	BCL	C1B-NB	4.70	1.39	1.35
13	bk	105	BCL	C1B-NB	4.70	1.39	1.35
13	bi	103	BCL	C1B-NB	4.70	1.39	1.35
13	bi	103	BCL	MG-NA	4.70	2.17	2.06
13	bj	104	BCL	C1B-NB	4.69	1.39	1.35
13	AN	104	BCL	C1B-NB	4.69	1.39	1.35
13	BX	1004	BCL	C1B-NB	4.69	1.39	1.35
13	bg	104	BCL	C1B-NB	4.69	1.39	1.35
13	AI	103	BCL	C1B-NB	4.68	1.39	1.35
13	AK	102	BCL	C1B-NB	4.68	1.39	1.35
13	BP	1004	BCL	C1B-NB	4.67	1.39	1.35
13	AV	102	BCL	C1B-NB	4.67	1.39	1.35
13	L	303	BCL	MG-NA	4.67	2.17	2.06
13	am	1001	BCL	C1B-NB	4.66	1.39	1.35
13	BI	104	BCL	C1B-NB	4.66	1.39	1.35
13	BQ	1003	BCL	C1B-NB	4.66	1.39	1.35
13	AR	101	BCL	C1B-NB	4.66	1.39	1.35
13	BR	1003	BCL	MG-NA	4.66	2.17	2.06
15	BV	1001	V7N	C14-C13	4.66	1.42	1.35
15	bk	103	V7N	C21-C22	4.65	1.39	1.34
13	an	102	BCL	C1B-NB	4.65	1.39	1.35
13	BC	103	BCL	MG-NA	4.65	2.17	2.06
13	BK	1003	BCL	C1B-NB	4.65	1.39	1.35
13	BE	104	BCL	C1B-NB	4.64	1.39	1.35
27	ai	101	UYH	O8-C28	4.64	1.46	1.33
15	bo	101	V7N	C17-C18	4.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BN	1006	BCL	MG-NA	4.63	2.17	2.06
15	AT	103	V7N	C21-C22	4.62	1.38	1.34
15	BD	101	V7N	C14-C13	4.61	1.41	1.35
13	AS	104	BCL	MG-NA	4.61	2.17	2.06
13	BV	1004	BCL	C1B-NB	4.61	1.39	1.35
13	BJ	1004	BCL	C1B-NB	4.60	1.39	1.35
13	BB	104	BCL	C1B-NB	4.60	1.39	1.35
13	L	308	BCL	MG-NA	4.60	2.17	2.06
13	BL	1004	BCL	MG-NA	4.59	2.17	2.06
13	M	403	BCL	MG-NA	4.59	2.17	2.06
15	bf	102	V7N	C17-C18	4.59	1.41	1.35
15	BW	1001	V7N	C14-C13	4.58	1.41	1.35
13	BF	104	BCL	MG-NA	4.58	2.17	2.06
15	BH	1001	V7N	C17-C18	4.58	1.41	1.35
15	bi	101	V7N	C17-C18	4.57	1.41	1.35
15	BQ	1001	V7N	C14-C13	4.57	1.41	1.35
15	be	101	V7N	C14-C13	4.57	1.41	1.35
15	BL	1001	V7N	C17-C18	4.57	1.41	1.35
15	bj	101	V7N	C17-C18	4.56	1.41	1.35
15	bc	104	V7N	C17-C18	4.56	1.41	1.35
15	BO	1001	V7N	C17-C18	4.55	1.41	1.35
15	BX	1001	V7N	C17-C18	4.55	1.41	1.35
15	BE	101	V7N	C17-C18	4.55	1.41	1.35
15	BB	101	V7N	C14-C13	4.54	1.41	1.35
15	bm	101	V7N	C17-C18	4.54	1.41	1.35
15	BJ	1001	V7N	C14-C13	4.52	1.41	1.35
15	bg	101	V7N	C17-C18	4.51	1.41	1.35
15	AE	1003	V7N	C17-C18	4.51	1.41	1.35
15	BN	1001	V7N	C14-C13	4.50	1.41	1.35
15	BS	1001	V7N	C14-C13	4.50	1.41	1.35
15	BC	101	V7N	C17-C18	4.50	1.41	1.35
15	bh	102	V7N	C17-C18	4.50	1.41	1.35
15	BP	1001	V7N	C14-C13	4.49	1.41	1.35
15	BA	101	V7N	C14-C13	4.49	1.41	1.35
13	AW	101	BCL	MG-NA	4.48	2.16	2.06
15	AH	105	V7N	C17-C18	4.48	1.41	1.35
15	BR	1001	V7N	C17-C18	4.48	1.41	1.35
13	M	405	BCL	C1B-NB	4.48	1.39	1.35
15	bl	102	V7N	C17-C18	4.47	1.41	1.35
15	BG	1001	V7N	C17-C18	4.47	1.41	1.35
27	ai	101	UYH	O7-C10	4.46	1.46	1.34
15	BV	1001	V7N	C17-C18	4.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bd	101	V7N	C17-C18	4.44	1.41	1.35
15	BT	1001	V7N	C17-C18	4.44	1.41	1.35
15	BM	1001	V7N	C14-C13	4.42	1.41	1.35
15	bp	102	V7N	C21-C22	4.36	1.38	1.34
15	BB	101	V7N	C17-C18	4.35	1.41	1.35
15	BQ	1001	V7N	C17-C18	4.33	1.41	1.35
15	BK	1001	V7N	C17-C18	4.32	1.41	1.35
15	AT	103	V7N	C6-C5	4.31	1.41	1.35
15	bb	101	V7N	C21-C22	4.31	1.38	1.34
15	ba	101	V7N	C21-C22	4.29	1.38	1.34
15	BW	1001	V7N	C17-C18	4.27	1.41	1.35
15	be	101	V7N	C17-C18	4.27	1.41	1.35
15	BJ	1001	V7N	C17-C18	4.27	1.41	1.35
15	bn	101	V7N	C21-C22	4.23	1.38	1.34
15	BK	1001	V7N	C21-C22	4.22	1.38	1.34
15	BS	1001	V7N	C17-C18	4.22	1.41	1.35
15	BM	1001	V7N	C17-C18	4.21	1.41	1.35
15	BD	101	V7N	C17-C18	4.21	1.41	1.35
15	BG	1001	V7N	C21-C22	4.19	1.38	1.34
15	BN	1001	V7N	C17-C18	4.19	1.41	1.35
15	bc	104	V7N	C21-C22	4.19	1.38	1.34
15	bo	101	V7N	C21-C22	4.19	1.38	1.34
15	BH	1001	V7N	C21-C22	4.17	1.38	1.34
15	BE	101	V7N	C21-C22	4.15	1.38	1.34
15	bl	102	V7N	C21-C22	4.15	1.38	1.34
15	bj	101	V7N	C21-C22	4.14	1.38	1.34
15	bi	101	V7N	C21-C22	4.14	1.38	1.34
15	BA	101	V7N	C17-C18	4.13	1.41	1.35
15	BX	1001	V7N	C21-C22	4.13	1.38	1.34
15	bf	102	V7N	C21-C22	4.13	1.38	1.34
15	BL	1001	V7N	C21-C22	4.10	1.38	1.34
15	BV	1001	V7N	C21-C22	4.09	1.38	1.34
15	BC	101	V7N	C21-C22	4.08	1.38	1.34
15	BO	1001	V7N	C21-C22	4.07	1.38	1.34
15	bk	103	V7N	C6-C5	4.05	1.41	1.35
15	bm	101	V7N	C21-C22	4.05	1.38	1.34
15	BT	1001	V7N	C21-C22	4.04	1.38	1.34
15	bg	101	V7N	C21-C22	4.04	1.38	1.34
15	BP	1001	V7N	C17-C18	4.04	1.41	1.35
15	AE	1003	V7N	C21-C22	4.03	1.38	1.34
15	bn	101	V7N	C6-C5	4.00	1.41	1.35
15	AH	105	V7N	C21-C22	4.00	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	ba	101	V7N	C6-C5	3.99	1.41	1.35
15	bb	101	V7N	C6-C5	3.99	1.41	1.35
15	bh	102	V7N	C21-C22	3.98	1.38	1.34
15	BQ	1001	V7N	C21-C22	3.95	1.38	1.34
15	bd	101	V7N	C21-C22	3.90	1.38	1.34
15	BR	1001	V7N	C21-C22	3.89	1.38	1.34
15	be	101	V7N	C21-C22	3.88	1.38	1.34
15	BD	101	V7N	C21-C22	3.87	1.38	1.34
15	bl	102	V7N	C6-C5	3.85	1.40	1.35
15	bo	101	V7N	C6-C5	3.84	1.40	1.35
15	BJ	1001	V7N	C21-C22	3.82	1.38	1.34
13	AO	101	BCL	MG-NC	3.79	2.15	2.06
15	BP	1001	V7N	C21-C22	3.78	1.38	1.34
15	bc	104	V7N	C6-C5	3.78	1.40	1.35
20	H1	1002	0V9	P-O2P	-3.78	1.37	1.50
15	BS	1001	V7N	C21-C22	3.77	1.38	1.34
15	BW	1001	V7N	C21-C22	3.77	1.38	1.34
15	bm	101	V7N	C6-C5	3.77	1.40	1.35
15	bi	101	V7N	C6-C5	3.77	1.40	1.35
15	BD	101	V7N	C6-C5	3.76	1.40	1.35
15	bf	102	V7N	C6-C5	3.76	1.40	1.35
15	bg	101	V7N	C6-C5	3.72	1.40	1.35
20	bj	103	0V9	P-O2P	-3.72	1.37	1.50
15	BE	101	V7N	C6-C5	3.72	1.40	1.35
15	bp	102	V7N	C6-C5	3.72	1.40	1.35
20	L	310	0V9	P-O2P	-3.71	1.37	1.50
20	bi	102	0V9	P-O2P	-3.71	1.37	1.50
20	bk	102	0V9	P-O2P	-3.71	1.37	1.50
20	ba	102	0V9	P-O2P	-3.70	1.37	1.50
20	bb	104	0V9	P-O2P	-3.70	1.37	1.50
20	be	103	0V9	P-O2P	-3.70	1.37	1.50
20	bc	102	0V9	P-O2P	-3.70	1.37	1.50
20	bo	104	0V9	P-O2P	-3.69	1.37	1.50
20	bl	103	0V9	P-O2P	-3.69	1.37	1.50
20	bg	102	0V9	P-O2P	-3.69	1.37	1.50
20	ba	104	0V9	P-O2P	-3.68	1.37	1.50
20	be	102	0V9	P-O2P	-3.68	1.37	1.50
15	BX	1001	V7N	C6-C5	3.67	1.40	1.35
20	bm	102	0V9	P-O2P	-3.67	1.37	1.50
20	bn	104	0V9	P-O2P	-3.67	1.37	1.50
20	bf	103	0V9	P-O2P	-3.67	1.37	1.50
20	aj	101	0V9	P-O2P	-3.67	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	bk	104	OV9	P-O2P	-3.66	1.37	1.50
20	bh	104	OV9	P-O2P	-3.66	1.37	1.50
13	AC	1002	BCL	MG-NC	3.66	2.15	2.06
15	bh	102	V7N	C6-C5	3.65	1.40	1.35
15	BR	1001	V7N	C6-C5	3.65	1.40	1.35
15	bj	101	V7N	C6-C5	3.64	1.40	1.35
13	AK	103	BCL	MG-NC	3.63	2.14	2.06
15	BM	1001	V7N	C6-C5	3.63	1.40	1.35
15	BH	1001	V7N	C6-C5	3.63	1.40	1.35
27	ai	101	UYH	O1-C1	3.63	1.46	1.40
18	M	409	V75	O2-C2	-3.62	1.40	1.46
13	bn	103	BCL	MG-NC	3.61	2.14	2.06
15	BV	1001	V7N	C6-C5	3.61	1.40	1.35
15	BA	101	V7N	C21-C22	3.59	1.37	1.34
13	AN	102	BCL	MG-NC	3.59	2.14	2.06
15	BG	1001	V7N	C6-C5	3.59	1.40	1.35
13	AD	1002	BCL	MG-NC	3.58	2.14	2.06
13	AE	1001	BCL	MG-NC	3.58	2.14	2.06
13	AL	103	BCL	MG-NC	3.58	2.14	2.06
13	AX	101	BCL	MG-NC	3.57	2.14	2.06
15	BB	101	V7N	C21-C22	3.57	1.37	1.34
15	BO	1001	V7N	C6-C5	3.56	1.40	1.35
13	AJ	101	BCL	MG-NC	3.56	2.14	2.06
15	BN	1001	V7N	C21-C22	3.56	1.37	1.34
15	bd	101	V7N	C6-C5	3.56	1.40	1.35
13	AQ	103	BCL	MG-NC	3.56	2.14	2.06
13	AJ	102	BCL	MG-NC	3.55	2.14	2.06
15	BM	1001	V7N	C21-C22	3.54	1.37	1.34
13	AB	101	BCL	MG-NC	3.54	2.14	2.06
13	AG	102	BCL	MG-NC	3.53	2.14	2.06
15	AH	105	V7N	C6-C5	3.53	1.40	1.35
15	BT	1001	V7N	C6-C5	3.53	1.40	1.35
15	BB	101	V7N	C6-C5	3.52	1.40	1.35
13	AF	1002	BCL	MG-NC	3.52	2.14	2.06
13	AM	102	BCL	MG-NC	3.52	2.14	2.06
13	AW	104	BCL	MG-NC	3.52	2.14	2.06
15	AE	1003	V7N	C6-C5	3.52	1.40	1.35
13	bc	103	BCL	MG-NC	3.52	2.14	2.06
15	BP	1001	V7N	C6-C5	3.51	1.40	1.35
13	ap	1001	BCL	MG-NC	3.51	2.14	2.06
13	AV	102	BCL	MG-NC	3.51	2.14	2.06
13	AS	101	BCL	MG-NC	3.50	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AQ	102	BCL	MG-NC	3.50	2.14	2.06
13	AV	103	BCL	MG-NC	3.50	2.14	2.06
13	AI	102	BCL	MG-NC	3.50	2.14	2.06
13	bp	103	BCL	MG-NC	3.50	2.14	2.06
13	AU	102	BCL	MG-NC	3.49	2.14	2.06
15	BC	101	V7N	C6-C5	3.49	1.40	1.35
15	BN	1001	V7N	C6-C5	3.48	1.40	1.35
13	AH	101	BCL	MG-NC	3.48	2.14	2.06
15	BQ	1001	V7N	C6-C5	3.48	1.40	1.35
13	bk	105	BCL	MG-NC	3.48	2.14	2.06
15	BK	1001	V7N	C6-C5	3.47	1.40	1.35
15	BL	1001	V7N	C6-C5	3.47	1.40	1.35
13	af	102	BCL	MG-NC	3.47	2.14	2.06
15	BW	1001	V7N	C6-C5	3.47	1.40	1.35
13	bm	103	BCL	MG-NC	3.47	2.14	2.06
13	AF	1001	BCL	MG-NC	3.46	2.14	2.06
13	AU	103	BCL	MG-NC	3.46	2.14	2.06
13	bd	103	BCL	MG-NC	3.46	2.14	2.06
13	BM	1004	BCL	MG-NC	3.44	2.14	2.06
13	AP	101	BCL	MG-NC	3.44	2.14	2.06
13	bf	105	BCL	MG-NC	3.44	2.14	2.06
13	aa	1001	BCL	MG-NC	3.44	2.14	2.06
15	BJ	1001	V7N	C6-C5	3.43	1.40	1.35
13	AB	103	BCL	MG-NC	3.43	2.14	2.06
13	AG	103	BCL	MG-NC	3.43	2.14	2.06
13	AR	101	BCL	MG-NC	3.42	2.14	2.06
13	bj	104	BCL	MG-NC	3.42	2.14	2.06
13	AA	1002	BCL	MG-NC	3.42	2.14	2.06
13	bb	103	BCL	MG-NC	3.42	2.14	2.06
13	AW	103	BCL	MG-NC	3.41	2.14	2.06
13	AN	104	BCL	MG-NC	3.41	2.14	2.06
13	al	1001	BCL	MG-NC	3.41	2.14	2.06
15	BS	1001	V7N	C6-C5	3.41	1.40	1.35
13	ae	1001	BCL	MG-NC	3.41	2.14	2.06
13	L	303	BCL	MG-NC	3.41	2.14	2.06
13	AA	1001	BCL	MG-NC	3.40	2.14	2.06
13	AS	104	BCL	MG-NC	3.40	2.14	2.06
13	AH	102	BCL	MG-NC	3.40	2.14	2.06
13	AK	102	BCL	MG-NC	3.40	2.14	2.06
13	an	102	BCL	MG-NC	3.40	2.14	2.06
13	BW	1003	BCL	MG-NC	3.40	2.14	2.06
13	AC	1001	BCL	MG-NC	3.40	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AT	102	BCL	MG-NC	3.40	2.14	2.06
13	bo	102	BCL	MG-NC	3.39	2.14	2.06
13	AE	1002	BCL	MG-NC	3.39	2.14	2.06
18	M	409	V75	O5-C5	-3.39	1.40	1.43
13	ab	1001	BCL	MG-NC	3.39	2.14	2.06
27	ai	101	UYH	C4-C5	3.38	1.60	1.53
13	ba	103	BCL	MG-NC	3.38	2.14	2.06
13	AL	101	BCL	MG-NC	3.38	2.14	2.06
13	ac	102	BCL	MG-NC	3.38	2.14	2.06
13	bl	105	BCL	MG-NC	3.38	2.14	2.06
13	BB	104	BCL	MG-NC	3.38	2.14	2.06
13	AO	102	BCL	MG-NC	3.37	2.14	2.06
13	bg	104	BCL	MG-NC	3.37	2.14	2.06
13	BD	106	BCL	MG-NC	3.36	2.14	2.06
13	BU	1004	BCL	MG-NC	3.36	2.14	2.06
13	ak	1001	BCL	MG-NC	3.36	2.14	2.06
13	AQ	101	BCL	MG-NC	3.35	2.14	2.06
13	be	104	BCL	MG-NC	3.35	2.14	2.06
13	ad	102	BCL	MG-NC	3.35	2.14	2.06
13	bh	105	BCL	MG-NC	3.35	2.14	2.06
15	be	101	V7N	C6-C5	3.35	1.40	1.35
13	ao	1001	BCL	MG-NC	3.34	2.14	2.06
13	aj	102	BCL	MG-NC	3.34	2.14	2.06
27	ai	101	UYH	C29-C28	3.34	1.60	1.50
15	BA	101	V7N	C6-C5	3.34	1.40	1.35
27	ai	101	UYH	C3-C2	3.33	1.60	1.52
13	BH	1003	BCL	MG-NC	3.33	2.14	2.06
13	AW	101	BCL	MG-NC	3.33	2.14	2.06
13	am	1001	BCL	MG-NC	3.33	2.14	2.06
13	BI	104	BCL	MG-NC	3.33	2.14	2.06
13	BG	1004	BCL	MG-NC	3.33	2.14	2.06
13	BX	1004	BCL	MG-NC	3.33	2.14	2.06
13	AI	103	BCL	MG-NC	3.33	2.14	2.06
13	ah	1001	BCL	MG-NC	3.33	2.14	2.06
13	BR	1003	BCL	MG-NC	3.33	2.14	2.06
13	AD	1001	BCL	MG-NC	3.32	2.14	2.06
13	BJ	1004	BCL	MG-NC	3.32	2.14	2.06
13	AS	102	BCL	MG-NC	3.32	2.14	2.06
13	BE	104	BCL	MG-NC	3.31	2.14	2.06
13	BV	1004	BCL	MG-NC	3.30	2.14	2.06
13	BP	1004	BCL	MG-NC	3.30	2.14	2.06
18	C	1006	V75	O2-C2	-3.30	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AM	101	BCL	MG-NC	3.30	2.14	2.06
13	AP	103	BCL	MG-NC	3.30	2.14	2.06
13	M	403	BCL	MG-NC	3.29	2.14	2.06
13	BO	1004	BCL	MG-NC	3.29	2.14	2.06
13	BQ	1003	BCL	MG-NC	3.28	2.14	2.06
13	bi	103	BCL	MG-NC	3.28	2.14	2.06
13	ag	1001	BCL	MG-NC	3.28	2.14	2.06
13	BK	1003	BCL	MG-NC	3.28	2.14	2.06
13	BL	1004	BCL	MG-NC	3.27	2.14	2.06
27	ai	101	UYH	C3-C4	3.27	1.60	1.52
13	ai	102	BCL	MG-NC	3.27	2.14	2.06
13	BS	1005	BCL	MG-NC	3.23	2.13	2.06
13	BT	1004	BCL	MG-NC	3.23	2.13	2.06
13	BN	1006	BCL	MG-NC	3.20	2.13	2.06
13	BA	104	BCL	MG-NC	3.20	2.13	2.06
13	BC	103	BCL	MG-NC	3.20	2.13	2.06
27	ai	101	UYH	C11-C10	3.16	1.60	1.50
13	BF	104	BCL	MG-NC	3.16	2.13	2.06
13	L	308	BCL	MG-NC	3.15	2.13	2.06
18	M	409	V75	O3-C3	-3.13	1.40	1.44
18	C	1006	V75	O5-C5	-3.09	1.40	1.43
18	C	1006	V75	O3-C3	-3.06	1.40	1.44
27	ai	101	UYH	C9-C8	3.01	1.59	1.50
13	M	405	BCL	MG-NC	2.98	2.13	2.06
27	ai	101	UYH	C7-C8	2.90	1.59	1.50
27	ai	101	UYH	C1-C2	2.89	1.60	1.52
22	M	406	BPH	C3D-CAD	-2.77	1.41	1.47
14	BW	1005	LMT	O3'-C3'	-2.77	1.36	1.43
14	AK	101	LMT	O3'-C3'	-2.76	1.36	1.43
14	BA	106	LMT	O3'-C3'	-2.76	1.36	1.43
22	L	301	BPH	C3D-CAD	-2.76	1.41	1.47
14	BD	105	LMT	O3'-C3'	-2.74	1.36	1.43
14	BE	102	LMT	O3'-C3'	-2.71	1.36	1.43
14	M	402	LMT	O3'-C3'	-2.71	1.36	1.43
14	AD	1004	LMT	O3'-C3'	-2.69	1.36	1.43
14	BR	1006	LMT	O3'-C3'	-2.68	1.36	1.43
14	BC	102	LMT	O3'-C3'	-2.68	1.36	1.43
14	BL	1003	LMT	O3'-C3'	-2.68	1.36	1.43
14	bk	101	LMT	O3'-C3'	-2.68	1.36	1.43
14	L	307	LMT	O3'-C3'	-2.68	1.36	1.43
14	BP	1006	LMT	O3'-C3'	-2.68	1.36	1.43
14	BK	1005	LMT	O3'-C3'	-2.67	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AW	102	LMT	O3'-C3'	-2.67	1.36	1.43
14	bf	101	LMT	O3'-C3'	-2.67	1.36	1.43
14	AJ	103	LMT	O3'-C3'	-2.66	1.36	1.43
14	bj	102	LMT	O3'-C3'	-2.66	1.36	1.43
14	ac	101	LMT	O3'-C3'	-2.66	1.36	1.43
14	AU	101	LMT	O3'-C3'	-2.66	1.36	1.43
14	BL	1002	LMT	O2'-C2'	-2.66	1.36	1.43
14	BR	1005	LMT	O3'-C3'	-2.66	1.36	1.43
14	AB	102	LMT	O3'-C3'	-2.65	1.36	1.43
14	bo	103	LMT	O3'-C3'	-2.65	1.36	1.43
14	bg	103	LMT	O3'-C3'	-2.65	1.36	1.43
14	BD	103	LMT	O3'-C3'	-2.65	1.36	1.43
14	bf	104	LMT	O3'-C3'	-2.65	1.36	1.43
14	BP	1002	LMT	O3'-C3'	-2.64	1.36	1.43
14	BF	101	LMT	O3'-C3'	-2.64	1.36	1.43
14	BO	1002	LMT	O3'-C3'	-2.64	1.36	1.43
14	AI	101	LMT	O3'-C3'	-2.64	1.36	1.43
14	BG	1003	LMT	O3'-C3'	-2.64	1.36	1.43
14	bn	102	LMT	O3'-C3'	-2.64	1.36	1.43
14	AS	103	LMT	O3'-C3'	-2.64	1.36	1.43
14	BF	103	LMT	O3'-C3'	-2.64	1.36	1.43
14	BT	1002	LMT	O3'-C3'	-2.63	1.36	1.43
14	BX	1002	LMT	O3'-C3'	-2.63	1.36	1.43
14	BH	1005	LMT	O3'-C3'	-2.63	1.36	1.43
14	BI	105	LMT	O3'-C3'	-2.63	1.36	1.43
14	BR	1002	LMT	O3'-C3'	-2.63	1.36	1.43
14	BH	1004	LMT	O3'-C3'	-2.63	1.36	1.43
14	bb	102	LMT	O3'-C3'	-2.63	1.36	1.43
14	bd	102	LMT	O3'-C3'	-2.63	1.36	1.43
14	BK	1002	LMT	O3'-C3'	-2.63	1.36	1.43
14	BD	102	LMT	O3'-C3'	-2.63	1.36	1.43
14	BE	106	LMT	O3'-C3'	-2.63	1.36	1.43
14	AG	101	LMT	O3'-C3'	-2.63	1.36	1.43
14	BU	1003	LMT	O3'-C3'	-2.62	1.36	1.43
14	BH	1002	LMT	O3'-C3'	-2.62	1.36	1.43
14	BN	1002	LMT	O3'-C3'	-2.62	1.36	1.43
14	BO	1003	LMT	O3'-C3'	-2.62	1.36	1.43
14	BW	1002	LMT	O3'-C3'	-2.62	1.36	1.43
14	L	306	LMT	O3'-C3'	-2.61	1.36	1.43
14	bh	101	LMT	O3'-C3'	-2.61	1.36	1.43
14	BG	1002	LMT	O3'-C3'	-2.61	1.36	1.43
14	L	305	LMT	O3'-C3'	-2.60	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AU	101	LMT	O2'-C2'	-2.60	1.36	1.43
14	BI	101	LMT	O3'-C3'	-2.60	1.36	1.43
14	BU	1002	LMT	O3'-C3'	-2.60	1.36	1.43
14	BJ	1003	LMT	O3'-C3'	-2.60	1.36	1.43
15	bk	103	V7N	C11-C12	2.60	1.41	1.34
14	BM	1002	LMT	O3'-C3'	-2.60	1.36	1.43
14	AD	1003	LMT	O3'-C3'	-2.60	1.36	1.43
14	AL	102	LMT	O3'-C3'	-2.60	1.36	1.43
14	BP	1003	LMT	O3'-C3'	-2.59	1.36	1.43
14	AP	102	LMT	O3'-C3'	-2.59	1.36	1.43
14	BT	1005	LMT	O3'-C3'	-2.59	1.36	1.43
14	BW	1004	LMT	O3'-C3'	-2.59	1.36	1.43
14	AH	104	LMT	O3'-C3'	-2.59	1.36	1.43
14	BN	1005	LMT	O3'-C3'	-2.59	1.36	1.43
14	BA	103	LMT	O3'-C3'	-2.59	1.36	1.43
14	BA	105	LMT	O3'-C3'	-2.59	1.36	1.43
14	BI	103	LMT	O3'-C3'	-2.59	1.36	1.43
14	bc	101	LMT	O3'-C3'	-2.58	1.36	1.43
14	L	302	LMT	O3'-C3'	-2.58	1.36	1.43
14	BA	102	LMT	O3'-C3'	-2.58	1.36	1.43
14	bl	104	LMT	O3'-C3'	-2.58	1.36	1.43
14	BS	1002	LMT	O3'-C3'	-2.58	1.36	1.43
14	BD	104	LMT	O3'-C3'	-2.58	1.36	1.43
14	BQ	1004	LMT	O3'-C3'	-2.58	1.36	1.43
14	BB	102	LMT	O3'-C3'	-2.58	1.36	1.43
14	AB	104	LMT	O3'-C3'	-2.58	1.36	1.43
14	bh	103	LMT	O3'-C3'	-2.58	1.36	1.43
15	AT	103	V7N	C11-C12	2.58	1.41	1.34
14	AH	103	LMT	O3'-C3'	-2.58	1.36	1.43
14	BT	1003	LMT	O3'-C3'	-2.58	1.36	1.43
14	AV	101	LMT	O3'-C3'	-2.57	1.36	1.43
14	BS	1003	LMT	O3'-C3'	-2.57	1.36	1.43
14	BE	103	LMT	O3'-C3'	-2.57	1.36	1.43
14	BI	102	LMT	O3'-C3'	-2.57	1.36	1.43
14	BL	1005	LMT	O3'-C3'	-2.57	1.36	1.43
22	M	406	BPH	C1B-C2B	-2.57	1.40	1.45
14	bm	104	LMT	O3'-C3'	-2.57	1.36	1.43
14	BP	1005	LMT	O3'-C3'	-2.57	1.36	1.43
14	AN	103	LMT	O3'-C3'	-2.57	1.36	1.43
14	L	304	LMT	O3'-C3'	-2.56	1.36	1.43
14	BU	1001	LMT	O3'-C3'	-2.56	1.36	1.43
14	BS	1004	LMT	O3'-C3'	-2.56	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	AR	102	LMT	O3'-C3'	-2.55	1.37	1.43
14	AN	101	LMT	O3'-C3'	-2.55	1.37	1.43
14	AO	103	LMT	O3'-C3'	-2.55	1.37	1.43
14	AA	1003	LMT	O3'-C3'	-2.55	1.37	1.43
14	BV	1002	LMT	O3'-C3'	-2.55	1.37	1.43
14	AF	1003	LMT	O3'-C3'	-2.55	1.37	1.43
14	BQ	1002	LMT	O3'-C3'	-2.54	1.37	1.43
14	BX	1003	LMT	O3'-C3'	-2.54	1.37	1.43
14	BM	1003	LMT	O3'-C3'	-2.54	1.37	1.43
13	AM	101	BCL	O1A-CGA	-2.53	1.15	1.22
14	BE	105	LMT	O3'-C3'	-2.53	1.37	1.43
14	BK	1004	LMT	O3'-C3'	-2.53	1.37	1.43
14	BK	1006	LMT	O3'-C3'	-2.53	1.37	1.43
27	ai	101	UYH	C6-C5	2.52	1.60	1.51
15	bn	101	V7N	C11-C12	2.52	1.41	1.34
14	BV	1003	LMT	O3'-C3'	-2.51	1.37	1.43
14	AT	101	LMT	O3'-C3'	-2.51	1.37	1.43
14	BB	103	LMT	O3'-C3'	-2.50	1.37	1.43
14	BC	104	LMT	O3'-C3'	-2.50	1.37	1.43
14	AH	106	LMT	O3'-C3'	-2.50	1.37	1.43
14	BN	1003	LMT	O3'-C3'	-2.50	1.37	1.43
26	af	101	V7B	O8-C28	2.49	1.40	1.33
14	BJ	1002	LMT	O3'-C3'	-2.48	1.37	1.43
14	BN	1004	LMT	O3'-C3'	-2.48	1.37	1.43
14	BW	1006	LMT	O3'-C3'	-2.48	1.37	1.43
14	AN	101	LMT	O2'-C2'	-2.47	1.37	1.43
14	BF	102	LMT	O3'-C3'	-2.47	1.37	1.43
14	bp	101	LMT	O3'-C3'	-2.46	1.37	1.43
26	ag	1002	V7B	O7-C8	-2.46	1.40	1.46
15	bb	101	V7N	C11-C12	2.45	1.40	1.34
15	bp	102	V7N	C11-C12	2.45	1.40	1.34
14	BL	1003	LMT	O2'-C2'	-2.45	1.37	1.43
14	BR	1004	LMT	O3'-C3'	-2.45	1.37	1.43
14	AH	103	LMT	O2'-C2'	-2.44	1.37	1.43
15	BM	1001	V7N	C12-C13	-2.44	1.40	1.45
15	bo	101	V7N	C11-C12	2.43	1.40	1.34
26	af	101	V7B	O7-C8	-2.43	1.40	1.46
14	bb	102	LMT	O2'-C2'	-2.42	1.37	1.43
14	BR	1005	LMT	O2'-C2'	-2.42	1.37	1.43
14	AH	106	LMT	O2'-C2'	-2.42	1.37	1.43
14	BL	1002	LMT	O3'-C3'	-2.41	1.37	1.43
15	BE	101	V7N	C11-C12	2.41	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bl	101	LMT	O3'-C3'	-2.40	1.37	1.43
15	BA	101	V7N	C12-C13	-2.40	1.40	1.45
14	AK	101	LMT	O2'-C2'	-2.40	1.37	1.43
15	bk	103	V7N	C7-C8	2.40	1.40	1.34
14	BP	1002	LMT	O2'-C2'	-2.40	1.37	1.43
14	bk	101	LMT	O2'-C2'	-2.39	1.37	1.43
14	bl	104	LMT	O2'-C2'	-2.39	1.37	1.43
22	L	301	BPH	C1B-C2B	-2.39	1.40	1.45
14	BP	1003	LMT	O2'-C2'	-2.39	1.37	1.43
14	BK	1002	LMT	O2'-C2'	-2.39	1.37	1.43
14	bp	101	LMT	O3B-C3B	-2.39	1.37	1.43
14	AF	1003	LMT	O2'-C2'	-2.39	1.37	1.43
15	bb	101	V7N	C7-C8	2.38	1.40	1.34
15	ba	101	V7N	C11-C12	2.38	1.40	1.34
13	AO	101	BCL	C4B-NB	2.38	1.37	1.35
14	BW	1002	LMT	O2'-C2'	-2.38	1.37	1.43
15	bc	104	V7N	C11-C12	2.38	1.40	1.34
15	bn	101	V7N	C7-C8	2.38	1.40	1.34
14	AB	102	LMT	O2'-C2'	-2.38	1.37	1.43
14	BH	1005	LMT	O2'-C2'	-2.38	1.37	1.43
14	AD	1004	LMT	O3B-C3B	-2.38	1.37	1.43
14	AR	102	LMT	O3B-C3B	-2.38	1.37	1.43
14	bd	102	LMT	O2'-C2'	-2.38	1.37	1.43
15	BJ	1001	V7N	C12-C13	-2.37	1.40	1.45
15	bh	102	V7N	C11-C12	2.37	1.40	1.34
15	be	101	V7N	C12-C13	-2.37	1.40	1.45
14	bg	103	LMT	O2'-C2'	-2.37	1.37	1.43
14	BN	1002	LMT	O2'-C2'	-2.37	1.37	1.43
14	BF	103	LMT	O2'-C2'	-2.37	1.37	1.43
14	BT	1002	LMT	O2'-C2'	-2.36	1.37	1.43
15	bf	102	V7N	C11-C12	2.36	1.40	1.34
14	AL	102	LMT	O2'-C2'	-2.36	1.37	1.43
15	bi	101	V7N	C11-C12	2.36	1.40	1.34
15	bg	101	V7N	C11-C12	2.36	1.40	1.34
15	ba	101	V7N	C7-C8	2.36	1.40	1.34
14	AI	101	LMT	O2'-C2'	-2.36	1.37	1.43
14	BD	105	LMT	O2'-C2'	-2.36	1.37	1.43
14	BL	1003	LMT	O3B-C3B	-2.35	1.37	1.43
14	bl	101	LMT	O2'-C2'	-2.35	1.37	1.43
14	BN	1005	LMT	O2'-C2'	-2.35	1.37	1.43
15	BG	1001	V7N	C11-C12	2.35	1.40	1.34
14	BE	102	LMT	O2'-C2'	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BX	1002	LMT	O2'-C2'	-2.35	1.37	1.43
14	bj	102	LMT	O2'-C2'	-2.35	1.37	1.43
14	BS	1004	LMT	O2'-C2'	-2.35	1.37	1.43
14	BU	1002	LMT	O2'-C2'	-2.35	1.37	1.43
14	BI	105	LMT	O2'-C2'	-2.35	1.37	1.43
14	AN	103	LMT	O2B-C2B	-2.35	1.37	1.43
15	BL	1001	V7N	C11-C12	2.35	1.40	1.34
14	ac	101	LMT	O2'-C2'	-2.35	1.37	1.43
14	AT	101	LMT	O2'-C2'	-2.35	1.37	1.43
15	BO	1001	V7N	C11-C12	2.34	1.40	1.34
14	AW	102	LMT	O3B-C3B	-2.34	1.37	1.43
15	bd	101	V7N	C11-C12	2.34	1.40	1.34
14	BT	1003	LMT	O2'-C2'	-2.34	1.37	1.43
14	bh	101	LMT	O2'-C2'	-2.34	1.37	1.43
14	BA	105	LMT	O2'-C2'	-2.34	1.37	1.43
14	bc	101	LMT	O3B-C3B	-2.34	1.37	1.43
14	bo	103	LMT	O2'-C2'	-2.34	1.37	1.43
14	bf	104	LMT	O2B-C2B	-2.34	1.37	1.43
14	BV	1002	LMT	O2'-C2'	-2.34	1.37	1.43
14	ac	101	LMT	O3B-C3B	-2.34	1.37	1.43
14	bn	102	LMT	O3B-C3B	-2.34	1.37	1.43
14	BU	1002	LMT	O3B-C3B	-2.34	1.37	1.43
18	C	1006	V75	O2-C2A	2.34	1.40	1.35
14	AV	101	LMT	O2B-C2B	-2.33	1.37	1.43
14	BS	1002	LMT	O3B-C3B	-2.33	1.37	1.43
14	AH	103	LMT	O2B-C2B	-2.33	1.37	1.43
14	BP	1005	LMT	O2'-C2'	-2.33	1.37	1.43
14	AG	101	LMT	O2B-C2B	-2.33	1.37	1.43
15	AH	105	V7N	C11-C12	2.33	1.40	1.34
15	BD	101	V7N	C11-C12	2.33	1.40	1.34
15	BV	1001	V7N	C11-C12	2.33	1.40	1.34
14	BD	103	LMT	O2'-C2'	-2.33	1.37	1.43
14	AN	103	LMT	O3B-C3B	-2.33	1.37	1.43
14	BO	1002	LMT	O3B-C3B	-2.33	1.37	1.43
14	AN	101	LMT	O3B-C3B	-2.33	1.37	1.43
14	AN	101	LMT	O2B-C2B	-2.33	1.37	1.43
14	bc	101	LMT	O2'-C2'	-2.33	1.37	1.43
15	BS	1001	V7N	C12-C13	-2.33	1.40	1.45
14	AR	102	LMT	O2B-C2B	-2.32	1.37	1.43
14	BK	1005	LMT	O3B-C3B	-2.32	1.37	1.43
14	BT	1002	LMT	O3B-C3B	-2.32	1.37	1.43
14	BE	106	LMT	O3B-C3B	-2.32	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BX	1001	V7N	C11-C12	2.32	1.40	1.34
15	bj	101	V7N	C11-C12	2.32	1.40	1.34
14	bk	101	LMT	O3B-C3B	-2.32	1.37	1.43
15	BA	101	V7N	C8-C9	-2.32	1.40	1.45
14	BI	101	LMT	O3B-C3B	-2.32	1.37	1.43
14	BW	1004	LMT	O2'-C2'	-2.32	1.37	1.43
14	bm	104	LMT	O2'-C2'	-2.32	1.37	1.43
14	AG	101	LMT	O3B-C3B	-2.32	1.37	1.43
15	BH	1001	V7N	C11-C12	2.32	1.40	1.34
15	BS	1001	V7N	C8-C9	-2.32	1.40	1.45
14	BA	102	LMT	O2'-C2'	-2.32	1.37	1.43
14	BK	1005	LMT	O2'-C2'	-2.32	1.37	1.43
14	AV	101	LMT	O2'-C2'	-2.31	1.37	1.43
14	BH	1002	LMT	O2'-C2'	-2.31	1.37	1.43
14	BX	1003	LMT	O3B-C3B	-2.31	1.37	1.43
14	BQ	1002	LMT	O2B-C2B	-2.31	1.37	1.43
14	bf	104	LMT	O2'-C2'	-2.31	1.37	1.43
15	bm	101	V7N	C11-C12	2.31	1.40	1.34
15	bl	102	V7N	C11-C12	2.31	1.40	1.34
14	AH	106	LMT	O3B-C3B	-2.31	1.37	1.43
14	AV	101	LMT	O3B-C3B	-2.31	1.37	1.43
14	BD	103	LMT	O3B-C3B	-2.31	1.37	1.43
15	BP	1001	V7N	C12-C13	-2.31	1.41	1.45
14	BC	102	LMT	O3B-C3B	-2.31	1.37	1.43
14	BW	1002	LMT	O3B-C3B	-2.31	1.37	1.43
14	BN	1005	LMT	O3B-C3B	-2.31	1.37	1.43
14	BD	102	LMT	O3B-C3B	-2.31	1.37	1.43
15	BN	1001	V7N	C12-C13	-2.31	1.41	1.45
15	be	101	V7N	C8-C9	-2.31	1.40	1.45
15	bg	101	V7N	C7-C8	2.31	1.40	1.34
14	BG	1002	LMT	O2'-C2'	-2.30	1.37	1.43
27	ai	101	UYH	C12-C11	2.30	1.60	1.52
14	BC	102	LMT	O2'-C2'	-2.30	1.37	1.43
14	BA	106	LMT	O3B-C3B	-2.30	1.37	1.43
14	bd	102	LMT	O3B-C3B	-2.30	1.37	1.43
26	ag	1002	V7B	O8-C9	-2.30	1.39	1.45
14	BA	105	LMT	O3B-C3B	-2.30	1.37	1.43
14	BA	106	LMT	O2'-C2'	-2.30	1.37	1.43
14	BX	1002	LMT	O3B-C3B	-2.30	1.37	1.43
14	AB	104	LMT	O2'-C2'	-2.30	1.37	1.43
14	BI	102	LMT	O3B-C3B	-2.30	1.37	1.43
14	L	302	LMT	O2'-C2'	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	307	LMT	O2'-C2'	-2.30	1.37	1.43
15	BR	1001	V7N	C11-C12	2.30	1.40	1.34
14	L	304	LMT	O2'-C2'	-2.30	1.37	1.43
14	L	305	LMT	O2'-C2'	-2.30	1.37	1.43
14	AF	1003	LMT	O3B-C3B	-2.30	1.37	1.43
15	BJ	1001	V7N	C8-C9	-2.30	1.40	1.45
14	ac	101	LMT	O2B-C2B	-2.30	1.37	1.43
14	BR	1002	LMT	O3B-C3B	-2.30	1.37	1.43
14	bh	101	LMT	O3B-C3B	-2.30	1.37	1.43
14	BB	103	LMT	O2'-C2'	-2.30	1.37	1.43
14	bf	101	LMT	O2B-C2B	-2.30	1.37	1.43
14	BD	103	LMT	O2B-C2B	-2.30	1.37	1.43
15	BB	101	V7N	C12-C13	-2.30	1.41	1.45
15	BT	1001	V7N	C11-C12	2.30	1.40	1.34
14	AD	1003	LMT	O2'-C2'	-2.29	1.37	1.43
14	AH	106	LMT	O2B-C2B	-2.29	1.37	1.43
14	AP	102	LMT	O2'-C2'	-2.29	1.37	1.43
15	bp	102	V7N	C7-C8	2.29	1.40	1.34
14	BI	101	LMT	O2'-C2'	-2.29	1.37	1.43
15	be	101	V7N	C11-C12	2.29	1.40	1.34
14	BU	1003	LMT	O3B-C3B	-2.29	1.37	1.43
14	AJ	103	LMT	O3B-C3B	-2.29	1.37	1.43
14	AS	103	LMT	O2'-C2'	-2.29	1.37	1.43
14	BE	106	LMT	O2'-C2'	-2.29	1.37	1.43
14	BA	102	LMT	O3B-C3B	-2.29	1.37	1.43
14	BQ	1004	LMT	O3B-C3B	-2.29	1.37	1.43
14	bf	104	LMT	O3B-C3B	-2.29	1.37	1.43
15	bo	101	V7N	C7-C8	2.29	1.40	1.34
14	BD	105	LMT	O3B-C3B	-2.29	1.37	1.43
14	BT	1005	LMT	O3B-C3B	-2.29	1.37	1.43
14	AO	103	LMT	O3B-C3B	-2.29	1.37	1.43
14	AP	102	LMT	O3B-C3B	-2.29	1.37	1.43
14	BR	1004	LMT	O3B-C3B	-2.29	1.37	1.43
14	L	305	LMT	O2B-C2B	-2.29	1.37	1.43
14	bn	102	LMT	O2B-C2B	-2.29	1.37	1.43
15	BK	1001	V7N	C11-C12	2.29	1.40	1.34
14	BP	1003	LMT	O3B-C3B	-2.29	1.37	1.43
14	BR	1002	LMT	O2'-C2'	-2.28	1.37	1.43
14	BX	1003	LMT	O2B-C2B	-2.28	1.37	1.43
14	AJ	103	LMT	O2'-C2'	-2.28	1.37	1.43
14	L	304	LMT	O3B-C3B	-2.28	1.37	1.43
14	bh	103	LMT	O3B-C3B	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bf	101	LMT	O3B-C3B	-2.28	1.37	1.43
15	AE	1003	V7N	C11-C12	2.28	1.40	1.34
15	BC	101	V7N	C11-C12	2.28	1.40	1.34
14	BP	1002	LMT	O3B-C3B	-2.28	1.37	1.43
14	L	306	LMT	O2B-C2B	-2.28	1.37	1.43
14	BW	1004	LMT	O3B-C3B	-2.28	1.37	1.43
14	AH	104	LMT	O3B-C3B	-2.28	1.37	1.43
14	AB	102	LMT	O3B-C3B	-2.28	1.37	1.43
14	bb	102	LMT	O3B-C3B	-2.28	1.37	1.43
14	BC	104	LMT	O2'-C2'	-2.28	1.37	1.43
26	ag	1002	V7B	O6-C5	-2.28	1.38	1.44
14	BI	105	LMT	O3B-C3B	-2.28	1.37	1.43
14	BP	1006	LMT	O2'-C2'	-2.28	1.37	1.43
14	BK	1002	LMT	O3B-C3B	-2.28	1.37	1.43
14	M	402	LMT	O2'-C2'	-2.28	1.37	1.43
14	bm	104	LMT	O3B-C3B	-2.28	1.37	1.43
14	L	302	LMT	O3B-C3B	-2.27	1.37	1.43
26	af	101	V7B	O7-C10	2.27	1.40	1.34
15	BW	1001	V7N	C12-C13	-2.27	1.41	1.45
14	AA	1003	LMT	O2B-C2B	-2.27	1.37	1.43
14	AD	1004	LMT	O2B-C2B	-2.27	1.37	1.43
14	BE	106	LMT	O2B-C2B	-2.27	1.37	1.43
15	BQ	1001	V7N	C11-C12	2.27	1.40	1.34
14	AS	103	LMT	O3B-C3B	-2.27	1.37	1.43
14	BI	101	LMT	O2B-C2B	-2.27	1.37	1.43
14	BH	1005	LMT	O3B-C3B	-2.27	1.37	1.43
15	bi	101	V7N	C7-C8	2.27	1.40	1.34
14	AO	103	LMT	O2'-C2'	-2.27	1.37	1.43
14	AH	104	LMT	O2'-C2'	-2.27	1.37	1.43
14	BD	102	LMT	O2B-C2B	-2.27	1.37	1.43
14	bn	102	LMT	O2'-C2'	-2.27	1.37	1.43
14	BL	1002	LMT	O3B-C3B	-2.27	1.37	1.43
14	BM	1003	LMT	O2'-C2'	-2.27	1.37	1.43
14	BN	1003	LMT	O2B-C2B	-2.27	1.37	1.43
14	BW	1006	LMT	O3B-C3B	-2.27	1.37	1.43
14	AI	101	LMT	O2B-C2B	-2.27	1.37	1.43
14	BS	1003	LMT	O3B-C3B	-2.27	1.37	1.43
14	AB	104	LMT	O2B-C2B	-2.27	1.37	1.43
14	AI	101	LMT	O3B-C3B	-2.27	1.37	1.43
14	BN	1002	LMT	O3B-C3B	-2.27	1.37	1.43
14	AB	102	LMT	O2B-C2B	-2.27	1.37	1.43
14	AT	101	LMT	O2B-C2B	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BN	1003	LMT	O3B-C3B	-2.27	1.37	1.43
14	bo	103	LMT	O3B-C3B	-2.27	1.37	1.43
14	BP	1005	LMT	O3B-C3B	-2.27	1.37	1.43
14	BU	1001	LMT	O3B-C3B	-2.27	1.37	1.43
15	BW	1001	V7N	C8-C9	-2.26	1.41	1.45
14	AU	101	LMT	O2B-C2B	-2.26	1.37	1.43
14	AU	101	LMT	O3B-C3B	-2.26	1.37	1.43
14	bl	101	LMT	O3B-C3B	-2.26	1.37	1.43
15	BB	101	V7N	C11-C12	2.26	1.40	1.34
14	BD	104	LMT	O3B-C3B	-2.26	1.37	1.43
14	BA	105	LMT	O2B-C2B	-2.26	1.37	1.43
14	BE	103	LMT	O3B-C3B	-2.26	1.37	1.43
15	BQ	1001	V7N	C12-C13	-2.26	1.41	1.45
14	BS	1002	LMT	O2'-C2'	-2.26	1.37	1.43
14	bl	104	LMT	O2B-C2B	-2.26	1.37	1.43
14	bp	101	LMT	O2'-C2'	-2.26	1.37	1.43
15	BL	1001	V7N	C8-C9	-2.26	1.41	1.45
14	BD	104	LMT	O2'-C2'	-2.26	1.37	1.43
14	BV	1002	LMT	O2B-C2B	-2.26	1.37	1.43
14	bh	101	LMT	O2B-C2B	-2.26	1.37	1.43
14	AS	103	LMT	O2B-C2B	-2.26	1.37	1.43
14	BF	103	LMT	O3B-C3B	-2.26	1.37	1.43
14	BP	1006	LMT	O2B-C2B	-2.26	1.37	1.43
14	BR	1006	LMT	O3B-C3B	-2.26	1.37	1.43
14	BW	1006	LMT	O2'-C2'	-2.26	1.37	1.43
14	BX	1002	LMT	O2B-C2B	-2.26	1.37	1.43
14	bg	103	LMT	O3B-C3B	-2.26	1.37	1.43
14	bg	103	LMT	O2B-C2B	-2.26	1.37	1.43
14	BH	1004	LMT	O3B-C3B	-2.26	1.37	1.43
14	BJ	1002	LMT	O2B-C2B	-2.26	1.37	1.43
14	L	307	LMT	O3B-C3B	-2.26	1.37	1.43
14	bc	101	LMT	O2B-C2B	-2.26	1.37	1.43
14	AP	102	LMT	O2B-C2B	-2.26	1.37	1.43
15	BP	1001	V7N	C8-C9	-2.26	1.41	1.45
14	BE	105	LMT	O2'-C2'	-2.26	1.37	1.43
14	BH	1005	LMT	O2B-C2B	-2.26	1.37	1.43
14	L	306	LMT	O3B-C3B	-2.26	1.37	1.43
14	bh	103	LMT	O2B-C2B	-2.26	1.37	1.43
14	BQ	1002	LMT	O2'-C2'	-2.25	1.37	1.43
14	AA	1003	LMT	O3B-C3B	-2.25	1.37	1.43
14	BC	104	LMT	O3B-C3B	-2.25	1.37	1.43
14	BR	1005	LMT	O3B-C3B	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bd	101	V7N	C8-C9	-2.25	1.41	1.45
14	BA	103	LMT	O2'-C2'	-2.25	1.37	1.43
14	bm	104	LMT	O2B-C2B	-2.25	1.37	1.43
14	AT	101	LMT	O3B-C3B	-2.25	1.37	1.43
14	BP	1006	LMT	O3B-C3B	-2.25	1.37	1.43
14	BW	1005	LMT	O3B-C3B	-2.25	1.37	1.43
14	AH	103	LMT	O3B-C3B	-2.25	1.37	1.43
15	AT	103	V7N	C20-C19	2.25	1.40	1.34
14	M	402	LMT	O2B-C2B	-2.25	1.37	1.43
15	BD	101	V7N	C7-C8	2.25	1.40	1.34
14	BI	103	LMT	O2B-C2B	-2.25	1.37	1.43
14	BT	1005	LMT	O2B-C2B	-2.25	1.37	1.43
14	BM	1002	LMT	O3B-C3B	-2.25	1.37	1.43
14	BS	1003	LMT	O2B-C2B	-2.25	1.37	1.43
14	AK	101	LMT	O4'-C4B	-2.25	1.37	1.43
14	BN	1004	LMT	O3B-C3B	-2.25	1.37	1.43
14	M	402	LMT	O3B-C3B	-2.25	1.37	1.43
15	BC	101	V7N	C12-C13	-2.25	1.41	1.45
14	BF	101	LMT	O3B-C3B	-2.25	1.37	1.43
14	AK	101	LMT	O3B-C3B	-2.25	1.37	1.43
14	BL	1003	LMT	O2B-C2B	-2.25	1.37	1.43
14	BE	102	LMT	O3B-C3B	-2.25	1.37	1.43
14	BH	1002	LMT	O3B-C3B	-2.24	1.37	1.43
14	BF	102	LMT	O3B-C3B	-2.24	1.37	1.43
14	AB	104	LMT	O3B-C3B	-2.24	1.37	1.43
14	BK	1005	LMT	O2B-C2B	-2.24	1.37	1.43
14	BJ	1003	LMT	O3B-C3B	-2.24	1.37	1.43
14	bl	104	LMT	O3B-C3B	-2.24	1.37	1.43
14	bh	103	LMT	O2'-C2'	-2.24	1.37	1.43
13	AC	1002	BCL	OBD-CAD	2.24	1.25	1.22
15	bl	102	V7N	C7-C8	2.24	1.40	1.34
13	AI	102	BCL	C4B-NB	2.24	1.37	1.35
15	BC	101	V7N	C8-C9	-2.24	1.41	1.45
15	BD	101	V7N	C12-C13	-2.24	1.41	1.45
14	AD	1003	LMT	O3B-C3B	-2.24	1.37	1.43
14	BV	1002	LMT	O3B-C3B	-2.24	1.37	1.43
14	BC	104	LMT	O2B-C2B	-2.24	1.37	1.43
14	BA	103	LMT	O3B-C3B	-2.24	1.37	1.43
14	AR	102	LMT	O2'-C2'	-2.24	1.37	1.43
14	BI	103	LMT	O3B-C3B	-2.24	1.37	1.43
14	bd	102	LMT	O2B-C2B	-2.24	1.37	1.43
14	BG	1003	LMT	O2'-C2'	-2.24	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BK	1004	LMT	O2'-C2'	-2.24	1.37	1.43
14	BM	1002	LMT	O2B-C2B	-2.24	1.37	1.43
14	BP	1002	LMT	O2B-C2B	-2.24	1.37	1.43
14	BW	1005	LMT	O2'-C2'	-2.24	1.37	1.43
14	BG	1003	LMT	O3B-C3B	-2.24	1.37	1.43
14	BR	1006	LMT	O2B-C2B	-2.24	1.37	1.43
14	AO	103	LMT	O2B-C2B	-2.24	1.37	1.43
14	BE	102	LMT	O2B-C2B	-2.23	1.37	1.43
14	L	302	LMT	O2B-C2B	-2.23	1.37	1.43
18	M	409	V75	O5-C1	-2.23	1.40	1.43
14	BS	1004	LMT	O2B-C2B	-2.23	1.37	1.43
14	BL	1005	LMT	O2B-C2B	-2.23	1.37	1.43
14	BB	103	LMT	O3B-C3B	-2.23	1.37	1.43
14	BG	1003	LMT	O2B-C2B	-2.23	1.37	1.43
13	AQ	103	BCL	OBD-CAD	2.23	1.25	1.22
14	BU	1001	LMT	O2B-C2B	-2.23	1.37	1.43
14	BV	1003	LMT	O2'-C2'	-2.23	1.37	1.43
14	BO	1003	LMT	O3B-C3B	-2.23	1.37	1.43
15	BW	1001	V7N	C11-C12	2.23	1.40	1.34
14	BK	1006	LMT	O2'-C2'	-2.23	1.37	1.43
14	BU	1003	LMT	O2B-C2B	-2.23	1.37	1.43
14	AH	104	LMT	O2B-C2B	-2.23	1.37	1.43
14	BG	1002	LMT	O3B-C3B	-2.23	1.37	1.43
14	BS	1002	LMT	O2B-C2B	-2.23	1.37	1.43
15	bc	104	V7N	C7-C8	2.23	1.40	1.34
14	AL	102	LMT	O3B-C3B	-2.23	1.37	1.43
14	BI	103	LMT	O2'-C2'	-2.23	1.37	1.43
14	BM	1003	LMT	O2B-C2B	-2.23	1.37	1.43
14	BK	1006	LMT	O2B-C2B	-2.23	1.37	1.43
14	BK	1002	LMT	O2B-C2B	-2.23	1.37	1.43
15	bm	101	V7N	C12-C13	-2.23	1.41	1.45
15	BL	1001	V7N	C12-C13	-2.23	1.41	1.45
15	bf	102	V7N	C7-C8	2.22	1.40	1.34
14	BN	1004	LMT	O2B-C2B	-2.22	1.37	1.43
14	AF	1003	LMT	O2B-C2B	-2.22	1.37	1.43
14	BR	1004	LMT	O2'-C2'	-2.22	1.37	1.43
14	BT	1005	LMT	O2'-C2'	-2.22	1.37	1.43
14	BX	1003	LMT	O2'-C2'	-2.22	1.37	1.43
14	bj	102	LMT	O3B-C3B	-2.22	1.37	1.43
14	BN	1005	LMT	O2B-C2B	-2.22	1.37	1.43
14	BJ	1002	LMT	O2'-C2'	-2.22	1.37	1.43
14	BK	1004	LMT	O3B-C3B	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AL	103	BCL	C4B-NB	2.22	1.37	1.35
14	L	305	LMT	O3B-C3B	-2.22	1.37	1.43
14	BE	105	LMT	O3B-C3B	-2.22	1.37	1.43
14	BN	1004	LMT	O2'-C2'	-2.22	1.37	1.43
15	BT	1001	V7N	C12-C13	-2.22	1.41	1.45
14	BB	102	LMT	O2'-C2'	-2.22	1.37	1.43
14	L	306	LMT	O2'-C2'	-2.22	1.37	1.43
14	BB	102	LMT	O3B-C3B	-2.22	1.37	1.43
14	BW	1004	LMT	O2B-C2B	-2.22	1.37	1.43
27	ai	101	UYH	C30-C29	2.22	1.60	1.52
14	BF	102	LMT	O2B-C2B	-2.22	1.37	1.43
14	BI	102	LMT	O2B-C2B	-2.22	1.37	1.43
18	C	1006	V75	O3-C3A	2.22	1.40	1.35
15	bk	103	V7N	C20-C19	2.22	1.40	1.34
14	bj	102	LMT	O2B-C2B	-2.22	1.37	1.43
14	AD	1004	LMT	O2'-C2'	-2.21	1.37	1.43
14	BE	103	LMT	O2B-C2B	-2.21	1.37	1.43
15	BA	101	V7N	C11-C12	2.21	1.40	1.34
26	ag	1002	V7B	O8-C28	2.21	1.39	1.33
15	BK	1001	V7N	C12-C13	-2.21	1.41	1.45
14	BH	1004	LMT	O2B-C2B	-2.21	1.37	1.43
15	BX	1001	V7N	C12-C13	-2.21	1.41	1.45
15	BO	1001	V7N	C12-C13	-2.21	1.41	1.45
14	BG	1002	LMT	O2B-C2B	-2.21	1.37	1.43
14	BH	1002	LMT	O2B-C2B	-2.21	1.37	1.43
14	BH	1004	LMT	O2'-C2'	-2.21	1.37	1.43
14	BL	1005	LMT	O2'-C2'	-2.21	1.37	1.43
14	BU	1002	LMT	O2B-C2B	-2.21	1.37	1.43
14	AW	102	LMT	O2'-C2'	-2.21	1.37	1.43
14	BM	1002	LMT	O2'-C2'	-2.21	1.37	1.43
14	BS	1004	LMT	O3B-C3B	-2.21	1.37	1.43
14	BT	1002	LMT	O2B-C2B	-2.21	1.37	1.43
26	ag	1002	V7B	O7-C10	2.21	1.40	1.34
14	BS	1003	LMT	O2'-C2'	-2.21	1.37	1.43
14	BV	1003	LMT	O2B-C2B	-2.21	1.37	1.43
14	BQ	1004	LMT	O2'-C2'	-2.21	1.37	1.43
15	BS	1001	V7N	C11-C12	2.21	1.40	1.34
15	AE	1003	V7N	C8-C9	-2.21	1.41	1.45
14	BF	103	LMT	O2B-C2B	-2.20	1.37	1.43
14	BL	1005	LMT	O3B-C3B	-2.20	1.37	1.43
15	BT	1001	V7N	C8-C9	-2.20	1.41	1.45
15	BN	1001	V7N	C19-C18	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BR	1002	LMT	O2B-C2B	-2.20	1.37	1.43
14	BN	1003	LMT	O2'-C2'	-2.20	1.37	1.43
14	BV	1003	LMT	O3B-C3B	-2.20	1.37	1.43
15	bk	103	V7N	C16-C15	2.20	1.41	1.36
14	BK	1006	LMT	O3B-C3B	-2.20	1.37	1.43
15	AT	103	V7N	C7-C8	2.20	1.40	1.34
15	AE	1003	V7N	C12-C13	-2.20	1.41	1.45
13	AU	102	BCL	OBD-CAD	2.20	1.25	1.22
14	BF	101	LMT	O2B-C2B	-2.20	1.37	1.43
14	bl	101	LMT	O2B-C2B	-2.20	1.37	1.43
14	BE	103	LMT	O2'-C2'	-2.20	1.37	1.43
15	BK	1001	V7N	C8-C9	-2.20	1.41	1.45
14	BD	104	LMT	O2B-C2B	-2.20	1.37	1.43
14	BT	1003	LMT	O3B-C3B	-2.20	1.37	1.43
14	BW	1002	LMT	O2B-C2B	-2.20	1.37	1.43
14	BQ	1002	LMT	O3B-C3B	-2.20	1.37	1.43
15	bd	101	V7N	C12-C13	-2.20	1.41	1.45
14	bb	102	LMT	O2B-C2B	-2.19	1.37	1.43
18	M	409	V75	O3-C3A	2.19	1.40	1.35
14	BN	1002	LMT	O2B-C2B	-2.19	1.37	1.43
15	BM	1001	V7N	C11-C12	2.19	1.40	1.34
15	bj	101	V7N	C7-C8	2.19	1.40	1.34
15	bh	102	V7N	C7-C8	2.19	1.40	1.34
13	aa	1001	BCL	C4B-NB	2.18	1.37	1.35
14	BO	1002	LMT	O2B-C2B	-2.18	1.37	1.43
15	BN	1001	V7N	C11-C12	2.18	1.40	1.34
14	BD	105	LMT	O2B-C2B	-2.18	1.37	1.43
14	BP	1005	LMT	O2B-C2B	-2.18	1.37	1.43
14	BT	1003	LMT	O2B-C2B	-2.18	1.37	1.43
15	BP	1001	V7N	C11-C12	2.18	1.40	1.34
15	BJ	1001	V7N	C11-C12	2.18	1.40	1.34
14	AD	1003	LMT	O2B-C2B	-2.18	1.37	1.43
14	BR	1005	LMT	O4'-C4B	-2.18	1.37	1.43
14	BW	1005	LMT	O2B-C2B	-2.18	1.37	1.43
14	BW	1006	LMT	O2B-C2B	-2.18	1.37	1.43
15	BV	1001	V7N	C12-C13	-2.18	1.41	1.45
15	bf	102	V7N	C12-C13	-2.18	1.41	1.45
14	AK	101	LMT	O2B-C2B	-2.18	1.37	1.43
22	M	406	BPH	CHC-C1C	2.18	1.41	1.36
15	BE	101	V7N	C7-C8	2.18	1.40	1.34
14	BJ	1003	LMT	O2B-C2B	-2.18	1.37	1.43
15	BQ	1001	V7N	C8-C9	-2.18	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BG	1001	V7N	C7-C8	2.17	1.40	1.34
14	BJ	1003	LMT	O2'-C2'	-2.17	1.37	1.43
14	BM	1003	LMT	O3B-C3B	-2.17	1.37	1.43
15	BR	1001	V7N	C7-C8	2.17	1.40	1.34
15	AH	105	V7N	C8-C9	-2.17	1.41	1.45
15	BV	1001	V7N	C8-C9	-2.17	1.41	1.45
14	AA	1003	LMT	O2'-C2'	-2.17	1.37	1.43
15	bj	101	V7N	C8-C9	-2.17	1.41	1.45
15	BH	1001	V7N	C7-C8	2.17	1.40	1.34
13	AQ	103	BCL	C4B-NB	2.17	1.37	1.35
15	bm	101	V7N	C7-C8	2.17	1.40	1.34
14	BJ	1002	LMT	O3B-C3B	-2.17	1.37	1.43
15	bd	101	V7N	C7-C8	2.17	1.40	1.34
15	AH	105	V7N	C12-C13	-2.17	1.41	1.45
14	BR	1005	LMT	O2B-C2B	-2.17	1.37	1.43
14	bf	101	LMT	O2'-C2'	-2.17	1.37	1.43
14	BI	102	LMT	O2'-C2'	-2.17	1.37	1.43
15	BG	1001	V7N	C8-C9	-2.17	1.41	1.45
14	AJ	103	LMT	O2B-C2B	-2.17	1.37	1.43
14	BK	1004	LMT	O2B-C2B	-2.17	1.37	1.43
14	BA	102	LMT	O2B-C2B	-2.16	1.37	1.43
14	AL	102	LMT	O2B-C2B	-2.16	1.37	1.43
15	BR	1001	V7N	C12-C13	-2.16	1.41	1.45
14	BB	103	LMT	O2B-C2B	-2.16	1.37	1.43
14	BU	1003	LMT	O2'-C2'	-2.16	1.37	1.43
15	BX	1001	V7N	C8-C9	-2.16	1.41	1.45
14	BE	105	LMT	O2B-C2B	-2.16	1.37	1.43
14	BL	1002	LMT	O2B-C2B	-2.16	1.37	1.43
15	BO	1001	V7N	C8-C9	-2.16	1.41	1.45
14	AG	101	LMT	O2'-C2'	-2.16	1.37	1.43
14	BF	101	LMT	O2'-C2'	-2.16	1.37	1.43
14	bk	101	LMT	O2B-C2B	-2.16	1.37	1.43
14	BB	102	LMT	O2B-C2B	-2.16	1.37	1.43
15	BB	101	V7N	C8-C9	-2.16	1.41	1.45
15	AE	1003	V7N	C7-C8	2.16	1.40	1.34
15	BN	1001	V7N	C8-C9	-2.16	1.41	1.45
14	BO	1003	LMT	O2'-C2'	-2.15	1.37	1.43
18	M	409	V75	O2-C2A	2.15	1.40	1.35
14	BA	103	LMT	O2B-C2B	-2.15	1.37	1.43
14	BP	1003	LMT	O2B-C2B	-2.15	1.37	1.43
14	BQ	1004	LMT	O2B-C2B	-2.15	1.37	1.43
15	bp	102	V7N	C20-C19	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bf	104	LMT	O4'-C4B	-2.15	1.37	1.43
13	AO	101	BCL	OBD-CAD	2.15	1.25	1.22
15	BE	101	V7N	C12-C13	-2.15	1.41	1.45
15	BG	1001	V7N	C12-C13	-2.15	1.41	1.45
14	BF	102	LMT	O2'-C2'	-2.15	1.37	1.43
15	BH	1001	V7N	C12-C13	-2.15	1.41	1.45
15	bl	102	V7N	C12-C13	-2.15	1.41	1.45
15	AT	103	V7N	C27-C26	2.15	1.50	1.45
13	AI	103	BCL	C4B-NB	2.15	1.37	1.35
14	BA	106	LMT	O2B-C2B	-2.14	1.37	1.43
15	BV	1001	V7N	C7-C8	2.14	1.40	1.34
14	BR	1006	LMT	O2'-C2'	-2.14	1.37	1.43
13	AB	103	BCL	OBD-CAD	2.14	1.25	1.22
15	BX	1001	V7N	C7-C8	2.14	1.40	1.34
13	AI	102	BCL	OBD-CAD	2.14	1.25	1.22
14	bn	102	LMT	O4'-C4B	-2.14	1.37	1.43
13	AC	1002	BCL	C4B-NB	2.14	1.37	1.35
14	BU	1001	LMT	O2'-C2'	-2.13	1.38	1.43
13	AK	103	BCL	OBD-CAD	2.13	1.25	1.22
14	BI	105	LMT	O4'-C4B	-2.13	1.38	1.43
13	ah	1001	BCL	C4B-NB	2.13	1.37	1.35
14	BI	105	LMT	O2B-C2B	-2.13	1.38	1.43
15	AT	103	V7N	C16-C15	2.13	1.41	1.36
15	BA	101	V7N	C19-C18	-2.13	1.41	1.45
14	AN	103	LMT	O2'-C2'	-2.13	1.38	1.43
14	BE	106	LMT	O4'-C4B	-2.13	1.38	1.43
15	bp	102	V7N	C16-C15	2.13	1.41	1.36
15	bh	102	V7N	C8-C9	-2.13	1.41	1.45
14	BD	102	LMT	O2'-C2'	-2.12	1.38	1.43
14	BO	1002	LMT	O2'-C2'	-2.12	1.38	1.43
14	L	307	LMT	O2B-C2B	-2.12	1.38	1.43
14	L	304	LMT	O2B-C2B	-2.12	1.38	1.43
15	BB	101	V7N	C19-C18	-2.12	1.41	1.45
14	BT	1002	LMT	O4'-C4B	-2.12	1.38	1.43
14	bp	101	LMT	O2B-C2B	-2.12	1.38	1.43
15	BM	1001	V7N	C8-C9	-2.12	1.41	1.45
15	BT	1001	V7N	C7-C8	2.12	1.40	1.34
15	bg	101	V7N	C12-C13	-2.12	1.41	1.45
14	BS	1002	LMT	O4'-C4B	-2.12	1.38	1.43
15	BE	101	V7N	C8-C9	-2.12	1.41	1.45
15	AH	105	V7N	C7-C8	2.12	1.40	1.34
13	AU	103	BCL	C4B-NB	2.12	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BH	1001	V7N	C8-C9	-2.12	1.41	1.45
14	bb	102	LMT	O4'-C4B	-2.11	1.38	1.43
14	BO	1003	LMT	O2B-C2B	-2.11	1.38	1.43
15	bj	101	V7N	C12-C13	-2.11	1.41	1.45
15	BM	1001	V7N	C19-C18	-2.11	1.41	1.45
14	AD	1003	LMT	O4'-C4B	-2.11	1.38	1.43
14	BH	1005	LMT	O4'-C4B	-2.11	1.38	1.43
14	BC	102	LMT	O2B-C2B	-2.11	1.38	1.43
14	bo	103	LMT	O2B-C2B	-2.11	1.38	1.43
13	AL	103	BCL	OBD-CAD	2.11	1.25	1.22
14	bd	102	LMT	O4'-C4B	-2.11	1.38	1.43
13	AH	101	BCL	OBD-CAD	2.11	1.25	1.22
15	bh	102	V7N	C12-C13	-2.11	1.41	1.45
15	BC	101	V7N	C7-C8	2.11	1.40	1.34
15	bb	101	V7N	C16-C15	2.10	1.41	1.36
15	BL	1001	V7N	C7-C8	2.10	1.40	1.34
15	BR	1001	V7N	C8-C9	-2.10	1.41	1.45
14	BN	1002	LMT	O4'-C4B	-2.10	1.38	1.43
15	bo	101	V7N	C16-C15	2.10	1.41	1.36
13	AF	1002	BCL	OBD-CAD	2.10	1.25	1.22
13	AW	104	BCL	OBD-CAD	2.10	1.25	1.22
14	AJ	103	LMT	O4'-C4B	-2.10	1.38	1.43
14	BR	1004	LMT	O2B-C2B	-2.10	1.38	1.43
13	af	102	BCL	C4B-NB	2.10	1.37	1.35
13	AN	102	BCL	OBD-CAD	2.10	1.25	1.22
15	BM	1001	V7N	C7-C8	2.10	1.40	1.34
15	BP	1001	V7N	C19-C18	-2.10	1.41	1.45
15	BN	1001	V7N	C7-C8	2.10	1.40	1.34
13	ab	1001	BCL	C4B-NB	2.10	1.37	1.35
15	bg	101	V7N	C8-C9	-2.09	1.41	1.45
14	BE	102	LMT	O4'-C4B	-2.09	1.38	1.43
15	bi	101	V7N	C20-C19	2.09	1.40	1.34
13	AE	1001	BCL	OBD-CAD	2.09	1.25	1.22
15	BP	1001	V7N	C7-C8	2.09	1.40	1.34
15	bc	104	V7N	C12-C13	-2.09	1.41	1.45
14	BL	1003	LMT	O4'-C4B	-2.09	1.38	1.43
14	BI	101	LMT	O4'-C4B	-2.09	1.38	1.43
15	BQ	1001	V7N	C7-C8	2.09	1.40	1.34
14	BF	102	LMT	O4'-C4B	-2.09	1.38	1.43
13	al	1001	BCL	C4B-NB	2.09	1.37	1.35
14	L	306	LMT	O4'-C4B	-2.09	1.38	1.43
15	bo	101	V7N	C20-C19	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	1006	V75	O5-C1	-2.09	1.40	1.43
13	AS	102	BCL	C4B-NB	2.09	1.37	1.35
15	BO	1001	V7N	C7-C8	2.08	1.39	1.34
14	AG	101	LMT	O4'-C4B	-2.08	1.38	1.43
14	AW	102	LMT	O4'-C4B	-2.08	1.38	1.43
15	bf	102	V7N	C8-C9	-2.08	1.41	1.45
14	BE	105	LMT	O4'-C4B	-2.08	1.38	1.43
14	BV	1003	LMT	O4'-C4B	-2.08	1.38	1.43
15	bi	101	V7N	C12-C13	-2.08	1.41	1.45
15	BB	101	V7N	C7-C8	2.08	1.39	1.34
15	ba	101	V7N	C12-C13	-2.08	1.41	1.45
14	BK	1004	LMT	O4'-C4B	-2.08	1.38	1.43
15	BK	1001	V7N	C7-C8	2.07	1.39	1.34
15	BW	1001	V7N	C19-C18	-2.07	1.41	1.45
15	bn	101	V7N	C20-C19	2.07	1.39	1.34
14	BL	1005	LMT	O4'-C4B	-2.07	1.38	1.43
14	BW	1002	LMT	O4'-C4B	-2.07	1.38	1.43
14	bl	104	LMT	O4'-C4B	-2.07	1.38	1.43
15	BS	1001	V7N	C7-C8	2.07	1.39	1.34
14	BR	1004	LMT	O4'-C4B	-2.07	1.38	1.43
13	AC	1001	BCL	C4B-NB	2.07	1.37	1.35
14	BK	1002	LMT	O4'-C4B	-2.07	1.38	1.43
14	BN	1003	LMT	O4'-C4B	-2.07	1.38	1.43
14	bh	103	LMT	O4'-C4B	-2.07	1.38	1.43
13	AR	101	BCL	C4B-NB	2.07	1.37	1.35
15	bl	102	V7N	C8-C9	-2.07	1.41	1.45
15	BJ	1001	V7N	C19-C18	-2.06	1.41	1.45
15	bf	102	V7N	C16-C15	2.06	1.41	1.36
13	ap	1001	BCL	C4B-NB	2.06	1.37	1.35
15	bp	102	V7N	C8-C9	-2.06	1.41	1.45
14	BM	1002	LMT	O4'-C4B	-2.06	1.38	1.43
13	AN	104	BCL	C4B-NB	2.06	1.37	1.35
15	BK	1001	V7N	C20-C19	2.06	1.39	1.34
14	BH	1002	LMT	O4'-C4B	-2.06	1.38	1.43
14	BN	1005	LMT	O4'-C4B	-2.06	1.38	1.43
13	AU	102	BCL	C4B-NB	2.06	1.37	1.35
14	BF	101	LMT	O4'-C4B	-2.06	1.38	1.43
13	AD	1001	BCL	OBD-CAD	2.06	1.25	1.22
15	bc	104	V7N	C8-C9	-2.06	1.41	1.45
15	bn	101	V7N	C16-C15	2.05	1.41	1.36
14	BB	102	LMT	O4'-C4B	-2.05	1.38	1.43
15	bb	101	V7N	C20-C19	2.05	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AW	104	BCL	C4B-NB	2.05	1.37	1.35
15	bc	104	V7N	C20-C19	2.05	1.39	1.34
13	ak	1001	BCL	C4B-NB	2.05	1.37	1.35
14	BA	106	LMT	O4'-C4B	-2.05	1.38	1.43
14	BB	103	LMT	O4'-C4B	-2.05	1.38	1.43
14	BD	103	LMT	O4'-C4B	-2.05	1.38	1.43
14	bg	103	LMT	O4'-C4B	-2.05	1.38	1.43
14	L	305	LMT	O4'-C4B	-2.05	1.38	1.43
15	bo	101	V7N	C12-C13	-2.05	1.41	1.45
14	BP	1003	LMT	O4'-C4B	-2.05	1.38	1.43
15	BL	1001	V7N	C20-C19	2.05	1.39	1.34
14	AH	103	LMT	O4'-C4B	-2.05	1.38	1.43
14	BM	1003	LMT	O4'-C4B	-2.05	1.38	1.43
14	AS	103	LMT	O4'-C4B	-2.05	1.38	1.43
14	L	302	LMT	O4'-C4B	-2.05	1.38	1.43
13	AG	102	BCL	OBD-CAD	2.05	1.25	1.22
13	AM	101	BCL	OBD-CAD	2.05	1.25	1.22
15	be	101	V7N	C7-C8	2.05	1.39	1.34
14	BF	103	LMT	O4'-C4B	-2.04	1.38	1.43
14	AF	1003	LMT	O4'-C4B	-2.04	1.38	1.43
14	BD	102	LMT	O4'-C4B	-2.04	1.38	1.43
14	BX	1003	LMT	O4'-C4B	-2.04	1.38	1.43
13	AW	101	BCL	OBD-CAD	2.04	1.25	1.22
14	BR	1002	LMT	O4'-C4B	-2.04	1.38	1.43
15	ba	101	V7N	C20-C19	2.04	1.39	1.34
14	M	402	LMT	O4'-C4B	-2.04	1.38	1.43
15	BE	101	V7N	C20-C19	2.04	1.39	1.34
15	BJ	1001	V7N	C7-C8	2.04	1.39	1.34
13	ag	1001	BCL	C4B-NB	2.04	1.37	1.35
14	BA	103	LMT	O4'-C4B	-2.04	1.38	1.43
14	BO	1003	LMT	O4'-C4B	-2.04	1.38	1.43
15	BW	1001	V7N	C7-C8	2.04	1.39	1.34
15	bg	101	V7N	C19-C18	-2.04	1.41	1.45
13	AO	102	BCL	C4B-NB	2.04	1.37	1.35
13	AS	102	BCL	OBD-CAD	2.04	1.25	1.22
15	BE	101	V7N	C16-C15	2.03	1.41	1.36
13	AL	101	BCL	C4B-NB	2.03	1.37	1.35
14	bk	101	LMT	O4'-C4B	-2.03	1.38	1.43
14	BT	1003	LMT	O4'-C4B	-2.03	1.38	1.43
15	bm	101	V7N	C8-C9	-2.03	1.41	1.45
22	L	301	BPH	C2C-C1C	-2.03	1.48	1.52
14	AU	101	LMT	O4'-C4B	-2.03	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BN	1004	LMT	O4'-C4B	-2.03	1.38	1.43
13	ae	1001	BCL	C4B-NB	2.03	1.37	1.35
15	BG	1001	V7N	C20-C19	2.03	1.39	1.34
15	bf	102	V7N	C20-C19	2.03	1.39	1.34
14	BR	1006	LMT	O4'-C4B	-2.03	1.38	1.43
14	AB	104	LMT	O4'-C4B	-2.03	1.38	1.43
13	AV	102	BCL	C4B-NB	2.03	1.37	1.35
15	BD	101	V7N	C19-C18	-2.03	1.41	1.45
14	bj	102	LMT	O4'-C4B	-2.03	1.38	1.43
13	an	102	BCL	C4B-NB	2.03	1.37	1.35
15	bk	103	V7N	C4-C3	2.03	1.37	1.32
14	BQ	1004	LMT	O4'-C4B	-2.03	1.38	1.43
15	BV	1001	V7N	C20-C19	2.03	1.39	1.34
14	BP	1005	LMT	O4'-C4B	-2.03	1.38	1.43
13	AQ	102	BCL	OBD-CAD	2.03	1.25	1.22
14	BI	102	LMT	O4'-C4B	-2.02	1.38	1.43
14	BT	1005	LMT	O4'-C4B	-2.02	1.38	1.43
14	BV	1002	LMT	O4'-C4B	-2.02	1.38	1.43
14	BJ	1002	LMT	O4'-C4B	-2.02	1.38	1.43
13	AM	102	BCL	C4B-NB	2.02	1.37	1.35
14	AH	106	LMT	O4'-C4B	-2.02	1.38	1.43
14	BS	1003	LMT	O4'-C4B	-2.02	1.38	1.43
14	BU	1002	LMT	O4'-C4B	-2.02	1.38	1.43
14	AN	103	LMT	O4'-C4B	-2.02	1.38	1.43
15	bo	101	V7N	C8-C9	-2.02	1.41	1.45
15	bl	102	V7N	C4-C3	2.02	1.37	1.32
14	BW	1005	LMT	O4'-C4B	-2.02	1.38	1.43
15	BT	1001	V7N	C20-C19	2.02	1.39	1.34
14	BH	1004	LMT	O4'-C4B	-2.02	1.38	1.43
14	bo	103	LMT	O4'-C4B	-2.02	1.38	1.43
15	BA	101	V7N	C7-C8	2.01	1.39	1.34
15	BX	1001	V7N	C20-C19	2.01	1.39	1.34
14	AO	103	LMT	O4'-C4B	-2.01	1.38	1.43
14	BX	1002	LMT	O4'-C4B	-2.01	1.38	1.43
13	AP	101	BCL	C4B-NB	2.01	1.37	1.35
14	AT	101	LMT	O4'-C4B	-2.01	1.38	1.43
14	BI	103	LMT	O4'-C4B	-2.01	1.38	1.43
14	bf	101	LMT	O4'-C4B	-2.01	1.38	1.43
15	BH	1001	V7N	C20-C19	2.01	1.39	1.34
14	BU	1003	LMT	O4'-C4B	-2.01	1.38	1.43
14	bc	101	LMT	O4'-C4B	-2.01	1.38	1.43
15	BH	1001	V7N	C16-C15	2.01	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	BJ	1003	LMT	O4'-C4B	-2.01	1.38	1.43
14	BK	1006	LMT	O4'-C4B	-2.01	1.38	1.43
14	BO	1002	LMT	O4'-C4B	-2.01	1.38	1.43
14	BD	105	LMT	O4'-C4B	-2.01	1.38	1.43
15	bc	104	V7N	C16-C15	2.01	1.41	1.36
14	BE	103	LMT	O4'-C4B	-2.01	1.38	1.43
15	AE	1003	V7N	C20-C19	2.01	1.39	1.34
14	AP	102	LMT	O4'-C4B	-2.01	1.38	1.43
14	BK	1005	LMT	O4'-C4B	-2.01	1.38	1.43
15	BO	1001	V7N	C20-C19	2.01	1.39	1.34
14	BC	102	LMT	O4'-C4B	-2.01	1.38	1.43
13	BS	1005	BCL	OBD-CAD	2.00	1.25	1.22
15	bi	101	V7N	C8-C9	-2.00	1.41	1.45
15	be	101	V7N	C19-C18	-2.00	1.41	1.45
14	AA	1003	LMT	O4'-C4B	-2.00	1.38	1.43
15	ba	101	V7N	C16-C15	2.00	1.41	1.36
15	bb	101	V7N	C12-C13	-2.00	1.41	1.45
15	bo	101	V7N	C4-C3	2.00	1.37	1.32
15	BS	1001	V7N	C19-C18	-2.00	1.41	1.45

