



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:54 PM EDT

PDB ID : 2WSF / pdb\_00002wsf  
Title : Improved Model of Plant Photosystem I  
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.  
Deposited on : 2009-09-05  
Resolution : 3.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : **FAILED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	165	1264	822	208	230	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	176	1374	899	226	245	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	153	1186	781	193	207	5	0	0	0

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	166	1319	861	219	236	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	730	5745	3766	974	987	18	0	0	0

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B	733	5848	3843	997	995	13	0	0	0

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	C	81	619	384	108	115	12	0	0	0

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	D	138	1095	704	189	198	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	E	65	520	332	93	95	0	0	0

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	F	154	1221	794	207	217	3	0	0	0

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	G	95	740	481	120	137	2	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	H	69	529	344	82	103	0	0	0

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	I	30	229	158	34	35	2	0	0	0

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

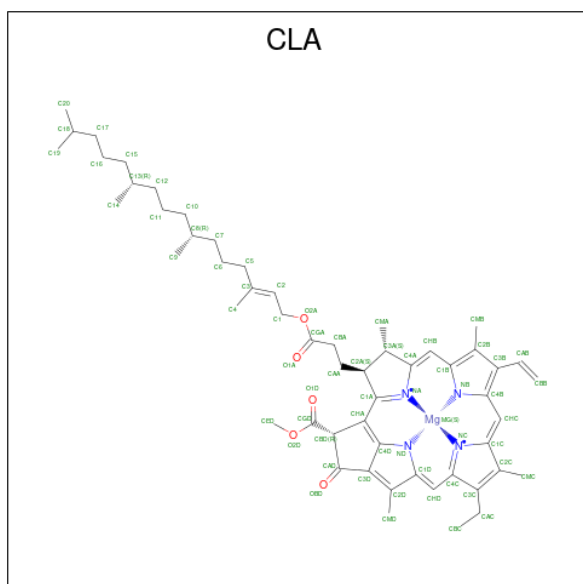
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			23	12	11			
19	O	2	Total	C	O	0	0	0
			22	12	10			
19	P	2	Total	C	O	0	0	0
			23	12	11			
19	Q	2	Total	C	O	0	0	0
			23	12	11			
19	S	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	T	2	Total	C	O	0	0	0
			23	12	11			
19	U	2	Total	C	O	0	0	0
			23	12	11			
19	V	2	Total	C	O	0	0	0
			23	12	11			
19	W	2	Total	C	O	0	0	0
			23	12	11			
19	X	2	Total	C	O	0	0	0
			22	12	10			
19	Y	2	Total	C	O	0	0	0
			23	12	11			
19	Z	2	Total	C	O	0	0	0
			23	12	11			
19	a	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	3	1	Total	C	Mg	N	0	0	
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			25	20	1	4			
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		

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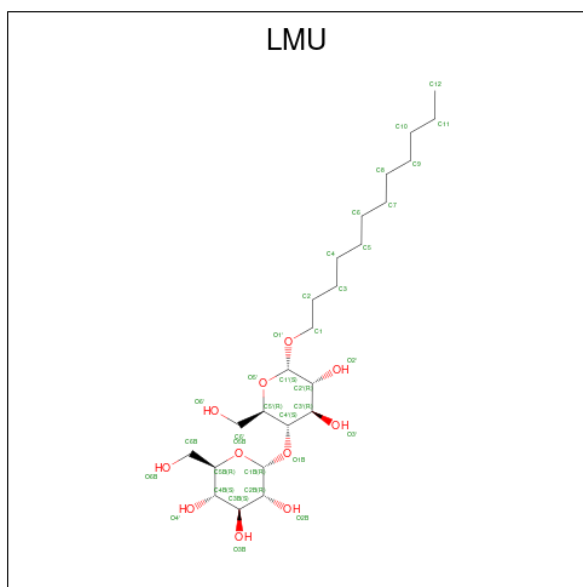
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		

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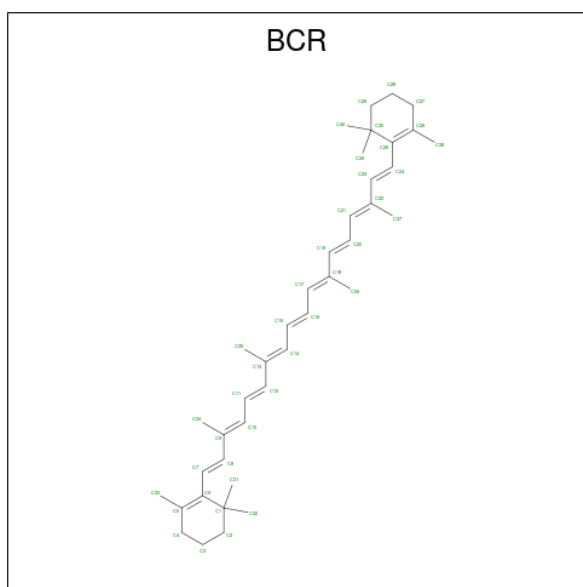
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			25	14	11		
21	C	1	Total	C	O	0	0
			35	24	11		
21	D	1	Total	C	O	0	0
			35	24	11		
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		
21	G	1	Total	C	O	0	0
			35	24	11		
21	G	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	G	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



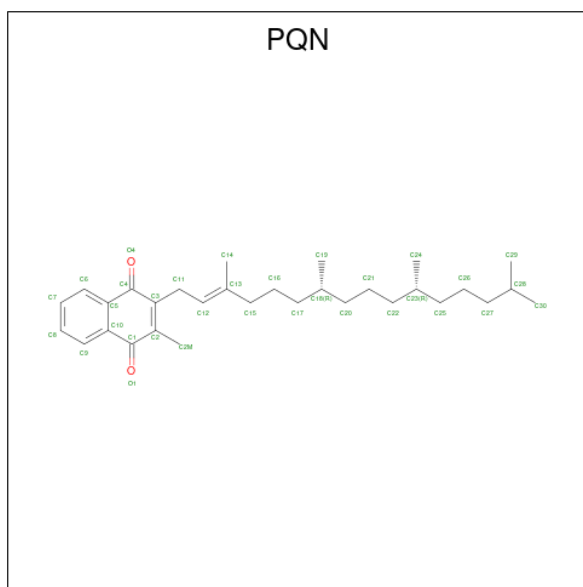
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	2	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	I	1	Total C 39 39	0	0
22	I	1	Total C 40 40	0	0

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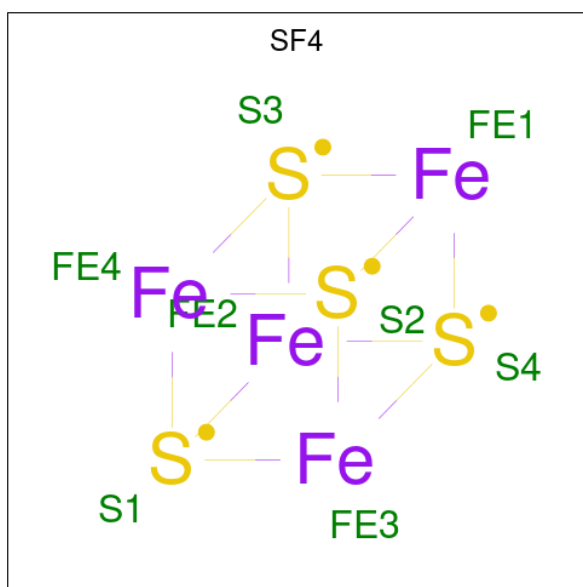
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



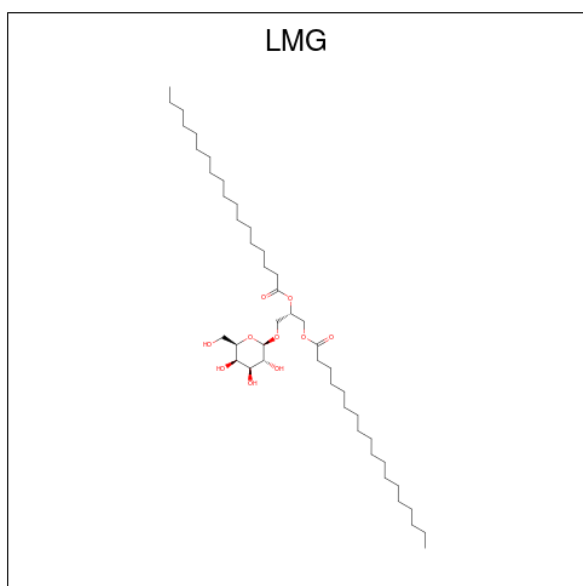
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	Fe S	0	0
			8	4 4		
24	C	1	Total	Fe S	0	0
			8	4 4		
24	C	1	Total	Fe S	0	0
			8	4 4		

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48	Depositor
% Data completeness (in resolution range)	96.4 (50.00-3.48)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.391 , 0.425	Depositor
Wilson B-factor (Å <sup>2</sup> )	81.0	Xtrriage
Anisotropy	0.408	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtrriage
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	GLC	M	1	19	11,11,12	0.53	0	15,15,17	2.21	2 (13%)
19	FRU	M	2	19	11,12,12	0.66	0	10,18,18	0.75	0
19	GLC	O	1	19	10,10,12	0.91	0	14,14,17	2.18	3 (21%)
19	FRU	O	2	19	11,12,12	0.60	0	10,18,18	1.14	1 (10%)
19	GLC	P	1	19	11,11,12	0.51	0	15,15,17	1.67	4 (26%)
19	FRU	P	2	19	11,12,12	0.71	0	10,18,18	1.21	2 (20%)
19	GLC	Q	1	19	11,11,12	0.58	0	15,15,17	2.28	5 (33%)
19	FRU	Q	2	19	11,12,12	0.72	0	10,18,18	1.21	1 (10%)
19	GLC	S	1	19	11,11,12	0.61	0	15,15,17	0.96	0
19	FRU	S	2	19	11,12,12	0.81	0	10,18,18	1.49	2 (20%)
19	GLC	T	1	19	11,11,12	0.50	0	15,15,17	0.76	1 (6%)
19	FRU	T	2	19	11,12,12	0.64	0	10,18,18	1.25	1 (10%)
19	GLC	U	1	19	11,11,12	0.64	0	15,15,17	2.54	4 (26%)
19	FRU	U	2	19	11,12,12	0.67	0	10,18,18	1.37	2 (20%)
19	GLC	V	1	19	11,11,12	0.55	0	15,15,17	1.80	4 (26%)
19	FRU	V	2	19	11,12,12	0.70	0	10,18,18	1.23	1 (10%)
19	GLC	W	1	19	11,11,12	0.57	0	15,15,17	0.91	0
19	FRU	W	2	19	11,12,12	0.49	0	10,18,18	1.18	0
19	GLC	X	1	19	10,10,12	0.90	0	14,14,17	1.88	5 (35%)
19	FRU	X	2	19	11,12,12	0.54	0	10,18,18	0.61	0
19	GLC	Y	1	19	11,11,12	1.64	3 (27%)	15,15,17	2.37	6 (40%)
19	FRU	Y	2	19	11,12,12	1.38	1 (9%)	10,18,18	1.45	2 (20%)
19	GLC	Z	1	19	11,11,12	0.41	0	15,15,17	0.98	1 (6%)
19	FRU	Z	2	19	11,12,12	0.66	0	10,18,18	1.11	0
19	GLC	a	1	19	11,11,12	0.76	0	15,15,17	1.32	1 (6%)
19	FRU	a	2	19	11,12,12	0.44	0	10,18,18	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	M	1	19	-	2/2/19/22	0/1/1/1
19	FRU	M	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	O	1	19	-	-	0/1/1/1
19	FRU	O	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	P	1	19	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	5/5/24/24	0/1/1/1
19	GLC	S	1	19	-	2/2/19/22	0/1/1/1
19	FRU	S	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	U	1	19	-	1/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	V	1	19	-	2/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	2/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	X	1	19	-	-	0/1/1/1
19	FRU	X	2	19	1/1/4/4	5/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	1/2/19/22	0/1/1/1
19	FRU	Z	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	a	1	19	-	0/2/19/22	0/1/1/1
19	FRU	a	2	19	1/1/4/4	4/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	2	FRU	O2-C2	4.23	1.48	1.40
19	Y	1	GLC	C1-C2	3.20	1.59	1.52
19	Y	1	GLC	C2-C3	2.89	1.56	1.52
19	Y	1	GLC	O2-C2	2.28	1.48	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	1	GLC	C1-O5-C5	7.93	122.82	112.19
19	U	1	GLC	C1-O5-C5	7.81	122.65	112.19
19	O	1	GLC	C1-C2-C3	6.00	118.38	109.64
19	Y	1	GLC	C6-C5-C4	5.70	127.01	113.02
19	V	1	GLC	C1-O5-C5	4.79	118.61	112.19
19	Q	1	GLC	C1-O5-C5	4.70	118.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	1	GLC	C3-C4-C5	-4.35	102.34	110.23
19	X	1	GLC	C1-C2-C3	-3.88	104.00	109.64
19	a	1	GLC	C1-C2-C3	-3.72	104.23	109.64
19	Q	1	GLC	C2-C3-C4	-3.58	104.57	110.86
19	Q	1	GLC	O3-C3-C2	3.39	116.97	110.05
19	X	1	GLC	C3-C4-C5	3.37	114.93	109.81
19	U	1	GLC	C2-C3-C4	-3.28	105.09	110.86
19	Y	1	GLC	O5-C5-C4	-3.26	102.89	110.83
19	S	2	FRU	O1-C1-C2	-3.20	104.60	111.67
19	P	1	GLC	C2-C3-C4	-3.12	105.37	110.86
19	U	1	GLC	O5-C5-C6	3.02	113.54	107.66
19	Y	1	GLC	C1-O5-C5	-3.00	108.16	112.19
19	V	1	GLC	O5-C5-C6	2.98	113.47	107.66
19	Y	2	FRU	C6-C5-C4	-2.91	108.23	115.10
19	O	1	GLC	O2-C2-C3	-2.83	104.28	110.15
19	Y	1	GLC	O5-C5-C6	2.81	113.12	107.66
19	O	2	FRU	O4-C4-C3	-2.80	103.75	112.16
19	U	1	GLC	C3-C4-C5	-2.74	105.27	110.23
19	Y	1	GLC	O2-C2-C1	2.69	115.37	109.22
19	Y	2	FRU	O2-C2-O5	2.68	114.47	109.33
19	T	2	FRU	C6-C5-C4	-2.62	108.91	115.10
19	P	1	GLC	O3-C3-C4	2.59	116.49	110.38
19	Y	1	GLC	O5-C1-C2	-2.58	104.63	110.79
19	X	1	GLC	C6-C5-C4	-2.57	108.38	113.08
19	S	2	FRU	O2-C2-O5	-2.55	104.43	109.33
19	U	2	FRU	O5-C5-C6	2.51	115.73	108.89
19	Q	2	FRU	O2-C2-O5	2.48	114.09	109.33
19	O	1	GLC	O5-C5-C4	-2.48	105.09	109.55
19	X	1	GLC	C1-O5-C5	-2.43	107.23	112.97
19	V	1	GLC	C6-C5-C4	-2.41	107.10	113.02
19	Z	1	GLC	C1-O5-C5	2.39	115.39	112.19
19	P	1	GLC	C1-C2-C3	-2.38	106.18	109.64
19	P	2	FRU	O1-C1-C2	-2.38	106.42	111.67
19	X	1	GLC	O5-C1-C2	-2.28	105.35	110.79
19	U	2	FRU	O3-C3-C4	-2.24	105.34	113.25
19	M	1	GLC	O5-C5-C4	2.23	116.24	110.83
19	Q	1	GLC	O5-C1-C2	2.19	116.01	110.79
19	V	2	FRU	O4-C4-C5	-2.17	104.84	111.08
19	V	1	GLC	C1-C2-C3	2.15	112.77	109.64
19	P	2	FRU	O2-C2-O5	2.12	113.39	109.33
19	T	1	GLC	C1-O5-C5	2.10	115.01	112.19
19	P	1	GLC	C1-O5-C5	2.01	114.89	112.19

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2
19	Q	2	FRU	C2
19	S	2	FRU	C2
19	T	2	FRU	C2
19	U	2	FRU	C2
19	V	2	FRU	C2
19	W	2	FRU	C2
19	X	2	FRU	C2
19	Y	2	FRU	C2
19	Z	2	FRU	C2
19	a	2	FRU	C2

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	P	2	FRU	C4-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	V	2	FRU	O1-C1-C2-C3
19	V	2	FRU	O1-C1-C2-O2
19	V	2	FRU	O1-C1-C2-O5
19	W	2	FRU	O1-C1-C2-C3
19	W	2	FRU	O1-C1-C2-O2
19	W	2	FRU	O1-C1-C2-O5
19	X	2	FRU	O1-C1-C2-C3
19	X	2	FRU	O1-C1-C2-O2
19	X	2	FRU	O1-C1-C2-O5
19	Y	2	FRU	C4-C5-C6-O6
19	Q	2	FRU	O5-C5-C6-O6
19	V	1	GLC	C4-C5-C6-O6
19	Q	2	FRU	C4-C5-C6-O6
19	X	2	FRU	C4-C5-C6-O6
19	Y	2	FRU	O5-C5-C6-O6
19	W	1	GLC	C4-C5-C6-O6
19	X	2	FRU	O5-C5-C6-O6
19	S	1	GLC	O5-C5-C6-O6
19	V	1	GLC	O5-C5-C6-O6
19	W	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	C4-C5-C6-O6

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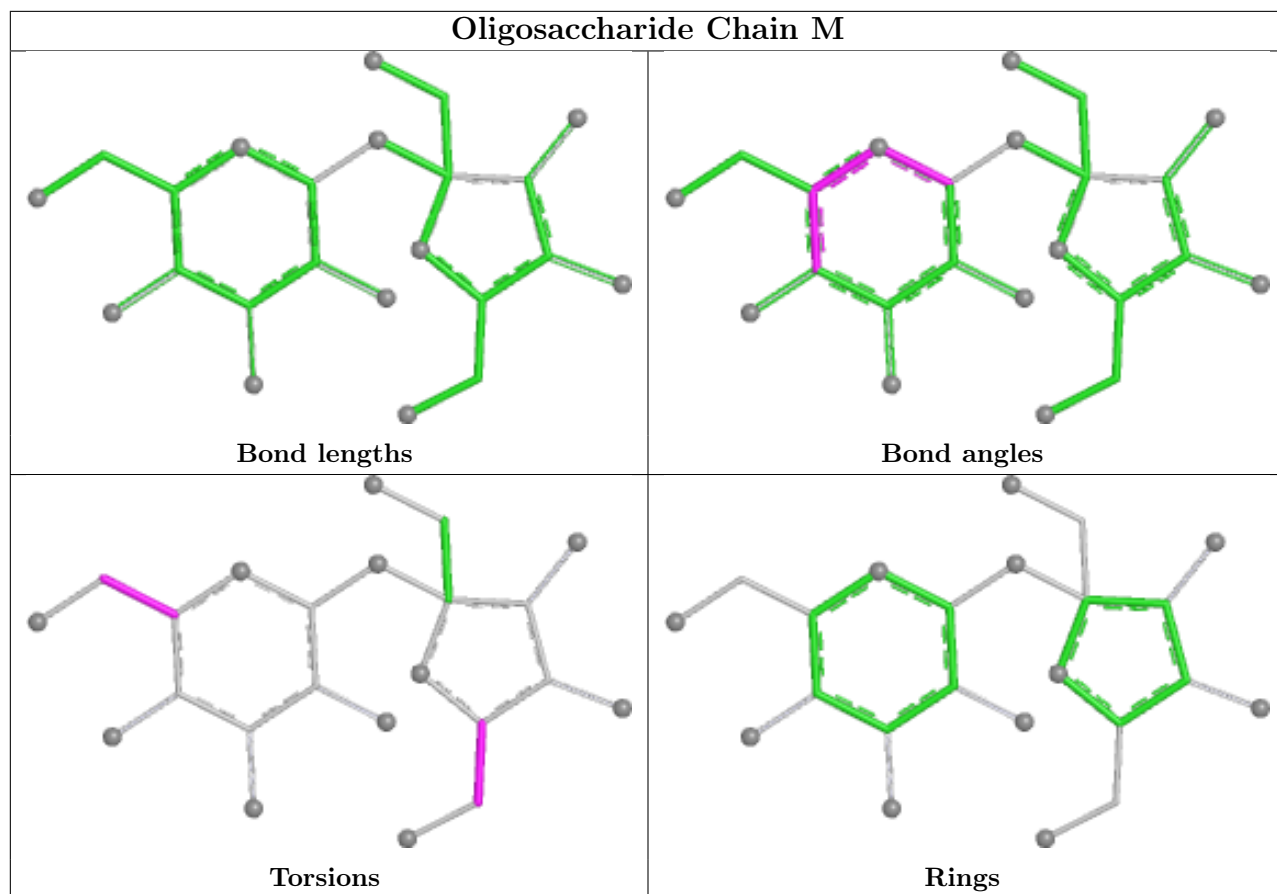
Mol	Chain	Res	Type	Atoms
19	S	1	GLC	C4-C5-C6-O6
19	Q	2	FRU	O1-C1-C2-O5
19	T	1	GLC	C4-C5-C6-O6
19	Q	1	GLC	O5-C5-C6-O6
19	T	1	GLC	O5-C5-C6-O6
19	a	2	FRU	O1-C1-C2-O5
19	U	1	GLC	O5-C5-C6-O6
19	Z	1	GLC	O5-C5-C6-O6
19	T	2	FRU	O1-C1-C2-O5
19	M	1	GLC	O5-C5-C6-O6
19	M	2	FRU	O5-C5-C6-O6
19	a	2	FRU	O1-C1-C2-C3
19	a	2	FRU	O5-C5-C6-O6
19	Y	2	FRU	O1-C1-C2-C3
19	a	2	FRU	O1-C1-C2-O2
19	M	1	GLC	C4-C5-C6-O6
19	S	2	FRU	O1-C1-C2-C3

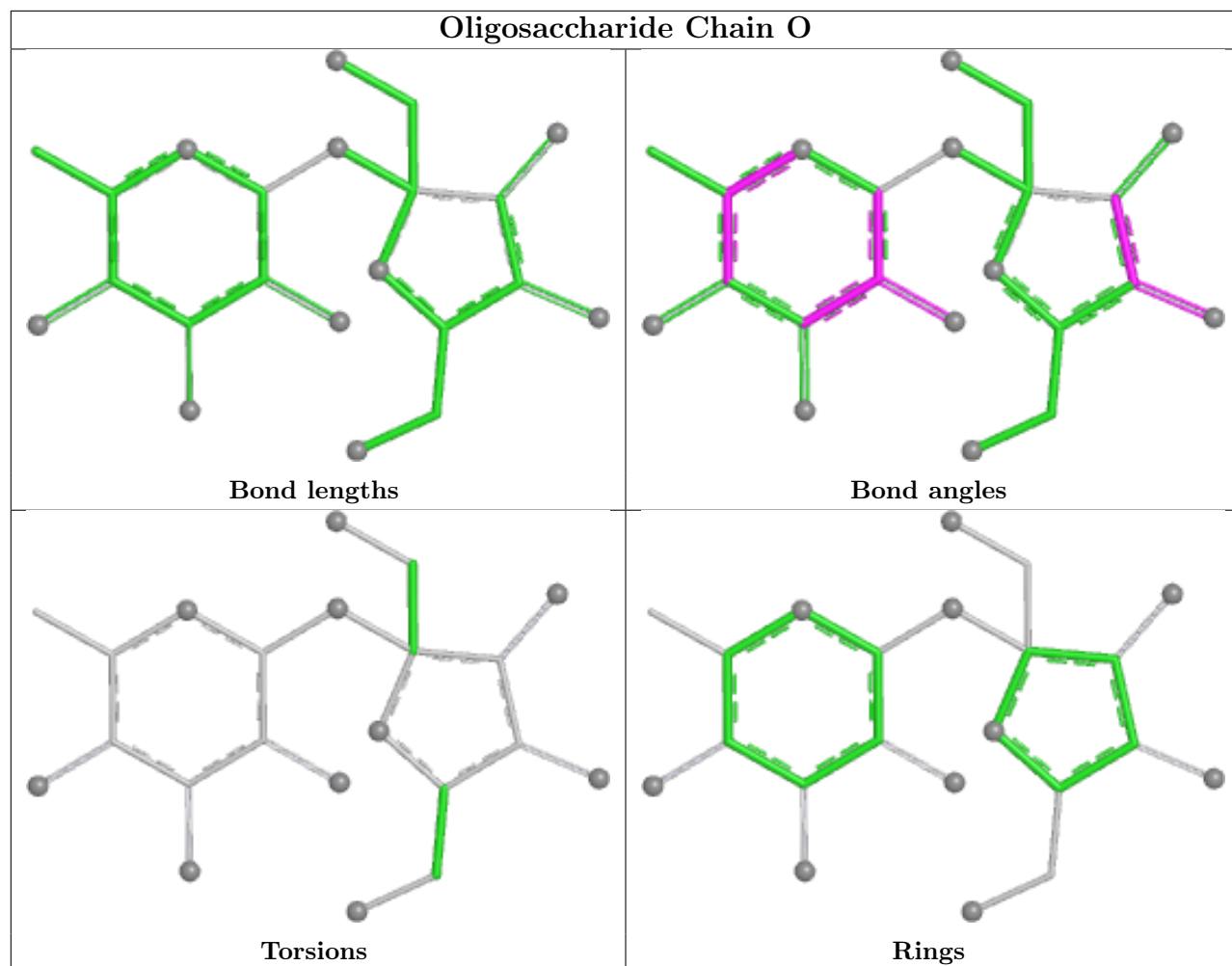
There are no ring outliers.

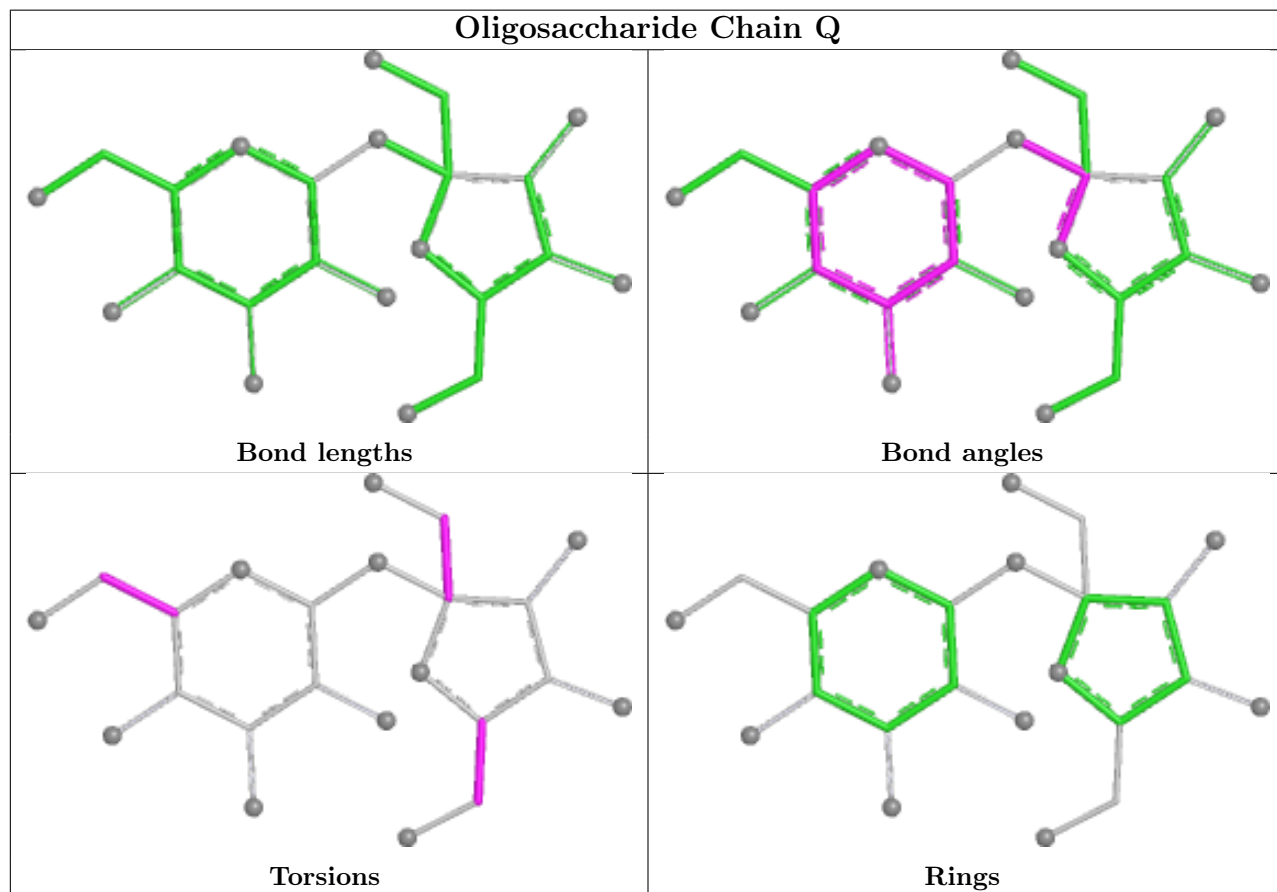
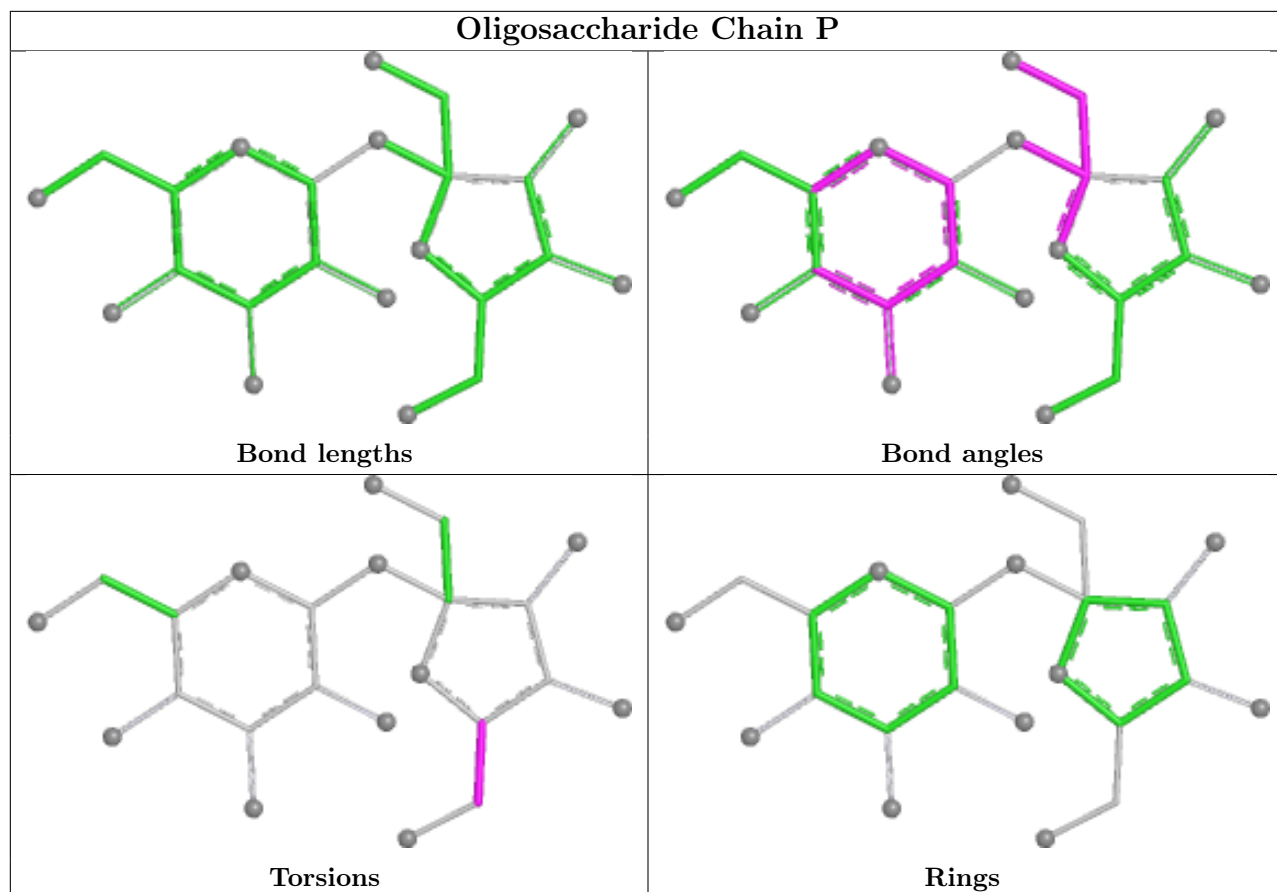
2 monomers are involved in 41 short contacts:

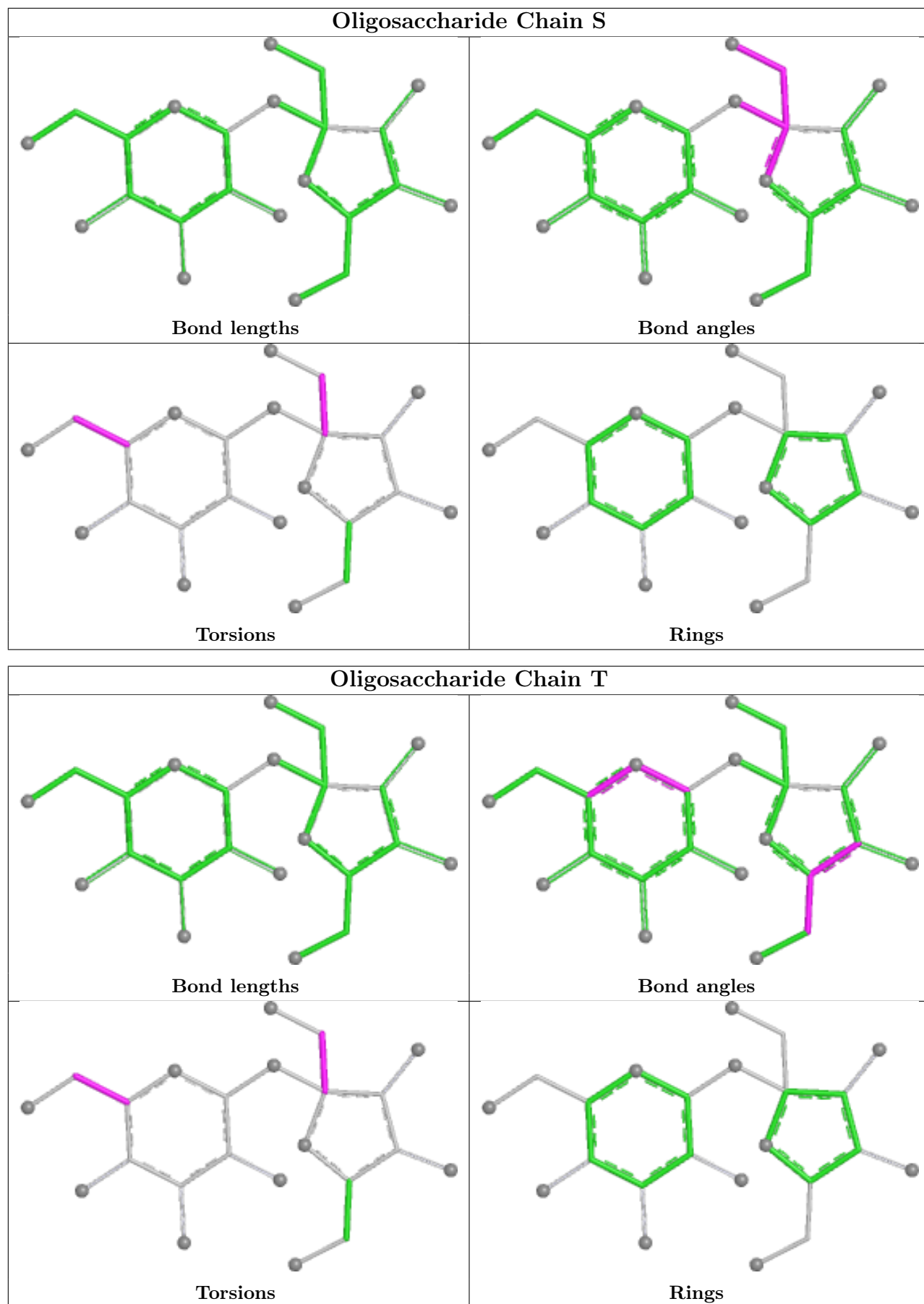
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Y	1	GLC	0	22
19	Y	2	FRU	0	19

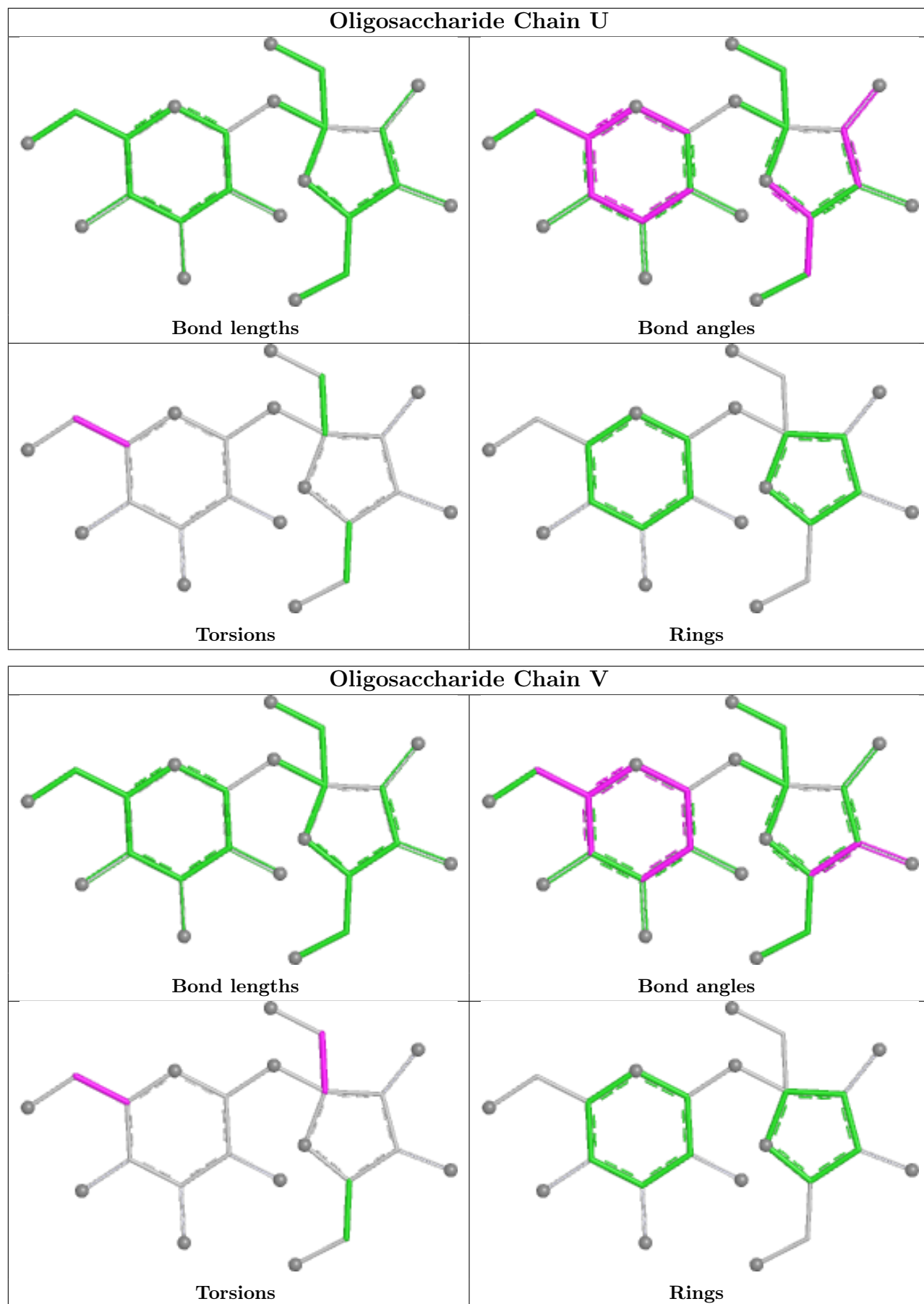
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

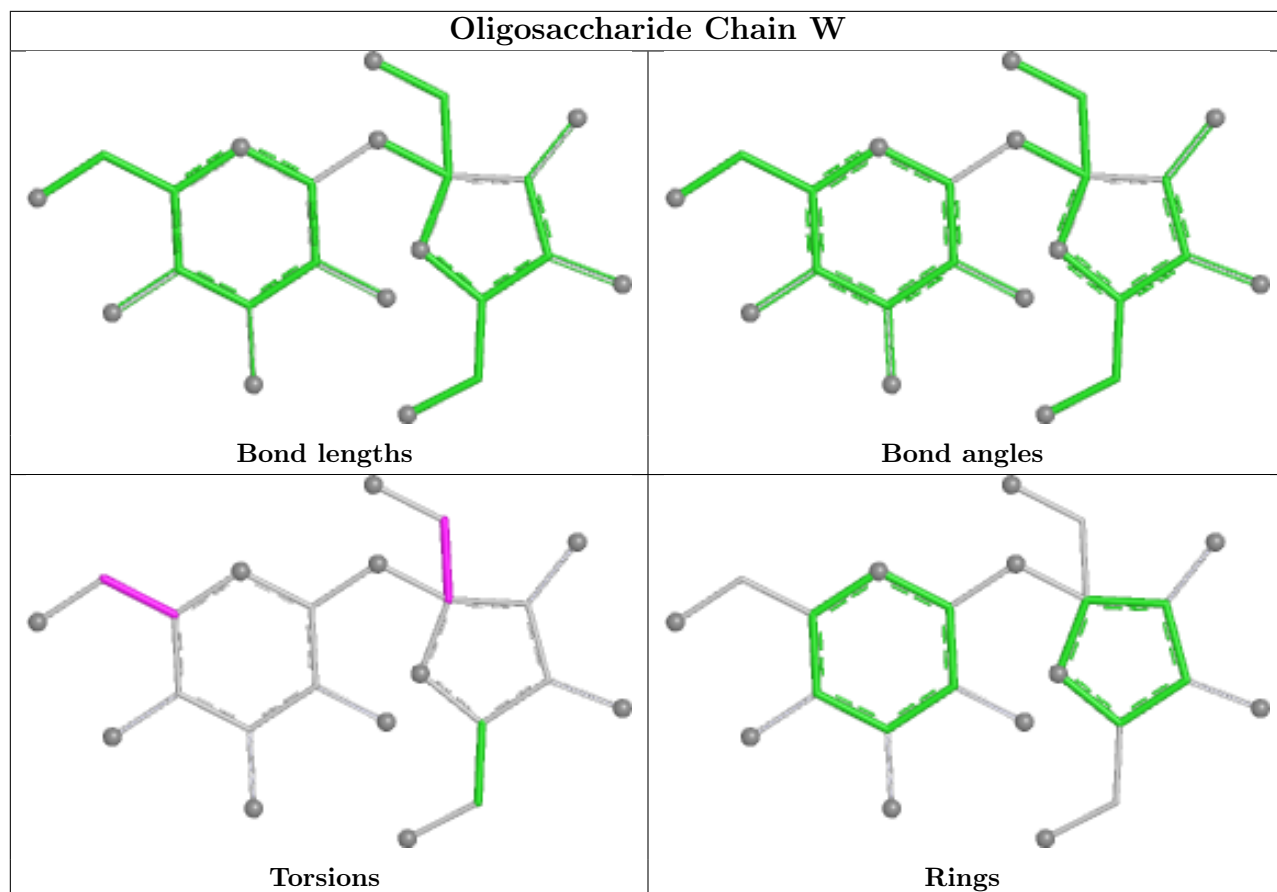


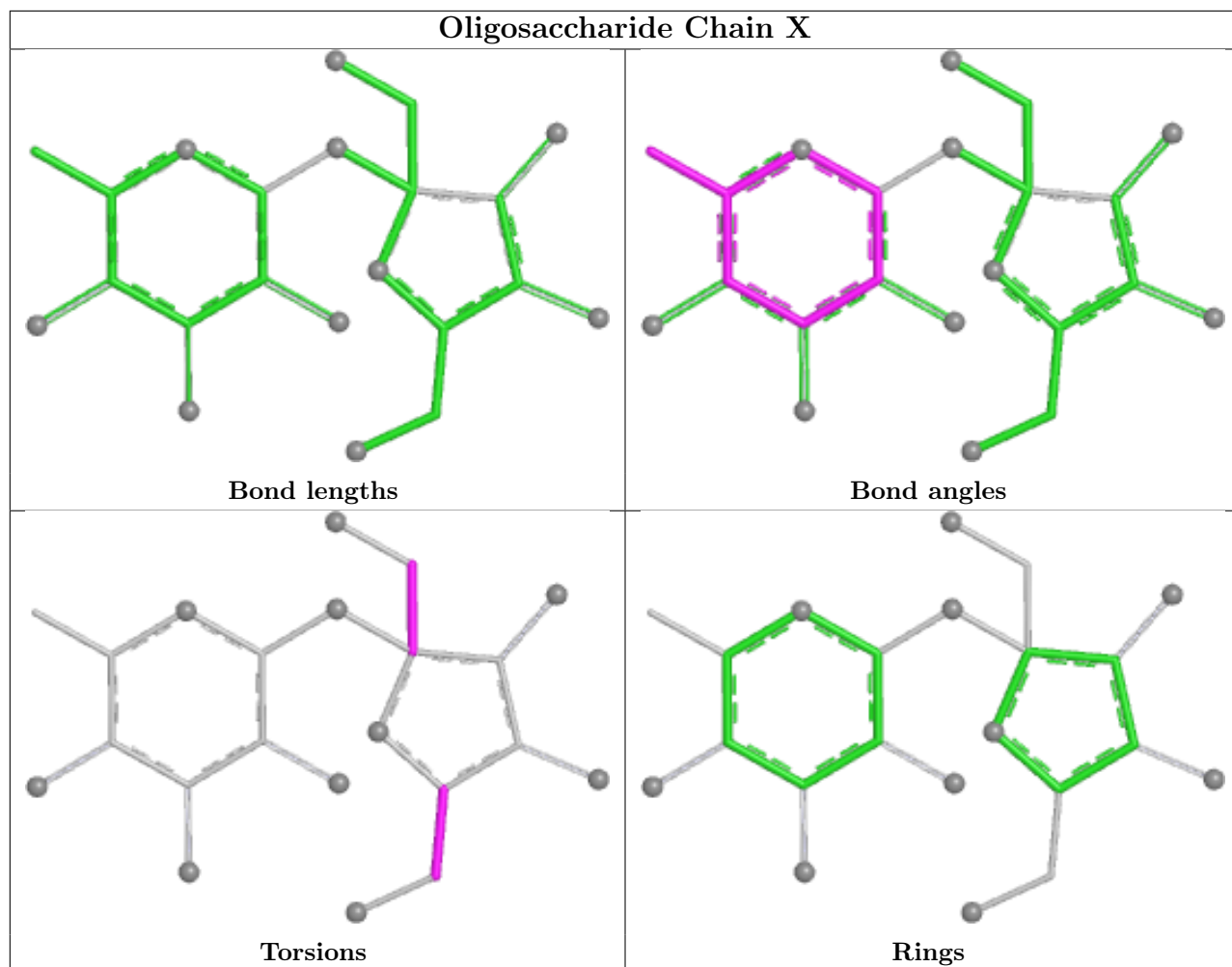


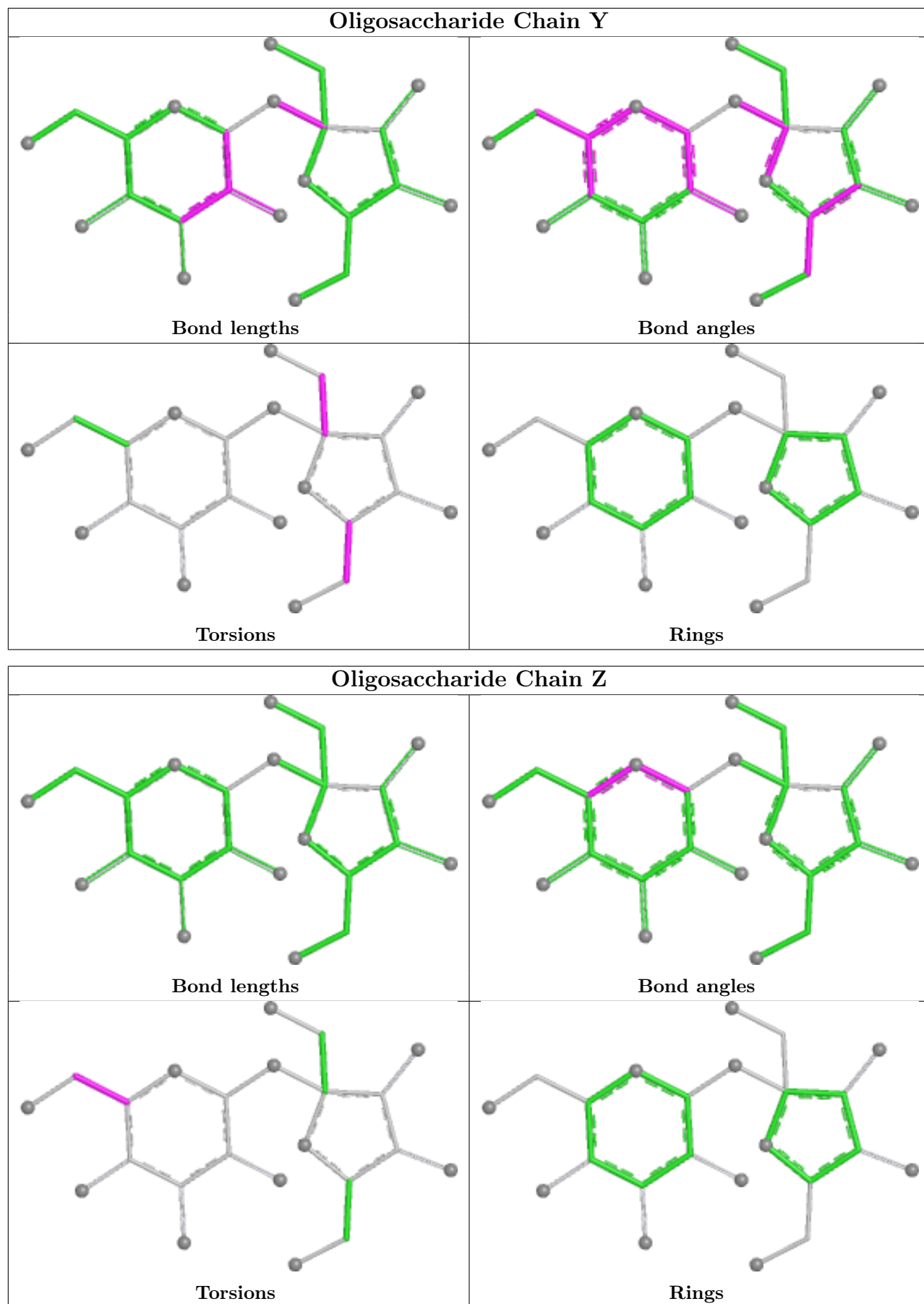


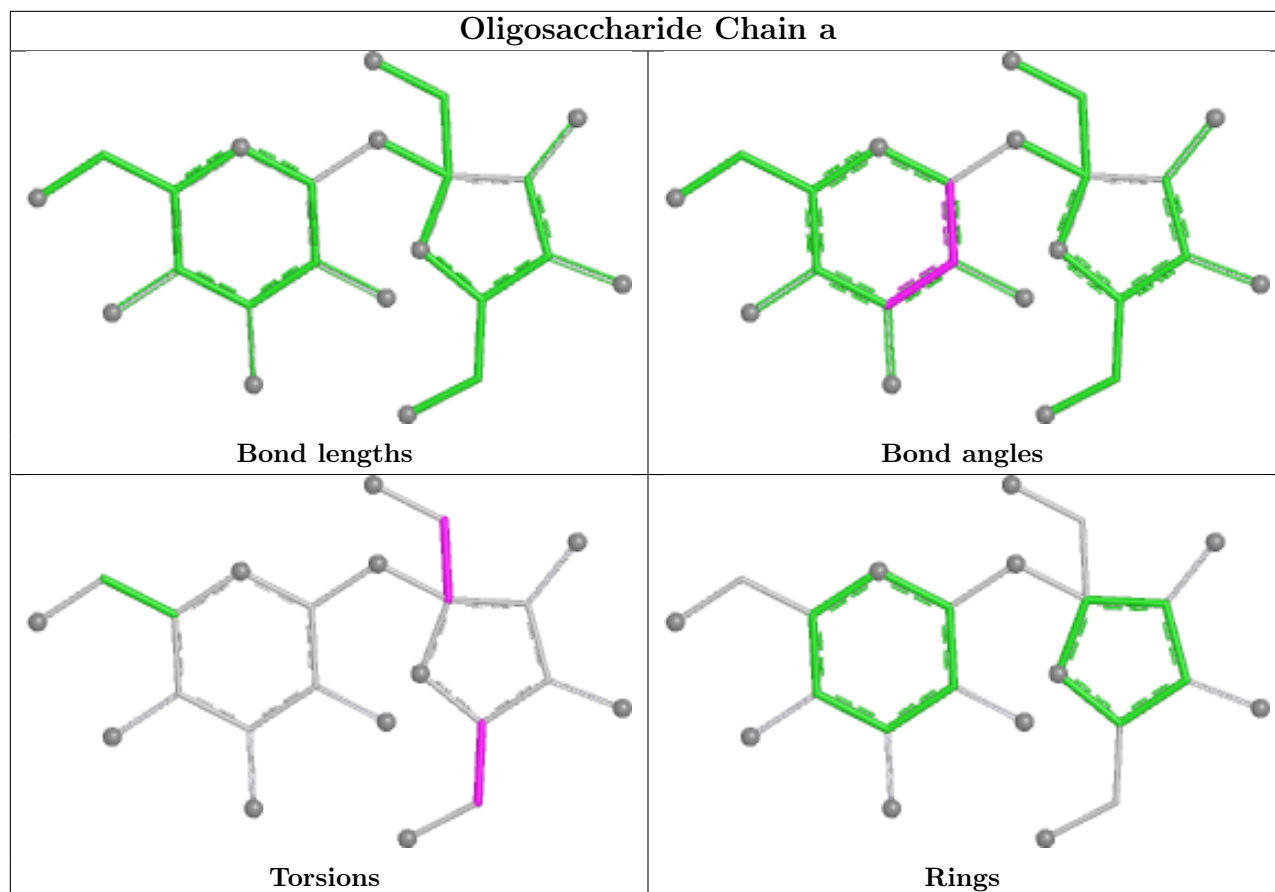












## 4.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 1 is unknown - leaving 243 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	CLA	A	823	-	62,66,73	2.23	14 (22%)	73,104,113	2.61	24 (32%)
20	CLA	H	108	-	62,66,73	2.48	22 (35%)	73,104,113	2.94	30 (41%)
20	CLA	2	307	-	69,73,73	2.16	16 (23%)	82,113,113	2.73	30 (36%)
21	LMU	R	105	-	36,36,36	0.75	1 (2%)	47,47,47	1.40	8 (17%)
20	CLA	B	835	-	49,53,73	2.60	15 (30%)	58,89,113	2.89	22 (37%)
20	CLA	A	851	-	69,73,73	2.23	15 (21%)	82,113,113	2.70	27 (32%)
20	CLA	B	819	-	45,49,73	2.93	22 (48%)	54,84,113	3.45	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	BCR	L	209	-	41,41,41	1.71	3 (7%)	56,56,56	5.79	17 (30%)
23	PQN	B	843	-	34,34,34	1.69	2 (5%)	43,45,45	1.35	6 (13%)
20	CLA	4	302	-	38,44,73	3.02	15 (39%)	52,78,113	3.39	24 (46%)
20	CLA	4	308	-	24,32,73	2.38	10 (41%)	31,54,113	2.88	18 (58%)
20	CLA	1	206	-	65,69,73	2.21	14 (21%)	77,108,113	2.67	30 (38%)
20	CLA	4	307	-	24,32,73	2.38	9 (37%)	31,54,113	2.82	17 (54%)
21	LMU	R	109	-	36,36,36	0.49	0	47,47,47	0.83	1 (2%)
20	CLA	A	802	-	24,32,73	2.40	8 (33%)	31,54,113	3.00	18 (58%)
21	LMU	A	852	-	36,36,36	0.56	1 (2%)	47,47,47	0.86	1 (2%)
21	LMU	G	102	-	36,36,36	0.61	0	47,47,47	1.61	8 (17%)
22	BCR	B	845	-	41,41,41	1.56	3 (7%)	56,56,56	4.89	19 (33%)
22	BCR	F	203	-	41,41,41	1.72	3 (7%)	56,56,56	5.62	19 (33%)
20	CLA	3	317	-	38,44,73	2.84	13 (34%)	52,78,113	3.29	26 (50%)
20	CLA	3	301	-	38,44,73	2.82	13 (34%)	52,78,113	3.38	24 (46%)
20	CLA	1	203	-	51,55,73	2.62	18 (35%)	60,91,113	3.39	29 (48%)
25	LMG	B	848	-	49,49,55	0.99	2 (4%)	57,57,63	1.09	3 (5%)
20	CLA	A	809	-	56,60,73	2.36	14 (25%)	65,97,113	2.86	30 (46%)
20	CLA	F	201	-	54,58,73	2.49	20 (37%)	64,95,113	3.14	26 (40%)
20	CLA	1	212	-	24,32,73	2.36	8 (33%)	31,54,113	2.83	18 (58%)
20	CLA	2	311	-	54,58,73	2.46	15 (27%)	64,95,113	2.94	28 (43%)
20	CLA	B	850	-	69,73,73	2.14	16 (23%)	82,113,113	2.70	34 (41%)
20	CLA	B	833	-	54,58,73	2.44	17 (31%)	64,95,113	3.01	26 (40%)
22	BCR	B	846	-	41,41,41	1.69	4 (9%)	56,56,56	5.71	23 (41%)
20	CLA	A	814	-	24,32,73	2.37	10 (41%)	31,54,113	2.99	19 (61%)
21	LMU	H	106	-	36,36,36	0.61	1 (2%)	47,47,47	1.59	11 (23%)
22	BCR	F	204	-	41,41,41	1.85	5 (12%)	56,56,56	5.90	23 (41%)
20	CLA	F	205	-	38,44,73	2.79	15 (39%)	52,78,113	3.13	25 (48%)
20	CLA	L	204	-	59,63,73	2.35	14 (23%)	70,101,113	2.74	29 (41%)
22	BCR	B	844	-	41,41,41	1.65	5 (12%)	56,56,56	5.31	24 (42%)
20	CLA	B	836	-	55,59,73	2.45	20 (36%)	64,96,113	3.12	24 (37%)
21	LMU	2	319	-	36,36,36	0.82	1 (2%)	47,47,47	1.58	11 (23%)
20	CLA	2	306	-	24,32,73	2.26	8 (33%)	31,54,113	2.78	17 (54%)
21	LMU	K	105	-	36,36,36	0.67	1 (2%)	47,47,47	1.56	8 (17%)
20	CLA	3	312	-	24,32,73	2.40	8 (33%)	31,54,113	2.82	18 (58%)
21	LMU	3	319	-	36,36,36	0.44	0	47,47,47	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LMU	K	107	-	36,36,36	0.53	0	47,47,47	1.32	7 (14%)
20	CLA	A	828	-	69,73,73	2.14	14 (20%)	82,113,113	2.56	27 (32%)
20	CLA	4	309	-	24,32,73	2.37	8 (33%)	31,54,113	2.89	19 (61%)
20	CLA	A	824	-	63,67,73	2.25	16 (25%)	74,105,113	2.73	27 (36%)
20	CLA	B	838	-	69,73,73	2.10	14 (20%)	82,113,113	2.55	26 (31%)
20	CLA	K	102	-	54,58,73	2.45	16 (29%)	64,95,113	2.95	24 (37%)
20	CLA	A	850	-	69,73,73	2.18	16 (23%)	82,113,113	2.61	26 (31%)
22	BCR	B	847	-	41,41,41	1.67	3 (7%)	56,56,56	5.60	18 (32%)
20	CLA	B	839	-	51,55,73	2.69	22 (43%)	60,91,113	3.56	28 (46%)
20	CLA	2	301	-	24,32,73	2.32	8 (33%)	31,54,113	2.86	19 (61%)
24	SF4	C	102	7	0,12,12	-	-	-	-	-
20	CLA	A	818	-	64,68,73	2.37	21 (32%)	76,107,113	2.95	32 (42%)
22	BCR	A	844	-	41,41,41	1.71	3 (7%)	56,56,56	5.71	21 (37%)
22	BCR	G	104	-	41,41,41	1.63	3 (7%)	56,56,56	5.88	19 (33%)
20	CLA	B	812	-	58,62,73	2.67	23 (39%)	71,100,113	3.18	29 (40%)
20	CLA	A	836	-	51,55,73	2.51	14 (27%)	60,91,113	2.75	22 (36%)
20	CLA	B	809	-	69,73,73	2.18	15 (21%)	82,113,113	2.88	30 (36%)
20	CLA	B	803	-	69,73,73	2.17	14 (20%)	82,113,113	2.63	28 (34%)
20	CLA	L	207	-	51,55,73	2.51	13 (25%)	60,91,113	3.13	26 (43%)
21	LMU	D	201	-	36,36,36	0.47	0	47,47,47	1.45	6 (12%)
21	LMU	A	853	-	36,36,36	0.50	0	47,47,47	1.43	7 (14%)
20	CLA	A	830	-	69,73,73	2.17	15 (21%)	82,113,113	2.56	21 (25%)
20	CLA	3	316	-	24,32,73	2.39	8 (33%)	31,54,113	2.96	18 (58%)
23	PQN	A	842	-	34,34,34	1.73	2 (5%)	43,45,45	1.22	4 (9%)
21	LMU	G	103	-	36,36,36	0.50	0	47,47,47	0.95	2 (4%)
20	CLA	B	817	-	50,54,73	2.45	13 (26%)	59,90,113	2.92	27 (45%)
20	CLA	A	840	-	59,63,73	2.29	14 (23%)	70,101,113	2.87	24 (34%)
20	CLA	L	208	-	54,58,73	2.49	17 (31%)	64,95,113	3.11	24 (37%)
21	LMU	A	854	-	36,36,36	0.52	0	47,47,47	1.28	7 (14%)
20	CLA	A	839	-	63,67,73	2.45	20 (31%)	74,105,113	2.96	32 (43%)
20	CLA	J	103	-	65,69,73	2.25	20 (30%)	77,108,113	2.55	22 (28%)
20	CLA	K	104	-	60,64,73	2.38	19 (31%)	71,102,113	2.97	26 (36%)
21	LMU	1	217	-	36,36,36	0.57	0	47,47,47	1.01	1 (2%)
20	CLA	4	312	-	24,32,73	2.43	8 (33%)	31,54,113	2.87	20 (64%)
20	CLA	A	827	-	59,63,73	2.31	15 (25%)	70,101,113	2.79	26 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	812	-	58,62,73	2.32	15 (25%)	68,99,113	2.63	23 (33%)
20	CLA	B	818	-	57,61,73	2.39	14 (24%)	67,98,113	2.69	22 (32%)
20	CLA	2	312	-	65,69,73	2.27	19 (29%)	77,108,113	2.89	30 (38%)
20	CLA	A	803	-	50,54,73	2.62	20 (40%)	59,90,113	3.33	24 (40%)
21	LMU	2	318	-	36,36,36	0.57	0	47,47,47	0.69	0
21	LMU	H	103	-	36,36,36	0.85	1 (2%)	47,47,47	2.15	13 (27%)
21	LMU	H	104	-	36,36,36	0.60	0	47,47,47	1.65	7 (14%)
20	CLA	4	317	-	56,60,73	2.44	17 (30%)	65,97,113	3.16	30 (46%)
20	CLA	2	309	-	24,32,73	2.34	9 (37%)	31,54,113	2.78	19 (61%)
20	CLA	A	807	-	50,54,73	2.52	16 (32%)	59,90,113	2.91	24 (40%)
20	CLA	B	827	-	69,73,73	2.14	16 (23%)	82,113,113	2.54	24 (29%)
20	CLA	B	834	-	49,53,73	2.60	15 (30%)	58,89,113	2.94	21 (36%)
20	CLA	L	202	-	59,63,73	2.35	16 (27%)	70,101,113	2.82	25 (35%)
20	CLA	B	830	-	69,73,73	2.16	15 (21%)	82,113,113	2.73	29 (35%)
20	CLA	A	835	-	69,73,73	2.22	16 (23%)	82,113,113	2.73	29 (35%)
20	CLA	A	819	-	62,66,73	2.30	16 (25%)	73,104,113	2.74	25 (34%)
21	LMU	4	320	-	36,36,36	0.78	1 (2%)	47,47,47	1.29	6 (12%)
20	CLA	A	810	-	49,53,73	2.62	14 (28%)	58,89,113	3.20	25 (43%)
20	CLA	B	807	-	49,53,73	2.61	16 (32%)	58,89,113	3.05	20 (34%)
20	CLA	A	817	-	56,60,73	2.40	15 (26%)	65,97,113	2.93	24 (36%)
20	CLA	B	810	-	64,68,73	2.29	16 (25%)	76,107,113	2.76	26 (34%)
21	LMU	2	321	-	36,36,36	0.82	1 (2%)	47,47,47	1.20	4 (8%)
24	SF4	C	103	-	0,12,12	-	-	-	-	-
21	LMU	2	313	-	36,36,36	0.52	0	47,47,47	1.61	6 (12%)
20	CLA	A	813	-	54,58,73	2.39	15 (27%)	64,95,113	2.86	27 (42%)
20	CLA	K	103	-	54,58,73	2.56	19 (35%)	64,95,113	2.97	26 (40%)
21	LMU	K	106	-	36,36,36	0.37	0	47,47,47	1.07	3 (6%)
20	CLA	B	828	-	69,73,73	2.23	15 (21%)	82,113,113	2.69	27 (32%)
22	BCR	I	103	-	41,41,41	1.88	5 (12%)	56,56,56	6.31	27 (48%)
20	CLA	B	820	-	65,69,73	2.16	15 (23%)	77,108,113	2.73	25 (32%)
20	CLA	A	833	5	49,53,73	2.61	15 (30%)	58,89,113	3.16	26 (44%)
20	CLA	4	306	-	56,60,73	2.63	20 (35%)	65,97,113	3.20	34 (52%)
21	LMU	4	319	-	35,35,36	0.80	2 (5%)	46,46,47	1.83	11 (23%)
21	LMU	H	105	-	36,36,36	0.73	1 (2%)	47,47,47	1.67	9 (19%)
20	CLA	J	101	-	52,56,73	2.47	16 (30%)	61,92,113	2.92	21 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	4	305	-	54,58,73	2.50	18 (33%)	64,95,113	2.95	26 (40%)
20	CLA	B	822	-	50,54,73	2.48	15 (30%)	59,90,113	3.10	19 (32%)
20	CLA	4	311	-	24,32,73	2.33	9 (37%)	31,54,113	2.93	18 (58%)
20	CLA	L	203	-	69,73,73	2.10	13 (18%)	82,113,113	2.69	28 (34%)
21	LMU	4	316	-	36,36,36	0.73	1 (2%)	47,47,47	1.09	3 (6%)
22	BCR	A	843	-	41,41,41	1.66	3 (7%)	56,56,56	5.62	21 (37%)
20	CLA	B	824	-	69,73,73	2.39	21 (30%)	82,113,113	2.71	26 (31%)
20	CLA	3	304	-	24,32,73	2.34	9 (37%)	31,54,113	3.06	19 (61%)
20	CLA	B	814	-	69,73,73	2.18	15 (21%)	82,113,113	2.48	26 (31%)
20	CLA	A	837	-	55,59,73	2.41	15 (27%)	64,96,113	3.12	27 (42%)
21	LMU	R	101	-	36,36,36	0.85	2 (5%)	47,47,47	2.10	11 (23%)
20	CLA	4	314	4	24,32,73	2.36	8 (33%)	31,54,113	2.71	18 (58%)
20	CLA	K	101	-	50,54,73	2.58	17 (34%)	59,90,113	2.96	22 (37%)
20	CLA	B	840	-	69,73,73	2.16	14 (20%)	82,113,113	2.58	26 (31%)
20	CLA	3	306	-	24,32,73	2.34	8 (33%)	31,54,113	2.85	18 (58%)
21	LMU	2	320	-	36,36,36	0.46	0	47,47,47	1.28	3 (6%)
20	CLA	A	829	-	54,58,73	2.46	13 (24%)	64,95,113	2.91	23 (35%)
20	CLA	B	825	-	58,62,73	2.38	16 (27%)	68,99,113	2.78	25 (36%)
20	CLA	A	820	-	55,59,73	2.44	14 (25%)	64,96,113	2.95	23 (35%)
20	CLA	G	105	-	55,59,73	2.47	18 (32%)	64,96,113	2.96	24 (37%)
20	CLA	L	201	-	64,68,73	2.27	15 (23%)	76,107,113	2.59	26 (34%)
22	BCR	J	102	-	41,41,41	1.64	3 (7%)	56,56,56	5.69	19 (33%)
20	CLA	3	310	-	69,73,73	2.23	20 (28%)	82,113,113	2.77	31 (37%)
20	CLA	B	813	-	59,63,73	2.27	15 (25%)	70,101,113	2.75	26 (37%)
20	CLA	1	207	-	55,59,73	2.49	17 (30%)	64,96,113	3.36	26 (40%)
20	CLA	B	829	-	69,73,73	2.11	14 (20%)	82,113,113	2.72	29 (35%)
20	CLA	H	110	16	54,58,73	2.45	13 (24%)	64,95,113	2.83	26 (40%)
20	CLA	4	304	-	59,63,73	2.31	14 (23%)	70,101,113	2.79	25 (35%)
20	CLA	3	315	-	24,32,73	2.42	9 (37%)	31,54,113	3.01	19 (61%)
21	LMU	3	318	-	36,36,36	0.49	1 (2%)	47,47,47	0.73	1 (2%)
20	CLA	2	303	-	62,66,73	2.39	20 (32%)	73,104,113	3.09	31 (42%)
20	CLA	2	315	-	24,32,73	2.36	8 (33%)	31,54,113	2.76	18 (58%)
20	CLA	A	822	-	54,58,73	2.44	16 (29%)	64,95,113	2.79	22 (34%)
20	CLA	2	308	-	24,32,73	2.37	10 (41%)	31,54,113	3.06	18 (58%)
20	CLA	3	303	-	38,44,73	2.89	11 (28%)	52,78,113	3.18	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	4	303	-	69,73,73	2.23	18 (26%)	82,113,113	2.96	30 (36%)
20	CLA	A	811	20	69,73,73	2.16	12 (17%)	82,113,113	2.77	29 (35%)
21	LMU	A	846	-	36,36,36	0.70	0	47,47,47	1.29	7 (14%)
21	LMU	L	205	-	36,36,36	0.64	1 (2%)	47,47,47	1.96	13 (27%)
21	LMU	C	101	-	36,36,36	0.70	1 (2%)	47,47,47	1.26	4 (8%)
20	CLA	A	834	-	50,54,73	2.54	15 (30%)	59,90,113	2.98	25 (42%)
20	CLA	A	831	-	69,73,73	2.29	23 (33%)	82,113,113	3.14	30 (36%)
20	CLA	A	832	-	54,58,73	2.43	15 (27%)	64,95,113	2.82	26 (40%)
20	CLA	1	205	-	38,44,73	2.94	13 (34%)	52,78,113	3.15	23 (44%)
20	CLA	A	808	5	64,68,73	2.28	16 (25%)	76,107,113	2.78	30 (39%)
20	CLA	B	811	6	24,32,73	2.37	9 (37%)	31,54,113	2.67	16 (51%)
20	CLA	B	815	-	64,68,73	2.24	13 (20%)	76,107,113	2.62	25 (32%)
20	CLA	A	821	5	46,50,73	2.51	12 (26%)	53,85,113	3.30	24 (45%)
20	CLA	A	805	-	58,62,73	2.29	13 (22%)	68,99,113	2.84	25 (36%)
20	CLA	4	301	-	59,63,73	2.35	16 (27%)	70,101,113	2.82	25 (35%)
20	CLA	B	816	-	64,68,73	2.20	12 (18%)	76,107,113	2.57	27 (35%)
21	LMU	L	206	-	36,36,36	0.51	0	47,47,47	1.02	3 (6%)
21	LMU	B	849	-	26,26,36	0.78	1 (3%)	37,37,47	1.30	6 (16%)
20	CLA	1	211	-	55,59,73	2.57	20 (36%)	64,96,113	3.43	29 (45%)
20	CLA	2	316	-	69,73,73	2.30	22 (31%)	82,113,113	2.76	25 (30%)
20	CLA	B	837	-	64,68,73	2.20	13 (20%)	76,107,113	2.71	22 (28%)
20	CLA	B	842	-	38,44,73	2.87	13 (34%)	52,78,113	3.35	28 (53%)
21	LMU	F	202	-	35,35,36	0.58	0	46,46,47	1.38	5 (10%)
20	CLA	3	302	-	24,32,73	2.37	8 (33%)	31,54,113	2.80	18 (58%)
20	CLA	H	101	-	59,63,73	2.39	15 (25%)	70,101,113	2.86	27 (38%)
20	CLA	F	207	-	57,61,73	2.68	23 (40%)	67,98,113	3.04	30 (44%)
21	LMU	R	103	-	36,36,36	0.71	1 (2%)	47,47,47	1.48	6 (12%)
20	CLA	3	313	-	54,58,73	2.46	12 (22%)	64,95,113	2.72	24 (37%)
20	CLA	B	802	-	58,62,73	2.33	14 (24%)	68,99,113	2.92	27 (39%)
20	CLA	3	311	-	69,73,73	2.18	15 (21%)	82,113,113	2.65	25 (30%)
21	LMU	E	101	-	36,36,36	0.62	0	47,47,47	1.91	13 (27%)
22	BCR	B	801	-	41,41,41	2.05	4 (9%)	56,56,56	6.23	22 (39%)
20	CLA	A	849	-	69,73,73	2.11	17 (24%)	82,113,113	2.75	27 (32%)
21	LMU	1	218	-	36,36,36	0.70	0	47,47,47	1.69	9 (19%)
21	LMU	R	106	-	36,36,36	0.52	0	47,47,47	1.23	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	BCR	2	317	-	41,41,41	1.68	3 (7%)	56,56,56	5.84	18 (32%)
20	CLA	3	309	-	24,32,73	2.33	9 (37%)	31,54,113	3.11	18 (58%)
20	CLA	B	831	-	54,58,73	2.50	15 (27%)	64,95,113	2.76	26 (40%)
20	CLA	B	832	-	63,67,73	2.31	16 (25%)	74,105,113	2.89	26 (35%)
20	CLA	1	215	-	55,59,73	2.49	22 (40%)	64,96,113	3.07	26 (40%)
20	CLA	3	307	-	46,50,73	2.67	15 (32%)	53,85,113	3.35	26 (49%)
20	CLA	A	841	-	24,32,73	2.40	8 (33%)	31,54,113	2.93	16 (51%)
20	CLA	A	816	-	58,62,73	2.42	19 (32%)	68,99,113	2.93	25 (36%)
21	LMU	1	216	-	36,36,36	0.46	0	47,47,47	1.40	6 (12%)
20	CLA	A	838	-	69,73,73	2.18	15 (21%)	82,113,113	2.62	32 (39%)
21	LMU	A	847	-	36,36,36	0.68	1 (2%)	47,47,47	1.43	7 (14%)
20	CLA	1	213	-	55,59,73	2.71	25 (45%)	64,96,113	3.19	28 (43%)
21	LMU	A	848	-	36,36,36	0.49	0	47,47,47	0.86	3 (6%)
20	CLA	2	304	-	24,32,73	2.35	10 (41%)	31,54,113	2.92	19 (61%)
20	CLA	1	208	-	24,32,73	2.31	8 (33%)	31,54,113	2.75	17 (54%)
20	CLA	F	206	-	45,49,73	2.68	15 (33%)	54,84,113	3.09	23 (42%)
20	CLA	B	808	-	65,69,73	2.23	20 (30%)	77,108,113	2.70	28 (36%)
21	LMU	G	101	-	36,36,36	1.09	3 (8%)	47,47,47	2.05	11 (23%)
20	CLA	A	804	20	59,63,73	2.37	14 (23%)	70,101,113	2.93	28 (40%)
21	LMU	R	102	-	36,36,36	0.57	0	47,47,47	1.51	9 (19%)
20	CLA	3	308	-	24,32,73	2.33	8 (33%)	31,54,113	2.97	18 (58%)
20	CLA	B	821	-	54,58,73	2.40	14 (25%)	64,95,113	2.94	27 (42%)
20	CLA	2	314	-	54,58,73	2.51	19 (35%)	64,95,113	3.27	25 (39%)
20	CLA	1	209	-	24,32,73	2.40	8 (33%)	31,54,113	2.83	20 (64%)
20	CLA	A	801	-	50,54,73	2.70	16 (32%)	61,90,113	3.63	31 (50%)
20	CLA	3	314	-	69,73,73	2.25	23 (33%)	82,113,113	2.85	27 (32%)
21	LMU	4	321	-	36,36,36	0.46	0	47,47,47	1.46	7 (14%)
20	CLA	H	109	-	59,63,73	2.35	14 (23%)	70,101,113	2.68	24 (34%)
20	CLA	R	107	-	61,65,73	2.31	13 (21%)	72,103,113	2.81	27 (37%)
21	LMU	B	805	-	36,36,36	0.68	1 (2%)	47,47,47	1.69	12 (25%)
21	LMU	A	855	-	36,36,36	0.66	1 (2%)	47,47,47	1.42	7 (14%)
20	CLA	4	313	-	38,44,73	2.80	13 (34%)	52,78,113	3.39	26 (50%)
20	CLA	1	201	-	50,54,73	2.52	18 (36%)	59,90,113	3.45	29 (49%)
20	CLA	1	204	-	50,54,73	2.69	20 (40%)	59,90,113	3.39	27 (45%)
21	LMU	L	210	-	36,36,36	0.71	1 (2%)	47,47,47	1.30	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	2	310	2	54,58,73	2.59	17 (31%)	64,95,113	3.03	26 (40%)
21	LMU	B	804	-	36,36,36	0.69	0	47,47,47	1.77	12 (25%)
20	CLA	B	841	-	69,73,73	2.08	15 (21%)	82,113,113	2.64	26 (31%)
20	CLA	A	806	-	60,64,73	2.28	14 (23%)	71,102,113	2.90	28 (39%)
20	CLA	B	823	-	59,63,73	2.38	16 (27%)	70,101,113	2.68	24 (34%)
21	LMU	R	104	-	36,36,36	0.57	1 (2%)	47,47,47	1.32	6 (12%)
20	CLA	3	305	-	24,32,73	2.29	8 (33%)	31,54,113	2.80	15 (48%)
20	CLA	A	826	-	69,73,73	2.15	16 (23%)	82,113,113	2.64	27 (32%)
20	CLA	2	305	-	54,58,73	2.44	13 (24%)	64,95,113	2.69	26 (40%)
20	CLA	B	806	-	69,73,73	2.16	15 (21%)	82,113,113	2.66	27 (32%)
22	BCR	A	845	-	41,41,41	1.73	4 (9%)	56,56,56	5.85	25 (44%)
20	CLA	H	102	-	59,63,73	2.31	13 (22%)	70,101,113	2.85	26 (37%)
20	CLA	I	102	-	64,68,73	2.24	14 (21%)	76,107,113	2.66	22 (28%)
20	CLA	B	826	-	62,66,73	2.28	16 (25%)	73,104,113	2.70	23 (31%)
20	CLA	R	108	-	69,73,73	2.17	13 (18%)	82,113,113	2.56	28 (34%)
20	CLA	4	310	-	54,58,73	2.48	19 (35%)	64,95,113	3.09	24 (37%)
20	CLA	1	214	-	24,32,73	2.36	8 (33%)	31,54,113	3.02	19 (61%)
20	CLA	A	815	-	54,58,73	2.48	13 (24%)	64,95,113	2.85	27 (42%)
20	CLA	4	318	-	51,55,73	2.54	19 (37%)	60,91,113	3.18	29 (48%)
22	BCR	I	101	-	39,40,41	1.38	3 (7%)	51,53,56	4.37	19 (37%)
24	SF4	A	856	5,6	0,12,12	-	-	-	-	-
20	CLA	4	315	-	50,54,73	2.51	18 (36%)	59,90,113	2.94	24 (40%)
20	CLA	2	302	-	55,59,73	2.58	20 (36%)	64,96,113	3.08	26 (40%)
20	CLA	1	202	-	45,49,73	2.66	15 (33%)	54,84,113	2.99	20 (37%)
20	CLA	1	210	1	38,44,73	2.83	12 (31%)	52,78,113	3.21	24 (46%)
20	CLA	A	825	-	69,73,73	2.14	16 (23%)	82,113,113	2.40	22 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	823	-	2/2/13/20	13/31/107/115	-
20	CLA	H	108	-	2/2/13/20	17/31/107/115	-
20	CLA	2	307	-	2/2/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	R	105	-	-	14/21/61/61	0/2/2/2
20	CLA	B	835	-	1/1/11/20	7/15/91/115	-
20	CLA	A	851	-	2/2/15/20	22/39/115/115	-
20	CLA	B	819	-	1/1/10/20	2/10/86/115	-
22	BCR	L	209	-	-	10/29/63/63	0/2/2/2
23	PQN	B	843	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	4	302	-	1/1/9/20	-	-
20	CLA	4	308	-	1/1/4/20	-	-
20	CLA	1	206	-	2/2/14/20	21/35/111/115	-
20	CLA	4	307	-	1/1/4/20	-	-
21	LMU	R	109	-	-	14/21/61/61	0/2/2/2
20	CLA	A	802	-	1/1/4/20	-	-
21	LMU	A	852	-	-	20/21/61/61	0/2/2/2
21	LMU	G	102	-	-	13/21/61/61	0/2/2/2
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
22	BCR	F	203	-	-	13/29/63/63	0/2/2/2
20	CLA	3	317	-	1/1/9/20	-	-
20	CLA	3	301	-	1/1/9/20	-	-
20	CLA	1	203	-	1/1/11/20	8/18/94/115	-
25	LMG	B	848	-	-	27/44/64/70	0/1/1/1
20	CLA	A	809	-	1/1/12/20	11/24/100/115	-
20	CLA	F	201	-	1/1/12/20	11/21/97/115	-
20	CLA	1	212	-	1/1/4/20	-	-
20	CLA	2	311	-	1/1/12/20	9/21/97/115	-
20	CLA	B	850	-	2/2/15/20	20/39/115/115	-
20	CLA	B	833	-	1/1/12/20	7/21/97/115	-
22	BCR	B	846	-	-	14/29/63/63	0/2/2/2
20	CLA	A	814	-	1/1/4/20	-	-
21	LMU	H	106	-	-	9/21/61/61	0/2/2/2
22	BCR	F	204	-	-	9/29/63/63	0/2/2/2
20	CLA	F	205	-	1/1/9/20	-	-
20	CLA	L	204	-	2/2/13/20	8/27/103/115	-
22	BCR	B	844	-	-	5/29/63/63	0/2/2/2
20	CLA	B	836	-	1/1/12/20	12/23/99/115	-
21	LMU	2	319	-	-	12/21/61/61	0/2/2/2
20	CLA	2	306	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	K	105	-	-	12/21/61/61	0/2/2/2
20	CLA	3	312	-	1/1/4/20	-	-
21	LMU	3	319	-	-	11/21/61/61	0/2/2/2
21	LMU	K	107	-	-	17/21/61/61	0/2/2/2
20	CLA	A	828	-	2/2/15/20	19/39/115/115	-
20	CLA	4	309	-	1/1/4/20	-	-
20	CLA	A	824	-	2/2/13/20	15/32/108/115	-
20	CLA	B	838	-	2/2/15/20	11/39/115/115	-
20	CLA	K	102	-	1/1/12/20	5/21/97/115	-
20	CLA	A	850	-	2/2/15/20	17/39/115/115	-
22	BCR	B	847	-	-	11/29/63/63	0/2/2/2
20	CLA	B	839	-	1/1/11/20	12/18/94/115	-
20	CLA	2	301	-	1/1/4/20	-	-
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	A	818	-	2/2/14/20	14/33/109/115	-
22	BCR	A	844	-	-	14/29/63/63	0/2/2/2
22	BCR	G	104	-	-	14/29/63/63	0/2/2/2
20	CLA	B	812	-	2/2/13/20	7/25/101/115	-
20	CLA	A	836	-	1/1/11/20	8/18/94/115	-
20	CLA	B	809	-	2/2/15/20	19/39/115/115	-
20	CLA	B	803	-	2/2/15/20	17/39/115/115	-
20	CLA	L	207	-	1/1/11/20	11/18/94/115	-
21	LMU	D	201	-	-	9/21/61/61	0/2/2/2
21	LMU	A	853	-	-	11/21/61/61	0/2/2/2
20	CLA	A	830	-	2/2/15/20	19/39/115/115	-
20	CLA	3	316	-	1/1/4/20	-	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
21	LMU	G	103	-	-	14/21/61/61	0/2/2/2
20	CLA	B	817	-	1/1/11/20	12/17/93/115	-
20	CLA	A	840	-	2/2/13/20	8/27/103/115	-
20	CLA	L	208	-	2/2/12/20	10/21/97/115	-
21	LMU	A	854	-	-	16/21/61/61	0/2/2/2
20	CLA	A	839	-	2/2/13/20	14/31/107/115	-
20	CLA	J	103	-	2/2/14/20	21/35/111/115	-
20	CLA	K	104	-	2/2/13/20	11/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	1	217	-	-	9/21/61/61	0/2/2/2
20	CLA	4	312	-	1/1/4/20	-	-
20	CLA	A	827	-	2/2/13/20	9/27/103/115	-
20	CLA	A	812	-	1/1/12/20	12/26/102/115	-
20	CLA	B	818	-	1/1/12/20	10/25/101/115	-
20	CLA	2	312	-	2/2/14/20	20/35/111/115	-
20	CLA	A	803	-	1/1/11/20	4/17/93/115	-
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
21	LMU	H	103	-	-	14/21/61/61	0/2/2/2
21	LMU	H	104	-	-	12/21/61/61	0/2/2/2
20	CLA	4	317	-	1/1/12/20	11/24/100/115	-
20	CLA	2	309	-	1/1/4/20	-	-
20	CLA	A	807	-	1/1/11/20	9/17/93/115	-
20	CLA	B	827	-	2/2/15/20	21/39/115/115	-
20	CLA	B	834	-	1/1/11/20	10/15/91/115	-
20	CLA	L	202	-	2/2/13/20	14/27/103/115	-
20	CLA	B	830	-	2/2/15/20	26/39/115/115	-
20	CLA	A	835	-	2/2/15/20	14/39/115/115	-
20	CLA	A	819	-	2/2/13/20	10/31/107/115	-
21	LMU	4	320	-	-	16/21/61/61	0/2/2/2
20	CLA	A	810	-	1/1/11/20	5/15/91/115	-
20	CLA	B	807	-	1/1/11/20	6/15/91/115	-
20	CLA	A	817	-	1/1/12/20	12/24/100/115	-
20	CLA	B	810	-	2/2/14/20	11/33/109/115	-
21	LMU	2	321	-	-	8/21/61/61	0/2/2/2
24	SF4	C	103	-	-	-	0/6/5/5
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	A	813	-	1/1/12/20	9/21/97/115	-
20	CLA	K	103	-	1/1/12/20	11/21/97/115	-
21	LMU	K	106	-	-	13/21/61/61	0/2/2/2
20	CLA	B	828	-	2/2/15/20	17/39/115/115	-
22	BCR	I	103	-	-	15/29/63/63	0/2/2/2
20	CLA	B	820	-	2/2/14/20	17/35/111/115	-
20	CLA	A	833	5	1/1/11/20	7/15/91/115	-
20	CLA	4	306	-	2/2/12/20	8/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	319	-	-	13/20/60/61	0/2/2/2
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	J	101	-	1/1/11/20	9/19/95/115	-
20	CLA	4	305	-	1/1/12/20	10/21/97/115	-
20	CLA	B	822	-	1/1/11/20	12/17/93/115	-
20	CLA	4	311	-	1/1/4/20	-	-
20	CLA	L	203	-	2/2/15/20	15/39/115/115	-
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
22	BCR	A	843	-	-	14/29/63/63	0/2/2/2
20	CLA	B	824	-	2/2/15/20	19/39/115/115	-
20	CLA	3	304	-	1/1/4/20	-	-
20	CLA	B	814	-	2/2/15/20	19/39/115/115	-
20	CLA	A	837	-	1/1/12/20	14/23/99/115	-
21	LMU	R	101	-	-	13/21/61/61	0/2/2/2
20	CLA	4	314	4	1/1/4/20	-	-
20	CLA	K	101	-	1/1/11/20	6/17/93/115	-
20	CLA	B	840	-	2/2/15/20	16/39/115/115	-
20	CLA	3	306	-	1/1/4/20	-	-
21	LMU	2	320	-	-	18/21/61/61	0/2/2/2
20	CLA	A	829	-	1/1/12/20	6/21/97/115	-
20	CLA	B	825	-	1/1/12/20	9/26/102/115	-
20	CLA	A	820	-	1/1/12/20	9/23/99/115	-
20	CLA	G	105	-	1/1/12/20	7/23/99/115	-
20	CLA	L	201	-	2/2/14/20	12/33/109/115	-
22	BCR	J	102	-	-	11/29/63/63	0/2/2/2
20	CLA	3	310	-	2/2/15/20	17/39/115/115	-
20	CLA	B	813	-	2/2/13/20	11/27/103/115	-
20	CLA	1	207	-	2/2/12/20	10/23/99/115	-
20	CLA	B	829	-	2/2/15/20	18/39/115/115	-
20	CLA	H	110	16	1/1/12/20	9/21/97/115	-
20	CLA	4	304	-	2/2/13/20	13/27/103/115	-
20	CLA	3	315	-	1/1/4/20	-	-
21	LMU	3	318	-	-	12/21/61/61	0/2/2/2
20	CLA	2	303	-	2/2/13/20	15/31/107/115	-
20	CLA	2	315	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	822	-	1/1/12/20	7/21/97/115	-
20	CLA	2	308	-	1/1/4/20	-	-
20	CLA	3	303	-	1/1/9/20	-	-
20	CLA	4	303	-	3/3/15/20	20/39/115/115	-
20	CLA	A	811	20	2/2/15/20	22/39/115/115	-
21	LMU	A	846	-	-	16/21/61/61	0/2/2/2
21	LMU	L	205	-	-	13/21/61/61	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	834	-	1/1/11/20	8/17/93/115	-
20	CLA	A	831	-	2/2/15/20	20/39/115/115	-
20	CLA	A	832	-	1/1/12/20	13/21/97/115	-
20	CLA	1	205	-	1/1/9/20	-	-
20	CLA	A	808	5	2/2/14/20	14/33/109/115	-
20	CLA	B	811	6	1/1/4/20	-	-
20	CLA	B	815	-	2/2/14/20	19/33/109/115	-
20	CLA	A	821	5	1/1/10/20	3/12/88/115	-
20	CLA	A	805	-	1/1/12/20	13/26/102/115	-
20	CLA	4	301	-	2/2/13/20	15/27/103/115	-
20	CLA	B	816	-	2/2/14/20	13/33/109/115	-
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
21	LMU	B	849	-	-	5/11/51/61	0/2/2/2
20	CLA	1	211	-	2/2/12/20	9/23/99/115	-
20	CLA	2	316	-	2/2/15/20	16/39/115/115	-
20	CLA	B	837	-	2/2/14/20	16/33/109/115	-
20	CLA	B	842	-	1/1/9/20	-	-
21	LMU	F	202	-	-	13/20/60/61	0/2/2/2
20	CLA	3	302	-	1/1/4/20	-	-
20	CLA	H	101	-	3/3/13/20	12/27/103/115	-
20	CLA	F	207	-	4/4/12/20	12/25/101/115	-
21	LMU	R	103	-	-	11/21/61/61	0/2/2/2
20	CLA	3	313	-	1/1/12/20	8/21/97/115	-
20	CLA	B	802	-	1/1/12/20	12/26/102/115	-
20	CLA	3	311	-	2/2/15/20	22/39/115/115	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
22	BCR	B	801	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	849	-	2/2/15/20	21/39/115/115	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
21	LMU	R	106	-	-	12/21/61/61	0/2/2/2
22	BCR	2	317	-	-	15/29/63/63	0/2/2/2
20	CLA	3	309	-	1/1/4/20	-	-
20	CLA	B	831	-	1/1/12/20	8/21/97/115	-
20	CLA	B	832	-	2/2/13/20	17/32/108/115	-
20	CLA	1	215	-	2/2/12/20	9/23/99/115	-
20	CLA	3	307	-	1/1/10/20	9/12/88/115	-
20	CLA	A	841	-	1/1/4/20	-	-
20	CLA	A	816	-	1/1/12/20	11/26/102/115	-
21	LMU	1	216	-	-	9/21/61/61	0/2/2/2
20	CLA	A	838	-	2/2/15/20	18/39/115/115	-
21	LMU	A	847	-	-	13/21/61/61	0/2/2/2
20	CLA	1	213	-	3/3/12/20	11/23/99/115	-
21	LMU	A	848	-	-	11/21/61/61	0/2/2/2
20	CLA	2	304	-	1/1/4/20	-	-
20	CLA	1	208	-	1/1/4/20	-	-
20	CLA	F	206	-	1/1/10/20	6/10/86/115	-
20	CLA	B	808	-	2/2/14/20	19/35/111/115	-
21	LMU	G	101	-	-	13/21/61/61	0/2/2/2
20	CLA	A	804	20	2/2/13/20	11/27/103/115	-
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
20	CLA	3	308	-	1/1/4/20	-	-
20	CLA	B	821	-	1/1/12/20	7/21/97/115	-
20	CLA	2	314	-	1/1/12/20	8/21/97/115	-
20	CLA	1	209	-	1/1/4/20	-	-
20	CLA	A	801	-	3/3/11/20	11/16/92/115	-
20	CLA	3	314	-	2/2/15/20	17/39/115/115	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	H	109	-	2/2/13/20	8/27/103/115	-
20	CLA	R	107	-	2/2/13/20	15/30/106/115	-
21	LMU	B	805	-	-	14/21/61/61	0/2/2/2
21	LMU	A	855	-	-	13/21/61/61	0/2/2/2
20	CLA	4	313	-	1/1/9/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	201	-	1/1/11/20	12/17/93/115	-
20	CLA	1	204	-	1/1/11/20	9/17/93/115	-
21	LMU	L	210	-	-	16/21/61/61	0/2/2/2
20	CLA	2	310	2	1/1/12/20	6/21/97/115	-
21	LMU	B	804	-	-	16/21/61/61	0/2/2/2
20	CLA	B	841	-	2/2/15/20	17/39/115/115	-
20	CLA	A	806	-	2/2/13/20	7/29/105/115	-
20	CLA	B	823	-	2/2/13/20	11/27/103/115	-
21	LMU	R	104	-	-	14/21/61/61	0/2/2/2
20	CLA	3	305	-	1/1/4/20	-	-
20	CLA	A	826	-	2/2/15/20	14/39/115/115	-
20	CLA	2	305	-	1/1/12/20	7/21/97/115	-
20	CLA	B	806	-	2/2/15/20	19/39/115/115	-
22	BCR	A	845	-	-	10/29/63/63	0/2/2/2
20	CLA	H	102	-	2/2/13/20	14/27/103/115	-
20	CLA	I	102	-	2/2/14/20	12/33/109/115	-
20	CLA	B	826	-	2/2/13/20	18/31/107/115	-
20	CLA	R	108	-	2/2/15/20	22/39/115/115	-
20	CLA	4	310	-	1/1/12/20	13/21/97/115	-
20	CLA	1	214	-	1/1/4/20	-	-
20	CLA	A	815	-	1/1/12/20	9/21/97/115	-
20	CLA	4	318	-	1/1/11/20	13/18/94/115	-
22	BCR	I	101	-	-	10/29/60/63	0/2/2/2
24	SF4	A	856	5,6	-	-	0/6/5/5
20	CLA	4	315	-	1/1/11/20	10/17/93/115	-
20	CLA	2	302	-	1/1/12/20	13/23/99/115	-
20	CLA	1	202	-	1/1/10/20	5/10/86/115	-
20	CLA	1	210	1	1/1/9/20	-	-
20	CLA	A	825	-	2/2/15/20	23/39/115/115	-

