



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:01 AM UTC

PDB ID : 9H22 / pdb_00009h22
EMDB ID : EMD-51788
Title : Cryo EM structure of RC-dLH complex model II from Gemmatimonas groenlandica
Authors : Gardiner, A.T.; Jing, Y.; Bina, D.; Mujakic, I.; Gardian, Z.; Kaftan, D.; Joosten, M.; Jakobi, A.; Castro-Hartmann, P.; Qian, P.; Koblizek, M.
Deposited on : 2024-10-10
Resolution : 2.30 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

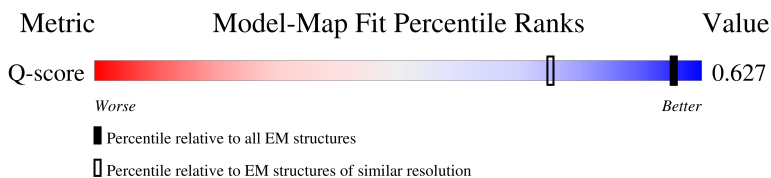
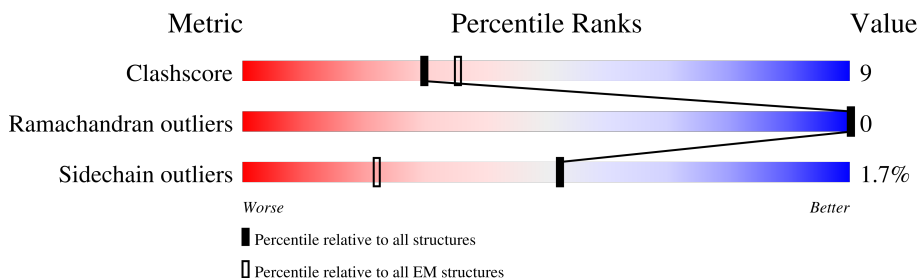
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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

Mol	Chain	Length	Quality of chain
1	S	204	
2	L	274	
3	M	392	


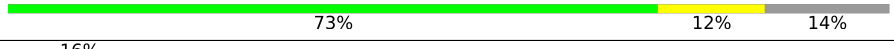
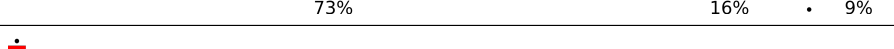
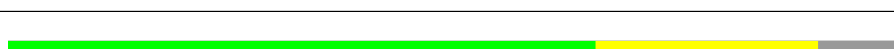



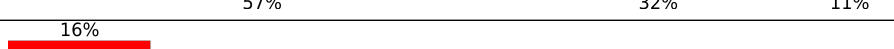



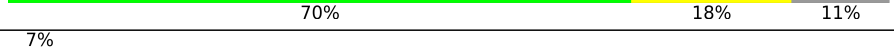

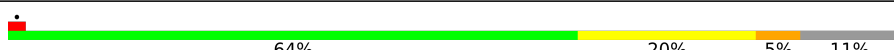


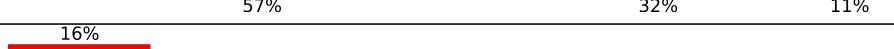







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Mol	Chain	Length	Quality of chain
4	H	66	
5	K	180	
6	C	373	
7	AA	56	
7	AB	56	
7	AC	56	
7	AD	56	
7	AE	56	
7	AF	56	
7	AG	56	
7	AH	56	
7	AI	56	
7	AJ	56	
7	AK	56	
7	AL	56	
7	AM	56	
7	AN	56	
7	AO	56	
7	AP	56	
7	AQ	56	
7	AR	56	
7	AS	56	
7	AT	56	
7	AU	56	
7	AV	56	

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Mol	Chain	Length	Quality of chain
7	AW	56	
7	AX	56	
8	BA	44	
8	BB	44	
8	BC	44	
8	BD	44	
8	BE	44	
8	BF	44	
8	BG	44	
8	BH	44	
8	BI	44	
8	BJ	44	
8	BK	44	
8	BL	44	
8	BM	44	
8	BN	44	
8	BO	44	
8	BP	44	
8	BQ	44	
8	BR	44	
8	BS	44	
8	BT	44	
8	BU	44	
8	BV	44	
8	BW	44	








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Mol	Chain	Length	Quality of chain
8	BX	44	
8	Ba	44	
8	Bb	44	
8	Bc	44	
8	Bd	44	
8	Be	44	
8	Bf	44	
8	Bg	44	
8	Bh	44	
8	Bi	44	
8	Bj	44	
8	Bk	44	
8	Bl	44	
8	Bm	44	
8	Bn	44	
8	Bo	44	
8	Bp	44	
9	Aa	71	
9	Ab	71	
9	Ac	71	
9	Ad	71	
9	Ae	71	
9	Af	71	
9	Ag	71	
9	Ah	71	

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Mol	Chain	Length	Quality of chain
9	Ai	71	
9	Aj	71	
9	Ak	71	
9	Al	71	
9	Am	71	
9	An	71	
9	Ao	71	
9	Ap	71	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49816 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 reaction centre S sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	103	Total	C	N	O	S	0	0
			800	498	150	148	4		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	271	Total	C	N	O	S	0	0
			2134	1435	346	342	11		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	335	Total	C	N	O	S	0	0
			2697	1789	441	457	10		

- Molecule 4 is a protein called reaction centre Ht su unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	60	Total	C	N	O	S	0	0
			510	338	85	85	2		

- Molecule 5 is a protein called reaction centre Hc sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	179	Total	C	N	O	S	0	0
			1373	873	231	262	7		

- Molecule 6 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	298	Total	C	N	O	S	0	0
			2330	1463	421	429	17		

- Molecule 7 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AA	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AB	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AC	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AD	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AE	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AF	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AG	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AH	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AI	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AJ	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AK	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
7	AL	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AM	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AN	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
7	AO	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AP	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AQ	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AR	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AS	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AT	48	Total	C	N	O	S	0	0
			392	262	66	61	3		
7	AU	48	Total	C	N	O	S	0	0
			392	262	66	61	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	AV	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
7	AW	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
7	AX	48	Total	C	N	O	S	0	0
			391	262	65	60	4		

- Molecule 8 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BA	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BB	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BC	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BD	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BE	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	BF	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BG	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BH	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BI	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	BJ	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BK	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BL	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BM	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BN	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BO	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BP	40	Total	C	N	O	S	0	0
			332	222	57	52	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	BQ	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BR	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BS	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BT	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BU	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
8	BV	41	Total	C	N	O	S	0	0
			341	228	59	53	1		
8	BW	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	BX	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
8	Ba	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bb	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bc	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bd	37	Total	C	N	O		0	0
			316	213	54	49			
8	Be	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bf	34	Total	C	N	O		0	0
			292	200	51	41			
8	Bg	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bh	36	Total	C	N	O		0	0
			309	209	53	47			
8	Bi	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bj	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bk	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bl	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bm	38	Total	C	N	O	S	0	0
			324	218	55	50	1		

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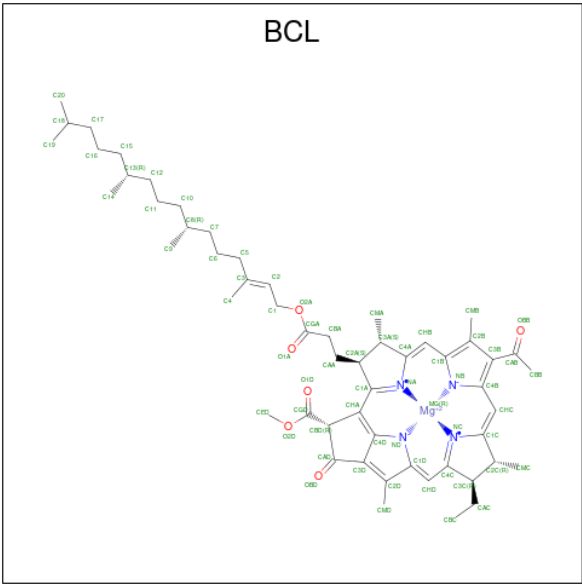
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Bn	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bo	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
8	Bp	35	Total	C	N	O		0	0
			300	204	52	44			

- Molecule 9 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aa	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
9	Ab	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
9	Ac	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
9	Ad	54	Total	C	N	O	S	0	0
			426	281	75	67	3		
9	Ae	59	Total	C	N	O	S	0	0
			454	298	80	73	3		
9	Af	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
9	Ag	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
9	Ah	53	Total	C	N	O	S	0	0
			411	272	69	67	3		
9	Ai	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
9	Aj	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
9	Ak	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
9	Al	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
9	Am	52	Total	C	N	O	S	0	0
			417	276	73	65	3		
9	An	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
9	Ao	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
9	Ap	55	Total	C	N	O	S	0	0
			432	284	76	69	3		

- Molecule 10 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
10	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
10	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BR	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BT	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BW	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ac	1	Total 66	C 55	Mg 1	N 4	O 6	0

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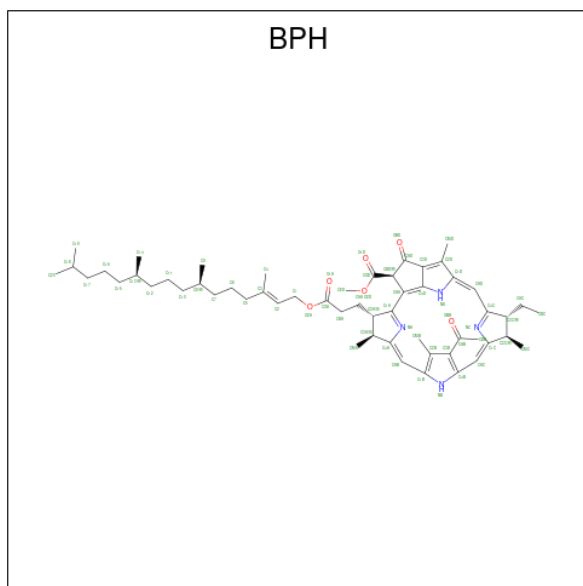
Mol	Chain	Residues	Atoms					AltConf
10	Bc	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Be	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Af	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bf	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bf	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bg	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bh	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bh	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bi	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bj	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bk	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Al	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Bl	1	Total 66	C 55	Mg 1	N 4	O 6	0

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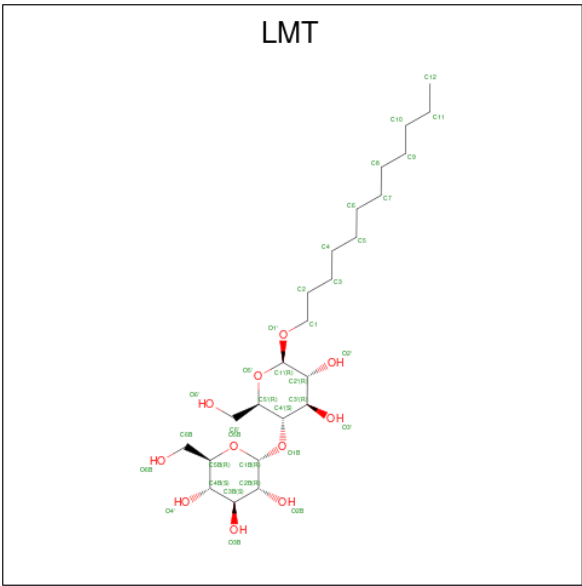
Mol	Chain	Residues	Atoms					AltConf
10	Bl	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Am	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Bm	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	An	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Bn	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Ao	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Bo	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	M	1	Total	C	O	0
			35	24	11	
12	BA	1	Total	C	O	0
			35	24	11	
12	BB	1	Total	C	O	0
			35	24	11	
12	AB	1	Total	C	O	0
			35	24	11	
12	BC	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	

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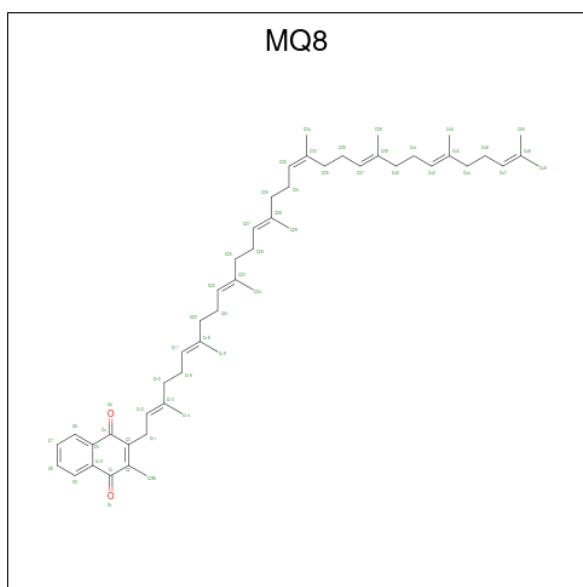
Mol	Chain	Residues	Atoms			AltConf
12	BG	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	AK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	
12	BM	1	Total	C	O	0
			35	24	11	
12	BN	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BP	1	Total	C	O	0
			35	24	11	
12	AQ	1	Total	C	O	0
			35	24	11	
12	BQ	1	Total	C	O	0
			35	24	11	
12	BR	1	Total	C	O	0
			35	24	11	
12	BS	1	Total	C	O	0
			35	24	11	
12	BT	1	Total	C	O	0
			35	24	11	
12	BU	1	Total	C	O	0
			35	24	11	
12	BV	1	Total	C	O	0
			35	24	11	
12	BX	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	BX	1	Total	C	O	0
			35	24	11	
12	Ba	1	Total	C	O	0
			35	24	11	
12	Bc	1	Total	C	O	0
			35	24	11	
12	Bc	1	Total	C	O	0
			35	24	11	
12	Bd	1	Total	C	O	0
			35	24	11	
12	Bg	1	Total	C	O	0
			35	24	11	
12	Bg	1	Total	C	O	0
			35	24	11	
12	Bi	1	Total	C	O	0
			35	24	11	
12	Bj	1	Total	C	O	0
			35	24	11	
12	Bk	1	Total	C	O	0
			35	24	11	
12	Bl	1	Total	C	O	0
			35	24	11	
12	Bm	1	Total	C	O	0
			35	24	11	
12	Bo	1	Total	C	O	0
			35	24	11	
12	Bp	1	Total	C	O	0
			35	24	11	

- Molecule 13 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).

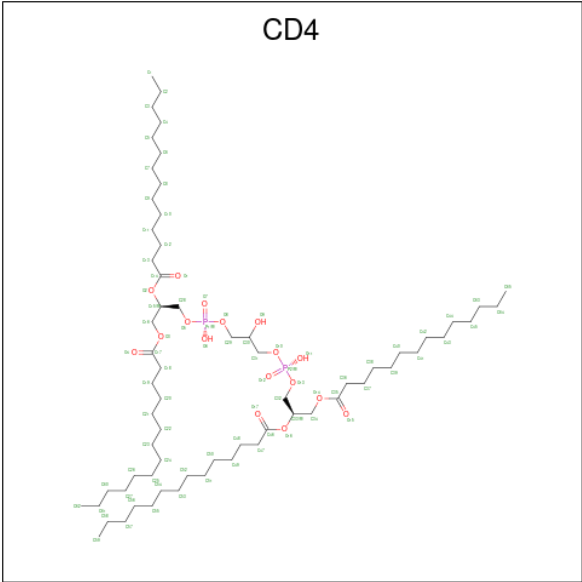


Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			53	51	2	
13	M	1	Total	C	O	0
			53	51	2	
13	Ad	1	Total	C	O	0
			53	51	2	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

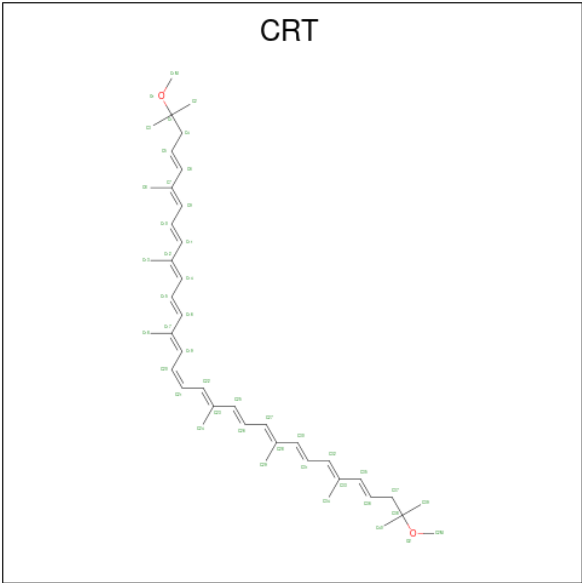
Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



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

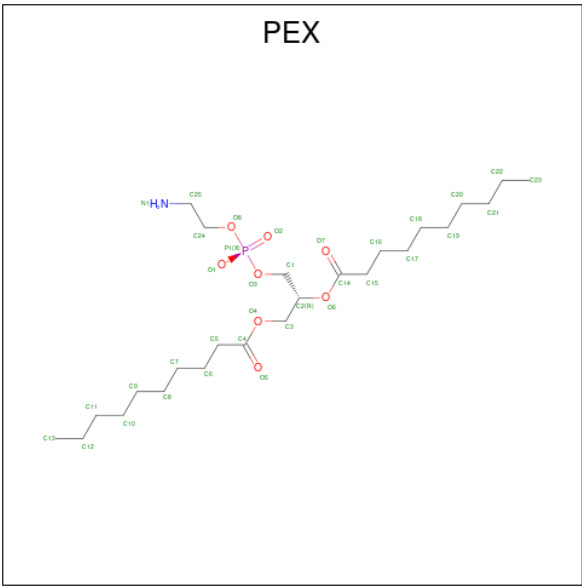
- Molecule 16 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



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

- Molecule 17 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD

ID: PEX) (formula: C₂₅H₄₉NO₈P).



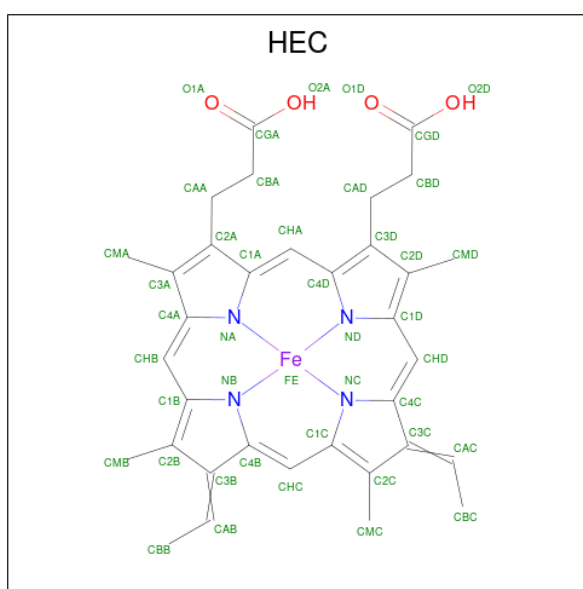
Mol	Chain	Residues	Atoms					AltConf
17	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	AG	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	AO	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	AT	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Ba	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bb	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bd	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Be	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bf	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bg	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bi	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bj	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bk	1	Total	C	N	O	P	0
			35	25	1	8	1	

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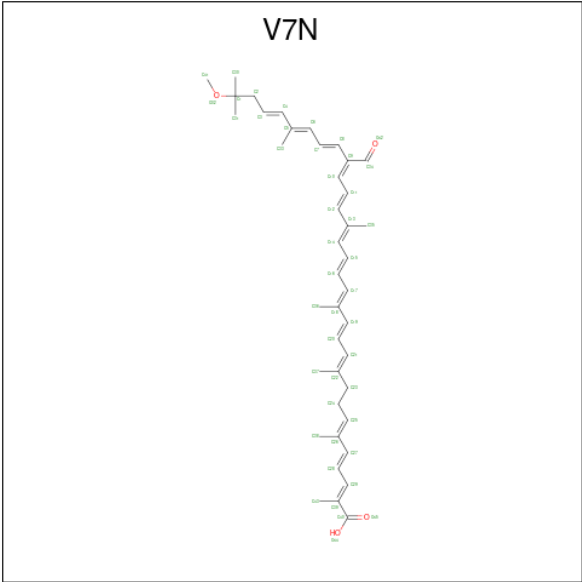
Mol	Chain	Residues	Atoms					AltConf
17	Bl	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bm	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bn	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	Bp	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 19 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: $C_{41}H_{54}O_4$).



Mol	Chain	Residues	Atoms			AltConf
19	BB	1	Total	C	O	0
			45	41	4	
19	BC	1	Total	C	O	0
			45	41	4	
19	BD	1	Total	C	O	0
			45	41	4	
19	BE	1	Total	C	O	0
			45	41	4	
19	BF	1	Total	C	O	0
			45	41	4	
19	AF	1	Total	C	O	0
			45	41	4	
19	AH	1	Total	C	O	0
			45	41	4	
19	AI	1	Total	C	O	0
			45	41	4	
19	AI	1	Total	C	O	0
			45	41	4	
19	BK	1	Total	C	O	0
			45	41	4	
19	AL	1	Total	C	O	0
			45	41	4	
19	BL	1	Total	C	O	0
			45	41	4	
19	BN	1	Total	C	O	0
			45	41	4	
19	BO	1	Total	C	O	0
			45	41	4	

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Mol	Chain	Residues	Atoms			AltConf
19	BP	1	Total	C	O	0
			45	41	4	
19	AP	1	Total	C	O	0
			45	41	4	
19	BR	1	Total	C	O	0
			45	41	4	
19	BS	1	Total	C	O	0
			45	41	4	
19	BT	1	Total	C	O	0
			45	41	4	
19	AT	1	Total	C	O	0
			45	41	4	
19	BV	1	Total	C	O	0
			45	41	4	
19	BW	1	Total	C	O	0
			45	41	4	
19	AX	1	Total	C	O	0
			45	41	4	
19	BX	1	Total	C	O	0
			45	41	4	
19	Ba	1	Total	C	O	0
			45	41	4	
19	Bb	1	Total	C	O	0
			45	41	4	
19	Bc	1	Total	C	O	0
			45	41	4	
19	Ad	1	Total	C	O	0
			45	41	4	
19	Bd	1	Total	C	O	0
			45	41	4	
19	Bf	1	Total	C	O	0
			45	41	4	
19	Ag	1	Total	C	O	0
			45	41	4	
19	Bg	1	Total	C	O	0
			45	41	4	
19	Bi	1	Total	C	O	0
			45	41	4	
19	Bj	1	Total	C	O	0
			45	41	4	
19	Bk	1	Total	C	O	0
			45	41	4	

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Mol	Chain	Residues	Atoms			AltConf
19	Bl	1	Total	C	O	0
			45	41	4	
19	Am	1	Total	C	O	0
			45	41	4	
19	Bm	1	Total	C	O	0
			45	41	4	
19	An	1	Total	C	O	0
			45	41	4	
19	Bp	1	Total	C	O	0
			45	41	4	

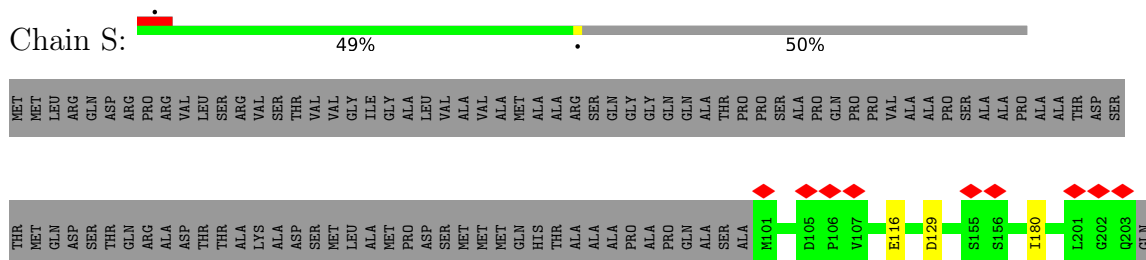
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	S	4	Total	O	0
			4	4	
20	L	11	Total	O	0
			11	11	
20	M	12	Total	O	0
			12	12	
20	K	1	Total	O	0
			1	1	
20	C	1	Total	O	0
			1	1	
20	Ad	1	Total	O	0
			1	1	
20	Ae	1	Total	O	0
			1	1	
20	Ah	1	Total	O	0
			1	1	
20	Aj	1	Total	O	0
			1	1	
20	Ak	2	Total	O	0
			2	2	
20	Al	1	Total	O	0
			1	1	
20	Am	2	Total	O	0
			2	2	

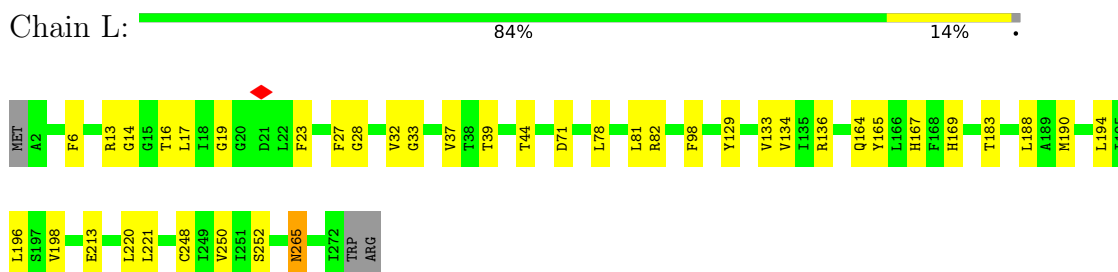
3 Residue-property plots

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

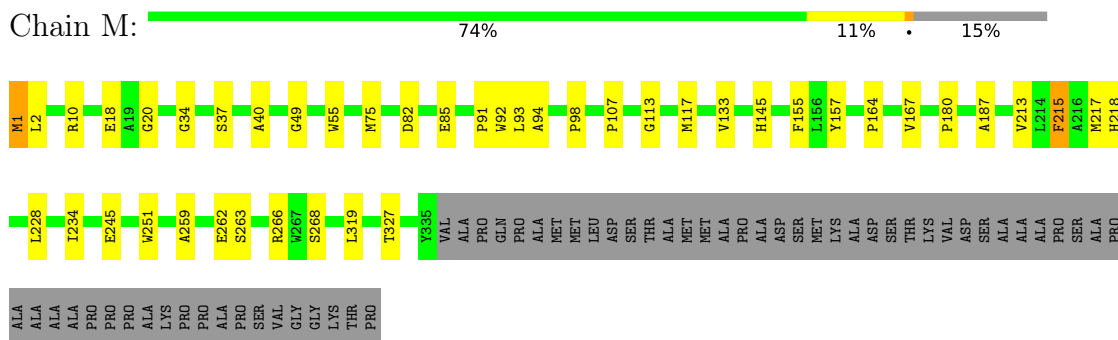
- Molecule 1: reaction centre S sub unit



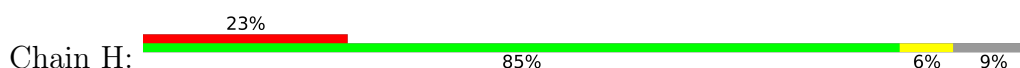
- Molecule 2: Reaction center protein L chain

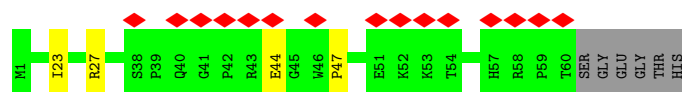


- Molecule 3: Reaction center protein M chain

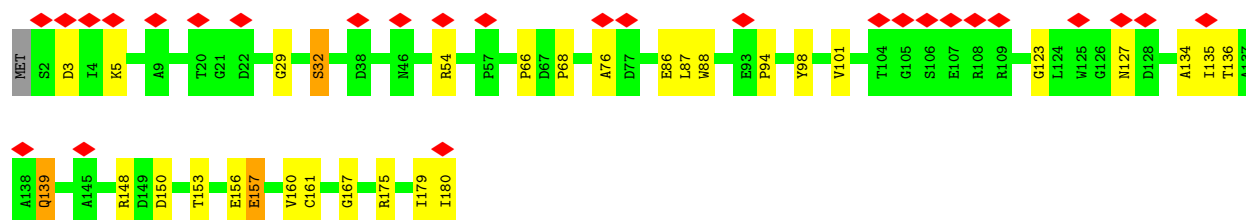
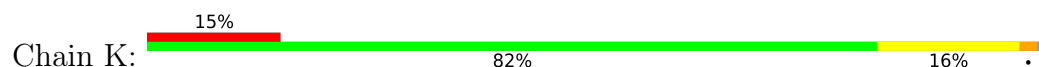


- Molecule 4: reaction centre Ht su unit

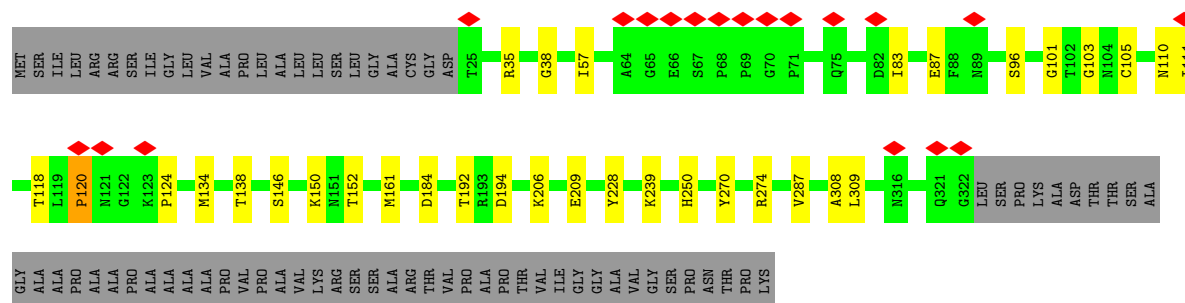




- Molecule 5: reaction centre Hc sub unit



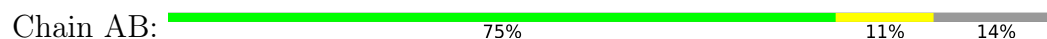
- Molecule 6: Photosynthetic reaction center cytochrome c subunit



- Molecule 7: Light-harvesting protein



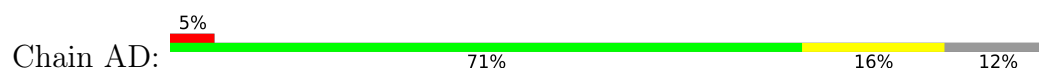
- Molecule 7: Light-harvesting protein



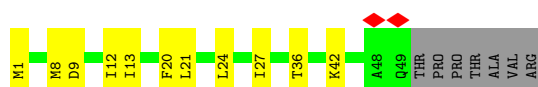
- Molecule 7: Light-harvesting protein



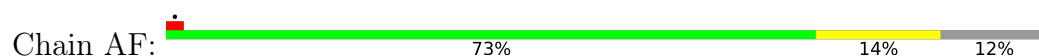
- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein



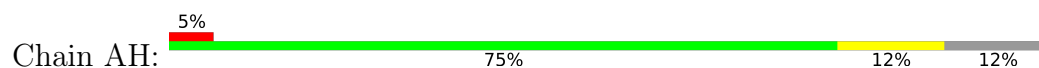
- Molecule 7: Light-harvesting protein



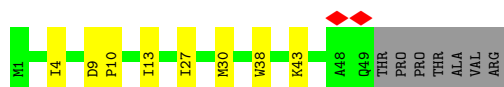
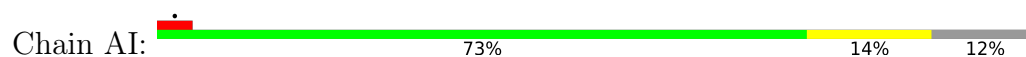
- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein

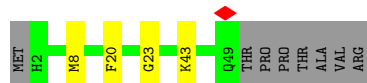
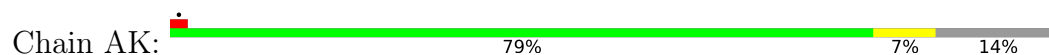


- Molecule 7: Light-harvesting protein





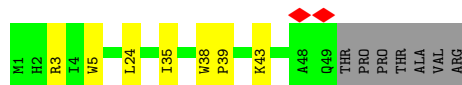
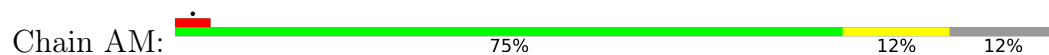
- Molecule 7: Light-harvesting protein



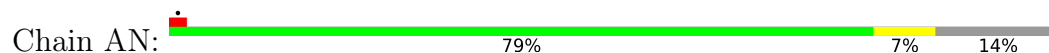
- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein



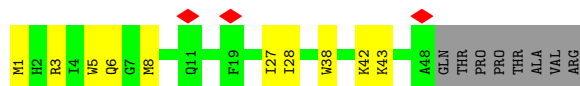
- Molecule 7: Light-harvesting protein



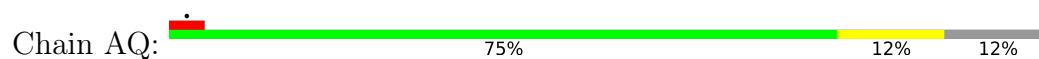
- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein



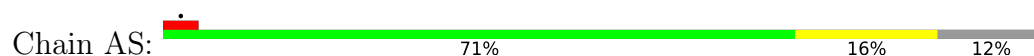
- Molecule 7: Light-harvesting protein



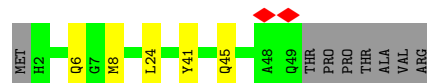
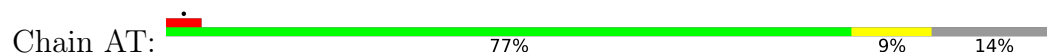
- Molecule 7: Light-harvesting protein



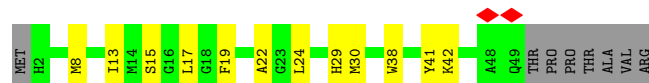
- Molecule 7: Light-harvesting protein



- Molecule 7: Light-harvesting protein



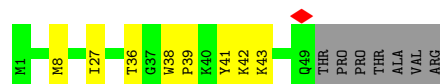
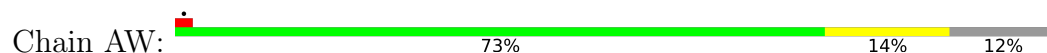
- Molecule 7: Light-harvesting protein




- Molecule 7: Light-harvesting protein

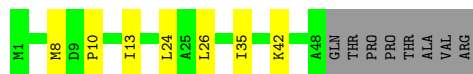


- Molecule 7: Light-harvesting protein




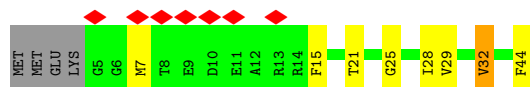
- Molecule 7: Light-harvesting protein

Chain AX:  73% 12% 14%




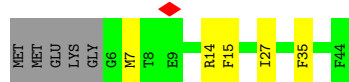
- Molecule 8: Light-harvesting protein

Chain BA:  16% 73% 16% 9%



- Molecule 8: Light-harvesting protein

Chain BB:  77% 11% 11%




- Molecule 8: Light-harvesting protein

Chain BC:  66% 25% 9%



- Molecule 8: Light-harvesting protein

Chain BD:  7% 73% 18% 9%



- Molecule 8: Light-harvesting protein

Chain BE:  5% 64% 20% 14%

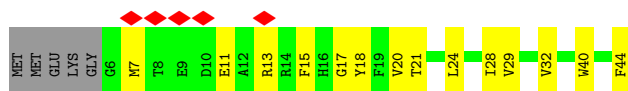


- Molecule 8: Light-harvesting protein

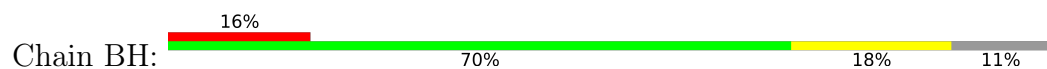
Chain BF:  5% 64% 25% 11%



- Molecule 8: Light-harvesting protein



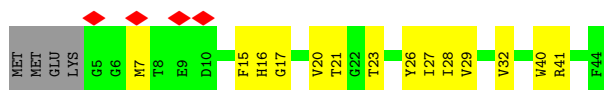
- Molecule 8: Light-harvesting protein



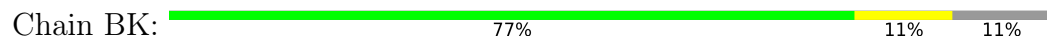
- Molecule 8: Light-harvesting protein



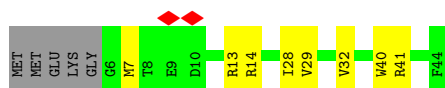
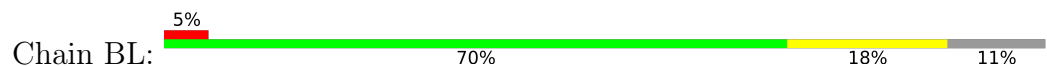
- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



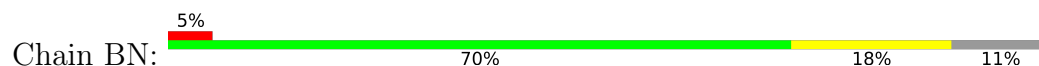
- Molecule 8: Light-harvesting protein



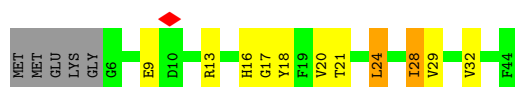
- Molecule 8: Light-harvesting protein



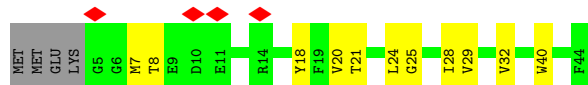
- Molecule 8: Light-harvesting protein



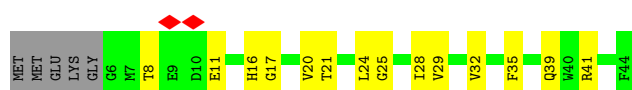
- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



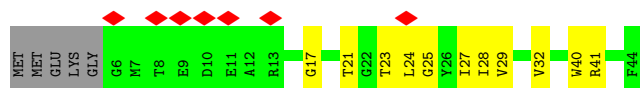
- Molecule 8: Light-harvesting protein



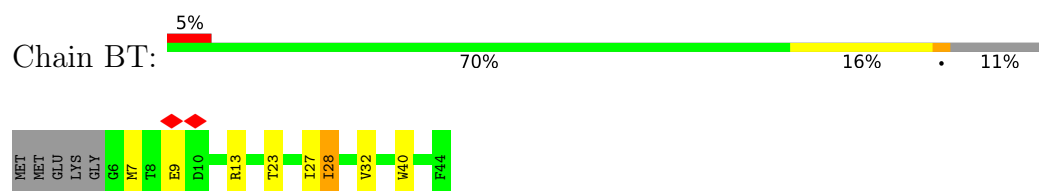
- Molecule 8: Light-harvesting protein



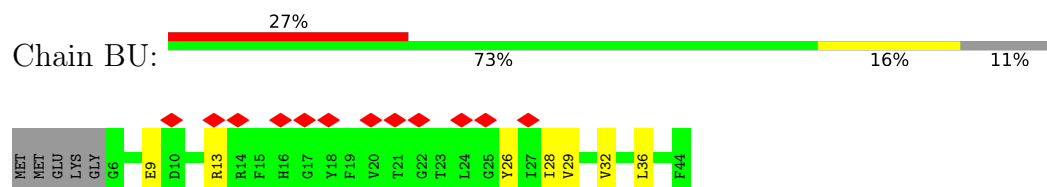
- Molecule 8: Light-harvesting protein



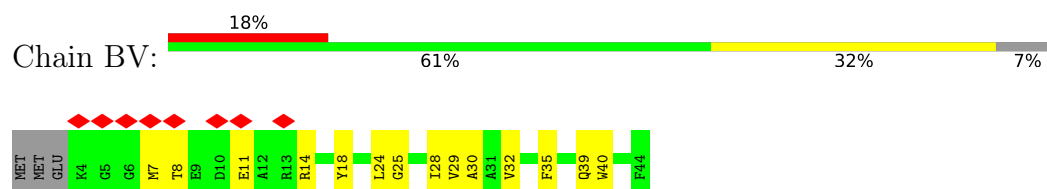
• Molecule 8: Light-harvesting protein



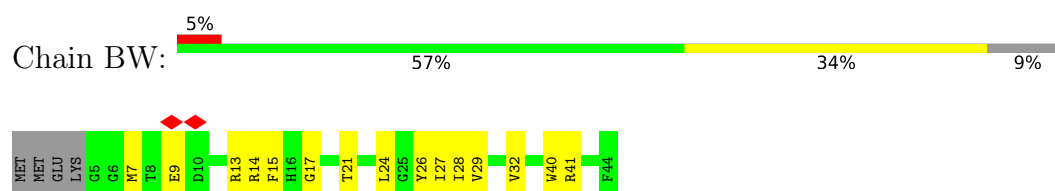
• Molecule 8: Light-harvesting protein



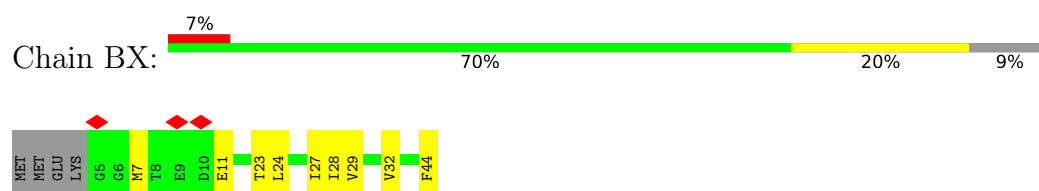
• Molecule 8: Light-harvesting protein



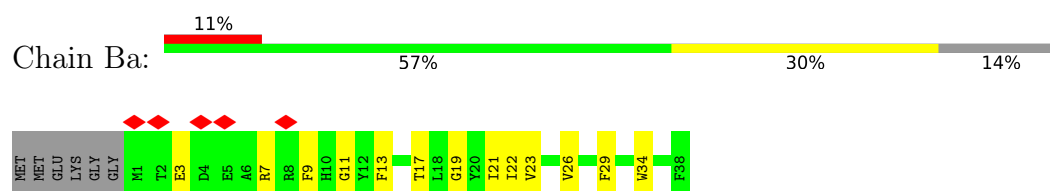
• Molecule 8: Light-harvesting protein



• Molecule 8: Light-harvesting protein

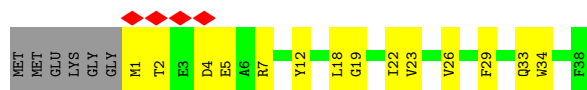


• Molecule 8: Light-harvesting protein



• Molecule 8: Light-harvesting protein





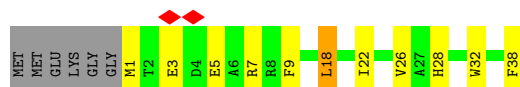
- Molecule 8: Light-harvesting protein



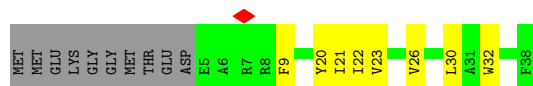
- Molecule 8: Light-harvesting protein



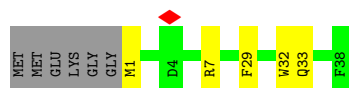
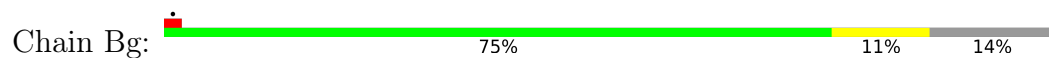
- Molecule 8: Light-harvesting protein



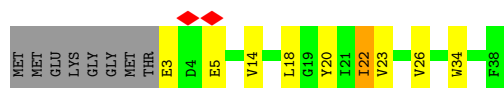
- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



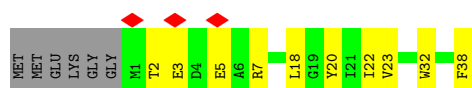
- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



- Molecule 8: Light-harvesting protein



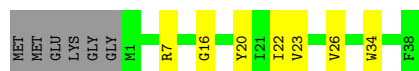
- Molecule 8: Light-harvesting protein



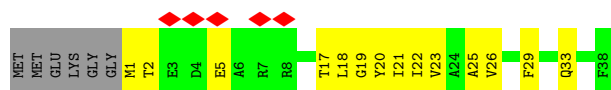
- Molecule 8: Light-harvesting protein



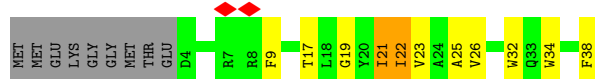
- Molecule 8: Light-harvesting protein



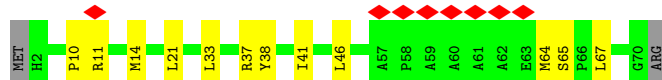
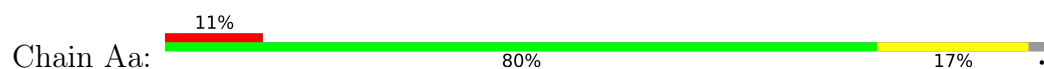
- Molecule 8: Light-harvesting protein



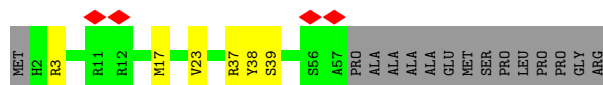
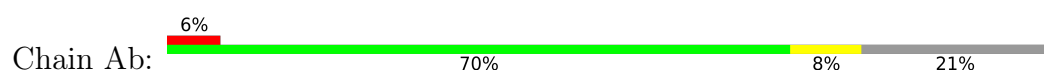
- Molecule 8: Light-harvesting protein



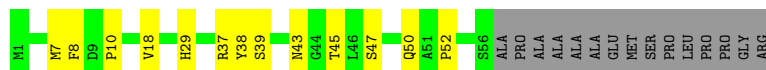
- Molecule 9: Light-harvesting protein



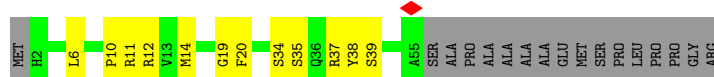
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



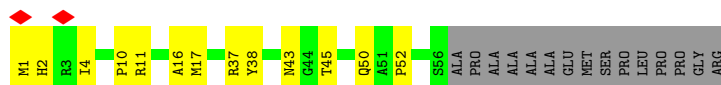
- Molecule 9: Light-harvesting protein



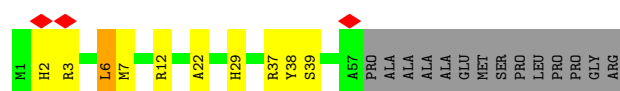
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



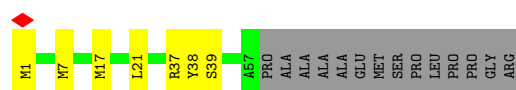
• Molecule 9: Light-harvesting protein



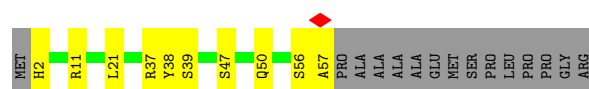
• Molecule 9: Light-harvesting protein



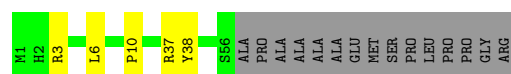
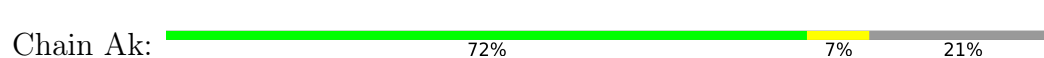
• Molecule 9: Light-harvesting protein



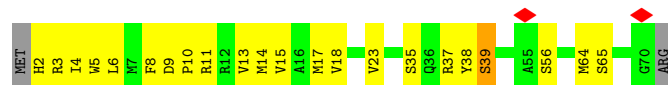
• Molecule 9: Light-harvesting protein



• Molecule 9: Light-harvesting protein



• Molecule 9: Light-harvesting protein

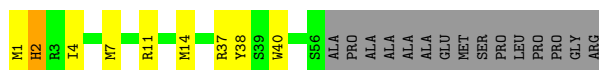


• Molecule 9: Light-harvesting protein

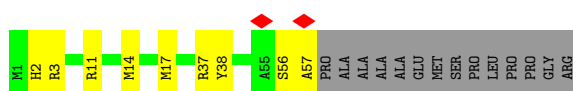




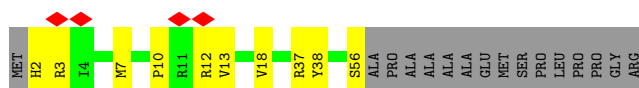
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF collection was performed within cryosparc	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0687	Depositor
Map size (\AA)	439.19998, 439.19998, 439.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.732, 0.732, 0.732	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V7N, PEX, MQ8, LMT, CD4, FE, BCL, CRT, HEC, BPH

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	S	0.14	0/819	0.26	0/1112
2	L	0.18	0/2217	0.33	0/3031
3	M	0.20	0/2796	0.36	0/3821
4	H	0.15	0/529	0.34	0/716
5	K	0.15	0/1408	0.34	0/1925
6	C	0.36	3/2395 (0.1%)	0.66	3/3268 (0.1%)
7	AA	0.20	0/405	0.39	0/547
7	AB	0.20	0/405	0.35	0/547
7	AC	0.20	0/405	0.39	0/547
7	AD	0.20	0/414	0.40	0/559
7	AE	0.19	0/414	0.34	0/559
7	AF	0.22	0/414	0.43	0/559
7	AG	0.19	0/414	0.40	0/559
7	AH	0.19	0/414	0.34	0/559
7	AI	0.19	0/414	0.41	0/559
7	AJ	0.23	0/405	0.48	0/547
7	AK	0.21	0/406	0.42	0/549
7	AL	0.20	0/405	0.40	0/547
7	AM	0.20	0/414	0.39	0/559
7	AN	0.26	0/406	0.53	0/549
7	AO	0.20	0/405	0.39	0/547
7	AP	0.20	0/405	0.41	0/547
7	AQ	0.18	0/414	0.34	0/559
7	AR	0.21	0/405	0.40	0/547
7	AS	0.24	0/414	0.41	0/559
7	AT	0.20	0/406	0.41	0/549
7	AU	0.22	0/406	0.39	0/549
7	AV	0.20	0/405	0.40	0/547
7	AW	0.20	0/414	0.41	0/559
7	AX	0.18	0/405	0.34	0/547
8	BA	0.18	0/346	0.33	0/471
8	BB	0.18	0/342	0.28	0/466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	BC	0.19	0/346	0.31	0/471
8	BD	0.19	0/346	0.36	0/471
8	BE	0.20	0/338	0.35	0/461
8	BF	0.17	0/342	0.30	0/466
8	BG	0.21	0/342	0.43	0/466
8	BH	0.21	0/342	0.35	0/466
8	BI	0.22	0/338	0.38	0/461
8	BJ	0.19	0/346	0.33	0/471
8	BK	0.21	0/342	0.38	0/466
8	BL	0.20	0/342	0.33	0/466
8	BM	0.20	0/346	0.31	0/471
8	BN	0.19	0/342	0.30	0/466
8	BO	0.20	0/342	0.38	0/466
8	BP	0.18	0/346	0.37	0/471
8	BQ	0.18	0/342	0.38	0/466
8	BR	0.21	0/342	0.41	0/466
8	BS	0.19	0/342	0.38	0/466
8	BT	0.17	0/342	0.34	0/466
8	BU	0.20	0/342	0.40	0/466
8	BV	0.19	0/355	0.45	0/482
8	BW	0.22	0/346	0.40	0/471
8	BX	0.20	0/346	0.33	0/471
8	Ba	0.20	0/338	0.32	0/461
8	Bb	0.20	0/338	0.39	0/461
8	Bc	0.21	0/338	0.31	0/461
8	Bd	0.26	0/330	0.42	0/451
8	Be	0.21	0/338	0.43	0/461
8	Bf	0.22	0/306	0.42	0/418
8	Bg	0.20	0/338	0.28	0/461
8	Bh	0.20	0/323	0.39	0/441
8	Bi	0.25	0/338	0.35	0/461
8	Bj	0.31	0/338	0.45	0/461
8	Bk	0.21	0/338	0.29	0/461
8	Bl	0.24	0/338	0.59	3/461 (0.7%)
8	Bm	0.19	0/338	0.27	0/461
8	Bn	0.19	0/338	0.29	0/461
8	Bo	0.21	0/338	0.38	0/461
8	Bp	0.27	0/314	0.68	2/429 (0.5%)
9	Aa	0.18	0/535	0.35	0/731
9	Ab	0.17	0/448	0.29	0/609
9	Ac	0.19	0/451	0.33	0/612
9	Ad	0.20	0/437	0.36	0/594
9	Ae	0.20	0/466	0.33	0/635

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	Af	0.19	0/451	0.38	0/612
9	Ag	0.19	0/456	0.34	0/619
9	Ah	0.18	0/421	0.31	0/573
9	Ai	0.18	0/456	0.36	0/619
9	Aj	0.18	0/448	0.33	0/609
9	Ak	0.19	0/451	0.31	0/612
9	Al	0.21	0/535	0.34	0/731
9	Am	0.22	0/428	0.32	0/582
9	An	0.20	0/451	0.35	0/612
9	Ao	0.18	0/456	0.28	0/619
9	Ap	0.17	0/443	0.30	0/602
All	All	0.21	3/40885 (0.0%)	0.39	8/55601 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AN	0	1
8	Bl	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	120	PRO	CG-CD	-11.97	1.10	1.50
6	C	120	PRO	N-CA	5.98	1.55	1.47
6	C	120	PRO	CB-CG	-5.03	1.24	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	120	PRO	N-CD-CG	-20.45	72.53	103.20
6	C	120	PRO	CA-CB-CG	-18.07	70.17	104.50
6	C	120	PRO	CB-CG-CD	15.47	155.61	106.10
8	Bp	21	ILE	CA-C-N	-6.29	112.71	122.09
8	Bp	21	ILE	C-N-CA	-6.29	112.71	122.09
8	Bl	22	ILE	CA-CB-CG1	6.18	120.92	110.40
8	Bl	21	ILE	CA-C-N	-5.25	115.42	122.72
8	Bl	21	ILE	C-N-CA	-5.25	115.42	122.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AN	19	PHE	Sidechain
8	BI	22	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	800	0	793	3	0
2	L	2134	0	2107	30	0
3	M	2697	0	2621	39	0
4	H	510	0	500	3	0
5	K	1373	0	1347	21	0
6	C	2330	0	2253	23	0
7	AA	391	0	394	7	0
7	AB	391	0	394	6	0
7	AC	391	0	394	8	0
7	AD	400	0	402	8	0
7	AE	400	0	402	13	0
7	AF	400	0	402	10	0
7	AG	400	0	402	10	0
7	AH	400	0	402	7	0
7	AI	400	0	402	8	0
7	AJ	391	0	394	8	0
7	AK	392	0	390	4	0
7	AL	391	0	394	12	0
7	AM	400	0	402	10	0
7	AN	392	0	390	2	0
7	AO	391	0	394	11	0
7	AP	391	0	394	10	0
7	AQ	400	0	402	7	0
7	AR	391	0	394	14	0
7	AS	400	0	402	10	0
7	AT	392	0	390	4	0
7	AU	392	0	390	10	0
7	AV	391	0	394	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AW	400	0	402	10	0
7	AX	391	0	394	7	0
8	BA	332	0	308	7	0
8	BB	328	0	305	4	0
8	BC	332	0	308	9	0
8	BD	332	0	308	7	0
8	BE	324	0	305	10	0
8	BF	328	0	305	10	0
8	BG	328	0	305	12	0
8	BH	328	0	305	8	0
8	BI	324	0	305	13	0
8	BJ	332	0	308	9	0
8	BK	328	0	305	5	0
8	BL	328	0	305	7	0
8	BM	332	0	308	11	0
8	BN	328	0	305	6	0
8	BO	328	0	305	7	0
8	BP	332	0	308	11	0
8	BQ	328	0	305	11	0
8	BR	328	0	305	14	0
8	BS	328	0	305	10	0
8	BT	328	0	305	7	0
8	BU	328	0	305	5	0
8	BV	341	0	321	10	0
8	BW	332	0	308	13	0
8	BX	332	0	308	7	0
8	Ba	324	0	305	14	0
8	Bb	324	0	305	13	0
8	Bc	324	0	305	6	0
8	Bd	316	0	293	6	0
8	Be	324	0	305	10	0
8	Bf	292	0	276	10	0
8	Bg	324	0	305	4	0
8	Bh	309	0	286	11	0
8	Bi	324	0	305	12	0
8	Bj	324	0	305	15	0
8	Bk	324	0	305	6	0
8	Bl	324	0	305	14	0
8	Bm	324	0	305	5	0
8	Bn	324	0	305	6	0
8	Bo	324	0	305	12	0
8	Bp	300	0	280	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Aa	520	0	532	13	0
9	Ab	437	0	450	6	0
9	Ac	440	0	457	9	0
9	Ad	426	0	440	12	0
9	Ae	454	0	467	12	0
9	Af	440	0	457	17	0
9	Ag	445	0	462	9	0
9	Ah	411	0	425	6	0
9	Ai	445	0	462	4	0
9	Aj	437	0	450	6	0
9	Ak	440	0	457	4	0
9	Al	520	0	532	18	0
9	Am	417	0	432	10	0
9	An	440	0	457	8	0
9	Ao	445	0	462	7	0
9	Ap	432	0	445	8	0
10	AB	66	0	71	4	0
10	AC	66	0	74	3	0
10	AD	66	0	70	2	0
10	AE	66	0	74	4	0
10	AF	66	0	74	5	0
10	AH	66	0	74	2	0
10	AI	66	0	74	4	0
10	AK	66	0	74	5	0
10	AL	66	0	74	2	0
10	AM	66	0	74	4	0
10	AN	66	0	74	1	0
10	AO	66	0	74	7	0
10	AP	66	0	72	5	0
10	AQ	132	0	142	9	0
10	AR	66	0	74	6	0
10	AT	132	0	145	2	0
10	AU	132	0	146	6	0
10	AV	66	0	74	3	0
10	AW	66	0	74	4	0
10	AX	66	0	74	2	0
10	Aa	66	0	74	7	0
10	Ac	66	0	74	4	0
10	Ae	66	0	74	2	0
10	Af	66	0	74	4	0
10	Ag	66	0	74	1	0
10	Ah	66	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Ai	66	0	74	3	0
10	Aj	66	0	74	6	0
10	Ak	66	0	72	1	0
10	Al	66	0	74	1	0
10	Am	66	0	74	2	0
10	An	66	0	74	4	0
10	Ao	66	0	74	1	0
10	BA	66	0	74	0	0
10	BB	66	0	74	2	0
10	BC	66	0	74	1	0
10	BD	66	0	74	2	0
10	BE	66	0	74	2	0
10	BF	66	0	74	2	0
10	BG	66	0	74	1	0
10	BH	66	0	74	1	0
10	BI	66	0	74	2	0
10	BJ	66	0	74	0	0
10	BK	66	0	74	0	0
10	BL	66	0	74	2	0
10	BM	66	0	74	2	0
10	BN	66	0	74	2	0
10	BO	66	0	74	1	0
10	BP	132	0	147	6	0
10	BQ	66	0	74	2	0
10	BR	66	0	74	2	0
10	BS	66	0	74	2	0
10	BT	66	0	74	0	0
10	BV	66	0	74	3	0
10	BW	66	0	74	2	0
10	BX	66	0	74	1	0
10	Ba	66	0	74	6	0
10	Bc	66	0	72	6	0
10	Bd	132	0	143	4	0
10	Be	66	0	72	4	0
10	Bf	132	0	146	14	0
10	Bg	66	0	74	4	0
10	Bh	132	0	146	9	0
10	Bi	66	0	74	6	0
10	Bj	66	0	72	11	0
10	Bk	66	0	74	4	0
10	Bl	132	0	146	8	0
10	Bm	66	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Bn	66	0	74	6	0
10	Bo	66	0	74	4	0
10	Bp	132	0	146	22	0
10	L	132	0	148	6	0
10	M	132	0	148	7	0
11	L	65	0	76	3	0
11	M	65	0	76	3	0
12	AB	35	0	45	1	0
12	AK	35	0	44	2	0
12	AQ	35	0	44	1	0
12	BA	35	0	45	0	0
12	BB	35	0	41	0	0
12	BC	35	0	44	2	0
12	BD	35	0	44	1	0
12	BF	35	0	45	0	0
12	BG	70	0	90	2	0
12	BH	35	0	45	0	0
12	BI	70	0	89	5	0
12	BK	70	0	89	2	0
12	BL	35	0	44	2	0
12	BM	35	0	46	1	0
12	BN	35	0	44	2	0
12	BO	35	0	45	2	0
12	BP	35	0	44	1	0
12	BQ	35	0	45	0	0
12	BR	35	0	45	2	0
12	BS	35	0	46	2	0
12	BT	35	0	44	3	0
12	BU	35	0	45	2	0
12	BV	35	0	45	0	0
12	BX	70	0	90	2	0
12	Ba	35	0	44	1	0
12	Bc	70	0	88	2	0
12	Bd	35	0	45	0	0
12	Bg	70	0	89	2	0
12	Bi	35	0	45	3	0
12	Bj	35	0	45	3	0
12	Bk	35	0	44	1	0
12	Bl	35	0	45	1	0
12	Bm	35	0	44	2	0
12	Bo	35	0	43	0	0
12	Bp	35	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	210	0	273	2	0
12	M	35	0	44	0	0
13	Ad	53	0	72	6	0
13	L	53	0	72	6	0
13	M	53	0	72	10	0
14	M	1	0	0	0	0
15	Af	84	0	124	11	0
15	M	84	0	124	3	0
16	M	44	0	60	0	0
17	AG	35	0	49	2	0
17	AO	35	0	49	4	0
17	AT	35	0	47	3	0
17	Ba	35	0	46	2	0
17	Bb	35	0	49	4	0
17	Bd	35	0	49	1	0
17	Be	35	0	47	5	0
17	Bf	35	0	49	4	0
17	Bg	35	0	49	3	0
17	Bi	35	0	49	5	0
17	Bj	35	0	49	3	0
17	Bk	35	0	47	4	0
17	Bl	35	0	49	3	0
17	Bm	35	0	49	3	0
17	Bn	35	0	49	2	0
17	Bp	35	0	49	1	0
17	M	35	0	49	0	0
18	C	172	0	121	2	0
19	AF	45	0	0	0	0
19	AH	45	0	0	0	0
19	AI	90	0	0	0	0
19	AL	45	0	0	0	0
19	AP	45	0	0	0	0
19	AT	45	0	0	0	0
19	AX	45	0	0	0	0
19	Ad	45	0	0	0	0
19	Ag	45	0	0	0	0
19	Am	45	0	0	1	0
19	An	45	0	0	0	0
19	BB	45	0	0	1	0
19	BC	45	0	0	2	0
19	BD	45	0	0	0	0
19	BE	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	BF	45	0	0	0	0
19	BK	45	0	0	0	0
19	BL	45	0	0	0	0
19	BN	45	0	0	1	0
19	BO	45	0	0	0	0
19	BP	45	0	0	0	0
19	BR	45	0	0	0	0
19	BS	45	0	0	0	0
19	BT	45	0	0	0	0
19	BV	45	0	0	1	0
19	BW	45	0	0	0	0
19	BX	45	0	0	0	0
19	Ba	45	0	0	0	0
19	Bb	45	0	0	0	0
19	Bc	45	0	0	0	0
19	Bd	45	0	0	1	0
19	Bf	45	0	0	1	0
19	Bg	45	0	0	0	0
19	Bi	45	0	0	0	0
19	Bj	45	0	0	0	0
19	Bk	45	0	0	0	0
19	Bl	45	0	0	0	0
19	Bm	45	0	0	0	0
19	Bp	45	0	0	1	0
20	Ad	1	0	0	0	0
20	Ae	1	0	0	0	0
20	Ah	1	0	0	0	0
20	Aj	1	0	0	0	0
20	Ak	2	0	0	0	0
20	Al	1	0	0	0	0
20	Am	2	0	0	0	0
20	C	1	0	0	0	0
20	K	1	0	0	1	0
20	L	11	0	0	0	0
20	M	12	0	0	1	0
20	S	4	0	0	0	0
All	All	49816	0	48619	894	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (894) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Bp:1001:BCL:C15	10:Bp:1001:BCL:C16	1.76	1.58
10:Bp:1001:BCL:C16	10:Bp:1001:BCL:C13	2.21	1.17
10:Bp:1001:BCL:H162	10:Bp:1001:BCL:H122	1.40	1.04
3:M:259:ALA:H	13:M:409:MQ8:H2M3	1.19	1.03
10:AQ:103:BCL:H172	8:Bb:19:GLY:HA3	1.57	0.87
10:Aj:101:BCL:CED	8:Bj:23:VAL:HG12	2.09	0.83
8:Bl:22:ILE:HG21	10:Bl:101:BCL:H193	1.61	0.82
10:Bp:1001:BCL:H162	10:Bp:1001:BCL:C12	2.10	0.81
8:Bh:22:ILE:HG21	10:Bh:101:BCL:H172	1.62	0.80
7:AL:19:PHE:HB2	8:Be:18:LEU:HG	1.64	0.80
7:AF:19:PHE:HB2	8:Bi:18:LEU:HD12	1.62	0.80
9:Ae:22:ALA:HB2	10:Ae:101:BCL:H43	1.64	0.79
10:Bi:1203:BCL:H71	12:Bj:102:LMT:H121	1.64	0.79
7:AE:27:ILE:HD12	10:Bj:101:BCL:H143	1.66	0.78
10:Bp:1001:BCL:C16	10:Bp:1001:BCL:C12	2.62	0.78
10:Bp:1001:BCL:C16	10:Bp:1001:BCL:H122	2.13	0.77
8:BO:9:GLU:OE2	8:BO:13:ARG:NH2	2.15	0.76
8:BW:9:GLU:OE1	8:BW:13:ARG:NH2	2.19	0.75
8:BD:24:LEU:HD13	8:BD:28:ILE:HD11	1.69	0.75
10:Aj:101:BCL:HED1	8:Bj:23:VAL:HG12	1.69	0.74
9:Ag:2:HIS:HA	8:Bg:7:ARG:HH22	1.52	0.73
7:AB:24:LEU:HB2	10:Bl:101:BCL:H143	1.71	0.72
8:Bc:1:MET:N	8:Bc:5:GLU:OE2	2.23	0.72
10:Bi:1203:BCL:H201	17:Bi:1204:PEX:H48	1.55	0.72
9:Af:16:ALA:HB2	15:Af:101:CD4:H86	1.70	0.72
8:BV:30:ALA:HB1	10:BV:102:BCL:HBA2	1.71	0.71
5:K:68:PRO:HG2	5:K:87:LEU:HD11	1.73	0.71
8:Bf:22:ILE:HB	10:Bf:101:BCL:H143	1.71	0.71
10:Aj:101:BCL:H62	10:Aj:101:BCL:H142	1.72	0.71
10:AK:101:BCL:H162	7:AL:23:GLY:HA3	1.73	0.71
7:AH:6:GLN:HG3	8:BH:7:MET:HB2	1.72	0.70
9:Ad:20:PHE:HD2	13:Ad:101:MQ8:H2M2	1.55	0.70
7:AF:12:ILE:HD11	8:Bi:11:GLY:HA2	1.74	0.70
10:AO:101:BCL:HED1	8:BO:29:VAL:HG12	1.73	0.70
8:BC:14:ARG:NH1	19:BC:103:V7N:O44	2.25	0.70
2:L:19:GLY:HA2	9:Ad:12:ARG:HD3	1.73	0.69
3:M:94:ALA:HB2	3:M:180:PRO:HG2	1.74	0.69
7:AW:43:LYS:HG2	7:AX:35:ILE:HA	1.74	0.68
3:M:1:MET:SD	3:M:1:MET:N	2.62	0.68
17:Bm:103:PEX:O1	12:Bm:104:LMT:O6'	2.12	0.68
8:BS:17:GLY:O	8:BS:21:THR:HG23	1.94	0.68
9:Am:7:MET:O	9:An:11:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:10:PRO:HA	7:AI:13:ILE:HD12	1.75	0.68
8:Bf:21:ILE:HG12	10:Bf:103:BCL:H12	1.76	0.67
7:AL:26:LEU:HD23	17:Be:102:PEX:H38	1.76	0.67
10:Bm:102:BCL:H93	10:An:101:BCL:H72	1.77	0.67
9:Al:2:HIS:HA	8:Bl:7:ARG:NH1	2.10	0.67
10:An:101:BCL:HED1	8:Bn:23:VAL:HG12	1.77	0.67
9:Aa:21:LEU:HB3	10:Aa:101:BCL:H2	1.77	0.67
7:AX:10:PRO:HD3	8:BX:7:MET:HG3	1.76	0.66
10:Ac:101:BCL:H171	8:Bc:19:GLY:HA3	1.77	0.66
10:Bh:102:BCL:H143	10:Ai:101:BCL:H172	1.76	0.66
8:Bp:19:GLY:O	8:Bp:23:VAL:HG12	1.96	0.66
7:AW:43:LYS:NZ	7:AW:43:LYS:HB3	2.11	0.66
8:Bl:21:ILE:HG22	8:Bl:22:ILE:HG23	1.76	0.66
7:AB:26:LEU:HD21	10:AB:101:BCL:H93	1.78	0.66
10:Aa:101:BCL:H122	10:Bp:1004:BCL:H151	1.78	0.66
8:BU:9:GLU:OE1	8:BU:13:ARG:NH1	2.29	0.66
7:AV:5:TRP:HA	7:AV:8:MET:HE2	1.77	0.66
8:BE:3:GLU:OE2	8:BE:7:ARG:NH2	2.28	0.66
9:Af:11:ARG:NH1	15:Af:101:CD4:O12	2.29	0.65
7:AU:30:MET:HE2	8:Bo:29:PHE:HD1	1.61	0.65
9:Al:3:ARG:HA	9:Al:6:LEU:HD23	1.78	0.65
10:Aa:101:BCL:H152	10:Bp:1004:BCL:H172	1.77	0.65
9:Ac:43:ASN:O	9:Ac:45:THR:N	2.27	0.64
9:Ag:6:LEU:HD23	8:Bg:1:MET:HG2	1.79	0.63
8:BJ:16:HIS:O	8:BJ:20:VAL:HG23	1.98	0.63
8:BV:24:LEU:O	8:BV:28:ILE:HD12	1.98	0.63
8:Bh:18:LEU:O	8:Bh:22:ILE:HG23	1.98	0.63
8:Bj:18:LEU:HG	8:Bj:22:ILE:HD11	1.81	0.63
3:M:262:GLU:OE2	20:M:501:HOH:O	2.15	0.63
5:K:88:TRP:HB2	5:K:98:TYR:HB2	1.80	0.63
8:Bj:18:LEU:HG	8:Bj:22:ILE:CD1	2.28	0.63
8:BJ:29:VAL:HG12	10:Bf:101:BCL:HED3	1.81	0.63
8:BD:29:VAL:HG22	10:Bj:101:BCL:HED1	1.81	0.63
7:AF:19:PHE:HB2	8:Bi:18:LEU:CD1	2.28	0.62
8:Ba:21:ILE:HG23	10:Ba:102:BCL:H12	1.81	0.62
9:Ab:3:ARG:HH22	8:Bb:7:ARG:HD2	1.64	0.62
17:Bl:104:PEX:H1	12:Bl:105:LMT:H12	1.81	0.62
8:BE:18:LEU:O	8:BE:22:ILE:HD12	1.99	0.62
10:AK:101:BCL:HED3	8:BK:29:VAL:HG12	1.80	0.62
7:AM:5:TRP:HE1	8:BM:16:HIS:CD2	2.17	0.62
12:Bg:1205:LMT:H22	8:Bh:34:TRP:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Bh:101:BCL:H41	10:Bh:101:BCL:H72	1.82	0.62
9:Al:2:HIS:HB3	9:Al:4:ILE:HG22	1.79	0.62
3:M:34:GLY:HA2	3:M:49:GLY:HA2	1.81	0.62
17:Bb:102:PEX:O1	12:Bc:1201:LMT:O6'	2.18	0.62
8:Bo:17:THR:O	8:Bo:21:ILE:HG12	2.00	0.62
7:Al:30:MET:HE1	17:Bg:1204:PEX:H6	1.82	0.62
7:AV:9:ASP:HB3	7:AV:12:ILE:HG22	1.82	0.62
10:Bp:1001:BCL:C16	10:Bp:1001:BCL:H13	2.23	0.61
10:Bf:103:BCL:H203	17:Bf:104:PEX:H10	1.81	0.61
17:AO:102:PEX:H22	10:Bc:1203:BCL:H8	1.82	0.61
10:Ba:102:BCL:H18	17:Ba:103:PEX:H4	1.83	0.61
8:BV:8:THR:OG1	8:BV:11:GLU:OE2	2.19	0.61
10:Be:101:BCL:HAA1	17:Be:102:PEX:H23	1.82	0.61
9:Af:43:ASN:O	9:Af:45:THR:N	2.32	0.61
6:C:96:SER:OG	6:C:101:GLY:O	2.18	0.60
6:C:110:ASN:HD22	6:C:120:PRO:HD3	1.66	0.60
8:BT:7:MET:HE2	7:AT:8:MET:O	2.01	0.60
8:Bp:34:TRP:HB2	12:Bp:1002:LMT:H21	1.83	0.60
10:AC:101:BCL:HED3	8:BC:29:VAL:HG12	1.83	0.60
8:BC:17:GLY:O	8:BC:21:THR:HG23	2.02	0.60
17:AO:102:PEX:H26	17:AO:102:PEX:H10	1.84	0.60
7:AQ:1:MET:HE2	8:BQ:16:HIS:HE2	1.67	0.60
12:Bj:102:LMT:H5B	12:Bj:102:LMT:H6D	1.83	0.60
7:Al:27:ILE:HG12	17:Bg:1204:PEX:H24	1.83	0.60
8:Bp:22:ILE:HB	10:Bp:1001:BCL:C16	2.31	0.60
7:AC:34:SER:HB2	17:Bk:1204:PEX:H47	1.82	0.60
8:BC:27:ILE:HD13	10:BC:101:BCL:H2	1.84	0.60
7:AO:1:MET:HE3	7:AO:1:MET:HA	1.84	0.60
7:AE:1:MET:HA	7:AE:1:MET:HE2	1.84	0.59
8:BX:27:ILE:HG12	10:BX:103:BCL:H12	1.84	0.59
9:Al:2:HIS:HA	8:Bl:7:ARG:HH12	1.67	0.59
8:BP:28:ILE:O	8:BP:32:VAL:HG23	2.03	0.59
10:AQ:101:BCL:H202	10:Ba:102:BCL:H8	1.85	0.59
8:BF:9:GLU:OE2	8:BF:13:ARG:NH2	2.35	0.59
8:BJ:26:TYR:OH	10:Bf:101:BCL:O1A	2.21	0.59
10:Bn:101:BCL:H122	10:Bn:101:BCL:H18	1.85	0.59
3:M:259:ALA:N	13:M:409:MQ8:H2M3	2.04	0.59
9:Af:11:ARG:NH2	15:Af:101:CD4:O6	2.32	0.59
8:Bi:21:ILE:HD13	10:Bi:1203:BCL:H2	1.85	0.59
8:BD:28:ILE:O	8:BD:32:VAL:HG23	2.03	0.58
7:AV:26:LEU:HD11	17:Bn:102:PEX:H24	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AO:9:ASP:OD1	7:AO:11:GLN:NE2	2.37	0.58
7:AE:20:PHE:HA	10:Bj:101:BCL:H202	1.85	0.58
10:AE:101:BCL:H13	10:AE:101:BCL:H203	1.85	0.58
8:BR:28:ILE:O	8:BR:32:VAL:HG23	2.03	0.58
5:K:135:ILE:HG23	5:K:139:GLN:HB2	1.85	0.58
7:AF:8:MET:HE3	7:AF:13:ILE:HD11	1.86	0.58
8:BC:33:ALA:HB1	12:BC:102:LMT:H101	1.85	0.58
8:BV:35:PHE:O	8:BV:39:GLN:HG2	2.04	0.58
10:AW:101:BCL:H8	7:AX:24:LEU:HD13	1.86	0.58
7:AL:43:LYS:HG2	7:AM:35:ILE:HA	1.86	0.57
13:Ad:101:MQ8:H251	13:Ad:101:MQ8:H293	1.85	0.57
10:Bi:1203:BCL:H162	17:Bi:1204:PEX:H4	1.85	0.57
8:BB:14:ARG:NH1	19:BB:102:V7N:O44	2.38	0.57
12:AK:102:LMT:H5B	12:AK:102:LMT:H6D	1.87	0.57
7:AX:26:LEU:HD23	17:Bm:103:PEX:H14	1.87	0.57
8:Be:1:MET:HA	8:Be:1:MET:HE2	1.87	0.57
7:AK:23:GLY:HA3	10:Bf:101:BCL:H141	1.85	0.57
7:AN:11:GLN:NE2	7:AO:4:ILE:O	2.38	0.56
3:M:145:HIS:NE2	15:M:402:CD4:O7	2.37	0.56
5:K:156:GLU:O	5:K:160:VAL:HG23	2.05	0.56
10:AQ:101:BCL:HED3	8:BQ:29:VAL:HG22	1.88	0.56
8:BV:14:ARG:HG2	8:BV:18:TYR:CE2	2.40	0.56
3:M:10:ARG:NH1	5:K:123:GLY:O	2.35	0.56
8:BD:40:TRP:HB2	12:BD:102:LMT:H21	1.86	0.56
8:BM:8:THR:OG1	8:BM:11:GLU:OE1	2.13	0.56
7:AR:29:HIS:HE1	10:AR:101:BCL:NA	2.01	0.56
7:AU:19:PHE:HB2	8:Bo:18:LEU:HG	1.86	0.56
9:Al:56:SER:OG	9:Am:36:GLN:NE2	2.35	0.56
10:An:101:BCL:H172	8:Bn:16:GLY:HA2	1.88	0.56
4:H:44:GLU:O	9:Ag:12:ARG:NH1	2.39	0.56
9:Ae:18:VAL:HG13	10:Ae:101:BCL:H51	1.88	0.56
9:An:2:HIS:HD2	8:Bn:7:ARG:HG3	1.71	0.56
6:C:96:SER:OG	6:C:103:GLY:O	2.19	0.56
10:AE:101:BCL:HED3	8:BE:23:VAL:HG12	1.86	0.56
9:Ae:35:SER:O	9:Ae:39:SER:OG	2.22	0.56
8:BA:28:ILE:O	8:BA:32:VAL:HG23	2.06	0.56
7:AR:30:MET:HE2	8:Ba:29:PHE:HD1	1.70	0.56
9:Ak:3:ARG:HG3	9:Ak:6:LEU:HD12	1.88	0.56
1:S:129:ASP:OD2	6:C:35:ARG:NH1	2.39	0.56
2:L:194:LEU:HD11	2:L:213:GLU:HB3	1.87	0.56
7:AE:21:LEU:HB2	10:AE:101:BCL:H42	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Bp:1001:BCL:H101	10:Bp:1001:BCL:H172	1.89	0.55
8:BI:17:THR:O	8:BI:21:ILE:HG12	2.07	0.55
7:AC:30:MET:HE1	17:Bk:1204:PEX:H10	1.88	0.55
8:BC:35:PHE:CE2	8:BC:39:GLN:NE2	2.74	0.55
8:BO:16:HIS:O	8:BO:20:VAL:HG23	2.06	0.55
8:BP:25:GLY:O	8:BP:29:VAL:HG12	2.06	0.55
8:BT:40:TRP:HB2	12:BT:103:LMT:H21	1.88	0.55
10:AV:1001:BCL:HED1	8:BV:29:VAL:HG22	1.87	0.55
8:Bj:18:LEU:O	8:Bj:22:ILE:HG13	2.06	0.55
10:Bl:101:BCL:H13	10:Bl:101:BCL:H18	1.89	0.55
8:BA:25:GLY:O	8:BA:29:VAL:HG12	2.06	0.55
7:AD:3:ARG:HD2	7:AD:6:GLN:HE21	1.71	0.55
8:BQ:20:VAL:O	8:BQ:24:LEU:HD13	2.07	0.55
10:Af:102:BCL:H141	10:Af:102:BCL:H18	1.87	0.55
13:M:409:MQ8:H141	13:M:409:MQ8:C17	2.37	0.55
9:Ai:37:ARG:HG2	9:Ai:38:TYR:CE2	2.42	0.55
7:AW:39:PRO:O	7:AW:43:LYS:HG3	2.07	0.55
10:Bc:1203:BCL:H121	10:Bd:101:BCL:H93	1.87	0.55
7:AU:24:LEU:HG	10:AU:101:BCL:CED	2.37	0.55
10:BQ:101:BCL:H61	10:BQ:101:BCL:HHB	1.88	0.55
7:AM:38:TRP:HB2	8:BM:40:TRP:HH2	1.72	0.54
7:AQ:12:ILE:HD11	8:Bb:12:TYR:CE2	2.42	0.54
8:BS:25:GLY:O	8:BS:29:VAL:HG12	2.07	0.54
9:Ag:3:ARG:HG3	9:Ag:6:LEU:HD12	1.89	0.54
17:Be:102:PEX:H9	17:Be:102:PEX:O7	2.08	0.54
10:Bn:101:BCL:H72	10:Bn:101:BCL:H41	1.89	0.54
3:M:218:HIS:HD1	13:M:409:MQ8:C6	2.19	0.54
10:AM:101:BCL:HED3	8:BM:29:VAL:HG12	1.90	0.54
8:BR:35:PHE:CE1	8:BR:39:GLN:NE2	2.75	0.54
17:Bj:104:PEX:O1	12:Bk:1201:LMT:O6'	2.24	0.54
10:Bo:1202:BCL:H8	10:Bo:1202:BCL:H152	1.89	0.54
5:K:29:GLY:O	5:K:32:SER:OG	2.25	0.54
8:BN:29:VAL:HG12	10:AN:101:BCL:HED3	1.89	0.54
8:BT:28:ILE:O	8:BT:32:VAL:HG23	2.08	0.54
8:BP:7:MET:HB3	7:AP:6:GLN:HA	1.89	0.54
8:BP:20:VAL:O	8:BP:24:LEU:HG	2.08	0.54
10:AR:101:BCL:H18	7:AS:27:ILE:HD11	1.89	0.54
3:M:82:ASP:HB3	3:M:85:GLU:HB2	1.89	0.54
8:BL:40:TRP:CE2	8:BL:41:ARG:HG3	2.42	0.54
9:Ad:37:ARG:HG2	9:Ad:38:TYR:CE2	2.43	0.54
8:BB:27:ILE:HD11	10:BB:101:BCL:H11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:VAL:HG22	13:M:409:MQ8:H401	1.90	0.53
7:AQ:22:ALA:HA	10:AQ:101:BCL:H12	1.90	0.53
7:AI:43:LYS:NZ	7:AI:43:LYS:HB3	2.23	0.53
8:BJ:23:THR:O	8:BJ:27:ILE:HG12	2.09	0.53
8:Bf:32:TRP:CG	17:Bf:104:PEX:H7	2.43	0.53
7:AX:10:PRO:HA	7:AX:13:ILE:HD12	1.90	0.53
9:Ae:37:ARG:HG2	9:Ae:38:TYR:CE2	2.43	0.53
7:AH:20:PHE:HD1	10:Bh:101:BCL:H171	1.72	0.53
9:Ai:21:LEU:HB3	10:Ai:101:BCL:C2	2.39	0.53
17:Bm:103:PEX:H31	17:Bm:103:PEX:H6	1.90	0.53
8:BG:28:ILE:O	8:BG:32:VAL:HG23	2.09	0.53
8:BO:18:TYR:HE2	7:AP:1:MET:H1	1.56	0.53
17:AT:103:PEX:H13	7:AU:30:MET:HE1	1.91	0.53
8:BQ:25:GLY:O	8:BQ:29:VAL:HG12	2.09	0.53
2:L:169:HIS:NE2	10:L:301:BCL:HBB2	2.24	0.53
9:Af:1:MET:HE3	9:Af:1:MET:N	2.24	0.53
9:Am:37:ARG:HG2	9:Am:38:TYR:CE2	2.44	0.53
7:AJ:9:ASP:OD1	7:AJ:11:GLN:N	2.33	0.53
7:AS:22:ALA:HB2	10:Bp:1001:BCL:H51	1.90	0.53
9:Af:1:MET:SD	9:Af:2:HIS:ND1	2.81	0.53
8:BE:14:VAL:O	8:BE:18:LEU:HG	2.09	0.53
10:AI:102:BCL:O1A	8:BI:20:TYR:OH	2.22	0.53
9:Ac:37:ARG:HG2	9:Ac:38:TYR:CE2	2.43	0.53
7:AQ:1:MET:HE2	8:BQ:16:HIS:NE2	2.23	0.53
7:AQ:36:THR:O	8:BQ:41:ARG:NH1	2.41	0.53
17:Bf:104:PEX:O1	12:Bg:1201:LMT:O6'	2.22	0.53
9:Ah:37:ARG:HG2	9:Ah:38:TYR:CE2	2.44	0.53
9:Ai:7:MET:SD	9:Aj:11:ARG:HG3	2.48	0.53
9:Al:37:ARG:HG2	9:Al:38:TYR:CE2	2.44	0.53
9:An:7:MET:HG2	9:Ao:11:ARG:HG3	1.90	0.53
8:Bh:22:ILE:HB	10:Bh:101:BCL:H141	1.91	0.52
8:BH:40:TRP:HB2	12:BI:1101:LMT:H22	1.92	0.52
10:Aj:101:BCL:HED3	8:Bj:23:VAL:HG12	1.89	0.52
2:L:82:ARG:NH2	9:Ae:39:SER:OG	2.42	0.52
8:BI:21:ILE:HG23	10:BI:1102:BCL:H12	1.92	0.52
8:BQ:35:PHE:O	8:BQ:39:GLN:HG2	2.08	0.52
8:BR:18:TYR:HA	8:BR:21:THR:HG22	1.91	0.52
7:AU:29:HIS:HE1	10:AU:102:BCL:NA	2.00	0.52
3:M:263:SER:HA	3:M:266:ARG:HG3	1.91	0.52
7:AE:8:MET:HB2	7:AE:13:ILE:HD11	1.92	0.52
8:BN:14:ARG:NH1	19:BN:103:V7N:O45	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BW:28:ILE:O	8:BW:32:VAL:HG23	2.09	0.52
12:BM:102:LMT:H92	10:BN:101:BCL:H143	1.90	0.52
9:Af:10:PRO:HB3	8:Bf:9:PHE:CZ	2.45	0.52
9:Ao:56:SER:OG	9:Ao:57:ALA:N	2.43	0.52
7:AI:38:TRP:HB2	8:BI:34:TRP:HH2	1.74	0.52
10:AK:101:BCL:H192	10:Be:101:BCL:H92	1.91	0.52
8:BS:41:ARG:NH1	7:AS:36:THR:O	2.43	0.52
10:Aa:101:BCL:H143	10:Bp:1004:BCL:H202	1.92	0.52
3:M:157:TYR:HB2	10:M:404:BCL:H62	1.92	0.52
5:K:98:TYR:OH	5:K:157:GLU:HG3	2.10	0.52
8:BG:29:VAL:HG12	10:Bh:101:BCL:HED3	1.91	0.52
10:Bc:1203:BCL:H13	10:Bc:1203:BCL:H71	1.90	0.52
8:BC:35:PHE:O	8:BC:39:GLN:HG2	2.09	0.52
7:AE:36:THR:O	8:BE:35:ARG:NH1	2.42	0.52
8:BI:29:PHE:O	8:BI:33:GLN:HG2	2.09	0.52
8:Bl:2:THR:OG1	8:Bl:3:GLU:N	2.43	0.52
7:AC:22:ALA:HB2	10:AC:101:BCL:H51	1.91	0.52
9:Al:13:VAL:HG23	9:Al:14:MET:HE2	1.91	0.52
8:Bm:17:THR:O	8:Bm:21:ILE:HG12	2.09	0.52
2:L:136:ARG:NH1	2:L:252:SER:O	2.43	0.52
8:Bf:22:ILE:O	8:Bf:26:VAL:HG23	2.10	0.52
2:L:6:PHE:CD1	3:M:245:GLU:HG2	2.45	0.51
6:C:192:THR:HG22	6:C:194:ASP:H	1.74	0.51
7:AF:14:MET:HA	7:AF:14:MET:HE2	1.92	0.51
7:AJ:10:PRO:HD3	8:BJ:7:MET:HE2	1.92	0.51
9:Ae:3:ARG:HG3	8:Be:7:ARG:HH22	1.76	0.51
8:BF:24:LEU:O	8:BF:28:ILE:HG23	2.10	0.51
8:BO:28:ILE:O	8:BO:32:VAL:HG23	2.11	0.51
8:BR:35:PHE:O	8:BR:39:GLN:HG2	2.11	0.51
8:BS:24:LEU:O	8:BS:28:ILE:HD12	2.09	0.51
9:Af:1:MET:SD	9:Af:2:HIS:N	2.84	0.51
11:L:303:BPH:HBB3	11:L:303:BPH:HHC	1.92	0.51
7:AB:24:LEU:HD13	10:Bl:101:BCL:H121	1.93	0.51
7:AH:6:GLN:NE2	8:BH:7:MET:O	2.44	0.51
10:AH:101:BCL:HMA3	12:BI:1101:LMT:H123	1.91	0.51
7:AU:8:MET:HE3	7:AU:13:ILE:HD11	1.93	0.51
9:Ag:37:ARG:HG2	9:Ag:38:TYR:CE2	2.45	0.51
3:M:217:MET:CE	13:M:409:MQ8:H143	2.41	0.51
10:AB:101:BCL:H11	19:BC:103:V7N:C34	2.40	0.51
8:BM:23:THR:O	8:BM:27:ILE:HG12	2.11	0.51
8:BT:9:GLU:HG2	7:AT:6:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Bh:3:GLU:HG2	8:Bh:5:GLU:H	1.75	0.51
9:Al:9:ASP:OD1	9:Al:11:ARG:NH1	2.44	0.51
6:C:184:ASP:N	6:C:184:ASP:OD1	2.43	0.51
7:AB:22:ALA:HA	10:AB:101:BCL:H62	1.93	0.51
9:Ag:22:ALA:HA	10:Ag:101:BCL:H2	1.93	0.51
10:AO:101:BCL:HMA3	12:BO:103:LMT:H122	1.94	0.50
9:Ak:37:ARG:HG2	9:Ak:38:TYR:CE2	2.46	0.50
7:AB:11:GLN:NE2	7:AC:4:ILE:O	2.43	0.50
7:AC:26:LEU:HD23	17:Bk:1204:PEX:H18	1.93	0.50
8:BP:29:VAL:O	10:BP:104:BCL:HED3	2.10	0.50
7:AW:27:ILE:HD13	17:Bn:102:PEX:H17	1.93	0.50
10:Bp:1001:BCL:C15	10:Bp:1001:BCL:H161	2.19	0.50
2:L:190:MET:HE2	13:L:310:MQ8:H2M1	1.94	0.50
8:BG:7:MET:HB3	8:BG:11:GLU:HB3	1.92	0.50
7:Al:43:LYS:HG2	7:AJ:35:ILE:HA	1.93	0.50
8:BT:13:ARG:N	8:BT:13:ARG:HD2	2.26	0.50
9:Aa:37:ARG:HG2	9:Aa:38:TYR:CE2	2.47	0.50
9:An:1:MET:O	9:An:4:ILE:HG22	2.11	0.50
8:BI:22:ILE:O	8:BI:26:VAL:HG23	2.11	0.50
9:Aj:37:ARG:HG2	9:Aj:38:TYR:CE2	2.46	0.50
10:BD:101:BCL:HED3	7:AD:24:LEU:HD23	1.93	0.50
7:AJ:30:MET:HG3	10:Bf:103:BCL:H193	1.94	0.50
8:BR:26:TYR:HE1	10:BR:101:BCL:HBA1	1.77	0.50
8:Ba:3:GLU:OE2	8:Ba:3:GLU:HA	2.12	0.50
9:Ac:10:PRO:HB3	8:Bc:9:PHE:CZ	2.46	0.50
8:Bk:25:ALA:HB1	17:Bk:1204:PEX:H19	1.94	0.50
10:Bp:1001:BCL:C15	10:Bp:1001:BCL:H162	2.19	0.50
6:C:150:LYS:C	6:C:152:THR:H	2.19	0.50
10:AW:101:BCL:H202	10:Bm:102:BCL:H51	1.93	0.50
9:Ao:37:ARG:HG2	9:Ao:38:TYR:CE2	2.46	0.50
7:AL:2:HIS:CG	8:BL:13:ARG:HG2	2.47	0.50
12:Bm:104:LMT:H22	8:Bn:34:TRP:HB2	1.94	0.50
3:M:155:PHE:HB2	15:M:402:CD4:H83	1.93	0.50
11:M:405:BPH:HBC3	11:M:405:BPH:HHD	1.94	0.50
7:AB:8:MET:HG3	7:AB:13:ILE:HD11	1.93	0.50
7:AE:20:PHE:HD1	10:Bj:101:BCL:H193	1.77	0.50
8:BH:24:LEU:O	8:BH:28:ILE:HG23	2.12	0.50
9:Af:37:ARG:HG2	9:Af:38:TYR:CE2	2.47	0.50
8:Bi:15:THR:O	8:Bi:18:LEU:HB3	2.11	0.50
7:AO:8:MET:HE3	7:AO:13:ILE:HD11	1.94	0.49
10:Bc:1203:BCL:H203	10:Bd:101:BCL:H62	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Ah:101:BCL:H143	8:Bh:20:TYR:HB2	1.94	0.49
2:L:23:PHE:O	2:L:33:GLY:HA2	2.12	0.49
5:K:66:PRO:HG3	5:K:127:ASN:HD22	1.76	0.49
8:BP:28:ILE:HG13	8:BP:29:VAL:N	2.27	0.49
8:BQ:28:ILE:O	8:BQ:32:VAL:HG23	2.12	0.49
12:BT:103:LMT:H121	10:Au:101:BCL:H72	1.94	0.49
10:Aj:101:BCL:H143	8:Bj:20:TYR:HB2	1.93	0.49
8:Bp:22:ILE:O	8:Bp:26:VAL:HG23	2.12	0.49
7:AW:36:THR:O	8:BW:41:ARG:NH1	2.45	0.49
8:BF:9:GLU:OE1	7:AF:3:ARG:NH2	2.46	0.49
7:AM:5:TRP:HE1	8:BM:16:HIS:HD2	1.58	0.49
10:AP:102:BCL:H142	10:Ac:101:BCL:H111	1.94	0.49
8:Be:3:GLU:O	8:Be:7:ARG:HG2	2.11	0.49
9:Ah:21:LEU:HB3	10:Ah:101:BCL:H12	1.94	0.49
8:Bp:25:ALA:HB3	10:Bp:1001:BCL:H161	1.94	0.49
9:Ap:37:ARG:HG2	9:Ap:38:TYR:CE2	2.47	0.49
6:C:206:LYS:HB3	9:Al:64:MET:HE1	1.94	0.49
8:BB:35:PHE:HB2	10:BB:101:BCL:H191	1.93	0.49
8:BV:25:GLY:O	8:BV:29:VAL:HG12	2.12	0.49
9:Aa:10:PRO:HB2	9:Ap:7:MET:HE1	1.94	0.49
7:AT:24:LEU:HD13	10:Bp:1001:BCL:C11	2.43	0.49
10:AW:101:BCL:HED3	8:BW:29:VAL:HG12	1.94	0.49
9:Ab:23:VAL:HG21	13:Ad:101:MQ8:H502	1.95	0.49
8:Be:28:HIS:HB3	17:Be:102:PEX:H32	1.94	0.49
9:Am:4:ILE:HD13	19:Am:102:V7N:C38	2.42	0.49
9:Am:10:PRO:HG2	8:Bm:1:MET:HE1	1.95	0.49
2:L:188:LEU:HD11	3:M:268:SER:HB3	1.95	0.49
5:K:167:GLY:O	5:K:175:ARG:NH1	2.42	0.49
7:AO:5:TRP:HA	7:AO:8:MET:HE2	1.94	0.49
8:BR:7:MET:HE3	7:AR:10:PRO:HG3	1.94	0.49
3:M:113:GLY:O	3:M:117:MET:HG3	2.13	0.49
10:AE:101:BCL:CED	8:BE:23:VAL:HG12	2.43	0.49
9:Aa:11:ARG:HH21	9:Ap:12:ARG:NH2	2.11	0.49
8:Bd:19:GLY:O	8:Bd:23:VAL:HG23	2.12	0.49
12:AB:102:LMT:H22	8:Bl:34:TRP:HB2	1.95	0.49
7:AM:38:TRP:HB2	8:BM:40:TRP:CH2	2.48	0.49
8:BP:24:LEU:O	8:BP:28:ILE:HG23	2.13	0.49
9:Ad:10:PRO:HB3	8:Bd:9:PHE:CZ	2.48	0.49
9:Af:11:ARG:HH22	15:Af:101:CD4:H58	1.78	0.49
10:Ah:101:BCL:CED	8:Bh:23:VAL:HG12	2.43	0.49
10:AQ:103:BCL:CED	8:Bb:23:VAL:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AQ:103:BCL:HED1	8:Bb:23:VAL:HG12	1.95	0.48
8:BS:25:GLY:HA2	8:BS:28:ILE:HD12	1.93	0.48
8:BS:28:ILE:O	8:BS:32:VAL:HG23	2.13	0.48
8:BD:24:LEU:O	8:BD:28:ILE:HD12	2.13	0.48
8:BD:41:ARG:NH1	7:AD:36:THR:O	2.46	0.48
12:BT:103:LMT:H101	10:AU:101:BCL:HBB2	1.95	0.48
9:Ae:13:VAL:HG22	15:Af:101:CD4:O4	2.13	0.48
8:Bm:19:GLY:O	8:Bm:23:VAL:HG23	2.13	0.48
9:An:37:ARG:HG2	9:An:38:TYR:CE2	2.48	0.48
4:H:27:ARG:HB3	4:H:27:ARG:NH1	2.28	0.48
10:AT:104:BCL:HED1	8:Bp:23:VAL:HG22	1.95	0.48
9:Ab:17:MET:HE2	9:Ab:17:MET:HB3	1.70	0.48
9:Ab:37:ARG:HG2	9:Ab:38:TYR:CD2	2.48	0.48
9:Ad:19:GLY:HA3	13:Ad:101:MQ8:H171	1.94	0.48
9:Af:1:MET:HE3	9:Af:1:MET:H3	1.78	0.48
9:Am:21:LEU:HB3	10:Am:101:BCL:H2	1.94	0.48
9:Ao:37:ARG:HG2	9:Ao:38:TYR:CD2	2.49	0.48
8:Bl:22:ILE:HB	10:Bl:101:BCL:H171	1.94	0.48
6:C:138:THR:HG21	6:C:309:LEU:HD13	1.95	0.48
8:BN:28:ILE:O	8:BN:32:VAL:HG23	2.14	0.48
5:K:179:ILE:HG23	5:K:180:ILE:HD13	1.95	0.48
7:AE:24:LEU:HA	10:Bj:101:BCL:H142	1.94	0.48
7:AM:39:PRO:O	7:AM:43:LYS:HB3	2.13	0.48
8:BV:28:ILE:O	8:BV:32:VAL:HG23	2.13	0.48
8:BX:7:MET:HA	8:BX:11:GLU:HG3	1.95	0.48
9:Al:10:PRO:HA	9:Al:13:VAL:HG22	1.94	0.48
2:L:164:GLN:NE2	6:C:38:GLY:O	2.38	0.48
7:AU:22:ALA:HB1	10:AU:102:BCL:H62	1.96	0.48
10:Af:102:BCL:HED1	8:Bf:23:VAL:HG12	1.95	0.48
10:Ah:101:BCL:HED3	8:Bh:23:VAL:HG12	1.95	0.48
8:Bh:22:ILE:O	8:Bh:26:VAL:HG23	2.14	0.48
9:Al:5:TRP:HZ3	9:Al:13:VAL:HG21	1.78	0.48
10:Am:101:BCL:H62	10:Am:101:BCL:H41	1.71	0.48
13:M:409:MQ8:H211	13:M:409:MQ8:H191	1.55	0.48
12:BL:103:LMT:H6D	8:BM:38:TRP:HZ2	1.79	0.48
8:BR:17:GLY:O	8:BR:20:VAL:HG12	2.13	0.48
13:L:310:MQ8:H311	13:L:310:MQ8:H291	1.66	0.48
8:Ba:19:GLY:O	8:Ba:23:VAL:HG23	2.14	0.48
10:Ah:101:BCL:H203	10:Ah:101:BCL:H13	1.96	0.48
7:AE:9:ASP:HB3	7:AE:12:ILE:HG12	1.96	0.47
8:BX:28:ILE:O	8:BX:32:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ba:23:VAL:HG11	10:Bp:1004:BCL:H121	1.95	0.47
10:Bi:1203:BCL:H62	10:Bi:1203:BCL:H41	1.70	0.47
8:BS:29:VAL:HG22	10:Bp:1001:BCL:CED	2.45	0.47
7:AP:42:LYS:HD2	7:AP:42:LYS:HA	1.74	0.47
9:Ab:37:ARG:HG2	9:Ab:38:TYR:CE2	2.49	0.47
6:C:270:TYR:HB3	6:C:274:ARG:HB2	1.95	0.47
10:BE:102:BCL:H62	10:BE:102:BCL:H41	1.77	0.47
10:BP:104:BCL:H61	10:BP:104:BCL:H41	1.76	0.47
8:BR:29:VAL:HG11	10:BS:101:BCL:H92	1.94	0.47
8:Bc:32:TRP:HH2	8:Bc:38:PHE:HB2	1.79	0.47
11:L:303:BPH:NC	3:M:213:VAL:HG22	2.29	0.47
10:BH:102:BCL:H52	10:BH:102:BCL:H11	1.72	0.47
10:AL:101:BCL:HED3	8:BL:29:VAL:HG12	1.96	0.47
10:AQ:101:BCL:H101	7:AR:20:PHE:HE1	1.79	0.47
9:Ad:35:SER:O	9:Ad:39:SER:OG	2.20	0.47
13:M:409:MQ8:H311	13:M:409:MQ8:H291	1.47	0.47
17:AG:1101:PEX:H2	12:Bi:1201:LMT:H12	1.95	0.47
8:BM:35:PHE:O	8:BM:39:GLN:HG2	2.15	0.47
8:BS:23:THR:O	8:BS:27:ILE:HG12	2.14	0.47
9:Aa:14:MET:HE2	9:Aa:14:MET:HA	1.95	0.47
10:L:301:BCL:HHC	10:L:301:BCL:HBB3	1.96	0.47
10:M:403:BCL:HBB2	10:M:403:BCL:HHC	1.97	0.47
7:AA:8:MET:HE2	7:AA:8:MET:HB3	1.82	0.47
8:BJ:28:ILE:O	8:BJ:32:VAL:HG23	2.14	0.47
10:M:403:BCL:HBB3	10:M:404:BCL:H61	1.97	0.47
8:Ba:34:TRP:HB2	12:Ba:104:LMT:H31	1.95	0.47
8:Bl:22:ILE:HA	8:Bl:25:ALA:H	1.80	0.47
3:M:75:MET:HG2	3:M:93:LEU:HB3	1.97	0.47
8:BG:40:TRP:HB2	12:BG:103:LMT:H22	1.97	0.47
5:K:179:ILE:O	5:K:180:ILE:HD12	2.15	0.47
3:M:228:LEU:HD23	5:K:161:CYS:HB3	1.97	0.46
5:K:153:THR:HG22	5:K:156:GLU:HG3	1.97	0.46
10:Bg:1203:BCL:H61	10:Bg:1203:BCL:H102	1.46	0.46
8:Bo:2:THR:O	8:Bo:5:GLU:HG2	2.15	0.46
8:Bo:21:ILE:HD12	10:Bo:1202:BCL:H11	1.98	0.46
10:AD:101:BCL:HED1	9:Aj:21:LEU:HD22	1.98	0.46
10:BF:102:BCL:H62	10:BF:102:BCL:H41	1.75	0.46
9:Ag:37:ARG:HG2	9:Ag:38:TYR:CD2	2.50	0.46
9:Ac:29:HIS:CE1	10:Bc:1203:BCL:HMD3	2.50	0.46
17:Bd:104:PEX:H10	17:Bd:104:PEX:H17	1.75	0.46
3:M:37:SER:HB3	3:M:40:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BF:29:VAL:HG12	10:AF:101:BCL:CED	2.45	0.46
10:AI:102:BCL:H11	10:AI:102:BCL:HBA2	1.63	0.46
8:BI:34:TRP:HB2	12:BI:1103:LMT:H21	1.97	0.46
9:AK:37:ARG:HG2	9:AK:38:TYR:CD2	2.51	0.46
9:AI:8:PHE:HB3	9:AI:13:VAL:HG11	1.96	0.46
8:BO:17:GLY:O	8:BO:21:THR:HG22	2.16	0.46
10:BW:102:BCL:H52	10:BW:102:BCL:H11	1.62	0.46
9:AI:17:MET:HE2	9:AI:17:MET:HB3	1.82	0.46
8:BI:32:TRP:HH2	8:BI:38:PHE:HB2	1.80	0.46
10:AN:101:BCL:H102	8:BN:20:TYR:HD1	1.81	0.46
12:BN:102:LMT:H121	12:BN:102:LMT:H92	1.81	0.46
9:Aa:21:LEU:HB3	10:Aa:101:BCL:C2	2.45	0.46
3:M:217:MET:HE1	13:M:409:MQ8:H143	1.98	0.46
7:AF:13:ILE:HG22	7:AF:14:MET:CE	2.45	0.46
8:BK:40:TRP:HB2	12:BK:103:LMT:H32	1.98	0.46
10:BP:104:BCL:H152	17:Bb:102:PEX:H20	1.98	0.46
10:AR:101:BCL:HBA2	10:AR:101:BCL:H11	1.59	0.46
7:AS:26:LEU:O	7:AS:30:MET:HG2	2.16	0.46
8:Bk:19:GLY:O	8:Bk:23:VAL:HG23	2.16	0.46
6:C:118:THR:HG22	6:C:124:PRO:HA	1.96	0.46
8:BE:22:ILE:O	8:BE:26:VAL:HG23	2.15	0.46
9:Ac:37:ARG:HG2	9:Ac:38:TYR:CD2	2.51	0.46
9:Ap:37:ARG:HG2	9:Ap:38:TYR:CD2	2.50	0.46
2:L:196:LEU:HD21	3:M:266:ARG:HG2	1.98	0.46
8:Bc:17:THR:O	8:Bc:21:ILE:HG12	2.16	0.46
9:Ah:4:ILE:HG13	9:Ah:5:TRP:H	1.80	0.46
12:L:309:LMT:H21	12:L:309:LMT:H51	1.70	0.46
5:K:3:ASP:HA	5:K:5:LYS:HE2	1.97	0.46
7:AF:26:LEU:HD23	17:Bi:1204:PEX:H17	1.97	0.46
7:AK:8:MET:HE2	7:AK:8:MET:HB2	1.82	0.46
8:BL:28:ILE:O	8:BL:32:VAL:HG23	2.16	0.46
12:BS:102:LMT:H102	12:BS:102:LMT:H71	1.55	0.46
12:BU:101:LMT:H12	12:BU:101:LMT:H41	1.73	0.46
10:Ah:101:BCL:H122	10:Ah:101:BCL:H8	1.75	0.46
8:Bj:32:TRP:HH2	8:Bj:38:PHE:HB2	1.80	0.46
2:L:27:PHE:CD1	15:Af:101:CD4:H57	2.52	0.45
6:C:83:ILE:HD11	6:C:87:GLU:HG2	1.97	0.45
8:BE:7:ARG:HH11	8:BE:7:ARG:HG3	1.80	0.45
15:Af:101:CD4:H28	15:Af:101:CD4:H27	1.35	0.45
9:Aj:2:HIS:HA	8:Bj:7:ARG:HH12	1.81	0.45
7:AE:20:PHE:CD1	10:Bj:101:BCL:H193	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:8:MET:HB2	7:AH:13:ILE:HD11	1.97	0.45
10:AQ:101:BCL:H52	10:AQ:101:BCL:H11	1.68	0.45
10:Aj:101:BCL:H193	10:Aj:101:BCL:H162	1.79	0.45
6:C:83:ILE:HD12	6:C:308:ALA:HB2	1.99	0.45
10:BI:1102:BCL:H62	10:BI:1102:BCL:H41	1.81	0.45
7:AQ:5:TRP:CD1	8:BQ:16:HIS:HB2	2.51	0.45
10:AU:102:BCL:H202	7:AV:27:ILE:HD11	1.99	0.45
9:Ae:57:ALA:HB3	9:Ae:58:PRO:HD3	1.98	0.45
8:BK:10:ASP:C	8:BK:10:ASP:OD1	2.59	0.45
8:BL:14:ARG:HH12	7:AM:3:ARG:HD2	1.81	0.45
8:BO:24:LEU:O	8:BO:28:ILE:HD12	2.17	0.45
9:Aa:10:PRO:HB3	8:Ba:9:PHE:CZ	2.52	0.45
13:Ad:101:MQ8:H461	13:Ad:101:MQ8:H451	1.43	0.45
10:Bg:1203:BCL:H202	8:Bh:23:VAL:HG22	1.97	0.45
9:Ao:17:MET:HE2	9:Ao:17:MET:HB3	1.74	0.45
19:Bp:1003:V7N:C10	10:Bp:1004:BCL:H2	2.46	0.45
8:BP:40:TRP:HH2	7:AP:38:TRP:HB2	1.80	0.45
8:Bb:18:LEU:O	8:Bb:22:ILE:HG23	2.15	0.45
8:Bb:22:ILE:O	8:Bb:26:VAL:HG23	2.17	0.45
19:Bf:102:V7N:C12	10:Bf:103:BCL:H2	2.46	0.45
17:Bi:1204:PEX:O1	12:Bj:102:LMT:O6'	2.34	0.45
8:Bo:29:PHE:O	8:Bo:33:GLN:HG2	2.16	0.45
8:Bp:21:ILE:HG22	8:Bp:22:ILE:HG22	1.98	0.45
8:BA:29:VAL:HG22	10:Bl:101:BCL:CED	2.46	0.45
7:AK:20:PHE:HD1	10:Bf:101:BCL:C17	2.29	0.45
7:AL:27:ILE:HG23	10:Be:101:BCL:H18	1.98	0.45
8:BP:7:MET:HG3	8:BP:8:THR:H	1.82	0.45
10:BP:104:BCL:H161	10:BP:104:BCL:H192	1.71	0.45
12:BR:102:LMT:H123	10:AR:101:BCL:HED1	1.98	0.45
7:AR:9:ASP:OD1	8:Ba:7:ARG:NH2	2.49	0.45
7:AV:38:TRP:HA	7:AV:41:TYR:CD2	2.52	0.45
17:Bb:102:PEX:H2	12:Bc:1201:LMT:H12	1.98	0.45
10:AD:101:BCL:H72	17:Bj:104:PEX:H42	1.98	0.45
7:AF:13:ILE:HG22	7:AF:14:MET:HE2	1.99	0.45
10:AP:102:BCL:H11	10:AP:102:BCL:H52	1.78	0.45
8:Bd:23:VAL:HG12	10:Bd:101:BCL:HED1	1.99	0.45
8:Bn:22:ILE:O	8:Bn:26:VAL:HG23	2.17	0.45
7:AA:10:PRO:HD3	8:BA:7:MET:HE2	1.99	0.45
8:BM:28:ILE:O	8:BM:32:VAL:HG23	2.17	0.45
12:AQ:102:LMT:H22	8:Bb:34:TRP:HB2	1.97	0.45
8:BU:26:TYR:HA	8:BU:29:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Bf:103:BCL:H61	10:Bf:103:BCL:H41	1.88	0.45
9:Am:29:HIS:CE1	10:Bm:102:BCL:HMD3	2.51	0.45
10:AF:101:BCL:H112	7:AG:20:PHE:HE1	1.81	0.45
8:BS:40:TRP:HH2	7:AS:38:TRP:HB2	1.82	0.45
8:BU:36:LEU:HD11	12:BU:101:LMT:O5'	2.17	0.45
10:Bc:1203:BCL:H93	10:Bc:1203:BCL:H41	1.99	0.45
5:K:76:ALA:HB3	5:K:136:THR:HG22	1.98	0.45
8:BF:28:ILE:O	8:BF:32:VAL:HG23	2.17	0.45
10:AH:101:BCL:HED3	8:BH:29:VAL:HG12	1.98	0.45
7:AR:12:ILE:HD11	8:Ba:11:GLY:HA2	1.98	0.45
8:BW:14:ARG:NH1	8:BW:14:ARG:HB2	2.32	0.45
9:Ad:37:ARG:HG2	9:Ad:38:TYR:CD2	2.51	0.45
9:An:37:ARG:HG2	9:An:38:TYR:CD2	2.52	0.45
5:K:148:ARG:HH21	5:K:150:ASP:CG	2.24	0.44
7:AO:43:LYS:HE3	7:AO:43:LYS:HB2	1.74	0.44
9:Ae:37:ARG:HG2	9:Ae:38:TYR:CD2	2.52	0.44
9:Ap:2:HIS:HB3	9:Ap:3:ARG:H	1.56	0.44
8:BG:20:VAL:O	8:BG:24:LEU:HD22	2.17	0.44
10:AO:101:BCL:H18	7:AP:27:ILE:HD11	1.99	0.44
7:AP:3:ARG:HA	7:AP:6:GLN:HG3	1.98	0.44
10:Bf:103:BCL:H122	17:Bf:104:PEX:H31	1.99	0.44
1:S:180:ILE:HB	2:L:265:ASN:OD1	2.17	0.44
8:BR:35:PHE:CZ	8:BR:39:GLN:NE2	2.85	0.44
8:BW:17:GLY:O	8:BW:21:THR:HG22	2.18	0.44
13:Ad:101:MQ8:H141	13:Ad:101:MQ8:H161	1.62	0.44
9:Am:37:ARG:HG2	9:Am:38:TYR:CD2	2.52	0.44
13:L:310:MQ8:H493	3:M:2:LEU:CD1	2.48	0.44
8:BU:28:ILE:O	8:BU:32:VAL:HG12	2.18	0.44
8:Bi:8:ARG:HH11	8:Bi:8:ARG:HG2	1.82	0.44
2:L:98:PHE:CZ	10:L:301:BCL:H102	2.52	0.44
7:AA:23:GLY:HA3	10:AX:102:BCL:H141	1.98	0.44
8:BI:3:GLU:OE2	8:BI:7:ARG:NH2	2.50	0.44
8:BR:15:PHE:HE2	7:AR:10:PRO:HB3	1.81	0.44
10:Af:102:BCL:H62	8:Bf:20:TYR:CE1	2.53	0.44
10:L:301:BCL:H52	10:L:302:BCL:HBB3	2.00	0.44
8:BI:34:TRP:CD2	8:BI:35:ARG:HG2	2.53	0.44
7:AV:12:ILE:HD13	9:An:1:MET:HG3	1.99	0.44
8:Bk:17:THR:O	8:Bk:21:ILE:HG12	2.17	0.44
12:L:304:LMT:H71	12:L:304:LMT:H41	1.79	0.44
10:AF:101:BCL:H61	10:AF:101:BCL:H102	1.94	0.44
12:BX:101:LMT:H12	12:BX:101:LMT:H2'	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Bc:22:ILE:O	8:Bc:26:VAL:HG23	2.18	0.44
10:AI:102:BCL:H91	10:AI:102:BCL:H112	1.78	0.44
7:AN:42:LYS:HD2	7:AN:42:LYS:HA	1.71	0.44
7:AO:38:TRP:HA	7:AO:41:TYR:CD2	2.53	0.44
8:BQ:8:THR:N	8:BQ:11:GLU:OE1	2.48	0.44
7:AV:19:PHE:HE2	10:Bn:101:BCL:H93	1.83	0.44
9:Aa:37:ARG:HG2	9:Aa:38:TYR:CD2	2.52	0.44
10:Bn:101:BCL:H11	10:Bn:101:BCL:H52	1.80	0.44
10:AI:102:BCL:HED3	8:BI:23:VAL:HG12	1.99	0.44
7:AO:22:ALA:HA	10:AO:101:BCL:H52	2.00	0.44
19:BV:101:V7N:O42	10:BV:102:BCL:H72	2.18	0.44
9:Aa:65:SER:OG	9:Aa:67:LEU:O	2.34	0.44
8:Ba:21:ILE:HD12	10:Ba:102:BCL:H12	1.99	0.44
10:Bi:1203:BCL:H121	17:Bi:1204:PEX:H28	1.98	0.44
10:Ao:101:BCL:H62	8:Bo:20:TYR:HE1	1.83	0.44
7:AA:30:MET:HG2	17:Bl:104:PEX:O2	2.18	0.43
17:AO:102:PEX:H9	17:AO:102:PEX:H14	1.75	0.43
8:BW:14:ARG:HB2	8:BW:14:ARG:HH11	1.83	0.43
10:Af:102:BCL:CED	8:Bf:23:VAL:HG12	2.48	0.43
9:Ag:29:HIS:CE1	10:Bg:1203:BCL:HMD3	2.53	0.43
10:Bg:1203:BCL:H11	10:Bg:1203:BCL:HBA1	1.77	0.43
12:BO:103:LMT:H1B	12:BO:103:LMT:H3'	1.73	0.43
7:AW:8:MET:O	8:BW:7:MET:HG3	2.17	0.43
8:Bf:22:ILE:HG21	10:Bf:101:BCL:C16	2.48	0.43
10:Bj:101:BCL:H101	10:Bj:101:BCL:H13	1.79	0.43
10:Ak:101:BCL:H11	10:Ak:101:BCL:H51	1.81	0.43
8:Bm:21:ILE:HD12	10:Bm:102:BCL:H11	2.00	0.43
2:L:213:GLU:OE1	3:M:234:ILE:HD11	2.18	0.43
3:M:55:TRP:CD1	9:Al:15:VAL:HG21	2.53	0.43
3:M:75:MET:HG2	3:M:93:LEU:CB	2.48	0.43
8:BG:44:PHE:CE1	12:BG:101:LMT:H42	2.54	0.43
8:BR:15:PHE:CD1	8:BR:15:PHE:C	2.96	0.43
8:Bb:2:THR:HG23	8:Bb:4:ASP:H	1.84	0.43
9:Ac:7:MET:HE1	9:Ad:10:PRO:HB2	2.00	0.43
9:Ad:10:PRO:HB3	8:Bd:9:PHE:CE2	2.52	0.43
8:Bd:23:VAL:HG12	10:Bd:101:BCL:CED	2.49	0.43
8:Bo:22:ILE:O	8:Bo:26:VAL:HG23	2.18	0.43
10:M:404:BCL:H141	11:M:405:BPH:H4C2	1.99	0.43
8:BF:14:ARG:HH21	7:AG:3:ARG:HD2	1.83	0.43
8:BG:17:GLY:O	8:BG:21:THR:HG22	2.19	0.43
8:BI:18:LEU:O	8:BI:22:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AM:101:BCL:H41	10:AM:101:BCL:H61	1.80	0.43
10:AO:101:BCL:H61	10:AO:101:BCL:H41	1.88	0.43
8:BU:29:VAL:HA	8:BU:32:VAL:HG12	2.01	0.43
7:AU:42:LYS:HA	7:AU:42:LYS:HD3	1.78	0.43
2:L:78:LEU:O	9:Ad:34:SER:OG	2.32	0.43
8:BB:7:MET:HE1	8:BB:15:PHE:HB2	2.01	0.43
17:AG:1101:PEX:O1	12:Bi:1201:LMT:O6'	2.36	0.43
8:BH:9:GLU:OE1	8:BH:13:ARG:HD2	2.19	0.43
10:BO:102:BCL:H62	10:BO:102:BCL:H41	1.77	0.43
9:Af:11:ARG:NH2	15:Af:101:CD4:H58	2.33	0.43
8:Bh:22:ILE:HB	10:Bh:101:BCL:C14	2.49	0.43
8:Bo:19:GLY:O	8:Bo:23:VAL:HG23	2.19	0.43
2:L:133:VAL:HG23	2:L:134:VAL:HG23	2.01	0.43
10:AP:102:BCL:H102	10:AP:102:BCL:H61	1.77	0.43
12:BR:102:LMT:O3'	12:BR:102:LMT:O2B	2.32	0.43
7:AV:19:PHE:CE2	10:Bn:101:BCL:H93	2.53	0.43
9:Am:36:GLN:O	9:Am:43:ASN:ND2	2.52	0.43
2:L:17:LEU:O	5:K:179:ILE:HG22	2.19	0.43
2:L:71:ASP:OD2	6:C:35:ARG:HB3	2.19	0.43
7:AP:5:TRP:HA	7:AP:8:MET:HE2	2.01	0.43
7:AV:40:LYS:HB3	7:AV:40:LYS:HE3	1.63	0.43
8:Be:22:ILE:O	8:Be:26:VAL:HG23	2.19	0.43
10:AF:101:BCL:H62	10:AF:101:BCL:H41	1.89	0.43
8:BP:18:TYR:HA	8:BP:21:THR:HG22	1.99	0.43
7:AQ:5:TRP:HA	7:AQ:8:MET:HE2	2.01	0.43
8:Ba:22:ILE:O	8:Ba:26:VAL:HG23	2.19	0.43
9:Ac:47:SER:OG	9:Ac:50:GLN:HG3	2.18	0.43
8:Bi:17:THR:O	8:Bi:21:ILE:HG13	2.18	0.43
9:Ao:14:MET:HB3	9:Ao:14:MET:HE3	1.80	0.43
5:K:54:ARG:HH12	5:K:86:GLU:HB2	1.83	0.43
8:BA:44:PHE:O	7:AX:42:LYS:HE2	2.19	0.43
7:AH:11:GLN:NE2	7:AI:4:ILE:O	2.49	0.43
12:BI:1101:LMT:H5B	12:BI:1101:LMT:H6E	2.01	0.43
7:AL:43:LYS:HB3	7:AL:43:LYS:HE2	1.48	0.43
9:Ao:2:HIS:CE1	9:Ao:3:ARG:HD3	2.54	0.43
7:AE:20:PHE:HA	10:Bj:101:BCL:C20	2.48	0.43
7:AI:38:TRP:HB2	8:BI:34:TRP:CH2	2.53	0.43
7:AP:43:LYS:HB3	7:AP:43:LYS:HE3	1.79	0.43
10:BS:101:BCL:O1D	7:AS:28:ILE:HD12	2.19	0.43
10:AX:102:BCL:HED3	8:BX:29:VAL:HG12	2.01	0.43
9:Ab:3:ARG:NH2	8:Bb:7:ARG:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ac:8:PHE:CE1	9:Ad:11:ARG:HG3	2.53	0.43
9:Af:17:MET:HE2	9:Af:17:MET:HB3	1.86	0.43
9:Ah:37:ARG:HG2	9:Ah:38:TYR:CD2	2.53	0.43
8:Bl:21:ILE:HG22	8:Bl:22:ILE:CG2	2.47	0.43
10:L:302:BCL:H3A	10:L:302:BCL:HBA2	1.82	0.42
6:C:134:MET:HE1	18:C:1001:HEC:C4D	2.48	0.42
8:BF:27:ILE:HD12	10:BF:102:BCL:H2	2.01	0.42
7:AG:2:HIS:CD2	8:BG:13:ARG:HB2	2.54	0.42
8:BR:13:ARG:HG3	8:BR:13:ARG:HH11	1.83	0.42
10:AV:1001:BCL:H162	10:AV:1001:BCL:H192	1.75	0.42
8:BV:30:ALA:CB	10:BV:102:BCL:HBA2	2.45	0.42
8:Bb:29:PHE:O	8:Bb:33:GLN:HG2	2.19	0.42
10:Be:101:BCL:CAB	17:Be:102:PEX:H10	2.49	0.42
10:Bk:1203:BCL:H192	10:Bk:1203:BCL:H162	1.81	0.42
8:Bo:1:MET:N	8:Bo:5:GLU:OE2	2.41	0.42
2:L:13:ARG:HG2	2:L:14:GLY:N	2.34	0.42
3:M:98:PRO:HG3	3:M:107:PRO:HG3	2.01	0.42
7:AG:38:TRP:CE3	7:AG:39:PRO:HD3	2.53	0.42
10:BP:101:BCL:O1D	7:AP:28:ILE:HD12	2.19	0.42
12:BP:102:LMT:H102	10:BQ:101:BCL:HBB2	2.01	0.42
8:Bi:31:ALA:HB2	12:Bi:1201:LMT:H62	2.00	0.42
10:Bo:1202:BCL:H41	10:Bo:1202:BCL:H71	2.01	0.42
10:AC:101:BCL:H72	7:AD:20:PHE:HE1	1.84	0.42
8:BF:18:TYR:HA	8:BF:21:THR:HG22	2.01	0.42
7:AG:43:LYS:O	7:AG:47:ASN:HB2	2.19	0.42
10:AM:101:BCL:H93	10:AM:101:BCL:H13	2.01	0.42
10:Aa:101:BCL:H71	10:Aa:101:BCL:H41	2.01	0.42
10:Bh:101:BCL:H121	10:Bh:101:BCL:H162	1.48	0.42
10:Bk:1203:BCL:H12	10:Bk:1203:BCL:H51	1.80	0.42
9:Al:37:ARG:HG2	9:Al:38:TYR:CD2	2.54	0.42
8:Bp:17:THR:O	8:Bp:21:ILE:HG12	2.19	0.42
17:Bp:1005:PEX:H6	17:Bp:1005:PEX:H12	1.53	0.42
7:AL:38:TRP:HA	7:AL:41:TYR:CD2	2.54	0.42
2:L:28:GLY:HA3	15:Af:101:CD4:H62	2.01	0.42
2:L:188:LEU:HD13	3:M:215:PHE:CG	2.55	0.42
10:AB:101:BCL:H12	10:AB:101:BCL:H61	2.01	0.42
7:AC:38:TRP:HA	7:AC:41:TYR:CE2	2.55	0.42
8:BE:7:ARG:HG3	8:BE:7:ARG:NH1	2.34	0.42
8:BH:9:GLU:O	8:BH:13:ARG:HG3	2.20	0.42
12:BI:1103:LMT:H72	12:BI:1103:LMT:H41	1.92	0.42
8:BJ:17:GLY:O	8:BJ:21:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BN:17:GLY:O	8:BN:21:THR:HG22	2.19	0.42
7:AW:42:LYS:HA	7:AW:42:LYS:HD2	1.84	0.42
10:AW:101:BCL:O1A	8:BW:26:TYR:OH	2.31	0.42
8:Bi:32:TRP:HH2	8:Bi:38:PHE:HB2	1.84	0.42
7:AG:10:PRO:HB3	8:BG:15:PHE:CE1	2.54	0.42
12:BL:103:LMT:H6D	8:BM:38:TRP:CZ2	2.55	0.42
10:AP:102:BCL:H151	10:AP:102:BCL:H18	1.68	0.42
7:AS:22:ALA:HA	10:Bp:1001:BCL:H2	2.00	0.42
12:BX:104:LMT:H3'	12:BX:104:LMT:H1B	1.80	0.42
13:L:310:MQ8:H2M1	13:L:310:MQ8:H111	1.68	0.42
6:C:118:THR:HA	6:C:124:PRO:HA	2.02	0.42
8:BP:40:TRP:CH2	7:AP:38:TRP:HB2	2.54	0.42
9:Ah:7:MET:HE3	9:Ah:7:MET:HB2	1.86	0.42
3:M:164:PRO:HA	3:M:167:VAL:HG22	2.02	0.42
8:BE:12:TYR:HA	8:BE:15:THR:HG22	2.01	0.42
7:AH:43:LYS:HB2	7:AH:43:LYS:HE3	1.77	0.42
10:AO:101:BCL:H162	10:AO:101:BCL:H141	1.75	0.42
10:AR:101:BCL:H112	7:AS:24:LEU:HD13	2.02	0.42
7:AU:15:SER:O	8:Bo:18:LEU:HD11	2.20	0.42
8:Bb:5:GLU:OE1	8:Bb:5:GLU:N	2.53	0.42
10:Ai:101:BCL:CED	8:Bi:23:VAL:HG12	2.50	0.42
10:Bl:103:BCL:CAB	17:Bl:104:PEX:H30	2.50	0.42
2:L:190:MET:CE	13:L:310:MQ8:H111	2.50	0.42
7:AC:38:TRP:CE3	7:AC:39:PRO:HG3	2.55	0.42
8:BD:7:MET:HE1	7:AD:13:ILE:HD12	2.02	0.42
8:BF:23:THR:O	8:BF:27:ILE:HG12	2.20	0.42
7:AR:30:MET:HE2	8:Ba:29:PHE:CD1	2.52	0.42
7:AR:43:LYS:HB3	7:AR:43:LYS:HE2	1.78	0.42
15:M:402:CD4:H64	15:M:402:CD4:H71	1.83	0.42
10:BD:101:BCL:HMD3	7:AD:29:HIS:CE1	2.55	0.42
8:BI:18:LEU:HD23	8:BI:18:LEU:HA	1.88	0.42
10:AM:101:BCL:H161	10:AM:101:BCL:H122	1.80	0.42
7:AO:21:LEU:HB3	10:AO:101:BCL:H12	2.01	0.42
8:BR:13:ARG:HG2	7:AR:2:HIS:CD2	2.55	0.42
7:AU:38:TRP:HA	7:AU:41:TYR:CD2	2.54	0.42
9:Ae:56:SER:HB3	9:Af:52:PRO:HG3	2.02	0.42
9:Af:1:MET:O	9:Af:4:ILE:HG22	2.20	0.42
8:Bg:32:TRP:CD2	17:Bg:1204:PEX:H7	2.55	0.42
9:Aj:47:SER:OG	9:Aj:50:GLN:HG3	2.20	0.42
8:Bj:18:LEU:HD11	10:Bj:101:BCL:H191	2.02	0.42
8:Bl:21:ILE:O	8:Bl:24:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:94:PRO:O	20:K:201:HOH:O	2.22	0.41
7:AD:22:ALA:HB2	10:Bj:101:BCL:H51	2.03	0.41
8:BG:18:TYR:CE1	7:AH:1:MET:HB3	2.54	0.41
9:Aa:46:LEU:HD13	9:Ap:56:SER:HB3	2.02	0.41
8:Bj:32:TRP:CG	17:Bj:104:PEX:H9	2.55	0.41
9:Ak:10:PRO:HB3	8:Bk:9:PHE:CZ	2.55	0.41
1:S:116:GLU:HB2	9:Af:50:GLN:NE2	2.35	0.41
7:AD:26:LEU:HD21	10:Bj:101:BCL:H111	2.01	0.41
7:AG:38:TRP:HB2	8:BG:40:TRP:CH2	2.56	0.41
10:AK:101:BCL:CED	8:BK:29:VAL:HG12	2.49	0.41
8:BN:24:LEU:HD23	8:BN:24:LEU:HA	1.94	0.41
7:AO:27:ILE:HG23	17:AO:102:PEX:H8	2.01	0.41
12:BS:102:LMT:H3'	12:BS:102:LMT:H1B	1.76	0.41
7:AW:38:TRP:CD1	8:BX:44:PHE:HB3	2.55	0.41
2:L:129:TYR:CD1	10:L:302:BCL:HBB1	2.55	0.41
3:M:157:TYR:HD1	10:M:403:BCL:HBB1	1.85	0.41
11:M:405:BPH:HBB3	11:M:405:BPH:HHC	2.02	0.41
7:AE:42:LYS:HA	7:AE:42:LYS:HD2	1.76	0.41
10:BR:101:BCL:HED3	7:AR:24:LEU:HD23	2.02	0.41
7:AR:1:MET:HE3	7:AR:1:MET:HB3	1.96	0.41
9:Ae:17:MET:HE3	9:Ae:17:MET:HB2	1.73	0.41
8:Bj:2:THR:HG23	8:Bj:5:GLU:H	1.84	0.41
10:Bm:102:BCL:H11	10:Bm:102:BCL:H52	1.77	0.41
6:C:228:TYR:OH	18:C:1003:HEC:O2A	2.38	0.41
7:AG:42:LYS:HD2	7:AG:42:LYS:HA	1.75	0.41
7:AJ:4:ILE:HD12	7:AJ:4:ILE:HA	1.94	0.41
12:AK:102:LMT:H21	8:Bf:30:LEU:HD22	2.01	0.41
8:BK:28:ILE:O	8:BK:32:VAL:HG23	2.19	0.41
8:BN:40:TRP:CD1	12:BN:102:LMT:H11	2.55	0.41
8:BR:40:TRP:HH2	7:AR:38:TRP:HB2	1.86	0.41
10:AT:104:BCL:H43	9:Ap:18:VAL:HG13	2.02	0.41
3:M:91:PRO:HG2	3:M:92:TRP:CE3	2.56	0.41
5:K:134:ALA:O	5:K:175:ARG:NH1	2.49	0.41
7:AA:42:LYS:NZ	7:AA:45:GLN:OE1	2.52	0.41
8:BJ:15:PHE:CD2	8:BJ:15:PHE:C	2.98	0.41
10:BL:102:BCL:H52	10:BL:102:BCL:H11	1.83	0.41
8:Ba:17:THR:O	8:Ba:21:ILE:HG12	2.21	0.41
9:Ac:37:ARG:HD2	9:Ac:52:PRO:O	2.21	0.41
9:Ae:10:PRO:HB3	8:Be:9:PHE:CE2	2.56	0.41
9:Ai:37:ARG:HG2	9:Ai:38:TYR:CD2	2.55	0.41
10:M:404:BCL:HBD	10:M:404:BCL:HAA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AJ:26:LEU:HG	10:Bf:103:BCL:C19	2.49	0.41
10:BN:101:BCL:H12	10:BN:101:BCL:H52	1.89	0.41
10:AQ:101:BCL:H111	10:AQ:101:BCL:H152	1.86	0.41
7:AS:4:ILE:HD12	7:AS:4:ILE:HA	1.84	0.41
10:Aa:101:BCL:CHC	10:Bp:1004:BCL:HBB3	2.50	0.41
8:Bb:1:MET:N	8:Bb:1:MET:SD	2.92	0.41
10:Ac:101:BCL:H162	10:Ac:101:BCL:H192	1.86	0.41
9:Ad:14:MET:HE1	19:Bd:102:V7N:C38	2.50	0.41
9:Al:10:PRO:HG2	8:Bl:1:MET:HE1	2.02	0.41
8:Bp:21:ILE:HD13	8:Bp:21:ILE:HA	1.78	0.41
2:L:221:LEU:HD12	13:L:310:MQ8:H142	2.01	0.41
3:M:98:PRO:HB3	3:M:107:PRO:HB3	2.03	0.41
3:M:251:TRP:CG	13:M:409:MQ8:H112	2.55	0.41
8:BA:15:PHE:CD2	8:BA:15:PHE:C	2.99	0.41
8:BC:28:ILE:O	8:BC:32:VAL:HG23	2.21	0.41
7:AG:3:ARG:HG2	7:AG:6:GLN:OE1	2.21	0.41
12:BK:101:LMT:H102	12:BK:101:LMT:H71	1.88	0.41
8:BS:40:TRP:CH2	7:AS:38:TRP:HB2	2.55	0.41
9:Aa:33:LEU:HD11	9:Aa:41:ILE:HD12	2.03	0.41
8:Be:22:ILE:HD13	8:Be:22:ILE:HA	1.86	0.41
9:Af:37:ARG:HG2	9:Af:38:TYR:CD2	2.56	0.41
9:Ap:10:PRO:HB3	8:Bp:9:PHE:CZ	2.56	0.41
11:L:303:BPH:H6C1	11:L:303:BPH:H102	1.72	0.41
7:AC:38:TRP:HA	7:AC:41:TYR:CD2	2.55	0.41
7:AG:38:TRP:HA	7:AG:41:TYR:CD2	2.56	0.41
10:AK:101:BCL:H142	10:AK:101:BCL:H112	1.80	0.41
7:AV:38:TRP:HB2	8:BV:40:TRP:CH2	2.55	0.41
10:Ac:101:BCL:H62	10:Ac:101:BCL:H41	1.81	0.41
8:Bj:2:THR:OG1	8:Bj:3:GLU:N	2.54	0.41
10:Bk:1203:BCL:H162	10:Bk:1203:BCL:H141	1.81	0.41
10:Bk:1203:BCL:H152	8:Bl:20:TYR:HB2	2.03	0.41
8:Bp:32:TRP:HH2	8:Bp:38:PHE:HB2	1.86	0.41
2:L:44:THR:HG21	15:Af:101:CD4:H6	2.03	0.41
3:M:327:THR:HG22	9:Al:65:SER:HB2	2.03	0.41
4:H:23:ILE:HG23	4:H:47:PRO:HG3	2.02	0.41
6:C:239:LYS:HE3	6:C:239:LYS:HB3	1.66	0.41
7:AA:38:TRP:HA	7:AA:41:TYR:CD2	2.56	0.41
8:BG:15:PHE:CD2	8:BG:15:PHE:C	2.99	0.41
10:BG:102:BCL:H62	10:BG:102:BCL:H41	1.80	0.41
7:AJ:24:LEU:O	7:AJ:28:ILE:HG13	2.21	0.41
7:AL:28:ILE:HD12	10:BL:102:BCL:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AL:101:BCL:H8	7:AM:24:LEU:HD13	2.03	0.41
8:BL:14:ARG:HH12	7:AM:3:ARG:CD	2.34	0.41
10:BP:104:BCL:H122	17:Bb:102:PEX:H22	2.02	0.41
10:AP:102:BCL:H141	10:AP:102:BCL:H162	1.84	0.41
7:AV:42:LYS:HD2	7:AV:42:LYS:HA	1.92	0.41
10:Ba:102:BCL:H151	17:Ba:103:PEX:H25	2.02	0.41
10:Bf:101:BCL:H61	10:Bf:101:BCL:H41	1.85	0.41
9:Ah:17:MET:HE2	9:Ah:17:MET:HB3	1.75	0.41
8:Bi:22:ILE:O	8:Bi:26:VAL:HG23	2.20	0.41
8:Bj:18:LEU:CG	8:Bj:22:ILE:HD11	2.48	0.41
8:Bk:22:ILE:O	8:Bk:26:VAL:HG23	2.20	0.41
10:Al:101:BCL:H193	10:Al:101:BCL:H161	1.82	0.41
2:L:165:TYR:O	2:L:167:HIS:N	2.53	0.41
6:C:161:MET:HE3	6:C:161:MET:HB3	1.95	0.41
7:AF:9:ASP:HB3	7:AF:12:ILE:HB	2.03	0.41
7:AO:38:TRP:HA	7:AO:41:TYR:CE2	2.56	0.41
9:Ag:3:ARG:CG	9:Ag:6:LEU:HD12	2.50	0.41
8:Bg:29:PHE:O	8:Bg:33:GLN:HG2	2.21	0.41
5:K:179:ILE:C	5:K:180:ILE:HD12	2.46	0.40
8:BA:29:VAL:HG22	10:Bl:101:BCL:HED3	2.02	0.40
8:BF:24:LEU:HD13	8:BF:24:LEU:HA	1.92	0.40
8:BQ:17:GLY:O	8:BQ:21:THR:HG22	2.21	0.40
7:AW:38:TRP:HA	7:AW:41:TYR:CE2	2.56	0.40
7:AW:38:TRP:HB2	8:BW:40:TRP:CH2	2.57	0.40
8:BW:7:MET:HE1	8:BW:15:PHE:CG	2.56	0.40
7:AX:8:MET:HB3	7:AX:13:ILE:HD11	2.03	0.40
9:Am:8:PHE:HE1	9:An:14:MET:HE3	1.85	0.40
7:AA:24:LEU:O	7:AA:28:ILE:HG13	2.22	0.40
7:AE:24:LEU:HD23	10:BE:102:BCL:HED3	2.03	0.40
10:AF:101:BCL:H122	8:Bi:26:VAL:HG21	2.02	0.40
7:AK:43:LYS:HB2	7:AK:43:LYS:HE3	1.62	0.40
7:AL:42:LYS:HD2	7:AL:42:LYS:HA	1.63	0.40
10:BM:101:BCL:CGA	10:BM:101:BCL:H3A	2.51	0.40
10:BM:101:BCL:H61	10:BM:101:BCL:H41	1.97	0.40
8:BT:9:GLU:OE1	8:BT:13:ARG:HD3	2.21	0.40
8:BT:23:THR:O	8:BT:27:ILE:HG13	2.20	0.40
8:Be:32:TRP:HH2	8:Be:38:PHE:HB2	1.87	0.40
9:Aj:56:SER:OG	9:Aj:57:ALA:N	2.53	0.40
9:Al:35:SER:O	9:Al:39:SER:HB2	2.21	0.40
2:L:37:VAL:HG22	15:Af:101:CD4:H19	2.04	0.40
2:L:220:LEU:HD11	3:M:133:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:187:ALA:HB2	6:C:209:GLU:HG3	2.03	0.40
3:M:319:LEU:HD21	6:C:250:HIS:NE2	2.37	0.40
10:M:403:BCL:H111	10:M:403:BCL:H162	2.03	0.40
8:BH:39:GLN:H	8:BH:39:GLN:HG2	1.65	0.40
7:AL:7:GLY:HA2	8:BL:7:MET:H	1.85	0.40
7:AM:38:TRP:CE3	7:AM:39:PRO:HD3	2.56	0.40
17:AT:103:PEX:H43	8:Bo:25:ALA:HB2	2.03	0.40
17:AT:103:PEX:H3	12:Bp:1002:LMT:H12	2.03	0.40
7:AV:9:ASP:O	7:AV:13:ILE:HG12	2.20	0.40
8:Bd:2:THR:O	8:Bd:5:GLU:HG3	2.21	0.40
10:Bh:102:BCL:H8	10:Bh:102:BCL:H121	1.97	0.40
10:Bn:101:BCL:H192	10:Bn:101:BCL:H161	1.86	0.40
10:Bo:1202:BCL:H92	10:Bo:1202:BCL:H62	1.84	0.40
3:M:18:GLU:OE1	3:M:20:GLY:N	2.54	0.40
8:BC:40:TRP:HB2	12:BC:102:LMT:H32	2.04	0.40
8:BJ:40:TRP:CE2	8:BJ:41:ARG:HG3	2.56	0.40
7:AT:41:TYR:O	7:AT:45:GLN:HG3	2.21	0.40
10:AV:1001:BCL:HBB3	10:BW:102:BCL:C4B	2.52	0.40
8:BW:24:LEU:O	8:BW:28:ILE:HD12	2.21	0.40
8:BW:27:ILE:HD13	8:BW:27:ILE:HA	1.95	0.40
10:Ba:102:BCL:H11	10:Ba:102:BCL:H52	1.88	0.40
8:Be:1:MET:N	8:Be:5:GLU:OE2	2.46	0.40
8:Bj:7:ARG:HA	8:Bj:7:ARG:HD3	1.81	0.40
8:Bl:12:TYR:HA	8:Bl:15:THR:HG22	2.04	0.40
6:C:57:ILE:HD11	9:Aa:64:MET:SD	2.60	0.40
7:AJ:9:ASP:OD1	7:AJ:9:ASP:C	2.64	0.40
7:AL:38:TRP:HA	7:AL:41:TYR:CE2	2.56	0.40
7:AR:29:HIS:HE1	10:AR:101:BCL:C1A	2.33	0.40
8:BX:23:THR:HG22	8:BX:27:ILE:HD12	2.02	0.40
9:Aa:14:MET:HE1	8:Ba:13:PHE:HE1	1.85	0.40
8:Bk:8:ARG:HG2	8:Bk:8:ARG:HH11	1.87	0.40
8:Bm:1:MET:HG2	8:Bm:5:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	101/204 (50%)	98 (97%)	3 (3%)	0	100	100
2	L	269/274 (98%)	262 (97%)	7 (3%)	0	100	100
3	M	333/392 (85%)	328 (98%)	5 (2%)	0	100	100
4	H	58/66 (88%)	57 (98%)	1 (2%)	0	100	100
5	K	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
6	C	296/373 (79%)	280 (95%)	16 (5%)	0	100	100
7	AA	46/56 (82%)	46 (100%)	0	0	100	100
7	AB	46/56 (82%)	46 (100%)	0	0	100	100
7	AC	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
7	AD	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
7	AE	47/56 (84%)	47 (100%)	0	0	100	100
7	AF	47/56 (84%)	47 (100%)	0	0	100	100
7	AG	47/56 (84%)	47 (100%)	0	0	100	100
7	AH	47/56 (84%)	47 (100%)	0	0	100	100
7	AI	47/56 (84%)	47 (100%)	0	0	100	100
7	AJ	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
7	AK	46/56 (82%)	46 (100%)	0	0	100	100
7	AL	46/56 (82%)	46 (100%)	0	0	100	100
7	AM	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
7	AN	46/56 (82%)	46 (100%)	0	0	100	100
7	AO	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
7	AP	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
7	AQ	47/56 (84%)	47 (100%)	0	0	100	100
7	AR	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
7	AS	47/56 (84%)	47 (100%)	0	0	100	100
7	AT	46/56 (82%)	46 (100%)	0	0	100	100
7	AU	46/56 (82%)	46 (100%)	0	0	100	100
7	AV	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
7	AW	47/56 (84%)	46 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AX	46/56 (82%)	46 (100%)	0	0	100	100
8	BA	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	BB	37/44 (84%)	37 (100%)	0	0	100	100
8	BC	38/44 (86%)	38 (100%)	0	0	100	100
8	BD	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	BE	36/44 (82%)	36 (100%)	0	0	100	100
8	BF	37/44 (84%)	37 (100%)	0	0	100	100
8	BG	37/44 (84%)	37 (100%)	0	0	100	100
8	BH	37/44 (84%)	37 (100%)	0	0	100	100
8	BI	36/44 (82%)	36 (100%)	0	0	100	100
8	BJ	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	BK	37/44 (84%)	37 (100%)	0	0	100	100
8	BL	37/44 (84%)	37 (100%)	0	0	100	100
8	BM	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	BN	37/44 (84%)	37 (100%)	0	0	100	100
8	BO	37/44 (84%)	37 (100%)	0	0	100	100
8	BP	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
8	BQ	37/44 (84%)	37 (100%)	0	0	100	100
8	BR	37/44 (84%)	37 (100%)	0	0	100	100
8	BS	37/44 (84%)	37 (100%)	0	0	100	100
8	BT	37/44 (84%)	35 (95%)	2 (5%)	0	100	100
8	BU	37/44 (84%)	37 (100%)	0	0	100	100
8	BV	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
8	BW	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	BX	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
8	Ba	36/44 (82%)	36 (100%)	0	0	100	100
8	Bb	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
8	Bc	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
8	Bd	35/44 (80%)	35 (100%)	0	0	100	100
8	Be	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
8	Bf	32/44 (73%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Bg	36/44 (82%)	36 (100%)	0	0	100	100
8	Bh	34/44 (77%)	33 (97%)	1 (3%)	0	100	100
8	Bi	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
8	Bj	36/44 (82%)	36 (100%)	0	0	100	100
8	Bk	36/44 (82%)	36 (100%)	0	0	100	100
8	Bl	36/44 (82%)	36 (100%)	0	0	100	100
8	Bm	36/44 (82%)	36 (100%)	0	0	100	100
8	Bn	36/44 (82%)	36 (100%)	0	0	100	100
8	Bo	36/44 (82%)	36 (100%)	0	0	100	100
8	Bp	33/44 (75%)	33 (100%)	0	0	100	100
9	Aa	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
9	Ab	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
9	Ac	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
9	Ad	52/71 (73%)	52 (100%)	0	0	100	100
9	Ae	57/71 (80%)	57 (100%)	0	0	100	100
9	Af	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
9	Ag	55/71 (78%)	55 (100%)	0	0	100	100
9	Ah	51/71 (72%)	48 (94%)	3 (6%)	0	100	100
9	Ai	55/71 (78%)	53 (96%)	2 (4%)	0	100	100
9	Aj	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
9	Ak	54/71 (76%)	54 (100%)	0	0	100	100
9	Al	67/71 (94%)	63 (94%)	4 (6%)	0	100	100
9	Am	50/71 (70%)	50 (100%)	0	0	100	100
9	An	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
9	Ao	55/71 (78%)	55 (100%)	0	0	100	100
9	Ap	53/71 (75%)	53 (100%)	0	0	100	100
All	All	4696/5729 (82%)	4606 (98%)	90 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	84/158 (53%)	84 (100%)	0	100	100
2	L	213/216 (99%)	205 (96%)	8 (4%)	29	44
3	M	272/311 (88%)	270 (99%)	2 (1%)	76	87
4	H	51/55 (93%)	51 (100%)	0	100	100
5	K	146/147 (99%)	142 (97%)	4 (3%)	39	58
6	C	251/302 (83%)	247 (98%)	4 (2%)	55	73
7	AA	38/45 (84%)	38 (100%)	0	100	100
7	AB	38/45 (84%)	38 (100%)	0	100	100
7	AC	38/45 (84%)	36 (95%)	2 (5%)	20	30
7	AD	18/45 (40%)	18 (100%)	0	100	100
7	AE	17/45 (38%)	17 (100%)	0	100	100
7	AF	39/45 (87%)	39 (100%)	0	100	100
7	AG	39/45 (87%)	39 (100%)	0	100	100
7	AH	39/45 (87%)	39 (100%)	0	100	100
7	AI	39/45 (87%)	38 (97%)	1 (3%)	40	59
7	AJ	38/45 (84%)	35 (92%)	3 (8%)	11	15
7	AK	38/45 (84%)	38 (100%)	0	100	100
7	AL	38/45 (84%)	37 (97%)	1 (3%)	40	59
7	AM	39/45 (87%)	39 (100%)	0	100	100
7	AN	38/45 (84%)	37 (97%)	1 (3%)	40	59
7	AO	38/45 (84%)	38 (100%)	0	100	100
7	AP	38/45 (84%)	38 (100%)	0	100	100
7	AQ	39/45 (87%)	38 (97%)	1 (3%)	40	59
7	AR	38/45 (84%)	38 (100%)	0	100	100
7	AS	39/45 (87%)	39 (100%)	0	100	100
7	AT	38/45 (84%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AU	38/45 (84%)	37 (97%)	1 (3%)	40	59
7	AV	38/45 (84%)	37 (97%)	1 (3%)	40	59
7	AW	39/45 (87%)	39 (100%)	0	100	100
7	AX	38/45 (84%)	38 (100%)	0	100	100
8	BA	30/34 (88%)	28 (93%)	2 (7%)	15	21
8	BB	30/34 (88%)	30 (100%)	0	100	100
8	BC	30/34 (88%)	30 (100%)	0	100	100
8	BD	9/34 (26%)	8 (89%)	1 (11%)	6	7
8	BE	24/34 (71%)	23 (96%)	1 (4%)	26	40
8	BF	30/34 (88%)	30 (100%)	0	100	100
8	BG	25/34 (74%)	25 (100%)	0	100	100
8	BH	30/34 (88%)	30 (100%)	0	100	100
8	BI	30/34 (88%)	30 (100%)	0	100	100
8	BJ	30/34 (88%)	30 (100%)	0	100	100
8	BK	30/34 (88%)	30 (100%)	0	100	100
8	BL	30/34 (88%)	30 (100%)	0	100	100
8	BM	30/34 (88%)	29 (97%)	1 (3%)	33	50
8	BN	30/34 (88%)	30 (100%)	0	100	100
8	BO	30/34 (88%)	28 (93%)	2 (7%)	15	21
8	BP	30/34 (88%)	30 (100%)	0	100	100
8	BQ	30/34 (88%)	30 (100%)	0	100	100
8	BR	30/34 (88%)	30 (100%)	0	100	100
8	BS	30/34 (88%)	30 (100%)	0	100	100
8	BT	30/34 (88%)	29 (97%)	1 (3%)	33	50
8	BU	30/34 (88%)	30 (100%)	0	100	100
8	BV	31/34 (91%)	30 (97%)	1 (3%)	34	51
8	BW	30/34 (88%)	30 (100%)	0	100	100
8	BX	30/34 (88%)	29 (97%)	1 (3%)	33	50
8	Ba	30/34 (88%)	30 (100%)	0	100	100
8	Bb	30/34 (88%)	30 (100%)	0	100	100
8	Bc	30/34 (88%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Bd	29/34 (85%)	28 (97%)	1 (3%)	32	49
8	Be	30/34 (88%)	29 (97%)	1 (3%)	33	50
8	Bf	26/34 (76%)	26 (100%)	0	100	100
8	Bg	30/34 (88%)	30 (100%)	0	100	100
8	Bh	28/34 (82%)	26 (93%)	2 (7%)	13	19
8	Bi	30/34 (88%)	30 (100%)	0	100	100
8	Bj	30/34 (88%)	30 (100%)	0	100	100
8	Bk	30/34 (88%)	30 (100%)	0	100	100
8	Bl	30/34 (88%)	28 (93%)	2 (7%)	15	21
8	Bm	30/34 (88%)	29 (97%)	1 (3%)	33	50
8	Bn	30/34 (88%)	30 (100%)	0	100	100
8	Bo	30/34 (88%)	30 (100%)	0	100	100
8	Bp	27/34 (79%)	26 (96%)	1 (4%)	30	45
9	Aa	53/55 (96%)	53 (100%)	0	100	100
9	Ab	45/55 (82%)	44 (98%)	1 (2%)	45	65
9	Ac	46/55 (84%)	44 (96%)	2 (4%)	26	39
9	Ad	44/55 (80%)	43 (98%)	1 (2%)	44	63
9	Ae	46/55 (84%)	46 (100%)	0	100	100
9	Af	46/55 (84%)	46 (100%)	0	100	100
9	Ag	46/55 (84%)	43 (94%)	3 (6%)	15	22
9	Ah	43/55 (78%)	42 (98%)	1 (2%)	44	63
9	Ai	46/55 (84%)	43 (94%)	3 (6%)	15	22
9	Aj	45/55 (82%)	44 (98%)	1 (2%)	45	65
9	Ak	46/55 (84%)	46 (100%)	0	100	100
9	Al	53/55 (96%)	50 (94%)	3 (6%)	18	27
9	Am	44/55 (80%)	43 (98%)	1 (2%)	44	63
9	An	46/55 (84%)	44 (96%)	2 (4%)	26	39
9	Ao	46/55 (84%)	46 (100%)	0	100	100
9	Ap	45/55 (82%)	44 (98%)	1 (2%)	45	65
All	All	3795/4509 (84%)	3729 (98%)	66 (2%)	52	72