All (1771) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BA	104	BCL	C1-C2-C3	6.57	137.41	126.04
13	AQ	103	BCL	C1-O2A-CGA	6.47	133.42	116.44
15	bb	101	V7N	C28-C27-C26	-6.45	108.29	126.42
15	BG	1001	V7N	C28-C27-C26	-6.35	108.57	126.42
14	BW	1005	LMT	C1-O1'-C1'	5.92	123.66	113.84
15	BN	1001	V7N	C28-C27-C26	-5.82	110.08	126.42
15	bg	101	V7N	C28-C27-C26	-5.34	111.42	126.42
16	C	1003	HEC	CMC-C2C-C1C	-5.25	120.40	128.46
16	C	1001	HEC	CMC-C2C-C1C	-5.24	120.42	128.46
15	AE	1003	V7N	C28-C27-C26	-5.18	111.88	126.42
15	BC	101	V7N	C28-C27-C26	-5.11	112.06	126.42
16	C	1004	HEC	CMC-C2C-C1C	-5.07	120.67	128.46
13	AL	103	BCL	C1-C2-C3	-5.04	117.32	126.04
21	ai	103	CD4	O2-C14-C13	5.03	122.35	111.50
15	be	101	V7N	C29-C28-C27	-5.02	107.56	123.22
15	BD	101	V7N	C28-C27-C26	-4.94	112.53	126.42
15	BM	1001	V7N	C28-C27-C26	-4.92	112.60	126.42
15	bk	103	V7N	C29-C28-C27	-4.89	107.97	123.22
15	bp	102	V7N	C28-C27-C26	-4.88	112.69	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AT	103	V7N	C28-C27-C26	-4.85	112.79	126.42
15	BX	1001	V7N	C28-C27-C26	-4.78	112.99	126.42
15	BT	1001	V7N	C29-C28-C27	-4.74	108.41	123.22
16	C	1002	HEC	CMC-C2C-C1C	-4.71	121.22	128.46
15	bc	104	V7N	C29-C28-C27	-4.70	108.54	123.22
15	BV	1001	V7N	C28-C27-C26	-4.67	113.29	126.42
15	bj	101	V7N	C29-C28-C27	-4.67	108.64	123.22
15	AH	105	V7N	C28-C27-C26	-4.67	113.31	126.42
26	ag	1002	V7B	O1-C7-C8	4.62	122.04	110.90
15	bf	102	V7N	C29-C28-C27	-4.57	108.96	123.22
15	bo	101	V7N	C29-C28-C27	-4.54	109.05	123.22
15	BJ	1001	V7N	C28-C27-C26	-4.51	113.73	126.42
15	BE	101	V7N	C28-C27-C26	-4.51	113.75	126.42
13	ag	1001	BCL	CMB-C2B-C1B	-4.51	121.53	128.46
15	bi	101	V7N	C29-C28-C27	-4.50	109.17	123.22
13	ak	1001	BCL	CMB-C2B-C1B	-4.49	121.56	128.46
18	C	1006	V75	O2-C2A-C2B	4.48	119.34	111.09
15	bh	102	V7N	C29-C28-C27	-4.48	109.23	123.22
15	BP	1001	V7N	C29-C28-C27	-4.47	109.26	123.22
15	BL	1001	V7N	C28-C27-C26	-4.46	113.88	126.42
13	ad	102	BCL	CMB-C2B-C1B	-4.44	121.64	128.46
15	bd	101	V7N	C29-C28-C27	-4.43	109.39	123.22
15	BR	1001	V7N	C28-C27-C26	-4.43	113.98	126.42
13	AO	101	BCL	CMB-C2B-C1B	-4.40	121.70	128.46
13	M	405	BCL	CMB-C2B-C1B	-4.39	121.71	128.46
18	M	409	V75	O3-C3A-C3B	4.39	119.17	111.09
26	af	101	V7B	C43-O52-C47	4.39	122.30	113.69
15	BH	1001	V7N	C29-C28-C27	-4.39	109.53	123.22
21	M	404	CD4	O2-C14-C13	4.38	120.95	111.50
18	C	1006	V75	O3-C3A-C3B	4.37	119.13	111.09
15	BQ	1001	V7N	C29-C28-C27	-4.37	109.59	123.22
13	ap	1001	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
13	am	1001	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
15	BW	1001	V7N	C29-C28-C27	-4.36	109.61	123.22
15	bm	101	V7N	C29-C28-C27	-4.36	109.62	123.22
21	af	104	CD4	C15-O2-C14	4.36	128.52	117.79
16	C	1004	HEC	CBD-CAD-C3D	-4.35	104.45	112.49
13	ba	103	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
13	ao	1001	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
13	ae	1001	BCL	CMB-C2B-C1B	-4.34	121.79	128.46
15	BS	1001	V7N	C29-C28-C27	-4.33	109.69	123.22
13	ac	102	BCL	CMB-C2B-C1B	-4.33	121.82	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bm	103	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
15	BO	1001	V7N	C29-C28-C27	-4.32	109.75	123.22
13	ah	1001	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
13	al	1001	BCL	CMB-C2B-C1B	-4.30	121.85	128.46
13	ai	102	BCL	CMB-C2B-C1B	-4.30	121.86	128.46
13	AD	1001	BCL	CMB-C2B-C1B	-4.29	121.86	128.46
13	bd	103	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
13	AC	1002	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
14	BK	1004	LMT	C1-O1'-C1'	4.29	120.95	113.84
13	BM	1004	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
13	bj	104	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
13	AB	101	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
13	AN	102	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
13	AW	104	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
13	AS	102	BCL	CMB-C2B-C1B	-4.25	121.94	128.46
13	AS	104	BCL	CMB-C2B-C1B	-4.24	121.94	128.46
13	AB	103	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
13	AG	102	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
13	aj	102	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
13	AI	102	BCL	CMB-C2B-C1B	-4.23	121.97	128.46
18	M	409	V75	O2-C2A-C2B	4.23	118.87	111.09
15	BP	1001	V7N	C28-C27-C26	-4.23	114.54	126.42
13	bh	105	BCL	CMB-C2B-C1B	-4.23	121.97	128.46
13	af	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
13	AE	1001	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
13	BS	1005	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
13	AJ	102	BCL	CMB-C2B-C1B	-4.21	122.00	128.46
13	BN	1006	BCL	CMB-C2B-C1B	-4.21	122.00	128.46
15	BB	101	V7N	C28-C27-C26	-4.20	114.61	126.42
13	BK	1003	BCL	CMB-C2B-C1B	-4.20	122.01	128.46
13	BE	104	BCL	CMB-C2B-C1B	-4.20	122.01	128.46
13	AM	101	BCL	CMB-C2B-C1B	-4.19	122.02	128.46
13	L	303	BCL	CMB-C2B-C1B	-4.19	122.02	128.46
15	BR	1001	V7N	C29-C28-C27	-4.19	110.14	123.22
13	AL	103	BCL	CMB-C2B-C1B	-4.18	122.04	128.46
13	BF	104	BCL	CMB-C2B-C1B	-4.18	122.05	128.46
13	AW	101	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
15	AT	103	V7N	C7-C6-C5	4.16	133.25	127.31
13	AP	103	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
13	AV	103	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
13	AK	103	BCL	CMB-C2B-C1B	-4.15	122.08	128.46
13	an	102	BCL	CMB-C2B-C1B	-4.15	122.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AH	101	BCL	CMB-C2B-C1B	-4.15	122.08	128.46
13	BI	104	BCL	CMB-C2B-C1B	-4.15	122.08	128.46
15	BN	1001	V7N	C15-C14-C13	-4.15	121.39	127.31
13	BJ	1004	BCL	CMB-C2B-C1B	-4.15	122.09	128.46
13	AQ	102	BCL	CMB-C2B-C1B	-4.14	122.10	128.46
15	bn	101	V7N	C29-C28-C27	-4.13	110.33	123.22
13	bp	103	BCL	CMB-C2B-C1B	-4.13	122.12	128.46
13	bo	102	BCL	CMB-C2B-C1B	-4.13	122.12	128.46
13	bl	105	BCL	CMB-C2B-C1B	-4.12	122.13	128.46
13	BC	103	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
13	BV	1004	BCL	CMB-C2B-C1B	-4.11	122.15	128.46
13	bf	105	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
13	BU	1004	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
13	AU	102	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
13	BL	1004	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
13	AA	1002	BCL	CMB-C2B-C1B	-4.09	122.17	128.46
13	BD	106	BCL	CMB-C2B-C1B	-4.08	122.19	128.46
13	bi	103	BCL	CMB-C2B-C1B	-4.08	122.19	128.46
15	BH	1001	V7N	C28-C27-C26	-4.08	114.96	126.42
13	AD	1002	BCL	CMB-C2B-C1B	-4.07	122.21	128.46
13	BG	1004	BCL	CMB-C2B-C1B	-4.07	122.21	128.46
15	BK	1001	V7N	C29-C28-C27	-4.06	110.53	123.22
14	BK	1006	LMT	C1-O1'-C1'	4.06	120.57	113.84
13	bb	103	BCL	CMB-C2B-C1B	-4.06	122.23	128.46
15	BS	1001	V7N	C28-C27-C26	-4.06	115.02	126.42
15	BB	101	V7N	C29-C28-C27	-4.04	110.60	123.22
13	bc	103	BCL	CMB-C2B-C1B	-4.04	122.25	128.46
13	BB	104	BCL	CMB-C2B-C1B	-4.04	122.26	128.46
13	bn	103	BCL	CMB-C2B-C1B	-4.04	122.26	128.46
13	AQ	103	BCL	CMB-C2B-C1B	-4.03	122.26	128.46
13	BX	1004	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
13	BR	1003	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
13	BA	104	BCL	CMB-C2B-C1B	-4.02	122.28	128.46
13	be	104	BCL	CMB-C2B-C1B	-4.02	122.28	128.46
13	bk	105	BCL	CMB-C2B-C1B	-4.02	122.28	128.46
13	BH	1003	BCL	CMB-C2B-C1B	-4.02	122.29	128.46
15	BA	101	V7N	C28-C27-C26	-4.02	115.13	126.42
13	AF	1002	BCL	CMB-C2B-C1B	-4.01	122.29	128.46
13	BW	1003	BCL	CMB-C2B-C1B	-4.01	122.29	128.46
21	ad	101	CD4	O2-C14-C13	4.01	120.14	111.50
13	bg	104	BCL	CMB-C2B-C1B	-4.01	122.31	128.46
15	BN	1001	V7N	C7-C6-C5	-4.00	121.60	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AJ	102	BCL	C1-C2-C3	-4.00	119.13	126.04
13	BT	1004	BCL	CMB-C2B-C1B	-3.99	122.34	128.46
15	BJ	1001	V7N	C29-C28-C27	-3.98	110.78	123.22
13	BP	1004	BCL	CMB-C2B-C1B	-3.98	122.35	128.46
13	AS	102	BCL	C4A-NA-C1A	3.97	108.49	106.71
15	BR	1001	V7N	C7-C6-C5	-3.96	121.65	127.31
15	BQ	1001	V7N	C28-C27-C26	-3.96	115.29	126.42
15	BM	1001	V7N	C15-C14-C13	-3.96	121.66	127.31
14	bc	101	LMT	C1-O1'-C1'	3.96	120.40	113.84
13	BQ	1003	BCL	CMB-C2B-C1B	-3.95	122.39	128.46
15	bf	102	V7N	C28-C27-C26	-3.95	115.31	126.42
13	AS	101	BCL	CMB-C2B-C1B	-3.95	122.39	128.46
15	bl	102	V7N	C28-C27-C26	-3.94	115.34	126.42
16	C	1004	HEC	CMB-C2B-C1B	-3.94	122.41	128.46
16	C	1003	HEC	CMB-C2B-C1B	-3.93	122.42	128.46
13	AJ	102	BCL	C1-O2A-CGA	3.93	126.75	116.44
15	BW	1001	V7N	C28-C27-C26	-3.92	115.41	126.42
21	H1	1003	CD4	O2-C14-C13	3.91	119.94	111.50
13	BO	1004	BCL	CMB-C2B-C1B	-3.91	122.45	128.46
13	AK	102	BCL	CMB-C2B-C1B	-3.91	122.45	128.46
13	AJ	101	BCL	CMB-C2B-C1B	-3.90	122.46	128.46
15	bm	101	V7N	C28-C27-C26	-3.90	115.47	126.42
13	AU	103	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
13	ab	1001	BCL	C4A-NA-C1A	3.89	108.46	106.71
13	ae	1001	BCL	C4A-NA-C1A	3.89	108.46	106.71
13	AM	102	BCL	CMB-C2B-C1B	-3.88	122.49	128.46
15	BD	101	V7N	C29-C28-C27	-3.88	111.10	123.22
13	AI	103	BCL	CMB-C2B-C1B	-3.88	122.50	128.46
13	M	405	BCL	C4A-NA-C1A	3.88	108.45	106.71
13	AG	103	BCL	CMB-C2B-C1B	-3.88	122.51	128.46
13	AV	102	BCL	CMB-C2B-C1B	-3.86	122.53	128.46
13	AN	104	BCL	CMB-C2B-C1B	-3.86	122.53	128.46
13	AP	103	BCL	C4A-NA-C1A	3.85	108.44	106.71
13	AH	102	BCL	CMB-C2B-C1B	-3.85	122.54	128.46
15	BM	1001	V7N	C29-C28-C27	-3.85	111.20	123.22
15	BO	1001	V7N	C28-C27-C26	-3.85	115.60	126.42
13	AX	101	BCL	CMB-C2B-C1B	-3.84	122.56	128.46
13	AW	103	BCL	CMB-C2B-C1B	-3.84	122.56	128.46
13	AF	1001	BCL	CMB-C2B-C1B	-3.83	122.57	128.46
15	BK	1001	V7N	C28-C27-C26	-3.83	115.66	126.42
13	AT	102	BCL	CMB-C2B-C1B	-3.83	122.58	128.46
14	AG	101	LMT	C3'-C4'-C5'	-3.83	102.14	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	af	103	CD4	O2-C14-C13	3.83	119.75	111.50
13	AL	101	BCL	CMB-C2B-C1B	-3.82	122.58	128.46
13	AO	102	BCL	CMB-C2B-C1B	-3.82	122.59	128.46
13	AR	101	BCL	CMB-C2B-C1B	-3.82	122.59	128.46
15	bh	102	V7N	C28-C27-C26	-3.81	115.71	126.42
13	an	102	BCL	C4A-NA-C1A	3.81	108.42	106.71
13	ab	1001	BCL	CMB-C2B-C1B	-3.79	122.64	128.46
16	C	1001	HEC	CMB-C2B-C1B	-3.79	122.64	128.46
13	AU	102	BCL	C1-C2-C3	-3.78	119.50	126.04
13	AP	101	BCL	CMB-C2B-C1B	-3.77	122.66	128.46
13	AC	1001	BCL	CMB-C2B-C1B	-3.77	122.68	128.46
13	am	1001	BCL	C4A-NA-C1A	3.76	108.40	106.71
20	bj	103	OV9	C2-O2-C10	3.76	127.05	117.79
13	AA	1001	BCL	CMB-C2B-C1B	-3.76	122.69	128.46
13	AW	104	BCL	C4A-NA-C1A	3.75	108.39	106.71
13	ao	1001	BCL	C4A-NA-C1A	3.75	108.39	106.71
13	BS	1005	BCL	C4A-NA-C1A	3.74	108.39	106.71
13	AV	103	BCL	C4A-NA-C1A	3.74	108.39	106.71
13	aa	1001	BCL	CMB-C2B-C1B	-3.73	122.73	128.46
26	af	101	V7B	O7-C10-C11	3.72	119.51	111.50
15	BH	1001	V7N	C7-C6-C5	-3.71	122.02	127.31
15	bn	101	V7N	C28-C27-C26	-3.71	116.00	126.42
13	AQ	101	BCL	CMB-C2B-C1B	-3.71	122.77	128.46
15	BE	101	V7N	C29-C28-C27	-3.70	111.66	123.22
14	BJ	1002	LMT	C1-O1'-C1'	3.70	119.98	113.84
13	al	1001	BCL	C4A-NA-C1A	3.69	108.36	106.71
13	ah	1001	BCL	C4A-NA-C1A	3.67	108.36	106.71
15	BL	1001	V7N	C29-C28-C27	-3.67	111.77	123.22
13	AA	1002	BCL	C4A-NA-C1A	3.65	108.35	106.71
13	AG	103	BCL	C4A-NA-C1A	3.64	108.34	106.71
13	AC	1002	BCL	C2A-C1A-CHA	3.64	130.23	123.86
13	BG	1004	BCL	C4A-NA-C1A	3.63	108.34	106.71
13	af	102	BCL	C4A-NA-C1A	3.63	108.34	106.71
19	H1	1001	PGW	C02-O01-C1	3.61	126.67	117.79
13	AN	102	BCL	C4A-NA-C1A	3.60	108.33	106.71
13	bk	105	BCL	C4A-NA-C1A	3.59	108.32	106.71
14	AA	1003	LMT	C3'-C4'-C5'	-3.59	102.69	110.93
13	AB	103	BCL	C4A-NA-C1A	3.59	108.32	106.71
13	ac	102	BCL	C4A-NA-C1A	3.59	108.32	106.71
13	AW	103	BCL	C4A-NA-C1A	3.59	108.32	106.71
13	ai	102	BCL	C4A-NA-C1A	3.59	108.32	106.71
13	BE	104	BCL	C1-C2-C3	-3.59	119.84	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	1002	HEC	CMB-C2B-C1B	-3.58	122.95	128.46
16	C	1001	HEC	CBD-CAD-C3D	-3.58	105.88	112.49
15	ba	101	V7N	C29-C28-C27	-3.58	112.05	123.22
13	AE	1002	BCL	CMB-C2B-C1B	-3.58	122.97	128.46
15	BD	101	V7N	C15-C14-C13	-3.57	122.21	127.31
15	bd	101	V7N	C28-C27-C26	-3.57	116.39	126.42
13	BT	1004	BCL	C4A-NA-C1A	3.57	108.31	106.71
13	aj	102	BCL	C4A-NA-C1A	3.57	108.31	106.71
13	AD	1002	BCL	C4A-NA-C1A	3.56	108.31	106.71
13	AO	102	BCL	C4A-NA-C1A	3.56	108.31	106.71
13	BV	1004	BCL	C4A-NA-C1A	3.55	108.30	106.71
13	AH	102	BCL	C4A-NA-C1A	3.55	108.30	106.71
13	M	405	BCL	CAD-C3D-C4D	-3.54	106.49	108.47
13	BO	1004	BCL	C4A-NA-C1A	3.54	108.30	106.71
15	BP	1001	V7N	C15-C14-C13	-3.54	122.26	127.31
13	L	308	BCL	CMB-C2B-C1B	-3.53	123.03	128.46
13	BH	1003	BCL	C4A-NA-C1A	3.53	108.29	106.71
15	AT	103	V7N	C35-C13-C14	-3.53	117.98	122.92
13	AF	1002	BCL	C4A-NA-C1A	3.53	108.29	106.71
13	AC	1001	BCL	C4A-NA-C1A	3.52	108.29	106.71
15	bl	102	V7N	C29-C28-C27	-3.52	112.23	123.22
13	AL	103	BCL	C4A-NA-C1A	3.52	108.29	106.71
14	L	302	LMT	C1-O1'-C1'	3.51	119.67	113.84
13	BQ	1003	BCL	C4A-NA-C1A	3.51	108.29	106.71
15	BX	1001	V7N	C15-C14-C13	-3.51	122.30	127.31
13	ad	102	BCL	C4A-NA-C1A	3.51	108.28	106.71
13	AT	102	BCL	C4A-NA-C1A	3.51	108.28	106.71
15	BC	101	V7N	C15-C14-C13	-3.50	122.32	127.31
13	BW	1003	BCL	C4A-NA-C1A	3.49	108.28	106.71
15	be	101	V7N	C28-C27-C26	-3.49	116.60	126.42
15	BB	101	V7N	C15-C14-C13	-3.49	122.33	127.31
15	bi	101	V7N	C28-C27-C26	-3.48	116.64	126.42
13	ap	1001	BCL	C4A-NA-C1A	3.48	108.27	106.71
16	C	1003	HEC	CMB-C2B-C3B	3.48	129.91	125.82
13	AU	103	BCL	C4A-NA-C1A	3.48	108.27	106.71
15	bo	101	V7N	C28-C27-C26	-3.47	116.66	126.42
13	AR	101	BCL	C4A-NA-C1A	3.47	108.27	106.71
13	AH	101	BCL	C1-C2-C3	-3.46	120.05	126.04
13	AX	101	BCL	CHA-C1A-NA	-3.46	118.47	126.40
13	AK	102	BCL	C4A-NA-C1A	3.46	108.26	106.71
14	BU	1003	LMT	C1-O1'-C1'	3.46	119.57	113.84
13	BB	104	BCL	C4A-NA-C1A	3.44	108.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AL	101	BCL	C4A-NA-C1A	3.44	108.25	106.71
20	be	102	OV9	C2-O2-C10	3.43	126.24	117.79
13	AN	104	BCL	C4A-NA-C1A	3.43	108.25	106.71
13	ad	102	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
13	AQ	103	BCL	C4A-NA-C1A	3.42	108.24	106.71
21	ad	101	CD4	O16-C46-C47	3.41	118.86	111.50
13	L	308	BCL	CAD-C3D-C4D	-3.41	106.57	108.47
13	AP	101	BCL	OBD-CAD-CBD	-3.41	121.03	125.89
13	bf	105	BCL	OBD-CAD-CBD	-3.41	121.03	125.89
21	af	103	CD4	C15-O2-C14	3.40	126.17	117.79
16	C	1001	HEC	CMB-C2B-C3B	3.40	129.82	125.82
13	be	104	BCL	OBD-CAD-CBD	-3.39	121.05	125.89
14	BF	101	LMT	C3'-C4'-C5'	-3.39	103.15	110.93
14	BR	1006	LMT	C3'-C4'-C5'	-3.39	103.15	110.93
13	AU	102	BCL	C1-O2A-CGA	3.39	125.34	116.44
15	bb	101	V7N	C36-C18-C17	-3.39	118.18	122.92
14	AB	104	LMT	C1-O1'-C1'	3.38	119.45	113.84
13	bk	105	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
13	ak	1001	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
13	ao	1001	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
13	AG	103	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
13	ae	1001	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
13	AS	101	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
13	AB	101	BCL	C4A-NA-C1A	3.38	108.22	106.71
13	AT	102	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
13	AU	103	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
13	ah	1001	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
13	AM	102	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
13	aa	1001	BCL	C4A-NA-C1A	3.37	108.22	106.71
13	AD	1002	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
13	AH	102	BCL	OBD-CAD-CBD	-3.37	121.09	125.89
13	an	102	BCL	OBD-CAD-CBD	-3.37	121.09	125.89
15	BS	1001	V7N	C15-C14-C13	-3.36	122.51	127.31
13	BN	1006	BCL	C4A-NA-C1A	3.36	108.22	106.71
13	ai	102	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
13	AJ	101	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
13	AL	101	BCL	CAD-C3D-C4D	-3.36	106.60	108.47
13	AK	102	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
13	AI	103	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
13	al	1001	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
13	AC	1002	BCL	CHA-C1A-NA	-3.36	118.71	126.40
13	BJ	1004	BCL	OBD-CAD-CBD	-3.36	121.10	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BK	1003	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
13	AD	1001	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
13	AG	102	BCL	CAD-C3D-C4D	-3.35	106.60	108.47
13	BT	1004	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	AV	102	BCL	C4A-NA-C1A	3.35	108.21	106.71
13	AO	102	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	AR	101	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BH	1003	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BL	1004	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BV	1004	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BD	106	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BG	1004	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	AF	1001	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	BQ	1003	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
13	AL	101	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
13	BE	104	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
22	M	406	BPH	OBD-CAD-CBD	-3.34	121.12	125.89
13	AV	102	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
13	L	308	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
13	ac	102	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
13	AQ	101	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
15	BD	101	V7N	C35-C13-C14	-3.34	118.25	122.92
13	AA	1001	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
13	AB	101	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
13	AV	103	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
13	ab	1001	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
13	bb	103	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
13	BF	104	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	BS	1005	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	aa	1001	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	BP	1004	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	af	102	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	ap	1001	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	AB	101	BCL	C1-C2-C3	3.33	131.80	126.04
14	BN	1003	LMT	C1-O1'-C1'	3.33	119.36	113.84
13	BR	1003	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	BU	1004	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
13	BO	1004	BCL	OBD-CAD-CBD	-3.32	121.14	125.89
15	ba	101	V7N	C28-C27-C26	-3.32	117.08	126.42
13	AS	104	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
13	BW	1003	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
13	BC	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AW	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
14	bk	101	LMT	C3'-C4'-C5'	-3.32	103.31	110.93
13	AG	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
13	AW	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
21	ai	103	CD4	O3-C16-C15	-3.32	98.77	108.43
13	aj	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
13	ba	103	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
13	AO	102	BCL	CAD-C3D-C4D	-3.32	106.62	108.47
13	AU	102	BCL	C4A-NA-C1A	3.32	108.20	106.71
13	AA	1002	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
13	BB	104	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
13	AM	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
13	ag	1001	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
13	AI	102	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
13	AP	103	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
13	bp	103	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
13	AN	104	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
13	AJ	101	BCL	C4A-NA-C1A	3.31	108.19	106.71
13	AX	101	BCL	CAD-C3D-C4D	-3.31	106.62	108.47
13	AB	103	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
13	BM	1004	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
13	bj	104	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
22	L	301	BPH	OBD-CAD-CBD	-3.31	121.17	125.89
23	an	101	MQ8	C12-C11-C3	3.30	120.95	112.05
15	bp	102	V7N	C29-C28-C27	-3.30	112.91	123.22
13	bc	103	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	AE	1002	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	AS	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	bl	105	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	bo	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	AN	104	BCL	CAD-C3D-C4D	-3.30	106.63	108.47
13	am	1001	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	AU	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	bm	103	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
13	BA	104	BCL	OBD-CAD-CBD	-3.30	121.19	125.89
13	AU	103	BCL	CAD-C3D-C4D	-3.30	106.63	108.47
13	BX	1004	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	AN	102	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	BN	1006	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	BI	104	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	bi	103	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	AC	1001	BCL	OBD-CAD-CBD	-3.29	121.19	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AQ	103	BCL	CAD-C3D-C4D	-3.29	106.64	108.47
13	AW	104	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
13	AX	101	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
15	BN	1001	V7N	C33-C5-C6	-3.29	118.32	122.92
13	AJ	102	BCL	OBD-CAD-CBD	-3.29	121.20	125.89
16	C	1004	HEC	CMB-C2B-C3B	3.28	129.68	125.82
13	AE	1002	BCL	C4A-NA-C1A	3.28	108.18	106.71
13	AM	102	BCL	C4A-NA-C1A	3.28	108.18	106.71
13	BP	1004	BCL	C4A-NA-C1A	3.28	108.18	106.71
13	aj	102	BCL	C1-C2-C3	3.28	131.72	126.04
13	bn	103	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
13	AQ	102	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
13	bh	105	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
13	AH	101	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
14	AK	101	LMT	C3'-C4'-C5'	-3.28	103.42	110.93
13	bg	104	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
13	AX	101	BCL	C4A-NA-C1A	3.27	108.18	106.71
13	ag	1001	BCL	C4A-NA-C1A	3.27	108.18	106.71
13	BE	104	BCL	C4A-NA-C1A	3.27	108.17	106.71
13	AE	1001	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
13	ak	1001	BCL	C4A-NA-C1A	3.26	108.17	106.71
13	AK	103	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
13	L	303	BCL	OBD-CAD-CBD	-3.26	121.24	125.89
13	AA	1001	BCL	C4A-NA-C1A	3.26	108.17	106.71
13	BD	106	BCL	C4A-NA-C1A	3.26	108.17	106.71
13	M	403	BCL	CMB-C2B-C1B	-3.26	123.46	128.46
13	AJ	102	BCL	C4A-NA-C1A	3.25	108.17	106.71
21	af	104	CD4	O16-C46-C47	3.24	118.49	111.50
13	AW	103	BCL	CAD-C3D-C4D	-3.24	106.66	108.47
13	AF	1002	BCL	OBD-CAD-CBD	-3.24	121.27	125.89
13	bd	103	BCL	OBD-CAD-CBD	-3.24	121.27	125.89
13	ag	1001	BCL	CMB-C2B-C3B	3.23	130.73	124.68
15	AH	105	V7N	C29-C28-C27	-3.23	113.13	123.22
13	M	405	BCL	CHA-C1A-NA	-3.23	119.00	126.40
13	AI	103	BCL	C4A-NA-C1A	3.23	108.16	106.71
26	ag	1002	V7B	C7-O1-C1	3.22	120.04	113.74
14	BA	106	LMT	C1-O1'-C1'	3.22	119.19	113.84
13	AT	102	BCL	CAD-C3D-C4D	-3.22	106.67	108.47
15	BX	1001	V7N	C35-C13-C14	-3.22	118.41	122.92
13	M	405	BCL	OBD-CAD-CBD	-3.22	121.29	125.89
13	M	403	BCL	OBD-CAD-CBD	-3.22	121.30	125.89
13	BM	1004	BCL	CHA-C1A-NA	-3.22	119.03	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AF	1001	BCL	C4A-NA-C1A	3.22	108.15	106.71
13	AC	1002	BCL	OBD-CAD-CBD	-3.21	121.31	125.89
14	BK	1005	LMT	C3'-C4'-C5'	-3.21	103.56	110.93
15	bc	104	V7N	C28-C27-C26	-3.21	117.41	126.42
14	BP	1006	LMT	C1-O1'-C1'	3.20	119.15	113.84
14	BW	1005	LMT	O5'-C1'-O1'	-3.20	102.39	109.97
23	an	101	MQ8	C11-C3-C4	3.20	121.92	118.50
13	AP	101	BCL	C4A-NA-C1A	3.20	108.14	106.71
13	AC	1002	BCL	CAD-C3D-C4D	-3.20	106.69	108.47
13	ad	102	BCL	CMB-C2B-C3B	3.19	130.65	124.68
13	AJ	101	BCL	CAD-C3D-C4D	-3.18	106.69	108.47
13	bp	103	BCL	CAD-C3D-C4D	-3.18	106.70	108.47
13	AO	102	BCL	CHA-C1A-NA	-3.18	119.12	126.40
13	M	405	BCL	CMB-C2B-C3B	3.17	130.61	124.68
13	BX	1004	BCL	CHA-C1A-NA	-3.17	119.13	126.40
13	AQ	103	BCL	OBD-CAD-CBD	-3.17	121.36	125.89
13	BO	1004	BCL	CHA-C1A-NA	-3.17	119.15	126.40
13	ai	102	BCL	CAD-C3D-C4D	-3.16	106.71	108.47
13	ak	1001	BCL	CMB-C2B-C3B	3.16	130.59	124.68
13	AH	102	BCL	CHA-C1A-NA	-3.16	119.16	126.40
13	AM	102	BCL	CHA-C1A-NA	-3.15	119.17	126.40
13	AL	101	BCL	CHA-C1A-NA	-3.15	119.18	126.40
13	BA	104	BCL	CHA-C1A-NA	-3.15	119.18	126.40
13	AO	101	BCL	CMB-C2B-C3B	3.15	130.57	124.68
13	AL	103	BCL	OBD-CAD-CBD	-3.15	121.40	125.89
13	af	102	BCL	CAD-C3D-C4D	-3.15	106.72	108.47
13	bf	105	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
13	AA	1001	BCL	CHA-C1A-NA	-3.14	119.20	126.40
13	AE	1002	BCL	CHA-C1A-NA	-3.14	119.20	126.40
13	BI	104	BCL	CHA-C1A-NA	-3.14	119.20	126.40
13	AD	1002	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
14	BF	102	LMT	C1-O1'-C1'	3.14	119.05	113.84
13	AW	101	BCL	CHA-C1A-NA	-3.14	119.20	126.40
13	AI	103	BCL	CHA-C1A-NA	-3.14	119.20	126.40
13	BM	1004	BCL	C4A-NA-C1A	3.14	108.12	106.71
13	ao	1001	BCL	CMB-C2B-C3B	3.14	130.55	124.68
13	AQ	101	BCL	CHA-C1A-NA	-3.14	119.21	126.40
22	L	301	BPH	C1C-NC-C4C	-3.14	107.78	110.54
13	AW	101	BCL	CAD-C3D-C4D	-3.13	106.72	108.47
13	AW	104	BCL	CAD-C3D-C4D	-3.13	106.72	108.47
13	AD	1001	BCL	CMB-C2B-C3B	3.13	130.54	124.68
13	AP	101	BCL	CHA-C1A-NA	-3.13	119.22	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BU	1004	BCL	CHA-C1A-NA	-3.13	119.22	126.40
13	AH	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
15	BN	1001	V7N	C35-C13-C14	-3.13	118.54	122.92
13	ap	1001	BCL	CMB-C2B-C3B	3.13	130.53	124.68
13	AB	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
13	AD	1002	BCL	CHA-C1A-NA	-3.12	119.24	126.40
13	AT	102	BCL	CHA-C1A-NA	-3.12	119.24	126.40
13	BB	104	BCL	CHA-C1A-NA	-3.12	119.24	126.40
13	ba	103	BCL	CHA-C1A-NA	-3.12	119.24	126.40
13	AE	1001	BCL	CHA-C1A-NA	-3.12	119.25	126.40
13	AC	1002	BCL	CMB-C2B-C3B	3.12	130.52	124.68
13	AK	102	BCL	CHA-C1A-NA	-3.12	119.25	126.40
13	AN	104	BCL	CHA-C1A-NA	-3.12	119.25	126.40
13	BK	1003	BCL	CHA-C1A-NA	-3.12	119.25	126.40
13	AK	103	BCL	CAD-C3D-C4D	-3.12	106.73	108.47
13	AV	102	BCL	CHA-C1A-NA	-3.12	119.25	126.40
15	BM	1001	V7N	C35-C13-C14	-3.12	118.55	122.92
15	BR	1001	V7N	C33-C5-C6	-3.12	118.55	122.92
13	AS	102	BCL	CHA-C1A-NA	-3.12	119.26	126.40
15	AE	1003	V7N	C15-C14-C13	-3.12	122.86	127.31
15	BC	101	V7N	C35-C13-C14	-3.12	118.56	122.92
15	bp	102	V7N	C35-C13-C14	-3.12	118.56	122.92
13	M	403	BCL	CAD-C3D-C4D	-3.11	106.73	108.47
13	ag	1001	BCL	CAD-C3D-C4D	-3.11	106.73	108.47
13	AG	103	BCL	CAD-C3D-C4D	-3.11	106.73	108.47
13	BC	103	BCL	CAD-C3D-C4D	-3.11	106.73	108.47
13	BC	103	BCL	CHA-C1A-NA	-3.11	119.27	126.40
13	AA	1001	BCL	CAD-C3D-C4D	-3.11	106.74	108.47
13	AF	1001	BCL	CAD-C3D-C4D	-3.11	106.74	108.47
13	BE	104	BCL	CHA-C1A-NA	-3.11	119.29	126.40
13	AE	1001	BCL	CAD-C3D-C4D	-3.10	106.74	108.47
13	AG	103	BCL	CHA-C1A-NA	-3.10	119.30	126.40
13	BL	1004	BCL	CHA-C1A-NA	-3.10	119.30	126.40
13	AQ	101	BCL	C4A-NA-C1A	3.10	108.10	106.71
13	BI	104	BCL	C4A-NA-C1A	3.10	108.10	106.71
13	AG	102	BCL	CMB-C2B-C3B	3.10	130.48	124.68
15	AE	1003	V7N	C35-C13-C14	-3.10	118.58	122.92
13	AC	1001	BCL	CHA-C1A-NA	-3.10	119.30	126.40
13	BR	1003	BCL	CHA-C1A-NA	-3.10	119.30	126.40
15	bg	101	V7N	C36-C18-C17	-3.10	118.58	122.92
13	AF	1001	BCL	CHA-C1A-NA	-3.10	119.31	126.40
13	bm	103	BCL	CMB-C2B-C3B	3.10	130.47	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AB	101	BCL	CMB-C2B-C3B	3.09	130.47	124.68
13	BW	1003	BCL	CHA-C1A-NA	-3.09	119.31	126.40
15	BT	1001	V7N	C28-C27-C26	-3.09	117.72	126.42
13	AS	104	BCL	CMB-C2B-C3B	3.09	130.47	124.68
13	AW	103	BCL	CHA-C1A-NA	-3.09	119.32	126.40
13	AS	101	BCL	CHA-C1A-NA	-3.09	119.32	126.40
13	AR	101	BCL	CHA-C1A-NA	-3.09	119.32	126.40
15	BM	1001	V7N	C38-C26-C27	-3.09	113.21	118.08
13	ba	103	BCL	CMB-C2B-C3B	3.09	130.46	124.68
13	am	1001	BCL	CMB-C2B-C3B	3.09	130.45	124.68
13	BM	1004	BCL	CAA-CBA-CGA	3.09	122.27	113.25
13	ac	102	BCL	CMB-C2B-C3B	3.09	130.45	124.68
13	AJ	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
13	AW	104	BCL	CMB-C2B-C3B	3.08	130.44	124.68
13	AU	103	BCL	CHA-C1A-NA	-3.08	119.35	126.40
13	ae	1001	BCL	CMB-C2B-C3B	3.08	130.43	124.68
13	AB	103	BCL	CMB-C2B-C3B	3.07	130.43	124.68
13	ai	102	BCL	CMB-C2B-C3B	3.07	130.43	124.68
13	AB	103	BCL	C1-O2A-CGA	3.07	124.50	116.44
13	AM	101	BCL	C4A-NA-C1A	3.07	108.08	106.71
13	BA	104	BCL	C4A-NA-C1A	3.07	108.08	106.71
13	BJ	1004	BCL	CHA-C1A-NA	-3.06	119.39	126.40
13	AI	102	BCL	CAD-C3D-C4D	-3.06	106.76	108.47
13	be	104	BCL	CAD-C3D-C4D	-3.06	106.76	108.47
13	AS	101	BCL	CAD-C3D-C4D	-3.06	106.76	108.47
15	BP	1001	V7N	C36-C18-C19	3.06	122.90	118.08
13	bh	105	BCL	CMB-C2B-C3B	3.05	130.39	124.68
13	aj	102	BCL	CMB-C2B-C3B	3.05	130.39	124.68
13	bj	104	BCL	CMB-C2B-C3B	3.05	130.39	124.68
14	BW	1005	LMT	O1'-C1'-C2'	3.05	113.07	108.30
13	ah	1001	BCL	CMB-C2B-C3B	3.05	130.38	124.68
13	AH	101	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
13	BG	1004	BCL	CHA-C1A-NA	-3.05	119.42	126.40
13	AN	102	BCL	CMB-C2B-C3B	3.05	130.38	124.68
13	AH	102	BCL	CAD-C3D-C4D	-3.04	106.77	108.47
13	AM	102	BCL	CAD-C3D-C4D	-3.04	106.77	108.47
13	BX	1004	BCL	CAD-C3D-C4D	-3.04	106.77	108.47
13	AI	102	BCL	CMB-C2B-C3B	3.04	130.37	124.68
13	bl	105	BCL	CAD-C3D-C4D	-3.04	106.77	108.47
13	AK	103	BCL	CMB-C2B-C3B	3.04	130.37	124.68
13	al	1001	BCL	CMB-C2B-C3B	3.04	130.37	124.68
13	AL	103	BCL	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AJ	102	BCL	CAD-C3D-C4D	-3.04	106.78	108.47
13	bk	105	BCL	CAD-C3D-C4D	-3.04	106.78	108.47
13	AO	101	BCL	OBD-CAD-CBD	-3.04	121.55	125.89
13	bm	103	BCL	CHA-C1A-NA	-3.04	119.44	126.40
13	BV	1004	BCL	CHA-C1A-NA	-3.04	119.44	126.40
13	AS	102	BCL	CMB-C2B-C3B	3.04	130.36	124.68
13	af	102	BCL	CMB-C2B-C3B	3.04	130.36	124.68
13	AJ	102	BCL	CMB-C2B-C3B	3.03	130.35	124.68
13	BK	1003	BCL	CAD-C3D-C4D	-3.03	106.78	108.47
13	AS	101	BCL	C4A-NA-C1A	3.03	108.07	106.71
13	BT	1004	BCL	CHA-C1A-NA	-3.03	119.46	126.40
15	BA	101	V7N	C15-C14-C13	-3.03	122.98	127.31
13	AQ	103	BCL	CHA-C1A-NA	-3.03	119.46	126.40
13	AW	101	BCL	CMB-C2B-C3B	3.03	130.34	124.68
15	bb	101	V7N	C16-C17-C18	-3.03	122.99	127.31
13	AM	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
13	BP	1004	BCL	CHA-C1A-NA	-3.02	119.48	126.40
13	BF	104	BCL	CHA-C1A-NA	-3.02	119.48	126.40
15	BK	1001	V7N	C36-C18-C17	-3.02	118.69	122.92
13	aa	1001	BCL	CAD-C3D-C4D	-3.02	106.79	108.47
13	BM	1004	BCL	CMB-C2B-C3B	3.02	130.33	124.68
13	AA	1002	BCL	C1-C2-C3	-3.02	120.83	126.04
13	BM	1004	BCL	C2A-C1A-CHA	3.02	129.13	123.86
13	bc	103	BCL	C4A-NA-C1A	3.02	108.06	106.71
13	bd	103	BCL	CMB-C2B-C3B	3.02	130.32	124.68
13	BD	106	BCL	CHA-C1A-NA	-3.02	119.49	126.40
13	BH	1003	BCL	CHA-C1A-NA	-3.02	119.49	126.40
13	AB	103	BCL	C1-C2-C3	-3.01	120.83	126.04
15	bj	101	V7N	C28-C27-C26	-3.01	117.95	126.42
13	AA	1002	BCL	CHA-C1A-NA	-3.01	119.50	126.40
13	bk	105	BCL	C1-O2A-CGA	3.01	124.35	116.44
13	AP	103	BCL	CHA-C1A-NA	-3.01	119.50	126.40
13	bd	103	BCL	CHA-C1A-NA	-3.01	119.50	126.40
13	AV	103	BCL	CHA-C1A-NA	-3.01	119.50	126.40
13	AS	104	BCL	CAD-C3D-C4D	-3.01	106.79	108.47
13	AE	1001	BCL	CMB-C2B-C3B	3.01	130.31	124.68
13	AV	103	BCL	CMB-C2B-C3B	3.01	130.31	124.68
13	AI	102	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	AJ	102	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	BQ	1003	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	bo	102	BCL	CHA-C1A-NA	-3.01	119.51	126.40
15	bc	104	V7N	C35-C13-C14	-3.01	118.71	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AQ	101	BCL	CAD-C3D-C4D	-3.01	106.79	108.47
13	AG	102	BCL	C4A-NA-C1A	3.01	108.06	106.71
13	bd	103	BCL	C4A-NA-C1A	3.01	108.06	106.71
13	AS	104	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	BN	1006	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	AD	1001	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	bg	104	BCL	CHA-C1A-NA	-3.01	119.52	126.40
13	an	102	BCL	CHA-C1A-NA	-3.00	119.52	126.40
13	AO	101	BCL	CHA-C1A-NA	-3.00	119.52	126.40
14	BN	1002	LMT	C1-O1'-C1'	3.00	118.82	113.84
21	H1	1003	CD4	O16-C46-C47	3.00	117.97	111.50
13	al	1001	BCL	CAD-C3D-C4D	-3.00	106.80	108.47
13	AP	103	BCL	CMB-C2B-C3B	3.00	130.29	124.68
13	L	303	BCL	CMB-C2B-C3B	3.00	130.29	124.68
13	L	303	BCL	CAD-C3D-C4D	-3.00	106.80	108.47
13	AR	101	BCL	CAD-C3D-C4D	-3.00	106.80	108.47
13	bl	105	BCL	CMB-C2B-C3B	3.00	130.28	124.68
13	BS	1005	BCL	CHA-C1A-NA	-2.99	119.54	126.40
13	bp	103	BCL	CHA-C1A-NA	-2.99	119.54	126.40
13	BS	1005	BCL	CMB-C2B-C3B	2.99	130.28	124.68
13	ac	102	BCL	CHA-C1A-NA	-2.99	119.54	126.40
13	bj	104	BCL	CHA-C1A-NA	-2.99	119.55	126.40
13	bc	103	BCL	CHA-C1A-NA	-2.99	119.55	126.40
13	AK	102	BCL	CAD-C3D-C4D	-2.99	106.80	108.47
13	aj	102	BCL	CHA-C1A-NA	-2.99	119.55	126.40
16	C	1002	HEC	CMB-C2B-C3B	2.99	129.34	125.82
13	AB	101	BCL	CAD-C3D-C4D	-2.99	106.80	108.47
13	ak	1001	BCL	CHA-C1A-NA	-2.99	119.55	126.40
13	AK	103	BCL	CHA-C1A-NA	-2.99	119.56	126.40
13	AM	101	BCL	CMB-C2B-C3B	2.99	130.27	124.68
13	BE	104	BCL	CMB-C2B-C3B	2.98	130.26	124.68
13	BN	1006	BCL	CMB-C2B-C3B	2.98	130.26	124.68
13	AP	103	BCL	CAD-C3D-C4D	-2.98	106.81	108.47
13	AA	1002	BCL	CMB-C2B-C3B	2.98	130.25	124.68
15	BB	101	V7N	C35-C13-C14	-2.98	118.75	122.92
13	AQ	102	BCL	CHA-C1A-NA	-2.98	119.58	126.40
15	bl	102	V7N	C35-C13-C12	2.98	122.77	118.08
13	BK	1003	BCL	CMB-C2B-C3B	2.98	130.25	124.68
13	an	102	BCL	CMB-C2B-C3B	2.97	130.24	124.68
13	bl	105	BCL	CHA-C1A-NA	-2.97	119.59	126.40
13	bi	103	BCL	CHA-C1A-NA	-2.97	119.59	126.40
13	AH	101	BCL	CMB-C2B-C3B	2.97	130.24	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AD	1002	BCL	CMB-C2B-C3B	2.97	130.24	124.68
13	ap	1001	BCL	CAD-C3D-C4D	-2.97	106.81	108.47
15	BT	1001	V7N	C35-C13-C14	-2.97	118.77	122.92
13	bi	103	BCL	C4A-NA-C1A	2.97	108.04	106.71
13	bi	103	BCL	CMB-C2B-C3B	2.97	130.23	124.68
13	AI	103	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
13	ad	102	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
13	bb	103	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
13	bk	105	BCL	O2A-C1-C2	-2.96	100.84	108.64
13	am	1001	BCL	CHA-C1A-NA	-2.96	119.61	126.40
14	L	307	LMT	O5B-C5B-C4B	2.96	115.08	109.69
13	BF	104	BCL	CMB-C2B-C3B	2.96	130.22	124.68
15	BD	101	V7N	C36-C18-C19	2.96	122.75	118.08
13	bn	103	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
13	bp	103	BCL	CMB-C2B-C3B	2.96	130.22	124.68
13	BJ	1004	BCL	CAD-C3D-C4D	-2.96	106.82	108.47
14	bh	101	LMT	C1-O1'-C1'	2.96	118.75	113.84
14	BW	1005	LMT	C3'-C4'-C5'	-2.96	104.15	110.93
13	af	102	BCL	CHA-C1A-NA	-2.96	119.63	126.40
15	BW	1001	V7N	C15-C14-C13	-2.96	123.09	127.31
15	bg	101	V7N	C35-C13-C14	-2.96	118.78	122.92
13	bn	103	BCL	CHA-C1A-NA	-2.95	119.63	126.40
13	aa	1001	BCL	C1-O2A-CGA	2.95	124.19	116.44
13	AF	1002	BCL	CAD-C3D-C4D	-2.95	106.82	108.47
13	bh	105	BCL	CHA-C1A-NA	-2.95	119.64	126.40
13	BL	1004	BCL	CMB-C2B-C3B	2.95	130.20	124.68
13	AQ	102	BCL	CMB-C2B-C3B	2.95	130.20	124.68
13	bf	105	BCL	CHA-C1A-NA	-2.95	119.64	126.40
13	ao	1001	BCL	CHA-C1A-NA	-2.95	119.64	126.40
13	ap	1001	BCL	CHA-C1A-NA	-2.95	119.64	126.40
13	be	104	BCL	CHA-C1A-NA	-2.95	119.64	126.40
13	AN	102	BCL	CHA-C1A-NA	-2.95	119.65	126.40
13	AG	102	BCL	CHA-C1A-NA	-2.95	119.65	126.40
13	bg	104	BCL	CAD-C3D-C4D	-2.95	106.83	108.47
13	BC	103	BCL	C4A-NA-C1A	2.94	108.03	106.71
13	aa	1001	BCL	CHA-C1A-NA	-2.94	119.66	126.40
13	ah	1001	BCL	CHA-C1A-NA	-2.94	119.66	126.40
13	BJ	1004	BCL	CMB-C2B-C3B	2.94	130.18	124.68
13	bn	103	BCL	CMB-C2B-C3B	2.94	130.18	124.68
13	BU	1004	BCL	CMB-C2B-C3B	2.94	130.18	124.68
13	al	1001	BCL	CHA-C1A-NA	-2.94	119.67	126.40
13	AC	1001	BCL	CAD-C3D-C4D	-2.94	106.83	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ae	1001	BCL	CAD-C3D-C4D	-2.94	106.83	108.47
14	BB	103	LMT	O1'-C1'-C2'	2.93	112.88	108.30
13	bg	104	BCL	CMB-C2B-C3B	2.93	130.16	124.68
15	BS	1001	V7N	C35-C13-C14	-2.93	118.82	122.92
13	AM	102	BCL	C2A-C1A-CHA	2.93	128.98	123.86
13	ah	1001	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
13	bf	105	BCL	CMB-C2B-C3B	2.93	130.16	124.68
13	AD	1001	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
13	bm	103	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
13	L	308	BCL	CHA-C1A-NA	-2.92	119.70	126.40
13	AF	1002	BCL	CMB-C2B-C3B	2.92	130.15	124.68
13	AU	102	BCL	CMB-C2B-C3B	2.92	130.14	124.68
15	BV	1001	V7N	C35-C13-C14	-2.92	118.83	122.92
13	ai	102	BCL	CHA-C1A-NA	-2.92	119.71	126.40
15	BA	101	V7N	C29-C28-C27	-2.92	114.10	123.22
13	AA	1002	BCL	CAD-C3D-C4D	-2.92	106.84	108.47
13	BO	1004	BCL	CAD-C3D-C4D	-2.92	106.84	108.47
13	AT	102	BCL	C2A-C1A-CHA	2.92	128.96	123.86
15	BQ	1001	V7N	C15-C14-C13	-2.92	123.15	127.31
13	BE	104	BCL	CAD-C3D-C4D	-2.91	106.84	108.47
13	bo	102	BCL	CAD-C3D-C4D	-2.91	106.85	108.47
13	AO	102	BCL	C2A-C1A-CHA	2.91	128.95	123.86
15	bh	102	V7N	C35-C13-C12	2.91	122.66	118.08
13	BJ	1004	BCL	C4A-NA-C1A	2.91	108.01	106.71
13	BW	1003	BCL	CMB-C2B-C3B	2.91	130.12	124.68
13	BE	104	BCL	C1-O2A-CGA	2.91	124.07	116.44
13	BI	104	BCL	CMB-C2B-C3B	2.91	130.12	124.68
13	be	104	BCL	CMB-C2B-C3B	2.91	130.12	124.68
13	BC	103	BCL	CMB-C2B-C3B	2.91	130.12	124.68
13	bh	105	BCL	C4A-NA-C1A	2.91	108.01	106.71
13	bo	102	BCL	CMB-C2B-C3B	2.91	130.12	124.68
13	BD	106	BCL	CAD-C3D-C4D	-2.91	106.85	108.47
13	BF	104	BCL	CAD-C3D-C4D	-2.91	106.85	108.47
15	BP	1001	V7N	C35-C13-C14	-2.91	118.85	122.92
13	ad	102	BCL	CHA-C1A-NA	-2.90	119.75	126.40
13	BL	1004	BCL	CAD-C3D-C4D	-2.90	106.85	108.47
26	ag	1002	V7B	O7-C10-C11	2.90	117.75	111.50
13	BR	1003	BCL	CMB-C2B-C3B	2.90	130.10	124.68
15	BA	101	V7N	C36-C18-C19	2.90	122.65	118.08
13	BV	1004	BCL	CMB-C2B-C3B	2.90	130.10	124.68
13	AW	104	BCL	CBA-CAA-C2A	2.90	122.41	113.86
13	ae	1001	BCL	CHA-C1A-NA	-2.89	119.77	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BR	1003	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
13	bp	103	BCL	C4A-NA-C1A	2.89	108.01	106.71
13	AQ	103	BCL	CMB-C2B-C3B	2.89	130.09	124.68
13	bb	103	BCL	CHA-C1A-NA	-2.89	119.78	126.40
13	bb	103	BCL	CMB-C2B-C3B	2.89	130.09	124.68
13	BT	1004	BCL	CMB-C2B-C3B	2.89	130.09	124.68
13	bh	105	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
15	be	101	V7N	C35-C13-C12	2.89	122.63	118.08
13	ag	1001	BCL	CHA-C1A-NA	-2.89	119.78	126.40
13	BG	1004	BCL	CMB-C2B-C3B	2.89	130.08	124.68
13	BA	104	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
13	AP	101	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
13	BU	1004	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
13	AU	102	BCL	CAD-C3D-C4D	-2.88	106.86	108.47
13	AH	102	BCL	C2A-C1A-CHA	2.88	128.90	123.86
14	BF	101	LMT	C1-O1'-C1'	2.88	118.62	113.84
13	BD	106	BCL	CMB-C2B-C3B	2.88	130.07	124.68
13	bc	103	BCL	CMB-C2B-C3B	2.88	130.07	124.68
13	ao	1001	BCL	CAD-C3D-C4D	-2.88	106.86	108.47
13	AF	1002	BCL	CHA-C1A-NA	-2.88	119.80	126.40
13	AU	102	BCL	CHA-C1A-NA	-2.88	119.81	126.40
15	BH	1001	V7N	C33-C5-C6	-2.88	118.89	122.92
13	BK	1003	BCL	C4A-NA-C1A	2.88	108.00	106.71
13	BP	1004	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
14	AW	102	LMT	C3'-C4'-C5'	-2.87	104.34	110.93
13	BI	104	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
13	ba	103	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
15	ba	101	V7N	C35-C13-C12	2.87	122.60	118.08
15	BW	1001	V7N	C35-C13-C14	-2.87	118.90	122.92
14	BL	1002	LMT	O1'-C1'-C2'	2.87	112.78	108.30
13	ab	1001	BCL	CHA-C1A-NA	-2.87	119.83	126.40
15	bb	101	V7N	C33-C5-C6	-2.87	118.91	122.92
13	bk	105	BCL	CHA-C1A-NA	-2.87	119.83	126.40
13	BH	1003	BCL	CMB-C2B-C3B	2.87	130.04	124.68
13	AV	103	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
13	BH	1003	BCL	C1-O2A-CGA	2.87	123.96	116.44
13	AB	103	BCL	CHA-C1A-NA	-2.86	119.84	126.40
13	AL	103	BCL	CHA-C1A-NA	-2.86	119.84	126.40
13	AE	1002	BCL	CAD-C3D-C4D	-2.86	106.87	108.47
13	AV	102	BCL	CAD-C3D-C4D	-2.86	106.87	108.47
13	AL	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
14	M	402	LMT	C1-O1'-C1'	2.86	118.58	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AQ	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
13	BB	104	BCL	CMB-C2B-C3B	2.86	130.03	124.68
15	BK	1001	V7N	C35-C13-C14	-2.86	118.92	122.92
15	bb	101	V7N	C35-C13-C14	-2.86	118.92	122.92
13	L	303	BCL	CHA-C1A-NA	-2.85	119.86	126.40
14	bb	102	LMT	C3'-C4'-C5'	-2.85	104.38	110.93
13	AK	102	BCL	C2A-C1A-CHA	2.85	128.85	123.86
14	AS	103	LMT	C3'-C4'-C5'	-2.85	104.39	110.93
15	bk	103	V7N	C35-C13-C14	-2.85	118.93	122.92
13	AQ	103	BCL	CAA-CBA-CGA	2.85	121.59	113.25
13	BA	104	BCL	CMB-C2B-C3B	2.85	130.01	124.68
13	AF	1001	BCL	C1-C2-C3	2.85	130.97	126.04
13	bb	103	BCL	C4A-NA-C1A	2.85	107.99	106.71
13	bg	104	BCL	C4A-NA-C1A	2.85	107.99	106.71
15	be	101	V7N	C33-C5-C4	2.85	122.57	118.08
13	BX	1004	BCL	CMB-C2B-C3B	2.85	130.01	124.68
13	AI	102	BCL	C4A-NA-C1A	2.85	107.99	106.71
13	AA	1001	BCL	C2A-C1A-CHA	2.85	128.84	123.86
14	BT	1005	LMT	C3'-C4'-C5'	-2.85	104.40	110.93
13	BP	1004	BCL	CMB-C2B-C3B	2.85	130.00	124.68
13	bj	104	BCL	C4A-NA-C1A	2.84	107.98	106.71
14	BC	102	LMT	C3'-C4'-C5'	-2.84	104.42	110.93
15	BT	1001	V7N	C15-C14-C13	-2.84	123.26	127.31
13	bi	103	BCL	CAD-C3D-C4D	-2.84	106.89	108.47
15	BR	1001	V7N	C35-C13-C14	-2.84	118.95	122.92
13	bk	105	BCL	CMB-C2B-C3B	2.84	129.99	124.68
15	BL	1001	V7N	C35-C13-C14	-2.84	118.95	122.92
13	AW	103	BCL	C2A-C1A-CHA	2.84	128.82	123.86
13	an	102	BCL	CAD-C3D-C4D	-2.84	106.89	108.47
13	BQ	1003	BCL	CMB-C2B-C3B	2.83	129.98	124.68
13	AV	102	BCL	C2A-C1A-CHA	2.83	128.81	123.86
13	BO	1004	BCL	CMB-C2B-C3B	2.83	129.97	124.68
15	bj	101	V7N	C33-C5-C4	2.83	122.53	118.08
15	AT	103	V7N	C36-C18-C17	-2.82	118.97	122.92
13	AM	101	BCL	CAD-C3D-C4D	-2.82	106.89	108.47
13	AS	101	BCL	C2A-C1A-CHA	2.82	128.79	123.86
13	M	405	BCL	C2A-C1A-CHA	2.82	128.79	123.86
15	bh	102	V7N	C33-C5-C4	2.82	122.52	118.08
13	am	1001	BCL	CAD-C3D-C4D	-2.81	106.90	108.47
15	BG	1001	V7N	C35-C13-C14	-2.81	118.98	122.92
13	BB	104	BCL	CAD-C3D-C4D	-2.81	106.90	108.47
13	ak	1001	BCL	CAD-C3D-C4D	-2.81	106.90	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	104	BCL	C2A-C1A-CHA	2.81	128.77	123.86
13	BV	1004	BCL	CAD-C3D-C4D	-2.81	106.90	108.47
15	BE	101	V7N	C35-C13-C14	-2.81	118.99	122.92
15	BJ	1001	V7N	C36-C18-C19	2.81	122.50	118.08
13	M	403	BCL	CHA-C1A-NA	-2.80	119.98	126.40
13	AW	104	BCL	CHA-C1A-NA	-2.80	119.98	126.40
15	bn	101	V7N	C33-C5-C6	-2.80	119.00	122.92
14	AN	103	LMT	O5B-C5B-C4B	2.80	114.78	109.69
13	AD	1002	BCL	C2A-C1A-CHA	2.80	128.75	123.86
15	BQ	1001	V7N	C35-C13-C14	-2.80	119.00	122.92
13	bd	103	BCL	CAD-C3D-C4D	-2.79	106.91	108.47
14	BF	103	LMT	C3'-C4'-C5'	-2.79	104.53	110.93
14	BI	101	LMT	C3'-C4'-C5'	-2.79	104.53	110.93
13	BG	1004	BCL	CAD-C3D-C4D	-2.79	106.92	108.47
14	bl	101	LMT	O1'-C1'-C2'	2.79	112.66	108.30
13	bj	104	BCL	CAD-C3D-C4D	-2.79	106.92	108.47
13	bn	103	BCL	C4A-NA-C1A	2.78	107.96	106.71
13	AI	103	BCL	C2A-C1A-CHA	2.78	128.73	123.86
13	BN	1006	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
13	AS	102	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
14	L	306	LMT	C3'-C4'-C5'	-2.78	104.56	110.93
13	AQ	102	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
13	bc	103	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
13	AU	103	BCL	C2A-C1A-CHA	2.78	128.71	123.86
15	bo	101	V7N	C35-C13-C14	-2.77	119.04	122.92
13	BQ	1003	BCL	CAD-C3D-C4D	-2.77	106.92	108.47
23	an	101	MQ8	C15-C16-C17	2.77	120.98	111.88
13	AQ	103	BCL	O2D-CGD-CBD	2.77	116.19	111.27
15	BP	1001	V7N	C38-C26-C27	-2.77	113.72	118.08
13	aj	102	BCL	C1-O2A-CGA	2.77	123.71	116.44
15	bi	101	V7N	C35-C13-C14	-2.77	119.05	122.92
13	AG	103	BCL	C2A-C1A-CHA	2.77	128.70	123.86
13	AR	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
21	ad	101	CD4	O3-C17-C18	2.76	120.58	111.91
13	bl	105	BCL	C4A-NA-C1A	2.76	107.95	106.71
14	bp	101	LMT	O5'-C1'-C2'	-2.76	104.50	110.35
13	aj	102	BCL	CAD-C3D-C4D	-2.76	106.93	108.47
15	BO	1001	V7N	C35-C13-C12	2.76	122.42	118.08
13	BE	104	BCL	C2A-C1A-CHA	2.76	128.68	123.86
13	AJ	101	BCL	C2A-C1A-CHA	2.76	128.68	123.86
15	bm	101	V7N	C35-C13-C12	2.76	122.42	118.08
13	BJ	1004	BCL	C1-O2A-CGA	2.76	123.67	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BK	1001	V7N	C15-C14-C13	-2.75	123.38	127.31
14	BW	1006	LMT	O5'-C5'-C4'	2.75	115.56	109.75
14	AH	106	LMT	O1'-C1'-C2'	2.75	112.60	108.30
13	BT	1004	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
13	AE	1002	BCL	C2A-C1A-CHA	2.75	128.67	123.86
16	C	1001	HEC	C1D-C2D-C3D	-2.75	105.08	107.00
13	BX	1004	BCL	C4A-NA-C1A	2.74	107.94	106.71
15	bm	101	V7N	C33-C5-C4	2.74	122.40	118.08
13	AS	104	BCL	C17-C16-C15	2.74	125.84	113.24
15	bg	101	V7N	C16-C17-C18	-2.74	123.40	127.31
14	BA	106	LMT	C3'-C4'-C5'	-2.74	104.64	110.93
26	ag	1002	V7B	C43-O4-C4	-2.74	111.19	117.96
14	BE	103	LMT	C3'-C4'-C5'	-2.74	104.65	110.93
15	BS	1001	V7N	C36-C18-C19	2.74	122.39	118.08
13	AC	1002	BCL	C4A-NA-C1A	2.74	107.94	106.71
13	BU	1004	BCL	C4A-NA-C1A	2.73	107.93	106.71
15	BA	101	V7N	C35-C13-C14	-2.73	119.10	122.92
13	AW	101	BCL	C1-C2-C3	2.73	130.76	126.04
14	AV	101	LMT	O5'-C1'-C2'	-2.73	104.58	110.35
19	H1	1001	PGW	O01-C1-C2	2.73	117.38	111.50
13	bf	105	BCL	C4A-NA-C1A	2.72	107.93	106.71
14	BH	1004	LMT	C3'-C4'-C5'	-2.72	104.68	110.93
13	BS	1005	BCL	CAD-C3D-C4D	-2.72	106.95	108.47
14	AV	101	LMT	O5'-C5'-C4'	2.72	115.49	109.75
13	AH	101	BCL	C2A-C1A-CHA	2.72	128.62	123.86
13	AQ	102	BCL	C4A-NA-C1A	2.72	107.93	106.71
15	bn	101	V7N	C35-C13-C12	2.72	122.36	118.08
13	BW	1003	BCL	CAD-C3D-C4D	-2.72	106.96	108.47
13	ab	1001	BCL	CAD-C3D-C4D	-2.71	106.96	108.47
13	AC	1001	BCL	C2A-C1A-CHA	2.71	128.60	123.86
13	BJ	1004	BCL	C2A-C1A-CHA	2.71	128.60	123.86
15	AH	105	V7N	C35-C13-C12	2.71	122.34	118.08
13	AL	103	BCL	CBA-CAA-C2A	2.71	121.86	113.86
15	bd	101	V7N	C35-C13-C14	-2.71	119.13	122.92
13	BF	104	BCL	C4A-NA-C1A	2.71	107.92	106.71
23	an	101	MQ8	C20-C21-C22	2.70	120.76	111.88
14	bl	101	LMT	O5'-C1'-C2'	-2.70	104.63	110.35
15	BR	1001	V7N	C15-C14-C13	-2.70	123.46	127.31
14	BU	1003	LMT	C3'-C4'-C5'	-2.70	104.74	110.93
13	AL	103	BCL	CAD-C3D-C4D	-2.70	106.97	108.47
15	be	101	V7N	C36-C18-C19	2.70	122.33	118.08
14	AR	102	LMT	O1'-C1'-C2'	2.70	112.51	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BM	1001	V7N	C36-C18-C19	2.69	122.32	118.08
13	bm	103	BCL	C4A-NA-C1A	2.69	107.92	106.71
13	AN	102	BCL	CAD-C3D-C4D	-2.69	106.97	108.47
14	L	304	LMT	O5B-C5B-C4B	2.69	114.58	109.69
13	BM	1004	BCL	CAD-C3D-C4D	-2.69	106.97	108.47
15	AE	1003	V7N	C36-C18-C17	-2.69	119.16	122.92
21	af	103	CD4	O16-C46-C47	2.69	117.30	111.50
21	ad	101	CD4	O3-C16-C15	2.69	116.25	108.43
15	bk	103	V7N	C36-C18-C17	-2.68	119.16	122.92
13	AB	103	BCL	CAD-C3D-C4D	-2.68	106.97	108.47
13	aj	102	BCL	C2A-C1A-CHA	2.68	128.55	123.86
13	ac	102	BCL	CAD-C3D-C4D	-2.68	106.97	108.47
14	BO	1003	LMT	C3'-C4'-C5'	-2.68	104.78	110.93
15	BV	1001	V7N	C29-C28-C27	-2.68	114.85	123.22
13	BR	1003	BCL	C4A-NA-C1A	2.68	107.91	106.71
15	bp	102	V7N	C33-C5-C4	2.68	122.30	118.08
15	bc	104	V7N	C33-C5-C4	2.67	122.29	118.08
14	BP	1006	LMT	C3'-C4'-C5'	-2.67	104.80	110.93
13	AX	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
16	C	1002	HEC	C1D-C2D-C3D	-2.67	105.14	107.00
14	BR	1004	LMT	C1-O1'-C1'	2.67	118.26	113.84
13	AS	102	BCL	C2A-C1A-CHA	2.67	128.52	123.86
13	AG	102	BCL	C2A-C1A-CHA	2.66	128.52	123.86
14	BU	1003	LMT	O5'-C1'-O1'	-2.66	103.67	109.97
13	BH	1003	BCL	CAD-C3D-C4D	-2.66	106.99	108.47
13	AJ	102	BCL	CBA-CAA-C2A	2.66	121.71	113.86
13	L	303	BCL	C2A-C1A-CHA	2.66	128.51	123.86
15	bc	104	V7N	C15-C14-C13	-2.66	123.52	127.31
13	AP	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
15	BC	101	V7N	C29-C28-C27	-2.65	114.94	123.22
15	bh	102	V7N	C35-C13-C14	-2.65	119.21	122.92
13	AF	1002	BCL	C2A-C1A-CHA	2.65	128.50	123.86
14	BD	102	LMT	C3'-C4'-C5'	-2.65	104.85	110.93
13	AW	104	BCL	C1-O2A-CGA	2.65	123.39	116.44
13	AO	101	BCL	CAD-C3D-C4D	-2.65	106.99	108.47
13	BK	1003	BCL	C2A-C1A-CHA	2.65	128.49	123.86
13	AM	101	BCL	C6-C5-C3	2.65	120.40	113.45
13	bo	102	BCL	C4A-NA-C1A	2.65	107.90	106.71
13	AQ	103	BCL	CED-O2D-CGD	2.65	121.92	115.94
13	AQ	103	BCL	C2A-C1A-CHA	2.65	128.49	123.86
15	AH	105	V7N	C35-C13-C14	-2.64	119.22	122.92
13	BX	1004	BCL	C2A-C1A-CHA	2.64	128.48	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bl	102	V7N	C33-C5-C4	2.63	122.22	118.08
14	BL	1005	LMT	C3'-C4'-C5'	-2.63	104.90	110.93
15	AH	105	V7N	C36-C18-C19	2.63	122.22	118.08
14	BB	103	LMT	C1'-O5'-C5'	-2.63	108.53	113.69
13	AD	1001	BCL	C4A-NA-C1A	2.63	107.89	106.71
15	bd	101	V7N	C35-C13-C12	2.63	122.22	118.08
13	be	104	BCL	C4A-NA-C1A	2.63	107.89	106.71
14	BI	103	LMT	C1-O1'-C1'	2.63	118.19	113.84
14	bg	103	LMT	O5B-C5B-C4B	2.63	114.46	109.69
13	M	403	BCL	C4A-NA-C1A	2.62	107.89	106.71
15	bo	101	V7N	C1-C2-C3	2.62	120.00	113.06
15	BR	1001	V7N	C3-C4-C5	2.62	129.85	125.89
13	AE	1001	BCL	C2A-C1A-CHA	2.62	128.44	123.86
15	bn	101	V7N	C35-C13-C14	-2.62	119.26	122.92
15	bb	101	V7N	C7-C6-C5	-2.62	123.58	127.31
21	af	104	CD4	O14-C35-C36	2.62	120.11	111.91
15	BL	1001	V7N	C36-C18-C17	-2.61	119.26	122.92
15	bo	101	V7N	C36-C18-C17	-2.61	119.26	122.92
14	M	402	LMT	C3'-C4'-C5'	-2.61	104.94	110.93
13	AK	102	BCL	CMB-C2B-C3B	2.61	129.56	124.68
14	AD	1003	LMT	C3'-C4'-C5'	-2.61	104.94	110.93
13	ac	102	BCL	C2A-C1A-CHA	2.61	128.43	123.86
15	ba	101	V7N	C33-C5-C4	2.61	122.19	118.08
13	BI	104	BCL	C2A-C1A-CHA	2.61	128.42	123.86
13	BA	104	BCL	C2A-C1A-CHA	2.61	128.42	123.86
13	AN	104	BCL	OBB-CAB-CBB	-2.61	114.30	120.17
13	AP	101	BCL	OBB-CAB-CBB	-2.61	114.30	120.17
13	AC	1002	BCL	CBA-CAA-C2A	2.61	121.56	113.86
13	AK	103	BCL	C2A-C1A-CHA	2.61	128.42	123.86
15	BX	1001	V7N	C29-C28-C27	-2.61	115.08	123.22
13	BU	1004	BCL	C2A-C1A-CHA	2.61	128.41	123.86
13	AA	1001	BCL	OBB-CAB-CBB	-2.61	114.31	120.17
26	ag	1002	V7B	O1-C1-C2	2.60	112.37	108.30
13	AO	102	BCL	OBB-CAB-CBB	-2.60	114.31	120.17
15	BJ	1001	V7N	C38-C26-C27	-2.60	113.98	118.08
13	AJ	101	BCL	CMB-C2B-C3B	2.60	129.54	124.68
13	AS	101	BCL	OBB-CAB-CBB	-2.60	114.32	120.17
13	AT	102	BCL	OBB-CAB-CBB	-2.60	114.32	120.17
15	BS	1001	V7N	C38-C26-C27	-2.60	113.98	118.08
13	AG	103	BCL	OBB-CAB-CBB	-2.60	114.32	120.17
15	bj	101	V7N	C35-C13-C14	-2.60	119.29	122.92
23	L	309	MQ8	C11-C3-C4	-2.59	115.72	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BB	104	BCL	C2A-C1A-CHA	2.59	128.39	123.86
15	BC	101	V7N	C36-C18-C17	-2.59	119.29	122.92
13	AD	1001	BCL	C2A-C1A-CHA	2.59	128.39	123.86
13	AJ	101	BCL	OBB-CAB-CBB	-2.59	114.35	120.17
15	bf	102	V7N	C35-C13-C14	-2.59	119.30	122.92
13	AU	103	BCL	OBB-CAB-CBB	-2.59	114.35	120.17
13	AS	101	BCL	CMB-C2B-C3B	2.59	129.52	124.68
13	BW	1003	BCL	C2A-C1A-CHA	2.59	128.38	123.86
15	BD	101	V7N	C38-C26-C27	-2.58	114.00	118.08
15	BO	1001	V7N	C35-C13-C14	-2.58	119.31	122.92
14	BT	1002	LMT	C3'-C4'-C5'	-2.58	105.01	110.93
13	AL	101	BCL	OBB-CAB-CBB	-2.58	114.36	120.17
15	bc	104	V7N	C36-C18-C17	-2.58	119.31	122.92
13	AB	101	BCL	C2A-C1A-CHA	2.58	128.37	123.86
13	AW	101	BCL	C2A-C1A-CHA	2.58	128.36	123.86
13	AN	102	BCL	C2A-C1A-CHA	2.58	128.36	123.86
13	AG	103	BCL	CMB-C2B-C3B	2.57	129.50	124.68
14	BW	1006	LMT	C1B-O1B-C4'	2.57	124.33	117.96
13	AX	101	BCL	CMB-C2B-C3B	2.57	129.49	124.68
13	AH	102	BCL	CMB-C2B-C3B	2.57	129.49	124.68
13	AF	1001	BCL	OBB-CAB-CBB	-2.57	114.38	120.17
13	AI	103	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
13	AW	103	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
15	BV	1001	V7N	C36-C18-C17	-2.57	119.33	122.92
15	BT	1001	V7N	C33-C5-C4	2.57	122.12	118.08
15	BO	1001	V7N	C36-C18-C19	2.57	122.12	118.08
13	AV	102	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
13	AR	101	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
15	bp	102	V7N	C36-C18-C17	-2.57	119.33	122.92
13	L	308	BCL	C2A-C1A-CHA	2.56	128.34	123.86
13	AH	102	BCL	OBB-CAB-CBB	-2.56	114.40	120.17
13	AM	102	BCL	OBB-CAB-CBB	-2.56	114.40	120.17
15	bd	101	V7N	C33-C5-C4	2.56	122.12	118.08
13	AM	102	BCL	CMB-C2B-C3B	2.56	129.47	124.68
15	BS	1001	V7N	C33-C5-C4	2.56	122.11	118.08
14	BA	102	LMT	O1'-C1'-C2'	2.56	112.30	108.30
15	BX	1001	V7N	C36-C18-C17	-2.56	119.34	122.92
15	BL	1001	V7N	C33-C5-C4	2.56	122.11	118.08
13	AK	102	BCL	OBB-CAB-CBB	-2.56	114.41	120.17
13	M	403	BCL	C1-O2A-CGA	2.56	123.16	116.44
13	AI	103	BCL	CMB-C2B-C3B	2.56	129.46	124.68
13	AT	102	BCL	CMB-C2B-C3B	2.56	129.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bh	105	BCL	CMD-C2D-C3D	2.56	129.46	124.68
13	AU	103	BCL	CMB-C2B-C3B	2.56	129.46	124.68
15	BG	1001	V7N	C36-C18-C17	-2.55	119.34	122.92
15	BA	101	V7N	C35-C13-C12	2.55	122.10	118.08
15	bf	102	V7N	C33-C5-C4	2.55	122.10	118.08
15	BJ	1001	V7N	C33-C5-C4	2.55	122.10	118.08
13	AK	103	BCL	C4A-NA-C1A	2.55	107.85	106.71
13	AB	101	BCL	OBB-CAB-CBB	-2.55	114.43	120.17
14	BQ	1004	LMT	C3'-C4'-C5'	-2.55	105.08	110.93
15	BE	101	V7N	C35-C13-C12	2.55	122.09	118.08
13	AF	1001	BCL	C2A-C1A-CHA	2.54	128.31	123.86
13	AL	103	BCL	C1-O2A-CGA	2.54	123.12	116.44
15	BH	1001	V7N	C35-C13-C14	-2.54	119.36	122.92
15	ba	101	V7N	C35-C13-C14	-2.54	119.36	122.92
13	AO	101	BCL	CBA-CAA-C2A	2.54	121.36	113.86
15	bb	101	V7N	C35-C13-C12	2.54	122.08	118.08
13	AW	103	BCL	CMB-C2B-C3B	2.54	129.43	124.68
13	AA	1002	BCL	C2A-C1A-CHA	2.54	128.30	123.86
13	ba	103	BCL	C2A-C1A-CHA	2.54	128.30	123.86
13	AL	103	BCL	C2A-C1A-CHA	2.54	128.30	123.86
15	be	101	V7N	C35-C13-C14	-2.54	119.37	122.92
13	AX	101	BCL	OBB-CAB-CBB	-2.54	114.46	120.17
15	bi	101	V7N	C35-C13-C12	2.54	122.07	118.08
13	bl	105	BCL	CMD-C2D-C3D	2.54	129.42	124.68
15	BB	101	V7N	C36-C18-C19	2.53	122.07	118.08
14	BK	1002	LMT	C3'-C4'-C5'	-2.53	105.12	110.93
15	ba	101	V7N	C36-C18-C17	-2.53	119.38	122.92
13	BO	1004	BCL	C2A-C1A-CHA	2.53	128.29	123.86
13	AF	1001	BCL	CMB-C2B-C3B	2.53	129.41	124.68
13	AS	104	BCL	C1C-NC-C4C	2.53	107.84	106.71
14	BA	103	LMT	C3'-C4'-C5'	-2.53	105.12	110.93
13	bo	102	BCL	CMD-C2D-C3D	2.53	129.41	124.68
13	BD	106	BCL	C2A-C1A-CHA	2.53	128.28	123.86
15	bl	102	V7N	C35-C13-C14	-2.53	119.38	122.92
13	AN	104	BCL	CMB-C2B-C3B	2.53	129.41	124.68
15	bi	101	V7N	C36-C18-C17	-2.53	119.38	122.92
14	AH	106	LMT	C1'-O5'-C5'	-2.53	108.73	113.69
15	bm	101	V7N	C36-C18-C17	-2.53	119.38	122.92
13	AV	103	BCL	C2A-C1A-CHA	2.53	128.28	123.86
23	an	101	MQ8	C35-C36-C37	2.53	120.19	111.88
13	am	1001	BCL	OBB-CAB-CBB	-2.53	114.48	120.17
14	BA	102	LMT	C1'-O5'-C5'	-2.53	108.73	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BW	1001	V7N	C35-C13-C12	2.53	122.06	118.08
13	AQ	101	BCL	OBB-CAB-CBB	-2.53	114.48	120.17
13	ap	1001	BCL	C2A-C1A-CHA	2.53	128.28	123.86
13	BP	1004	BCL	O2A-C1-C2	-2.52	102.00	108.64
15	BM	1001	V7N	C33-C5-C4	2.52	122.05	118.08
13	aa	1001	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
13	AL	101	BCL	CMB-C2B-C3B	2.52	129.39	124.68
14	BM	1002	LMT	C3'-C4'-C5'	-2.52	105.15	110.93
14	AR	102	LMT	O5B-C5B-C4B	2.52	114.26	109.69
13	al	1001	BCL	OBB-CAB-CBB	-2.52	114.51	120.17
21	M	404	CD4	O3-C16-C15	-2.51	101.11	108.43
13	AD	1002	BCL	OBB-CAB-CBB	-2.51	114.51	120.17
13	an	102	BCL	C2A-C1A-CHA	2.51	128.25	123.86
15	BE	101	V7N	C36-C18-C19	2.51	122.04	118.08
15	bj	101	V7N	C35-C13-C12	2.51	122.04	118.08
13	bb	103	BCL	CMD-C2D-C3D	2.51	129.38	124.68
13	AC	1001	BCL	OBB-CAB-CBB	-2.51	114.52	120.17
13	bp	103	BCL	CMD-C2D-C3D	2.51	129.38	124.68
14	BK	1004	LMT	O5'-C5'-C4'	2.51	115.05	109.75
13	AB	103	BCL	C2A-C1A-CHA	2.51	128.25	123.86
14	BQ	1002	LMT	O1'-C1'-C2'	2.51	112.22	108.30
13	bd	103	BCL	CMD-C2D-C3D	2.51	129.37	124.68
13	AA	1001	BCL	CMB-C2B-C3B	2.51	129.37	124.68
13	bn	103	BCL	CMD-C2D-C3D	2.51	129.37	124.68
13	BV	1004	BCL	CBA-CAA-C2A	2.51	121.26	113.86
14	BR	1004	LMT	O5'-C1'-C2'	-2.51	105.04	110.35
13	ak	1001	BCL	C2A-C1A-CHA	2.51	128.24	123.86
26	af	101	V7B	C1-O6-C5	2.50	118.60	113.69
15	bf	102	V7N	C36-C18-C17	-2.50	119.42	122.92
14	BA	103	LMT	C1'-O5'-C5'	-2.50	108.77	113.69
14	AJ	103	LMT	C3'-C4'-C5'	-2.50	105.19	110.93
15	BV	1001	V7N	C36-C18-C19	2.50	122.02	118.08
13	ab	1001	BCL	CMB-C2B-C3B	2.50	129.36	124.68
13	AO	102	BCL	CMB-C2B-C3B	2.50	129.36	124.68
13	AR	101	BCL	CMB-C2B-C3B	2.50	129.35	124.68
13	AD	1002	BCL	C4B-C3B-CAB	-2.50	122.31	127.13
13	ab	1001	BCL	OBB-CAB-CBB	-2.50	114.55	120.17
13	AV	102	BCL	CMB-C2B-C3B	2.49	129.35	124.68
22	M	406	BPH	CHC-C1C-NC	-2.49	122.24	125.20
15	BA	101	V7N	C33-C5-C4	2.49	122.00	118.08
13	an	102	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
15	bm	101	V7N	C36-C18-C19	2.49	122.00	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AE	1003	V7N	C29-C28-C27	-2.49	115.44	123.22
13	am	1001	BCL	C2A-C1A-CHA	2.49	128.21	123.86
13	AL	103	BCL	OBB-CAB-CBB	-2.49	114.57	120.17
22	M	406	BPH	C1C-NC-C4C	-2.49	108.35	110.54
13	L	308	BCL	C1-O2A-CGA	2.49	122.97	116.44
13	ae	1001	BCL	OBB-CAB-CBB	-2.49	114.58	120.17
15	bl	102	V7N	C36-C18-C17	-2.49	119.44	122.92
13	AQ	101	BCL	CMB-C2B-C3B	2.48	129.32	124.68
14	BN	1002	LMT	C3'-C4'-C5'	-2.48	105.23	110.93
15	bm	101	V7N	C35-C13-C14	-2.48	119.44	122.92
27	ai	101	UYH	O1-C7-C8	-2.48	104.91	110.90
14	bb	102	LMT	O5'-C1'-O1'	-2.48	104.10	109.97
13	AM	101	BCL	C1-C2-C3	-2.48	121.76	126.04
14	BS	1002	LMT	O1'-C1'-C2'	2.48	112.17	108.30
15	bg	101	V7N	C33-C5-C4	2.48	121.98	118.08
13	AP	101	BCL	CMB-C2B-C3B	2.48	129.31	124.68
14	BQ	1004	LMT	O5'-C1'-O1'	-2.48	104.11	109.97
15	bk	103	V7N	C35-C13-C12	2.47	121.97	118.08
13	ad	102	BCL	OBB-CAB-CBB	-2.47	114.60	120.17
15	bd	101	V7N	C36-C18-C19	2.47	121.97	118.08
15	bg	101	V7N	C15-C14-C13	-2.47	123.78	127.31
14	AN	101	LMT	O1'-C1'-C2'	2.47	112.16	108.30
14	bf	101	LMT	O1'-C1'-C2'	2.47	112.16	108.30
15	BJ	1001	V7N	C35-C13-C14	-2.47	119.47	122.92
13	ak	1001	BCL	OBB-CAB-CBB	-2.47	114.62	120.17
13	aa	1001	BCL	CMB-C2B-C3B	2.47	129.29	124.68
13	bf	105	BCL	CMD-C2D-C3D	2.46	129.29	124.68
13	af	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
13	bm	103	BCL	CMD-C2D-C3D	2.46	129.28	124.68
13	bi	103	BCL	CMD-C2D-C3D	2.46	129.28	124.68
13	bc	103	BCL	C2A-C1A-CHA	2.46	128.16	123.86
13	ai	102	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
15	bi	101	V7N	C36-C18-C19	2.46	121.95	118.08
13	BG	1004	BCL	C2A-C1A-CHA	2.45	128.15	123.86
14	AN	101	LMT	C1'-O5'-C5'	-2.45	108.87	113.69
15	bi	101	V7N	C33-C5-C4	2.45	121.94	118.08
13	ao	1001	BCL	OBB-CAB-CBB	-2.45	114.65	120.17
13	M	403	BCL	C2A-C1A-CHA	2.45	128.15	123.86
13	ap	1001	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
13	ad	102	BCL	C2A-C1A-CHA	2.45	128.14	123.86
15	BH	1001	V7N	C36-C18-C19	2.45	121.94	118.08
13	AC	1002	BCL	C1C-NC-C4C	2.45	107.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	105	LMT	C1-O1'-C1'	2.45	117.90	113.84
13	AQ	102	BCL	C2A-C1A-CHA	2.45	128.14	123.86
13	AS	104	BCL	C2A-C1A-CHA	2.45	128.14	123.86
20	bk	104	0V9	O2-C10-O4	-2.45	117.79	123.70
15	bj	101	V7N	C36-C18-C17	-2.45	119.50	122.92
13	AC	1001	BCL	CMB-C2B-C3B	2.45	129.25	124.68
13	BP	1004	BCL	C2A-C1A-CHA	2.44	128.13	123.86
15	bn	101	V7N	C36-C18-C17	-2.44	119.50	122.92
13	bp	103	BCL	C2A-C1A-CHA	2.44	128.13	123.86
13	AO	101	BCL	OBB-CAB-CBB	-2.44	114.68	120.17
13	ah	1001	BCL	OBB-CAB-CBB	-2.44	114.68	120.17
13	AP	103	BCL	C2A-C1A-CHA	2.44	128.13	123.86
13	bg	104	BCL	CMD-C2D-C3D	2.44	129.24	124.68
13	be	104	BCL	CMD-C2D-C3D	2.44	129.24	124.68
22	L	301	BPH	CHC-C1C-NC	-2.44	122.31	125.20
13	BL	1004	BCL	C4A-NA-C1A	2.44	107.80	106.71
13	AE	1002	BCL	OBB-CAB-CBB	-2.44	114.68	120.17
13	bd	103	BCL	OBB-CAB-CBB	-2.44	114.69	120.17
13	ac	102	BCL	OBB-CAB-CBB	-2.44	114.69	120.17
13	BS	1005	BCL	C2A-C1A-CHA	2.43	128.12	123.86
13	AN	102	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
13	M	405	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
14	BP	1002	LMT	C3'-C4'-C5'	-2.43	105.35	110.93
15	BJ	1001	V7N	C35-C13-C12	2.43	121.91	118.08
15	BQ	1001	V7N	C36-C18-C19	2.43	121.91	118.08
13	BE	104	BCL	CAA-CBA-CGA	2.43	120.36	113.25
13	al	1001	BCL	C2A-C1A-CHA	2.43	128.11	123.86
14	ac	101	LMT	C3'-C4'-C5'	-2.43	105.35	110.93
13	bk	105	BCL	CBA-CAA-C2A	2.43	121.03	113.86
13	af	102	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
13	BV	1004	BCL	C2A-C1A-CHA	2.43	128.10	123.86
15	BG	1001	V7N	C35-C13-C12	2.43	121.90	118.08
20	L	310	0V9	O3-C30-O5	-2.43	117.47	123.59
13	ai	102	BCL	C1-C2-C3	2.42	130.24	126.04
13	ag	1001	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
13	aj	102	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
15	BR	1001	V7N	C36-C18-C19	2.42	121.89	118.08
13	bj	104	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
15	bo	101	V7N	C33-C5-C4	2.42	121.89	118.08
13	bd	103	BCL	C2A-C1A-CHA	2.42	128.09	123.86
14	BE	102	LMT	C3'-C4'-C5'	-2.41	105.39	110.93
15	BK	1001	V7N	C36-C18-C19	2.41	121.88	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	ae	1001	BCL	C2A-C1A-CHA	2.41	128.07	123.86
13	bc	103	BCL	CMD-C2D-C3D	2.41	129.18	124.68
13	BQ	1003	BCL	C2A-C1A-CHA	2.41	128.07	123.86
14	bk	101	LMT	C1-O1'-C1'	2.41	117.83	113.84
13	AI	102	BCL	OBB-CAB-CBB	-2.41	114.75	120.17
13	AW	101	BCL	OBB-CAB-CBB	-2.41	114.75	120.17
13	ba	103	BCL	OBB-CAB-CBB	-2.41	114.75	120.17
15	BR	1001	V7N	C35-C13-C12	2.40	121.87	118.08
16	C	1004	HEC	C1D-C2D-C3D	-2.40	105.32	107.00
13	BH	1003	BCL	C2A-C1A-CHA	2.40	128.06	123.86
13	ba	103	BCL	CMD-C2D-C3D	2.40	129.17	124.68
13	AJ	102	BCL	C2A-C1A-CHA	2.40	128.06	123.86
15	BO	1001	V7N	C33-C5-C4	2.40	121.86	118.08
14	BL	1002	LMT	O2'-C2'-C3'	-2.40	104.80	110.35
15	AE	1003	V7N	C36-C18-C19	2.40	121.86	118.08
14	BX	1003	LMT	C1-O1'-C1'	2.40	117.82	113.84
13	AE	1001	BCL	C1C-NC-C4C	2.40	107.78	106.71
14	BO	1002	LMT	C3'-C4'-C5'	-2.40	105.43	110.93
14	BW	1006	LMT	O5'-C1'-C2'	-2.40	105.28	110.35
13	BL	1004	BCL	C2A-C1A-CHA	2.40	128.05	123.86
13	AW	104	BCL	C2A-C1A-CHA	2.40	128.05	123.86
15	BP	1001	V7N	C33-C5-C4	2.40	121.85	118.08
13	AU	102	BCL	C2A-C1A-CHA	2.40	128.05	123.86
15	BQ	1001	V7N	C36-C18-C17	-2.40	119.57	122.92
14	BO	1003	LMT	O5B-C5B-C4B	2.39	114.04	109.69
13	BL	1004	BCL	C4B-C3B-CAB	-2.39	122.50	127.13
13	bj	104	BCL	CMD-C2D-C3D	2.39	129.15	124.68
15	bk	103	V7N	C28-C27-C26	-2.39	119.70	126.42
13	BF	104	BCL	CMD-C2D-C3D	2.39	129.15	124.68
14	bl	101	LMT	O5'-C5'-C4'	2.39	114.80	109.75
14	bh	101	LMT	O5'-C1'-O1'	-2.39	104.31	109.97
15	bl	102	V7N	C36-C18-C19	2.39	121.84	118.08
13	ab	1001	BCL	C4-C3-C5	-2.39	111.25	115.27
21	af	103	CD4	O3-C16-C15	-2.39	101.48	108.43
15	BP	1001	V7N	C35-C13-C12	2.39	121.84	118.08
26	af	101	V7B	O4-C4-C3	2.39	113.64	107.28
15	BW	1001	V7N	C36-C18-C19	2.39	121.84	118.08
13	BW	1003	BCL	CBA-CAA-C2A	2.39	120.91	113.86
13	bk	105	BCL	CMD-C2D-C3D	2.39	129.14	124.68
21	ad	101	CD4	C15-O2-C14	2.38	123.66	117.79
15	BG	1001	V7N	C33-C5-C4	2.38	121.83	118.08
15	BE	101	V7N	C36-C18-C17	-2.38	119.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BJ	1004	BCL	CMD-C2D-C3D	2.38	129.14	124.68
13	ae	1001	BCL	CMD-C2D-C3D	2.38	129.14	124.68
15	BT	1001	V7N	C36-C18-C19	2.38	121.83	118.08
14	BK	1004	LMT	O5'-C5'-C6'	2.38	112.36	106.44
13	BU	1004	BCL	CMD-C2D-C3D	2.38	129.13	124.68
13	L	308	BCL	CMD-C2D-C3D	2.38	129.13	124.68
13	AB	101	BCL	C4B-C3B-CAB	-2.38	122.53	127.13
13	AE	1002	BCL	CMB-C2B-C3B	2.38	129.13	124.68
15	bh	102	V7N	C36-C18-C17	-2.38	119.59	122.92
15	BC	101	V7N	C36-C18-C19	2.38	121.82	118.08
13	L	308	BCL	C4A-NA-C1A	2.38	107.77	106.71
13	BM	1004	BCL	CMD-C2D-C3D	2.38	129.12	124.68
15	BL	1001	V7N	C36-C18-C19	2.37	121.81	118.08
13	AM	101	BCL	OBB-CAB-CBB	-2.37	114.83	120.17
13	AI	102	BCL	C2A-C1A-CHA	2.37	128.00	123.86
13	AD	1001	BCL	OBB-CAB-CBB	-2.37	114.83	120.17
13	AH	101	BCL	C1-O2A-CGA	2.37	122.66	116.44
13	BP	1004	BCL	C1-O2A-CGA	2.37	122.66	116.44
13	BC	103	BCL	C2A-C1A-CHA	2.37	128.00	123.86
21	ai	103	CD4	C16-O3-C17	2.37	125.89	117.12
20	be	102	OV9	O3P-P-O2P	2.37	118.31	109.07
15	BW	1001	V7N	C33-C5-C4	2.37	121.81	118.08
13	BN	1006	BCL	CMD-C2D-C3D	2.37	129.10	124.68
15	BC	101	V7N	C33-C5-C4	2.36	121.80	118.08
13	ai	102	BCL	C2A-C1A-CHA	2.36	127.99	123.86
15	BB	101	V7N	C35-C13-C12	2.36	121.80	118.08
13	BR	1003	BCL	CMD-C2D-C3D	2.36	129.10	124.68
14	BH	1005	LMT	C1-O1'-C1'	2.36	117.76	113.84
14	bp	101	LMT	C2'-C3'-C4'	2.36	115.07	109.68
20	bk	104	OV9	O3-C30-O5	-2.36	117.64	123.59
15	BG	1001	V7N	C36-C18-C19	2.36	121.79	118.08
13	AW	104	BCL	OBB-CAB-CBB	-2.36	114.86	120.17
20	bo	104	OV9	O3P-P-O2P	2.36	118.27	109.07
13	AS	104	BCL	OBB-CAB-CBB	-2.36	114.87	120.17
13	BS	1005	BCL	OBB-CAB-CBB	-2.36	114.87	120.17
13	BM	1004	BCL	OBB-CAB-CBB	-2.35	114.87	120.17
23	an	101	MQ8	O4-C4-C3	2.35	124.34	120.56
13	AB	101	BCL	CMD-C2D-C3D	2.35	129.08	124.68
13	AK	103	BCL	CMD-C2D-C3D	2.35	129.08	124.68
15	BB	101	V7N	C33-C5-C4	2.35	121.78	118.08
20	bf	103	OV9	O3P-P-O2P	2.35	118.26	109.07
15	BX	1001	V7N	C36-C18-C19	2.35	121.78	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BH	1001	V7N	C36-C18-C17	-2.35	119.63	122.92
13	AQ	102	BCL	OBB-CAB-CBB	-2.35	114.88	120.17
13	bh	105	BCL	C2A-C1A-CHA	2.35	127.97	123.86
13	AS	104	BCL	CMD-C2D-C3D	2.35	129.07	124.68
13	ao	1001	BCL	C2A-C1A-CHA	2.35	127.96	123.86
14	bh	103	LMT	C1-O1'-C1'	2.35	117.73	113.84
13	ag	1001	BCL	C2A-C1A-CHA	2.35	127.96	123.86
13	L	308	BCL	CMB-C2B-C3B	2.35	129.07	124.68
13	bj	104	BCL	C2A-C1A-CHA	2.35	127.96	123.86
13	ao	1001	BCL	CMD-C2D-C3D	2.35	129.07	124.68
15	BT	1001	V7N	C36-C18-C17	-2.35	119.64	122.92
17	C	1005	NDG	C1-O5-C5	2.35	115.37	112.19
13	BE	104	BCL	CMD-C2D-C3D	2.34	129.06	124.68
15	bd	101	V7N	C36-C18-C17	-2.34	119.64	122.92
15	BN	1001	V7N	C36-C18-C17	-2.34	119.64	122.92
13	BN	1006	BCL	C2A-C1A-CHA	2.34	127.95	123.86
13	BO	1004	BCL	CMD-C2D-C3D	2.34	129.06	124.68
14	AR	102	LMT	C3'-C4'-C5'	-2.34	105.56	110.93
13	bh	105	BCL	OBB-CAB-CBB	-2.34	114.91	120.17
14	BD	103	LMT	C3'-C4'-C5'	-2.34	105.57	110.93
15	BS	1001	V7N	C36-C18-C17	-2.34	119.65	122.92
13	AD	1002	BCL	CMD-C2D-C3D	2.33	129.05	124.68
13	BA	104	BCL	CMD-C2D-C3D	2.33	129.04	124.68
13	BT	1004	BCL	O2A-C1-C2	-2.33	102.50	108.64
13	AC	1002	BCL	OBB-CAB-CBB	-2.33	114.92	120.17
13	ab	1001	BCL	C2A-C1A-CHA	2.33	127.94	123.86
13	AG	102	BCL	CMD-C2D-C3D	2.33	129.04	124.68
13	BC	103	BCL	CMD-C2D-C3D	2.33	129.04	124.68
15	BX	1001	V7N	C33-C5-C4	2.33	121.75	118.08
13	ad	102	BCL	CMD-C2D-C3D	2.33	129.04	124.68
15	AH	105	V7N	C33-C5-C4	2.33	121.75	118.08
13	AS	102	BCL	OBB-CAB-CBB	-2.33	114.92	120.17
13	BI	104	BCL	CMD-C2D-C3D	2.33	129.04	124.68
13	BP	1004	BCL	CMD-C2D-C3D	2.33	129.04	124.68
15	AH	105	V7N	C36-C18-C17	-2.33	119.66	122.92
14	bl	104	LMT	C1-O1'-C1'	2.33	117.70	113.84
13	AP	103	BCL	OBB-CAB-CBB	-2.33	114.93	120.17
13	AJ	102	BCL	C1C-NC-C4C	2.33	107.75	106.71
13	AJ	101	BCL	CMD-C2D-C3D	2.33	129.03	124.68
13	BO	1004	BCL	C4B-C3B-CAB	-2.33	122.64	127.13
14	AD	1004	LMT	C1-O1'-C1'	2.32	117.69	113.84
14	BK	1006	LMT	O5'-C1'-C2'	-2.32	105.43	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AP	103	BCL	CMD-C2D-C3D	2.32	129.02	124.68
13	AL	101	BCL	CMD-C2D-C3D	2.32	129.02	124.68
15	bn	101	V7N	C7-C6-C5	-2.32	124.00	127.31
13	AP	101	BCL	CMD-C2D-C3D	2.32	129.02	124.68
13	BT	1004	BCL	C1-O2A-CGA	2.32	122.53	116.44
13	BG	1004	BCL	CMD-C2D-C3D	2.32	129.02	124.68
15	bn	101	V7N	C3-C4-C5	2.32	129.40	125.89
13	BJ	1004	BCL	CAA-CBA-CGA	2.32	120.03	113.25
13	AR	101	BCL	CMD-C2D-C3D	2.32	129.02	124.68
13	AM	102	BCL	CMD-C2D-C3D	2.32	129.01	124.68
13	BL	1004	BCL	CMD-C2D-C3D	2.32	129.01	124.68
13	AV	102	BCL	CMD-C2D-C3D	2.32	129.01	124.68
13	AC	1001	BCL	CMD-C2D-C3D	2.32	129.01	124.68
15	BD	101	V7N	C36-C18-C17	-2.32	119.68	122.92
13	AI	102	BCL	CMD-C2D-C3D	2.32	129.01	124.68
13	AB	103	BCL	OBB-CAB-CBB	-2.32	114.96	120.17
21	M	404	CD4	O16-C46-C47	2.32	116.49	111.50
15	BV	1001	V7N	C15-C14-C13	-2.31	124.01	127.31
21	ai	103	CD4	O14-C35-C36	2.31	119.17	111.91
13	ah	1001	BCL	C2A-C1A-CHA	2.31	127.90	123.86
13	AG	103	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	AW	104	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	ac	102	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	bi	103	BCL	C2A-C1A-CHA	2.31	127.90	123.86
13	AE	1002	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	AI	103	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	AT	102	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	BD	106	BCL	CMD-C2D-C3D	2.31	129.00	124.68
17	C1	301	NDG	C1-O5-C5	2.31	115.32	112.19
13	aa	1001	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	AU	102	BCL	OBB-CAB-CBB	-2.31	114.97	120.17
15	BN	1001	V7N	C36-C18-C19	2.31	121.72	118.08
15	BL	1001	V7N	C15-C14-C13	-2.31	124.02	127.31
13	M	405	BCL	CMD-C2D-C3D	2.31	129.00	124.68
13	BE	104	BCL	OBB-CAB-CBB	-2.31	114.98	120.17
13	AS	101	BCL	CMD-C2D-C3D	2.31	128.99	124.68
13	BK	1003	BCL	CMD-C2D-C3D	2.31	128.99	124.68
13	AQ	101	BCL	CMD-C2D-C3D	2.31	128.99	124.68
22	L	301	BPH	CMD-C2D-C3D	2.31	128.99	124.68
13	AF	1001	BCL	CMD-C2D-C3D	2.31	128.99	124.68
13	AK	102	BCL	CMD-C2D-C3D	2.30	128.99	124.68
16	C	1002	HEC	CAA-CBA-CGA	-2.30	108.81	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BF	104	BCL	OBB-CAB-CBB	-2.30	114.98	120.17
13	AO	102	BCL	CMD-C2D-C3D	2.30	128.99	124.68
13	ag	1001	BCL	CMD-C2D-C3D	2.30	128.99	124.68
13	BC	103	BCL	C4B-C3B-CAB	-2.30	122.68	127.13
13	AA	1001	BCL	CMD-C2D-C3D	2.30	128.98	124.68
13	aj	102	BCL	CMD-C2D-C3D	2.30	128.98	124.68
13	an	102	BCL	CMD-C2D-C3D	2.30	128.98	124.68
15	BV	1001	V7N	C33-C5-C4	2.30	121.70	118.08
14	AD	1004	LMT	C3'-C4'-C5'	-2.30	105.65	110.93
15	BS	1001	V7N	C35-C13-C12	2.30	121.70	118.08
14	BA	106	LMT	O5B-C5B-C4B	2.30	113.87	109.69
14	BP	1005	LMT	C3'-C4'-C5'	-2.30	105.66	110.93
20	bf	103	OV9	O2-C10-O4	-2.30	118.15	123.70
13	bg	104	BCL	C2A-C1A-CHA	2.30	127.88	123.86
21	af	104	CD4	O2-C15-C28	2.30	116.72	108.40
13	AH	101	BCL	CMD-C2D-C3D	2.30	128.98	124.68
13	AA	1002	BCL	CMD-C2D-C3D	2.30	128.97	124.68
14	AH	106	LMT	C1-O1'-C1'	2.30	117.65	113.84
15	bc	104	V7N	C35-C13-C12	2.30	121.69	118.08
13	BX	1004	BCL	CMD-C2D-C3D	2.29	128.97	124.68
13	AL	103	BCL	C4B-C3B-CAB	-2.29	122.70	127.13
13	BN	1006	BCL	OBB-CAB-CBB	-2.29	115.01	120.17
13	BV	1004	BCL	CMD-C2D-C3D	2.29	128.97	124.68
13	BB	104	BCL	CMD-C2D-C3D	2.29	128.96	124.68
13	ak	1001	BCL	CMD-C2D-C3D	2.29	128.96	124.68
13	am	1001	BCL	CMD-C2D-C3D	2.29	128.96	124.68
13	BS	1005	BCL	CMD-C2D-C3D	2.29	128.96	124.68
13	AV	103	BCL	OBB-CAB-CBB	-2.29	115.02	120.17
13	BW	1003	BCL	CMD-C2D-C3D	2.29	128.96	124.68
19	H1	1001	PGW	O03-C01-C02	2.29	115.09	108.43
13	AQ	102	BCL	CMD-C2D-C3D	2.29	128.96	124.68
15	bj	101	V7N	C36-C18-C19	2.29	121.68	118.08
13	bc	103	BCL	CBA-CAA-C2A	2.29	120.61	113.86
13	BA	104	BCL	OBB-CAB-CBB	-2.29	115.03	120.17
13	AE	1001	BCL	CMD-C2D-C3D	2.28	128.95	124.68
13	ai	102	BCL	CMD-C2D-C3D	2.28	128.95	124.68
13	BU	1004	BCL	C4B-C3B-CAB	-2.28	122.72	127.13
13	AH	102	BCL	CMD-C2D-C3D	2.28	128.95	124.68
13	BQ	1003	BCL	CMD-C2D-C3D	2.28	128.95	124.68
14	BE	106	LMT	C3B-C4B-C5B	-2.28	106.17	110.24
15	bf	102	V7N	C35-C13-C12	2.28	121.67	118.08
13	AV	103	BCL	CMD-C2D-C3D	2.28	128.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bm	103	BCL	OBB-CAB-CBB	-2.28	115.04	120.17
13	AA	1001	BCL	C11-C10-C8	2.28	123.29	115.92
15	BK	1001	V7N	C35-C13-C12	2.28	121.67	118.08
15	BD	101	V7N	C33-C5-C4	2.28	121.67	118.08
13	af	102	BCL	CMD-C2D-C3D	2.28	128.94	124.68
13	AD	1001	BCL	CMD-C2D-C3D	2.28	128.94	124.68
13	BJ	1004	BCL	OBB-CAB-CBB	-2.28	115.04	120.17
13	AJ	102	BCL	OBB-CAB-CBB	-2.28	115.04	120.17
13	L	303	BCL	OBB-CAB-CBB	-2.28	115.04	120.17
13	BT	1004	BCL	CMD-C2D-C3D	2.28	128.94	124.68
14	bh	101	LMT	O1'-C1'-C2'	2.28	111.86	108.30
13	BT	1004	BCL	C2A-C1A-CHA	2.28	127.84	123.86
13	bo	102	BCL	C2A-C1A-CHA	2.28	127.84	123.86
14	BE	102	LMT	C1-O1'-C1'	2.28	117.61	113.84
13	AN	102	BCL	CMD-C2D-C3D	2.28	128.94	124.68
13	BH	1003	BCL	CBA-CAA-C2A	2.28	120.58	113.86
13	ba	103	BCL	C4A-NA-C1A	2.28	107.73	106.71
13	ah	1001	BCL	CMD-C2D-C3D	2.28	128.94	124.68
14	BK	1002	LMT	C1-O1'-C1'	2.27	117.61	113.84
14	bp	101	LMT	O5'-C5'-C4'	2.27	114.55	109.75
15	BJ	1001	V7N	C36-C18-C17	-2.27	119.74	122.92
13	al	1001	BCL	CMD-C2D-C3D	2.27	128.93	124.68
13	ap	1001	BCL	CMD-C2D-C3D	2.27	128.93	124.68
20	H1	1002	0V9	O3-C30-O5	-2.27	117.86	123.59
13	AO	101	BCL	C4A-NA-C1A	2.27	107.73	106.71
15	BV	1001	V7N	C35-C13-C12	2.27	121.65	118.08
13	AN	102	BCL	C1C-NC-C4C	2.27	107.73	106.71
13	AW	103	BCL	CMD-C2D-C3D	2.27	128.92	124.68
20	be	102	0V9	O3-C30-O5	-2.27	117.87	123.59
14	BJ	1003	LMT	C3'-C4'-C5'	-2.27	105.73	110.93
14	bo	103	LMT	C3'-C4'-C5'	-2.27	105.73	110.93
13	BT	1004	BCL	C11-C10-C8	2.27	123.25	115.92
14	BL	1005	LMT	O5B-C5B-C4B	2.27	113.81	109.69
13	bk	105	BCL	OBB-CAB-CBB	-2.26	115.07	120.17
13	BH	1003	BCL	CMD-C2D-C3D	2.26	128.91	124.68
22	M	406	BPH	CHD-C4C-NC	-2.26	122.51	125.20
13	BD	106	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
13	AS	104	BCL	CAA-CBA-CGA	2.26	119.86	113.25
13	BV	1004	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
15	AT	103	V7N	C15-C14-C13	-2.26	124.08	127.31
13	AX	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
13	AU	103	BCL	CMD-C2D-C3D	2.26	128.91	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bl	105	BCL	C2A-C1A-CHA	2.26	127.81	123.86
15	BT	1001	V7N	C35-C13-C12	2.26	121.64	118.08
13	AE	1001	BCL	OBB-CAB-CBB	-2.26	115.09	120.17
14	bc	101	LMT	C3'-C4'-C5'	-2.26	105.75	110.93
14	BU	1001	LMT	C1-O1'-C1'	2.26	117.58	113.84
13	AJ	102	BCL	CMD-C2D-C3D	2.26	128.90	124.68
21	H1	1003	CD4	O14-C35-C36	2.25	118.98	111.91
13	bp	103	BCL	OBB-CAB-CBB	-2.25	115.10	120.17
13	BG	1004	BCL	OBB-CAB-CBB	-2.25	115.10	120.17
15	AE	1003	V7N	C33-C5-C4	2.25	121.62	118.08
13	BK	1003	BCL	OBB-CAB-CBB	-2.25	115.10	120.17
20	bn	104	OV9	C2-O2-C10	2.25	123.33	117.79
13	AG	102	BCL	OBB-CAB-CBB	-2.25	115.11	120.17
13	aa	1001	BCL	C2A-C1A-CHA	2.25	127.79	123.86
13	AM	101	BCL	CMD-C2D-C3D	2.25	128.88	124.68
20	bi	102	OV9	O3P-P-O2P	2.25	117.84	109.07
13	BS	1005	BCL	C4B-C3B-CAB	-2.24	122.79	127.13
13	bm	103	BCL	C2A-C1A-CHA	2.24	127.78	123.86
13	ab	1001	BCL	CMD-C2D-C3D	2.24	128.88	124.68
22	L	301	BPH	OBB-CAB-CBB	-2.24	114.76	119.73
13	L	303	BCL	CMD-C2D-C3D	2.24	128.87	124.68
23	L	309	MQ8	C20-C21-C22	2.24	119.25	111.88
14	BD	104	LMT	C3'-C4'-C5'	-2.24	105.79	110.93
13	BP	1004	BCL	C4B-C3B-CAB	-2.24	122.80	127.13
15	bo	101	V7N	C36-C18-C19	2.24	121.61	118.08
15	BH	1001	V7N	C35-C13-C12	2.24	121.60	118.08
13	BH	1003	BCL	OBB-CAB-CBB	-2.24	115.13	120.17
14	BF	102	LMT	O5'-C1'-C2'	-2.24	105.61	110.35
14	bj	102	LMT	C3'-C4'-C5'	-2.24	105.80	110.93
13	AW	101	BCL	CBA-CAA-C2A	2.24	120.46	113.86
13	bp	103	BCL	C11-C10-C8	-2.24	108.69	115.92
13	BB	104	BCL	OBB-CAB-CBB	-2.24	115.14	120.17
23	an	101	MQ8	C21-C20-C18	-2.24	105.62	112.98
13	AF	1002	BCL	CMD-C2D-C3D	2.24	128.86	124.68
15	bp	102	V7N	C35-C13-C12	2.24	121.60	118.08
22	M	406	BPH	CMD-C2D-C3D	2.24	128.86	124.68
13	AL	103	BCL	CMD-C2D-C3D	2.23	128.85	124.68
13	ai	102	BCL	C11-C10-C8	2.23	123.14	115.92
13	bo	102	BCL	OBB-CAB-CBB	-2.23	115.15	120.17
15	bc	104	V7N	C36-C18-C19	2.23	121.59	118.08
14	BA	105	LMT	O1'-C1'-C2'	2.23	111.78	108.30
13	BI	104	BCL	C4B-C3B-CAB	-2.23	122.82	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BF	101	LMT	O5'-C1'-O1'	-2.23	104.69	109.97
14	AD	1003	LMT	C3B-C4B-C5B	-2.23	106.26	110.24
13	bf	105	BCL	OBB-CAB-CBB	-2.23	115.16	120.17
14	BX	1002	LMT	C3'-C4'-C5'	-2.23	105.82	110.93
13	BA	104	BCL	C4B-C3B-CAB	-2.23	122.83	127.13
15	bh	102	V7N	C36-C18-C19	2.23	121.58	118.08
13	bi	103	BCL	OBB-CAB-CBB	-2.23	115.16	120.17
13	bg	104	BCL	C1C-NC-C4C	2.22	107.71	106.71
13	BM	1004	BCL	C4B-C3B-CAB	-2.22	122.83	127.13
26	ag	1002	V7B	C9-C8-C7	2.22	117.05	111.79
13	M	403	BCL	C1C-NC-C4C	2.22	107.70	106.71
13	AA	1002	BCL	OBB-CAB-CBB	-2.22	115.17	120.17
13	BT	1004	BCL	OBB-CAB-CBB	-2.22	115.17	120.17
13	AS	102	BCL	CMD-C2D-C3D	2.22	128.83	124.68
15	BO	1001	V7N	C36-C18-C17	-2.22	119.81	122.92
14	BM	1003	LMT	O1'-C1'-C2'	2.22	111.77	108.30
15	bg	101	V7N	C1-C2-C3	2.22	118.94	113.06
15	BN	1001	V7N	C35-C13-C12	2.22	121.57	118.08
15	bm	101	V7N	C1-C2-C3	2.22	118.93	113.06
15	bg	101	V7N	C35-C13-C12	2.22	121.57	118.08
13	AK	103	BCL	OBB-CAB-CBB	-2.22	115.18	120.17
15	BW	1001	V7N	C36-C18-C17	-2.22	119.82	122.92
13	BR	1003	BCL	C4B-C3B-CAB	-2.22	122.85	127.13
15	bo	101	V7N	C35-C13-C12	2.22	121.57	118.08
20	H1	1002	0V9	O2-C10-O4	-2.21	118.35	123.70
13	BR	1003	BCL	C2A-C1A-CHA	2.21	127.73	123.86
13	bg	104	BCL	C4B-C3B-CAB	-2.21	122.85	127.13
26	af	101	V7B	O8-C9-C8	2.21	114.88	108.43
15	AT	103	V7N	C36-C18-C19	2.21	121.56	118.08
15	BP	1001	V7N	C36-C18-C17	-2.21	119.83	122.92
13	BW	1003	BCL	C4B-C3B-CAB	-2.21	122.86	127.13
13	M	403	BCL	CMD-C2D-C3D	2.21	128.81	124.68
15	BK	1001	V7N	C33-C5-C4	2.21	121.56	118.08
13	BW	1003	BCL	OBB-CAB-CBB	-2.21	115.19	120.17
14	AT	101	LMT	C3'-C4'-C5'	-2.21	105.86	110.93
14	BD	102	LMT	C1-O1'-C1'	2.21	117.50	113.84
13	BL	1004	BCL	OBB-CAB-CBB	-2.21	115.20	120.17
13	AB	103	BCL	CMD-C2D-C3D	2.20	128.80	124.68
20	aj	101	0V9	C2-O2-C10	2.20	123.22	117.79
20	bg	102	0V9	O3P-P-O2P	2.20	117.67	109.07
14	BV	1002	LMT	O5'-C1'-C2'	-2.20	105.69	110.35
27	ai	101	UYH	O7-C10-C11	2.20	116.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BG	1004	BCL	CBA-CAA-C2A	2.20	120.36	113.86
13	AH	101	BCL	OBB-CAB-CBB	-2.20	115.22	120.17
13	bc	103	BCL	OBB-CAB-CBB	-2.20	115.22	120.17
13	BX	1004	BCL	CBA-CAA-C2A	2.20	120.36	113.86
13	AO	101	BCL	C2A-C1A-CHA	2.20	127.70	123.86
13	bn	103	BCL	C2A-C1A-CHA	2.20	127.70	123.86
13	AN	102	BCL	C4B-C3B-CAB	-2.20	122.88	127.13
13	AS	104	BCL	C4A-NA-C1A	2.20	107.69	106.71
13	AQ	103	BCL	CMD-C2D-C3D	2.20	128.79	124.68
13	AK	103	BCL	C1C-NC-C4C	2.20	107.69	106.71
13	an	102	BCL	C4B-C3B-CAB	-2.19	122.89	127.13
21	M	404	CD4	O3-C17-C18	2.19	118.79	111.91
13	BC	103	BCL	OBB-CAB-CBB	-2.19	115.23	120.17
13	BI	104	BCL	OBB-CAB-CBB	-2.19	115.23	120.17
15	BQ	1001	V7N	C35-C13-C12	2.19	121.53	118.08
13	AW	101	BCL	C4B-C3B-CAB	-2.19	122.89	127.13
15	BM	1001	V7N	C36-C18-C17	-2.19	119.85	122.92
13	ba	103	BCL	C1C-NC-C4C	2.19	107.69	106.71
14	BW	1006	LMT	C2'-C3'-C4'	2.19	114.68	109.68
13	AW	101	BCL	CMD-C2D-C3D	2.19	128.78	124.68
13	BN	1006	BCL	C1C-NC-C4C	2.19	107.69	106.71
20	bm	102	OV9	O3P-P-O2P	2.19	117.62	109.07
13	ag	1001	BCL	C1C-NC-C4C	2.18	107.69	106.71
13	BP	1004	BCL	OBB-CAB-CBB	-2.18	115.25	120.17
14	AB	104	LMT	C3'-C4'-C5'	-2.18	105.92	110.93
13	AK	103	BCL	C4B-C3B-CAB	-2.18	122.91	127.13
13	AU	102	BCL	CMD-C2D-C3D	2.18	128.76	124.68
13	AN	104	BCL	CMD-C2D-C3D	2.18	128.75	124.68
14	BL	1003	LMT	O5B-C5B-C4B	2.18	113.65	109.69
13	BD	106	BCL	C4B-C3B-CAB	-2.18	122.92	127.13
13	bi	103	BCL	C4B-C3B-CAB	-2.18	122.92	127.13
14	BE	106	LMT	C3'-C4'-C5'	-2.18	105.94	110.93
14	AH	106	LMT	O5'-C1'-C2'	-2.18	105.75	110.35
14	BT	1003	LMT	C1-O1'-C1'	2.17	117.45	113.84
22	M	406	BPH	C6-C5-C3	2.17	119.16	113.45
15	bb	101	V7N	C3-C4-C5	2.17	129.18	125.89
13	BX	1004	BCL	OBB-CAB-CBB	-2.17	115.28	120.17
15	ba	101	V7N	C36-C18-C19	2.17	121.50	118.08
14	bn	102	LMT	C3'-C4'-C5'	-2.17	105.95	110.93
13	AF	1002	BCL	C4B-C3B-CAB	-2.17	122.94	127.13
13	AV	103	BCL	C4B-C3B-CAB	-2.17	122.94	127.13
13	BB	104	BCL	C6-C5-C3	2.17	119.14	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AC	1002	BCL	CMD-C2D-C3D	2.17	128.74	124.68
13	bb	103	BCL	C2A-C1A-CHA	2.17	127.65	123.86
15	be	101	V7N	C36-C18-C17	-2.17	119.89	122.92
15	BQ	1001	V7N	C33-C5-C4	2.17	121.49	118.08
13	bk	105	BCL	C1C-NC-C4C	2.17	107.68	106.71
13	M	403	BCL	CMB-C2B-C3B	2.17	128.73	124.68
13	BO	1004	BCL	OBB-CAB-CBB	-2.16	115.30	120.17
13	AV	103	BCL	C1C-NC-C4C	2.16	107.68	106.71
14	L	307	LMT	C1-O1'-C1'	2.16	117.43	113.84
14	BV	1003	LMT	O1'-C1'-C2'	2.16	111.68	108.30
13	AG	102	BCL	C4B-C3B-CAB	-2.16	122.95	127.13
13	bo	102	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
13	bg	104	BCL	OBB-CAB-CBB	-2.16	115.32	120.17
13	bp	103	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
21	af	103	CD4	C33-O16-C46	2.16	123.10	117.79
13	bh	105	BCL	C4B-C3B-CAB	-2.16	122.97	127.13
13	bf	105	BCL	C2A-C1A-CHA	2.15	127.62	123.86
16	C	1002	HEC	CAD-CBD-CGD	-2.15	109.06	112.67
13	bb	103	BCL	OBB-CAB-CBB	-2.15	115.33	120.17
14	BB	102	LMT	C3'-C4'-C5'	-2.15	105.99	110.93
13	bn	103	BCL	OBB-CAB-CBB	-2.15	115.33	120.17
13	aj	102	BCL	O2A-C1-C2	-2.15	102.99	108.64
15	BD	101	V7N	C35-C13-C12	2.15	121.46	118.08
13	AB	103	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
13	bj	104	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
13	BR	1003	BCL	OBB-CAB-CBB	-2.15	115.34	120.17
13	bj	104	BCL	C1C-NC-C4C	2.14	107.67	106.71
13	BF	104	BCL	C2A-C1A-CHA	2.14	127.61	123.86
13	BU	1004	BCL	OBB-CAB-CBB	-2.14	115.36	120.17
15	bf	102	V7N	C36-C18-C19	2.14	121.44	118.08
13	AQ	102	BCL	C4B-C3B-CAB	-2.14	123.00	127.13
14	BS	1002	LMT	C1'-O5'-C5'	-2.14	109.49	113.69
14	BQ	1002	LMT	C3'-C4'-C5'	-2.14	106.03	110.93
13	AU	102	BCL	CAA-CBA-CGA	2.14	119.50	113.25
13	bk	105	BCL	C2A-C1A-CHA	2.14	127.59	123.86
26	ag	1002	V7B	O8-C28-C29	2.14	118.61	111.91
13	bl	105	BCL	OBB-CAB-CBB	-2.14	115.36	120.17
13	BF	104	BCL	C4B-C3B-CAB	-2.13	123.00	127.13
14	AN	101	LMT	C1-O1'-C1'	2.13	117.38	113.84
13	L	303	BCL	C1C-NC-C4C	2.13	107.67	106.71
14	BD	105	LMT	C3'-C4'-C5'	-2.13	106.04	110.93
14	AF	1003	LMT	C3'-C4'-C5'	-2.13	106.04	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AF	1002	BCL	OBB-CAB-CBB	-2.13	115.37	120.17
13	BT	1004	BCL	C1-C2-C3	-2.13	122.36	126.04
13	AD	1001	BCL	C4B-C3B-CAB	-2.13	123.01	127.13
13	AU	102	BCL	CBA-CAA-C2A	2.13	120.15	113.86
13	bi	103	BCL	C1C-NC-C4C	2.13	107.66	106.71
14	AB	102	LMT	C1'-O5'-C5'	-2.13	109.51	113.69
13	AP	103	BCL	C4B-C3B-CAB	-2.13	123.02	127.13
13	BV	1004	BCL	C4B-C3B-CAB	-2.13	123.02	127.13
13	BX	1004	BCL	C4B-C3B-CAB	-2.13	123.02	127.13
13	AW	104	BCL	C1-C2-C3	-2.12	122.37	126.04
14	BR	1002	LMT	C3'-C4'-C5'	-2.12	106.06	110.93
13	be	104	BCL	OBB-CAB-CBB	-2.12	115.39	120.17
14	bm	104	LMT	C3'-C4'-C5'	-2.12	106.07	110.93
15	bl	102	V7N	C1-C2-C3	2.12	118.67	113.06
13	BQ	1003	BCL	OBB-CAB-CBB	-2.12	115.40	120.17
14	AT	101	LMT	C1'-O5'-C5'	-2.12	109.53	113.69
15	BR	1001	V7N	C36-C18-C17	-2.12	119.95	122.92
20	bn	104	0V9	O1P-P-O4P	-2.12	97.91	107.75
14	bm	104	LMT	O5B-C5B-C4B	2.12	113.54	109.69
13	bc	103	BCL	C1C-NC-C4C	2.12	107.66	106.71
13	bm	103	BCL	C1C-NC-C4C	2.12	107.66	106.71
13	AG	102	BCL	C1-O2A-CGA	2.12	122.00	116.44
14	BC	104	LMT	O5B-C5B-C4B	2.12	113.54	109.69
13	ai	102	BCL	C4B-C3B-CAB	-2.12	123.04	127.13
14	BS	1004	LMT	O5'-C1'-C2'	-2.12	105.87	110.35
13	L	303	BCL	C4A-NA-C1A	2.12	107.66	106.71
14	bl	104	LMT	C1'-O5'-C5'	-2.11	109.54	113.69
14	BP	1003	LMT	C3'-C4'-C5'	-2.11	106.08	110.93
27	ai	101	UYH	C12-C11-C10	-2.11	105.94	113.62
20	ba	102	0V9	O2-C10-O4	-2.11	118.60	123.70
13	bl	105	BCL	C1C-NC-C4C	2.11	107.65	106.71
13	L	308	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
17	C	1005	NDG	O4-C4-C3	-2.11	105.48	110.35
13	bn	103	BCL	C4B-C3B-CAB	-2.11	123.06	127.13
13	BB	104	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
14	BU	1002	LMT	C3'-C4'-C5'	-2.10	106.10	110.93
14	BJ	1002	LMT	O5'-C1'-C2'	-2.10	105.89	110.35
13	AA	1002	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
13	BE	104	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
13	AB	103	BCL	CBA-CAA-C2A	2.10	120.07	113.86
13	BJ	1004	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
14	BH	1005	LMT	C3'-C4'-C5'	-2.10	106.11	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	be	104	BCL	C2A-C1A-CHA	2.10	127.53	123.86
13	AQ	103	BCL	OBB-CAB-CBB	-2.10	115.44	120.17
16	C	1003	HEC	C1D-C2D-C3D	-2.10	105.54	107.00
20	bc	102	0V9	O2-C10-O4	-2.10	118.63	123.70
14	BL	1002	LMT	O5'-C1'-C2'	-2.10	105.91	110.35
14	bf	104	LMT	C1'-O5'-C5'	-2.09	109.58	113.69
13	AM	101	BCL	CBA-CAA-C2A	2.09	120.04	113.86
15	bn	101	V7N	C36-C18-C19	2.09	121.37	118.08
13	BH	1003	BCL	C4B-C3B-CAB	-2.09	123.09	127.13
14	bb	102	LMT	C1-O1'-C1'	2.09	117.30	113.84
21	M	404	CD4	C48-C47-C46	-2.09	106.03	113.62
15	bp	102	V7N	C36-C18-C19	2.09	121.36	118.08
14	BG	1003	LMT	C1'-O5'-C5'	-2.08	109.60	113.69
14	bl	101	LMT	C2'-C3'-C4'	2.08	114.44	109.68
14	AW	102	LMT	O1B-C1B-C2B	2.08	113.49	108.10
15	bg	101	V7N	C29-C28-C27	-2.08	116.72	123.22
13	AS	104	BCL	C4B-C3B-CAB	-2.08	123.11	127.13
13	AQ	102	BCL	C1C-NC-C4C	2.08	107.64	106.71
15	bk	103	V7N	C36-C18-C19	2.08	121.35	118.08
14	BK	1005	LMT	C1-O1'-C1'	2.08	117.28	113.84
14	bf	101	LMT	O5'-C1'-O1'	-2.08	105.06	109.97
13	bh	105	BCL	C1C-NC-C4C	2.08	107.64	106.71
13	AJ	102	BCL	C4B-C3B-CAB	-2.07	123.12	127.13
15	ba	101	V7N	C30-C1-C2	-2.07	107.68	110.86
20	bj	103	0V9	O3-C30-O5	-2.07	118.36	123.59
22	L	301	BPH	C1-O2A-CGA	2.07	121.87	116.44
13	AP	103	BCL	C6-C5-C3	2.07	118.88	113.45
14	BN	1005	LMT	C3B-C4B-C5B	-2.07	106.55	110.24
14	bd	102	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
15	AT	103	V7N	C35-C13-C12	2.07	121.33	118.08
13	bd	103	BCL	C4B-C3B-CAB	-2.07	123.14	127.13
13	AA	1002	BCL	C1C-NC-C4C	2.07	107.64	106.71
20	bg	102	0V9	O3-C30-O5	-2.06	118.38	123.59
15	AT	103	V7N	C4-C5-C6	-2.06	115.78	118.94
21	ai	103	CD4	O16-C46-C47	2.06	115.94	111.50
13	ab	1001	BCL	C1-O2A-CGA	2.06	121.85	116.44
14	AH	106	LMT	O5'-C5'-C4'	2.06	114.09	109.75
14	bc	101	LMT	O5B-C5B-C4B	2.06	113.43	109.69
14	BI	105	LMT	C3'-C4'-C5'	-2.06	106.21	110.93
13	AM	101	BCL	C1C-NC-C4C	2.06	107.63	106.71
13	be	104	BCL	C1C-NC-C4C	2.06	107.63	106.71
13	BB	104	BCL	C1-C2-C3	2.05	129.60	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	bc	101	LMT	O5'-C1'-O1'	-2.05	105.11	109.97
14	bl	101	LMT	C1'-O5'-C5'	-2.05	109.66	113.69
14	BN	1003	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
20	bh	104	0V9	O2-C10-O4	-2.05	118.75	123.70
20	aj	101	0V9	O3P-P-O2P	2.05	117.08	109.07
15	AT	103	V7N	C29-C28-C27	-2.05	116.82	123.22
13	bi	103	BCL	C1-C2-C3	-2.05	122.50	126.04
13	bb	103	BCL	C1C-NC-C4C	2.05	107.63	106.71
13	BA	104	BCL	C7-C6-C5	2.05	118.92	113.36
15	BH	1001	V7N	C3-C4-C5	2.05	128.98	125.89
15	BG	1001	V7N	C15-C14-C13	-2.05	124.39	127.31
14	AV	101	LMT	O1'-C1'-C2'	2.05	111.50	108.30
13	bc	103	BCL	C4B-C3B-CAB	-2.04	123.18	127.13
21	ai	103	CD4	C33-O16-C46	2.04	122.82	117.79
14	BR	1006	LMT	C1-O1'-C1'	2.04	117.22	113.84
13	AS	102	BCL	C4B-C3B-CAB	-2.04	123.19	127.13
15	bf	102	V7N	C1-C2-C3	2.04	118.46	113.06
21	ai	103	CD4	O2-C14-O1	-2.04	118.78	123.70
20	bk	104	0V9	O3P-P-O2P	2.04	117.03	109.07
13	bb	103	BCL	C4B-C3B-CAB	-2.04	123.19	127.13
13	ak	1001	BCL	C6-C5-C3	2.04	118.80	113.45
14	bf	104	LMT	C3'-C4'-C5'	-2.04	106.26	110.93
13	AF	1002	BCL	C1-O2A-CGA	2.04	121.78	116.44
13	AW	104	BCL	C1C-NC-C4C	2.04	107.62	106.71
15	BA	101	V7N	C36-C18-C17	-2.03	120.07	122.92
15	BN	1001	V7N	C38-C26-C27	-2.03	114.87	118.08
20	bk	102	0V9	O3P-P-O2P	2.03	117.00	109.07
14	AG	101	LMT	C1'-O5'-C5'	-2.03	109.70	113.69
13	AM	101	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
20	bi	102	0V9	O3-C30-O5	-2.03	118.47	123.59
14	AD	1003	LMT	C1'-O5'-C5'	-2.03	109.71	113.69
20	bc	102	0V9	O3P-P-O2P	2.03	116.98	109.07
14	BL	1003	LMT	C1'-O5'-C5'	-2.03	109.71	113.69
14	bj	102	LMT	O5'-C1'-O1'	-2.03	105.18	109.97
13	BS	1005	BCL	C1-C2-C3	2.03	129.55	126.04
14	AN	103	LMT	C3'-C4'-C5'	-2.02	106.28	110.93
13	BG	1004	BCL	C4B-C3B-CAB	-2.02	123.22	127.13
26	ag	1002	V7B	O6-C5-C4	-2.02	105.49	109.75
14	BT	1002	LMT	C3B-C4B-C5B	-2.02	106.63	110.24
14	BQ	1002	LMT	C1'-O5'-C5'	-2.02	109.72	113.69
15	bi	101	V7N	C15-C14-C13	-2.02	124.43	127.31
14	AS	103	LMT	C1'-O5'-C5'	-2.02	109.72	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	bd	101	V7N	C15-C14-C13	-2.02	124.43	127.31
23	L	309	MQ8	C16-C17-C18	-2.02	122.80	127.66
20	bf	103	0V9	O3-C30-O5	-2.02	118.50	123.59
14	AB	102	LMT	O1'-C1'-C2'	2.02	111.45	108.30
13	BP	1004	BCL	CBA-CAA-C2A	2.02	119.82	113.86
22	L	301	BPH	C3A-C4A-CHB	2.02	125.31	121.83
13	M	403	BCL	OBB-CAB-CBB	-2.02	115.63	120.17
13	BT	1004	BCL	CBA-CAA-C2A	2.01	119.81	113.86
13	AF	1001	BCL	C6-C5-C3	2.01	118.74	113.45
14	BN	1005	LMT	C3'-C4'-C5'	-2.01	106.31	110.93
14	BA	105	LMT	C1'-O5'-C5'	-2.01	109.74	113.69
14	BX	1002	LMT	C1'-O5'-C5'	-2.01	109.74	113.69
13	ac	102	BCL	C4B-C3B-CAB	-2.01	123.24	127.13
20	ba	104	0V9	O1P-P-O4P	-2.01	98.40	107.75
13	bf	105	BCL	C1C-NC-C4C	2.01	107.61	106.71
13	AE	1001	BCL	CBA-CAA-C2A	2.01	119.80	113.86
13	BT	1004	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
13	aj	102	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
13	AW	101	BCL	C1C-NC-C4C	2.01	107.61	106.71
14	AG	101	LMT	C3B-C4B-C5B	-2.01	106.66	110.24
13	BO	1004	BCL	CBA-CAA-C2A	2.01	119.79	113.86
14	BT	1005	LMT	O5B-C5B-C4B	2.01	113.34	109.69
15	BE	101	V7N	C33-C5-C4	2.01	121.24	118.08
14	BE	105	LMT	C1'-O5'-C5'	-2.01	109.75	113.69
20	bb	104	0V9	O3P-P-O2P	2.01	116.90	109.07
20	bc	102	0V9	O3-C30-O5	-2.00	118.53	123.59
14	bg	103	LMT	C3'-C4'-C5'	-2.00	106.33	110.93
13	af	102	BCL	C4B-C3B-CAB	-2.00	123.26	127.13
14	AW	102	LMT	C1-O1'-C1'	2.00	117.16	113.84
20	bh	104	0V9	O3-C30-O5	-2.00	118.54	123.59

There are no chirality outliers.