All (2653) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	BCR	C20-C21	-9.11	1.14	1.43
20	1	205	CLA	CAB-C3B	-8.53	1.33	1.50
20	B	812	CLA	CAB-C3B	-8.43	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	843	BCR	C20-C21	-8.28	1.17	1.43
22	A	844	BCR	C20-C21	-8.25	1.17	1.43
22	F	203	BCR	C20-C21	-8.21	1.17	1.43
22	L	209	BCR	C20-C21	-8.21	1.17	1.43
22	F	204	BCR	C20-C21	-8.20	1.17	1.43
20	4	302	CLA	CAB-C3B	-8.19	1.34	1.50
22	A	845	BCR	C20-C21	-8.17	1.17	1.43
22	2	317	BCR	C20-C21	-8.16	1.17	1.43
23	B	843	PQN	C3-C2	8.10	1.49	1.35
22	B	847	BCR	C20-C21	-8.10	1.18	1.43
22	B	846	BCR	C20-C21	-8.05	1.18	1.43
22	J	102	BCR	C20-C21	-8.05	1.18	1.43
23	A	842	PQN	C3-C2	8.04	1.49	1.35
20	B	842	CLA	CAB-C3B	-7.94	1.34	1.50
22	I	103	BCR	C20-C21	-7.93	1.18	1.43
22	G	104	BCR	C20-C21	-7.92	1.18	1.43
20	1	210	CLA	CAB-C3B	-7.86	1.34	1.50
20	3	317	CLA	CAB-C3B	-7.81	1.34	1.50
20	3	301	CLA	CAB-C3B	-7.79	1.34	1.50
20	3	303	CLA	CHC-C1C	7.72	1.53	1.38
20	A	801	CLA	CAB-C3B	-7.72	1.35	1.50
20	4	313	CLA	CAB-C3B	-7.67	1.35	1.50
20	3	303	CLA	CAB-C3B	-7.65	1.35	1.50
22	B	844	BCR	C20-C21	-7.52	1.19	1.43
22	B	845	BCR	C20-C21	-7.25	1.20	1.43
20	B	819	CLA	C3A-C2A	-7.05	1.48	1.54
20	3	313	CLA	CHC-C1C	6.81	1.52	1.38
20	2	305	CLA	CHC-C1C	6.79	1.52	1.38
20	A	809	CLA	CHD-C1D	6.75	1.51	1.38
20	A	810	CLA	CHC-C1C	6.73	1.52	1.38
20	B	807	CLA	CHC-C1C	6.73	1.52	1.38
20	B	814	CLA	CHC-C1C	6.69	1.51	1.38
20	A	815	CLA	CHD-C1D	6.66	1.51	1.38
20	H	110	CLA	CHC-C1C	6.63	1.51	1.38
20	A	819	CLA	CHC-C1C	6.61	1.51	1.38
20	A	820	CLA	CHC-C1C	6.58	1.51	1.38
20	B	816	CLA	CHC-C1C	6.55	1.51	1.38
20	B	831	CLA	CHD-C1D	6.54	1.51	1.38
20	B	806	CLA	CHC-C1C	6.53	1.51	1.38
20	B	832	CLA	CHC-C1C	6.52	1.51	1.38
20	1	203	CLA	CHC-C1C	6.52	1.51	1.38
20	A	804	CLA	CHC-C1C	6.52	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	811	CLA	CHD-C1D	6.51	1.51	1.38
20	B	828	CLA	CHC-C1C	6.51	1.51	1.38
20	1	210	CLA	CHC-C1C	6.50	1.51	1.38
20	1	207	CLA	CHC-C1C	6.50	1.51	1.38
20	I	102	CLA	CHC-C1C	6.49	1.51	1.38
20	4	304	CLA	CHD-C1D	6.49	1.51	1.38
20	4	312	CLA	CHC-C1C	6.48	1.51	1.38
20	A	808	CLA	CHC-C1C	6.48	1.51	1.38
20	G	105	CLA	CHC-C1C	6.46	1.51	1.38
20	A	851	CLA	CHD-C1D	6.46	1.51	1.38
20	3	312	CLA	CHC-C1C	6.46	1.51	1.38
20	B	831	CLA	CHC-C1C	6.45	1.51	1.38
20	3	313	CLA	CHD-C1D	6.45	1.51	1.38
20	H	101	CLA	CHD-C1D	6.45	1.51	1.38
20	A	801	CLA	CHD-C1D	6.44	1.51	1.38
20	A	838	CLA	CHC-C1C	6.42	1.51	1.38
20	B	840	CLA	CHC-C1C	6.41	1.51	1.38
20	L	204	CLA	CHC-C1C	6.40	1.51	1.38
20	H	109	CLA	CHC-C1C	6.39	1.51	1.38
20	A	835	CLA	CHC-C1C	6.38	1.51	1.38
20	4	314	CLA	CHC-C1C	6.37	1.51	1.38
20	B	818	CLA	CHC-C1C	6.37	1.51	1.38
20	4	302	CLA	CHC-C1C	6.37	1.51	1.38
20	A	830	CLA	CHD-C1D	6.37	1.50	1.38
20	A	813	CLA	CHC-C1C	6.36	1.51	1.38
20	B	821	CLA	CHC-C1C	6.35	1.51	1.38
20	1	215	CLA	CHC-C1C	6.35	1.51	1.38
20	L	201	CLA	CHC-C1C	6.34	1.51	1.38
20	3	302	CLA	CHC-C1C	6.34	1.51	1.38
20	A	840	CLA	CHC-C1C	6.34	1.51	1.38
20	A	810	CLA	CHD-C1D	6.34	1.50	1.38
20	A	836	CLA	CHC-C1C	6.33	1.51	1.38
20	A	815	CLA	CHC-C1C	6.32	1.51	1.38
20	F	205	CLA	CHC-C1C	6.32	1.51	1.38
20	H	109	CLA	CHD-C1D	6.32	1.50	1.38
20	2	305	CLA	CHD-C1D	6.32	1.50	1.38
20	B	835	CLA	CHC-C1C	6.31	1.51	1.38
20	3	316	CLA	CHC-C1C	6.31	1.50	1.38
20	A	824	CLA	CHC-C1C	6.31	1.51	1.38
20	A	829	CLA	CHD-C1D	6.30	1.50	1.38
20	K	101	CLA	CHC-C1C	6.30	1.51	1.38
20	A	823	CLA	CHC-C1C	6.29	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	318	CLA	CHD-C1D	6.29	1.50	1.38
20	B	819	CLA	C3D-C4D	-6.28	1.30	1.44
20	B	803	CLA	CHC-C1C	6.28	1.51	1.38
20	B	807	CLA	CHD-C1D	6.27	1.50	1.38
20	4	301	CLA	CHC-C1C	6.27	1.51	1.38
20	B	815	CLA	CHC-C1C	6.27	1.51	1.38
20	L	202	CLA	CHC-C1C	6.27	1.51	1.38
20	R	108	CLA	CHC-C1C	6.27	1.51	1.38
20	A	829	CLA	CHC-C1C	6.27	1.51	1.38
20	A	821	CLA	CHD-C1D	6.27	1.50	1.38
20	A	827	CLA	CHC-C1C	6.26	1.51	1.38
20	B	810	CLA	CHD-C1D	6.26	1.50	1.38
20	A	822	CLA	CHD-C1D	6.26	1.50	1.38
20	L	208	CLA	CHC-C1C	6.26	1.51	1.38
20	1	205	CLA	CHD-C1D	6.25	1.50	1.38
20	B	802	CLA	CHC-C1C	6.25	1.51	1.38
20	A	819	CLA	CHD-C1D	6.24	1.50	1.38
20	B	823	CLA	CHD-C1D	6.24	1.50	1.38
20	B	839	CLA	CHC-C1C	6.23	1.51	1.38
20	H	102	CLA	CHC-C1C	6.23	1.51	1.38
20	H	101	CLA	CHC-C1C	6.23	1.51	1.38
20	B	836	CLA	CHC-C1C	6.23	1.51	1.38
20	B	817	CLA	CHC-C1C	6.22	1.50	1.38
20	B	803	CLA	CHD-C1D	6.22	1.50	1.38
20	B	822	CLA	CHC-C1C	6.22	1.50	1.38
20	3	317	CLA	CHC-C1C	6.22	1.50	1.38
20	3	301	CLA	CHC-C1C	6.21	1.50	1.38
20	F	205	CLA	CAB-C3B	-6.21	1.38	1.50
20	B	834	CLA	CHC-C1C	6.21	1.50	1.38
20	2	302	CLA	CHC-C1C	6.20	1.50	1.38
20	L	207	CLA	CHC-C1C	6.20	1.50	1.38
20	3	307	CLA	CHD-C1D	6.20	1.50	1.38
20	2	315	CLA	CHC-C1C	6.20	1.50	1.38
20	A	832	CLA	CHC-C1C	6.20	1.50	1.38
20	1	208	CLA	CHC-C1C	6.19	1.50	1.38
20	B	839	CLA	C3D-C4D	-6.18	1.30	1.44
20	1	206	CLA	CHC-C1C	6.18	1.50	1.38
20	A	828	CLA	CHC-C1C	6.18	1.50	1.38
20	A	815	CLA	CHD-C4C	6.18	1.53	1.39
20	R	107	CLA	CHC-C1C	6.17	1.50	1.38
20	3	311	CLA	CHC-C1C	6.17	1.50	1.38
20	B	812	CLA	C3D-C4D	-6.17	1.30	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	312	CLA	CHC-C1C	6.17	1.50	1.38
20	1	212	CLA	CHC-C1C	6.17	1.50	1.38
20	A	811	CLA	CHD-C4C	6.16	1.53	1.39
20	A	832	CLA	CHD-C1D	6.16	1.50	1.38
20	A	820	CLA	CHD-C1D	6.15	1.50	1.38
20	A	807	CLA	CHD-C1D	6.15	1.50	1.38
20	A	817	CLA	CHC-C1C	6.15	1.50	1.38
20	B	827	CLA	CHC-C1C	6.15	1.50	1.38
20	B	842	CLA	CHC-C1C	6.15	1.50	1.38
20	1	214	CLA	CHC-C1C	6.15	1.50	1.38
20	A	834	CLA	CHC-C1C	6.15	1.50	1.38
20	1	202	CLA	CHD-C1D	6.15	1.50	1.38
20	B	828	CLA	CHD-C1D	6.15	1.50	1.38
20	A	851	CLA	CHD-C4C	6.15	1.53	1.39
20	1	210	CLA	CHD-C1D	6.14	1.50	1.38
20	H	102	CLA	CHD-C1D	6.14	1.50	1.38
20	A	810	CLA	CHD-C4C	6.13	1.53	1.39
20	A	831	CLA	C3D-C4D	-6.13	1.30	1.44
20	4	315	CLA	CHC-C1C	6.13	1.50	1.38
20	B	850	CLA	CHC-C1C	6.13	1.50	1.38
20	A	825	CLA	CHC-C1C	6.12	1.50	1.38
20	2	311	CLA	CHC-C1C	6.12	1.50	1.38
20	1	202	CLA	O2D-CGD	6.12	1.48	1.33
20	3	308	CLA	CHC-C1C	6.11	1.50	1.38
20	A	806	CLA	CHC-C1C	6.11	1.50	1.38
20	L	207	CLA	CHD-C1D	6.10	1.50	1.38
20	1	209	CLA	CHC-C1C	6.10	1.50	1.38
20	2	310	CLA	CHD-C1D	6.10	1.50	1.38
20	1	205	CLA	CHC-C1C	6.10	1.50	1.38
20	B	809	CLA	CHD-C1D	6.10	1.50	1.38
20	4	317	CLA	CHD-C1D	6.10	1.50	1.38
20	4	309	CLA	CHC-C1C	6.10	1.50	1.38
20	H	109	CLA	CHD-C4C	6.09	1.53	1.39
20	L	201	CLA	CHD-C1D	6.09	1.50	1.38
20	A	812	CLA	CHC-C1C	6.09	1.50	1.38
20	A	816	CLA	CHC-C1C	6.09	1.50	1.38
20	4	313	CLA	CHC-C1C	6.08	1.50	1.38
20	4	306	CLA	CHC-C1C	6.08	1.50	1.38
20	A	849	CLA	CHC-C1C	6.08	1.50	1.38
20	A	817	CLA	CHD-C1D	6.08	1.50	1.38
20	L	203	CLA	CHC-C1C	6.08	1.50	1.38
20	H	108	CLA	C3D-C4D	-6.08	1.30	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	306	CLA	CHC-C1C	6.07	1.50	1.38
20	A	801	CLA	CHC-C1C	6.07	1.50	1.38
20	2	304	CLA	CHC-C1C	6.07	1.50	1.38
20	2	316	CLA	C3D-C4D	-6.07	1.30	1.44
20	A	830	CLA	CHC-C1C	6.06	1.50	1.38
20	B	815	CLA	CHD-C1D	6.06	1.50	1.38
20	A	850	CLA	CHC-C1C	6.06	1.50	1.38
20	B	826	CLA	CHC-C1C	6.06	1.50	1.38
20	A	826	CLA	CHC-C1C	6.06	1.50	1.38
20	3	301	CLA	CHD-C1D	6.05	1.50	1.38
20	R	108	CLA	CHD-C1D	6.05	1.50	1.38
20	3	317	CLA	CHD-C1D	6.05	1.50	1.38
20	B	812	CLA	CHC-C1C	6.04	1.50	1.38
20	A	807	CLA	CHC-C1C	6.04	1.50	1.38
20	K	103	CLA	CHD-C1D	6.03	1.50	1.38
20	B	810	CLA	CHC-C1C	6.03	1.50	1.38
20	A	826	CLA	CHD-C1D	6.03	1.50	1.38
20	A	821	CLA	CHD-C4C	6.02	1.52	1.39
20	J	101	CLA	CHC-C1C	6.02	1.50	1.38
20	A	835	CLA	CHD-C1D	6.02	1.50	1.38
20	B	823	CLA	CHC-C1C	6.02	1.50	1.38
20	4	305	CLA	CHC-C1C	6.02	1.50	1.38
20	B	840	CLA	CHD-C1D	6.02	1.50	1.38
20	B	824	CLA	C3D-C4D	-6.01	1.30	1.44
20	A	840	CLA	CHD-C1D	6.01	1.50	1.38
20	B	818	CLA	CHD-C1D	6.01	1.50	1.38
20	L	201	CLA	CHD-C4C	6.01	1.52	1.39
20	A	836	CLA	CHD-C1D	6.01	1.50	1.38
20	B	837	CLA	CHC-C1C	6.00	1.50	1.38
20	B	838	CLA	CHD-C1D	6.00	1.50	1.38
20	3	307	CLA	CHD-C4C	6.00	1.52	1.39
20	B	831	CLA	CHD-C4C	6.00	1.52	1.39
20	B	828	CLA	CHD-C4C	6.00	1.52	1.39
20	A	833	CLA	CHC-C1C	5.99	1.50	1.38
20	A	811	CLA	CHC-C1C	5.99	1.50	1.38
20	A	822	CLA	CHC-C1C	5.99	1.50	1.38
20	K	104	CLA	CHD-C1D	5.99	1.50	1.38
20	A	818	CLA	CAB-C3B	-5.98	1.31	1.47
20	K	102	CLA	CHD-C1D	5.98	1.50	1.38
20	A	823	CLA	CHD-C1D	5.98	1.50	1.38
20	B	820	CLA	CHC-C1C	5.98	1.50	1.38
20	A	827	CLA	CHD-C1D	5.97	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	CHD-C1D	5.97	1.50	1.38
20	3	313	CLA	CHD-C4C	5.96	1.52	1.39
20	F	205	CLA	CHD-C1D	5.96	1.50	1.38
20	1	202	CLA	CHC-C1C	5.96	1.50	1.38
20	A	837	CLA	CHC-C1C	5.96	1.50	1.38
20	K	104	CLA	CHC-C1C	5.96	1.50	1.38
20	F	205	CLA	CHD-C4C	5.96	1.52	1.39
20	A	806	CLA	CHD-C1D	5.96	1.50	1.38
20	3	311	CLA	CHD-C1D	5.96	1.50	1.38
20	A	829	CLA	CHD-C4C	5.95	1.52	1.39
20	1	207	CLA	CHD-C1D	5.95	1.50	1.38
20	A	802	CLA	CHC-C1C	5.95	1.50	1.38
20	A	832	CLA	CHD-C4C	5.94	1.52	1.39
20	B	834	CLA	CHD-C1D	5.94	1.50	1.38
20	A	826	CLA	CHD-C4C	5.93	1.52	1.39
20	B	829	CLA	CHC-C1C	5.93	1.50	1.38
20	A	803	CLA	CAB-C3B	-5.93	1.31	1.47
20	B	830	CLA	CHC-C1C	5.93	1.50	1.38
20	H	101	CLA	O2D-CGD	5.92	1.47	1.33
20	A	801	CLA	CHD-C4C	5.92	1.52	1.39
20	B	806	CLA	CHD-C4C	5.92	1.52	1.39
20	B	837	CLA	CHD-C1D	5.91	1.50	1.38
20	B	802	CLA	CHD-C1D	5.90	1.50	1.38
20	3	303	CLA	CHD-C1D	5.90	1.50	1.38
20	4	308	CLA	CHC-C1C	5.90	1.50	1.38
20	B	818	CLA	CHD-C4C	5.89	1.52	1.39
20	A	822	CLA	CHD-C4C	5.89	1.52	1.39
20	A	833	CLA	CHD-C1D	5.89	1.49	1.38
20	F	206	CLA	CHC-C1C	5.89	1.50	1.38
20	4	307	CLA	CHC-C1C	5.89	1.50	1.38
20	A	808	CLA	CHD-C1D	5.88	1.49	1.38
20	A	833	CLA	O2A-CGA	5.88	1.50	1.30
20	H	101	CLA	CHD-C4C	5.88	1.52	1.39
20	L	207	CLA	CHD-C4C	5.88	1.52	1.39
20	B	810	CLA	CHD-C4C	5.88	1.52	1.39
20	B	809	CLA	CHC-C1C	5.88	1.50	1.38
20	B	813	CLA	CHC-C1C	5.88	1.50	1.38
20	A	805	CLA	CHD-C1D	5.88	1.49	1.38
20	A	812	CLA	CHD-C1D	5.87	1.49	1.38
20	A	820	CLA	CHD-C4C	5.87	1.52	1.39
20	3	314	CLA	C3D-C4D	-5.87	1.31	1.44
20	A	804	CLA	CHD-C4C	5.87	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	101	CLA	CHD-C1D	5.86	1.49	1.38
20	I	102	CLA	CHD-C1D	5.86	1.49	1.38
20	B	815	CLA	CHD-C4C	5.86	1.52	1.39
20	A	851	CLA	CHC-C1C	5.86	1.50	1.38
20	B	838	CLA	CHC-C1C	5.86	1.50	1.38
20	B	842	CLA	CHD-C1D	5.85	1.49	1.38
20	B	841	CLA	CHD-C1D	5.85	1.49	1.38
20	4	303	CLA	CHD-C4C	5.85	1.52	1.39
20	B	823	CLA	CHD-C4C	5.85	1.52	1.39
20	4	318	CLA	CHC-C1C	5.84	1.50	1.38
20	4	311	CLA	CHC-C1C	5.84	1.50	1.38
20	3	313	CLA	O2D-CGD	5.84	1.47	1.33
20	2	310	CLA	CHC-C1C	5.84	1.50	1.38
20	B	838	CLA	CHD-C4C	5.83	1.52	1.39
20	B	831	CLA	O2D-CGD	5.83	1.47	1.33
20	B	825	CLA	CHC-C1C	5.83	1.50	1.38
20	K	102	CLA	CHC-C1C	5.83	1.50	1.38
20	B	850	CLA	CHD-C1D	5.83	1.49	1.38
20	3	305	CLA	CHC-C1C	5.83	1.50	1.38
20	A	805	CLA	CHC-C1C	5.83	1.50	1.38
20	2	314	CLA	CHC-C1C	5.83	1.50	1.38
20	2	310	CLA	CHD-C4C	5.83	1.52	1.39
20	A	805	CLA	CHD-C4C	5.82	1.52	1.39
20	2	311	CLA	CHD-C1D	5.82	1.49	1.38
20	A	813	CLA	CHD-C1D	5.82	1.49	1.38
20	R	107	CLA	CHD-C1D	5.81	1.49	1.38
20	K	101	CLA	CHD-C1D	5.81	1.49	1.38
20	B	816	CLA	CHD-C1D	5.81	1.49	1.38
20	B	807	CLA	CHD-C4C	5.81	1.52	1.39
20	A	825	CLA	CHD-C1D	5.81	1.49	1.38
20	4	318	CLA	CHD-C4C	5.80	1.52	1.39
20	A	833	CLA	CHD-C4C	5.80	1.52	1.39
20	A	821	CLA	CHC-C1C	5.80	1.50	1.38
20	A	834	CLA	CHD-C1D	5.79	1.49	1.38
20	A	809	CLA	CHD-C4C	5.79	1.52	1.39
20	1	205	CLA	CHD-C4C	5.78	1.52	1.39
20	A	806	CLA	CHD-C4C	5.78	1.52	1.39
20	A	807	CLA	CHD-C4C	5.77	1.52	1.39
20	A	814	CLA	CHC-C1C	5.77	1.49	1.38
20	A	823	CLA	CHD-C4C	5.77	1.52	1.39
20	A	830	CLA	CHD-C4C	5.77	1.52	1.39
20	4	304	CLA	CHC-C1C	5.76	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	839	CLA	CAB-C3B	-5.76	1.32	1.47
20	B	827	CLA	CHD-C1D	5.76	1.49	1.38
20	4	303	CLA	CHC-C1C	5.76	1.50	1.38
20	K	104	CLA	C3D-C4D	-5.76	1.31	1.44
20	B	809	CLA	CHD-C4C	5.76	1.52	1.39
20	B	813	CLA	CHD-C1D	5.75	1.49	1.38
20	B	821	CLA	CHD-C1D	5.75	1.49	1.38
20	3	315	CLA	CHC-C1C	5.75	1.49	1.38
20	2	305	CLA	CHD-C4C	5.75	1.52	1.39
20	A	840	CLA	CHD-C4C	5.74	1.52	1.39
20	A	804	CLA	CHD-C1D	5.73	1.49	1.38
20	4	302	CLA	CHD-C1D	5.73	1.49	1.38
20	A	818	CLA	CHC-C1C	5.73	1.50	1.38
20	B	835	CLA	CHD-C1D	5.73	1.49	1.38
20	1	203	CLA	C3D-C4D	-5.72	1.31	1.44
20	B	830	CLA	CHD-C1D	5.72	1.49	1.38
20	4	317	CLA	CHC-C1C	5.72	1.49	1.38
20	A	831	CLA	CHC-C1C	5.72	1.49	1.38
20	A	839	CLA	O2D-CGD	5.72	1.47	1.33
20	A	801	CLA	O2D-CGD	5.72	1.47	1.33
20	B	826	CLA	CHD-C1D	5.71	1.49	1.38
20	2	301	CLA	CHC-C1C	5.71	1.49	1.38
20	K	103	CLA	CHC-C1C	5.71	1.49	1.38
20	A	819	CLA	CHD-C4C	5.71	1.52	1.39
20	R	107	CLA	O2D-CGD	5.70	1.47	1.33
20	J	103	CLA	CHC-C1C	5.70	1.49	1.38
20	H	110	CLA	CHD-C1D	5.70	1.49	1.38
20	A	815	CLA	O2D-CGD	5.70	1.47	1.33
20	L	202	CLA	CHD-C1D	5.69	1.49	1.38
20	B	824	CLA	CHC-C1C	5.69	1.49	1.38
22	B	801	BCR	C21-C22	-5.69	1.22	1.35
20	1	206	CLA	O2D-CGD	5.69	1.47	1.33
20	R	107	CLA	CHD-C4C	5.68	1.52	1.39
20	A	837	CLA	CHD-C1D	5.68	1.49	1.38
20	B	802	CLA	CHD-C4C	5.68	1.52	1.39
20	2	305	CLA	O2D-CGD	5.68	1.47	1.33
20	B	803	CLA	CHD-C4C	5.68	1.52	1.39
20	2	310	CLA	CAB-C3B	-5.68	1.32	1.47
20	A	850	CLA	CHD-C1D	5.68	1.49	1.38
20	B	814	CLA	CHD-C1D	5.68	1.49	1.38
20	B	833	CLA	CHD-C1D	5.68	1.49	1.38
20	4	304	CLA	CHD-C4C	5.68	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	206	CLA	CHD-C1D	5.68	1.49	1.38
20	A	828	CLA	CHD-C4C	5.67	1.52	1.39
20	4	313	CLA	CHD-C1D	5.67	1.49	1.38
20	F	207	CLA	C3D-C4D	-5.67	1.31	1.44
20	K	103	CLA	C3D-C4D	-5.67	1.31	1.44
20	A	827	CLA	CHD-C4C	5.66	1.52	1.39
20	2	309	CLA	CHC-C1C	5.66	1.49	1.38
20	A	835	CLA	CHD-C4C	5.66	1.52	1.39
20	B	841	CLA	CHC-C1C	5.66	1.49	1.38
20	H	102	CLA	O2D-CGD	5.65	1.47	1.33
20	A	812	CLA	CHD-C4C	5.65	1.52	1.39
20	1	211	CLA	CHC-C1C	5.65	1.49	1.38
20	A	818	CLA	C3D-C4D	-5.65	1.31	1.44
20	A	841	CLA	CHC-C1C	5.65	1.49	1.38
20	B	840	CLA	CHD-C4C	5.65	1.52	1.39
20	A	810	CLA	O2D-CGD	5.64	1.47	1.33
20	B	837	CLA	CHD-C4C	5.64	1.52	1.39
20	H	102	CLA	CHD-C4C	5.64	1.52	1.39
20	A	808	CLA	CHD-C4C	5.64	1.52	1.39
20	4	310	CLA	CHC-C1C	5.64	1.49	1.38
20	A	836	CLA	CHD-C4C	5.64	1.52	1.39
20	B	834	CLA	CHD-C4C	5.63	1.52	1.39
20	K	103	CLA	O2D-CGD	5.63	1.47	1.33
20	B	808	CLA	CHC-C1C	5.62	1.49	1.38
20	1	213	CLA	C3D-C4D	-5.62	1.31	1.44
20	A	824	CLA	CHD-C1D	5.62	1.49	1.38
20	H	110	CLA	O2D-CGD	5.62	1.47	1.33
20	4	301	CLA	O2D-CGD	5.62	1.47	1.33
20	3	317	CLA	CHD-C4C	5.62	1.52	1.39
20	F	207	CLA	CHD-C1D	5.61	1.49	1.38
20	B	819	CLA	CHC-C1C	5.61	1.49	1.38
20	A	838	CLA	CHD-C1D	5.61	1.49	1.38
20	4	303	CLA	O2D-CGD	5.61	1.47	1.33
20	B	809	CLA	CAB-C3B	-5.61	1.32	1.47
20	4	306	CLA	C3D-C4D	-5.61	1.31	1.44
20	B	817	CLA	CHD-C1D	5.60	1.49	1.38
20	B	850	CLA	CHD-C4C	5.60	1.52	1.39
20	A	828	CLA	CHD-C1D	5.60	1.49	1.38
20	B	806	CLA	CHD-C1D	5.60	1.49	1.38
20	R	108	CLA	O2D-CGD	5.59	1.47	1.33
20	A	813	CLA	CHD-C4C	5.59	1.51	1.39
20	3	311	CLA	CHD-C4C	5.58	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	836	CLA	C3D-C4D	-5.58	1.31	1.44
20	A	817	CLA	CHD-C4C	5.58	1.51	1.39
20	L	203	CLA	CHD-C1D	5.58	1.49	1.38
20	B	817	CLA	CHD-C4C	5.58	1.51	1.39
20	2	306	CLA	CHC-C1C	5.58	1.49	1.38
20	3	304	CLA	CHC-C1C	5.58	1.49	1.38
20	B	816	CLA	O2D-CGD	5.58	1.46	1.33
20	2	307	CLA	CHD-C4C	5.58	1.51	1.39
20	B	821	CLA	CHD-C4C	5.57	1.51	1.39
20	2	311	CLA	O2D-CGD	5.57	1.46	1.33
20	B	815	CLA	O2D-CGD	5.57	1.46	1.33
20	1	215	CLA	O2D-CGD	5.57	1.46	1.33
20	B	833	CLA	CHC-C1C	5.57	1.49	1.38
20	1	204	CLA	O2D-CGD	5.57	1.46	1.33
20	R	108	CLA	CHD-C4C	5.57	1.51	1.39
20	1	210	CLA	CHD-C4C	5.57	1.51	1.39
20	B	827	CLA	CHD-C4C	5.56	1.51	1.39
20	A	816	CLA	C3D-C4D	-5.56	1.31	1.44
20	B	825	CLA	CHD-C1D	5.56	1.49	1.38
20	L	208	CLA	CHD-C4C	5.55	1.51	1.39
20	4	317	CLA	CHD-C4C	5.55	1.51	1.39
20	1	203	CLA	CHD-C1D	5.55	1.49	1.38
20	L	208	CLA	O2D-CGD	5.55	1.46	1.33
20	3	307	CLA	C3D-C4D	-5.55	1.31	1.44
20	L	202	CLA	CHD-C4C	5.54	1.51	1.39
20	B	825	CLA	CHD-C4C	5.54	1.51	1.39
20	1	202	CLA	CHD-C4C	5.54	1.51	1.39
20	1	207	CLA	CHD-C4C	5.54	1.51	1.39
20	K	103	CLA	CHD-C4C	5.54	1.51	1.39
20	1	201	CLA	CHD-C1D	5.54	1.49	1.38
20	B	816	CLA	CHD-C4C	5.54	1.51	1.39
20	A	835	CLA	CAB-C3B	-5.54	1.32	1.47
20	H	109	CLA	O2D-CGD	5.54	1.46	1.33
20	B	828	CLA	C3D-C4D	-5.54	1.31	1.44
20	2	307	CLA	CHD-C1D	5.54	1.49	1.38
20	A	839	CLA	CHC-C1C	5.54	1.49	1.38
20	B	822	CLA	CHD-C4C	5.54	1.51	1.39
20	A	840	CLA	O2D-CGD	5.54	1.46	1.33
20	2	316	CLA	CHC-C1C	5.53	1.49	1.38
20	3	301	CLA	CHD-C4C	5.53	1.51	1.39
20	A	805	CLA	O2D-CGD	5.53	1.46	1.33
20	A	803	CLA	C3D-C4D	-5.53	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	303	CLA	CHC-C1C	5.53	1.49	1.38
20	B	839	CLA	C4C-C3C	-5.53	1.35	1.45
20	L	204	CLA	CHD-C1D	5.53	1.49	1.38
20	2	303	CLA	C3D-C4D	-5.53	1.31	1.44
20	B	823	CLA	O2D-CGD	5.53	1.46	1.33
20	1	204	CLA	CHD-C1D	5.53	1.49	1.38
20	G	105	CLA	CHD-C1D	5.52	1.49	1.38
20	A	834	CLA	CHD-C4C	5.52	1.51	1.39
20	I	102	CLA	CHD-C4C	5.52	1.51	1.39
20	K	104	CLA	CHD-C4C	5.52	1.51	1.39
20	A	819	CLA	O2D-CGD	5.52	1.46	1.33
20	A	824	CLA	CHD-C4C	5.52	1.51	1.39
20	H	110	CLA	CHD-C4C	5.52	1.51	1.39
20	B	835	CLA	CHD-C4C	5.52	1.51	1.39
22	I	101	BCR	C20-C21	-5.52	1.26	1.43
20	L	204	CLA	O2D-CGD	5.51	1.46	1.33
20	3	303	CLA	CHD-C4C	5.50	1.51	1.39
20	J	101	CLA	CHD-C4C	5.50	1.51	1.39
20	4	310	CLA	C3D-C4D	-5.50	1.31	1.44
20	B	826	CLA	CHD-C4C	5.50	1.51	1.39
20	L	203	CLA	CHD-C4C	5.49	1.51	1.39
20	B	829	CLA	CHD-C1D	5.49	1.49	1.38
20	H	108	CLA	CHC-C1C	5.49	1.49	1.38
20	F	206	CLA	CHC-C4B	5.49	1.51	1.39
20	B	806	CLA	O2D-CGD	5.49	1.46	1.33
20	4	306	CLA	CHD-C1D	5.49	1.49	1.38
20	K	101	CLA	CHD-C4C	5.49	1.51	1.39
20	K	102	CLA	CHD-C4C	5.48	1.51	1.39
20	A	838	CLA	CHD-C4C	5.48	1.51	1.39
20	4	306	CLA	CHD-C4C	5.47	1.51	1.39
20	2	303	CLA	CHD-C1D	5.47	1.49	1.38
20	B	824	CLA	CAB-C3B	-5.47	1.32	1.47
20	3	310	CLA	C3D-C4D	-5.46	1.31	1.44
20	A	803	CLA	CHC-C1C	5.46	1.49	1.38
20	A	837	CLA	CHD-C4C	5.46	1.51	1.39
20	B	814	CLA	CHD-C4C	5.46	1.51	1.39
20	F	207	CLA	CHC-C1C	5.46	1.49	1.38
20	4	317	CLA	O2D-CGD	5.46	1.46	1.33
20	4	301	CLA	CHD-C1D	5.45	1.49	1.38
20	1	204	CLA	C3D-C4D	-5.45	1.31	1.44
20	B	813	CLA	CHD-C4C	5.45	1.51	1.39
20	A	832	CLA	O2D-CGD	5.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	822	CLA	O2D-CGD	5.45	1.46	1.33
20	B	832	CLA	CHD-C4C	5.44	1.51	1.39
20	A	820	CLA	O2D-CGD	5.44	1.46	1.33
20	B	822	CLA	O2D-CGD	5.44	1.46	1.33
20	1	204	CLA	CHD-C4C	5.43	1.51	1.39
20	A	850	CLA	CHD-C4C	5.43	1.51	1.39
20	A	833	CLA	O2D-CGD	5.43	1.46	1.33
20	G	105	CLA	CHD-C4C	5.43	1.51	1.39
20	1	204	CLA	CHC-C1C	5.43	1.49	1.38
20	A	825	CLA	CHD-C4C	5.43	1.51	1.39
20	B	835	CLA	CAB-C3B	-5.42	1.32	1.47
20	3	307	CLA	O2D-CGD	5.42	1.46	1.33
20	A	806	CLA	O2D-CGD	5.42	1.46	1.33
20	4	310	CLA	O2D-CGD	5.42	1.46	1.33
20	A	851	CLA	CAB-C3B	-5.41	1.32	1.47
20	B	842	CLA	CHD-C4C	5.41	1.51	1.39
20	A	812	CLA	O2D-CGD	5.41	1.46	1.33
20	F	206	CLA	CHD-C4C	5.41	1.51	1.39
20	A	838	CLA	O2D-CGD	5.41	1.46	1.33
20	3	309	CLA	CHC-C1C	5.41	1.49	1.38
20	2	310	CLA	C3D-C4D	-5.40	1.32	1.44
20	B	834	CLA	O2D-CGD	5.39	1.46	1.33
20	L	207	CLA	O2D-CGD	5.39	1.46	1.33
20	B	818	CLA	O2D-CGD	5.39	1.46	1.33
20	L	201	CLA	O2D-CGD	5.39	1.46	1.33
20	A	821	CLA	O2D-CGD	5.39	1.46	1.33
20	B	814	CLA	CHC-C4B	5.38	1.51	1.39
20	L	204	CLA	CHD-C4C	5.38	1.51	1.39
20	B	808	CLA	C3D-C4D	-5.38	1.32	1.44
20	2	314	CLA	O2D-CGD	5.38	1.46	1.33
20	B	825	CLA	CAB-C3B	-5.38	1.33	1.47
20	B	832	CLA	CAB-C3B	-5.38	1.33	1.47
20	3	313	CLA	CHC-C4B	5.37	1.51	1.39
20	3	307	CLA	CHC-C1C	5.37	1.49	1.38
20	1	213	CLA	CHD-C4C	5.37	1.51	1.39
20	4	301	CLA	CHD-C4C	5.37	1.51	1.39
20	A	802	CLA	CHD-C1D	5.36	1.51	1.38
20	3	311	CLA	O2D-CGD	5.35	1.46	1.33
20	B	840	CLA	O2D-CGD	5.35	1.46	1.33
20	2	312	CLA	C3D-C4D	-5.35	1.32	1.44
20	2	302	CLA	C3D-C4D	-5.35	1.32	1.44
20	4	302	CLA	C3D-C4D	-5.35	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	K	101	CLA	C3D-C4D	-5.35	1.32	1.44
20	1	213	CLA	CHC-C1C	5.35	1.49	1.38
20	K	102	CLA	C3D-C4D	-5.34	1.32	1.44
20	A	841	CLA	CHD-C1D	5.34	1.51	1.38
20	A	834	CLA	C3D-C4D	-5.34	1.32	1.44
20	B	832	CLA	CHC-C4B	5.34	1.51	1.39
20	B	814	CLA	CAB-C3B	-5.33	1.33	1.47
20	J	101	CLA	O2D-CGD	5.33	1.46	1.33
20	A	807	CLA	O2D-CGD	5.33	1.46	1.33
20	B	810	CLA	O2D-CGD	5.33	1.46	1.33
20	J	103	CLA	CAB-C3B	-5.33	1.33	1.47
20	2	307	CLA	O2D-CGD	5.33	1.46	1.33
20	F	207	CLA	O2D-CGD	5.33	1.46	1.33
20	B	817	CLA	O2D-CGD	5.33	1.46	1.33
20	B	835	CLA	O2D-CGD	5.33	1.46	1.33
20	B	826	CLA	C3D-C4D	-5.33	1.32	1.44
20	A	849	CLA	O2D-CGD	5.32	1.46	1.33
20	1	201	CLA	C3D-C4D	-5.32	1.32	1.44
20	K	102	CLA	O2D-CGD	5.32	1.46	1.33
20	G	105	CLA	O2D-CGD	5.32	1.46	1.33
20	A	817	CLA	O2D-CGD	5.32	1.46	1.33
20	4	305	CLA	C3D-C4D	-5.32	1.32	1.44
20	B	803	CLA	O2D-CGD	5.32	1.46	1.33
20	J	103	CLA	C3D-C4D	-5.31	1.32	1.44
20	B	830	CLA	O2D-CGD	5.31	1.46	1.33
20	B	833	CLA	CHD-C4C	5.31	1.51	1.39
20	1	210	CLA	CHC-C4B	5.31	1.51	1.39
20	B	825	CLA	O2D-CGD	5.31	1.46	1.33
20	H	110	CLA	CHC-C4B	5.31	1.51	1.39
20	1	211	CLA	O2D-CGD	5.30	1.46	1.33
20	4	313	CLA	CHD-C4C	5.30	1.51	1.39
20	B	826	CLA	CAB-C3B	-5.29	1.33	1.47
20	A	837	CLA	CAB-C3B	-5.29	1.33	1.47
20	4	306	CLA	O2D-CGD	5.29	1.46	1.33
20	B	823	CLA	CAB-C3B	-5.29	1.33	1.47
20	B	824	CLA	C4C-C3C	-5.29	1.36	1.45
20	1	204	CLA	CAB-C3B	-5.29	1.33	1.47
20	L	208	CLA	CHD-C1D	5.29	1.48	1.38
20	1	211	CLA	CAB-C3B	-5.29	1.33	1.47
20	A	834	CLA	O2D-CGD	5.29	1.46	1.33
20	A	808	CLA	CAB-C3B	-5.29	1.33	1.47
20	L	207	CLA	CHC-C4B	5.29	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	816	CLA	CHD-C1D	5.29	1.48	1.38
20	2	311	CLA	CHD-C4C	5.28	1.51	1.39
20	A	824	CLA	CAB-C3B	-5.28	1.33	1.47
20	3	314	CLA	CHD-C4C	5.28	1.51	1.39
20	4	304	CLA	O2D-CGD	5.28	1.46	1.33
20	B	833	CLA	O2D-CGD	5.28	1.46	1.33
20	4	302	CLA	CHD-C4C	5.28	1.51	1.39
20	G	105	CLA	C3D-C4D	-5.28	1.32	1.44
20	4	318	CLA	CAB-C3B	-5.28	1.33	1.47
20	B	813	CLA	O2D-CGD	5.28	1.46	1.33
20	A	825	CLA	C3D-C4D	-5.27	1.32	1.44
20	B	824	CLA	CHD-C1D	5.27	1.48	1.38
20	2	308	CLA	CHC-C1C	5.27	1.48	1.38
20	3	310	CLA	C4C-C3C	-5.27	1.36	1.45
20	4	313	CLA	CHC-C4B	5.27	1.51	1.39
20	1	213	CLA	CHD-C1D	5.27	1.48	1.38
20	B	806	CLA	CAB-C3B	-5.26	1.33	1.47
20	A	804	CLA	O2A-CGA	5.26	1.48	1.33
20	A	849	CLA	CHC-C4B	5.26	1.51	1.39
20	B	811	CLA	CHD-C1D	5.26	1.51	1.38
20	2	307	CLA	C3D-C4D	-5.26	1.32	1.44
20	A	810	CLA	C3D-C4D	-5.26	1.32	1.44
20	F	207	CLA	CHD-C4C	5.26	1.51	1.39
20	A	811	CLA	O2D-CGD	5.26	1.46	1.33
20	A	808	CLA	C3D-C4D	-5.26	1.32	1.44
20	B	810	CLA	CAB-C3B	-5.25	1.33	1.47
20	H	108	CLA	CAB-C3B	-5.25	1.33	1.47
20	B	807	CLA	O2D-CGD	5.25	1.46	1.33
20	B	834	CLA	C3D-C4D	-5.24	1.32	1.44
20	B	829	CLA	CHD-C4C	5.24	1.51	1.39
20	L	203	CLA	O2D-CGD	5.24	1.46	1.33
20	2	314	CLA	C3D-C4D	-5.23	1.32	1.44
20	I	102	CLA	O2D-CGD	5.23	1.46	1.33
20	B	831	CLA	C3D-C4D	-5.23	1.32	1.44
20	I	102	CLA	CHC-C4B	5.23	1.51	1.39
20	B	820	CLA	CHD-C1D	5.23	1.48	1.38
20	L	202	CLA	O2D-CGD	5.23	1.46	1.33
20	B	841	CLA	CHD-C4C	5.23	1.51	1.39
20	A	828	CLA	O2D-CGD	5.22	1.46	1.33
20	1	211	CLA	C3D-C4D	-5.22	1.32	1.44
20	A	819	CLA	CHC-C4B	5.22	1.51	1.39
20	L	208	CLA	CHC-C4B	5.22	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	830	CLA	C3D-C4D	-5.21	1.32	1.44
20	B	802	CLA	O2D-CGD	5.21	1.46	1.33
20	F	207	CLA	C3A-C2A	-5.21	1.40	1.54
20	A	820	CLA	CHC-C4B	5.21	1.51	1.39
20	3	314	CLA	CHD-C1D	5.21	1.48	1.38
20	A	849	CLA	CHD-C4C	5.21	1.51	1.39
20	B	833	CLA	C3D-C4D	-5.20	1.32	1.44
20	2	310	CLA	O2D-CGD	5.20	1.46	1.33
20	3	310	CLA	CHC-C1C	5.20	1.48	1.38
20	B	819	CLA	CHD-C1D	5.20	1.48	1.38
20	A	827	CLA	CAB-C3B	-5.20	1.33	1.47
20	A	839	CLA	O2A-CGA	5.20	1.48	1.33
20	1	206	CLA	CHD-C4C	5.19	1.51	1.39
20	B	828	CLA	O2D-CGD	5.19	1.46	1.33
20	A	826	CLA	CAB-C3B	-5.19	1.33	1.47
20	A	839	CLA	CHD-C1D	5.19	1.48	1.38
20	L	202	CLA	C3D-C4D	-5.19	1.32	1.44
20	A	824	CLA	C3D-C4D	-5.19	1.32	1.44
20	B	820	CLA	CHD-C4C	5.19	1.51	1.39
20	B	830	CLA	CHD-C4C	5.19	1.51	1.39
20	3	310	CLA	O2D-CGD	5.19	1.46	1.33
20	4	312	CLA	CHD-C1D	5.19	1.51	1.38
20	3	303	CLA	CHC-C4B	5.18	1.51	1.39
20	1	203	CLA	CAB-C3B	-5.18	1.33	1.47
20	A	836	CLA	O2D-CGD	5.18	1.46	1.33
20	B	836	CLA	CAB-C3B	-5.18	1.33	1.47
20	1	213	CLA	O2D-CGD	5.18	1.46	1.33
20	1	203	CLA	CHD-C4C	5.18	1.51	1.39
20	F	201	CLA	C4C-C3C	-5.18	1.36	1.45
20	A	850	CLA	O2D-CGD	5.18	1.46	1.33
20	2	311	CLA	C3D-C4D	-5.18	1.32	1.44
20	A	833	CLA	C3D-C4D	-5.18	1.32	1.44
20	B	802	CLA	CAB-C3B	-5.17	1.33	1.47
20	A	803	CLA	CHD-C1D	5.17	1.48	1.38
20	H	101	CLA	O2A-CGA	5.17	1.48	1.33
20	1	213	CLA	C3A-C2A	-5.17	1.40	1.54
20	A	803	CLA	CHD-C4C	5.17	1.51	1.39
20	A	829	CLA	O2D-CGD	5.17	1.45	1.33
20	B	827	CLA	CAB-C3B	-5.16	1.33	1.47
20	2	312	CLA	O2D-CGD	5.16	1.45	1.33
20	4	317	CLA	CAB-C3B	-5.16	1.33	1.47
20	F	206	CLA	O2D-CGD	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	314	CLA	C4C-C3C	-5.16	1.36	1.45
20	B	828	CLA	CHC-C4B	5.16	1.51	1.39
20	B	837	CLA	CAB-C3B	-5.16	1.33	1.47
20	A	838	CLA	CHC-C4B	5.16	1.51	1.39
20	B	836	CLA	CHD-C4C	5.16	1.50	1.39
20	A	816	CLA	O2D-CGD	5.16	1.45	1.33
20	4	318	CLA	C3D-C4D	-5.16	1.32	1.44
20	F	201	CLA	C3D-C4D	-5.16	1.32	1.44
20	A	827	CLA	O2D-CGD	5.15	1.45	1.33
20	B	816	CLA	CHC-C4B	5.15	1.51	1.39
20	2	303	CLA	CHD-C4C	5.15	1.50	1.39
23	A	842	PQN	C10-C5	5.15	1.49	1.40
20	A	829	CLA	C3D-C4D	-5.15	1.32	1.44
20	A	805	CLA	O2A-CGA	5.15	1.48	1.33
20	B	809	CLA	C3D-C4D	-5.15	1.32	1.44
20	B	808	CLA	CHD-C1D	5.15	1.48	1.38
20	4	302	CLA	C3A-C2A	-5.15	1.49	1.54
20	1	201	CLA	CHD-C4C	5.15	1.50	1.39
20	1	203	CLA	O2D-CGD	5.15	1.45	1.33
20	1	207	CLA	CHC-C4B	5.15	1.51	1.39
20	3	311	CLA	C3D-C4D	-5.15	1.32	1.44
20	B	821	CLA	O2D-CGD	5.15	1.45	1.33
20	3	314	CLA	O2D-CGD	5.14	1.45	1.33
20	2	302	CLA	CHC-C4B	5.14	1.50	1.39
20	B	829	CLA	CAB-C3B	-5.14	1.33	1.47
20	A	810	CLA	CHC-C4B	5.14	1.50	1.39
20	3	310	CLA	CAB-C3B	-5.14	1.33	1.47
20	A	812	CLA	CHC-C4B	5.13	1.50	1.39
20	A	834	CLA	CAB-C3B	-5.13	1.33	1.47
20	A	851	CLA	O2D-CGD	5.13	1.45	1.33
20	B	808	CLA	CHD-C4C	5.13	1.50	1.39
20	B	834	CLA	CAB-C3B	-5.13	1.33	1.47
20	K	104	CLA	CAB-C3B	-5.13	1.33	1.47
20	A	839	CLA	C3D-C4D	-5.13	1.32	1.44
20	B	815	CLA	CAB-C3B	-5.12	1.33	1.47
20	B	822	CLA	CHD-C1D	5.12	1.48	1.38
20	4	306	CLA	C4C-C3C	-5.11	1.36	1.45
20	B	842	CLA	CHC-C4B	5.11	1.50	1.39
20	A	808	CLA	O2D-CGD	5.11	1.45	1.33
20	4	306	CLA	C1B-NB	-5.11	1.31	1.37
20	3	301	CLA	CHC-C4B	5.11	1.50	1.39
20	B	817	CLA	CHC-C4B	5.11	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	809	CLA	O2D-CGD	5.10	1.45	1.33
20	4	306	CLA	CAB-C3B	-5.10	1.33	1.47
20	B	838	CLA	CAB-C3B	-5.10	1.33	1.47
20	A	838	CLA	C3D-C4D	-5.10	1.32	1.44
20	F	206	CLA	C3D-C4D	-5.10	1.32	1.44
20	J	101	CLA	C3D-C4D	-5.10	1.32	1.44
20	B	819	CLA	CHD-C4C	5.09	1.50	1.39
20	K	101	CLA	O2D-CGD	5.09	1.45	1.33
20	I	102	CLA	C3D-C4D	-5.09	1.32	1.44
20	L	203	CLA	C3D-C4D	-5.09	1.32	1.44
20	4	303	CLA	CHD-C1D	5.09	1.48	1.38
20	2	302	CLA	O2D-CGD	5.09	1.45	1.33
20	2	303	CLA	O2D-CGD	5.09	1.45	1.33
20	F	201	CLA	O2D-CGD	5.09	1.45	1.33
20	A	837	CLA	O2D-CGD	5.09	1.45	1.33
20	A	831	CLA	C4C-C3C	-5.08	1.36	1.45
20	H	109	CLA	CHC-C4B	5.08	1.50	1.39
20	2	314	CLA	CAB-C3B	-5.08	1.33	1.47
20	A	849	CLA	CHD-C1D	5.08	1.48	1.38
20	2	312	CLA	CHD-C4C	5.08	1.50	1.39
20	A	804	CLA	CAB-C3B	-5.08	1.33	1.47
20	B	811	CLA	CHC-C1C	5.08	1.48	1.38
20	B	840	CLA	CHC-C4B	5.08	1.50	1.39
20	1	206	CLA	CHC-C4B	5.08	1.50	1.39
20	B	808	CLA	CAB-C3B	-5.07	1.33	1.47
20	A	835	CLA	C3D-C4D	-5.07	1.32	1.44
20	B	835	CLA	C3D-C4D	-5.07	1.32	1.44
20	2	303	CLA	CAB-C3B	-5.07	1.33	1.47
20	A	836	CLA	C3D-C4D	-5.07	1.32	1.44
20	F	205	CLA	C3D-C4D	-5.06	1.32	1.44
20	F	206	CLA	C3A-C2A	-5.06	1.50	1.54
20	A	835	CLA	O2D-CGD	5.06	1.45	1.33
20	A	823	CLA	C3D-C4D	-5.06	1.32	1.44
20	1	206	CLA	CHD-C1D	5.06	1.48	1.38
20	1	205	CLA	CHC-C4B	5.06	1.50	1.39
20	4	305	CLA	O2D-CGD	5.06	1.45	1.33
20	A	809	CLA	CHC-C1C	5.06	1.48	1.38
20	R	108	CLA	CHC-C4B	5.05	1.50	1.39
20	J	103	CLA	CHD-C1D	5.05	1.48	1.38
20	B	823	CLA	C3D-C4D	-5.05	1.32	1.44
20	4	309	CLA	CHD-C1D	5.05	1.50	1.38
20	A	850	CLA	CAB-C3B	-5.05	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	302	CLA	CAB-C3B	-5.05	1.33	1.47
20	A	816	CLA	CHD-C4C	5.05	1.50	1.39
20	B	807	CLA	CHC-C4B	5.05	1.50	1.39
20	B	814	CLA	O2D-CGD	5.05	1.45	1.33
20	4	307	CLA	CHD-C1D	5.05	1.50	1.38
20	B	829	CLA	O2D-CGD	5.04	1.45	1.33
20	3	317	CLA	CHC-C4B	5.04	1.50	1.39
20	B	803	CLA	CAB-C3B	-5.04	1.33	1.47
20	2	311	CLA	O2A-CGA	5.04	1.48	1.33
20	A	829	CLA	O2A-CGA	5.04	1.48	1.33
20	B	812	CLA	CHC-C4B	5.04	1.50	1.39
20	A	851	CLA	C3D-C4D	-5.04	1.32	1.44
20	2	312	CLA	CHC-C4B	5.04	1.50	1.39
20	B	812	CLA	CHD-C4C	5.04	1.50	1.39
20	2	305	CLA	CHC-C4B	5.03	1.50	1.39
20	2	316	CLA	CHD-C4C	5.03	1.50	1.39
20	A	823	CLA	CHC-C4B	5.03	1.50	1.39
20	K	101	CLA	CHC-C4B	5.02	1.50	1.39
20	1	203	CLA	CHC-C4B	5.02	1.50	1.39
20	A	820	CLA	C3D-C4D	-5.02	1.32	1.44
20	L	204	CLA	CHC-C4B	5.02	1.50	1.39
20	B	837	CLA	O2D-CGD	5.02	1.45	1.33
20	B	841	CLA	O2D-CGD	5.02	1.45	1.33
20	2	312	CLA	CAB-C3B	-5.02	1.34	1.47
20	F	201	CLA	CAB-C3B	-5.02	1.34	1.47
20	B	836	CLA	CHD-C1D	5.02	1.48	1.38
20	B	822	CLA	CHC-C4B	5.01	1.50	1.39
20	2	316	CLA	CAB-C3B	-5.01	1.34	1.47
20	4	303	CLA	CAB-C3B	-5.01	1.34	1.47
20	A	836	CLA	CAB-C3B	-5.01	1.34	1.47
20	B	819	CLA	CAB-C3B	-5.01	1.34	1.47
20	4	301	CLA	C3D-C4D	-5.01	1.32	1.44
20	A	804	CLA	CHC-C4B	5.01	1.50	1.39
20	A	839	CLA	CHD-C4C	5.01	1.50	1.39
20	A	832	CLA	C3D-C4D	-5.01	1.32	1.44
20	H	102	CLA	CHC-C4B	5.01	1.50	1.39
20	2	316	CLA	O2D-CGD	5.00	1.45	1.33
20	1	207	CLA	O2D-CGD	5.00	1.45	1.33
20	J	103	CLA	CHD-C4C	5.00	1.50	1.39
20	A	834	CLA	CHC-C4B	5.00	1.50	1.39
20	4	301	CLA	CAB-C3B	-5.00	1.34	1.47
20	B	820	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	O2D-CGD	4.99	1.45	1.33
20	A	850	CLA	O2A-CGA	4.99	1.47	1.33
20	B	850	CLA	C3D-C4D	-4.99	1.33	1.44
20	B	827	CLA	C3D-C4D	-4.99	1.33	1.44
20	A	815	CLA	CHC-C4B	4.99	1.50	1.39
20	4	315	CLA	CAB-C3B	-4.99	1.34	1.47
20	B	806	CLA	CHC-C4B	4.98	1.50	1.39
20	2	307	CLA	CHC-C1C	4.98	1.48	1.38
20	B	821	CLA	CHC-C4B	4.98	1.50	1.39
20	L	202	CLA	CHC-C4B	4.98	1.50	1.39
20	A	807	CLA	C3D-C4D	-4.98	1.33	1.44
20	B	838	CLA	C3D-C4D	-4.98	1.33	1.44
20	A	818	CLA	C4C-C3C	-4.98	1.36	1.45
20	A	823	CLA	O2D-CGD	4.98	1.45	1.33
20	B	818	CLA	CHC-C4B	4.97	1.50	1.39
20	A	809	CLA	O2D-CGD	4.97	1.45	1.33
20	B	827	CLA	O2D-CGD	4.97	1.45	1.33
20	3	307	CLA	CAB-C3B	-4.97	1.34	1.47
20	L	201	CLA	CHC-C4B	4.96	1.50	1.39
20	L	207	CLA	CAB-C3B	-4.96	1.34	1.47
20	3	301	CLA	C3D-C4D	-4.96	1.33	1.44
20	1	215	CLA	C4C-C3C	-4.96	1.36	1.45
20	B	840	CLA	C3D-C4D	-4.96	1.33	1.44
20	2	314	CLA	CHD-C4C	4.96	1.50	1.39
20	B	831	CLA	CHC-C4B	4.96	1.50	1.39
20	A	817	CLA	CHC-C4B	4.96	1.50	1.39
20	R	108	CLA	O2A-CGA	4.96	1.47	1.33
20	A	811	CLA	CAB-C3B	-4.96	1.34	1.47
20	A	826	CLA	CHC-C4B	4.95	1.50	1.39
20	B	834	CLA	CHC-C4B	4.95	1.50	1.39
20	1	215	CLA	CHC-C4B	4.95	1.50	1.39
20	4	315	CLA	CHC-C4B	4.95	1.50	1.39
20	B	802	CLA	C3D-C4D	-4.95	1.33	1.44
20	4	310	CLA	CHD-C4C	4.95	1.50	1.39
20	4	305	CLA	CHD-C1D	4.94	1.48	1.38
20	G	105	CLA	CHC-C4B	4.94	1.50	1.39
20	A	813	CLA	O2D-CGD	4.94	1.45	1.33
20	3	311	CLA	CHC-C4B	4.94	1.50	1.39
20	L	204	CLA	OBD-CAD	4.94	1.31	1.22
20	A	804	CLA	C3D-C4D	-4.94	1.33	1.44
20	R	107	CLA	CHC-C4B	4.94	1.50	1.39
20	B	828	CLA	CAB-C3B	-4.94	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	C3D-C4D	-4.93	1.33	1.44
20	B	841	CLA	CAB-C3B	-4.93	1.34	1.47
20	B	829	CLA	C3D-C4D	-4.93	1.33	1.44
20	B	824	CLA	CHD-C4C	4.93	1.50	1.39
20	H	110	CLA	C3D-C4D	-4.93	1.33	1.44
20	4	305	CLA	CAB-C3B	-4.93	1.34	1.47
20	J	101	CLA	CAB-C3B	-4.93	1.34	1.47
20	A	828	CLA	C3D-C4D	-4.93	1.33	1.44
20	B	820	CLA	CHC-C4B	4.93	1.50	1.39
20	F	205	CLA	CHC-C4B	4.93	1.50	1.39
20	G	105	CLA	CAB-C3B	-4.93	1.34	1.47
20	3	306	CLA	CHD-C1D	4.93	1.50	1.38
20	I	102	CLA	CAB-C3B	-4.93	1.34	1.47
20	2	307	CLA	CAB-C3B	-4.93	1.34	1.47
20	A	851	CLA	CHC-C4B	4.92	1.50	1.39
20	2	312	CLA	CHD-C1D	4.92	1.48	1.38
20	1	212	CLA	CHD-C1D	4.92	1.50	1.38
20	2	302	CLA	CHD-C4C	4.92	1.50	1.39
20	3	317	CLA	C3D-C4D	-4.92	1.33	1.44
20	1	201	CLA	O2D-CGD	4.92	1.45	1.33
20	A	818	CLA	CHD-C4C	4.92	1.50	1.39
20	3	309	CLA	CHD-C1D	4.92	1.50	1.38
20	B	839	CLA	CAB-C3B	-4.92	1.34	1.47
20	B	807	CLA	C3D-C4D	-4.91	1.33	1.44
20	4	302	CLA	CHC-C4B	4.91	1.50	1.39
20	3	302	CLA	CHD-C1D	4.91	1.50	1.38
20	B	833	CLA	CAB-C3B	-4.91	1.34	1.47
20	1	209	CLA	CHD-C1D	4.91	1.50	1.38
20	A	808	CLA	CHC-C4B	4.91	1.50	1.39
20	R	107	CLA	O2A-CGA	4.91	1.47	1.33
20	L	203	CLA	CAB-C3B	-4.91	1.34	1.47
20	A	809	CLA	CAB-C3B	-4.91	1.34	1.47
20	L	202	CLA	CAB-C3B	-4.90	1.34	1.47
20	A	826	CLA	C3D-C4D	-4.90	1.33	1.44
20	B	820	CLA	C3D-C4D	-4.90	1.33	1.44
20	B	827	CLA	CHC-C4B	4.90	1.50	1.39
20	A	824	CLA	O2D-CGD	4.90	1.45	1.33
20	A	817	CLA	C3D-C4D	-4.90	1.33	1.44
20	B	815	CLA	CHC-C4B	4.90	1.50	1.39
20	1	213	CLA	CAB-C3B	-4.90	1.34	1.47
20	A	807	CLA	CAB-C3B	-4.90	1.34	1.47
20	A	823	CLA	CAB-C3B	-4.89	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	K	104	CLA	O2D-CGD	4.89	1.45	1.33
20	A	817	CLA	CAB-C3B	-4.89	1.34	1.47
20	A	805	CLA	C3D-C4D	-4.89	1.33	1.44
20	A	824	CLA	CHC-C4B	4.89	1.50	1.39
20	A	822	CLA	O2A-CGA	4.89	1.47	1.33
20	L	204	CLA	CAB-C3B	-4.89	1.34	1.47
20	I	102	CLA	O2A-CGA	4.89	1.47	1.33
20	L	208	CLA	CAB-C3B	-4.89	1.34	1.47
20	A	806	CLA	C3D-C4D	-4.89	1.33	1.44
20	2	316	CLA	CHD-C1D	4.88	1.48	1.38
20	A	809	CLA	C3D-C4D	-4.88	1.33	1.44
20	B	850	CLA	O2D-CGD	4.88	1.45	1.33
20	H	108	CLA	C1B-NB	-4.88	1.31	1.37
20	3	311	CLA	CAB-C3B	-4.88	1.34	1.47
20	A	812	CLA	C3D-C4D	-4.88	1.33	1.44
20	A	827	CLA	O2A-CGA	4.87	1.47	1.33
20	F	201	CLA	CHC-C1C	4.87	1.48	1.38
20	4	308	CLA	CHD-C1D	4.87	1.50	1.38
20	B	837	CLA	C3D-C4D	-4.87	1.33	1.44
20	B	836	CLA	O2D-CGD	4.87	1.45	1.33
20	A	830	CLA	C3D-C4D	-4.87	1.33	1.44
20	B	835	CLA	CHC-C4B	4.87	1.50	1.39
20	A	804	CLA	O2D-CGD	4.87	1.45	1.33
20	A	818	CLA	O2D-CGD	4.87	1.45	1.33
23	B	843	PQN	C10-C5	4.87	1.48	1.40
20	4	317	CLA	C3D-C4D	-4.87	1.33	1.44
20	K	103	CLA	CAB-C3B	-4.86	1.34	1.47
22	F	204	BCR	C21-C22	-4.86	1.24	1.35
20	2	302	CLA	CHD-C1D	4.86	1.47	1.38
20	B	812	CLA	CHD-C1D	4.86	1.47	1.38
20	B	838	CLA	O2D-CGD	4.86	1.45	1.33
20	1	205	CLA	C3D-C4D	-4.86	1.33	1.44
20	A	822	CLA	CHC-C4B	4.86	1.50	1.39
20	L	204	CLA	C3D-C4D	-4.86	1.33	1.44
20	L	201	CLA	CAB-C3B	-4.86	1.34	1.47
20	4	301	CLA	CHC-C4B	4.86	1.50	1.39
20	B	826	CLA	O2D-CGD	4.86	1.45	1.33
20	B	818	CLA	O2A-CGA	4.86	1.47	1.33
20	4	315	CLA	C3D-C4D	-4.85	1.33	1.44
20	K	101	CLA	CAB-C3B	-4.85	1.34	1.47
20	B	831	CLA	CAB-C3B	-4.85	1.34	1.47
20	A	803	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	CHC-C4B	4.85	1.50	1.39
20	3	315	CLA	CHD-C1D	4.85	1.50	1.38
20	A	840	CLA	CHC-C4B	4.85	1.50	1.39
20	B	850	CLA	CAB-C3B	-4.85	1.34	1.47
20	A	821	CLA	CAB-C3B	-4.84	1.34	1.47
20	1	201	CLA	CHC-C1C	4.84	1.48	1.38
20	B	802	CLA	CHC-C4B	4.84	1.50	1.39
20	3	312	CLA	CHD-C1D	4.84	1.50	1.38
20	B	825	CLA	C3D-C4D	-4.84	1.33	1.44
20	A	815	CLA	C3D-C4D	-4.84	1.33	1.44
20	B	820	CLA	CAB-C3B	-4.84	1.34	1.47
20	A	850	CLA	CHC-C4B	4.84	1.50	1.39
20	B	829	CLA	CHC-C4B	4.84	1.50	1.39
20	1	210	CLA	C3D-C4D	-4.84	1.33	1.44
20	B	841	CLA	C3D-C4D	-4.84	1.33	1.44
20	B	806	CLA	C3D-C4D	-4.83	1.33	1.44
20	4	315	CLA	CHD-C1D	4.83	1.47	1.38
20	J	101	CLA	CHC-C4B	4.83	1.50	1.39
20	R	107	CLA	C3D-C4D	-4.83	1.33	1.44
20	A	825	CLA	O2D-CGD	4.83	1.45	1.33
20	4	315	CLA	CHD-C4C	4.83	1.50	1.39
20	A	806	CLA	CHC-C4B	4.83	1.50	1.39
20	A	838	CLA	CAB-C3B	-4.83	1.34	1.47
20	1	215	CLA	C3D-C4D	-4.83	1.33	1.44
20	A	849	CLA	CAB-C3B	-4.83	1.34	1.47
20	2	310	CLA	C1B-NB	-4.83	1.31	1.37
20	B	836	CLA	CHC-C4B	4.83	1.50	1.39
20	F	206	CLA	CAB-C3B	-4.82	1.34	1.47
20	A	811	CLA	CHC-C4B	4.82	1.50	1.39
20	A	807	CLA	CHC-C4B	4.82	1.50	1.39
20	1	211	CLA	CHD-C4C	4.82	1.50	1.39
20	A	830	CLA	CAB-C3B	-4.82	1.34	1.47
20	3	303	CLA	C3D-C4D	-4.81	1.33	1.44
20	2	311	CLA	CHC-C4B	4.81	1.50	1.39
20	B	822	CLA	C3D-C4D	-4.81	1.33	1.44
20	B	821	CLA	CAB-C3B	-4.81	1.34	1.47
20	H	109	CLA	C3D-C4D	-4.81	1.33	1.44
20	B	839	CLA	CHD-C4C	4.81	1.50	1.39
20	A	801	CLA	O2A-CGA	4.81	1.47	1.33
20	2	302	CLA	C4C-C3C	-4.81	1.36	1.45
20	H	108	CLA	O2D-CGD	4.80	1.45	1.33
20	4	303	CLA	C3D-C4D	-4.80	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	813	CLA	C3D-C4D	-4.80	1.33	1.44
20	3	304	CLA	CHD-C1D	4.80	1.50	1.38
20	1	211	CLA	O2A-CGA	4.80	1.47	1.33
20	A	840	CLA	CAB-C3B	-4.80	1.34	1.47
20	A	816	CLA	CHC-C4B	4.80	1.50	1.39
20	A	819	CLA	C3D-C4D	-4.80	1.33	1.44
20	4	304	CLA	CAB-C3B	-4.79	1.34	1.47
20	3	308	CLA	CHD-C1D	4.79	1.50	1.38
20	B	813	CLA	C3D-C4D	-4.79	1.33	1.44
20	A	828	CLA	CHC-C4B	4.79	1.50	1.39
20	1	207	CLA	C3D-C4D	-4.79	1.33	1.44
20	B	815	CLA	C3D-C4D	-4.79	1.33	1.44
20	B	816	CLA	C3D-C4D	-4.79	1.33	1.44
20	A	811	CLA	O2A-CGA	4.79	1.47	1.33
20	1	207	CLA	CAB-C3B	-4.79	1.34	1.47
20	3	310	CLA	CHD-C1D	4.78	1.47	1.38
20	A	811	CLA	C3D-C4D	-4.78	1.33	1.44
20	A	827	CLA	CHC-C4B	4.78	1.50	1.39
20	A	814	CLA	CHD-C1D	4.78	1.50	1.38
20	L	207	CLA	C3D-C4D	-4.78	1.33	1.44
20	A	816	CLA	CAB-C3B	-4.78	1.34	1.47
20	B	814	CLA	C3D-C4D	-4.78	1.33	1.44
20	A	808	CLA	O2A-CGA	4.78	1.47	1.33
20	K	102	CLA	CAB-C3B	-4.78	1.34	1.47
20	1	207	CLA	O2A-CGA	4.77	1.47	1.33
20	B	815	CLA	O2A-CGA	4.77	1.47	1.33
20	H	101	CLA	CHC-C4B	4.77	1.50	1.39
20	A	835	CLA	CHC-C4B	4.77	1.50	1.39
20	A	812	CLA	O2A-CGA	4.77	1.47	1.33
20	2	301	CLA	CHD-C1D	4.77	1.50	1.38
20	B	826	CLA	CHC-C4B	4.77	1.50	1.39
20	3	313	CLA	C3D-C4D	-4.77	1.33	1.44
20	B	818	CLA	C3D-C4D	-4.77	1.33	1.44
20	1	206	CLA	CAB-C3B	-4.77	1.34	1.47
20	1	206	CLA	C3D-C4D	-4.76	1.33	1.44
20	A	829	CLA	CAB-C3B	-4.76	1.34	1.47
20	B	837	CLA	O2A-CGA	4.76	1.47	1.33
20	B	810	CLA	O2A-CGA	4.76	1.47	1.33
20	H	102	CLA	C3D-C4D	-4.76	1.33	1.44
20	B	807	CLA	CAB-C3B	-4.76	1.34	1.47
20	2	314	CLA	CHD-C1D	4.75	1.47	1.38
20	F	207	CLA	CAB-C3B	-4.75	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	807	CLA	O2A-CGA	4.75	1.46	1.30
20	A	826	CLA	O2D-CGD	4.75	1.44	1.33
20	1	213	CLA	OBD-CAD	4.75	1.30	1.22
20	A	829	CLA	CHC-C4B	4.75	1.50	1.39
20	1	208	CLA	CHD-C1D	4.75	1.50	1.38
20	4	305	CLA	CHD-C4C	4.74	1.50	1.39
20	B	822	CLA	O2A-CGA	4.74	1.47	1.33
20	4	315	CLA	O2D-CGD	4.74	1.44	1.33
20	B	824	CLA	CHC-C4B	4.74	1.50	1.39
20	2	305	CLA	CAB-C3B	-4.74	1.34	1.47
20	4	304	CLA	O2A-CGA	4.74	1.47	1.33
20	A	830	CLA	CHC-C4B	4.74	1.50	1.39
20	B	842	CLA	C3D-C4D	-4.74	1.33	1.44
20	2	307	CLA	O2A-CGA	4.73	1.47	1.33
20	B	824	CLA	C1B-NB	-4.73	1.31	1.37
20	L	204	CLA	O2A-CGA	4.73	1.47	1.33
20	A	825	CLA	CHC-C4B	4.73	1.50	1.39
20	1	202	CLA	C3D-C4D	-4.73	1.33	1.44
20	A	822	CLA	C3D-C4D	-4.73	1.33	1.44
20	K	102	CLA	CHC-C4B	4.72	1.50	1.39
20	A	833	CLA	CHC-C4B	4.72	1.50	1.39
20	B	840	CLA	O2A-CGA	4.72	1.47	1.33
20	1	201	CLA	CAB-C3B	-4.72	1.34	1.47
20	B	825	CLA	CHC-C4B	4.72	1.50	1.39
20	A	810	CLA	O2A-CGA	4.71	1.46	1.30
20	L	203	CLA	CHC-C4B	4.71	1.50	1.39
20	A	813	CLA	CHC-C4B	4.71	1.50	1.39
20	B	820	CLA	O2A-CGA	4.71	1.47	1.33
20	B	825	CLA	OBD-CAD	4.71	1.30	1.22
20	A	821	CLA	C3D-C4D	-4.71	1.33	1.44
20	1	211	CLA	C4C-C3C	-4.71	1.37	1.45
22	A	844	BCR	C21-C22	-4.70	1.24	1.35
20	4	314	CLA	CHD-C1D	4.70	1.49	1.38
20	J	103	CLA	O2D-CGD	4.70	1.44	1.33
20	L	201	CLA	C3D-C4D	-4.70	1.33	1.44
20	B	823	CLA	CHC-C4B	4.70	1.50	1.39
20	A	837	CLA	C3D-C4D	-4.70	1.33	1.44
20	L	201	CLA	O2A-CGA	4.69	1.47	1.33
20	4	304	CLA	C3D-C4D	-4.69	1.33	1.44
20	2	305	CLA	C3D-C4D	-4.69	1.33	1.44
20	B	817	CLA	C3D-C4D	-4.69	1.33	1.44
20	H	101	CLA	CAB-C3B	-4.69	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	108	CLA	CAB-C3B	-4.69	1.34	1.47
20	B	821	CLA	C3D-C4D	-4.68	1.33	1.44
20	K	104	CLA	CHC-C4B	4.68	1.49	1.39
20	A	817	CLA	O2A-CGA	4.68	1.47	1.33
20	H	109	CLA	CAB-C3B	-4.68	1.34	1.47
20	1	214	CLA	CHD-C1D	4.68	1.49	1.38
20	A	850	CLA	C3D-C4D	-4.68	1.33	1.44
20	4	310	CLA	CHD-C1D	4.68	1.47	1.38
20	A	822	CLA	CAB-C3B	-4.67	1.34	1.47
20	A	832	CLA	CHC-C4B	4.67	1.49	1.39
20	B	818	CLA	CAB-C3B	-4.67	1.34	1.47
20	B	819	CLA	CHC-C4B	4.67	1.49	1.39
20	B	832	CLA	O2A-CGA	4.67	1.47	1.33
20	3	310	CLA	CHD-C4C	4.67	1.49	1.39
20	B	837	CLA	CHC-C4B	4.67	1.49	1.39
20	1	211	CLA	CHD-C1D	4.67	1.47	1.38
20	B	831	CLA	O2A-CGA	4.66	1.46	1.33
20	3	305	CLA	CHD-C1D	4.66	1.49	1.38
20	1	206	CLA	OBD-CAD	4.66	1.30	1.22
20	H	108	CLA	CHD-C1D	4.66	1.47	1.38
20	A	819	CLA	CAB-C3B	-4.65	1.35	1.47
20	2	303	CLA	O2A-CGA	4.65	1.46	1.33
22	B	801	BCR	C20-C19	-4.65	1.22	1.34
20	A	831	CLA	CHD-C1D	4.65	1.47	1.38
20	H	108	CLA	CHD-C4C	4.65	1.49	1.39
20	B	839	CLA	O2D-CGD	4.65	1.44	1.33
20	B	810	CLA	CHC-C4B	4.65	1.49	1.39
20	A	832	CLA	CAB-C3B	-4.65	1.35	1.47
20	4	313	CLA	C3D-C4D	-4.64	1.33	1.44
20	B	813	CLA	CHC-C4B	4.64	1.49	1.39
20	A	836	CLA	CHC-C4B	4.64	1.49	1.39
20	H	102	CLA	CAB-C3B	-4.64	1.35	1.47
20	4	310	CLA	CAB-C3B	-4.64	1.35	1.47
20	B	839	CLA	CHC-C4B	4.64	1.49	1.39
20	H	109	CLA	O2A-CGA	4.64	1.46	1.33
20	A	820	CLA	O2A-CGA	4.63	1.46	1.33
20	A	809	CLA	O2A-CGA	4.63	1.46	1.33
20	2	305	CLA	O2A-CGA	4.63	1.46	1.33
20	B	821	CLA	O2A-CGA	4.63	1.46	1.33
20	B	802	CLA	O2A-CGA	4.63	1.46	1.33
20	R	108	CLA	C3D-C4D	-4.63	1.33	1.44
20	A	810	CLA	CAB-C3B	-4.63	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	819	CLA	O2D-CGD	4.62	1.44	1.33
20	A	830	CLA	O2D-CGD	4.62	1.44	1.33
20	4	305	CLA	C4C-C3C	-4.62	1.37	1.45
20	4	310	CLA	C4C-C3C	-4.62	1.37	1.45
20	H	110	CLA	O2A-CGA	4.61	1.46	1.33
20	A	813	CLA	CAB-C3B	-4.61	1.35	1.47
20	B	803	CLA	CHC-C4B	4.61	1.49	1.39
20	L	207	CLA	O2A-CGA	4.61	1.46	1.33
20	H	102	CLA	O2A-CGA	4.61	1.46	1.33
22	I	103	BCR	C21-C22	-4.61	1.25	1.35
20	A	836	CLA	OBD-CAD	4.61	1.30	1.22
20	1	202	CLA	CAB-C3B	-4.60	1.35	1.47
20	A	825	CLA	O2A-CGA	4.60	1.46	1.33
22	F	203	BCR	C21-C22	-4.60	1.25	1.35
20	A	815	CLA	O2A-CGA	4.59	1.46	1.33
20	1	206	CLA	O2A-CGA	4.59	1.46	1.33
20	4	318	CLA	O2D-CGD	4.59	1.44	1.33
20	A	815	CLA	CAB-C3B	-4.59	1.35	1.47
20	B	816	CLA	O2A-CGA	4.59	1.46	1.33
20	A	832	CLA	O2A-CGA	4.58	1.46	1.33
20	B	841	CLA	O2A-CGA	4.58	1.46	1.33
20	B	825	CLA	O2A-CGA	4.58	1.46	1.33
20	A	835	CLA	O2A-CGA	4.58	1.46	1.33
20	B	816	CLA	CAB-C3B	-4.58	1.35	1.47
20	A	821	CLA	CHC-C4B	4.57	1.49	1.39
20	K	103	CLA	CHC-C4B	4.57	1.49	1.39
20	2	303	CLA	C4C-C3C	-4.57	1.37	1.45
20	B	813	CLA	O2A-CGA	4.57	1.46	1.33
20	B	810	CLA	C3D-C4D	-4.57	1.33	1.44
20	A	833	CLA	CAB-C3B	-4.57	1.35	1.47
20	4	311	CLA	CHD-C1D	4.57	1.49	1.38
20	A	805	CLA	CAB-C3B	-4.57	1.35	1.47
20	L	208	CLA	C3D-C4D	-4.57	1.33	1.44
20	L	208	CLA	O2A-CGA	4.57	1.46	1.33
20	A	827	CLA	C3D-C4D	-4.56	1.33	1.44
20	J	103	CLA	CHC-C4B	4.56	1.49	1.39
20	A	828	CLA	O2A-CGA	4.56	1.46	1.33
20	A	831	CLA	O2D-CGD	4.56	1.44	1.33
20	B	833	CLA	CHC-C4B	4.56	1.49	1.39
20	F	201	CLA	CHD-C4C	4.55	1.49	1.39
20	B	817	CLA	CAB-C3B	-4.55	1.35	1.47
20	B	834	CLA	O2A-CGA	4.55	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	211	CLA	CHC-C4B	4.55	1.49	1.39
20	3	314	CLA	CHC-C1C	4.54	1.47	1.38
22	B	846	BCR	C21-C22	-4.54	1.25	1.35
22	A	845	BCR	C21-C22	-4.54	1.25	1.35
20	A	825	CLA	CAB-C3B	-4.53	1.35	1.47
20	B	830	CLA	CAB-C3B	-4.53	1.35	1.47
20	B	814	CLA	O2A-CGA	4.53	1.46	1.33
20	2	311	CLA	CAB-C3B	-4.53	1.35	1.47
20	4	314	CLA	CHC-C4B	4.53	1.51	1.39
20	B	841	CLA	CHC-C4B	4.53	1.49	1.39
20	B	835	CLA	O2A-CGA	4.53	1.45	1.30
20	A	801	CLA	CHC-C4B	4.52	1.49	1.39
20	L	202	CLA	O2A-CGA	4.52	1.46	1.33
20	B	803	CLA	C3D-C4D	-4.51	1.34	1.44
20	H	110	CLA	CAB-C3B	-4.51	1.35	1.47
20	A	819	CLA	O2A-CGA	4.51	1.46	1.33
20	F	207	CLA	CHC-C4B	4.51	1.49	1.39
20	3	313	CLA	O2A-CGA	4.51	1.46	1.33
20	B	808	CLA	CHC-C4B	4.51	1.49	1.39
20	B	803	CLA	O2A-CGA	4.51	1.46	1.33
20	R	107	CLA	CAB-C3B	-4.50	1.35	1.47
20	B	819	CLA	C4C-C3C	-4.50	1.37	1.45
20	B	839	CLA	CHD-C1D	4.50	1.47	1.38
20	A	820	CLA	CAB-C3B	-4.50	1.35	1.47
20	1	215	CLA	O2A-CGA	4.50	1.46	1.33
20	4	305	CLA	CHC-C4B	4.49	1.49	1.39
20	A	840	CLA	C3D-C4D	-4.49	1.34	1.44
22	A	843	BCR	C21-C22	-4.49	1.25	1.35
20	A	838	CLA	O2A-CGA	4.48	1.46	1.33
20	B	839	CLA	O2A-CGA	4.48	1.46	1.33
20	A	830	CLA	O2A-CGA	4.47	1.46	1.33
20	A	828	CLA	CAB-C3B	-4.47	1.35	1.47
20	A	813	CLA	O2A-CGA	4.47	1.46	1.33
20	H	108	CLA	O2A-CGA	4.47	1.46	1.33
20	3	313	CLA	CAB-C3B	-4.47	1.35	1.47
20	1	202	CLA	CHC-C4B	4.47	1.49	1.39
22	2	317	BCR	C21-C22	-4.47	1.25	1.35
20	K	104	CLA	O2A-CGA	4.45	1.46	1.33
20	1	203	CLA	C4C-C3C	-4.45	1.37	1.45
20	B	830	CLA	CHC-C4B	4.45	1.49	1.39
20	4	302	CLA	OBD-CAD	4.45	1.30	1.22
20	A	805	CLA	CHC-C4B	4.44	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	215	CLA	CAB-C3B	-4.44	1.35	1.47
20	1	205	CLA	OBD-CAD	4.44	1.30	1.22
20	B	824	CLA	O2D-CGD	4.44	1.44	1.33
20	1	213	CLA	O2A-CGA	4.43	1.46	1.33
22	L	209	BCR	C21-C22	-4.42	1.25	1.35
20	R	108	CLA	OBD-CAD	4.42	1.30	1.22
20	J	101	CLA	O2A-CGA	4.42	1.46	1.33
20	B	809	CLA	CHC-C4B	4.42	1.49	1.39
20	B	828	CLA	O2A-CGA	4.41	1.46	1.33
20	B	826	CLA	O2A-CGA	4.41	1.46	1.33
20	3	310	CLA	CHC-C4B	4.41	1.49	1.39
22	J	102	BCR	C21-C22	-4.41	1.25	1.35
20	A	837	CLA	CHC-C4B	4.41	1.49	1.39
20	1	202	CLA	OBD-CAD	4.40	1.30	1.22
20	B	840	CLA	CAB-C3B	-4.40	1.35	1.47
20	A	806	CLA	CAB-C3B	-4.40	1.35	1.47
20	3	310	CLA	O2A-CGA	4.39	1.46	1.33
20	2	309	CLA	CHD-C1D	4.39	1.49	1.38
20	A	839	CLA	CHC-C4B	4.38	1.49	1.39
22	B	847	BCR	C21-C22	-4.38	1.25	1.35
20	A	804	CLA	OBD-CAD	4.38	1.30	1.22
20	2	303	CLA	CHC-C4B	4.38	1.49	1.39
20	1	213	CLA	C1B-NB	-4.38	1.32	1.37
20	A	851	CLA	OBD-CAD	4.38	1.30	1.22
20	3	311	CLA	O2A-CGA	4.37	1.46	1.33
20	1	215	CLA	CHD-C1D	4.37	1.46	1.38
20	2	314	CLA	CHC-C4B	4.37	1.49	1.39
20	A	831	CLA	CHD-C4C	4.37	1.49	1.39
20	4	304	CLA	CHC-C4B	4.37	1.49	1.39
20	A	806	CLA	OBD-CAD	4.36	1.30	1.22
20	A	840	CLA	O2A-CGA	4.36	1.46	1.33
25	B	848	LMG	O8-C28	4.36	1.46	1.33
20	3	307	CLA	C1C-C2C	-4.35	1.35	1.44
20	L	208	CLA	OBD-CAD	4.35	1.30	1.22
20	B	822	CLA	CAB-C3B	-4.35	1.35	1.47
20	4	304	CLA	OBD-CAD	4.35	1.30	1.22
20	B	808	CLA	C4C-C3C	-4.35	1.37	1.45
20	H	108	CLA	C4C-C3C	-4.35	1.37	1.45
20	H	109	CLA	OBD-CAD	4.34	1.30	1.22
20	4	306	CLA	CHC-C4B	4.34	1.49	1.39
20	4	318	CLA	CHC-C4B	4.34	1.49	1.39
20	2	316	CLA	CHC-C4B	4.34	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	838	CLA	CHC-C4B	4.34	1.49	1.39
20	G	105	CLA	O2A-CGA	4.34	1.46	1.33
20	2	308	CLA	MG-NA	-4.34	1.96	2.06
20	B	827	CLA	O2A-CGA	4.34	1.46	1.33
20	A	834	CLA	O2A-CGA	4.34	1.46	1.33
20	A	821	CLA	OBD-CAD	4.34	1.29	1.22
20	A	837	CLA	O2A-CGA	4.34	1.46	1.33
20	4	318	CLA	O2A-CGA	4.33	1.46	1.33
20	A	818	CLA	CHC-C4B	4.33	1.49	1.39
20	B	806	CLA	O2A-CGA	4.33	1.46	1.33
20	4	301	CLA	O2A-CGA	4.33	1.46	1.33
20	1	215	CLA	CHD-C4C	4.33	1.49	1.39
20	B	838	CLA	O2A-CGA	4.32	1.45	1.33
20	B	842	CLA	OBD-CAD	4.32	1.29	1.22
20	4	305	CLA	O2A-CGA	4.32	1.45	1.33
20	A	807	CLA	O2A-CGA	4.31	1.46	1.33
20	B	815	CLA	OBD-CAD	4.31	1.29	1.22
20	A	818	CLA	CHD-C1D	4.31	1.46	1.38
20	4	313	CLA	C3A-C2A	-4.30	1.50	1.54
20	1	204	CLA	C1B-NB	-4.30	1.32	1.37
20	4	317	CLA	CHC-C4B	4.30	1.49	1.39
20	K	103	CLA	C1B-NB	-4.30	1.32	1.37
20	2	306	CLA	CHD-C1D	4.30	1.48	1.38
20	B	822	CLA	OBD-CAD	4.28	1.29	1.22
25	B	848	LMG	O7-C10	4.28	1.46	1.34
20	B	812	CLA	O2A-CGA	4.28	1.45	1.33
20	4	306	CLA	O2A-CGA	4.28	1.45	1.33
20	B	812	CLA	C4C-C3C	-4.28	1.37	1.45
20	3	317	CLA	OBD-CAD	4.28	1.29	1.22
20	2	310	CLA	CHC-C4B	4.27	1.49	1.39
20	2	315	CLA	CHD-C1D	4.27	1.48	1.38
20	3	316	CLA	CHD-C1D	4.27	1.48	1.38
20	A	806	CLA	O2A-CGA	4.27	1.45	1.33
20	B	833	CLA	O2A-CGA	4.27	1.45	1.33
20	A	801	CLA	C3D-C4D	-4.26	1.34	1.44
20	A	836	CLA	O2A-CGA	4.26	1.45	1.33
20	A	823	CLA	O2A-CGA	4.26	1.45	1.33
20	3	303	CLA	OBD-CAD	4.26	1.29	1.22
20	A	849	CLA	C3D-C4D	-4.26	1.34	1.44
20	B	842	CLA	C3A-C2A	-4.26	1.50	1.54
20	B	824	CLA	O2A-CGA	4.25	1.45	1.33
20	2	302	CLA	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	314	CLA	C1C-C2C	-4.25	1.35	1.44
20	B	823	CLA	O2A-CGA	4.25	1.45	1.33
20	H	101	CLA	C3D-C4D	-4.25	1.34	1.44
20	A	803	CLA	O2A-CGA	4.24	1.46	1.33
20	B	817	CLA	OBD-CAD	4.24	1.29	1.22
20	1	201	CLA	O2A-CGA	4.24	1.46	1.33
20	2	316	CLA	O2A-CGA	4.23	1.45	1.33
20	A	816	CLA	C4C-C3C	-4.23	1.37	1.45
20	3	312	CLA	CHC-C4B	4.22	1.51	1.39
20	A	809	CLA	CHC-C4B	4.22	1.48	1.39
20	B	830	CLA	O2A-CGA	4.20	1.45	1.33
20	A	812	CLA	CAB-C3B	-4.20	1.36	1.47
20	2	304	CLA	CHD-C1D	4.20	1.48	1.38
20	B	808	CLA	O2D-CGD	4.20	1.43	1.33
20	B	829	CLA	O2A-CGA	4.20	1.45	1.33
20	R	108	CLA	CHB-C1B	4.19	1.48	1.39
20	B	812	CLA	O2D-CGD	4.19	1.43	1.33
20	H	108	CLA	CHC-C4B	4.19	1.48	1.39
20	A	824	CLA	O2A-CGA	4.19	1.45	1.33
20	4	310	CLA	CHC-C4B	4.18	1.48	1.39
20	F	207	CLA	C4C-C3C	-4.18	1.37	1.45
20	3	315	CLA	MG-NA	-4.18	1.96	2.06
20	B	807	CLA	OBD-CAD	4.18	1.29	1.22
20	4	303	CLA	O2A-CGA	4.17	1.45	1.33
20	1	211	CLA	OBD-CAD	4.17	1.29	1.22
20	L	203	CLA	CHB-C1B	4.17	1.48	1.39
20	2	316	CLA	C4C-C3C	-4.16	1.38	1.45
20	K	102	CLA	O2A-CGA	4.16	1.45	1.33
20	4	303	CLA	CHC-C4B	4.16	1.48	1.39
20	A	803	CLA	C4C-C3C	-4.16	1.38	1.45
20	F	201	CLA	CHD-C1D	4.16	1.46	1.38
20	2	314	CLA	O2A-CGA	4.15	1.45	1.33
20	A	818	CLA	O2A-CGA	4.15	1.45	1.33
20	1	213	CLA	CHC-C4B	4.14	1.48	1.39
20	F	201	CLA	C1B-NB	-4.14	1.32	1.37
20	4	315	CLA	O2A-CGA	4.14	1.45	1.33
20	A	839	CLA	C1B-NB	-4.14	1.32	1.37
20	2	316	CLA	C1B-NB	-4.13	1.32	1.37
20	A	849	CLA	O2A-CGA	4.13	1.45	1.33
20	A	826	CLA	O2A-CGA	4.13	1.45	1.33
20	3	314	CLA	CAB-C3B	-4.13	1.36	1.47
20	A	815	CLA	OBD-CAD	4.13	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	209	CLA	CHC-C4B	4.12	1.50	1.39
22	G	104	BCR	C21-C22	-4.12	1.26	1.35
20	4	310	CLA	O2A-CGA	4.12	1.45	1.33
20	2	307	CLA	CHB-C1B	4.12	1.48	1.39
20	A	834	CLA	OBD-CAD	4.11	1.29	1.22
22	I	101	BCR	C21-C22	-4.11	1.26	1.35
20	F	201	CLA	CHC-C4B	4.11	1.48	1.39
20	J	103	CLA	O2A-CGA	4.11	1.45	1.33
20	3	302	CLA	CHC-C4B	4.11	1.50	1.39
20	2	311	CLA	OBD-CAD	4.11	1.29	1.22
20	A	851	CLA	O2A-CGA	4.10	1.45	1.33
20	R	107	CLA	OBD-CAD	4.10	1.29	1.22
20	4	303	CLA	C1B-NB	-4.10	1.32	1.37
20	B	817	CLA	O2A-CGA	4.10	1.45	1.33
20	1	201	CLA	C1B-NB	-4.09	1.32	1.37
20	1	206	CLA	CHB-C1B	4.09	1.48	1.39
20	B	818	CLA	OBD-CAD	4.09	1.29	1.22
20	3	313	CLA	OBD-CAD	4.08	1.29	1.22
20	F	201	CLA	O2A-CGA	4.08	1.45	1.33
20	1	201	CLA	OBD-CAD	4.08	1.29	1.22
20	F	207	CLA	OBD-CAD	4.08	1.29	1.22
20	J	103	CLA	C1B-NB	-4.08	1.32	1.37
20	L	201	CLA	OBD-CAD	4.07	1.29	1.22
20	2	316	CLA	C4B-NB	-4.07	1.32	1.37
20	2	310	CLA	O2A-CGA	4.07	1.45	1.33
20	A	816	CLA	O2A-CGA	4.07	1.45	1.33
20	B	808	CLA	O2A-CGA	4.07	1.45	1.33
20	B	813	CLA	CAB-C3B	-4.06	1.36	1.47
20	A	835	CLA	OBD-CAD	4.05	1.29	1.22
20	3	311	CLA	OBD-CAD	4.05	1.29	1.22
20	B	829	CLA	CHB-C1B	4.05	1.48	1.39
20	B	809	CLA	O2A-CGA	4.05	1.45	1.33
20	A	803	CLA	CHC-C4B	4.05	1.48	1.39
20	1	204	CLA	MG-NA	-4.04	1.96	2.06
20	A	810	CLA	OBD-CAD	4.04	1.29	1.22
20	3	314	CLA	C4C-C3C	-4.04	1.38	1.45
20	2	314	CLA	C1B-NB	-4.03	1.32	1.37
22	I	103	BCR	C30-C25	-4.03	1.48	1.53
20	L	202	CLA	OBD-CAD	4.03	1.29	1.22
20	G	105	CLA	C4C-C3C	-4.03	1.38	1.45
20	B	850	CLA	O2A-CGA	4.02	1.45	1.33
20	A	831	CLA	CHC-C4B	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	307	CLA	CHC-C4B	4.02	1.48	1.39
20	A	840	CLA	OBD-CAD	4.02	1.29	1.22
20	4	315	CLA	C4C-C3C	-4.01	1.38	1.45
20	K	103	CLA	O2A-CGA	4.01	1.45	1.33
20	A	801	CLA	CHB-C1B	4.01	1.48	1.39
20	H	110	CLA	OBD-CAD	4.01	1.29	1.22
20	1	207	CLA	OBD-CAD	4.01	1.29	1.22
20	4	303	CLA	OBD-CAD	3.99	1.29	1.22
20	F	206	CLA	OBD-CAD	3.99	1.29	1.22
20	A	828	CLA	OBD-CAD	3.99	1.29	1.22
20	F	205	CLA	OBD-CAD	3.99	1.29	1.22
20	A	821	CLA	CHB-C1B	3.99	1.48	1.39
20	1	204	CLA	CHC-C4B	3.99	1.48	1.39
20	B	813	CLA	OBD-CAD	3.99	1.29	1.22
20	1	208	CLA	CHC-C4B	3.99	1.50	1.39
20	A	831	CLA	C1B-NB	-3.99	1.32	1.37
20	K	101	CLA	O2A-CGA	3.98	1.45	1.33
20	4	309	CLA	CHC-C4B	3.98	1.50	1.39
20	A	803	CLA	C1B-NB	-3.98	1.32	1.37
20	3	314	CLA	C1B-NB	-3.98	1.32	1.37
20	3	309	CLA	MG-NA	-3.97	1.96	2.06
20	B	823	CLA	OBD-CAD	3.97	1.29	1.22
20	4	317	CLA	C1B-NB	-3.97	1.32	1.37
20	A	830	CLA	OBD-CAD	3.97	1.29	1.22
20	B	840	CLA	OBD-CAD	3.97	1.29	1.22
20	2	308	CLA	CHD-C1D	3.97	1.48	1.38
20	L	207	CLA	OBD-CAD	3.97	1.29	1.22
20	B	806	CLA	OBD-CAD	3.97	1.29	1.22
20	A	831	CLA	O2A-CGA	3.96	1.44	1.33
20	1	212	CLA	CHC-C4B	3.96	1.50	1.39
20	L	204	CLA	CHB-C1B	3.96	1.48	1.39
20	1	211	CLA	CHB-C1B	3.95	1.48	1.39
20	B	820	CLA	CHB-C1B	3.95	1.48	1.39
20	A	814	CLA	CHC-C4B	3.95	1.50	1.39
20	4	312	CLA	CHC-C4B	3.94	1.50	1.39
20	K	102	CLA	OBD-CAD	3.94	1.29	1.22
20	2	302	CLA	C1B-NB	-3.94	1.32	1.37
20	A	833	CLA	OBD-CAD	3.94	1.29	1.22
20	B	838	CLA	CHB-C1B	3.93	1.48	1.39
20	A	849	CLA	C4C-C3C	-3.93	1.38	1.45
20	1	211	CLA	C1B-NB	-3.93	1.32	1.37
20	A	812	CLA	OBD-CAD	3.93	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	204	CLA	O2A-CGA	3.93	1.45	1.33
20	A	837	CLA	C4C-C3C	-3.92	1.38	1.45
20	B	814	CLA	C4C-C3C	-3.92	1.38	1.45
20	A	807	CLA	OBD-CAD	3.92	1.29	1.22
20	3	307	CLA	CHC-C4B	3.91	1.48	1.39
20	1	204	CLA	C4C-C3C	-3.91	1.38	1.45
20	L	203	CLA	OBD-CAD	3.91	1.29	1.22
20	A	831	CLA	C1C-C2C	-3.90	1.36	1.44
20	1	202	CLA	C1B-NB	-3.90	1.32	1.37
20	A	814	CLA	MG-NA	-3.90	1.97	2.06
20	4	301	CLA	OBD-CAD	3.90	1.29	1.22
20	F	207	CLA	O2A-CGA	3.89	1.44	1.33
20	3	307	CLA	C1B-NB	-3.89	1.32	1.37
20	3	306	CLA	CHC-C4B	3.89	1.50	1.39
20	B	830	CLA	OBD-CAD	3.89	1.29	1.22
20	H	102	CLA	OBD-CAD	3.89	1.29	1.22
20	4	305	CLA	OBD-CAD	3.89	1.29	1.22
20	B	836	CLA	O2A-CGA	3.89	1.44	1.33
20	3	316	CLA	MG-NA	-3.88	1.97	2.06
20	H	110	CLA	CHB-C1B	3.87	1.48	1.39
20	A	839	CLA	OBD-CAD	3.87	1.29	1.22
20	L	203	CLA	O2A-CGA	3.87	1.44	1.33
20	F	205	CLA	C3A-C2A	-3.87	1.51	1.54
20	1	215	CLA	C1B-NB	-3.86	1.32	1.37
20	A	816	CLA	C1B-NB	-3.86	1.32	1.37
20	H	101	CLA	OBD-CAD	3.86	1.29	1.22
20	A	820	CLA	OBD-CAD	3.85	1.29	1.22
20	4	313	CLA	OBD-CAD	3.85	1.29	1.22
20	2	307	CLA	OBD-CAD	3.85	1.29	1.22
20	B	835	CLA	OBD-CAD	3.85	1.29	1.22
20	3	304	CLA	MG-NA	-3.85	1.97	2.06
20	3	305	CLA	CHC-C4B	3.84	1.50	1.39
20	B	841	CLA	CHB-C1B	3.84	1.48	1.39
20	A	838	CLA	OBD-CAD	3.84	1.29	1.22
20	A	822	CLA	OBD-CAD	3.84	1.29	1.22
20	B	837	CLA	CHB-C1B	3.84	1.48	1.39
20	3	308	CLA	CHC-C4B	3.83	1.50	1.39
20	4	318	CLA	C1B-NB	-3.83	1.32	1.37
20	G	105	CLA	OBD-CAD	3.83	1.29	1.22
20	B	834	CLA	OBD-CAD	3.83	1.29	1.22
20	A	809	CLA	CHB-C1B	3.83	1.48	1.39
20	4	305	CLA	CHB-C1B	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	213	CLA	C4C-C3C	-3.82	1.38	1.45
20	B	812	CLA	C1B-NB	-3.82	1.32	1.37
20	A	801	CLA	OBD-CAD	3.82	1.29	1.22
20	1	214	CLA	MG-NA	-3.81	1.97	2.06
20	3	307	CLA	OBD-CAD	3.81	1.29	1.22
20	4	311	CLA	CHC-C4B	3.81	1.50	1.39
20	3	314	CLA	C4B-NB	-3.81	1.32	1.37
20	3	301	CLA	CHB-C1B	3.81	1.48	1.39
20	2	302	CLA	OBD-CAD	3.80	1.29	1.22
20	B	810	CLA	OBD-CAD	3.79	1.29	1.22
20	A	850	CLA	OBD-CAD	3.79	1.29	1.22
20	3	314	CLA	O2A-CGA	3.79	1.44	1.33
20	F	201	CLA	C1C-C2C	-3.78	1.36	1.44
20	4	303	CLA	C4C-C3C	-3.78	1.38	1.45
22	A	844	BCR	C20-C19	-3.78	1.24	1.34
20	A	838	CLA	C4C-C3C	-3.78	1.38	1.45
20	1	203	CLA	OBD-CAD	3.78	1.29	1.22
20	A	826	CLA	OBD-CAD	3.78	1.29	1.22
20	4	317	CLA	C4C-C3C	-3.78	1.38	1.45
20	A	817	CLA	OBD-CAD	3.77	1.29	1.22
20	B	802	CLA	OBD-CAD	3.77	1.29	1.22
20	J	103	CLA	OBD-CAD	3.77	1.29	1.22
20	3	310	CLA	C4B-NB	-3.77	1.32	1.37
20	B	816	CLA	OBD-CAD	3.77	1.29	1.22
20	2	303	CLA	C1B-NB	-3.76	1.32	1.37
20	B	826	CLA	OBD-CAD	3.76	1.29	1.22
22	B	844	BCR	C21-C22	-3.76	1.27	1.35
20	A	819	CLA	OBD-CAD	3.76	1.29	1.22
20	A	839	CLA	C4C-C3C	-3.76	1.38	1.45
20	A	831	CLA	OBD-CAD	3.76	1.28	1.22
20	3	315	CLA	CHC-C4B	3.75	1.49	1.39
20	B	850	CLA	OBD-CAD	3.75	1.28	1.22
20	A	805	CLA	CHB-C1B	3.75	1.47	1.39
20	1	214	CLA	CHC-C4B	3.75	1.49	1.39
20	H	102	CLA	CHB-C1B	3.75	1.47	1.39
20	A	837	CLA	OBD-CAD	3.75	1.28	1.22
20	B	830	CLA	CHB-C1B	3.75	1.47	1.39
20	4	306	CLA	C1C-C2C	-3.75	1.36	1.44
20	3	314	CLA	OBD-CAD	3.75	1.28	1.22
20	2	310	CLA	C4C-C3C	-3.75	1.38	1.45
20	4	307	CLA	CHC-C4B	3.73	1.49	1.39
20	4	317	CLA	O2A-CGA	3.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	304	CLA	CHC-C4B	3.73	1.49	1.39
20	L	204	CLA	C4C-C3C	-3.72	1.38	1.45
20	B	832	CLA	OBD-CAD	3.72	1.28	1.22
20	2	315	CLA	CHC-C4B	3.72	1.49	1.39
20	B	821	CLA	CHB-C1B	3.72	1.47	1.39
20	3	316	CLA	CHC-C4B	3.72	1.49	1.39
20	A	829	CLA	OBD-CAD	3.71	1.28	1.22
20	K	102	CLA	C4C-C3C	-3.71	1.38	1.45
20	A	802	CLA	MG-NA	-3.71	1.97	2.06
20	3	301	CLA	OBD-CAD	3.71	1.28	1.22
20	B	842	CLA	CHB-C1B	3.71	1.47	1.39
20	B	817	CLA	CHB-C1B	3.71	1.47	1.39
20	4	303	CLA	C1C-C2C	-3.71	1.37	1.44
20	B	829	CLA	OBD-CAD	3.70	1.28	1.22
20	A	802	CLA	CHC-C4B	3.70	1.49	1.39
20	K	101	CLA	O2A-C1	3.70	1.53	1.45
20	2	312	CLA	OBD-CAD	3.70	1.28	1.22
20	B	833	CLA	OBD-CAD	3.70	1.28	1.22
20	B	824	CLA	C1D-ND	-3.70	1.33	1.37
20	A	841	CLA	CHC-C4B	3.69	1.49	1.39
20	J	101	CLA	OBD-CAD	3.69	1.28	1.22
20	1	210	CLA	CHB-C1B	3.69	1.47	1.39
20	1	201	CLA	CHC-C4B	3.69	1.47	1.39
20	A	807	CLA	CHB-C1B	3.69	1.47	1.39
20	A	829	CLA	CHB-C1B	3.68	1.47	1.39
20	B	831	CLA	OBD-CAD	3.68	1.28	1.22
20	R	107	CLA	CHB-C1B	3.68	1.47	1.39
20	K	104	CLA	C1B-NB	-3.68	1.33	1.37
20	3	307	CLA	CHB-C1B	3.68	1.47	1.39
20	B	834	CLA	C4C-C3C	-3.68	1.38	1.45
20	4	308	CLA	MG-NA	-3.68	1.97	2.06
20	2	312	CLA	O2A-CGA	3.68	1.44	1.33
20	A	809	CLA	OBD-CAD	3.68	1.28	1.22
20	1	215	CLA	OBD-CAD	3.67	1.28	1.22
20	2	302	CLA	MG-NA	-3.67	1.97	2.06
20	1	202	CLA	C3A-C2A	-3.67	1.51	1.54
22	F	203	BCR	C20-C19	-3.67	1.25	1.34
20	A	813	CLA	OBD-CAD	3.67	1.28	1.22
22	L	209	BCR	C20-C19	-3.66	1.25	1.34
20	B	824	CLA	C9-C8	3.66	1.64	1.52
20	B	836	CLA	OBD-CAD	3.66	1.28	1.22
20	3	314	CLA	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	830	CLA	C4C-C3C	-3.66	1.38	1.45
22	B	845	BCR	C21-C22	-3.66	1.27	1.35
20	A	841	CLA	MG-NA	-3.65	1.97	2.06
20	3	317	CLA	CHB-C1B	3.65	1.47	1.39
20	K	103	CLA	C1C-C2C	-3.65	1.37	1.44
20	2	312	CLA	C4C-C3C	-3.65	1.38	1.45
20	2	303	CLA	OBD-CAD	3.65	1.28	1.22
20	A	809	CLA	C1C-C2C	-3.65	1.37	1.44
20	A	834	CLA	CHB-C1B	3.64	1.47	1.39
20	A	832	CLA	OBD-CAD	3.63	1.28	1.22
20	4	310	CLA	CHB-C1B	3.62	1.47	1.39
20	A	802	CLA	CHD-C4C	3.62	1.52	1.40
20	1	205	CLA	CHB-C1B	3.62	1.47	1.39
20	1	213	CLA	C1C-C2C	-3.62	1.37	1.44
20	2	307	CLA	C4C-C3C	-3.62	1.38	1.45
20	A	825	CLA	CHB-C1B	3.61	1.47	1.39
20	H	108	CLA	C1C-C2C	-3.61	1.37	1.44
20	B	813	CLA	CHB-C1B	3.61	1.47	1.39
20	F	207	CLA	C1B-NB	-3.60	1.33	1.37
20	A	839	CLA	C1C-C2C	-3.60	1.37	1.44
20	1	205	CLA	C3A-C2A	-3.60	1.51	1.54
20	A	815	CLA	CHB-C1B	3.60	1.47	1.39
20	A	841	CLA	CHD-C4C	3.60	1.52	1.40
20	A	828	CLA	CHB-C1B	3.59	1.47	1.39
20	A	827	CLA	OBD-CAD	3.59	1.28	1.22
20	J	103	CLA	C1C-C2C	-3.59	1.37	1.44
20	K	103	CLA	OBD-CAD	3.59	1.28	1.22
20	B	816	CLA	CHB-C1B	3.59	1.47	1.39
20	B	822	CLA	C4C-C3C	-3.59	1.38	1.45
20	A	831	CLA	CAB-C3B	-3.59	1.37	1.47
20	B	811	CLA	CHC-C4B	3.58	1.49	1.39
20	B	826	CLA	CHB-C1B	3.58	1.47	1.39
20	4	305	CLA	C1B-NB	-3.58	1.33	1.37
20	2	304	CLA	MG-NA	-3.58	1.97	2.06
20	F	201	CLA	CHB-C1B	3.58	1.47	1.39
20	B	837	CLA	OBD-CAD	3.58	1.28	1.22
20	A	820	CLA	CHB-C1B	3.57	1.47	1.39
20	G	105	CLA	C1B-NB	-3.57	1.33	1.37
20	H	108	CLA	MG-NA	-3.57	1.97	2.06
20	B	835	CLA	C1B-NB	-3.57	1.33	1.37
20	1	204	CLA	C1C-C2C	-3.57	1.37	1.44
20	4	318	CLA	OBD-CAD	3.57	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	817	CLA	CHB-C1B	3.57	1.47	1.39
20	3	309	CLA	CHC-C4B	3.57	1.49	1.39
20	2	309	CLA	CHC-C4B	3.56	1.49	1.39
20	A	803	CLA	CHB-C1B	3.56	1.47	1.39
20	A	850	CLA	C1B-NB	-3.56	1.33	1.37
22	F	204	BCR	C20-C19	-3.55	1.25	1.34
20	B	836	CLA	C4C-C3C	-3.55	1.39	1.45
20	3	310	CLA	OBD-CAD	3.55	1.28	1.22
20	2	309	CLA	MG-NA	-3.54	1.97	2.06
20	1	204	CLA	OBD-CAD	3.54	1.28	1.22
20	B	819	CLA	C1C-C2C	-3.54	1.37	1.44
20	2	305	CLA	OBD-CAD	3.54	1.28	1.22
20	B	827	CLA	C4C-C3C	-3.54	1.39	1.45
20	B	833	CLA	CHB-C1B	3.54	1.47	1.39
22	2	317	BCR	C20-C19	-3.54	1.25	1.34
20	1	207	CLA	CHB-C1B	3.53	1.47	1.39
20	2	314	CLA	OBD-CAD	3.52	1.28	1.22
20	2	303	CLA	MG-NA	-3.52	1.97	2.06
20	A	831	CLA	C1D-ND	-3.51	1.33	1.37
20	B	821	CLA	OBD-CAD	3.51	1.28	1.22
20	A	833	CLA	CHB-C1B	3.51	1.47	1.39
20	3	310	CLA	CHB-C1B	3.51	1.47	1.39
20	F	207	CLA	CAA-C2A	-3.50	1.47	1.54
20	A	825	CLA	C4C-C3C	-3.50	1.39	1.45
20	2	305	CLA	CHB-C1B	3.50	1.47	1.39
20	B	829	CLA	C4C-C3C	-3.50	1.39	1.45
22	A	843	BCR	C20-C19	-3.49	1.25	1.34
20	4	315	CLA	CHB-C1B	3.49	1.47	1.39
20	K	102	CLA	CHB-C1B	3.49	1.47	1.39
20	J	103	CLA	C4C-C3C	-3.49	1.39	1.45
20	B	818	CLA	C1B-NB	-3.49	1.33	1.37
20	4	307	CLA	MG-NA	-3.48	1.98	2.06
22	A	845	BCR	C20-C19	-3.48	1.25	1.34
20	B	839	CLA	C1B-NB	-3.48	1.33	1.37
20	B	803	CLA	OBD-CAD	3.48	1.28	1.22
20	3	313	CLA	CHB-C1B	3.48	1.47	1.39
20	A	818	CLA	MG-NA	-3.48	1.98	2.06
20	2	308	CLA	CHC-C4B	3.48	1.49	1.39
20	K	103	CLA	C4C-C3C	-3.48	1.39	1.45
20	A	838	CLA	CHB-C1B	3.47	1.47	1.39
20	H	108	CLA	C1D-ND	-3.47	1.33	1.37
20	A	808	CLA	OBD-CAD	3.47	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	841	CLA	OBD-CAD	3.47	1.28	1.22
20	4	315	CLA	OBD-CAD	3.46	1.28	1.22
20	B	806	CLA	CHB-C1B	3.46	1.47	1.39
20	2	306	CLA	CHC-C4B	3.46	1.49	1.39
20	4	310	CLA	C1C-C2C	-3.46	1.37	1.44
20	3	310	CLA	C1B-NB	-3.46	1.33	1.37
20	K	101	CLA	CHB-C1B	3.46	1.47	1.39
20	3	311	CLA	C4C-C3C	-3.46	1.39	1.45
20	L	202	CLA	C4C-C3C	-3.46	1.39	1.45
20	3	303	CLA	CHB-C1B	3.45	1.47	1.39
20	A	811	CLA	OBD-CAD	3.45	1.28	1.22
20	2	307	CLA	C1C-C2C	-3.45	1.37	1.44
22	B	847	BCR	C20-C19	-3.44	1.25	1.34
20	H	110	CLA	C4C-C3C	-3.44	1.39	1.45
22	B	846	BCR	C20-C19	-3.44	1.25	1.34
20	4	306	CLA	MG-NA	-3.44	1.98	2.06
20	3	308	CLA	MG-NA	-3.43	1.98	2.06
20	A	831	CLA	C4B-NB	-3.43	1.33	1.37
20	1	209	CLA	MG-NA	-3.43	1.98	2.06
20	B	819	CLA	C1B-NB	-3.43	1.33	1.37
20	B	814	CLA	C1B-NB	-3.43	1.33	1.37
20	A	810	CLA	CHB-C1B	3.43	1.47	1.39
20	B	832	CLA	C4C-C3C	-3.43	1.39	1.45
20	3	303	CLA	C3A-C2A	-3.43	1.51	1.54
20	4	310	CLA	C1B-NB	-3.43	1.33	1.37
20	1	201	CLA	C1C-C2C	-3.42	1.37	1.44
20	B	812	CLA	OBD-CAD	3.42	1.28	1.22
20	I	102	CLA	CHB-C1B	3.41	1.47	1.39
20	B	825	CLA	C1B-NB	-3.41	1.33	1.37
20	A	813	CLA	C4C-C3C	-3.41	1.39	1.45
20	A	830	CLA	C4C-C3C	-3.41	1.39	1.45
20	K	101	CLA	C4C-C3C	-3.41	1.39	1.45
20	B	824	CLA	CHB-C1B	3.41	1.47	1.39
20	A	824	CLA	OBD-CAD	3.40	1.28	1.22
20	B	823	CLA	CHB-C1B	3.40	1.47	1.39
20	K	101	CLA	OBD-CAD	3.40	1.28	1.22
20	2	301	CLA	CHC-C4B	3.40	1.48	1.39
20	4	304	CLA	CHB-C1B	3.40	1.47	1.39
20	B	827	CLA	OBD-CAD	3.40	1.28	1.22
20	B	820	CLA	C4C-C3C	-3.40	1.39	1.45
20	A	840	CLA	CHB-C1B	3.40	1.47	1.39
20	2	311	CLA	C1B-NB	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	CHB-C1B	3.40	1.47	1.39
20	2	315	CLA	MG-NA	-3.39	1.98	2.06
20	B	838	CLA	C4C-C3C	-3.39	1.39	1.45
20	4	301	CLA	CHB-C1B	3.39	1.47	1.39
20	B	833	CLA	C4C-C3C	-3.39	1.39	1.45
20	A	849	CLA	CHB-C1B	3.39	1.47	1.39
20	A	851	CLA	C4C-C3C	-3.39	1.39	1.45
20	A	803	CLA	C1C-C2C	-3.39	1.37	1.44
20	B	835	CLA	C4C-C3C	-3.39	1.39	1.45
20	4	302	CLA	CHB-C1B	3.39	1.47	1.39
20	1	201	CLA	C4C-C3C	-3.38	1.39	1.45
20	B	811	CLA	CHD-C4C	3.38	1.51	1.40
20	2	314	CLA	MG-NA	-3.38	1.98	2.06
20	A	818	CLA	C1C-C2C	-3.38	1.37	1.44
20	F	207	CLA	CHB-C1B	3.38	1.47	1.39
20	K	102	CLA	C1B-NB	-3.38	1.33	1.37
20	4	306	CLA	C1B-C2B	-3.37	1.35	1.43
20	B	839	CLA	C1C-C2C	-3.37	1.37	1.44
20	K	104	CLA	C4C-C3C	-3.37	1.39	1.45
20	B	826	CLA	C4C-C3C	-3.37	1.39	1.45
20	2	302	CLA	C1C-C2C	-3.37	1.37	1.44
20	A	849	CLA	OBD-CAD	3.37	1.28	1.22
20	L	208	CLA	CHB-C1B	3.37	1.47	1.39
20	B	835	CLA	CHB-C1B	3.36	1.47	1.39
20	A	818	CLA	C1B-NB	-3.36	1.33	1.37
20	A	850	CLA	C4C-C3C	-3.36	1.39	1.45
20	A	833	CLA	C4C-C3C	-3.35	1.39	1.45
20	A	830	CLA	C1B-NB	-3.35	1.33	1.37
20	F	206	CLA	C4C-C3C	-3.35	1.39	1.45
20	B	818	CLA	CHB-C1B	3.35	1.46	1.39
20	B	839	CLA	MG-NA	-3.34	1.98	2.06
20	B	827	CLA	C1B-NB	-3.34	1.33	1.37
20	1	203	CLA	CHB-C1B	3.34	1.46	1.39
20	B	828	CLA	CHB-C1B	3.34	1.46	1.39
20	A	827	CLA	CHB-C1B	3.34	1.46	1.39
20	B	823	CLA	C1B-NB	-3.33	1.33	1.37
20	L	202	CLA	CHB-C1B	3.33	1.46	1.39
20	F	206	CLA	CHB-C1B	3.33	1.46	1.39
20	B	828	CLA	OBD-CAD	3.33	1.28	1.22
20	4	308	CLA	CHC-C4B	3.33	1.48	1.39
20	H	108	CLA	OBD-CAD	3.33	1.28	1.22
20	1	213	CLA	C4B-NB	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	836	CLA	C1B-NB	-3.33	1.33	1.37
20	A	836	CLA	CHB-C1B	3.33	1.46	1.39
20	K	104	CLA	C1C-C2C	-3.33	1.37	1.44
20	B	850	CLA	C4C-C3C	-3.33	1.39	1.45
22	J	102	BCR	C20-C19	-3.33	1.26	1.34
20	L	201	CLA	CHB-C1B	3.33	1.46	1.39
20	B	815	CLA	CHB-C1B	3.33	1.46	1.39
20	J	101	CLA	CHB-C1B	3.32	1.46	1.39
20	4	311	CLA	MG-NA	-3.32	1.98	2.06
20	4	309	CLA	CHD-C4C	3.32	1.51	1.40
20	H	109	CLA	CHB-C1B	3.32	1.46	1.39
20	A	812	CLA	CHB-C1B	3.32	1.46	1.39
20	A	824	CLA	CHB-C1B	3.32	1.46	1.39
20	K	104	CLA	OBD-CAD	3.32	1.28	1.22
20	B	803	CLA	C4C-C3C	-3.32	1.39	1.45
20	B	808	CLA	C1B-NB	-3.31	1.33	1.37
20	B	850	CLA	CHB-C1B	3.31	1.46	1.39
20	2	303	CLA	C4B-NB	-3.31	1.33	1.37
20	B	828	CLA	C4C-C3C	-3.31	1.39	1.45
20	3	311	CLA	C1B-NB	-3.31	1.33	1.37
20	A	823	CLA	CHB-C1B	3.31	1.46	1.39
20	B	833	CLA	C1C-C2C	-3.31	1.37	1.44
20	I	102	CLA	C4C-C3C	-3.30	1.39	1.45
20	4	301	CLA	C4C-C3C	-3.30	1.39	1.45
20	4	315	CLA	C1B-NB	-3.30	1.33	1.37
20	B	840	CLA	CHB-C1B	3.30	1.46	1.39
20	B	802	CLA	CHB-C1B	3.29	1.46	1.39
20	A	828	CLA	C4C-C3C	-3.29	1.39	1.45
20	A	806	CLA	CHB-C1B	3.29	1.46	1.39
20	A	839	CLA	C3A-C2A	-3.29	1.45	1.54
20	3	312	CLA	CHD-C4C	3.29	1.51	1.40
20	B	810	CLA	C1B-NB	-3.29	1.33	1.37
20	B	809	CLA	C1C-C2C	-3.29	1.37	1.44
20	1	207	CLA	C2A-C1A	-3.28	1.44	1.52
20	B	810	CLA	CHB-C1B	3.28	1.46	1.39
20	B	813	CLA	C1B-NB	-3.27	1.33	1.37
20	1	214	CLA	CHD-C4C	3.27	1.51	1.40
20	B	834	CLA	C1B-NB	-3.27	1.33	1.37
20	B	808	CLA	CHB-C1B	3.27	1.46	1.39
20	B	834	CLA	CHB-C1B	3.27	1.46	1.39
20	4	304	CLA	C1B-NB	-3.27	1.33	1.37
20	B	832	CLA	CHB-C1B	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	314	CLA	C1C-C2C	-3.27	1.37	1.44
20	2	310	CLA	C1C-C2C	-3.26	1.37	1.44
20	1	203	CLA	MG-NA	-3.26	1.98	2.06
20	1	207	CLA	C4C-C3C	-3.26	1.39	1.45
22	G	104	BCR	C20-C19	-3.26	1.26	1.34
20	A	832	CLA	CHB-C1B	3.26	1.46	1.39
20	A	851	CLA	C1B-NB	-3.25	1.33	1.37
20	A	825	CLA	OBD-CAD	3.25	1.28	1.22
20	A	816	CLA	OBD-CAD	3.25	1.28	1.22
20	3	304	CLA	CHC-C4B	3.25	1.48	1.39
20	4	317	CLA	CHB-C1B	3.25	1.46	1.39
20	4	310	CLA	C1D-ND	-3.25	1.33	1.37
20	A	830	CLA	CHB-C1B	3.25	1.46	1.39
20	2	303	CLA	C1C-C2C	-3.25	1.37	1.44
20	A	818	CLA	C4B-NB	-3.25	1.33	1.37
20	B	833	CLA	C1B-NB	-3.24	1.33	1.37
20	4	317	CLA	C1C-C2C	-3.24	1.37	1.44
20	B	807	CLA	C4C-C3C	-3.24	1.39	1.45
20	A	835	CLA	C4C-C3C	-3.23	1.39	1.45
20	B	810	CLA	C1C-C2C	-3.23	1.38	1.44
20	3	302	CLA	CHD-C4C	3.23	1.51	1.40
20	A	813	CLA	CHB-C1B	3.23	1.46	1.39
20	2	307	CLA	C1B-NB	-3.23	1.33	1.37
20	B	820	CLA	OBD-CAD	3.22	1.28	1.22
20	1	212	CLA	CHD-C4C	3.22	1.51	1.40
20	A	804	CLA	CHB-C1B	3.22	1.46	1.39
20	4	301	CLA	C1B-NB	-3.22	1.33	1.37
20	A	832	CLA	C1B-NB	-3.22	1.33	1.37
20	J	101	CLA	C4C-C3C	-3.22	1.39	1.45
20	B	812	CLA	C1C-C2C	-3.22	1.38	1.44
20	B	809	CLA	OBD-CAD	3.22	1.28	1.22
20	L	208	CLA	C4C-C3C	-3.22	1.39	1.45
20	1	204	CLA	C4B-NB	-3.21	1.33	1.37
20	B	803	CLA	C1C-C2C	-3.21	1.38	1.44
20	A	822	CLA	CHB-C1B	3.21	1.46	1.39
20	B	838	CLA	OBD-CAD	3.21	1.28	1.22
20	3	305	CLA	CHD-C4C	3.21	1.51	1.40
20	H	101	CLA	C1B-NB	-3.21	1.33	1.37
20	A	811	CLA	CHB-C1B	3.21	1.46	1.39
20	1	208	CLA	CHD-C4C	3.21	1.51	1.40
20	4	312	CLA	MG-NA	-3.21	1.98	2.06
22	I	103	BCR	C20-C19	-3.21	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	304	CLA	CHD-C4C	3.20	1.51	1.40
20	2	302	CLA	C4B-NB	-3.20	1.33	1.37
20	4	317	CLA	OBD-CAD	3.19	1.28	1.22
20	2	310	CLA	MG-NA	-3.19	1.98	2.06
20	B	809	CLA	C4C-C3C	-3.19	1.39	1.45
20	A	824	CLA	C4C-C3C	-3.19	1.39	1.45
20	A	812	CLA	C4C-C3C	-3.19	1.39	1.45
20	1	203	CLA	O2A-CGA	3.19	1.42	1.33
20	2	311	CLA	CHB-C1B	3.19	1.46	1.39
20	A	826	CLA	C4C-C3C	-3.19	1.39	1.45
20	F	207	CLA	C2A-C1A	-3.19	1.45	1.52
20	B	814	CLA	CHB-C1B	3.19	1.46	1.39
20	B	840	CLA	C4C-C3C	-3.19	1.39	1.45
20	2	301	CLA	MG-NA	-3.18	1.98	2.06
20	J	101	CLA	C1B-NB	-3.18	1.33	1.37
20	A	837	CLA	C1C-C2C	-3.18	1.38	1.44
20	3	311	CLA	CHB-C1B	3.18	1.46	1.39
20	4	313	CLA	CHB-C1B	3.18	1.46	1.39
20	A	811	CLA	C1C-C2C	-3.18	1.38	1.44
20	4	304	CLA	C1C-C2C	-3.18	1.38	1.44
20	A	851	CLA	CHB-C1B	3.18	1.46	1.39
20	A	805	CLA	OBD-CAD	3.18	1.28	1.22
20	4	306	CLA	OBD-CAD	3.17	1.27	1.22
20	1	202	CLA	CHB-C1B	3.17	1.46	1.39
22	B	844	BCR	C20-C19	-3.17	1.26	1.34
20	B	814	CLA	OBD-CAD	3.16	1.27	1.22
20	B	812	CLA	MG-NA	-3.16	1.98	2.06
20	B	821	CLA	C4C-C3C	-3.16	1.39	1.45
20	B	831	CLA	C1B-NB	-3.16	1.33	1.37
20	3	307	CLA	MG-NA	-3.16	1.98	2.06
20	4	314	CLA	CHD-C4C	3.16	1.51	1.40
20	K	102	CLA	C1C-C2C	-3.16	1.38	1.44
20	3	309	CLA	CHD-C4C	3.16	1.51	1.40
20	A	811	CLA	C4C-C3C	-3.15	1.39	1.45
20	B	807	CLA	C1B-NB	-3.15	1.33	1.37
20	B	812	CLA	C4B-NB	-3.15	1.33	1.37
20	A	803	CLA	C4B-NB	-3.15	1.33	1.37
20	3	301	CLA	C3A-C2A	-3.15	1.51	1.54
20	2	312	CLA	C1B-NB	-3.15	1.33	1.37
20	B	836	CLA	C1C-C2C	-3.15	1.38	1.44
20	4	312	CLA	CHD-C4C	3.14	1.51	1.40
20	A	837	CLA	CHB-C1B	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	824	CLA	C1B-NB	-3.14	1.33	1.37
20	H	101	CLA	CHB-C1B	3.14	1.46	1.39
20	1	211	CLA	C1C-C2C	-3.14	1.38	1.44
20	L	202	CLA	C1B-NB	-3.14	1.33	1.37
20	B	808	CLA	C1C-C2C	-3.14	1.38	1.44
20	4	309	CLA	MG-NA	-3.14	1.98	2.06
20	1	215	CLA	C1D-C2D	-3.14	1.39	1.45
22	F	204	BCR	C30-C25	-3.14	1.49	1.53
20	B	811	CLA	MG-NA	-3.14	1.98	2.06
20	3	308	CLA	CHD-C4C	3.13	1.51	1.40
20	4	311	CLA	CHD-C4C	3.13	1.51	1.40
20	2	314	CLA	CHB-C1B	3.13	1.46	1.39
20	A	806	CLA	C4C-C3C	-3.13	1.39	1.45
20	B	836	CLA	CHB-C1B	3.13	1.46	1.39
20	A	833	CLA	C1C-C2C	-3.13	1.38	1.44
20	B	803	CLA	CHB-C1B	3.12	1.46	1.39
20	F	207	CLA	C4B-NB	-3.12	1.33	1.37
20	2	306	CLA	MG-NA	-3.12	1.98	2.06
20	B	825	CLA	C4C-C3C	-3.12	1.39	1.45
20	R	107	CLA	C1B-NB	-3.12	1.33	1.37
20	B	822	CLA	CHB-C1B	3.12	1.46	1.39
20	4	307	CLA	CHD-C4C	3.11	1.50	1.40
20	F	201	CLA	C1D-ND	-3.11	1.33	1.37
20	B	839	CLA	C1D-ND	-3.11	1.33	1.37
20	A	836	CLA	C4C-C3C	-3.11	1.39	1.45
20	B	810	CLA	C4C-C3C	-3.11	1.39	1.45
20	A	823	CLA	OBD-CAD	3.11	1.27	1.22
20	A	819	CLA	CHB-C1B	3.11	1.46	1.39
20	1	213	CLA	C1B-C2B	-3.11	1.35	1.43
20	A	807	CLA	C4C-C3C	-3.10	1.39	1.45
20	K	101	CLA	C1B-NB	-3.10	1.33	1.37
20	B	802	CLA	C4C-C3C	-3.10	1.39	1.45
20	R	108	CLA	C1B-NB	-3.10	1.33	1.37
20	K	104	CLA	CHB-C1B	3.10	1.46	1.39
20	A	808	CLA	C4C-C3C	-3.10	1.39	1.45
20	B	838	CLA	C1B-NB	-3.10	1.33	1.37
20	2	316	CLA	C1C-C2C	-3.10	1.38	1.44
20	F	206	CLA	C1B-NB	-3.10	1.33	1.37
20	B	839	CLA	CHB-C1B	3.09	1.46	1.39
20	A	836	CLA	C1B-NB	-3.09	1.33	1.37
20	A	826	CLA	CHB-C1B	3.09	1.46	1.39
20	B	819	CLA	C1D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	312	CLA	MG-NA	-3.09	1.98	2.06
20	L	201	CLA	C4C-C3C	-3.09	1.39	1.45
20	A	822	CLA	C1B-NB	-3.09	1.33	1.37
20	B	811	CLA	C3D-C4D	-3.08	1.36	1.44
20	4	305	CLA	C1C-C2C	-3.08	1.38	1.44
20	A	828	CLA	C1B-NB	-3.08	1.33	1.37
20	4	318	CLA	CHB-C1B	3.08	1.46	1.39
20	A	831	CLA	MG-ND	-3.08	1.99	2.05
20	A	814	CLA	CHD-C4C	3.07	1.50	1.40
20	1	210	CLA	C3A-C2A	-3.07	1.51	1.54
20	L	207	CLA	CHB-C1B	3.07	1.46	1.39
20	3	315	CLA	CHD-C4C	3.07	1.50	1.40
20	1	210	CLA	OBD-CAD	3.07	1.27	1.22
20	A	839	CLA	CHB-C1B	3.07	1.46	1.39
20	A	817	CLA	C4C-C3C	-3.07	1.39	1.45
20	4	308	CLA	CHD-C4C	3.07	1.50	1.40
20	F	207	CLA	C1C-C2C	-3.06	1.38	1.44
20	A	825	CLA	C1B-NB	-3.06	1.33	1.37
20	A	837	CLA	C1B-NB	-3.06	1.33	1.37
20	A	805	CLA	C1C-C2C	-3.06	1.38	1.44
20	4	317	CLA	MG-NA	-3.06	1.99	2.06
20	A	822	CLA	C4C-C3C	-3.05	1.39	1.45
20	L	201	CLA	C1B-NB	-3.05	1.33	1.37
20	A	827	CLA	C1B-NB	-3.05	1.33	1.37
20	2	311	CLA	C4C-C3C	-3.05	1.39	1.45
20	2	310	CLA	CHB-C1B	3.05	1.46	1.39
20	3	306	CLA	CHD-C4C	3.04	1.50	1.40
20	H	108	CLA	C4B-NB	-3.04	1.33	1.37
20	2	316	CLA	OBD-CAD	3.04	1.27	1.22
20	L	208	CLA	C1B-NB	-3.04	1.33	1.37
20	B	826	CLA	C1B-NB	-3.04	1.33	1.37
20	H	108	CLA	CHB-C4A	-3.03	1.30	1.37
20	2	306	CLA	CHD-C4C	3.03	1.50	1.40
20	B	821	CLA	C1B-NB	-3.03	1.33	1.37
20	K	103	CLA	C1B-C2B	-3.03	1.36	1.43
20	2	301	CLA	CHD-C4C	3.03	1.50	1.40
20	A	851	CLA	C1C-C2C	-3.03	1.38	1.44
20	A	813	CLA	C1C-C2C	-3.02	1.38	1.44
20	1	201	CLA	CHB-C1B	3.02	1.46	1.39
20	K	103	CLA	MG-NA	-3.02	1.99	2.06
20	B	806	CLA	C4C-C3C	-3.02	1.39	1.45
20	4	314	CLA	CHB-C1B	3.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	316	CLA	C1C-NC	-3.01	1.33	1.37
20	1	212	CLA	MG-NA	-3.01	1.99	2.06
20	A	835	CLA	C1B-NB	-3.00	1.33	1.37
20	B	825	CLA	CHB-C1B	3.00	1.46	1.39
20	I	102	CLA	OBD-CAD	3.00	1.27	1.22
20	A	820	CLA	C1B-NB	-3.00	1.33	1.37
20	B	824	CLA	MG-NA	-2.99	1.99	2.06
20	2	303	CLA	CHB-C1B	2.99	1.46	1.39
20	2	306	CLA	CHB-C1B	2.99	1.47	1.39
20	B	809	CLA	CHB-C1B	2.99	1.46	1.39
20	4	306	CLA	CHB-C4A	-2.99	1.30	1.37
20	4	302	CLA	C1B-NB	-2.98	1.33	1.37
20	A	830	CLA	C1C-C2C	-2.98	1.38	1.44
20	3	302	CLA	MG-NA	-2.98	1.99	2.06
20	3	314	CLA	MG-NA	-2.98	1.99	2.06
20	A	810	CLA	C4C-C3C	-2.98	1.40	1.45
20	B	830	CLA	C1C-C2C	-2.98	1.38	1.44
20	L	203	CLA	C4C-C3C	-2.98	1.40	1.45
20	B	817	CLA	C4C-C3C	-2.97	1.40	1.45
20	B	808	CLA	MG-NA	-2.97	1.99	2.06
20	2	302	CLA	C1B-C2B	-2.97	1.36	1.43
21	H	105	LMU	O1'-C1'	2.97	1.45	1.40
21	2	321	LMU	O1'-C1'	2.97	1.45	1.40
20	A	820	CLA	C4C-C3C	-2.97	1.40	1.45
20	A	840	CLA	C1B-NB	-2.97	1.34	1.37
20	J	103	CLA	MG-NA	-2.96	1.99	2.06
20	B	803	CLA	C1B-NB	-2.96	1.34	1.37
20	1	206	CLA	C4C-C3C	-2.96	1.40	1.45
20	A	801	CLA	C1C-C2C	-2.95	1.38	1.44
20	3	305	CLA	MG-NA	-2.95	1.99	2.06
20	1	215	CLA	CHB-C1B	2.95	1.46	1.39
20	B	831	CLA	CHB-C1B	2.94	1.46	1.39
20	4	310	CLA	OBD-CAD	2.94	1.27	1.22
20	R	107	CLA	C4C-C3C	-2.94	1.40	1.45
20	2	310	CLA	OBD-CAD	2.94	1.27	1.22
20	F	205	CLA	CHB-C1B	2.94	1.46	1.39
20	B	809	CLA	MG-NA	-2.93	1.99	2.06
20	1	203	CLA	C1C-C2C	-2.93	1.38	1.44
20	3	307	CLA	C4C-C3C	-2.93	1.40	1.45
20	H	101	CLA	C4C-C3C	-2.93	1.40	1.45
20	1	209	CLA	CHD-C4C	2.93	1.50	1.40
20	4	318	CLA	C1C-C2C	-2.92	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	C1C-C2C	-2.92	1.38	1.44
20	A	850	CLA	CHB-C1B	2.92	1.46	1.39
20	A	834	CLA	C4C-C3C	-2.92	1.40	1.45
20	A	835	CLA	CHB-C1B	2.92	1.46	1.39
20	A	804	CLA	C4C-C3C	-2.91	1.40	1.45
20	A	808	CLA	CHB-C1B	2.91	1.46	1.39
20	B	830	CLA	C1B-NB	-2.91	1.34	1.37
20	A	819	CLA	C4C-C3C	-2.91	1.40	1.45
20	1	211	CLA	C3D-CAD	-2.91	1.35	1.45
20	B	807	CLA	CHB-C1B	2.90	1.45	1.39
20	B	819	CLA	C4B-NB	-2.90	1.34	1.37
20	2	315	CLA	CHB-C1B	2.90	1.47	1.39
20	3	312	CLA	MG-NA	-2.90	1.99	2.06
20	1	206	CLA	C1B-NB	-2.89	1.34	1.37
20	B	819	CLA	MG-NA	-2.89	1.99	2.06
20	A	831	CLA	CHB-C1B	2.89	1.45	1.39
20	H	108	CLA	MG-ND	-2.89	2.00	2.05
20	A	803	CLA	OBD-CAD	2.89	1.27	1.22
20	F	201	CLA	C4B-NB	-2.89	1.34	1.37
20	A	817	CLA	C1B-NB	-2.89	1.34	1.37
20	B	850	CLA	C1D-ND	-2.89	1.34	1.37
20	H	110	CLA	C1B-NB	-2.89	1.34	1.37
21	G	101	LMU	C4B-C3B	2.88	1.59	1.52
20	3	302	CLA	CHB-C1B	2.88	1.47	1.39
20	A	816	CLA	C1C-C2C	-2.88	1.38	1.44
20	A	831	CLA	MG-NA	-2.88	1.99	2.06
20	2	316	CLA	C1D-C2D	-2.88	1.39	1.45
20	L	208	CLA	CBD-CAD	-2.88	1.43	1.56
21	4	320	LMU	O1'-C1'	2.88	1.45	1.40
20	2	309	CLA	CHD-C4C	2.88	1.50	1.40
20	B	839	CLA	OBD-CAD	2.87	1.27	1.22
20	A	839	CLA	MG-NA	-2.87	1.99	2.06
20	B	819	CLA	CHB-C1B	2.87	1.45	1.39
20	1	211	CLA	CBD-CGD	-2.87	1.43	1.52
20	R	108	CLA	C4C-C3C	-2.87	1.40	1.45
20	B	822	CLA	C1B-NB	-2.87	1.34	1.37
20	3	306	CLA	MG-NA	-2.87	1.99	2.06
20	H	108	CLA	C1B-C2B	-2.87	1.36	1.43
20	1	203	CLA	C1D-ND	-2.87	1.34	1.37
20	B	824	CLA	OBD-CAD	2.87	1.27	1.22
20	3	316	CLA	CHD-C4C	2.86	1.50	1.40
20	A	816	CLA	C4B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	208	CLA	CHB-C1B	2.86	1.47	1.39
20	1	202	CLA	C4C-C3C	-2.86	1.40	1.45
20	A	807	CLA	C1B-NB	-2.86	1.34	1.37
20	B	809	CLA	C1B-NB	-2.86	1.34	1.37
20	3	312	CLA	CHA-C1A	2.86	1.49	1.41
20	B	828	CLA	C1B-NB	-2.86	1.34	1.37
20	B	820	CLA	C1B-NB	-2.86	1.34	1.37
20	B	809	CLA	C4B-NB	-2.85	1.34	1.37
20	3	305	CLA	CHB-C1B	2.85	1.47	1.39
20	A	818	CLA	CHB-C1B	2.85	1.45	1.39
20	A	831	CLA	C1D-C2D	-2.85	1.39	1.45
20	4	307	CLA	CHB-C1B	2.85	1.47	1.39
20	4	309	CLA	CHB-C1B	2.85	1.47	1.39
20	4	303	CLA	MG-NA	-2.85	1.99	2.06
20	A	839	CLA	C1D-ND	-2.85	1.34	1.37
20	J	101	CLA	C1C-C2C	-2.85	1.38	1.44
20	A	837	CLA	MG-NA	-2.84	1.99	2.06
20	3	306	CLA	CHB-C1B	2.84	1.47	1.39
20	4	302	CLA	C4C-C3C	-2.84	1.38	1.44
20	A	821	CLA	C1C-C2C	-2.84	1.38	1.44
20	A	809	CLA	C1B-NB	-2.84	1.34	1.37
20	3	314	CLA	CHB-C1B	2.84	1.45	1.39
20	J	103	CLA	CHB-C1B	2.84	1.45	1.39
20	4	315	CLA	C1C-C2C	-2.84	1.38	1.44
20	H	102	CLA	C4C-C3C	-2.84	1.40	1.45
20	A	818	CLA	C1B-C2B	-2.84	1.36	1.43
20	B	840	CLA	C1B-NB	-2.84	1.34	1.37
20	2	305	CLA	C4C-C3C	-2.84	1.40	1.45
20	2	305	CLA	C1B-NB	-2.84	1.34	1.37
20	1	213	CLA	CAA-CBA	2.84	1.61	1.52
20	F	207	CLA	CMA-C3A	2.84	1.59	1.53
20	F	201	CLA	OBD-CAD	2.84	1.27	1.22
20	B	813	CLA	C1C-C2C	-2.83	1.38	1.44
20	B	818	CLA	C4C-C3C	-2.83	1.40	1.45
20	3	315	CLA	C3D-C4D	-2.83	1.37	1.44
20	2	312	CLA	CHB-C1B	2.83	1.45	1.39
20	2	315	CLA	CHD-C4C	2.82	1.49	1.40
20	4	312	CLA	C3D-C4D	-2.82	1.37	1.44
20	A	815	CLA	C4C-C3C	-2.82	1.40	1.45
20	3	312	CLA	CHB-C1B	2.82	1.47	1.39
20	B	802	CLA	C1B-NB	-2.81	1.34	1.37
20	A	833	CLA	C1B-NB	-2.81	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	C1B-NB	-2.81	1.34	1.37
20	2	316	CLA	CHB-C1B	2.81	1.45	1.39
22	B	845	BCR	C20-C19	-2.81	1.27	1.34
20	B	823	CLA	C4C-C3C	-2.81	1.40	1.45
20	1	205	CLA	C1B-NB	-2.80	1.34	1.37
20	1	210	CLA	C1B-NB	-2.80	1.34	1.37
20	B	842	CLA	C1B-NB	-2.80	1.34	1.37
20	4	311	CLA	CHB-C1B	2.80	1.47	1.39
20	A	818	CLA	C1D-ND	-2.80	1.34	1.37
20	A	816	CLA	MG-NA	-2.80	1.99	2.06
20	B	824	CLA	C1C-C2C	-2.80	1.38	1.44
20	H	108	CLA	C1D-C2D	-2.80	1.39	1.45
20	2	312	CLA	C1D-ND	-2.80	1.34	1.37
20	2	315	CLA	C3D-C4D	-2.79	1.37	1.44
20	A	829	CLA	C1B-NB	-2.79	1.34	1.37
20	4	305	CLA	C1D-ND	-2.79	1.34	1.37
20	2	304	CLA	CHD-C4C	2.79	1.49	1.40
20	1	212	CLA	CHB-C1B	2.79	1.47	1.39
20	3	310	CLA	MG-NA	-2.79	1.99	2.06
21	B	849	LMU	O1'-C1'	2.79	1.44	1.40
20	B	813	CLA	C4C-C3C	-2.79	1.40	1.45
20	1	201	CLA	MG-NA	-2.79	1.99	2.06
20	2	316	CLA	MG-NA	-2.78	1.99	2.06
20	3	317	CLA	C1B-NB	-2.78	1.34	1.37
20	A	835	CLA	MG-NA	-2.77	1.99	2.06
20	2	310	CLA	C1B-C2B	-2.77	1.36	1.43
20	A	816	CLA	C1B-C2B	-2.77	1.36	1.43
20	B	824	CLA	C4B-NB	-2.77	1.34	1.37
22	I	101	BCR	C20-C19	-2.76	1.27	1.34
21	B	805	LMU	O1'-C1'	2.76	1.44	1.40
20	B	819	CLA	C1C-NC	-2.76	1.33	1.37
20	A	819	CLA	C1B-NB	-2.76	1.34	1.37
20	B	824	CLA	C1B-C2B	-2.76	1.36	1.43
20	B	830	CLA	MG-NA	-2.76	1.99	2.06
20	B	817	CLA	C1C-C2C	-2.76	1.38	1.44
20	B	823	CLA	C1C-C2C	-2.76	1.38	1.44
20	H	109	CLA	C1B-NB	-2.75	1.34	1.37
20	B	836	CLA	MG-NA	-2.75	1.99	2.06
20	3	306	CLA	CHA-C1A	2.75	1.49	1.41
20	B	812	CLA	C1D-ND	-2.75	1.34	1.37
20	1	208	CLA	CHA-C1A	2.75	1.49	1.41
20	F	201	CLA	MG-NA	-2.75	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	C1C-C2C	-2.75	1.38	1.44
20	1	203	CLA	C1B-NB	-2.75	1.34	1.37
20	A	826	CLA	C1B-NB	-2.75	1.34	1.37
20	L	204	CLA	C1B-NB	-2.75	1.34	1.37
20	B	838	CLA	C1C-C2C	-2.75	1.38	1.44
20	4	305	CLA	MG-NA	-2.75	1.99	2.06
20	A	840	CLA	C4C-C3C	-2.75	1.40	1.45
20	B	835	CLA	C1B-C2B	-2.75	1.36	1.43
20	A	835	CLA	C1C-C2C	-2.74	1.39	1.44
20	B	816	CLA	C4C-C3C	-2.74	1.40	1.45
20	B	839	CLA	C3D-CAD	-2.74	1.36	1.45
20	F	205	CLA	C1C-C2C	-2.74	1.39	1.44
20	A	821	CLA	C4C-C3C	-2.74	1.40	1.45
20	B	832	CLA	C1B-NB	-2.73	1.34	1.37
20	I	102	CLA	C1B-NB	-2.73	1.34	1.37
20	4	312	CLA	CHB-C1B	2.73	1.47	1.39
20	3	317	CLA	C4C-C3C	-2.72	1.39	1.44
20	A	834	CLA	C1C-C2C	-2.72	1.39	1.44
20	3	314	CLA	C1C-NC	-2.72	1.33	1.37
20	A	826	CLA	C4B-NB	-2.72	1.34	1.37
20	B	837	CLA	C4C-C3C	-2.72	1.40	1.45
20	B	812	CLA	CHB-C1B	2.71	1.45	1.39
20	G	105	CLA	CHB-C1B	2.71	1.45	1.39
20	A	816	CLA	CHB-C1B	2.71	1.45	1.39
20	4	305	CLA	C1D-C2D	-2.71	1.40	1.45
20	B	803	CLA	MG-NA	-2.71	1.99	2.06
20	2	312	CLA	C1D-C2D	-2.71	1.40	1.45
20	B	836	CLA	C1D-ND	-2.71	1.34	1.37
21	2	319	LMU	O1'-C1'	2.70	1.44	1.40
20	J	103	CLA	C1D-ND	-2.70	1.34	1.37
20	3	317	CLA	C3A-C2A	-2.70	1.52	1.54
20	1	212	CLA	CHA-C1A	2.70	1.49	1.41
20	2	302	CLA	C1C-NC	-2.70	1.33	1.37
20	3	313	CLA	C4C-C3C	-2.70	1.40	1.45
21	4	316	LMU	O1'-C1'	2.70	1.44	1.40
20	A	829	CLA	C1C-C2C	-2.70	1.39	1.44
20	B	850	CLA	C1C-C2C	-2.70	1.39	1.44
20	A	839	CLA	C4B-NB	-2.70	1.34	1.37
20	A	801	CLA	C1B-NB	-2.70	1.34	1.37
20	A	806	CLA	C1B-NB	-2.70	1.34	1.37
20	4	303	CLA	C1B-C2B	-2.69	1.36	1.43
20	A	814	CLA	CHB-C1B	2.69	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	204	CLA	C1D-ND	-2.69	1.34	1.37
20	3	311	CLA	C1C-C2C	-2.69	1.39	1.44
20	A	808	CLA	C1B-NB	-2.68	1.34	1.37
20	1	205	CLA	C1C-C2C	-2.68	1.39	1.44
20	4	302	CLA	C4B-NB	-2.68	1.34	1.37
20	4	306	CLA	C4B-NB	-2.68	1.34	1.37
20	A	815	CLA	C1B-NB	-2.68	1.34	1.37
20	H	102	CLA	C1B-NB	-2.68	1.34	1.37
20	K	103	CLA	C1D-ND	-2.68	1.34	1.37
20	4	314	CLA	CHA-C1A	2.68	1.48	1.41
20	3	317	CLA	C1C-C2C	-2.68	1.39	1.44
21	H	103	LMU	O1'-C1'	2.67	1.44	1.40
20	2	307	CLA	C1D-ND	-2.67	1.34	1.37
20	4	307	CLA	C3D-C4D	-2.67	1.37	1.44
20	3	314	CLA	C1B-C2B	-2.67	1.36	1.43
20	3	310	CLA	C1D-ND	-2.67	1.34	1.37
20	1	215	CLA	MG-NA	-2.67	1.99	2.06
20	1	204	CLA	CHB-C1B	2.67	1.45	1.39
20	A	817	CLA	C1C-C2C	-2.67	1.39	1.44
20	B	818	CLA	C1C-C2C	-2.67	1.39	1.44
20	3	309	CLA	CHA-C1A	2.66	1.48	1.41
20	B	819	CLA	C1D-C2D	-2.66	1.40	1.45
20	L	207	CLA	C4C-C3C	-2.66	1.40	1.45
20	A	806	CLA	C1C-C2C	-2.66	1.39	1.44
20	A	824	CLA	C1C-C2C	-2.66	1.39	1.44
20	3	305	CLA	CHA-C1A	2.66	1.48	1.41
20	2	310	CLA	C1D-ND	-2.66	1.34	1.37
20	A	825	CLA	C1C-C2C	-2.65	1.39	1.44
20	A	812	CLA	C1B-NB	-2.65	1.34	1.37
20	1	208	CLA	MG-NA	-2.65	2.00	2.06
20	L	207	CLA	C1B-NB	-2.65	1.34	1.37
20	F	201	CLA	C1D-C2D	-2.65	1.40	1.45
20	A	832	CLA	C1C-C2C	-2.65	1.39	1.44
20	4	315	CLA	MG-NA	-2.65	2.00	2.06
20	A	826	CLA	C1C-C2C	-2.64	1.39	1.44
20	A	805	CLA	C4C-C3C	-2.64	1.40	1.45
20	B	831	CLA	C4C-C3C	-2.64	1.40	1.45
20	2	308	CLA	C3C-C4C	-2.64	1.36	1.43
20	2	309	CLA	C3D-C4D	-2.64	1.37	1.44
20	A	818	CLA	C1D-C2D	-2.64	1.40	1.45
20	3	316	CLA	C3D-C4D	-2.64	1.37	1.44
20	1	211	CLA	CBD-CAD	-2.64	1.44	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	815	CLA	C4C-C3C	-2.64	1.40	1.45
20	4	301	CLA	C1C-C2C	-2.64	1.39	1.44
20	1	211	CLA	C4B-NB	-2.64	1.34	1.37
20	1	209	CLA	C3D-C4D	-2.63	1.37	1.44
20	2	316	CLA	C1D-ND	-2.63	1.34	1.37
20	3	303	CLA	C1B-NB	-2.63	1.34	1.37
20	F	206	CLA	C1C-C2C	-2.63	1.39	1.44
20	A	803	CLA	MG-NA	-2.63	2.00	2.06
20	A	822	CLA	C1C-C2C	-2.63	1.39	1.44
20	A	849	CLA	C1B-NB	-2.62	1.34	1.37
20	A	812	CLA	C1C-C2C	-2.62	1.39	1.44
20	A	832	CLA	C4C-C3C	-2.62	1.40	1.45
20	2	301	CLA	C3D-C4D	-2.62	1.37	1.44
20	1	202	CLA	C1C-C2C	-2.62	1.39	1.44
20	2	312	CLA	C1C-C2C	-2.62	1.39	1.44
20	1	201	CLA	C4B-NB	-2.62	1.34	1.37
20	A	836	CLA	C1C-C2C	-2.61	1.39	1.44
20	B	812	CLA	C1D-C2D	-2.61	1.40	1.45
20	2	316	CLA	C1B-C2B	-2.61	1.37	1.43
20	K	103	CLA	CHB-C1B	2.61	1.45	1.39
20	A	851	CLA	MG-NA	-2.60	2.00	2.06
20	4	310	CLA	MG-NA	-2.60	2.00	2.06
20	4	313	CLA	C1B-NB	-2.60	1.34	1.37
20	2	306	CLA	CHA-C1A	2.60	1.48	1.41
20	3	302	CLA	CHA-C1A	2.60	1.48	1.41
20	B	825	CLA	C1C-C2C	-2.60	1.39	1.44
20	4	303	CLA	C4B-NB	-2.59	1.34	1.37
20	A	818	CLA	OBD-CAD	2.59	1.26	1.22
20	B	819	CLA	C1B-C2B	-2.58	1.37	1.43
20	2	303	CLA	C1C-NC	-2.58	1.33	1.37
20	A	827	CLA	C4C-C3C	-2.58	1.40	1.45
20	J	103	CLA	C1D-C2D	-2.58	1.40	1.45
20	A	823	CLA	C1B-NB	-2.58	1.34	1.37
20	B	837	CLA	C1B-NB	-2.58	1.34	1.37
20	K	101	CLA	MG-NA	-2.58	2.00	2.06
20	3	310	CLA	C1C-C2C	-2.58	1.39	1.44
20	A	841	CLA	C3D-C4D	-2.58	1.37	1.44
20	A	834	CLA	C1B-NB	-2.57	1.34	1.37
20	A	809	CLA	C4B-NB	-2.57	1.34	1.37
20	F	207	CLA	C1D-ND	-2.57	1.34	1.37
20	4	303	CLA	CHB-C4A	-2.56	1.31	1.37
20	1	207	CLA	C3A-C2A	-2.56	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	203	CLA	C2A-C1A	-2.56	1.46	1.52
20	B	828	CLA	C1C-C2C	-2.56	1.39	1.44
20	B	831	CLA	C1C-C2C	-2.55	1.39	1.44
20	B	840	CLA	C1C-C2C	-2.55	1.39	1.44
20	A	827	CLA	C1C-C2C	-2.55	1.39	1.44
20	A	813	CLA	C1B-NB	-2.55	1.34	1.37
20	L	207	CLA	C1C-C2C	-2.55	1.39	1.44
20	1	213	CLA	MG-NA	-2.55	2.00	2.06
20	H	108	CLA	C1C-NC	-2.55	1.33	1.37
20	A	810	CLA	C1C-C2C	-2.55	1.39	1.44
20	K	101	CLA	C1C-C2C	-2.55	1.39	1.44
20	1	213	CLA	MG-ND	-2.55	2.00	2.05
20	A	841	CLA	CHA-C1A	2.54	1.48	1.41
20	1	215	CLA	C1D-ND	-2.54	1.34	1.37
20	1	213	CLA	C1C-NC	-2.54	1.33	1.37
20	3	303	CLA	C4C-C3C	-2.54	1.39	1.44
20	3	316	CLA	CHB-C1B	2.54	1.46	1.39
20	G	105	CLA	C4B-NB	-2.54	1.34	1.37
20	4	315	CLA	C4B-NB	-2.54	1.34	1.37
20	4	318	CLA	C1D-ND	-2.54	1.34	1.37
20	4	303	CLA	CHB-C1B	2.53	1.45	1.39
20	H	101	CLA	C1C-C2C	-2.53	1.39	1.44
20	A	823	CLA	C4C-C3C	-2.53	1.40	1.45
20	B	824	CLA	C4D-CHA	-2.53	1.29	1.38
20	B	815	CLA	C1C-C2C	-2.53	1.39	1.44
22	B	801	BCR	C17-C18	-2.53	1.30	1.35
20	B	826	CLA	C1C-C2C	-2.53	1.39	1.44
20	A	850	CLA	C1C-C2C	-2.53	1.39	1.44
20	2	304	CLA	CHB-C1B	2.53	1.46	1.39
20	A	813	CLA	MG-NA	-2.53	2.00	2.06
20	B	812	CLA	CHB-C4A	-2.52	1.31	1.37
20	B	837	CLA	C1C-C2C	-2.52	1.39	1.44
20	G	105	CLA	C1B-C2B	-2.52	1.37	1.43
20	B	839	CLA	C4D-CHA	-2.52	1.29	1.38
20	3	314	CLA	C1D-ND	-2.52	1.34	1.37
20	1	213	CLA	CHB-C4A	-2.52	1.31	1.37
20	2	308	CLA	CHD-C4C	2.52	1.48	1.40
20	A	850	CLA	C1B-C2B	-2.51	1.37	1.43
20	A	809	CLA	C4C-C3C	-2.51	1.40	1.45
20	3	311	CLA	MG-NA	-2.51	2.00	2.06
20	2	302	CLA	CHB-C4A	-2.51	1.31	1.37
20	1	201	CLA	C1D-C2D	-2.51	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	819	CLA	CHB-C4A	-2.51	1.31	1.37
20	K	104	CLA	C1B-C2B	-2.50	1.37	1.43
20	F	206	CLA	C4B-NB	-2.50	1.34	1.37
20	1	210	CLA	C4C-C3C	-2.50	1.39	1.44
20	2	304	CLA	C3D-C4D	-2.50	1.38	1.44
20	4	318	CLA	C4C-C3C	-2.50	1.40	1.45
20	3	304	CLA	CHB-C1B	2.50	1.46	1.39
21	G	101	LMU	C6B-C5B	2.49	1.60	1.51
20	B	825	CLA	C4B-NB	-2.49	1.34	1.37
20	B	812	CLA	C3D-CAD	-2.49	1.36	1.45
20	3	304	CLA	C3D-C4D	-2.49	1.38	1.44
20	2	301	CLA	CHA-C1A	2.49	1.48	1.41
20	2	301	CLA	CHB-C1B	2.49	1.46	1.39
20	3	313	CLA	C1B-NB	-2.49	1.34	1.37
20	A	849	CLA	C1D-C2D	-2.49	1.40	1.45
20	A	828	CLA	C1C-C2C	-2.49	1.39	1.44
20	A	849	CLA	C1D-ND	-2.49	1.34	1.37
20	2	307	CLA	MG-NA	-2.49	2.00	2.06
20	L	202	CLA	C1C-C2C	-2.49	1.39	1.44
20	3	307	CLA	C1D-ND	-2.48	1.34	1.37
20	A	838	CLA	C1D-ND	-2.48	1.34	1.37
20	4	308	CLA	C3D-C4D	-2.48	1.38	1.44
20	A	815	CLA	C1C-C2C	-2.48	1.39	1.44
20	F	205	CLA	C4C-C3C	-2.48	1.39	1.44
20	2	308	CLA	C2C-C1C	-2.48	1.37	1.43
20	4	315	CLA	C1B-C2B	-2.48	1.37	1.43
20	3	301	CLA	C1B-NB	-2.47	1.34	1.37
20	4	309	CLA	CHA-C1A	2.47	1.48	1.41
22	F	204	BCR	C1-C6	-2.47	1.50	1.53
20	G	105	CLA	C1C-C2C	-2.47	1.39	1.44
22	A	845	BCR	C30-C25	-2.46	1.50	1.53
20	4	308	CLA	CHA-C1A	2.46	1.48	1.41
20	B	835	CLA	C1C-C2C	-2.46	1.39	1.44
20	A	802	CLA	CHA-C1A	2.46	1.48	1.41
20	A	805	CLA	C1B-NB	-2.46	1.34	1.37
20	1	213	CLA	CHB-C1B	2.46	1.44	1.39
20	B	811	CLA	CHB-C1B	2.46	1.46	1.39
20	4	311	CLA	CHA-C1A	2.46	1.48	1.41
20	1	205	CLA	C4C-C3C	-2.46	1.39	1.44
20	A	802	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	818	CLA	C1C-NC	-2.45	1.34	1.37
20	2	308	CLA	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	103	BCR	C1-C6	-2.45	1.50	1.53
20	A	838	CLA	C1B-NB	-2.45	1.34	1.37
20	2	312	CLA	C4B-NB	-2.45	1.34	1.37
20	4	305	CLA	C4B-NB	-2.45	1.34	1.37
20	B	808	CLA	C1D-ND	-2.44	1.34	1.37
20	B	839	CLA	C1B-C2B	-2.44	1.37	1.43
20	4	311	CLA	C3D-C4D	-2.44	1.38	1.44
20	L	208	CLA	C4B-NB	-2.44	1.34	1.37
20	2	308	CLA	C1C-NC	-2.44	1.32	1.38
20	A	823	CLA	C1C-C2C	-2.44	1.39	1.44
20	B	834	CLA	MG-NA	-2.44	2.00	2.06
20	F	207	CLA	C1B-C2B	-2.44	1.37	1.43
20	4	302	CLA	C1C-C2C	-2.43	1.39	1.44
20	G	105	CLA	MG-NA	-2.43	2.00	2.06
20	1	214	CLA	CHB-C1B	2.43	1.46	1.39
20	B	841	CLA	C4C-C3C	-2.43	1.40	1.45
20	1	204	CLA	C1B-C2B	-2.43	1.37	1.43
20	B	808	CLA	OBD-CAD	2.43	1.26	1.22
20	A	821	CLA	C1B-NB	-2.43	1.34	1.37
20	A	850	CLA	C4B-NB	-2.43	1.34	1.37
20	1	214	CLA	C3D-C4D	-2.42	1.38	1.44
20	B	822	CLA	C1C-C2C	-2.42	1.39	1.44
20	G	105	CLA	CHB-C4A	-2.42	1.31	1.37
20	3	315	CLA	CHB-C1B	2.42	1.46	1.39
20	2	304	CLA	CHA-C1A	2.42	1.48	1.41
20	A	808	CLA	MG-NA	-2.42	2.00	2.06
20	3	308	CLA	CHA-C1A	2.42	1.48	1.41
22	B	846	BCR	C30-C25	-2.41	1.50	1.53
20	A	802	CLA	CHB-C1B	2.41	1.46	1.39
20	K	104	CLA	C4B-NB	-2.41	1.34	1.37
20	F	207	CLA	MG-NA	-2.41	2.00	2.06
20	B	827	CLA	C1C-C2C	-2.41	1.39	1.44
20	B	833	CLA	C4B-NB	-2.40	1.34	1.37
20	A	819	CLA	C1B-C2B	-2.40	1.37	1.43
20	1	202	CLA	C1B-C2B	-2.40	1.37	1.43
20	B	811	CLA	CHA-C1A	2.40	1.48	1.41
20	B	836	CLA	C1B-C2B	-2.40	1.37	1.43
20	A	839	CLA	C1B-C2B	-2.40	1.37	1.43
20	2	316	CLA	C3D-CAD	-2.40	1.37	1.45
20	B	812	CLA	C1B-C2B	-2.40	1.37	1.43
20	L	202	CLA	MG-NA	-2.40	2.00	2.06
20	A	834	CLA	C1D-ND	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	839	CLA	C1C-NC	-2.39	1.34	1.37
20	A	814	CLA	C3D-C4D	-2.39	1.38	1.44
20	R	107	CLA	C1C-C2C	-2.39	1.39	1.44
20	3	308	CLA	C3D-C4D	-2.39	1.38	1.44
20	3	304	CLA	CHA-C1A	2.39	1.48	1.41
20	K	104	CLA	MG-NA	-2.39	2.00	2.06
20	B	850	CLA	MG-NA	-2.39	2.00	2.06
20	1	213	CLA	C1D-C2D	-2.39	1.40	1.45
20	A	832	CLA	MG-NA	-2.39	2.00	2.06
20	2	306	CLA	C3D-C4D	-2.38	1.38	1.44
20	F	201	CLA	C1C-NC	-2.38	1.34	1.37
20	B	807	CLA	MG-NA	-2.38	2.00	2.06
20	A	831	CLA	C1B-C2B	-2.38	1.37	1.43
20	4	313	CLA	C1C-C2C	-2.38	1.39	1.44
20	4	314	CLA	MG-NA	-2.38	2.00	2.06
20	B	832	CLA	C1B-C2B	-2.37	1.37	1.43
20	F	205	CLA	C1B-NB	-2.37	1.34	1.37
20	1	206	CLA	C1C-C2C	-2.37	1.39	1.44
20	B	841	CLA	C1C-C2C	-2.37	1.39	1.44
20	A	806	CLA	MG-NA	-2.37	2.00	2.06
20	A	839	CLA	C2A-C1A	-2.37	1.46	1.52
20	4	302	CLA	C1B-C2B	-2.37	1.37	1.43
20	L	203	CLA	C1B-NB	-2.37	1.34	1.37
20	2	312	CLA	CHB-C4A	-2.36	1.31	1.37
20	4	308	CLA	CHB-C1B	2.36	1.46	1.39
20	3	314	CLA	C3D-CAD	-2.36	1.37	1.45
20	B	827	CLA	C1B-C2B	-2.36	1.37	1.43
20	A	824	CLA	MG-NA	-2.36	2.00	2.06
20	B	827	CLA	MG-NA	-2.36	2.00	2.06
20	2	311	CLA	C1C-C2C	-2.36	1.39	1.44
20	A	825	CLA	MG-NA	-2.35	2.00	2.06
20	L	201	CLA	C1C-C2C	-2.35	1.39	1.44
20	A	804	CLA	C1B-NB	-2.35	1.34	1.37
20	1	215	CLA	C1C-C2C	-2.35	1.39	1.44
20	B	832	CLA	C1C-C2C	-2.35	1.39	1.44
20	2	302	CLA	C1D-ND	-2.35	1.34	1.37
20	B	828	CLA	MG-NA	-2.35	2.00	2.06
20	L	208	CLA	CBD-CGD	-2.35	1.45	1.52
20	B	819	CLA	OBD-CAD	2.35	1.26	1.22
20	B	808	CLA	C1D-C2D	-2.35	1.40	1.45
20	B	836	CLA	C4B-NB	-2.34	1.34	1.37
20	A	808	CLA	C1B-C2B	-2.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	814	CLA	C2C-C1C	-2.34	1.37	1.43
20	A	835	CLA	C1B-C2B	-2.34	1.37	1.43
20	I	102	CLA	C1C-C2C	-2.34	1.39	1.44
20	B	807	CLA	C1B-C2B	-2.34	1.37	1.43
20	B	802	CLA	C1C-C2C	-2.34	1.39	1.44
20	A	803	CLA	C1D-ND	-2.34	1.34	1.37
20	1	207	CLA	C1C-C2C	-2.33	1.39	1.44
20	J	101	CLA	MG-NA	-2.33	2.00	2.06
20	A	841	CLA	CHB-C1B	2.33	1.46	1.39
21	R	105	LMU	O1'-C1'	2.33	1.44	1.40
20	3	310	CLA	C1B-C2B	-2.33	1.37	1.43
20	K	103	CLA	CHB-C4A	-2.33	1.31	1.37
20	F	205	CLA	C1B-C2B	-2.33	1.37	1.43
20	J	103	CLA	C4B-NB	-2.33	1.34	1.37
20	H	101	CLA	MG-NA	-2.33	2.00	2.06
20	A	833	CLA	MG-NA	-2.33	2.00	2.06
20	K	103	CLA	C4B-NB	-2.33	1.34	1.37
20	A	820	CLA	C1C-C2C	-2.33	1.39	1.44
20	B	826	CLA	C4B-NB	-2.32	1.34	1.37
20	L	203	CLA	C1C-C2C	-2.32	1.39	1.44
20	4	301	CLA	MG-NA	-2.32	2.00	2.06
20	B	821	CLA	C1C-C2C	-2.32	1.39	1.44
20	2	309	CLA	CHA-C1A	2.32	1.47	1.41
20	1	203	CLA	C1B-C2B	-2.32	1.37	1.43
20	B	818	CLA	C1B-C2B	-2.32	1.37	1.43
20	4	318	CLA	MG-NA	-2.32	2.00	2.06
20	1	215	CLA	C3D-CAD	-2.32	1.37	1.45
20	2	308	CLA	CHA-C1A	2.31	1.47	1.41
20	4	317	CLA	C4B-NB	-2.31	1.34	1.37
20	A	831	CLA	CHB-C4A	-2.31	1.31	1.37
20	2	309	CLA	CHB-C1B	2.31	1.46	1.39
20	K	102	CLA	MG-NA	-2.31	2.00	2.06
20	1	213	CLA	C1D-ND	-2.31	1.34	1.37
20	4	318	CLA	C1B-C2B	-2.31	1.37	1.43
20	1	215	CLA	MG-ND	-2.31	2.01	2.05
20	B	814	CLA	C1C-C2C	-2.31	1.39	1.44
20	4	310	CLA	C4B-NB	-2.31	1.34	1.37
20	A	838	CLA	C1C-C2C	-2.30	1.39	1.44
20	2	314	CLA	C3D-CAD	-2.30	1.37	1.45
20	2	302	CLA	CHB-C1B	2.30	1.44	1.39
20	L	201	CLA	C1B-C2B	-2.30	1.37	1.43
20	1	212	CLA	C3D-C4D	-2.30	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	849	CLA	C1C-C2C	-2.30	1.39	1.44
20	B	829	CLA	C1C-C2C	-2.29	1.39	1.44
20	H	102	CLA	C1C-C2C	-2.29	1.39	1.44
20	F	206	CLA	MG-NA	-2.29	2.00	2.06
20	R	108	CLA	C1C-C2C	-2.29	1.39	1.44
20	2	316	CLA	CAA-C2A	-2.29	1.49	1.54
20	A	829	CLA	C4C-C3C	-2.29	1.41	1.45
20	H	109	CLA	C1C-C2C	-2.29	1.39	1.44
20	1	210	CLA	C1C-C2C	-2.29	1.39	1.44
20	1	215	CLA	CHB-C4A	-2.29	1.32	1.37
20	1	215	CLA	C4B-NB	-2.29	1.34	1.37
20	3	308	CLA	CHB-C1B	2.29	1.46	1.39
20	3	309	CLA	C3D-C4D	-2.29	1.38	1.44
20	B	841	CLA	C1B-NB	-2.28	1.34	1.37
20	B	819	CLA	MG-ND	-2.28	2.01	2.05
20	B	833	CLA	MG-NA	-2.28	2.00	2.06
20	B	831	CLA	C1B-C2B	-2.28	1.37	1.43
20	A	803	CLA	C1B-C2B	-2.28	1.37	1.43
20	B	825	CLA	C1B-C2B	-2.28	1.37	1.43
20	4	314	CLA	C3D-C4D	-2.28	1.38	1.44
20	A	808	CLA	C1C-C2C	-2.27	1.39	1.44
20	4	312	CLA	CHA-C1A	2.27	1.47	1.41
20	H	109	CLA	C4C-C3C	-2.27	1.41	1.45
20	1	207	CLA	C1B-NB	-2.27	1.34	1.37
20	B	817	CLA	C1B-NB	-2.27	1.34	1.37
20	A	804	CLA	C1C-C2C	-2.27	1.39	1.44
20	1	207	CLA	MG-NA	-2.27	2.00	2.06
20	L	204	CLA	C1C-C2C	-2.27	1.39	1.44
20	A	840	CLA	C1C-C2C	-2.27	1.39	1.44
21	4	319	LMU	O6B-C6B	2.26	1.51	1.42
20	3	315	CLA	CHA-C1A	2.26	1.47	1.41
20	A	810	CLA	C1B-NB	-2.26	1.34	1.37
20	4	306	CLA	C3A-C2A	-2.26	1.48	1.54
20	B	810	CLA	MG-NA	-2.25	2.00	2.06
20	B	808	CLA	MG-ND	-2.25	2.01	2.05
20	1	213	CLA	C3A-C4A	-2.25	1.44	1.51
20	3	301	CLA	C1C-C2C	-2.25	1.40	1.44
20	B	814	CLA	MG-NA	-2.25	2.00	2.06
20	3	314	CLA	CHB-C4A	-2.25	1.32	1.37
20	B	850	CLA	C1D-C2D	-2.25	1.40	1.45
20	A	835	CLA	CHB-C4A	-2.25	1.32	1.37
20	B	842	CLA	C1C-C2C	-2.24	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	312	CLA	C3D-C4D	-2.24	1.38	1.44
20	2	304	CLA	C3C-C4C	-2.24	1.37	1.43
20	2	314	CLA	C4B-NB	-2.24	1.34	1.37
20	4	309	CLA	C3D-C4D	-2.24	1.38	1.44
20	B	808	CLA	C1B-C2B	-2.24	1.37	1.43
20	A	838	CLA	MG-NA	-2.24	2.00	2.06
20	B	823	CLA	MG-NA	-2.24	2.00	2.06
20	2	316	CLA	CHB-C4A	-2.24	1.32	1.37
20	3	314	CLA	C3B-C4B	-2.24	1.36	1.42
20	B	814	CLA	C1B-C2B	-2.24	1.37	1.43
20	B	823	CLA	C4B-NB	-2.24	1.34	1.37
20	B	811	CLA	C2C-C1C	-2.23	1.37	1.43
20	A	803	CLA	C3D-CAD	-2.23	1.37	1.45
20	B	810	CLA	C4B-NB	-2.23	1.34	1.37
20	B	806	CLA	C1D-ND	-2.23	1.34	1.37
20	B	839	CLA	C1D-C2D	-2.23	1.40	1.45
20	L	208	CLA	C1B-C2B	-2.23	1.37	1.43
20	4	317	CLA	C1B-C2B	-2.23	1.37	1.43
20	A	819	CLA	C4B-NB	-2.23	1.34	1.37
20	A	830	CLA	MG-NA	-2.22	2.01	2.06
20	B	821	CLA	MG-NA	-2.22	2.01	2.06
20	B	824	CLA	C1C-NC	-2.22	1.34	1.37
20	4	304	CLA	MG-NA	-2.22	2.01	2.06
20	A	816	CLA	CHB-C4A	-2.22	1.32	1.37
20	1	214	CLA	CHA-C1A	2.22	1.47	1.41
20	B	807	CLA	C1C-C2C	-2.22	1.40	1.44
20	3	315	CLA	C2C-C1C	-2.22	1.37	1.43
20	A	827	CLA	MG-NA	-2.22	2.01	2.06
20	B	808	CLA	C4B-NB	-2.22	1.34	1.37
20	4	305	CLA	C1C-NC	-2.22	1.34	1.37
20	3	307	CLA	C4B-NB	-2.22	1.34	1.37
20	3	301	CLA	C4C-C3C	-2.22	1.40	1.44
20	A	808	CLA	C1D-ND	-2.22	1.34	1.37
21	4	319	LMU	O1'-C1'	2.22	1.43	1.40
21	H	106	LMU	O1'-C1'	2.21	1.43	1.40
20	1	204	CLA	CHB-C4A	-2.21	1.32	1.37
20	B	812	CLA	C1C-NC	-2.21	1.34	1.37
20	L	202	CLA	C1B-C2B	-2.21	1.37	1.43
20	3	310	CLA	C1D-C2D	-2.21	1.41	1.45
20	A	810	CLA	MG-NA	-2.21	2.01	2.06
20	B	840	CLA	MG-NA	-2.21	2.01	2.06
20	3	302	CLA	C3D-C4D	-2.21	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	308	CLA	C3C-C4C	-2.21	1.37	1.43
20	3	310	CLA	C1C-NC	-2.20	1.34	1.37
21	A	847	LMU	O1'-C1'	2.20	1.43	1.40
20	4	313	CLA	MG-NA	-2.20	2.01	2.06
20	A	826	CLA	C1B-C2B	-2.20	1.38	1.43
20	1	215	CLA	C1B-C2B	-2.20	1.38	1.43
20	1	209	CLA	CHA-C1A	2.20	1.47	1.41
20	4	304	CLA	C4C-C3C	-2.20	1.41	1.45
20	B	842	CLA	C4C-C3C	-2.20	1.40	1.44
20	3	309	CLA	CHB-C1B	2.20	1.45	1.39
20	4	311	CLA	C3C-C4C	-2.20	1.37	1.43
20	4	315	CLA	C1D-ND	-2.20	1.35	1.37
20	2	302	CLA	MG-ND	-2.19	2.01	2.05
20	J	103	CLA	C1B-C2B	-2.19	1.38	1.43
20	3	304	CLA	C2C-C1C	-2.19	1.37	1.43
20	B	806	CLA	C1C-C2C	-2.19	1.40	1.44
20	B	832	CLA	C4B-NB	-2.19	1.35	1.37
20	B	822	CLA	C1B-C2B	-2.19	1.38	1.43
20	B	819	CLA	C3D-CAD	-2.19	1.37	1.45
20	1	207	CLA	CAA-C2A	-2.19	1.50	1.54
20	A	831	CLA	C1C-NC	-2.19	1.34	1.37
20	A	814	CLA	CHA-C1A	2.18	1.47	1.41
20	B	816	CLA	C1C-C2C	-2.18	1.40	1.44
20	B	826	CLA	MG-NA	-2.18	2.01	2.06
20	2	305	CLA	C1C-C2C	-2.18	1.40	1.44
20	A	804	CLA	C1B-C2B	-2.18	1.38	1.43
20	A	816	CLA	C3D-CAD	-2.18	1.38	1.45
20	J	103	CLA	CHB-C4A	-2.18	1.32	1.37
20	1	209	CLA	CHB-C1B	2.18	1.45	1.39
20	A	822	CLA	C1B-C2B	-2.18	1.38	1.43
20	A	831	CLA	C3D-CAD	-2.18	1.38	1.45
20	1	203	CLA	C4D-CHA	-2.18	1.31	1.38
20	B	807	CLA	CHB-C4A	-2.17	1.32	1.37
20	3	314	CLA	MG-ND	-2.17	2.01	2.05
20	4	318	CLA	C4B-NB	-2.17	1.35	1.37
20	A	819	CLA	MG-NA	-2.17	2.01	2.06
20	A	803	CLA	C1C-NC	-2.17	1.34	1.37
20	A	801	CLA	C4C-C3C	-2.17	1.41	1.45
20	B	829	CLA	C1D-C2D	-2.16	1.41	1.45
20	K	101	CLA	C1B-C2B	-2.16	1.38	1.43
20	A	820	CLA	MG-NA	-2.16	2.01	2.06
20	3	317	CLA	MG-NA	-2.16	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	813	CLA	MG-NA	-2.16	2.01	2.06
20	2	303	CLA	C3D-CAD	-2.16	1.38	1.45
20	2	312	CLA	C1B-C2B	-2.16	1.38	1.43
20	A	830	CLA	C1B-C2B	-2.16	1.38	1.43
20	A	822	CLA	MG-NA	-2.15	2.01	2.06
20	3	311	CLA	C1B-C2B	-2.15	1.38	1.43
20	1	201	CLA	C1D-ND	-2.15	1.35	1.37
20	3	309	CLA	C2C-C1C	-2.15	1.38	1.43
20	A	807	CLA	MG-NA	-2.15	2.01	2.06
20	B	820	CLA	C1C-C2C	-2.15	1.40	1.44
20	4	310	CLA	C1B-C2B	-2.15	1.38	1.43
20	4	310	CLA	C1C-NC	-2.15	1.34	1.37
20	B	806	CLA	MG-NA	-2.15	2.01	2.06
20	4	307	CLA	CHA-C1A	2.15	1.47	1.41
20	4	306	CLA	C1D-ND	-2.14	1.35	1.37
20	F	207	CLA	CHB-C4A	-2.14	1.32	1.37
20	4	315	CLA	C1D-C2D	-2.14	1.41	1.45
20	B	824	CLA	C1D-C2D	-2.14	1.41	1.45
21	L	210	LMU	O1'-C1'	2.14	1.43	1.40
20	A	834	CLA	MG-NA	-2.14	2.01	2.06
20	A	849	CLA	C1B-C2B	-2.14	1.38	1.43
20	4	306	CLA	CAA-C2A	-2.14	1.50	1.54
20	F	205	CLA	CHB-C4A	-2.14	1.32	1.37
20	4	301	CLA	C4B-NB	-2.13	1.35	1.37
20	K	104	CLA	C3D-CAD	-2.13	1.38	1.45
20	B	835	CLA	MG-NA	-2.13	2.01	2.06
20	A	828	CLA	C1B-C2B	-2.13	1.38	1.43
20	A	823	CLA	C1B-C2B	-2.13	1.38	1.43
20	4	313	CLA	C4C-C3C	-2.13	1.40	1.44
20	B	812	CLA	C3A-C2A	-2.13	1.48	1.54
20	F	201	CLA	C3D-CAD	-2.13	1.38	1.45
21	C	101	LMU	O1'-C1'	2.13	1.43	1.40
20	A	824	CLA	C1B-C2B	-2.13	1.38	1.43
20	F	205	CLA	MG-NA	-2.13	2.01	2.06
20	B	812	CLA	C4D-CHA	-2.13	1.31	1.38
20	K	103	CLA	MG-ND	-2.12	2.01	2.05
20	4	308	CLA	C2C-C1C	-2.12	1.38	1.43
20	A	837	CLA	C4B-NB	-2.12	1.35	1.37
20	3	306	CLA	C3D-C2D	2.12	1.40	1.35
20	2	309	CLA	C2D-C1D	-2.12	1.38	1.44
20	H	110	CLA	C1C-C2C	-2.12	1.40	1.44
20	B	827	CLA	C4B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	C1B-C2B	-2.12	1.38	1.43
20	A	818	CLA	C3A-C2A	-2.12	1.48	1.54
20	B	806	CLA	C1B-NB	-2.12	1.35	1.37
21	R	103	LMU	O1'-C1'	2.12	1.43	1.40
20	B	820	CLA	C1D-ND	-2.12	1.35	1.37
20	L	208	CLA	C1C-C2C	-2.11	1.40	1.44
20	3	314	CLA	MG-NB	-2.11	2.01	2.05
20	A	807	CLA	C1C-C2C	-2.11	1.40	1.44
20	A	801	CLA	C2A-C1A	-2.11	1.47	1.52
20	4	303	CLA	C3A-C2A	-2.11	1.48	1.54
20	B	830	CLA	C1D-ND	-2.11	1.35	1.37
20	A	826	CLA	MG-NA	-2.11	2.01	2.06
20	B	822	CLA	MG-NA	-2.11	2.01	2.06
21	A	852	LMU	O1'-C1'	2.11	1.43	1.40
20	A	831	CLA	C3A-C2A	-2.11	1.48	1.54
20	4	310	CLA	C1D-C2D	-2.11	1.41	1.45
20	K	102	CLA	C4B-NB	-2.11	1.35	1.37
22	B	844	BCR	C1-C6	-2.10	1.51	1.53
20	A	850	CLA	CHB-C4A	-2.10	1.32	1.37
20	B	831	CLA	C1D-ND	-2.10	1.35	1.37
20	3	310	CLA	C3B-C4B	-2.10	1.36	1.42
20	B	829	CLA	MG-NA	-2.10	2.01	2.06
20	3	305	CLA	C3D-C4D	-2.10	1.39	1.44
20	1	206	CLA	MG-NA	-2.10	2.01	2.06
20	B	833	CLA	C1C-NC	-2.10	1.34	1.37
20	K	101	CLA	C1D-ND	-2.10	1.35	1.37
20	B	802	CLA	MG-NA	-2.10	2.01	2.06
21	K	105	LMU	O1'-C1'	2.09	1.43	1.40
20	A	807	CLA	C4B-NB	-2.09	1.35	1.37
20	1	208	CLA	C3D-C4D	-2.09	1.39	1.44
20	A	814	CLA	C3C-C4C	-2.09	1.38	1.43
21	R	101	LMU	O1'-C1'	2.09	1.43	1.40
20	1	201	CLA	C3D-CAD	-2.09	1.38	1.45
20	2	307	CLA	C4B-NB	-2.09	1.35	1.37
20	B	823	CLA	C1D-ND	-2.09	1.35	1.37
21	A	855	LMU	O1'-C1'	2.09	1.43	1.40
20	B	841	CLA	C1D-ND	-2.09	1.35	1.37
20	1	211	CLA	C1D-C2D	-2.09	1.41	1.45
20	A	818	CLA	CHB-C4A	-2.09	1.32	1.37
20	A	812	CLA	MG-NA	-2.09	2.01	2.06
20	B	839	CLA	CHB-C4A	-2.09	1.32	1.37
20	4	318	CLA	CHB-C4A	-2.09	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	108	CLA	C3D-CAD	-2.08	1.38	1.45
20	F	201	CLA	C1B-C2B	-2.08	1.38	1.43
20	H	101	CLA	C3A-C2A	-2.08	1.48	1.54
20	K	102	CLA	C1B-C2B	-2.08	1.38	1.43
20	A	801	CLA	C3A-C2A	-2.08	1.48	1.54
20	4	302	CLA	MG-NA	-2.08	2.01	2.06
20	L	201	CLA	MG-NA	-2.08	2.01	2.06
20	B	836	CLA	C1D-C2D	-2.08	1.41	1.45
20	A	825	CLA	C1B-C2B	-2.08	1.38	1.43
20	A	832	CLA	C4B-NB	-2.08	1.35	1.37
21	R	101	LMU	O2B-C2B	2.07	1.48	1.43
20	2	303	CLA	C1D-ND	-2.07	1.35	1.37
20	3	316	CLA	C3C-C4C	-2.07	1.38	1.43
20	J	101	CLA	C1B-C2B	-2.07	1.38	1.43
20	B	842	CLA	MG-NA	-2.07	2.01	2.06
20	2	311	CLA	C4B-NB	-2.07	1.35	1.37
20	B	839	CLA	C4B-NB	-2.07	1.35	1.37
20	2	314	CLA	C1D-ND	-2.07	1.35	1.37
20	A	833	CLA	C1B-C2B	-2.07	1.38	1.43
20	2	303	CLA	C3A-C2A	-2.07	1.48	1.54
20	A	801	CLA	CBD-CAD	-2.07	1.47	1.56
20	A	816	CLA	C1C-NC	-2.07	1.34	1.37
20	L	202	CLA	C4B-NB	-2.07	1.35	1.37
20	A	817	CLA	MG-NA	-2.06	2.01	2.06
20	B	834	CLA	C1B-C2B	-2.06	1.38	1.43
20	G	105	CLA	C3D-CAD	-2.06	1.38	1.45
20	2	314	CLA	C1D-C2D	-2.06	1.41	1.45
20	B	813	CLA	C1D-ND	-2.06	1.35	1.37
20	4	306	CLA	CHB-C1B	2.06	1.44	1.39
20	2	310	CLA	C4B-NB	-2.06	1.35	1.37
20	A	803	CLA	C1D-C2D	-2.05	1.41	1.45
20	2	314	CLA	CHB-C4A	-2.05	1.32	1.37
20	K	104	CLA	CHB-C4A	-2.05	1.32	1.37
20	B	836	CLA	MG-ND	-2.05	2.01	2.05
20	A	807	CLA	C1B-C2B	-2.05	1.38	1.43
20	B	836	CLA	CHB-C4A	-2.04	1.32	1.37
20	A	822	CLA	C4B-NB	-2.04	1.35	1.37
20	4	307	CLA	C2C-C1C	-2.04	1.38	1.43
20	A	839	CLA	MG-ND	-2.04	2.01	2.05
20	4	317	CLA	C3D-CAD	-2.04	1.38	1.45
20	2	304	CLA	C2C-C1C	-2.04	1.38	1.43
20	F	207	CLA	CBD-CAD	-2.04	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	318	LMU	O1'-C1'	2.04	1.43	1.40
20	A	836	CLA	C4B-NB	-2.04	1.35	1.37
20	B	826	CLA	C1B-C2B	-2.03	1.38	1.43
20	A	824	CLA	C4B-NB	-2.03	1.35	1.37
20	1	213	CLA	MG-NB	-2.03	2.01	2.05
20	A	827	CLA	C1B-C2B	-2.03	1.38	1.43
20	B	838	CLA	C4B-NB	-2.03	1.35	1.37
20	1	204	CLA	C2A-C1A	-2.03	1.47	1.52
21	L	205	LMU	O1'-C1'	2.03	1.43	1.40
20	J	101	CLA	C4B-NB	-2.03	1.35	1.37
20	2	311	CLA	C1D-C2D	-2.03	1.41	1.45
20	4	301	CLA	C1B-C2B	-2.03	1.38	1.43
20	1	211	CLA	C1C-NC	-2.03	1.34	1.37
20	B	825	CLA	C1D-C2D	-2.03	1.41	1.45
20	A	840	CLA	MG-NA	-2.03	2.01	2.06
20	A	812	CLA	C1B-C2B	-2.03	1.38	1.43
20	A	849	CLA	MG-NA	-2.03	2.01	2.06
20	4	318	CLA	C1D-C2D	-2.03	1.41	1.45
20	1	202	CLA	CAA-C2A	2.03	1.57	1.53
20	3	301	CLA	MG-NA	-2.02	2.01	2.06
20	B	841	CLA	MG-NA	-2.02	2.01	2.06
20	2	315	CLA	C2D-C1D	-2.02	1.39	1.44
20	1	211	CLA	MG-NA	-2.02	2.01	2.06
20	A	825	CLA	C4B-NB	-2.02	1.35	1.37
20	A	817	CLA	C4B-NB	-2.02	1.35	1.37
20	A	851	CLA	C4B-NB	-2.02	1.35	1.37
20	B	833	CLA	C1D-C2D	-2.02	1.41	1.45
21	R	104	LMU	O1'-C1'	2.02	1.43	1.40
20	1	215	CLA	C1C-NC	-2.02	1.34	1.37
20	B	810	CLA	C1B-C2B	-2.01	1.38	1.43
20	H	108	CLA	C3A-C2A	-2.01	1.49	1.54
20	H	109	CLA	C1B-C2B	-2.01	1.38	1.43
20	1	205	CLA	C1B-C2B	-2.01	1.38	1.43
20	2	303	CLA	CHB-C4A	-2.01	1.32	1.37
22	B	844	BCR	C30-C25	-2.01	1.51	1.53
20	B	815	CLA	C1B-NB	-2.01	1.35	1.37
20	I	102	CLA	C1B-C2B	-2.01	1.38	1.43
20	1	204	CLA	C4D-CHA	-2.01	1.31	1.38
20	K	104	CLA	C1D-ND	-2.01	1.35	1.37
20	L	204	CLA	MG-NA	-2.01	2.01	2.06
21	G	101	LMU	C4B-C5B	2.01	1.57	1.53
20	A	813	CLA	C1B-C2B	-2.00	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	103	CLA	MG-ND	-2.00	2.01	2.05
20	B	808	CLA	C4D-CHA	-2.00	1.31	1.38
20	B	820	CLA	C1D-C2D	-2.00	1.41	1.45
20	B	832	CLA	CHB-C4A	-2.00	1.32	1.37