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	16	THR
2	L	39	THR
2	L	81	LEU
2	L	183	THR
2	L	198	VAL
2	L	248	CYS
2	L	250	VAL
2	L	265	ASN
3	M	1	MET
3	M	215	PHE
5	K	32	SER
5	K	101	VAL
5	K	139	GLN
5	K	157	GLU
6	C	105	CYS
6	C	111	ILE
6	C	146	SER
6	C	287	VAL
8	BA	21	THR
8	BA	32	VAL
7	AC	1	MET
7	AC	17	LEU
8	BD	13	ARG
8	BE	22	ILE
7	AI	9	ASP
7	AJ	11	GLN
7	AJ	26	LEU
7	AJ	38	TRP
7	AL	4	ILE
8	BM	21	THR
7	AN	8	MET
8	BO	24	LEU
8	BO	28	ILE
7	AQ	19	PHE
8	BT	28	ILE
7	AU	17	LEU
7	AV	15	SER
8	BV	7	MET
8	BX	24	LEU
9	Ab	39	SER
9	Ac	18	VAL
9	Ac	39	SER
9	Ad	6	LEU

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Mol	Chain	Res	Type
8	Bd	14	VAL
8	Be	18	LEU
9	Ag	6	LEU
9	Ag	7	MET
9	Ag	39	SER
9	Ah	4	ILE
8	Bh	14	VAL
8	Bh	22	ILE
9	Ai	1	MET
9	Ai	17	MET
9	Ai	39	SER
9	Aj	39	SER
9	Al	18	VAL
9	Al	23	VAL
9	Al	39	SER
8	Bl	2	THR
8	Bl	5	GLU
9	Am	50	GLN
8	Bm	22	ILE
9	An	2	HIS
9	An	40	TRP
9	Ap	13	VAL
8	Bp	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	184	ASN
3	M	141	ASN
3	M	292	ASN
5	K	121	ASN
5	K	139	GLN
5	K	151	GLN
6	C	31	GLN
6	C	181	HIS
6	C	201	ASN
6	C	260	GLN
6	C	267	GLN
6	C	293	ASN
8	BA	16	HIS
8	BI	33	GLN
7	AJ	6	GLN

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Mol	Chain	Res	Type
7	AJ	11	GLN
7	AJ	47	ASN
7	AK	6	GLN
8	BM	16	HIS
7	AO	11	GLN
7	AR	45	GLN
7	AS	11	GLN
7	AS	47	ASN
7	AT	6	GLN
8	BU	39	GLN
7	AX	11	GLN
8	Ba	33	GLN
9	Ac	36	GLN
9	Ac	50	GLN
9	Al	36	GLN
9	Al	50	GLN
9	An	36	GLN
9	Ao	36	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 1 is monoatomic - leaving 201 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$
10	BCL	AW	101	-	69,74,74	1.13	7 (10%)	79,115,115	1.35	9 (11%)
10	BCL	Bd	101	10	69,74,74	1.27	8 (11%)	79,115,115	1.59	12 (15%)
19	V7N	Am	102	-	44,44,44	1.66	6 (13%)	48,54,54	1.77	15 (31%)
10	BCL	Ak	101	10	69,74,74	1.15	6 (8%)	79,115,115	1.41	11 (13%)
19	V7N	AL	102	-	44,44,44	1.65	7 (15%)	48,54,54	1.58	11 (22%)
10	BCL	AT	104	-	69,74,74	1.16	6 (8%)	79,115,115	1.43	11 (13%)
10	BCL	AU	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.41	10 (12%)
10	BCL	BK	102	-	69,74,74	1.07	6 (8%)	79,115,115	1.44	10 (12%)
10	BCL	Ag	101	-	69,74,74	1.18	6 (8%)	79,115,115	1.46	12 (15%)
12	LMT	L	306	-	36,36,36	1.13	4 (11%)	47,47,47	1.03	4 (8%)
10	BCL	Aa	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.45	12 (15%)
10	BCL	BG	102	-	69,74,74	1.09	5 (7%)	79,115,115	1.32	7 (8%)
12	LMT	BC	102	-	36,36,36	1.21	6 (16%)	47,47,47	0.94	2 (4%)
12	LMT	BN	102	-	36,36,36	1.19	6 (16%)	47,47,47	1.02	3 (6%)
12	LMT	BB	103	10	36,36,36	1.16	6 (16%)	47,47,47	0.99	2 (4%)
10	BCL	Bk	1203	-	69,74,74	1.15	5 (7%)	79,115,115	1.29	6 (7%)
12	LMT	BQ	102	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	2 (4%)
12	LMT	Bl	105	-	36,36,36	1.16	5 (13%)	47,47,47	1.09	2 (4%)
18	HEC	C	1002	6	46,50,50	1.85	5 (10%)	58,82,82	1.84	5 (8%)
10	BCL	L	302	-	69,74,74	1.15	6 (8%)	79,115,115	1.45	8 (10%)
19	V7N	Bp	1003	-	44,44,44	1.65	8 (18%)	48,54,54	1.58	10 (20%)
10	BCL	AR	101	-	69,74,74	1.12	8 (11%)	79,115,115	1.41	12 (15%)
12	LMT	AQ	102	-	36,36,36	1.15	6 (16%)	47,47,47	1.07	2 (4%)
17	PEX	Bb	102	-	34,34,34	0.56	0	37,39,39	0.51	0
17	PEX	Bp	1005	-	34,34,34	0.55	0	37,39,39	0.48	0
10	BCL	BF	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.32	8 (10%)
10	BCL	BC	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.39	10 (12%)
10	BCL	BH	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.42	11 (13%)
10	BCL	AX	102	-	69,74,74	1.17	7 (10%)	79,115,115	1.38	10 (12%)
13	MQ8	Ad	101	-	54,54,54	0.30	0	67,69,69	0.64	2 (2%)
12	LMT	Bc	1201	-	36,36,36	1.17	6 (16%)	47,47,47	1.04	3 (6%)
10	BCL	AM	101	-	69,74,74	1.14	7 (10%)	79,115,115	1.41	9 (11%)
10	BCL	BV	102	-	69,74,74	1.09	5 (7%)	79,115,115	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	Bp	1004	-	69,74,74	1.16	5 (7%)	79,115,115	1.29	7 (8%)
17	PEX	Bn	102	-	34,34,34	0.55	0	37,39,39	0.50	0
10	BCL	BP	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.40	10 (12%)
10	BCL	Ao	101	-	69,74,74	1.19	6 (8%)	79,115,115	1.53	11 (13%)
10	BCL	Ae	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.38	10 (12%)
12	LMT	Bj	102	-	36,36,36	1.19	5 (13%)	47,47,47	0.98	2 (4%)
10	BCL	An	101	-	69,74,74	1.17	6 (8%)	79,115,115	1.48	11 (13%)
19	V7N	BS	103	-	44,44,44	1.65	7 (15%)	48,54,54	1.60	11 (22%)
19	V7N	AT	102	-	44,44,44	1.64	6 (13%)	48,54,54	1.77	12 (25%)
17	PEX	Bd	104	-	34,34,34	0.56	0	37,39,39	0.50	0
10	BCL	Bp	1001	-	69,74,74	1.40	8 (11%)	79,115,115	1.93	15 (18%)
19	V7N	Bf	102	-	44,44,44	1.67	7 (15%)	48,54,54	1.70	11 (22%)
10	BCL	Ai	101	-	69,74,74	1.16	6 (8%)	79,115,115	1.33	9 (11%)
12	LMT	Bm	104	-	36,36,36	1.15	5 (13%)	47,47,47	1.15	3 (6%)
13	MQ8	L	310	-	54,54,54	0.32	0	67,69,69	0.68	2 (2%)
19	V7N	BW	101	-	44,44,44	1.64	8 (18%)	48,54,54	1.65	10 (20%)
10	BCL	Bl	103	-	69,74,74	1.12	6 (8%)	79,115,115	1.61	10 (12%)
12	LMT	BD	102	-	36,36,36	1.20	6 (16%)	47,47,47	1.01	3 (6%)
10	BCL	BE	102	-	69,74,74	1.11	6 (8%)	79,115,115	1.32	8 (10%)
10	BCL	Bh	101	-	69,74,74	1.22	8 (11%)	79,115,115	1.63	11 (13%)
12	LMT	BS	102	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)
10	BCL	AI	102	-	69,74,74	1.13	7 (10%)	79,115,115	1.47	11 (13%)
10	BCL	BN	101	-	69,74,74	1.13	6 (8%)	79,115,115	1.36	11 (13%)
10	BCL	Be	101	17	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
19	V7N	An	102	-	44,44,44	1.66	8 (18%)	48,54,54	1.64	11 (22%)
12	LMT	L	305	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
10	BCL	BM	101	-	69,74,74	1.13	5 (7%)	79,115,115	1.38	9 (11%)
12	LMT	BL	103	-	36,36,36	1.18	6 (16%)	47,47,47	1.03	2 (4%)
10	BCL	BB	101	-	69,74,74	1.13	5 (7%)	79,115,115	1.42	13 (16%)
12	LMT	BG	103	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	2 (4%)
19	V7N	BC	103	-	44,44,44	1.63	5 (11%)	48,54,54	1.77	11 (22%)
10	BCL	BS	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.31	7 (8%)
10	BCL	BD	101	-	69,74,74	1.12	5 (7%)	79,115,115	1.36	11 (13%)
10	BCL	Bf	101	-	69,74,74	1.21	7 (10%)	79,115,115	1.61	11 (13%)
12	LMT	BT	103	-	36,36,36	1.18	5 (13%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LMT	BG	101	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	2 (4%)
19	V7N	BD	103	-	44,44,44	1.65	6 (13%)	48,54,54	1.64	12 (25%)
19	V7N	BE	101	-	44,44,44	1.64	8 (18%)	48,54,54	1.76	12 (25%)
19	V7N	BR	103	-	44,44,44	1.64	6 (13%)	48,54,54	1.68	10 (20%)
19	V7N	Ba	101	-	44,44,44	1.65	7 (15%)	48,54,54	1.79	14 (29%)
19	V7N	Bd	102	-	44,44,44	1.64	6 (13%)	48,54,54	1.78	12 (25%)
10	BCL	BW	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.46	11 (13%)
10	BCL	Ba	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.58	10 (12%)
12	LMT	Bc	1204	-	36,36,36	1.18	6 (16%)	47,47,47	1.04	3 (6%)
12	LMT	Bp	1002	-	36,36,36	1.18	6 (16%)	47,47,47	0.99	2 (4%)
17	PEX	Ba	103	10	34,34,34	0.56	0	37,39,39	0.52	0
17	PEX	AO	102	-	34,34,34	0.56	0	37,39,39	0.53	0
19	V7N	Ag	102	-	44,44,44	1.71	7 (15%)	48,54,54	1.47	10 (20%)
10	BCL	Bh	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.33	8 (10%)
19	V7N	BX	102	-	44,44,44	1.67	5 (11%)	48,54,54	1.72	11 (22%)
15	CD4	Af	101	-	83,83,83	0.39	0	89,95,95	0.38	0
10	BCL	Bg	1203	-	69,74,74	1.15	6 (8%)	79,115,115	1.35	9 (11%)
12	LMT	BP	102	-	36,36,36	1.20	6 (16%)	47,47,47	0.98	2 (4%)
10	BCL	AT	101	-	69,74,74	1.13	5 (7%)	79,115,115	1.36	9 (11%)
12	LMT	BO	103	-	36,36,36	1.18	6 (16%)	47,47,47	1.00	2 (4%)
17	PEX	AT	103	-	34,34,34	0.55	0	37,39,39	0.74	2 (5%)
10	BCL	M	403	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	8 (10%)
10	BCL	Bn	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.48	11 (13%)
10	BCL	BQ	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
17	PEX	Be	102	10	34,34,34	0.55	0	37,39,39	0.57	0
12	LMT	BK	103	-	36,36,36	1.17	6 (16%)	47,47,47	0.89	0
12	LMT	BU	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.95	1 (2%)
12	LMT	AB	102	-	36,36,36	1.17	6 (16%)	47,47,47	1.10	4 (8%)
19	V7N	AI	101	-	44,44,44	1.66	8 (18%)	48,54,54	1.72	11 (22%)
10	BCL	Bc	1203	10	69,74,74	1.17	6 (8%)	79,115,115	1.37	12 (15%)
12	LMT	BX	101	-	36,36,36	1.14	4 (11%)	47,47,47	1.00	2 (4%)
12	LMT	L	304	-	36,36,36	1.11	5 (13%)	47,47,47	0.93	1 (2%)
10	BCL	BL	102	-	69,74,74	1.12	6 (8%)	79,115,115	1.40	10 (12%)
11	BPH	M	405	-	59,70,70	1.11	3 (5%)	59,101,101	1.90	10 (16%)
12	LMT	L	307	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HEC	C	1001	6	46,50,50	1.84	6 (13%)	58,82,82	1.92	4 (6%)
10	BCL	BJ	101	-	69,74,74	1.12	5 (7%)	79,115,115	1.36	11 (13%)
10	BCL	L	301	10	69,74,74	1.14	5 (7%)	79,115,115	1.36	9 (11%)
10	BCL	AH	101	-	69,74,74	1.15	7 (10%)	79,115,115	1.41	9 (11%)
10	BCL	Ah	101	-	69,74,74	1.21	7 (10%)	79,115,115	1.42	11 (13%)
17	PEX	Bm	103	-	34,34,34	0.56	0	37,39,39	0.47	0
12	LMT	Bg	1201	-	36,36,36	1.16	6 (16%)	47,47,47	1.08	3 (6%)
19	V7N	BK	104	-	44,44,44	1.66	8 (18%)	48,54,54	1.66	9 (18%)
17	PEX	Bf	104	-	34,34,34	0.54	0	37,39,39	0.67	0
10	BCL	Bl	101	-	69,74,74	1.32	9 (13%)	79,115,115	1.69	11 (13%)
10	BCL	Bj	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.71	17 (21%)
12	LMT	M	407	-	36,36,36	1.21	6 (16%)	47,47,47	1.02	3 (6%)
10	BCL	AU	102	-	69,74,74	1.11	6 (8%)	79,115,115	1.37	9 (11%)
19	V7N	AX	101	-	44,44,44	1.67	8 (18%)	48,54,54	1.64	9 (18%)
12	LMT	BF	101	-	36,36,36	1.16	6 (16%)	47,47,47	1.02	2 (4%)
12	LMT	BI	1101	-	36,36,36	1.16	4 (11%)	47,47,47	0.96	1 (2%)
19	V7N	Ad	102	-	44,44,44	1.66	6 (13%)	48,54,54	1.66	10 (20%)
10	BCL	AF	101	-	69,74,74	1.14	7 (10%)	79,115,115	1.35	9 (11%)
19	V7N	BF	103	-	44,44,44	1.63	6 (13%)	48,54,54	1.77	10 (20%)
18	HEC	C	1000	6	46,50,50	1.84	5 (10%)	58,82,82	1.91	5 (8%)
10	BCL	BA	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.37	11 (13%)
10	BCL	BP	104	-	69,74,74	1.17	7 (10%)	79,115,115	1.42	10 (12%)
10	BCL	BT	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.31	6 (7%)
12	LMT	Bk	1201	-	36,36,36	1.15	5 (13%)	47,47,47	1.18	3 (6%)
10	BCL	Al	101	-	69,74,74	1.20	6 (8%)	79,115,115	1.39	10 (12%)
12	LMT	BH	101	-	36,36,36	1.15	5 (13%)	47,47,47	1.05	2 (4%)
10	BCL	Bf	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.36	8 (10%)
10	BCL	Bo	1202	-	69,74,74	1.13	4 (5%)	79,115,115	1.30	9 (11%)
19	V7N	AI	103	-	44,44,44	1.66	5 (11%)	48,54,54	1.71	10 (20%)
18	HEC	C	1003	6	46,50,50	1.84	4 (8%)	58,82,82	1.90	4 (6%)
19	V7N	BP	103	-	44,44,44	1.65	6 (13%)	48,54,54	1.62	9 (18%)
12	LMT	L	308	-	36,36,36	1.14	5 (13%)	47,47,47	1.00	1 (2%)
12	LMT	L	309	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	3 (6%)
10	BCL	Bd	103	-	69,74,74	1.15	7 (10%)	79,115,115	1.31	9 (11%)
10	BCL	AD	101	10	69,74,74	1.16	5 (7%)	79,115,115	1.34	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MQ8	M	409	-	54,54,54	0.48	1 (1%)	67,69,69	0.56	2 (2%)
19	V7N	Bi	1202	-	44,44,44	1.66	8 (18%)	48,54,54	1.68	13 (27%)
19	V7N	BL	101	-	44,44,44	1.67	8 (18%)	48,54,54	1.65	11 (22%)
15	CD4	M	402	-	83,83,83	0.54	1 (1%)	89,95,95	0.40	0
12	LMT	BX	104	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
10	BCL	BI	1102	-	69,74,74	1.14	6 (8%)	79,115,115	1.50	10 (12%)
10	BCL	AQ	101	17	69,74,74	1.13	6 (8%)	79,115,115	1.47	12 (15%)
17	PEX	M	408	-	34,34,34	0.54	0	37,39,39	0.64	1 (2%)
19	V7N	Bl	102	-	44,44,44	1.67	7 (15%)	48,54,54	1.61	11 (22%)
12	LMT	BV	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.94	1 (2%)
10	BCL	AO	101	-	69,74,74	1.13	6 (8%)	79,115,115	1.45	12 (15%)
10	BCL	BR	101	-	69,74,74	1.13	6 (8%)	79,115,115	1.40	11 (13%)
17	PEX	Bk	1204	10	34,34,34	0.57	0	37,39,39	0.55	0
19	V7N	AH	102	-	44,44,44	1.66	6 (13%)	48,54,54	1.62	9 (18%)
19	V7N	AF	102	-	44,44,44	1.66	6 (13%)	48,54,54	1.60	9 (18%)
19	V7N	Bk	1202	-	44,44,44	1.67	7 (15%)	48,54,54	1.70	11 (22%)
12	LMT	Bi	1201	-	36,36,36	1.15	6 (16%)	47,47,47	1.13	2 (4%)
12	LMT	AK	102	-	36,36,36	1.18	6 (16%)	47,47,47	1.06	2 (4%)
10	BCL	AE	101	-	69,74,74	1.15	7 (10%)	79,115,115	1.42	11 (13%)
19	V7N	Bm	101	-	44,44,44	1.65	6 (13%)	48,54,54	1.71	11 (22%)
12	LMT	Ba	104	-	36,36,36	1.15	6 (16%)	47,47,47	1.05	2 (4%)
11	BPH	L	303	-	59,70,70	1.17	5 (8%)	59,101,101	1.88	10 (16%)
10	BCL	AB	101	17,12	69,74,74	1.16	7 (10%)	79,115,115	1.39	11 (13%)
10	BCL	AC	101	-	69,74,74	1.15	6 (8%)	79,115,115	1.48	11 (13%)
17	PEX	Bi	1204	-	34,34,34	0.55	0	37,39,39	0.58	0
19	V7N	BO	101	-	44,44,44	1.66	6 (13%)	48,54,54	1.70	11 (22%)
19	V7N	Bg	1202	-	44,44,44	1.65	6 (13%)	48,54,54	1.78	11 (22%)
12	LMT	BR	102	-	36,36,36	1.19	6 (16%)	47,47,47	0.99	2 (4%)
12	LMT	BI	1103	-	36,36,36	1.17	6 (16%)	47,47,47	0.99	1 (2%)
12	LMT	Bg	1205	-	36,36,36	1.17	6 (16%)	47,47,47	0.97	2 (4%)
19	V7N	BN	103	-	44,44,44	1.64	7 (15%)	48,54,54	1.61	9 (18%)
19	V7N	BB	102	-	44,44,44	1.64	6 (13%)	48,54,54	1.77	13 (27%)
10	BCL	AV	1001	-	69,74,74	1.14	6 (8%)	79,115,115	1.37	8 (10%)
10	BCL	Bi	1203	-	69,74,74	1.13	5 (7%)	79,115,115	1.32	7 (8%)
10	BCL	AK	101	-	69,74,74	1.15	6 (8%)	79,115,115	1.45	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	Ac	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.60	11 (13%)
12	LMT	BM	102	-	36,36,36	1.19	6 (16%)	47,47,47	1.04	3 (6%)
10	BCL	AL	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.32	8 (10%)
12	LMT	Bd	105	-	36,36,36	1.18	6 (16%)	47,47,47	1.03	2 (4%)
10	BCL	BX	103	-	69,74,74	1.11	4 (5%)	79,115,115	1.43	9 (11%)
17	PEX	Bl	104	-	34,34,34	0.55	0	37,39,39	0.49	0
12	LMT	BA	102	-	36,36,36	1.16	6 (16%)	47,47,47	0.98	1 (2%)
17	PEX	AG	1101	-	34,34,34	0.55	0	37,39,39	0.48	0
17	PEX	Bg	1204	-	34,34,34	0.53	0	37,39,39	0.55	0
10	BCL	AP	102	-	69,74,74	1.17	6 (8%)	79,115,115	1.46	12 (15%)
19	V7N	Bb	101	-	44,44,44	1.65	6 (13%)	48,54,54	1.70	10 (20%)
19	V7N	Bc	1202	-	44,44,44	1.65	6 (13%)	48,54,54	1.67	13 (27%)
16	CRT	M	406	-	43,43,43	0.41	0	48,54,54	0.76	2 (4%)
19	V7N	Bj	103	-	44,44,44	1.66	8 (18%)	48,54,54	1.73	15 (31%)
10	BCL	Bm	102	-	69,74,74	1.14	4 (5%)	79,115,115	1.30	7 (8%)
12	LMT	BK	101	-	36,36,36	1.16	6 (16%)	47,47,47	1.05	4 (8%)
10	BCL	Af	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.66	12 (15%)
10	BCL	BO	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.35	8 (10%)
10	BCL	Aj	101	-	69,74,74	1.17	7 (10%)	79,115,115	1.43	9 (11%)
19	V7N	AP	101	-	44,44,44	1.68	6 (13%)	48,54,54	1.79	12 (25%)
17	PEX	Bj	104	-	34,34,34	0.55	0	37,39,39	0.50	0
19	V7N	BV	101	-	44,44,44	1.65	8 (18%)	48,54,54	1.69	11 (22%)
10	BCL	M	404	10	69,74,74	1.15	6 (8%)	79,115,115	1.62	14 (17%)
19	V7N	BT	102	-	44,44,44	1.66	8 (18%)	48,54,54	1.57	8 (16%)
10	BCL	AQ	103	-	69,74,74	1.15	6 (8%)	79,115,115	1.46	11 (13%)
10	BCL	AN	101	-	69,74,74	1.14	7 (10%)	79,115,115	1.32	8 (10%)
12	LMT	Bo	1201	-	36,36,36	1.18	6 (16%)	47,47,47	1.03	3 (6%)
10	BCL	Am	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.44	12 (15%)

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
10	BCL	AW	101	-	-	7/41/137/137	-
10	BCL	Bd	101	10	-	5/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	V7N	Am	102	-	-	18/53/53/53	-
10	BCL	Ak	101	10	-	5/41/137/137	-
19	V7N	AL	102	-	-	8/53/53/53	-
10	BCL	AT	104	-	-	5/41/137/137	-
10	BCL	AU	101	-	-	7/41/137/137	-
10	BCL	BK	102	-	-	2/41/137/137	-
10	BCL	Ag	101	-	-	2/41/137/137	-
12	LMT	L	306	-	-	11/21/61/61	0/2/2/2
10	BCL	Aa	101	-	-	7/41/137/137	-
10	BCL	BG	102	-	-	2/41/137/137	-
12	LMT	BC	102	-	-	11/21/61/61	0/2/2/2
12	LMT	BN	102	-	-	11/21/61/61	0/2/2/2
12	LMT	BB	103	10	-	9/21/61/61	0/2/2/2
10	BCL	Bk	1203	-	-	5/41/137/137	-
12	LMT	BQ	102	-	-	9/21/61/61	0/2/2/2
12	LMT	Bl	105	-	-	13/21/61/61	0/2/2/2
18	HEC	C	1002	6	-	4/14/54/54	-
10	BCL	L	302	-	-	6/41/137/137	-
19	V7N	Bp	1003	-	-	10/53/53/53	-
10	BCL	AR	101	-	-	5/41/137/137	-
12	LMT	AQ	102	-	-	4/21/61/61	0/2/2/2
17	PEX	Bb	102	-	-	11/38/38/38	-
17	PEX	Bp	1005	-	-	18/38/38/38	-
10	BCL	BF	102	-	-	4/41/137/137	-
10	BCL	BC	101	-	-	2/41/137/137	-
10	BCL	BH	102	-	-	4/41/137/137	-
10	BCL	AX	102	-	-	4/41/137/137	-
13	MQ8	Ad	101	-	-	26/47/67/67	0/2/2/2
12	LMT	Bc	1201	-	-	7/21/61/61	0/2/2/2
10	BCL	AM	101	-	-	6/41/137/137	-
10	BCL	BV	102	-	-	7/41/137/137	-
10	BCL	Bp	1004	-	-	5/41/137/137	-
17	PEX	Bn	102	-	-	15/38/38/38	-
10	BCL	BP	101	-	-	3/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	Ao	101	-	-	4/41/137/137	-
10	BCL	Ae	101	-	-	3/41/137/137	-
12	LMT	Bj	102	-	-	5/21/61/61	0/2/2/2
10	BCL	An	101	-	-	9/41/137/137	-
19	V7N	BS	103	-	-	6/53/53/53	-
19	V7N	AT	102	-	-	6/53/53/53	-
17	PEX	Bd	104	-	-	15/38/38/38	-
10	BCL	Bp	1001	-	-	6/41/137/137	-
19	V7N	Bf	102	-	-	13/53/53/53	-
10	BCL	Ai	101	-	-	5/41/137/137	-
12	LMT	Bm	104	-	-	3/21/61/61	0/2/2/2
13	MQ8	L	310	-	-	25/47/67/67	0/2/2/2
19	V7N	BW	101	-	-	6/53/53/53	-
10	BCL	Bl	103	-	-	2/41/137/137	-
12	LMT	BD	102	-	-	9/21/61/61	0/2/2/2
10	BCL	BE	102	-	-	5/41/137/137	-
10	BCL	Bh	101	-	-	7/41/137/137	-
12	LMT	BS	102	-	-	7/21/61/61	0/2/2/2
10	BCL	AI	102	-	-	3/41/137/137	-
10	BCL	BN	101	-	-	3/41/137/137	-
10	BCL	Be	101	17	-	6/41/137/137	-
19	V7N	An	102	-	-	18/53/53/53	-
12	LMT	L	305	-	-	5/21/61/61	0/2/2/2
10	BCL	BM	101	-	-	3/41/137/137	-
12	LMT	BL	103	-	-	10/21/61/61	0/2/2/2
10	BCL	BB	101	-	-	4/41/137/137	-
12	LMT	BG	103	-	-	2/21/61/61	0/2/2/2
19	V7N	BC	103	-	-	4/53/53/53	-
10	BCL	BS	101	-	-	5/41/137/137	-
10	BCL	BD	101	-	-	1/41/137/137	-
10	BCL	Bf	101	-	-	4/41/137/137	-
12	LMT	BT	103	-	-	7/21/61/61	0/2/2/2
12	LMT	BG	101	-	-	6/21/61/61	0/2/2/2
19	V7N	BD	103	-	-	6/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	V7N	BE	101	-	-	10/53/53/53	-
19	V7N	BR	103	-	-	5/53/53/53	-
19	V7N	Ba	101	-	-	18/53/53/53	-
19	V7N	Bd	102	-	-	15/53/53/53	-
10	BCL	BW	102	-	-	4/41/137/137	-
10	BCL	Ba	102	-	-	8/41/137/137	-
12	LMT	Bc	1204	-	-	8/21/61/61	0/2/2/2
12	LMT	Bp	1002	-	-	9/21/61/61	0/2/2/2
17	PEX	Ba	103	10	-	16/38/38/38	-
17	PEX	AO	102	-	-	13/38/38/38	-
19	V7N	Ag	102	-	-	16/53/53/53	-
10	BCL	Bh	102	-	-	4/41/137/137	-
19	V7N	BX	102	-	-	14/53/53/53	-
15	CD4	Af	101	-	-	22/94/94/94	-
10	BCL	Bg	1203	-	-	13/41/137/137	-
12	LMT	BP	102	-	-	11/21/61/61	0/2/2/2
10	BCL	AT	101	-	-	5/41/137/137	-
12	LMT	BO	103	-	-	10/21/61/61	0/2/2/2
17	PEX	AT	103	-	-	19/38/38/38	-
10	BCL	M	403	-	-	6/41/137/137	-
10	BCL	Bn	101	-	-	10/41/137/137	-
10	BCL	BQ	101	-	-	2/41/137/137	-
17	PEX	Be	102	10	-	11/38/38/38	-
12	LMT	BK	103	-	-	9/21/61/61	0/2/2/2
12	LMT	BU	101	-	-	7/21/61/61	0/2/2/2
12	LMT	AB	102	-	-	8/21/61/61	0/2/2/2
19	V7N	AI	101	-	-	12/53/53/53	-
10	BCL	Bc	1203	10	-	10/41/137/137	-
12	LMT	BX	101	-	-	11/21/61/61	0/2/2/2
12	LMT	L	304	-	-	9/21/61/61	0/2/2/2
10	BCL	BL	102	-	-	7/41/137/137	-
11	BPH	M	405	-	-	5/37/105/105	0/5/6/6
12	LMT	L	307	-	-	9/21/61/61	0/2/2/2
18	HEC	C	1001	6	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	BJ	101	-	-	3/41/137/137	-
10	BCL	L	301	10	-	1/41/137/137	-
10	BCL	AH	101	-	-	5/41/137/137	-
10	BCL	Ah	101	-	-	6/41/137/137	-
17	PEX	Bm	103	-	-	15/38/38/38	-
12	LMT	Bg	1201	-	-	5/21/61/61	0/2/2/2
19	V7N	BK	104	-	-	10/53/53/53	-
17	PEX	Bf	104	-	-	21/38/38/38	-
10	BCL	Bl	101	-	-	10/41/137/137	-
10	BCL	Bj	101	-	-	6/41/137/137	-
12	LMT	M	407	-	-	10/21/61/61	0/2/2/2
10	BCL	AU	102	-	-	4/41/137/137	-
19	V7N	AX	101	-	-	13/53/53/53	-
12	LMT	BF	101	-	-	10/21/61/61	0/2/2/2
12	LMT	BI	1101	-	-	7/21/61/61	0/2/2/2
19	V7N	Ad	102	-	-	17/53/53/53	-
10	BCL	AF	101	-	-	8/41/137/137	-
19	V7N	BF	103	-	-	5/53/53/53	-
18	HEC	C	1000	6	-	6/14/54/54	-
10	BCL	BA	101	-	-	3/41/137/137	-
10	BCL	BP	104	-	-	7/41/137/137	-
10	BCL	BT	101	-	-	5/41/137/137	-
12	LMT	Bk	1201	-	-	5/21/61/61	0/2/2/2
10	BCL	Al	101	-	-	0/41/137/137	-
12	LMT	BH	101	-	-	6/21/61/61	0/2/2/2
10	BCL	Bf	103	-	-	9/41/137/137	-
10	BCL	Bo	1202	-	-	9/41/137/137	-
19	V7N	AI	103	-	-	12/53/53/53	-
18	HEC	C	1003	6	-	4/14/54/54	-
19	V7N	BP	103	-	-	6/53/53/53	-
12	LMT	L	308	-	-	9/21/61/61	0/2/2/2
12	LMT	L	309	-	-	8/21/61/61	0/2/2/2
10	BCL	Bd	103	-	-	5/41/137/137	-
10	BCL	AD	101	10	-	11/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQ8	M	409	-	-	25/47/67/67	0/2/2/2
19	V7N	Bi	1202	-	-	14/53/53/53	-
19	V7N	BL	101	-	-	12/53/53/53	-
15	CD4	M	402	-	-	18/94/94/94	-
12	LMT	BX	104	-	-	7/21/61/61	0/2/2/2
10	BCL	BI	1102	-	-	5/41/137/137	-
10	BCL	AQ	101	17	-	7/41/137/137	-
17	PEX	M	408	-	-	13/38/38/38	-
19	V7N	Bl	102	-	-	12/53/53/53	-
12	LMT	BV	103	-	-	9/21/61/61	0/2/2/2
10	BCL	AO	101	-	-	3/41/137/137	-
10	BCL	BR	101	-	-	4/41/137/137	-
17	PEX	Bk	1204	10	-	16/38/38/38	-
19	V7N	AH	102	-	-	7/53/53/53	-
19	V7N	AF	102	-	-	7/53/53/53	-
19	V7N	Bk	1202	-	-	10/53/53/53	-
12	LMT	Bi	1201	-	-	11/21/61/61	0/2/2/2
12	LMT	AK	102	-	-	8/21/61/61	0/2/2/2
10	BCL	AE	101	-	-	3/41/137/137	-
19	V7N	Bm	101	-	-	12/53/53/53	-
12	LMT	Ba	104	-	-	11/21/61/61	0/2/2/2
11	BPH	L	303	-	-	4/37/105/105	0/5/6/6
10	BCL	AB	101	17,12	-	10/41/137/137	-
10	BCL	AC	101	-	-	7/41/137/137	-
17	PEX	Bi	1204	-	-	11/38/38/38	-
19	V7N	BO	101	-	-	4/53/53/53	-
19	V7N	Bg	1202	-	-	14/53/53/53	-
12	LMT	BR	102	-	-	5/21/61/61	0/2/2/2
12	LMT	BI	1103	-	-	11/21/61/61	0/2/2/2
12	LMT	Bg	1205	-	-	2/21/61/61	0/2/2/2
19	V7N	BN	103	-	-	4/53/53/53	-
19	V7N	BB	102	-	-	5/53/53/53	-
10	BCL	AV	1001	-	-	0/41/137/137	-
10	BCL	Bi	1203	-	-	4/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	AK	101	-	-	4/41/137/137	-
10	BCL	Ac	101	-	-	5/41/137/137	-
12	LMT	BM	102	-	-	5/21/61/61	0/2/2/2
10	BCL	AL	101	-	-	5/41/137/137	-
12	LMT	Bd	105	-	-	3/21/61/61	0/2/2/2
10	BCL	BX	103	-	-	3/41/137/137	-
17	PEX	Bl	104	-	-	20/38/38/38	-
12	LMT	BA	102	-	-	8/21/61/61	0/2/2/2
17	PEX	AG	1101	-	-	22/38/38/38	-
17	PEX	Bg	1204	-	-	22/38/38/38	-
10	BCL	AP	102	-	-	3/41/137/137	-
19	V7N	Bb	101	-	-	11/53/53/53	-
19	V7N	Bc	1202	-	-	15/53/53/53	-
16	CRT	M	406	-	-	3/51/51/51	-
19	V7N	Bj	103	-	-	14/53/53/53	-
10	BCL	Bm	102	-	-	6/41/137/137	-
12	LMT	BK	101	-	-	6/21/61/61	0/2/2/2
10	BCL	Af	102	-	-	5/41/137/137	-
10	BCL	BO	102	-	-	5/41/137/137	-
10	BCL	Aj	101	-	-	6/41/137/137	-
19	V7N	AP	101	-	-	6/53/53/53	-
17	PEX	Bj	104	-	-	17/38/38/38	-
19	V7N	BV	101	-	-	9/53/53/53	-
10	BCL	M	404	10	-	0/41/137/137	-
19	V7N	BT	102	-	-	7/53/53/53	-
10	BCL	AQ	103	-	-	3/41/137/137	-
10	BCL	AN	101	-	-	9/41/137/137	-
12	LMT	Bo	1201	-	-	12/21/61/61	0/2/2/2
10	BCL	Am	101	-	-	5/41/137/137	-

All (1057) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Ag	102	V7N	C28-C27	6.95	1.52	1.34
19	Bi	1202	V7N	C28-C27	6.81	1.52	1.34
19	Am	102	V7N	C28-C27	6.77	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Ad	102	V7N	C28-C27	6.76	1.52	1.34
19	BO	101	V7N	C28-C27	6.75	1.52	1.34
19	BL	101	V7N	C28-C27	6.75	1.52	1.34
19	An	102	V7N	C28-C27	6.74	1.52	1.34
19	Bf	102	V7N	C28-C27	6.74	1.52	1.34
19	Bg	1202	V7N	C28-C27	6.74	1.52	1.34
19	Bk	1202	V7N	C28-C27	6.73	1.52	1.34
19	Bm	101	V7N	C28-C27	6.73	1.52	1.34
19	BK	104	V7N	C28-C27	6.73	1.52	1.34
19	BV	101	V7N	C28-C27	6.73	1.52	1.34
19	AX	101	V7N	C28-C27	6.72	1.52	1.34
19	Bl	102	V7N	C28-C27	6.72	1.52	1.34
19	BD	103	V7N	C28-C27	6.72	1.52	1.34
19	BX	102	V7N	C28-C27	6.71	1.52	1.34
19	Ba	101	V7N	C28-C27	6.71	1.52	1.34
19	Bp	1003	V7N	C28-C27	6.71	1.52	1.34
19	AF	102	V7N	C28-C27	6.70	1.52	1.34
19	Bj	103	V7N	C28-C27	6.69	1.52	1.34
19	AI	101	V7N	C28-C27	6.68	1.52	1.34
19	BS	103	V7N	C28-C27	6.68	1.52	1.34
19	AP	101	V7N	C28-C27	6.67	1.52	1.34
19	Bb	101	V7N	C28-C27	6.67	1.52	1.34
19	BP	103	V7N	C28-C27	6.67	1.52	1.34
19	BT	102	V7N	C28-C27	6.65	1.52	1.34
19	Bc	1202	V7N	C28-C27	6.65	1.52	1.34
19	AH	102	V7N	C28-C27	6.65	1.52	1.34
19	AI	103	V7N	C28-C27	6.63	1.52	1.34
19	BR	103	V7N	C28-C27	6.62	1.52	1.34
19	Bd	102	V7N	C28-C27	6.62	1.52	1.34
19	AL	102	V7N	C28-C27	6.62	1.51	1.34
19	AT	102	V7N	C28-C27	6.61	1.51	1.34
19	BB	102	V7N	C28-C27	6.61	1.51	1.34
19	BW	101	V7N	C28-C27	6.60	1.51	1.34
19	BN	103	V7N	C28-C27	6.59	1.51	1.34
19	BE	101	V7N	C28-C27	6.55	1.51	1.34
19	BC	103	V7N	C28-C27	6.55	1.51	1.34
19	BF	103	V7N	C28-C27	6.54	1.51	1.34
18	C	1002	HEC	CAC-C3C	6.40	1.55	1.35
18	C	1001	HEC	CAC-C3C	6.31	1.55	1.35
18	C	1003	HEC	CAC-C3C	6.30	1.55	1.35
18	C	1001	HEC	CAB-C3B	6.25	1.55	1.35
18	C	1002	HEC	CAB-C3B	6.23	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	1003	HEC	CAB-C3B	6.20	1.55	1.35
18	C	1000	HEC	CAC-C3C	6.18	1.55	1.35
18	C	1000	HEC	CAB-C3B	6.13	1.54	1.35
10	Bp	1001	BCL	C16-C15	5.88	1.76	1.52
18	C	1001	HEC	C3D-C2D	5.68	1.53	1.38
18	C	1003	HEC	C3D-C2D	5.62	1.53	1.38
18	C	1000	HEC	C3D-C2D	5.60	1.53	1.38
18	C	1002	HEC	C3D-C2D	5.48	1.53	1.38
10	L	302	BCL	MG-NA	5.19	2.18	2.06
10	Ag	101	BCL	MG-NA	5.17	2.18	2.06
10	Ac	101	BCL	MG-NA	5.16	2.18	2.06
10	BI	1102	BCL	MG-NA	5.15	2.18	2.06
10	Ao	101	BCL	MG-NA	5.11	2.18	2.06
10	AT	104	BCL	MG-NA	5.10	2.18	2.06
10	Am	101	BCL	MG-NA	5.07	2.18	2.06
10	AX	102	BCL	MG-NA	5.07	2.18	2.06
10	Al	101	BCL	MG-NA	5.07	2.18	2.06
10	Ah	101	BCL	MG-NA	5.05	2.18	2.06
10	Af	102	BCL	MG-NA	5.02	2.18	2.06
10	Ai	101	BCL	MG-NA	5.01	2.18	2.06
10	Ae	101	BCL	MG-NA	5.00	2.18	2.06
10	Aj	101	BCL	MG-NA	5.00	2.18	2.06
10	AI	102	BCL	MG-NA	4.98	2.18	2.06
10	AC	101	BCL	MG-NA	4.96	2.18	2.06
10	BB	101	BCL	MG-NA	4.96	2.18	2.06
10	AQ	101	BCL	MG-NA	4.96	2.18	2.06
10	BW	102	BCL	MG-NA	4.95	2.18	2.06
10	AV	1001	BCL	MG-NA	4.95	2.18	2.06
10	BL	102	BCL	MG-NA	4.95	2.18	2.06
10	M	403	BCL	MG-NA	4.95	2.18	2.06
10	Ak	101	BCL	MG-NA	4.94	2.18	2.06
10	Bd	101	BCL	MG-NA	4.93	2.18	2.06
10	AE	101	BCL	MG-NA	4.93	2.18	2.06
10	AM	101	BCL	MG-NA	4.92	2.18	2.06
10	AK	101	BCL	MG-NA	4.92	2.18	2.06
10	Aa	101	BCL	MG-NA	4.91	2.17	2.06
10	AT	101	BCL	MG-NA	4.90	2.17	2.06
10	Bl	101	BCL	MG-NA	4.90	2.17	2.06
10	AN	101	BCL	MG-NA	4.89	2.17	2.06
10	Bc	1203	BCL	MG-NA	4.89	2.17	2.06
10	Bd	103	BCL	MG-NA	4.89	2.17	2.06
10	BP	104	BCL	MG-NA	4.88	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AL	101	BCL	MG-NA	4.88	2.17	2.06
10	AQ	103	BCL	MG-NA	4.88	2.17	2.06
10	Bh	101	BCL	MG-NA	4.88	2.17	2.06
10	BO	102	BCL	MG-NA	4.87	2.17	2.06
10	AB	101	BCL	MG-NA	4.87	2.17	2.06
10	BM	101	BCL	MG-NA	4.87	2.17	2.06
10	AH	101	BCL	MG-NA	4.86	2.17	2.06
10	Bm	102	BCL	MG-NA	4.85	2.17	2.06
10	AO	101	BCL	MG-NA	4.85	2.17	2.06
10	Bp	1001	BCL	MG-NA	4.84	2.17	2.06
10	AF	101	BCL	MG-NA	4.83	2.17	2.06
10	Bp	1004	BCL	MG-NA	4.83	2.17	2.06
10	AD	101	BCL	MG-NA	4.83	2.17	2.06
10	Bi	1203	BCL	MG-NA	4.82	2.17	2.06
10	Bl	103	BCL	MG-NA	4.82	2.17	2.06
10	An	101	BCL	MG-NA	4.82	2.17	2.06
10	Bf	101	BCL	MG-NA	4.82	2.17	2.06
10	BR	101	BCL	MG-NA	4.81	2.17	2.06
10	AW	101	BCL	MG-NA	4.81	2.17	2.06
10	Bk	1203	BCL	MG-NA	4.80	2.17	2.06
10	BP	101	BCL	MG-NA	4.79	2.17	2.06
10	BD	101	BCL	MG-NA	4.79	2.17	2.06
10	AP	102	BCL	MG-NA	4.79	2.17	2.06
10	Bg	1203	BCL	MG-NA	4.78	2.17	2.06
10	Ba	102	BCL	MG-NA	4.77	2.17	2.06
10	Bj	101	BCL	MG-NA	4.77	2.17	2.06
10	Bn	101	BCL	MG-NA	4.77	2.17	2.06
10	M	404	BCL	MG-NA	4.76	2.17	2.06
10	Bf	103	BCL	MG-NA	4.75	2.17	2.06
10	BQ	101	BCL	MG-NA	4.74	2.17	2.06
10	BC	101	BCL	MG-NA	4.74	2.17	2.06
10	BX	103	BCL	MG-NA	4.74	2.17	2.06
10	BE	102	BCL	MG-NA	4.72	2.17	2.06
10	Bh	102	BCL	MG-NA	4.71	2.17	2.06
10	BV	102	BCL	MG-NA	4.71	2.17	2.06
10	Be	101	BCL	MG-NA	4.70	2.17	2.06
10	BF	102	BCL	MG-NA	4.70	2.17	2.06
10	BA	101	BCL	MG-NA	4.70	2.17	2.06
10	Bo	1202	BCL	MG-NA	4.69	2.17	2.06
10	BT	101	BCL	MG-NA	4.69	2.17	2.06
10	BN	101	BCL	MG-NA	4.69	2.17	2.06
10	BS	101	BCL	MG-NA	4.69	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AU	101	BCL	MG-NA	4.68	2.17	2.06
10	BJ	101	BCL	MG-NA	4.67	2.17	2.06
10	BG	102	BCL	MG-NA	4.66	2.17	2.06
10	L	301	BCL	MG-NA	4.65	2.17	2.06
10	BK	102	BCL	MG-NA	4.65	2.17	2.06
10	BH	102	BCL	MG-NA	4.64	2.17	2.06
11	M	405	BPH	CBD-CGD	-4.44	1.46	1.52
11	L	303	BPH	CBD-CGD	-4.30	1.47	1.52
10	AU	102	BCL	MG-NA	4.23	2.16	2.06
10	AR	101	BCL	MG-NA	4.20	2.16	2.06
10	Bl	101	BCL	C16-C17	4.01	1.68	1.52
10	Bp	1004	BCL	MG-NC	3.62	2.14	2.06
10	Bn	101	BCL	MG-NC	3.59	2.14	2.06
10	Bl	103	BCL	MG-NC	3.58	2.14	2.06
10	Bd	103	BCL	MG-NC	3.56	2.14	2.06
11	L	303	BPH	C3B-C4B	3.55	1.47	1.41
10	BQ	101	BCL	MG-NC	3.54	2.14	2.06
10	Bi	1203	BCL	MG-NC	3.54	2.14	2.06
10	AT	104	BCL	MG-NC	3.54	2.14	2.06
10	BM	101	BCL	MG-NC	3.52	2.14	2.06
10	Bo	1202	BCL	MG-NC	3.52	2.14	2.06
10	AD	101	BCL	MG-NC	3.52	2.14	2.06
10	Bh	102	BCL	MG-NC	3.52	2.14	2.06
10	Be	101	BCL	MG-NC	3.51	2.14	2.06
10	Ae	101	BCL	MG-NC	3.51	2.14	2.06
10	Bk	1203	BCL	MG-NC	3.51	2.14	2.06
10	L	302	BCL	MG-NC	3.50	2.14	2.06
10	Am	101	BCL	MG-NC	3.50	2.14	2.06
10	AU	101	BCL	MG-NC	3.50	2.14	2.06
10	L	301	BCL	MG-NC	3.49	2.14	2.06
10	Ao	101	BCL	MG-NC	3.49	2.14	2.06
10	BT	101	BCL	MG-NC	3.49	2.14	2.06
10	BS	101	BCL	MG-NC	3.49	2.14	2.06
10	Ac	101	BCL	MG-NC	3.48	2.14	2.06
10	Ak	101	BCL	MG-NC	3.48	2.14	2.06
10	BC	101	BCL	MG-NC	3.48	2.14	2.06
10	BB	101	BCL	MG-NC	3.47	2.14	2.06
10	Al	101	BCL	MG-NC	3.47	2.14	2.06
10	Bm	102	BCL	MG-NC	3.46	2.14	2.06
10	Ba	102	BCL	MG-NC	3.46	2.14	2.06
10	Bg	1203	BCL	MG-NC	3.46	2.14	2.06
10	BG	102	BCL	MG-NC	3.46	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Aj	101	BCL	MG-NC	3.46	2.14	2.06
10	Bc	1203	BCL	MG-NC	3.46	2.14	2.06
10	Ag	101	BCL	MG-NC	3.46	2.14	2.06
10	BX	103	BCL	MG-NC	3.45	2.14	2.06
10	Bd	101	BCL	MG-NC	3.45	2.14	2.06
10	BA	101	BCL	MG-NC	3.44	2.14	2.06
10	BV	102	BCL	MG-NC	3.44	2.14	2.06
10	BJ	101	BCL	MG-NC	3.43	2.14	2.06
10	AP	102	BCL	MG-NC	3.43	2.14	2.06
10	BD	101	BCL	MG-NC	3.42	2.14	2.06
10	Ai	101	BCL	MG-NC	3.41	2.14	2.06
10	BF	102	BCL	MG-NC	3.41	2.14	2.06
10	BN	101	BCL	MG-NC	3.40	2.14	2.06
10	Af	102	BCL	MG-NC	3.38	2.14	2.06
10	BL	102	BCL	MG-NC	3.37	2.14	2.06
10	Bf	103	BCL	MG-NC	3.37	2.14	2.06
10	M	403	BCL	MG-NC	3.36	2.14	2.06
10	An	101	BCL	MG-NC	3.36	2.14	2.06
10	BP	101	BCL	MG-NC	3.36	2.14	2.06
10	BK	102	BCL	MG-NC	3.36	2.14	2.06
10	BH	102	BCL	MG-NC	3.36	2.14	2.06
10	Ah	101	BCL	MG-NC	3.35	2.14	2.06
10	AV	1001	BCL	MG-NC	3.35	2.14	2.06
10	Bl	101	BCL	MG-NC	3.31	2.14	2.06
10	BR	101	BCL	MG-NC	3.30	2.14	2.06
10	Bp	1001	BCL	MG-NC	3.30	2.14	2.06
10	BP	104	BCL	MG-NC	3.30	2.14	2.06
10	Bh	101	BCL	MG-NC	3.30	2.14	2.06
10	AI	102	BCL	MG-NC	3.29	2.14	2.06
10	BI	1102	BCL	MG-NC	3.28	2.14	2.06
10	BE	102	BCL	MG-NC	3.28	2.14	2.06
10	AQ	103	BCL	MG-NC	3.28	2.14	2.06
10	Aa	101	BCL	MG-NC	3.28	2.14	2.06
11	M	405	BPH	C3D-CAD	-3.26	1.41	1.47
10	AT	101	BCL	MG-NC	3.25	2.14	2.06
10	AX	102	BCL	MG-NC	3.24	2.14	2.06
11	L	303	BPH	C3D-CAD	-3.24	1.41	1.47
10	Bf	101	BCL	MG-NC	3.24	2.14	2.06
10	AE	101	BCL	MG-NC	3.23	2.14	2.06
10	AK	101	BCL	MG-NC	3.23	2.13	2.06
10	AL	101	BCL	MG-NC	3.23	2.13	2.06
10	AQ	101	BCL	MG-NC	3.23	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BO	102	BCL	MG-NC	3.22	2.13	2.06
10	AM	101	BCL	MG-NC	3.21	2.13	2.06
10	AN	101	BCL	MG-NC	3.19	2.13	2.06
10	AO	101	BCL	MG-NC	3.19	2.13	2.06
10	AC	101	BCL	MG-NC	3.18	2.13	2.06
10	Bj	101	BCL	MG-NC	3.18	2.13	2.06
10	AB	101	BCL	MG-NC	3.18	2.13	2.06
10	AF	101	BCL	MG-NC	3.15	2.13	2.06
10	AH	101	BCL	MG-NC	3.15	2.13	2.06
10	AW	101	BCL	MG-NC	3.15	2.13	2.06
10	BW	102	BCL	MG-NC	3.14	2.13	2.06
12	BD	102	LMT	O2'-C2'	-3.03	1.35	1.43
10	L	301	BCL	C3B-C4B	3.03	1.47	1.41
12	BC	102	LMT	O2'-C2'	-2.95	1.35	1.43
10	M	404	BCL	MG-NC	2.95	2.13	2.06
10	AX	102	BCL	O1A-CGA	-2.86	1.14	1.22
12	M	407	LMT	O2'-C2'	-2.82	1.36	1.43
10	Al	101	BCL	O1A-CGA	-2.81	1.14	1.22
10	AR	101	BCL	MG-NC	2.78	2.12	2.06
10	Bh	101	BCL	C16-C15	2.77	1.63	1.52
10	An	101	BCL	C3B-C4B	2.77	1.46	1.41
19	Ag	102	V7N	C14-C13	2.76	1.42	1.35
10	Ag	101	BCL	C3B-C4B	2.76	1.46	1.41
12	BT	103	LMT	O2'-C2'	-2.76	1.36	1.43
15	M	402	CD4	O13-C32	-2.76	1.34	1.44
10	Ah	101	BCL	O1A-CGA	-2.73	1.14	1.22
12	Bk	1201	LMT	O2'-C2'	-2.73	1.36	1.43
19	AL	102	V7N	C14-C13	2.71	1.42	1.35
19	Bf	102	V7N	C14-C13	2.70	1.42	1.35
12	BK	103	LMT	O3'-C3'	-2.70	1.36	1.43
12	BV	103	LMT	O3'-C3'	-2.69	1.36	1.43
19	Bp	1003	V7N	C14-C13	2.68	1.42	1.35
12	BL	103	LMT	O3'-C3'	-2.68	1.36	1.43
10	AU	102	BCL	MG-NC	2.68	2.12	2.06
12	BP	102	LMT	O3'-C3'	-2.68	1.36	1.43
12	BC	102	LMT	O3'-C3'	-2.67	1.36	1.43
12	BG	101	LMT	O3'-C3'	-2.67	1.36	1.43
12	BN	102	LMT	O3'-C3'	-2.67	1.36	1.43
12	BX	101	LMT	O3'-C3'	-2.67	1.36	1.43
10	AU	102	BCL	C3B-C4B	2.67	1.46	1.41
12	Bo	1201	LMT	O2'-C2'	-2.67	1.36	1.43
10	Bj	101	BCL	C3B-C4B	2.67	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AX	101	V7N	C14-C13	2.66	1.41	1.35
12	BL	103	LMT	O2'-C2'	-2.65	1.36	1.43
10	M	403	BCL	C3B-C4B	2.65	1.46	1.41
12	BI	1101	LMT	O3'-C3'	-2.65	1.36	1.43
19	Ag	102	V7N	C17-C18	2.65	1.41	1.35
12	Bp	1002	LMT	O3'-C3'	-2.64	1.36	1.43
12	BT	103	LMT	O3'-C3'	-2.63	1.36	1.43
12	Bk	1201	LMT	O3'-C3'	-2.63	1.36	1.43
12	BF	101	LMT	O3'-C3'	-2.63	1.36	1.43
10	Aj	101	BCL	C3B-C4B	2.63	1.46	1.41
12	BH	101	LMT	O3'-C3'	-2.62	1.36	1.43
12	Bm	104	LMT	O3'-C3'	-2.62	1.36	1.43
12	BK	103	LMT	O2'-C2'	-2.62	1.36	1.43
12	BR	102	LMT	O3'-C3'	-2.62	1.36	1.43
10	Af	102	BCL	C3B-C4B	2.62	1.46	1.41
19	AX	101	V7N	C17-C18	2.62	1.41	1.35
19	BE	101	V7N	C14-C13	2.61	1.41	1.35
12	Bg	1201	LMT	O3'-C3'	-2.60	1.36	1.43
12	AB	102	LMT	O3'-C3'	-2.60	1.36	1.43
19	Bf	102	V7N	C17-C18	2.60	1.41	1.35
10	M	404	BCL	C3B-C4B	2.60	1.46	1.41
19	BP	103	V7N	C14-C13	2.60	1.41	1.35
19	BL	101	V7N	C14-C13	2.60	1.41	1.35
10	Al	101	BCL	C3B-C4B	2.60	1.46	1.41
12	L	309	LMT	O3'-C3'	-2.59	1.36	1.43
12	BG	103	LMT	O3'-C3'	-2.59	1.36	1.43
19	BT	102	V7N	C14-C13	2.59	1.41	1.35
19	BW	101	V7N	C14-C13	2.59	1.41	1.35
19	BN	103	V7N	C14-C13	2.59	1.41	1.35
10	Bd	101	BCL	C17-C18	2.59	1.68	1.51
12	Bj	102	LMT	O3'-C3'	-2.59	1.36	1.43
19	Bj	103	V7N	C14-C13	2.59	1.41	1.35
19	BX	102	V7N	C12-C13	-2.59	1.40	1.46
12	AK	102	LMT	O3'-C3'	-2.59	1.36	1.43
12	Bo	1201	LMT	O3'-C3'	-2.59	1.36	1.43
19	AH	102	V7N	C14-C13	2.58	1.41	1.35
12	BP	102	LMT	O2'-C2'	-2.58	1.36	1.43
19	Bp	1003	V7N	C17-C18	2.57	1.41	1.35
12	BO	103	LMT	O3'-C3'	-2.57	1.36	1.43
10	Ak	101	BCL	C3B-C4B	2.57	1.46	1.41
10	AN	101	BCL	C3B-C4B	2.57	1.46	1.41
10	AC	101	BCL	C3B-C4B	2.57	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BK	104	V7N	C14-C13	2.57	1.41	1.35
12	BA	102	LMT	O3'-C3'	-2.56	1.36	1.43
19	AF	102	V7N	C14-C13	2.56	1.41	1.35
12	Bp	1002	LMT	O2'-C2'	-2.56	1.36	1.43
12	M	407	LMT	O3'-C3'	-2.56	1.36	1.43
12	AQ	102	LMT	O3'-C3'	-2.56	1.36	1.43
12	BB	103	LMT	O3'-C3'	-2.56	1.36	1.43
19	BS	103	V7N	C14-C13	2.55	1.41	1.35
10	AR	101	BCL	C3B-C4B	2.55	1.46	1.41
10	AW	101	BCL	C3B-C4B	2.55	1.46	1.41
12	BX	104	LMT	O3'-C3'	-2.55	1.36	1.43
10	BP	104	BCL	C3B-C4B	2.55	1.46	1.41
19	An	102	V7N	C14-C13	2.55	1.41	1.35
10	AO	101	BCL	C3B-C4B	2.55	1.46	1.41
10	Bh	101	BCL	C3B-C4B	2.54	1.46	1.41
10	BJ	101	BCL	C3B-C4B	2.54	1.46	1.41
10	BR	101	BCL	C1D-C2D	-2.54	1.40	1.45
12	Ba	104	LMT	O3'-C3'	-2.54	1.36	1.43
10	AK	101	BCL	O1A-CGA	-2.54	1.14	1.22
19	Bb	101	V7N	C14-C13	2.54	1.41	1.35
19	Bi	1202	V7N	C14-C13	2.53	1.41	1.35
19	BC	103	V7N	C12-C13	-2.53	1.40	1.46
12	BN	102	LMT	O2'-C2'	-2.53	1.36	1.43
19	Bk	1202	V7N	C12-C13	-2.53	1.40	1.46
12	Bc	1204	LMT	O3'-C3'	-2.53	1.36	1.43
19	Bg	1202	V7N	C14-C13	2.53	1.41	1.35
10	Aa	101	BCL	C3B-C4B	2.53	1.46	1.41
12	BG	101	LMT	O1'-C1'	-2.52	1.36	1.40
19	BD	103	V7N	C14-C13	2.52	1.41	1.35
12	Bl	105	LMT	O3'-C3'	-2.52	1.36	1.43
12	Bg	1205	LMT	O3'-C3'	-2.52	1.36	1.43
19	BS	103	V7N	C17-C18	2.51	1.41	1.35
19	Bl	102	V7N	C14-C13	2.51	1.41	1.35
12	BD	102	LMT	O3'-C3'	-2.51	1.36	1.43
12	BQ	102	LMT	O3'-C3'	-2.51	1.36	1.43
19	AL	102	V7N	C17-C18	2.51	1.41	1.35
12	BU	101	LMT	O3'-C3'	-2.51	1.36	1.43
19	AH	102	V7N	C17-C18	2.50	1.41	1.35
10	AT	104	BCL	C3B-C4B	2.50	1.46	1.41
12	L	306	LMT	O3'-C3'	-2.50	1.36	1.43
10	Ao	101	BCL	C3B-C4B	2.50	1.46	1.41
19	BE	101	V7N	C17-C18	2.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Bm	101	V7N	C14-C13	2.49	1.41	1.35
19	Ad	102	V7N	C14-C13	2.49	1.41	1.35
12	Ba	104	LMT	O2'-C2'	-2.49	1.36	1.43
12	Bg	1201	LMT	O2'-C2'	-2.49	1.36	1.43
19	Ba	101	V7N	C14-C13	2.48	1.41	1.35
10	Bd	101	BCL	O1A-CGA	-2.48	1.15	1.22
19	Bj	103	V7N	C17-C18	2.48	1.41	1.35
12	L	307	LMT	O3'-C3'	-2.48	1.36	1.43
19	AI	101	V7N	C14-C13	2.48	1.41	1.35
12	Bc	1201	LMT	O3'-C3'	-2.48	1.36	1.43
19	Bc	1202	V7N	C14-C13	2.48	1.41	1.35
12	BF	101	LMT	O2'-C2'	-2.48	1.36	1.43
12	BI	1103	LMT	O3'-C3'	-2.47	1.36	1.43
10	Bc	1203	BCL	C3B-C4B	2.47	1.46	1.41
19	Am	102	V7N	C12-C13	-2.47	1.40	1.46
10	Bd	101	BCL	C3B-C4B	2.47	1.46	1.41
19	AT	102	V7N	C12-C13	-2.47	1.40	1.46
10	BL	102	BCL	C3B-C4B	2.47	1.46	1.41
13	M	409	MQ8	C11-C12	-2.47	1.46	1.50
10	Bf	101	BCL	C3B-C4B	2.46	1.46	1.41
19	AP	101	V7N	C14-C13	2.46	1.41	1.35
19	Bi	1202	V7N	C17-C18	2.46	1.41	1.35
10	BI	1102	BCL	C1D-C2D	-2.46	1.40	1.45
12	BM	102	LMT	O3'-C3'	-2.46	1.36	1.43
12	Bl	105	LMT	O2'-C2'	-2.46	1.36	1.43
19	BL	101	V7N	C17-C18	2.46	1.41	1.35
12	L	305	LMT	O3'-C3'	-2.46	1.36	1.43
10	AQ	101	BCL	C3B-C4B	2.45	1.46	1.41
12	BG	101	LMT	O2'-C2'	-2.45	1.36	1.43
10	Bf	101	BCL	C16-C15	2.45	1.62	1.52
12	Bi	1201	LMT	O3'-C3'	-2.45	1.36	1.43
10	AE	101	BCL	C3B-C4B	2.45	1.46	1.41
19	BO	101	V7N	C12-C13	-2.45	1.40	1.46
19	BR	103	V7N	C12-C13	-2.45	1.40	1.46
12	Bj	102	LMT	O2'-C2'	-2.45	1.36	1.43
19	An	102	V7N	C17-C18	2.45	1.41	1.35
10	AB	101	BCL	C3B-C4B	2.45	1.45	1.41
10	AI	102	BCL	C3B-C4B	2.44	1.45	1.41
10	BP	104	BCL	O1A-CGA	-2.44	1.15	1.22
12	BI	1103	LMT	O2'-C2'	-2.44	1.36	1.43
10	AX	102	BCL	C3B-C4B	2.44	1.45	1.41
12	Bd	105	LMT	O3'-C3'	-2.44	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BV	101	V7N	C14-C13	2.44	1.41	1.35
19	Bd	102	V7N	C17-C18	2.44	1.41	1.35
12	Bc	1204	LMT	O2'-C2'	-2.44	1.36	1.43
19	BB	102	V7N	C14-C13	2.44	1.41	1.35
10	Ac	101	BCL	C3B-C4B	2.44	1.45	1.41
12	AQ	102	LMT	O2'-C2'	-2.44	1.36	1.43
12	AK	102	LMT	O2'-C2'	-2.43	1.36	1.43
19	AT	102	V7N	C19-C18	-2.43	1.40	1.46
12	AB	102	LMT	O2'-C2'	-2.43	1.36	1.43
12	Bd	105	LMT	O2'-C2'	-2.43	1.36	1.43
10	Ae	101	BCL	C3B-C4B	2.43	1.45	1.41
10	Bl	101	BCL	C16-C15	2.43	1.62	1.52
19	Bg	1202	V7N	C17-C18	2.43	1.41	1.35
12	BV	103	LMT	O2'-C2'	-2.42	1.37	1.43
10	Ah	101	BCL	CBD-CGD	-2.42	1.45	1.52
12	BK	101	LMT	O3'-C3'	-2.42	1.37	1.43
19	Bc	1202	V7N	C12-C13	-2.42	1.40	1.46
10	M	404	BCL	CHD-C1D	2.42	1.43	1.38
12	BI	1101	LMT	O2'-C2'	-2.42	1.37	1.43
10	Ah	101	BCL	C3B-C4B	2.42	1.45	1.41
19	BT	102	V7N	C17-C18	2.42	1.41	1.35
19	Bd	102	V7N	C14-C13	2.42	1.41	1.35
12	BR	102	LMT	O2'-C2'	-2.42	1.37	1.43
12	L	308	LMT	O3'-C3'	-2.42	1.37	1.43
19	Bc	1202	V7N	C17-C18	2.41	1.41	1.35
19	Ad	102	V7N	C12-C13	-2.41	1.40	1.46
19	BF	103	V7N	C12-C13	-2.41	1.40	1.46
19	Ba	101	V7N	C17-C18	2.41	1.41	1.35
10	Bp	1001	BCL	C3B-C4B	2.41	1.45	1.41
10	AU	101	BCL	CBD-CGD	-2.41	1.45	1.52
11	M	405	BPH	C3B-C4B	2.41	1.45	1.41
10	AT	101	BCL	C3B-C4B	2.41	1.45	1.41
10	Bp	1001	BCL	C16-C17	2.41	1.62	1.52
12	Bl	105	LMT	O2B-C2B	-2.40	1.37	1.43
19	AP	101	V7N	C17-C18	2.40	1.41	1.35
10	AQ	103	BCL	C3B-C4B	2.40	1.45	1.41
12	Bm	104	LMT	O2'-C2'	-2.40	1.37	1.43
19	AF	102	V7N	C17-C18	2.40	1.41	1.35
19	BR	103	V7N	C14-C13	2.40	1.41	1.35
12	L	309	LMT	O2'-C2'	-2.40	1.37	1.43
12	BA	102	LMT	O2'-C2'	-2.40	1.37	1.43
12	BG	101	LMT	O2B-C2B	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AF	101	BCL	C3B-C4B	2.40	1.45	1.41
19	Bb	101	V7N	C17-C18	2.40	1.41	1.35
10	Ai	101	BCL	C3B-C4B	2.39	1.45	1.41
19	Bl	102	V7N	C17-C18	2.39	1.41	1.35
12	Bc	1201	LMT	O2'-C2'	-2.39	1.37	1.43
10	M	403	BCL	CHD-C1D	2.39	1.43	1.38
19	BB	102	V7N	C12-C13	-2.39	1.40	1.46
19	BP	103	V7N	C12-C13	-2.39	1.40	1.46
10	Bf	103	BCL	C3B-C4B	2.39	1.45	1.41
10	Bl	101	BCL	C3B-C4B	2.38	1.45	1.41
10	Bk	1203	BCL	O1A-CGA	-2.38	1.15	1.22
10	BR	101	BCL	C3B-C4B	2.38	1.45	1.41
19	BV	101	V7N	C17-C18	2.38	1.41	1.35
19	AT	102	V7N	C14-C13	2.38	1.41	1.35
10	L	302	BCL	C3B-C4B	2.38	1.45	1.41
12	M	407	LMT	O2B-C2B	-2.38	1.37	1.43
10	Bd	103	BCL	C3B-C4B	2.38	1.45	1.41
10	BD	101	BCL	C3B-C4B	2.37	1.45	1.41
19	Am	102	V7N	C14-C13	2.37	1.41	1.35
19	BW	101	V7N	C12-C13	-2.37	1.40	1.46
12	BA	102	LMT	O2B-C2B	-2.37	1.37	1.43
19	AI	101	V7N	C17-C18	2.36	1.41	1.35
12	BF	101	LMT	O2B-C2B	-2.36	1.37	1.43
12	BU	101	LMT	O2'-C2'	-2.36	1.37	1.43
12	BS	102	LMT	O3'-C3'	-2.36	1.37	1.43
10	BN	101	BCL	C3B-C4B	2.36	1.45	1.41
12	Bm	104	LMT	O3B-C3B	-2.36	1.37	1.43
19	AI	103	V7N	C12-C13	-2.36	1.40	1.46
19	BX	102	V7N	C14-C13	2.36	1.41	1.35
12	Bg	1205	LMT	O2'-C2'	-2.36	1.37	1.43
10	Bl	103	BCL	C3B-C4B	2.36	1.45	1.41
10	AH	101	BCL	C3B-C4B	2.36	1.45	1.41
19	BF	103	V7N	C14-C13	2.35	1.41	1.35
10	Am	101	BCL	C3B-C4B	2.35	1.45	1.41
12	Bg	1201	LMT	O1'-C1'	-2.35	1.36	1.40
19	BN	103	V7N	C17-C18	2.35	1.41	1.35
10	Aj	101	BCL	O1A-CGA	-2.35	1.15	1.22
19	An	102	V7N	C12-C13	-2.35	1.40	1.46
19	BW	101	V7N	C17-C18	2.35	1.41	1.35
10	Bg	1203	BCL	C3D-C4D	-2.35	1.38	1.44
12	Ba	104	LMT	O2B-C2B	-2.35	1.37	1.43
10	L	301	BCL	O1A-CGA	-2.35	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AB	101	BCL	C5-C3	2.35	1.56	1.51
12	BG	103	LMT	O1'-C1'	-2.35	1.36	1.40
19	Bk	1202	V7N	C14-C13	2.35	1.41	1.35
12	L	309	LMT	O2B-C2B	-2.34	1.37	1.43
12	AQ	102	LMT	O3B-C3B	-2.34	1.37	1.43
12	Bo	1201	LMT	O1'-C1'	-2.34	1.36	1.40
19	Bf	102	V7N	C11-C12	2.34	1.40	1.34
19	Bm	101	V7N	C17-C18	2.34	1.41	1.35
10	Be	101	BCL	C3D-C4D	-2.34	1.38	1.44
19	BP	103	V7N	C17-C18	2.34	1.41	1.35
10	BQ	101	BCL	C1D-C2D	-2.34	1.40	1.45
10	Bd	103	BCL	C3D-C4D	-2.34	1.38	1.44
19	Ad	102	V7N	C17-C18	2.34	1.41	1.35
12	L	307	LMT	O2'-C2'	-2.34	1.37	1.43
10	AV	1001	BCL	C3B-C4B	2.33	1.45	1.41
12	BM	102	LMT	O2'-C2'	-2.33	1.37	1.43
12	BU	101	LMT	O2B-C2B	-2.33	1.37	1.43
19	Bl	102	V7N	C12-C13	-2.33	1.41	1.46
12	BB	103	LMT	O2'-C2'	-2.33	1.37	1.43
10	BD	101	BCL	C3D-C4D	-2.33	1.38	1.44
10	BW	102	BCL	C3B-C4B	2.33	1.45	1.41
19	BX	102	V7N	C17-C18	2.33	1.41	1.35
12	BX	101	LMT	O2B-C2B	-2.33	1.37	1.43
12	BO	103	LMT	O1'-C1'	-2.33	1.36	1.40
19	BX	102	V7N	C19-C18	-2.33	1.41	1.46
12	L	304	LMT	O3'-C3'	-2.33	1.37	1.43
10	BT	101	BCL	C1D-C2D	-2.32	1.40	1.45
10	BE	102	BCL	C3B-C4B	2.32	1.45	1.41
12	L	308	LMT	O2B-C2B	-2.32	1.37	1.43
12	BR	102	LMT	O1'-C1'	-2.32	1.36	1.40
19	BO	101	V7N	C17-C18	2.32	1.41	1.35
10	Bm	102	BCL	C1D-C2D	-2.32	1.40	1.45
19	AI	103	V7N	C14-C13	2.32	1.41	1.35
12	AK	102	LMT	O2B-C2B	-2.32	1.37	1.43
10	BH	102	BCL	C3B-C4B	2.32	1.45	1.41
12	BV	103	LMT	O2B-C2B	-2.32	1.37	1.43
19	BC	103	V7N	C19-C18	-2.32	1.41	1.46
19	AX	101	V7N	C11-C12	2.32	1.40	1.34
10	BX	103	BCL	C3B-C4B	2.32	1.45	1.41
19	BK	104	V7N	C12-C13	-2.32	1.41	1.46
19	AI	101	V7N	C12-C13	-2.31	1.41	1.46
19	AP	101	V7N	C12-C13	-2.31	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Bi	1201	LMT	O2'-C2'	-2.31	1.37	1.43
12	Bm	104	LMT	O2B-C2B	-2.31	1.37	1.43
19	BD	103	V7N	C17-C18	2.31	1.41	1.35
12	BX	101	LMT	O2'-C2'	-2.31	1.37	1.43
10	AU	102	BCL	C1D-C2D	-2.31	1.40	1.45
10	Bg	1203	BCL	O1A-CGA	-2.31	1.15	1.22
19	Bm	101	V7N	C12-C13	-2.31	1.41	1.46
10	BA	101	BCL	C1D-C2D	-2.31	1.40	1.45
10	Bo	1202	BCL	C3D-C4D	-2.31	1.39	1.44
12	BK	103	LMT	O2B-C2B	-2.31	1.37	1.43
19	BD	103	V7N	C12-C13	-2.31	1.41	1.46
19	BK	104	V7N	C17-C18	2.31	1.41	1.35
12	BB	103	LMT	O3B-C3B	-2.31	1.37	1.43
10	AD	101	BCL	C3B-C4B	2.31	1.45	1.41
10	AL	101	BCL	C3B-C4B	2.31	1.45	1.41
10	Bp	1004	BCL	C3B-C4B	2.31	1.45	1.41
12	BS	102	LMT	O2B-C2B	-2.31	1.37	1.43
10	Ah	101	BCL	C3D-C4D	-2.30	1.39	1.44
10	Bc	1203	BCL	C3D-C4D	-2.30	1.39	1.44
12	AK	102	LMT	O3B-C3B	-2.30	1.37	1.43
12	BO	103	LMT	O2B-C2B	-2.30	1.37	1.43
12	BX	104	LMT	O2B-C2B	-2.30	1.37	1.43
12	BX	104	LMT	O3B-C3B	-2.30	1.37	1.43
12	BN	102	LMT	O3B-C3B	-2.30	1.37	1.43
10	AM	101	BCL	C3B-C4B	2.30	1.45	1.41
10	Bl	103	BCL	C3D-C4D	-2.30	1.39	1.44
19	BC	103	V7N	C14-C13	2.29	1.41	1.35
10	BP	104	BCL	C3D-C4D	-2.29	1.39	1.44
19	AI	103	V7N	C17-C18	2.29	1.41	1.35
19	BB	102	V7N	C19-C18	-2.29	1.41	1.46
19	BF	103	V7N	C19-C18	-2.29	1.41	1.46
19	Ag	102	V7N	C11-C12	2.29	1.40	1.34
10	Bh	102	BCL	C3D-C4D	-2.29	1.39	1.44
12	BP	102	LMT	O2B-C2B	-2.29	1.37	1.43
10	Bg	1203	BCL	C1D-C2D	-2.29	1.40	1.45
12	AK	102	LMT	O1'-C1'	-2.29	1.36	1.40
10	AR	101	BCL	CHD-C1D	2.29	1.42	1.38
12	L	304	LMT	O2B-C2B	-2.29	1.37	1.43
10	Bi	1203	BCL	C3B-C4B	2.29	1.45	1.41
10	Bm	102	BCL	C3D-C4D	-2.28	1.39	1.44
10	BE	102	BCL	C1D-C2D	-2.28	1.40	1.45
10	BG	102	BCL	C3D-C4D	-2.28	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BT	103	LMT	O1'-C1'	-2.28	1.36	1.40
12	BQ	102	LMT	O3B-C3B	-2.28	1.37	1.43
10	AU	101	BCL	C3D-C4D	-2.28	1.39	1.44
10	BF	102	BCL	C3D-C4D	-2.28	1.39	1.44
10	BO	102	BCL	C1D-C2D	-2.28	1.40	1.45
12	BK	103	LMT	O3B-C3B	-2.28	1.37	1.43
12	Bk	1201	LMT	O1'-C1'	-2.28	1.36	1.40
10	Bn	101	BCL	C3D-C4D	-2.28	1.39	1.44
19	Bk	1202	V7N	C19-C18	-2.28	1.41	1.46
12	BS	102	LMT	O3B-C3B	-2.28	1.37	1.43
12	Bl	105	LMT	O1'-C1'	-2.28	1.36	1.40
10	BS	101	BCL	C3D-C4D	-2.28	1.39	1.44
19	Bd	102	V7N	C12-C13	-2.27	1.41	1.46
12	BL	103	LMT	O3B-C3B	-2.27	1.37	1.43
12	Bd	105	LMT	O3B-C3B	-2.27	1.37	1.43
10	BX	103	BCL	C3D-C4D	-2.27	1.39	1.44
10	Bf	103	BCL	C3D-C4D	-2.27	1.39	1.44
12	Bp	1002	LMT	O1'-C1'	-2.27	1.36	1.40
19	BL	101	V7N	C11-C12	2.27	1.40	1.34
10	AX	102	BCL	C3D-C4D	-2.27	1.39	1.44
12	BI	1103	LMT	O1'-C1'	-2.27	1.36	1.40
10	Ba	102	BCL	C3B-C4B	2.27	1.45	1.41
19	AF	102	V7N	C12-C13	-2.27	1.41	1.46
12	Bp	1002	LMT	O2B-C2B	-2.27	1.37	1.43
10	AE	101	BCL	CBD-CGD	-2.27	1.45	1.52
10	AN	101	BCL	C3D-C4D	-2.27	1.39	1.44
10	Bk	1203	BCL	C3D-C4D	-2.27	1.39	1.44
10	AD	101	BCL	C3D-C4D	-2.27	1.39	1.44
19	BV	101	V7N	C11-C12	2.27	1.40	1.34
19	BO	101	V7N	C14-C13	2.27	1.41	1.35
10	BO	102	BCL	C3B-C4B	2.27	1.45	1.41
12	BI	1103	LMT	O3B-C3B	-2.27	1.37	1.43
12	BO	103	LMT	O2'-C2'	-2.27	1.37	1.43
19	Bb	101	V7N	C19-C18	-2.27	1.41	1.46
10	Bh	102	BCL	C3B-C4B	2.27	1.45	1.41
10	BA	101	BCL	C3B-C4B	2.26	1.45	1.41
10	BP	101	BCL	C1D-C2D	-2.26	1.40	1.45
12	BQ	102	LMT	O2'-C2'	-2.26	1.37	1.43
12	BS	102	LMT	O1'-C1'	-2.26	1.36	1.40
19	BK	104	V7N	C19-C18	-2.26	1.41	1.46
10	AM	101	BCL	C3D-C4D	-2.26	1.39	1.44
19	Am	102	V7N	C17-C18	2.26	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AB	102	LMT	O3B-C3B	-2.26	1.37	1.43
10	AF	101	BCL	C3D-C4D	-2.26	1.39	1.44
12	Bc	1201	LMT	O3B-C3B	-2.26	1.37	1.43
12	BB	103	LMT	O2B-C2B	-2.26	1.37	1.43
12	BQ	102	LMT	O2B-C2B	-2.26	1.37	1.43
10	Am	101	BCL	C3D-C4D	-2.26	1.39	1.44
12	Bj	102	LMT	O1'-C1'	-2.26	1.36	1.40
12	Bj	102	LMT	O3B-C3B	-2.26	1.37	1.43
10	AK	101	BCL	C3B-C4B	2.26	1.45	1.41
10	AP	102	BCL	C3D-C4D	-2.25	1.39	1.44
10	BB	101	BCL	C3B-C4B	2.25	1.45	1.41
10	BP	101	BCL	C3D-C4D	-2.25	1.39	1.44
10	BL	102	BCL	C3D-C4D	-2.25	1.39	1.44
19	AH	102	V7N	C12-C13	-2.25	1.41	1.46
10	L	302	BCL	CHD-C1D	2.25	1.42	1.38
19	Bi	1202	V7N	C12-C13	-2.25	1.41	1.46
12	BK	101	LMT	O3B-C3B	-2.25	1.37	1.43
19	Bg	1202	V7N	C12-C13	-2.25	1.41	1.46
10	Bp	1004	BCL	C3D-C4D	-2.25	1.39	1.44
12	AB	102	LMT	O2B-C2B	-2.25	1.37	1.43
12	Bp	1002	LMT	O3B-C3B	-2.25	1.37	1.43
19	BR	103	V7N	C17-C18	2.25	1.41	1.35
12	Bc	1201	LMT	O2B-C2B	-2.24	1.37	1.43
10	BK	102	BCL	C1D-C2D	-2.24	1.40	1.45
12	Bi	1201	LMT	O2B-C2B	-2.24	1.37	1.43
12	AQ	102	LMT	O2B-C2B	-2.24	1.37	1.43
10	L	302	BCL	O1A-CGA	-2.24	1.15	1.22
19	Bp	1003	V7N	C11-C12	2.24	1.40	1.34
19	BR	103	V7N	C19-C18	-2.24	1.41	1.46
10	BI	1102	BCL	C3D-C4D	-2.24	1.39	1.44
12	L	309	LMT	O1'-C1'	-2.24	1.36	1.40
10	AD	101	BCL	C1D-C2D	-2.24	1.40	1.45
10	BS	101	BCL	C1D-C2D	-2.24	1.40	1.45
12	L	308	LMT	O2'-C2'	-2.24	1.37	1.43
10	BN	101	BCL	C3D-C4D	-2.24	1.39	1.44
19	BN	103	V7N	C12-C13	-2.24	1.41	1.46
12	L	304	LMT	O3B-C3B	-2.24	1.37	1.43
10	Ac	101	BCL	C1D-C2D	-2.24	1.40	1.45
19	Bj	103	V7N	C11-C12	2.24	1.40	1.34
12	BC	102	LMT	O1'-C1'	-2.23	1.36	1.40
10	AQ	103	BCL	CBD-CGD	-2.23	1.45	1.52
10	AL	101	BCL	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Bi	1201	LMT	O3B-C3B	-2.23	1.37	1.43
10	BH	102	BCL	C3D-C4D	-2.23	1.39	1.44
12	AB	102	LMT	O1'-C1'	-2.23	1.36	1.40
19	AL	102	V7N	C12-C13	-2.23	1.41	1.46
10	BV	102	BCL	C3B-C4B	2.23	1.45	1.41
19	BT	102	V7N	C11-C12	2.23	1.40	1.34
19	Bk	1202	V7N	C17-C18	2.23	1.41	1.35
12	M	407	LMT	O1'-C1'	-2.23	1.36	1.40
19	BS	103	V7N	C12-C13	-2.23	1.41	1.46
12	BV	103	LMT	O3B-C3B	-2.23	1.37	1.43
10	BJ	101	BCL	C3D-C4D	-2.23	1.39	1.44
12	BI	1101	LMT	O3B-C3B	-2.23	1.37	1.43
10	BE	102	BCL	C3D-C4D	-2.23	1.39	1.44
10	BC	101	BCL	C3B-C4B	2.22	1.45	1.41
10	Bp	1001	BCL	C3D-C4D	-2.22	1.39	1.44
18	C	1000	HEC	C3B-C2B	-2.22	1.33	1.41
10	BL	102	BCL	C1D-C2D	-2.22	1.40	1.45
12	AB	102	LMT	O4'-C4B	-2.22	1.37	1.43
10	AU	102	BCL	C3D-C4D	-2.22	1.39	1.44
12	L	306	LMT	O2B-C2B	-2.22	1.37	1.43
12	BL	103	LMT	O2B-C2B	-2.22	1.37	1.43
19	AT	102	V7N	C17-C18	2.22	1.40	1.35
10	BF	102	BCL	C1D-C2D	-2.22	1.41	1.45
19	BT	102	V7N	C12-C13	-2.22	1.41	1.46
12	Bg	1201	LMT	O3B-C3B	-2.21	1.37	1.43
12	BA	102	LMT	O1'-C1'	-2.21	1.36	1.40
10	AT	104	BCL	O1A-CGA	-2.21	1.15	1.22
12	BN	102	LMT	O2B-C2B	-2.21	1.37	1.43
12	BR	102	LMT	O3B-C3B	-2.21	1.37	1.43
12	BG	103	LMT	O2B-C2B	-2.21	1.37	1.43
12	BR	102	LMT	O2B-C2B	-2.21	1.37	1.43
12	Bg	1201	LMT	O2B-C2B	-2.21	1.37	1.43
10	BQ	101	BCL	C3D-C4D	-2.21	1.39	1.44
19	AX	101	V7N	C7-C8	2.21	1.40	1.34
12	BQ	102	LMT	O1'-C1'	-2.21	1.36	1.40
12	Bd	105	LMT	O1'-C1'	-2.21	1.36	1.40
12	Bl	105	LMT	O3B-C3B	-2.21	1.37	1.43
19	Am	102	V7N	C19-C18	-2.21	1.41	1.46
10	Bg	1203	BCL	C3B-C4B	2.21	1.45	1.41
19	Bg	1202	V7N	C11-C12	2.21	1.40	1.34
12	BD	102	LMT	O1'-C1'	-2.21	1.36	1.40
12	BM	102	LMT	O2B-C2B	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	BCL	C3D-C4D	-2.21	1.39	1.44
10	Bi	1203	BCL	C3D-C4D	-2.21	1.39	1.44
10	BR	101	BCL	O1A-CGA	-2.21	1.15	1.22
10	Bd	101	BCL	C19-C18	2.21	1.63	1.51
10	Ao	101	BCL	C3D-C4D	-2.21	1.39	1.44
19	Bf	102	V7N	C12-C13	-2.21	1.41	1.46
10	BG	102	BCL	C3B-C4B	2.21	1.45	1.41
10	BV	102	BCL	C3D-C4D	-2.21	1.39	1.44
19	BT	102	V7N	C19-C18	-2.21	1.41	1.46
10	BT	101	BCL	C3D-C4D	-2.21	1.39	1.44
10	AU	101	BCL	C3B-C4B	2.21	1.45	1.41
19	Ba	101	V7N	C12-C13	-2.21	1.41	1.46
12	Bk	1201	LMT	O3B-C3B	-2.20	1.37	1.43
10	AT	101	BCL	C3D-C4D	-2.20	1.39	1.44
19	Bd	102	V7N	C19-C18	-2.20	1.41	1.46
12	BD	102	LMT	O2B-C2B	-2.20	1.37	1.43
10	Bn	101	BCL	C3B-C4B	2.20	1.45	1.41
12	BF	101	LMT	O3B-C3B	-2.20	1.37	1.43
10	BB	101	BCL	C3D-C4D	-2.20	1.39	1.44
10	BJ	101	BCL	C1D-C2D	-2.20	1.41	1.45
10	AH	101	BCL	C3D-C4D	-2.20	1.39	1.44
10	BI	1102	BCL	C3B-C4B	2.20	1.45	1.41
12	BL	103	LMT	O1'-C1'	-2.20	1.36	1.40
10	BQ	101	BCL	C3B-C4B	2.20	1.45	1.41
10	AW	101	BCL	C3D-C4D	-2.20	1.39	1.44
19	BE	101	V7N	C11-C12	2.20	1.40	1.34
10	Bh	101	BCL	C3D-C4D	-2.20	1.39	1.44
19	AX	101	V7N	C6-C5	2.20	1.40	1.35
10	M	404	BCL	O2A-CGA	-2.20	1.27	1.33
12	Ba	104	LMT	O3B-C3B	-2.20	1.37	1.43
12	BG	101	LMT	O3B-C3B	-2.20	1.37	1.43
19	Bb	101	V7N	C12-C13	-2.20	1.41	1.46
10	BA	101	BCL	C3D-C4D	-2.20	1.39	1.44
10	Ba	102	BCL	C3D-C4D	-2.20	1.39	1.44
10	Be	101	BCL	C3B-C4B	2.20	1.45	1.41
12	BT	103	LMT	O3B-C3B	-2.20	1.37	1.43
12	Bo	1201	LMT	O2B-C2B	-2.20	1.37	1.43
12	Bo	1201	LMT	O3B-C3B	-2.20	1.37	1.43
10	BR	101	BCL	C3D-C4D	-2.19	1.39	1.44
12	Bc	1204	LMT	O2B-C2B	-2.19	1.37	1.43
12	L	307	LMT	O3B-C3B	-2.19	1.37	1.43
10	AQ	103	BCL	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AL	102	V7N	C11-C12	2.19	1.40	1.34
12	BG	103	LMT	O3B-C3B	-2.19	1.37	1.43
10	Bp	1004	BCL	C1D-C2D	-2.19	1.41	1.45
10	Al	101	BCL	C3D-C4D	-2.19	1.39	1.44
12	L	309	LMT	O3B-C3B	-2.19	1.37	1.43
10	BC	101	BCL	C3D-C4D	-2.19	1.39	1.44
12	BG	103	LMT	O2'-C2'	-2.19	1.37	1.43
12	BH	101	LMT	O1'-C1'	-2.19	1.36	1.40
19	BE	101	V7N	C19-C18	-2.19	1.41	1.46
19	AI	103	V7N	C19-C18	-2.19	1.41	1.46
12	Bc	1204	LMT	O1'-C1'	-2.19	1.36	1.40
12	Bg	1205	LMT	O1'-C1'	-2.19	1.36	1.40
10	Bd	103	BCL	C1D-C2D	-2.19	1.41	1.45
19	Bi	1202	V7N	C11-C12	2.18	1.40	1.34
19	AI	101	V7N	C19-C18	-2.18	1.41	1.46
10	Aa	101	BCL	CHD-C1D	2.18	1.42	1.38
10	BM	101	BCL	C3D-C4D	-2.18	1.39	1.44
10	Am	101	BCL	O1A-CGA	-2.18	1.16	1.22
10	AR	101	BCL	C3D-C4D	-2.18	1.39	1.44
19	BK	104	V7N	C11-C12	2.18	1.40	1.34
10	BK	102	BCL	C3D-C4D	-2.18	1.39	1.44
10	AB	101	BCL	C3D-C4D	-2.18	1.39	1.44
12	Bk	1201	LMT	O2B-C2B	-2.18	1.37	1.43
10	Ak	101	BCL	C3D-C4D	-2.18	1.39	1.44
12	BC	102	LMT	O3B-C3B	-2.18	1.37	1.43
19	BN	103	V7N	C11-C12	2.18	1.40	1.34
10	AN	101	BCL	CBD-CGD	-2.18	1.45	1.52
10	AX	102	BCL	CBD-CGD	-2.18	1.45	1.52
12	BD	102	LMT	O3B-C3B	-2.18	1.37	1.43
10	AI	102	BCL	CBD-CGD	-2.18	1.45	1.52
10	Bc	1203	BCL	C1D-C2D	-2.18	1.41	1.45
10	L	302	BCL	C3D-C4D	-2.18	1.39	1.44
12	BH	101	LMT	O3B-C3B	-2.18	1.37	1.43
12	BV	103	LMT	O1'-C1'	-2.18	1.36	1.40
19	Bp	1003	V7N	C6-C5	2.18	1.40	1.35
10	Ah	101	BCL	C1D-C2D	-2.18	1.41	1.45
19	BB	102	V7N	C17-C18	2.18	1.40	1.35
19	Ba	101	V7N	C11-C12	2.17	1.40	1.34
10	AV	1001	BCL	C3D-C4D	-2.17	1.39	1.44
12	BN	102	LMT	O1'-C1'	-2.17	1.36	1.40
12	BP	102	LMT	O1'-C1'	-2.17	1.36	1.40
12	BU	101	LMT	O3B-C3B	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Bc	1204	LMT	O3B-C3B	-2.17	1.37	1.43
12	Bj	102	LMT	O2B-C2B	-2.17	1.37	1.43
10	Ai	101	BCL	C3D-C4D	-2.17	1.39	1.44
12	BP	102	LMT	O3B-C3B	-2.17	1.37	1.43
10	AQ	101	BCL	CHD-C1D	2.17	1.42	1.38
10	AC	101	BCL	C3D-C4D	-2.17	1.39	1.44
10	AQ	101	BCL	C3D-C4D	-2.17	1.39	1.44
12	M	407	LMT	O3B-C3B	-2.17	1.37	1.43
10	AR	101	BCL	C1D-C2D	-2.17	1.41	1.45
10	BF	102	BCL	C3B-C4B	2.17	1.45	1.41
19	Bl	102	V7N	C19-C18	-2.17	1.41	1.46
12	BI	1101	LMT	O2B-C2B	-2.17	1.37	1.43
12	Bg	1201	LMT	O4'-C4B	-2.17	1.37	1.43
19	An	102	V7N	C11-C12	2.17	1.40	1.34
19	AI	101	V7N	C11-C12	2.17	1.40	1.34
12	BX	104	LMT	O1'-C1'	-2.17	1.36	1.40
10	BK	102	BCL	C3B-C4B	2.17	1.45	1.41
12	BM	102	LMT	O3B-C3B	-2.16	1.37	1.43
10	Bo	1202	BCL	C3B-C4B	2.16	1.45	1.41
10	Bf	101	BCL	C3D-C4D	-2.16	1.39	1.44
11	L	303	BPH	CHA-CBD	2.16	1.54	1.51
12	BH	101	LMT	O2'-C2'	-2.16	1.37	1.43
10	Bk	1203	BCL	C3B-C4B	2.16	1.45	1.41
10	Bh	101	BCL	CHD-C1D	2.16	1.42	1.38
10	AH	101	BCL	CBD-CGD	-2.16	1.45	1.52
12	BO	103	LMT	O3B-C3B	-2.16	1.37	1.43
12	BC	102	LMT	O2B-C2B	-2.16	1.37	1.43
19	BN	103	V7N	C19-C18	-2.16	1.41	1.46
10	Ac	101	BCL	C3D-C4D	-2.16	1.39	1.44
12	Bc	1201	LMT	O4'-C4B	-2.16	1.37	1.43
19	BV	101	V7N	C12-C13	-2.16	1.41	1.46
19	BC	103	V7N	C17-C18	2.16	1.40	1.35
10	AP	102	BCL	C3B-C4B	2.15	1.45	1.41
10	AK	101	BCL	CBD-CGD	-2.15	1.45	1.52
19	Bb	101	V7N	C11-C12	2.15	1.40	1.34
12	BK	101	LMT	O2B-C2B	-2.15	1.37	1.43
19	BF	103	V7N	C17-C18	2.15	1.40	1.35
12	BO	103	LMT	O4'-C4B	-2.15	1.37	1.43
19	Ag	102	V7N	C7-C8	2.15	1.40	1.34
19	AI	101	V7N	C6-C5	2.15	1.40	1.35
12	BI	1103	LMT	O2B-C2B	-2.15	1.37	1.43
10	Bj	101	BCL	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AO	101	BCL	CHD-C1D	2.15	1.42	1.38
12	Bc	1201	LMT	O1'-C1'	-2.15	1.36	1.40
19	Bl	102	V7N	C11-C12	2.15	1.40	1.34
10	AO	101	BCL	C3D-C4D	-2.15	1.39	1.44
12	BB	103	LMT	O1'-C1'	-2.15	1.36	1.40
10	AE	101	BCL	CHD-C1D	2.15	1.42	1.38
10	BW	102	BCL	C3D-C4D	-2.15	1.39	1.44
12	BA	102	LMT	O3B-C3B	-2.15	1.37	1.43
10	Bn	101	BCL	C1D-C2D	-2.15	1.41	1.45
10	Aj	101	BCL	C3D-C4D	-2.15	1.39	1.44
10	Aa	101	BCL	C3D-C4D	-2.15	1.39	1.44
10	Af	102	BCL	C3D-C4D	-2.15	1.39	1.44
10	AI	102	BCL	C3D-C4D	-2.15	1.39	1.44
10	Bl	101	BCL	C3D-C4D	-2.14	1.39	1.44
19	Bm	101	V7N	C11-C12	2.14	1.40	1.34
12	BF	101	LMT	O1'-C1'	-2.14	1.36	1.40
19	BE	101	V7N	C12-C13	-2.14	1.41	1.46
19	BV	101	V7N	C19-C18	-2.14	1.41	1.46
12	Bm	104	LMT	O1'-C1'	-2.14	1.36	1.40
10	Be	101	BCL	C1D-C2D	-2.14	1.41	1.45
12	L	305	LMT	O4'-C4B	-2.14	1.37	1.43
10	AF	101	BCL	CBD-CGD	-2.14	1.46	1.52
10	AE	101	BCL	C3D-C4D	-2.14	1.39	1.44
12	BL	103	LMT	O4'-C4B	-2.14	1.37	1.43
19	AH	102	V7N	C11-C12	2.14	1.40	1.34
10	AK	101	BCL	C3D-C4D	-2.14	1.39	1.44
12	AQ	102	LMT	O1'-C1'	-2.14	1.36	1.40
12	L	305	LMT	O3B-C3B	-2.14	1.37	1.43
18	C	1000	HEC	C3C-C2C	-2.14	1.34	1.41
10	Ae	101	BCL	C3D-C4D	-2.14	1.39	1.44
12	L	305	LMT	O2B-C2B	-2.14	1.37	1.43
10	AO	101	BCL	O1A-CGA	-2.14	1.16	1.22
12	L	304	LMT	O2'-C2'	-2.14	1.37	1.43
10	AB	101	BCL	O1A-CGA	-2.13	1.16	1.22
19	Bd	102	V7N	C11-C12	2.13	1.40	1.34
10	BT	101	BCL	C3B-C4B	2.13	1.45	1.41
10	BD	101	BCL	C1D-C2D	-2.13	1.41	1.45
12	BT	103	LMT	O2B-C2B	-2.13	1.37	1.43
10	Bf	101	BCL	CBD-CGD	-2.13	1.46	1.52
12	BK	103	LMT	O1'-C1'	-2.13	1.36	1.40
19	BL	101	V7N	C12-C13	-2.13	1.41	1.46
10	BV	102	BCL	C1D-C2D	-2.13	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BE	101	V7N	C6-C5	2.13	1.40	1.35
12	BD	102	LMT	O4'-C4B	-2.13	1.37	1.43
10	AF	101	BCL	CHD-C1D	2.13	1.42	1.38
12	BX	101	LMT	O3B-C3B	-2.13	1.37	1.43
12	L	306	LMT	O2'-C2'	-2.13	1.37	1.43
19	BL	101	V7N	C6-C5	2.12	1.40	1.35
12	Bd	105	LMT	O2B-C2B	-2.12	1.37	1.43
19	BD	103	V7N	C11-C12	2.12	1.40	1.34
12	M	407	LMT	O4'-C4B	-2.12	1.37	1.43
12	BB	103	LMT	O4'-C4B	-2.12	1.37	1.43
10	Bd	101	BCL	C3D-C4D	-2.12	1.39	1.44
12	L	306	LMT	O3B-C3B	-2.12	1.37	1.43
12	Bi	1201	LMT	O4'-C4B	-2.12	1.37	1.43
10	BG	102	BCL	C1D-C2D	-2.12	1.41	1.45
10	Ba	102	BCL	C1D-C2D	-2.12	1.41	1.45
19	Bm	101	V7N	C19-C18	-2.12	1.41	1.46
12	BM	102	LMT	O1'-C1'	-2.12	1.36	1.40
12	L	307	LMT	O2B-C2B	-2.12	1.37	1.43
10	BW	102	BCL	C1D-C2D	-2.12	1.41	1.45
10	BM	101	BCL	C1D-C2D	-2.12	1.41	1.45
19	BS	103	V7N	C11-C12	2.12	1.40	1.34
19	Bp	1003	V7N	C7-C8	2.12	1.40	1.34
18	C	1002	HEC	C3B-C2B	-2.12	1.34	1.41
19	Bp	1003	V7N	C12-C13	-2.12	1.41	1.46
10	BS	101	BCL	C3B-C4B	2.11	1.45	1.41
19	Bc	1202	V7N	C11-C12	2.11	1.40	1.34
18	C	1003	HEC	C3B-C2B	-2.11	1.34	1.41
12	BC	102	LMT	O4'-C4B	-2.11	1.37	1.43
19	AF	102	V7N	C11-C12	2.11	1.40	1.34
12	Bd	105	LMT	O4'-C4B	-2.11	1.37	1.43
12	BG	101	LMT	O4'-C4B	-2.11	1.37	1.43
11	L	303	BPH	C1D-C2D	2.11	1.41	1.39
10	BO	102	BCL	C3D-C4D	-2.11	1.39	1.44
19	AF	102	V7N	C19-C18	-2.11	1.41	1.46
10	An	101	BCL	CBD-CGD	-2.11	1.46	1.52
10	AV	1001	BCL	O1A-CGA	-2.11	1.16	1.22
10	BW	102	BCL	CHD-C1D	2.11	1.42	1.38
12	Bg	1205	LMT	O3B-C3B	-2.11	1.37	1.43
10	Bh	101	BCL	CBD-CGD	-2.11	1.46	1.52
19	Ag	102	V7N	C12-C13	-2.10	1.41	1.46
10	AP	102	BCL	C1D-C2D	-2.10	1.41	1.45
19	BO	101	V7N	C8-C9	-2.10	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bl	101	BCL	O1A-CGA	-2.10	1.16	1.22
12	BX	104	LMT	O2'-C2'	-2.10	1.37	1.43
10	BC	101	BCL	CHD-C1D	2.10	1.42	1.38
10	BP	104	BCL	CHD-C1D	2.10	1.42	1.38
19	Bj	103	V7N	C7-C8	2.10	1.40	1.34
12	L	308	LMT	O3B-C3B	-2.10	1.37	1.43
19	Ag	102	V7N	C6-C5	2.10	1.40	1.35
12	Bi	1201	LMT	O1'-C1'	-2.10	1.36	1.40
19	AP	101	V7N	C19-C18	-2.10	1.41	1.46
19	AX	101	V7N	C12-C13	-2.10	1.41	1.46
12	L	304	LMT	O4'-C4B	-2.10	1.37	1.43
19	BL	101	V7N	C7-C8	2.10	1.40	1.34
19	BN	103	V7N	C7-C8	2.10	1.40	1.34
19	BO	101	V7N	C19-C18	-2.09	1.41	1.46
19	Bg	1202	V7N	C19-C18	-2.09	1.41	1.46
12	Ba	104	LMT	O4'-C4B	-2.09	1.37	1.43
19	Bj	103	V7N	C12-C13	-2.09	1.41	1.46
10	M	404	BCL	C3D-C4D	-2.09	1.39	1.44
10	Ag	101	BCL	CHD-C1D	2.09	1.42	1.38
10	An	101	BCL	C3D-C4D	-2.09	1.39	1.44
19	BS	103	V7N	C7-C8	2.09	1.40	1.34
10	BI	1102	BCL	CHD-C1D	2.09	1.42	1.38
19	BP	103	V7N	C11-C12	2.09	1.40	1.34
10	Ai	101	BCL	CHD-C1D	2.09	1.42	1.38
19	BS	103	V7N	C6-C5	2.09	1.40	1.35
10	BL	102	BCL	CHD-C1D	2.09	1.42	1.38
19	Bj	103	V7N	C19-C18	-2.09	1.41	1.46
10	Af	102	BCL	CBD-CGD	-2.09	1.46	1.52
19	Ad	102	V7N	C19-C18	-2.09	1.41	1.46
10	BP	101	BCL	C3B-C4B	2.08	1.45	1.41
10	Bh	102	BCL	C1D-C2D	-2.08	1.41	1.45
12	L	305	LMT	O2'-C2'	-2.08	1.37	1.43
10	Ao	101	BCL	CBD-CGD	-2.08	1.46	1.52
10	Bl	103	BCL	C1D-C2D	-2.08	1.41	1.45
19	Ba	101	V7N	C19-C18	-2.08	1.41	1.46
12	BN	102	LMT	O4'-C4B	-2.08	1.37	1.43
10	AC	101	BCL	CBD-CGD	-2.08	1.46	1.52
19	BE	101	V7N	C7-C8	2.08	1.40	1.34
10	AM	101	BCL	C1D-C2D	-2.08	1.41	1.45
19	AI	101	V7N	C7-C8	2.08	1.40	1.34
10	AW	101	BCL	O1A-CGA	-2.08	1.16	1.22
10	Bd	103	BCL	O1A-CGA	-2.08	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BP	102	LMT	O4'-C4B	-2.08	1.37	1.43
19	BW	101	V7N	C11-C12	2.08	1.40	1.34
19	AX	101	V7N	C19-C18	-2.08	1.41	1.46
10	AW	101	BCL	CHD-C1D	2.08	1.42	1.38
19	Bi	1202	V7N	C7-C8	2.08	1.40	1.34
10	AB	101	BCL	CHD-C1D	2.08	1.42	1.38
10	AT	104	BCL	C3D-C4D	-2.08	1.39	1.44
12	Bg	1205	LMT	O2B-C2B	-2.08	1.37	1.43
12	BA	102	LMT	O4'-C4B	-2.08	1.37	1.43
12	Bg	1205	LMT	O4'-C4B	-2.07	1.37	1.43
19	BP	103	V7N	C19-C18	-2.07	1.41	1.46
12	Bp	1002	LMT	O4'-C4B	-2.07	1.37	1.43
10	AR	101	BCL	CBD-CGD	-2.07	1.46	1.52
19	AL	102	V7N	C6-C5	2.07	1.40	1.35
19	BW	101	V7N	C19-C18	-2.07	1.41	1.46
10	An	101	BCL	CHD-C1D	2.07	1.42	1.38
10	Ak	101	BCL	CHD-C1D	2.07	1.42	1.38
10	AR	101	BCL	O1A-CGA	-2.07	1.16	1.22
10	Bd	101	BCL	CBD-CGD	-2.07	1.46	1.52
10	BN	101	BCL	CHD-C1D	2.07	1.42	1.38
19	Bf	102	V7N	C19-C18	-2.07	1.41	1.46
19	BV	101	V7N	C7-C8	2.06	1.40	1.34
12	Ba	104	LMT	O1'-C1'	-2.06	1.36	1.40
19	AL	102	V7N	C7-C8	2.06	1.40	1.34
10	BH	102	BCL	C1D-C2D	-2.06	1.41	1.45
10	Bl	101	BCL	CBD-CGD	-2.06	1.46	1.52
10	BB	101	BCL	C1D-C2D	-2.06	1.41	1.45
10	AI	102	BCL	CHD-C1D	2.06	1.42	1.38
10	Ag	101	BCL	O1A-CGA	-2.06	1.16	1.22
10	AU	102	BCL	CHD-C1D	2.06	1.42	1.38
12	AK	102	LMT	O4'-C4B	-2.06	1.37	1.43
10	Bi	1203	BCL	C1D-C2D	-2.06	1.41	1.45
12	L	309	LMT	O4'-C4B	-2.06	1.37	1.43
10	BN	101	BCL	C1D-C2D	-2.06	1.41	1.45
19	Bj	103	V7N	C6-C5	2.06	1.40	1.35
10	Ag	101	BCL	C3D-C4D	-2.06	1.39	1.44
12	BI	1103	LMT	O4'-C4B	-2.06	1.37	1.43
10	BA	101	BCL	O1A-CGA	-2.06	1.16	1.22
19	Ad	102	V7N	C11-C12	2.05	1.40	1.34
19	Bc	1202	V7N	C19-C18	-2.05	1.41	1.46
10	Bc	1203	BCL	CHD-C1D	2.05	1.42	1.38
19	AH	102	V7N	C19-C18	-2.05	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BT	102	V7N	C6-C5	2.05	1.40	1.35
19	BV	101	V7N	C6-C5	2.05	1.40	1.35
10	AX	102	BCL	CHD-C1D	2.05	1.42	1.38
12	BK	101	LMT	O1'-C1'	-2.05	1.36	1.40
10	AF	101	BCL	C1D-C2D	-2.05	1.41	1.45
19	BW	101	V7N	C7-C8	2.05	1.40	1.34
18	C	1001	HEC	C3C-C2C	-2.05	1.34	1.41
19	BL	101	V7N	C19-C18	-2.05	1.41	1.46
10	Aj	101	BCL	CHD-C1D	2.05	1.42	1.38
12	BM	102	LMT	O5'-C5'	-2.05	1.39	1.44
19	Bi	1202	V7N	C6-C5	2.05	1.40	1.35
12	BS	102	LMT	O2'-C2'	-2.05	1.37	1.43
10	Ao	101	BCL	O1A-CGA	-2.05	1.16	1.22
10	AM	101	BCL	CBD-CGD	-2.05	1.46	1.52
19	Bk	1202	V7N	C8-C9	-2.04	1.40	1.45
10	BK	102	BCL	CHD-C1D	2.04	1.42	1.38
10	Ae	101	BCL	CHD-C1D	2.04	1.42	1.38
10	Bp	1001	BCL	CBD-CGD	-2.04	1.46	1.52
10	AM	101	BCL	CHD-C1D	2.04	1.42	1.38
10	Ak	101	BCL	C1D-C2D	-2.04	1.41	1.45
10	AI	102	BCL	O1A-CGA	-2.04	1.16	1.22
19	BF	103	V7N	C11-C12	2.04	1.40	1.34
19	An	102	V7N	C19-C18	-2.04	1.41	1.46
10	AE	101	BCL	O1A-CGA	-2.04	1.16	1.22
12	BF	101	LMT	O4'-C4B	-2.04	1.37	1.43
12	AQ	102	LMT	O4'-C4B	-2.04	1.37	1.43
18	C	1001	HEC	C3B-C2B	-2.04	1.34	1.41
10	Al	101	BCL	CHD-C1D	2.04	1.42	1.38
19	Bl	102	V7N	C7-C8	2.04	1.40	1.34
10	L	301	BCL	CHD-C1D	2.04	1.42	1.38
19	An	102	V7N	C7-C8	2.04	1.40	1.34
10	Bl	101	BCL	CHD-C1D	2.03	1.42	1.38
18	C	1001	HEC	CMB-C2B	2.03	1.54	1.50
10	AT	101	BCL	CHD-C1D	2.03	1.42	1.38
19	BT	102	V7N	C7-C8	2.03	1.40	1.34
12	BK	101	LMT	O2'-C2'	-2.03	1.37	1.43
12	Bc	1204	LMT	O4'-C4B	-2.03	1.37	1.43
10	AV	1001	BCL	CHD-C1D	2.03	1.42	1.38
12	BK	103	LMT	O4'-C4B	-2.03	1.37	1.43
19	An	102	V7N	C6-C5	2.03	1.40	1.35
10	AQ	103	BCL	C1D-C2D	-2.03	1.41	1.45
10	Am	101	BCL	C1D-C2D	-2.03	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AN	101	BCL	C1D-C2D	-2.03	1.41	1.45
10	AH	101	BCL	C1D-C2D	-2.03	1.41	1.45
12	BQ	102	LMT	O4'-C4B	-2.03	1.37	1.43
10	Bh	101	BCL	C5-C3	2.03	1.55	1.51
10	AL	101	BCL	CHD-C1D	2.03	1.42	1.38
10	Bl	103	BCL	CHD-C1D	2.03	1.42	1.38
10	AT	104	BCL	C1D-C2D	-2.03	1.41	1.45
10	AQ	101	BCL	O1A-CGA	-2.03	1.16	1.22
19	BK	104	V7N	C7-C8	2.03	1.40	1.34
19	BR	103	V7N	C11-C12	2.03	1.40	1.34
19	BB	102	V7N	C11-C12	2.03	1.40	1.34
19	Bp	1003	V7N	C19-C18	-2.03	1.41	1.46
12	BR	102	LMT	O4'-C4B	-2.02	1.37	1.43
19	BD	103	V7N	C19-C18	-2.02	1.41	1.46
12	BH	101	LMT	O2B-C2B	-2.02	1.37	1.43
19	Bf	102	V7N	C7-C8	2.02	1.40	1.34
12	L	308	LMT	O4'-C4B	-2.02	1.37	1.43
12	Bo	1201	LMT	O4'-C4B	-2.02	1.38	1.43
10	AN	101	BCL	CHD-C1D	2.02	1.42	1.38
10	BC	101	BCL	C1D-C2D	-2.02	1.41	1.45
19	AT	102	V7N	C11-C12	2.02	1.39	1.34
18	C	1002	HEC	C3C-C2C	-2.02	1.34	1.41
10	Aj	101	BCL	CBD-CGD	-2.02	1.46	1.52
10	AW	101	BCL	CBD-CGD	-2.02	1.46	1.52
10	AP	102	BCL	O1A-CGA	-2.02	1.16	1.22
10	Ai	101	BCL	C1D-C2D	-2.01	1.41	1.45
10	Bd	103	BCL	CHD-C1D	2.01	1.42	1.38
10	AH	101	BCL	CHD-C1D	2.01	1.42	1.38
10	AL	101	BCL	CBD-CGD	-2.01	1.46	1.52
19	Ba	101	V7N	C7-C8	2.01	1.39	1.34
10	Bj	101	BCL	CHD-C1D	2.01	1.42	1.38
19	BK	104	V7N	C6-C5	2.01	1.40	1.35
19	Bk	1202	V7N	C11-C12	2.01	1.39	1.34
10	Bf	103	BCL	C1D-C2D	-2.01	1.41	1.45
19	AP	101	V7N	C8-C9	-2.01	1.40	1.45
10	BP	104	BCL	CBD-CGD	-2.01	1.46	1.52
10	AC	101	BCL	CHD-C1D	2.01	1.42	1.38
10	BE	102	BCL	CHD-C1D	2.01	1.42	1.38
19	Am	102	V7N	C11-C12	2.01	1.39	1.34
12	BK	101	LMT	O5'-C5'	-2.01	1.39	1.44
10	Bp	1001	BCL	CHD-C1D	2.00	1.42	1.38
10	BM	101	BCL	CHD-C1D	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Bi	1202	V7N	C19-C18	-2.00	1.41	1.46
12	BU	101	LMT	O4'-C4B	-2.00	1.38	1.43
10	Bf	101	BCL	CHD-C1D	2.00	1.42	1.38
19	BW	101	V7N	C6-C5	2.00	1.40	1.35