All (1852) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	AB	103	BCL	C1A-C2A-CAA-CBA
13	AB	103	BCL	C3A-C2A-CAA-CBA
13	AD	1001	BCL	C3A-C2A-CAA-CBA
13	AF	1002	BCL	C1A-C2A-CAA-CBA
13	AG	102	BCL	C1A-C2A-CAA-CBA
13	AG	102	BCL	CHA-CBD-CGD-O1D
13	AJ	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	AJ	102	BCL	C3A-C2A-CAA-CBA
13	AJ	102	BCL	CHA-CBD-CGD-O1D
13	AJ	102	BCL	CHA-CBD-CGD-O2D
13	AK	103	BCL	CHA-CBD-CGD-O1D
13	AK	103	BCL	CHA-CBD-CGD-O2D
13	AL	103	BCL	C3A-C2A-CAA-CBA
13	AN	102	BCL	CHA-CBD-CGD-O1D
13	AN	102	BCL	CHA-CBD-CGD-O2D
13	AO	101	BCL	C1A-C2A-CAA-CBA
13	AO	101	BCL	C3A-C2A-CAA-CBA
13	AQ	103	BCL	CBD-CGD-O2D-CED
13	AQ	103	BCL	O1D-CGD-O2D-CED
13	AS	104	BCL	C3A-C2A-CAA-CBA
13	AS	104	BCL	CHA-CBD-CGD-O1D
13	AU	102	BCL	C1A-C2A-CAA-CBA
13	AU	102	BCL	C3A-C2A-CAA-CBA
13	AW	101	BCL	O2A-C1-C2-C3
13	AW	104	BCL	C1A-C2A-CAA-CBA
13	AW	104	BCL	C3A-C2A-CAA-CBA
13	AW	104	BCL	CHA-CBD-CGD-O1D
13	BA	104	BCL	O2A-C1-C2-C3
13	BC	103	BCL	O2A-C1-C2-C3
13	BF	104	BCL	C1A-C2A-CAA-CBA
13	BG	1004	BCL	O2A-C1-C2-C3
13	BK	1003	BCL	CHA-CBD-CGD-O1D
13	BK	1003	BCL	O2A-C1-C2-C3
13	BL	1004	BCL	C1A-C2A-CAA-CBA
13	BN	1006	BCL	O2A-C1-C2-C3
13	BR	1003	BCL	C1A-C2A-CAA-CBA
13	BS	1005	BCL	O2A-C1-C2-C3
13	aa	1001	BCL	O2A-C1-C2-C3
13	bc	103	BCL	C1A-C2A-CAA-CBA
13	bc	103	BCL	C3A-C2A-CAA-CBA
13	bf	105	BCL	C1A-C2A-CAA-CBA
13	bf	105	BCL	C3A-C2A-CAA-CBA
13	bk	105	BCL	C1A-C2A-CAA-CBA
13	bk	105	BCL	C3A-C2A-CAA-CBA
13	bl	105	BCL	C1A-C2A-CAA-CBA
14	AA	1003	LMT	C2'-C1'-O1'-C1
14	AA	1003	LMT	O5'-C1'-O1'-C1
14	AN	101	LMT	C2'-C1'-O1'-C1
14	AN	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
14	AO	103	LMT	C2-C1-O1'-C1'
14	AR	102	LMT	C2'-C1'-O1'-C1
14	AR	102	LMT	O5'-C1'-O1'-C1
14	AR	102	LMT	C2-C1-O1'-C1'
14	AV	101	LMT	C2-C1-O1'-C1'
14	BA	102	LMT	C2-C1-O1'-C1'
14	BA	103	LMT	C2'-C1'-O1'-C1
14	BA	103	LMT	O5'-C1'-O1'-C1
14	BA	106	LMT	C2'-C1'-O1'-C1
14	BC	102	LMT	C2-C1-O1'-C1'
14	BE	102	LMT	C2-C1-O1'-C1'
14	BE	103	LMT	C2'-C1'-O1'-C1
14	BE	103	LMT	O5'-C1'-O1'-C1
14	BF	101	LMT	O5'-C1'-O1'-C1
14	BF	101	LMT	C2-C1-O1'-C1'
14	BI	103	LMT	C2-C1-O1'-C1'
14	BL	1002	LMT	O5'-C1'-O1'-C1
14	BL	1005	LMT	C2'-C1'-O1'-C1
14	BL	1005	LMT	O5'-C1'-O1'-C1
14	BP	1006	LMT	C2-C1-O1'-C1'
14	BT	1005	LMT	O5'-C1'-O1'-C1
14	BU	1001	LMT	C2'-C1'-O1'-C1
14	BU	1001	LMT	O5'-C1'-O1'-C1
14	BU	1003	LMT	C2'-C1'-O1'-C1
14	BU	1003	LMT	O5'-C1'-O1'-C1
14	BU	1003	LMT	C2-C1-O1'-C1'
14	BW	1005	LMT	C2'-C1'-O1'-C1
14	BW	1005	LMT	O5'-C1'-O1'-C1
14	BW	1006	LMT	C2'-C1'-O1'-C1
14	BW	1006	LMT	O5'-C1'-O1'-C1
14	L	305	LMT	C2'-C1'-O1'-C1
14	L	305	LMT	O5'-C1'-O1'-C1
14	bc	101	LMT	O5'-C1'-O1'-C1
14	bc	101	LMT	C2-C1-O1'-C1'
14	bd	102	LMT	C2'-C1'-O1'-C1
14	bd	102	LMT	O5'-C1'-O1'-C1
14	bg	103	LMT	C2-C1-O1'-C1'
14	bh	101	LMT	C2'-C1'-O1'-C1
14	bh	101	LMT	O5'-C1'-O1'-C1
14	bl	104	LMT	C2-C1-O1'-C1'
15	AE	1003	V7N	C27-C28-C29-C39
15	AH	105	V7N	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
15	AH	105	V7N	C38-C26-C27-C28
15	AH	105	V7N	C3-C4-C5-C33
15	AH	105	V7N	C3-C4-C5-C6
15	AT	103	V7N	C25-C26-C27-C28
15	AT	103	V7N	C38-C26-C27-C28
15	AT	103	V7N	C7-C8-C9-C10
15	BA	101	V7N	C25-C26-C27-C28
15	BA	101	V7N	C38-C26-C27-C28
15	BA	101	V7N	C27-C28-C29-C39
15	BC	101	V7N	C27-C28-C29-C39
15	BD	101	V7N	C25-C26-C27-C28
15	BD	101	V7N	C38-C26-C27-C28
15	BE	101	V7N	C25-C26-C27-C28
15	BE	101	V7N	C38-C26-C27-C28
15	BG	1001	V7N	C25-C26-C27-C28
15	BG	1001	V7N	C38-C26-C27-C28
15	BG	1001	V7N	C27-C28-C29-C39
15	BJ	1001	V7N	C25-C26-C27-C28
15	BL	1001	V7N	O42-C34-C9-C10
15	BL	1001	V7N	O42-C34-C9-C8
15	BM	1001	V7N	C25-C26-C27-C28
15	BM	1001	V7N	C38-C26-C27-C28
15	BN	1001	V7N	C27-C28-C29-C39
15	BS	1001	V7N	C25-C26-C27-C28
15	BS	1001	V7N	C38-C26-C27-C28
15	BV	1001	V7N	C26-C27-C28-C29
15	BV	1001	V7N	C27-C28-C29-C39
15	BX	1001	V7N	C27-C28-C29-C39
15	BX	1001	V7N	O42-C34-C9-C10
15	ba	101	V7N	C25-C26-C27-C28
15	ba	101	V7N	C38-C26-C27-C28
15	ba	101	V7N	C27-C28-C29-C39
15	bb	101	V7N	C30-C1-C2-C3
15	bb	101	V7N	C31-C1-C2-C3
15	bb	101	V7N	O32-C1-C2-C3
15	bb	101	V7N	O42-C34-C9-C10
15	bc	104	V7N	C25-C26-C27-C28
15	bc	104	V7N	C38-C26-C27-C28
15	be	101	V7N	C38-C26-C27-C28
15	be	101	V7N	O42-C34-C9-C10
15	be	101	V7N	O42-C34-C9-C8
15	bg	101	V7N	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
15	bh	102	V7N	C25-C26-C27-C28
15	bh	102	V7N	C38-C26-C27-C28
15	bh	102	V7N	C3-C4-C5-C33
15	bj	101	V7N	C25-C26-C27-C28
15	bj	101	V7N	C38-C26-C27-C28
15	bl	102	V7N	O32-C1-C2-C3
15	bl	102	V7N	C25-C26-C27-C28
15	bl	102	V7N	C38-C26-C27-C28
15	bl	102	V7N	C27-C28-C29-C39
15	bm	101	V7N	C25-C26-C27-C28
15	bm	101	V7N	C38-C26-C27-C28
15	bn	101	V7N	C25-C26-C27-C28
15	bn	101	V7N	C38-C26-C27-C28
15	bn	101	V7N	C3-C4-C5-C6
15	bo	101	V7N	C25-C26-C27-C28
15	bo	101	V7N	C38-C26-C27-C28
15	bp	102	V7N	C25-C26-C27-C28
15	bp	102	V7N	C38-C26-C27-C28
15	bp	102	V7N	C3-C4-C5-C33
15	bp	102	V7N	C3-C4-C5-C6
19	H1	1001	PGW	C02-C03-O11-P
20	L	310	0V9	C4-O4P-P-O2P
20	aj	101	0V9	C5-C4-O4P-P
20	aj	101	0V9	C4-O4P-P-O2P
20	ba	102	0V9	C2-C1-O3P-P
20	ba	102	0V9	C5-C4-O4P-P
20	ba	104	0V9	C2-C1-O3P-P
20	ba	104	0V9	C5-C4-O4P-P
20	ba	104	0V9	C1-O3P-P-O2P
20	ba	104	0V9	C1-O3P-P-O4P
20	bb	104	0V9	O2-C2-C3-O3
20	bb	104	0V9	C2-C1-O3P-P
20	bc	102	0V9	O2-C2-C3-O3
20	bc	102	0V9	C2-C1-O3P-P
20	bc	102	0V9	C4-O4P-P-O2P
20	bc	102	0V9	C4-O4P-P-O3P
20	be	102	0V9	C5-C4-O4P-P
20	be	102	0V9	C4-O4P-P-O2P
20	be	103	0V9	O2-C2-C3-O3
20	be	103	0V9	C2-C1-O3P-P
20	bf	103	0V9	C2-C1-O3P-P
20	bf	103	0V9	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
20	bg	102	0V9	C5-C4-O4P-P
20	bh	104	0V9	C2-C1-O3P-P
20	bh	104	0V9	C4-O4P-P-O1P
20	bh	104	0V9	C4-O4P-P-O2P
20	bj	103	0V9	C2-C1-O3P-P
20	bk	102	0V9	C1-O3P-P-O2P
20	bk	104	0V9	C2-C1-O3P-P
20	bk	104	0V9	C1-O3P-P-O4P
20	bl	103	0V9	C2-C1-O3P-P
20	bl	103	0V9	C5-C4-O4P-P
20	bn	104	0V9	C5-C4-O4P-P
20	bn	104	0V9	C1-O3P-P-O2P
20	bn	104	0V9	C1-O3P-P-O4P
21	H1	1003	CD4	C29-O8-P1-O5
21	H1	1003	CD4	C29-O8-P1-O6
21	H1	1003	CD4	C29-O8-P1-O7
21	M	404	CD4	C13-C14-O2-C15
21	M	404	CD4	C29-O8-P1-O7
21	ad	101	CD4	C13-C14-O2-C15
21	ad	101	CD4	C29-O8-P1-O5
21	ad	101	CD4	C29-O8-P1-O7
21	af	103	CD4	C16-C15-O2-C14
21	af	103	CD4	C15-C28-O5-P1
21	ai	103	CD4	C13-C14-O2-C15
22	M	406	BPH	C4B-C3B-CAB-OBB
23	L	309	MQ8	C27-C28-C30-C31
23	L	309	MQ8	C29-C28-C30-C31
23	an	101	MQ8	C12-C11-C3-C2
23	an	101	MQ8	C12-C11-C3-C4
23	an	101	MQ8	C13-C15-C16-C17
14	BL	1003	LMT	O5B-C1B-O1B-C4'
14	BL	1005	LMT	O5B-C1B-O1B-C4'
14	bp	101	LMT	O5B-C1B-O1B-C4'
26	af	101	V7B	O52-C43-O4-C4
14	AW	102	LMT	O5B-C1B-O1B-C4'
21	ad	101	CD4	O1-C14-O2-C15
21	af	103	CD4	O1-C14-O2-C15
21	ai	103	CD4	O1-C14-O2-C15
14	AW	102	LMT	C2B-C1B-O1B-C4'
14	bp	101	LMT	C2B-C1B-O1B-C4'
13	AK	103	BCL	C3-C5-C6-C7
13	AU	103	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	BV	1004	BCL	C3-C5-C6-C7
13	ao	1001	BCL	C3-C5-C6-C7
13	bk	105	BCL	C3-C5-C6-C7
14	BW	1006	LMT	O5B-C1B-O1B-C4'
14	L	304	LMT	O5B-C1B-O1B-C4'
14	BW	1006	LMT	C5'-C4'-O1B-C1B
13	AC	1002	BCL	C2A-CAA-CBA-CGA
13	BC	103	BCL	C2A-CAA-CBA-CGA
13	BX	1004	BCL	C2A-CAA-CBA-CGA
13	AE	1001	BCL	C3-C5-C6-C7
14	BA	106	LMT	O5B-C1B-O1B-C4'
14	BO	1003	LMT	O5B-C1B-O1B-C4'
21	M	404	CD4	O1-C14-O2-C15
15	bg	101	V7N	C27-C28-C29-C39
14	BW	1006	LMT	C2B-C1B-O1B-C4'
14	AU	101	LMT	O5'-C5'-C6'-O6'
21	ad	101	CD4	O9-C30-C31-O10
13	bl	105	BCL	C3-C5-C6-C7
14	L	304	LMT	C2B-C1B-O1B-C4'
14	AF	1003	LMT	O5'-C5'-C6'-O6'
14	AG	101	LMT	O5'-C5'-C6'-O6'
14	bf	101	LMT	O5'-C5'-C6'-O6'
14	BR	1004	LMT	O5B-C1B-O1B-C4'
14	bg	103	LMT	O5B-C1B-O1B-C4'
14	BM	1003	LMT	O5'-C5'-C6'-O6'
14	BX	1002	LMT	O5'-C5'-C6'-O6'
14	bc	101	LMT	O5B-C5B-C6B-O6B
14	BE	106	LMT	O5B-C1B-O1B-C4'
14	BO	1003	LMT	C2B-C1B-O1B-C4'
14	BF	102	LMT	O5'-C5'-C6'-O6'
14	BG	1003	LMT	O5'-C5'-C6'-O6'
14	bd	102	LMT	O5B-C5B-C6B-O6B
14	AB	104	LMT	O5B-C5B-C6B-O6B
14	AP	102	LMT	O5'-C5'-C6'-O6'
14	BQ	1004	LMT	O5'-C5'-C6'-O6'
14	bh	101	LMT	O5'-C5'-C6'-O6'
20	aj	101	OV9	C2-C1-O3P-P
20	bn	104	OV9	C2-C1-O3P-P
14	AL	102	LMT	O5'-C5'-C6'-O6'
14	BW	1006	LMT	O5'-C5'-C6'-O6'
14	ac	101	LMT	O5'-C5'-C6'-O6'
14	BA	106	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
14	BW	1002	LMT	O5'-C1'-O1'-C1
23	L	309	MQ8	C33-C35-C36-C37
13	AC	1001	BCL	C3-C5-C6-C7
14	BI	105	LMT	O5B-C1B-O1B-C4'
14	BR	1005	LMT	O5B-C1B-O1B-C4'
14	AU	101	LMT	C4'-C5'-C6'-O6'
14	BD	103	LMT	O5'-C5'-C6'-O6'
14	bm	104	LMT	O5B-C5B-C6B-O6B
21	ad	101	CD4	C29-C30-C31-O10
26	af	101	V7B	O52-C47-C48-O53
14	BW	1006	LMT	C4'-C5'-C6'-O6'
14	AL	102	LMT	C4B-C5B-C6B-O6B
14	BR	1004	LMT	C5'-C4'-O1B-C1B
14	L	307	LMT	O5B-C1B-O1B-C4'
14	BG	1002	LMT	O5'-C5'-C6'-O6'
14	BN	1003	LMT	O5'-C5'-C6'-O6'
14	AF	1003	LMT	C4'-C5'-C6'-O6'
13	AE	1002	BCL	C15-C16-C17-C18
21	af	104	CD4	O8-C29-C30-O9
14	AH	106	LMT	C2'-C1'-O1'-C1
14	BE	105	LMT	C2'-C1'-O1'-C1
14	BF	101	LMT	C2'-C1'-O1'-C1
14	BT	1005	LMT	C2'-C1'-O1'-C1
14	bc	101	LMT	C2'-C1'-O1'-C1
20	bf	103	OV9	C12-C13-C14-C15
13	AA	1002	BCL	C6-C7-C8-C9
13	AC	1002	BCL	C11-C12-C13-C14
13	BA	104	BCL	C6-C7-C8-C9
13	BS	1005	BCL	C11-C10-C8-C9
13	M	403	BCL	C11-C10-C8-C9
13	ab	1001	BCL	C6-C7-C8-C9
15	AE	1003	V7N	C38-C26-C27-C28
15	BC	101	V7N	C38-C26-C27-C28
15	BH	1001	V7N	C38-C26-C27-C28
15	BH	1001	V7N	C3-C4-C5-C33
15	BJ	1001	V7N	C38-C26-C27-C28
15	BK	1001	V7N	C38-C26-C27-C28
15	BL	1001	V7N	C38-C26-C27-C28
15	BN	1001	V7N	C38-C26-C27-C28
15	BN	1001	V7N	C3-C4-C5-C33
15	BO	1001	V7N	C38-C26-C27-C28
15	BP	1001	V7N	C38-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
15	BR	1001	V7N	C38-C26-C27-C28
15	BR	1001	V7N	C3-C4-C5-C33
15	BS	1001	V7N	C3-C4-C5-C33
15	BT	1001	V7N	C38-C26-C27-C28
15	BW	1001	V7N	C38-C26-C27-C28
15	BX	1001	V7N	C38-C26-C27-C28
15	bb	101	V7N	C38-C26-C27-C28
15	bb	101	V7N	C3-C4-C5-C33
15	bf	102	V7N	C38-C26-C27-C28
15	bg	101	V7N	C38-C26-C27-C28
15	bk	103	V7N	C38-C26-C27-C28
15	AE	1003	V7N	C25-C26-C27-C28
15	BB	101	V7N	C25-C26-C27-C28
15	BC	101	V7N	C25-C26-C27-C28
15	BH	1001	V7N	C25-C26-C27-C28
15	BH	1001	V7N	C3-C4-C5-C6
15	BK	1001	V7N	C25-C26-C27-C28
15	BL	1001	V7N	C25-C26-C27-C28
15	BN	1001	V7N	C25-C26-C27-C28
15	BN	1001	V7N	C3-C4-C5-C6
15	BO	1001	V7N	C25-C26-C27-C28
15	BP	1001	V7N	C25-C26-C27-C28
15	BR	1001	V7N	C25-C26-C27-C28
15	BR	1001	V7N	C3-C4-C5-C6
15	BT	1001	V7N	C25-C26-C27-C28
15	BW	1001	V7N	C25-C26-C27-C28
15	BX	1001	V7N	C25-C26-C27-C28
15	bb	101	V7N	C25-C26-C27-C28
15	bb	101	V7N	C3-C4-C5-C6
15	be	101	V7N	C25-C26-C27-C28
15	bg	101	V7N	C25-C26-C27-C28
15	bk	103	V7N	C25-C26-C27-C28
14	M	402	LMT	O5'-C5'-C6'-O6'
14	bd	102	LMT	O5'-C5'-C6'-O6'
14	bp	101	LMT	O5'-C5'-C6'-O6'
14	BG	1003	LMT	C4'-C5'-C6'-O6'
14	BX	1002	LMT	C4'-C5'-C6'-O6'
14	bk	101	LMT	C2B-C1B-O1B-C4'
13	bg	104	BCL	C5-C6-C7-C8
14	BS	1003	LMT	O5'-C5'-C6'-O6'
14	BS	1004	LMT	O5'-C5'-C6'-O6'
14	ac	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
14	BD	105	LMT	O5B-C1B-O1B-C4'
14	AJ	103	LMT	C2B-C1B-O1B-C4'
14	bj	102	LMT	O5'-C5'-C6'-O6'
13	AH	101	BCL	C10-C11-C12-C13
13	AS	104	BCL	C5-C6-C7-C8
13	AX	101	BCL	C13-C15-C16-C17
14	L	307	LMT	C2B-C1B-O1B-C4'
14	bb	102	LMT	O5B-C5B-C6B-O6B
13	BL	1004	BCL	C5-C6-C7-C8
13	ap	1001	BCL	C8-C10-C11-C12
14	BL	1002	LMT	C5'-C4'-O1B-C1B
14	BR	1002	LMT	O5B-C1B-O1B-C4'
14	BO	1002	LMT	O5'-C5'-C6'-O6'
14	AG	101	LMT	C1-C2-C3-C4
14	bo	103	LMT	O1'-C1-C2-C3
13	AI	103	BCL	C10-C11-C12-C13
14	AD	1003	LMT	O5B-C1B-O1B-C4'
14	AJ	103	LMT	O5B-C1B-O1B-C4'
14	BF	102	LMT	C4'-C5'-C6'-O6'
13	ab	1001	BCL	C6-C7-C8-C10
13	bn	103	BCL	C6-C7-C8-C10
14	L	302	LMT	C1-C2-C3-C4
20	ba	104	0V9	C38-C39-C40-C41
15	AH	105	V7N	C27-C28-C29-C39
15	AT	103	V7N	C27-C28-C29-C39
15	bb	101	V7N	C27-C28-C29-C39
15	bf	102	V7N	C27-C28-C29-C39
15	bi	101	V7N	C27-C28-C29-C39
15	bn	101	V7N	C27-C28-C29-C39
15	bp	102	V7N	C27-C28-C29-C39
13	AH	101	BCL	C2A-CAA-CBA-CGA
13	AR	101	BCL	C5-C6-C7-C8
14	AB	104	LMT	C4B-C5B-C6B-O6B
26	ag	1002	V7B	O52-C47-C48-O53
14	AP	102	LMT	C4'-C5'-C6'-O6'
14	bf	101	LMT	C4'-C5'-C6'-O6'
14	AH	106	LMT	O5'-C1'-O1'-C1
14	BD	105	LMT	O5'-C1'-O1'-C1
14	BP	1003	LMT	O1'-C1-C2-C3
14	BT	1002	LMT	O5B-C1B-O1B-C4'
15	BN	1001	V7N	C26-C27-C28-C29
15	BQ	1001	V7N	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
14	BF	103	LMT	O1'-C1-C2-C3
14	BB	103	LMT	O5'-C5'-C6'-O6'
14	BV	1003	LMT	O5'-C5'-C6'-O6'
14	L	304	LMT	O5B-C5B-C6B-O6B
13	AQ	102	BCL	C5-C6-C7-C8
14	BT	1003	LMT	O1'-C1-C2-C3
20	bl	103	0V9	C30-C31-C32-C33
13	AB	103	BCL	C15-C16-C17-C18
13	AG	102	BCL	C5-C6-C7-C8
13	BD	106	BCL	C5-C6-C7-C8
13	BG	1004	BCL	C15-C16-C17-C18
13	M	403	BCL	C8-C10-C11-C12
13	an	102	BCL	C13-C15-C16-C17
13	bb	103	BCL	C10-C11-C12-C13
13	bc	103	BCL	C8-C10-C11-C12
14	bk	101	LMT	O5B-C1B-O1B-C4'
14	BM	1003	LMT	C4'-C5'-C6'-O6'
21	af	103	CD4	C13-C14-O2-C15
13	AL	101	BCL	C10-C11-C12-C13
13	AO	101	BCL	C10-C11-C12-C13
13	AP	103	BCL	C10-C11-C12-C13
13	AU	103	BCL	C10-C11-C12-C13
13	BJ	1004	BCL	C15-C16-C17-C18
13	bi	103	BCL	C8-C10-C11-C12
22	M	406	BPH	C13-C15-C16-C17
26	af	101	V7B	C18-C19-C20-C21
20	L	310	0V9	C4-O4P-P-O3P
20	aj	101	0V9	C4-O4P-P-O3P
20	be	102	0V9	C4-O4P-P-O3P
20	be	103	0V9	C4-O4P-P-O3P
20	bf	103	0V9	C1-O3P-P-O4P
20	bg	102	0V9	C4-O4P-P-O3P
20	bk	102	0V9	C1-O3P-P-O4P
21	af	104	CD4	C32-O13-P2-O10
26	ag	1002	V7B	O6-C5-C6-O5
14	AR	102	LMT	O5B-C5B-C6B-O6B
14	BS	1002	LMT	O5B-C1B-O1B-C4'
13	AO	101	BCL	C4-C3-C5-C6
14	BL	1002	LMT	C3'-C4'-O1B-C1B
14	BA	103	LMT	O5B-C1B-O1B-C4'
13	BR	1003	BCL	C2A-CAA-CBA-CGA
13	bj	104	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	BH	1002	LMT	O5'-C5'-C6'-O6'
13	AI	103	BCL	C3-C5-C6-C7
13	AR	101	BCL	C3-C5-C6-C7
13	AS	101	BCL	C8-C10-C11-C12
15	be	101	V7N	C27-C28-C29-C39
20	bm	102	0V9	C10-C11-C12-C13
21	H1	1003	CD4	C11-C12-C13-C14
14	AD	1003	LMT	C1-C2-C3-C4
13	BD	106	BCL	C8-C10-C11-C12
14	BJ	1002	LMT	C2-C3-C4-C5
14	BR	1004	LMT	C3'-C4'-O1B-C1B
14	L	306	LMT	C7-C8-C9-C10
20	bh	104	0V9	C11-C12-C13-C14
13	AG	103	BCL	C16-C17-C18-C20
14	bg	103	LMT	C2-C3-C4-C5
20	bg	102	0V9	C34-C35-C36-C37
21	af	103	CD4	C5-C6-C7-C8
21	M	404	CD4	C16-C15-O2-C14
13	BR	1003	BCL	C13-C15-C16-C17
21	af	104	CD4	C46-C47-C48-C49
26	ag	1002	V7B	C31-C32-C33-C34
21	M	404	CD4	C26-C27-C60-C61
14	AG	101	LMT	C4'-C5'-C6'-O6'
14	AS	103	LMT	C1-C2-C3-C4
21	H1	1003	CD4	C49-C50-C51-C52
14	AK	101	LMT	C2'-C1'-O1'-C1
14	BD	105	LMT	C2'-C1'-O1'-C1
14	AU	101	LMT	C6-C7-C8-C9
13	AQ	103	BCL	C15-C16-C17-C18
13	ae	1001	BCL	C10-C11-C12-C13
13	AB	103	BCL	C4-C3-C5-C6
13	ah	1001	BCL	C4-C3-C5-C6
13	al	1001	BCL	C4-C3-C5-C6
13	AA	1002	BCL	C2-C3-C5-C6
13	BS	1005	BCL	C6-C7-C8-C9
13	L	303	BCL	C14-C13-C15-C16
13	ae	1001	BCL	C14-C13-C15-C16
13	ag	1001	BCL	C14-C13-C15-C16
13	al	1001	BCL	C6-C7-C8-C9
13	ao	1001	BCL	C11-C12-C13-C14
13	bc	103	BCL	C14-C13-C15-C16
13	be	104	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	bj	104	BCL	C11-C10-C8-C9
13	AM	102	BCL	C10-C11-C12-C13
13	ba	103	BCL	C10-C11-C12-C13
14	AK	101	LMT	O5B-C5B-C6B-O6B
14	AL	102	LMT	O5B-C5B-C6B-O6B
13	AQ	103	BCL	C2A-CAA-CBA-CGA
15	BB	101	V7N	C38-C26-C27-C28
15	BQ	1001	V7N	C38-C26-C27-C28
15	bd	101	V7N	C38-C26-C27-C28
15	bi	101	V7N	C38-C26-C27-C28
15	bn	101	V7N	C3-C4-C5-C33
14	AR	102	LMT	C5'-C4'-O1B-C1B
15	BQ	1001	V7N	C25-C26-C27-C28
15	bd	101	V7N	C25-C26-C27-C28
15	bf	102	V7N	C25-C26-C27-C28
15	bh	102	V7N	C3-C4-C5-C6
15	bi	101	V7N	C25-C26-C27-C28
13	AC	1002	BCL	C3-C5-C6-C7
13	BA	104	BCL	C3-C5-C6-C7
13	bc	103	BCL	C13-C15-C16-C17
20	bg	102	0V9	C19-C20-C21-C22
20	bc	102	0V9	C10-C11-C12-C13
14	BB	103	LMT	C5-C6-C7-C8
14	ac	101	LMT	C11-C10-C9-C8
19	H1	1001	PGW	C15-C16-C17-C18
14	BR	1004	LMT	C1-C2-C3-C4
14	AD	1003	LMT	O5'-C5'-C6'-O6'
14	BP	1003	LMT	O5'-C1'-O1'-C1
20	bf	103	0V9	O4P-C4-C5-N
20	ba	104	0V9	C31-C32-C33-C34
20	H1	1002	0V9	C10-C11-C12-C13
20	bk	104	0V9	C10-C11-C12-C13
13	AA	1002	BCL	C10-C11-C12-C13
13	AG	102	BCL	C13-C15-C16-C17
13	AJ	102	BCL	C13-C15-C16-C17
13	AW	104	BCL	C10-C11-C12-C13
14	BF	102	LMT	O1'-C1-C2-C3
13	AF	1002	BCL	C3A-C2A-CAA-CBA
13	BF	104	BCL	C3A-C2A-CAA-CBA
13	BL	1004	BCL	C3A-C2A-CAA-CBA
13	BR	1003	BCL	C3A-C2A-CAA-CBA
13	BW	1003	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	bl	105	BCL	C3A-C2A-CAA-CBA
13	AA	1002	BCL	C15-C16-C17-C18
13	AK	103	BCL	C8-C10-C11-C12
13	aa	1001	BCL	C8-C10-C11-C12
13	ad	102	BCL	C8-C10-C11-C12
13	ae	1001	BCL	C5-C6-C7-C8
13	bd	103	BCL	C8-C10-C11-C12
13	be	104	BCL	C15-C16-C17-C18
13	bg	104	BCL	C10-C11-C12-C13
14	AI	101	LMT	C2-C1-O1'-C1'
14	BC	104	LMT	C2-C1-O1'-C1'
14	BN	1002	LMT	C2-C1-O1'-C1'
14	BN	1003	LMT	C2-C1-O1'-C1'
14	BQ	1004	LMT	C2-C1-O1'-C1'
14	BX	1003	LMT	C2-C1-O1'-C1'
14	M	402	LMT	C2-C1-O1'-C1'
14	bb	102	LMT	C2-C1-O1'-C1'
14	bh	101	LMT	C2-C1-O1'-C1'
14	bk	101	LMT	C2-C1-O1'-C1'
14	AN	103	LMT	O1'-C1-C2-C3
14	BS	1004	LMT	C3-C4-C5-C6
20	bk	102	0V9	C35-C36-C37-C38
21	af	103	CD4	C6-C7-C8-C9
14	bh	101	LMT	O5B-C5B-C6B-O6B
13	AF	1001	BCL	C3-C5-C6-C7
13	ba	103	BCL	C3-C5-C6-C7
21	ai	103	CD4	C53-C54-C55-C56
13	bk	105	BCL	C15-C16-C17-C18
13	AU	102	BCL	C4-C3-C5-C6
13	AB	103	BCL	C2-C3-C5-C6
13	AU	102	BCL	C2-C3-C5-C6
14	bg	103	LMT	C5'-C4'-O1B-C1B
13	BH	1003	BCL	C2A-CAA-CBA-CGA
13	BH	1003	BCL	C8-C10-C11-C12
13	bk	105	BCL	C8-C10-C11-C12
26	ag	1002	V7B	C11-C12-C13-C14
14	bm	104	LMT	C5'-C4'-O1B-C1B
21	H1	1003	CD4	C18-C19-C20-C21
21	M	404	CD4	O8-C29-C30-O9
14	BL	1002	LMT	O5'-C5'-C6'-O6'
14	BQ	1004	LMT	C4'-C5'-C6'-O6'
13	AM	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	AD	1003	LMT	C7-C8-C9-C10
14	BH	1004	LMT	C3-C4-C5-C6
14	AK	101	LMT	C1-C2-C3-C4
13	BE	104	BCL	C2-C1-O2A-CGA
13	BJ	1004	BCL	C2-C1-O2A-CGA
14	BL	1002	LMT	C2-C3-C4-C5
21	ad	101	CD4	C4-C5-C6-C7
14	L	302	LMT	O5B-C5B-C6B-O6B
13	AN	102	BCL	C13-C15-C16-C17
20	bk	104	OV9	C11-C10-O2-C2
14	bf	104	LMT	C6-C7-C8-C9
20	bb	104	OV9	C38-C39-C40-C41
21	ad	101	CD4	C44-C45-C63-C64
14	AH	104	LMT	O5'-C5'-C6'-O6'
14	BR	1004	LMT	O5'-C5'-C6'-O6'
14	bg	103	LMT	O5B-C5B-C6B-O6B
26	ag	1002	V7B	C10-C11-C12-C13
13	ak	1001	BCL	C10-C11-C12-C13
14	BV	1002	LMT	O5'-C5'-C6'-O6'
13	AA	1002	BCL	C4-C3-C5-C6
13	AL	103	BCL	C4-C3-C5-C6
13	AS	104	BCL	C4-C3-C5-C6
13	ba	103	BCL	C4-C3-C5-C6
13	AA	1002	BCL	C6-C7-C8-C10
13	AC	1001	BCL	C11-C10-C8-C7
13	AO	101	BCL	C2-C3-C5-C6
13	BA	104	BCL	C6-C7-C8-C10
13	BG	1004	BCL	C2-C3-C5-C6
13	M	403	BCL	C11-C10-C8-C7
13	M	405	BCL	C12-C13-C15-C16
13	ah	1001	BCL	C2-C3-C5-C6
13	al	1001	BCL	C6-C7-C8-C10
13	ao	1001	BCL	C11-C12-C13-C15
13	be	104	BCL	C6-C7-C8-C10
13	bj	104	BCL	C11-C10-C8-C7
13	bl	105	BCL	C12-C13-C15-C16
13	AM	101	BCL	C5-C6-C7-C8
20	bo	104	OV9	C19-C20-C21-C22
13	BB	104	BCL	C2A-CAA-CBA-CGA
14	AU	101	LMT	C4-C5-C6-C7
21	M	404	CD4	C38-C39-C40-C41
21	ai	103	CD4	C44-C45-C63-C64

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Mol	Chain	Res	Type	Atoms
20	bi	102	0V9	C30-C31-C32-C33
14	AN	103	LMT	O5'-C5'-C6'-O6'
14	BI	103	LMT	O1'-C1-C2-C3
14	bl	104	LMT	C1-C2-C3-C4
14	bk	101	LMT	O5'-C5'-C6'-O6'
14	AL	102	LMT	C4'-C5'-C6'-O6'
14	AF	1003	LMT	O5'-C1'-O1'-C1
13	AV	103	BCL	C10-C11-C12-C13
13	bd	103	BCL	C15-C16-C17-C18
14	BJ	1002	LMT	C5-C6-C7-C8
20	bm	102	0V9	C11-C10-O2-C2
27	ai	101	UYH	C11-C10-O7-C8
21	ad	101	CD4	O13-C32-C33-O16
21	af	103	CD4	O2-C15-C28-O5
14	bm	104	LMT	C4B-C5B-C6B-O6B
13	AG	102	BCL	C3-C5-C6-C7
20	aj	101	0V9	C10-C11-C12-C13
14	AH	104	LMT	C7-C8-C9-C10
14	BK	1004	LMT	O1'-C1-C2-C3
14	AF	1003	LMT	C2'-C1'-O1'-C1
14	BP	1003	LMT	C2'-C1'-O1'-C1
13	bh	105	BCL	C8-C10-C11-C12
20	bf	103	0V9	O2-C2-C3-O3
20	bk	104	0V9	O2-C2-C3-O3
27	ai	101	UYH	O7-C8-C9-O8
14	AB	104	LMT	O5'-C5'-C6'-O6'
14	BP	1003	LMT	O5'-C5'-C6'-O6'
14	BI	102	LMT	C5-C6-C7-C8
20	bo	104	0V9	C22-C23-C24-C25
20	be	103	0V9	C34-C35-C36-C37
14	AA	1003	LMT	O5B-C5B-C6B-O6B
20	bl	103	0V9	C15-C16-C17-C18
13	BI	104	BCL	C4-C3-C5-C6
13	AS	104	BCL	C2-C3-C5-C6
13	ba	103	BCL	C2-C3-C5-C6
23	L	309	MQ8	C37-C38-C40-C41
13	AC	1001	BCL	C11-C10-C8-C9
13	AW	101	BCL	C6-C7-C8-C9
13	BO	1004	BCL	C11-C10-C8-C9
13	BQ	1003	BCL	C11-C10-C8-C9
13	M	405	BCL	C14-C13-C15-C16
13	ac	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	ap	1001	BCL	C6-C7-C8-C9
13	bk	105	BCL	C6-C7-C8-C9
13	bl	105	BCL	C14-C13-C15-C16
13	bn	103	BCL	C6-C7-C8-C9
14	BN	1004	LMT	O5'-C5'-C6'-O6'
13	AO	101	BCL	C3-C5-C6-C7
13	BT	1004	BCL	C3-C5-C6-C7
14	BT	1005	LMT	O5B-C1B-O1B-C4'
13	ba	103	BCL	C2A-CAA-CBA-CGA
14	BU	1001	LMT	O1'-C1-C2-C3
14	AP	102	LMT	O5B-C5B-C6B-O6B
14	BX	1003	LMT	O5'-C5'-C6'-O6'
14	AV	101	LMT	C7-C8-C9-C10
13	AD	1001	BCL	C1A-C2A-CAA-CBA
13	AE	1001	BCL	C1A-C2A-CAA-CBA
13	AK	103	BCL	C1A-C2A-CAA-CBA
13	AL	103	BCL	C1A-C2A-CAA-CBA
13	AQ	102	BCL	C1A-C2A-CAA-CBA
13	AQ	103	BCL	C1A-C2A-CAA-CBA
13	AS	104	BCL	C1A-C2A-CAA-CBA
13	AW	101	BCL	C1A-C2A-CAA-CBA
13	AG	103	BCL	C16-C17-C18-C19
20	bm	102	0V9	O4-C10-O2-C2
27	ai	101	UYH	O9-C10-O7-C8
20	ba	102	0V9	C11-C10-O2-C2
14	bd	102	LMT	C4B-C5B-C6B-O6B
13	bn	103	BCL	C8-C10-C11-C12
20	bh	104	0V9	C4-O4P-P-O3P
21	M	404	CD4	C29-O8-P1-O5
21	ai	103	CD4	C29-O8-P1-O5
14	AP	102	LMT	C6-C7-C8-C9
21	ai	103	CD4	C11-C12-C13-C14
14	BG	1002	LMT	C1-C2-C3-C4
20	bk	102	0V9	O3P-C1-C2-C3
14	BS	1004	LMT	C4'-C5'-C6'-O6'
20	bl	103	0V9	C13-C14-C15-C16
14	bh	101	LMT	C4'-C5'-C6'-O6'
14	bf	101	LMT	C11-C10-C9-C8
14	BX	1003	LMT	C5'-C4'-O1B-C1B
14	bd	102	LMT	C4-C5-C6-C7
21	M	404	CD4	O8-C29-C30-C31
13	BG	1004	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	BS	1005	BCL	C4-C3-C5-C6
23	L	309	MQ8	C39-C38-C40-C41
14	BU	1003	LMT	O1'-C1-C2-C3
14	bo	103	LMT	C7-C8-C9-C10
20	bk	102	0V9	C39-C40-C41-C42
13	AQ	102	BCL	C8-C10-C11-C12
21	ai	103	CD4	C40-C41-C42-C43
13	BI	104	BCL	C2A-CAA-CBA-CGA
14	bk	101	LMT	O5B-C5B-C6B-O6B
14	BD	104	LMT	C3-C4-C5-C6
20	bb	104	0V9	C1-C2-C3-O3
20	be	103	0V9	C1-C2-C3-O3
20	bm	102	0V9	C1-C2-C3-O3
14	AR	102	LMT	O5'-C5'-C6'-O6'
14	BG	1002	LMT	C4'-C5'-C6'-O6'
14	BS	1003	LMT	O1'-C1-C2-C3
13	BM	1004	BCL	C10-C11-C12-C13
14	AI	101	LMT	O5B-C5B-C6B-O6B
14	AT	101	LMT	O5B-C5B-C6B-O6B
14	BB	102	LMT	O5'-C5'-C6'-O6'
14	BC	104	LMT	O5B-C5B-C6B-O6B
20	bg	102	0V9	C10-C11-C12-C13
15	bb	101	V7N	C2-C1-O32-C41
15	bc	104	V7N	C2-C1-O32-C41
15	bk	103	V7N	C2-C1-O32-C41
25	M	408	CRT	C37-C38-O2-C2M
14	AS	103	LMT	O5B-C5B-C6B-O6B
14	AW	102	LMT	O5'-C5'-C6'-O6'
14	L	306	LMT	O5'-C5'-C6'-O6'
14	bf	101	LMT	O5B-C5B-C6B-O6B
14	BX	1003	LMT	C1-C2-C3-C4
20	bl	103	0V9	C2-C3-O3-C30
21	af	103	CD4	C22-C23-C24-C25
13	AF	1001	BCL	C5-C6-C7-C8
14	AA	1003	LMT	O5'-C5'-C6'-O6'
14	L	307	LMT	C2-C3-C4-C5
20	bc	102	0V9	C11-C10-O2-C2
14	AH	103	LMT	O5'-C5'-C6'-O6'
14	AS	103	LMT	O5'-C5'-C6'-O6'
14	BD	105	LMT	O5'-C5'-C6'-O6'
14	BI	102	LMT	O5'-C5'-C6'-O6'
14	BK	1006	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
14	BO	1003	LMT	O5B-C5B-C6B-O6B
14	BT	1002	LMT	O5'-C5'-C6'-O6'
13	AE	1001	BCL	C4-C3-C5-C6
13	AF	1002	BCL	C4-C3-C5-C6
13	AS	101	BCL	C4-C3-C5-C6
20	bh	104	0V9	C31-C30-O3-C3
13	ak	1001	BCL	C5-C6-C7-C8
14	BN	1003	LMT	C4'-C5'-C6'-O6'
20	bj	103	0V9	C1-C2-O2-C10
21	ad	101	CD4	C28-C15-O2-C14
21	af	104	CD4	C28-C15-O2-C14
14	AU	101	LMT	O5B-C5B-C6B-O6B
20	ba	102	0V9	O4-C10-O2-C2
13	AJ	102	BCL	C2-C1-O2A-CGA
13	ad	102	BCL	C2-C1-O2A-CGA
13	ai	102	BCL	C2-C1-O2A-CGA
13	ap	1001	BCL	C2-C1-O2A-CGA
14	AB	102	LMT	C3-C4-C5-C6
14	AD	1003	LMT	C4-C5-C6-C7
19	H1	1001	PGW	C27-C15-C16-C17
14	BJ	1002	LMT	C4-C5-C6-C7
14	bf	101	LMT	C6-C7-C8-C9
20	bj	103	0V9	O3P-C1-C2-O2
26	af	101	V7B	C19-C20-C21-C23
27	ai	101	UYH	C30-C31-C32-C33
14	AV	101	LMT	C2'-C1'-O1'-C1
14	BL	1002	LMT	C2'-C1'-O1'-C1
15	bb	101	V7N	C30-C1-O32-C41
15	bb	101	V7N	C31-C1-O32-C41
15	bc	104	V7N	C30-C1-O32-C41
15	bc	104	V7N	C31-C1-O32-C41
15	bk	103	V7N	C31-C1-O32-C41
25	M	408	CRT	C39-C38-O2-C2M
25	M	408	CRT	C40-C38-O2-C2M
20	be	102	0V9	O2-C2-C3-O3
13	AG	103	BCL	C10-C11-C12-C13
15	bk	103	V7N	C30-C1-C2-C3
15	bk	103	V7N	C31-C1-C2-C3
14	BD	105	LMT	C5'-C4'-O1B-C1B
14	BC	104	LMT	O5'-C5'-C6'-O6'
14	BN	1002	LMT	O5B-C1B-O1B-C4'
13	AM	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	ai	102	BCL	C4-C3-C5-C6
13	AC	1001	BCL	C6-C7-C8-C10
13	AC	1002	BCL	C11-C12-C13-C15
13	AE	1001	BCL	C2-C3-C5-C6
13	AM	101	BCL	C2-C3-C5-C6
13	AS	101	BCL	C6-C7-C8-C10
13	AW	101	BCL	C6-C7-C8-C10
13	AX	101	BCL	C11-C10-C8-C7
13	BN	1006	BCL	C11-C10-C8-C7
13	BO	1004	BCL	C11-C10-C8-C7
13	BP	1004	BCL	C6-C7-C8-C10
13	BQ	1003	BCL	C11-C10-C8-C7
13	ac	102	BCL	C11-C10-C8-C7
13	ai	102	BCL	C2-C3-C5-C6
13	bk	105	BCL	C6-C7-C8-C10
13	bo	102	BCL	C11-C10-C8-C7
13	AO	101	BCL	C6-C7-C8-C9
13	AV	102	BCL	C6-C7-C8-C9
13	AX	101	BCL	C11-C10-C8-C9
13	BH	1003	BCL	C11-C12-C13-C14
13	BN	1006	BCL	C11-C10-C8-C9
13	BP	1004	BCL	C6-C7-C8-C9
13	an	102	BCL	C6-C7-C8-C9
13	bo	102	BCL	C11-C10-C8-C9
15	BP	1001	V7N	C27-C28-C29-C39
20	bn	104	0V9	C33-C34-C35-C36
15	bm	101	V7N	O32-C1-C2-C3
14	BH	1005	LMT	O5B-C1B-O1B-C4'
15	BV	1001	V7N	C38-C26-C27-C28
14	bb	102	LMT	C4'-C5'-C6'-O6'
14	AS	103	LMT	O5B-C1B-O1B-C4'
13	bm	103	BCL	C5-C6-C7-C8
14	bg	103	LMT	C3'-C4'-O1B-C1B
26	af	101	V7B	C5-C4-O4-C43
20	bg	102	0V9	C31-C30-O3-C3
14	BT	1003	LMT	C1-C2-C3-C4
14	AR	102	LMT	C3'-C4'-O1B-C1B
13	BH	1003	BCL	C13-C15-C16-C17
26	ag	1002	V7B	C4-C5-C6-O5
14	BW	1006	LMT	C3'-C4'-O1B-C1B
13	BK	1003	BCL	C10-C11-C12-C13
13	bj	104	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	H1	1001	PGW	C01-C02-C03-O11
20	H1	1002	0V9	O3P-C1-C2-C3
20	bl	103	0V9	O3P-C1-C2-C3
21	ad	101	CD4	O13-C32-C33-C34
13	al	1001	BCL	C3-C5-C6-C7
23	L	309	MQ8	C18-C20-C21-C22
26	af	101	V7B	C3-C4-O4-C43
14	BN	1003	LMT	O5B-C5B-C6B-O6B
14	L	306	LMT	C4-C5-C6-C7
13	AF	1002	BCL	C2-C3-C5-C6
13	AL	103	BCL	C2-C3-C5-C6
13	AS	101	BCL	C2-C3-C5-C6
14	bm	104	LMT	C3'-C4'-O1B-C1B
13	bm	103	BCL	C10-C11-C12-C13
20	bg	102	0V9	O5-C30-O3-C3
14	BD	103	LMT	O1'-C1-C2-C3
13	af	102	BCL	C3-C5-C6-C7
13	AE	1001	BCL	C16-C17-C18-C20
13	bp	103	BCL	C16-C17-C18-C20
14	bl	104	LMT	C3-C4-C5-C6
20	bg	102	0V9	C2-C1-O3P-P
13	AE	1001	BCL	C3A-C2A-CAA-CBA
13	AH	101	BCL	C3A-C2A-CAA-CBA
13	AM	101	BCL	C3A-C2A-CAA-CBA
13	AW	101	BCL	C3A-C2A-CAA-CBA
13	BK	1003	BCL	C3A-C2A-CAA-CBA
13	BO	1004	BCL	C3A-C2A-CAA-CBA
13	BQ	1003	BCL	C3A-C2A-CAA-CBA
13	BV	1004	BCL	C3A-C2A-CAA-CBA
13	aj	102	BCL	C3A-C2A-CAA-CBA
13	be	104	BCL	C3A-C2A-CAA-CBA
13	bn	103	BCL	C3A-C2A-CAA-CBA
14	ac	101	LMT	C2-C3-C4-C5
14	bd	102	LMT	C4'-C5'-C6'-O6'
14	BL	1002	LMT	O5B-C1B-O1B-C4'
15	bc	104	V7N	C27-C28-C29-C39
14	AA	1003	LMT	C2-C1-O1'-C1'
14	AB	104	LMT	C2-C1-O1'-C1'
14	BA	106	LMT	C2-C1-O1'-C1'
14	BB	103	LMT	C2-C1-O1'-C1'
14	BF	102	LMT	C2-C1-O1'-C1'
14	BJ	1002	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
14	BK	1004	LMT	C2-C1-O1'-C1'
14	BK	1005	LMT	C2-C1-O1'-C1'
14	BK	1006	LMT	C2-C1-O1'-C1'
14	BP	1003	LMT	C2-C1-O1'-C1'
14	BR	1004	LMT	C2-C1-O1'-C1'
14	BT	1002	LMT	C2-C1-O1'-C1'
14	BT	1003	LMT	C2-C1-O1'-C1'
14	BU	1001	LMT	C2-C1-O1'-C1'
14	BW	1005	LMT	C2-C1-O1'-C1'
14	L	302	LMT	C2-C1-O1'-C1'
14	L	305	LMT	C2-C1-O1'-C1'
14	bj	102	LMT	C2-C1-O1'-C1'
14	bm	104	LMT	C2-C1-O1'-C1'
14	bo	103	LMT	C2-C1-O1'-C1'
14	BA	103	LMT	C5'-C4'-O1B-C1B
14	BA	105	LMT	C3-C4-C5-C6
14	BP	1002	LMT	C9-C10-C11-C12
13	AT	102	BCL	C10-C11-C12-C13
14	BN	1004	LMT	C3-C4-C5-C6
13	AE	1001	BCL	C16-C17-C18-C19
26	af	101	V7B	C19-C20-C21-C22
14	BW	1002	LMT	O1'-C1-C2-C3
20	be	103	0V9	C33-C34-C35-C36
13	bl	105	BCL	C8-C10-C11-C12
20	bc	102	0V9	C1-C2-C3-O3
20	be	102	0V9	C1-C2-C3-O3
20	bf	103	0V9	C1-C2-C3-O3
20	bk	104	0V9	C1-C2-C3-O3
21	M	404	CD4	C28-C15-C16-O3
21	af	104	CD4	C28-C15-C16-O3
21	ai	103	CD4	C28-C15-C16-O3
27	ai	101	UYH	C7-C8-C9-O8
21	af	104	CD4	C42-C43-C44-C45
14	AR	102	LMT	C3-C4-C5-C6
13	BH	1003	BCL	O2A-C1-C2-C3
13	BO	1004	BCL	O2A-C1-C2-C3
14	M	402	LMT	C4'-C5'-C6'-O6'
14	BW	1004	LMT	O5B-C1B-O1B-C4'
20	ba	104	0V9	C35-C36-C37-C38
15	BP	1001	V7N	C23-C24-C25-C26
14	BK	1002	LMT	O5B-C5B-C6B-O6B
14	L	302	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
14	bc	101	LMT	C4B-C5B-C6B-O6B
21	af	103	CD4	C48-C49-C50-C51
20	bk	102	0V9	O3P-C1-C2-O2
21	M	404	CD4	O2-C15-C28-O5
21	af	103	CD4	O13-C32-C33-O16
13	bp	103	BCL	C16-C17-C18-C19
14	AS	103	LMT	C5-C6-C7-C8
13	AF	1001	BCL	C10-C11-C12-C13
20	bh	104	0V9	O5-C30-O3-C3
15	BX	1001	V7N	O42-C34-C9-C8
15	ba	101	V7N	O42-C34-C9-C8
15	bb	101	V7N	O42-C34-C9-C8
20	bm	102	0V9	O2-C2-C3-O3
21	af	103	CD4	O2-C15-C16-O3
21	af	104	CD4	O2-C15-C16-O3
13	AQ	103	BCL	CBA-CGA-O2A-C1
14	BK	1004	LMT	C5'-C4'-O1B-C1B
15	AT	103	V7N	C5-C6-C7-C8
14	bh	101	LMT	O5B-C1B-O1B-C4'
14	BO	1002	LMT	C2B-C1B-O1B-C4'
13	AG	102	BCL	C11-C10-C8-C9
13	AI	102	BCL	C6-C7-C8-C9
13	BJ	1004	BCL	C11-C12-C13-C14
13	BP	1004	BCL	C11-C12-C13-C14
13	BU	1004	BCL	C6-C7-C8-C9
14	BT	1005	LMT	O1'-C1-C2-C3
14	bf	104	LMT	C1-C2-C3-C4
13	AP	103	BCL	C8-C10-C11-C12
13	ao	1001	BCL	C13-C15-C16-C17
21	af	103	CD4	C30-C29-O8-P1
14	AO	103	LMT	C5'-C4'-O1B-C1B
14	AR	102	LMT	O1'-C1-C2-C3
13	AX	101	BCL	C2A-CAA-CBA-CGA
13	BB	104	BCL	C16-C17-C18-C19
13	BB	104	BCL	C16-C17-C18-C20
13	AE	1001	BCL	C13-C15-C16-C17
14	BK	1002	LMT	O1'-C1-C2-C3
13	AG	102	BCL	C4C-C3C-CAC-CBC
13	AS	102	BCL	C4C-C3C-CAC-CBC
13	BN	1006	BCL	C4C-C3C-CAC-CBC
15	BS	1001	V7N	C3-C4-C5-C6
14	AN	103	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
26	af	101	V7B	C33-C34-C35-C36
20	bk	104	0V9	O4-C10-O2-C2
14	bf	104	LMT	C2-C3-C4-C5
13	AJ	102	BCL	C5-C6-C7-C8
14	BP	1005	LMT	C9-C10-C11-C12
14	BJ	1002	LMT	C9-C10-C11-C12
20	bi	102	0V9	C31-C32-C33-C34
20	ba	104	0V9	O3P-C1-C2-C3
20	be	102	0V9	O3P-C1-C2-C3
21	ai	103	CD4	C16-C15-C28-O5
14	BL	1005	LMT	C5'-C4'-O1B-C1B
13	AK	103	BCL	C6-C7-C8-C10
13	AV	102	BCL	C6-C7-C8-C10
13	AV	103	BCL	C6-C7-C8-C10
13	AW	104	BCL	C11-C10-C8-C7
13	BH	1003	BCL	C11-C12-C13-C15
13	BP	1004	BCL	C11-C12-C13-C15
13	BV	1004	BCL	C11-C12-C13-C15
13	L	303	BCL	C12-C13-C15-C16
13	M	403	BCL	C6-C7-C8-C10
13	ag	1001	BCL	C11-C12-C13-C15
13	ag	1001	BCL	C12-C13-C15-C16
13	ah	1001	BCL	C12-C13-C15-C16
13	an	102	BCL	C6-C7-C8-C10
13	ap	1001	BCL	C6-C7-C8-C10
13	ap	1001	BCL	C11-C12-C13-C15
13	bc	103	BCL	C12-C13-C15-C16
13	bg	104	BCL	C11-C10-C8-C7
13	bm	103	BCL	C6-C7-C8-C10
19	H1	1001	PGW	C07-C06-C10-C9
14	bf	101	LMT	C7-C8-C9-C10
22	M	406	BPH	C4B-C3B-CAB-CBB
13	am	1001	BCL	C8-C10-C11-C12
15	BT	1001	V7N	C27-C28-C29-C39
15	bk	103	V7N	C27-C28-C29-C39
13	AK	103	BCL	C16-C17-C18-C19
14	BW	1004	LMT	O5'-C5'-C6'-O6'
13	AS	102	BCL	C5-C6-C7-C8
13	AV	103	BCL	C5-C6-C7-C8
14	BL	1003	LMT	C4-C5-C6-C7
20	bn	104	0V9	C11-C10-O2-C2
14	AT	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
13	ae	1001	BCL	C13-C15-C16-C17
14	BX	1003	LMT	C3'-C4'-O1B-C1B
20	L	310	0V9	C10-C11-C12-C13
19	H1	1001	PGW	C20-C19-O03-C01
20	be	102	0V9	C39-C40-C41-C42
14	BP	1002	LMT	C4-C5-C6-C7
13	BI	104	BCL	C5-C6-C7-C8
13	bl	105	BCL	C10-C11-C12-C13
13	AQ	102	BCL	CAD-CBD-CGD-O2D
14	bh	101	LMT	C2B-C1B-O1B-C4'
14	BO	1002	LMT	O5B-C5B-C6B-O6B
13	AA	1001	BCL	C10-C11-C12-C13
13	AL	103	BCL	C15-C16-C17-C18
13	AS	101	BCL	C15-C16-C17-C18
13	ba	103	BCL	C8-C10-C11-C12
26	af	101	V7B	C46-C47-C48-O53
14	BX	1003	LMT	O1'-C1-C2-C3
14	bc	101	LMT	O5'-C5'-C6'-O6'
14	BK	1002	LMT	O5'-C1'-O1'-C1
14	BK	1004	LMT	O5'-C1'-O1'-C1
14	BN	1005	LMT	O5'-C1'-O1'-C1
13	ao	1001	BCL	C5-C6-C7-C8
14	BI	102	LMT	O1'-C1-C2-C3
20	H1	1002	0V9	C1-C2-C3-O3
20	bk	102	0V9	C2-C1-O3P-P
20	bo	104	0V9	C2-C1-O3P-P
21	af	103	CD4	C28-C15-C16-O3
19	H1	1001	PGW	O01-C02-C03-O11
20	aj	101	0V9	O3P-C1-C2-O2
20	ba	104	0V9	O3P-C1-C2-O2
20	bl	103	0V9	O3P-C1-C2-O2
21	M	404	CD4	O13-C32-C33-O16
14	BS	1003	LMT	C3-C4-C5-C6
13	AE	1001	BCL	C15-C16-C17-C18
14	AH	103	LMT	C2-C3-C4-C5
20	H1	1002	0V9	C14-C15-C16-C17
13	AG	102	BCL	CHA-CBD-CGD-O2D
13	AH	101	BCL	CHA-CBD-CGD-O1D
13	AH	101	BCL	CHA-CBD-CGD-O2D
13	AS	104	BCL	CHA-CBD-CGD-O2D
13	AW	104	BCL	CHA-CBD-CGD-O2D
13	BK	1003	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	L	307	LMT	C4'-C5'-C6'-O6'
21	M	404	CD4	O2-C15-C16-O3
21	ad	101	CD4	O2-C15-C16-O3
13	AQ	103	BCL	O1A-CGA-O2A-C1
14	BJ	1003	LMT	C3-C4-C5-C6
13	AK	103	BCL	C16-C17-C18-C20
14	AF	1003	LMT	C4-C5-C6-C7
21	af	103	CD4	C19-C20-C21-C22
21	af	104	CD4	C9-C10-C11-C12
15	BM	1001	V7N	C23-C24-C25-C26
13	al	1001	BCL	C2-C3-C5-C6
14	BE	103	LMT	O5B-C5B-C6B-O6B
26	af	101	V7B	C35-C36-C37-C38
13	AI	103	BCL	C14-C13-C15-C16
13	AV	103	BCL	C6-C7-C8-C9
14	BK	1004	LMT	C3'-C4'-O1B-C1B
21	H1	1003	CD4	C43-C44-C45-C63
13	AP	103	BCL	C15-C16-C17-C18
14	BA	106	LMT	C5'-C4'-O1B-C1B
21	M	404	CD4	C36-C37-C38-C39
15	BO	1001	V7N	C3-C4-C5-C33
14	BD	105	LMT	C3'-C4'-O1B-C1B
14	BI	105	LMT	C4-C5-C6-C7
14	BX	1002	LMT	C4-C5-C6-C7
15	BV	1001	V7N	C25-C26-C27-C28
14	BG	1003	LMT	C5-C6-C7-C8
13	AH	101	BCL	C1A-C2A-CAA-CBA
13	AS	102	BCL	C1A-C2A-CAA-CBA
13	BW	1003	BCL	C1A-C2A-CAA-CBA
13	bb	103	BCL	C1A-C2A-CAA-CBA
13	be	104	BCL	C1A-C2A-CAA-CBA
13	bi	103	BCL	C1A-C2A-CAA-CBA
13	bn	103	BCL	C1A-C2A-CAA-CBA
13	AQ	103	BCL	C2-C1-O2A-CGA
13	AK	103	BCL	CBD-CGD-O2D-CED
14	bl	101	LMT	O5'-C5'-C6'-O6'
20	bi	102	OV9	C13-C14-C15-C16
19	H1	1001	PGW	C03-O11-P-O12
21	af	104	CD4	C31-O10-P2-O13
13	AA	1002	BCL	CBD-CGD-O2D-CED
21	af	104	CD4	C5-C6-C7-C8
13	AW	104	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	L	309	MQ8	C14-C13-C15-C16
20	L	310	0V9	C2-C1-O3P-P
20	be	102	0V9	C2-C1-O3P-P
20	bm	102	0V9	C2-C1-O3P-P
19	H1	1001	PGW	C03-O11-P-O14
20	L	310	0V9	C4-O4P-P-O1P
20	bc	102	0V9	C4-O4P-P-O1P
20	be	102	0V9	C4-O4P-P-O1P
20	be	103	0V9	C4-O4P-P-O2P
20	bg	102	0V9	C4-O4P-P-O2P
20	bk	102	0V9	C1-O3P-P-O1P
20	bk	104	0V9	C1-O3P-P-O2P
20	bm	102	0V9	C1-O3P-P-O1P
21	af	104	CD4	C32-O13-P2-O12
13	BI	104	BCL	C16-C17-C18-C19
14	AI	101	LMT	O1'-C1-C2-C3
21	H1	1003	CD4	O13-C32-C33-C34
21	M	404	CD4	O13-C32-C33-C34
21	af	103	CD4	C16-C15-C28-O5
21	af	103	CD4	O13-C32-C33-C34
21	af	103	CD4	C23-C24-C25-C26
20	bh	104	0V9	C40-C41-C42-C43
20	H1	1002	0V9	C5-C4-O4P-P
20	L	310	0V9	C5-C4-O4P-P
20	bh	104	0V9	C5-C4-O4P-P
20	bi	102	0V9	C5-C4-O4P-P
20	bk	102	0V9	C5-C4-O4P-P
20	bm	102	0V9	C5-C4-O4P-P
20	bo	104	0V9	C5-C4-O4P-P
14	L	305	LMT	C1-C2-C3-C4
14	BP	1005	LMT	O5'-C5'-C6'-O6'
14	bb	102	LMT	O5'-C5'-C6'-O6'
20	aj	101	0V9	C33-C34-C35-C36
20	be	103	0V9	C2-C3-O3-C30
14	BH	1005	LMT	C4-C5-C6-C7
14	bm	104	LMT	C6-C7-C8-C9
21	af	104	CD4	O8-C29-C30-C31
14	BN	1002	LMT	O1'-C1-C2-C3
14	BV	1002	LMT	C5-C6-C7-C8
20	aj	101	0V9	C40-C41-C42-C43
20	ba	104	0V9	C32-C33-C34-C35
20	be	102	0V9	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	AG	102	BCL	C11-C12-C13-C15
13	AI	103	BCL	C12-C13-C15-C16
13	BG	1004	BCL	C11-C10-C8-C7
13	BJ	1004	BCL	C6-C7-C8-C10
13	ak	1001	BCL	C12-C13-C15-C16
13	ba	103	BCL	C11-C10-C8-C7
13	bh	105	BCL	C12-C13-C15-C16
13	bi	103	BCL	C3A-C2A-CAA-CBA
20	H1	1002	0V9	O3P-C1-C2-O2
21	af	104	CD4	O13-C32-C33-O16
21	ai	103	CD4	O2-C15-C28-O5
15	BL	1001	V7N	C27-C28-C29-C39
14	BD	105	LMT	C2-C1-O1'-C1'
14	BH	1005	LMT	C2-C1-O1'-C1'
13	BT	1004	BCL	C10-C11-C12-C13
13	BV	1004	BCL	C10-C11-C12-C13
20	aj	101	0V9	C14-C15-C16-C17
15	AT	103	V7N	O42-C34-C9-C10
15	BO	1001	V7N	O42-C34-C9-C10
15	ba	101	V7N	O42-C34-C9-C10
20	bg	102	0V9	C33-C34-C35-C36
21	M	404	CD4	C55-C56-C57-C58
21	ad	101	CD4	C28-C15-C16-O3
21	ai	103	CD4	O2-C15-C16-O3
21	ai	103	CD4	O16-C33-C34-O14
14	BP	1006	LMT	O1'-C1-C2-C3
14	bn	102	LMT	C3-C4-C5-C6
13	bj	104	BCL	O2A-C1-C2-C3
26	ag	1002	V7B	C8-C7-O1-C1
20	bi	102	0V9	C2-C1-O3P-P
21	af	104	CD4	C15-C28-O5-P1
21	ai	103	CD4	C30-C31-O10-P2
13	ah	1001	BCL	C15-C16-C17-C18
13	AC	1002	BCL	C4-C3-C5-C6
13	bm	103	BCL	C4-C3-C5-C6
21	M	404	CD4	C44-C45-C63-C64
21	ad	101	CD4	C11-C10-C9-C8
20	bj	103	0V9	C35-C36-C37-C38
13	BB	104	BCL	C15-C16-C17-C18
13	AK	103	BCL	C6-C7-C8-C9
13	AW	104	BCL	C11-C10-C8-C9
13	BJ	1004	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	BV	1004	BCL	C11-C12-C13-C14
13	ag	1001	BCL	C11-C12-C13-C14
13	ah	1001	BCL	C14-C13-C15-C16
13	ap	1001	BCL	C11-C12-C13-C14
13	bg	104	BCL	C11-C10-C8-C9
14	BS	1002	LMT	C4-C5-C6-C7
13	BI	104	BCL	C16-C17-C18-C20
21	af	103	CD4	C20-C21-C22-C23
14	BD	103	LMT	O5'-C1'-O1'-C1
21	ai	103	CD4	C17-C18-C19-C20
14	BD	103	LMT	C4'-C5'-C6'-O6'
20	bk	104	0V9	C35-C36-C37-C38
26	af	101	V7B	C15-C16-C17-C18
14	BU	1002	LMT	C4-C5-C6-C7
20	bj	103	0V9	C31-C32-C33-C34
15	BL	1001	V7N	C3-C4-C5-C33
15	bb	101	V7N	C36-C18-C19-C20
13	bj	104	BCL	C16-C17-C18-C19
14	BW	1004	LMT	C4-C5-C6-C7
13	AK	103	BCL	C15-C16-C17-C18
14	AR	102	LMT	C6-C7-C8-C9
14	bp	101	LMT	C2-C3-C4-C5
14	BT	1005	LMT	C2B-C1B-O1B-C4'
20	bc	102	0V9	O4-C10-O2-C2
13	AW	101	BCL	C4-C3-C5-C6
13	BF	104	BCL	C4-C3-C5-C6
15	bl	102	V7N	C37-C22-C23-C24
13	AM	101	BCL	CAA-CBA-CGA-O2A
13	BS	1005	BCL	C2-C3-C5-C6
13	BA	104	BCL	C5-C6-C7-C8
14	bf	101	LMT	C2-C3-C4-C5
20	bo	104	0V9	C33-C34-C35-C36
14	BE	102	LMT	O5B-C1B-O1B-C4'
13	AA	1001	BCL	C8-C10-C11-C12
14	AH	103	LMT	C4-C5-C6-C7
19	H1	1001	PGW	C03-C02-O01-C1
20	be	102	0V9	C1-C2-O2-C10
20	bl	103	0V9	C3-C2-O2-C10
20	bn	104	0V9	C3-C2-O2-C10
21	ai	103	CD4	C28-C15-O2-C14
21	af	104	CD4	O13-C32-C33-C34
13	BA	104	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	BL	1004	BCL	C2A-CAA-CBA-CGA
13	BP	1004	BCL	C2A-CAA-CBA-CGA
13	BS	1005	BCL	C2A-CAA-CBA-CGA
14	AB	104	LMT	C4-C5-C6-C7
14	BA	102	LMT	C4-C5-C6-C7
14	bj	102	LMT	C4'-C5'-C6'-O6'
14	bp	101	LMT	C3'-C4'-O1B-C1B
13	AQ	103	BCL	C3-C5-C6-C7
14	BR	1002	LMT	C4-C5-C6-C7
20	aj	101	0V9	C36-C37-C38-C39
14	BN	1002	LMT	C5'-C4'-O1B-C1B
15	BJ	1001	V7N	C27-C28-C29-C39
21	H1	1003	CD4	O13-C32-C33-O16
14	BA	103	LMT	C3'-C4'-O1B-C1B
14	BR	1005	LMT	C4-C5-C6-C7
13	BO	1004	BCL	C4-C3-C5-C6
13	ap	1001	BCL	C4-C3-C5-C6
14	AO	103	LMT	C3'-C4'-O1B-C1B
13	AA	1002	BCL	C3-C5-C6-C7
13	AC	1002	BCL	C2-C3-C5-C6
13	AW	104	BCL	C2-C3-C5-C6
13	bm	103	BCL	C2-C3-C5-C6
14	bb	102	LMT	C4-C5-C6-C7
14	L	305	LMT	C7-C8-C9-C10
27	ai	101	UYH	C28-C29-C30-C31
14	AA	1003	LMT	C5'-C4'-O1B-C1B
14	bp	101	LMT	C4-C5-C6-C7
13	BQ	1003	BCL	C2A-CAA-CBA-CGA
15	bk	103	V7N	C30-C1-O32-C41
21	ad	101	CD4	C54-C55-C56-C57
20	bb	104	0V9	C2-C3-O3-C30
14	BD	102	LMT	C4'-C5'-C6'-O6'
20	aj	101	0V9	O2-C2-C3-O3
14	BE	106	LMT	C4-C5-C6-C7
20	H1	1002	0V9	C4-O4P-P-O3P
20	ba	102	0V9	C1-O3P-P-O4P
20	bi	102	0V9	C1-O3P-P-O4P
20	bk	102	0V9	C4-O4P-P-O3P
20	bo	104	0V9	C1-O3P-P-O4P
21	af	103	CD4	C29-O8-P1-O5
14	BW	1005	LMT	C9-C10-C11-C12
14	bp	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
15	bl	102	V7N	C30-C1-C2-C3
14	AK	101	LMT	C7-C8-C9-C10
14	BB	102	LMT	C2-C3-C4-C5
21	M	404	CD4	C1-C2-C3-C4
20	aj	101	0V9	C1-C2-C3-O3
13	aj	102	BCL	C5-C6-C7-C8
13	ae	1001	BCL	C12-C13-C15-C16
13	M	405	BCL	CAA-CBA-CGA-O2A
13	AC	1001	BCL	C6-C7-C8-C9
13	AS	101	BCL	C6-C7-C8-C9
13	M	403	BCL	C6-C7-C8-C9
13	ak	1001	BCL	C14-C13-C15-C16
13	ba	103	BCL	C11-C10-C8-C9
13	bm	103	BCL	C6-C7-C8-C9
14	BN	1004	LMT	C1-C2-C3-C4
13	AO	101	BCL	C16-C17-C18-C20
14	AO	103	LMT	C6-C7-C8-C9
14	BH	1004	LMT	O5B-C1B-O1B-C4'
14	bc	101	LMT	O5B-C1B-O1B-C4'
13	BV	1004	BCL	C2A-CAA-CBA-CGA
14	AI	101	LMT	C7-C8-C9-C10
15	BM	1001	V7N	O32-C1-C2-C3
15	BN	1001	V7N	O32-C1-C2-C3
14	AP	102	LMT	O1'-C1-C2-C3
14	BL	1005	LMT	C3'-C4'-O1B-C1B
14	bp	101	LMT	C5'-C4'-O1B-C1B
15	BW	1001	V7N	C3-C4-C5-C33
14	AN	103	LMT	C3'-C4'-O1B-C1B
20	bc	102	0V9	C31-C32-C33-C34
21	H1	1003	CD4	C15-C28-O5-P1
14	AG	101	LMT	C11-C10-C9-C8
20	aj	101	0V9	C16-C17-C18-C19
14	BG	1002	LMT	C9-C10-C11-C12
20	bl	103	0V9	C32-C33-C34-C35
13	ak	1001	BCL	C3-C5-C6-C7
14	AD	1004	LMT	O5B-C5B-C6B-O6B
14	BO	1002	LMT	O5B-C1B-O1B-C4'
14	L	307	LMT	C7-C8-C9-C10
14	AS	103	LMT	C2B-C1B-O1B-C4'
15	BJ	1001	V7N	C23-C24-C25-C26
15	BS	1001	V7N	C23-C24-C25-C26
14	BS	1003	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
13	BI	104	BCL	C2-C3-C5-C6
23	L	309	MQ8	C12-C13-C15-C16
14	BE	102	LMT	O1'-C1-C2-C3
20	bo	104	0V9	C20-C21-C22-C23
13	bj	104	BCL	C16-C17-C18-C20
14	BT	1005	LMT	C5'-C4'-O1B-C1B
13	AK	103	BCL	O1D-CGD-O2D-CED
14	BU	1001	LMT	O5B-C5B-C6B-O6B
13	AC	1002	BCL	C15-C16-C17-C18
13	AV	102	BCL	C13-C15-C16-C17
20	aj	101	0V9	O3P-C1-C2-C3
20	aj	101	0V9	O4P-C4-C5-N
20	ba	102	0V9	O4P-C4-C5-N
20	bg	102	0V9	C32-C33-C34-C35
14	BK	1004	LMT	O5B-C1B-O1B-C4'
14	BL	1002	LMT	C2B-C1B-O1B-C4'
13	AA	1002	BCL	O1D-CGD-O2D-CED
14	BR	1002	LMT	C5'-C4'-O1B-C1B
15	ba	101	V7N	C37-C22-C23-C24
13	AK	102	BCL	C8-C10-C11-C12
13	BB	104	BCL	C2-C3-C5-C6
19	H1	1001	PGW	O04-C19-O03-C01
20	ba	104	0V9	C16-C17-C18-C19
21	ai	103	CD4	O9-C30-C31-O10
20	bn	104	0V9	C2-C3-O3-C30
20	bb	104	0V9	C12-C13-C14-C15
21	ad	101	CD4	C10-C11-C12-C13
26	ag	1002	V7B	C15-C16-C17-C18
14	bk	101	LMT	O1'-C1-C2-C3
14	bf	104	LMT	O1'-C1-C2-C3
13	BG	1004	BCL	C2A-CAA-CBA-CGA
14	BL	1002	LMT	C5-C6-C7-C8
14	BL	1003	LMT	C5'-C4'-O1B-C1B
13	AK	103	BCL	C3A-C2A-CAA-CBA
13	BI	104	BCL	C3A-C2A-CAA-CBA
13	bb	103	BCL	C3A-C2A-CAA-CBA
26	ag	1002	V7B	O9-C10-O7-C8
13	AN	102	BCL	CBD-CGD-O2D-CED
21	af	104	CD4	C43-C44-C45-C63
14	BM	1002	LMT	O5'-C5'-C6'-O6'
14	AG	101	LMT	C7-C8-C9-C10
14	BW	1004	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	AB	104	LMT	C5'-C4'-O1B-C1B
14	bh	103	LMT	C7-C8-C9-C10
13	AG	102	BCL	C11-C12-C13-C14
13	AS	104	BCL	C11-C12-C13-C14
13	bm	103	BCL	C14-C13-C15-C16
14	BA	105	LMT	C2-C3-C4-C5
13	AF	1002	BCL	C15-C16-C17-C18
21	af	103	CD4	C52-C53-C54-C55
14	bl	101	LMT	C4B-C5B-C6B-O6B
14	bc	101	LMT	C5-C6-C7-C8
21	H1	1003	CD4	C37-C38-C39-C40
14	BK	1005	LMT	C4-C5-C6-C7
14	L	302	LMT	C4'-C5'-C6'-O6'
14	BX	1003	LMT	O5B-C1B-O1B-C4'
13	AO	101	BCL	C16-C17-C18-C19
13	AC	1002	BCL	O2A-C1-C2-C3
13	BX	1004	BCL	O2A-C1-C2-C3
13	af	102	BCL	O2A-C1-C2-C3
13	bd	103	BCL	O2A-C1-C2-C3
22	L	301	BPH	O2A-C1-C2-C3
14	bb	102	LMT	C6-C7-C8-C9
20	bh	104	0V9	C34-C35-C36-C37
14	L	305	LMT	O5B-C5B-C6B-O6B
20	H1	1002	0V9	C32-C33-C34-C35
14	BF	102	LMT	C1-C2-C3-C4
13	ap	1001	BCL	C5-C6-C7-C8
13	bb	103	BCL	C15-C16-C17-C18
20	bh	104	0V9	C35-C36-C37-C38
21	af	103	CD4	C34-C33-O16-C46
13	AJ	102	BCL	C10-C11-C12-C13
13	AK	103	BCL	C5-C6-C7-C8
13	AW	103	BCL	C4-C3-C5-C6
13	AM	101	BCL	C1A-C2A-CAA-CBA
13	AP	103	BCL	C1A-C2A-CAA-CBA
13	AV	103	BCL	C1A-C2A-CAA-CBA
13	BK	1003	BCL	C1A-C2A-CAA-CBA
13	BO	1004	BCL	C1A-C2A-CAA-CBA
13	BU	1004	BCL	C1A-C2A-CAA-CBA
13	BV	1004	BCL	C1A-C2A-CAA-CBA
13	bg	104	BCL	C1A-C2A-CAA-CBA
13	bh	105	BCL	C1A-C2A-CAA-CBA
13	bj	104	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	bo	102	BCL	C1A-C2A-CAA-CBA
13	bp	103	BCL	C1A-C2A-CAA-CBA
20	bm	102	0V9	C13-C14-C15-C16
14	AB	102	LMT	C4B-C5B-C6B-O6B
20	bn	104	0V9	O4-C10-O2-C2
13	AM	102	BCL	C6-C7-C8-C10
13	ae	1001	BCL	C11-C10-C8-C7
14	BH	1005	LMT	C2B-C1B-O1B-C4'
27	ai	101	UYH	C15-C16-C17-C18
15	BD	101	V7N	C23-C24-C25-C26
15	bm	101	V7N	C27-C28-C29-C39
13	AJ	102	BCL	C15-C16-C17-C18
14	BA	106	LMT	O1'-C1-C2-C3
21	ai	103	CD4	C50-C51-C52-C53
14	AP	102	LMT	C3-C4-C5-C6
21	H1	1003	CD4	C56-C57-C58-C59
13	AP	101	BCL	C15-C16-C17-C18
13	BS	1005	BCL	C5-C6-C7-C8
13	AG	102	BCL	C2A-CAA-CBA-CGA
13	AQ	101	BCL	C15-C16-C17-C18
13	AR	101	BCL	C13-C15-C16-C17
14	BN	1002	LMT	C4-C5-C6-C7
21	af	104	CD4	O2-C15-C28-O5
14	AN	103	LMT	C5-C6-C7-C8
13	AC	1001	BCL	C5-C6-C7-C8
26	ag	1002	V7B	C29-C28-O8-C9
14	BD	104	LMT	C6-C7-C8-C9
21	H1	1003	CD4	C36-C37-C38-C39
21	af	103	CD4	C37-C38-C39-C40
13	BV	1004	BCL	C4-C3-C5-C6
15	bd	101	V7N	C37-C22-C23-C24
13	AI	102	BCL	C5-C6-C7-C8
15	ba	101	V7N	C21-C22-C23-C24
14	BA	103	LMT	C5-C6-C7-C8
14	bk	101	LMT	C7-C8-C9-C10
13	ai	102	BCL	C8-C10-C11-C12
20	bf	103	0V9	C10-C11-C12-C13
14	BN	1002	LMT	C2B-C1B-O1B-C4'
20	bg	102	0V9	C38-C39-C40-C41
14	BI	102	LMT	C2-C3-C4-C5
14	bd	102	LMT	C5-C6-C7-C8
15	BR	1001	V7N	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
15	bd	101	V7N	C27-C28-C29-C39
13	aj	102	BCL	C15-C16-C17-C18
22	M	406	BPH	C10-C11-C12-C13
14	BR	1004	LMT	C5-C6-C7-C8
15	BN	1001	V7N	C23-C24-C25-C26
20	be	102	0V9	C10-C11-C12-C13
14	BC	102	LMT	C4-C5-C6-C7
13	AN	102	BCL	O1D-CGD-O2D-CED
13	bg	104	BCL	C4-C3-C5-C6
15	bg	101	V7N	C37-C22-C23-C24
14	BS	1003	LMT	O5B-C1B-O1B-C4'
13	BF	104	BCL	C2-C3-C5-C6
15	bl	102	V7N	C21-C22-C23-C24
14	bf	104	LMT	C5-C6-C7-C8
20	H1	1002	0V9	C16-C17-C18-C19
13	AD	1001	BCL	C14-C13-C15-C16
13	AL	103	BCL	C6-C7-C8-C9
13	AM	101	BCL	C11-C12-C13-C14
14	BI	101	LMT	C5'-C4'-O1B-C1B
14	BG	1003	LMT	C1-C2-C3-C4
14	BA	105	LMT	C6-C7-C8-C9
14	AB	104	LMT	O5B-C1B-O1B-C4'
14	bc	101	LMT	C5'-C4'-O1B-C1B
13	AQ	102	BCL	C10-C11-C12-C13
13	bp	103	BCL	C5-C6-C7-C8
14	BI	101	LMT	C4-C5-C6-C7
13	af	102	BCL	C5-C6-C7-C8
14	AB	102	LMT	O5'-C5'-C6'-O6'
14	BK	1002	LMT	C5'-C4'-O1B-C1B
14	BN	1003	LMT	C9-C10-C11-C12
13	BM	1004	BCL	CAA-CBA-CGA-O2A
14	BP	1002	LMT	C4'-C5'-C6'-O6'
15	bc	104	V7N	C13-C14-C15-C16
13	BN	1006	BCL	C4-C3-C5-C6
13	bk	105	BCL	C4-C3-C5-C6
15	BG	1001	V7N	C37-C22-C23-C24
15	bb	101	V7N	C37-C22-C23-C24
13	AH	101	BCL	C4C-C3C-CAC-CBC
13	AW	101	BCL	C4C-C3C-CAC-CBC
13	BD	106	BCL	C4C-C3C-CAC-CBC
13	BT	1004	BCL	C4C-C3C-CAC-CBC
13	BU	1004	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	L	301	BPH	C4C-C3C-CAC-CBC
13	AW	101	BCL	C2-C3-C5-C6
13	BO	1004	BCL	C2-C3-C5-C6
13	ap	1001	BCL	C2-C3-C5-C6
13	AF	1001	BCL	C8-C10-C11-C12
27	ai	101	UYH	C8-C7-O1-C1
21	af	103	CD4	C2-C3-C4-C5
14	bc	101	LMT	C6-C7-C8-C9
21	H1	1003	CD4	C23-C24-C25-C26
13	BU	1004	BCL	C16-C17-C18-C19
20	bk	102	0V9	C16-C17-C18-C19
20	be	102	0V9	O3P-C1-C2-O2
14	bm	104	LMT	C1-C2-C3-C4
21	af	103	CD4	C33-C34-O14-C35
13	BK	1003	BCL	C2A-CAA-CBA-CGA
13	bd	103	BCL	C2A-CAA-CBA-CGA
13	AM	102	BCL	C15-C16-C17-C18
14	BJ	1002	LMT	C3-C4-C5-C6
14	BH	1002	LMT	C4'-C5'-C6'-O6'
14	BA	103	LMT	C2B-C1B-O1B-C4'
14	BP	1002	LMT	O5B-C1B-O1B-C4'
14	BA	105	LMT	C5'-C4'-O1B-C1B
20	bj	103	0V9	O3P-C1-C2-C3
13	BU	1004	BCL	C4-C3-C5-C6
13	bh	105	BCL	C4-C3-C5-C6
15	be	101	V7N	C37-C22-C23-C24
26	ag	1002	V7B	C11-C10-O7-C8
13	AF	1001	BCL	C11-C12-C13-C15
13	AH	101	BCL	C2-C3-C5-C6
13	AI	102	BCL	C6-C7-C8-C10
13	AM	101	BCL	C11-C12-C13-C15
13	AO	101	BCL	C6-C7-C8-C10
13	bm	103	BCL	C12-C13-C15-C16
13	bp	103	BCL	C2-C3-C5-C6
20	L	310	0V9	O4P-C4-C5-N
20	bl	103	0V9	O4P-C4-C5-N
26	ag	1002	V7B	O10-C28-O8-C9
14	AR	102	LMT	C4-C5-C6-C7
14	BT	1002	LMT	C4-C5-C6-C7
15	BM	1001	V7N	C13-C14-C15-C16
21	ad	101	CD4	C39-C40-C41-C42
21	af	103	CD4	O8-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
14	BJ	1003	LMT	C2-C3-C4-C5
14	BP	1005	LMT	C2-C3-C4-C5
13	ad	102	BCL	C5-C6-C7-C8
13	AH	101	BCL	CAA-CBA-CGA-O2A
20	be	102	0V9	O3-C30-C31-C32
14	BR	1006	LMT	O5B-C1B-O1B-C4'
14	BR	1002	LMT	C4'-C5'-C6'-O6'
14	AN	103	LMT	C4-C5-C6-C7
20	bc	102	0V9	C16-C17-C18-C19
20	bm	102	0V9	C16-C17-C18-C19
13	AS	102	BCL	CAA-CBA-CGA-O2A
13	ag	1001	BCL	C4-C3-C5-C6
13	ao	1001	BCL	C4-C3-C5-C6
15	BA	101	V7N	C37-C22-C23-C24
15	bh	102	V7N	C37-C22-C23-C24
13	AW	103	BCL	C2-C3-C5-C6
13	AF	1001	BCL	C11-C12-C13-C14
13	AP	101	BCL	C6-C7-C8-C9
13	AQ	101	BCL	C6-C7-C8-C9
13	BG	1004	BCL	C11-C10-C8-C9
13	BI	104	BCL	C11-C12-C13-C14
13	BK	1003	BCL	C11-C12-C13-C14
13	bh	105	BCL	C14-C13-C15-C16
14	BW	1005	LMT	C3-C4-C5-C6
13	BU	1004	BCL	C8-C10-C11-C12
21	H1	1003	CD4	C38-C39-C40-C41
13	AC	1002	BCL	C3A-C2A-CAA-CBA
13	AG	102	BCL	C3A-C2A-CAA-CBA
13	BG	1004	BCL	C3A-C2A-CAA-CBA
13	BH	1003	BCL	C3A-C2A-CAA-CBA
13	BN	1006	BCL	C3A-C2A-CAA-CBA
13	BT	1004	BCL	C3A-C2A-CAA-CBA
13	BU	1004	BCL	C3A-C2A-CAA-CBA
13	bg	104	BCL	C3A-C2A-CAA-CBA
13	bj	104	BCL	C3A-C2A-CAA-CBA
13	bo	102	BCL	C3A-C2A-CAA-CBA
13	bp	103	BCL	C3A-C2A-CAA-CBA
14	BB	103	LMT	C5'-C4'-O1B-C1B
13	ab	1001	BCL	CAA-CBA-CGA-O2A
20	bi	102	0V9	C18-C19-C20-C21
14	BA	106	LMT	C3'-C4'-O1B-C1B
14	BC	102	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
14	BW	1002	LMT	C5'-C4'-O1B-C1B
13	AC	1002	BCL	CAD-CBD-CGD-O2D
13	AO	101	BCL	CAD-CBD-CGD-O2D
13	L	303	BCL	CAD-CBD-CGD-O2D
13	L	308	BCL	CAD-CBD-CGD-O2D
13	bc	103	BCL	CAD-CBD-CGD-O2D
14	AT	101	LMT	C5'-C4'-O1B-C1B
14	BS	1003	LMT	C5'-C4'-O1B-C1B
21	ad	101	CD4	C24-C25-C26-C27
13	bb	103	BCL	C2A-CAA-CBA-CGA
14	BB	103	LMT	O5B-C1B-O1B-C4'
13	AW	104	BCL	CAA-CBA-CGA-O2A
13	ai	102	BCL	CAA-CBA-CGA-O2A
21	ad	101	CD4	C12-C13-C14-O2
13	AH	101	BCL	C4-C3-C5-C6
23	an	101	MQ8	C24-C23-C25-C26
13	BN	1006	BCL	C2-C3-C5-C6
13	BV	1004	BCL	C2-C3-C5-C6
15	BG	1001	V7N	C21-C22-C23-C24
15	bd	101	V7N	C21-C22-C23-C24
13	AL	103	BCL	CAA-CBA-CGA-O2A
13	ae	1001	BCL	CAA-CBA-CGA-O2A
13	ap	1001	BCL	CAA-CBA-CGA-O2A
20	bc	102	0V9	O2-C10-C11-C12
20	be	103	0V9	O2-C10-C11-C12
14	bf	104	LMT	C5'-C4'-O1B-C1B
14	bh	101	LMT	C7-C8-C9-C10
15	BL	1001	V7N	C3-C4-C5-C6
15	BO	1001	V7N	C3-C4-C5-C6
15	BW	1001	V7N	C3-C4-C5-C6
14	BN	1002	LMT	O5B-C5B-C6B-O6B
20	bb	104	0V9	C18-C19-C20-C21
21	af	103	CD4	C50-C51-C52-C53
14	AK	101	LMT	C11-C10-C9-C8
13	AP	103	BCL	CAA-CBA-CGA-O2A
13	BX	1004	BCL	CAA-CBA-CGA-O2A
20	bf	103	0V9	O2-C10-C11-C12
20	bn	104	0V9	O3-C30-C31-C32
19	H1	1001	PGW	C16-C15-C27-C26
13	AI	102	BCL	O2A-C1-C2-C3
13	BP	1004	BCL	O2A-C1-C2-C3
13	BT	1004	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	ba	103	BCL	O2A-C1-C2-C3
13	bi	103	BCL	O2A-C1-C2-C3
13	bl	105	BCL	O2A-C1-C2-C3
14	AS	103	LMT	C4-C5-C6-C7
20	bg	102	0V9	C31-C32-C33-C34
13	BO	1004	BCL	C2A-CAA-CBA-CGA
13	BT	1004	BCL	C2A-CAA-CBA-CGA
13	bp	103	BCL	C2A-CAA-CBA-CGA
13	BE	104	BCL	C5-C6-C7-C8
14	AA	1003	LMT	C9-C10-C11-C12
14	AH	106	LMT	C5-C6-C7-C8
14	BO	1003	LMT	O1'-C1-C2-C3
26	ag	1002	V7B	C14-C15-C16-C17
20	be	103	0V9	C16-C17-C18-C19
20	bk	102	0V9	C18-C19-C20-C21
13	AW	104	BCL	C16-C17-C18-C19
14	BP	1002	LMT	C5'-C4'-O1B-C1B
14	BT	1003	LMT	C4-C5-C6-C7
14	L	302	LMT	C5-C6-C7-C8
14	BT	1002	LMT	C2B-C1B-O1B-C4'
14	bc	101	LMT	C2B-C1B-O1B-C4'
14	BD	102	LMT	C5-C6-C7-C8
13	AA	1001	BCL	CHA-CBD-CGD-O2D
13	AB	103	BCL	CHA-CBD-CGD-O1D
13	AB	103	BCL	CHA-CBD-CGD-O2D
13	AD	1001	BCL	CHA-CBD-CGD-O1D
13	AD	1001	BCL	CHA-CBD-CGD-O2D
13	AD	1002	BCL	CHA-CBD-CGD-O1D
13	AD	1002	BCL	CHA-CBD-CGD-O2D
13	AE	1001	BCL	CHA-CBD-CGD-O1D
13	AE	1001	BCL	CHA-CBD-CGD-O2D
13	AF	1002	BCL	CHA-CBD-CGD-O1D
13	AF	1002	BCL	CHA-CBD-CGD-O2D
13	AI	102	BCL	CHA-CBD-CGD-O1D
13	AI	102	BCL	CHA-CBD-CGD-O2D
13	AM	101	BCL	CHA-CBD-CGD-O2D
13	AM	102	BCL	CHA-CBD-CGD-O1D
13	AM	102	BCL	CHA-CBD-CGD-O2D
13	AO	102	BCL	CHA-CBD-CGD-O1D
13	AO	102	BCL	CHA-CBD-CGD-O2D
13	AP	101	BCL	CHA-CBD-CGD-O2D
13	AU	103	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	AU	103	BCL	CHA-CBD-CGD-O2D
13	BA	104	BCL	CHA-CBD-CGD-O1D
13	BA	104	BCL	CHA-CBD-CGD-O2D
13	BB	104	BCL	CHA-CBD-CGD-O1D
13	BB	104	BCL	CHA-CBD-CGD-O2D
13	BD	106	BCL	CHA-CBD-CGD-O1D
13	BD	106	BCL	CHA-CBD-CGD-O2D
13	BE	104	BCL	CHA-CBD-CGD-O2D
13	BF	104	BCL	CHA-CBD-CGD-O1D
13	BF	104	BCL	CHA-CBD-CGD-O2D
13	BG	1004	BCL	CHA-CBD-CGD-O1D
13	BG	1004	BCL	CHA-CBD-CGD-O2D
13	BH	1003	BCL	CHA-CBD-CGD-O2D
13	BI	104	BCL	CHA-CBD-CGD-O1D
13	BI	104	BCL	CHA-CBD-CGD-O2D
13	BM	1004	BCL	CHA-CBD-CGD-O2D
13	BP	1004	BCL	CHA-CBD-CGD-O1D
13	BP	1004	BCL	CHA-CBD-CGD-O2D
13	BQ	1003	BCL	CHA-CBD-CGD-O1D
13	BQ	1003	BCL	CHA-CBD-CGD-O2D
13	BR	1003	BCL	CHA-CBD-CGD-O1D
13	BR	1003	BCL	CHA-CBD-CGD-O2D
13	BS	1005	BCL	CHA-CBD-CGD-O2D
13	BT	1004	BCL	CHA-CBD-CGD-O1D
13	BT	1004	BCL	CHA-CBD-CGD-O2D
13	BU	1004	BCL	CHA-CBD-CGD-O1D
13	BU	1004	BCL	CHA-CBD-CGD-O2D
13	BW	1003	BCL	CHA-CBD-CGD-O1D
13	BW	1003	BCL	CHA-CBD-CGD-O2D
13	BX	1004	BCL	CHA-CBD-CGD-O1D
13	BX	1004	BCL	CHA-CBD-CGD-O2D
13	BK	1003	BCL	C4-C3-C5-C6
20	L	310	0V9	O3-C30-C31-C32
20	bc	102	0V9	O3-C30-C31-C32
15	bb	101	V7N	C21-C22-C23-C24
21	af	103	CD4	C53-C54-C55-C56
14	bn	102	LMT	C7-C8-C9-C10
13	AI	103	BCL	C16-C17-C18-C19
13	ak	1001	BCL	C8-C10-C11-C12
13	bf	105	BCL	C10-C11-C12-C13
14	BC	104	LMT	C7-C8-C9-C10
20	bg	102	0V9	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
20	bl	103	0V9	O2-C2-C3-O3
26	af	101	V7B	O1-C7-C8-O7
20	be	103	0V9	C10-C11-C12-C13
21	M	404	CD4	C17-C18-C19-C20
13	BG	1004	BCL	C8-C10-C11-C12
19	H1	1001	PGW	O01-C1-C2-C3
20	bb	104	0V9	O3-C30-C31-C32
13	BN	1006	BCL	C2A-CAA-CBA-CGA
15	BM	1001	V7N	C31-C1-C2-C3
15	bl	102	V7N	C31-C1-C2-C3
21	af	103	CD4	O16-C46-C47-C48
23	L	309	MQ8	C45-C43-C44-C46
14	BP	1006	LMT	C4-C5-C6-C7
13	BH	1003	BCL	C15-C16-C17-C18
13	AJ	102	BCL	C11-C12-C13-C15
13	AS	102	BCL	C12-C13-C15-C16
13	BI	104	BCL	C11-C12-C13-C15
13	BU	1004	BCL	C2-C3-C5-C6
22	M	406	BPH	C11-C12-C13-C15
21	M	404	CD4	C15-C28-O5-P1
13	bi	103	BCL	CAA-CBA-CGA-O2A
14	BP	1005	LMT	C6-C7-C8-C9
13	AB	101	BCL	C6-C7-C8-C9
13	AM	102	BCL	C6-C7-C8-C9
13	bp	103	BCL	C11-C12-C13-C14
15	BB	101	V7N	C13-C14-C15-C16
15	BK	1001	V7N	C27-C28-C29-C39
15	BM	1001	V7N	C27-C28-C29-C39
15	bo	101	V7N	C27-C28-C29-C39
14	BB	102	LMT	C5-C6-C7-C8
14	BH	1004	LMT	C2-C3-C4-C5
14	BQ	1002	LMT	C9-C10-C11-C12
13	AW	104	BCL	C16-C17-C18-C20
21	H1	1003	CD4	C10-C11-C12-C13
13	AP	101	BCL	C8-C10-C11-C12
13	be	104	BCL	C2A-CAA-CBA-CGA
15	BE	101	V7N	C23-C24-C25-C26
13	AU	102	BCL	CAA-CBA-CGA-O2A
20	bm	102	0V9	O2-C10-C11-C12
26	ag	1002	V7B	C46-C47-C48-O53
13	AL	103	BCL	CAA-CBA-CGA-O1A
13	AS	102	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	AI	102	BCL	C13-C15-C16-C17
14	BR	1002	LMT	C2B-C1B-O1B-C4'
20	bb	104	0V9	C11-C12-C13-C14
13	bg	104	BCL	C2-C3-C5-C6
13	AS	104	BCL	CAA-CBA-CGA-O2A
20	be	102	0V9	O2-C10-C11-C12
14	bj	102	LMT	O1'-C1-C2-C3
13	bi	103	BCL	CAA-CBA-CGA-O1A
20	bf	103	0V9	O4-C10-C11-C12
13	AN	102	BCL	C1A-C2A-CAA-CBA
13	BD	106	BCL	C1A-C2A-CAA-CBA
13	BG	1004	BCL	C1A-C2A-CAA-CBA
13	BI	104	BCL	C1A-C2A-CAA-CBA
13	BN	1006	BCL	C1A-C2A-CAA-CBA
13	BQ	1003	BCL	C1A-C2A-CAA-CBA
13	BT	1004	BCL	C1A-C2A-CAA-CBA
13	aa	1001	BCL	C1A-C2A-CAA-CBA
13	aj	102	BCL	C1A-C2A-CAA-CBA
13	ba	103	BCL	C1A-C2A-CAA-CBA
13	BU	1004	BCL	C10-C11-C12-C13
14	BS	1002	LMT	C2B-C1B-O1B-C4'
13	L	303	BCL	C2-C1-O2A-CGA
14	L	305	LMT	O5'-C5'-C6'-O6'
13	AU	102	BCL	CAA-CBA-CGA-O1A
13	ab	1001	BCL	CAA-CBA-CGA-O1A
13	ai	102	BCL	CAA-CBA-CGA-O1A
14	BD	102	LMT	C3-C4-C5-C6
14	AD	1003	LMT	C2B-C1B-O1B-C4'
21	ai	103	CD4	C32-C33-C34-O14
26	af	101	V7B	O1-C7-C8-C9
13	AV	103	BCL	C13-C15-C16-C17
13	AF	1002	BCL	C2A-CAA-CBA-CGA
20	ba	102	0V9	C13-C14-C15-C16
13	AI	103	BCL	C16-C17-C18-C20
13	ap	1001	BCL	CAA-CBA-CGA-O1A
20	L	310	0V9	O5-C30-C31-C32
20	be	102	0V9	O5-C30-C31-C32
14	BN	1004	LMT	C5'-C4'-O1B-C1B
26	af	101	V7B	C8-C9-O8-C28
20	bg	102	0V9	C11-C12-C13-C14
13	bp	103	BCL	C4-C3-C5-C6
14	AG	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	BH	1004	LMT	C6-C7-C8-C9
14	BW	1005	LMT	C2-C3-C4-C5
13	AH	101	BCL	CAA-CBA-CGA-O1A
14	AP	102	LMT	C1-C2-C3-C4
14	BK	1004	LMT	C9-C10-C11-C12
19	H1	1001	PGW	C03-O11-P-O13
20	L	310	0V9	C1-O3P-P-O2P
20	ba	104	0V9	C1-O3P-P-O1P
20	bn	104	0V9	C1-O3P-P-O1P
21	M	404	CD4	C32-O13-P2-O12
21	ad	101	CD4	C32-O13-P2-O12
21	af	103	CD4	C29-O8-P1-O7
21	af	104	CD4	C29-O8-P1-O6
21	ai	103	CD4	C31-O10-P2-O12
20	H1	1002	0V9	O2-C2-C3-O3
13	AP	103	BCL	CAA-CBA-CGA-O1A
13	BX	1004	BCL	CAA-CBA-CGA-O1A
20	bc	102	0V9	O5-C30-C31-C32
13	AW	103	BCL	C15-C16-C17-C18
13	AW	104	BCL	C13-C15-C16-C17
13	BL	1004	BCL	C10-C11-C12-C13
13	am	1001	BCL	C5-C6-C7-C8
13	AW	104	BCL	CAA-CBA-CGA-O1A
19	H1	1001	PGW	O02-C1-C2-C3
21	ad	101	CD4	C12-C13-C14-O1
21	af	103	CD4	O17-C46-C47-C48
14	BE	102	LMT	C5'-C4'-O1B-C1B
21	H1	1003	CD4	C50-C51-C52-C53
20	bk	104	0V9	C19-C20-C21-C22
15	bb	101	V7N	C26-C27-C28-C29
13	ae	1001	BCL	CAA-CBA-CGA-O1A
20	bc	102	0V9	O4-C10-C11-C12
14	AL	102	LMT	C4-C5-C6-C7
14	L	307	LMT	O1'-C1-C2-C3
13	AG	103	BCL	CAA-CBA-CGA-O2A
20	bk	104	0V9	O2-C10-C11-C12
20	aj	101	0V9	C2-C3-O3-C30
13	BK	1003	BCL	C2-C3-C5-C6
13	AF	1002	BCL	CAD-CBD-CGD-O1D
13	AI	102	BCL	CAD-CBD-CGD-O1D
13	AQ	101	BCL	CAD-CBD-CGD-O1D
13	BU	1004	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	BW	1003	BCL	CAD-CBD-CGD-O1D
13	M	405	BCL	CAD-CBD-CGD-O1D
20	be	103	0V9	C5-C4-O4P-P
20	bf	103	0V9	C5-C4-O4P-P
14	BE	102	LMT	C2B-C1B-O1B-C4'
13	AG	103	BCL	C11-C12-C13-C14
13	AJ	102	BCL	C11-C12-C13-C14
13	AS	102	BCL	C6-C7-C8-C9
13	BJ	1004	BCL	C11-C10-C8-C9
13	BK	1003	BCL	C14-C13-C15-C16
13	ad	102	BCL	C14-C13-C15-C16
13	ae	1001	BCL	C11-C10-C8-C9
13	aj	102	BCL	C14-C13-C15-C16
13	al	1001	BCL	C14-C13-C15-C16
22	M	406	BPH	C11-C12-C13-C14
13	AO	102	BCL	C8-C10-C11-C12
14	AS	103	LMT	C5'-C4'-O1B-C1B
14	bj	102	LMT	C1-C2-C3-C4
13	AW	103	BCL	C16-C17-C18-C20
13	BL	1004	BCL	CAA-CBA-CGA-O2A
13	ad	102	BCL	CAA-CBA-CGA-O2A
14	bp	101	LMT	C1-C2-C3-C4
15	AH	105	V7N	C1-C2-C3-C4
15	BS	1001	V7N	C1-C2-C3-C4
15	BW	1001	V7N	C1-C2-C3-C4
15	bc	104	V7N	C1-C2-C3-C4
14	BK	1006	LMT	C4-C5-C6-C7
20	bn	104	0V9	C31-C32-C33-C34
20	bb	104	0V9	O5-C30-C31-C32
14	BX	1003	LMT	C2B-C1B-O1B-C4'
13	BR	1003	BCL	C4-C3-C5-C6
13	bj	104	BCL	C4-C3-C5-C6
22	L	301	BPH	C4-C3-C5-C6
20	bo	104	0V9	C31-C32-C33-C34
13	AB	101	BCL	C6-C7-C8-C10
13	AF	1001	BCL	C11-C10-C8-C7
13	AN	104	BCL	C12-C13-C15-C16
13	AP	101	BCL	C6-C7-C8-C10
13	AQ	102	BCL	C3A-C2A-CAA-CBA
13	AQ	103	BCL	C3A-C2A-CAA-CBA
13	AU	102	BCL	C12-C13-C15-C16
13	BJ	1004	BCL	C11-C10-C8-C7

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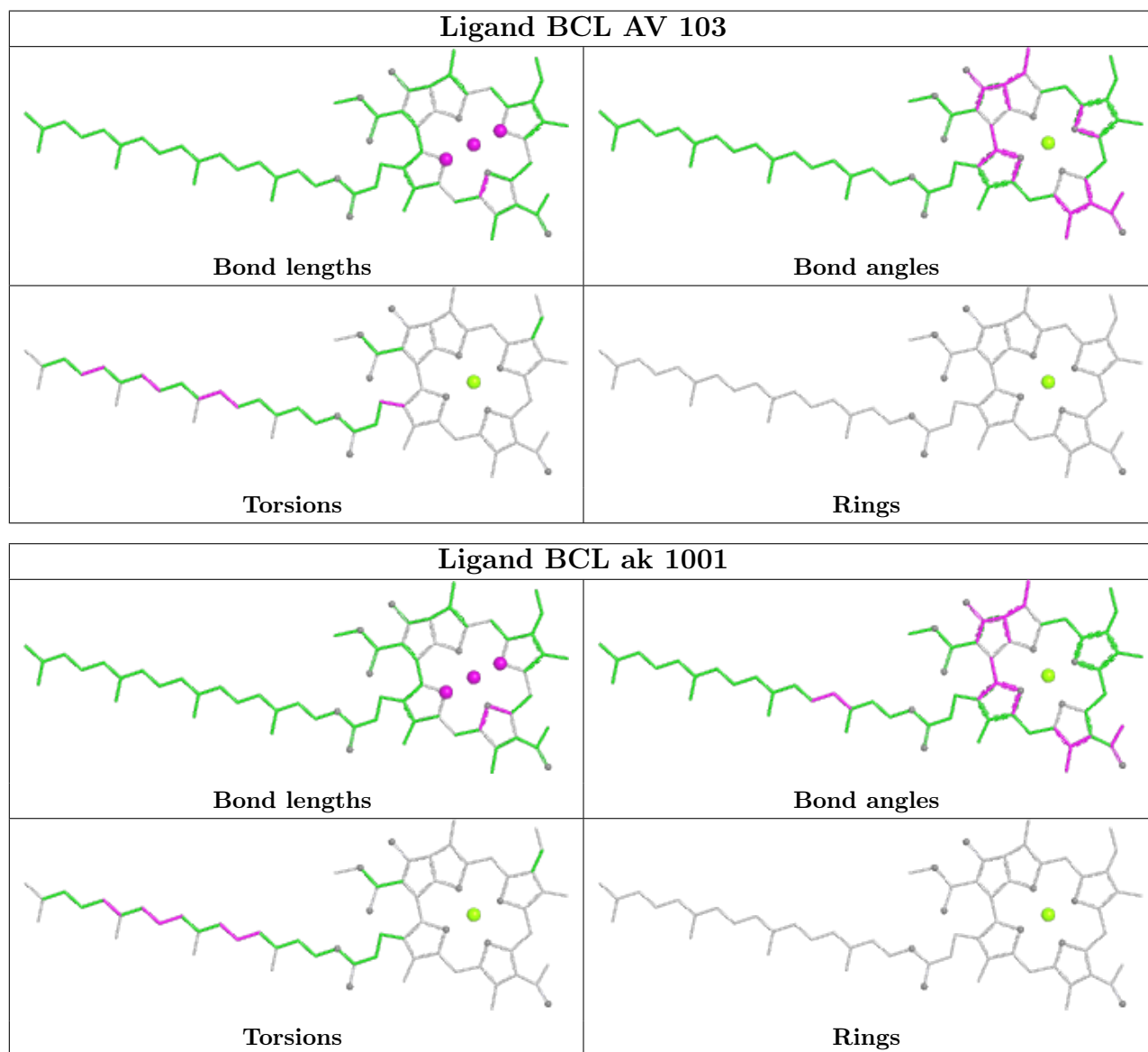
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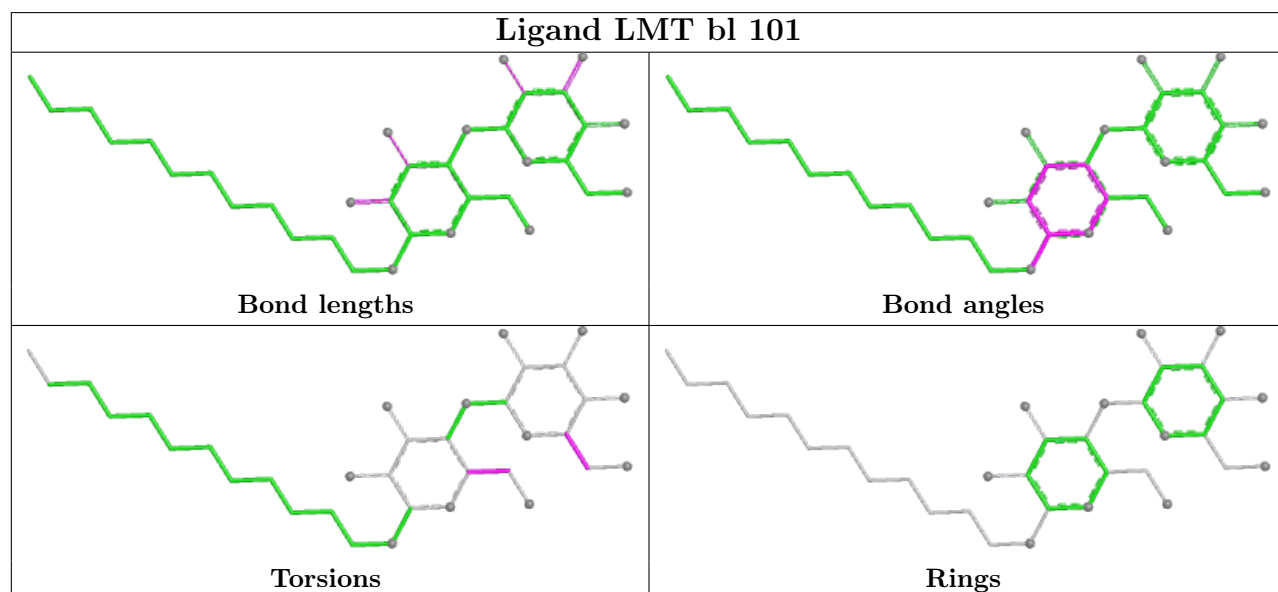
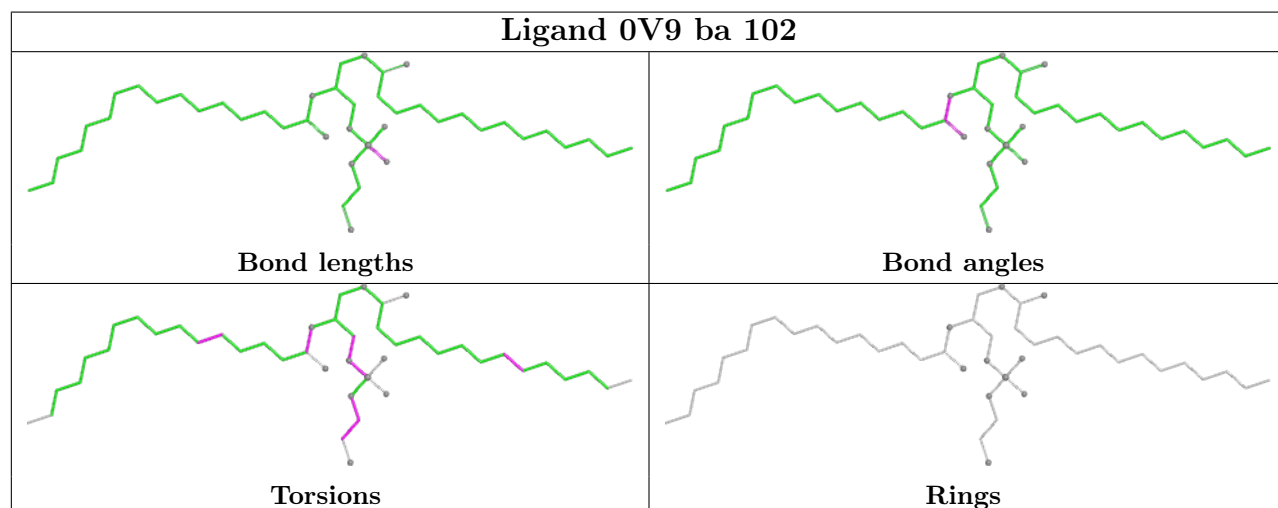
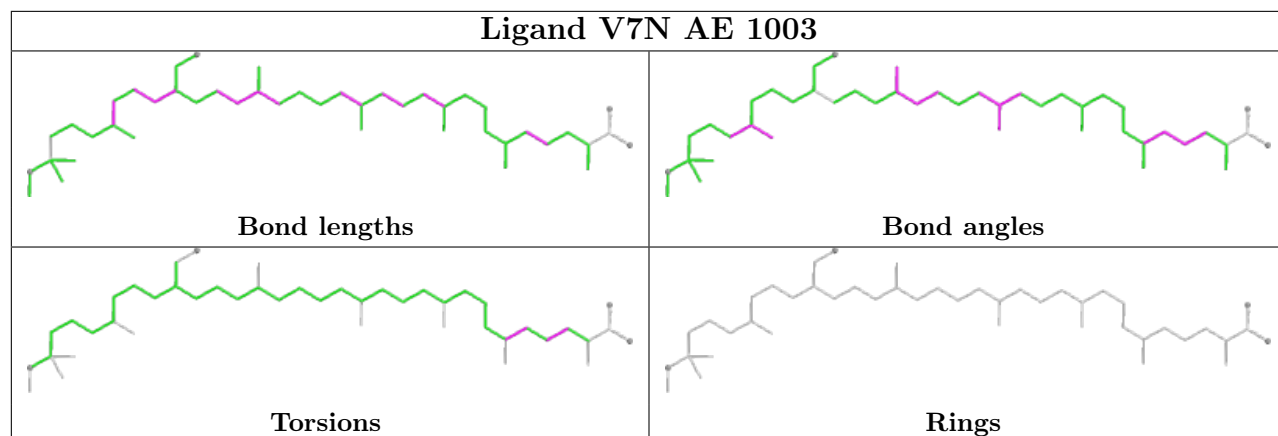
Mol	Chain	Res	Type	Atoms
13	BJ	1004	BCL	C11-C12-C13-C15
13	BK	1003	BCL	C11-C12-C13-C15
13	bh	105	BCL	C3A-C2A-CAA-CBA
13	bp	103	BCL	C11-C10-C8-C7
13	bp	103	BCL	C11-C12-C13-C15
13	ad	102	BCL	CAA-CBA-CGA-O1A
13	ah	1001	BCL	CAA-CBA-CGA-O1A
14	BR	1006	LMT	C5-C6-C7-C8
13	ah	1001	BCL	CAA-CBA-CGA-O2A
26	ag	1002	V7B	O7-C10-C11-C12
15	BQ	1001	V7N	C3-C4-C5-C6
15	BV	1001	V7N	C3-C4-C5-C6
15	BO	1001	V7N	C27-C28-C29-C39
14	BC	104	LMT	C1-C2-C3-C4
14	BK	1002	LMT	C2-C1-O1'-C1'
14	BL	1002	LMT	C2-C1-O1'-C1'
14	BN	1005	LMT	C2-C1-O1'-C1'
14	BW	1006	LMT	C2-C1-O1'-C1'
21	af	104	CD4	O14-C35-C36-C37
14	BE	105	LMT	O5'-C1'-O1'-C1
22	L	301	BPH	C8-C10-C11-C12
21	af	104	CD4	O1-C14-O2-C15
14	BO	1002	LMT	C4'-C5'-C6'-O6'
14	BR	1005	LMT	C5'-C4'-O1B-C1B
13	AH	101	BCL	C8-C10-C11-C12
15	bc	104	V7N	C23-C24-C25-C26
15	bg	101	V7N	C23-C24-C25-C26
23	L	309	MQ8	C44-C46-C47-C48
14	BC	104	LMT	C5'-C4'-O1B-C1B
20	ba	102	OV9	C36-C37-C38-C39
13	BC	103	BCL	CAA-CBA-CGA-O2A
27	ai	101	UYH	C37-C38-C39-C40
13	AS	101	BCL	C10-C11-C12-C13
13	AF	1002	BCL	C13-C15-C16-C17
13	BA	104	BCL	C10-C11-C12-C13
13	ao	1001	BCL	C15-C16-C17-C18
14	BL	1003	LMT	C3'-C4'-O1B-C1B
14	BD	105	LMT	C2B-C1B-O1B-C4'
14	BN	1002	LMT	C3'-C4'-O1B-C1B

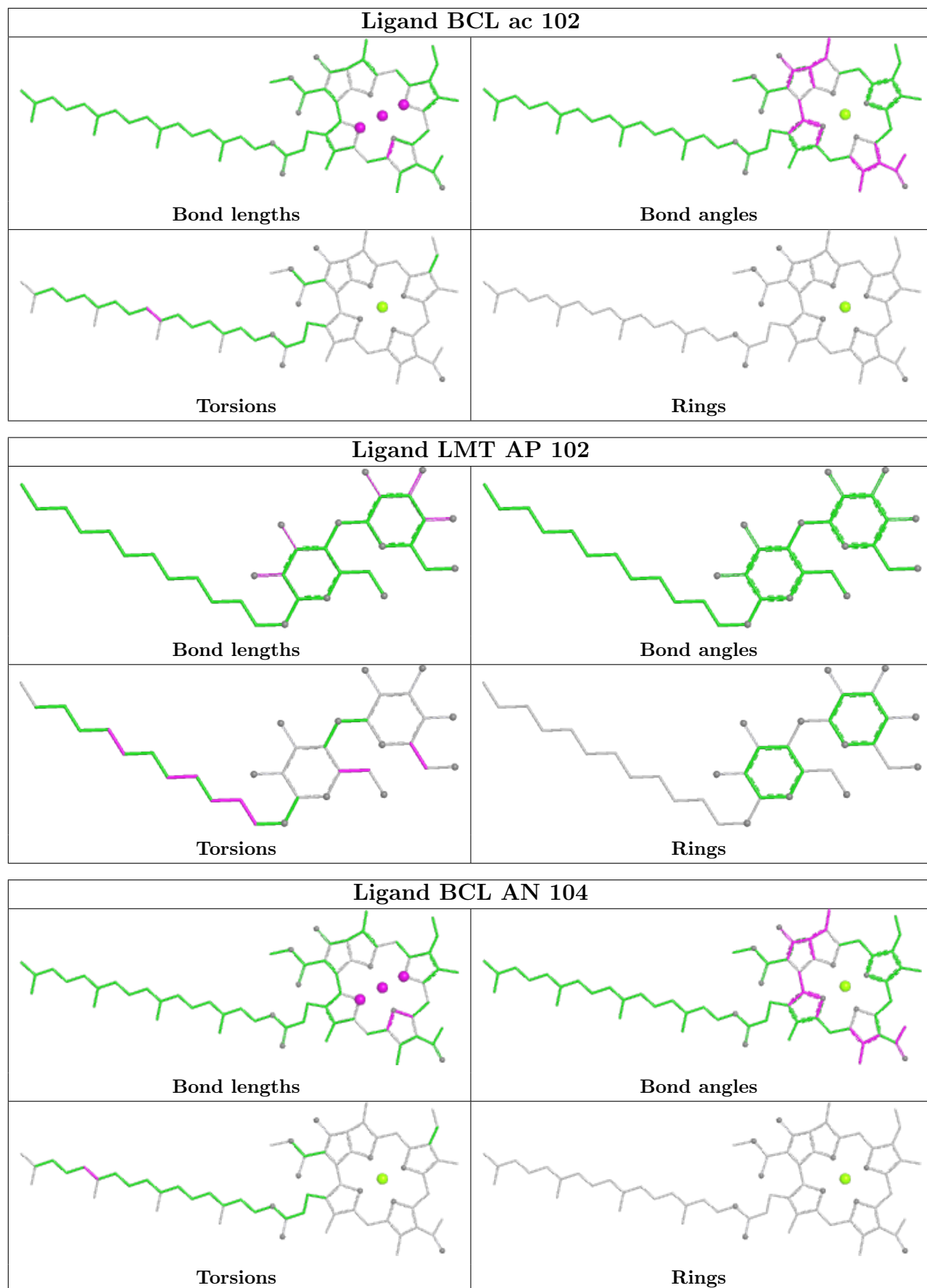
There are no ring outliers.