All (4943) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	104	BCR	C20-C21-C22	36.93	179.07	127.28
22	L	209	BCR	C20-C21-C22	36.44	178.38	127.28
22	A	845	BCR	C20-C21-C22	36.19	178.03	127.28
22	J	102	BCR	C20-C21-C22	36.12	177.93	127.28
22	B	846	BCR	C20-C21-C22	36.04	177.82	127.28
22	A	844	BCR	C20-C21-C22	35.98	177.74	127.28
22	F	204	BCR	C20-C21-C22	35.87	177.59	127.28
22	I	103	BCR	C20-C21-C22	35.84	177.54	127.28
22	A	843	BCR	C20-C21-C22	35.42	176.95	127.28
22	2	317	BCR	C20-C21-C22	35.24	176.70	127.28
22	B	801	BCR	C20-C21-C22	35.10	176.50	127.28
22	F	203	BCR	C20-C21-C22	35.01	176.38	127.28
22	B	847	BCR	C20-C21-C22	34.88	176.20	127.28
22	B	844	BCR	C20-C21-C22	31.64	171.65	127.28
22	B	845	BCR	C20-C21-C22	29.91	169.23	127.28
22	I	101	BCR	C20-C21-C22	20.82	156.47	127.28
22	A	845	BCR	C21-C20-C19	19.04	178.37	123.20
22	B	847	BCR	C21-C20-C19	18.99	178.22	123.20
22	L	209	BCR	C21-C20-C19	18.88	177.89	123.20
22	G	104	BCR	C21-C20-C19	18.86	177.84	123.20
22	I	103	BCR	C21-C20-C19	18.83	177.76	123.20
22	2	317	BCR	C21-C20-C19	18.70	177.39	123.20
22	B	801	BCR	C21-C20-C19	18.54	176.93	123.20
22	F	203	BCR	C21-C20-C19	18.43	176.60	123.20
22	B	846	BCR	C21-C20-C19	18.22	175.98	123.20
22	J	102	BCR	C21-C20-C19	18.19	175.90	123.20
22	F	204	BCR	C21-C20-C19	18.15	175.80	123.20
22	A	843	BCR	C21-C20-C19	17.72	174.54	123.20
22	A	844	BCR	C21-C20-C19	16.83	171.97	123.20
22	B	845	BCR	C21-C20-C19	15.64	168.52	123.20
22	B	844	BCR	C21-C20-C19	15.56	168.29	123.20
20	2	316	CLA	OBD-CAD-C3D	-11.88	100.66	128.42
22	I	101	BCR	C24-C23-C22	-11.86	108.69	126.23
20	A	801	CLA	CAB-C3B-C4B	-11.78	107.49	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	831	CLA	OBD-CAD-C3D	-11.76	100.92	128.42
20	2	303	CLA	OBD-CAD-C3D	-11.68	101.12	128.42
20	4	302	CLA	CAB-C3B-C4B	-11.50	107.91	125.42
20	B	812	CLA	CAB-C3B-C4B	-11.48	107.94	125.42
20	B	839	CLA	OBD-CAD-C3D	-11.46	101.62	128.42
20	3	301	CLA	CAB-C3B-C4B	-11.43	108.01	125.42
20	B	842	CLA	CAB-C3B-C4B	-11.34	108.15	125.42
20	4	313	CLA	CAB-C3B-C4B	-11.26	108.28	125.42
20	3	314	CLA	OBD-CAD-C3D	-11.18	102.28	128.42
22	B	801	BCR	C7-C8-C9	-10.62	110.52	126.23
20	2	310	CLA	OBD-CAD-C3D	-10.57	103.70	128.42
20	B	828	CLA	OBD-CAD-C3D	-10.53	103.80	128.42
20	A	803	CLA	OBD-CAD-C3D	-10.51	103.86	128.42
20	1	210	CLA	CAB-C3B-C4B	-10.49	109.45	125.42
22	B	801	BCR	C15-C16-C17	-10.48	102.08	123.52
20	1	211	CLA	OBD-CAD-C3D	-10.45	103.99	128.42
20	1	213	CLA	OBD-CAD-C3D	-10.44	104.02	128.42
22	I	101	BCR	C21-C20-C19	10.43	153.42	123.20
20	A	833	CLA	OBD-CAD-C3D	-10.37	104.17	128.42
20	K	104	CLA	OBD-CAD-C3D	-10.37	104.19	128.42
20	A	840	CLA	CBB-CAB-C3B	10.31	179.06	127.53
20	3	307	CLA	CBB-CAB-C3B	10.30	178.97	127.53
20	B	823	CLA	CBB-CAB-C3B	10.20	178.50	127.53
20	I	102	CLA	CBB-CAB-C3B	10.16	178.29	127.53
20	L	208	CLA	CBB-CAB-C3B	10.13	178.12	127.53
20	J	103	CLA	CBB-CAB-C3B	10.11	178.03	127.53
20	A	817	CLA	CBB-CAB-C3B	10.09	177.95	127.53
20	A	830	CLA	CBB-CAB-C3B	10.08	177.87	127.53
20	3	310	CLA	OBD-CAD-C3D	-10.08	104.87	128.42
20	H	101	CLA	CBB-CAB-C3B	10.07	177.83	127.53
20	4	317	CLA	CBB-CAB-C3B	10.07	177.81	127.53
20	3	311	CLA	CBB-CAB-C3B	10.06	177.79	127.53
20	2	312	CLA	CBB-CAB-C3B	10.04	177.71	127.53
20	1	201	CLA	CBB-CAB-C3B	10.04	177.69	127.53
20	A	801	CLA	OBD-CAD-C3D	-10.04	104.95	128.42
20	B	812	CLA	OBD-CAD-C3D	-10.03	104.97	128.42
20	K	101	CLA	CBB-CAB-C3B	10.02	177.61	127.53
20	A	849	CLA	CBB-CAB-C3B	9.98	177.40	127.53
20	3	317	CLA	CAB-C3B-C4B	-9.98	110.23	125.42
20	A	815	CLA	CBB-CAB-C3B	9.97	177.36	127.53
20	4	301	CLA	CBB-CAB-C3B	9.95	177.26	127.53
20	A	816	CLA	OBD-CAD-C3D	-9.95	105.15	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	822	CLA	CBB-CAB-C3B	9.95	177.24	127.53
20	4	301	CLA	OBD-CAD-C3D	-9.95	105.17	128.42
20	B	824	CLA	CBB-CAB-C3B	9.94	177.18	127.53
20	R	108	CLA	CBB-CAB-C3B	9.94	177.18	127.53
20	A	820	CLA	OBD-CAD-C3D	-9.93	105.20	128.42
20	3	313	CLA	CBB-CAB-C3B	9.93	177.12	127.53
20	B	820	CLA	CBB-CAB-C3B	9.91	177.03	127.53
20	4	305	CLA	CBB-CAB-C3B	9.89	176.95	127.53
20	A	851	CLA	CBB-CAB-C3B	9.89	176.94	127.53
20	B	803	CLA	CBB-CAB-C3B	9.88	176.88	127.53
20	A	829	CLA	CBB-CAB-C3B	9.87	176.86	127.53
20	F	201	CLA	CBB-CAB-C3B	9.86	176.80	127.53
20	B	819	CLA	OBD-CAD-C3D	-9.86	105.37	128.42
20	A	850	CLA	CBB-CAB-C3B	9.84	176.71	127.53
20	B	822	CLA	OBD-CAD-C3D	-9.84	105.41	128.42
20	R	107	CLA	CBB-CAB-C3B	9.81	176.54	127.53
20	A	832	CLA	CBB-CAB-C3B	9.81	176.52	127.53
20	A	829	CLA	OBD-CAD-C3D	-9.80	105.50	128.42
20	2	314	CLA	CBB-CAB-C3B	9.79	176.46	127.53
20	J	101	CLA	CBB-CAB-C3B	9.79	176.45	127.53
20	A	826	CLA	CBB-CAB-C3B	9.76	176.29	127.53
20	B	834	CLA	CBB-CAB-C3B	9.75	176.24	127.53
20	K	102	CLA	CBB-CAB-C3B	9.74	176.21	127.53
20	B	833	CLA	OBD-CAD-C3D	-9.74	105.65	128.42
20	H	110	CLA	CBB-CAB-C3B	9.73	176.13	127.53
20	L	202	CLA	CBB-CAB-C3B	9.72	176.10	127.53
20	A	836	CLA	CBB-CAB-C3B	9.70	176.01	127.53
20	A	824	CLA	OBD-CAD-C3D	-9.70	105.74	128.42
20	A	833	CLA	CBB-CAB-C3B	9.70	176.00	127.53
20	B	825	CLA	CBB-CAB-C3B	9.70	175.99	127.53
20	F	206	CLA	CBB-CAB-C3B	9.69	175.94	127.53
20	1	203	CLA	CBB-CAB-C3B	9.67	175.82	127.53
20	B	826	CLA	CBB-CAB-C3B	9.66	175.80	127.53
20	A	810	CLA	OBD-CAD-C3D	-9.66	105.83	128.42
20	1	204	CLA	CBB-CAB-C3B	9.65	175.75	127.53
20	B	821	CLA	CBB-CAB-C3B	9.64	175.70	127.53
20	2	311	CLA	OBD-CAD-C3D	-9.62	105.93	128.42
20	A	808	CLA	OBD-CAD-C3D	-9.62	105.93	128.42
20	A	805	CLA	OBD-CAD-C3D	-9.60	105.98	128.42
20	4	303	CLA	OBD-CAD-C3D	-9.59	106.00	128.42
20	G	105	CLA	OBD-CAD-C3D	-9.59	106.01	128.42
20	F	207	CLA	OBD-CAD-C3D	-9.58	106.03	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	203	CLA	OBD-CAD-C3D	-9.58	106.03	128.42
20	A	806	CLA	CBB-CAB-C3B	9.58	175.37	127.53
20	B	818	CLA	CBB-CAB-C3B	9.57	175.35	127.53
20	B	809	CLA	CBB-CAB-C3B	9.56	175.31	127.53
20	B	837	CLA	CBB-CAB-C3B	9.55	175.25	127.53
20	1	203	CLA	OBD-CAD-C3D	-9.54	106.11	128.42
20	H	102	CLA	CBB-CAB-C3B	9.53	175.14	127.53
20	A	819	CLA	OBD-CAD-C3D	-9.52	106.16	128.42
20	H	101	CLA	OBD-CAD-C3D	-9.52	106.17	128.42
20	L	201	CLA	CBB-CAB-C3B	9.51	175.05	127.53
20	L	202	CLA	OBD-CAD-C3D	-9.51	106.19	128.42
20	3	307	CLA	OBD-CAD-C3D	-9.50	106.21	128.42
20	B	810	CLA	CBB-CAB-C3B	9.49	174.94	127.53
20	L	208	CLA	OBD-CAD-C3D	-9.48	106.26	128.42
20	A	810	CLA	CBB-CAB-C3B	9.47	174.86	127.53
20	B	850	CLA	OBD-CAD-C3D	-9.47	106.28	128.42
20	A	826	CLA	OBD-CAD-C3D	-9.47	106.28	128.42
20	A	834	CLA	CBB-CAB-C3B	9.47	174.83	127.53
20	1	211	CLA	CBB-CAB-C3B	9.47	174.82	127.53
20	2	316	CLA	CBB-CAB-C3B	9.47	174.82	127.53
20	L	207	CLA	CBB-CAB-C3B	9.46	174.78	127.53
20	L	204	CLA	CBB-CAB-C3B	9.45	174.76	127.53
20	4	306	CLA	OBD-CAD-C3D	-9.42	106.39	128.42
20	B	839	CLA	CBB-CAB-C3B	9.42	174.60	127.53
20	B	826	CLA	OBD-CAD-C3D	-9.41	106.42	128.42
20	A	837	CLA	CBB-CAB-C3B	9.41	174.52	127.53
20	2	307	CLA	OBD-CAD-C3D	-9.40	106.45	128.42
20	B	815	CLA	CBB-CAB-C3B	9.40	174.47	127.53
20	K	102	CLA	OBD-CAD-C3D	-9.36	106.54	128.42
20	H	109	CLA	CBB-CAB-C3B	9.35	174.25	127.53
20	B	802	CLA	CBB-CAB-C3B	9.31	174.04	127.53
20	B	806	CLA	CBB-CAB-C3B	9.31	174.04	127.53
20	A	835	CLA	CBB-CAB-C3B	9.31	174.03	127.53
20	A	817	CLA	OBD-CAD-C3D	-9.31	106.66	128.42
20	B	837	CLA	OBD-CAD-C3D	-9.30	106.67	128.42
20	4	315	CLA	CBB-CAB-C3B	9.30	173.97	127.53
20	B	836	CLA	CBB-CAB-C3B	9.29	173.95	127.53
20	1	215	CLA	OBD-CAD-C3D	-9.29	106.71	128.42
22	I	103	BCR	C24-C23-C22	-9.26	112.54	126.23
20	L	203	CLA	CBB-CAB-C3B	9.25	173.72	127.53
20	F	206	CLA	OBD-CAD-C3D	-9.23	106.83	128.42
20	B	827	CLA	CBB-CAB-C3B	9.23	173.66	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	807	CLA	CBB-CAB-C3B	9.23	173.66	127.53
20	1	204	CLA	OBD-CAD-C3D	-9.22	106.88	128.42
20	3	311	CLA	OBD-CAD-C3D	-9.21	106.88	128.42
20	2	302	CLA	CBB-CAB-C3B	9.19	173.43	127.53
20	I	102	CLA	OBD-CAD-C3D	-9.19	106.95	128.42
20	B	832	CLA	CAA-C2A-C3A	-9.18	88.19	113.00
20	3	317	CLA	OBD-CAD-C3D	-9.18	106.96	128.42
20	A	830	CLA	OBD-CAD-C3D	-9.17	106.99	128.42
20	1	207	CLA	CBB-CAB-C3B	9.16	173.27	127.53
20	B	813	CLA	CBB-CAB-C3B	9.15	173.26	127.53
20	K	103	CLA	CBB-CAB-C3B	9.15	173.23	127.53
20	R	107	CLA	OBD-CAD-C3D	-9.15	107.03	128.42
20	H	109	CLA	OBD-CAD-C3D	-9.14	107.05	128.42
20	A	813	CLA	CBB-CAB-C3B	9.14	173.20	127.53
20	B	802	CLA	OBD-CAD-C3D	-9.14	107.05	128.42
20	A	825	CLA	OBD-CAD-C3D	-9.13	107.07	128.42
20	B	809	CLA	OBD-CAD-C3D	-9.12	107.10	128.42
20	B	831	CLA	CBB-CAB-C3B	9.10	172.97	127.53
20	1	202	CLA	CBB-CAB-C3B	9.09	172.95	127.53
20	2	310	CLA	CBB-CAB-C3B	9.08	172.88	127.53
20	B	819	CLA	CBB-CAB-C3B	9.07	172.84	127.53
20	A	850	CLA	OBD-CAD-C3D	-9.06	107.23	128.42
20	1	213	CLA	CBB-CAB-C3B	9.06	172.81	127.53
20	4	302	CLA	OBD-CAD-C3D	-9.06	107.24	128.42
20	A	822	CLA	OBD-CAD-C3D	-9.05	107.25	128.42
20	A	824	CLA	CBB-CAB-C3B	9.03	172.66	127.53
20	A	820	CLA	CBB-CAB-C3B	9.03	172.65	127.53
20	K	101	CLA	OBD-CAD-C3D	-9.03	107.32	128.42
20	A	828	CLA	OBD-CAD-C3D	-9.02	107.33	128.42
20	A	837	CLA	OBD-CAD-C3D	-9.01	107.37	128.42
20	B	813	CLA	OBD-CAD-C3D	-9.00	107.37	128.42
20	K	103	CLA	OBD-CAD-C3D	-9.00	107.38	128.42
20	2	311	CLA	CBB-CAB-C3B	8.99	172.43	127.53
20	3	303	CLA	OBD-CAD-C3D	-8.99	107.41	128.42
22	B	801	BCR	C15-C14-C13	-8.97	114.69	127.28
20	2	312	CLA	OBD-CAD-C3D	-8.97	107.44	128.42
20	4	318	CLA	CBB-CAB-C3B	8.95	172.22	127.53
20	B	835	CLA	CBB-CAB-C3B	8.94	172.20	127.53
20	3	314	CLA	CBB-CAB-C3B	8.94	172.18	127.53
20	A	806	CLA	OBD-CAD-C3D	-8.93	107.54	128.42
20	4	305	CLA	OBD-CAD-C3D	-8.93	107.55	128.42
20	A	827	CLA	CBB-CAB-C3B	8.92	172.10	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	832	CLA	CBB-CAB-C3B	8.90	171.99	127.53
20	2	303	CLA	CBB-CAB-C3B	8.89	171.96	127.53
20	F	201	CLA	OBD-CAD-C3D	-8.89	107.64	128.42
20	A	851	CLA	OBD-CAD-C3D	-8.88	107.66	128.42
20	B	834	CLA	OBD-CAD-C3D	-8.88	107.66	128.42
20	A	812	CLA	CBB-CAB-C3B	8.87	171.83	127.53
20	A	811	CLA	CBB-CAB-C3B	8.85	171.75	127.53
20	B	828	CLA	CBB-CAB-C3B	8.85	171.74	127.53
20	H	108	CLA	CBB-CAB-C3B	8.83	171.65	127.53
20	J	101	CLA	OBD-CAD-C3D	-8.81	107.83	128.42
20	L	208	CLA	O2D-CGD-CBD	8.79	126.60	111.23
20	2	305	CLA	CBB-CAB-C3B	8.77	171.34	127.53
20	A	819	CLA	CBB-CAB-C3B	8.77	171.32	127.53
20	B	816	CLA	CBB-CAB-C3B	8.76	171.31	127.53
20	B	814	CLA	CBB-CAB-C3B	8.76	171.30	127.53
20	1	205	CLA	OBD-CAD-C3D	-8.76	107.94	128.42
20	B	821	CLA	OBD-CAD-C3D	-8.76	107.95	128.42
20	L	207	CLA	OBD-CAD-C3D	-8.75	107.96	128.42
20	B	827	CLA	OBD-CAD-C3D	-8.75	107.97	128.42
22	2	317	BCR	C16-C17-C18	-8.74	115.02	127.28
20	2	302	CLA	OBD-CAD-C3D	-8.72	108.03	128.42
20	A	803	CLA	CBB-CAB-C3B	8.72	171.08	127.53
20	B	830	CLA	CBB-CAB-C3B	8.70	171.01	127.53
20	B	829	CLA	CBB-CAB-C3B	8.70	171.00	127.53
20	A	821	CLA	CBB-CAB-C3B	8.70	170.99	127.53
20	B	807	CLA	CBB-CAB-C3B	8.69	170.97	127.53
20	1	206	CLA	CBB-CAB-C3B	8.69	170.96	127.53
22	I	101	BCR	C7-C8-C9	-8.69	113.38	126.23
20	A	838	CLA	CBB-CAB-C3B	8.67	170.87	127.53
20	1	201	CLA	OBD-CAD-C3D	-8.64	108.22	128.42
20	B	808	CLA	CBB-CAB-C3B	8.62	170.61	127.53
20	2	314	CLA	OBD-CAD-C3D	-8.57	108.39	128.42
20	A	809	CLA	CBB-CAB-C3B	8.56	170.28	127.53
20	B	836	CLA	OBD-CAD-C3D	-8.56	108.42	128.42
20	B	835	CLA	OBD-CAD-C3D	-8.53	108.47	128.42
20	1	205	CLA	CAB-C3B-C4B	-8.53	112.43	125.42
20	H	110	CLA	OBD-CAD-C3D	-8.53	108.48	128.42
20	A	816	CLA	CBB-CAB-C3B	8.52	170.08	127.53
20	4	303	CLA	CBB-CAB-C3B	8.52	170.08	127.53
20	A	822	CLA	CBB-CAB-C3B	8.51	170.02	127.53
20	K	104	CLA	CBB-CAB-C3B	8.50	169.98	127.53
20	A	823	CLA	CBB-CAB-C3B	8.47	169.82	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	301	CLA	OBD-CAD-C3D	-8.46	108.63	128.42
20	B	841	CLA	CBB-CAB-C3B	8.46	169.78	127.53
20	B	824	CLA	OBD-CAD-C3D	-8.43	108.72	128.42
22	B	844	BCR	C24-C23-C22	-8.39	113.82	126.23
20	A	801	CLA	C4D-C3D-CAD	8.37	117.20	108.11
20	B	816	CLA	OBD-CAD-C3D	-8.35	108.89	128.42
20	2	307	CLA	CBB-CAB-C3B	8.30	169.02	127.53
20	B	850	CLA	CBB-CAB-C3B	8.29	168.96	127.53
20	A	838	CLA	OBD-CAD-C3D	-8.27	109.08	128.42
20	A	804	CLA	CBB-CAB-C3B	8.27	168.85	127.53
20	H	102	CLA	OBD-CAD-C3D	-8.26	109.10	128.42
20	4	313	CLA	OBD-CAD-C3D	-8.26	109.12	128.42
20	A	839	CLA	CBB-CAB-C3B	8.23	168.65	127.53
20	B	833	CLA	CBB-CAB-C3B	8.22	168.59	127.53
20	A	807	CLA	OBD-CAD-C3D	-8.20	109.25	128.42
20	1	207	CLA	OBD-CAD-C3D	-8.16	109.35	128.42
20	B	803	CLA	OBD-CAD-C3D	-8.14	109.39	128.42
20	4	304	CLA	CBB-CAB-C3B	8.13	168.16	127.53
20	A	827	CLA	OBD-CAD-C3D	-8.11	109.45	128.42
20	B	820	CLA	OBD-CAD-C3D	-8.11	109.47	128.42
20	B	840	CLA	OBD-CAD-C3D	-8.10	109.48	128.42
20	1	211	CLA	CMD-C2D-C1D	8.10	139.00	124.73
22	I	103	BCR	C30-C25-C26	-8.10	111.57	122.64
20	A	831	CLA	CBB-CAB-C3B	8.09	167.94	127.53
20	A	808	CLA	CBB-CAB-C3B	8.08	167.91	127.53
20	A	815	CLA	OBD-CAD-C3D	-8.07	109.55	128.42
20	4	304	CLA	OBD-CAD-C3D	-8.07	109.56	128.42
20	A	835	CLA	OBD-CAD-C3D	-8.06	109.57	128.42
20	B	840	CLA	CBB-CAB-C3B	8.06	167.81	127.53
20	B	807	CLA	OBD-CAD-C3D	-8.06	109.57	128.42
20	1	215	CLA	C4D-C3D-CAD	8.06	116.86	108.11
20	A	803	CLA	O2D-CGD-CBD	8.05	125.31	111.23
20	B	817	CLA	CBB-CAB-C3B	8.05	167.75	127.53
20	B	838	CLA	CBB-CAB-C3B	8.03	167.67	127.53
20	B	823	CLA	OBD-CAD-C3D	-8.02	109.67	128.42
20	3	303	CLA	CAB-C3B-C4B	-8.00	113.24	125.42
20	A	840	CLA	OBD-CAD-C3D	-7.96	109.82	128.42
20	F	207	CLA	CBB-CAB-C3B	7.95	167.22	127.53
20	1	207	CLA	C3A-C2A-C1A	7.94	113.24	101.34
20	1	210	CLA	OBD-CAD-C3D	-7.94	109.87	128.42
20	B	839	CLA	CMD-C2D-C1D	7.93	138.69	124.73
20	B	831	CLA	OBD-CAD-C3D	-7.92	109.89	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	204	CLA	OBD-CAD-C3D	-7.88	110.00	128.42
20	A	818	CLA	OBD-CAD-C3D	-7.87	110.02	128.42
20	1	206	CLA	OBD-CAD-C3D	-7.86	110.05	128.42
20	A	849	CLA	OBD-CAD-C3D	-7.85	110.06	128.42
20	1	201	CLA	C4A-NA-C1A	7.84	110.25	106.68
20	A	812	CLA	OBD-CAD-C3D	-7.83	110.12	128.42
20	B	838	CLA	OBD-CAD-C3D	-7.83	110.12	128.42
20	B	832	CLA	OBD-CAD-C3D	-7.83	110.13	128.42
20	4	310	CLA	OBD-CAD-C3D	-7.82	110.13	128.42
20	A	849	CLA	C4D-C3D-CAD	7.82	116.59	108.11
20	4	317	CLA	OBD-CAD-C3D	-7.81	110.17	128.42
20	4	318	CLA	O2D-CGD-CBD	7.80	124.87	111.23
20	B	810	CLA	O2D-CGD-CBD	7.80	124.86	111.23
20	B	842	CLA	OBD-CAD-C3D	-7.79	110.20	128.42
20	1	204	CLA	CMD-C2D-C1D	7.78	138.43	124.73
20	B	841	CLA	OBD-CAD-C3D	-7.78	110.24	128.42
20	4	318	CLA	C4D-C3D-CAD	7.77	116.54	108.11
20	A	828	CLA	CBB-CAB-C3B	7.68	165.90	127.53
20	A	827	CLA	O2D-CGD-CBD	7.68	124.65	111.23
20	A	839	CLA	OBD-CAD-C3D	-7.67	110.50	128.42
20	A	821	CLA	O2D-CGD-CBD	7.65	124.60	111.23
20	1	215	CLA	C1D-CHD-C4C	-7.62	109.82	126.02
20	1	202	CLA	OBD-CAD-C3D	-7.61	110.63	128.42
20	B	817	CLA	OBD-CAD-C3D	-7.60	110.65	128.42
20	4	318	CLA	OBD-CAD-C3D	-7.59	110.67	128.42
20	A	834	CLA	OBD-CAD-C3D	-7.57	110.72	128.42
20	A	813	CLA	OBD-CAD-C3D	-7.56	110.75	128.42
20	B	839	CLA	O2D-CGD-CBD	7.52	124.38	111.23
20	B	830	CLA	OBD-CAD-C3D	-7.51	110.86	128.42
20	A	825	CLA	CBB-CAB-C3B	7.49	164.94	127.53
20	A	823	CLA	OBD-CAD-C3D	-7.47	110.96	128.42
20	A	821	CLA	OBD-CAD-C3D	-7.46	110.97	128.42
22	I	103	BCR	C16-C15-C14	-7.45	108.28	123.52
20	A	809	CLA	OBD-CAD-C3D	-7.43	111.05	128.42
20	1	213	CLA	CAA-C2A-C1A	7.43	136.32	111.97
20	A	832	CLA	OBD-CAD-C3D	-7.42	111.08	128.42
20	B	814	CLA	OBD-CAD-C3D	-7.42	111.08	128.42
20	B	829	CLA	OBD-CAD-C3D	-7.41	111.10	128.42
20	B	839	CLA	C4D-C3D-CAD	7.41	116.15	108.11
21	L	205	LMU	C1B-O1B-C4'	-7.36	100.53	117.98
21	G	101	LMU	O1'-C1'-C2'	7.33	119.41	108.27
20	K	104	CLA	O2D-CGD-CBD	7.32	124.03	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	306	CLA	CBB-CAB-C3B	7.31	164.05	127.53
20	A	831	CLA	C1D-CHD-C4C	-7.31	110.48	126.02
20	A	839	CLA	CMD-C2D-C1D	7.30	137.59	124.73
20	B	818	CLA	OBD-CAD-C3D	-7.29	111.37	128.42
22	I	103	BCR	C16-C17-C18	-7.27	117.08	127.28
20	4	317	CLA	C4A-NA-C1A	7.25	109.99	106.68
20	1	203	CLA	CMD-C2D-C1D	7.24	137.47	124.73
20	F	205	CLA	OBD-CAD-C3D	-7.20	111.58	128.42
20	K	104	CLA	CMD-C2D-C1D	7.20	137.41	124.73
20	2	314	CLA	C4D-C3D-CAD	7.20	115.93	108.11
20	2	302	CLA	C1D-CHD-C4C	-7.20	110.72	126.02
20	1	204	CLA	C4D-C3D-CAD	7.18	115.90	108.11
20	4	317	CLA	C4D-C3D-CAD	7.15	115.88	108.11
20	B	836	CLA	O2D-CGD-CBD	7.14	123.72	111.23
20	3	310	CLA	O2D-CGD-CBD	7.13	123.70	111.23
20	F	201	CLA	O2D-CGD-CBD	7.13	123.70	111.23
20	1	207	CLA	CMD-C2D-C1D	7.11	137.25	124.73
20	G	105	CLA	O2D-CGD-CBD	7.09	123.62	111.23
20	B	829	CLA	O2D-CGD-CBD	7.08	123.60	111.23
20	3	314	CLA	CMD-C2D-C1D	7.07	137.18	124.73
20	B	808	CLA	OBD-CAD-C3D	-7.06	111.91	128.42
20	2	314	CLA	CMD-C2D-C1D	7.06	137.15	124.73
20	A	818	CLA	C1D-CHD-C4C	-7.02	111.10	126.02
20	4	310	CLA	C4D-C3D-CAD	7.01	115.72	108.11
20	A	805	CLA	CBB-CAB-C3B	6.98	162.39	127.53
20	H	102	CLA	CMD-C2D-C1D	6.97	137.00	124.73
20	B	837	CLA	O2D-CGD-CBD	6.95	123.39	111.23
22	F	204	BCR	C15-C14-C13	-6.95	117.53	127.28
20	A	835	CLA	O2D-CGD-CBD	6.88	123.26	111.23
20	2	303	CLA	O2D-CGD-CBD	6.88	123.25	111.23
20	B	830	CLA	O2D-CGD-CBD	6.88	123.25	111.23
20	A	820	CLA	CMD-C2D-C1D	6.87	136.83	124.73
21	H	103	LMU	C3 <sup>1</sup> -C4 <sup>1</sup> -C5 <sup>1</sup>	-6.87	95.71	110.93
20	2	307	CLA	O2D-CGD-CBD	6.86	123.22	111.23
20	L	201	CLA	OBD-CAD-C3D	-6.86	112.38	128.42
20	4	315	CLA	OBD-CAD-C3D	-6.85	112.40	128.42
20	1	215	CLA	CHD-C4C-C3C	-6.85	114.78	124.77
20	4	303	CLA	C1D-CHD-C4C	-6.82	111.52	126.02
20	1	203	CLA	C4D-C3D-CAD	6.81	115.50	108.11
20	B	822	CLA	CMD-C2D-C1D	6.80	136.71	124.73
20	A	801	CLA	CMD-C2D-C1D	6.80	136.70	124.73
20	G	105	CLA	CMD-C2D-C1D	6.80	136.70	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	812	CLA	C1D-CHD-C4C	-6.79	111.60	126.02
20	B	838	CLA	O2D-CGD-CBD	6.78	123.09	111.23
20	G	105	CLA	CBB-CAB-C3B	6.78	161.41	127.53
20	1	201	CLA	C4D-C3D-CAD	6.77	115.46	108.11
20	A	836	CLA	O2D-CGD-CBD	6.77	123.06	111.23
20	A	831	CLA	C3B-C2B-C1B	-6.77	99.19	107.17
20	A	811	CLA	CMD-C2D-C1D	6.76	136.63	124.73
20	B	840	CLA	CMD-C2D-C1D	6.75	136.62	124.73
20	B	821	CLA	CMD-C2D-C1D	6.75	136.61	124.73
20	4	310	CLA	C1D-CHD-C4C	-6.74	111.69	126.02
20	B	809	CLA	O2D-CGD-CBD	6.74	123.01	111.23
20	B	837	CLA	CMD-C2D-C1D	6.73	136.57	124.73
20	A	839	CLA	C4D-C3D-CAD	6.72	115.41	108.11
20	B	815	CLA	OBD-CAD-C3D	-6.72	112.72	128.42
20	2	314	CLA	CHD-C4C-NC	6.72	134.65	124.23
20	B	839	CLA	CHD-C4C-NC	6.71	134.64	124.23
20	4	303	CLA	CGD-CBD-CAD	6.71	132.57	110.85
20	4	304	CLA	O2D-CGD-CBD	6.70	122.95	111.23
22	B	801	BCR	C10-C11-C12	-6.70	103.78	123.20
20	A	811	CLA	C3B-C2B-C1B	-6.69	99.28	107.17
20	B	826	CLA	CMD-C2D-C1D	6.69	136.51	124.73
20	B	807	CLA	CMD-C2D-C1D	6.69	136.51	124.73
20	1	207	CLA	C4D-C3D-CAD	6.69	115.37	108.11
20	B	825	CLA	O2D-CGD-CBD	6.68	122.92	111.23
20	A	819	CLA	CMD-C2D-C1D	6.67	136.47	124.73
20	B	815	CLA	CMD-C2D-C1D	6.67	136.47	124.73
20	1	211	CLA	C4D-C3D-CAD	6.67	115.34	108.11
20	K	102	CLA	CMD-C2D-C1D	6.66	136.46	124.73
20	2	303	CLA	CMD-C2D-C1D	6.66	136.46	124.73
20	F	205	CLA	CMD-C2D-C1D	6.65	136.43	124.73
20	1	213	CLA	C1D-CHD-C4C	-6.64	111.91	126.02
20	A	851	CLA	CMD-C2D-C1D	6.63	136.41	124.73
20	A	818	CLA	CHD-C4C-NC	6.63	134.51	124.23
20	A	839	CLA	O2D-CGD-CBD	6.62	122.80	111.23
20	A	821	CLA	C4D-C3D-CAD	6.62	115.29	108.11
20	2	305	CLA	OBD-CAD-C3D	-6.59	113.00	128.42
20	B	812	CLA	CAB-C3B-C2B	-6.59	106.02	123.53
20	3	317	CLA	CMD-C2D-C1D	6.58	136.31	124.73
20	B	807	CLA	O2D-CGD-CBD	6.58	122.73	111.23
20	B	839	CLA	C1D-CHD-C4C	-6.57	112.05	126.02
20	R	107	CLA	CMD-C2D-C1D	6.57	136.30	124.73
20	G	105	CLA	C1D-CHD-C4C	-6.56	112.08	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	310	CLA	CHD-C4C-NC	6.55	134.39	124.23
20	A	818	CLA	CMD-C2D-C1D	6.55	136.25	124.73
20	1	211	CLA	C1D-CHD-C4C	-6.54	112.12	126.02
20	A	851	CLA	C4D-C3D-CAD	6.54	115.20	108.11
22	B	801	BCR	C3-C4-C5	-6.52	102.43	114.06
20	L	202	CLA	CMD-C2D-C1D	6.52	136.20	124.73
20	4	310	CLA	CMD-C2D-C1D	6.52	136.20	124.73
20	2	316	CLA	C1D-CHD-C4C	-6.51	112.19	126.02
20	3	310	CLA	CHD-C4C-C3C	-6.50	115.29	124.77
20	H	101	CLA	C4D-C3D-CAD	6.49	115.16	108.11
20	1	201	CLA	CMD-C2D-C1D	6.49	136.16	124.73
20	A	840	CLA	O2D-CGD-CBD	6.49	122.58	111.23
20	4	301	CLA	CMD-C2D-C1D	6.49	136.15	124.73
20	2	314	CLA	C1D-CHD-C4C	-6.49	112.23	126.02
20	A	804	CLA	OBD-CAD-C3D	-6.49	113.26	128.42
20	1	210	CLA	CMD-C2D-C1D	6.49	136.15	124.73
20	3	313	CLA	OBD-CAD-C3D	-6.49	113.26	128.42
20	4	306	CLA	C1D-CHD-C4C	-6.48	112.24	126.02
20	4	317	CLA	CMD-C2D-C1D	6.48	136.15	124.73
20	J	103	CLA	OBD-CAD-C3D	-6.48	113.28	128.42
20	4	303	CLA	CMD-C2D-C1D	6.47	136.12	124.73
20	B	812	CLA	CMD-C2D-C1D	6.47	136.12	124.73
20	B	830	CLA	CMD-C2D-C1D	6.47	136.12	124.73
20	B	828	CLA	CMD-C2D-C1D	6.47	136.12	124.73
20	A	811	CLA	OBD-CAD-C3D	-6.47	113.31	128.42
20	A	829	CLA	O2D-CGD-CBD	6.46	122.53	111.23
20	B	821	CLA	C4D-C3D-CAD	6.46	115.12	108.11
20	A	817	CLA	CMD-C2D-C1D	6.46	136.10	124.73
20	B	834	CLA	CMD-C2D-C1D	6.45	136.09	124.73
20	B	830	CLA	C4D-C3D-CAD	6.45	115.11	108.11
20	H	108	CLA	C1D-CHD-C4C	-6.45	112.31	126.02
20	4	306	CLA	CHD-C4C-NC	6.45	134.22	124.23
20	4	302	CLA	C1D-CHD-C4C	-6.44	112.33	126.02
20	3	314	CLA	C1D-CHD-C4C	-6.44	112.34	126.02
20	4	305	CLA	C1D-CHD-C4C	-6.43	112.35	126.02
20	R	107	CLA	C4D-C3D-CAD	6.43	115.09	108.11
21	R	101	LMU	C4B-C3B-C2B	-6.43	99.55	110.83
20	A	835	CLA	CMD-C2D-C1D	6.42	136.04	124.73
20	A	803	CLA	CMD-C2D-C1D	6.42	136.04	124.73
20	A	828	CLA	O2D-CGD-CBD	6.42	122.45	111.23
20	B	820	CLA	O2D-CGD-CBD	6.41	122.44	111.23
20	B	819	CLA	C1D-CHD-C4C	-6.40	112.41	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	206	CLA	CMD-C2D-C1D	6.40	136.00	124.73
20	H	108	CLA	C2B-C1B-NB	6.40	116.96	110.33
20	K	103	CLA	CMD-C2D-C1D	6.39	135.99	124.73
20	R	108	CLA	CMD-C2D-C1D	6.38	135.96	124.73
20	B	817	CLA	CMD-C2D-C1D	6.37	135.95	124.73
20	2	305	CLA	CMD-C2D-C1D	6.37	135.95	124.73
20	A	810	CLA	CMD-C2D-C1D	6.37	135.95	124.73
20	A	832	CLA	CMD-C2D-C1D	6.37	135.94	124.73
20	H	110	CLA	O2D-CGD-CBD	6.36	122.36	111.23
20	F	207	CLA	CMA-C3A-C4A	6.36	128.88	111.77
20	3	310	CLA	C1D-CHD-C4C	-6.36	112.51	126.02
20	1	210	CLA	CAB-C3B-C2B	-6.35	106.66	123.53
20	A	804	CLA	CMD-C2D-C1D	6.35	135.91	124.73
20	A	822	CLA	C4D-C3D-CAD	6.35	115.00	108.11
20	B	806	CLA	CMD-C2D-C1D	6.34	135.90	124.73
20	F	205	CLA	C1B-C2B-C3B	-6.34	101.06	107.03
20	1	202	CLA	CMD-C2D-C1D	6.34	135.90	124.73
20	A	824	CLA	CMD-C2D-C1D	6.34	135.89	124.73
20	1	215	CLA	CBB-CAB-C3B	6.34	159.18	127.53
22	2	317	BCR	C11-C10-C9	-6.33	118.40	127.28
20	B	833	CLA	C4D-C3D-CAD	6.33	114.98	108.11
20	B	812	CLA	C4D-C3D-CAD	6.33	114.98	108.11
20	A	816	CLA	CMD-C2D-C1D	6.33	135.87	124.73
20	B	813	CLA	CMD-C2D-C1D	6.32	135.86	124.73
20	2	316	CLA	CMD-C2D-C1D	6.31	135.85	124.73
20	B	835	CLA	CMD-C2D-C1D	6.30	135.82	124.73
20	3	310	CLA	CHD-C4C-NC	6.30	133.99	124.23
20	A	806	CLA	CMD-C2D-C1D	6.30	135.81	124.73
20	A	818	CLA	O2D-CGD-CBD	6.29	122.23	111.23
20	B	836	CLA	CMD-C2D-C1D	6.29	135.81	124.73
20	3	303	CLA	CMD-C2D-C1D	6.29	135.80	124.73
20	A	823	CLA	CMD-C2D-C1D	6.29	135.80	124.73
20	A	816	CLA	C1D-CHD-C4C	-6.28	112.67	126.02
20	J	101	CLA	CMD-C2D-C1D	6.28	135.78	124.73
20	1	206	CLA	C4D-C3D-CAD	6.27	114.92	108.11
20	4	304	CLA	CMD-C2D-C1D	6.27	135.77	124.73
20	A	837	CLA	CMD-C2D-C1D	6.27	135.76	124.73
20	L	201	CLA	CMD-C2D-C1D	6.26	135.76	124.73
20	2	312	CLA	C1D-CHD-C4C	-6.26	112.72	126.02
20	4	310	CLA	O2D-CGD-CBD	6.26	122.17	111.23
20	R	108	CLA	OBD-CAD-C3D	-6.26	113.80	128.42
20	A	837	CLA	C4D-C3D-CAD	6.25	114.90	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	108	CLA	O2D-CGD-CBD	6.25	122.16	111.23
20	A	834	CLA	CMD-C2D-C1D	6.25	135.74	124.73
20	4	304	CLA	C4D-C3D-CAD	6.25	114.89	108.11
20	B	820	CLA	C4D-C3D-CAD	6.25	114.89	108.11
20	B	833	CLA	CMD-C2D-C1D	6.24	135.72	124.73
20	A	833	CLA	CMD-C2D-C1D	6.24	135.72	124.73
20	B	806	CLA	C3B-C2B-C1B	-6.24	99.81	107.17
20	A	804	CLA	C3B-C2B-C1B	-6.24	99.81	107.17
20	1	215	CLA	CHD-C4C-NC	6.23	133.90	124.23
20	3	307	CLA	CHC-C1C-NC	6.23	133.69	124.31
20	B	836	CLA	C1D-CHD-C4C	-6.23	112.78	126.02
20	2	302	CLA	CMD-C2D-C1D	6.22	135.69	124.73
20	4	306	CLA	CMD-C2D-C1D	6.22	135.68	124.73
20	A	822	CLA	CMD-C2D-C1D	6.22	135.68	124.73
20	B	828	CLA	O2D-CGD-CBD	6.21	122.09	111.23
20	2	302	CLA	CHD-C4C-NC	6.21	133.86	124.23
20	1	211	CLA	CHD-C4C-NC	6.21	133.86	124.23
20	B	832	CLA	O2D-CGD-CBD	6.20	122.08	111.23
21	1	218	LMU	C1B-O1B-C4'	-6.20	103.29	117.98
20	F	207	CLA	C1D-CHD-C4C	-6.19	112.86	126.02
20	L	203	CLA	CMD-C2D-C1D	6.19	135.63	124.73
20	1	205	CLA	CMD-C2D-C1D	6.18	135.62	124.73
20	1	207	CLA	CBA-CAA-C2A	-6.18	95.40	113.79
20	B	832	CLA	CMD-C2D-C1D	6.18	135.61	124.73
20	A	801	CLA	CAB-C3B-C2B	-6.17	107.14	123.53
20	4	315	CLA	C1D-CHD-C4C	-6.17	112.90	126.02
20	F	207	CLA	O2D-CGD-CBD	6.17	122.02	111.23
20	2	312	CLA	O2D-CGD-CBD	6.17	122.02	111.23
20	L	207	CLA	CMD-C2D-C1D	6.16	135.58	124.73
20	B	808	CLA	C1D-CHD-C4C	-6.16	112.92	126.02
20	B	819	CLA	CAA-C2A-C3A	-6.16	102.10	116.23
20	L	207	CLA	O2D-CGD-CBD	6.16	122.00	111.23
20	3	311	CLA	CMD-C2D-C1D	6.16	135.58	124.73
20	B	839	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
20	4	302	CLA	C4D-C3D-CAD	6.15	114.79	108.11
20	B	813	CLA	C4D-C3D-CAD	6.14	114.78	108.11
20	B	807	CLA	C4D-C3D-CAD	6.14	114.78	108.11
20	3	301	CLA	C4D-C3D-CAD	6.14	114.78	108.11
20	B	840	CLA	C4D-C3D-CAD	6.13	114.77	108.11
20	B	809	CLA	CMD-C2D-C1D	6.13	135.53	124.73
20	A	801	CLA	O2D-CGD-CBD	6.13	121.94	111.23
20	F	201	CLA	C1D-CHD-C4C	-6.12	113.00	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	820	CLA	O2D-CGD-CBD	6.12	121.94	111.23
20	1	211	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
20	4	303	CLA	CHD-C4C-NC	6.12	133.71	124.23
20	B	841	CLA	C4D-C3D-CAD	6.12	114.75	108.11
20	A	821	CLA	CMD-C2D-C1D	6.11	135.49	124.73
20	A	830	CLA	CMD-C2D-C1D	6.11	135.49	124.73
20	3	310	CLA	CBB-CAB-C3B	6.11	158.04	127.53
20	L	208	CLA	C1D-CHD-C4C	-6.11	113.04	126.02
20	1	202	CLA	C4D-C3D-CAD	6.10	114.73	108.11
20	1	201	CLA	O2D-CGD-CBD	6.10	121.89	111.23
20	1	205	CLA	C4D-C3D-CAD	6.10	114.73	108.11
22	B	844	BCR	C1-C6-C5	-6.10	114.30	122.64
20	F	205	CLA	CAB-C3B-C4B	-6.10	116.14	125.42
20	4	313	CLA	C4D-C3D-CAD	6.09	114.72	108.11
20	4	306	CLA	CAA-C2A-C1A	6.09	131.93	111.97
20	A	812	CLA	CMD-C2D-C1D	6.09	135.44	124.73
20	B	803	CLA	C4D-C3D-CAD	6.08	114.71	108.11
20	K	104	CLA	C4D-C3D-CAD	6.08	114.71	108.11
20	J	101	CLA	C4D-C3D-CAD	6.07	114.70	108.11
20	A	817	CLA	C4D-C3D-CAD	6.06	114.69	108.11
20	H	109	CLA	O2D-CGD-CBD	6.06	121.83	111.23
20	B	803	CLA	CMD-C2D-C1D	6.06	135.40	124.73
20	A	820	CLA	C4D-C3D-CAD	6.06	114.69	108.11
20	A	801	CLA	CAA-C2A-C3A	6.05	129.36	113.00
20	B	838	CLA	CMD-C2D-C1D	6.05	135.39	124.73
20	F	201	CLA	CHD-C4C-NC	6.05	133.61	124.23
20	B	810	CLA	OBD-CAD-C3D	-6.05	114.28	128.42
20	2	302	CLA	C4D-C3D-CAD	6.04	114.67	108.11
20	A	805	CLA	CMD-C2D-C1D	6.04	135.36	124.73
20	K	103	CLA	C4D-C3D-CAD	6.04	114.67	108.11
20	A	815	CLA	CMD-C2D-C1D	6.04	135.36	124.73
20	B	822	CLA	C4D-C3D-CAD	6.04	114.66	108.11
20	B	829	CLA	C4D-C3D-CAD	6.03	114.66	108.11
20	H	101	CLA	CMD-C2D-C1D	6.03	135.34	124.73
20	A	830	CLA	C4D-C3D-CAD	6.03	114.65	108.11
20	A	807	CLA	CMD-C2D-C1D	6.03	135.34	124.73
20	A	818	CLA	C4D-C3D-CAD	6.03	114.65	108.11
20	B	850	CLA	C4D-C3D-CAD	6.02	114.65	108.11
20	A	828	CLA	C4D-C3D-CAD	6.02	114.65	108.11
20	1	213	CLA	O2D-CGD-CBD	6.02	121.76	111.23
20	B	817	CLA	O2D-CGD-CBD	6.02	121.76	111.23
20	J	103	CLA	C1D-CHD-C4C	-6.02	113.22	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	312	CLA	C4D-C3D-CAD	6.02	114.64	108.11
20	2	305	CLA	C4D-C3D-CAD	6.02	114.64	108.11
20	I	102	CLA	CMD-C2D-C1D	6.01	135.32	124.73
20	B	806	CLA	OBD-CAD-C3D	-6.01	114.37	128.42
20	B	842	CLA	CAB-C3B-C2B	-6.01	107.57	123.53
20	B	823	CLA	C4D-C3D-CAD	6.01	114.63	108.11
20	F	201	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
20	2	303	CLA	C4D-C3D-CAD	6.01	114.63	108.11
20	B	842	CLA	CMD-C2D-C1D	6.00	135.30	124.73
20	B	833	CLA	O2D-CGD-CBD	6.00	121.72	111.23
20	A	826	CLA	CMD-C2D-C1D	6.00	135.29	124.73
20	B	822	CLA	C1D-CHD-C4C	-5.99	113.30	126.02
20	B	826	CLA	C4D-C3D-CAD	5.98	114.61	108.11
20	H	102	CLA	C4D-C3D-CAD	5.98	114.61	108.11
20	3	301	CLA	CMD-C2D-C1D	5.98	135.26	124.73
20	L	203	CLA	C4D-C3D-CAD	5.98	114.60	108.11
20	B	823	CLA	CMD-C2D-C1D	5.98	135.26	124.73
20	2	311	CLA	C1D-CHD-C4C	-5.98	113.31	126.02
20	K	101	CLA	C1D-CHD-C4C	-5.97	113.33	126.02
20	L	208	CLA	C4D-C3D-CAD	5.97	114.59	108.11
20	A	835	CLA	C4D-C3D-CAD	5.96	114.58	108.11
20	A	810	CLA	O2D-CGD-CBD	5.96	121.65	111.23
20	4	310	CLA	CBB-CAB-C3B	5.96	157.31	127.53
20	B	819	CLA	C4D-C3D-CAD	5.96	114.58	108.11
20	F	206	CLA	C4D-C3D-CAD	5.96	114.58	108.11
20	B	814	CLA	C1D-CHD-C4C	-5.95	113.38	126.02
20	B	802	CLA	CMD-C2D-C1D	5.94	135.19	124.73
20	A	818	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
20	4	302	CLA	CMD-C2D-C1D	5.93	135.18	124.73
20	B	833	CLA	C1D-CHD-C4C	-5.93	113.42	126.02
20	4	301	CLA	C4D-C3D-CAD	5.93	114.55	108.11
20	B	836	CLA	C4D-C3D-CAD	5.93	114.54	108.11
20	B	818	CLA	CMD-C2D-C1D	5.92	135.16	124.73
20	A	809	CLA	O2D-CGD-CBD	5.92	121.58	111.23
20	A	850	CLA	C1D-CHD-C4C	-5.91	113.46	126.02
20	G	105	CLA	CHD-C4C-NC	5.91	133.39	124.23
20	B	835	CLA	C4D-C3D-CAD	5.91	114.52	108.11
20	B	837	CLA	C4D-C3D-CAD	5.90	114.52	108.11
20	L	202	CLA	C4D-C3D-CAD	5.90	114.51	108.11
20	1	215	CLA	CMD-C2D-C1D	5.90	135.12	124.73
20	A	825	CLA	C1D-CHD-C4C	-5.90	113.48	126.02
20	A	834	CLA	C4D-C3D-CAD	5.90	114.51	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	313	CLA	CMD-C2D-C1D	5.90	135.11	124.73
20	L	208	CLA	CMD-C2D-C1D	5.89	135.10	124.73
20	A	831	CLA	O2D-CGD-CBD	5.89	121.52	111.23
20	A	808	CLA	CMD-C2D-C1D	5.88	135.09	124.73
20	B	812	CLA	O2D-CGD-CBD	5.88	121.51	111.23
20	2	316	CLA	C4D-C3D-CAD	5.88	114.49	108.11
20	4	315	CLA	O2D-CGD-CBD	5.88	121.51	111.23
20	B	841	CLA	C3B-C2B-C1B	-5.88	100.24	107.17
20	B	808	CLA	C4D-C3D-CAD	5.88	114.49	108.11
20	4	318	CLA	CMD-C2D-C1D	5.88	135.08	124.73
20	B	827	CLA	CMD-C2D-C1D	5.88	135.08	124.73
20	A	809	CLA	CMD-C2D-C1D	5.88	135.08	124.73
20	I	102	CLA	C1D-CHD-C4C	-5.88	113.53	126.02
20	B	820	CLA	CMD-C2D-C1D	5.87	135.07	124.73
20	A	806	CLA	C4D-C3D-CAD	5.87	114.48	108.11
20	K	101	CLA	C4D-C3D-CAD	5.87	114.48	108.11
20	R	108	CLA	C4D-C3D-CAD	5.87	114.48	108.11
20	B	830	CLA	C1D-CHD-C4C	-5.87	113.55	126.02
20	1	201	CLA	C1D-CHD-C4C	-5.86	113.56	126.02
20	B	825	CLA	C1D-CHD-C4C	-5.86	113.57	126.02
20	B	832	CLA	C4D-C3D-CAD	5.86	114.47	108.11
20	L	204	CLA	CMD-C2D-C1D	5.86	135.04	124.73
20	B	814	CLA	CMD-C2D-C1D	5.85	135.03	124.73
20	2	302	CLA	O2D-CGD-CBD	5.84	121.44	111.23
20	2	310	CLA	C4D-C3D-CAD	5.84	114.45	108.11
20	1	206	CLA	CMD-C2D-C1D	5.84	135.01	124.73
20	4	303	CLA	C4D-CHA-C1A	5.84	128.21	121.24
20	A	807	CLA	O2D-CGD-CBD	5.84	121.43	111.23
21	G	101	LMU	C1'-O5'-C5'	-5.83	102.33	113.72
20	L	207	CLA	CAA-C2A-C3A	-5.83	97.25	113.00
20	B	824	CLA	CHD-C4C-C3C	-5.83	116.28	124.77
20	3	311	CLA	C4D-C3D-CAD	5.83	114.44	108.11
20	B	810	CLA	C4D-C3D-CAD	5.82	114.43	108.11
20	A	840	CLA	CMD-C2D-C1D	5.82	134.97	124.73
20	B	829	CLA	C1D-CHD-C4C	-5.82	113.66	126.02
20	2	310	CLA	CMD-C2D-C1D	5.81	134.97	124.73
20	A	803	CLA	C1D-CHD-C4C	-5.81	113.66	126.02
20	3	303	CLA	C1D-CHD-C4C	-5.81	113.67	126.02
20	F	205	CLA	C4D-C3D-CAD	5.81	114.42	108.11
20	B	815	CLA	C4D-C3D-CAD	5.81	114.41	108.11
20	L	204	CLA	O2D-CGD-CBD	5.81	121.38	111.23
20	A	813	CLA	CMD-C2D-C1D	5.80	134.95	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	303	CLA	C1D-CHD-C4C	-5.80	113.70	126.02
20	B	827	CLA	C1D-CHD-C4C	-5.80	113.70	126.02
20	B	807	CLA	C2B-C1B-NB	5.80	116.34	110.33
20	A	828	CLA	CMD-C2D-C1D	5.79	134.93	124.73
20	B	829	CLA	C4A-NA-C1A	5.79	109.32	106.68
20	3	317	CLA	C4D-C3D-CAD	5.79	114.39	108.11
20	B	817	CLA	C4D-C3D-CAD	5.77	114.38	108.11
20	B	834	CLA	C4D-C3D-CAD	5.77	114.38	108.11
20	3	311	CLA	C1D-CHD-C4C	-5.77	113.75	126.02
20	A	831	CLA	CHD-C4C-NC	5.77	133.18	124.23
20	B	808	CLA	CMD-C2D-C1D	5.77	134.88	124.73
20	A	840	CLA	C4D-C3D-CAD	5.77	114.37	108.11
20	H	110	CLA	C4D-C3D-CAD	5.76	114.36	108.11
20	A	813	CLA	C1D-CHD-C4C	-5.76	113.78	126.02
20	A	849	CLA	C3B-C2B-C1B	-5.76	100.38	107.17
20	F	206	CLA	C1D-CHD-C4C	-5.75	113.80	126.02
20	1	203	CLA	CHD-C4C-NC	5.75	133.14	124.23
20	B	819	CLA	CMD-C2D-C1D	5.75	134.85	124.73
20	A	839	CLA	C1D-CHD-C4C	-5.74	113.81	126.02
20	H	108	CLA	C3B-C2B-C1B	-5.74	100.41	107.17
20	1	205	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
20	3	309	CLA	C3A-C4A-CHB	-5.73	116.89	123.91
20	A	815	CLA	C4D-C3D-CAD	5.72	114.32	108.11
20	B	841	CLA	CMD-C2D-C1D	5.72	134.80	124.73
20	J	101	CLA	C1D-CHD-C4C	-5.72	113.87	126.02
20	2	308	CLA	CHD-C4C-NC	5.71	132.92	124.24
20	1	206	CLA	C1D-CHD-C4C	-5.71	113.88	126.02
20	H	108	CLA	OBD-CAD-C3D	-5.71	115.07	128.42
20	A	826	CLA	C4D-C3D-CAD	5.71	114.31	108.11
20	A	819	CLA	C4D-C3D-CAD	5.71	114.30	108.11
20	3	311	CLA	O2D-CGD-CBD	5.71	121.21	111.23
20	A	833	CLA	C1D-CHD-C4C	-5.71	113.89	126.02
20	A	811	CLA	C4D-C3D-CAD	5.70	114.30	108.11
20	2	307	CLA	C1D-CHD-C4C	-5.70	113.90	126.02
20	4	305	CLA	C4D-C3D-CAD	5.70	114.30	108.11
20	B	842	CLA	C4D-C3D-CAD	5.70	114.30	108.11
20	3	303	CLA	C4D-C3D-CAD	5.70	114.29	108.11
22	I	103	BCR	C1-C6-C5	-5.69	114.86	122.64
20	3	310	CLA	CMD-C2D-C1D	5.68	134.73	124.73
20	K	102	CLA	C1D-CHD-C4C	-5.67	113.96	126.02
20	A	849	CLA	CMD-C2D-C1D	5.67	134.72	124.73
20	H	108	CLA	CMD-C2D-C1D	5.67	134.71	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	844	BCR	C30-C25-C26	-5.67	114.89	122.64
20	B	828	CLA	C4D-C3D-CAD	5.66	114.25	108.11
20	A	838	CLA	C4D-C3D-CAD	5.65	114.25	108.11
20	4	313	CLA	C1D-CHD-C4C	-5.65	114.00	126.02
20	K	102	CLA	C4D-C3D-CAD	5.65	114.24	108.11
20	B	824	CLA	CHD-C4C-NC	5.65	132.99	124.23
20	3	315	CLA	C3A-C4A-CHB	-5.65	117.00	123.91
20	4	303	CLA	C4D-C3D-CAD	5.65	114.24	108.11
20	B	824	CLA	CMD-C2D-C1D	5.64	134.67	124.73
20	A	829	CLA	CMD-C2D-C1D	5.64	134.67	124.73
20	A	824	CLA	O2D-CGD-CBD	5.64	121.09	111.23
20	L	202	CLA	O2D-CGD-CBD	5.63	121.08	111.23
20	L	204	CLA	C1D-CHD-C4C	-5.63	114.05	126.02
20	B	832	CLA	C1D-CHD-C4C	-5.63	114.05	126.02
20	2	302	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
20	1	210	CLA	C4D-C3D-CAD	5.63	114.22	108.11
20	4	303	CLA	CHC-C1C-NC	5.62	132.78	124.31
20	A	806	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
20	F	207	CLA	CMD-C2D-C1D	5.62	134.62	124.73
20	L	203	CLA	O2D-CGD-CBD	5.61	121.05	111.23
20	3	317	CLA	C1D-CHD-C4C	-5.61	114.09	126.02
20	3	301	CLA	CAB-C3B-C2B	-5.61	108.63	123.53
20	B	834	CLA	C1D-CHD-C4C	-5.61	114.09	126.02
20	2	308	CLA	C3A-C4A-CHB	-5.61	117.04	123.91
20	3	304	CLA	C4A-NA-C1A	5.61	109.24	106.68
20	A	817	CLA	O2D-CGD-CBD	5.61	121.03	111.23
20	4	313	CLA	CAB-C3B-C2B	-5.60	108.65	123.53
20	B	820	CLA	C1D-CHD-C4C	-5.60	114.11	126.02
20	B	827	CLA	C4D-C3D-CAD	5.60	114.19	108.11
20	A	819	CLA	C1D-CHD-C4C	-5.60	114.12	126.02
20	A	803	CLA	C4D-C3D-CAD	5.60	114.18	108.11
20	L	202	CLA	C1D-CHD-C4C	-5.59	114.13	126.02
20	1	204	CLA	C1D-CHD-C4C	-5.59	114.13	126.02
20	B	809	CLA	C1D-CHD-C4C	-5.59	114.13	126.02
20	4	310	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
20	F	205	CLA	C1D-CHD-C4C	-5.59	114.14	126.02
20	1	210	CLA	C1D-CHD-C4C	-5.59	114.14	126.02
20	4	301	CLA	C1D-CHD-C4C	-5.59	114.14	126.02
20	A	817	CLA	C1D-CHD-C4C	-5.59	114.14	126.02
20	L	207	CLA	C4D-C3D-CAD	5.58	114.17	108.11
20	A	805	CLA	C4D-C3D-CAD	5.58	114.17	108.11
20	A	807	CLA	C4D-C3D-CAD	5.58	114.17	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	201	CLA	C4A-NA-C1A	5.58	109.22	106.68
20	A	837	CLA	C1D-CHD-C4C	-5.57	114.17	126.02
20	B	822	CLA	CHD-C4C-NC	5.57	132.87	124.23
20	A	825	CLA	C4D-C3D-CAD	5.57	114.15	108.11
20	A	811	CLA	C1D-CHD-C4C	-5.56	114.19	126.02
20	B	835	CLA	O2D-CGD-CBD	5.56	120.96	111.23
20	B	816	CLA	C1D-CHD-C4C	-5.56	114.20	126.02
20	4	313	CLA	CMD-C2D-C1D	5.56	134.52	124.73
20	B	802	CLA	O2D-CGD-CBD	5.56	120.94	111.23
20	A	813	CLA	C4D-C3D-CAD	5.55	114.14	108.11
20	B	814	CLA	CHD-C4C-NC	5.55	132.84	124.23
20	A	812	CLA	C1D-CHD-C4C	-5.54	114.24	126.02
20	A	818	CLA	CBB-CAB-C3B	5.54	155.21	127.53
20	2	314	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
20	L	201	CLA	O2D-CGD-CBD	5.54	120.91	111.23
20	A	808	CLA	C4D-C3D-CAD	5.53	114.11	108.11
20	A	805	CLA	C1D-CHD-C4C	-5.53	114.27	126.02
20	A	826	CLA	C1D-CHD-C4C	-5.53	114.27	126.02
20	A	828	CLA	C1D-CHD-C4C	-5.52	114.30	126.02
20	2	311	CLA	C4D-C3D-CAD	5.52	114.10	108.11
20	A	824	CLA	C4D-C3D-CAD	5.51	114.09	108.11
20	H	110	CLA	C1D-CHD-C4C	-5.51	114.30	126.02
20	B	819	CLA	O2D-CGD-CBD	5.51	120.86	111.23
20	1	209	CLA	C3A-C4A-CHB	-5.51	117.16	123.91
20	A	831	CLA	CMD-C2D-C1D	5.51	134.42	124.73
22	I	101	BCR	C3-C4-C5	-5.50	104.24	114.06
20	A	833	CLA	O2D-CGD-CBD	5.50	120.85	111.23
20	F	205	CLA	C2B-C1B-NB	5.50	116.03	110.33
20	L	207	CLA	C1D-CHD-C4C	-5.50	114.34	126.02
20	4	310	CLA	CHC-C1C-NC	5.49	132.59	124.31
20	B	826	CLA	C1D-CHD-C4C	-5.49	114.34	126.02
20	3	309	CLA	C4A-NA-C1A	5.49	109.18	106.68
20	B	803	CLA	C1D-CHD-C4C	-5.49	114.36	126.02
20	3	317	CLA	CAB-C3B-C2B	-5.47	108.99	123.53
20	B	837	CLA	C1D-CHD-C4C	-5.47	114.39	126.02
21	H	104	LMU	C1B-O5B-C5B	5.47	124.41	113.72
20	B	814	CLA	C4D-C3D-CAD	5.47	114.05	108.11
21	R	101	LMU	O1B-C1B-C2B	5.47	121.55	108.09
20	K	101	CLA	CMD-C2D-C1D	5.47	134.36	124.73
20	B	835	CLA	C1D-CHD-C4C	-5.47	114.39	126.02
20	A	825	CLA	O2D-CGD-CBD	5.47	120.79	111.23
20	1	213	CLA	CMD-C2D-C1D	5.46	134.35	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	306	CLA	CHC-C1C-NC	5.46	132.54	124.31
20	1	207	CLA	C1D-CHD-C4C	-5.46	114.42	126.02
20	3	314	CLA	CHC-C1C-NC	5.46	132.53	124.31
20	B	825	CLA	OBD-CAD-C3D	-5.46	115.66	128.42
20	B	807	CLA	C1D-CHD-C4C	-5.46	114.42	126.02
20	A	832	CLA	C4D-C3D-CAD	5.46	114.03	108.11
20	A	806	CLA	O2D-CGD-CBD	5.45	120.77	111.23
22	I	103	BCR	C11-C10-C9	-5.45	119.63	127.28
20	H	109	CLA	CMD-C2D-C1D	5.45	134.33	124.73
20	H	102	CLA	C1D-CHD-C4C	-5.45	114.44	126.02
20	A	830	CLA	C1D-CHD-C4C	-5.44	114.45	126.02
20	1	206	CLA	O2D-CGD-CBD	5.44	120.75	111.23
20	1	207	CLA	CGD-CBD-CAD	-5.44	93.22	110.85
22	F	204	BCR	C24-C23-C22	-5.44	118.18	126.23
20	A	836	CLA	C1D-CHD-C4C	-5.44	114.46	126.02
20	B	814	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
21	E	101	LMU	C1B-O5B-C5B	-5.44	103.10	113.72
20	B	838	CLA	C4D-C3D-CAD	5.44	114.01	108.11
20	B	821	CLA	C1D-CHD-C4C	-5.43	114.47	126.02
20	3	301	CLA	C1D-CHD-C4C	-5.43	114.47	126.02
20	A	838	CLA	C1D-CHD-C4C	-5.43	114.47	126.02
20	A	834	CLA	O2D-CGD-CBD	5.43	120.72	111.23
20	B	825	CLA	CMD-C2D-C1D	5.43	134.28	124.73
20	A	823	CLA	C1D-CHD-C4C	-5.42	114.50	126.02
20	A	840	CLA	C1D-CHD-C4C	-5.42	114.50	126.02
20	A	816	CLA	C4D-C3D-CAD	5.42	113.99	108.11
20	A	850	CLA	CMD-C2D-C1D	5.41	134.26	124.73
20	A	827	CLA	C1D-CHD-C4C	-5.41	114.52	126.02
20	A	823	CLA	C4D-C3D-CAD	5.41	113.98	108.11
20	B	822	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
20	3	313	CLA	C1D-CHD-C4C	-5.41	114.53	126.02
20	A	849	CLA	CHD-C4C-C3C	-5.40	116.89	124.77
20	B	806	CLA	C2B-C1B-NB	5.39	115.91	110.33
20	B	828	CLA	C1D-CHD-C4C	-5.39	114.57	126.02
20	2	307	CLA	CHD-C4C-NC	5.39	132.58	124.23
20	4	303	CLA	CAA-C2A-C3A	-5.39	98.44	113.00
20	H	109	CLA	C1D-CHD-C4C	-5.39	114.57	126.02
20	A	838	CLA	O2D-CGD-CBD	5.39	120.65	111.23
22	A	845	BCR	C11-C10-C9	-5.39	119.72	127.28
20	A	809	CLA	C4D-C3D-CAD	5.38	113.95	108.11
20	2	310	CLA	C4B-CHC-C1C	-5.38	113.59	126.25
20	A	824	CLA	C1D-CHD-C4C	-5.38	114.58	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	805	LMU	C1B-O1B-C4'	-5.38	105.22	117.98
20	2	304	CLA	CHD-C4C-NC	5.38	132.42	124.24
20	3	314	CLA	CHD-C4C-NC	5.38	132.57	124.23
20	B	850	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
20	3	313	CLA	O2D-CGD-CBD	5.38	120.63	111.23
20	A	808	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
20	4	305	CLA	CMD-C2D-C1D	5.37	134.19	124.73
20	A	810	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
22	G	104	BCR	C11-C10-C9	-5.37	119.74	127.28
20	3	307	CLA	CMD-C2D-C1D	5.37	134.18	124.73
20	4	317	CLA	C1D-CHD-C4C	-5.37	114.61	126.02
20	G	105	CLA	CHD-C4C-C3C	-5.36	116.95	124.77
20	A	816	CLA	O2D-CGD-CBD	5.36	120.61	111.23
20	3	307	CLA	C4B-CHC-C1C	-5.36	113.64	126.25
20	A	833	CLA	C4D-C3D-CAD	5.36	113.93	108.11
20	B	827	CLA	O2D-CGD-CBD	5.36	120.60	111.23
20	A	827	CLA	C4D-C3D-CAD	5.35	113.92	108.11
20	L	203	CLA	C1D-CHD-C4C	-5.35	114.65	126.02
20	H	108	CLA	CHD-C4C-NC	5.35	132.53	124.23
20	J	101	CLA	O2D-CGD-CBD	5.35	120.58	111.23
20	2	303	CLA	CHD-C4C-NC	5.35	132.52	124.23
20	A	809	CLA	C1D-CHD-C4C	-5.35	114.66	126.02
20	B	823	CLA	C1D-CHD-C4C	-5.35	114.66	126.02
20	B	819	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
20	A	803	CLA	C4A-NA-C1A	5.34	109.12	106.68
20	B	802	CLA	C1D-CHD-C4C	-5.34	114.66	126.02
20	2	311	CLA	O2D-CGD-CBD	5.34	120.57	111.23
20	B	818	CLA	C4D-C3D-CAD	5.34	113.91	108.11
20	4	315	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
20	A	821	CLA	C1D-CHD-C4C	-5.34	114.67	126.02
20	A	831	CLA	C4D-C3D-CAD	5.34	113.91	108.11
20	A	849	CLA	C1D-CHD-C4C	-5.34	114.67	126.02
20	A	820	CLA	C1D-CHD-C4C	-5.34	114.68	126.02
20	R	107	CLA	C1D-CHD-C4C	-5.33	114.68	126.02
20	A	837	CLA	CHD-C4C-NC	5.33	132.50	124.23
20	A	803	CLA	CHD-C4C-NC	5.33	132.50	124.23
20	H	109	CLA	C4D-C3D-CAD	5.33	113.90	108.11
20	B	842	CLA	CBD-CAD-C3D	-5.33	101.14	108.25
20	3	310	CLA	C4D-C3D-CAD	5.32	113.89	108.11
20	A	804	CLA	C2B-C1B-NB	5.32	115.84	110.33
20	A	835	CLA	C1D-CHD-C4C	-5.32	114.71	126.02
20	3	308	CLA	C4A-NA-C1A	5.32	109.11	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	204	CLA	C4D-C3D-CAD	5.32	113.88	108.11
20	1	203	CLA	C1D-CHD-C4C	-5.32	114.72	126.02
20	4	311	CLA	CHD-C4C-NC	5.32	132.32	124.24
20	B	824	CLA	C1D-CHD-C4C	-5.31	114.73	126.02
20	B	831	CLA	O2D-CGD-CBD	5.31	120.51	111.23
20	B	809	CLA	C4D-C3D-CAD	5.31	113.87	108.11
20	2	314	CLA	C4A-NA-C1A	5.31	109.10	106.68
20	K	103	CLA	O2D-CGD-CBD	5.31	120.51	111.23
22	A	844	BCR	C16-C17-C18	-5.31	119.84	127.28
20	2	307	CLA	C4B-CHC-C1C	-5.30	113.78	126.25
20	A	836	CLA	CMD-C2D-C1D	5.30	134.06	124.73
20	I	102	CLA	C4D-C3D-CAD	5.30	113.86	108.11
22	2	317	BCR	C38-C26-C25	-5.30	118.70	124.48
20	B	822	CLA	O2D-CGD-CBD	5.30	120.49	111.23
20	A	839	CLA	CHC-C1C-NC	5.29	132.28	124.31
20	4	315	CLA	CMD-C2D-C1D	5.29	134.04	124.73
20	A	825	CLA	CMD-C2D-C1D	5.29	134.04	124.73
20	B	831	CLA	C4D-C3D-CAD	5.29	113.85	108.11
20	B	818	CLA	O2D-CGD-CBD	5.29	120.47	111.23
20	4	306	CLA	C4D-C3D-CAD	5.29	113.85	108.11
20	3	303	CLA	CHD-C4C-NC	5.29	132.43	124.23
20	B	812	CLA	CHD-C4C-NC	5.29	132.43	124.23
20	3	314	CLA	C4B-CHC-C1C	-5.28	113.83	126.25
20	B	806	CLA	C4D-C3D-CAD	5.28	113.84	108.11
20	A	832	CLA	C1D-CHD-C4C	-5.27	114.81	126.02
20	K	104	CLA	C1D-CHD-C4C	-5.27	114.81	126.02
20	I	102	CLA	O2D-CGD-CBD	5.27	120.45	111.23
20	B	817	CLA	C1D-CHD-C4C	-5.27	114.81	126.02
20	H	101	CLA	C1D-CHD-C4C	-5.27	114.82	126.02
20	A	831	CLA	CHC-C1C-NC	5.27	132.24	124.31
20	4	302	CLA	CBD-CAD-C3D	-5.26	101.22	108.25
20	3	314	CLA	O2D-CGD-CBD	5.26	120.43	111.23
22	I	103	BCR	C8-C9-C10	5.26	127.29	119.01
20	A	808	CLA	O2D-CGD-CBD	5.26	120.43	111.23
20	B	838	CLA	C1D-CHD-C4C	-5.26	114.84	126.02
20	3	303	CLA	CHD-C4C-C3C	-5.26	116.72	125.03
20	A	837	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
20	A	822	CLA	C1D-CHD-C4C	-5.26	114.85	126.02
20	A	804	CLA	C1D-CHD-C4C	-5.25	114.86	126.02
20	B	824	CLA	C4D-C3D-CAD	5.25	113.81	108.11
20	A	811	CLA	C2B-C1B-NB	5.25	115.77	110.33
20	3	303	CLA	CAB-C3B-C2B	-5.25	109.60	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	812	CLA	C4D-C3D-CAD	5.24	113.80	108.11
20	B	842	CLA	C1D-CHD-C4C	-5.24	114.88	126.02
20	4	315	CLA	CHD-C4C-NC	5.24	132.35	124.23
20	B	806	CLA	O2D-CGD-CBD	5.24	120.39	111.23
20	B	819	CLA	CHD-C4C-NC	5.24	132.35	124.23
20	1	202	CLA	C1D-CHD-C4C	-5.24	114.89	126.02
20	4	313	CLA	CBD-CAD-C3D	-5.23	101.27	108.25
20	K	101	CLA	O2D-CGD-CBD	5.23	120.37	111.23
20	B	802	CLA	C4D-C3D-CAD	5.23	113.78	108.11
20	B	802	CLA	C4-C3-C5	5.22	124.30	115.23
20	B	810	CLA	C1D-CHD-C4C	-5.22	114.92	126.02
20	3	315	CLA	C2A-C1A-CHA	-5.22	113.73	122.63
20	B	827	CLA	CHD-C4C-NC	5.22	132.33	124.23
20	B	841	CLA	CHC-C4B-NB	5.22	131.88	124.05
20	K	103	CLA	C1D-CHD-C4C	-5.22	114.92	126.02
20	1	212	CLA	C3A-C4A-CHB	-5.22	117.52	123.91
21	R	101	LMU	O2B-C2B-C3B	5.22	122.67	110.38
20	F	207	CLA	CHD-C4C-NC	5.21	132.31	124.23
20	A	841	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
20	B	825	CLA	C4D-C3D-CAD	5.21	113.77	108.11
20	1	201	CLA	C4B-CHC-C1C	-5.21	114.00	126.25
20	A	814	CLA	C4A-NA-C1A	5.21	109.06	106.68
20	A	851	CLA	O2D-CGD-CBD	5.21	120.34	111.23
20	A	816	CLA	CHD-C4C-NC	5.20	132.30	124.23
20	A	850	CLA	C4D-C3D-CAD	5.20	113.75	108.11
20	B	829	CLA	CMD-C2D-C1D	5.20	133.88	124.73
22	B	845	BCR	C24-C23-C22	-5.20	118.55	126.23
20	4	308	CLA	C3A-C4A-CHB	-5.19	117.55	123.91
20	1	207	CLA	C4A-NA-C1A	5.19	109.05	106.68
20	K	102	CLA	CHD-C4C-NC	5.19	132.28	124.23
20	1	204	CLA	CHD-C4C-NC	5.19	132.28	124.23
20	A	802	CLA	C2A-C1A-CHA	-5.19	113.79	122.63
22	F	204	BCR	C30-C25-C26	-5.19	115.55	122.64
20	A	806	CLA	C1D-CHD-C4C	-5.18	115.00	126.02
20	A	816	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
20	B	818	CLA	C1D-CHD-C4C	-5.18	115.01	126.02
21	E	101	LMU	C4B-C3B-C2B	-5.18	101.74	110.83
20	2	312	CLA	CMD-C2D-C1D	5.18	133.85	124.73
20	A	810	CLA	C4D-C3D-CAD	5.18	113.73	108.11
20	L	201	CLA	C1D-CHD-C4C	-5.17	115.02	126.02
20	A	831	CLA	C2B-C1B-NB	5.17	115.69	110.33
20	4	302	CLA	CHD-C4C-NC	5.17	132.25	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	808	CLA	C1D-CHD-C4C	-5.17	115.03	126.02
20	B	831	CLA	CMD-C2D-C1D	5.17	133.83	124.73
20	B	809	CLA	C2B-C1B-NB	5.16	115.68	110.33
20	R	108	CLA	C1D-CHD-C4C	-5.16	115.05	126.02
20	B	841	CLA	C1D-CHD-C4C	-5.16	115.05	126.02
20	B	808	CLA	CHD-C4C-NC	5.16	132.23	124.23
21	H	103	LMU	O5'-C5'-C6'	5.16	119.22	106.44
20	B	819	CLA	C2B-C1B-NB	5.16	115.67	110.33
20	1	211	CLA	O2A-CGA-CBA	5.15	127.55	111.83
20	A	834	CLA	C1D-CHD-C4C	-5.15	115.07	126.02
20	A	829	CLA	C1D-CHD-C4C	-5.15	115.08	126.02
20	A	849	CLA	CHD-C4C-NC	5.15	132.21	124.23
20	B	810	CLA	CMD-C2D-C1D	5.15	133.79	124.73
20	F	205	CLA	CHD-C4C-NC	5.14	132.21	124.23
20	B	813	CLA	C1D-CHD-C4C	-5.14	115.09	126.02
20	1	211	CLA	C4A-NA-C1A	5.14	109.03	106.68
20	B	830	CLA	C4A-NA-C1A	5.14	109.03	106.68
20	4	315	CLA	C4D-C3D-CAD	5.14	113.69	108.11
20	B	837	CLA	O2D-CGD-O1D	-5.14	113.85	123.85
20	4	318	CLA	CAA-C2A-C1A	5.14	128.81	111.97
20	2	309	CLA	C3A-C4A-CHB	-5.14	117.62	123.91
20	2	316	CLA	CHD-C4C-NC	5.13	132.19	124.23
20	3	305	CLA	CHD-C4C-NC	5.13	132.04	124.24
20	2	311	CLA	CMD-C2D-C1D	5.13	133.76	124.73
20	1	204	CLA	C4B-CHC-C1C	-5.13	114.19	126.25
20	2	314	CLA	C4B-CHC-C1C	-5.12	114.20	126.25
20	B	816	CLA	CMD-C2D-C1D	5.12	133.75	124.73
20	3	310	CLA	CHC-C4B-NB	5.12	131.73	124.05
21	2	320	LMU	C4B-C3B-C2B	-5.12	101.84	110.83
20	2	310	CLA	CHC-C1C-NC	5.12	132.02	124.31
20	H	110	CLA	CMD-C2D-C1D	5.12	133.74	124.73
20	2	311	CLA	C4A-NA-C1A	5.12	109.01	106.68
20	4	306	CLA	C3A-C2A-C1A	5.11	109.00	101.34
20	A	814	CLA	C2A-C1A-CHA	-5.11	113.92	122.63
20	F	201	CLA	C4B-CHC-C1C	-5.11	114.23	126.25
20	A	808	CLA	C2B-C1B-NB	5.11	115.62	110.33
20	A	851	CLA	C1D-CHD-C4C	-5.11	115.16	126.02
21	A	855	LMU	O1B-C4'-C3'	5.11	120.22	107.23
20	2	307	CLA	CMD-C2D-C1D	5.11	133.72	124.73
20	1	204	CLA	CMD-C2D-C3D	-5.11	115.98	127.69
20	A	801	CLA	C1D-CHD-C4C	-5.11	115.17	126.02
20	L	204	CLA	CHD-C4C-NC	5.11	132.15	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	205	CLA	CBD-CAD-C3D	-5.10	101.43	108.25
20	A	835	CLA	C2B-C1B-NB	5.10	115.62	110.33
20	A	831	CLA	C4B-CHC-C1C	-5.10	114.25	126.25
20	B	816	CLA	C4D-C3D-CAD	5.10	113.64	108.11
20	B	809	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
20	A	838	CLA	CMD-C2D-C1D	5.10	133.70	124.73
20	A	815	CLA	C1D-CHD-C4C	-5.09	115.19	126.02
20	3	306	CLA	C3A-C4A-CHB	-5.09	117.67	123.91
20	B	840	CLA	O2D-CGD-CBD	5.09	120.13	111.23
22	G	104	BCR	C15-C14-C13	-5.09	120.14	127.28
20	3	308	CLA	C3A-C4A-CHB	-5.09	117.68	123.91
20	4	317	CLA	CHD-C4C-NC	5.09	132.12	124.23
20	A	818	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
20	3	304	CLA	CHC-C1C-NC	5.09	131.81	124.33
20	L	208	CLA	CHD-C4C-NC	5.07	132.10	124.23
20	3	301	CLA	CBD-CAD-C3D	-5.06	101.49	108.25
20	A	838	CLA	CHD-C4C-NC	5.06	132.07	124.23
20	G	105	CLA	C2B-C1B-NB	5.06	115.57	110.33
20	3	316	CLA	C2A-C1A-CHA	-5.06	114.01	122.63
20	A	802	CLA	C3A-C4A-CHB	-5.06	117.72	123.91
20	A	809	CLA	CHC-C1C-NC	5.05	131.92	124.31
20	A	833	CLA	CHD-C4C-NC	5.05	132.06	124.23
21	H	105	LMU	C1B-O5B-C5B	5.05	123.58	113.72
20	2	310	CLA	O2D-CGD-CBD	5.05	120.05	111.23
20	1	213	CLA	CHD-C4C-NC	5.04	132.05	124.23
20	B	839	CLA	CMD-C2D-C3D	-5.04	116.12	127.69
20	A	814	CLA	C1B-NB-C4B	-5.04	102.77	106.31
20	1	203	CLA	C2A-C1A-CHA	-5.04	115.12	123.87
20	B	821	CLA	CHD-C4C-NC	5.04	132.04	124.23
20	3	316	CLA	C3A-C4A-CHB	-5.03	117.75	123.91
20	2	307	CLA	CHC-C1C-NC	5.03	131.88	124.31
20	A	810	CLA	C1D-CHD-C4C	-5.03	115.34	126.02
20	2	301	CLA	C3A-C4A-CHB	-5.02	117.76	123.91
20	2	312	CLA	C1-C2-C3	-5.02	117.97	126.20
20	H	108	CLA	CHC-C1C-NC	5.02	131.87	124.31
20	2	302	CLA	C2B-C1B-NB	5.02	115.53	110.33
20	A	818	CLA	C1-C2-C3	-5.02	117.98	126.20
20	3	313	CLA	C4D-C3D-CAD	5.02	113.56	108.11
22	A	844	BCR	C15-C14-C13	-5.01	120.25	127.28
22	I	101	BCR	C23-C22-C21	5.01	126.89	119.01
20	A	837	CLA	C2B-C1B-NB	5.01	115.53	110.33
20	B	816	CLA	O2D-CGD-CBD	5.01	119.99	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	314	CLA	C4D-C3D-CAD	5.01	113.55	108.11
20	L	208	CLA	CHD-C4C-C3C	-5.01	117.47	124.77
20	3	304	CLA	CHD-C4C-NC	5.01	131.85	124.24
20	A	832	CLA	O2D-CGD-CBD	5.01	119.98	111.23
20	A	829	CLA	C4D-C3D-CAD	5.00	113.54	108.11
20	1	214	CLA	C2A-C1A-CHA	-5.00	114.10	122.63
21	D	201	LMU	C1'-O5'-C5'	-5.00	103.96	113.72
20	A	804	CLA	C1-O2A-CGA	5.00	128.75	116.65
20	A	831	CLA	C4-C3-C5	5.00	123.90	115.23
20	B	850	CLA	C2B-C1B-NB	5.00	115.51	110.33
20	3	306	CLA	CHD-C4C-NC	5.00	131.83	124.24
20	2	308	CLA	C4C-CHD-C1D	-4.99	111.76	125.98
20	A	801	CLA	C3A-C2A-C1A	4.99	108.81	101.34
20	A	813	CLA	CHD-C4C-NC	4.99	131.96	124.23
20	2	305	CLA	C1D-CHD-C4C	-4.98	115.44	126.02
20	A	807	CLA	C1D-CHD-C4C	-4.98	115.44	126.02
23	B	843	PQN	C11-C12-C13	-4.98	118.26	126.83
20	4	305	CLA	CHD-C4C-NC	4.97	131.94	124.23
20	A	819	CLA	C2B-C1B-NB	4.97	115.48	110.33
20	B	806	CLA	CHD-C4C-NC	4.97	131.94	124.23
20	1	203	CLA	CMD-C2D-C3D	-4.97	116.29	127.69
20	A	836	CLA	C2B-C1B-NB	4.97	115.48	110.33
20	B	810	CLA	C4A-NA-C1A	4.97	108.94	106.68
20	A	804	CLA	CHD-C4C-NC	4.97	131.93	124.23
20	4	306	CLA	C2B-C1B-NB	4.97	115.48	110.33
20	2	310	CLA	CHD-C4C-NC	4.96	131.93	124.23
20	2	312	CLA	CHD-C4C-NC	4.96	131.92	124.23
20	A	839	CLA	C4B-CHC-C1C	-4.96	114.59	126.25
22	F	203	BCR	C11-C10-C9	-4.96	120.33	127.28
20	B	836	CLA	CHD-C4C-NC	4.96	131.92	124.23
20	B	816	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
20	A	813	CLA	CHC-C1C-NC	4.96	131.78	124.31
20	4	307	CLA	C2A-C1A-CHA	-4.96	114.18	122.63
20	B	850	CLA	C1D-CHD-C4C	-4.95	115.49	126.02
22	B	847	BCR	C15-C14-C13	-4.95	120.33	127.28
20	B	806	CLA	C1D-CHD-C4C	-4.95	115.49	126.02
20	A	850	CLA	C2B-C1B-NB	4.95	115.46	110.33
20	3	317	CLA	CHD-C4C-NC	4.95	131.90	124.23
20	3	312	CLA	C3A-C4A-CHB	-4.95	117.85	123.91
22	F	204	BCR	C10-C11-C12	-4.94	108.89	123.20
20	A	831	CLA	C4B-C3B-C2B	4.94	113.44	107.30
20	2	312	CLA	CHD-C4C-C3C	-4.93	117.58	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	821	CLA	O2D-CGD-CBD	4.93	119.85	111.23
20	3	311	CLA	CHD-C4C-NC	4.93	131.88	124.23
20	B	820	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
21	B	804	LMU	C3'-C4'-C5'	-4.93	100.00	110.93
20	2	307	CLA	C4D-C3D-CAD	4.93	113.46	108.11
21	R	103	LMU	O1B-C4'-C3'	4.93	119.75	107.23
20	B	835	CLA	CHD-C4C-NC	4.93	131.87	124.23
20	R	107	CLA	O2D-CGD-CBD	4.92	119.84	111.23
20	1	214	CLA	C3A-C4A-CHB	-4.92	117.88	123.91
22	2	317	BCR	C16-C15-C14	-4.92	113.45	123.52
20	F	205	CLA	CBD-CAD-C3D	-4.92	101.68	108.25
20	A	835	CLA	CHD-C4C-NC	4.92	131.85	124.23
20	3	314	CLA	CHC-C4B-NB	4.91	131.42	124.05
20	B	828	CLA	C2B-C1B-NB	4.91	115.42	110.33
20	1	203	CLA	O2D-CGD-CBD	4.91	119.81	111.23
20	4	302	CLA	CAB-C3B-C2B	-4.90	110.52	123.53
22	A	844	BCR	C24-C23-C22	-4.90	118.99	126.23
20	3	303	CLA	CBD-CAD-C3D	-4.90	101.71	108.25
20	A	839	CLA	CHD-C4C-NC	4.90	131.82	124.23
21	H	105	LMU	C1B-C2B-C3B	-4.90	99.71	110.01
20	F	201	CLA	C4D-C3D-CAD	4.89	113.42	108.11
20	4	317	CLA	CHC-C1C-NC	4.89	131.68	124.31
20	B	808	CLA	CHD-C4C-C3C	-4.89	117.64	124.77
20	J	103	CLA	CMD-C2D-C1D	4.89	133.34	124.73
20	3	307	CLA	C1D-CHD-C4C	-4.88	115.64	126.02
20	2	316	CLA	CHD-C4C-C3C	-4.88	117.65	124.77
20	2	306	CLA	C1C-CHC-C4B	-4.88	113.17	126.04
20	A	804	CLA	C3B-C4B-NB	-4.88	106.17	110.53
20	A	806	CLA	C2B-C1B-NB	4.88	115.39	110.33
20	1	208	CLA	C3A-C4A-CHB	-4.88	117.94	123.91
20	K	104	CLA	C4-C3-C5	4.88	123.69	115.23
21	H	103	LMU	C1B-O1B-C4'	-4.88	106.42	117.98
20	1	207	CLA	C2A-C3A-C4A	-4.88	93.99	101.87
20	L	204	CLA	CHD-C4C-C3C	-4.87	117.67	124.77
20	B	820	CLA	CHD-C4C-NC	4.87	131.78	124.23
20	A	850	CLA	O2D-CGD-CBD	4.87	119.74	111.23
20	A	826	CLA	C2B-C1B-NB	4.86	115.37	110.33
20	1	206	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
20	1	204	CLA	CAA-C2A-C3A	-4.86	99.86	113.00
20	B	836	CLA	C2B-C1B-NB	4.86	115.36	110.33
20	B	829	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
20	B	834	CLA	CHD-C4C-NC	4.85	131.76	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	303	CLA	C2B-C1B-NB	4.85	115.36	110.33
20	G	105	CLA	C4D-C3D-CAD	4.85	113.38	108.11
20	2	303	CLA	C4A-NA-C1A	4.85	108.89	106.68
20	2	314	CLA	C1-C2-C3	-4.85	118.91	126.76
22	L	209	BCR	C7-C8-C9	-4.85	119.06	126.23
20	A	838	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
20	K	103	CLA	CHC-C1C-NC	4.84	131.60	124.31
20	3	305	CLA	C3A-C4A-CHB	-4.84	117.98	123.91
20	A	850	CLA	CHD-C4C-NC	4.84	131.74	124.23
20	B	838	CLA	CHD-C4C-NC	4.84	131.74	124.23
20	2	314	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
20	H	108	CLA	CHD-C4C-C3C	-4.84	117.72	124.77
20	2	305	CLA	C2B-C1B-NB	4.84	115.35	110.33
20	L	201	CLA	CHD-C4C-NC	4.84	131.73	124.23
20	1	204	CLA	CHC-C1C-NC	4.84	131.60	124.31
20	B	839	CLA	CHC-C1C-NC	4.84	131.59	124.31
20	B	815	CLA	C1D-CHD-C4C	-4.84	115.74	126.02
20	A	805	CLA	C4B-CHC-C1C	-4.84	114.88	126.25
20	A	831	CLA	CHD-C4C-C3C	-4.83	117.72	124.77
20	L	202	CLA	CHD-C4C-NC	4.83	131.73	124.23
20	B	831	CLA	C1D-CHD-C4C	-4.83	115.75	126.02
20	1	207	CLA	O2D-CGD-CBD	4.83	119.67	111.23
20	B	807	CLA	CHD-C4C-NC	4.83	131.72	124.23
20	4	304	CLA	C4B-CHC-C1C	-4.83	114.89	126.25
21	G	102	LMU	C1B-O5B-C5B	-4.82	104.30	113.72
20	A	804	CLA	C4D-C3D-CAD	4.82	113.35	108.11
20	4	312	CLA	C2A-C1A-CHA	-4.82	114.41	122.63
20	4	304	CLA	CHC-C1C-NC	4.82	131.57	124.31
21	H	103	LMU	O1B-C1B-C2B	4.82	119.95	108.09
20	4	301	CLA	CHD-C4C-NC	4.82	131.70	124.23
20	4	305	CLA	CHD-C4C-C3C	-4.82	117.75	124.77
20	4	308	CLA	C3B-C2B-C1B	-4.82	101.45	106.81
20	H	108	CLA	C4D-C3D-CAD	4.81	113.33	108.11
20	1	205	CLA	CHD-C4C-NC	4.81	131.69	124.23
20	B	840	CLA	C2B-C1B-NB	4.81	115.32	110.33
20	A	825	CLA	CHD-C4C-NC	4.81	131.69	124.23
20	B	830	CLA	CHD-C4C-NC	4.81	131.69	124.23
20	2	314	CLA	C2B-C1B-NB	4.81	115.31	110.33
20	A	837	CLA	C4B-CHC-C1C	-4.81	114.94	126.25
20	4	310	CLA	C4B-CHC-C1C	-4.81	114.95	126.25
20	1	211	CLA	O2D-CGD-CBD	4.80	119.63	111.23
20	A	851	CLA	CHD-C4C-NC	4.80	131.68	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	315	CLA	CHD-C4C-NC	4.80	131.54	124.24
20	4	311	CLA	C3A-C4A-CHB	-4.80	118.03	123.91
20	4	318	CLA	C1D-CHD-C4C	-4.80	115.81	126.02
20	A	826	CLA	CHD-C4C-NC	4.80	131.68	124.23
21	D	201	LMU	O1'-C1'-C2'	4.80	115.56	108.27
20	A	813	CLA	C2B-C1B-NB	4.80	115.30	110.33
22	B	801	BCR	C36-C18-C19	4.79	125.41	118.09
20	2	310	CLA	C1D-CHD-C4C	-4.79	115.83	126.02
20	1	201	CLA	CHC-C1C-NC	4.79	131.53	124.31
22	A	843	BCR	C15-C14-C13	-4.79	120.56	127.28
20	A	837	CLA	CHC-C1C-NC	4.79	131.52	124.31
20	K	101	CLA	CHD-C4C-NC	4.79	131.66	124.23
20	H	108	CLA	C4B-CHC-C1C	-4.79	114.99	126.25
20	A	803	CLA	CHC-C1C-NC	4.79	131.52	124.31
20	A	805	CLA	CHC-C1C-NC	4.79	131.52	124.31
20	J	101	CLA	CHD-C4C-NC	4.79	131.65	124.23
20	1	213	CLA	CHC-C1C-NC	4.79	131.52	124.31
20	2	314	CLA	CHC-C1C-NC	4.79	131.52	124.31
20	4	314	CLA	C3A-C4A-CHB	-4.78	118.06	123.91
20	B	850	CLA	C4B-CHC-C1C	-4.78	115.01	126.25
20	H	110	CLA	CHD-C4C-NC	4.78	131.64	124.23
22	I	101	BCR	C4-C5-C6	-4.78	116.25	122.70
20	B	824	CLA	O2D-CGD-CBD	4.78	119.58	111.23
20	A	833	CLA	CHC-C1C-NC	4.77	131.50	124.31
20	A	828	CLA	CHD-C4C-NC	4.77	131.63	124.23
22	B	844	BCR	C28-C27-C26	-4.77	105.55	114.06
21	4	319	LMU	C1B-O1B-C4'	-4.76	106.68	117.98
20	A	811	CLA	CMB-C2B-C1B	4.76	132.67	125.42
20	2	304	CLA	C3A-C4A-CHB	-4.76	118.08	123.91
22	I	103	BCR	C7-C8-C9	4.76	133.28	126.23
20	4	313	CLA	C1B-C2B-C3B	-4.76	102.56	107.03
20	3	309	CLA	C1B-NB-C4B	-4.76	102.97	106.31
20	3	304	CLA	C2A-C1A-CHA	-4.76	114.52	122.63
20	1	201	CLA	CHC-C4B-NB	4.76	131.19	124.05
20	A	819	CLA	O2D-CGD-CBD	4.75	119.54	111.23
20	A	839	CLA	CMD-C2D-C3D	-4.75	116.79	127.69
20	B	809	CLA	CHC-C1C-NC	4.75	131.47	124.31
20	B	840	CLA	C1D-CHD-C4C	-4.75	115.92	126.02
20	B	802	CLA	CHD-C4C-NC	4.75	131.59	124.23
20	A	849	CLA	C4B-CHC-C1C	-4.74	115.10	126.25
20	B	815	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
20	B	841	CLA	C4B-CHC-C1C	-4.73	115.12	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	O2D-CGD-CBD	4.73	119.50	111.23
20	1	210	CLA	CBD-CAD-C3D	-4.73	101.93	108.25
20	4	305	CLA	O2D-CGD-CBD	4.73	119.50	111.23
20	2	303	CLA	CHD-C4C-C3C	-4.73	117.88	124.77
21	2	313	LMU	O1'-C1'-C2'	4.72	115.45	108.27
20	3	317	CLA	CBD-CAD-C3D	-4.72	101.94	108.25
20	3	308	CLA	C2A-C1A-CHA	-4.72	114.58	122.63
20	B	836	CLA	C4-C3-C5	4.72	121.68	116.13
20	H	110	CLA	CHD-C4C-C3C	-4.72	117.89	124.77
20	L	207	CLA	C2B-C1B-NB	4.72	115.22	110.33
20	K	102	CLA	O2D-CGD-CBD	4.72	119.47	111.23
20	K	103	CLA	C4B-CHC-C1C	-4.71	115.16	126.25
20	A	811	CLA	C4B-C3B-C2B	4.71	113.16	107.30
20	A	801	CLA	CMD-C2D-C3D	-4.71	116.88	127.69
20	H	101	CLA	C2B-C1B-NB	4.71	115.21	110.33
20	B	828	CLA	CHD-C4C-NC	4.71	131.53	124.23
20	4	317	CLA	C4B-CHC-C1C	-4.71	115.17	126.25
20	A	831	CLA	CMB-C2B-C1B	4.70	132.58	125.42
20	F	206	CLA	CHD-C4C-NC	4.70	131.52	124.23
20	A	838	CLA	C2B-C1B-NB	4.70	115.20	110.33
20	A	813	CLA	O2D-CGD-CBD	4.70	119.44	111.23
20	I	102	CLA	CHD-C4C-NC	4.69	131.51	124.23
20	4	309	CLA	C2A-C1A-CHA	-4.69	114.63	122.63
20	K	103	CLA	C2B-C1B-NB	4.69	115.19	110.33
20	B	830	CLA	CHC-C4B-NB	4.69	131.09	124.05
20	A	804	CLA	C4B-CHC-C1C	-4.69	115.22	126.25
20	3	313	CLA	C2B-C1B-NB	4.69	115.19	110.33
20	A	804	CLA	O2A-CGA-CBA	4.69	126.14	111.83
20	A	837	CLA	O2D-CGD-CBD	4.69	119.43	111.23
20	1	207	CLA	CHD-C4C-NC	4.69	131.50	124.23
20	B	803	CLA	C2B-C1B-NB	4.69	115.19	110.33
20	L	207	CLA	CHD-C4C-NC	4.68	131.49	124.23
20	A	804	CLA	O2D-CGD-CBD	4.68	119.41	111.23
20	B	812	CLA	CHD-C4C-C3C	-4.68	117.95	124.77
20	B	826	CLA	CHD-C4C-NC	4.68	131.48	124.23
20	4	308	CLA	CHD-C4C-NC	4.68	131.35	124.24
20	A	809	CLA	C4B-CHC-C1C	-4.67	115.26	126.25
20	A	812	CLA	CHD-C4C-NC	4.67	131.47	124.23
20	1	207	CLA	CAA-C2A-C3A	4.67	125.61	113.00
20	F	201	CLA	CMD-C2D-C1D	4.67	132.95	124.73
20	A	823	CLA	O2D-CGD-CBD	4.67	119.39	111.23
20	A	835	CLA	CHC-C1C-NC	4.67	131.34	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	304	CLA	C1C-CHC-C4B	-4.67	113.73	126.04
20	B	819	CLA	CHD-C4C-C3C	-4.66	117.97	124.77
20	A	821	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
20	B	832	CLA	CHD-C4C-NC	4.66	131.46	124.23
20	L	201	CLA	C4D-C3D-CAD	4.66	113.17	108.11
20	A	850	CLA	CHD-C4C-C3C	-4.66	117.98	124.77
20	1	202	CLA	C4A-NA-C1A	4.66	108.81	106.68
20	A	806	CLA	CHD-C4C-NC	4.66	131.46	124.23
20	K	104	CLA	CMD-C2D-C3D	-4.66	117.00	127.69
20	A	805	CLA	CHD-C4C-NC	4.66	131.45	124.23
20	B	833	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
20	B	811	CLA	C2A-C1A-CHA	-4.66	114.69	122.63
20	A	849	CLA	C3B-C4B-NB	-4.65	106.38	110.53
20	A	810	CLA	CHD-C4C-NC	4.65	131.44	124.23
20	B	803	CLA	CHC-C1C-NC	4.65	131.31	124.31
20	A	803	CLA	C4B-CHC-C1C	-4.65	115.32	126.25
20	F	201	CLA	CHC-C4B-NB	4.65	131.02	124.05
20	1	205	CLA	CAB-C3B-C2B	-4.64	111.20	123.53
20	B	829	CLA	CHD-C4C-NC	4.64	131.43	124.23
20	B	802	CLA	C2B-C1B-NB	4.64	115.14	110.33
20	A	804	CLA	C4B-C3B-C2B	4.64	113.07	107.30
20	B	834	CLA	O2D-CGD-CBD	4.64	119.34	111.23
20	A	841	CLA	C1C-CHC-C4B	-4.64	113.81	126.04
20	3	305	CLA	CHC-C1C-NC	4.64	131.14	124.33
20	1	214	CLA	C4A-NA-C1A	4.64	108.79	106.68
20	4	318	CLA	C4B-CHC-C1C	-4.63	115.36	126.25
20	A	801	CLA	O2D-CGD-O1D	-4.63	114.84	123.85
20	B	827	CLA	CHD-C4C-C3C	-4.63	118.02	124.77
20	3	309	CLA	CHD-C4C-NC	4.63	131.27	124.24
22	F	203	BCR	C15-C14-C13	-4.63	120.79	127.28
20	4	306	CLA	C4B-CHC-C1C	-4.63	115.37	126.25
20	2	316	CLA	CAA-CBA-CGA	-4.63	100.07	113.21
20	2	308	CLA	C4A-NA-C1A	4.62	108.79	106.68
20	A	851	CLA	CMD-C2D-C3D	-4.62	117.09	127.69
20	J	103	CLA	CHC-C1C-NC	4.62	131.27	124.31
20	A	851	CLA	C2B-C1B-NB	4.62	115.11	110.33
20	1	214	CLA	CHD-C4C-NC	4.61	131.25	124.24
20	3	316	CLA	CHD-C4C-NC	4.61	131.25	124.24
20	A	812	CLA	O2D-CGD-CBD	4.61	119.30	111.23
20	2	308	CLA	CHC-C1C-NC	4.61	131.11	124.33
20	B	830	CLA	C4B-CHC-C1C	-4.61	115.40	126.25
20	A	830	CLA	CHD-C4C-NC	4.61	131.38	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	803	CLA	O2D-CGD-O1D	-4.61	114.88	123.85
20	A	831	CLA	C3B-C4B-NB	-4.61	106.42	110.53
20	4	302	CLA	CHD-C4C-C3C	-4.61	117.75	125.03
20	1	210	CLA	CHD-C4C-NC	4.61	131.38	124.23
20	1	204	CLA	O2D-CGD-CBD	4.61	119.28	111.23
20	1	202	CLA	C4B-CHC-C1C	-4.61	115.41	126.25
20	B	840	CLA	CHD-C4C-NC	4.61	131.37	124.23
20	B	807	CLA	CMD-C2D-C3D	-4.61	117.13	127.69
20	4	310	CLA	C4A-NA-C1A	4.60	108.78	106.68
20	A	827	CLA	CMD-C2D-C1D	4.60	132.82	124.73
20	B	809	CLA	CHD-C4C-NC	4.60	131.36	124.23
20	2	307	CLA	CHD-C4C-C3C	-4.59	118.07	124.77
20	B	833	CLA	CHD-C4C-NC	4.59	131.35	124.23
20	2	312	CLA	C2B-C1B-NB	4.59	115.09	110.33
20	2	314	CLA	CMD-C2D-C3D	-4.59	117.16	127.69
20	A	824	CLA	CHD-C4C-NC	4.59	131.35	124.23
20	B	803	CLA	CHD-C4C-NC	4.59	131.35	124.23
22	B	801	BCR	C8-C9-C10	4.59	126.23	119.01
20	A	821	CLA	C4A-NA-C1A	4.59	108.77	106.68
20	A	838	CLA	CHD-C4C-C3C	-4.59	118.08	124.77
20	3	315	CLA	C1C-CHC-C4B	-4.59	113.94	126.04
20	A	810	CLA	C2B-C1B-NB	4.59	115.08	110.33
20	F	207	CLA	C1-C2-C3	-4.59	118.68	126.20
20	4	306	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
20	A	811	CLA	CHC-C1C-NC	4.58	131.21	124.31
20	A	801	CLA	CHC-C1C-NC	4.58	131.21	124.31
20	B	836	CLA	CHC-C1C-NC	4.58	131.21	124.31
20	H	102	CLA	O2D-CGD-CBD	4.58	119.23	111.23
20	4	303	CLA	C2B-C1B-NB	4.58	115.07	110.33
20	1	213	CLA	C4-C3-C5	4.58	121.51	116.13
20	2	304	CLA	CHC-C1C-NC	4.58	131.06	124.33
20	3	310	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
20	B	815	CLA	O2D-CGD-CBD	4.57	119.22	111.23
20	A	823	CLA	C2B-C1B-NB	4.57	115.06	110.33
20	A	819	CLA	CMD-C2D-C3D	-4.57	117.22	127.69
20	F	206	CLA	O2D-CGD-CBD	4.57	119.21	111.23
20	B	825	CLA	CHD-C4C-NC	4.56	131.31	124.23
20	B	808	CLA	C4B-CHC-C1C	-4.56	115.52	126.25
20	A	818	CLA	CHC-C1C-NC	4.56	131.18	124.31
20	1	203	CLA	C4B-CHC-C1C	-4.56	115.52	126.25
20	4	303	CLA	C4B-CHC-C1C	-4.56	115.52	126.25
21	B	805	LMU	O5B-C5B-C4B	-4.56	101.48	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	102	CLA	CHD-C4C-NC	4.56	131.30	124.23
20	3	302	CLA	CHD-C4C-NC	4.56	131.17	124.24
20	3	304	CLA	C3A-C4A-CHB	-4.56	118.33	123.91
20	4	309	CLA	CHD-C4C-NC	4.56	131.17	124.24
20	1	201	CLA	CHD-C4C-NC	4.56	131.30	124.23
20	L	201	CLA	C2B-C1B-NB	4.56	115.05	110.33
20	A	811	CLA	CHD-C4C-NC	4.56	131.29	124.23
20	1	209	CLA	C2A-C1A-CHA	-4.56	114.86	122.63
20	A	830	CLA	O2D-CGD-CBD	4.55	119.19	111.23
20	4	308	CLA	C1B-NB-C4B	-4.55	103.12	106.31
20	2	304	CLA	C4A-NA-C1A	4.55	108.76	106.68
20	A	840	CLA	C2B-C1B-NB	4.55	115.05	110.33
20	B	826	CLA	O2D-CGD-CBD	4.55	119.19	111.23
20	B	809	CLA	C4A-NA-C1A	4.55	108.75	106.68
20	2	311	CLA	CHD-C4C-C3C	-4.55	118.14	124.77
20	A	849	CLA	CHC-C4B-NB	4.55	130.87	124.05
20	A	811	CLA	CMD-C2D-C3D	-4.55	117.26	127.69
20	B	810	CLA	O1D-CGD-CBD	-4.55	115.55	124.52
20	3	309	CLA	CHC-C1C-NC	4.55	131.01	124.33
20	A	822	CLA	C2B-C1B-NB	4.54	115.04	110.33
20	A	802	CLA	C1C-CHC-C4B	-4.54	114.06	126.04
22	B	801	BCR	C34-C9-C10	-4.54	115.46	122.82
20	A	805	CLA	C4A-NA-C1A	4.54	108.75	106.68
20	3	307	CLA	CAC-C3C-C4C	4.54	130.69	124.79
22	F	204	BCR	C8-C7-C6	-4.54	114.88	127.00
20	A	815	CLA	C2B-C1B-NB	4.53	115.03	110.33
20	A	841	CLA	CHC-C1C-NC	4.53	130.99	124.33
20	3	306	CLA	C4C-CHD-C1D	-4.53	113.07	125.98
20	A	836	CLA	CHD-C4C-NC	4.53	131.25	124.23
20	1	207	CLA	CHD-C4C-C3C	-4.52	118.18	124.77
20	B	840	CLA	C4B-CHC-C1C	-4.52	115.61	126.25
20	3	315	CLA	CHC-C1C-NC	4.52	130.98	124.33
20	B	832	CLA	C2B-C1B-NB	4.52	115.02	110.33
20	4	304	CLA	C4A-NA-C1A	4.52	108.74	106.68
20	3	312	CLA	CHD-C4C-NC	4.52	131.11	124.24
20	B	825	CLA	C2B-C1B-NB	4.52	115.01	110.33
20	4	306	CLA	C4A-NA-C1A	4.52	108.74	106.68
20	A	802	CLA	C2D-C3D-C4D	-4.52	101.86	107.35
20	1	206	CLA	CHD-C4C-NC	4.51	131.23	124.23
20	A	839	CLA	C2B-C1B-NB	4.51	115.00	110.33
20	3	307	CLA	CHD-C4C-NC	4.51	131.22	124.23
20	A	808	CLA	CHD-C4C-NC	4.51	131.22	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	841	CLA	C2A-C1A-CHA	-4.51	114.94	122.63
20	B	816	CLA	CHD-C4C-NC	4.51	131.22	124.23
20	A	815	CLA	O2D-CGD-CBD	4.51	119.11	111.23
20	A	825	CLA	CHD-C4C-C3C	-4.51	118.20	124.77
20	B	831	CLA	C2B-C1B-NB	4.50	115.00	110.33
22	L	209	BCR	C11-C10-C9	-4.50	120.97	127.28
20	2	307	CLA	CHC-C4B-NB	4.50	130.79	124.05
20	B	808	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
20	4	318	CLA	CHC-C1C-NC	4.49	131.08	124.31
20	A	820	CLA	CHD-C4C-NC	4.49	131.20	124.23
20	B	824	CLA	C4B-CHC-C1C	-4.49	115.68	126.25
20	4	312	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
20	B	824	CLA	C6-C5-C3	-4.49	102.53	113.47
20	A	819	CLA	CHD-C4C-NC	4.49	131.19	124.23
20	L	203	CLA	CHD-C4C-C3C	-4.49	118.23	124.77
20	1	204	CLA	CHC-C4B-NB	4.48	130.78	124.05
20	B	816	CLA	C2B-C1B-NB	4.48	114.98	110.33
22	A	844	BCR	C11-C10-C9	-4.48	120.99	127.28
20	3	310	CLA	C4B-CHC-C1C	-4.48	115.70	126.25
20	B	842	CLA	CHD-C4C-NC	4.48	131.18	124.23
20	2	304	CLA	C4C-CHD-C1D	-4.48	113.21	125.98
20	1	214	CLA	CHC-C1C-NC	4.48	130.92	124.33
22	B	847	BCR	C16-C17-C18	-4.48	120.99	127.28
20	B	817	CLA	CHD-C4C-NC	4.48	131.18	124.23
21	K	105	LMU	O1'-C1'-C2'	4.48	115.08	108.27
20	A	839	CLA	CHD-C4C-C3C	-4.48	118.25	124.77
20	A	834	CLA	CMD-C2D-C3D	-4.47	117.43	127.69
20	4	318	CLA	C2B-C1B-NB	4.47	114.96	110.33
20	A	803	CLA	CHD-C4C-C3C	-4.47	118.25	124.77
20	2	301	CLA	C2A-C1A-CHA	-4.47	115.01	122.63
20	A	826	CLA	C1-C2-C3	-4.47	118.88	126.20
20	B	806	CLA	CMD-C2D-C3D	-4.47	117.44	127.69
20	B	808	CLA	CAA-C2A-C3A	-4.47	100.93	113.00
20	1	211	CLA	C4B-CHC-C1C	-4.47	115.74	126.25
20	B	830	CLA	CHD-C4C-C3C	-4.47	118.26	124.77
20	A	834	CLA	C4B-CHC-C1C	-4.46	115.75	126.25
20	J	103	CLA	CHD-C4C-NC	4.46	131.15	124.23
20	A	821	CLA	C4B-CHC-C1C	-4.46	115.75	126.25
20	4	311	CLA	C4C-CHD-C1D	-4.46	113.26	125.98
20	A	818	CLA	C2B-C1B-NB	4.46	114.95	110.33
20	4	310	CLA	CMD-C2D-C3D	-4.46	117.46	127.69
20	2	315	CLA	C4C-CHD-C1D	-4.46	113.27	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	801	CLA	C4A-NA-C1A	4.46	108.71	106.68
20	A	827	CLA	C2B-C1B-NB	4.46	114.95	110.33
20	B	812	CLA	C1B-C2B-C3B	-4.45	102.84	107.03
20	3	302	CLA	C2A-C1A-CHA	-4.45	115.05	122.63
20	R	107	CLA	CHD-C4C-NC	4.45	131.12	124.23
20	F	207	CLA	C4D-C3D-CAD	4.45	112.93	108.11
20	B	832	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
20	K	103	CLA	CMD-C2D-C3D	-4.44	117.50	127.69
20	B	833	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
20	1	213	CLA	CMA-C3A-C4A	4.44	123.71	111.77
20	1	212	CLA	CHD-C4C-NC	4.44	130.99	124.24
20	2	310	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
20	A	828	CLA	C4A-NA-C1A	4.44	108.70	106.68
20	4	309	CLA	CHC-C1C-NC	4.44	130.85	124.33
20	3	311	CLA	C2B-C1B-NB	4.44	114.93	110.33
20	A	835	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
20	A	802	CLA	C4A-NA-C1A	4.43	108.70	106.68
20	3	307	CLA	C4D-C3D-CAD	4.43	112.92	108.11
20	4	311	CLA	CHC-C1C-NC	4.43	130.84	124.33
20	4	306	CLA	O2A-CGA-CBA	4.43	125.34	111.83
20	4	313	CLA	C2B-C1B-NB	4.43	114.92	110.33
20	F	201	CLA	CHC-C1C-NC	4.43	130.98	124.31
20	1	213	CLA	C4B-CHC-C1C	-4.43	115.84	126.25
20	4	315	CLA	C4A-NA-C1A	4.43	108.70	106.68
20	B	838	CLA	C4B-CHC-C1C	-4.43	115.84	126.25
20	A	849	CLA	C2B-C1B-NB	4.42	114.91	110.33
20	1	201	CLA	CMD-C2D-C3D	-4.42	117.55	127.69
20	4	315	CLA	C2B-C1B-NB	4.42	114.91	110.33
20	K	104	CLA	C2B-C1B-NB	4.42	114.91	110.33
20	J	103	CLA	C4D-C3D-CAD	4.42	112.90	108.11
20	4	304	CLA	C2B-C1B-NB	4.42	114.91	110.33
21	2	319	LMU	C1B-O1B-C4'	-4.42	107.51	117.98
20	2	315	CLA	CHC-C1C-NC	4.41	130.82	124.33
20	4	303	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
20	A	836	CLA	OBD-CAD-C3D	-4.41	118.10	128.42
20	2	302	CLA	CGD-CBD-CAD	4.41	125.13	110.85
20	H	102	CLA	CMD-C2D-C3D	-4.41	117.57	127.69
22	J	102	BCR	C11-C10-C9	-4.41	121.09	127.28
20	B	806	CLA	C4B-C3B-C2B	4.41	112.79	107.30
20	A	834	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
20	A	822	CLA	CHD-C4C-NC	4.41	131.07	124.23
20	1	203	CLA	CHC-C1C-NC	4.41	130.95	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	308	CLA	CHD-C4C-NC	4.41	130.94	124.24
20	3	313	CLA	CHD-C4C-NC	4.41	131.06	124.23
20	1	211	CLA	CMD-C2D-C3D	-4.41	117.58	127.69
21	R	101	LMU	C1'-C2'-C3'	-4.40	100.75	110.01
20	J	103	CLA	O2D-CGD-CBD	4.40	118.92	111.23
20	B	836	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
20	2	315	CLA	CHA-C4D-ND	4.40	131.06	124.84
20	B	821	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
20	3	302	CLA	C3A-C4A-CHB	-4.40	118.52	123.91
20	B	822	CLA	C2B-C1B-NB	4.40	114.89	110.33
20	B	840	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
20	B	815	CLA	CMD-C2D-C3D	-4.40	117.60	127.69
20	B	836	CLA	C1-C2-C3	-4.40	118.99	126.20
20	A	805	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
20	K	102	CLA	C4B-CHC-C1C	-4.40	115.91	126.25
20	B	835	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
20	1	202	CLA	CHC-C1C-NC	4.39	130.93	124.31
20	B	840	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
20	3	316	CLA	CHC-C1C-NC	4.39	130.79	124.33
20	A	828	CLA	CHD-C4C-C3C	-4.39	118.37	124.77
20	K	102	CLA	CHC-C1C-NC	4.39	130.92	124.31
20	K	104	CLA	O2D-CGD-O1D	-4.39	115.31	123.85
20	3	301	CLA	CHD-C4C-NC	4.39	131.03	124.23
20	A	818	CLA	C4B-CHC-C1C	-4.39	115.93	126.25
20	B	829	CLA	CMB-C2B-C1B	4.39	132.10	125.42
20	A	840	CLA	CHD-C4C-NC	4.39	131.03	124.23
20	1	207	CLA	CMD-C2D-C3D	-4.39	117.63	127.69
20	1	209	CLA	C3B-C2B-C1B	-4.38	101.93	106.81
20	A	830	CLA	C4B-CHC-C1C	-4.38	115.94	126.25
20	4	309	CLA	C3A-C4A-CHB	-4.38	118.55	123.91
20	A	817	CLA	CHD-C4C-NC	4.38	131.02	124.23
20	L	202	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
20	R	108	CLA	O2A-CGA-CBA	4.38	125.17	111.83
21	3	319	LMU	C1B-O1B-C4'	-4.37	107.61	117.98
20	R	108	CLA	CHD-C4C-NC	4.37	131.01	124.23
20	2	306	CLA	CHC-C4B-NB	4.37	130.40	124.08
20	A	820	CLA	CMD-C2D-C3D	-4.37	117.67	127.69
25	B	848	LMG	O7-C10-C11	4.37	120.93	111.48
22	F	203	BCR	C7-C8-C9	-4.37	119.77	126.23
20	2	308	CLA	C2A-C1A-CHA	-4.37	115.18	122.63
20	2	303	CLA	CHC-C1C-NC	4.37	130.89	124.31
20	3	311	CLA	CHD-C4C-C3C	-4.37	118.41	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	821	CLA	CHD-C4C-NC	4.37	131.00	124.23
20	A	834	CLA	CHD-C4C-NC	4.37	131.00	124.23
20	4	305	CLA	O2A-CGA-CBA	4.37	125.15	111.83
20	J	103	CLA	C4B-CHC-C1C	-4.36	115.99	126.25
20	1	202	CLA	C2B-C1B-NB	4.36	114.85	110.33
22	I	103	BCR	C27-C26-C25	-4.36	116.81	122.70
20	3	302	CLA	CHC-C1C-NC	4.36	130.74	124.33
20	A	826	CLA	O2D-CGD-CBD	4.36	118.85	111.23
22	J	102	BCR	C15-C14-C13	-4.36	121.16	127.28
20	K	104	CLA	CHC-C1C-NC	4.36	130.88	124.31
20	B	815	CLA	C4B-CHC-C1C	-4.36	116.00	126.25
20	3	309	CLA	C2A-C1A-CHA	-4.36	115.20	122.63
20	1	203	CLA	CHD-C4C-C3C	-4.36	118.42	124.77
20	B	818	CLA	CHD-C4C-NC	4.35	130.98	124.23
22	A	845	BCR	C15-C14-C13	-4.35	121.17	127.28
20	B	817	CLA	C4A-NA-C1A	4.35	108.66	106.68
20	B	814	CLA	O2D-CGD-CBD	4.35	118.83	111.23
20	B	837	CLA	CHD-C4C-NC	4.35	130.97	124.23
20	F	206	CLA	CHD-C4C-C3C	-4.35	118.44	124.77
20	3	305	CLA	C4A-NA-C1A	4.35	108.66	106.68
20	3	305	CLA	C4C-CHD-C1D	-4.35	113.60	125.98
20	A	835	CLA	CMD-C2D-C3D	-4.34	117.73	127.69
20	A	810	CLA	C4B-CHC-C1C	-4.34	116.03	126.25
20	A	815	CLA	CHD-C4C-NC	4.34	130.96	124.23
20	3	306	CLA	CHC-C1C-NC	4.34	130.71	124.33
20	2	304	CLA	C2A-C1A-CHA	-4.34	115.23	122.63
21	2	313	LMU	C1-O1'-C1'	-4.34	106.27	113.68
20	2	302	CLA	CHC-C1C-NC	4.34	130.85	124.31
20	A	806	CLA	C4B-CHC-C1C	-4.34	116.04	126.25
20	4	313	CLA	CHD-C4C-NC	4.34	130.96	124.23
20	3	304	CLA	C1B-NB-C4B	-4.34	103.27	106.31
22	B	846	BCR	C11-C10-C9	-4.34	121.19	127.28
20	1	204	CLA	C2B-C1B-NB	4.34	114.82	110.33
20	1	212	CLA	CHC-C1C-NC	4.34	130.71	124.33
20	1	211	CLA	O2A-CGA-O1A	-4.33	112.79	123.63
20	4	317	CLA	C2B-C1B-NB	4.33	114.82	110.33
20	A	810	CLA	CMD-C2D-C3D	-4.33	117.76	127.69
20	B	850	CLA	CHD-C4C-NC	4.33	130.94	124.23
20	B	807	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
20	3	307	CLA	O2D-CGD-CBD	4.33	118.80	111.23
20	2	309	CLA	C4C-CHD-C1D	-4.33	113.65	125.98
20	R	108	CLA	O2D-CGD-CBD	4.33	118.79	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	205	CLA	CMD-C2D-C3D	-4.32	117.77	127.69
20	A	807	CLA	CHD-C4C-NC	4.32	130.94	124.23
21	G	102	LMU	C1B-C2B-C3B	-4.32	100.92	110.01
20	2	306	CLA	CHC-C1C-NC	4.32	130.68	124.33
20	A	821	CLA	CHC-C1C-NC	4.32	130.82	124.31
20	B	819	CLA	CHC-C1C-NC	4.32	130.82	124.31
20	B	835	CLA	C4B-CHC-C1C	-4.32	116.09	126.25
20	4	317	CLA	CAA-C2A-C3A	-4.32	101.33	113.00
20	L	203	CLA	CHD-C4C-NC	4.32	130.92	124.23
20	A	841	CLA	C3B-C2B-C1B	-4.32	102.01	106.81
20	1	215	CLA	C2B-C1B-NB	4.31	114.80	110.33
20	1	214	CLA	C1B-NB-C4B	-4.31	103.28	106.31
20	B	839	CLA	C4B-CHC-C1C	-4.31	116.11	126.25
20	A	849	CLA	C4B-C3B-C2B	4.31	112.66	107.30
20	B	836	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
20	A	819	CLA	CHC-C1C-NC	4.31	130.80	124.31
20	A	809	CLA	CHC-C4B-NB	4.31	130.51	124.05
20	B	823	CLA	CHD-C4C-NC	4.31	130.91	124.23
20	4	317	CLA	CHD-C4C-C3C	-4.31	118.49	124.77
20	A	823	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
20	I	102	CLA	CHD-C4C-C3C	-4.31	118.49	124.77
20	3	307	CLA	C2A-C1A-CHA	-4.30	116.40	123.87
22	2	317	BCR	C11-C12-C13	-4.30	114.58	126.36
20	A	827	CLA	CHD-C4C-NC	4.30	130.90	124.23
22	I	103	BCR	C29-C30-C25	-4.30	104.19	110.44
20	B	836	CLA	C4B-CHC-C1C	-4.30	116.14	126.25
20	B	806	CLA	C3B-C4B-NB	-4.30	106.69	110.53
20	4	311	CLA	C2A-C1A-CHA	-4.30	115.31	122.63
20	4	301	CLA	CHD-C4C-C3C	-4.30	118.51	124.77
20	B	810	CLA	C4B-CHC-C1C	-4.30	116.15	126.25
20	4	307	CLA	C3A-C4A-CHB	-4.29	118.65	123.91
22	2	317	BCR	C33-C5-C6	-4.29	119.80	124.48
20	A	811	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
20	A	822	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
20	1	210	CLA	CMD-C2D-C3D	-4.29	117.86	127.69
20	3	303	CLA	C1B-C2B-C3B	-4.29	103.00	107.03
20	B	834	CLA	CMD-C2D-C3D	-4.28	117.86	127.69
20	B	836	CLA	O2D-CGD-O1D	-4.28	115.51	123.85
20	B	850	CLA	CHC-C1C-NC	4.28	130.76	124.31
20	2	305	CLA	CMD-C2D-C3D	-4.28	117.87	127.69
20	4	308	CLA	C4C-CHD-C1D	-4.28	113.78	125.98
20	H	109	CLA	C2B-C1B-NB	4.28	114.77	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	317	CLA	CMD-C2D-C3D	-4.28	117.87	127.69
20	A	816	CLA	C2B-C1B-NB	4.28	114.76	110.33
20	3	312	CLA	C2A-C1A-CHA	-4.28	115.34	122.63
20	B	809	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
20	B	840	CLA	CMD-C2D-C3D	-4.28	117.88	127.69
20	1	213	CLA	CHD-C4C-C3C	-4.28	118.54	124.77
20	A	840	CLA	C4A-NA-C1A	4.28	108.63	106.68
20	2	309	CLA	CHD-C4C-NC	4.28	130.74	124.24
20	B	841	CLA	O2A-CGA-CBA	4.27	124.87	111.83
20	H	110	CLA	C2B-C1B-NB	4.27	114.76	110.33
20	B	828	CLA	CMD-C2D-C3D	-4.27	117.89	127.69
20	B	814	CLA	C2B-C1B-NB	4.27	114.75	110.33
20	A	836	CLA	CHC-C1C-NC	4.27	130.74	124.31
20	R	108	CLA	C4B-CHC-C1C	-4.27	116.21	126.25
20	1	208	CLA	CHD-C4C-NC	4.27	130.73	124.24
20	H	101	CLA	CHD-C4C-NC	4.27	130.85	124.23
20	B	807	CLA	CHD-C4C-C3C	-4.27	118.55	124.77
20	A	814	CLA	C2D-C3D-C4D	-4.27	102.17	107.35
20	4	314	CLA	CHD-C4C-NC	4.26	130.72	124.24
20	A	815	CLA	CMD-C2D-C3D	-4.26	117.91	127.69
20	K	102	CLA	CMD-C2D-C3D	-4.26	117.92	127.69
20	B	810	CLA	CHC-C1C-NC	4.26	130.73	124.31
20	2	315	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
20	B	810	CLA	C2B-C1B-NB	4.26	114.74	110.33
20	A	829	CLA	CHC-C1C-NC	4.26	130.72	124.31
20	A	833	CLA	C4B-CHC-C1C	-4.25	116.25	126.25
20	B	816	CLA	CHD-C4C-C3C	-4.25	118.58	124.77
20	4	317	CLA	C1-C2-C3	-4.25	119.23	126.20
21	L	210	LMU	C3B-C4B-C5B	4.25	117.94	110.23
20	A	837	CLA	CAA-CBA-CGA	-4.25	101.14	113.21
20	B	830	CLA	CMD-C2D-C3D	-4.25	117.95	127.69
20	2	304	CLA	C1B-NB-C4B	-4.25	103.33	106.31
20	1	201	CLA	CHB-C4A-NA	4.25	130.53	124.40
22	I	103	BCR	C38-C26-C27	4.24	122.64	113.60
20	A	804	CLA	CMD-C2D-C3D	-4.24	117.96	127.69
20	1	203	CLA	CGD-CBD-CAD	-4.24	97.12	110.85
20	4	308	CLA	C2A-C1A-CHA	-4.24	115.40	122.63
20	A	827	CLA	C4B-CHC-C1C	-4.24	116.28	126.25
20	3	314	CLA	CHD-C4C-C3C	-4.24	118.59	124.77
20	4	301	CLA	CED-O2D-CGD	4.24	125.53	115.92
20	B	833	CLA	C2B-C1B-NB	4.24	114.72	110.33
20	4	314	CLA	C2A-C1A-CHA	-4.24	115.41	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	317	CLA	CHD-C4C-C3C	-4.24	118.34	125.03
20	4	302	CLA	C1B-C2B-C3B	-4.24	103.05	107.03
20	1	207	CLA	C2B-C1B-NB	4.24	114.72	110.33
20	1	204	CLA	C4A-NA-C1A	4.24	108.61	106.68
20	A	821	CLA	O1D-CGD-CBD	-4.24	116.16	124.52
20	B	812	CLA	C2B-C1B-NB	4.24	114.72	110.33
20	A	832	CLA	CHD-C4C-NC	4.24	130.80	124.23
20	B	841	CLA	C4B-C3B-C2B	4.23	112.57	107.30
20	4	304	CLA	CMD-C2D-C3D	-4.23	117.98	127.69
20	4	318	CLA	CMD-C2D-C3D	-4.23	117.98	127.69
20	3	301	CLA	C4B-CHC-C1C	-4.23	116.29	126.25
22	F	204	BCR	C34-C9-C8	4.23	124.55	118.09
20	K	101	CLA	CHD-C4C-C3C	-4.23	118.61	124.77
20	A	835	CLA	C4B-CHC-C1C	-4.23	116.30	126.25
20	4	313	CLA	CBD-CHA-C1A	4.23	133.76	127.38
20	4	307	CLA	C1B-NB-C4B	-4.23	103.35	106.31
20	B	803	CLA	O2D-CGD-CBD	4.23	118.62	111.23
20	A	802	CLA	CHC-C1C-NC	4.23	130.54	124.33
20	A	804	CLA	CHC-C1C-NC	4.22	130.67	124.31
22	G	104	BCR	C7-C8-C9	-4.22	119.99	126.23
20	2	311	CLA	C4B-CHC-C1C	-4.22	116.32	126.25
22	B	847	BCR	C11-C10-C9	-4.22	121.36	127.28
20	3	309	CLA	C2D-C3D-C4D	-4.22	102.22	107.35
20	3	308	CLA	C3B-C2B-C1B	-4.22	102.11	106.81
20	2	308	CLA	C3B-C2B-C1B	-4.22	102.12	106.81
20	B	826	CLA	CMD-C2D-C3D	-4.22	118.02	127.69
20	H	102	CLA	CHD-C4C-C3C	-4.21	118.63	124.77
20	A	801	CLA	C4B-CHC-C1C	-4.21	116.34	126.25
20	B	841	CLA	CHD-C4C-C3C	-4.21	118.63	124.77
20	2	306	CLA	CHD-C4C-NC	4.21	130.64	124.24
20	2	305	CLA	O2D-CGD-CBD	4.21	118.59	111.23
20	F	205	CLA	CHC-C1C-NC	4.21	130.65	124.31
20	A	837	CLA	CHD-C4C-C3C	-4.21	118.64	124.77
20	4	312	CLA	CHA-C4D-ND	4.21	130.79	124.84
20	A	851	CLA	C4B-CHC-C1C	-4.21	116.35	126.25
20	2	305	CLA	CHD-C4C-NC	4.21	130.76	124.23
20	R	107	CLA	C4B-CHC-C1C	-4.20	116.36	126.25
20	K	103	CLA	CHD-C4C-NC	4.20	130.75	124.23
20	3	316	CLA	C4A-NA-C1A	4.20	108.60	106.68
20	1	203	CLA	CAA-CBA-CGA	-4.20	101.28	113.21
20	3	301	CLA	CBD-CHA-C1A	4.20	133.72	127.38
20	L	208	CLA	C2B-C1B-NB	4.20	114.68	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	315	CLA	C2D-C3D-C4D	-4.20	102.25	107.35
20	B	821	CLA	CMD-C2D-C3D	-4.20	118.07	127.69
20	A	810	CLA	C3B-C4B-NB	-4.20	106.78	110.53
20	H	101	CLA	CHC-C1C-NC	4.19	130.63	124.31
20	B	813	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
20	B	833	CLA	C4B-CHC-C1C	-4.19	116.39	126.25
20	2	303	CLA	C2B-C1B-NB	4.19	114.67	110.33
20	B	821	CLA	C4B-CHC-C1C	-4.19	116.40	126.25
20	B	837	CLA	CMD-C2D-C3D	-4.19	118.09	127.69
20	A	834	CLA	CAA-C2A-C3A	-4.19	101.69	113.00
21	4	319	LMU	C3B-C4B-C5B	4.18	117.82	110.23
20	F	207	CLA	CBC-CAC-C3C	-4.18	101.08	112.42
20	B	838	CLA	CHC-C1C-NC	4.18	130.61	124.31
20	B	826	CLA	CHD-C4C-C3C	-4.18	118.68	124.77
20	B	813	CLA	CHC-C1C-NC	4.18	130.61	124.31
20	A	827	CLA	CHC-C1C-NC	4.18	130.61	124.31
22	A	844	BCR	C7-C8-C9	-4.18	120.05	126.23
20	3	315	CLA	CHD-C4C-NC	4.18	130.59	124.24
20	2	316	CLA	CMD-C2D-C3D	-4.18	118.11	127.69
20	4	309	CLA	C4A-NA-C1A	4.18	108.58	106.68
20	3	316	CLA	C4C-CHD-C1D	-4.17	114.09	125.98
20	B	839	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
22	F	204	BCR	C16-C17-C18	-4.17	121.43	127.28
20	A	812	CLA	C2B-C1B-NB	4.17	114.65	110.33
20	F	206	CLA	C2B-C1B-NB	4.17	114.65	110.33
20	K	104	CLA	CHD-C4C-NC	4.17	130.69	124.23
21	B	804	LMU	C1B-O5B-C5B	4.17	121.86	113.72
20	R	107	CLA	CHD-C4C-C3C	-4.17	118.70	124.77
20	B	819	CLA	C4B-CHC-C1C	-4.17	116.45	126.25
20	L	203	CLA	C4B-CHC-C1C	-4.17	116.45	126.25
20	A	813	CLA	CHD-C4C-C3C	-4.17	118.70	124.77
20	2	311	CLA	CHD-C4C-NC	4.16	130.68	124.23
20	B	802	CLA	CHD-C4C-C3C	-4.16	118.71	124.77
20	K	101	CLA	C4B-CHC-C1C	-4.16	116.47	126.25
20	A	830	CLA	CHC-C1C-NC	4.15	130.57	124.31
20	H	102	CLA	C4B-CHC-C1C	-4.15	116.48	126.25
20	A	821	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	B	818	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	I	102	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	L	202	CLA	CMD-C2D-C3D	-4.15	118.17	127.69
20	B	806	CLA	C4B-CHC-C1C	-4.15	116.49	126.25
21	4	319	LMU	O5B-C5B-C4B	4.15	117.18	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	839	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	B	830	CLA	CHC-C1C-NC	4.15	130.56	124.31
20	B	821	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	1	205	CLA	C1B-C2B-C3B	-4.15	103.13	107.03
20	1	211	CLA	CHC-C1C-NC	4.15	130.56	124.31
20	A	832	CLA	CMD-C2D-C3D	-4.15	118.18	127.69
20	A	817	CLA	C2B-C1B-NB	4.15	114.62	110.33
20	B	841	CLA	CMB-C2B-C1B	4.14	131.73	125.42
21	1	216	LMU	C1'-O5'-C5'	-4.14	105.63	113.72
20	1	215	CLA	C4A-NA-C1A	4.14	108.57	106.68
20	A	807	CLA	C4B-CHC-C1C	-4.14	116.51	126.25
20	3	317	CLA	C4B-CHC-C1C	-4.14	116.51	126.25
20	A	829	CLA	C4B-CHC-C1C	-4.14	116.52	126.25
20	B	815	CLA	CHD-C4C-NC	4.14	130.65	124.23
20	1	210	CLA	CHD-C4C-C3C	-4.14	118.50	125.03
20	B	818	CLA	C4B-CHC-C1C	-4.14	116.52	126.25
20	R	108	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
20	F	207	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
20	2	315	CLA	C1C-CHC-C4B	-4.13	115.14	126.04
20	A	832	CLA	C2B-C1B-NB	4.13	114.61	110.33
20	A	804	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
20	A	819	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
20	B	823	CLA	C4B-CHC-C1C	-4.13	116.53	126.25
20	4	312	CLA	C3D-C4D-CHA	-4.13	115.98	125.20
20	1	214	CLA	C3B-C2B-C1B	-4.13	102.22	106.81
20	B	850	CLA	C4A-NA-C1A	4.13	108.56	106.68
20	A	823	CLA	CMD-C2D-C3D	-4.12	118.23	127.69
20	2	316	CLA	O2D-CGD-CBD	4.12	118.44	111.23
20	4	301	CLA	C2B-C1B-NB	4.12	114.60	110.33
20	B	850	CLA	O2D-CGD-CBD	4.12	118.44	111.23
20	A	806	CLA	CMD-C2D-C3D	-4.12	118.24	127.69
22	I	103	BCR	C15-C16-C17	4.12	131.95	123.52
20	A	802	CLA	C3B-C2B-C1B	-4.12	102.22	106.81
20	A	823	CLA	CHD-C4C-NC	4.12	130.62	124.23
20	4	312	CLA	CHD-C4C-NC	4.12	130.50	124.24
21	F	202	LMU	C1B-O1B-C4'	-4.12	108.21	117.98
20	4	309	CLA	C4C-CHD-C1D	-4.12	114.25	125.98
20	J	101	CLA	CHD-C4C-C3C	-4.12	118.77	124.77
20	A	811	CLA	C4A-NA-C1A	4.12	108.56	106.68
20	1	211	CLA	CHC-C4B-NB	4.12	130.23	124.05
20	B	825	CLA	O2D-CGD-O1D	-4.12	115.83	123.85
20	A	820	CLA	C2B-C1B-NB	4.12	114.60	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	829	CLA	C3B-C2B-C1B	-4.12	102.32	107.17
21	H	104	LMU	C3'-C4'-C5'	-4.12	101.81	110.93
20	L	201	CLA	C4B-CHC-C1C	-4.12	116.57	126.25
20	B	813	CLA	CMD-C2D-C3D	-4.12	118.25	127.69
20	A	802	CLA	C1B-NB-C4B	-4.11	103.42	106.31
20	A	817	CLA	CHD-C4C-C3C	-4.11	118.77	124.77
20	A	805	CLA	CHC-C4B-NB	4.11	130.22	124.05
20	A	813	CLA	C4A-NA-C1A	4.11	108.56	106.68
20	A	808	CLA	C4B-CHC-C1C	-4.11	116.58	126.25
20	A	814	CLA	CHD-C4C-NC	4.11	130.49	124.24
20	H	101	CLA	C4B-CHC-C1C	-4.11	116.58	126.25
20	A	840	CLA	CHD-C4C-C3C	-4.11	118.78	124.77
20	1	212	CLA	C4A-NA-C1A	4.11	108.55	106.68
20	B	828	CLA	O2A-CGA-CBA	4.11	124.36	111.83
20	A	806	CLA	CHD-C4C-C3C	-4.11	118.79	124.77
20	B	842	CLA	CAA-C2A-C3A	-4.11	106.81	116.23
20	B	807	CLA	CHC-C1C-NC	4.11	130.50	124.31
20	A	810	CLA	CHC-C1C-NC	4.10	130.49	124.31
20	B	840	CLA	CHC-C1C-NC	4.10	130.49	124.31
20	3	307	CLA	CHC-C1C-C2C	-4.10	115.29	126.95
20	A	830	CLA	C2B-C1B-NB	4.10	114.58	110.33
22	F	204	BCR	C8-C9-C10	-4.10	112.56	119.01
20	B	818	CLA	CHC-C1C-NC	4.10	130.48	124.31
20	A	823	CLA	C4B-CHC-C1C	-4.10	116.61	126.25
20	4	310	CLA	CED-O2D-CGD	4.10	125.21	115.92
20	B	810	CLA	C1-C2-C3	-4.10	119.48	126.20
20	A	817	CLA	CMD-C2D-C3D	-4.10	118.30	127.69
20	B	831	CLA	C4B-CHC-C1C	-4.10	116.62	126.25
20	A	820	CLA	CHD-C4C-C3C	-4.09	118.80	124.77
20	1	202	CLA	CHD-C4C-NC	4.09	130.58	124.23
20	B	806	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
20	1	213	CLA	C2B-C1B-NB	4.09	114.57	110.33
20	3	314	CLA	CMD-C2D-C3D	-4.09	118.31	127.69
20	A	837	CLA	CMD-C2D-C3D	-4.09	118.31	127.69
20	R	107	CLA	CMD-C2D-C3D	-4.09	118.31	127.69
20	A	833	CLA	C2B-C1B-NB	4.09	114.56	110.33
21	1	217	LMU	O1B-C4'-C3'	4.09	117.62	107.23
20	A	814	CLA	CHC-C1C-NC	4.09	130.34	124.33
20	G	105	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
20	1	207	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
20	4	317	CLA	CMD-C2D-C3D	-4.09	118.32	127.69
22	B	801	BCR	C24-C23-C22	-4.09	120.19	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	312	CLA	C4C-CHD-C1D	-4.08	114.34	125.98
20	1	206	CLA	CAC-C3C-C4C	4.08	130.10	124.79
20	3	309	CLA	C1C-CHC-C4B	-4.08	115.27	126.04
20	4	310	CLA	O1D-CGD-CBD	-4.08	116.46	124.52
20	B	842	CLA	C4A-NA-C1A	4.08	108.54	106.68
20	L	202	CLA	C2B-C1B-NB	4.08	114.56	110.33
20	B	822	CLA	C4B-CHC-C1C	-4.08	116.65	126.25
20	3	312	CLA	C4A-NA-C1A	4.07	108.54	106.68
20	4	303	CLA	CMD-C2D-C3D	-4.07	118.34	127.69
20	3	309	CLA	C3B-C2B-C1B	-4.07	102.28	106.81
20	1	212	CLA	C4C-CHD-C1D	-4.07	114.37	125.98
20	A	841	CLA	CHC-C4B-NB	4.07	129.97	124.08
20	1	203	CLA	C2B-C1B-NB	4.07	114.55	110.33
20	A	834	CLA	C2B-C1B-NB	4.07	114.55	110.33
20	L	204	CLA	C4A-NA-C1A	4.07	108.54	106.68
20	A	821	CLA	CMD-C2D-C3D	-4.07	118.35	127.69
20	A	825	CLA	CHC-C1C-NC	4.07	130.44	124.31
20	B	813	CLA	CHD-C4C-NC	4.07	130.54	124.23
20	K	104	CLA	C4B-CHC-C1C	-4.07	116.68	126.25
20	B	822	CLA	CMD-C2D-C3D	-4.07	118.36	127.69
20	A	836	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
20	3	308	CLA	CHC-C1C-NC	4.07	130.31	124.33
20	3	302	CLA	C4C-CHD-C1D	-4.07	114.39	125.98
20	B	834	CLA	CHD-C4C-C3C	-4.07	118.85	124.77
20	B	817	CLA	CAC-C3C-C4C	4.06	130.08	124.79
20	4	312	CLA	CHC-C1C-NC	4.06	130.30	124.33
21	H	106	LMU	C1B-O5B-C5B	4.06	121.65	113.72
21	R	102	LMU	C3'-C4'-C5'	-4.06	101.93	110.93
20	A	833	CLA	CMD-C2D-C3D	-4.06	118.38	127.69
22	L	209	BCR	C15-C16-C17	-4.06	115.21	123.52
20	B	833	CLA	CMD-C2D-C3D	-4.06	118.38	127.69
21	C	101	LMU	O1'-C1'-C2'	4.06	114.44	108.27
20	B	828	CLA	CHD-C4C-C3C	-4.06	118.85	124.77
20	B	827	CLA	C4B-CHC-C1C	-4.06	116.70	126.25
20	B	817	CLA	CHD-C4C-C3C	-4.06	118.86	124.77
20	B	830	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
20	A	813	CLA	C4B-CHC-C1C	-4.06	116.71	126.25
20	A	841	CLA	C2D-C3D-C4D	-4.06	102.42	107.35
20	B	841	CLA	C4A-NA-C1A	4.06	108.53	106.68
20	L	207	CLA	C4B-CHC-C1C	-4.05	116.72	126.25
20	4	311	CLA	C1C-CHC-C4B	-4.05	115.35	126.04
20	1	209	CLA	C4C-CHD-C1D	-4.05	114.44	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	101	CLA	CHC-C1C-NC	4.05	130.41	124.31
20	A	824	CLA	C4B-CHC-C1C	-4.05	116.72	126.25
20	2	309	CLA	CHC-C4B-NB	4.05	129.93	124.08
20	A	822	CLA	CMD-C2D-C3D	-4.05	118.40	127.69
20	R	108	CLA	CMD-C2D-C3D	-4.05	118.40	127.69
20	B	842	CLA	CHD-C4C-C3C	-4.05	118.64	125.03
20	B	811	CLA	C1C-CHC-C4B	-4.05	115.36	126.04
20	A	818	CLA	CMD-C2D-C3D	-4.05	118.41	127.69
20	B	807	CLA	O2D-CGD-O1D	-4.05	115.97	123.85
20	A	828	CLA	C4B-CHC-C1C	-4.05	116.73	126.25
20	3	308	CLA	C1B-NB-C4B	-4.05	103.47	106.31
20	B	817	CLA	CHC-C1C-NC	4.05	130.41	124.31
20	A	841	CLA	CHD-C4C-NC	4.05	130.39	124.24
21	R	103	LMU	C1B-O5B-C5B	4.05	121.62	113.72
20	1	206	CLA	C4B-CHC-C1C	-4.04	116.74	126.25
20	2	301	CLA	C3B-C2B-C1B	-4.04	102.31	106.81
20	B	823	CLA	CHC-C1C-NC	4.04	130.40	124.31
20	A	832	CLA	CHC-C1C-NC	4.04	130.40	124.31
20	2	312	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
20	B	823	CLA	CMD-C2D-C3D	-4.04	118.43	127.69
20	A	825	CLA	C4B-CHC-C1C	-4.03	116.76	126.25
20	3	301	CLA	CHD-C4C-C3C	-4.03	118.66	125.03
20	3	311	CLA	CHC-C1C-NC	4.03	130.39	124.31
20	B	811	CLA	CHC-C4B-NB	4.03	129.91	124.08
20	A	850	CLA	C4B-CHC-C1C	-4.03	116.76	126.25
20	A	809	CLA	CMD-C2D-C3D	-4.03	118.44	127.69
20	A	812	CLA	CHD-C4C-C3C	-4.03	118.89	124.77
20	1	211	CLA	CGD-CBD-CAD	-4.03	97.79	110.85
20	2	307	CLA	O2A-CGA-CBA	4.03	124.13	111.83
20	A	836	CLA	C4B-CHC-C1C	-4.03	116.77	126.25
20	4	301	CLA	CHC-C1C-NC	4.03	130.38	124.31
20	B	820	CLA	C4B-CHC-C1C	-4.03	116.77	126.25
20	A	811	CLA	CAA-C2A-C3A	-4.03	102.12	113.00
20	1	201	CLA	C2B-C1B-NB	4.03	114.50	110.33
20	1	212	CLA	C2A-C1A-CHA	-4.02	115.77	122.63
20	B	811	CLA	C3A-C4A-CHB	-4.02	118.98	123.91
20	A	832	CLA	C4B-CHC-C1C	-4.02	116.78	126.25
20	A	811	CLA	CHC-C4B-NB	4.02	130.09	124.05
20	B	833	CLA	CHC-C1C-NC	4.02	130.37	124.31
20	B	834	CLA	C4B-CHC-C1C	-4.02	116.79	126.25
20	A	830	CLA	CMD-C2D-C3D	-4.02	118.47	127.69
20	3	311	CLA	C4B-CHC-C1C	-4.02	116.80	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	305	CLA	C4A-NA-C1A	4.02	108.51	106.68
21	4	320	LMU	C2'-C3'-C4'	4.02	118.80	109.68
20	4	308	CLA	CHC-C1C-NC	4.02	130.23	124.33
21	G	102	LMU	O1B-C1B-C2B	4.02	117.97	108.09
22	J	102	BCR	C7-C8-C9	-4.02	120.29	126.23
20	K	102	CLA	C2B-C1B-NB	4.02	114.49	110.33
22	B	801	BCR	C19-C18-C17	-4.01	112.69	119.01
20	B	815	CLA	C2B-C1B-NB	4.01	114.49	110.33
20	4	314	CLA	C4C-CHD-C1D	-4.01	114.55	125.98
20	B	824	CLA	C2A-C1A-CHA	-4.01	116.90	123.87
20	J	101	CLA	CMD-C2D-C3D	-4.01	118.49	127.69
20	4	309	CLA	C1C-CHC-C4B	-4.01	115.47	126.04
20	2	311	CLA	CHC-C4B-NB	4.01	130.06	124.05
20	A	807	CLA	CMD-C2D-C3D	-4.01	118.49	127.69
20	K	101	CLA	CMD-C2D-C3D	-4.01	118.50	127.69
20	1	205	CLA	CMD-C2D-C3D	-4.01	118.50	127.69
20	B	810	CLA	CHD-C4C-NC	4.01	130.44	124.23
20	L	203	CLA	C3B-C2B-C1B	-4.01	102.45	107.17
20	B	819	CLA	CMD-C2D-C3D	-4.01	118.50	127.69
20	J	101	CLA	C4B-CHC-C1C	-4.01	116.83	126.25
20	B	802	CLA	C4B-CHC-C1C	-4.00	116.83	126.25
20	B	803	CLA	CHD-C4C-C3C	-4.00	118.94	124.77
20	1	205	CLA	CHD-C4C-C3C	-4.00	118.71	125.03
20	B	835	CLA	CMD-C2D-C3D	-4.00	118.51	127.69
20	B	802	CLA	C4A-NA-C1A	4.00	108.50	106.68
20	2	310	CLA	C2B-C1B-NB	4.00	114.47	110.33
20	B	808	CLA	C2B-C1B-NB	4.00	114.47	110.33
20	2	306	CLA	C3A-C4A-CHB	-4.00	119.01	123.91
20	1	202	CLA	CMD-C2D-C3D	-4.00	118.52	127.69
20	L	203	CLA	C6-C5-C3	-4.00	103.73	113.47
20	4	312	CLA	C1C-CHC-C4B	-3.99	115.50	126.04
20	J	103	CLA	C2B-C1B-NB	3.99	114.47	110.33
22	G	104	BCR	C16-C17-C18	-3.99	121.68	127.28
20	B	825	CLA	C4B-CHC-C1C	-3.99	116.86	126.25
20	2	306	CLA	C2A-C1A-CHA	-3.99	115.83	122.63
20	3	301	CLA	CMD-C2D-C3D	-3.99	118.54	127.69
20	B	836	CLA	CMD-C2D-C3D	-3.99	118.54	127.69
20	1	205	CLA	C4B-CHC-C1C	-3.99	116.87	126.25
20	B	823	CLA	C2B-C1B-NB	3.99	114.46	110.33
20	A	802	CLA	CHC-C4B-NB	3.99	129.84	124.08
20	B	803	CLA	CMD-C2D-C3D	-3.99	118.54	127.69
20	1	202	CLA	CHD-C4C-C3C	-3.99	118.96	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	305	CLA	CHC-C1C-NC	3.99	130.32	124.31
20	A	805	CLA	C2B-C1B-NB	3.99	114.46	110.33
20	4	306	CLA	CMD-C2D-C3D	-3.99	118.55	127.69
20	4	302	CLA	C2B-C1B-NB	3.99	114.46	110.33
20	B	850	CLA	CMD-C2D-C1D	3.99	131.75	124.73
20	H	102	CLA	C4-C3-C5	3.99	122.15	115.23
20	A	841	CLA	C1B-NB-C4B	-3.98	103.52	106.31
20	H	102	CLA	C4A-NA-C1A	3.98	108.50	106.68
21	F	202	LMU	C2'-C3'-C4'	-3.98	100.64	109.68
20	3	306	CLA	C2A-C1A-CHA	-3.98	115.84	122.63
20	A	824	CLA	C2B-C1B-NB	3.98	114.46	110.33
20	4	307	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
20	1	214	CLA	C1C-CHC-C4B	-3.98	115.54	126.04
22	A	845	BCR	C33-C5-C6	-3.98	120.14	124.48
20	1	208	CLA	C4C-CHD-C1D	-3.98	114.63	125.98
20	B	831	CLA	C3B-C2B-C1B	-3.98	102.47	107.17
20	2	303	CLA	C4B-CHC-C1C	-3.98	116.89	126.25
20	B	829	CLA	C4B-CHC-C1C	-3.98	116.89	126.25
20	3	305	CLA	C1C-CHC-C4B	-3.98	115.55	126.04
20	A	815	CLA	CHC-C1C-NC	3.98	130.30	124.31
20	A	816	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
20	2	303	CLA	CMB-C2B-C1B	3.98	131.47	125.42
20	L	202	CLA	C4B-CHC-C1C	-3.97	116.90	126.25
22	A	845	BCR	C24-C23-C22	-3.97	120.36	126.23
20	A	833	CLA	C4A-NA-C1A	3.97	108.49	106.68
20	B	829	CLA	O2D-CGD-O1D	-3.97	116.11	123.85
20	4	301	CLA	C4B-CHC-C1C	-3.97	116.91	126.25
20	A	827	CLA	C3B-C2B-C1B	-3.97	102.49	107.17
20	H	109	CLA	C4B-CHC-C1C	-3.97	116.91	126.25
20	J	103	CLA	C4A-NA-C1A	3.97	108.49	106.68
20	B	834	CLA	C2B-C1B-NB	3.97	114.44	110.33
20	4	302	CLA	CMD-C2D-C3D	-3.97	118.59	127.69
20	F	205	CLA	C4B-CHC-C1C	-3.96	116.92	126.25
20	1	207	CLA	C4B-CHC-C1C	-3.96	116.92	126.25
20	4	315	CLA	C4B-CHC-C1C	-3.96	116.93	126.25
20	3	311	CLA	CMD-C2D-C3D	-3.96	118.60	127.69
22	B	845	BCR	C30-C25-C26	-3.96	117.22	122.64
20	B	809	CLA	C4B-CHC-C1C	-3.96	116.93	126.25
22	G	104	BCR	C33-C5-C6	-3.96	120.16	124.48
20	A	838	CLA	C4B-CHC-C1C	-3.96	116.93	126.25
20	K	101	CLA	C2B-C1B-NB	3.96	114.43	110.33
20	1	208	CLA	C2A-C1A-CHA	-3.96	115.88	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	838	CLA	CMD-C2D-C3D	-3.96	118.61	127.69
20	B	808	CLA	CHC-C1C-NC	3.96	130.27	124.31
20	A	803	CLA	CMA-C3A-C4A	-3.96	101.14	111.77
20	3	305	CLA	C2A-C1A-CHA	-3.96	115.89	122.63
20	A	850	CLA	CAA-C2A-C1A	3.96	124.94	111.97
20	B	809	CLA	CMD-C2D-C3D	-3.96	118.62	127.69
20	B	826	CLA	C4B-CHC-C1C	-3.96	116.94	126.25
20	2	305	CLA	C4B-CHC-C1C	-3.96	116.95	126.25
20	1	209	CLA	CHD-C4C-NC	3.95	130.25	124.24
20	4	312	CLA	C4C-CHD-C1D	-3.95	114.72	125.98
20	A	824	CLA	CMD-C2D-C3D	-3.95	118.63	127.69
20	A	834	CLA	CHC-C1C-NC	3.95	130.26	124.31
20	B	828	CLA	C3B-C2B-C1B	-3.95	102.52	107.17
20	2	314	CLA	CHC-C4B-NB	3.95	129.97	124.05
20	2	302	CLA	CMD-C2D-C3D	-3.95	118.64	127.69
20	L	201	CLA	CHD-C4C-C3C	-3.95	119.02	124.77
22	B	847	BCR	C24-C23-C22	-3.95	120.40	126.23
20	4	309	CLA	CHA-C4D-ND	3.95	130.41	124.84
20	4	307	CLA	C4A-NA-C1A	3.95	108.48	106.68
20	1	211	CLA	CBA-CAA-C2A	3.95	125.53	113.79
20	2	309	CLA	CHA-C4D-ND	3.94	130.41	124.84
20	3	312	CLA	CHC-C1C-NC	3.94	130.13	124.33
20	B	818	CLA	CMD-C2D-C3D	-3.94	118.65	127.69
20	A	806	CLA	CHC-C1C-NC	3.94	130.25	124.31
20	A	824	CLA	CHC-C1C-NC	3.94	130.25	124.31
20	L	207	CLA	CHC-C1C-NC	3.94	130.25	124.31
20	2	301	CLA	C4A-NA-C1A	3.94	108.48	106.68
20	A	831	CLA	CHC-C4B-NB	3.94	129.96	124.05
20	4	315	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
20	2	309	CLA	C1C-CHC-C4B	-3.94	115.65	126.04
20	3	306	CLA	C3B-C2B-C1B	-3.94	102.43	106.81
20	A	826	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
20	B	819	CLA	CGD-CBD-CAD	-3.94	98.10	110.85
20	1	214	CLA	C4C-CHD-C1D	-3.94	114.76	125.98
20	A	820	CLA	C4B-CHC-C1C	-3.94	116.99	126.25
20	4	312	CLA	C2D-C3D-C4D	-3.94	102.57	107.35
20	A	824	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
20	3	315	CLA	CHC-C4B-NB	3.93	129.77	124.08
20	1	203	CLA	C3B-C2B-C1B	-3.93	102.53	107.17
20	4	304	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
20	L	203	CLA	C4A-NA-C1A	3.93	108.47	106.68
20	F	206	CLA	CMD-C2D-C3D	-3.93	118.67	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	826	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
20	H	101	CLA	CHB-C4A-NA	3.93	130.07	124.40
20	A	818	CLA	C6-C5-C3	-3.93	103.90	113.47
20	A	814	CLA	C3A-C4A-CHB	-3.93	119.10	123.91
20	L	208	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
20	4	301	CLA	CMD-C2D-C3D	-3.93	118.69	127.69
20	3	306	CLA	C4A-NA-C1A	3.93	108.47	106.68
20	4	307	CLA	C3D-C4D-CHA	-3.92	116.44	125.20
20	A	808	CLA	CHD-C4C-C3C	-3.92	119.05	124.77
22	A	844	BCR	C33-C5-C6	-3.92	120.20	124.48
20	H	109	CLA	CHD-C4C-NC	3.92	130.31	124.23
20	B	815	CLA	CHC-C4B-NB	3.92	129.93	124.05
20	3	313	CLA	CHD-C4C-C3C	-3.92	119.06	124.77
20	3	301	CLA	C1B-C2B-C3B	-3.92	103.35	107.03
20	A	814	CLA	C1C-CHC-C4B	-3.92	115.71	126.04
20	3	317	CLA	C2B-C1B-NB	3.92	114.39	110.33
20	B	824	CLA	CAA-C2A-C1A	-3.92	99.15	111.97
20	1	204	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
20	F	201	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
21	2	321	LMU	O1B-C4'-C5'	3.91	119.74	109.48
20	B	834	CLA	CHC-C1C-NC	3.91	130.20	124.31
20	L	203	CLA	CMD-C2D-C3D	-3.91	118.72	127.69
20	A	821	CLA	CHC-C4B-NB	3.91	129.91	124.05
20	3	315	CLA	C4A-NA-C1A	3.91	108.46	106.68
20	4	317	CLA	CHB-C4A-NA	3.91	130.04	124.40
20	2	309	CLA	C2A-C1A-CHA	-3.91	115.97	122.63
20	A	807	CLA	CHD-C4C-C3C	-3.91	119.08	124.77
20	2	303	CLA	CMD-C2D-C3D	-3.91	118.73	127.69
20	1	205	CLA	CBD-CHA-C1A	3.91	133.28	127.38
20	A	814	CLA	C3D-C4D-CHA	-3.91	116.48	125.20
20	R	107	CLA	C2B-C1B-NB	3.91	114.38	110.33
20	B	835	CLA	CHC-C1C-NC	3.91	130.19	124.31
20	2	310	CLA	C4A-NA-C1A	3.91	108.46	106.68
20	1	208	CLA	CHC-C1C-NC	3.91	130.07	124.33
20	H	108	CLA	O2A-CGA-CBA	3.90	123.74	111.83
20	B	802	CLA	CHC-C1C-NC	3.90	130.19	124.31
20	3	307	CLA	CAC-C3C-C2C	-3.90	120.39	127.56
20	1	202	CLA	O2D-CGD-CBD	3.90	118.05	111.23
20	B	832	CLA	C4B-CHC-C1C	-3.90	117.08	126.25
20	B	803	CLA	C4B-CHC-C1C	-3.90	117.08	126.25
20	J	101	CLA	C2B-C1B-NB	3.90	114.37	110.33
20	4	318	CLA	O1D-CGD-CBD	-3.90	116.83	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	214	CLA	C2D-C3D-C4D	-3.90	102.61	107.35
20	4	306	CLA	C2A-C3A-C4A	-3.90	95.58	101.87
20	2	315	CLA	C3D-C4D-CHA	-3.89	116.50	125.20
20	2	303	CLA	CAA-C2A-C3A	-3.89	102.48	113.00
20	3	312	CLA	C3B-C2B-C1B	-3.89	102.48	106.81
22	A	843	BCR	C16-C17-C18	-3.89	121.82	127.28
20	B	817	CLA	C4B-CHC-C1C	-3.89	117.09	126.25
20	4	314	CLA	CHA-C4D-ND	3.89	130.34	124.84
20	3	302	CLA	C4A-NA-C1A	3.89	108.45	106.68
20	2	316	CLA	C2B-C1B-NB	3.89	114.36	110.33
20	3	312	CLA	C1B-NB-C4B	-3.89	103.58	106.31
20	L	208	CLA	O1D-CGD-CBD	-3.89	116.85	124.52
20	A	812	CLA	C4B-CHC-C1C	-3.89	117.10	126.25
20	1	205	CLA	C2B-C1B-NB	3.89	114.36	110.33
20	1	209	CLA	CHA-C4D-ND	3.89	130.33	124.84
20	B	815	CLA	CHC-C1C-NC	3.89	130.16	124.31
20	R	107	CLA	CHC-C1C-NC	3.89	130.16	124.31
20	A	829	CLA	CHD-C4C-NC	3.88	130.25	124.23
20	B	842	CLA	CBD-CHA-C1A	3.88	133.24	127.38
20	4	314	CLA	CHC-C1C-NC	3.88	130.04	124.33
20	G	105	CLA	CHC-C1C-NC	3.88	130.16	124.31
20	3	308	CLA	C4C-CHD-C1D	-3.88	114.92	125.98
20	3	302	CLA	C1C-CHC-C4B	-3.88	115.81	126.04
20	3	302	CLA	C1B-NB-C4B	-3.88	103.59	106.31
20	2	301	CLA	CHC-C4B-NB	3.88	129.69	124.08
20	A	851	CLA	CHC-C1C-NC	3.88	130.15	124.31
20	B	832	CLA	CMD-C2D-C3D	-3.88	118.80	127.69
21	L	205	LMU	C4B-C3B-C2B	3.87	117.63	110.83
20	B	850	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
20	B	813	CLA	C4A-NA-C1A	3.87	108.45	106.68
20	3	316	CLA	C1C-CHC-C4B	-3.87	115.83	126.04
20	H	101	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
20	A	836	CLA	C3B-C2B-C1B	-3.87	102.61	107.17
20	B	811	CLA	C2D-C3D-C4D	-3.87	102.65	107.35
20	1	209	CLA	C3D-C4D-CHA	-3.87	116.56	125.20
20	3	303	CLA	CMD-C2D-C3D	-3.87	118.82	127.69
20	A	817	CLA	CHC-C1C-NC	3.86	130.13	124.31
21	H	103	LMU	O1B-C4'-C3'	3.86	117.05	107.23
20	3	301	CLA	CHC-C4B-NB	3.86	129.84	124.05
20	1	208	CLA	C3B-C2B-C1B	-3.86	102.51	106.81
20	A	805	CLA	CMD-C2D-C3D	-3.86	118.83	127.69
20	L	207	CLA	CMD-C2D-C3D	-3.86	118.83	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	101	LMU	C1B-O1B-C4'	-3.86	108.82	117.98
20	A	807	CLA	C2B-C1B-NB	3.86	114.33	110.33
20	H	109	CLA	CHC-C1C-NC	3.86	130.13	124.31
22	B	846	BCR	C16-C17-C18	-3.86	121.86	127.28
22	B	846	BCR	C7-C8-C9	-3.86	120.53	126.23
20	B	838	CLA	C2B-C1B-NB	3.86	114.33	110.33
20	B	841	CLA	CHD-C4C-NC	3.86	130.21	124.23
20	F	205	CLA	CHD-C4C-C3C	-3.85	118.94	125.03
20	L	201	CLA	CHC-C1C-NC	3.85	130.12	124.31
20	A	830	CLA	CHD-C4C-C3C	-3.85	119.16	124.77
20	2	305	CLA	CHC-C1C-NC	3.85	130.11	124.31
20	A	812	CLA	CHC-C1C-NC	3.85	130.11	124.31
22	A	843	BCR	C7-C8-C9	-3.85	120.54	126.23
20	3	315	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
20	B	838	CLA	CHD-C4C-C3C	-3.85	119.16	124.77
20	3	317	CLA	C1B-C2B-C3B	-3.85	103.41	107.03
20	A	822	CLA	O2D-CGD-CBD	3.85	117.96	111.23
20	4	305	CLA	C4B-CHC-C1C	-3.85	117.20	126.25
22	I	103	BCR	C34-C9-C10	-3.85	116.58	122.82
20	F	207	CLA	C4B-CHC-C1C	-3.85	117.20	126.25
20	4	307	CLA	CHC-C1C-NC	3.85	129.98	124.33
20	K	101	CLA	CHC-C1C-NC	3.85	130.10	124.31
20	2	306	CLA	CHA-C4D-ND	3.84	130.27	124.84
20	A	805	CLA	O2D-CGD-CBD	3.84	117.95	111.23
20	B	814	CLA	C4B-CHC-C1C	-3.84	117.21	126.25
20	B	817	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
20	B	837	CLA	CHD-C4C-C3C	-3.84	119.17	124.77
20	B	808	CLA	CHC-C4B-NB	3.84	129.81	124.05
20	B	837	CLA	C4B-CHC-C1C	-3.84	117.22	126.25
20	B	829	CLA	CHC-C4B-NB	3.84	129.81	124.05
20	A	828	CLA	CHC-C1C-NC	3.84	130.09	124.31
20	1	215	CLA	C1-C2-C3	-3.84	119.91	126.20
20	B	803	CLA	CHB-C4A-NA	3.84	129.94	124.40
21	R	105	LMU	O5B-C1B-C2B	3.84	118.25	110.37
20	4	307	CLA	C1C-CHC-C4B	-3.83	115.93	126.04
20	2	301	CLA	C1C-CHC-C4B	-3.83	115.93	126.04
22	B	844	BCR	C38-C26-C27	3.83	121.77	113.60
20	A	840	CLA	CHC-C1C-NC	3.83	130.08	124.31
20	H	108	CLA	CHB-C4A-NA	3.83	129.93	124.40
21	K	105	LMU	C3B-C4B-C5B	-3.83	103.28	110.23
20	A	851	CLA	C3B-C2B-C1B	-3.83	102.66	107.17
20	4	309	CLA	C3D-C4D-CHA	-3.83	116.65	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	102	CLA	C2B-C1B-NB	3.83	114.30	110.33
20	3	315	CLA	C3D-C4D-CHA	-3.83	116.65	125.20
20	2	312	CLA	C4B-CHC-C1C	-3.83	117.24	126.25
20	B	809	CLA	C6-C5-C3	-3.83	104.15	113.47
20	A	822	CLA	CHC-C1C-NC	3.83	130.07	124.31
20	3	313	CLA	CMD-C2D-C3D	-3.82	118.92	127.69
20	A	834	CLA	CHC-C4B-NB	3.82	129.78	124.05
20	B	809	CLA	CHB-C4A-NA	3.82	129.91	124.40
20	4	308	CLA	C4A-NA-C1A	3.82	108.42	106.68
20	H	101	CLA	CMD-C2D-C3D	-3.82	118.93	127.69
22	A	843	BCR	C11-C10-C9	-3.82	121.92	127.28
21	1	218	LMU	O5'-C1'-C2'	3.82	118.22	110.37
20	2	312	CLA	C4-C3-C5	3.82	121.85	115.23
20	3	308	CLA	C1C-CHC-C4B	-3.82	115.97	126.04
20	A	823	CLA	CHD-C4C-C3C	-3.82	119.21	124.77
20	B	842	CLA	C4B-CHC-C1C	-3.82	117.27	126.25
21	4	321	LMU	C4B-C3B-C2B	3.82	117.53	110.83
20	B	830	CLA	CMB-C2B-C1B	3.82	131.23	125.42
20	A	809	CLA	CHC-C1C-C2C	-3.81	116.11	126.95
20	L	207	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
20	A	817	CLA	C4B-CHC-C1C	-3.81	117.29	126.25
20	1	210	CLA	C2B-C1B-NB	3.81	114.28	110.33
20	4	302	CLA	CAA-C2A-C3A	-3.81	107.50	116.23
20	H	108	CLA	CAA-C2A-C1A	3.81	124.45	111.97
20	F	201	CLA	CGD-CBD-CAD	-3.81	98.52	110.85
20	A	840	CLA	C4B-CHC-C1C	-3.81	117.30	126.25
20	B	803	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
20	1	204	CLA	CHD-C4C-C3C	-3.80	119.23	124.77
20	3	316	CLA	C3D-C4D-CHA	-3.80	116.70	125.20
20	1	212	CLA	C1C-CHC-C4B	-3.80	116.01	126.04
20	B	825	CLA	CHD-C4C-C3C	-3.80	119.23	124.77
20	L	201	CLA	CMD-C2D-C3D	-3.80	118.97	127.69
20	A	801	CLA	O2A-CGA-CBA	3.80	123.42	111.83
20	A	826	CLA	CMD-C2D-C3D	-3.80	118.97	127.69
22	G	104	BCR	C24-C23-C22	-3.80	120.62	126.23
20	A	803	CLA	C2B-C1B-NB	3.80	114.26	110.33
20	4	310	CLA	CBA-CAA-C2A	-3.80	102.50	113.79
20	4	303	CLA	CED-O2D-CGD	3.80	124.53	115.92
20	B	820	CLA	C2B-C1B-NB	3.79	114.26	110.33
20	B	814	CLA	CHC-C1C-NC	3.79	130.03	124.31
20	L	202	CLA	CHC-C1C-NC	3.79	130.02	124.31
20	B	833	CLA	CHC-C4B-NB	3.79	129.74	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	812	CLA	CMD-C2D-C3D	-3.79	119.00	127.69
20	F	207	CLA	CBA-CAA-C2A	-3.79	102.52	113.79
20	A	816	CLA	C1-C2-C3	-3.79	119.99	126.20
20	2	301	CLA	CHA-C4D-ND	3.79	130.19	124.84
20	A	825	CLA	C2B-C1B-NB	3.79	114.25	110.33
20	2	316	CLA	C3B-C2B-C1B	-3.78	102.71	107.17
20	1	214	CLA	C3D-C4D-CHA	-3.78	116.75	125.20
20	K	102	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
22	B	845	BCR	C16-C17-C18	-3.78	121.97	127.28
20	B	809	CLA	CMB-C2B-C1B	3.78	131.17	125.42
20	B	808	CLA	O2D-CGD-CBD	3.78	117.83	111.23
20	B	811	CLA	C3D-C4D-CHA	-3.78	116.76	125.20
22	A	845	BCR	C30-C25-C26	-3.78	117.47	122.64
20	2	301	CLA	CHD-C4C-NC	3.78	129.98	124.24
20	A	802	CLA	C3D-C4D-CHA	-3.78	116.77	125.20
20	4	313	CLA	CHD-C4C-C3C	-3.77	119.07	125.03
20	3	306	CLA	C1C-CHC-C4B	-3.77	116.09	126.04
21	A	854	LMU	C2'-C3'-C4'	3.77	118.25	109.68
20	A	815	CLA	C4B-CHC-C1C	-3.77	117.38	126.25
20	4	311	CLA	C4A-NA-C1A	3.77	108.40	106.68
20	B	827	CLA	CMD-C2D-C3D	-3.77	119.04	127.69
20	B	831	CLA	CMD-C2D-C3D	-3.77	119.04	127.69
20	B	831	CLA	CHC-C1C-NC	3.77	129.99	124.31
20	B	822	CLA	CHC-C1C-NC	3.77	129.99	124.31
21	B	804	LMU	C1'-O5'-C5'	3.77	121.08	113.72
20	L	204	CLA	C4B-CHC-C1C	-3.77	117.39	126.25
20	4	314	CLA	C1C-CHC-C4B	-3.77	116.11	126.04
20	H	102	CLA	CHC-C1C-NC	3.77	129.98	124.31
20	A	805	CLA	CHD-C4C-C3C	-3.77	119.28	124.77
20	A	851	CLA	CHD-C4C-C3C	-3.77	119.28	124.77
20	1	201	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
20	3	301	CLA	C4A-NA-C1A	3.77	108.40	106.68
21	1	218	LMU	C3B-C4B-C5B	3.77	117.06	110.23
20	4	307	CLA	CHA-C4D-ND	3.76	130.16	124.84
20	B	821	CLA	CHC-C1C-NC	3.76	129.98	124.31
22	B	844	BCR	C27-C26-C25	-3.76	117.62	122.70
21	R	101	LMU	C1B-O1B-C4'	-3.76	109.06	117.98
20	A	849	CLA	CMD-C2D-C3D	-3.76	119.06	127.69
22	2	317	BCR	C7-C8-C9	-3.76	120.67	126.23
20	1	207	CLA	CHC-C1C-NC	3.76	129.97	124.31
20	A	840	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
20	2	305	CLA	CHD-C4C-C3C	-3.76	119.29	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	212	CLA	C1B-NB-C4B	-3.76	103.68	106.31
20	B	827	CLA	C2B-C1B-NB	3.76	114.22	110.33
20	3	317	CLA	CHC-C1C-NC	3.76	129.97	124.31
21	L	205	LMU	C1'-O5'-C5'	3.76	121.05	113.72
20	A	811	CLA	O2D-CGD-CBD	3.75	117.79	111.23
20	A	850	CLA	CHC-C1C-NC	3.75	129.96	124.31
20	B	818	CLA	CHD-C4C-C3C	-3.75	119.31	124.77
20	1	207	CLA	CAA-CBA-CGA	3.75	123.85	113.21
21	H	103	LMU	C2'-C3'-C4'	-3.75	101.17	109.68
20	R	108	CLA	C1-C2-C3	3.75	132.34	126.20
20	B	817	CLA	C2B-C1B-NB	3.75	114.21	110.33
20	1	210	CLA	C4B-CHC-C1C	-3.75	117.44	126.25
22	I	103	BCR	C8-C7-C6	-3.75	116.99	127.00
20	B	806	CLA	CHC-C1C-NC	3.75	129.95	124.31
20	B	812	CLA	CHC-C1C-NC	3.75	129.95	124.31
21	4	316	LMU	C1B-O5B-C5B	3.75	121.03	113.72
20	1	205	CLA	CHC-C1C-NC	3.74	129.95	124.31
20	A	812	CLA	CMD-C2D-C3D	-3.74	119.10	127.69
20	3	304	CLA	C4C-CHD-C1D	-3.74	115.31	125.98
20	A	850	CLA	O2A-CGA-CBA	3.74	123.25	111.83
20	A	823	CLA	CHC-C1C-NC	3.74	129.95	124.31
20	3	316	CLA	CHA-C4D-ND	3.74	130.13	124.84
20	2	301	CLA	C2D-C3D-C4D	-3.74	102.81	107.35
20	3	316	CLA	C3B-C2B-C1B	-3.74	102.65	106.81
20	A	839	CLA	C3A-C2A-C1A	3.74	106.94	101.34
20	L	201	CLA	C4-C3-C5	3.74	121.72	115.23
20	A	814	CLA	CHB-C1B-NB	-3.74	118.68	124.08
22	B	845	BCR	C27-C26-C25	-3.73	117.66	122.70
20	3	304	CLA	CHC-C4B-NB	3.73	129.47	124.08
20	B	832	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
20	A	835	CLA	CHD-C4C-C3C	-3.73	119.33	124.77
20	2	305	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
20	A	834	CLA	CHD-C4C-C3C	-3.73	119.34	124.77
20	L	207	CLA	CHD-C4C-C3C	-3.73	119.34	124.77
20	H	101	CLA	O2D-CGD-CBD	3.73	117.75	111.23
20	H	108	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
20	H	110	CLA	C4B-CHC-C1C	-3.73	117.48	126.25
20	K	104	CLA	CAC-C3C-C4C	3.73	129.64	124.79
20	4	313	CLA	C4A-NA-C1A	3.73	108.38	106.68
20	B	810	CLA	C3B-C2B-C1B	-3.73	102.78	107.17
22	I	101	BCR	C16-C15-C14	-3.73	115.90	123.52
21	R	102	LMU	C1B-O5B-C5B	3.73	121.00	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	103	CLA	O2A-CGA-CBA	3.72	123.19	111.83
20	4	311	CLA	C3B-C2B-C1B	-3.72	102.67	106.81
20	A	850	CLA	C3B-C2B-C1B	-3.72	102.78	107.17
20	A	820	CLA	CHC-C1C-NC	3.72	129.91	124.31
20	A	816	CLA	C4B-CHC-C1C	-3.72	117.50	126.25
20	1	209	CLA	C2D-C3D-C4D	-3.71	102.84	107.35
20	B	819	CLA	C3B-C4B-NB	-3.71	107.21	110.53
20	A	817	CLA	O2A-CGA-CBA	3.71	123.15	111.83
20	1	210	CLA	CHC-C1C-NC	3.71	129.90	124.31
20	2	307	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
20	A	831	CLA	CBC-CAC-C3C	-3.71	102.36	112.42
20	2	310	CLA	CMD-C2D-C3D	-3.71	119.18	127.69
20	A	829	CLA	C2B-C1B-NB	3.71	114.17	110.33
20	B	826	CLA	C2B-C1B-NB	3.71	114.17	110.33
20	B	838	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
20	4	302	CLA	CHC-C1C-NC	3.71	129.89	124.31
20	J	103	CLA	CHD-C4C-C3C	-3.71	119.37	124.77
21	2	313	LMU	C1'-C2'-C3'	-3.70	102.22	110.01
22	L	209	BCR	C36-C18-C19	3.70	123.75	118.09
20	4	309	CLA	C1B-NB-C4B	-3.70	103.71	106.31
20	A	803	CLA	CMD-C2D-C3D	-3.70	119.20	127.69
20	1	208	CLA	C1B-NB-C4B	-3.70	103.72	106.31
20	2	309	CLA	CHC-C1C-NC	3.70	129.76	124.33
20	1	206	CLA	CHC-C1C-NC	3.70	129.88	124.31
20	A	810	CLA	C4B-C3B-C2B	3.69	111.90	107.30
20	F	207	CLA	CHC-C4B-NB	3.69	129.59	124.05
20	A	829	CLA	CMD-C2D-C3D	-3.69	119.22	127.69
20	L	201	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
20	A	806	CLA	CHC-C4B-NB	3.69	129.59	124.05
20	B	838	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
20	A	805	CLA	CMB-C2B-C1B	3.69	131.04	125.42
20	B	841	CLA	C2B-C1B-NB	3.69	114.15	110.33
20	B	807	CLA	C4B-CHC-C1C	-3.69	117.58	126.25
20	A	813	CLA	CMD-C2D-C3D	-3.69	119.24	127.69
20	A	836	CLA	CHD-C4C-C3C	-3.68	119.40	124.77
20	A	828	CLA	CMD-C2D-C3D	-3.68	119.24	127.69
20	A	840	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
20	2	315	CLA	C3A-C4A-CHB	-3.68	119.40	123.91
20	B	813	CLA	C2B-C1B-NB	3.68	114.14	110.33
20	J	103	CLA	CHB-C4A-NA	3.68	129.71	124.40
20	H	102	CLA	CHC-C4B-NB	3.68	129.57	124.05
20	1	211	CLA	C1-C2-C3	-3.68	120.17	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	314	CLA	CHC-C1C-C2C	-3.68	116.49	126.95
20	1	215	CLA	CMA-C3A-C4A	-3.68	101.89	111.77
20	A	840	CLA	C4-C3-C5	3.68	121.61	115.23
20	B	826	CLA	CHC-C1C-NC	3.68	129.85	124.31
20	A	816	CLA	CMD-C2D-C3D	-3.68	119.25	127.69
20	2	311	CLA	CHC-C1C-NC	3.68	129.85	124.31
20	B	838	CLA	C4-C3-C5	3.68	121.61	115.23
22	L	209	BCR	C30-C25-C26	-3.68	117.61	122.64
20	3	314	CLA	C3B-C2B-C1B	-3.67	102.84	107.17
20	F	207	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
20	B	832	CLA	CHC-C1C-NC	3.67	129.84	124.31
20	B	803	CLA	CGD-CBD-CAD	3.67	122.74	110.85
20	B	827	CLA	C4-C3-C5	3.67	121.60	115.23
20	3	305	CLA	C3B-C2B-C1B	-3.67	102.72	106.81
22	I	103	BCR	C38-C26-C25	-3.67	120.48	124.48
20	B	828	CLA	C4B-CHC-C1C	-3.67	117.62	126.25
20	B	827	CLA	CHC-C1C-NC	3.67	129.84	124.31
20	B	814	CLA	CMD-C2D-C3D	-3.67	119.28	127.69
20	K	103	CLA	CHB-C4A-NA	3.67	129.69	124.40
22	B	844	BCR	C38-C26-C25	-3.67	120.48	124.48
20	B	839	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
20	2	308	CLA	C1C-CHC-C4B	-3.67	116.37	126.04
20	B	816	CLA	C4B-CHC-C1C	-3.67	117.62	126.25
22	A	843	BCR	C33-C5-C6	-3.67	120.48	124.48
20	A	809	CLA	C2B-C1B-NB	3.66	114.13	110.33
20	4	310	CLA	CMB-C2B-C1B	3.66	131.00	125.42
20	A	819	CLA	C4B-CHC-C1C	-3.66	117.63	126.25
22	B	845	BCR	C34-C9-C10	-3.66	116.88	122.82
20	3	304	CLA	C3B-C2B-C1B	-3.66	102.74	106.81
20	B	850	CLA	CHC-C4B-NB	3.66	129.54	124.05
20	B	808	CLA	CMD-C2D-C3D	-3.66	119.30	127.69
20	A	804	CLA	CHC-C4B-NB	3.66	129.54	124.05
20	B	837	CLA	CHC-C1C-NC	3.66	129.82	124.31
20	B	824	CLA	CHC-C4B-NB	3.66	129.53	124.05
20	3	305	CLA	C1B-NB-C4B	-3.65	103.75	106.31
20	A	841	CLA	C3D-C4D-CHA	-3.65	117.04	125.20
20	1	201	CLA	CHD-C4C-C3C	-3.65	119.45	124.77
20	4	312	CLA	CHC-C4B-NB	3.65	129.36	124.08
20	B	823	CLA	O2D-CGD-CBD	3.65	117.61	111.23
20	4	312	CLA	C3B-C2B-C1B	-3.65	102.75	106.81
20	A	813	CLA	C3B-C2B-C1B	-3.65	102.86	107.17
20	1	201	CLA	CAC-C3C-C4C	3.65	129.54	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	301	CLA	C3D-C4D-CHA	-3.65	117.05	125.20
20	B	811	CLA	CHC-C1C-NC	3.65	129.70	124.33
20	4	315	CLA	CHC-C1C-NC	3.65	129.81	124.31
20	F	207	CLA	CED-O2D-CGD	3.65	124.19	115.92
20	A	803	CLA	CHB-C4A-NA	3.65	129.67	124.40
20	A	831	CLA	C5-C3-C2	-3.65	112.98	121.17
20	A	849	CLA	CED-O2D-CGD	3.65	124.19	115.92
21	H	105	LMU	C2'-C3'-C4'	3.65	117.96	109.68
20	R	108	CLA	CHC-C1C-NC	3.65	129.80	124.31
20	4	309	CLA	C3B-C2B-C1B	-3.64	102.75	106.81
20	B	841	CLA	CHC-C1C-NC	3.64	129.80	124.31
20	A	837	CLA	CHC-C4B-NB	3.64	129.51	124.05
20	L	203	CLA	CHC-C4B-NB	3.64	129.51	124.05
22	L	209	BCR	C24-C23-C22	-3.64	120.85	126.23
20	4	313	CLA	C4B-CHC-C1C	-3.64	117.69	126.25
20	A	802	CLA	CHD-C4C-NC	3.64	129.77	124.24
20	A	811	CLA	C3B-C4B-NB	-3.64	107.28	110.53
20	L	207	CLA	O2D-CGD-O1D	-3.63	116.77	123.85
20	B	825	CLA	C4A-NA-C1A	3.63	108.34	106.68
21	H	106	LMU	O5B-C5B-C4B	3.63	116.25	109.70
20	3	301	CLA	CHC-C1C-NC	3.63	129.78	124.31
20	1	211	CLA	CMB-C2B-C1B	3.63	130.95	125.42
20	3	307	CLA	CMD-C2D-C3D	-3.63	119.36	127.69
20	G	105	CLA	CMD-C2D-C3D	-3.63	119.37	127.69
20	4	307	CLA	CHD-C4C-NC	3.62	129.75	124.24
20	1	201	CLA	CHC-C1C-C2C	-3.62	116.65	126.95
20	A	801	CLA	CBA-CAA-C2A	3.62	124.57	113.79
20	B	820	CLA	CMD-C2D-C3D	-3.62	119.38	127.69
20	A	835	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
20	B	828	CLA	CHC-C1C-NC	3.62	129.76	124.31
20	A	808	CLA	CMD-C2D-C3D	-3.62	119.39	127.69
20	A	841	CLA	C4A-NA-C1A	3.62	108.33	106.68
21	L	206	LMU	C1B-O1B-C4'	-3.62	109.40	117.98
20	B	802	CLA	CMD-C2D-C3D	-3.62	119.40	127.69
20	3	313	CLA	C4B-CHC-C1C	-3.61	117.75	126.25
20	B	820	CLA	C1-C2-C3	-3.61	120.28	126.20
20	2	301	CLA	C4C-CHD-C1D	-3.61	115.69	125.98
20	4	302	CLA	C4B-CHC-C1C	-3.61	117.75	126.25
20	B	812	CLA	C4B-CHC-C1C	-3.61	117.75	126.25
20	B	811	CLA	CHD-C4C-NC	3.61	129.73	124.24
20	1	202	CLA	CED-O2D-CGD	3.61	124.10	115.92
20	B	810	CLA	CHC-C4B-NB	3.61	129.46	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	842	PQN	C14-C13-C15	3.61	121.49	115.23
20	A	822	CLA	CHD-C4C-C3C	-3.61	119.52	124.77
20	A	837	CLA	C4A-NA-C1A	3.60	108.32	106.68
20	A	807	CLA	C3B-C2B-C1B	-3.60	102.92	107.17
20	3	308	CLA	CHA-C4D-ND	3.60	129.93	124.84
20	B	810	CLA	CMD-C2D-C3D	-3.60	119.43	127.69
20	3	307	CLA	C2B-C1B-NB	3.60	114.06	110.33
20	2	301	CLA	CHC-C1C-NC	3.60	129.62	124.33
20	4	314	CLA	C3D-C4D-CHA	-3.60	117.16	125.20
20	I	102	CLA	CMD-C2D-C3D	-3.60	119.44	127.69
21	G	101	LMU	C1B-C2B-C3B	-3.60	102.44	110.01
20	4	306	CLA	O2D-CGD-CBD	3.60	117.52	111.23
20	1	208	CLA	C1C-CHC-C4B	-3.59	116.56	126.04
20	3	314	CLA	C2B-C1B-NB	3.59	114.05	110.33
20	3	309	CLA	C3D-C4D-ND	3.59	114.41	109.50
20	A	839	CLA	C3B-C2B-C1B	-3.59	102.94	107.17
20	B	841	CLA	CMD-C2D-C3D	-3.59	119.45	127.69
20	3	302	CLA	CHA-C4D-ND	3.59	129.91	124.84
20	A	810	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
20	4	307	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
20	A	822	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
20	1	212	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
20	B	825	CLA	O2A-CGA-CBA	3.58	122.75	111.83
20	L	203	CLA	C1-C2-C3	-3.58	120.33	126.20
20	B	842	CLA	C2B-C1B-NB	3.58	114.04	110.33
20	4	311	CLA	CHA-C4D-ND	3.58	129.90	124.84
20	2	312	CLA	CHC-C1C-NC	3.57	129.69	124.31
21	A	847	LMU	O5B-C1B-C2B	3.57	117.71	110.37
20	4	304	CLA	CHC-C1C-C2C	-3.57	116.80	126.95
20	4	313	CLA	CMD-C2D-C3D	-3.57	119.50	127.69
20	2	304	CLA	C1C-CHC-C4B	-3.57	116.63	126.04
21	C	101	LMU	C1B-C2B-C3B	3.57	117.52	110.01
20	2	308	CLA	C1B-NB-C4B	-3.57	103.81	106.31
20	I	102	CLA	C4B-CHC-C1C	-3.57	117.86	126.25
22	J	102	BCR	C24-C23-C22	-3.57	120.96	126.23
20	4	304	CLA	CHC-C4B-NB	3.57	129.40	124.05
20	A	840	CLA	C1-C2-C3	-3.56	120.36	126.20
20	B	835	CLA	C2B-C1B-NB	3.56	114.02	110.33
21	L	205	LMU	O5B-C5B-C4B	-3.56	103.28	109.70
20	2	307	CLA	C4A-NA-C1A	3.56	108.30	106.68
20	K	103	CLA	O2A-CGA-CBA	3.56	122.69	111.83
20	3	309	CLA	C4C-CHD-C1D	-3.56	115.84	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	312	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
20	I	102	CLA	CHC-C1C-NC	3.56	129.67	124.31
20	4	314	CLA	CHC-C4B-NB	3.56	129.22	124.08
20	L	204	CLA	CMD-C2D-C3D	-3.56	119.53	127.69
20	2	302	CLA	C3B-C2B-C1B	-3.56	102.98	107.17
20	3	306	CLA	CHC-C4B-NB	3.56	129.22	124.08
20	H	109	CLA	CMD-C2D-C3D	-3.55	119.54	127.69
20	1	215	CLA	C4B-CHC-C1C	-3.55	117.89	126.25
20	3	305	CLA	CHC-C4B-NB	3.55	129.21	124.08
20	2	307	CLA	CHC-C1C-C2C	-3.55	116.85	126.95
20	A	827	CLA	C1-O2A-CGA	3.55	125.25	116.65
20	B	831	CLA	CHD-C4C-NC	3.55	129.74	124.23
20	3	302	CLA	C3D-C4D-CHA	-3.55	117.27	125.20
20	L	203	CLA	CHC-C1C-NC	3.55	129.66	124.31
20	3	308	CLA	C3D-C4D-CHA	-3.55	117.28	125.20
20	1	206	CLA	C2B-C1B-NB	3.55	114.00	110.33
20	B	824	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
22	I	101	BCR	C38-C26-C25	-3.54	120.62	124.46
20	A	827	CLA	CHD-C4C-C3C	-3.54	119.61	124.77
22	A	845	BCR	C16-C17-C18	-3.54	122.31	127.28
20	A	807	CLA	CHC-C4B-NB	3.54	129.36	124.05
22	B	845	BCR	C8-C9-C10	3.54	124.58	119.01
20	A	839	CLA	O2A-CGA-CBA	3.54	122.63	111.83
20	A	801	CLA	CHD-C4C-NC	3.54	129.72	124.23
20	4	318	CLA	C4A-NA-C1A	3.54	108.29	106.68
20	2	302	CLA	C4B-CHC-C1C	-3.54	117.92	126.25
21	2	313	LMU	O5'-C5'-C4'	-3.54	102.41	109.72
20	B	810	CLA	O2A-CGA-CBA	3.54	122.61	111.83
20	B	842	CLA	CMD-C2D-C3D	-3.53	119.58	127.69
22	B	844	BCR	C3-C4-C5	-3.53	107.75	114.06
20	4	311	CLA	C1B-NB-C4B	-3.53	103.83	106.31
20	2	306	CLA	C4C-CHD-C1D	-3.53	115.91	125.98
20	4	311	CLA	C3D-C4D-CHA	-3.53	117.31	125.20
20	A	819	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
20	3	314	CLA	C4A-NA-C1A	3.53	108.29	106.68
20	A	818	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
20	F	207	CLA	CMD-C2D-C3D	-3.52	119.61	127.69
20	4	311	CLA	CHC-C4B-NB	3.52	129.17	124.08
20	A	826	CLA	O2A-CGA-CBA	3.52	122.57	111.83
20	3	303	CLA	CBD-CHA-C1A	3.52	132.69	127.38
20	3	313	CLA	CHC-C1C-NC	3.52	129.61	124.31
20	B	842	CLA	C1B-C2B-C3B	-3.52	103.72	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	201	CLA	C1-O2A-CGA	3.52	125.17	116.65
20	B	825	CLA	CHC-C1C-NC	3.52	129.61	124.31
20	4	314	CLA	C4A-NA-C1A	3.52	108.28	106.68
20	4	310	CLA	C2B-C1B-NB	3.52	113.97	110.33
20	A	838	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
20	A	839	CLA	CHC-C4B-NB	3.52	129.32	124.05
20	A	815	CLA	CHD-C4C-C3C	-3.52	119.65	124.77
20	B	837	CLA	C2B-C1B-NB	3.52	113.97	110.33
20	3	312	CLA	C1C-CHC-C4B	-3.52	116.77	126.04
20	L	207	CLA	CHB-C4A-NA	3.52	129.47	124.40
22	I	103	BCR	C15-C14-C13	3.52	132.21	127.28
22	F	203	BCR	C33-C5-C6	-3.51	120.65	124.48
20	4	317	CLA	CAA-CBA-CGA	-3.51	103.23	113.21
20	B	802	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
20	A	816	CLA	C4-C3-C5	3.51	121.32	115.23
20	B	829	CLA	O2A-CGA-CBA	3.51	122.54	111.83
21	A	853	LMU	O1'-C1'-C2'	3.51	113.61	108.27
20	B	825	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
20	A	808	CLA	CHC-C1C-NC	3.51	129.60	124.31
20	3	309	CLA	CHC-C4B-NB	3.51	129.15	124.08
20	1	215	CLA	CED-O2D-CGD	3.51	123.88	115.92
20	3	308	CLA	C2D-C3D-C4D	-3.51	103.09	107.35
20	A	830	CLA	CHC-C4B-NB	3.50	129.30	124.05
22	L	209	BCR	C27-C26-C25	-3.50	117.97	122.70
20	B	811	CLA	CHA-C4D-ND	3.50	129.79	124.84
20	1	208	CLA	C4A-NA-C1A	3.50	108.28	106.68
20	B	833	CLA	C4A-NA-C1A	3.50	108.28	106.68
20	1	206	CLA	CMD-C2D-C3D	-3.50	119.67	127.69
20	A	823	CLA	C4-C3-C5	3.50	121.30	115.23
20	1	208	CLA	C2D-C3D-C4D	-3.50	103.10	107.35
20	L	203	CLA	CMB-C2B-C1B	3.50	130.74	125.42
20	A	809	CLA	O2A-CGA-CBA	3.50	122.49	111.83
20	1	212	CLA	C2D-C3D-C4D	-3.50	103.10	107.35
21	A	847	LMU	C3B-C4B-C5B	-3.50	103.89	110.23
20	2	309	CLA	C3D-C4D-CHA	-3.49	117.40	125.20
20	3	316	CLA	C1B-NB-C4B	-3.49	103.86	106.31
20	3	316	CLA	C2D-C3D-C4D	-3.49	103.11	107.35
20	B	821	CLA	C4A-NA-C1A	3.49	108.27	106.68
20	H	108	CLA	CAA-C2A-C3A	-3.48	103.58	113.00
20	B	825	CLA	CMD-C2D-C3D	-3.48	119.70	127.69
20	A	821	CLA	CMB-C2B-C1B	3.48	130.72	125.42
20	B	824	CLA	C2B-C1B-NB	3.48	113.94	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	832	CLA	C4-C3-C5	3.48	121.27	115.23
20	B	829	CLA	CHC-C1C-NC	3.48	129.55	124.31
20	3	303	CLA	C4B-CHC-C1C	-3.48	118.07	126.25
20	H	110	CLA	CHC-C1C-NC	3.48	129.55	124.31
20	A	809	CLA	CHD-C4C-NC	3.48	129.62	124.23
20	B	830	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
20	A	821	CLA	CAA-C2A-C1A	3.47	119.83	112.14
20	4	304	CLA	CAC-C3C-C4C	3.47	129.31	124.79
20	A	816	CLA	C4A-NA-C1A	3.47	108.26	106.68
20	3	312	CLA	C2D-C3D-C4D	-3.47	103.13	107.35
20	A	832	CLA	CHD-C4C-C3C	-3.47	119.71	124.77
21	R	106	LMU	C1B-O5B-C5B	3.47	120.50	113.72
20	H	101	CLA	CMA-C3A-C2A	-3.47	100.57	113.98
20	3	301	CLA	C2B-C1B-NB	3.47	113.92	110.33
20	B	850	CLA	O2A-CGA-CBA	3.47	122.41	111.83
20	B	808	CLA	O2A-CGA-CBA	3.47	122.41	111.83
21	G	101	LMU	C1-O1'-C1'	-3.47	107.76	113.68
20	1	204	CLA	CED-O2D-CGD	3.47	123.78	115.92
20	H	110	CLA	CED-O2D-CGD	3.47	123.78	115.92
20	3	310	CLA	C4A-NA-C1A	3.47	108.26	106.68
20	A	821	CLA	CHD-C4C-C3C	-3.47	119.72	124.77
20	2	304	CLA	C2D-C3D-C4D	-3.46	103.14	107.35
20	I	102	CLA	O2A-CGA-CBA	3.46	122.39	111.83
20	A	815	CLA	O2A-CGA-CBA	3.46	122.39	111.83
21	B	804	LMU	O1B-C4'-C3'	3.46	116.03	107.23
20	1	210	CLA	C1B-C2B-C3B	-3.46	103.78	107.03
20	A	809	CLA	C3B-C2B-C1B	-3.46	103.09	107.17
20	2	316	CLA	CHC-C4B-NB	3.46	129.24	124.05
20	F	206	CLA	C4B-CHC-C1C	-3.46	118.11	126.25
20	1	215	CLA	CMD-C2D-C3D	-3.46	119.76	127.69
20	B	839	CLA	C1D-ND-C4D	-3.46	103.89	106.31
20	3	315	CLA	CHA-C4D-ND	3.46	129.73	124.84
20	A	831	CLA	CAC-C3C-C4C	3.46	129.29	124.79
20	B	824	CLA	CMD-C2D-C3D	-3.45	119.77	127.69
20	1	209	CLA	C1B-NB-C4B	-3.45	103.89	106.31
20	1	213	CLA	CBA-CAA-C2A	-3.45	103.52	113.79
20	1	215	CLA	CHB-C4A-NA	3.45	129.38	124.40
20	2	306	CLA	C1B-NB-C4B	-3.45	103.89	106.31
21	B	805	LMU	O1B-C1B-C2B	3.45	116.58	108.09
20	1	212	CLA	C3D-C4D-CHA	-3.45	117.49	125.20
20	B	811	CLA	C4A-NA-C1A	3.45	108.25	106.68
20	4	305	CLA	CAC-C3C-C4C	3.45	129.27	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	802	CLA	C3D-C4D-ND	3.45	114.21	109.50
21	H	104	LMU	O1B-C1B-C2B	3.45	116.57	108.09
20	A	816	CLA	CHC-C1C-NC	3.45	129.50	124.31
21	A	853	LMU	C2'-C3'-C4'	3.44	117.49	109.68
20	A	808	CLA	CAA-C2A-C1A	-3.44	100.70	111.97
20	A	818	CLA	CHC-C4B-NB	3.44	129.21	124.05
20	B	842	CLA	CHC-C1C-NC	3.44	129.49	124.31
20	F	206	CLA	C3B-C2B-C1B	-3.44	103.12	107.17
20	B	816	CLA	CHC-C1C-NC	3.44	129.49	124.31
20	A	838	CLA	O2A-CGA-CBA	3.44	122.32	111.83
20	G	105	CLA	C4B-CHC-C1C	-3.43	118.17	126.25
20	B	820	CLA	C3B-C2B-C1B	-3.43	103.12	107.17
20	B	821	CLA	C3B-C2B-C1B	-3.43	103.12	107.17
20	4	313	CLA	CHC-C1C-NC	3.43	129.48	124.31
21	H	103	LMU	O1B-C4'-C5'	3.43	118.47	109.48
20	R	107	CLA	CED-O2D-CGD	3.43	123.69	115.92
20	F	206	CLA	CMA-C3A-C2A	-3.43	108.37	116.23
20	H	108	CLA	C1-C2-C3	3.43	131.81	126.20
20	3	304	CLA	C3D-C4D-CHA	-3.43	117.55	125.20
20	B	813	CLA	CHD-C4C-C3C	-3.43	119.78	124.77
20	B	820	CLA	CHC-C4B-NB	3.42	129.19	124.05
20	A	818	CLA	C3B-C4B-NB	-3.42	107.47	110.53
20	R	108	CLA	CHC-C4B-NB	3.42	129.18	124.05
20	A	826	CLA	CHC-C1C-NC	3.42	129.47	124.31
20	4	309	CLA	C2D-C3D-C4D	-3.42	103.20	107.35
20	A	809	CLA	C4A-NA-C1A	3.42	108.24	106.68
20	B	820	CLA	C4A-NA-C1A	3.42	108.24	106.68
20	A	839	CLA	C1-O2A-CGA	3.42	124.92	116.65
20	3	309	CLA	CHB-C4A-NA	3.42	129.29	124.43
20	1	215	CLA	CHC-C1C-NC	3.42	129.46	124.31
20	A	839	CLA	CHC-C1C-C2C	-3.42	117.24	126.95
20	4	312	CLA	C4A-NA-C1A	3.41	108.24	106.68
20	1	208	CLA	C3D-C4D-CHA	-3.41	117.58	125.20
20	2	311	CLA	C2B-C1B-NB	3.41	113.86	110.33
20	1	203	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
20	H	102	CLA	C3B-C2B-C1B	-3.41	103.15	107.17
22	I	101	BCR	C38-C26-C27	3.41	120.87	113.60
20	A	839	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
22	F	203	BCR	C16-C17-C18	-3.41	122.50	127.28
20	4	318	CLA	CHB-C4A-NA	3.41	129.32	124.40
20	A	808	CLA	C3B-C4B-NB	-3.41	107.49	110.53
20	2	303	CLA	C3B-C2B-C1B	-3.41	103.15	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	838	CLA	CHC-C4B-NB	3.41	129.16	124.05
20	B	831	CLA	C1-O2A-CGA	3.41	124.89	116.65
20	A	816	CLA	CHC-C4B-NB	3.40	129.16	124.05
20	3	302	CLA	C3B-C2B-C1B	-3.40	103.02	106.81
20	1	213	CLA	CHC-C4B-NB	3.40	129.15	124.05
22	B	846	BCR	C24-C23-C22	-3.40	121.20	126.23
21	F	202	LMU	C1B-O5B-C5B	3.40	120.36	113.72
20	R	107	CLA	O2A-CGA-CBA	3.40	122.20	111.83
20	L	203	CLA	C2B-C1B-NB	3.40	113.85	110.33
20	3	312	CLA	C3D-C4D-CHA	-3.40	117.61	125.20
20	B	802	CLA	CHB-C4A-NA	3.40	129.30	124.40
20	1	206	CLA	C3B-C2B-C1B	-3.40	103.17	107.17
20	H	108	CLA	CMD-C2D-C3D	-3.40	119.90	127.69
20	2	301	CLA	C1B-NB-C4B	-3.39	103.93	106.31
20	3	314	CLA	C1-C2-C3	-3.39	120.64	126.20
20	B	809	CLA	C1-C2-C3	-3.39	120.64	126.20
20	A	807	CLA	CHC-C1C-NC	3.39	129.42	124.31
22	I	101	BCR	C37-C22-C21	-3.39	117.32	122.82
20	2	306	CLA	C3D-C4D-CHA	-3.39	117.62	125.20
21	G	101	LMU	C1'-C2'-C3'	-3.39	102.87	110.01
20	2	312	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
20	2	316	CLA	C4B-CHC-C1C	-3.39	118.27	126.25
20	3	308	CLA	CHC-C4B-NB	3.39	128.98	124.08
20	A	823	CLA	CHC-C4B-NB	3.39	129.13	124.05
20	2	307	CLA	CMD-C2D-C3D	-3.39	119.92	127.69
20	1	206	CLA	C4A-NA-C1A	3.39	108.22	106.68
20	1	206	CLA	CHC-C4B-NB	3.39	129.13	124.05
21	R	105	LMU	C2'-C3'-C4'	3.39	117.37	109.68
21	R	104	LMU	O1B-C4'-C3'	3.39	115.84	107.23
21	K	105	LMU	C1B-C2B-C3B	3.39	117.14	110.01
20	4	309	CLA	CHC-C4B-NB	3.38	128.97	124.08
22	B	847	BCR	C7-C8-C9	-3.38	121.23	126.23
20	A	851	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
22	2	317	BCR	C15-C14-C13	-3.38	122.53	127.28
20	J	103	CLA	CHC-C4B-NB	3.38	129.12	124.05
20	A	818	CLA	O2A-CGA-CBA	3.38	122.14	111.83
22	B	844	BCR	C16-C17-C18	-3.38	122.54	127.28
20	L	202	CLA	C1-C2-C3	-3.38	120.66	126.20
20	3	306	CLA	CHA-C4D-ND	3.38	129.61	124.84
20	1	210	CLA	CBD-CHA-C1A	3.38	132.47	127.38
21	K	107	LMU	C1B-O1B-C4'	-3.37	109.98	117.98
20	4	318	CLA	CHD-C4C-NC	3.37	129.46	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	814	CLA	C3D-C4D-ND	3.37	114.11	109.50
20	A	818	CLA	C4A-NA-C1A	3.37	108.22	106.68
20	F	207	CLA	CHC-C1C-NC	3.37	129.39	124.31
20	L	208	CLA	C4B-CHC-C1C	-3.37	118.32	126.25
20	4	308	CLA	C1C-CHC-C4B	-3.37	117.15	126.04
20	A	815	CLA	C3B-C2B-C1B	-3.37	103.20	107.17
20	A	801	CLA	C2B-C1B-NB	3.37	113.82	110.33
20	B	832	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
20	B	829	CLA	C1-C2-C3	-3.37	120.68	126.20
20	3	315	CLA	C4C-CHD-C1D	-3.37	116.39	125.98
21	B	805	LMU	C3B-C4B-C5B	-3.37	104.13	110.23
20	B	811	CLA	C3B-C2B-C1B	-3.36	103.07	106.81
20	4	310	CLA	O2A-CGA-CBA	3.36	122.08	111.83
20	K	101	CLA	CHC-C4B-NB	3.36	129.09	124.05
20	B	840	CLA	O2A-CGA-CBA	3.36	122.07	111.83
20	4	303	CLA	O2A-CGA-CBA	3.36	122.07	111.83
20	B	823	CLA	CHD-C4C-C3C	-3.36	119.88	124.77
22	I	103	BCR	C2-C1-C6	-3.36	105.56	110.44
20	B	825	CLA	CHC-C4B-NB	3.36	129.08	124.05
20	3	317	CLA	CBD-CHA-C1A	3.36	132.44	127.38
21	A	853	LMU	C1B-C2B-C3B	3.35	117.07	110.01
20	L	208	CLA	CMD-C2D-C3D	-3.35	120.00	127.69
20	B	815	CLA	CMB-C2B-C1B	3.35	130.53	125.42
20	A	833	CLA	CHD-C4C-C3C	-3.35	119.89	124.77
20	3	305	CLA	CHA-C4D-ND	3.35	129.58	124.84
20	B	818	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
20	4	305	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
21	A	846	LMU	C1B-O5B-C5B	3.35	120.26	113.72
20	B	821	CLA	CHC-C4B-NB	3.35	129.07	124.05
20	A	808	CLA	CHC-C4B-NB	3.35	129.07	124.05
20	3	314	CLA	C4-C3-C5	3.35	121.04	115.23
21	R	102	LMU	C1B-C2B-C3B	3.35	117.05	110.01
20	A	838	CLA	CMD-C2D-C3D	-3.35	120.01	127.69
20	3	304	CLA	C2D-C3D-C4D	-3.35	103.28	107.35
20	A	822	CLA	CHC-C4B-NB	3.35	129.07	124.05
20	3	312	CLA	CHA-C4D-ND	3.35	129.57	124.84
20	3	311	CLA	O2A-CGA-CBA	3.35	122.04	111.83
20	B	836	CLA	CAA-CBA-CGA	-3.35	103.71	113.21
20	A	814	CLA	C3B-C2B-C1B	-3.35	103.09	106.81
21	R	104	LMU	O1B-C1B-C2B	3.35	116.32	108.09
20	2	315	CLA	C1B-NB-C4B	-3.35	103.97	106.31
20	K	103	CLA	CMA-C3A-C4A	-3.34	102.79	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	850	CLA	CHB-C4A-NA	3.34	129.22	124.40
20	B	817	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
20	B	850	CLA	CAA-C2A-C3A	-3.34	103.97	113.00
21	4	319	LMU	C1'-C2'-C3'	3.34	117.04	110.01
20	A	812	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
20	B	824	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
20	F	201	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
20	B	841	CLA	O2D-CGD-CBD	3.34	117.07	111.23
20	A	824	CLA	CAC-C3C-C4C	3.34	129.13	124.79
20	3	317	CLA	CHC-C4B-NB	3.34	129.06	124.05
20	3	313	CLA	C3B-C2B-C1B	-3.34	103.24	107.17
21	K	105	LMU	O5B-C5B-C6B	3.33	114.70	106.44
20	4	313	CLA	CAA-C2A-C3A	-3.33	108.58	116.23
21	H	106	LMU	C1B-C2B-C3B	3.33	117.02	110.01
20	B	831	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
20	R	108	CLA	C4A-NA-C1A	3.33	108.20	106.68
22	B	846	BCR	C28-C27-C26	-3.33	108.11	114.06
22	B	801	BCR	C33-C5-C6	-3.33	120.85	124.48
20	G	105	CLA	C3B-C2B-C1B	-3.33	103.24	107.17
20	A	801	CLA	CHC-C1C-C2C	-3.33	117.48	126.95
20	3	307	CLA	CHC-C4B-NB	3.33	129.04	124.05
20	B	813	CLA	CHC-C4B-NB	3.33	129.04	124.05
20	B	831	CLA	CHC-C4B-NB	3.33	129.04	124.05
20	3	304	CLA	CHA-C4D-ND	3.33	129.54	124.84
20	B	822	CLA	CHB-C4A-NA	3.33	129.20	124.40
20	B	806	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
20	A	827	CLA	O1D-CGD-CBD	-3.32	117.96	124.52
20	A	827	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
20	A	810	CLA	CHC-C4B-NB	3.32	129.04	124.05
20	2	309	CLA	C3B-C2B-C1B	-3.32	103.11	106.81
20	L	204	CLA	CHC-C1C-NC	3.32	129.32	124.31
20	3	310	CLA	C2B-C1B-NB	3.32	113.77	110.33
20	A	831	CLA	CMD-C2D-C3D	-3.32	120.08	127.69
20	1	212	CLA	CHA-C4D-ND	3.32	129.53	124.84
20	4	313	CLA	CMB-C2B-C1B	3.32	130.47	125.42
20	A	829	CLA	O2A-CGA-CBA	3.32	121.95	111.83
20	B	822	CLA	C3B-C2B-C1B	-3.32	103.26	107.17
20	A	838	CLA	C4A-NA-C1A	3.31	108.19	106.68
20	A	840	CLA	C3B-C2B-C1B	-3.31	103.27	107.17
20	4	308	CLA	C2D-C3D-C4D	-3.31	103.33	107.35
22	A	844	BCR	C30-C25-C26	-3.31	118.11	122.64
22	F	203	BCR	C38-C26-C25	-3.31	120.88	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	829	CLA	CHB-C4A-NA	3.31	129.17	124.40
20	A	838	CLA	CAA-C2A-C3A	-3.31	104.07	113.00
20	1	203	CLA	C3D-C4D-ND	3.31	115.36	109.99
20	A	811	CLA	CHD-C4C-C3C	-3.30	119.95	124.77
20	2	308	CLA	CHA-C4D-ND	3.30	129.51	124.84
21	K	105	LMU	O5B-C5B-C4B	-3.30	103.75	109.70
20	4	308	CLA	C3D-C4D-CHA	-3.30	117.82	125.20
20	B	810	CLA	CHB-C4A-NA	3.30	129.17	124.40
21	H	106	LMU	O5B-C1B-C2B	3.30	117.15	110.37
20	2	310	CLA	CHC-C1C-C2C	-3.30	117.57	126.95
20	1	214	CLA	CHA-C4D-ND	3.30	129.50	124.84
20	1	212	CLA	CHC-C4B-NB	3.30	128.84	124.08
20	2	308	CLA	C3C-C4C-CHD	-3.30	116.67	125.23
20	B	837	CLA	CHC-C4B-NB	3.30	128.99	124.05
20	A	818	CLA	CMB-C2B-C1B	3.29	130.44	125.42
20	A	826	CLA	C4B-CHC-C1C	-3.29	118.50	126.25
20	3	301	CLA	CMB-C2B-C1B	3.29	130.43	125.42
20	1	208	CLA	CHA-C4D-ND	3.29	129.49	124.84
21	A	855	LMU	C3'-C4'-C5'	-3.29	103.64	110.93
20	1	203	CLA	C4A-NA-C1A	3.29	108.18	106.68
20	2	309	CLA	C2D-C3D-C4D	-3.29	103.35	107.35
20	4	318	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
20	A	810	CLA	C2A-C1A-CHA	-3.28	118.17	123.87
20	1	203	CLA	CAA-C2A-C1A	-3.28	101.22	111.97
20	2	311	CLA	CAA-C2A-C1A	3.28	122.73	111.97
20	A	812	CLA	CHC-C4B-NB	3.28	128.97	124.05
20	B	835	CLA	CHC-C4B-NB	3.28	128.97	124.05
20	I	102	CLA	C3B-C2B-C1B	-3.28	103.30	107.17
20	A	813	CLA	C1-C2-C3	-3.28	121.46	126.76
20	4	317	CLA	CHC-C4B-NB	3.28	128.97	124.05
20	A	830	CLA	C3B-C2B-C1B	-3.28	103.31	107.17
20	2	308	CLA	C3D-C4D-CHA	-3.28	117.88	125.20
20	A	836	CLA	CMD-C2D-C3D	-3.28	120.18	127.69
20	B	842	CLA	CMA-C3A-C2A	-3.28	108.72	116.23
20	R	108	CLA	C2B-C1B-NB	3.27	113.72	110.33
20	A	808	CLA	C4B-C3B-C2B	3.27	111.37	107.30
22	F	204	BCR	C3-C4-C5	-3.27	108.22	114.06
20	1	213	CLA	CMD-C2D-C3D	-3.27	120.18	127.69
20	A	839	CLA	CGD-CBD-CAD	-3.27	100.25	110.85
20	2	315	CLA	CHC-C4B-NB	3.27	128.81	124.08
21	A	847	LMU	O1'-C1'-C2'	3.27	113.24	108.27
20	A	832	CLA	C4A-NA-C1A	3.27	108.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	827	CLA	CMD-C2D-C3D	-3.27	120.19	127.69
20	A	832	CLA	CHB-C4A-NA	3.27	129.12	124.40
20	A	817	CLA	C3B-C2B-C1B	-3.27	103.32	107.17
22	A	843	BCR	C24-C23-C22	-3.27	121.40	126.23
20	A	825	CLA	CMD-C2D-C3D	-3.27	120.20	127.69
20	B	803	CLA	C1-O2A-CGA	3.27	124.56	116.65
20	A	805	CLA	CHC-C1C-C2C	-3.27	117.67	126.95
20	1	202	CLA	CHC-C4B-NB	3.27	128.95	124.05
20	B	826	CLA	C3B-C2B-C1B	-3.27	103.32	107.17
20	A	850	CLA	CMD-C2D-C3D	-3.26	120.20	127.69
20	K	103	CLA	CHD-C4C-C3C	-3.26	120.02	124.77
20	B	806	CLA	CED-O2D-CGD	3.26	123.31	115.92
20	A	803	CLA	CHC-C1C-C2C	-3.26	117.68	126.95
20	3	309	CLA	C3D-C4D-CHA	-3.26	117.92	125.20
20	4	313	CLA	CHC-C4B-NB	3.26	128.94	124.05
20	B	815	CLA	CHD-C4C-C3C	-3.26	120.02	124.77
20	2	308	CLA	CHC-C4B-NB	3.26	128.79	124.08
20	B	839	CLA	C4A-NA-C1A	3.26	108.17	106.68
20	2	311	CLA	O2A-CGA-CBA	3.26	121.76	111.83
21	2	320	LMU	C3B-C4B-C5B	-3.26	104.33	110.23
21	2	319	LMU	O1'-C1'-C2'	3.25	113.21	108.27
20	1	205	CLA	CHC-C4B-NB	3.25	128.92	124.05
20	B	819	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
20	A	811	CLA	C1-C2-C3	-3.25	120.88	126.20
20	3	303	CLA	CHC-C1C-NC	3.24	129.20	124.31
20	K	102	CLA	CHC-C4B-NB	3.24	128.91	124.05
20	B	823	CLA	CHC-C4B-NB	3.24	128.91	124.05
20	A	841	CLA	C4C-CHD-C1D	-3.24	116.75	125.98
20	A	835	CLA	C1-C2-C3	-3.24	120.89	126.20
20	A	827	CLA	CHC-C4B-NB	3.24	128.91	124.05
20	1	203	CLA	C1D-ND-C4D	-3.24	104.04	106.31
20	A	830	CLA	O2A-CGA-CBA	3.24	121.71	111.83
20	1	209	CLA	CHC-C4B-NB	3.24	128.76	124.08
20	A	814	CLA	CHA-C4D-ND	3.24	129.42	124.84
21	R	105	LMU	C1B-O5B-C5B	3.24	120.04	113.72
20	L	208	CLA	C3B-C2B-C1B	-3.24	103.35	107.17
20	B	812	CLA	C4A-NA-C1A	3.24	108.16	106.68
20	B	827	CLA	CHC-C4B-NB	3.24	128.90	124.05
22	B	801	BCR	C1-C6-C7	3.24	124.43	115.65
20	B	809	CLA	O2A-CGA-CBA	3.23	121.70	111.83
20	B	802	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
20	A	838	CLA	CHC-C1C-NC	3.23	129.18	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	843	PQN	C2M-C2-C3	-3.23	119.14	124.45
20	1	209	CLA	C1C-CHC-C4B	-3.23	117.52	126.04
20	1	206	CLA	O2A-CGA-CBA	3.23	121.69	111.83
20	2	304	CLA	C3B-C2B-C1B	-3.23	103.21	106.81
20	3	306	CLA	C3D-C4D-CHA	-3.23	117.98	125.20
20	J	101	CLA	C4A-NA-C1A	3.23	108.15	106.68
20	4	304	CLA	C3B-C2B-C1B	-3.23	103.36	107.17
20	3	311	CLA	C3B-C2B-C1B	-3.23	103.36	107.17
20	F	201	CLA	CMB-C2B-C1B	3.23	130.34	125.42
20	B	828	CLA	O1D-CGD-CBD	-3.23	118.15	124.52
20	A	851	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	B	814	CLA	C4A-NA-C1A	3.23	108.15	106.68
20	2	302	CLA	O2A-CGA-CBA	3.23	121.68	111.83
21	B	804	LMU	C2 <sup>1</sup> -C3 <sup>1</sup> -C4 <sup>1</sup>	-3.23	102.35	109.68
20	A	824	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
20	K	101	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
20	4	315	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	1	207	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	R	107	CLA	C4-C3-C5	3.22	120.83	115.23
20	2	310	CLA	CHC-C4B-NB	3.22	128.89	124.05
20	H	108	CLA	C6-C5-C3	-3.22	105.61	113.47
20	A	829	CLA	CHC-C4B-NB	3.22	128.88	124.05
20	B	841	CLA	C3B-C4B-NB	-3.22	107.65	110.53
20	3	309	CLA	C4D-ND-C1D	-3.22	104.05	106.31
20	B	806	CLA	C4-C3-C5	3.22	120.82	115.23
20	H	102	CLA	O2A-CGA-CBA	3.22	121.65	111.83
20	2	316	CLA	CHC-C1C-NC	3.22	129.16	124.31
20	2	304	CLA	C3D-C4D-CHA	-3.22	118.02	125.20
20	A	828	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
21	H	104	LMU	O2B-C2B-C1B	3.22	117.74	110.08
21	C	101	LMU	C4B-C3B-C2B	3.22	116.47	110.83
20	B	808	CLA	C4A-NA-C1A	3.22	108.15	106.68
20	2	307	CLA	C1-O2A-CGA	3.22	124.43	116.65
20	4	305	CLA	CMD-C2D-C3D	-3.21	120.32	127.69
20	K	104	CLA	CHD-C4C-C3C	-3.21	120.09	124.77
20	R	107	CLA	CHC-C4B-NB	3.21	128.87	124.05
20	2	306	CLA	C4A-NA-C1A	3.21	108.14	106.68
20	B	812	CLA	CMB-C2B-C1B	3.21	130.31	125.42
21	1	216	LMU	O1 <sup>1</sup> -C1 <sup>1</sup> -C2 <sup>1</sup>	3.21	113.15	108.27
20	1	213	CLA	CHC-C1C-C2C	-3.21	117.83	126.95
20	H	101	CLA	O2A-CGA-CBA	3.20	121.61	111.83
21	4	319	LMU	C2 <sup>1</sup> -C3 <sup>1</sup> -C4 <sup>1</sup>	3.20	116.95	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	103	CLA	CHC-C1C-C2C	-3.20	117.84	126.95
22	B	846	BCR	C15-C14-C13	-3.20	122.78	127.28
21	4	319	LMU	O2'-C2'-C3'	-3.20	102.83	110.38
20	2	310	CLA	C1-C2-C3	-3.20	121.58	126.76
20	A	831	CLA	O2A-CGA-CBA	3.20	121.59	111.83
20	A	813	CLA	CHB-C4A-NA	3.20	129.02	124.40
20	A	809	CLA	CAC-C3C-C4C	3.20	128.95	124.79
20	2	303	CLA	CHB-C4A-NA	3.20	129.01	124.40
20	B	840	CLA	CHC-C4B-NB	3.20	128.84	124.05
20	A	806	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
20	H	110	CLA	CMD-C2D-C3D	-3.19	120.37	127.69
20	4	311	CLA	C2D-C3D-C4D	-3.19	103.47	107.35
20	1	208	CLA	CHC-C4B-NB	3.19	128.69	124.08
20	A	816	CLA	O2A-CGA-CBA	3.18	121.55	111.83
20	L	207	CLA	C4A-NA-C1A	3.18	108.13	106.68
21	A	853	LMU	C1'-O5'-C5'	-3.18	107.50	113.72
20	4	303	CLA	CHC-C1C-C2C	-3.18	117.90	126.95
21	A	847	LMU	C1B-O5B-C5B	3.18	119.93	113.72
20	A	832	CLA	C3B-C2B-C1B	-3.18	103.42	107.17
20	3	311	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
20	A	825	CLA	C3B-C2B-C1B	-3.18	103.42	107.17
20	A	850	CLA	CHB-C4A-NA	3.18	128.99	124.40
20	4	318	CLA	CBA-CAA-C2A	-3.18	104.33	113.79
20	4	318	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
20	K	101	CLA	C3B-C2B-C1B	-3.18	103.42	107.17
20	3	308	CLA	CHB-C4A-NA	3.18	128.95	124.43
20	A	820	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
20	B	842	CLA	CHC-C4B-NB	3.18	128.82	124.05
20	B	837	CLA	C1-O2A-CGA	3.18	124.34	116.65
20	A	801	CLA	CED-O2D-CGD	3.18	123.12	115.92
20	4	301	CLA	C4A-NA-C1A	3.18	108.13	106.68
21	H	106	LMU	C1'-C2'-C3'	3.18	116.69	110.01
20	A	829	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
20	B	809	CLA	CHD-C4C-C3C	-3.17	120.15	124.77
20	L	201	CLA	O2A-CGA-CBA	3.17	121.51	111.83
20	1	215	CLA	C3B-C2B-C1B	-3.17	103.43	107.17
20	B	826	CLA	CHC-C4B-NB	3.17	128.81	124.05
20	B	825	CLA	CHB-C4A-NA	3.17	128.98	124.40
20	A	821	CLA	CHC-C1C-C2C	-3.17	117.95	126.95
20	K	104	CLA	C3B-C2B-C1B	-3.16	103.44	107.17
20	B	818	CLA	O2A-CGA-CBA	3.16	121.48	111.83
20	3	316	CLA	CHC-C4B-NB	3.16	128.65	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	824	CLA	C3B-C2B-C1B	-3.16	103.44	107.17
22	2	317	BCR	C23-C24-C25	-3.16	118.55	127.00
21	G	101	LMU	O5B-C5B-C4B	-3.16	104.00	109.70
20	2	311	CLA	CHB-C4A-NA	3.16	128.96	124.40
20	B	831	CLA	CED-O2D-CGD	3.16	123.08	115.92
20	A	818	CLA	C4B-C3B-C2B	3.16	111.23	107.30
20	B	818	CLA	C1-C2-C3	-3.16	121.02	126.20
21	4	321	LMU	C1B-O5B-C5B	-3.16	107.55	113.72
20	F	205	CLA	CAB-C3B-C2B	-3.16	115.15	123.53
20	A	815	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
20	3	302	CLA	CHC-C4B-NB	3.16	128.64	124.08
20	B	818	CLA	C4A-NA-C1A	3.16	108.12	106.68
20	B	820	CLA	O1D-CGD-CBD	-3.16	118.29	124.52
20	3	306	CLA	C1B-NB-C4B	-3.15	104.10	106.31
20	4	304	CLA	CHB-C4A-NA	3.15	128.95	124.40
20	B	811	CLA	C4C-CHD-C1D	-3.15	117.00	125.98
20	A	837	CLA	CAA-C2A-C1A	-3.15	101.64	111.97
20	2	306	CLA	C1C-NC-C4C	-3.15	105.24	106.68
20	B	827	CLA	C1-C2-C3	-3.15	121.03	126.20
20	A	832	CLA	C1-C2-C3	-3.15	121.67	126.76
20	B	829	CLA	CMD-C2D-C3D	-3.15	120.47	127.69
20	A	801	CLA	CHC-C4B-NB	3.15	128.77	124.05
20	1	214	CLA	CHC-C4B-NB	3.15	128.63	124.08
20	2	311	CLA	CMD-C2D-C3D	-3.15	120.47	127.69
20	3	310	CLA	CMD-C2D-C3D	-3.15	120.47	127.69
20	B	808	CLA	C6-C5-C3	-3.14	105.81	113.47
20	B	837	CLA	C3B-C2B-C1B	-3.14	103.47	107.17
21	B	805	LMU	O3'-C3'-C2'	-3.14	102.97	110.38
20	B	850	CLA	C4B-C3B-C2B	3.14	111.21	107.30
20	L	204	CLA	CHC-C4B-NB	3.14	128.76	124.05
20	B	802	CLA	C5-C3-C2	-3.14	114.12	121.17
20	1	203	CLA	CHC-C4B-NB	3.14	128.75	124.05
20	B	809	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
20	B	808	CLA	CGD-CBD-CAD	-3.14	100.69	110.85
20	A	827	CLA	CMB-C2B-C1B	3.14	130.19	125.42
20	4	307	CLA	CHB-C1B-NB	-3.14	119.55	124.08
21	A	846	LMU	C2'-C3'-C4'	3.14	116.80	109.68
20	A	841	CLA	C3D-C4D-ND	3.14	113.78	109.50
20	B	812	CLA	CHC-C4B-NB	3.14	128.75	124.05
20	J	103	CLA	CMD-C2D-C3D	-3.13	120.50	127.69
20	A	804	CLA	CMB-C2B-C1B	3.13	130.19	125.42
20	1	206	CLA	C4-C3-C5	3.13	120.67	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	101	LMU	O5B-C5B-C6B	3.13	114.20	106.44
20	4	315	CLA	O1D-CGD-CBD	-3.13	118.35	124.52
20	A	812	CLA	C4A-NA-C1A	3.13	108.11	106.68
20	1	201	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
22	A	845	BCR	C7-C8-C9	-3.13	121.61	126.23
20	L	204	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
20	4	317	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
20	F	206	CLA	CHC-C1C-NC	3.13	129.02	124.31
21	H	105	LMU	C3B-C4B-C5B	-3.12	104.57	110.23
20	F	205	CLA	C4B-C3B-C2B	3.12	109.97	107.03
20	B	834	CLA	CHC-C4B-NB	3.12	128.74	124.05
20	B	820	CLA	CHC-C1C-NC	3.12	129.01	124.31
22	B	801	BCR	C37-C22-C23	3.12	122.86	118.09
20	4	307	CLA	C4C-CHD-C1D	-3.12	117.08	125.98
20	3	312	CLA	CHC-C4B-NB	3.12	128.59	124.08
20	A	803	CLA	CHC-C4B-NB	3.12	128.73	124.05
20	H	109	CLA	CHD-C4C-C3C	-3.12	120.22	124.77
20	A	803	CLA	C3B-C2B-C1B	-3.12	103.49	107.17
22	A	843	BCR	C33-C5-C4	3.12	120.25	113.60
20	A	806	CLA	C4B-C3B-C2B	3.12	111.18	107.30
20	A	824	CLA	CHC-C4B-NB	3.12	128.73	124.05
20	B	824	CLA	CBA-CAA-C2A	3.12	123.07	113.79
20	1	202	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
20	B	823	CLA	C3B-C2B-C1B	-3.12	103.50	107.17
20	B	830	CLA	C2A-C1A-CHA	-3.12	118.46	123.87
20	1	209	CLA	CHC-C1C-NC	3.12	128.91	124.33
20	4	314	CLA	C2D-C3D-C4D	-3.12	103.56	107.35
20	3	307	CLA	C3D-C4D-ND	3.11	115.05	109.99
20	3	307	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
20	B	834	CLA	C3B-C2B-C1B	-3.11	103.50	107.17
20	3	310	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
21	2	320	LMU	O1B-C1B-C2B	3.11	115.75	108.09
22	I	101	BCR	C27-C26-C25	-3.11	118.51	122.68
20	A	829	CLA	C3B-C2B-C1B	-3.11	103.50	107.17
20	A	836	CLA	C4D-C3D-CAD	3.11	111.48	108.11
20	A	833	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
21	R	101	LMU	O1'-C1'-C2'	3.11	113.00	108.27
20	A	828	CLA	CHC-C4B-NB	3.11	128.71	124.05
20	A	832	CLA	CHC-C4B-NB	3.11	128.71	124.05
20	1	214	CLA	C3D-C4D-ND	3.11	113.74	109.50
20	4	301	CLA	C1-C2-C3	-3.10	121.11	126.20
20	2	306	CLA	C2C-C1C-CHC	-3.10	117.71	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	831	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
20	G	105	CLA	CHB-C4A-NA	3.10	128.88	124.40
20	B	810	CLA	CHD-C4C-C3C	-3.10	120.25	124.77
20	2	307	CLA	C4-C3-C5	3.10	120.61	115.23
20	4	304	CLA	C4-C3-C5	3.10	120.61	115.23
20	2	314	CLA	CMB-C2B-C1B	3.10	130.14	125.42
20	A	838	CLA	CHC-C4B-NB	3.10	128.70	124.05
20	3	315	CLA	C1B-NB-C4B	-3.10	104.14	106.31
22	B	801	BCR	C33-C5-C4	3.10	120.20	113.60
20	B	829	CLA	C2B-C1B-NB	3.10	113.54	110.33
20	4	304	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
20	A	832	CLA	CMB-C2B-C1B	3.10	130.13	125.42
20	4	308	CLA	CHA-C4D-ND	3.09	129.21	124.84
21	4	321	LMU	O2B-C2B-C3B	-3.09	103.08	110.38
20	F	205	CLA	CMB-C2B-C3B	3.09	131.75	123.53
20	L	208	CLA	CHC-C1C-NC	3.09	128.97	124.31
20	B	829	CLA	CHB-C1B-NB	-3.09	119.41	124.05
20	B	809	CLA	CHC-C4B-NB	3.09	128.69	124.05
22	A	844	BCR	C33-C5-C4	3.09	120.18	113.60
20	3	302	CLA	C2D-C3D-C4D	-3.09	103.60	107.35
20	1	201	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
20	A	801	CLA	C1B-C2B-C3B	-3.09	104.13	107.03
20	A	815	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
20	H	108	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
20	B	819	CLA	CMB-C2B-C1B	3.08	130.11	125.42
20	A	808	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
20	B	817	CLA	CHC-C4B-NB	3.08	128.67	124.05
20	J	101	CLA	CHC-C4B-NB	3.08	128.67	124.05
20	4	301	CLA	C3B-C2B-C1B	-3.08	103.54	107.17
20	4	303	CLA	C3B-C2B-C1B	-3.08	103.54	107.17
20	2	311	CLA	CGD-CBD-CAD	-3.08	100.87	110.85
20	H	101	CLA	C1-O2A-CGA	3.08	124.11	116.65
22	B	844	BCR	C11-C10-C9	-3.08	122.96	127.28
20	H	101	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
20	H	102	CLA	CMB-C2B-C1B	3.08	130.10	125.42
20	H	109	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
20	A	831	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
20	A	824	CLA	O2A-CGA-CBA	3.08	121.22	111.83
21	E	101	LMU	O4'-C4B-C5B	3.08	116.90	109.32
20	K	103	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
20	A	833	CLA	CHC-C4B-NB	3.07	128.66	124.05
20	A	849	CLA	CHC-C1C-NC	3.07	128.94	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	306	CLA	C2D-C3D-C4D	-3.07	103.62	107.35
21	2	313	LMU	O1B-C4'-C5'	3.07	117.53	109.48
20	B	813	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
20	L	207	CLA	CGD-CBD-CAD	-3.07	100.91	110.85
20	2	312	CLA	CHC-C4B-NB	3.07	128.65	124.05
20	L	204	CLA	C2B-C1B-NB	3.07	113.51	110.33
20	F	205	CLA	CHB-C4A-NA	3.07	128.83	124.40
20	A	841	CLA	CHA-C4D-ND	3.07	129.17	124.84
20	A	805	CLA	C4-C3-C5	3.06	120.55	115.23
20	3	310	CLA	C4-C3-C5	3.06	120.55	115.23
22	J	102	BCR	C38-C26-C25	-3.06	121.14	124.48
22	B	847	BCR	C11-C12-C13	-3.06	117.97	126.36
20	4	305	CLA	CMB-C2B-C1B	3.06	130.08	125.42
20	L	207	CLA	CHC-C4B-NB	3.06	128.64	124.05
20	B	822	CLA	O1D-CGD-CBD	-3.06	118.49	124.52
20	F	205	CLA	CBD-CHA-C1A	3.06	131.99	127.38
20	4	306	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
20	B	816	CLA	CHC-C4B-NB	3.06	128.63	124.05
20	A	840	CLA	CED-O2D-CGD	3.05	122.84	115.92
21	B	849	LMU	O1'-C1'-C2'	3.05	112.91	108.27
22	J	102	BCR	C16-C17-C18	-3.05	123.00	127.28
22	F	204	BCR	C33-C5-C6	-3.05	121.15	124.48
20	2	308	CLA	CHB-C4A-NA	3.05	128.77	124.43
20	3	317	CLA	C4A-NA-C1A	3.05	108.07	106.68
20	A	824	CLA	C4A-NA-C1A	3.05	108.07	106.68
20	A	825	CLA	CHC-C4B-NB	3.05	128.63	124.05
20	3	310	CLA	O1D-CGD-CBD	-3.05	118.50	124.52
20	L	202	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
20	B	819	CLA	C4B-C3B-C2B	3.05	111.09	107.30
20	B	816	CLA	CMD-C2D-C3D	-3.04	120.71	127.69
20	B	809	CLA	CHB-C1B-NB	-3.04	119.48	124.05
20	2	303	CLA	O2A-CGA-CBA	3.04	121.11	111.83
20	B	812	CLA	CBA-CAA-C2A	-3.04	104.74	113.79
20	L	204	CLA	O2A-CGA-CBA	3.04	121.11	111.83
20	2	312	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	3	304	CLA	C2C-C1C-CHC	-3.04	117.88	125.84
21	4	319	LMU	O1B-C4'-C5'	-3.04	101.50	109.48
20	2	302	CLA	CHB-C4A-NA	3.04	128.78	124.40
22	B	846	BCR	C38-C26-C25	-3.04	121.17	124.48
20	B	839	CLA	C3B-C4B-NB	-3.04	107.82	110.53
20	2	312	CLA	C4A-NA-C1A	3.04	108.06	106.68
20	A	805	CLA	CED-O2D-CGD	3.04	122.80	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	303	CLA	C1-C2-C3	-3.04	121.22	126.20
20	K	103	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
20	B	813	CLA	C4-C3-C2	-3.03	115.84	123.63
21	B	804	LMU	O5'-C1'-C2'	3.03	116.60	110.37
20	F	205	CLA	C4A-NA-C1A	3.03	108.06	106.68
20	3	316	CLA	CHB-C4A-NA	3.03	128.74	124.43
20	1	213	CLA	C4D-C3D-CAD	3.03	111.40	108.11
20	1	201	CLA	CBA-CAA-C2A	-3.03	104.78	113.79
20	A	808	CLA	C6-C5-C3	-3.03	106.09	113.47
21	R	103	LMU	O1'-C1'-C2'	3.03	112.87	108.27
20	3	313	CLA	O2A-CGA-CBA	3.03	121.07	111.83
20	B	830	CLA	CHC-C1C-C2C	-3.03	118.35	126.95
20	4	310	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
22	A	843	BCR	C23-C24-C25	-3.02	118.92	127.00
20	B	836	CLA	CHC-C4B-NB	3.02	128.58	124.05
22	A	845	BCR	C40-C30-C25	-3.02	105.50	110.24
20	A	825	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
20	K	103	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
20	B	803	CLA	C4A-NA-C1A	3.02	108.06	106.68
20	L	201	CLA	CHC-C4B-NB	3.02	128.58	124.05
20	3	315	CLA	C3D-C4D-ND	3.02	113.62	109.50
20	A	802	CLA	CHB-C4A-NA	3.02	128.72	124.43
20	2	312	CLA	CHB-C4A-NA	3.02	128.75	124.40
20	A	814	CLA	C4C-CHD-C1D	-3.02	117.39	125.98
20	2	312	CLA	CMD-C2D-C3D	-3.02	120.77	127.69
20	A	811	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
20	A	837	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
21	L	205	LMU	C1B-O5B-C5B	-3.01	107.83	113.72
20	A	817	CLA	C1-O2A-CGA	3.01	123.95	116.65
20	4	318	CLA	CHC-C4B-NB	3.01	128.57	124.05
20	K	102	CLA	O2A-CGA-CBA	3.01	121.02	111.83
20	2	303	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
20	4	310	CLA	C1D-ND-C4D	-3.01	104.20	106.31
21	B	804	LMU	O5B-C5B-C4B	3.01	115.12	109.70
21	A	847	LMU	C2'-C3'-C4'	3.01	116.51	109.68
20	A	820	CLA	CHC-C4B-NB	3.01	128.56	124.05
21	H	103	LMU	O5'-C1'-C2'	3.01	116.55	110.37
20	3	307	CLA	C4A-NA-C1A	3.01	108.05	106.68
20	4	304	CLA	O2A-CGA-CBA	3.01	121.00	111.83
20	F	201	CLA	C2B-C1B-NB	3.01	113.44	110.33
20	3	311	CLA	O2A-CGA-O1A	-3.01	116.11	123.63
20	A	835	CLA	O2A-CGA-CBA	3.01	121.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	848	LMG	O8-C28-C29	3.00	121.00	111.83
20	3	311	CLA	C4-C3-C5	3.00	120.44	115.23
22	F	204	BCR	C15-C16-C17	-3.00	117.37	123.52
20	L	201	CLA	C1-O2A-CGA	3.00	123.92	116.65
20	H	101	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
20	A	804	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
20	1	215	CLA	CMB-C2B-C1B	3.00	129.99	125.42
20	4	306	CLA	CHB-C4A-NA	3.00	128.73	124.40
20	2	310	CLA	O2A-CGA-CBA	3.00	120.99	111.83
20	A	851	CLA	CHB-C4A-NA	3.00	128.73	124.40
20	K	102	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
20	4	301	CLA	C4-C3-C5	3.00	120.43	115.23
20	B	850	CLA	CMD-C2D-C3D	-3.00	120.81	127.69
20	L	202	CLA	C3B-C2B-C1B	-3.00	103.64	107.17
21	K	107	LMU	C4B-C3B-C2B	-3.00	105.57	110.83
20	A	805	CLA	C1-O2A-CGA	3.00	123.90	116.65
20	2	303	CLA	CHC-C4B-NB	3.00	128.54	124.05
20	B	821	CLA	O2A-CGA-CBA	3.00	120.97	111.83
20	B	813	CLA	CAC-C3C-C4C	2.99	128.69	124.79
21	2	319	LMU	C2'-C3'-C4'	2.99	116.48	109.68
20	F	207	CLA	C2B-C1B-NB	2.99	113.43	110.33
20	B	841	CLA	CHB-C1B-NB	-2.99	119.56	124.05
20	A	829	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
20	4	314	CLA	C3B-C2B-C1B	-2.99	103.48	106.81
20	A	808	CLA	CHB-C4A-NA	2.99	128.71	124.40
20	B	815	CLA	C4B-C3B-C2B	2.99	111.02	107.30
20	1	213	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	A	828	CLA	C4-C3-C5	2.99	120.41	115.23
20	A	806	CLA	C1-C2-C3	-2.99	121.30	126.20
20	B	824	CLA	C3D-C4D-ND	2.99	114.84	109.99
20	1	204	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
22	B	845	BCR	C37-C22-C21	-2.99	117.98	122.82
20	B	822	CLA	C4A-NA-C1A	2.99	108.04	106.68
20	2	312	CLA	CBA-CAA-C2A	-2.98	104.91	113.79
20	2	316	CLA	CHB-C4A-NA	2.98	128.71	124.40
20	A	828	CLA	C1-C2-C3	-2.98	121.31	126.20
20	A	811	CLA	C11-C12-C13	-2.98	106.06	115.97
20	A	817	CLA	CHC-C4B-NB	2.98	128.52	124.05
20	4	315	CLA	CMD-C2D-C3D	-2.98	120.86	127.69
20	A	811	CLA	CHB-C4A-NA	2.98	128.70	124.40
20	A	833	CLA	CHB-C4A-NA	2.97	128.69	124.40
20	A	820	CLA	C3B-C2B-C1B	-2.97	103.66	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	824	CLA	CHC-C1C-NC	2.97	128.79	124.31
20	B	810	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
20	4	315	CLA	CGD-CBD-CAD	-2.97	101.23	110.85
20	H	110	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	A	818	CLA	C6-C7-C8	-2.97	106.09	115.97
20	L	208	CLA	C4D-CHA-C1A	2.97	124.78	121.24
20	L	202	CLA	CHC-C4B-NB	2.97	128.50	124.05
20	R	107	CLA	C4A-NA-C1A	2.97	108.03	106.68
20	B	827	CLA	C3B-C2B-C1B	-2.97	103.67	107.17
20	2	304	CLA	C3C-C4C-CHD	-2.97	117.53	125.23
20	F	201	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
20	A	822	CLA	C1-C2-C3	-2.97	121.96	126.76
22	I	103	BCR	C30-C25-C24	2.97	123.69	115.65
20	H	109	CLA	C3B-C2B-C1B	-2.97	103.67	107.17
20	K	102	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
20	F	206	CLA	CHC-C4B-NB	2.96	128.50	124.05
20	I	102	CLA	C4A-NA-C1A	2.96	108.03	106.68
20	J	103	CLA	C3B-C2B-C1B	-2.96	103.68	107.17
20	2	307	CLA	C2A-C1A-CHA	-2.96	118.73	123.87
21	2	319	LMU	C1'-C2'-C3'	2.96	116.24	110.01
20	A	802	CLA	CHA-C4D-ND	2.96	129.02	124.84
20	A	840	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	B	822	CLA	CHC-C4B-NB	2.96	128.49	124.05
20	A	804	CLA	O2A-CGA-O1A	-2.96	116.23	123.63
20	B	850	CLA	CBA-CAA-C2A	-2.96	104.99	113.79
20	B	833	CLA	O1D-CGD-CBD	-2.96	118.69	124.52
20	L	201	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	F	204	BCR	C2-C1-C6	2.96	114.73	110.44
20	A	816	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	4	308	CLA	CHC-C4B-NB	2.96	128.35	124.08
20	A	849	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	K	102	CLA	C4A-NA-C1A	2.95	108.03	106.68
20	B	830	CLA	CMA-C3A-C2A	-2.95	102.56	113.98
21	R	102	LMU	C1-O1'-C1'	-2.95	108.64	113.68
20	B	823	CLA	C4-C3-C5	2.95	120.35	115.23
20	F	207	CLA	C4A-NA-C1A	2.95	108.03	106.68
20	A	831	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	R	107	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
20	A	801	CLA	CAC-C3C-C4C	2.95	128.63	124.79
20	B	831	CLA	CHD-C4C-C3C	-2.95	120.47	124.77
20	A	838	CLA	CHB-C4A-NA	2.95	128.66	124.40
20	B	832	CLA	CHC-C4B-NB	2.95	128.47	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	211	CLA	CAA-C2A-C1A	-2.95	102.32	111.97
20	B	807	CLA	C4A-NA-C1A	2.95	108.02	106.68
20	J	101	CLA	C3B-C2B-C1B	-2.95	103.70	107.17
20	A	816	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
20	A	830	CLA	CHC-C1C-C2C	-2.95	118.58	126.95
21	E	101	LMU	C3B-C4B-C5B	-2.94	104.89	110.23
20	F	207	CLA	CHB-C4A-NA	2.94	128.65	124.40
20	1	207	CLA	O2A-CGA-CBA	2.94	120.81	111.83
21	A	854	LMU	O1'-C1'-C2'	2.94	112.74	108.27
20	A	829	CLA	CHD-C4C-C3C	-2.94	120.48	124.77
20	K	103	CLA	CHC-C4B-NB	2.94	128.46	124.05
20	2	309	CLA	C1B-NB-C4B	-2.94	104.25	106.31
21	R	105	LMU	C1'-C2'-C3'	2.94	116.19	110.01
20	4	317	CLA	C3B-C2B-C1B	-2.94	103.71	107.17
20	A	809	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	2	311	CLA	C3B-C2B-C1B	-2.94	103.71	107.17
21	K	106	LMU	O1B-C1B-C2B	2.94	115.31	108.09
20	A	851	CLA	CMB-C2B-C1B	2.93	129.89	125.42
20	3	311	CLA	C4A-NA-C1A	2.93	108.02	106.68
20	A	810	CLA	CMA-C3A-C2A	-2.93	102.64	113.98
20	K	103	CLA	C3B-C2B-C1B	-2.93	103.71	107.17
22	I	101	BCR	C10-C11-C12	-2.93	114.70	123.20
20	2	314	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
20	B	807	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	A	836	CLA	O2A-CGA-CBA	2.93	120.76	111.83
21	R	105	LMU	O5'-C5'-C6'	2.93	113.69	106.44
20	A	818	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
20	B	806	CLA	CHC-C4B-NB	2.93	128.44	124.05
21	4	319	LMU	O1B-C4'-C3'	-2.92	99.80	107.23
22	2	317	BCR	C35-C13-C12	2.92	122.56	118.09
20	4	307	CLA	CHC-C4B-NB	2.92	128.31	124.08
20	B	803	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
20	B	841	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
20	B	810	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
20	1	213	CLA	CGD-CBD-CAD	-2.92	101.39	110.85
20	J	101	CLA	O2A-CGA-CBA	2.92	120.74	111.83
20	3	314	CLA	C4D-CHA-C1A	2.92	124.73	121.24
20	H	101	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
21	R	103	LMU	C1B-O1B-C4'	2.92	124.90	117.98
20	A	801	CLA	C2A-C3A-C4A	-2.92	97.16	101.87
20	2	311	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
20	2	303	CLA	O1D-CGD-CBD	-2.92	118.77	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	102	CLA	C1-O2A-CGA	2.92	123.71	116.65
20	A	814	CLA	C4D-ND-C1D	-2.92	104.27	106.31
20	2	316	CLA	C4A-NA-C1A	2.92	108.01	106.68
20	3	305	CLA	C2C-C1C-CHC	-2.91	118.20	125.84
20	2	314	CLA	CHB-C1B-NB	-2.91	119.68	124.05
20	H	110	CLA	C3B-C2B-C1B	-2.91	103.73	107.17
21	E	101	LMU	O1B-C1B-O5B	2.91	118.36	110.69
20	4	318	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	F	203	BCR	C1-C6-C5	-2.91	118.66	122.64
21	2	319	LMU	C6B-C5B-C4B	2.91	120.17	113.02
20	B	833	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
20	A	833	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
20	1	206	CLA	C1-O2A-CGA	2.91	123.69	116.65
20	H	108	CLA	CHC-C4B-NB	2.91	128.41	124.05
20	3	310	CLA	CHC-C1C-NC	2.91	128.69	124.31
20	4	313	CLA	CHB-C4A-NA	2.91	128.59	124.40
20	A	828	CLA	CMB-C2B-C1B	2.90	129.84	125.42
20	B	838	CLA	C4A-NA-C1A	2.90	108.00	106.68
21	H	105	LMU	C3'-C4'-C5'	2.90	117.37	110.93
20	B	820	CLA	O2A-CGA-CBA	2.90	120.69	111.83
21	L	205	LMU	O5B-C5B-C6B	2.90	113.64	106.44
20	1	213	CLA	C3B-C2B-C1B	-2.90	103.75	107.17
20	3	313	CLA	CED-O2D-CGD	2.90	122.50	115.92
20	B	802	CLA	C1-O2A-CGA	2.90	123.67	116.65
20	3	314	CLA	CHB-C4A-NA	2.90	128.59	124.40
22	A	845	BCR	C33-C5-C4	2.90	119.78	113.60
20	A	851	CLA	O2A-CGA-CBA	2.90	120.67	111.83
21	4	319	LMU	C3'-C4'-C5'	2.90	117.36	110.93
20	A	812	CLA	O2A-CGA-CBA	2.90	120.67	111.83
20	L	204	CLA	C1D-ND-C4D	-2.90	104.28	106.31
20	2	308	CLA	C2D-C3D-C4D	-2.90	103.83	107.35
20	L	207	CLA	O2A-CGA-CBA	2.90	120.67	111.83
20	B	850	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	2	314	CLA	CHB-C4A-NA	2.90	128.58	124.40
20	B	838	CLA	CMB-C2B-C1B	2.90	129.83	125.42
20	A	830	CLA	C4A-NA-C1A	2.90	108.00	106.68
20	A	822	CLA	CHB-C4A-NA	2.89	128.58	124.40
20	B	816	CLA	O2A-CGA-CBA	2.89	120.66	111.83
22	I	101	BCR	C28-C27-C26	-2.89	108.89	114.06
20	A	813	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
22	F	203	BCR	C23-C24-C25	-2.89	119.27	127.00
20	A	834	CLA	O2D-CGD-O1D	-2.89	118.22	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	309	CLA	C1C-NC-C4C	-2.89	105.36	106.68
20	A	832	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
20	2	302	CLA	C1-C2-C3	-2.89	121.46	126.20
20	4	305	CLA	CHC-C4B-NB	2.89	128.39	124.05
20	A	840	CLA	CMB-C2B-C1B	2.89	129.82	125.42
20	4	317	CLA	CHB-C1B-NB	-2.89	119.71	124.05
20	4	306	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
20	B	811	CLA	C3D-C4D-ND	2.89	113.45	109.50
20	F	206	CLA	CAA-C2A-C3A	-2.89	109.61	116.23
21	K	106	LMU	C4B-C3B-C2B	-2.89	105.76	110.83
20	4	312	CLA	C1B-NB-C4B	-2.89	104.29	106.31
20	4	313	CLA	CMA-C3A-C2A	-2.89	109.61	116.23
20	A	826	CLA	CHB-C4A-NA	2.89	128.56	124.40
20	2	306	CLA	C2D-C3D-C4D	-2.88	103.84	107.35
20	3	315	CLA	CHB-C4A-NA	2.88	128.53	124.43
20	A	851	CLA	C1-C2-C3	2.88	130.92	126.20
20	R	107	CLA	C3B-C2B-C1B	-2.88	103.77	107.17
20	4	303	CLA	CHC-C4B-NB	2.88	128.37	124.05
20	K	104	CLA	C4-C3-C2	-2.88	116.23	123.63
20	B	830	CLA	C2B-C1B-NB	2.88	113.31	110.33
20	4	317	CLA	O2D-CGD-CBD	2.88	116.27	111.23
20	L	207	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
21	R	101	LMU	O5'-C1'-O1'	2.88	116.85	110.04
20	K	103	CLA	C1-C2-C3	-2.88	122.10	126.76
20	1	210	CLA	C4A-NA-C1A	2.88	107.99	106.68
20	1	214	CLA	CHB-C4A-NA	2.88	128.52	124.43
20	B	836	CLA	CAC-C3C-C4C	2.88	128.53	124.79
20	A	823	CLA	O2A-CGA-CBA	2.88	120.61	111.83
20	B	838	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
20	4	302	CLA	CHC-C4B-NB	2.88	128.36	124.05
20	H	101	CLA	C4A-NA-C1A	2.88	107.99	106.68
20	B	823	CLA	CED-O2D-CGD	2.87	122.44	115.92
20	4	305	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
20	F	207	CLA	CMA-C3A-C2A	2.87	125.10	113.98
20	H	109	CLA	O2A-CGA-CBA	2.87	120.59	111.83
22	G	104	BCR	C38-C26-C25	-2.87	121.35	124.48
21	R	102	LMU	O5B-C1B-C2B	2.87	116.27	110.37
20	F	205	CLA	CHC-C4B-NB	2.87	128.35	124.05
20	2	304	CLA	C3D-C4D-ND	2.87	113.42	109.50
20	3	307	CLA	C3C-C4C-NC	-2.87	106.76	110.43
20	H	108	CLA	CMA-C3A-C4A	-2.87	104.07	111.77
20	B	826	CLA	CAC-C3C-C4C	2.87	128.52	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	849	CLA	C4A-NA-C1A	2.86	107.99	106.68
20	B	823	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
20	4	318	CLA	O2A-CGA-CBA	2.86	120.56	111.83
20	J	103	CLA	C4-C3-C5	2.86	120.19	115.23
21	A	846	LMU	O5'-C5'-C4'	2.86	115.63	109.72
20	4	301	CLA	O2A-CGA-CBA	2.86	120.55	111.83
20	4	307	CLA	C3D-C4D-ND	2.86	113.41	109.50
20	A	828	CLA	C2B-C1B-NB	2.86	113.29	110.33
20	B	834	CLA	C4A-NA-C1A	2.86	107.98	106.68
20	B	815	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	G	104	BCR	C33-C5-C4	2.85	119.68	113.60
20	B	816	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
20	1	207	CLA	C1D-ND-C4D	-2.85	104.31	106.31
21	A	853	LMU	C4B-C3B-C2B	2.85	115.84	110.83
20	A	849	CLA	CAA-C2A-C3A	-2.85	105.29	113.00
20	B	815	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
21	L	206	LMU	O1'-C1'-C2'	2.85	112.61	108.27
20	3	310	CLA	C6-C5-C3	-2.85	106.52	113.47
20	1	210	CLA	CMB-C2B-C1B	2.85	129.76	125.42
20	A	825	CLA	C4A-NA-C1A	2.85	107.98	106.68
20	A	827	CLA	C4A-NA-C1A	2.85	107.98	106.68
20	B	803	CLA	O2A-CGA-CBA	2.85	120.53	111.83
20	3	311	CLA	CHC-C4B-NB	2.85	128.32	124.05
20	A	835	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
20	4	303	CLA	CBC-CAC-C3C	-2.85	104.70	112.42
20	4	304	CLA	CHD-C4C-NC	2.85	128.64	124.23
20	A	827	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
20	A	806	CLA	C4A-NA-C1A	2.85	107.98	106.68
20	2	314	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
20	B	839	CLA	O1D-CGD-CBD	-2.84	118.91	124.52
20	B	832	CLA	CHB-C4A-NA	2.84	128.50	124.40
21	G	101	LMU	O5B-C5B-C6B	2.84	113.49	106.44
20	B	817	CLA	C1D-ND-C4D	-2.84	104.32	106.31
20	4	311	CLA	C2C-C1C-CHC	-2.84	118.39	125.84
20	A	832	CLA	CMA-C3A-C4A	-2.84	104.13	111.77
20	A	820	CLA	O2A-CGA-CBA	2.84	120.50	111.83
20	4	301	CLA	CHC-C4B-NB	2.84	128.31	124.05
21	L	210	LMU	O5B-C5B-C4B	2.84	114.82	109.70
20	1	215	CLA	CAA-C2A-C1A	2.84	121.28	111.97
20	A	850	CLA	CHC-C4B-NB	2.84	128.31	124.05
20	B	836	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
20	B	816	CLA	C4-C3-C5	2.84	120.16	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	807	CLA	C2A-C1A-CHA	-2.84	118.94	123.87
20	A	836	CLA	CHC-C1C-C2C	-2.83	118.89	126.95
20	B	850	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
20	3	310	CLA	C1-O2A-CGA	2.83	123.51	116.65
20	H	109	CLA	CHC-C4B-NB	2.83	128.30	124.05
20	G	105	CLA	C4A-NA-C1A	2.83	107.97	106.68
22	L	209	BCR	C33-C5-C6	-2.83	121.40	124.48
20	1	205	CLA	C4A-NA-C1A	2.83	107.97	106.68
20	B	838	CLA	CBC-CAC-C3C	-2.83	104.75	112.42
20	B	833	CLA	O2A-CGA-CBA	2.83	120.45	111.83
20	B	840	CLA	C4A-NA-C1A	2.83	107.97	106.68
20	B	817	CLA	O1D-CGD-CBD	-2.82	118.95	124.52
21	E	101	LMU	O5 <sup>1</sup> -C5 <sup>3</sup> -C6 <sup>7</sup>	2.82	113.44	106.44
20	A	837	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
21	1	218	LMU	C4B-C3B-C2B	2.82	115.78	110.83
20	2	312	CLA	CAA-CBA-CGA	-2.82	105.20	113.21
21	R	106	LMU	C1 <sup>1</sup> -C2 <sup>2</sup> -C3 <sup>7</sup>	2.82	115.94	110.01
20	1	203	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	H	109	CLA	CHB-C4A-NA	2.82	128.47	124.40
21	4	319	LMU	C1B-C2B-C3B	-2.82	104.08	110.01
20	F	207	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
21	R	101	LMU	O5B-C5B-C6B	2.82	113.42	106.44
20	I	102	CLA	CHC-C4B-NB	2.82	128.27	124.05
22	B	801	BCR	C7-C6-C5	-2.82	115.07	121.56
20	1	211	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
21	D	201	LMU	O5B-C5B-C6B	2.82	113.42	106.44
23	A	842	PQN	C21-C20-C18	-2.81	106.61	115.97
21	1	216	LMU	C1B-O5B-C5B	-2.81	108.23	113.72
20	1	204	CLA	CAA-C2A-C1A	-2.81	102.76	111.97
20	3	310	CLA	O2A-CGA-CBA	2.81	120.41	111.83
20	3	309	CLA	C2C-C1C-CHC	-2.81	118.48	125.84
20	K	102	CLA	CBC-CAC-C3C	-2.81	104.81	112.42
20	3	304	CLA	CHB-C4A-NA	2.81	128.42	124.43
20	B	825	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
20	A	802	CLA	C4C-CHD-C1D	-2.80	117.99	125.98
20	3	301	CLA	CAA-C2A-C3A	-2.80	109.80	116.23
22	I	101	BCR	C33-C5-C4	2.80	119.57	113.60
20	L	208	CLA	CAA-C2A-C1A	2.80	121.16	111.97
20	A	806	CLA	C2A-C1A-CHA	-2.80	119.00	123.87
20	3	310	CLA	CMC-C2C-C1C	2.80	129.41	125.03
22	J	102	BCR	C30-C25-C26	-2.80	118.81	122.64
20	A	821	CLA	CHB-C1B-NB	-2.80	119.85	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	315	CLA	CHB-C4A-NA	2.80	128.44	124.40
22	A	844	BCR	C11-C12-C13	-2.80	118.69	126.36
20	A	818	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
20	F	206	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
20	B	808	CLA	C11-C10-C8	-2.79	106.68	115.97
22	A	845	BCR	C1-C6-C5	-2.79	118.82	122.64
20	A	850	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
21	D	201	LMU	C1'-C2'-C3'	-2.79	104.14	110.01
20	A	830	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	1	202	CLA	CAA-C2A-C1A	2.79	118.70	111.81
20	B	815	CLA	C4A-NA-C1A	2.79	107.95	106.68
20	3	312	CLA	CHB-C4A-NA	2.79	128.40	124.43
20	2	315	CLA	C3C-C4C-CHD	-2.79	117.98	125.23
20	B	825	CLA	CGD-CBD-CAD	-2.79	101.82	110.85
20	A	833	CLA	CAC-C3C-C4C	2.79	128.42	124.79
20	A	809	CLA	C4-C3-C5	2.79	120.06	115.23
22	A	845	BCR	C27-C26-C25	-2.79	118.94	122.70
20	3	315	CLA	C2C-C1C-CHC	-2.79	118.54	125.84
20	1	204	CLA	CHB-C4A-NA	2.78	128.42	124.40
20	B	814	CLA	C3B-C2B-C1B	-2.78	103.89	107.17
20	B	840	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
20	A	805	CLA	O2A-CGA-CBA	2.78	120.31	111.83
20	K	104	CLA	CHC-C4B-NB	2.78	128.22	124.05
20	J	101	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	H	108	CLA	O2A-C1-C2	2.78	118.81	108.11
20	1	204	CLA	C3D-C4D-ND	2.78	114.50	109.99
22	B	801	BCR	C4-C5-C6	-2.78	118.95	122.70
20	B	816	CLA	CMB-C2B-C1B	2.78	129.65	125.42
20	1	213	CLA	O2A-CGA-CBA	2.78	120.31	111.83
20	3	311	CLA	CHB-C4A-NA	2.78	128.41	124.40
20	B	828	CLA	CHB-C4A-NA	2.78	128.41	124.40
20	B	802	CLA	CHC-C4B-NB	2.78	128.21	124.05
22	B	844	BCR	C34-C9-C10	-2.78	118.32	122.82
20	3	316	CLA	C3C-C4C-CHD	-2.78	118.02	125.23
20	K	104	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
20	2	302	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
20	J	101	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
20	1	210	CLA	CHC-C4B-NB	2.77	128.21	124.05
20	4	305	CLA	C2B-C1B-NB	2.77	113.20	110.33
21	E	101	LMU	O2'-C2'-C1'	-2.77	103.47	110.08
20	2	303	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
20	3	314	CLA	O2D-CGD-O1D	-2.77	118.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	201	CLA	CMB-C2B-C1B	2.77	129.64	125.42
20	B	814	CLA	CBA-CAA-C2A	-2.77	105.55	113.79
21	4	316	LMU	O1'-C1'-C2'	2.77	112.48	108.27
20	A	801	CLA	CAA-C2A-C1A	2.77	121.04	111.97
20	B	837	CLA	CMB-C2B-C1B	2.77	129.63	125.42
20	B	802	CLA	CAA-C2A-C1A	2.77	121.04	111.97
20	A	806	CLA	C3B-C4B-NB	-2.76	108.06	110.53
20	A	827	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	3	306	CLA	C3C-C4C-CHD	-2.76	118.06	125.23
20	2	308	CLA	C2C-C1C-CHC	-2.76	118.61	125.84
20	A	801	CLA	CHD-C4C-C3C	-2.76	120.75	124.77
20	2	304	CLA	C2C-C1C-CHC	-2.76	118.61	125.84
20	H	101	CLA	CHC-C4B-NB	2.76	128.19	124.05
20	B	831	CLA	C1-C2-C3	-2.76	122.30	126.76
21	1	216	LMU	O5'-C1'-C2'	-2.76	104.71	110.37
20	1	202	CLA	C3B-C2B-C1B	-2.75	103.92	107.17
21	H	105	LMU	C4B-C3B-C2B	-2.75	106.00	110.83
20	B	812	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
20	2	303	CLA	C1D-ND-C4D	-2.75	104.38	106.31
21	A	846	LMU	C3B-C4B-C5B	2.75	115.22	110.23
23	A	842	PQN	C2M-C2-C3	-2.75	119.93	124.45
20	B	824	CLA	O2A-CGA-CBA	2.75	120.22	111.83
20	2	305	CLA	C4A-NA-C1A	2.75	107.93	106.68
20	B	819	CLA	CHC-C4B-NB	2.75	128.17	124.05
20	R	108	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
20	A	835	CLA	CAA-C2A-C1A	-2.75	102.97	111.97
20	2	301	CLA	CHB-C4A-NA	2.75	128.33	124.43
20	B	811	CLA	C1B-NB-C4B	-2.74	104.39	106.31
20	A	817	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
20	R	108	CLA	O2A-C1-C2	2.74	118.66	108.11
20	2	305	CLA	CHB-C4A-NA	2.74	128.36	124.40
21	G	101	LMU	O1B-C1B-C2B	2.74	114.83	108.09
20	H	109	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
21	4	320	LMU	C3'-C4'-C5'	2.74	117.00	110.93
22	B	844	BCR	C1-C6-C7	2.74	123.08	115.65
20	B	834	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	2	312	CLA	C11-C10-C8	-2.74	106.86	115.97
20	F	207	CLA	C3B-C2B-C1B	-2.74	103.94	107.17
20	2	310	CLA	C1D-ND-C4D	-2.74	104.39	106.31
21	A	846	LMU	C3'-C4'-C5'	2.74	117.00	110.93
21	2	319	LMU	O1B-C1B-C2B	2.74	114.82	108.09
20	1	206	CLA	C1D-ND-C4D	-2.74	104.39	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	208	CLA	O2A-CGA-CBA	2.74	120.18	111.83
20	B	841	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
20	4	301	CLA	CAC-C3C-C4C	2.73	128.34	124.79
20	1	204	CLA	C1D-ND-C4D	-2.73	104.39	106.31
22	B	846	BCR	C33-C5-C6	-2.73	121.50	124.48
20	R	108	CLA	C4-C3-C2	-2.73	116.61	123.63
21	L	205	LMU	C3B-C4B-C5B	2.73	115.19	110.23
20	B	809	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
20	H	109	CLA	C4-C3-C5	2.73	119.97	115.23
20	A	812	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	2	307	CLA	C3D-C4D-ND	2.73	114.42	109.99
20	A	806	CLA	O2A-CGA-CBA	2.73	120.16	111.83
20	A	819	CLA	CED-O2D-CGD	2.73	122.11	115.92
20	A	823	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	4	312	CLA	C3D-C4D-ND	2.73	113.23	109.50
20	B	824	CLA	C1D-ND-C4D	-2.73	104.40	106.31
20	G	105	CLA	C1-C2-C3	-2.73	121.73	126.20
20	A	840	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
20	F	205	CLA	CAA-C2A-C3A	-2.73	109.98	116.23
22	F	204	BCR	C27-C26-C25	-2.73	119.02	122.70
20	B	818	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
20	4	304	CLA	C1-O2A-CGA	2.73	123.25	116.65
20	A	811	CLA	CAA-C2A-C1A	-2.73	103.05	111.97
20	L	204	CLA	CMB-C2B-C1B	2.72	129.56	125.42
20	4	303	CLA	O2D-CGD-CBD	2.72	115.99	111.23
20	B	813	CLA	C3B-C2B-C1B	-2.72	103.96	107.17
20	B	832	CLA	CAA-CBA-CGA	-2.72	105.49	113.21
20	A	815	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
20	B	808	CLA	CMB-C2B-C1B	2.72	129.56	125.42
20	B	812	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	A	843	BCR	C8-C7-C6	-2.72	119.74	127.00
20	1	201	CLA	CAC-C3C-C2C	-2.72	122.57	127.56
20	B	837	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
20	4	301	CLA	CHB-C4A-NA	2.72	128.32	124.40
20	R	107	CLA	CHC-C1C-C2C	-2.71	119.23	126.95
20	A	814	CLA	CHB-C4A-NA	2.71	128.29	124.43
21	H	106	LMU	C1'-O5'-C5'	2.71	119.02	113.72
20	1	204	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
20	B	812	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	F	204	BCR	C1-C6-C5	-2.71	118.93	122.64
20	A	805	CLA	CAC-C3C-C4C	2.71	128.31	124.79
21	F	202	LMU	O5B-C5B-C6B	2.71	113.15	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	839	CLA	CMB-C2B-C1B	2.71	129.54	125.42
20	3	305	CLA	CHB-C4A-NA	2.71	128.28	124.43
22	L	209	BCR	C38-C26-C27	2.71	119.37	113.60
20	B	816	CLA	CED-O2D-CGD	2.71	122.06	115.92
20	A	806	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
20	A	820	CLA	CED-O2D-CGD	2.71	122.05	115.92
20	A	834	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
20	H	101	CLA	CED-O2D-CGD	2.70	122.05	115.92
21	H	104	LMU	O1B-C4'-C5'	2.70	116.57	109.48
20	B	831	CLA	CHC-C1C-C2C	-2.70	119.26	126.95
22	G	104	BCR	C23-C24-C25	-2.70	119.79	127.00
20	2	314	CLA	O2D-CGD-CBD	2.70	115.94	111.23
20	B	815	CLA	CHB-C4A-NA	2.70	128.29	124.40
21	4	321	LMU	O1'-C1'-C2'	2.70	112.37	108.27
20	B	830	CLA	CHB-C1B-NB	-2.70	120.01	124.05
20	A	826	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
20	2	304	CLA	CHB-C4A-NA	2.69	128.26	124.43
20	1	201	CLA	CHB-C1B-NB	-2.69	120.01	124.05
20	F	201	CLA	CHB-C1B-NB	-2.69	120.01	124.05
22	F	204	BCR	C37-C22-C21	-2.69	118.45	122.82
20	3	305	CLA	C3D-C4D-CHA	-2.69	119.19	125.20
20	K	104	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	A	835	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
20	H	101	CLA	CMA-C3A-C4A	-2.69	104.54	111.77
22	B	845	BCR	C15-C14-C13	-2.69	123.51	127.28
21	2	313	LMU	O1B-C1B-C2B	2.69	114.71	108.09
22	L	209	BCR	C3-C4-C5	-2.69	109.26	114.06
20	R	108	CLA	CMB-C2B-C1B	2.69	129.51	125.42
20	B	821	CLA	C1D-ND-C4D	-2.69	104.43	106.31
20	A	827	CLA	O2A-CGA-CBA	2.69	120.03	111.83
20	1	206	CLA	C1-C2-C3	-2.69	121.80	126.20
20	3	316	CLA	C3D-C4D-ND	2.69	113.17	109.50
20	2	310	CLA	C3D-C4D-ND	2.68	114.35	109.99
20	A	823	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
20	B	802	CLA	CAC-C3C-C4C	2.68	128.28	124.79
20	2	315	CLA	C2C-C1C-CHC	-2.68	118.81	125.84
20	4	304	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
22	A	845	BCR	C3-C4-C5	-2.68	109.28	114.06
20	B	808	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	A	819	CLA	C4-C3-C5	2.68	119.88	115.23
20	A	808	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
20	3	317	CLA	CMB-C2B-C1B	2.68	129.50	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	808	CLA	C1-O2A-CGA	2.68	123.13	116.65
20	B	817	CLA	CHB-C4A-NA	2.68	128.26	124.40
21	B	849	LMU	C2'-C3'-C4'	2.68	115.75	109.68
20	2	307	CLA	C3B-C2B-C1B	-2.67	104.02	107.17
20	2	301	CLA	C1C-NC-C4C	-2.67	105.46	106.68
20	A	826	CLA	C4A-NA-C1A	2.67	107.90	106.68
20	4	315	CLA	C1D-ND-C4D	-2.67	104.44	106.31
20	A	812	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
20	B	813	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
20	4	306	CLA	CBA-CAA-C2A	-2.67	105.85	113.79
20	A	839	CLA	CAA-C2A-C3A	2.67	120.22	113.00
20	A	836	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	A	851	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
20	B	817	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
21	2	319	LMU	C1'-O5'-C5'	2.67	118.93	113.72
20	A	819	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
20	4	317	CLA	CAA-C2A-C1A	-2.67	103.24	111.97
20	A	814	CLA	C2C-C1C-CHC	-2.67	118.85	125.84
20	3	311	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
20	A	806	CLA	CED-O2D-CGD	2.67	121.96	115.92
21	B	849	LMU	O5B-C5B-C4B	2.66	114.50	109.70
20	4	310	CLA	C3B-C2B-C1B	-2.66	104.03	107.17
20	A	801	CLA	CHC-C4B-C3B	-2.66	119.70	127.43
20	4	318	CLA	CHD-C4C-C3C	-2.66	120.89	124.77
20	A	825	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
20	B	818	CLA	CHC-C4B-NB	2.66	128.04	124.05
21	4	320	LMU	C1'-C2'-C3'	2.66	115.61	110.01
20	2	304	CLA	C4D-ND-C1D	-2.66	104.45	106.31
20	F	206	CLA	CMB-C2B-C1B	2.66	129.47	125.42
22	I	101	BCR	C24-C25-C26	-2.66	115.43	121.56
20	A	806	CLA	CHB-C4A-NA	2.66	128.24	124.40
20	B	808	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
20	A	838	CLA	C3B-C4B-NB	-2.66	108.16	110.53
20	4	310	CLA	C3D-C4D-ND	2.66	114.30	109.99
20	A	840	CLA	CHC-C4B-NB	2.66	128.03	124.05
22	L	209	BCR	C37-C22-C21	-2.66	118.51	122.82
22	B	844	BCR	C33-C5-C6	-2.65	121.59	124.48
21	R	106	LMU	C2'-C3'-C4'	2.65	115.70	109.68
21	B	804	LMU	O1B-C1B-C2B	2.65	114.61	108.09
22	B	845	BCR	C38-C26-C27	2.65	119.25	113.60
21	D	201	LMU	C4B-C3B-C2B	-2.65	106.17	110.83
20	2	309	CLA	CHD-C1D-ND	2.65	128.59	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	302	CLA	C3D-C4D-ND	2.65	114.29	109.99
20	A	818	CLA	C1D-ND-C4D	-2.65	104.45	106.31
20	A	851	CLA	C2A-C1A-CHA	-2.65	119.28	123.87
20	B	802	CLA	CMB-C2B-C1B	2.65	129.45	125.42
20	B	810	CLA	CMB-C2B-C1B	2.65	129.45	125.42
20	2	311	CLA	C1-O2A-CGA	2.64	123.05	116.65
20	2	303	CLA	CHB-C1B-NB	-2.64	120.08	124.05
22	I	103	BCR	C35-C13-C12	2.64	122.12	118.09
20	1	206	CLA	CHB-C1B-NB	-2.64	120.08	124.05
20	1	212	CLA	C2C-C1C-CHC	-2.64	118.92	125.84
20	4	303	CLA	C11-C10-C8	-2.64	107.18	115.97
21	G	103	LMU	C1B-O1B-C4'	-2.64	111.72	117.98
21	1	218	LMU	C3'-C4'-C5'	-2.64	105.08	110.93
22	2	317	BCR	C38-C26-C27	2.64	119.23	113.60
20	3	317	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
20	A	839	CLA	CHB-C1B-NB	-2.64	120.09	124.05
20	H	108	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	H	102	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
20	3	306	CLA	CHB-C4A-NA	2.64	128.18	124.43
20	K	102	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
20	2	306	CLA	C3B-C2B-C1B	-2.64	103.87	106.81
20	3	307	CLA	CHB-C4A-NA	2.64	128.21	124.40
20	A	826	CLA	CMA-C3A-C4A	-2.64	104.69	111.77
20	A	835	CLA	CAA-C2A-C3A	-2.64	105.88	113.00
20	1	209	CLA	C3D-C4D-ND	2.64	113.10	109.50
20	L	208	CLA	CHC-C4B-NB	2.64	128.00	124.05
20	3	303	CLA	CAA-C2A-C3A	-2.63	110.19	116.23
20	3	307	CLA	CHB-C1B-NB	-2.63	120.10	124.05
20	B	831	CLA	CGD-CBD-CAD	2.63	119.37	110.85
20	2	304	CLA	CHA-C4D-ND	2.63	128.56	124.84
20	4	309	CLA	CHB-C4A-NA	2.63	128.17	124.43
20	1	211	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
20	A	811	CLA	CAA-CBA-CGA	2.63	120.68	113.21
20	3	305	CLA	C3C-C4C-CHD	-2.63	118.40	125.23
20	H	102	CLA	CED-O2D-CGD	2.63	121.88	115.92
20	A	805	CLA	CHB-C1B-NB	-2.63	120.11	124.05
20	A	801	CLA	CGD-CBD-CAD	2.63	119.35	110.85
20	3	301	CLA	CHB-C4A-NA	2.63	128.19	124.40
20	B	828	CLA	C4-C3-C5	2.63	119.78	115.23
20	B	841	CLA	CHB-C4A-NA	2.62	128.19	124.40
21	B	805	LMU	O1'-C1'-C2'	2.62	112.26	108.27
20	A	802	CLA	C4D-ND-C1D	-2.62	104.47	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	310	CLA	CHC-C4B-NB	2.62	127.98	124.05
20	4	313	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
20	A	815	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	A	851	CLA	C4A-NA-C1A	2.62	107.87	106.68
20	2	309	CLA	C2C-C1C-CHC	-2.62	118.98	125.84
22	F	203	BCR	C20-C19-C18	-2.62	119.19	126.36
20	1	203	CLA	CMB-C2B-C1B	2.62	129.40	125.42
20	A	841	CLA	C2C-C1C-CHC	-2.62	118.98	125.84
20	1	214	CLA	C4D-ND-C1D	-2.62	104.48	106.31
20	L	204	CLA	C4-C3-C5	2.61	119.77	115.23
20	4	308	CLA	CHB-C4A-NA	2.61	128.15	124.43
22	A	844	BCR	C8-C7-C6	-2.61	120.01	127.00
20	1	202	CLA	CHB-C4A-NA	2.61	128.17	124.40
20	3	313	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
20	A	822	CLA	CHC-C1C-C2C	-2.61	119.52	126.95
20	4	303	CLA	C3D-C4D-ND	2.61	114.23	109.99
20	A	804	CLA	C4-C3-C5	2.61	119.76	115.23
20	R	108	CLA	CAA-CBA-CGA	2.61	120.63	113.21
21	K	107	LMU	C1'-C2'-C3'	-2.61	104.52	110.01
21	G	101	LMU	O4'-C4B-C5B	2.61	115.76	109.32
20	A	810	CLA	C3D-C4D-ND	2.61	114.23	109.99
20	B	806	CLA	C3D-C4D-ND	2.61	114.23	109.99
20	B	833	CLA	CAA-CBA-CGA	-2.61	105.80	113.21
20	2	309	CLA	C4A-NA-C1A	2.61	107.87	106.68
20	A	822	CLA	C4A-NA-C1A	2.61	107.87	106.68
20	1	212	CLA	CHB-C4A-NA	2.61	128.14	124.43
20	A	831	CLA	C11-C10-C8	-2.61	107.30	115.97
20	4	305	CLA	CHB-C1B-NB	-2.61	120.14	124.05
20	L	202	CLA	C1-O2A-CGA	2.61	122.96	116.65
20	3	301	CLA	CHC-C4B-C3B	-2.60	119.86	127.43
20	2	307	CLA	C2B-C1B-NB	2.60	113.03	110.33
20	B	839	CLA	CAA-CBA-CGA	-2.60	105.81	113.21
20	B	840	CLA	C4-C3-C5	2.60	119.75	115.23
20	H	110	CLA	C4A-NA-C1A	2.60	107.87	106.68
20	L	204	CLA	C3B-C2B-C1B	-2.60	104.10	107.17
22	B	847	BCR	C30-C25-C26	-2.60	119.08	122.64
20	B	808	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	1	209	CLA	CHB-C4A-NA	2.60	128.13	124.43
20	G	105	CLA	O2A-CGA-CBA	2.60	119.77	111.83
20	A	835	CLA	C4A-NA-C1A	2.60	107.87	106.68
20	A	832	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
21	L	205	LMU	O5'-C5'-C6'	2.60	112.88	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	817	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	A	811	CLA	O2A-CGA-CBA	2.60	119.76	111.83
20	A	839	CLA	C4A-NA-C1A	2.60	107.86	106.68
20	B	840	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
20	A	812	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
20	A	815	CLA	C1-O2A-CGA	2.60	122.94	116.65
20	4	314	CLA	CHB-C4A-NA	2.60	128.12	124.43
20	B	842	CLA	CMB-C2B-C1B	2.60	129.37	125.42
20	B	820	CLA	C4-C3-C5	2.59	119.73	115.23
20	4	318	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
20	B	816	CLA	C4B-C3B-C2B	2.59	110.53	107.30
21	B	804	LMU	O5'-C5'-C6'	2.59	112.87	106.44
20	B	832	CLA	C4A-NA-C1A	2.59	107.86	106.68
20	2	301	CLA	C2C-C1C-CHC	-2.59	119.05	125.84
20	1	215	CLA	C4-C3-C5	2.59	119.18	116.13
20	4	302	CLA	CMA-C3A-C2A	-2.59	110.29	116.23
20	1	215	CLA	O2D-CGD-CBD	2.59	115.76	111.23
21	K	105	LMU	O1B-C4'-C5'	2.59	116.27	109.48
20	B	842	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	A	809	CLA	O2A-C1-C2	2.59	118.07	108.11
20	A	836	CLA	CMB-C2B-C1B	2.59	129.36	125.42
20	B	803	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
22	I	103	BCR	C33-C5-C6	-2.59	121.66	124.48
20	B	839	CLA	C3D-C4D-ND	2.59	114.19	109.99
20	B	803	CLA	CMB-C2B-C1B	2.59	129.36	125.42
20	A	835	CLA	C3D-C4D-ND	2.59	114.19	109.99
20	A	835	CLA	CHC-C4B-NB	2.59	127.93	124.05
20	B	829	CLA	CHC-C1C-C2C	-2.58	119.60	126.95
20	L	202	CLA	C4A-NA-C1A	2.58	107.86	106.68
20	2	305	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
20	L	203	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
20	A	830	CLA	CHB-C4A-NA	2.58	128.13	124.40
20	J	103	CLA	C1-C2-C3	-2.58	121.97	126.20
20	2	305	CLA	O2A-CGA-CBA	2.58	119.70	111.83
20	4	307	CLA	C2C-C1C-CHC	-2.58	119.08	125.84
20	1	213	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	K	104	CLA	C1-C2-C3	-2.58	121.97	126.20
20	B	850	CLA	CHB-C1B-NB	-2.58	120.18	124.05
20	F	207	CLA	CMB-C2B-C1B	2.58	129.35	125.42
20	2	315	CLA	C3B-C2B-C1B	-2.58	103.94	106.81
20	A	850	CLA	CED-O2D-CGD	2.58	121.77	115.92
20	1	205	CLA	CHC-C1C-C2C	-2.58	119.62	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	840	CLA	CHB-C1B-NB	-2.58	120.18	124.05
20	A	837	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	2	315	CLA	C4A-NA-C1A	2.58	107.86	106.68
20	A	840	CLA	C1-O2A-CGA	2.58	122.89	116.65
20	A	801	CLA	CMB-C2B-C1B	2.58	129.34	125.42
20	B	819	CLA	CMA-C3A-C2A	-2.58	110.32	116.23
22	I	101	BCR	C35-C13-C12	2.58	122.02	118.09
20	B	816	CLA	C3B-C4B-NB	-2.58	108.23	110.53
21	A	854	LMU	C1'-O5'-C5'	-2.57	108.69	113.72
22	B	846	BCR	C38-C26-C27	2.57	119.08	113.60
20	3	303	CLA	C4A-NA-C1A	2.57	107.85	106.68
20	A	808	CLA	C4A-NA-C1A	2.57	107.85	106.68
20	3	306	CLA	C2C-C1C-CHC	-2.57	119.11	125.84
20	A	810	CLA	CED-O2D-CGD	2.57	121.74	115.92
20	4	309	CLA	C2C-C1C-CHC	-2.57	119.11	125.84
20	A	814	CLA	CHC-C4B-NB	2.57	127.79	124.08
20	H	102	CLA	CGD-CBD-CAD	-2.57	102.53	110.85
20	3	303	CLA	C1D-ND-C4D	-2.57	104.51	106.31
20	2	304	CLA	CHC-C4B-NB	2.57	127.79	124.08
20	I	102	CLA	C1-O2A-CGA	2.57	122.86	116.65
21	L	205	LMU	O5'-C1'-C2'	2.57	115.64	110.37
20	A	807	CLA	C3D-C4D-ND	2.56	114.16	109.99
20	A	824	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
20	B	834	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
22	F	204	BCR	C33-C5-C4	2.56	119.06	113.60
20	A	823	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
22	A	844	BCR	C27-C26-C25	-2.56	119.24	122.70
20	A	828	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
20	B	827	CLA	O2A-CGA-CBA	2.56	119.65	111.83
20	1	211	CLA	CED-O2D-CGD	2.56	121.73	115.92
20	4	301	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
20	A	810	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
21	H	106	LMU	C6'-C5'-C4'	-2.56	106.18	113.38
20	B	806	CLA	CHB-C4A-NA	2.56	128.09	124.40
20	1	203	CLA	C4D-CHA-C1A	-2.56	118.19	121.24
20	I	102	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
20	A	808	CLA	C1-C2-C3	-2.56	122.01	126.20
22	B	845	BCR	C23-C22-C21	2.56	123.03	119.01
20	4	313	CLA	CHB-C1B-NB	-2.56	120.22	124.05
21	4	321	LMU	C1B-O1B-C4'	-2.56	111.92	117.98
20	A	819	CLA	CHB-C4A-NA	2.55	128.09	124.40
20	B	814	CLA	O2A-CGA-CBA	2.55	119.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	103	LMU	O3'-C3'-C2'	2.55	116.40	110.38
20	A	804	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
20	F	205	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
20	A	832	CLA	O2A-CGA-CBA	2.55	119.62	111.83
20	A	810	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
21	R	103	LMU	C6B-C5B-C4B	-2.55	106.75	113.02
20	A	817	CLA	C4A-NA-C1A	2.55	107.84	106.68
20	A	820	CLA	C4A-NA-C1A	2.55	107.84	106.68
21	E	101	LMU	O1B-C1B-C2B	2.55	114.37	108.09
20	A	838	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
20	A	831	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
20	3	301	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
20	A	850	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
20	R	107	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
20	B	814	CLA	C4-C3-C5	2.55	119.65	115.23
20	A	849	CLA	CMB-C2B-C1B	2.55	129.30	125.42
20	B	823	CLA	C4A-NA-C1A	2.55	107.84	106.68
21	A	855	LMU	O5'-C1'-C2'	2.55	115.61	110.37
20	A	807	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
22	J	102	BCR	C8-C7-C6	-2.55	120.19	127.00
20	B	813	CLA	C5-C3-C2	2.55	126.89	121.17
20	A	826	CLA	C1-O2A-CGA	2.55	122.82	116.65
20	4	306	CLA	CMA-C3A-C4A	-2.55	104.93	111.77
20	A	839	CLA	CHB-C4A-NA	2.55	128.07	124.40
20	B	815	CLA	CAC-C3C-C4C	2.55	128.10	124.79
20	B	839	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
20	3	302	CLA	C3C-C4C-CHD	-2.55	118.62	125.23
21	K	107	LMU	C1'-O5'-C5'	-2.55	108.75	113.72
22	A	843	BCR	C4-C5-C6	-2.55	119.26	122.70
20	2	316	CLA	C4-C3-C5	2.55	119.65	115.23
20	H	108	CLA	C4A-NA-C1A	2.54	107.84	106.68
20	3	302	CLA	C2C-C1C-CHC	-2.54	119.17	125.84
20	2	310	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
20	L	204	CLA	CHB-C1B-NB	-2.54	120.23	124.05
20	B	813	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	A	829	CLA	CMB-C2B-C1B	2.54	129.29	125.42
20	1	212	CLA	C3D-C4D-ND	2.54	112.97	109.50
20	1	204	CLA	O2A-CGA-O1A	-2.54	115.61	123.20
20	K	101	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
20	B	831	CLA	CAC-C3C-C4C	2.54	128.10	124.79
20	J	101	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	A	850	CLA	O1D-CGD-CBD	-2.54	119.51	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	831	CLA	CMB-C2B-C1B	2.54	129.29	125.42
21	G	101	LMU	O5'-C1'-C2'	-2.54	105.15	110.37
20	I	102	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	B	836	CLA	O2A-CGA-CBA	2.54	119.58	111.83
20	B	829	CLA	C4B-C3B-C2B	2.54	110.46	107.30
20	A	829	CLA	CAC-C3C-C4C	2.54	128.09	124.79
20	B	839	CLA	CED-O2D-CGD	2.54	121.67	115.92
20	1	211	CLA	CHB-C1B-NB	-2.54	120.24	124.05
20	A	810	CLA	CHC-C1C-C2C	-2.54	119.74	126.95
20	2	307	CLA	C1D-ND-C4D	-2.54	104.53	106.31
20	B	809	CLA	C16-C15-C13	-2.54	107.54	115.97
21	R	105	LMU	O1'-C1'-C2'	2.54	112.12	108.27
20	A	839	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
20	B	823	CLA	CHB-C4A-NA	2.53	128.06	124.40
20	4	308	CLA	C3D-C4D-ND	2.53	112.96	109.50
20	B	833	CLA	CED-O2D-CGD	2.53	121.66	115.92
20	L	203	CLA	CAC-C3C-C4C	2.53	128.09	124.79
20	B	829	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
20	A	805	CLA	CHB-C4A-NA	2.53	128.06	124.40
20	2	304	CLA	CHB-C1B-NB	-2.53	120.42	124.08
20	1	214	CLA	C2C-C1C-CHC	-2.53	119.21	125.84
20	B	824	CLA	C9-C8-C10	2.53	120.30	111.27
20	3	307	CLA	C3B-C2B-C1B	-2.53	104.19	107.17
20	1	203	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
21	4	320	LMU	O5'-C5'-C4'	2.53	114.95	109.72
20	2	310	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	H	108	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
20	3	316	CLA	C2C-C1C-CHC	-2.53	119.21	125.84
20	B	821	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
22	A	843	BCR	C38-C26-C25	-2.53	121.73	124.48
20	4	306	CLA	CED-O2D-CGD	2.53	121.65	115.92
23	B	843	PQN	C16-C15-C13	-2.53	107.31	113.47
22	A	845	BCR	C38-C26-C27	2.53	118.98	113.60
21	H	104	LMU	O5B-C5B-C6B	2.53	112.70	106.44
20	2	307	CLA	CGD-CBD-CAD	2.53	119.02	110.85
20	3	310	CLA	C6-C7-C8	-2.53	107.57	115.97
20	1	209	CLA	C4A-NA-C1A	2.53	107.83	106.68
20	A	835	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	A	827	CLA	C4-C3-C5	2.52	119.61	115.23
20	B	826	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
20	B	828	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
20	B	819	CLA	CHC-C1C-C2C	-2.52	119.78	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	844	BCR	C23-C24-C25	-2.52	120.26	127.00
22	F	203	BCR	C30-C25-C26	-2.52	119.19	122.64
20	B	850	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
20	4	317	CLA	C4D-CHA-C1A	-2.52	118.24	121.24
20	4	305	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
20	L	203	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
20	3	310	CLA	C2A-C1A-CHA	-2.52	119.50	123.87
21	R	101	LMU	O2B-C2B-C1B	2.52	116.07	110.08
20	A	837	CLA	C4-C3-C5	2.52	119.09	116.13
20	H	110	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
22	I	101	BCR	C16-C17-C18	-2.52	123.75	127.28
20	1	207	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
20	4	309	CLA	C3D-C4D-ND	2.51	112.94	109.50
20	A	834	CLA	C3D-C4D-ND	2.51	114.07	109.99
20	B	842	CLA	CHC-C1C-C2C	-2.51	119.80	126.95
20	2	305	CLA	CED-O2D-CGD	2.51	121.62	115.92
20	A	803	CLA	CHB-C1B-NB	-2.51	120.28	124.05
20	B	835	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
20	F	206	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
20	3	307	CLA	CED-O2D-CGD	2.51	121.61	115.92
20	1	208	CLA	C3D-C4D-ND	2.51	112.93	109.50
20	A	806	CLA	CAA-C2A-C1A	-2.51	103.75	111.97
20	A	802	CLA	C2C-C1C-CHC	-2.51	119.26	125.84
20	3	302	CLA	CHB-C4A-NA	2.51	128.00	124.43
20	A	824	CLA	CHB-C4A-NA	2.51	128.02	124.40
21	L	205	LMU	O4'-C4B-C5B	-2.51	103.14	109.32
20	A	836	CLA	CHC-C4B-NB	2.51	127.81	124.05
20	4	306	CLA	C3B-C2B-C1B	-2.51	104.21	107.17
20	L	202	CLA	O2A-CGA-CBA	2.51	119.48	111.83
20	2	315	CLA	CHD-C1D-ND	2.51	128.38	124.84
22	I	103	BCR	C29-C28-C27	2.51	116.79	111.28
20	A	807	CLA	O1D-CGD-CBD	-2.51	119.58	124.52
20	H	110	CLA	C1D-ND-C4D	-2.51	104.55	106.31
20	1	206	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
20	A	827	CLA	CGD-CBD-CAD	2.50	118.95	110.85
20	4	314	CLA	C3C-C4C-CHD	-2.50	118.73	125.23
20	2	315	CLA	C2D-C3D-C4D	-2.50	104.31	107.35
20	3	317	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	F	203	BCR	C33-C5-C4	2.50	118.93	113.60
20	B	820	CLA	CAA-C2A-C1A	2.50	120.17	111.97
20	B	815	CLA	O2A-CGA-CBA	2.50	119.46	111.83
20	B	822	CLA	CHC-C1C-C2C	-2.50	119.84	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	202	LMU	C4B-C3B-C2B	-2.50	106.44	110.83
20	A	807	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
20	3	308	CLA	C2C-C1C-CHC	-2.50	119.29	125.84
20	I	102	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
20	2	307	CLA	CMB-C2B-C1B	2.50	129.22	125.42
20	B	815	CLA	CED-O2D-CGD	2.50	121.58	115.92
20	3	304	CLA	C3D-C4D-ND	2.50	112.91	109.50
22	G	104	BCR	C8-C7-C6	-2.50	120.33	127.00
20	B	818	CLA	CHB-C4A-NA	2.50	128.00	124.40
20	2	311	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
20	B	838	CLA	O2A-CGA-CBA	2.49	119.44	111.83
20	B	811	CLA	C2C-C1C-CHC	-2.49	119.31	125.84
20	A	823	CLA	C4A-NA-C1A	2.49	107.82	106.68
20	2	303	CLA	CAA-C2A-C1A	-2.49	103.81	111.97
20	R	108	CLA	CHB-C1B-NB	-2.49	120.31	124.05
20	B	803	CLA	CHC-C4B-NB	2.49	127.79	124.05
20	L	201	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
20	4	311	CLA	CHB-C4A-NA	2.49	127.97	124.43
20	B	825	CLA	CBC-CAC-C3C	-2.49	105.68	112.42
20	A	809	CLA	CMB-C2B-C1B	2.49	129.21	125.42
22	J	102	BCR	C38-C26-C27	2.49	118.90	113.60
20	4	312	CLA	CHD-C1D-ND	2.49	128.35	124.84
20	R	107	CLA	C1D-ND-C4D	-2.49	104.57	106.31
20	A	804	CLA	CBA-CAA-C2A	2.49	121.19	113.79
20	A	839	CLA	CMB-C2B-C1B	2.48	129.20	125.42
21	G	101	LMU	O1B-C1B-O5B	2.48	117.23	110.69
20	L	202	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
20	1	204	CLA	CAC-C3C-C4C	2.48	128.02	124.79
20	A	820	CLA	C4-C3-C5	2.48	119.05	116.13
20	A	837	CLA	C4B-C3B-C2B	2.48	110.39	107.30
20	A	849	CLA	O2A-CGA-CBA	2.48	119.39	111.83
20	4	306	CLA	C3D-C4D-ND	2.48	114.02	109.99
20	B	850	CLA	CMB-C2B-C1B	2.48	129.19	125.42
20	B	829	CLA	C11-C12-C13	-2.48	107.74	115.97
20	A	838	CLA	C4B-C3B-C2B	2.47	110.38	107.30
21	R	102	LMU	C1'-O5'-C5'	-2.47	108.89	113.72
20	A	817	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
20	B	840	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
20	B	809	CLA	CAC-C3C-C4C	2.47	128.00	124.79
21	4	319	LMU	O5'-C5'-C6'	2.47	112.56	106.44
20	1	208	CLA	C3C-C4C-CHD	-2.47	118.82	125.23
22	A	843	BCR	C1-C6-C5	-2.47	119.27	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	CLA	CGD-CBD-CAD	2.47	118.83	110.85
20	A	809	CLA	CHD-C4C-C3C	-2.47	121.18	124.77
20	B	806	CLA	O2A-CGA-CBA	2.47	119.35	111.83
20	A	828	CLA	CAA-C2A-C1A	-2.47	103.89	111.97
20	A	818	CLA	CGD-CBD-CAD	2.47	118.83	110.85
20	3	313	CLA	CHB-C4A-NA	2.47	127.96	124.40
20	1	208	CLA	CHB-C4A-NA	2.46	127.93	124.43
20	1	211	CLA	C1D-ND-C4D	-2.46	104.58	106.31
21	3	319	LMU	O1'-C1'-C2'	2.46	112.01	108.27
20	A	826	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
20	B	802	CLA	O2A-CGA-CBA	2.46	119.34	111.83
20	A	815	CLA	C1-C2-C3	-2.46	122.78	126.76
20	B	835	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
20	B	825	CLA	CMB-C2B-C1B	2.46	129.16	125.42
20	B	830	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
20	B	827	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
22	B	801	BCR	C37-C22-C21	-2.46	118.83	122.82
20	J	103	CLA	C1-O2A-CGA	2.46	122.60	116.65
20	A	820	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	A	821	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	3	312	CLA	C2C-C1C-CHC	-2.46	119.40	125.84
20	K	101	CLA	C4A-NA-C1A	2.46	107.80	106.68
20	4	317	CLA	C1D-ND-C4D	-2.46	104.59	106.31
20	B	818	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
20	B	829	CLA	CMA-C3A-C2A	-2.46	104.49	113.98
20	A	813	CLA	C3D-C4D-ND	2.46	113.98	109.99
20	A	808	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
20	B	840	CLA	CHB-C4A-NA	2.46	127.94	124.40
20	4	304	CLA	CHB-C1B-NB	-2.46	120.37	124.05
21	A	855	LMU	O5'-C5'-C4'	-2.46	104.65	109.72
20	K	103	CLA	C4A-NA-C1A	2.45	107.80	106.68
22	B	846	BCR	C11-C12-C13	-2.45	119.63	126.36
21	R	105	LMU	O5B-C5B-C6B	2.45	112.52	106.44
20	A	819	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
21	A	848	LMU	C1B-O1B-C4'	-2.45	112.16	117.98
20	B	816	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	B	807	CLA	C3D-C4D-ND	2.45	113.97	109.99
20	2	305	CLA	CHC-C4B-NB	2.45	127.73	124.05
20	L	203	CLA	CHB-C1B-NB	-2.45	120.37	124.05
20	2	314	CLA	CED-O2D-CGD	2.45	121.48	115.92
20	2	309	CLA	C3C-C4C-CHD	-2.45	118.86	125.23
20	1	206	CLA	O2D-CGD-O1D	-2.45	119.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	201	CLA	C4A-NA-C1A	2.45	107.80	106.68
20	F	205	CLA	C3D-C4D-ND	2.45	113.97	109.99
20	B	803	CLA	C3D-C4D-ND	2.45	113.97	109.99
20	2	305	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
20	A	824	CLA	C1-C2-C3	-2.45	122.19	126.20
20	F	207	CLA	C4-C3-C5	2.45	119.48	115.23
21	R	105	LMU	C3B-C4B-C5B	-2.45	105.79	110.23
22	B	801	BCR	C23-C24-C25	-2.45	120.46	127.00
21	H	106	LMU	O1B-C4'-C3'	2.45	113.45	107.23
20	B	814	CLA	CHC-C4B-NB	2.45	127.72	124.05
20	B	839	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
20	1	205	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	B	806	CLA	C2A-C1A-CHA	-2.45	119.62	123.87
22	G	104	BCR	C38-C26-C27	2.44	118.81	113.60
20	B	830	CLA	CHB-C4A-NA	2.44	127.93	124.40
20	B	832	CLA	O2A-CGA-CBA	2.44	119.28	111.83
20	K	101	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
22	A	845	BCR	C28-C27-C26	-2.44	109.70	114.06
20	2	303	CLA	C3D-C4D-ND	2.44	113.96	109.99
20	B	814	CLA	C1D-ND-C4D	-2.44	104.60	106.31
21	1	216	LMU	C1B-O1B-C4'	-2.44	112.19	117.98
20	1	209	CLA	C3C-C4C-CHD	-2.44	118.89	125.23
20	A	825	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	F	201	CLA	O2A-CGA-CBA	2.44	119.27	111.83
20	2	302	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
20	B	803	CLA	CHB-C1B-NB	-2.44	120.39	124.05
20	F	206	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	4	308	CLA	C3C-C4C-CHD	-2.44	118.90	125.23
21	4	321	LMU	C1B-C2B-C3B	2.43	115.13	110.01
20	1	214	CLA	C3C-C4C-CHD	-2.43	118.91	125.23
20	A	828	CLA	O2A-CGA-CBA	2.43	119.25	111.83
20	2	302	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
20	B	821	CLA	C3D-C4D-ND	2.43	113.94	109.99
20	R	108	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
20	4	311	CLA	C3C-C4C-CHD	-2.43	118.92	125.23
20	4	309	CLA	C3C-C4C-CHD	-2.43	118.92	125.23
22	A	843	BCR	C28-C27-C26	-2.43	109.72	114.06
20	A	813	CLA	C1D-ND-C4D	-2.43	104.61	106.31
20	B	817	CLA	CHB-C1B-NB	-2.43	120.40	124.05
20	A	850	CLA	C4-C3-C5	2.43	119.44	115.23
20	B	828	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
20	3	313	CLA	CHC-C4B-NB	2.43	127.69	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	312	CLA	C3D-C4D-ND	2.43	112.82	109.50
20	2	310	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
20	H	110	CLA	C1-O2A-CGA	2.43	122.53	116.65
22	B	844	BCR	C29-C30-C25	-2.43	106.91	110.44
20	R	108	CLA	C3B-C2B-C1B	-2.43	104.31	107.17
22	B	844	BCR	C30-C25-C24	2.43	122.23	115.65
20	1	210	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
20	2	312	CLA	C4-C3-C2	-2.43	117.40	123.63
20	1	208	CLA	C2C-C1C-CHC	-2.43	119.48	125.84
20	3	302	CLA	C3D-C4D-ND	2.43	112.81	109.50
20	A	850	CLA	C1-C2-C3	-2.42	122.22	126.20
20	B	808	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
20	B	826	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
20	A	832	CLA	CHB-C1B-NB	-2.42	120.41	124.05
22	B	846	BCR	C23-C24-C25	-2.42	120.53	127.00
20	J	103	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
20	3	303	CLA	CHB-C4A-NA	2.42	127.89	124.40
21	2	319	LMU	O5'-C5'-C6'	2.42	112.44	106.44
20	B	839	CLA	CHC-C4B-NB	2.42	127.68	124.05
20	K	102	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	3	304	CLA	C3C-C4C-CHD	-2.42	118.95	125.23
20	A	803	CLA	CMB-C2B-C1B	2.42	129.10	125.42
22	B	844	BCR	C33-C5-C4	2.42	118.75	113.60
21	L	206	LMU	O5B-C5B-C6B	2.42	112.43	106.44
20	4	314	CLA	C2C-C1C-CHC	-2.42	119.51	125.84
20	2	310	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
22	B	844	BCR	C37-C22-C21	-2.42	118.90	122.82
20	B	835	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
20	B	832	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
20	A	818	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
20	2	316	CLA	C4-C3-C2	-2.41	117.43	123.63
21	1	218	LMU	O5'-C5'-C6'	2.41	112.42	106.44
20	H	108	CLA	CMB-C2B-C3B	2.41	132.22	126.55
20	3	303	CLA	CMC-C2C-C1C	2.41	128.80	125.03
20	B	827	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	B	803	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
20	3	308	CLA	C3D-C4D-ND	2.41	112.80	109.50
20	4	311	CLA	C3D-C4D-ND	2.41	112.79	109.50
20	B	819	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	B	840	CLA	C1-C2-C3	-2.41	122.25	126.20
20	A	820	CLA	CHC-C1C-C2C	-2.41	120.10	126.95
20	B	820	CLA	CHC-C1C-C2C	-2.41	120.10	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	303	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
20	B	810	CLA	CHB-C1B-NB	-2.41	120.44	124.05
20	3	313	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
20	A	836	CLA	C4A-NA-C1A	2.40	107.78	106.68
20	B	807	CLA	C1D-ND-C4D	-2.40	104.62	106.31
20	A	833	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	A	823	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	B	816	CLA	C4-C3-C2	-2.40	117.45	123.63
20	B	813	CLA	O2A-CGA-CBA	2.40	119.16	111.83
20	K	101	CLA	CHB-C4A-NA	2.40	127.87	124.40
20	A	831	CLA	CAC-C3C-C2C	-2.40	123.14	127.56
20	L	201	CLA	C3D-C4D-ND	2.40	113.89	109.99
20	A	833	CLA	CAC-C3C-C2C	-2.40	123.15	127.56
20	3	313	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
20	4	308	CLA	C2C-C1C-CHC	-2.40	119.56	125.84
20	L	204	CLA	C1-O2A-CGA	2.40	122.45	116.65
20	3	317	CLA	CHC-C4B-C3B	-2.40	120.47	127.43
20	4	315	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
20	A	829	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
20	B	842	CLA	CHC-C4B-C3B	-2.39	120.48	127.43
20	L	202	CLA	CHB-C4A-NA	2.39	127.85	124.40
21	G	102	LMU	O5B-C5B-C6B	-2.39	100.51	106.44
20	1	214	CLA	CHB-C1B-NB	-2.39	120.62	124.08
20	4	312	CLA	C3C-C4C-CHD	-2.39	119.02	125.23
20	2	316	CLA	O2A-CGA-CBA	2.39	119.12	111.83
20	A	841	CLA	CHB-C4A-NA	2.39	127.83	124.43
20	L	208	CLA	C1-C2-C3	-2.39	122.90	126.76
20	B	828	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
20	A	804	CLA	CHB-C4A-NA	2.39	127.85	124.40
20	A	813	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
20	A	807	CLA	CAC-C3C-C4C	2.39	127.90	124.79
22	A	844	BCR	C28-C27-C26	-2.39	109.80	114.06
20	B	802	CLA	CHC-C1C-C2C	-2.39	120.17	126.95
21	A	847	LMU	C1'-C2'-C3'	2.39	115.03	110.01
20	A	803	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
21	H	105	LMU	O5'-C1'-C2'	-2.39	105.47	110.37
20	2	301	CLA	C3D-C4D-ND	2.39	112.76	109.50
20	B	806	CLA	C1D-ND-C4D	-2.38	104.64	106.31
20	B	842	CLA	CHB-C1B-NB	-2.38	120.47	124.05
22	A	843	BCR	C15-C16-C17	-2.38	118.64	123.52
20	A	823	CLA	CMB-C2B-C1B	2.38	129.05	125.42
21	2	321	LMU	C1'-O5'-C5'	2.38	118.37	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	103	CLA	C2D-C1D-ND	-2.38	107.77	110.13
20	L	201	CLA	CHB-C4A-NA	2.38	127.84	124.40
22	2	317	BCR	C8-C7-C6	-2.38	120.63	127.00
21	H	106	LMU	O5'-C1'-C2'	2.38	115.26	110.37
21	K	106	LMU	C1B-O5B-C5B	-2.38	109.07	113.72
21	A	855	LMU	O5'-C5'-C6'	2.38	112.34	106.44
20	1	207	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
20	B	806	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
20	A	819	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
20	2	306	CLA	C3B-C4B-CHC	-2.38	118.33	126.76
22	B	846	BCR	C29-C30-C25	-2.38	106.98	110.44
20	4	317	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
20	A	838	CLA	C1D-ND-C4D	-2.38	104.64	106.31
21	H	104	LMU	C3B-C4B-C5B	-2.38	105.92	110.23
20	1	204	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
20	L	203	CLA	C6-C7-C8	-2.38	108.06	115.97
22	A	845	BCR	C8-C7-C6	-2.38	120.65	127.00
20	A	811	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
20	B	832	CLA	C1-O2A-CGA	2.38	122.40	116.65
22	A	844	BCR	C38-C26-C27	2.38	118.66	113.60
20	A	811	CLA	CHB-C1B-NB	-2.37	120.49	124.05
20	B	826	CLA	C4A-NA-C1A	2.37	107.76	106.68
20	1	215	CLA	CHD-C1D-ND	2.37	128.14	124.80
20	4	312	CLA	CHB-C4A-NA	2.37	127.81	124.43
20	A	821	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
20	A	822	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
21	H	106	LMU	O5'-C5'-C6'	2.37	112.32	106.44
20	4	301	CLA	C1D-ND-C4D	-2.37	104.65	106.31
20	A	827	CLA	CAC-C3C-C4C	2.37	127.88	124.79
20	A	835	CLA	CMB-C2B-C1B	2.37	129.03	125.42
20	A	807	CLA	CMC-C2C-C1C	2.37	128.74	125.03
20	K	104	CLA	C1-O2A-CGA	2.37	122.39	116.65
20	L	204	CLA	C4-C3-C2	-2.37	117.54	123.63
20	3	312	CLA	C3C-C4C-CHD	-2.37	119.08	125.23
20	R	107	CLA	C1-O2A-CGA	2.37	122.38	116.65
21	B	805	LMU	O5B-C1B-C2B	2.37	115.23	110.37
20	A	809	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
20	B	807	CLA	CMB-C2B-C1B	2.37	129.02	125.42
20	4	302	CLA	CBD-CHA-C1A	2.37	130.95	127.38
22	L	209	BCR	C8-C7-C6	-2.37	120.68	127.00
20	B	838	CLA	CHB-C1B-NB	-2.37	120.50	124.05
20	2	306	CLA	C3C-C4C-CHD	-2.36	119.09	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	210	LMU	O5'-C5'-C6'	2.36	112.30	106.44
20	1	201	CLA	C4D-CHA-C1A	-2.36	118.42	121.24
20	2	303	CLA	CED-O2D-CGD	2.36	121.28	115.92
20	1	211	CLA	CHB-C4A-NA	2.36	127.81	124.40
20	4	306	CLA	CHB-C1B-C2B	-2.36	120.57	127.43
20	B	827	CLA	C4A-NA-C1A	2.36	107.76	106.68
21	A	855	LMU	O1B-C4'-C5'	2.36	115.67	109.48
20	A	826	CLA	CHC-C4B-NB	2.36	127.59	124.05
20	B	841	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
20	4	306	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
22	B	844	BCR	C23-C22-C21	2.36	122.72	119.01
20	B	816	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
20	4	317	CLA	C4-C3-C5	2.36	119.33	115.23
20	A	838	CLA	C2A-C1A-CHA	-2.36	119.77	123.87
21	1	216	LMU	C1B-C2B-C3B	-2.36	105.05	110.01
20	B	831	CLA	CHB-C4A-NA	2.36	127.80	124.40
20	B	827	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
20	B	840	CLA	C3B-C4B-NB	-2.36	108.42	110.53
22	J	102	BCR	C30-C25-C24	2.36	122.05	115.65
20	B	828	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
20	B	820	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
20	B	817	CLA	CMB-C2B-C1B	2.36	129.01	125.42
20	A	816	CLA	C1-O2A-CGA	2.36	122.35	116.65
20	B	821	CLA	CMA-C3A-C2A	-2.36	104.88	113.98
22	B	847	BCR	C20-C19-C18	-2.35	119.91	126.36
20	4	303	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
20	B	807	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
20	A	834	CLA	C2A-C1A-CHA	-2.35	119.78	123.87
20	3	308	CLA	C3C-C4C-CHD	-2.35	119.12	125.23
20	J	101	CLA	CED-O2D-CGD	2.35	121.25	115.92
20	1	211	CLA	C2B-C1B-NB	2.35	112.76	110.33
20	B	828	CLA	CHC-C4B-NB	2.35	127.57	124.05
23	B	843	PQN	C14-C13-C15	2.35	119.30	115.23
20	4	315	CLA	CBA-CAA-C2A	-2.35	106.81	113.79
20	B	808	CLA	C4B-C3B-C2B	2.35	110.22	107.30
20	4	310	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
20	A	835	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
20	4	312	CLA	C2C-C1C-CHC	-2.34	119.70	125.84
21	A	848	LMU	O5'-C5'-C6'	2.34	112.25	106.44
20	B	835	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
20	A	816	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
20	B	817	CLA	O2D-CGD-O1D	-2.34	119.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	103	LMU	O5'-C5'-C4'	-2.34	104.89	109.72
21	B	804	LMU	C6B-C5B-C4B	-2.34	107.28	113.02
21	2	319	LMU	C3'-C4'-C5'	2.34	116.11	110.93
20	K	102	CLA	CED-O2D-CGD	2.34	121.22	115.92
20	A	809	CLA	CHB-C1B-NB	-2.34	120.54	124.05
20	B	826	CLA	O2A-CGA-CBA	2.34	118.96	111.83
20	A	833	CLA	CED-O2D-CGD	2.34	121.22	115.92
20	A	815	CLA	CHC-C4B-NB	2.34	127.56	124.05
22	A	845	BCR	C23-C24-C25	-2.34	120.75	127.00
20	2	312	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
20	B	810	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
20	F	206	CLA	C4A-NA-C1A	2.34	107.75	106.68
20	2	316	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
20	B	812	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
20	B	824	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
20	A	823	CLA	C1-C2-C3	-2.33	122.37	126.20
20	4	303	CLA	C1D-ND-C4D	-2.33	104.67	106.31
20	A	851	CLA	CHB-C1B-NB	-2.33	120.55	124.05
20	B	824	CLA	C10-C8-C7	2.33	123.89	112.07
20	A	833	CLA	C3D-C4D-ND	2.33	113.78	109.99
20	A	819	CLA	O2A-CGA-CBA	2.33	118.95	111.83
20	G	105	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
20	1	210	CLA	CHB-C4A-NA	2.33	127.77	124.40
20	2	305	CLA	C1-O2A-CGA	2.33	122.30	116.65
20	B	832	CLA	C1-C2-C3	-2.33	122.38	126.20
20	A	808	CLA	CMB-C2B-C1B	2.33	128.97	125.42
20	4	306	CLA	CGD-CBD-CAD	2.33	118.39	110.85
20	A	816	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
20	A	839	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
20	2	312	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
20	A	828	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	B	827	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	4	318	CLA	CAA-C2A-C3A	2.33	119.29	113.00
20	A	817	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
20	H	102	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	H	109	CLA	CED-O2D-CGD	2.33	121.20	115.92
20	4	305	CLA	C1-C2-C3	-2.33	123.00	126.76
20	A	838	CLA	C3D-C4D-ND	2.33	113.77	109.99
20	L	204	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
20	3	314	CLA	C11-C10-C8	-2.32	108.24	115.97
20	B	837	CLA	O2A-CGA-CBA	2.32	118.92	111.83
20	A	810	CLA	CMB-C2B-C1B	2.32	128.96	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	818	CLA	CED-O2D-CGD	2.32	121.18	115.92
22	J	102	BCR	C23-C24-C25	-2.32	120.79	127.00
20	B	819	CLA	C2D-C1D-ND	-2.32	107.83	110.13
20	1	215	CLA	C1-O2A-CGA	2.32	122.27	116.65
21	K	105	LMU	O3B-C3B-C4B	-2.32	104.90	110.38
20	F	201	CLA	C1D-ND-C4D	-2.32	104.68	106.31
20	3	306	CLA	CHD-C1D-ND	2.32	128.12	124.84
20	B	812	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
20	2	316	CLA	CED-O2D-CGD	2.32	121.17	115.92
20	B	806	CLA	CMB-C2B-C1B	2.32	128.95	125.42
20	A	805	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
20	3	307	CLA	CMB-C2B-C1B	2.32	128.95	125.42
20	2	302	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
20	4	302	CLA	CMB-C2B-C3B	2.32	129.69	123.53
20	B	838	CLA	C3D-C4D-ND	2.32	113.75	109.99
20	1	209	CLA	CHD-C1D-ND	2.32	128.12	124.84
20	1	201	CLA	CGD-CBD-CAD	-2.32	103.35	110.85
20	1	211	CLA	C3B-C2B-C1B	-2.32	104.44	107.17
20	B	803	CLA	CED-O2D-CGD	2.32	121.17	115.92
20	A	825	CLA	O2A-CGA-CBA	2.32	118.89	111.83
20	F	201	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
22	F	203	BCR	C11-C12-C13	-2.31	120.02	126.36
20	A	815	CLA	CGD-CBD-CAD	2.31	118.34	110.85
22	F	203	BCR	C24-C23-C22	-2.31	122.81	126.23
20	A	818	CLA	CAA-C2A-C1A	-2.31	104.39	111.97
20	A	807	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
20	A	804	CLA	C3D-C4D-ND	2.31	113.75	109.99
20	4	302	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
20	H	110	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
20	L	204	CLA	C3D-C4D-ND	2.31	113.74	109.99
25	B	848	LMG	O7-C10-O9	-2.31	118.30	123.70
22	F	203	BCR	C37-C22-C21	-2.31	119.07	122.82
22	B	846	BCR	C33-C5-C4	2.31	118.52	113.60
20	A	828	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
20	A	815	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
22	A	844	BCR	C3-C4-C5	-2.31	109.94	114.06
20	A	813	CLA	CHC-C4B-NB	2.31	127.51	124.05
20	4	308	CLA	CHB-C1B-NB	-2.31	120.75	124.08
20	B	817	CLA	C3D-C4D-ND	2.31	113.74	109.99
20	B	830	CLA	O2A-CGA-CBA	2.31	118.87	111.83
20	A	822	CLA	CAC-C3C-C4C	2.31	127.79	124.79
21	4	320	LMU	O5B-C5B-C6B	2.31	112.16	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	CLA	CHB-C1B-NB	-2.31	120.59	124.05
20	A	804	CLA	C1D-ND-C4D	-2.31	104.69	106.31
20	A	833	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
20	3	311	CLA	C1-C2-C3	-2.30	122.42	126.20
20	L	201	CLA	C1D-ND-C4D	-2.30	104.70	106.31
20	4	312	CLA	C3D-C2D-C1D	2.30	110.14	107.35
20	2	310	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
22	I	101	BCR	C12-C13-C14	-2.30	115.39	119.01
20	A	828	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
21	B	849	LMU	O1B-C4'-C3'	2.30	113.07	107.23
21	2	321	LMU	O1'-C1'-C2'	2.30	111.76	108.27
22	B	846	BCR	C37-C22-C23	2.30	121.60	118.09
20	B	828	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
20	3	301	CLA	CHB-C1B-NB	-2.30	120.60	124.05
20	3	317	CLA	CAA-C2A-C3A	-2.30	110.96	116.23
20	A	851	CLA	C3D-C4D-ND	2.30	113.72	109.99
20	F	207	CLA	C3D-C4D-ND	2.29	113.72	109.99
20	F	201	CLA	O1D-CGD-CBD	-2.29	119.99	124.52
20	1	213	CLA	CMA-C3A-C2A	2.29	122.85	113.98
20	L	204	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
21	A	846	LMU	O1'-C1'-C2'	2.29	111.75	108.27
20	G	105	CLA	CMB-C2B-C1B	2.29	128.91	125.42
20	A	829	CLA	C1-O2A-CGA	2.29	122.20	116.65
20	B	825	CLA	C1-O2A-CGA	2.29	122.20	116.65
20	2	307	CLA	CHB-C1B-NB	-2.29	120.61	124.05
21	L	205	LMU	O1B-C1B-C2B	2.29	113.73	108.09
21	3	318	LMU	C1B-O1B-C4'	-2.29	112.55	117.98
22	A	844	BCR	C4-C5-C6	-2.29	119.61	122.70
20	4	302	CLA	CHB-C4A-NA	2.29	127.70	124.40
20	A	812	CLA	CED-O2D-CGD	2.29	121.11	115.92
20	1	203	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
20	4	314	CLA	CHD-C1D-ND	2.29	128.07	124.84
20	A	826	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
20	F	206	CLA	C2A-C1A-CHA	-2.29	119.90	123.86
20	L	203	CLA	O2A-CGA-CBA	2.29	118.81	111.83
20	G	105	CLA	C4-C3-C5	2.29	118.82	116.13
20	A	849	CLA	CMC-C2C-C1C	2.29	128.60	125.03
22	A	845	BCR	C1-C6-C7	2.28	121.85	115.65
21	A	852	LMU	O5'-C5'-C6'	2.28	112.10	106.44
20	B	820	CLA	CMC-C2C-C1C	2.28	128.60	125.03
20	A	806	CLA	C3D-C4D-ND	2.28	113.70	109.99
22	A	843	BCR	C1-C6-C7	2.28	121.84	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	209	CLA	C1C-NC-C4C	-2.28	105.64	106.68
20	B	830	CLA	C3D-C4D-ND	2.28	113.69	109.99
22	B	844	BCR	C36-C18-C19	2.28	121.57	118.09
21	R	103	LMU	O5B-C5B-C4B	2.28	113.81	109.70
20	A	819	CLA	CGD-CBD-CAD	2.28	118.22	110.85
20	B	840	CLA	C1D-ND-C4D	-2.28	104.71	106.31
20	H	108	CLA	C4B-C3B-C2B	2.28	110.13	107.30
20	B	841	CLA	C4-C3-C5	2.28	119.18	115.23
20	B	834	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
21	A	846	LMU	O5B-C5B-C4B	2.28	113.80	109.70
20	A	835	CLA	C1D-ND-C4D	-2.28	104.72	106.31
22	A	845	BCR	C11-C12-C13	-2.28	120.12	126.36
20	4	317	CLA	O2A-CGA-CBA	2.28	118.77	111.83
22	A	844	BCR	C15-C16-C17	-2.28	118.86	123.52
21	R	102	LMU	O1'-C1'-C2'	2.28	111.73	108.27
20	4	318	CLA	CMB-C2B-C1B	2.27	128.88	125.42
20	B	842	CLA	CGD-CBD-CAD	-2.27	104.97	114.30
20	A	816	CLA	CED-O2D-CGD	2.27	121.08	115.92
20	B	821	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	A	837	CLA	CBC-CAC-C3C	-2.27	106.25	112.42
20	2	308	CLA	C3D-C4D-ND	2.27	112.61	109.50
20	B	836	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	B	830	CLA	C1D-ND-C4D	-2.27	104.72	106.31
20	L	208	CLA	CAC-C3C-C4C	2.27	127.74	124.79
21	G	102	LMU	O5B-C1B-C2B	-2.27	105.71	110.37
20	B	832	CLA	CMB-C2B-C1B	2.27	128.87	125.42
20	A	818	CLA	CHB-C4A-NA	2.27	127.67	124.40
22	B	844	BCR	C15-C14-C13	-2.27	124.10	127.28
20	F	201	CLA	CHB-C4A-NA	2.27	127.67	124.40
20	1	203	CLA	C3B-C4B-NB	-2.27	108.51	110.53
20	A	839	CLA	C3D-C4D-ND	2.26	113.67	109.99
20	4	317	CLA	C3A-C2A-C1A	2.26	104.73	101.34
20	A	826	CLA	C7-C6-C5	-2.26	107.23	113.26
20	B	850	CLA	C3D-C4D-ND	2.26	113.67	109.99
20	K	103	CLA	C5-C3-C4	2.26	119.80	114.59
20	B	802	CLA	CHB-C1B-NB	-2.26	120.66	124.05
20	L	202	CLA	C4-C3-C5	2.26	119.16	115.23
20	A	819	CLA	C1-O2A-CGA	2.26	122.12	116.65
20	A	834	CLA	CHB-C4A-NA	2.26	127.66	124.40
20	B	813	CLA	CHB-C1B-NB	-2.26	120.66	124.05
20	B	814	CLA	C3D-C4D-ND	2.26	113.66	109.99
21	A	854	LMU	C1-O1'-C1'	-2.26	109.82	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	313	CLA	CAC-C3C-C4C	2.26	128.57	125.03
21	1	218	LMU	O5B-C5B-C6B	2.26	112.04	106.44
22	A	844	BCR	C1-C6-C7	2.26	121.78	115.65
20	4	306	CLA	C4-C3-C2	-2.26	117.82	123.63
22	B	844	BCR	C4-C5-C6	-2.26	119.65	122.70
22	2	317	BCR	C20-C19-C18	-2.26	120.17	126.36
20	3	304	CLA	CHB-C1B-NB	-2.26	120.82	124.08
20	K	101	CLA	C3D-C4D-ND	2.26	113.66	109.99
20	3	317	CLA	CHB-C1B-NB	-2.26	120.67	124.05
20	A	819	CLA	CHC-C4B-NB	2.26	127.43	124.05
20	1	210	CLA	CHB-C1B-NB	-2.26	120.67	124.05
20	A	816	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
22	A	843	BCR	C38-C26-C27	2.25	118.40	113.60
20	A	831	CLA	C11-C12-C13	-2.25	108.47	115.97
20	3	309	CLA	C3C-C4C-CHD	-2.25	119.38	125.23
20	F	207	CLA	O2A-CGA-CBA	2.25	118.70	111.83
22	I	103	BCR	C19-C18-C17	2.25	122.55	119.01
20	B	823	CLA	O2A-CGA-CBA	2.25	118.70	111.83
20	3	314	CLA	CHC-C4B-C3B	-2.25	117.60	127.37
20	A	850	CLA	O2A-C1-C2	2.25	116.77	108.11
20	L	201	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
22	B	846	BCR	C30-C25-C26	-2.25	119.56	122.64
22	B	845	BCR	C16-C15-C14	-2.25	118.92	123.52
20	B	826	CLA	CHB-C4A-NA	2.25	127.65	124.40
20	A	828	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
20	B	809	CLA	CMA-C3A-C2A	-2.25	105.29	113.98
20	B	817	CLA	O2A-CGA-CBA	2.25	120.63	112.14
20	A	815	CLA	C3D-C4D-ND	2.25	113.64	109.99
20	4	317	CLA	CMB-C2B-C1B	2.25	128.84	125.42
20	A	806	CLA	CMB-C2B-C1B	2.25	128.84	125.42
20	B	823	CLA	CAC-C3C-C4C	2.25	127.71	124.79
22	L	209	BCR	C28-C27-C26	-2.25	110.05	114.06
20	1	212	CLA	C3C-C4C-CHD	-2.24	119.40	125.23
20	A	801	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
20	1	215	CLA	O2A-CGA-CBA	2.24	118.68	111.83
20	A	826	CLA	C11-C10-C8	-2.24	108.51	115.97
20	B	809	CLA	C3D-C4D-ND	2.24	113.63	109.99
20	R	108	CLA	CGD-CBD-CAD	-2.24	103.59	110.85
22	A	843	BCR	C30-C25-C26	-2.24	119.57	122.64
20	B	840	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
20	A	829	CLA	CHB-C4A-NA	2.24	127.63	124.40
20	4	303	CLA	C6-C5-C3	-2.24	108.01	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	201	CLA	CED-O2D-CGD	2.24	120.99	115.92
20	2	311	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
20	H	102	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
20	A	832	CLA	CED-O2D-CGD	2.24	120.99	115.92
20	A	832	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
21	R	102	LMU	C3B-C4B-C5B	-2.24	106.18	110.23
21	B	804	LMU	O3'-C3'-C2'	2.24	115.64	110.38
20	A	838	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
20	4	304	CLA	CAC-C3C-C2C	-2.23	123.45	127.56
22	2	317	BCR	C37-C22-C23	2.23	121.50	118.09
20	4	318	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
20	L	203	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
20	1	205	CLA	CAA-C2A-C3A	-2.23	111.11	116.23
20	H	102	CLA	CHB-C1B-NB	-2.23	120.70	124.05
20	A	813	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
23	A	842	PQN	C12-C11-C3	-2.23	106.58	112.08
22	A	845	BCR	C38-C26-C25	-2.23	122.05	124.48
20	B	809	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
21	K	107	LMU	O5B-C5B-C6B	2.23	111.96	106.44
20	A	838	CLA	C6-C7-C8	-2.23	108.56	115.97
20	B	830	CLA	C4B-C3B-C2B	2.23	110.07	107.30
20	B	825	CLA	CAA-CBA-CGA	-2.23	106.88	113.21
22	B	801	BCR	C20-C19-C18	-2.23	120.26	126.36
22	A	845	BCR	C35-C13-C14	-2.23	119.21	122.82
22	2	317	BCR	C36-C18-C17	-2.22	119.22	122.82
20	1	213	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
20	2	307	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
20	A	808	CLA	O2A-CGA-CBA	2.22	118.61	111.83
20	4	305	CLA	C1D-ND-C4D	-2.22	104.75	106.31
20	A	809	CLA	CHC-C4B-C3B	-2.22	117.74	127.37
20	1	206	CLA	CED-O2D-CGD	2.22	120.95	115.92
20	B	827	CLA	C3D-C4D-ND	2.22	113.59	109.99
20	3	313	CLA	C3D-C4D-ND	2.22	113.59	109.99
20	A	851	CLA	CGD-CBD-CAD	2.22	118.03	110.85
20	H	110	CLA	O2A-CGA-CBA	2.22	118.60	111.83
20	B	813	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
20	4	303	CLA	C7-C6-C5	-2.22	107.35	113.26
21	E	101	LMU	C1'-C2'-C3'	2.22	114.67	110.01
20	B	833	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
20	2	314	CLA	C1D-ND-C4D	-2.22	104.76	106.31
21	L	205	LMU	O5B-C1B-C2B	2.22	114.92	110.37
20	4	301	CLA	CMB-C2B-C1B	2.22	128.79	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	834	CLA	CMB-C2B-C1B	2.22	128.79	125.42
20	A	815	CLA	CED-O2D-CGD	2.21	120.94	115.92
20	B	841	CLA	CAA-CBA-CGA	2.21	119.49	113.21
20	B	812	CLA	CAC-C3C-C4C	2.21	127.67	124.79
20	A	830	CLA	C3D-C4D-ND	2.21	113.58	109.99
20	L	208	CLA	CHB-C4A-NA	2.21	127.59	124.40
20	3	310	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
20	B	814	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
20	3	314	CLA	O2A-CGA-CBA	2.21	118.57	111.83
20	3	314	CLA	CMB-C2B-C1B	2.21	128.78	125.42
20	2	302	CLA	CHC-C4B-NB	2.21	127.36	124.05
20	A	849	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
20	A	806	CLA	CHB-C1B-NB	-2.21	120.74	124.05
20	K	104	CLA	C4A-NA-C1A	2.21	107.69	106.68
20	4	317	CLA	C4-C3-C2	-2.21	117.96	123.63
21	B	805	LMU	O3B-C3B-C2B	-2.21	105.17	110.38
20	H	110	CLA	CHC-C4B-NB	2.21	127.36	124.05
20	4	313	CLA	CHC-C4B-C3B	-2.21	121.02	127.43
20	R	107	CLA	CAA-CBA-CGA	2.21	119.47	113.21
20	1	206	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
20	A	849	CLA	CHB-C1B-NB	-2.21	120.74	124.05
20	B	831	CLA	C3D-C4D-ND	2.21	113.57	109.99
20	R	108	CLA	CAA-C2A-C1A	2.21	119.20	111.97
21	A	848	LMU	C1-O1'-C1'	-2.20	109.91	113.68
20	B	850	CLA	CAC-C3C-C4C	2.20	127.66	124.79
20	A	813	CLA	CHB-C1B-NB	-2.20	120.74	124.05
21	R	109	LMU	O1'-C1'-C2'	2.20	111.62	108.27
20	2	308	CLA	CHD-C1D-ND	2.20	127.95	124.84
20	3	303	CLA	CHC-C4B-NB	2.20	127.35	124.05
22	A	844	BCR	C38-C26-C25	-2.20	122.08	124.48
20	F	205	CLA	C1D-ND-C4D	-2.20	104.77	106.31
20	B	815	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
20	A	809	CLA	C3D-C4D-ND	2.20	113.56	109.99
20	A	825	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
20	3	313	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
20	2	301	CLA	C3C-C4C-CHD	-2.20	119.52	125.23
20	K	103	CLA	CED-O2D-CGD	2.20	120.90	115.92
20	2	302	CLA	C4D-CHA-C1A	2.20	123.87	121.24
20	A	817	CLA	C3D-C4D-ND	2.20	113.56	109.99
21	1	218	LMU	C1'-C2'-C3'	2.20	114.63	110.01
22	J	102	BCR	C33-C5-C6	-2.20	122.09	124.48
20	B	840	CLA	C3D-C4D-ND	2.20	113.56	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	307	CLA	CED-O2D-CGD	2.20	120.90	115.92
20	A	839	CLA	CED-O2D-CGD	2.20	120.90	115.92
22	F	203	BCR	C38-C26-C27	2.20	118.28	113.60
20	B	833	CLA	CMB-C2B-C1B	2.19	128.76	125.42
20	A	834	CLA	C3B-C4B-NB	-2.19	108.57	110.53
20	4	306	CLA	C4-C3-C5	2.19	119.04	115.23
21	3	319	LMU	C1'-O5'-C5'	2.19	118.00	113.72
20	4	314	CLA	C3D-C4D-ND	2.19	112.50	109.50
20	4	307	CLA	CHB-C4A-NA	2.19	127.55	124.43
20	A	851	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
20	K	104	CLA	CMB-C2B-C1B	2.19	128.76	125.42
22	I	103	BCR	C7-C6-C5	2.19	126.60	121.56
22	B	845	BCR	C1-C6-C7	2.19	121.59	115.65
20	B	810	CLA	CAC-C3C-C4C	2.19	127.64	124.79
20	A	836	CLA	CHB-C1B-NB	-2.19	120.76	124.05
22	B	847	BCR	C27-C26-C25	-2.19	119.75	122.70
20	B	810	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
20	B	833	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
21	R	101	LMU	O5B-C1B-C2B	-2.19	105.87	110.37
22	B	846	BCR	C27-C26-C25	-2.19	119.75	122.70
20	R	107	CLA	C3D-C4D-ND	2.19	113.54	109.99
21	D	201	LMU	O5'-C1'-C2'	-2.19	105.88	110.37
20	A	801	CLA	CHB-C1B-NB	-2.19	120.77	124.05
20	A	813	CLA	CMB-C2B-C1B	2.18	128.75	125.42
20	K	102	CLA	C3D-C4D-ND	2.18	113.54	109.99
20	4	303	CLA	CAC-C3C-C4C	2.18	127.63	124.79
20	1	213	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
20	A	813	CLA	C5-C3-C4	2.18	119.61	114.59
20	A	833	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
20	4	309	CLA	CHD-C1D-ND	2.18	127.92	124.84
20	K	102	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
20	A	837	CLA	C1-O2A-CGA	2.18	121.93	116.65
20	B	850	CLA	C7-C6-C5	-2.18	107.45	113.26
20	A	818	CLA	C3D-C4D-ND	2.18	113.53	109.99
20	B	822	CLA	O2A-CGA-CBA	2.18	120.37	112.14
20	B	815	CLA	C3D-C4D-ND	2.18	113.53	109.99
20	A	803	CLA	CBC-CAC-C3C	-2.18	106.51	112.42
21	H	103	LMU	O6'-C6'-C5'	-2.18	103.92	111.33
21	R	104	LMU	O1B-C1B-O5B	-2.18	104.96	110.69
20	B	827	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
21	E	101	LMU	O3B-C3B-C2B	2.18	115.51	110.38
20	A	818	CLA	C2A-C1A-CHA	-2.18	120.09	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	845	BCR	C20-C19-C18	-2.17	120.40	126.36
20	1	201	CLA	CHC-C4B-C3B	-2.17	117.93	127.37
20	4	315	CLA	CHB-C1B-NB	-2.17	120.79	124.05
20	I	102	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	2	302	CLA	C2A-C1A-CHA	-2.17	120.09	123.87
20	3	302	CLA	CHB-C1B-NB	-2.17	120.94	124.08
21	G	102	LMU	O5B-C5B-C4B	-2.17	105.78	109.70
21	L	210	LMU	O1B-C4'-C3'	2.17	112.75	107.23
22	G	104	BCR	C28-C27-C26	-2.17	110.18	114.06
20	B	826	CLA	CMB-C2B-C1B	2.17	128.72	125.42
20	1	201	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
20	B	821	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
20	1	210	CLA	CHC-C4B-C3B	-2.17	121.14	127.43
21	4	321	LMU	C3B-C4B-C5B	2.17	114.16	110.23
20	A	802	CLA	C3D-C2D-C1D	2.17	109.98	107.35
21	3	319	LMU	C1'-C2'-C3'	-2.17	105.45	110.01
20	A	803	CLA	O2A-CGA-CBA	2.17	120.32	112.14
22	F	204	BCR	C4-C5-C6	-2.16	119.78	122.70
20	A	811	CLA	C3A-C2A-C1A	2.16	104.58	101.34
21	A	853	LMU	C1-O1'-C1'	-2.16	109.98	113.68
22	J	102	BCR	C11-C12-C13	-2.16	120.43	126.36
21	H	103	LMU	O1'-C1'-C2'	2.16	111.56	108.27
20	1	206	CLA	C3D-C4D-ND	2.16	113.50	109.99
20	L	202	CLA	C3D-C4D-ND	2.16	113.50	109.99
22	J	102	BCR	C15-C16-C17	-2.16	119.09	123.52
20	2	315	CLA	CHB-C1B-NB	-2.16	120.95	124.08
20	3	303	CLA	C3D-C4D-ND	2.16	113.50	109.99
20	2	312	CLA	CMB-C2B-C1B	2.16	128.71	125.42
20	A	807	CLA	O2A-CGA-CBA	2.16	120.30	112.14
20	4	318	CLA	C2D-C1D-ND	-2.16	107.99	110.13
21	H	105	LMU	O1'-C1-C2	2.16	116.69	109.37
20	A	824	CLA	C3D-C4D-ND	2.16	113.50	109.99
20	B	823	CLA	C3D-C4D-ND	2.16	113.50	109.99
20	F	201	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
20	B	812	CLA	C1-C2-C3	-2.16	122.66	126.20
20	A	809	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
20	2	312	CLA	C11-C12-C13	-2.16	108.80	115.97
20	4	301	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	3	314	CLA	CED-O2D-CGD	2.16	120.81	115.92
20	A	839	CLA	C6-C5-C3	-2.16	108.22	113.47
20	L	208	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
20	B	829	CLA	O1D-CGD-CBD	-2.15	120.27	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	842	CLA	C1D-ND-C4D	-2.15	104.80	106.31
20	3	317	CLA	C3D-C4D-ND	2.15	113.49	109.99
20	A	824	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
21	R	104	LMU	C1B-O1B-C4'	2.15	123.08	117.98
20	B	833	CLA	CAC-C3C-C4C	2.15	127.59	124.79
20	2	315	CLA	C3D-C4D-ND	2.15	112.44	109.50
20	B	814	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
20	F	207	CLA	C2A-C3A-C4A	2.15	105.34	101.87
20	B	838	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
20	H	101	CLA	CAA-C2A-C1A	2.15	119.02	111.97
20	A	849	CLA	C6-C7-C8	-2.15	108.82	115.97
22	2	317	BCR	C24-C23-C22	-2.15	123.06	126.23
20	A	822	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
22	B	845	BCR	C2-C1-C6	2.15	113.56	110.44
20	L	204	CLA	CED-O2D-CGD	2.15	120.79	115.92
22	F	204	BCR	C35-C13-C14	-2.15	119.34	122.82
20	B	831	CLA	C2D-C1D-ND	-2.15	108.00	110.13
20	2	303	CLA	C6-C5-C3	-2.15	108.24	113.47
20	4	306	CLA	C3C-C4C-NC	-2.15	107.68	110.43
20	H	110	CLA	C3D-C4D-ND	2.14	113.47	109.99
20	A	849	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
20	A	837	CLA	C3D-C4D-ND	2.14	113.47	109.99
20	B	814	CLA	C3A-C2A-C1A	2.14	104.55	101.34
20	B	842	CLA	C3D-C4D-ND	2.14	113.47	109.99
20	2	307	CLA	CHC-C4B-C3B	-2.14	118.07	127.37
20	I	102	CLA	CMB-C2B-C1B	2.14	128.68	125.42
20	B	808	CLA	CBC-CAC-C3C	-2.14	106.61	112.42
20	B	808	CLA	C4-C3-C5	2.14	118.95	115.23
22	J	102	BCR	C20-C19-C18	-2.14	120.49	126.36
20	2	310	CLA	C5-C3-C4	2.14	119.52	114.59
21	2	319	LMU	O5'-C1'-C2'	2.14	114.77	110.37
20	2	307	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	L	202	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
21	C	101	LMU	O5B-C5B-C4B	-2.14	105.84	109.70
20	A	825	CLA	CMB-C2B-C1B	2.14	128.68	125.42
21	A	854	LMU	C3'-C4'-C5'	2.14	115.67	110.93
20	H	109	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
20	A	835	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	F	207	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
22	B	845	BCR	C33-C5-C6	-2.14	122.15	124.48
20	3	312	CLA	CHB-C1B-NB	-2.14	120.99	124.08
22	B	847	BCR	C1-C6-C5	-2.14	119.72	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	310	CLA	CHB-C4A-NA	2.13	127.48	124.40
20	B	812	CLA	CAA-CBA-CGA	-2.13	107.15	113.21
20	A	828	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
20	K	101	CLA	CMB-C2B-C1B	2.13	128.66	125.42
22	J	102	BCR	C28-C27-C26	-2.13	110.25	114.06
20	A	829	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	B	826	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
20	F	206	CLA	C3D-C4D-ND	2.13	113.45	109.99
21	K	107	LMU	O5'-C5'-C6'	2.13	111.72	106.44
20	1	210	CLA	C3D-C4D-ND	2.13	113.45	109.99
20	B	835	CLA	O2A-CGA-O1A	-2.13	117.85	123.33
20	1	205	CLA	CMB-C2B-C1B	2.13	128.66	125.42
21	B	805	LMU	C1'-C2'-C3'	2.13	114.49	110.01
20	A	809	CLA	C1-C2-C3	2.13	129.69	126.20
22	B	846	BCR	C16-C15-C14	-2.13	119.16	123.52
20	2	314	CLA	CAC-C3C-C4C	-2.13	122.02	124.79
20	B	835	CLA	CHB-C4A-NA	2.13	127.47	124.40
20	3	308	CLA	CHB-C1B-NB	-2.13	121.00	124.08
21	G	102	LMU	O4'-C4B-C3B	2.13	115.39	110.38
20	B	816	CLA	C3D-C4D-ND	2.13	113.44	109.99
20	B	829	CLA	C16-C15-C13	-2.13	108.90	115.97
21	B	849	LMU	C3B-C4B-C5B	2.13	114.09	110.23
20	2	311	CLA	CED-O2D-CGD	2.13	120.74	115.92
20	3	306	CLA	C3D-C4D-ND	2.13	112.41	109.50
20	A	836	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
20	H	102	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
20	B	850	CLA	C1D-ND-C4D	-2.12	104.82	106.31
20	B	836	CLA	C3D-C4D-ND	2.12	113.44	109.99
22	G	104	BCR	C11-C12-C13	-2.12	120.54	126.36
20	1	215	CLA	CMA-C3A-C2A	-2.12	105.78	113.98
20	1	215	CLA	CHC-C4B-NB	2.12	127.23	124.05
21	E	101	LMU	O1'-C1'-C2'	-2.12	105.05	108.27
20	B	826	CLA	C3D-C4D-ND	2.12	113.43	109.99
20	A	819	CLA	C3A-C2A-C1A	2.12	104.52	101.34
22	G	104	BCR	C27-C26-C25	-2.12	119.84	122.70
20	3	315	CLA	C3D-C2D-C1D	2.12	109.92	107.35
20	L	204	CLA	CMC-C2C-C1C	2.12	128.34	125.03
20	B	823	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
20	1	206	CLA	CBC-CAC-C3C	2.12	118.16	112.42
20	3	307	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
20	A	824	CLA	C4-C3-C5	2.12	118.90	115.23
20	B	850	CLA	C16-C17-C18	-2.12	106.49	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	854	LMU	O5B-C5B-C6B	2.12	111.68	106.44
20	B	850	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
20	3	301	CLA	C3D-C4D-ND	2.12	113.43	109.99
20	1	203	CLA	O2A-CGA-CBA	2.12	118.29	111.83
20	3	317	CLA	C2A-C1A-CHA	-2.12	120.19	123.86
20	3	315	CLA	C3C-C4C-CHD	-2.12	119.74	125.23
21	B	805	LMU	C1B-C2B-C3B	2.12	114.46	110.01
20	1	209	CLA	CHB-C1B-NB	-2.12	121.02	124.08
20	B	803	CLA	CMA-C3A-C2A	-2.11	105.81	113.98
20	2	303	CLA	C6-C7-C8	-2.11	108.94	115.97
22	B	845	BCR	C35-C13-C14	-2.11	119.39	122.82
20	A	817	CLA	CHB-C1B-NB	-2.11	120.88	124.05
20	B	811	CLA	CHB-C4A-NA	2.11	127.44	124.43
20	3	314	CLA	CAC-C3C-C4C	2.11	127.54	124.79
20	B	816	CLA	C4A-NA-C1A	2.11	107.64	106.68
20	A	838	CLA	CHB-C1B-NB	-2.11	120.88	124.05
20	4	306	CLA	CHC-C4B-NB	2.11	127.22	124.05
21	R	101	LMU	C1-O1'-C1'	-2.11	110.07	113.68
20	B	814	CLA	CHB-C4A-NA	2.11	127.45	124.40
20	L	203	CLA	CHB-C4A-NA	2.11	127.45	124.40
20	2	312	CLA	C2A-C1A-CHA	-2.11	120.20	123.87
20	B	839	CLA	CHB-C4A-NA	2.11	127.45	124.40
20	A	813	CLA	O2A-CGA-CBA	2.11	118.27	111.83
20	A	808	CLA	C2A-C1A-CHA	-2.11	120.20	123.87
20	B	806	CLA	C4A-NA-C1A	2.11	107.64	106.68
20	A	813	CLA	CAC-C3C-C4C	2.11	127.54	124.79
20	3	310	CLA	C1D-ND-C4D	-2.11	104.83	106.31
20	3	304	CLA	C3B-C4B-CHC	-2.11	119.28	126.76
20	L	204	CLA	CHB-C4A-NA	2.11	127.44	124.40
20	4	314	CLA	C1C-NC-C4C	-2.11	105.72	106.68
20	B	837	CLA	C4A-NA-C1A	2.11	107.64	106.68
20	A	826	CLA	C3D-C4D-ND	2.11	113.41	109.99
22	F	203	BCR	C8-C7-C6	-2.11	121.37	127.00
21	K	105	LMU	C4B-C3B-C2B	2.11	114.53	110.83
20	2	311	CLA	CHB-C1B-NB	-2.11	120.89	124.05
20	B	803	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
20	A	812	CLA	C3D-C4D-ND	2.10	113.41	109.99
20	A	821	CLA	C3D-C4D-ND	2.10	113.41	109.99
20	1	204	CLA	CHC-C4B-C3B	-2.10	118.24	127.37
20	A	831	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
20	J	101	CLA	C3D-C4D-ND	2.10	113.40	109.99
21	B	849	LMU	O5'-C5'-C4'	2.10	114.07	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	804	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
20	4	305	CLA	CHB-C4A-NA	2.10	127.43	124.40
20	B	820	CLA	CHB-C1B-NB	-2.10	120.90	124.05
20	B	833	CLA	CHB-C1B-NB	-2.10	120.90	124.05
20	B	802	CLA	CMC-C2C-C1C	2.10	128.31	125.03
20	4	302	CLA	C3D-C4D-ND	2.10	113.40	109.99
20	B	828	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
20	H	110	CLA	CHB-C4A-NA	2.10	127.43	124.40
20	1	202	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
20	B	850	CLA	C1-C2-C3	-2.10	122.76	126.20
22	A	843	BCR	C11-C12-C13	-2.10	120.61	126.36
20	2	305	CLA	C3D-C4D-ND	2.10	113.40	109.99
22	A	843	BCR	C27-C26-C25	-2.10	119.87	122.70
20	A	851	CLA	C16-C15-C13	-2.10	109.00	115.97
20	A	838	CLA	C4D-CHA-C1A	-2.09	118.75	121.24
20	A	822	CLA	O2A-CGA-CBA	2.09	118.22	111.83
20	A	815	CLA	C4A-NA-C1A	2.09	107.63	106.68
21	2	319	LMU	C3B-C4B-C5B	2.09	114.03	110.23
20	A	838	CLA	CMB-C2B-C1B	2.09	128.61	125.42
21	R	104	LMU	O5'-C5'-C4'	2.09	114.05	109.72
22	A	845	BCR	C37-C22-C21	-2.09	119.43	122.82
21	R	102	LMU	C6'-C5'-C4'	2.09	119.26	113.38
20	B	830	CLA	C1-O2A-CGA	2.09	121.71	116.65
20	A	839	CLA	C1D-ND-C4D	-2.09	104.85	106.31
20	3	303	CLA	CMB-C2B-C3B	2.09	129.08	123.53
20	A	820	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
21	A	854	LMU	C1B-C2B-C3B	2.09	114.40	110.01
20	1	206	CLA	CMB-C2B-C1B	2.09	128.60	125.42
20	B	821	CLA	CHB-C1B-NB	-2.09	120.92	124.05
20	2	311	CLA	C5-C3-C4	2.09	119.39	114.59
20	L	207	CLA	CMB-C2B-C1B	2.09	128.59	125.42
20	R	108	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
20	A	815	CLA	CHB-C1B-NB	-2.09	120.92	124.05
20	3	310	CLA	C11-C10-C8	-2.09	109.03	115.97
22	B	847	BCR	C28-C27-C26	-2.08	110.34	114.06
21	B	804	LMU	C4B-C3B-C2B	-2.08	107.17	110.83
20	3	313	CLA	CAA-C2A-C1A	2.08	118.80	111.97
20	B	835	CLA	C3D-C4D-ND	2.08	113.37	109.99
20	3	313	CLA	C4A-NA-C1A	2.08	107.63	106.68
20	B	818	CLA	C1-O2A-CGA	2.08	121.69	116.65
20	A	834	CLA	C4B-C3B-C2B	2.08	109.89	107.30
22	L	209	BCR	C30-C25-C24	2.08	121.29	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	837	CLA	CMB-C2B-C1B	2.08	128.59	125.42
20	4	315	CLA	CMB-C2B-C1B	2.08	128.58	125.42
20	H	110	CLA	CHB-C1B-NB	-2.08	120.93	124.05
20	A	849	CLA	CGD-CBD-CAD	2.08	117.57	110.85
20	4	304	CLA	C4D-CHA-C1A	-2.08	118.77	121.24
20	A	850	CLA	CMB-C2B-C1B	2.08	128.58	125.42
22	B	846	BCR	C20-C19-C18	-2.08	120.67	126.36
20	R	107	CLA	CHB-C4A-NA	2.08	127.40	124.40
22	B	847	BCR	C33-C5-C6	-2.08	122.22	124.48
20	4	305	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
20	A	832	CLA	C3D-C4D-ND	2.08	113.36	109.99
21	A	847	LMU	C1B-C2B-C3B	2.08	114.38	110.01
20	3	310	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
20	B	812	CLA	CHC-C4B-C3B	-2.08	121.40	127.43
23	B	843	PQN	C2M-C2-C1	2.08	120.50	116.68
22	F	204	BCR	C20-C19-C18	-2.08	120.67	126.36
20	B	809	CLA	C4-C3-C5	2.08	118.83	115.23
20	B	837	CLA	CHB-C4A-NA	2.07	127.39	124.40
20	4	301	CLA	C3D-C4D-ND	2.07	113.36	109.99
20	A	834	CLA	CED-O2D-CGD	2.07	120.62	115.92
21	2	321	LMU	C1B-C2B-C3B	2.07	114.37	110.01
20	1	205	CLA	CMA-C3A-C2A	-2.07	111.48	116.23
20	2	305	CLA	C1D-ND-C4D	-2.07	104.86	106.31
21	B	805	LMU	C2'-C3'-C4'	2.07	114.38	109.68
20	2	309	CLA	C3B-C4B-CHC	-2.07	119.43	126.76
20	G	105	CLA	CBA-CAA-C2A	-2.07	107.64	113.79
21	B	805	LMU	O2'-C2'-C3'	-2.07	105.50	110.38
20	K	104	CLA	O2A-CGA-CBA	2.07	118.14	111.83
22	I	103	BCR	C12-C13-C14	-2.07	115.76	119.01
22	B	847	BCR	C8-C7-C6	-2.07	121.48	127.00
22	G	104	BCR	C20-C19-C18	-2.07	120.70	126.36
20	H	109	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	A	819	CLA	C3D-C4D-ND	2.06	113.34	109.99
22	B	845	BCR	C8-C7-C6	-2.06	121.48	127.00
20	2	311	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
22	F	204	BCR	C28-C27-C26	-2.06	110.38	114.06
20	3	316	CLA	CHB-C1B-NB	-2.06	121.10	124.08
21	H	105	LMU	O5B-C5B-C6B	2.06	111.55	106.44
20	A	817	CLA	CMB-C2B-C1B	2.06	128.56	125.42
20	4	318	CLA	CAA-CBA-CGA	2.06	119.06	113.21
20	B	850	CLA	CGD-CBD-CAD	2.06	117.52	110.85
20	1	213	CLA	CHA-C4D-ND	2.06	136.80	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	839	CLA	C4B-C3B-C2B	2.06	109.86	107.30
20	L	202	CLA	C1D-ND-C4D	-2.06	104.87	106.31
20	2	316	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
20	2	303	CLA	C1-O2A-CGA	2.06	121.63	116.65
20	3	317	CLA	C1D-ND-C4D	-2.06	104.87	106.31
20	H	110	CLA	C2A-C1A-CHA	-2.06	120.30	123.87
22	A	845	BCR	C15-C16-C17	-2.06	119.31	123.52
20	1	205	CLA	CHC-C4B-C3B	-2.06	121.46	127.43
20	A	833	CLA	C1D-ND-C4D	-2.06	104.87	106.31
20	K	103	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
20	2	316	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
22	B	847	BCR	C38-C26-C27	2.05	117.98	113.60
20	1	209	CLA	C2C-C1C-CHC	-2.05	120.46	125.84
20	A	834	CLA	O2A-CGA-CBA	2.05	119.90	112.14
20	B	833	CLA	C1-O2A-CGA	2.05	121.62	116.65
20	A	828	CLA	CED-O2D-CGD	2.05	120.57	115.92
22	I	103	BCR	C23-C22-C21	2.05	122.24	119.01
20	3	311	CLA	C3D-C4D-ND	2.05	113.32	109.99
20	4	318	CLA	CAC-C3C-C4C	2.05	127.46	124.79
20	1	206	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	A	839	CLA	CAC-C3C-C4C	2.05	127.46	124.79
20	B	817	CLA	CAC-C3C-C2C	-2.05	123.79	127.56
20	A	824	CLA	C1D-ND-C4D	-2.05	104.87	106.31
20	A	808	CLA	C3D-C4D-ND	2.05	113.32	109.99
20	2	302	CLA	C1D-ND-C4D	-2.05	104.87	106.31
20	A	809	CLA	CMA-C3A-C4A	2.05	117.28	111.77
22	F	203	BCR	C3-C4-C5	-2.05	110.40	114.06
20	1	211	CLA	O2A-C1-C2	2.05	115.99	108.11
21	A	853	LMU	C1B-O1B-C4'	-2.05	113.12	117.98
20	B	821	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
20	B	824	CLA	C3B-C4B-NB	-2.05	108.70	110.53
20	4	311	CLA	CHD-C1D-ND	2.05	127.73	124.84
20	R	107	CLA	C4-C3-C2	-2.05	118.37	123.63
20	K	101	CLA	C2D-C1D-ND	-2.05	108.10	110.13
20	4	309	CLA	CHB-C1B-NB	-2.05	121.12	124.08
20	4	302	CLA	C2A-C1A-CHA	-2.05	120.32	123.86
20	G	105	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
20	B	814	CLA	C16-C15-C13	-2.05	109.17	115.97
20	B	834	CLA	CED-O2D-CGD	2.04	120.55	115.92
20	4	315	CLA	O2A-CGA-CBA	2.04	119.86	112.14
20	K	104	CLA	CAC-C3C-C2C	-2.04	123.80	127.56
21	K	107	LMU	O1B-C4'-C5'	2.04	114.83	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	106	LMU	O5B-C1B-C2B	2.04	114.57	110.37
20	B	835	CLA	O2A-CGA-CBA	2.04	120.45	114.00
20	B	821	CLA	C1-C2-C3	-2.04	123.46	126.76
20	3	310	CLA	C4-C3-C2	-2.04	118.39	123.63
20	A	821	CLA	C4B-C3B-C2B	2.04	109.84	107.30
20	B	812	CLA	CGD-CBD-CAD	-2.04	104.24	110.85
22	B	846	BCR	C1-C6-C7	2.04	121.18	115.65
20	4	303	CLA	CHA-C1A-NA	-2.04	121.77	126.39
20	1	213	CLA	CED-O2D-CGD	2.04	120.54	115.92
21	4	320	LMU	O2'-C2'-C3'	-2.04	105.57	110.38
20	A	838	CLA	CMC-C2C-C1C	2.04	128.22	125.03
20	A	824	CLA	C1-O2A-CGA	2.04	121.58	116.65
21	G	102	LMU	C4B-C3B-C2B	-2.04	107.25	110.83
20	B	842	CLA	CMC-C2C-C1C	2.04	128.22	125.03
20	4	305	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
20	B	823	CLA	CMB-C2B-C1B	2.04	128.52	125.42
20	B	832	CLA	C3A-C2A-C1A	2.04	104.39	101.34
20	A	833	CLA	CHB-C1B-NB	-2.04	120.99	124.05
22	G	104	BCR	C1-C6-C5	-2.04	119.85	122.64
20	B	825	CLA	CMC-C2C-C1C	2.04	128.22	125.03
20	B	834	CLA	C3D-C4D-ND	2.04	113.30	109.99
20	L	207	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
20	2	305	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
20	A	838	CLA	C1-C2-C3	-2.03	122.86	126.20
20	A	824	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	B	845	BCR	C3-C4-C5	-2.03	110.43	114.06
20	A	809	CLA	C2D-C1D-ND	-2.03	108.11	110.13
20	1	201	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
20	A	812	CLA	CHB-C1B-NB	-2.03	121.00	124.05
20	R	108	CLA	CHB-C4A-NA	2.03	127.33	124.40
21	4	316	LMU	O5'-C5'-C6'	2.03	111.47	106.44
20	1	212	CLA	CHD-C1D-ND	2.03	127.71	124.84
22	J	102	BCR	C27-C26-C25	-2.03	119.96	122.70
20	B	816	CLA	CAC-C3C-C4C	2.03	127.43	124.79
20	2	301	CLA	C3D-C2D-C1D	2.03	109.81	107.35
20	B	838	CLA	C2A-C1A-CHA	-2.03	120.35	123.87
20	1	210	CLA	C1D-ND-C4D	-2.03	104.89	106.31
21	1	218	LMU	O1B-C4'-C5'	-2.03	104.16	109.48
21	A	855	LMU	C1'-C2'-C3'	2.03	114.28	110.01
20	4	302	CLA	CHC-C4B-C3B	-2.03	121.54	127.43
20	L	207	CLA	CHB-C1B-NB	-2.03	121.01	124.05
20	B	831	CLA	CAA-C2A-C3A	-2.03	107.53	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	310	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
20	B	821	CLA	C1-O2A-CGA	2.02	121.55	116.65
20	2	316	CLA	CAC-C3C-C4C	2.02	127.42	124.79
20	B	828	CLA	C1-C2-C3	-2.02	122.88	126.20
22	B	847	BCR	C38-C26-C25	-2.02	122.28	124.48
21	H	103	LMU	O2B-C2B-C1B	2.02	114.90	110.08
20	B	828	CLA	C3D-C4D-ND	2.02	113.28	109.99
20	L	201	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
20	B	821	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
20	B	838	CLA	C1D-ND-C4D	-2.02	104.89	106.31
20	L	208	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
20	L	203	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
20	4	306	CLA	CAA-C2A-C3A	2.02	118.46	113.00
20	2	305	CLA	CMB-C2B-C1B	2.02	128.50	125.42
21	R	104	LMU	O5B-C1B-C2B	-2.02	106.22	110.37
20	2	314	CLA	O2A-CGA-CBA	2.02	118.00	111.83
20	B	813	CLA	C3D-C4D-ND	2.02	113.27	109.99
20	L	207	CLA	CAC-C3C-C4C	2.02	127.42	124.79
20	B	829	CLA	C3B-C4B-NB	-2.02	108.73	110.53
20	A	812	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
20	A	835	CLA	C3A-C2A-C1A	2.02	104.36	101.34
22	B	846	BCR	C4-C5-C6	-2.02	119.97	122.70
20	H	101	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
20	A	814	CLA	C3C-C4C-CHD	-2.02	119.99	125.23
20	G	105	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
20	A	820	CLA	C1-C2-C3	-2.02	122.89	126.20
20	B	828	CLA	CMB-C2B-C1B	2.02	128.49	125.42
20	B	850	CLA	C11-C10-C8	-2.02	109.26	115.97
21	L	205	LMU	O3'-C3'-C2'	-2.02	105.62	110.38
20	3	310	CLA	CHC-C4B-C3B	-2.02	118.61	127.37
20	H	109	CLA	C4-C3-C2	-2.02	118.45	123.63
20	B	839	CLA	O2A-CGA-CBA	2.02	117.98	111.83
20	A	808	CLA	CAA-CBA-CGA	2.02	118.93	113.21
20	B	830	CLA	C7-C6-C5	-2.02	107.89	113.26
20	A	826	CLA	CMB-C2B-C1B	2.02	128.49	125.42
20	A	823	CLA	CAC-C3C-C4C	2.02	127.41	124.79
20	A	825	CLA	C3D-C4D-ND	2.01	113.26	109.99
20	B	812	CLA	C6-C5-C3	-2.01	108.56	113.47
20	B	834	CLA	C2A-C1A-CHA	-2.01	120.37	123.87
20	B	814	CLA	C11-C10-C8	-2.01	109.27	115.97
22	B	844	BCR	C10-C11-C12	-2.01	117.37	123.20
22	B	846	BCR	C1-C6-C5	-2.01	119.89	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	315	CLA	CHB-C1B-NB	-2.01	121.17	124.08
20	F	205	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
22	L	209	BCR	C19-C18-C17	-2.01	115.84	119.01
22	B	847	BCR	C23-C24-C25	-2.01	121.62	127.00
20	A	830	CLA	C1-O2A-CGA	2.01	121.52	116.65
20	B	835	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
23	B	843	PQN	C11-C3-C2	-2.01	121.44	124.89
20	H	108	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
21	H	106	LMU	C4B-C3B-C2B	-2.01	107.31	110.83
20	1	207	CLA	C3D-C4D-ND	2.01	113.25	109.99
20	A	807	CLA	CHB-C4A-NA	2.01	127.30	124.40
20	3	311	CLA	CED-O2D-CGD	2.01	120.47	115.92
20	L	203	CLA	CED-O2D-CGD	2.01	120.47	115.92
20	L	207	CLA	CED-O2D-CGD	2.01	120.47	115.92
20	2	305	CLA	CHB-C1B-NB	-2.01	121.04	124.05
20	K	102	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
20	H	109	CLA	C1-O2A-CGA	2.01	121.51	116.65
20	3	311	CLA	C2A-C1A-CHA	-2.01	120.39	123.87
20	A	850	CLA	C4A-NA-C1A	2.01	107.59	106.68
20	B	836	CLA	C4-C3-C2	-2.01	118.48	123.63
20	B	837	CLA	CHB-C1B-NB	-2.01	121.04	124.05
22	F	204	BCR	C36-C18-C17	-2.00	119.57	122.82
20	A	827	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
20	B	813	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
20	A	810	CLA	CHB-C4A-NA	2.00	127.29	124.40
22	G	104	BCR	C3-C4-C5	-2.00	110.48	114.06
20	B	820	CLA	CHB-C4A-NA	2.00	127.29	124.40
20	3	309	CLA	CHA-C4D-ND	2.00	127.67	124.84
20	2	309	CLA	CHB-C4A-NA	2.00	127.28	124.43
22	B	801	BCR	C16-C17-C18	-2.00	124.47	127.28
20	2	311	CLA	CMB-C2B-C1B	2.00	128.47	125.42
20	4	306	CLA	C1D-ND-C4D	-2.00	104.91	106.31
20	A	837	CLA	C3B-C4B-NB	-2.00	108.74	110.53
21	G	103	LMU	O1'-C1'-C2'	2.00	111.31	108.27
20	4	313	CLA	CMC-C2C-C1C	2.00	128.16	125.03
20	4	312	CLA	CHB-C1B-NB	-2.00	121.19	124.08
20	B	817	CLA	CAA-C2A-C1A	2.00	118.53	111.97