All (1430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	405	BPH	C4D-CHA-CBD	-10.56	103.39	108.45
11	L	303	BPH	C4D-CHA-CBD	-10.21	103.56	108.45
10	Bp	1001	BCL	C16-C15-C13	-10.07	82.49	115.97
18	C	1000	HEC	CBC-CAC-C3C	-8.74	109.96	127.43
18	C	1001	HEC	CBC-CAC-C3C	-8.38	110.69	127.43
18	C	1003	HEC	CBB-CAB-C3B	-8.23	110.99	127.43
18	C	1003	HEC	CBC-CAC-C3C	-8.16	111.12	127.43
18	C	1000	HEC	CBB-CAB-C3B	-8.14	111.17	127.43
18	C	1001	HEC	CBB-CAB-C3B	-7.89	111.67	127.43
18	C	1002	HEC	CBC-CAC-C3C	-7.89	111.67	127.43
18	C	1002	HEC	CBB-CAB-C3B	-7.60	112.25	127.43
10	Bl	101	BCL	C17-C16-C15	-7.25	80.77	113.28
10	Bl	103	BCL	C1-C2-C3	-6.99	114.75	126.20
19	AP	101	V7N	C28-C27-C26	-6.54	108.43	126.36
19	BW	101	V7N	C28-C27-C26	-6.45	108.67	126.36
10	Ac	101	BCL	C1-O2A-CGA	6.38	132.08	116.65
10	Bf	101	BCL	C16-C15-C13	6.33	137.00	115.97
10	Bh	101	BCL	C16-C15-C13	-6.04	95.88	115.97
10	Bj	101	BCL	C17-C16-C15	5.98	140.06	113.28
19	BC	103	V7N	C28-C27-C26	-5.82	110.40	126.36
10	Af	102	BCL	C1-C2-C3	5.76	135.63	126.20
10	M	404	BCL	C4D-CHA-C1A	5.73	128.08	121.24
19	Ba	101	V7N	C28-C27-C26	-5.69	110.75	126.36
10	Ao	101	BCL	C1-C2-C3	5.69	135.52	126.20
19	BB	102	V7N	C28-C27-C26	-5.68	110.80	126.36
19	BE	101	V7N	C28-C27-C26	-5.67	110.83	126.36
19	AI	101	V7N	C28-C27-C26	-5.62	110.95	126.36
19	BV	101	V7N	C28-C27-C26	-5.62	110.96	126.36
19	AT	102	V7N	C28-C27-C26	-5.55	111.14	126.36
19	BS	103	V7N	C28-C27-C26	-5.53	111.19	126.36
10	L	302	BCL	C4D-CHA-C1A	5.52	127.83	121.24
19	AX	101	V7N	C28-C27-C26	-5.49	111.31	126.36
19	BF	103	V7N	C28-C27-C26	-5.41	111.54	126.36
19	AI	103	V7N	C28-C27-C26	-5.39	111.58	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AF	102	V7N	C28-C27-C26	-5.37	111.64	126.36
10	Ao	101	BCL	C4D-CHA-C1A	5.36	127.64	121.24
19	BR	103	V7N	C28-C27-C26	-5.34	111.73	126.36
10	AQ	103	BCL	C4D-CHA-C1A	5.32	127.59	121.24
19	Bf	102	V7N	C28-C27-C26	-5.32	111.79	126.36
10	An	101	BCL	C4D-CHA-C1A	5.30	127.56	121.24
10	Af	102	BCL	C4D-CHA-C1A	5.30	127.56	121.24
10	Ak	101	BCL	C4D-CHA-C1A	5.29	127.56	121.24
10	BW	102	BCL	C1-C2-C3	-5.28	117.55	126.20
19	BD	103	V7N	C28-C27-C26	-5.27	111.91	126.36
10	AT	104	BCL	C4D-CHA-C1A	5.27	127.52	121.24
10	Am	101	BCL	C4D-CHA-C1A	5.25	127.50	121.24
10	Bd	101	BCL	C4D-CHA-C1A	5.25	127.50	121.24
10	AT	101	BCL	C4D-CHA-C1A	5.24	127.49	121.24
10	Bk	1203	BCL	C4D-CHA-C1A	5.23	127.48	121.24
10	Bg	1203	BCL	C4D-CHA-C1A	5.22	127.47	121.24
10	Ac	101	BCL	C4D-CHA-C1A	5.22	127.47	121.24
10	Bj	101	BCL	C4D-CHA-C1A	5.22	127.47	121.24
10	Be	101	BCL	C4D-CHA-C1A	5.20	127.45	121.24
19	BL	101	V7N	C28-C27-C26	-5.20	112.11	126.36
10	Ah	101	BCL	C4D-CHA-C1A	5.20	127.44	121.24
10	Aj	101	BCL	C4D-CHA-C1A	5.19	127.43	121.24
10	AO	101	BCL	C4D-CHA-C1A	5.19	127.43	121.24
10	AV	1001	BCL	C4D-CHA-C1A	5.17	127.41	121.24
10	Bc	1203	BCL	C4D-CHA-C1A	5.16	127.40	121.24
10	Bo	1202	BCL	C4D-CHA-C1A	5.16	127.40	121.24
10	BN	101	BCL	C4D-CHA-C1A	5.16	127.39	121.24
10	M	403	BCL	C4D-CHA-C1A	5.15	127.39	121.24
10	Bf	103	BCL	C4D-CHA-C1A	5.15	127.38	121.24
10	Bm	102	BCL	C4D-CHA-C1A	5.15	127.38	121.24
19	Bg	1202	V7N	C28-C27-C26	-5.15	112.25	126.36
19	AH	102	V7N	C28-C27-C26	-5.14	112.26	126.36
10	AP	102	BCL	C4D-CHA-C1A	5.14	127.38	121.24
10	Bd	103	BCL	C4D-CHA-C1A	5.13	127.36	121.24
19	BP	103	V7N	C28-C27-C26	-5.13	112.31	126.36
10	BO	102	BCL	C4D-CHA-C1A	5.12	127.35	121.24
10	BB	101	BCL	C4D-CHA-C1A	5.11	127.34	121.24
10	BD	101	BCL	C4D-CHA-C1A	5.09	127.32	121.24
10	BI	1102	BCL	C4D-CHA-C1A	5.09	127.32	121.24
10	Bp	1001	BCL	C17-C16-C15	5.09	136.07	113.28
10	AU	102	BCL	C4D-CHA-C1A	5.08	127.30	121.24
10	Ai	101	BCL	C4D-CHA-C1A	5.08	127.30	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	101	BCL	C4D-CHA-C1A	5.07	127.29	121.24
10	Bh	102	BCL	C4D-CHA-C1A	5.07	127.29	121.24
10	Bn	101	BCL	C4D-CHA-C1A	5.06	127.28	121.24
10	BK	102	BCL	C4D-CHA-C1A	5.06	127.28	121.24
10	Ae	101	BCL	C4D-CHA-C1A	5.05	127.27	121.24
19	Bc	1202	V7N	C28-C27-C26	-5.05	112.53	126.36
10	Ba	102	BCL	C4D-CHA-C1A	5.04	127.25	121.24
10	AM	101	BCL	C11-C10-C8	5.04	132.71	115.97
19	Bj	103	V7N	C28-C27-C26	-5.03	112.56	126.36
10	BR	101	BCL	C4D-CHA-C1A	5.02	127.23	121.24
10	BQ	101	BCL	C4D-CHA-C1A	5.01	127.22	121.24
10	Bl	101	BCL	C4D-CHA-C1A	5.00	127.21	121.24
19	Bk	1202	V7N	C28-C27-C26	-5.00	112.66	126.36
10	AF	101	BCL	C4D-CHA-C1A	4.99	127.20	121.24
10	BM	101	BCL	C4D-CHA-C1A	4.99	127.20	121.24
10	AD	101	BCL	C4D-CHA-C1A	4.99	127.20	121.24
10	Bh	101	BCL	C17-C16-C15	4.99	135.62	113.28
19	AL	102	V7N	C28-C27-C26	-4.98	112.70	126.36
10	Ba	102	BCL	C16-C15-C13	4.98	132.51	115.97
10	Bf	101	BCL	C16-C17-C18	4.98	138.15	115.94
10	BH	102	BCL	C4D-CHA-C1A	4.96	127.16	121.24
10	BL	102	BCL	C4D-CHA-C1A	4.96	127.16	121.24
10	AH	101	BCL	C4D-CHA-C1A	4.95	127.15	121.24
10	AI	102	BCL	C4D-CHA-C1A	4.95	127.14	121.24
10	Bl	103	BCL	C4D-CHA-C1A	4.94	127.14	121.24
10	BC	101	BCL	C4D-CHA-C1A	4.93	127.13	121.24
10	BE	102	BCL	C4D-CHA-C1A	4.93	127.13	121.24
10	Ag	101	BCL	C4D-CHA-C1A	4.93	127.12	121.24
10	Al	101	BCL	C4D-CHA-C1A	4.92	127.11	121.24
19	Ad	102	V7N	C28-C27-C26	-4.91	112.90	126.36
19	Bm	101	V7N	C28-C27-C26	-4.91	112.91	126.36
19	BO	101	V7N	C28-C27-C26	-4.91	112.91	126.36
19	BX	102	V7N	C28-C27-C26	-4.90	112.92	126.36
10	BX	103	BCL	C4D-CHA-C1A	4.89	127.08	121.24
10	BA	101	BCL	C4D-CHA-C1A	4.88	127.07	121.24
19	BT	102	V7N	C28-C27-C26	-4.88	112.98	126.36
10	BS	101	BCL	C4D-CHA-C1A	4.88	127.06	121.24
19	Am	102	V7N	C28-C27-C26	-4.86	113.04	126.36
10	Aa	101	BCL	C4D-CHA-C1A	4.85	127.03	121.24
10	BF	102	BCL	C4D-CHA-C1A	4.85	127.03	121.24
10	BJ	101	BCL	C4D-CHA-C1A	4.83	127.00	121.24
10	AE	101	BCL	C4D-CHA-C1A	4.82	127.00	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Bp	1004	BCL	C4D-CHA-C1A	4.81	126.98	121.24
10	BV	102	BCL	C4D-CHA-C1A	4.80	126.97	121.24
19	Bb	101	V7N	C28-C27-C26	-4.79	113.22	126.36
19	An	102	V7N	C28-C27-C26	-4.79	113.23	126.36
10	AW	101	BCL	C4D-CHA-C1A	4.78	126.95	121.24
10	Bp	1001	BCL	C4D-CHA-C1A	4.77	126.94	121.24
10	Bi	1203	BCL	C4D-CHA-C1A	4.77	126.94	121.24
19	BN	103	V7N	C28-C27-C26	-4.77	113.28	126.36
10	AN	101	BCL	C4D-CHA-C1A	4.76	126.92	121.24
10	AM	101	BCL	C4D-CHA-C1A	4.75	126.91	121.24
10	AX	102	BCL	C4D-CHA-C1A	4.73	126.88	121.24
19	Bd	102	V7N	C28-C27-C26	-4.70	113.47	126.36
10	AB	101	BCL	C4D-CHA-C1A	4.69	126.83	121.24
10	AR	101	BCL	C4D-CHA-C1A	4.68	126.83	121.24
19	BK	104	V7N	C28-C27-C26	-4.67	113.56	126.36
10	Bh	101	BCL	C4D-CHA-C1A	4.67	126.81	121.24
10	BT	101	BCL	C4D-CHA-C1A	4.63	126.77	121.24
19	Bp	1003	V7N	C28-C27-C26	-4.63	113.68	126.36
10	BG	102	BCL	C4D-CHA-C1A	4.62	126.75	121.24
10	AC	101	BCL	C11-C10-C8	4.60	131.27	115.97
19	BX	102	V7N	C29-C28-C27	-4.60	109.88	123.20
19	Bd	102	V7N	C29-C28-C27	-4.60	109.89	123.20
19	Bi	1202	V7N	C28-C27-C26	-4.59	113.78	126.36
10	AC	101	BCL	C4D-CHA-C1A	4.59	126.71	121.24
10	Af	102	BCL	C16-C15-C13	4.58	131.20	115.97
10	AQ	101	BCL	C4D-CHA-C1A	4.58	126.70	121.24
10	M	404	BCL	C4A-NA-C1A	4.55	108.75	106.68
10	BW	102	BCL	C4D-CHA-C1A	4.54	126.66	121.24
19	BN	103	V7N	C29-C28-C27	-4.51	110.12	123.20
10	BP	101	BCL	C4D-CHA-C1A	4.49	126.60	121.24
19	Bl	102	V7N	C28-C27-C26	-4.45	114.17	126.36
10	L	301	BCL	C4D-CHA-C1A	4.44	126.54	121.24
10	BP	104	BCL	C4D-CHA-C1A	4.43	126.52	121.24
19	BT	102	V7N	C29-C28-C27	-4.42	110.38	123.20
10	AL	101	BCL	C4D-CHA-C1A	4.40	126.49	121.24
10	BI	1102	BCL	C1-O2A-CGA	4.38	127.25	116.65
19	BR	103	V7N	C29-C28-C27	-4.36	110.56	123.20
19	BP	103	V7N	C29-C28-C27	-4.35	110.59	123.20
10	Ba	102	BCL	C1-O2A-CGA	4.34	127.16	116.65
19	BF	103	V7N	C29-C28-C27	-4.33	110.67	123.20
10	AU	102	BCL	C1D-ND-C4D	-4.29	103.30	106.31
10	Bf	101	BCL	C4D-CHA-C1A	4.26	126.32	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AR	101	BCL	C1D-ND-C4D	-4.24	103.33	106.31
10	Bd	101	BCL	C1-C2-C3	4.24	133.15	126.20
19	Bc	1202	V7N	C20-C21-C22	-4.17	121.82	127.69
10	Bn	101	BCL	C16-C15-C13	4.17	129.83	115.97
19	BE	101	V7N	C29-C28-C27	-4.17	111.11	123.20
10	AU	101	BCL	C4D-CHA-C1A	4.16	126.20	121.24
10	Bl	103	BCL	C1-O2A-CGA	4.14	126.66	116.65
19	Ag	102	V7N	C28-C27-C26	-4.10	115.12	126.36
11	L	303	BPH	C4D-ND-C1D	-4.09	103.97	108.87
19	Bm	101	V7N	C29-C28-C27	-4.09	111.35	123.20
19	AI	103	V7N	C29-C28-C27	-4.08	111.39	123.20
10	AU	102	BCL	CHD-C1D-ND	-4.07	119.08	124.80
10	AR	101	BCL	CHD-C1D-ND	-4.03	119.13	124.80
11	M	405	BPH	C4D-ND-C1D	-4.02	104.06	108.87
10	L	302	BCL	C1D-ND-C4D	-4.01	103.50	106.31
10	M	403	BCL	CHD-C1D-ND	-4.00	119.17	124.80
19	BK	104	V7N	C29-C28-C27	-4.00	111.62	123.20
19	Bb	101	V7N	C29-C28-C27	-3.98	111.66	123.20
10	BH	102	BCL	CHD-C1D-ND	-3.97	119.21	124.80
19	AH	102	V7N	C29-C28-C27	-3.96	111.72	123.20
10	AP	102	BCL	C11-C10-C8	3.96	129.12	115.97
10	M	404	BCL	CHD-C1D-ND	-3.94	119.25	124.80
19	BB	102	V7N	C29-C28-C27	-3.91	111.87	123.20
10	AQ	101	BCL	C1-C2-C3	-3.91	119.79	126.20
10	Bl	101	BCL	C4A-NA-C1A	3.89	108.45	106.68
10	BP	101	BCL	C4A-NA-C1A	3.89	108.45	106.68
10	AF	101	BCL	C4A-NA-C1A	3.88	108.45	106.68
10	Bl	101	BCL	C16-C17-C18	3.88	133.24	115.94
19	BS	103	V7N	C29-C28-C27	-3.85	112.05	123.20
19	AL	102	V7N	C29-C28-C27	-3.84	112.06	123.20
10	Ah	101	BCL	C4A-NA-C1A	3.84	108.43	106.68
19	BD	103	V7N	C29-C28-C27	-3.83	112.09	123.20
19	AT	102	V7N	C29-C28-C27	-3.83	112.09	123.20
10	L	302	BCL	CHD-C1D-ND	-3.83	119.41	124.80
19	BC	103	V7N	C29-C28-C27	-3.83	112.11	123.20
10	AW	101	BCL	C4A-NA-C1A	3.82	108.42	106.68
10	AH	101	BCL	C4A-NA-C1A	3.82	108.42	106.68
10	Bd	101	BCL	C4A-NA-C1A	3.82	108.42	106.68
10	Ac	101	BCL	C4A-NA-C1A	3.82	108.42	106.68
10	AQ	101	BCL	C16-C15-C13	3.82	128.66	115.97
19	AF	102	V7N	C29-C28-C27	-3.81	112.16	123.20
10	Ae	101	BCL	C4A-NA-C1A	3.81	108.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	1001	HEC	C4D-ND-C1D	3.81	112.03	105.82
19	AI	101	V7N	C29-C28-C27	-3.81	112.17	123.20
18	C	1003	HEC	C4D-ND-C1D	3.79	112.00	105.82
19	An	102	V7N	C29-C28-C27	-3.79	112.22	123.20
10	Ak	101	BCL	C1-C2-C3	-3.79	119.99	126.20
19	Bk	1202	V7N	C20-C21-C22	-3.78	122.37	127.69
10	AM	101	BCL	C4A-NA-C1A	3.78	108.40	106.68
19	BO	101	V7N	C29-C28-C27	-3.77	112.29	123.20
10	Aj	101	BCL	C4A-NA-C1A	3.77	108.40	106.68
19	BL	101	V7N	C2-C3-C4	-3.75	119.64	124.91
10	AN	101	BCL	C4A-NA-C1A	3.75	108.39	106.68
10	BI	1102	BCL	CHD-C1D-ND	-3.74	119.54	124.80
10	Af	102	BCL	C4A-NA-C1A	3.73	108.38	106.68
19	BV	101	V7N	C29-C28-C27	-3.73	112.38	123.20
10	L	301	BCL	CHD-C1D-ND	-3.73	119.55	124.80
10	Ba	102	BCL	C17-C16-C15	3.73	129.97	113.28
10	M	403	BCL	C1D-ND-C4D	-3.73	103.70	106.31
10	AX	102	BCL	C4A-NA-C1A	3.72	108.38	106.68
10	Bh	101	BCL	C4A-NA-C1A	3.72	108.38	106.68
19	Bp	1003	V7N	C29-C28-C27	-3.72	112.42	123.20
10	Ag	101	BCL	C1D-ND-C4D	-3.72	103.70	106.31
10	AI	102	BCL	C4A-NA-C1A	3.71	108.37	106.68
19	Bi	1202	V7N	C2-C3-C4	-3.70	119.71	124.91
10	Bp	1001	BCL	C4A-NA-C1A	3.70	108.37	106.68
10	BP	104	BCL	CED-O2D-CGD	3.70	124.31	115.92
19	BB	102	V7N	C20-C21-C22	-3.70	122.49	127.69
10	AE	101	BCL	C4A-NA-C1A	3.70	108.37	106.68
10	Bn	101	BCL	C17-C16-C15	3.70	129.85	113.28
18	C	1002	HEC	C4D-ND-C1D	3.70	111.85	105.82
19	AP	101	V7N	C35-C13-C12	3.70	123.73	118.09
10	AQ	103	BCL	C4A-NA-C1A	3.69	108.36	106.68
10	BH	102	BCL	C1-C2-C3	-3.69	120.16	126.20
10	Am	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
10	BQ	101	BCL	CHD-C1D-ND	-3.68	119.62	124.80
19	Bc	1202	V7N	C29-C28-C27	-3.68	112.54	123.20
10	BS	101	BCL	CHD-C1D-ND	-3.68	119.63	124.80
10	Bo	1202	BCL	CHD-C1D-ND	-3.67	119.63	124.80
19	Bg	1202	V7N	C20-C21-C22	-3.67	122.53	127.69
10	AT	101	BCL	C4A-NA-C1A	3.67	108.35	106.68
10	Ba	102	BCL	C4A-NA-C1A	3.67	108.35	106.68
19	Bj	103	V7N	C29-C28-C27	-3.67	112.57	123.20
10	AO	101	BCL	C1D-ND-C4D	-3.66	103.74	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Bf	102	V7N	C29-C28-C27	-3.66	112.60	123.20
10	AO	101	BCL	C4A-NA-C1A	3.66	108.35	106.68
10	AQ	101	BCL	C4A-NA-C1A	3.66	108.35	106.68
10	BX	103	BCL	CHD-C1D-ND	-3.65	119.66	124.80
19	Bg	1202	V7N	C29-C28-C27	-3.65	112.64	123.20
10	BH	102	BCL	C4A-NA-C1A	3.63	108.34	106.68
10	AK	101	BCL	C4A-NA-C1A	3.63	108.34	106.68
10	Aa	101	BCL	CHD-C1D-ND	-3.63	119.69	124.80
10	Bk	1203	BCL	CHD-C1D-ND	-3.63	119.69	124.80
19	Bg	1202	V7N	C2-C3-C4	-3.63	119.82	124.91
10	Ai	101	BCL	C4A-NA-C1A	3.62	108.33	106.68
10	Ao	101	BCL	C4A-NA-C1A	3.62	108.33	106.68
10	Al	101	BCL	C4A-NA-C1A	3.62	108.33	106.68
10	Am	101	BCL	CHD-C1D-ND	-3.62	119.71	124.80
10	BV	102	BCL	CHD-C1D-ND	-3.61	119.72	124.80
19	Bl	102	V7N	C29-C28-C27	-3.61	112.74	123.20
10	BO	102	BCL	CHD-C1D-ND	-3.61	119.72	124.80
19	Bd	102	V7N	C7-C6-C5	-3.61	122.21	127.28
10	Ak	101	BCL	C1D-ND-C4D	-3.61	103.78	106.31
10	Bn	101	BCL	CHD-C1D-ND	-3.60	119.73	124.80
10	AL	101	BCL	C4A-NA-C1A	3.60	108.32	106.68
19	BL	101	V7N	C29-C28-C27	-3.60	112.77	123.20
10	BP	104	BCL	C4A-NA-C1A	3.60	108.32	106.68
10	AT	104	BCL	CHD-C1D-ND	-3.60	119.74	124.80
10	Bf	101	BCL	C4A-NA-C1A	3.59	108.32	106.68
10	M	404	BCL	C1D-ND-C4D	-3.59	103.79	106.31
10	BJ	101	BCL	CHD-C1D-ND	-3.59	119.74	124.80
10	Bd	101	BCL	C1D-ND-C4D	-3.59	103.79	106.31
19	Bk	1202	V7N	C29-C28-C27	-3.59	112.81	123.20
10	BP	104	BCL	C1D-ND-C4D	-3.58	103.80	106.31
10	Ao	101	BCL	CHD-C1D-ND	-3.58	119.76	124.80
19	AI	101	V7N	C2-C3-C4	-3.58	119.89	124.91
10	Aj	101	BCL	CHD-C1D-ND	-3.57	119.78	124.80
10	Ag	101	BCL	CHD-C1D-ND	-3.57	119.78	124.80
10	Be	101	BCL	CHD-C1D-ND	-3.57	119.78	124.80
19	Bg	1202	V7N	C7-C6-C5	-3.56	122.28	127.28
10	AV	1001	BCL	C4A-NA-C1A	3.56	108.30	106.68
10	BX	103	BCL	C4A-NA-C1A	3.56	108.30	106.68
10	Al	101	BCL	C1D-ND-C4D	-3.55	103.82	106.31
10	An	101	BCL	C1D-ND-C4D	-3.55	103.82	106.31
10	Af	102	BCL	C1D-ND-C4D	-3.55	103.82	106.31
10	AC	101	BCL	C4A-NA-C1A	3.55	108.30	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BB	101	BCL	CHD-C1D-ND	-3.55	119.81	124.80
19	BO	101	V7N	C35-C13-C12	3.55	123.51	118.09
11	L	303	BPH	C3D-C4D-ND	3.55	112.26	107.71
10	BL	102	BCL	CHD-C1D-ND	-3.55	119.81	124.80
10	Bd	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
10	Ae	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
10	AQ	103	BCL	C1D-ND-C4D	-3.53	103.83	106.31
19	Am	102	V7N	C29-C28-C27	-3.53	112.98	123.20
10	BR	101	BCL	CHD-C1D-ND	-3.53	119.84	124.80
10	Bg	1203	BCL	CHD-C1D-ND	-3.52	119.84	124.80
10	BA	101	BCL	CHD-C1D-ND	-3.52	119.85	124.80
10	AT	104	BCL	C1D-ND-C4D	-3.52	103.84	106.31
19	Bi	1202	V7N	C29-C28-C27	-3.52	113.00	123.20
10	BN	101	BCL	CHD-C1D-ND	-3.51	119.86	124.80
10	An	101	BCL	CHD-C1D-ND	-3.51	119.86	124.80
10	Bj	101	BCL	C4A-NA-C1A	3.51	108.28	106.68
10	BD	101	BCL	CHD-C1D-ND	-3.51	119.86	124.80
10	AT	101	BCL	C1D-ND-C4D	-3.51	103.85	106.31
10	Ae	101	BCL	C1D-ND-C4D	-3.51	103.85	106.31
10	Bj	101	BCL	CHD-C1D-ND	-3.51	119.86	124.80
10	Ak	101	BCL	CHD-C1D-ND	-3.51	119.87	124.80
19	Bd	102	V7N	C2-C3-C4	-3.51	119.99	124.91
10	Aa	101	BCL	C1D-ND-C4D	-3.50	103.86	106.31
19	Ba	101	V7N	C2-C3-C4	-3.50	120.00	124.91
10	Af	102	BCL	CHD-C1D-ND	-3.50	119.88	124.80
19	BV	101	V7N	C35-C13-C12	3.49	123.42	118.09
10	BC	101	BCL	CHD-C1D-ND	-3.49	119.89	124.80
10	Bi	1203	BCL	CHD-C1D-ND	-3.49	119.89	124.80
10	Ai	101	BCL	C1D-ND-C4D	-3.49	103.86	106.31
10	Al	101	BCL	CHD-C1D-ND	-3.49	119.89	124.80
10	Bh	102	BCL	CHD-C1D-ND	-3.49	119.89	124.80
10	Ac	101	BCL	C1D-ND-C4D	-3.49	103.86	106.31
10	BG	102	BCL	CHD-C1D-ND	-3.49	119.89	124.80
10	Ba	102	BCL	CHD-C1D-ND	-3.48	119.90	124.80
10	BT	101	BCL	CHD-C1D-ND	-3.48	119.91	124.80
10	BF	102	BCL	CHD-C1D-ND	-3.48	119.91	124.80
10	BP	101	BCL	CHD-C1D-ND	-3.48	119.91	124.80
10	Bf	103	BCL	CHD-C1D-ND	-3.48	119.91	124.80
10	Bp	1004	BCL	CHD-C1D-ND	-3.48	119.91	124.80
10	BK	102	BCL	CHD-C1D-ND	-3.47	119.91	124.80
10	L	301	BCL	C1D-ND-C4D	-3.47	103.88	106.31
10	AU	101	BCL	C1D-ND-C4D	-3.47	103.88	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Ao	101	BCL	C1D-ND-C4D	-3.47	103.88	106.31
10	BX	103	BCL	C17-C16-C15	3.47	128.84	113.28
10	AU	101	BCL	CHD-C1D-ND	-3.47	119.92	124.80
19	AX	101	V7N	C2-C3-C4	-3.47	120.04	124.91
10	Aj	101	BCL	C1D-ND-C4D	-3.47	103.88	106.31
19	Ag	102	V7N	O44-C40-O45	-3.47	115.65	123.90
19	Bj	103	V7N	C7-C6-C5	-3.47	122.42	127.28
10	BW	102	BCL	C4A-NA-C1A	3.47	108.26	106.68
11	M	405	BPH	C3D-C4D-ND	3.46	112.15	107.71
18	C	1000	HEC	C4D-ND-C1D	3.46	111.47	105.82
10	Aa	101	BCL	C2A-C1A-CHA	3.46	129.87	123.87
10	Bc	1203	BCL	CHD-C1D-ND	-3.46	119.93	124.80
10	Bf	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
10	Bf	101	BCL	CHD-C1D-ND	-3.45	119.94	124.80
10	Am	101	BCL	C4A-NA-C1A	3.45	108.25	106.68
10	An	101	BCL	C4A-NA-C1A	3.45	108.25	106.68
10	Bj	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
10	AD	101	BCL	CHD-C1D-ND	-3.45	119.94	124.80
10	AB	101	BCL	CHD-C1D-ND	-3.45	119.95	124.80
19	Ad	102	V7N	C2-C3-C4	-3.45	120.07	124.91
10	AE	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
19	BE	101	V7N	C7-C6-C5	-3.45	122.45	127.28
12	L	308	LMT	C3'-C4'-C5'	-3.44	103.29	110.93
10	Bp	1001	BCL	CHD-C1D-ND	-3.44	119.95	124.80
10	AO	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
10	Bm	102	BCL	CHD-C1D-ND	-3.44	119.96	124.80
19	AX	101	V7N	C29-C28-C27	-3.44	113.22	123.20
10	BR	101	BCL	C1D-ND-C4D	-3.44	103.90	106.31
19	BF	103	V7N	C2-C3-C4	-3.44	120.08	124.91
10	AT	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
10	Bl	103	BCL	CHD-C1D-ND	-3.44	119.97	124.80
10	AW	101	BCL	CHD-C1D-ND	-3.43	119.98	124.80
10	BM	101	BCL	CHD-C1D-ND	-3.43	119.98	124.80
10	AQ	103	BCL	CHD-C1D-ND	-3.43	119.98	124.80
10	Bd	103	BCL	CHD-C1D-ND	-3.43	119.98	124.80
19	BX	102	V7N	C7-C6-C5	-3.42	122.47	127.28
10	AW	101	BCL	C1D-ND-C4D	-3.42	103.91	106.31
10	Bh	102	BCL	C1-C2-C3	-3.42	120.59	126.20
10	Ai	101	BCL	CHD-C1D-ND	-3.42	119.99	124.80
10	Ac	101	BCL	CHD-C1D-ND	-3.41	120.00	124.80
10	BG	102	BCL	C1D-ND-C4D	-3.41	103.92	106.31
10	BX	103	BCL	C1D-ND-C4D	-3.41	103.92	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AX	102	BCL	CHD-C1D-ND	-3.41	120.01	124.80
10	Bl	101	BCL	CHD-C1D-ND	-3.41	120.01	124.80
19	Ba	101	V7N	C29-C28-C27	-3.40	113.34	123.20
10	Ah	101	BCL	C1D-ND-C4D	-3.40	103.93	106.31
10	BL	102	BCL	C4A-NA-C1A	3.40	108.23	106.68
10	AI	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
10	BW	102	BCL	C1D-ND-C4D	-3.40	103.93	106.31
10	AL	101	BCL	CHD-C1D-ND	-3.40	120.02	124.80
19	Ad	102	V7N	C29-C28-C27	-3.40	113.36	123.20
19	BT	102	V7N	C35-C13-C12	3.40	123.28	118.09
10	BE	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
10	AU	101	BCL	C1-C2-C3	-3.39	120.64	126.20
10	Bl	101	BCL	C6-C5-C3	3.39	121.74	113.47
10	AT	104	BCL	C4A-NA-C1A	3.39	108.23	106.68
10	Ba	102	BCL	C1D-ND-C4D	-3.39	103.93	106.31
10	Ah	101	BCL	CHD-C1D-ND	-3.39	120.03	124.80
10	BS	101	BCL	C1D-ND-C4D	-3.39	103.94	106.31
10	BL	102	BCL	C1D-ND-C4D	-3.38	103.94	106.31
10	BQ	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
10	AC	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
10	AV	1001	BCL	CHD-C1D-ND	-3.38	120.04	124.80
10	AM	101	BCL	CHD-C1D-ND	-3.38	120.05	124.80
10	BP	104	BCL	CHD-C1D-ND	-3.38	120.05	124.80
10	Bh	101	BCL	CHD-C1D-ND	-3.38	120.05	124.80
10	BO	102	BCL	C1D-ND-C4D	-3.38	103.94	106.31
10	BI	1102	BCL	C1D-ND-C4D	-3.38	103.94	106.31
10	BJ	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
19	BK	104	V7N	C7-C6-C5	-3.38	122.54	127.28
10	Bp	1001	BCL	C1D-ND-C4D	-3.37	103.94	106.31
19	BX	102	V7N	O44-C40-O45	-3.37	115.87	123.90
10	AV	1001	BCL	C1D-ND-C4D	-3.37	103.95	106.31
10	BW	102	BCL	CHD-C1D-ND	-3.37	120.06	124.80
10	AE	101	BCL	CHD-C1D-ND	-3.36	120.07	124.80
10	BP	101	BCL	C1D-ND-C4D	-3.36	103.95	106.31
10	Bo	1202	BCL	C1D-ND-C4D	-3.36	103.95	106.31
10	Bm	102	BCL	C1D-ND-C4D	-3.36	103.95	106.31
19	Bd	102	V7N	C35-C13-C12	3.36	123.22	118.09
10	AC	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
10	AN	101	BCL	CHD-C1D-ND	-3.35	120.08	124.80
10	AX	102	BCL	C1D-ND-C4D	-3.35	103.96	106.31
10	AK	101	BCL	CHD-C1D-ND	-3.35	120.09	124.80
10	AQ	101	BCL	CHD-C1D-ND	-3.35	120.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Bm	101	V7N	C35-C13-C12	3.35	123.20	118.09
10	AP	102	BCL	CHD-C1D-ND	-3.34	120.10	124.80
10	Bd	103	BCL	C1D-ND-C4D	-3.34	103.97	106.31
10	AF	101	BCL	CHD-C1D-ND	-3.34	120.11	124.80
19	AT	102	V7N	C35-C13-C12	3.34	123.18	118.09
10	BK	102	BCL	C1D-ND-C4D	-3.33	103.97	106.31
19	Bb	101	V7N	C20-C21-C22	-3.33	123.00	127.69
10	BI	1102	BCL	C4A-NA-C1A	3.33	108.20	106.68
10	Bc	1203	BCL	C1D-ND-C4D	-3.33	103.98	106.31
10	Bn	101	BCL	C1D-ND-C4D	-3.33	103.98	106.31
10	AF	101	BCL	C1D-ND-C4D	-3.33	103.98	106.31
10	AD	101	BCL	C1D-ND-C4D	-3.32	103.98	106.31
10	AH	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
10	AU	102	BCL	CHA-C1A-NA	-3.32	118.87	126.39
19	BC	103	V7N	C35-C13-C12	3.32	123.16	118.09
10	BT	101	BCL	C1D-ND-C4D	-3.32	103.98	106.31
19	AI	103	V7N	C35-C13-C12	3.32	123.16	118.09
10	Be	101	BCL	C1D-ND-C4D	-3.32	103.98	106.31
10	BC	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	BR	101	BCL	C4A-NA-C1A	3.31	108.19	106.68
10	AL	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	AN	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	AM	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	BF	102	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	AI	102	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	Bk	1203	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	AB	101	BCL	C1D-ND-C4D	-3.31	103.99	106.31
10	AP	102	BCL	C1D-ND-C4D	-3.30	103.99	106.31
10	AE	101	BCL	CHA-C1A-NA	-3.30	118.92	126.39
19	Bm	101	V7N	C2-C3-C4	-3.30	120.28	124.91
10	BN	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31
10	AQ	101	BCL	C1D-ND-C4D	-3.29	104.00	106.31
19	AI	103	V7N	C2-C3-C4	-3.29	120.29	124.91
19	Bf	102	V7N	C15-C14-C13	-3.29	122.67	127.28
10	AH	101	BCL	C1D-ND-C4D	-3.29	104.01	106.31
10	Bh	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	BI	1102	BCL	C16-C15-C13	3.28	126.87	115.97
19	Bb	101	V7N	C2-C3-C4	-3.28	120.31	124.91
10	BE	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	Bl	101	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	Bf	103	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	Ac	101	BCL	CHA-C1A-NA	-3.28	118.97	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Bl	103	BCL	C1D-ND-C4D	-3.28	104.01	106.31
19	BP	103	V7N	C20-C21-C22	-3.28	123.08	127.69
10	BB	101	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	Bi	1203	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	AC	101	BCL	C1-C2-C3	3.27	131.55	126.20
10	AI	102	BCL	CHA-C1A-NA	-3.27	118.99	126.39
19	BK	104	V7N	O44-C40-O45	-3.27	116.12	123.90
10	L	302	BCL	CHA-C1A-NA	-3.26	119.00	126.39
10	AK	101	BCL	CHA-C1A-NA	-3.26	119.00	126.39
10	AT	104	BCL	C17-C16-C15	3.26	127.89	113.28
10	BA	101	BCL	C1D-ND-C4D	-3.26	104.03	106.31
10	AK	101	BCL	C1D-ND-C4D	-3.26	104.03	106.31
10	Bd	101	BCL	C16-C15-C13	3.26	126.79	115.97
10	Bl	103	BCL	C4A-NA-C1A	3.26	108.17	106.68
10	Bp	1004	BCL	C1D-ND-C4D	-3.26	104.03	106.31
19	AL	102	V7N	O44-C40-O45	-3.26	116.15	123.90
10	AK	101	BCL	C17-C16-C15	3.26	127.86	113.28
10	BW	102	BCL	C1-O2A-CGA	3.25	124.53	116.65
10	BV	102	BCL	C4A-NA-C1A	3.25	108.16	106.68
19	BV	101	V7N	O44-C40-O45	-3.25	116.17	123.90
10	BD	101	BCL	C1D-ND-C4D	-3.25	104.03	106.31
10	BV	102	BCL	C1D-ND-C4D	-3.24	104.04	106.31
10	BH	102	BCL	C1D-ND-C4D	-3.24	104.04	106.31
10	AB	101	BCL	C4A-NA-C1A	3.24	108.16	106.68
19	Bf	102	V7N	O44-C40-O45	-3.23	116.20	123.90
10	AV	1001	BCL	CHA-C1A-NA	-3.23	119.08	126.39
10	Ag	101	BCL	C4A-NA-C1A	3.22	108.15	106.68
19	AF	102	V7N	C35-C13-C12	3.22	123.01	118.09
10	Bj	101	BCL	C6-C7-C8	-3.22	105.27	115.97
10	BM	101	BCL	C1D-ND-C4D	-3.22	104.05	106.31
10	BM	101	BCL	C2A-C1A-CHA	3.22	129.45	123.87
10	AE	101	BCL	C17-C16-C15	3.22	127.69	113.28
10	AX	102	BCL	CHA-C1A-NA	-3.22	119.11	126.39
10	AH	101	BCL	CHA-C1A-NA	-3.21	119.11	126.39
10	Bh	101	BCL	C1D-ND-C4D	-3.21	104.06	106.31
10	Ag	101	BCL	CHA-C1A-NA	-3.21	119.12	126.39
11	M	405	BPH	OBD-CAD-CBD	-3.21	121.11	125.82
10	AM	101	BCL	CHA-C1A-NA	-3.21	119.13	126.39
19	Bb	101	V7N	C35-C13-C12	3.20	122.97	118.09
10	AR	101	BCL	CHA-C1A-NA	-3.19	119.16	126.39
12	Bi	1201	LMT	C1'-O5'-C5'	-3.18	107.50	113.72
19	BD	103	V7N	C35-C13-C12	3.18	122.95	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Bp	1004	BCL	C17-C16-C15	3.18	127.54	113.28
10	Ah	101	BCL	CHA-C1A-NA	-3.18	119.19	126.39
19	AT	102	V7N	O44-C40-O45	-3.17	116.34	123.90
19	Bi	1202	V7N	O44-C40-O45	-3.17	116.34	123.90
19	AX	101	V7N	O44-C40-O45	-3.17	116.35	123.90
12	Bm	104	LMT	C3'-C4'-C5'	-3.17	103.91	110.93
11	L	303	BPH	OBD-CAD-CBD	-3.17	121.17	125.82
19	Ad	102	V7N	O44-C40-O45	-3.17	116.36	123.90
10	AP	102	BCL	C4A-NA-C1A	3.17	108.12	106.68
10	AN	101	BCL	CHA-C1A-NA	-3.16	119.22	126.39
19	Bl	102	V7N	O44-C40-O45	-3.16	116.37	123.90
19	BF	103	V7N	O44-C40-O45	-3.16	116.37	123.90
19	BO	101	V7N	O44-C40-O45	-3.16	116.37	123.90
10	Bf	101	BCL	CHA-C1A-NA	-3.16	119.23	126.39
10	Bg	1203	BCL	C1D-ND-C4D	-3.16	104.09	106.31
19	Ba	101	V7N	O44-C40-O45	-3.16	116.37	123.90
19	AP	101	V7N	C27-C26-C25	3.16	122.89	118.49
19	AP	101	V7N	O44-C40-O45	-3.16	116.38	123.90
12	BH	101	LMT	C3'-C4'-C5'	-3.16	103.93	110.93
19	BF	103	V7N	C35-C13-C12	3.15	122.91	118.09
10	Af	102	BCL	CHA-C1A-NA	-3.15	119.26	126.39
19	AX	101	V7N	C35-C13-C12	3.15	122.90	118.09
10	AF	101	BCL	CHA-C1A-NA	-3.15	119.27	126.39
19	AH	102	V7N	C35-C13-C12	3.15	122.89	118.09
19	Bj	103	V7N	C35-C13-C12	3.14	122.89	118.09
19	BO	101	V7N	C2-C3-C4	-3.14	120.50	124.91
19	Bc	1202	V7N	O44-C40-O45	-3.14	116.42	123.90
10	AC	101	BCL	CHA-C1A-NA	-3.14	119.28	126.39
10	An	101	BCL	CHA-C1A-NA	-3.14	119.28	126.39
10	Bp	1004	BCL	CHA-C1A-NA	-3.14	119.29	126.39
19	An	102	V7N	O44-C40-O45	-3.14	116.43	123.90
10	AL	101	BCL	C1-C2-C3	-3.13	121.06	126.20
19	Bi	1202	V7N	C35-C13-C12	3.13	122.87	118.09
19	BS	103	V7N	C35-C13-C12	3.13	122.87	118.09
10	Ak	101	BCL	CHA-C1A-NA	-3.13	119.31	126.39
19	Bd	102	V7N	O44-C40-O45	-3.13	116.45	123.90
19	Ba	101	V7N	C7-C6-C5	-3.13	122.89	127.28
10	Bd	103	BCL	CHA-C1A-NA	-3.12	119.32	126.39
19	Bm	101	V7N	O44-C40-O45	-3.12	116.46	123.90
19	BW	101	V7N	O44-C40-O45	-3.12	116.47	123.90
19	Bk	1202	V7N	C35-C13-C12	3.12	122.85	118.09
10	Al	101	BCL	CHA-C1A-NA	-3.12	119.33	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AO	101	BCL	CHA-C1A-NA	-3.12	119.33	126.39
19	BR	103	V7N	C35-C13-C12	3.11	122.84	118.09
10	Bp	1001	BCL	CHA-C1A-NA	-3.11	119.34	126.39
10	BB	101	BCL	C4A-NA-C1A	3.11	108.10	106.68
10	M	404	BCL	CHA-C1A-NA	-3.11	119.35	126.39
10	AT	104	BCL	CHA-C1A-NA	-3.11	119.35	126.39
10	BM	101	BCL	CHA-C1A-NA	-3.11	119.35	126.39
19	BO	101	V7N	C33-C5-C4	3.11	122.84	118.09
19	BL	101	V7N	C35-C13-C12	3.10	122.83	118.09
19	Bg	1202	V7N	O44-C40-O45	-3.10	116.51	123.90
10	AQ	103	BCL	CHA-C1A-NA	-3.10	119.37	126.39
19	AI	101	V7N	O44-C40-O45	-3.10	116.52	123.90
10	Bl	101	BCL	CHA-C1A-NA	-3.10	119.37	126.39
19	BL	101	V7N	O44-C40-O45	-3.10	116.52	123.90
12	M	407	LMT	C1'-O5'-C5'	-3.10	107.67	113.72
19	BD	103	V7N	O44-C40-O45	-3.10	116.53	123.90
19	AF	102	V7N	O44-C40-O45	-3.10	116.53	123.90
19	BC	103	V7N	O44-C40-O45	-3.09	116.53	123.90
19	BW	101	V7N	C20-C21-C22	-3.09	123.34	127.69
10	AO	101	BCL	C11-C10-C8	-3.09	105.69	115.97
19	BE	101	V7N	C2-C3-C4	-3.09	120.58	124.91
12	BR	102	LMT	C3'-C4'-C5'	-3.09	104.09	110.93
10	Bh	101	BCL	C6-C5-C3	3.09	120.99	113.47
19	Ad	102	V7N	C36-C18-C19	3.08	122.80	118.09
19	BB	102	V7N	O44-C40-O45	-3.08	116.56	123.90
10	Bi	1203	BCL	CHA-C1A-NA	-3.08	119.42	126.39
10	BT	101	BCL	C2A-C1A-CHA	3.08	129.21	123.87
10	AV	1001	BCL	C2A-C1A-CHA	3.08	129.21	123.87
19	Am	102	V7N	C27-C26-C25	3.08	122.78	118.49
19	Bb	101	V7N	O44-C40-O45	-3.08	116.58	123.90
19	BP	103	V7N	O44-C40-O45	-3.07	116.58	123.90
19	BT	102	V7N	O44-C40-O45	-3.07	116.58	123.90
10	Bh	101	BCL	CHA-C1A-NA	-3.07	119.43	126.39
19	BS	103	V7N	O44-C40-O45	-3.07	116.59	123.90
10	Bg	1203	BCL	CHA-C1A-NA	-3.07	119.44	126.39
10	BB	101	BCL	CHA-C1A-NA	-3.07	119.44	126.39
10	BF	102	BCL	C2A-C1A-CHA	3.07	129.19	123.87
10	Ag	101	BCL	C6-C7-C8	3.07	126.16	115.97
10	BO	102	BCL	C4A-NA-C1A	3.07	108.08	106.68
10	BF	102	BCL	CHA-C1A-NA	-3.06	119.45	126.39
19	BB	102	V7N	C35-C13-C12	3.06	122.77	118.09
10	BS	101	BCL	CHA-C1A-NA	-3.06	119.46	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Bp	1003	V7N	O44-C40-O45	-3.06	116.61	123.90
19	AI	103	V7N	O44-C40-O45	-3.06	116.61	123.90
10	Aa	101	BCL	CHA-C1A-NA	-3.06	119.46	126.39
10	AT	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
19	BE	101	V7N	O44-C40-O45	-3.05	116.63	123.90
10	BT	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
10	Ao	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
10	AW	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
19	AT	102	V7N	C33-C5-C4	3.05	122.75	118.09
19	BE	101	V7N	C35-C13-C12	3.05	122.74	118.09
10	Bc	1203	BCL	CHA-C1A-NA	-3.05	119.49	126.39
12	Bk	1201	LMT	O5B-C5B-C4B	3.05	115.19	109.70
10	Bh	102	BCL	CHA-C1A-NA	-3.05	119.50	126.39
19	BN	103	V7N	O44-C40-O45	-3.05	116.65	123.90
10	BQ	101	BCL	CHA-C1A-NA	-3.04	119.50	126.39
13	L	310	MQ8	C11-C3-C2	-3.04	119.67	124.89
10	BE	102	BCL	C4A-NA-C1A	3.04	108.07	106.68
10	AI	102	BCL	C11-C10-C8	-3.04	105.86	115.97
10	AL	101	BCL	CHA-C1A-NA	-3.04	119.51	126.39
10	Aj	101	BCL	CHA-C1A-NA	-3.03	119.52	126.39
10	Ai	101	BCL	CHA-C1A-NA	-3.03	119.52	126.39
19	Bj	103	V7N	O44-C40-O45	-3.03	116.68	123.90
10	Bk	1203	BCL	CHA-C1A-NA	-3.03	119.53	126.39
10	AD	101	BCL	CHA-C1A-NA	-3.03	119.53	126.39
10	AU	101	BCL	CED-O2D-CGD	3.03	122.79	115.92
10	Bj	101	BCL	CHA-C1A-NA	-3.03	119.53	126.39
10	BX	103	BCL	C1-C2-C3	-3.03	121.24	126.20
19	Bl	102	V7N	C20-C21-C22	-3.03	123.44	127.69
10	AU	101	BCL	C4A-NA-C1A	3.02	108.06	106.68
10	Bm	102	BCL	C4A-NA-C1A	3.02	108.06	106.68
10	BP	101	BCL	CHA-C1A-NA	-3.02	119.54	126.39
10	BC	101	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	AQ	101	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	Bd	101	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	AB	101	BCL	CHA-C1A-NA	-3.02	119.56	126.39
10	AP	102	BCL	CHA-C1A-NA	-3.01	119.57	126.39
19	Bl	102	V7N	C35-C13-C12	3.01	122.69	118.09
10	Bl	103	BCL	CHA-C1A-NA	-3.01	119.57	126.39
19	AI	103	V7N	C20-C21-C22	-3.01	123.46	127.69
10	L	301	BCL	C11-C10-C8	3.01	125.97	115.97
10	Bk	1203	BCL	C4A-NA-C1A	3.01	108.05	106.68
10	Bn	101	BCL	CHA-C1A-NA	-3.01	119.58	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AT	102	V7N	C2-C3-C4	-3.01	120.69	124.91
10	Bg	1203	BCL	C17-C16-C15	3.00	126.73	113.28
10	Bf	103	BCL	CHA-C1A-NA	-3.00	119.59	126.39
10	Bo	1202	BCL	CHA-C1A-NA	-3.00	119.60	126.39
10	Bc	1203	BCL	C4A-NA-C1A	3.00	108.05	106.68
19	Ba	101	V7N	C35-C13-C12	3.00	122.67	118.09
12	L	309	LMT	C3'-C4'-C5'	-3.00	104.29	110.93
19	Am	102	V7N	C35-C13-C12	2.99	122.66	118.09
19	Bg	1202	V7N	C35-C13-C12	2.99	122.65	118.09
10	BG	102	BCL	CHA-C1A-NA	-2.99	119.63	126.39
10	BD	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	Be	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
19	AH	102	V7N	O44-C40-O45	-2.98	116.80	123.90
19	AI	101	V7N	C35-C13-C12	2.98	122.64	118.09
10	BA	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	BN	101	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	BH	102	BCL	C1-O2A-CGA	2.98	123.86	116.65
19	Bp	1003	V7N	C2-C3-C4	-2.98	120.73	124.91
10	Am	101	BCL	CHA-C1A-NA	-2.98	119.65	126.39
19	Bk	1202	V7N	O44-C40-O45	-2.98	116.81	123.90
10	M	403	BCL	C2A-C1A-CHA	2.98	129.03	123.87
10	BC	101	BCL	C4A-NA-C1A	2.97	108.03	106.68
10	Bm	102	BCL	CHA-C1A-NA	-2.97	119.67	126.39
19	BN	103	V7N	C2-C3-C4	-2.96	120.75	124.91
10	BM	101	BCL	C4A-NA-C1A	2.96	108.03	106.68
19	BN	103	V7N	C35-C13-C12	2.96	122.61	118.09
10	BJ	101	BCL	CHA-C1A-NA	-2.96	119.69	126.39
10	BK	102	BCL	CHA-C1A-NA	-2.96	119.69	126.39
10	BV	102	BCL	CHA-C1A-NA	-2.96	119.70	126.39
19	BC	103	V7N	C33-C5-C4	2.95	122.59	118.09
10	BK	102	BCL	C4A-NA-C1A	2.95	108.03	106.68
10	Ae	101	BCL	CHA-C1A-NA	-2.95	119.71	126.39
10	BC	101	BCL	C2A-C1A-CHA	2.95	128.98	123.87
10	Ba	102	BCL	CHA-C1A-NA	-2.95	119.72	126.39
10	AD	101	BCL	C4A-NA-C1A	2.95	108.02	106.68
19	Am	102	V7N	C2-C3-C4	-2.94	120.78	124.91
10	BO	102	BCL	CHA-C1A-NA	-2.94	119.72	126.39
19	Bj	103	V7N	C2-C3-C4	-2.94	120.78	124.91
10	Be	101	BCL	C4A-NA-C1A	2.94	108.02	106.68
19	BE	101	V7N	C20-C21-C22	-2.93	123.57	127.69
10	Bd	101	BCL	C11-C10-C8	-2.93	106.23	115.97
10	M	403	BCL	C4A-NA-C1A	2.93	108.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BI	1102	BCL	CHA-C1A-NA	-2.92	119.77	126.39
10	M	403	BCL	CHA-C1A-NA	-2.92	119.78	126.39
10	BG	102	BCL	C2A-C1A-CHA	2.92	128.94	123.87
19	BR	103	V7N	O44-C40-O45	-2.92	116.95	123.90
19	Bc	1202	V7N	C35-C13-C12	2.91	122.53	118.09
13	Ad	101	MQ8	C11-C3-C2	-2.91	119.91	124.89
19	Am	102	V7N	O44-C40-O45	-2.91	116.98	123.90
10	BE	102	BCL	CHA-C1A-NA	-2.91	119.81	126.39
10	BR	101	BCL	CHA-C1A-NA	-2.91	119.81	126.39
10	AQ	103	BCL	C2A-C1A-CHA	2.90	128.91	123.87
10	L	302	BCL	C11-C10-C8	-2.90	106.33	115.97
10	AO	101	BCL	C2A-C1A-CHA	2.90	128.90	123.87
10	AQ	103	BCL	C16-C15-C13	2.90	125.60	115.97
10	BQ	101	BCL	C4A-NA-C1A	2.90	108.00	106.68
10	M	404	BCL	CAA-CBA-CGA	-2.89	105.00	113.21
10	L	302	BCL	C1-C2-C3	-2.88	121.48	126.20
10	AI	102	BCL	O2A-CGA-O1A	-2.88	116.43	123.63
19	BK	104	V7N	C2-C3-C4	-2.88	120.87	124.91
10	BK	102	BCL	C2A-C1A-CHA	2.88	128.86	123.87
10	AO	101	BCL	C1-C2-C3	-2.88	121.48	126.20
10	BN	101	BCL	C4A-NA-C1A	2.88	107.99	106.68
10	BB	101	BCL	CAA-CBA-CGA	2.87	121.37	113.21
19	BD	103	V7N	C36-C18-C19	2.87	122.48	118.09
19	Bp	1003	V7N	C35-C13-C12	2.87	122.47	118.09
10	AF	101	BCL	C2A-C1A-CHA	2.87	128.85	123.87
10	BH	102	BCL	CHA-C1A-NA	-2.87	119.89	126.39
19	Am	102	V7N	C7-C6-C5	-2.87	123.25	127.28
19	BC	103	V7N	C36-C18-C19	2.86	122.46	118.09
19	BC	103	V7N	C2-C3-C4	-2.86	120.90	124.91
12	BX	101	LMT	C3'-C4'-C5'	-2.85	104.60	110.93
19	BX	102	V7N	C35-C13-C12	2.85	122.45	118.09
10	BP	104	BCL	CHA-C1A-NA	-2.85	119.94	126.39
10	AQ	103	BCL	C17-C16-C15	-2.85	100.52	113.28
10	BL	102	BCL	CHA-C1A-NA	-2.85	119.95	126.39
10	BJ	101	BCL	C4A-NA-C1A	2.85	107.98	106.68
10	Ac	101	BCL	C2A-C1A-CHA	2.84	128.80	123.87
10	Bl	101	BCL	C2A-C1A-CHA	2.84	128.79	123.87
10	Aa	101	BCL	CAA-CBA-CGA	-2.83	105.17	113.21
19	Bk	1202	V7N	C36-C18-C19	2.83	122.41	118.09
19	BW	101	V7N	C35-C13-C12	2.83	122.41	118.09
19	Am	102	V7N	C36-C18-C19	2.83	122.41	118.09
10	BL	102	BCL	C1-C2-C3	-2.83	121.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BK	104	V7N	C35-C13-C12	2.83	122.41	118.09
10	BA	101	BCL	C4A-NA-C1A	2.83	107.97	106.68
10	AU	102	BCL	C4A-NA-C1A	2.83	107.97	106.68
10	L	302	BCL	C4A-NA-C1A	2.82	107.97	106.68
19	An	102	V7N	C35-C13-C12	2.82	122.40	118.09
19	BF	103	V7N	C36-C18-C19	2.82	122.39	118.09
10	BK	102	BCL	C16-C15-C13	2.82	125.33	115.97
12	BK	101	LMT	C3'-C4'-C5'	-2.82	104.69	110.93
19	Bl	102	V7N	C2-C3-C4	-2.81	120.96	124.91
19	BC	103	V7N	C20-C21-C22	-2.81	123.73	127.69
19	Bi	1202	V7N	C36-C18-C19	2.81	122.39	118.09
10	An	101	BCL	C2A-C1A-CHA	2.81	128.75	123.87
10	AH	101	BCL	C6-C5-C3	2.81	120.32	113.47
12	BF	101	LMT	C1'-O5'-C5'	-2.81	108.23	113.72
10	BW	102	BCL	CHA-C1A-NA	-2.81	120.03	126.39
19	BF	103	V7N	C33-C5-C4	2.81	122.38	118.09
19	Bm	101	V7N	C36-C18-C19	2.81	122.38	118.09
12	AQ	102	LMT	C3'-C4'-C5'	-2.80	104.72	110.93
19	Bf	102	V7N	C35-C13-C14	-2.80	118.28	122.82
19	An	102	V7N	C36-C18-C19	2.80	122.36	118.09
19	Bk	1202	V7N	C33-C5-C4	2.79	122.36	118.09
12	BF	101	LMT	C3'-C4'-C5'	-2.79	104.74	110.93
10	BD	101	BCL	C4A-NA-C1A	2.79	107.95	106.68
10	Bn	101	BCL	C4A-NA-C1A	2.79	107.95	106.68
10	BG	102	BCL	C4A-NA-C1A	2.79	107.95	106.68
19	Ad	102	V7N	C35-C13-C12	2.79	122.35	118.09
10	AU	101	BCL	CHA-C1A-NA	-2.79	120.08	126.39
10	Bd	101	BCL	C19-C18-C17	2.79	128.04	111.55
19	An	102	V7N	C11-C10-C9	-2.78	123.70	127.28
12	BM	102	LMT	C1'-O5'-C5'	-2.78	108.29	113.72
12	Bc	1204	LMT	C1'-O5'-C5'	-2.78	108.29	113.72
10	BX	103	BCL	CHA-C1A-NA	-2.78	120.09	126.39
19	AP	101	V7N	C2-C3-C4	-2.78	121.01	124.91
10	Aj	101	BCL	C17-C16-C15	2.78	125.73	113.28
10	BB	101	BCL	C2A-C1A-CHA	2.78	128.69	123.87
19	Ad	102	V7N	C11-C10-C9	-2.77	123.71	127.28
10	Bi	1203	BCL	C2A-C1A-CHA	2.77	128.68	123.87
19	AP	101	V7N	C29-C28-C27	-2.77	115.17	123.20
19	AX	101	V7N	C35-C13-C14	-2.77	118.33	122.82
10	BP	101	BCL	C16-C15-C13	2.77	125.17	115.97
13	M	409	MQ8	C2M-C2-C3	-2.77	119.90	124.45
10	BV	102	BCL	C2A-C1A-CHA	2.77	128.67	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Bf	103	BCL	C4A-NA-C1A	2.77	107.94	106.68
10	Aa	101	BCL	CBA-CAA-C2A	2.77	122.02	113.79
19	Bi	1202	V7N	C7-C6-C5	-2.77	123.40	127.28
10	Bd	103	BCL	C4A-NA-C1A	2.76	107.94	106.68
10	Bp	1001	BCL	C14-C13-C15	-2.76	101.45	111.27
10	AI	102	BCL	C2A-C1A-CHA	2.76	128.65	123.87
19	BE	101	V7N	C35-C13-C14	-2.75	118.36	122.82
10	Af	102	BCL	C17-C16-C15	2.75	125.59	113.28
10	AU	102	BCL	C2A-C1A-CHA	2.75	128.63	123.87
12	BU	101	LMT	C3'-C4'-C5'	-2.75	104.84	110.93
10	BS	101	BCL	C4A-NA-C1A	2.74	107.93	106.68
10	Ao	101	BCL	C2A-C1A-CHA	2.74	128.63	123.87
10	Aj	101	BCL	C2A-C1A-CHA	2.74	128.63	123.87
19	AL	102	V7N	C27-C26-C25	2.74	122.31	118.49
12	Bd	105	LMT	C1'-O5'-C5'	-2.74	108.37	113.72
19	BD	103	V7N	C20-C21-C22	-2.74	123.84	127.69
19	BB	102	V7N	C33-C5-C4	2.74	122.27	118.09
19	Bm	101	V7N	C7-C6-C5	-2.74	123.44	127.28
10	AR	101	BCL	C2A-C1A-CHA	2.73	128.61	123.87
12	BN	102	LMT	C1'-O5'-C5'	-2.73	108.38	113.72
19	BR	103	V7N	C33-C5-C4	2.73	122.26	118.09
10	BA	101	BCL	C2A-C1A-CHA	2.73	128.60	123.87
18	C	1001	HEC	C2A-C1A-NA	-2.73	107.69	110.32
19	Am	102	V7N	C38-C26-C25	-2.73	119.01	123.73
12	Bl	105	LMT	C1'-O5'-C5'	-2.72	108.40	113.72
19	An	102	V7N	C2-C3-C4	-2.72	121.09	124.91
10	Bi	1203	BCL	C4A-NA-C1A	2.72	107.92	106.68
10	BI	1102	BCL	C2A-C1A-CHA	2.72	128.59	123.87
10	BO	102	BCL	C2A-C1A-CHA	2.72	128.59	123.87
10	Bj	101	BCL	C2A-C1A-CHA	2.72	128.59	123.87
19	Ag	102	V7N	C35-C13-C12	2.72	122.24	118.09
10	L	301	BCL	C2A-C1A-CHA	2.72	128.58	123.87
10	Bg	1203	BCL	C4A-NA-C1A	2.72	107.92	106.68
10	Bh	101	BCL	C2A-C1A-CHA	2.71	128.58	123.87
10	Af	102	BCL	C2A-C1A-CHA	2.71	128.57	123.87
12	BT	103	LMT	C1'-O5'-C5'	-2.71	108.42	113.72
10	An	101	BCL	C17-C16-C15	2.71	125.41	113.28
19	BR	103	V7N	C36-C18-C19	2.71	122.22	118.09
10	BD	101	BCL	C2A-C1A-CHA	2.71	128.56	123.87
10	BJ	101	BCL	C2A-C1A-CHA	2.70	128.56	123.87
19	AF	102	V7N	C2-C3-C4	-2.70	121.12	124.91
10	L	301	BCL	CHA-C1A-NA	-2.70	120.27	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AM	101	BCL	C2A-C1A-CHA	2.70	128.55	123.87
19	BL	101	V7N	C35-C13-C14	-2.70	118.44	122.82
19	Ba	101	V7N	C35-C13-C14	-2.70	118.44	122.82
19	BO	101	V7N	C36-C18-C19	2.70	122.21	118.09
19	Am	102	V7N	C11-C10-C9	-2.69	123.81	127.28
10	Ae	101	BCL	C6-C5-C3	2.69	120.02	113.47
12	BI	1103	LMT	C1'-O5'-C5'	-2.69	108.47	113.72
12	L	305	LMT	C1'-O5'-C5'	-2.69	108.47	113.72
12	BG	103	LMT	C1'-O5'-C5'	-2.69	108.47	113.72
19	BV	101	V7N	C2-C3-C4	-2.69	121.14	124.91
19	BX	102	V7N	O45-C40-C39	2.69	129.02	122.09
10	Bo	1202	BCL	C4A-NA-C1A	2.68	107.90	106.68
10	Bf	101	BCL	C1-C2-C3	-2.68	121.80	126.20
12	BB	103	LMT	C1'-O5'-C5'	-2.68	108.48	113.72
10	AB	101	BCL	C1-O2A-CGA	-2.68	110.16	116.65
10	Bd	101	BCL	C2A-C1A-CHA	2.68	128.51	123.87
19	AT	102	V7N	C36-C18-C19	2.68	122.18	118.09
10	AN	101	BCL	C2A-C1A-CHA	2.67	128.50	123.87
10	BE	102	BCL	C2A-C1A-CHA	2.67	128.50	123.87
10	Ah	101	BCL	C2A-C1A-CHA	2.66	128.49	123.87
10	Bl	103	BCL	C2A-C1A-CHA	2.66	128.49	123.87
19	BK	104	V7N	C20-C21-C22	-2.66	123.95	127.69
19	BV	101	V7N	C20-C21-C22	-2.66	123.96	127.69
10	AU	101	BCL	C6-C7-C8	2.65	124.79	115.97
10	Bh	102	BCL	C4A-NA-C1A	2.65	107.89	106.68
10	Bj	101	BCL	C1-C2-C3	2.64	130.52	126.20
19	BN	103	V7N	C33-C5-C4	2.64	122.12	118.09
12	Bi	1201	LMT	O5B-C5B-C4B	2.64	114.45	109.70
19	Bb	101	V7N	C7-C6-C5	-2.63	123.58	127.28
12	BQ	102	LMT	C1'-O5'-C5'	-2.63	108.58	113.72
12	AK	102	LMT	C1'-O5'-C5'	-2.63	108.58	113.72
19	Ba	101	V7N	C36-C18-C19	2.63	122.11	118.09
10	M	404	BCL	C2A-C1A-CHA	2.63	128.43	123.87
10	Am	101	BCL	C16-C15-C13	2.62	124.69	115.97
11	M	405	BPH	C2D-C1D-ND	2.62	111.33	109.43
19	AH	102	V7N	C36-C18-C19	2.62	122.09	118.09
10	AE	101	BCL	C2A-C1A-CHA	2.62	128.41	123.87
10	BR	101	BCL	C2A-C1A-CHA	2.62	128.41	123.87
10	BN	101	BCL	C2A-C1A-CHA	2.62	128.41	123.87
10	L	301	BCL	C16-C15-C13	2.61	124.65	115.97
12	BP	102	LMT	C3'-C4'-C5'	-2.61	105.14	110.93
12	Bk	1201	LMT	C1'-O5'-C5'	-2.61	108.62	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	101	V7N	C20-C21-C22	-2.61	124.02	127.69
19	BP	103	V7N	C35-C13-C12	2.61	122.07	118.09
10	AR	101	BCL	C16-C15-C13	2.60	124.62	115.97
10	Bf	103	BCL	C1-O2A-CGA	2.60	122.95	116.65
12	AB	102	LMT	C3B-C4B-C5B	-2.60	105.52	110.23
10	BT	101	BCL	C4A-NA-C1A	2.60	107.86	106.68
19	Ag	102	V7N	C7-C6-C5	-2.60	123.64	127.28
19	AI	103	V7N	C36-C18-C19	2.60	122.06	118.09
10	AR	101	BCL	C4A-NA-C1A	2.60	107.86	106.68
12	BH	101	LMT	C1'-O5'-C5'	-2.59	108.66	113.72
10	AI	102	BCL	O2A-CGA-CBA	2.59	119.73	111.83
12	Bm	104	LMT	C1'-O5'-C5'	-2.58	108.68	113.72
19	BV	101	V7N	C36-C18-C19	2.58	122.03	118.09
19	AL	102	V7N	C35-C13-C12	2.58	122.03	118.09
19	BP	103	V7N	C36-C18-C19	2.58	122.03	118.09
10	Ak	101	BCL	C4A-NA-C1A	2.58	107.86	106.68
19	BV	101	V7N	C35-C13-C14	-2.58	118.64	122.82
19	Bj	103	V7N	C20-C21-C22	-2.58	124.06	127.69
19	Bj	103	V7N	C33-C5-C6	-2.57	118.65	122.82
10	Ag	101	BCL	CAA-CBA-CGA	-2.57	105.91	113.21
10	Al	101	BCL	C2A-C1A-CHA	2.57	128.33	123.87
10	BK	102	BCL	CAA-CBA-CGA	2.57	120.50	113.21
10	Be	101	BCL	C2A-C1A-CHA	2.56	128.32	123.87
19	Bc	1202	V7N	C33-C5-C4	2.56	122.00	118.09
19	Bp	1003	V7N	C20-C21-C22	-2.56	124.09	127.69
12	AK	102	LMT	C3'-C4'-C5'	-2.56	105.25	110.93
19	Am	102	V7N	C20-C21-C22	-2.56	124.09	127.69
10	L	301	BCL	C4A-NA-C1A	2.56	107.85	106.68
10	BL	102	BCL	C2A-C1A-CHA	2.56	128.31	123.87
10	Bp	1001	BCL	C2A-C1A-CHA	2.56	128.31	123.87
12	Bc	1201	LMT	C3'-C4'-C5'	-2.55	105.27	110.93
12	L	309	LMT	C1'-O5'-C5'	-2.55	108.73	113.72
19	AH	102	V7N	C27-C26-C25	2.55	122.05	118.49
10	AW	101	BCL	C2A-C1A-CHA	2.55	128.30	123.87
10	AK	101	BCL	C6-C5-C3	2.55	119.68	113.47
10	Bf	101	BCL	C2A-C1A-CHA	2.55	128.29	123.87
10	AK	101	BCL	C2A-C1A-CHA	2.55	128.29	123.87
10	Bj	101	BCL	CBA-CAA-C2A	-2.55	106.21	113.79
19	Bd	102	V7N	C36-C18-C19	2.55	121.98	118.09
19	BX	102	V7N	C15-C14-C13	-2.55	123.71	127.28
10	BP	101	BCL	C2A-C1A-CHA	2.55	128.29	123.87
12	Bd	105	LMT	C3'-C4'-C5'	-2.55	105.29	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BK	101	LMT	C1'-O5'-C5'	-2.54	108.75	113.72
13	L	310	MQ8	C2M-C2-C3	-2.54	120.27	124.45
10	M	403	BCL	C16-C15-C13	2.54	124.42	115.97
10	AT	101	BCL	C2A-C1A-CHA	2.54	128.27	123.87
19	BV	101	V7N	C33-C5-C4	2.54	121.96	118.09
10	Bp	1001	BCL	C15-C13-C12	2.53	124.91	112.07
10	AH	101	BCL	C2A-C1A-CHA	2.53	128.26	123.87
12	L	306	LMT	C1'-O5'-C5'	-2.53	108.78	113.72
10	M	404	BCL	O2A-CGA-O1A	-2.53	117.30	123.63
19	BN	103	V7N	C36-C18-C19	2.53	121.95	118.09
19	Bf	102	V7N	C35-C13-C12	2.53	121.95	118.09
19	Bf	102	V7N	C36-C18-C19	2.53	121.95	118.09
19	Bj	103	V7N	C27-C26-C25	2.53	122.01	118.49
19	AF	102	V7N	C36-C18-C19	2.53	121.95	118.09
19	AI	101	V7N	C7-C6-C5	-2.53	123.74	127.28
10	AT	104	BCL	C2A-C1A-CHA	2.53	128.25	123.87
10	AQ	103	BCL	C16-C17-C18	2.52	127.20	115.94
19	Bl	102	V7N	C36-C18-C19	2.52	121.94	118.09
10	BO	102	BCL	C16-C15-C13	2.52	124.35	115.97
19	Bf	102	V7N	C7-C6-C5	-2.52	123.74	127.28
19	AL	102	V7N	C36-C18-C19	2.52	121.94	118.09
19	AL	102	V7N	C2-C3-C4	-2.52	121.38	124.91
10	AP	102	BCL	C2A-C1A-CHA	2.52	128.23	123.87
10	BQ	101	BCL	C2A-C1A-CHA	2.51	128.23	123.87
10	Ag	101	BCL	C2A-C1A-CHA	2.51	128.23	123.87
19	BS	103	V7N	C36-C18-C19	2.51	121.93	118.09
10	An	101	BCL	C16-C15-C13	2.51	124.31	115.97
12	L	304	LMT	C1'-O5'-C5'	-2.51	108.82	113.72
19	AH	102	V7N	C35-C13-C14	-2.51	118.75	122.82
10	AL	101	BCL	C2A-C1A-CHA	2.51	128.22	123.87
10	AX	102	BCL	C2A-C1A-CHA	2.51	128.22	123.87
10	BQ	101	BCL	C11-C10-C8	2.51	124.30	115.97
10	Al	101	BCL	OBB-CAB-CBB	-2.51	114.16	119.77
10	Bp	1004	BCL	C2A-C1A-CHA	2.51	128.22	123.87
10	Ak	101	BCL	C2A-C1A-CHA	2.50	128.21	123.87
10	Ai	101	BCL	C2A-C1A-CHA	2.50	128.21	123.87
19	Ag	102	V7N	C36-C18-C19	2.50	121.91	118.09
10	Bj	101	BCL	C6-C5-C3	2.50	119.56	113.47
10	BJ	101	BCL	C17-C16-C15	2.50	124.47	113.28
12	Bo	1201	LMT	C1'-O5'-C5'	-2.50	108.84	113.72
10	BA	101	BCL	C11-C10-C8	2.50	124.26	115.97
19	Ba	101	V7N	C20-C21-C22	-2.50	124.18	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301	BCL	OBB-CAB-CBB	-2.49	114.19	119.77
10	Aa	101	BCL	C6-C5-C3	2.49	119.53	113.47
12	Bc	1201	LMT	C1'-O5'-C5'	-2.49	108.86	113.72
11	L	303	BPH	C2D-C1D-ND	2.49	111.23	109.43
19	An	102	V7N	C20-C21-C22	-2.48	124.20	127.69
12	Bl	105	LMT	O5B-C5B-C4B	2.48	114.17	109.70
19	BW	101	V7N	C33-C5-C4	2.48	121.88	118.09
10	BP	104	BCL	C16-C15-C13	2.48	124.20	115.97
19	BR	103	V7N	C2-C3-C4	-2.48	121.43	124.91
13	Ad	101	MQ8	C2M-C2-C3	-2.48	120.38	124.45
12	Bo	1201	LMT	C3'-C4'-C5'	-2.48	105.44	110.93
10	BW	102	BCL	C2A-C1A-CHA	2.48	128.16	123.87
19	BB	102	V7N	C2-C3-C4	-2.47	121.44	124.91
10	Am	101	BCL	C2A-C1A-CHA	2.47	128.16	123.87
18	C	1000	HEC	C2A-C1A-NA	-2.47	107.94	110.32
10	BC	101	BCL	C16-C15-C13	2.47	124.18	115.97
10	Bm	102	BCL	C2A-C1A-CHA	2.47	128.15	123.87
10	Bc	1203	BCL	C2A-C1A-CHA	2.47	128.15	123.87
19	BB	102	V7N	C36-C18-C19	2.47	121.86	118.09
12	BD	102	LMT	C3'-C4'-C5'	-2.47	105.46	110.93
19	Ba	101	V7N	C15-C14-C13	-2.47	123.82	127.28
10	Ae	101	BCL	C2A-C1A-CHA	2.46	128.14	123.87
12	AB	102	LMT	C3'-C4'-C5'	-2.46	105.47	110.93
10	BF	102	BCL	C4A-NA-C1A	2.46	107.80	106.68
10	BX	103	BCL	C2A-C1A-CHA	2.46	128.14	123.87
10	AD	101	BCL	C6-C5-C3	2.46	119.46	113.47
19	AT	102	V7N	C20-C21-C22	-2.46	124.23	127.69
19	BL	101	V7N	C7-C6-C5	-2.46	123.83	127.28
10	Al	101	BCL	CMB-C2B-C1B	-2.45	121.69	125.42
19	AH	102	V7N	C2-C3-C4	-2.45	121.47	124.91
11	L	303	BPH	OBB-CAB-CBB	-2.45	114.97	120.19
10	AU	101	BCL	C2A-C1A-CHA	2.45	128.12	123.87
19	BP	103	V7N	C2-C3-C4	-2.45	121.47	124.91
17	AT	103	PEX	C3-C2-C1	2.45	117.49	111.78
19	BF	103	V7N	C15-C14-C13	-2.45	123.85	127.28
10	AI	102	BCL	C16-C15-C13	2.44	124.09	115.97
19	AL	102	V7N	C33-C5-C4	2.44	121.82	118.09
19	AH	102	V7N	C33-C5-C4	2.44	121.82	118.09
17	AT	103	PEX	C2-O6-C14	2.44	123.64	117.80
10	AQ	101	BCL	C2A-C1A-CHA	2.44	128.10	123.87
12	AB	102	LMT	C1'-O5'-C5'	-2.44	108.96	113.72
10	M	404	BCL	OBB-CAB-CBB	-2.44	114.31	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BR	103	V7N	C20-C21-C22	-2.43	124.27	127.69
10	Ac	101	BCL	C11-C10-C8	-2.43	107.89	115.97
10	BR	101	BCL	C1-O2A-CGA	2.43	122.53	116.65
10	BR	101	BCL	C1-C2-C3	-2.43	122.22	126.20
19	Bc	1202	V7N	C36-C18-C19	2.43	121.80	118.09
10	BP	104	BCL	C2A-C1A-CHA	2.43	128.08	123.87
19	BB	102	V7N	C27-C26-C25	2.43	121.87	118.49
19	Ag	102	V7N	C2-C3-C4	-2.42	121.51	124.91
12	BX	104	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
19	BS	103	V7N	C2-C3-C4	-2.42	121.52	124.91
12	L	306	LMT	C3'-C4'-C5'	-2.42	105.58	110.93
10	AT	101	BCL	C6-C5-C3	2.41	119.35	113.47
10	Bg	1203	BCL	C2A-C1A-CHA	2.41	128.05	123.87
19	Bm	101	V7N	C20-C21-C22	-2.41	124.30	127.69
10	BN	101	BCL	C16-C15-C13	2.41	123.98	115.97
19	Bg	1202	V7N	C27-C26-C25	2.41	121.84	118.49
10	Bo	1202	BCL	C2A-C1A-CHA	2.41	128.04	123.87
12	Bm	104	LMT	C3B-C4B-C5B	-2.40	105.87	110.23
10	AB	101	BCL	C1-C2-C3	-2.40	122.26	126.20
10	Bd	103	BCL	C2A-C1A-CHA	2.40	128.04	123.87
12	BV	103	LMT	C3'-C4'-C5'	-2.40	105.61	110.93
12	BA	102	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
19	AP	101	V7N	C33-C5-C4	2.40	121.75	118.09
10	M	404	BCL	CMB-C2B-C1B	-2.40	121.77	125.42
10	BH	102	BCL	C2A-C1A-CHA	2.40	128.03	123.87
19	Bm	101	V7N	C35-C13-C14	-2.40	118.94	122.82
11	M	405	BPH	OBB-CAB-C3B	2.39	123.98	119.99
16	M	406	CRT	C20-C21-C22	2.39	128.40	123.52
19	BK	104	V7N	C16-C17-C18	-2.39	123.93	127.28
18	C	1003	HEC	C2A-C1A-NA	-2.39	108.02	110.32
12	BX	104	LMT	C1'-O5'-C5'	-2.39	109.06	113.72
10	AD	101	BCL	C2A-C1A-CHA	2.39	128.01	123.87
12	BD	102	LMT	C1'-O5'-C5'	-2.39	109.06	113.72
19	BW	101	V7N	C2-C3-C4	-2.38	121.57	124.91
10	AV	1001	BCL	C6-C5-C3	2.38	119.27	113.47
12	Bk	1201	LMT	C1B-O5B-C5B	2.38	118.37	113.72
10	An	101	BCL	C1-C2-C3	2.38	130.10	126.20
10	Ba	102	BCL	C2A-C1A-CHA	2.38	128.00	123.87
19	BW	101	V7N	C29-C28-C27	-2.38	116.30	123.20
10	Aj	101	BCL	CMB-C2B-C1B	-2.38	121.79	125.42
12	L	306	LMT	C3B-C4B-C5B	-2.38	105.92	110.23
10	Ac	101	BCL	OBB-CAB-CBB	-2.38	114.44	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AI	101	V7N	C36-C18-C19	2.38	121.72	118.09
19	BX	102	V7N	C2-C3-C4	-2.38	121.58	124.91
12	BC	102	LMT	C1'-O5'-C5'	-2.38	109.08	113.72
10	Ae	101	BCL	OBb-CAB-CBB	-2.37	114.45	119.77
10	Bp	1001	BCL	C11-C10-C8	-2.37	108.08	115.97
12	BL	103	LMT	C3'-C4'-C5'	-2.37	105.67	110.93
10	Aa	101	BCL	C4A-NA-C1A	2.37	107.76	106.68
12	BN	102	LMT	C3'-C4'-C5'	-2.37	105.67	110.93
10	M	404	BCL	C1-O2A-CGA	-2.37	110.91	116.65
19	AI	103	V7N	C35-C13-C14	-2.37	118.98	122.82
12	BC	102	LMT	C3'-C4'-C5'	-2.36	105.69	110.93
10	Aa	101	BCL	C17-C16-C15	2.36	123.86	113.28
10	Bn	101	BCL	C6-C5-C3	2.36	119.22	113.47
19	BD	103	V7N	C33-C5-C4	2.36	121.69	118.09
12	BB	103	LMT	C3'-C4'-C5'	-2.36	105.70	110.93
10	Bf	103	BCL	C2A-C1A-CHA	2.36	127.96	123.87
10	AQ	101	BCL	CMB-C2B-C1B	-2.36	121.83	125.42
19	BT	102	V7N	C33-C5-C4	2.36	121.69	118.09
12	BO	103	LMT	C1'-O5'-C5'	-2.36	109.12	113.72
12	Bg	1201	LMT	C1'-O5'-C5'	-2.36	109.12	113.72
19	Bl	102	V7N	C35-C13-C14	-2.35	119.00	122.82
10	AR	101	BCL	O2A-CGA-O1A	-2.35	117.74	123.63
19	AI	101	V7N	C35-C13-C14	-2.35	119.00	122.82
10	An	101	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
10	M	404	BCL	O2A-CGA-CBA	2.35	119.00	111.83
19	An	102	V7N	C7-C6-C5	-2.35	123.98	127.28
10	Bn	101	BCL	C2A-C1A-CHA	2.35	127.94	123.87
19	AI	103	V7N	C15-C14-C13	-2.35	123.98	127.28
10	An	101	BCL	OBb-CAB-CBB	-2.34	114.52	119.77
12	M	407	LMT	C3'-C4'-C5'	-2.34	105.74	110.93
19	Bf	102	V7N	C33-C5-C4	2.34	121.67	118.09
12	BD	102	LMT	C3B-C4B-C5B	-2.34	105.99	110.23
10	BE	102	BCL	C1C-NC-C4C	2.34	107.75	106.68
10	Ao	101	BCL	CMB-C2B-C1B	-2.34	121.86	125.42
12	BT	103	LMT	C3'-C4'-C5'	-2.34	105.75	110.93
12	Ba	104	LMT	C3'-C4'-C5'	-2.34	105.75	110.93
19	BL	101	V7N	C15-C14-C13	-2.33	124.01	127.28
10	AN	101	BCL	OBb-CAB-CBB	-2.33	114.56	119.77
10	Bp	1004	BCL	C4A-NA-C1A	2.32	107.74	106.68
10	BS	101	BCL	C2A-C1A-CHA	2.32	127.89	123.87
10	AR	101	BCL	C11-C10-C8	-2.32	108.26	115.97
10	Ao	101	BCL	OBb-CAB-CBB	-2.32	114.58	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AX	101	V7N	C7-C6-C5	-2.32	124.03	127.28
12	BX	101	LMT	C1'-O5'-C5'	-2.32	109.20	113.72
10	AN	101	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
19	BX	102	V7N	C35-C13-C14	-2.31	119.07	122.82
10	AB	101	BCL	CED-O2D-CGD	2.31	121.16	115.92
19	BB	102	V7N	C35-C13-C14	-2.31	119.07	122.82
12	BO	103	LMT	C3'-C4'-C5'	-2.31	105.81	110.93
12	BR	102	LMT	C1'-O5'-C5'	-2.31	109.21	113.72
19	Bg	1202	V7N	C35-C13-C14	-2.31	119.08	122.82
10	AW	101	BCL	OBB-CAB-CBB	-2.30	114.61	119.77
19	BF	103	V7N	C35-C13-C14	-2.30	119.09	122.82
19	AX	101	V7N	C27-C26-C25	2.30	121.69	118.49
19	AP	101	V7N	C20-C21-C22	-2.30	124.45	127.69
10	Aj	101	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
10	Bj	101	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
10	BK	102	BCL	C1C-NC-C4C	2.30	107.73	106.68
10	AX	102	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
10	Bk	1203	BCL	C2A-C1A-CHA	2.30	127.85	123.87
10	Aa	101	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
19	BS	103	V7N	C33-C5-C4	2.29	121.59	118.09
19	Ba	101	V7N	C11-C10-C9	-2.29	124.33	127.28
11	L	303	BPH	O2D-CGD-CBD	2.29	113.46	110.95
19	BT	102	V7N	C36-C18-C19	2.29	121.59	118.09
19	Bj	103	V7N	C3-C4-C5	2.29	129.35	125.89
10	BI	1102	BCL	C1-C2-C3	-2.29	122.45	126.20
10	BM	101	BCL	CAB-C3B-C2B	2.29	132.50	127.74
10	BJ	101	BCL	C16-C15-C13	2.29	123.57	115.97
10	BN	101	BCL	C17-C16-C15	2.29	123.53	113.28
19	Bd	102	V7N	C33-C5-C6	-2.29	119.11	122.82
10	BM	101	BCL	C6-C5-C3	2.28	119.03	113.47
12	Ba	104	LMT	C1'-O5'-C5'	-2.28	109.26	113.72
10	AU	102	BCL	CMB-C2B-C1B	-2.28	121.94	125.42
10	Ak	101	BCL	CMB-C2B-C1B	-2.28	121.94	125.42
19	BT	102	V7N	C2-C3-C4	-2.28	121.71	124.91
19	BL	101	V7N	C36-C18-C19	2.28	121.57	118.09
19	AP	101	V7N	C36-C18-C19	2.28	121.57	118.09
19	An	102	V7N	O45-C40-C39	2.28	127.97	122.09
10	BL	102	BCL	C1C-NC-C4C	2.28	107.72	106.68
10	BR	101	BCL	CMB-C2B-C1B	-2.28	121.95	125.42
10	Ak	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
10	AC	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
19	Bc	1202	V7N	C36-C18-C17	-2.28	119.13	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BQ	101	BCL	CAB-C3B-C2B	2.28	132.47	127.74
19	Bc	1202	V7N	C16-C17-C18	-2.28	124.08	127.28
19	BD	103	V7N	C27-C26-C25	2.28	121.66	118.49
10	M	404	BCL	CAB-C3B-C2B	2.28	132.47	127.74
10	AV	1001	BCL	C1-C2-C3	-2.28	122.47	126.20
19	Bd	102	V7N	C35-C13-C14	-2.28	119.13	122.82
19	Bj	103	V7N	C35-C13-C14	-2.27	119.13	122.82
12	BN	102	LMT	O1'-C1'-C2'	2.27	111.73	108.27
10	BL	102	BCL	C16-C15-C13	2.27	123.52	115.97
12	Bp	1002	LMT	C1'-O5'-C5'	-2.27	109.28	113.72
10	Ag	101	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
19	BD	103	V7N	C2-C3-C4	-2.27	121.72	124.91
19	BS	103	V7N	C27-C26-C25	2.27	121.65	118.49
11	L	303	BPH	CMB-C2B-C3B	2.27	129.22	124.68
13	M	409	MQ8	C11-C3-C2	-2.27	121.00	124.89
19	BV	101	V7N	C27-C26-C25	2.27	121.65	118.49
11	M	405	BPH	CMD-C2D-C3D	2.26	129.21	124.68
10	Bp	1001	BCL	C14-C13-C12	-2.26	103.21	111.27
10	Bf	103	BCL	C1C-NC-C4C	2.26	107.71	106.68
19	BL	101	V7N	C20-C21-C22	-2.26	124.51	127.69
12	BG	101	LMT	C3'-C4'-C5'	-2.26	105.92	110.93
19	AT	102	V7N	C15-C14-C13	-2.26	124.11	127.28
10	Bh	102	BCL	C2A-C1A-CHA	2.26	127.79	123.87
10	Bf	101	BCL	CMB-C2B-C1B	-2.26	121.98	125.42
10	AP	102	BCL	C1C-NC-C4C	2.26	107.71	106.68
10	BB	101	BCL	O2A-CGA-O1A	-2.26	117.98	123.63
19	Ag	102	V7N	C27-C26-C25	2.26	121.63	118.49
10	Am	101	BCL	OBB-CAB-CBB	-2.25	114.72	119.77
12	BM	102	LMT	C3B-C4B-C5B	-2.25	106.15	110.23
10	AE	101	BCL	OBB-CAB-CBB	-2.25	114.72	119.77
10	Am	101	BCL	C17-C16-C15	-2.25	103.19	113.28
12	BP	102	LMT	C1'-O5'-C5'	-2.25	109.32	113.72
10	AR	101	BCL	O2A-CGA-CBA	2.25	118.70	111.83
19	Bl	102	V7N	C15-C14-C13	-2.25	124.13	127.28
12	L	305	LMT	C3'-C4'-C5'	-2.25	105.95	110.93
10	Ag	101	BCL	OBB-CAB-CBB	-2.25	114.74	119.77
10	Bj	101	BCL	OBB-CAB-CBB	-2.24	114.74	119.77
12	BS	102	LMT	C3B-C4B-C5B	-2.24	106.16	110.23
10	AQ	101	BCL	OBB-CAB-CBB	-2.24	114.74	119.77
19	BK	104	V7N	C35-C13-C14	-2.24	119.18	122.82
10	AT	101	BCL	OBB-CAB-CBB	-2.24	114.75	119.77
19	BW	101	V7N	C36-C18-C19	2.24	121.51	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BR	101	BCL	OBB-CAB-CBB	-2.24	114.75	119.77
10	AE	101	BCL	CAB-C3B-C2B	2.24	132.40	127.74
10	AT	104	BCL	OBB-CAB-CBB	-2.24	114.75	119.77
19	Bb	101	V7N	C35-C13-C14	-2.24	119.19	122.82
10	BN	101	BCL	C6-C5-C3	2.24	118.92	113.47
19	BP	103	V7N	C33-C5-C4	2.24	121.50	118.09
12	BL	103	LMT	C1'-O5'-C5'	-2.24	109.36	113.72
10	BJ	101	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
10	Bm	102	BCL	C1C-NC-C4C	2.23	107.70	106.68
19	BX	102	V7N	C20-C21-C22	-2.23	124.55	127.69
10	BV	102	BCL	C1-C2-C3	-2.23	122.54	126.20
10	Af	102	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
10	Ai	101	BCL	CAB-C3B-C2B	2.23	132.38	127.74
10	Af	102	BCL	OBB-CAB-CBB	-2.23	114.77	119.77
10	Bp	1001	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
18	C	1002	HEC	C2A-C1A-NA	-2.23	108.17	110.32
10	AT	104	BCL	CAB-C3B-C2B	2.23	132.37	127.74
10	Bj	101	BCL	C16-C17-C18	-2.22	106.01	115.94
10	Be	101	BCL	CAB-C3B-C2B	2.22	132.36	127.74
10	Ao	101	BCL	C11-C10-C8	2.22	123.36	115.97
10	AC	101	BCL	C2A-C1A-CHA	2.22	127.72	123.87
19	AF	102	V7N	C33-C5-C4	2.22	121.48	118.09
10	Ah	101	BCL	C11-C10-C8	-2.22	108.59	115.97
10	Ac	101	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
12	Bj	102	LMT	C3'-C4'-C5'	-2.22	106.02	110.93
12	Bj	102	LMT	C1'-O5'-C5'	-2.21	109.40	113.72
19	BN	103	V7N	C35-C13-C14	-2.21	119.23	122.82
19	Bp	1003	V7N	C35-C13-C14	-2.21	119.23	122.82
19	AT	102	V7N	C35-C13-C14	-2.21	119.23	122.82
10	Ah	101	BCL	C17-C16-C15	2.21	123.17	113.28
10	AW	101	BCL	CMB-C2B-C1B	-2.21	122.06	125.42
10	Bh	101	BCL	CMB-C2B-C1B	-2.21	122.06	125.42
10	BA	101	BCL	C1C-NC-C4C	2.21	107.69	106.68
19	AP	101	V7N	C35-C13-C14	-2.21	119.24	122.82
10	Am	101	BCL	CAB-C3B-C2B	2.21	132.32	127.74
10	BN	101	BCL	C1C-NC-C4C	2.20	107.68	106.68
19	Bl	102	V7N	C33-C5-C4	2.20	121.45	118.09
10	BH	102	BCL	CMB-C2B-C1B	-2.20	122.07	125.42
10	BA	101	BCL	CAB-C3B-C2B	2.20	132.31	127.74
10	M	403	BCL	C1C-NC-C4C	2.20	107.68	106.68
10	Ai	101	BCL	OBB-CAB-CBB	-2.20	114.85	119.77
19	Ad	102	V7N	C27-C26-C25	2.20	121.55	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BR	101	BCL	CAB-C3B-C2B	2.20	132.31	127.74
19	Bg	1202	V7N	C36-C18-C19	2.20	121.44	118.09
12	Bc	1204	LMT	C3'-C4'-C5'	-2.20	106.06	110.93
19	Bp	1003	V7N	C3-C4-C5	2.20	129.21	125.89
10	Ae	101	BCL	CAB-C3B-C2B	2.20	132.30	127.74
19	Bi	1202	V7N	C35-C13-C14	-2.19	119.26	122.82
10	Ac	101	BCL	CAB-C3B-C2B	2.19	132.30	127.74
12	L	309	LMT	C3B-C4B-C5B	-2.19	106.25	110.23
10	AQ	101	BCL	C15-C13-C12	-2.19	100.95	112.07
10	Am	101	BCL	C1-O2A-CGA	2.19	121.96	116.65
19	Bk	1202	V7N	C2-C3-C4	-2.19	121.83	124.91
19	BE	101	V7N	C15-C14-C13	-2.19	124.20	127.28
10	BI	1102	BCL	C17-C16-C15	2.19	123.10	113.28
19	Bc	1202	V7N	O45-C40-C39	2.19	127.74	122.09
19	An	102	V7N	C35-C13-C14	-2.19	119.27	122.82
10	AT	101	BCL	CMB-C2B-C1B	-2.19	122.08	125.42
16	M	406	CRT	C21-C22-C23	-2.19	124.21	127.28
10	AE	101	BCL	C6-C5-C3	2.19	118.80	113.47
19	BD	103	V7N	O45-C40-C39	2.19	127.73	122.09
10	Bj	101	BCL	CAA-CBA-CGA	2.19	119.42	113.21
12	L	306	LMT	O5B-C5B-C6B	2.19	111.86	106.44
10	Am	101	BCL	CMB-C2B-C1B	-2.19	122.09	125.42
19	Bi	1202	V7N	C27-C26-C25	2.18	121.53	118.49
19	Bd	102	V7N	C27-C26-C25	2.18	121.53	118.49
12	Bg	1205	LMT	C1'-O5'-C5'	-2.18	109.46	113.72
10	BW	102	BCL	C1C-NC-C4C	2.18	107.67	106.68
19	BD	103	V7N	C35-C13-C14	-2.18	119.28	122.82
10	BD	101	BCL	C17-C16-C15	2.18	123.05	113.28
10	Bd	101	BCL	OBB-CAB-CBB	-2.18	114.89	119.77
17	M	408	PEX	C2-O6-C14	2.18	123.01	117.80
19	Bg	1202	V7N	C33-C5-C6	-2.18	119.29	122.82
10	Al	101	BCL	C16-C15-C13	-2.18	108.73	115.97
11	M	405	BPH	C1-O2A-CGA	2.18	121.92	116.65
10	Aa	101	BCL	OBB-CAB-CBB	-2.17	114.90	119.77
19	BO	101	V7N	C36-C18-C17	-2.17	119.30	122.82
10	AI	102	BCL	C11-C12-C13	-2.17	108.74	115.97
10	AF	101	BCL	CMB-C2B-C1B	-2.17	122.11	125.42
19	Bp	1003	V7N	C36-C18-C19	2.17	121.40	118.09
10	Bo	1202	BCL	C6-C5-C3	2.17	118.75	113.47
19	BS	103	V7N	C35-C13-C14	-2.17	119.30	122.82
10	AX	102	BCL	OBB-CAB-CBB	-2.17	114.92	119.77
10	Ao	101	BCL	CAB-C3B-C2B	2.17	132.24	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AC	101	BCL	C6-C5-C3	2.16	118.74	113.47
10	L	302	BCL	CAA-CBA-CGA	2.16	119.35	113.21
19	Ag	102	V7N	C35-C13-C14	-2.16	119.31	122.82
18	C	1000	HEC	CAD-CBD-CGD	-2.16	107.93	113.67
19	AI	101	V7N	C27-C26-C25	2.16	121.50	118.49
10	BX	103	BCL	C16-C15-C13	2.16	123.15	115.97
10	Ah	101	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
10	BG	102	BCL	CAA-CBA-CGA	2.16	119.34	113.21
19	BX	102	V7N	C36-C18-C19	2.16	121.39	118.09
10	AR	101	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
10	AC	101	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
10	AM	101	BCL	CMB-C2B-C1B	-2.16	122.14	125.42
10	BH	102	BCL	CAB-C3B-C2B	2.16	132.22	127.74
19	Bk	1202	V7N	C27-C26-C25	2.16	121.49	118.49
10	BJ	101	BCL	C11-C10-C8	2.15	123.12	115.97
12	BG	103	LMT	C3'-C4'-C5'	-2.15	106.17	110.93
19	BC	103	V7N	O45-C40-C39	2.15	127.63	122.09
19	BD	103	V7N	C36-C18-C17	-2.15	119.33	122.82
10	AP	102	BCL	C16-C15-C13	2.14	123.09	115.97
10	Ae	101	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
19	Bb	101	V7N	C36-C18-C19	2.14	121.36	118.09
10	AU	102	BCL	OBB-CAB-CBB	-2.14	114.99	119.77
10	BP	104	BCL	CMB-C2B-C1B	-2.14	122.17	125.42
19	AP	101	V7N	C28-C29-C39	-2.14	120.60	126.64
10	AF	101	BCL	OBB-CAB-CBB	-2.13	114.99	119.77
10	Bc	1203	BCL	C14-C13-C15	-2.13	103.67	111.27
19	AL	102	V7N	C20-C21-C22	-2.13	124.69	127.69
19	Bk	1202	V7N	C15-C14-C13	-2.13	124.29	127.28
10	BC	101	BCL	C6-C5-C3	2.13	118.66	113.47
10	AQ	103	BCL	OBB-CAB-CBB	-2.13	114.99	119.77
19	Am	102	V7N	C33-C5-C6	-2.13	119.36	122.82
10	AQ	103	BCL	CAB-C3B-C2B	2.13	132.17	127.74
18	C	1002	HEC	CBD-CAD-C3D	-2.13	106.64	112.53
19	BR	103	V7N	C16-C17-C18	-2.13	124.29	127.28
10	BA	101	BCL	C17-C16-C15	2.13	122.83	113.28
19	Bf	102	V7N	O45-C40-C39	2.13	127.58	122.09
19	Am	102	V7N	C15-C14-C13	-2.13	124.29	127.28
10	Bo	1202	BCL	C1C-NC-C4C	2.13	107.65	106.68
19	AT	102	V7N	C27-C26-C25	2.13	121.45	118.49
10	Bj	101	BCL	C20-C18-C17	2.13	124.14	111.55
10	AX	102	BCL	O2A-CGA-CBA	2.13	118.32	111.83
10	BP	104	BCL	OBB-CAB-CBB	-2.13	115.01	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	101	BCL	OBB-CAB-CBB	-2.13	115.01	119.77
10	Af	102	BCL	CAB-C3B-C2B	2.12	132.16	127.74
10	BB	101	BCL	O2A-CGA-CBA	2.12	118.31	111.83
19	Ag	102	V7N	C28-C29-C39	-2.12	120.64	126.64
19	Bj	103	V7N	C16-C17-C18	-2.12	124.30	127.28
10	Ai	101	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
12	Bp	1002	LMT	C3'-C4'-C5'	-2.12	106.23	110.93
10	AM	101	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
19	BW	101	V7N	C35-C13-C14	-2.12	119.38	122.82
19	BC	103	V7N	C15-C14-C13	-2.12	124.31	127.28
10	BS	101	BCL	O2D-CGD-O1D	-2.12	119.72	123.85
10	Bd	103	BCL	CMB-C2B-C1B	-2.12	122.19	125.42
10	BO	102	BCL	C1C-NC-C4C	2.12	107.64	106.68
19	Bj	103	V7N	C36-C18-C17	-2.11	119.39	122.82
19	AI	103	V7N	C36-C18-C17	-2.11	119.39	122.82
12	Bg	1201	LMT	C3'-C4'-C5'	-2.11	106.25	110.93
19	Bi	1202	V7N	O45-C40-C39	2.11	127.54	122.09
10	Bh	101	BCL	OBB-CAB-CBB	-2.11	115.04	119.77
10	Ah	101	BCL	OBB-CAB-CBB	-2.11	115.04	119.77
19	BO	101	V7N	C3-C4-C5	2.11	129.08	125.89
12	AQ	102	LMT	C1'-O5'-C5'	-2.11	109.60	113.72
19	Bm	101	V7N	C33-C5-C4	2.11	121.31	118.09
19	AF	102	V7N	C35-C13-C14	-2.11	119.40	122.82
10	Ag	101	BCL	CAB-C3B-C2B	2.11	132.12	127.74
10	AK	101	BCL	CMB-C2B-C1B	-2.11	122.21	125.42
12	M	407	LMT	C3B-C4B-C5B	-2.11	106.41	110.23
19	AI	101	V7N	C3-C4-C5	2.11	129.07	125.89
19	BB	102	V7N	C15-C14-C13	-2.10	124.33	127.28
10	Bg	1203	BCL	C1-C2-C3	-2.10	122.75	126.20
10	BD	101	BCL	C11-C10-C8	2.10	122.95	115.97
10	BE	102	BCL	OBB-CAB-CBB	-2.10	115.07	119.77
19	Ag	102	V7N	C29-C28-C27	-2.10	117.12	123.20
10	AD	101	BCL	OBB-CAB-CBB	-2.10	115.07	119.77
11	M	405	BPH	C1-C2-C3	-2.10	122.76	126.20
19	Bk	1202	V7N	C35-C13-C14	-2.10	119.42	122.82
10	Bl	103	BCL	OBB-CAB-CBB	-2.10	115.07	119.77
19	Ba	101	V7N	O45-C40-C39	2.10	127.50	122.09
19	Ad	102	V7N	C20-C21-C22	-2.10	124.74	127.69
10	Bh	102	BCL	CAB-C3B-C2B	2.10	132.10	127.74
10	Ak	101	BCL	CAB-C3B-C2B	2.10	132.10	127.74
12	BM	102	LMT	O5B-C5B-C6B	2.09	111.63	106.44
12	AB	102	LMT	O5B-C5B-C6B	2.09	111.62	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BW	101	V7N	C27-C26-C25	2.09	121.40	118.49
12	BK	101	LMT	O5'-C1'-O1'	-2.09	105.10	110.04
10	AU	102	BCL	C1-C2-C3	-2.09	122.78	126.20
10	Bf	101	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
12	Bc	1204	LMT	O5B-C5B-C4B	2.09	113.46	109.70
10	AO	101	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
10	AT	104	BCL	CMB-C2B-C1B	-2.09	122.24	125.42
10	Ag	101	BCL	C1-C2-C3	2.09	129.62	126.20
10	AW	101	BCL	C11-C10-C8	-2.09	109.03	115.97
12	BI	1101	LMT	C1'-O5'-C5'	-2.09	109.65	113.72
10	Bc	1203	BCL	OBB-CAB-CBB	-2.09	115.10	119.77
10	Bp	1001	BCL	OBB-CAB-CBB	-2.09	115.10	119.77
10	Bn	101	BCL	O2D-CGD-O1D	-2.09	119.79	123.85
10	Bd	103	BCL	OBB-CAB-CBB	-2.08	115.10	119.77
10	Be	101	BCL	C11-C10-C8	-2.08	109.04	115.97
10	Al	101	BCL	CAB-C3B-C2B	2.08	132.07	127.74
10	AK	101	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
10	Bn	101	BCL	C1C-NC-C4C	2.08	107.63	106.68
19	BN	103	V7N	C20-C21-C22	-2.08	124.76	127.69
10	M	404	BCL	C6-C7-C8	-2.08	109.05	115.97
10	AB	101	BCL	CAA-CBA-CGA	-2.08	107.30	113.21
10	Bg	1203	BCL	C16-C15-C13	2.08	122.88	115.97
19	Bi	1202	V7N	C3-C4-C5	2.08	129.03	125.89
10	BD	101	BCL	C1C-NC-C4C	2.08	107.63	106.68
19	AT	102	V7N	O45-C40-C39	2.08	127.45	122.09
10	AB	101	BCL	OBB-CAB-CBB	-2.08	115.12	119.77
19	BS	103	V7N	O45-C40-C39	2.08	127.44	122.09
10	Bc	1203	BCL	CMB-C2B-C1B	-2.07	122.26	125.42
10	AH	101	BCL	OBB-CAB-CBB	-2.07	115.13	119.77
19	BV	101	V7N	O45-C40-C39	2.07	127.43	122.09
10	Bl	101	BCL	OBB-CAB-CBB	-2.07	115.13	119.77
19	Bd	102	V7N	O45-C40-C39	2.07	127.43	122.09
10	BB	101	BCL	C17-C16-C15	2.07	122.54	113.28
10	BD	101	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
10	Bl	101	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
10	AD	101	BCL	C16-C15-C13	2.07	122.83	115.97
12	Bg	1201	LMT	C3B-C4B-C5B	-2.07	106.49	110.23
10	Ah	101	BCL	CAB-C3B-C2B	2.07	132.03	127.74
19	Bb	101	V7N	O45-C40-C39	2.07	127.42	122.09
19	BT	102	V7N	C35-C13-C14	-2.07	119.47	122.82
10	Bi	1203	BCL	C1-C2-C3	2.06	129.58	126.20
19	BE	101	V7N	C33-C5-C6	-2.06	119.47	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BB	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
10	BA	101	BCL	OBB-CAB-CBB	-2.06	115.15	119.77
19	BL	101	V7N	C27-C26-C25	2.06	121.36	118.49
11	L	303	BPH	CMD-C2D-C3D	2.06	128.80	124.68
19	Bf	102	V7N	C7-C8-C9	-2.06	123.80	127.30
19	BS	103	V7N	C36-C18-C17	-2.06	119.48	122.82
10	BC	101	BCL	C17-C16-C15	2.06	122.51	113.28
10	AP	102	BCL	C11-C12-C13	2.06	122.81	115.97
19	BR	103	V7N	C36-C18-C17	-2.06	119.48	122.82
10	BL	102	BCL	CMB-C2B-C1B	-2.06	122.29	125.42
10	AU	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
10	BP	101	BCL	CAB-C3B-C2B	2.06	132.01	127.74
10	BF	102	BCL	C1C-NC-C4C	2.05	107.62	106.68
19	BO	101	V7N	O45-C40-C39	2.05	127.39	122.09
19	Bd	102	V7N	C20-C21-C22	-2.05	124.80	127.69
19	Am	102	V7N	C35-C13-C14	-2.05	119.49	122.82
10	AO	101	BCL	CMB-C2B-C1B	-2.05	122.29	125.42
10	Bj	101	BCL	CAB-C3B-C2B	2.05	132.00	127.74
12	BG	101	LMT	C1'-O5'-C5'	-2.05	109.72	113.72
12	Bo	1201	LMT	O5B-C5B-C4B	2.05	113.39	109.70
10	Bd	101	BCL	CMB-C2B-C1B	-2.05	122.30	125.42
10	BD	101	BCL	OBB-CAB-CBB	-2.05	115.19	119.77
10	Bl	103	BCL	CAB-C3B-C2B	2.05	131.99	127.74
10	Bp	1001	BCL	C12-C11-C10	2.05	122.44	113.28
10	BB	101	BCL	CAB-C3B-C2B	2.04	131.99	127.74
11	L	303	BPH	C6-C5-C3	2.04	118.45	113.47
19	BC	103	V7N	C35-C13-C14	-2.04	119.50	122.82
10	AP	102	BCL	C6-C5-C3	2.04	118.45	113.47
10	AE	101	BCL	CMB-C2B-C1B	-2.04	122.31	125.42
19	AL	102	V7N	C36-C18-C17	-2.04	119.51	122.82
19	Bi	1202	V7N	C33-C5-C6	-2.04	119.51	122.82
10	AH	101	BCL	CMB-C2B-C1B	-2.04	122.31	125.42
10	AX	102	BCL	C1-C2-C3	-2.04	122.85	126.20
10	BH	102	BCL	OBB-CAB-CBB	-2.04	115.20	119.77
19	Bl	102	V7N	C27-C26-C25	2.04	121.33	118.49
10	Ba	102	BCL	C1C-NC-C4C	2.04	107.61	106.68
19	AL	102	V7N	O45-C40-C39	2.04	127.35	122.09
10	AK	101	BCL	CAB-C3B-C2B	2.04	131.97	127.74
10	Bc	1203	BCL	C6-C5-C3	2.04	118.43	113.47
10	AF	101	BCL	C1-C2-C3	-2.04	122.86	126.20
12	Bg	1205	LMT	C3'-C4'-C5'	-2.04	106.42	110.93
19	Am	102	V7N	O45-C40-C39	2.04	127.34	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	102	V7N	C16-C17-C18	-2.03	124.42	127.28
10	AP	102	BCL	C1-C2-C3	-2.03	122.86	126.20
10	AR	101	BCL	OBB-CAB-CBB	-2.03	115.22	119.77
19	BE	101	V7N	O45-C40-C39	2.03	127.33	122.09
19	Bc	1202	V7N	C2-C3-C4	-2.03	122.06	124.91
10	AT	104	BCL	O2D-CGD-O1D	-2.03	119.90	123.85
19	Bj	103	V7N	O45-C40-C39	2.03	127.32	122.09
11	M	405	BPH	O2D-CGD-CBD	2.03	113.17	110.95
19	Bj	103	V7N	C36-C18-C19	2.02	121.18	118.09
10	BF	102	BCL	O2D-CGD-O1D	-2.02	119.91	123.85
19	Ad	102	V7N	C7-C6-C5	-2.02	124.44	127.28
12	BS	102	LMT	O5'-C1'-O1'	-2.02	105.26	110.04
19	BF	103	V7N	O45-C40-C39	2.02	127.31	122.09
12	BQ	102	LMT	O5B-C5B-C6B	2.02	111.45	106.44
10	BC	101	BCL	O2D-CGD-O1D	-2.02	119.91	123.85
19	AX	101	V7N	C36-C18-C19	2.02	121.18	118.09
12	BK	101	LMT	O6'-C6'-C5'	-2.02	104.45	111.33
19	Bm	101	V7N	C15-C14-C13	-2.02	124.44	127.28
10	BP	101	BCL	O2D-CGD-O1D	-2.02	119.92	123.85
10	AL	101	BCL	OBB-CAB-CBB	-2.02	115.25	119.77
10	BK	102	BCL	C1-C2-C3	-2.02	122.89	126.20
19	Ba	101	V7N	C36-C18-C17	-2.02	119.55	122.82
10	Bd	103	BCL	CAB-C3B-C2B	2.02	131.93	127.74
19	Bp	1003	V7N	C33-C5-C6	-2.02	119.55	122.82
12	L	307	LMT	C1'-O5'-C5'	-2.02	109.78	113.72
12	Bc	1201	LMT	C3B-C4B-C5B	-2.01	106.58	110.23
10	AQ	101	BCL	CAB-C3B-C2B	2.01	131.93	127.74
19	Bi	1202	V7N	C20-C21-C22	-2.01	124.86	127.69
10	BB	101	BCL	OBB-CAB-CBB	-2.01	115.26	119.77
10	Bo	1202	BCL	CAB-C3B-C2B	2.01	131.92	127.74
10	BM	101	BCL	CAA-CBA-CGA	2.01	118.92	113.21
19	BE	101	V7N	C36-C18-C19	2.01	121.16	118.09
10	AO	101	BCL	O2D-CGD-O1D	-2.01	119.93	123.85
19	AF	102	V7N	O45-C40-C39	2.01	127.28	122.09
10	Bc	1203	BCL	C1C-NC-C4C	2.01	107.60	106.68
19	Ba	101	V7N	C33-C5-C6	-2.01	119.56	122.82
10	BJ	101	BCL	OBB-CAB-CBB	-2.01	115.27	119.77
19	BB	102	V7N	C36-C18-C17	-2.01	119.56	122.82
10	Ak	101	BCL	C17-C16-C15	2.01	122.28	113.28
19	BO	101	V7N	C4-C5-C6	-2.01	115.85	119.01
19	Bc	1202	V7N	C35-C13-C14	-2.01	119.57	122.82
10	Bc	1203	BCL	C16-C15-C13	2.01	122.63	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BW	102	BCL	O2D-CGD-O1D	-2.01	119.94	123.85
19	AP	101	V7N	C36-C18-C17	-2.00	119.57	122.82
10	AB	101	BCL	CMB-C2B-C1B	-2.00	122.37	125.42
10	BP	101	BCL	C1C-NC-C4C	2.00	107.59	106.68
19	Bc	1202	V7N	C27-C26-C25	2.00	121.28	118.49
10	AD	101	BCL	CAB-C3B-C2B	2.00	131.90	127.74
10	BN	101	BCL	CMB-C2B-C1B	-2.00	122.37	125.42
19	BP	103	V7N	C36-C18-C17	-2.00	119.57	122.82
10	BW	102	BCL	CMB-C2B-C1B	-2.00	122.37	125.42
10	AO	101	BCL	CAB-C3B-C2B	2.00	131.90	127.74