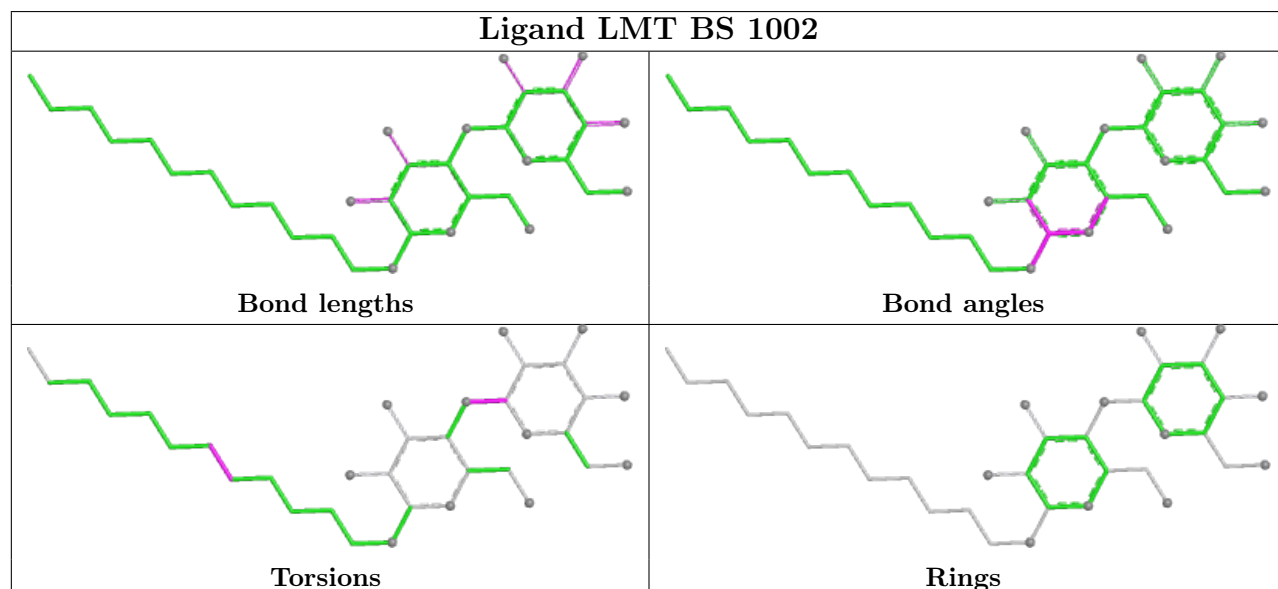
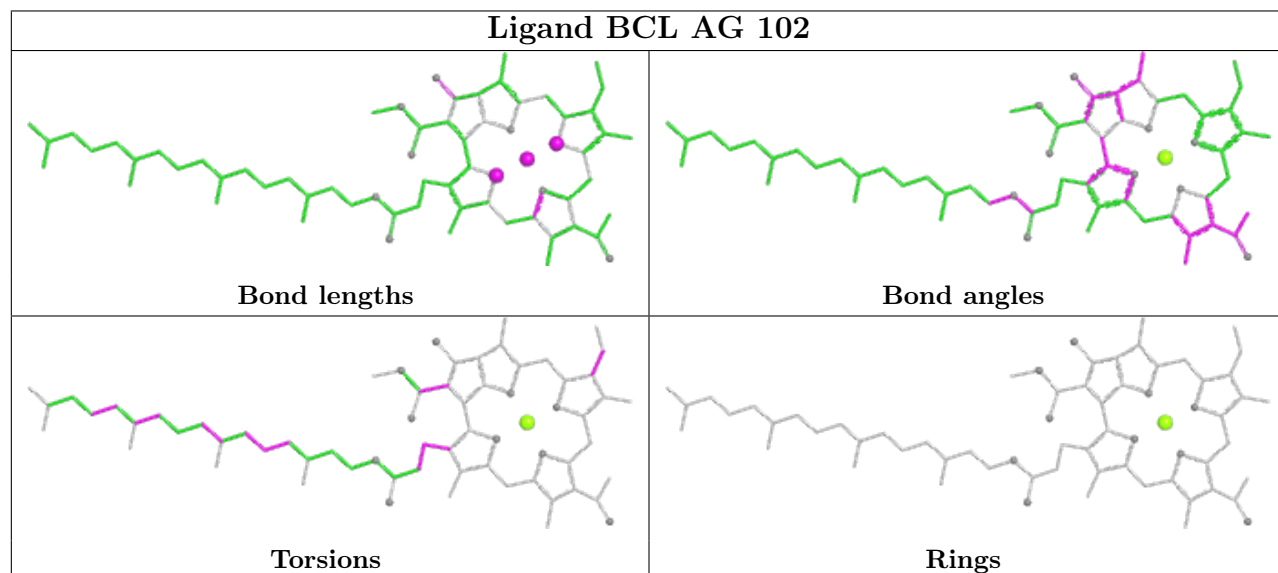
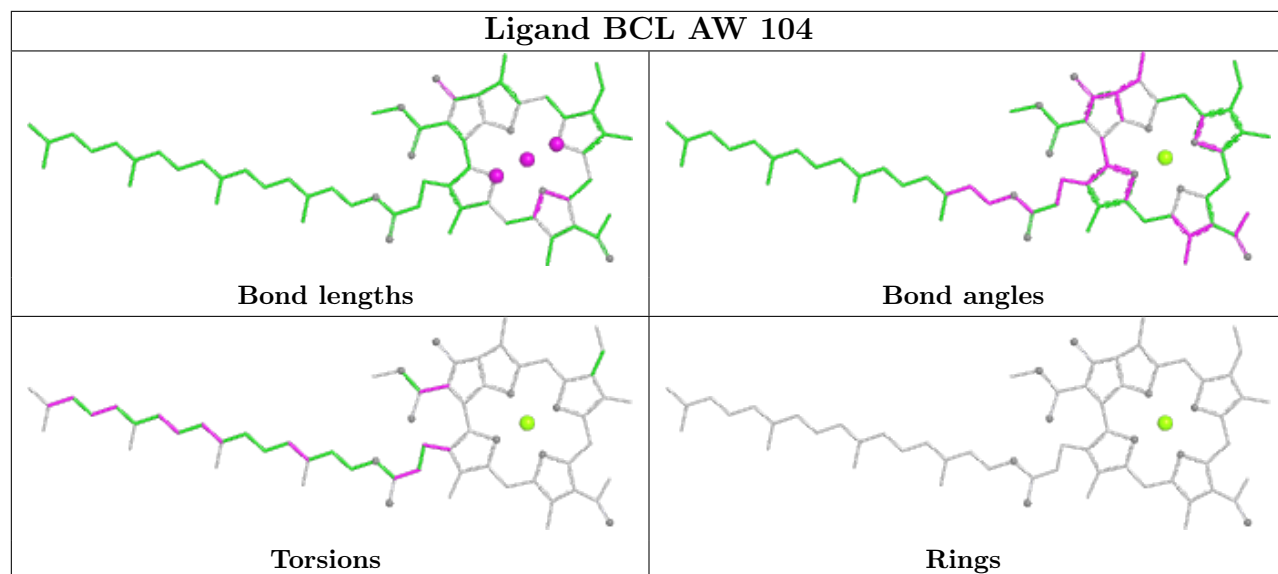
No monomer is involved in short contacts.

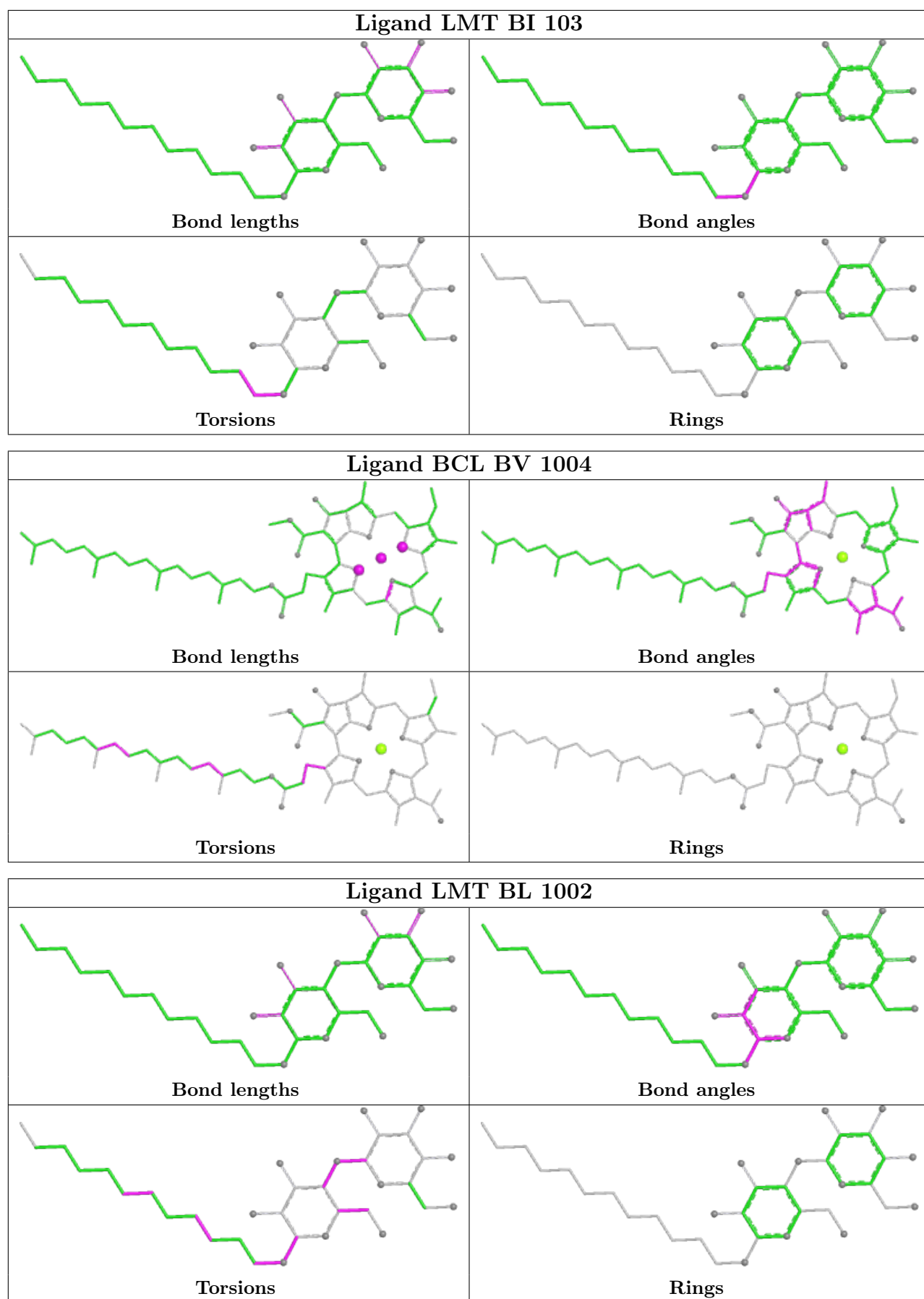
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

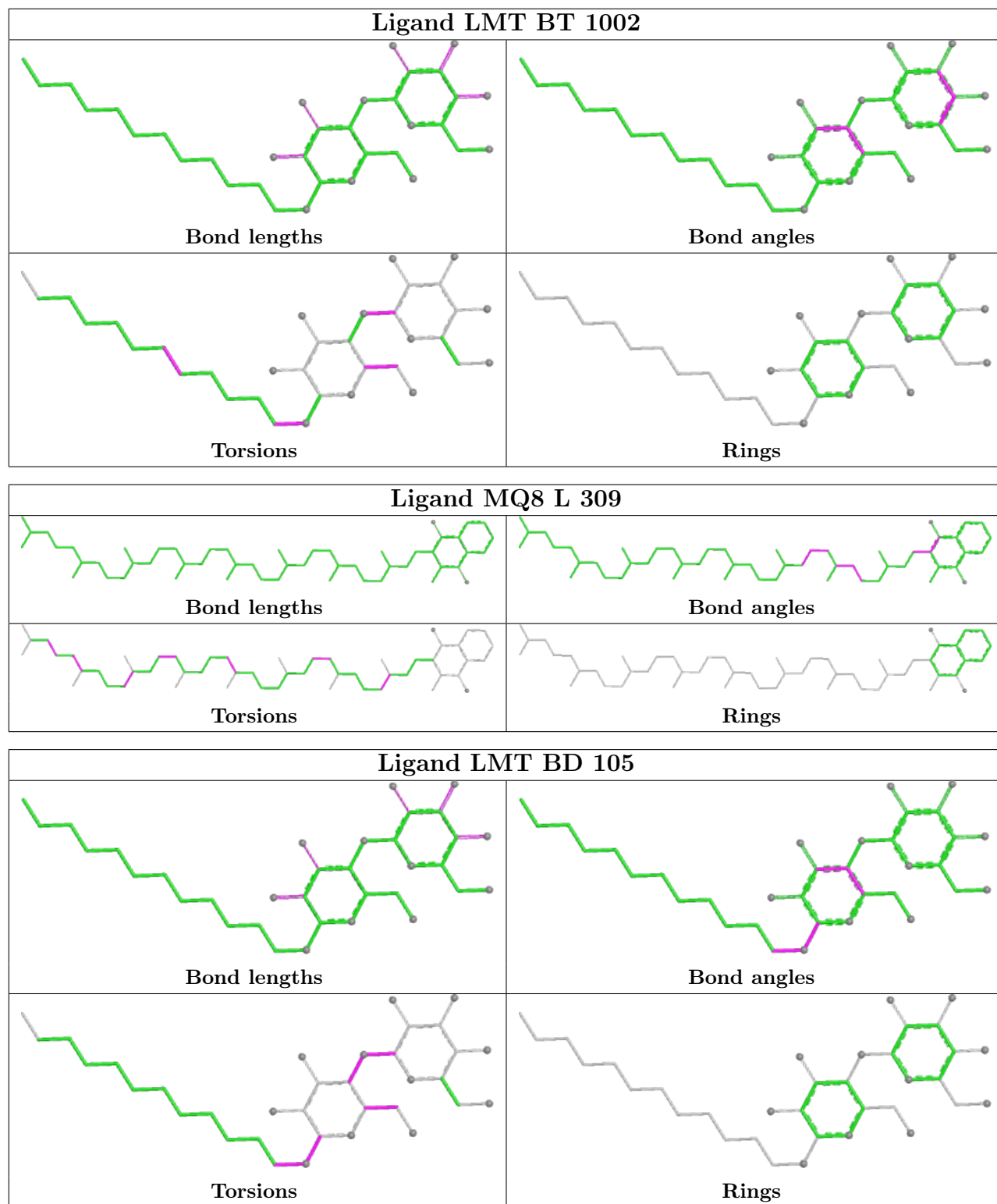




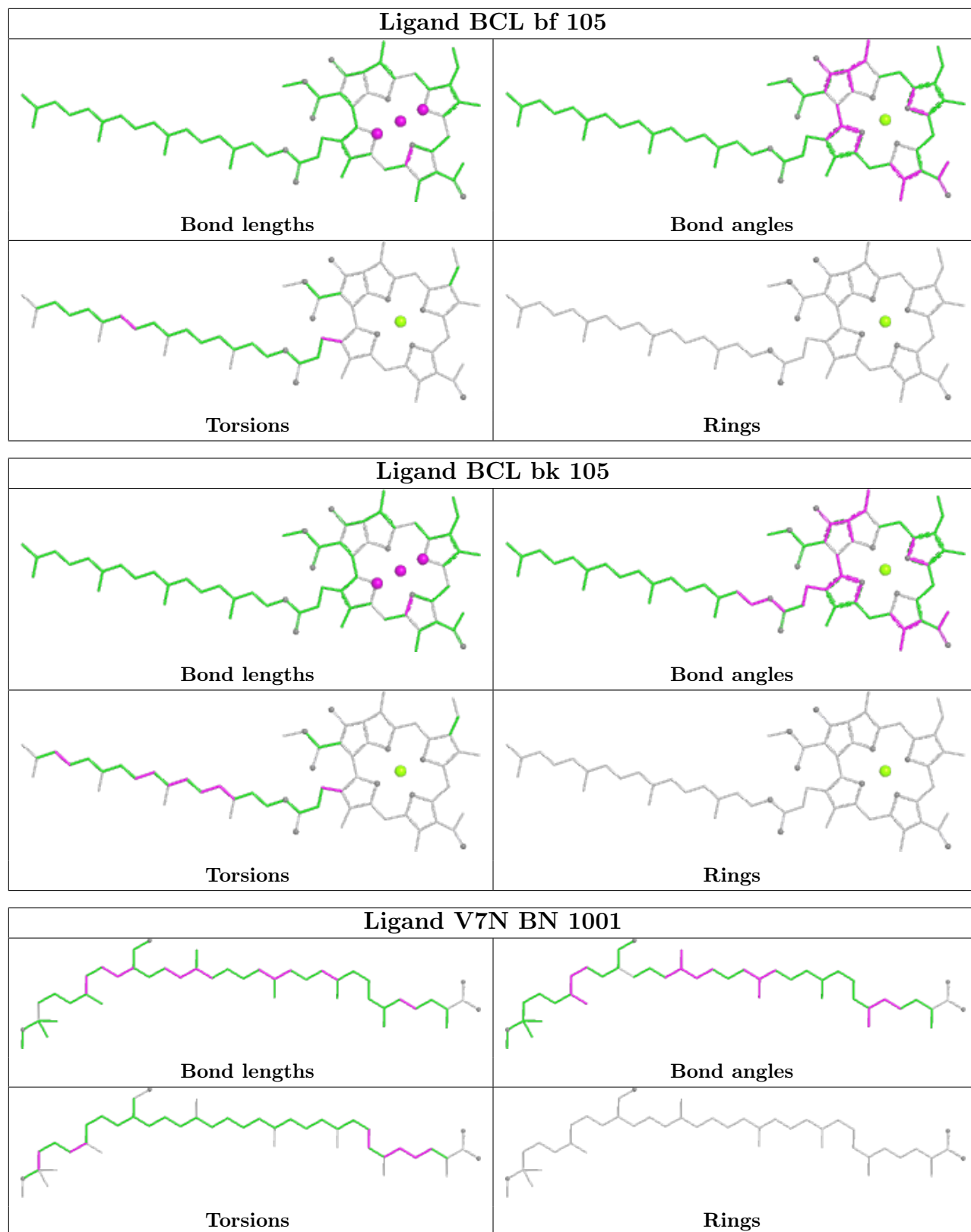


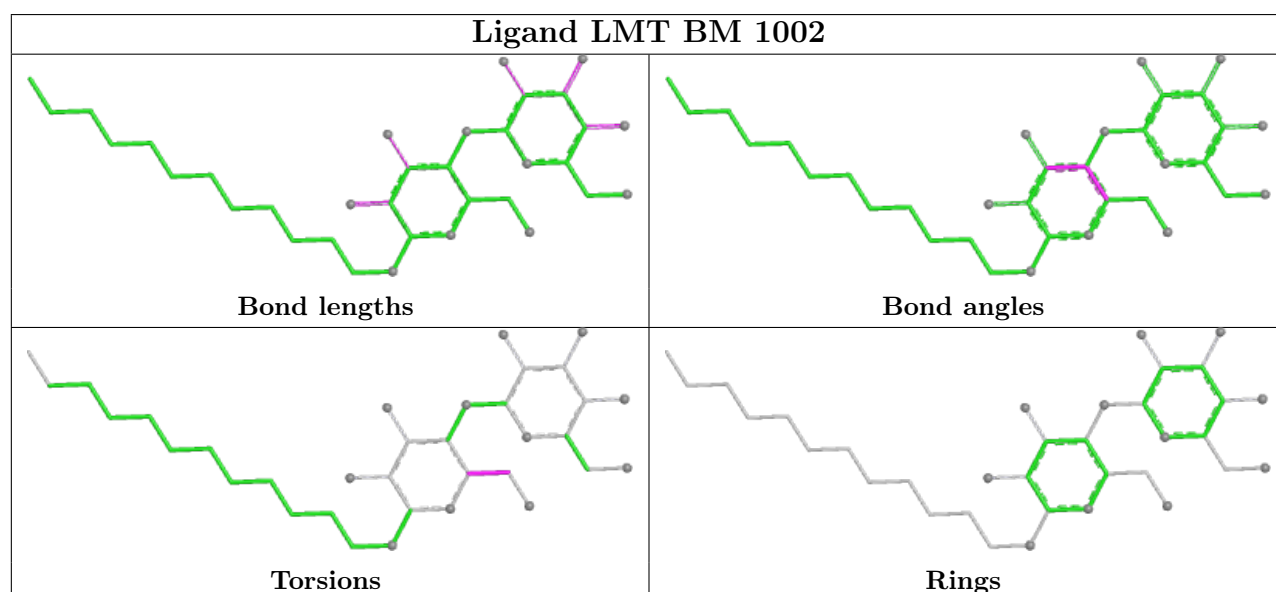
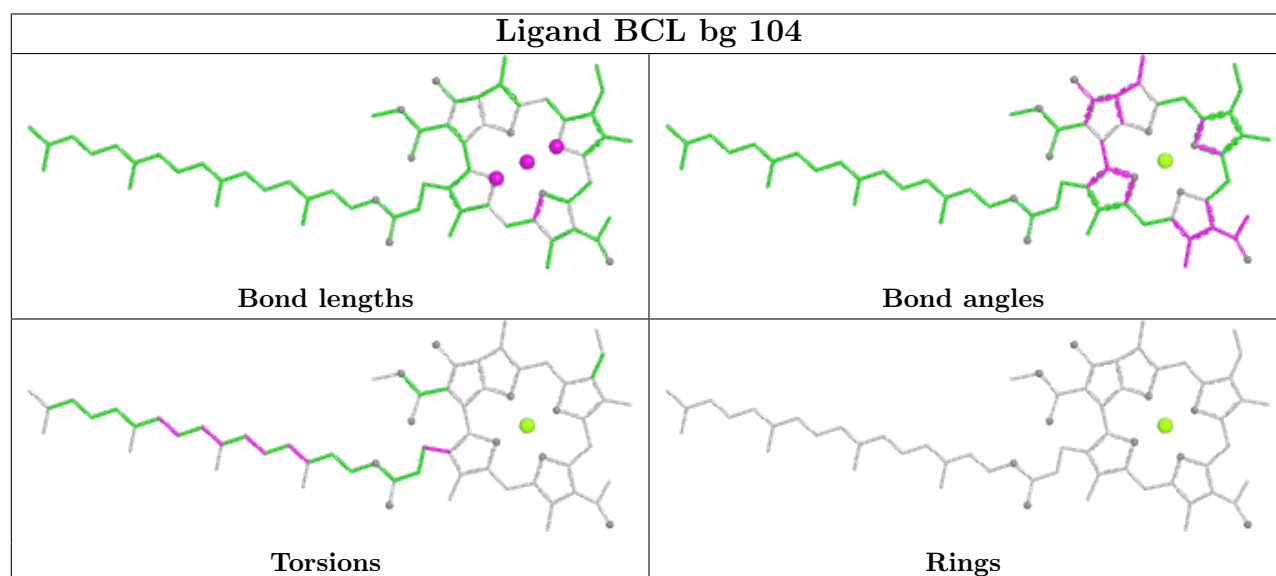
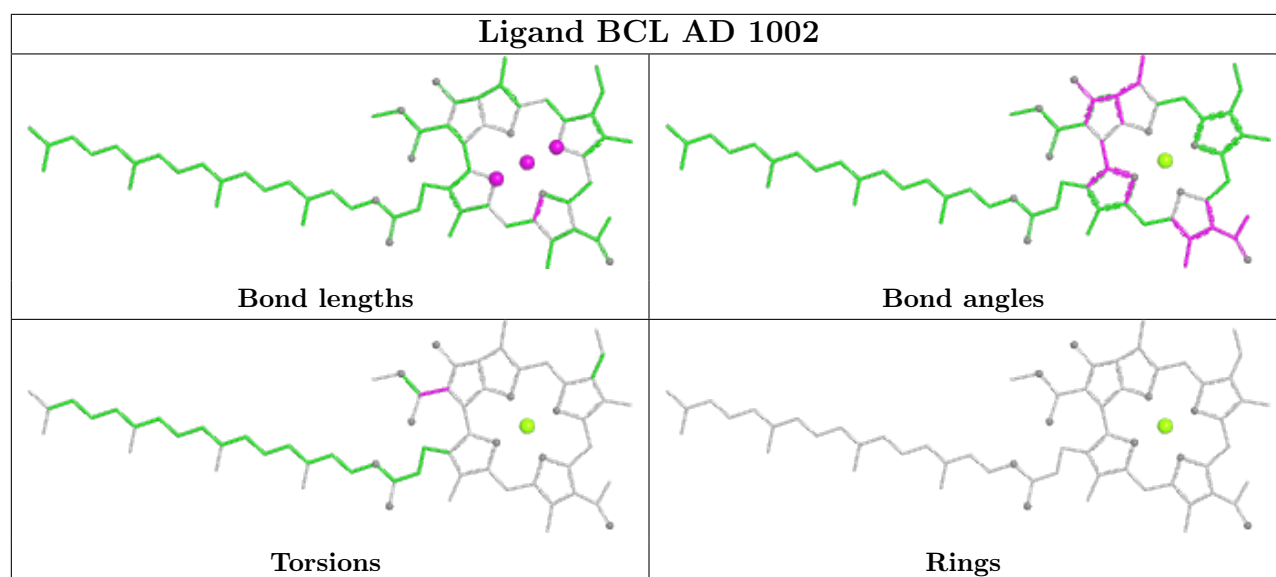


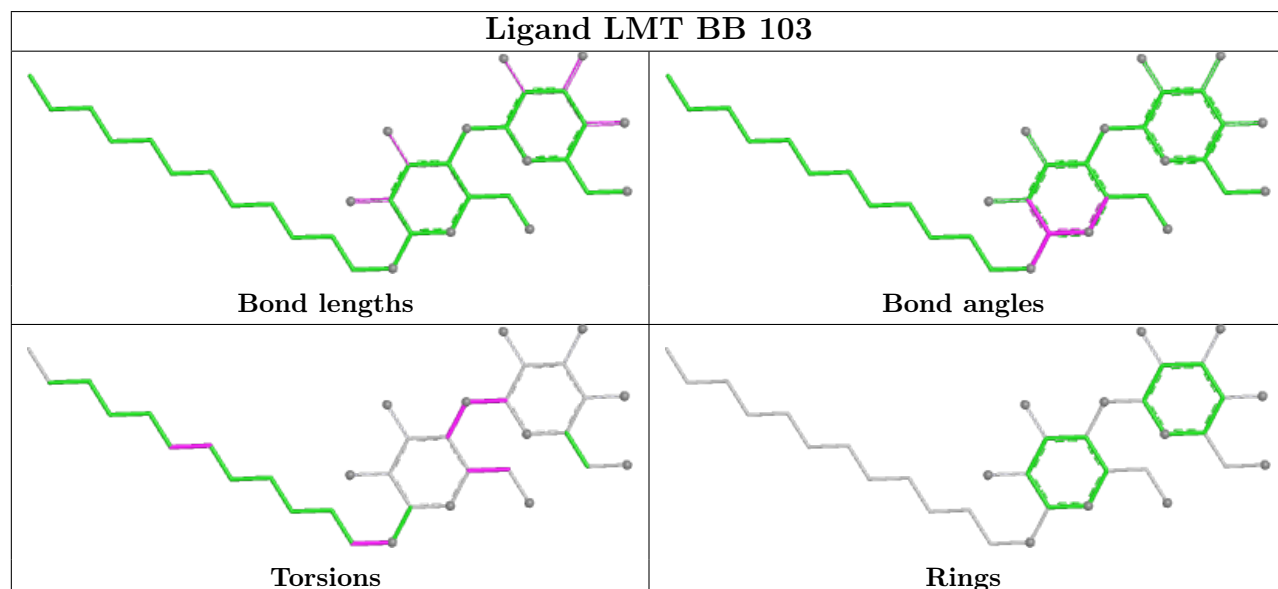
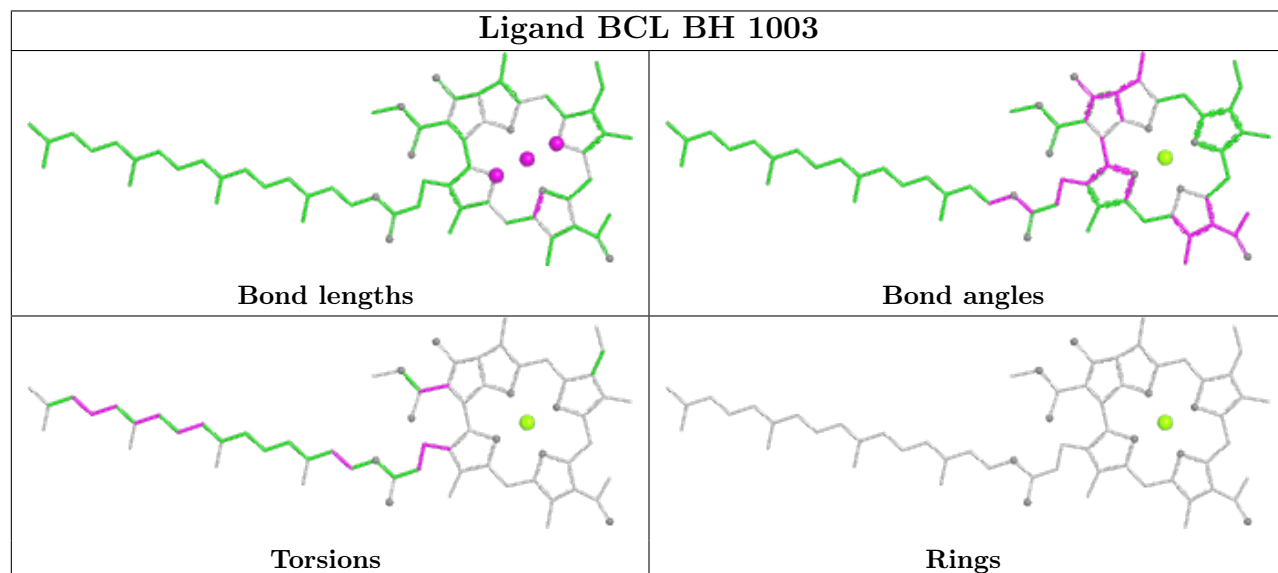
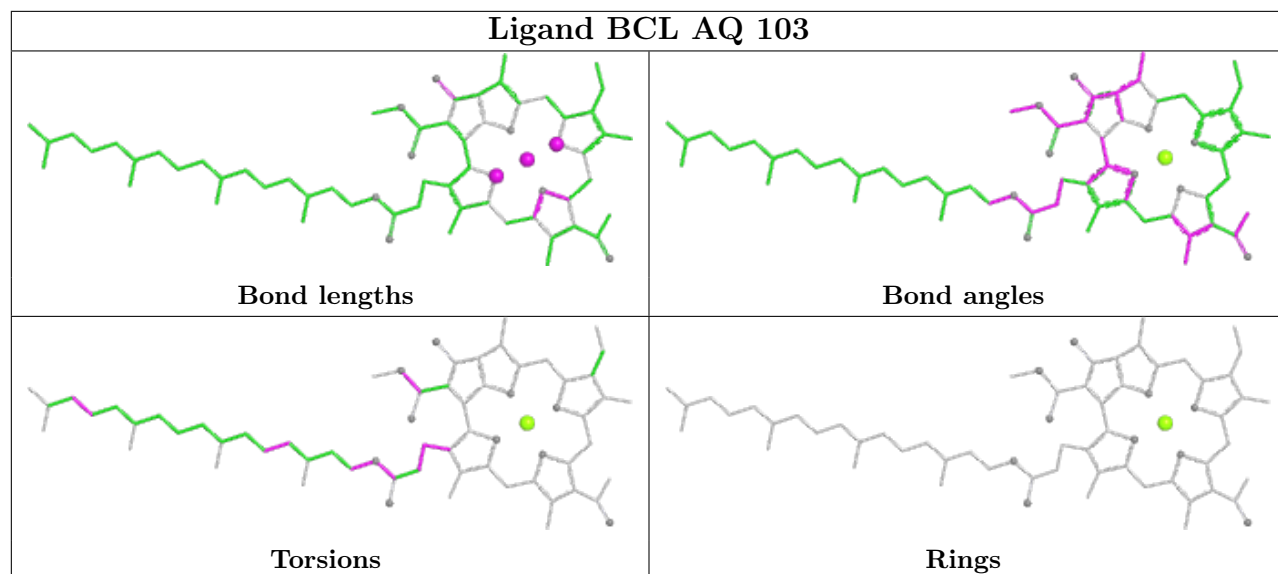


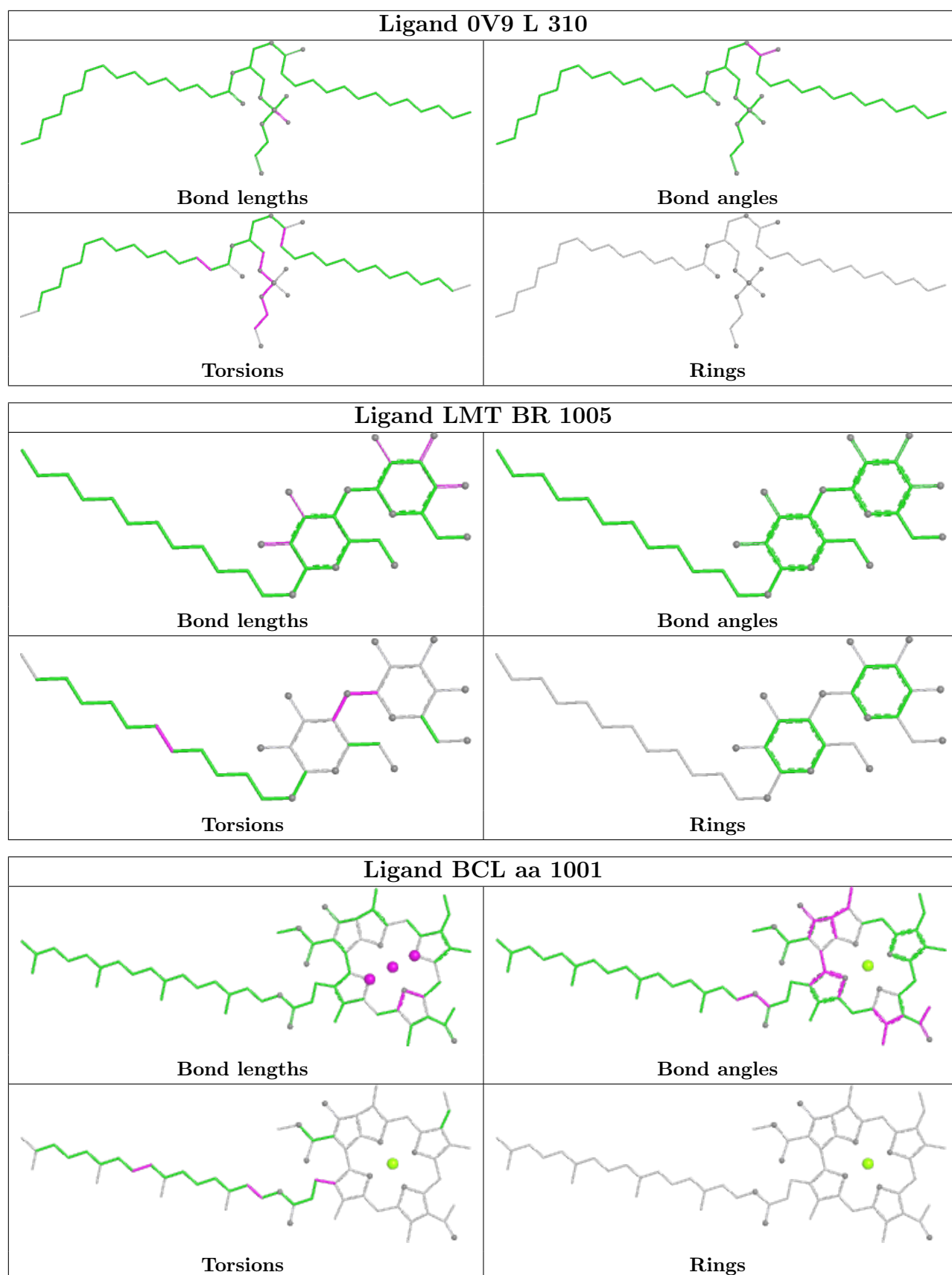


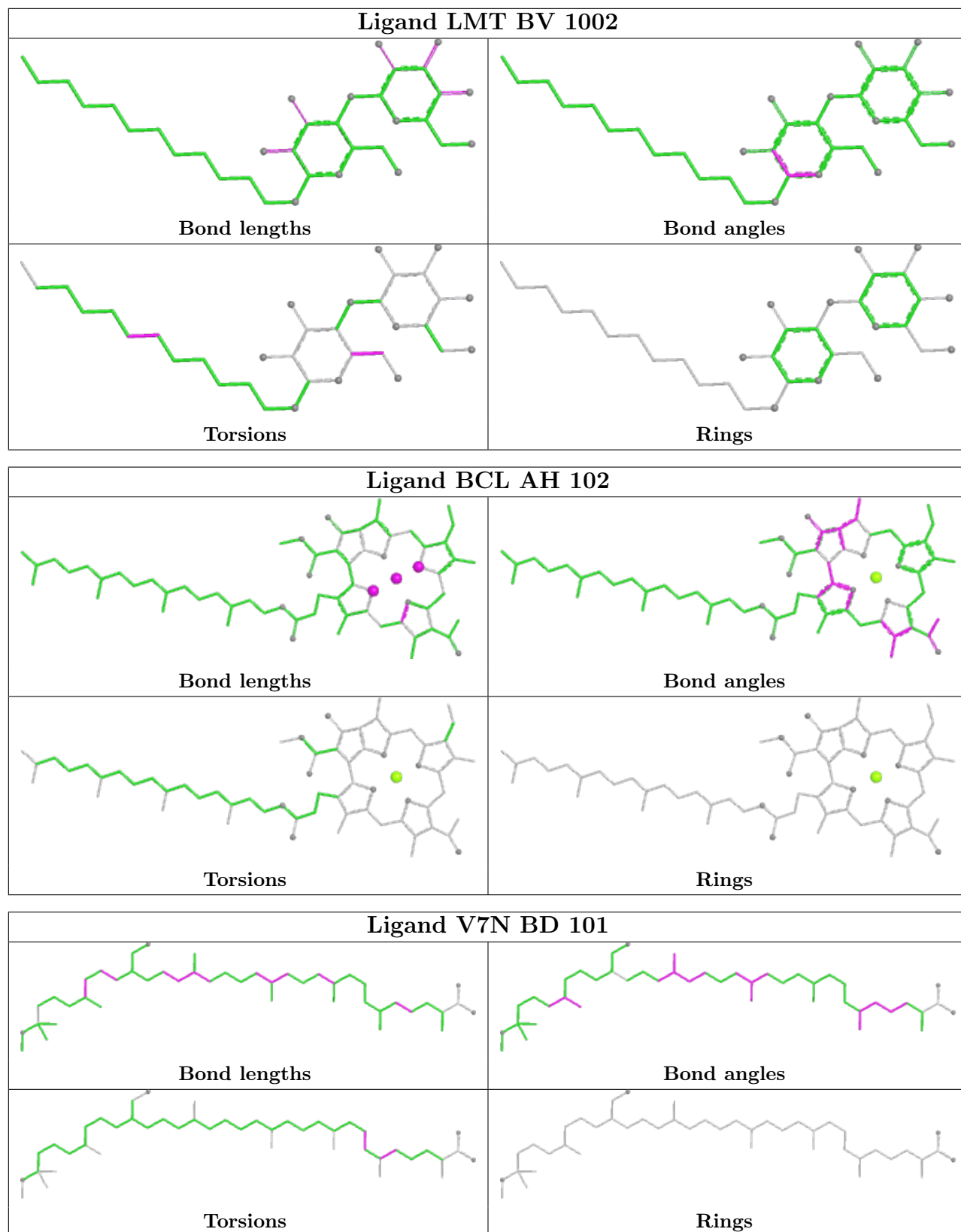


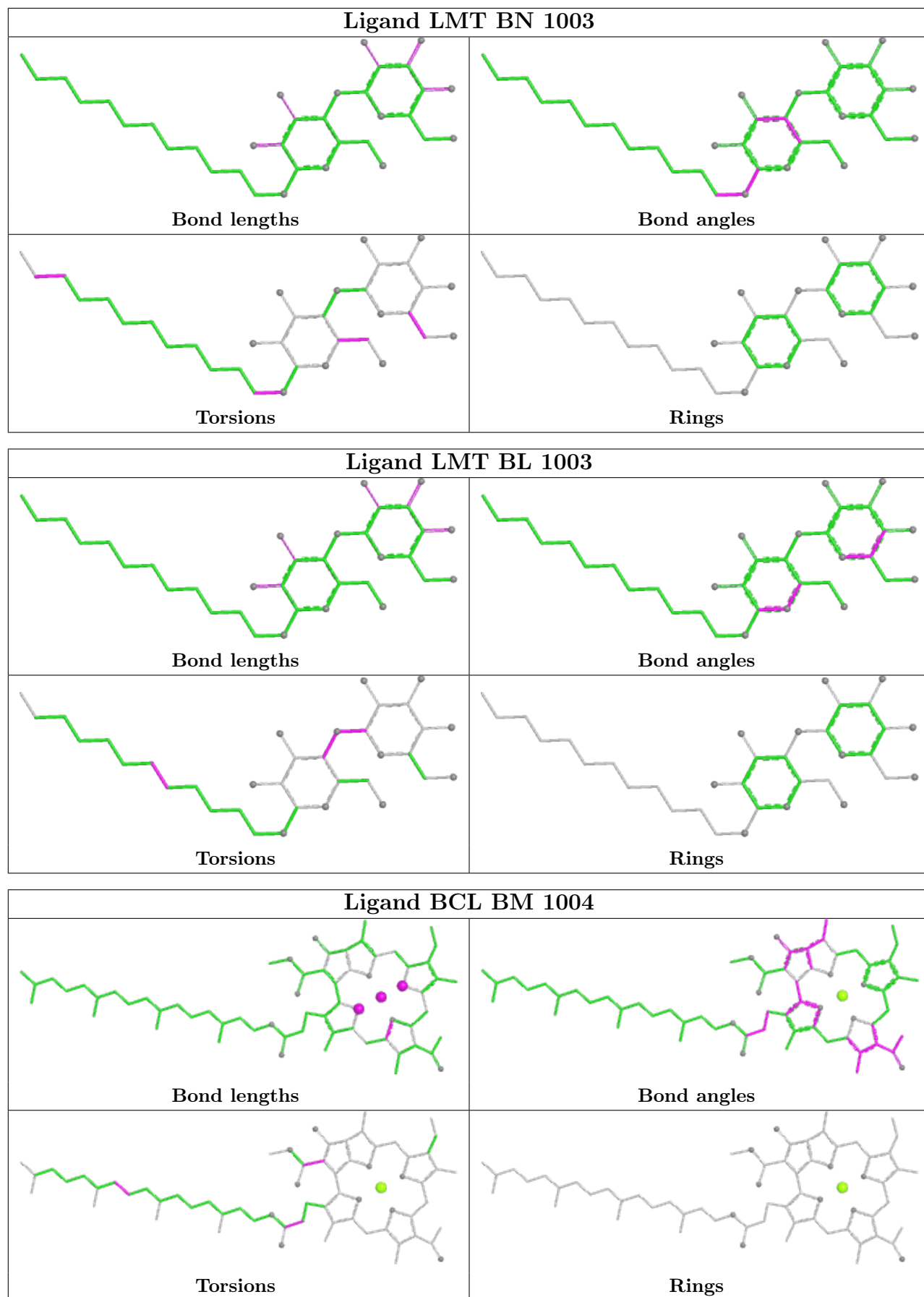


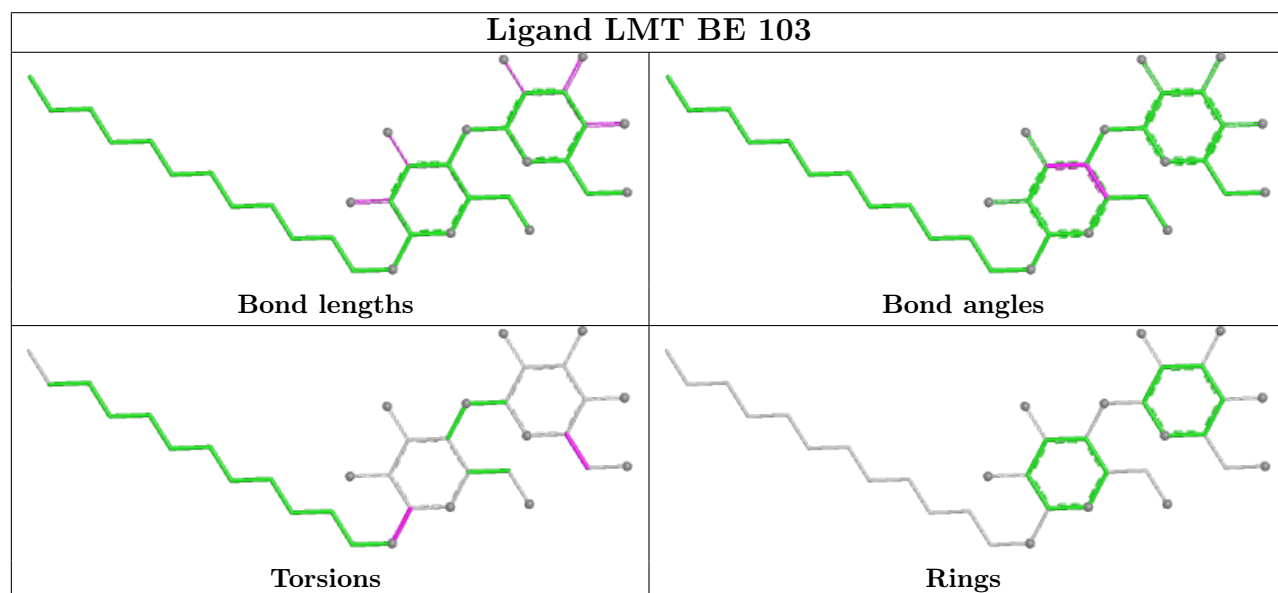
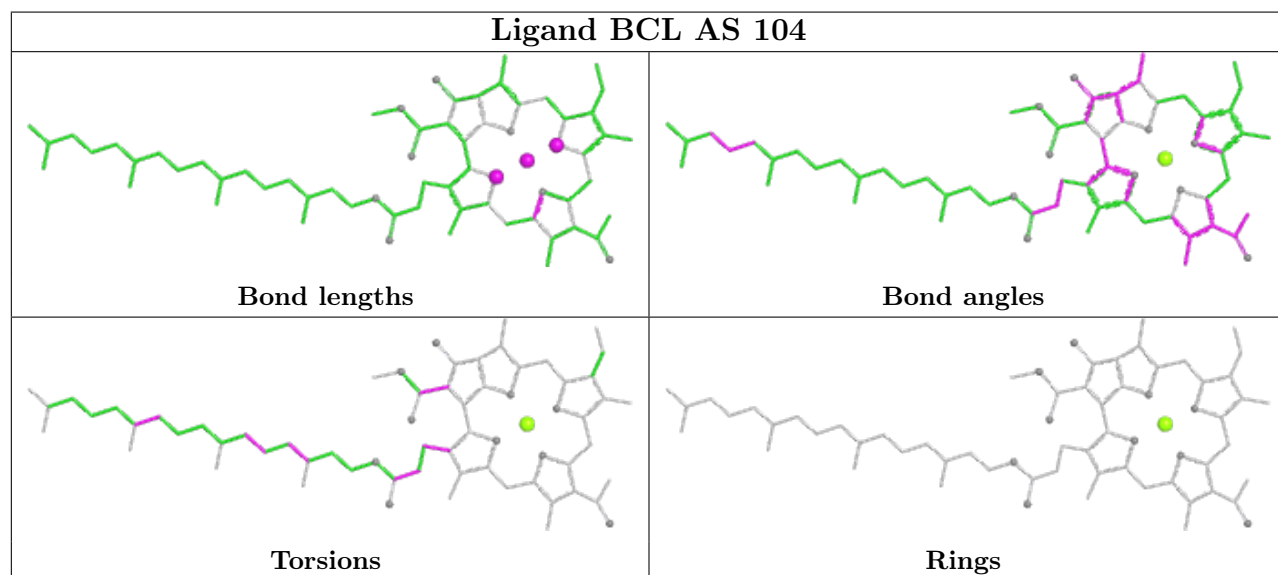
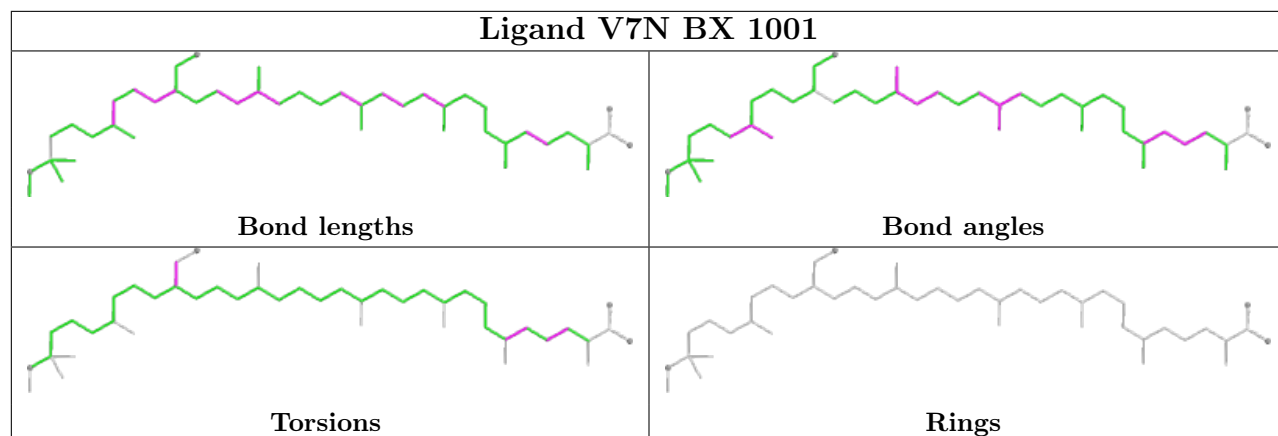


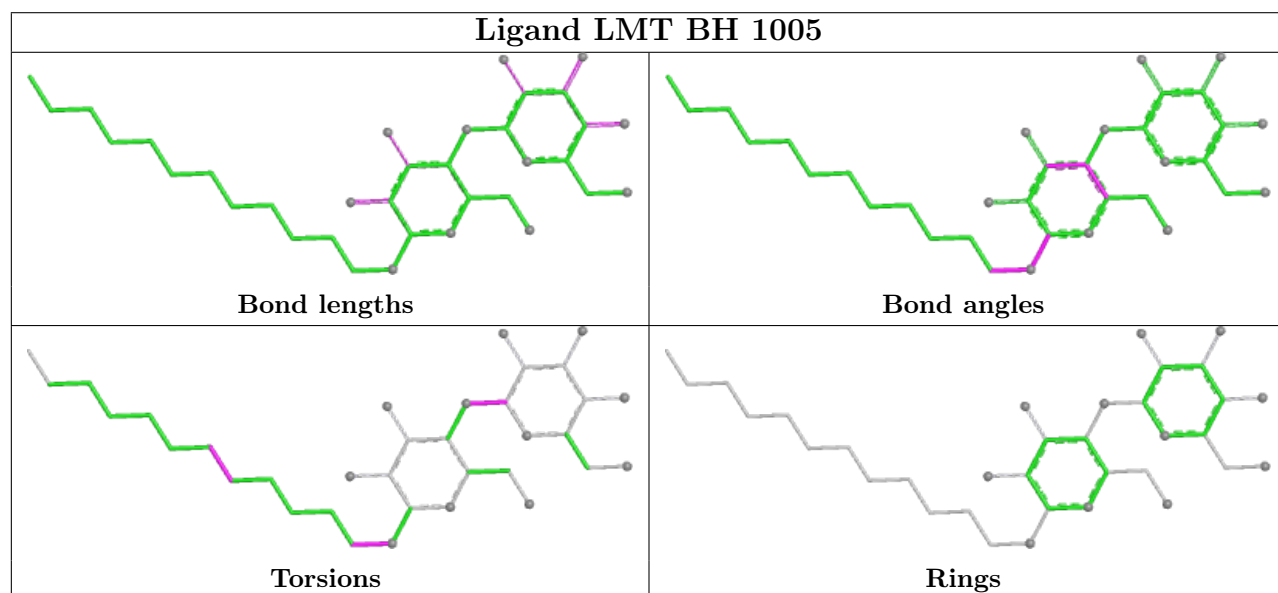
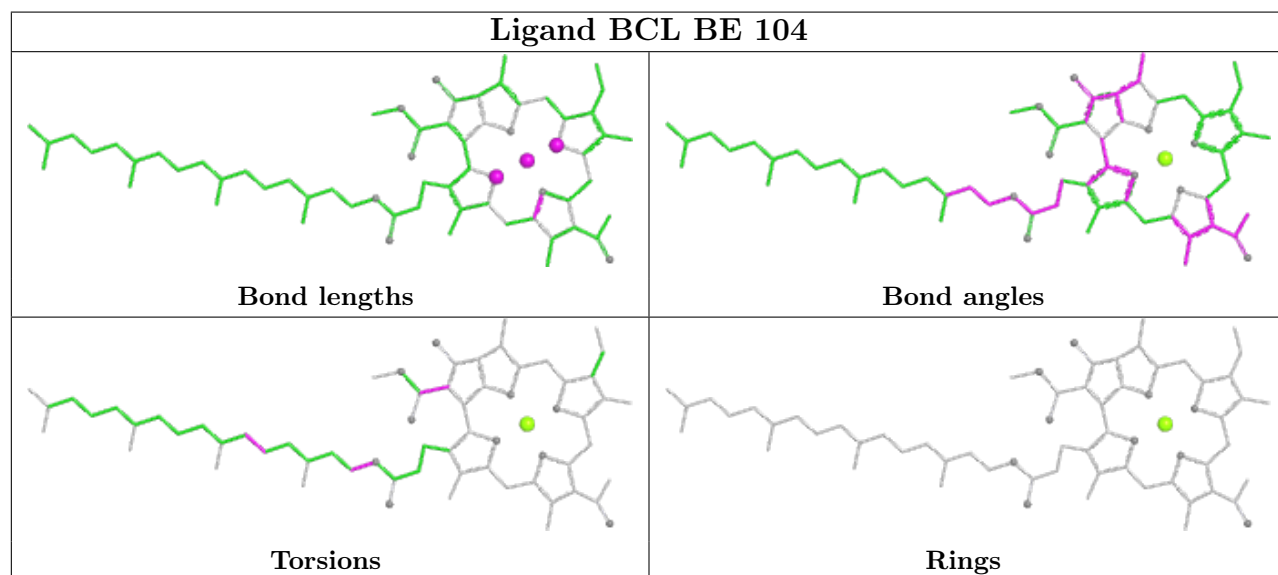
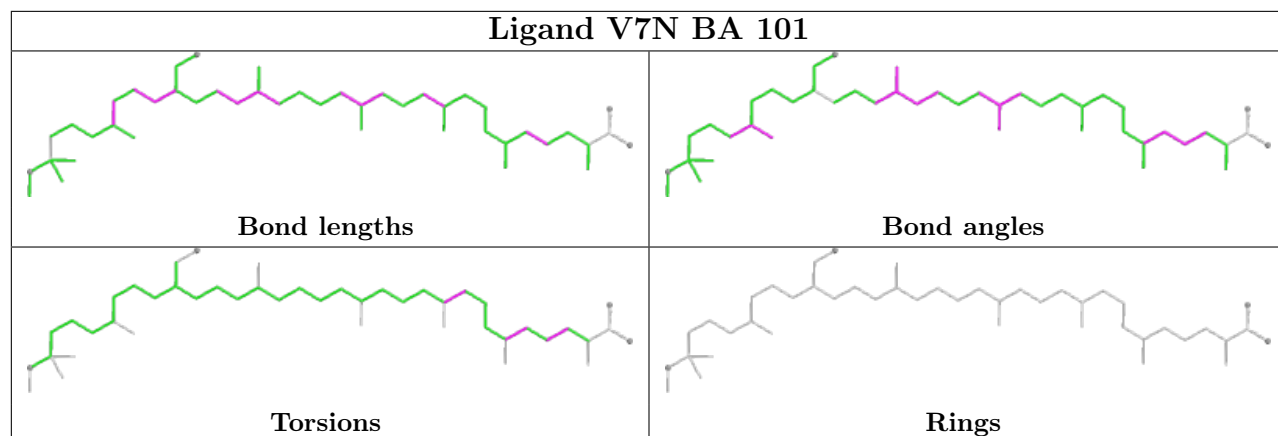




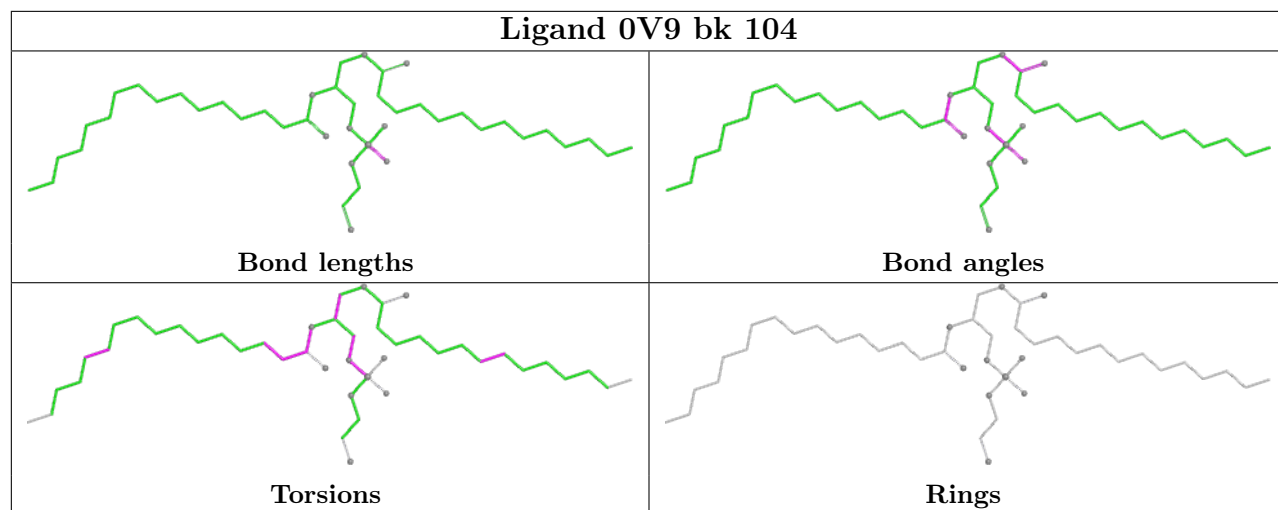


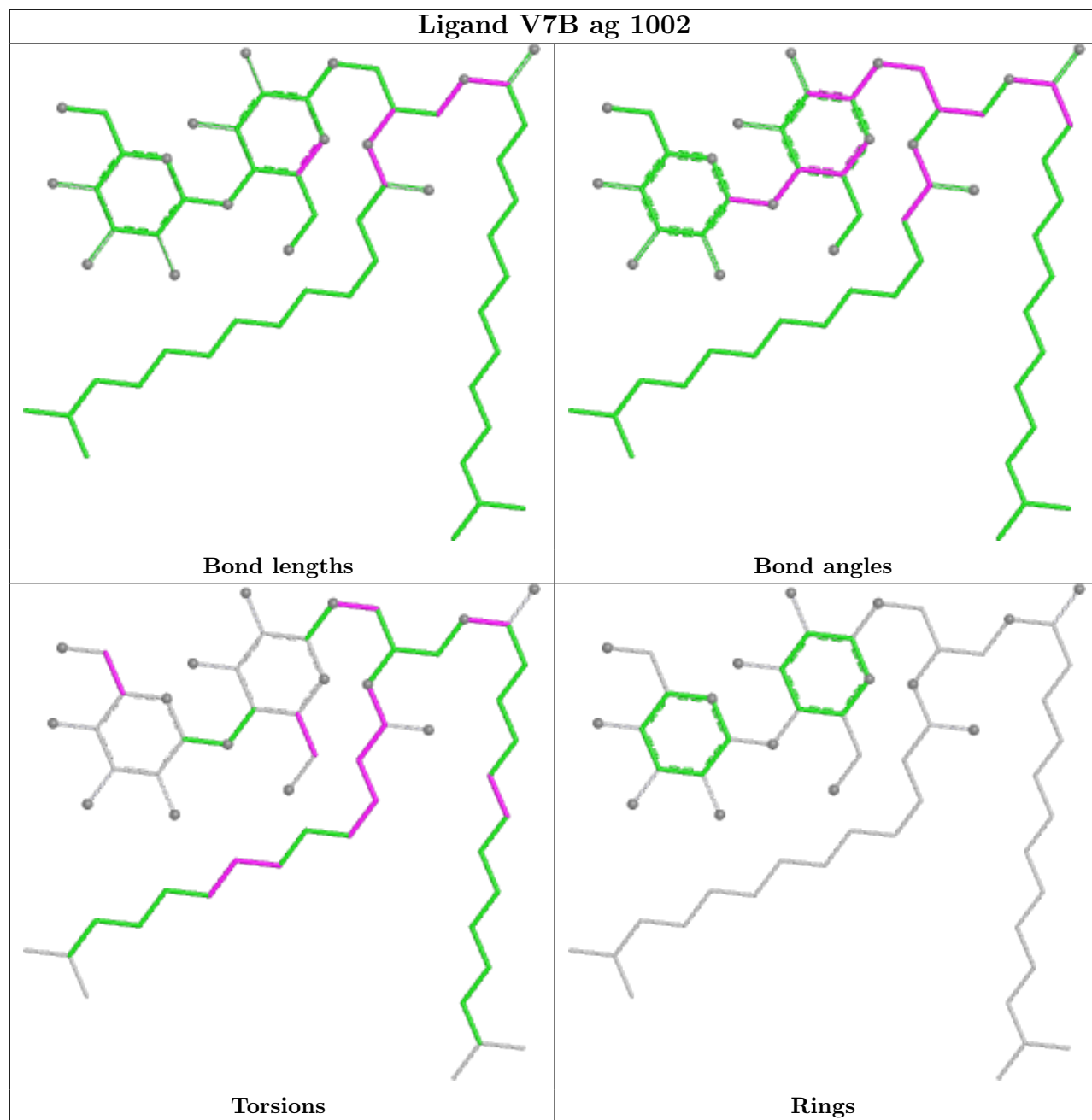


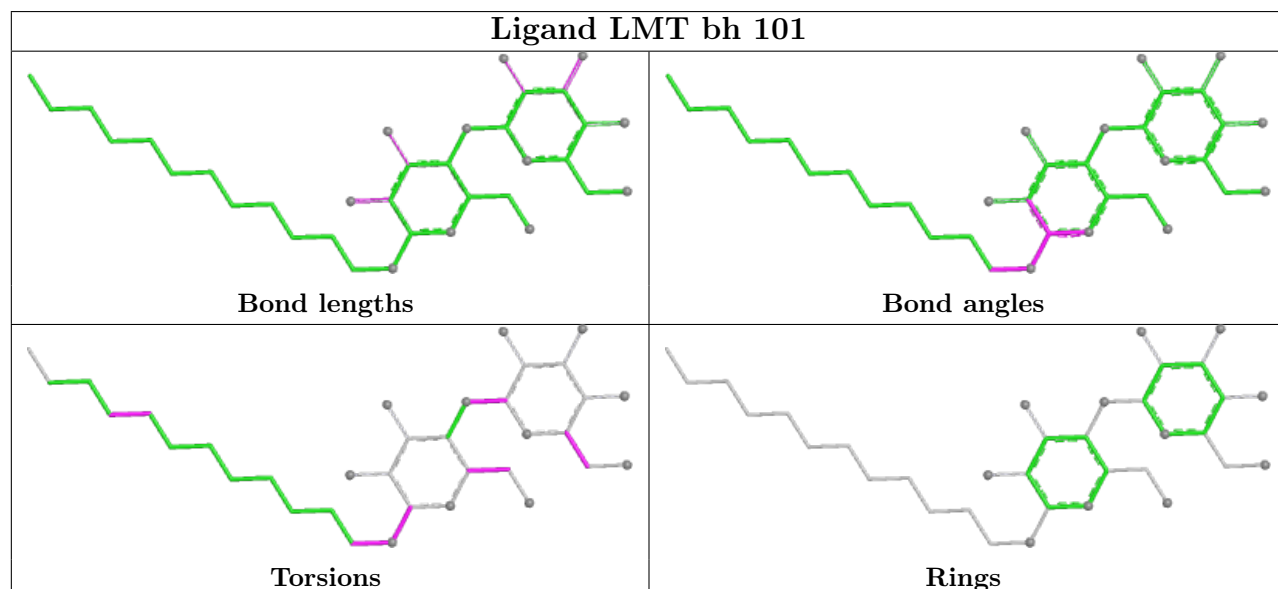
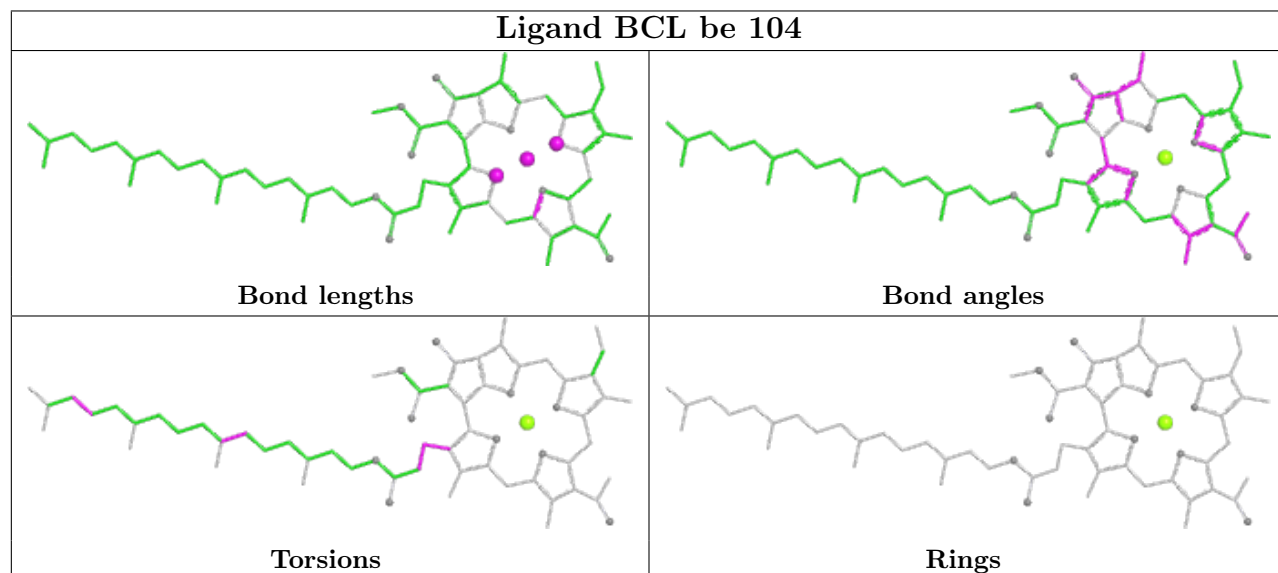
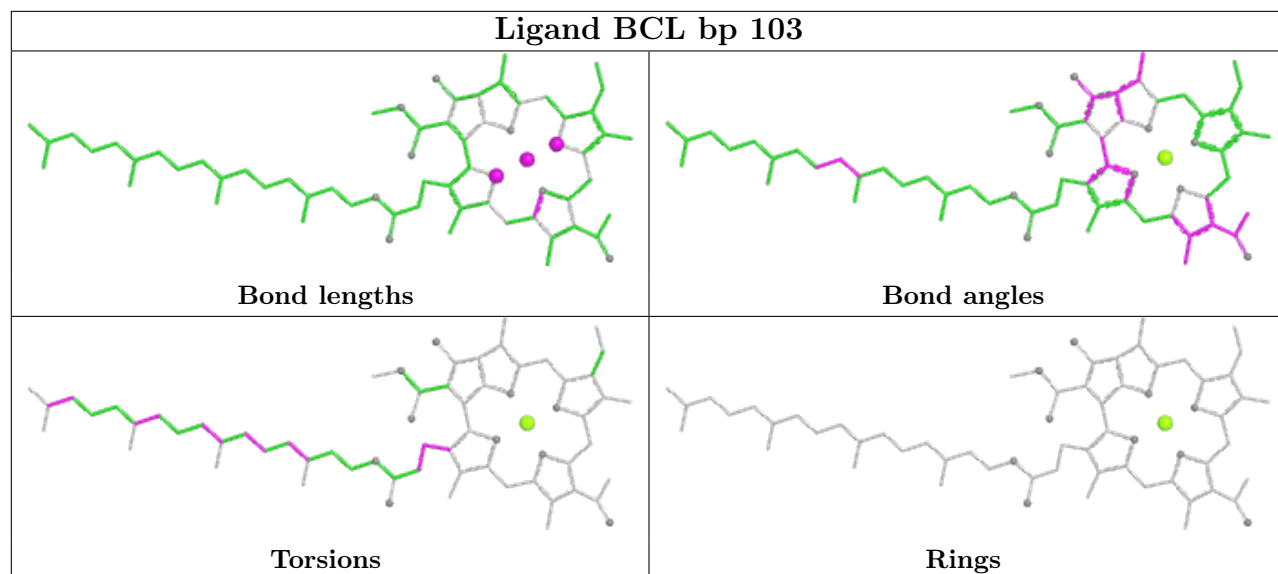


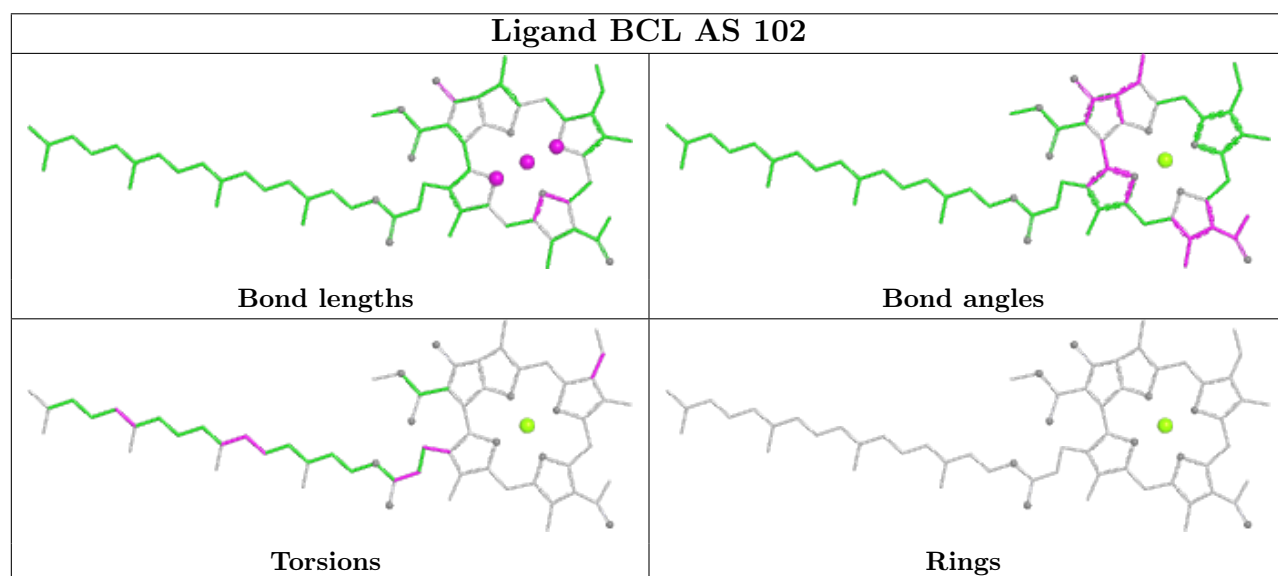
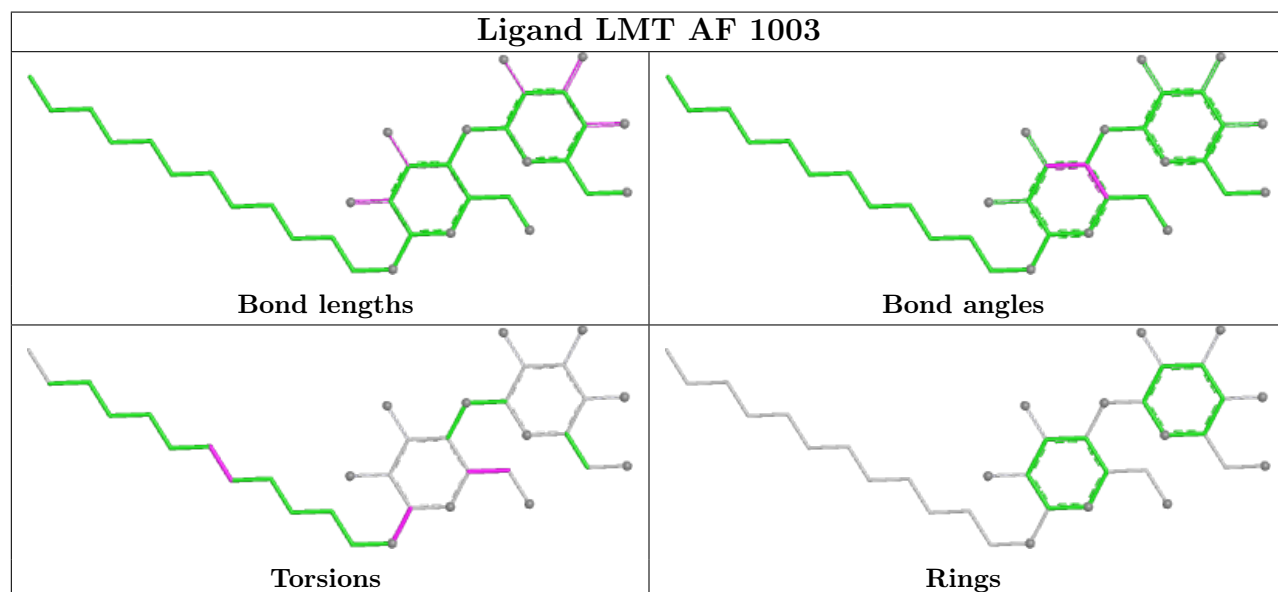
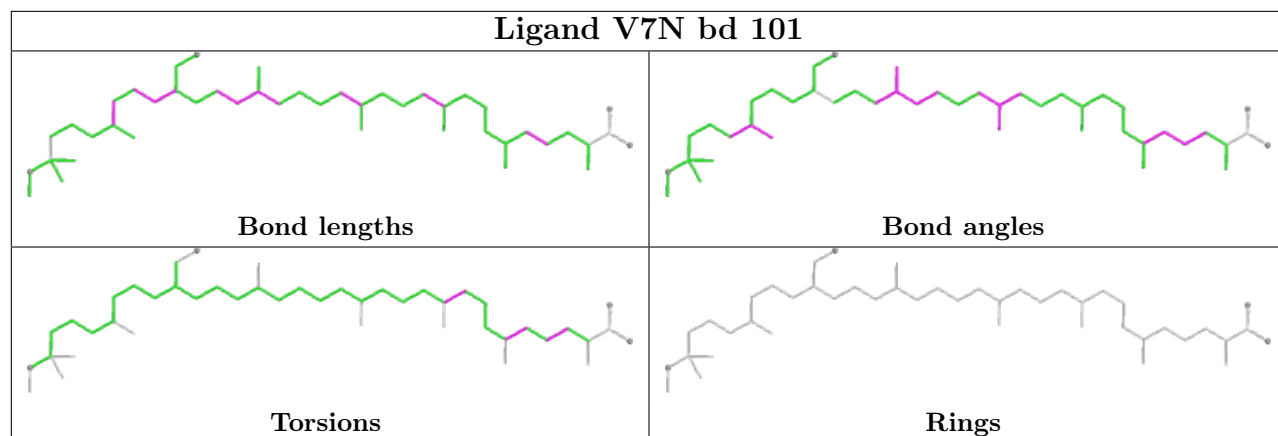


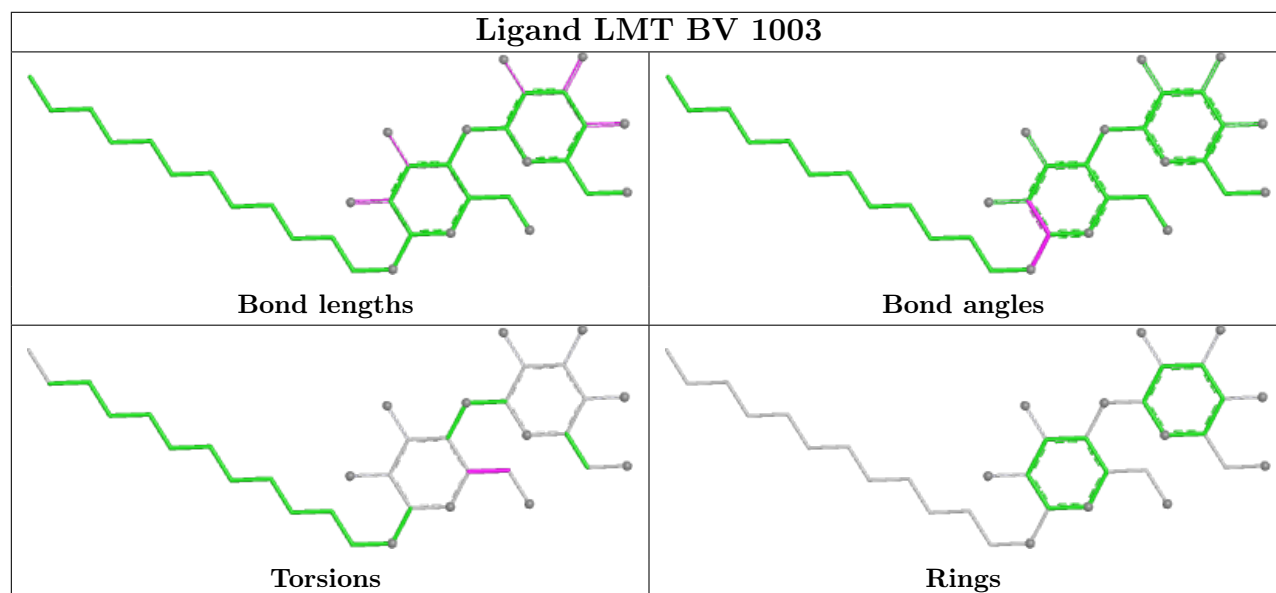
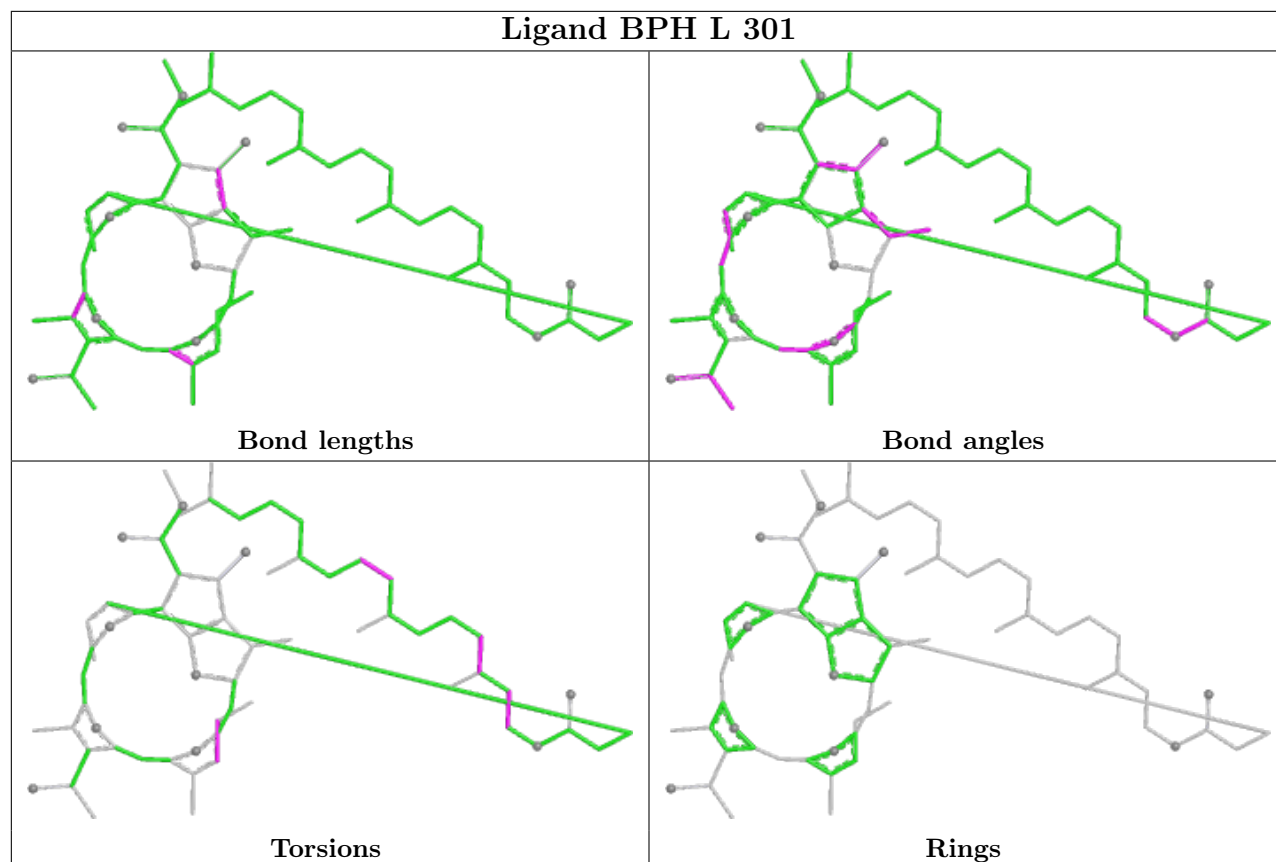


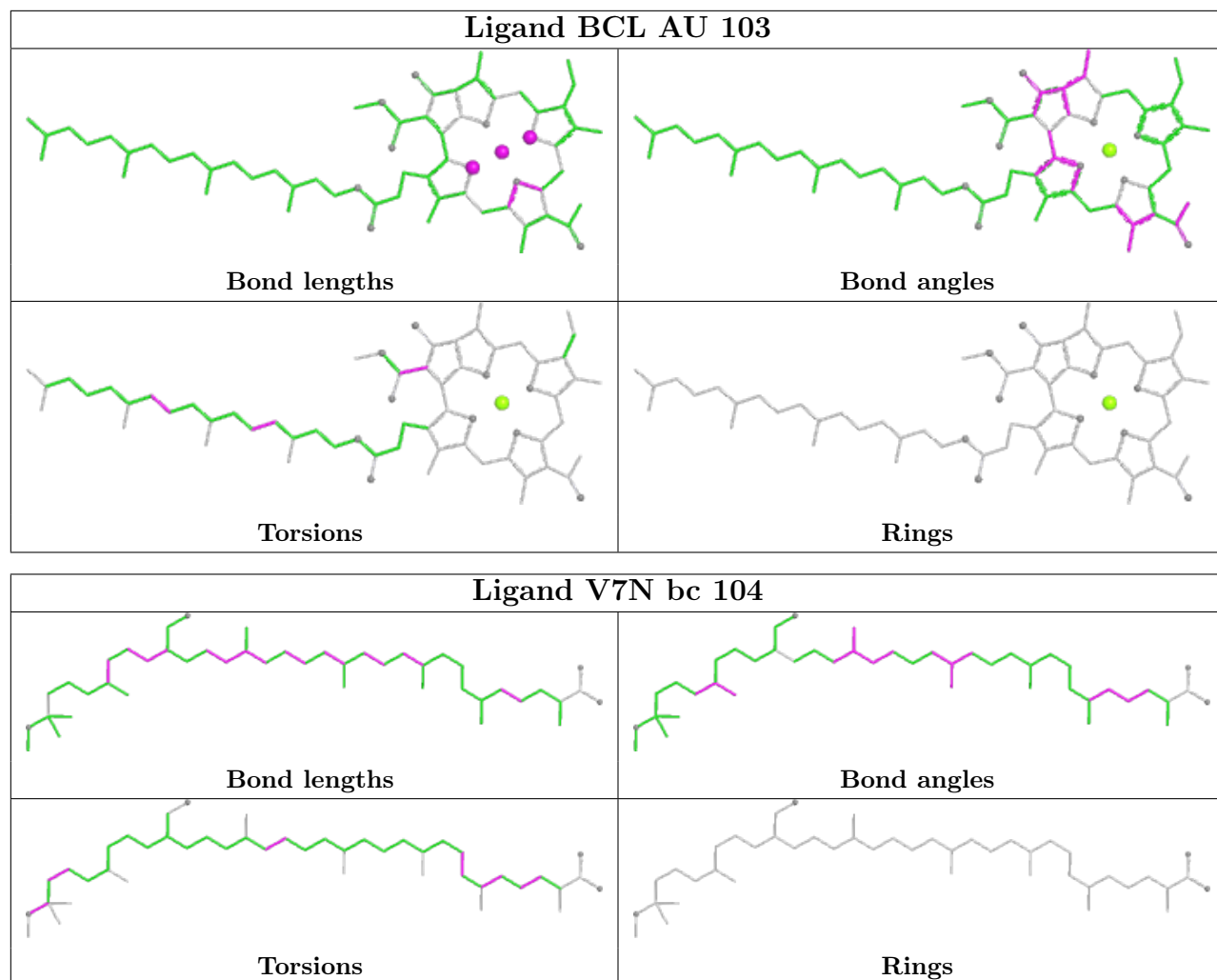


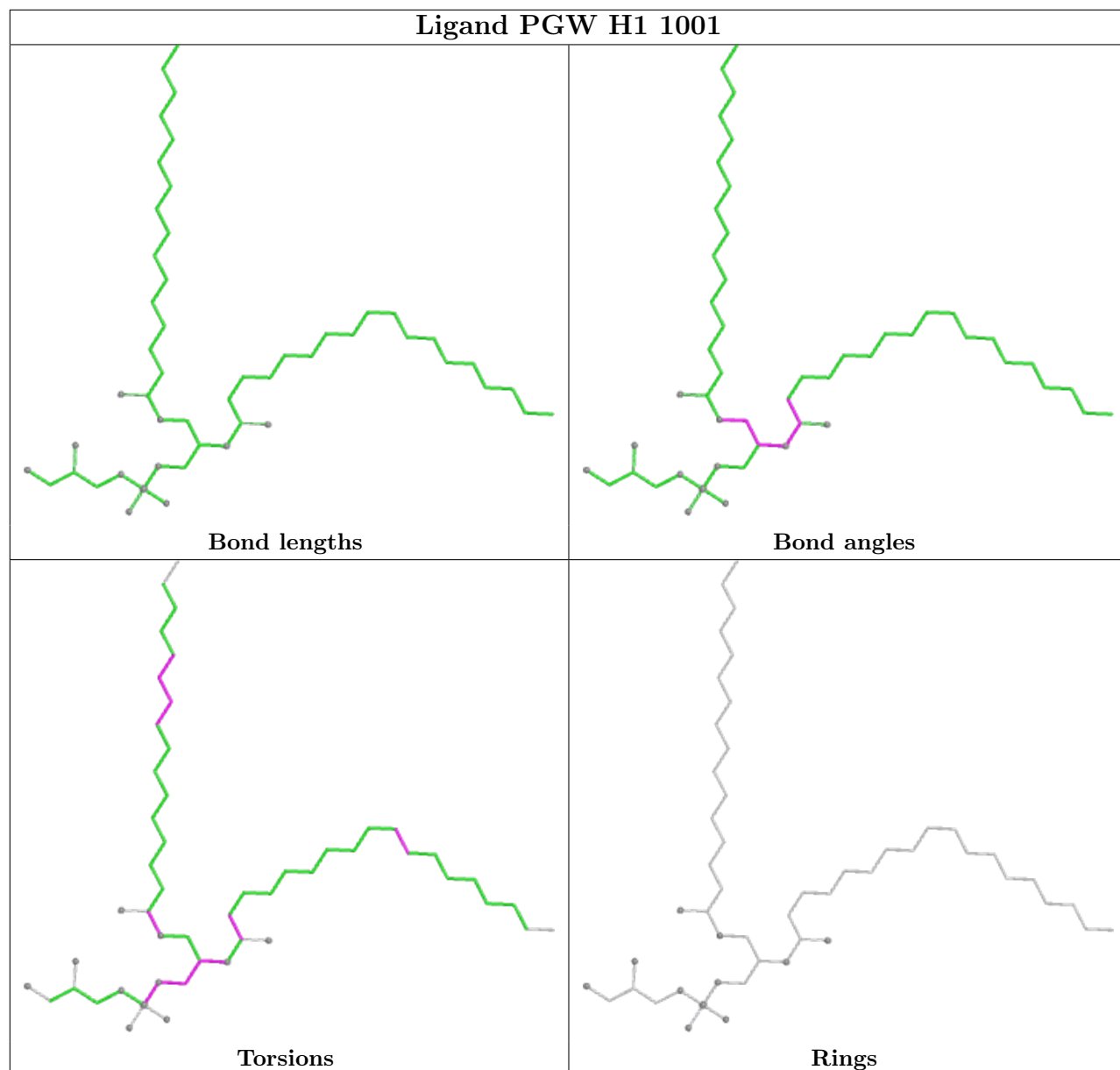


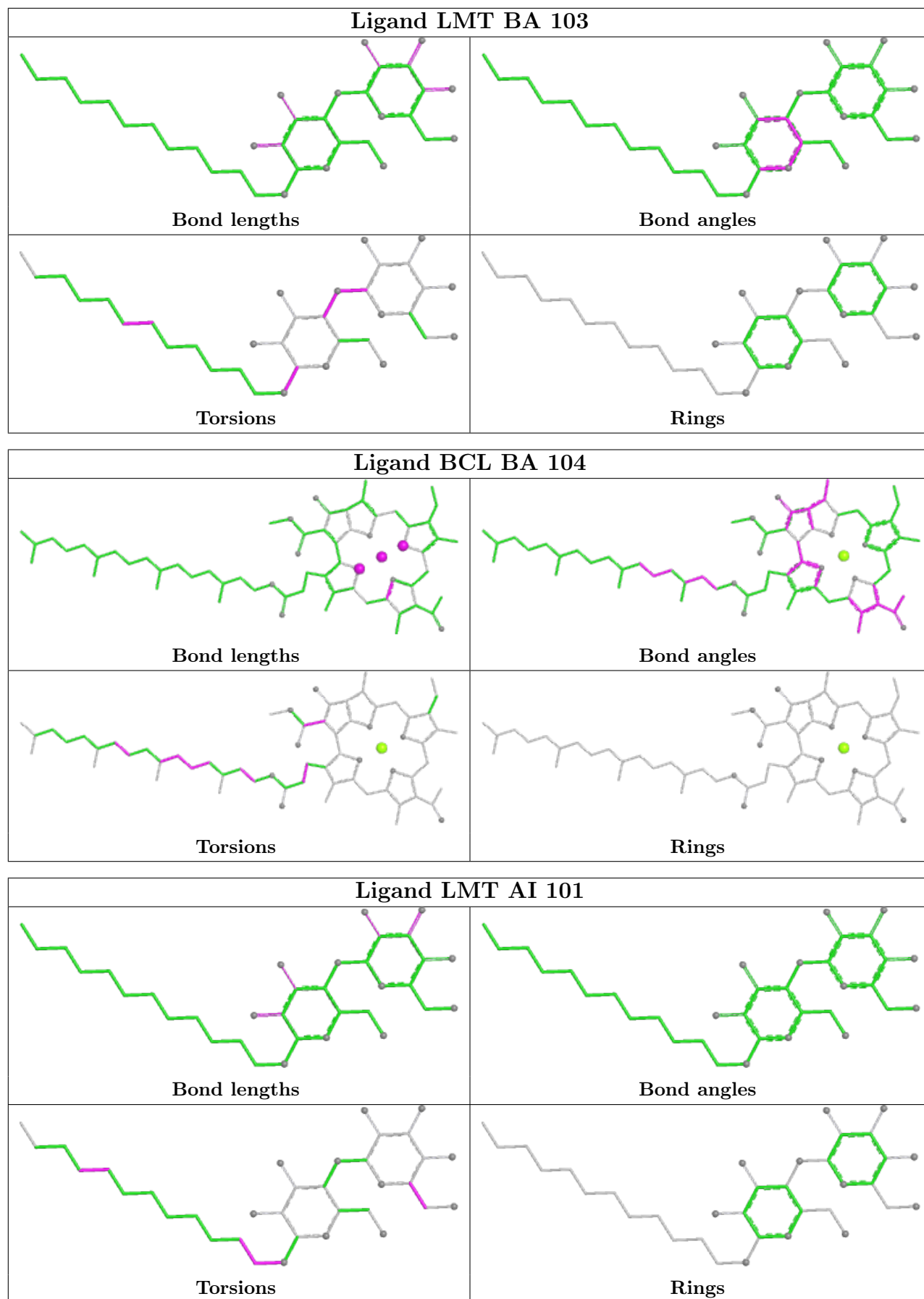




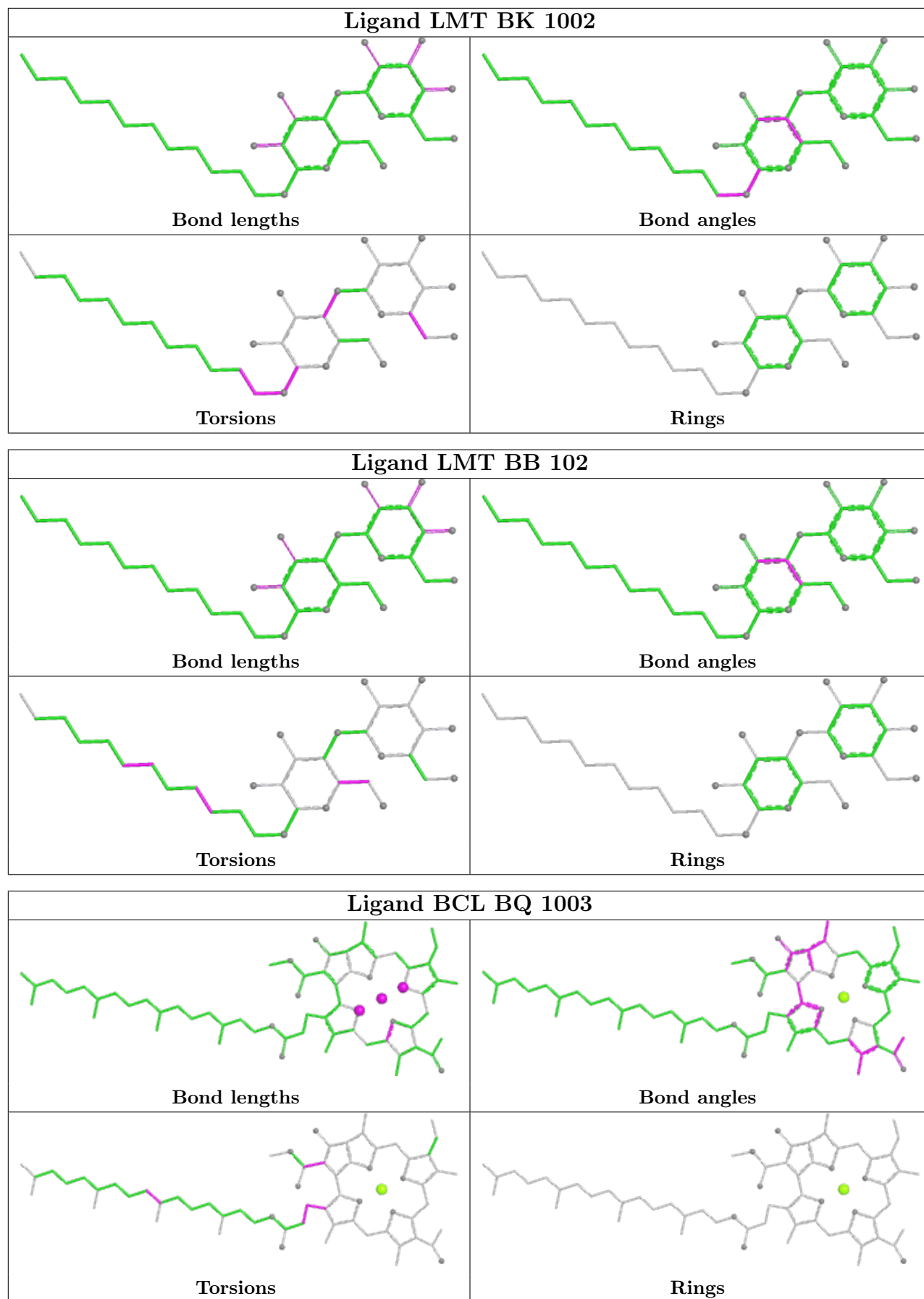


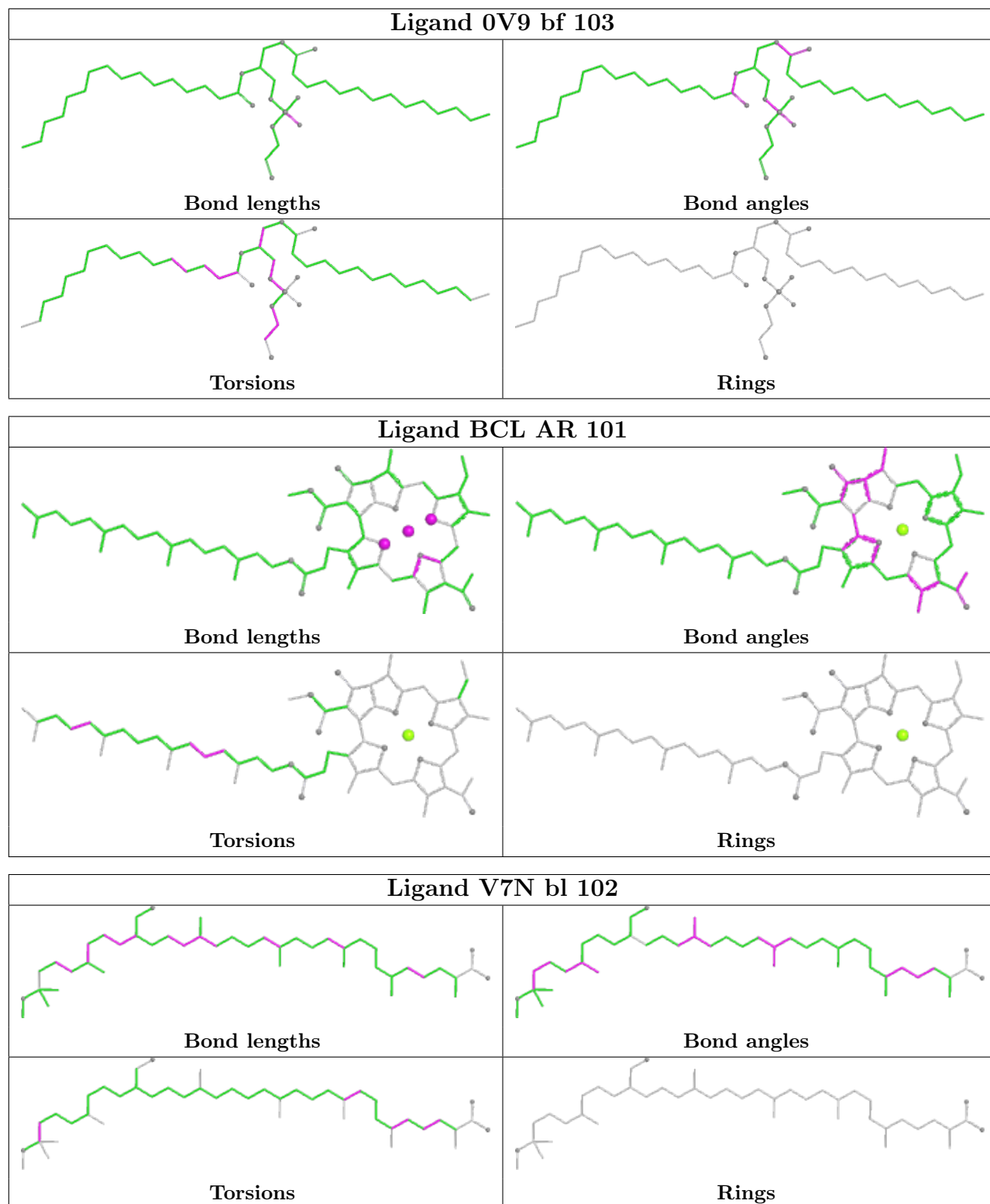


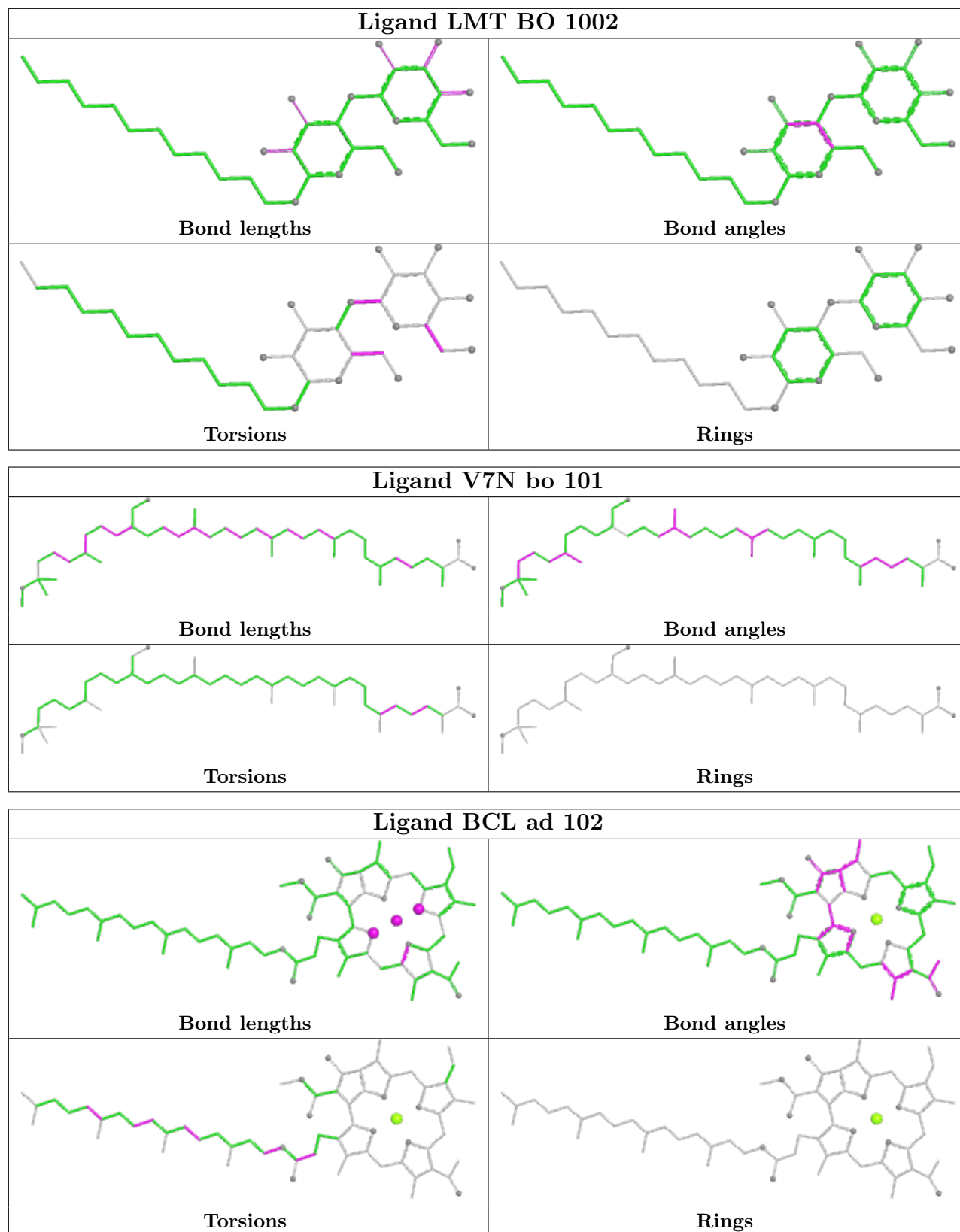


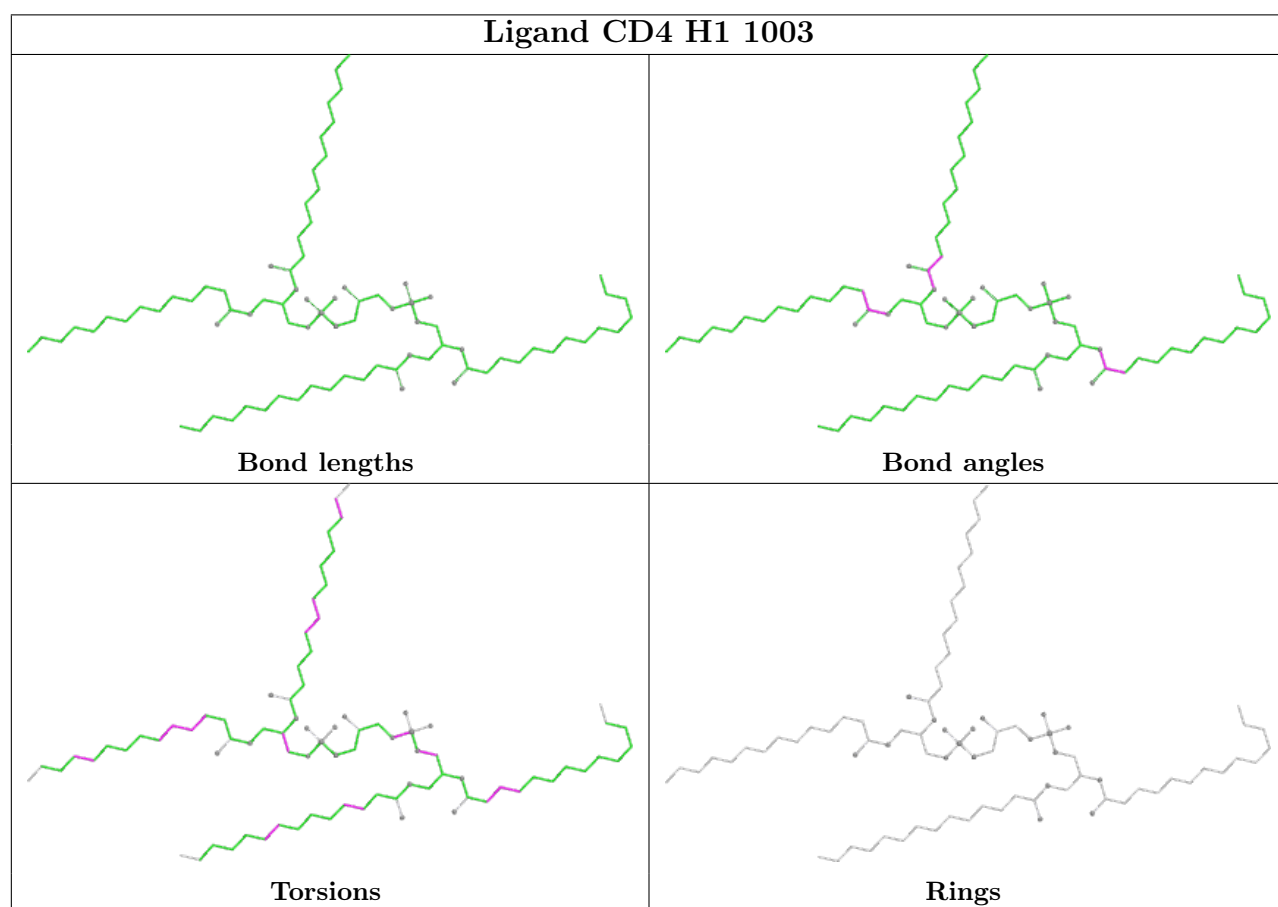
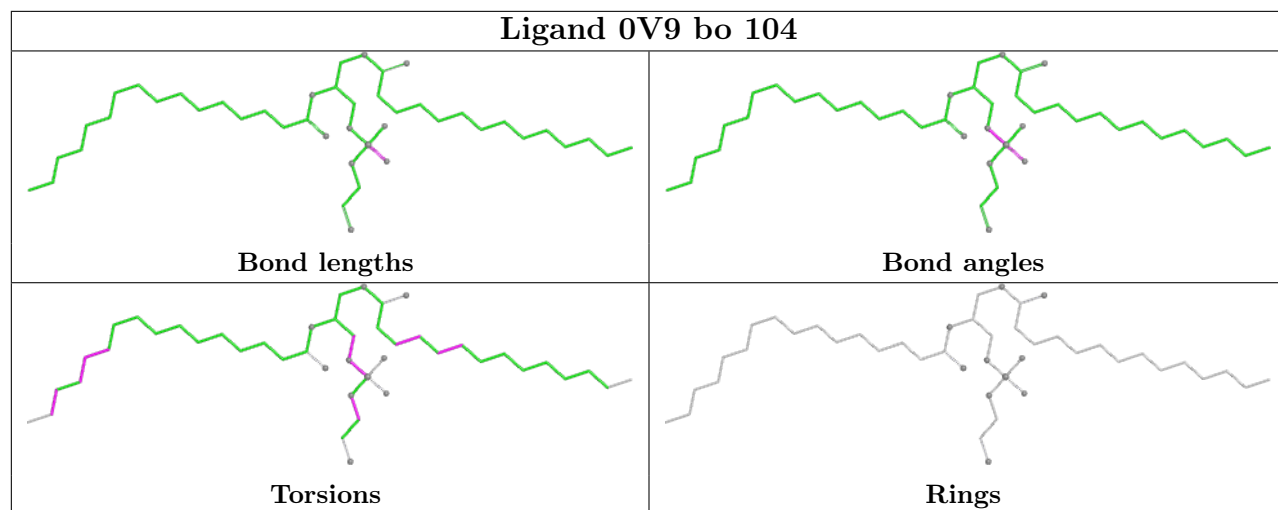