All (258) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	201	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	1	202	CLA	ND
20	1	203	CLA	ND
20	1	204	CLA	ND
20	1	205	CLA	ND
20	1	206	CLA	ND
20	1	206	CLA	C8
20	1	207	CLA	ND
20	1	207	CLA	C2A
20	1	208	CLA	ND
20	1	209	CLA	ND
20	1	210	CLA	ND
20	1	211	CLA	ND
20	1	211	CLA	CBD
20	1	212	CLA	ND
20	1	213	CLA	ND
20	1	213	CLA	C3A
20	1	213	CLA	C2A
20	1	214	CLA	ND
20	1	215	CLA	ND
20	1	215	CLA	CBD
20	2	301	CLA	ND
20	2	302	CLA	ND
20	2	303	CLA	ND
20	2	303	CLA	C8
20	2	304	CLA	ND
20	2	305	CLA	ND
20	2	306	CLA	ND
20	2	307	CLA	ND
20	2	307	CLA	C8
20	2	308	CLA	ND
20	2	309	CLA	ND
20	2	310	CLA	ND
20	2	311	CLA	ND
20	2	312	CLA	ND
20	2	312	CLA	C8
20	2	314	CLA	ND
20	2	315	CLA	ND
20	2	316	CLA	ND
20	2	316	CLA	C8
20	3	301	CLA	ND
20	3	302	CLA	ND
20	3	303	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	3	304	CLA	ND
20	3	305	CLA	ND
20	3	306	CLA	ND
20	3	307	CLA	ND
20	3	308	CLA	ND
20	3	309	CLA	ND
20	3	310	CLA	ND
20	3	310	CLA	C8
20	3	311	CLA	ND
20	3	311	CLA	C8
20	3	312	CLA	ND
20	3	313	CLA	ND
20	3	314	CLA	ND
20	3	314	CLA	C8
20	3	315	CLA	ND
20	3	316	CLA	ND
20	3	317	CLA	ND
20	4	301	CLA	ND
20	4	301	CLA	C8
20	4	302	CLA	ND
20	4	303	CLA	ND
20	4	303	CLA	CBD
20	4	303	CLA	C8
20	4	304	CLA	ND
20	4	304	CLA	C8
20	4	305	CLA	ND
20	4	306	CLA	ND
20	4	306	CLA	C2A
20	4	307	CLA	ND
20	4	308	CLA	ND
20	4	309	CLA	ND
20	4	310	CLA	ND
20	4	311	CLA	ND
20	4	312	CLA	ND
20	4	313	CLA	ND
20	4	314	CLA	ND
20	4	315	CLA	ND
20	4	317	CLA	ND
20	4	318	CLA	ND
20	A	801	CLA	ND
20	A	801	CLA	C2A
20	A	801	CLA	CBD

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	804	CLA	C8
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	806	CLA	C8
20	A	807	CLA	ND
20	A	808	CLA	ND
20	A	808	CLA	C8
20	A	809	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	811	CLA	C8
20	A	812	CLA	ND
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	816	CLA	ND
20	A	817	CLA	ND
20	A	818	CLA	ND
20	A	818	CLA	C8
20	A	819	CLA	ND
20	A	819	CLA	C8
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND
20	A	823	CLA	ND
20	A	823	CLA	C8
20	A	824	CLA	ND
20	A	824	CLA	C8
20	A	825	CLA	ND
20	A	825	CLA	C8
20	A	826	CLA	ND
20	A	826	CLA	C8
20	A	827	CLA	ND
20	A	827	CLA	C8
20	A	828	CLA	ND
20	A	828	CLA	C8
20	A	829	CLA	ND
20	A	830	CLA	ND
20	A	830	CLA	C8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	A	831	CLA	ND
20	A	831	CLA	C8
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	835	CLA	C8
20	A	836	CLA	ND
20	A	837	CLA	ND
20	A	838	CLA	ND
20	A	838	CLA	C8
20	A	839	CLA	ND
20	A	839	CLA	C2A
20	A	840	CLA	ND
20	A	840	CLA	C8
20	A	841	CLA	ND
20	A	849	CLA	ND
20	A	849	CLA	C8
20	A	850	CLA	ND
20	A	850	CLA	C8
20	A	851	CLA	ND
20	A	851	CLA	C8
20	B	802	CLA	ND
20	B	803	CLA	ND
20	B	803	CLA	C8
20	B	806	CLA	ND
20	B	806	CLA	C8
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	808	CLA	C8
20	B	809	CLA	ND
20	B	809	CLA	C8
20	B	810	CLA	ND
20	B	810	CLA	C8
20	B	811	CLA	ND
20	B	812	CLA	ND
20	B	812	CLA	C8
20	B	813	CLA	ND
20	B	813	CLA	C8
20	B	814	CLA	ND
20	B	814	CLA	C8
20	B	815	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	B	815	CLA	C8
20	B	816	CLA	ND
20	B	816	CLA	C8
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	820	CLA	ND
20	B	820	CLA	C8
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	823	CLA	C8
20	B	824	CLA	ND
20	B	824	CLA	C8
20	B	825	CLA	ND
20	B	826	CLA	ND
20	B	826	CLA	C8
20	B	827	CLA	ND
20	B	827	CLA	C8
20	B	828	CLA	ND
20	B	828	CLA	C8
20	B	829	CLA	ND
20	B	829	CLA	C8
20	B	830	CLA	ND
20	B	830	CLA	C8
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	832	CLA	C8
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	835	CLA	ND
20	B	836	CLA	ND
20	B	837	CLA	ND
20	B	837	CLA	C8
20	B	838	CLA	ND
20	B	838	CLA	C8
20	B	839	CLA	ND
20	B	840	CLA	ND
20	B	840	CLA	C8
20	B	841	CLA	ND
20	B	841	CLA	C8
20	B	842	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
20	B	850	CLA	ND
20	B	850	CLA	C8
20	F	201	CLA	ND
20	F	205	CLA	ND
20	F	206	CLA	ND
20	F	207	CLA	ND
20	F	207	CLA	C3A
20	F	207	CLA	CBD
20	F	207	CLA	C2A
20	G	105	CLA	ND
20	H	101	CLA	ND
20	H	101	CLA	CBD
20	H	101	CLA	C8
20	H	102	CLA	ND
20	H	102	CLA	C8
20	H	108	CLA	ND
20	H	108	CLA	C8
20	H	109	CLA	ND
20	H	109	CLA	C8
20	H	110	CLA	ND
20	I	102	CLA	ND
20	I	102	CLA	C8
20	J	101	CLA	ND
20	J	103	CLA	ND
20	J	103	CLA	C8
20	K	101	CLA	ND
20	K	102	CLA	ND
20	K	103	CLA	ND
20	K	104	CLA	ND
20	K	104	CLA	C8
20	L	201	CLA	ND
20	L	201	CLA	C8
20	L	202	CLA	ND
20	L	202	CLA	C8
20	L	203	CLA	ND
20	L	203	CLA	C8
20	L	204	CLA	ND
20	L	204	CLA	C8
20	L	207	CLA	ND
20	L	208	CLA	ND
20	L	208	CLA	CBD
20	R	107	CLA	ND

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Mol	Chain	Res	Type	Atom
20	R	107	CLA	C8
20	R	108	CLA	ND
20	R	108	CLA	C8
23	A	842	PQN	C23
23	B	843	PQN	C23