There are no chirality outliers.

All (1639) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	302	BCL	C1A-C2A-CAA-CBA
10	L	302	BCL	C3A-C2A-CAA-CBA
10	AD	101	BCL	C11-C10-C8-C9
10	BF	102	BCL	C4-C3-C5-C6
10	BG	102	BCL	C4-C3-C5-C6
10	AI	102	BCL	CBA-CGA-O2A-C1
10	AI	102	BCL	O1A-CGA-O2A-C1
10	AM	101	BCL	C2-C3-C5-C6
10	AM	101	BCL	C4-C3-C5-C6
10	BO	102	BCL	C2-C3-C5-C6
10	BO	102	BCL	C4-C3-C5-C6
10	AR	101	BCL	CBA-CGA-O2A-C1
10	AR	101	BCL	O1A-CGA-O2A-C1
10	Ac	101	BCL	C2-C1-O2A-CGA
10	Bd	101	BCL	O2A-C1-C2-C3
10	Be	101	BCL	C2-C3-C5-C6
10	Be	101	BCL	C4-C3-C5-C6
10	Af	102	BCL	O2A-C1-C2-C3
10	Bg	1203	BCL	CBA-CGA-O2A-C1
10	Bg	1203	BCL	O1A-CGA-O2A-C1
10	Bh	102	BCL	C1A-C2A-CAA-CBA
10	Ak	101	BCL	C1A-C2A-CAA-CBA
10	Ak	101	BCL	C3A-C2A-CAA-CBA
10	Bk	1203	BCL	C1A-C2A-CAA-CBA
10	Am	101	BCL	C2-C3-C5-C6
10	Am	101	BCL	C4-C3-C5-C6
10	Bn	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	Ao	101	BCL	O2A-C1-C2-C3
10	Bo	1202	BCL	C1A-C2A-CAA-CBA
10	Bo	1202	BCL	C3A-C2A-CAA-CBA
12	L	308	LMT	C2-C1-O1'-C1'
12	M	407	LMT	C2-C1-O1'-C1'
12	BB	103	LMT	O5'-C1'-O1'-C1
12	BF	101	LMT	C2-C1-O1'-C1'
12	BK	103	LMT	O5'-C1'-O1'-C1
12	BM	102	LMT	O5'-C1'-O1'-C1
12	BO	103	LMT	C3'-C4'-O1B-C1B
12	Ba	104	LMT	O5'-C1'-O1'-C1
13	L	310	MQ8	C26-C27-C28-C29
13	L	310	MQ8	C26-C27-C28-C30
13	L	310	MQ8	C31-C32-C33-C34
13	L	310	MQ8	C31-C32-C33-C35
13	L	310	MQ8	C41-C42-C43-C44
13	L	310	MQ8	C41-C42-C43-C45
13	M	409	MQ8	C16-C17-C18-C19
13	M	409	MQ8	C16-C17-C18-C20
13	M	409	MQ8	C19-C18-C20-C21
13	M	409	MQ8	C21-C22-C23-C24
13	M	409	MQ8	C21-C22-C23-C25
13	M	409	MQ8	C31-C32-C33-C34
13	M	409	MQ8	C31-C32-C33-C35
13	M	409	MQ8	C45-C43-C44-C46
13	Ad	101	MQ8	C25-C26-C27-C28
13	Ad	101	MQ8	C26-C27-C28-C29
13	Ad	101	MQ8	C31-C32-C33-C34
13	Ad	101	MQ8	C31-C32-C33-C35
13	Ad	101	MQ8	C32-C33-C35-C36
13	Ad	101	MQ8	C34-C33-C35-C36
15	M	402	CD4	C31-O10-P2-O12
15	M	402	CD4	C31-O10-P2-O13
15	M	402	CD4	C32-O13-P2-O12
15	M	402	CD4	O17-C46-O16-C33
15	M	402	CD4	C47-C46-O16-C33
15	Af	101	CD4	C13-C14-O2-C15
15	Af	101	CD4	O1-C14-O2-C15
15	Af	101	CD4	O4-C17-O3-C16
15	Af	101	CD4	C18-C17-O3-C16
15	Af	101	CD4	C28-O5-P1-O6
15	Af	101	CD4	C28-O5-P1-O7

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Mol	Chain	Res	Type	Atoms
15	Af	101	CD4	C28-O5-P1-O8
15	Af	101	CD4	O16-C33-C34-O14
17	M	408	PEX	C1-O3-P1-O1
17	M	408	PEX	C1-O3-P1-O8
17	M	408	PEX	C24-O8-P1-O1
17	M	408	PEX	C24-O8-P1-O3
17	M	408	PEX	C15-C14-O6-C2
17	AG	1101	PEX	C1-O3-P1-O2
17	AG	1101	PEX	C24-O8-P1-O1
17	AG	1101	PEX	C24-O8-P1-O3
17	AG	1101	PEX	C25-C24-O8-P1
17	AG	1101	PEX	O8-C24-C25-N1
17	AO	102	PEX	C1-O3-P1-O1
17	AO	102	PEX	C24-O8-P1-O1
17	AT	103	PEX	C1-O3-P1-O2
17	AT	103	PEX	C1-O3-P1-O8
17	AT	103	PEX	C24-O8-P1-O1
17	AT	103	PEX	C24-O8-P1-O2
17	AT	103	PEX	C24-O8-P1-O3
17	AT	103	PEX	C15-C14-O6-C2
17	AT	103	PEX	O8-C24-C25-N1
17	Ba	103	PEX	C1-O3-P1-O1
17	Ba	103	PEX	C1-O3-P1-O2
17	Ba	103	PEX	C1-O3-P1-O8
17	Ba	103	PEX	C24-O8-P1-O1
17	Ba	103	PEX	C24-O8-P1-O2
17	Ba	103	PEX	C24-O8-P1-O3
17	Ba	103	PEX	O3-C1-C2-O6
17	Ba	103	PEX	O7-C14-O6-C2
17	Ba	103	PEX	C15-C14-O6-C2
17	Bd	104	PEX	C1-O3-P1-O8
17	Bd	104	PEX	C24-O8-P1-O2
17	Bd	104	PEX	C24-O8-P1-O3
17	Be	102	PEX	C1-O3-P1-O2
17	Be	102	PEX	C1-O3-P1-O8
17	Be	102	PEX	C24-O8-P1-O1
17	Be	102	PEX	C15-C14-O6-C2
17	Be	102	PEX	O8-C24-C25-N1
17	Bf	104	PEX	C1-O3-P1-O1
17	Bf	104	PEX	C1-O3-P1-O8
17	Bf	104	PEX	C24-O8-P1-O3
17	Bf	104	PEX	C15-C14-O6-C2

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Mol	Chain	Res	Type	Atoms
17	Bg	1204	PEX	C1-O3-P1-O1
17	Bg	1204	PEX	C1-O3-P1-O8
17	Bg	1204	PEX	C24-O8-P1-O2
17	Bg	1204	PEX	O6-C2-C3-O4
17	Bg	1204	PEX	O8-C24-C25-N1
17	Bi	1204	PEX	C1-O3-P1-O2
17	Bi	1204	PEX	C1-O3-P1-O8
17	Bi	1204	PEX	C24-O8-P1-O1
17	Bi	1204	PEX	C24-O8-P1-O3
17	Bi	1204	PEX	C25-C24-O8-P1
17	Bj	104	PEX	C1-O3-P1-O1
17	Bj	104	PEX	C1-O3-P1-O8
17	Bj	104	PEX	C24-O8-P1-O1
17	Bj	104	PEX	C24-O8-P1-O3
17	Bj	104	PEX	C25-C24-O8-P1
17	Bk	1204	PEX	C1-O3-P1-O1
17	Bk	1204	PEX	C1-O3-P1-O8
17	Bk	1204	PEX	O8-C24-C25-N1
17	Bl	104	PEX	C1-O3-P1-O1
17	Bl	104	PEX	C1-O3-P1-O8
17	Bl	104	PEX	C24-O8-P1-O2
17	Bm	103	PEX	C24-O8-P1-O1
17	Bm	103	PEX	C24-O8-P1-O2
17	Bn	102	PEX	C24-O8-P1-O1
17	Bn	102	PEX	C24-O8-P1-O2
17	Bn	102	PEX	C24-O8-P1-O3
17	Bn	102	PEX	O8-C24-C25-N1
17	Bp	1005	PEX	C1-O3-P1-O1
17	Bp	1005	PEX	C1-O3-P1-O2
17	Bp	1005	PEX	C1-O3-P1-O8
17	Bp	1005	PEX	C24-O8-P1-O1
17	Bp	1005	PEX	C24-O8-P1-O2
17	Bp	1005	PEX	C24-O8-P1-O3
18	C	1000	HEC	C2B-C3B-CAB-CBB
18	C	1000	HEC	C4B-C3B-CAB-CBB
18	C	1000	HEC	C2C-C3C-CAC-CBC
18	C	1001	HEC	C2B-C3B-CAB-CBB
18	C	1001	HEC	C4B-C3B-CAB-CBB
18	C	1001	HEC	C2C-C3C-CAC-CBC
18	C	1002	HEC	C2B-C3B-CAB-CBB
18	C	1002	HEC	C4B-C3B-CAB-CBB
18	C	1002	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
18	C	1002	HEC	C4C-C3C-CAC-CBC
18	C	1003	HEC	C2B-C3B-CAB-CBB
18	C	1003	HEC	C4B-C3B-CAB-CBB
18	C	1003	HEC	C2C-C3C-CAC-CBC
19	BB	102	V7N	C26-C27-C28-C29
19	BB	102	V7N	O42-C34-C9-C10
19	BB	102	V7N	O42-C34-C9-C8
19	BC	103	V7N	O42-C34-C9-C10
19	BC	103	V7N	O42-C34-C9-C8
19	BD	103	V7N	C26-C27-C28-C29
19	BD	103	V7N	O42-C34-C9-C10
19	BD	103	V7N	O42-C34-C9-C8
19	BE	101	V7N	C30-C1-C2-C3
19	BE	101	V7N	C31-C1-C2-C3
19	BE	101	V7N	O32-C1-C2-C3
19	BE	101	V7N	C25-C26-C27-C28
19	BE	101	V7N	C38-C26-C27-C28
19	BE	101	V7N	O42-C34-C9-C10
19	BE	101	V7N	O42-C34-C9-C8
19	BF	103	V7N	C25-C26-C27-C28
19	BF	103	V7N	C38-C26-C27-C28
19	BF	103	V7N	O42-C34-C9-C10
19	BF	103	V7N	O42-C34-C9-C8
19	AF	102	V7N	C25-C26-C27-C28
19	AF	102	V7N	C38-C26-C27-C28
19	AF	102	V7N	O42-C34-C9-C8
19	AH	102	V7N	O42-C34-C9-C10
19	AH	102	V7N	O42-C34-C9-C8
19	AI	101	V7N	C30-C1-C2-C3
19	AI	101	V7N	C31-C1-C2-C3
19	AI	101	V7N	O32-C1-C2-C3
19	AI	101	V7N	C17-C18-C19-C20
19	AI	101	V7N	C25-C26-C27-C28
19	AI	101	V7N	C38-C26-C27-C28
19	AI	101	V7N	O42-C34-C9-C10
19	AI	101	V7N	O42-C34-C9-C8
19	AI	103	V7N	C30-C1-C2-C3
19	AI	103	V7N	C31-C1-C2-C3
19	AI	103	V7N	O32-C1-C2-C3
19	AI	103	V7N	C25-C26-C27-C28
19	AI	103	V7N	C38-C26-C27-C28
19	AI	103	V7N	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	AI	103	V7N	O42-C34-C9-C10
19	AI	103	V7N	O42-C34-C9-C8
19	BK	104	V7N	C30-C1-C2-C3
19	BK	104	V7N	C31-C1-C2-C3
19	BK	104	V7N	O32-C1-C2-C3
19	BK	104	V7N	O42-C34-C9-C10
19	BK	104	V7N	O42-C34-C9-C8
19	AL	102	V7N	C17-C18-C19-C20
19	AL	102	V7N	C26-C27-C28-C29
19	AL	102	V7N	O42-C34-C9-C10
19	AL	102	V7N	O42-C34-C9-C8
19	BL	101	V7N	C30-C1-C2-C3
19	BL	101	V7N	C31-C1-C2-C3
19	BL	101	V7N	O32-C1-C2-C3
19	BL	101	V7N	O42-C34-C9-C10
19	BL	101	V7N	O42-C34-C9-C8
19	BN	103	V7N	O42-C34-C9-C10
19	BO	101	V7N	O42-C34-C9-C10
19	BO	101	V7N	O42-C34-C9-C8
19	BP	103	V7N	C25-C26-C27-C28
19	BP	103	V7N	C38-C26-C27-C28
19	BP	103	V7N	O42-C34-C9-C10
19	BP	103	V7N	O42-C34-C9-C8
19	AP	101	V7N	C38-C26-C27-C28
19	AP	101	V7N	O42-C34-C9-C10
19	AP	101	V7N	O42-C34-C9-C8
19	BR	103	V7N	O42-C34-C9-C10
19	BR	103	V7N	O42-C34-C9-C8
19	BS	103	V7N	O42-C34-C9-C8
19	BT	102	V7N	O42-C34-C9-C10
19	BT	102	V7N	O42-C34-C9-C8
19	AT	102	V7N	C25-C26-C27-C28
19	AT	102	V7N	C38-C26-C27-C28
19	AT	102	V7N	O42-C34-C9-C10
19	AT	102	V7N	O42-C34-C9-C8
19	BV	101	V7N	C26-C27-C28-C29
19	BV	101	V7N	O42-C34-C9-C10
19	BV	101	V7N	O42-C34-C9-C8
19	BW	101	V7N	O42-C34-C9-C10
19	BW	101	V7N	O42-C34-C9-C8
19	AX	101	V7N	O32-C1-C2-C3
19	AX	101	V7N	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	AX	101	V7N	C38-C26-C27-C28
19	AX	101	V7N	O42-C34-C9-C10
19	AX	101	V7N	O42-C34-C9-C8
19	BX	102	V7N	O32-C1-C2-C3
19	BX	102	V7N	O42-C34-C9-C10
19	BX	102	V7N	O42-C34-C9-C8
19	Ba	101	V7N	C30-C1-C2-C3
19	Ba	101	V7N	C31-C1-C2-C3
19	Ba	101	V7N	O32-C1-C2-C3
19	Ba	101	V7N	O42-C34-C9-C10
19	Ba	101	V7N	O42-C34-C9-C8
19	Bb	101	V7N	C30-C1-C2-C3
19	Bb	101	V7N	C31-C1-C2-C3
19	Bb	101	V7N	O32-C1-C2-C3
19	Bb	101	V7N	C26-C27-C28-C29
19	Bb	101	V7N	O42-C34-C9-C10
19	Bb	101	V7N	O42-C34-C9-C8
19	Bc	1202	V7N	O32-C1-C2-C3
19	Bc	1202	V7N	C26-C27-C28-C29
19	Bc	1202	V7N	O42-C34-C9-C10
19	Bc	1202	V7N	O42-C34-C9-C8
19	Ad	102	V7N	O32-C1-C2-C3
19	Ad	102	V7N	C26-C27-C28-C29
19	Ad	102	V7N	O42-C34-C9-C10
19	Ad	102	V7N	O42-C34-C9-C8
19	Ad	102	V7N	C3-C4-C5-C33
19	Ad	102	V7N	C3-C4-C5-C6
19	Ad	102	V7N	C7-C8-C9-C10
19	Bd	102	V7N	C30-C1-C2-C3
19	Bd	102	V7N	C31-C1-C2-C3
19	Bd	102	V7N	O32-C1-C2-C3
19	Bd	102	V7N	C26-C27-C28-C29
19	Bd	102	V7N	O42-C34-C9-C10
19	Bd	102	V7N	O42-C34-C9-C8
19	Bf	102	V7N	C30-C1-C2-C3
19	Bf	102	V7N	C31-C1-C2-C3
19	Bf	102	V7N	O32-C1-C2-C3
19	Bf	102	V7N	C26-C27-C28-C29
19	Bf	102	V7N	O42-C34-C9-C10
19	Bf	102	V7N	O42-C34-C9-C8
19	Bf	102	V7N	C7-C8-C9-C10
19	Ag	102	V7N	C30-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	Ag	102	V7N	C31-C1-C2-C3
19	Ag	102	V7N	O32-C1-C2-C3
19	Ag	102	V7N	C25-C26-C27-C28
19	Ag	102	V7N	C26-C27-C28-C29
19	Ag	102	V7N	O42-C34-C9-C10
19	Ag	102	V7N	C7-C8-C9-C10
19	Bg	1202	V7N	C30-C1-C2-C3
19	Bg	1202	V7N	C31-C1-C2-C3
19	Bg	1202	V7N	O32-C1-C2-C3
19	Bg	1202	V7N	C26-C27-C28-C29
19	Bg	1202	V7N	O42-C34-C9-C10
19	Bg	1202	V7N	O42-C34-C9-C8
19	Bg	1202	V7N	C7-C8-C9-C34
19	Bi	1202	V7N	C30-C1-C2-C3
19	Bi	1202	V7N	C31-C1-C2-C3
19	Bi	1202	V7N	O32-C1-C2-C3
19	Bi	1202	V7N	C25-C26-C27-C28
19	Bi	1202	V7N	C26-C27-C28-C29
19	Bi	1202	V7N	C27-C28-C29-C39
19	Bi	1202	V7N	O42-C34-C9-C10
19	Bi	1202	V7N	O42-C34-C9-C8
19	Bj	103	V7N	C30-C1-C2-C3
19	Bj	103	V7N	C31-C1-C2-C3
19	Bj	103	V7N	O32-C1-C2-C3
19	Bj	103	V7N	C26-C27-C28-C29
19	Bj	103	V7N	O42-C34-C9-C10
19	Bj	103	V7N	O42-C34-C9-C8
19	Bj	103	V7N	C3-C4-C5-C6
19	Bk	1202	V7N	C26-C27-C28-C29
19	Bk	1202	V7N	O42-C34-C9-C10
19	Bk	1202	V7N	O42-C34-C9-C8
19	Bl	102	V7N	C30-C1-C2-C3
19	Bl	102	V7N	C31-C1-C2-C3
19	Bl	102	V7N	O32-C1-C2-C3
19	Bl	102	V7N	C26-C27-C28-C29
19	Bl	102	V7N	O42-C34-C9-C10
19	Bl	102	V7N	O42-C34-C9-C8
19	Am	102	V7N	C30-C1-C2-C3
19	Am	102	V7N	C31-C1-C2-C3
19	Am	102	V7N	O32-C1-C2-C3
19	Am	102	V7N	C11-C12-C13-C14
19	Am	102	V7N	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	Am	102	V7N	O42-C34-C9-C10
19	Am	102	V7N	O42-C34-C9-C8
19	Am	102	V7N	C7-C8-C9-C34
19	Bm	101	V7N	C30-C1-C2-C3
19	Bm	101	V7N	C31-C1-C2-C3
19	Bm	101	V7N	O32-C1-C2-C3
19	Bm	101	V7N	C30-C1-O32-C41
19	Bm	101	V7N	O42-C34-C9-C10
19	Bm	101	V7N	O42-C34-C9-C8
19	Bm	101	V7N	C3-C4-C5-C33
19	Bm	101	V7N	C3-C4-C5-C6
19	An	102	V7N	C30-C1-C2-C3
19	An	102	V7N	C31-C1-C2-C3
19	An	102	V7N	O32-C1-C2-C3
19	An	102	V7N	C25-C26-C27-C28
19	An	102	V7N	C38-C26-C27-C28
19	An	102	V7N	C26-C27-C28-C29
19	An	102	V7N	O42-C34-C9-C10
19	An	102	V7N	O42-C34-C9-C8
19	An	102	V7N	C7-C8-C9-C10
19	Bp	1003	V7N	C30-C1-C2-C3
19	Bp	1003	V7N	C31-C1-C2-C3
19	Bp	1003	V7N	O32-C1-C2-C3
19	Bp	1003	V7N	C22-C23-C24-C25
19	Bp	1003	V7N	C26-C27-C28-C29
19	Bp	1003	V7N	O42-C34-C9-C8
12	Bi	1201	LMT	O5B-C1B-O1B-C4'
17	Bf	104	PEX	O5-C4-O4-C3
12	Bk	1201	LMT	O5B-C1B-O1B-C4'
13	L	310	MQ8	C46-C47-C48-C49
13	M	409	MQ8	C46-C47-C48-C50
17	Bf	104	PEX	C5-C4-O4-C3
17	Bj	104	PEX	O5-C4-O4-C3
12	L	307	LMT	C3'-C4'-O1B-C1B
12	BS	102	LMT	C3'-C4'-O1B-C1B
12	BX	104	LMT	C3'-C4'-O1B-C1B
17	M	408	PEX	O7-C14-O6-C2
17	AT	103	PEX	O7-C14-O6-C2
17	Be	102	PEX	O7-C14-O6-C2
17	Bf	104	PEX	O7-C14-O6-C2
17	AT	103	PEX	C5-C4-O4-C3
17	Bj	104	PEX	C5-C4-O4-C3

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Mol	Chain	Res	Type	Atoms
12	L	304	LMT	C3'-C4'-O1B-C1B
12	AB	102	LMT	C4B-C5B-C6B-O6B
12	Bg	1201	LMT	O5B-C1B-O1B-C4'
12	BU	101	LMT	O5'-C5'-C6'-O6'
10	AD	101	BCL	C4-C3-C5-C6
10	AF	101	BCL	C4-C3-C5-C6
10	AL	101	BCL	C4-C3-C5-C6
10	BL	102	BCL	C4-C3-C5-C6
10	BM	101	BCL	C4-C3-C5-C6
10	AN	101	BCL	C4-C3-C5-C6
10	AO	101	BCL	C4-C3-C5-C6
10	BP	104	BCL	C4-C3-C5-C6
10	AT	101	BCL	C4-C3-C5-C6
10	AW	101	BCL	C4-C3-C5-C6
10	AX	102	BCL	C4-C3-C5-C6
10	Aa	101	BCL	C4-C3-C5-C6
10	Ac	101	BCL	C4-C3-C5-C6
10	Bf	101	BCL	C4-C3-C5-C6
10	Bf	103	BCL	C4-C3-C5-C6
10	Bi	1203	BCL	C4-C3-C5-C6
10	An	101	BCL	C4-C3-C5-C6
10	Bp	1004	BCL	C4-C3-C5-C6
13	M	409	MQ8	C29-C28-C30-C31
10	AD	101	BCL	C2-C3-C5-C6
10	BF	102	BCL	C2-C3-C5-C6
10	AF	101	BCL	C2-C3-C5-C6
10	BG	102	BCL	C2-C3-C5-C6
10	AL	101	BCL	C2-C3-C5-C6
10	BM	101	BCL	C2-C3-C5-C6
10	BP	104	BCL	C2-C3-C5-C6
10	AX	102	BCL	C2-C3-C5-C6
10	Aa	101	BCL	C2-C3-C5-C6
10	Ac	101	BCL	C2-C3-C5-C6
10	Bf	101	BCL	C2-C3-C5-C6
10	Bf	103	BCL	C2-C3-C5-C6
10	Bi	1203	BCL	C2-C3-C5-C6
10	An	101	BCL	C2-C3-C5-C6
13	M	409	MQ8	C17-C18-C20-C21
13	M	409	MQ8	C42-C43-C44-C46
12	AK	102	LMT	O5B-C5B-C6B-O6B
12	BP	102	LMT	O5'-C5'-C6'-O6'
12	Bo	1201	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
10	Bc	1203	BCL	C2A-CAA-CBA-CGA
10	Be	101	BCL	C2A-CAA-CBA-CGA
13	M	409	MQ8	C26-C27-C28-C29
13	Ad	101	MQ8	C11-C12-C13-C14
13	Ad	101	MQ8	C16-C17-C18-C19
13	Ad	101	MQ8	C36-C37-C38-C39
13	M	409	MQ8	C26-C27-C28-C30
13	Ad	101	MQ8	C11-C12-C13-C15
13	Ad	101	MQ8	C16-C17-C18-C20
13	Ad	101	MQ8	C26-C27-C28-C30
13	Ad	101	MQ8	C36-C37-C38-C40
12	L	309	LMT	O5B-C5B-C6B-O6B
12	AB	102	LMT	O5B-C5B-C6B-O6B
19	AP	101	V7N	C27-C28-C29-C39
19	BW	101	V7N	C27-C28-C29-C39
19	Bc	1202	V7N	C19-C20-C21-C22
19	Bd	102	V7N	C27-C28-C29-C39
12	BK	103	LMT	C3'-C4'-O1B-C1B
12	BV	103	LMT	C3'-C4'-O1B-C1B
12	BC	102	LMT	O5'-C5'-C6'-O6'
12	L	307	LMT	C4'-C5'-C6'-O6'
12	BX	101	LMT	C4B-C5B-C6B-O6B
13	L	310	MQ8	C46-C47-C48-C50
13	M	409	MQ8	C46-C47-C48-C49
17	AO	102	PEX	C5-C4-O4-C3
17	Bm	103	PEX	C5-C4-O4-C3
12	L	306	LMT	O5'-C5'-C6'-O6'
12	BB	103	LMT	O5B-C5B-C6B-O6B
12	Bc	1201	LMT	O5B-C5B-C6B-O6B
17	AT	103	PEX	O5-C4-O4-C3
12	L	304	LMT	C4B-C5B-C6B-O6B
12	BF	101	LMT	C4B-C5B-C6B-O6B
12	BH	101	LMT	C4'-C5'-C6'-O6'
12	AK	102	LMT	C4B-C5B-C6B-O6B
12	AQ	102	LMT	O5B-C1B-O1B-C4'
12	BN	102	LMT	O5'-C5'-C6'-O6'
10	BE	102	BCL	C4-C3-C5-C6
13	Ad	101	MQ8	C45-C43-C44-C46
10	AN	101	BCL	C2-C3-C5-C6
10	AO	101	BCL	C2-C3-C5-C6
10	AT	101	BCL	C2-C3-C5-C6
10	AW	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	Bp	1004	BCL	C2-C3-C5-C6
13	L	310	MQ8	C27-C28-C30-C31
13	Ad	101	MQ8	C42-C43-C44-C46
12	L	307	LMT	O5'-C5'-C6'-O6'
12	BF	101	LMT	O5B-C5B-C6B-O6B
13	M	409	MQ8	C28-C30-C31-C32
13	M	409	MQ8	C43-C44-C46-C47
13	Ad	101	MQ8	C43-C44-C46-C47
19	AI	103	V7N	C22-C23-C24-C25
19	BO	101	V7N	C22-C23-C24-C25
19	BV	101	V7N	C22-C23-C24-C25
19	BX	102	V7N	C22-C23-C24-C25
19	Bb	101	V7N	C22-C23-C24-C25
19	Bc	1202	V7N	C22-C23-C24-C25
19	Bf	102	V7N	C22-C23-C24-C25
19	Ag	102	V7N	C22-C23-C24-C25
19	Bg	1202	V7N	C22-C23-C24-C25
19	Bj	103	V7N	C22-C23-C24-C25
19	Bk	1202	V7N	C22-C23-C24-C25
19	Am	102	V7N	C22-C23-C24-C25
19	An	102	V7N	C22-C23-C24-C25
12	BU	101	LMT	C4'-C5'-C6'-O6'
12	L	304	LMT	O5B-C5B-C6B-O6B
12	BA	102	LMT	O5'-C5'-C6'-O6'
12	BP	102	LMT	O5B-C5B-C6B-O6B
12	L	309	LMT	C4B-C5B-C6B-O6B
12	BB	103	LMT	C4B-C5B-C6B-O6B
12	BP	102	LMT	C4'-C5'-C6'-O6'
12	Bc	1201	LMT	C4B-C5B-C6B-O6B
17	AO	102	PEX	O5-C4-O4-C3
17	Bm	103	PEX	O5-C4-O4-C3
12	L	304	LMT	O5'-C1'-O1'-C1
12	L	306	LMT	O5'-C1'-O1'-C1
12	BF	101	LMT	O5'-C1'-O1'-C1
12	Bc	1204	LMT	O5B-C5B-C6B-O6B
12	Bo	1201	LMT	O5B-C5B-C6B-O6B
12	BO	103	LMT	C4'-C5'-C6'-O6'
12	Bo	1201	LMT	C4'-C5'-C6'-O6'
13	L	310	MQ8	C40-C41-C42-C43
12	L	308	LMT	O5B-C5B-C6B-O6B
12	BG	101	LMT	O5B-C5B-C6B-O6B
12	BQ	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
12	Bm	104	LMT	O5B-C1B-O1B-C4'
13	L	310	MQ8	C21-C22-C23-C24
12	L	306	LMT	O5B-C5B-C6B-O6B
12	M	407	LMT	O5'-C5'-C6'-O6'
12	BG	101	LMT	O5'-C5'-C6'-O6'
12	BX	101	LMT	O5B-C5B-C6B-O6B
13	L	310	MQ8	C21-C22-C23-C25
12	BX	104	LMT	C4'-C5'-C6'-O6'
19	BO	101	V7N	C27-C28-C29-C39
19	Ba	101	V7N	C27-C28-C29-C39
19	Bm	101	V7N	C27-C28-C29-C39
12	BH	101	LMT	O5'-C5'-C6'-O6'
12	BI	1103	LMT	O5B-C5B-C6B-O6B
12	BL	103	LMT	O5'-C5'-C6'-O6'
12	M	407	LMT	C4'-C5'-C6'-O6'
12	BQ	102	LMT	C4'-C5'-C6'-O6'
12	Bo	1201	LMT	C4B-C5B-C6B-O6B
12	L	306	LMT	C4B-C5B-C6B-O6B
12	BG	101	LMT	C4'-C5'-C6'-O6'
10	BV	102	BCL	C4-C3-C5-C6
10	Bc	1203	BCL	C4-C3-C5-C6
13	L	310	MQ8	C29-C28-C30-C31
13	Ad	101	MQ8	C14-C13-C15-C16
19	Bd	102	V7N	C37-C22-C23-C24
10	BE	102	BCL	C2-C3-C5-C6
10	BL	102	BCL	C2-C3-C5-C6
10	BV	102	BCL	C2-C3-C5-C6
10	Bc	1203	BCL	C2-C3-C5-C6
13	M	409	MQ8	C27-C28-C30-C31
13	Ad	101	MQ8	C12-C13-C15-C16
19	Bd	102	V7N	C21-C22-C23-C24
10	BB	101	BCL	C11-C10-C8-C9
10	Bh	101	BCL	C11-C12-C13-C14
10	An	101	BCL	C11-C10-C8-C9
11	L	303	BPH	C14-C13-C15-C16
11	M	405	BPH	C6-C7-C8-C9
12	Bj	102	LMT	O5B-C5B-C6B-O6B
12	L	306	LMT	C4'-C5'-C6'-O6'
12	L	309	LMT	C4'-C5'-C6'-O6'
12	BP	102	LMT	C4B-C5B-C6B-O6B
12	L	304	LMT	C2'-C1'-O1'-C1
12	L	306	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
12	BF	101	LMT	C2'-C1'-O1'-C1
12	BB	103	LMT	O5'-C5'-C6'-O6'
12	BT	103	LMT	O5B-C5B-C6B-O6B
12	BC	102	LMT	C4B-C5B-C6B-O6B
12	AK	102	LMT	C4'-C5'-C6'-O6'
19	BB	102	V7N	C38-C26-C27-C28
19	BC	103	V7N	C38-C26-C27-C28
19	BD	103	V7N	C38-C26-C27-C28
19	BE	101	V7N	C3-C4-C5-C33
19	AH	102	V7N	C38-C26-C27-C28
19	AI	101	V7N	C36-C18-C19-C20
19	AL	102	V7N	C36-C18-C19-C20
19	BL	101	V7N	C38-C26-C27-C28
19	BR	103	V7N	C38-C26-C27-C28
19	BS	103	V7N	C38-C26-C27-C28
19	BT	102	V7N	C38-C26-C27-C28
19	AX	101	V7N	C36-C18-C19-C20
19	BX	102	V7N	C38-C26-C27-C28
19	BX	102	V7N	C3-C4-C5-C33
19	Ba	101	V7N	C38-C26-C27-C28
19	Bc	1202	V7N	C36-C18-C19-C20
19	Bf	102	V7N	C38-C26-C27-C28
19	Ag	102	V7N	C38-C26-C27-C28
19	Bg	1202	V7N	C3-C4-C5-C33
19	Bi	1202	V7N	C38-C26-C27-C28
19	Bl	102	V7N	C11-C12-C13-C35
19	Bl	102	V7N	C3-C4-C5-C33
19	Am	102	V7N	C11-C12-C13-C35
19	Am	102	V7N	C38-C26-C27-C28
19	BB	102	V7N	C25-C26-C27-C28
19	BC	103	V7N	C25-C26-C27-C28
19	BD	103	V7N	C25-C26-C27-C28
19	BE	101	V7N	C3-C4-C5-C6
19	AH	102	V7N	C25-C26-C27-C28
19	AP	101	V7N	C25-C26-C27-C28
19	BR	103	V7N	C25-C26-C27-C28
19	BX	102	V7N	C25-C26-C27-C28
19	BX	102	V7N	C3-C4-C5-C6
19	Ba	101	V7N	C25-C26-C27-C28
19	Bc	1202	V7N	C25-C26-C27-C28
19	Ad	102	V7N	C25-C26-C27-C28
19	Bf	102	V7N	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	Bg	1202	V7N	C3-C4-C5-C6
19	Bj	103	V7N	C25-C26-C27-C28
19	Bl	102	V7N	C3-C4-C5-C6
10	AC	101	BCL	C2A-CAA-CBA-CGA
17	AG	1101	PEX	C4-C5-C6-C7
12	M	407	LMT	C1-C2-C3-C4
12	BC	102	LMT	O5B-C5B-C6B-O6B
12	AK	102	LMT	O5'-C5'-C6'-O6'
12	BC	102	LMT	C4'-C5'-C6'-O6'
17	Bp	1005	PEX	C4-C5-C6-C7
10	BI	1102	BCL	C2-C1-O2A-CGA
10	Ba	102	BCL	C2-C1-O2A-CGA
12	BA	102	LMT	C4B-C5B-C6B-O6B
13	L	310	MQ8	C36-C37-C38-C39
10	Bf	101	BCL	C15-C16-C17-C18
10	Aj	101	BCL	C15-C16-C17-C18
12	BA	102	LMT	O5B-C5B-C6B-O6B
12	BI	1101	LMT	O5B-C5B-C6B-O6B
17	Bl	104	PEX	C4-C5-C6-C7
10	BM	101	BCL	C10-C11-C12-C13
12	BO	103	LMT	O5'-C5'-C6'-O6'
10	Bg	1203	BCL	C6-C7-C8-C10
12	BQ	102	LMT	O1'-C1-C2-C3
11	M	405	BPH	C4-C3-C5-C6
12	L	307	LMT	O5B-C5B-C6B-O6B
12	L	308	LMT	O5'-C5'-C6'-O6'
12	BN	102	LMT	O5B-C5B-C6B-O6B
12	BX	104	LMT	O5'-C5'-C6'-O6'
12	L	307	LMT	C4B-C5B-C6B-O6B
19	AI	103	V7N	C27-C28-C29-C39
19	BK	104	V7N	C27-C28-C29-C39
19	BL	101	V7N	C27-C28-C29-C39
19	BN	103	V7N	C27-C28-C29-C39
19	BP	103	V7N	C27-C28-C29-C39
19	BS	103	V7N	C27-C28-C29-C39
19	BT	102	V7N	C27-C28-C29-C39
12	BK	101	LMT	O1'-C1-C2-C3
12	Ba	104	LMT	O5B-C5B-C6B-O6B
13	L	310	MQ8	C13-C15-C16-C17
13	L	310	MQ8	C23-C25-C26-C27
13	L	310	MQ8	C38-C40-C41-C42
13	Ad	101	MQ8	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	Ad	101	MQ8	C28-C30-C31-C32
19	Ad	102	V7N	C22-C23-C24-C25
19	Bi	1202	V7N	C22-C23-C24-C25
19	Bl	102	V7N	C22-C23-C24-C25
12	BN	102	LMT	C4B-C5B-C6B-O6B
12	Bl	105	LMT	C4B-C5B-C6B-O6B
12	Bc	1201	LMT	O1'-C1-C2-C3
17	AT	103	PEX	C4-C5-C6-C7
10	Bf	101	BCL	C8-C10-C11-C12
18	C	1001	HEC	C3D-CAD-CBD-CGD
10	BJ	101	BCL	C2A-CAA-CBA-CGA
19	BS	103	V7N	C26-C27-C28-C29
19	BX	102	V7N	C26-C27-C28-C29
10	Bo	1202	BCL	C5-C6-C7-C8
17	Bf	104	PEX	C14-C15-C16-C17
17	Bj	104	PEX	C4-C5-C6-C7
12	Bl	105	LMT	O5B-C1B-O1B-C4'
12	M	407	LMT	O5'-C1'-O1'-C1
12	BN	102	LMT	O5'-C1'-O1'-C1
10	AK	101	BCL	C15-C16-C17-C18
10	Bc	1203	BCL	C8-C10-C11-C12
10	Bl	101	BCL	C15-C16-C17-C18
10	Bm	102	BCL	C13-C15-C16-C17
12	BA	102	LMT	O1'-C1-C2-C3
10	Ae	101	BCL	C13-C15-C16-C17
12	Bo	1201	LMT	O5B-C1B-O1B-C4'
12	Bk	1201	LMT	O1'-C1-C2-C3
12	Bo	1201	LMT	O1'-C1-C2-C3
17	AG	1101	PEX	C14-C15-C16-C17
12	Bl	105	LMT	O5B-C5B-C6B-O6B
17	Bd	104	PEX	C5-C4-O4-C3
17	Bp	1005	PEX	C5-C6-C7-C8
19	AH	102	V7N	C27-C28-C29-C39
19	Am	102	V7N	C19-C20-C21-C22
15	Af	101	CD4	C29-C30-C31-O10
10	BD	101	BCL	C2A-CAA-CBA-CGA
10	BN	101	BCL	C2A-CAA-CBA-CGA
10	BO	102	BCL	C2A-CAA-CBA-CGA
10	AQ	101	BCL	C2A-CAA-CBA-CGA
10	BS	101	BCL	C2A-CAA-CBA-CGA
10	AX	102	BCL	C2A-CAA-CBA-CGA
17	AG	1101	PEX	C5-C4-O4-C3

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Mol	Chain	Res	Type	Atoms
12	BC	102	LMT	O1'-C1-C2-C3
10	AQ	103	BCL	C10-C11-C12-C13
10	Aa	101	BCL	C15-C16-C17-C18
10	Bo	1202	BCL	C10-C11-C12-C13
17	Bl	104	PEX	C9-C10-C11-C12
12	BN	102	LMT	C4'-C5'-C6'-O6'
10	Bl	103	BCL	C13-C15-C16-C17
10	Bg	1203	BCL	C5-C6-C7-C8
10	L	302	BCL	C4B-C3B-CAB-OBB
10	L	302	BCL	C4B-C3B-CAB-CBB
10	M	403	BCL	C4B-C3B-CAB-OBB
10	M	403	BCL	C4B-C3B-CAB-CBB
10	Bc	1203	BCL	C6-C7-C8-C9
12	BU	101	LMT	C4B-C5B-C6B-O6B
13	M	409	MQ8	C41-C42-C43-C45
12	M	407	LMT	C2'-C1'-O1'-C1
12	BB	103	LMT	C2'-C1'-O1'-C1
12	BC	102	LMT	C2'-C1'-O1'-C1
12	BL	103	LMT	C2'-C1'-O1'-C1
12	BM	102	LMT	C2'-C1'-O1'-C1
12	BN	102	LMT	C2'-C1'-O1'-C1
12	BP	102	LMT	C2'-C1'-O1'-C1
12	BR	102	LMT	O1'-C1-C2-C3
12	L	309	LMT	O5'-C5'-C6'-O6'
12	BU	101	LMT	O5B-C5B-C6B-O6B
10	Bh	101	BCL	C10-C11-C12-C13
19	AI	101	V7N	C3-C4-C5-C33
19	BK	104	V7N	C36-C18-C19-C20
19	BK	104	V7N	C3-C4-C5-C33
19	BL	101	V7N	C3-C4-C5-C33
19	BV	101	V7N	C38-C26-C27-C28
19	AX	101	V7N	C3-C4-C5-C33
19	Bc	1202	V7N	C38-C26-C27-C28
19	Ad	102	V7N	C38-C26-C27-C28
19	Bd	102	V7N	C38-C26-C27-C28
19	Bj	103	V7N	C38-C26-C27-C28
19	Bj	103	V7N	C3-C4-C5-C33
19	AI	101	V7N	C3-C4-C5-C6
19	BK	104	V7N	C3-C4-C5-C6
19	BL	101	V7N	C3-C4-C5-C6
19	BS	103	V7N	C25-C26-C27-C28
19	BV	101	V7N	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	AX	101	V7N	C3-C4-C5-C6
19	Bd	102	V7N	C25-C26-C27-C28
19	Bl	102	V7N	C11-C12-C13-C14
19	Am	102	V7N	C25-C26-C27-C28
17	Bd	104	PEX	O5-C4-O4-C3
10	BA	101	BCL	C2A-CAA-CBA-CGA
10	BQ	101	BCL	C2A-CAA-CBA-CGA
10	BR	101	BCL	C2A-CAA-CBA-CGA
10	BW	102	BCL	C2A-CAA-CBA-CGA
12	BP	102	LMT	C4-C5-C6-C7
12	Bd	105	LMT	O1'-C1-C2-C3
12	BC	102	LMT	O5'-C1'-O1'-C1
12	BL	103	LMT	O5'-C1'-O1'-C1
12	BP	102	LMT	O5'-C1'-O1'-C1
12	Bc	1204	LMT	O5'-C1'-O1'-C1
10	Bf	103	BCL	C8-C10-C11-C12
17	Be	102	PEX	C14-C15-C16-C17
10	Bl	103	BCL	C2-C1-O2A-CGA
19	Ad	102	V7N	C43-C39-C40-O44
19	Ad	102	V7N	C43-C39-C40-O45
17	AG	1101	PEX	O5-C4-O4-C3
12	Bo	1201	LMT	C5-C6-C7-C8
17	Bf	104	PEX	C11-C10-C9-C8
17	Bg	1204	PEX	C6-C7-C8-C9
17	Bl	104	PEX	C18-C19-C20-C21
12	BF	101	LMT	C11-C10-C9-C8
12	BG	101	LMT	C3-C4-C5-C6
12	BK	101	LMT	C1-C2-C3-C4
12	BK	103	LMT	C5-C6-C7-C8
17	AT	103	PEX	C11-C10-C9-C8
12	BK	101	LMT	C2-C1-O1'-C1'
12	BP	102	LMT	C2-C1-O1'-C1'
12	BQ	102	LMT	C2-C1-O1'-C1'
12	BT	103	LMT	C2-C1-O1'-C1'
12	BV	103	LMT	C2-C1-O1'-C1'
12	BX	101	LMT	C2-C1-O1'-C1'
12	Bp	1002	LMT	C2-C1-O1'-C1'
17	Bk	1204	PEX	C7-C8-C9-C10
17	Bp	1005	PEX	C9-C10-C11-C12
17	Bk	1204	PEX	C18-C19-C20-C21
10	BX	103	BCL	C2A-CAA-CBA-CGA
17	Bg	1204	PEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	Bi	1204	PEX	C18-C19-C20-C21
17	Bl	104	PEX	C6-C7-C8-C9
17	Bg	1204	PEX	O3-C1-C2-C3
12	BK	103	LMT	C2-C3-C4-C5
17	Bk	1204	PEX	C16-C17-C18-C19
17	Bb	102	PEX	C4-C5-C6-C7
17	Bi	1204	PEX	C4-C5-C6-C7
17	Bn	102	PEX	C4-C5-C6-C7
12	Bi	1201	LMT	O5B-C5B-C6B-O6B
12	Bc	1201	LMT	C5-C6-C7-C8
12	Bk	1201	LMT	C7-C8-C9-C10
17	Bp	1005	PEX	C11-C10-C9-C8
12	BV	103	LMT	C4'-C5'-C6'-O6'
12	BX	101	LMT	C4'-C5'-C6'-O6'
12	Bc	1204	LMT	C4B-C5B-C6B-O6B
10	AB	101	BCL	C3A-C2A-CAA-CBA
10	Bf	103	BCL	C3A-C2A-CAA-CBA
10	Bh	102	BCL	C3A-C2A-CAA-CBA
10	Bk	1203	BCL	C3A-C2A-CAA-CBA
10	Bn	101	BCL	C3A-C2A-CAA-CBA
10	Bp	1004	BCL	C3A-C2A-CAA-CBA
12	L	306	LMT	C6-C7-C8-C9
12	M	407	LMT	C3-C4-C5-C6
12	BI	1101	LMT	C1-C2-C3-C4
12	BI	1103	LMT	C1-C2-C3-C4
12	Bl	105	LMT	C4-C5-C6-C7
12	Bl	105	LMT	O1'-C1-C2-C3
12	Bi	1201	LMT	C5-C6-C7-C8
12	BF	101	LMT	C3-C4-C5-C6
12	BX	104	LMT	C6-C7-C8-C9
12	Bp	1002	LMT	C3-C4-C5-C6
10	Bn	101	BCL	C8-C10-C11-C12
12	BI	1101	LMT	C3-C4-C5-C6
12	BL	103	LMT	C7-C8-C9-C10
12	BO	103	LMT	C4-C5-C6-C7
12	BV	103	LMT	C5'-C4'-O1B-C1B
12	L	309	LMT	C3-C4-C5-C6
17	Bn	102	PEX	C6-C7-C8-C9
12	Bi	1201	LMT	C4-C5-C6-C7
17	M	408	PEX	C18-C19-C20-C21
12	L	308	LMT	C1-C2-C3-C4
12	BC	102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	Bd	105	LMT	C5-C6-C7-C8
17	Bk	1204	PEX	C6-C7-C8-C9
12	Bm	104	LMT	C1-C2-C3-C4
12	BB	103	LMT	C5-C6-C7-C8
12	BX	101	LMT	C4-C5-C6-C7
12	BS	102	LMT	C3-C4-C5-C6
12	L	308	LMT	C4B-C5B-C6B-O6B
10	Bh	101	BCL	C4-C3-C5-C6
17	Bj	104	PEX	C18-C19-C20-C21
17	Bn	102	PEX	C19-C20-C21-C22
19	BR	103	V7N	C26-C27-C28-C29
19	AT	102	V7N	C26-C27-C28-C29
10	Bh	101	BCL	C2-C3-C5-C6
11	M	405	BPH	C2-C3-C5-C6
12	BK	103	LMT	O5B-C5B-C6B-O6B
12	BX	101	LMT	C5-C6-C7-C8
12	L	305	LMT	C2'-C1'-O1'-C1
17	M	408	PEX	C16-C17-C18-C19
12	BH	101	LMT	C1-C2-C3-C4
12	BX	101	LMT	C3-C4-C5-C6
12	AQ	102	LMT	C1-C2-C3-C4
12	BG	101	LMT	C4B-C5B-C6B-O6B
17	AG	1101	PEX	C16-C17-C18-C19
12	BK	101	LMT	C5-C6-C7-C8
12	BK	103	LMT	C5'-C4'-O1B-C1B
12	Bp	1002	LMT	O1'-C1-C2-C3
12	L	308	LMT	C6-C7-C8-C9
19	AX	101	V7N	C17-C18-C19-C20
12	Bj	102	LMT	C5-C6-C7-C8
12	BT	103	LMT	O1'-C1-C2-C3
10	AK	101	BCL	C2A-CAA-CBA-CGA
10	Bd	101	BCL	C16-C17-C18-C20
10	Bj	101	BCL	C3-C5-C6-C7
10	AR	101	BCL	C8-C10-C11-C12
10	Bj	101	BCL	C13-C15-C16-C17
12	BX	104	LMT	C4-C5-C6-C7
19	BL	101	V7N	C22-C23-C24-C25
12	BD	102	LMT	C1-C2-C3-C4
10	Bd	101	BCL	C8-C10-C11-C12
12	BL	103	LMT	C4-C5-C6-C7
17	Bj	104	PEX	C5-C6-C7-C8
12	BL	103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
17	Bk	1204	PEX	C11-C10-C9-C8
10	Bp	1001	BCL	C15-C16-C17-C18
12	L	308	LMT	C4-C5-C6-C7
10	BH	102	BCL	C2-C1-O2A-CGA
12	BX	104	LMT	O5B-C5B-C6B-O6B
12	BQ	102	LMT	C4-C5-C6-C7
12	Bo	1201	LMT	C4-C5-C6-C7
10	BL	102	BCL	C2A-CAA-CBA-CGA
12	AK	102	LMT	C1-C2-C3-C4
10	AI	102	BCL	C13-C15-C16-C17
10	Bh	102	BCL	C10-C11-C12-C13
10	Aj	101	BCL	C5-C6-C7-C8
17	Bn	102	PEX	C14-C15-C16-C17
12	BG	103	LMT	C1-C2-C3-C4
12	BT	103	LMT	C4B-C5B-C6B-O6B
12	Bj	102	LMT	C4B-C5B-C6B-O6B
17	Bb	102	PEX	C7-C8-C9-C10
10	AB	101	BCL	C1A-C2A-CAA-CBA
10	Bf	103	BCL	C1A-C2A-CAA-CBA
10	Bp	1004	BCL	C1A-C2A-CAA-CBA
10	AM	101	BCL	C8-C10-C11-C12
12	Bj	102	LMT	C4-C5-C6-C7
12	Bl	105	LMT	C5-C6-C7-C8
17	Bf	104	PEX	C16-C17-C18-C19
10	AP	102	BCL	C5-C6-C7-C8
12	BQ	102	LMT	O5B-C5B-C6B-O6B
10	BP	104	BCL	C6-C7-C8-C10
10	Be	101	BCL	C11-C12-C13-C15
10	Bo	1202	BCL	C11-C12-C13-C15
10	Bl	101	BCL	C16-C17-C18-C20
12	Bg	1201	LMT	O5B-C5B-C6B-O6B
19	BV	101	V7N	C30-C1-C2-C3
19	AX	101	V7N	C30-C1-C2-C3
19	BX	102	V7N	C30-C1-C2-C3
19	Bc	1202	V7N	C30-C1-C2-C3
19	Ad	102	V7N	C30-C1-C2-C3
17	AG	1101	PEX	C5-C6-C7-C8
10	AC	101	BCL	C10-C11-C12-C13
17	M	408	PEX	C5-C6-C7-C8
17	Bm	103	PEX	C15-C16-C17-C18
10	BE	102	BCL	C2A-CAA-CBA-CGA
10	Ak	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	AO	101	BCL	C11-C12-C13-C14
10	BV	102	BCL	C14-C13-C15-C16
10	Bg	1203	BCL	C11-C10-C8-C9
12	BV	103	LMT	O5'-C5'-C6'-O6'
12	AB	102	LMT	C1-C2-C3-C4
12	BQ	102	LMT	C5-C6-C7-C8
12	BX	101	LMT	C2'-C1'-O1'-C1
12	Bc	1204	LMT	C2'-C1'-O1'-C1
12	BX	101	LMT	O5'-C5'-C6'-O6'
15	M	402	CD4	C32-C33-C34-O14
15	Af	101	CD4	C32-C33-C34-O14
17	Bg	1204	PEX	C1-C2-C3-O4
12	BO	103	LMT	C7-C8-C9-C10
12	Bg	1205	LMT	C5-C6-C7-C8
12	BS	102	LMT	O5B-C5B-C6B-O6B
12	BD	102	LMT	C3-C4-C5-C6
19	Bk	1202	V7N	C2-C1-O32-C41
10	AN	101	BCL	C13-C15-C16-C17
12	Bd	105	LMT	C4-C5-C6-C7
17	Bm	103	PEX	C5-C6-C7-C8
12	Bk	1201	LMT	O5B-C5B-C6B-O6B
19	AL	102	V7N	C38-C26-C27-C28
19	Ba	101	V7N	C3-C4-C5-C33
19	Ag	102	V7N	C3-C4-C5-C33
19	Bi	1202	V7N	C3-C4-C5-C33
19	Am	102	V7N	C3-C4-C5-C33
19	Bp	1003	V7N	C3-C4-C5-C33
12	BU	101	LMT	C2-C3-C4-C5
19	BL	101	V7N	C25-C26-C27-C28
19	BT	102	V7N	C25-C26-C27-C28
19	Bd	102	V7N	C3-C4-C5-C6
19	Bf	102	V7N	C3-C4-C5-C6
17	AO	102	PEX	C15-C16-C17-C18
12	BN	102	LMT	C6-C7-C8-C9
10	L	302	BCL	C2B-C3B-CAB-OBB
10	L	302	BCL	C2B-C3B-CAB-CBB
10	M	403	BCL	C2B-C3B-CAB-OBB
10	M	403	BCL	C2B-C3B-CAB-CBB
10	An	101	BCL	O2A-C1-C2-C3
12	BI	1103	LMT	C4-C5-C6-C7
12	Bc	1201	LMT	C4-C5-C6-C7
17	Bp	1005	PEX	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	AH	102	V7N	C26-C27-C28-C29
10	Ai	101	BCL	C10-C11-C12-C13
12	BA	102	LMT	C4-C5-C6-C7
12	BF	101	LMT	C4-C5-C6-C7
17	Bj	104	PEX	C16-C17-C18-C19
10	AB	101	BCL	C3-C5-C6-C7
12	Bp	1002	LMT	C2-C3-C4-C5
12	BB	103	LMT	O1'-C1-C2-C3
17	AG	1101	PEX	O3-C1-C2-O6
17	Bb	102	PEX	C6-C7-C8-C9
17	Bk	1204	PEX	C9-C10-C11-C12
17	Bb	102	PEX	C9-C10-C11-C12
12	Bi	1201	LMT	C5'-C4'-O1B-C1B
10	BI	1102	BCL	C4-C3-C5-C6
10	AU	102	BCL	C2-C3-C5-C6
17	Bg	1204	PEX	C17-C18-C19-C20
12	BD	102	LMT	C2-C3-C4-C5
12	L	309	LMT	C9-C10-C11-C12
17	AT	103	PEX	C14-C15-C16-C17
12	BA	102	LMT	C4'-C5'-C6'-O6'
12	BM	102	LMT	C4B-C5B-C6B-O6B
10	BH	102	BCL	CAA-CBA-CGA-O2A
10	BL	102	BCL	CAA-CBA-CGA-O2A
17	Bd	104	PEX	C6-C7-C8-C9
12	Bi	1201	LMT	O1'-C1-C2-C3
12	L	306	LMT	C11-C10-C9-C8
12	BQ	102	LMT	C6-C7-C8-C9
19	Ad	102	V7N	C29-C39-C40-O44
19	Ad	102	V7N	C29-C39-C40-O45
19	An	102	V7N	C43-C39-C40-O44
19	An	102	V7N	C43-C39-C40-O45
12	BD	102	LMT	C4B-C5B-C6B-O6B
17	Bp	1005	PEX	C5-C4-O4-C3
16	M	406	CRT	C39-C38-O2-C2M
16	M	406	CRT	C40-C38-O2-C2M
19	Bk	1202	V7N	C30-C1-O32-C41
19	Bm	101	V7N	C31-C1-O32-C41
12	L	304	LMT	C5'-C4'-O1B-C1B
13	M	409	MQ8	C36-C37-C38-C39
12	BD	102	LMT	C5-C6-C7-C8
10	AN	101	BCL	C10-C11-C12-C13
10	AU	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	Bc	1202	V7N	C37-C22-C23-C24
12	BT	103	LMT	C9-C10-C11-C12
17	M	408	PEX	C5-C4-O4-C3
10	AM	101	BCL	C10-C11-C12-C13
12	L	309	LMT	C11-C10-C9-C8
12	L	304	LMT	C2-C1-O1'-C1'
12	BD	102	LMT	C2-C1-O1'-C1'
12	BI	1103	LMT	C2-C1-O1'-C1'
10	BP	104	BCL	C6-C7-C8-C9
10	AQ	101	BCL	C6-C7-C8-C9
10	Aa	101	BCL	C6-C7-C8-C9
10	Af	102	BCL	C11-C10-C8-C9
10	Aj	101	BCL	C11-C10-C8-C9
10	Bk	1203	BCL	C11-C10-C8-C9
10	Am	101	BCL	C11-C12-C13-C14
12	Bg	1201	LMT	C5-C6-C7-C8
17	AG	1101	PEX	C9-C10-C11-C12
10	Bm	102	BCL	C10-C11-C12-C13
10	AQ	101	BCL	C13-C15-C16-C17
12	BX	104	LMT	C5'-C4'-O1B-C1B
10	AD	101	BCL	C16-C17-C18-C20
10	An	101	BCL	C2A-CAA-CBA-CGA
17	Be	102	PEX	C15-C16-C17-C18
12	BK	103	LMT	C2'-C1'-O1'-C1
12	AQ	102	LMT	C5-C6-C7-C8
17	Ba	103	PEX	C11-C10-C9-C8
17	Ba	103	PEX	O3-C1-C2-C3
17	Bj	104	PEX	C11-C10-C9-C8
10	AD	101	BCL	C11-C10-C8-C7
10	AT	104	BCL	C11-C12-C13-C15
10	BV	102	BCL	C12-C13-C15-C16
10	Bg	1203	BCL	C11-C10-C8-C7
10	Aj	101	BCL	C11-C10-C8-C7
10	Bk	1203	BCL	C11-C10-C8-C7
10	An	101	BCL	C11-C10-C8-C7
10	Bo	1202	BCL	C12-C13-C15-C16
10	Ah	101	BCL	C15-C16-C17-C18
12	Bi	1201	LMT	O5'-C5'-C6'-O6'
10	Ah	101	BCL	C4-C3-C5-C6
17	Bd	104	PEX	C14-C15-C16-C17
17	Bm	103	PEX	C9-C10-C11-C12
19	Ba	101	V7N	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	Bf	102	V7N	C3-C4-C5-C33
12	BO	103	LMT	C3-C4-C5-C6
19	Ba	101	V7N	C3-C4-C5-C6
17	AG	1101	PEX	C11-C10-C9-C8
12	Bi	1201	LMT	C4'-C5'-C6'-O6'
17	Bg	1204	PEX	C20-C21-C22-C23
15	Af	101	CD4	C47-C48-C49-C50
17	AG	1101	PEX	C1-C2-C3-O4
17	Ba	103	PEX	C1-C2-C3-O4
17	Bd	104	PEX	C1-C2-C3-O4
10	Bd	101	BCL	C16-C17-C18-C19
17	Bm	103	PEX	C18-C19-C20-C21
19	Bc	1202	V7N	C21-C22-C23-C24
12	Ba	104	LMT	C5-C6-C7-C8
17	Bb	102	PEX	O3-C1-C2-O6
15	Af	101	CD4	O9-C30-C31-O10
12	BM	102	LMT	O5B-C5B-C6B-O6B
12	Bi	1201	LMT	C3'-C4'-O1B-C1B
17	Bf	104	PEX	C6-C7-C8-C9
12	BS	102	LMT	C6-C7-C8-C9
12	Ba	104	LMT	C3-C4-C5-C6
12	BC	102	LMT	C2-C3-C4-C5
15	M	402	CD4	O16-C33-C34-O14
15	Af	101	CD4	O2-C15-C16-O3
17	Bd	104	PEX	O6-C2-C3-O4
10	Ba	102	BCL	C8-C10-C11-C12
12	BN	102	LMT	C11-C10-C9-C8
10	Ah	101	BCL	C2-C3-C5-C6
12	Ba	104	LMT	C4-C5-C6-C7
12	Bp	1002	LMT	C5-C6-C7-C8
17	Be	102	PEX	C16-C17-C18-C19
12	Bi	1201	LMT	C3-C4-C5-C6
10	AB	101	BCL	C10-C11-C12-C13
10	AH	101	BCL	C15-C16-C17-C18
10	Bo	1202	BCL	C11-C12-C13-C14
12	BR	102	LMT	C11-C10-C9-C8
12	L	305	LMT	O5'-C1'-O1'-C1
12	BI	1101	LMT	O5'-C1'-O1'-C1
12	Bg	1201	LMT	O5'-C1'-O1'-C1
12	BI	1103	LMT	C4B-C5B-C6B-O6B
12	BI	1101	LMT	C4B-C5B-C6B-O6B
10	Bf	103	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	Ad	101	MQ8	C13-C15-C16-C17
19	Bm	101	V7N	C22-C23-C24-C25
10	AD	101	BCL	C4C-C3C-CAC-CBC
10	Bg	1203	BCL	C4C-C3C-CAC-CBC
10	BF	102	BCL	C2A-CAA-CBA-CGA
17	Bf	104	PEX	C4-C5-C6-C7
12	BK	103	LMT	O1'-C1-C2-C3
19	Bf	102	V7N	C13-C14-C15-C16
10	AD	101	BCL	C16-C17-C18-C19
12	L	306	LMT	C3-C4-C5-C6
12	Bl	105	LMT	C4'-C5'-C6'-O6'
10	AP	102	BCL	C13-C15-C16-C17
17	AG	1101	PEX	O3-C1-C2-C3
10	Bl	101	BCL	C16-C17-C18-C19
10	Bj	101	BCL	C5-C6-C7-C8
19	BW	101	V7N	C38-C26-C27-C28
19	Bb	101	V7N	C3-C4-C5-C33
19	Bd	102	V7N	C3-C4-C5-C33
19	Ag	102	V7N	C11-C12-C13-C35
19	An	102	V7N	C3-C4-C5-C33
12	AB	102	LMT	C3-C4-C5-C6
10	AC	101	BCL	C6-C7-C8-C10
10	Bc	1203	BCL	C12-C13-C15-C16
10	Bl	101	BCL	C11-C12-C13-C15
10	Bl	101	BCL	C12-C13-C15-C16
19	Ad	102	V7N	C1-C2-C3-C4
19	Bl	102	V7N	C1-C2-C3-C4
19	Bm	101	V7N	C1-C2-C3-C4
12	L	307	LMT	C11-C10-C9-C8
19	AL	102	V7N	C25-C26-C27-C28
19	BW	101	V7N	C25-C26-C27-C28
19	Bb	101	V7N	C3-C4-C5-C6
19	Bc	1202	V7N	C17-C18-C19-C20
19	Ag	102	V7N	C3-C4-C5-C6
19	Bi	1202	V7N	C3-C4-C5-C6
19	Am	102	V7N	C3-C4-C5-C6
19	An	102	V7N	C3-C4-C5-C6
19	Bp	1003	V7N	C3-C4-C5-C6
17	M	408	PEX	O5-C4-O4-C3
10	BT	101	BCL	C4-C3-C5-C6
13	L	310	MQ8	C24-C23-C25-C26
12	BA	102	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	AB	102	LMT	O5B-C1B-O1B-C4'
10	Aj	101	BCL	O2A-C1-C2-C3
17	Bf	104	PEX	C3-C2-O6-C14
19	Ba	101	V7N	C7-C8-C9-C10
19	Bd	102	V7N	C7-C8-C9-C10
19	Bg	1202	V7N	C7-C8-C9-C10
19	Bi	1202	V7N	C7-C8-C9-C10
19	Am	102	V7N	C7-C8-C9-C10
17	Bp	1005	PEX	O5-C4-O4-C3
12	L	308	LMT	C4'-C5'-C6'-O6'
12	AK	102	LMT	C5-C6-C7-C8
12	Bj	102	LMT	O1'-C1-C2-C3
12	L	306	LMT	C4-C5-C6-C7
12	BL	103	LMT	C4'-C5'-C6'-O6'
10	BE	102	BCL	CAA-CBA-CGA-O2A
15	M	402	CD4	O2-C15-C28-O5
17	Bg	1204	PEX	O3-C1-C2-O6
17	Bk	1204	PEX	O3-C1-C2-O6
12	L	307	LMT	O5'-C1'-O1'-C1
12	Bi	1201	LMT	O5'-C1'-O1'-C1
17	Bf	104	PEX	C1-C2-C3-O4
10	BI	1102	BCL	C2-C3-C5-C6
12	BC	102	LMT	C9-C10-C11-C12
12	BV	103	LMT	C4-C5-C6-C7
17	Bf	104	PEX	C25-C24-O8-P1
17	Bg	1204	PEX	C25-C24-O8-P1
19	AF	102	V7N	O42-C34-C9-C10
19	BS	103	V7N	O42-C34-C9-C10
19	Bp	1003	V7N	O42-C34-C9-C10
12	Bp	1002	LMT	C4'-C5'-C6'-O6'
10	Af	102	BCL	C15-C16-C17-C18
17	Bn	102	PEX	C18-C19-C20-C21
17	Bf	104	PEX	O6-C2-C3-O4
10	AC	101	BCL	C6-C7-C8-C9
10	AP	102	BCL	C14-C13-C15-C16
10	Bd	103	BCL	C6-C7-C8-C9
12	BQ	102	LMT	C7-C8-C9-C10
19	AF	102	V7N	O32-C1-C2-C3
19	Bk	1202	V7N	O32-C1-C2-C3
17	Ba	103	PEX	C7-C8-C9-C10
10	Bf	103	BCL	C2-C1-O2A-CGA
11	M	405	BPH	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
10	Bf	103	BCL	C15-C16-C17-C18
19	An	102	V7N	C29-C39-C40-O45
10	AQ	101	BCL	C8-C10-C11-C12
12	Bc	1204	LMT	C1-C2-C3-C4
12	BO	103	LMT	C5-C6-C7-C8
12	BS	102	LMT	C5'-C4'-O1B-C1B
17	Bm	103	PEX	C17-C18-C19-C20
10	Bm	102	BCL	C1A-C2A-CAA-CBA
10	Bn	101	BCL	C4-C3-C5-C6
13	L	310	MQ8	C14-C13-C15-C16
12	BK	101	LMT	C4B-C5B-C6B-O6B
19	BK	104	V7N	C17-C18-C19-C20
13	L	310	MQ8	C36-C37-C38-C40
12	BS	102	LMT	C4-C5-C6-C7
12	BN	102	LMT	C7-C8-C9-C10
15	Af	101	CD4	C22-C23-C24-C25
15	M	402	CD4	C16-C15-C28-O5
17	Bb	102	PEX	O3-C1-C2-C3
17	Bj	104	PEX	O3-C1-C2-C3
17	Bk	1204	PEX	O3-C1-C2-C3
12	Ba	104	LMT	O5B-C1B-O1B-C4'
10	Bh	101	BCL	C11-C12-C13-C15
10	An	101	BCL	C11-C12-C13-C15
17	Bj	104	PEX	C6-C7-C8-C9
12	L	305	LMT	O1'-C1-C2-C3
19	BV	101	V7N	C31-C1-C2-C3
19	BX	102	V7N	C31-C1-C2-C3
19	Ad	102	V7N	C31-C1-C2-C3
17	Ba	103	PEX	C18-C19-C20-C21
12	BI	1103	LMT	C5'-C4'-O1B-C1B
12	BI	1103	LMT	C2-C3-C4-C5
10	AK	101	BCL	C10-C11-C12-C13
12	BD	102	LMT	C6-C7-C8-C9
18	C	1000	HEC	C4C-C3C-CAC-CBC
18	C	1001	HEC	C4C-C3C-CAC-CBC
18	C	1003	HEC	C4C-C3C-CAC-CBC
12	BB	103	LMT	C4'-C5'-C6'-O6'
10	Bp	1001	BCL	C16-C17-C18-C19
12	L	307	LMT	C5'-C4'-O1B-C1B
17	AO	102	PEX	O3-C1-C2-O6
17	Bj	104	PEX	O3-C1-C2-O6
17	AG	1101	PEX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
12	BU	101	LMT	C1-C2-C3-C4
10	AT	104	BCL	C11-C12-C13-C14
10	Bg	1203	BCL	C6-C7-C8-C9
10	Bl	101	BCL	C11-C12-C13-C14
19	BL	101	V7N	C5-C6-C7-C8
19	AX	101	V7N	C27-C28-C29-C39
19	Am	102	V7N	C9-C10-C11-C12
15	M	402	CD4	C49-C50-C51-C52
17	AO	102	PEX	C19-C20-C21-C22
12	L	305	LMT	C7-C8-C9-C10
17	AG	1101	PEX	O6-C2-C3-O4
17	Bj	104	PEX	O6-C2-C3-O4
17	AO	102	PEX	C1-C2-C3-O4
17	Bl	104	PEX	C1-C2-C3-O4
17	Bp	1005	PEX	C1-C2-C3-O4
17	AO	102	PEX	C17-C18-C19-C20
17	Bg	1204	PEX	C15-C16-C17-C18
10	Bn	101	BCL	C3-C5-C6-C7
17	AO	102	PEX	C18-C19-C20-C21
10	BP	104	BCL	CAD-CBD-CGD-O2D
12	BF	101	LMT	C6-C7-C8-C9
17	Bg	1204	PEX	C5-C4-O4-C3
17	Bl	104	PEX	C5-C4-O4-C3
12	BI	1103	LMT	O5'-C1'-O1'-C1
12	L	304	LMT	C3-C4-C5-C6
12	BS	102	LMT	C7-C8-C9-C10
10	Bl	101	BCL	C5-C6-C7-C8
10	BP	104	BCL	CAD-CBD-CGD-O1D
15	M	402	CD4	C31-O10-P2-O11
15	Af	101	CD4	C32-O13-P2-O12
17	AT	103	PEX	C1-O3-P1-O1
17	Bd	104	PEX	C1-O3-P1-O2
17	Bd	104	PEX	C24-O8-P1-O1
17	Bf	104	PEX	C24-O8-P1-O2
17	Bf	104	PEX	O8-C24-C25-N1
17	Bg	1204	PEX	C24-O8-P1-O3
17	Bl	104	PEX	C24-O8-P1-O3
17	Bm	103	PEX	C1-O3-P1-O2
17	Bm	103	PEX	C24-O8-P1-O3
17	Bn	102	PEX	C1-O3-P1-O2
19	BE	101	V7N	C5-C6-C7-C8
19	BX	102	V7N	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	Bd	102	V7N	C13-C14-C15-C16
19	Am	102	V7N	C5-C6-C7-C8
12	Bk	1201	LMT	C6-C7-C8-C9
10	Bj	101	BCL	C4-C3-C5-C6
17	Bl	104	PEX	C15-C14-O6-C2
17	Bg	1204	PEX	C2-C1-O3-P1
19	Ag	102	V7N	C11-C12-C13-C14
17	Ba	103	PEX	C10-C11-C12-C13
12	BA	102	LMT	C3-C4-C5-C6
17	AT	103	PEX	C17-C18-C19-C20
12	BN	102	LMT	C3-C4-C5-C6
10	Bn	101	BCL	C10-C11-C12-C13
12	BD	102	LMT	O5B-C5B-C6B-O6B
12	Bo	1201	LMT	C5'-C4'-O1B-C1B
10	Bp	1004	BCL	O2A-C1-C2-C3
17	Be	102	PEX	C18-C19-C20-C21
10	BV	102	BCL	CAA-CBA-CGA-O2A
10	BO	102	BCL	C13-C15-C16-C17
12	BX	101	LMT	C7-C8-C9-C10
10	Bl	101	BCL	C14-C13-C15-C16
10	An	101	BCL	C11-C12-C13-C14
10	Bo	1202	BCL	C14-C13-C15-C16
11	M	405	BPH	C6-C7-C8-C10
10	BW	102	BCL	CAA-CBA-CGA-O2A
17	Bg	1204	PEX	O5-C4-O4-C3
12	BF	101	LMT	C4'-C5'-C6'-O6'
10	Bh	102	BCL	C13-C15-C16-C17
17	Bl	104	PEX	O5-C4-O4-C3
10	BT	101	BCL	C2-C3-C5-C6
12	BV	103	LMT	C6-C7-C8-C9
12	Bc	1201	LMT	O5B-C1B-O1B-C4'
12	Bp	1002	LMT	O5B-C5B-C6B-O6B
17	Bp	1005	PEX	O4-C4-C5-C6
10	Aa	101	BCL	C10-C11-C12-C13
19	AI	101	V7N	C5-C6-C7-C8
19	Bk	1202	V7N	C27-C28-C29-C39
17	Bn	102	PEX	C5-C6-C7-C8
17	Bf	104	PEX	C20-C21-C22-C23
12	BL	103	LMT	O5B-C5B-C6B-O6B
10	AU	101	BCL	C16-C17-C18-C19
10	AU	101	BCL	C16-C17-C18-C20
12	M	407	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
10	Bj	101	BCL	C10-C11-C12-C13
10	AD	101	BCL	C8-C10-C11-C12
10	BW	102	BCL	C2-C1-O2A-CGA
10	Ag	101	BCL	C2-C1-O2A-CGA
10	AC	101	BCL	C4-C3-C5-C6
13	Ad	101	MQ8	C39-C38-C40-C41
12	Bp	1002	LMT	C5'-C4'-O1B-C1B
19	Ba	101	V7N	C29-C39-C40-O44
19	Ba	101	V7N	C43-C39-C40-O44
19	An	102	V7N	C29-C39-C40-O44
10	Bl	101	BCL	C10-C11-C12-C13
13	M	409	MQ8	C18-C20-C21-C22
19	BN	103	V7N	C22-C23-C24-C25
10	Ai	101	BCL	C8-C10-C11-C12
19	AI	103	V7N	C30-C1-O32-C41
19	Bk	1202	V7N	C31-C1-O32-C41
15	M	402	CD4	C12-C13-C14-O2
12	L	309	LMT	C4-C5-C6-C7
10	BP	101	BCL	C2A-CAA-CBA-CGA
10	AU	101	BCL	C2A-CAA-CBA-CGA
16	M	406	CRT	C20-C21-C22-C23
19	Bb	101	V7N	C19-C20-C21-C22
19	Bb	101	V7N	C5-C6-C7-C8
19	Bg	1202	V7N	C5-C6-C7-C8
19	Bi	1202	V7N	C13-C14-C15-C16
12	Bl	105	LMT	O5'-C1'-O1'-C1
10	Bj	101	BCL	C2-C3-C5-C6
13	L	310	MQ8	C12-C13-C15-C16
10	BL	102	BCL	CAA-CBA-CGA-O1A
12	BC	102	LMT	C2-C1-O1'-C1'
12	BK	103	LMT	C2-C1-O1'-C1'
12	BL	103	LMT	C2-C1-O1'-C1'
12	BO	103	LMT	C2-C1-O1'-C1'
12	BR	102	LMT	C2-C1-O1'-C1'
10	BR	101	BCL	CAA-CBA-CGA-O2A
17	Bl	104	PEX	O4-C4-C5-C6
12	BG	101	LMT	C1-C2-C3-C4
10	AE	101	BCL	C11-C12-C13-C14
17	AT	103	PEX	C2-C1-O3-P1
12	BI	1101	LMT	C5-C6-C7-C8
17	Bg	1204	PEX	C9-C10-C11-C12
13	M	409	MQ8	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
12	BX	101	LMT	C6-C7-C8-C9
13	Ad	101	MQ8	C37-C38-C40-C41
17	Bl	104	PEX	C16-C17-C18-C19
12	Bg	1205	LMT	C5'-C4'-O1B-C1B
13	Ad	101	MQ8	C38-C40-C41-C42
19	BD	103	V7N	C27-C28-C29-C39
19	AL	102	V7N	C27-C28-C29-C39
19	BX	102	V7N	C19-C20-C21-C22
19	Bg	1202	V7N	C13-C14-C15-C16
12	Bl	105	LMT	C3-C4-C5-C6
10	BA	101	BCL	C12-C13-C15-C16
10	BB	101	BCL	C6-C7-C8-C10
10	BV	102	BCL	C11-C10-C8-C7
10	Aa	101	BCL	C11-C12-C13-C15
19	BN	103	V7N	O42-C34-C9-C8
19	Ag	102	V7N	O42-C34-C9-C8
10	AF	101	BCL	C15-C16-C17-C18
17	Bf	104	PEX	C9-C10-C11-C12
10	Bd	103	BCL	C3A-C2A-CAA-CBA
10	Bm	102	BCL	C3A-C2A-CAA-CBA
12	BP	102	LMT	C3-C4-C5-C6
10	AC	101	BCL	C2-C3-C5-C6
10	Bg	1203	BCL	C2A-CAA-CBA-CGA
12	Bc	1204	LMT	C5-C6-C7-C8
10	BL	102	BCL	C2-C1-O2A-CGA
10	AT	101	BCL	C2-C1-O2A-CGA
10	AW	101	BCL	C2-C1-O2A-CGA
11	L	303	BPH	C2C-C3C-CAC-CBC
12	Bm	104	LMT	C3-C4-C5-C6
12	BR	102	LMT	C3-C4-C5-C6
17	Bl	104	PEX	C17-C18-C19-C20
12	BO	103	LMT	O1'-C1-C2-C3
10	AB	101	BCL	C4-C3-C5-C6
10	Bg	1203	BCL	C4-C3-C5-C6
19	AF	102	V7N	C37-C22-C23-C24
17	Bd	104	PEX	C16-C17-C18-C19
10	BC	101	BCL	C13-C15-C16-C17
10	BN	101	BCL	C13-C15-C16-C17
10	BH	102	BCL	CAA-CBA-CGA-O1A
10	BC	101	BCL	C6-C7-C8-C9
10	AR	101	BCL	C11-C12-C13-C14
10	AW	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	Aa	101	BCL	C11-C12-C13-C14
10	Be	101	BCL	C14-C13-C15-C16
17	AT	103	PEX	C20-C21-C22-C23
12	BI	1103	LMT	C7-C8-C9-C10
12	BR	102	LMT	C1-C2-C3-C4
12	BH	101	LMT	C9-C10-C11-C12
17	M	408	PEX	C1-C2-O6-C14
17	Bl	104	PEX	O7-C14-O6-C2
17	Bb	102	PEX	C11-C10-C9-C8
10	AB	101	BCL	C2-C3-C5-C6
10	Bg	1203	BCL	C2-C3-C5-C6
10	AD	101	BCL	C1A-C2A-CAA-CBA
10	Ba	102	BCL	C1A-C2A-CAA-CBA
10	Bd	103	BCL	C1A-C2A-CAA-CBA
17	Bn	102	PEX	C5-C4-O4-C3
12	L	304	LMT	C4'-C5'-C6'-O6'
12	Ba	104	LMT	C4B-C5B-C6B-O6B
12	AB	102	LMT	C2B-C1B-O1B-C4'
10	Bn	101	BCL	C15-C16-C17-C18
10	AH	101	BCL	C10-C11-C12-C13
10	BS	101	BCL	C4-C3-C5-C6
19	BT	102	V7N	C37-C22-C23-C24
12	Bo	1201	LMT	C3-C4-C5-C6
17	Bd	104	PEX	C7-C8-C9-C10
10	AE	101	BCL	C11-C12-C13-C15
10	AF	101	BCL	C11-C10-C8-C7
10	BT	101	BCL	C11-C12-C13-C15
10	AW	101	BCL	C11-C12-C13-C15
10	Ah	101	BCL	C6-C7-C8-C10
12	BU	101	LMT	C3-C4-C5-C6
10	Ah	101	BCL	C16-C17-C18-C20
19	AX	101	V7N	C31-C1-C2-C3
19	Bc	1202	V7N	C31-C1-C2-C3
19	Bk	1202	V7N	C30-C1-C2-C3
19	An	102	V7N	C11-C12-C13-C35
17	AG	1101	PEX	O4-C4-C5-C6
13	L	310	MQ8	C22-C23-C25-C26
13	M	409	MQ8	C22-C23-C25-C26
19	AF	102	V7N	C21-C22-C23-C24
12	Ba	104	LMT	C2-C3-C4-C5
19	Ba	101	V7N	C43-C39-C40-O45
10	Ae	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	Bg	1203	BCL	C8-C10-C11-C12
17	AG	1101	PEX	C10-C11-C12-C13
12	BI	1103	LMT	C3-C4-C5-C6
17	Bl	104	PEX	C5-C6-C7-C8
12	BO	103	LMT	O5'-C1'-O1'-C1
10	Bp	1001	BCL	C4-C3-C5-C6
13	L	310	MQ8	C19-C18-C20-C21
19	BW	101	V7N	C37-C22-C23-C24
17	Bl	104	PEX	C2-C1-O3-P1
17	Bn	102	PEX	O5-C4-O4-C3
17	Bm	103	PEX	C19-C20-C21-C22
12	BI	1101	LMT	C2'-C1'-O1'-C1
19	BP	103	V7N	C22-C23-C24-C25
17	Bi	1204	PEX	C5-C6-C7-C8
12	AK	102	LMT	C5'-C4'-O1B-C1B
17	Bg	1204	PEX	O7-C14-O6-C2
19	BF	103	V7N	C37-C22-C23-C24
12	L	306	LMT	C5-C6-C7-C8
12	BV	103	LMT	C3-C4-C5-C6
10	Bp	1001	BCL	C2-C3-C5-C6
10	Ah	101	BCL	C16-C17-C18-C19
10	AK	101	BCL	C8-C10-C11-C12
17	Bg	1204	PEX	C7-C8-C9-C10
12	AK	102	LMT	O5B-C1B-O1B-C4'
10	AQ	103	BCL	C16-C17-C18-C20
12	AQ	102	LMT	O5B-C5B-C6B-O6B
10	BK	102	BCL	C10-C11-C12-C13
17	AO	102	PEX	O3-C1-C2-C3
12	BB	103	LMT	C9-C10-C11-C12
10	BW	102	BCL	C4-C3-C5-C6
15	Af	101	CD4	C7-C8-C9-C10
10	Bd	101	BCL	C15-C16-C17-C18
13	L	310	MQ8	C17-C18-C20-C21
12	BK	101	LMT	O5'-C1'-O1'-C1
17	Ba	103	PEX	C2-C1-O3-P1
12	Bo	1201	LMT	C2B-C1B-O1B-C4'
10	Bc	1203	BCL	C5-C6-C7-C8
17	AO	102	PEX	C10-C11-C12-C13
19	Ag	102	V7N	C5-C6-C7-C8
10	BT	101	BCL	C11-C12-C13-C14
10	AU	101	BCL	C11-C10-C8-C9
10	Ao	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	BP	102	LMT	C1-C2-C3-C4
15	M	402	CD4	C11-C10-C9-C8
10	Bg	1203	BCL	C15-C16-C17-C18
10	AD	101	BCL	C2-C1-O2A-CGA
10	BF	102	BCL	C2-C1-O2A-CGA
10	BN	101	BCL	C2-C1-O2A-CGA
10	AT	104	BCL	C2-C1-O2A-CGA
10	Ai	101	BCL	C2-C1-O2A-CGA
12	Bc	1204	LMT	C5'-C4'-O1B-C1B
10	AT	104	BCL	C4-C3-C5-C6
10	Bn	101	BCL	C2-C3-C5-C6
12	Ba	104	LMT	C2B-C1B-O1B-C4'
10	Ak	101	BCL	C5-C6-C7-C8
10	Ac	101	BCL	O2A-C1-C2-C3
10	Bc	1203	BCL	O2A-C1-C2-C3
10	Ag	101	BCL	O2A-C1-C2-C3
10	Am	101	BCL	O2A-C1-C2-C3
19	Ba	101	V7N	C26-C27-C28-C29
12	AB	102	LMT	C5'-C4'-O1B-C1B
17	Be	102	PEX	C7-C8-C9-C10
17	AO	102	PEX	C6-C7-C8-C9
13	M	409	MQ8	C41-C42-C43-C44
12	BI	1103	LMT	C3'-C4'-O1B-C1B
12	BT	103	LMT	C11-C10-C9-C8
17	Bl	104	PEX	C10-C11-C12-C13
17	Bd	104	PEX	O3-C1-C2-O6
12	BD	102	LMT	O5'-C1'-O1'-C1
12	BM	102	LMT	C7-C8-C9-C10
13	M	409	MQ8	C13-C15-C16-C17
17	Bj	104	PEX	C1-C2-C3-O4
10	AB	101	BCL	C5-C6-C7-C8
12	BH	101	LMT	C11-C10-C9-C8
15	M	402	CD4	C48-C49-C50-C51
17	Bb	102	PEX	C18-C19-C20-C21
12	BV	103	LMT	C1-C2-C3-C4
10	Bp	1001	BCL	C16-C17-C18-C20
17	AT	103	PEX	C16-C17-C18-C19
17	Bb	102	PEX	C5-C6-C7-C8
12	Bc	1204	LMT	O1'-C1-C2-C3
12	Ba	104	LMT	C5'-C4'-O1B-C1B
17	Bk	1204	PEX	O6-C2-C3-O4
10	AN	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	Af	102	BCL	C11-C12-C13-C14
10	Am	101	BCL	C14-C13-C15-C16
10	Bm	102	BCL	C14-C13-C15-C16
10	AQ	103	BCL	C16-C17-C18-C19
10	AT	101	BCL	CAA-CBA-CGA-O2A
17	Bn	102	PEX	O6-C14-C15-C16
12	BP	102	LMT	C9-C10-C11-C12
15	M	402	CD4	O13-C32-C33-C34
17	Bd	104	PEX	O3-C1-C2-C3
10	M	403	BCL	C15-C16-C17-C18
15	Af	101	CD4	C26-C27-C60-C61
19	BV	101	V7N	O32-C1-C2-C3
12	BN	102	LMT	C4-C5-C6-C7
12	Bl	105	LMT	C2B-C1B-O1B-C4'
10	BB	101	BCL	C11-C10-C8-C7
10	BR	101	BCL	C11-C12-C13-C15
11	L	303	BPH	C12-C13-C15-C16
17	Bg	1204	PEX	C15-C14-O6-C2
10	Bh	101	BCL	CAA-CBA-CGA-O2A
17	Bm	103	PEX	C16-C17-C18-C19
10	L	301	BCL	C2-C1-O2A-CGA
10	AN	101	BCL	C2-C1-O2A-CGA
10	Bd	103	BCL	C2-C1-O2A-CGA
10	Bi	1203	BCL	C2-C1-O2A-CGA
10	Bl	101	BCL	C2-C1-O2A-CGA
19	Ba	101	V7N	C29-C39-C40-O45
13	L	310	MQ8	C43-C44-C46-C47
10	AN	101	BCL	CAA-CBA-CGA-O2A
10	AU	102	BCL	CAA-CBA-CGA-O2A
10	Ba	102	BCL	CAA-CBA-CGA-O2A
17	Bb	102	PEX	O4-C4-C5-C6
12	L	305	LMT	C9-C10-C11-C12
13	Ad	101	MQ8	C29-C28-C30-C31
10	AH	101	BCL	CAA-CBA-CGA-O2A
10	BX	103	BCL	CAA-CBA-CGA-O2A
12	BL	103	LMT	C1-C2-C3-C4
13	Ad	101	MQ8	C27-C28-C30-C31
15	Af	101	CD4	C48-C49-C50-C51
19	AI	103	V7N	C31-C1-O32-C41
19	Bc	1202	V7N	C31-C1-O32-C41
19	Bj	103	V7N	C30-C1-O32-C41
19	Bj	103	V7N	C31-C1-O32-C41

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Mol	Chain	Res	Type	Atoms
10	AB	101	BCL	CAA-CBA-CGA-O2A
10	AL	101	BCL	CAA-CBA-CGA-O2A
10	AW	101	BCL	CAA-CBA-CGA-O2A
18	C	1000	HEC	CAA-CBA-CGA-O2A
10	AF	101	BCL	CAA-CBA-CGA-O2A
10	AM	101	BCL	CAA-CBA-CGA-O2A
10	Ai	101	BCL	CAA-CBA-CGA-O2A
17	Bi	1204	PEX	C17-C18-C19-C20
12	M	407	LMT	O1'-C1-C2-C3
12	M	407	LMT	C7-C8-C9-C10
17	Bp	1005	PEX	C16-C17-C18-C19
11	L	303	BPH	C8-C10-C11-C12
17	Bm	103	PEX	O6-C14-C15-C16
10	AF	101	BCL	C8-C10-C11-C12
10	Ae	101	BCL	C15-C16-C17-C18
18	C	1000	HEC	CAA-CBA-CGA-O1A
10	AF	101	BCL	C11-C10-C8-C9
10	BR	101	BCL	C11-C12-C13-C14
10	Bf	103	BCL	C14-C13-C15-C16
10	Ao	101	BCL	C14-C13-C15-C16
10	Bm	102	BCL	C5-C6-C7-C8
15	Af	101	CD4	C12-C13-C14-O2
10	BS	101	BCL	C1A-C2A-CAA-CBA
17	Bk	1204	PEX	C17-C18-C19-C20
10	AH	101	BCL	C4-C3-C5-C6
12	BH	101	LMT	O5'-C1'-O1'-C1
10	AQ	101	BCL	CAA-CBA-CGA-O2A
15	M	402	CD4	O3-C17-C18-C19
17	AG	1101	PEX	O6-C14-C15-C16
17	Bi	1204	PEX	O6-C14-C15-C16
10	BS	101	BCL	C2-C3-C5-C6
19	BT	102	V7N	C21-C22-C23-C24
18	C	1001	HEC	CAD-CBD-CGD-O2D
19	An	102	V7N	C11-C12-C13-C14
19	Ag	102	V7N	C13-C14-C15-C16
12	Bl	105	LMT	C6-C7-C8-C9
10	BP	101	BCL	CAA-CBA-CGA-O2A
10	BH	102	BCL	C2A-CAA-CBA-CGA
10	Bn	101	BCL	C2A-CAA-CBA-CGA
12	L	307	LMT	C2'-C1'-O1'-C1
12	Bg	1201	LMT	C2'-C1'-O1'-C1
10	Bk	1203	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	L	308	LMT	O1'-C1-C2-C3
10	BO	102	BCL	CAA-CBA-CGA-O2A
19	AX	101	V7N	C37-C22-C23-C24
10	AL	101	BCL	C2-C1-O2A-CGA
10	Be	101	BCL	C2-C1-O2A-CGA
10	Aj	101	BCL	C2-C1-O2A-CGA
10	An	101	BCL	C2-C1-O2A-CGA
10	Bn	101	BCL	C2-C1-O2A-CGA
10	AU	101	BCL	CAA-CBA-CGA-O2A
10	AT	104	BCL	C6-C7-C8-C10
10	AU	101	BCL	C11-C10-C8-C7
10	Ba	102	BCL	C11-C10-C8-C7
10	Ao	101	BCL	C6-C7-C8-C10
12	AB	102	LMT	C5-C6-C7-C8
10	Bo	1202	BCL	O2A-C1-C2-C3
17	Bl	104	PEX	C7-C8-C9-C10
12	Bl	105	LMT	C5'-C4'-O1B-C1B
10	BK	102	BCL	CAA-CBA-CGA-O2A
17	Bk	1204	PEX	O6-C14-C15-C16
17	M	408	PEX	C11-C10-C9-C8
10	BX	103	BCL	CAA-CBA-CGA-O1A
19	AT	102	V7N	C27-C28-C29-C39
10	BV	102	BCL	C2A-CAA-CBA-CGA
10	Ba	102	BCL	C2A-CAA-CBA-CGA
10	BT	101	BCL	C16-C17-C18-C20
10	BJ	101	BCL	CAA-CBA-CGA-O2A
12	Ba	104	LMT	O1'-C1-C2-C3
17	Bp	1005	PEX	C2-C1-O3-P1
10	AD	101	BCL	C3A-C2A-CAA-CBA
10	BJ	101	BCL	C4-C3-C5-C6
10	Ba	102	BCL	C3A-C2A-CAA-CBA
19	Bg	1202	V7N	C37-C22-C23-C24
10	BE	102	BCL	CAA-CBA-CGA-O1A
10	AH	101	BCL	CAA-CBA-CGA-O1A
10	Bh	101	BCL	CAA-CBA-CGA-O1A
10	Ai	101	BCL	CAA-CBA-CGA-O1A
10	Bp	1001	BCL	C10-C11-C12-C13
10	AX	102	BCL	C5-C6-C7-C8
12	Bl	105	LMT	O5'-C5'-C6'-O6'
19	AP	101	V7N	C23-C24-C25-C26
10	AT	101	BCL	CAA-CBA-CGA-O1A
10	AW	101	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	Bc	1201	LMT	C2B-C1B-O1B-C4'
10	M	403	BCL	C11-C10-C8-C9
10	Ba	102	BCL	C11-C10-C8-C9
10	Bc	1203	BCL	C11-C12-C13-C14
17	Bb	102	PEX	C15-C16-C17-C18
12	Bp	1002	LMT	O5B-C1B-O1B-C4'
10	AB	101	BCL	C8-C10-C11-C12
10	BI	1102	BCL	C5-C6-C7-C8
10	AB	101	BCL	CAA-CBA-CGA-O1A
10	AN	101	BCL	CAA-CBA-CGA-O1A
10	AU	102	BCL	CAA-CBA-CGA-O1A
19	Ba	101	V7N	C1-C2-C3-C4
19	Bp	1003	V7N	C1-C2-C3-C4
10	AF	101	BCL	CAA-CBA-CGA-O1A
10	AE	101	BCL	C10-C11-C12-C13
10	BB	101	BCL	CAA-CBA-CGA-O2A
19	AH	102	V7N	C17-C18-C19-C20
19	BX	102	V7N	C17-C18-C19-C20
17	Bn	102	PEX	O7-C14-C15-C16
10	BL	102	BCL	C13-C15-C16-C17
15	Af	101	CD4	C10-C11-C12-C13
10	BQ	101	BCL	CAA-CBA-CGA-O2A
15	M	402	CD4	O14-C35-C36-C37
17	Bf	104	PEX	O4-C4-C5-C6
15	Af	101	CD4	C28-C15-C16-O3
18	C	1001	HEC	CAD-CBD-CGD-O1D
17	Bm	103	PEX	O7-C14-C15-C16
10	AC	101	BCL	C5-C6-C7-C8
10	AN	101	BCL	C8-C10-C11-C12
10	BP	104	BCL	C5-C6-C7-C8
10	BA	101	BCL	CAA-CBA-CGA-O2A
12	Bo	1201	LMT	C3'-C4'-O1B-C1B
17	AG	1101	PEX	O7-C14-C15-C16
10	AR	101	BCL	CAD-CBD-CGD-O2D
10	Af	102	BCL	CAD-CBD-CGD-O2D
19	Bj	103	V7N	C2-C1-O32-C41
10	AL	101	BCL	CAA-CBA-CGA-O1A
10	AQ	101	BCL	CAA-CBA-CGA-O1A
10	BS	101	BCL	C5-C6-C7-C8
10	Bc	1203	BCL	C2-C1-O2A-CGA
17	Bi	1204	PEX	C11-C10-C9-C8
15	Af	101	CD4	C12-C13-C14-O1

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Mol	Chain	Res	Type	Atoms
10	BI	1102	BCL	CAA-CBA-CGA-O2A
17	Bk	1204	PEX	O4-C4-C5-C6
10	Bd	103	BCL	C2A-CAA-CBA-CGA
10	Bi	1203	BCL	C2A-CAA-CBA-CGA
12	BT	103	LMT	C5'-C4'-O1B-C1B
10	AU	101	BCL	CAA-CBA-CGA-O1A
10	AQ	101	BCL	C15-C16-C17-C18
10	BP	101	BCL	C4-C3-C5-C6
17	Bp	1005	PEX	O6-C14-C15-C16
12	BG	103	LMT	C5'-C4'-O1B-C1B
10	AM	101	BCL	CAA-CBA-CGA-O1A
17	Bk	1204	PEX	O7-C14-C15-C16
10	Ac	101	BCL	CAA-CBA-CGA-O2A
10	Ak	101	BCL	C10-C11-C12-C13
15	M	402	CD4	O4-C17-C18-C19
17	AT	103	PEX	C18-C19-C20-C21

There are no ring outliers.