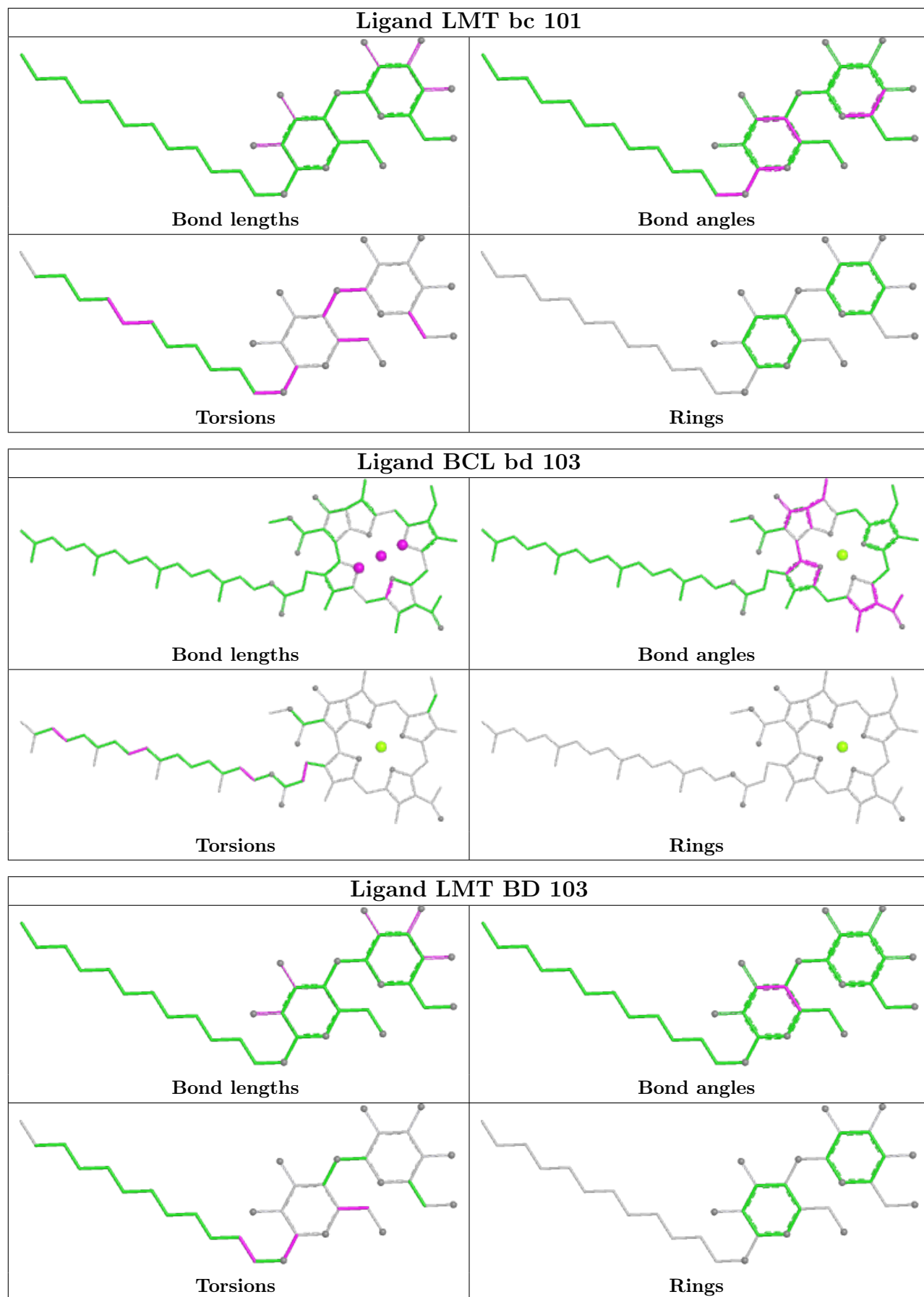


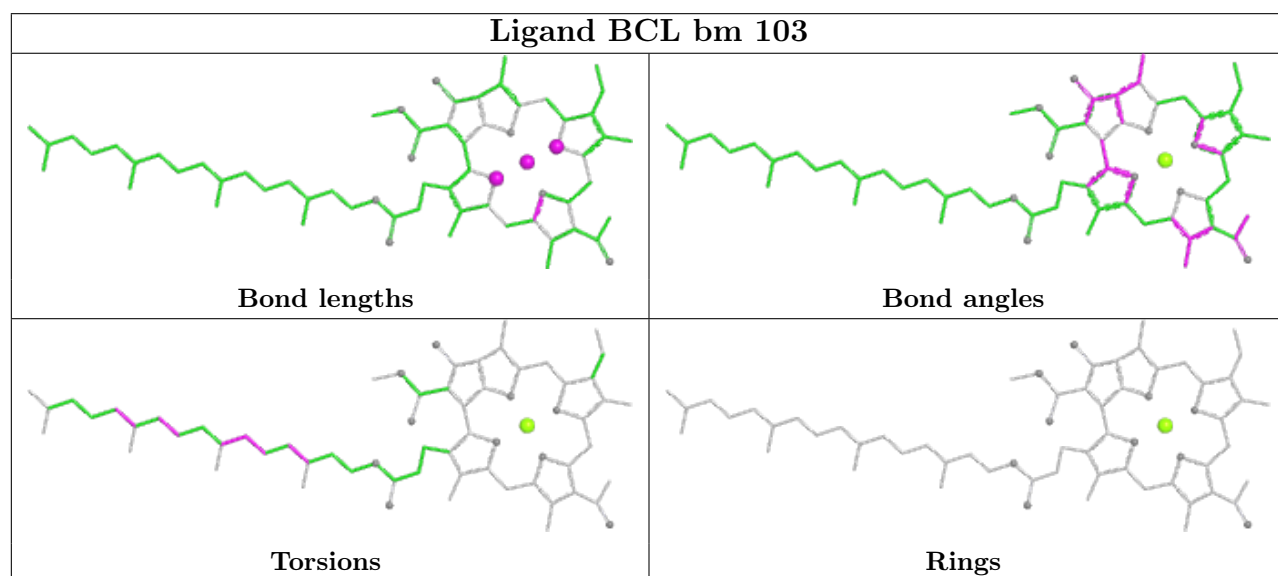
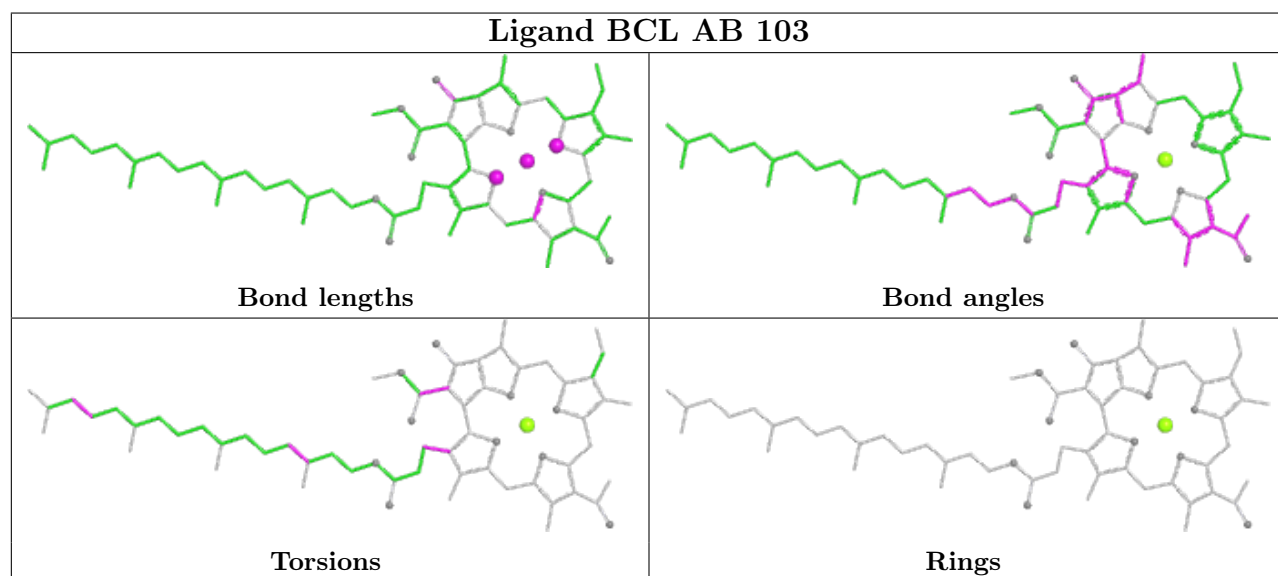
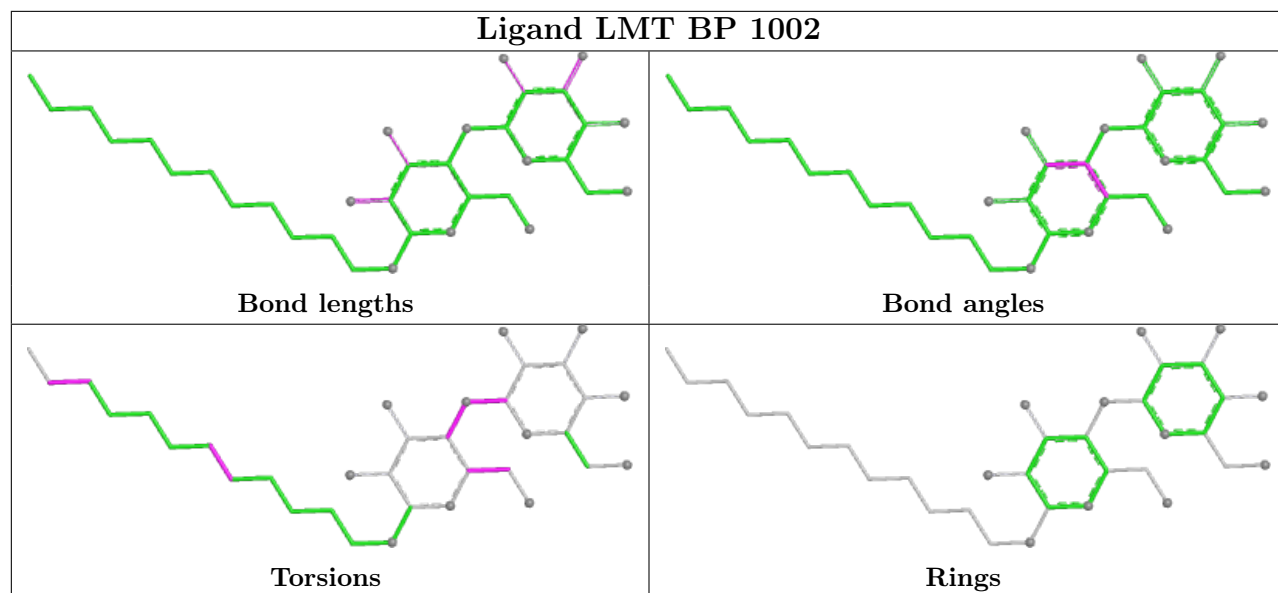


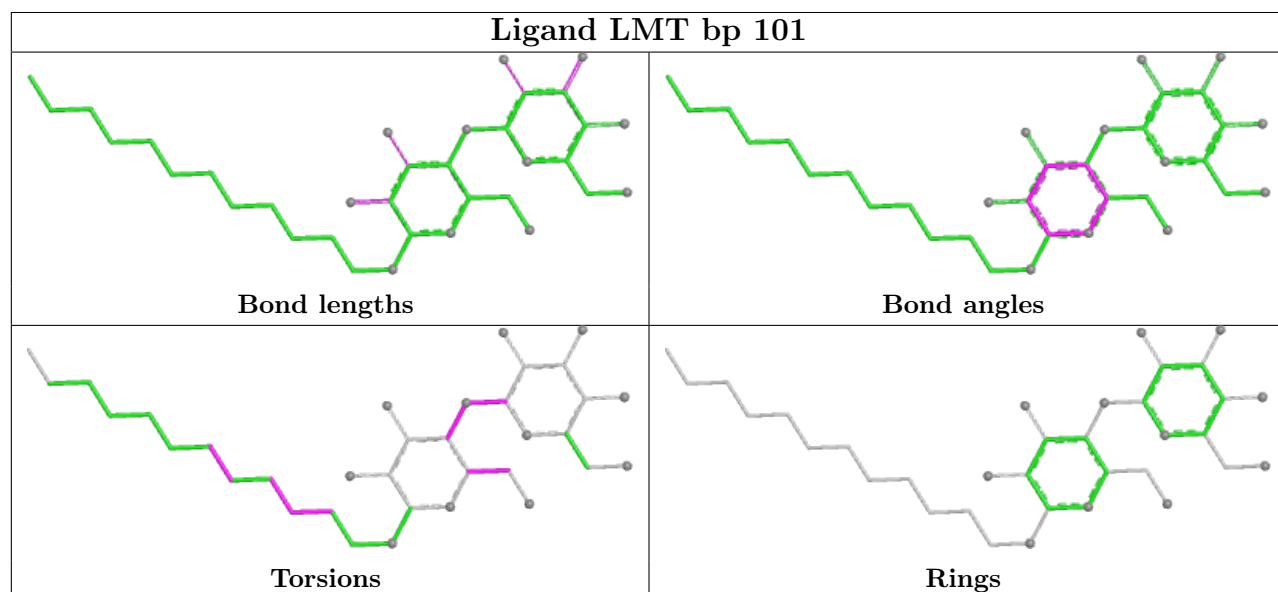
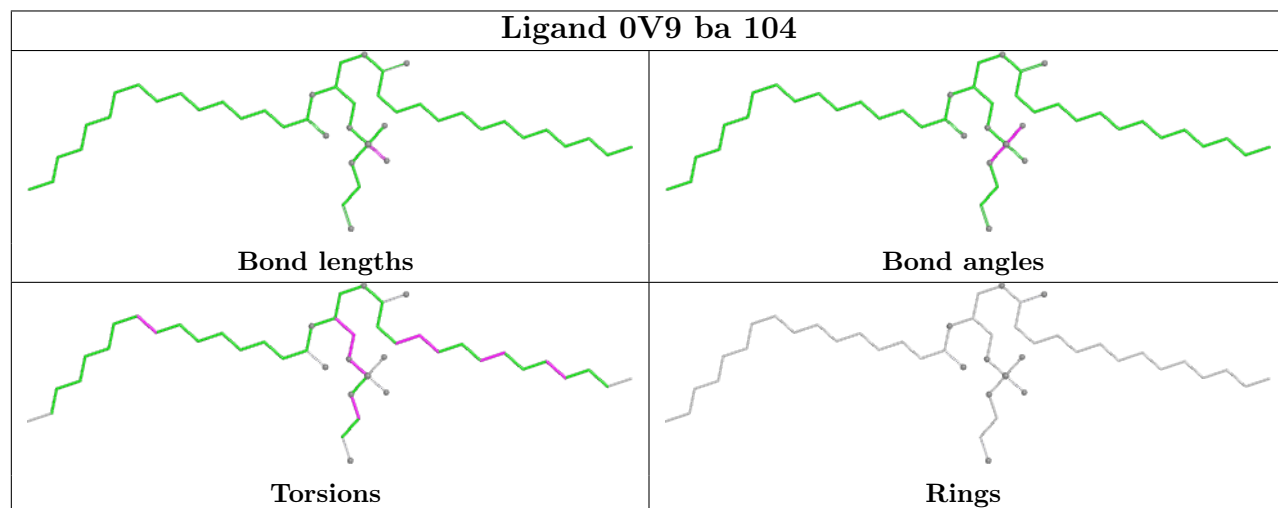
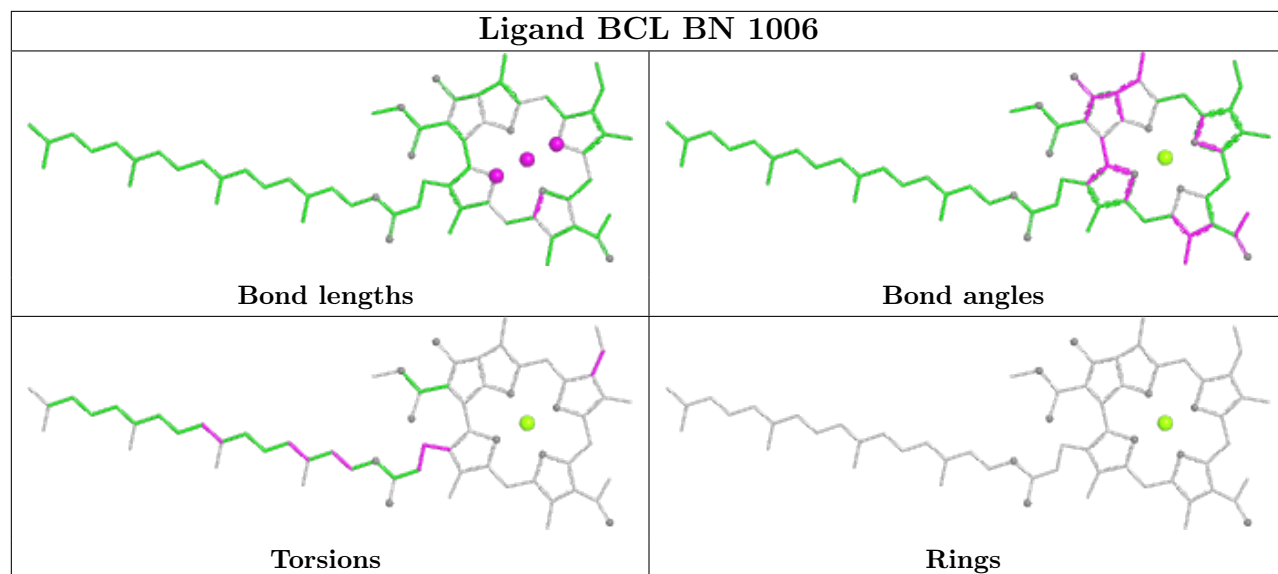


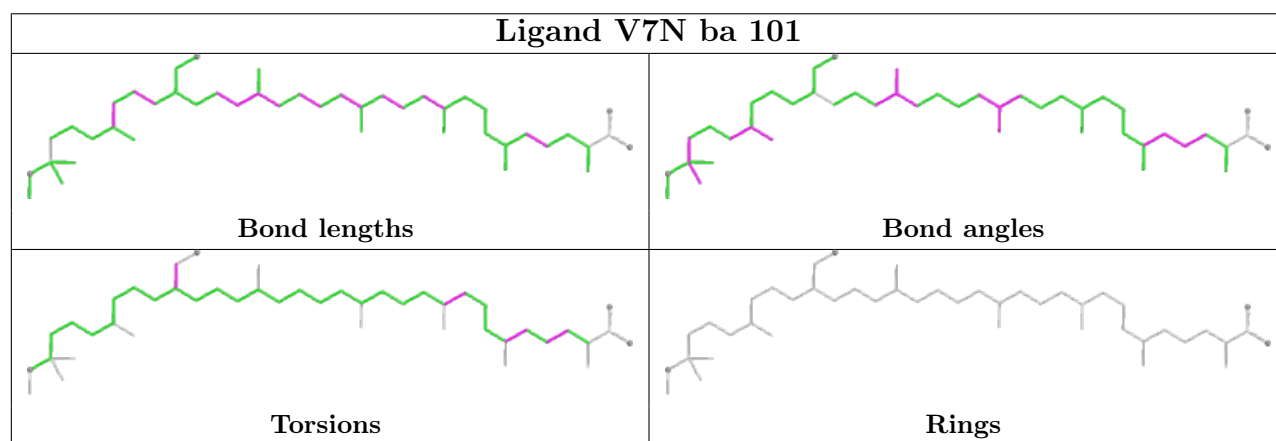
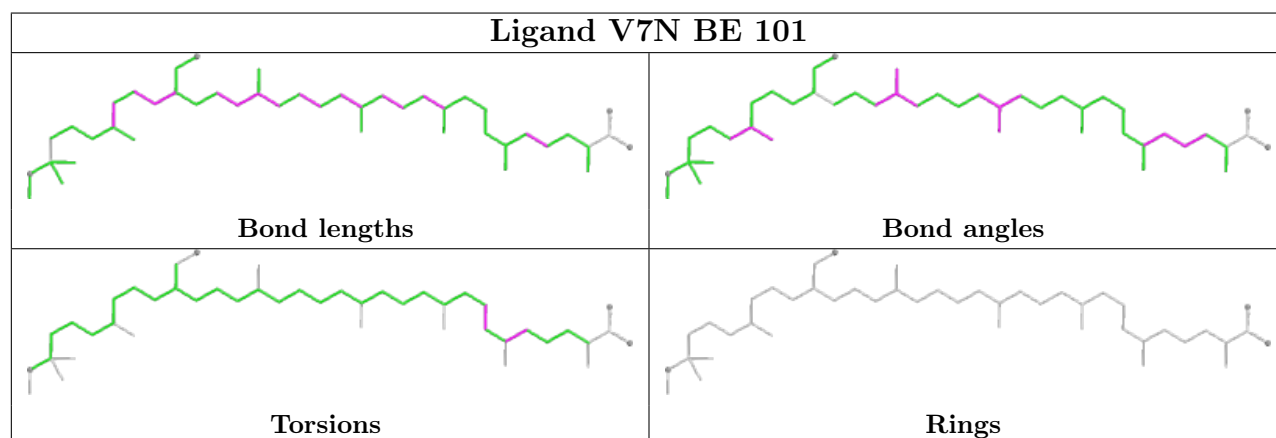
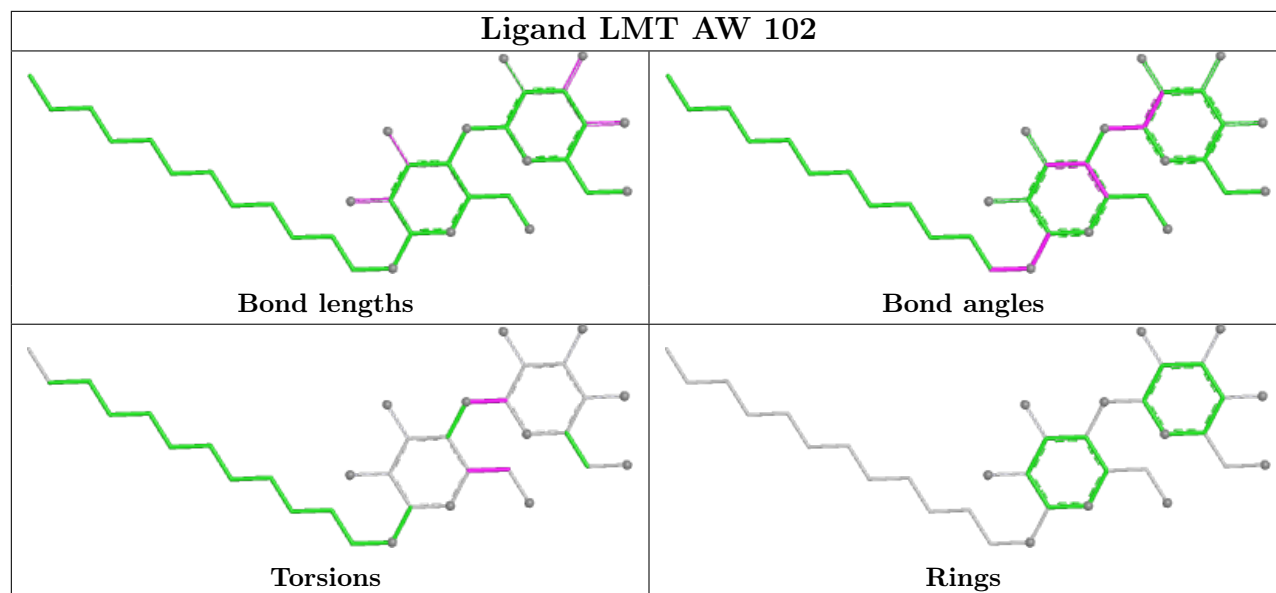




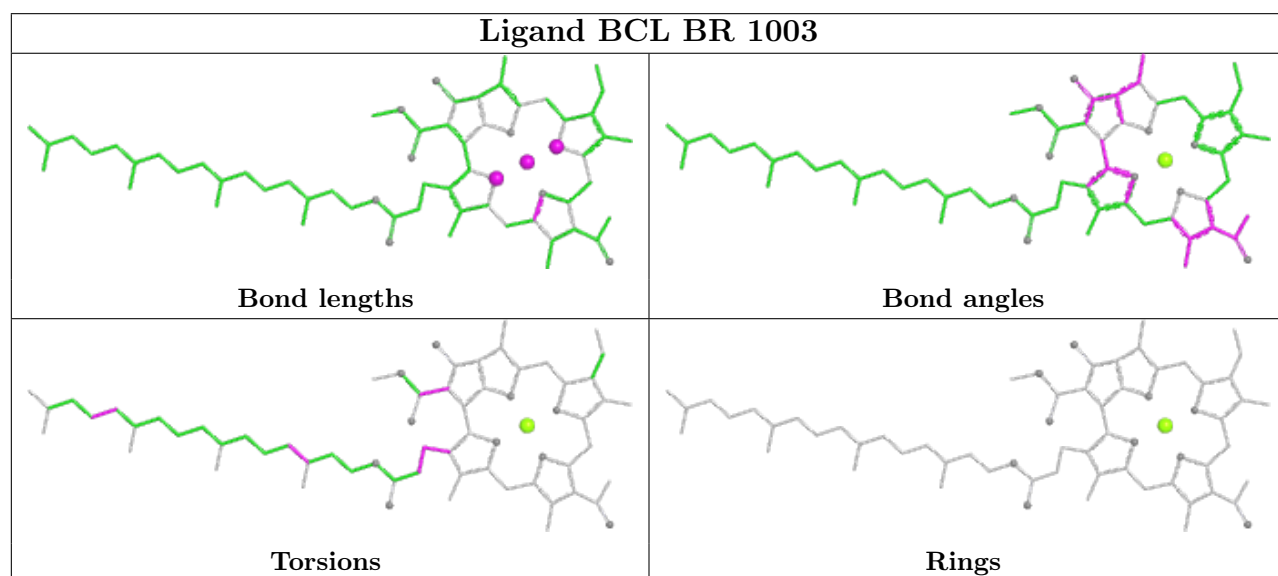
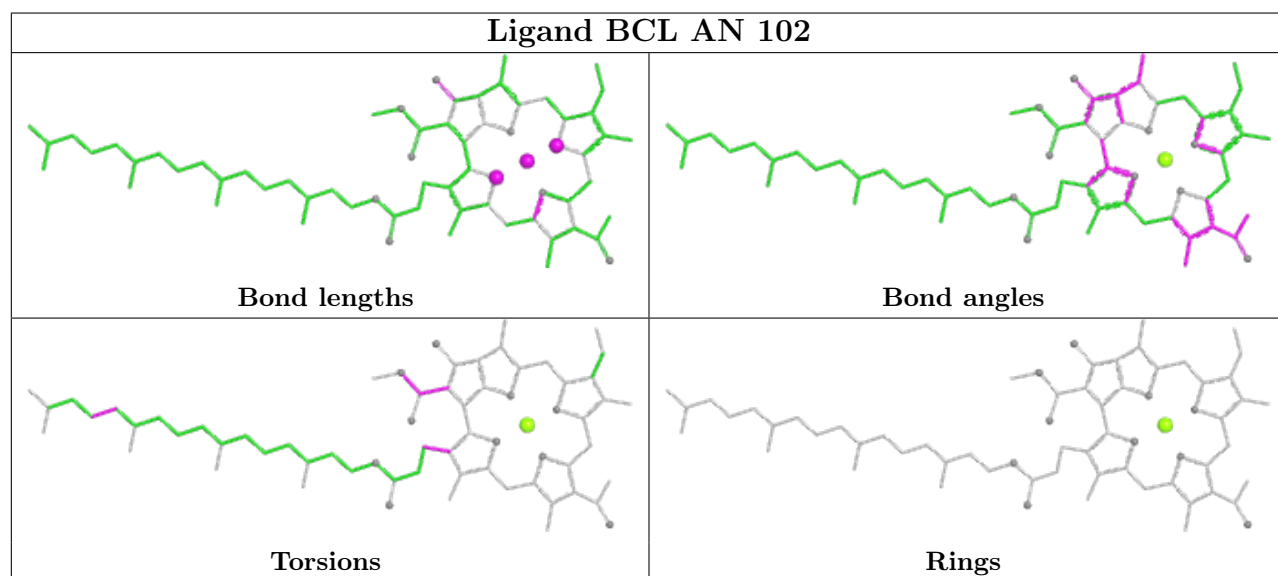
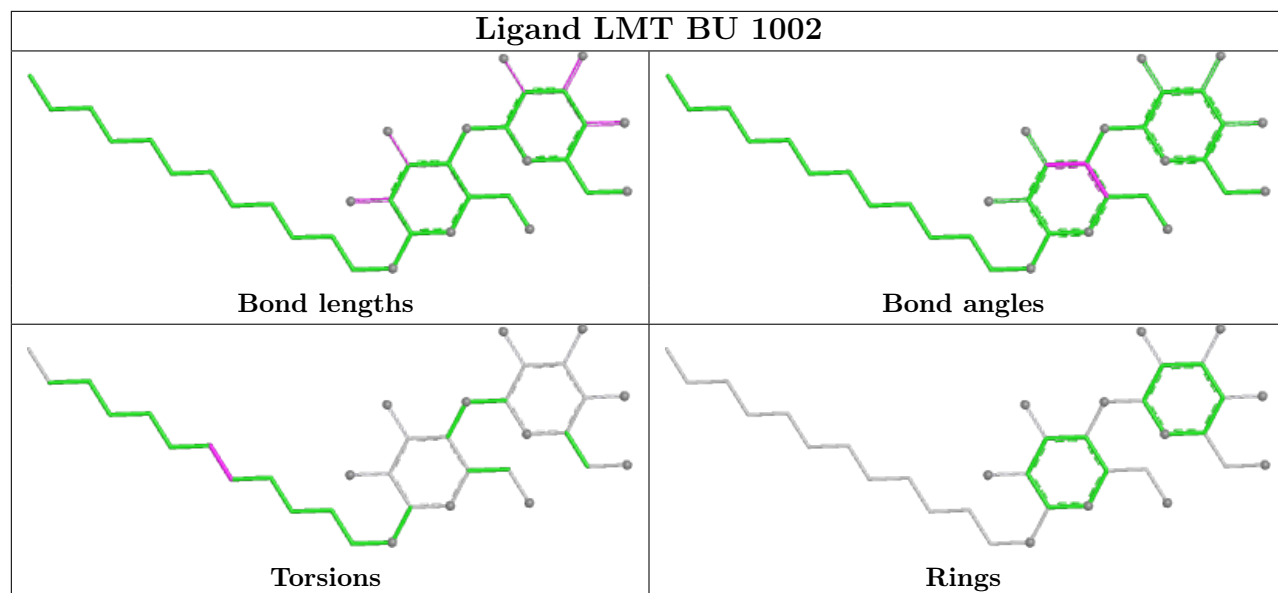


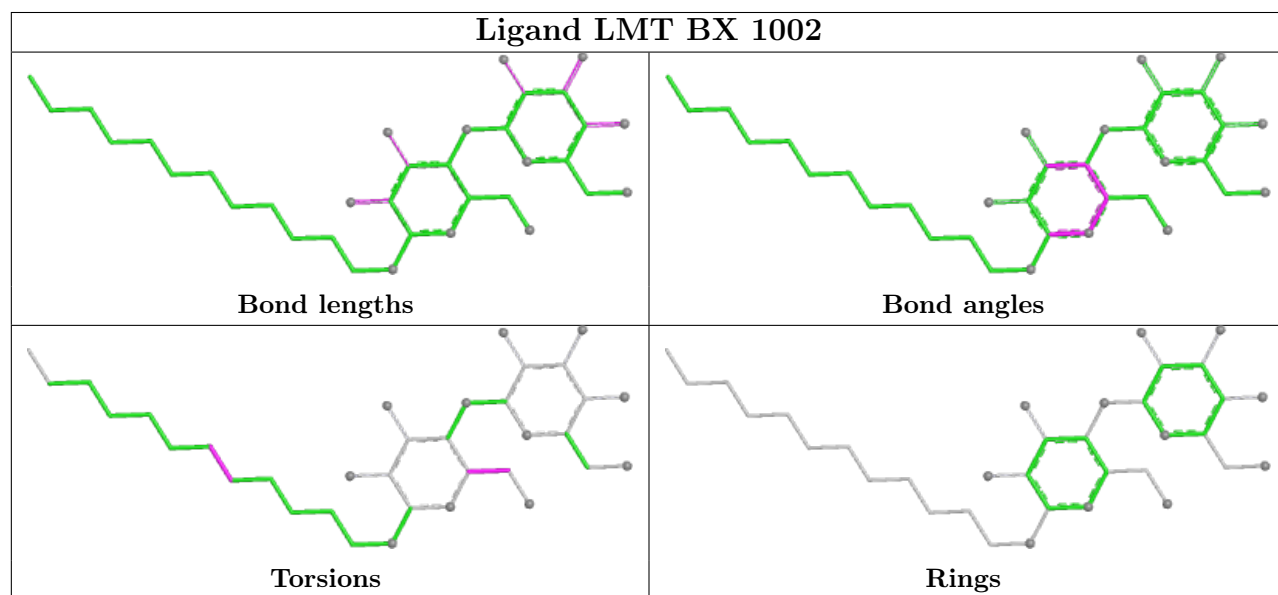
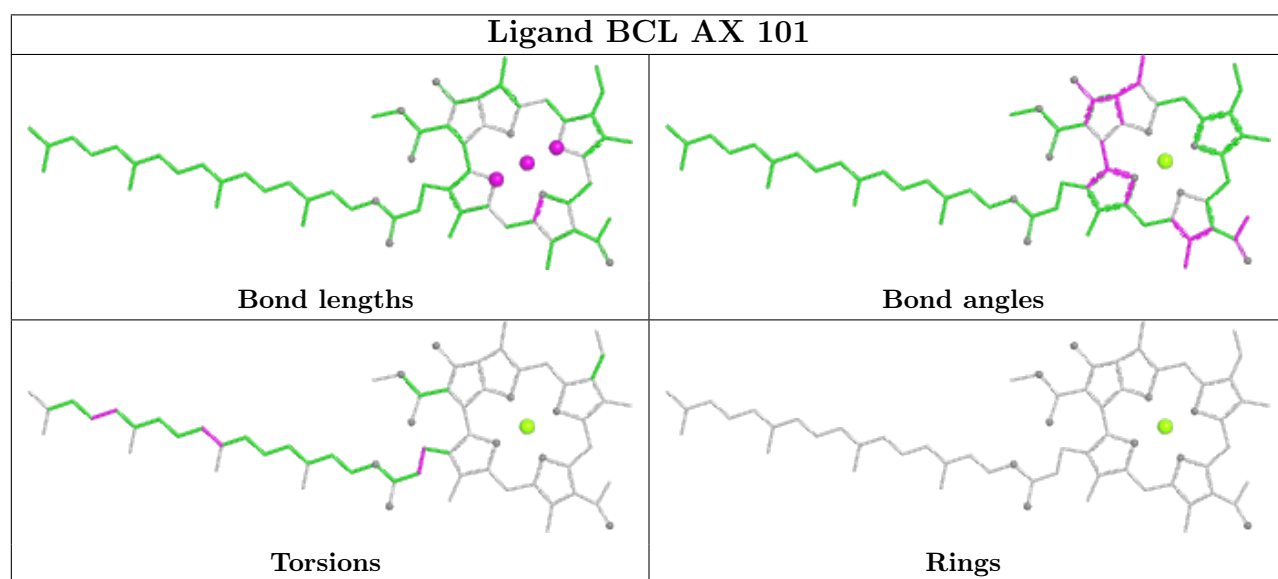
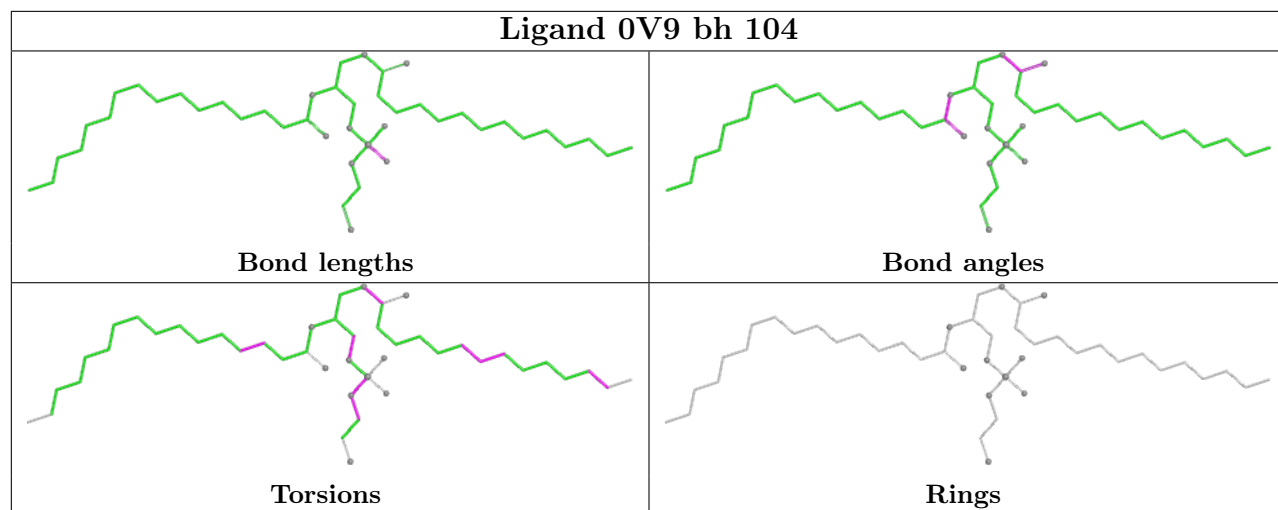


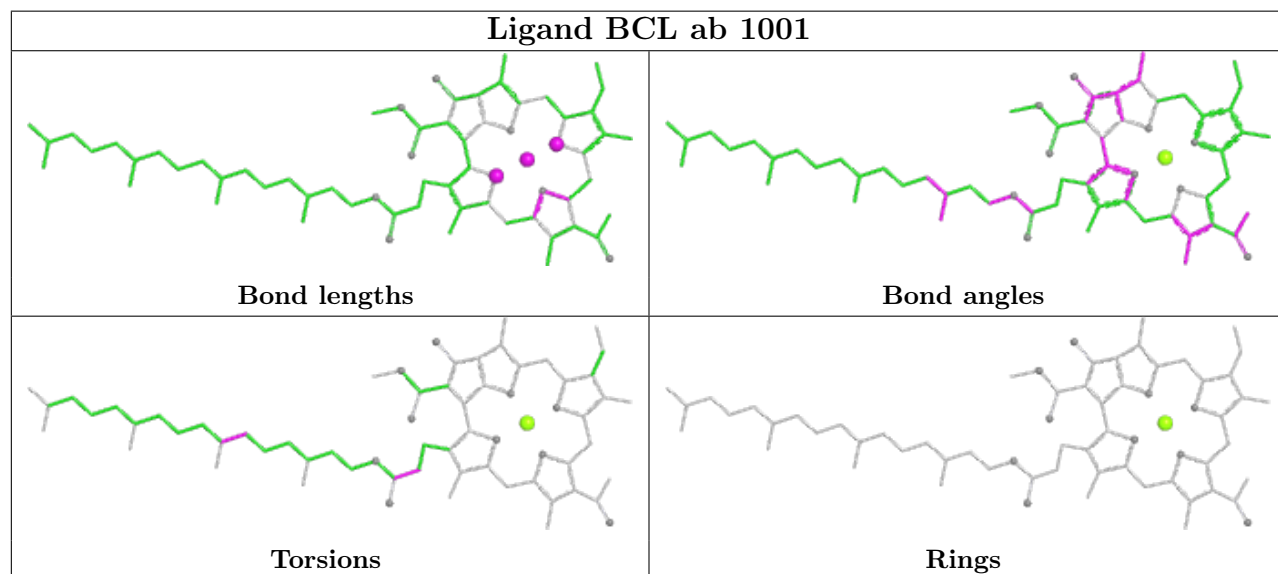
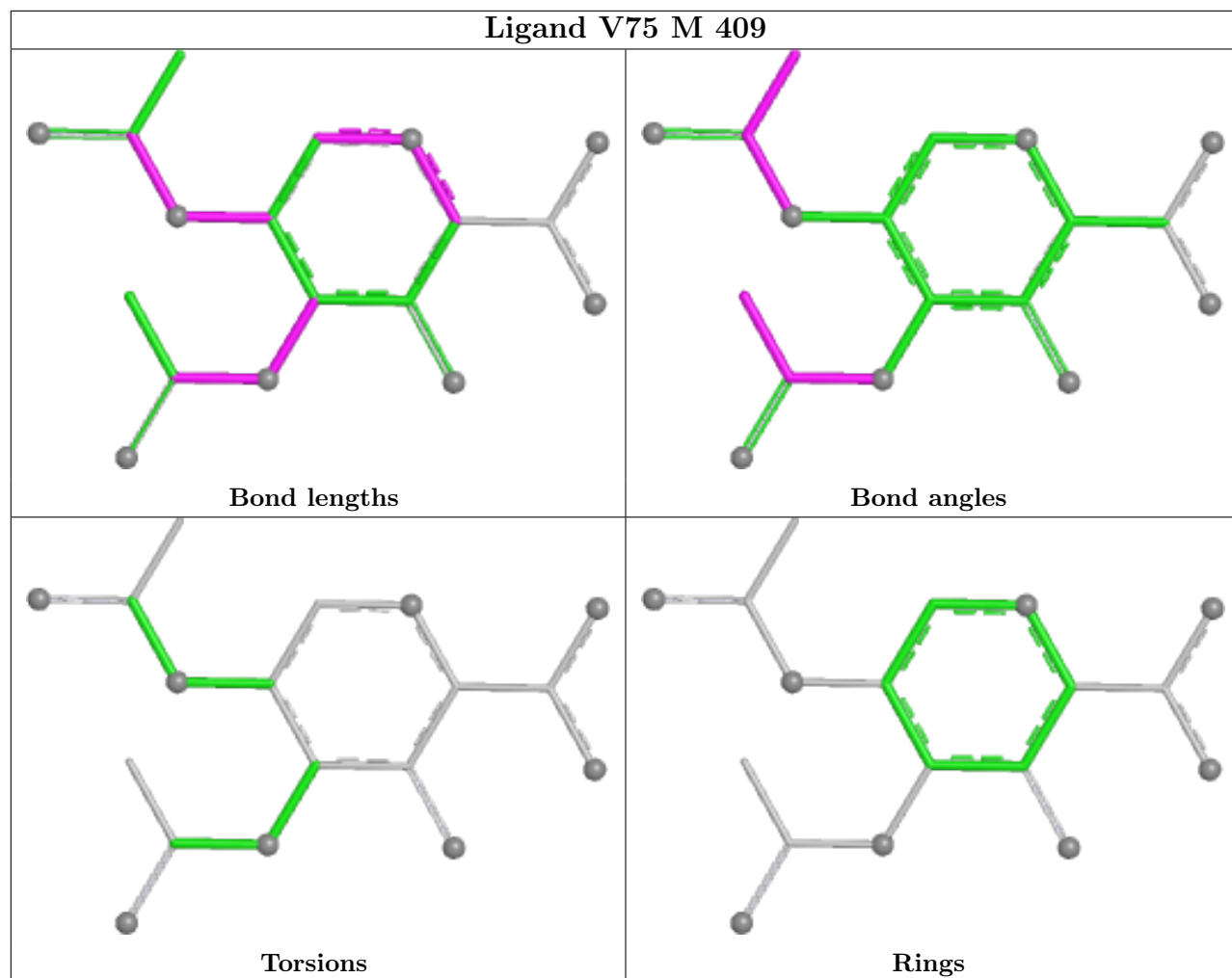


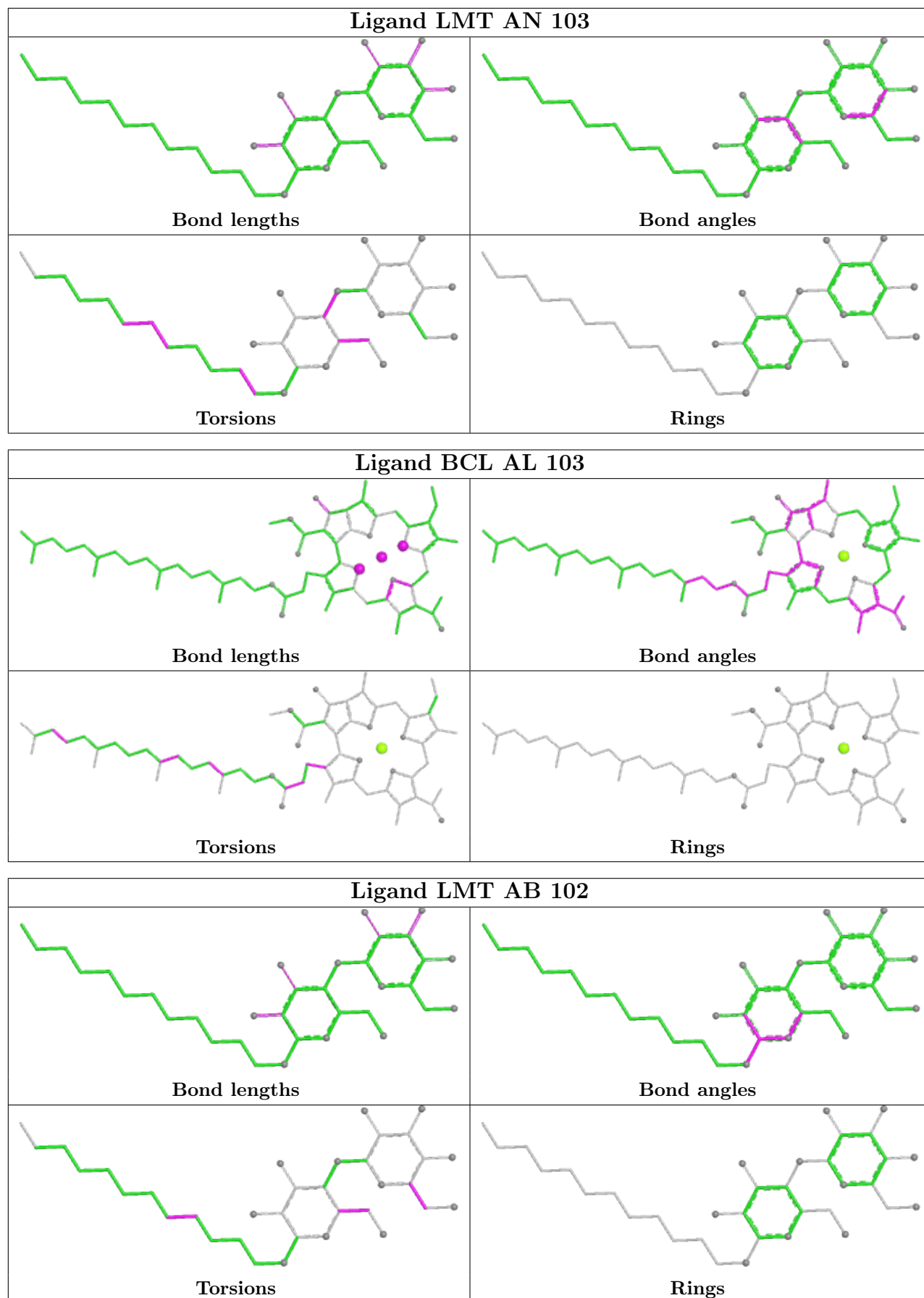


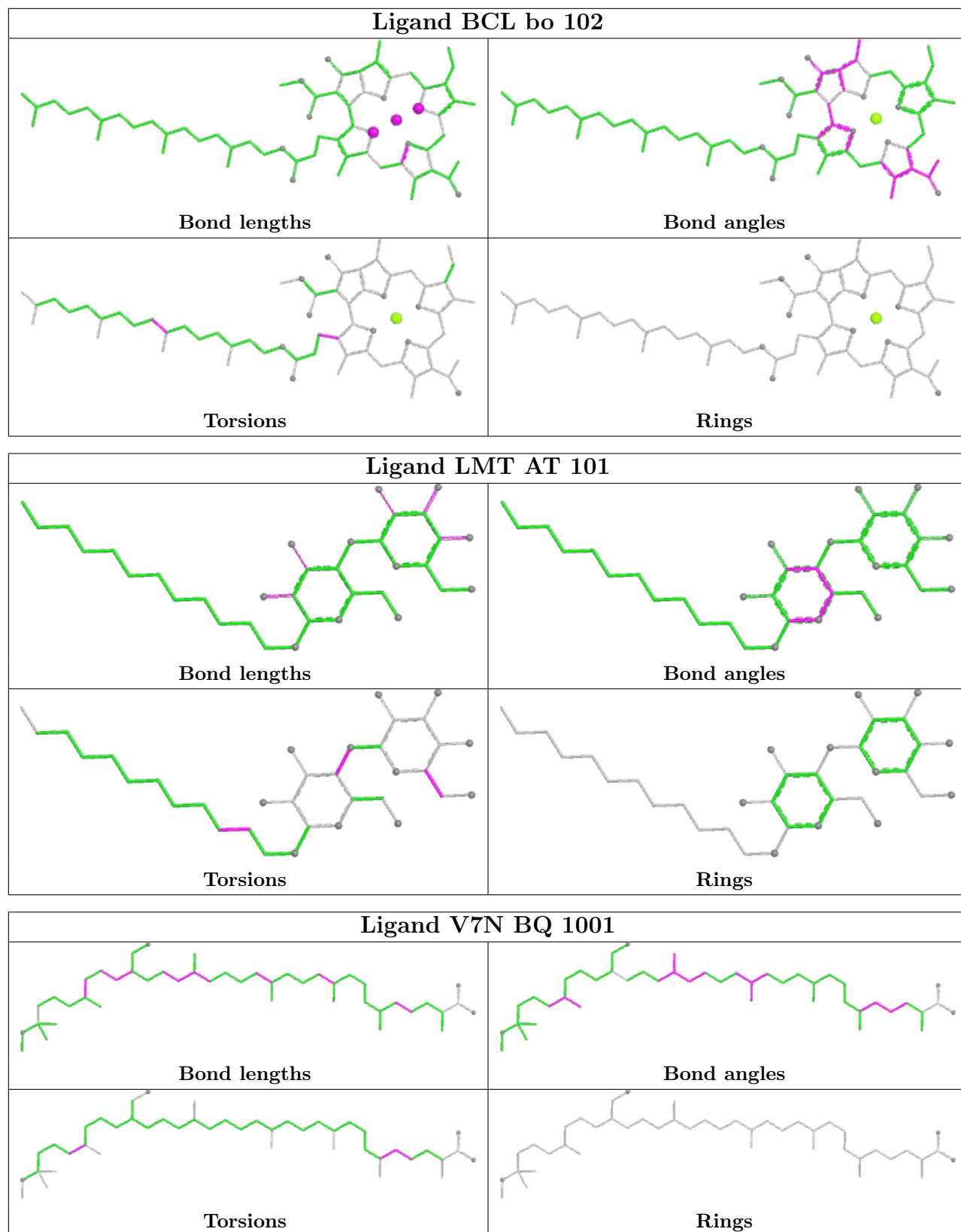


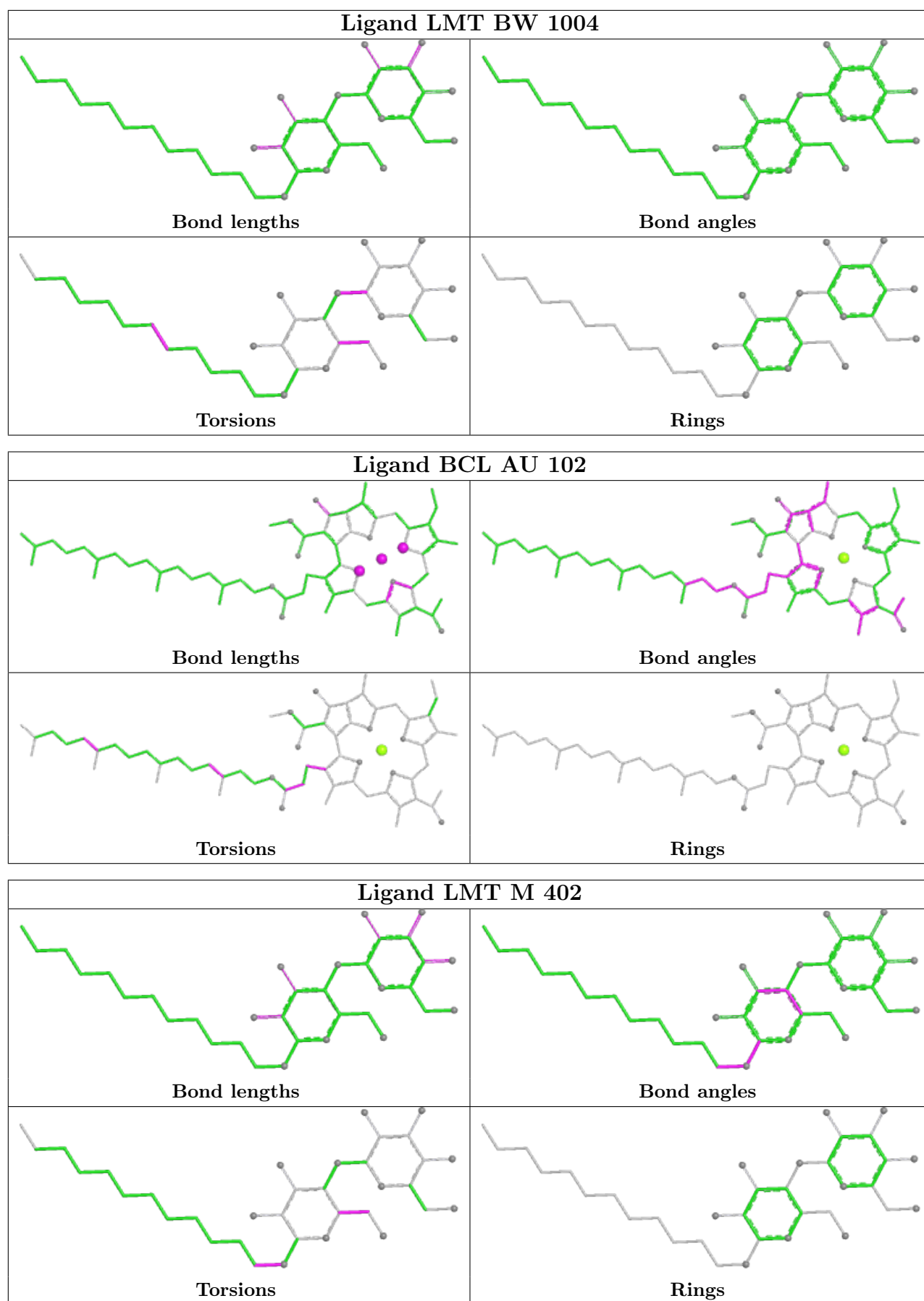


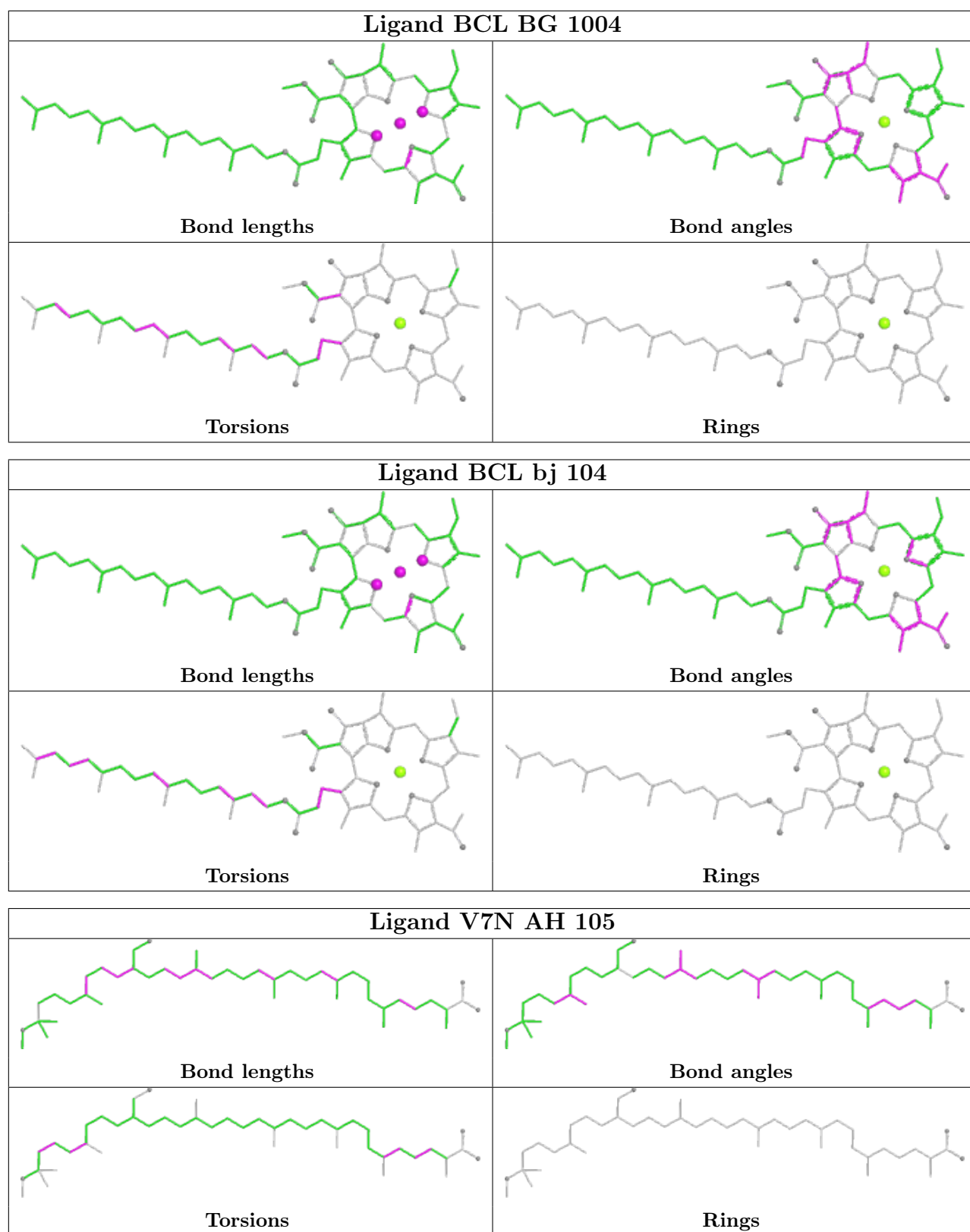


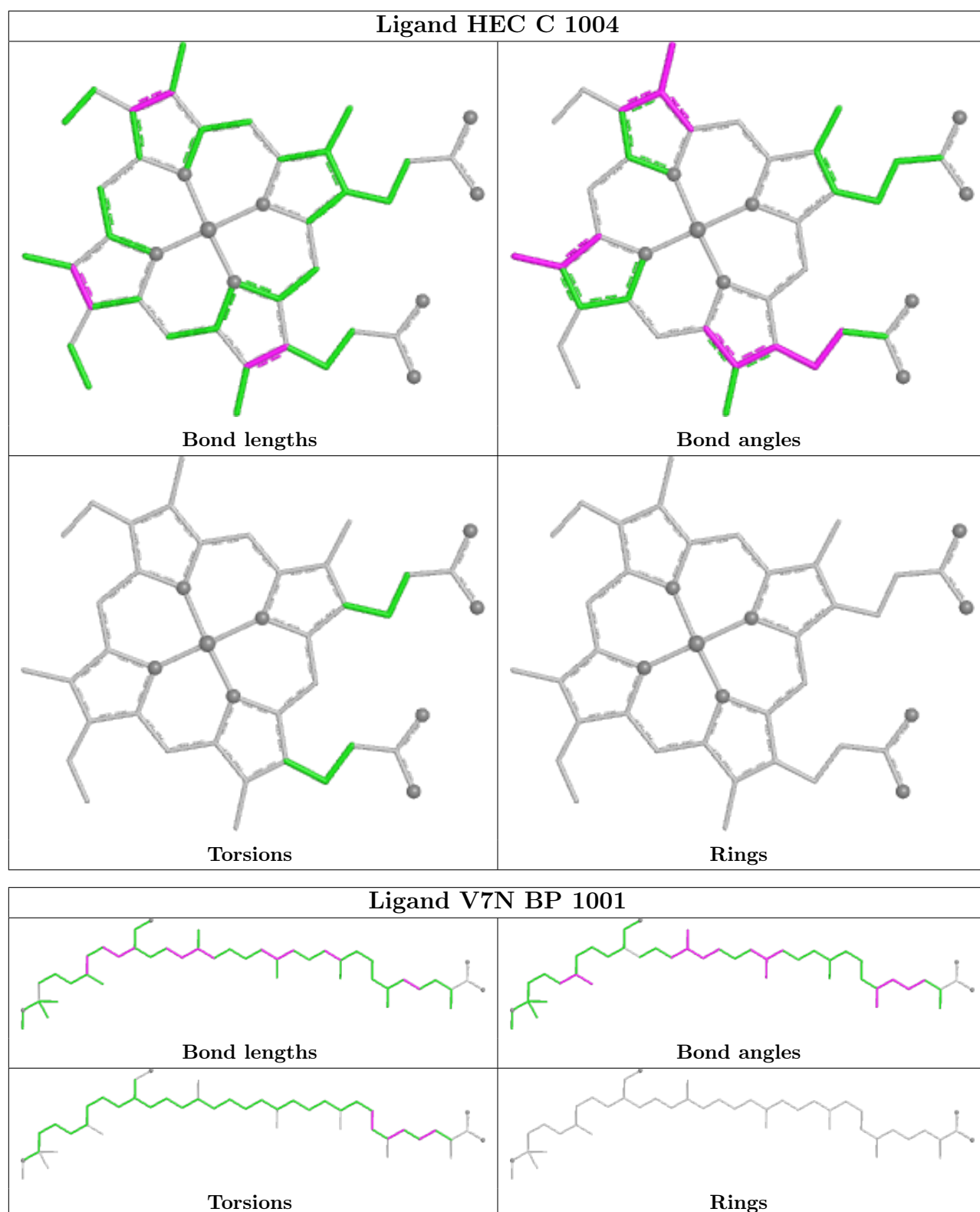




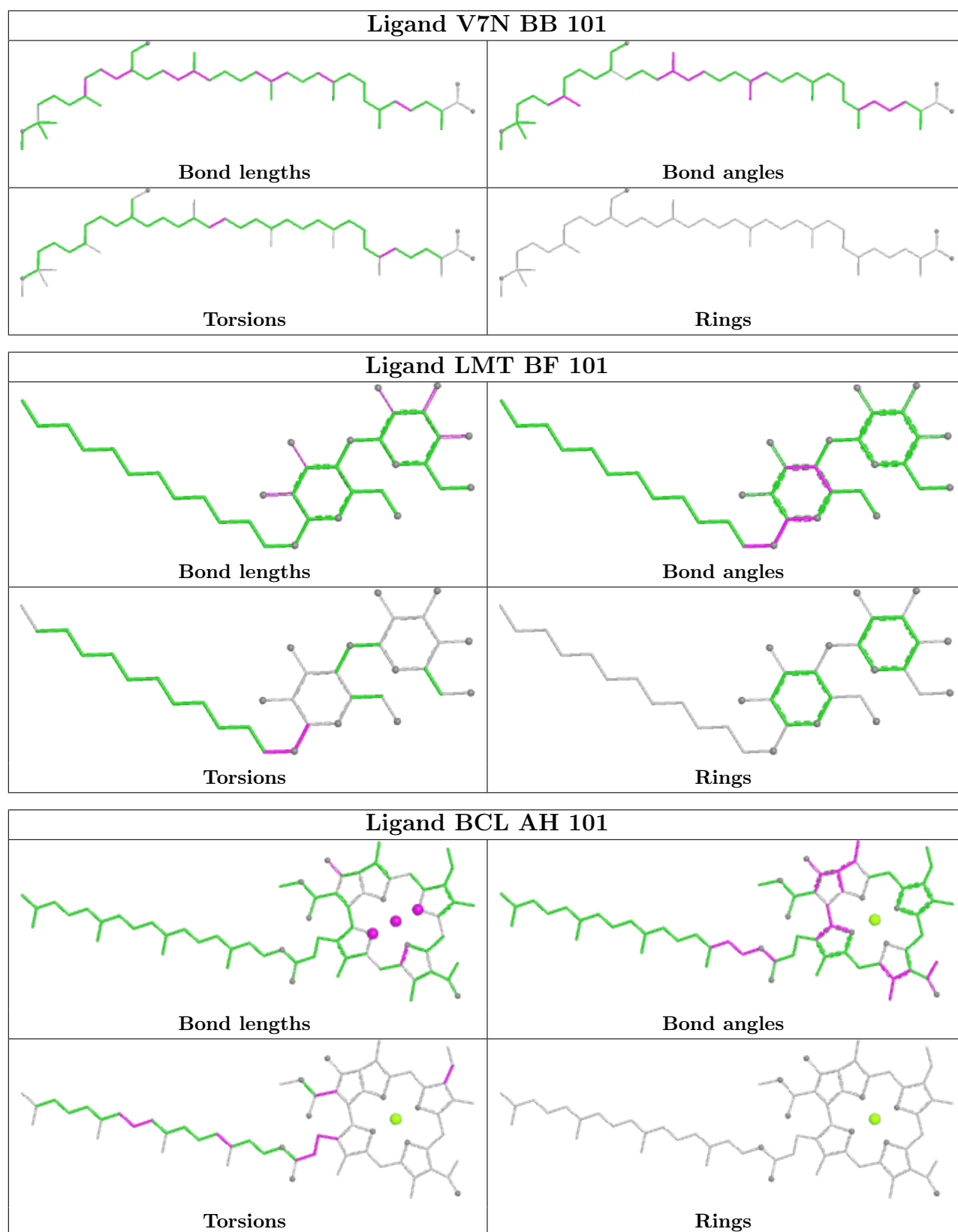


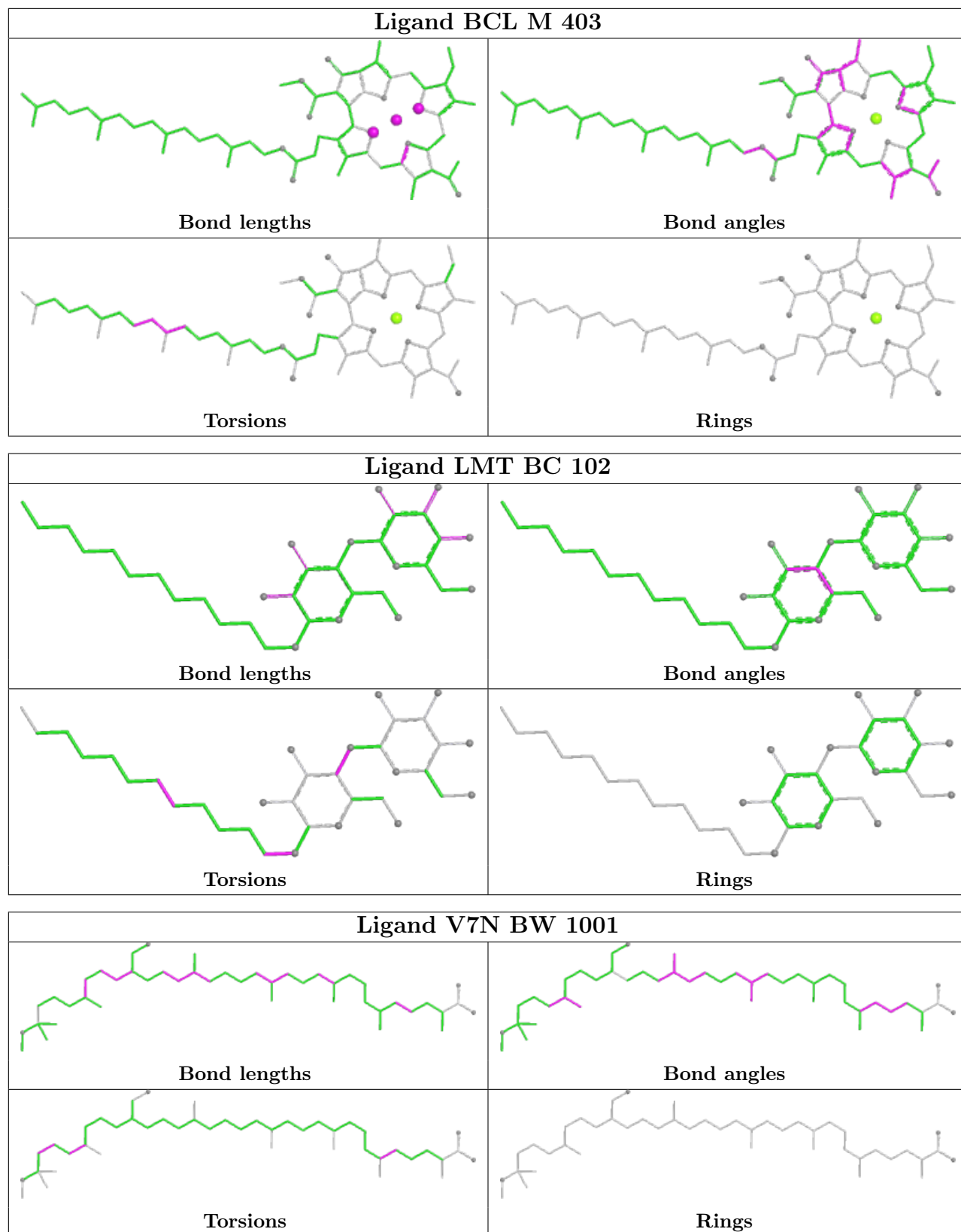


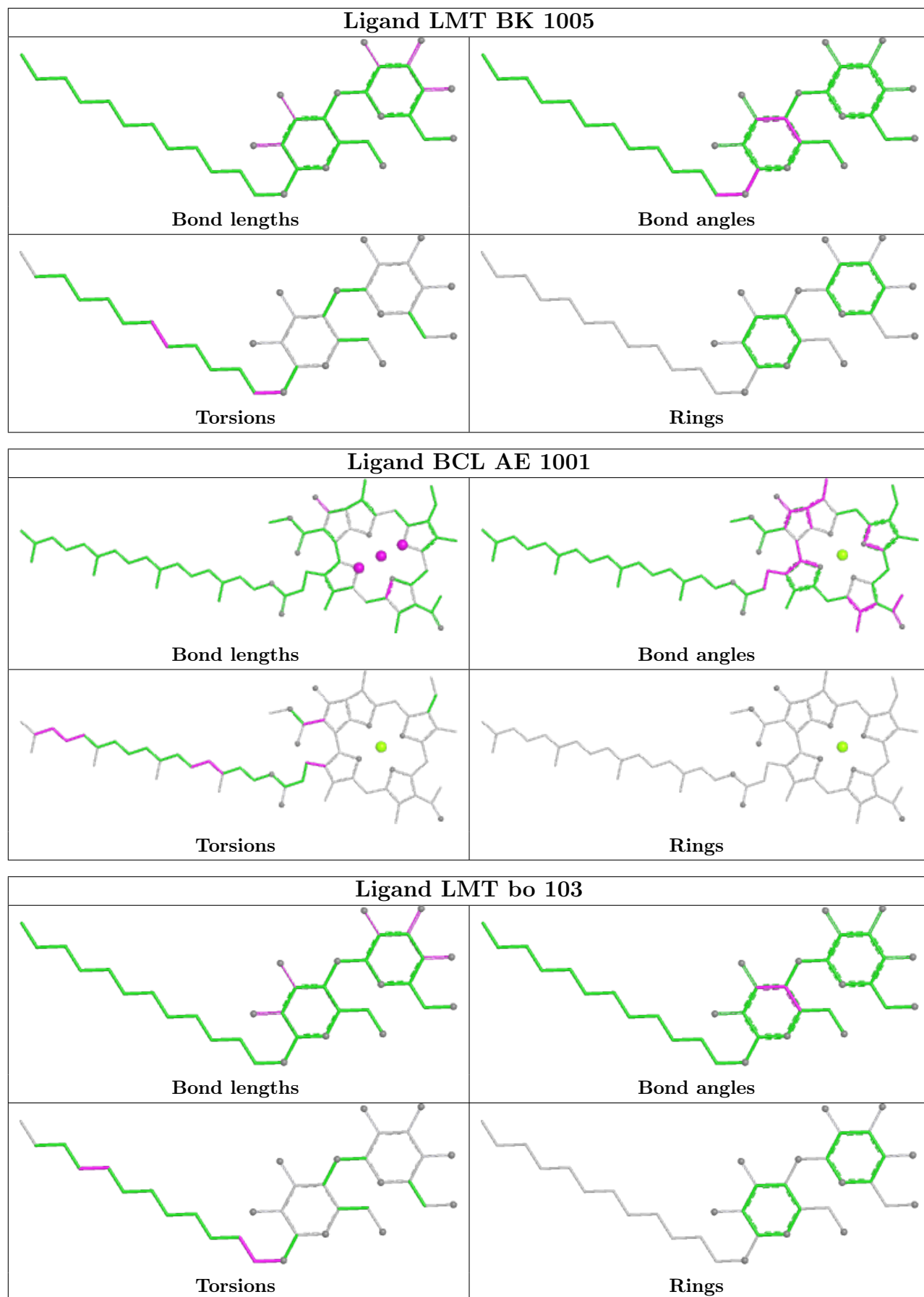


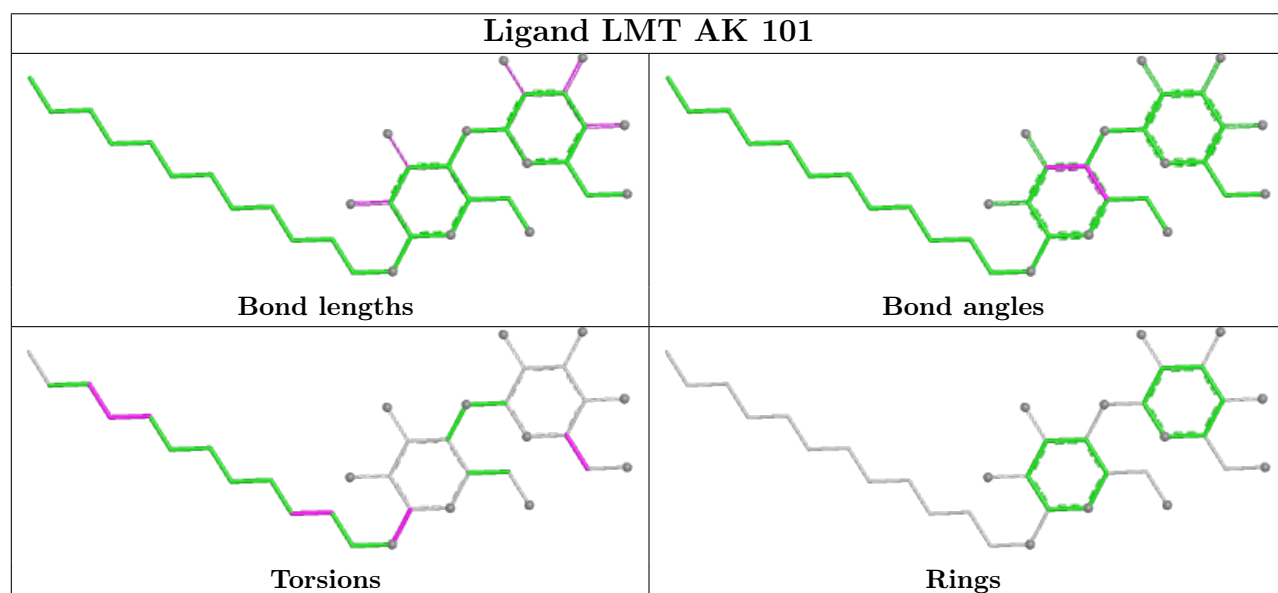
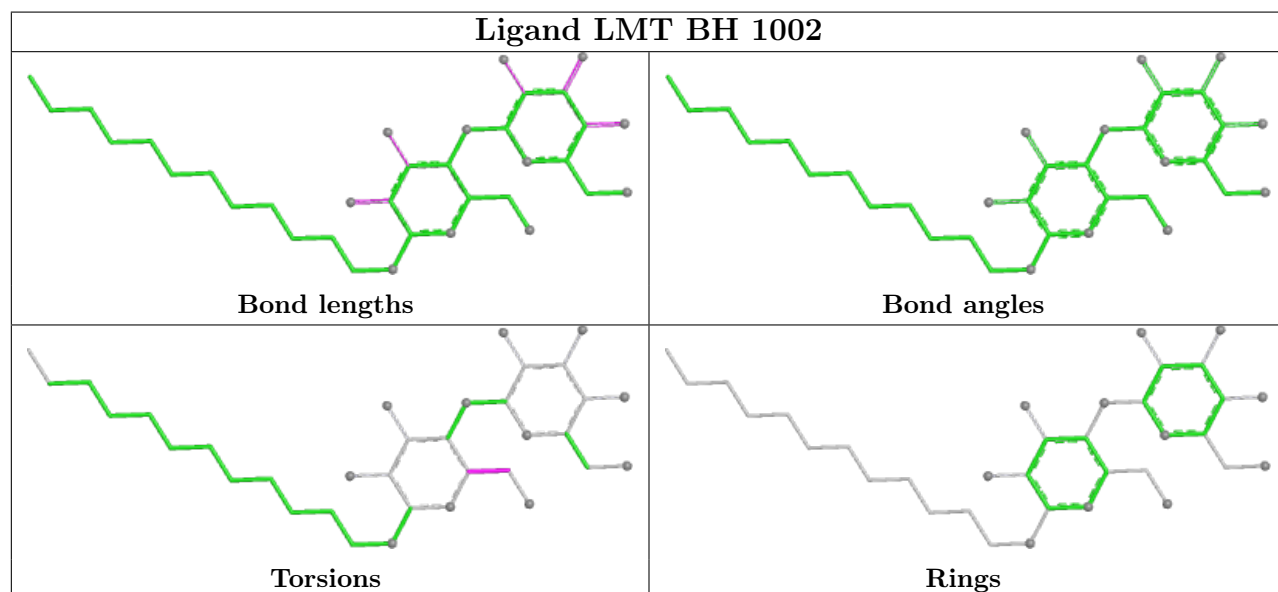
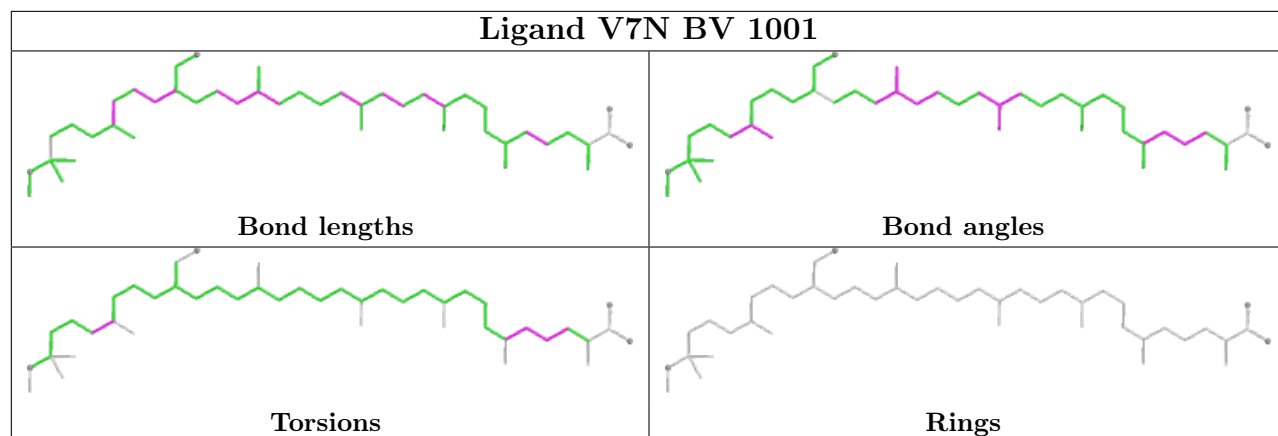


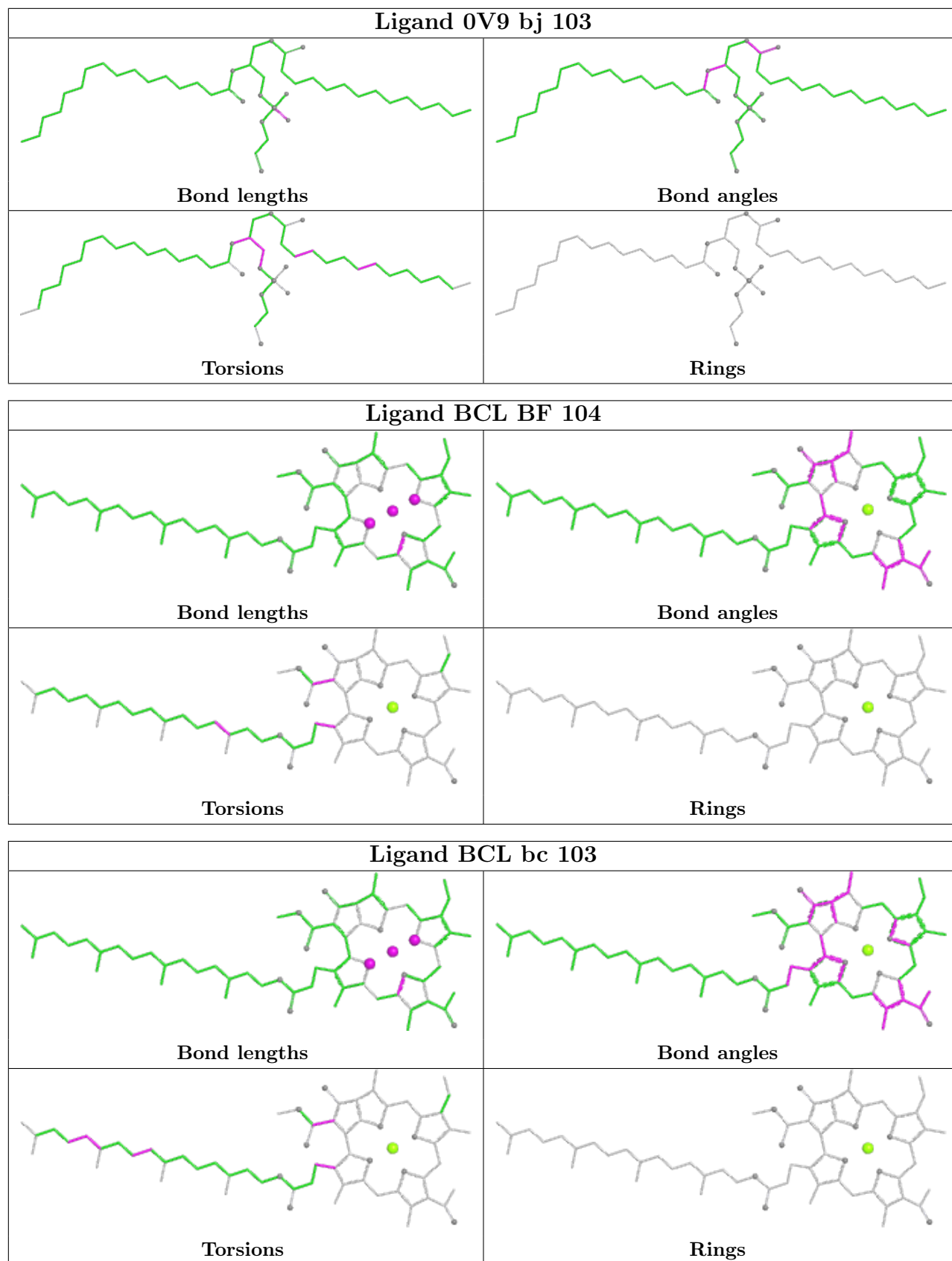


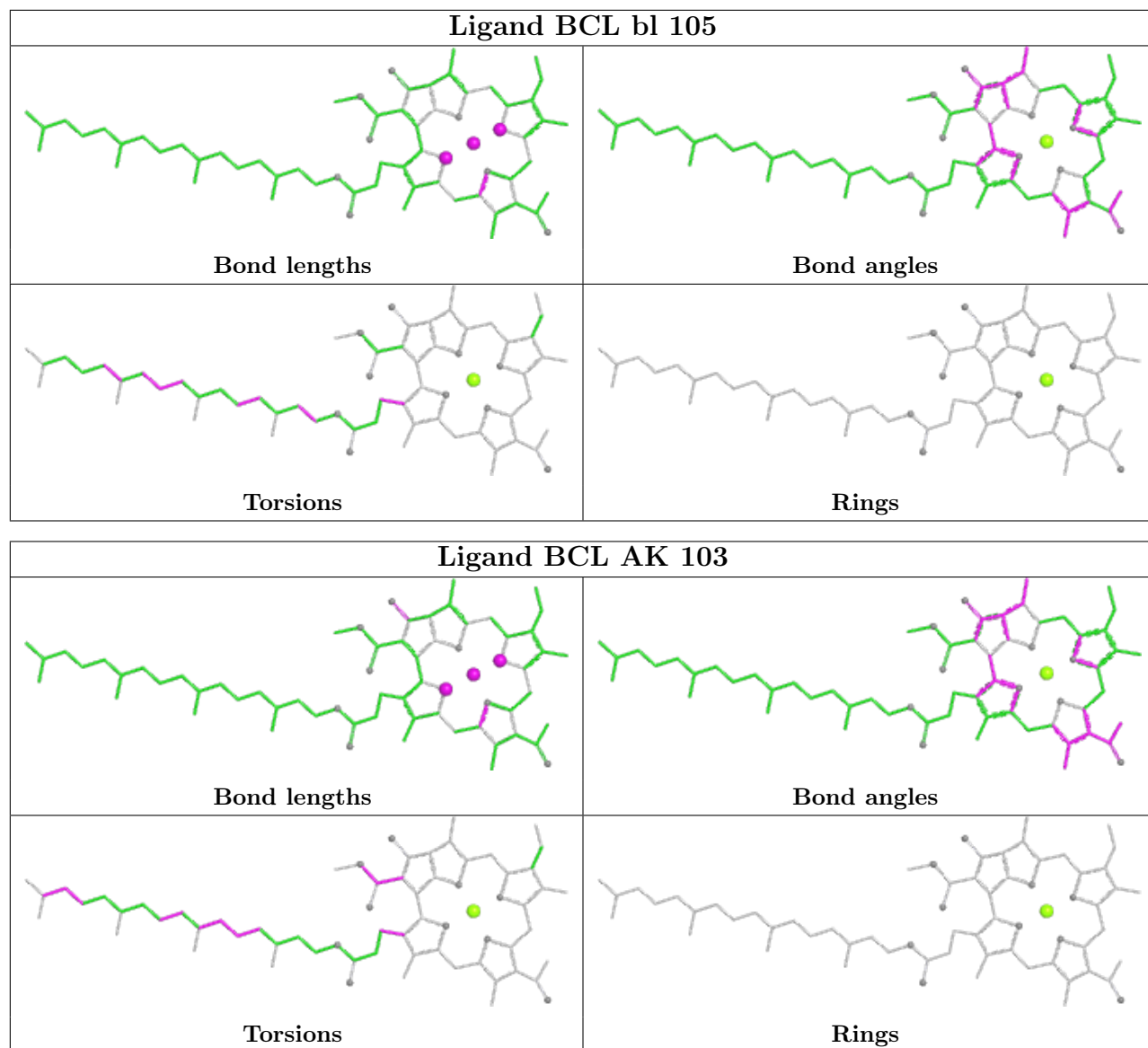


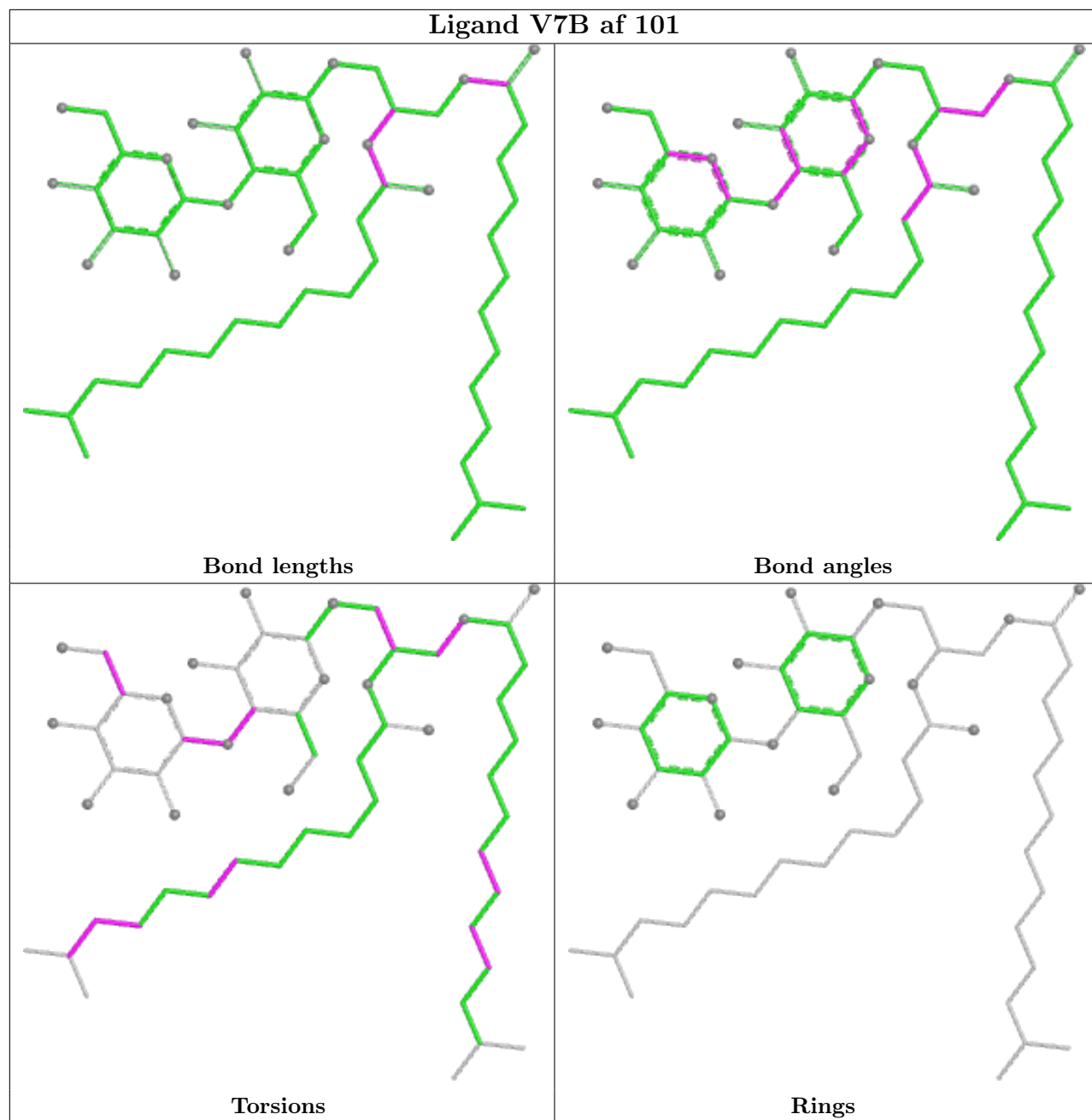


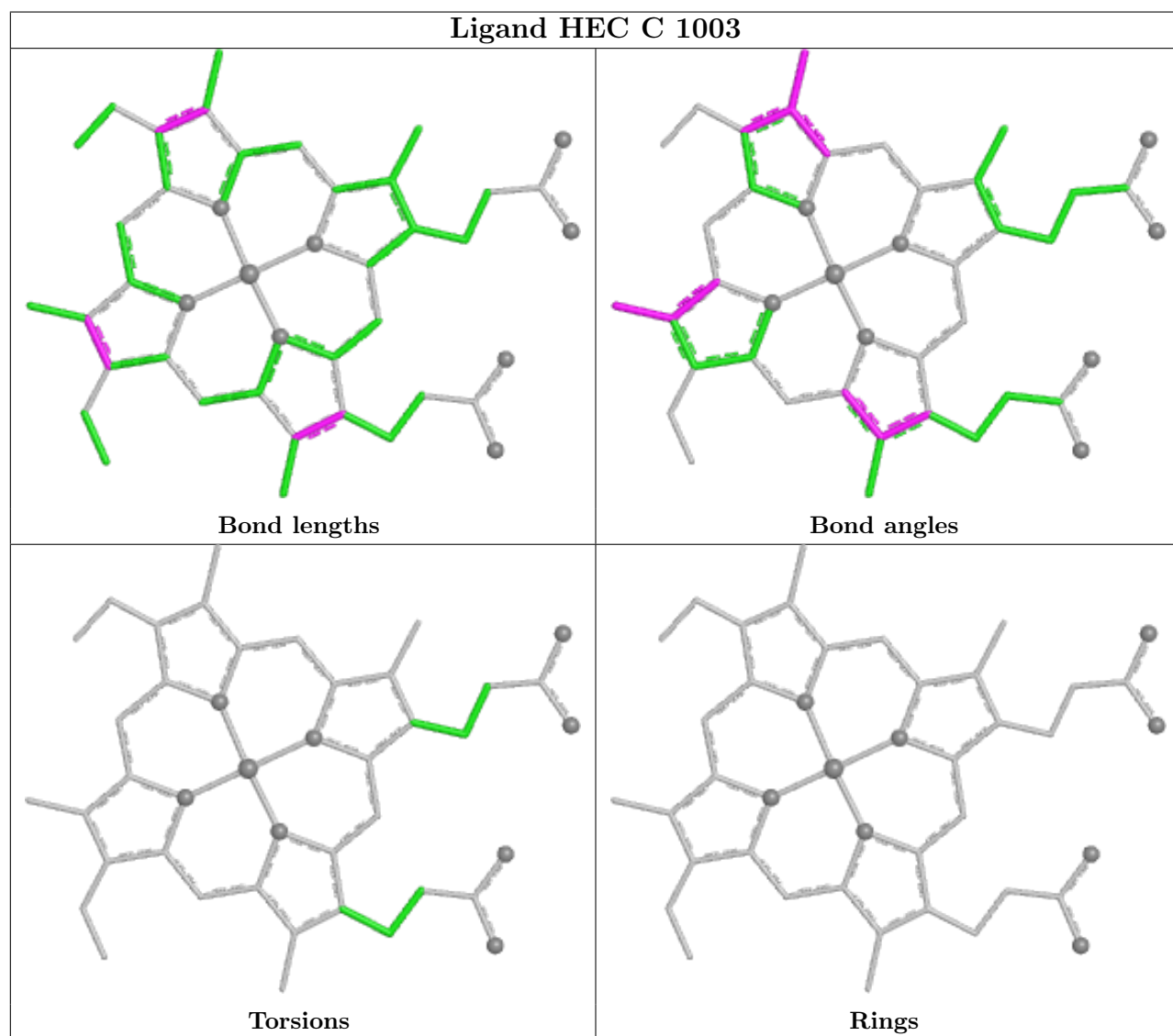
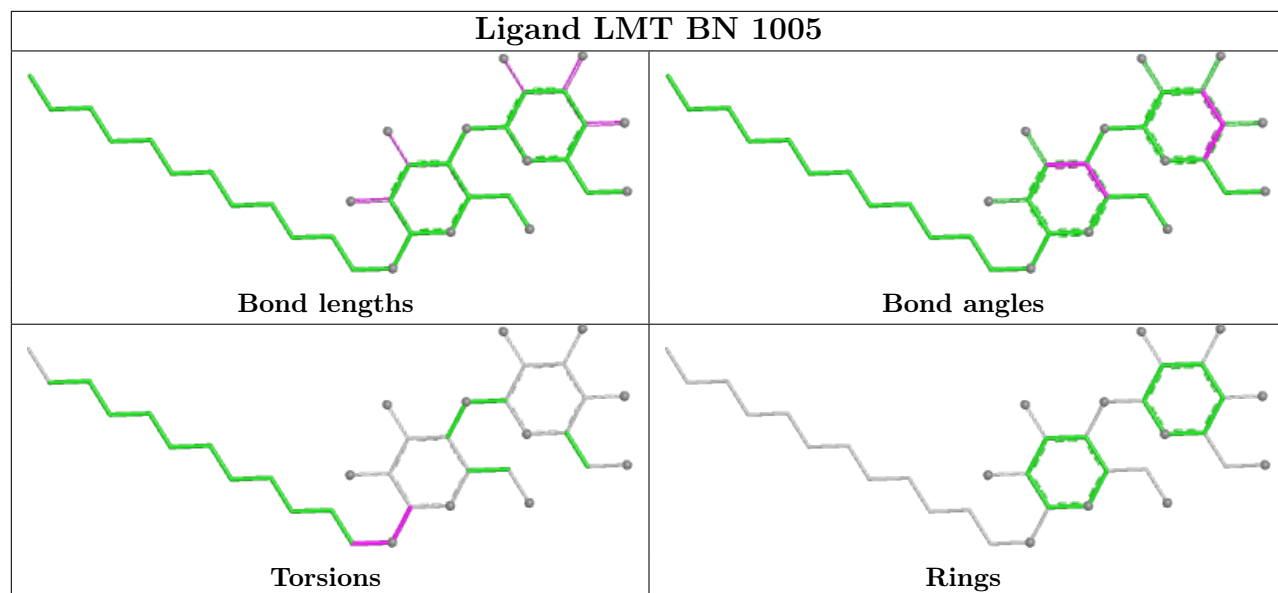




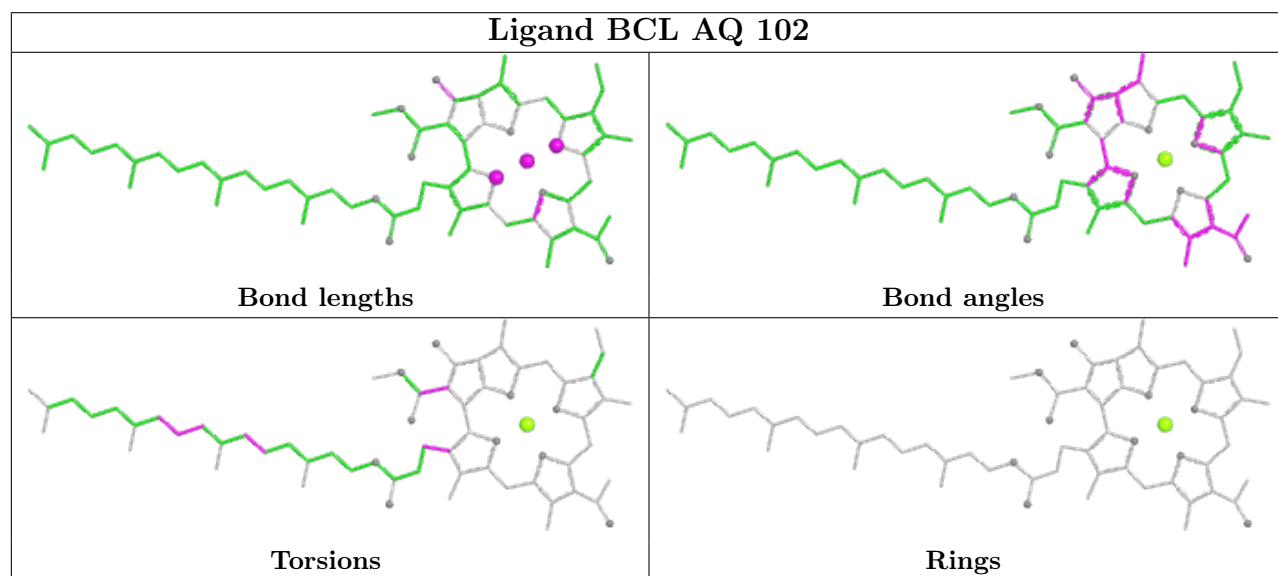
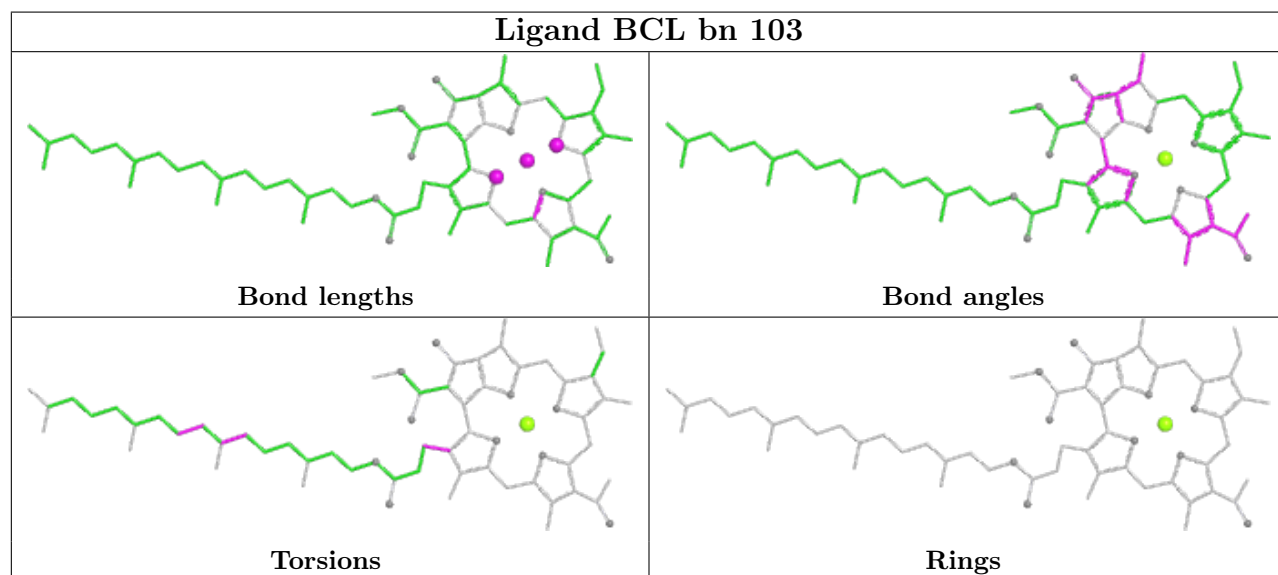
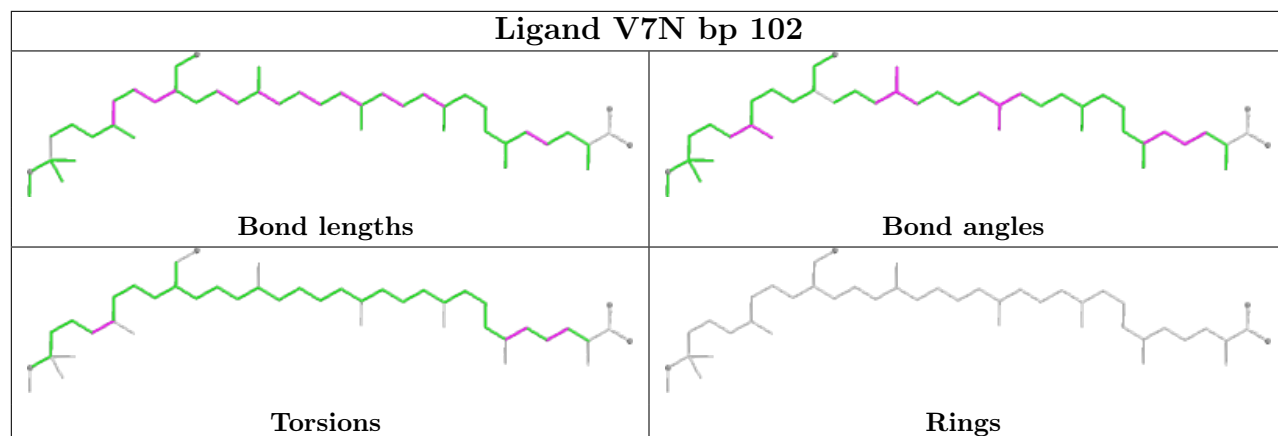