All (2566) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	201	CLA	C1A-C2A-CAA-CBA
20	1	201	CLA	C3A-C2A-CAA-CBA
20	1	201	CLA	CBA-CGA-O2A-C1
20	1	201	CLA	CHA-CBD-CGD-O1D
20	1	201	CLA	CHA-CBD-CGD-O2D
20	1	202	CLA	C4B-C3B-CAB-CBB
20	1	202	CLA	CBD-CGD-O2D-CED
20	1	203	CLA	C2B-C3B-CAB-CBB
20	1	203	CLA	CBD-CGD-O2D-CED
20	1	204	CLA	C1A-C2A-CAA-CBA
20	1	204	CLA	CBA-CGA-O2A-C1
20	1	204	CLA	O1A-CGA-O2A-C1
20	1	204	CLA	CBD-CGD-O2D-CED
20	1	206	CLA	C4B-C3B-CAB-CBB
20	1	206	CLA	C2C-C3C-CAC-CBC
20	1	206	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	CHA-CBD-CGD-O1D
20	1	206	CLA	CHA-CBD-CGD-O2D
20	1	207	CLA	C2B-C3B-CAB-CBB
20	1	207	CLA	CBD-CGD-O2D-CED
20	1	207	CLA	C2-C3-C5-C6
20	1	207	CLA	C4-C3-C5-C6
20	1	211	CLA	C2B-C3B-CAB-CBB
20	1	211	CLA	CBD-CGD-O2D-CED
20	1	213	CLA	C3A-C2A-CAA-CBA
20	1	213	CLA	C4B-C3B-CAB-CBB
20	1	213	CLA	C2-C3-C5-C6
20	1	213	CLA	C4-C3-C5-C6
20	1	215	CLA	C2B-C3B-CAB-CBB
20	1	215	CLA	CAD-CBD-CGD-O1D
20	1	215	CLA	CAD-CBD-CGD-O2D
20	1	215	CLA	C2-C3-C5-C6
20	1	215	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	2	302	CLA	C1A-C2A-CAA-CBA
20	2	302	CLA	C3A-C2A-CAA-CBA
20	2	302	CLA	C4B-C3B-CAB-CBB
20	2	302	CLA	O2A-C1-C2-C3
20	2	302	CLA	C2-C3-C5-C6
20	2	302	CLA	C4-C3-C5-C6
20	2	303	CLA	C1A-C2A-CAA-CBA
20	2	303	CLA	C3A-C2A-CAA-CBA
20	2	303	CLA	C2-C1-O2A-CGA
20	2	303	CLA	C4B-C3B-CAB-CBB
20	2	303	CLA	CAD-CBD-CGD-O1D
20	2	303	CLA	CAD-CBD-CGD-O2D
20	2	305	CLA	C2-C1-O2A-CGA
20	2	307	CLA	CBA-CGA-O2A-C1
20	2	307	CLA	O1A-CGA-O2A-C1
20	2	307	CLA	C6-C7-C8-C9
20	2	310	CLA	C4B-C3B-CAB-CBB
20	2	311	CLA	CBA-CGA-O2A-C1
20	2	311	CLA	O1A-CGA-O2A-C1
20	2	312	CLA	C4B-C3B-CAB-CBB
20	2	312	CLA	CAD-CBD-CGD-O1D
20	2	312	CLA	CAD-CBD-CGD-O2D
20	2	312	CLA	CBD-CGD-O2D-CED
20	2	314	CLA	C2B-C3B-CAB-CBB
20	2	314	CLA	CBD-CGD-O2D-CED
20	2	314	CLA	O1D-CGD-O2D-CED
20	2	316	CLA	C4B-C3B-CAB-CBB
20	2	316	CLA	CHA-CBD-CGD-O1D
20	2	316	CLA	CHA-CBD-CGD-O2D
20	3	307	CLA	C1A-C2A-CAA-CBA
20	3	307	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	CBD-CGD-O2D-CED
20	3	310	CLA	C1A-C2A-CAA-CBA
20	3	310	CLA	C3A-C2A-CAA-CBA
20	3	310	CLA	CAD-CBD-CGD-O1D
20	3	310	CLA	CAD-CBD-CGD-O2D
20	3	311	CLA	CHA-CBD-CGD-O1D
20	3	311	CLA	CHA-CBD-CGD-O2D
20	3	314	CLA	CBA-CGA-O2A-C1
20	3	314	CLA	O1A-CGA-O2A-C1
20	3	314	CLA	C2B-C3B-CAB-CBB
20	4	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	4	303	CLA	C6-C7-C8-C9
20	4	304	CLA	C4B-C3B-CAB-CBB
20	4	304	CLA	CHA-CBD-CGD-O1D
20	4	304	CLA	CHA-CBD-CGD-O2D
20	4	306	CLA	C2-C1-O2A-CGA
20	4	306	CLA	C2B-C3B-CAB-CBB
20	4	310	CLA	C1A-C2A-CAA-CBA
20	4	310	CLA	C2B-C3B-CAB-CBB
20	4	310	CLA	CBD-CGD-O2D-CED
20	4	315	CLA	C1A-C2A-CAA-CBA
20	4	315	CLA	C4B-C3B-CAB-CBB
20	4	317	CLA	C4B-C3B-CAB-CBB
20	4	318	CLA	C2B-C3B-CAB-CBB
20	4	318	CLA	CHA-CBD-CGD-O1D
20	4	318	CLA	CHA-CBD-CGD-O2D
20	4	318	CLA	CBD-CGD-O2D-CED
20	A	801	CLA	C1A-C2A-CAA-CBA
20	A	801	CLA	CAD-CBD-CGD-O1D
20	A	801	CLA	CAD-CBD-CGD-O2D
20	A	801	CLA	CBD-CGD-O2D-CED
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	O1A-CGA-O2A-C1
20	A	804	CLA	CBD-CGD-O2D-CED
20	A	805	CLA	C1A-C2A-CAA-CBA
20	A	805	CLA	C3A-C2A-CAA-CBA
20	A	805	CLA	C2B-C3B-CAB-CBB
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	O1A-CGA-O2A-C1
20	A	806	CLA	CBD-CGD-O2D-CED
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	807	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C3A-C2A-CAA-CBA
20	A	808	CLA	CHA-CBD-CGD-O1D
20	A	808	CLA	CHA-CBD-CGD-O2D
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	811	CLA	CBD-CGD-O2D-CED
20	A	812	CLA	C2B-C3B-CAB-CBB
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	813	CLA	CBD-CGD-O2D-CED
20	A	815	CLA	C1A-C2A-CAA-CBA
20	A	815	CLA	CBA-CGA-O2A-C1
20	A	815	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	CBD-CGD-O2D-CED
20	A	816	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	C2B-C3B-CAB-CBB
20	A	816	CLA	CBD-CGD-O2D-CED
20	A	817	CLA	C1A-C2A-CAA-CBA
20	A	817	CLA	C3A-C2A-CAA-CBA
20	A	817	CLA	C2B-C3B-CAB-CBB
20	A	818	CLA	C1A-C2A-CAA-CBA
20	A	818	CLA	C3A-C2A-CAA-CBA
20	A	818	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	C2B-C3B-CAB-CBB
20	A	820	CLA	C4B-C3B-CAB-CBB
20	A	820	CLA	CAD-CBD-CGD-O1D
20	A	820	CLA	CAD-CBD-CGD-O2D
20	A	821	CLA	C1A-C2A-CAA-CBA
20	A	821	CLA	C3A-C2A-CAA-CBA
20	A	821	CLA	C4B-C3B-CAB-CBB
20	A	822	CLA	C1A-C2A-CAA-CBA
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	C2B-C3B-CAB-CBB
20	A	824	CLA	C4B-C3B-CAB-CBB
20	A	824	CLA	CBD-CGD-O2D-CED
20	A	824	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	C1A-C2A-CAA-CBA
20	A	828	CLA	C3A-C2A-CAA-CBA
20	A	828	CLA	CHA-CBD-CGD-O1D
20	A	828	CLA	CHA-CBD-CGD-O2D
20	A	830	CLA	C2B-C3B-CAB-CBB
20	A	830	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	CHA-CBD-CGD-O1D
20	A	831	CLA	CHA-CBD-CGD-O2D
20	A	832	CLA	C1A-C2A-CAA-CBA
20	A	832	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	833	CLA	C1A-C2A-CAA-CBA
20	A	833	CLA	C3A-C2A-CAA-CBA
20	A	833	CLA	C4B-C3B-CAB-CBB
20	A	833	CLA	CBD-CGD-O2D-CED
20	A	834	CLA	C1A-C2A-CAA-CBA
20	A	834	CLA	C2B-C3B-CAB-CBB
20	A	834	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CAD-CBD-CGD-O1D
20	A	835	CLA	CAD-CBD-CGD-O2D
20	A	836	CLA	C2B-C3B-CAB-CBB
20	A	837	CLA	C4B-C3B-CAB-CBB
20	A	837	CLA	C2-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	A	838	CLA	C1A-C2A-CAA-CBA
20	A	838	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C2B-C3B-CAB-CBB
20	A	839	CLA	C1A-C2A-CAA-CBA
20	A	839	CLA	C3A-C2A-CAA-CBA
20	A	839	CLA	C2B-C3B-CAB-CBB
20	A	839	CLA	C2C-C3C-CAC-CBC
20	A	839	CLA	C4C-C3C-CAC-CBC
20	A	839	CLA	C2-C3-C5-C6
20	A	839	CLA	C4-C3-C5-C6
20	A	840	CLA	C3A-C2A-CAA-CBA
20	A	840	CLA	CBD-CGD-O2D-CED
20	A	849	CLA	C3A-C2A-CAA-CBA
20	A	849	CLA	CBA-CGA-O2A-C1
20	A	850	CLA	CBD-CGD-O2D-CED
20	A	850	CLA	O1D-CGD-O2D-CED
20	A	850	CLA	C6-C7-C8-C9
20	B	802	CLA	C4-C3-C5-C6
20	B	803	CLA	C2B-C3B-CAB-CBB
20	B	807	CLA	C1A-C2A-CAA-CBA
20	B	807	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	C1A-C2A-CAA-CBA
20	B	808	CLA	C2-C1-O2A-CGA
20	B	808	CLA	CAD-CBD-CGD-O1D
20	B	808	CLA	CAD-CBD-CGD-O2D
20	B	809	CLA	CAD-CBD-CGD-O1D
20	B	809	CLA	CAD-CBD-CGD-O2D
20	B	809	CLA	CBD-CGD-O2D-CED
20	B	810	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	810	CLA	CHA-CBD-CGD-O1D
20	B	810	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	C11-C10-C8-C9
20	B	812	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	CBD-CGD-O2D-CED
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C4B-C3B-CAB-CBB
20	B	814	CLA	CAD-CBD-CGD-O1D
20	B	814	CLA	CAD-CBD-CGD-O2D
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	815	CLA	C3A-C2A-CAA-CBA
20	B	815	CLA	C2B-C3B-CAB-CBB
20	B	816	CLA	C4B-C3B-CAB-CBB
20	B	816	CLA	CAD-CBD-CGD-O1D
20	B	816	CLA	CAD-CBD-CGD-O2D
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	817	CLA	C2C-C3C-CAC-CBC
20	B	817	CLA	C4C-C3C-CAC-CBC
20	B	817	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	O1D-CGD-O2D-CED
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	CBD-CGD-O2D-CED
20	B	820	CLA	C1A-C2A-CAA-CBA
20	B	820	CLA	C3A-C2A-CAA-CBA
20	B	821	CLA	C4B-C3B-CAB-CBB
20	B	821	CLA	CBD-CGD-O2D-CED
20	B	822	CLA	CHA-CBD-CGD-O1D
20	B	822	CLA	CHA-CBD-CGD-O2D
20	B	822	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	C4B-C3B-CAB-CBB
20	B	824	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	C2B-C3B-CAB-CBB
20	B	824	CLA	CBD-CGD-O2D-CED
20	B	826	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C4C-C3C-CAC-CBC
20	B	826	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	826	CLA	C4-C3-C5-C6
20	B	826	CLA	C11-C10-C8-C9
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C11-C12-C13-C14
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	CBD-CGD-O2D-CED
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C2B-C3B-CAB-CBB
20	B	830	CLA	C2B-C3B-CAB-CBB
20	B	830	CLA	CAD-CBD-CGD-O1D
20	B	830	CLA	CAD-CBD-CGD-O2D
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	831	CLA	C3A-C2A-CAA-CBA
20	B	831	CLA	C2B-C3B-CAB-CBB
20	B	831	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	O1D-CGD-O2D-CED
20	B	832	CLA	CBD-CGD-O2D-CED
20	B	833	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C4B-C3B-CAB-CBB
20	B	834	CLA	CAD-CBD-CGD-O2D
20	B	835	CLA	C2B-C3B-CAB-CBB
20	B	835	CLA	CBD-CGD-O2D-CED
20	B	836	CLA	C2B-C3B-CAB-CBB
20	B	836	CLA	C2C-C3C-CAC-CBC
20	B	836	CLA	C4C-C3C-CAC-CBC
20	B	836	CLA	C2-C3-C5-C6
20	B	836	CLA	C4-C3-C5-C6
20	B	837	CLA	C2B-C3B-CAB-CBB
20	B	839	CLA	CBA-CGA-O2A-C1
20	B	839	CLA	O1A-CGA-O2A-C1
20	B	839	CLA	CBD-CGD-O2D-CED
20	B	840	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C3A-C2A-CAA-CBA
20	B	850	CLA	C4B-C3B-CAB-CBB
20	F	201	CLA	C2C-C3C-CAC-CBC
20	F	201	CLA	C4C-C3C-CAC-CBC
20	F	206	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	F	207	CLA	C1A-C2A-CAA-CBA
20	F	207	CLA	C4B-C3B-CAB-CBB
20	F	207	CLA	CBD-CGD-O2D-CED
20	F	207	CLA	O1D-CGD-O2D-CED
20	G	105	CLA	C2B-C3B-CAB-CBB
20	G	105	CLA	CAD-CBD-CGD-O1D
20	G	105	CLA	CAD-CBD-CGD-O2D
20	G	105	CLA	CBD-CGD-O2D-CED
20	H	101	CLA	C1A-C2A-CAA-CBA
20	H	101	CLA	C3A-C2A-CAA-CBA
20	H	101	CLA	CBD-CGD-O2D-CED
20	H	102	CLA	C2B-C3B-CAB-CBB
20	H	108	CLA	C2B-C3B-CAB-CBB
20	H	109	CLA	CAD-CBD-CGD-O1D
20	H	109	CLA	CAD-CBD-CGD-O2D
20	H	109	CLA	CBD-CGD-O2D-CED
20	H	110	CLA	C1A-C2A-CAA-CBA
20	H	110	CLA	C3A-C2A-CAA-CBA
20	H	110	CLA	CBD-CGD-O2D-CED
20	I	102	CLA	C4B-C3B-CAB-CBB
20	J	101	CLA	C1A-C2A-CAA-CBA
20	J	101	CLA	CBD-CGD-O2D-CED
20	J	103	CLA	C3A-C2A-CAA-CBA
20	J	103	CLA	C4B-C3B-CAB-CBB
20	J	103	CLA	CHA-CBD-CGD-O1D
20	J	103	CLA	CHA-CBD-CGD-O2D
20	J	103	CLA	CBD-CGD-O2D-CED
20	J	103	CLA	O1D-CGD-O2D-CED
20	K	102	CLA	C2B-C3B-CAB-CBB
20	K	102	CLA	O2A-C1-C2-C3
20	K	104	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	CBD-CGD-O2D-CED
20	L	201	CLA	O1D-CGD-O2D-CED
20	L	201	CLA	C4-C3-C5-C6
20	L	202	CLA	C2-C1-O2A-CGA
20	L	202	CLA	CHA-CBD-CGD-O1D
20	L	202	CLA	CHA-CBD-CGD-O2D
20	L	202	CLA	CBD-CGD-O2D-CED
20	L	204	CLA	C2B-C3B-CAB-CBB
20	L	204	CLA	CBD-CGD-O2D-CED
20	L	207	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	L	207	CLA	CHA-CBD-CGD-O1D
20	L	207	CLA	CHA-CBD-CGD-O2D
20	L	207	CLA	CBD-CGD-O2D-CED
20	L	208	CLA	C1A-C2A-CAA-CBA
20	L	208	CLA	C2B-C3B-CAB-CBB
20	L	208	CLA	C4C-C3C-CAC-CBC
20	R	107	CLA	C1A-C2A-CAA-CBA
20	R	107	CLA	CHA-CBD-CGD-O1D
20	R	107	CLA	CHA-CBD-CGD-O2D
20	R	107	CLA	CBD-CGD-O2D-CED
20	R	108	CLA	C1A-C2A-CAA-CBA
20	R	108	CLA	O1A-CGA-O2A-C1
20	R	108	CLA	CAD-CBD-CGD-O2D
21	1	216	LMU	O5B-C1B-O1B-C4'
21	1	217	LMU	C2-C1-O1'-C1'
21	2	318	LMU	C2'-C1'-O1'-C1
21	2	318	LMU	O5'-C1'-O1'-C1
21	2	319	LMU	O5'-C1'-O1'-C1
21	2	320	LMU	C2B-C1B-O1B-C4'
21	2	320	LMU	C2'-C1'-O1'-C1
21	2	321	LMU	C2-C1-O1'-C1'
21	3	318	LMU	C2'-C1'-O1'-C1
21	3	318	LMU	O5'-C1'-O1'-C1
21	4	319	LMU	C2'-C1'-O1'-C1
21	4	319	LMU	O5'-C1'-O1'-C1
21	4	319	LMU	C2-C1-O1'-C1'
21	4	320	LMU	O5'-C1'-O1'-C1
21	4	321	LMU	C2-C1-O1'-C1'
21	A	847	LMU	C2-C1-O1'-C1'
21	A	848	LMU	C2'-C1'-O1'-C1
21	A	848	LMU	O5'-C1'-O1'-C1
21	A	848	LMU	C2-C1-O1'-C1'
21	A	852	LMU	O5'-C1'-O1'-C1
21	B	805	LMU	C2'-C1'-O1'-C1
21	B	805	LMU	O5'-C1'-O1'-C1
21	E	101	LMU	C2'-C1'-O1'-C1
21	E	101	LMU	O5'-C1'-O1'-C1
21	E	101	LMU	C2-C1-O1'-C1'
21	F	202	LMU	C2'-C1'-O1'-C1
21	F	202	LMU	O5'-C1'-O1'-C1
21	H	103	LMU	C2'-C1'-O1'-C1
21	H	104	LMU	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
21	H	104	LMU	C2-C1-O1'-C1'
21	H	105	LMU	O5'-C1'-O1'-C1
21	H	106	LMU	O5'-C1'-O1'-C1
21	K	106	LMU	C2B-C1B-O1B-C4'
21	K	106	LMU	O5'-C1'-O1'-C1
21	K	107	LMU	C3'-C4'-O1B-C1B
21	K	107	LMU	O5'-C1'-O1'-C1
21	L	206	LMU	C2-C1-O1'-C1'
21	L	210	LMU	C2-C1-O1'-C1'
21	R	102	LMU	C2-C1-O1'-C1'
21	R	104	LMU	O5'-C1'-O1'-C1
21	R	104	LMU	C2-C1-O1'-C1'
21	R	106	LMU	C2'-C1'-O1'-C1
21	R	106	LMU	O5'-C1'-O1'-C1
21	R	106	LMU	C2-C1-O1'-C1'
21	R	109	LMU	O5B-C1B-O1B-C4'
21	R	109	LMU	C2'-C1'-O1'-C1
21	R	109	LMU	O5'-C1'-O1'-C1
21	R	109	LMU	C2-C1-O1'-C1'
22	2	317	BCR	C36-C18-C19-C20
22	2	317	BCR	C18-C19-C20-C21
22	2	317	BCR	C20-C21-C22-C23
22	2	317	BCR	C20-C21-C22-C37
22	A	843	BCR	C7-C8-C9-C10
22	A	843	BCR	C7-C8-C9-C34
22	A	843	BCR	C18-C19-C20-C21
22	A	843	BCR	C20-C21-C22-C23
22	A	843	BCR	C20-C21-C22-C37
22	A	843	BCR	C21-C22-C23-C24
22	A	843	BCR	C37-C22-C23-C24
22	A	844	BCR	C11-C12-C13-C14
22	A	844	BCR	C17-C18-C19-C20
22	A	844	BCR	C36-C18-C19-C20
22	A	844	BCR	C21-C22-C23-C24
22	A	844	BCR	C37-C22-C23-C24
22	A	845	BCR	C18-C19-C20-C21
22	A	845	BCR	C23-C24-C25-C26
22	B	801	BCR	C11-C12-C13-C14
22	B	801	BCR	C11-C12-C13-C35
22	B	801	BCR	C13-C14-C15-C16
22	B	801	BCR	C15-C16-C17-C18
22	B	801	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	B	801	BCR	C20-C21-C22-C23
22	B	801	BCR	C20-C21-C22-C37
22	B	801	BCR	C21-C22-C23-C24
22	B	845	BCR	C19-C20-C21-C22
22	B	845	BCR	C20-C21-C22-C23
22	B	845	BCR	C20-C21-C22-C37
22	B	845	BCR	C21-C22-C23-C24
22	B	845	BCR	C37-C22-C23-C24
22	B	845	BCR	C23-C24-C25-C26
22	B	845	BCR	C23-C24-C25-C30
22	B	846	BCR	C11-C12-C13-C14
22	B	846	BCR	C11-C12-C13-C35
22	B	846	BCR	C17-C18-C19-C20
22	B	846	BCR	C36-C18-C19-C20
22	B	846	BCR	C18-C19-C20-C21
22	B	846	BCR	C20-C21-C22-C23
22	B	846	BCR	C20-C21-C22-C37
22	B	847	BCR	C5-C6-C7-C8
22	B	847	BCR	C7-C8-C9-C34
22	B	847	BCR	C18-C19-C20-C21
22	B	847	BCR	C20-C21-C22-C23
22	B	847	BCR	C20-C21-C22-C37
22	B	847	BCR	C21-C22-C23-C24
22	B	847	BCR	C37-C22-C23-C24
22	F	204	BCR	C7-C8-C9-C10
22	F	204	BCR	C9-C10-C11-C12
22	F	204	BCR	C18-C19-C20-C21
22	G	104	BCR	C7-C8-C9-C10
22	G	104	BCR	C17-C18-C19-C20
22	G	104	BCR	C36-C18-C19-C20
22	G	104	BCR	C18-C19-C20-C21
22	G	104	BCR	C20-C21-C22-C23
22	G	104	BCR	C20-C21-C22-C37
22	I	101	BCR	C5-C6-C7-C8
22	I	101	BCR	C9-C10-C11-C12
22	I	101	BCR	C21-C22-C23-C24
22	I	103	BCR	C9-C10-C11-C12
22	I	103	BCR	C11-C12-C13-C14
22	I	103	BCR	C17-C18-C19-C20
22	I	103	BCR	C36-C18-C19-C20
22	I	103	BCR	C18-C19-C20-C21
22	I	103	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	I	103	BCR	C20-C21-C22-C37
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
22	J	102	BCR	C17-C18-C19-C20
22	J	102	BCR	C18-C19-C20-C21
22	L	209	BCR	C7-C8-C9-C10
22	L	209	BCR	C7-C8-C9-C34
22	L	209	BCR	C20-C21-C22-C23
22	L	209	BCR	C20-C21-C22-C37
22	L	209	BCR	C21-C22-C23-C24
22	L	209	BCR	C37-C22-C23-C24
25	B	848	LMG	O6-C1-O1-C7
25	B	848	LMG	C11-C10-O7-C8
21	2	313	LMU	C5'-C4'-O1B-C1B
21	2	318	LMU	C5'-C4'-O1B-C1B
21	H	106	LMU	C3'-C4'-O1B-C1B
20	2	311	CLA	C4C-C3C-CAC-CBC
20	3	311	CLA	C4C-C3C-CAC-CBC
20	A	801	CLA	C4C-C3C-CAC-CBC
20	A	824	CLA	C4C-C3C-CAC-CBC
20	A	824	CLA	C2C-C3C-CAC-CBC
20	B	826	CLA	C2C-C3C-CAC-CBC
20	L	208	CLA	C2C-C3C-CAC-CBC
20	1	204	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	O1D-CGD-O2D-CED
20	1	207	CLA	O1D-CGD-O2D-CED
20	1	213	CLA	O1D-CGD-O2D-CED
20	4	315	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	O1D-CGD-O2D-CED
20	A	815	CLA	O1D-CGD-O2D-CED
20	A	816	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	O1D-CGD-O2D-CED
20	A	823	CLA	O1D-CGD-O2D-CED
20	A	837	CLA	O1D-CGD-O2D-CED
20	B	812	CLA	O1D-CGD-O2D-CED
20	B	816	CLA	O1D-CGD-O2D-CED
20	B	818	CLA	O1D-CGD-O2D-CED
20	B	821	CLA	O1D-CGD-O2D-CED
20	B	822	CLA	O1D-CGD-O2D-CED
20	B	833	CLA	O1D-CGD-O2D-CED
20	H	102	CLA	O1D-CGD-O2D-CED
20	L	202	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	L	204	CLA	O1D-CGD-O2D-CED
20	R	107	CLA	O1D-CGD-O2D-CED
21	K	107	LMU	O5B-C1B-O1B-C4'
21	1	217	LMU	C3'-C4'-O1B-C1B
21	4	321	LMU	C5'-C4'-O1B-C1B
21	B	849	LMU	C3'-C4'-O1B-C1B
21	R	101	LMU	C3'-C4'-O1B-C1B
21	R	103	LMU	C3'-C4'-O1B-C1B
20	A	825	CLA	C4C-C3C-CAC-CBC
20	H	101	CLA	C4C-C3C-CAC-CBC
20	2	311	CLA	C2C-C3C-CAC-CBC
20	3	311	CLA	C2C-C3C-CAC-CBC
20	4	301	CLA	C2C-C3C-CAC-CBC
20	A	825	CLA	C2C-C3C-CAC-CBC
20	1	202	CLA	O1D-CGD-O2D-CED
20	1	203	CLA	O1D-CGD-O2D-CED
20	2	312	CLA	O1D-CGD-O2D-CED
20	3	307	CLA	O1D-CGD-O2D-CED
20	A	801	CLA	O1D-CGD-O2D-CED
20	A	811	CLA	O1D-CGD-O2D-CED
20	A	826	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	O1D-CGD-O2D-CED
20	B	839	CLA	O1D-CGD-O2D-CED
20	F	206	CLA	O1D-CGD-O2D-CED
20	G	105	CLA	O1D-CGD-O2D-CED
20	H	101	CLA	O1D-CGD-O2D-CED
20	H	110	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	CBD-CGD-O2D-CED
20	1	213	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBD-CGD-O2D-CED
20	3	313	CLA	CBD-CGD-O2D-CED
20	4	305	CLA	CBD-CGD-O2D-CED
20	4	315	CLA	CBD-CGD-O2D-CED
20	A	807	CLA	CBD-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	817	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	CBD-CGD-O2D-CED
20	A	825	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	CBD-CGD-O2D-CED
20	A	828	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	832	CLA	CBD-CGD-O2D-CED
20	A	837	CLA	CBD-CGD-O2D-CED
20	A	839	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	B	816	CLA	CBD-CGD-O2D-CED
20	B	819	CLA	CBD-CGD-O2D-CED
20	B	820	CLA	CBD-CGD-O2D-CED
20	B	830	CLA	CBD-CGD-O2D-CED
20	B	833	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	CBD-CGD-O2D-CED
20	B	850	CLA	CBD-CGD-O2D-CED
20	H	102	CLA	CBD-CGD-O2D-CED
20	L	208	CLA	CBD-CGD-O2D-CED
21	D	201	LMU	O5B-C1B-O1B-C4'
21	G	102	LMU	O5B-C1B-O1B-C4'
21	H	103	LMU	O5B-C1B-O1B-C4'
21	E	101	LMU	C2B-C1B-O1B-C4'
20	2	316	CLA	O1A-CGA-O2A-C1
20	3	311	CLA	O1A-CGA-O2A-C1
20	4	317	CLA	O1A-CGA-O2A-C1
20	A	849	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	O1A-CGA-O2A-C1
20	H	102	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	O1A-CGA-O2A-C1
20	1	204	CLA	C4C-C3C-CAC-CBC
20	1	213	CLA	C4C-C3C-CAC-CBC
20	4	304	CLA	C4C-C3C-CAC-CBC
20	B	828	CLA	C4C-C3C-CAC-CBC
20	B	841	CLA	C4C-C3C-CAC-CBC
20	2	303	CLA	C2C-C3C-CAC-CBC
20	4	304	CLA	C2C-C3C-CAC-CBC
20	A	801	CLA	C2C-C3C-CAC-CBC
20	H	101	CLA	C2C-C3C-CAC-CBC
20	K	104	CLA	C2C-C3C-CAC-CBC
20	4	318	CLA	O1D-CGD-O2D-CED
20	A	830	CLA	O1D-CGD-O2D-CED
20	A	840	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	O1D-CGD-O2D-CED
20	L	207	CLA	O1D-CGD-O2D-CED
21	A	847	LMU	O5B-C1B-O1B-C4'
21	B	804	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
21	E	101	LMU	O5B-C1B-O1B-C4'
21	L	210	LMU	O5B-C1B-O1B-C4'
21	R	102	LMU	O5B-C1B-O1B-C4'
21	R	105	LMU	O5B-C1B-O1B-C4'
21	B	804	LMU	C2B-C1B-O1B-C4'
21	K	107	LMU	C2B-C1B-O1B-C4'
20	4	315	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1
20	K	101	CLA	CBA-CGA-O2A-C1
21	K	105	LMU	C5'-C4'-O1B-C1B
25	B	848	LMG	C8-C9-O8-C28
20	1	202	CLA	C4C-C3C-CAC-CBC
20	4	301	CLA	C4C-C3C-CAC-CBC
20	1	204	CLA	C2C-C3C-CAC-CBC
20	1	211	CLA	O1D-CGD-O2D-CED
20	4	305	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	O1D-CGD-O2D-CED
20	A	810	CLA	O1D-CGD-O2D-CED
20	B	826	CLA	O1D-CGD-O2D-CED
20	B	834	CLA	O1D-CGD-O2D-CED
20	2	316	CLA	CBA-CGA-O2A-C1
20	3	311	CLA	CBA-CGA-O2A-C1
20	4	317	CLA	CBA-CGA-O2A-C1
20	H	102	CLA	CBA-CGA-O2A-C1
20	R	108	CLA	CBA-CGA-O2A-C1
21	G	103	LMU	O5B-C1B-O1B-C4'
20	1	206	CLA	O1A-CGA-O2A-C1
20	1	207	CLA	O1A-CGA-O2A-C1
20	2	314	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	O1A-CGA-O2A-C1
20	A	826	CLA	O1A-CGA-O2A-C1
20	A	832	CLA	O1A-CGA-O2A-C1
20	A	851	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	850	CLA	O1A-CGA-O2A-C1
20	J	103	CLA	O1A-CGA-O2A-C1
20	K	102	CLA	O1A-CGA-O2A-C1
20	L	203	CLA	O1A-CGA-O2A-C1
20	R	107	CLA	O1A-CGA-O2A-C1
20	2	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	3	314	CLA	C15-C16-C17-C18
21	2	321	LMU	C5'-C4'-O1B-C1B
21	A	847	LMU	C5'-C4'-O1B-C1B
20	1	201	CLA	O1A-CGA-O2A-C1
20	4	315	CLA	O1A-CGA-O2A-C1
20	K	101	CLA	O1A-CGA-O2A-C1
20	4	318	CLA	C4C-C3C-CAC-CBC
20	A	819	CLA	C4C-C3C-CAC-CBC
20	B	803	CLA	C4C-C3C-CAC-CBC
20	B	824	CLA	C4C-C3C-CAC-CBC
20	B	839	CLA	C4C-C3C-CAC-CBC
20	K	103	CLA	C4C-C3C-CAC-CBC
20	K	104	CLA	C4C-C3C-CAC-CBC
20	1	213	CLA	C2C-C3C-CAC-CBC
20	A	819	CLA	C2C-C3C-CAC-CBC
20	B	828	CLA	C2C-C3C-CAC-CBC
21	A	846	LMU	C4B-C5B-C6B-O6B
20	A	807	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	O1D-CGD-O2D-CED
20	A	813	CLA	O1D-CGD-O2D-CED
20	A	834	CLA	O1D-CGD-O2D-CED
20	B	806	CLA	O1D-CGD-O2D-CED
20	B	824	CLA	O1D-CGD-O2D-CED
21	4	321	LMU	O5B-C1B-O1B-C4'
21	R	104	LMU	C3'-C4'-O1B-C1B
20	B	837	CLA	C4C-C3C-CAC-CBC
20	1	202	CLA	C2C-C3C-CAC-CBC
20	4	318	CLA	C2C-C3C-CAC-CBC
20	B	803	CLA	C2C-C3C-CAC-CBC
20	B	839	CLA	C2C-C3C-CAC-CBC
20	K	103	CLA	C2C-C3C-CAC-CBC
20	A	833	CLA	O1D-CGD-O2D-CED
20	B	835	CLA	O1D-CGD-O2D-CED
20	J	101	CLA	O1D-CGD-O2D-CED
21	4	316	LMU	O5'-C5'-C6'-O6'
20	1	203	CLA	C2-C1-O2A-CGA
21	A	855	LMU	C3'-C4'-O1B-C1B
20	A	832	CLA	C4C-C3C-CAC-CBC
20	B	830	CLA	C4C-C3C-CAC-CBC
20	A	832	CLA	C2C-C3C-CAC-CBC
20	B	822	CLA	C2C-C3C-CAC-CBC
20	B	824	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	B	841	CLA	C2C-C3C-CAC-CBC
25	B	848	LMG	O9-C10-O7-C8
20	B	817	CLA	CBA-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	2	307	CLA	C3-C5-C6-C7
20	2	316	CLA	C3-C5-C6-C7
20	3	314	CLA	C3-C5-C6-C7
20	4	301	CLA	C3-C5-C6-C7
20	4	304	CLA	C3-C5-C6-C7
20	A	805	CLA	C3-C5-C6-C7
20	A	818	CLA	C3-C5-C6-C7
20	A	819	CLA	C3-C5-C6-C7
20	A	828	CLA	C3-C5-C6-C7
20	A	838	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	B	840	CLA	C3-C5-C6-C7
20	H	102	CLA	C3-C5-C6-C7
20	2	303	CLA	C4C-C3C-CAC-CBC
20	B	830	CLA	C2C-C3C-CAC-CBC
20	H	109	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	CBA-CGA-O2A-C1
20	1	207	CLA	CBA-CGA-O2A-C1
20	2	314	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	CBA-CGA-O2A-C1
20	A	836	CLA	CBA-CGA-O2A-C1
20	A	851	CLA	CBA-CGA-O2A-C1
20	B	806	CLA	CBA-CGA-O2A-C1
20	B	813	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
20	B	825	CLA	CBA-CGA-O2A-C1
20	B	850	CLA	CBA-CGA-O2A-C1
20	J	103	CLA	CBA-CGA-O2A-C1
20	K	102	CLA	CBA-CGA-O2A-C1
20	L	203	CLA	CBA-CGA-O2A-C1
20	R	107	CLA	CBA-CGA-O2A-C1
21	1	218	LMU	O5'-C5'-C6'-O6'
21	B	805	LMU	C3'-C4'-O1B-C1B
20	4	304	CLA	CBD-CGD-O2D-CED
20	4	317	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	CBD-CGD-O2D-CED
20	B	808	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	815	CLA	CBD-CGD-O2D-CED
20	H	108	CLA	CBD-CGD-O2D-CED
20	I	102	CLA	CBD-CGD-O2D-CED
20	R	108	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	C2C-C3C-CAC-CBC
20	4	318	CLA	C2-C1-O2A-CGA
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	O1D-CGD-O2D-CED
20	B	832	CLA	O1D-CGD-O2D-CED
20	3	307	CLA	C2C-C3C-CAC-CBC
20	A	816	CLA	C2C-C3C-CAC-CBC
20	A	804	CLA	O1D-CGD-O2D-CED
20	A	805	CLA	C4-C3-C5-C6
20	B	820	CLA	C4-C3-C5-C6
20	H	102	CLA	C4-C3-C5-C6
20	L	204	CLA	C4-C3-C5-C6
20	R	107	CLA	C4-C3-C5-C6
23	A	842	PQN	C14-C13-C15-C16
23	B	843	PQN	C14-C13-C15-C16
20	A	805	CLA	C2-C3-C5-C6
20	B	802	CLA	C2-C3-C5-C6
20	B	820	CLA	C2-C3-C5-C6
20	B	826	CLA	C2-C3-C5-C6
20	H	102	CLA	C2-C3-C5-C6
20	L	201	CLA	C2-C3-C5-C6
20	L	204	CLA	C2-C3-C5-C6
20	R	107	CLA	C2-C3-C5-C6
21	1	218	LMU	C3'-C4'-O1B-C1B
21	A	852	LMU	C3'-C4'-O1B-C1B
20	A	834	CLA	CBA-CGA-O2A-C1
21	2	313	LMU	O5'-C5'-C6'-O6'
21	R	104	LMU	O5B-C5B-C6B-O6B
20	A	839	CLA	C2A-CAA-CBA-CGA
20	K	103	CLA	C2A-CAA-CBA-CGA
20	L	201	CLA	C2A-CAA-CBA-CGA
21	2	320	LMU	O5B-C1B-O1B-C4'
20	A	826	CLA	C3-C5-C6-C7
20	A	827	CLA	C3-C5-C6-C7
20	A	830	CLA	C3-C5-C6-C7
20	B	802	CLA	C3-C5-C6-C7
20	B	837	CLA	C3-C5-C6-C7
20	B	841	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	3	319	LMU	C3'-C4'-O1B-C1B
20	A	817	CLA	C2C-C3C-CAC-CBC
20	A	801	CLA	CBA-CGA-O2A-C1
20	A	809	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
20	A	832	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	G	105	CLA	CBA-CGA-O2A-C1
20	H	109	CLA	CBA-CGA-O2A-C1
20	L	208	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
21	K	106	LMU	O5B-C1B-O1B-C4'
21	R	103	LMU	C4B-C5B-C6B-O6B
20	B	822	CLA	C4C-C3C-CAC-CBC
21	A	854	LMU	O5B-C5B-C6B-O6B
21	4	320	LMU	C2B-C1B-O1B-C4'
21	4	321	LMU	C2B-C1B-O1B-C4'
21	K	106	LMU	C4'-C5'-C6'-O6'
22	A	843	BCR	C9-C10-C11-C12
22	B	846	BCR	C9-C10-C11-C12
22	F	203	BCR	C19-C20-C21-C22
22	I	101	BCR	C19-C20-C21-C22
22	J	102	BCR	C19-C20-C21-C22
22	L	209	BCR	C19-C20-C21-C22
20	A	828	CLA	O1A-CGA-O2A-C1
20	A	836	CLA	O1A-CGA-O2A-C1
20	F	207	CLA	O1A-CGA-O2A-C1
20	3	313	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	O1D-CGD-O2D-CED
21	4	319	LMU	C5'-C4'-O1B-C1B
20	A	834	CLA	O1A-CGA-O2A-C1
21	G	102	LMU	O5'-C5'-C6'-O6'
20	A	816	CLA	C4C-C3C-CAC-CBC
20	4	305	CLA	C2C-C3C-CAC-CBC
20	J	101	CLA	C2C-C3C-CAC-CBC
21	2	319	LMU	C4B-C5B-C6B-O6B
20	B	850	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	C3-C5-C6-C7
20	H	108	CLA	C3-C5-C6-C7
23	A	842	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	1	201	CLA	CBD-CGD-O2D-CED
20	3	311	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	CBD-CGD-O2D-CED
20	B	836	CLA	CBD-CGD-O2D-CED
21	G	102	LMU	C11-C10-C9-C8
21	4	320	LMU	O5B-C1B-O1B-C4'
20	B	830	CLA	O1D-CGD-O2D-CED
20	2	305	CLA	CBA-CGA-O2A-C1
20	4	310	CLA	CBA-CGA-O2A-C1
20	B	808	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	CBA-CGA-O2A-C1
25	B	848	LMG	C29-C28-O8-C9
21	1	216	LMU	O5'-C5'-C6'-O6'
21	B	804	LMU	O5B-C5B-C6B-O6B
21	R	106	LMU	O5B-C5B-C6B-O6B
20	A	801	CLA	O1A-CGA-O2A-C1
20	B	806	CLA	O1A-CGA-O2A-C1
20	B	813	CLA	O1A-CGA-O2A-C1
20	B	820	CLA	O1A-CGA-O2A-C1
20	L	208	CLA	O1A-CGA-O2A-C1
21	K	107	LMU	C4B-C5B-C6B-O6B
21	R	101	LMU	C4'-C5'-C6'-O6'
20	2	311	CLA	O1D-CGD-O2D-CED
21	4	320	LMU	O5B-C5B-C6B-O6B
21	F	202	LMU	O5'-C5'-C6'-O6'
21	R	105	LMU	O5B-C5B-C6B-O6B
21	2	313	LMU	C4'-C5'-C6'-O6'
21	4	316	LMU	C4'-C5'-C6'-O6'
21	B	849	LMU	C4'-C5'-C6'-O6'
20	A	805	CLA	CBD-CGD-O2D-CED
20	B	802	CLA	CBD-CGD-O2D-CED
20	B	825	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	C2C-C3C-CAC-CBC
20	A	836	CLA	C2C-C3C-CAC-CBC
21	2	318	LMU	O5B-C1B-O1B-C4'
20	H	109	CLA	O1A-CGA-O2A-C1
21	F	202	LMU	O5B-C5B-C6B-O6B
21	A	854	LMU	C4B-C5B-C6B-O6B
21	B	804	LMU	C4B-C5B-C6B-O6B
20	A	832	CLA	O1D-CGD-O2D-CED
20	B	820	CLA	O1D-CGD-O2D-CED
20	A	816	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	849	CLA	C3-C5-C6-C7
20	B	830	CLA	C3-C5-C6-C7
20	L	204	CLA	C3-C5-C6-C7
20	B	841	CLA	CBD-CGD-O2D-CED
21	4	320	LMU	O5'-C5'-C6'-O6'
21	K	105	LMU	O5'-C5'-C6'-O6'
21	R	105	LMU	O5'-C5'-C6'-O6'
20	B	840	CLA	C2C-C3C-CAC-CBC
21	A	846	LMU	C4'-C5'-C6'-O6'
21	F	202	LMU	C4'-C5'-C6'-O6'
21	G	102	LMU	C4'-C5'-C6'-O6'
20	3	313	CLA	CBA-CGA-O2A-C1
20	F	207	CLA	CBA-CGA-O2A-C1
21	A	846	LMU	C3'-C4'-O1B-C1B
20	2	307	CLA	C4-C3-C5-C6
20	A	831	CLA	C4-C3-C5-C6
20	A	850	CLA	C4-C3-C5-C6
20	2	307	CLA	C2-C3-C5-C6
20	A	831	CLA	C2-C3-C5-C6
20	A	850	CLA	C2-C3-C5-C6
23	A	842	PQN	C12-C13-C15-C16
20	2	305	CLA	O1A-CGA-O2A-C1
21	A	846	LMU	O5'-C5'-C6'-O6'
21	A	855	LMU	O5'-C5'-C6'-O6'
21	H	103	LMU	O5B-C5B-C6B-O6B
21	R	101	LMU	O5'-C5'-C6'-O6'
21	R	104	LMU	C4B-C5B-C6B-O6B
20	A	836	CLA	CBD-CGD-O2D-CED
21	K	107	LMU	O5B-C5B-C6B-O6B
21	L	206	LMU	O5B-C5B-C6B-O6B
21	1	218	LMU	C4'-C5'-C6'-O6'
21	R	106	LMU	C4B-C5B-C6B-O6B
20	4	317	CLA	C3-C5-C6-C7
20	A	805	CLA	C2A-CAA-CBA-CGA
20	B	815	CLA	C2A-CAA-CBA-CGA
21	G	101	LMU	C2B-C1B-O1B-C4'
21	K	105	LMU	C5-C6-C7-C8
20	B	837	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	O1A-CGA-O2A-C1
20	A	837	CLA	O1A-CGA-O2A-C1
20	B	808	CLA	O1A-CGA-O2A-C1
20	G	105	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	848	LMG	O10-C28-O8-C9
21	2	320	LMU	O5'-C1'-O1'-C1
21	4	316	LMU	O5'-C1'-O1'-C1
21	A	854	LMU	O5'-C1'-O1'-C1
21	C	101	LMU	O5'-C1'-O1'-C1
21	H	103	LMU	O5'-C1'-O1'-C1
21	L	210	LMU	O5'-C1'-O1'-C1
21	R	101	LMU	O5'-C1'-O1'-C1
21	R	105	LMU	O5'-C1'-O1'-C1
21	R	104	LMU	C11-C10-C9-C8
21	A	846	LMU	O5B-C5B-C6B-O6B
21	1	217	LMU	C1-C2-C3-C4
21	H	105	LMU	O1'-C1-C2-C3
20	A	837	CLA	CBA-CGA-O2A-C1
20	A	839	CLA	CBA-CGA-O2A-C1
20	K	104	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBD-CGD-O2D-CED
20	B	813	CLA	CBD-CGD-O2D-CED
21	2	319	LMU	O5B-C5B-C6B-O6B
21	3	318	LMU	O5'-C5'-C6'-O6'
21	A	852	LMU	O5'-C5'-C6'-O6'
21	B	849	LMU	O5'-C5'-C6'-O6'
21	L	205	LMU	O5B-C5B-C6B-O6B
21	L	205	LMU	O5'-C5'-C6'-O6'
20	1	201	CLA	C2C-C3C-CAC-CBC
20	1	207	CLA	C2C-C3C-CAC-CBC
21	3	319	LMU	C4-C5-C6-C7
21	A	853	LMU	C2-C3-C4-C5
21	K	106	LMU	O5'-C5'-C6'-O6'
21	R	103	LMU	O5B-C5B-C6B-O6B
21	3	318	LMU	C4'-C5'-C6'-O6'
21	A	855	LMU	C4'-C5'-C6'-O6'
21	H	106	LMU	C4B-C5B-C6B-O6B
21	R	106	LMU	C6-C7-C8-C9
21	R	109	LMU	C7-C8-C9-C10
20	3	307	CLA	C4C-C3C-CAC-CBC
20	A	817	CLA	C4C-C3C-CAC-CBC
21	D	201	LMU	O1'-C1-C2-C3
21	R	104	LMU	O5'-C5'-C6'-O6'
21	2	313	LMU	C4-C5-C6-C7
21	B	804	LMU	C6-C7-C8-C9
22	F	204	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	F	204	BCR	C15-C16-C17-C18
21	E	101	LMU	C1-C2-C3-C4
20	1	211	CLA	CBA-CGA-O2A-C1
20	2	310	CLA	CBA-CGA-O2A-C1
20	3	310	CLA	CBA-CGA-O2A-C1
20	4	304	CLA	CBA-CGA-O2A-C1
20	4	318	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBA-CGA-O2A-C1
20	A	838	CLA	CBA-CGA-O2A-C1
20	H	108	CLA	CBA-CGA-O2A-C1
20	H	110	CLA	CBA-CGA-O2A-C1
21	4	319	LMU	C7-C8-C9-C10
21	L	210	LMU	O5B-C5B-C6B-O6B
21	L	205	LMU	C4B-C5B-C6B-O6B
21	4	319	LMU	C5-C6-C7-C8
21	4	320	LMU	C7-C8-C9-C10
21	H	106	LMU	C7-C8-C9-C10
20	I	102	CLA	O1D-CGD-O2D-CED
21	2	313	LMU	C2-C3-C4-C5
21	A	846	LMU	C2-C3-C4-C5
21	A	853	LMU	C11-C10-C9-C8
21	R	104	LMU	C4'-C5'-C6'-O6'
21	R	105	LMU	C4'-C5'-C6'-O6'
21	R	102	LMU	C6-C7-C8-C9
20	3	311	CLA	C4-C3-C5-C6
20	B	827	CLA	C4-C3-C5-C6
20	3	311	CLA	C2-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
23	B	843	PQN	C12-C13-C15-C16
20	2	303	CLA	C11-C10-C8-C9
20	A	811	CLA	C14-C13-C15-C16
20	A	825	CLA	C11-C10-C8-C9
20	A	825	CLA	C14-C13-C15-C16
20	A	831	CLA	C6-C7-C8-C9
20	A	831	CLA	C11-C12-C13-C14
20	A	851	CLA	C6-C7-C8-C9
20	A	851	CLA	C11-C10-C8-C9
20	B	803	CLA	C14-C13-C15-C16
20	B	806	CLA	C11-C10-C8-C9
20	B	806	CLA	C14-C13-C15-C16
20	B	808	CLA	C11-C10-C8-C9
20	B	808	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	824	CLA	C11-C10-C8-C9
20	B	824	CLA	C14-C13-C15-C16
20	B	828	CLA	C6-C7-C8-C9
20	B	830	CLA	C11-C10-C8-C9
20	B	832	CLA	C11-C10-C8-C9
20	B	838	CLA	C11-C12-C13-C14
20	H	108	CLA	C6-C7-C8-C9
20	R	108	CLA	C11-C10-C8-C9
20	R	108	CLA	C11-C12-C13-C14
23	A	842	PQN	C21-C22-C23-C24
21	H	105	LMU	C5-C6-C7-C8
21	1	216	LMU	C4'-C5'-C6'-O6'
21	R	105	LMU	C4B-C5B-C6B-O6B
20	B	815	CLA	O1D-CGD-O2D-CED
20	L	208	CLA	O1D-CGD-O2D-CED
20	R	108	CLA	O1D-CGD-O2D-CED
21	4	316	LMU	C2'-C1'-O1'-C1
21	4	320	LMU	C2'-C1'-O1'-C1
21	4	321	LMU	C2'-C1'-O1'-C1
21	A	852	LMU	C2'-C1'-O1'-C1
21	A	854	LMU	C2'-C1'-O1'-C1
21	C	101	LMU	C2'-C1'-O1'-C1
21	G	101	LMU	C2'-C1'-O1'-C1
21	K	106	LMU	C2'-C1'-O1'-C1
21	L	210	LMU	C2'-C1'-O1'-C1
21	R	101	LMU	C2'-C1'-O1'-C1
21	R	105	LMU	C2'-C1'-O1'-C1
21	A	846	LMU	C5'-C4'-O1B-C1B
20	4	304	CLA	O1D-CGD-O2D-CED
21	4	316	LMU	O5B-C5B-C6B-O6B
20	3	313	CLA	O1A-CGA-O2A-C1
20	4	304	CLA	O1A-CGA-O2A-C1
20	A	838	CLA	O1A-CGA-O2A-C1
21	L	206	LMU	C4B-C5B-C6B-O6B
21	2	313	LMU	C2B-C1B-O1B-C4'
22	2	317	BCR	C37-C22-C23-C24
22	A	844	BCR	C11-C12-C13-C35
22	A	845	BCR	C7-C8-C9-C34
22	B	801	BCR	C37-C22-C23-C24
22	B	846	BCR	C37-C22-C23-C24
22	F	204	BCR	C7-C8-C9-C34
22	G	104	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	I	101	BCR	C36-C18-C19-C20
22	I	101	BCR	C37-C22-C23-C24
22	I	103	BCR	C11-C12-C13-C35
22	J	102	BCR	C36-C18-C19-C20
22	2	317	BCR	C17-C18-C19-C20
22	2	317	BCR	C21-C22-C23-C24
22	B	847	BCR	C7-C8-C9-C10
22	F	203	BCR	C21-C22-C23-C24
21	K	105	LMU	C4'-C5'-C6'-O6'
20	A	817	CLA	C3-C5-C6-C7
20	A	830	CLA	C2A-CAA-CBA-CGA
20	B	822	CLA	C2A-CAA-CBA-CGA
20	B	840	CLA	C2A-CAA-CBA-CGA
20	H	102	CLA	C2A-CAA-CBA-CGA
20	J	101	CLA	C4C-C3C-CAC-CBC
21	L	210	LMU	C5-C6-C7-C8
20	B	824	CLA	C3-C5-C6-C7
21	A	854	LMU	O5'-C5'-C6'-O6'
21	R	103	LMU	O5'-C5'-C6'-O6'
21	A	852	LMU	C4'-C5'-C6'-O6'
21	L	210	LMU	C4'-C5'-C6'-O6'
21	F	202	LMU	C4B-C5B-C6B-O6B
21	R	101	LMU	C4B-C5B-C6B-O6B
20	F	201	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	C5-C6-C7-C8
20	1	206	CLA	C2-C1-O2A-CGA
20	A	805	CLA	C2-C1-O2A-CGA
20	A	823	CLA	C2-C1-O2A-CGA
20	A	824	CLA	C2-C1-O2A-CGA
20	A	837	CLA	C2-C1-O2A-CGA
21	E	101	LMU	C3-C4-C5-C6
20	B	803	CLA	O1D-CGD-O2D-CED
20	K	103	CLA	CBD-CGD-O2D-CED
21	R	109	LMU	C3'-C4'-O1B-C1B
20	A	851	CLA	C2C-C3C-CAC-CBC
20	B	838	CLA	C13-C15-C16-C17
20	B	808	CLA	O1D-CGD-O2D-CED
21	L	206	LMU	O5'-C5'-C6'-O6'
20	2	310	CLA	O1A-CGA-O2A-C1
20	H	110	CLA	O1A-CGA-O2A-C1
20	2	305	CLA	C2C-C3C-CAC-CBC
21	B	849	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	2	312	CLA	C11-C12-C13-C15
20	2	316	CLA	C12-C13-C15-C16
20	3	314	CLA	C11-C10-C8-C7
20	4	303	CLA	C12-C13-C15-C16
20	A	849	CLA	C12-C13-C15-C16
20	B	815	CLA	C11-C10-C8-C7
20	B	824	CLA	C11-C12-C13-C15
20	L	203	CLA	C11-C10-C8-C7
20	4	317	CLA	O1D-CGD-O2D-CED
21	2	319	LMU	C3-C4-C5-C6
21	A	852	LMU	C2-C3-C4-C5
21	K	107	LMU	C3-C4-C5-C6
21	1	217	LMU	O1'-C1-C2-C3
21	F	202	LMU	O1'-C1-C2-C3
20	1	206	CLA	C4-C3-C5-C6
21	E	101	LMU	O5'-C5'-C6'-O6'
20	3	311	CLA	C13-C15-C16-C17
20	A	808	CLA	C5-C6-C7-C8
20	A	849	CLA	C10-C11-C12-C13
21	L	210	LMU	C4B-C5B-C6B-O6B
22	A	845	BCR	C19-C20-C21-C22
22	G	104	BCR	C19-C20-C21-C22
22	I	103	BCR	C19-C20-C21-C22
21	L	206	LMU	O1'-C1-C2-C3
20	K	104	CLA	O1A-CGA-O2A-C1
20	A	835	CLA	O1D-CGD-O2D-CED
21	H	103	LMU	C4B-C5B-C6B-O6B
21	K	107	LMU	C4'-C5'-C6'-O6'
20	A	819	CLA	C5-C6-C7-C8
20	A	831	CLA	C13-C15-C16-C17
20	A	851	CLA	C8-C10-C11-C12
20	B	806	CLA	C15-C16-C17-C18
20	B	815	CLA	C5-C6-C7-C8
20	B	815	CLA	C10-C11-C12-C13
20	B	828	CLA	C8-C10-C11-C12
20	B	840	CLA	C4C-C3C-CAC-CBC
21	2	313	LMU	O5B-C1B-O1B-C4'
21	1	216	LMU	O5B-C5B-C6B-O6B
20	A	812	CLA	O1A-CGA-O2A-C1
20	A	839	CLA	O1A-CGA-O2A-C1
20	H	108	CLA	O1A-CGA-O2A-C1
20	A	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	827	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	C5-C6-C7-C8
20	L	201	CLA	C5-C6-C7-C8
20	R	108	CLA	C8-C10-C11-C12
21	B	805	LMU	O5'-C5'-C6'-O6'
20	4	305	CLA	C4C-C3C-CAC-CBC
20	A	817	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	C2A-CAA-CBA-CGA
20	A	832	CLA	C2A-CAA-CBA-CGA
20	A	849	CLA	C2A-CAA-CBA-CGA
20	B	806	CLA	C2A-CAA-CBA-CGA
20	B	814	CLA	C2A-CAA-CBA-CGA
20	B	818	CLA	C2A-CAA-CBA-CGA
20	B	823	CLA	C2A-CAA-CBA-CGA
20	B	830	CLA	C2A-CAA-CBA-CGA
20	J	103	CLA	C2A-CAA-CBA-CGA
20	R	107	CLA	C2A-CAA-CBA-CGA
20	2	307	CLA	C5-C6-C7-C8
20	A	818	CLA	C5-C6-C7-C8
20	B	803	CLA	C13-C15-C16-C17
20	B	824	CLA	C13-C15-C16-C17
20	B	841	CLA	C15-C16-C17-C18
20	L	202	CLA	C5-C6-C7-C8
20	L	203	CLA	C8-C10-C11-C12
21	A	852	LMU	O1'-C1-C2-C3
20	4	318	CLA	O1A-CGA-O2A-C1
20	F	201	CLA	O1A-CGA-O2A-C1
21	4	321	LMU	O5'-C1'-O1'-C1
21	A	853	LMU	O5'-C1'-O1'-C1
21	G	101	LMU	O5'-C1'-O1'-C1
21	A	853	LMU	C4-C5-C6-C7
21	D	201	LMU	C2-C3-C4-C5
21	K	107	LMU	C5-C6-C7-C8
21	1	218	LMU	O1'-C1-C2-C3
21	H	104	LMU	O1'-C1-C2-C3
20	1	206	CLA	C8-C10-C11-C12
20	3	314	CLA	C10-C11-C12-C13
20	3	314	CLA	C13-C15-C16-C17
20	A	827	CLA	C5-C6-C7-C8
20	A	849	CLA	C5-C6-C7-C8
20	B	820	CLA	C10-C11-C12-C13
20	B	823	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	843	PQN	C18-C20-C21-C22
20	2	302	CLA	C2C-C3C-CAC-CBC
21	1	216	LMU	C7-C8-C9-C10
21	H	104	LMU	C3-C4-C5-C6
20	2	302	CLA	CBD-CGD-O2D-CED
20	1	211	CLA	O1A-CGA-O2A-C1
20	3	310	CLA	O1A-CGA-O2A-C1
20	B	840	CLA	C10-C11-C12-C13
20	I	102	CLA	C5-C6-C7-C8
23	A	842	PQN	C25-C26-C27-C28
21	R	105	LMU	O1'-C1-C2-C3
20	3	311	CLA	O1D-CGD-O2D-CED
21	G	101	LMU	O5B-C1B-O1B-C4'
20	A	831	CLA	C15-C16-C17-C18
20	A	851	CLA	C15-C16-C17-C18
20	B	827	CLA	C15-C16-C17-C18
23	B	843	PQN	C20-C21-C22-C23
21	2	313	LMU	O5B-C5B-C6B-O6B
21	H	106	LMU	O5B-C5B-C6B-O6B
21	L	210	LMU	O5'-C5'-C6'-O6'
21	A	854	LMU	O1'-C1-C2-C3
21	B	804	LMU	O1'-C1-C2-C3
21	K	107	LMU	O1'-C1-C2-C3
20	B	836	CLA	O1D-CGD-O2D-CED
20	H	108	CLA	O1D-CGD-O2D-CED
20	2	312	CLA	C2C-C3C-CAC-CBC
21	2	318	LMU	O1'-C1-C2-C3
20	A	811	CLA	C10-C11-C12-C13
20	A	838	CLA	C13-C15-C16-C17
20	B	803	CLA	C10-C11-C12-C13
20	B	810	CLA	C8-C10-C11-C12
20	B	813	CLA	C5-C6-C7-C8
23	B	843	PQN	C15-C16-C17-C18
20	B	830	CLA	CBA-CGA-O2A-C1
21	4	320	LMU	C4B-C5B-C6B-O6B
20	3	311	CLA	C3-C5-C6-C7
20	A	811	CLA	C3-C5-C6-C7
21	H	105	LMU	C3'-C4'-O1B-C1B
20	B	830	CLA	C15-C16-C17-C18
20	R	108	CLA	C5-C6-C7-C8
21	4	319	LMU	C4'-C5'-C6'-O6'
20	A	807	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	824	CLA	C2A-CAA-CBA-CGA
20	A	837	CLA	C2A-CAA-CBA-CGA
20	A	838	CLA	C2A-CAA-CBA-CGA
20	B	831	CLA	C2A-CAA-CBA-CGA
20	B	835	CLA	C2A-CAA-CBA-CGA
20	A	825	CLA	CBA-CGA-O2A-C1
21	R	103	LMU	C7-C8-C9-C10
20	A	826	CLA	C15-C16-C17-C18
20	A	850	CLA	C13-C15-C16-C17
20	B	806	CLA	C13-C15-C16-C17
20	B	814	CLA	C5-C6-C7-C8
20	B	838	CLA	C8-C10-C11-C12
21	R	109	LMU	C5'-C4'-O1B-C1B
20	A	820	CLA	O1D-CGD-O2D-CED
20	B	841	CLA	O1D-CGD-O2D-CED
20	A	830	CLA	C13-C15-C16-C17
20	B	814	CLA	C10-C11-C12-C13
20	A	805	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	C5-C6-C7-C8
20	A	851	CLA	C10-C11-C12-C13
20	H	102	CLA	C5-C6-C7-C8
20	L	203	CLA	C15-C16-C17-C18
20	B	802	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	C4C-C3C-CAC-CBC
20	R	107	CLA	C8-C10-C11-C12
20	3	311	CLA	C5-C6-C7-C8
20	A	828	CLA	C13-C15-C16-C17
20	A	849	CLA	C8-C10-C11-C12
20	A	828	CLA	C11-C10-C8-C9
20	B	850	CLA	C11-C12-C13-C14
21	2	313	LMU	C9-C10-C11-C12
21	H	105	LMU	C2'-C1'-O1'-C1
21	H	106	LMU	C2'-C1'-O1'-C1
21	L	206	LMU	C2'-C1'-O1'-C1
25	B	848	LMG	C2-C1-O1-C7
20	B	830	CLA	C5-C6-C7-C8
20	3	311	CLA	C16-C17-C18-C20
20	L	202	CLA	C6-C7-C8-C10
22	F	203	BCR	C20-C21-C22-C37
20	A	811	CLA	C4C-C3C-CAC-CBC
20	J	103	CLA	C3-C5-C6-C7
21	1	218	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	R	102	LMU	C11-C10-C9-C8
20	L	201	CLA	C10-C11-C12-C13
23	A	842	PQN	C20-C21-C22-C23
22	2	317	BCR	C11-C12-C13-C35
22	A	844	BCR	C7-C8-C9-C34
22	B	844	BCR	C7-C8-C9-C34
22	F	203	BCR	C37-C22-C23-C24
22	G	104	BCR	C37-C22-C23-C24
22	I	103	BCR	C37-C22-C23-C24
22	J	102	BCR	C37-C22-C23-C24
20	A	831	CLA	C2C-C3C-CAC-CBC
21	H	105	LMU	O5'-C5'-C6'-O6'
21	K	107	LMU	O5'-C5'-C6'-O6'
22	A	844	BCR	C7-C8-C9-C10
22	A	845	BCR	C7-C8-C9-C10
22	B	844	BCR	C7-C8-C9-C10
22	G	104	BCR	C21-C22-C23-C24
22	I	101	BCR	C17-C18-C19-C20
22	I	103	BCR	C21-C22-C23-C24
22	J	102	BCR	C21-C22-C23-C24
21	L	205	LMU	C4'-C5'-C6'-O6'
21	R	106	LMU	O1'-C1-C2-C3
20	1	211	CLA	C2A-CAA-CBA-CGA
20	3	313	CLA	C2A-CAA-CBA-CGA
20	4	305	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C2A-CAA-CBA-CGA
20	A	829	CLA	C2A-CAA-CBA-CGA
20	A	836	CLA	C2A-CAA-CBA-CGA
20	A	840	CLA	C2A-CAA-CBA-CGA
20	H	108	CLA	C2A-CAA-CBA-CGA
20	K	101	CLA	C2A-CAA-CBA-CGA
20	A	809	CLA	O2A-C1-C2-C3
20	A	825	CLA	O2A-C1-C2-C3
20	A	837	CLA	O2A-C1-C2-C3
20	R	108	CLA	O2A-C1-C2-C3
21	H	104	LMU	C5'-C4'-O1B-C1B
20	A	811	CLA	C16-C17-C18-C19
20	A	818	CLA	C11-C12-C13-C15
20	A	827	CLA	C6-C7-C8-C9
20	A	835	CLA	C16-C17-C18-C19
20	B	837	CLA	C11-C12-C13-C14
20	A	824	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	K	104	CLA	C3-C5-C6-C7
22	F	203	BCR	C20-C21-C22-C23
21	L	206	LMU	O5'-C1'-O1'-C1
21	D	201	LMU	O5B-C5B-C6B-O6B
21	R	101	LMU	O5B-C5B-C6B-O6B
21	1	218	LMU	C7-C8-C9-C10
20	B	825	CLA	O1D-CGD-O2D-CED
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	840	CLA	CBA-CGA-O2A-C1
20	K	103	CLA	CBA-CGA-O2A-C1
20	A	838	CLA	C10-C11-C12-C13
20	B	809	CLA	C10-C11-C12-C13
21	3	319	LMU	O5'-C5'-C6'-O6'
20	A	815	CLA	C2C-C3C-CAC-CBC
20	2	302	CLA	C2-C1-O2A-CGA
20	2	316	CLA	C2-C1-O2A-CGA
20	B	832	CLA	C2-C1-O2A-CGA
20	3	311	CLA	C16-C17-C18-C19
20	3	314	CLA	C16-C17-C18-C19
20	3	314	CLA	C16-C17-C18-C20
20	B	840	CLA	C16-C17-C18-C19
20	I	102	CLA	C11-C12-C13-C14
20	L	203	CLA	C16-C17-C18-C19
20	L	203	CLA	C16-C17-C18-C20
23	A	842	PQN	C26-C27-C28-C30
20	B	830	CLA	O1A-CGA-O2A-C1
20	1	207	CLA	C4C-C3C-CAC-CBC
20	2	310	CLA	C2C-C3C-CAC-CBC
20	B	807	CLA	C2C-C3C-CAC-CBC
21	4	320	LMU	C6-C7-C8-C9
21	4	321	LMU	C3-C4-C5-C6
25	B	848	LMG	C32-C33-C34-C35
21	2	313	LMU	C1-C2-C3-C4
21	R	102	LMU	C1-C2-C3-C4
21	4	316	LMU	C2-C3-C4-C5
21	A	848	LMU	C7-C8-C9-C10
21	K	107	LMU	C4-C5-C6-C7
20	A	831	CLA	C5-C6-C7-C8
21	4	321	LMU	C4'-C5'-C6'-O6'
21	A	855	LMU	C6-C7-C8-C9
21	B	805	LMU	C4-C5-C6-C7
21	H	103	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	K	107	LMU	C6-C7-C8-C9
21	L	205	LMU	C6-C7-C8-C9
21	L	210	LMU	C11-C10-C9-C8
21	R	101	LMU	C2-C3-C4-C5
21	R	103	LMU	O1'-C1-C2-C3
20	A	825	CLA	O1A-CGA-O2A-C1
20	1	201	CLA	O1D-CGD-O2D-CED
20	A	823	CLA	CBA-CGA-O2A-C1
21	3	318	LMU	C2-C3-C4-C5
21	3	318	LMU	C4-C5-C6-C7
21	4	321	LMU	C5-C6-C7-C8
21	C	101	LMU	C7-C8-C9-C10
21	E	101	LMU	C11-C10-C9-C8
21	L	205	LMU	C7-C8-C9-C10
21	L	206	LMU	C6-C7-C8-C9
21	A	846	LMU	C2-C1-O1'-C1'
21	D	201	LMU	C2-C1-O1'-C1'
21	G	102	LMU	C2-C1-O1'-C1'
21	L	205	LMU	C2-C1-O1'-C1'
20	4	306	CLA	CBD-CGD-O2D-CED
21	H	104	LMU	C4B-C5B-C6B-O6B
21	2	320	LMU	C4-C5-C6-C7
21	G	101	LMU	C7-C8-C9-C10
21	G	103	LMU	C2-C3-C4-C5
21	R	104	LMU	C5-C6-C7-C8
25	B	848	LMG	C33-C34-C35-C36
20	A	812	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	O1D-CGD-O2D-CED
20	3	310	CLA	C13-C15-C16-C17
20	1	201	CLA	C4B-C3B-CAB-CBB
20	2	307	CLA	C4B-C3B-CAB-CBB
20	3	313	CLA	C4B-C3B-CAB-CBB
20	4	301	CLA	C4B-C3B-CAB-CBB
20	A	803	CLA	C4B-C3B-CAB-CBB
20	A	807	CLA	C4B-C3B-CAB-CBB
20	A	811	CLA	C4B-C3B-CAB-CBB
20	A	834	CLA	C4B-C3B-CAB-CBB
20	B	809	CLA	C4B-C3B-CAB-CBB
20	B	815	CLA	C4B-C3B-CAB-CBB
20	B	817	CLA	C4B-C3B-CAB-CBB
20	B	818	CLA	C4B-C3B-CAB-CBB
20	B	822	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	825	CLA	C4B-C3B-CAB-CBB
20	B	829	CLA	C4B-C3B-CAB-CBB
20	B	830	CLA	C4B-C3B-CAB-CBB
20	B	833	CLA	C4B-C3B-CAB-CBB
20	F	201	CLA	C4B-C3B-CAB-CBB
20	H	108	CLA	C4B-C3B-CAB-CBB
20	R	107	CLA	C4B-C3B-CAB-CBB
21	K	106	LMU	O1'-C1-C2-C3
21	R	106	LMU	C2-C3-C4-C5
25	B	848	LMG	C17-C18-C19-C20
20	A	828	CLA	C16-C17-C18-C19
20	A	828	CLA	C16-C17-C18-C20
20	A	850	CLA	C16-C17-C18-C19
20	A	850	CLA	C16-C17-C18-C20
20	B	837	CLA	C11-C12-C13-C15
20	1	215	CLA	C2A-CAA-CBA-CGA
20	2	312	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	C2A-CAA-CBA-CGA
21	1	217	LMU	C3-C4-C5-C6
21	A	848	LMU	C5-C6-C7-C8
21	2	319	LMU	C1-C2-C3-C4
21	L	210	LMU	C1-C2-C3-C4
21	R	103	LMU	C1-C2-C3-C4
21	D	201	LMU	C11-C10-C9-C8
21	K	106	LMU	C4-C5-C6-C7
21	H	103	LMU	C6-C7-C8-C9
21	H	105	LMU	C5'-C4'-O1B-C1B
25	B	848	LMG	C10-C11-C12-C13
20	3	310	CLA	C10-C11-C12-C13
20	A	825	CLA	C8-C10-C11-C12
21	2	318	LMU	C7-C8-C9-C10
21	4	316	LMU	C7-C8-C9-C10
21	C	101	LMU	C11-C10-C9-C8
20	B	825	CLA	C3-C5-C6-C7
20	1	203	CLA	C3A-C2A-CAA-CBA
20	3	311	CLA	C3A-C2A-CAA-CBA
20	4	310	CLA	C3A-C2A-CAA-CBA
20	A	806	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	825	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	816	CLA	C3A-C2A-CAA-CBA
20	F	201	CLA	C3A-C2A-CAA-CBA
20	K	104	CLA	C3A-C2A-CAA-CBA
20	L	201	CLA	C3A-C2A-CAA-CBA
20	L	207	CLA	C3A-C2A-CAA-CBA
20	L	208	CLA	C3A-C2A-CAA-CBA
20	R	107	CLA	C3A-C2A-CAA-CBA
21	4	320	LMU	C3-C4-C5-C6
21	A	852	LMU	C7-C8-C9-C10
21	G	103	LMU	C5-C6-C7-C8
21	H	106	LMU	C6-C7-C8-C9
20	2	303	CLA	C5-C6-C7-C8
20	A	828	CLA	C8-C10-C11-C12
20	A	830	CLA	C15-C16-C17-C18
20	A	838	CLA	C5-C6-C7-C8
20	B	850	CLA	C10-C11-C12-C13
21	3	319	LMU	C5'-C4'-O1B-C1B
21	1	216	LMU	C4B-C5B-C6B-O6B
21	3	318	LMU	O1'-C1-C2-C3
21	A	852	LMU	C1-C2-C3-C4
21	R	109	LMU	C1-C2-C3-C4
21	2	320	LMU	C5-C6-C7-C8
21	A	847	LMU	C6-C7-C8-C9
21	A	853	LMU	O1'-C1-C2-C3
21	2	313	LMU	C11-C10-C9-C8
21	A	848	LMU	C6-C7-C8-C9
21	K	106	LMU	C3-C4-C5-C6
20	1	215	CLA	CBA-CGA-O2A-C1
21	4	321	LMU	C6-C7-C8-C9
21	H	105	LMU	C4-C5-C6-C7
20	3	314	CLA	C8-C10-C11-C12
21	4	316	LMU	C4-C5-C6-C7
21	A	846	LMU	C3-C4-C5-C6
21	A	847	LMU	C5-C6-C7-C8
21	A	854	LMU	C3-C4-C5-C6
21	G	101	LMU	C2-C3-C4-C5
21	K	107	LMU	C11-C10-C9-C8
21	L	210	LMU	C6-C7-C8-C9
25	B	848	LMG	C37-C38-C39-C40
21	1	218	LMU	C5'-C4'-O1B-C1B
21	2	321	LMU	C7-C8-C9-C10
21	B	804	LMU	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	F	202	LMU	C5-C6-C7-C8
20	B	813	CLA	O1D-CGD-O2D-CED
21	G	102	LMU	C4-C5-C6-C7
21	A	848	LMU	C11-C10-C9-C8
20	A	835	CLA	C16-C17-C18-C20
20	B	840	CLA	C16-C17-C18-C20
20	I	102	CLA	C11-C12-C13-C15
20	B	814	CLA	O1A-CGA-O2A-C1
21	2	320	LMU	O5'-C5'-C6'-O6'
20	2	311	CLA	C2B-C3B-CAB-CBB
20	3	307	CLA	C2B-C3B-CAB-CBB
20	A	813	CLA	C2B-C3B-CAB-CBB
20	A	825	CLA	C2B-C3B-CAB-CBB
20	A	828	CLA	C2B-C3B-CAB-CBB
20	A	829	CLA	C2B-C3B-CAB-CBB
20	B	802	CLA	C2B-C3B-CAB-CBB
20	B	816	CLA	C2B-C3B-CAB-CBB
20	B	833	CLA	C2B-C3B-CAB-CBB
20	H	110	CLA	C2B-C3B-CAB-CBB
20	K	101	CLA	C2B-C3B-CAB-CBB
20	L	203	CLA	C2B-C3B-CAB-CBB
20	L	207	CLA	C2B-C3B-CAB-CBB
22	2	317	BCR	C23-C24-C25-C26
22	2	317	BCR	C23-C24-C25-C30
22	A	843	BCR	C23-C24-C25-C26
22	A	843	BCR	C23-C24-C25-C30
22	A	844	BCR	C1-C6-C7-C8
22	A	844	BCR	C5-C6-C7-C8
22	A	844	BCR	C23-C24-C25-C26
22	A	845	BCR	C23-C24-C25-C30
22	B	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C23-C24-C25-C26
22	B	847	BCR	C23-C24-C25-C30
22	F	203	BCR	C1-C6-C7-C8
22	F	203	BCR	C5-C6-C7-C8
22	F	203	BCR	C23-C24-C25-C26
22	F	203	BCR	C23-C24-C25-C30
22	I	101	BCR	C1-C6-C7-C8
22	J	102	BCR	C1-C6-C7-C8
22	J	102	BCR	C5-C6-C7-C8
20	B	827	CLA	CBA-CGA-O2A-C1
20	2	303	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	852	LMU	C5-C6-C7-C8
21	C	101	LMU	C6-C7-C8-C9
21	G	101	LMU	C3-C4-C5-C6
21	L	210	LMU	C3-C4-C5-C6
21	3	319	LMU	C9-C10-C11-C12
21	R	109	LMU	C9-C10-C11-C12
21	G	103	LMU	C7-C8-C9-C10
20	B	827	CLA	C2A-CAA-CBA-CGA
20	B	838	CLA	C15-C16-C17-C18
20	B	825	CLA	C5-C6-C7-C8
21	B	805	LMU	C5-C6-C7-C8
20	A	823	CLA	O1A-CGA-O2A-C1
20	B	840	CLA	O1A-CGA-O2A-C1
21	L	206	LMU	C2-C3-C4-C5
20	A	851	CLA	C4C-C3C-CAC-CBC
20	F	207	CLA	C4-C3-C5-C6
21	4	316	LMU	C11-C10-C9-C8
21	A	855	LMU	C7-C8-C9-C10
22	B	844	BCR	C18-C19-C20-C21
20	1	206	CLA	C2-C3-C5-C6
20	L	202	CLA	C6-C7-C8-C9
21	4	321	LMU	C2-C3-C4-C5
21	A	846	LMU	C5-C6-C7-C8
21	A	846	LMU	C11-C10-C9-C8
21	A	854	LMU	C7-C8-C9-C10
21	B	805	LMU	C11-C10-C9-C8
21	G	101	LMU	C11-C10-C9-C8
21	H	105	LMU	C7-C8-C9-C10
20	A	813	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	A	839	CLA	C8-C10-C11-C12
21	4	319	LMU	C6-C7-C8-C9
21	G	103	LMU	C3-C4-C5-C6
21	R	105	LMU	C2-C3-C4-C5
21	R	105	LMU	C5-C6-C7-C8
20	B	820	CLA	C8-C10-C11-C12
20	H	101	CLA	C5-C6-C7-C8
21	3	319	LMU	C7-C8-C9-C10
21	A	855	LMU	C4-C5-C6-C7
21	R	105	LMU	C7-C8-C9-C10
21	R	109	LMU	C11-C10-C9-C8
21	A	855	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
20	B	814	CLA	C15-C16-C17-C18
21	3	318	LMU	C11-C10-C9-C8
21	K	105	LMU	C7-C8-C9-C10
21	R	105	LMU	C1-C2-C3-C4
21	H	104	LMU	C2-C3-C4-C5
21	1	218	LMU	C6-C7-C8-C9
21	2	320	LMU	C6-C7-C8-C9
21	R	109	LMU	C5-C6-C7-C8
20	1	201	CLA	C4C-C3C-CAC-CBC
21	L	205	LMU	C1-C2-C3-C4
21	R	106	LMU	C1-C2-C3-C4
22	F	203	BCR	C13-C14-C15-C16
21	A	852	LMU	O5B-C1B-O1B-C4'
20	B	829	CLA	C10-C11-C12-C13
20	I	102	CLA	C8-C10-C11-C12
20	R	108	CLA	C10-C11-C12-C13
21	C	101	LMU	O5'-C5'-C6'-O6'
21	R	104	LMU	O1'-C1-C2-C3
21	3	319	LMU	C3-C4-C5-C6
25	B	848	LMG	C35-C36-C37-C38
21	L	206	LMU	C4'-C5'-C6'-O6'
21	4	321	LMU	C1-C2-C3-C4
20	1	215	CLA	O1A-CGA-O2A-C1
20	B	803	CLA	C15-C16-C17-C18
21	R	103	LMU	C4'-C5'-C6'-O6'
21	L	206	LMU	C5-C6-C7-C8
22	2	317	BCR	C11-C12-C13-C14
22	B	846	BCR	C21-C22-C23-C24
21	1	217	LMU	C6-C7-C8-C9
21	A	852	LMU	C4-C5-C6-C7
20	2	314	CLA	C2A-CAA-CBA-CGA
20	A	827	CLA	C2A-CAA-CBA-CGA
20	A	811	CLA	C16-C17-C18-C20
20	B	813	CLA	C6-C7-C8-C9
20	B	838	CLA	C16-C17-C18-C19
21	B	804	LMU	C5-C6-C7-C8
25	B	848	LMG	C11-C12-C13-C14
20	4	301	CLA	C4-C3-C5-C6
20	K	103	CLA	O1A-CGA-O2A-C1
21	A	852	LMU	C2B-C1B-O1B-C4'
20	4	303	CLA	C8-C10-C11-C12
21	A	853	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	L	205	LMU	C4-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	A	831	CLA	C10-C11-C12-C13
20	B	850	CLA	C5-C6-C7-C8
21	2	320	LMU	C3-C4-C5-C6
21	A	853	LMU	C5-C6-C7-C8
20	3	310	CLA	C2C-C3C-CAC-CBC
20	3	314	CLA	C2C-C3C-CAC-CBC
21	4	316	LMU	C1-C2-C3-C4
21	A	852	LMU	C5'-C4'-O1B-C1B
21	A	847	LMU	C3-C4-C5-C6
21	F	202	LMU	C7-C8-C9-C10
21	2	321	LMU	O5B-C5B-C6B-O6B
21	R	102	LMU	O5'-C5'-C6'-O6'
21	R	109	LMU	C2-C3-C4-C5
25	B	848	LMG	C40-C41-C42-C43
20	4	304	CLA	C5-C6-C7-C8
20	B	841	CLA	C10-C11-C12-C13
20	4	304	CLA	C6-C7-C8-C10
21	G	102	LMU	C2-C3-C4-C5
20	B	827	CLA	O1A-CGA-O2A-C1
21	G	103	LMU	O5'-C5'-C6'-O6'
21	G	101	LMU	C1-C2-C3-C4
20	A	850	CLA	C15-C16-C17-C18
20	B	840	CLA	C8-C10-C11-C12
21	2	318	LMU	C5-C6-C7-C8
21	A	847	LMU	C2-C3-C4-C5
21	2	313	LMU	O1'-C1-C2-C3
20	A	808	CLA	C3-C5-C6-C7
20	A	831	CLA	C3-C5-C6-C7
21	A	854	LMU	C4'-C5'-C6'-O6'
20	B	803	CLA	CBA-CGA-O2A-C1
21	2	319	LMU	C2-C3-C4-C5
21	A	847	LMU	C11-C10-C9-C8
20	B	850	CLA	C8-C10-C11-C12
21	B	804	LMU	O5'-C5'-C6'-O6'
20	A	818	CLA	C11-C12-C13-C14
20	B	813	CLA	C6-C7-C8-C10
20	B	829	CLA	C16-C17-C18-C20
20	2	307	CLA	C10-C11-C12-C13
20	B	809	CLA	C8-C10-C11-C12
20	B	827	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	855	LMU	C11-C10-C9-C8
21	L	210	LMU	C7-C8-C9-C10
20	F	207	CLA	C2-C3-C5-C6
20	2	305	CLA	C4C-C3C-CAC-CBC
20	L	207	CLA	C2C-C3C-CAC-CBC
21	L	210	LMU	C2-C3-C4-C5
25	B	848	LMG	C15-C16-C17-C18
25	B	848	LMG	C39-C40-C41-C42
20	A	808	CLA	C2A-CAA-CBA-CGA
20	B	808	CLA	C2A-CAA-CBA-CGA
20	B	834	CLA	C2A-CAA-CBA-CGA
20	B	836	CLA	C2A-CAA-CBA-CGA
20	F	201	CLA	C2A-CAA-CBA-CGA
20	4	306	CLA	O1D-CGD-O2D-CED
20	4	303	CLA	C5-C6-C7-C8
21	A	848	LMU	O5B-C5B-C6B-O6B
21	1	217	LMU	C5-C6-C7-C8
21	G	101	LMU	C6-C7-C8-C9
21	K	105	LMU	C1-C2-C3-C4
20	A	813	CLA	O1A-CGA-O2A-C1
20	B	823	CLA	O1A-CGA-O2A-C1
20	1	206	CLA	C3-C5-C6-C7
21	3	318	LMU	C5-C6-C7-C8
21	A	852	LMU	C11-C10-C9-C8
21	R	105	LMU	C5'-C4'-O1B-C1B
21	K	106	LMU	C11-C10-C9-C8
20	1	203	CLA	C1A-C2A-CAA-CBA
20	1	206	CLA	C1A-C2A-CAA-CBA
20	1	213	CLA	C1A-C2A-CAA-CBA
20	3	313	CLA	C1A-C2A-CAA-CBA
20	4	303	CLA	C1A-C2A-CAA-CBA
20	4	318	CLA	C1A-C2A-CAA-CBA
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	820	CLA	C1A-C2A-CAA-CBA
20	A	825	CLA	C1A-C2A-CAA-CBA
20	A	837	CLA	C1A-C2A-CAA-CBA
20	A	840	CLA	C1A-C2A-CAA-CBA
20	A	849	CLA	C1A-C2A-CAA-CBA
20	B	802	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	839	CLA	C1A-C2A-CAA-CBA
20	B	841	CLA	C1A-C2A-CAA-CBA
20	F	201	CLA	C1A-C2A-CAA-CBA
20	J	103	CLA	C1A-C2A-CAA-CBA
20	A	827	CLA	CBD-CGD-O2D-CED
20	A	849	CLA	C13-C15-C16-C17
20	A	851	CLA	C13-C15-C16-C17
20	B	829	CLA	C5-C6-C7-C8
21	H	103	LMU	C2-C3-C4-C5
21	G	102	LMU	C5-C6-C7-C8
21	R	101	LMU	C11-C10-C9-C8
20	B	820	CLA	C5-C6-C7-C8
21	H	103	LMU	O5'-C5'-C6'-O6'
20	A	812	CLA	C5-C6-C7-C8
21	A	853	LMU	C6-C7-C8-C9
21	2	320	LMU	O1'-C1-C2-C3
20	R	108	CLA	C3-C5-C6-C7
20	2	303	CLA	C11-C10-C8-C7
20	3	311	CLA	C11-C10-C8-C7
20	A	825	CLA	C6-C7-C8-C10
20	B	806	CLA	C12-C13-C15-C16
20	B	808	CLA	C6-C7-C8-C10
20	B	809	CLA	C12-C13-C15-C16
20	B	815	CLA	C6-C7-C8-C10
20	B	820	CLA	C11-C12-C13-C15
20	B	826	CLA	C11-C10-C8-C7
20	B	830	CLA	C6-C7-C8-C10
20	B	837	CLA	C6-C7-C8-C10
20	B	840	CLA	C11-C10-C8-C7
20	R	108	CLA	C6-C7-C8-C10
20	R	108	CLA	C11-C10-C8-C7
20	R	108	CLA	C11-C12-C13-C15
21	1	218	LMU	C11-C10-C9-C8
21	4	319	LMU	C4-C5-C6-C7
21	L	205	LMU	C11-C10-C9-C8
20	B	815	CLA	C11-C12-C13-C15
20	B	809	CLA	C13-C15-C16-C17
21	H	104	LMU	C3'-C4'-O1B-C1B
20	A	825	CLA	C4-C3-C5-C6
20	B	808	CLA	C4-C3-C5-C6
21	A	852	LMU	C4B-C5B-C6B-O6B
20	B	808	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	815	CLA	C2-C3-C5-C6
21	2	319	LMU	C5-C6-C7-C8
20	2	312	CLA	C8-C10-C11-C12
20	4	301	CLA	C2A-CAA-CBA-CGA
20	B	829	CLA	C2A-CAA-CBA-CGA
20	2	312	CLA	C6-C7-C8-C9
20	2	312	CLA	C11-C10-C8-C9
20	4	303	CLA	C11-C12-C13-C14
20	A	818	CLA	C6-C7-C8-C9
20	A	823	CLA	C11-C10-C8-C9
20	A	825	CLA	C6-C7-C8-C9
20	A	851	CLA	C14-C13-C15-C16
20	B	815	CLA	C6-C7-C8-C9
20	B	820	CLA	C11-C10-C8-C9
20	B	829	CLA	C11-C12-C13-C14
20	B	837	CLA	C6-C7-C8-C9
20	J	103	CLA	C11-C10-C8-C9
21	2	319	LMU	C4-C5-C6-C7
21	H	104	LMU	C6-C7-C8-C9
22	B	801	BCR	C19-C20-C21-C22
21	A	854	LMU	C1-C2-C3-C4
21	B	804	LMU	C7-C8-C9-C10
20	4	305	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	CBA-CGA-O2A-C1
21	B	805	LMU	C5'-C4'-O1B-C1B
21	H	105	LMU	C9-C10-C11-C12
21	3	319	LMU	C2'-C1'-O1'-C1
21	K	107	LMU	C2'-C1'-O1'-C1
21	1	217	LMU	O5'-C5'-C6'-O6'
21	2	318	LMU	C4'-C5'-C6'-O6'
21	K	105	LMU	O5B-C5B-C6B-O6B
20	L	204	CLA	CBA-CGA-O2A-C1
21	E	101	LMU	O5B-C5B-C6B-O6B
20	2	307	CLA	C16-C17-C18-C20
20	A	827	CLA	C6-C7-C8-C10
20	A	830	CLA	C16-C17-C18-C19
23	B	843	PQN	C26-C27-C28-C30
21	B	804	LMU	C3-C4-C5-C6
21	K	105	LMU	C11-C10-C9-C8
21	R	103	LMU	C4-C5-C6-C7
20	A	809	CLA	C2C-C3C-CAC-CBC
21	4	319	LMU	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
20	K	103	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	O1A-CGA-O2A-C1
21	2	321	LMU	C2-C3-C4-C5
21	4	321	LMU	C11-C10-C9-C8
21	H	103	LMU	C7-C8-C9-C10
21	4	319	LMU	O1'-C1-C2-C3
20	A	825	CLA	C2-C3-C5-C6
20	B	828	CLA	C10-C11-C12-C13
22	I	103	BCR	C7-C8-C9-C34
21	A	848	LMU	C3-C4-C5-C6
20	4	305	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	C2A-CAA-CBA-CGA
20	B	826	CLA	C2A-CAA-CBA-CGA
21	3	319	LMU	O5B-C5B-C6B-O6B
21	B	805	LMU	O5B-C5B-C6B-O6B
20	2	316	CLA	C8-C10-C11-C12
20	2	302	CLA	CBA-CGA-O2A-C1
20	A	822	CLA	CBA-CGA-O2A-C1
20	J	101	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	O2A-C1-C2-C3
20	A	851	CLA	O2A-C1-C2-C3
20	B	833	CLA	O2A-C1-C2-C3
20	F	201	CLA	O2A-C1-C2-C3
21	2	319	LMU	C7-C8-C9-C10
21	L	205	LMU	C5-C6-C7-C8
22	A	844	BCR	C19-C20-C21-C22
20	H	102	CLA	C6-C7-C8-C9
21	K	105	LMU	C9-C10-C11-C12
21	A	847	LMU	O1'-C1-C2-C3
21	H	104	LMU	C11-C10-C9-C8
21	4	321	LMU	O5'-C5'-C6'-O6'
20	B	840	CLA	C5-C6-C7-C8
20	4	306	CLA	CBA-CGA-O2A-C1
20	B	841	CLA	CBA-CGA-O2A-C1
20	2	303	CLA	C10-C11-C12-C13
21	H	104	LMU	C9-C10-C11-C12
21	4	316	LMU	C4B-C5B-C6B-O6B
20	A	830	CLA	C2-C3-C5-C6
20	B	810	CLA	C2-C3-C5-C6
21	4	319	LMU	C11-C10-C9-C8
21	R	101	LMU	C9-C10-C11-C12
25	B	848	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
21	K	106	LMU	C6-C7-C8-C9
21	L	206	LMU	C11-C10-C9-C8
21	2	318	LMU	C2-C3-C4-C5
21	2	321	LMU	C6-C7-C8-C9
21	H	103	LMU	C3-C4-C5-C6
20	B	825	CLA	C6-C7-C8-C9
21	A	846	LMU	C9-C10-C11-C12
21	A	847	LMU	C9-C10-C11-C12
21	A	855	LMU	C5-C6-C7-C8
21	2	318	LMU	C9-C10-C11-C12
21	R	104	LMU	C9-C10-C11-C12
20	B	832	CLA	C10-C11-C12-C13
21	D	201	LMU	C3-C4-C5-C6
20	B	830	CLA	C13-C15-C16-C17
21	C	101	LMU	C5-C6-C7-C8
20	L	208	CLA	C2A-CAA-CBA-CGA
20	H	101	CLA	C3-C5-C6-C7
21	A	854	LMU	C4-C5-C6-C7
21	H	106	LMU	C11-C10-C9-C8
20	A	816	CLA	C6-C7-C8-C9
21	H	106	LMU	C9-C10-C11-C12
21	G	102	LMU	C5'-C4'-O1B-C1B
21	B	804	LMU	C4-C5-C6-C7
21	B	805	LMU	C1-C2-C3-C4
21	G	101	LMU	C4-C5-C6-C7
20	1	203	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	CBA-CGA-O2A-C1
21	B	849	LMU	O5B-C5B-C6B-O6B
21	R	105	LMU	C3'-C4'-O1B-C1B
20	A	829	CLA	CBD-CGD-O2D-CED
21	F	202	LMU	C11-C10-C9-C8
20	2	302	CLA	C4C-C3C-CAC-CBC
20	A	819	CLA	C10-C11-C12-C13
21	E	101	LMU	C9-C10-C11-C12
20	B	814	CLA	C13-C15-C16-C17
20	R	108	CLA	C13-C15-C16-C17
22	2	317	BCR	C19-C20-C21-C22
22	F	204	BCR	C19-C20-C21-C22
20	1	206	CLA	C14-C13-C15-C16
20	J	103	CLA	C14-C13-C15-C16
20	2	307	CLA	C16-C17-C18-C19
20	A	812	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	830	CLA	C4-C3-C5-C6
20	B	810	CLA	C4-C3-C5-C6
20	B	850	CLA	C4-C3-C5-C6
20	J	103	CLA	C4-C3-C5-C6
21	1	218	LMU	C1-C2-C3-C4
21	E	101	LMU	C4-C5-C6-C7
21	G	103	LMU	C3'-C4'-O1B-C1B
21	1	216	LMU	C5-C6-C7-C8
21	2	313	LMU	C2-C1-O1'-C1'
21	2	318	LMU	C2-C1-O1'-C1'
21	A	852	LMU	C2-C1-O1'-C1'
21	C	101	LMU	C2-C1-O1'-C1'
21	K	107	LMU	C2-C1-O1'-C1'
21	R	103	LMU	C2-C1-O1'-C1'
20	B	810	CLA	C3-C5-C6-C7
21	G	103	LMU	C1-C2-C3-C4
20	3	311	CLA	C11-C10-C8-C9
20	3	314	CLA	C11-C10-C8-C9
20	A	826	CLA	C6-C7-C8-C9
20	B	809	CLA	C6-C7-C8-C9
20	B	809	CLA	C14-C13-C15-C16
20	B	820	CLA	C11-C12-C13-C14
20	B	829	CLA	C6-C7-C8-C9
20	B	830	CLA	C6-C7-C8-C9
20	B	840	CLA	C11-C10-C8-C9
20	J	103	CLA	C6-C7-C8-C9
20	A	811	CLA	C8-C10-C11-C12
20	3	311	CLA	C4B-C3B-CAB-CBB
20	4	305	CLA	C4B-C3B-CAB-CBB
20	A	815	CLA	C4B-C3B-CAB-CBB
20	B	832	CLA	C4B-C3B-CAB-CBB
20	F	206	CLA	C4B-C3B-CAB-CBB
20	B	807	CLA	C4C-C3C-CAC-CBC
20	B	828	CLA	C5-C6-C7-C8
20	B	815	CLA	C11-C12-C13-C14
20	2	310	CLA	C4C-C3C-CAC-CBC
21	2	319	LMU	C2'-C1'-O1'-C1
21	R	104	LMU	C2'-C1'-O1'-C1
20	2	307	CLA	C6-C7-C8-C10
20	2	312	CLA	C6-C7-C8-C10
20	2	312	CLA	C11-C10-C8-C7
20	3	310	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	4	303	CLA	C11-C12-C13-C15
20	A	826	CLA	C6-C7-C8-C10
20	A	831	CLA	C6-C7-C8-C10
20	A	851	CLA	C11-C10-C8-C7
20	A	851	CLA	C11-C12-C13-C15
20	A	851	CLA	C12-C13-C15-C16
20	B	808	CLA	C11-C12-C13-C15
20	B	809	CLA	C6-C7-C8-C10
20	B	810	CLA	C11-C10-C8-C7
20	B	820	CLA	C11-C10-C8-C7
20	B	824	CLA	C6-C7-C8-C10
20	B	827	CLA	C11-C12-C13-C15
20	B	829	CLA	C6-C7-C8-C10
20	B	829	CLA	C11-C12-C13-C15
20	B	830	CLA	C12-C13-C15-C16
20	B	841	CLA	C11-C12-C13-C15
20	J	103	CLA	C6-C7-C8-C10
20	J	103	CLA	C11-C10-C8-C7
20	J	103	CLA	C11-C12-C13-C15
20	A	819	CLA	C8-C10-C11-C12
20	A	830	CLA	C16-C17-C18-C20
21	1	217	LMU	C7-C8-C9-C10
20	2	307	CLA	C3A-C2A-CAA-CBA
20	A	820	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C4-C3-C5-C6
20	B	815	CLA	C4-C3-C5-C6
20	B	830	CLA	C4-C3-C5-C6
20	F	207	CLA	C3A-C2A-CAA-CBA
20	H	108	CLA	C3A-C2A-CAA-CBA
20	B	812	CLA	C5-C6-C7-C8
20	A	835	CLA	C2-C3-C5-C6
21	2	321	LMU	O5'-C1'-O1'-C1
20	L	204	CLA	O1A-CGA-O2A-C1
22	A	843	BCR	C19-C20-C21-C22
22	B	844	BCR	C19-C20-C21-C22
22	G	104	BCR	C15-C16-C17-C18
22	I	101	BCR	C15-C16-C17-C18
21	G	102	LMU	C3'-C4'-O1B-C1B
21	A	855	LMU	C1-C2-C3-C4
20	2	302	CLA	O1A-CGA-O2A-C1
20	A	822	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	J	101	CLA	O1A-CGA-O2A-C1
21	G	101	LMU	C9-C10-C11-C12
21	H	105	LMU	C4B-C5B-C6B-O6B
21	1	216	LMU	C4-C5-C6-C7
21	2	318	LMU	C3-C4-C5-C6
20	2	312	CLA	C4C-C3C-CAC-CBC
20	A	820	CLA	CBA-CGA-O2A-C1
20	H	108	CLA	C8-C10-C11-C12
25	B	848	LMG	O1-C7-C8-C9
21	A	855	LMU	C2-C3-C4-C5
21	C	101	LMU	C9-C10-C11-C12
21	3	318	LMU	C7-C8-C9-C10
21	A	846	LMU	C6-C7-C8-C9
20	B	815	CLA	C8-C10-C11-C12
20	B	827	CLA	C13-C15-C16-C17
20	A	835	CLA	C4-C3-C5-C6
20	A	815	CLA	C4C-C3C-CAC-CBC
20	A	812	CLA	C2-C3-C5-C6
20	B	830	CLA	C2-C3-C5-C6
20	B	850	CLA	C2-C3-C5-C6
20	J	103	CLA	C2-C3-C5-C6
20	A	819	CLA	O1D-CGD-O2D-CED
20	A	805	CLA	C5-C6-C7-C8
20	A	838	CLA	C16-C17-C18-C20
21	D	201	LMU	C6-C7-C8-C9
25	B	848	LMG	C13-C14-C15-C16
21	A	846	LMU	O1'-C1-C2-C3
20	B	817	CLA	C2B-C3B-CAB-CBB
22	2	317	BCR	C5-C6-C7-C8
22	A	844	BCR	C23-C24-C25-C30
22	G	104	BCR	C23-C24-C25-C30
22	L	209	BCR	C1-C6-C7-C8
20	B	830	CLA	C8-C10-C11-C12
21	F	202	LMU	C2-C3-C4-C5
21	2	318	LMU	O5B-C5B-C6B-O6B
20	L	202	CLA	C3-C5-C6-C7
21	L	205	LMU	C2-C3-C4-C5
21	G	103	LMU	C5'-C4'-O1B-C1B
21	E	101	LMU	O1'-C1-C2-C3
21	R	102	LMU	C9-C10-C11-C12
21	L	206	LMU	C7-C8-C9-C10
21	2	320	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	A	842	PQN	C26-C27-C28-C29
23	B	843	PQN	C26-C27-C28-C29
20	B	809	CLA	C5-C6-C7-C8
21	A	854	LMU	C2-C3-C4-C5
20	3	311	CLA	C10-C11-C12-C13
20	2	312	CLA	C12-C13-C15-C16
20	B	813	CLA	C2-C3-C5-C6
21	G	103	LMU	C6-C7-C8-C9
20	B	810	CLA	C11-C12-C13-C15
20	A	824	CLA	C10-C11-C12-C13
20	4	315	CLA	C2C-C3C-CAC-CBC
20	3	314	CLA	C14-C13-C15-C16
20	A	838	CLA	C6-C7-C8-C9
20	B	841	CLA	C11-C12-C13-C14
20	J	103	CLA	C11-C12-C13-C14
21	2	321	LMU	C9-C10-C11-C12
21	1	216	LMU	O5'-C1'-O1'-C1
20	F	207	CLA	C5-C6-C7-C8
21	G	102	LMU	C9-C10-C11-C12
20	4	304	CLA	C6-C7-C8-C9
20	B	827	CLA	O1D-CGD-O2D-CED
21	C	101	LMU	C3'-C4'-O1B-C1B
21	C	101	LMU	C5'-C4'-O1B-C1B
20	B	835	CLA	C2C-C3C-CAC-CBC
21	K	105	LMU	C6-C7-C8-C9
20	B	826	CLA	C5-C6-C7-C8
21	L	206	LMU	C1-C2-C3-C4
22	A	843	BCR	C13-C14-C15-C16
22	F	203	BCR	C15-C16-C17-C18
20	4	310	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	C11-C12-C13-C15
20	B	838	CLA	C16-C17-C18-C20
20	A	811	CLA	C13-C15-C16-C17
20	A	838	CLA	C15-C16-C17-C18
20	A	823	CLA	C8-C10-C11-C12
20	A	811	CLA	O1A-CGA-O2A-C1
20	A	831	CLA	CBA-CGA-O2A-C1
20	B	832	CLA	CBA-CGA-O2A-C1
20	B	832	CLA	C8-C10-C11-C12
20	A	804	CLA	C6-C7-C8-C10
20	3	310	CLA	C6-C7-C8-C10
20	A	835	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	850	CLA	C6-C7-C8-C10
20	B	841	CLA	C12-C13-C15-C16
20	H	108	CLA	C6-C7-C8-C10
20	I	102	CLA	C11-C10-C8-C7
23	A	842	PQN	C22-C23-C25-C26
20	H	108	CLA	C2C-C3C-CAC-CBC
20	A	823	CLA	C3-C5-C6-C7
22	I	103	BCR	C7-C8-C9-C10
20	1	203	CLA	O1A-CGA-O2A-C1
20	4	306	CLA	O1A-CGA-O2A-C1
20	B	832	CLA	C11-C12-C13-C14
20	A	850	CLA	C5-C6-C7-C8
20	B	807	CLA	C2A-CAA-CBA-CGA
20	B	829	CLA	C16-C17-C18-C19
21	A	852	LMU	C6-C7-C8-C9
21	1	218	LMU	C9-C10-C11-C12
20	A	820	CLA	O1A-CGA-O2A-C1
20	A	830	CLA	O1A-CGA-O2A-C1
20	B	841	CLA	O1A-CGA-O2A-C1
20	4	301	CLA	C2-C3-C5-C6
21	2	313	LMU	C4B-C5B-C6B-O6B
20	B	828	CLA	C3-C5-C6-C7
25	B	848	LMG	C9-C8-O7-C10
21	3	319	LMU	C2-C3-C4-C5
21	G	102	LMU	C1-C2-C3-C4
23	B	843	PQN	C23-C25-C26-C27
20	4	303	CLA	C16-C17-C18-C20
20	H	108	CLA	C10-C11-C12-C13
21	A	854	LMU	C5-C6-C7-C8
20	B	850	CLA	C3-C5-C6-C7
20	B	808	CLA	C8-C10-C11-C12
20	B	802	CLA	C5-C6-C7-C8
20	3	314	CLA	CBD-CGD-O2D-CED
20	4	301	CLA	C6-C7-C8-C10
21	K	105	LMU	C2-C3-C4-C5
20	B	832	CLA	O1A-CGA-O2A-C1
20	4	317	CLA	C4-C3-C5-C6
20	2	307	CLA	C2A-CAA-CBA-CGA
21	2	320	LMU	C9-C10-C11-C12
20	B	816	CLA	C10-C11-C12-C13
21	2	313	LMU	C5-C6-C7-C8
20	3	310	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	827	CLA	C6-C7-C8-C9
20	A	831	CLA	C4C-C3C-CAC-CBC
20	A	849	CLA	C16-C17-C18-C19
21	H	103	LMU	C5-C6-C7-C8
21	G	103	LMU	C4-C5-C6-C7
20	A	831	CLA	O1A-CGA-O2A-C1
20	1	215	CLA	C2-C1-O2A-CGA
20	3	310	CLA	C2-C1-O2A-CGA
20	H	102	CLA	C6-C7-C8-C10
20	A	823	CLA	C5-C6-C7-C8
21	E	101	LMU	C7-C8-C9-C10
21	R	101	LMU	O1'-C1-C2-C3
21	R	106	LMU	C3'-C4'-O1B-C1B
20	2	316	CLA	C16-C17-C18-C20
20	A	808	CLA	C11-C12-C13-C14
20	B	806	CLA	C16-C17-C18-C19
21	H	105	LMU	O5B-C5B-C6B-O6B
21	G	102	LMU	O1'-C1-C2-C3
21	G	101	LMU	C2-C1-O1'-C1'
21	G	103	LMU	C2-C1-O1'-C1'
20	F	207	CLA	C3-C5-C6-C7
20	1	204	CLA	C4B-C3B-CAB-CBB
20	3	311	CLA	C1A-C2A-CAA-CBA
20	4	306	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C4B-C3B-CAB-CBB
20	A	849	CLA	C4-C3-C5-C6
21	C	101	LMU	O1'-C1-C2-C3
21	2	320	LMU	C5'-C4'-O1B-C1B
20	A	823	CLA	C10-C11-C12-C13
20	B	802	CLA	C2A-CAA-CBA-CGA
21	2	319	LMU	O5B-C1B-O1B-C4'
21	2	320	LMU	C7-C8-C9-C10
21	4	316	LMU	C3-C4-C5-C6
21	K	105	LMU	C3'-C4'-O1B-C1B
20	1	211	CLA	C2-C3-C5-C6
20	B	829	CLA	C3-C5-C6-C7
21	K	106	LMU	C1-C2-C3-C4
20	2	307	CLA	C11-C10-C8-C7
20	A	808	CLA	C11-C10-C8-C7
20	A	824	CLA	C11-C10-C8-C7
20	A	828	CLA	C6-C7-C8-C10
20	A	830	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	C12-C13-C15-C16
20	B	806	CLA	C11-C10-C8-C7
20	B	808	CLA	C11-C10-C8-C7
20	B	814	CLA	C11-C10-C8-C7
20	B	816	CLA	C11-C10-C8-C7
20	B	824	CLA	C12-C13-C15-C16
20	B	826	CLA	C6-C7-C8-C10
20	B	830	CLA	C11-C12-C13-C15
20	K	104	CLA	C6-C7-C8-C10
23	A	842	PQN	C21-C22-C23-C25
20	2	316	CLA	C16-C17-C18-C19
20	A	838	CLA	C16-C17-C18-C19
20	B	806	CLA	C16-C17-C18-C20
20	B	810	CLA	C11-C12-C13-C14
20	A	851	CLA	CBD-CGD-O2D-CED
21	R	109	LMU	O1'-C1-C2-C3
20	4	315	CLA	C3A-C2A-CAA-CBA
21	G	103	LMU	C11-C10-C9-C8
20	2	316	CLA	C11-C12-C13-C14
20	A	835	CLA	C14-C13-C15-C16
20	A	849	CLA	C14-C13-C15-C16
20	B	815	CLA	C11-C10-C8-C9
20	R	108	CLA	C14-C13-C15-C16
20	J	101	CLA	CAA-CBA-CGA-O2A
21	H	103	LMU	C11-C10-C9-C8
21	R	102	LMU	C4-C5-C6-C7
21	A	854	LMU	O5B-C1B-O1B-C4'
20	A	804	CLA	C2C-C3C-CAC-CBC
21	4	319	LMU	O5'-C5'-C6'-O6'
20	B	816	CLA	C11-C12-C13-C14
21	K	106	LMU	C9-C10-C11-C12
21	2	320	LMU	C11-C10-C9-C8
21	H	105	LMU	C2-C3-C4-C5
20	A	826	CLA	C13-C15-C16-C17
20	4	301	CLA	CAD-CBD-CGD-O2D
20	A	826	CLA	CAD-CBD-CGD-O2D
20	A	832	CLA	CAD-CBD-CGD-O2D
20	A	850	CLA	CAD-CBD-CGD-O2D
20	B	836	CLA	CAD-CBD-CGD-O2D
20	B	837	CLA	CAD-CBD-CGD-O2D
20	B	839	CLA	CAD-CBD-CGD-O2D
20	B	838	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	H	101	CLA	C2A-CAA-CBA-CGA
20	L	202	CLA	C2A-CAA-CBA-CGA
20	A	850	CLA	C8-C10-C11-C12
21	R	102	LMU	C7-C8-C9-C10
20	3	307	CLA	CAD-CBD-CGD-O1D
20	3	314	CLA	CAD-CBD-CGD-O1D
20	4	301	CLA	CAD-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O2D
20	A	826	CLA	CAD-CBD-CGD-O1D
20	A	832	CLA	CAD-CBD-CGD-O1D
20	A	850	CLA	CAD-CBD-CGD-O1D
20	B	802	CLA	CAD-CBD-CGD-O1D
20	B	818	CLA	CHA-CBD-CGD-O1D
20	B	820	CLA	CHA-CBD-CGD-O1D
20	B	820	CLA	CHA-CBD-CGD-O2D
20	B	834	CLA	CAD-CBD-CGD-O1D
20	B	836	CLA	CAD-CBD-CGD-O1D
20	B	837	CLA	CAD-CBD-CGD-O1D
20	B	839	CLA	CAD-CBD-CGD-O1D
20	F	206	CLA	CAD-CBD-CGD-O1D
20	H	101	CLA	CAD-CBD-CGD-O1D
20	R	108	CLA	CAD-CBD-CGD-O1D
22	2	317	BCR	C15-C16-C17-C18
22	A	844	BCR	C13-C14-C15-C16
22	B	844	BCR	C15-C16-C17-C18
22	I	101	BCR	C23-C24-C25-C30
20	A	804	CLA	C3-C5-C6-C7
20	A	811	CLA	C4-C3-C5-C6
20	1	201	CLA	C2B-C3B-CAB-CBB
20	A	803	CLA	C2B-C3B-CAB-CBB
20	A	807	CLA	C2B-C3B-CAB-CBB
20	A	811	CLA	C2B-C3B-CAB-CBB
20	B	807	CLA	C2B-C3B-CAB-CBB
20	B	809	CLA	C2B-C3B-CAB-CBB
20	F	206	CLA	C2B-C3B-CAB-CBB
20	4	317	CLA	C2-C3-C5-C6
20	A	835	CLA	C8-C10-C11-C12
20	B	803	CLA	C16-C17-C18-C20
20	3	310	CLA	C4C-C3C-CAC-CBC
21	A	854	LMU	C2B-C1B-O1B-C4'
20	3	310	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	A	824	CLA	C8-C10-C11-C12
20	A	840	CLA	C3-C5-C6-C7
20	B	824	CLA	C5-C6-C7-C8
22	G	104	BCR	C13-C14-C15-C16
20	A	849	CLA	C16-C17-C18-C20
20	2	316	CLA	C14-C13-C15-C16
20	3	310	CLA	C6-C7-C8-C9
20	A	831	CLA	C11-C10-C8-C9
20	A	851	CLA	C11-C12-C13-C14
20	B	814	CLA	C11-C10-C8-C9
20	B	828	CLA	C11-C10-C8-C9
20	B	841	CLA	C14-C13-C15-C16
20	L	203	CLA	C11-C12-C13-C14
23	A	842	PQN	C24-C23-C25-C26
23	B	843	PQN	C21-C22-C23-C24
20	2	312	CLA	C14-C13-C15-C16
20	2	316	CLA	C11-C12-C13-C15
20	B	809	CLA	C11-C10-C8-C7
20	B	837	CLA	C11-C10-C8-C7
20	A	840	CLA	C2C-C3C-CAC-CBC
20	B	806	CLA	C5-C6-C7-C8
20	B	809	CLA	C15-C16-C17-C18
20	B	813	CLA	C3-C5-C6-C7
20	A	801	CLA	CAA-CBA-CGA-O2A
20	L	207	CLA	C4C-C3C-CAC-CBC
20	L	203	CLA	C4-C3-C5-C6
21	R	106	LMU	C5'-C4'-O1B-C1B
20	A	819	CLA	CBA-CGA-O2A-C1
21	4	320	LMU	C4-C5-C6-C7
25	B	848	LMG	C38-C39-C40-C41
20	B	817	CLA	CAA-CBA-CGA-O2A
20	1	213	CLA	CBA-CGA-O2A-C1
22	B	801	BCR	C9-C10-C11-C12
21	L	205	LMU	C3'-C4'-O1B-C1B
21	4	320	LMU	C9-C10-C11-C12
20	A	819	CLA	O1A-CGA-O2A-C1
21	R	102	LMU	C3'-C4'-O1B-C1B
20	4	303	CLA	C2-C1-O2A-CGA
20	A	816	CLA	C2-C1-O2A-CGA
20	2	316	CLA	C4-C3-C5-C6
20	L	202	CLA	C2C-C3C-CAC-CBC
21	C	101	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	4	305	CLA	CAA-CBA-CGA-O2A
21	B	805	LMU	C4'-C5'-C6'-O6'
20	B	832	CLA	C3-C5-C6-C7
20	A	809	CLA	C4C-C3C-CAC-CBC
20	1	204	CLA	C2A-CAA-CBA-CGA
20	A	818	CLA	C2A-CAA-CBA-CGA
20	H	110	CLA	C2A-CAA-CBA-CGA
20	L	207	CLA	C2A-CAA-CBA-CGA
22	B	846	BCR	C19-C20-C21-C22
22	J	102	BCR	C15-C16-C17-C18
22	L	209	BCR	C15-C16-C17-C18
20	B	814	CLA	C4-C3-C5-C6
21	2	320	LMU	C2-C1-O1'-C1'
21	3	318	LMU	C2-C1-O1'-C1'
21	A	853	LMU	C2-C1-O1'-C1'
21	F	202	LMU	C2-C1-O1'-C1'
21	H	103	LMU	C2-C1-O1'-C1'
20	A	808	CLA	C11-C10-C8-C9
20	A	824	CLA	C11-C10-C8-C9
20	A	830	CLA	C11-C10-C8-C9
20	B	830	CLA	C14-C13-C15-C16
20	L	203	CLA	C11-C10-C8-C9
20	4	317	CLA	C2C-C3C-CAC-CBC
20	A	827	CLA	O1D-CGD-O2D-CED
21	A	847	LMU	C7-C8-C9-C10
20	A	825	CLA	C10-C11-C12-C13
20	A	812	CLA	C6-C7-C8-C9
20	A	824	CLA	C11-C12-C13-C14
20	L	203	CLA	C2-C3-C5-C6
21	F	202	LMU	C3'-C4'-O1B-C1B
20	A	811	CLA	C12-C13-C15-C16
20	A	825	CLA	C11-C12-C13-C15
20	A	835	CLA	C11-C10-C8-C7
20	A	849	CLA	C11-C10-C8-C7
20	L	203	CLA	C11-C12-C13-C15
20	3	311	CLA	C8-C10-C11-C12
20	A	810	CLA	CAA-CBA-CGA-O2A
20	2	307	CLA	C13-C15-C16-C17
20	B	850	CLA	CAA-CBA-CGA-O2A
20	1	213	CLA	O1A-CGA-O2A-C1
21	B	804	LMU	C2-C3-C4-C5
20	4	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	812	CLA	C3A-C2A-CAA-CBA
20	A	834	CLA	C3A-C2A-CAA-CBA
20	B	806	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	C3A-C2A-CAA-CBA
20	K	103	CLA	C3A-C2A-CAA-CBA
21	1	218	LMU	C2-C3-C4-C5
20	A	811	CLA	C2-C3-C5-C6
22	A	845	BCR	C35-C13-C14-C15
22	B	801	BCR	C11-C10-C9-C34
22	B	845	BCR	C11-C10-C9-C34
22	F	204	BCR	C16-C17-C18-C36
20	B	829	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	C2C-C3C-CAC-CBC
20	F	207	CLA	C2-C1-O2A-CGA
20	A	829	CLA	O1D-CGD-O2D-CED
21	H	105	LMU	C4'-C5'-C6'-O6'
20	1	211	CLA	C4-C3-C5-C6
20	2	307	CLA	C15-C16-C17-C18
20	B	832	CLA	C4-C3-C5-C6
21	2	320	LMU	C3'-C4'-O1B-C1B
20	B	828	CLA	CAA-CBA-CGA-O2A
20	A	849	CLA	C2-C3-C5-C6
20	A	851	CLA	C16-C17-C18-C19
20	B	824	CLA	C16-C17-C18-C20
21	H	105	LMU	O5B-C1B-O1B-C4'
20	B	835	CLA	CAA-CBA-CGA-O1A
20	A	830	CLA	C8-C10-C11-C12
20	A	810	CLA	CAA-CBA-CGA-O1A
20	4	303	CLA	C14-C13-C15-C16
20	A	811	CLA	C6-C7-C8-C9
20	B	809	CLA	C11-C10-C8-C9
20	B	809	CLA	C11-C12-C13-C14
20	B	814	CLA	C14-C13-C15-C16
20	B	824	CLA	C11-C12-C13-C14
20	B	830	CLA	C11-C12-C13-C14
20	B	850	CLA	C11-C10-C8-C9
20	H	108	CLA	C11-C10-C8-C9
20	K	104	CLA	C6-C7-C8-C9
20	L	201	CLA	C11-C10-C8-C9
20	4	303	CLA	C16-C17-C18-C19
20	A	804	CLA	C6-C7-C8-C9
20	A	826	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	F	203	BCR	C9-C10-C11-C12
20	A	833	CLA	CAA-CBA-CGA-O2A
20	A	824	CLA	CBA-CGA-O2A-C1
20	B	814	CLA	C2-C3-C5-C6
20	B	832	CLA	C2-C3-C5-C6
21	B	804	LMU	C9-C10-C11-C12
20	A	824	CLA	O1A-CGA-O2A-C1
20	A	835	CLA	C13-C15-C16-C17
20	B	835	CLA	CAA-CBA-CGA-O2A
20	A	850	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
21	K	107	LMU	C9-C10-C11-C12
20	2	307	CLA	C1A-C2A-CAA-CBA
20	A	806	CLA	C1A-C2A-CAA-CBA
20	B	832	CLA	C1A-C2A-CAA-CBA
20	B	837	CLA	C1A-C2A-CAA-CBA
20	H	108	CLA	C1A-C2A-CAA-CBA
20	K	103	CLA	C1A-C2A-CAA-CBA
22	A	845	BCR	C12-C13-C14-C15
22	B	801	BCR	C11-C10-C9-C8
22	B	845	BCR	C11-C10-C9-C8
22	F	204	BCR	C16-C17-C18-C19
20	A	840	CLA	C4C-C3C-CAC-CBC
21	A	852	LMU	O5B-C5B-C6B-O6B
21	H	104	LMU	O5B-C5B-C6B-O6B
20	4	303	CLA	C2B-C3B-CAB-CBB
20	A	808	CLA	C2B-C3B-CAB-CBB
20	A	809	CLA	C2B-C3B-CAB-CBB
20	A	835	CLA	C2B-C3B-CAB-CBB
20	B	806	CLA	C2B-C3B-CAB-CBB
20	B	808	CLA	C2B-C3B-CAB-CBB
20	B	828	CLA	C2B-C3B-CAB-CBB
20	B	850	CLA	C2B-C3B-CAB-CBB
20	F	201	CLA	C2B-C3B-CAB-CBB
20	H	109	CLA	C2B-C3B-CAB-CBB
20	K	103	CLA	C2B-C3B-CAB-CBB
22	2	317	BCR	C1-C6-C7-C8
22	G	104	BCR	C23-C24-C25-C26
22	L	209	BCR	C5-C6-C7-C8
20	B	803	CLA	C4-C3-C5-C6
20	B	825	CLA	C4-C3-C5-C6
20	B	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	4	320	LMU	C2-C3-C4-C5
20	A	825	CLA	C5-C6-C7-C8
20	4	303	CLA	C6-C7-C8-C10
20	4	303	CLA	C11-C10-C8-C7
20	A	825	CLA	C11-C10-C8-C7
20	A	825	CLA	C12-C13-C15-C16
20	A	838	CLA	C6-C7-C8-C10
20	A	849	CLA	C6-C7-C8-C10
20	A	851	CLA	C6-C7-C8-C10
20	B	828	CLA	C6-C7-C8-C10
20	B	828	CLA	C11-C10-C8-C7
20	B	832	CLA	C11-C10-C8-C7
20	B	838	CLA	C11-C10-C8-C7
20	B	840	CLA	C6-C7-C8-C10
20	B	850	CLA	C11-C10-C8-C7
20	H	108	CLA	C11-C10-C8-C7
23	B	843	PQN	C21-C22-C23-C25
20	A	851	CLA	C16-C17-C18-C20
21	B	804	LMU	C3'-C4'-O1B-C1B
20	1	206	CLA	C12-C13-C15-C16
20	J	103	CLA	C12-C13-C15-C16
22	A	843	BCR	C36-C18-C19-C20
20	A	826	CLA	C4-C3-C5-C6
20	B	814	CLA	CAA-CBA-CGA-O2A
20	B	831	CLA	CAA-CBA-CGA-O2A
20	2	312	CLA	C10-C11-C12-C13
20	A	804	CLA	C2-C1-O2A-CGA
20	B	838	CLA	C2-C1-O2A-CGA
20	A	830	CLA	C10-C11-C12-C13
20	A	811	CLA	C11-C12-C13-C14
20	B	803	CLA	C6-C7-C8-C9
20	A	833	CLA	CAA-CBA-CGA-O1A
25	B	848	LMG	C31-C32-C33-C34
20	2	316	CLA	C2-C3-C5-C6
21	R	101	LMU	C4-C5-C6-C7
21	A	852	LMU	C9-C10-C11-C12
21	A	848	LMU	C2-C3-C4-C5
20	A	829	CLA	O1A-CGA-O2A-C1
20	4	310	CLA	C2A-CAA-CBA-CGA
20	I	102	CLA	C2A-CAA-CBA-CGA
21	4	320	LMU	C4'-C5'-C6'-O6'
20	B	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	R	108	CLA	CAA-CBA-CGA-O2A
20	L	201	CLA	C11-C12-C13-C15
21	H	105	LMU	C2B-C1B-O1B-C4'
21	B	805	LMU	C9-C10-C11-C12
20	2	307	CLA	CBD-CGD-O2D-CED
21	R	104	LMU	C2-C3-C4-C5
20	3	307	CLA	C4B-C3B-CAB-CBB
20	B	824	CLA	C4B-C3B-CAB-CBB
20	K	103	CLA	C4B-C3B-CAB-CBB
21	A	847	LMU	C1-C2-C3-C4
21	B	804	LMU	C1-C2-C3-C4
21	A	855	LMU	C5'-C4'-O1B-C1B
20	A	851	CLA	O1D-CGD-O2D-CED
20	R	107	CLA	C5-C6-C7-C8
20	B	826	CLA	C10-C11-C12-C13
21	B	805	LMU	C3-C4-C5-C6
20	A	827	CLA	O1A-CGA-O2A-C1
20	4	301	CLA	C6-C7-C8-C9
21	A	853	LMU	O5'-C5'-C6'-O6'
20	B	850	CLA	C6-C7-C8-C10
21	R	101	LMU	C6-C7-C8-C9
21	R	103	LMU	C6-C7-C8-C9
20	4	303	CLA	CBA-CGA-O2A-C1
20	2	307	CLA	C11-C10-C8-C9
20	2	312	CLA	C11-C12-C13-C14
20	3	310	CLA	C11-C12-C13-C14
20	A	850	CLA	C11-C12-C13-C14
20	B	816	CLA	C11-C10-C8-C9
20	B	850	CLA	C14-C13-C15-C16
21	1	218	LMU	C5-C6-C7-C8
21	A	853	LMU	C7-C8-C9-C10
20	2	314	CLA	CAA-CBA-CGA-O2A
20	A	838	CLA	C2-C1-O2A-CGA
20	B	827	CLA	C2-C1-O2A-CGA
20	R	107	CLA	C2-C1-O2A-CGA
20	2	302	CLA	O1D-CGD-O2D-CED
21	A	846	LMU	C4-C5-C6-C7
20	1	206	CLA	C3A-C2A-CAA-CBA
20	2	305	CLA	C3A-C2A-CAA-CBA
20	4	301	CLA	C3A-C2A-CAA-CBA
20	B	837	CLA	C3A-C2A-CAA-CBA
25	B	848	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	B	827	CLA	C10-C11-C12-C13
20	3	314	CLA	C4C-C3C-CAC-CBC
20	B	826	CLA	O2A-C1-C2-C3
20	L	203	CLA	O2A-C1-C2-C3
20	4	303	CLA	O1A-CGA-O2A-C1
22	F	203	BCR	C18-C19-C20-C21
21	C	101	LMU	C1-C2-C3-C4
21	R	104	LMU	O5B-C1B-O1B-C4'
21	A	847	LMU	C4-C5-C6-C7
21	A	846	LMU	C1-C2-C3-C4
20	A	829	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	C4-C3-C5-C6
20	A	826	CLA	C2-C3-C5-C6
20	K	102	CLA	C2C-C3C-CAC-CBC
20	L	201	CLA	C11-C12-C13-C14
21	2	313	LMU	C3-C4-C5-C6
21	A	854	LMU	C9-C10-C11-C12
20	B	826	CLA	C6-C7-C8-C9
20	B	838	CLA	C11-C10-C8-C9
20	B	840	CLA	C14-C13-C15-C16
20	A	805	CLA	CAA-CBA-CGA-O2A
21	4	321	LMU	C7-C8-C9-C10
21	D	201	LMU	C4B-C5B-C6B-O6B
20	4	303	CLA	CAA-CBA-CGA-O2A
20	A	849	CLA	CAA-CBA-CGA-O2A
20	B	822	CLA	CAA-CBA-CGA-O2A
20	B	836	CLA	CAA-CBA-CGA-O2A
20	B	839	CLA	CAA-CBA-CGA-O2A
20	H	102	CLA	CAA-CBA-CGA-O2A
20	B	823	CLA	C6-C7-C8-C9
20	B	829	CLA	C2-C3-C5-C6
20	B	826	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	C6-C7-C8-C10
20	A	818	CLA	C11-C10-C8-C7
20	A	823	CLA	C11-C10-C8-C7
20	A	850	CLA	C11-C12-C13-C15
20	B	809	CLA	C11-C12-C13-C15
20	B	814	CLA	C12-C13-C15-C16
21	4	320	LMU	C1-C2-C3-C4
20	4	305	CLA	C2B-C3B-CAB-CBB
20	A	810	CLA	C2B-C3B-CAB-CBB
20	A	831	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	R	108	CLA	C2B-C3B-CAB-CBB
22	A	845	BCR	C5-C6-C7-C8
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	846	BCR	C23-C24-C25-C30
22	I	103	BCR	C1-C6-C7-C8
22	I	103	BCR	C5-C6-C7-C8
20	2	303	CLA	CAA-CBA-CGA-O2A
20	B	821	CLA	CAA-CBA-CGA-O2A
20	2	307	CLA	C2-C1-O2A-CGA
20	4	310	CLA	C2-C1-O2A-CGA
20	B	806	CLA	C2-C1-O2A-CGA
20	H	101	CLA	C2-C1-O2A-CGA
20	L	203	CLA	C2-C1-O2A-CGA
20	A	827	CLA	CBA-CGA-O2A-C1
20	F	201	CLA	O1D-CGD-O2D-CED
21	A	855	LMU	O5'-C1'-O1'-C1
25	B	848	LMG	C28-C29-C30-C31
20	2	311	CLA	CAA-CBA-CGA-O2A
20	I	102	CLA	CAA-CBA-CGA-O2A
20	L	202	CLA	CAA-CBA-CGA-O2A
21	3	319	LMU	C11-C10-C9-C8
20	B	812	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	C2A-CAA-CBA-CGA
20	A	851	CLA	C2A-CAA-CBA-CGA
20	B	839	CLA	C2A-CAA-CBA-CGA
25	B	848	LMG	C41-C42-C43-C44
20	1	206	CLA	CAA-CBA-CGA-O2A
20	B	806	CLA	CAA-CBA-CGA-O2A
20	B	818	CLA	CAA-CBA-CGA-O2A
20	B	827	CLA	CAA-CBA-CGA-O2A
21	H	105	LMU	C11-C10-C9-C8
21	R	102	LMU	C2-C3-C4-C5
20	B	826	CLA	O1A-CGA-O2A-C1
20	K	104	CLA	C11-C10-C8-C7
20	K	104	CLA	C11-C10-C8-C9
20	2	312	CLA	C4-C3-C5-C6
21	G	103	LMU	O1'-C1-C2-C3
20	A	839	CLA	C6-C7-C8-C10
20	A	837	CLA	CAA-CBA-CGA-O2A
20	B	834	CLA	CAA-CBA-CGA-O1A
20	A	838	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	4	310	CLA	CAA-CBA-CGA-O1A
21	4	320	LMU	C2-C1-O1'-C1'
20	A	828	CLA	C6-C7-C8-C9
20	I	102	CLA	C11-C10-C8-C9
21	L	210	LMU	C9-C10-C11-C12
20	1	207	CLA	C1A-C2A-CAA-CBA
20	2	305	CLA	C1A-C2A-CAA-CBA
20	A	830	CLA	C4B-C3B-CAB-CBB
20	B	813	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C4B-C3B-CAB-CBB
20	K	101	CLA	C1A-C2A-CAA-CBA
20	L	202	CLA	C1A-C2A-CAA-CBA
20	L	207	CLA	C4B-C3B-CAB-CBB
20	3	313	CLA	CAA-CBA-CGA-O2A
20	4	317	CLA	CAA-CBA-CGA-O2A
20	A	803	CLA	CAA-CBA-CGA-O2A
20	B	823	CLA	CAA-CBA-CGA-O2A
21	R	106	LMU	C3-C4-C5-C6
22	A	843	BCR	C17-C18-C19-C20
20	B	834	CLA	CAA-CBA-CGA-O2A
20	4	315	CLA	CAA-CBA-CGA-O2A
20	4	318	CLA	CAA-CBA-CGA-O2A
21	R	109	LMU	C3-C4-C5-C6
20	A	813	CLA	CAA-CBA-CGA-O2A
21	3	318	LMU	C9-C10-C11-C12
20	4	301	CLA	C2-C1-O2A-CGA
20	A	808	CLA	C2-C1-O2A-CGA
20	A	832	CLA	C2-C1-O2A-CGA
20	B	802	CLA	C2-C1-O2A-CGA
20	B	831	CLA	C2-C1-O2A-CGA
20	A	828	CLA	C11-C10-C8-C7
20	B	824	CLA	C11-C10-C8-C7
20	B	850	CLA	C11-C12-C13-C15
20	B	850	CLA	C12-C13-C15-C16
20	B	803	CLA	CAA-CBA-CGA-O2A
20	B	817	CLA	C2A-CAA-CBA-CGA
21	B	805	LMU	O5B-C1B-O1B-C4'
20	A	801	CLA	C2-C1-O2A-CGA
20	2	314	CLA	C3A-C2A-CAA-CBA
20	A	822	CLA	C3A-C2A-CAA-CBA
20	B	832	CLA	C3A-C2A-CAA-CBA
20	J	101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	K	101	CLA	C3A-C2A-CAA-CBA
20	R	108	CLA	C3A-C2A-CAA-CBA
20	I	102	CLA	CAA-CBA-CGA-O1A
20	4	301	CLA	O1A-CGA-O2A-C1
20	A	828	CLA	C10-C11-C12-C13
20	B	838	CLA	CAA-CBA-CGA-O2A
20	L	202	CLA	CAA-CBA-CGA-O1A
20	1	206	CLA	CAA-CBA-CGA-O1A
20	2	303	CLA	CAA-CBA-CGA-O1A
20	4	303	CLA	CAA-CBA-CGA-O1A
20	A	849	CLA	CAA-CBA-CGA-O1A
21	2	320	LMU	C2-C3-C4-C5
21	4	316	LMU	C6-C7-C8-C9
20	B	829	CLA	C13-C15-C16-C17
20	4	301	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	C11-C10-C8-C9
20	A	849	CLA	C6-C7-C8-C9
20	B	803	CLA	C11-C10-C8-C9
20	B	816	CLA	C6-C7-C8-C9
20	4	318	CLA	CAA-CBA-CGA-O1A
20	A	803	CLA	CAA-CBA-CGA-O1A
20	B	821	CLA	CAA-CBA-CGA-O1A
20	B	836	CLA	CAA-CBA-CGA-O1A
21	A	848	LMU	C2B-C1B-O1B-C4'
20	A	805	CLA	CAA-CBA-CGA-O1A
22	A	845	BCR	C17-C18-C19-C20
20	B	827	CLA	CAA-CBA-CGA-O1A
20	B	839	CLA	CAA-CBA-CGA-O1A
20	H	102	CLA	CAA-CBA-CGA-O1A
20	B	806	CLA	CAA-CBA-CGA-O1A
20	B	822	CLA	CAA-CBA-CGA-O1A
20	H	110	CLA	CAA-CBA-CGA-O2A
20	2	311	CLA	CAA-CBA-CGA-O1A
20	A	813	CLA	CAA-CBA-CGA-O1A
20	A	838	CLA	CAA-CBA-CGA-O1A
25	B	848	LMG	C42-C43-C44-C45
20	4	303	CLA	C15-C16-C17-C18
20	A	830	CLA	CAA-CBA-CGA-O2A
20	B	841	CLA	CAA-CBA-CGA-O2A
20	1	211	CLA	CAD-CBD-CGD-O2D
20	B	802	CLA	CAD-CBD-CGD-O2D
20	B	832	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

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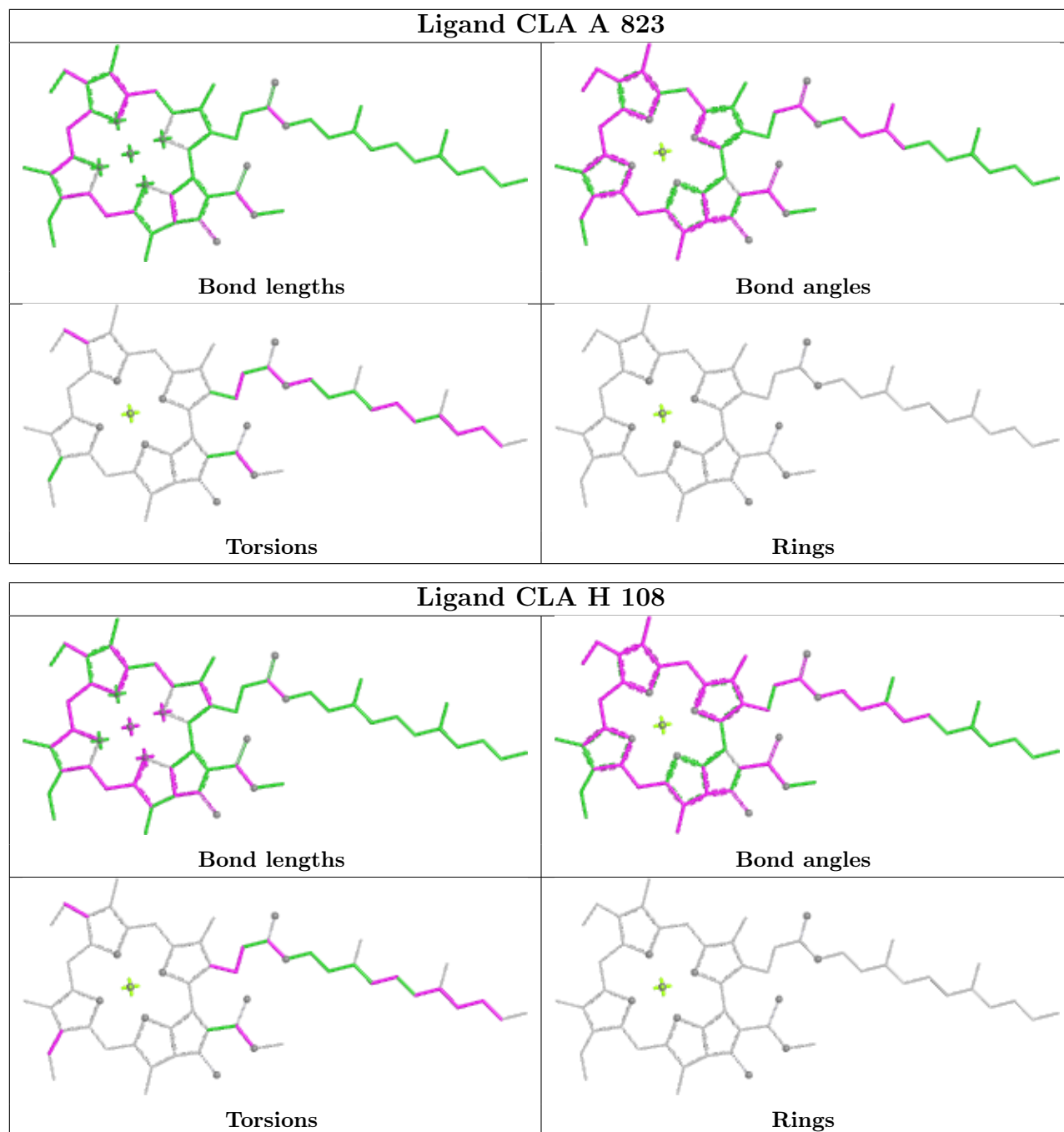
Mol	Chain	Res	Type	Atoms
20	F	206	CLA	CAD-CBD-CGD-O2D
20	H	101	CLA	CAD-CBD-CGD-O2D
20	A	825	CLA	CAA-CBA-CGA-O2A
20	4	315	CLA	CAA-CBA-CGA-O1A
20	4	317	CLA	CAA-CBA-CGA-O1A
20	A	837	CLA	CAA-CBA-CGA-O1A
20	B	830	CLA	C10-C11-C12-C13
20	2	310	CLA	C2-C1-O2A-CGA
20	A	809	CLA	C2-C1-O2A-CGA
20	B	823	CLA	CAA-CBA-CGA-O1A
20	A	811	CLA	CAA-CBA-CGA-O2A
21	2	319	LMU	C2B-C1B-O1B-C4'
20	H	109	CLA	CAA-CBA-CGA-O2A

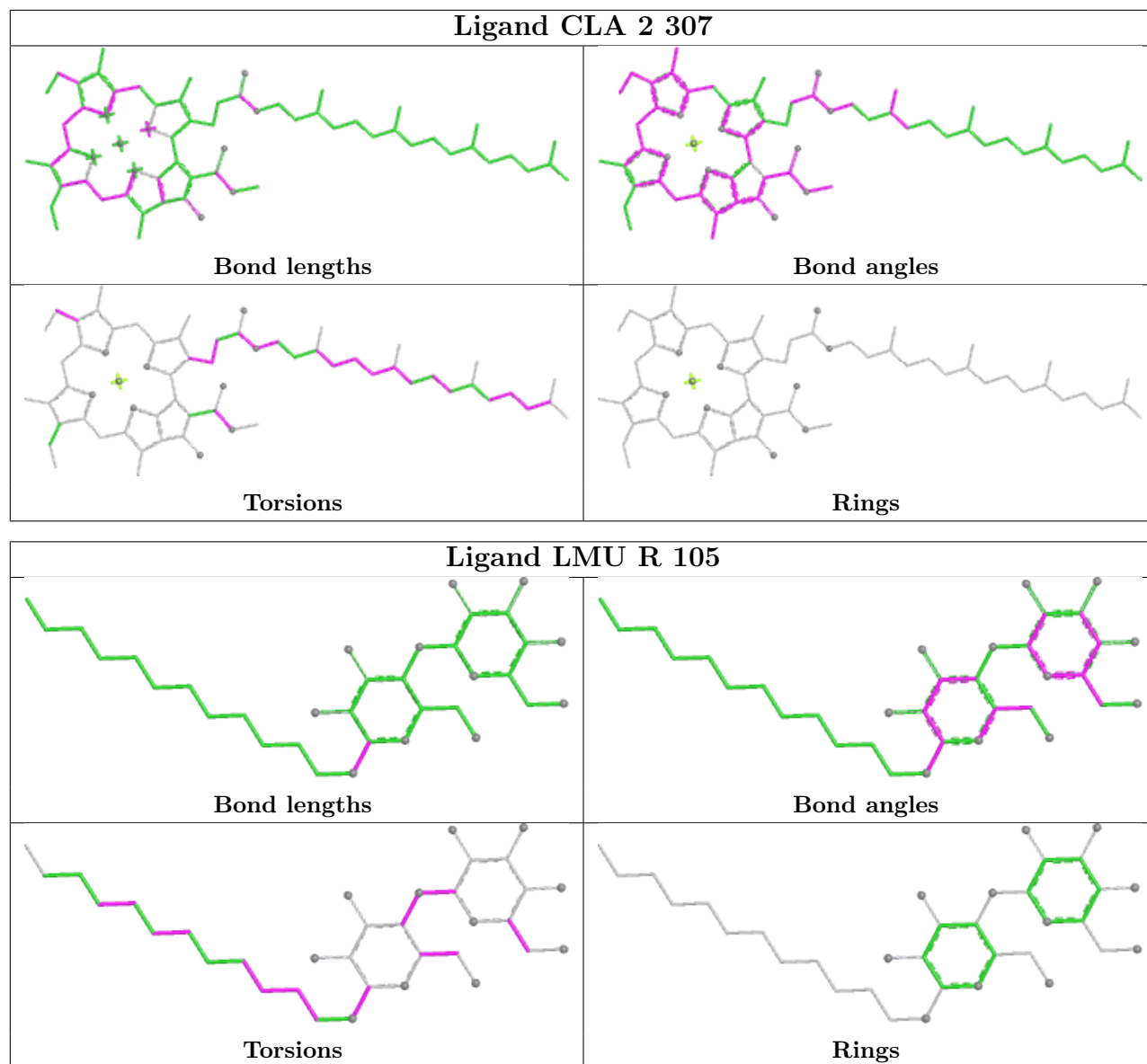
There are no ring outliers.

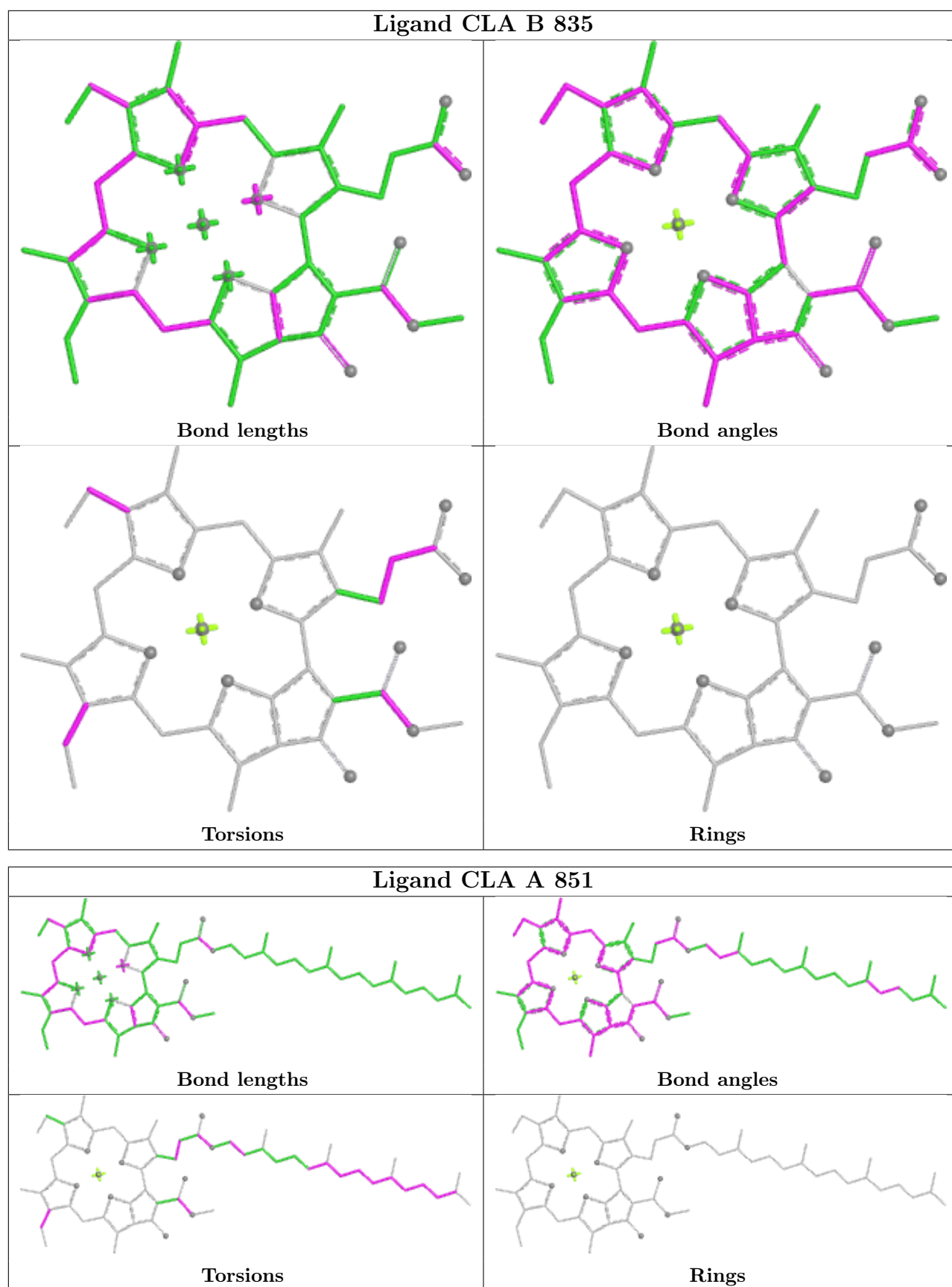
5 monomers are involved in 45 short contacts:

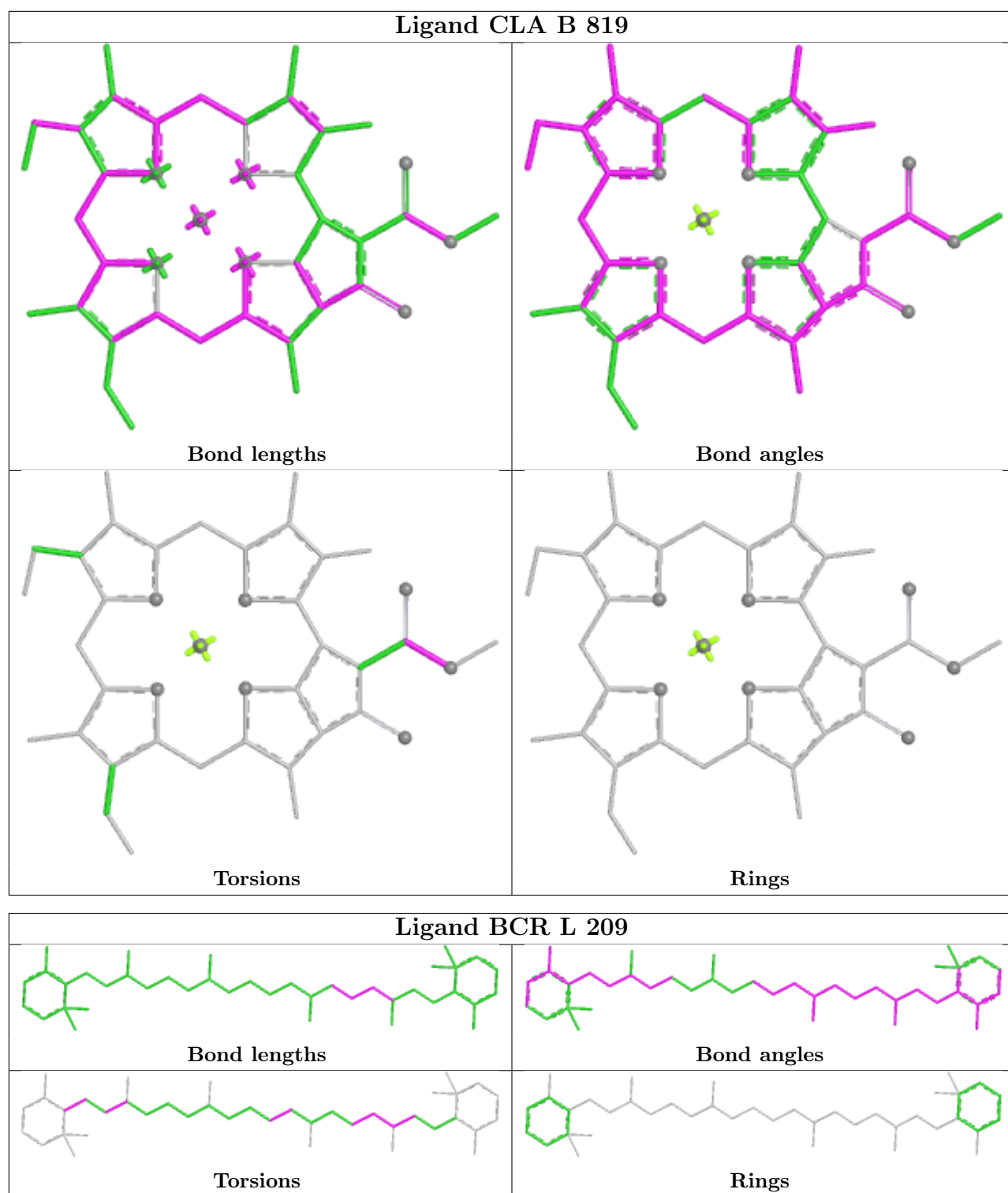
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	R	109	LMU	0	3
21	4	319	LMU	0	3
20	K	101	CLA	0	1
20	1	207	CLA	0	1
21	G	101	LMU	0	41

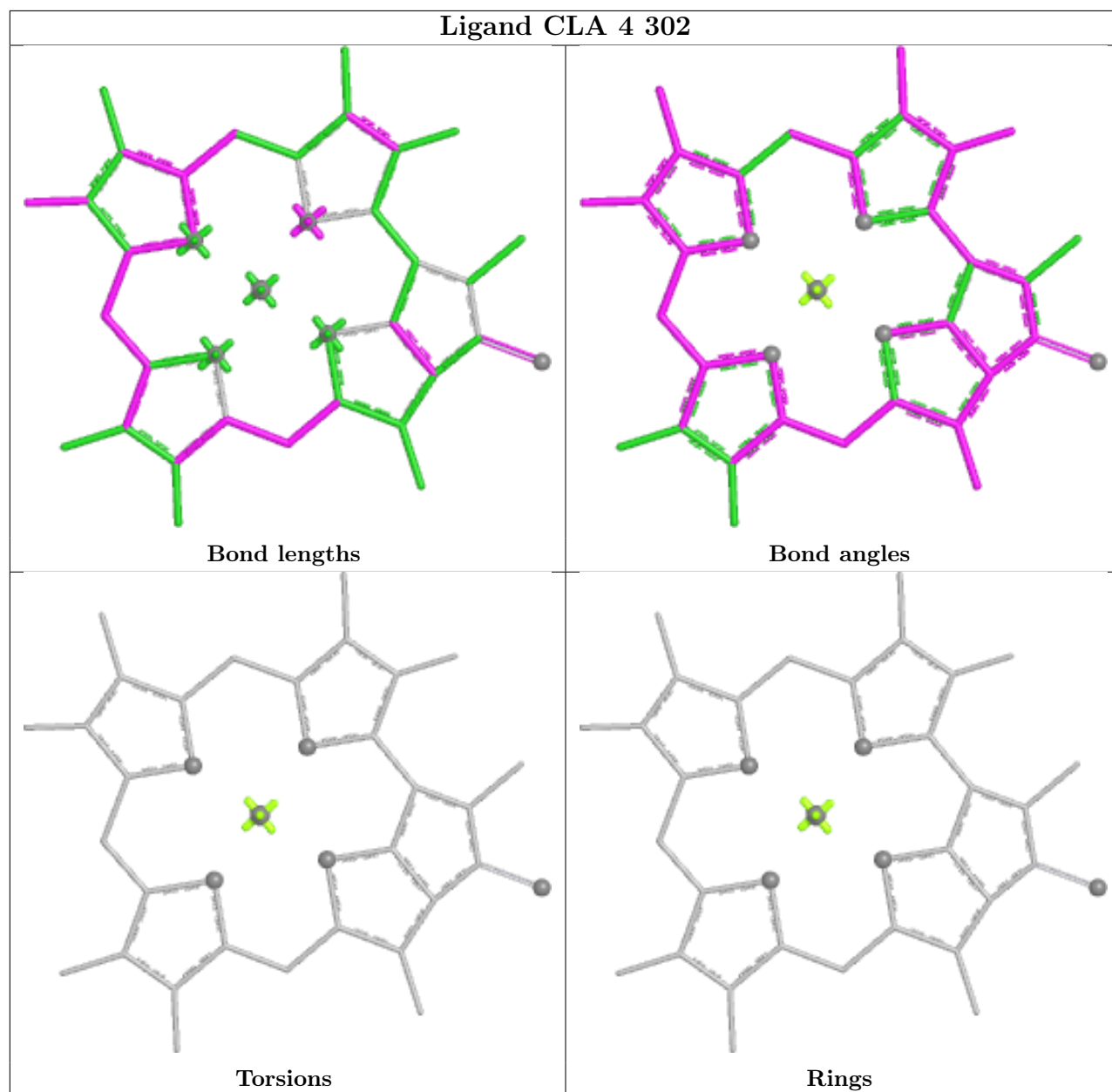
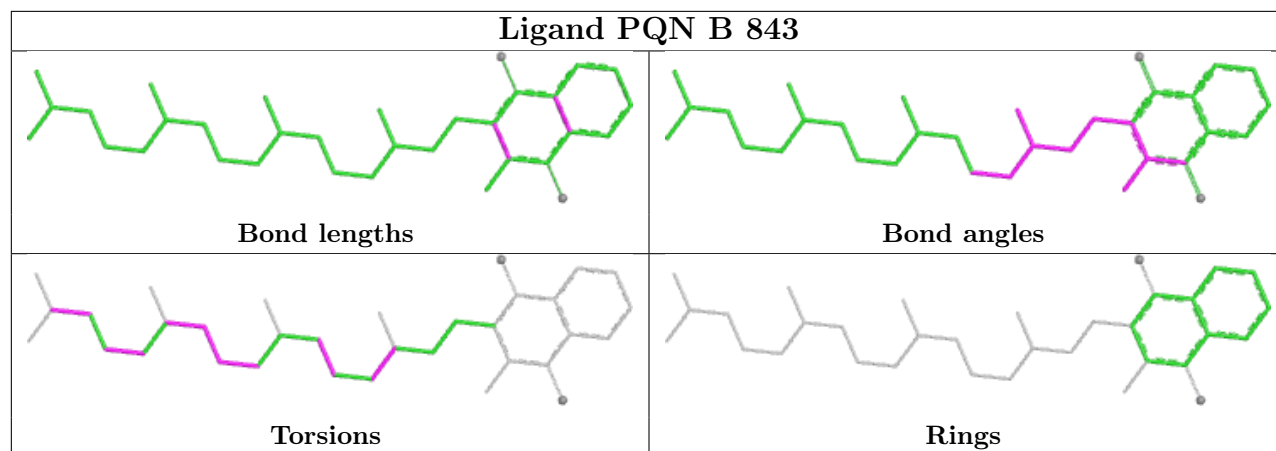
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



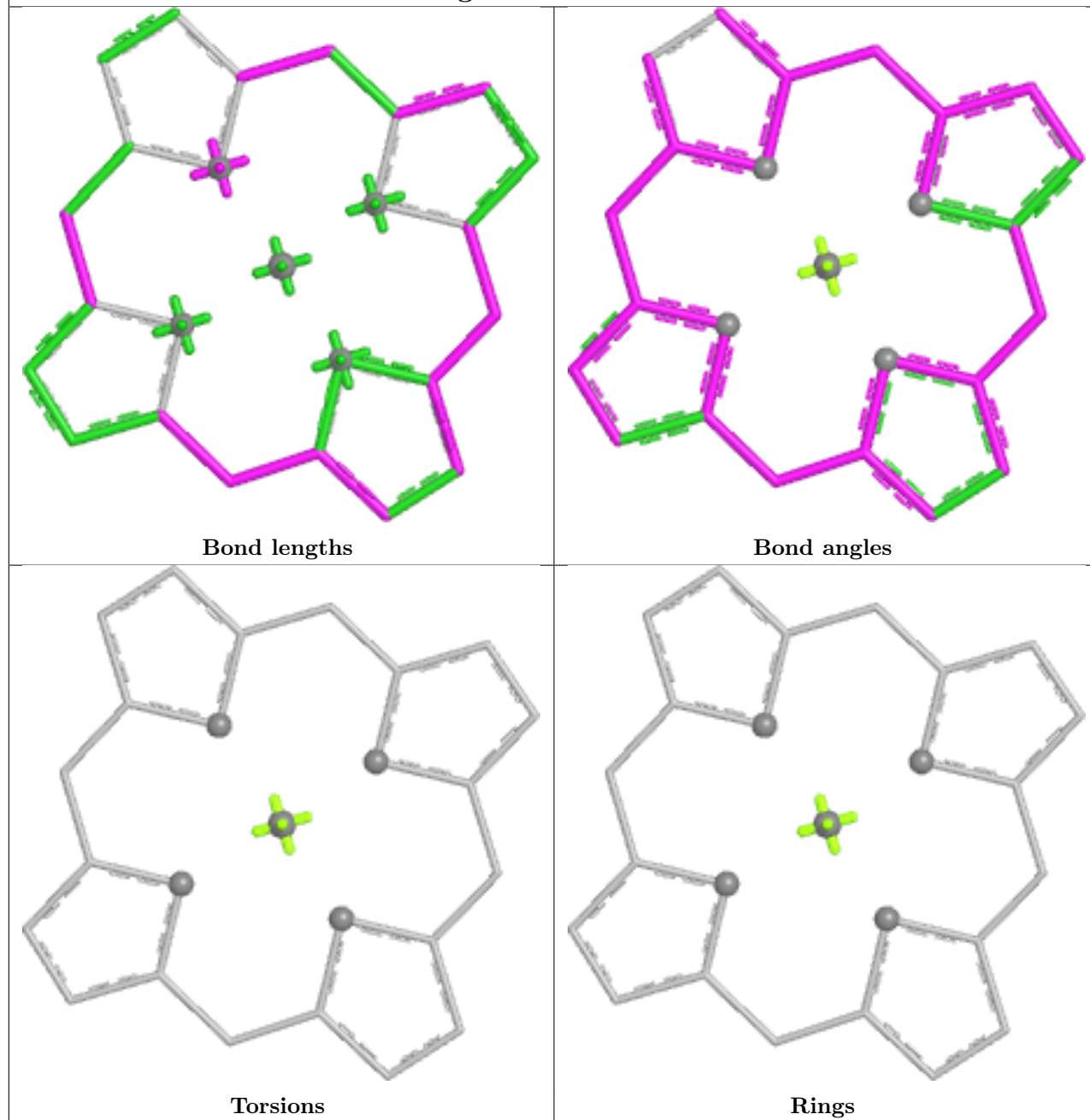


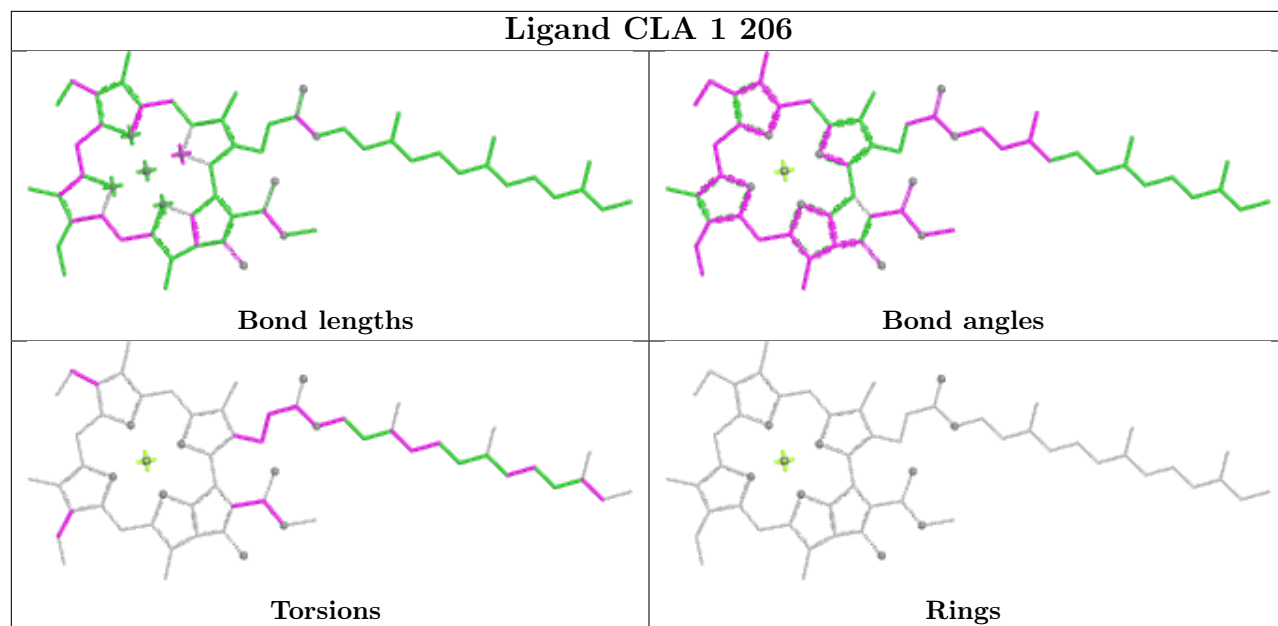




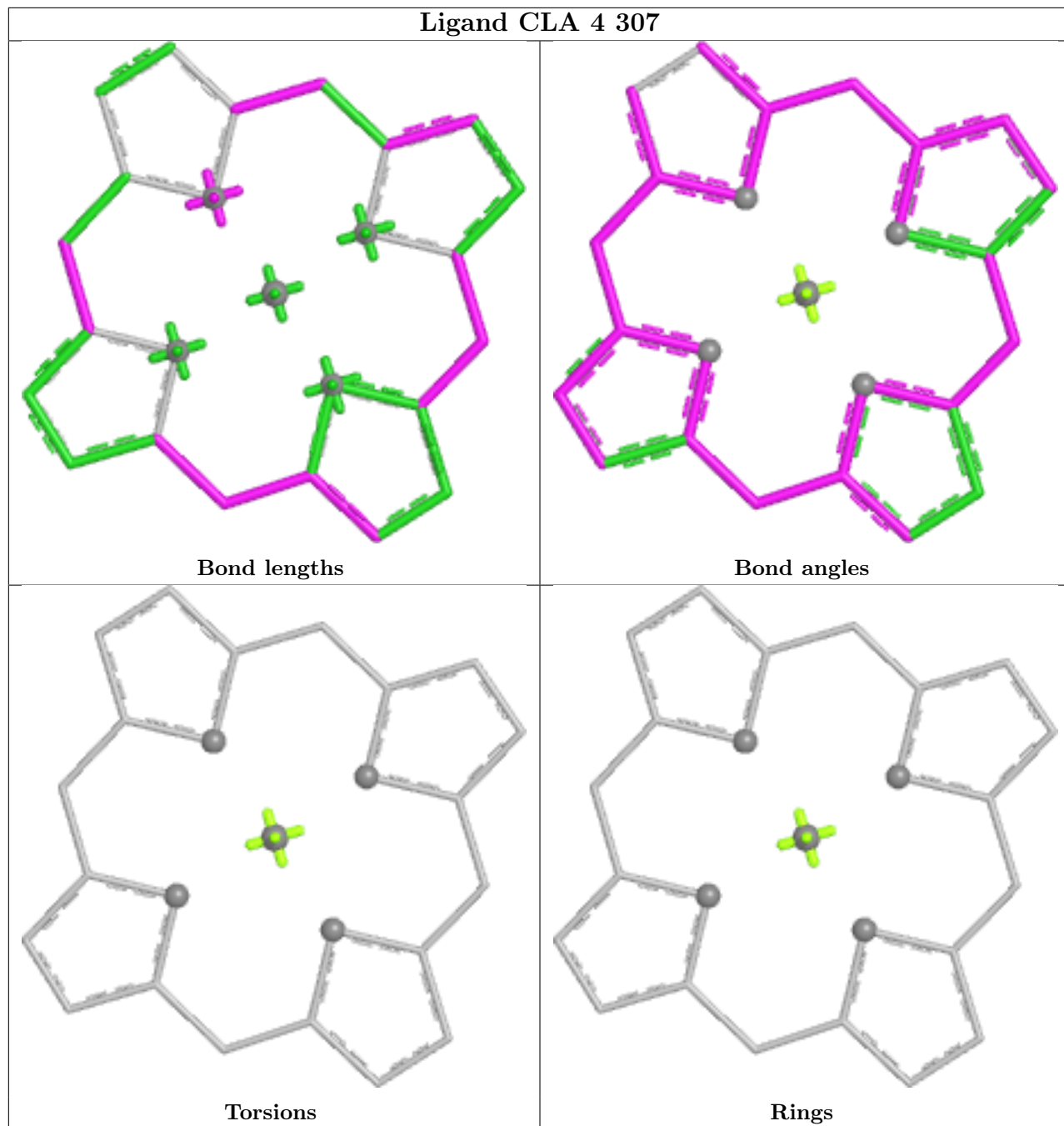


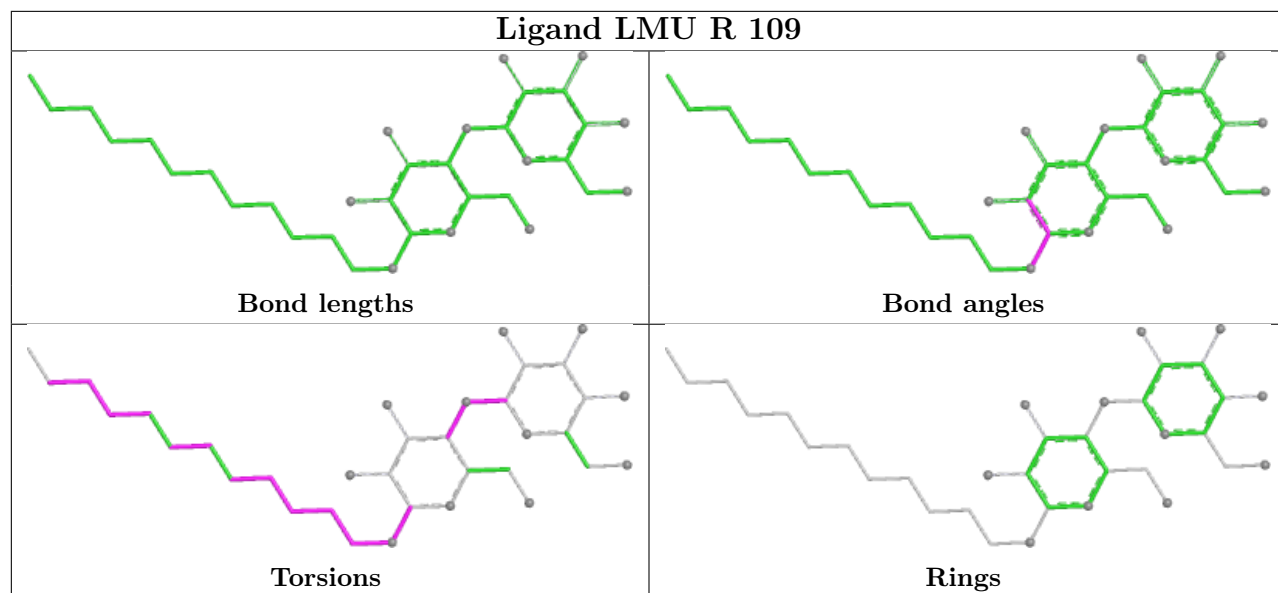
## Ligand CLA 4 308

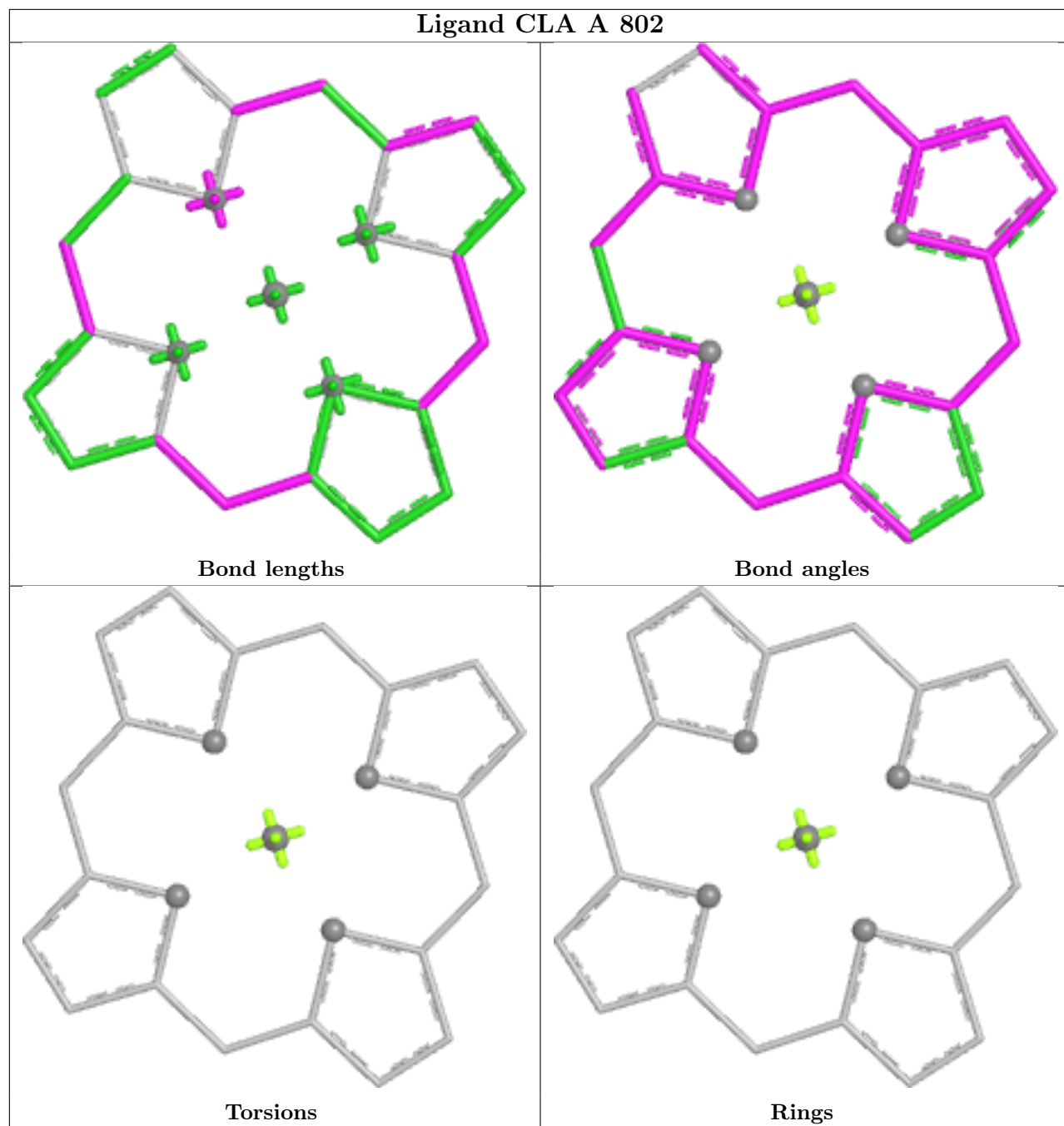


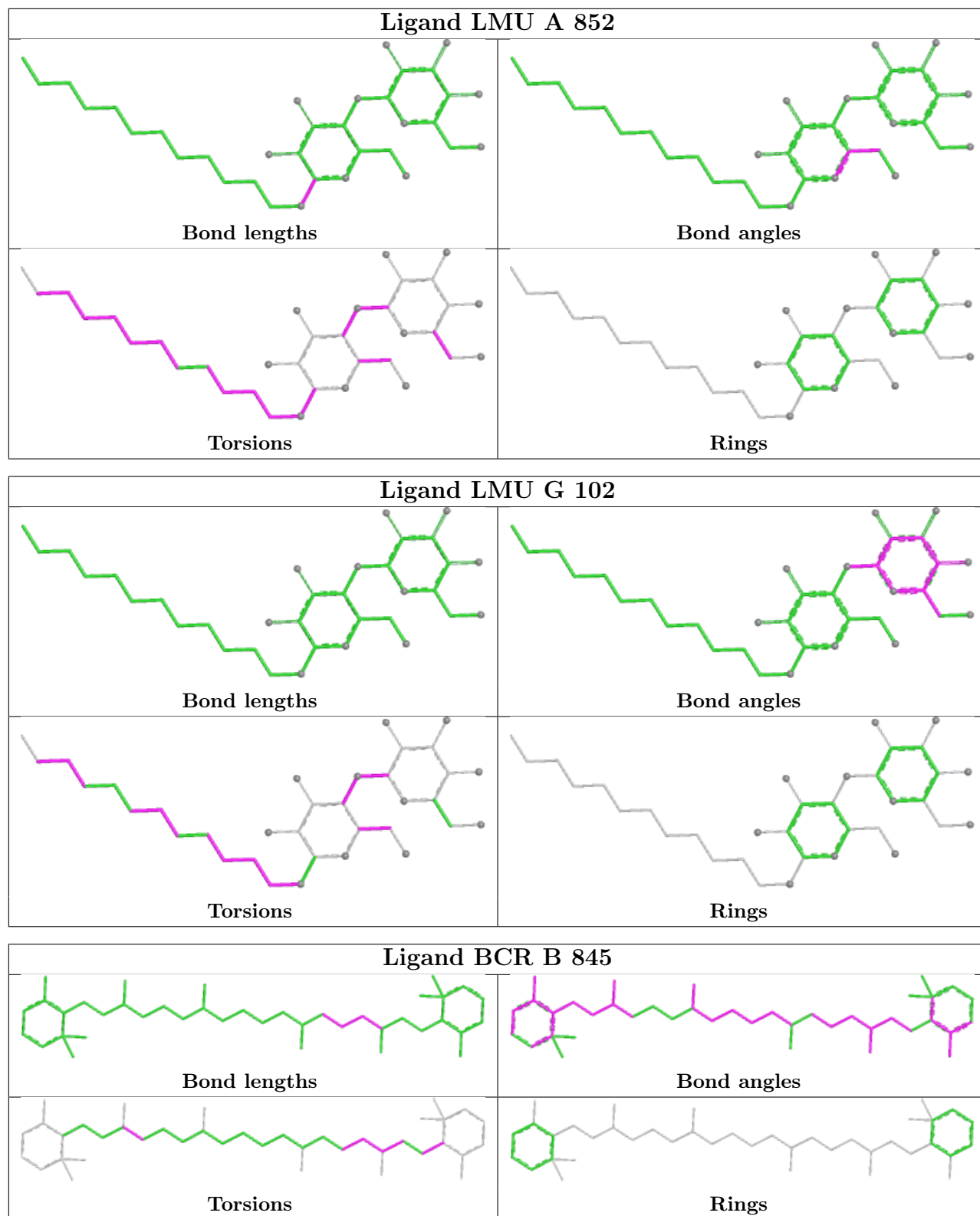


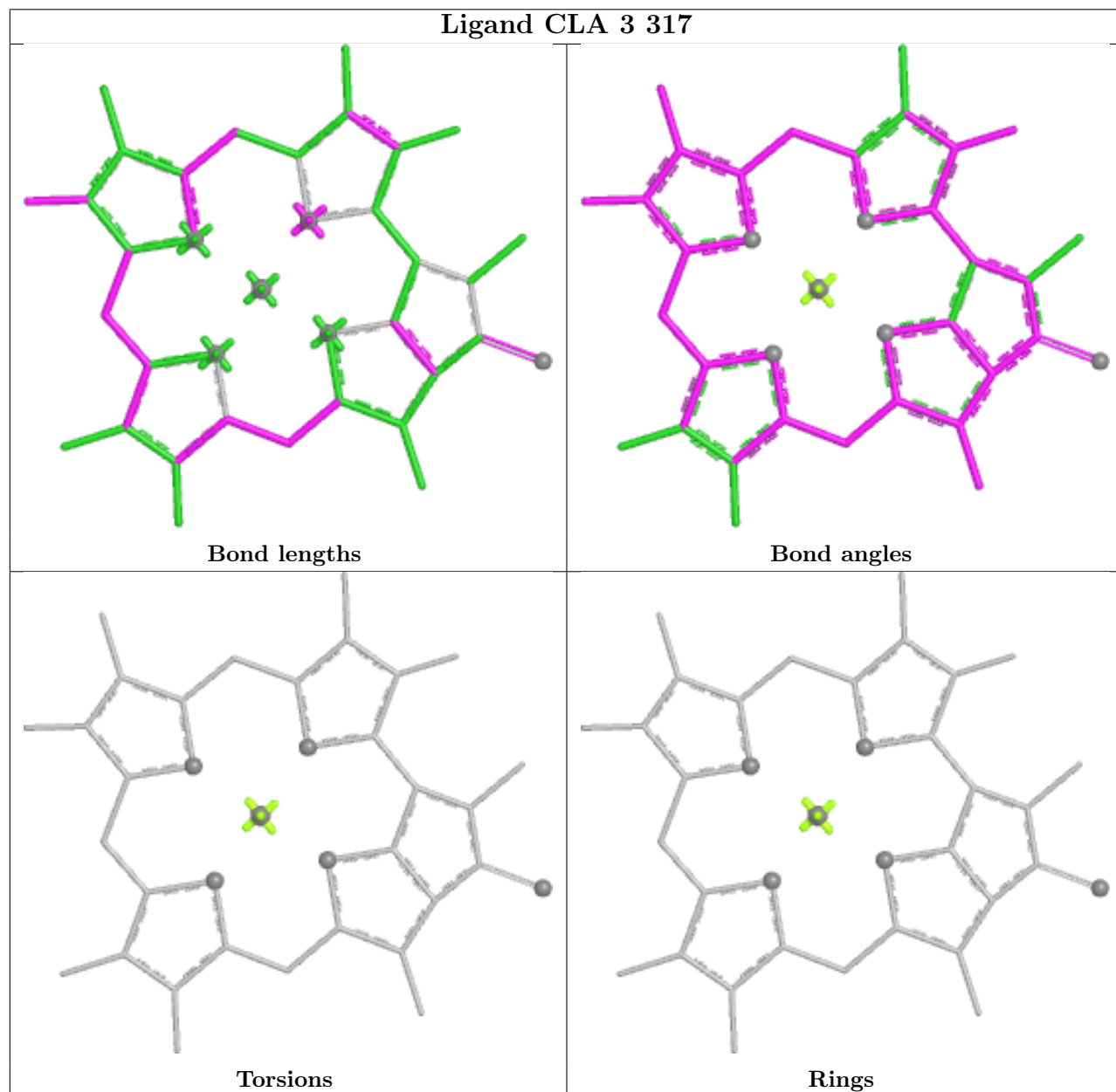
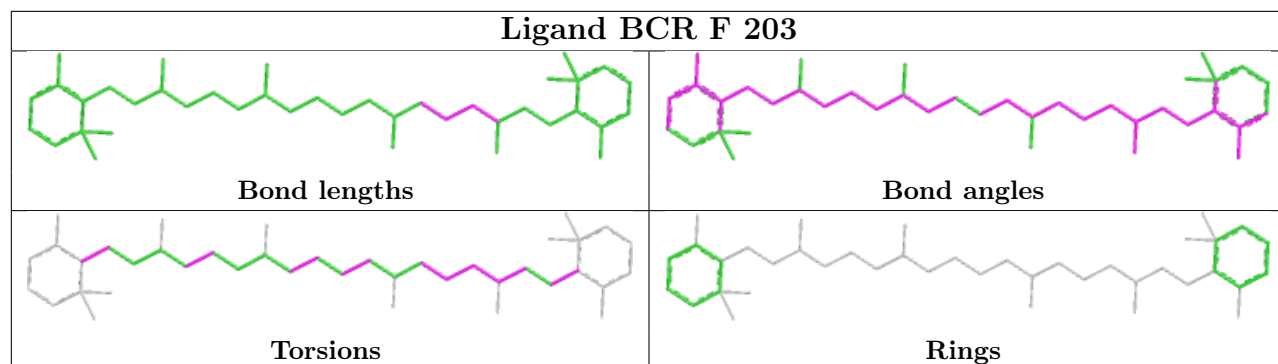
## Ligand CLA 4 307

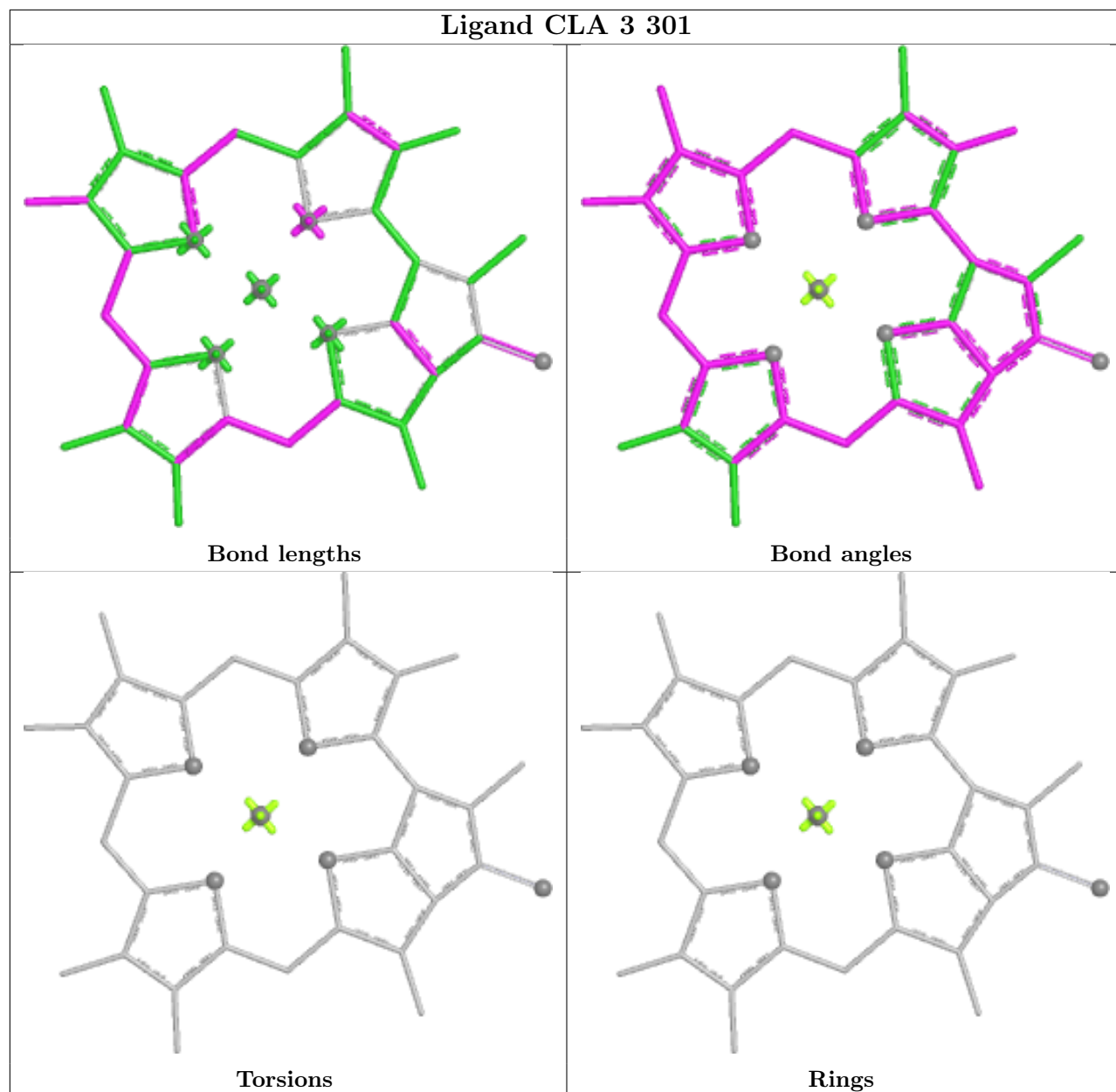


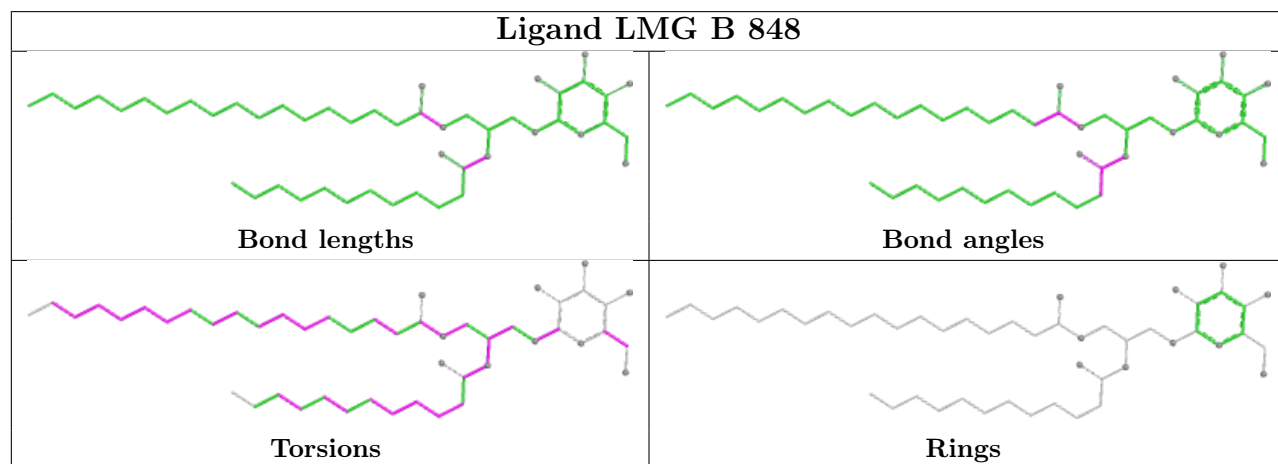
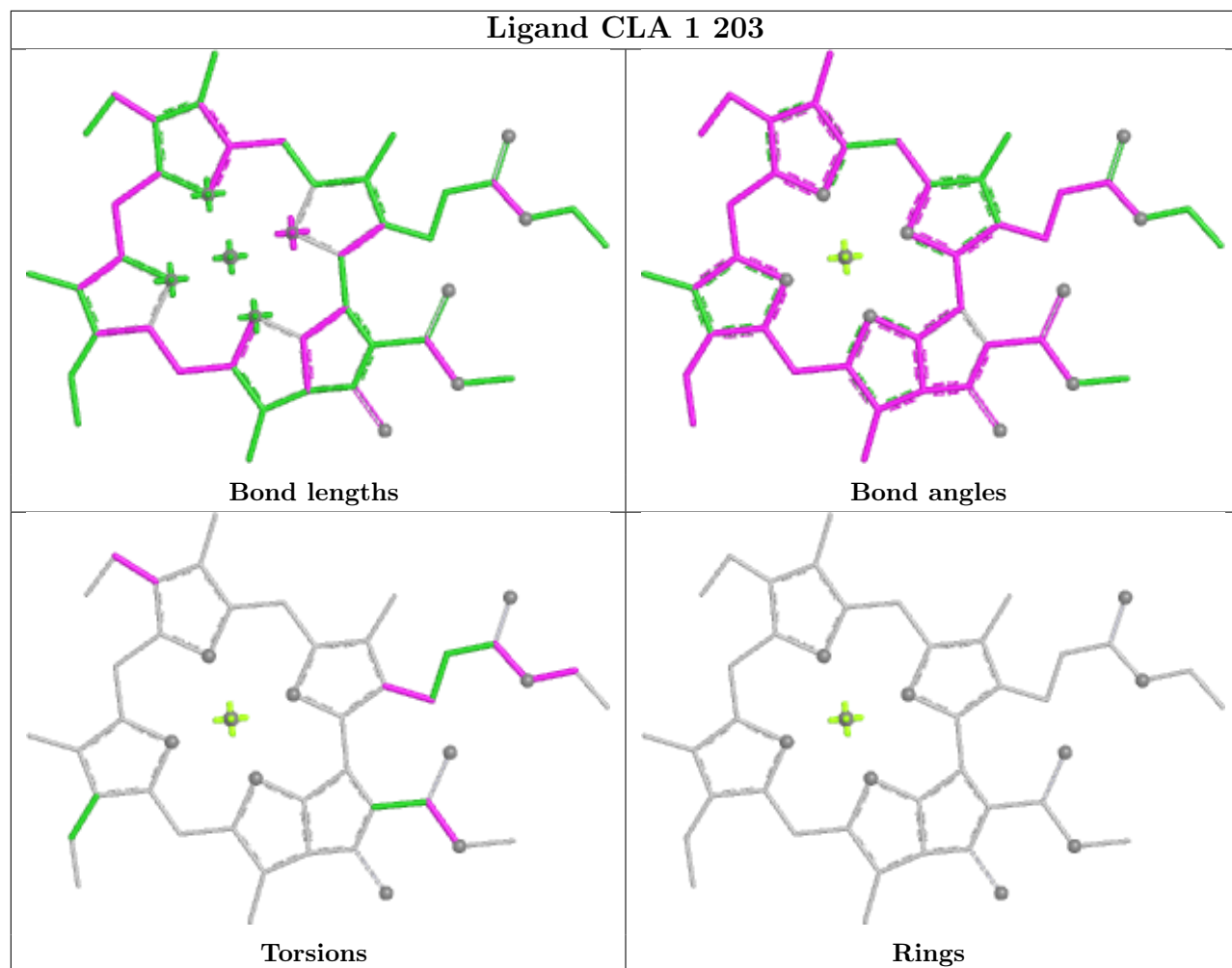


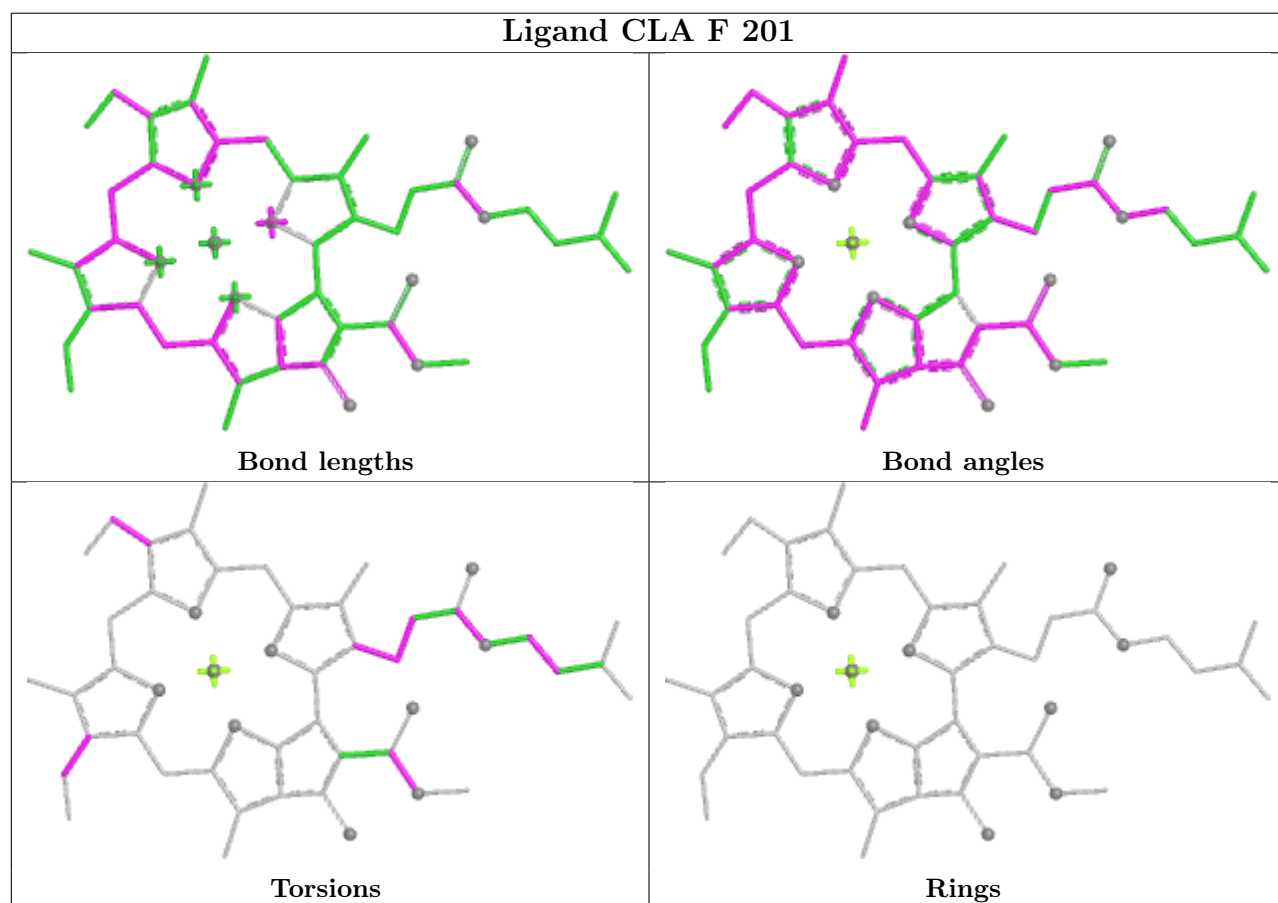
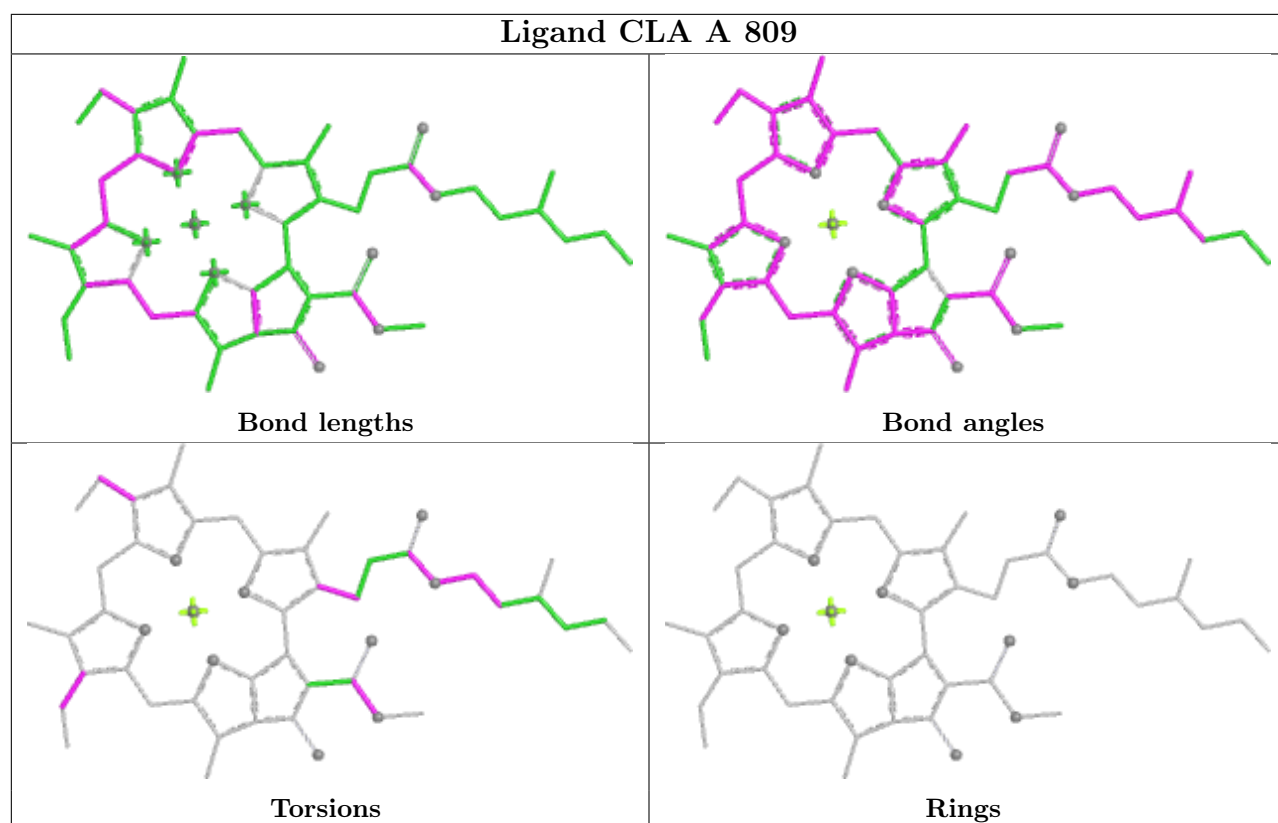