145 monomers are involved in 392 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AW	101	BCL	4	0
10	Bd	101	BCL	4	0
19	Am	102	V7N	1	0
10	Ak	101	BCL	1	0
10	AT	104	BCL	2	0
10	AU	101	BCL	3	0
10	Ag	101	BCL	1	0
10	Aa	101	BCL	7	0
10	BG	102	BCL	1	0
12	BC	102	LMT	2	0
12	BN	102	LMT	2	0
10	Bk	1203	BCL	4	0
12	Bl	105	LMT	1	0
10	L	302	BCL	3	0
19	Bp	1003	V7N	1	0
10	AR	101	BCL	6	0
12	AQ	102	LMT	1	0
17	Bb	102	PEX	4	0
17	Bp	1005	PEX	1	0
10	BF	102	BCL	2	0
10	BC	101	BCL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	BH	102	BCL	1	0
10	AX	102	BCL	2	0
13	Ad	101	MQ8	6	0
12	Bc	1201	LMT	2	0
10	AM	101	BCL	4	0
10	BV	102	BCL	3	0
10	Bp	1004	BCL	6	0
17	Bn	102	PEX	2	0
10	BP	101	BCL	1	0
10	Ao	101	BCL	1	0
10	Ae	101	BCL	2	0
12	Bj	102	LMT	3	0
10	An	101	BCL	4	0
17	Bd	104	PEX	1	0
10	Bp	1001	BCL	16	0
19	Bf	102	V7N	1	0
10	Ai	101	BCL	3	0
12	Bm	104	LMT	2	0
13	L	310	MQ8	6	0
10	Bl	103	BCL	1	0
12	BD	102	LMT	1	0
10	BE	102	BCL	2	0
10	Bh	101	BCL	7	0
12	BS	102	LMT	2	0
10	AI	102	BCL	4	0
10	BN	101	BCL	2	0
10	Be	101	BCL	4	0
10	BM	101	BCL	2	0
12	BL	103	LMT	2	0
10	BB	101	BCL	2	0
12	BG	103	LMT	1	0
19	BC	103	V7N	2	0
10	BS	101	BCL	2	0
10	BD	101	BCL	2	0
10	Bf	101	BCL	7	0
12	BT	103	LMT	3	0
12	BG	101	LMT	1	0
19	Bd	102	V7N	1	0
10	BW	102	BCL	2	0
10	Ba	102	BCL	6	0
12	Bp	1002	LMT	2	0
17	Ba	103	PEX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AO	102	PEX	4	0
10	Bh	102	BCL	2	0
15	Af	101	CD4	11	0
10	Bg	1203	BCL	4	0
12	BP	102	LMT	1	0
12	BO	103	LMT	2	0
17	AT	103	PEX	3	0
10	M	403	BCL	4	0
10	Bn	101	BCL	6	0
10	BQ	101	BCL	2	0
17	Be	102	PEX	5	0
12	BK	103	LMT	1	0
12	BU	101	LMT	2	0
12	AB	102	LMT	1	0
10	Bc	1203	BCL	6	0
12	BX	101	LMT	1	0
12	L	304	LMT	1	0
10	BL	102	BCL	2	0
11	M	405	BPH	3	0
18	C	1001	HEC	1	0
10	L	301	BCL	4	0
10	AH	101	BCL	2	0
10	Ah	101	BCL	6	0
17	Bm	103	PEX	3	0
12	Bg	1201	LMT	1	0
17	Bf	104	PEX	4	0
10	Bl	101	BCL	7	0
10	Bj	101	BCL	11	0
10	AU	102	BCL	3	0
12	BI	1101	LMT	3	0
10	AF	101	BCL	5	0
10	BP	104	BCL	5	0
12	Bk	1201	LMT	1	0
10	Al	101	BCL	1	0
10	Bf	103	BCL	7	0
10	Bo	1202	BCL	4	0
18	C	1003	HEC	1	0
12	L	309	LMT	1	0
10	AD	101	BCL	2	0
13	M	409	MQ8	10	0
15	M	402	CD4	3	0
12	BX	104	LMT	1	0

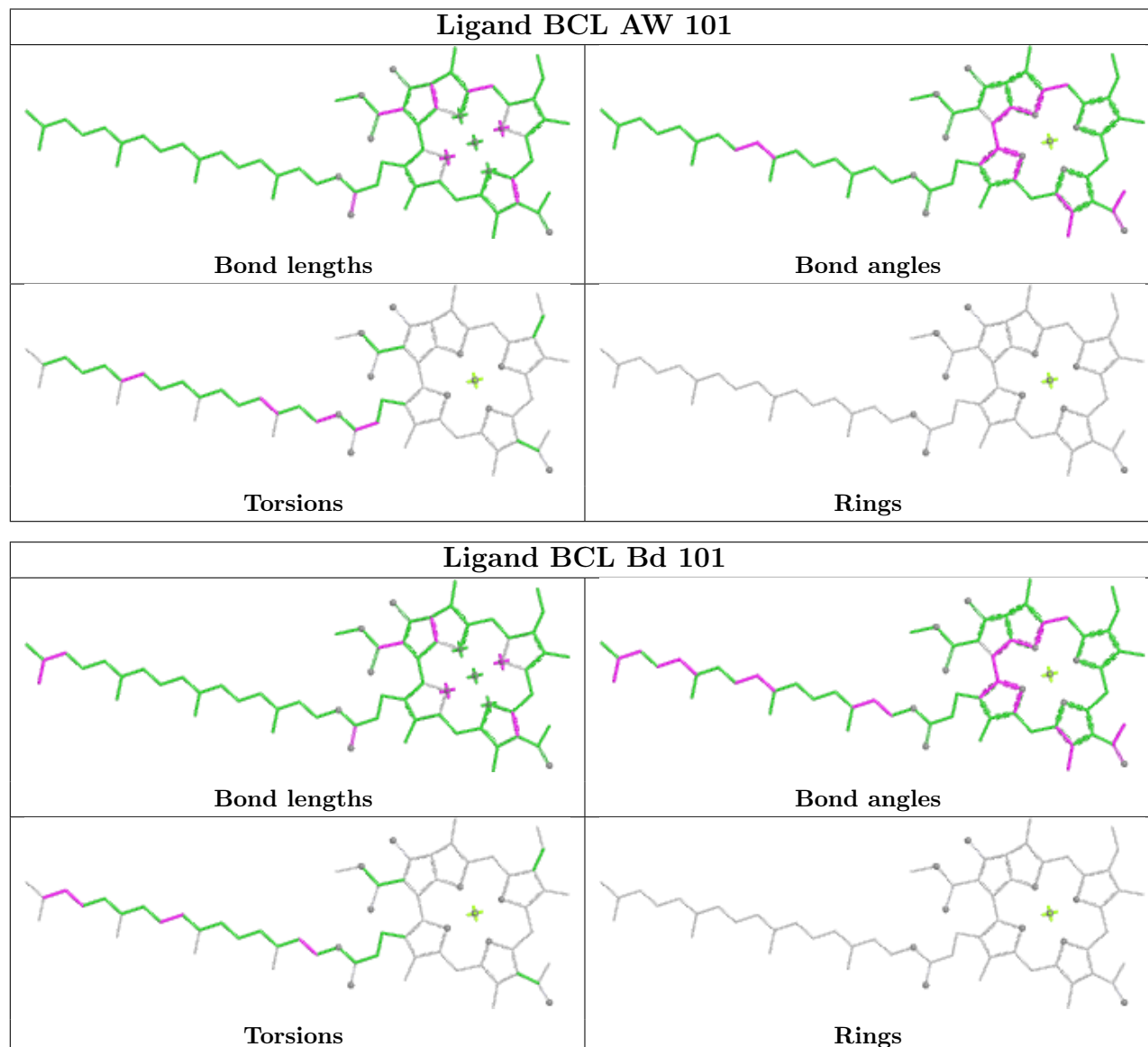
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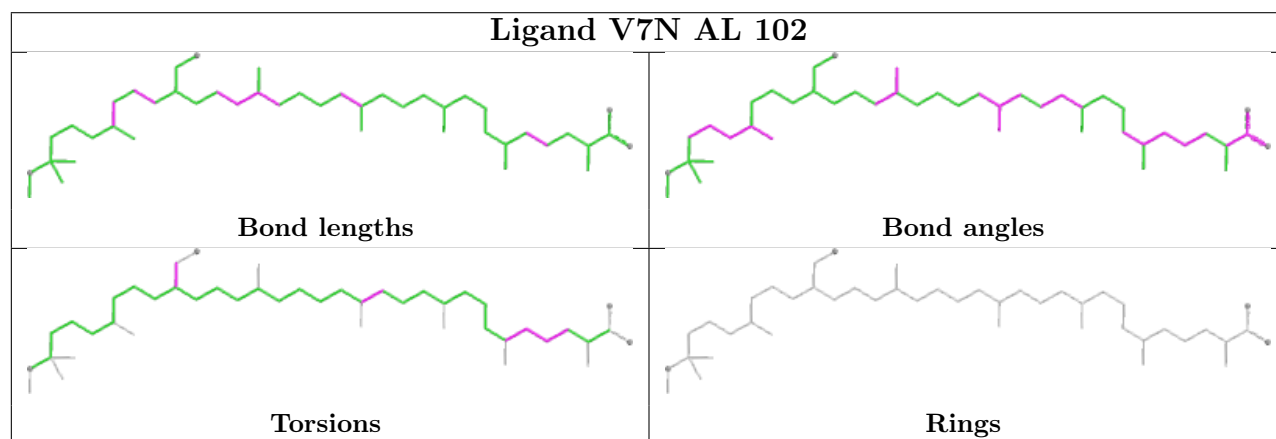
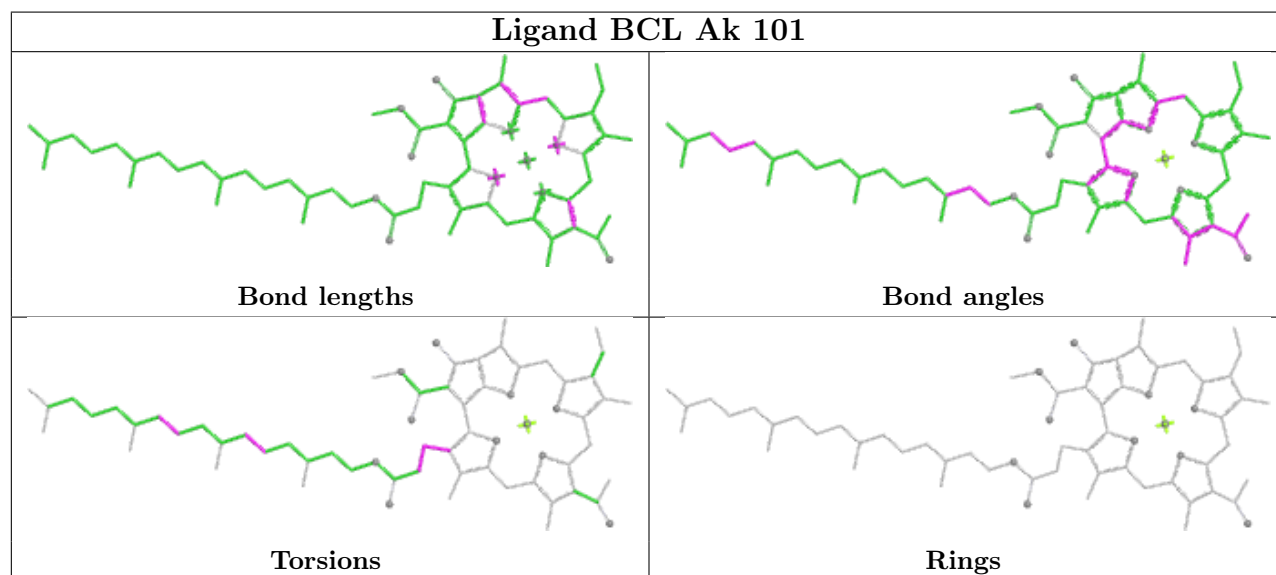
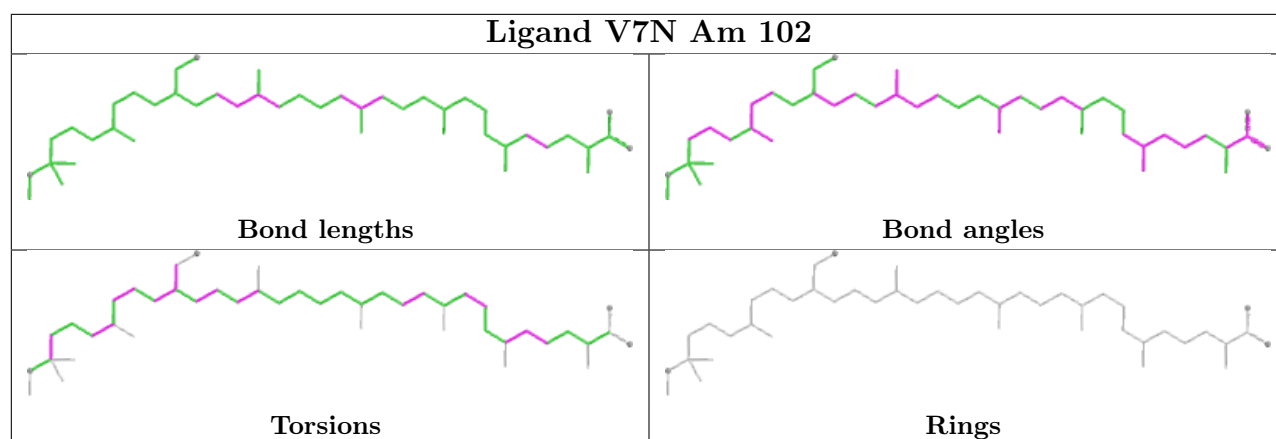
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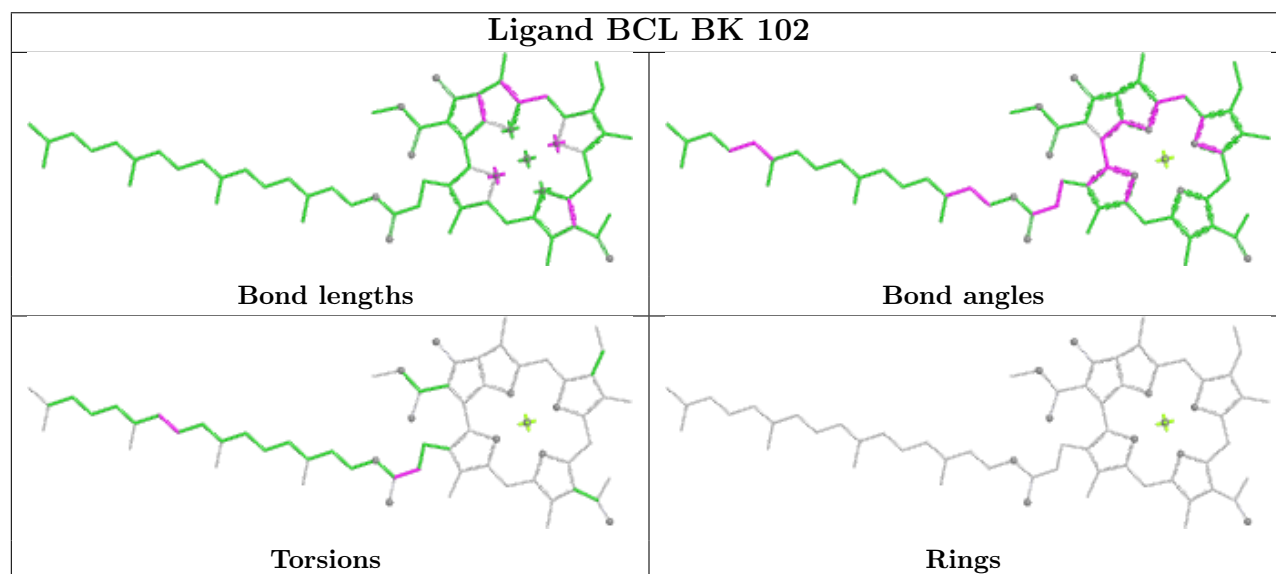
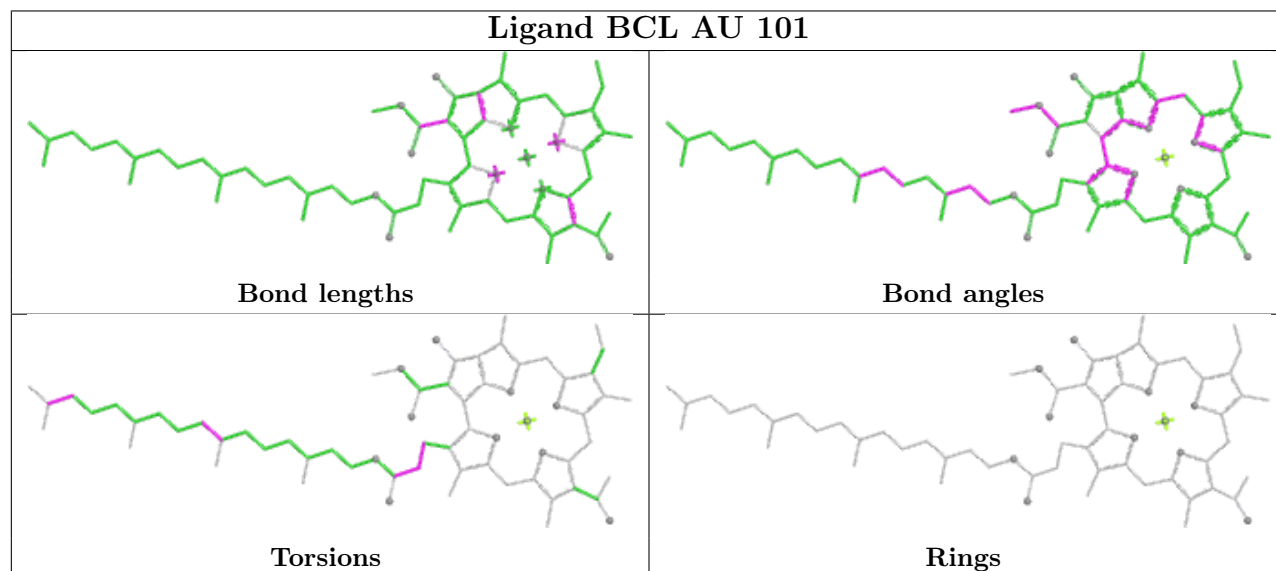
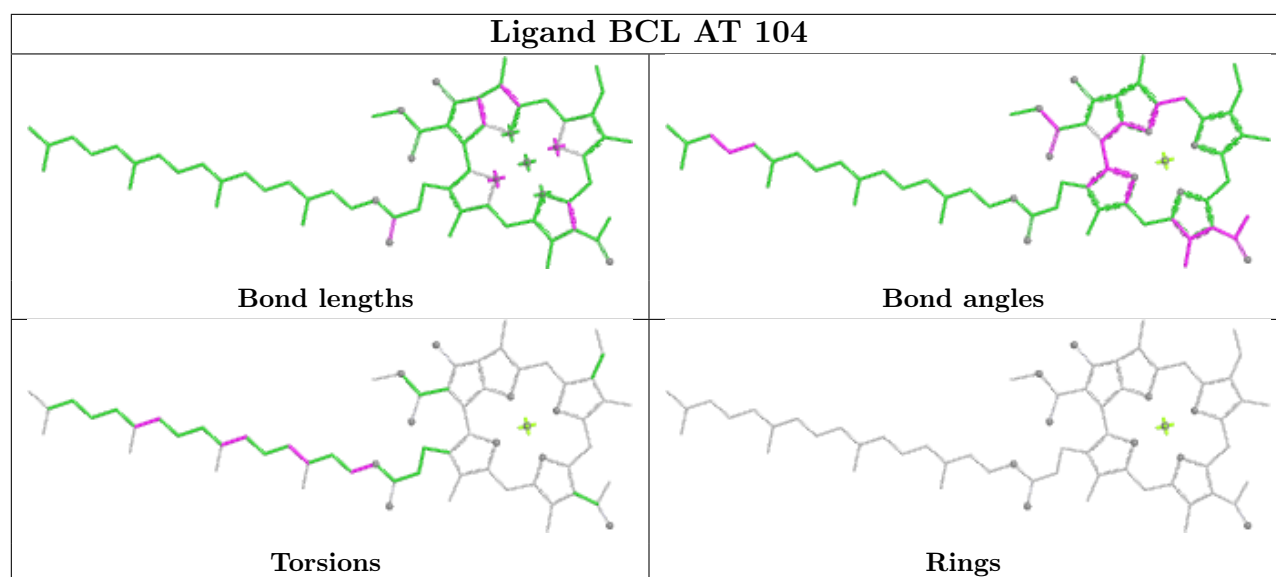
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	BI	1102	BCL	2	0
10	AQ	101	BCL	6	0
10	AO	101	BCL	7	0
10	BR	101	BCL	2	0
17	Bk	1204	PEX	4	0
12	Bi	1201	LMT	3	0
12	AK	102	LMT	2	0
10	AE	101	BCL	4	0
12	Ba	104	LMT	1	0
11	L	303	BPH	3	0
10	AB	101	BCL	4	0
10	AC	101	BCL	3	0
17	Bi	1204	PEX	5	0
12	BR	102	LMT	2	0
12	BI	1103	LMT	2	0
12	Bg	1205	LMT	1	0
19	BN	103	V7N	1	0
19	BB	102	V7N	1	0
10	AV	1001	BCL	3	0
10	Bi	1203	BCL	6	0
10	AK	101	BCL	5	0
10	Ac	101	BCL	4	0
12	BM	102	LMT	1	0
10	AL	101	BCL	2	0
10	BX	103	BCL	1	0
17	Bl	104	PEX	3	0
17	AG	1101	PEX	2	0
17	Bg	1204	PEX	3	0
10	AP	102	BCL	5	0
10	Bm	102	BCL	5	0
12	BK	101	LMT	1	0
10	Af	102	BCL	4	0
10	BO	102	BCL	1	0
10	Aj	101	BCL	6	0
17	Bj	104	PEX	3	0
19	BV	101	V7N	1	0
10	M	404	BCL	4	0
10	AQ	103	BCL	3	0
10	AN	101	BCL	1	0
10	Am	101	BCL	2	0

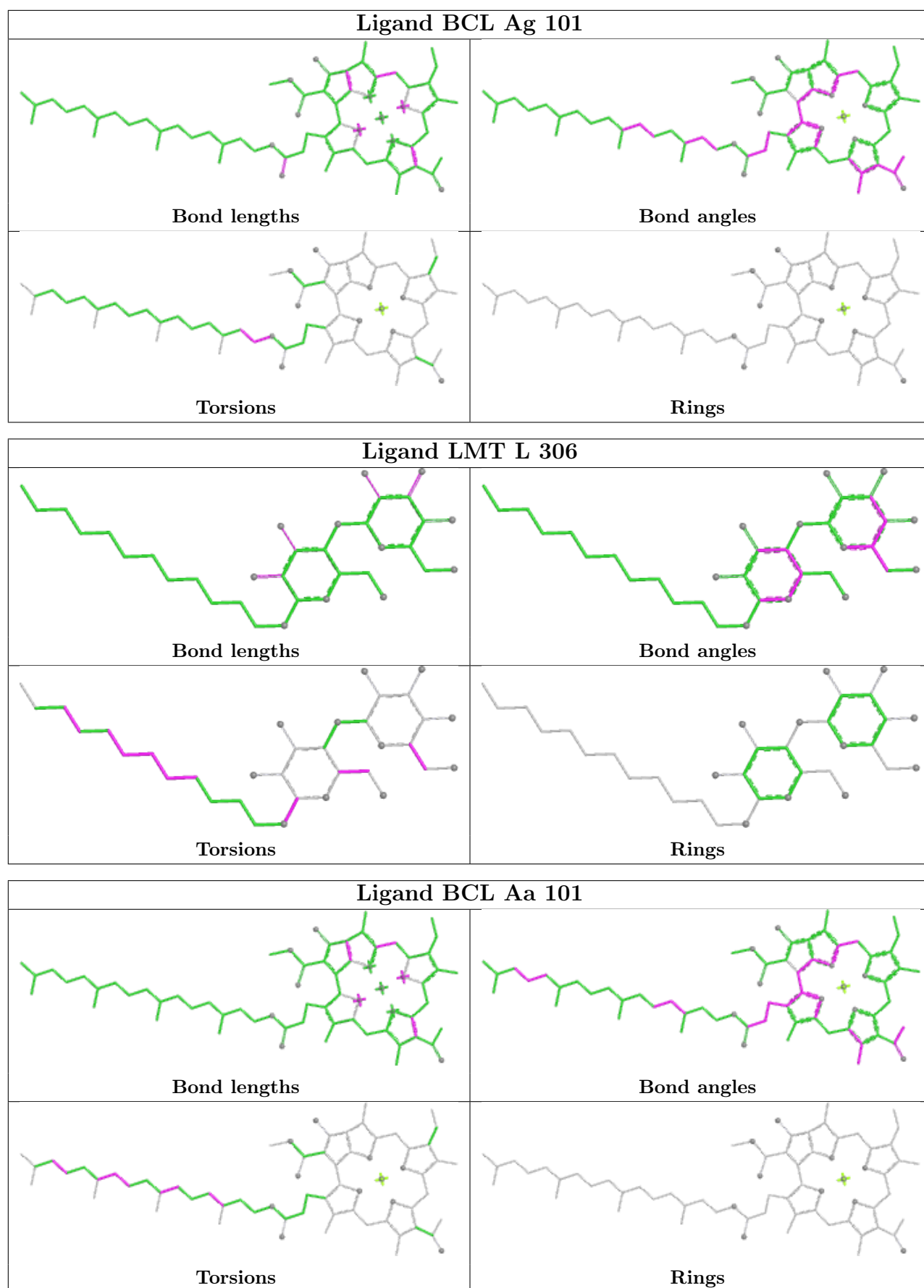
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

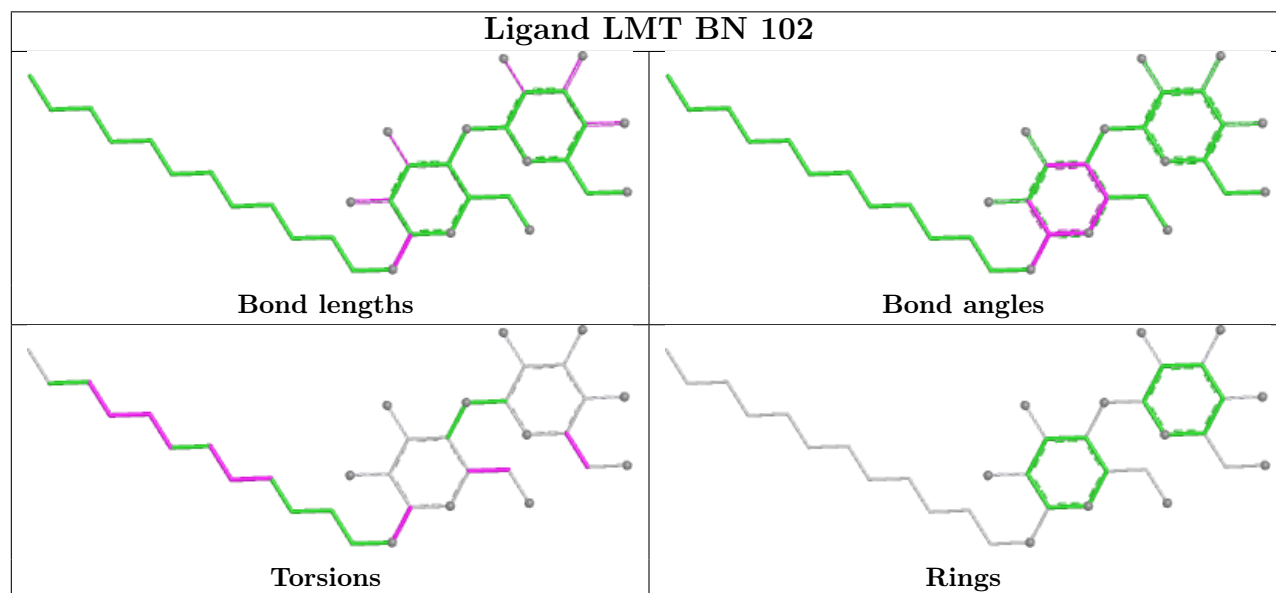
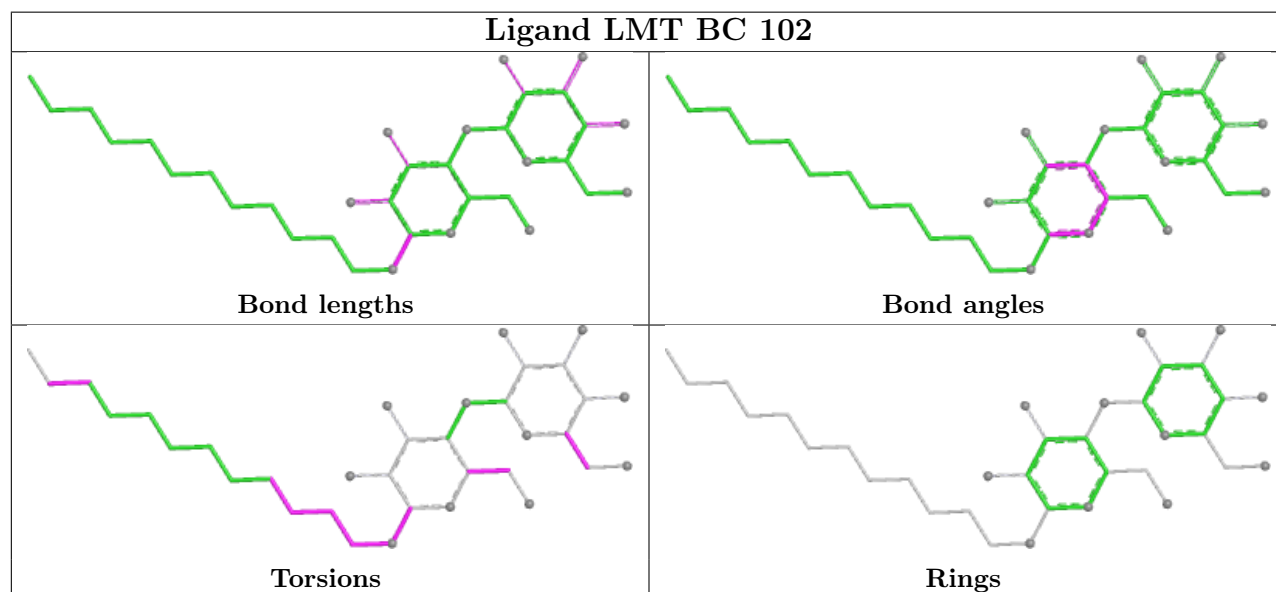
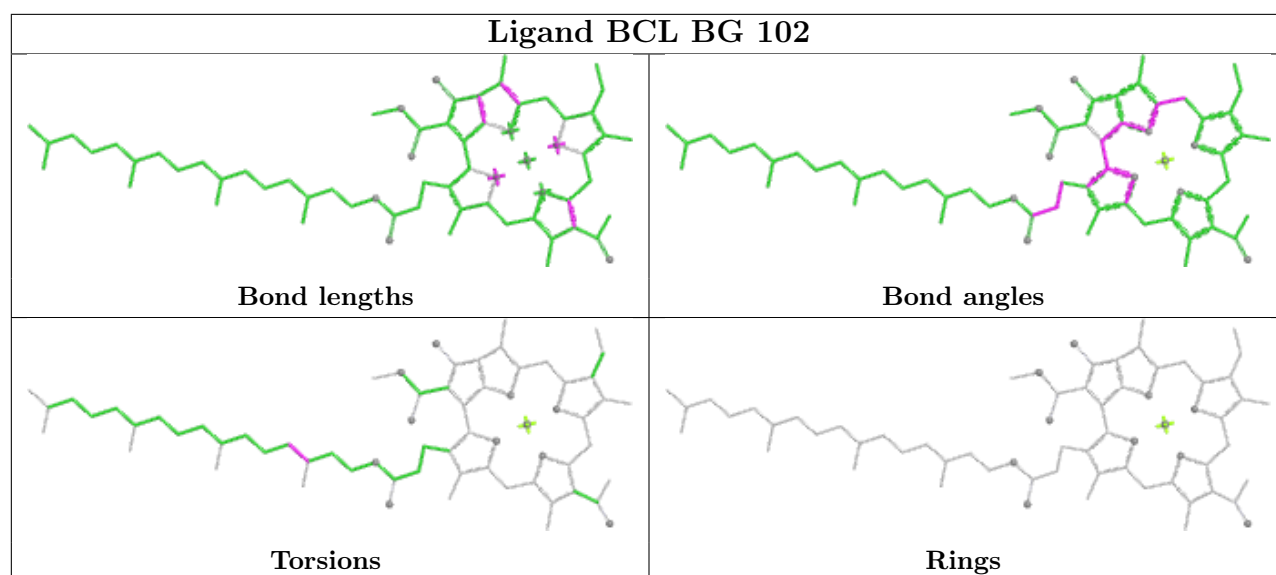
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

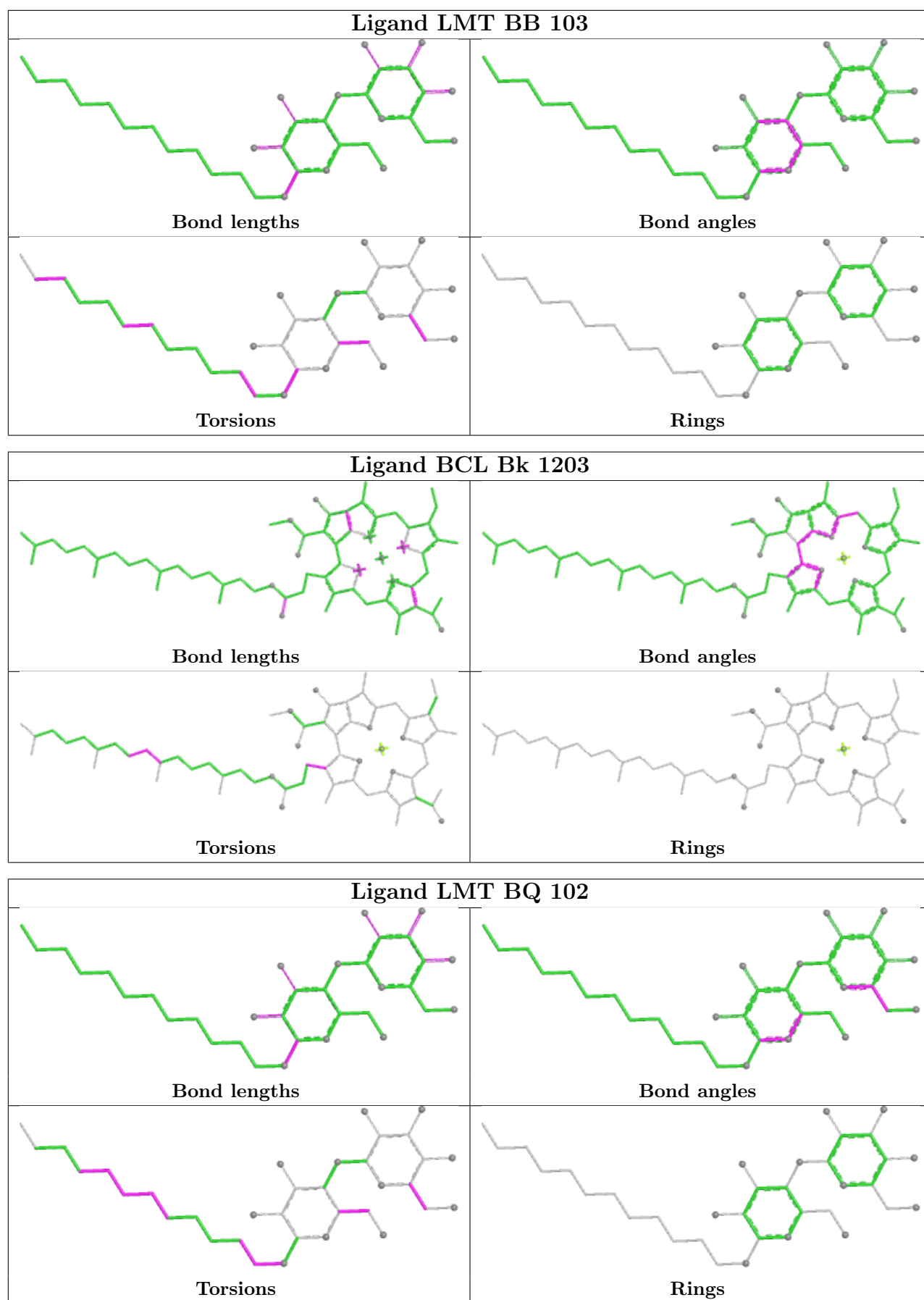


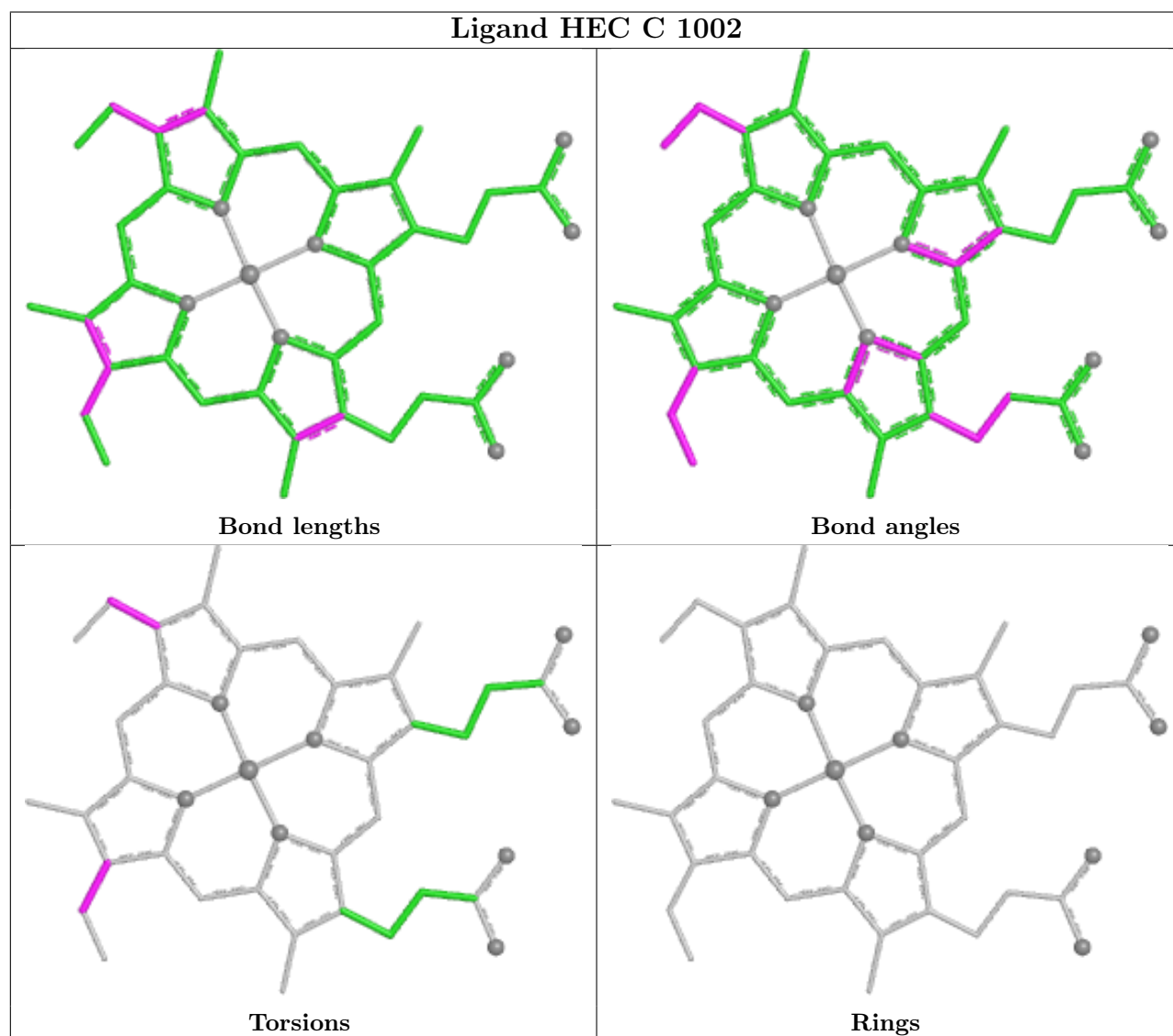
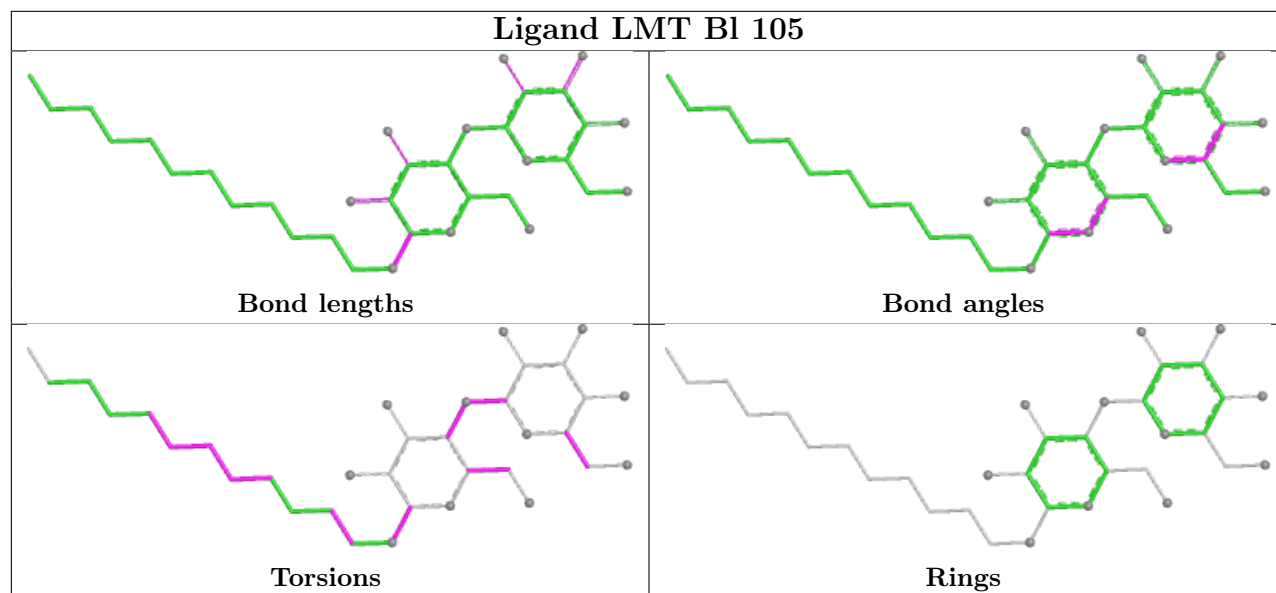


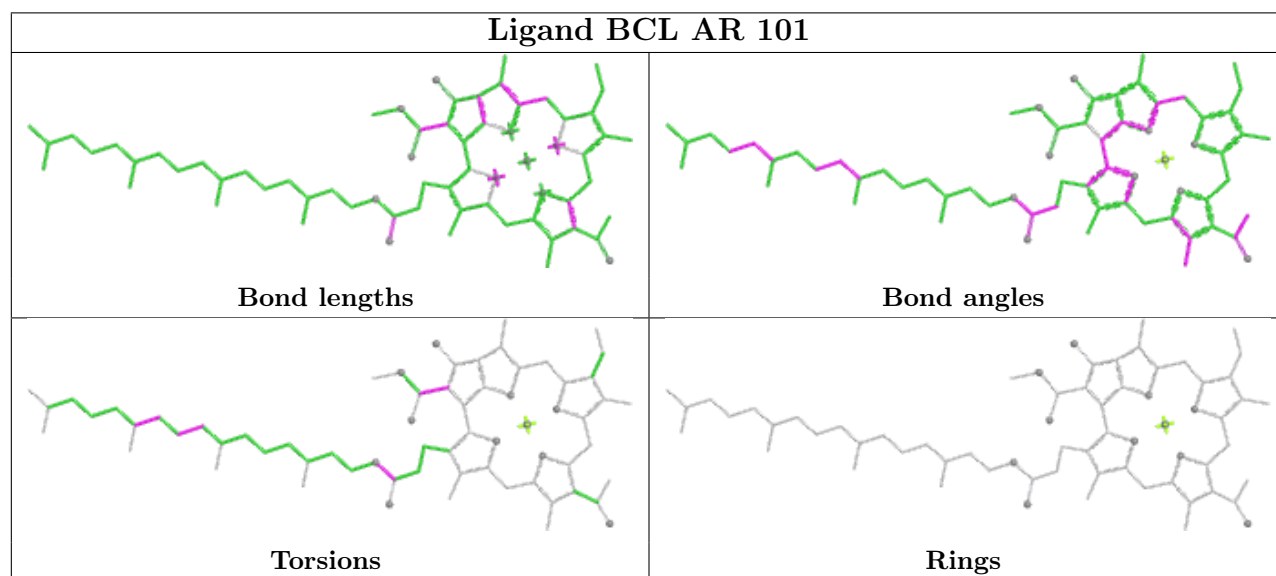
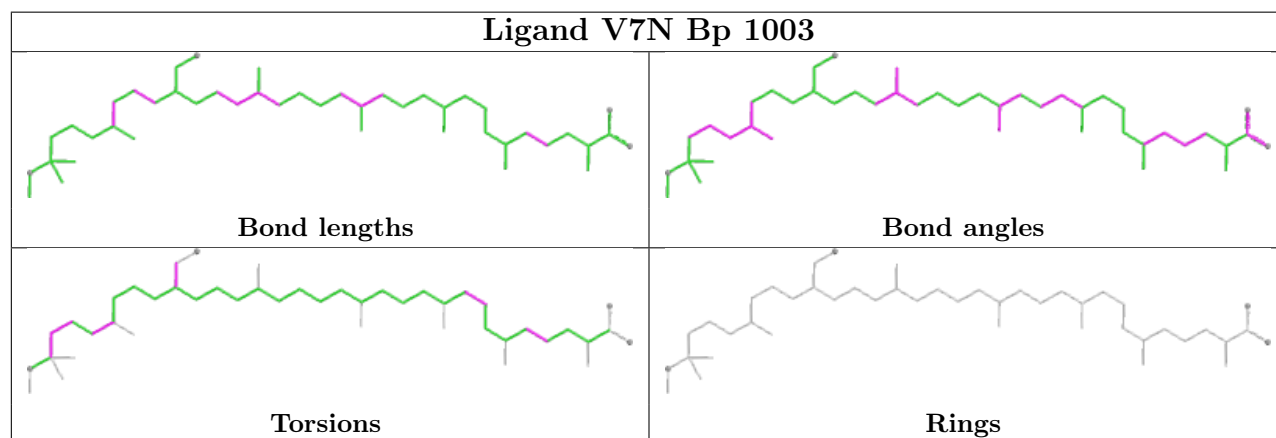
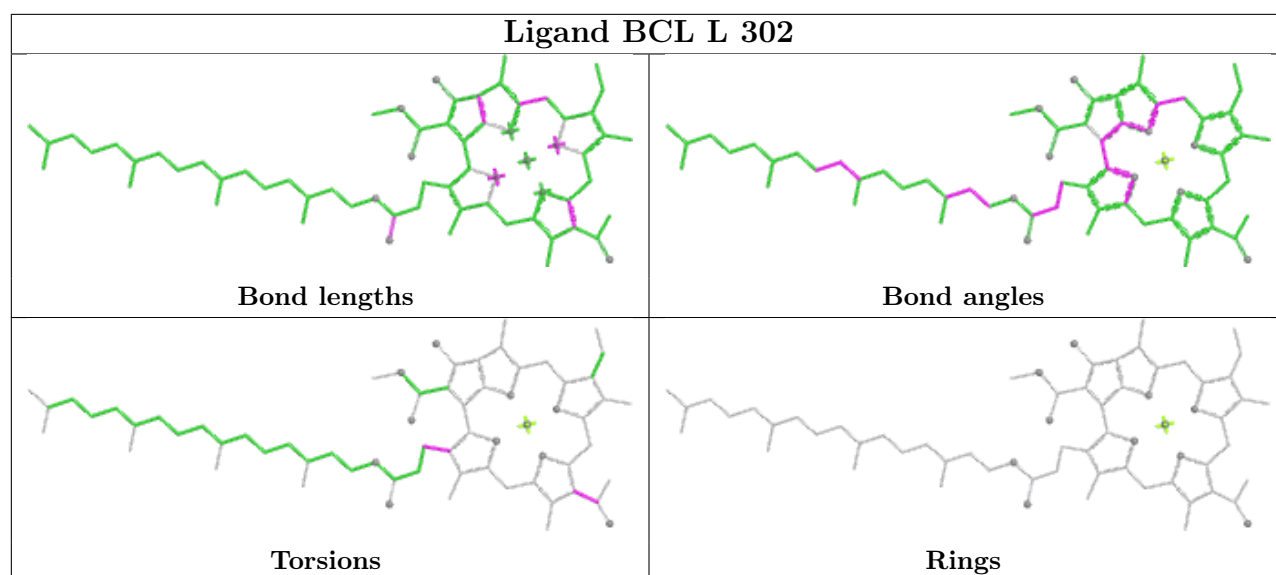


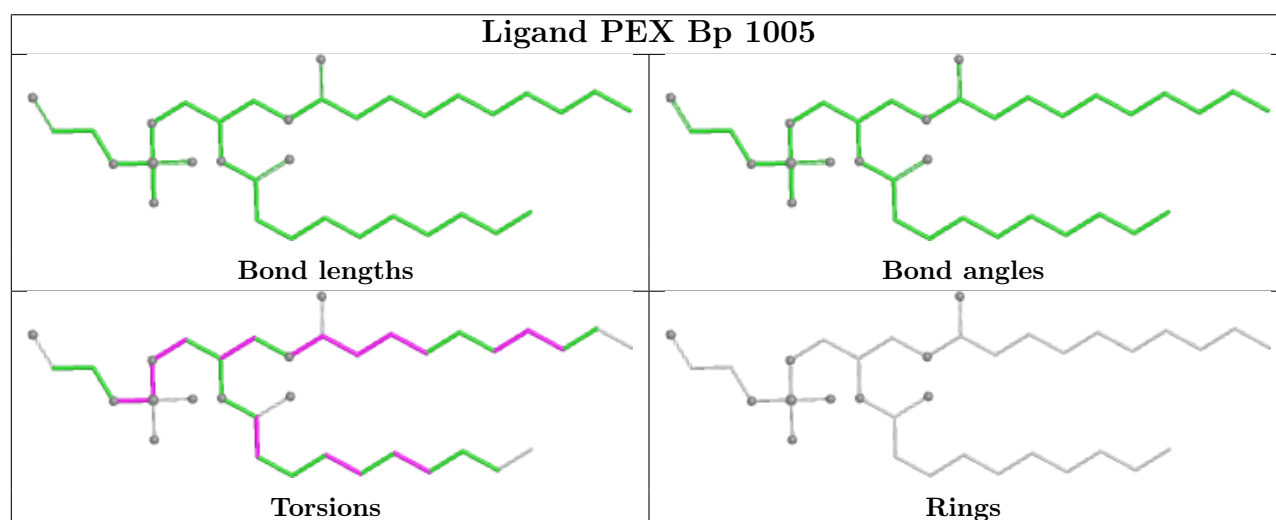
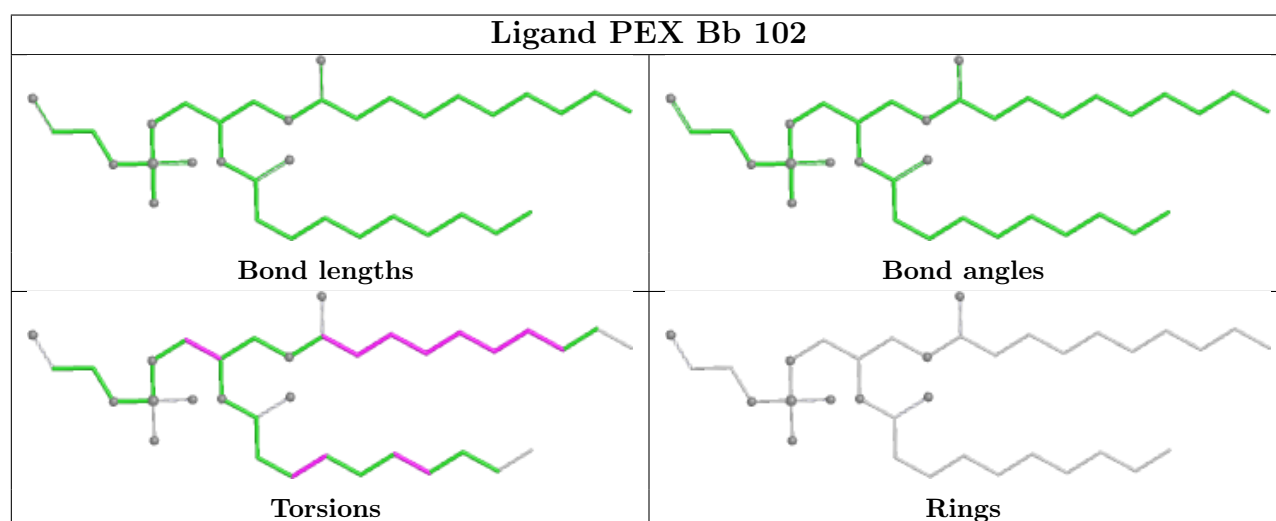
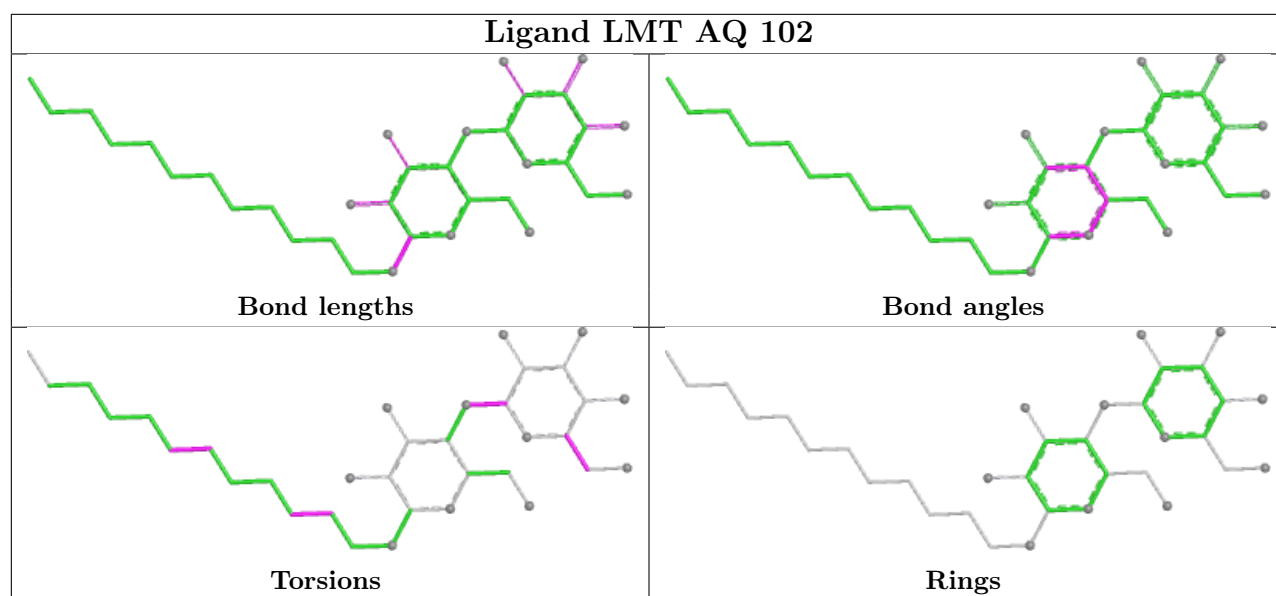


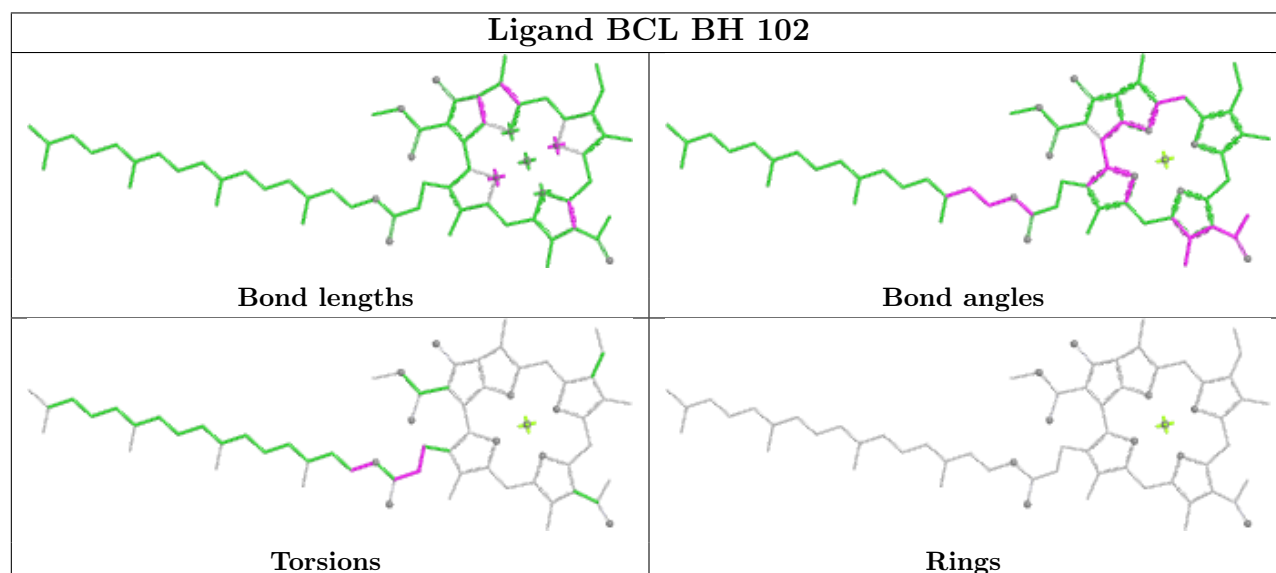
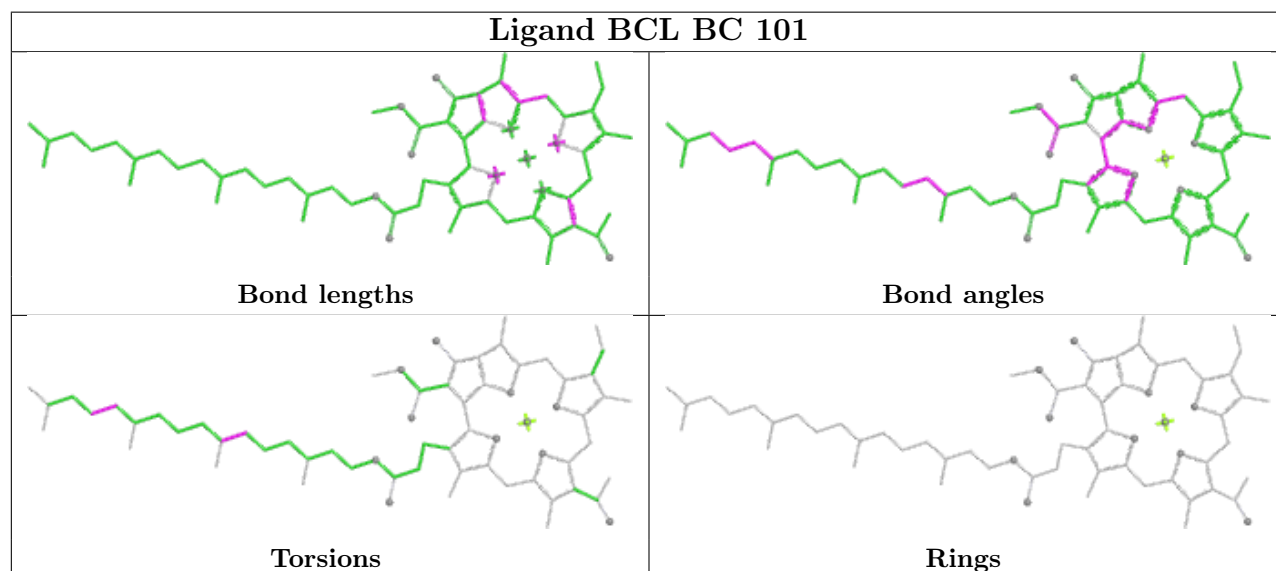
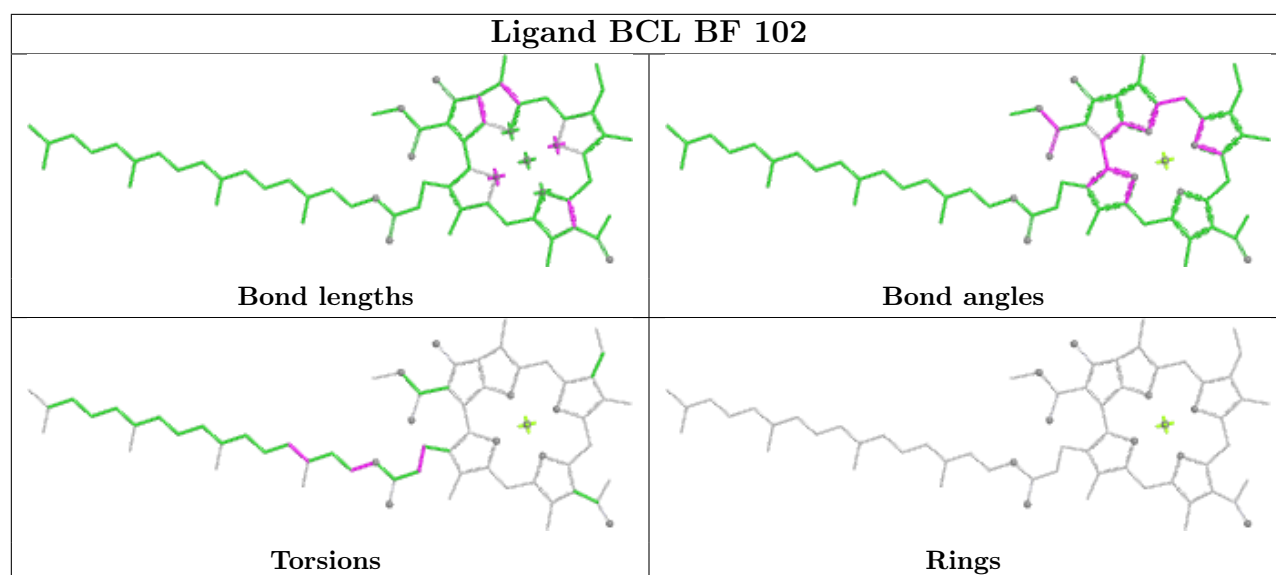


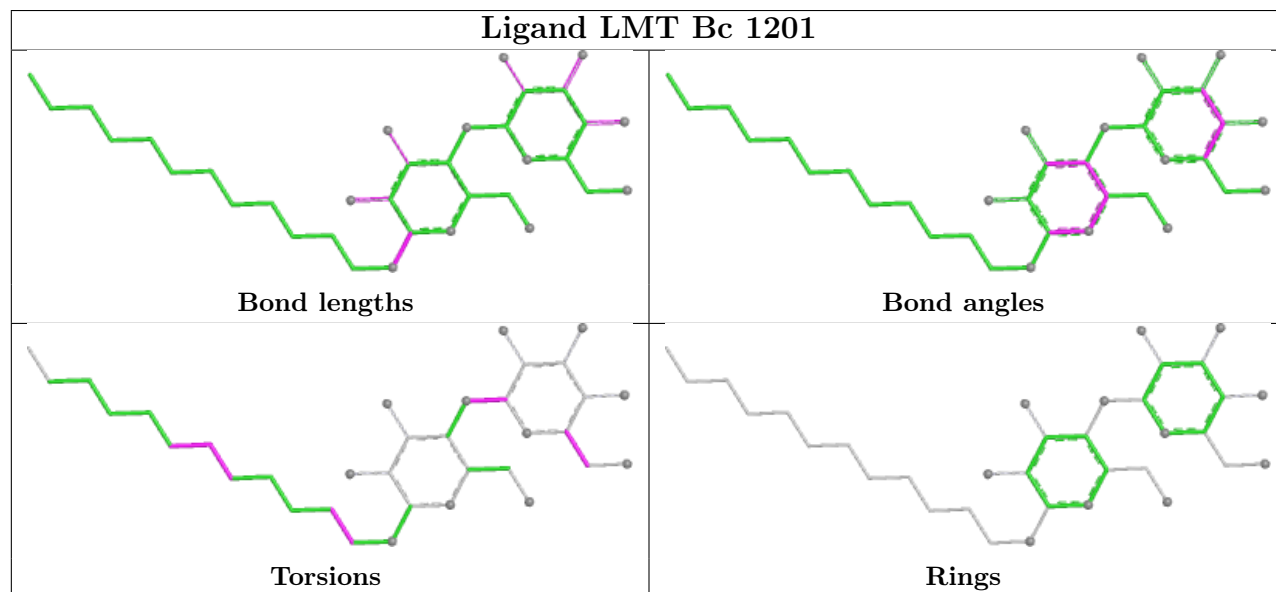
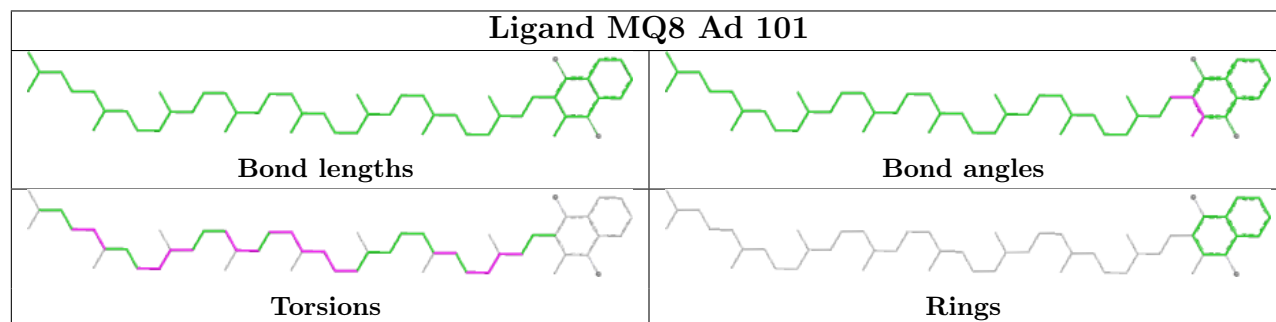
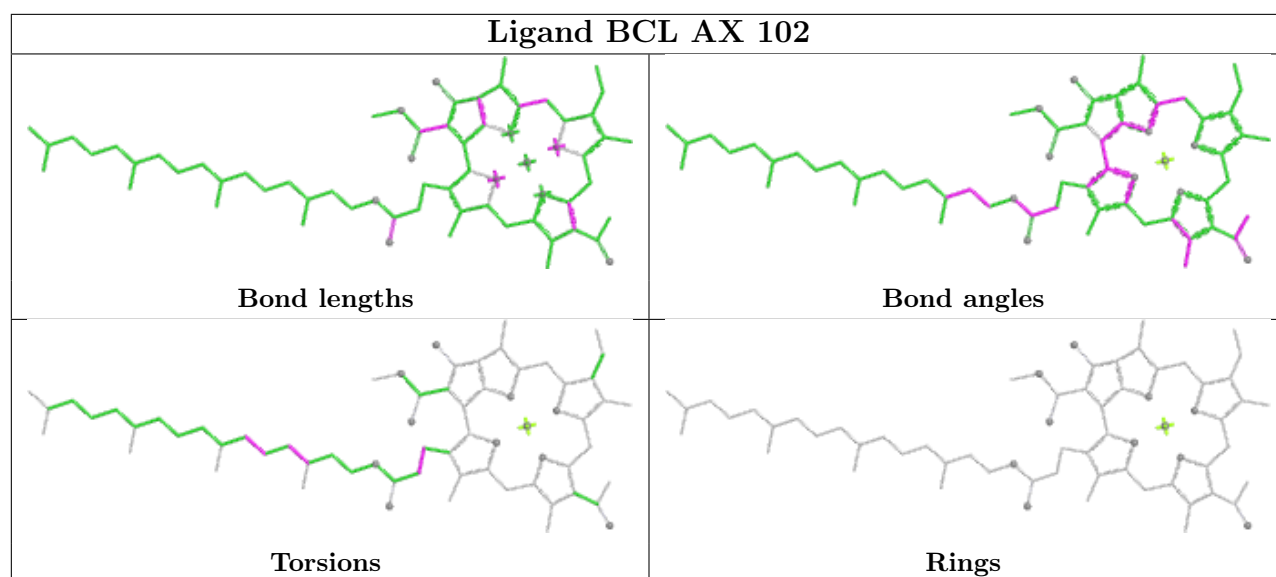


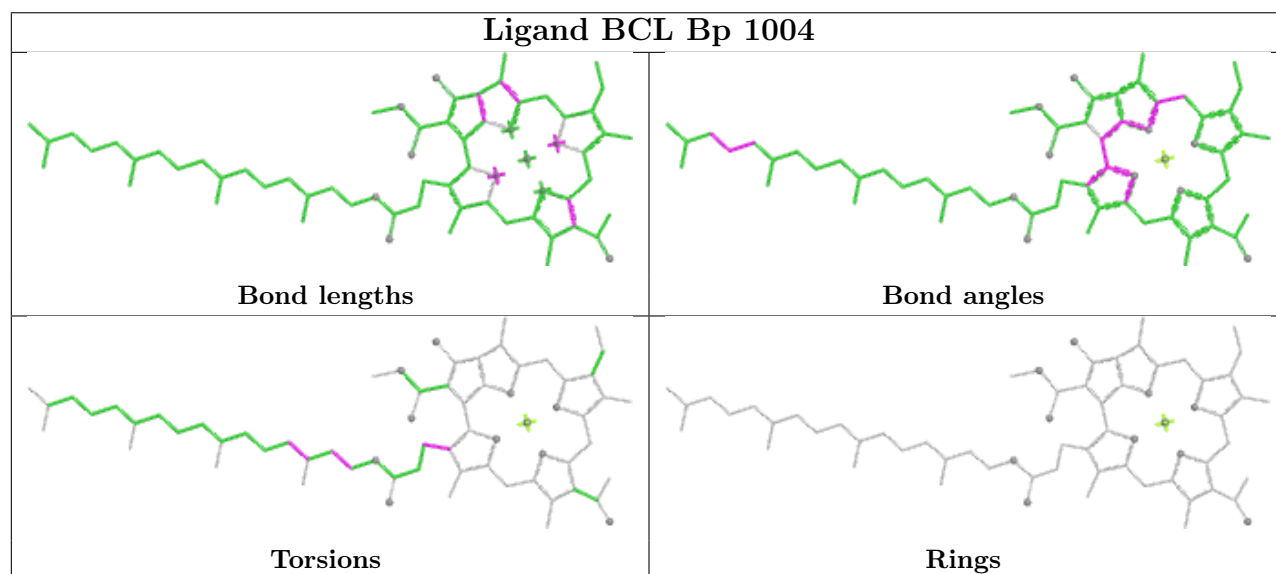
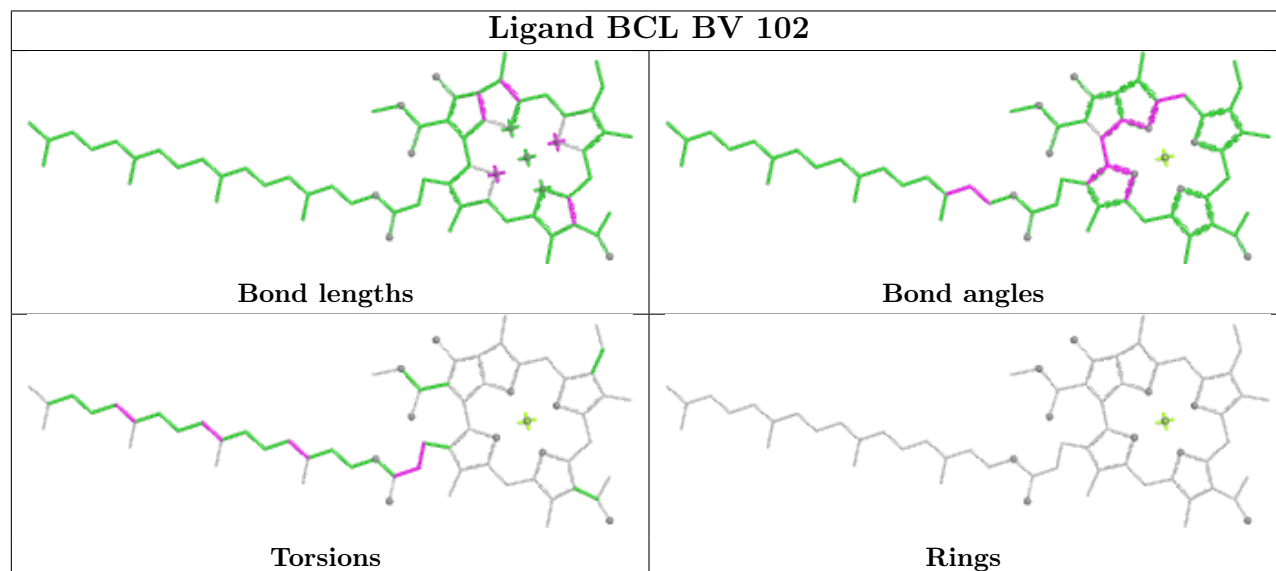
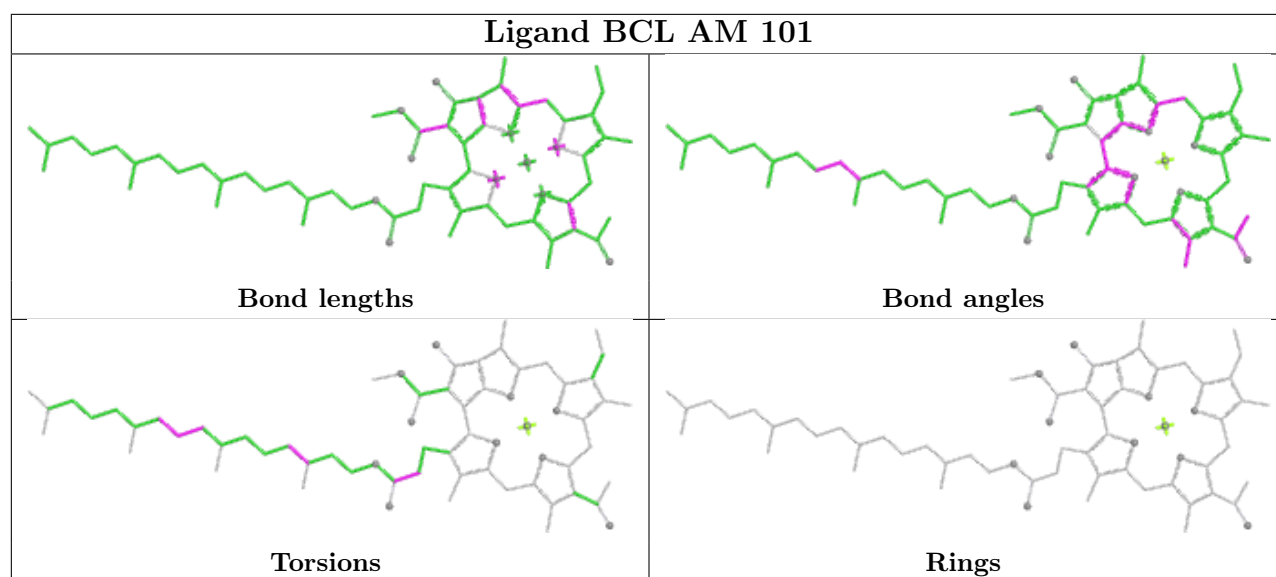


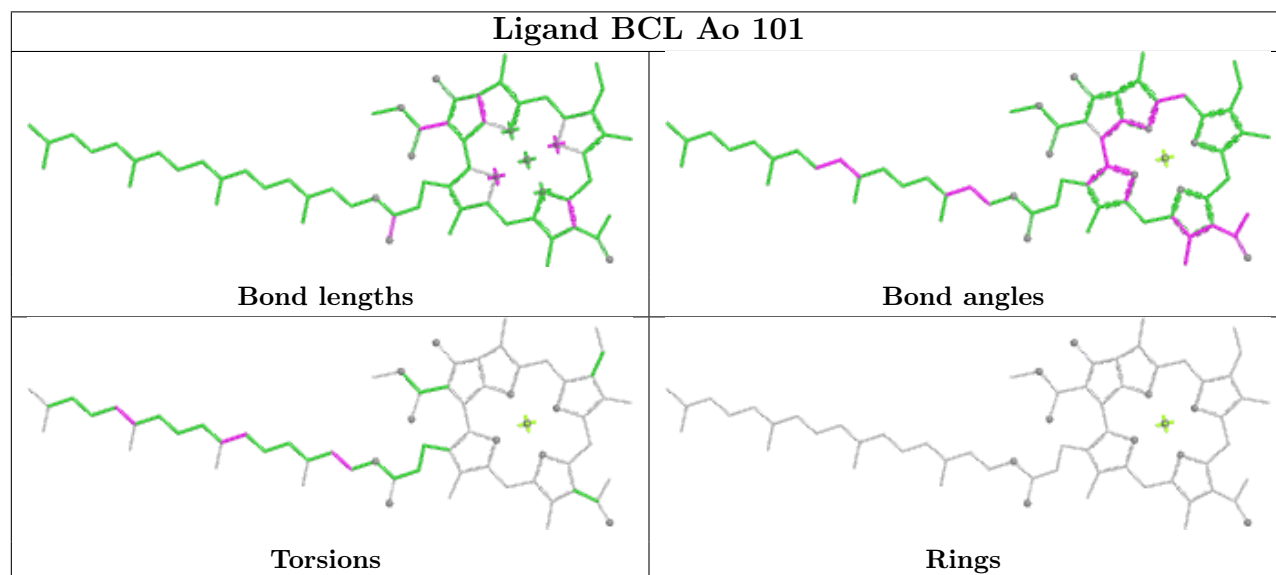
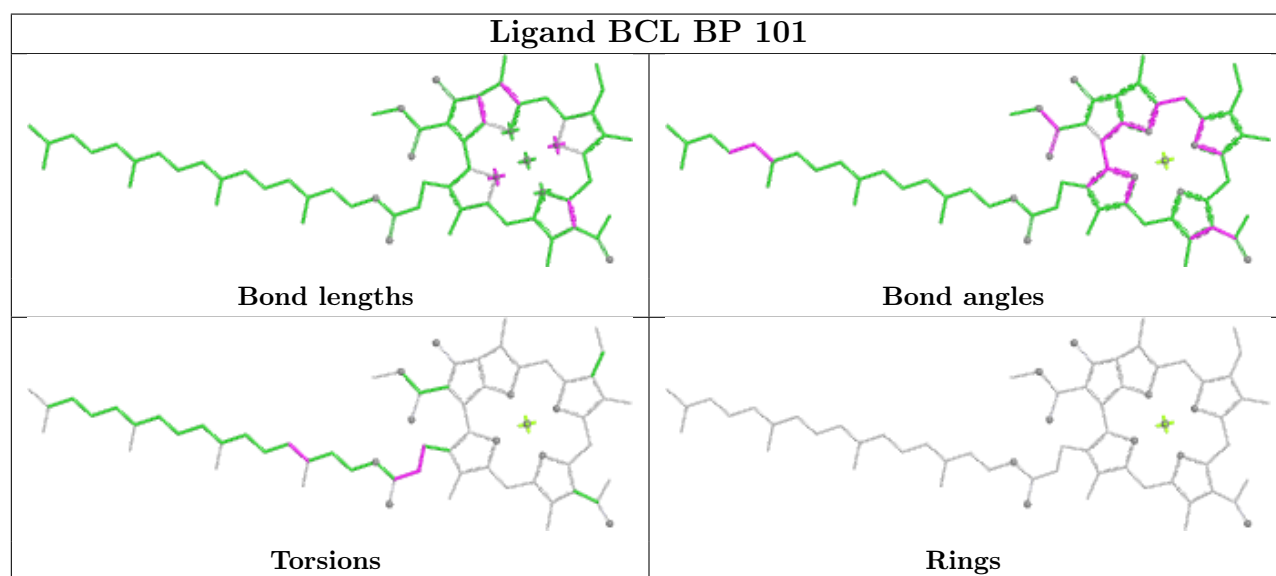
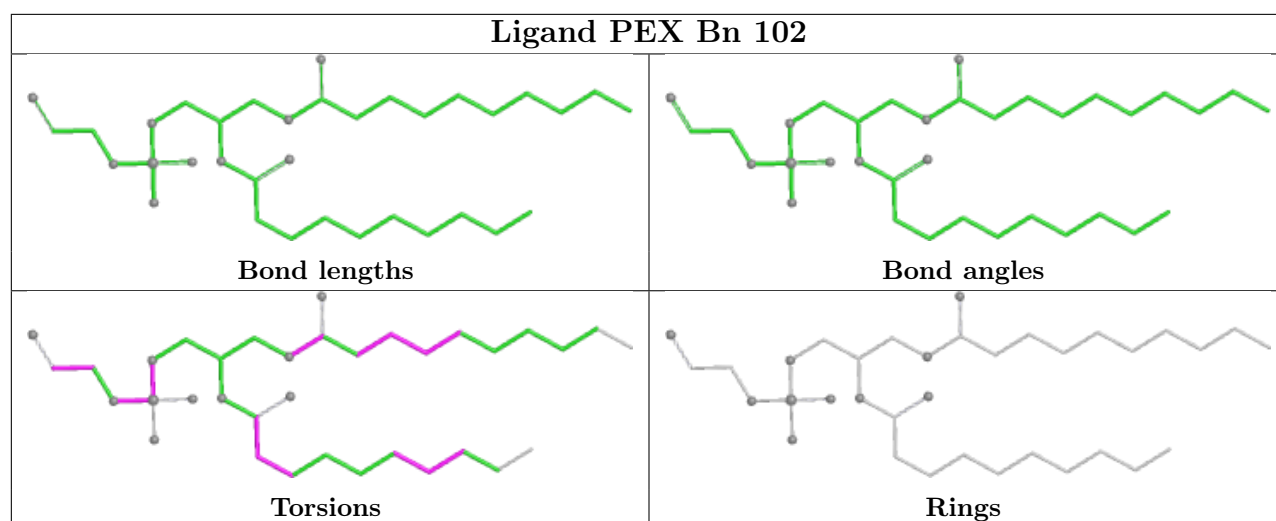


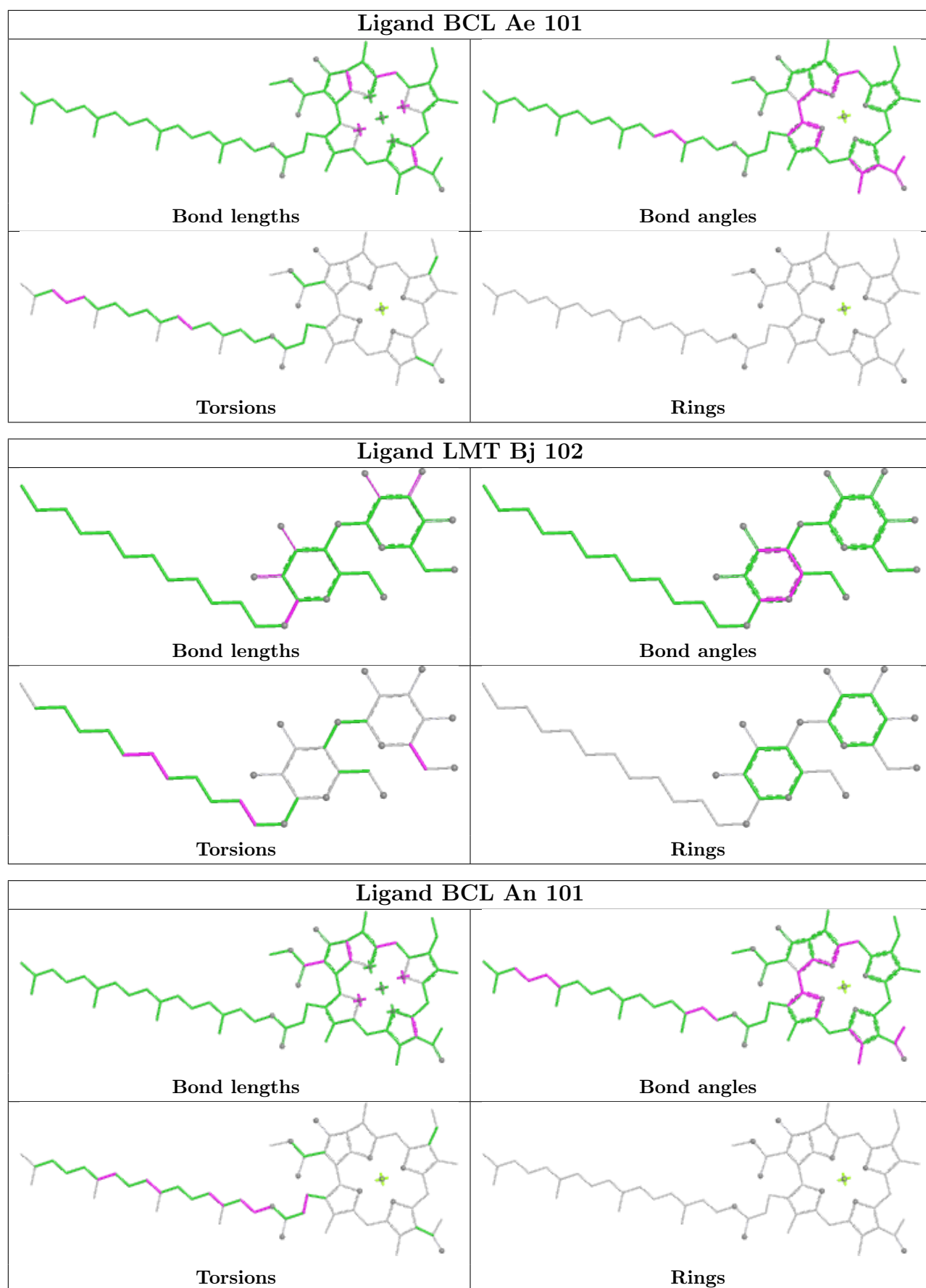


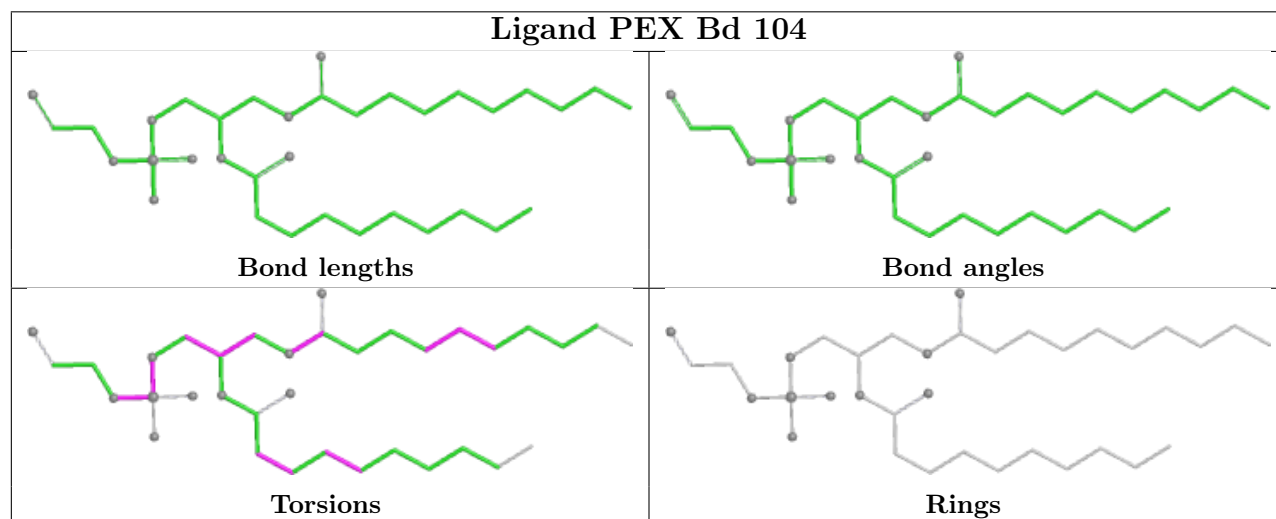
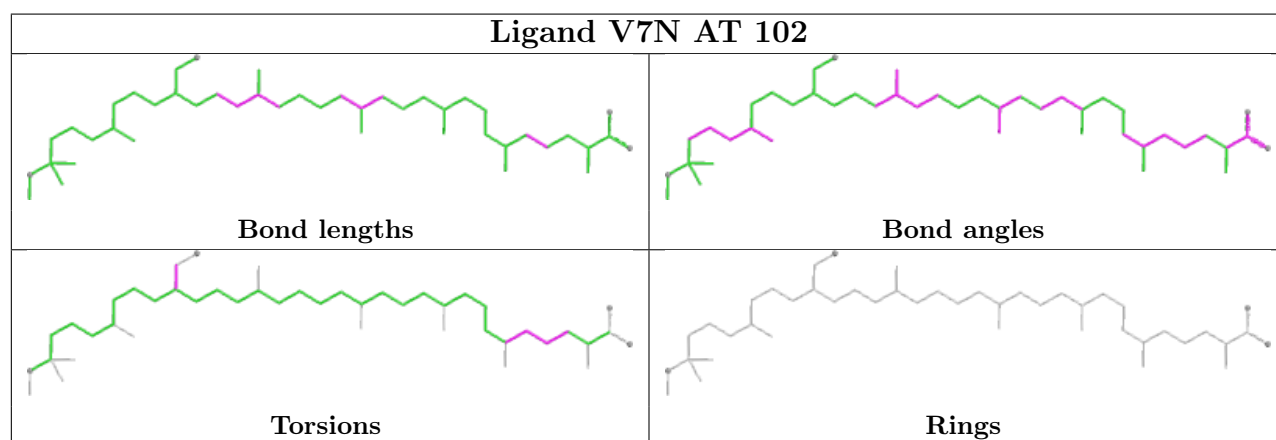
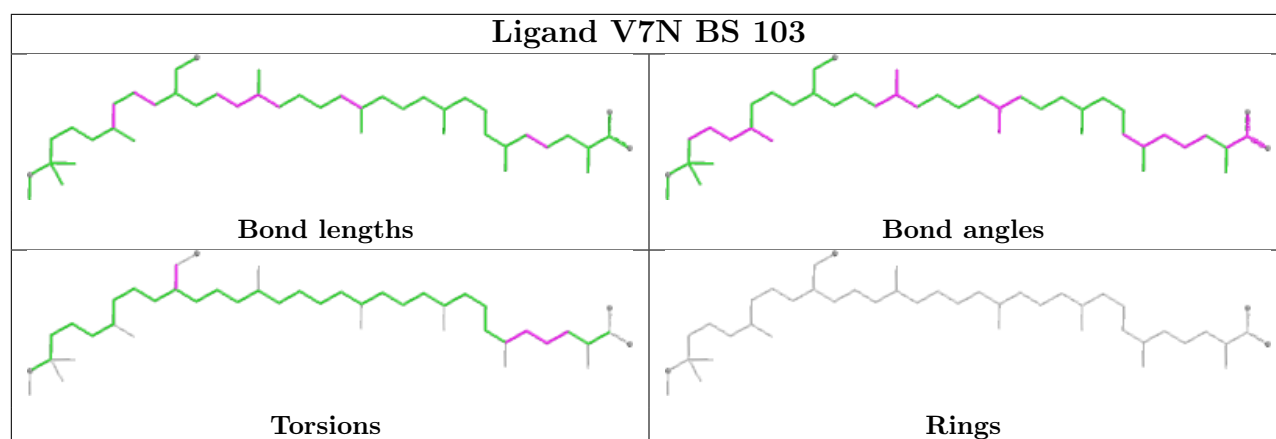