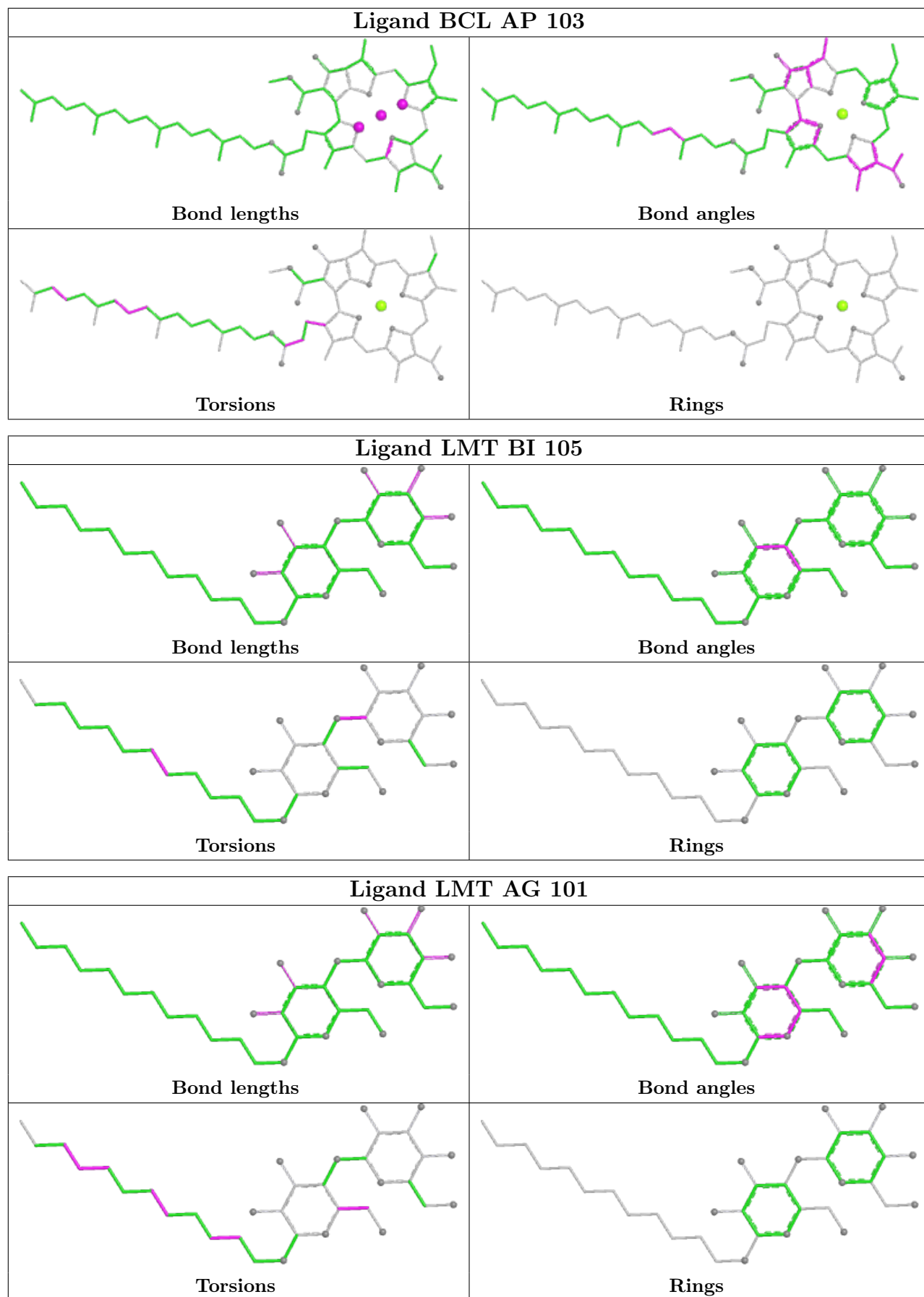


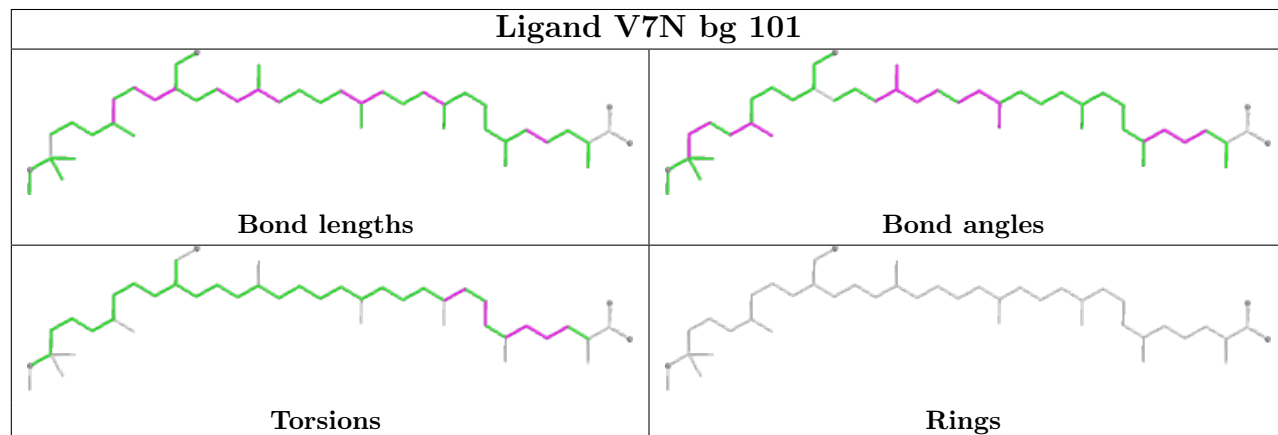
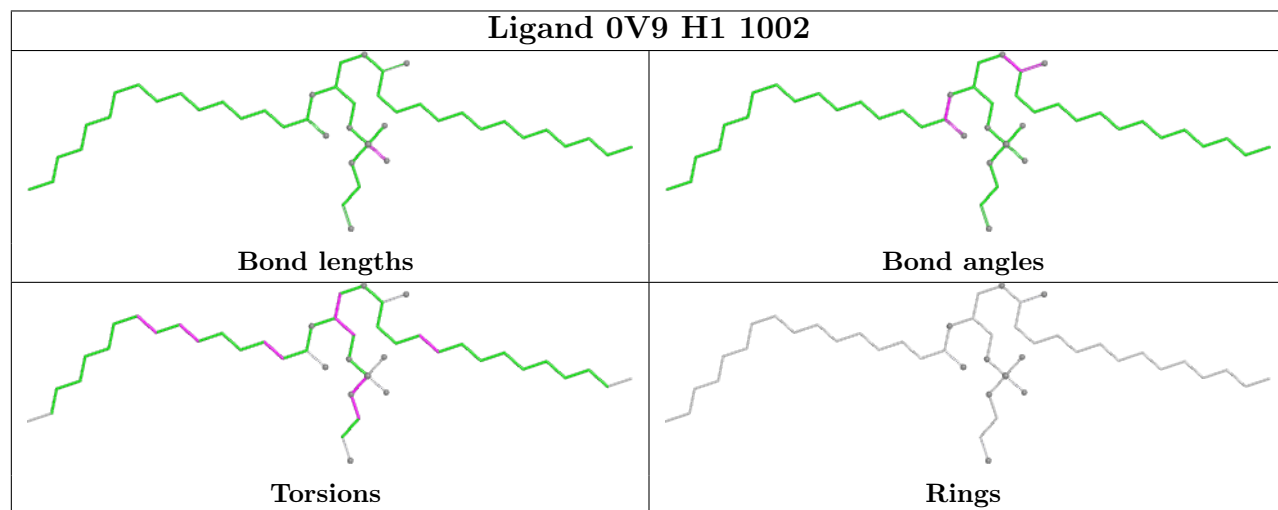
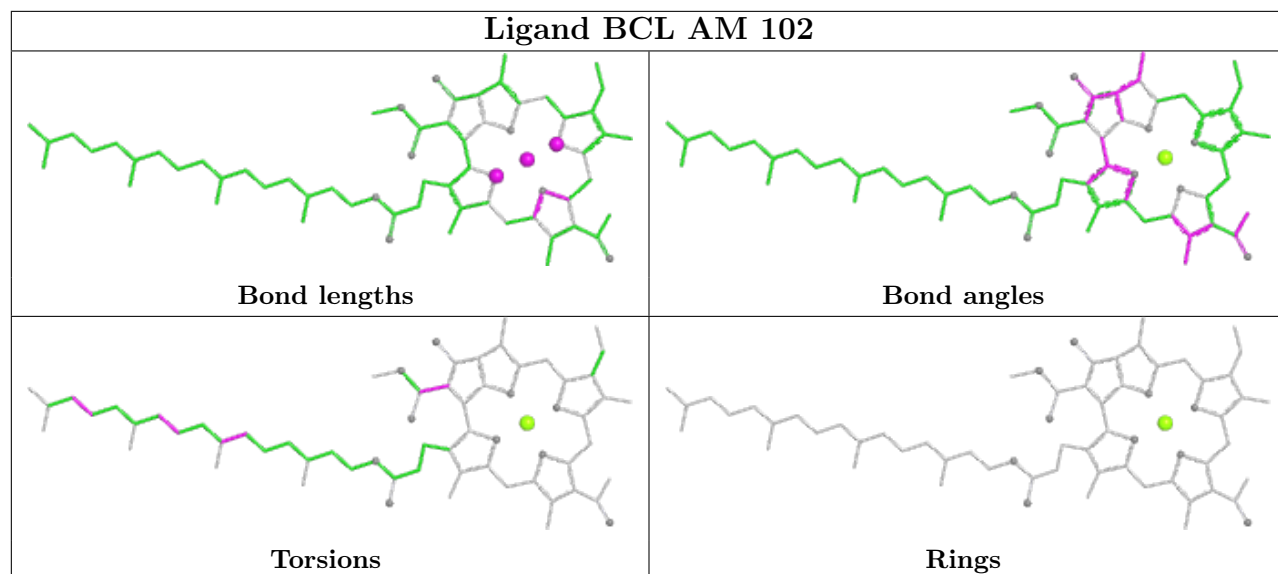


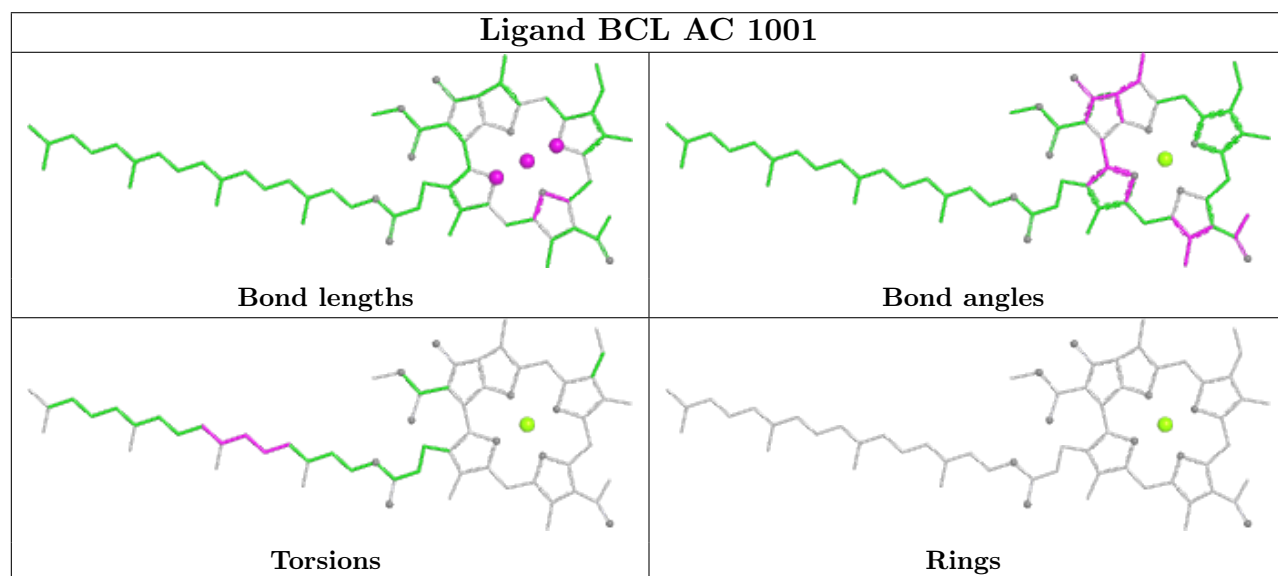
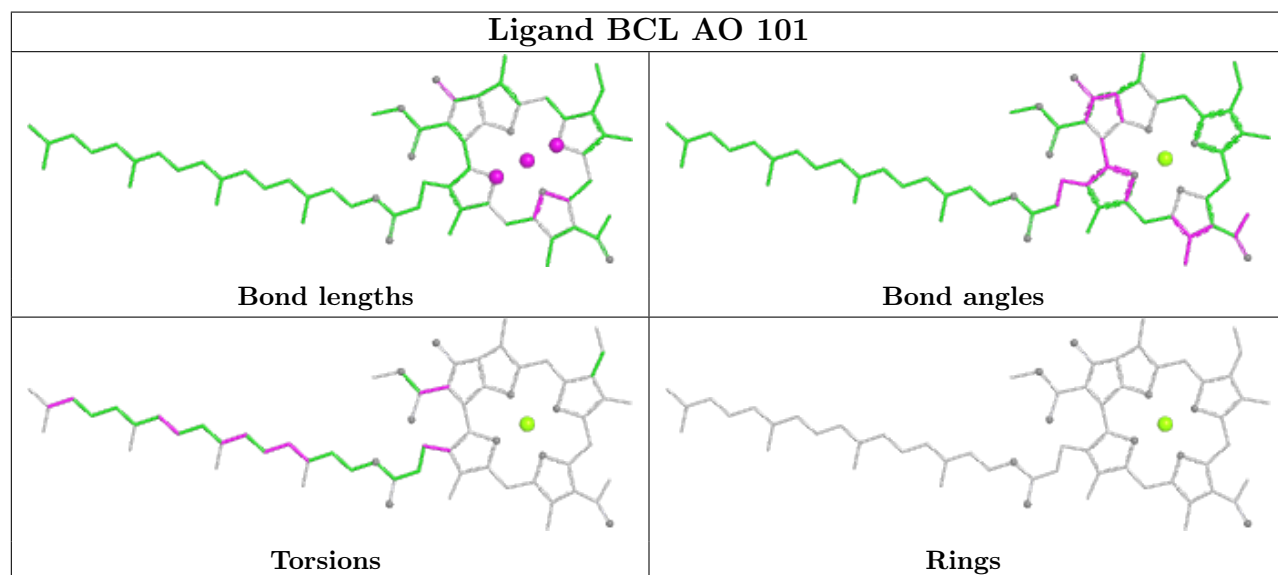
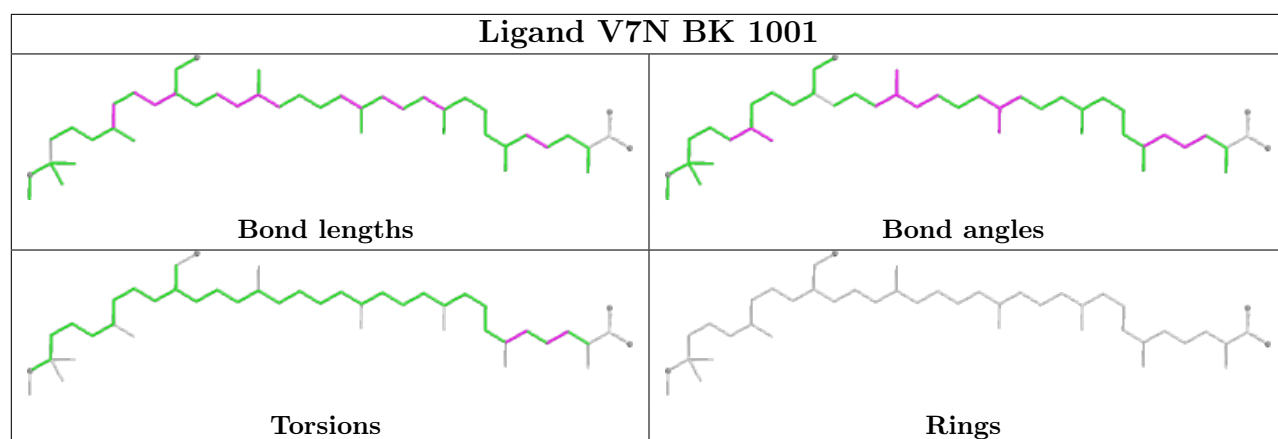


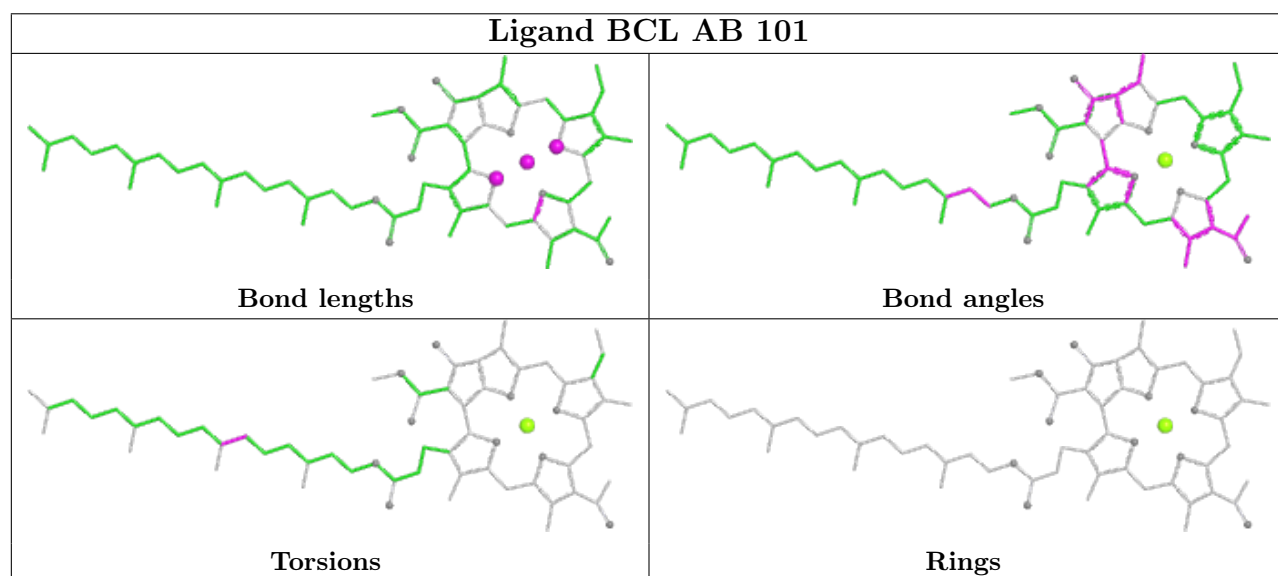
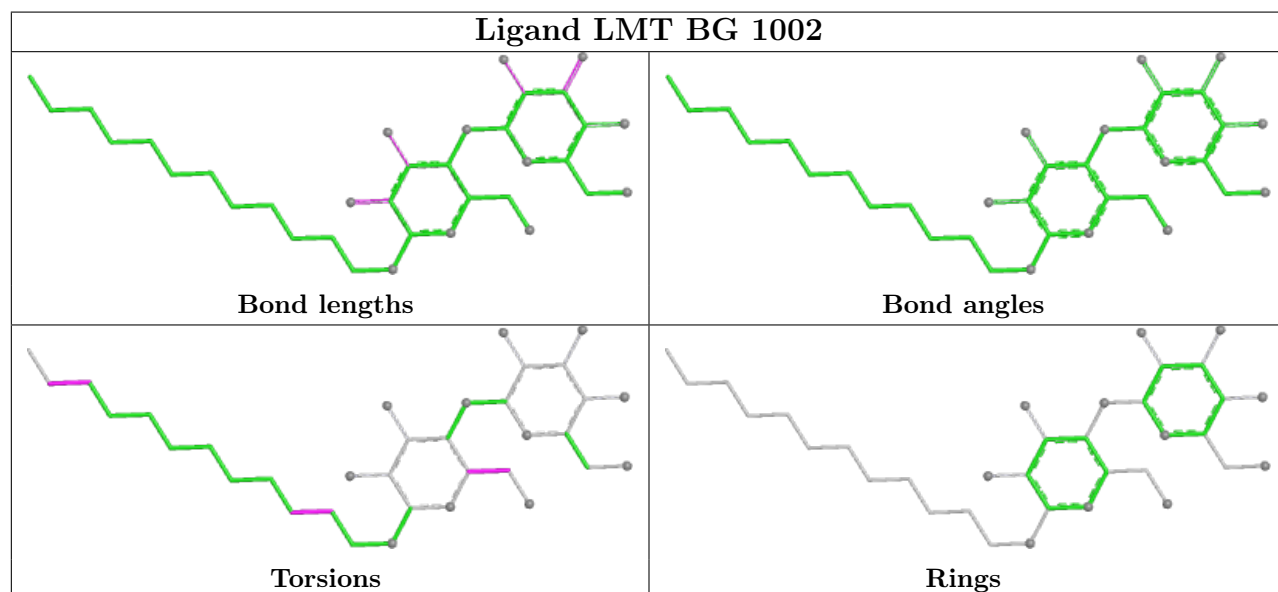
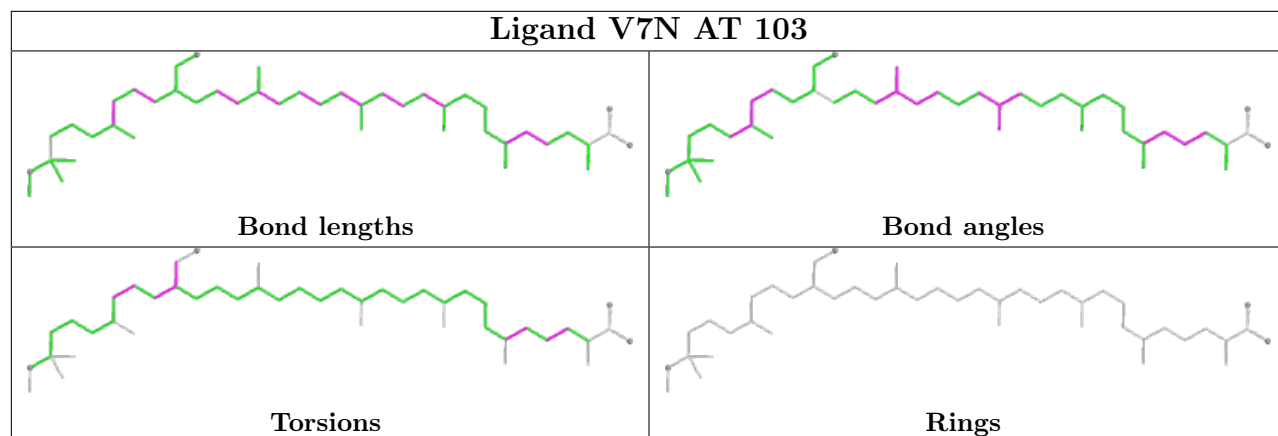


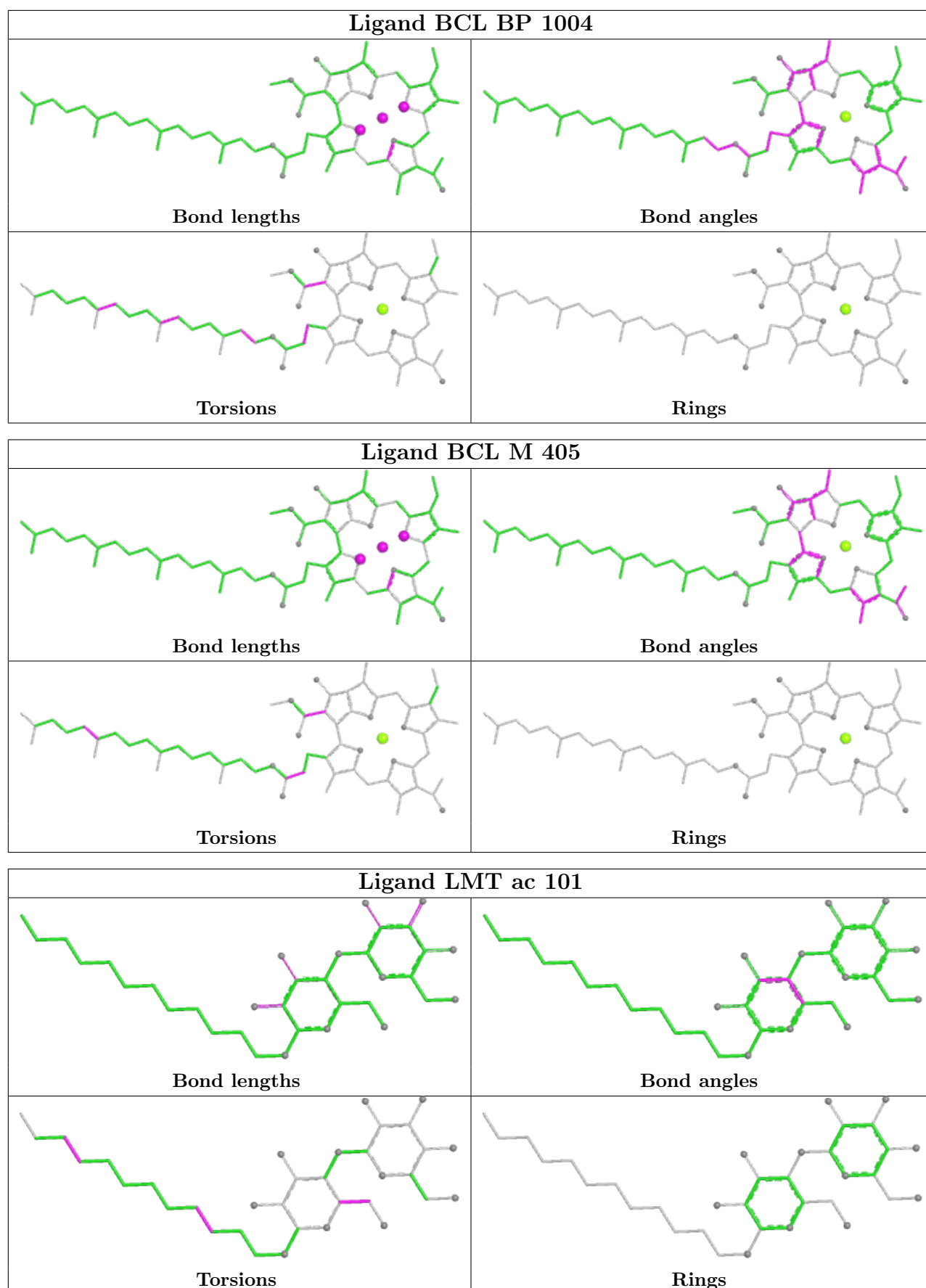


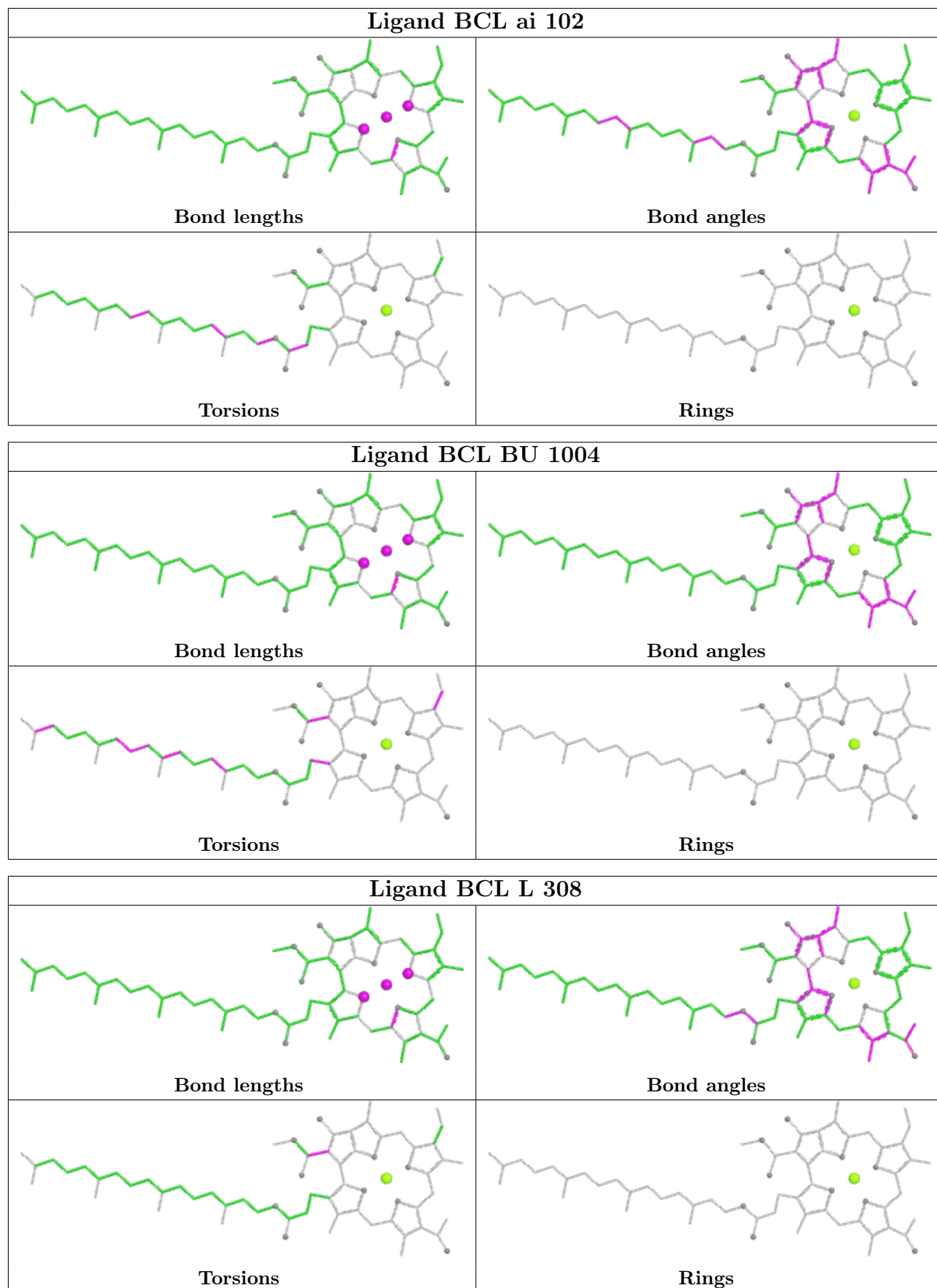


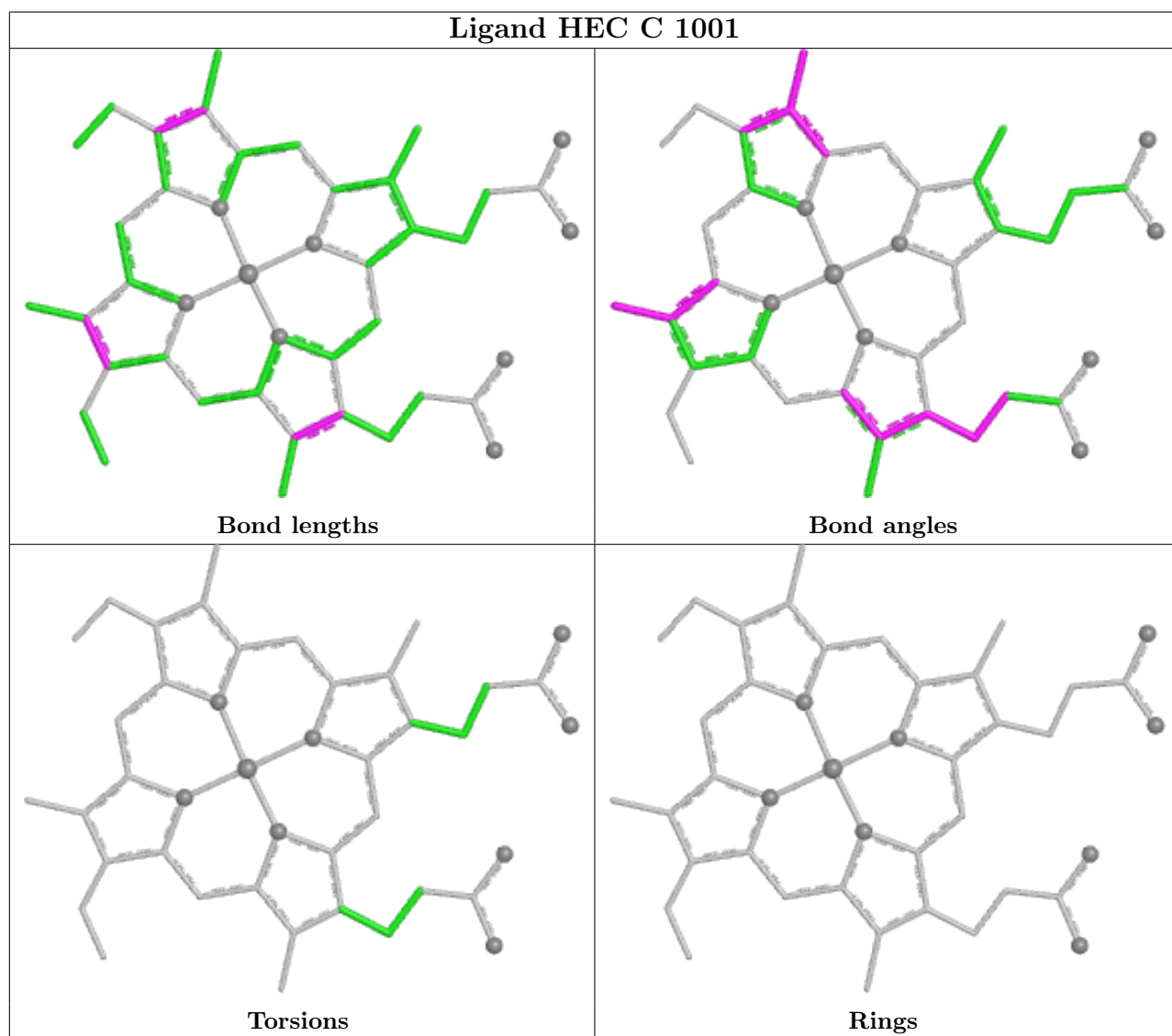
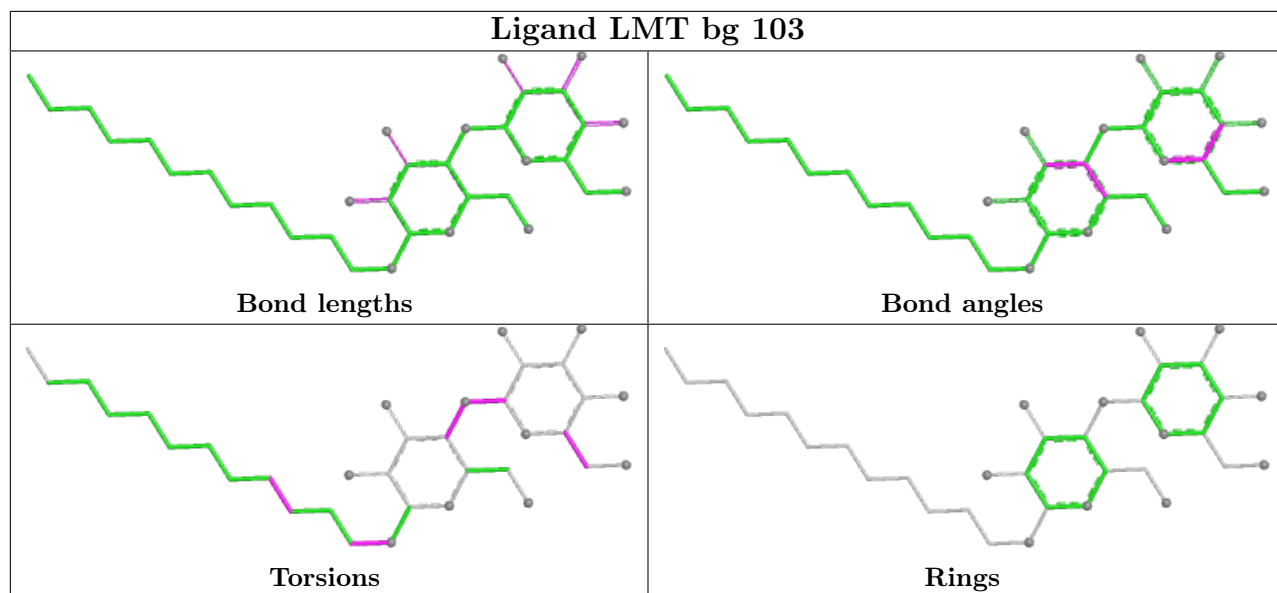




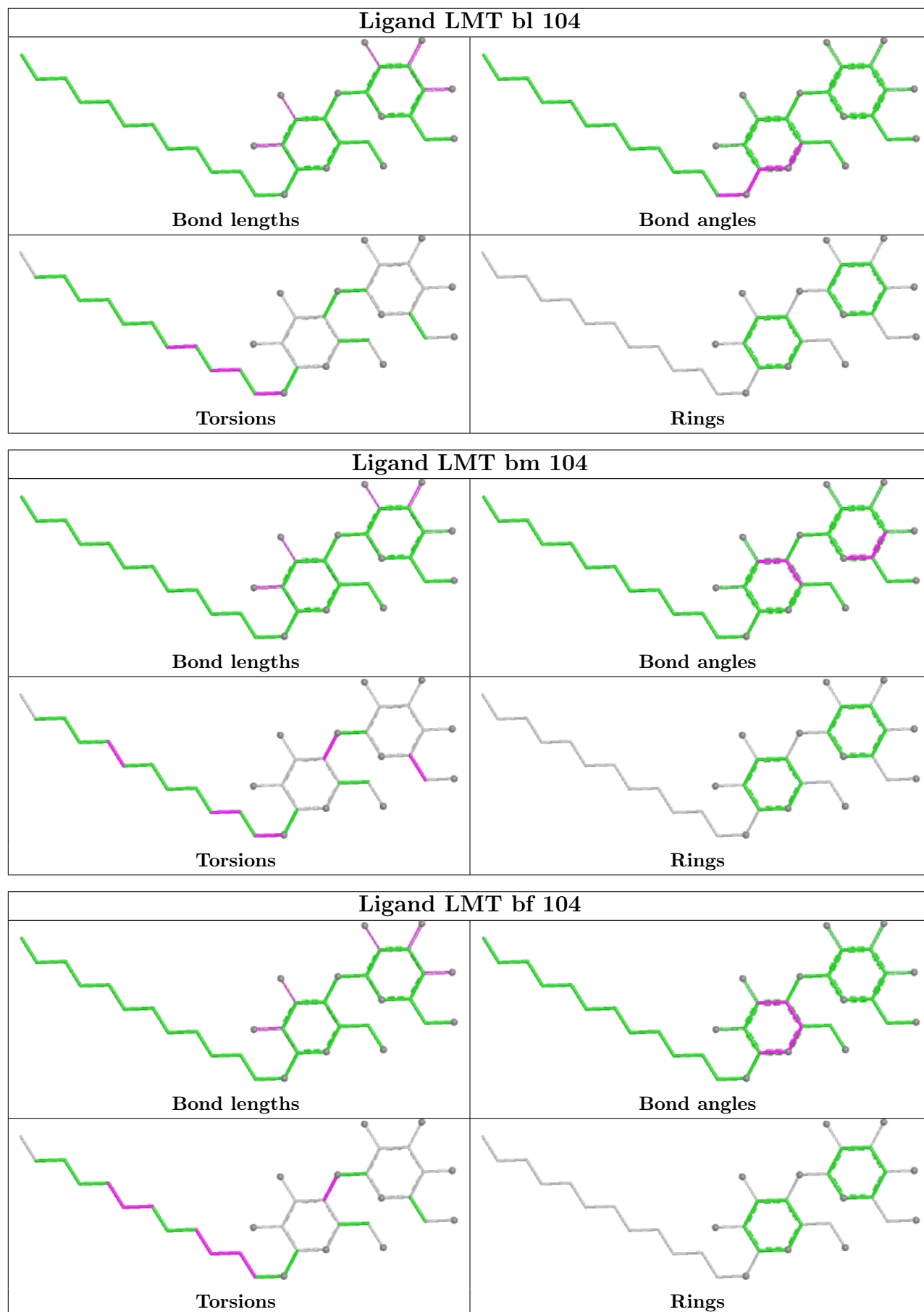


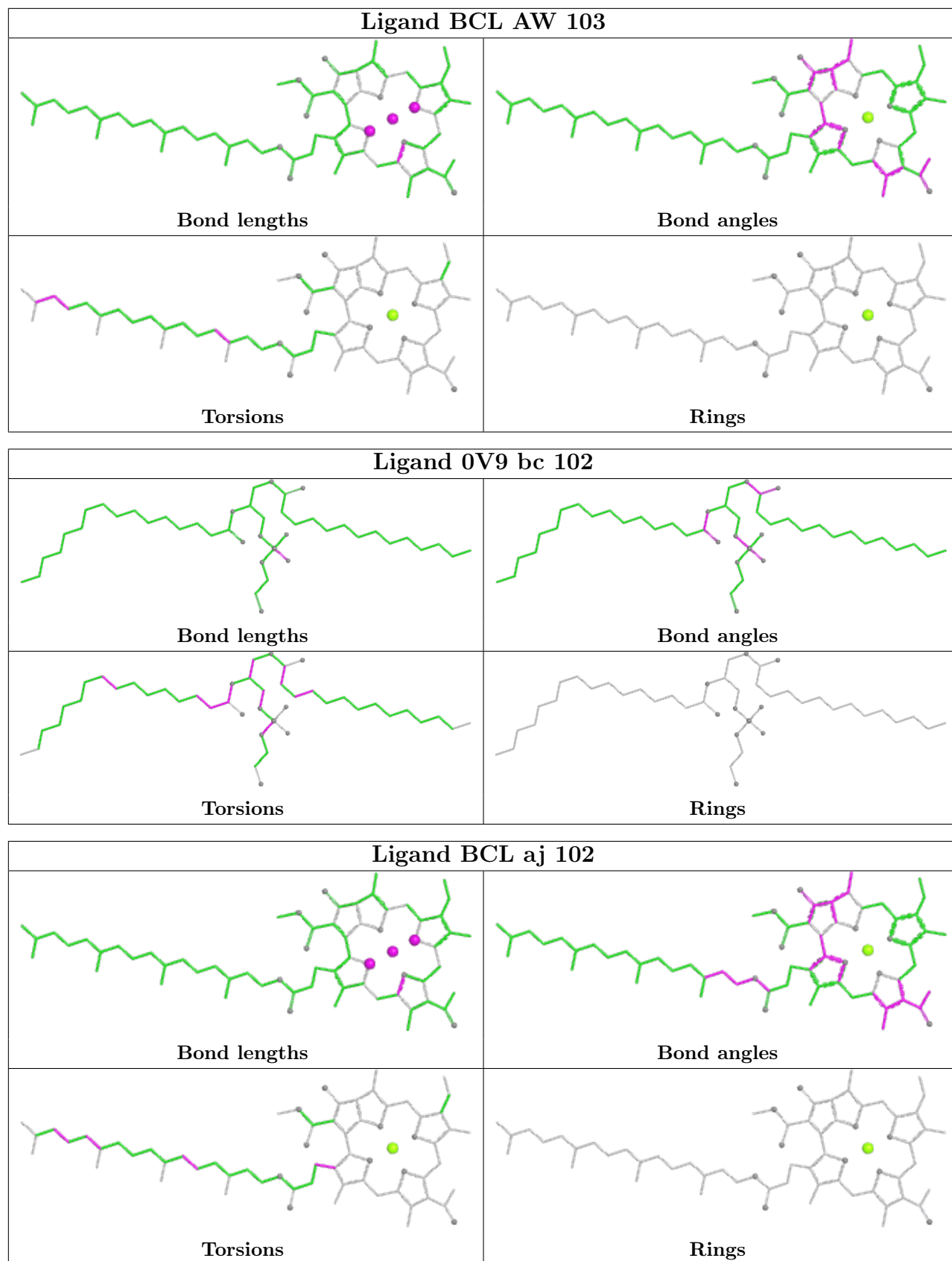


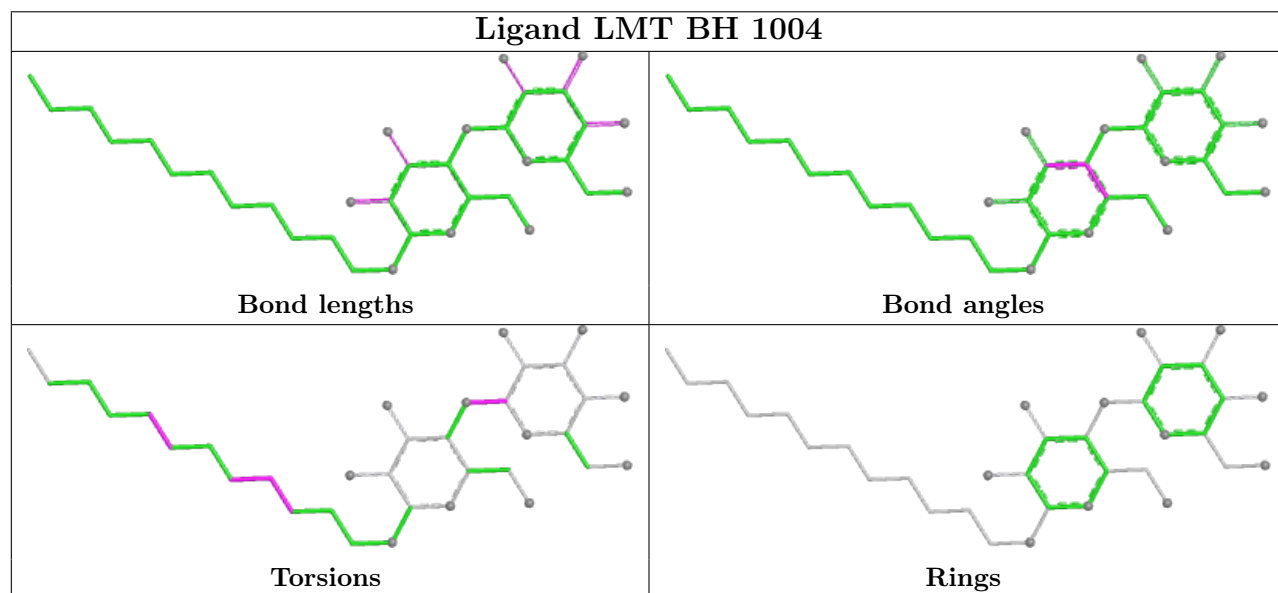
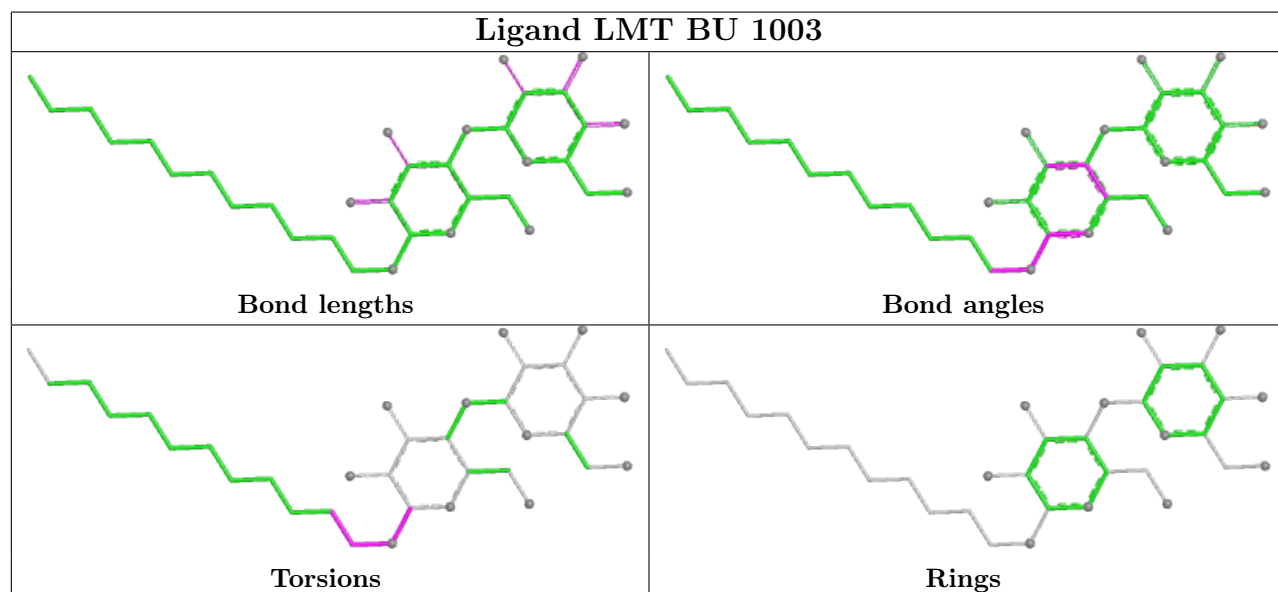
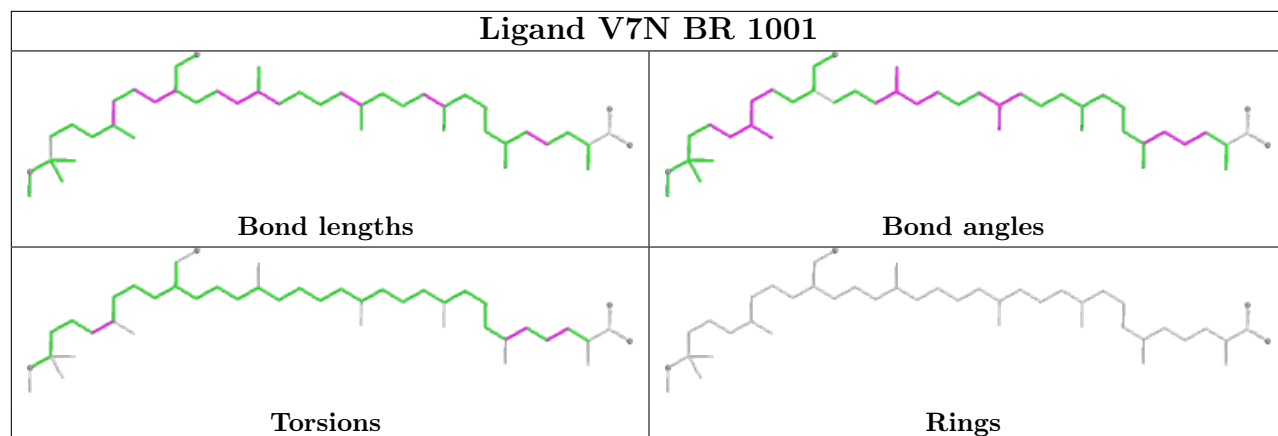


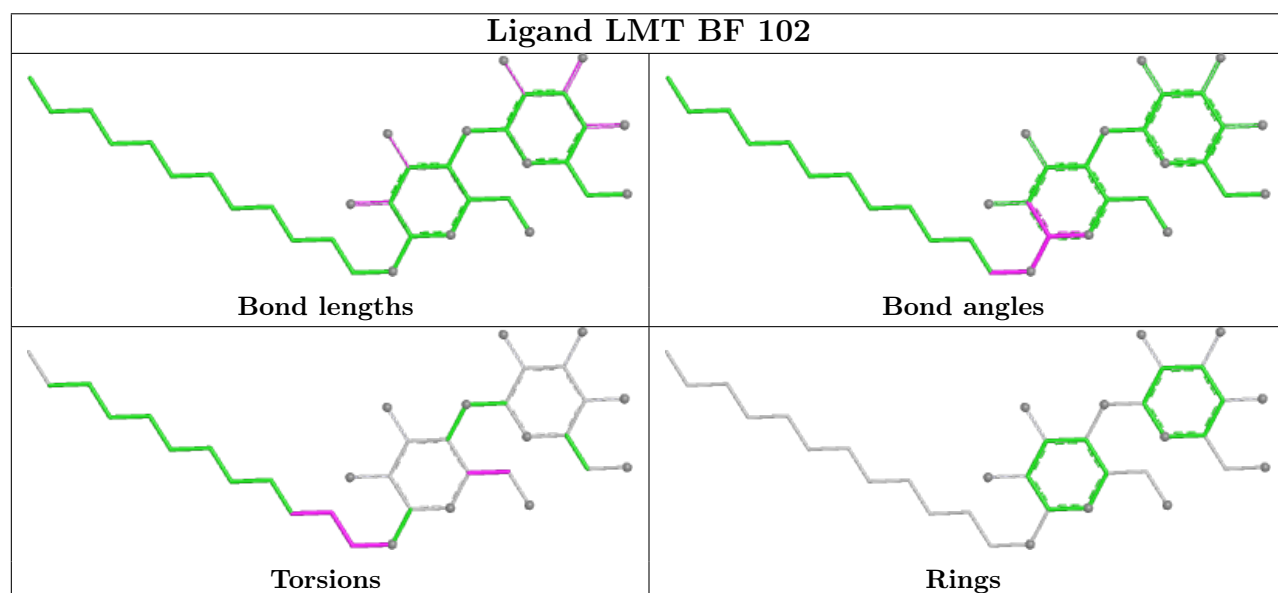
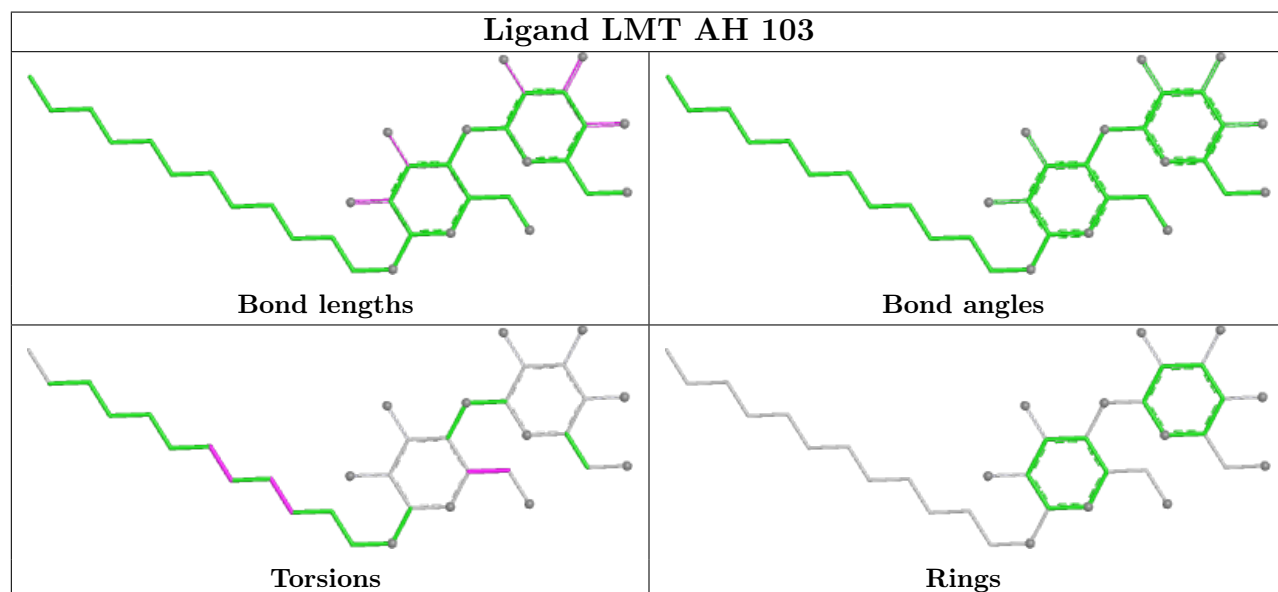
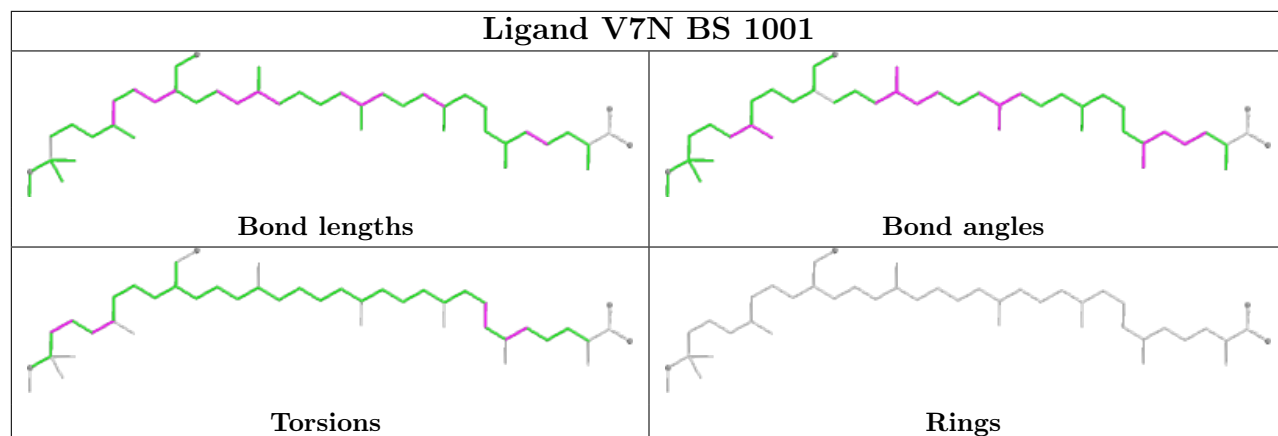


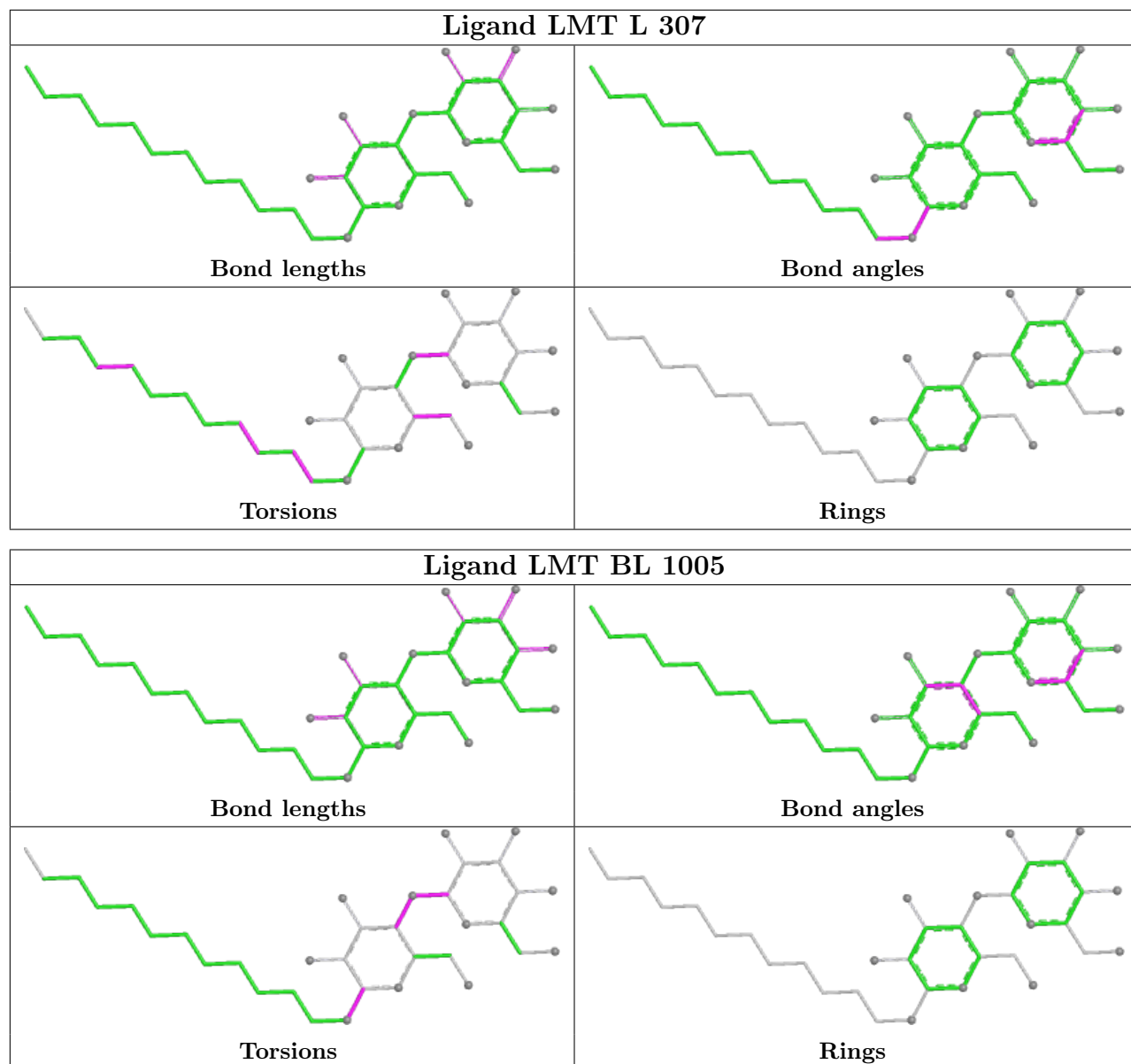


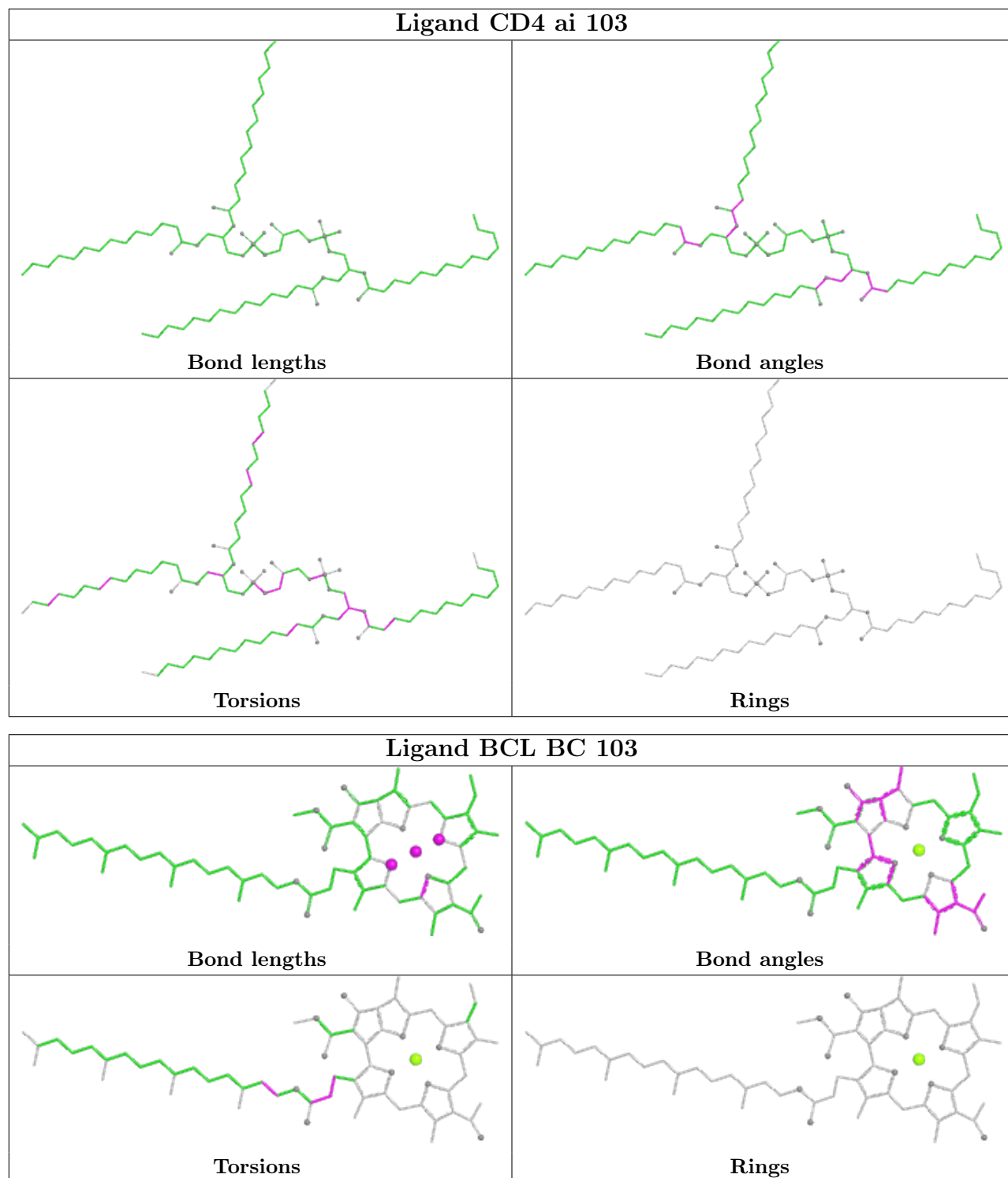


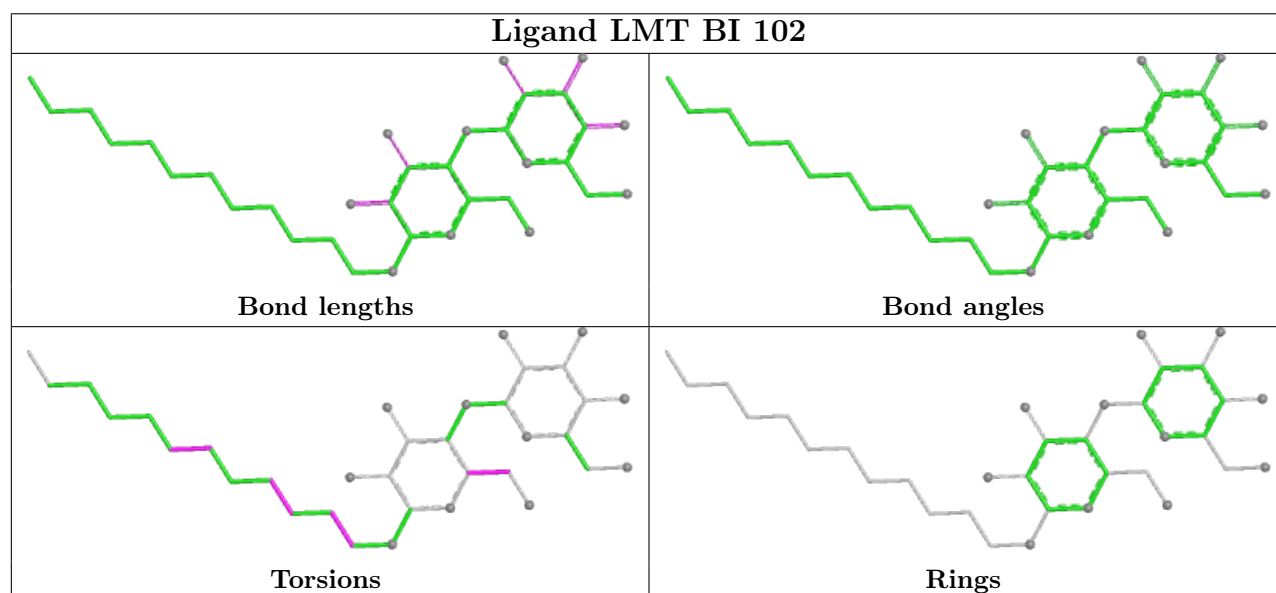
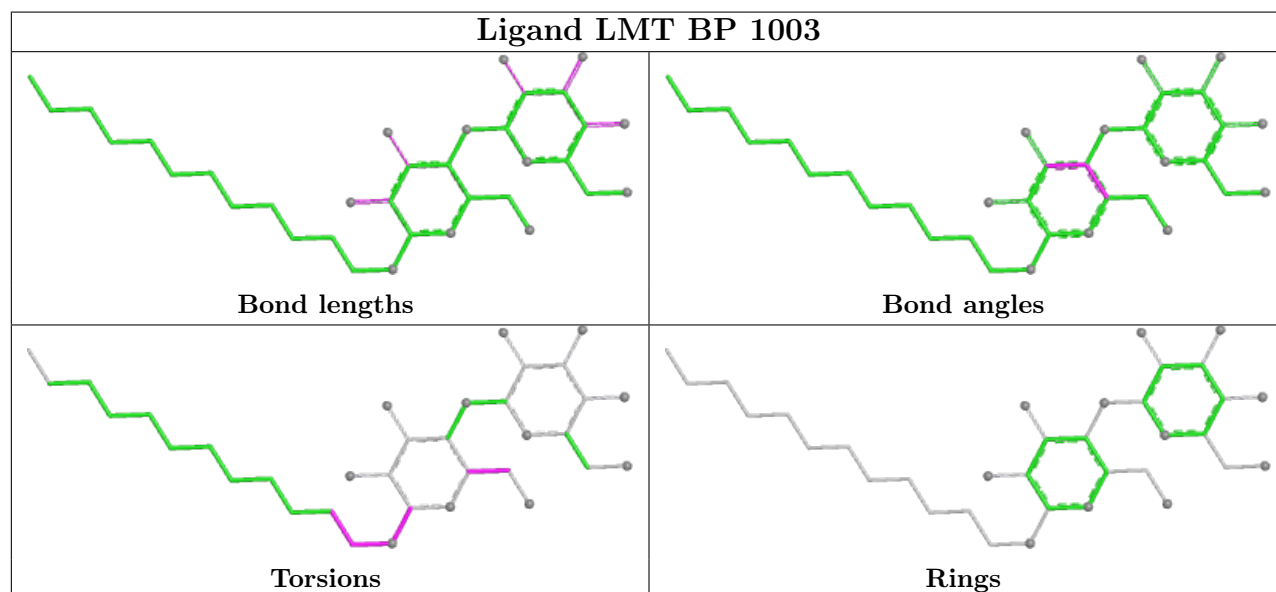
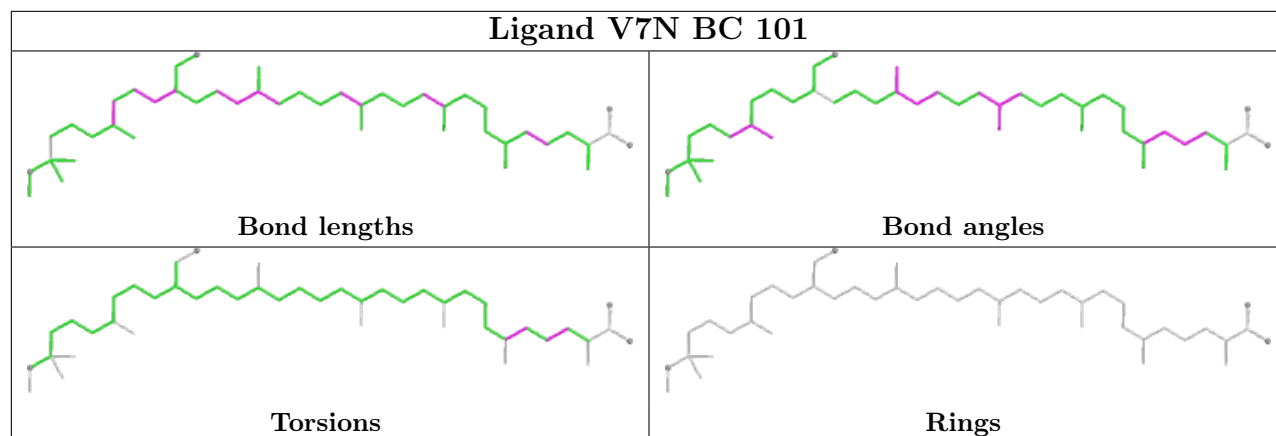


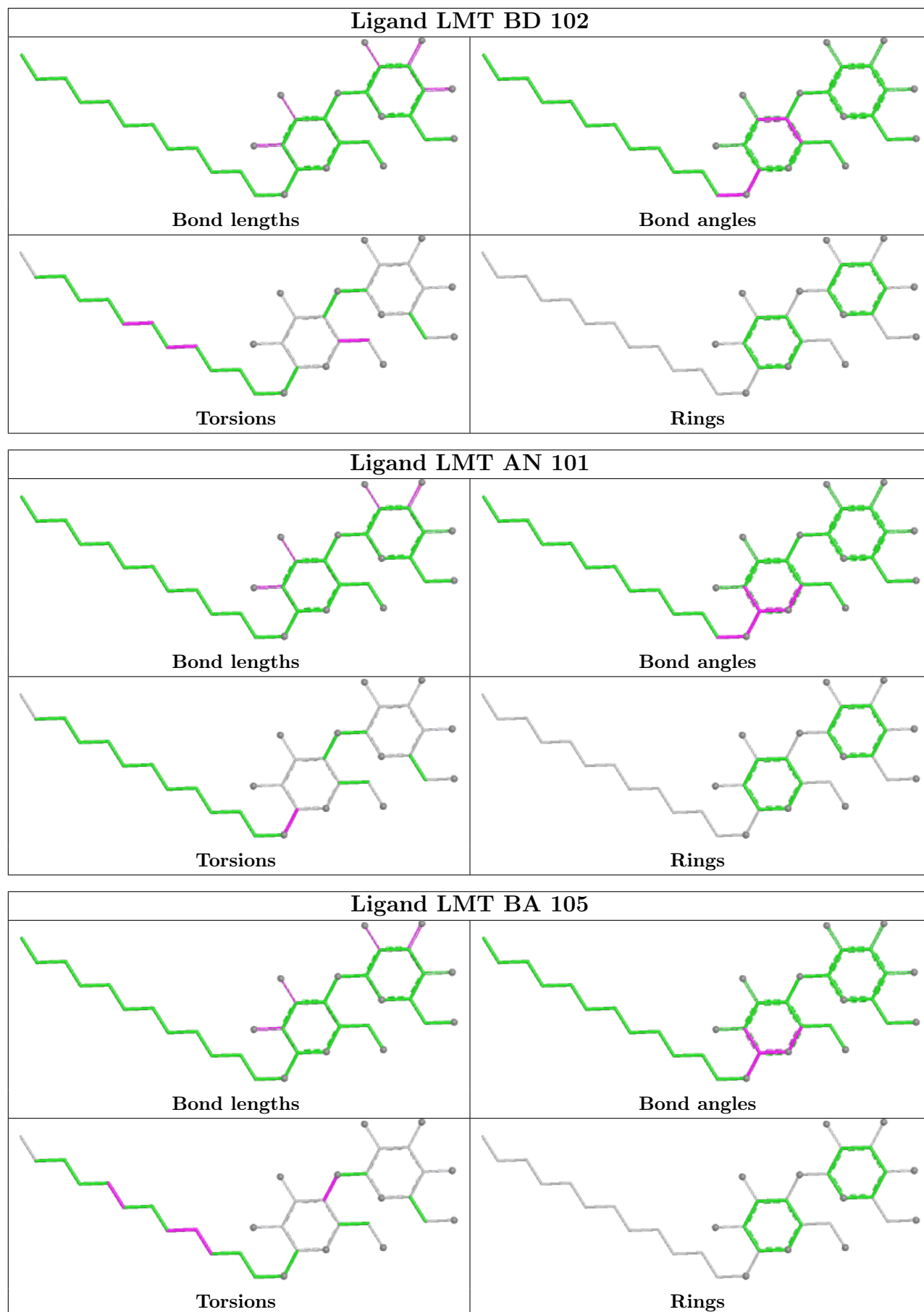




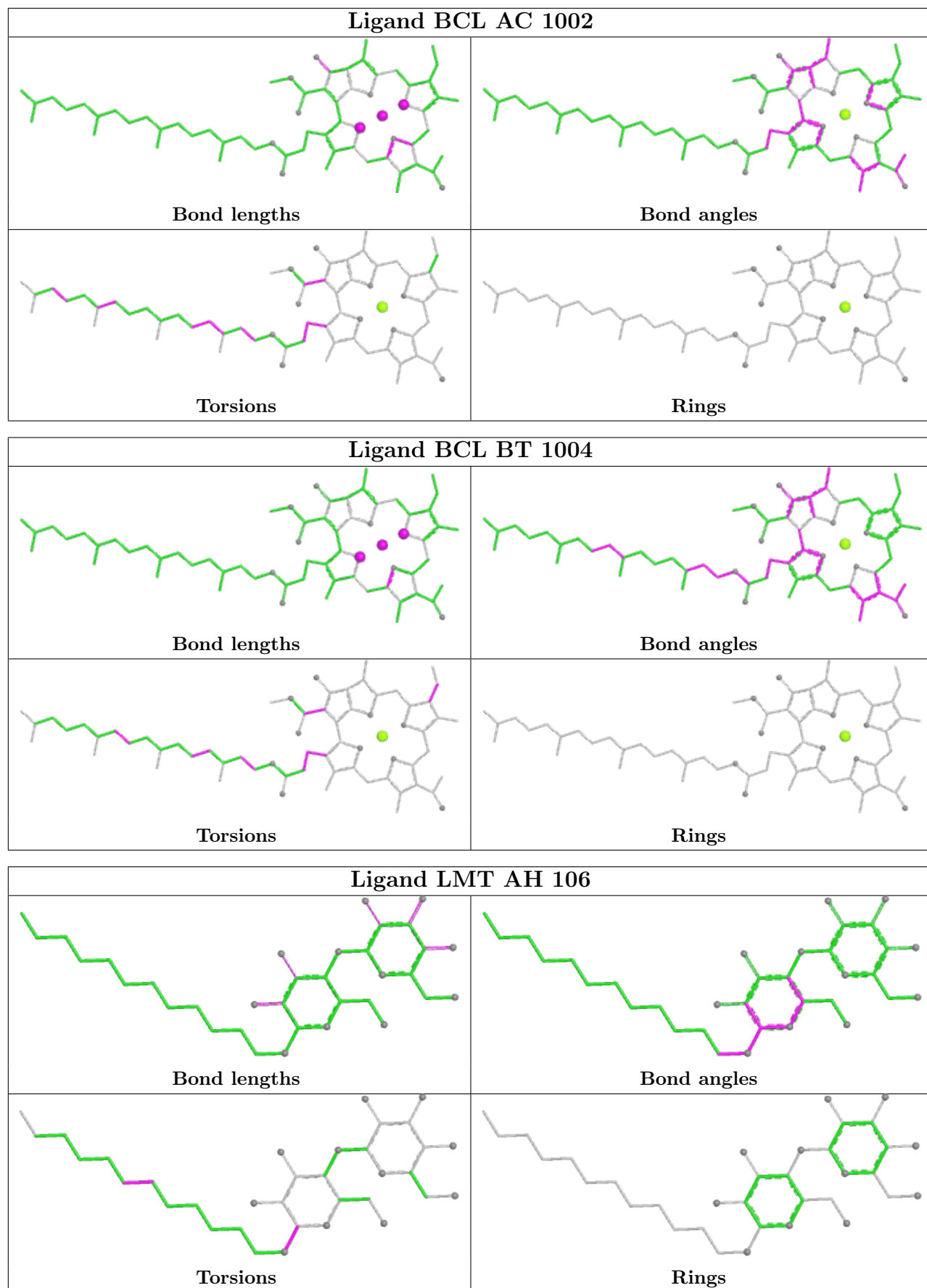


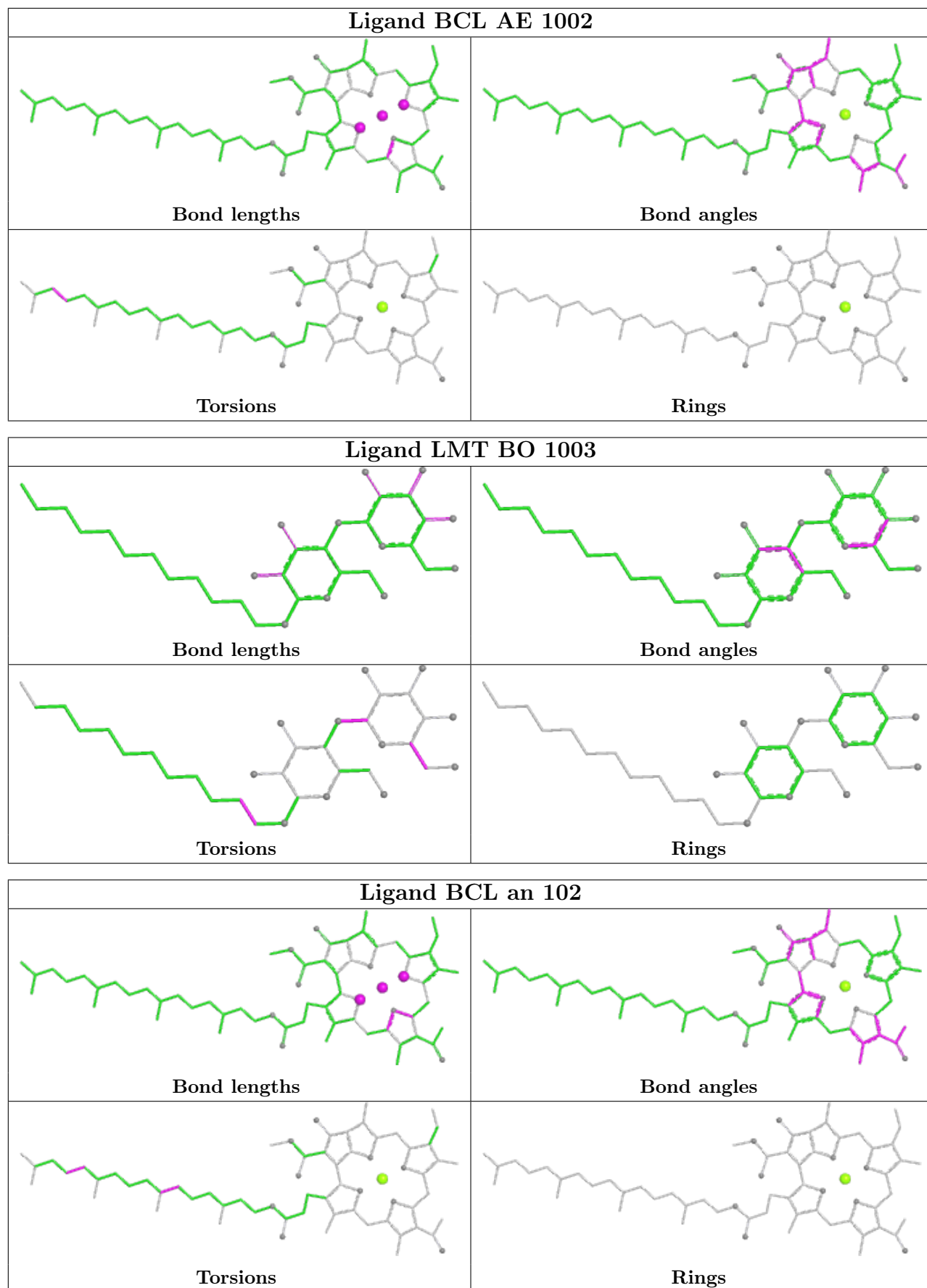


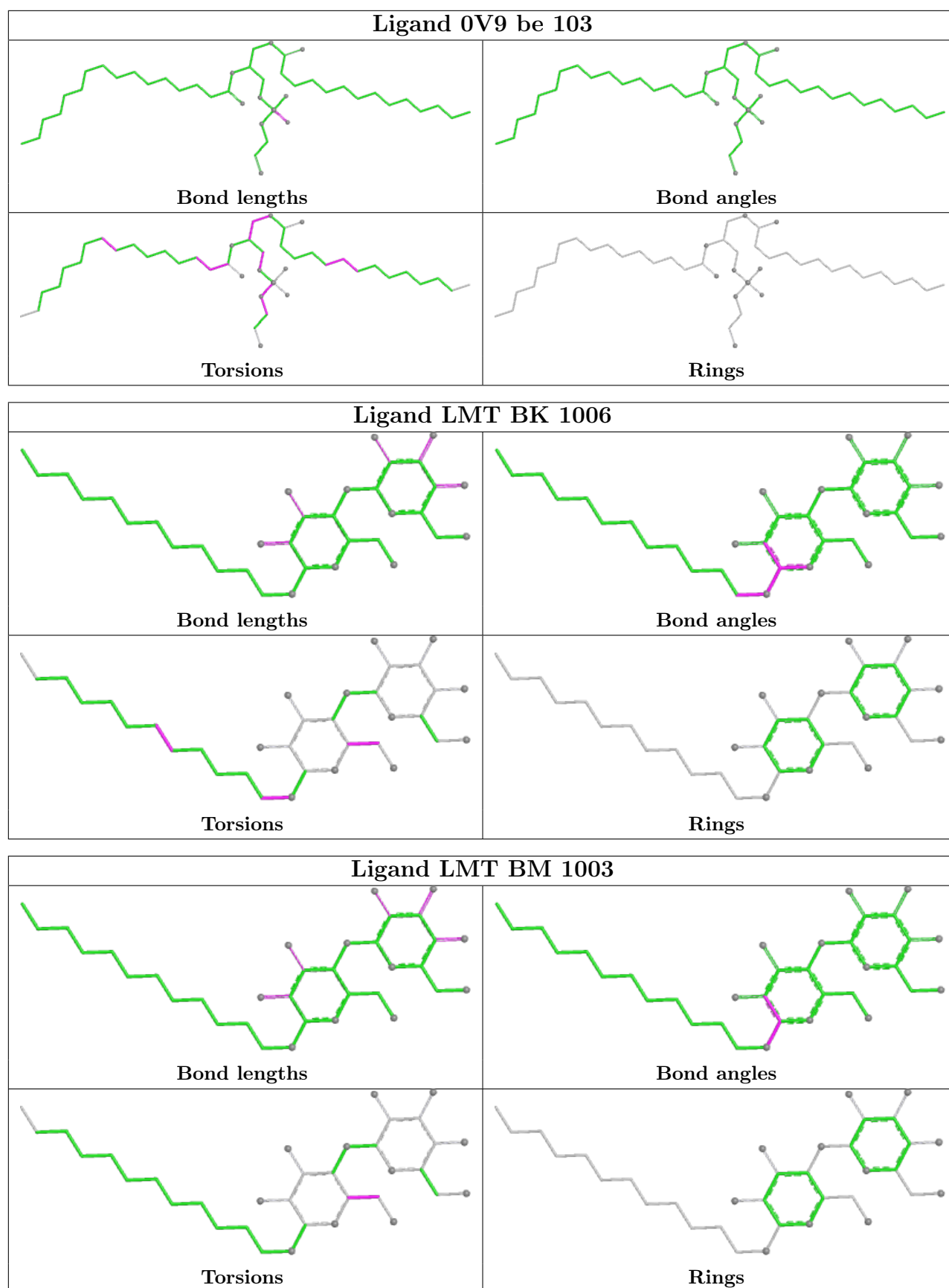


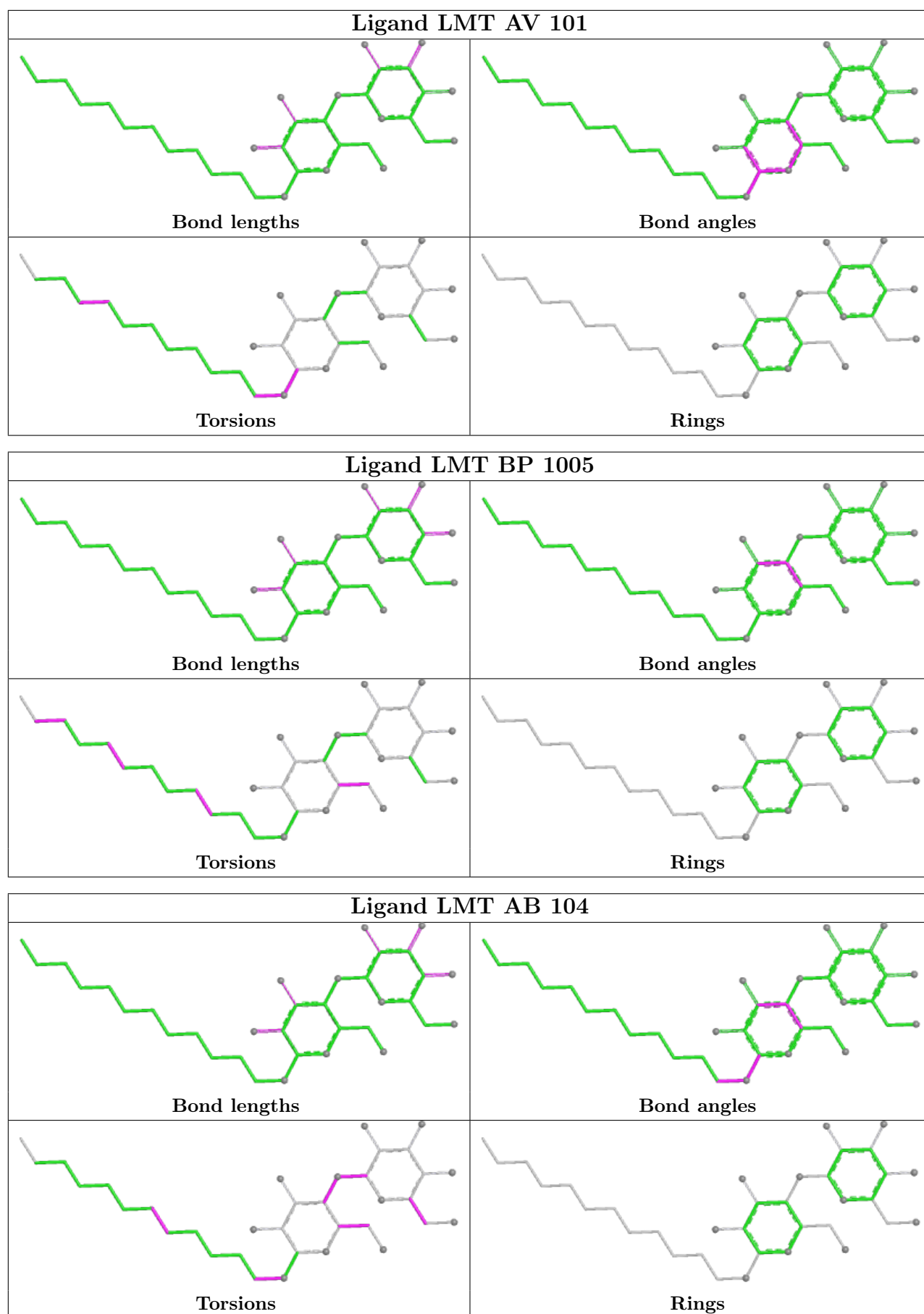


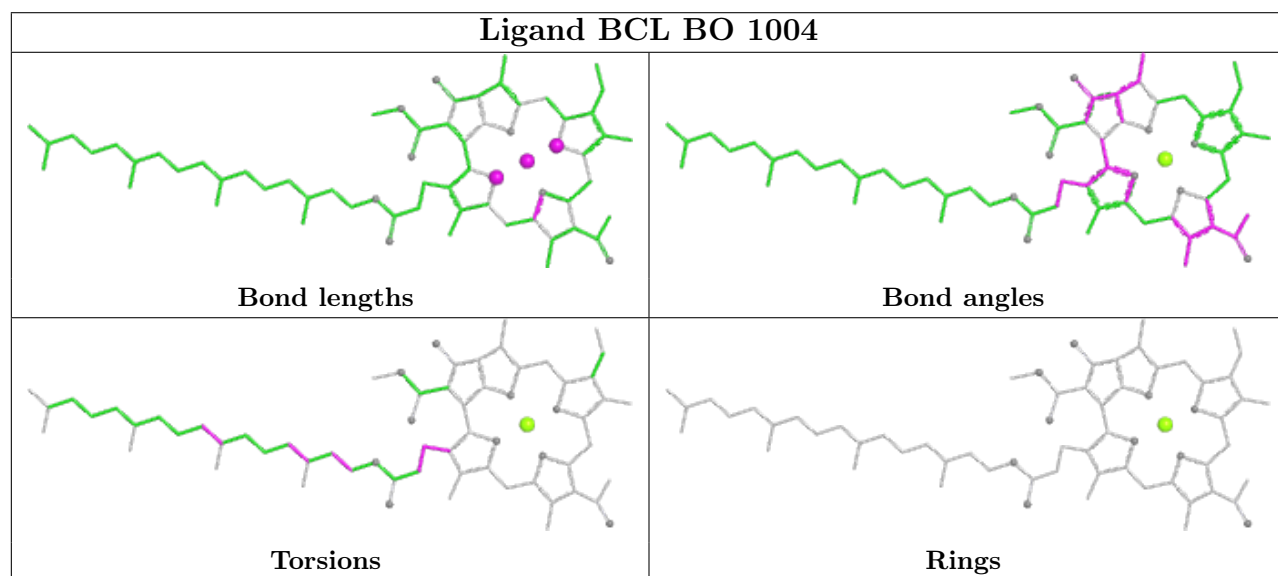
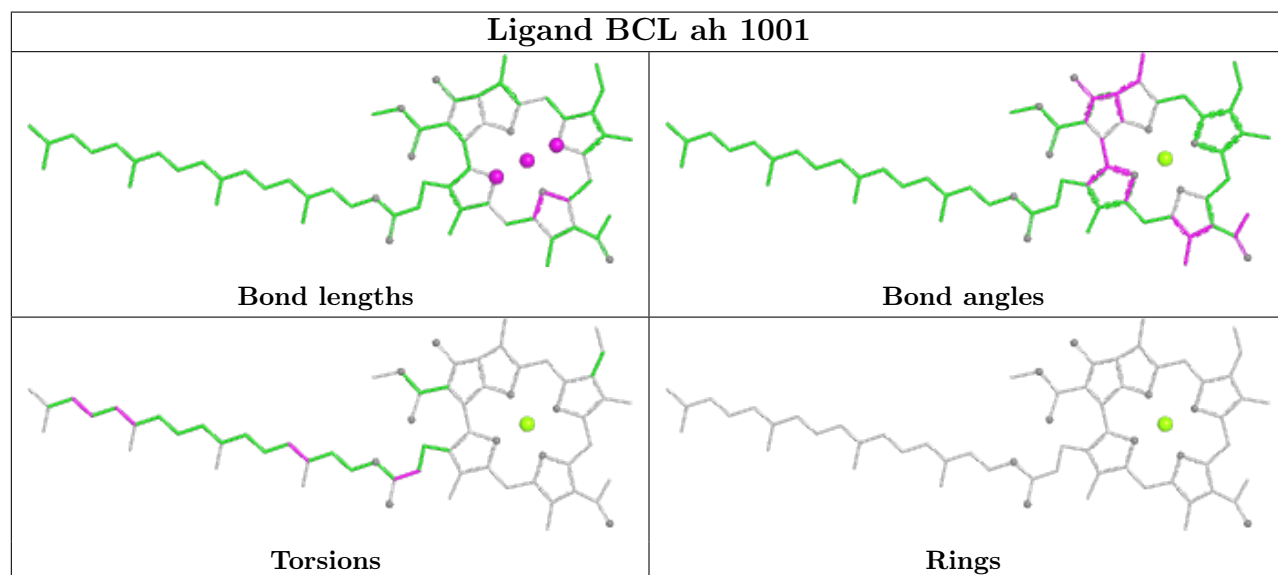
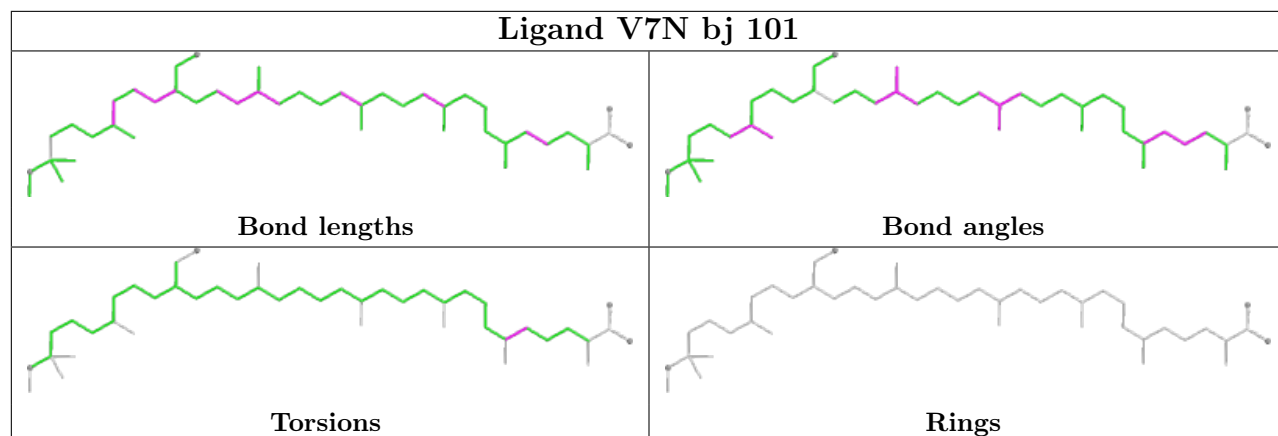