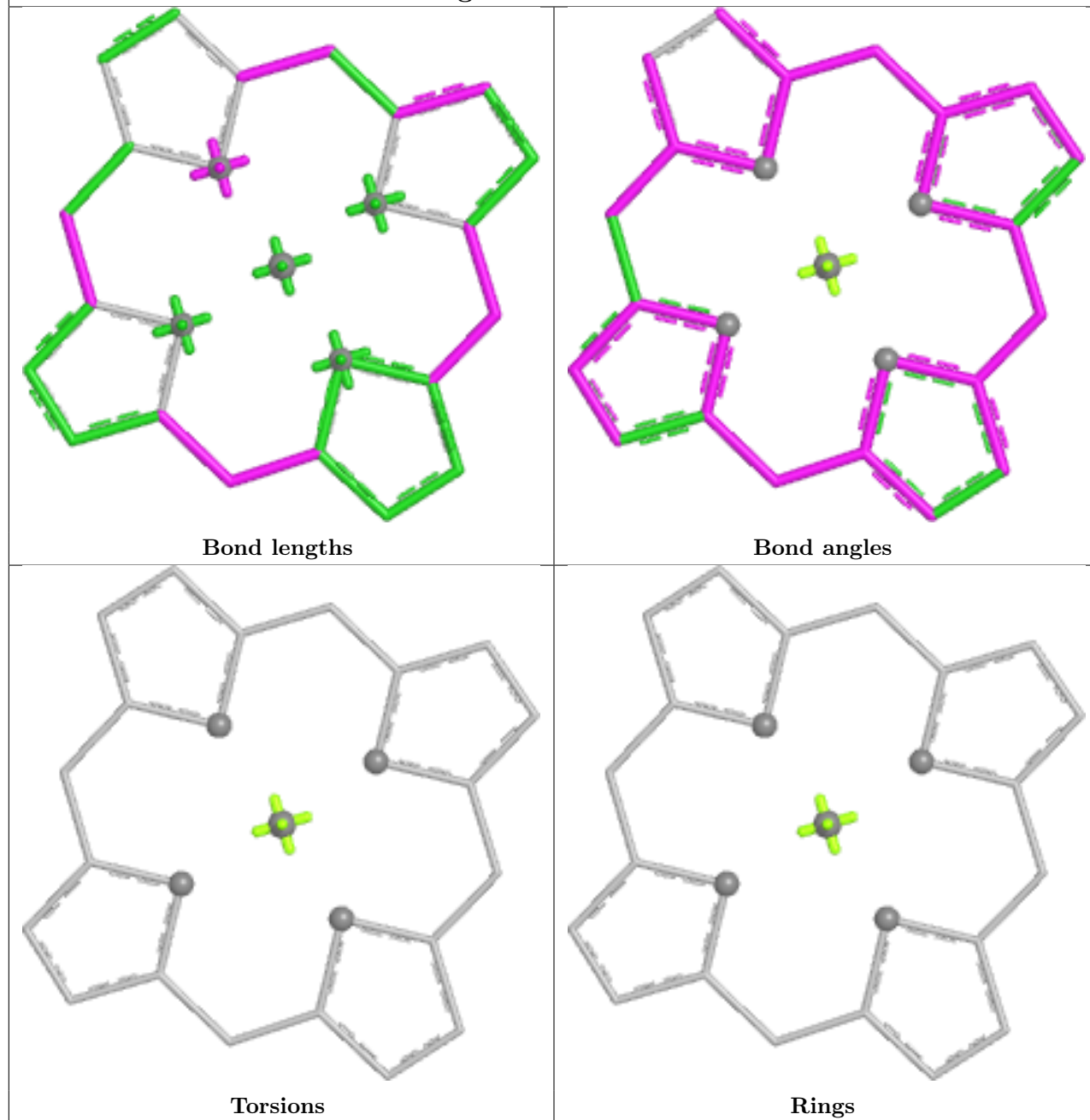


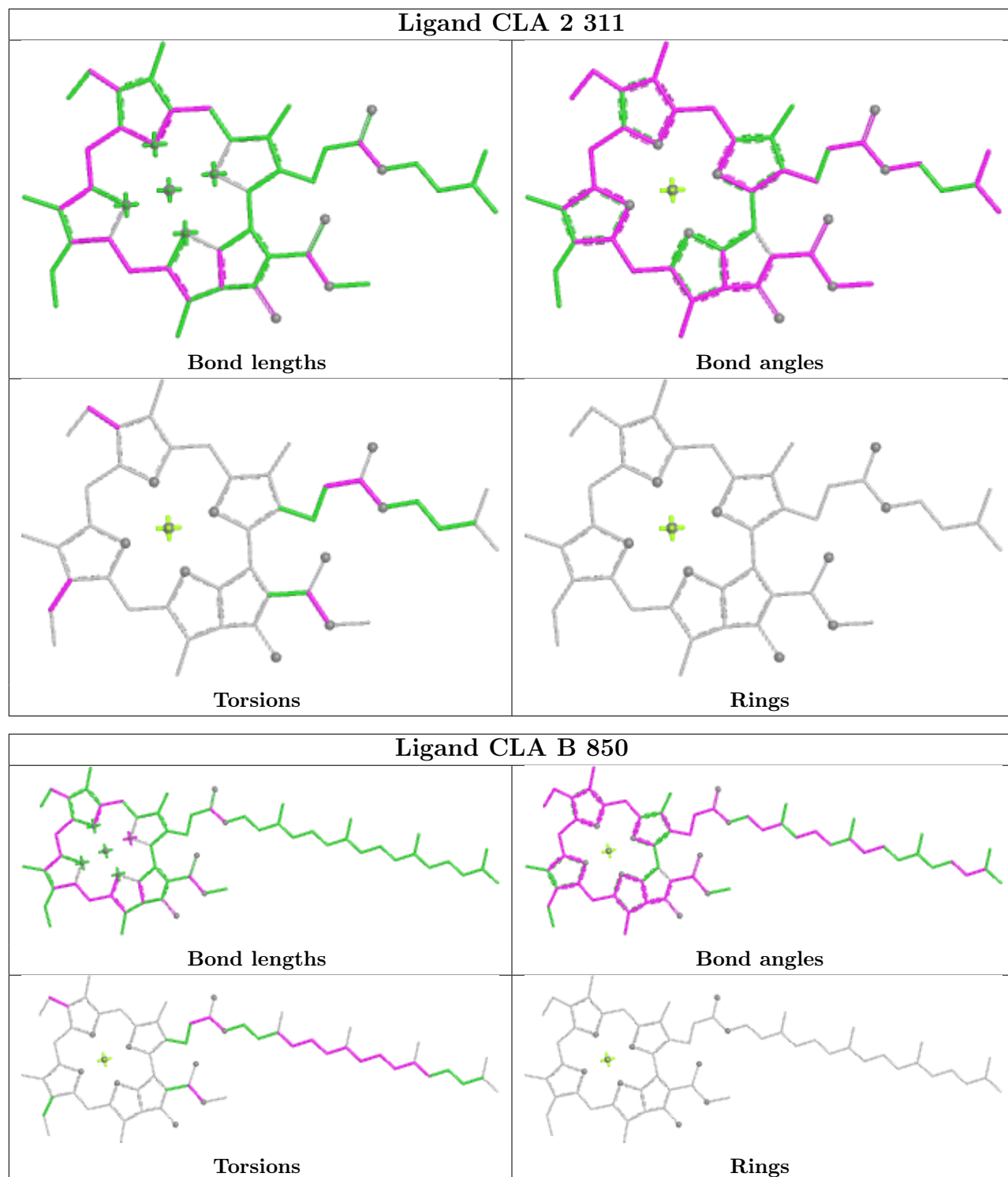


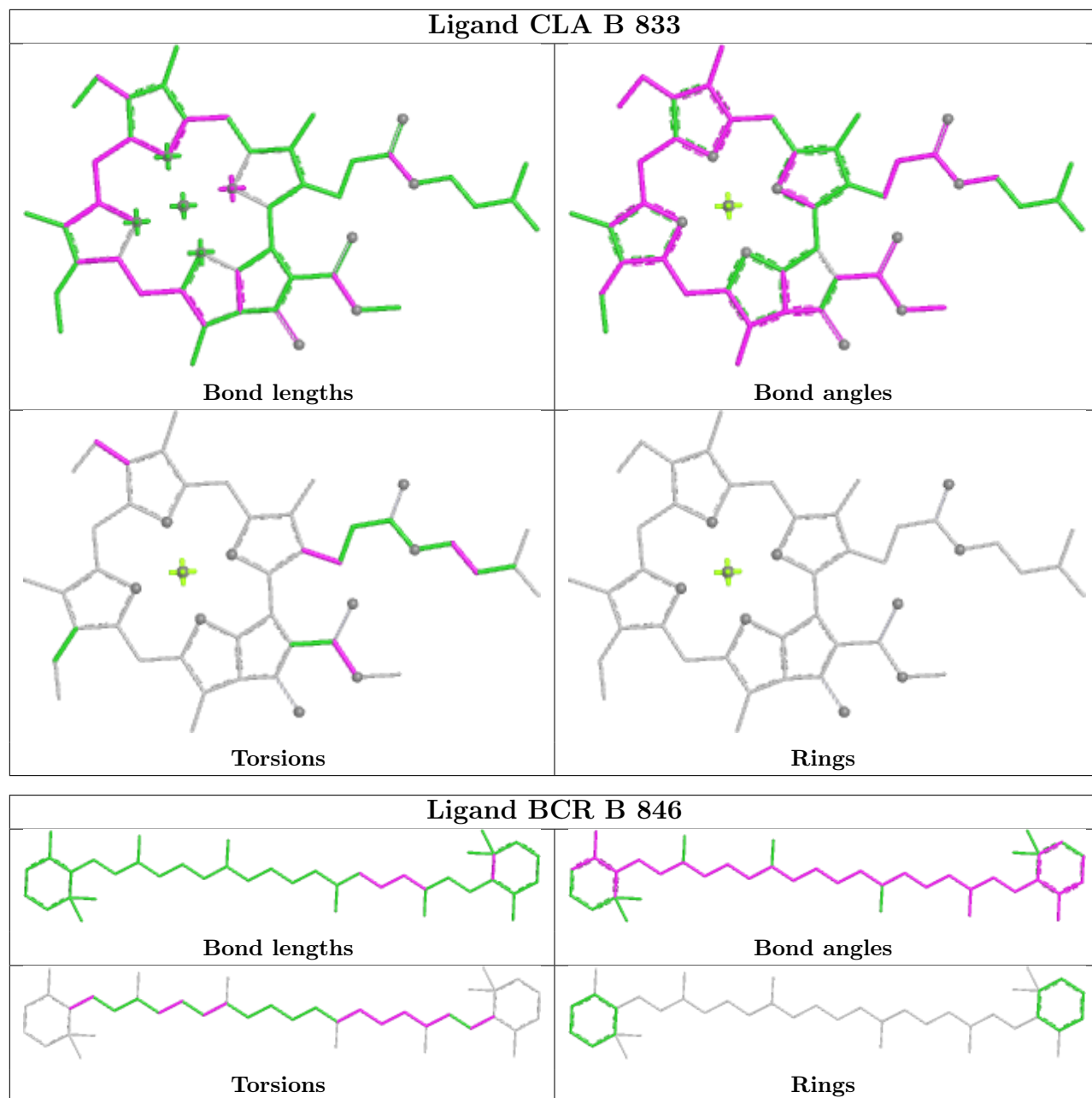




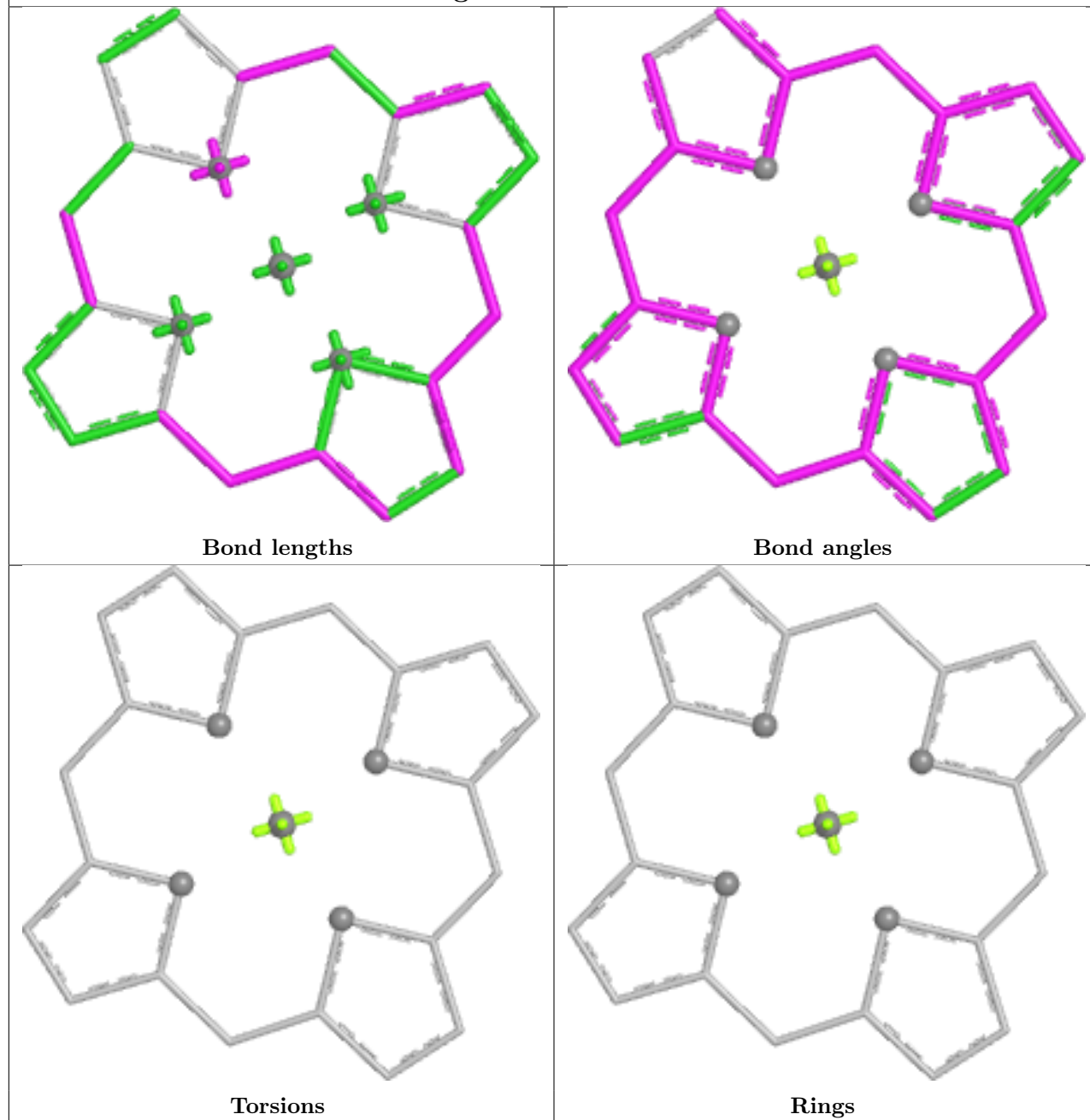
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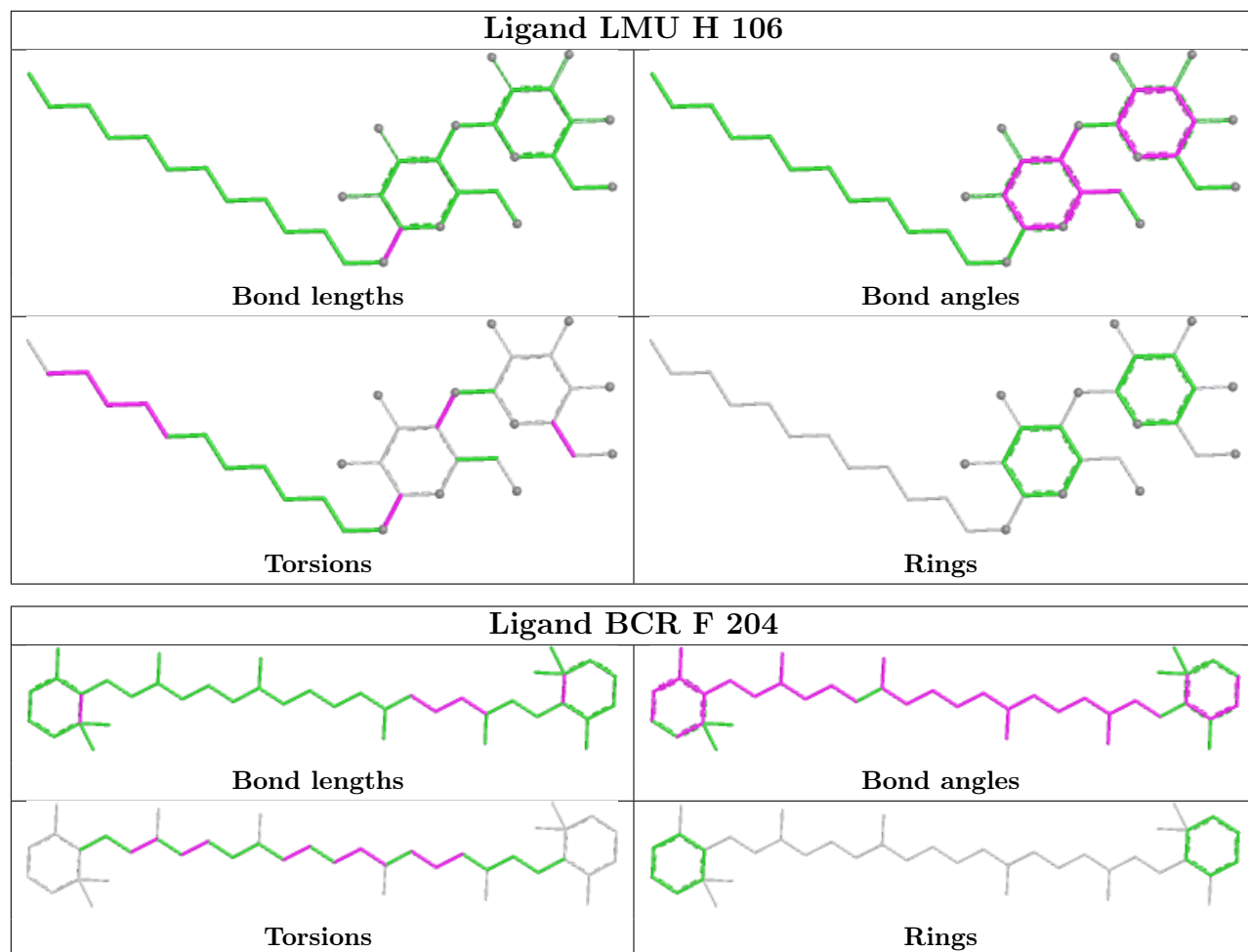


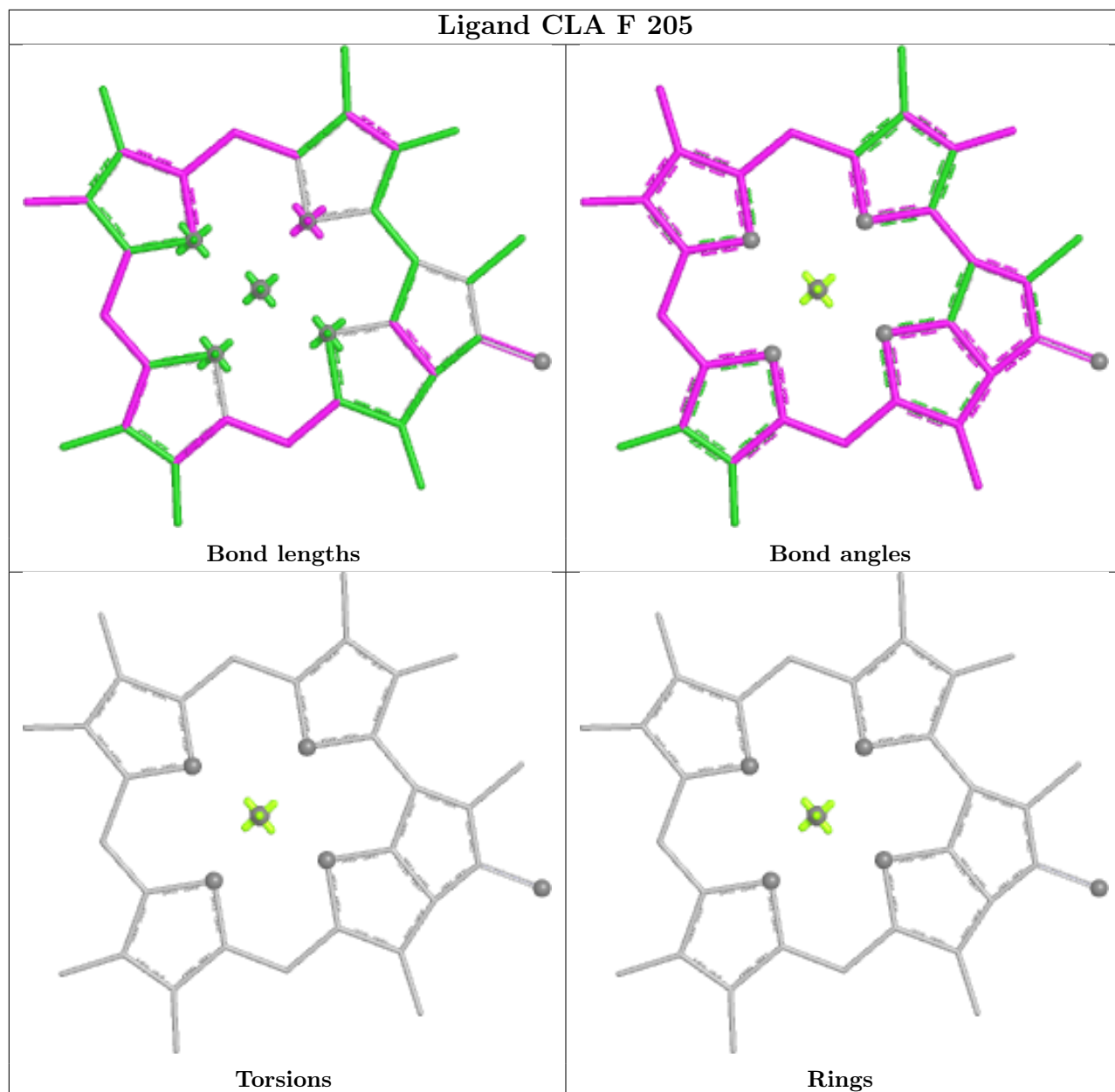


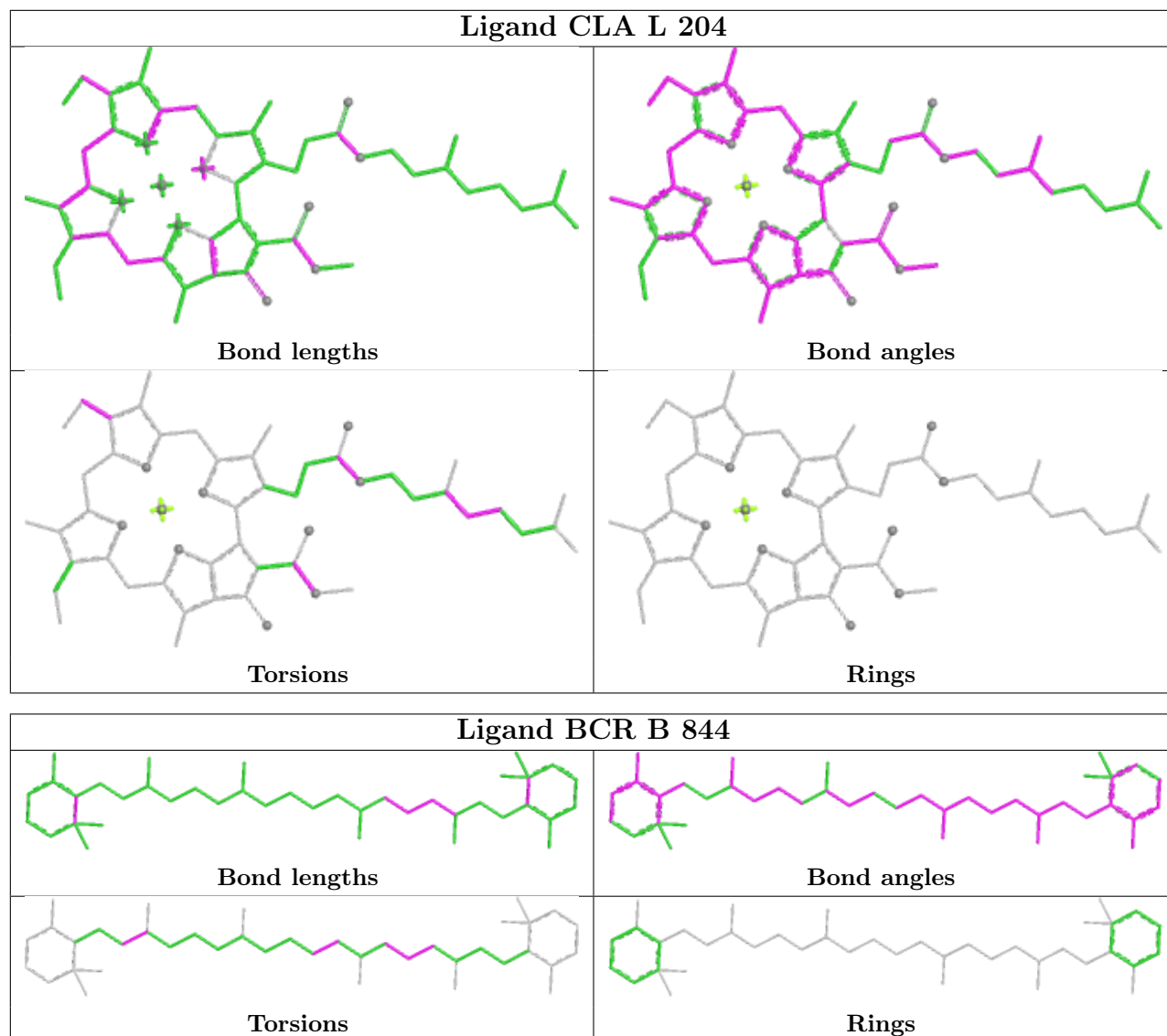


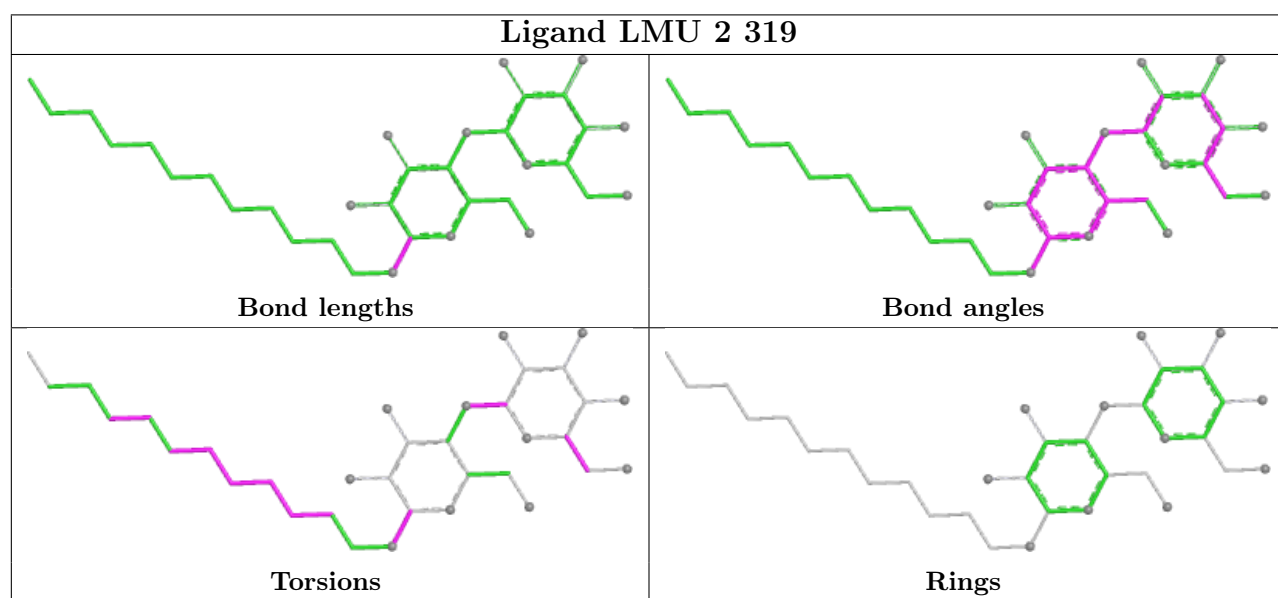
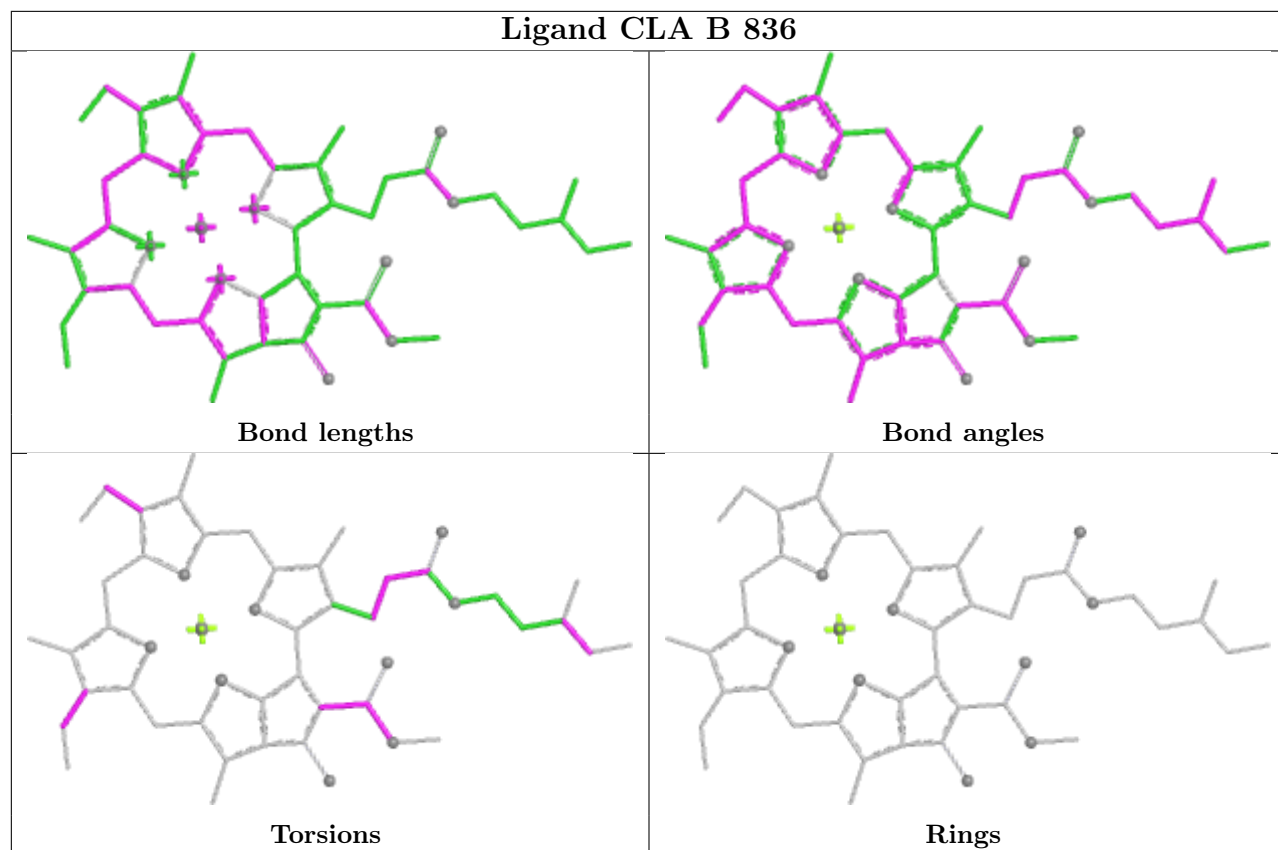
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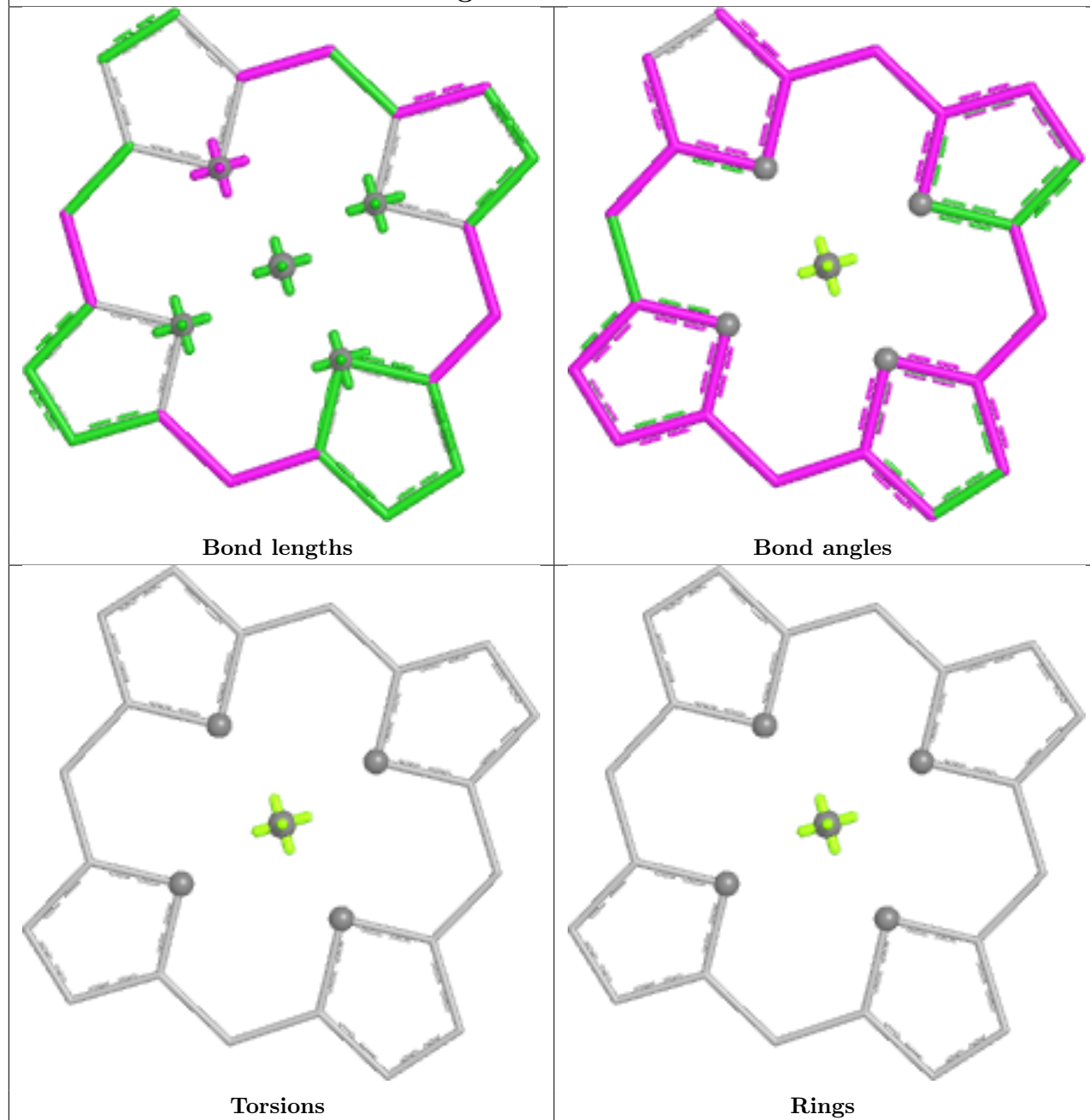


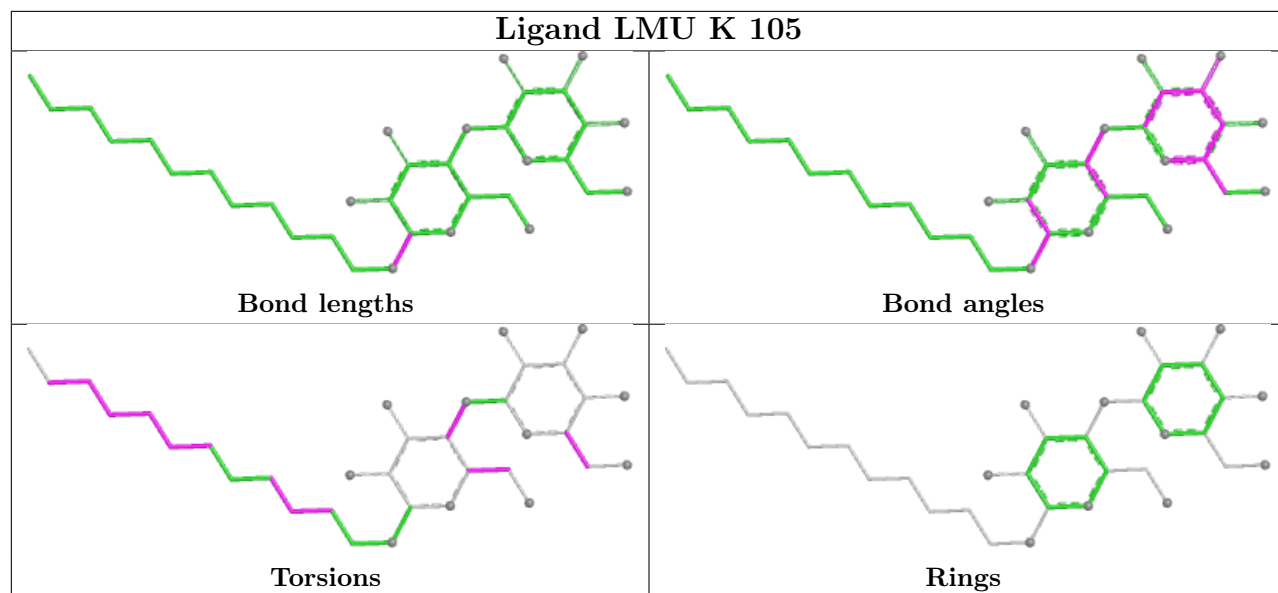




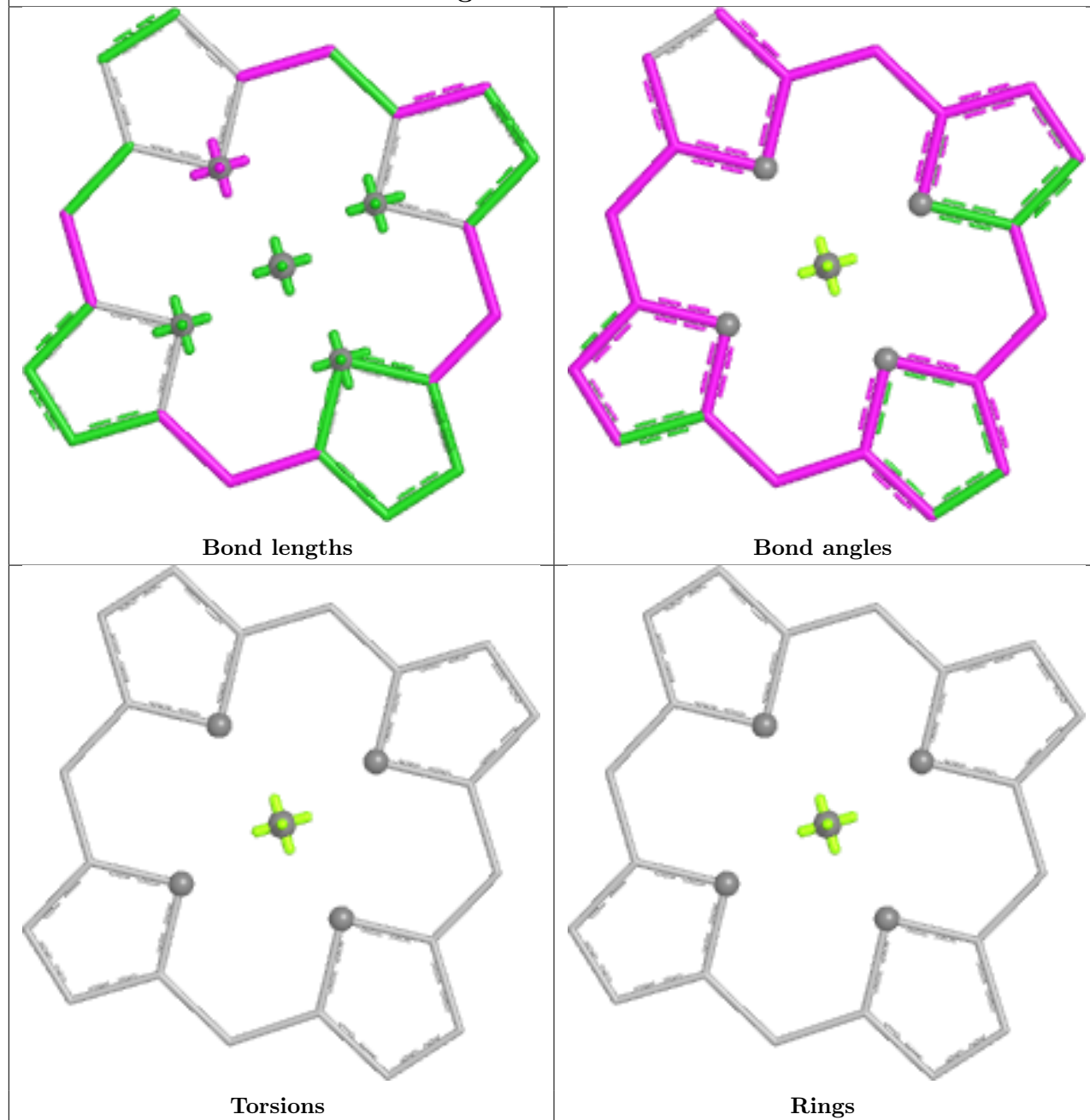


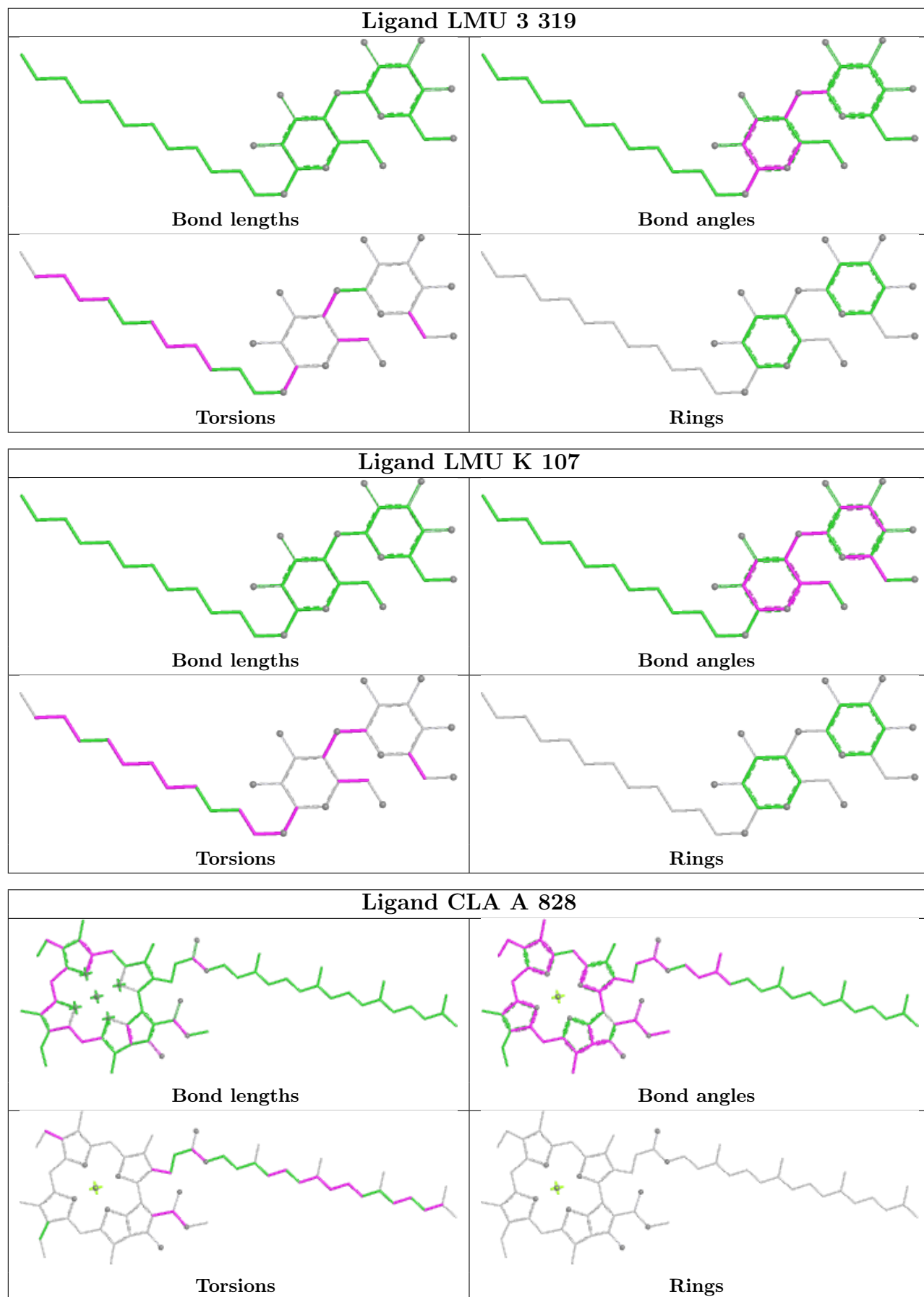
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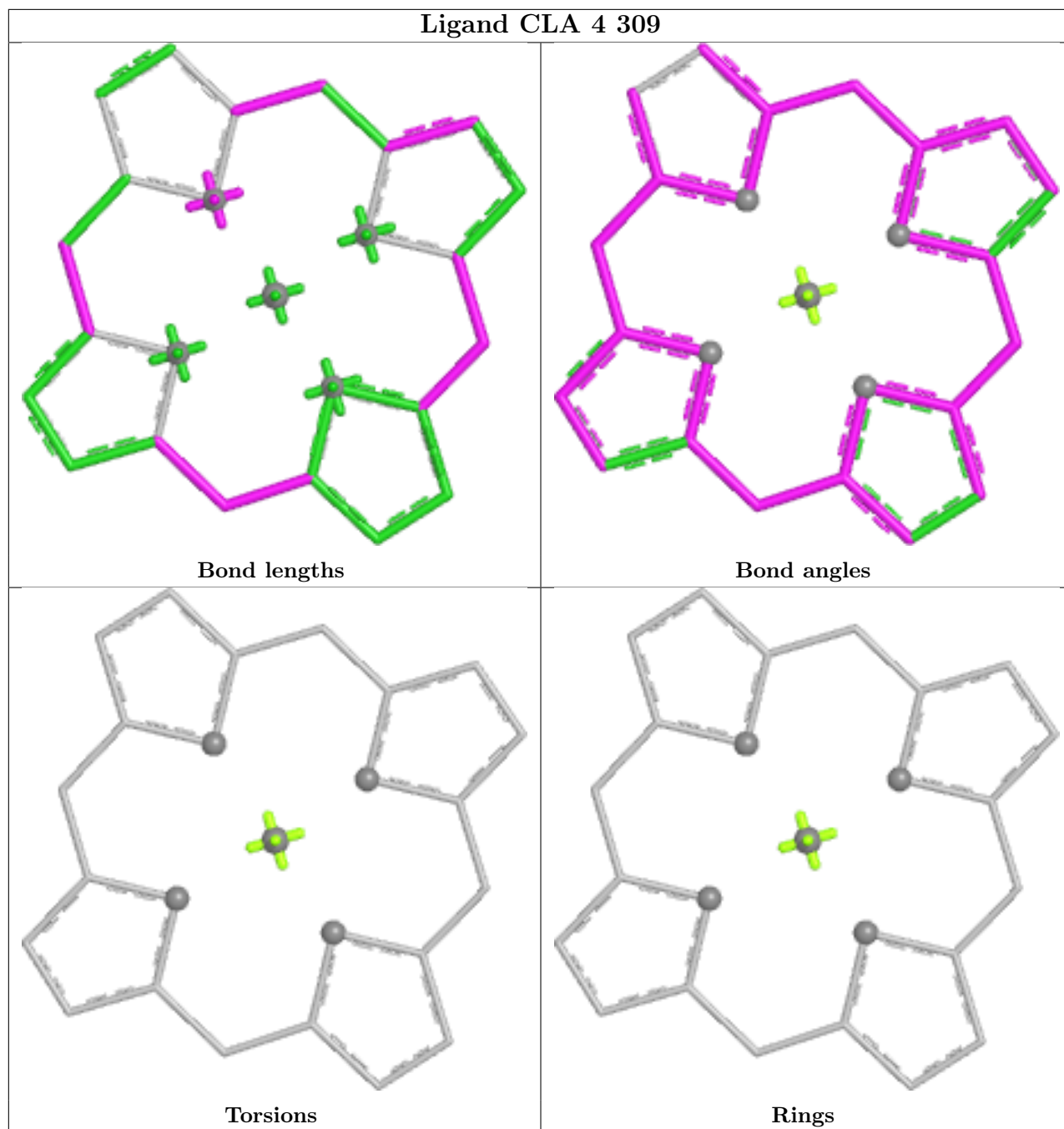


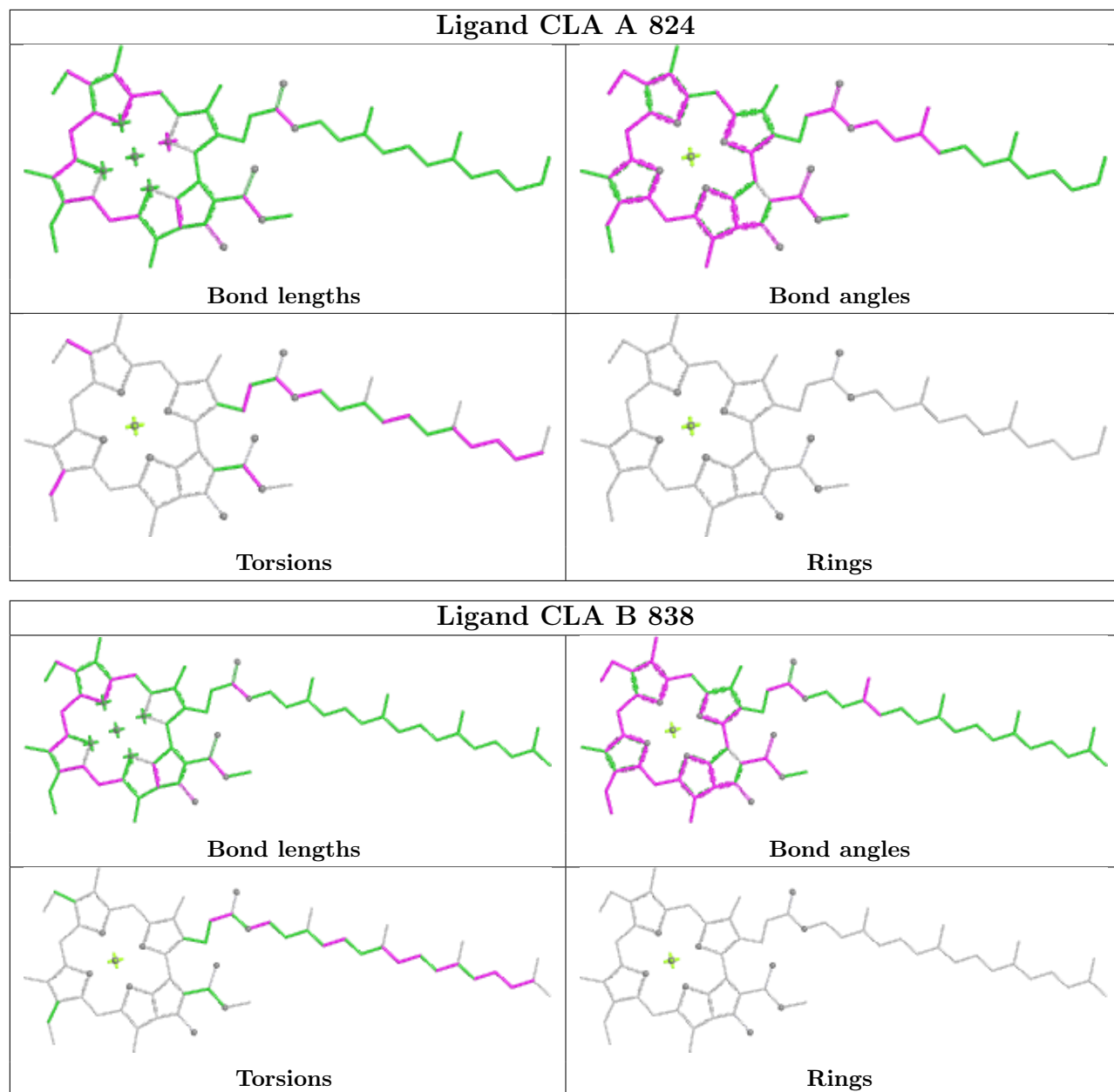
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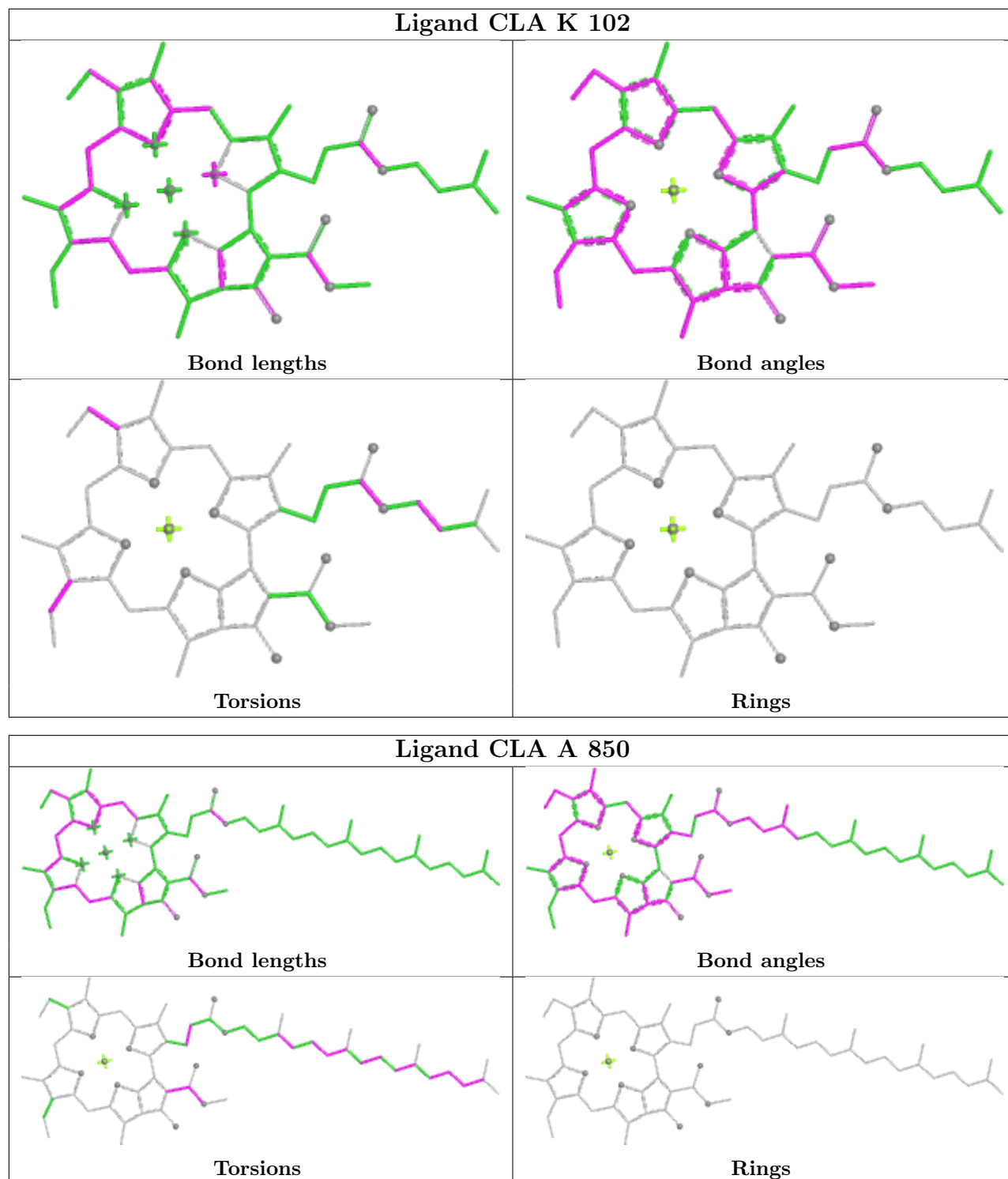


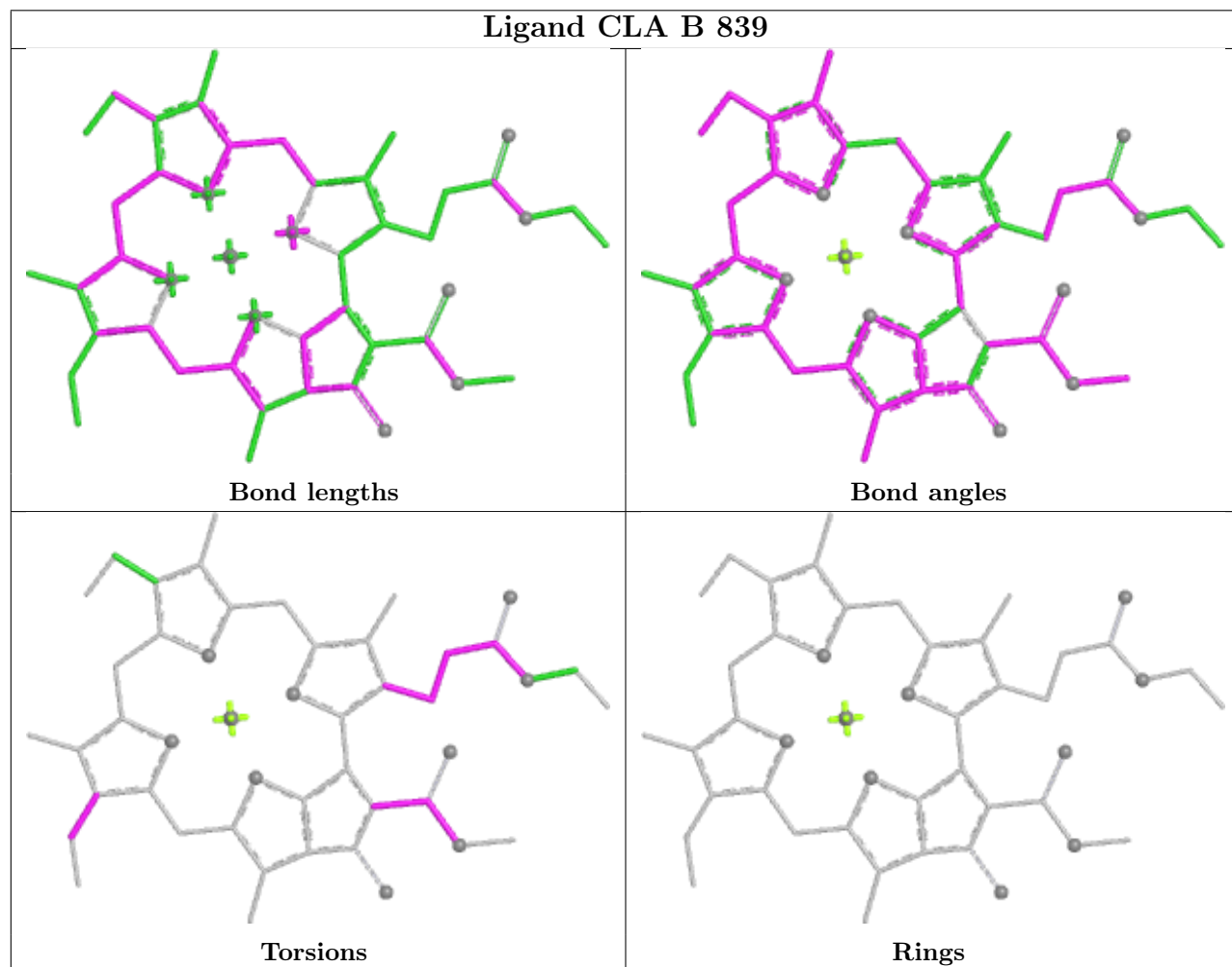
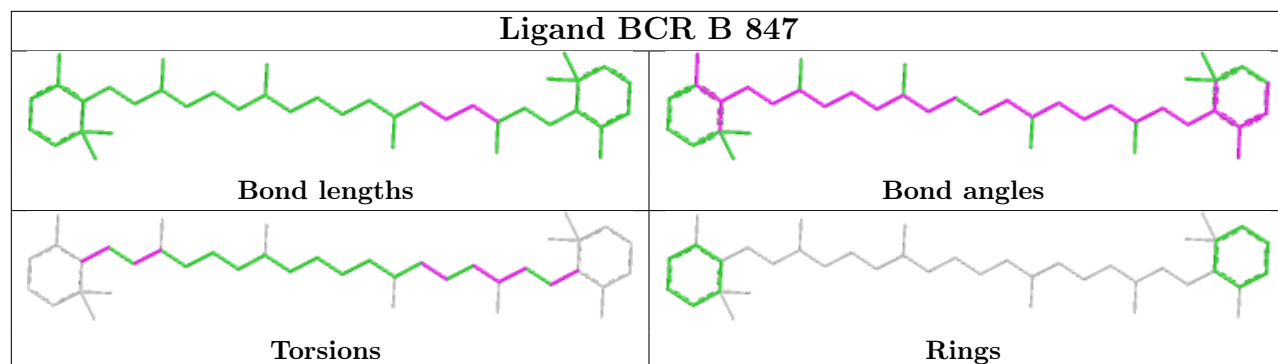


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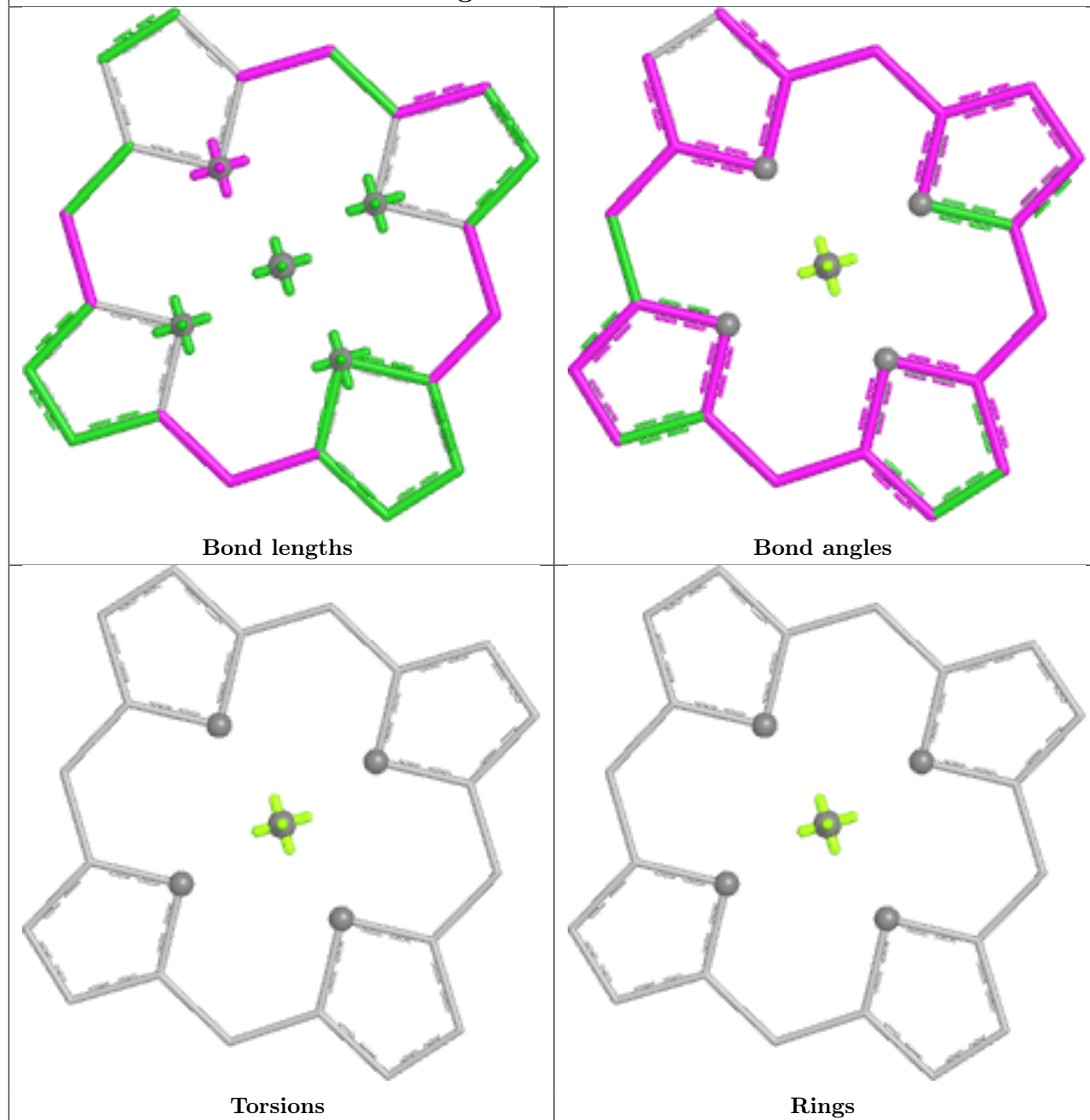


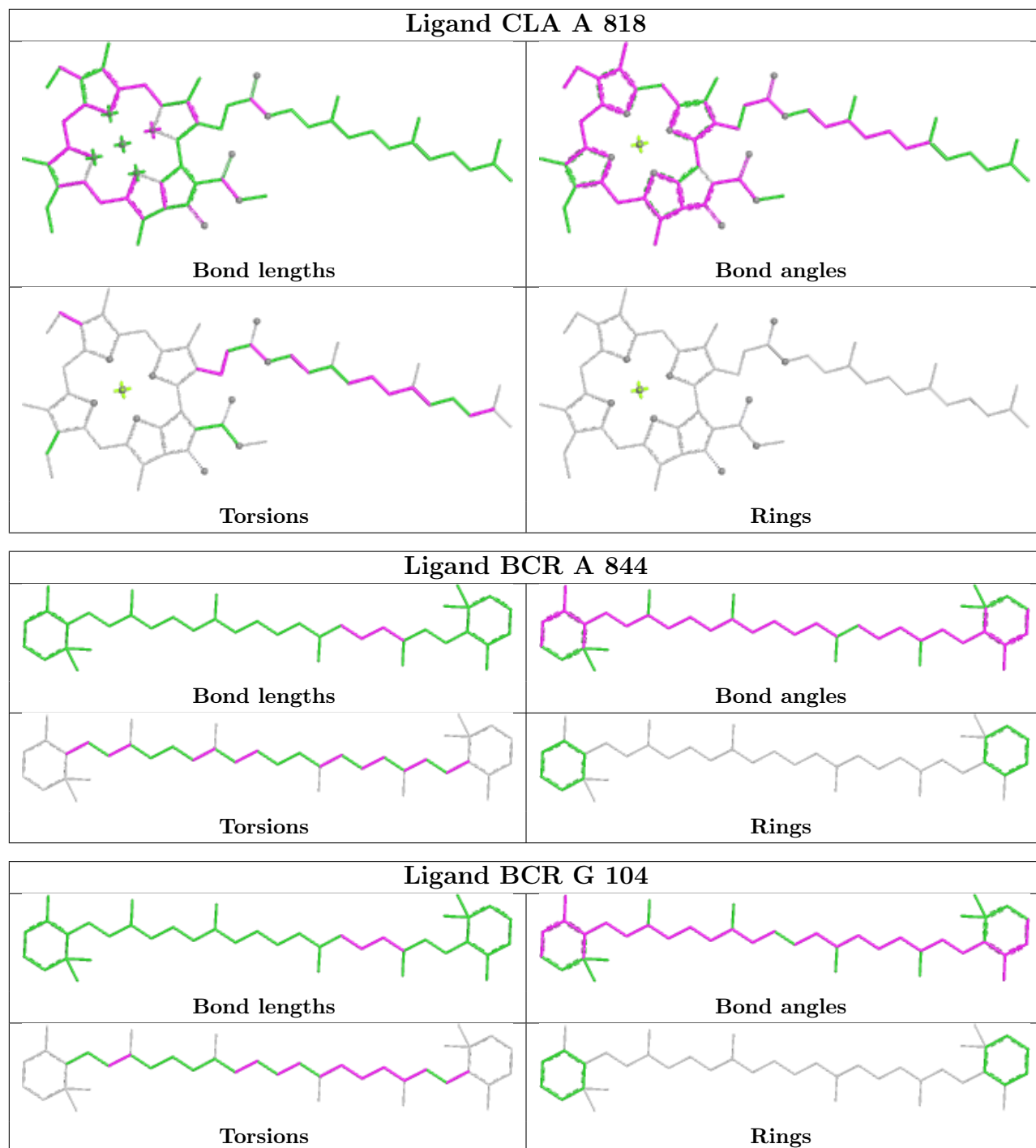


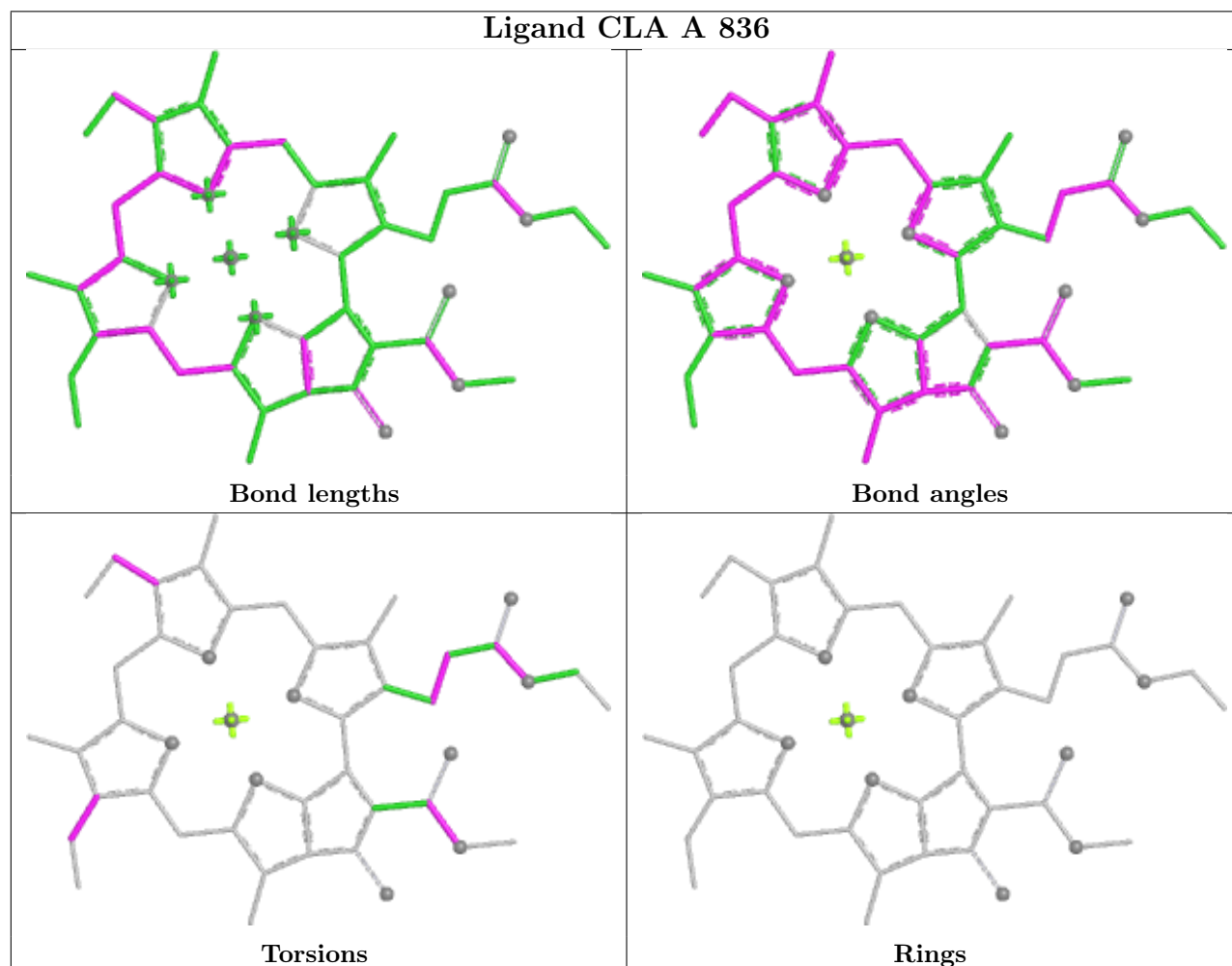
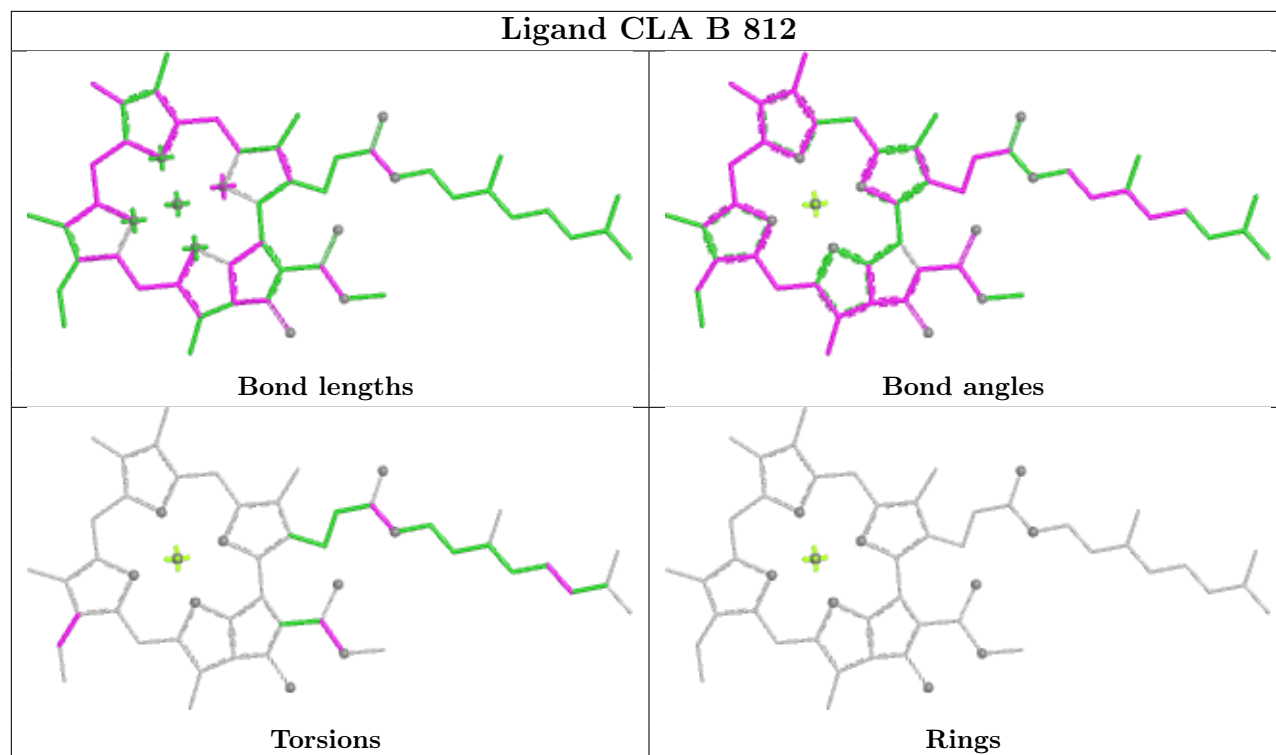


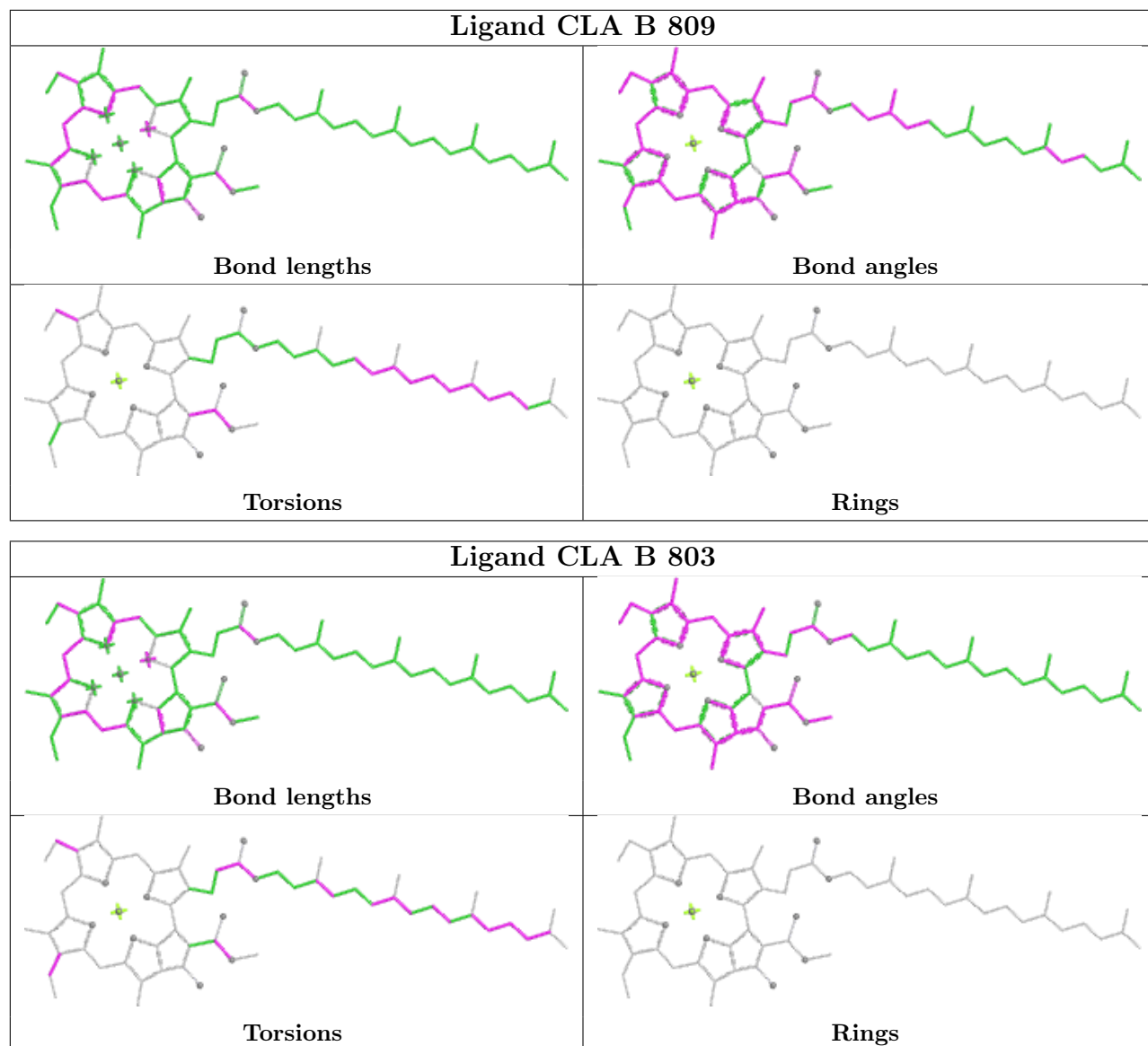


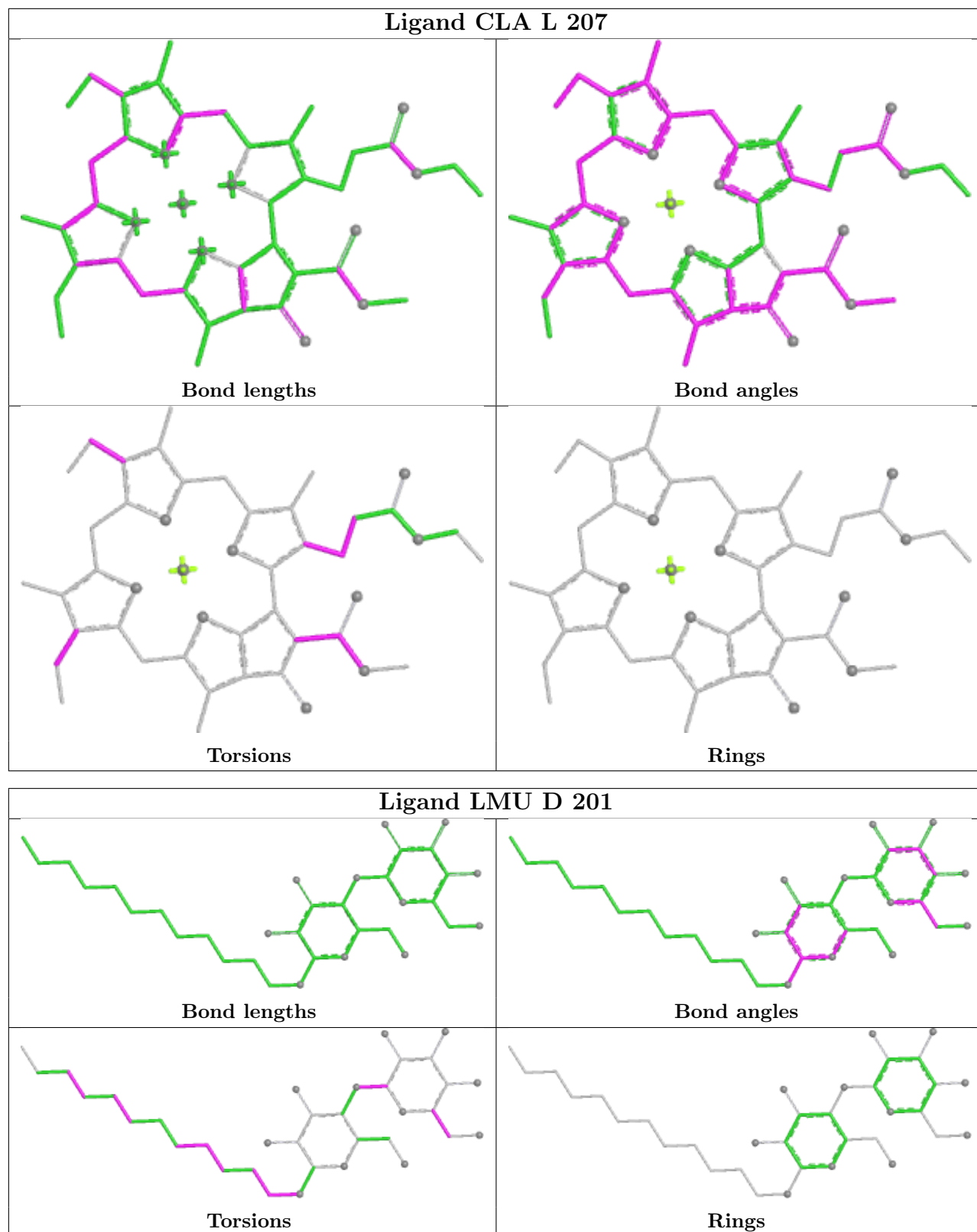
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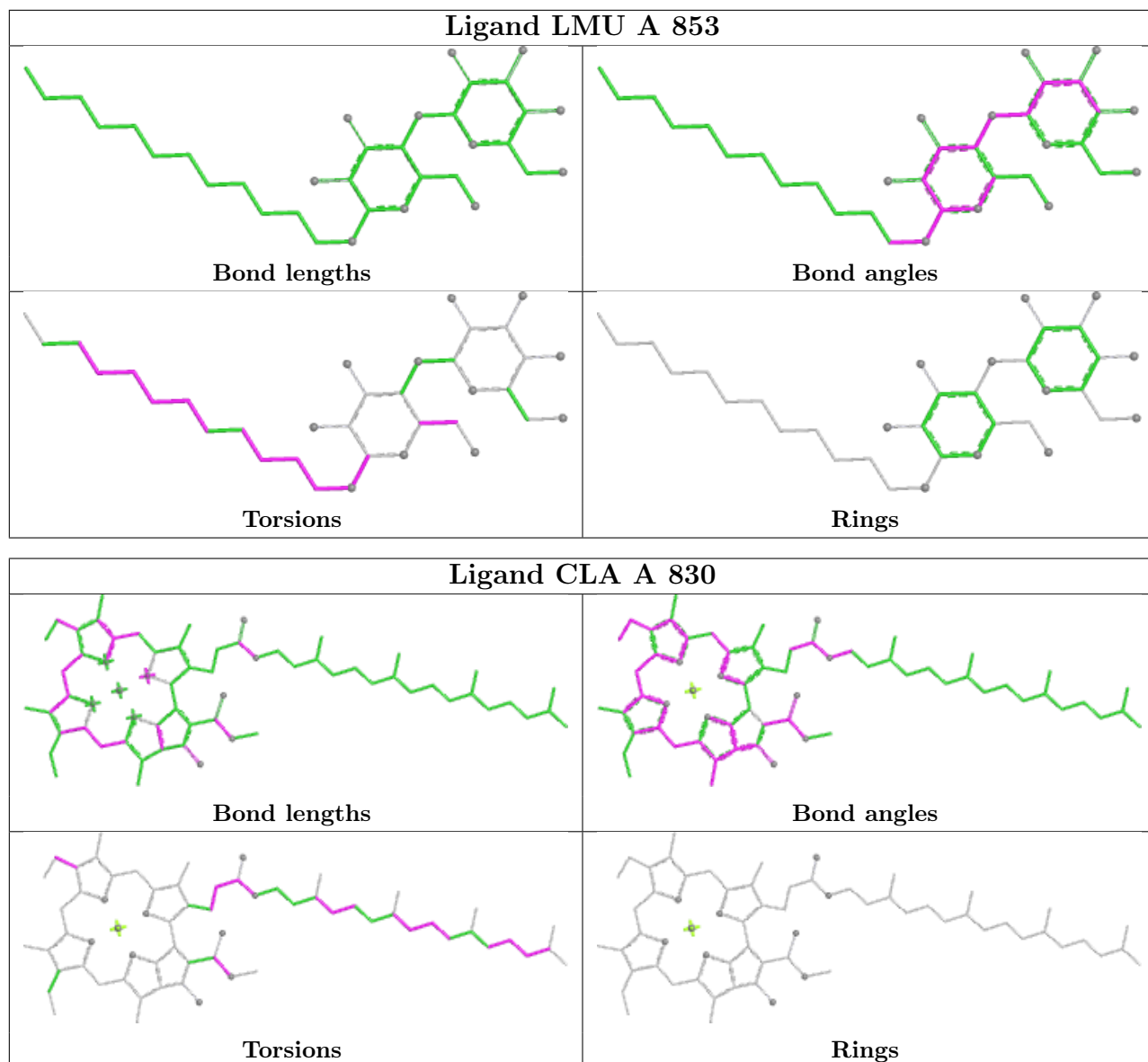


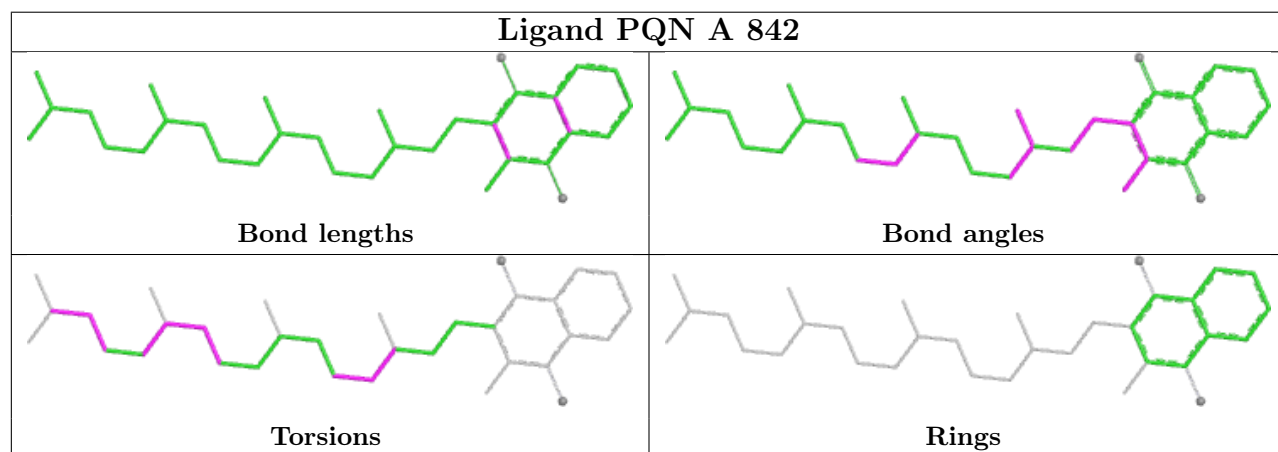
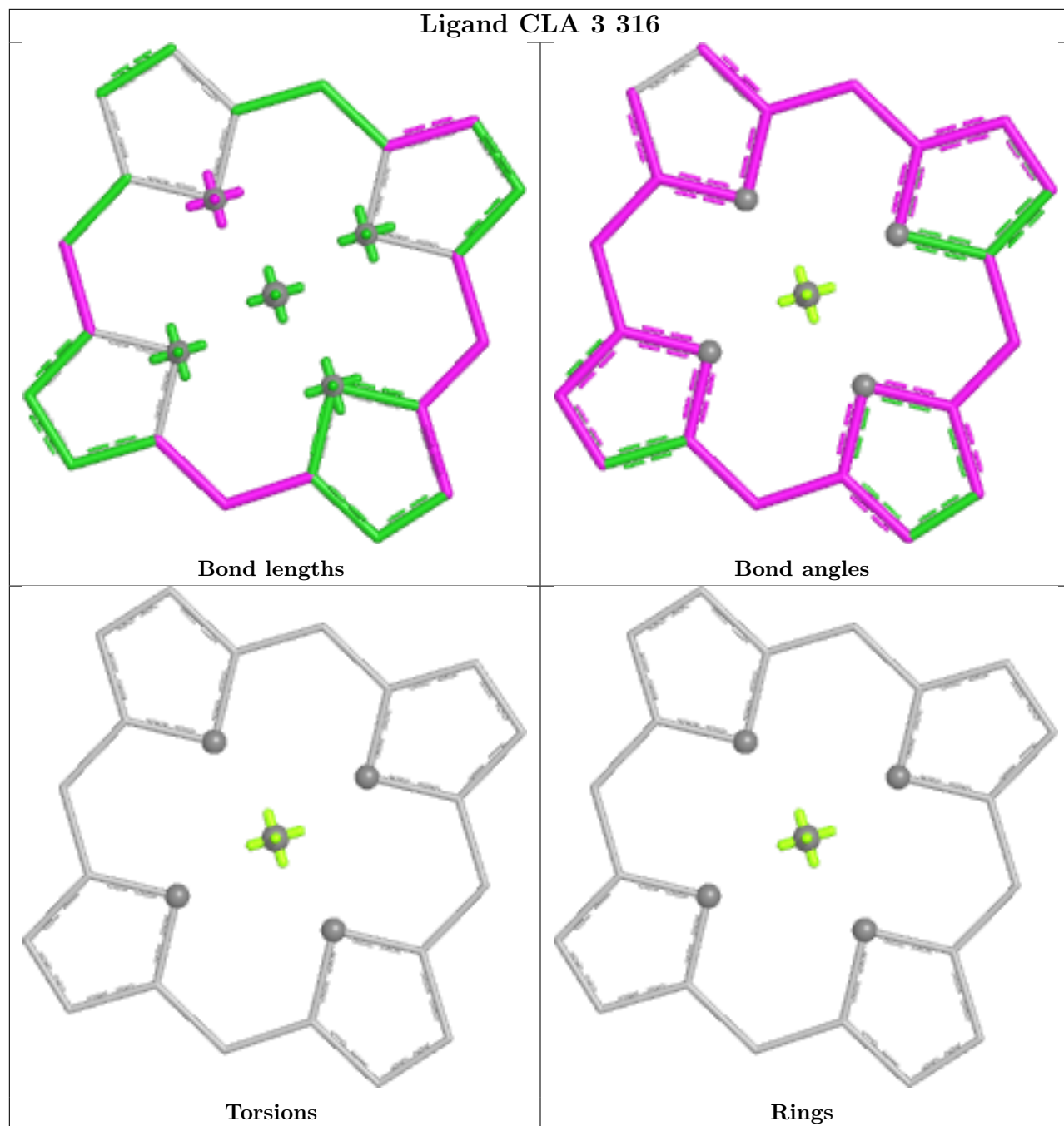


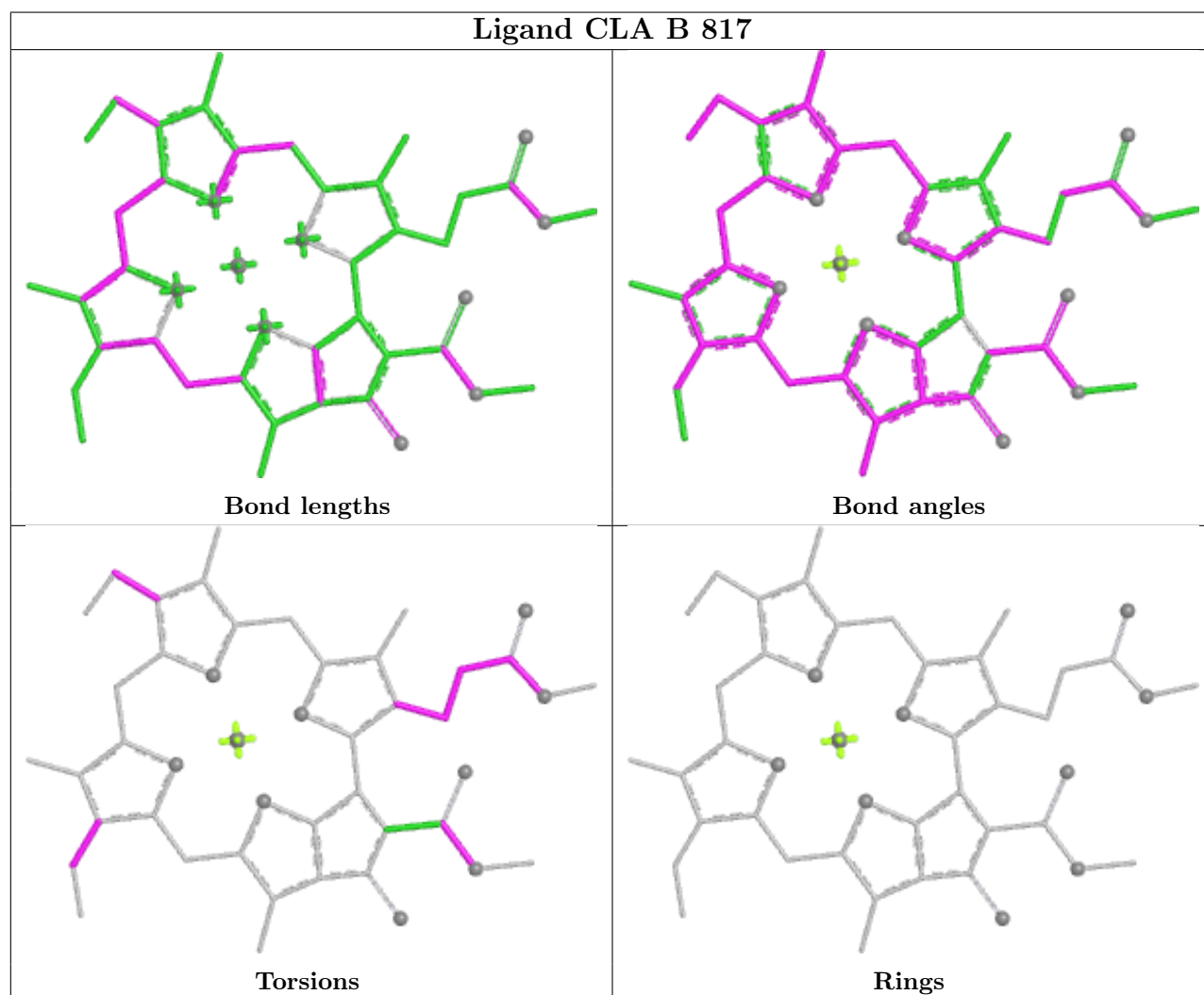
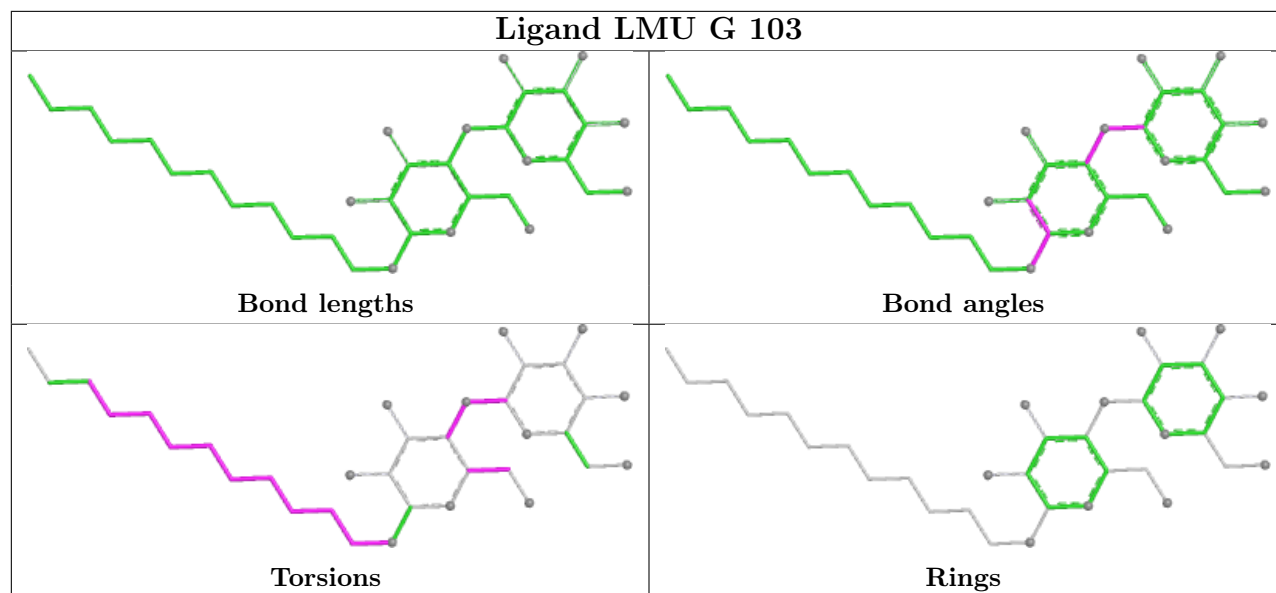


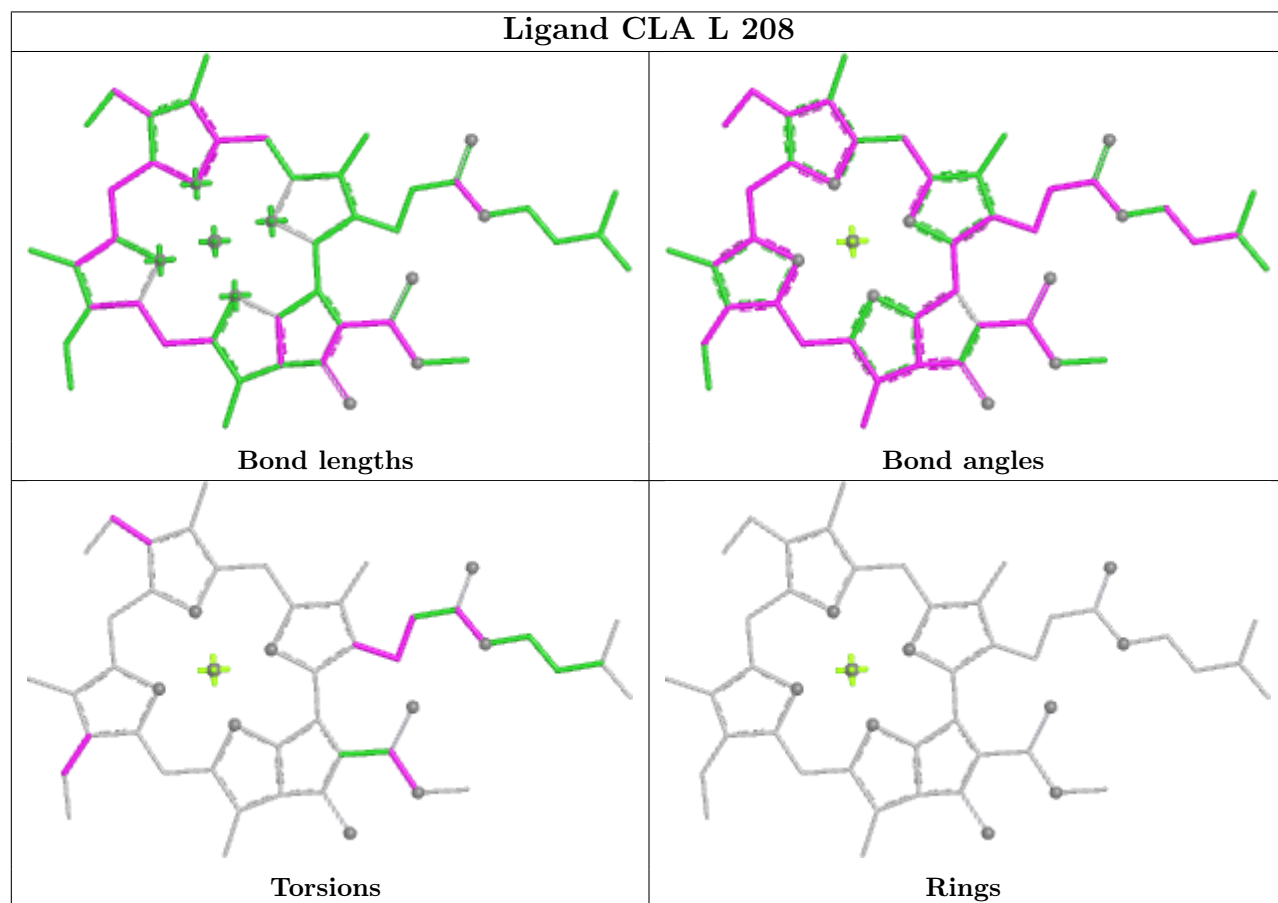
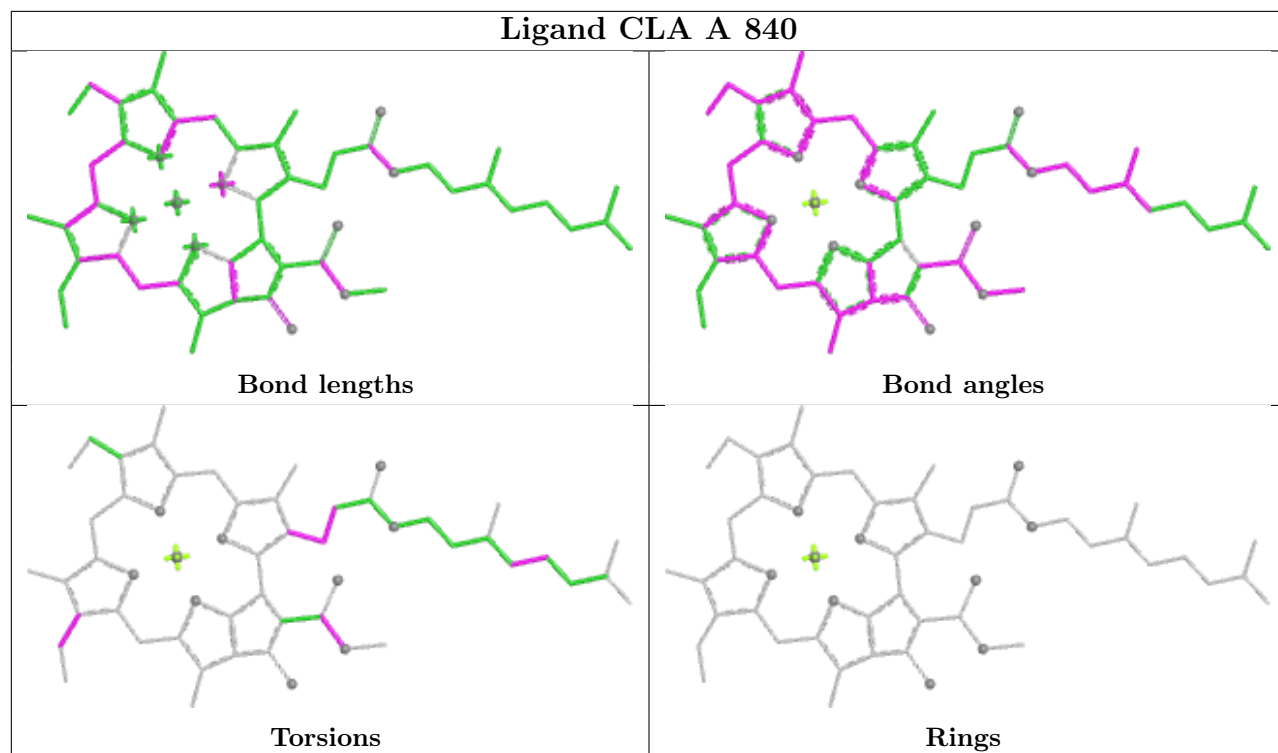


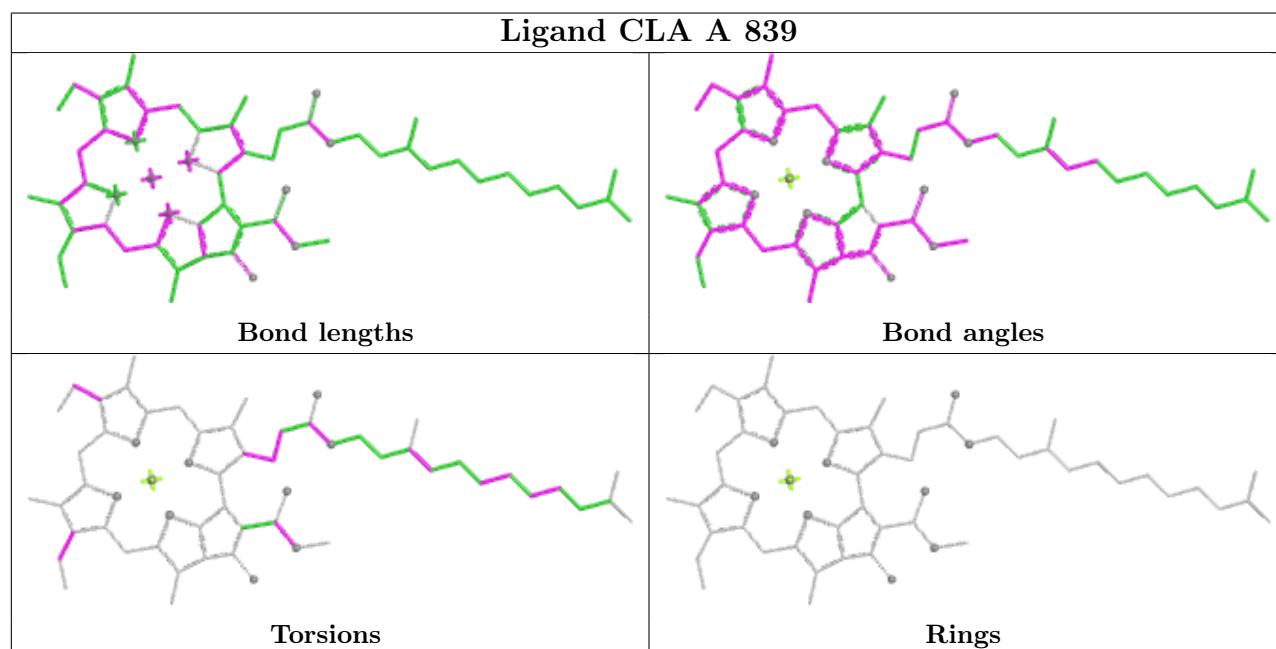
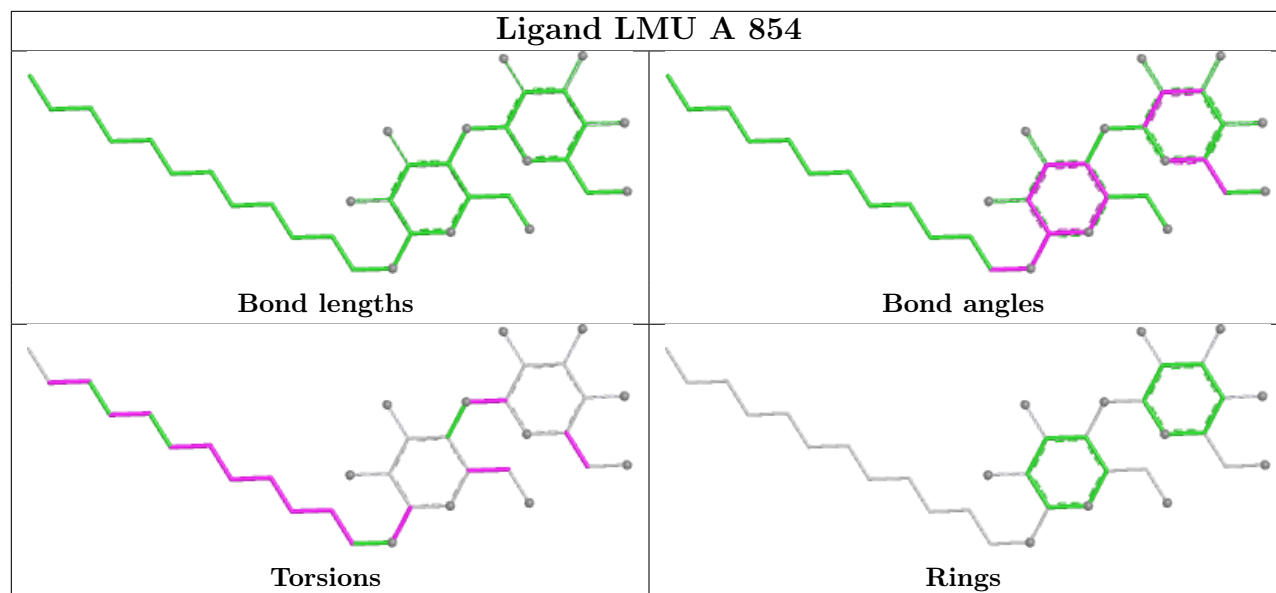


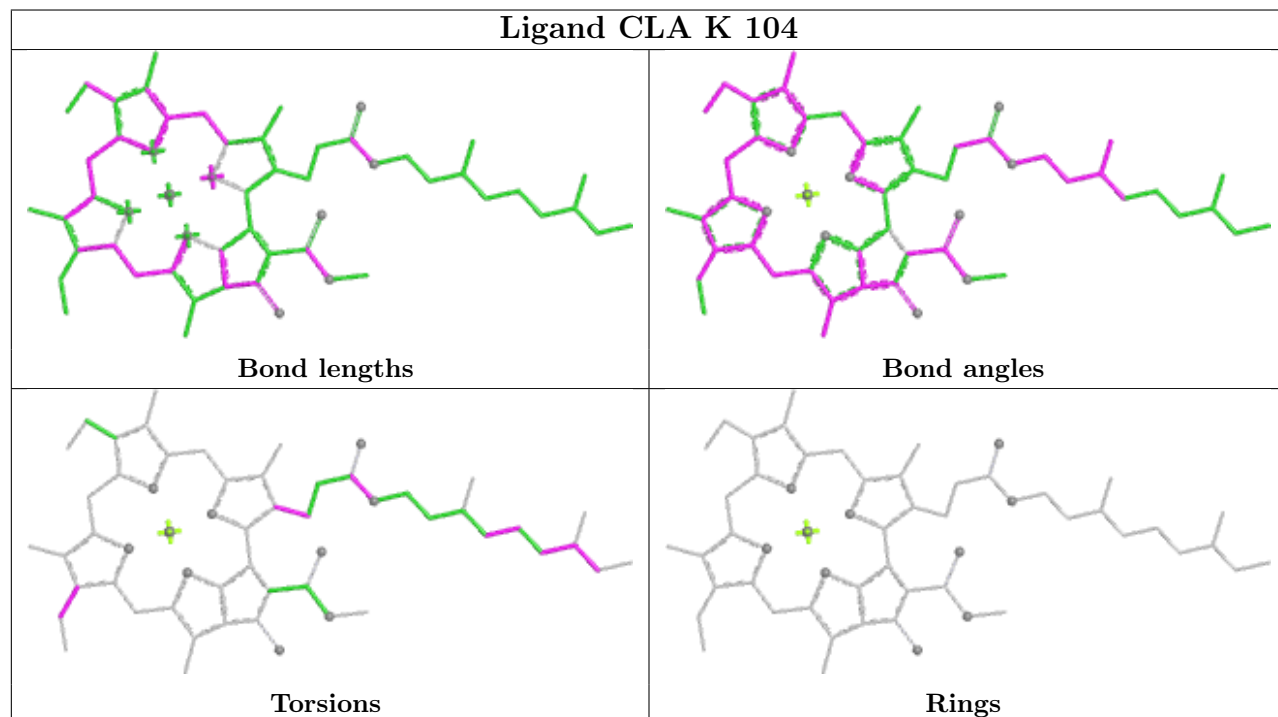
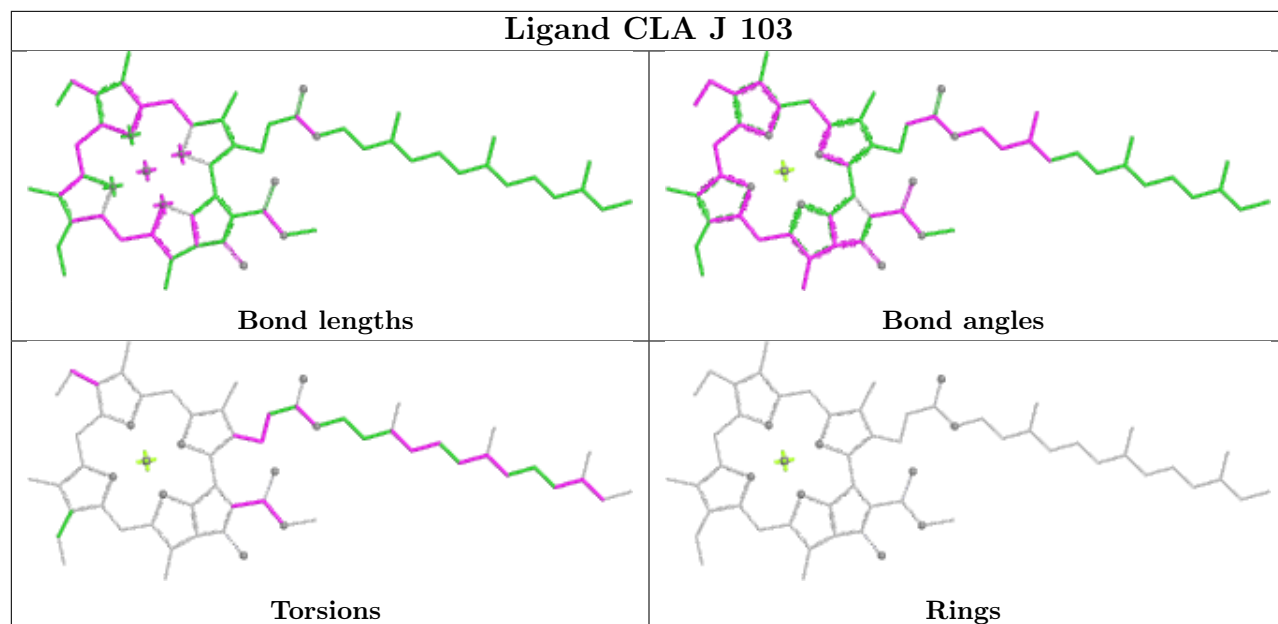


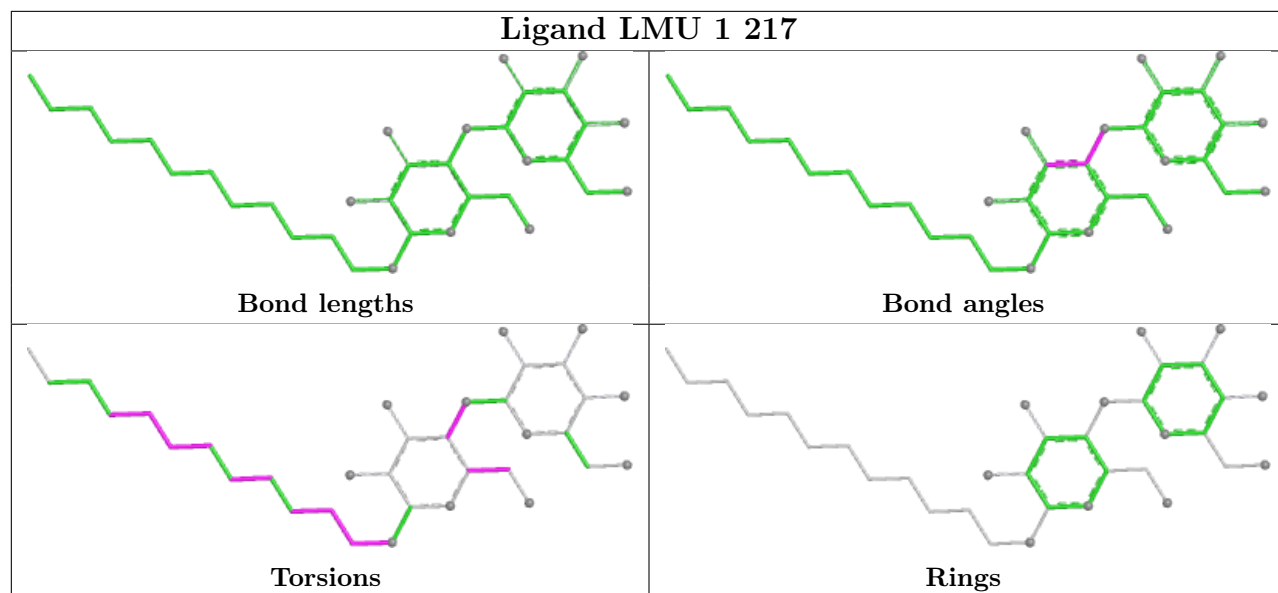




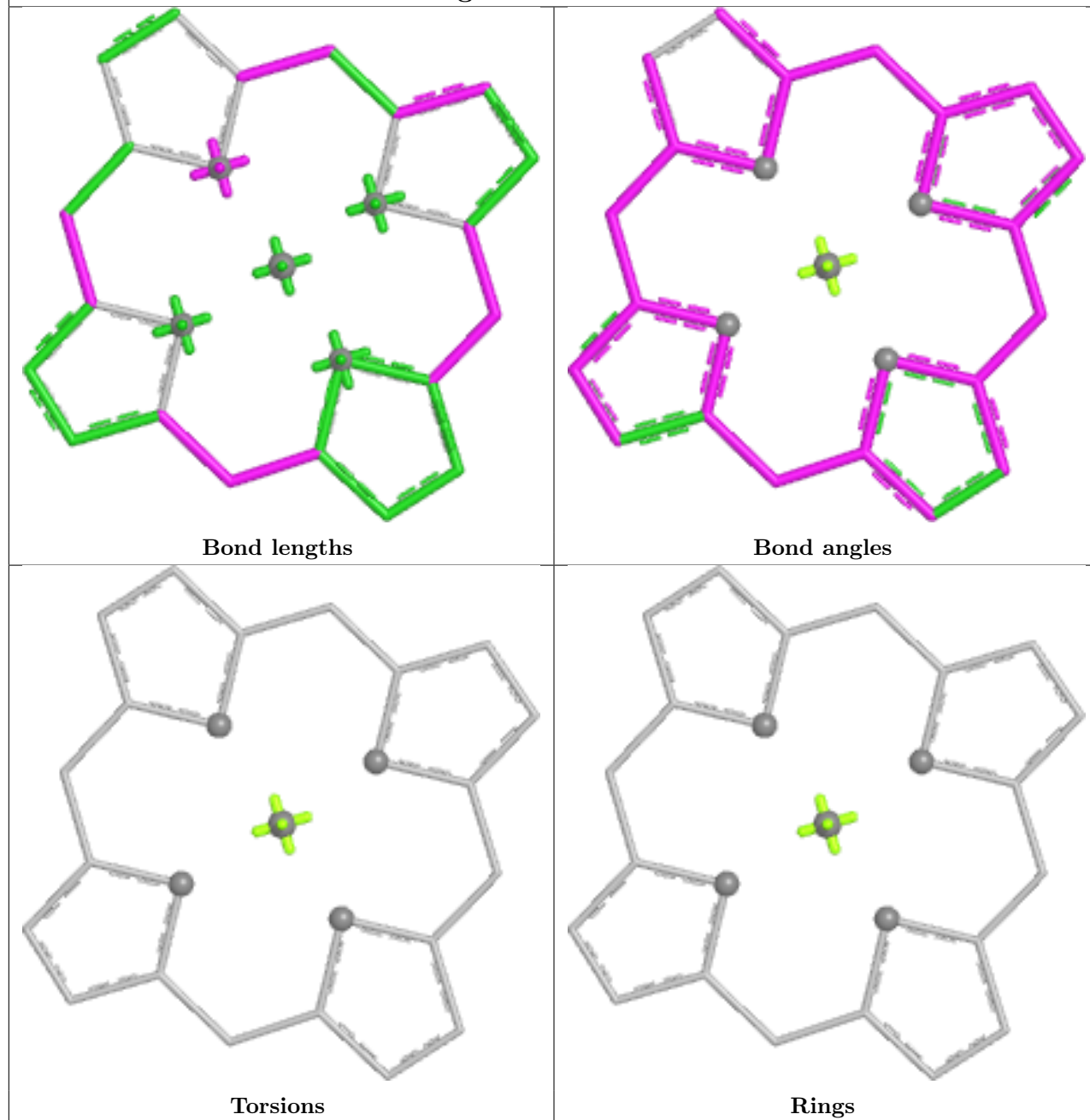


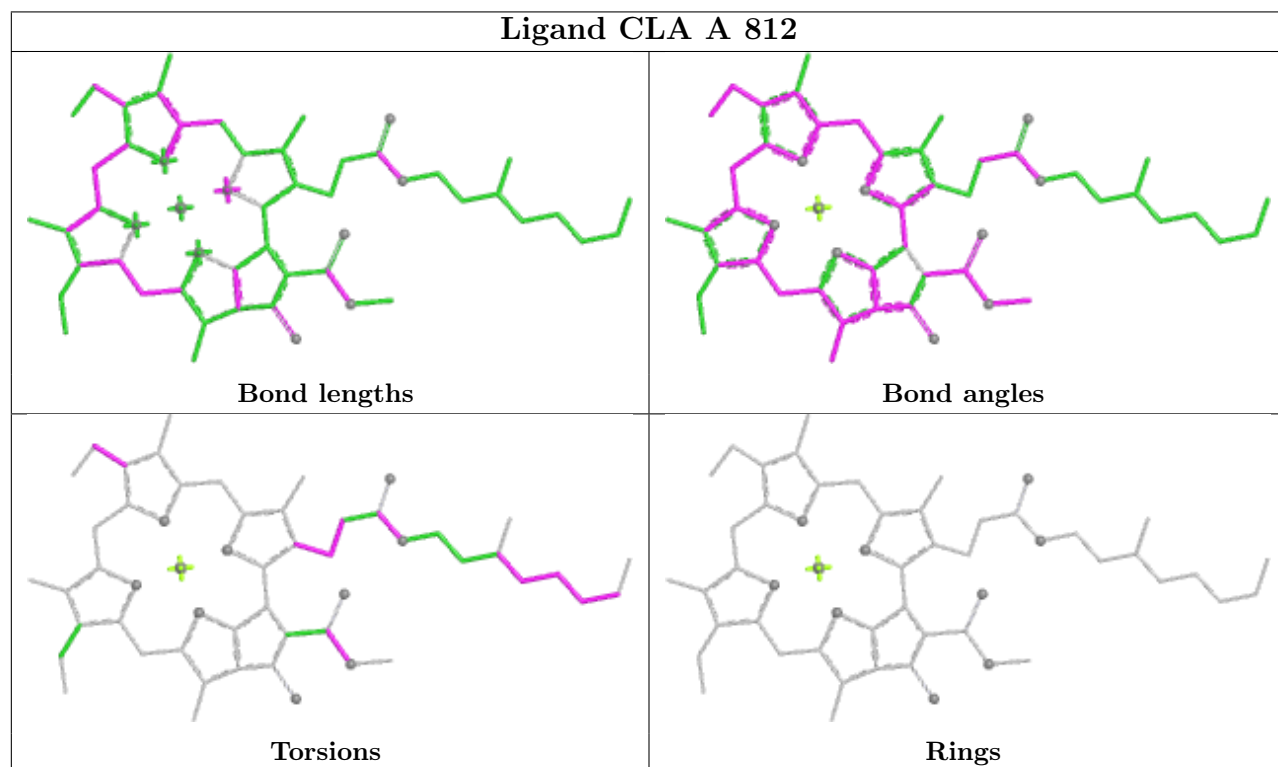
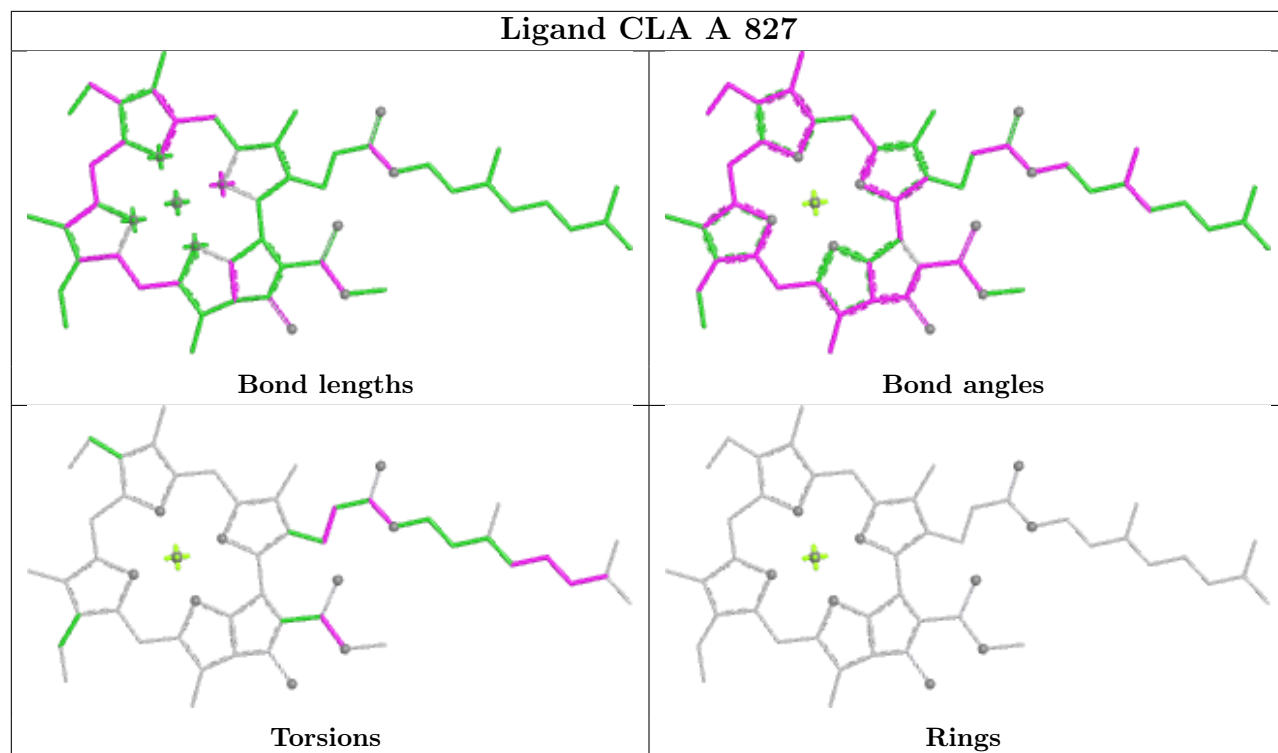


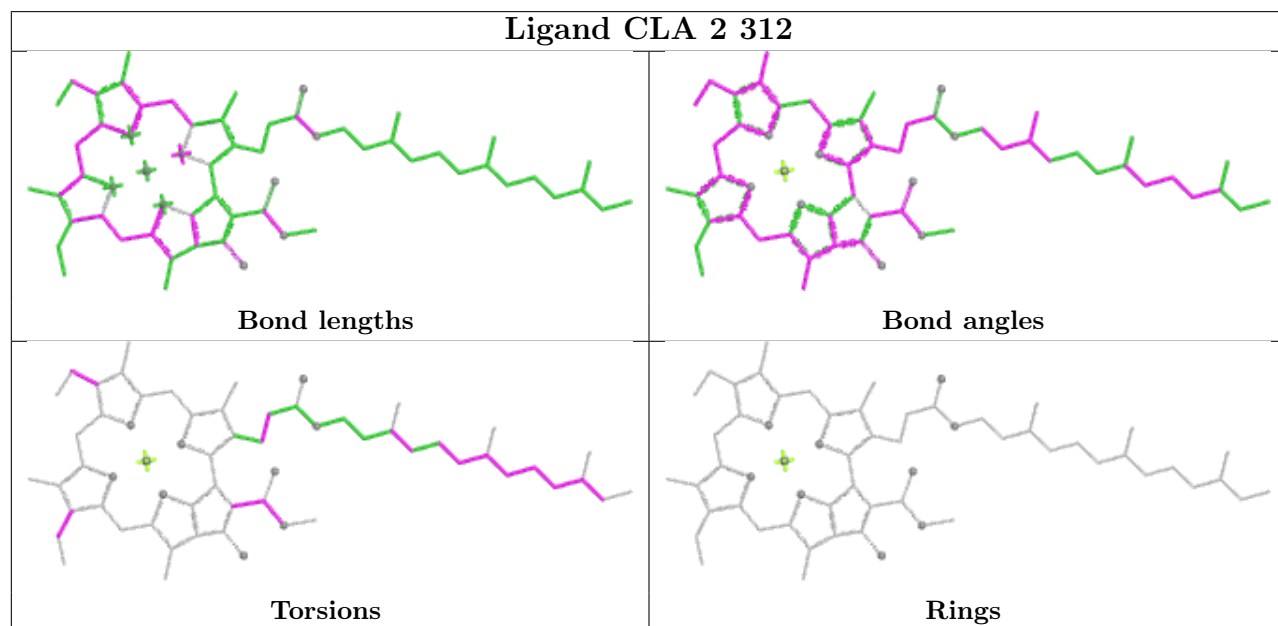
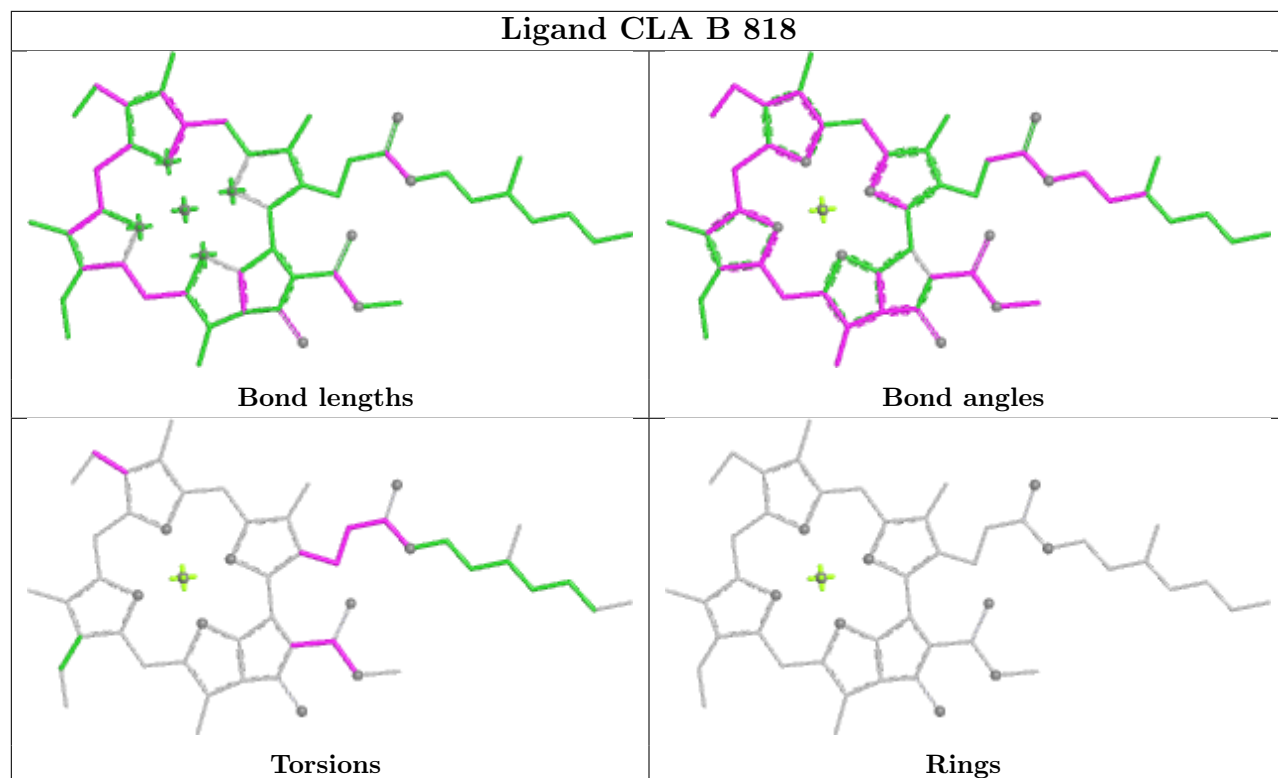


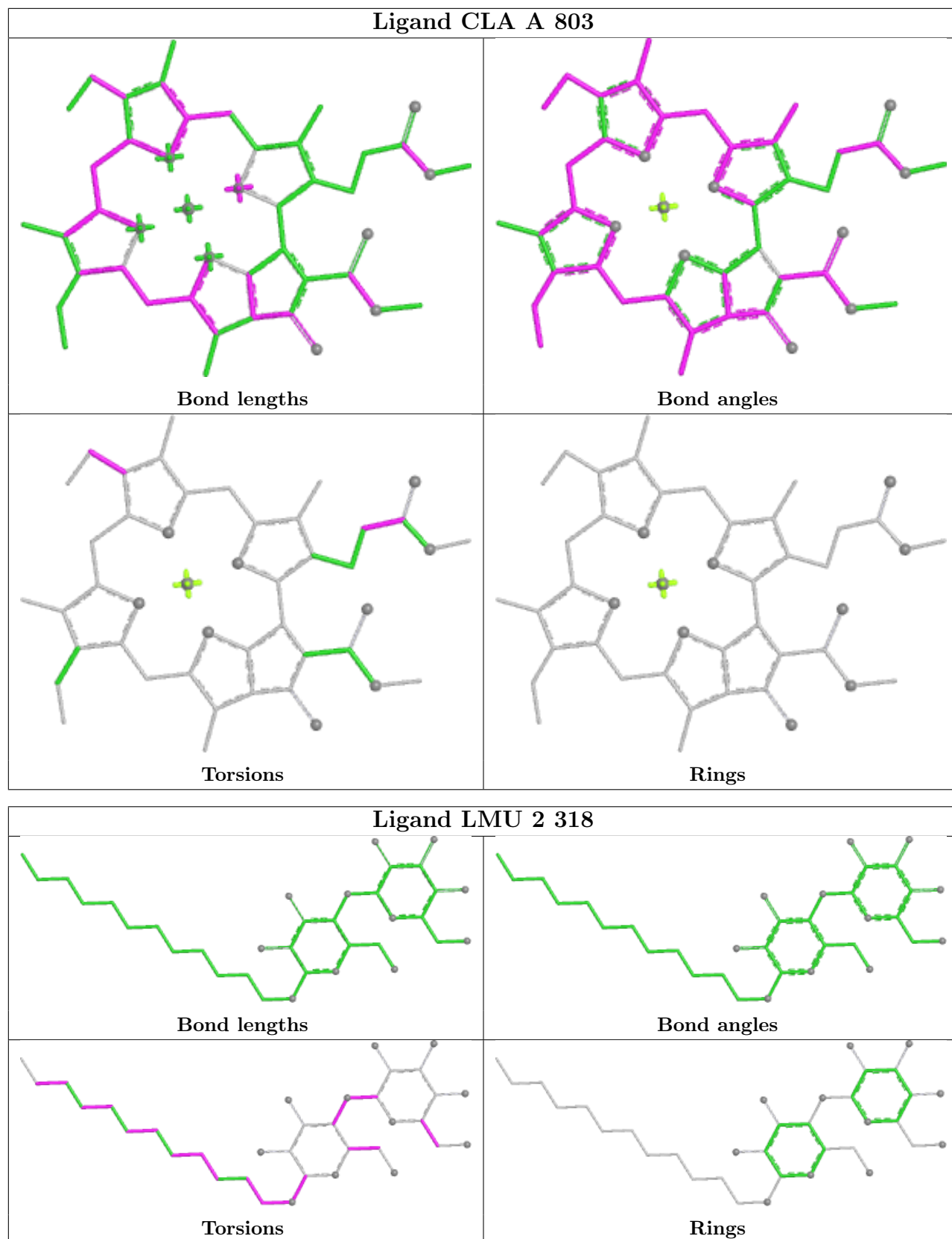


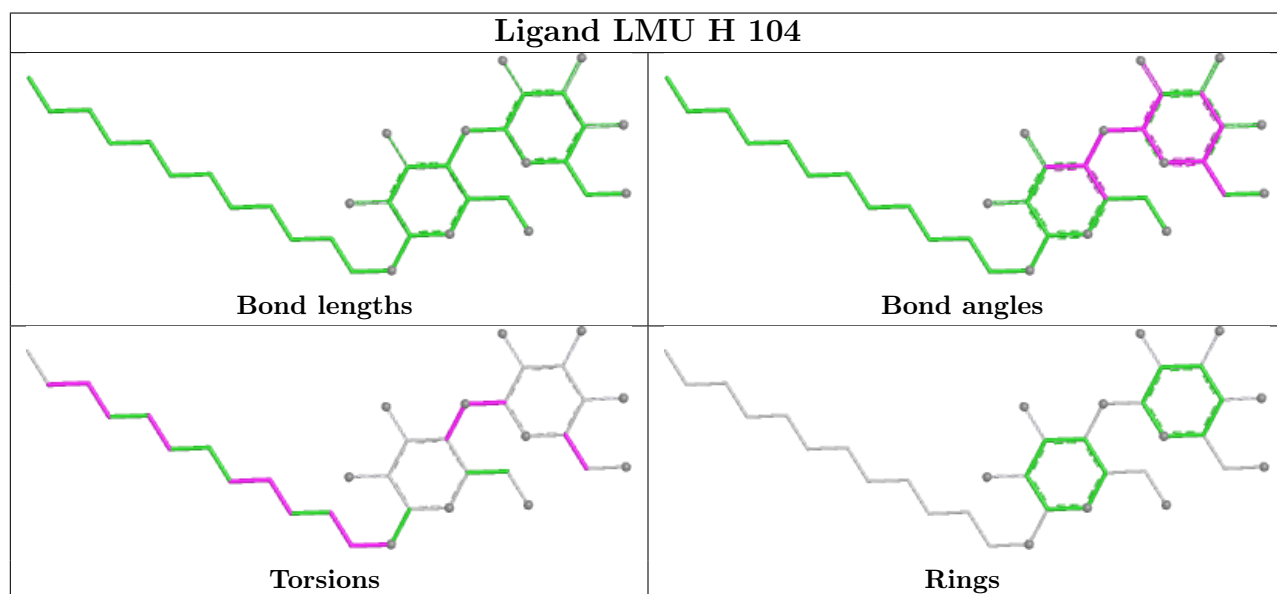
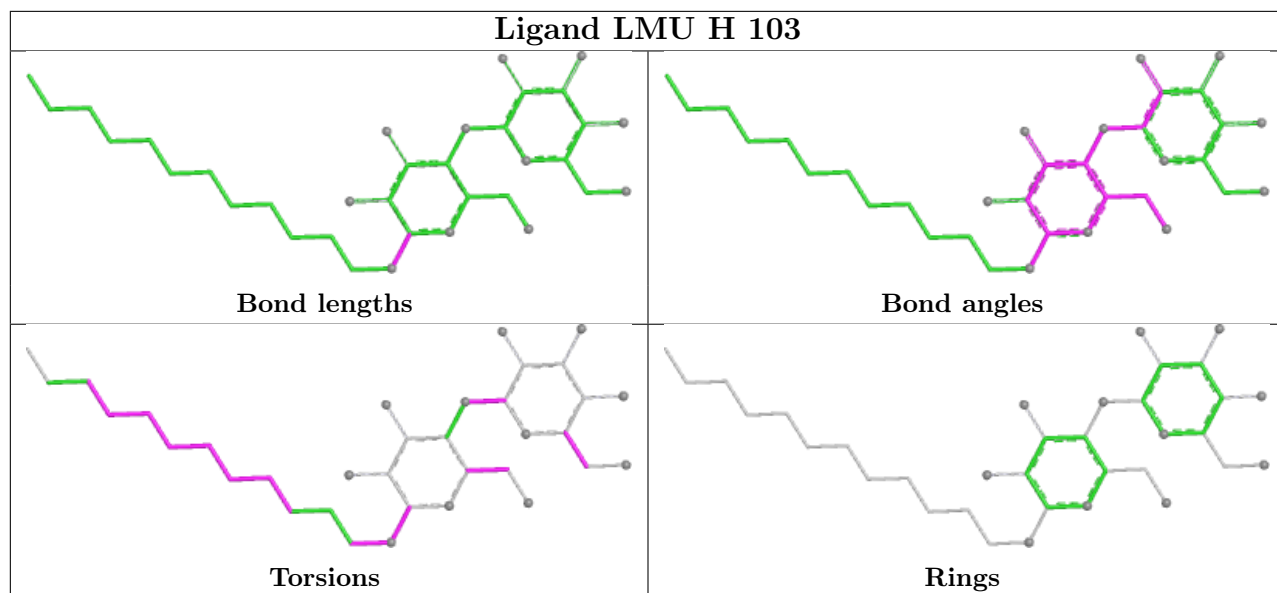
## Ligand CLA 4 312

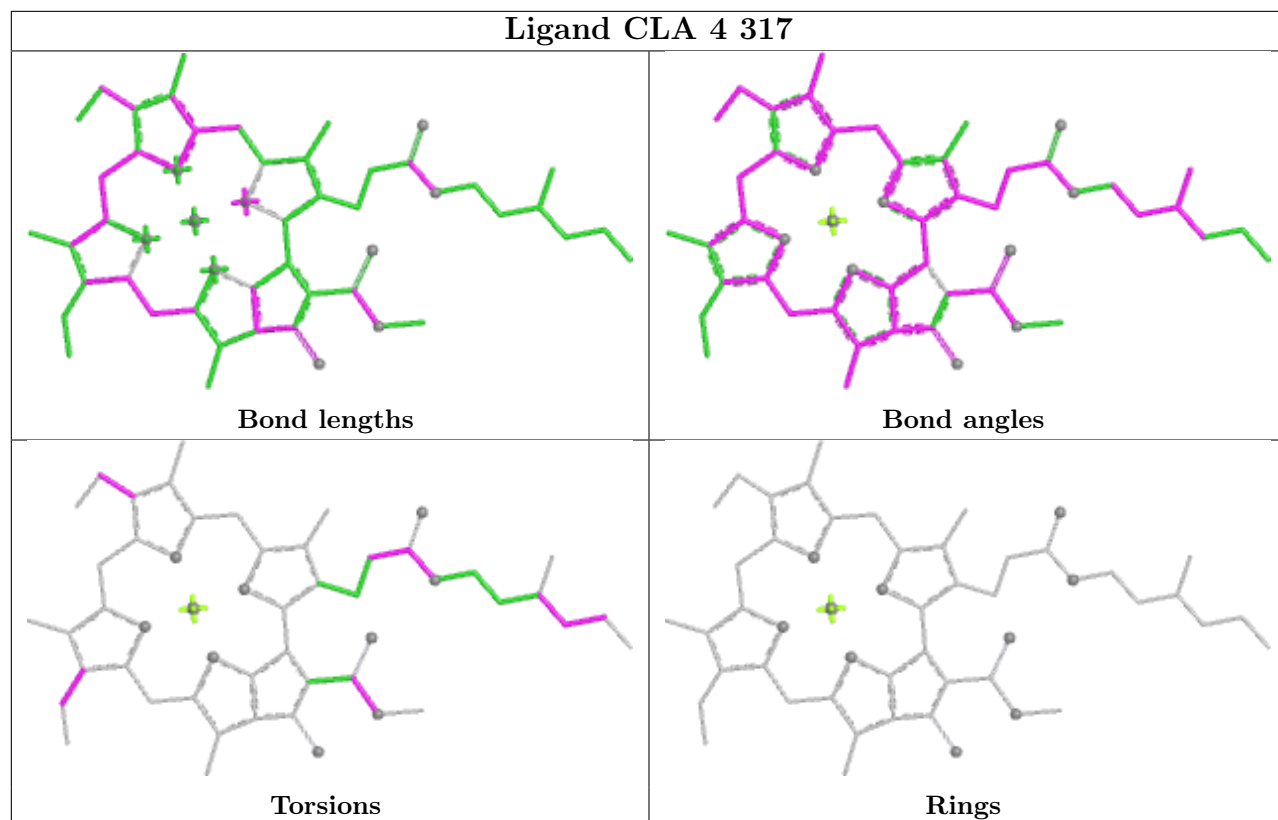




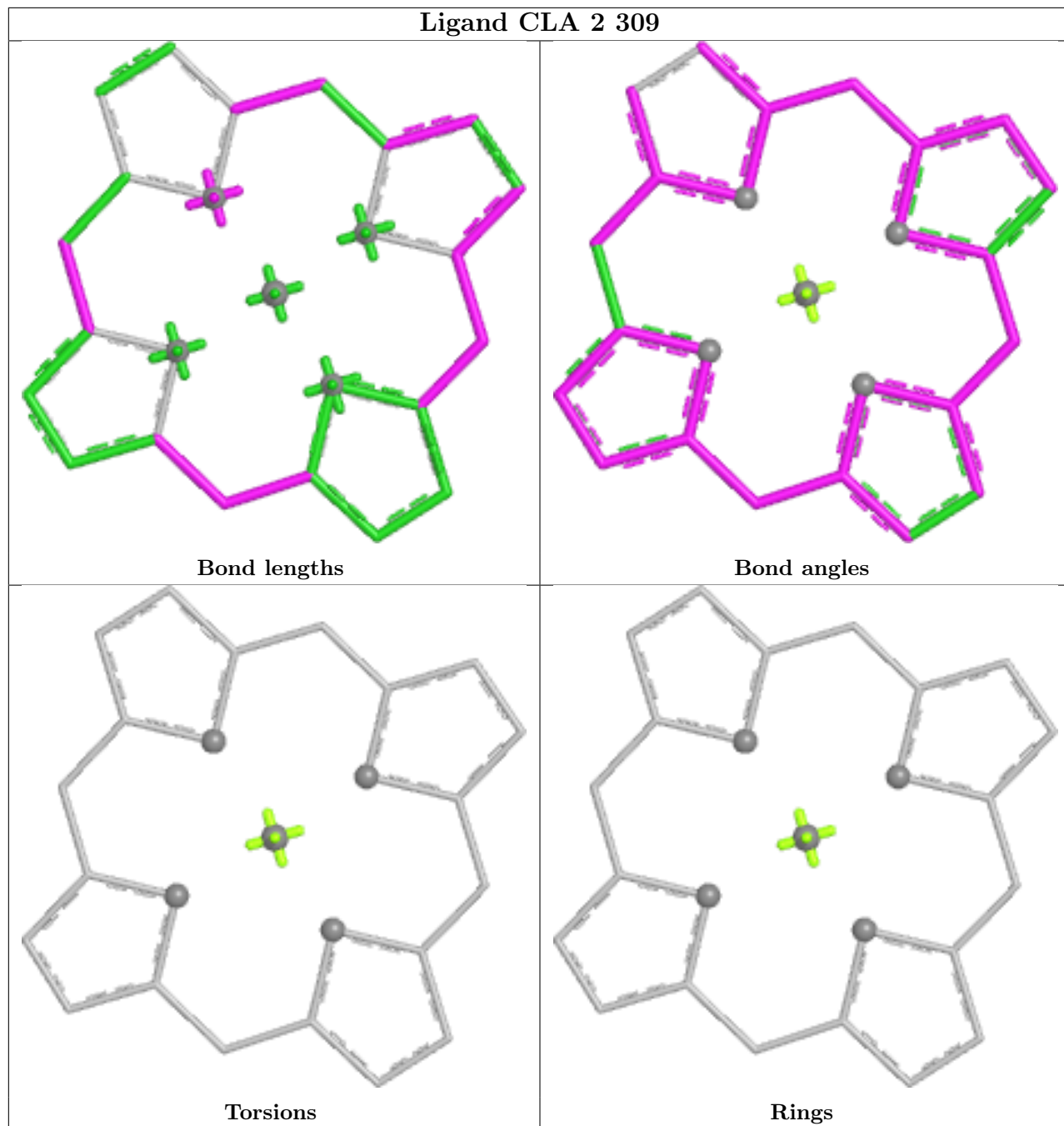


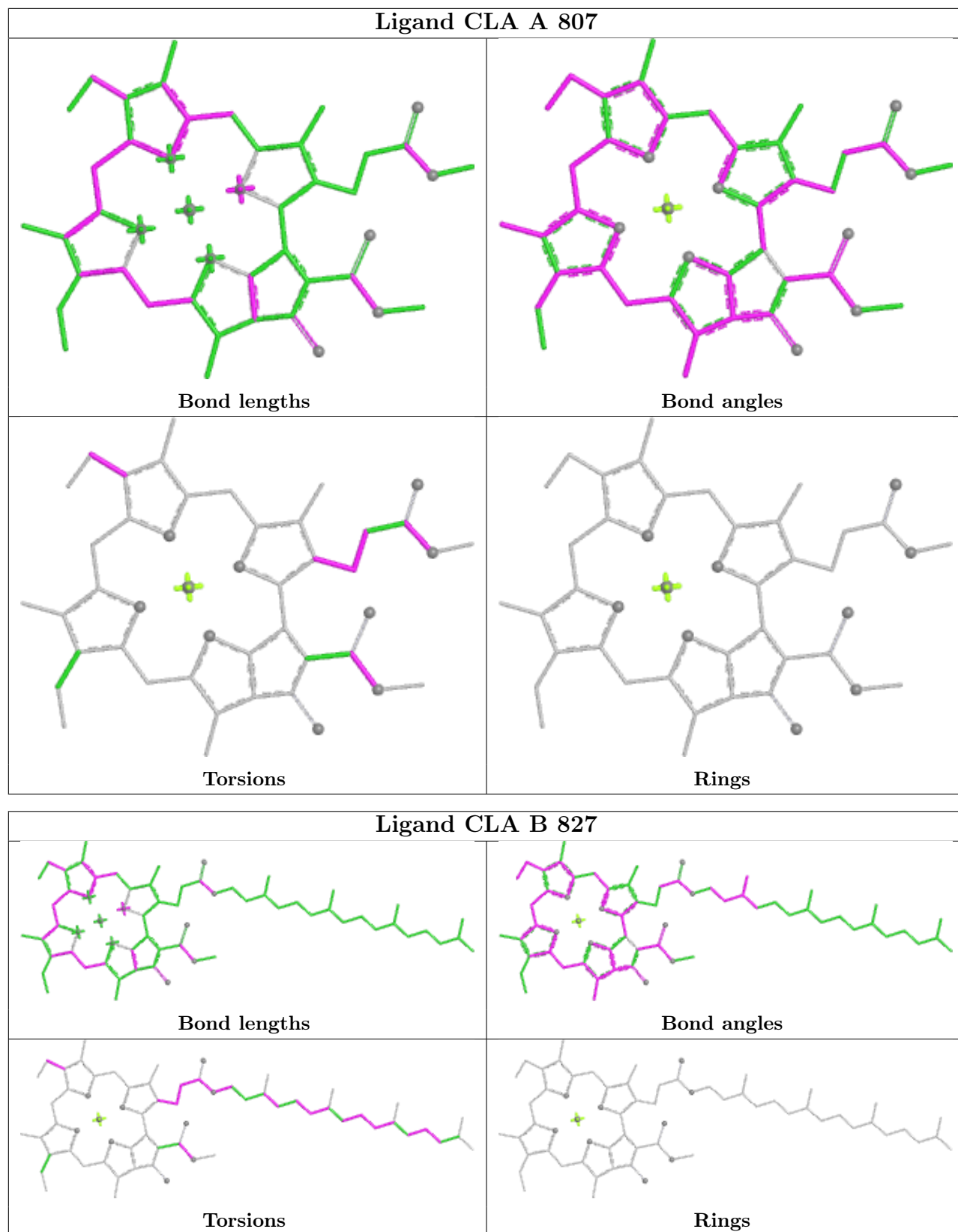


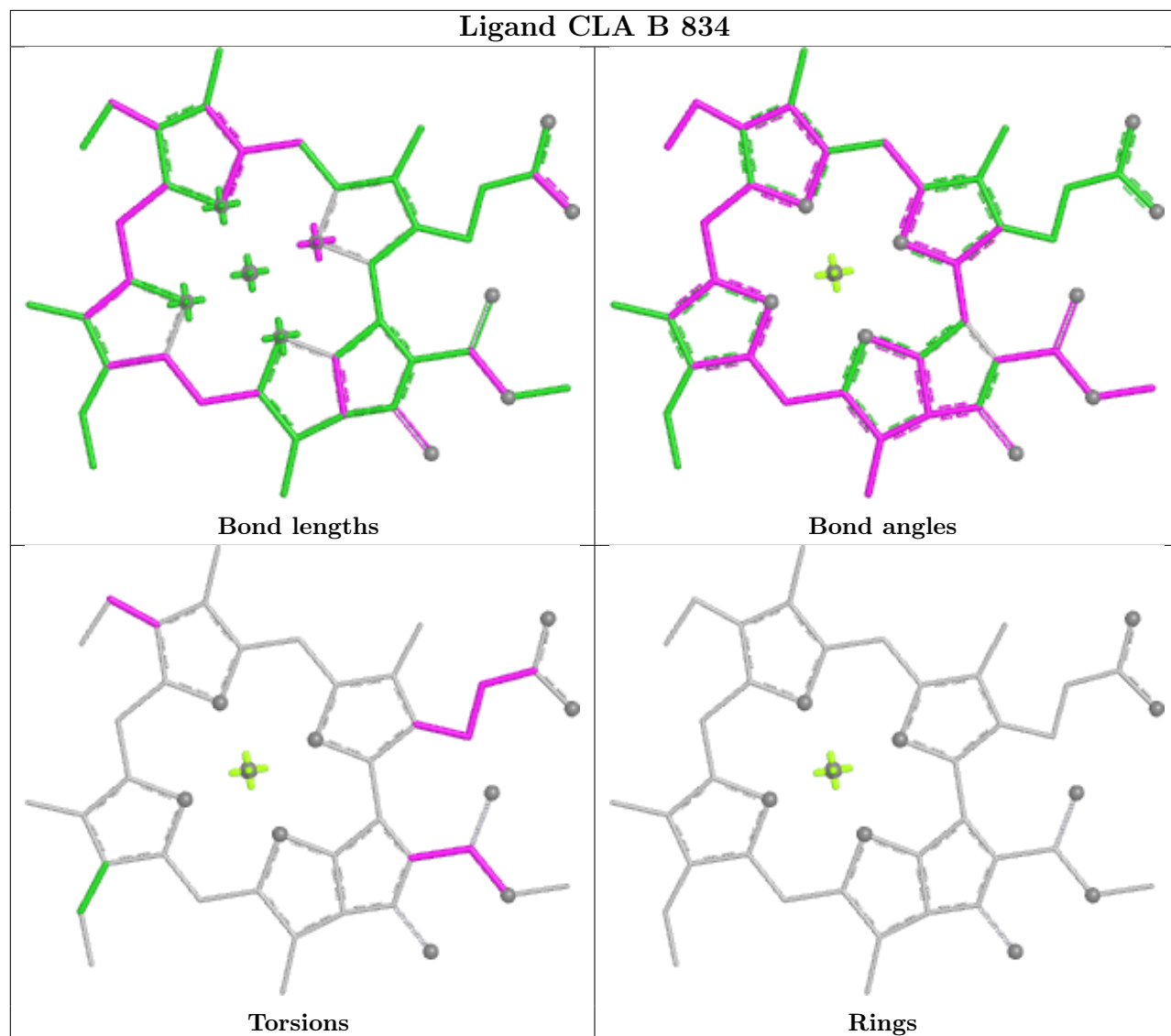


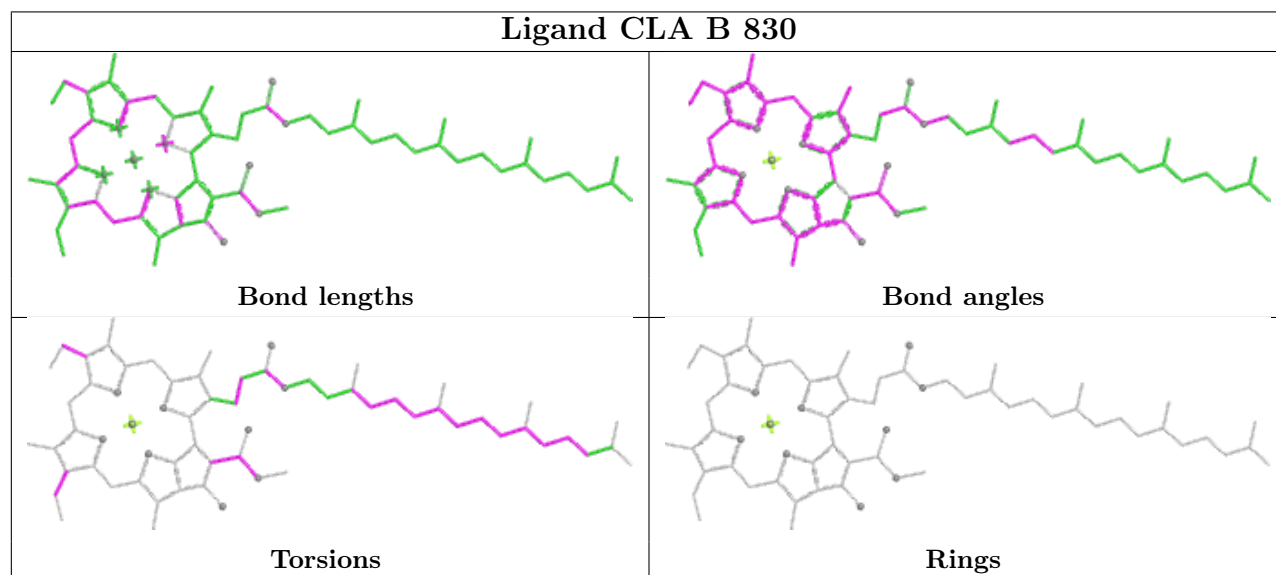
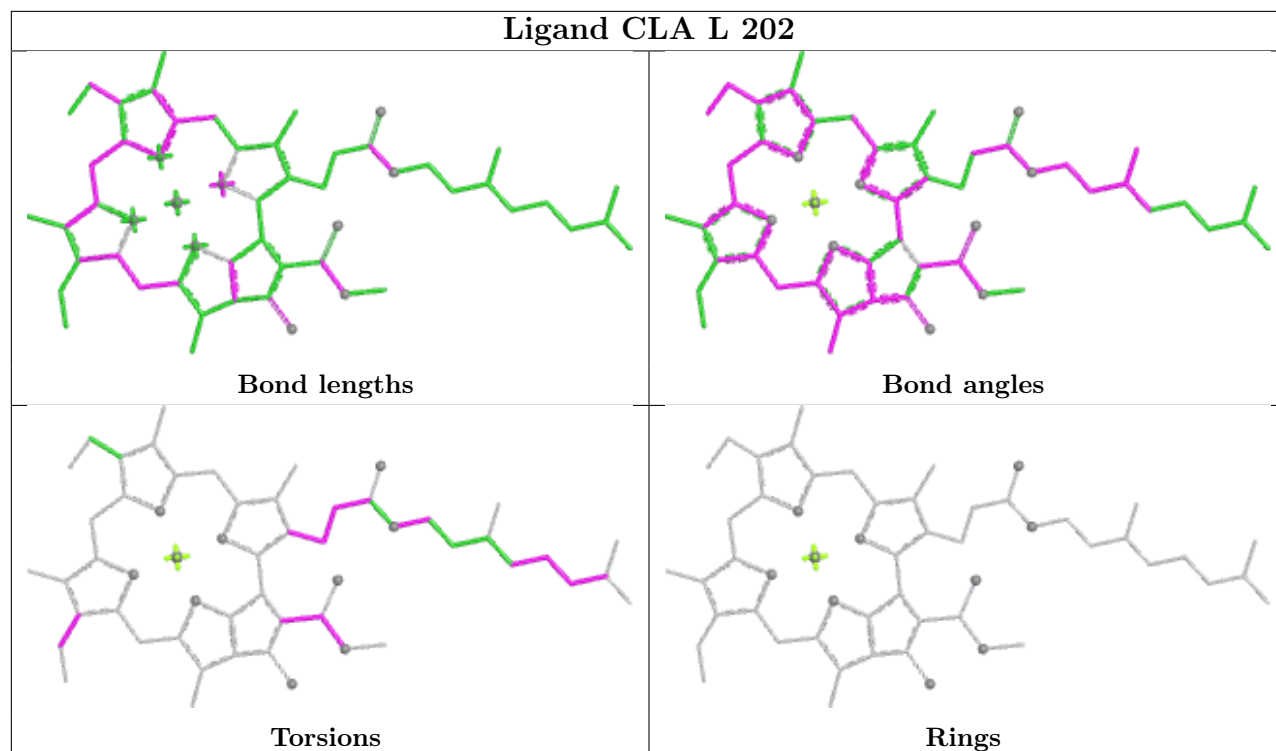


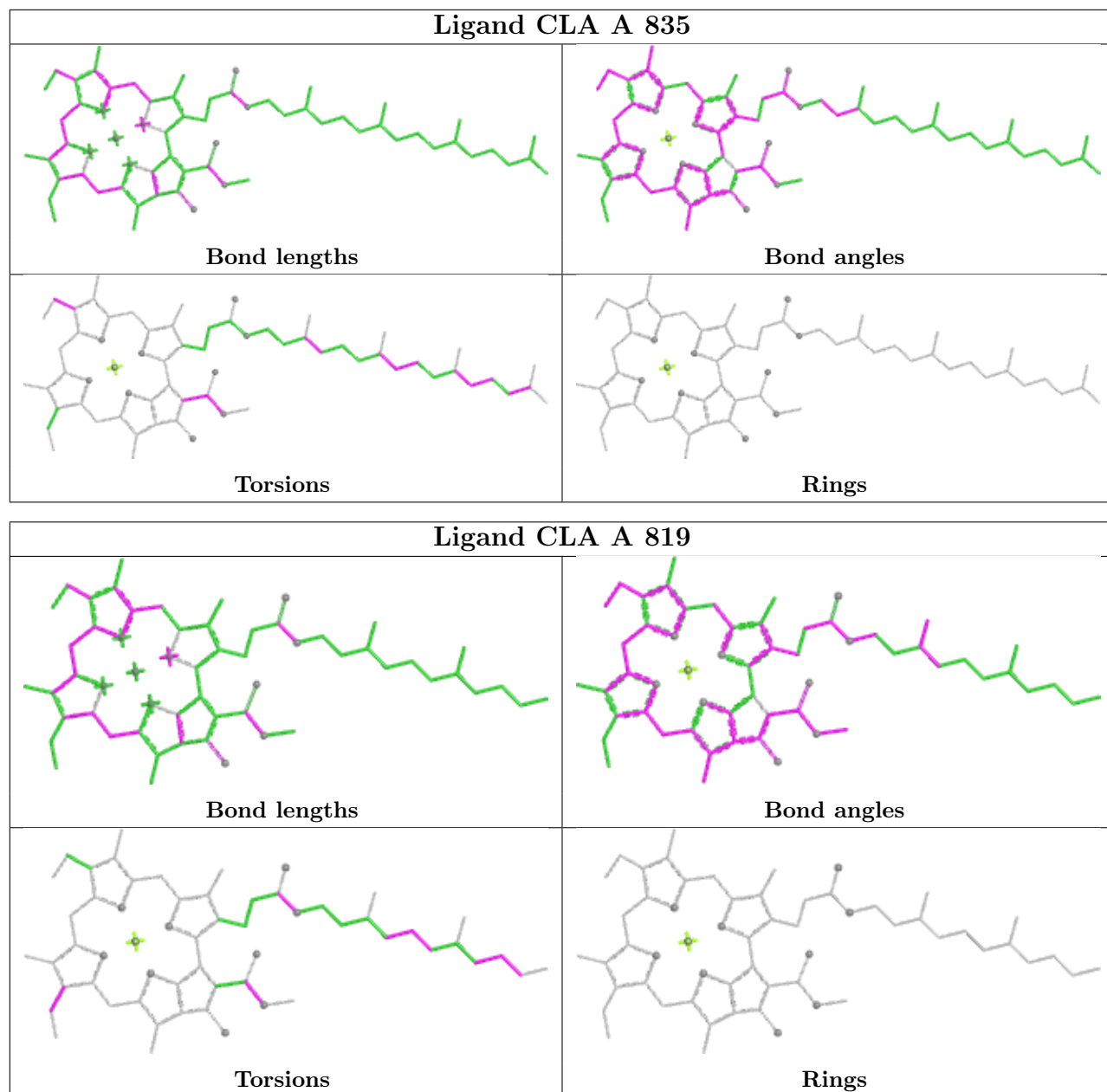
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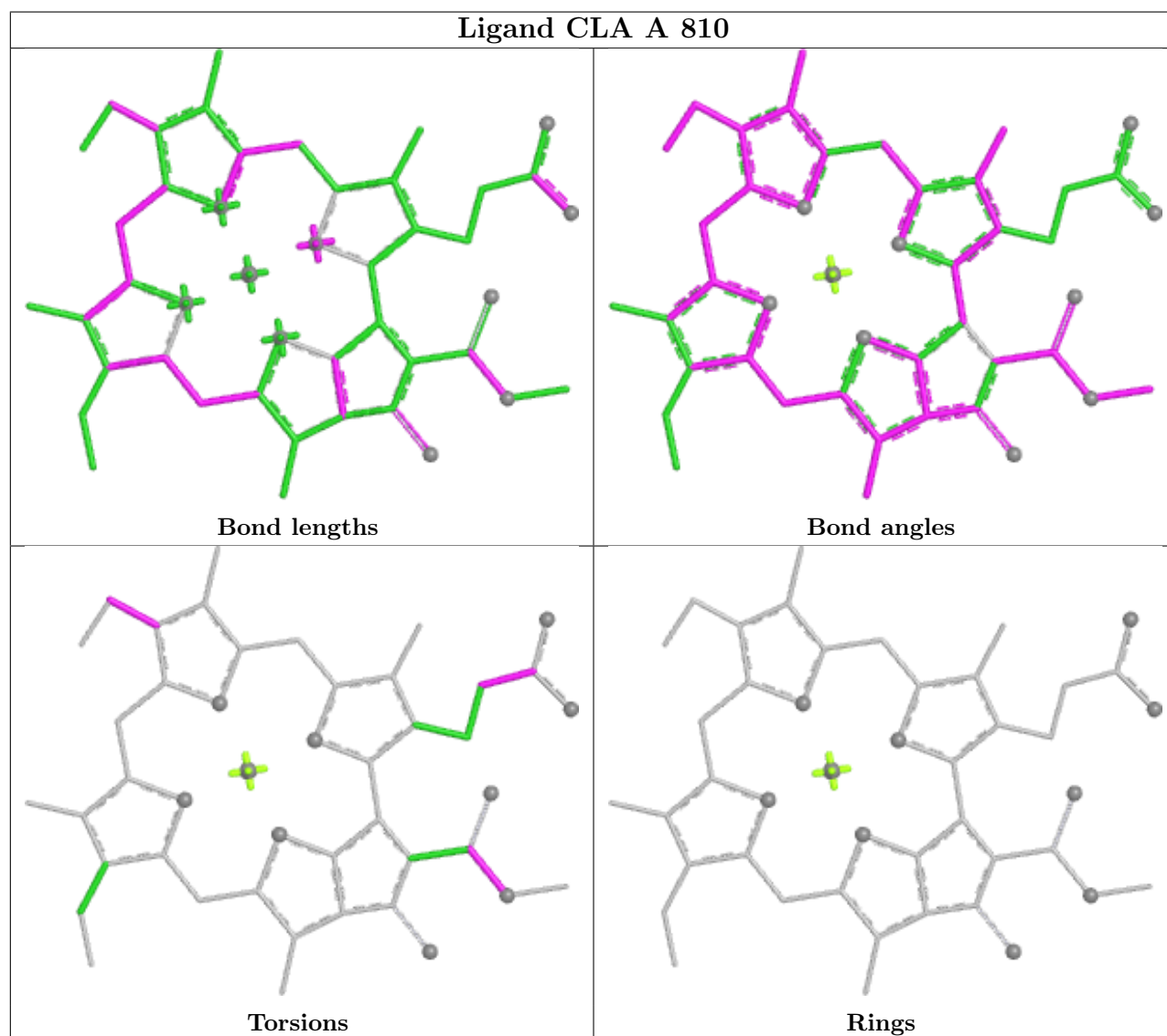
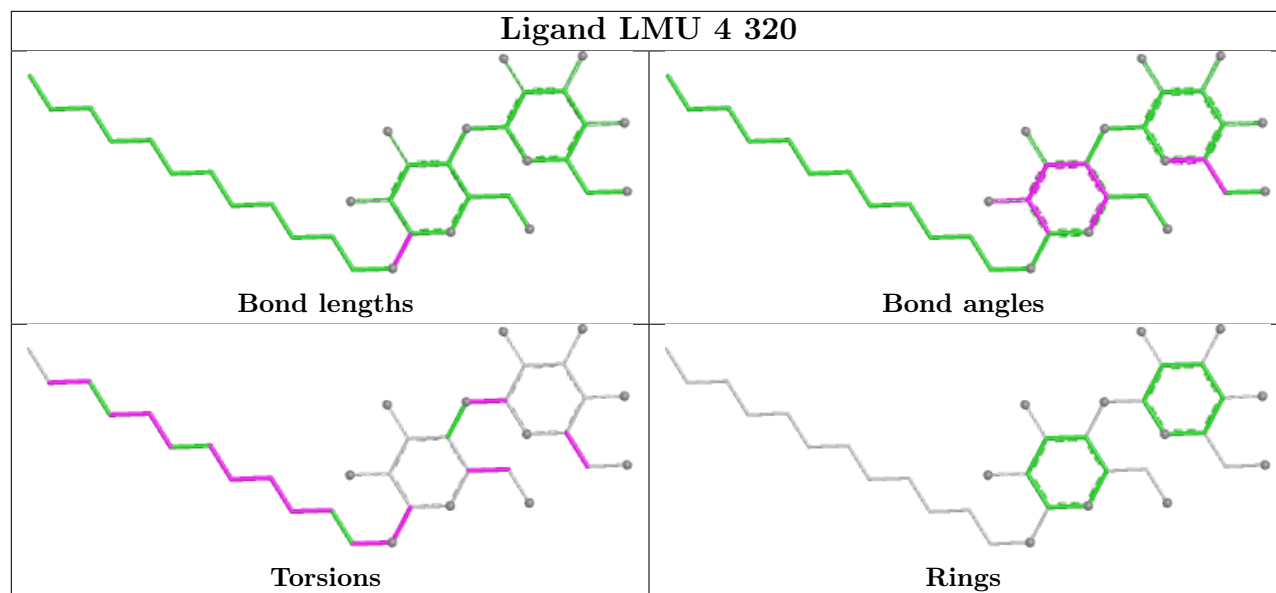


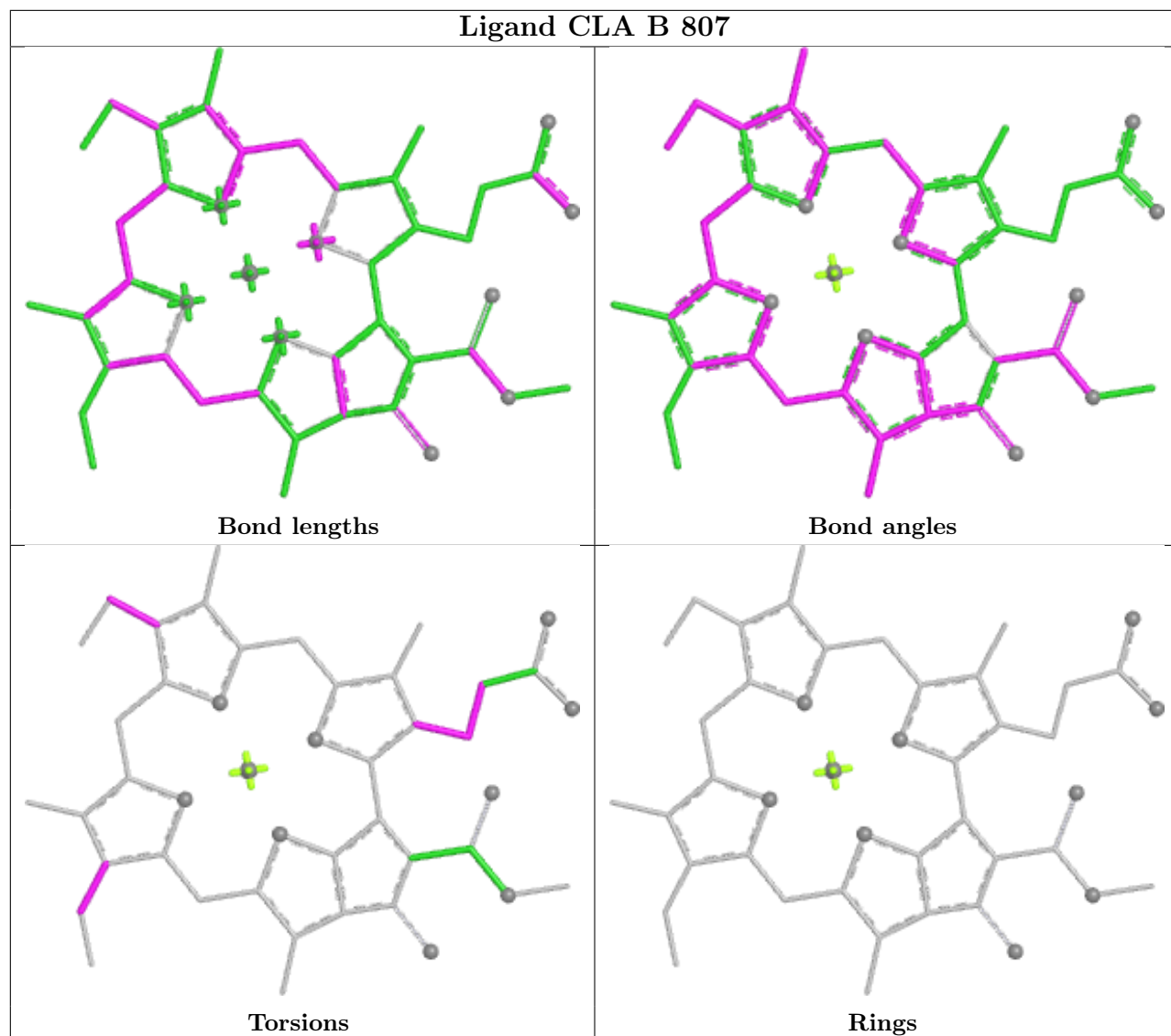


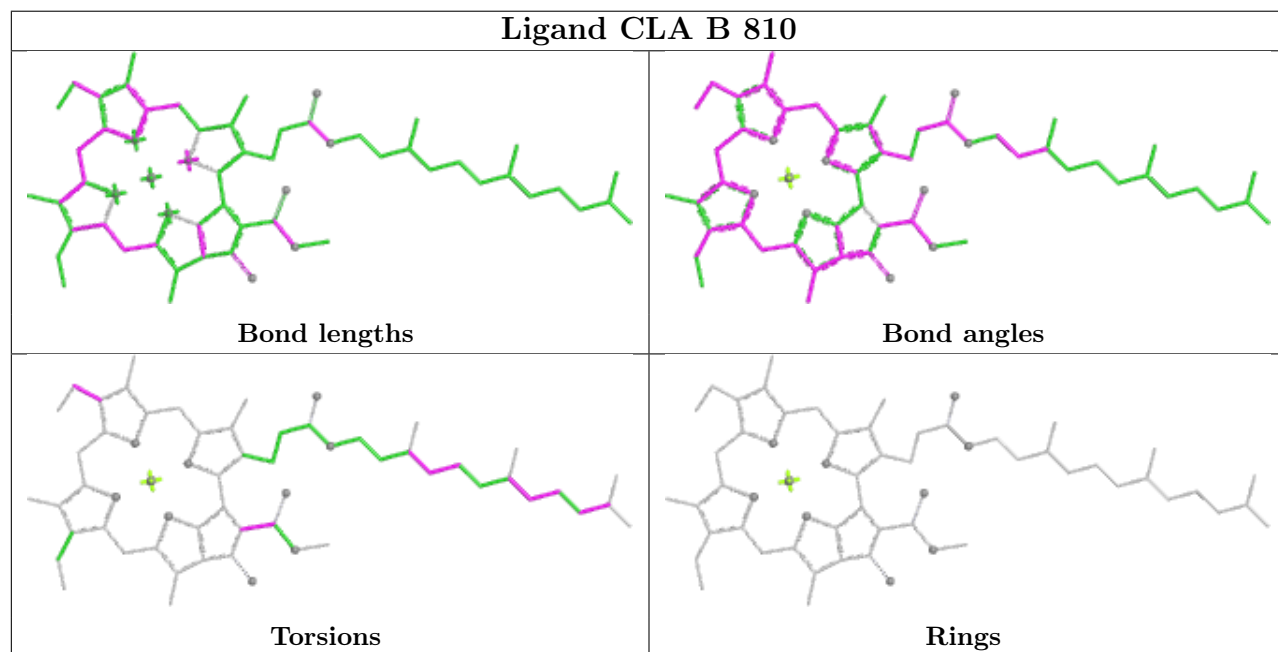
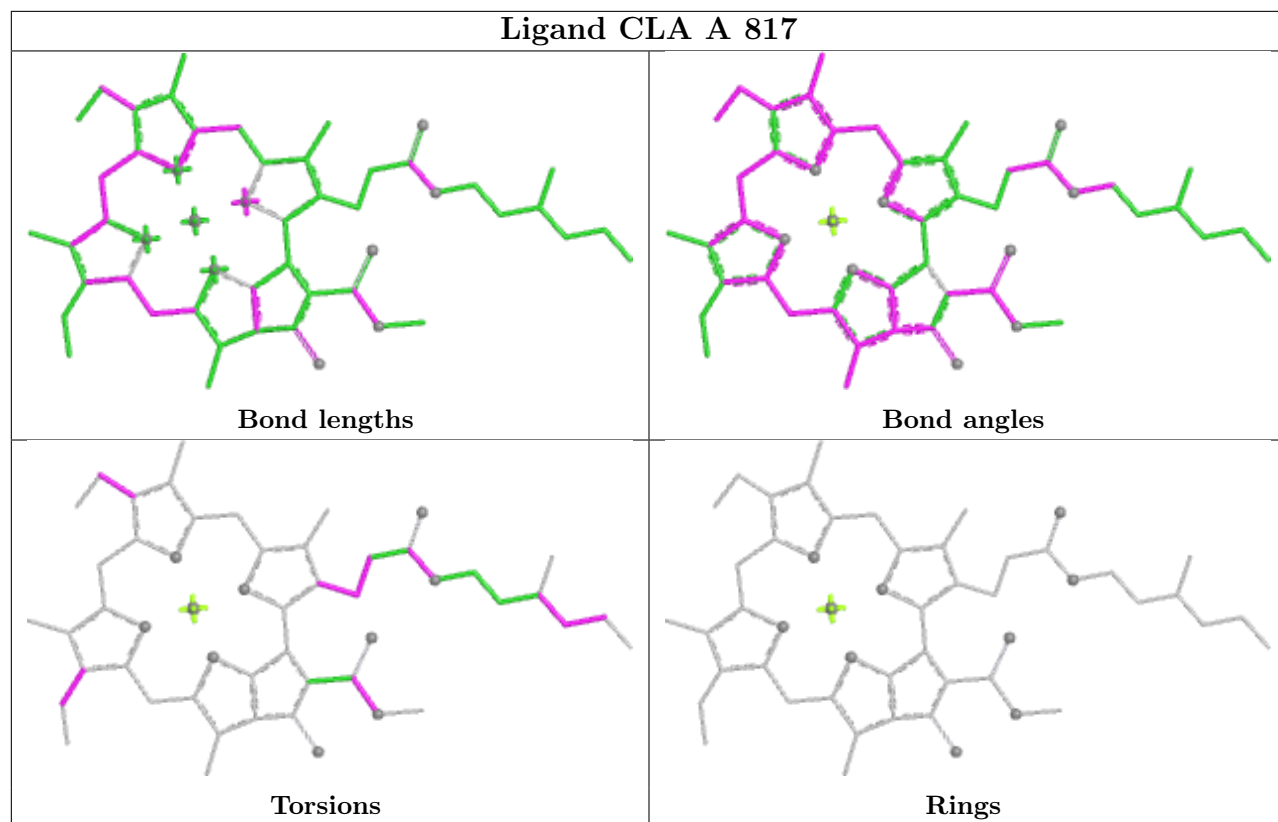