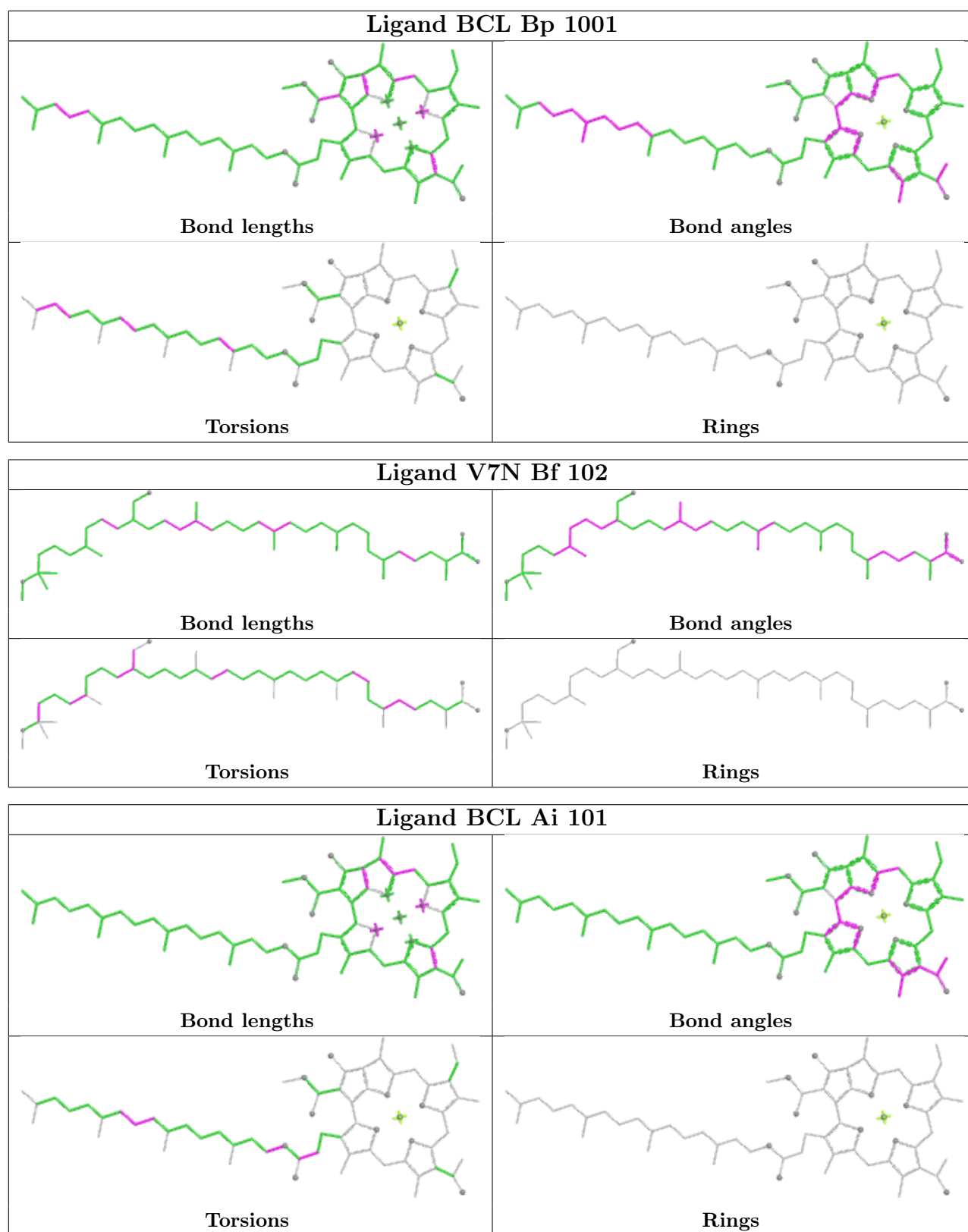


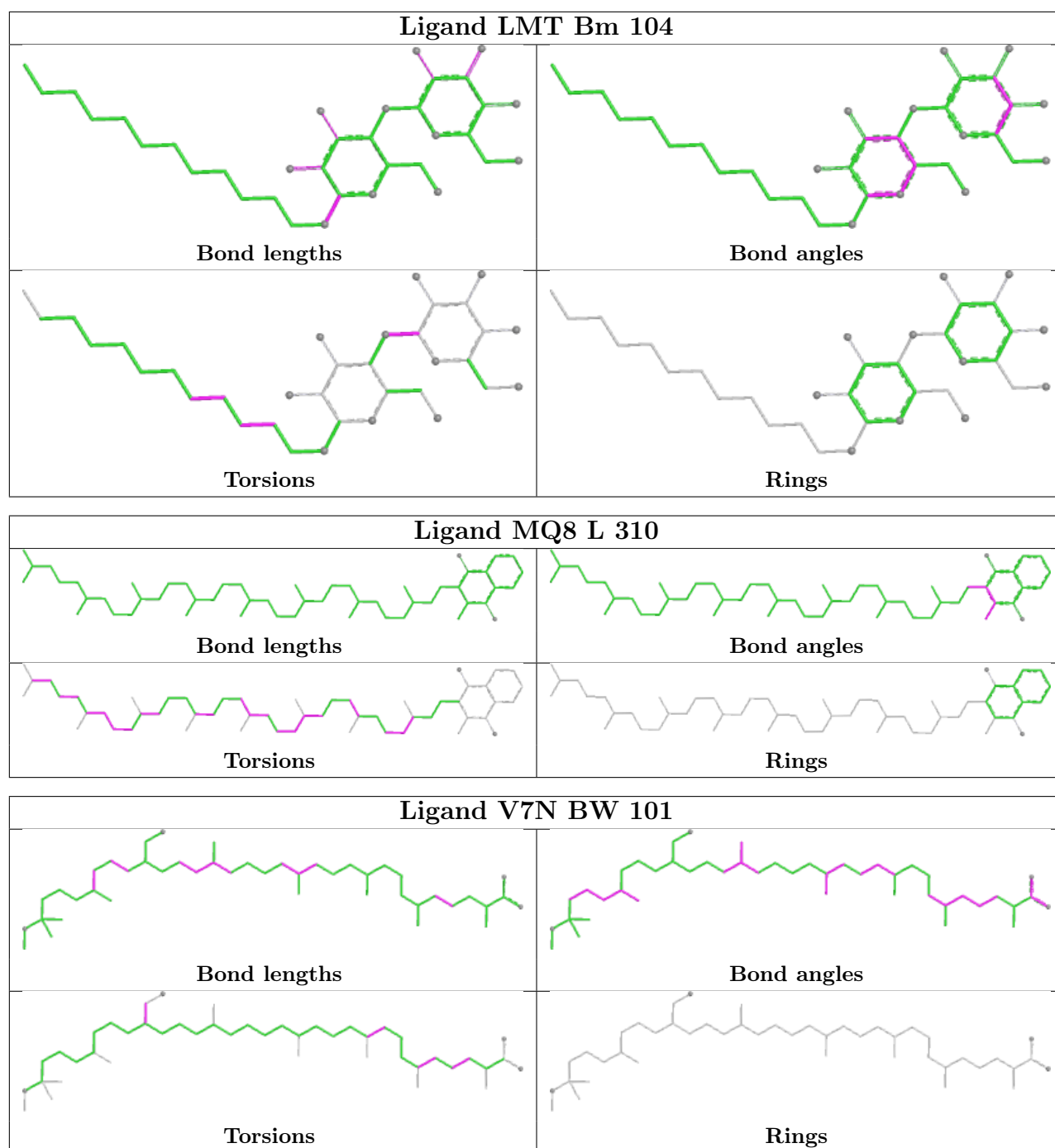


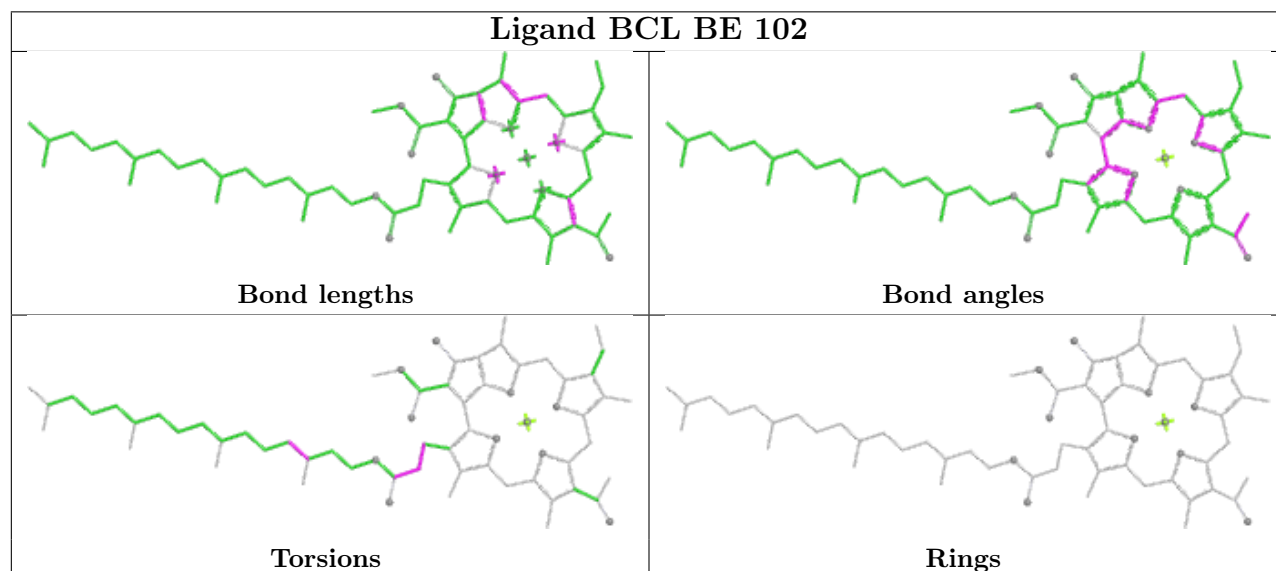
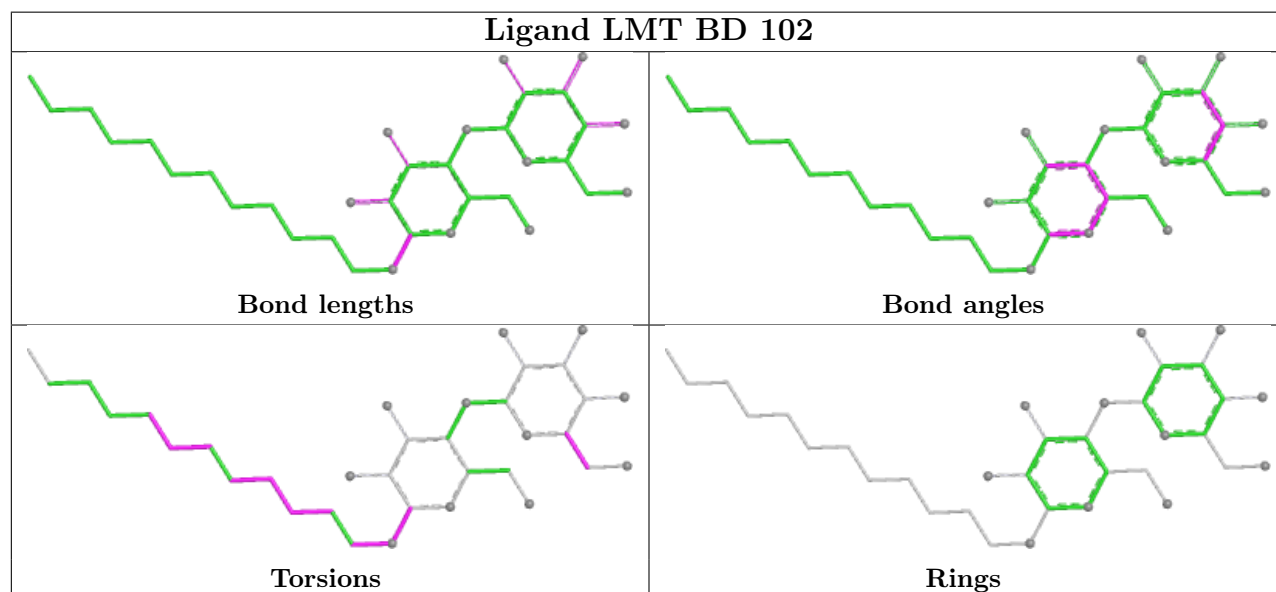
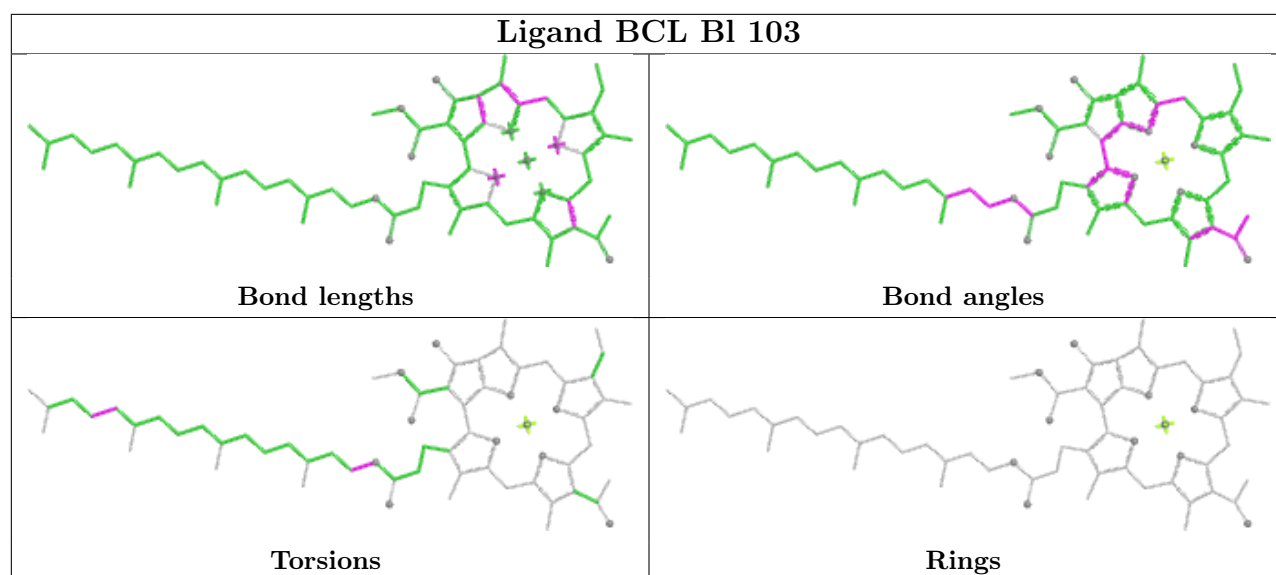


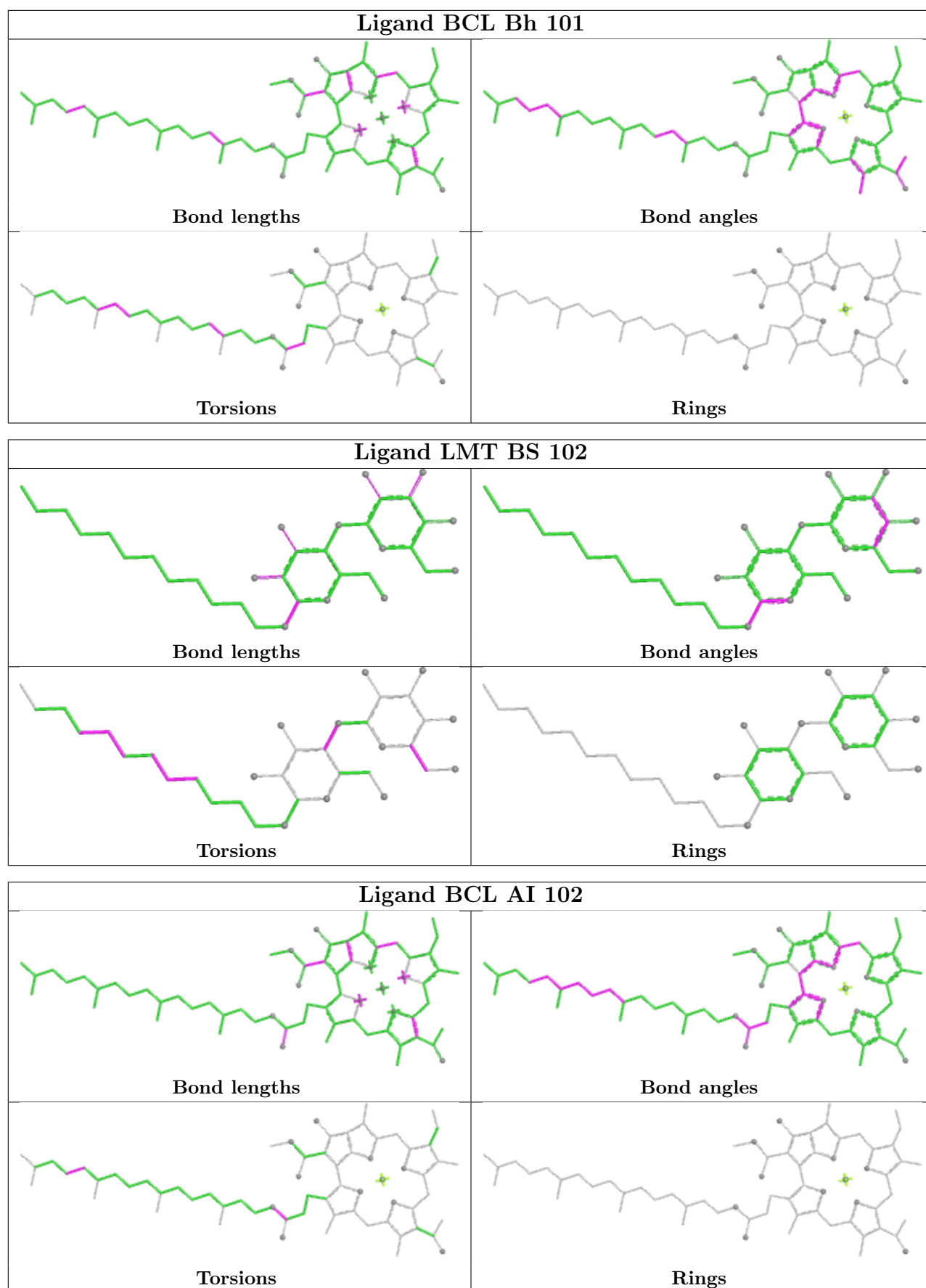


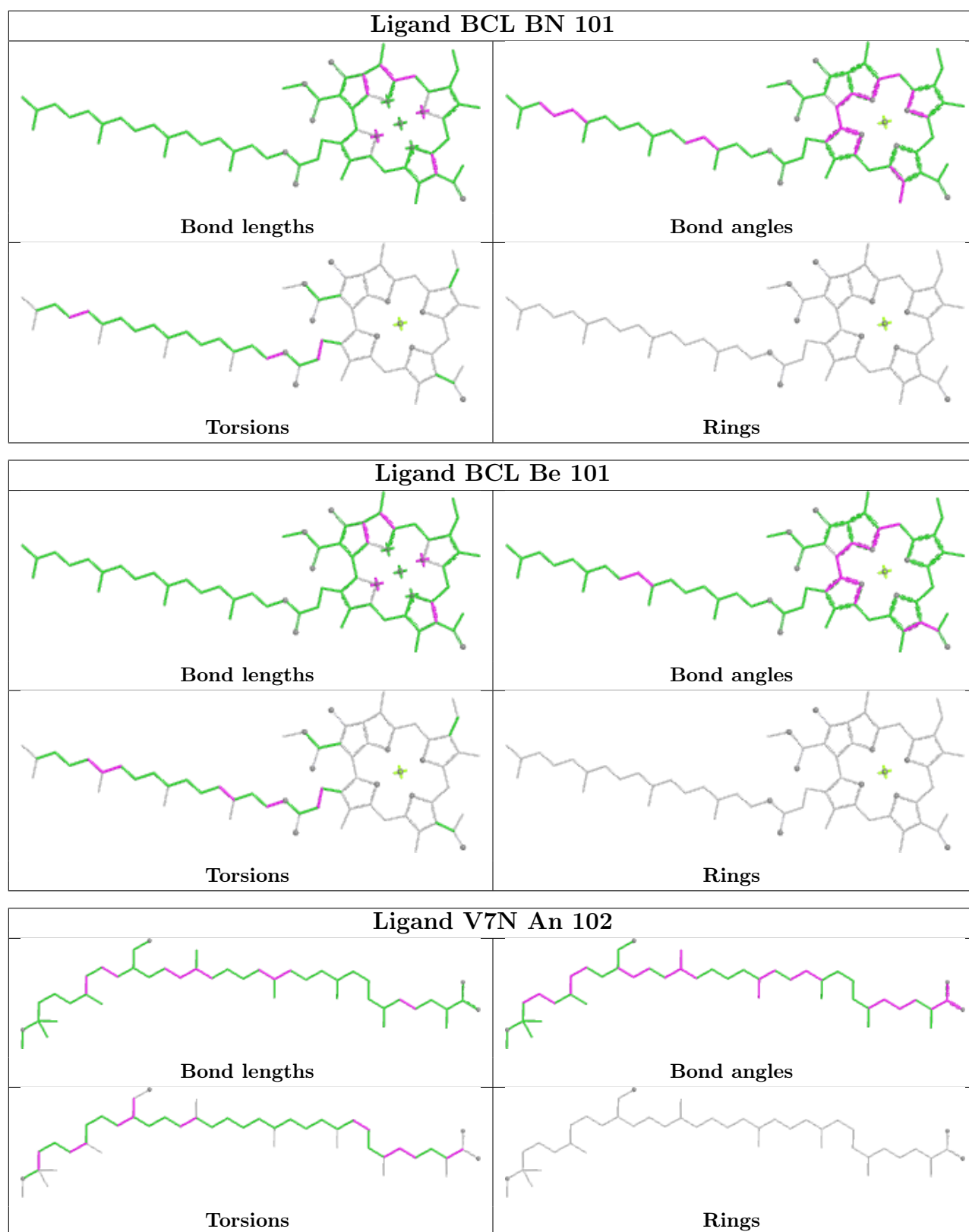


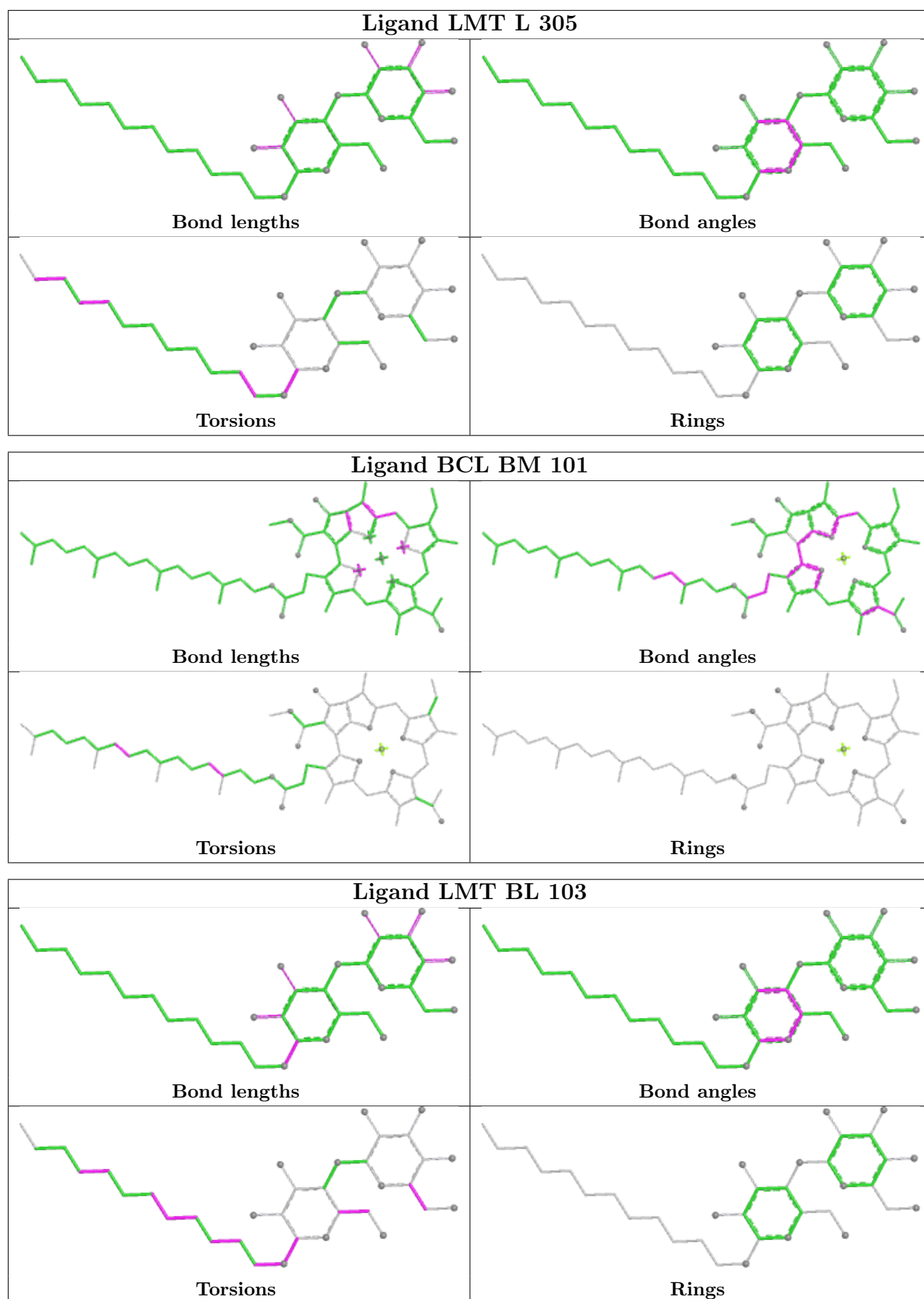


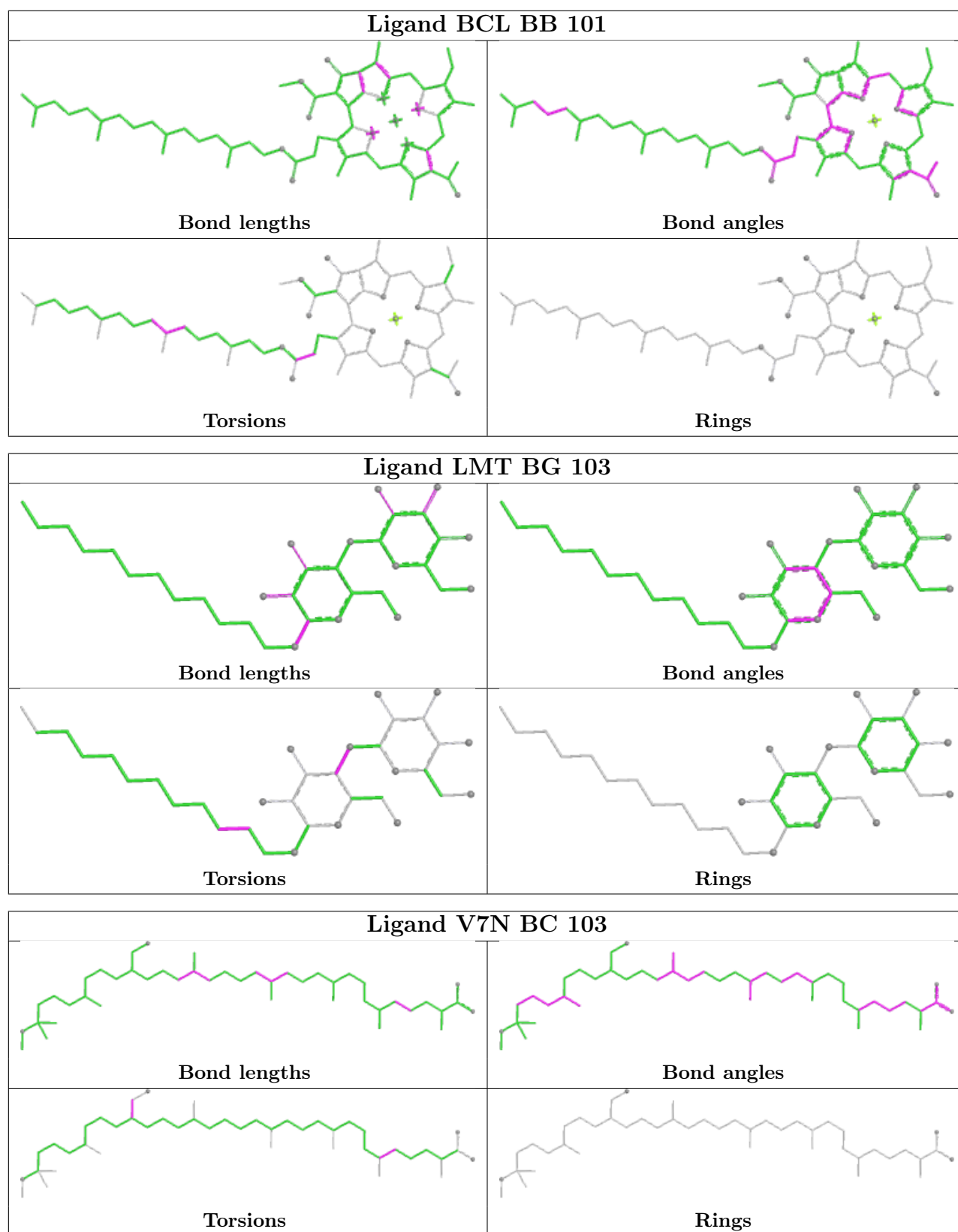


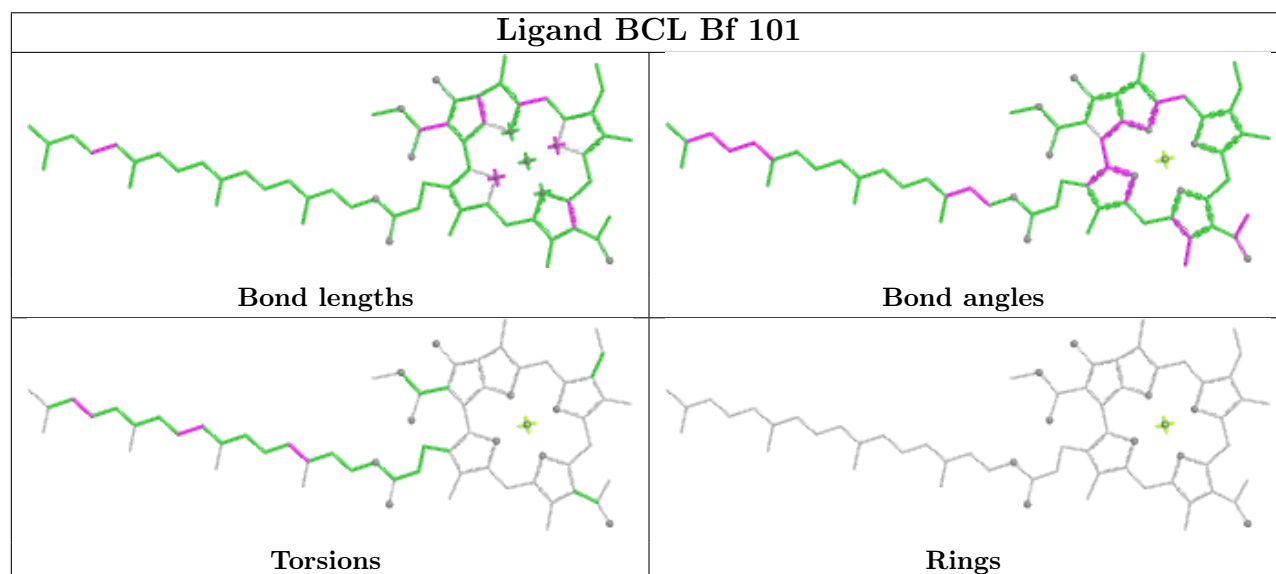
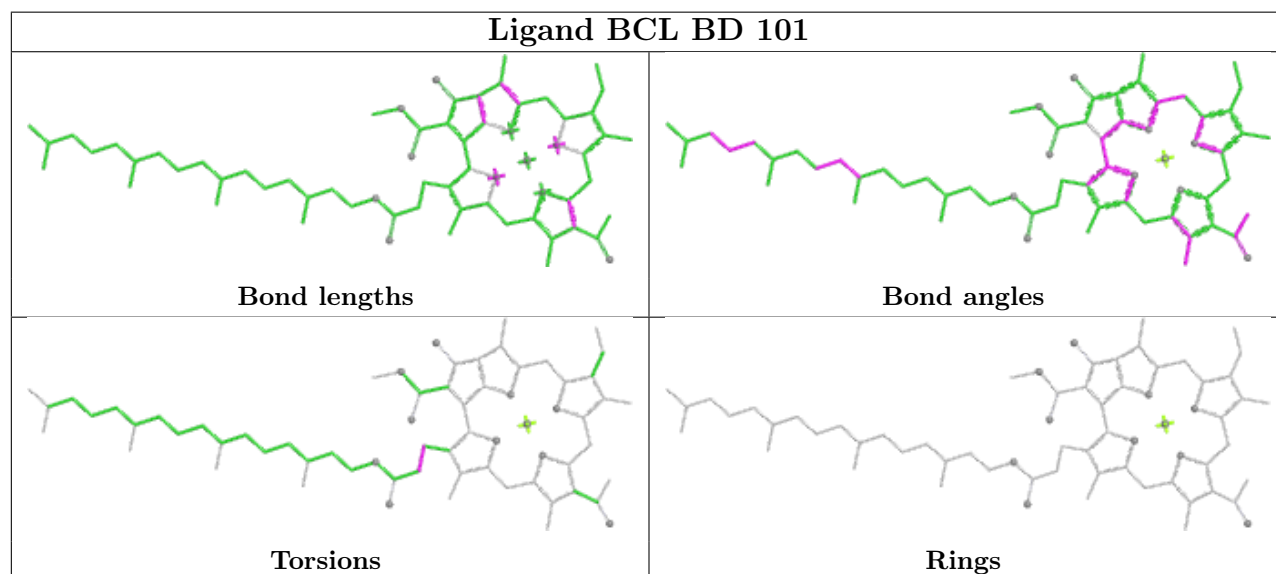
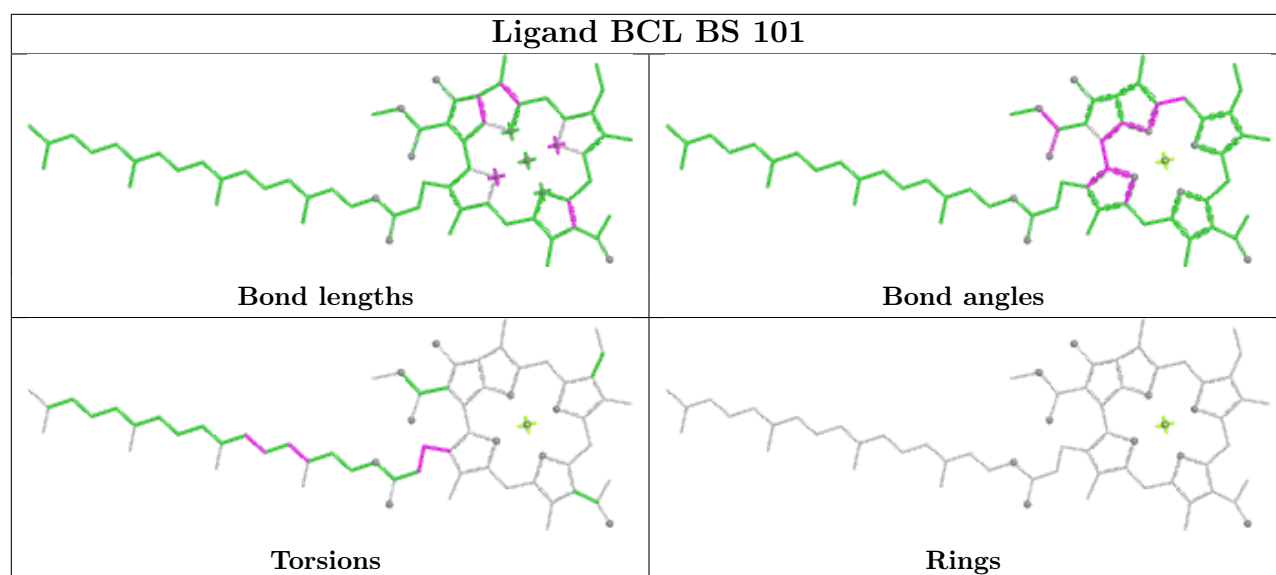


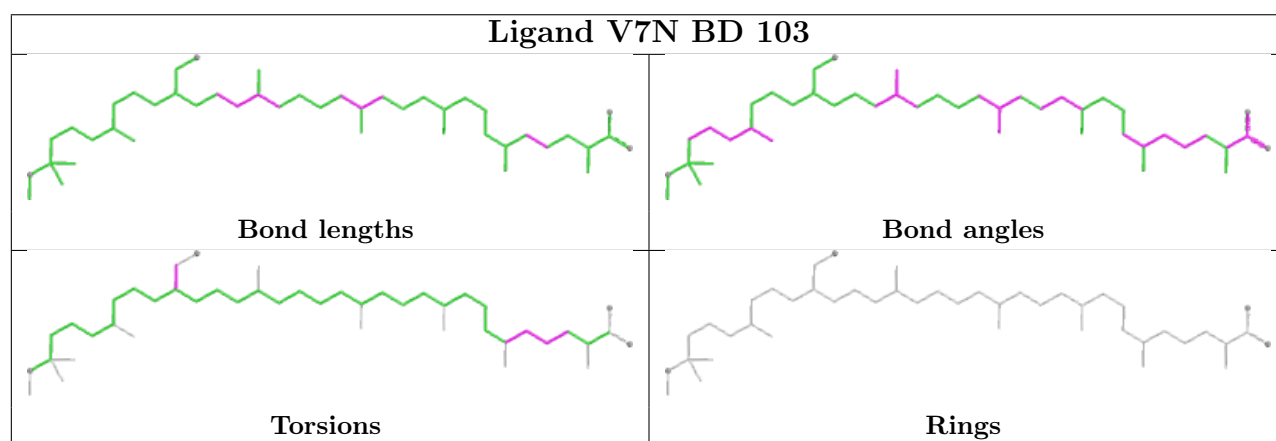
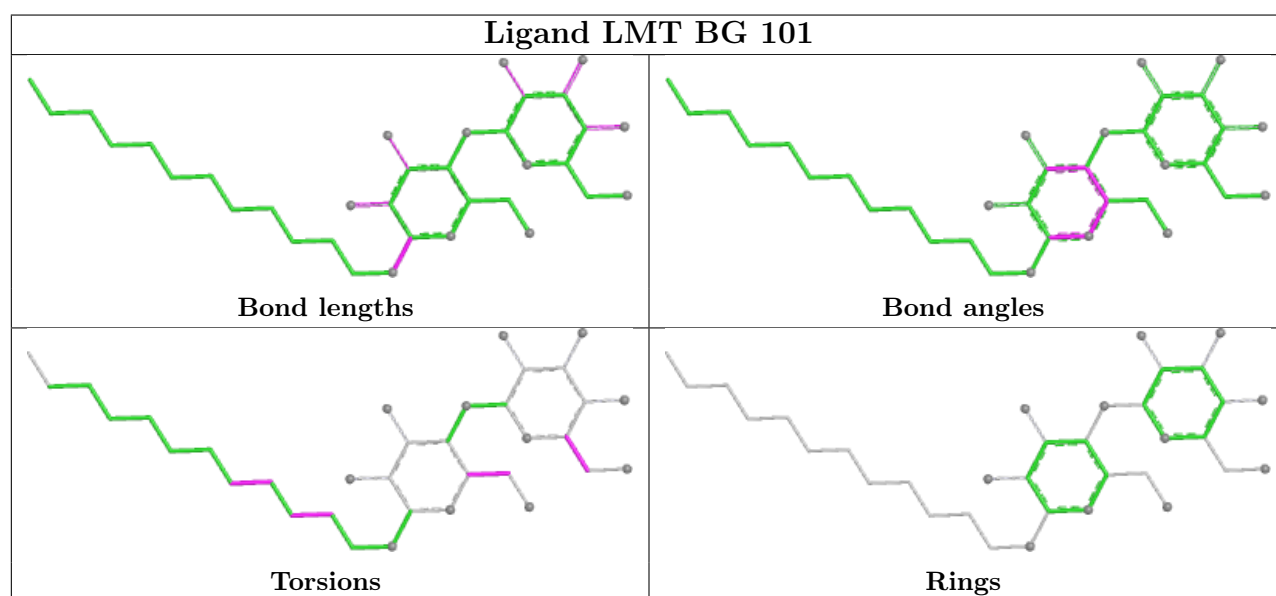
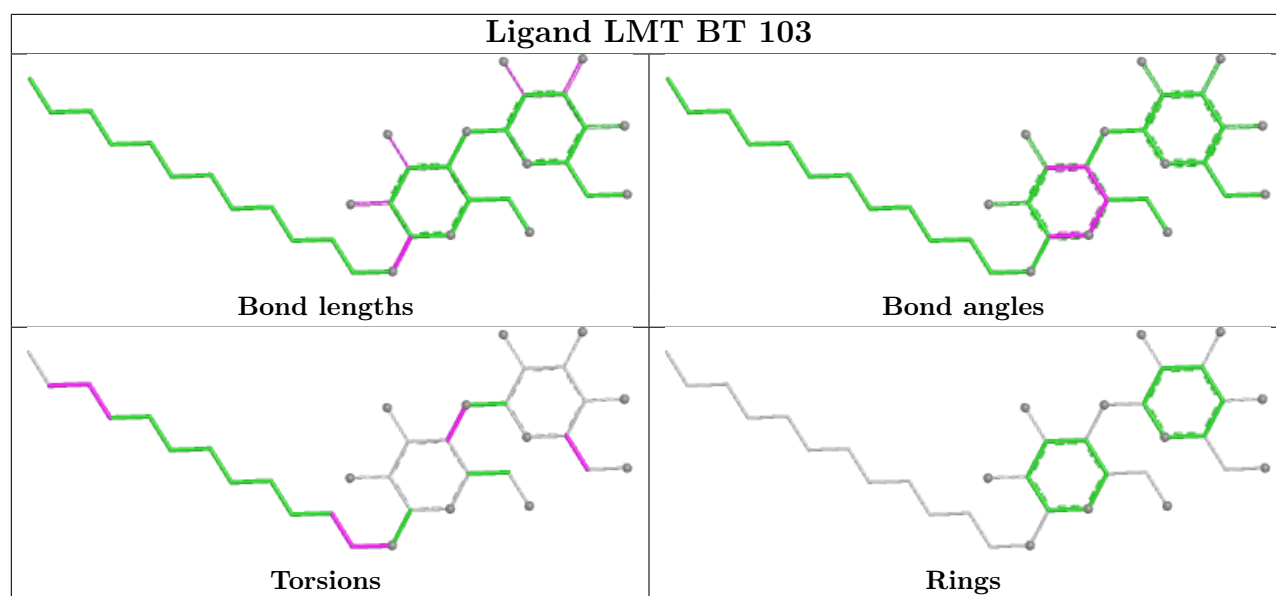


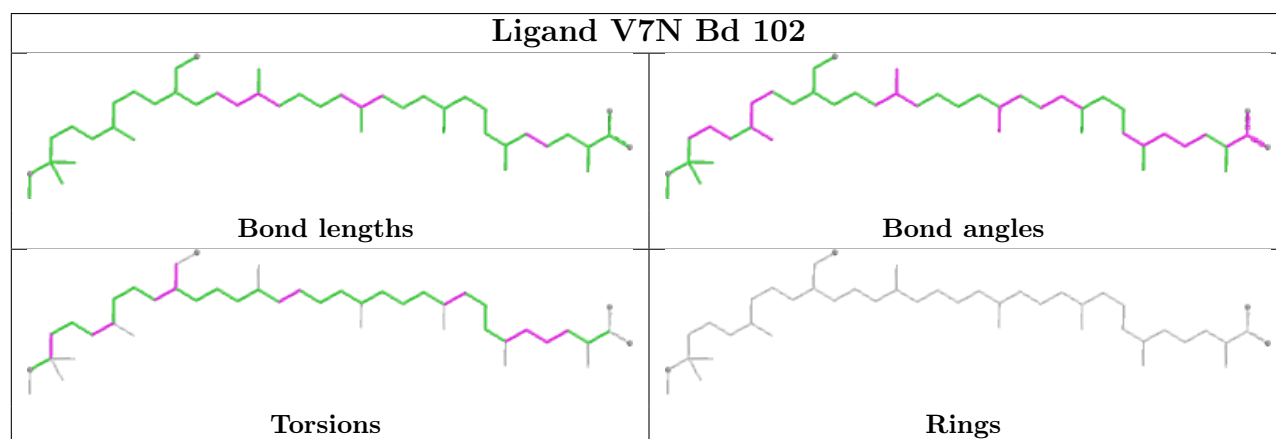
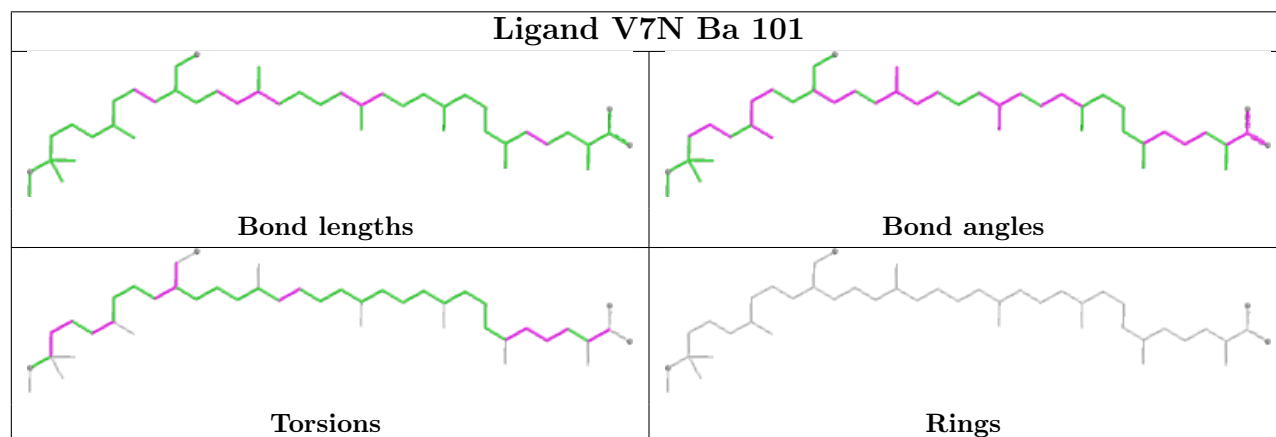
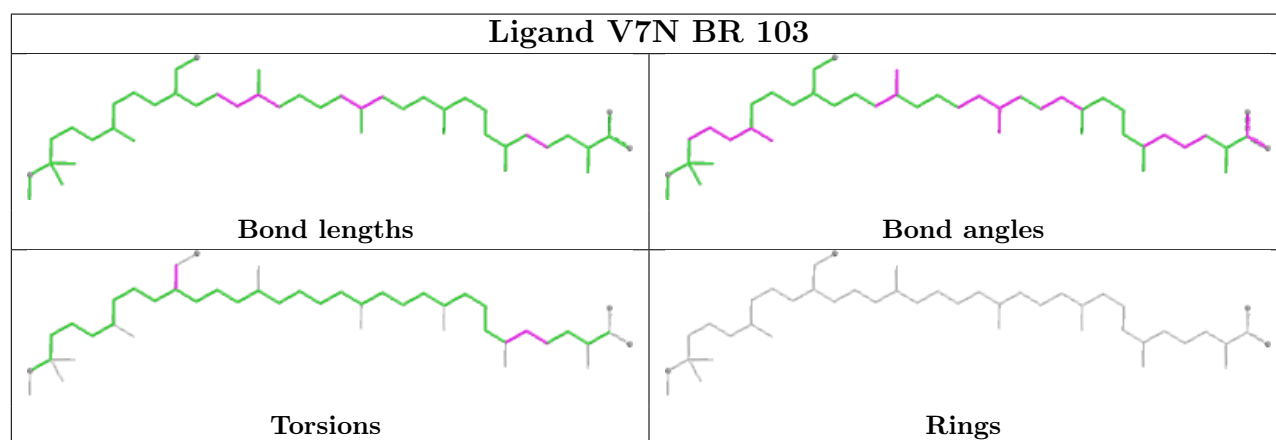
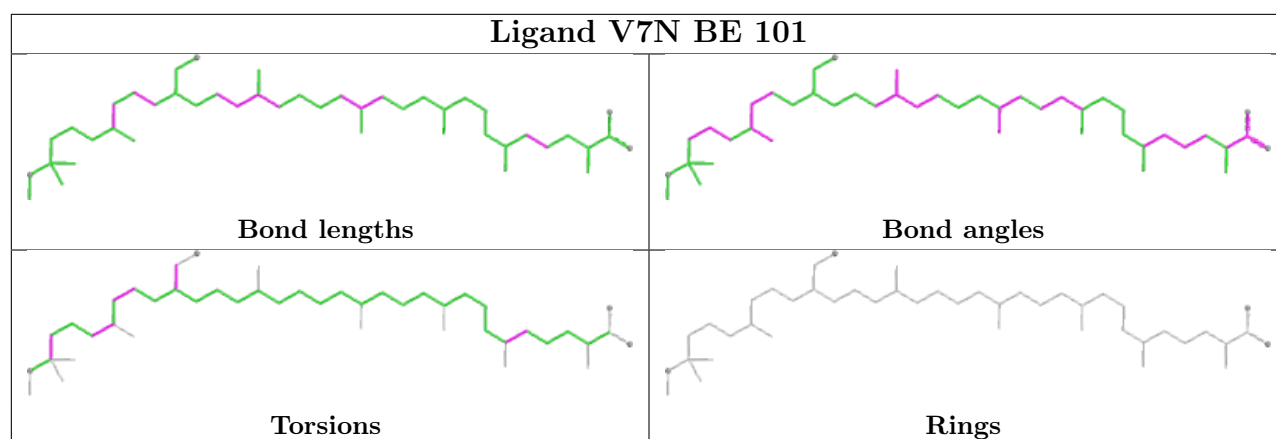


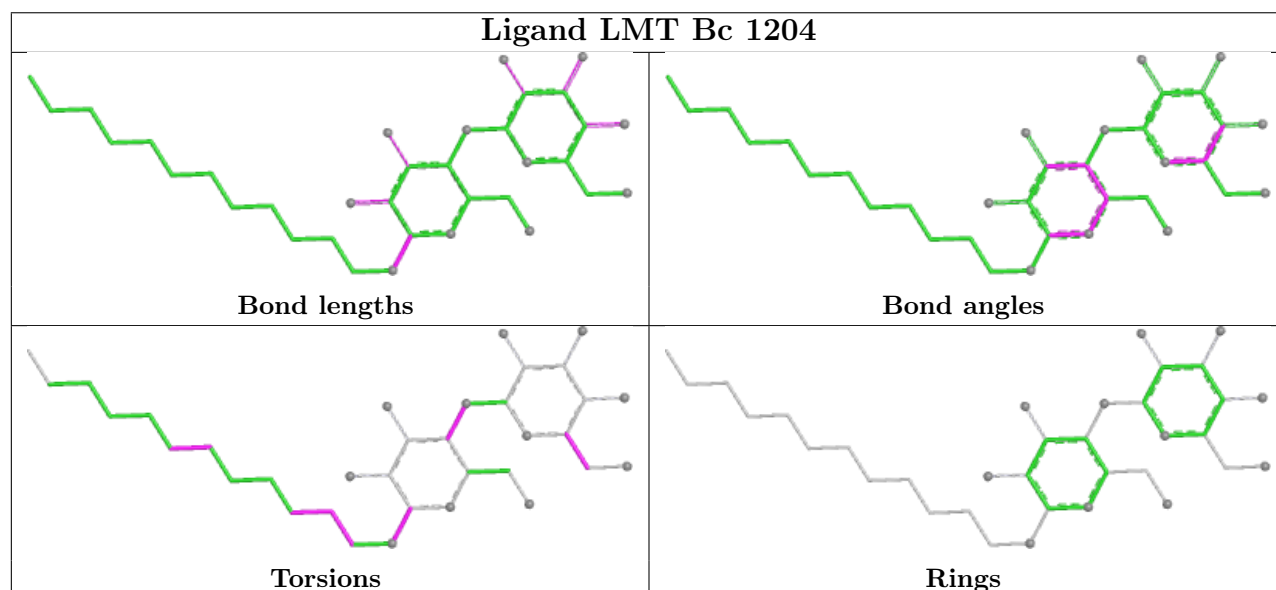
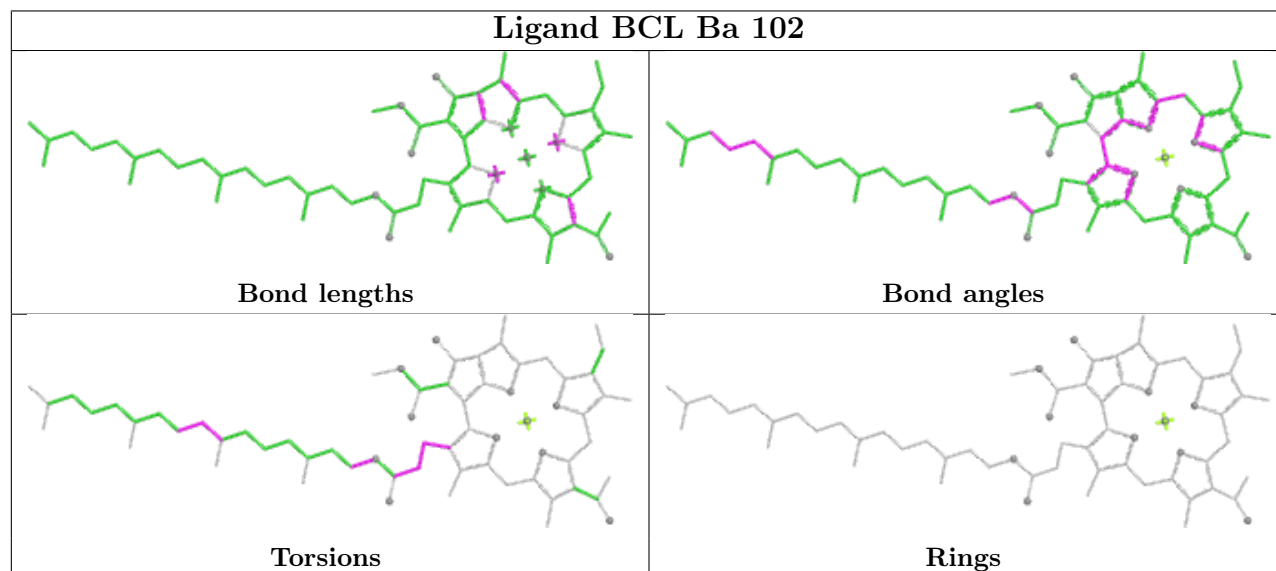
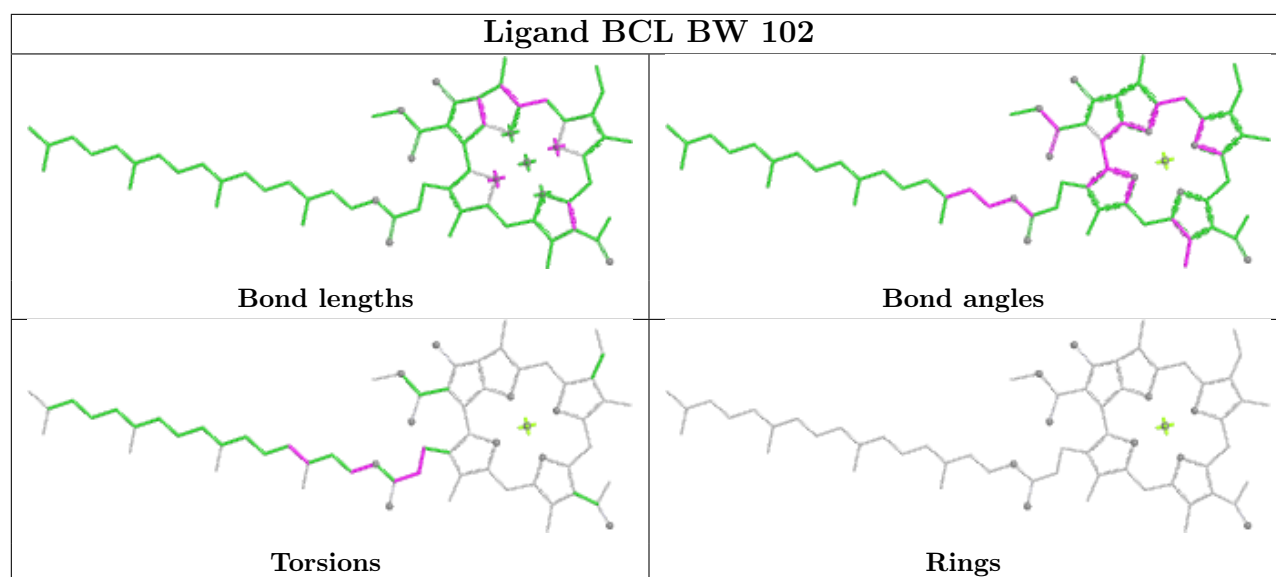


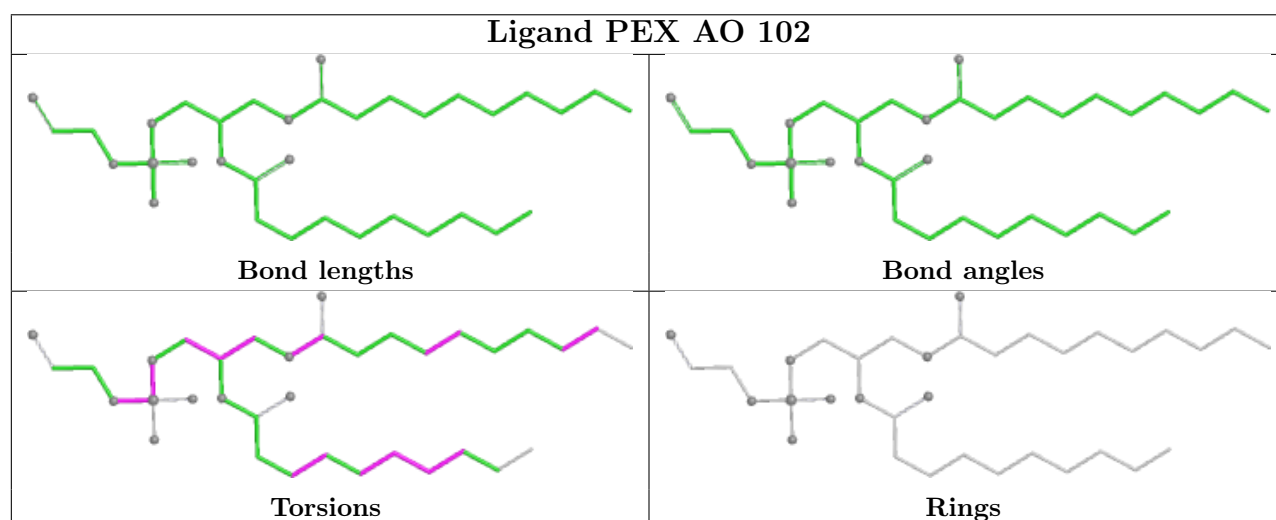
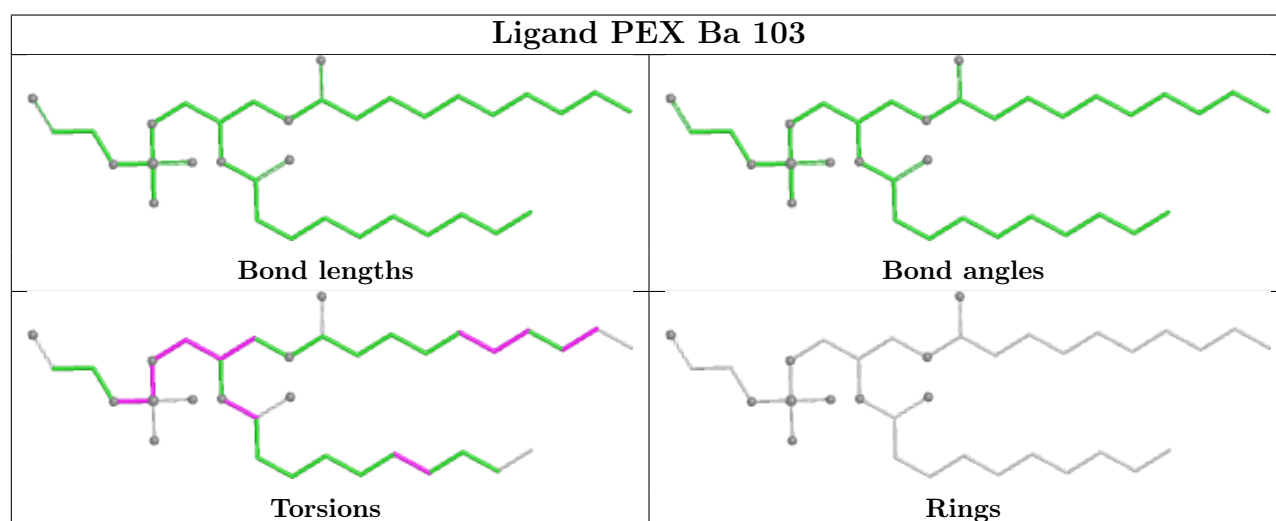
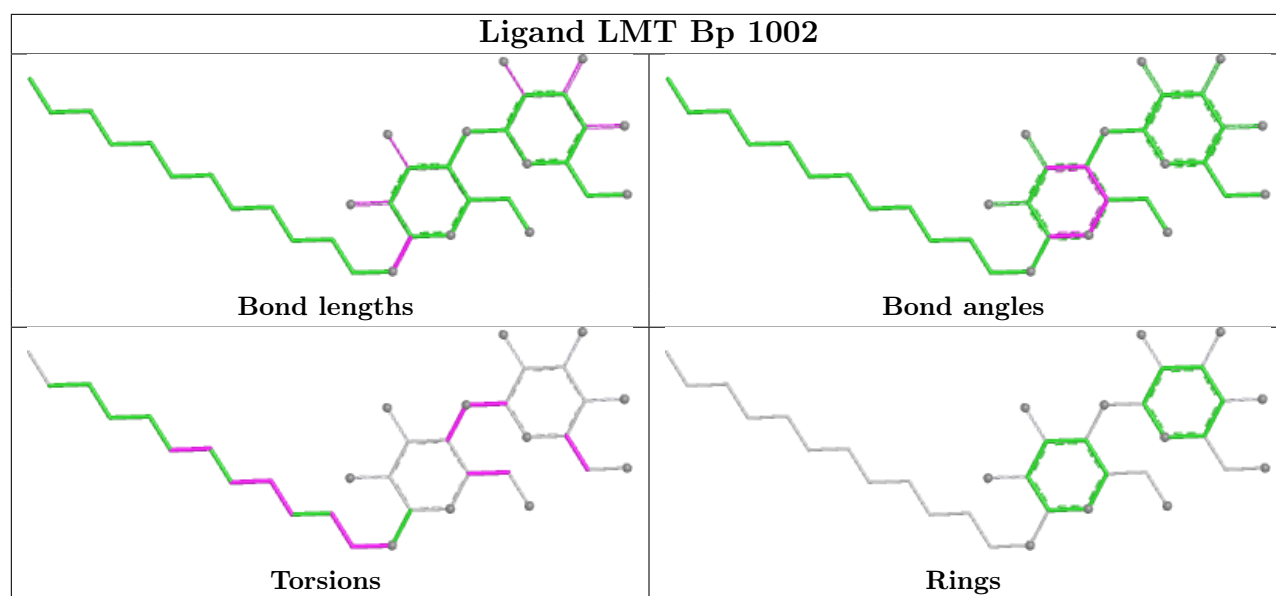


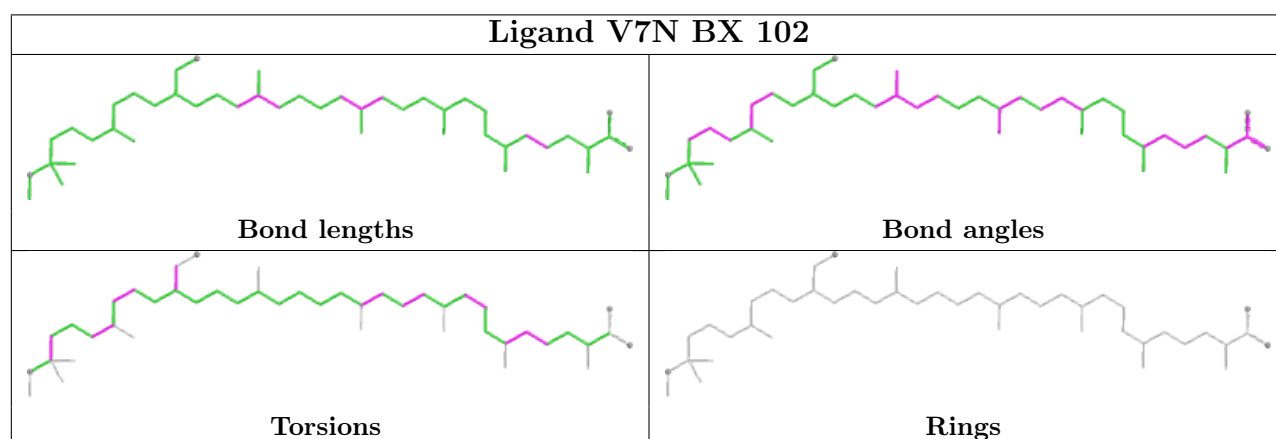
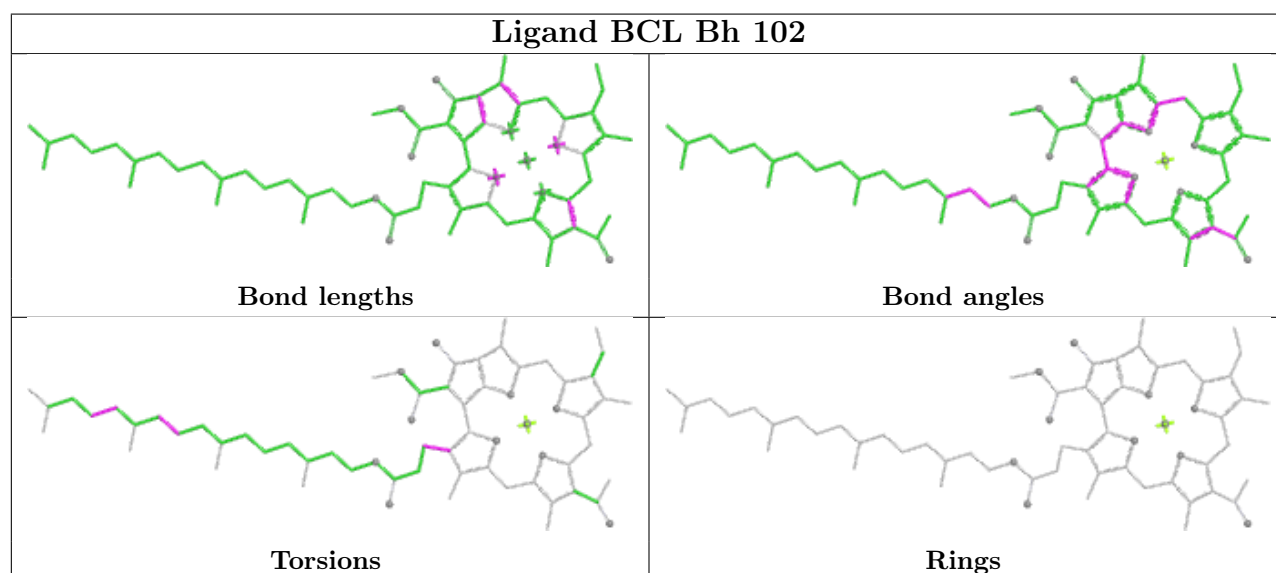
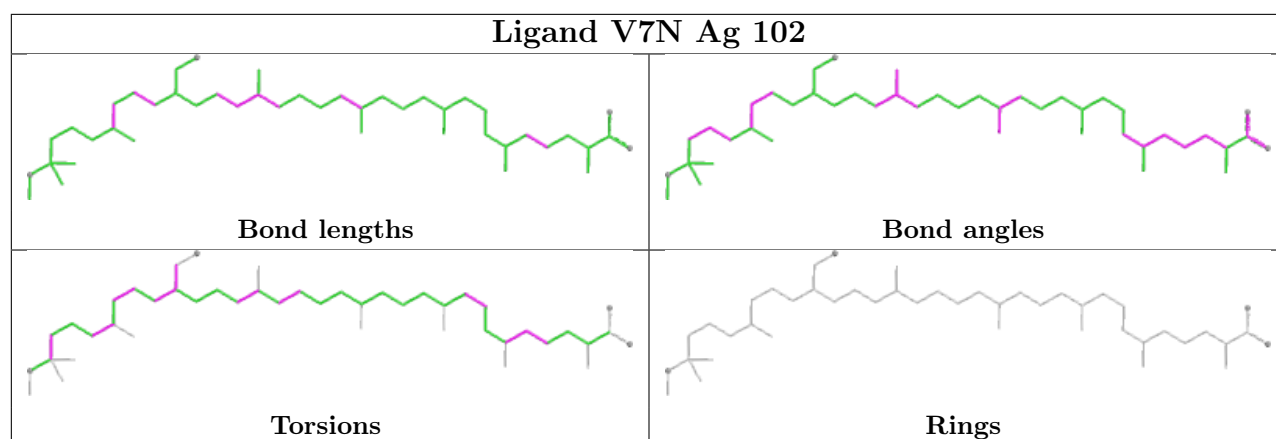


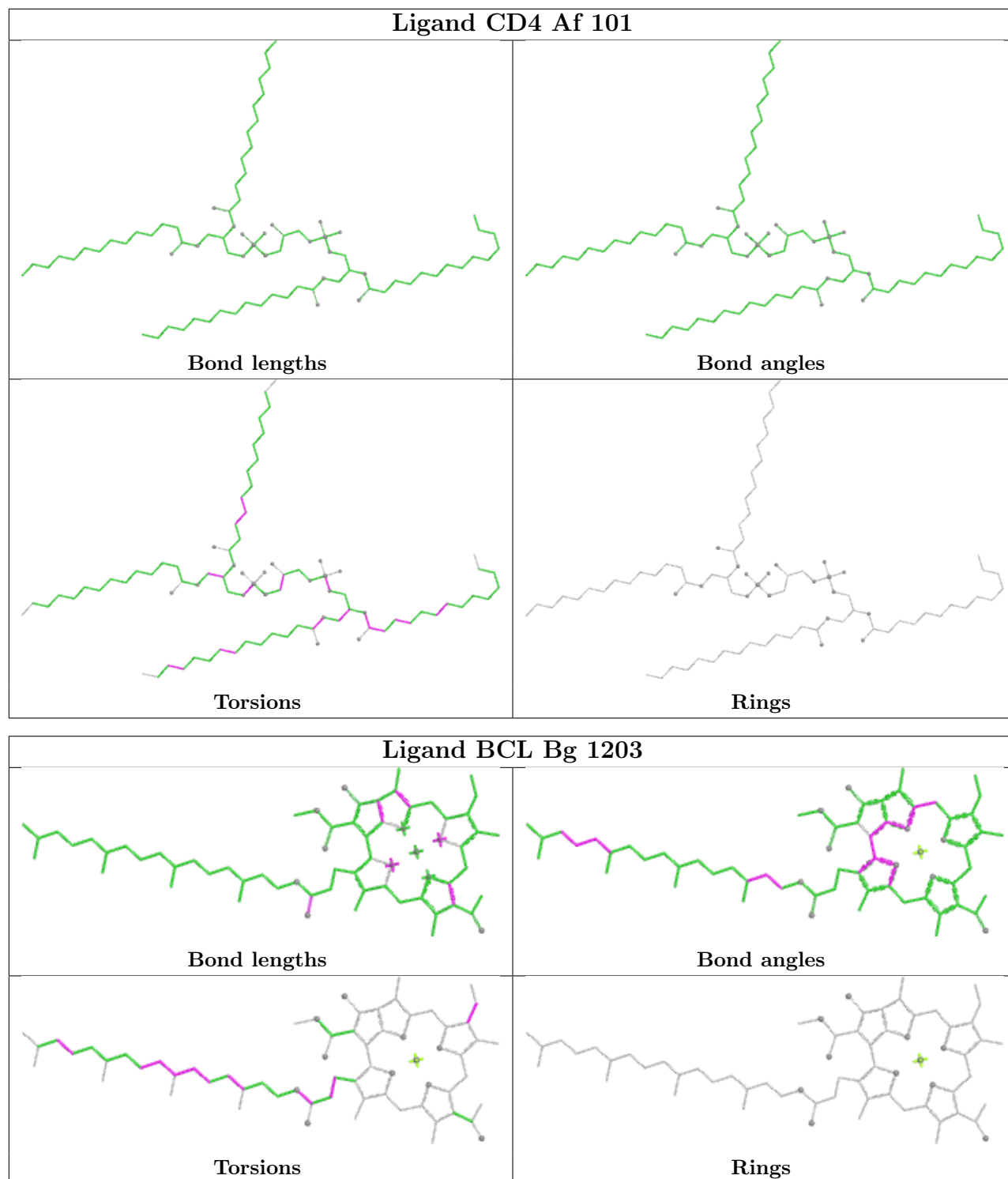


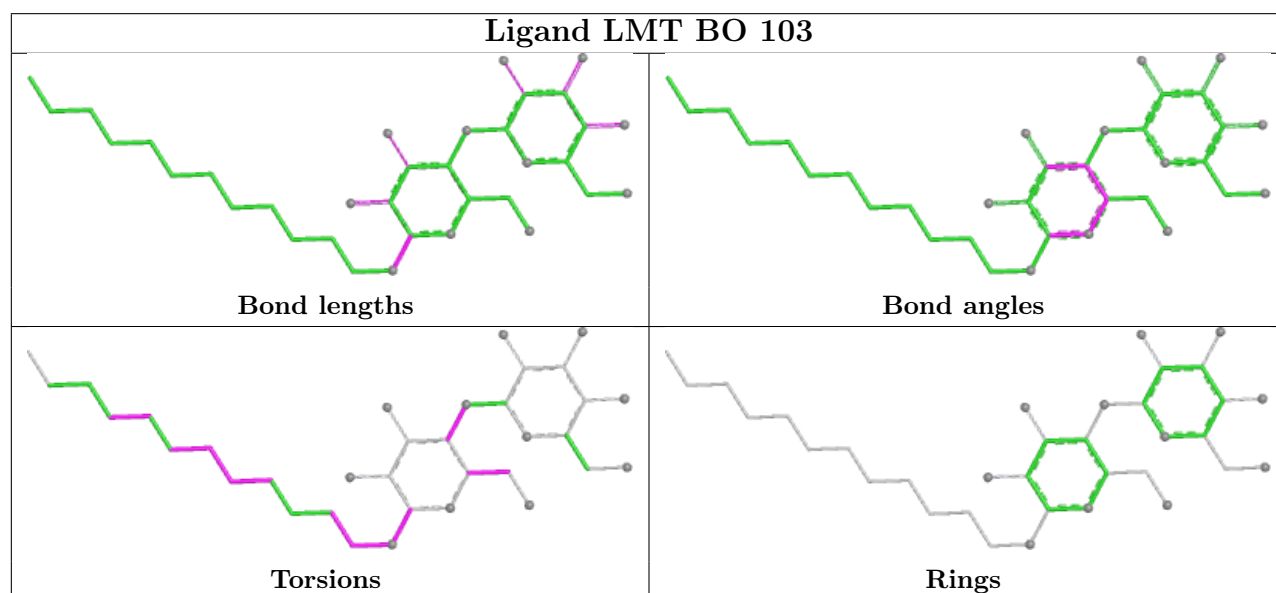
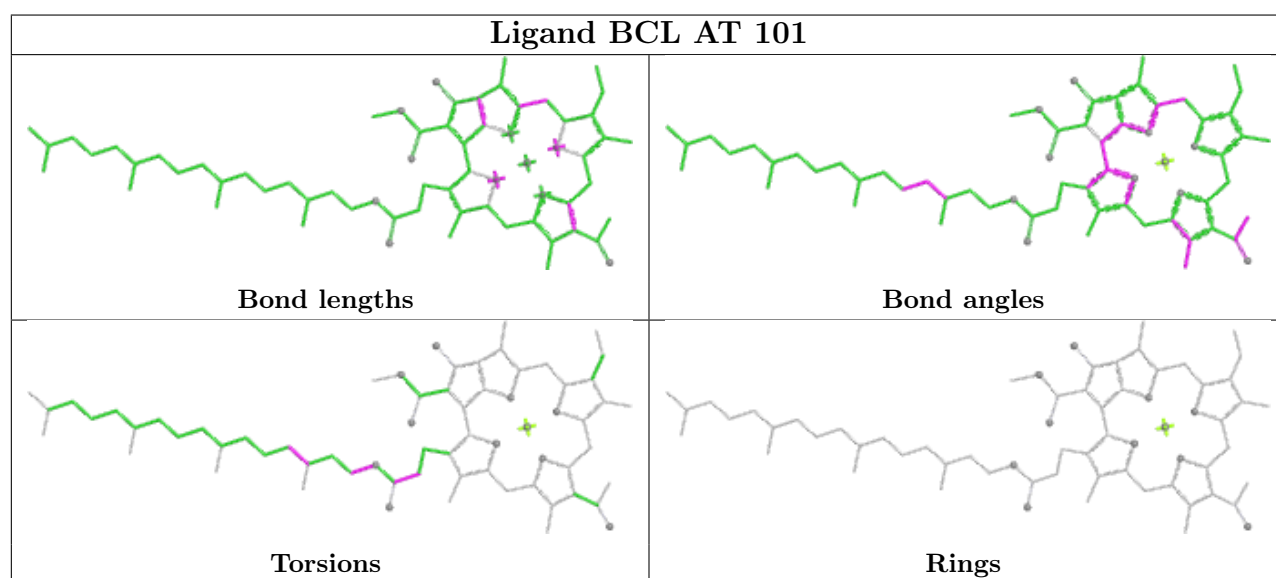
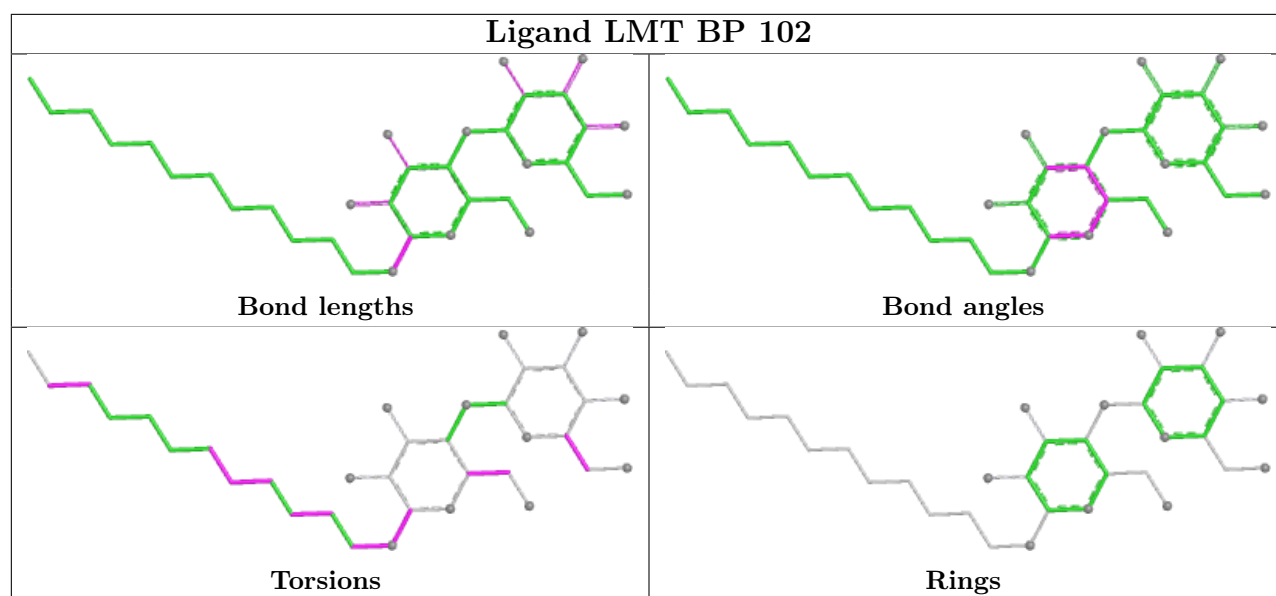


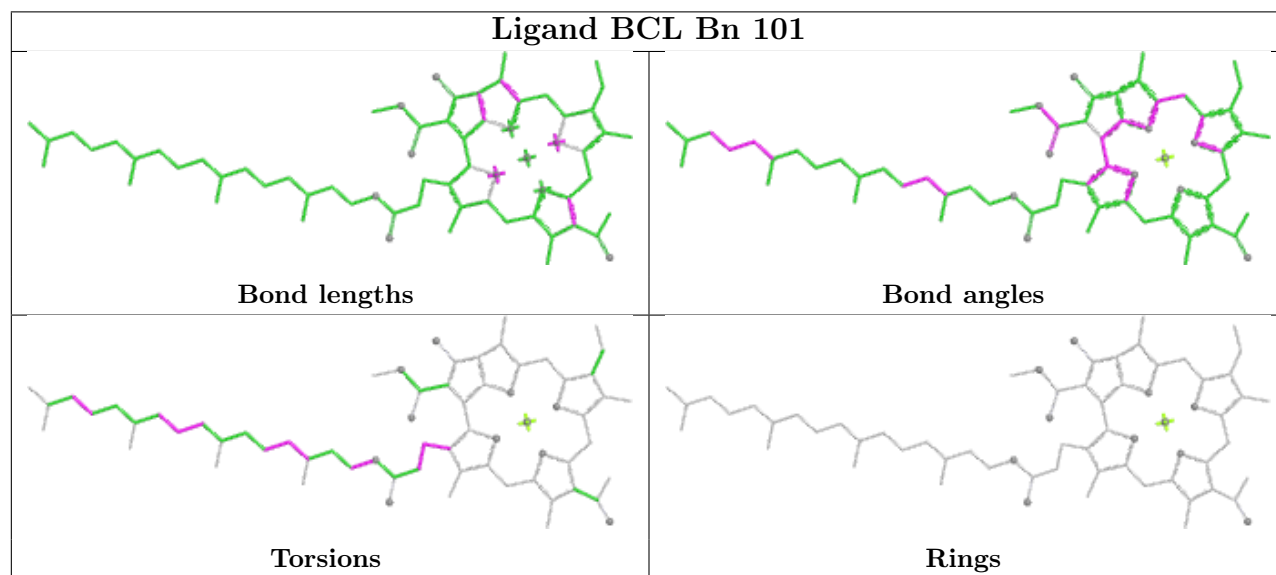
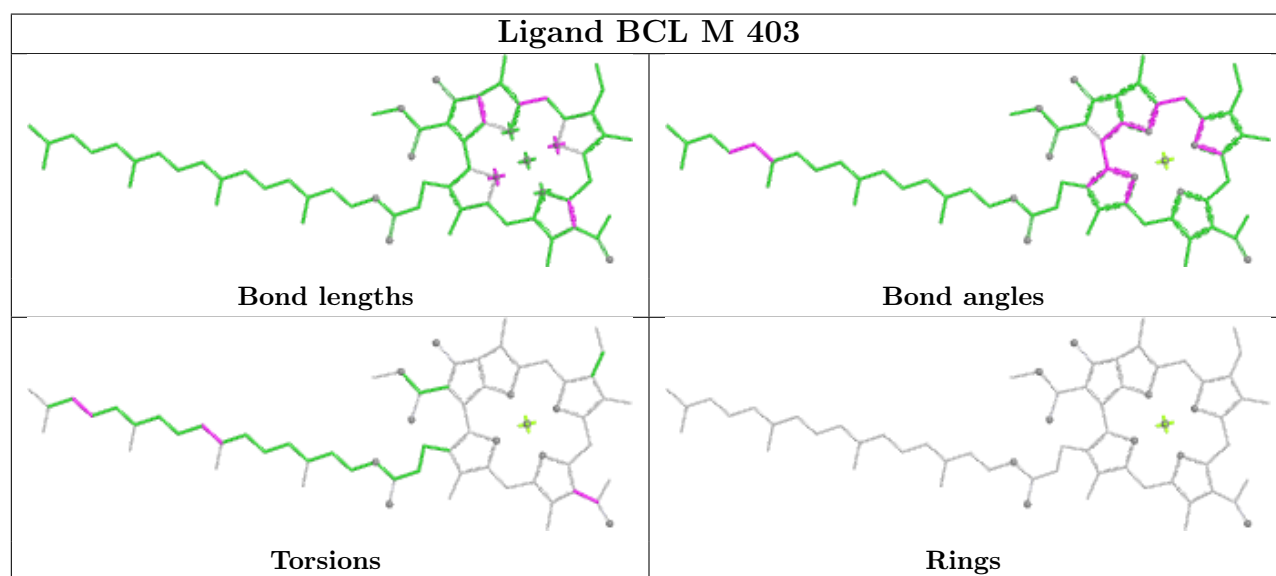
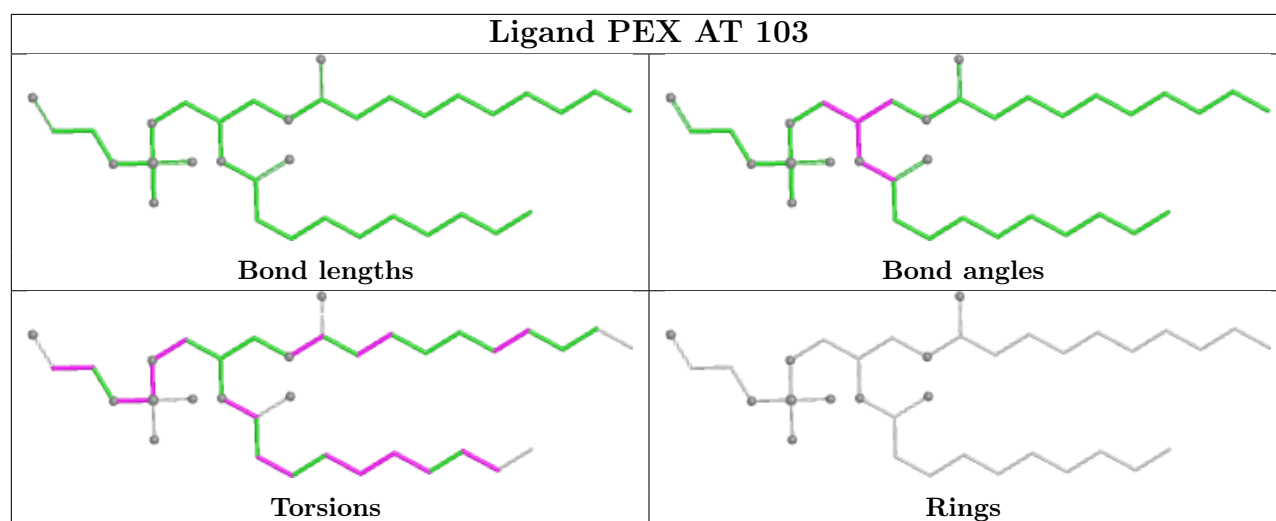


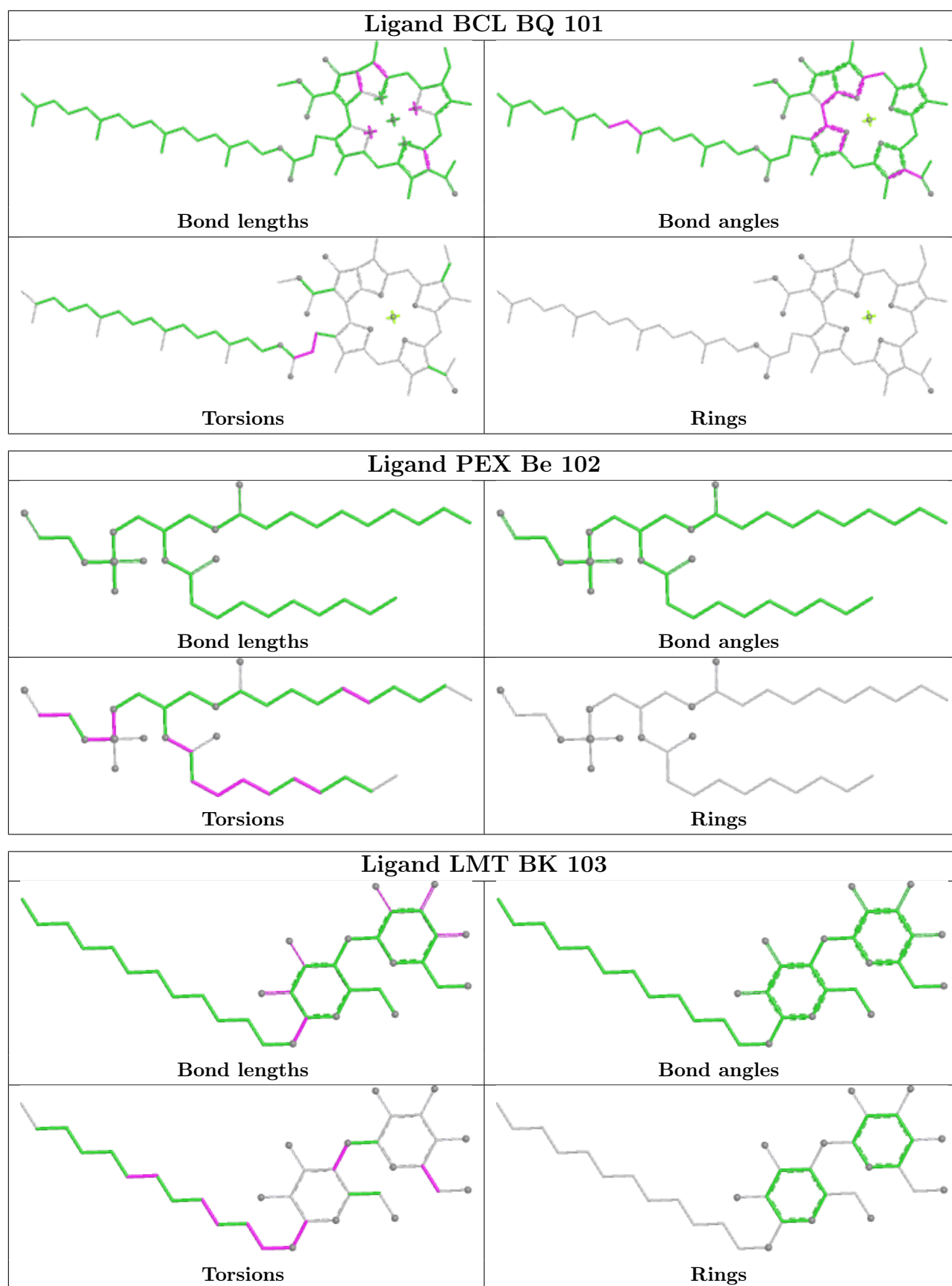


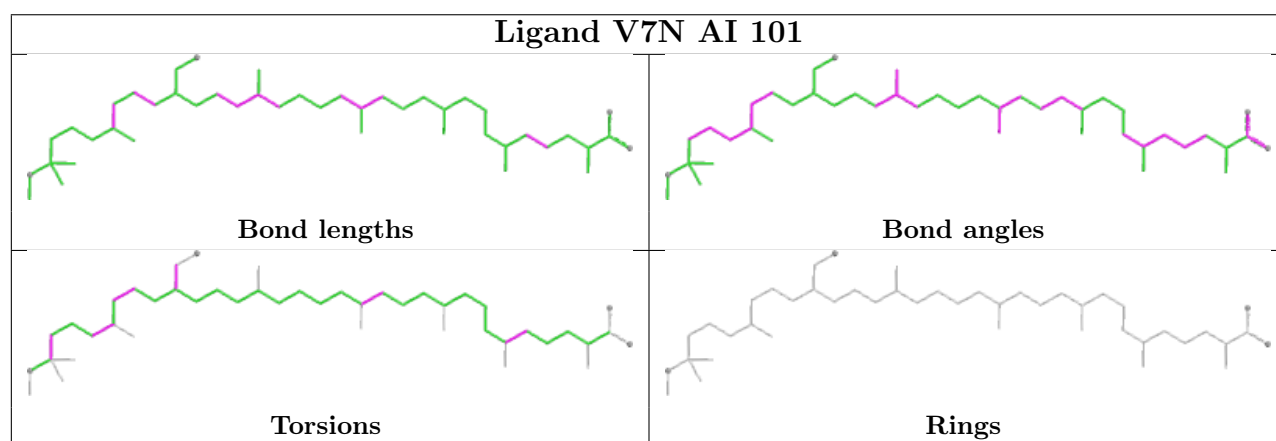
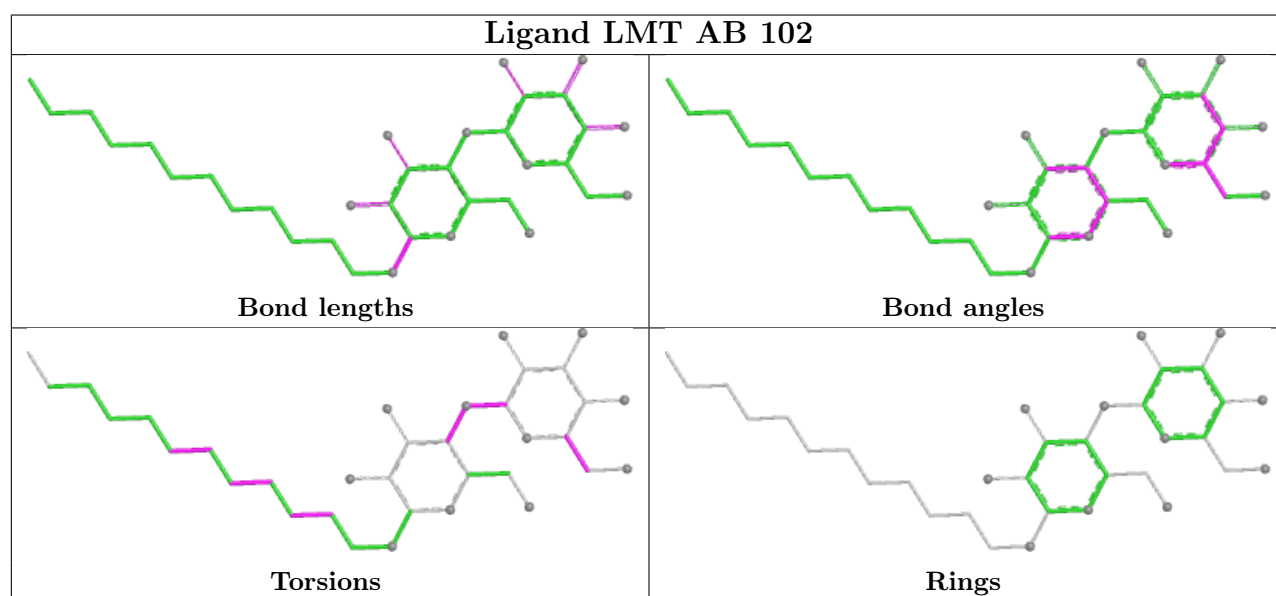
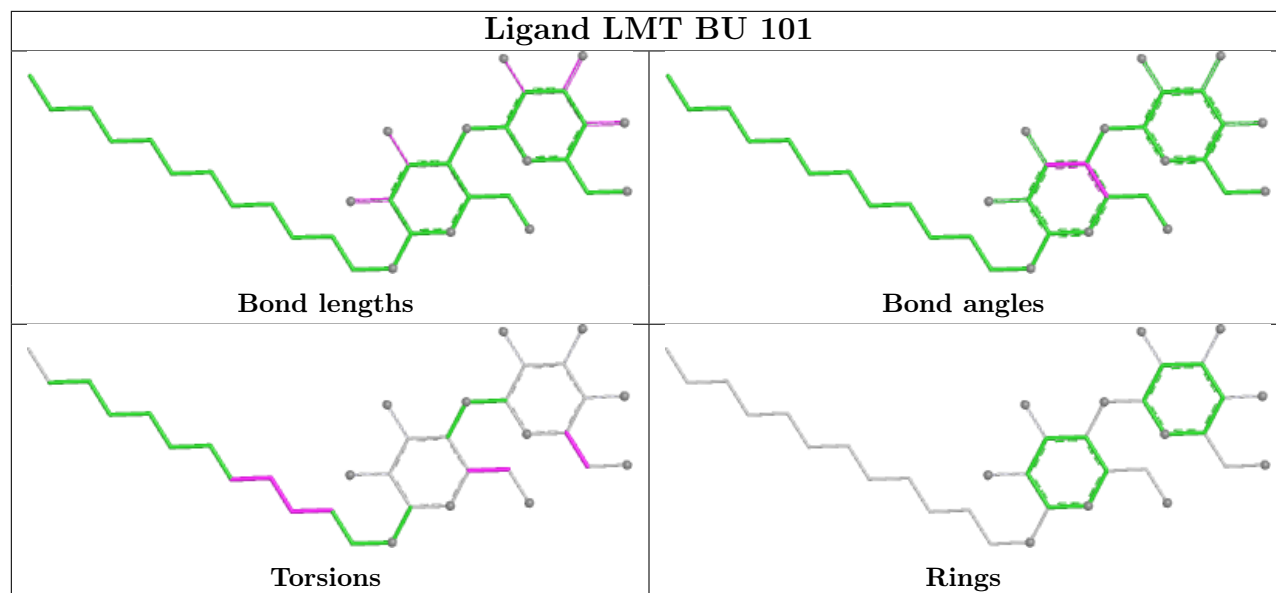


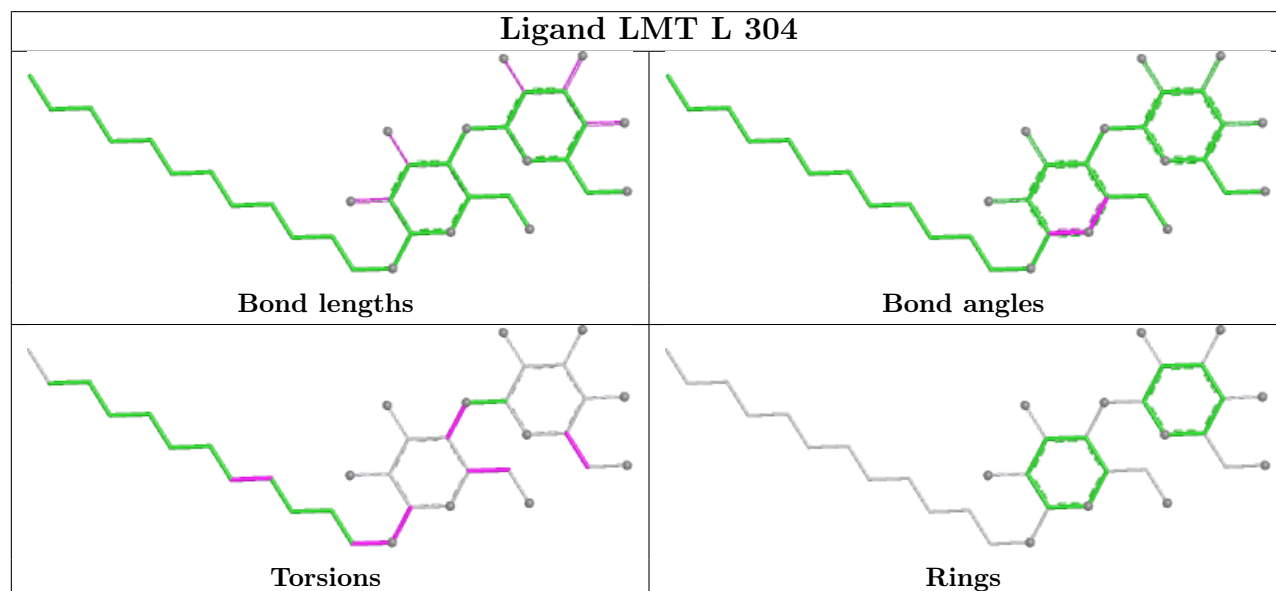
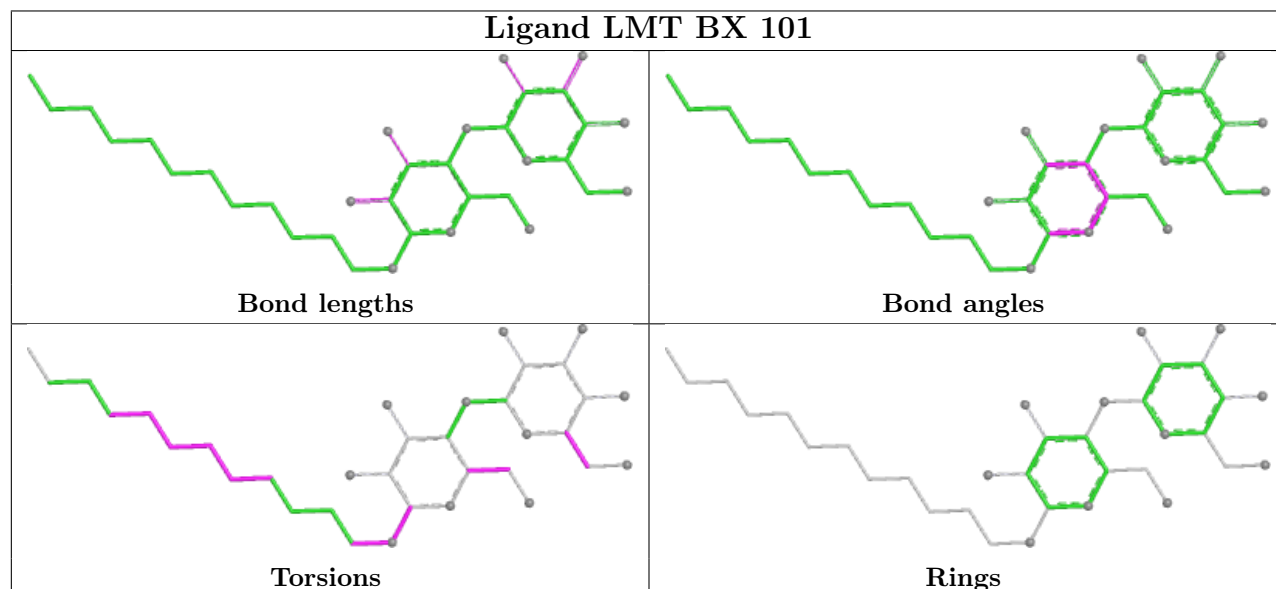
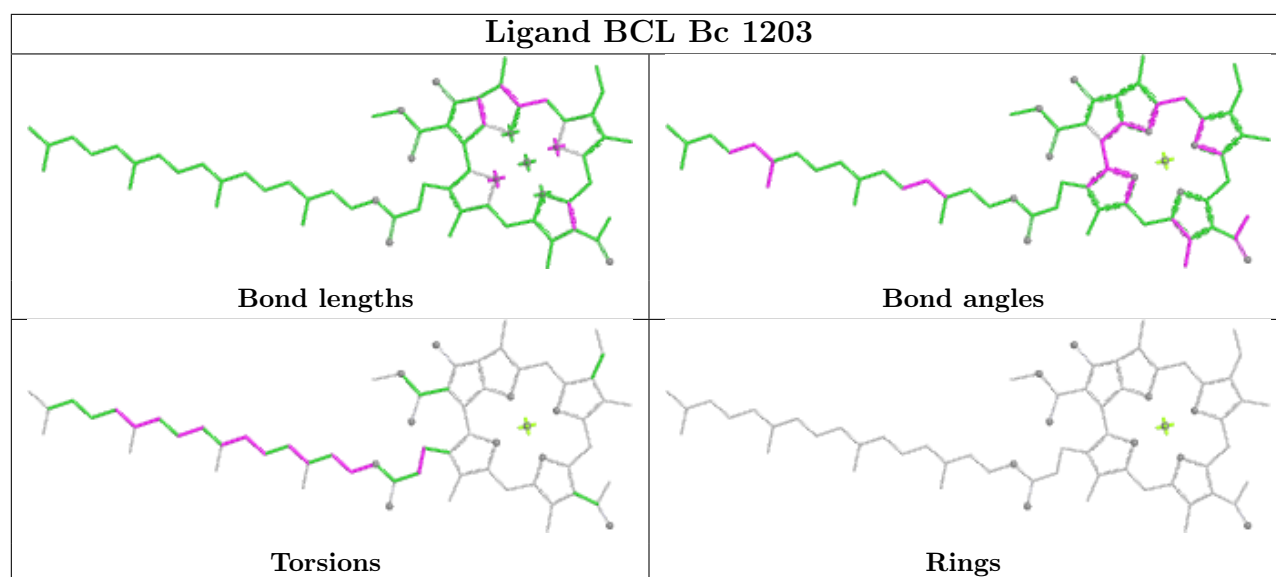


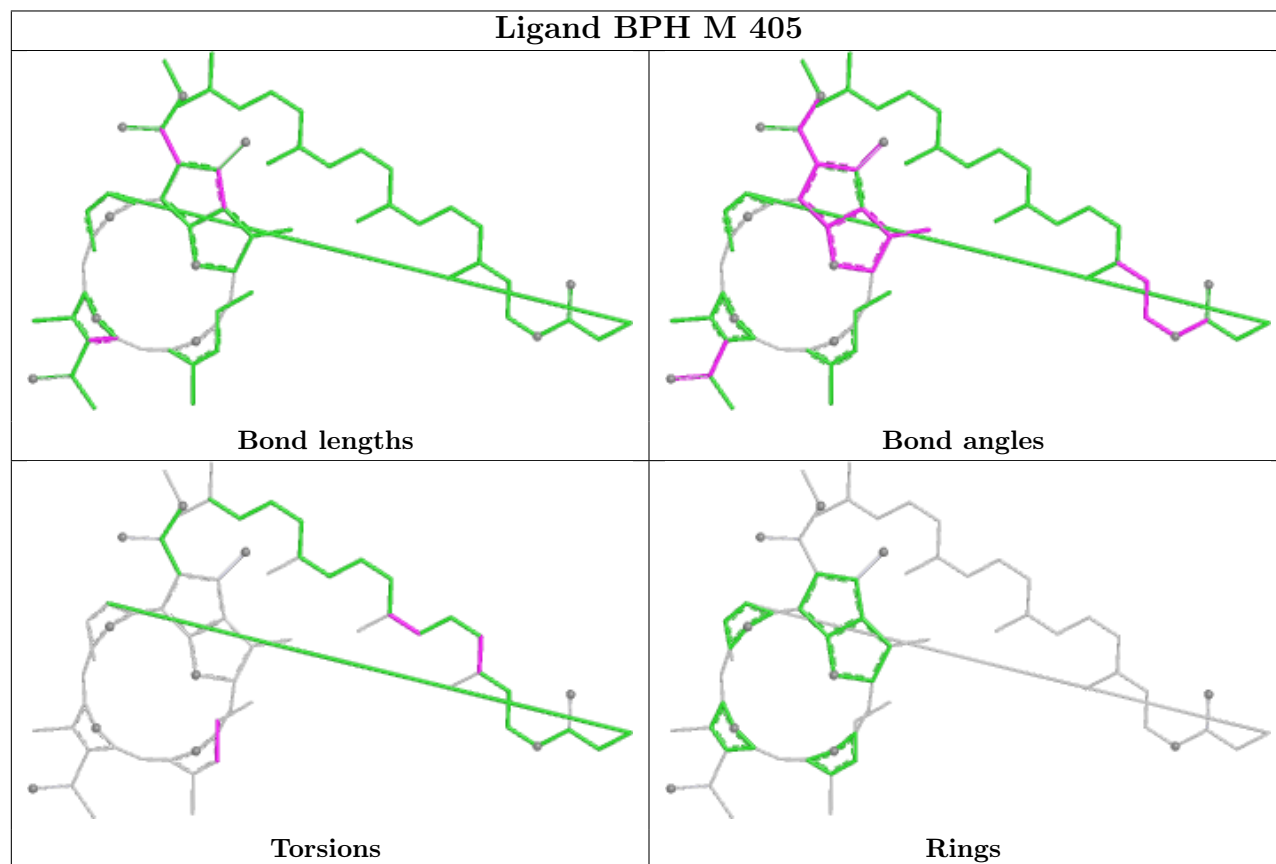
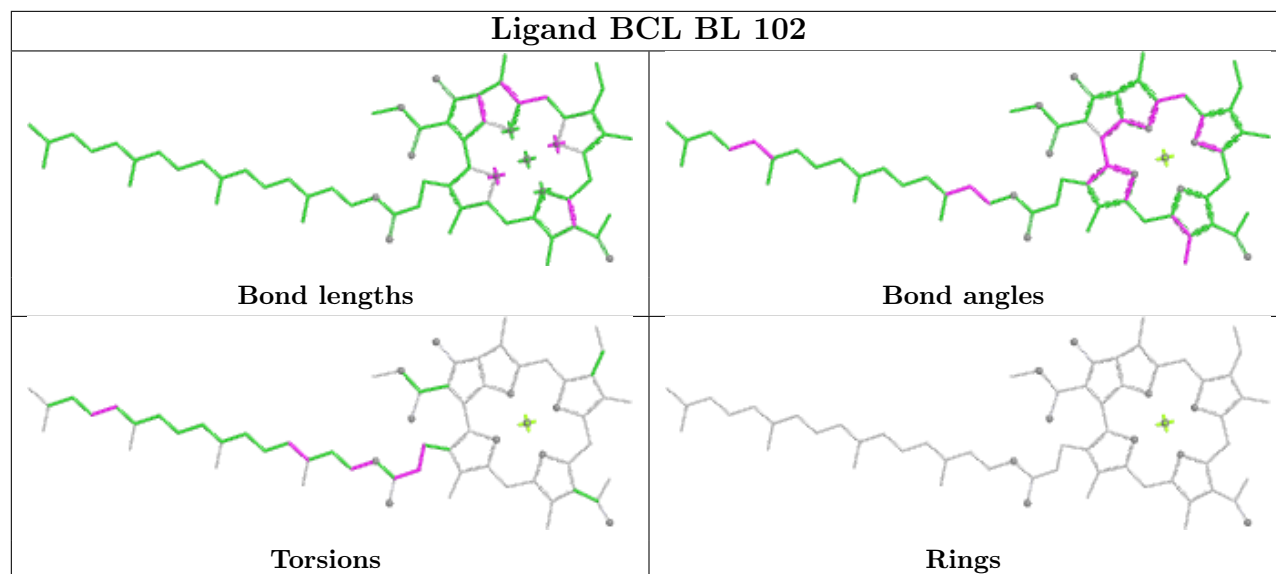


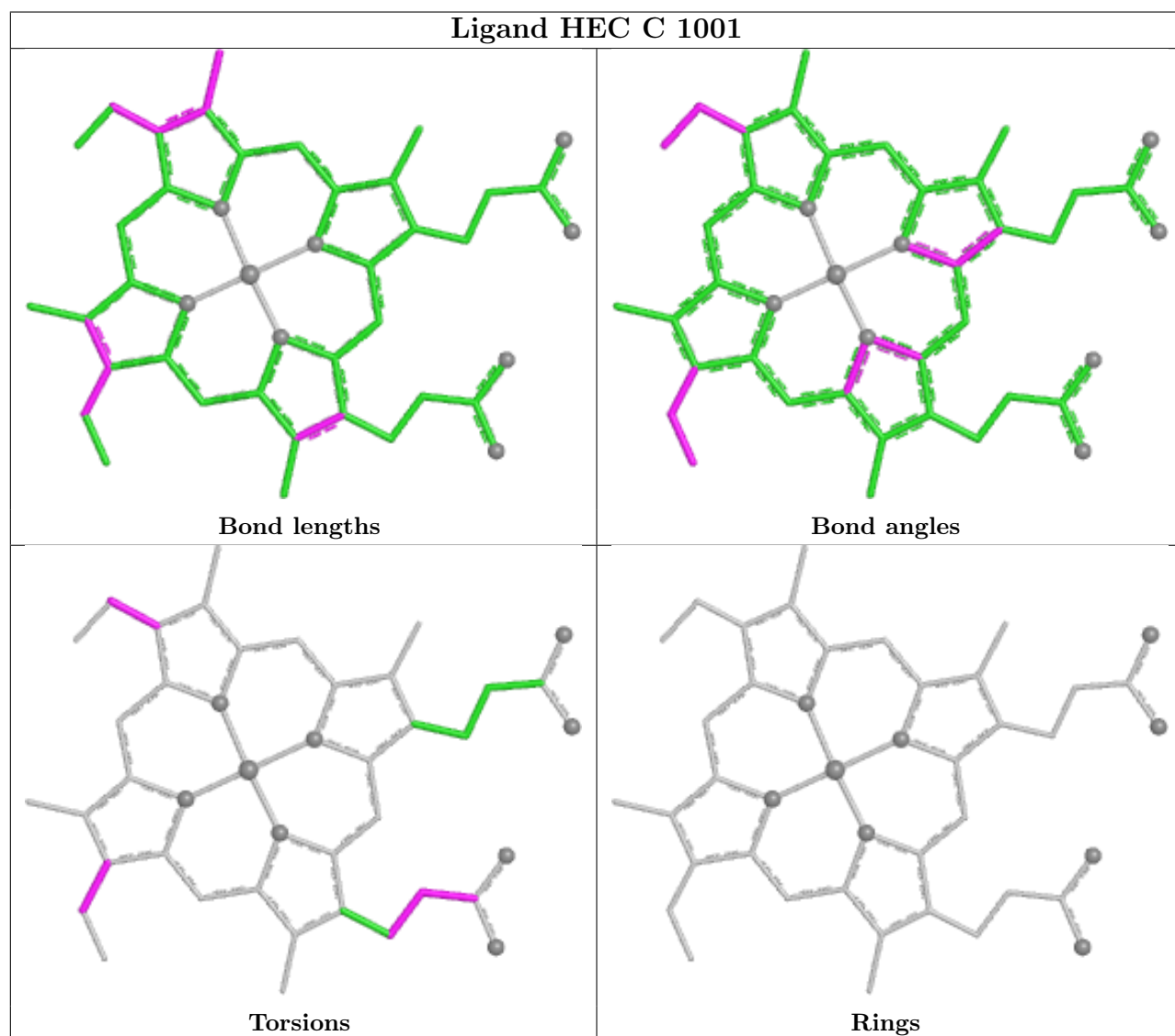
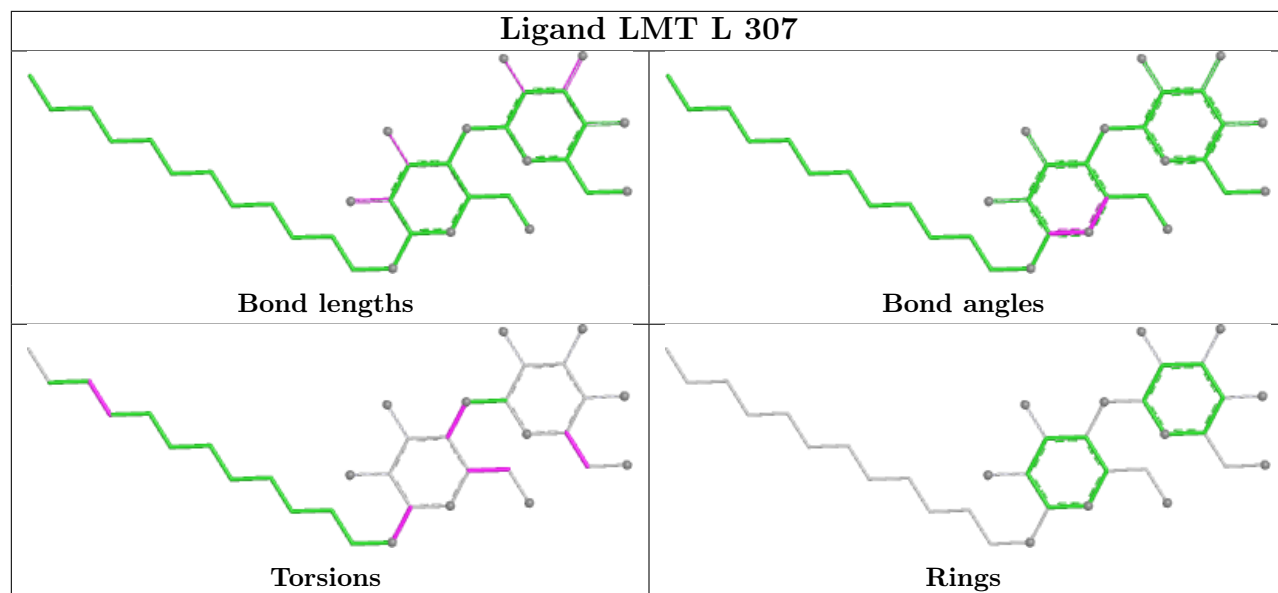