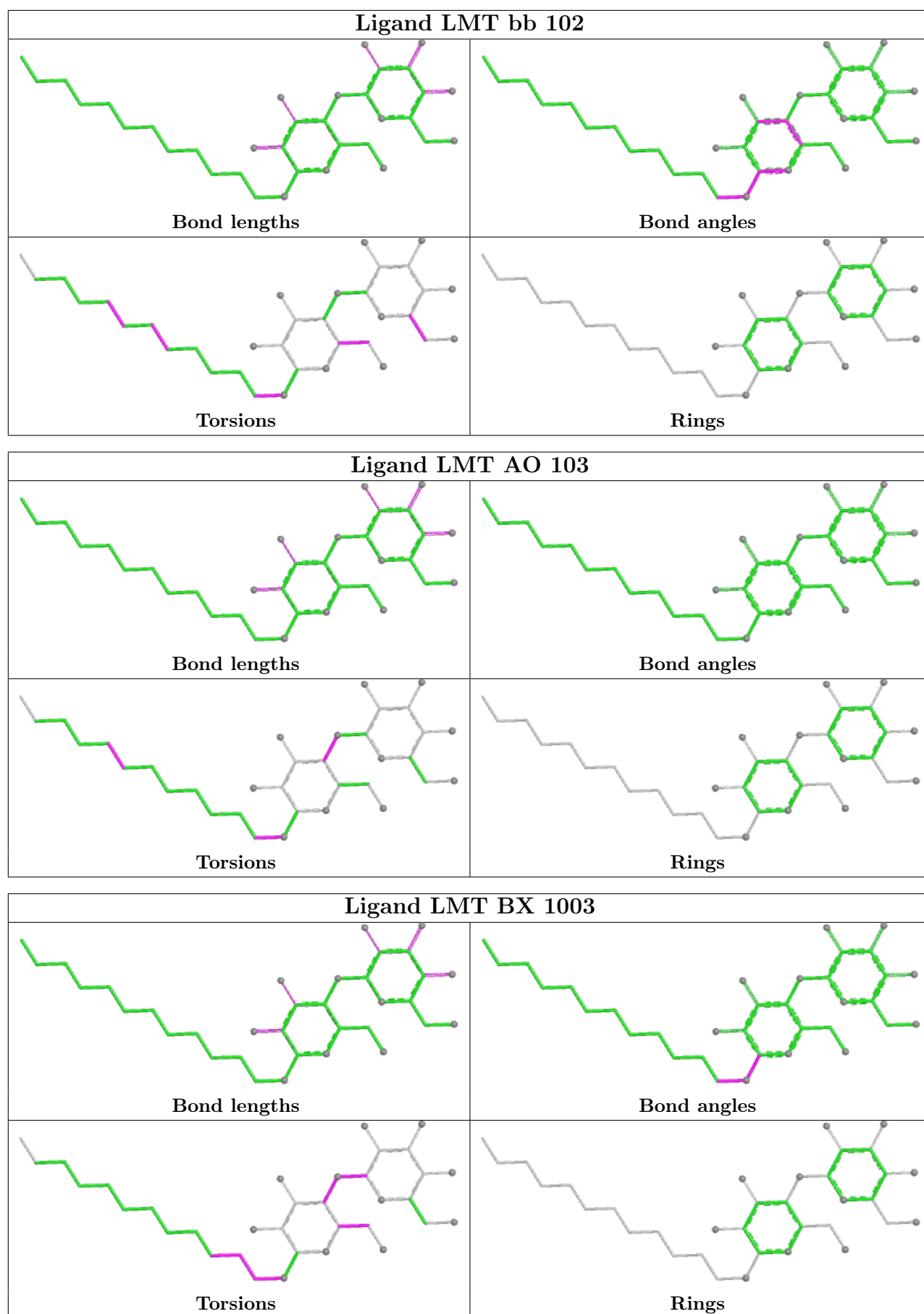


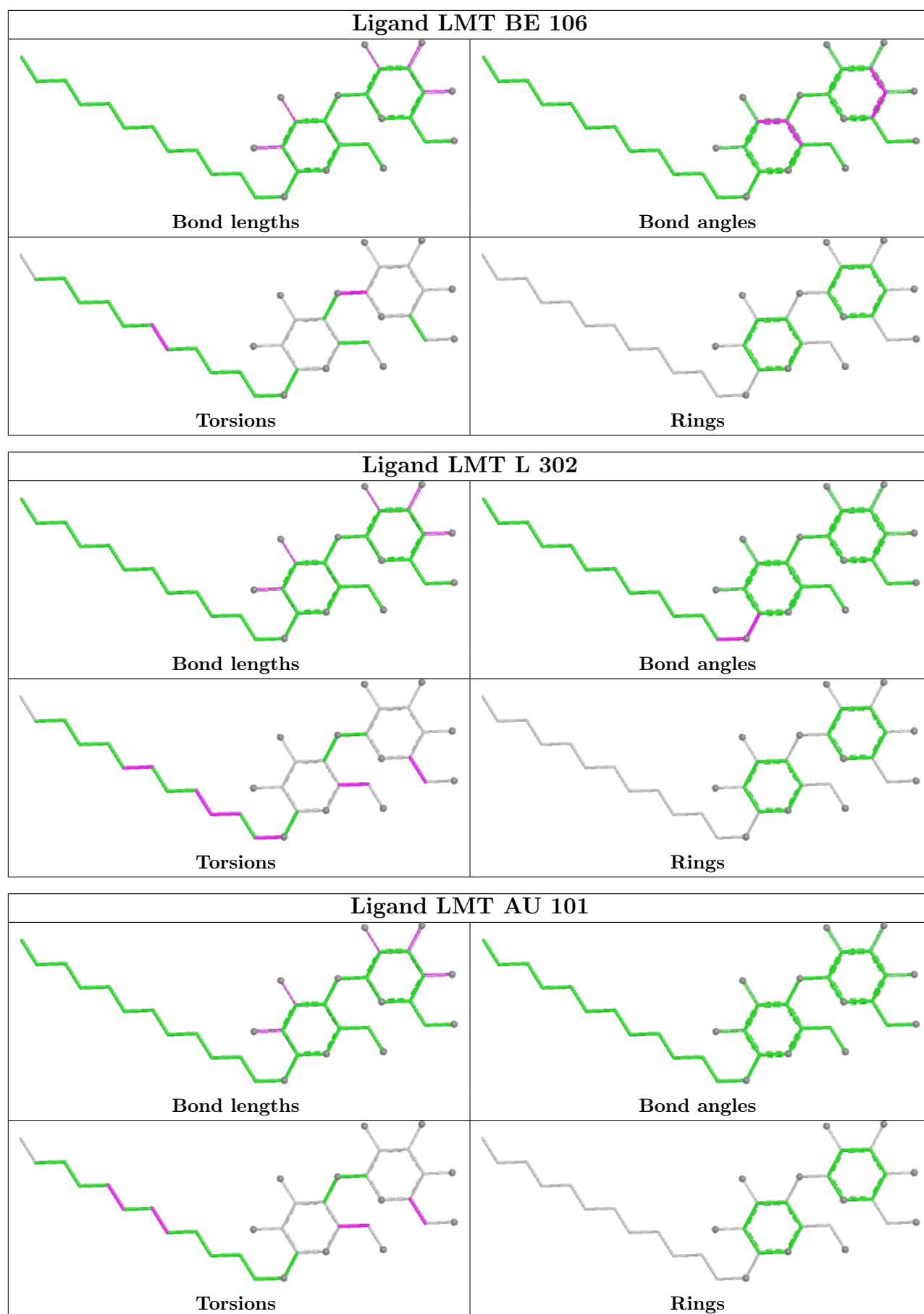


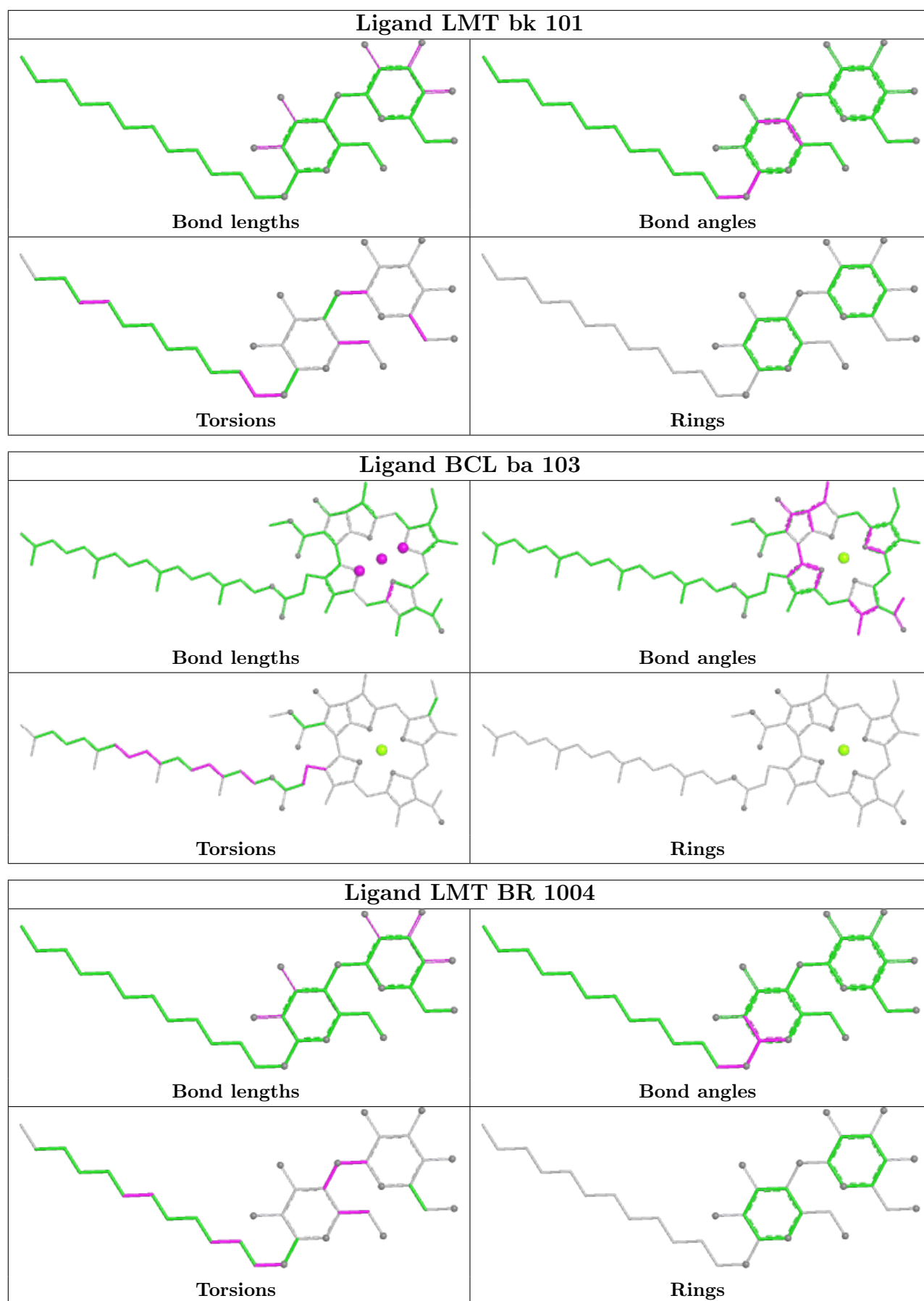




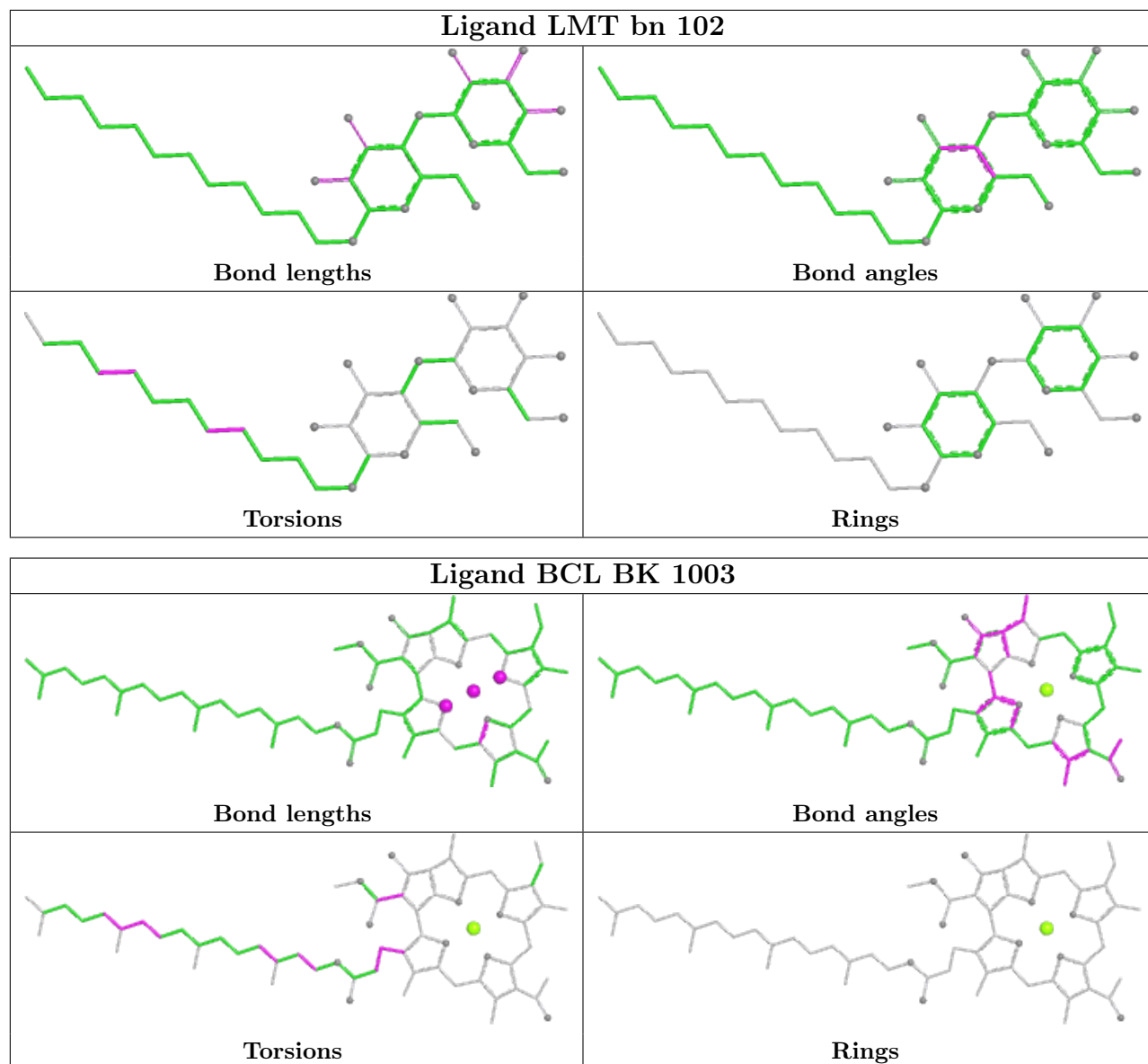


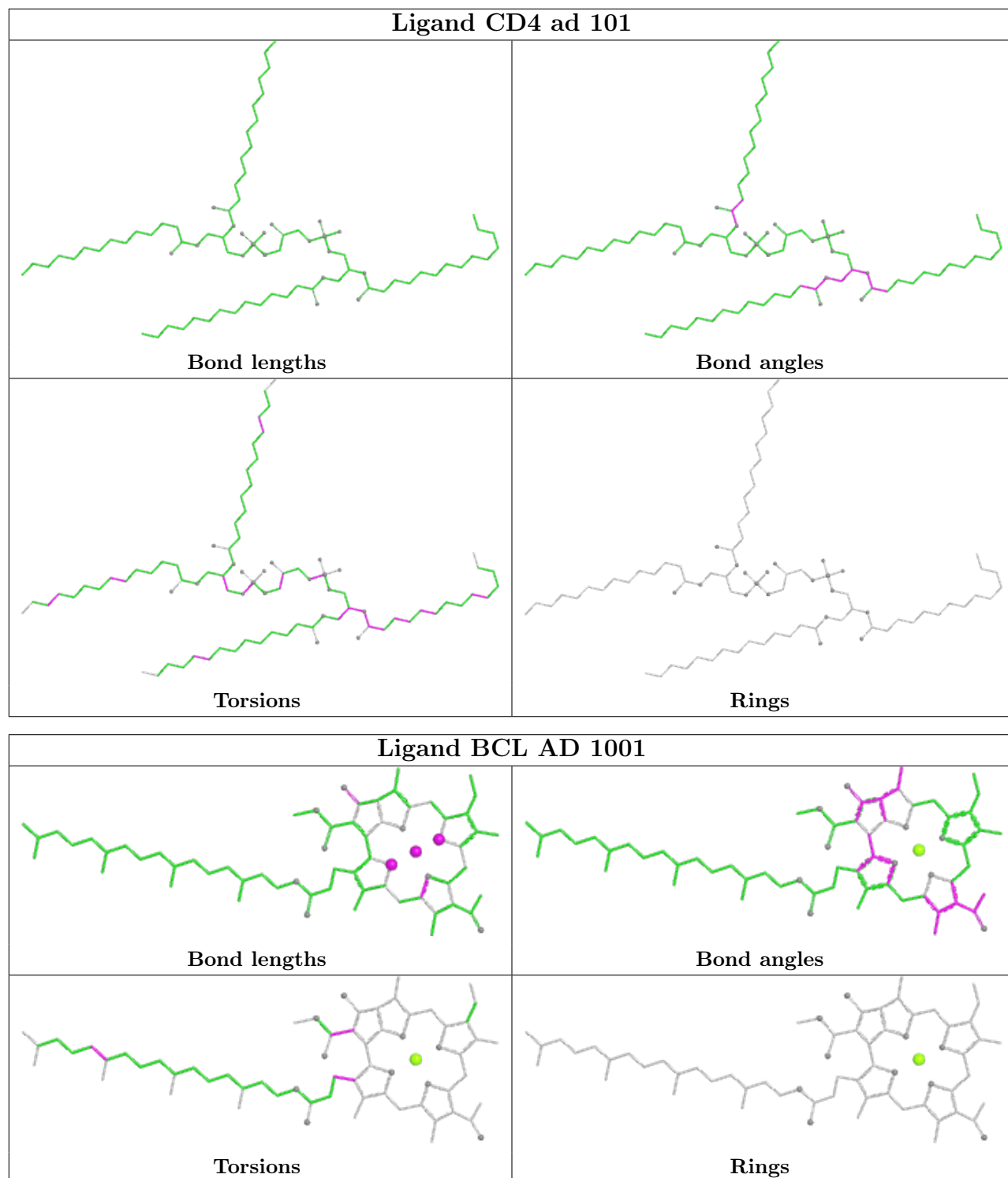


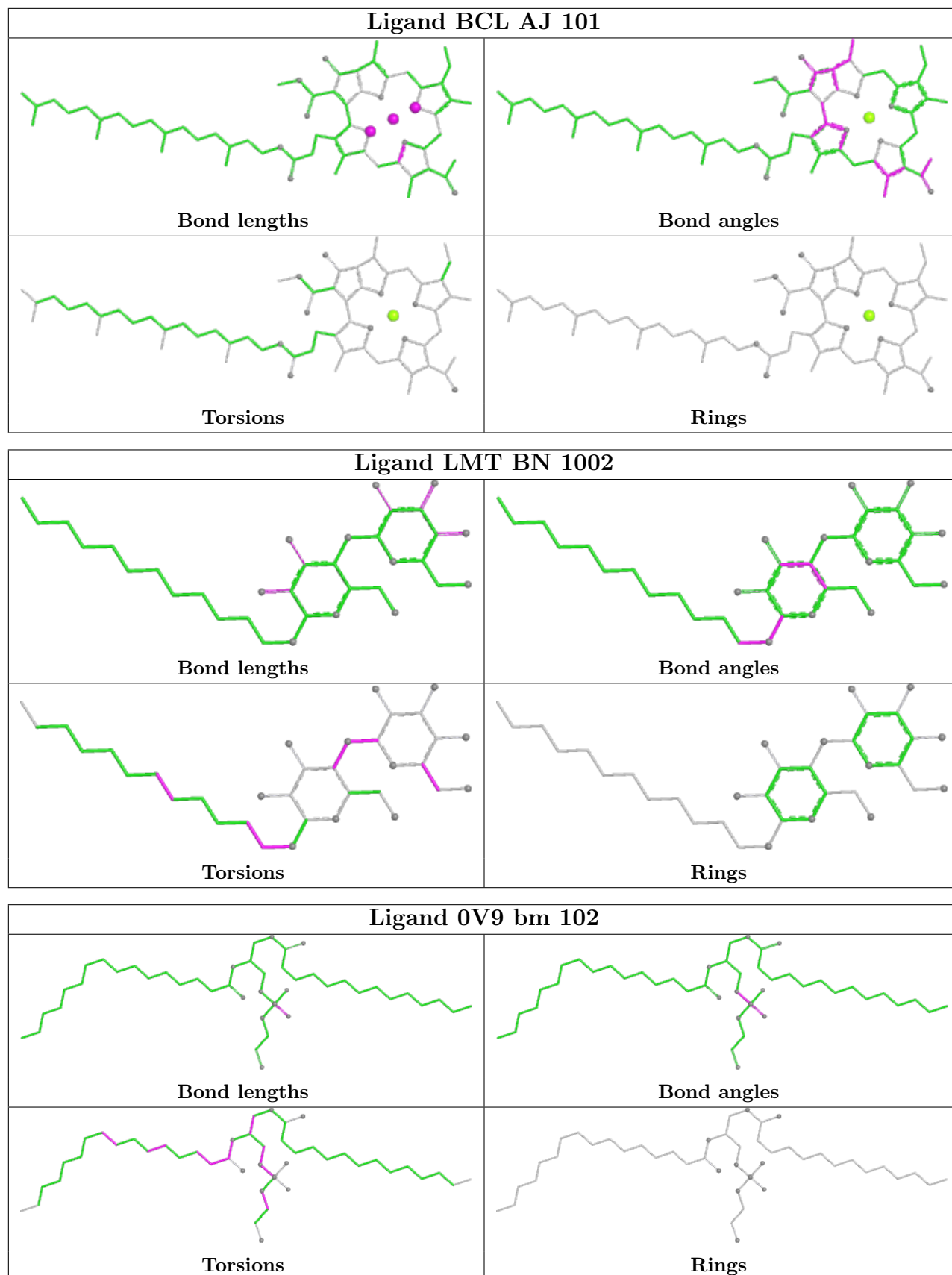


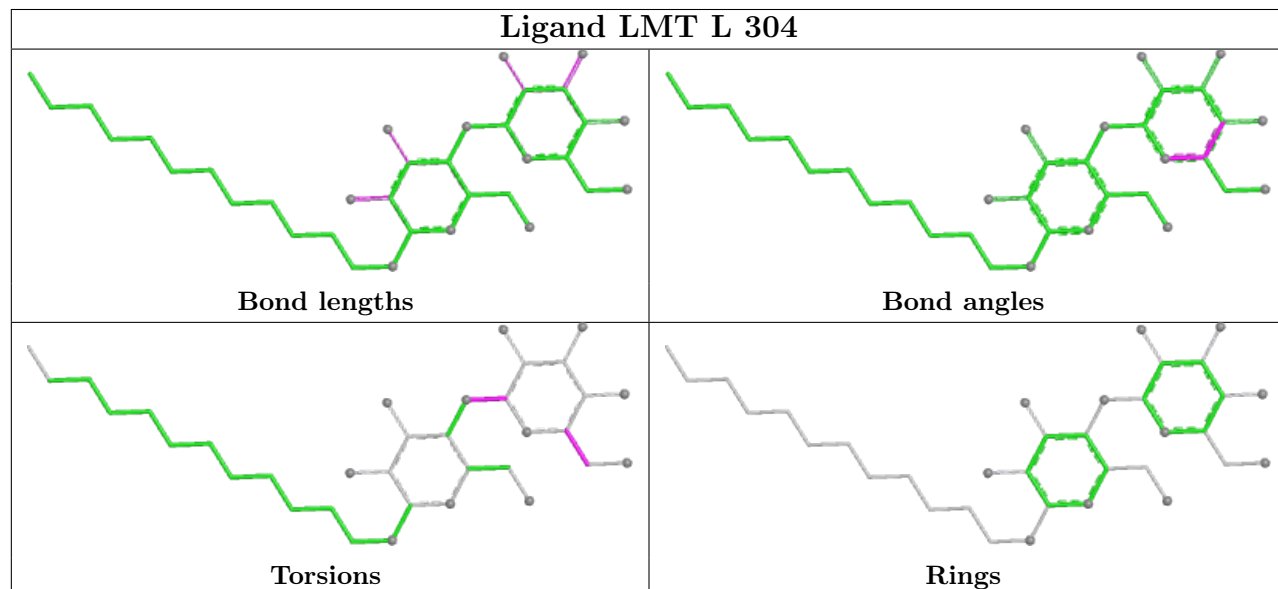
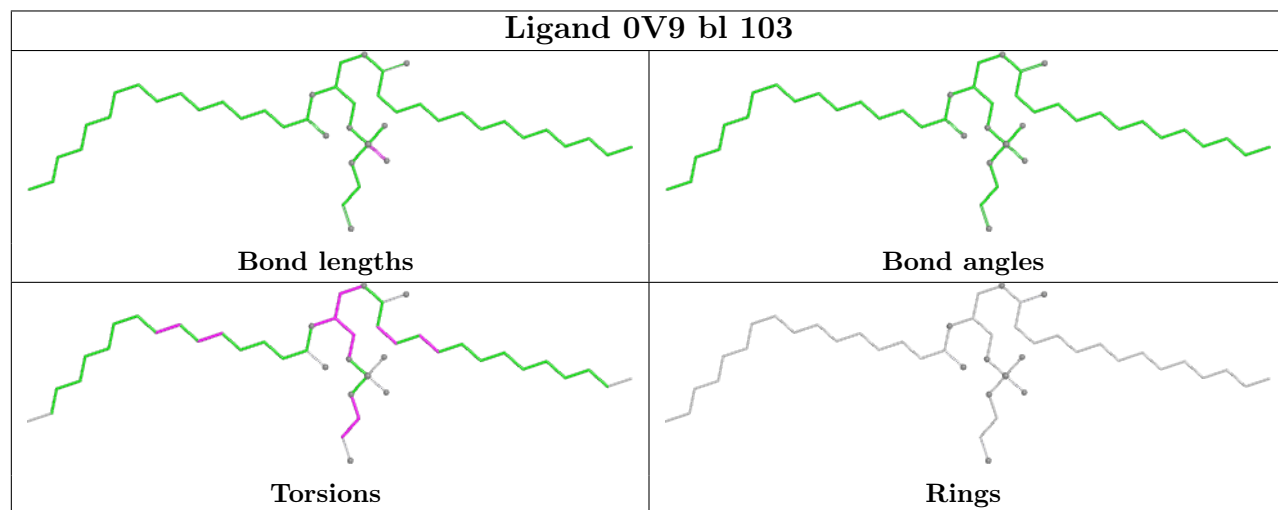
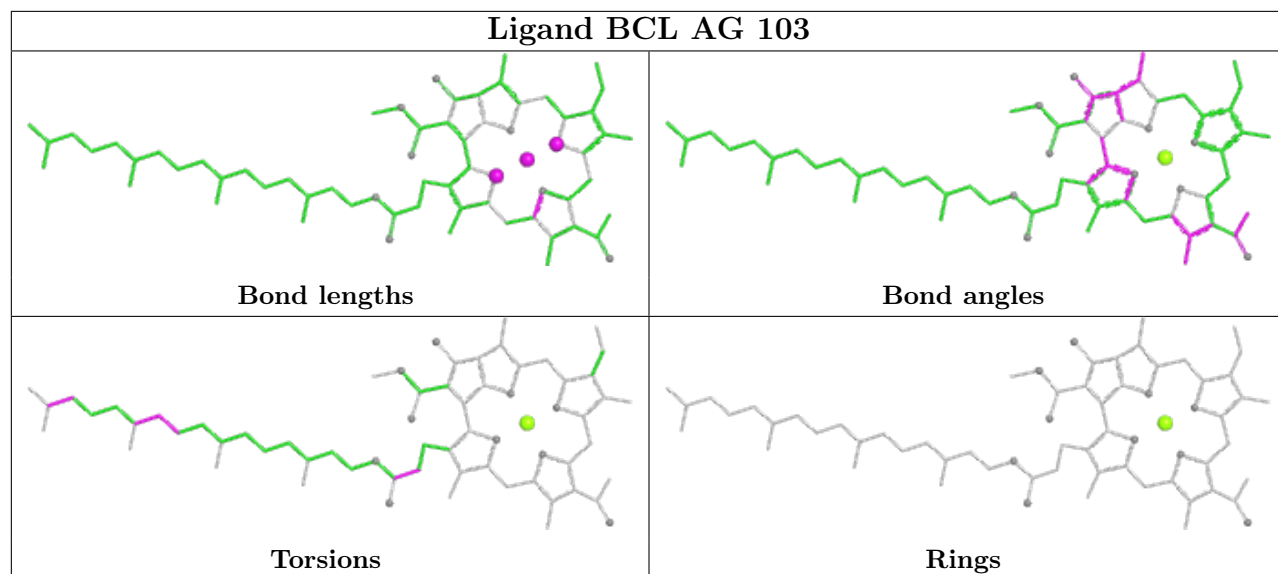


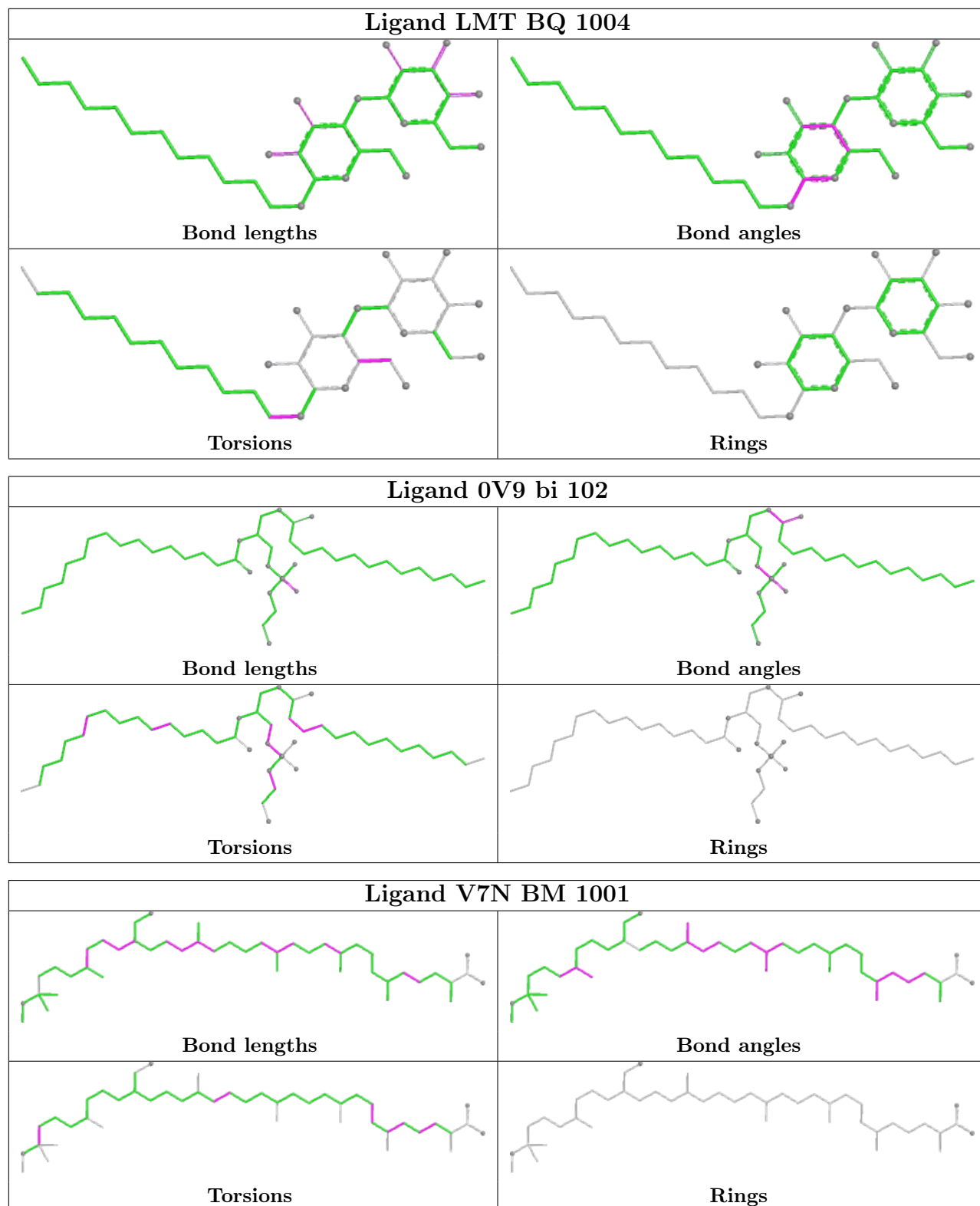


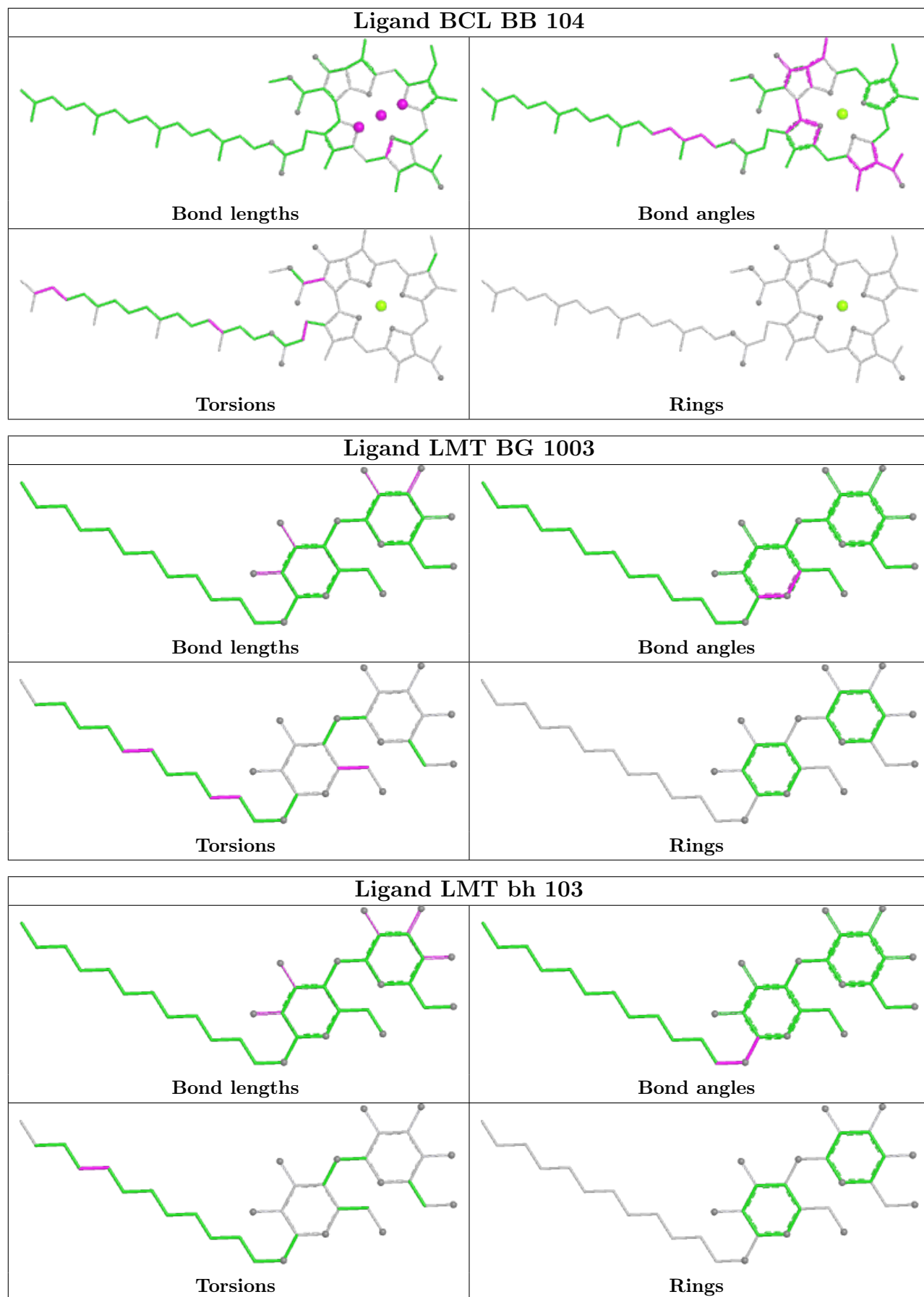


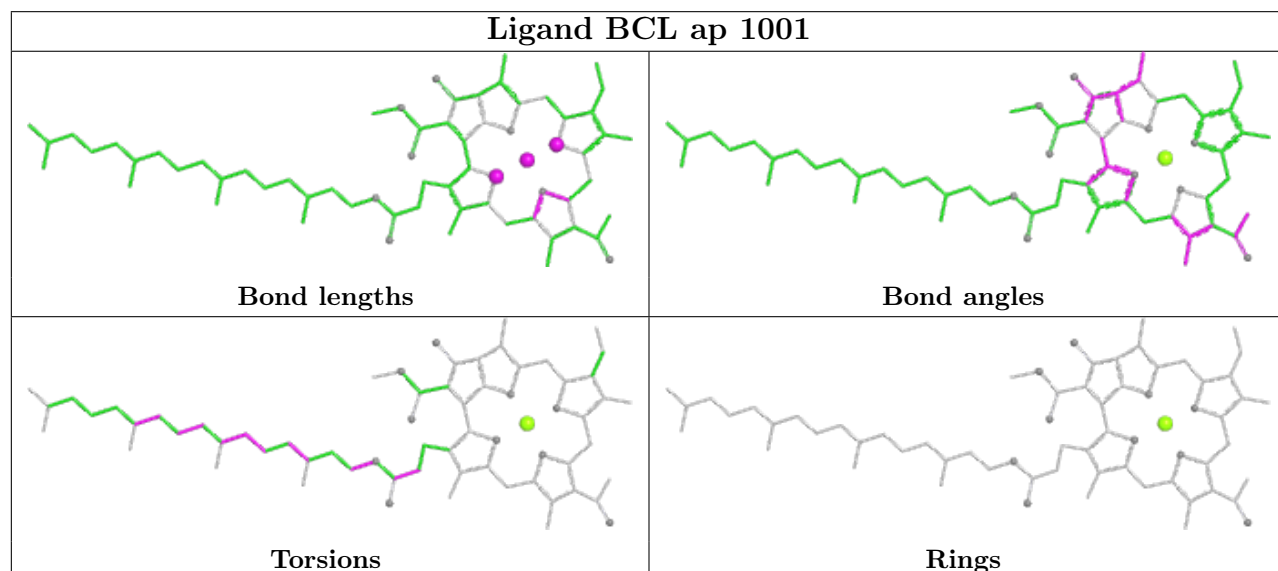
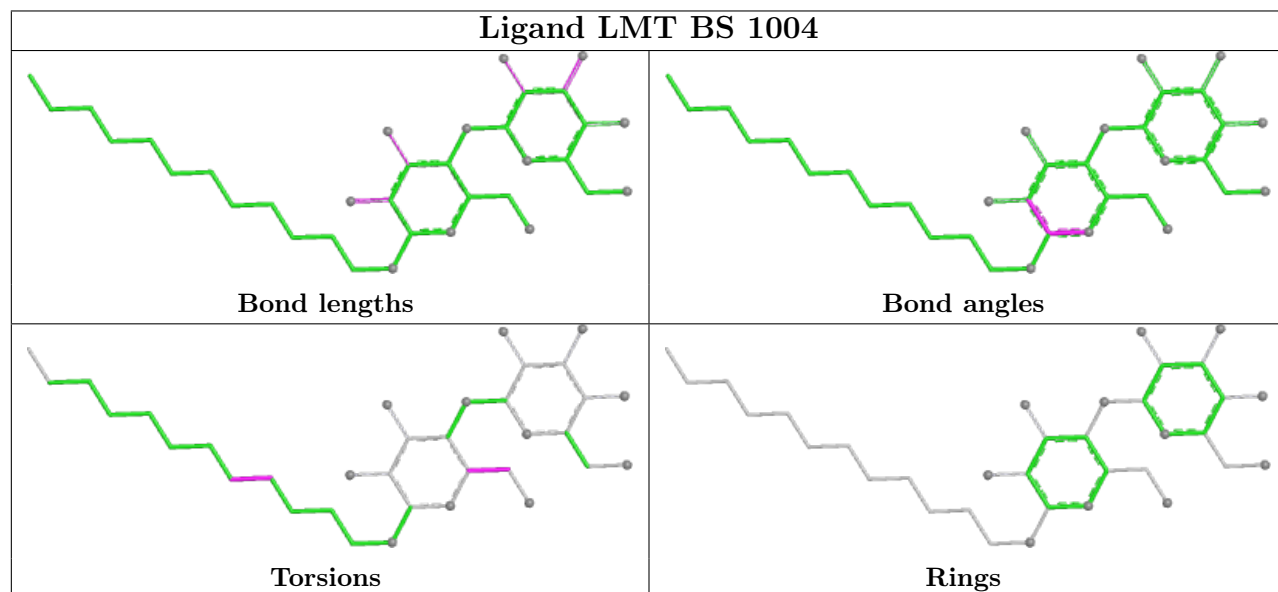
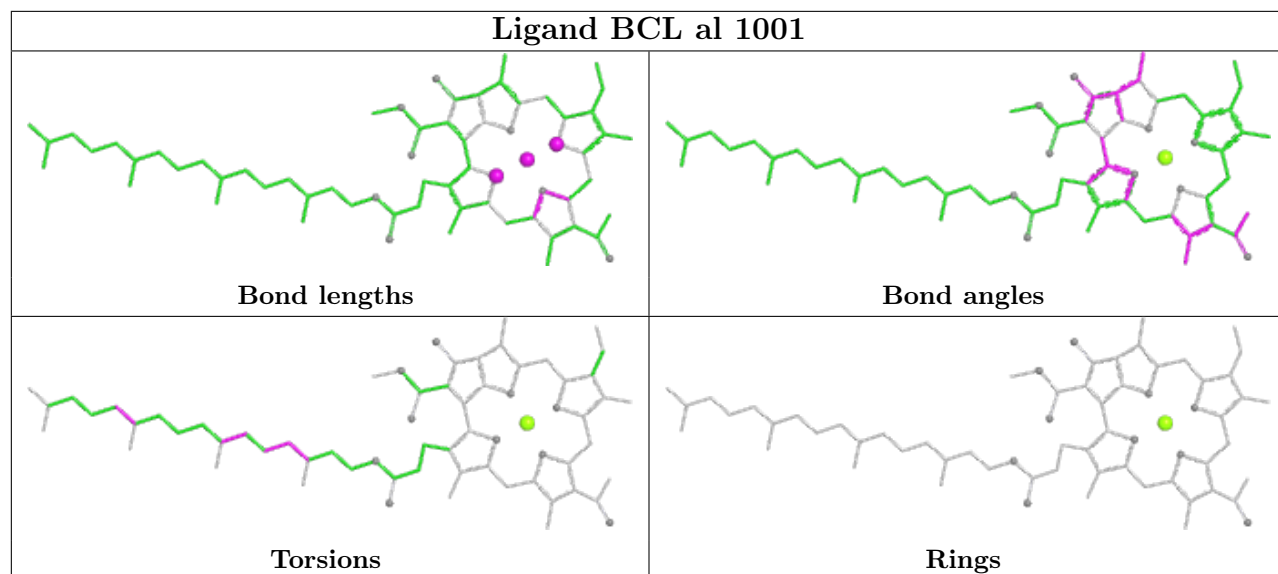


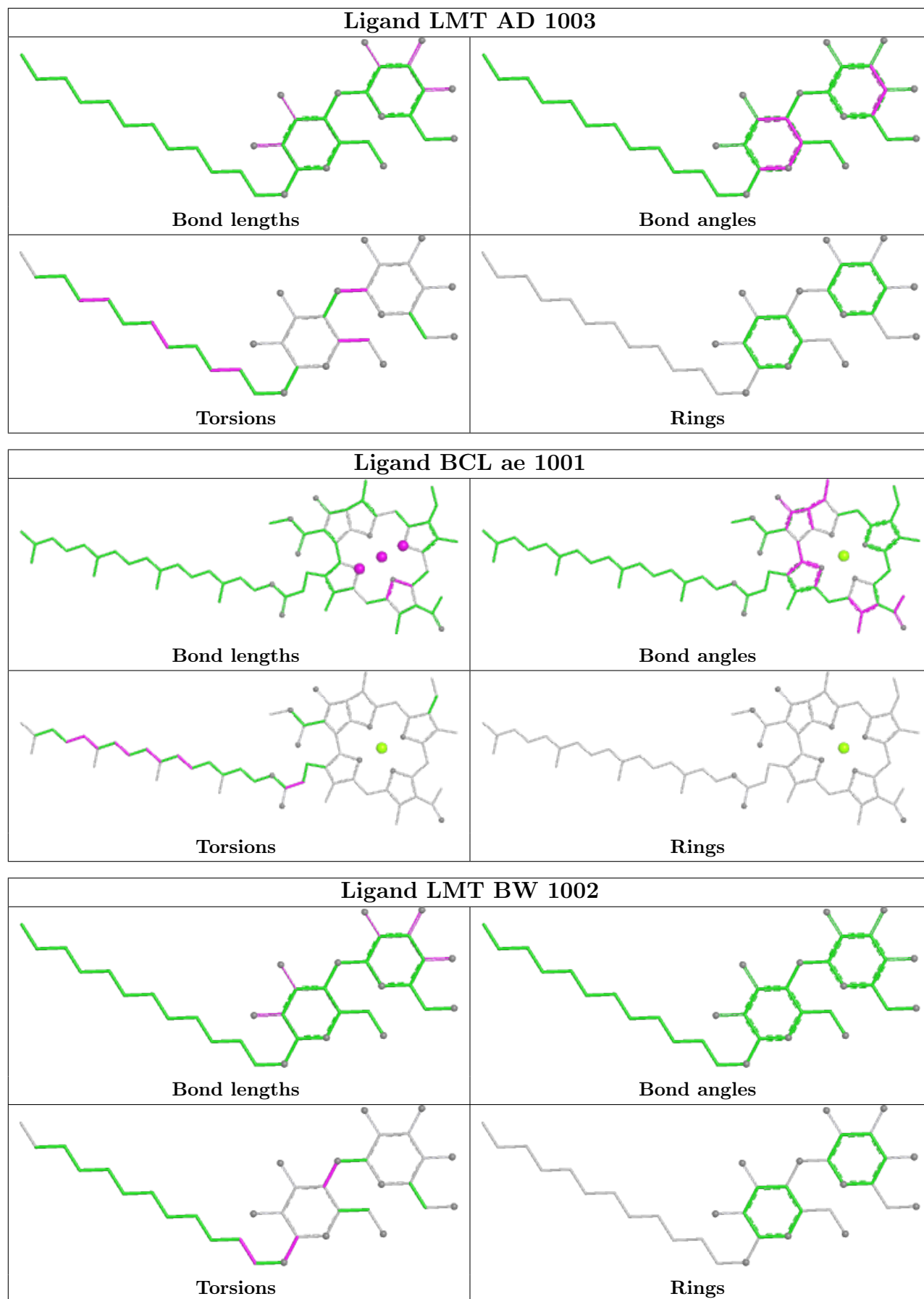




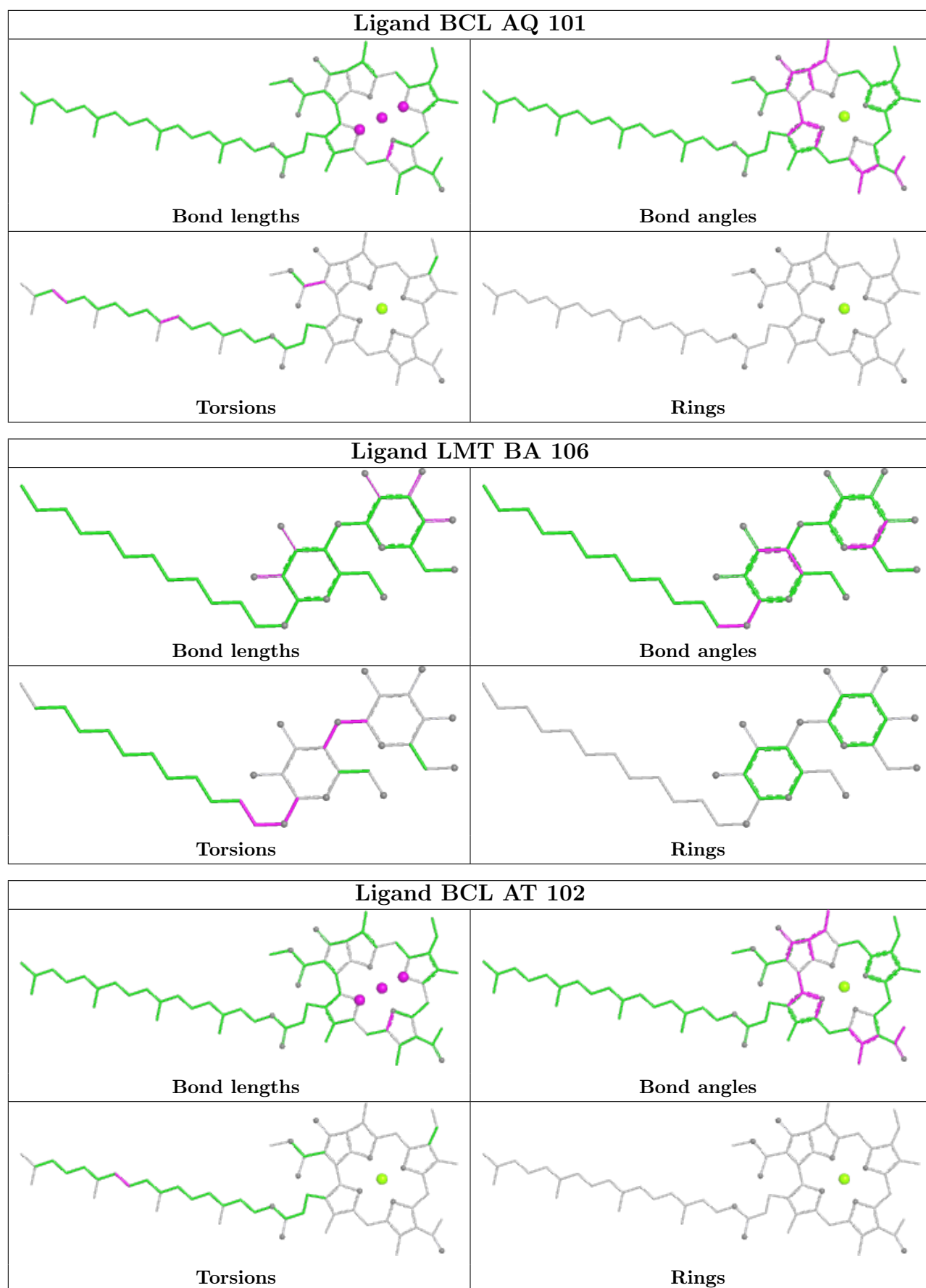


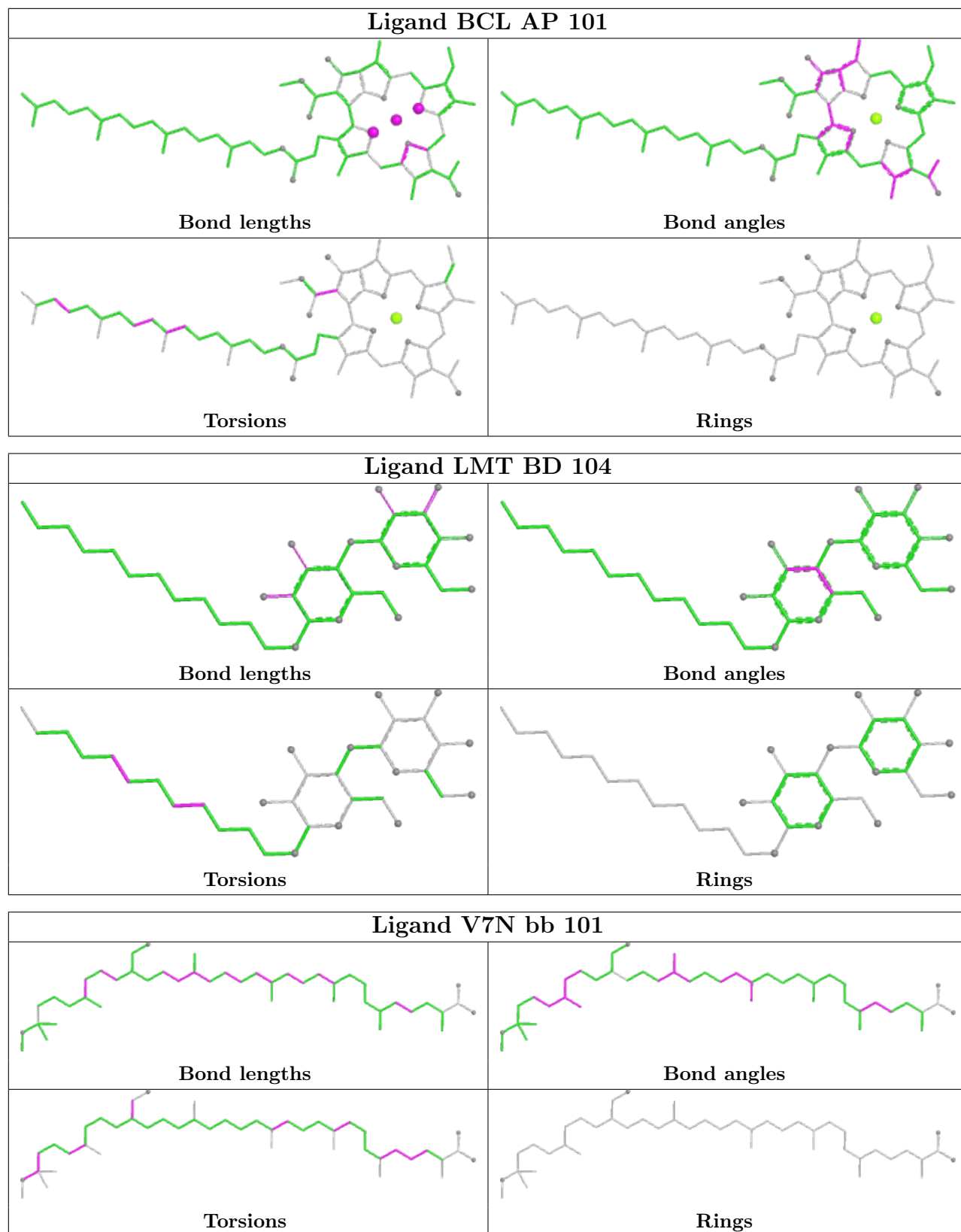


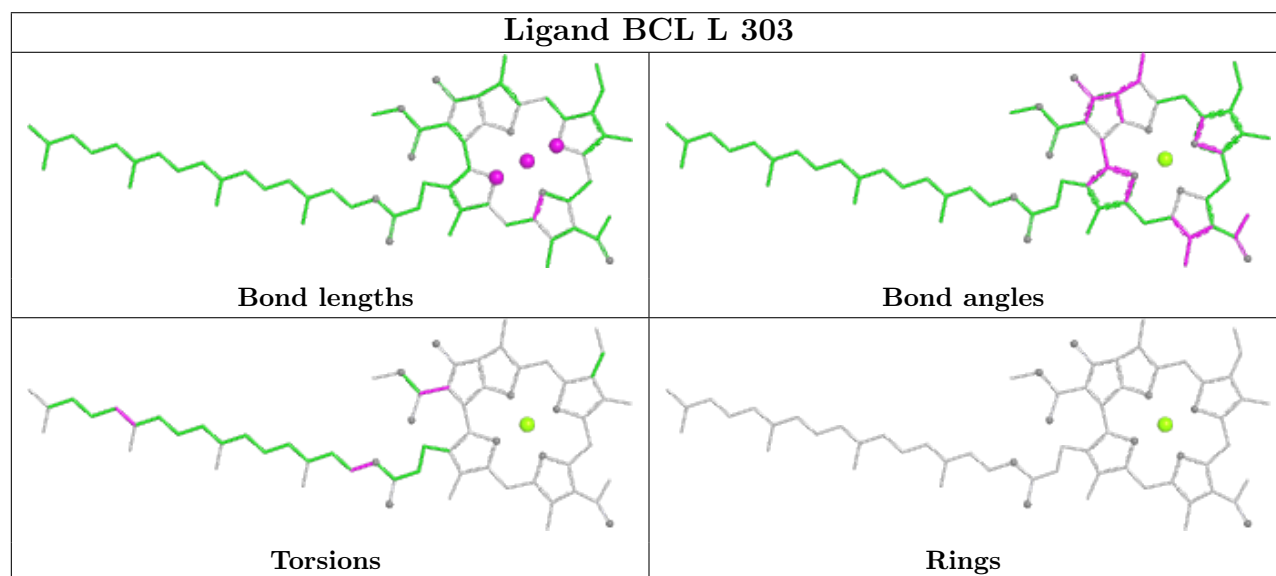
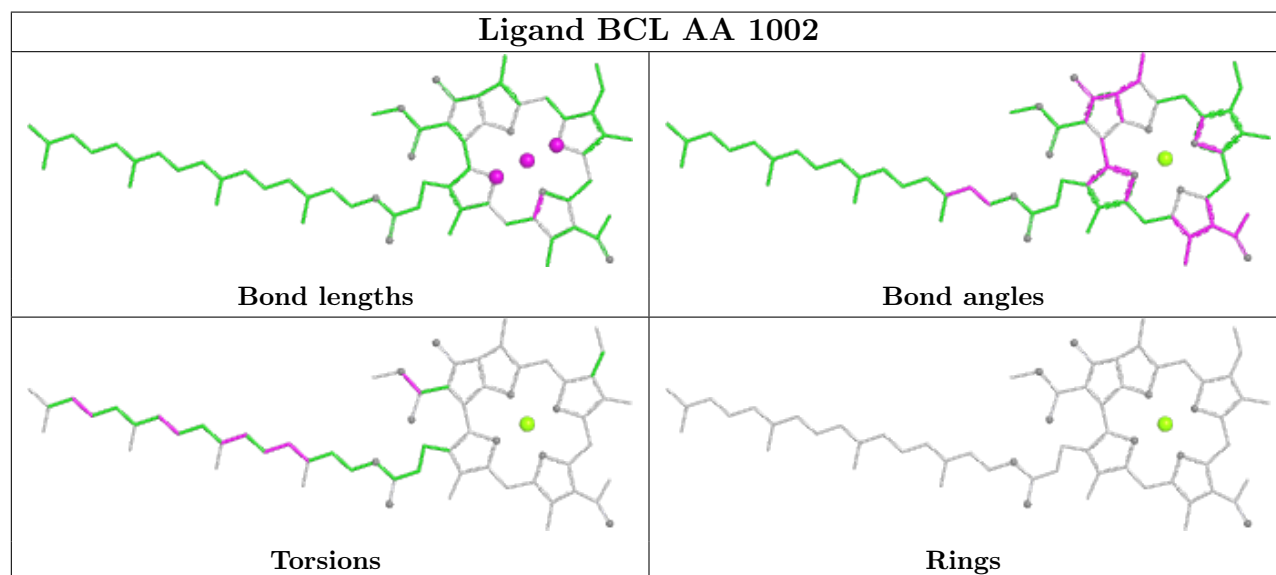
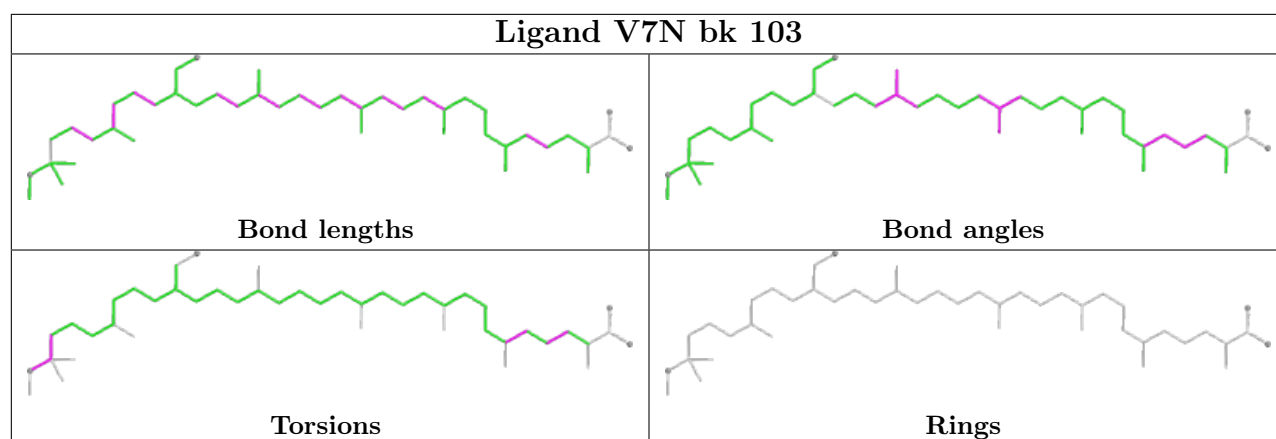


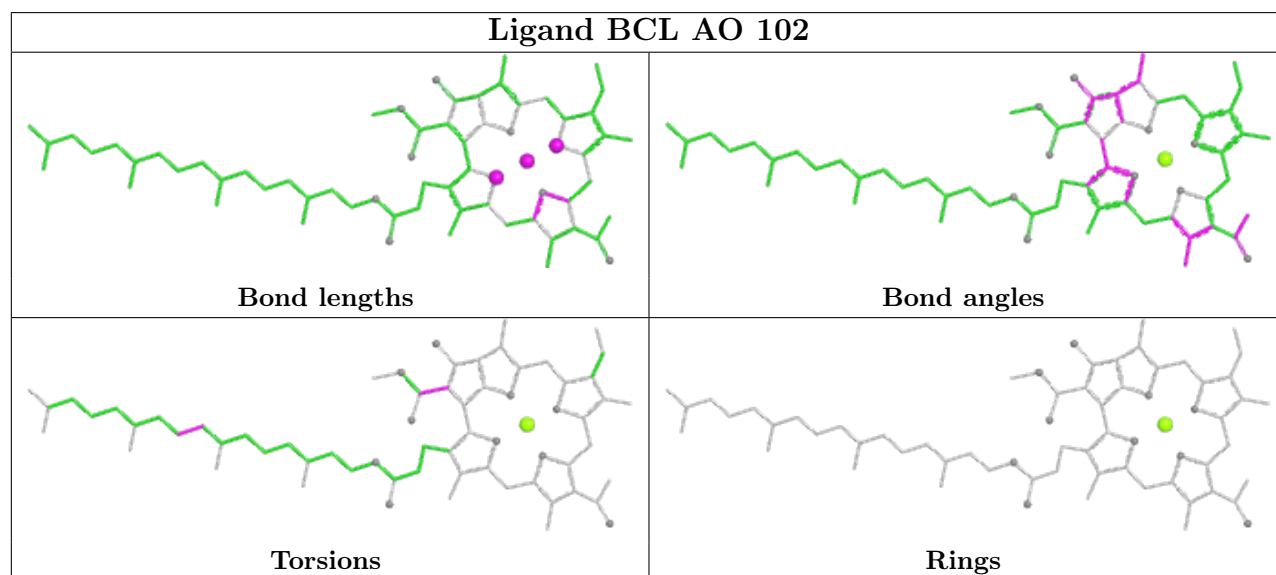
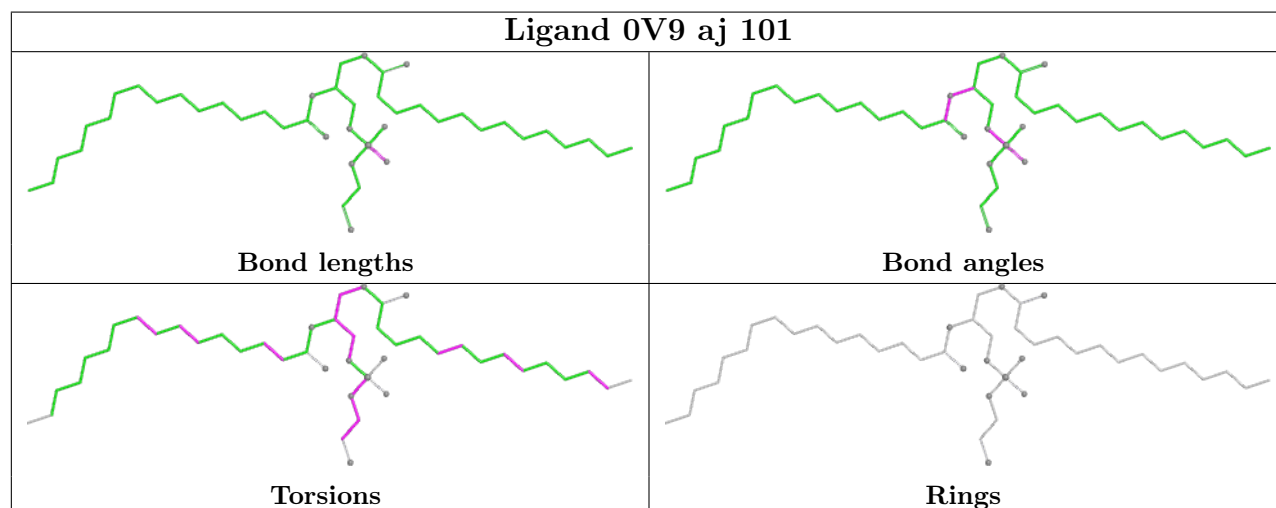
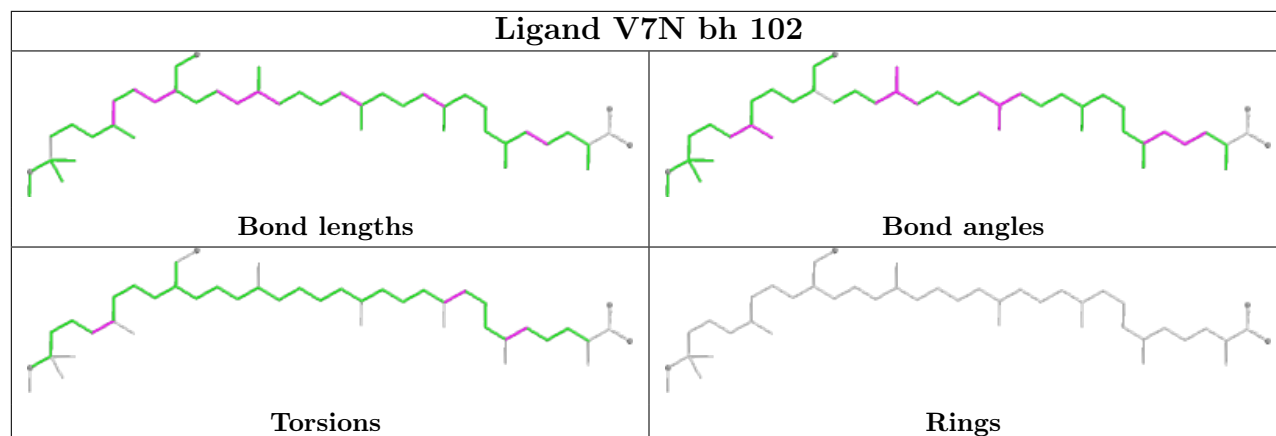


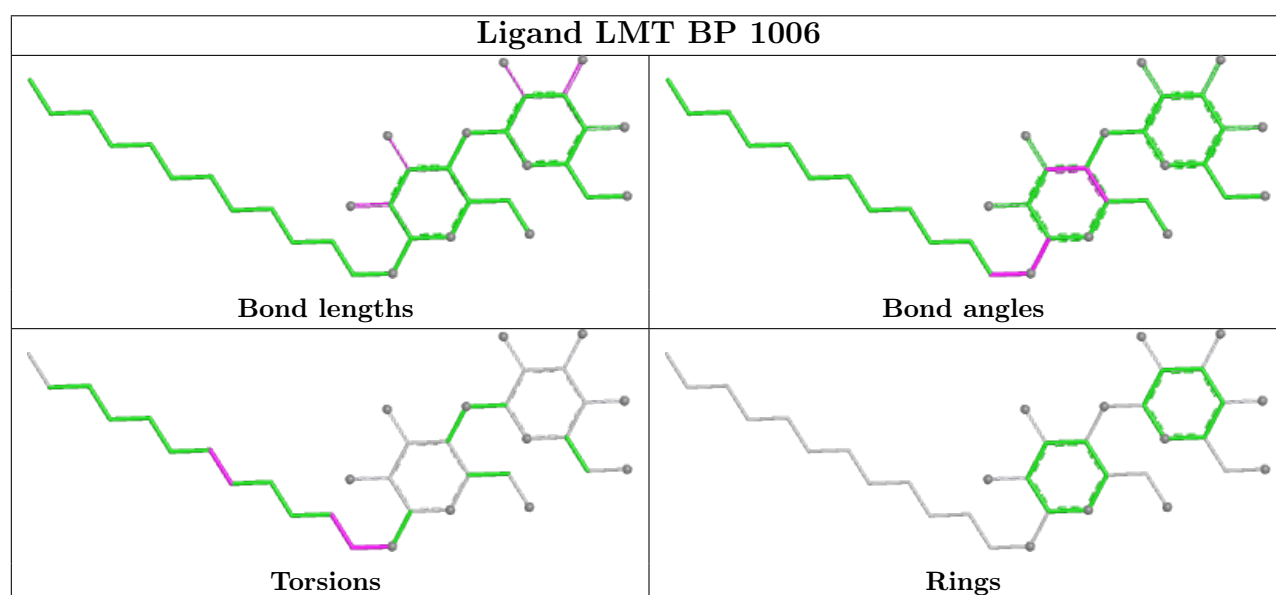
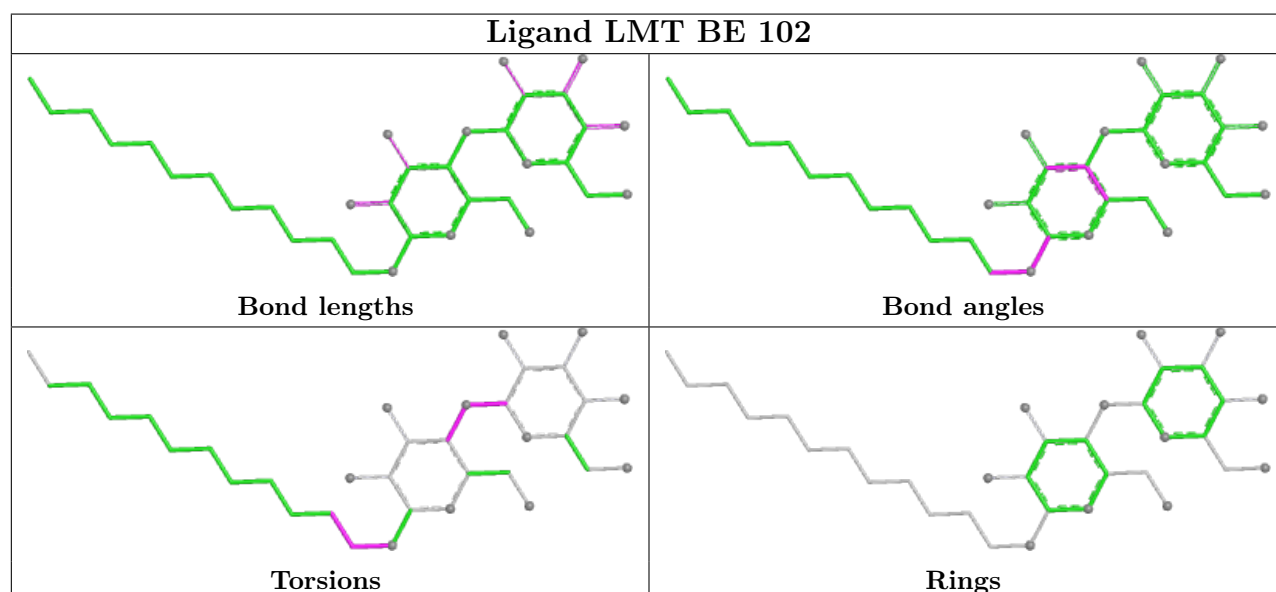
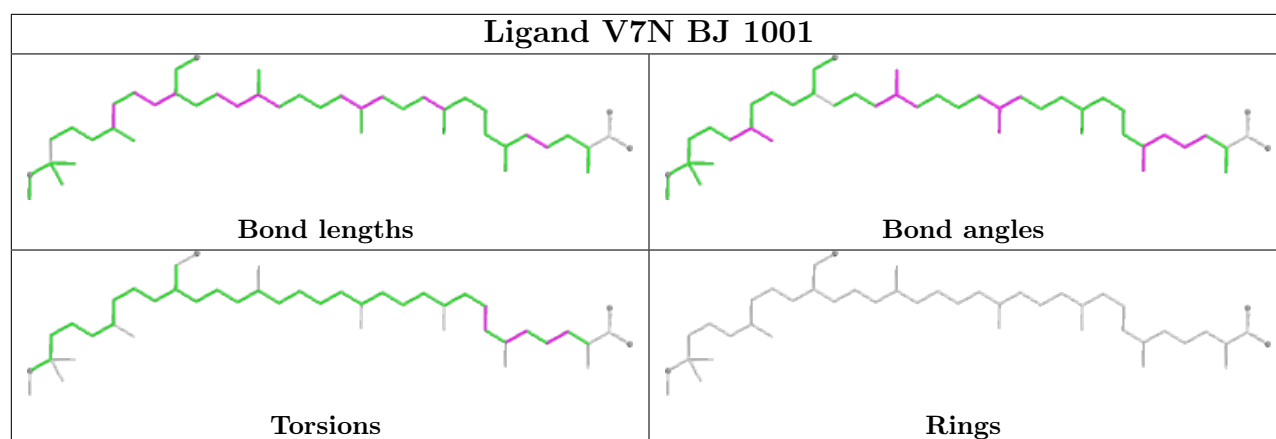


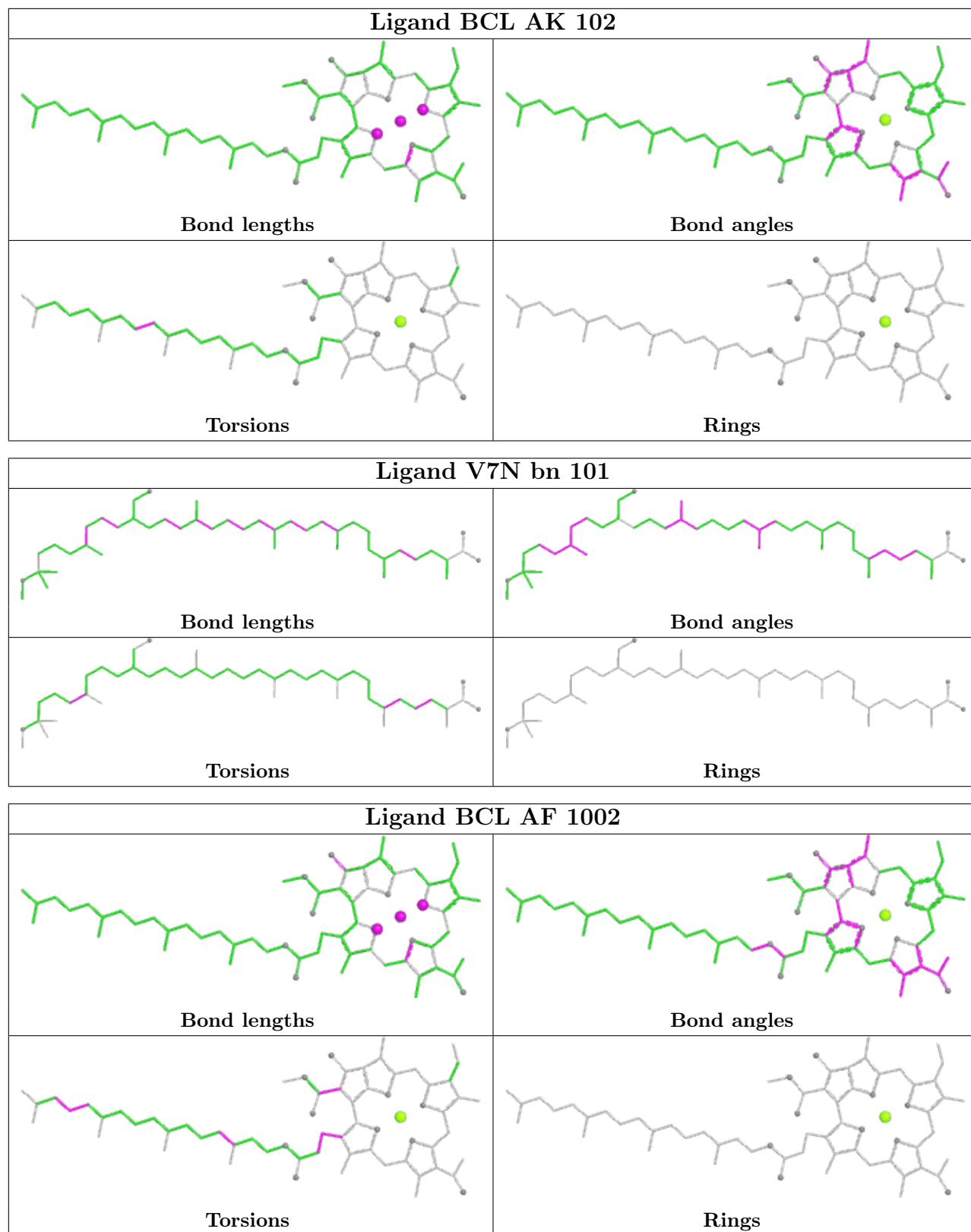


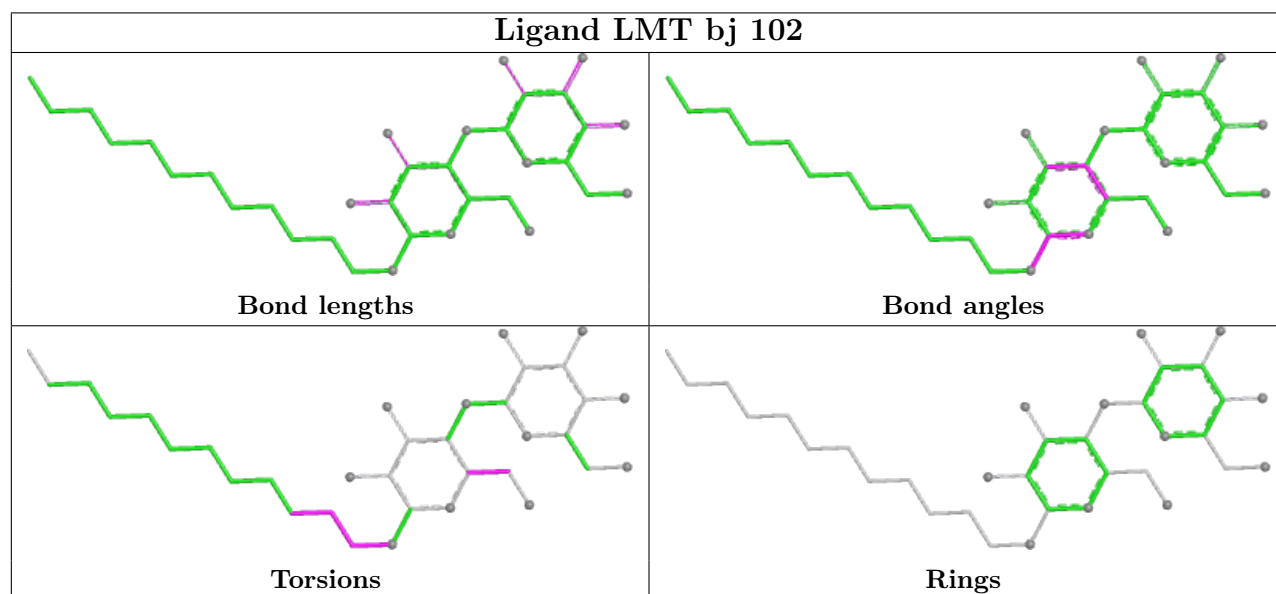
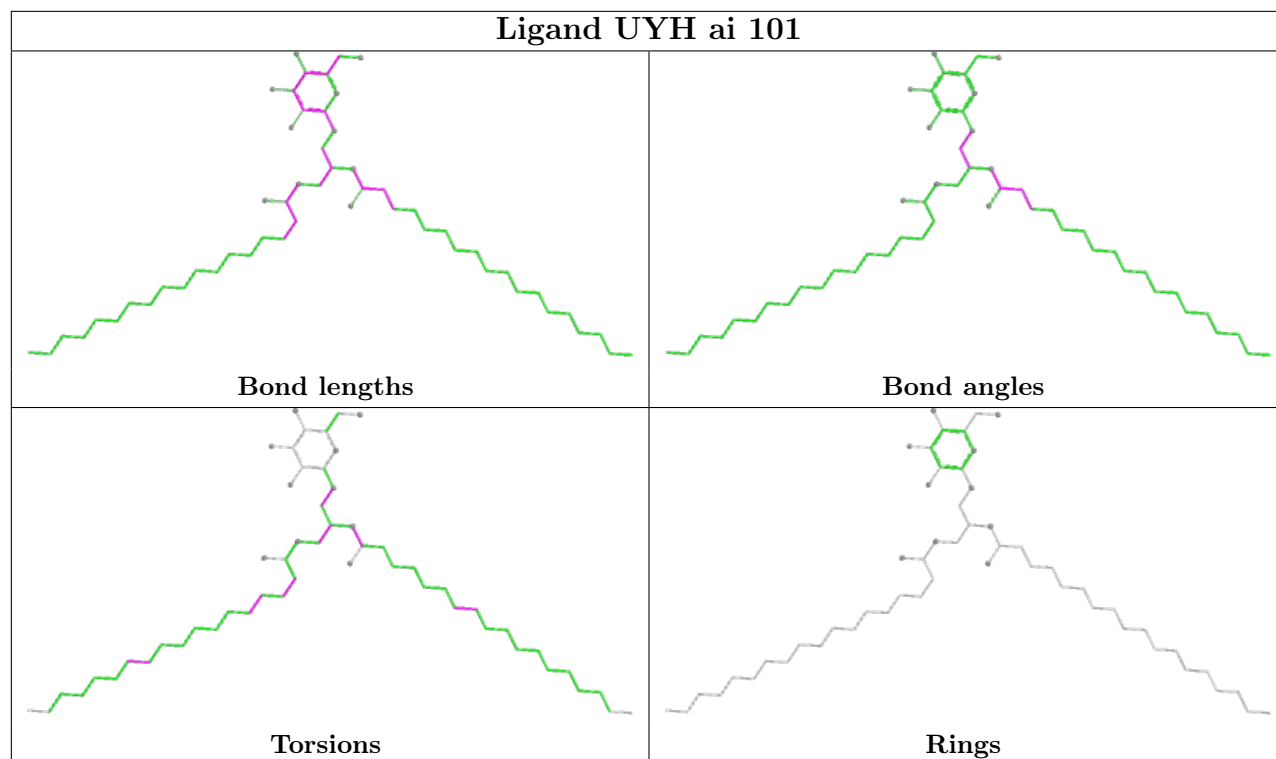


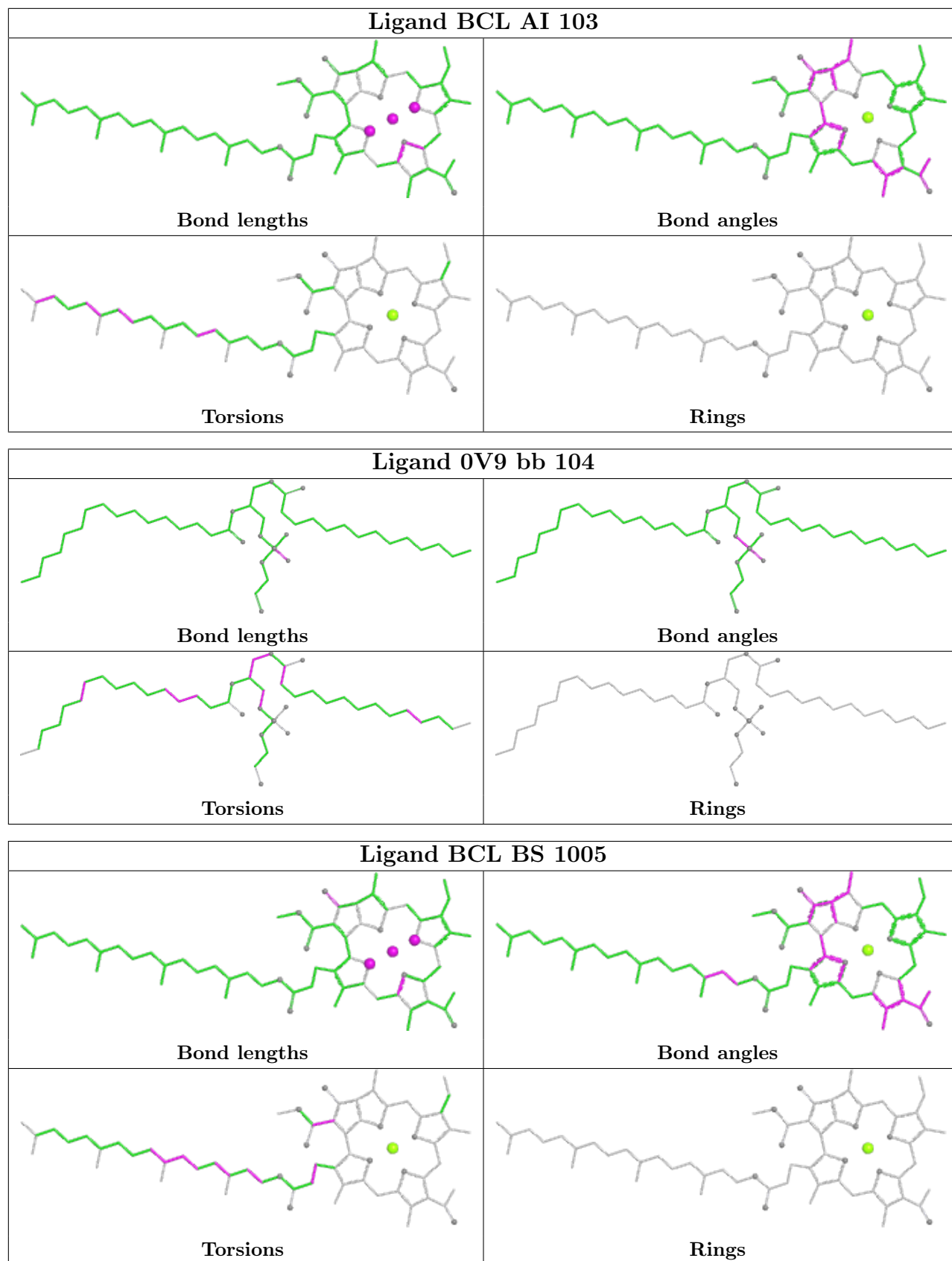




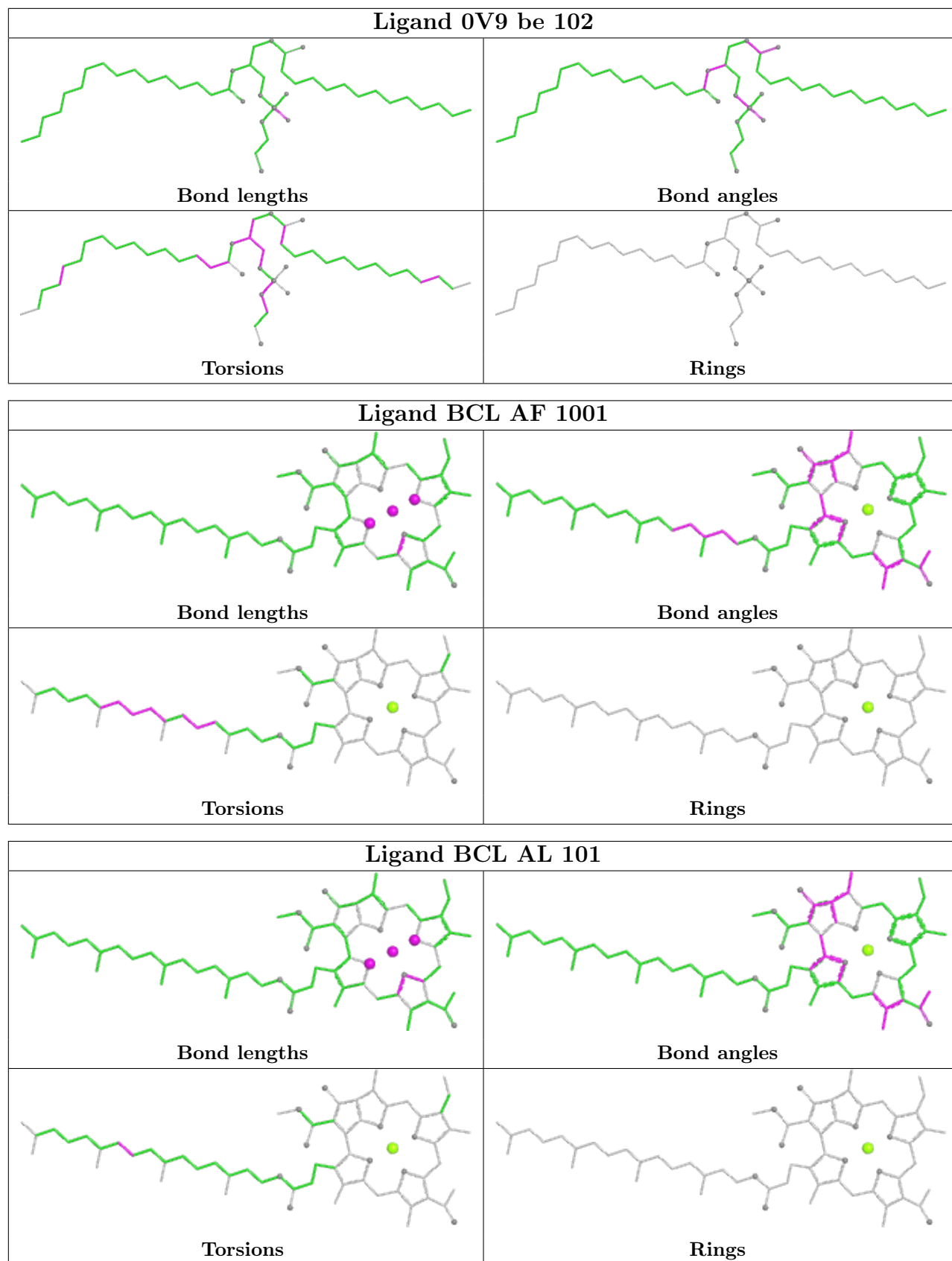


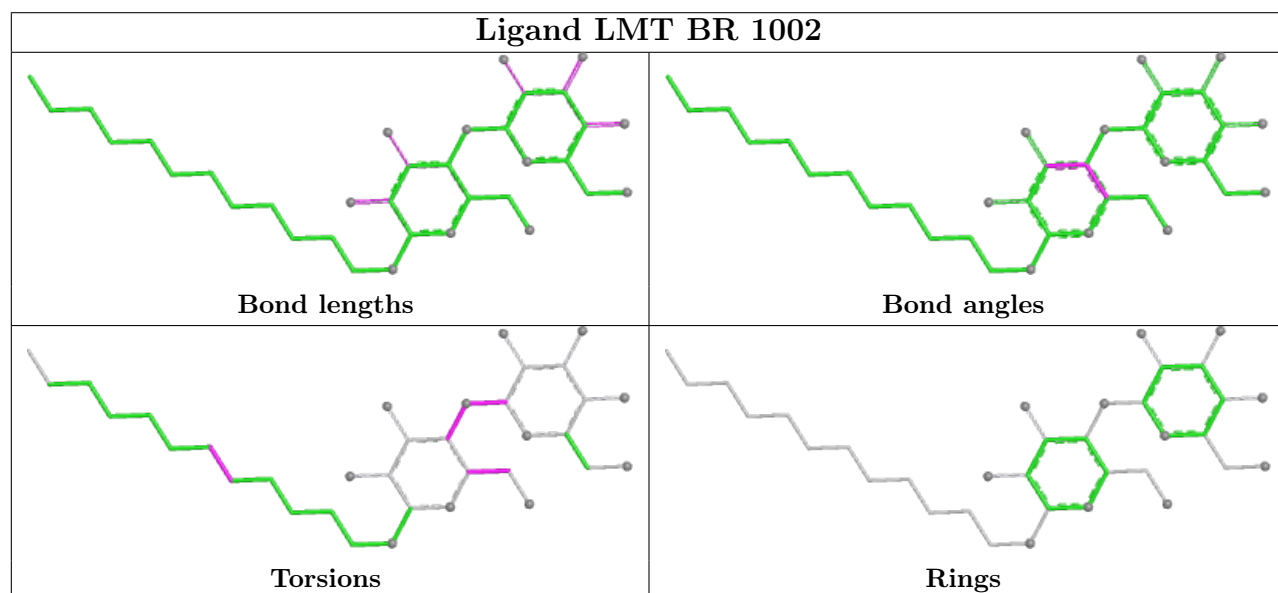
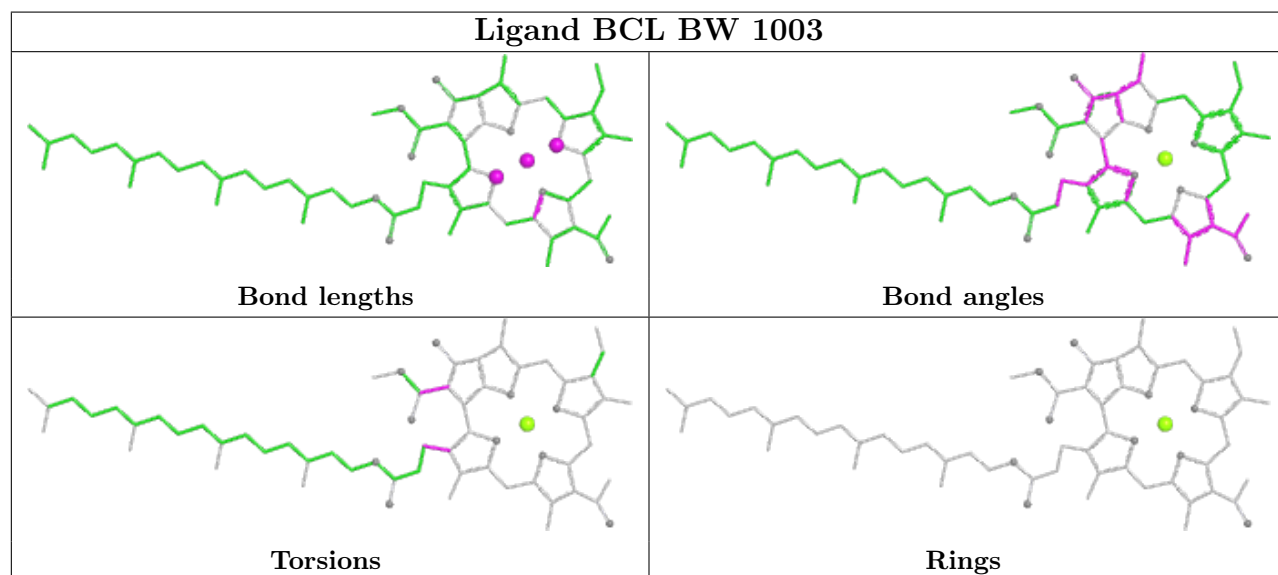
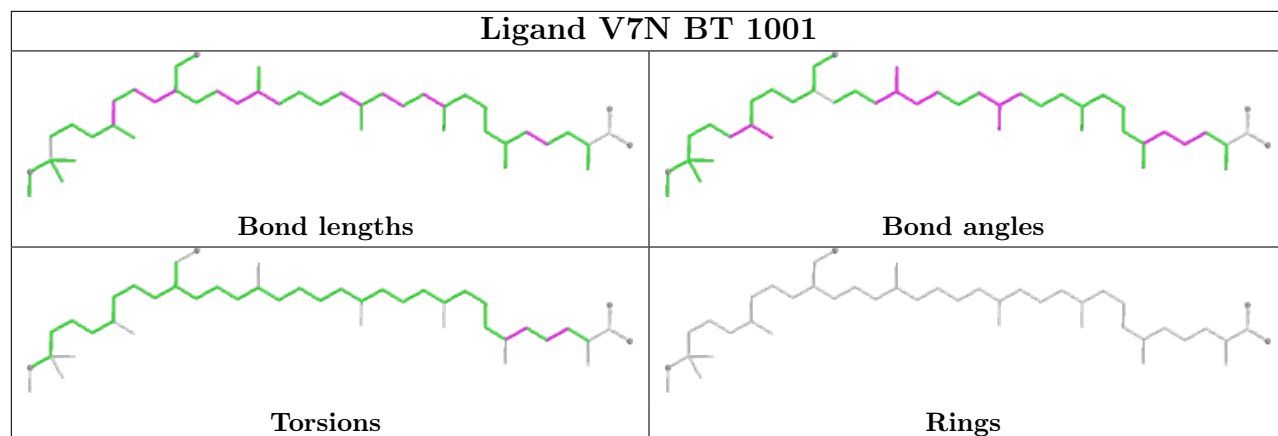


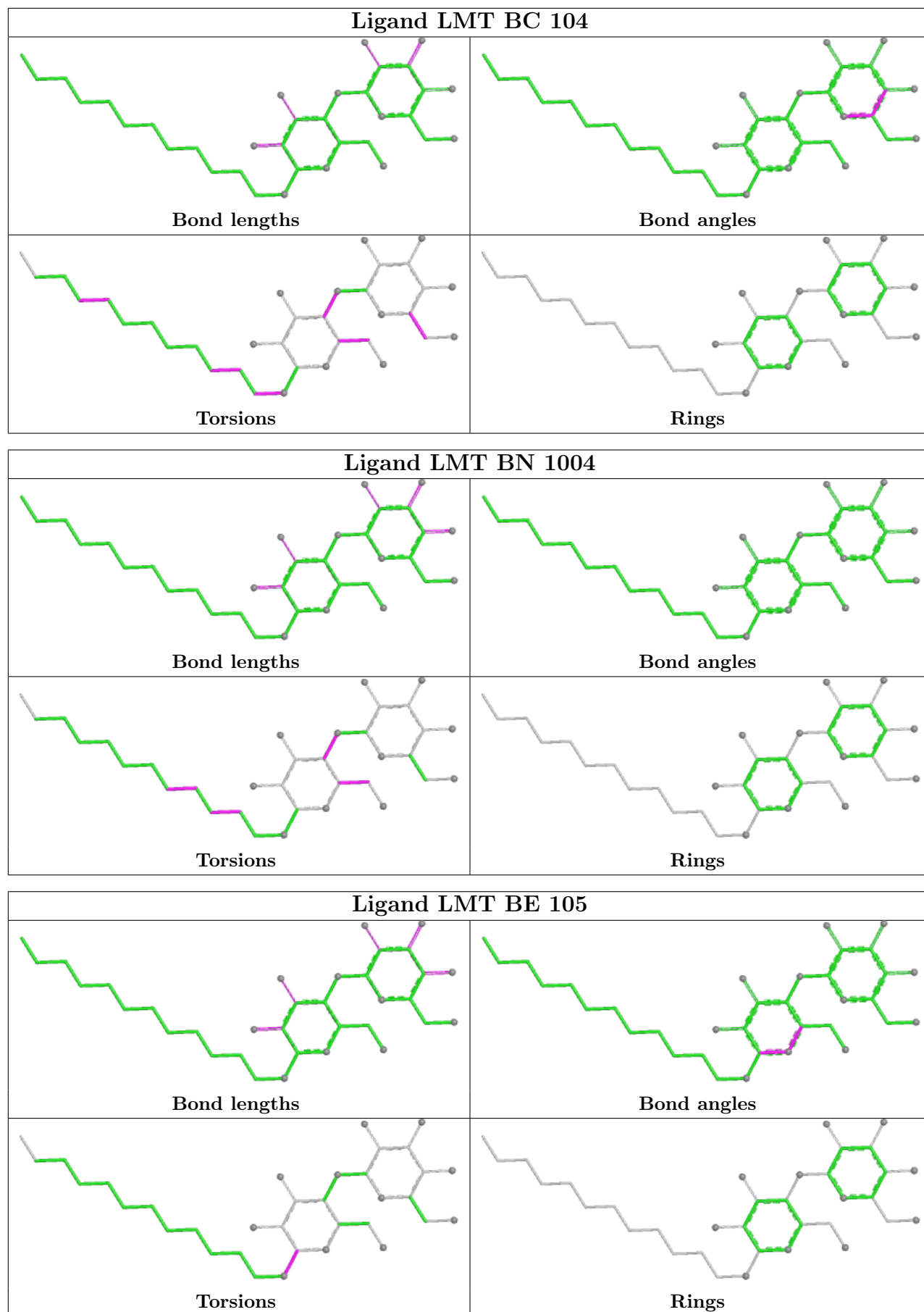


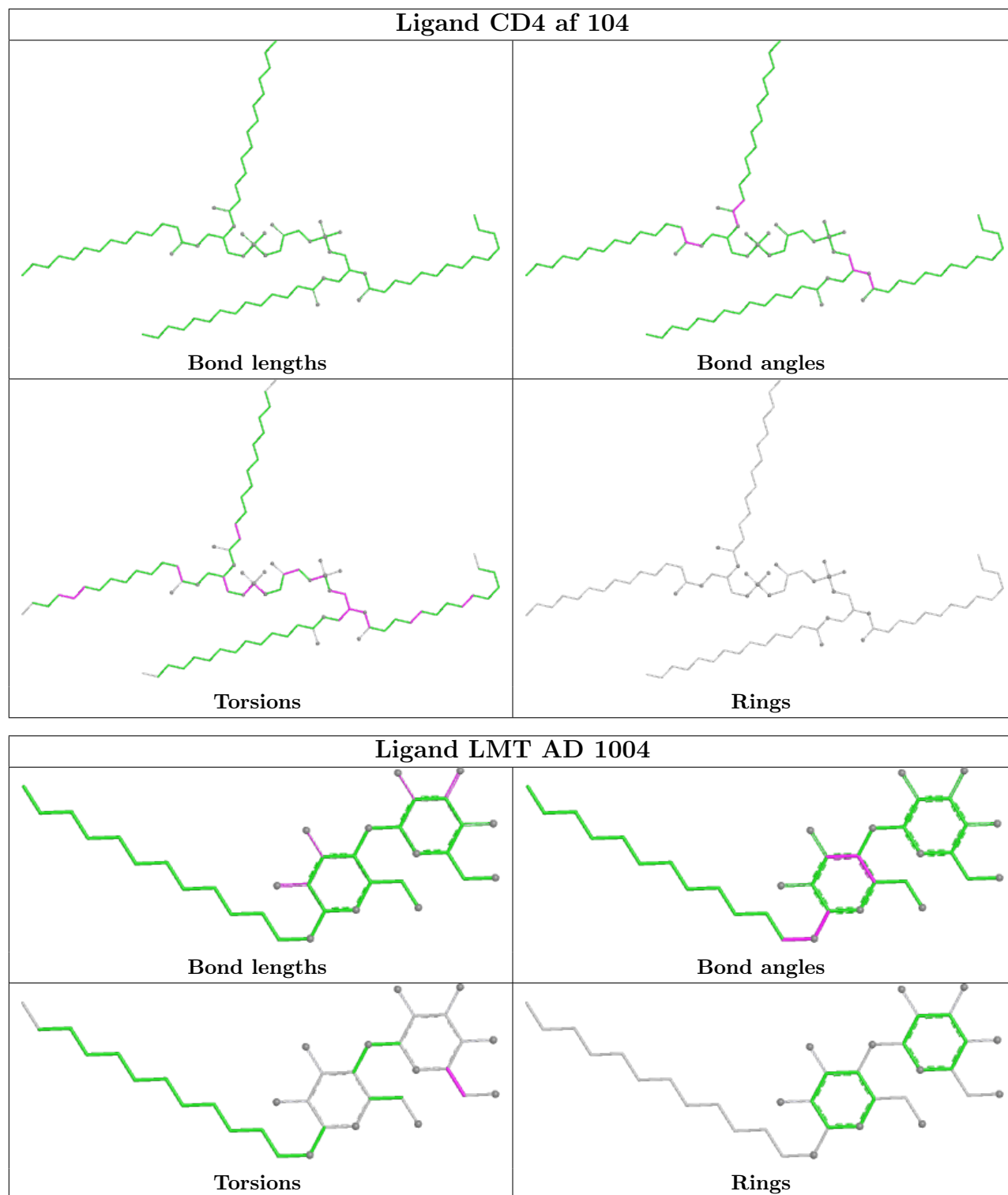


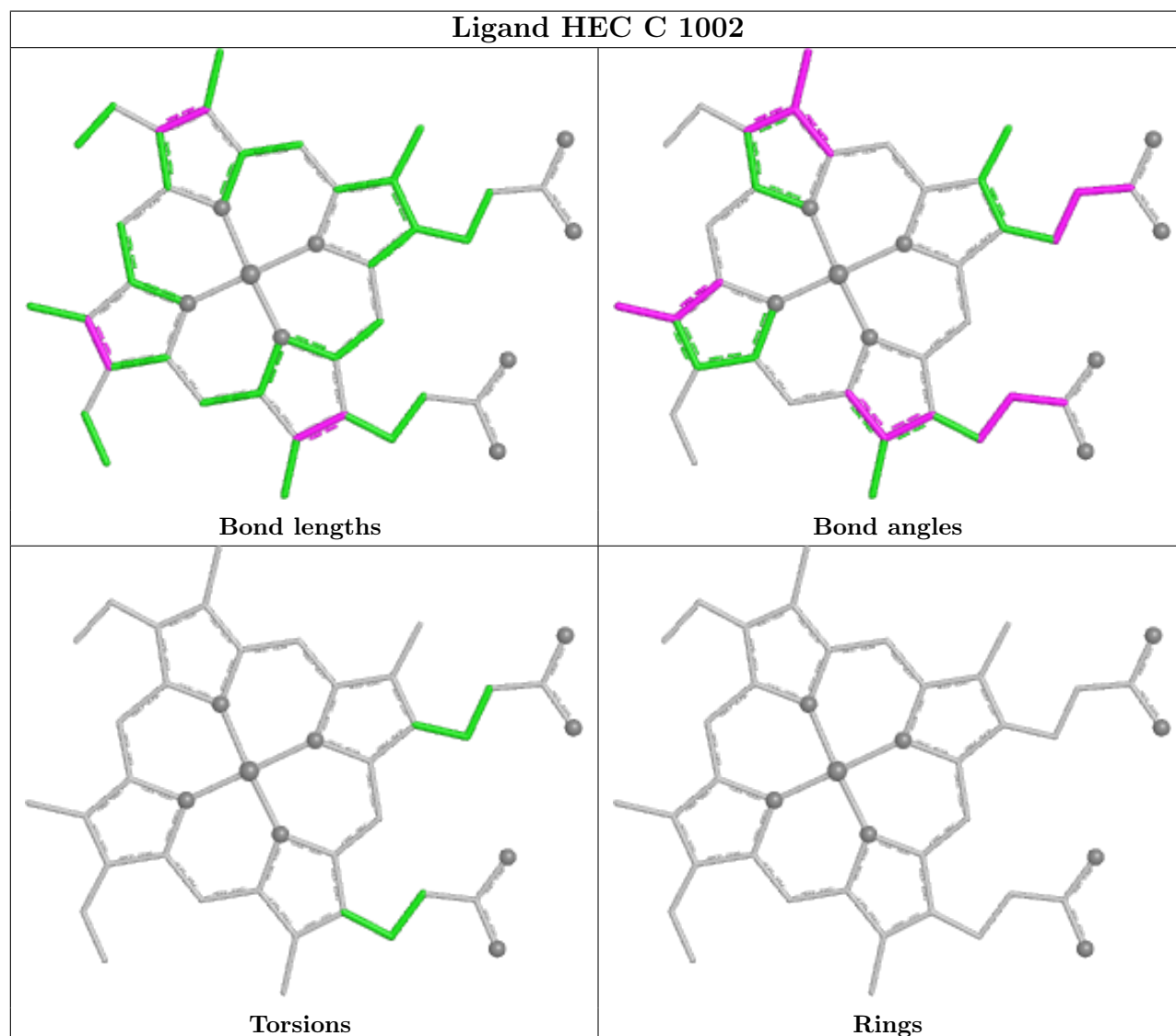
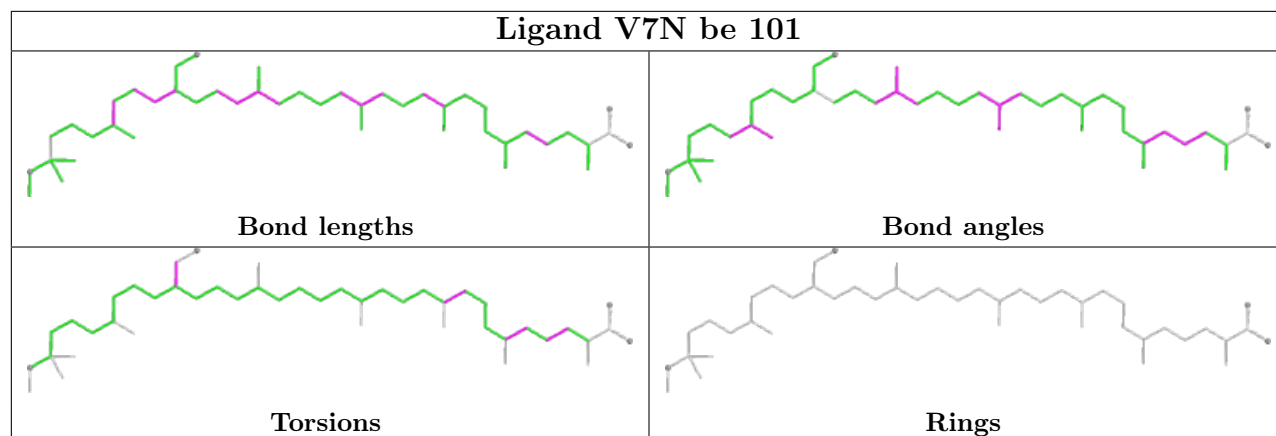


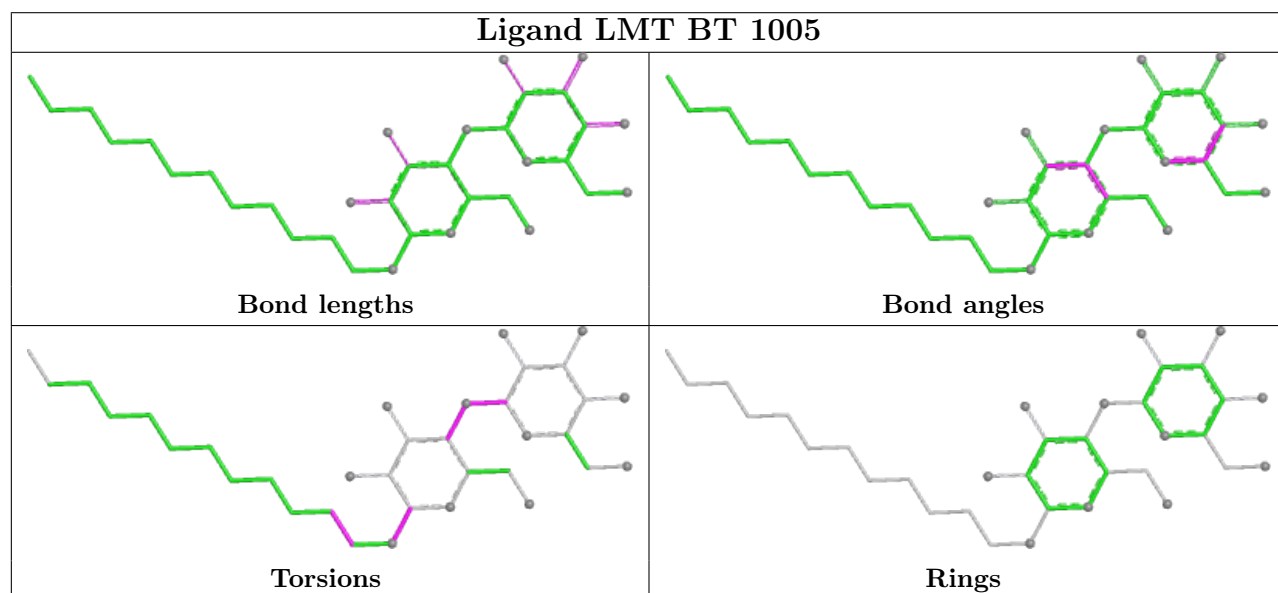
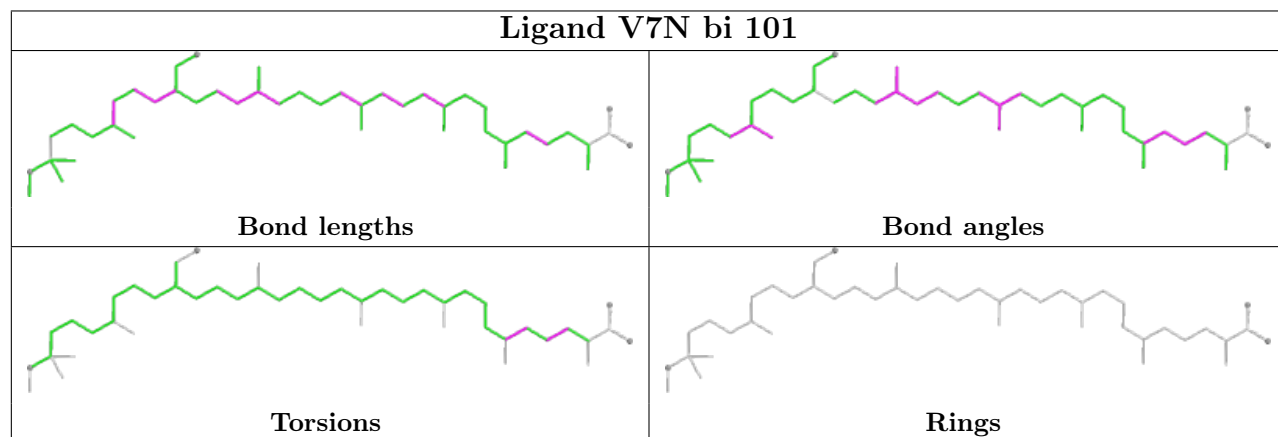
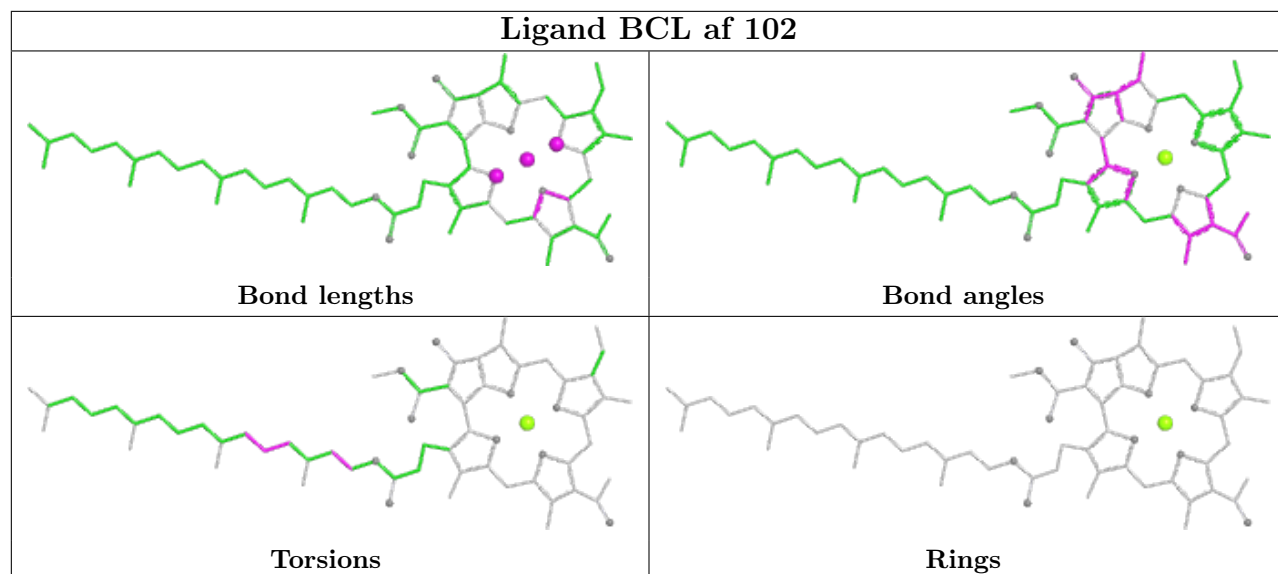


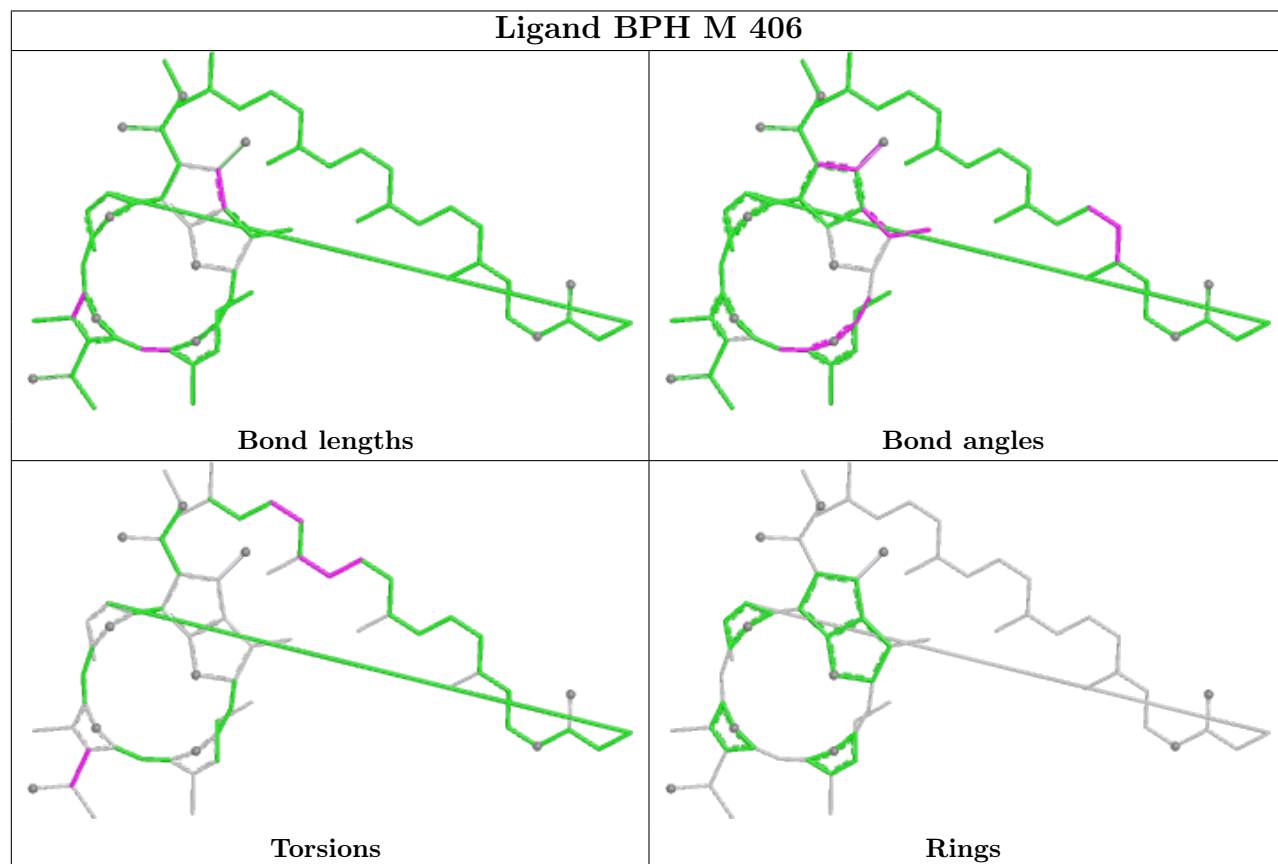
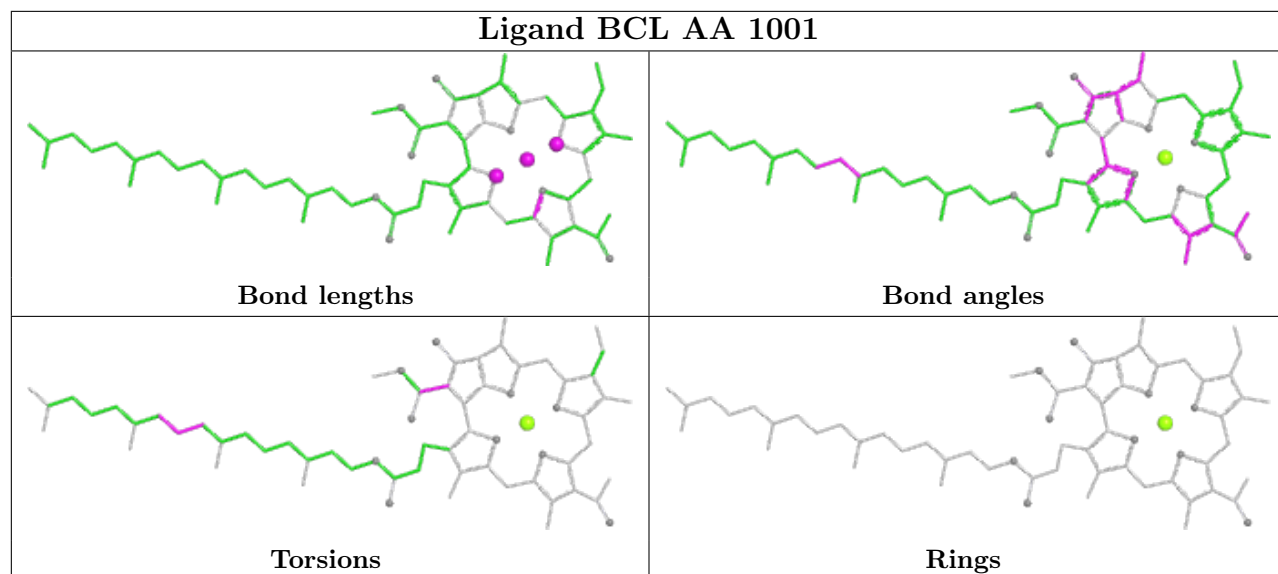