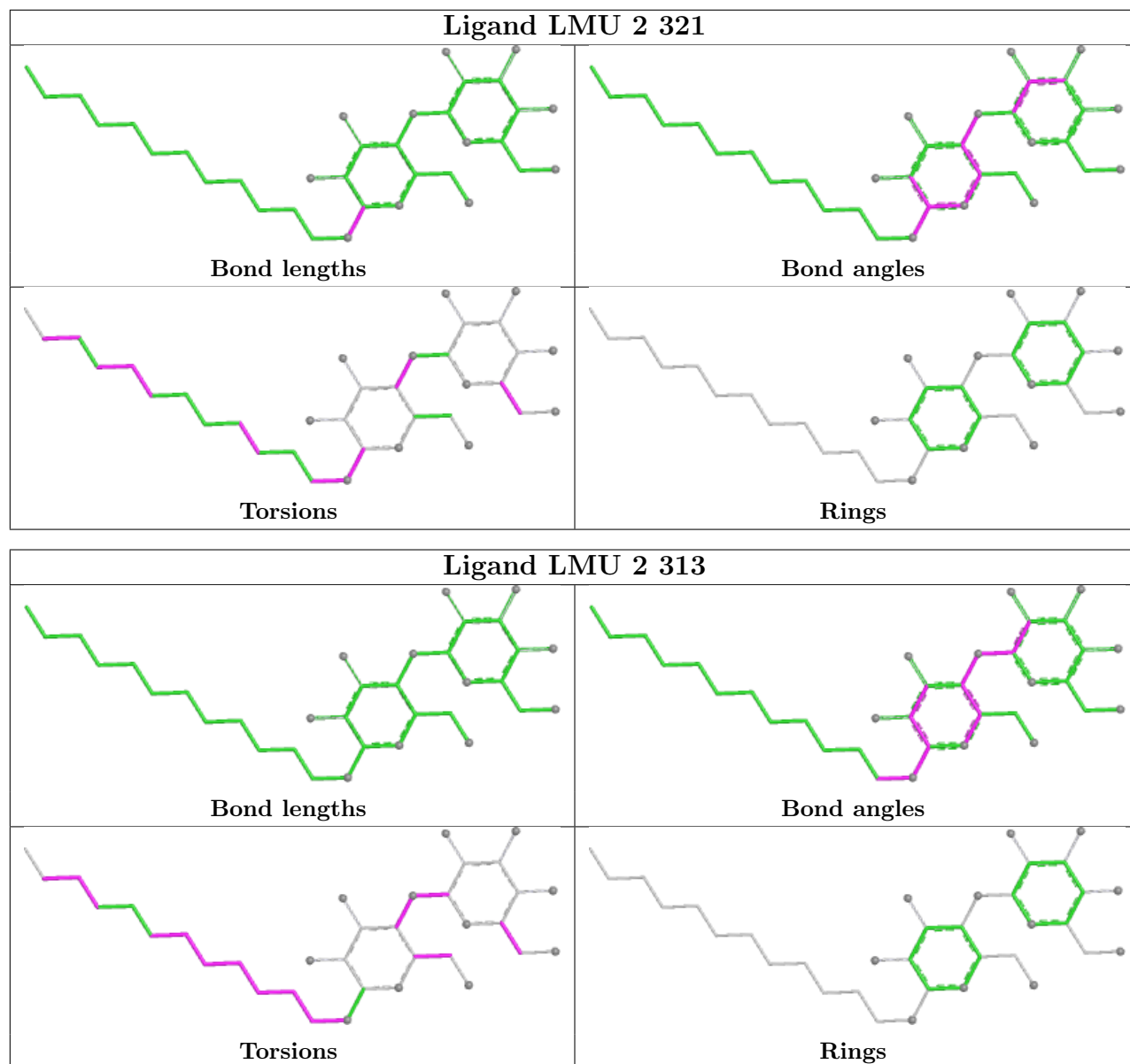


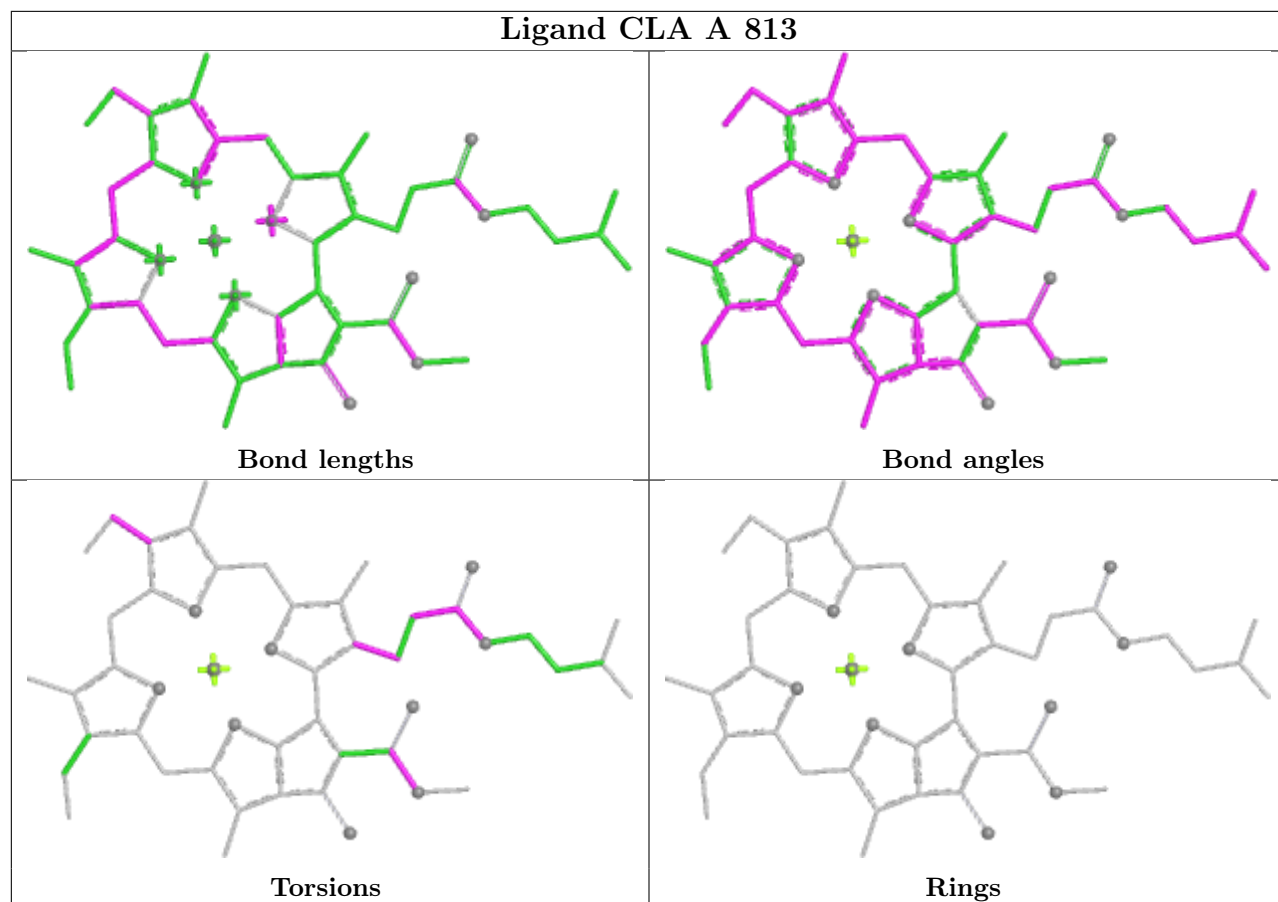


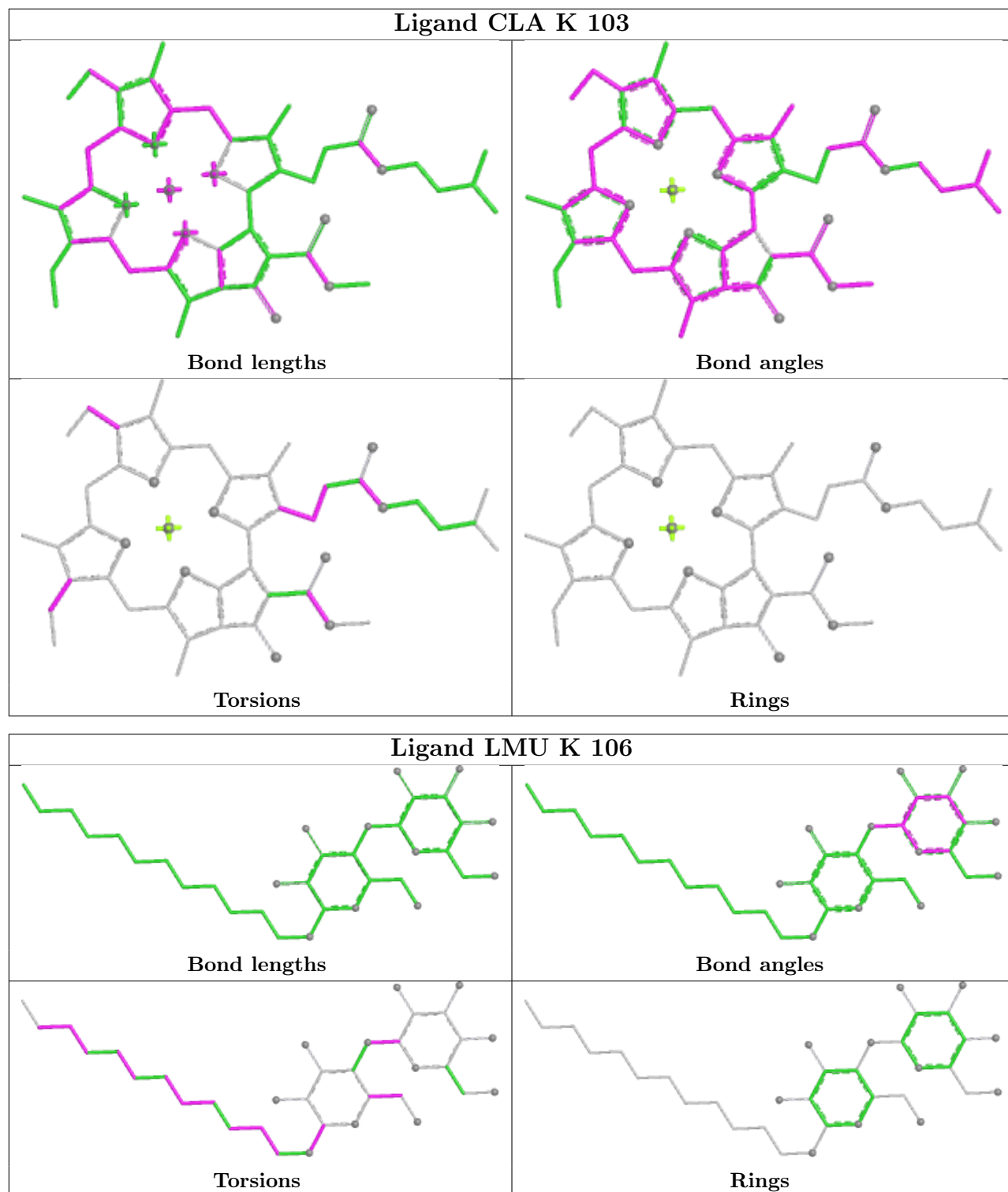


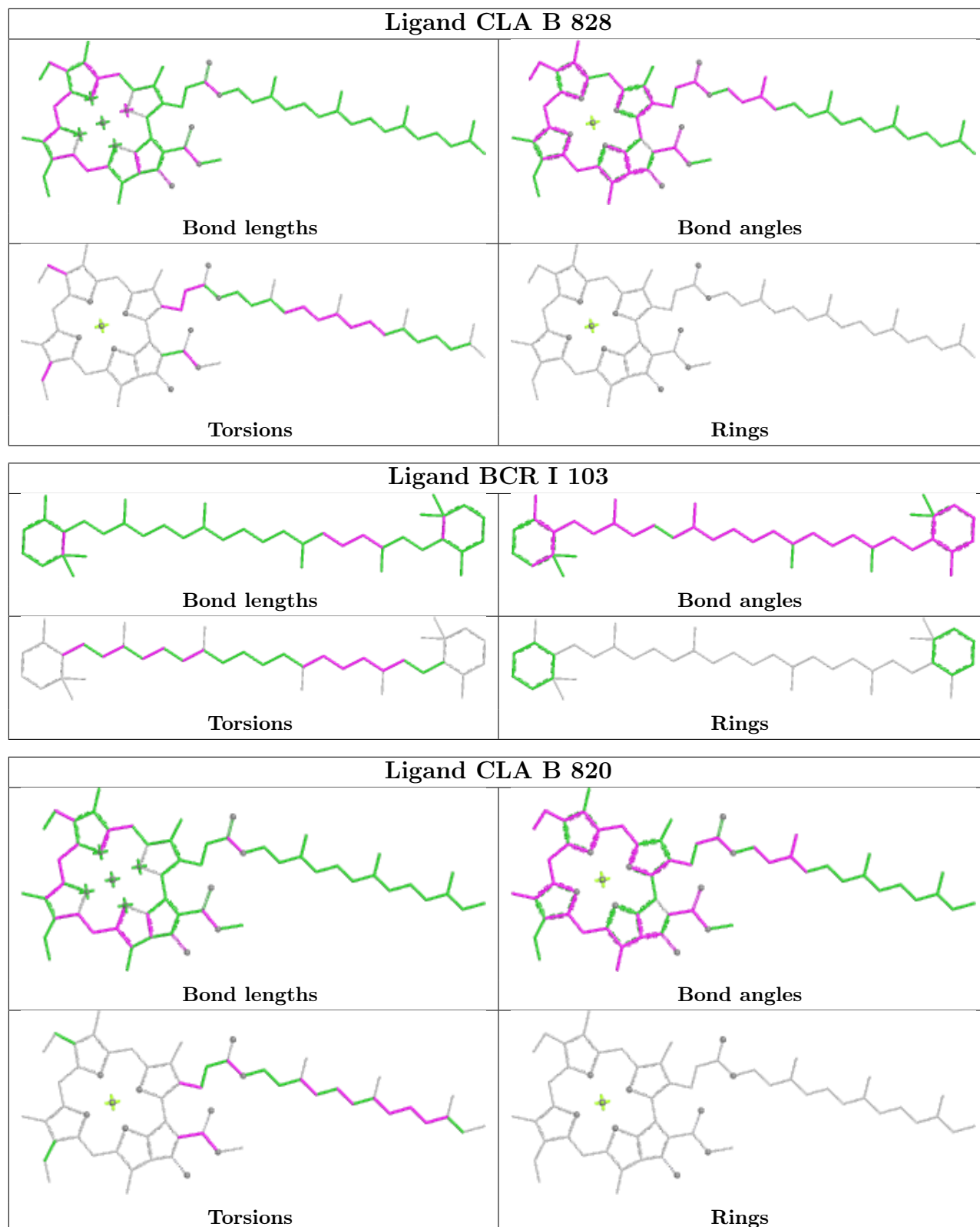


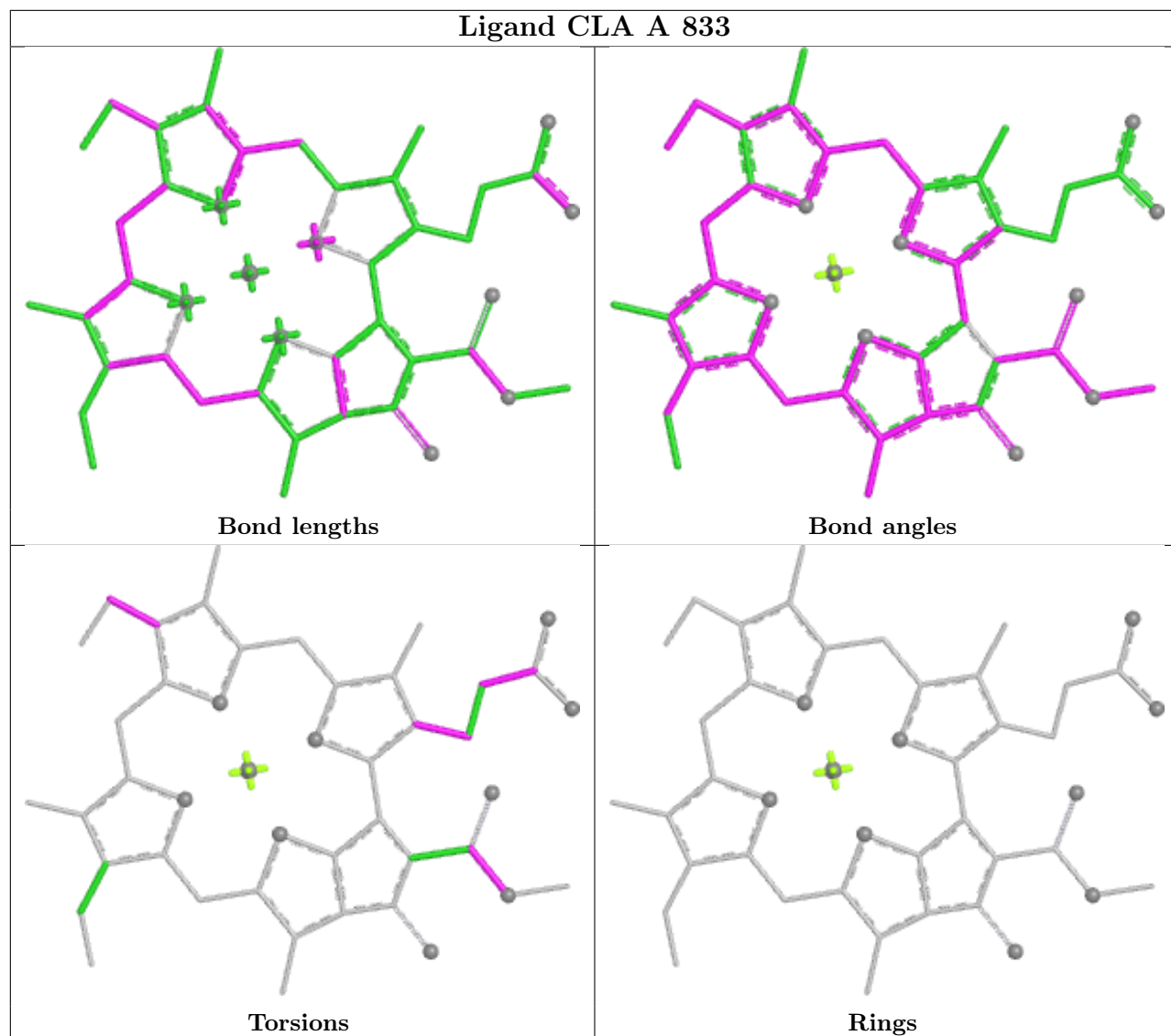


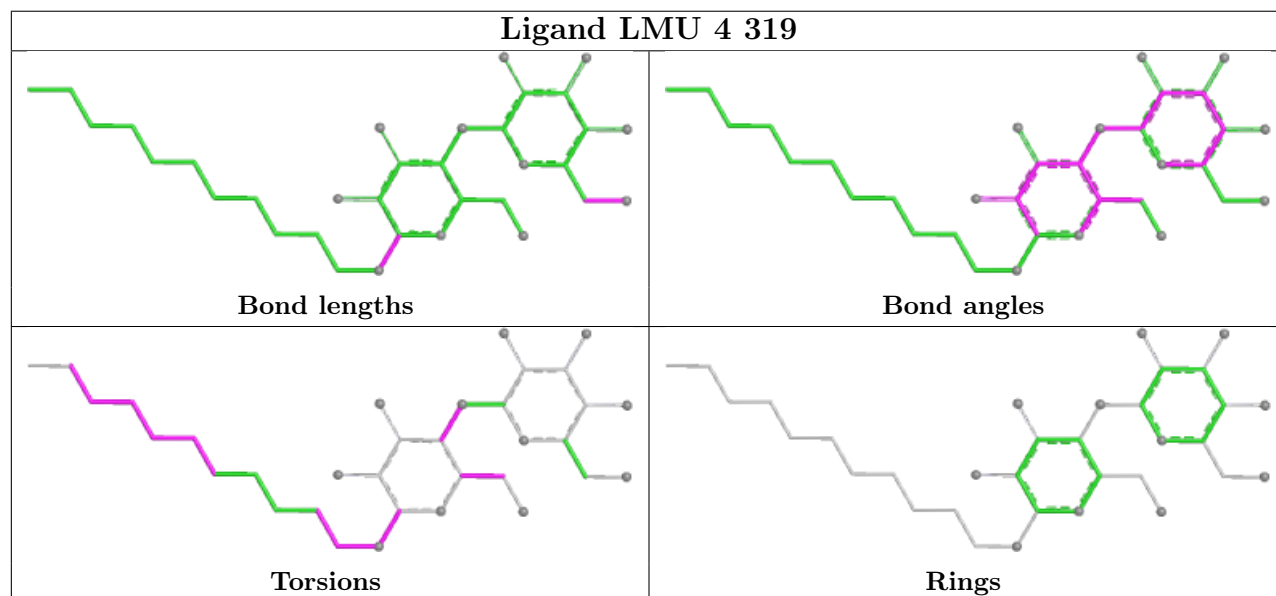
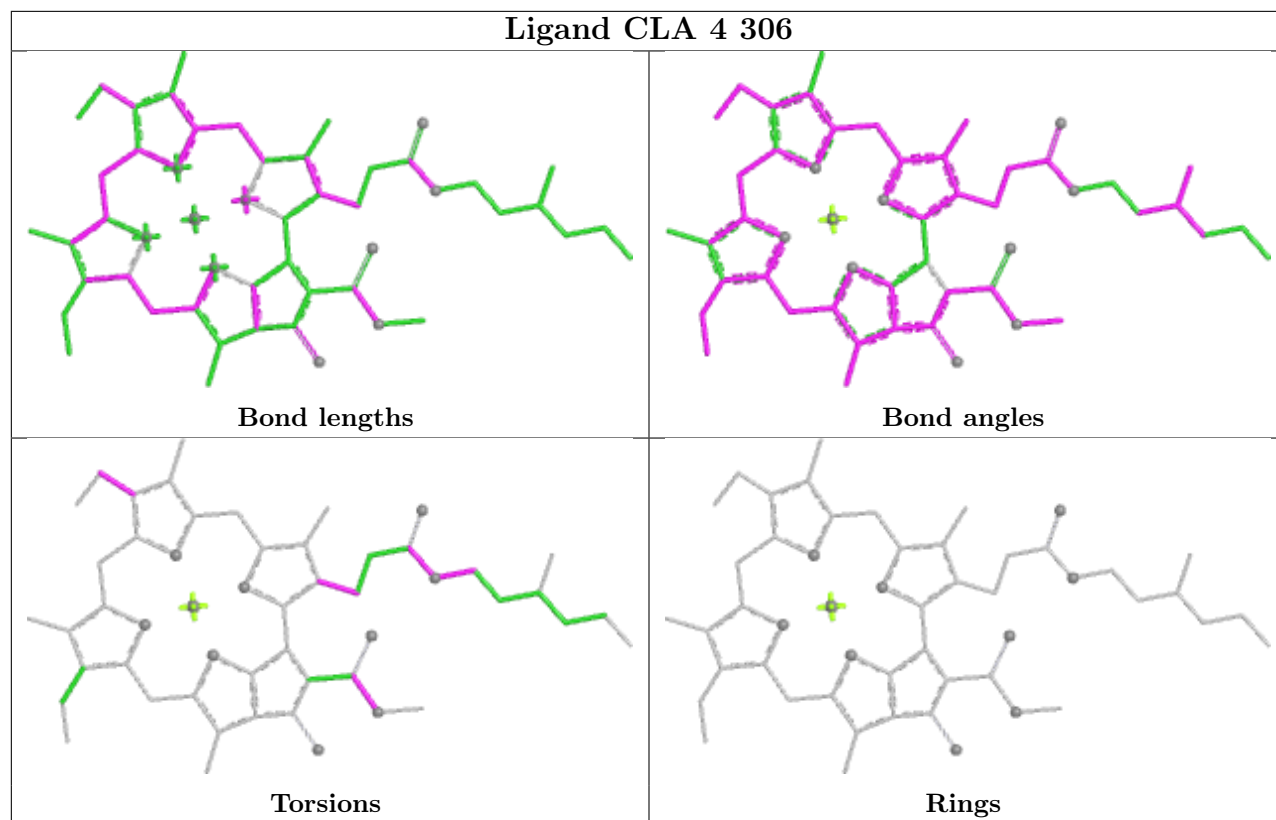


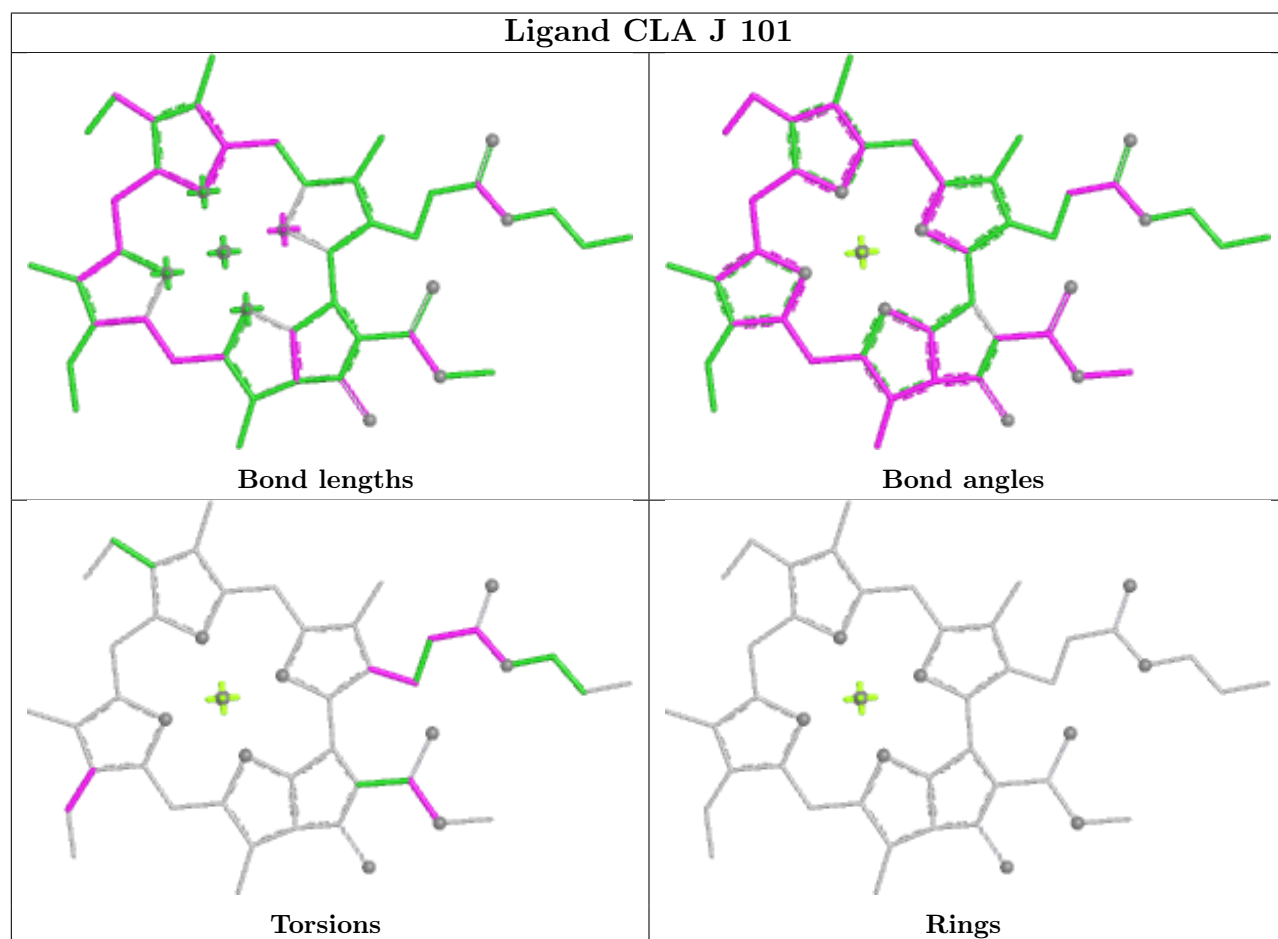
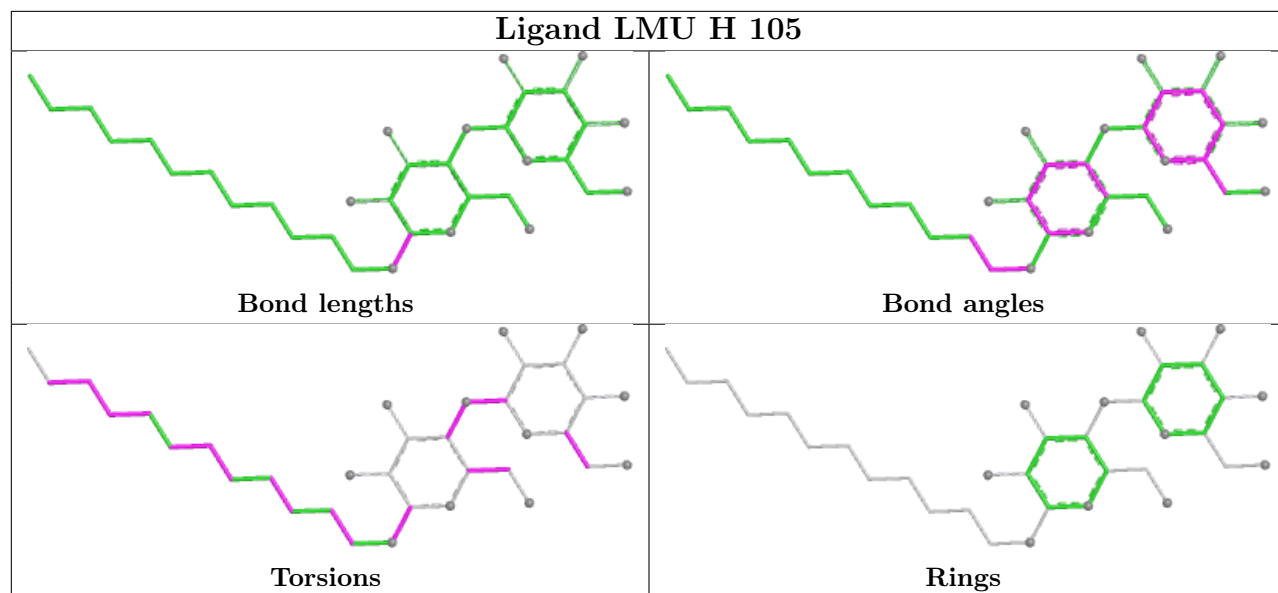


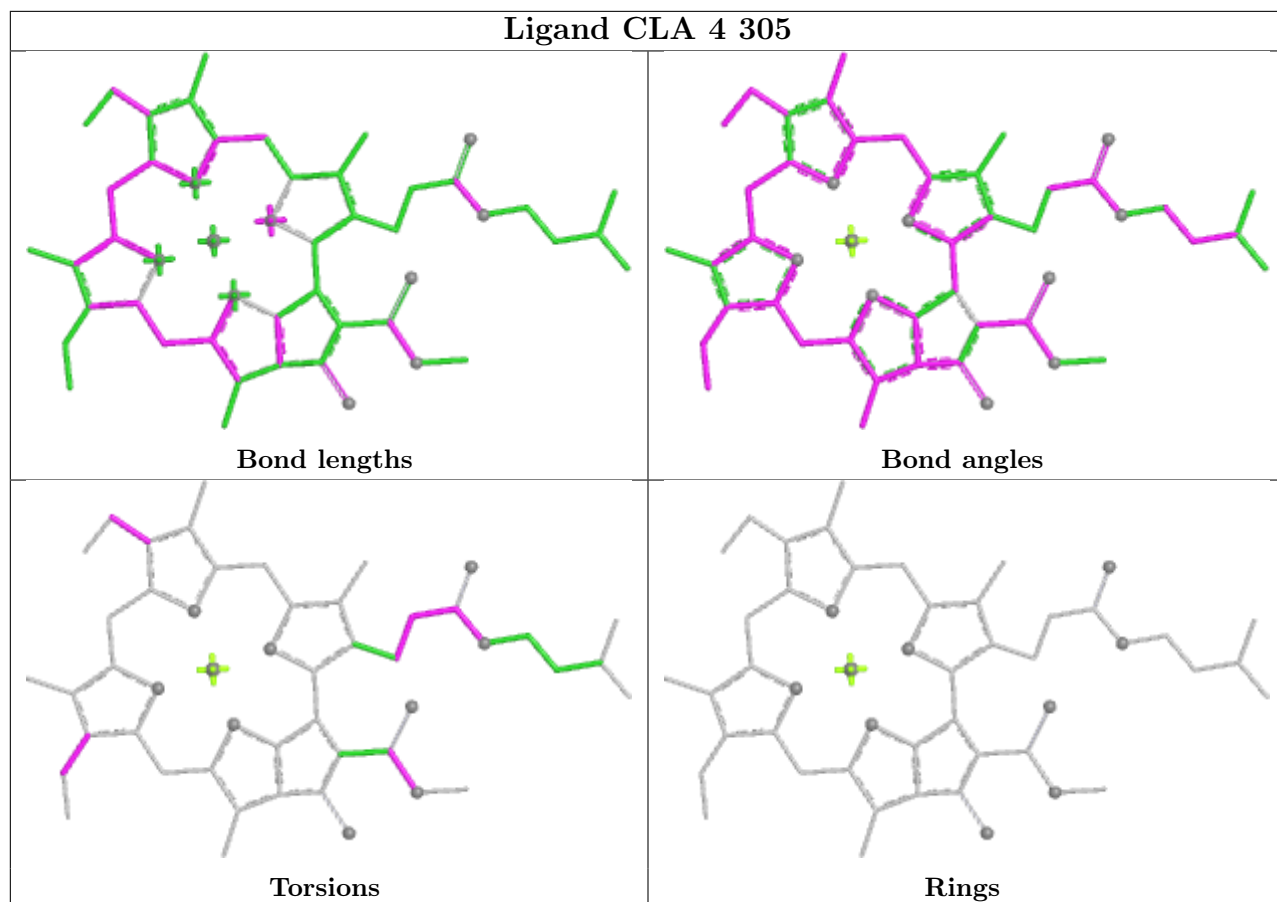


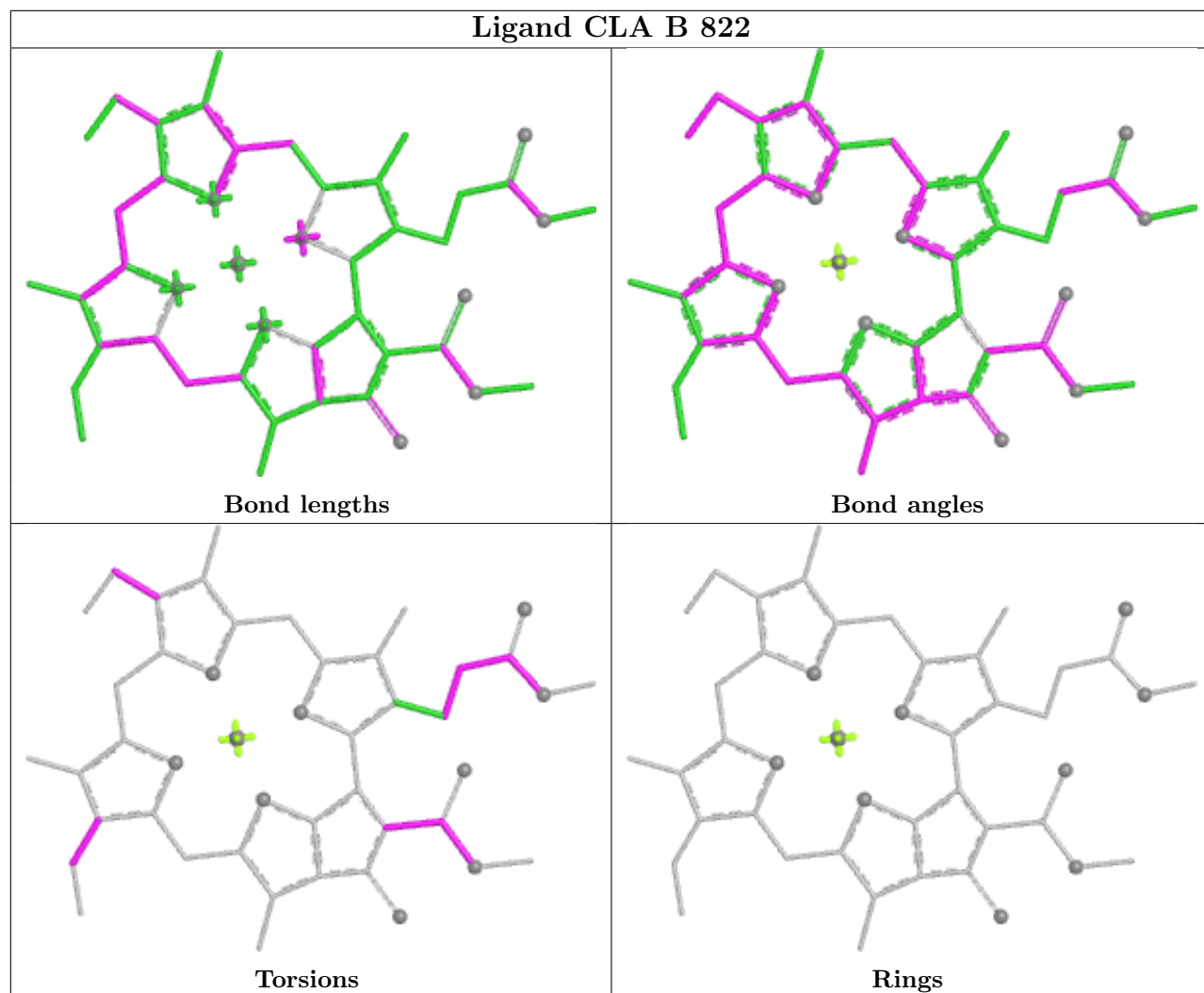




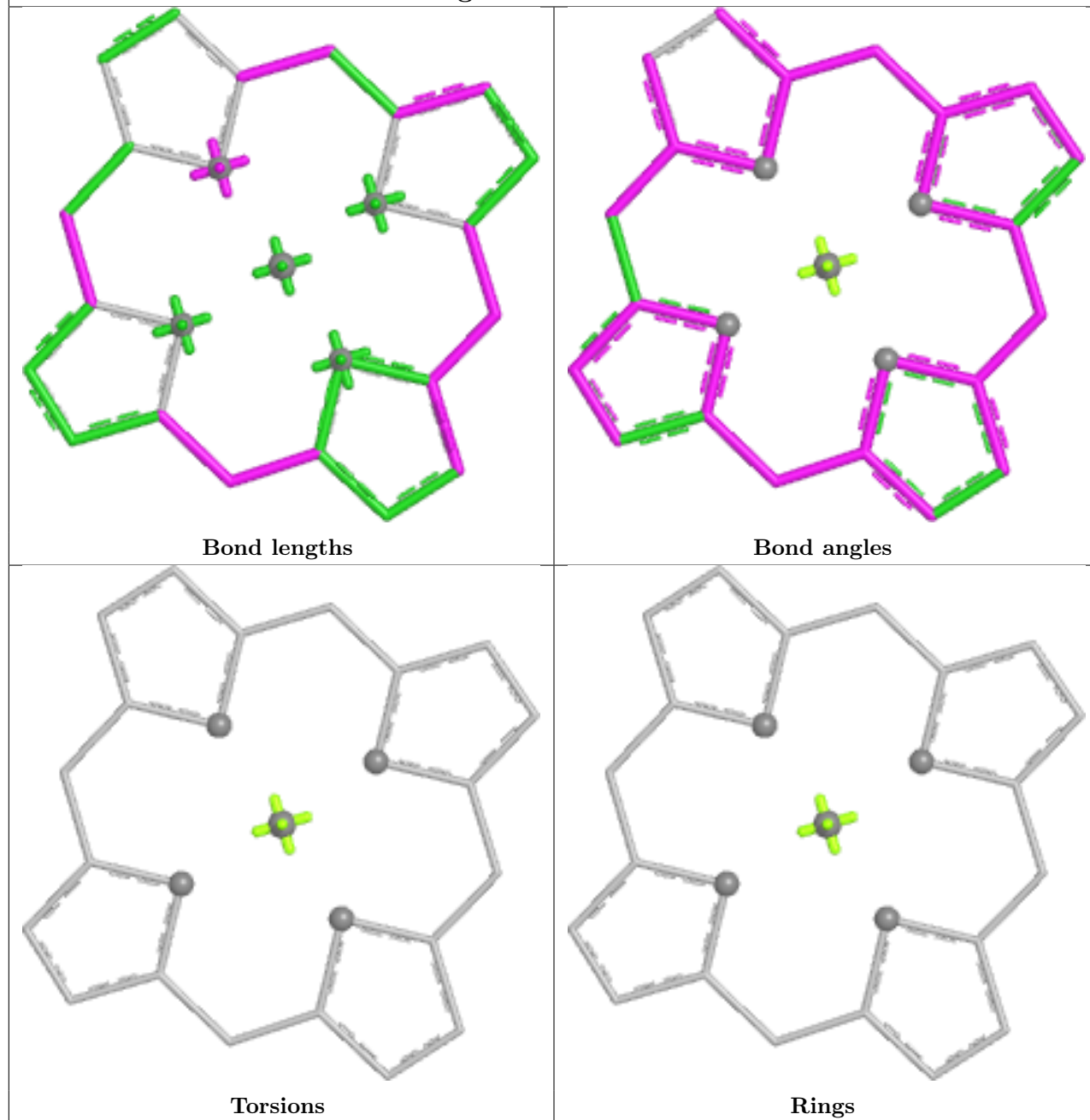


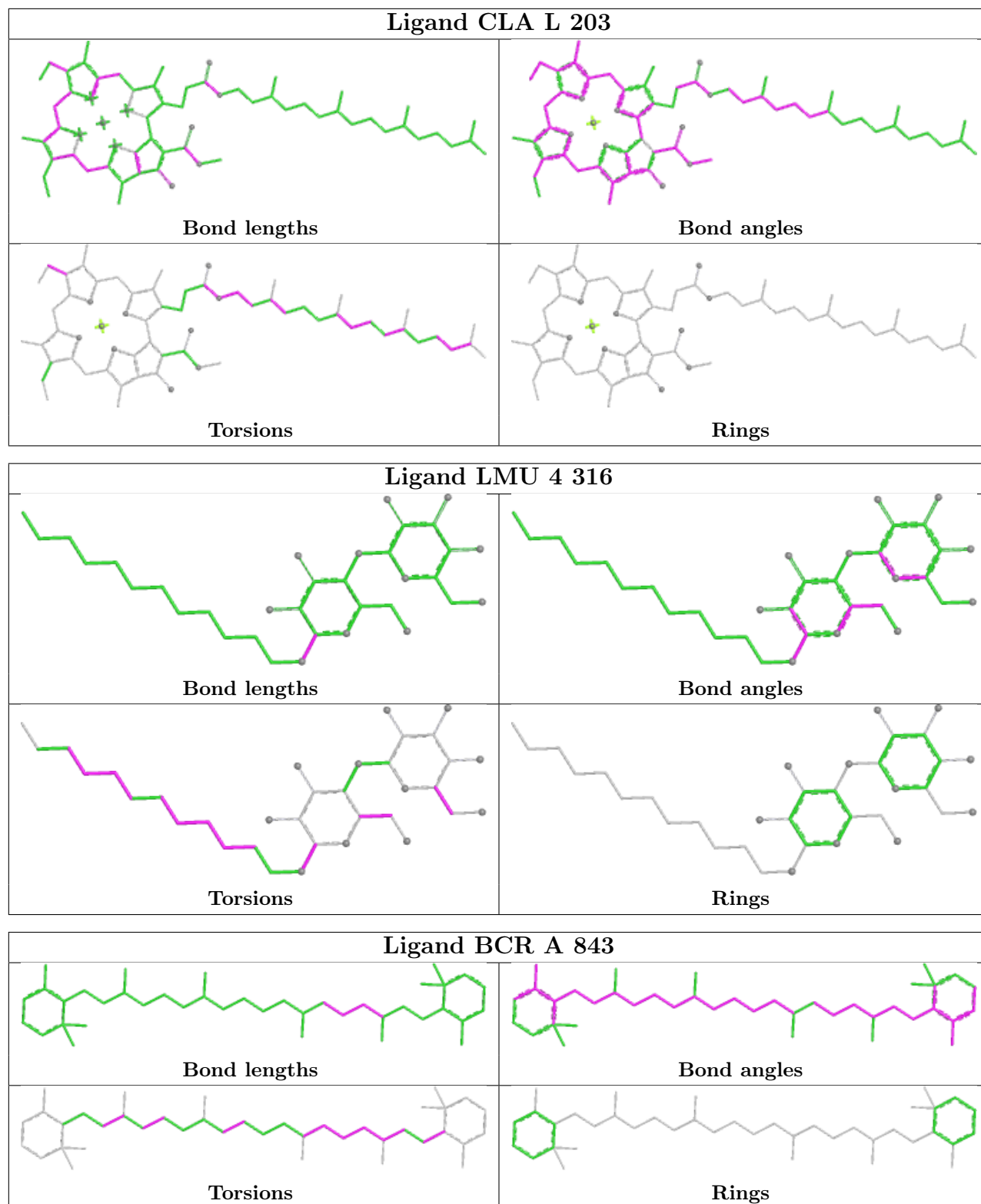


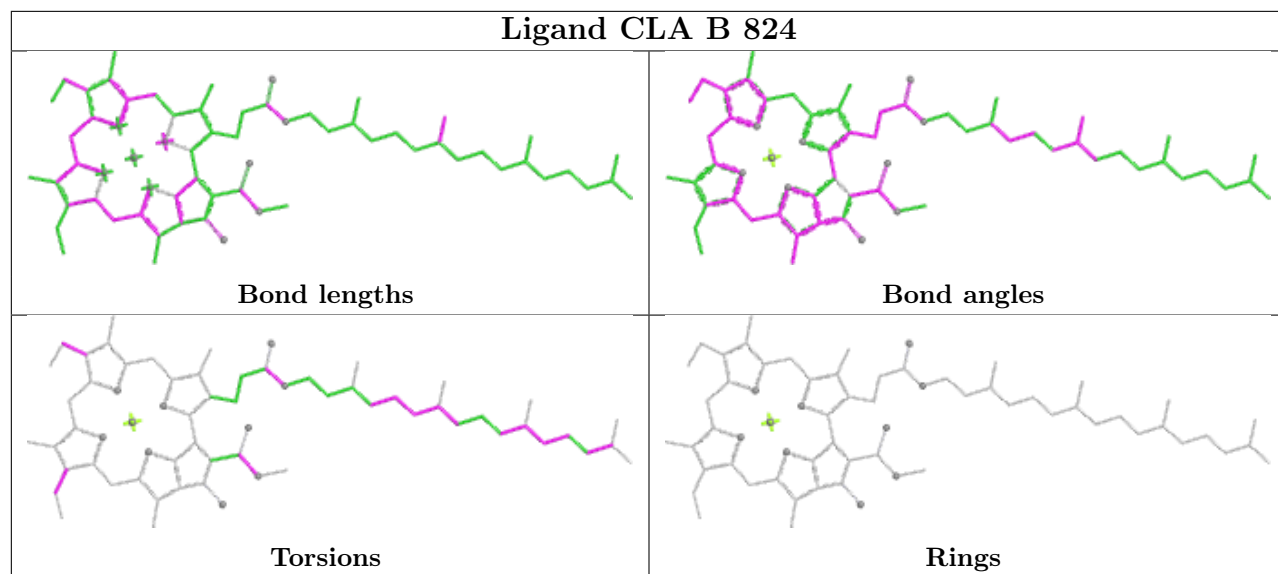




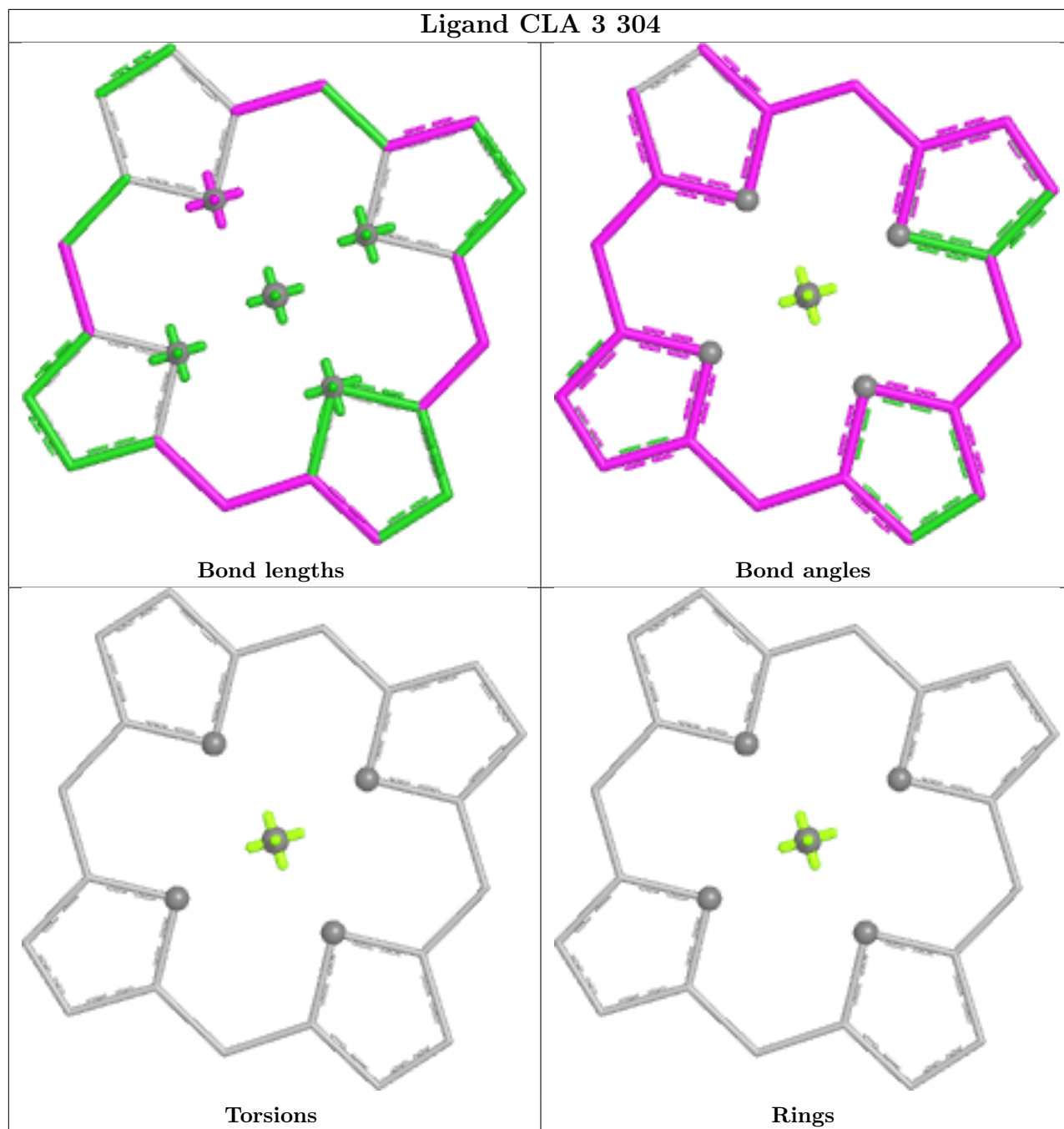
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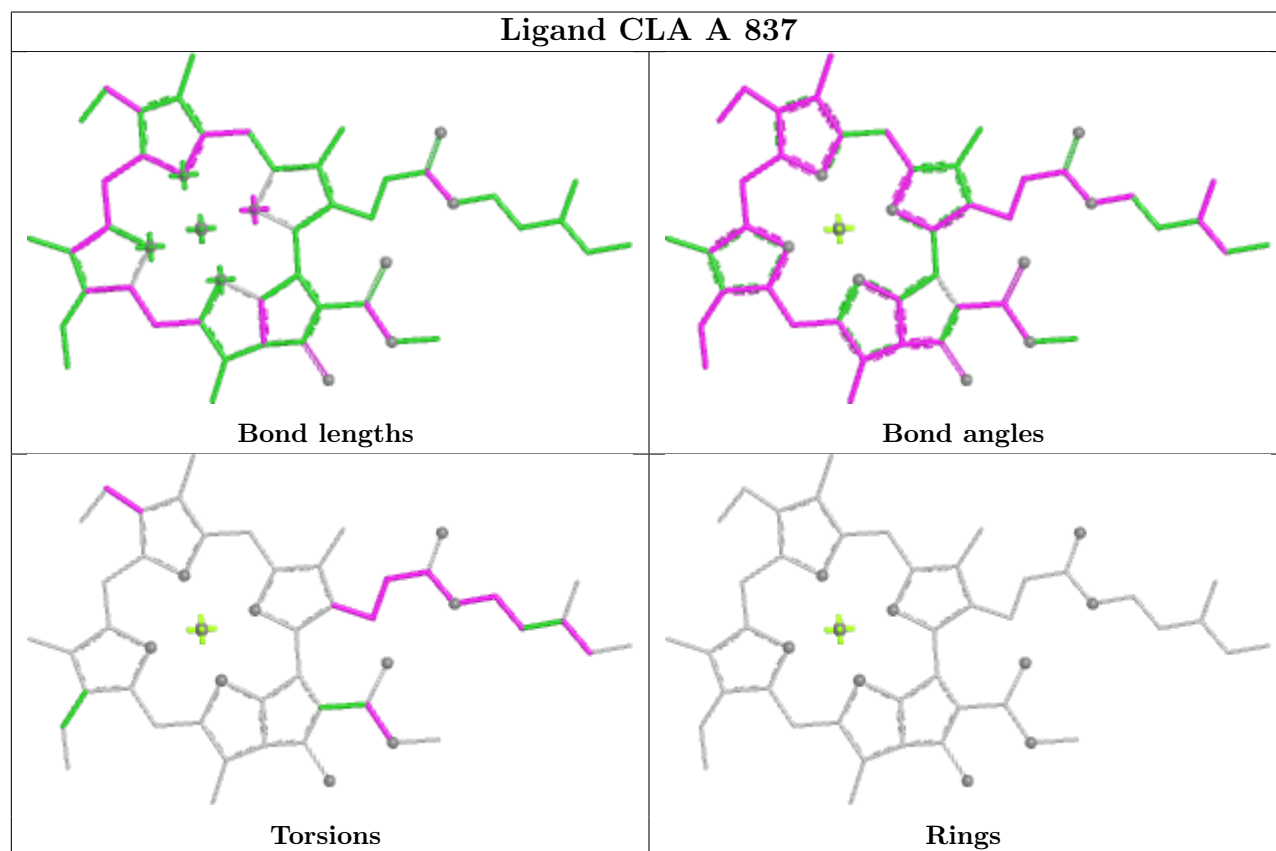
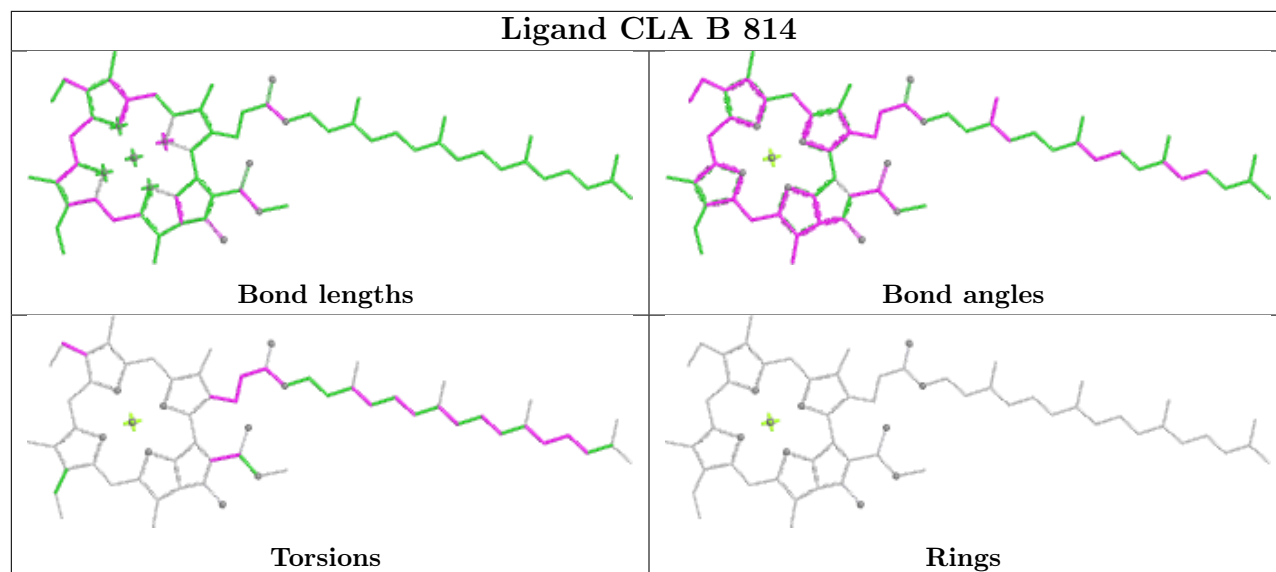


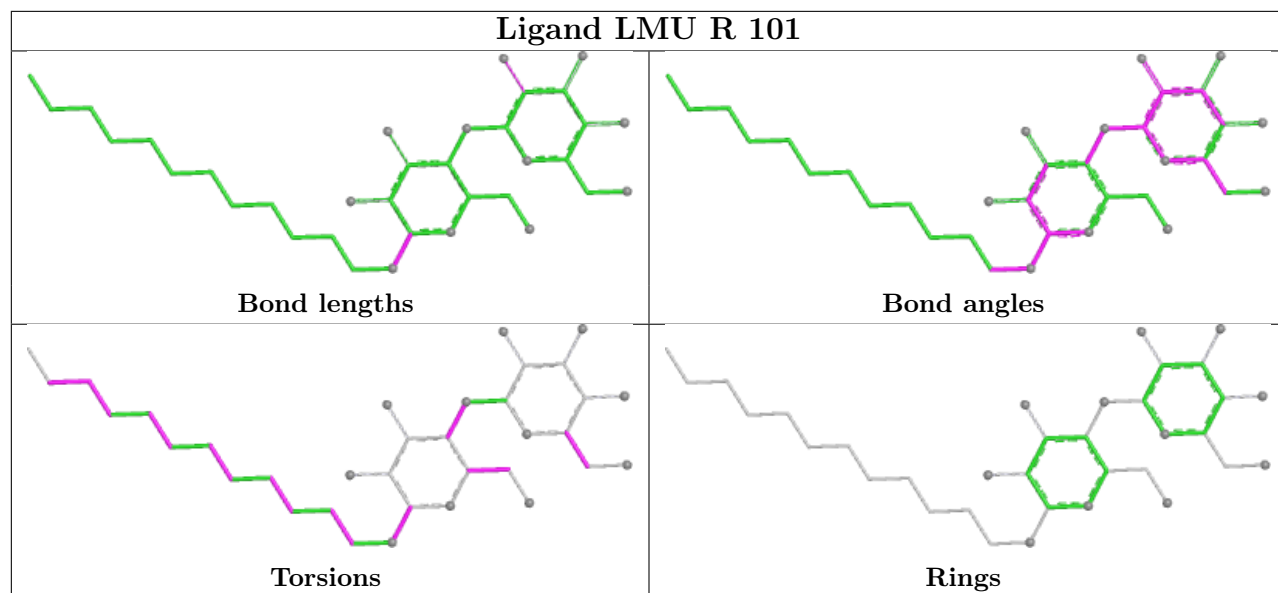




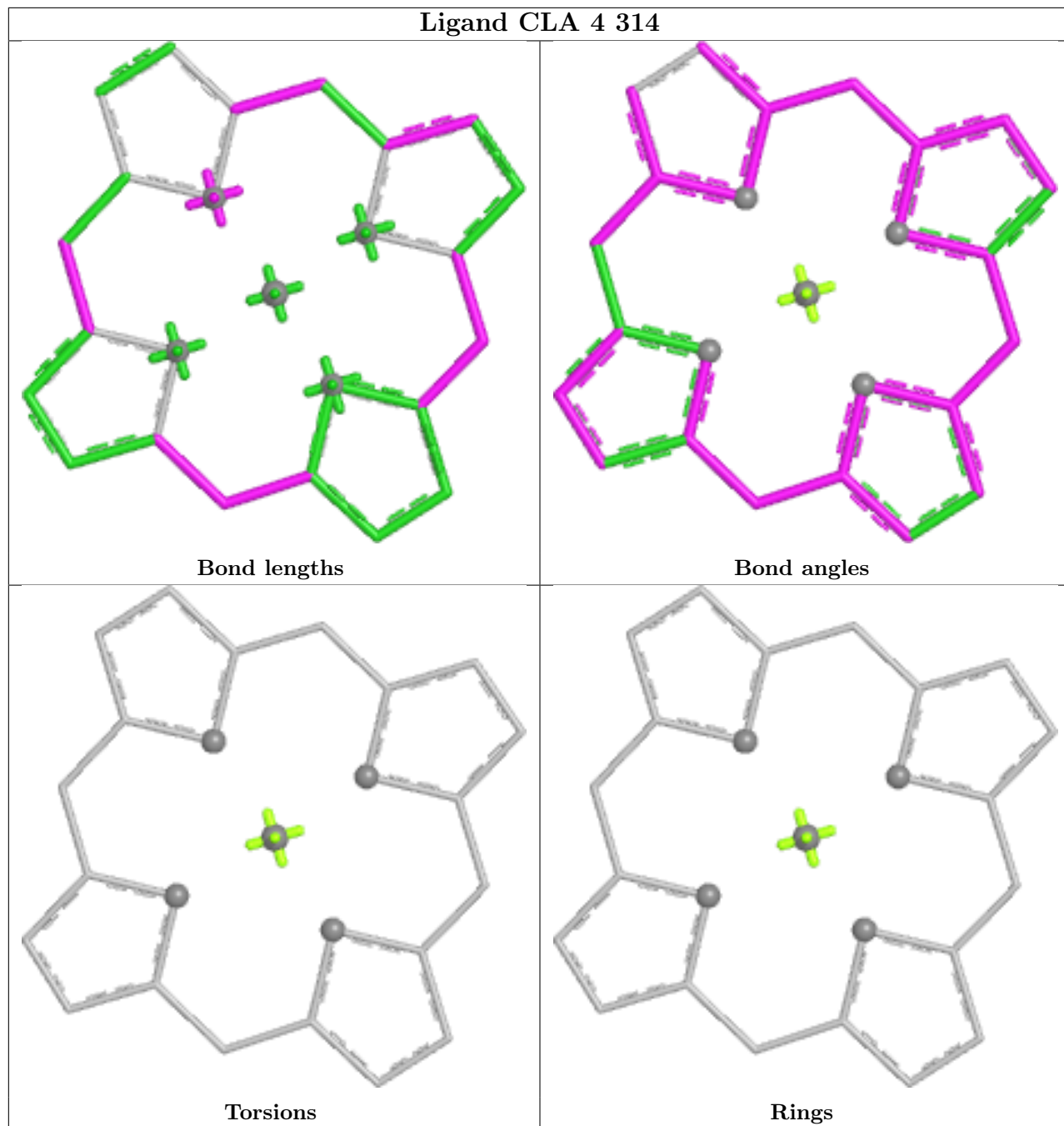
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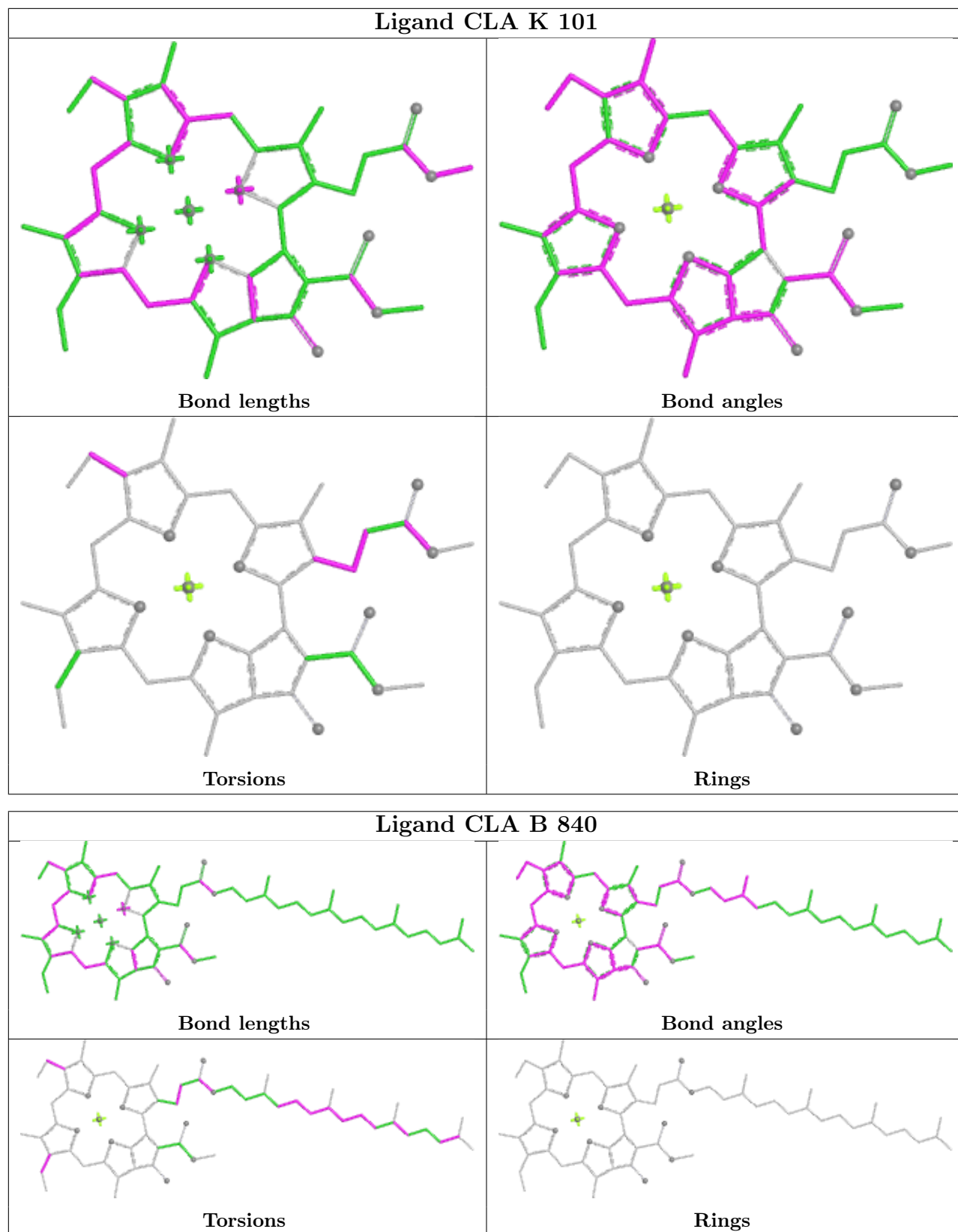




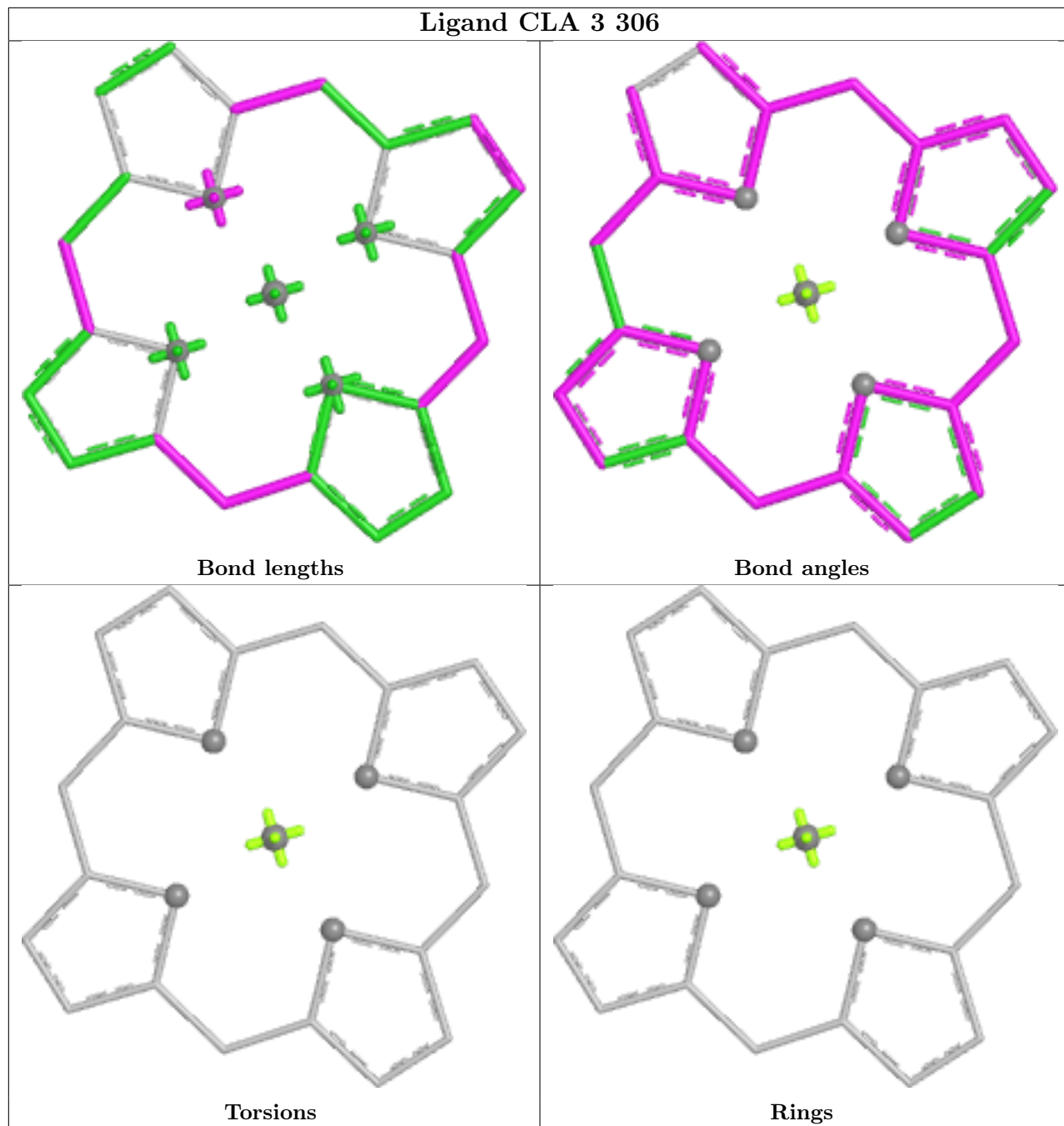


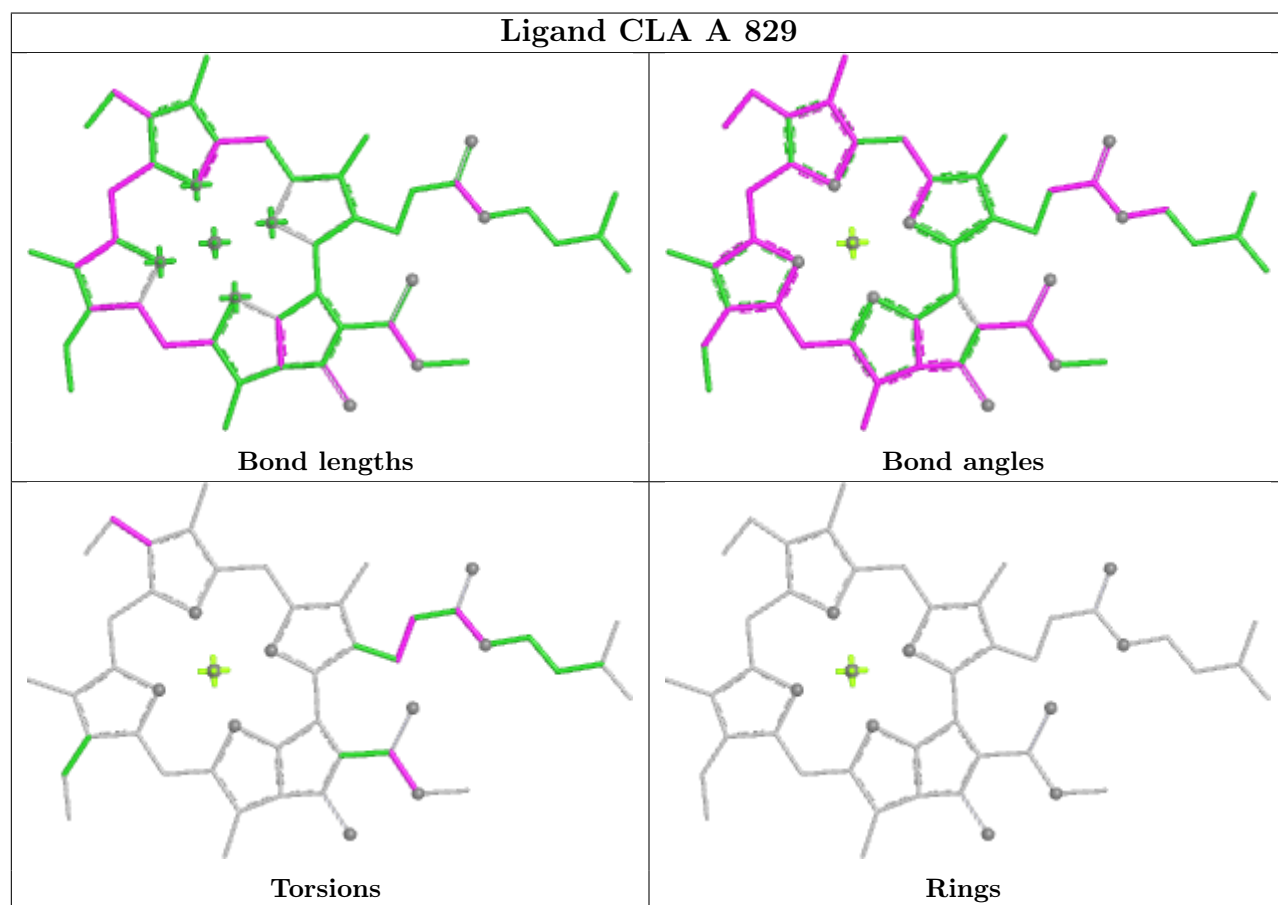
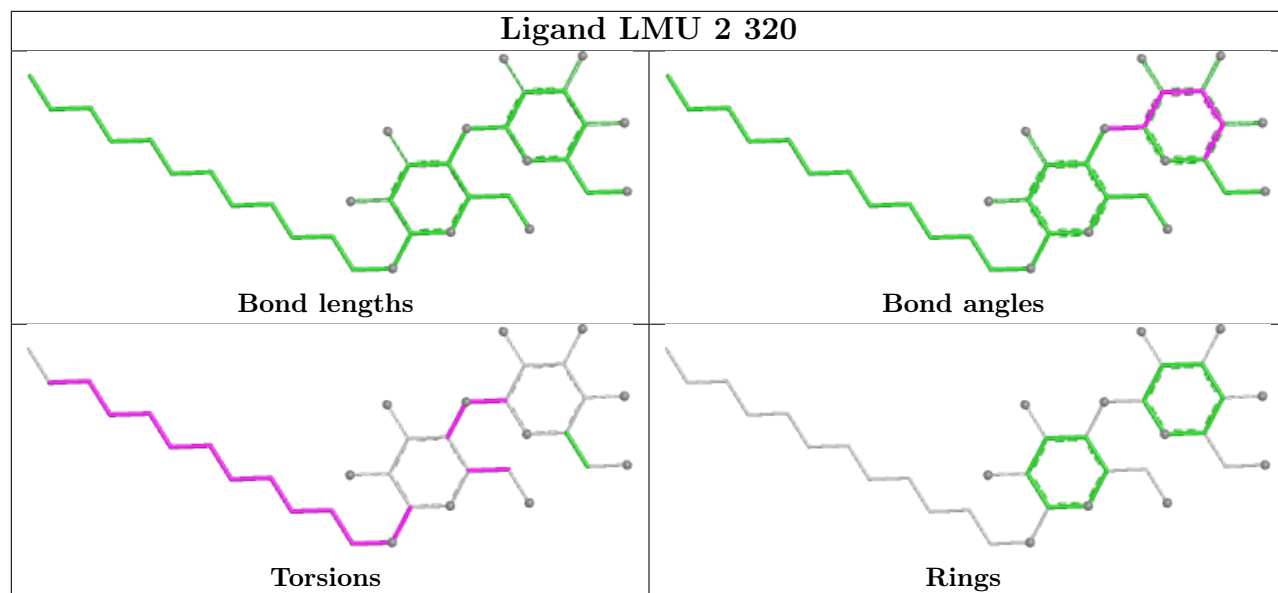
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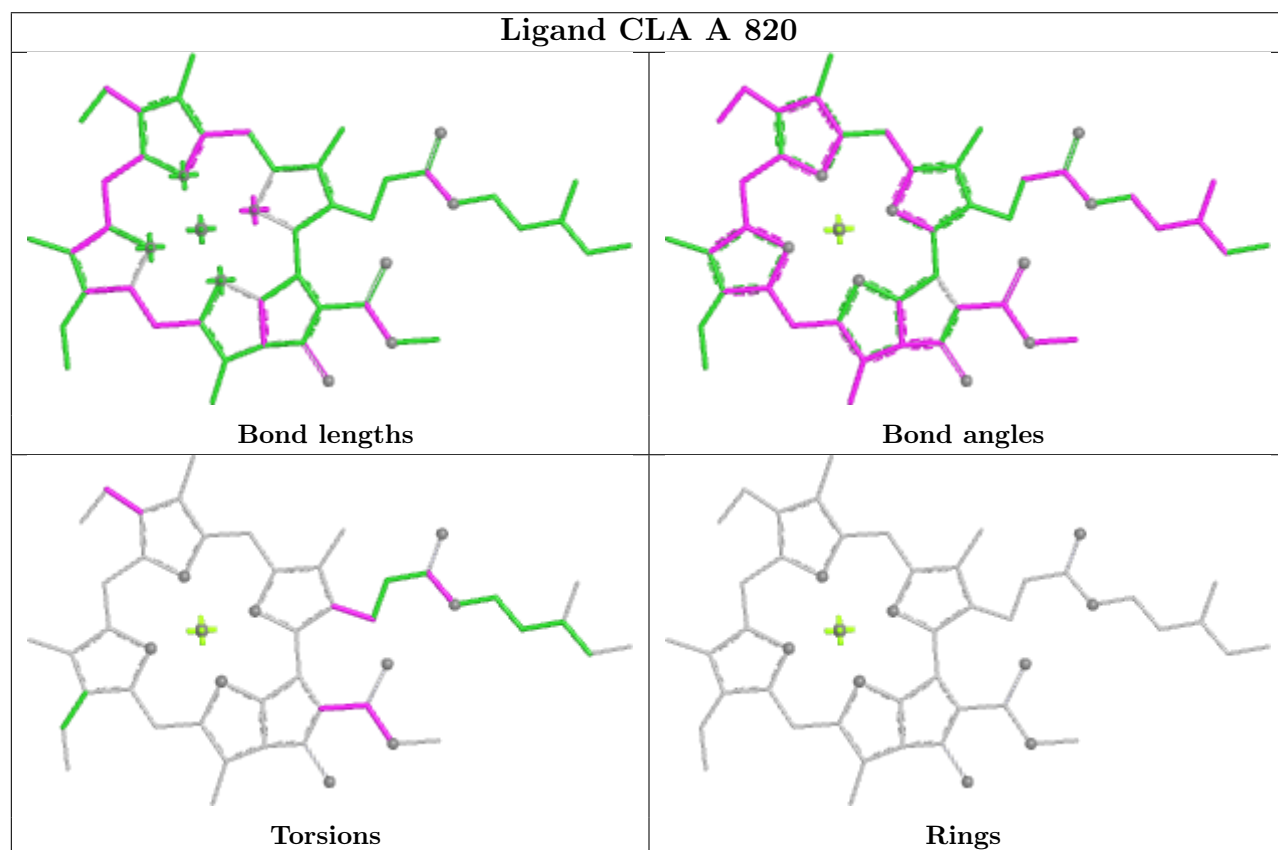
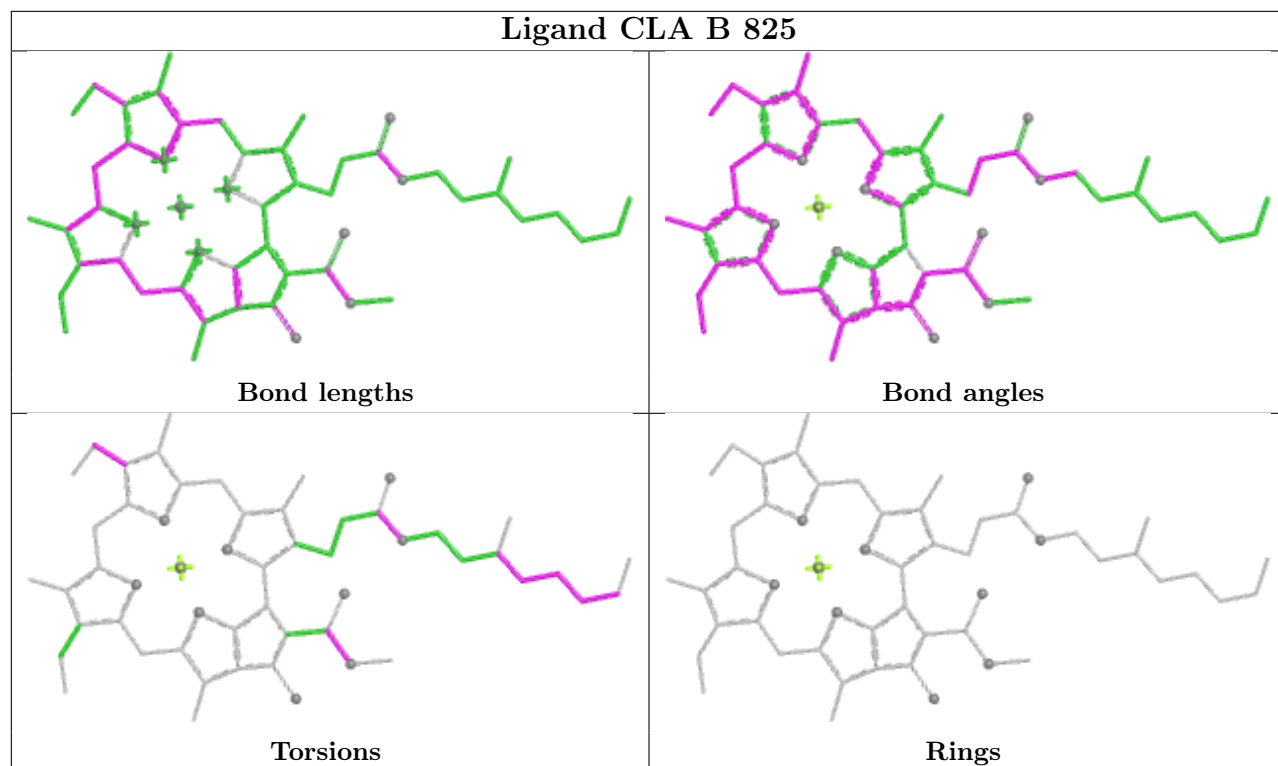


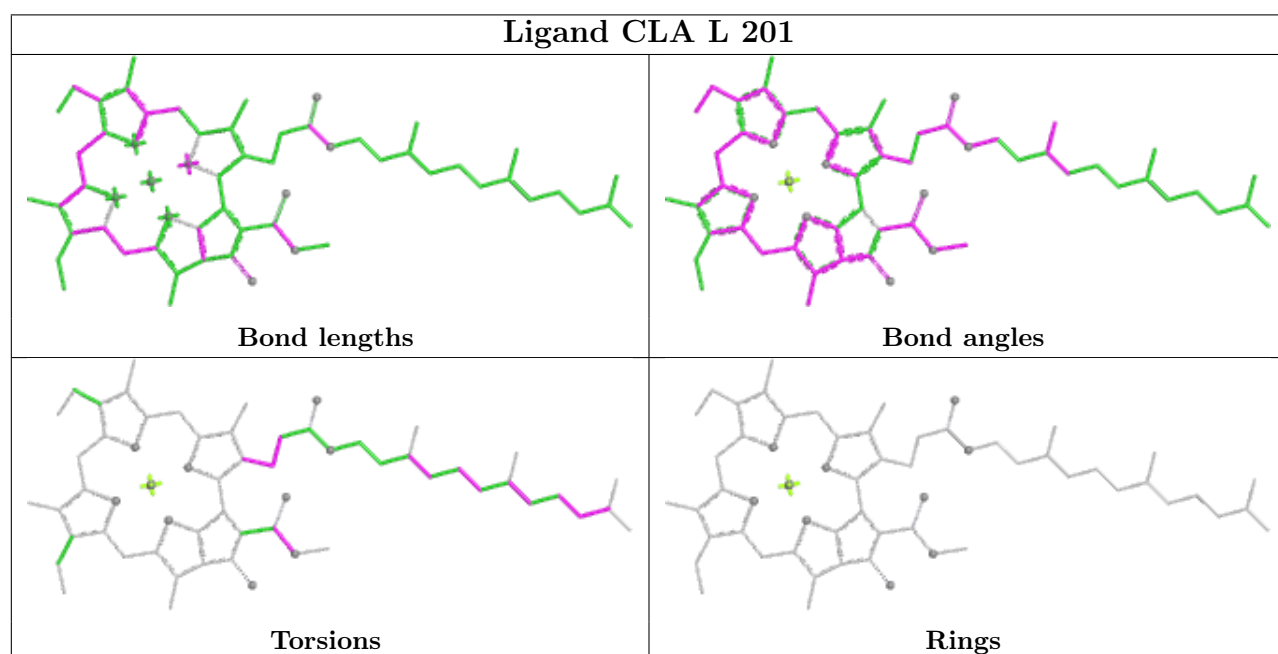
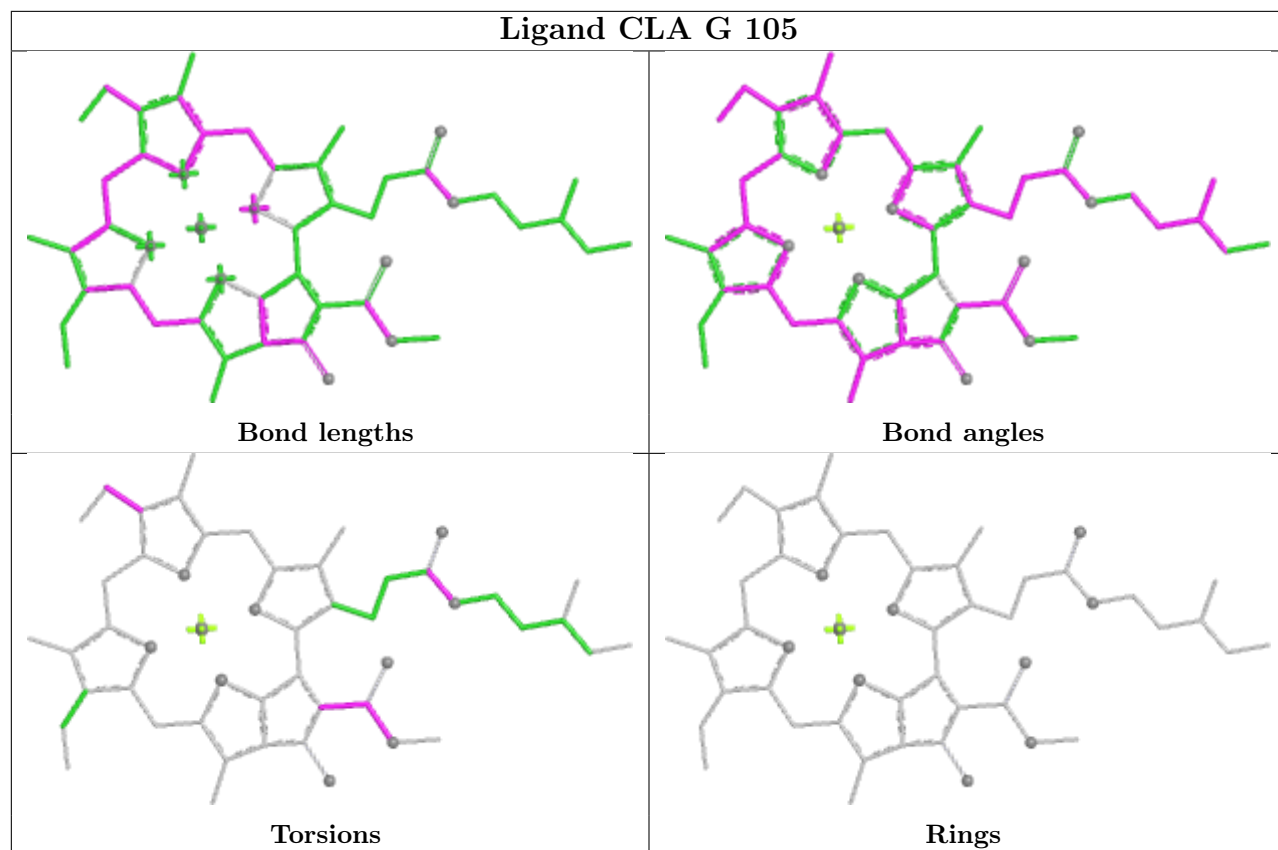


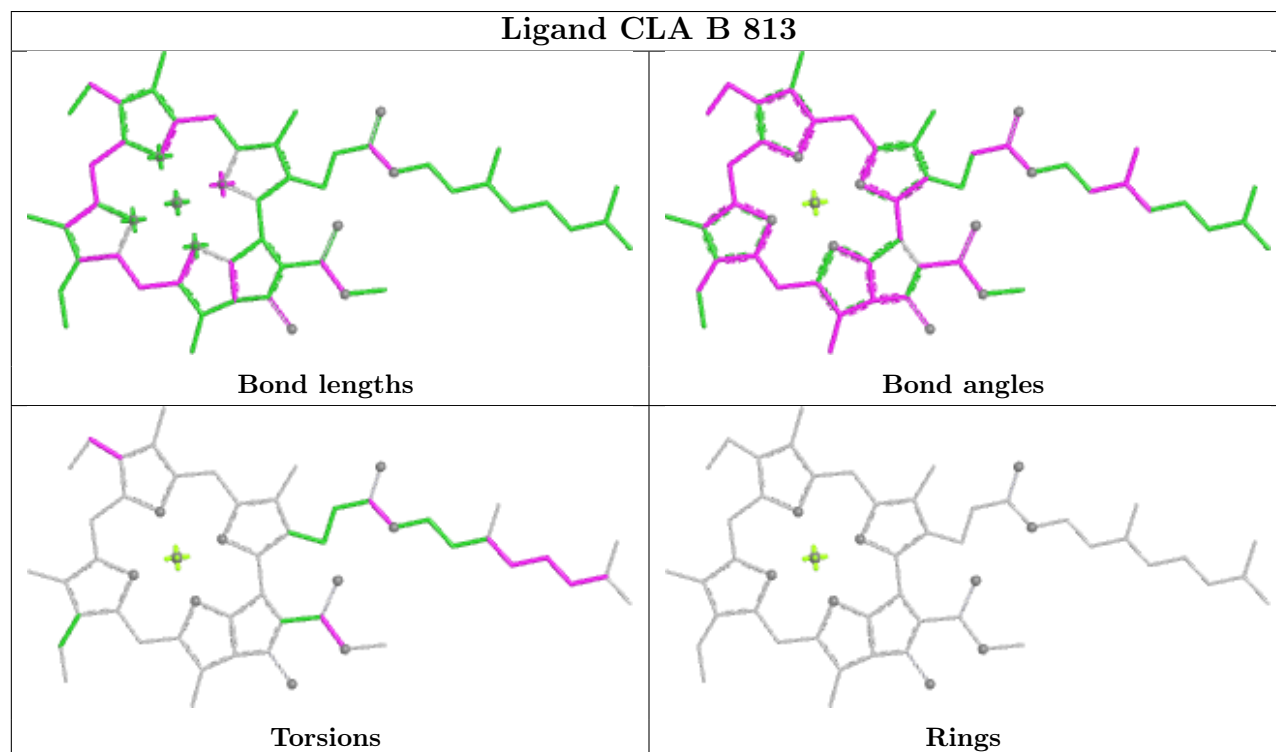
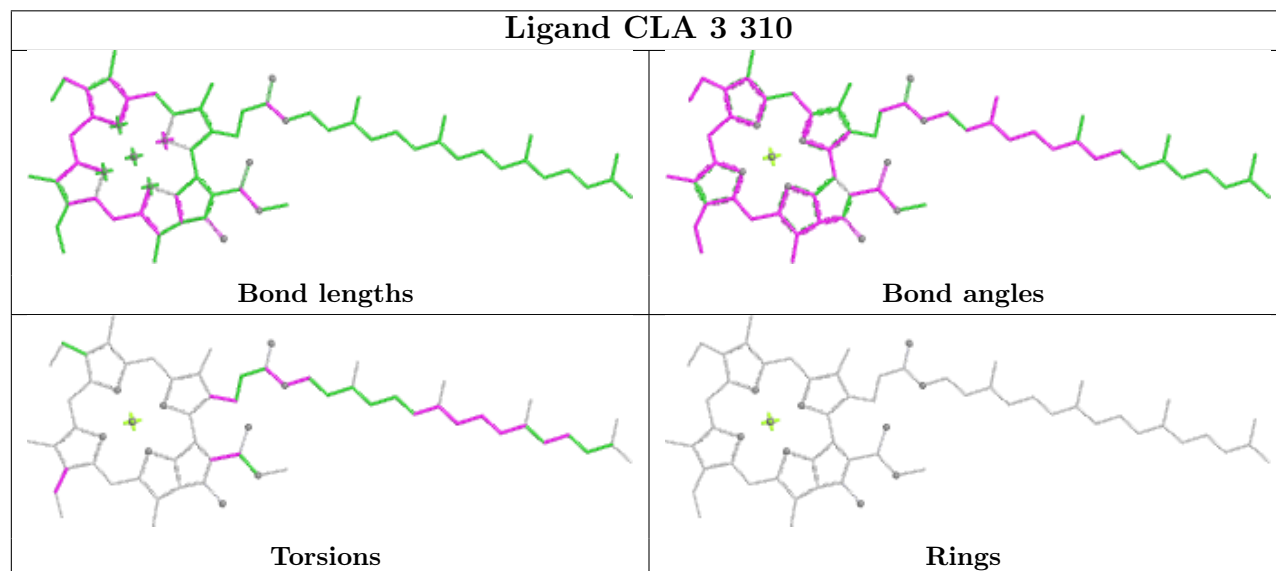
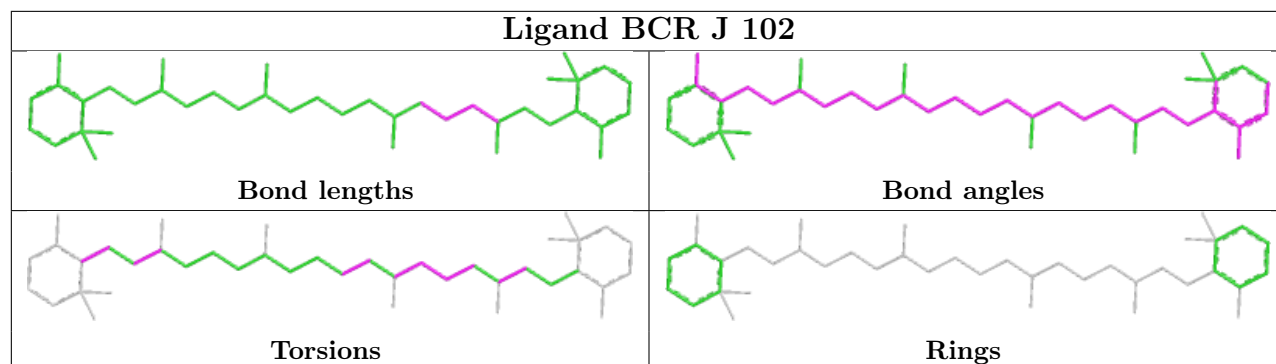
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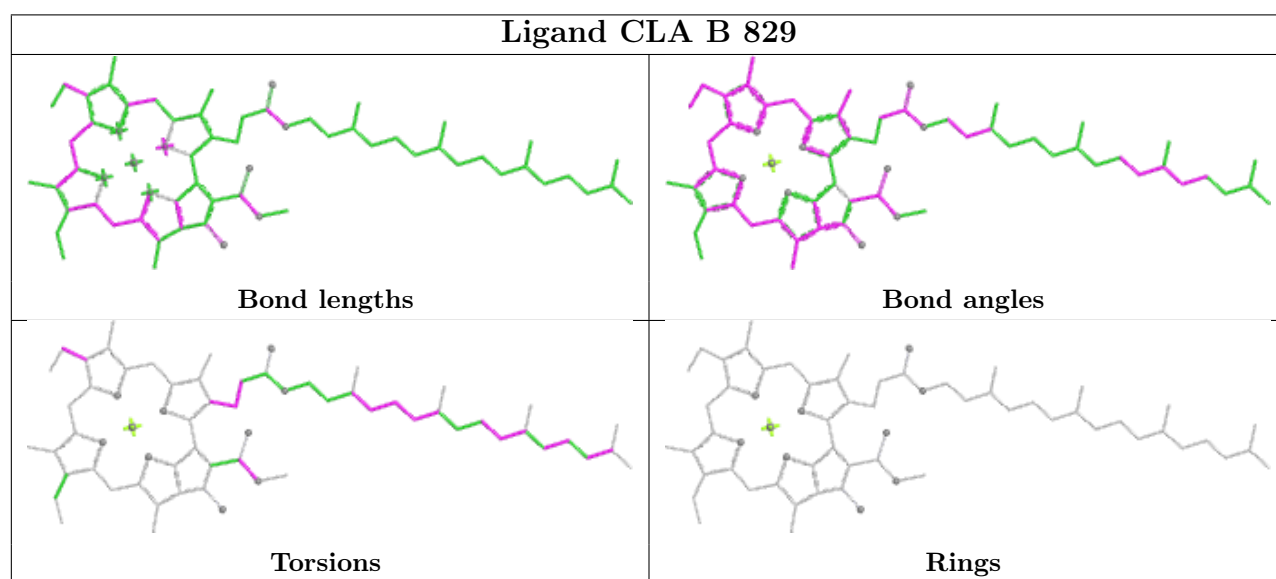
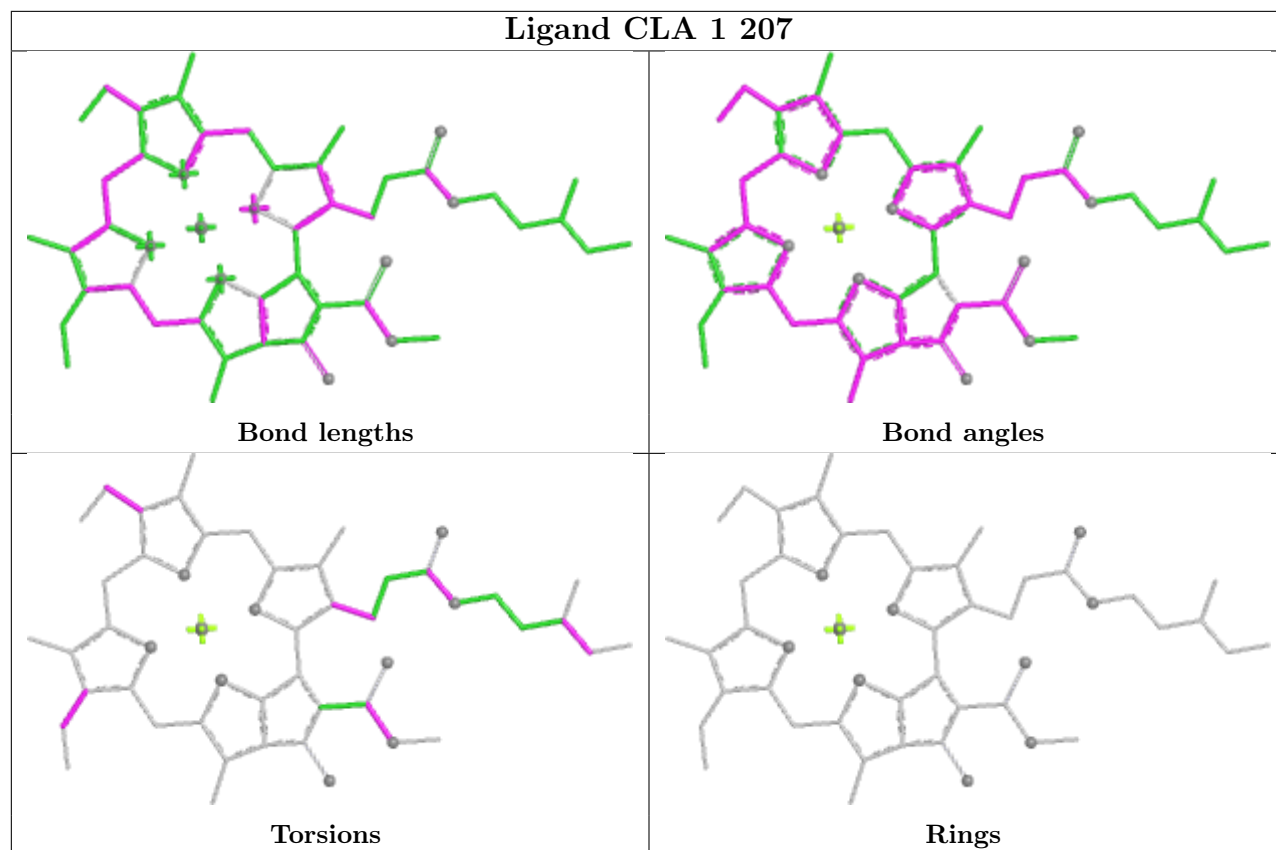


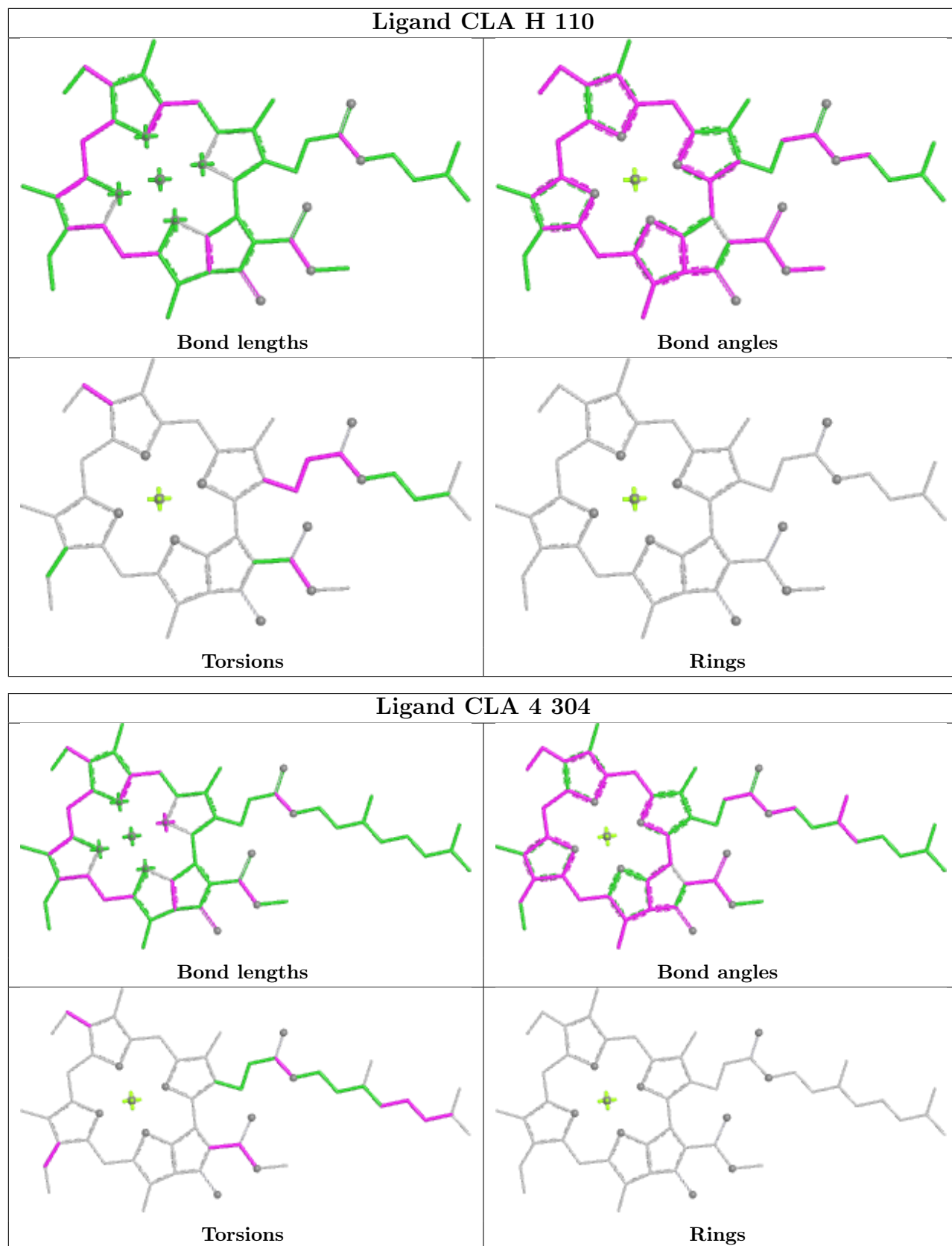




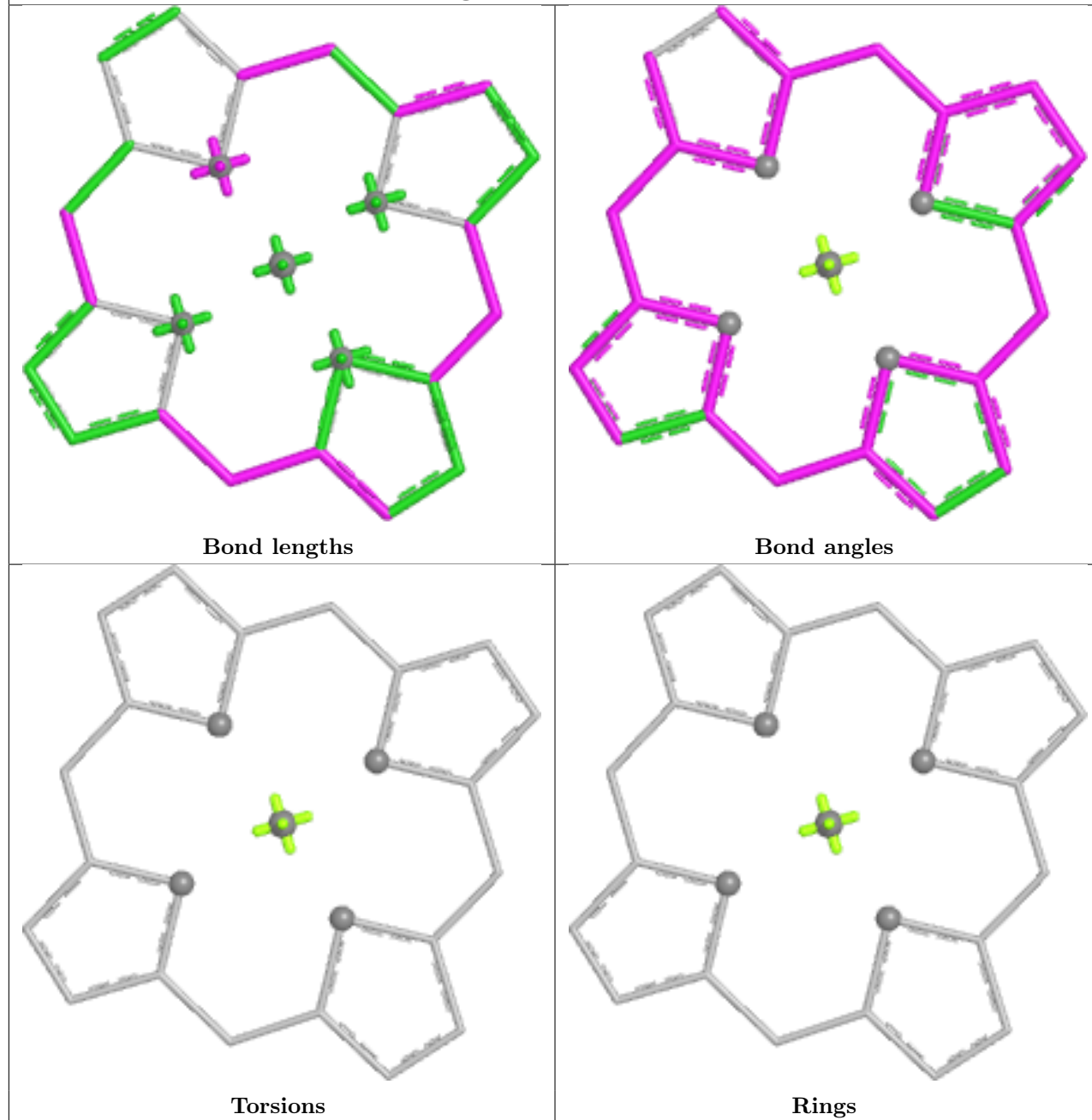


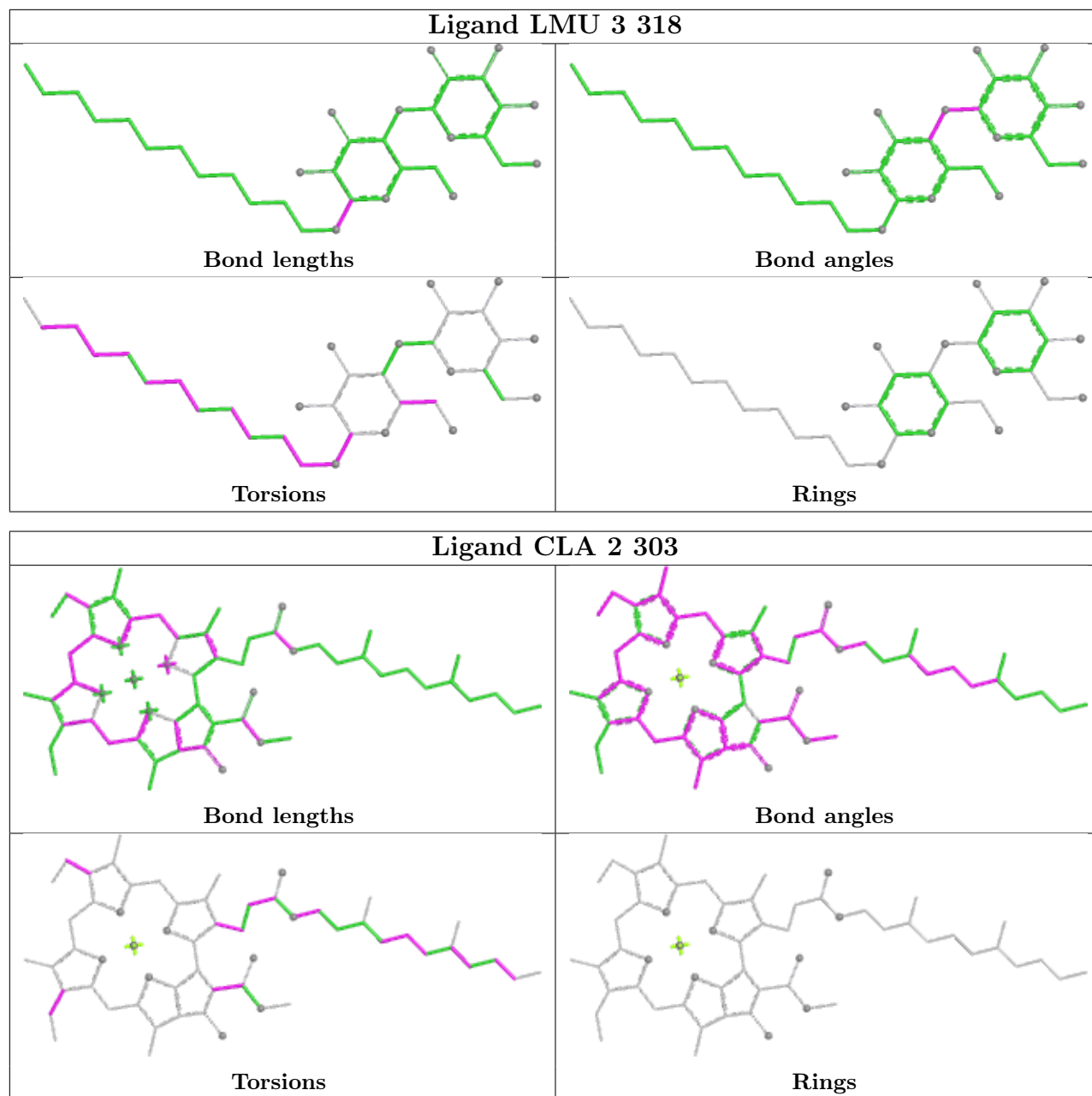




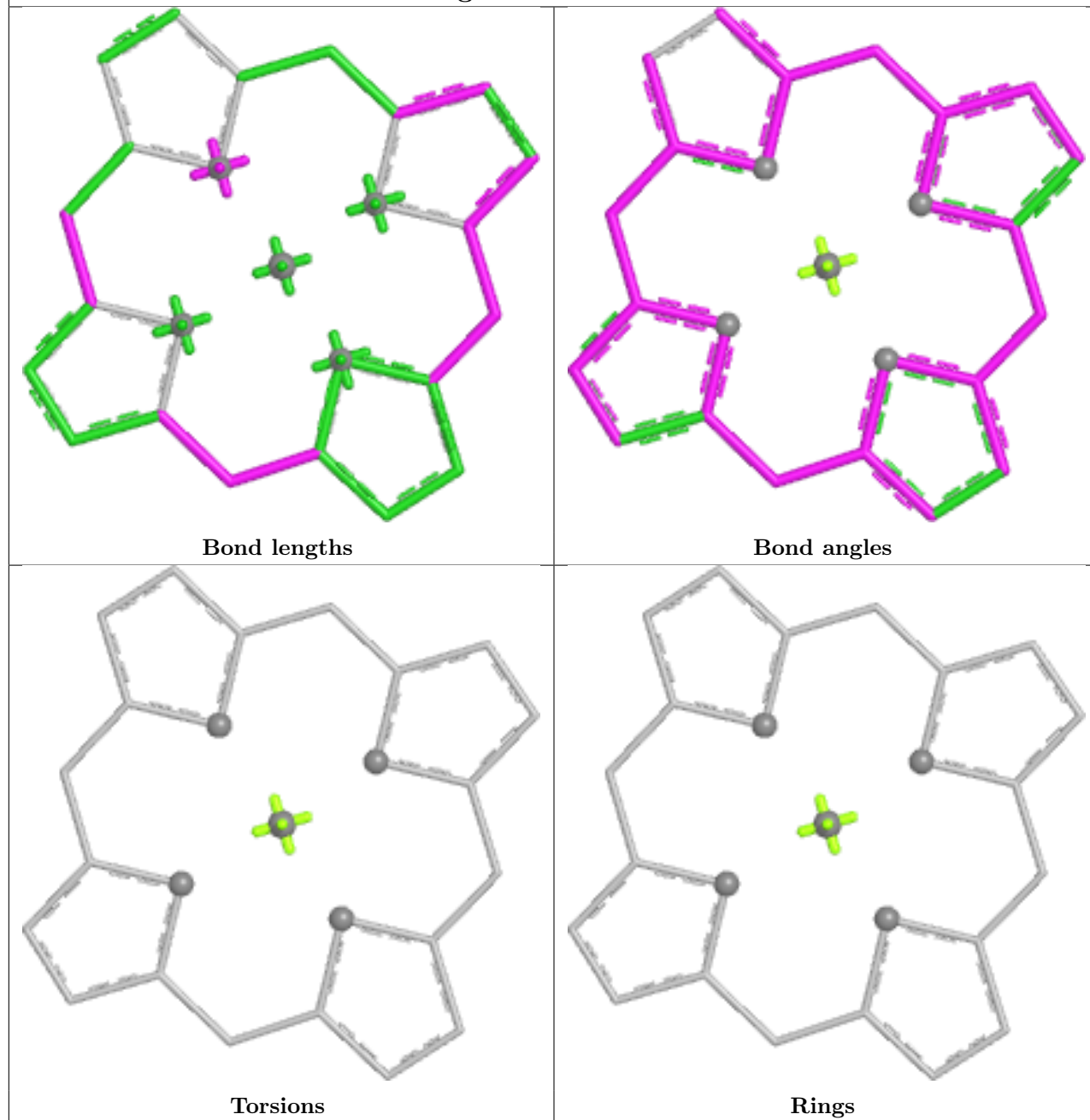


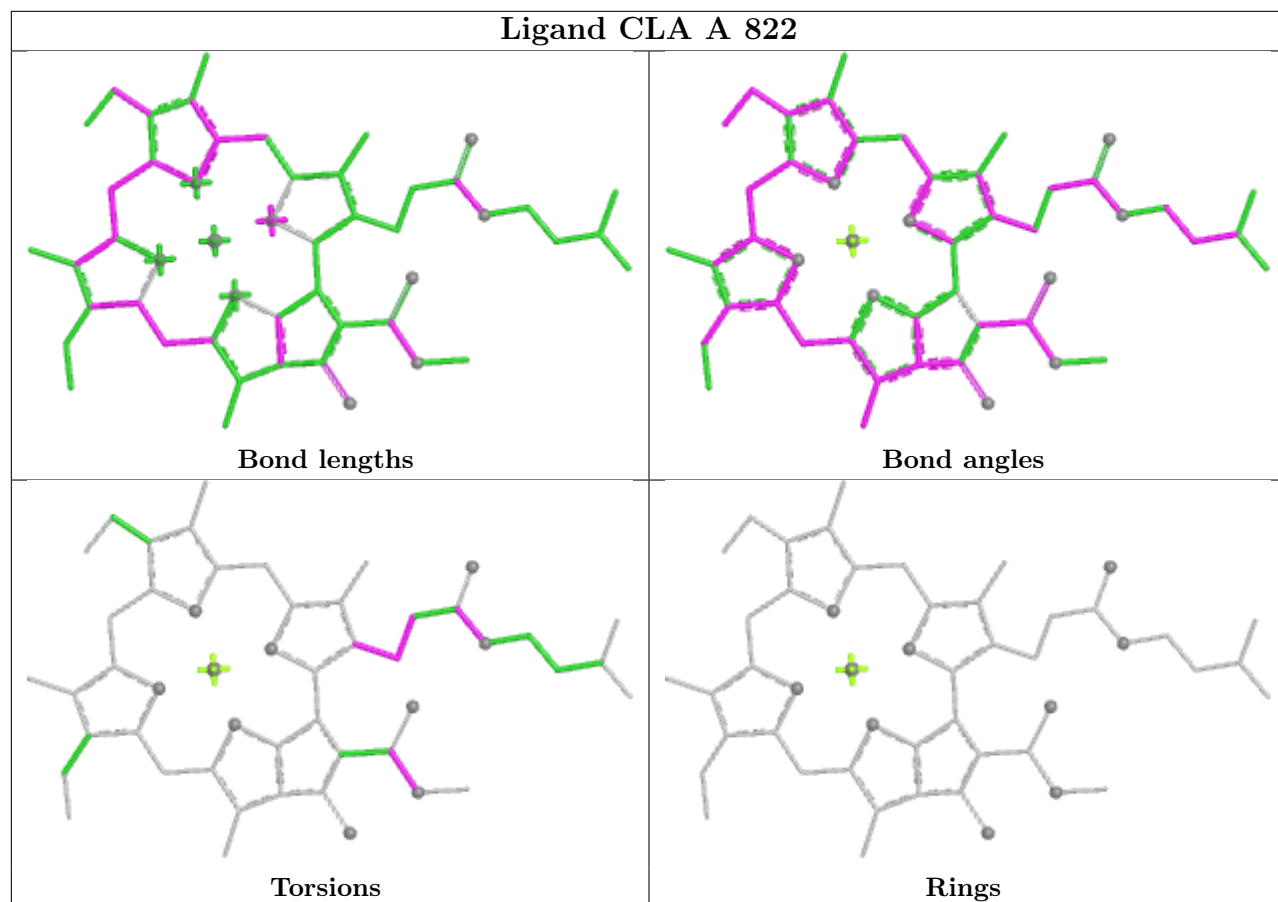
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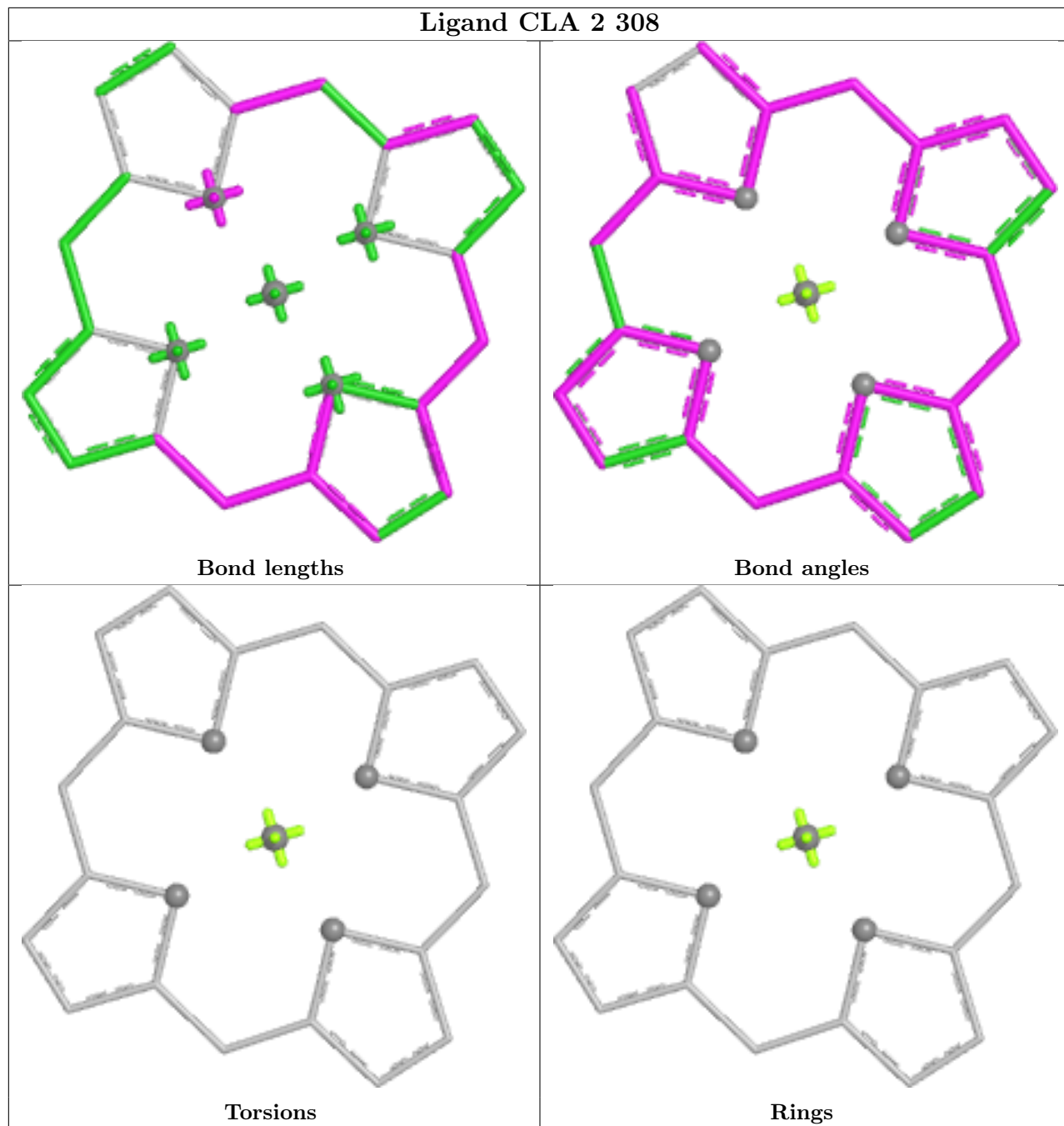


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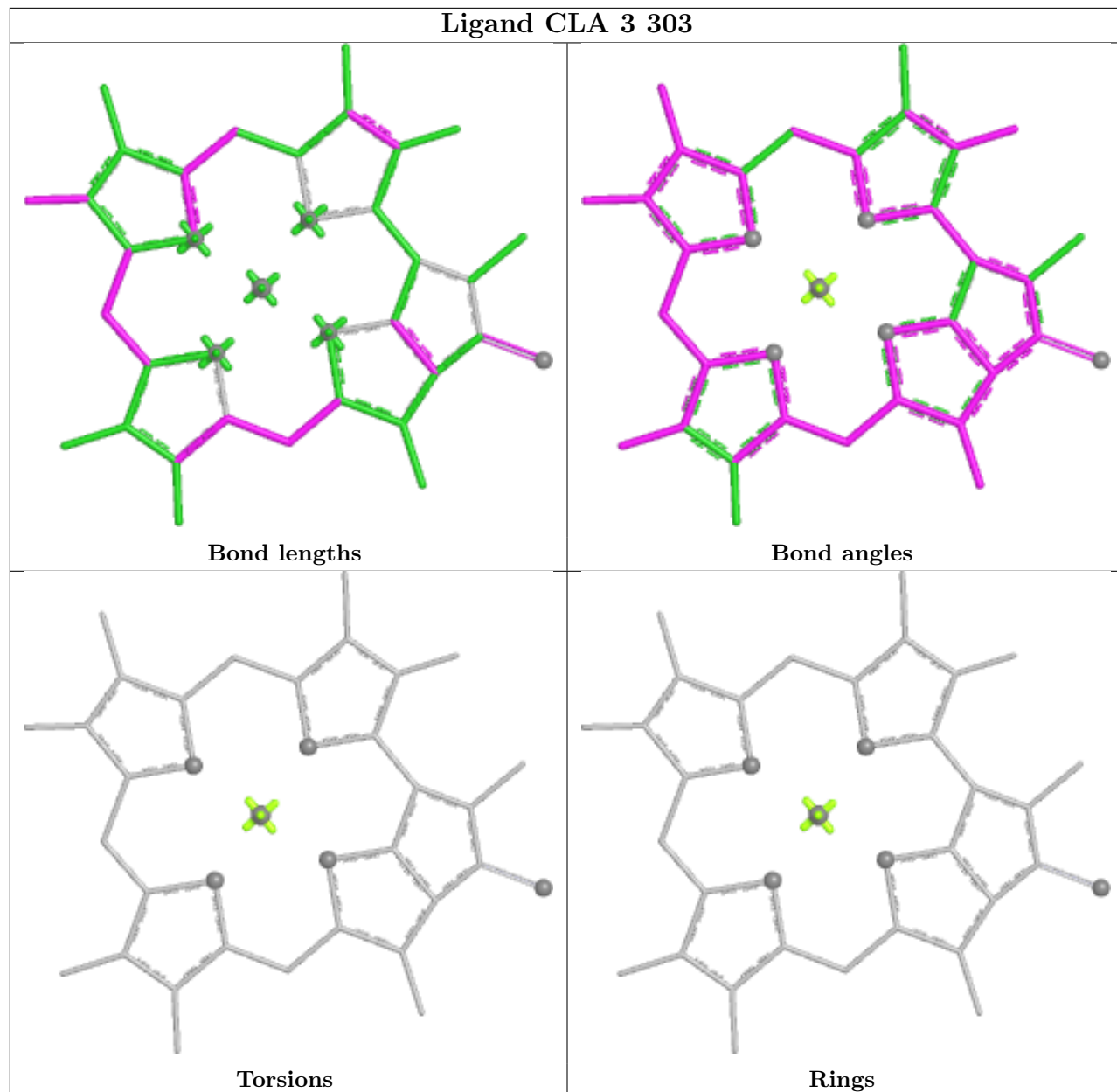


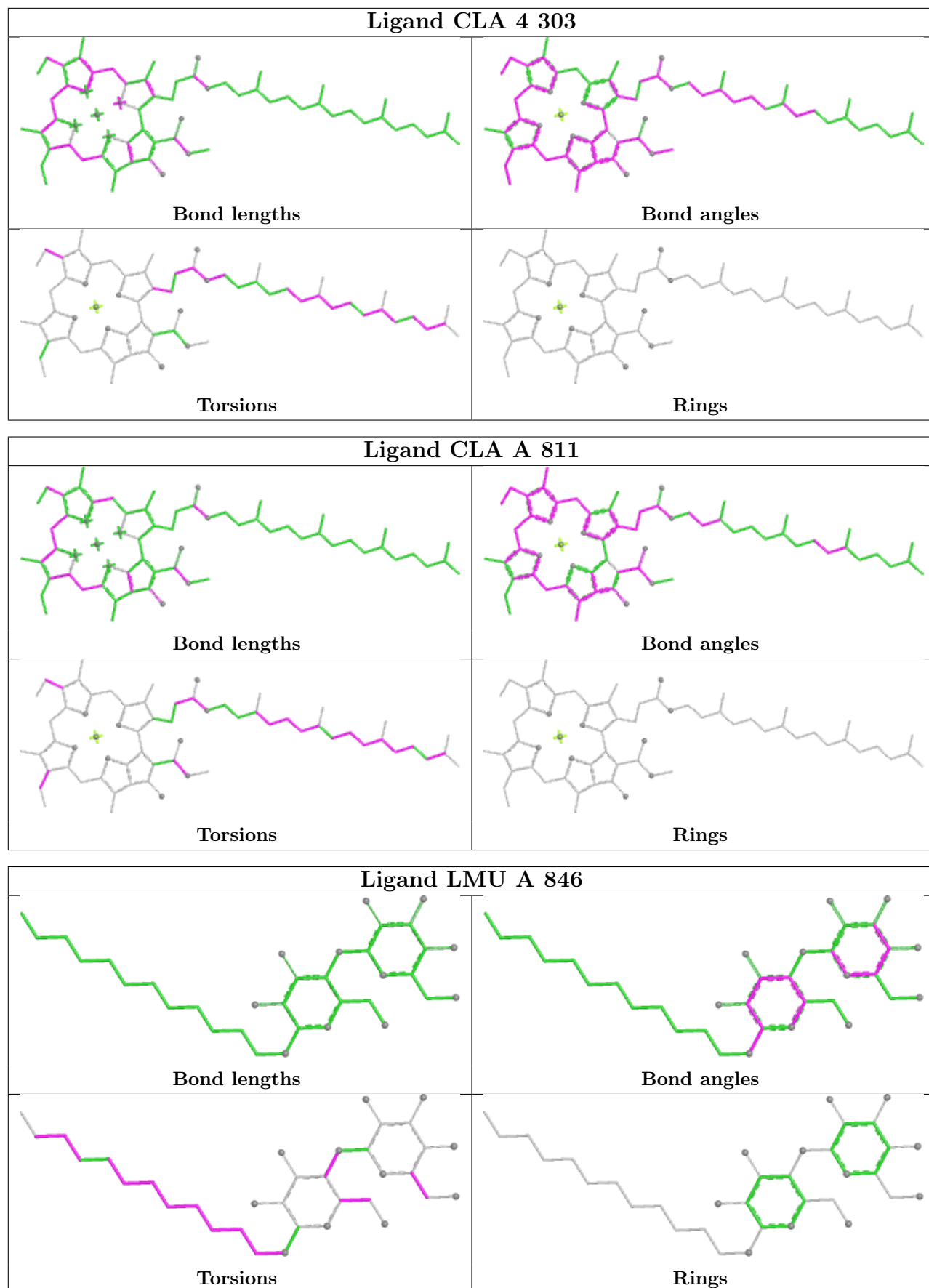


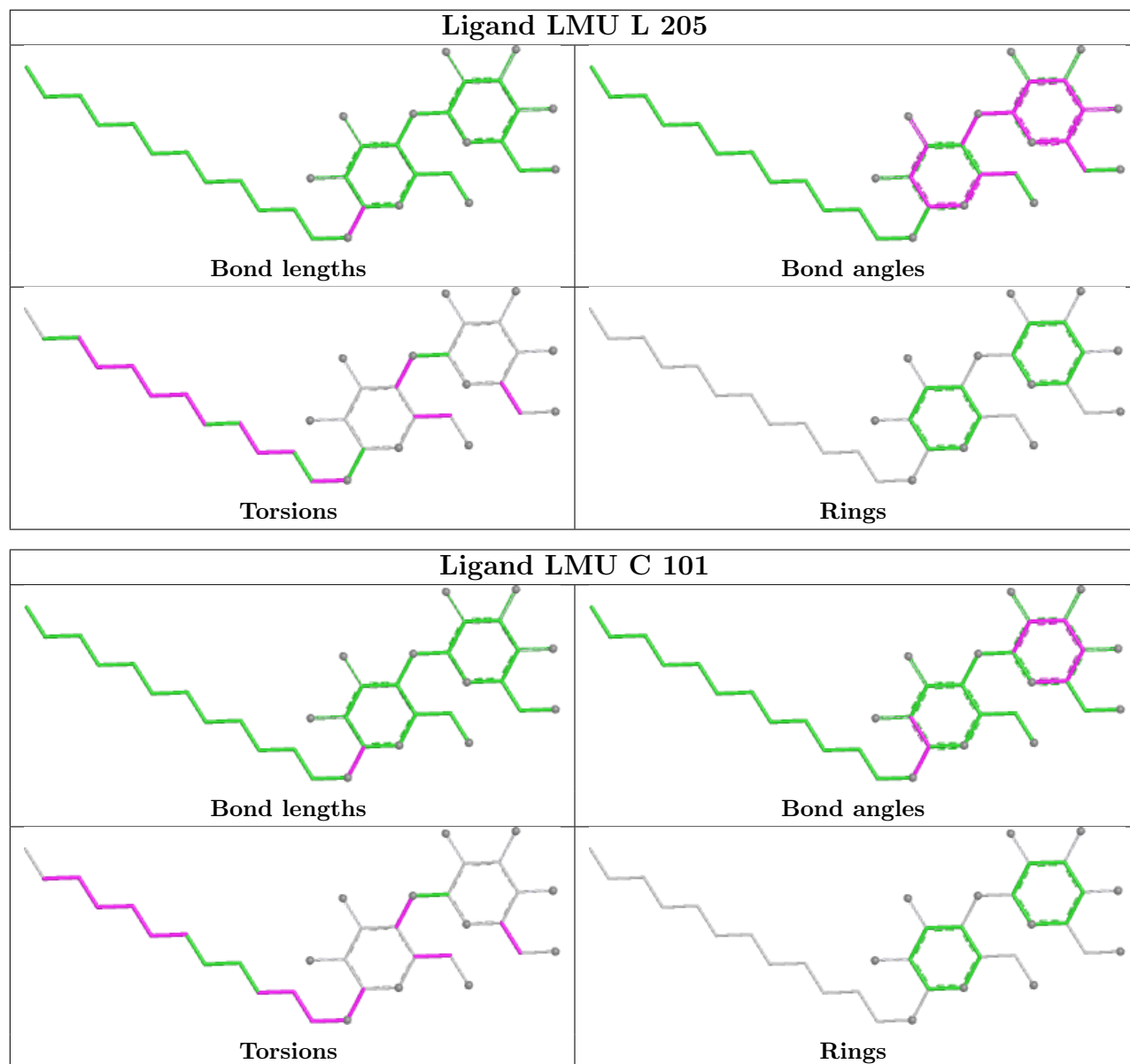
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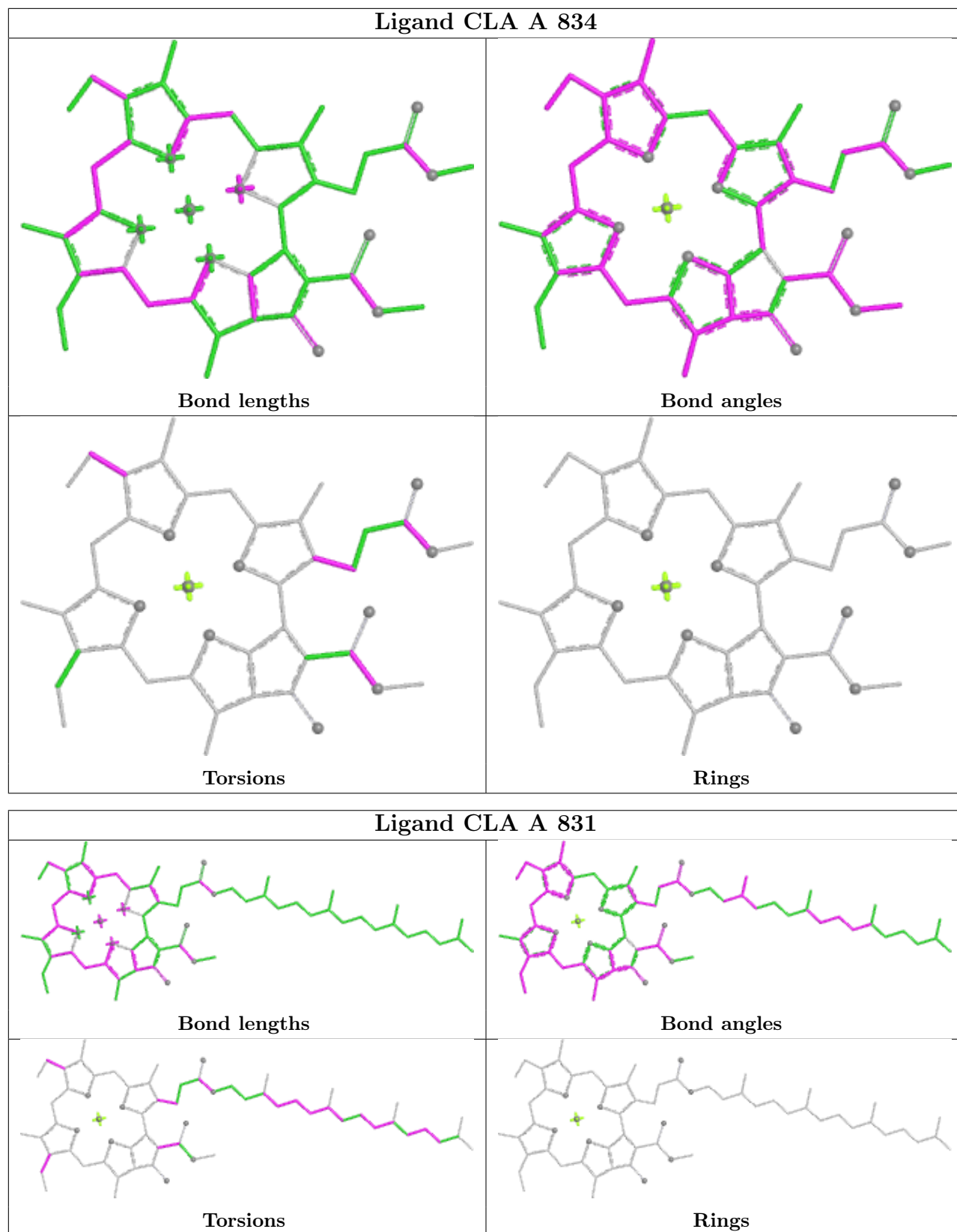


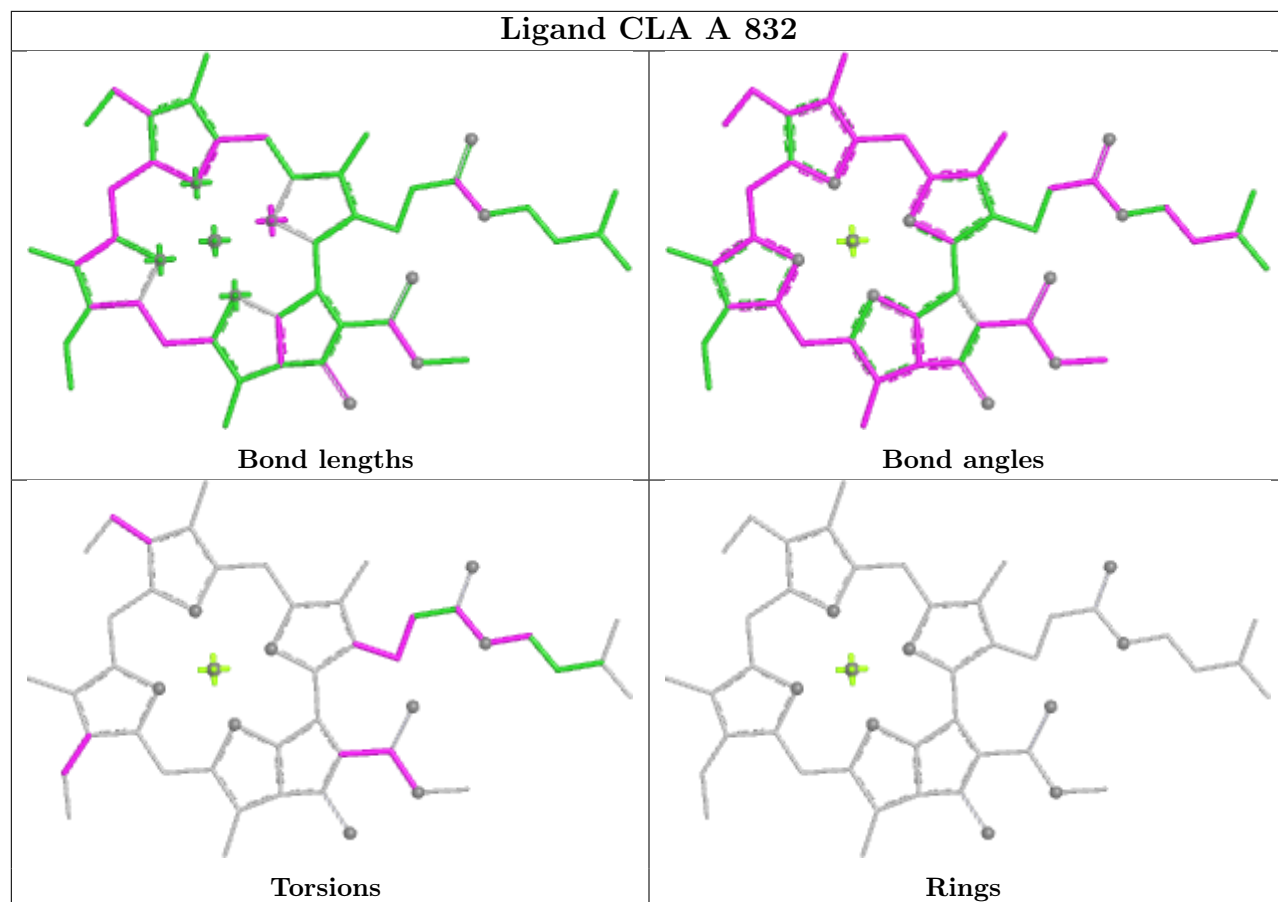
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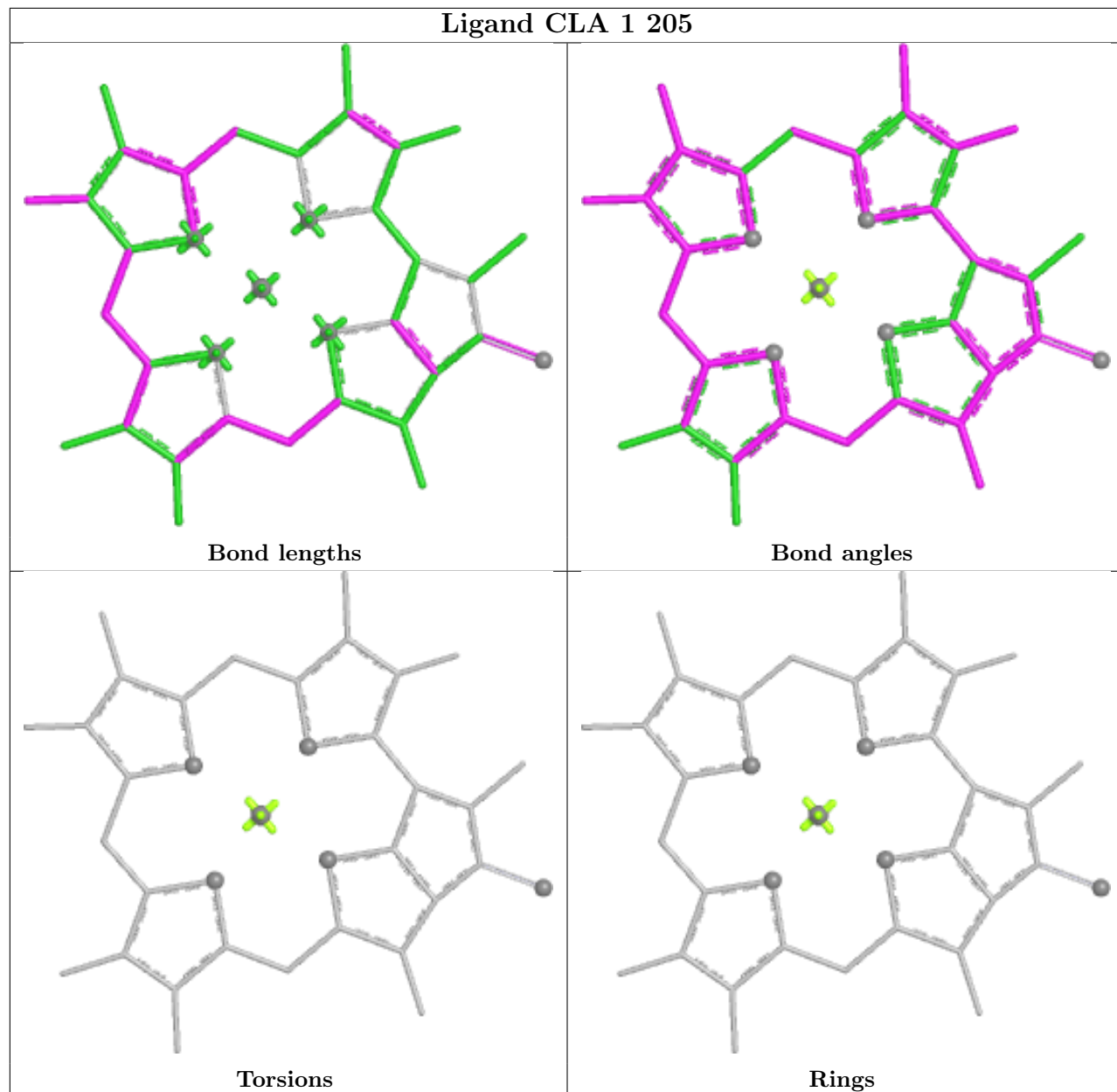


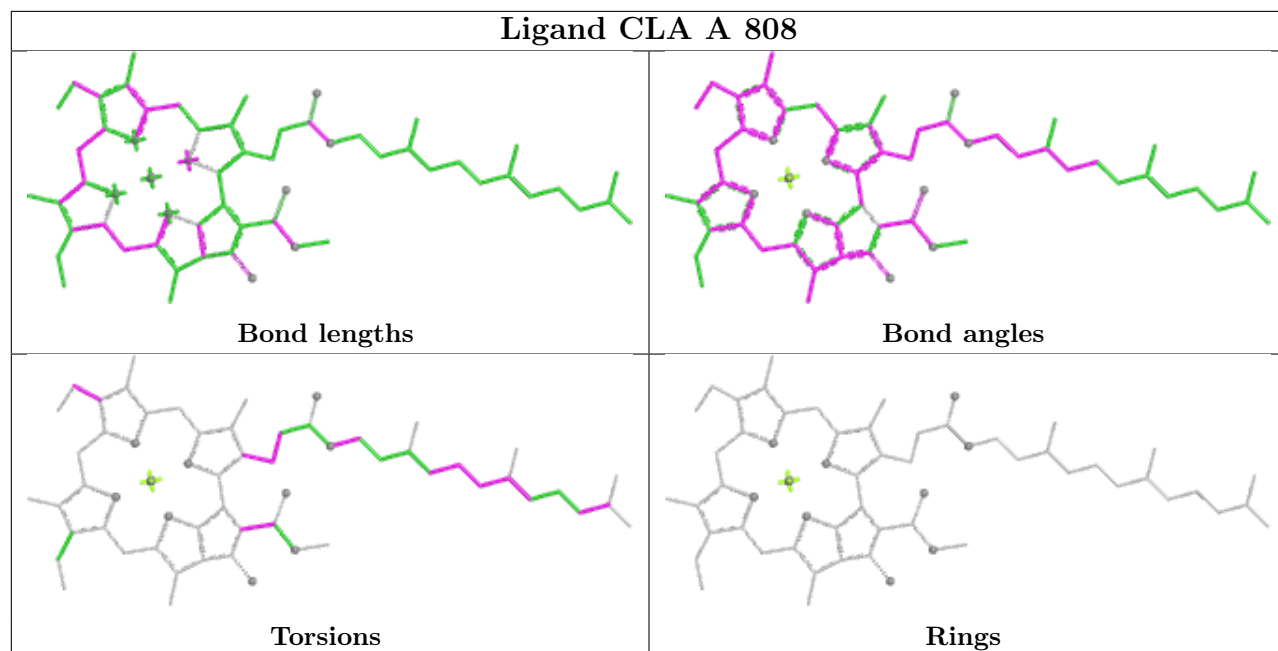




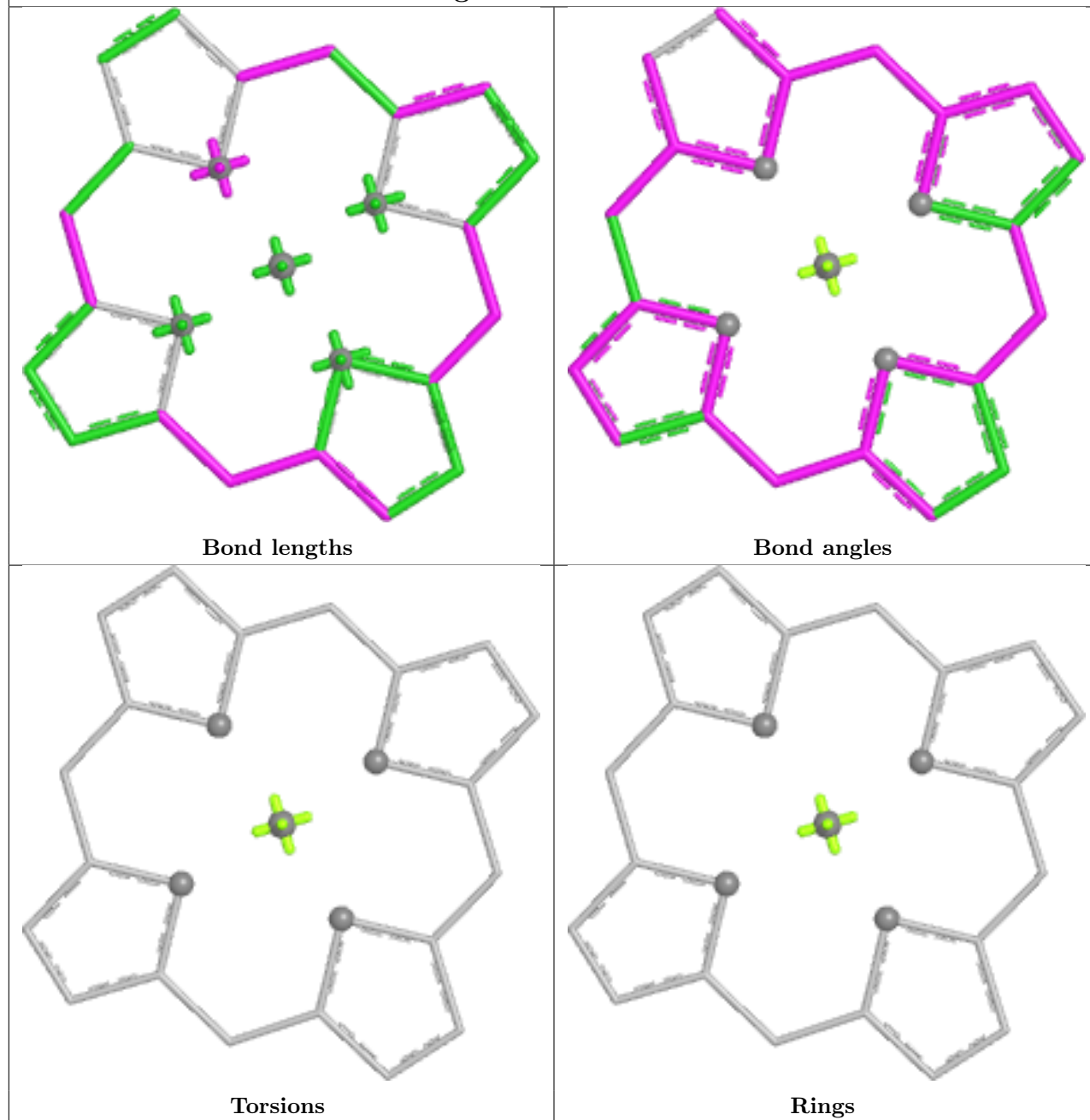


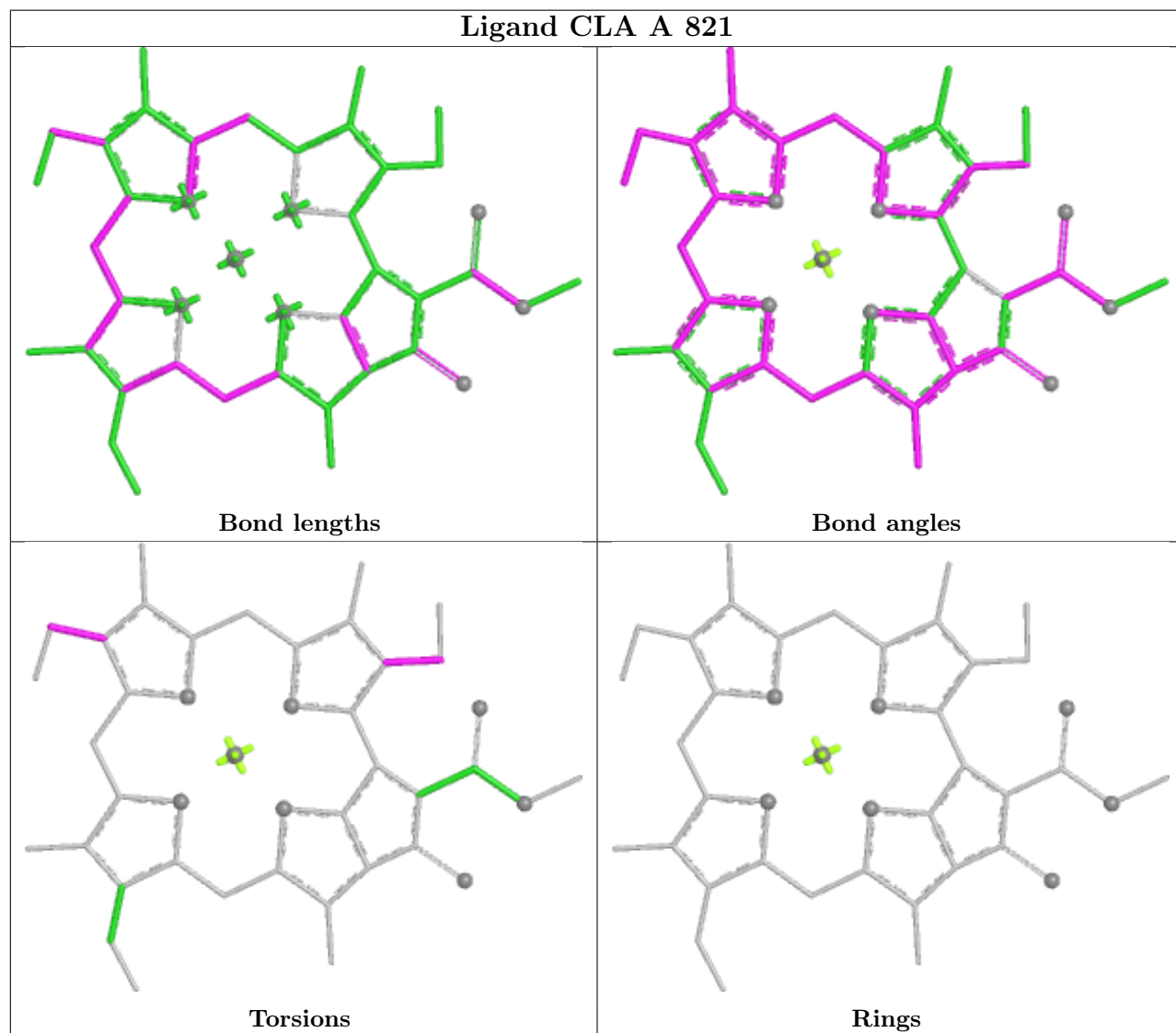
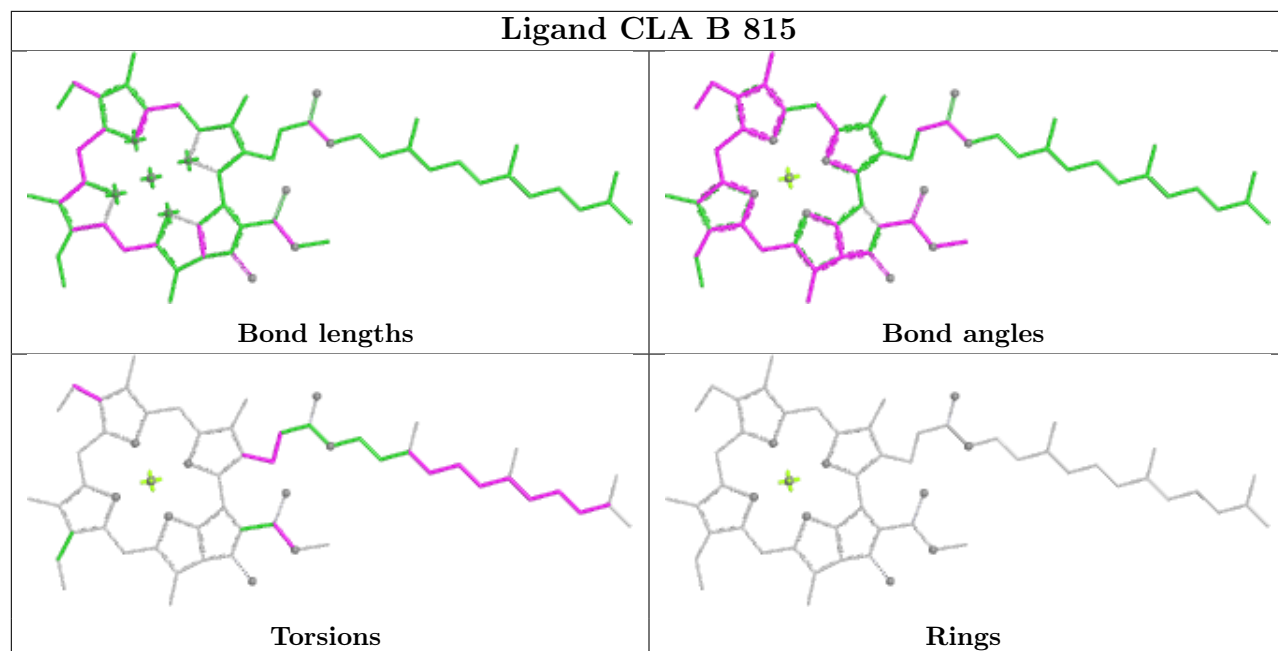
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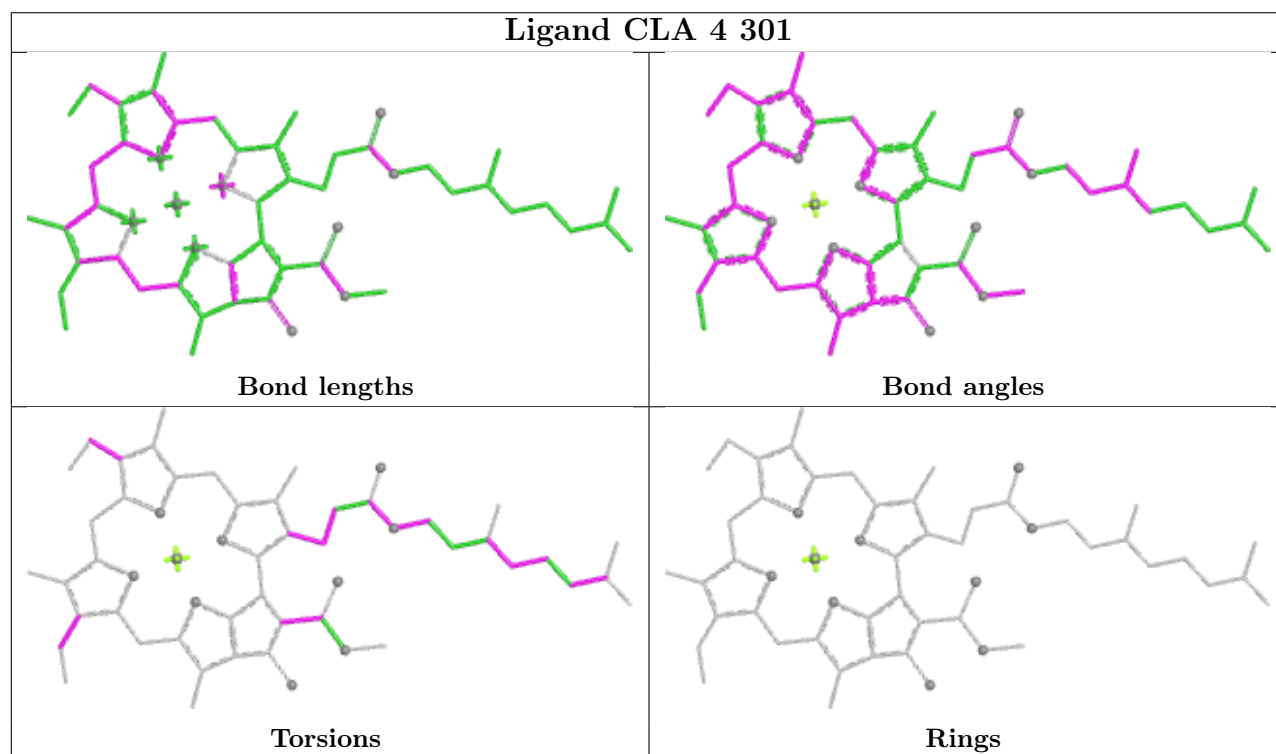
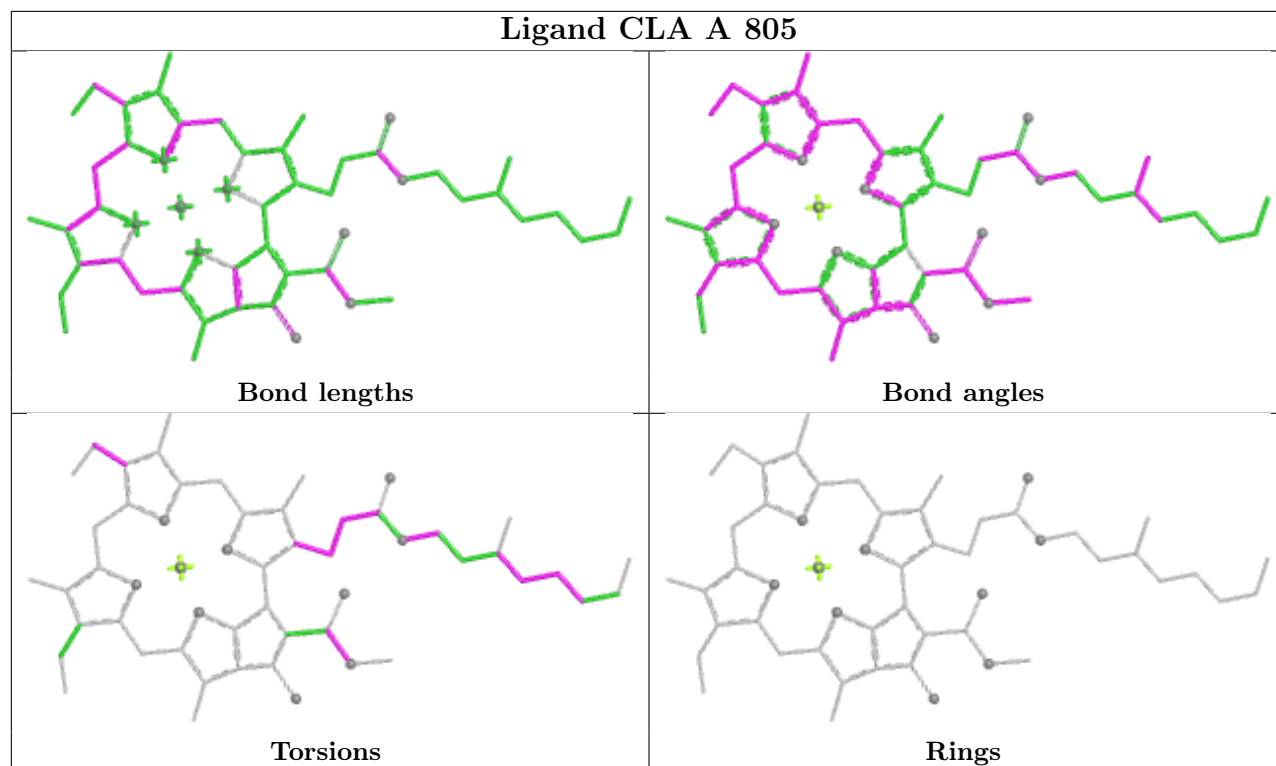