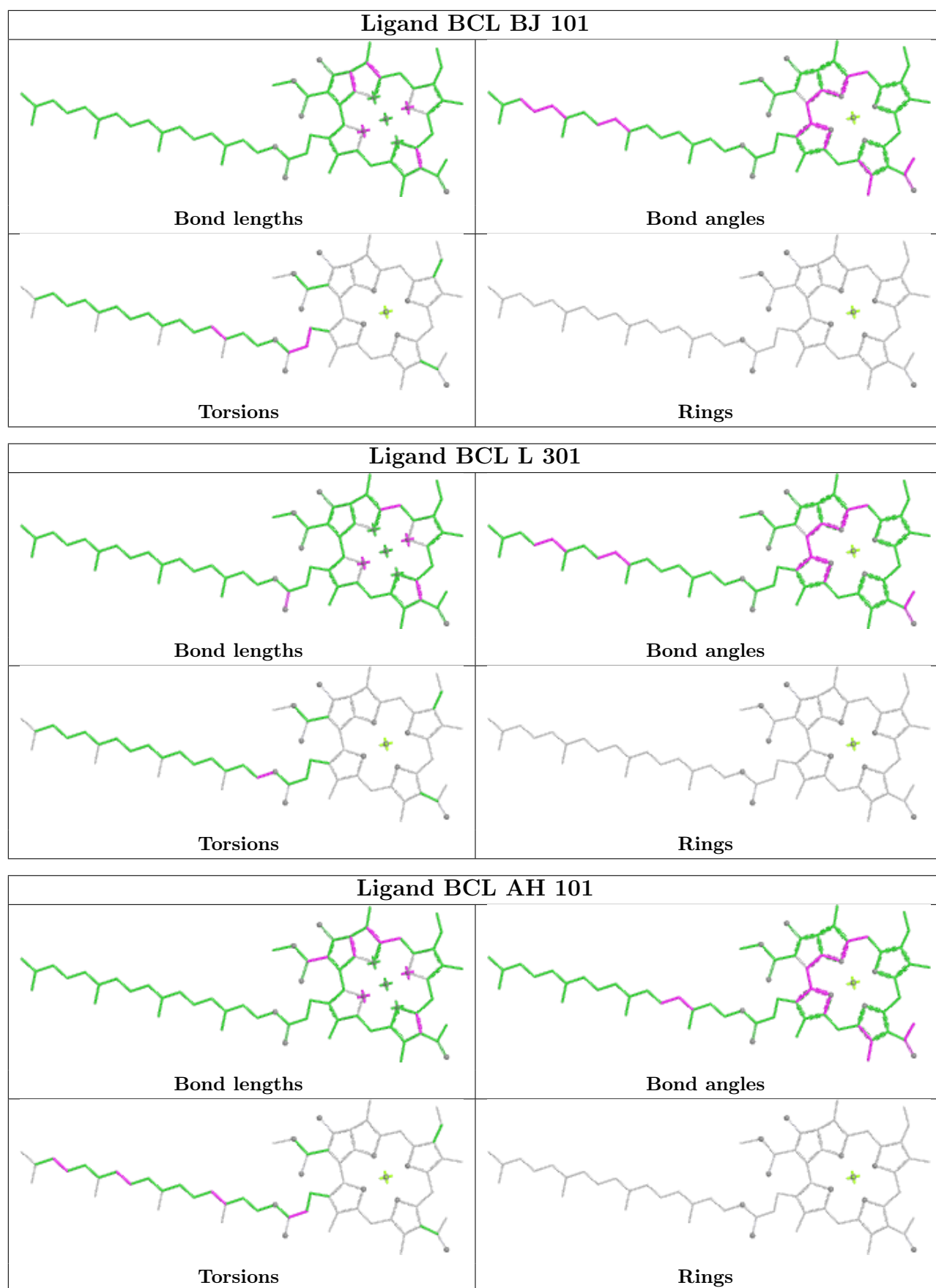


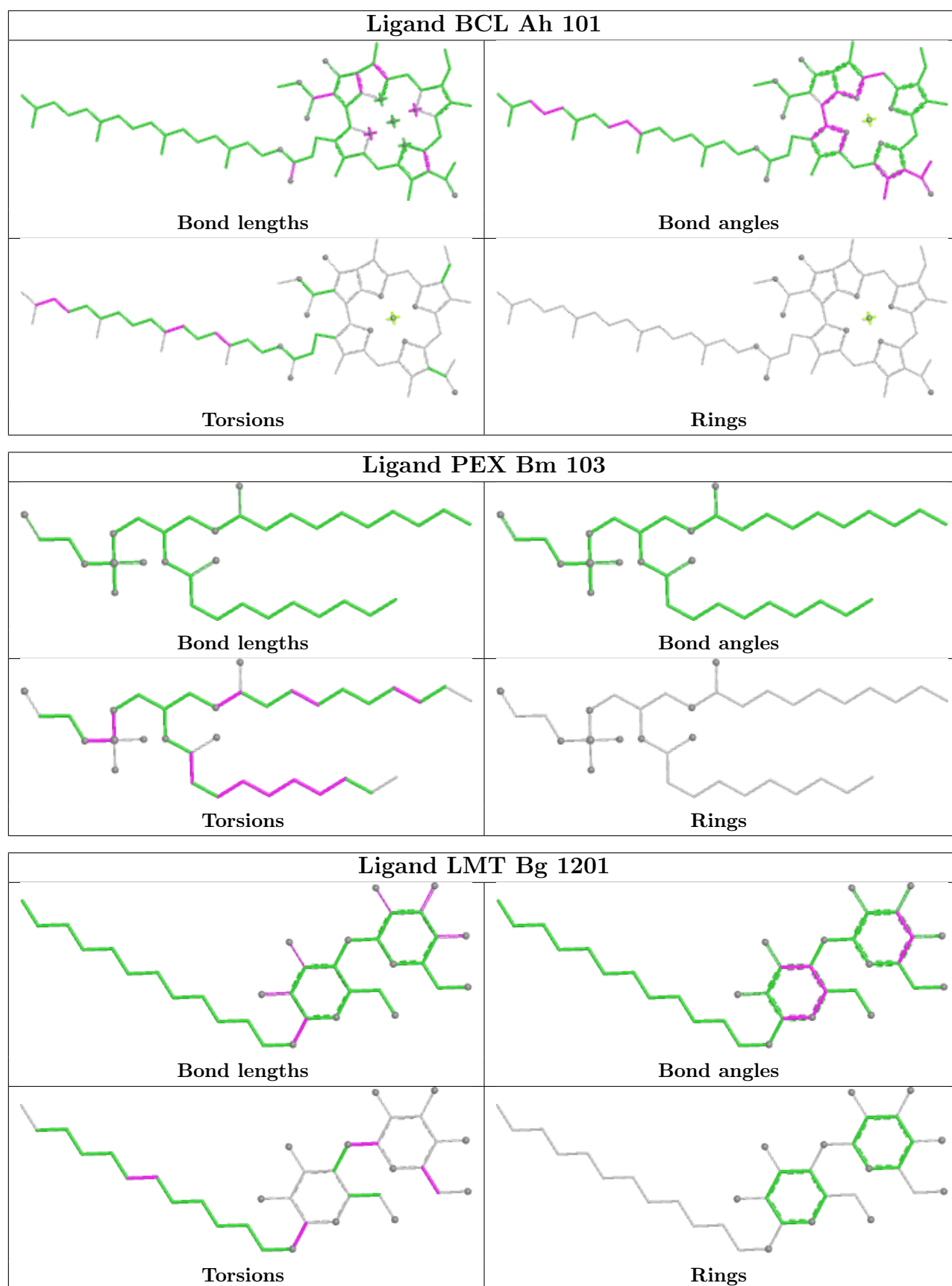


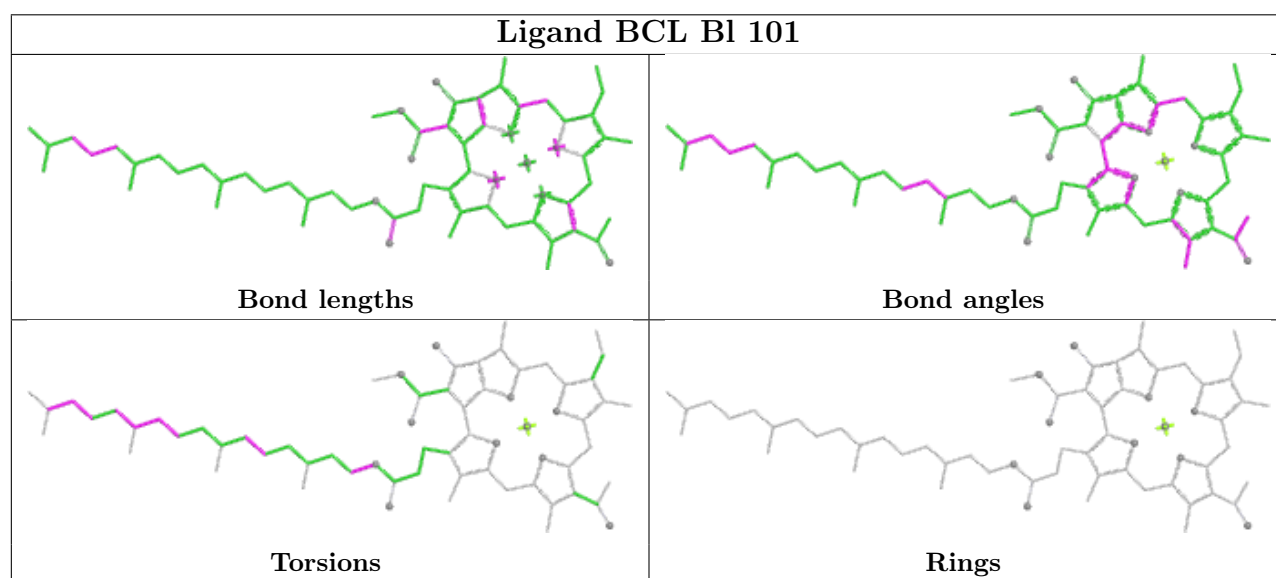
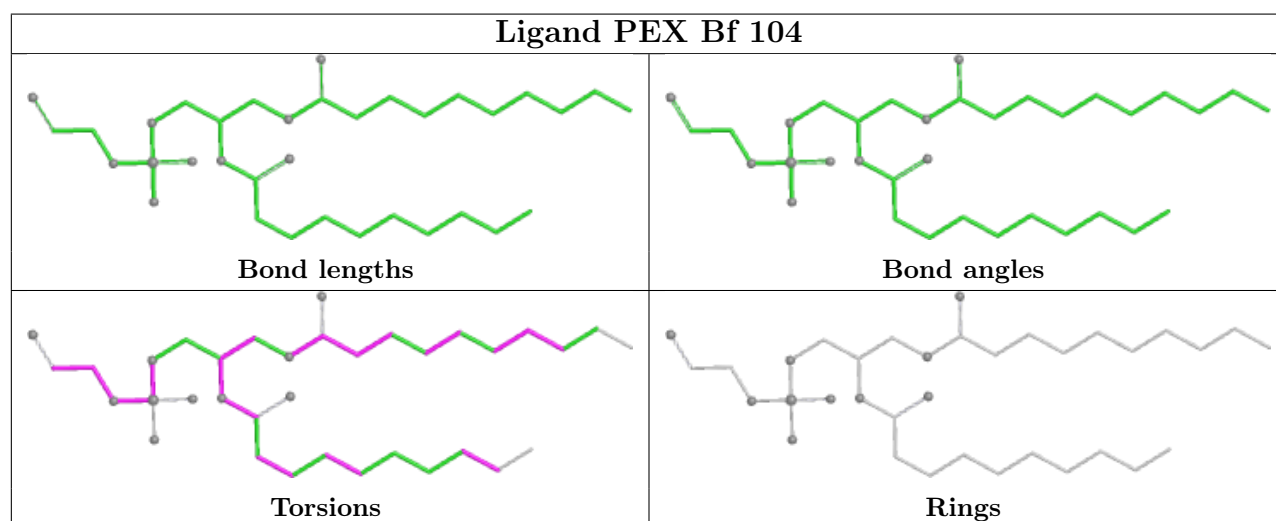
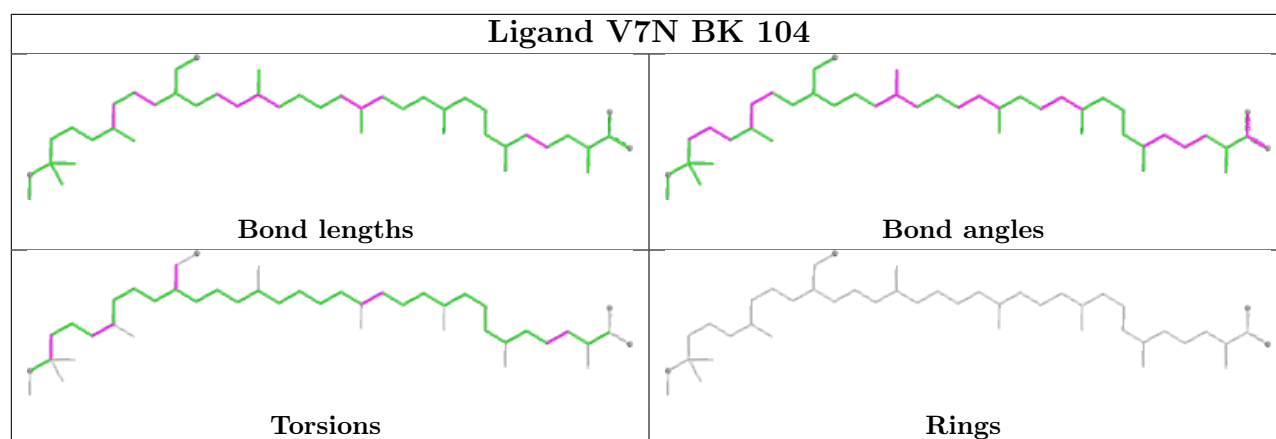


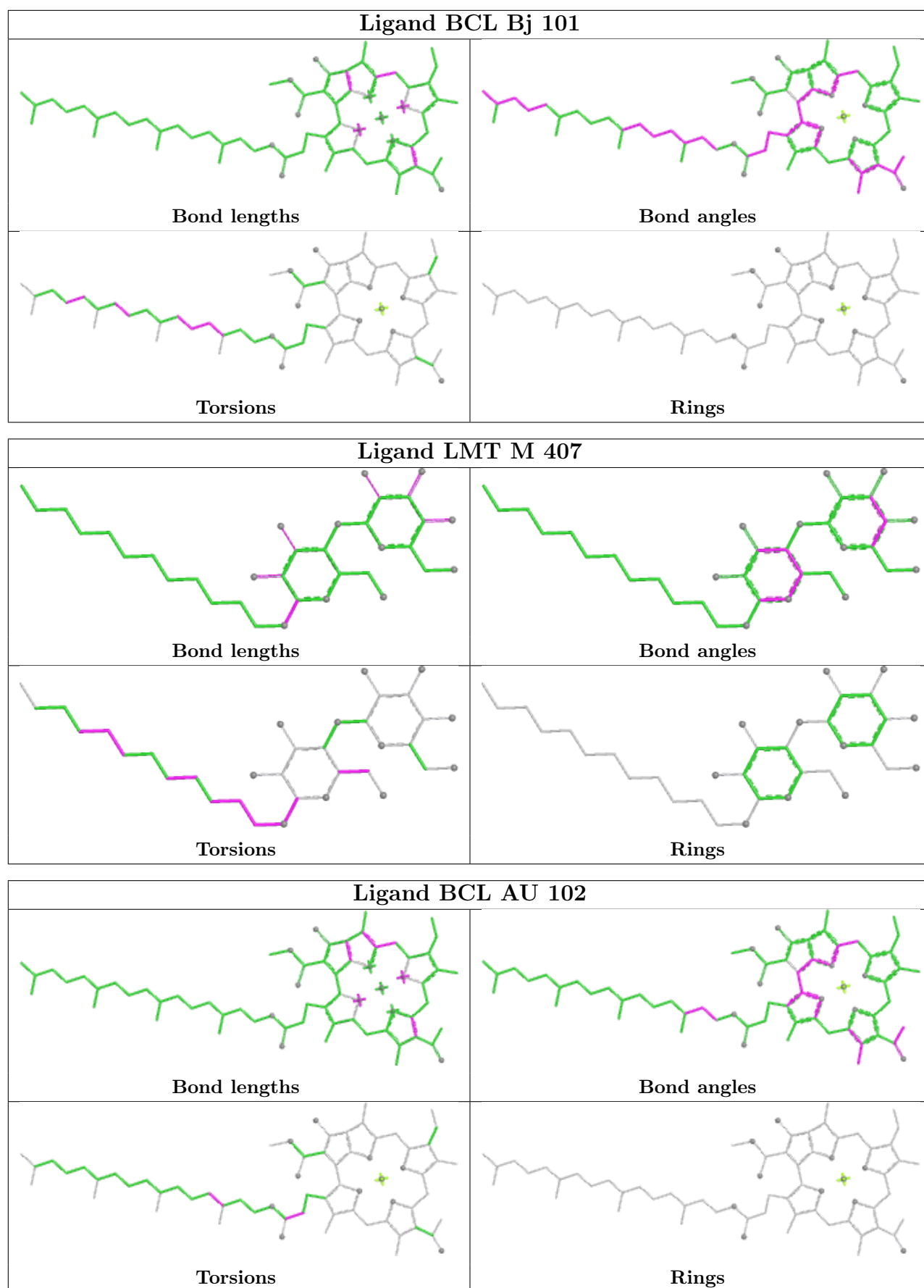


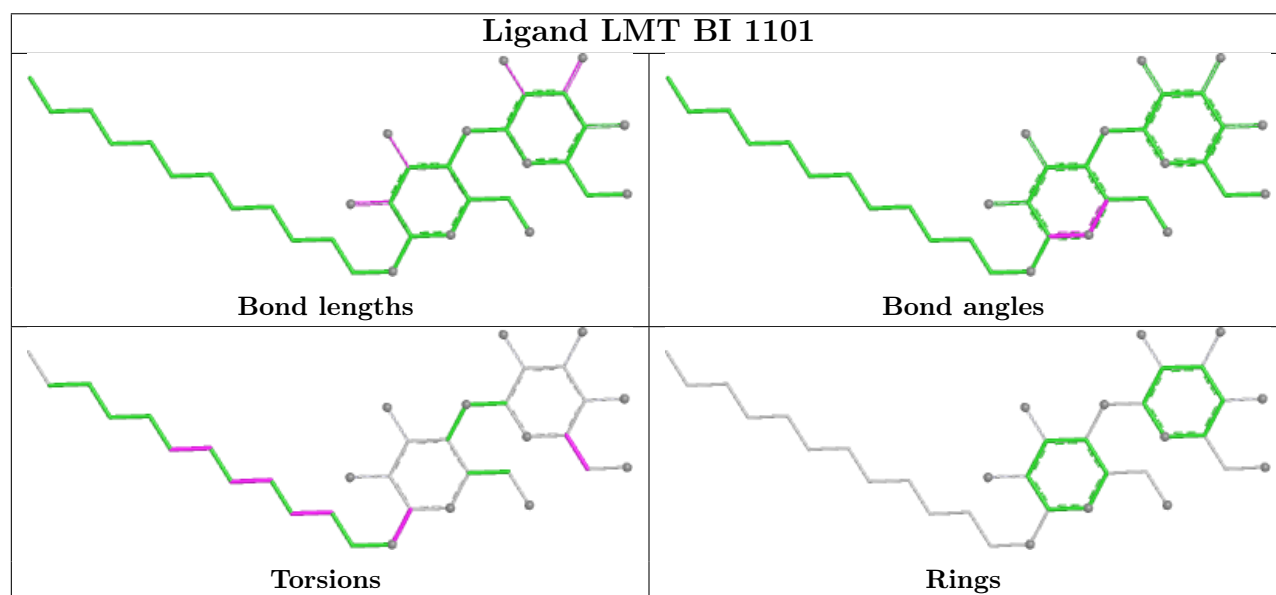
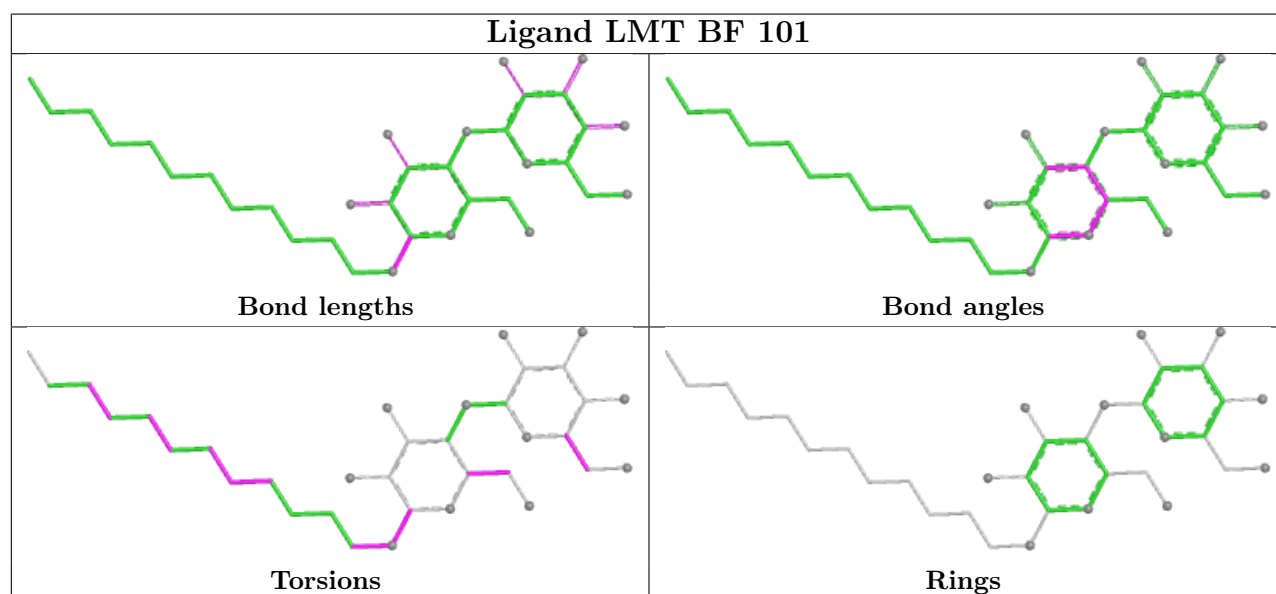
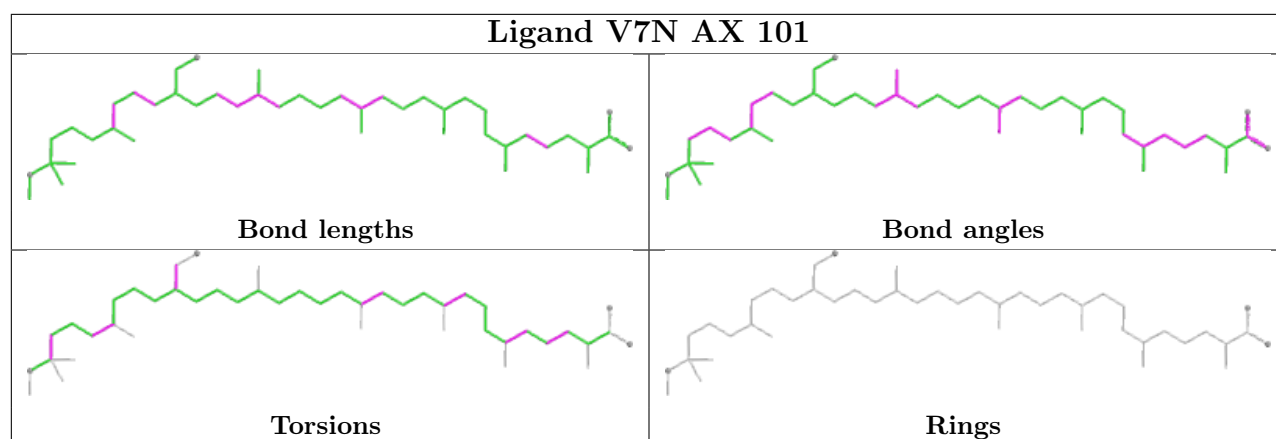


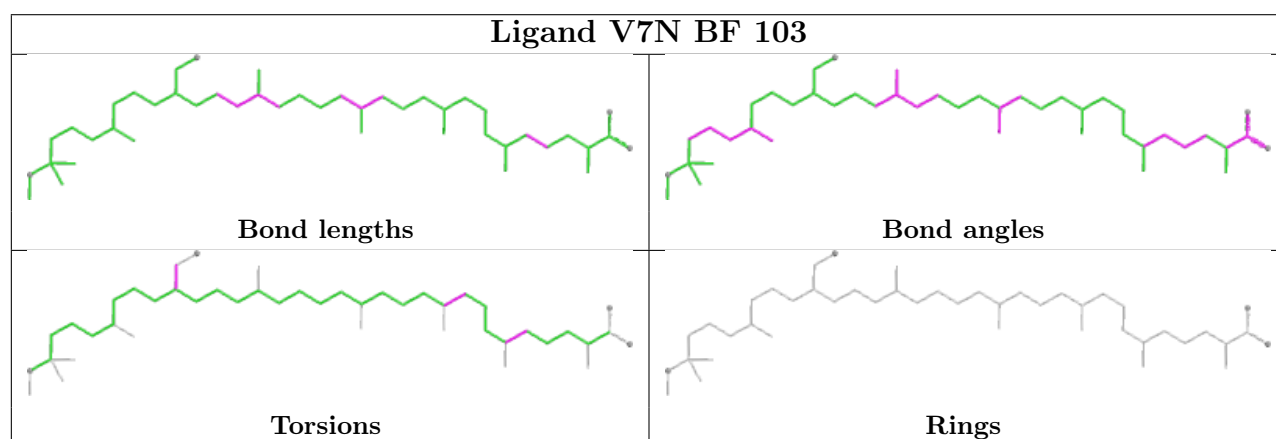
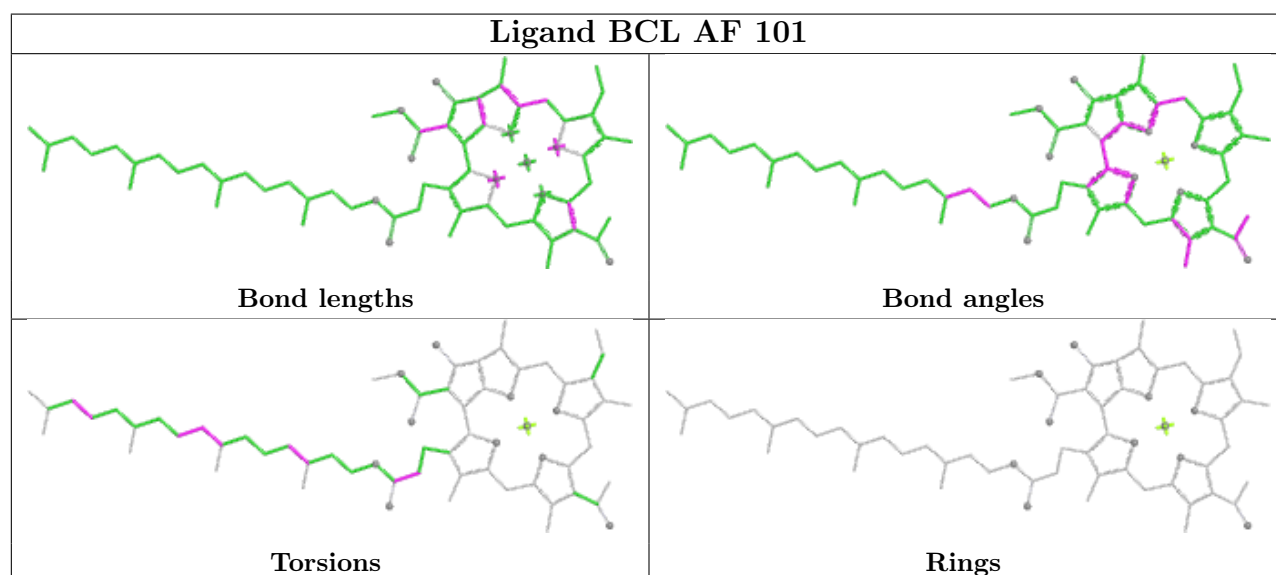
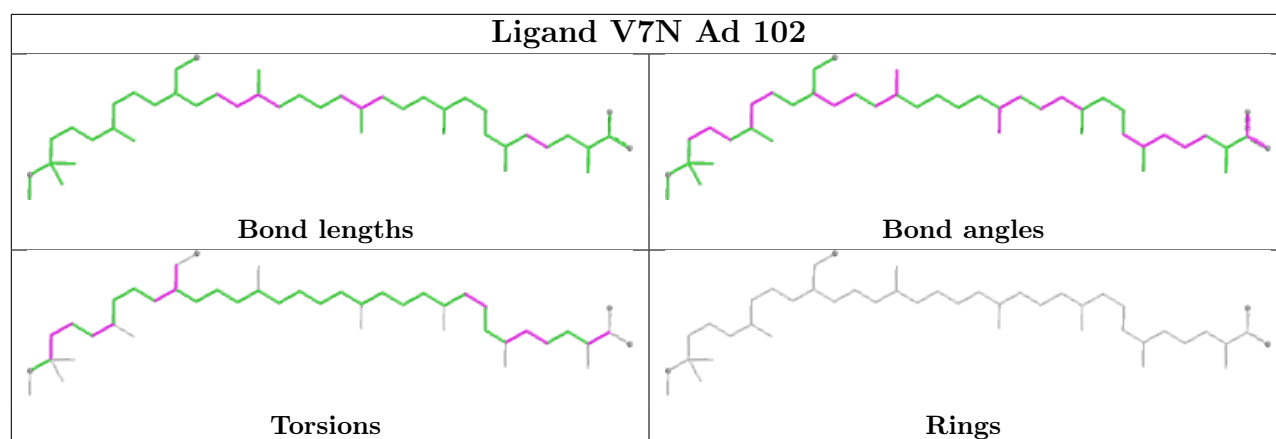


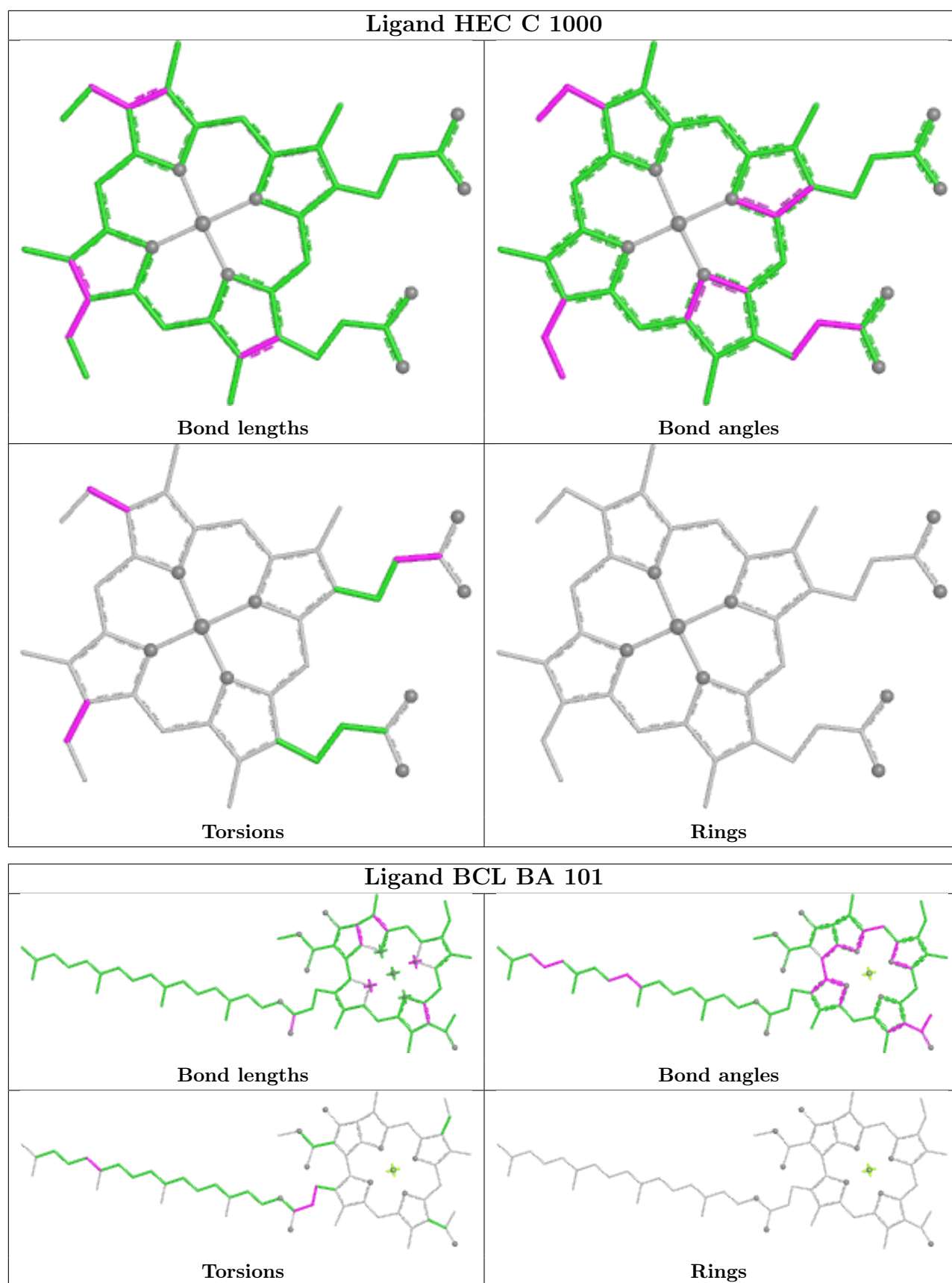


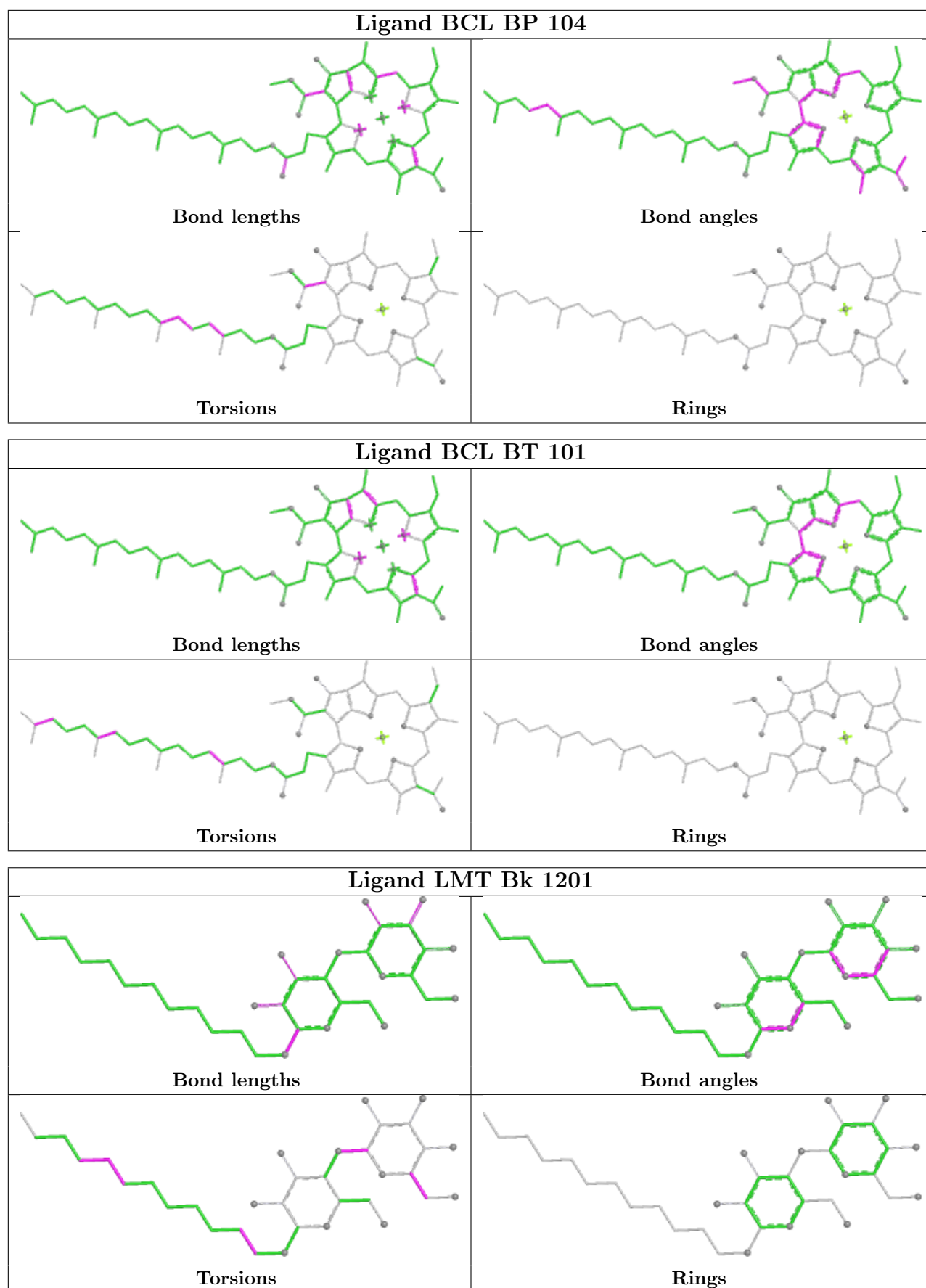


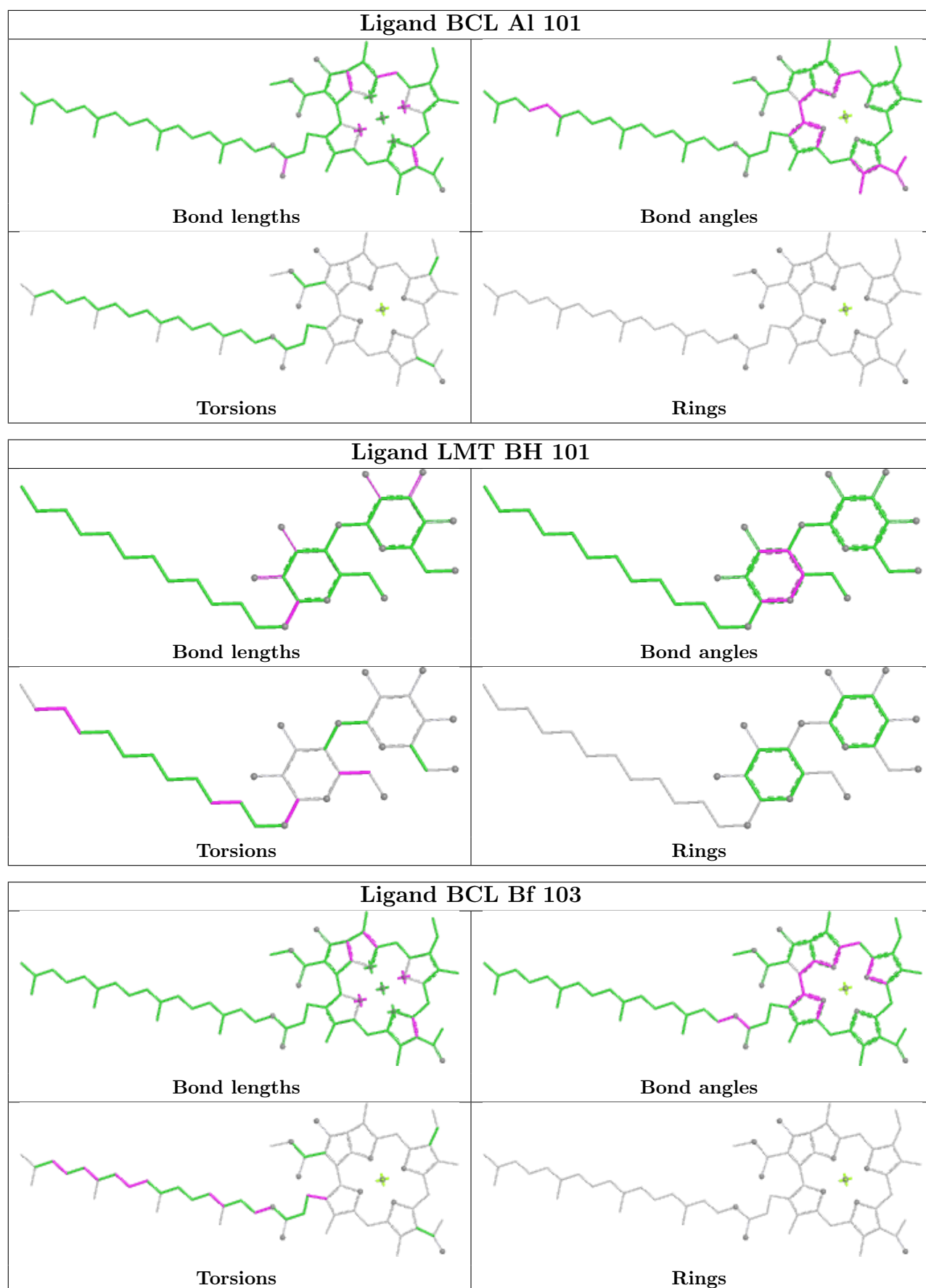


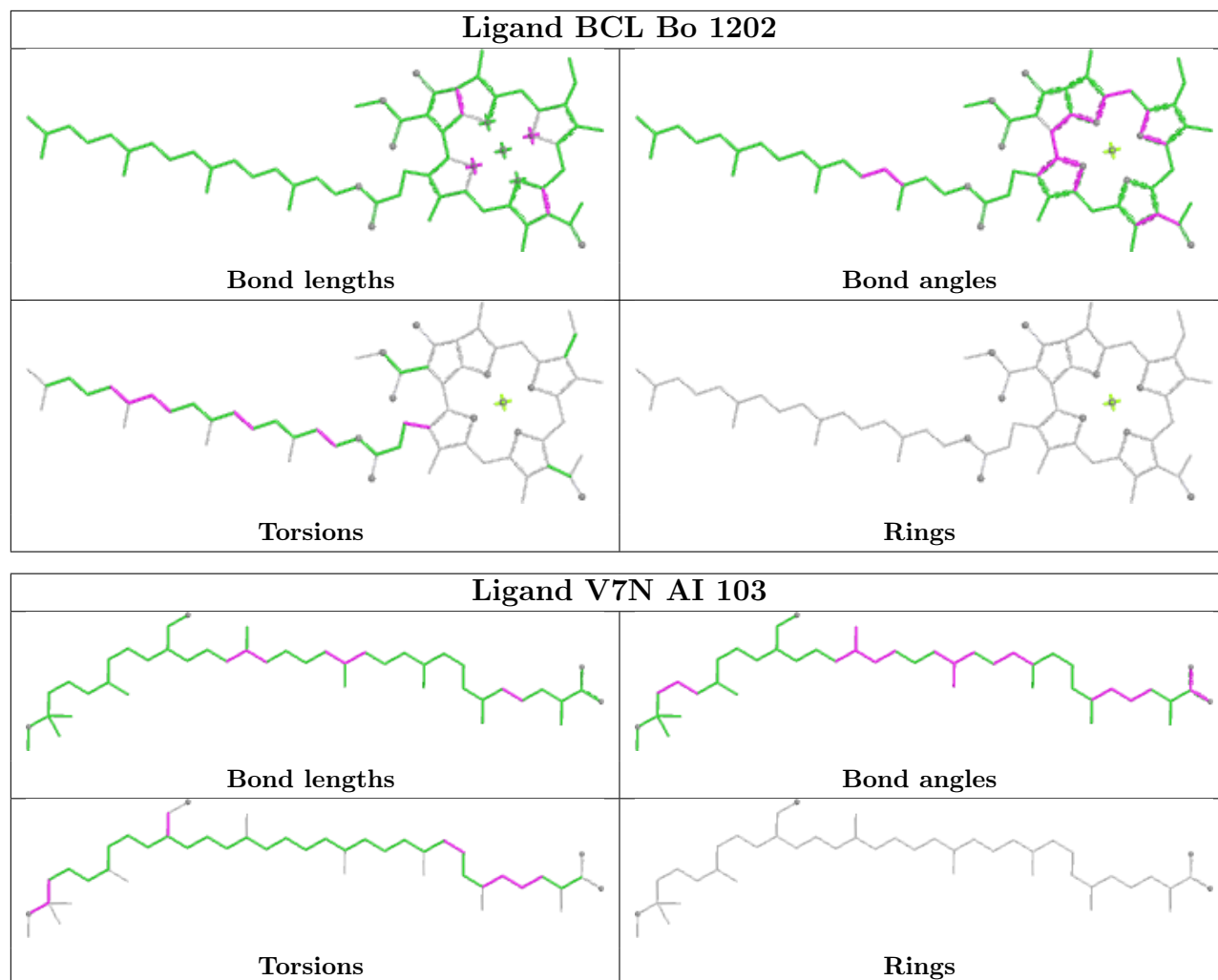




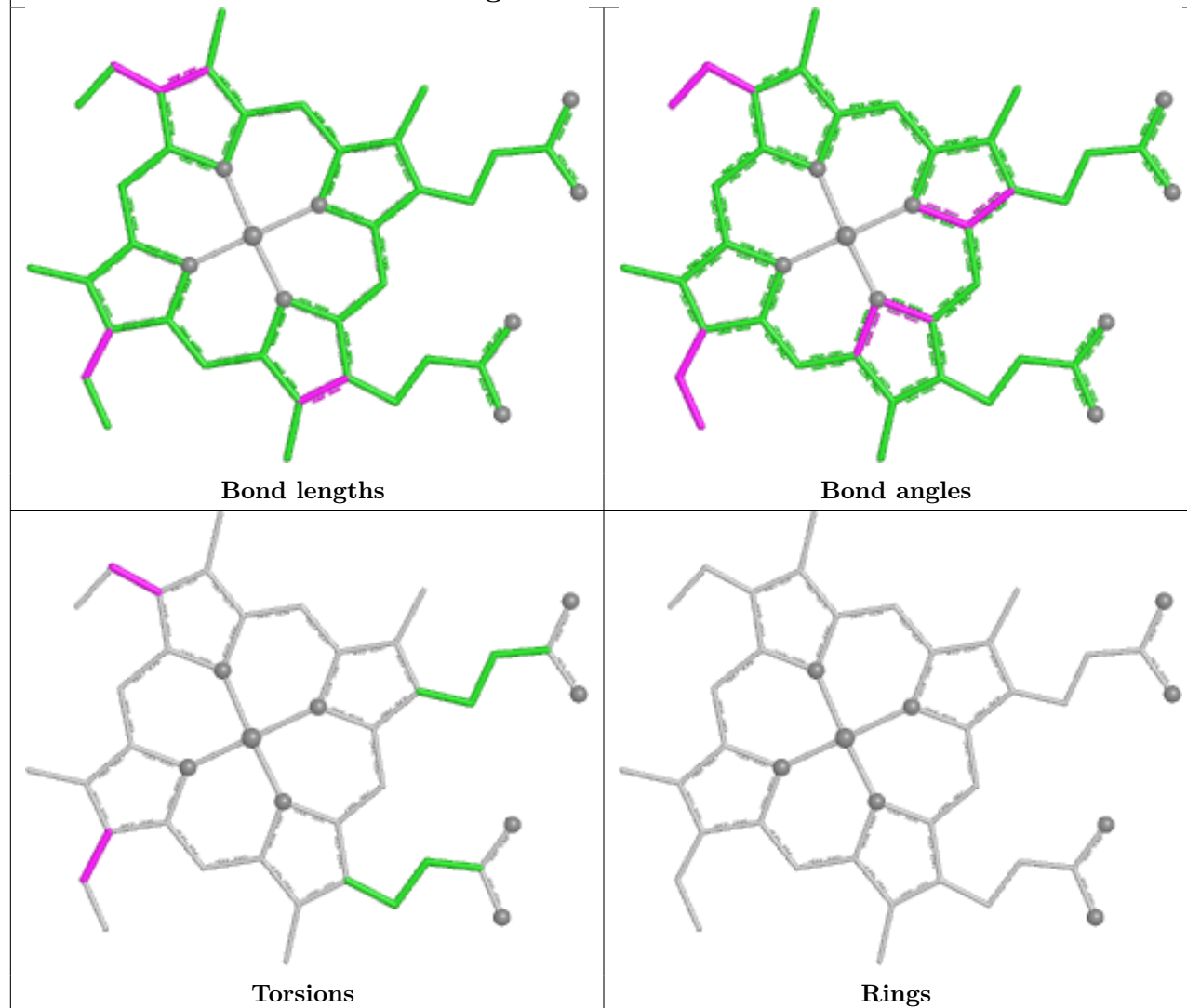




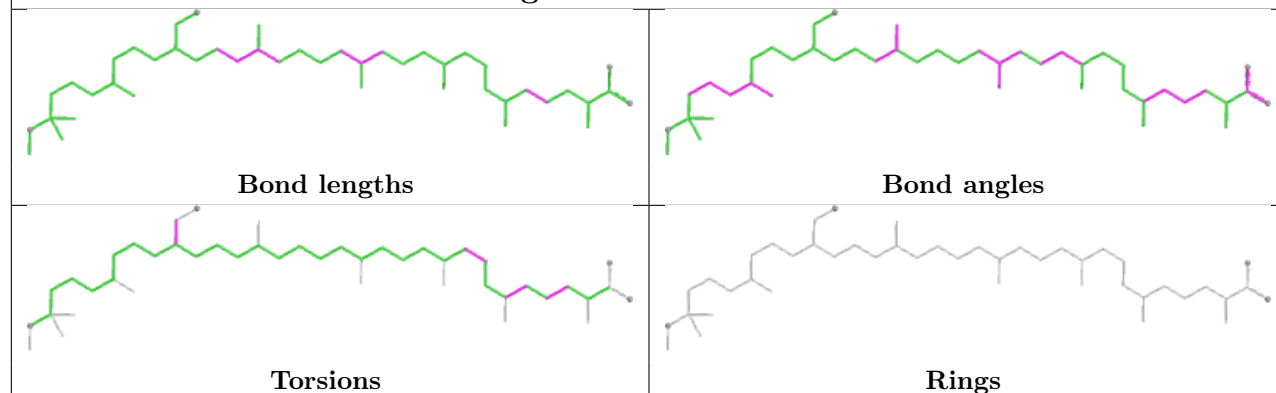


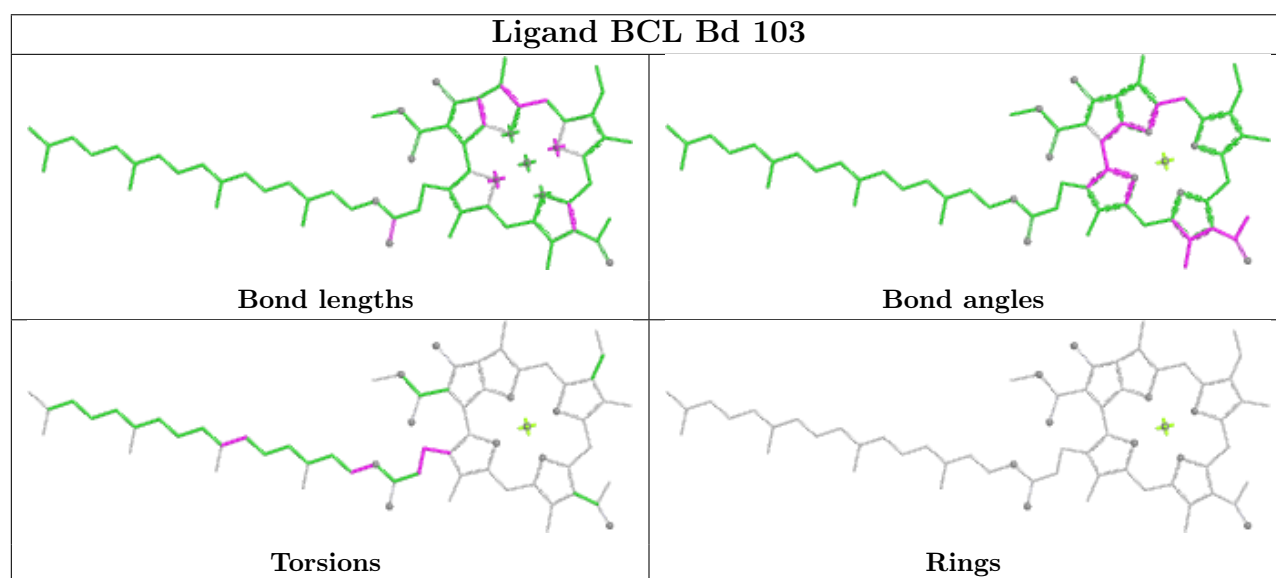
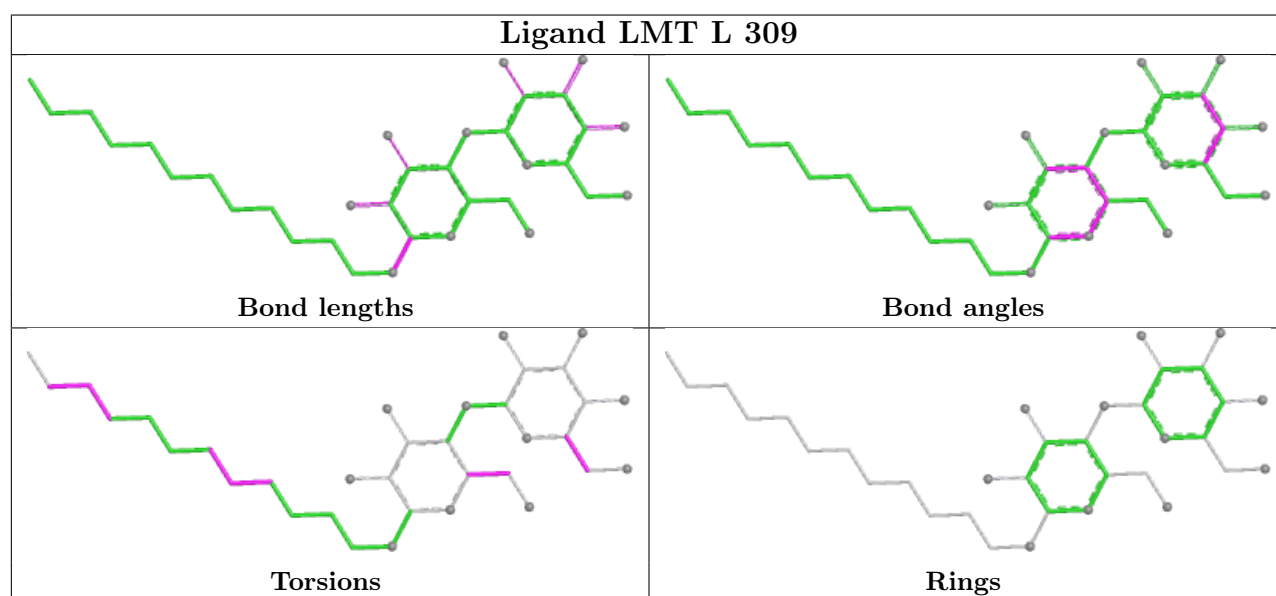
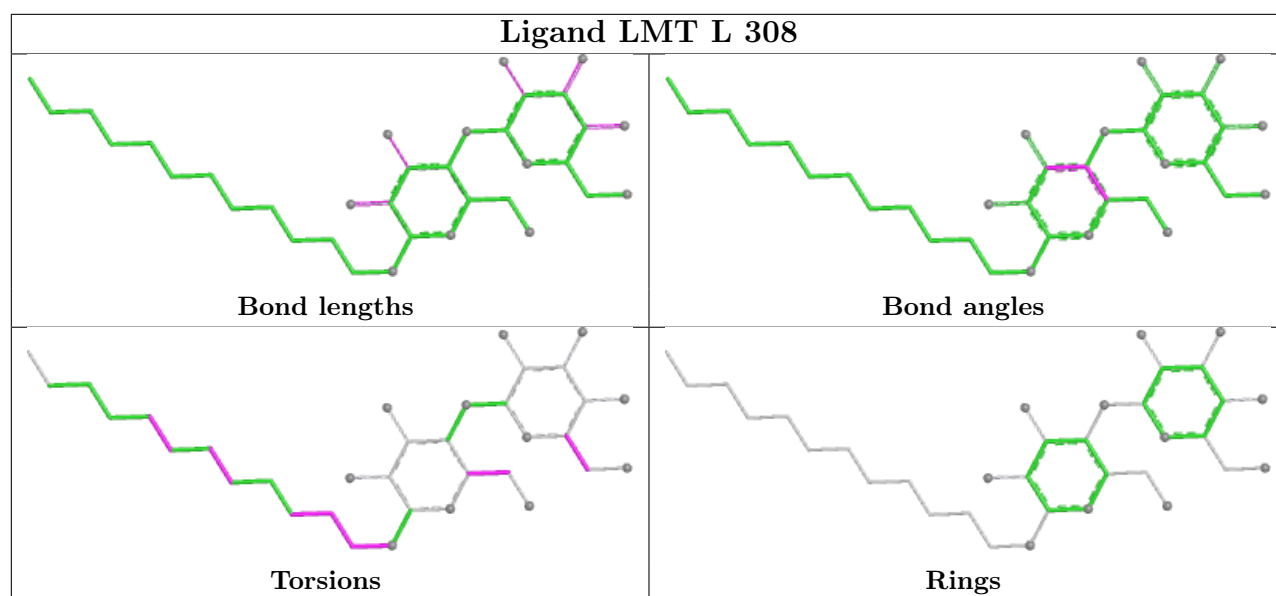


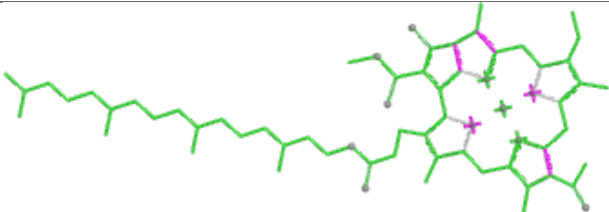
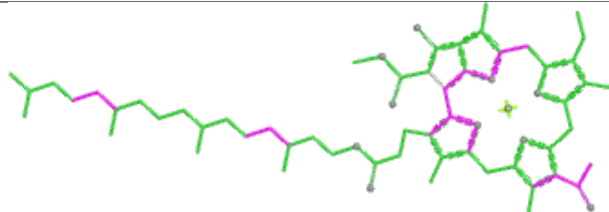
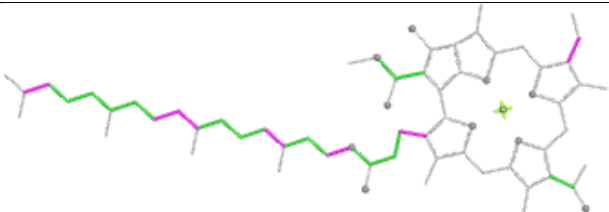
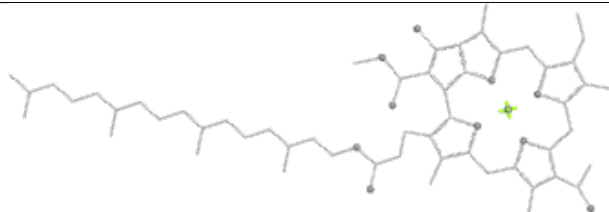
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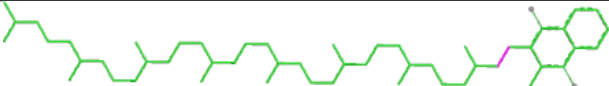





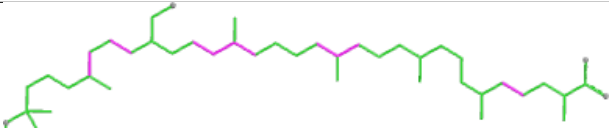
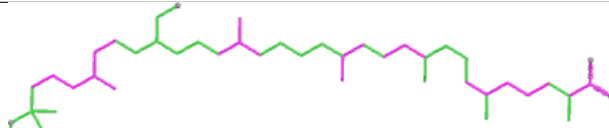
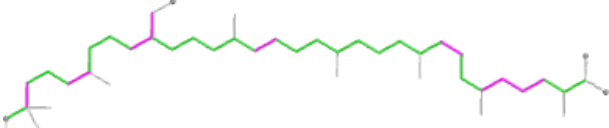
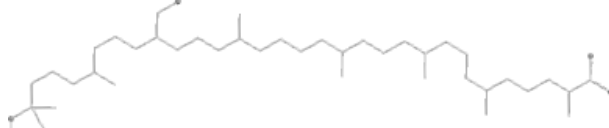
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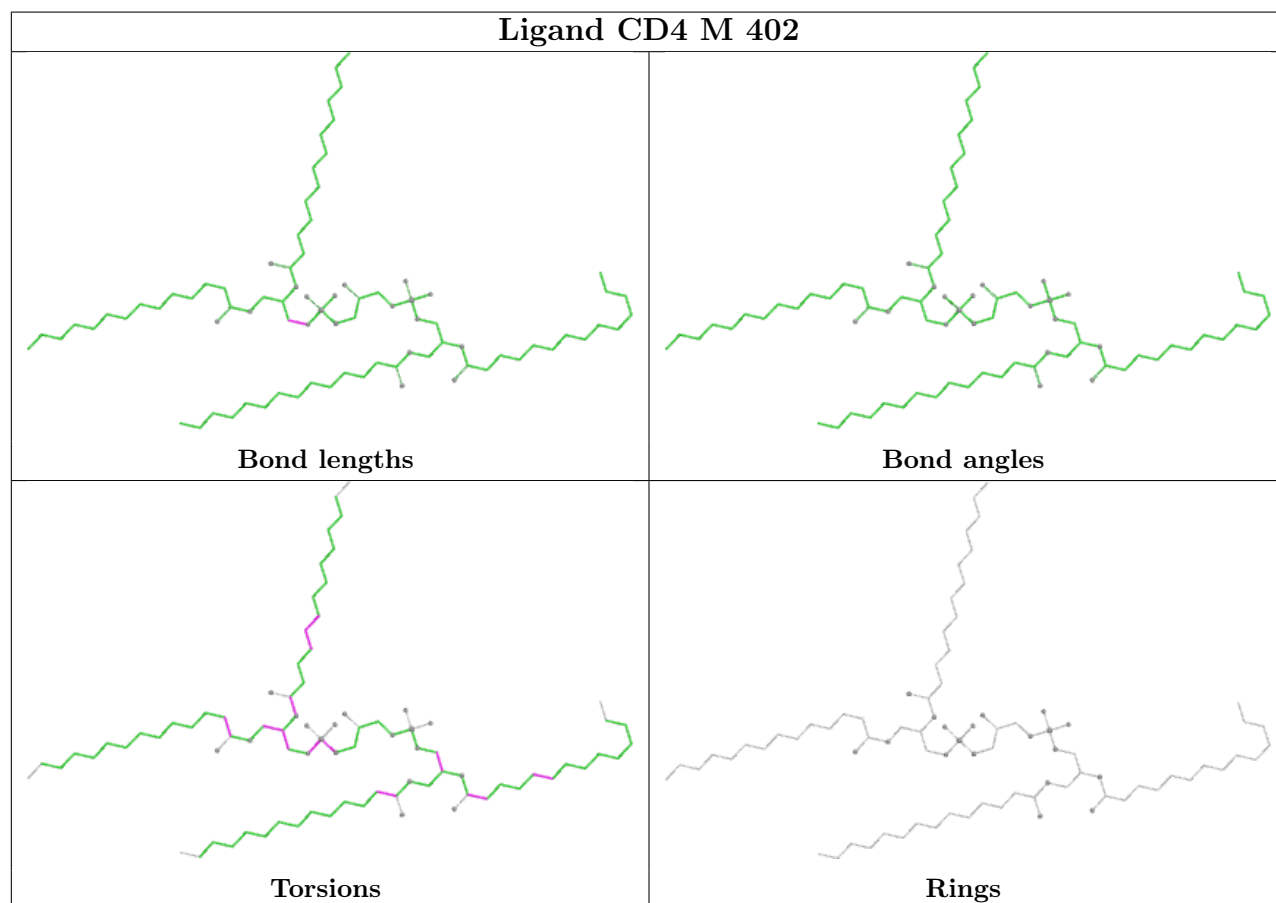
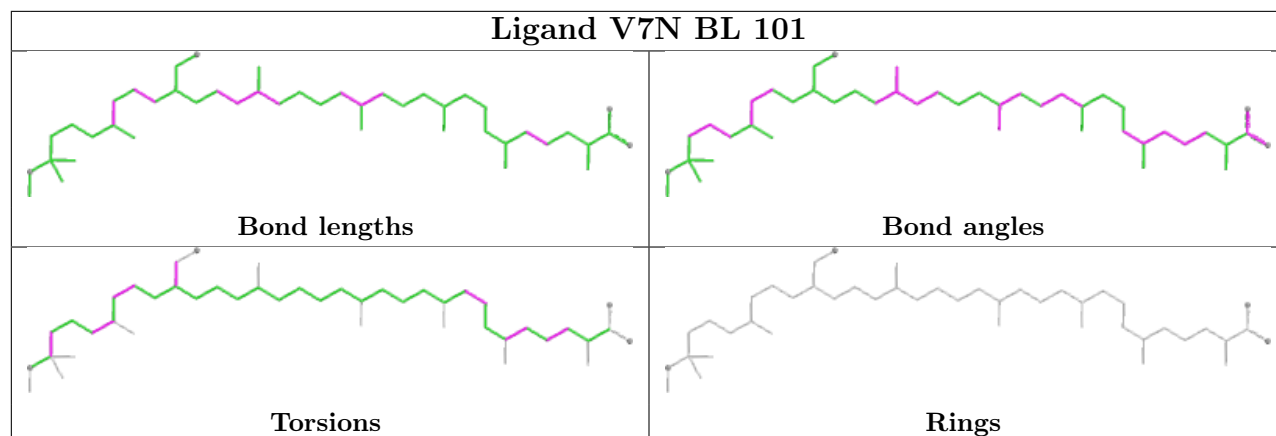


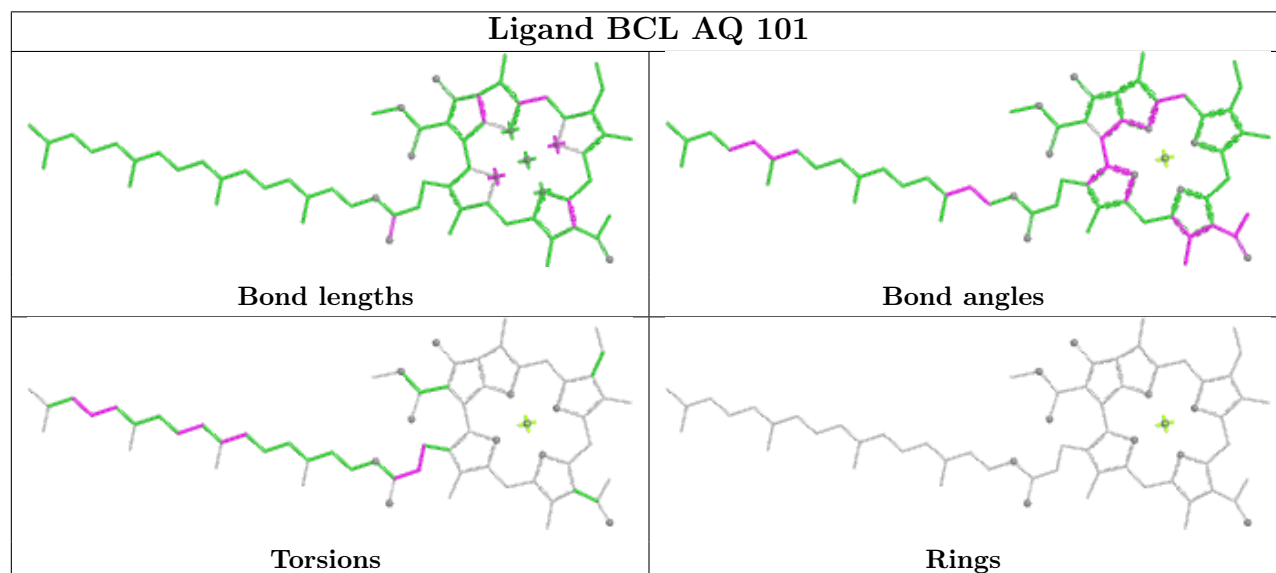
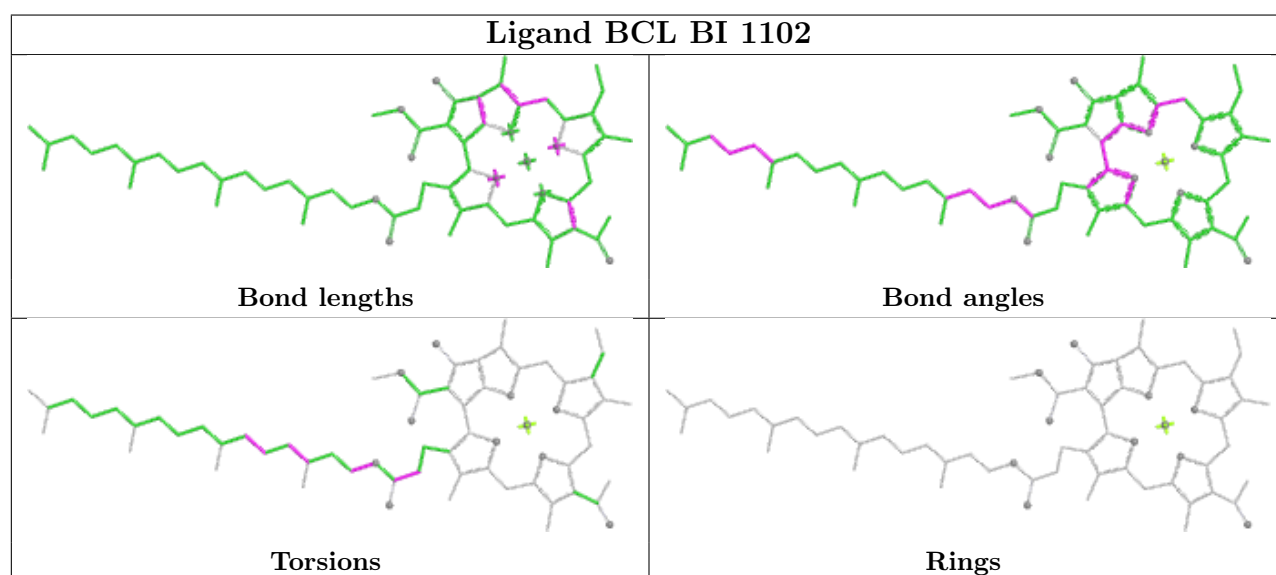
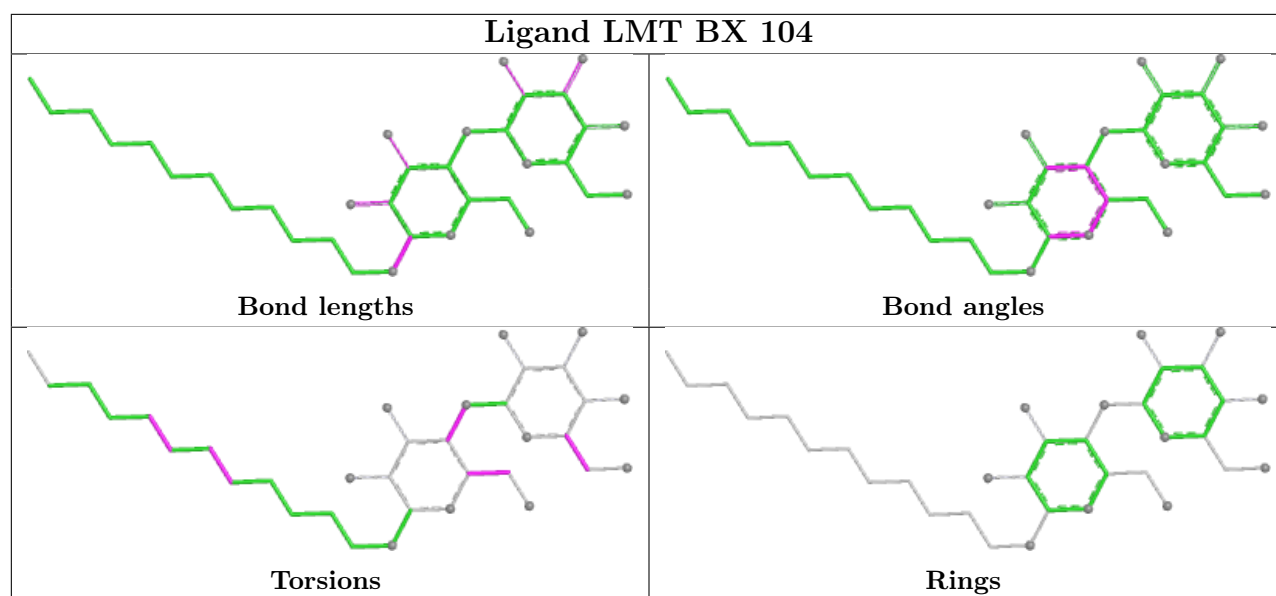


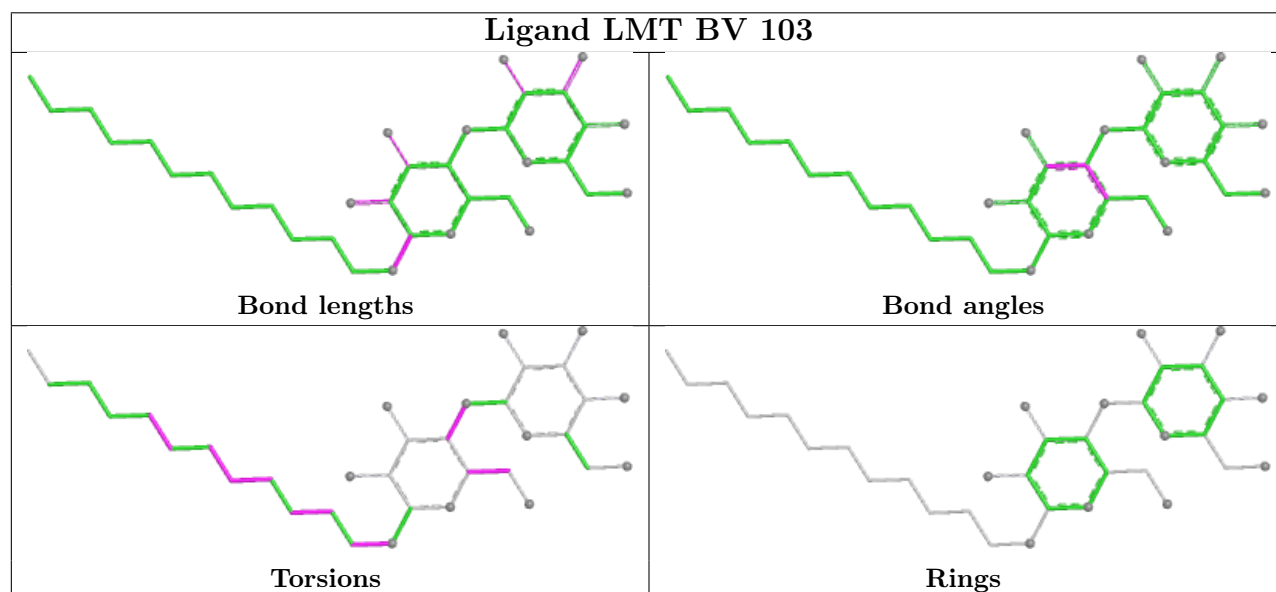
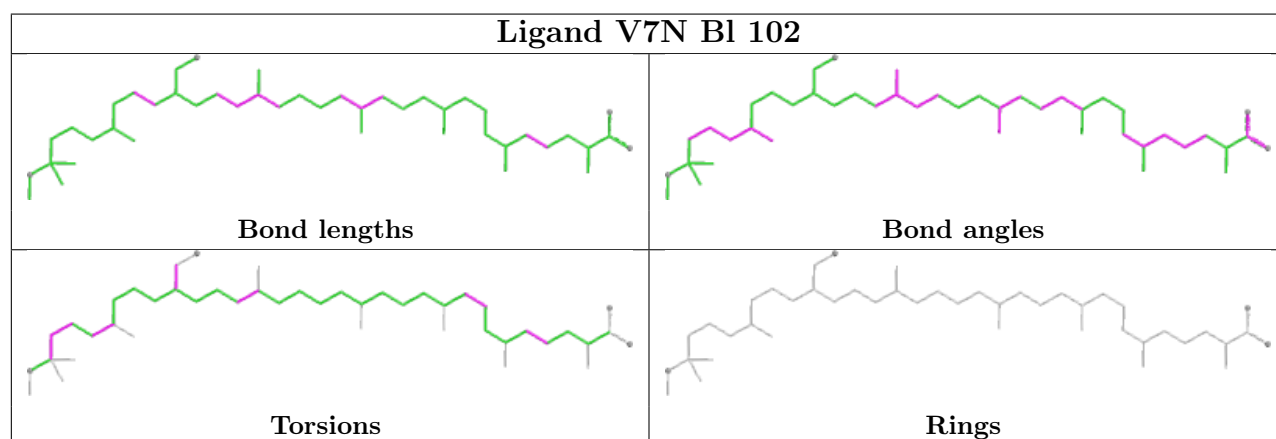
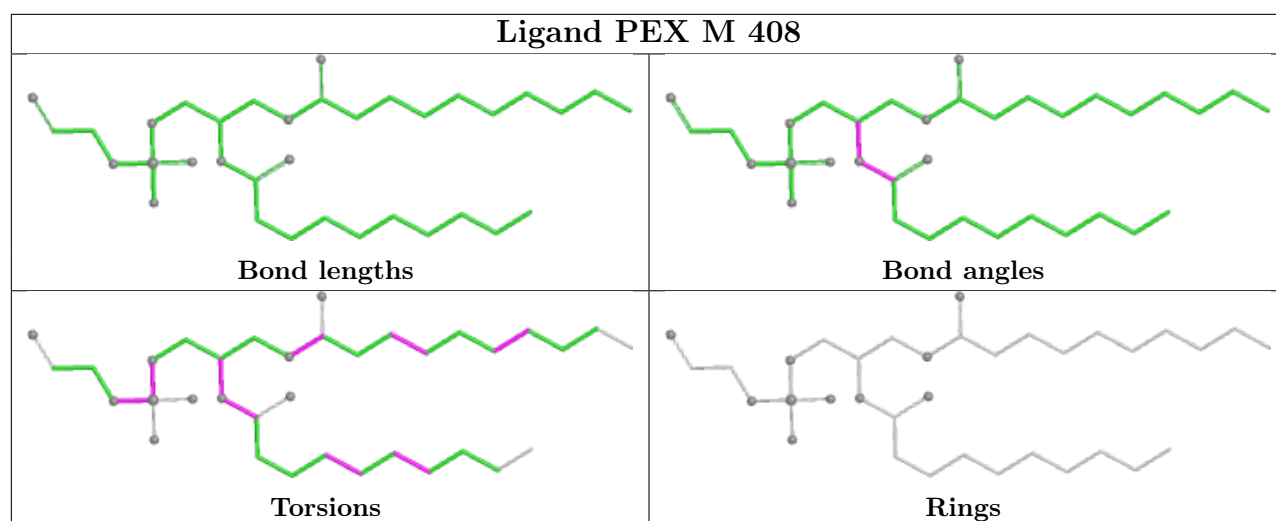
Ligand BCL AD 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

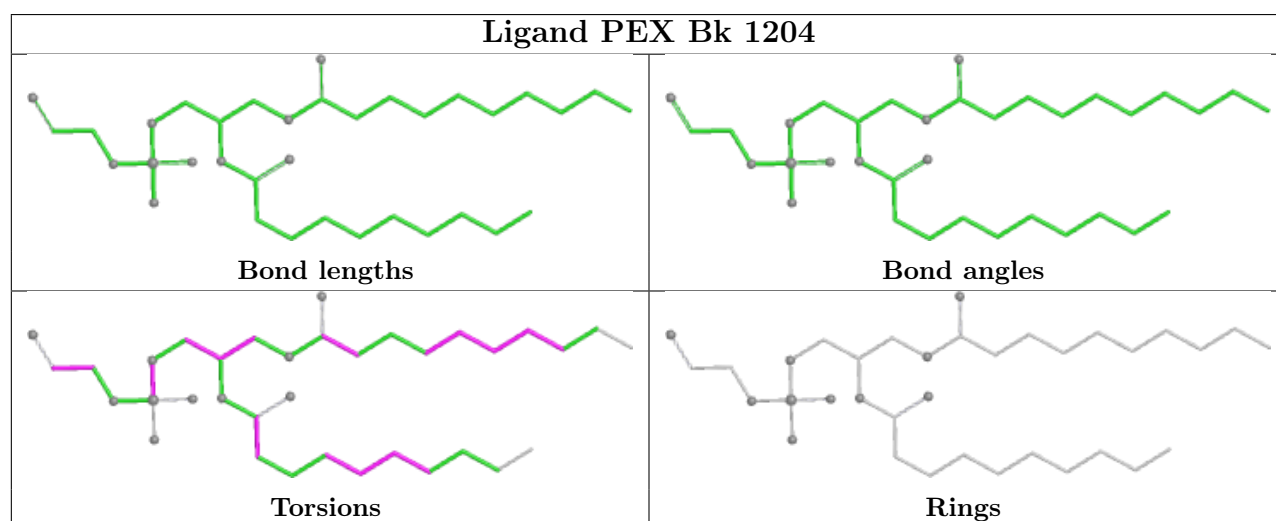
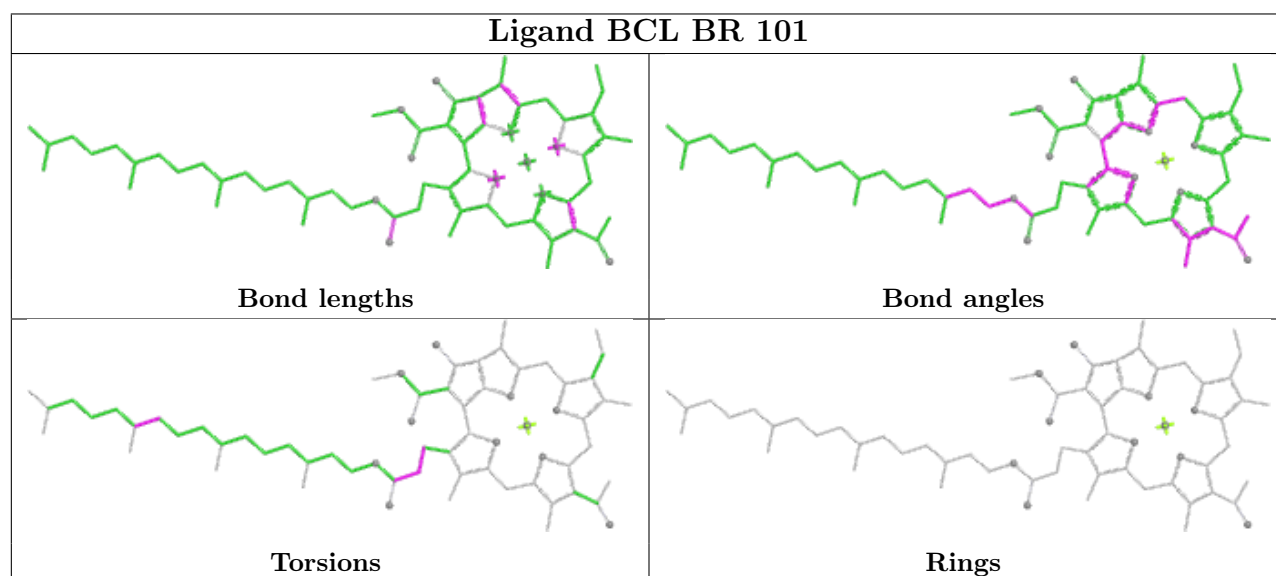
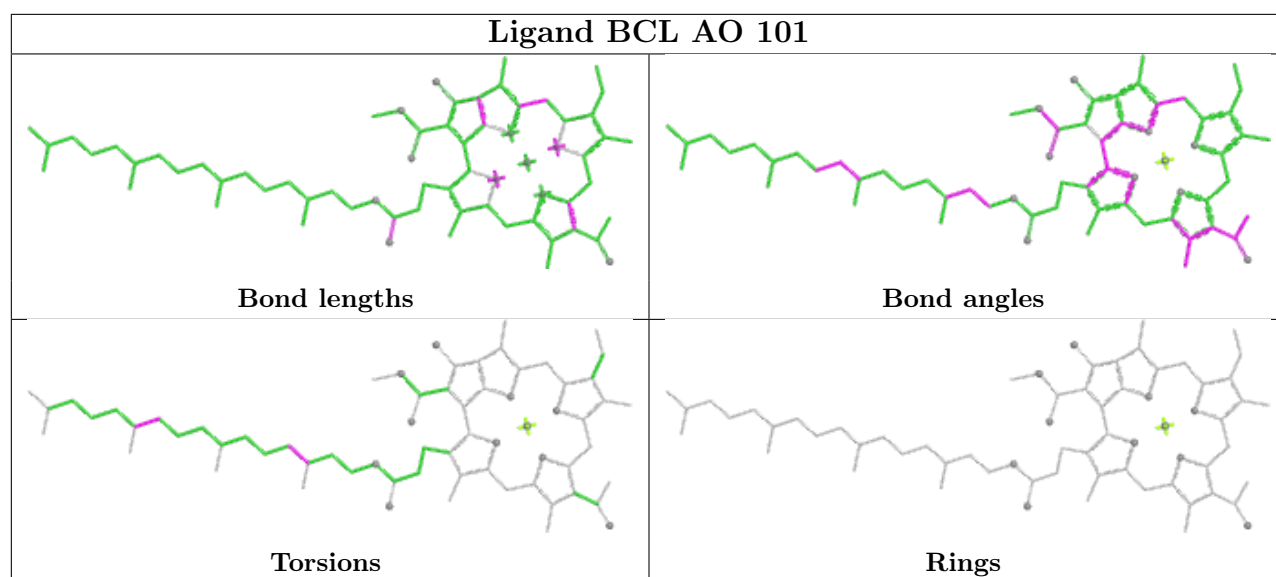
Ligand MQ8 M 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

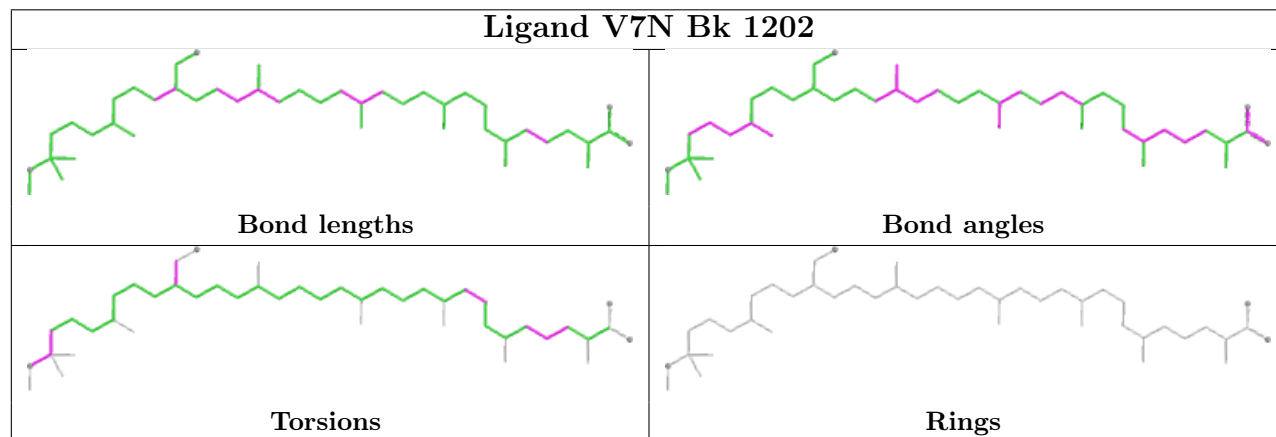
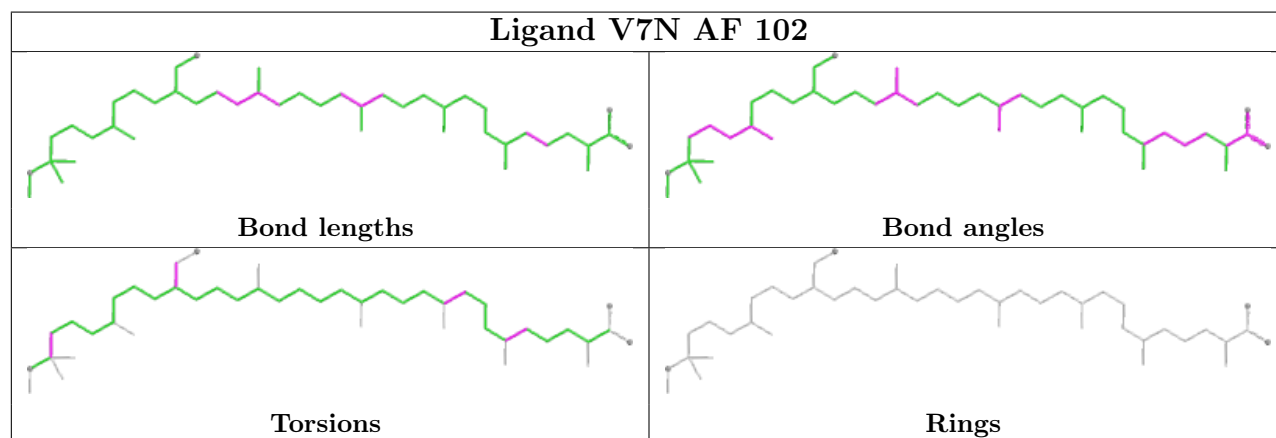
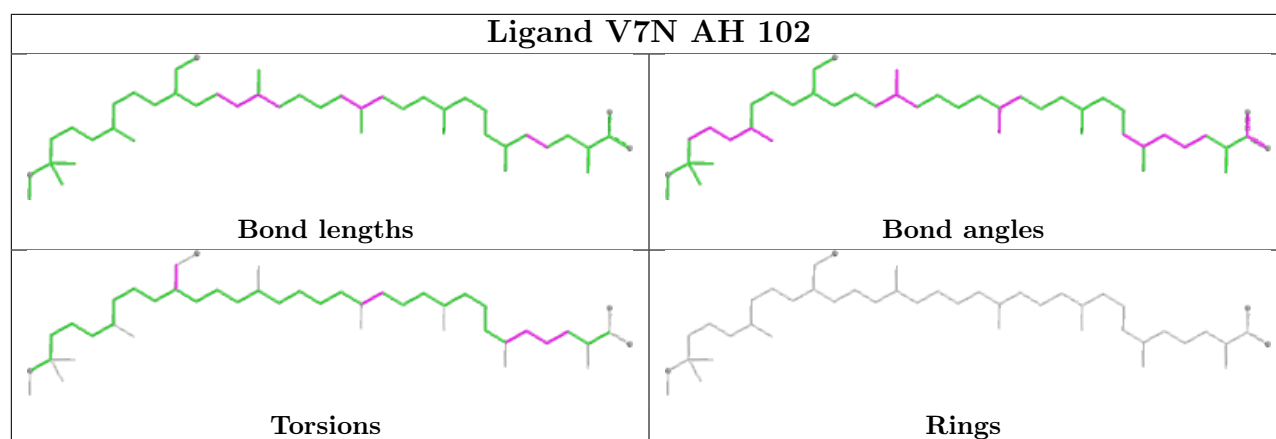
Ligand V7N Bi 1202	
	
Bond lengths	Bond angles
	
Torsions	Rings

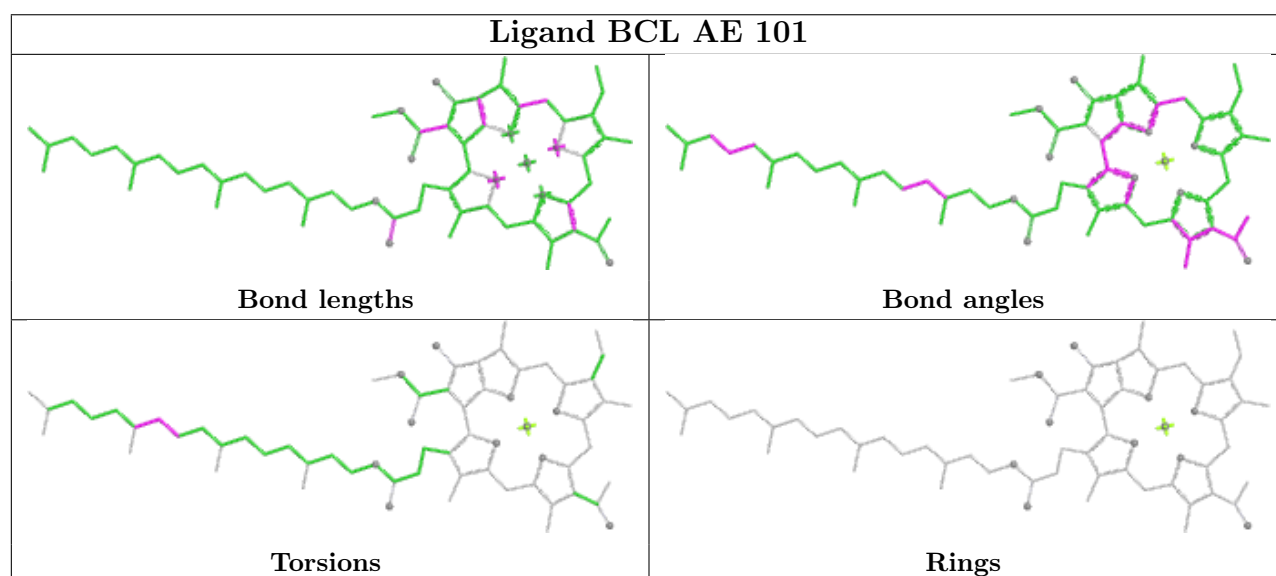
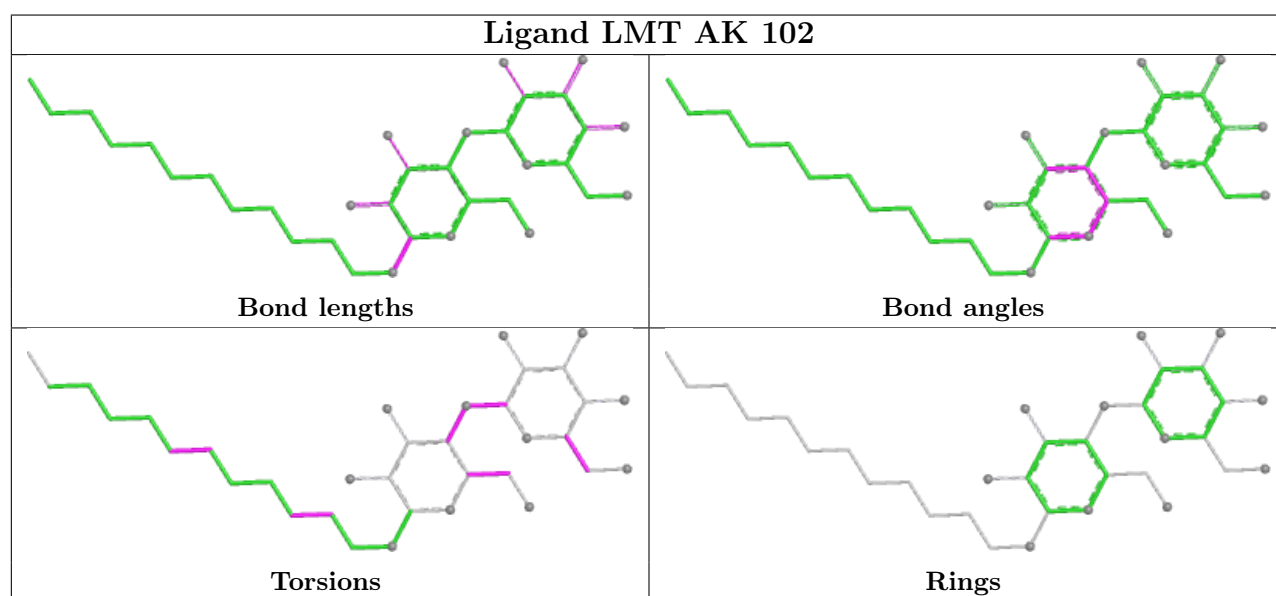
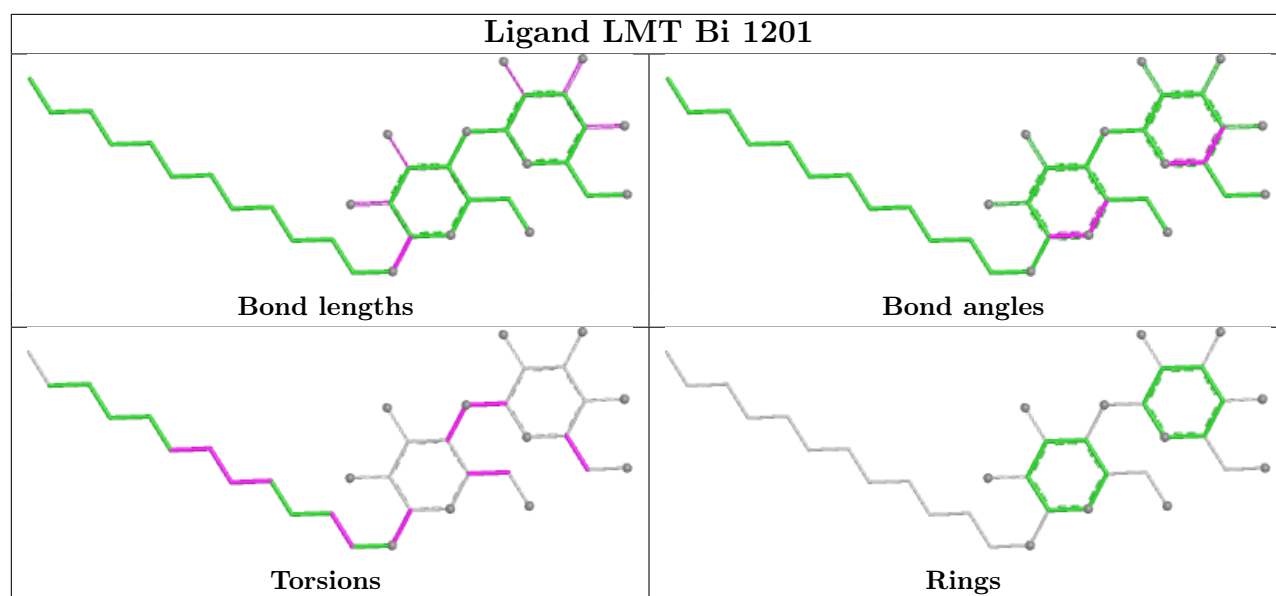


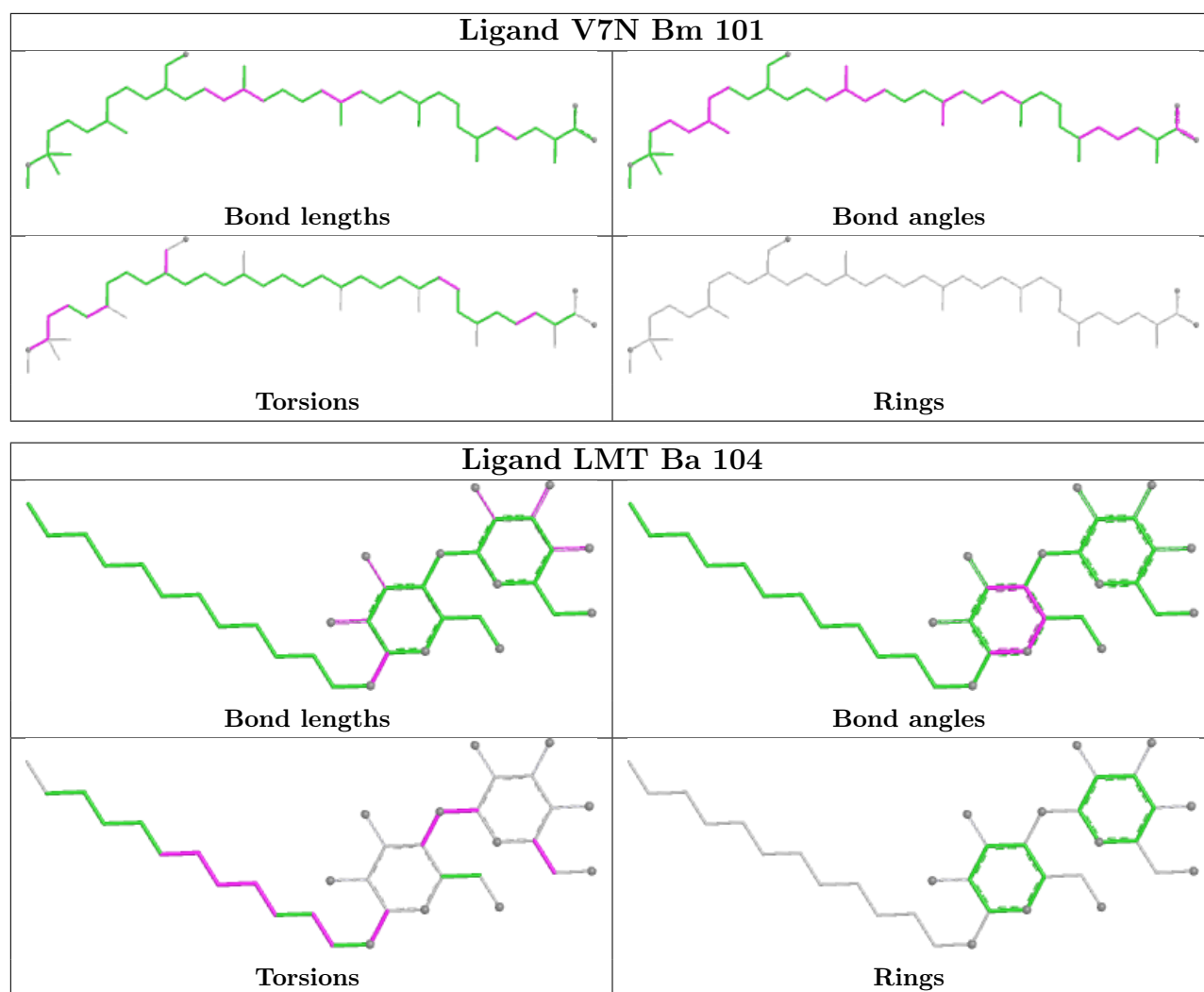




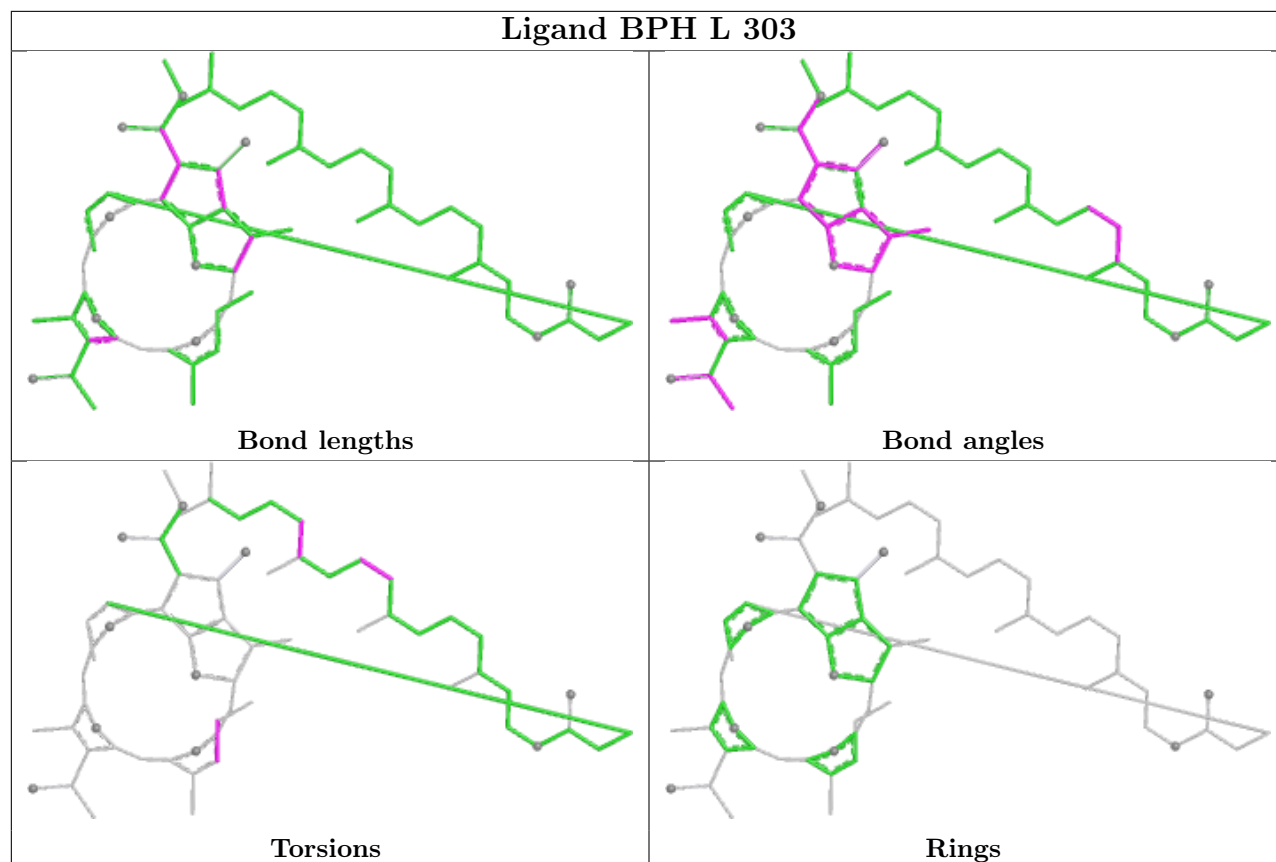




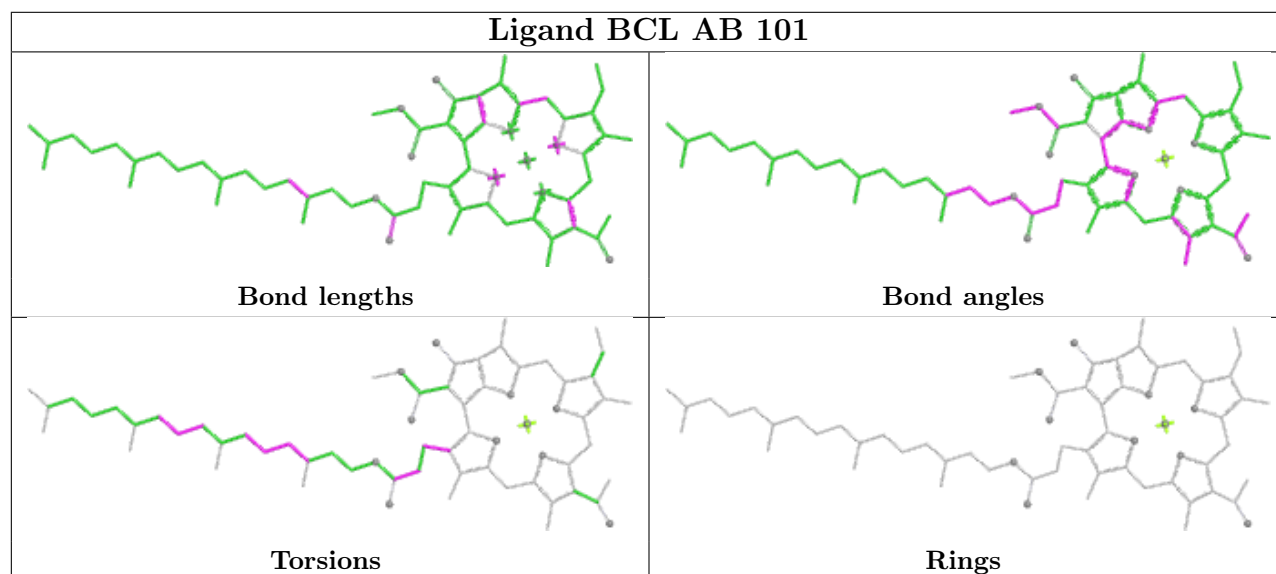


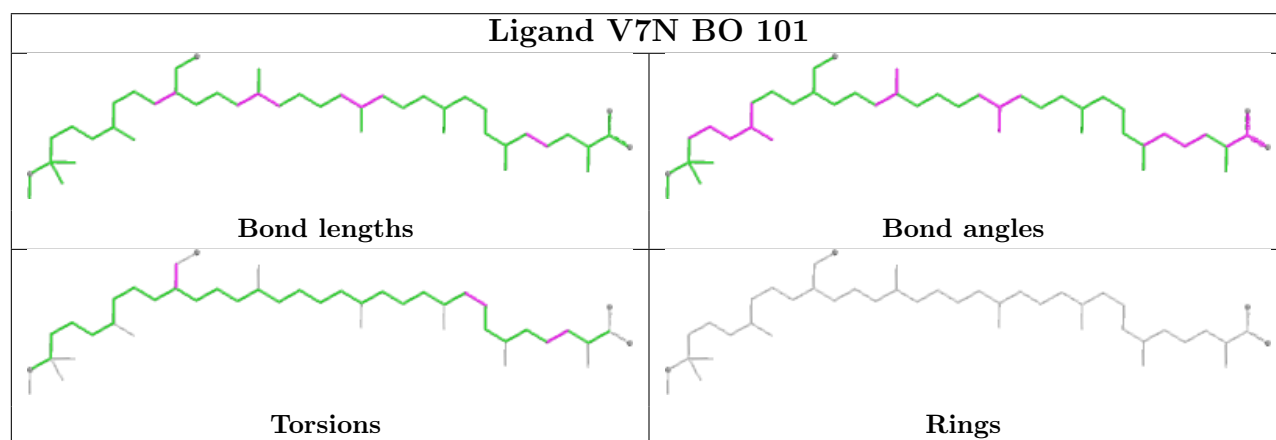
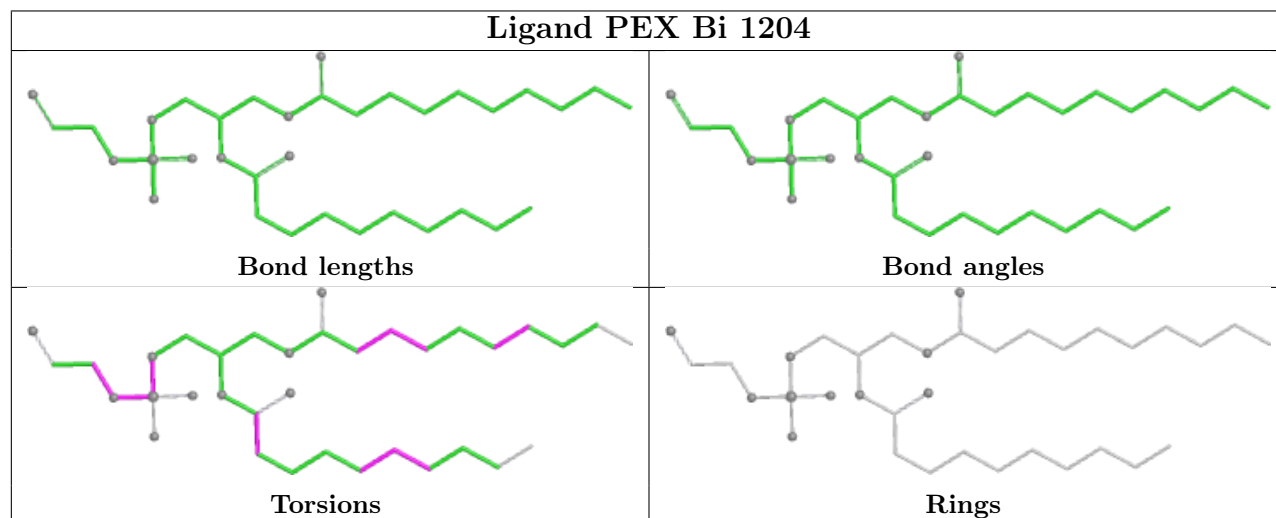
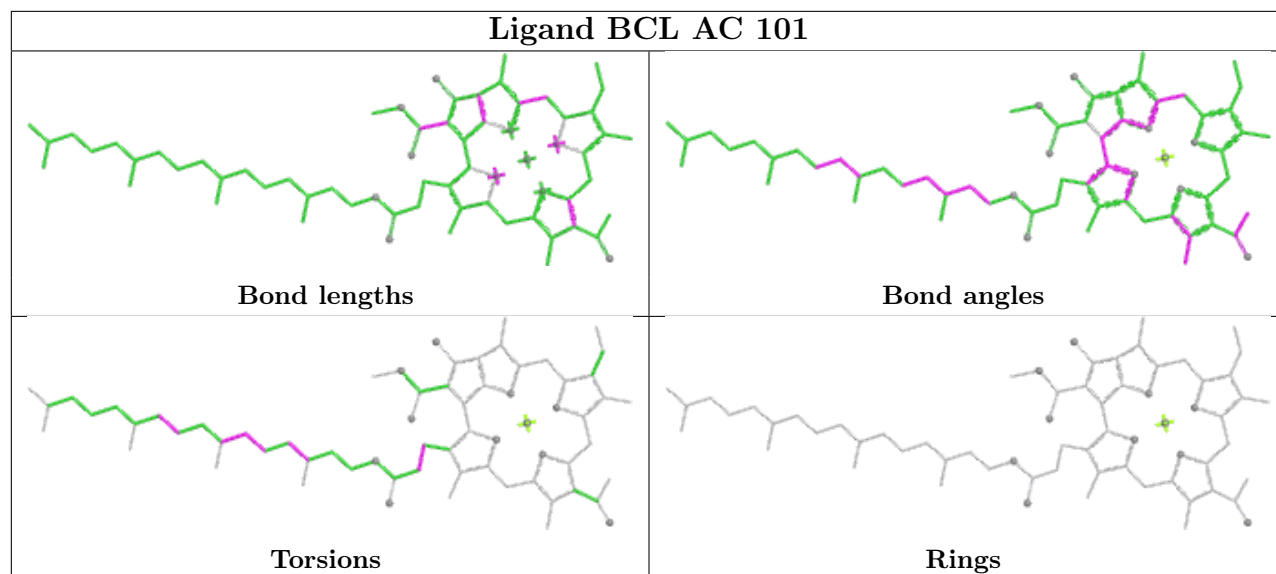


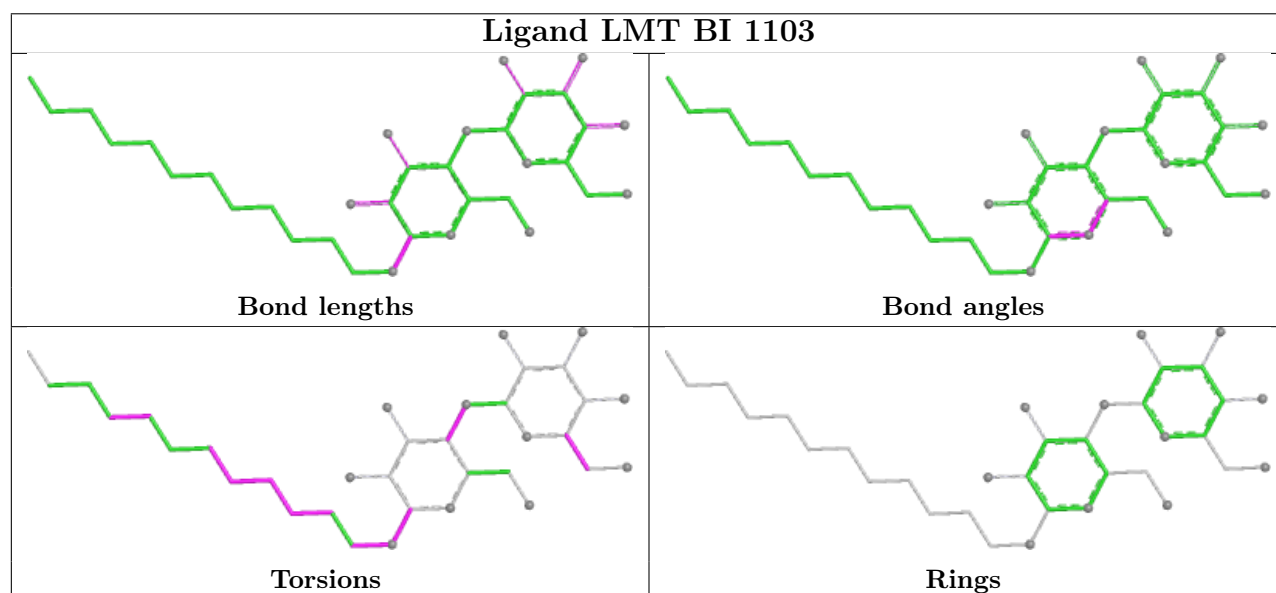
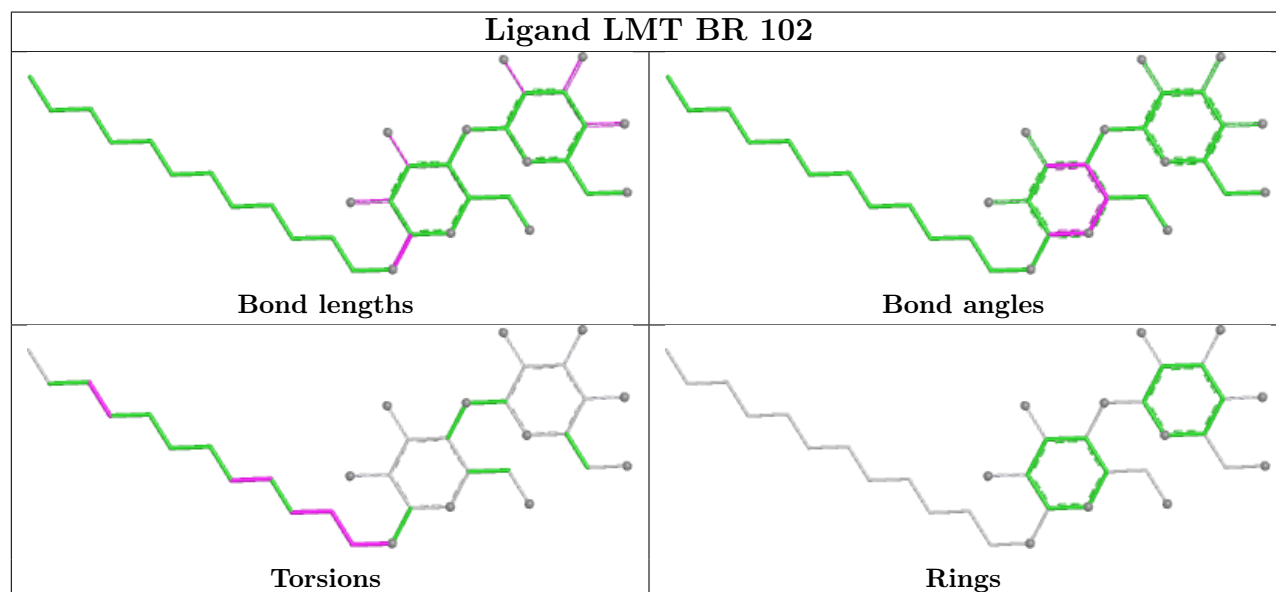
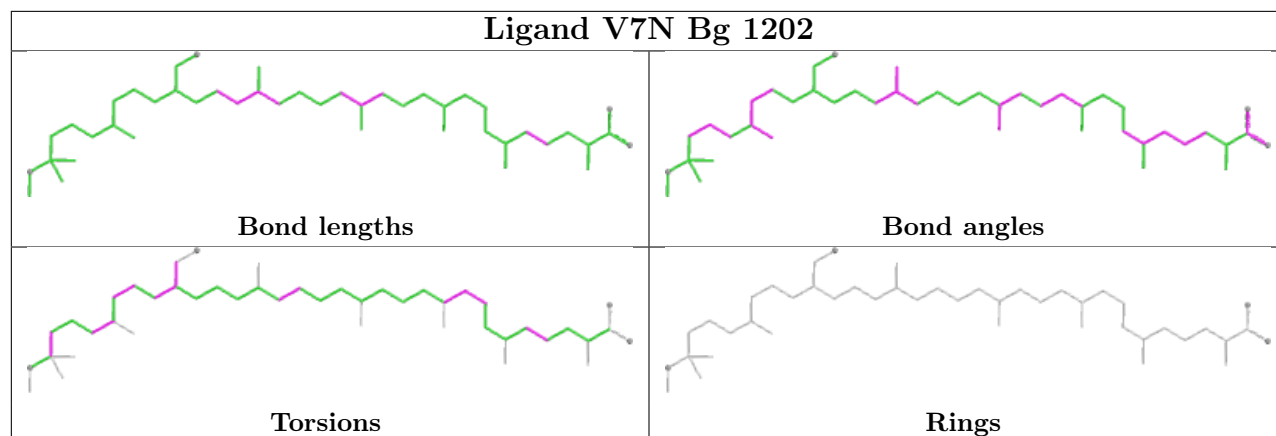
Ligand BPH L 303