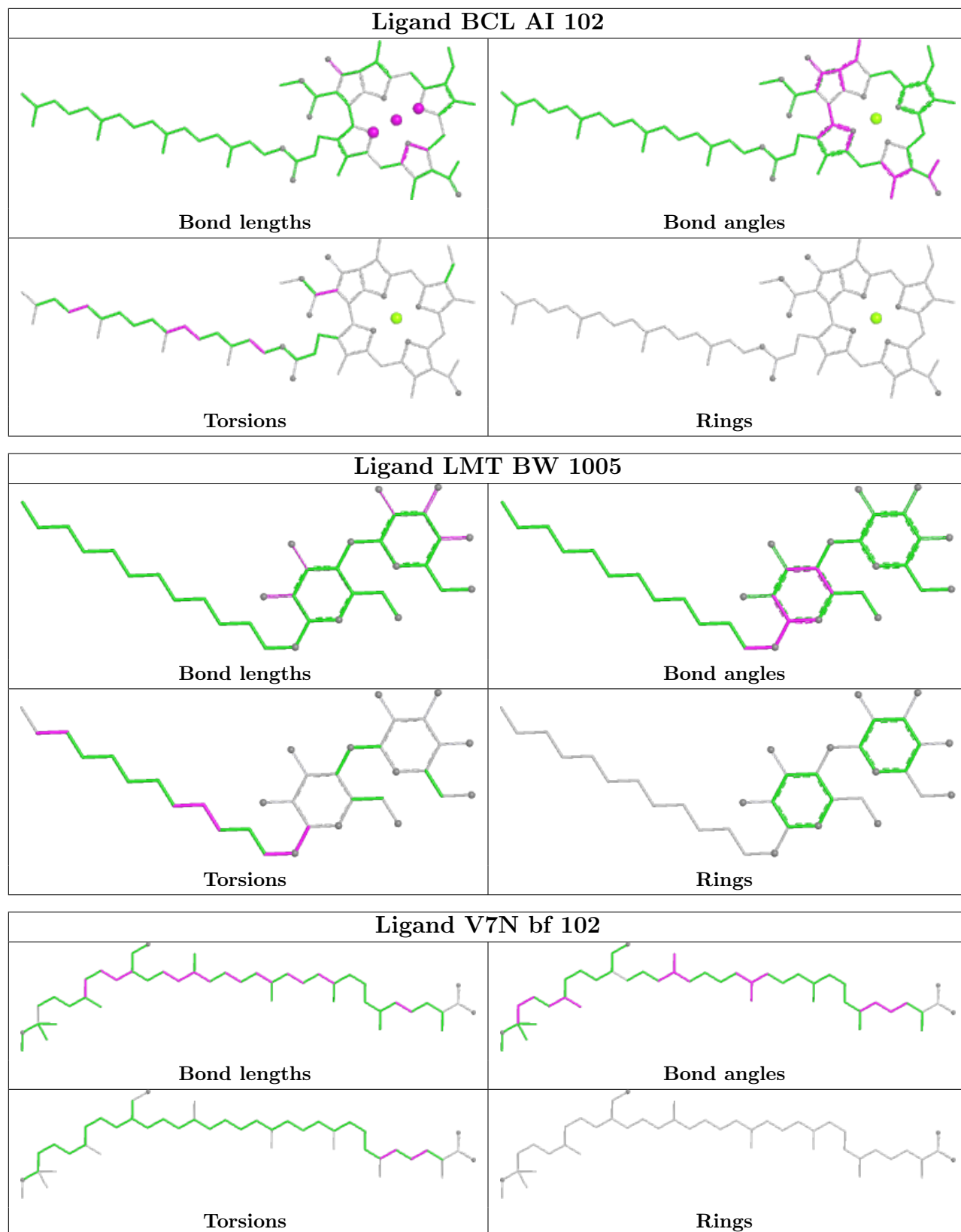




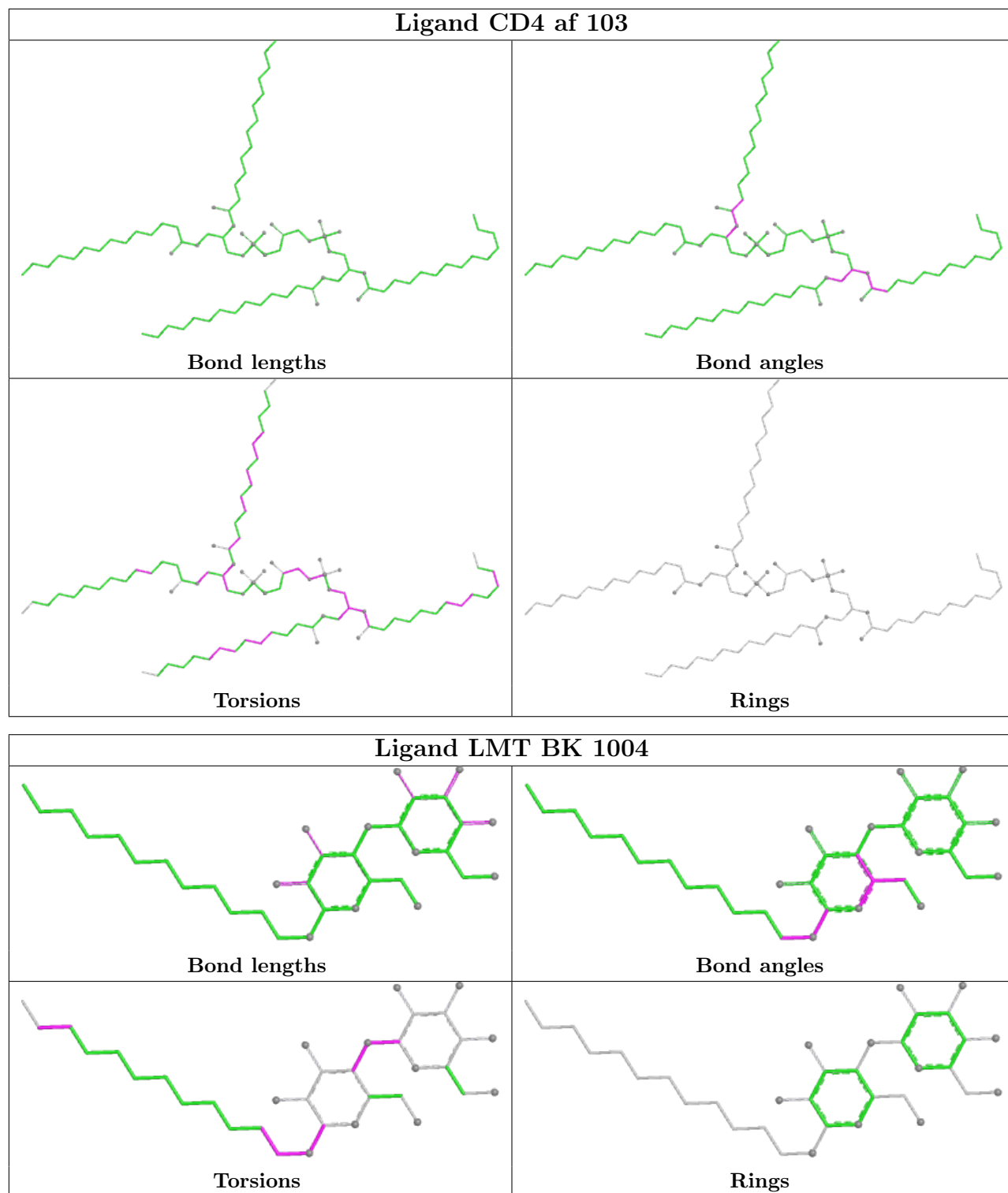


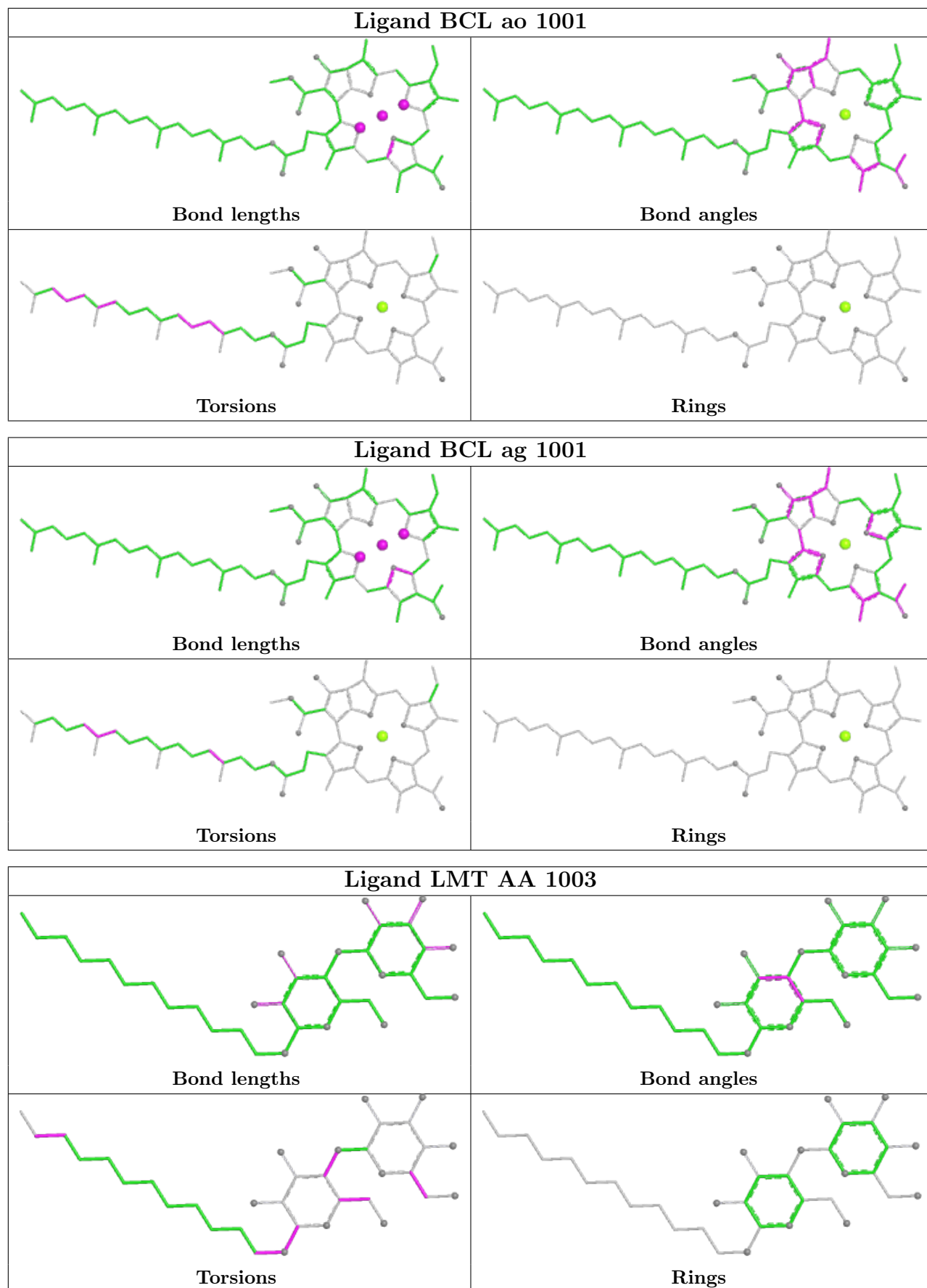


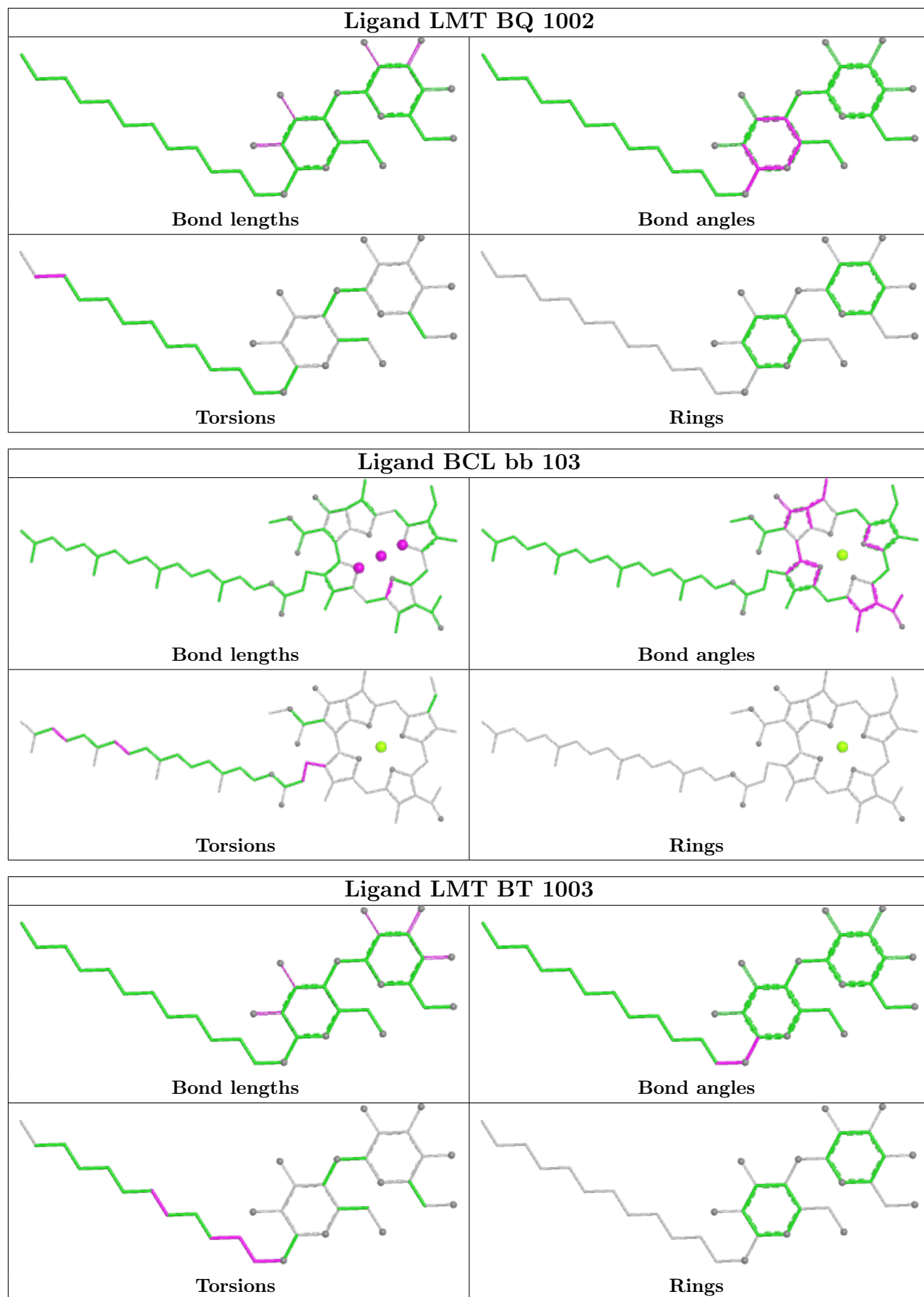


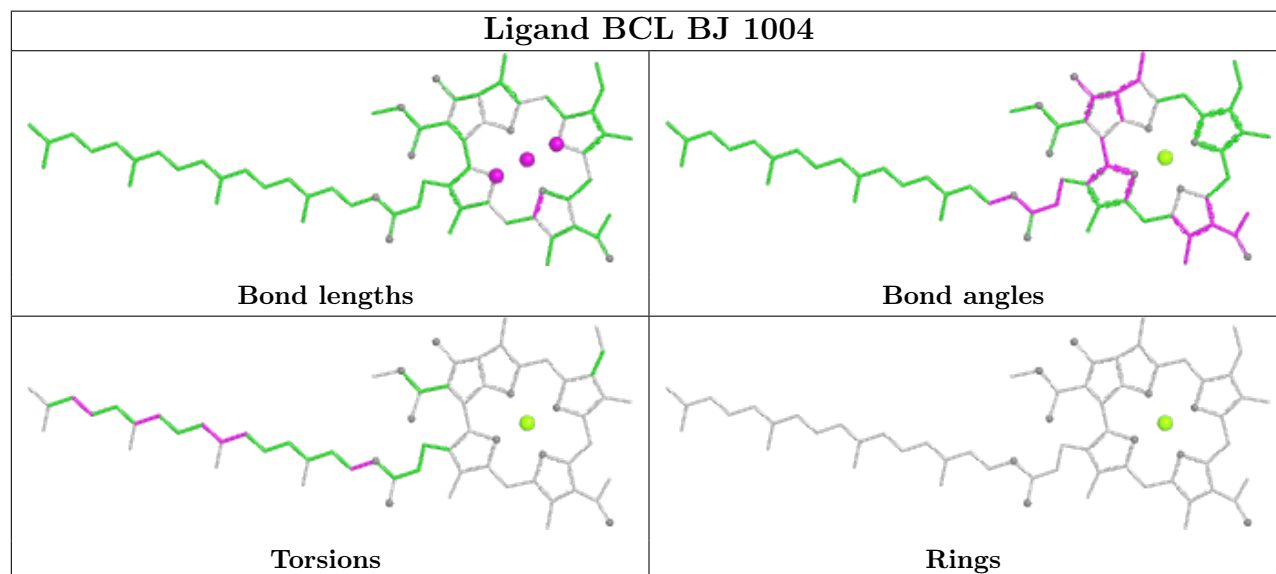
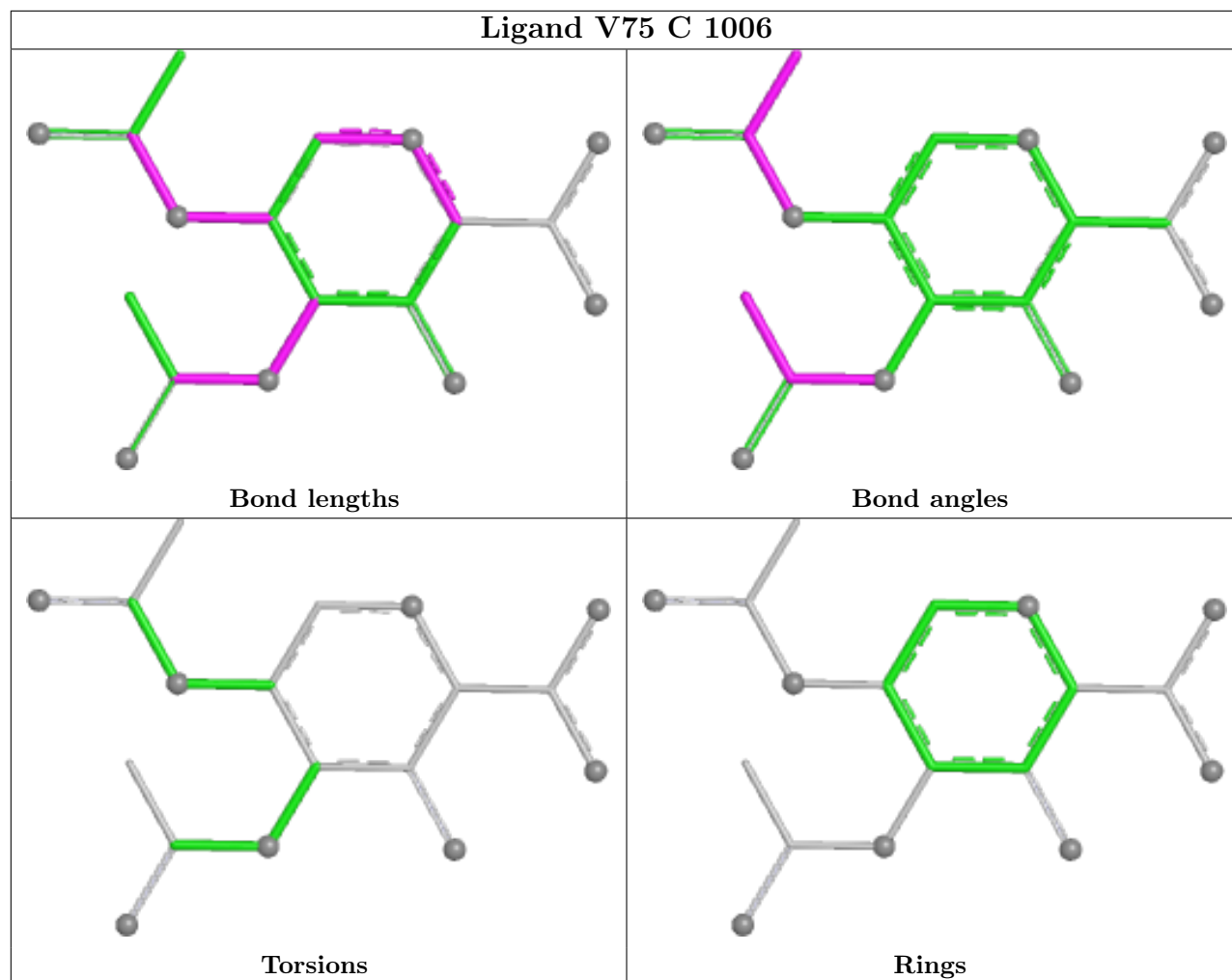


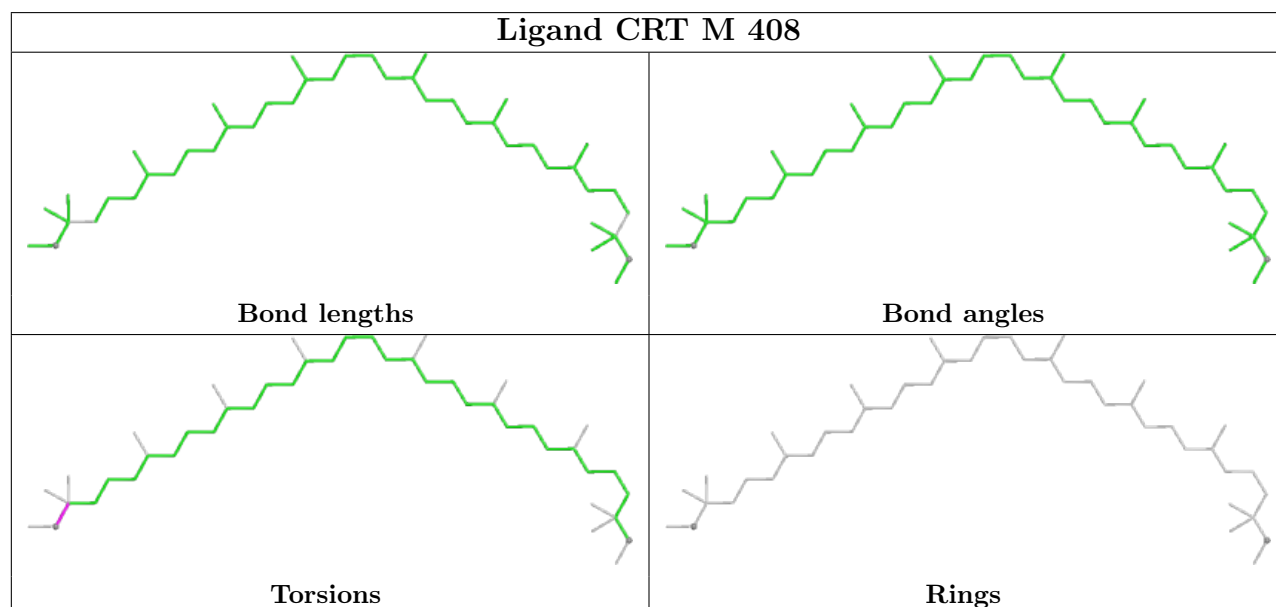
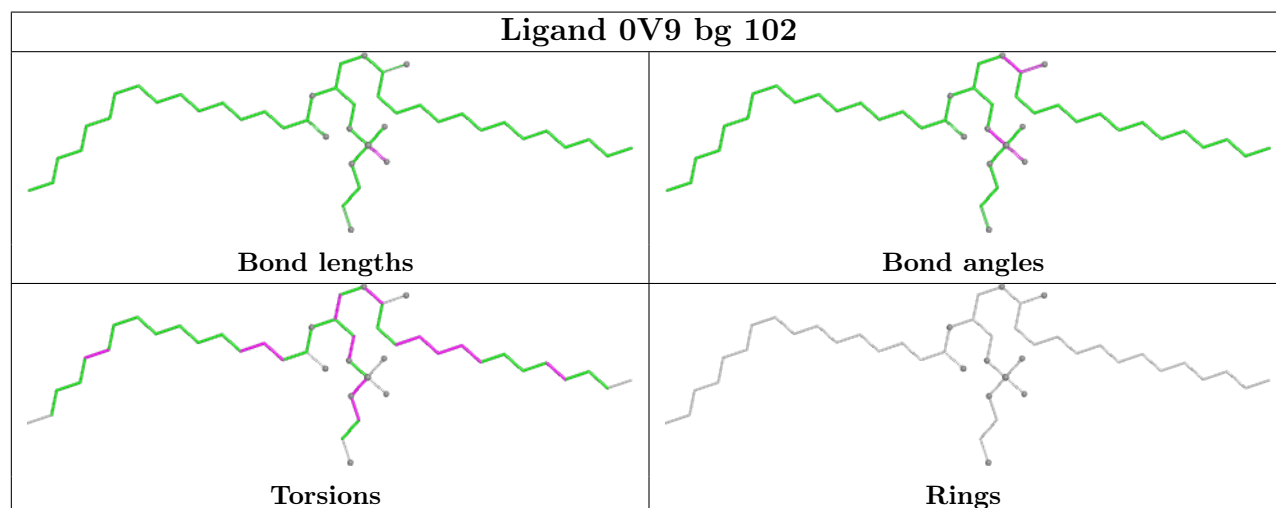
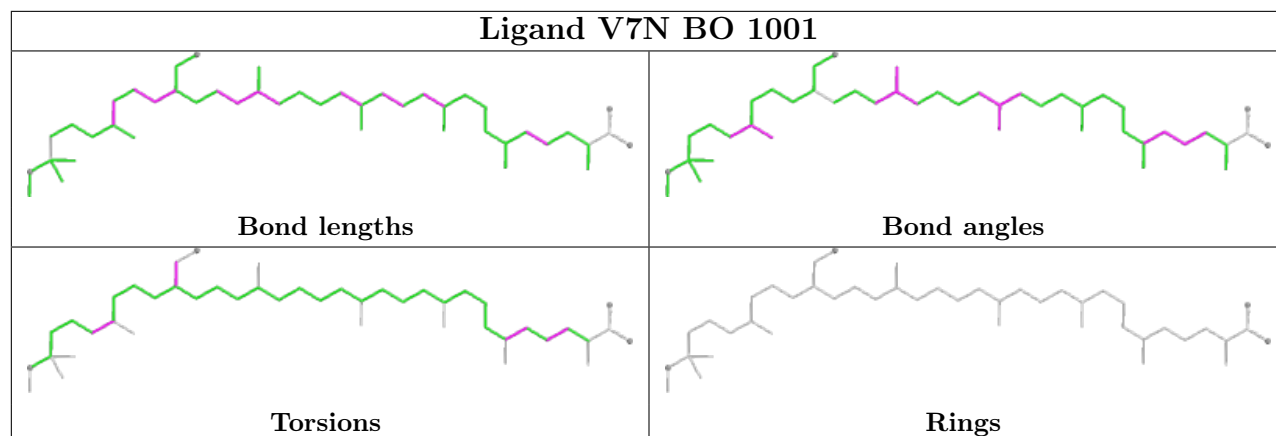


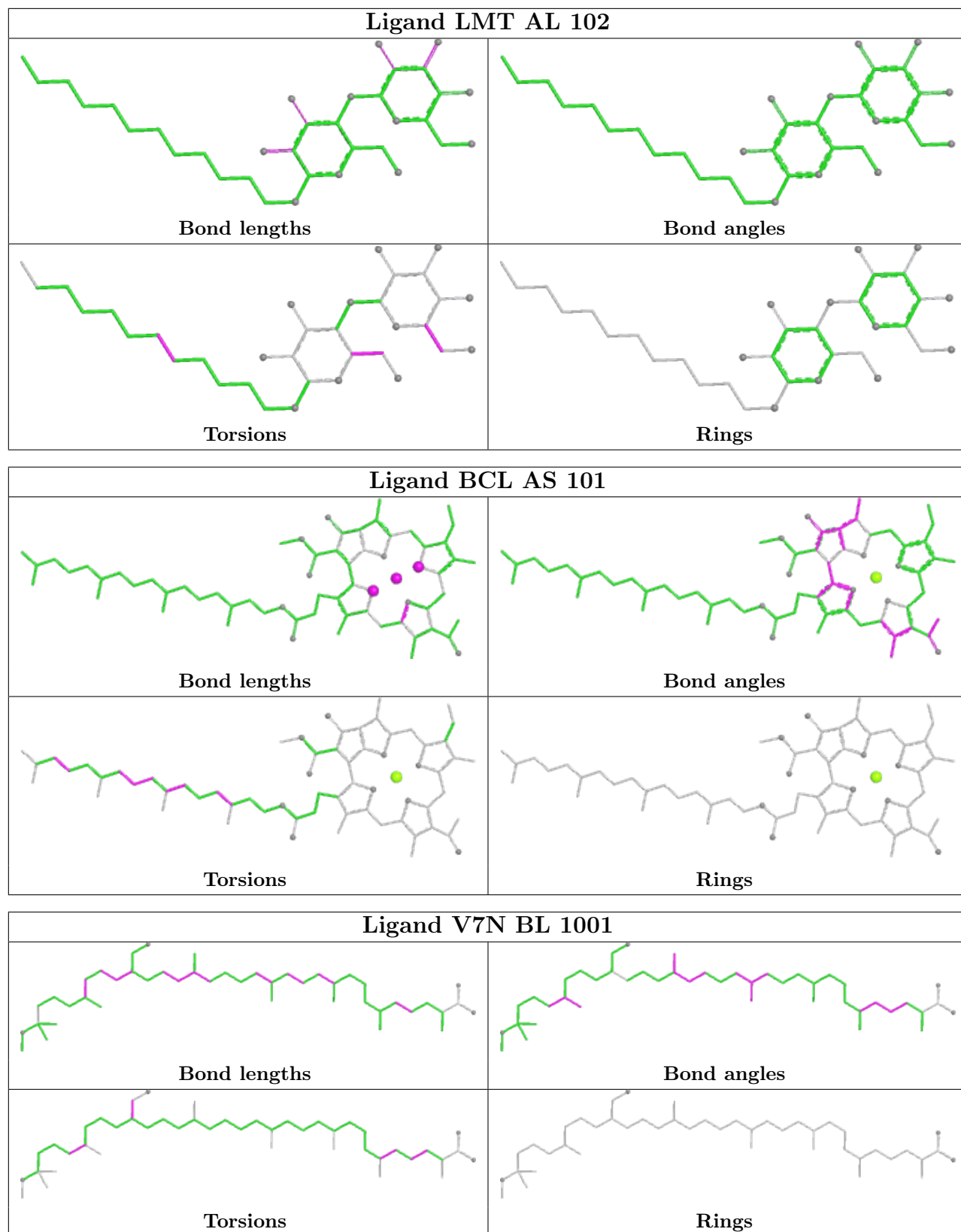


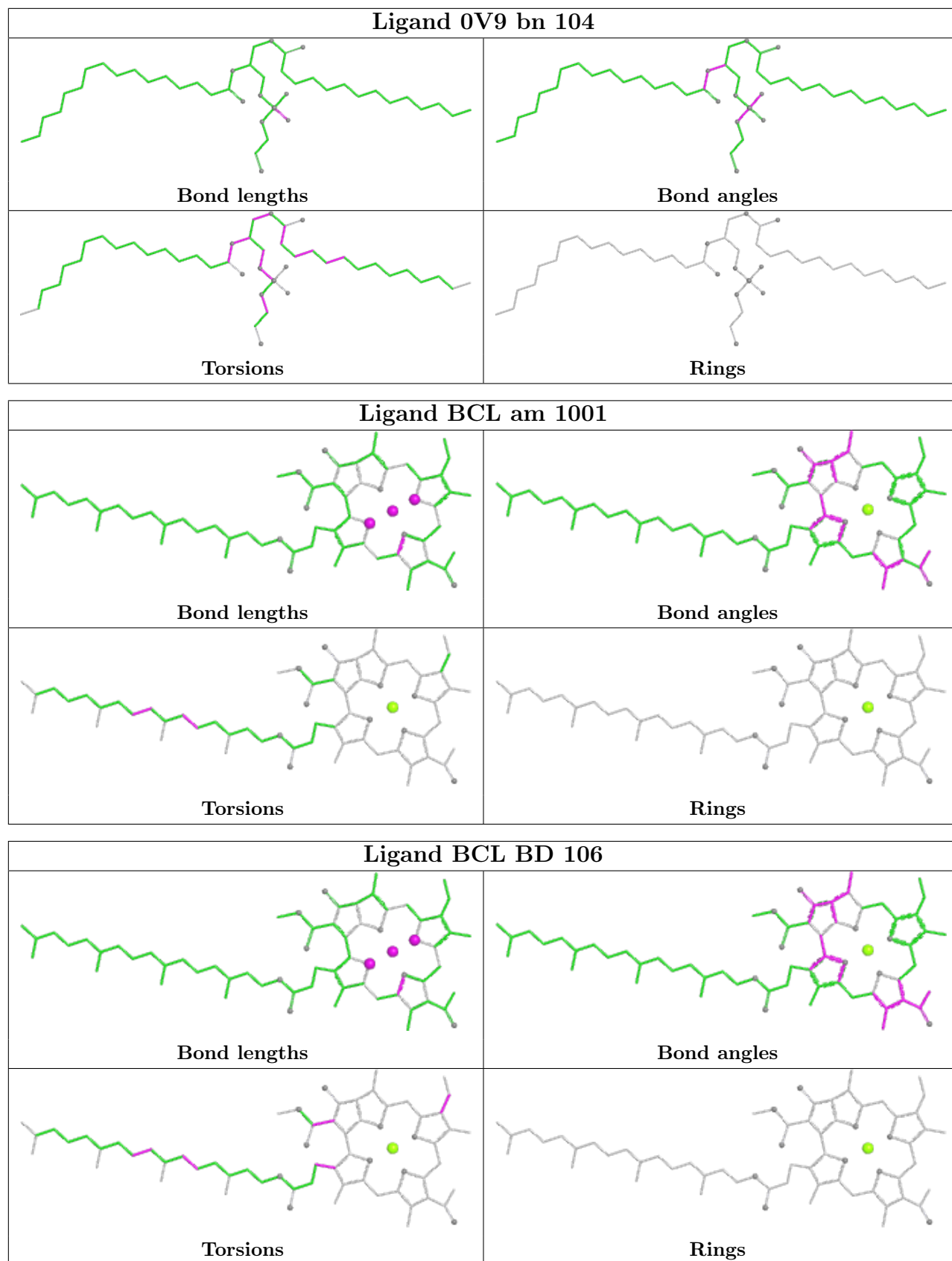


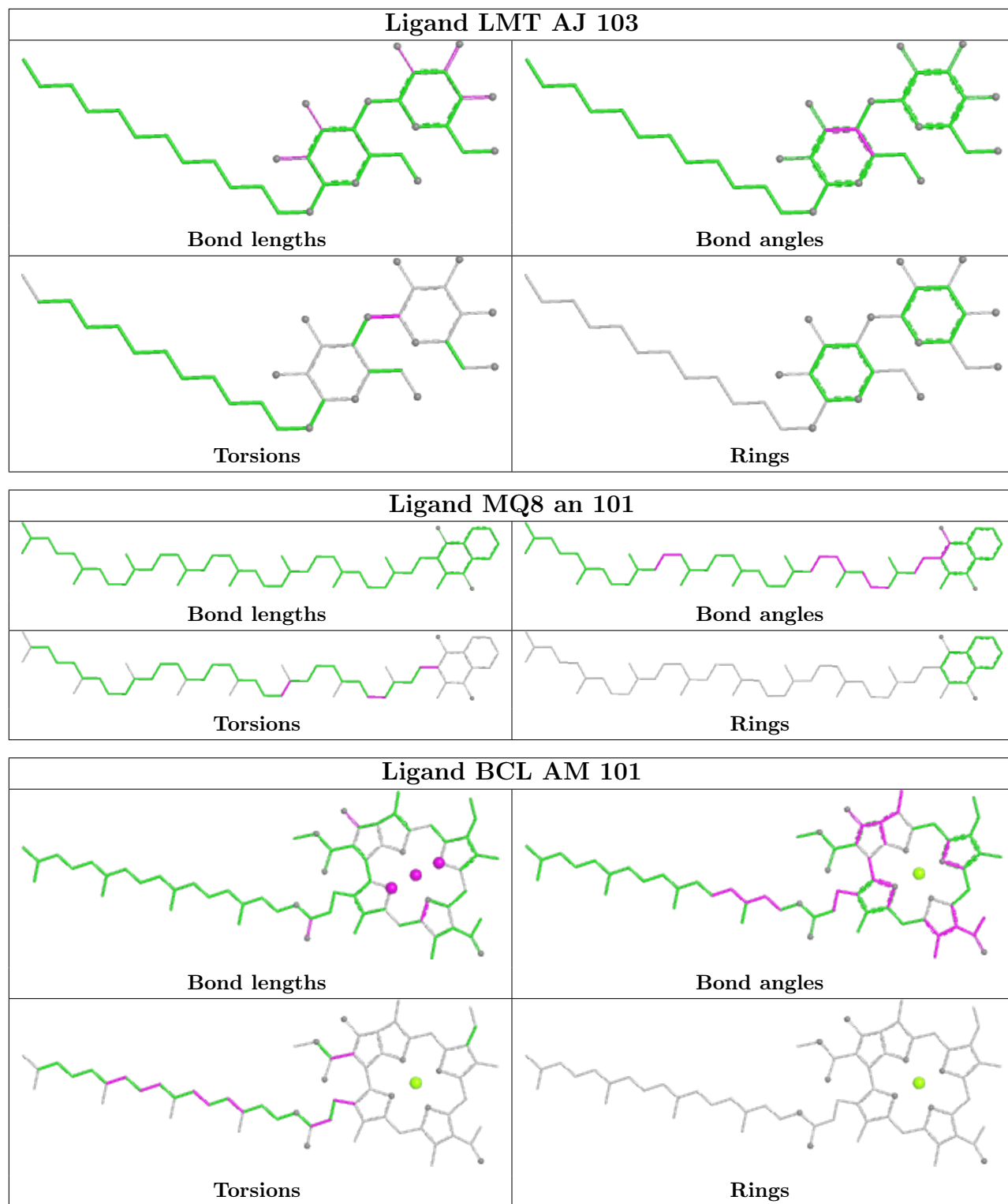




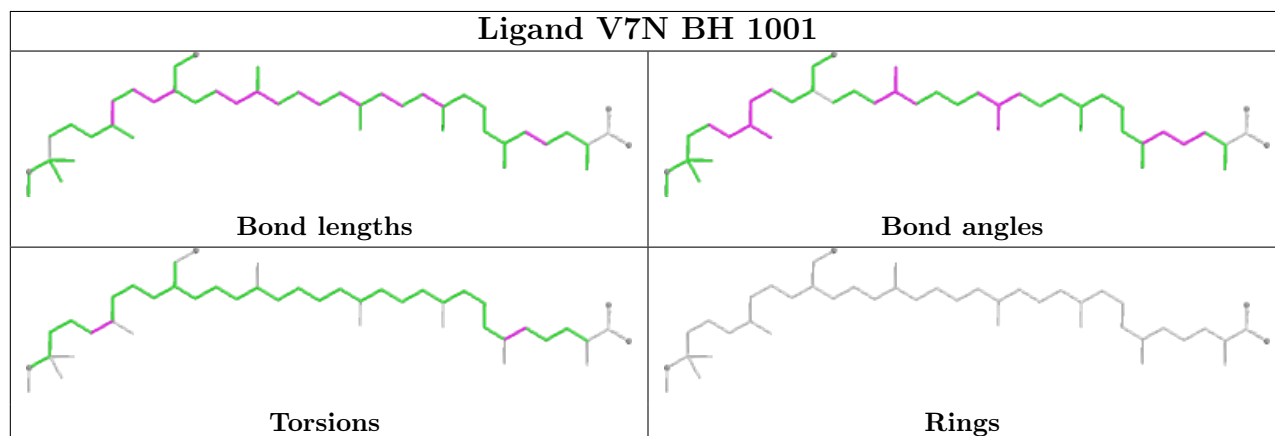
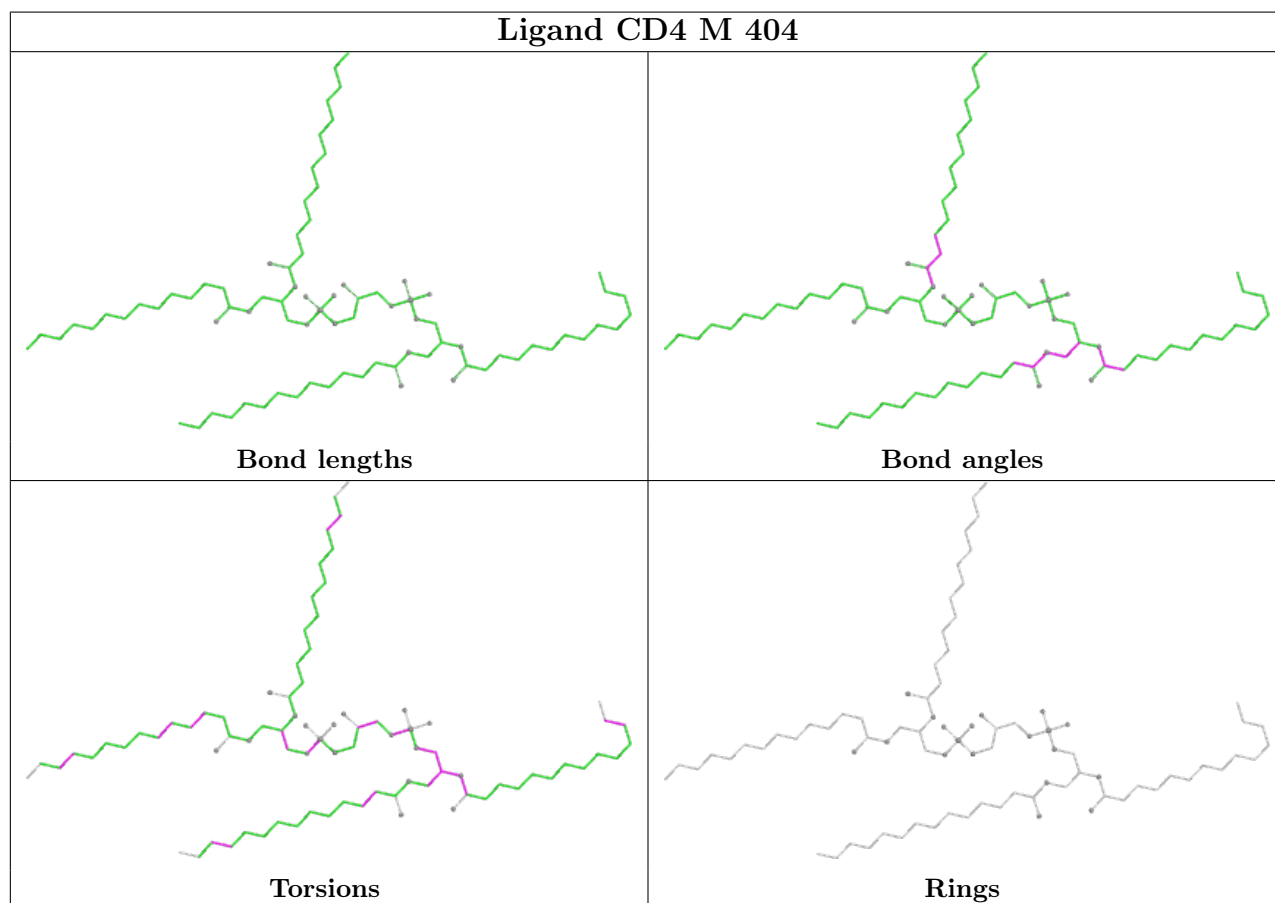
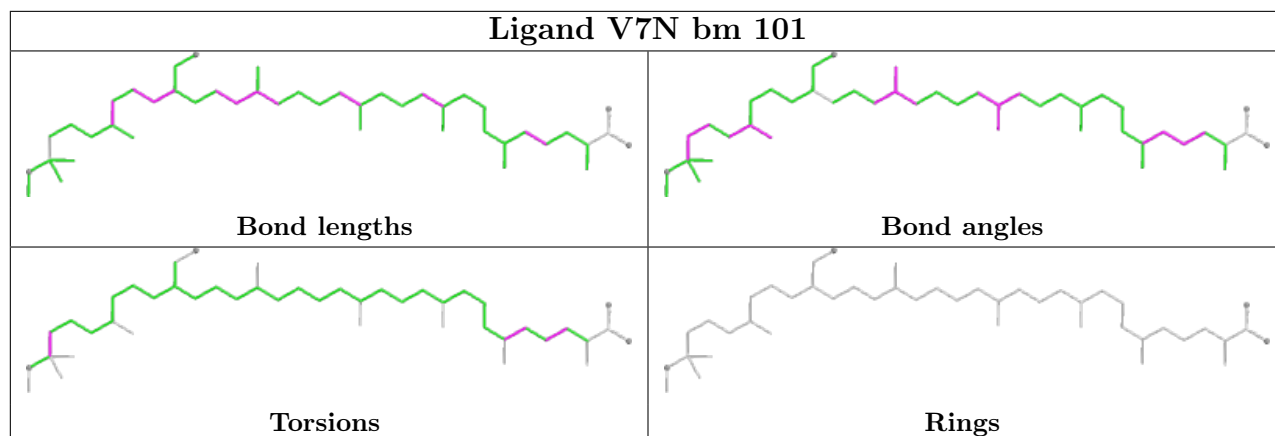


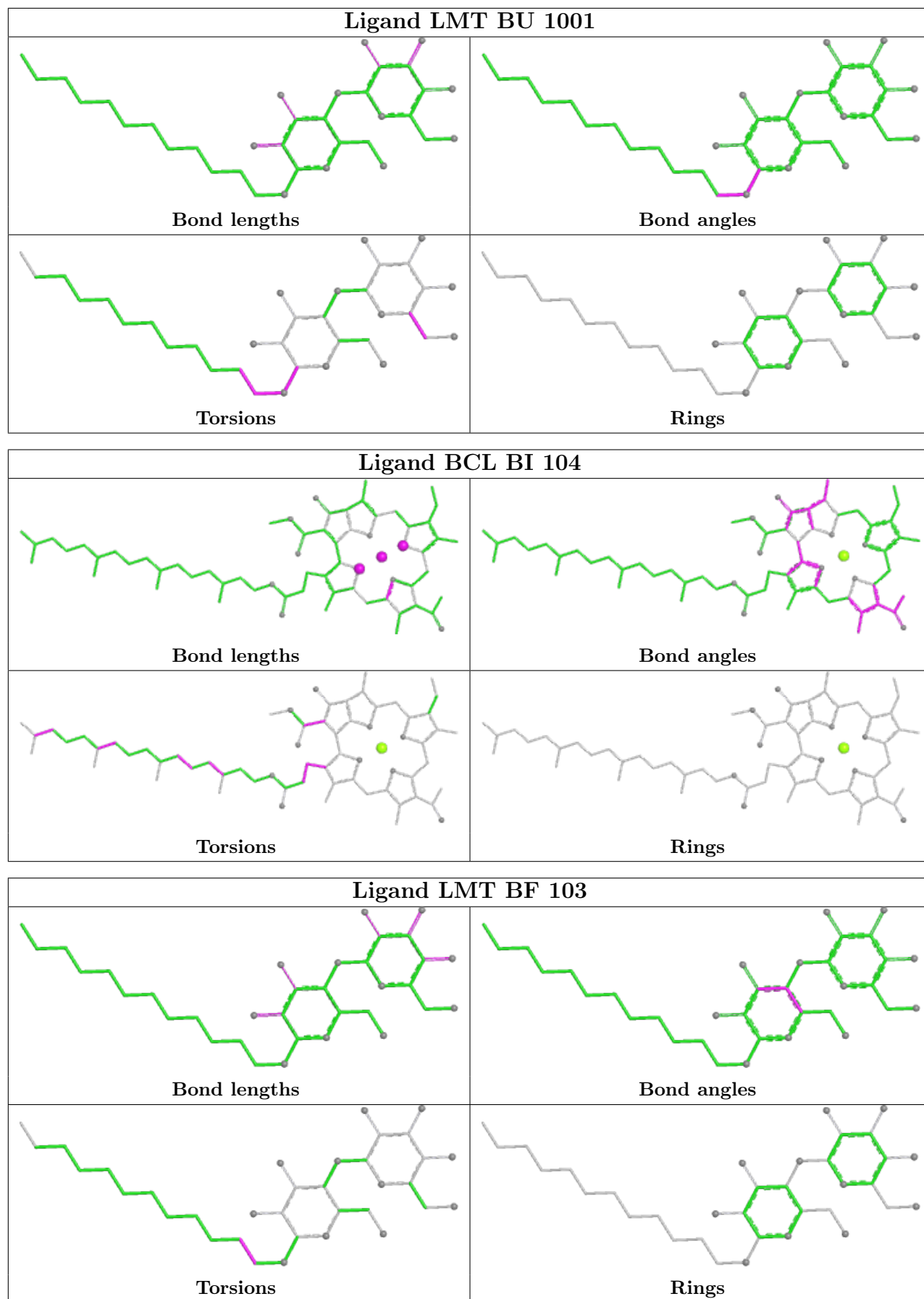


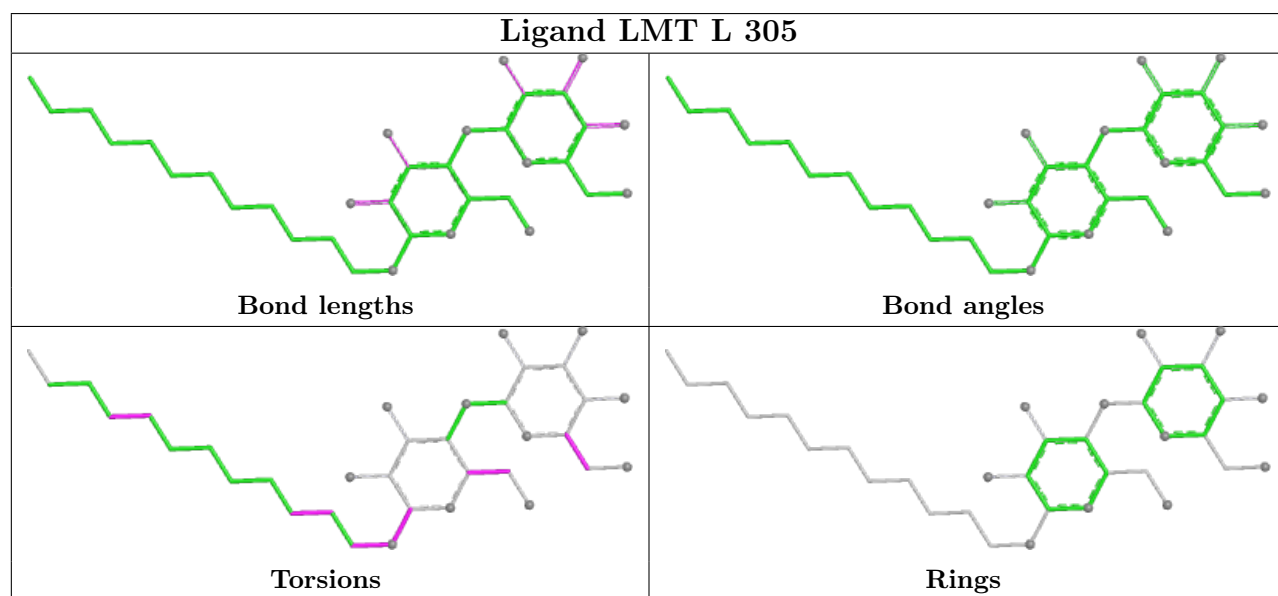
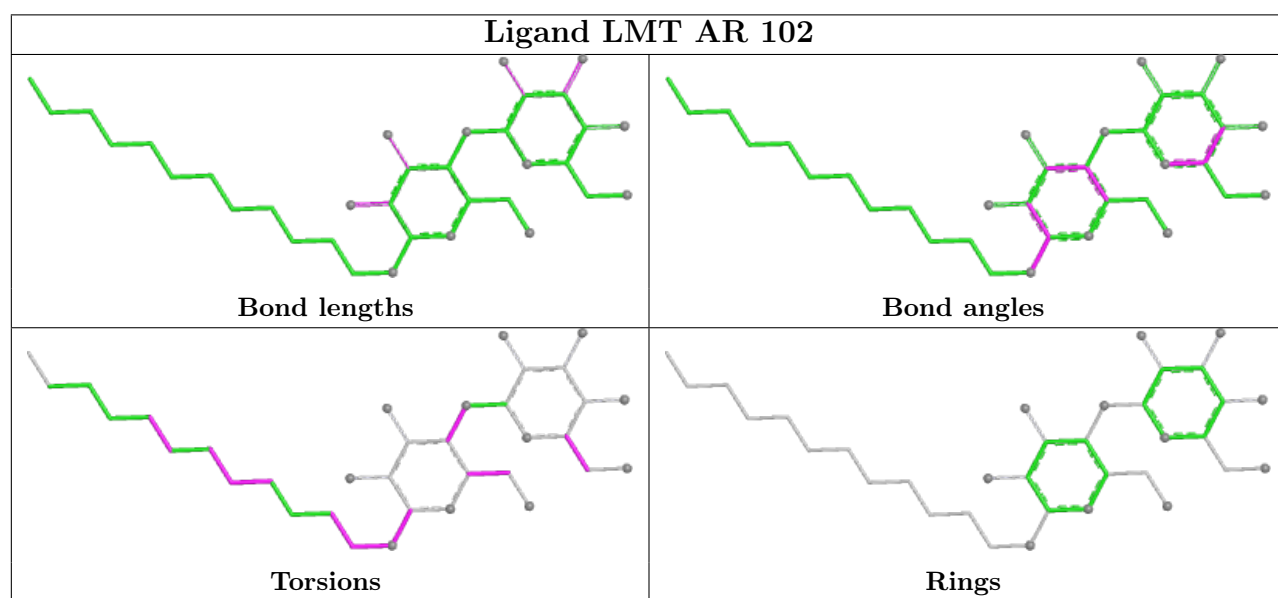
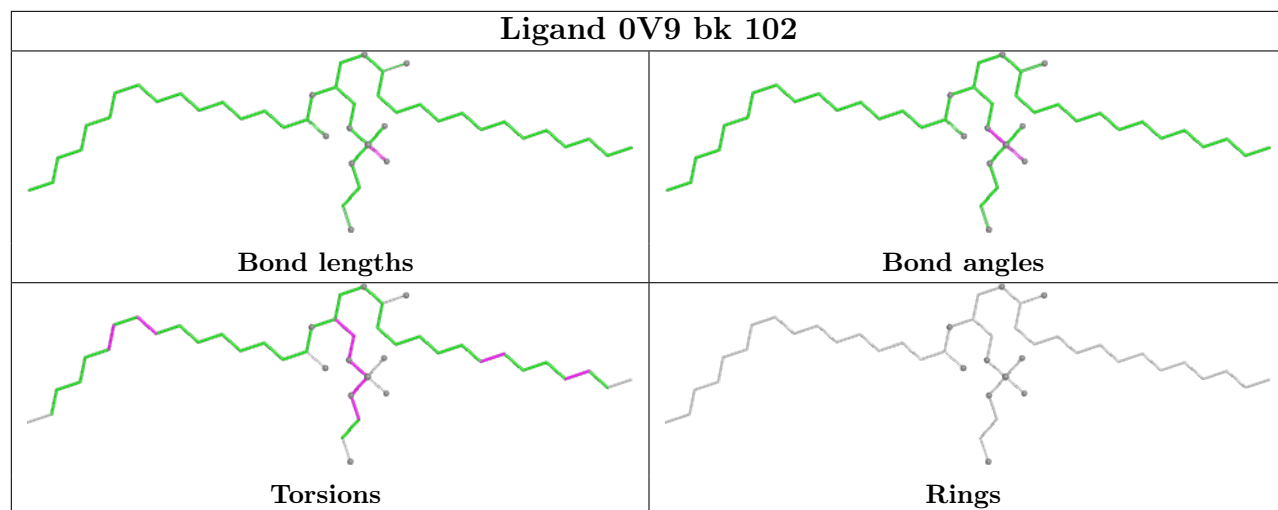


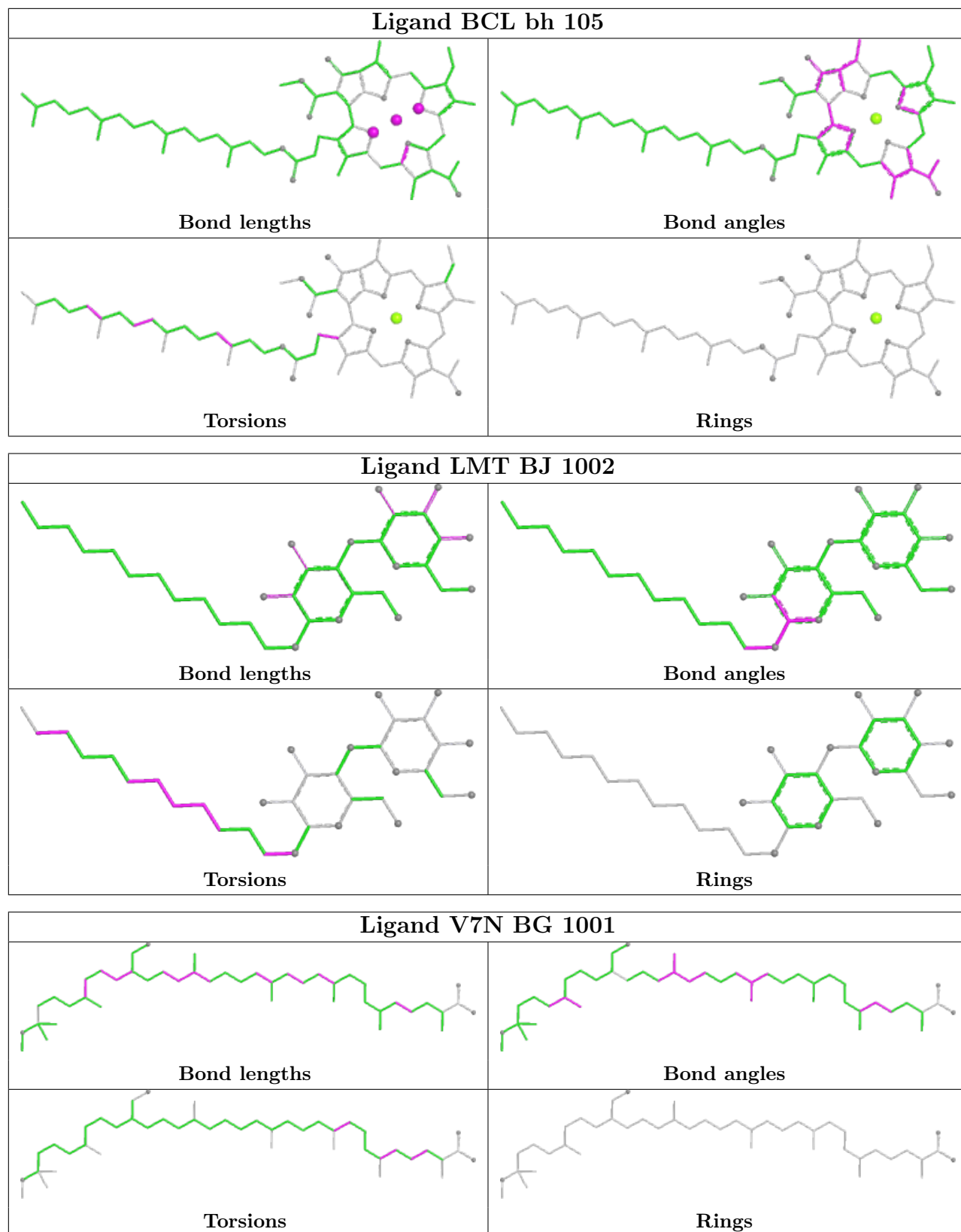


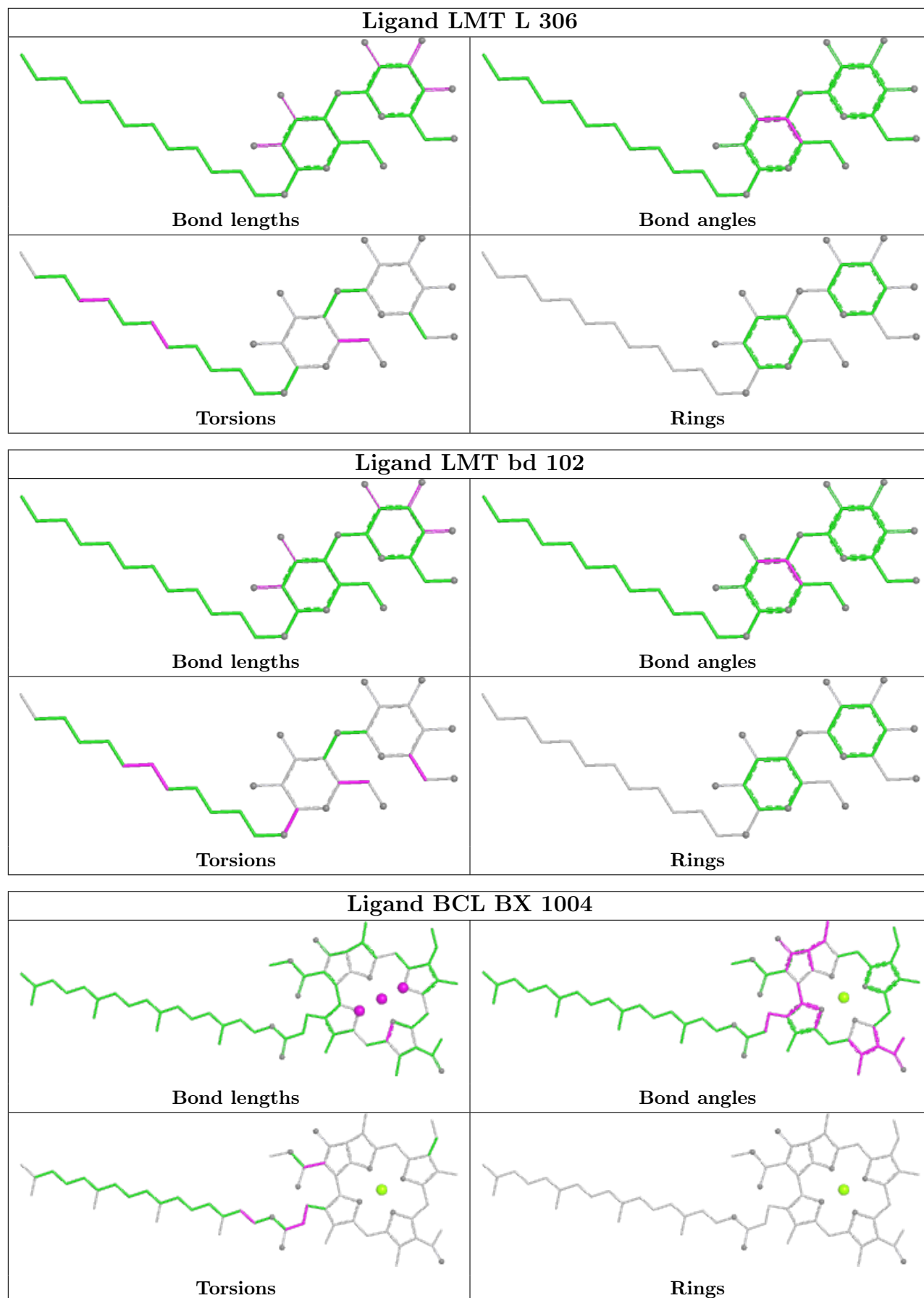


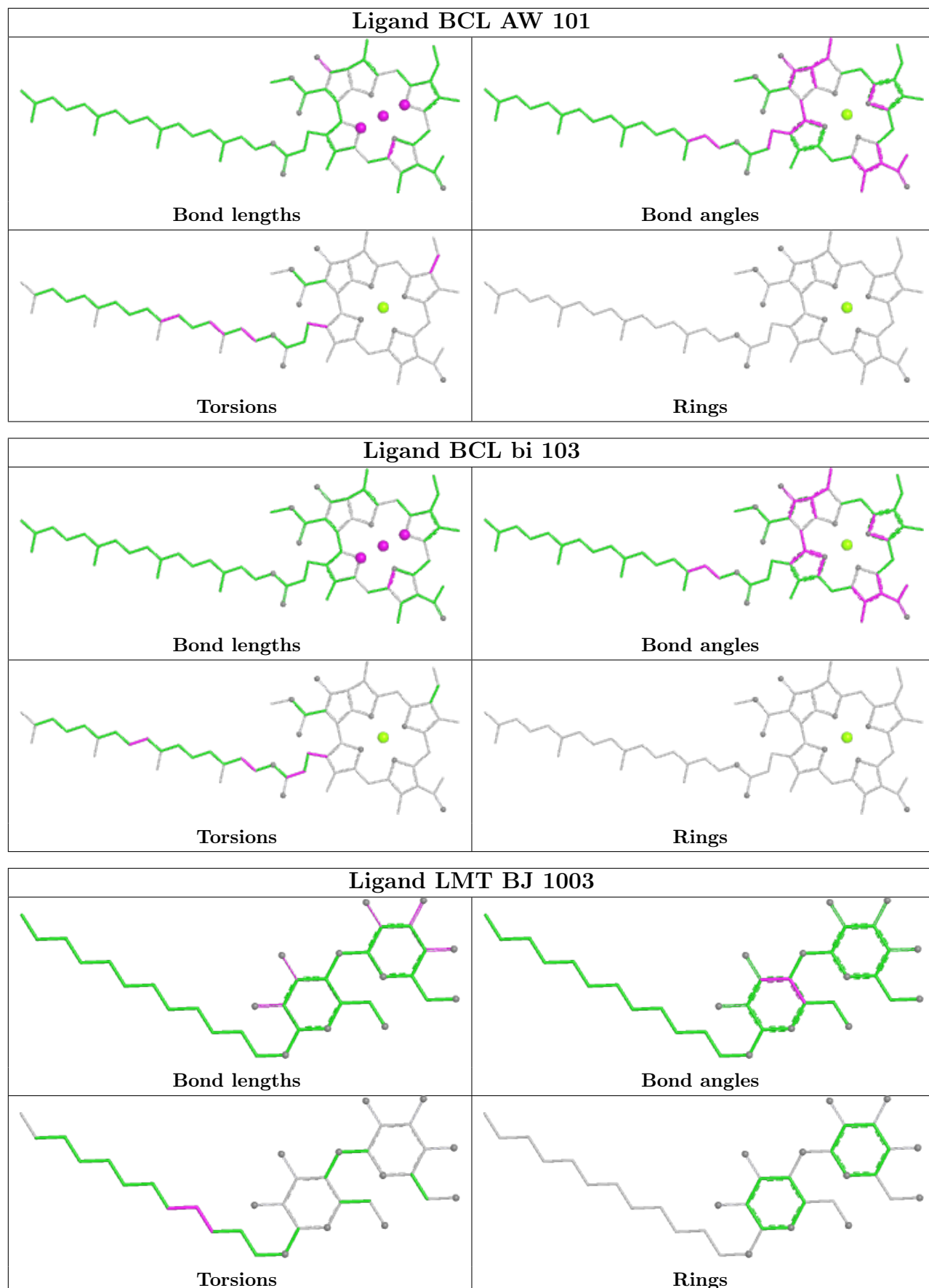


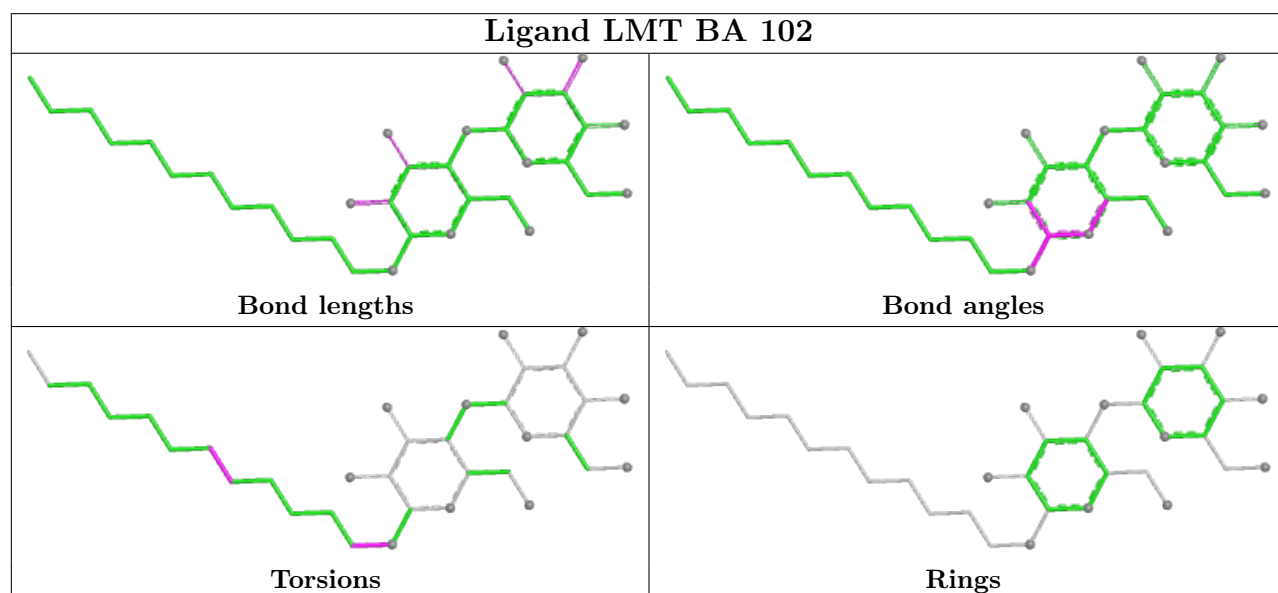
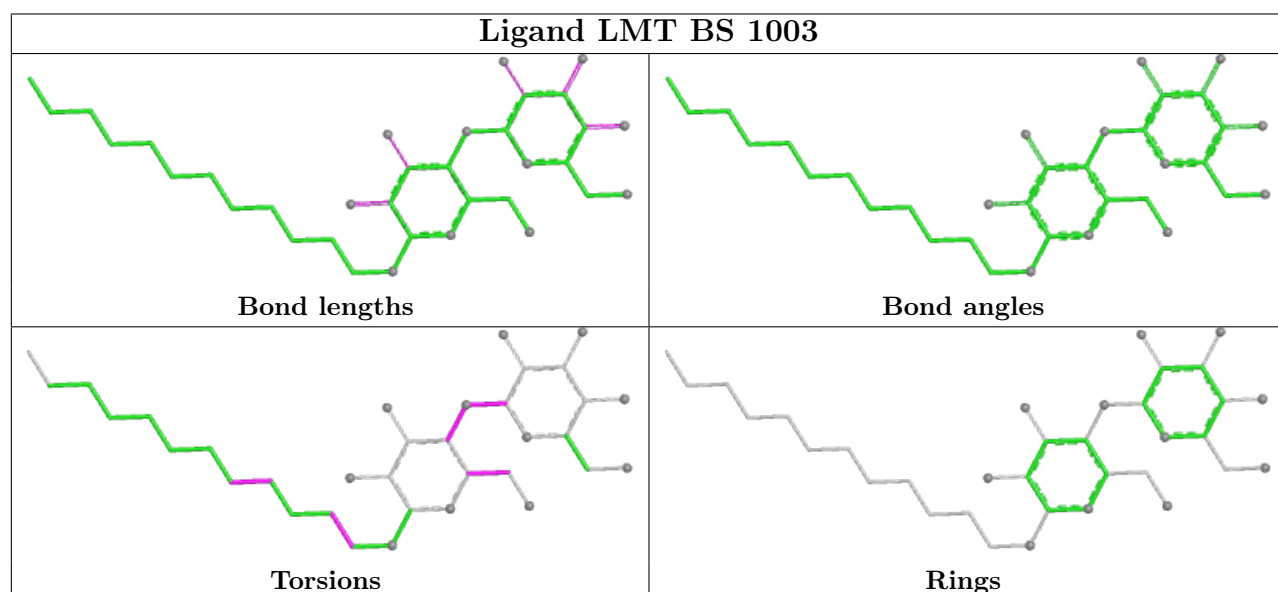
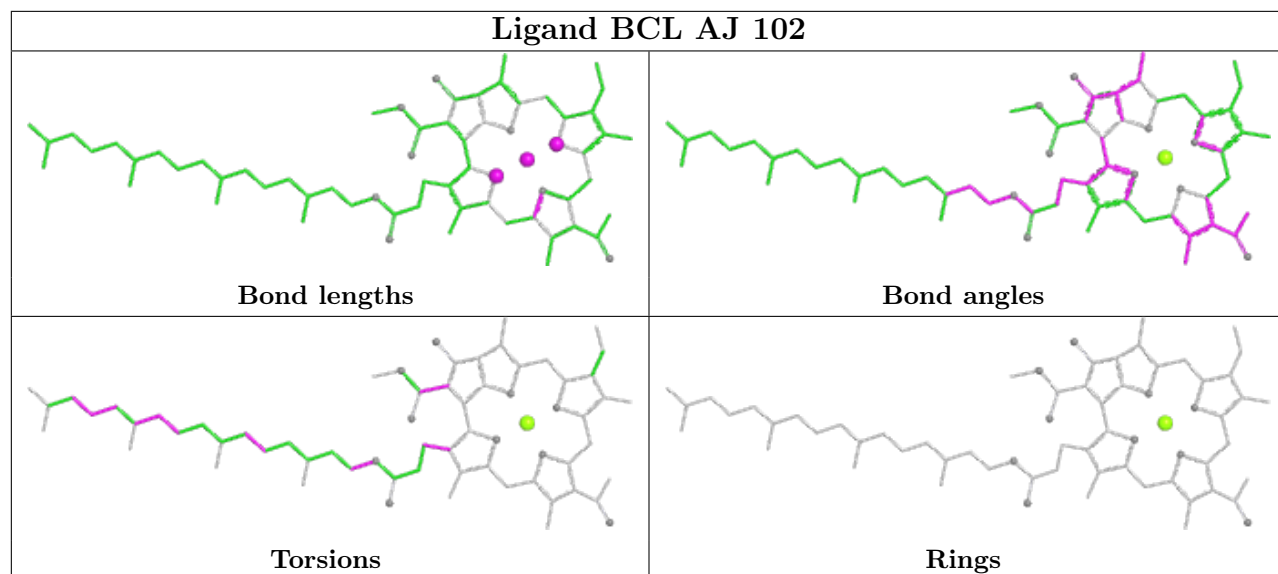


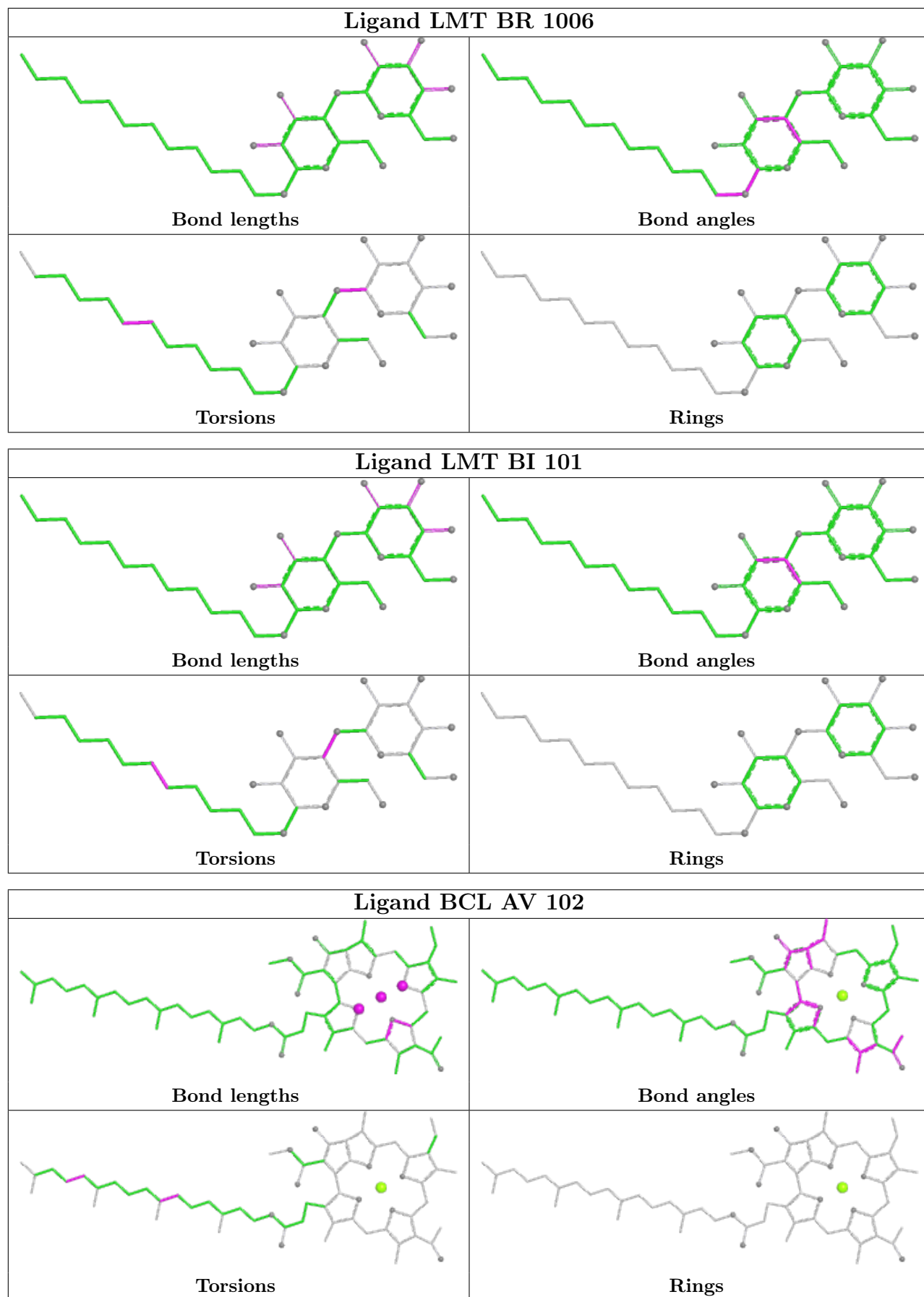




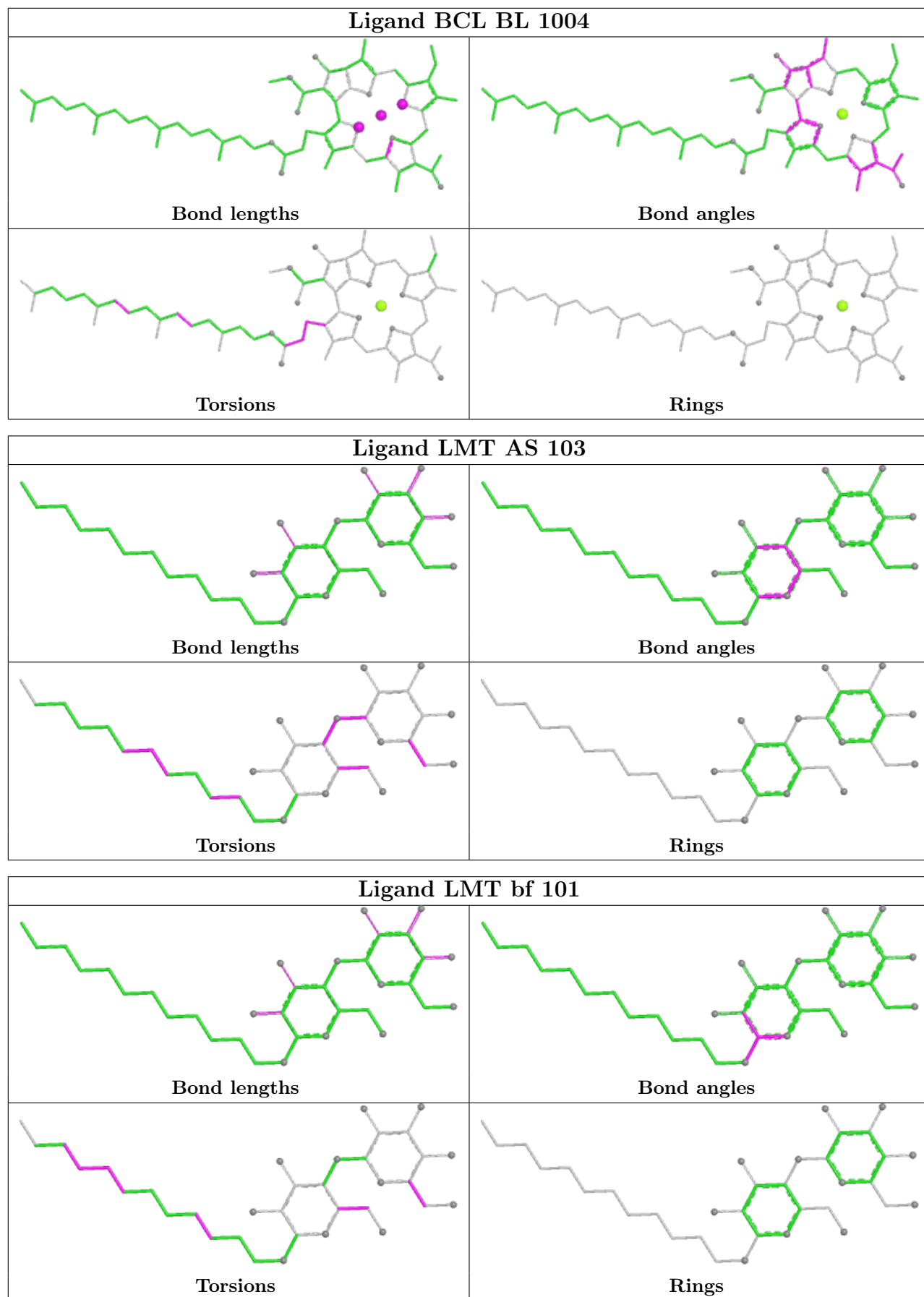


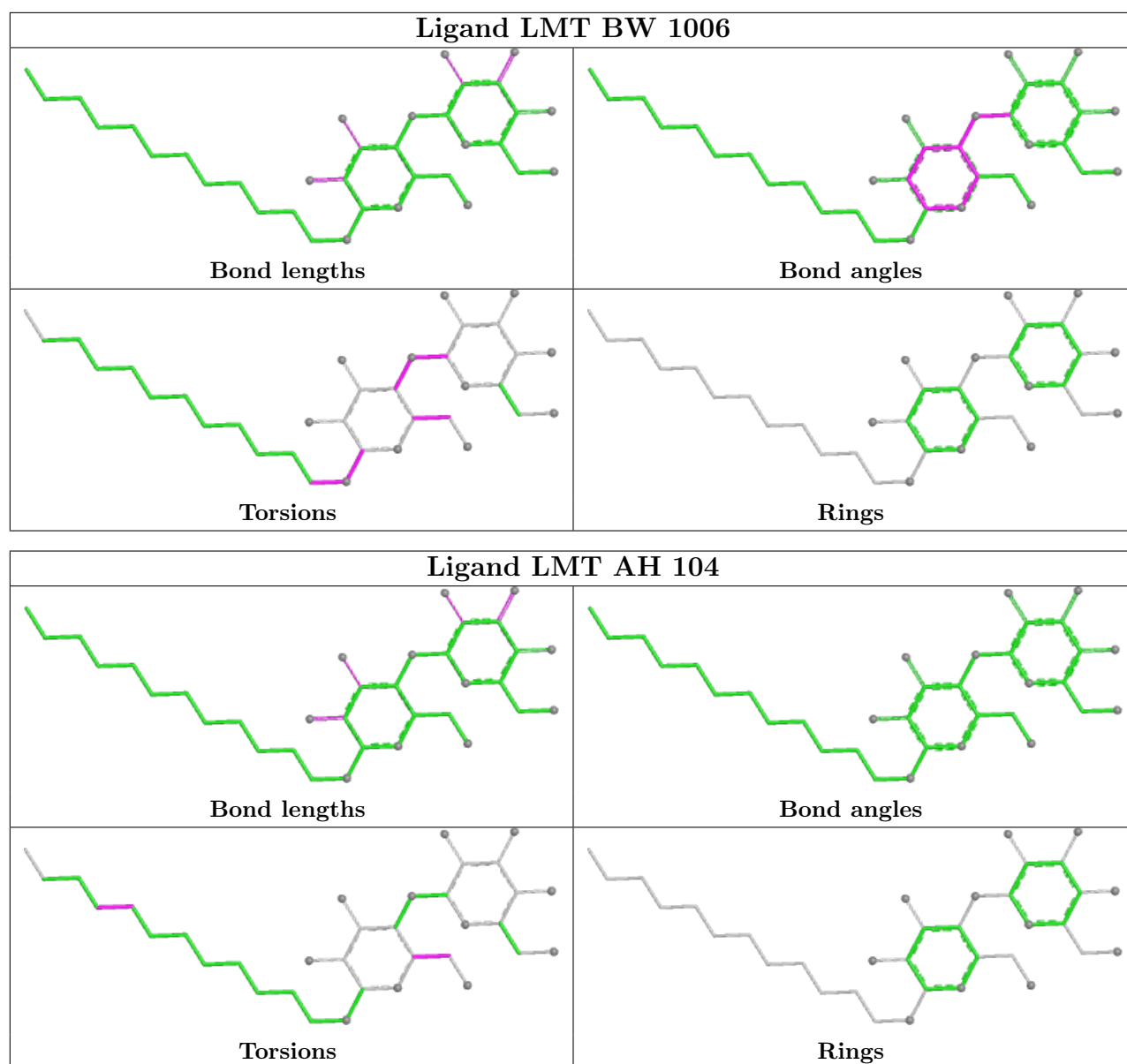












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

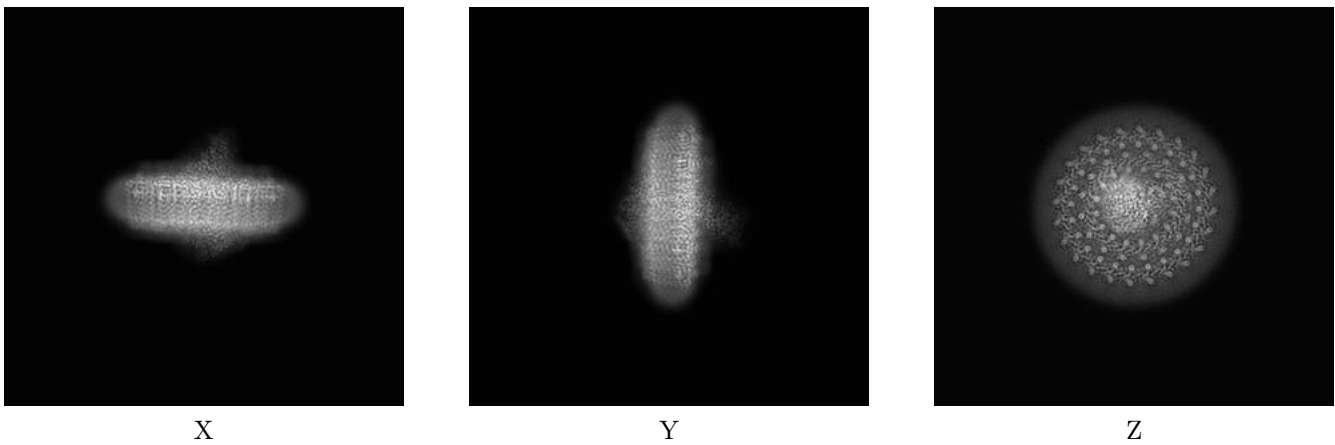
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12682. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

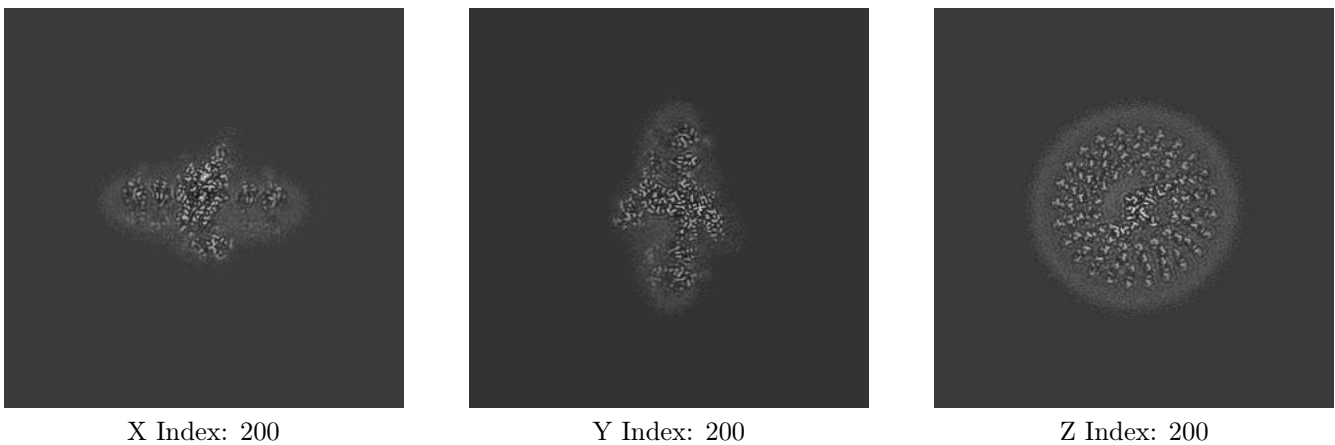
#### 6.1.1 Primary map



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

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

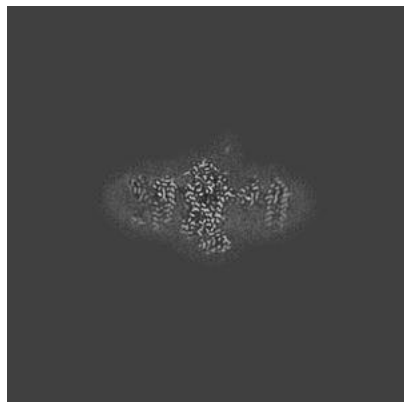
#### 6.2.1 Primary map



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

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

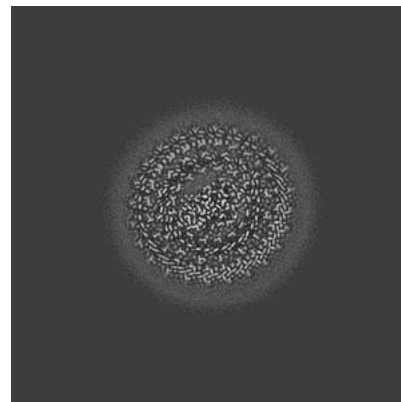
### 6.3.1 Primary map



X Index: 206



Y Index: 210

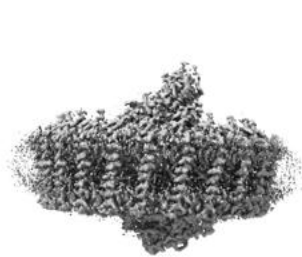


Z Index: 214

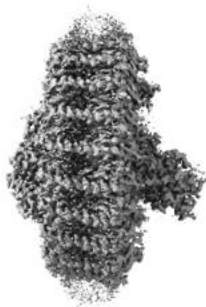
The images above show the largest variance slices of the map in three orthogonal directions.

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

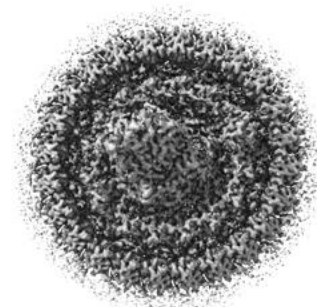
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

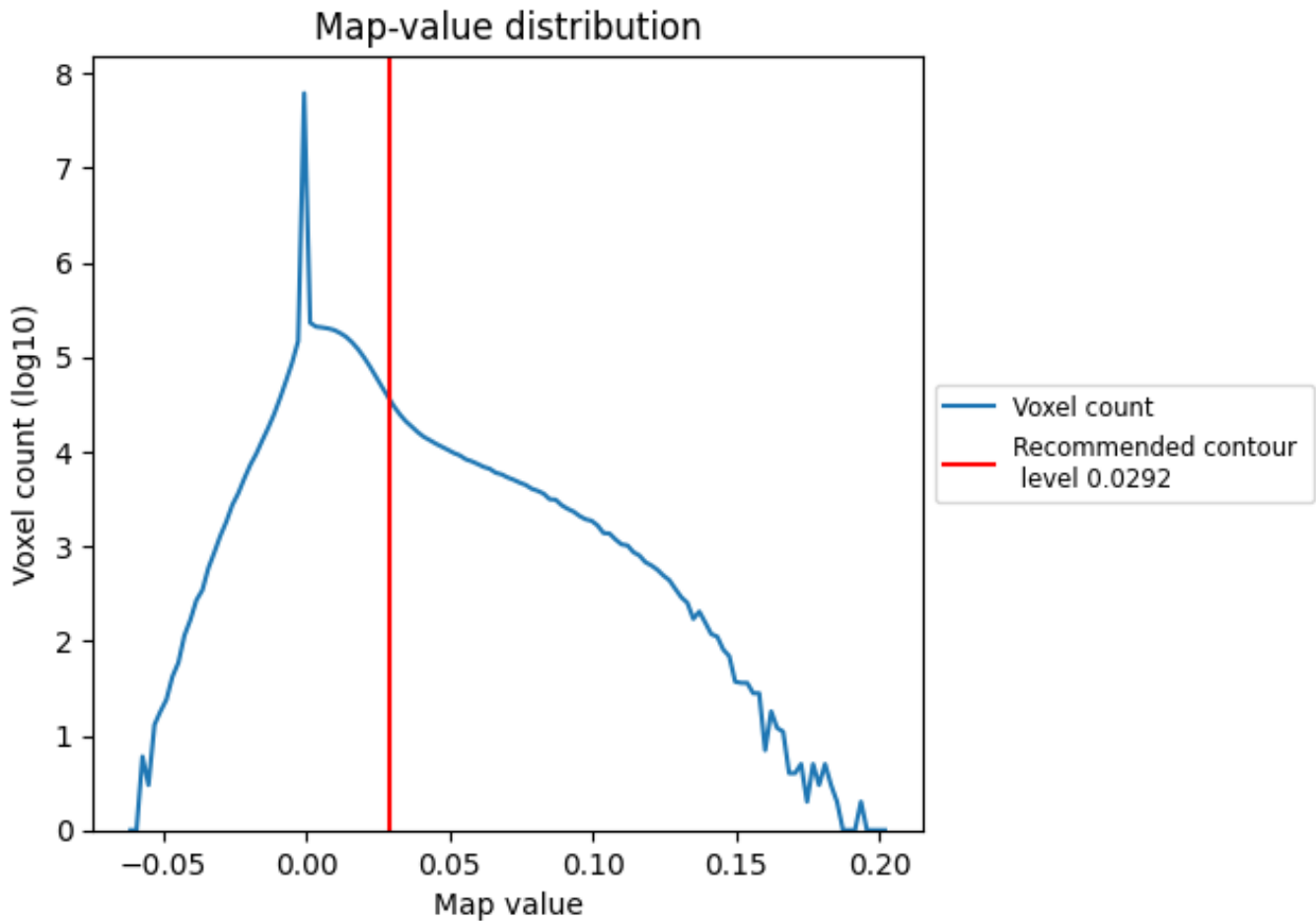
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

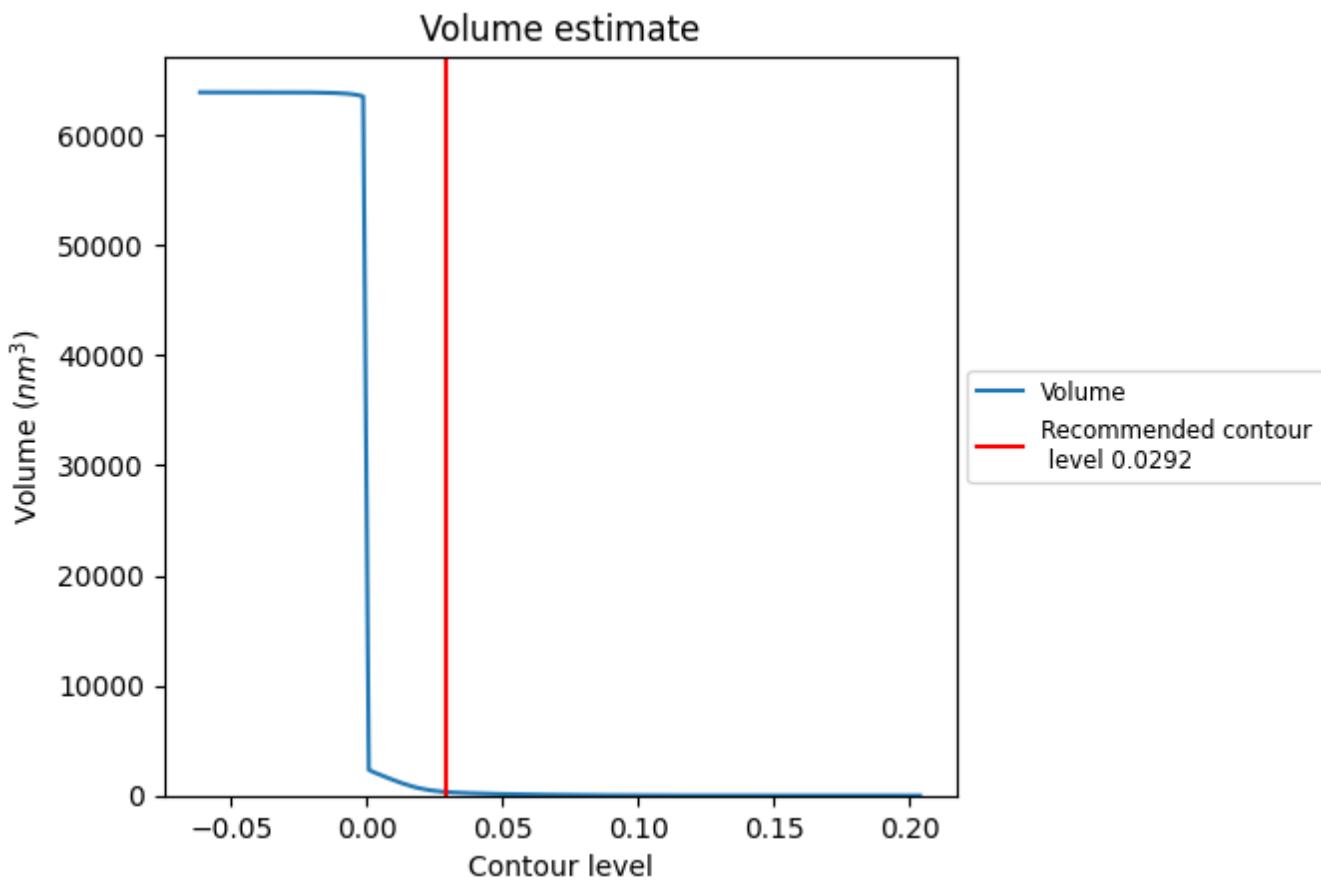
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

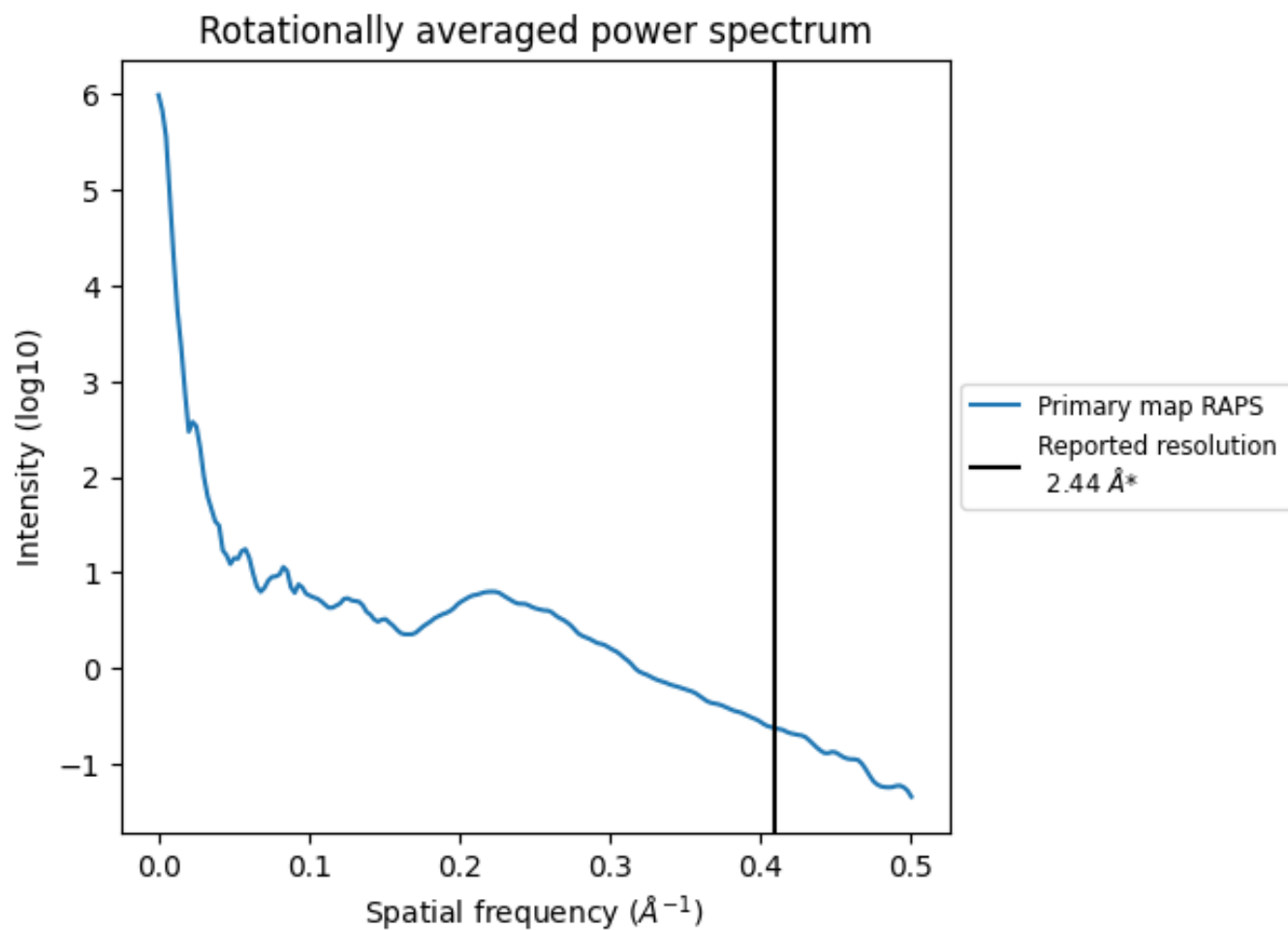
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm<sup>3</sup>; this corresponds to an approximate mass of 296 kDa.

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

### 7.3 Rotationally averaged power spectrum i



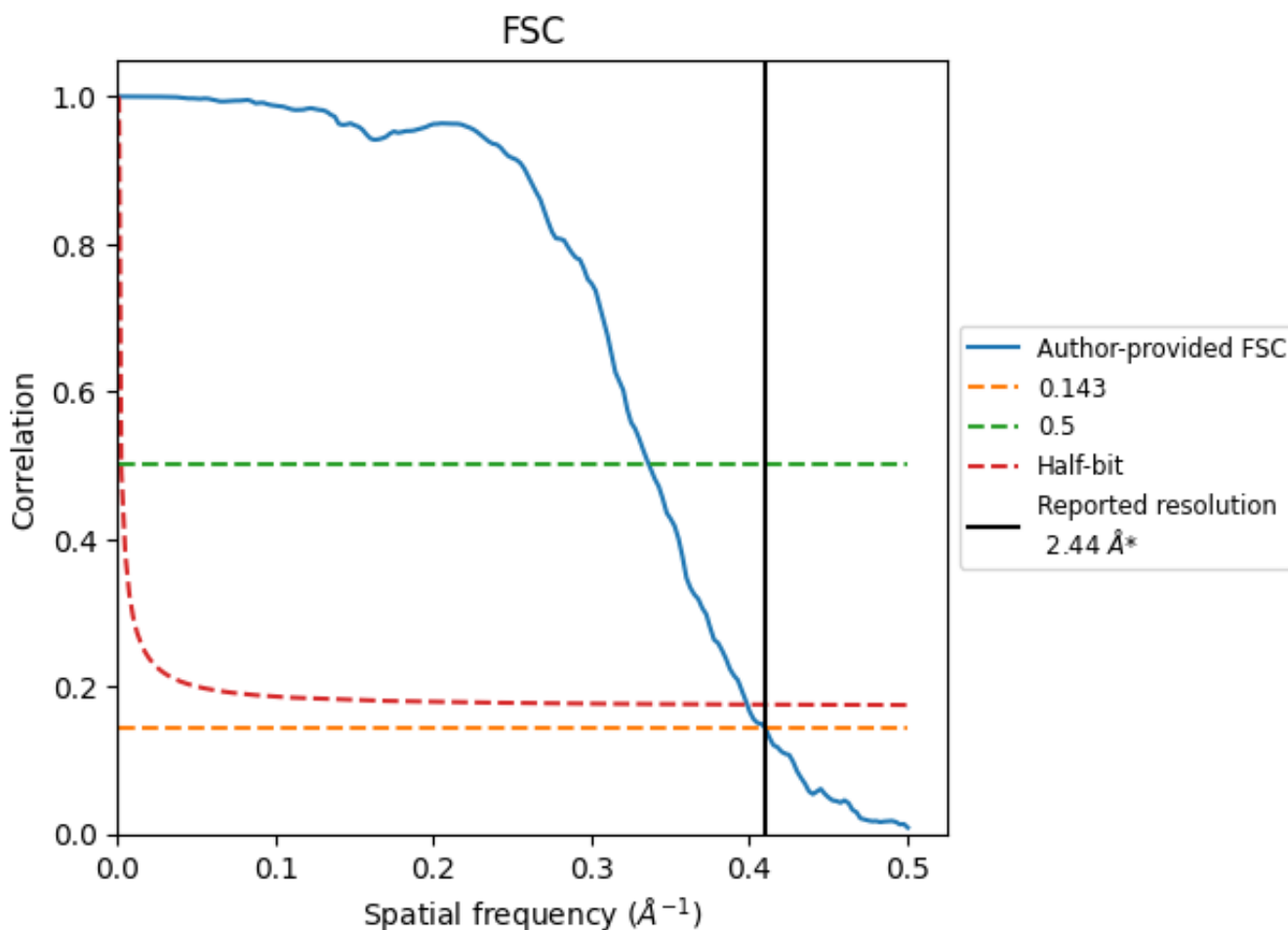
\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>



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

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

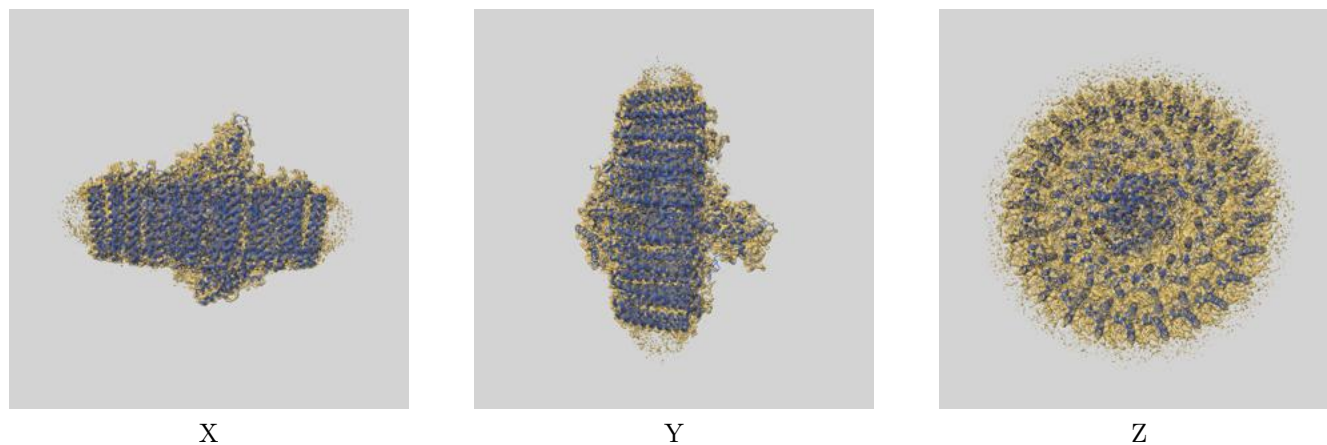
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.97	2.51
Unmasked-calculated*	-	-	-

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

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

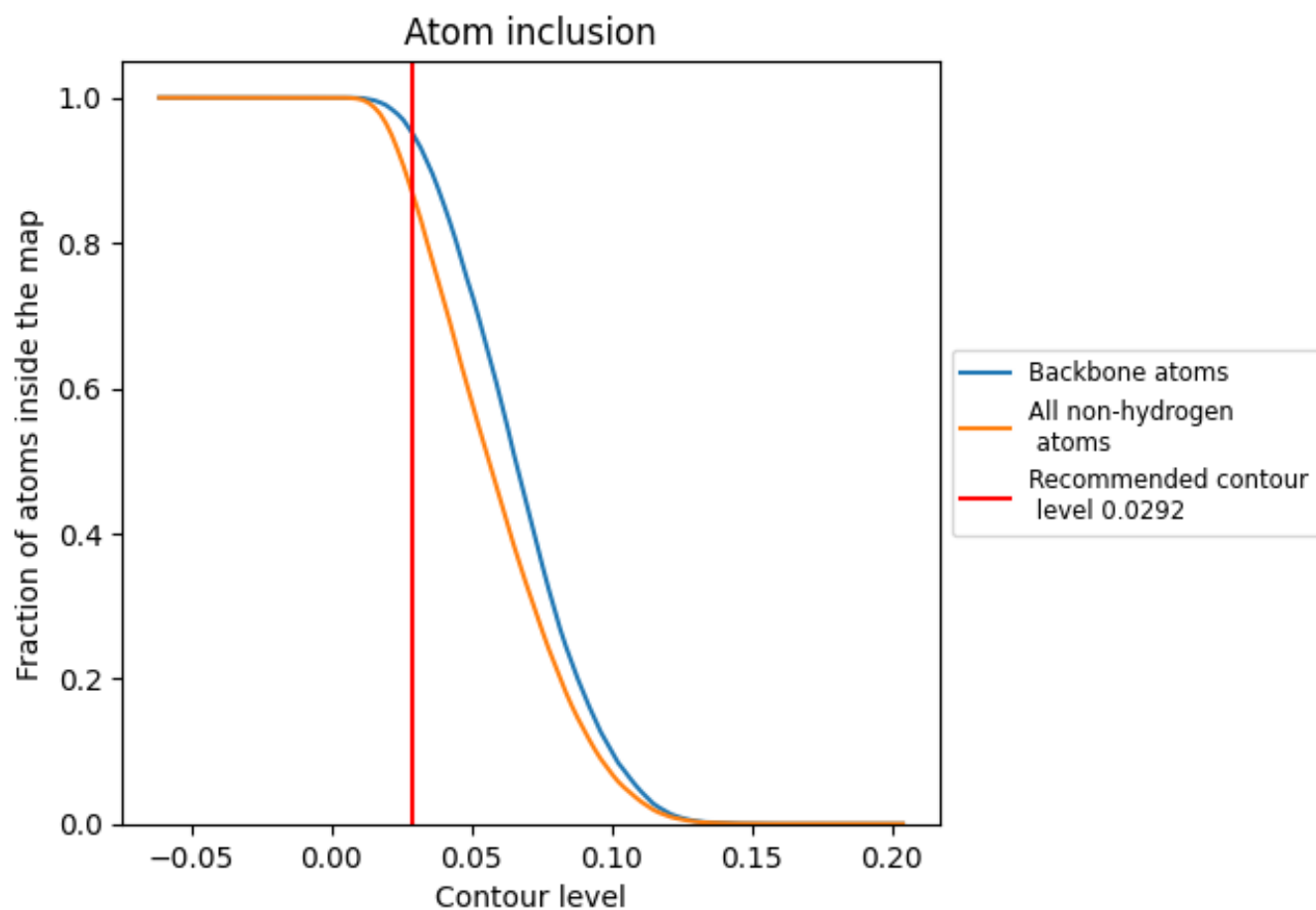
This section contains information regarding the fit between EMDB map EMD-12682 and PDB model 7O0X. Per-residue inclusion information can be found in section 3 on page 39.

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



The images above show the 3D surface view of the map at the recommended contour level 0.0292 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 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.