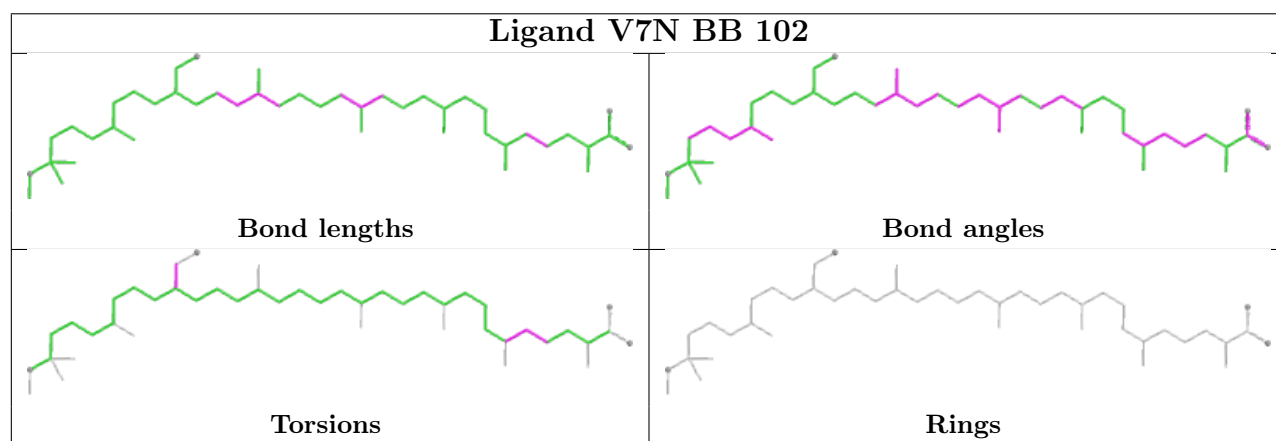
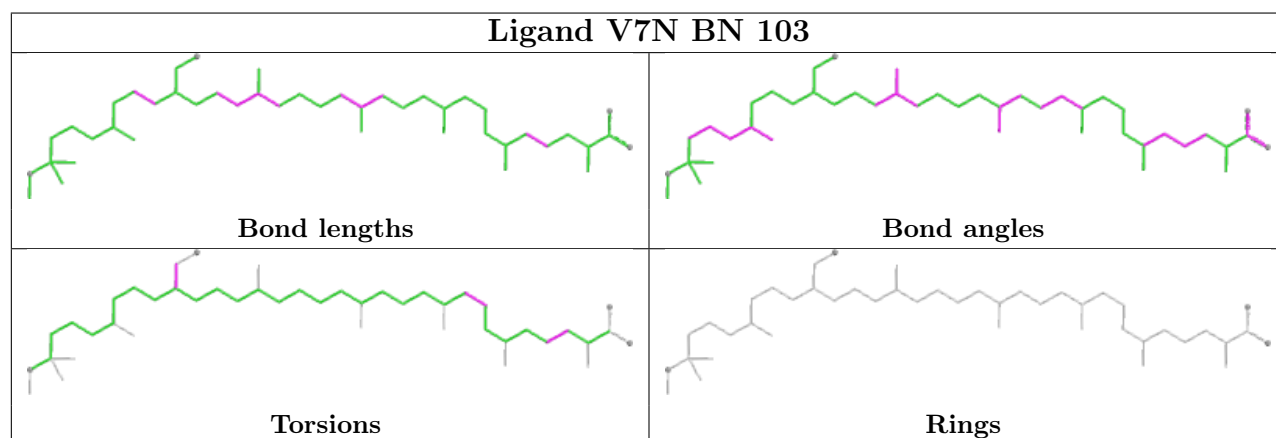
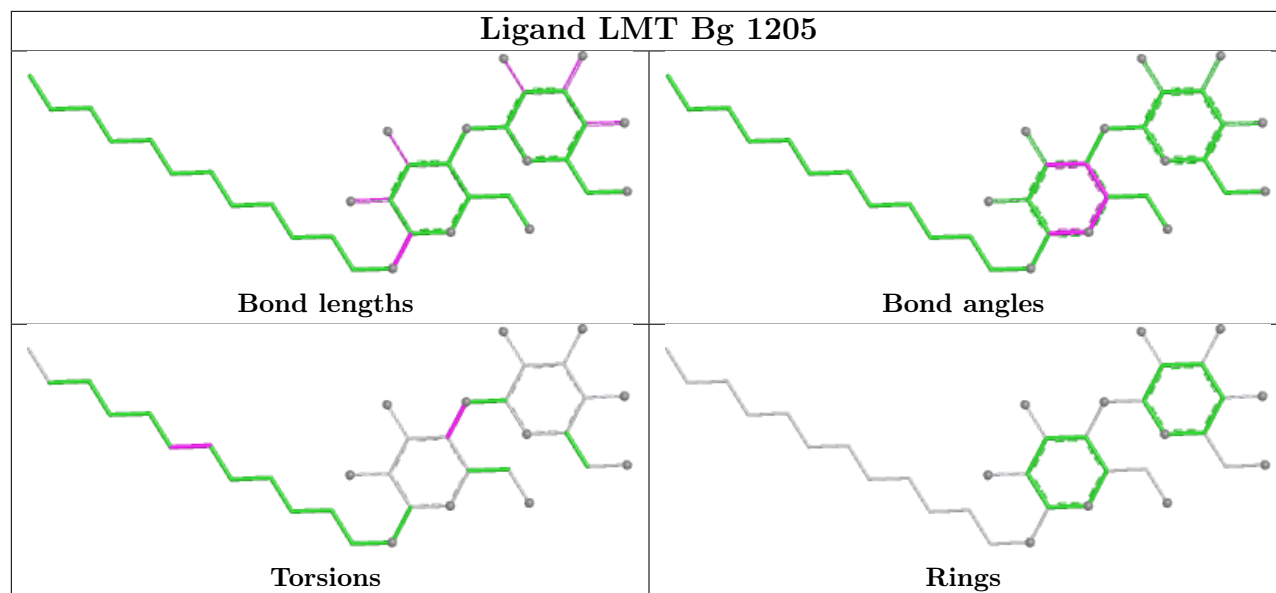


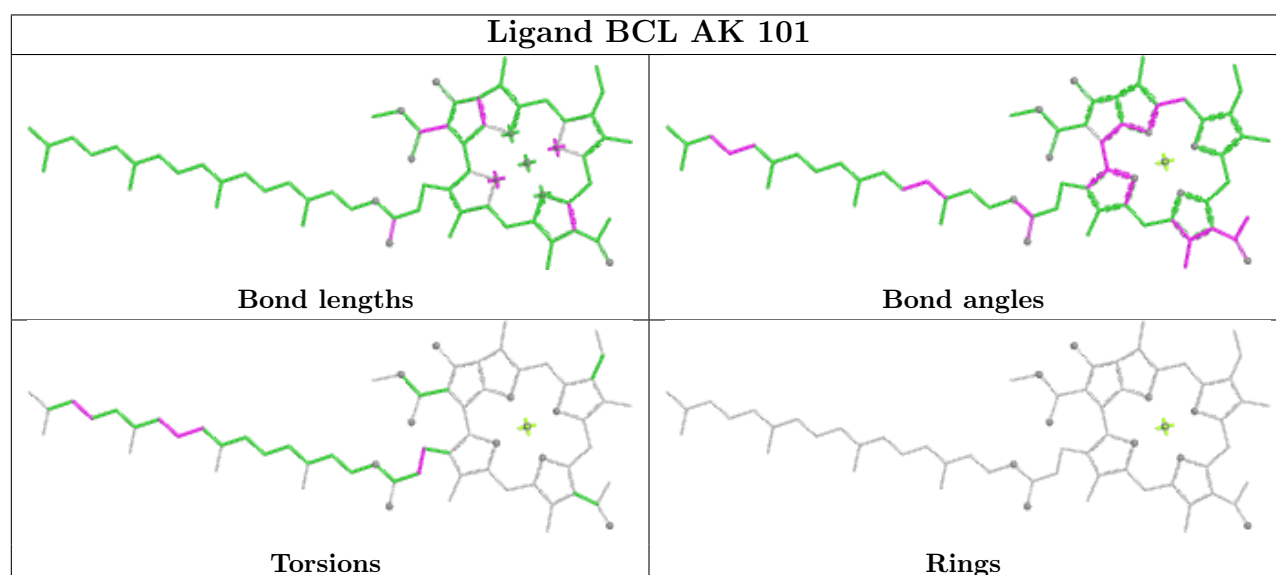
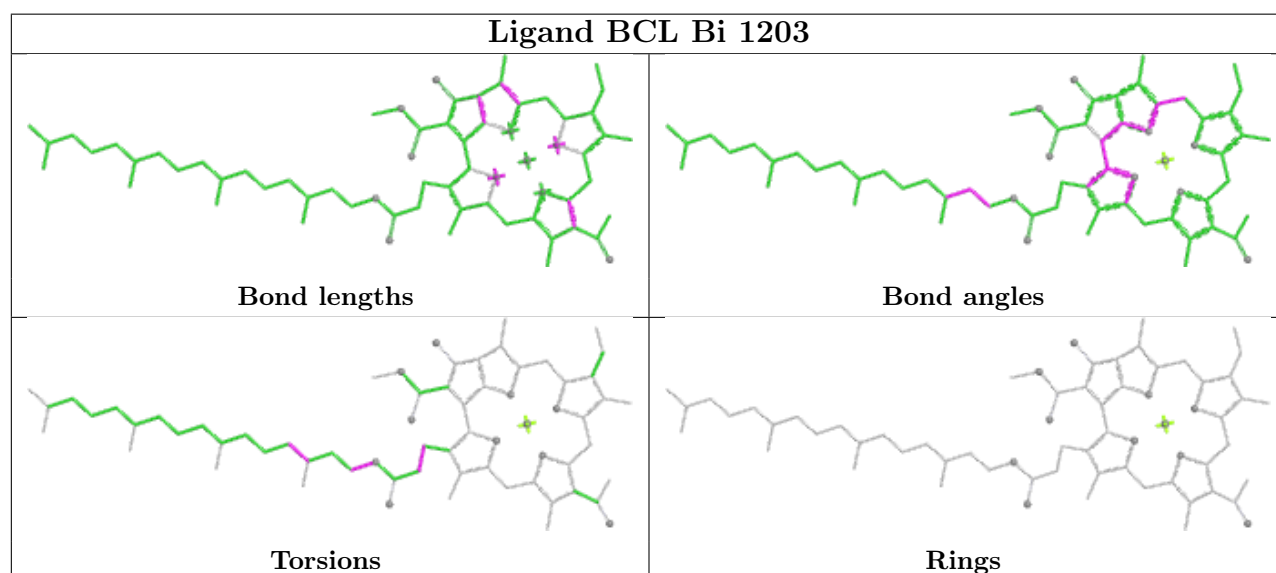
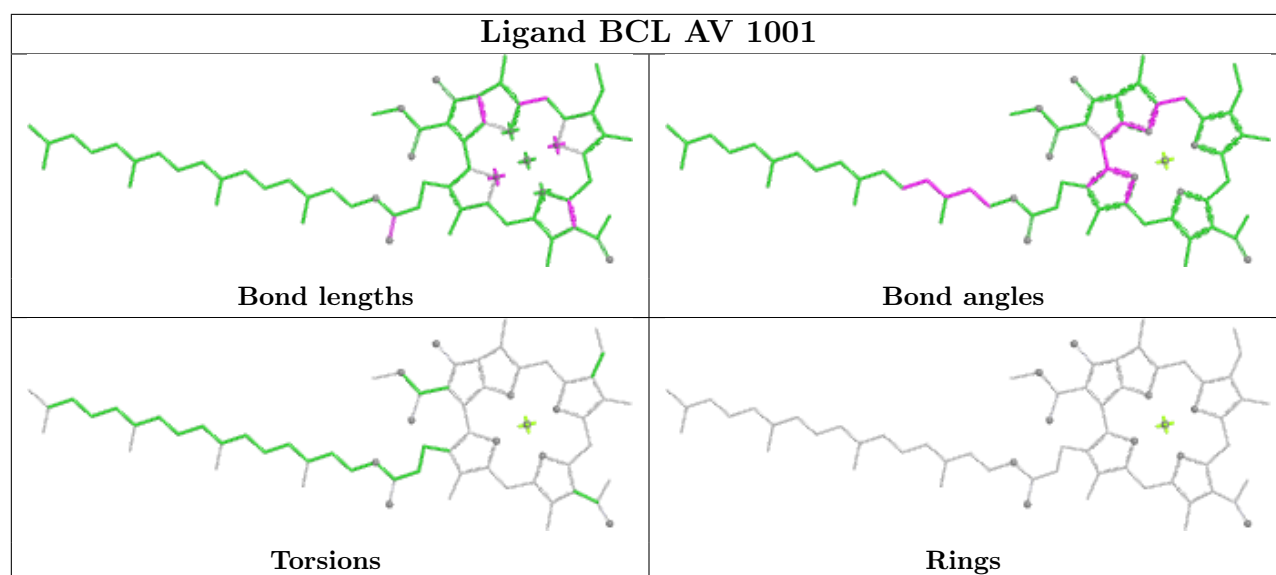
Ligand BCL AB 101

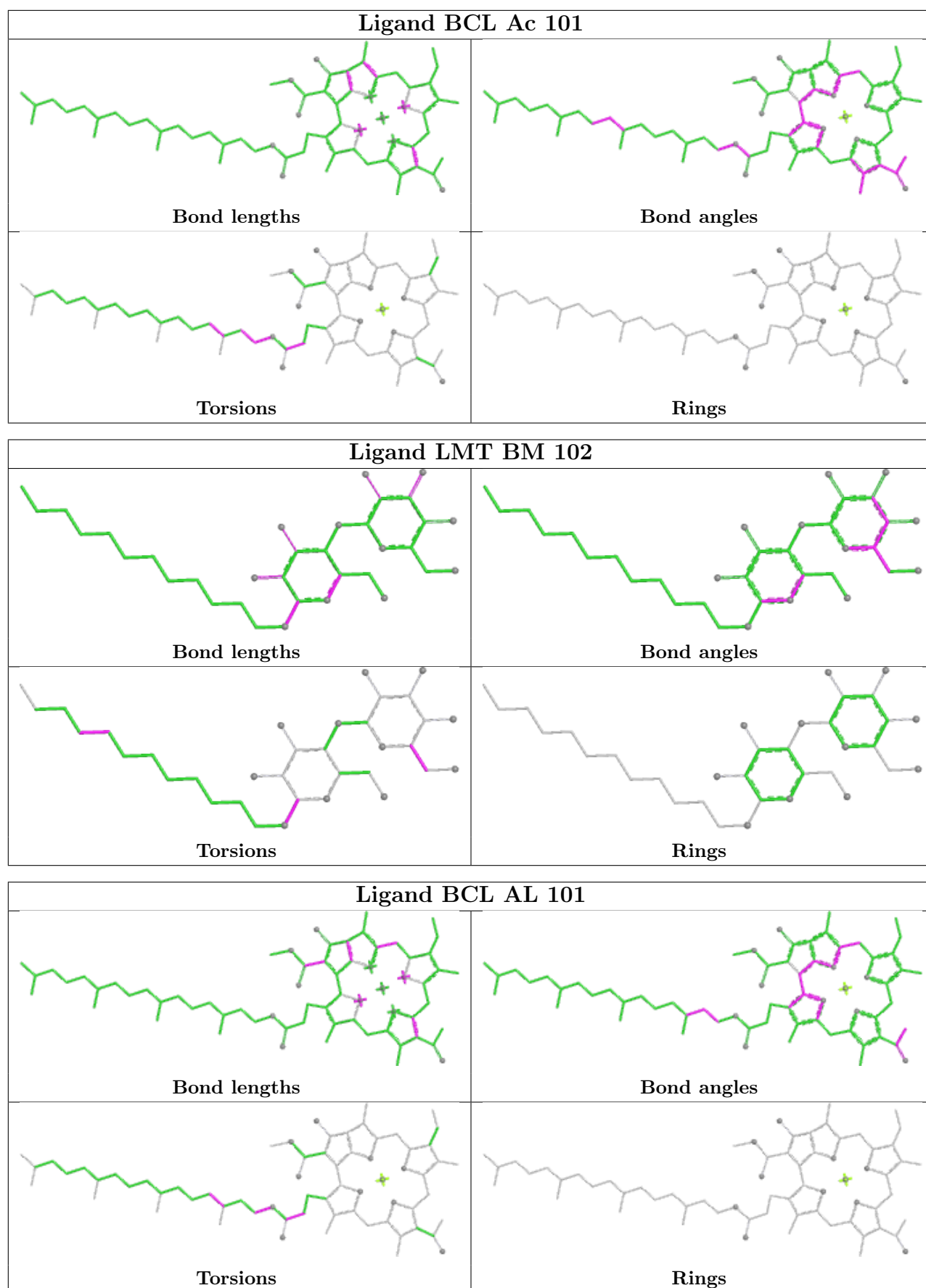


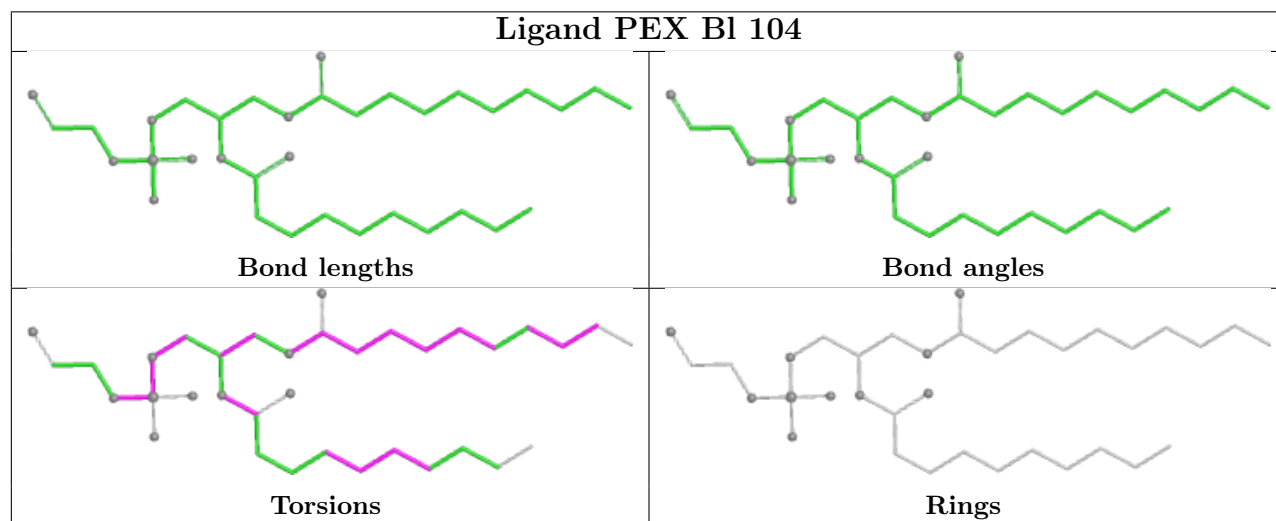
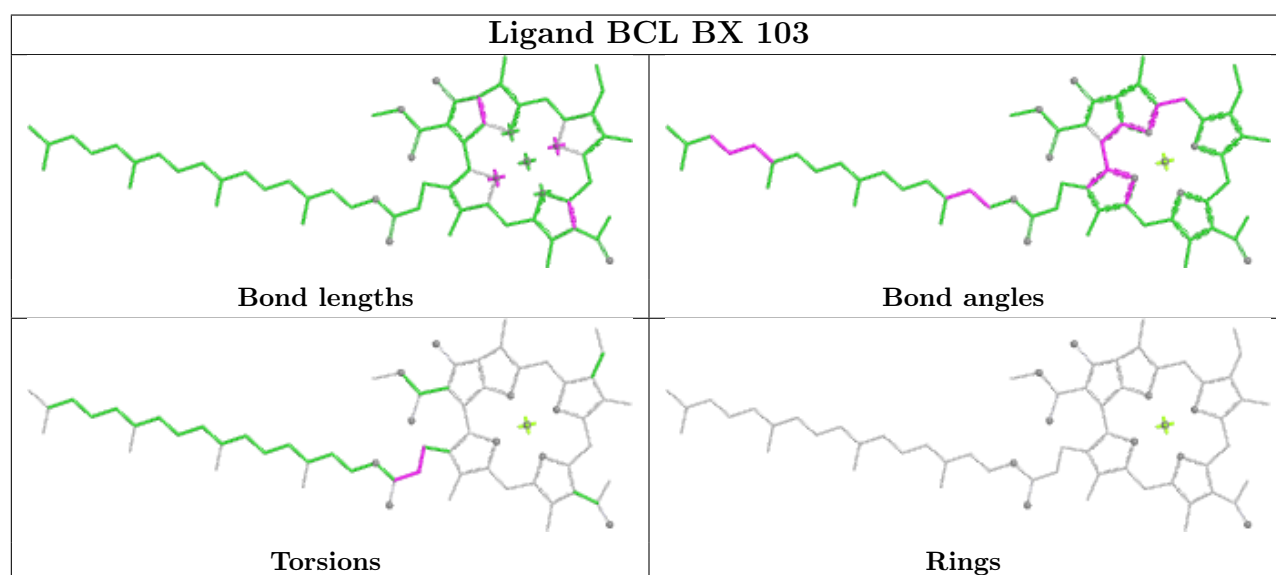
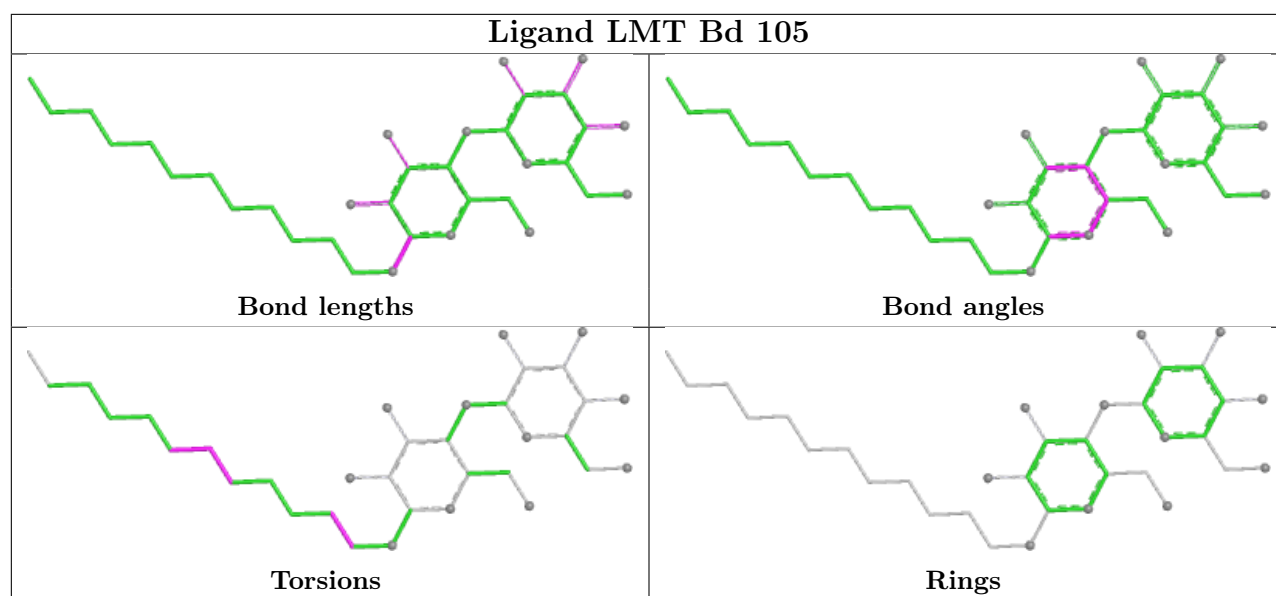


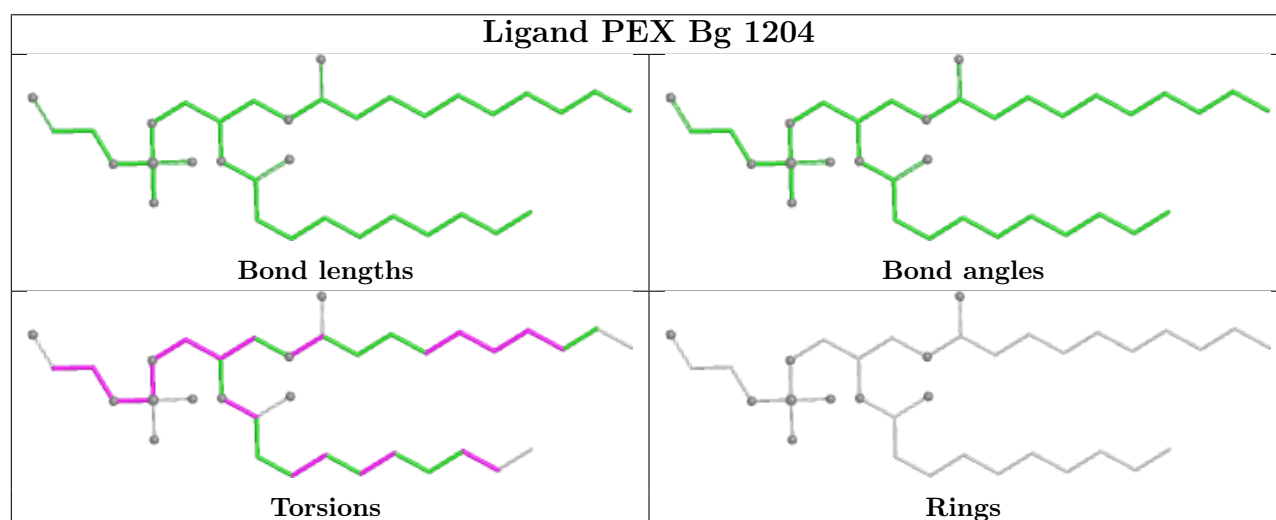
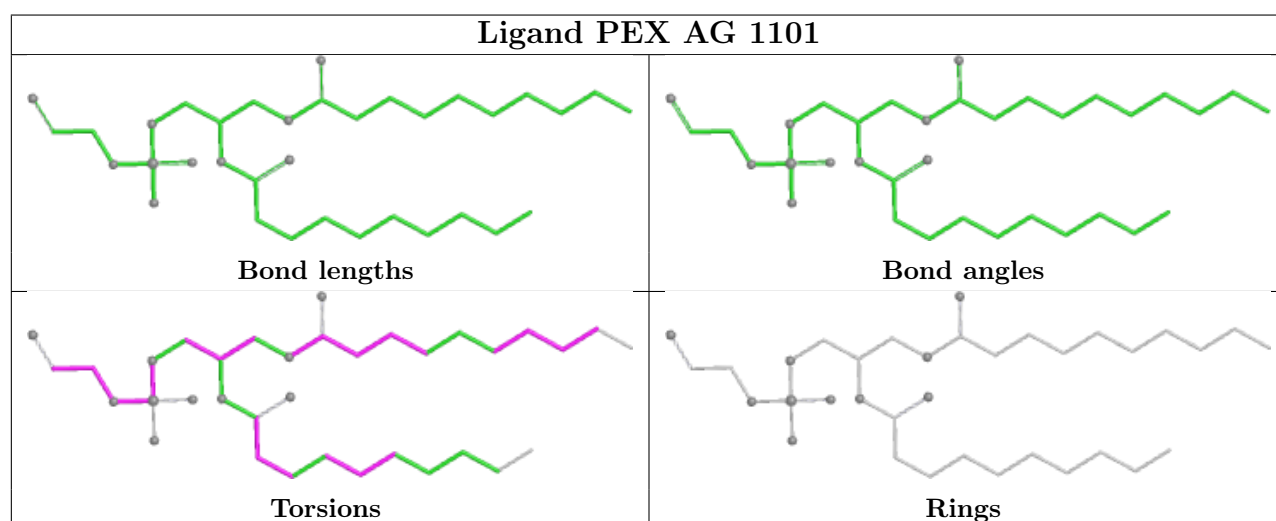
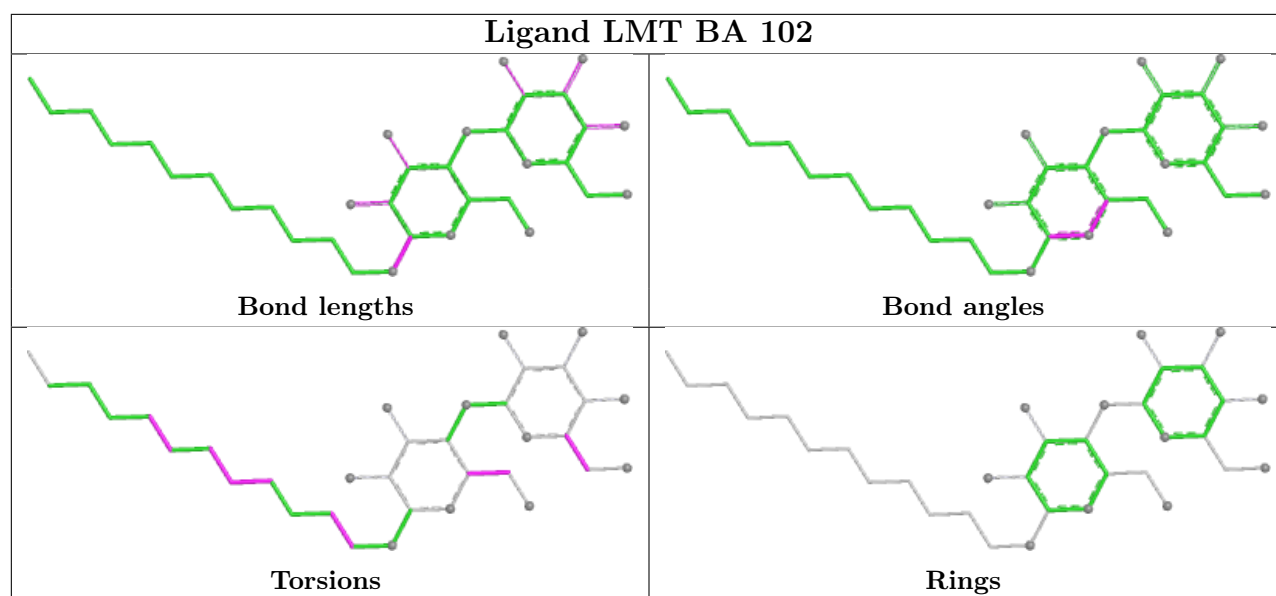


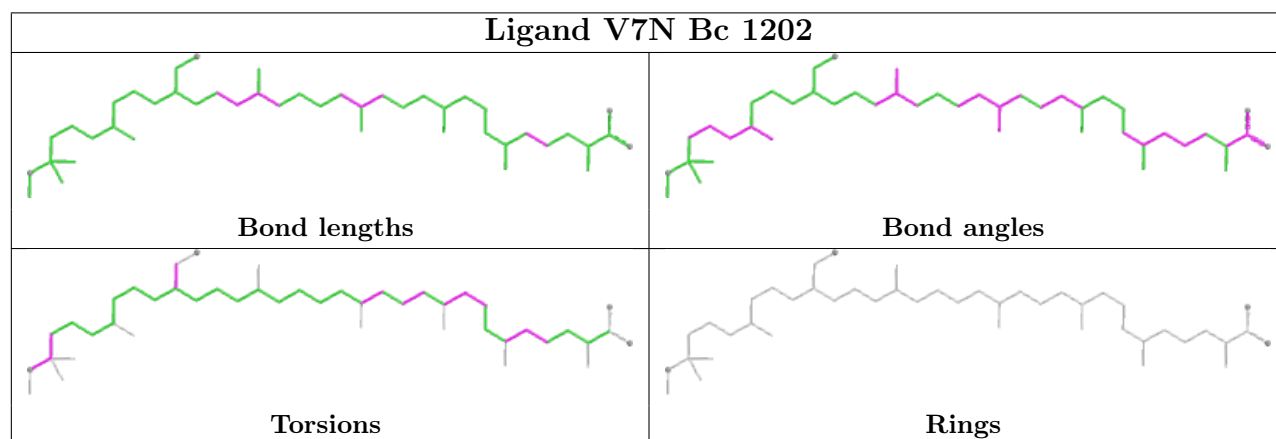
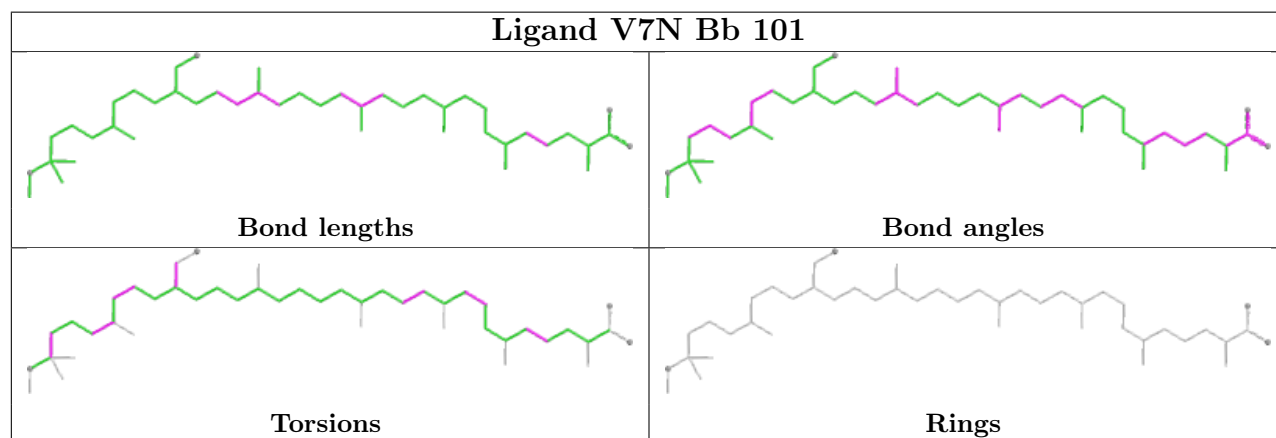
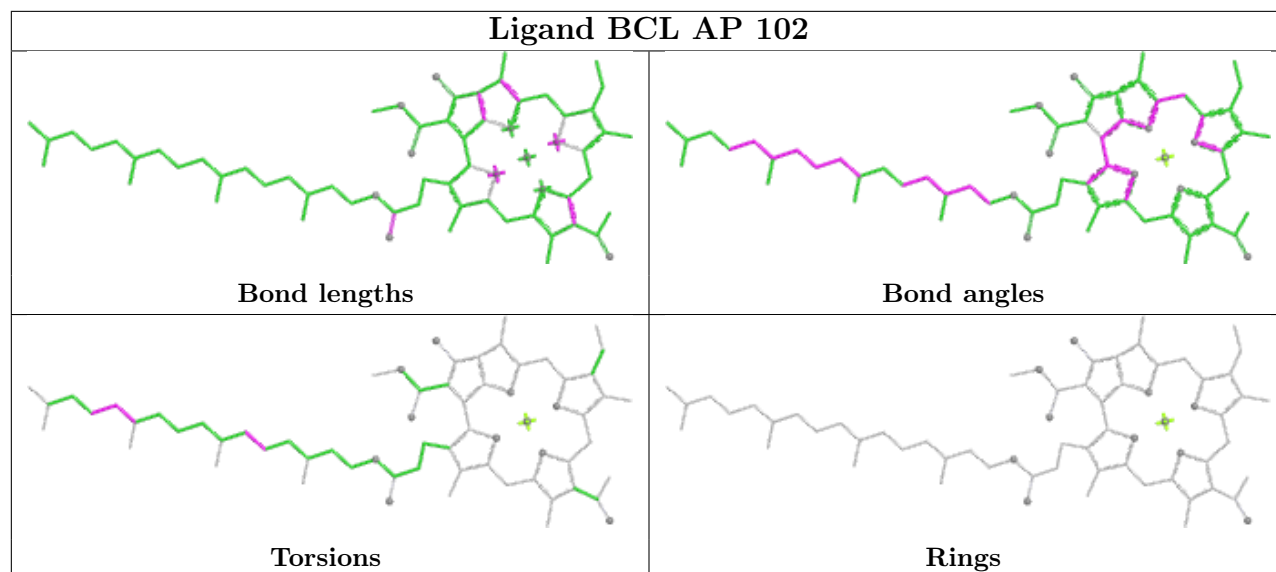


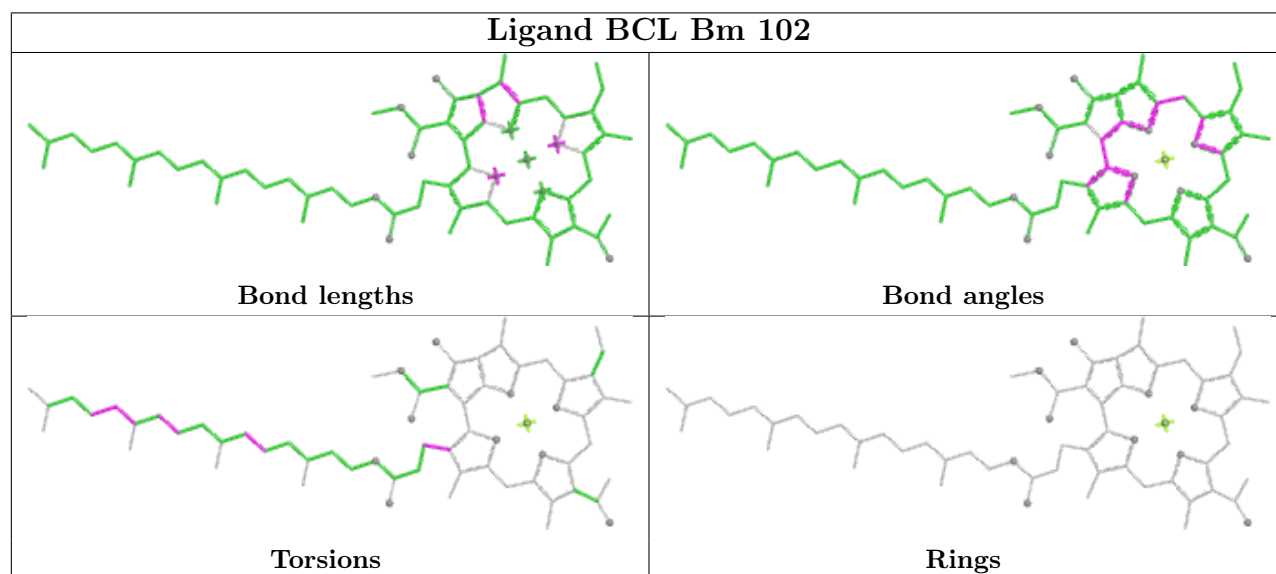
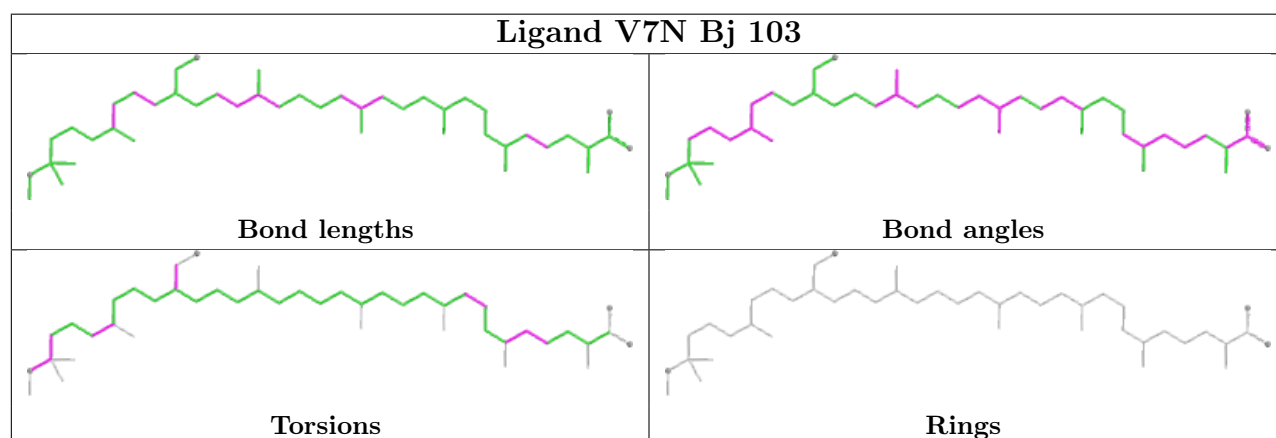
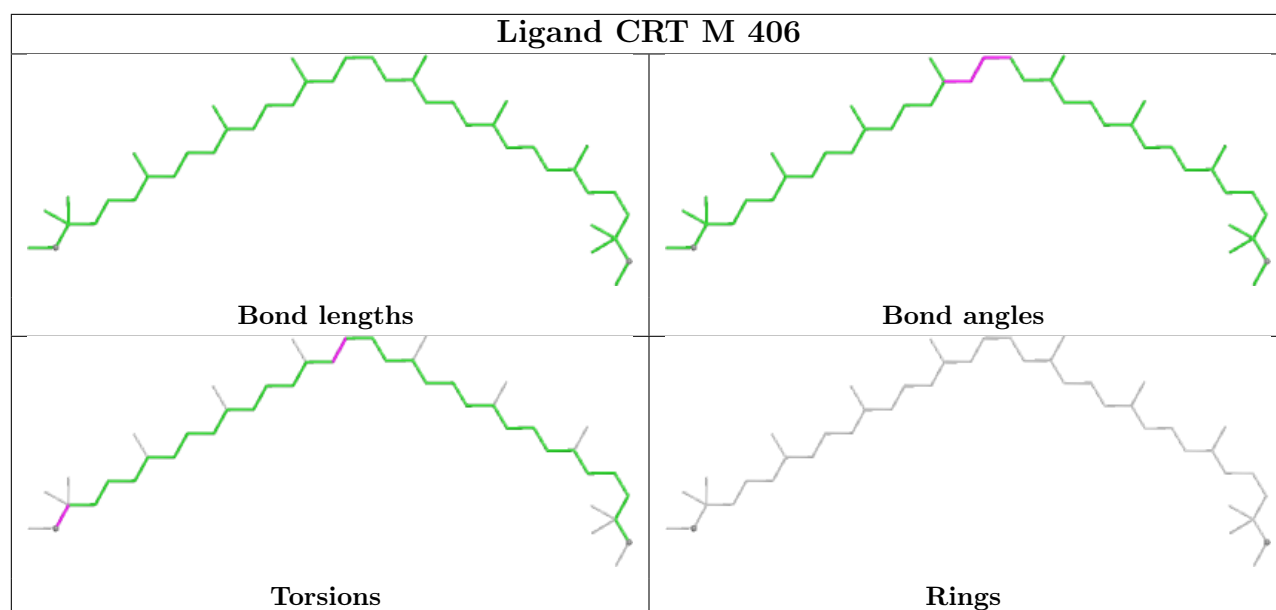


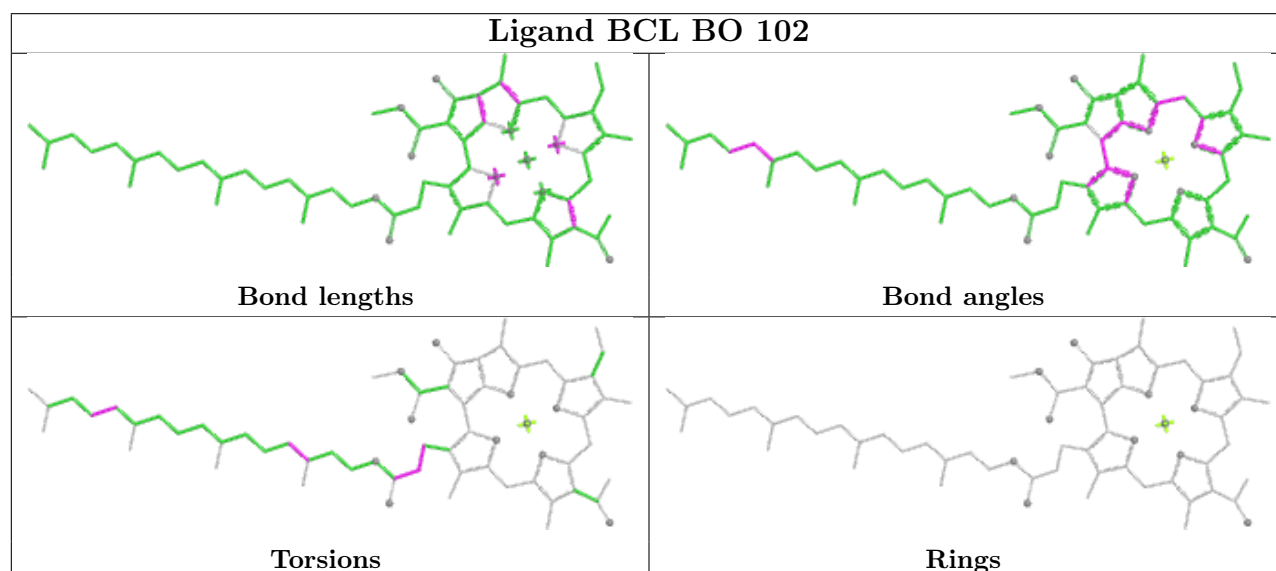
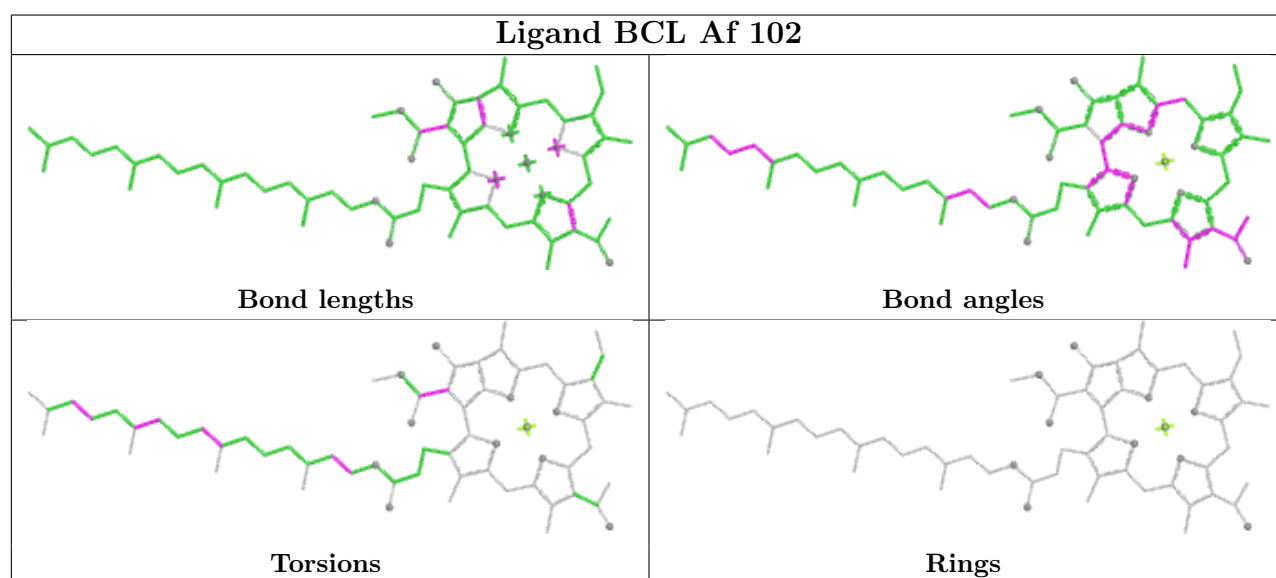
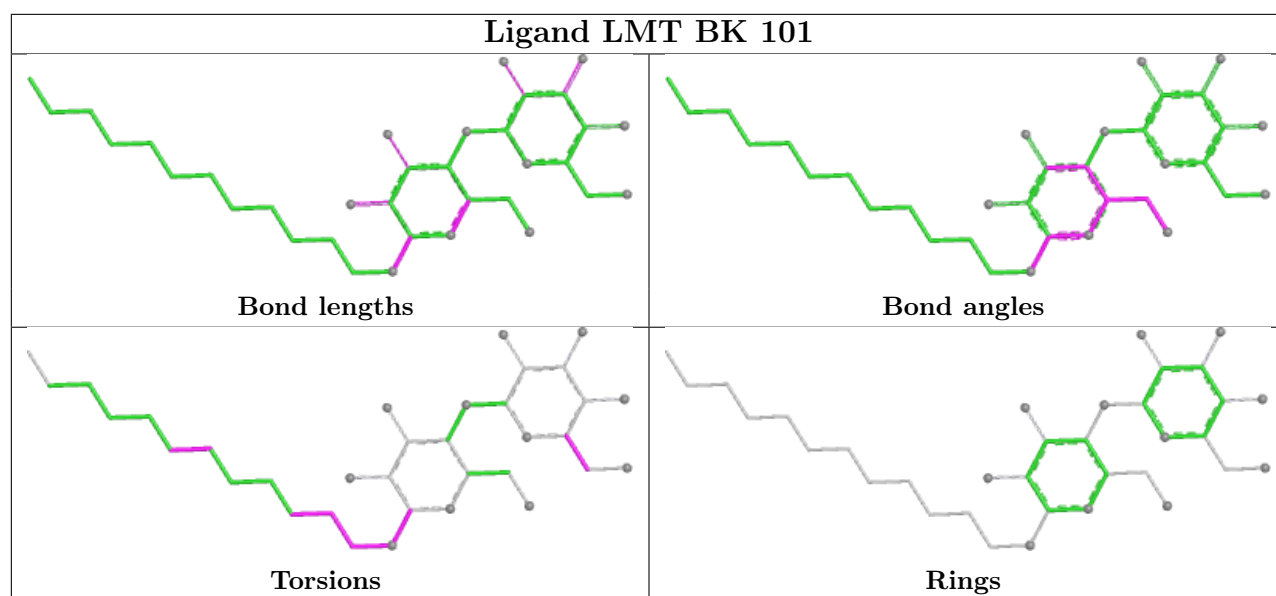


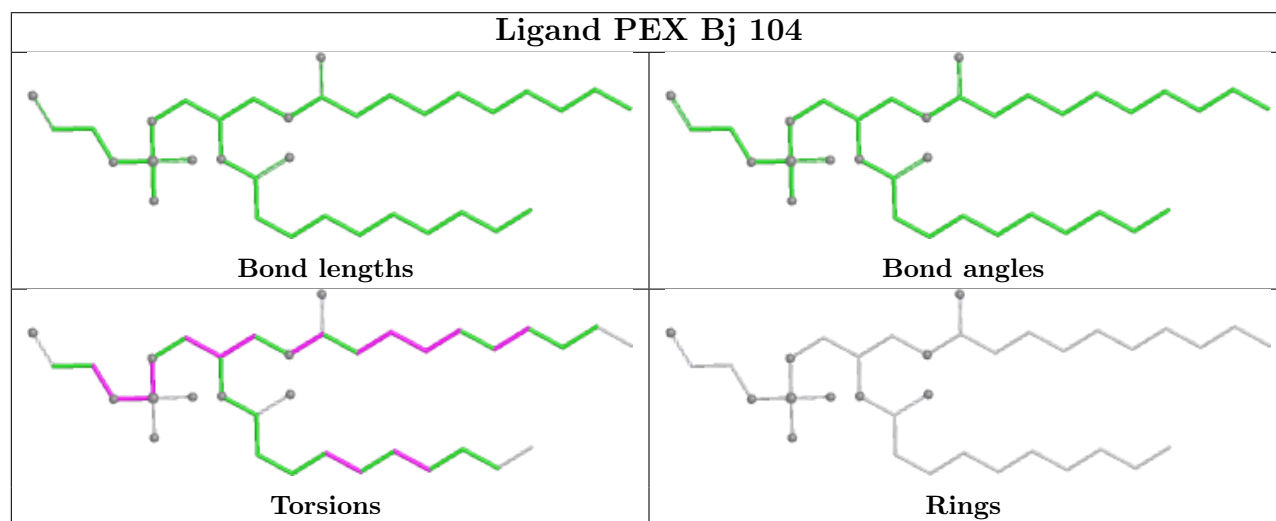
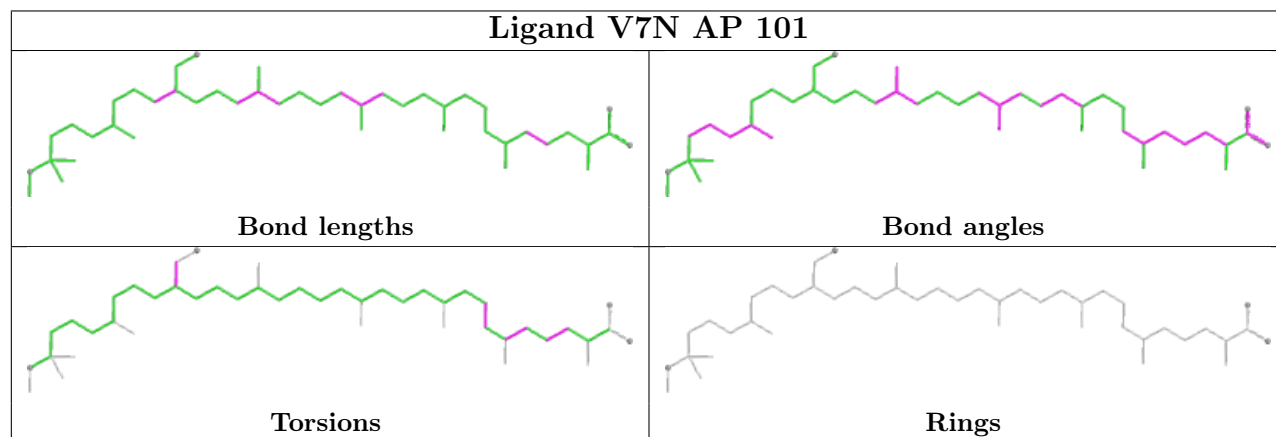
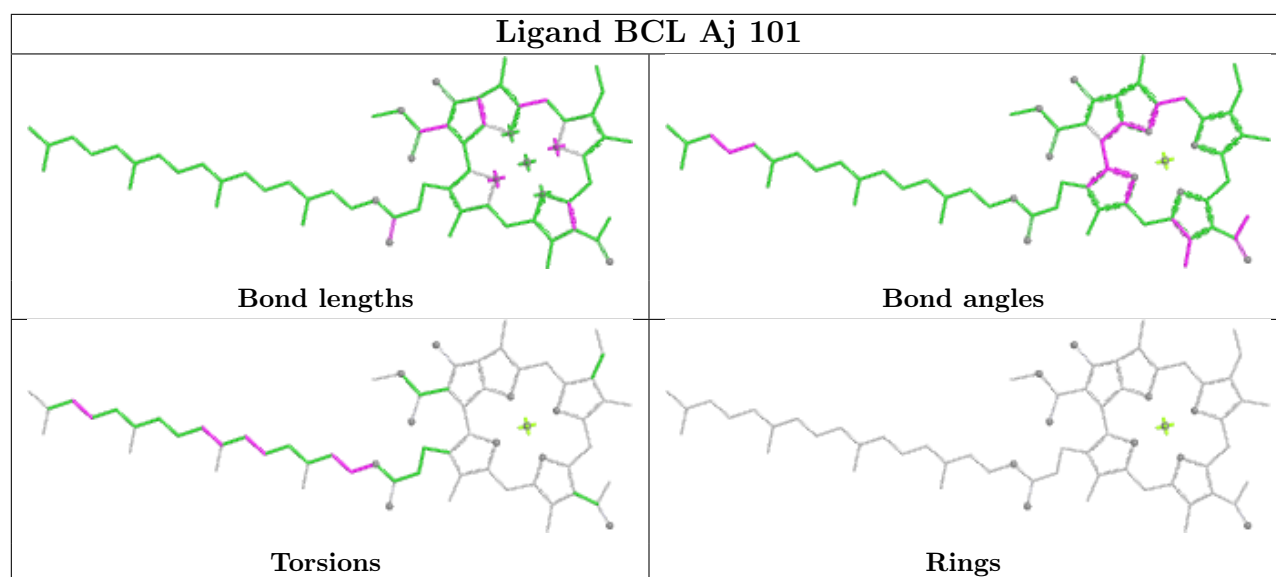


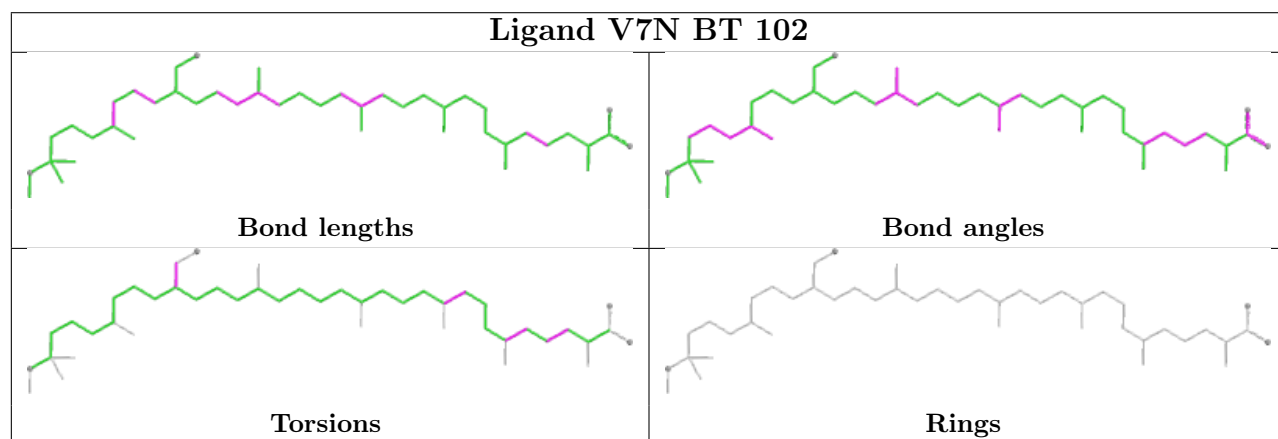
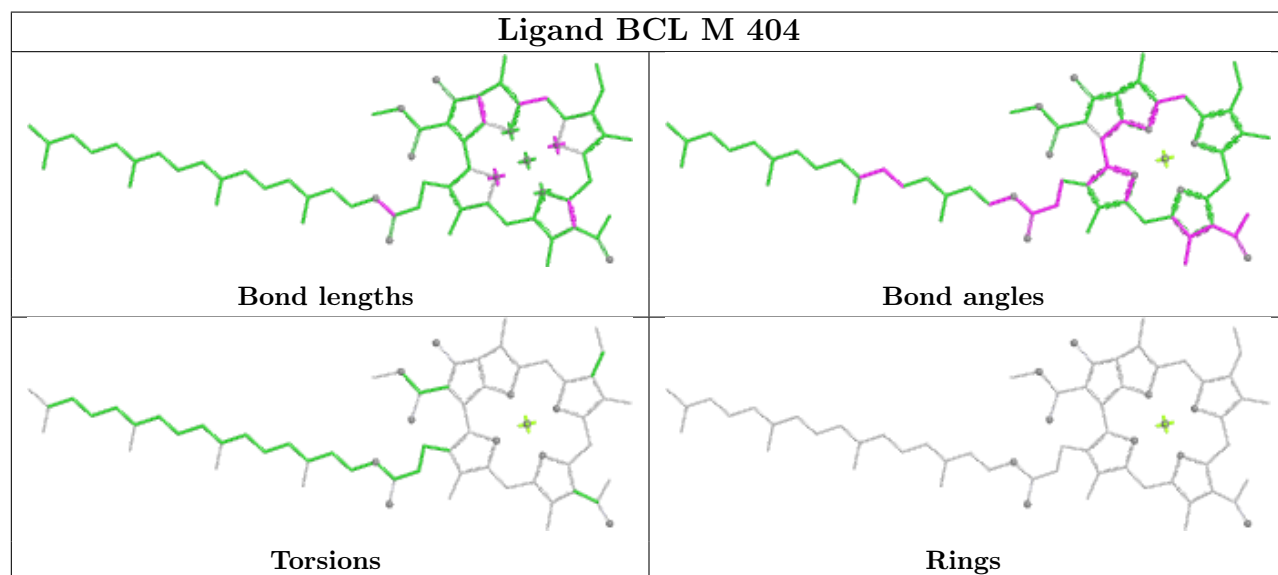
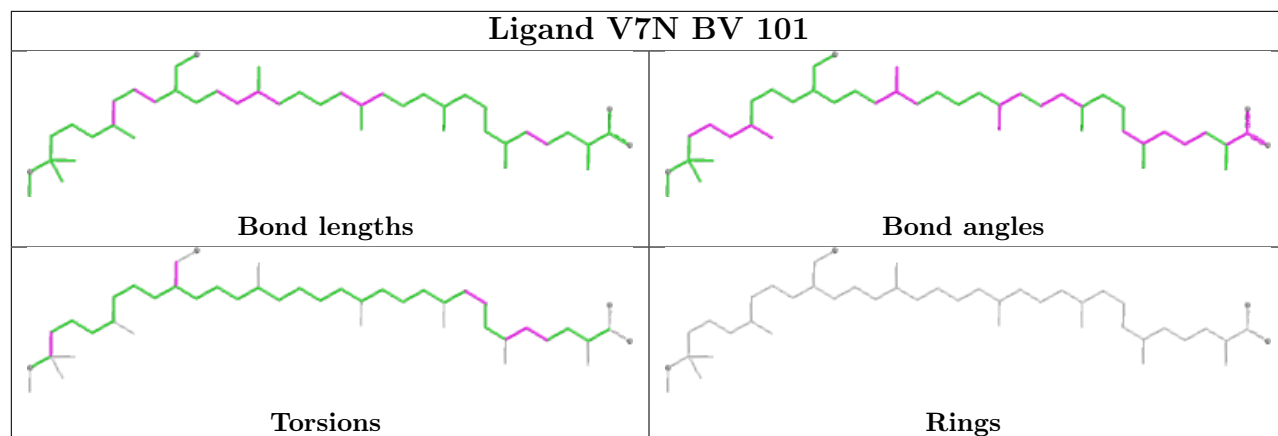


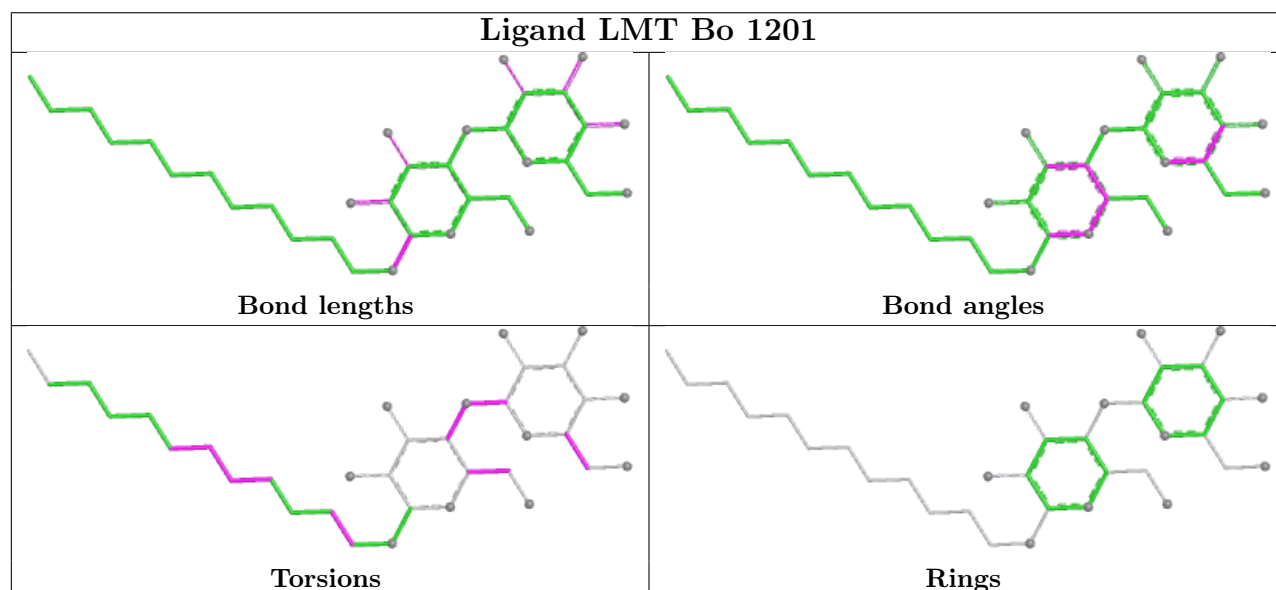
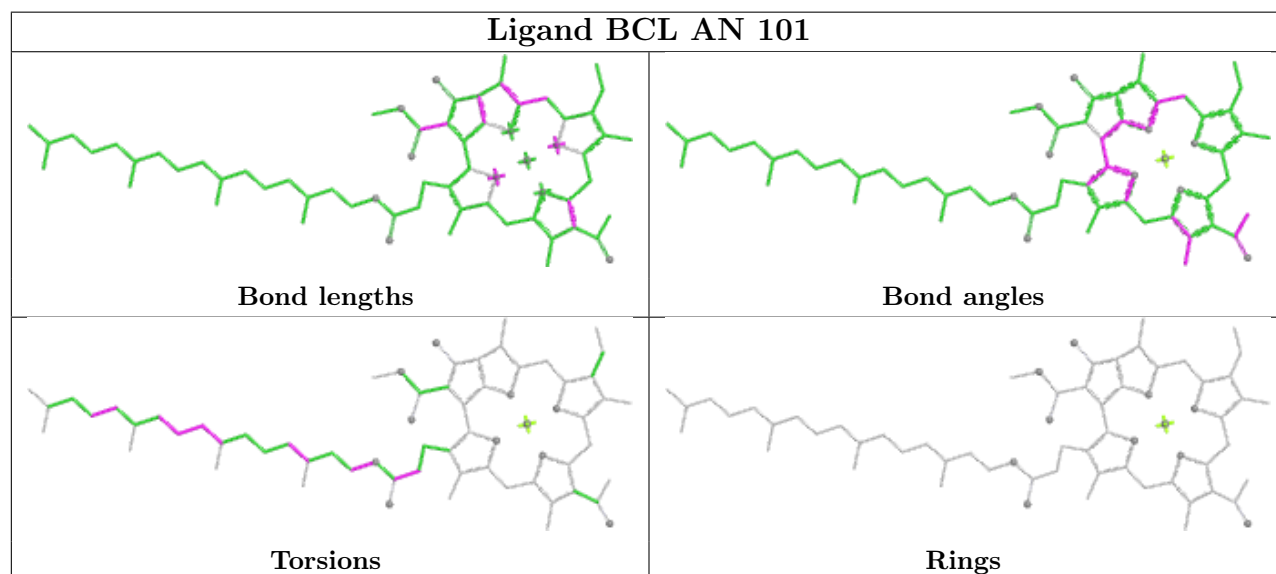
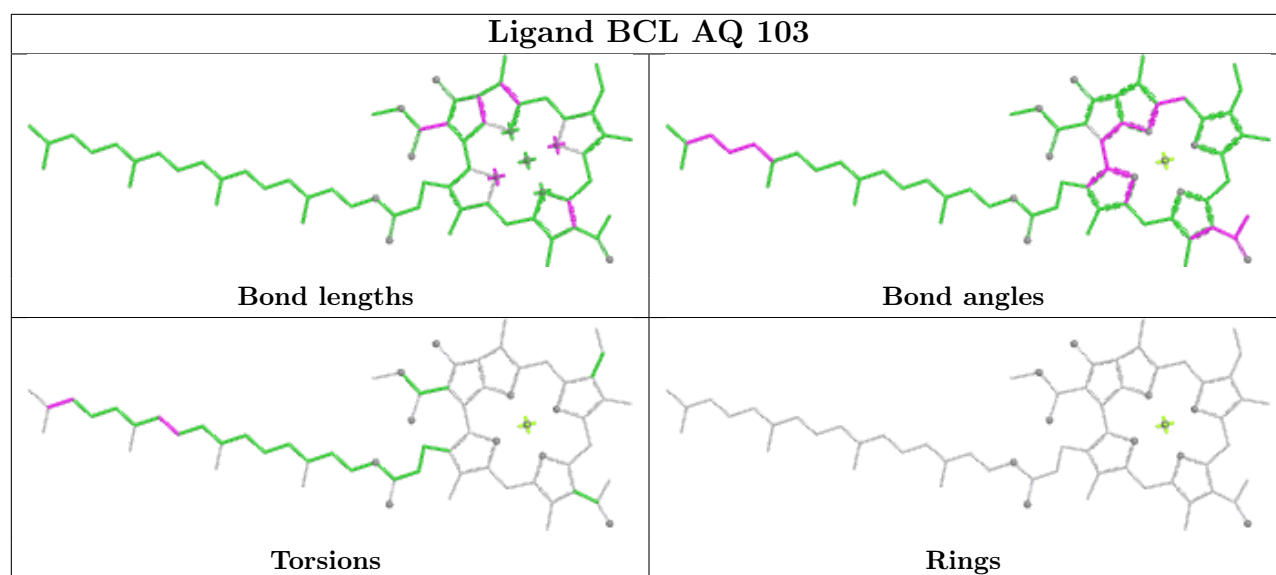


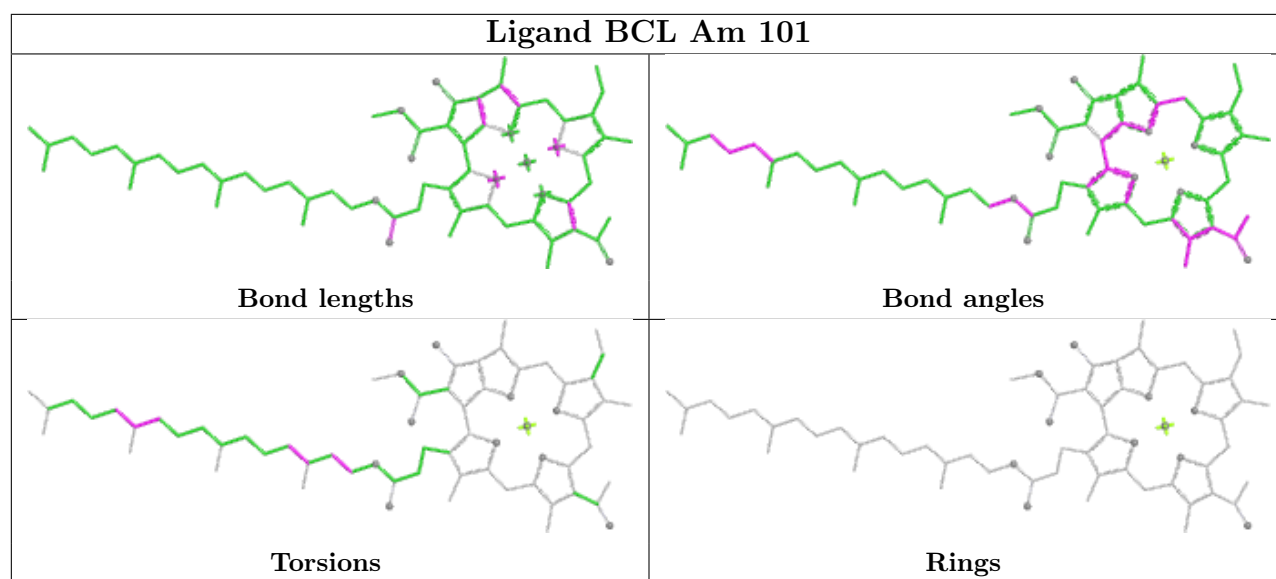












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

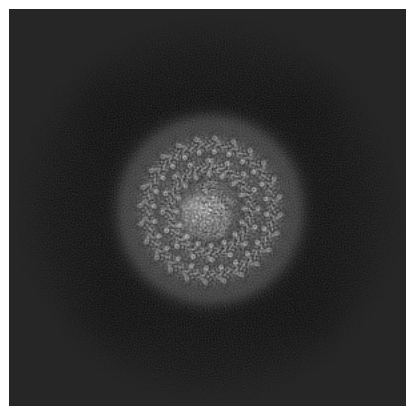
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51788. These allow visual inspection of the internal detail of the map and identification of artifacts.

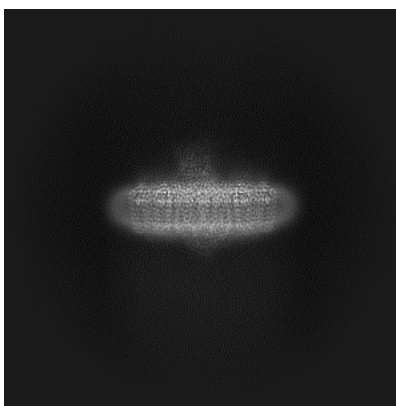
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

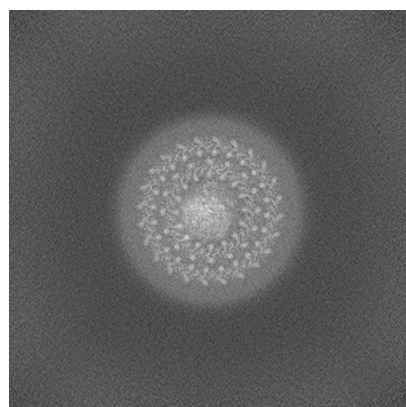


Y

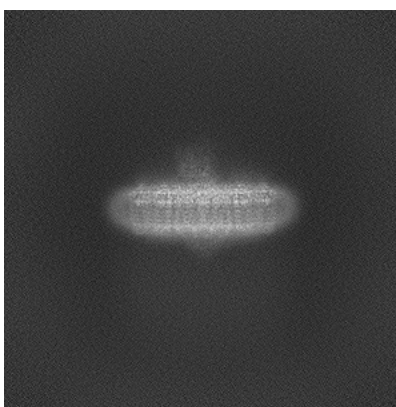


Z

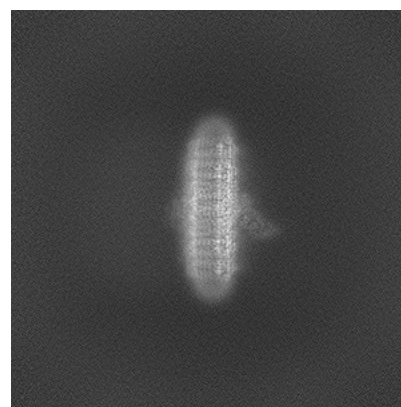
6.1.2 Raw map



X



Y

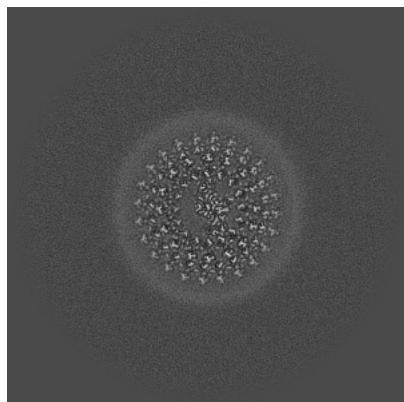


Z

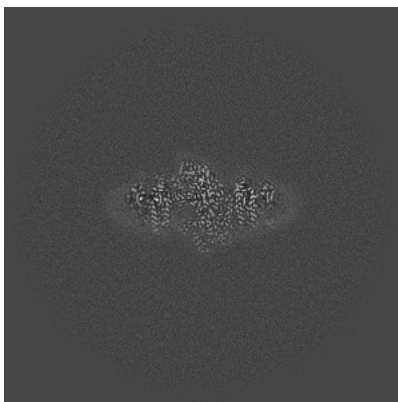
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

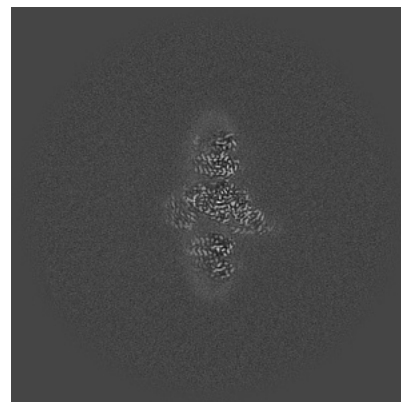
6.2.1 Primary map



X Index: 300

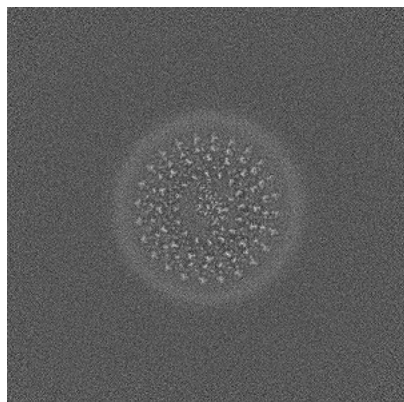


Y Index: 300

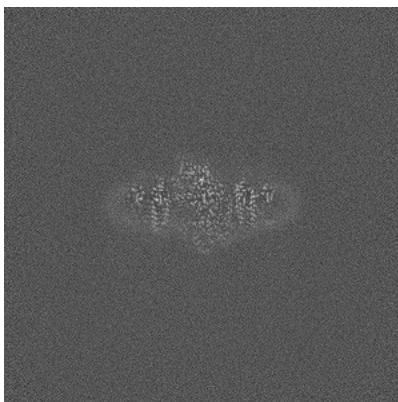


Z Index: 300

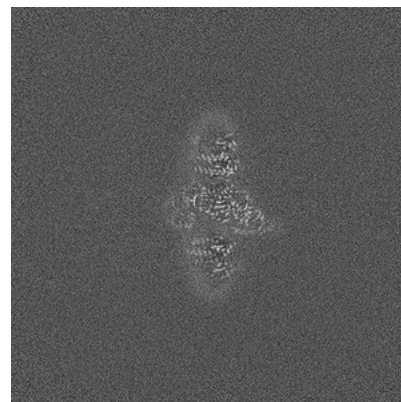
6.2.2 Raw map



X Index: 300



Y Index: 300

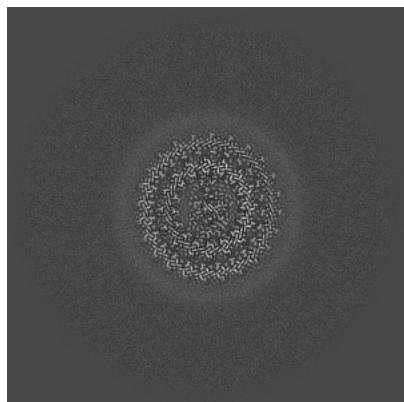


Z Index: 300

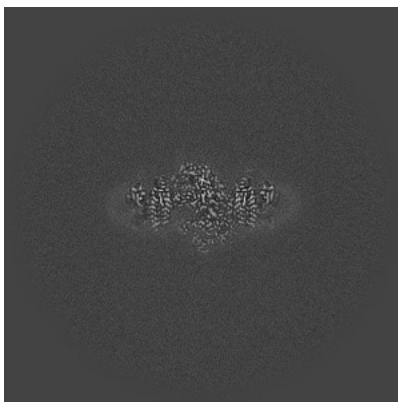
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

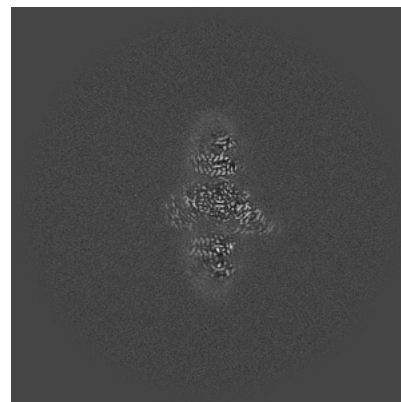
6.3.1 Primary map



X Index: 312

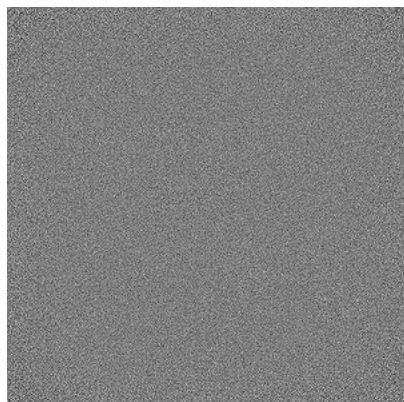


Y Index: 301

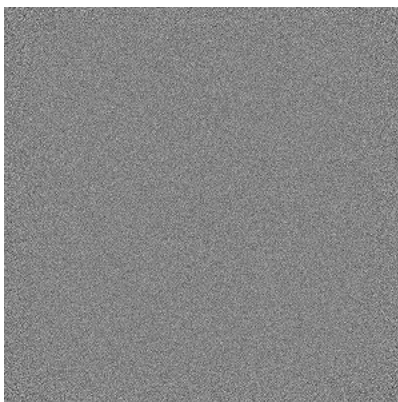


Z Index: 299

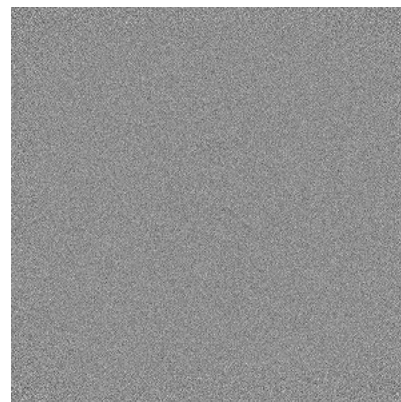
6.3.2 Raw map



X Index: 0



Y Index: 0

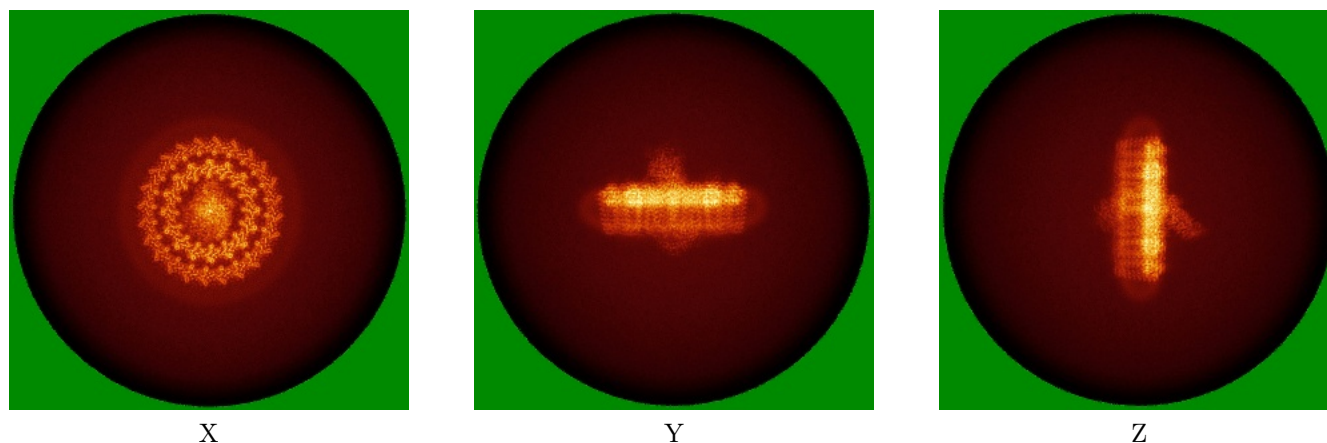


Z Index: 599

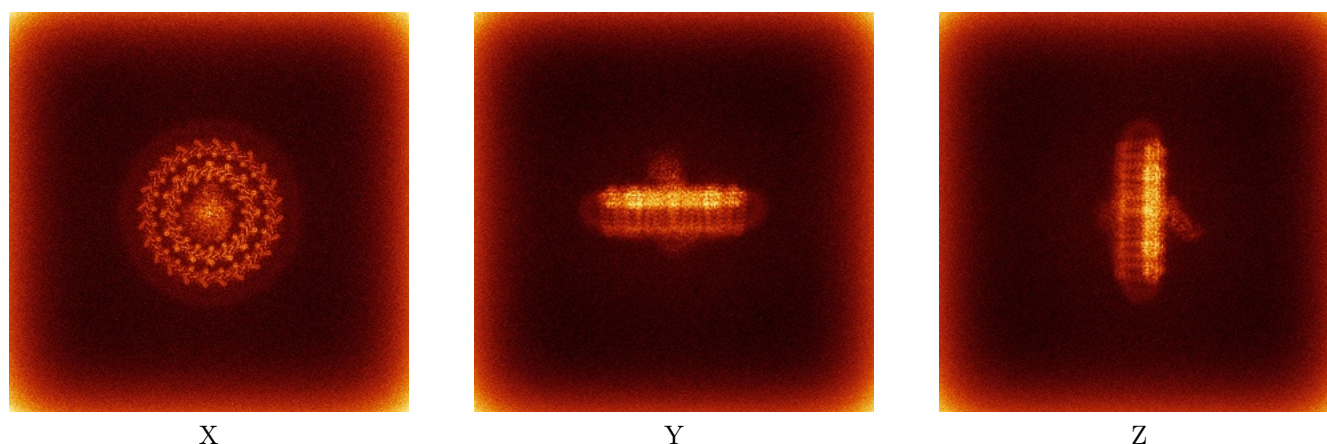
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

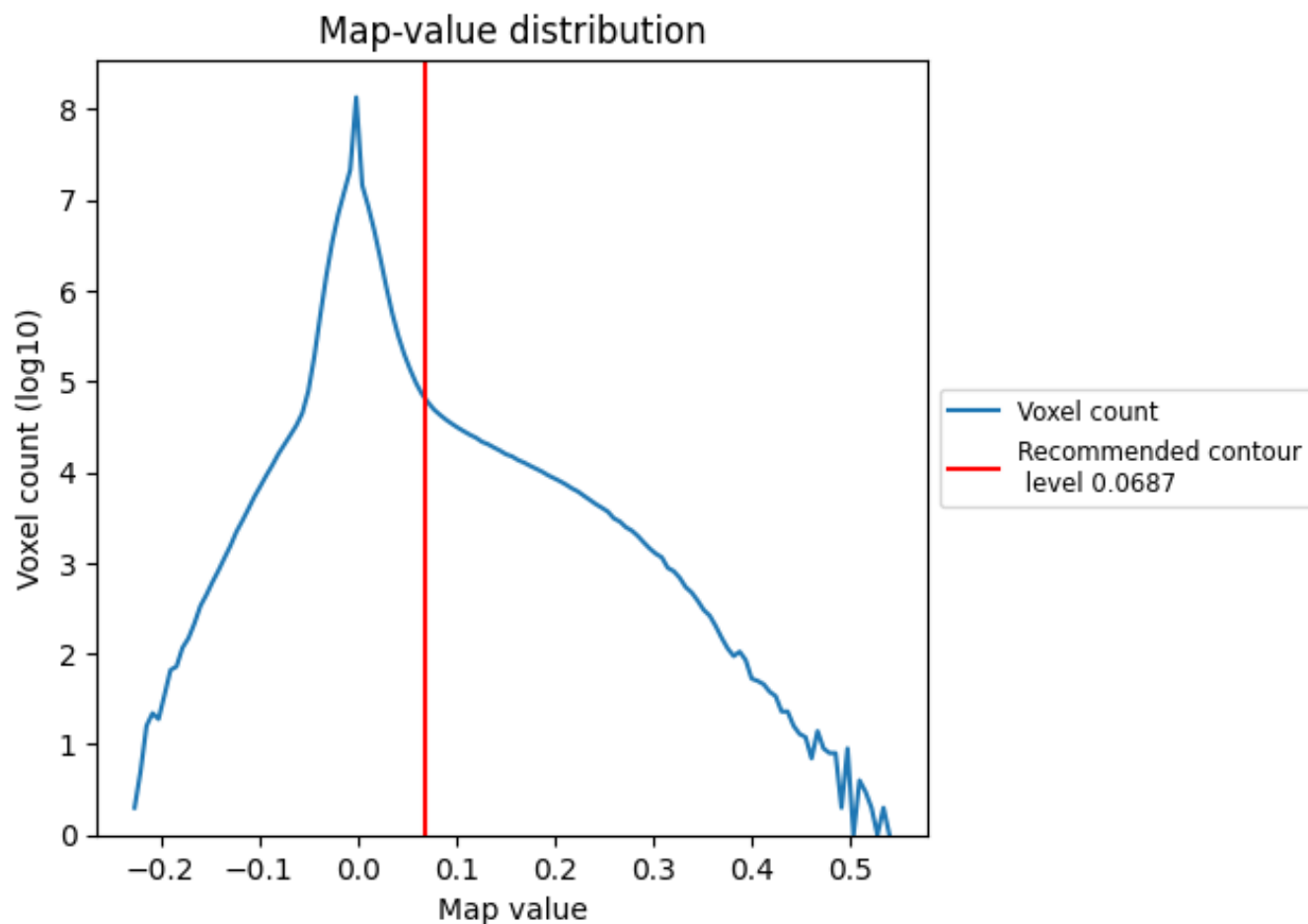
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

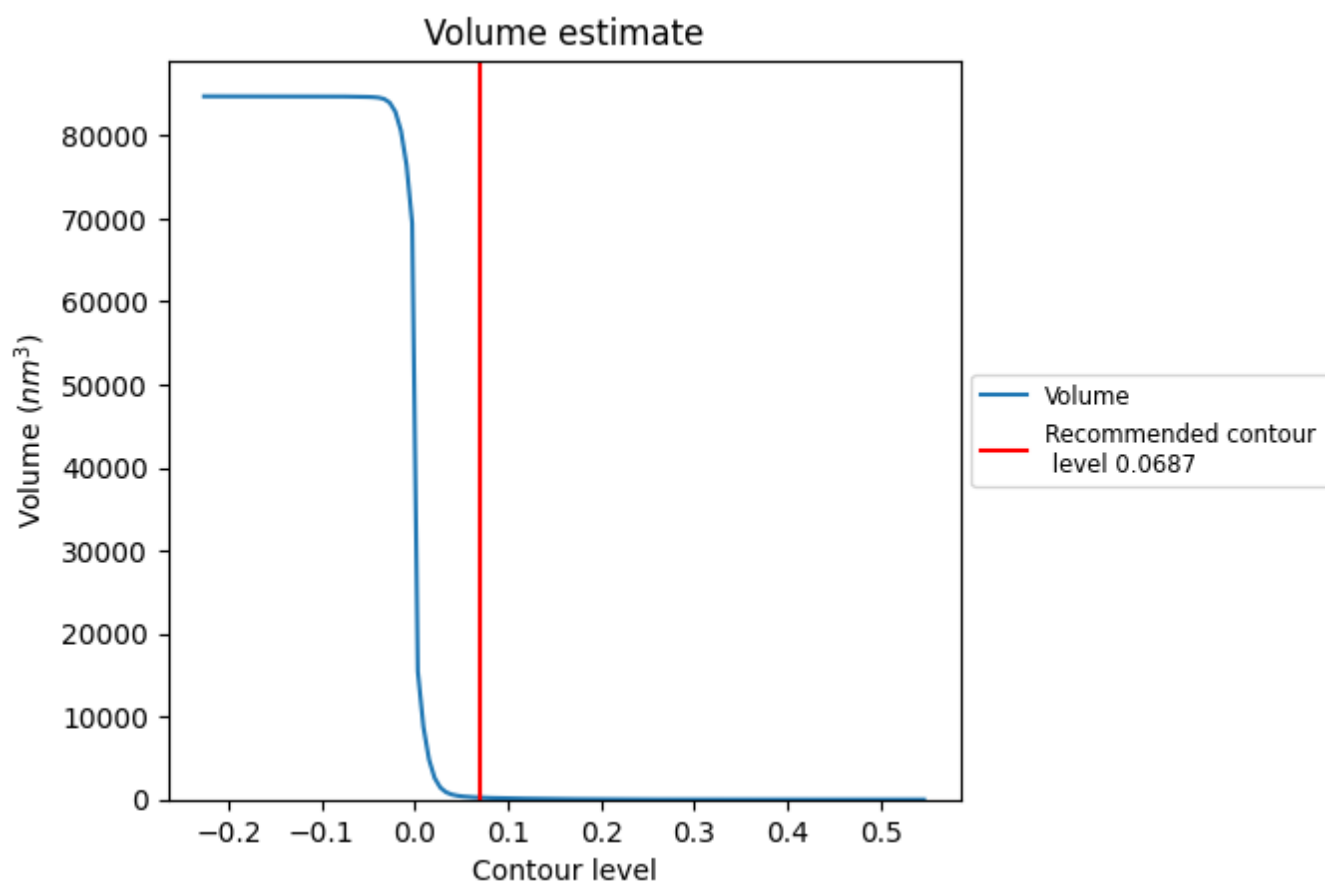
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

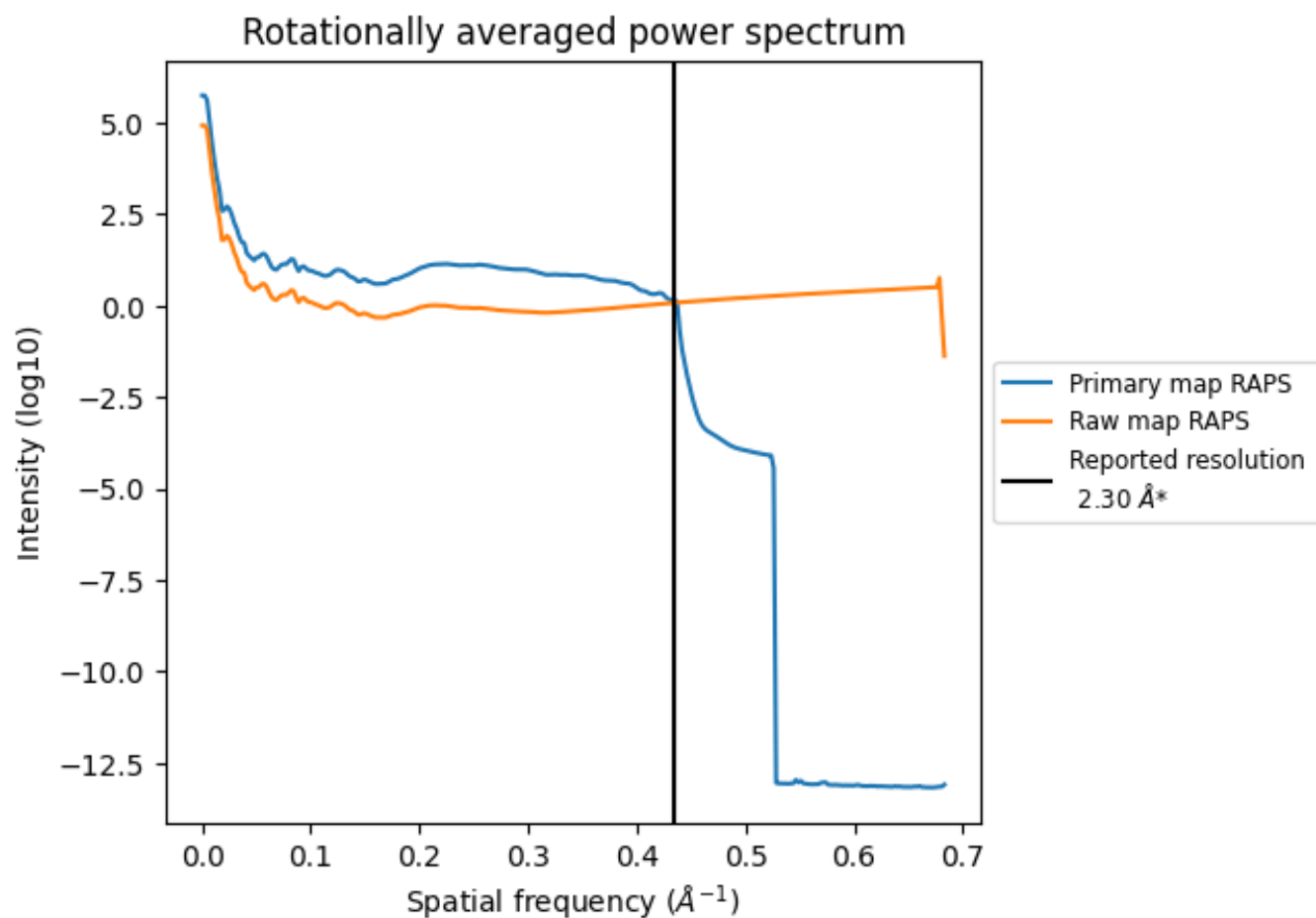
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm³; this corresponds to an approximate mass of 222 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

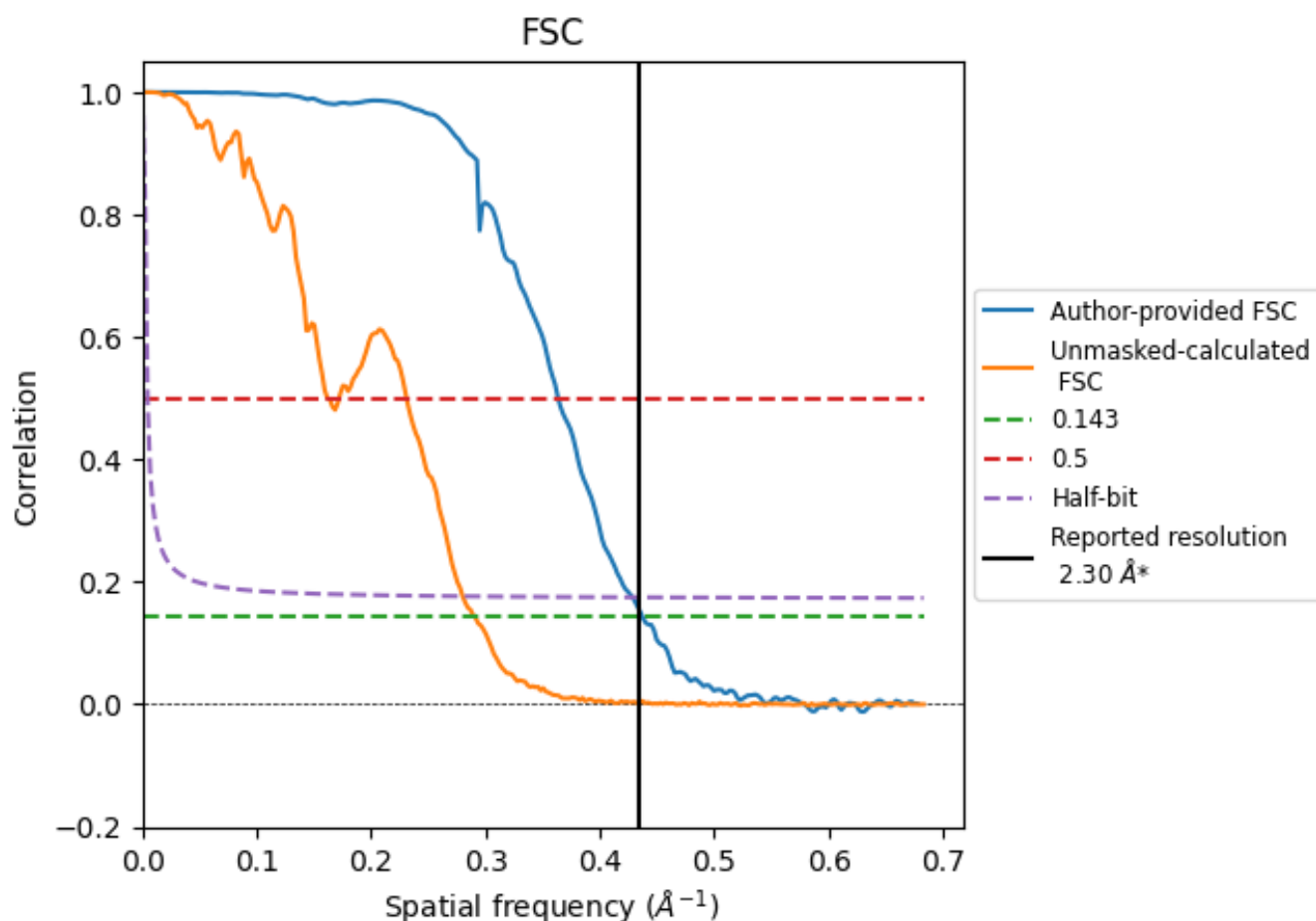


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

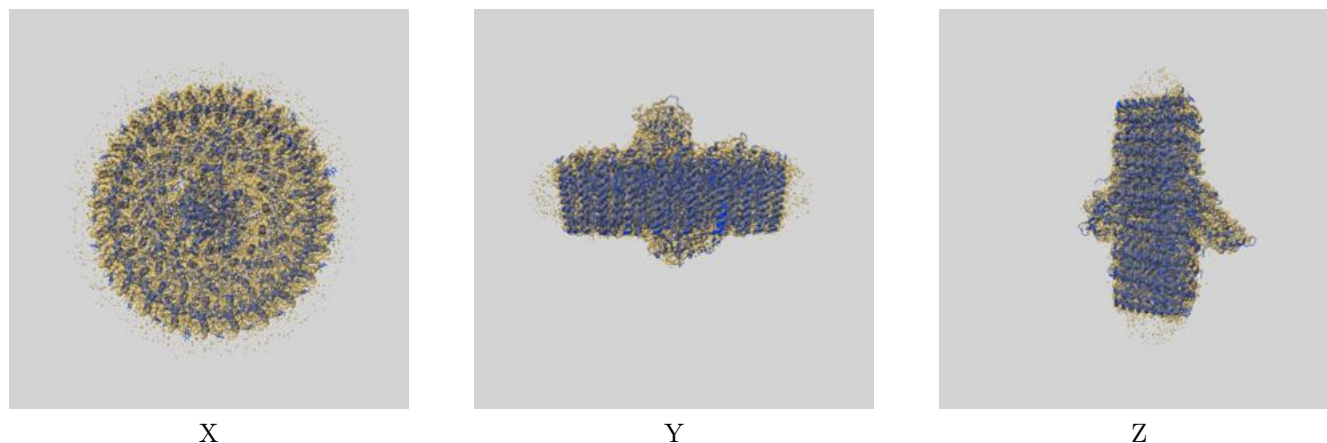
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.75	2.33
Unmasked-calculated*	3.44	6.17	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

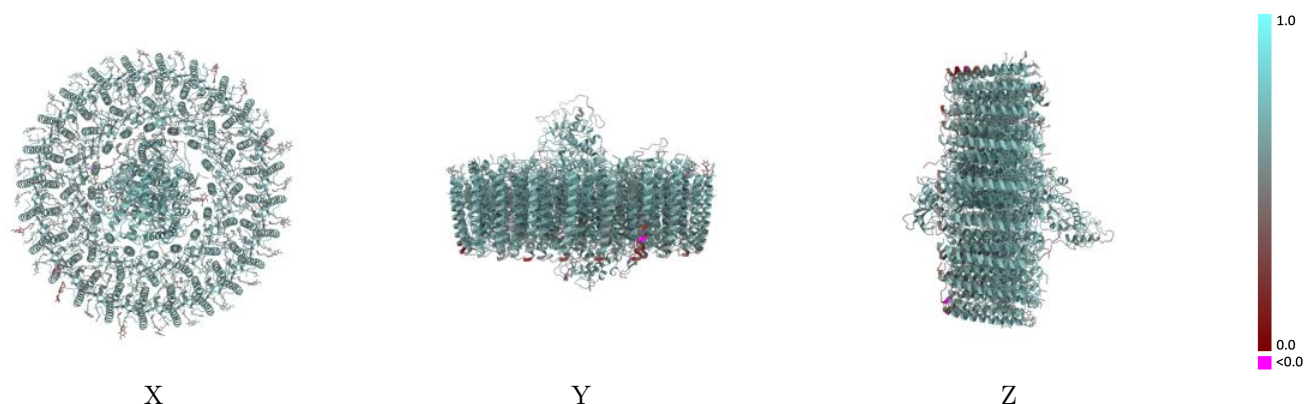
This section contains information regarding the fit between EMDB map EMD-51788 and PDB model 9H22. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



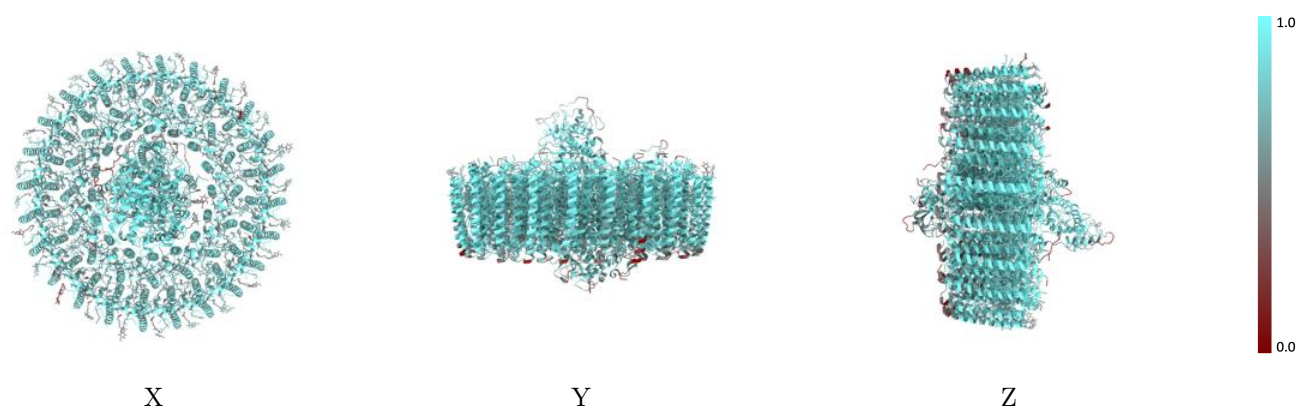
The images above show the 3D surface view of the map at the recommended contour level 0.0687 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



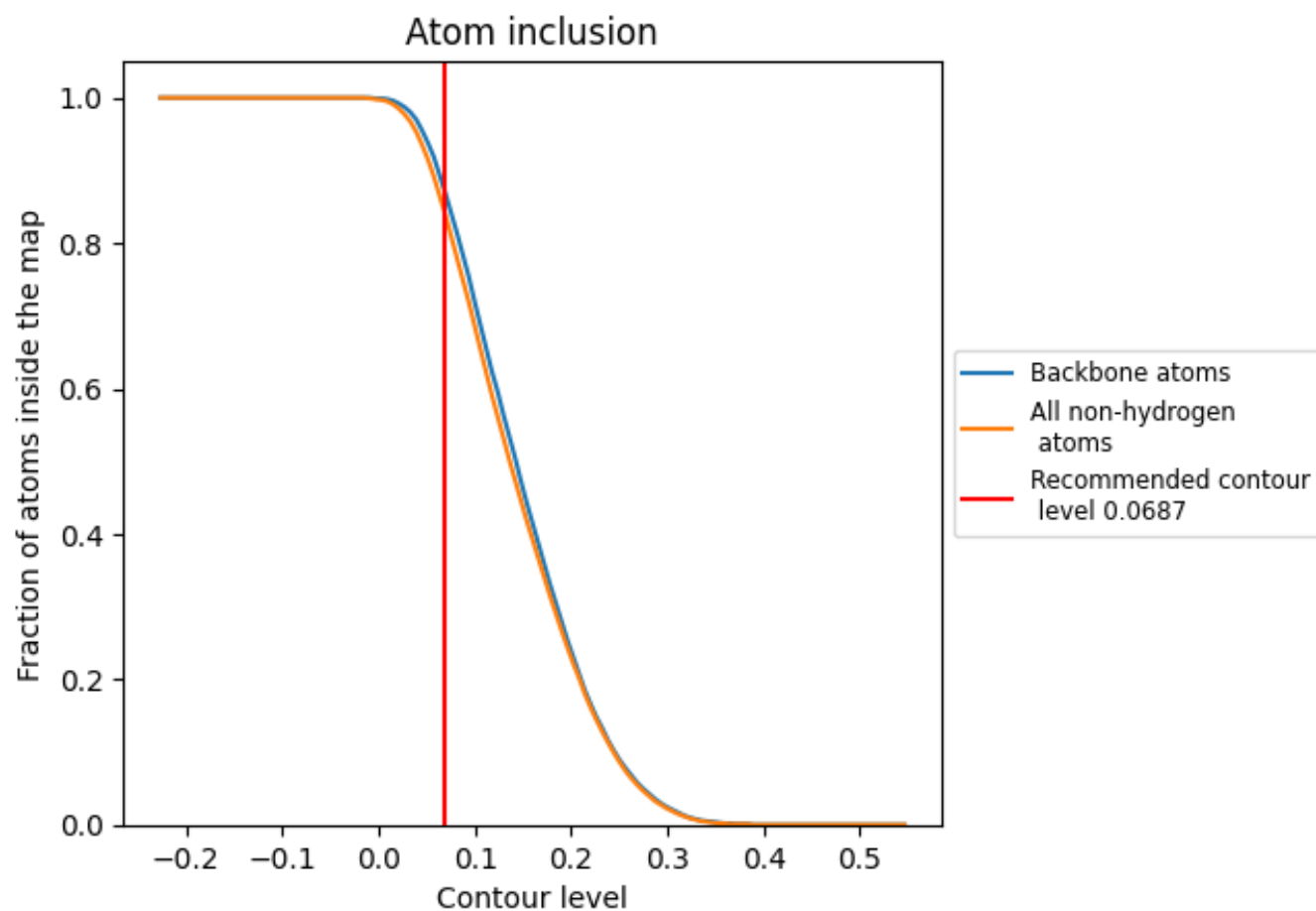
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0687).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0687) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.6270
AA	 0.8540	 0.6310
AB	 0.9020	 0.6520
AC	 0.9330	 0.6570
AD	 0.8150	 0.6160
AE	 0.8740	 0.6460
AF	 0.8920	 0.6490
AG	 0.8240	 0.6250
AH	 0.8740	 0.6380
AI	 0.8700	 0.6380
AJ	 0.8590	 0.6270
AK	 0.8840	 0.6380
AL	 0.9180	 0.6540
AM	 0.8330	 0.6190
AN	 0.8810	 0.6370
AO	 0.9020	 0.6400
AP	 0.8120	 0.6040
AQ	 0.8290	 0.6250
AR	 0.8850	 0.6320
AS	 0.8060	 0.6050
AT	 0.8090	 0.6090
AU	 0.8540	 0.6240
AV	 0.8160	 0.6160
AW	 0.8770	 0.6370
AX	 0.9260	 0.6600
Aa	 0.7850	 0.6030
Ab	 0.8730	 0.6440
Ac	 0.9100	 0.6610
Ad	 0.8340	 0.6280
Ae	 0.9090	 0.6530
Af	 0.8170	 0.6180
Ag	 0.8500	 0.6270
Ah	 0.8530	 0.6340
Ai	 0.8750	 0.6400
Aj	 0.8930	 0.6500























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Chain	Atom inclusion	Q-score
Ak	 0.9330	 0.6760
Al	 0.9190	 0.6620
Am	 0.9220	 0.6640
An	 0.9010	 0.6610
Ao	 0.8850	 0.6550
Ap	 0.8480	 0.6060
BA	 0.7580	 0.5470
BB	 0.8500	 0.6340
BC	 0.8470	 0.6300
BD	 0.7990	 0.5960
BE	 0.8410	 0.5970
BF	 0.8100	 0.5940
BG	 0.7620	 0.5900
BH	 0.6930	 0.4910
BI	 0.8200	 0.6060
BJ	 0.8090	 0.5950
BK	 0.8040	 0.6080
BL	 0.8580	 0.6260
BM	 0.7940	 0.6030
BN	 0.8540	 0.6370
BO	 0.8500	 0.6180
BP	 0.7350	 0.5560
BQ	 0.8210	 0.6040
BR	 0.8100	 0.6050
BS	 0.7230	 0.5380
BT	 0.8300	 0.5920
BU	 0.6020	 0.3810
BV	 0.7350	 0.5580
BW	 0.8390	 0.6030
BX	 0.7970	 0.5820
Ba	 0.7880	 0.5870
Bb	 0.8370	 0.6160
Bc	 0.8410	 0.6280
Bd	 0.8510	 0.6360
Be	 0.8830	 0.6460
Bf	 0.8540	 0.6370
Bg	 0.8080	 0.6180
Bh	 0.8510	 0.6290
Bi	 0.8000	 0.6090
Bj	 0.8310	 0.6270
Bk	 0.8960	 0.6590
Bl	 0.8350	 0.6300

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Chain	Atom inclusion	Q-score
Bm	 0.8590	 0.6500
Bn	 0.8830	 0.6440
Bo	 0.8050	 0.5950
Bp	 0.7990	 0.5980
C	 0.8800	 0.6520
H	 0.6980	 0.5850
K	 0.6920	 0.5910
L	 0.8940	 0.6590
M	 0.9300	 0.6770
S	 0.8390	 0.6700