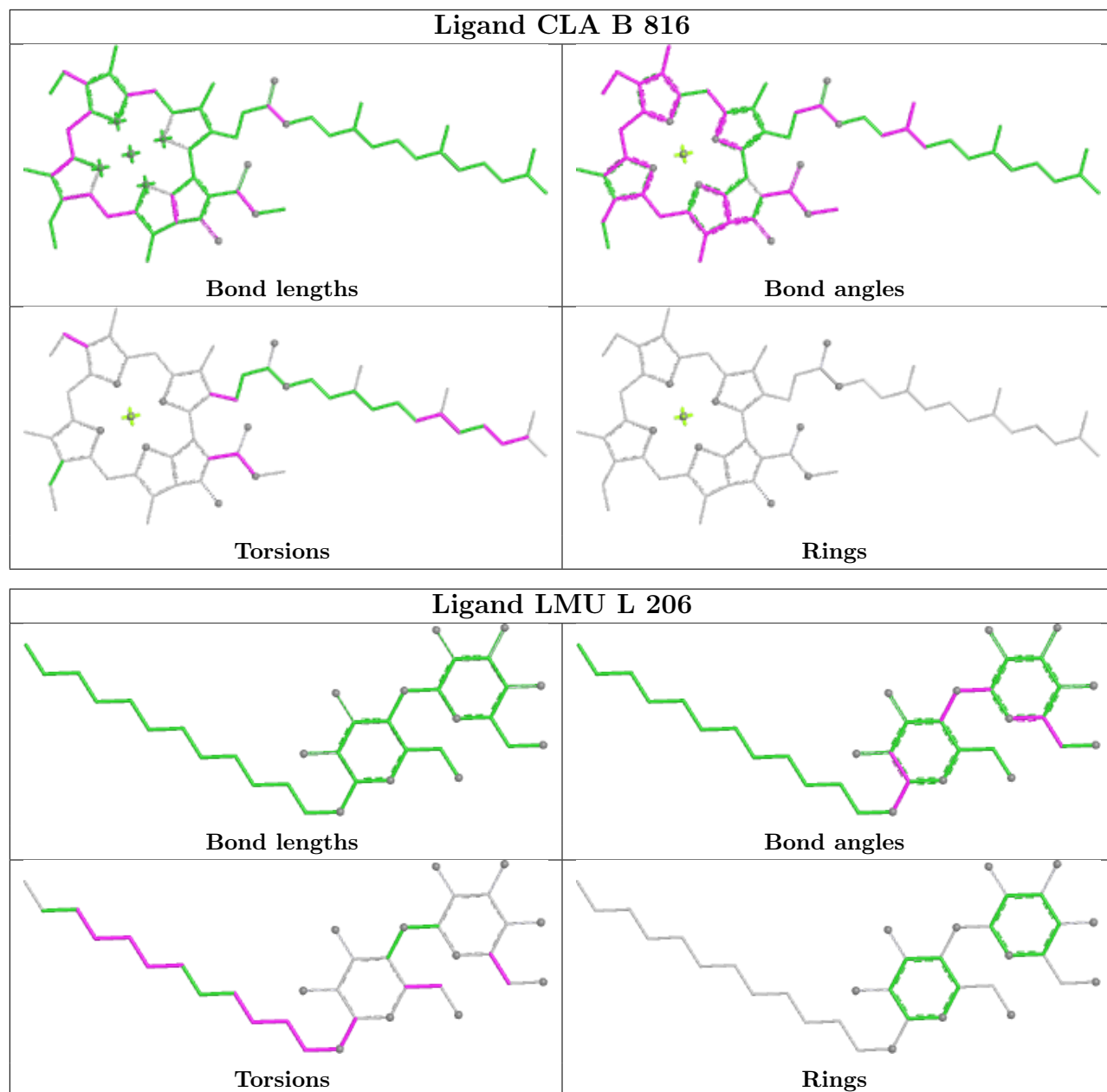


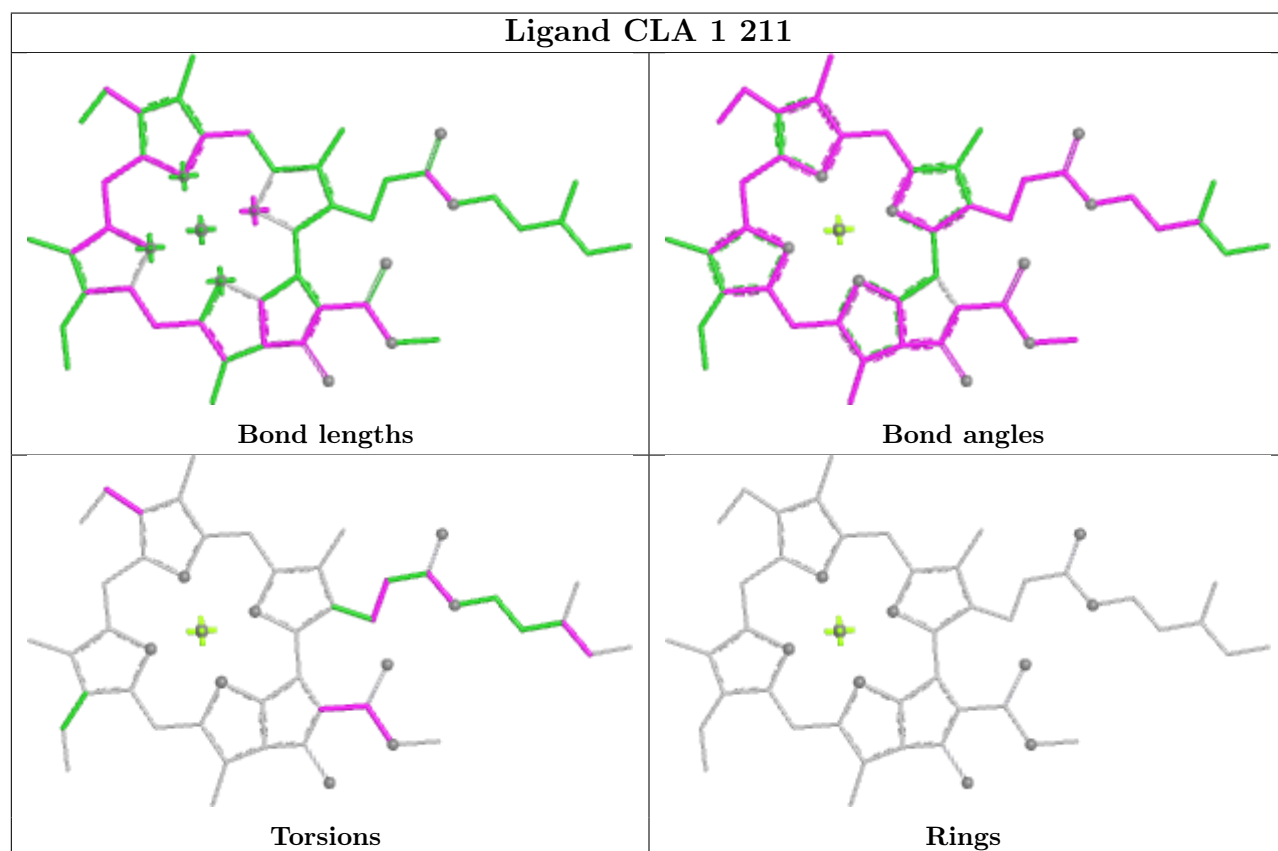
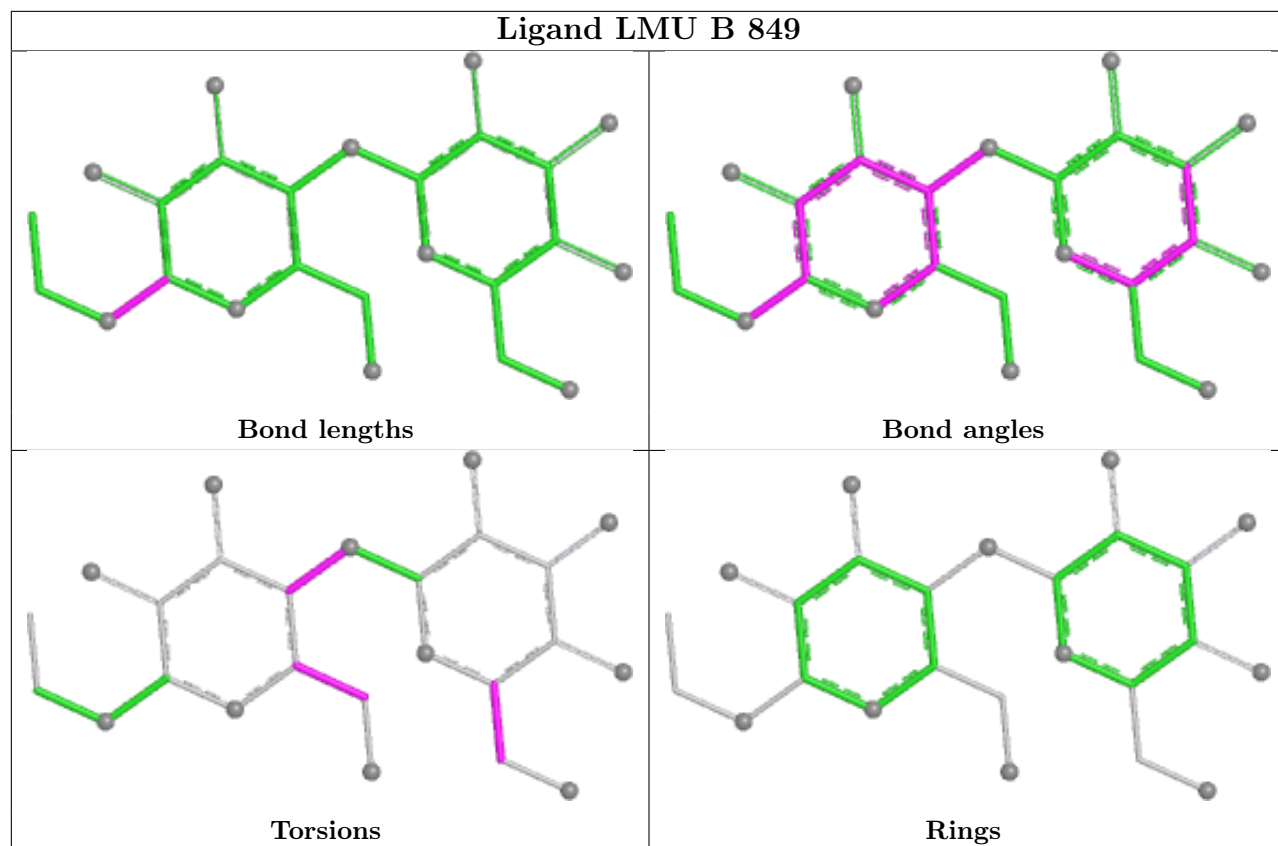
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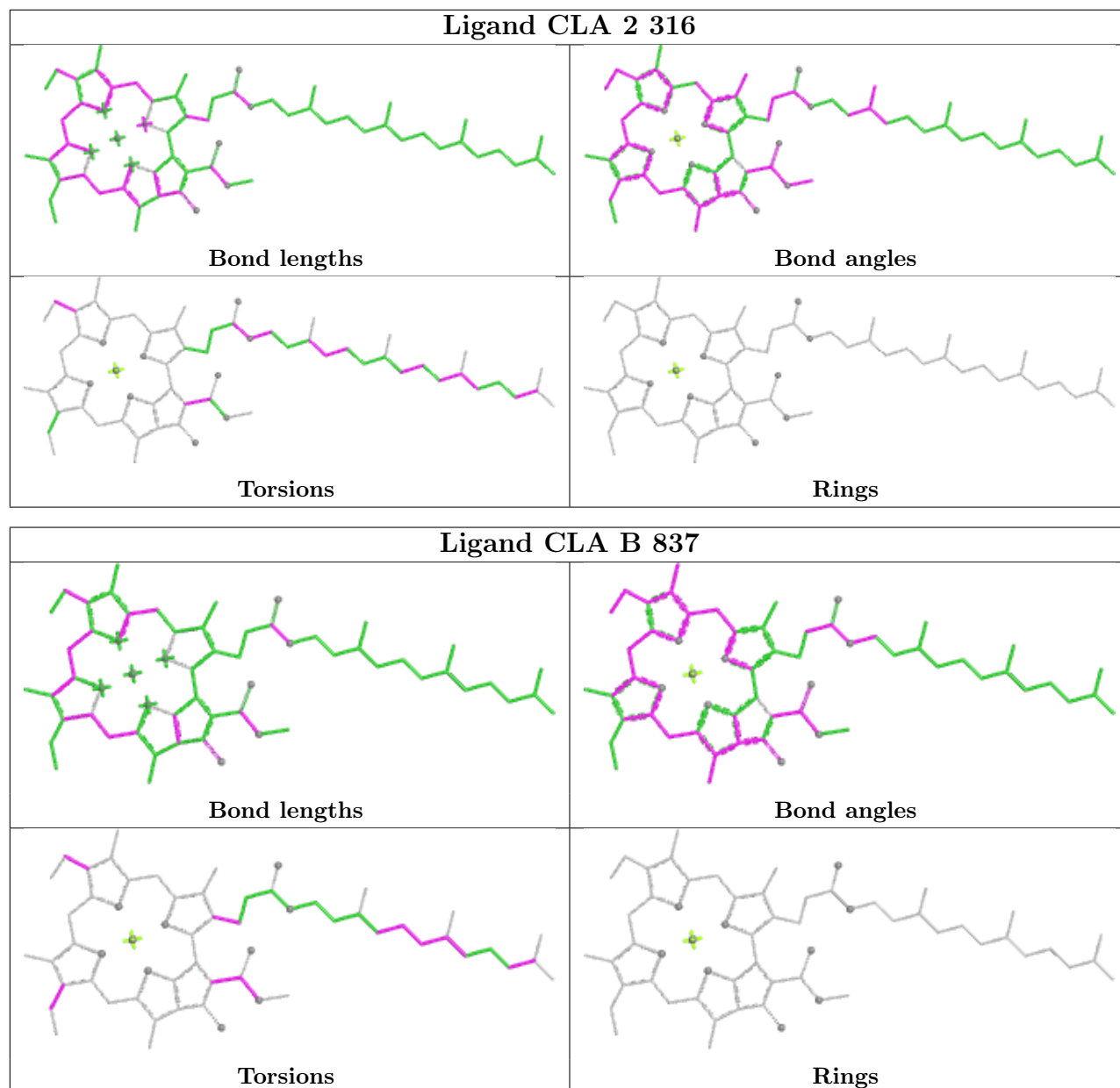


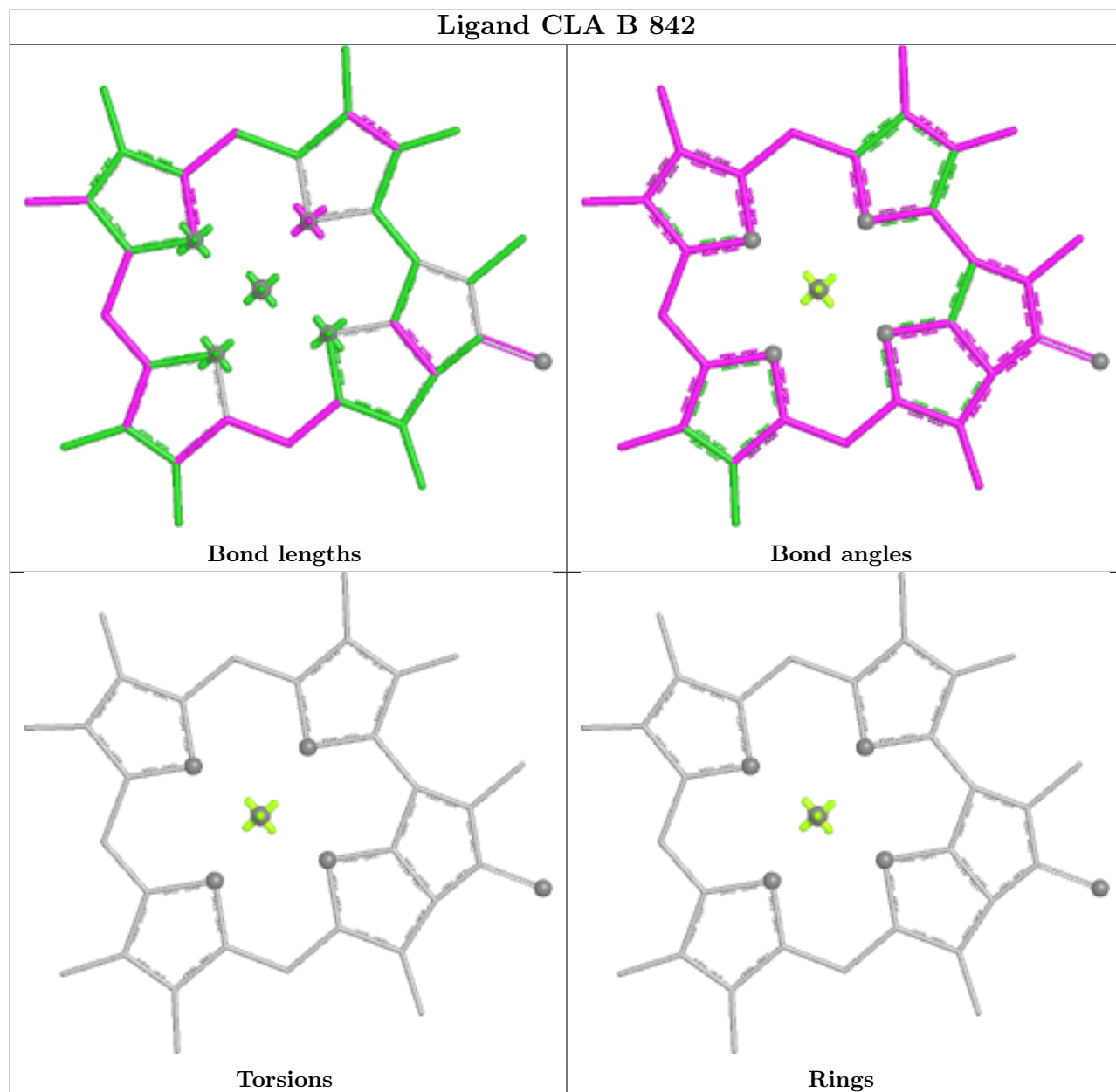


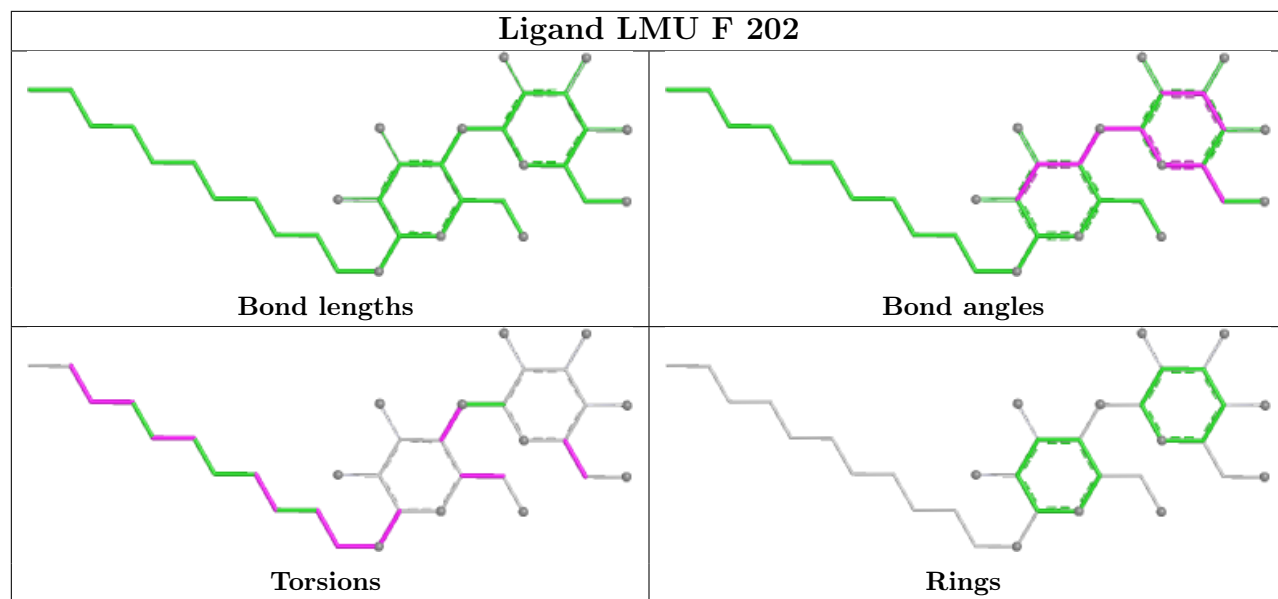




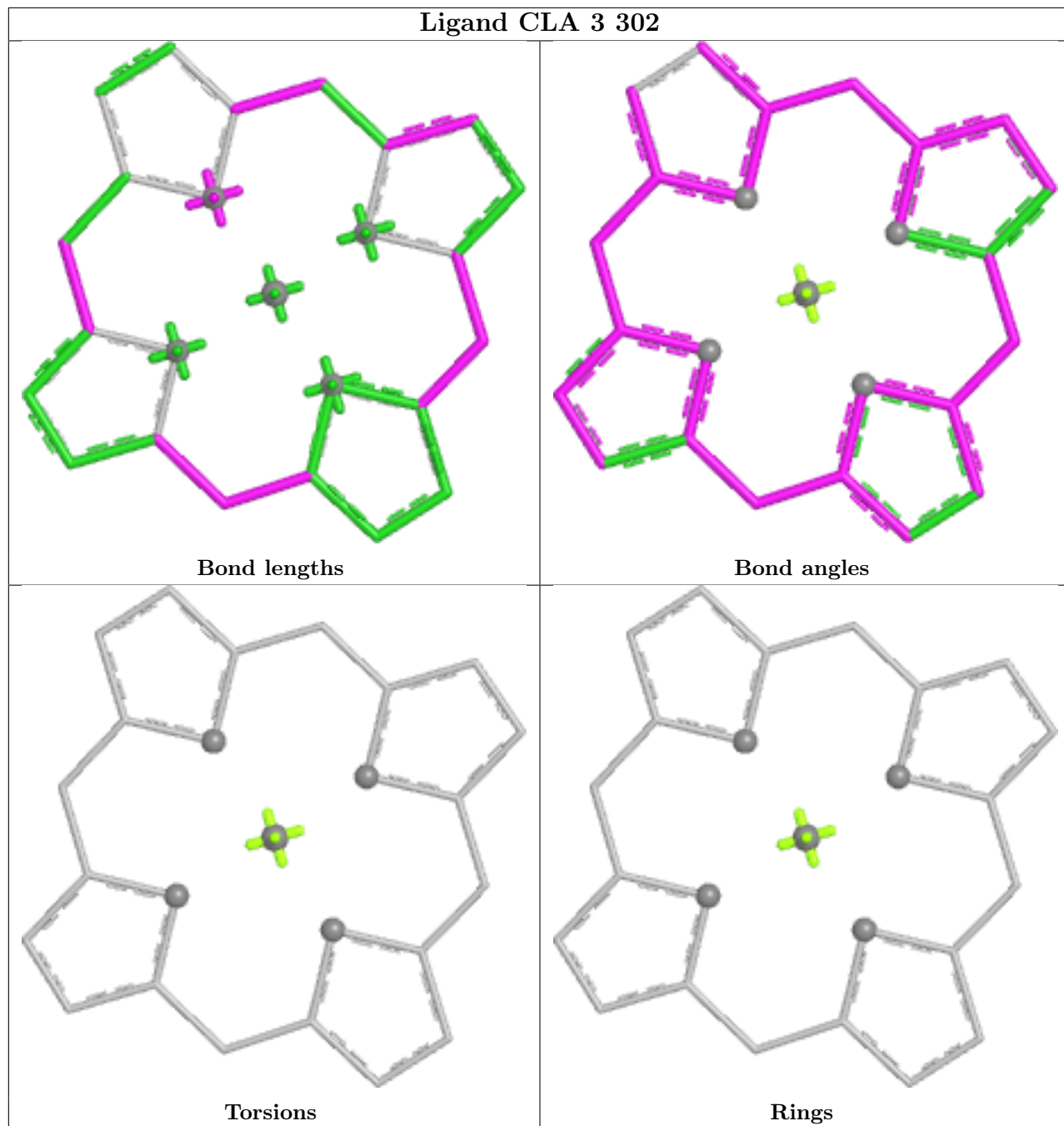


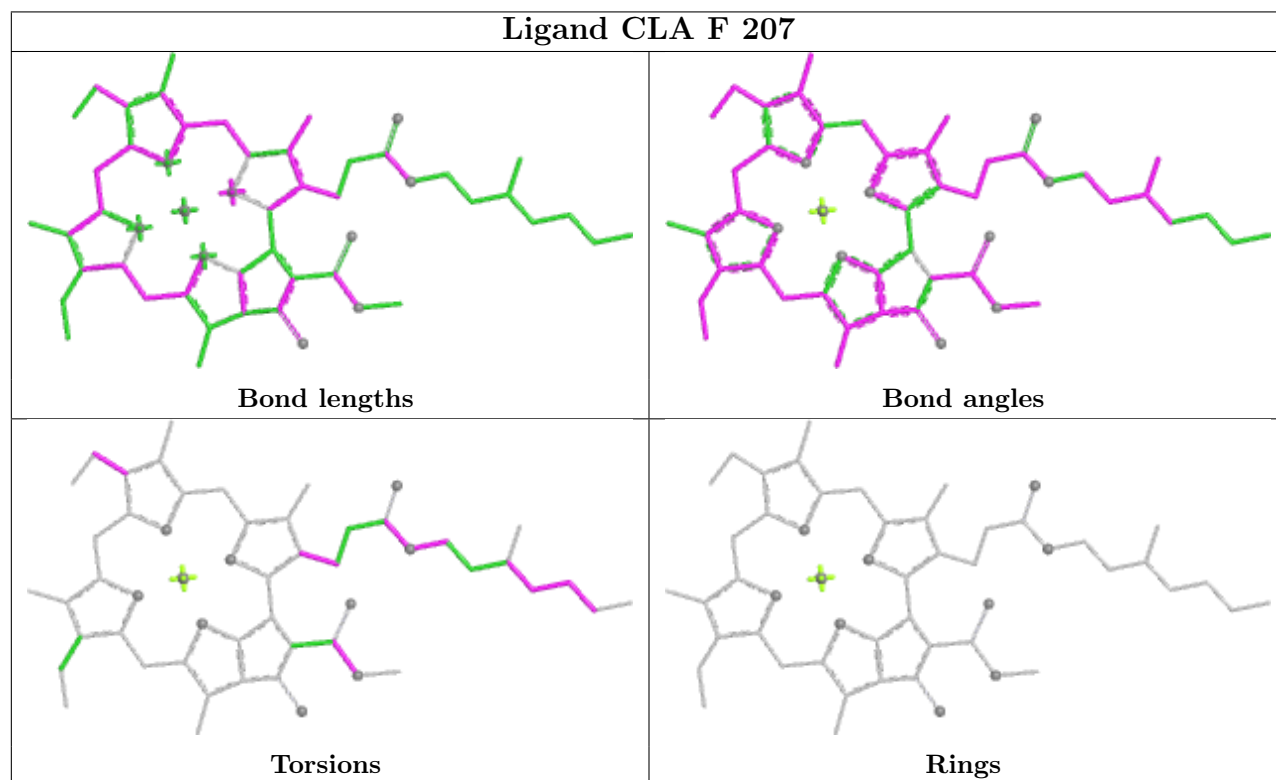
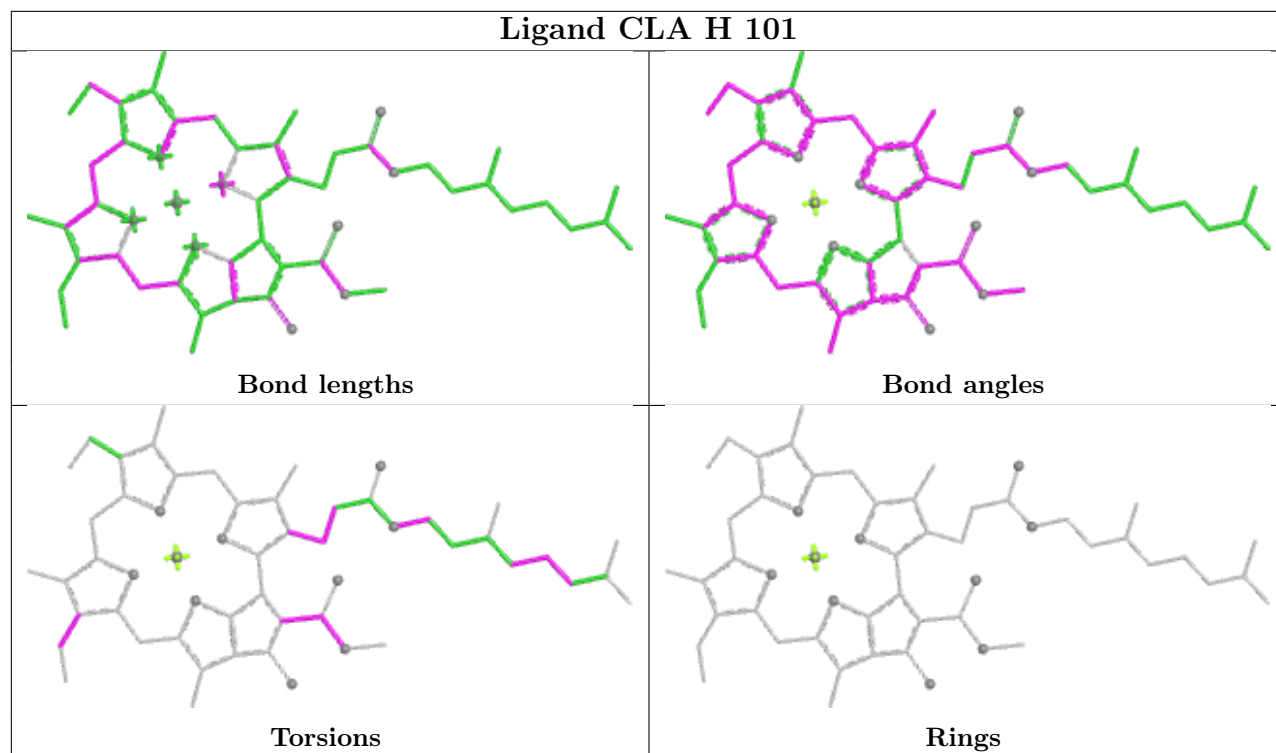


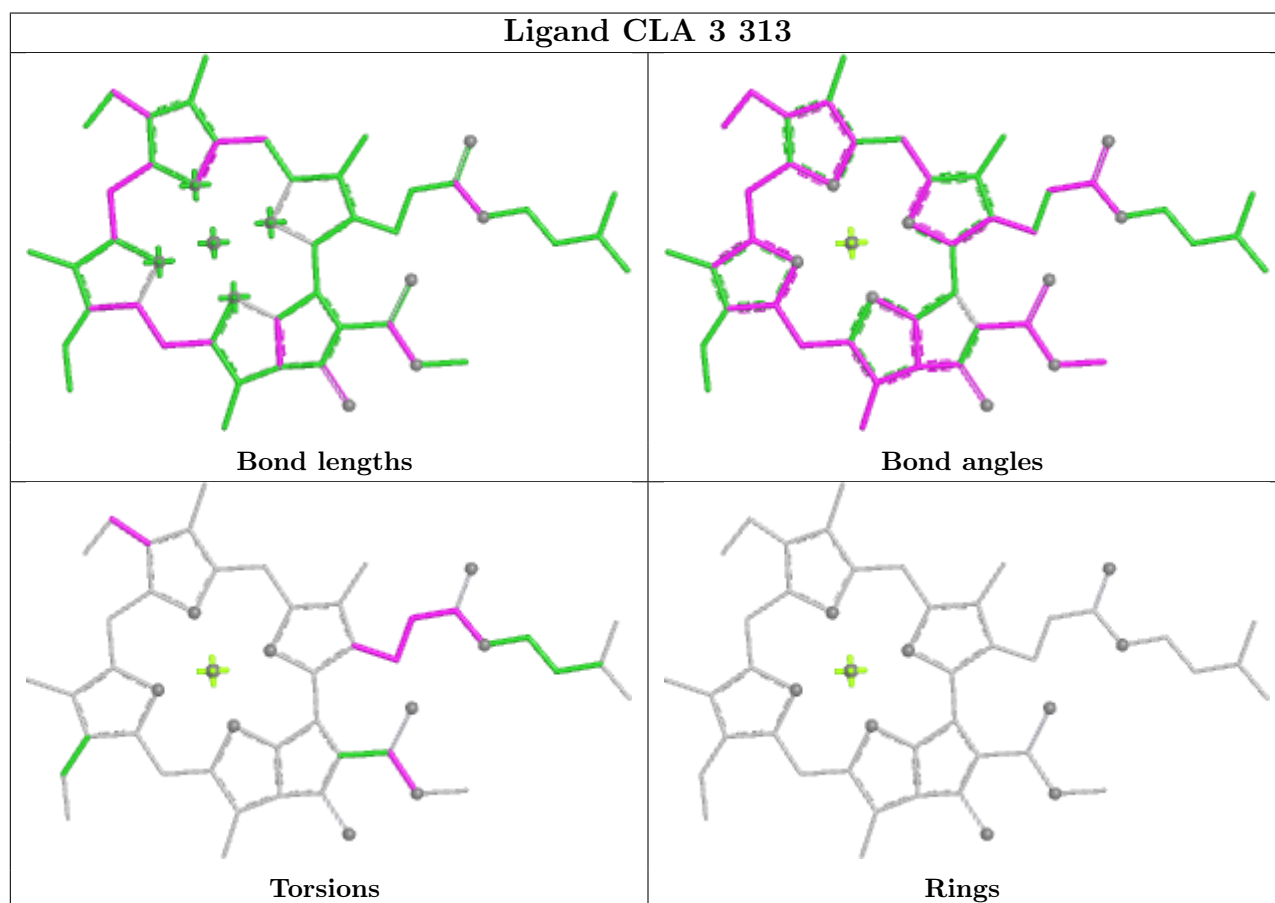
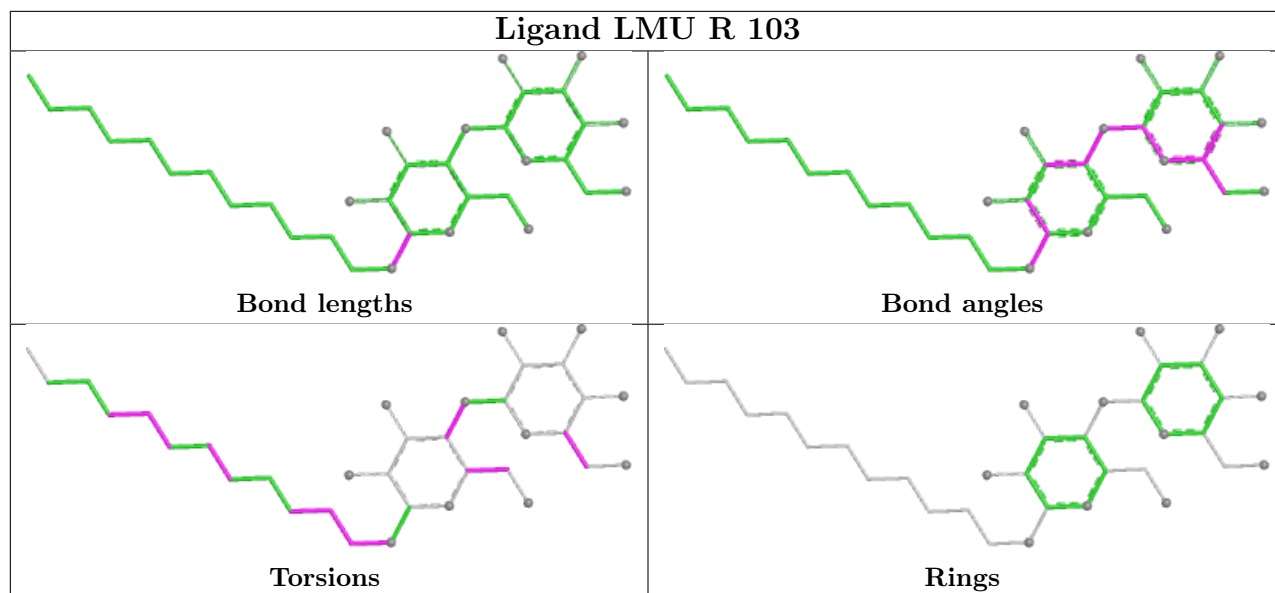


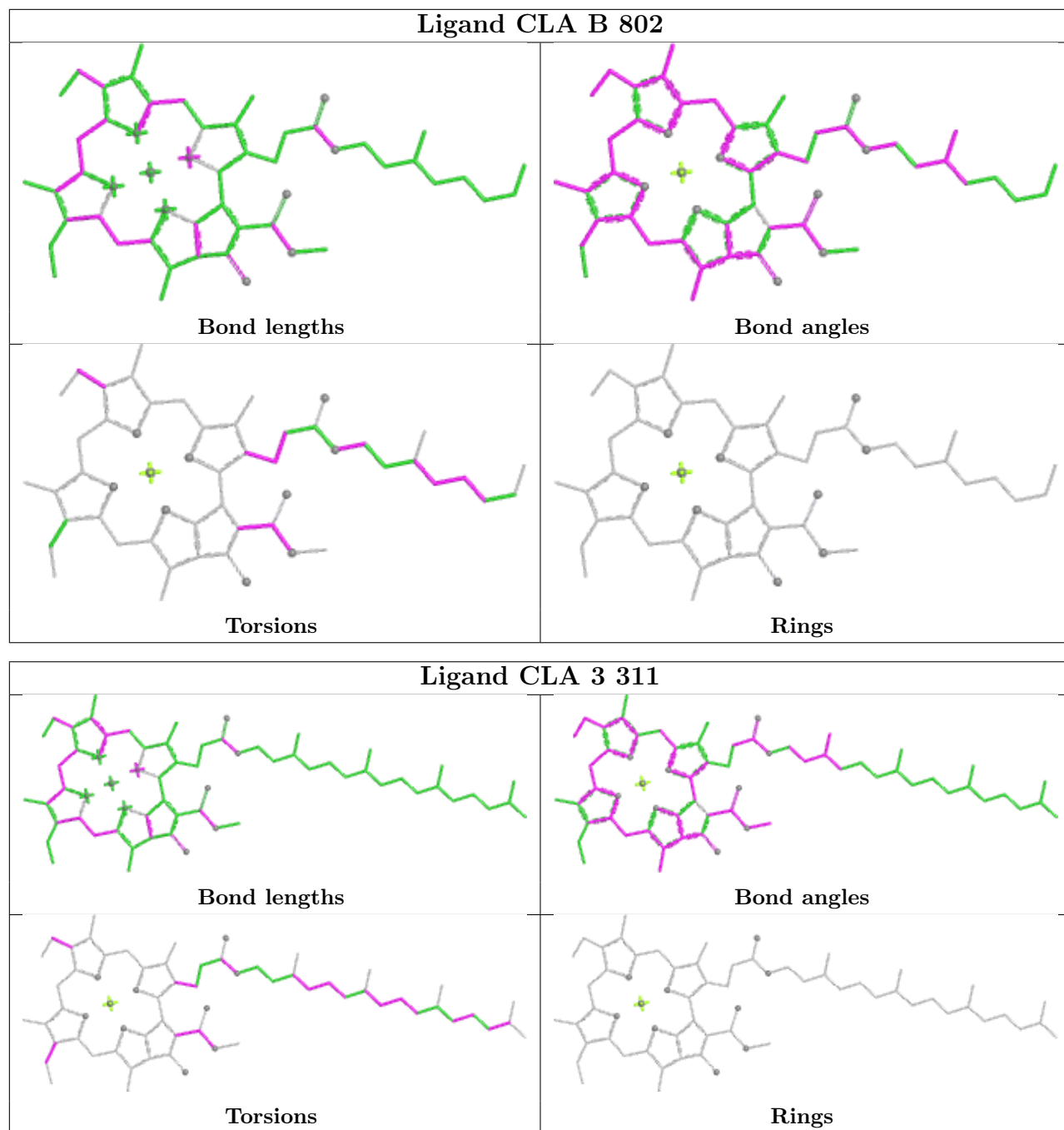


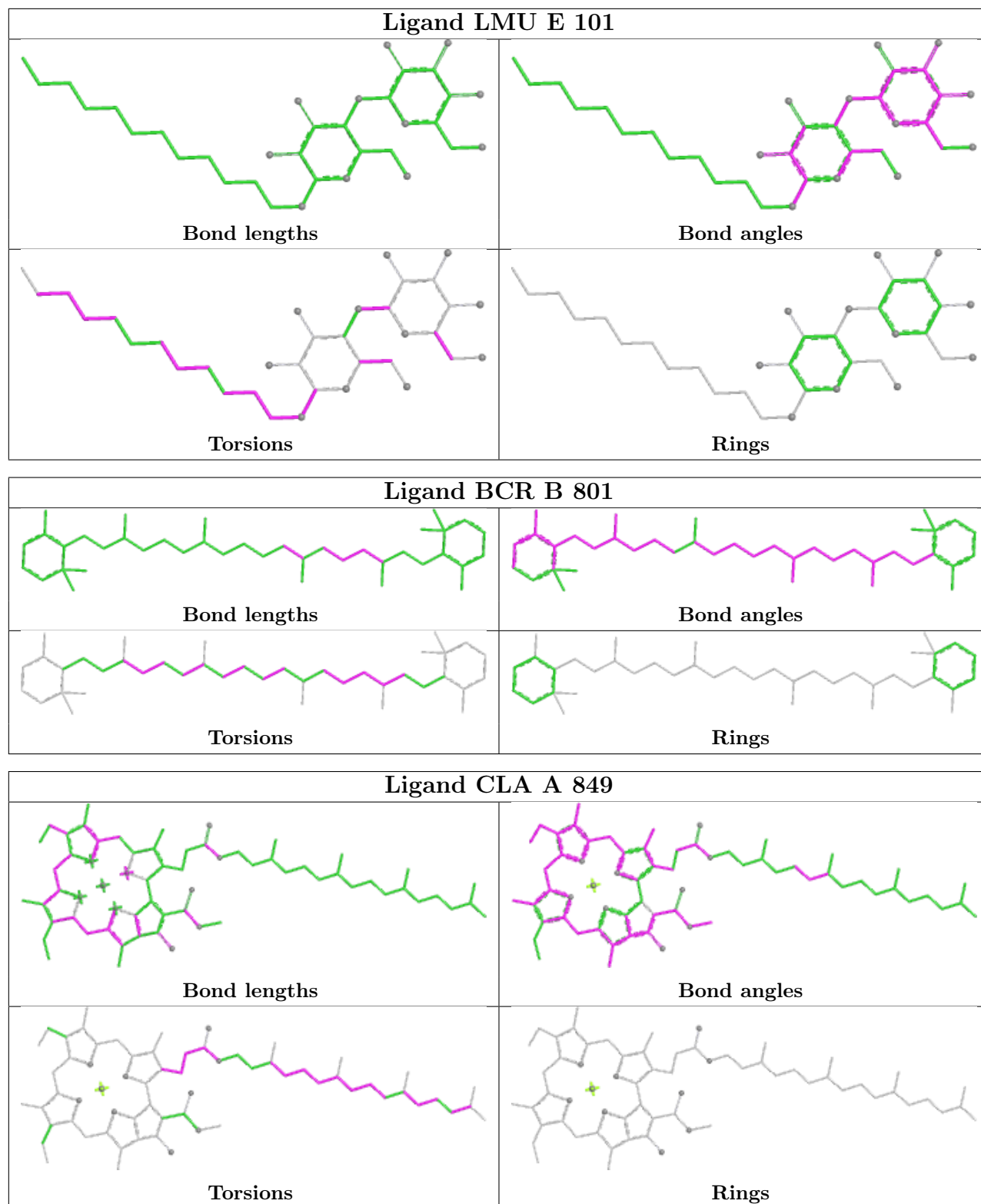
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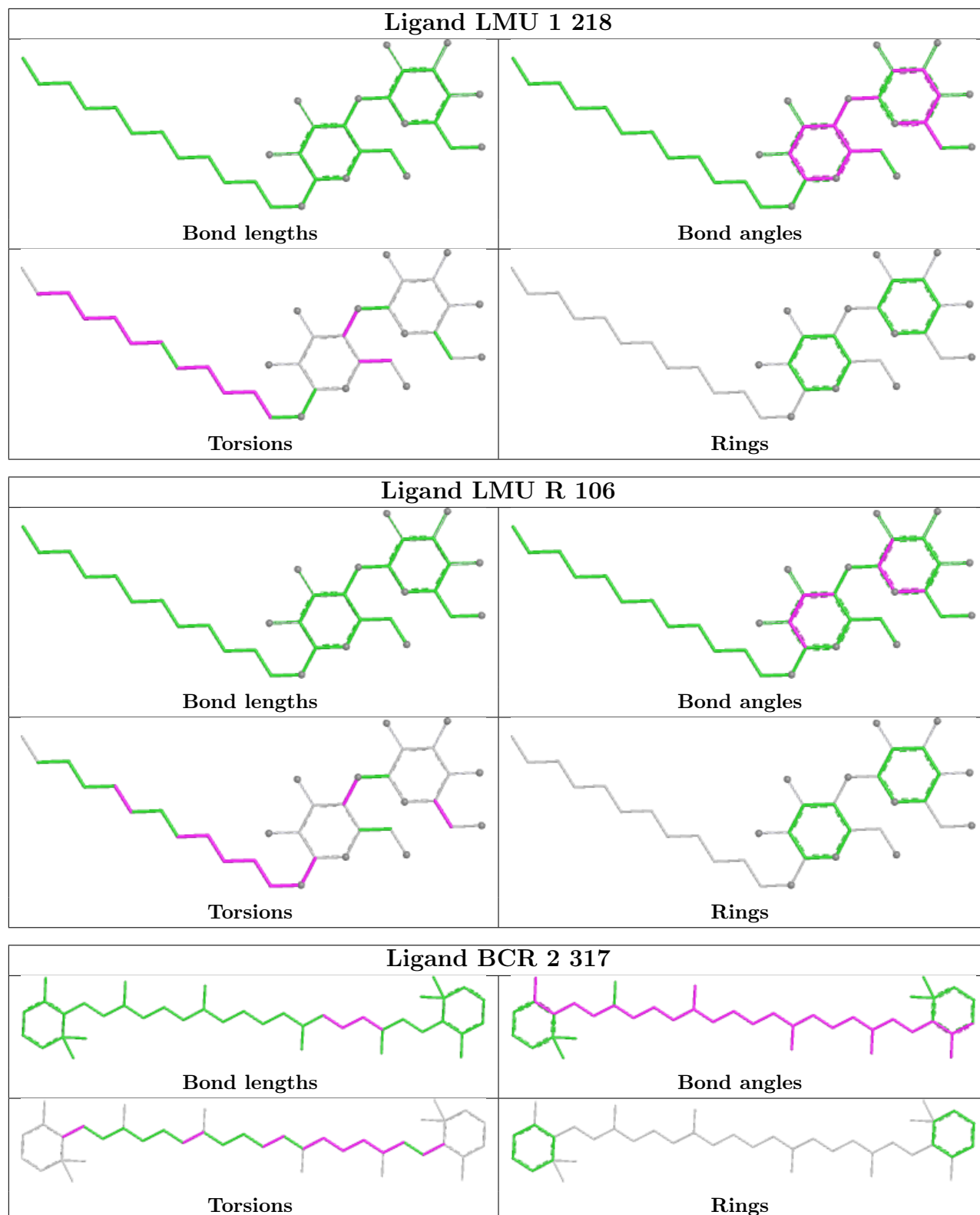




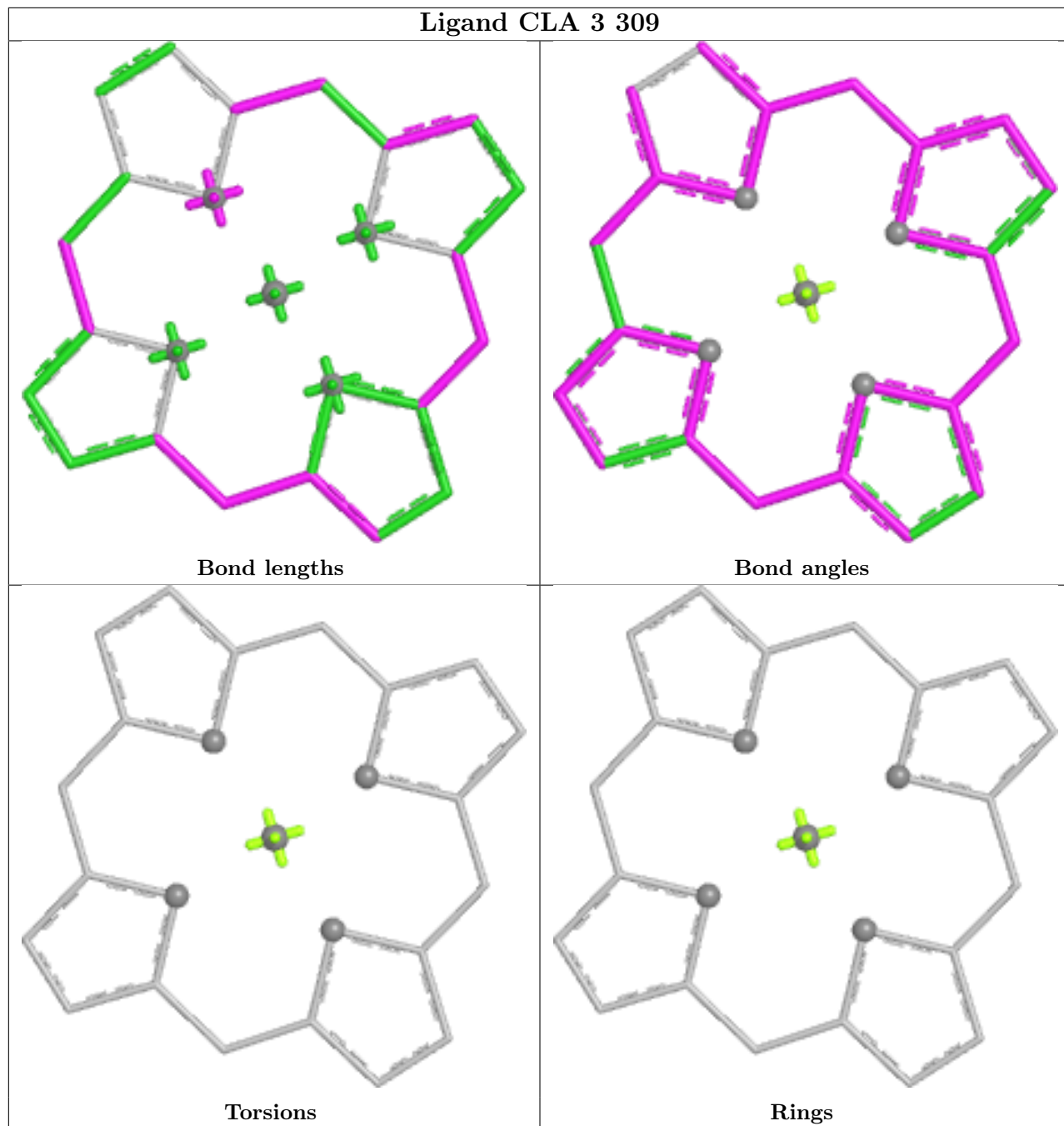


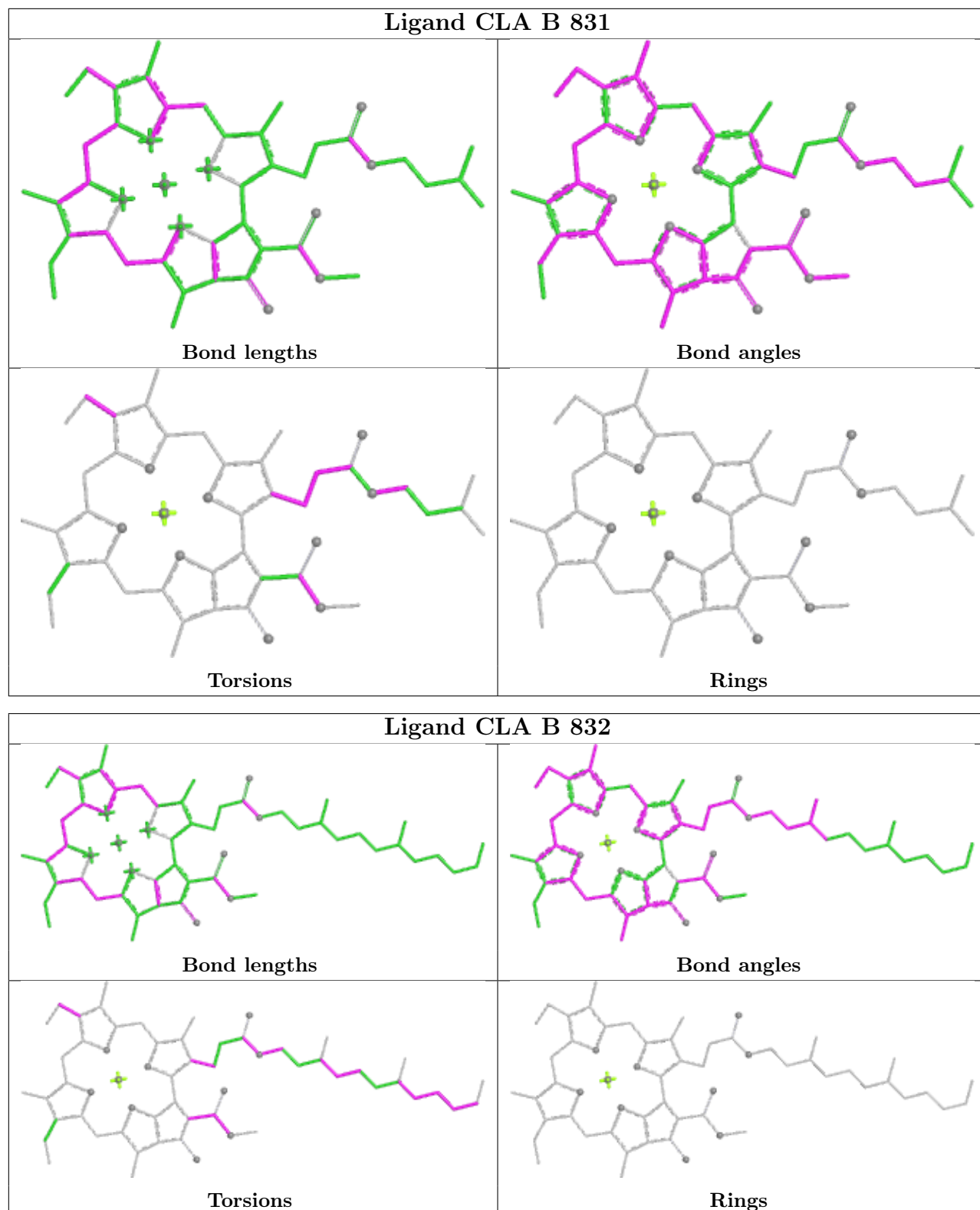


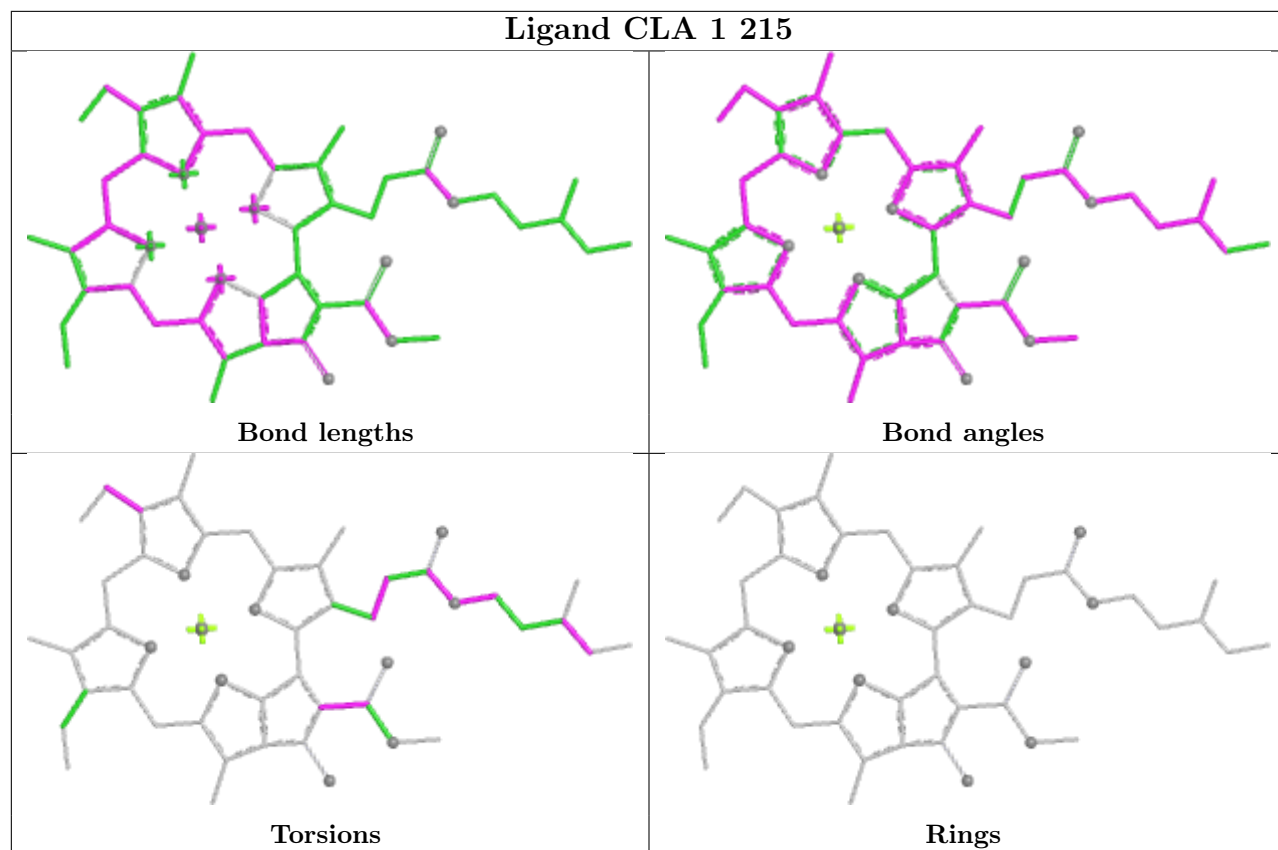


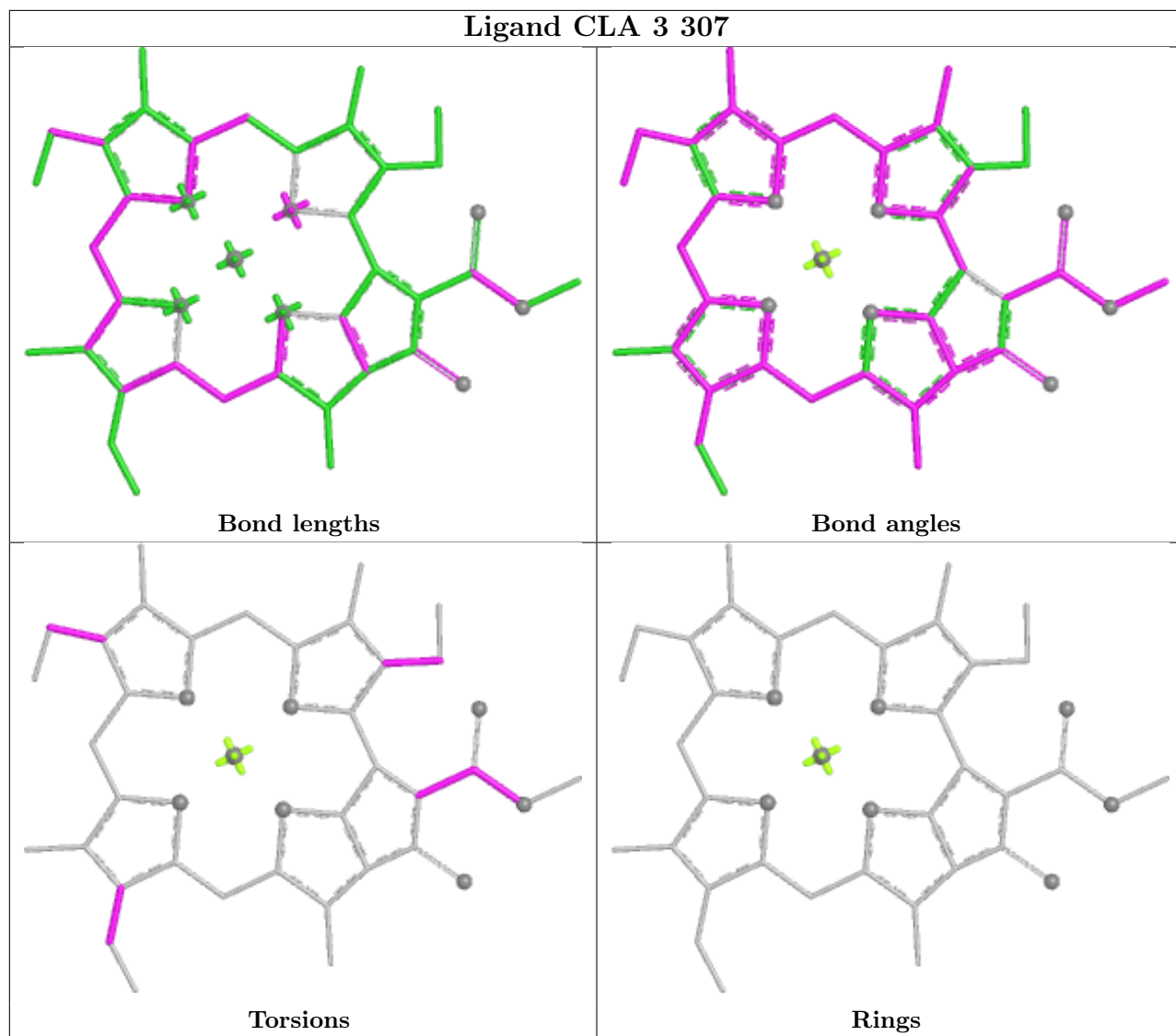


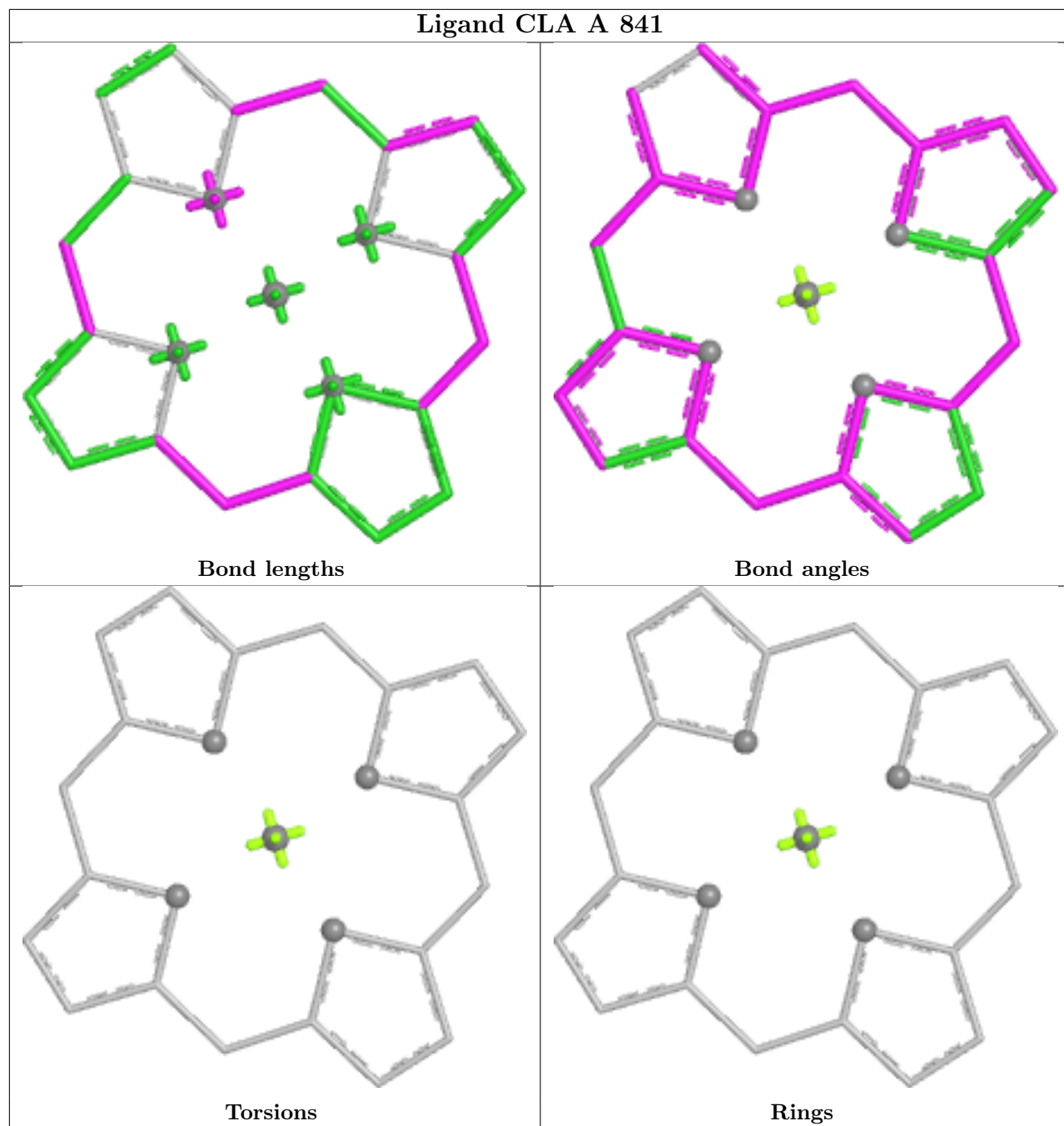
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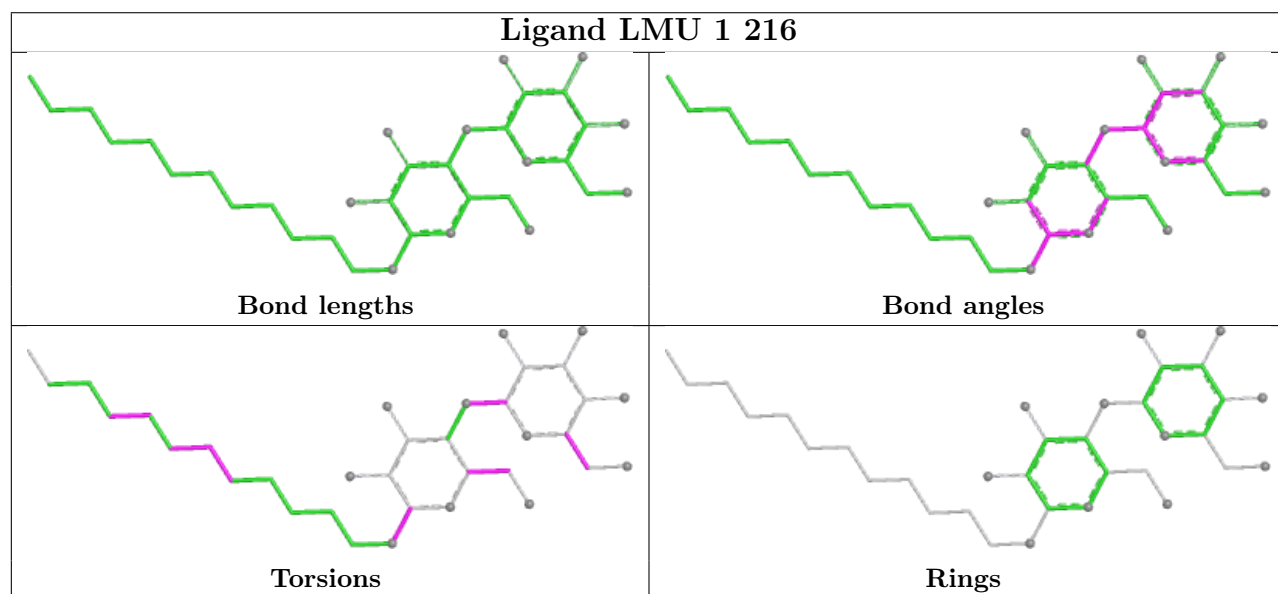
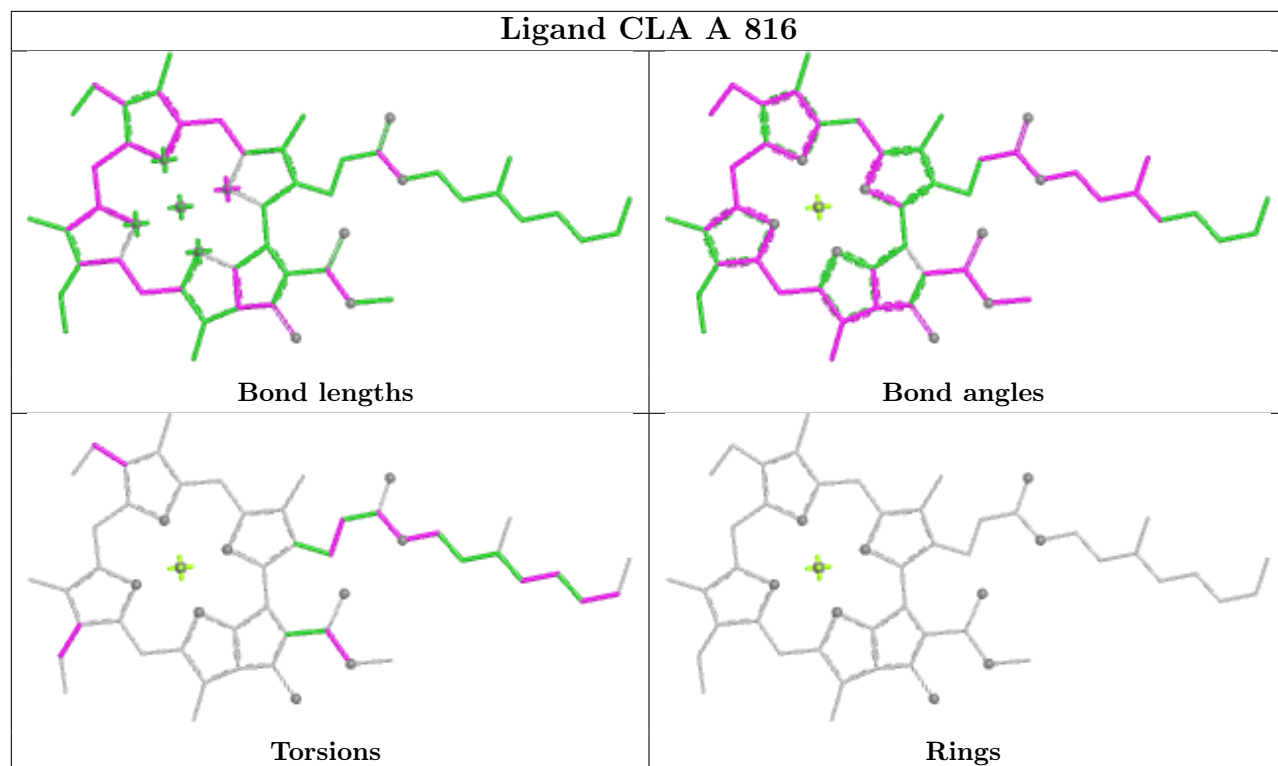


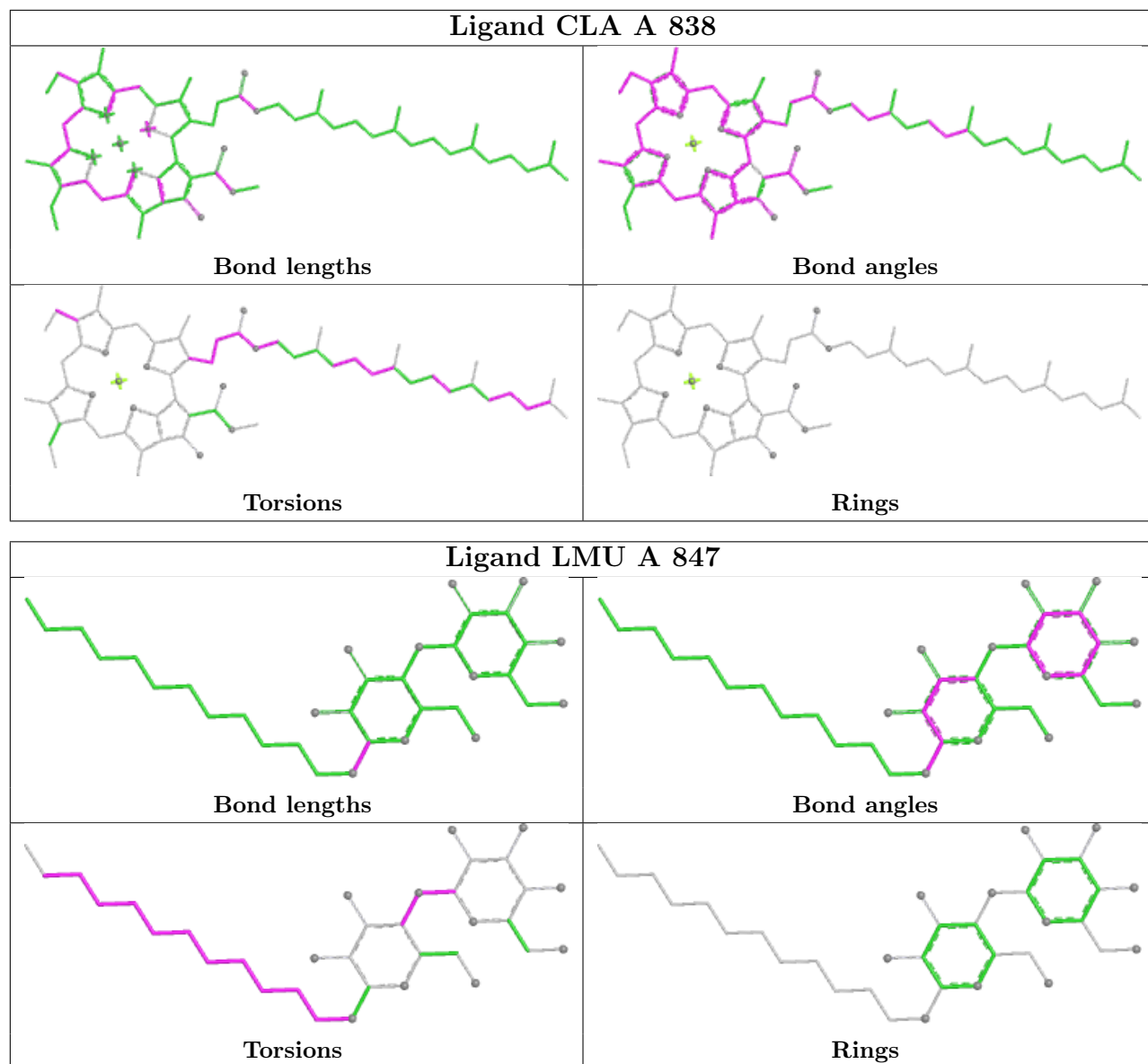


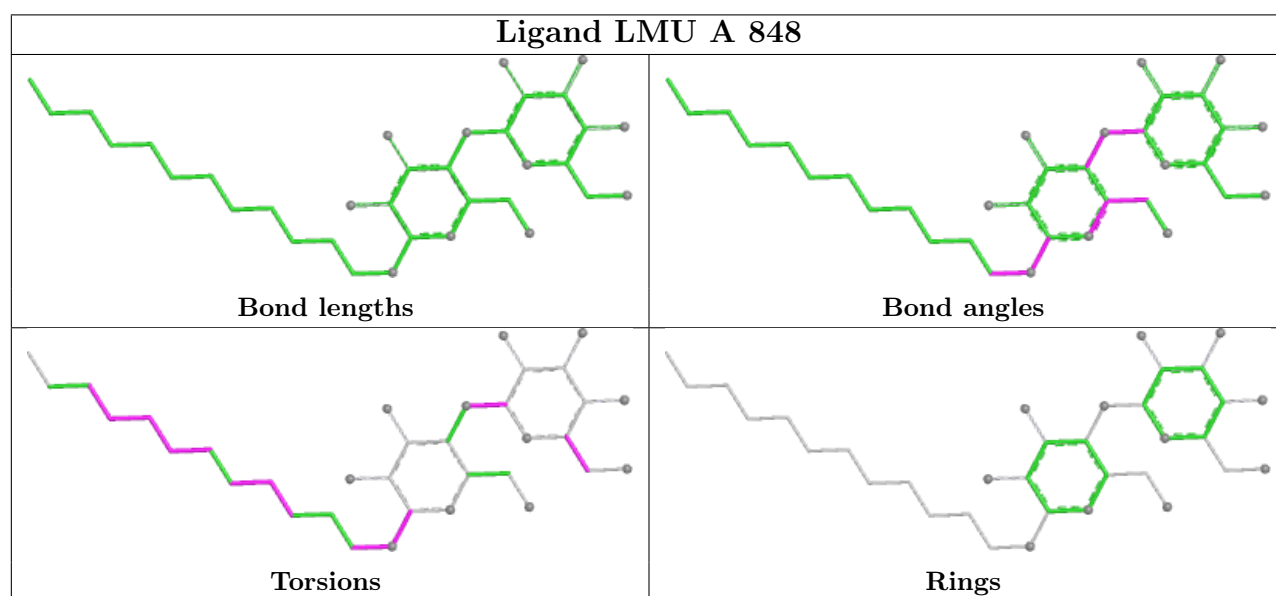
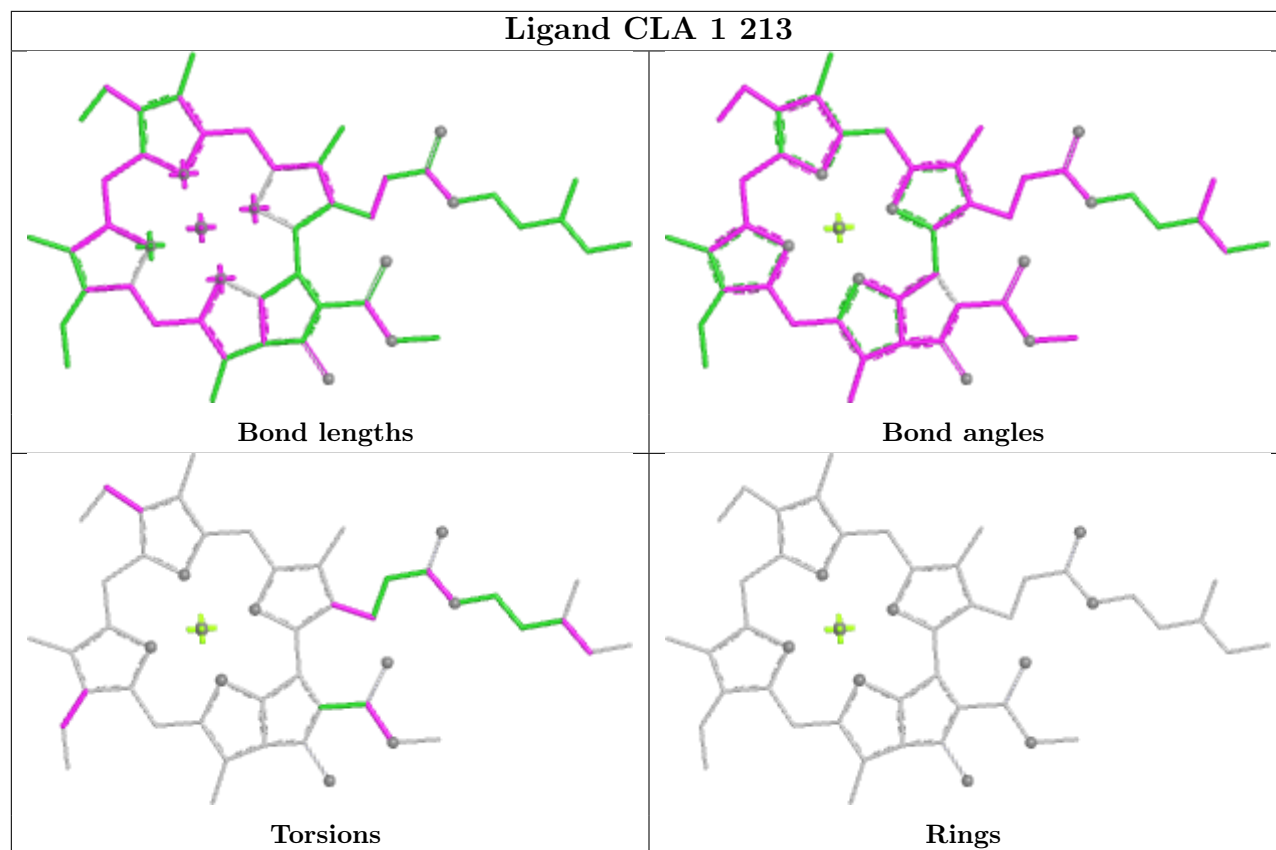




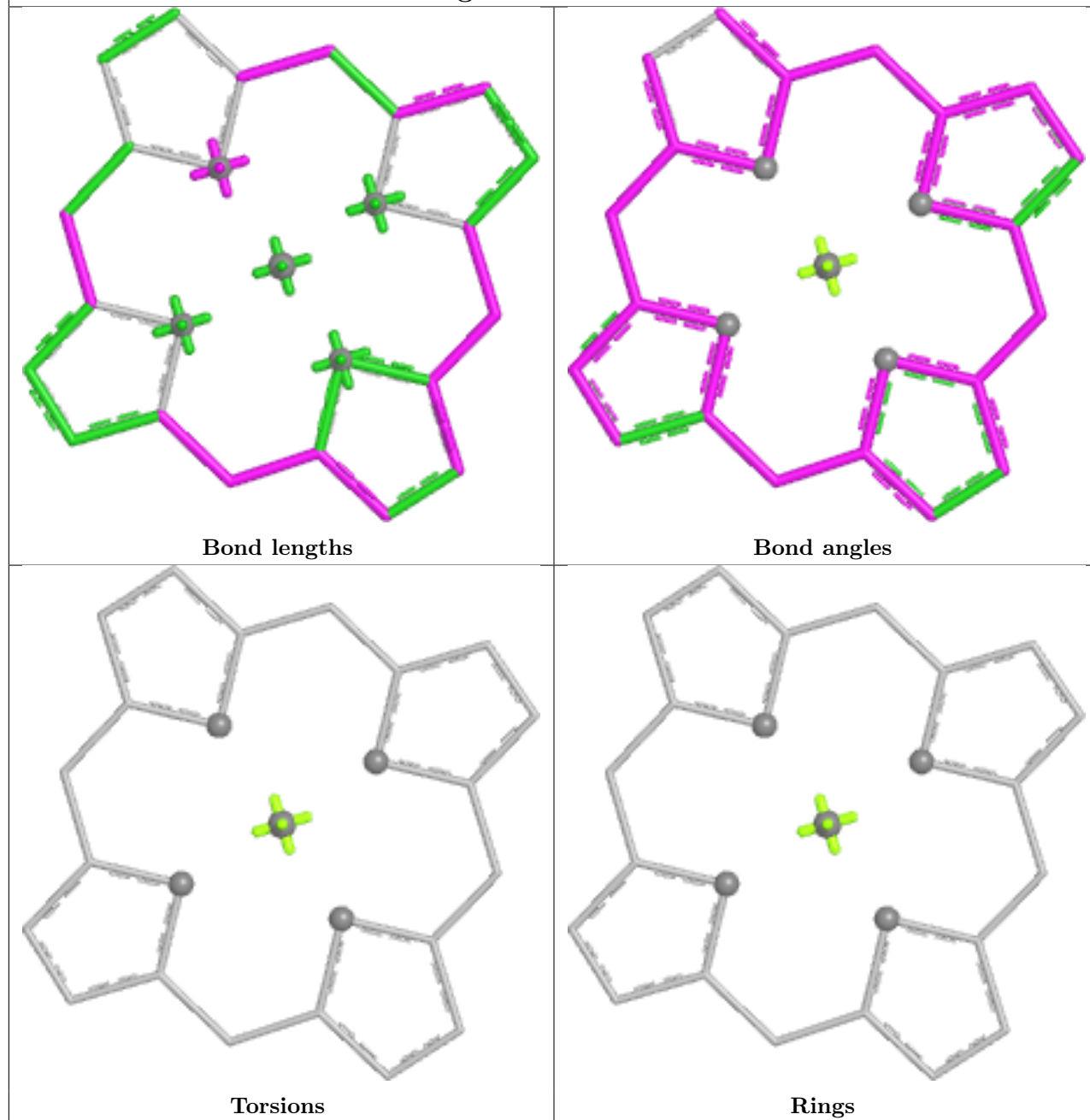




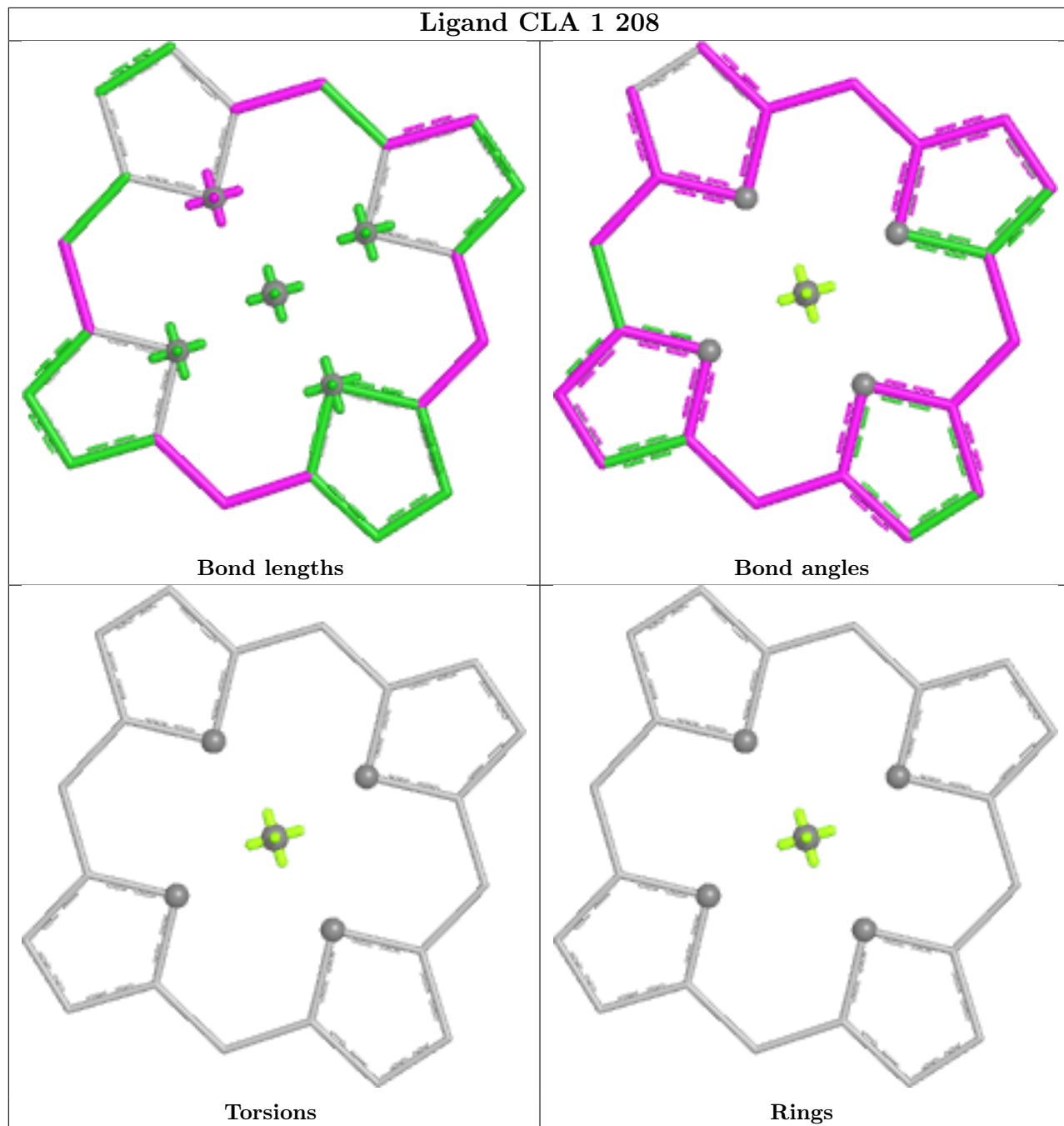


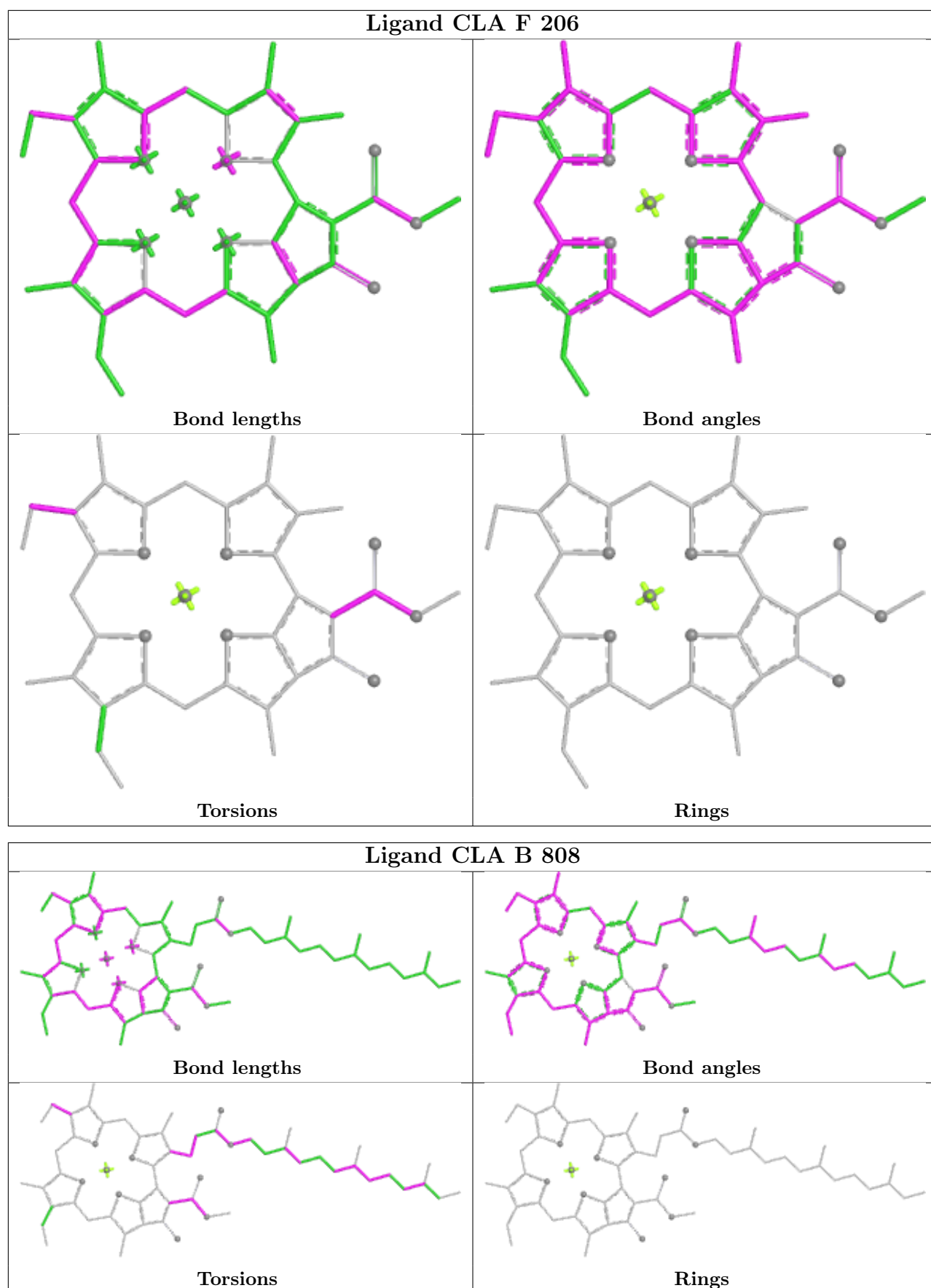


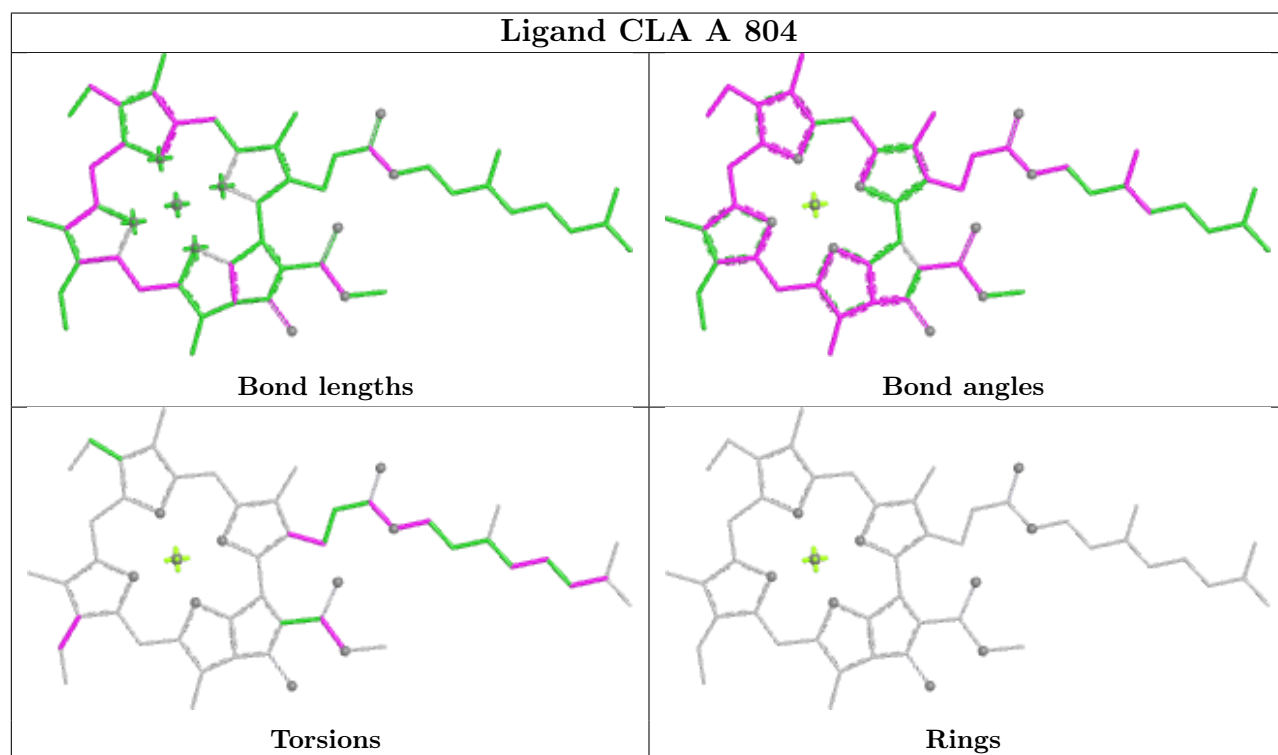
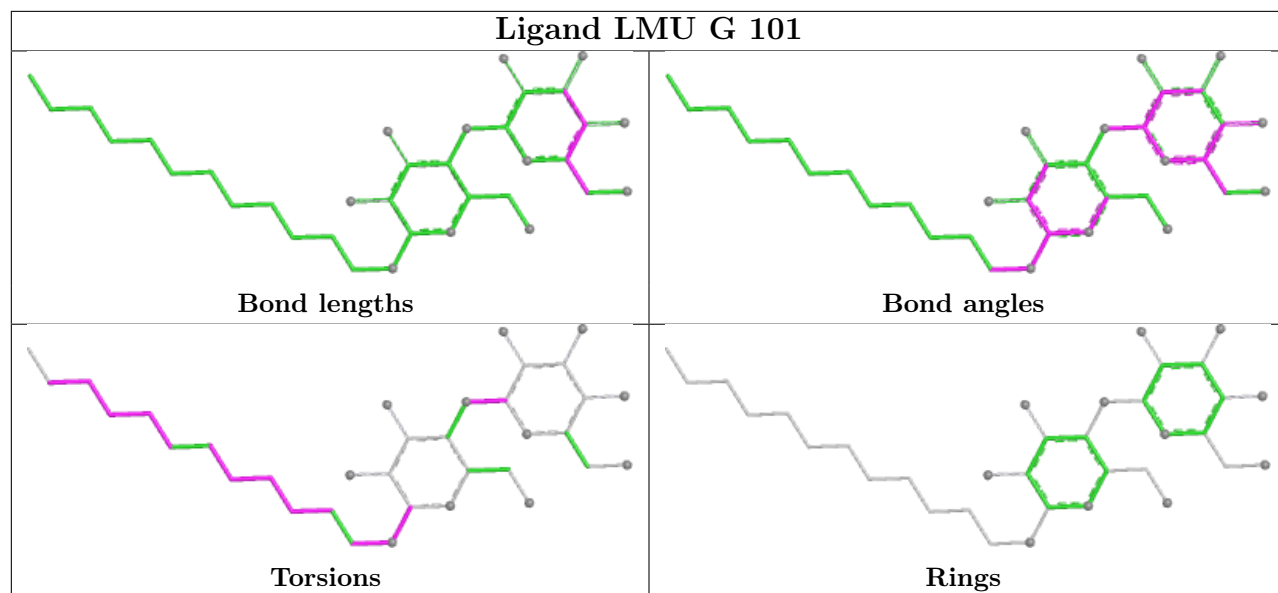
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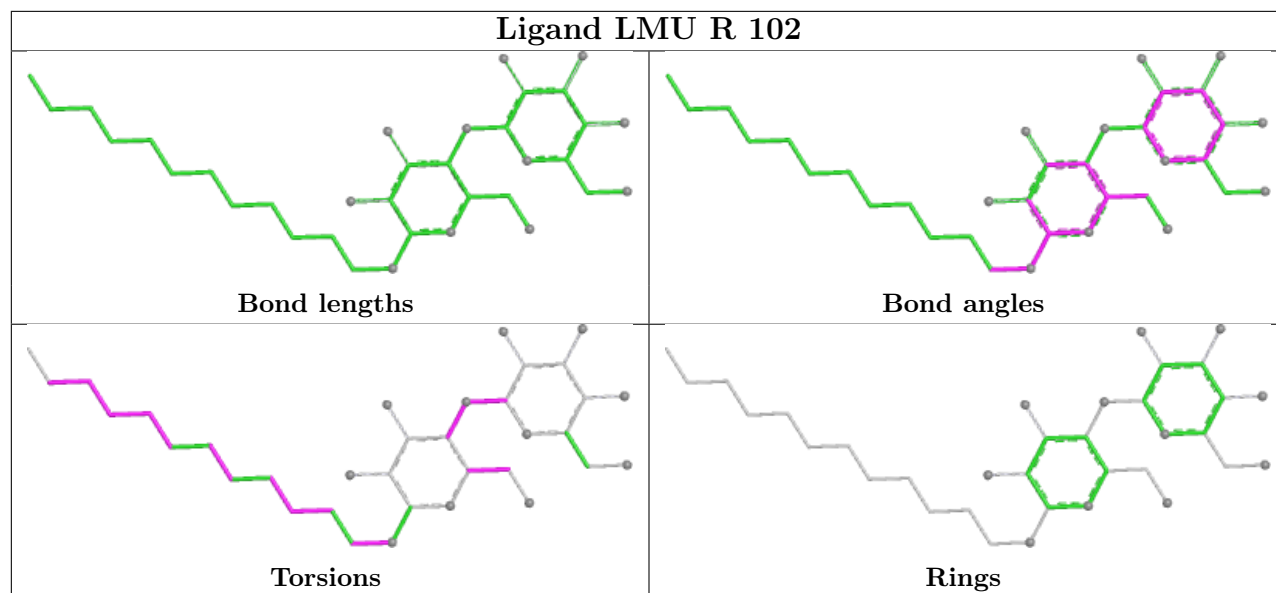


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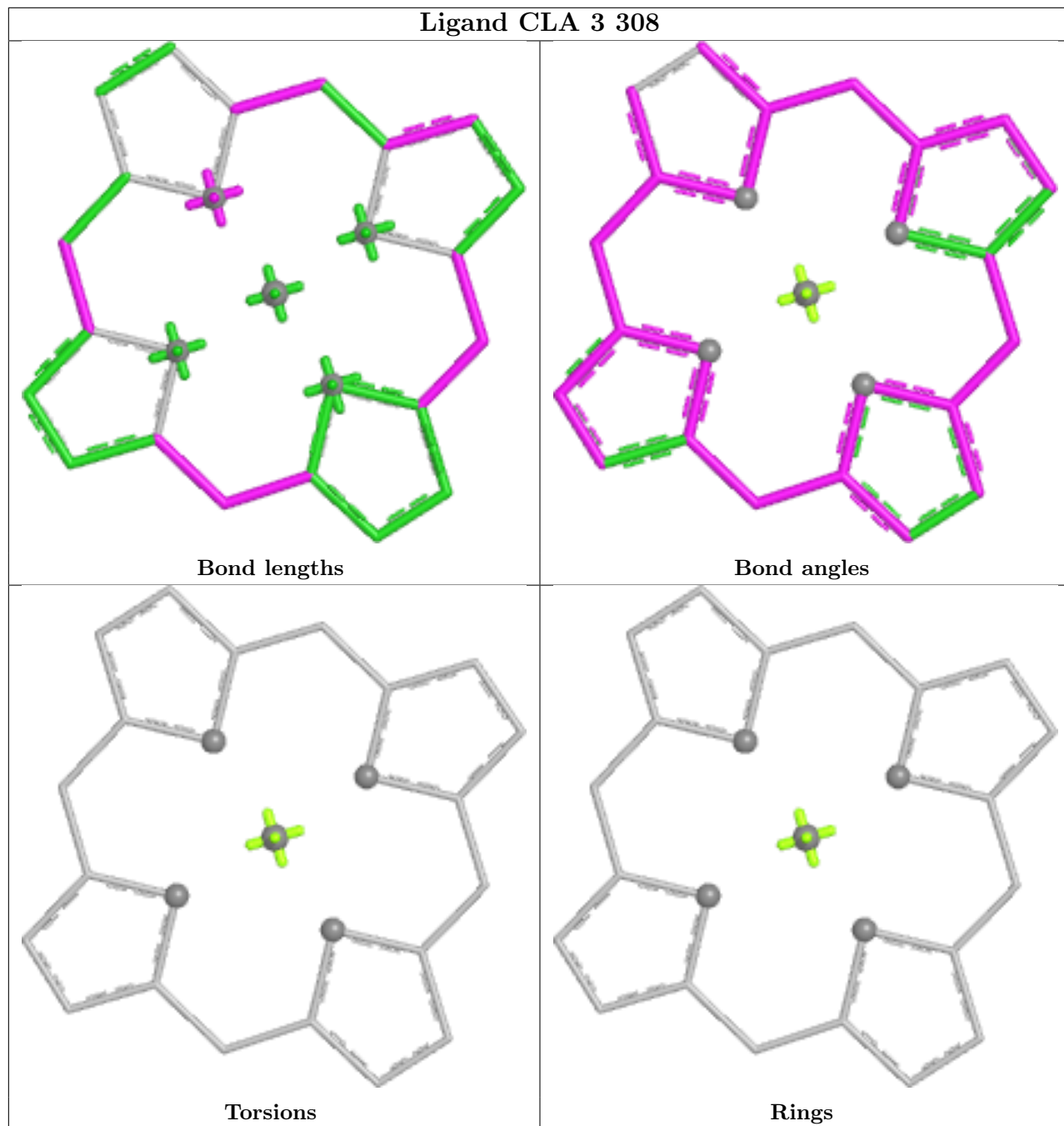


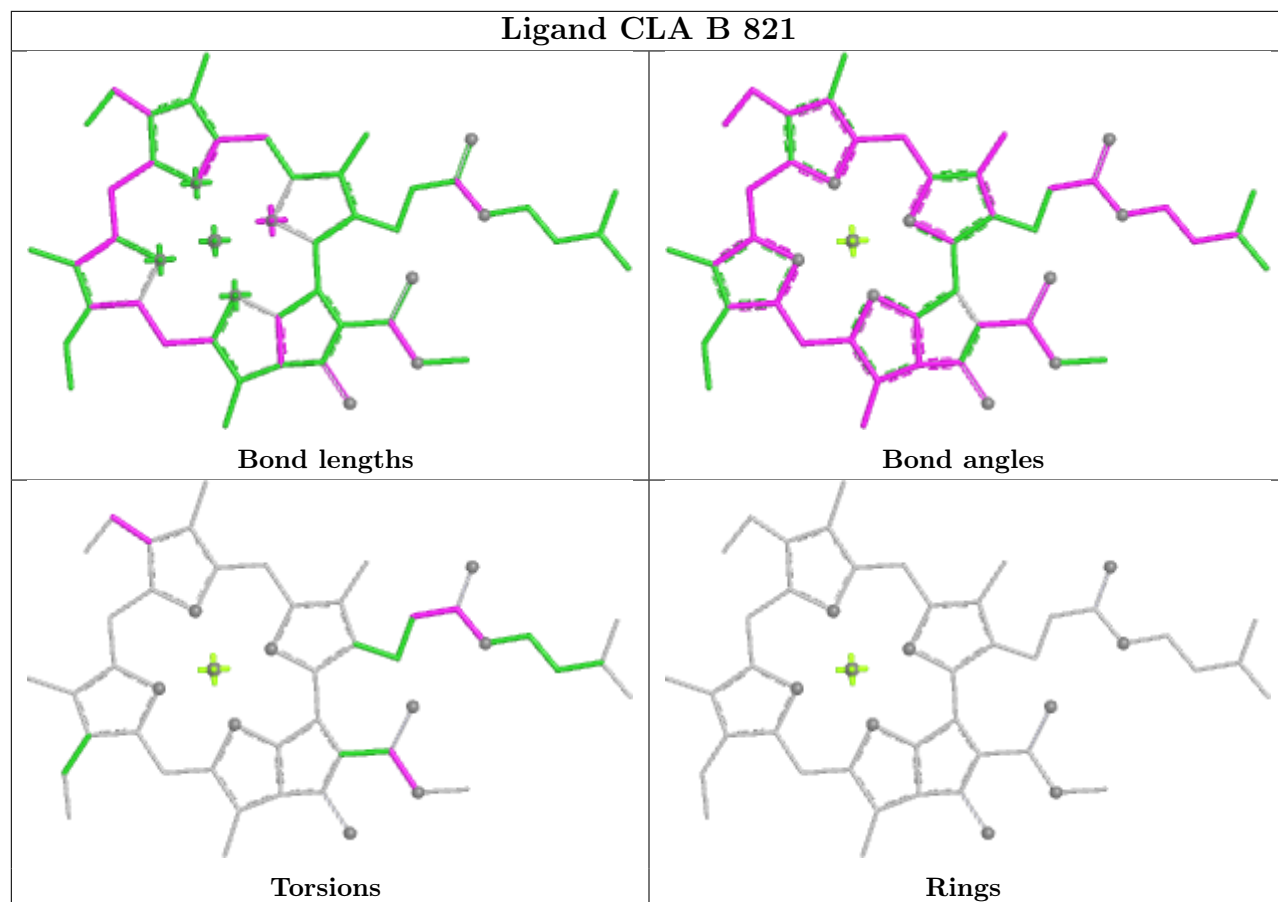


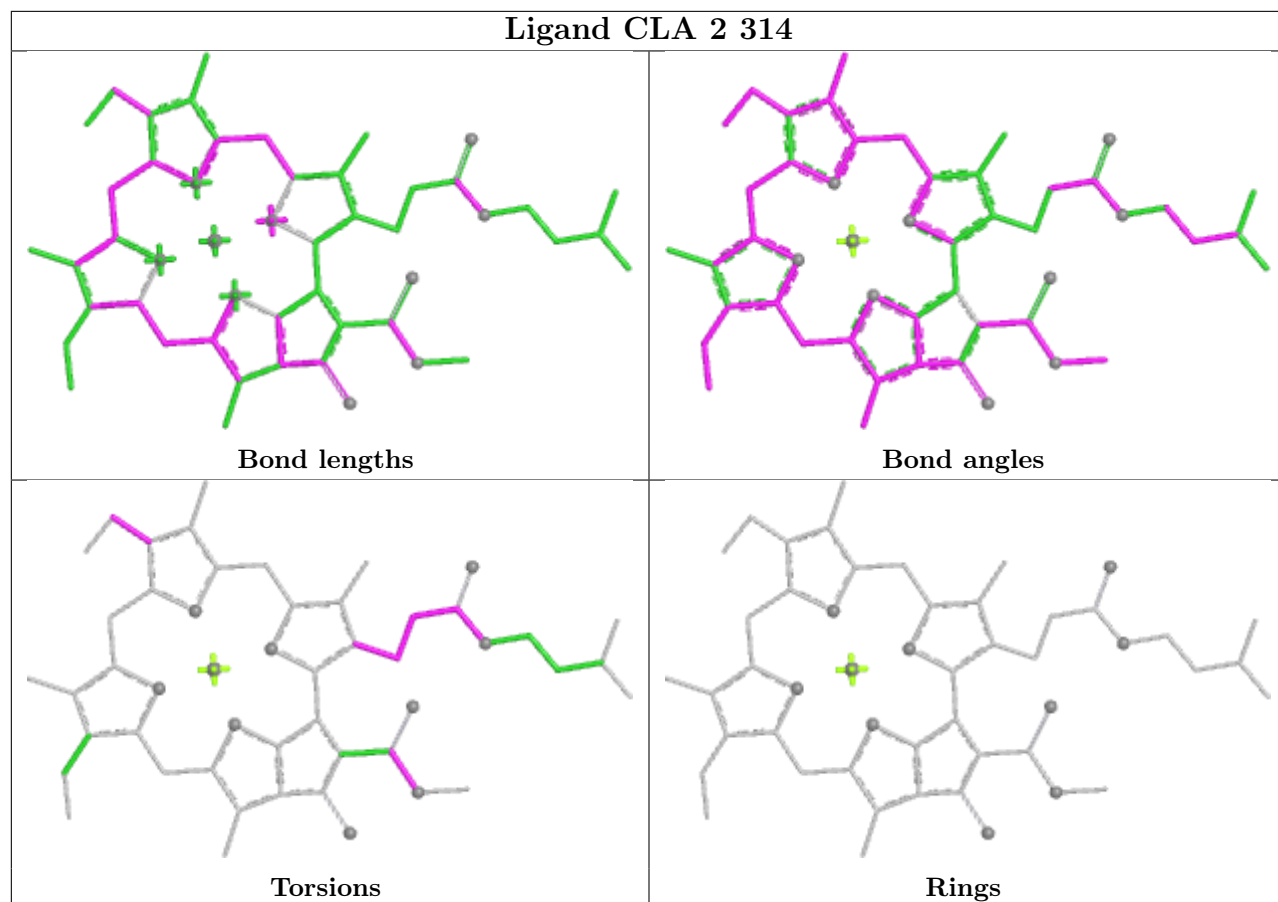




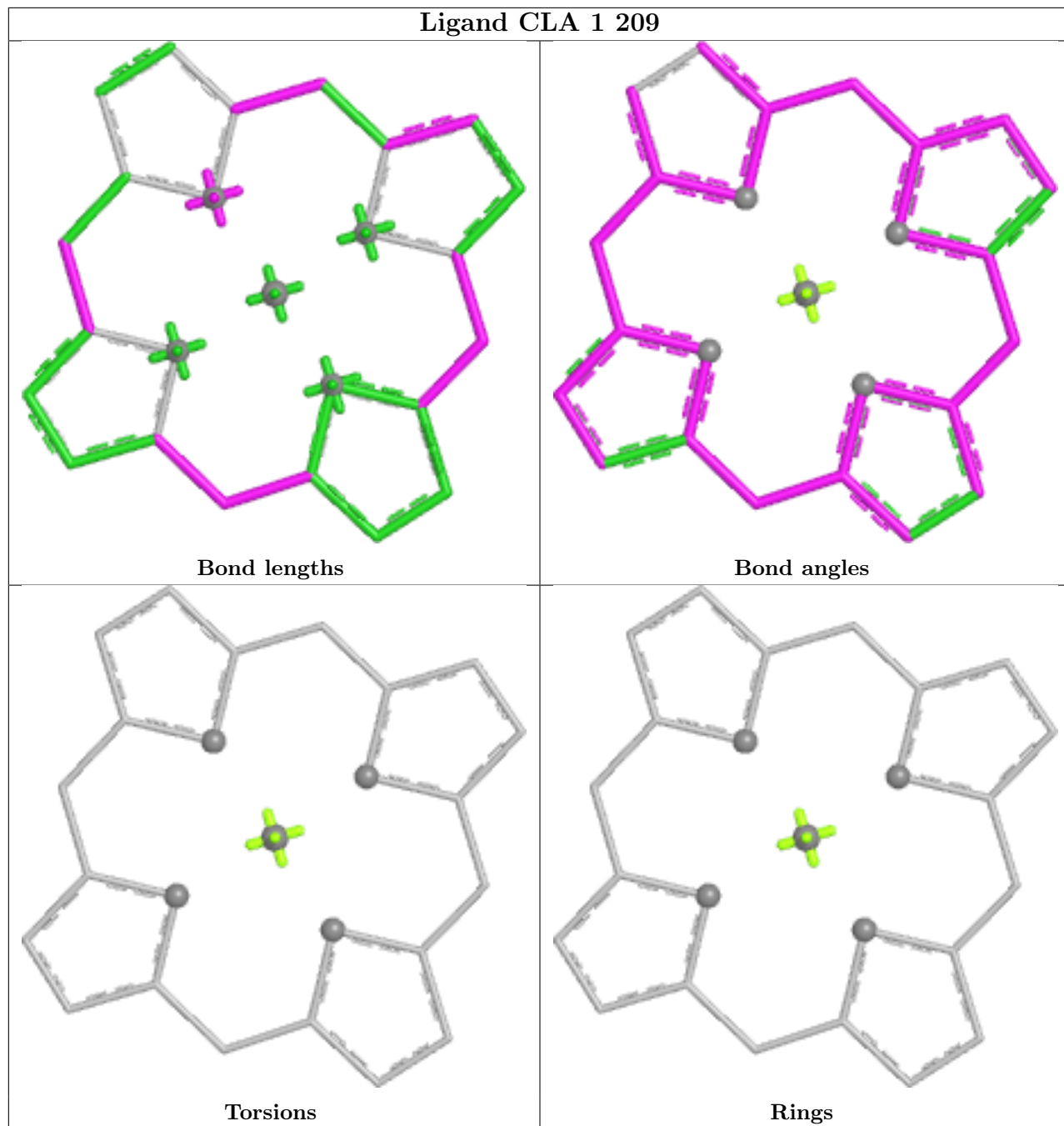
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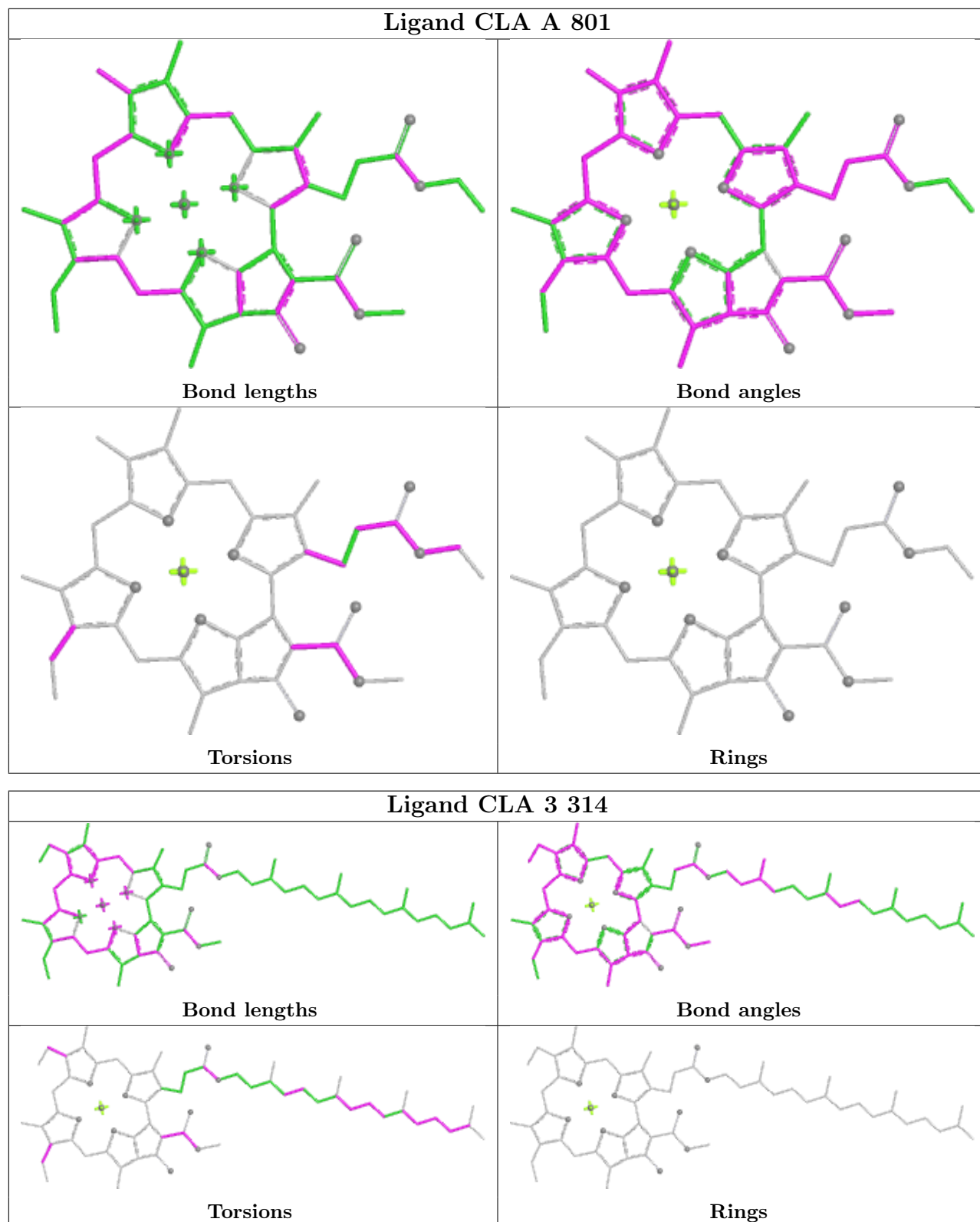


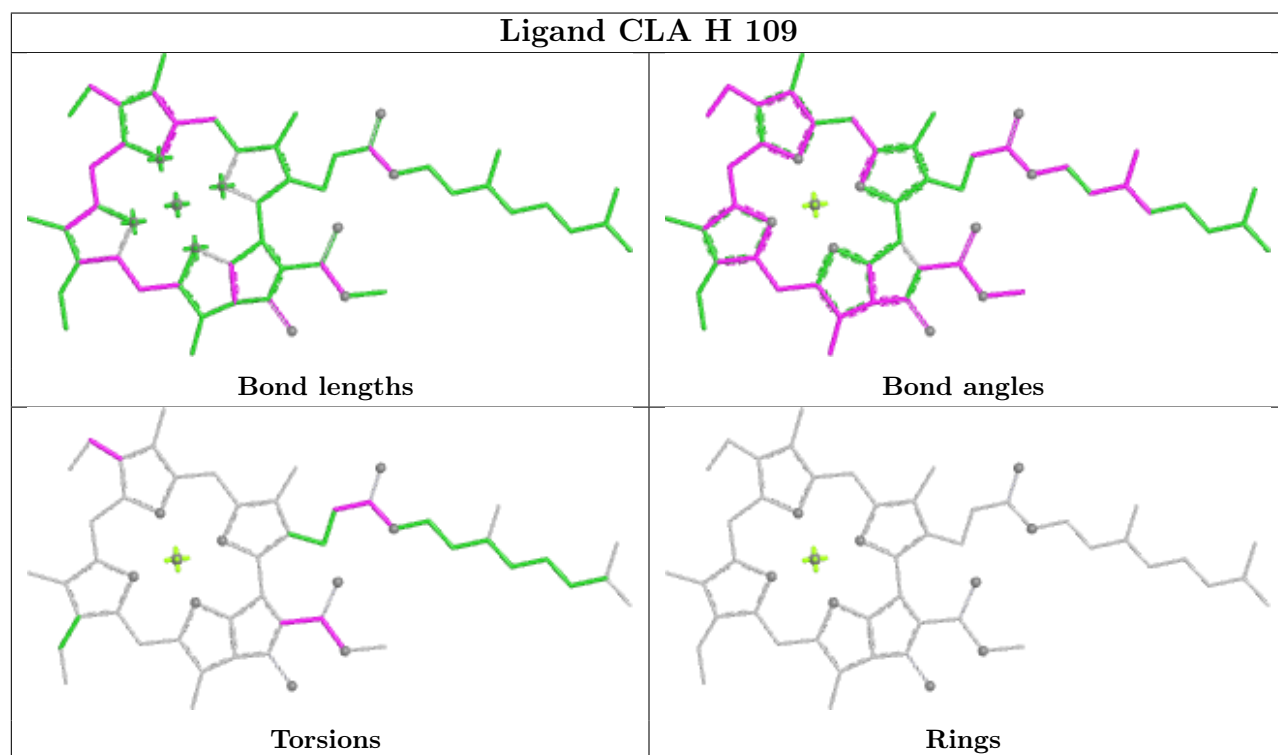
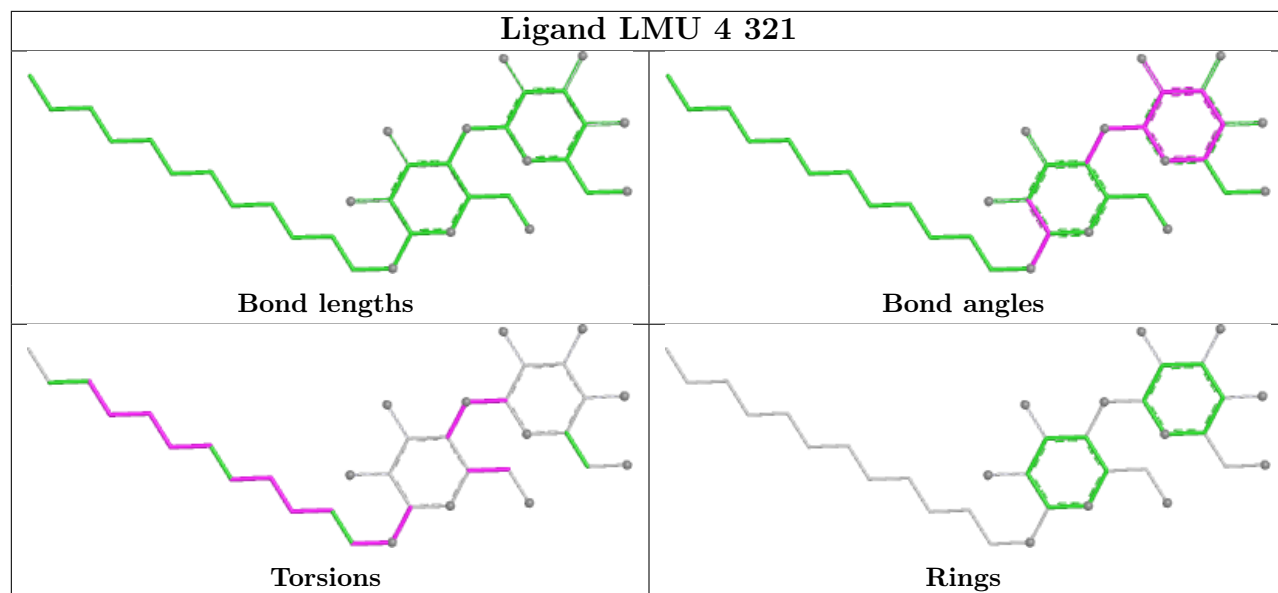


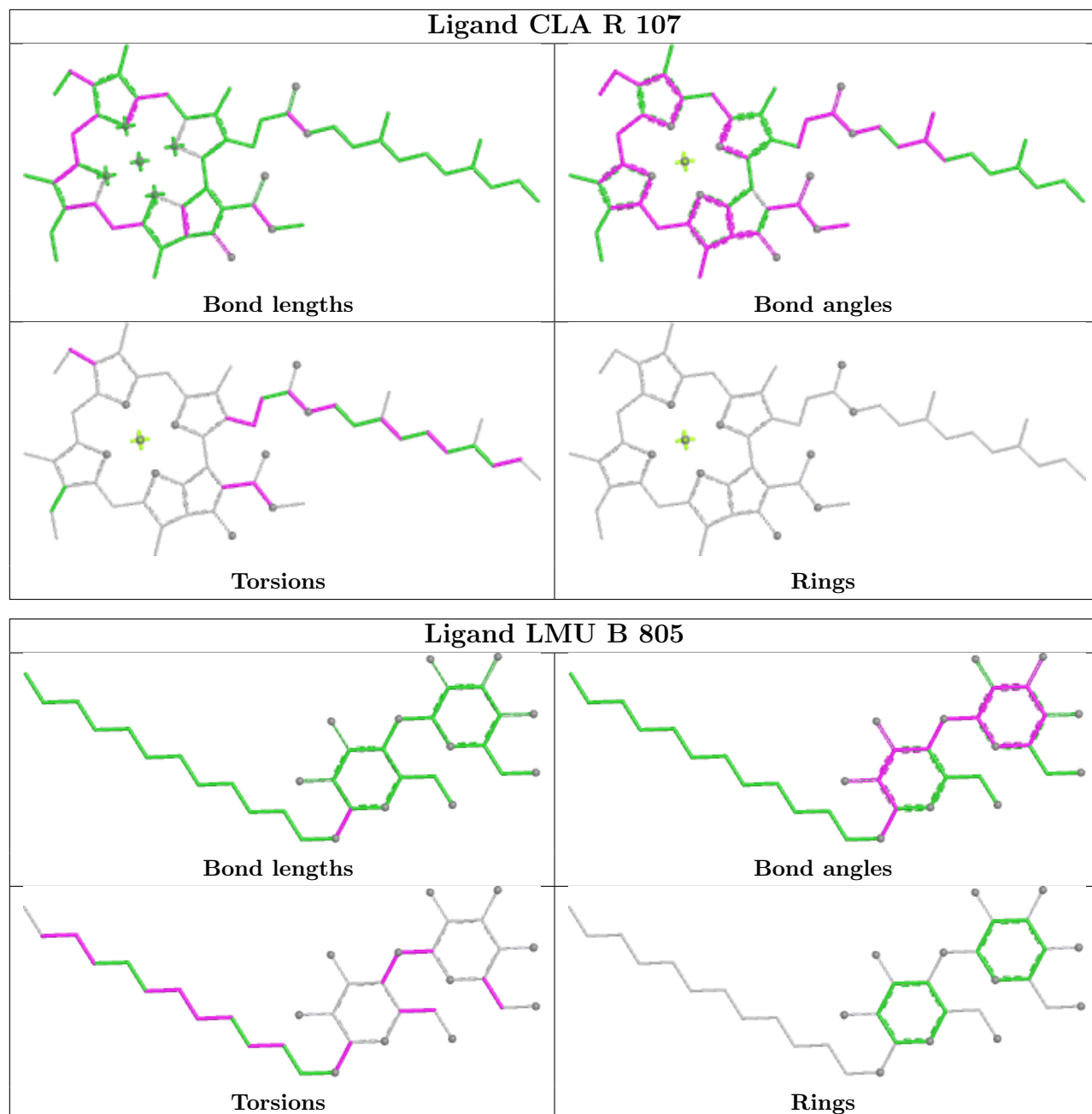


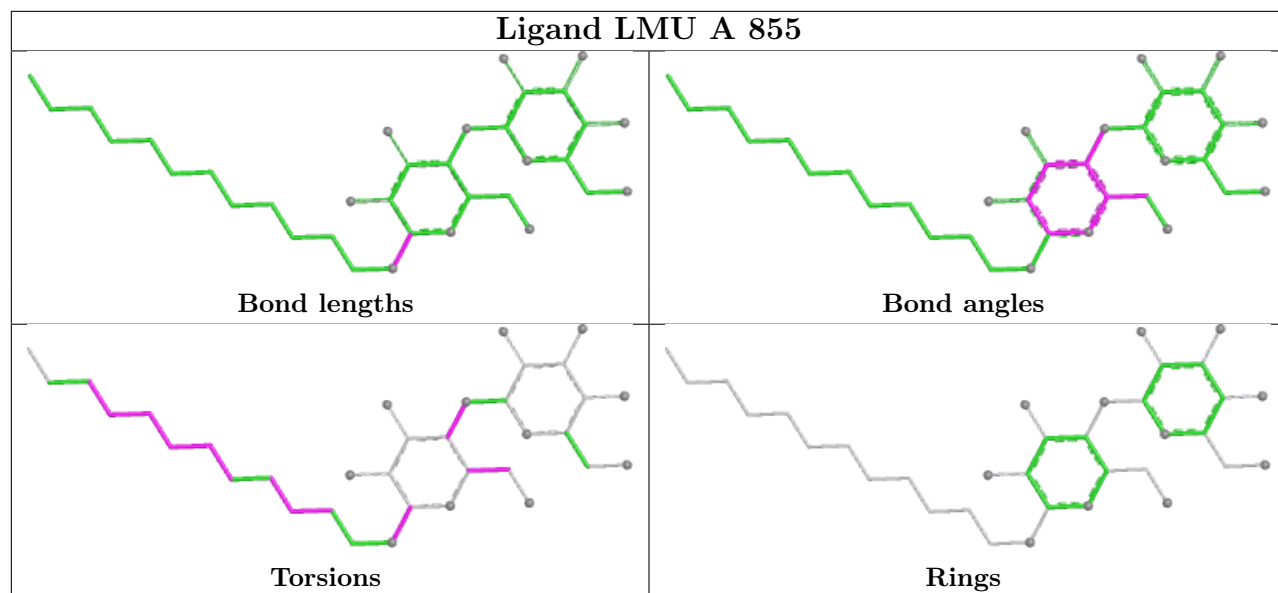
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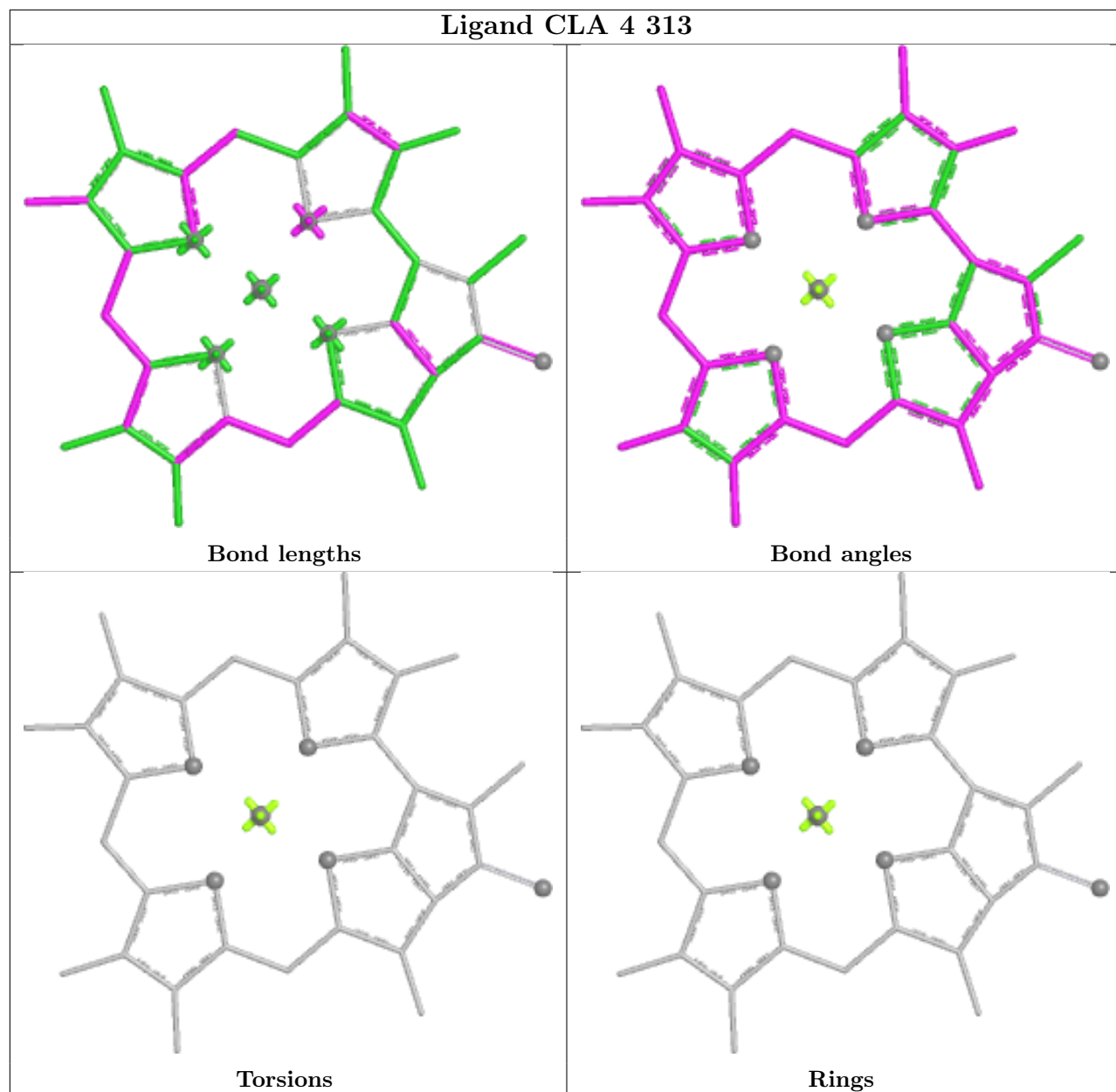


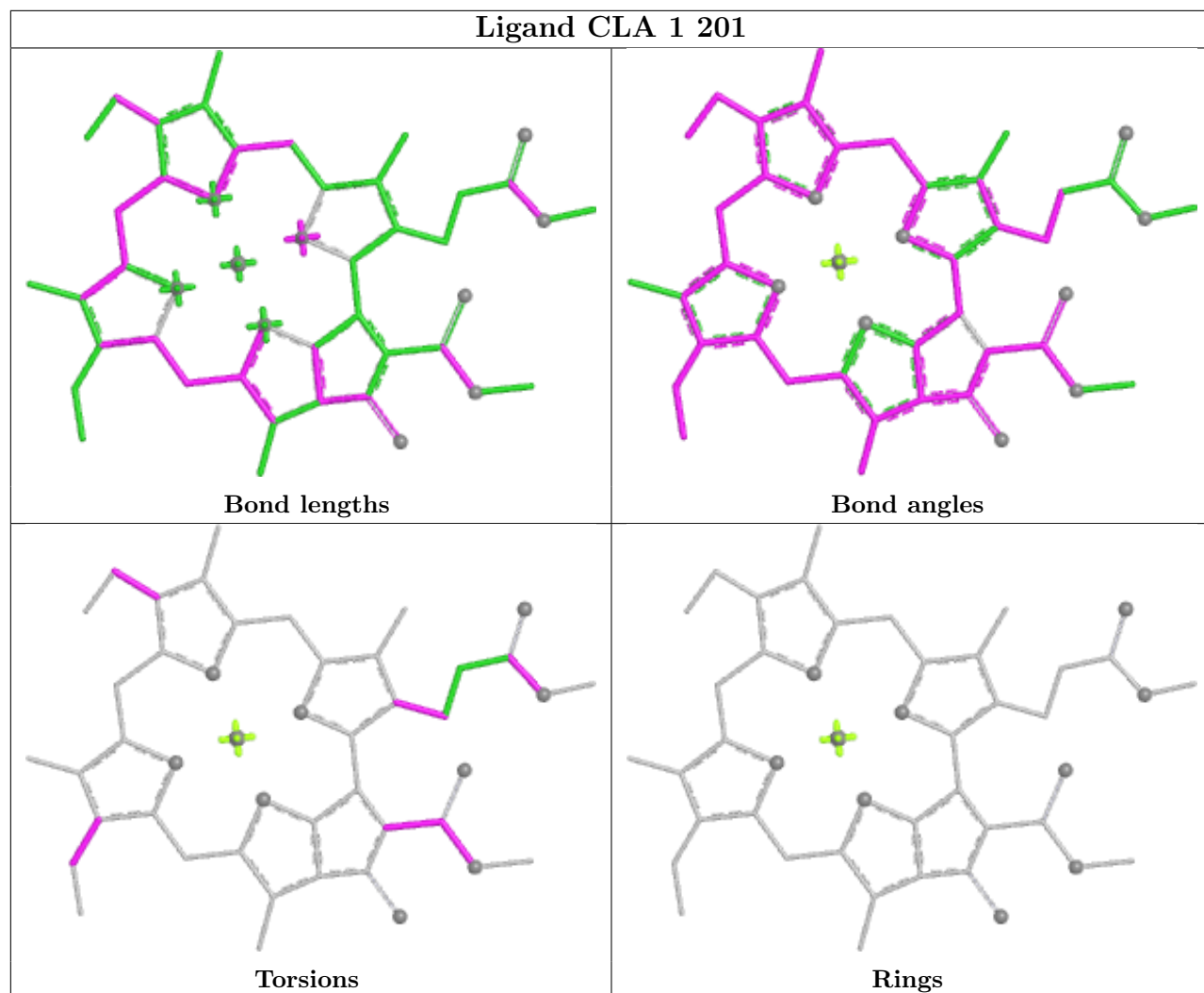


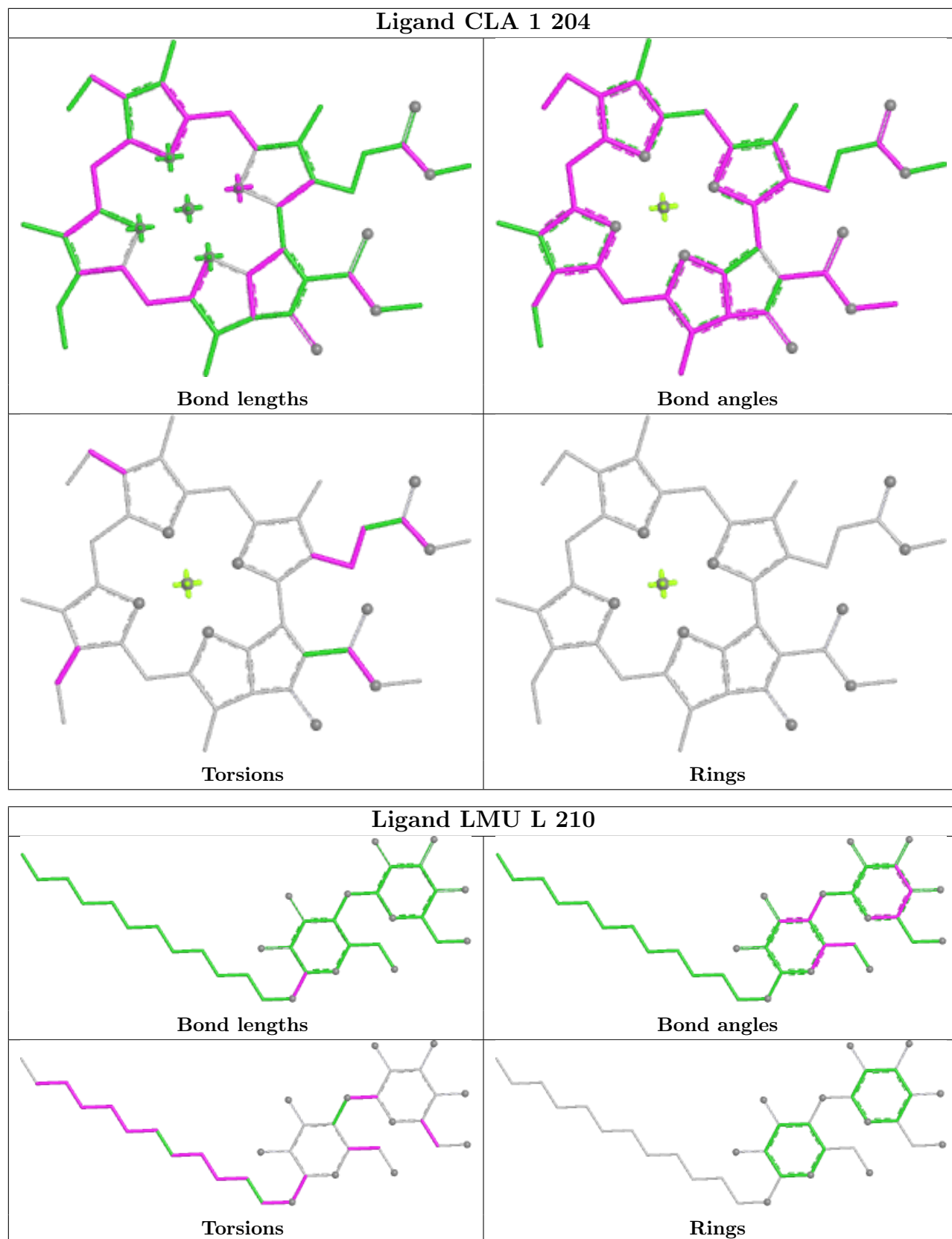


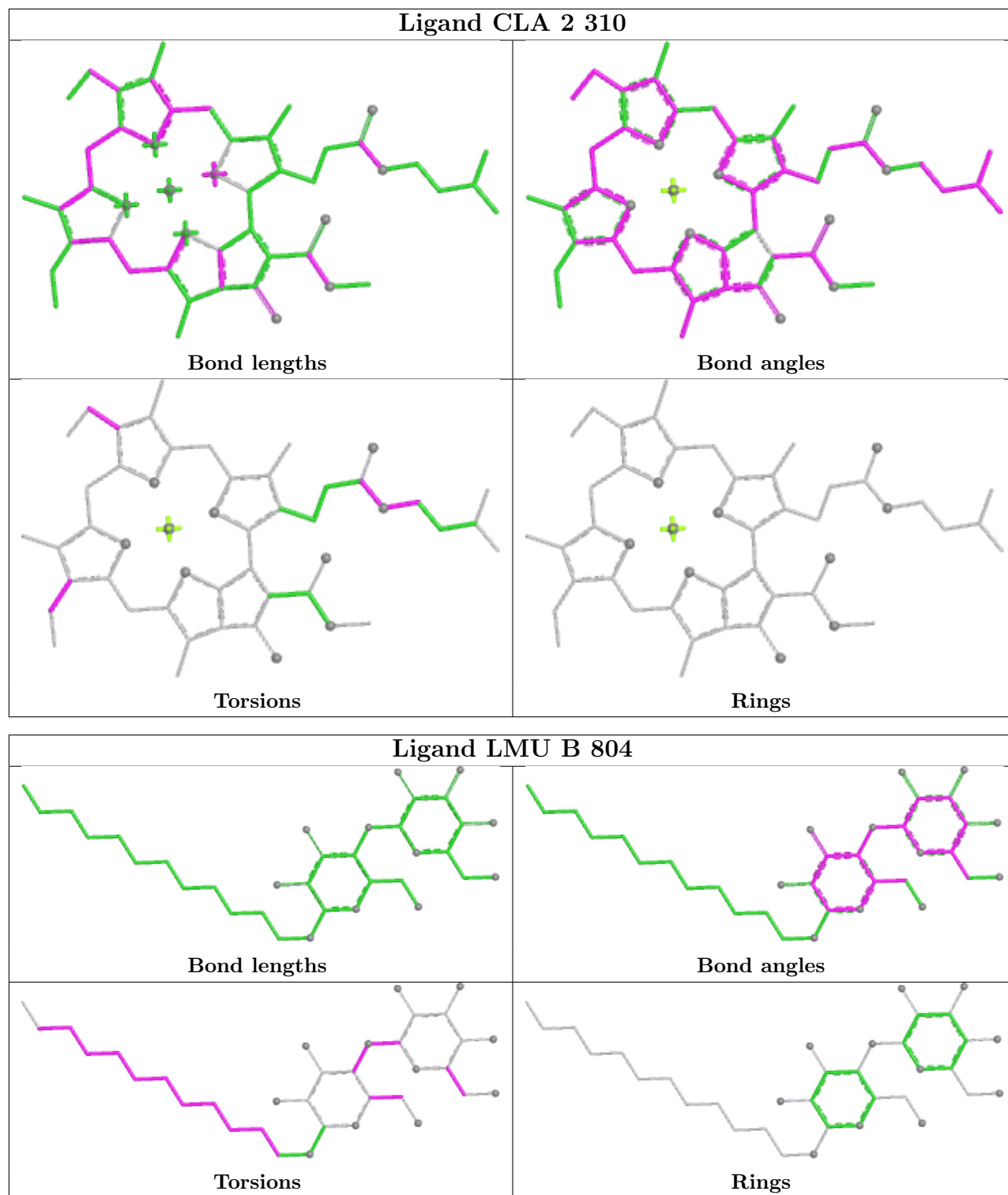


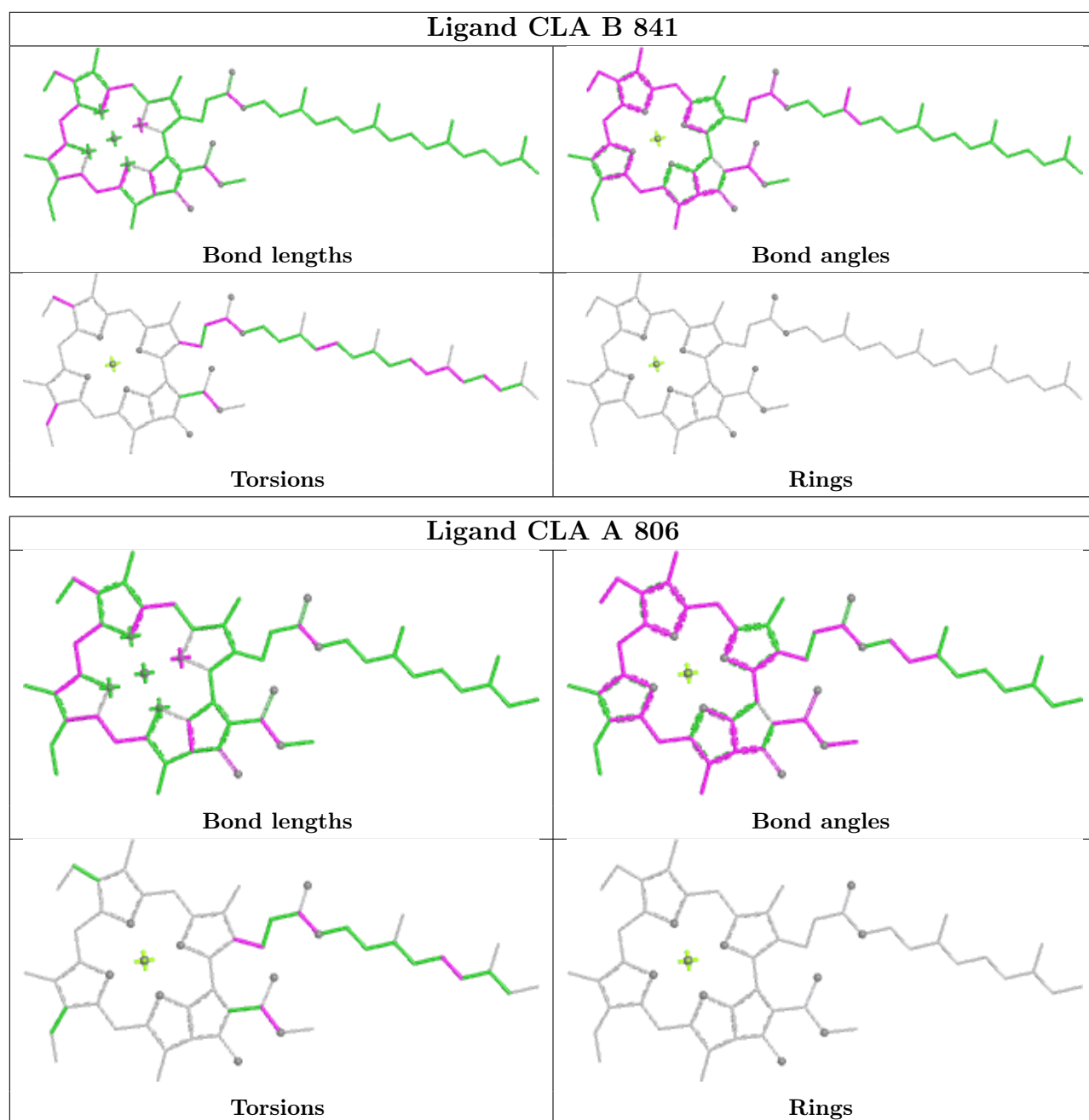


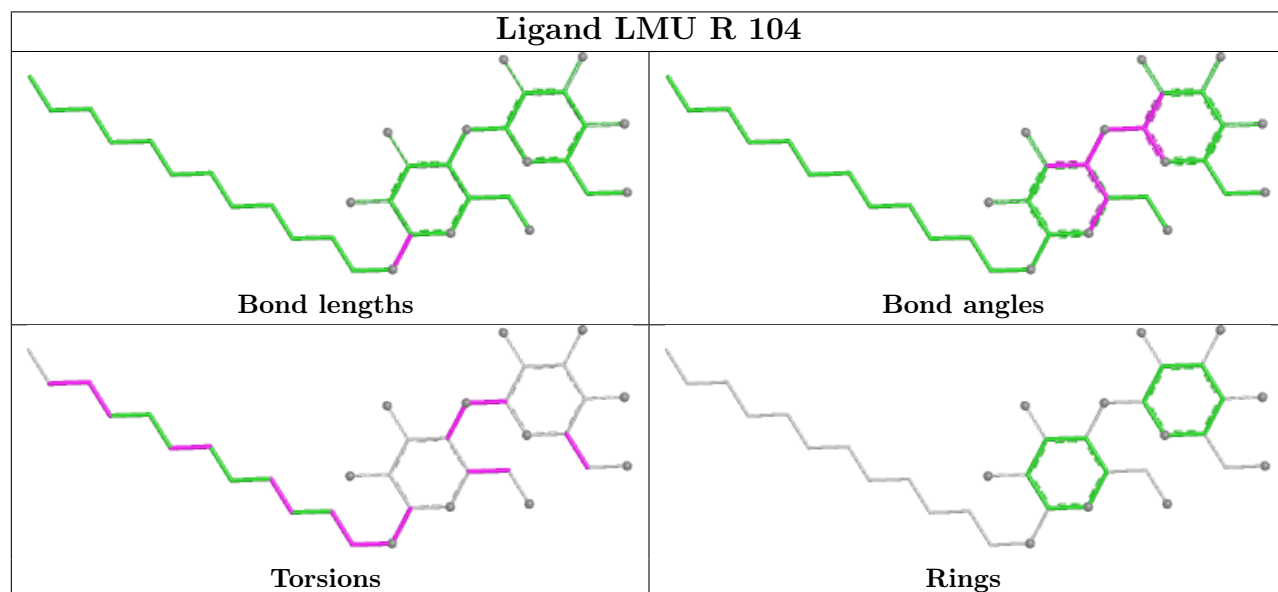
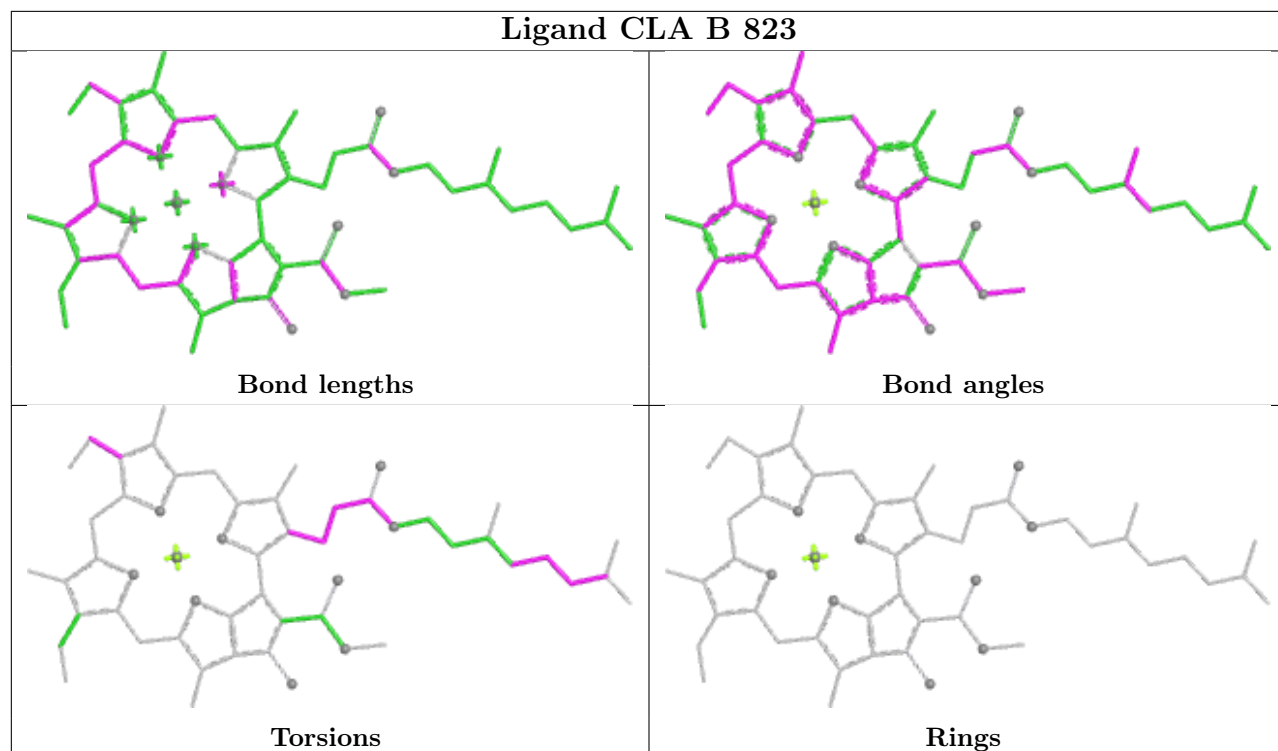




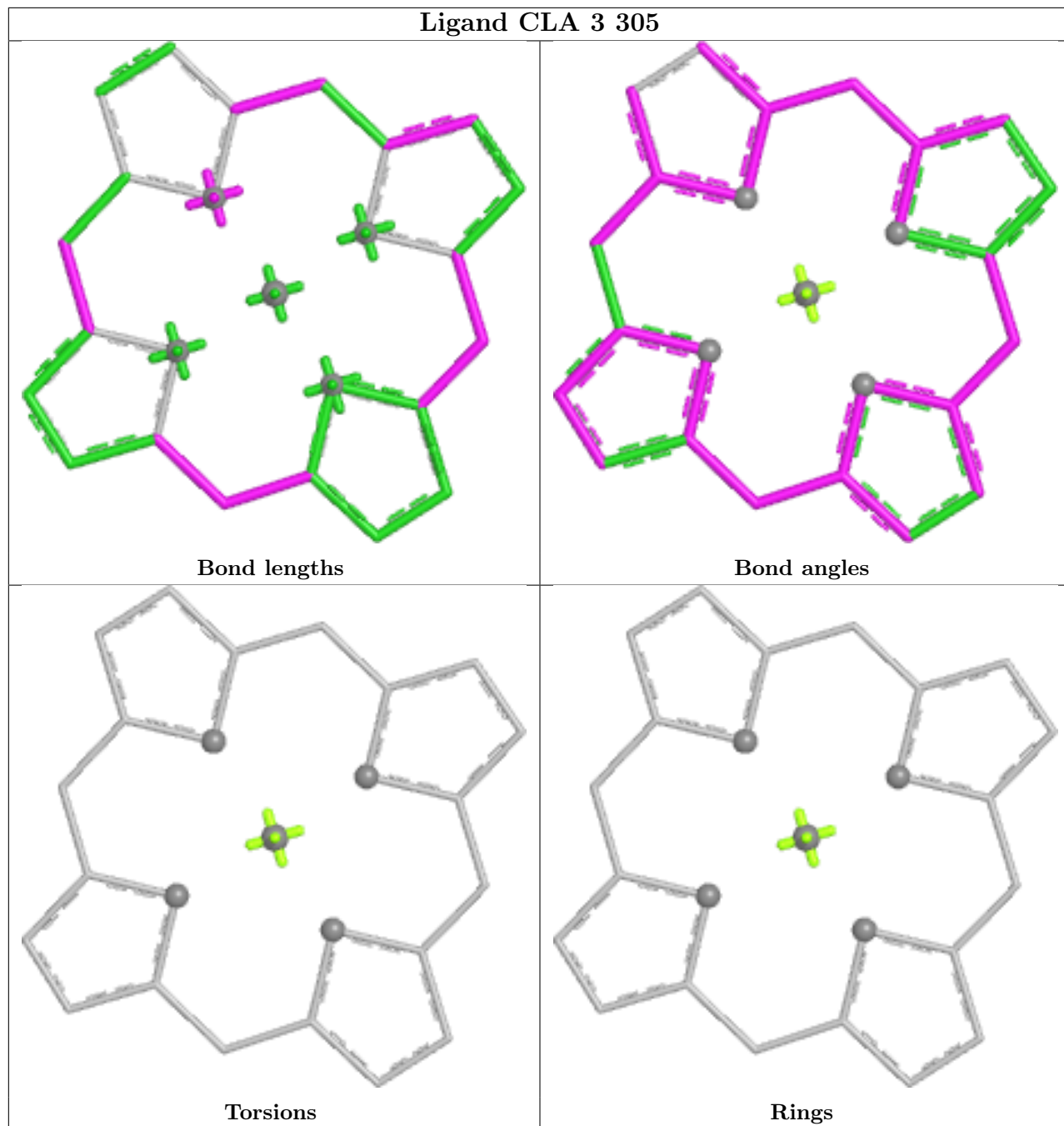


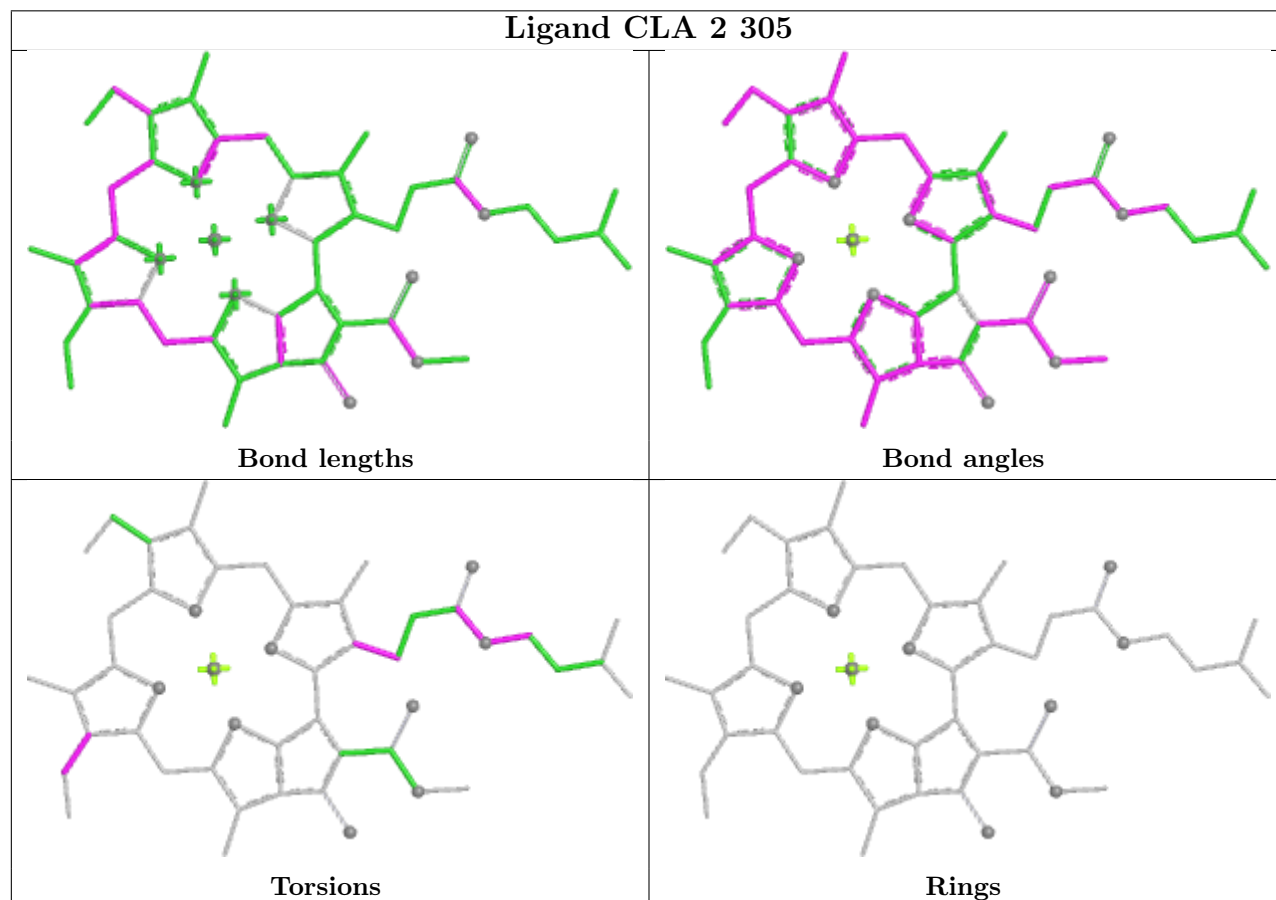
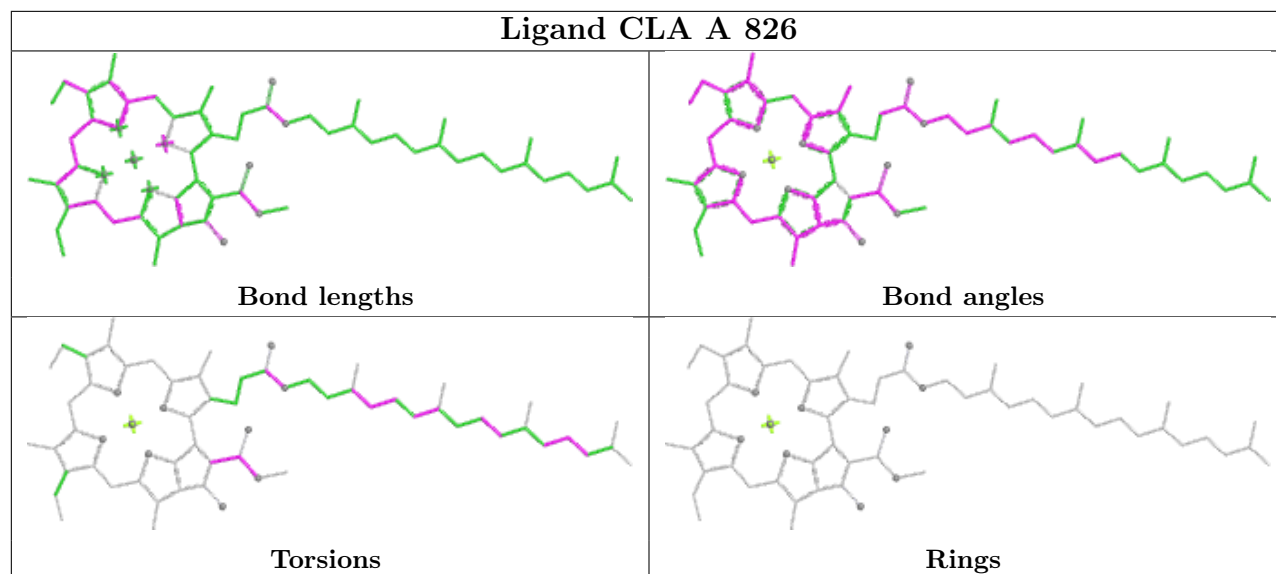


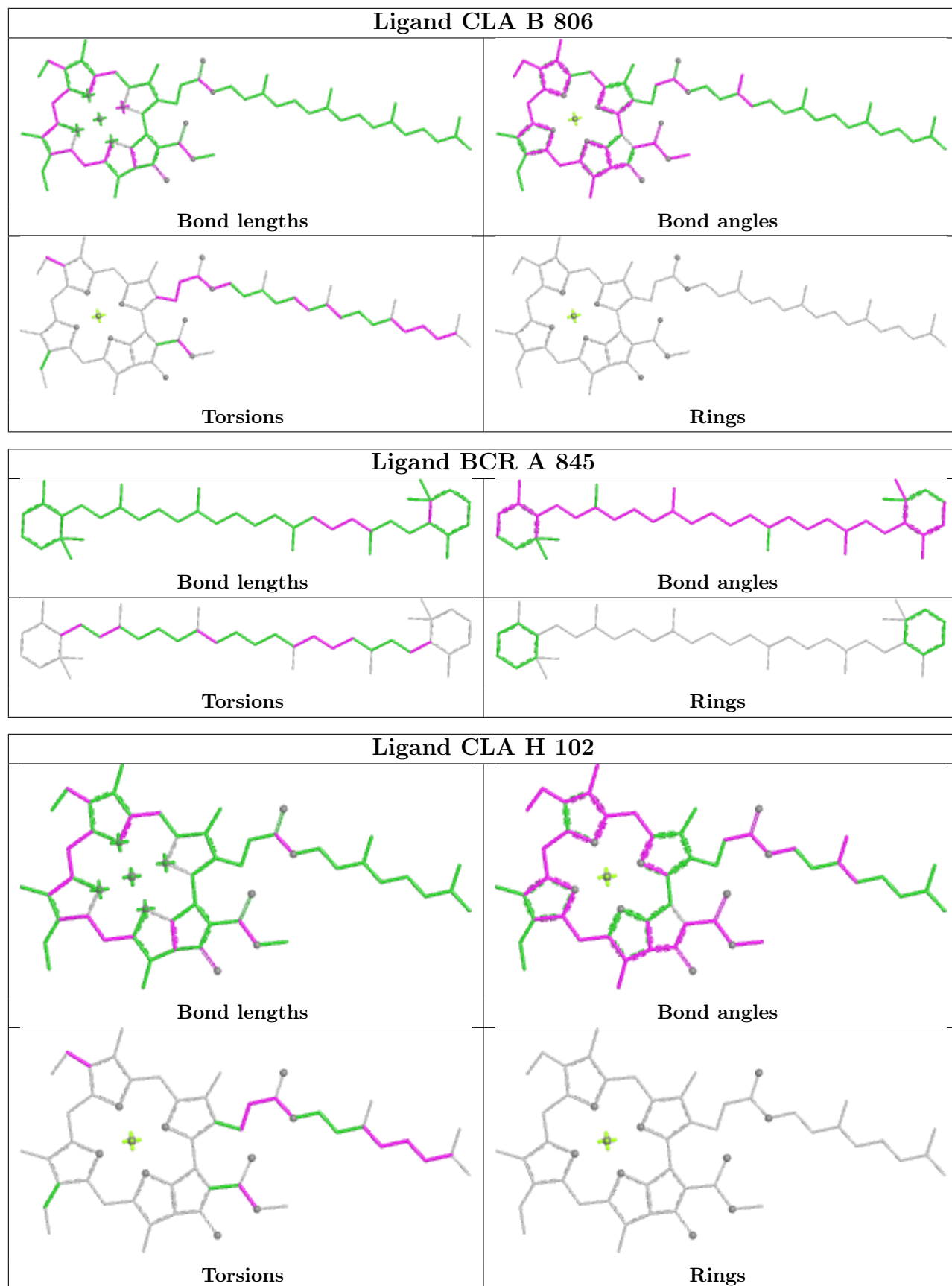


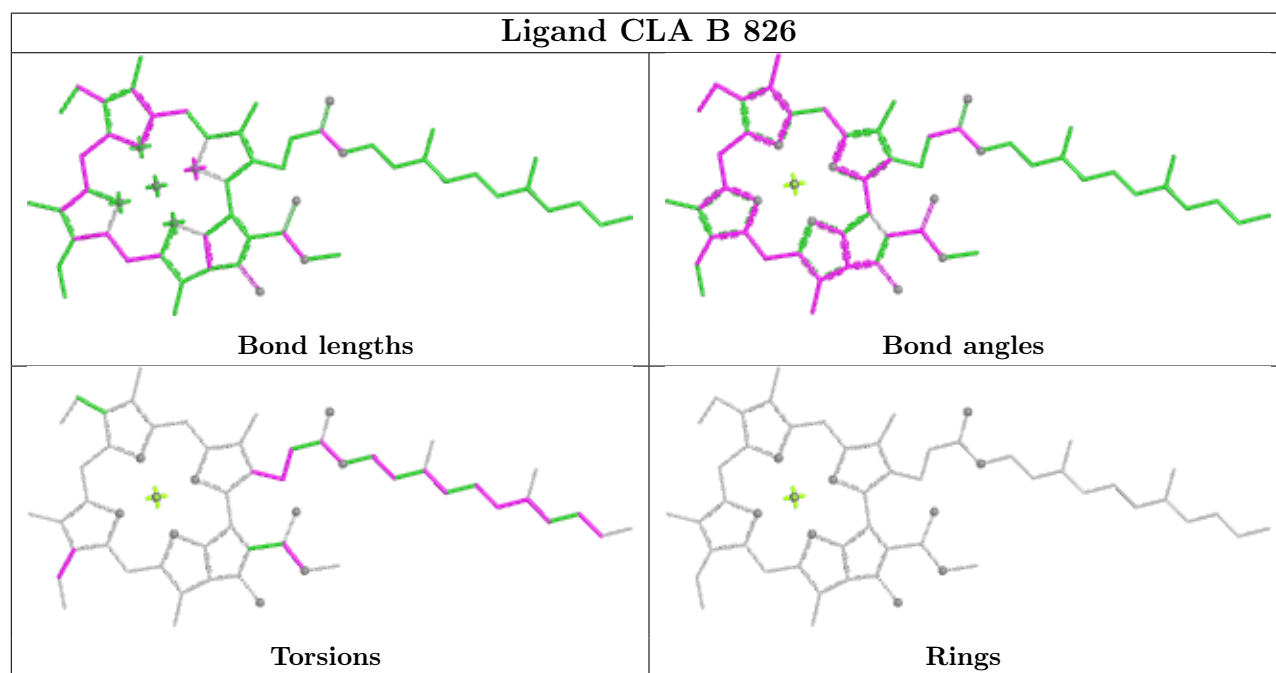
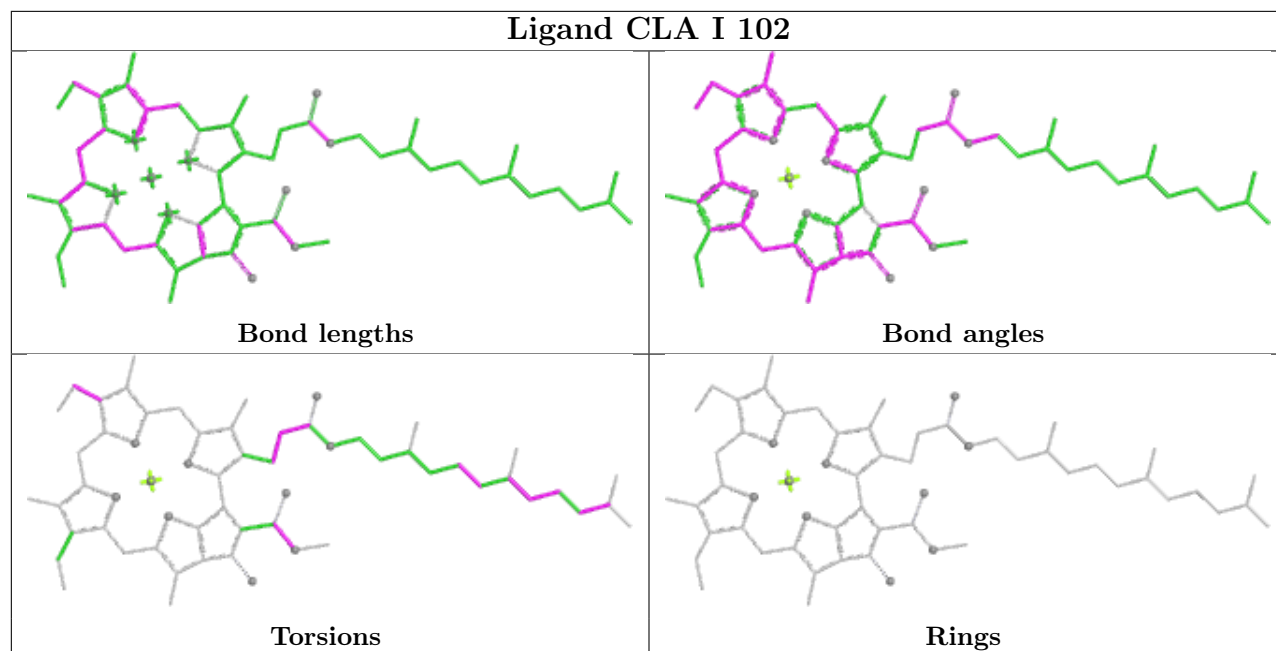


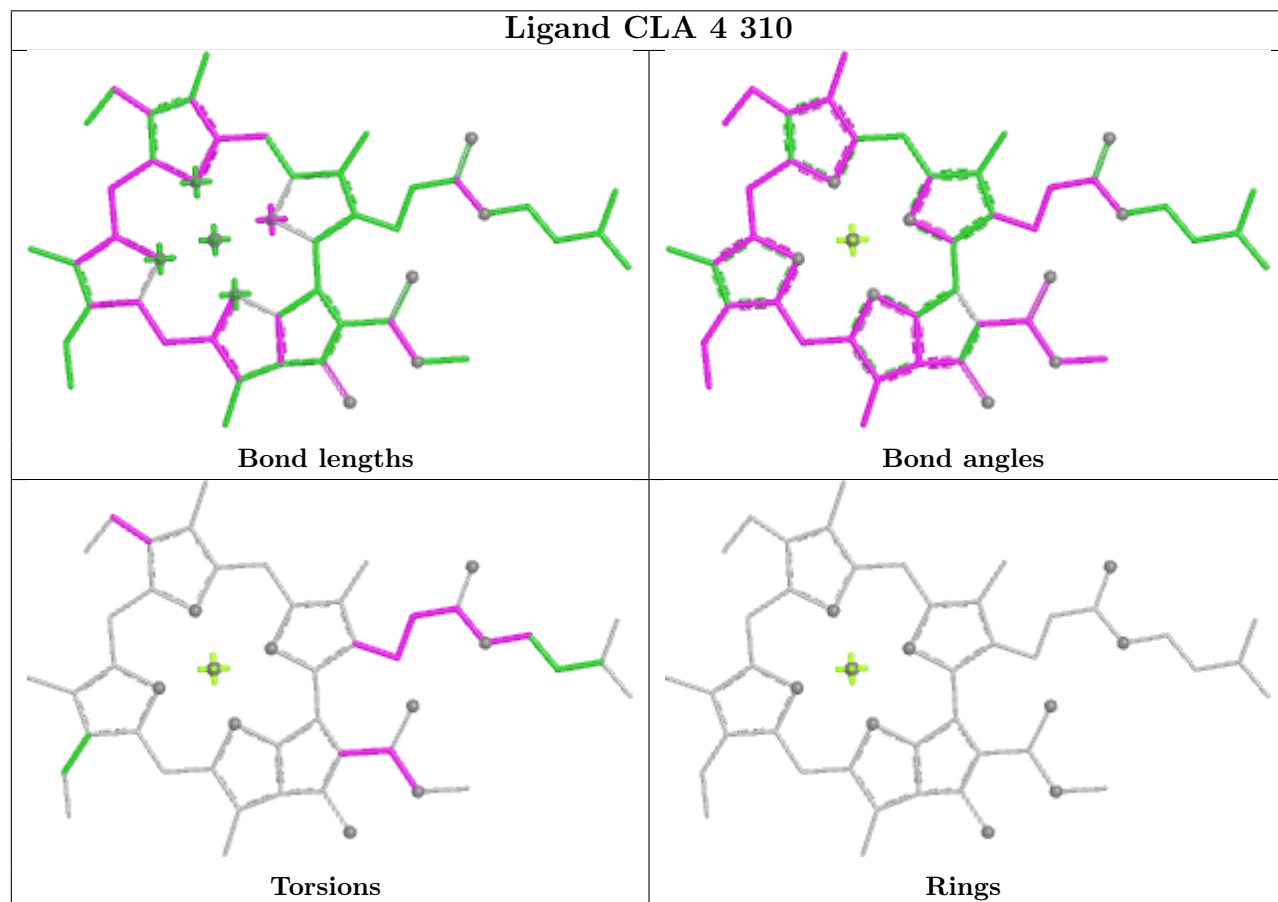
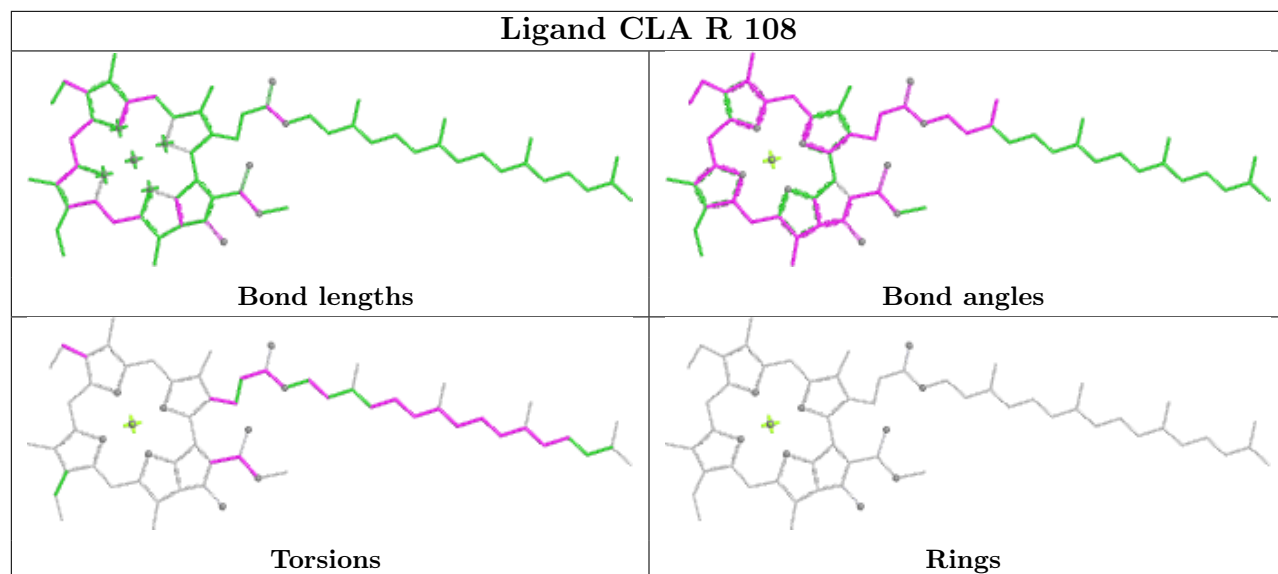
## Ligand CLA 3 305



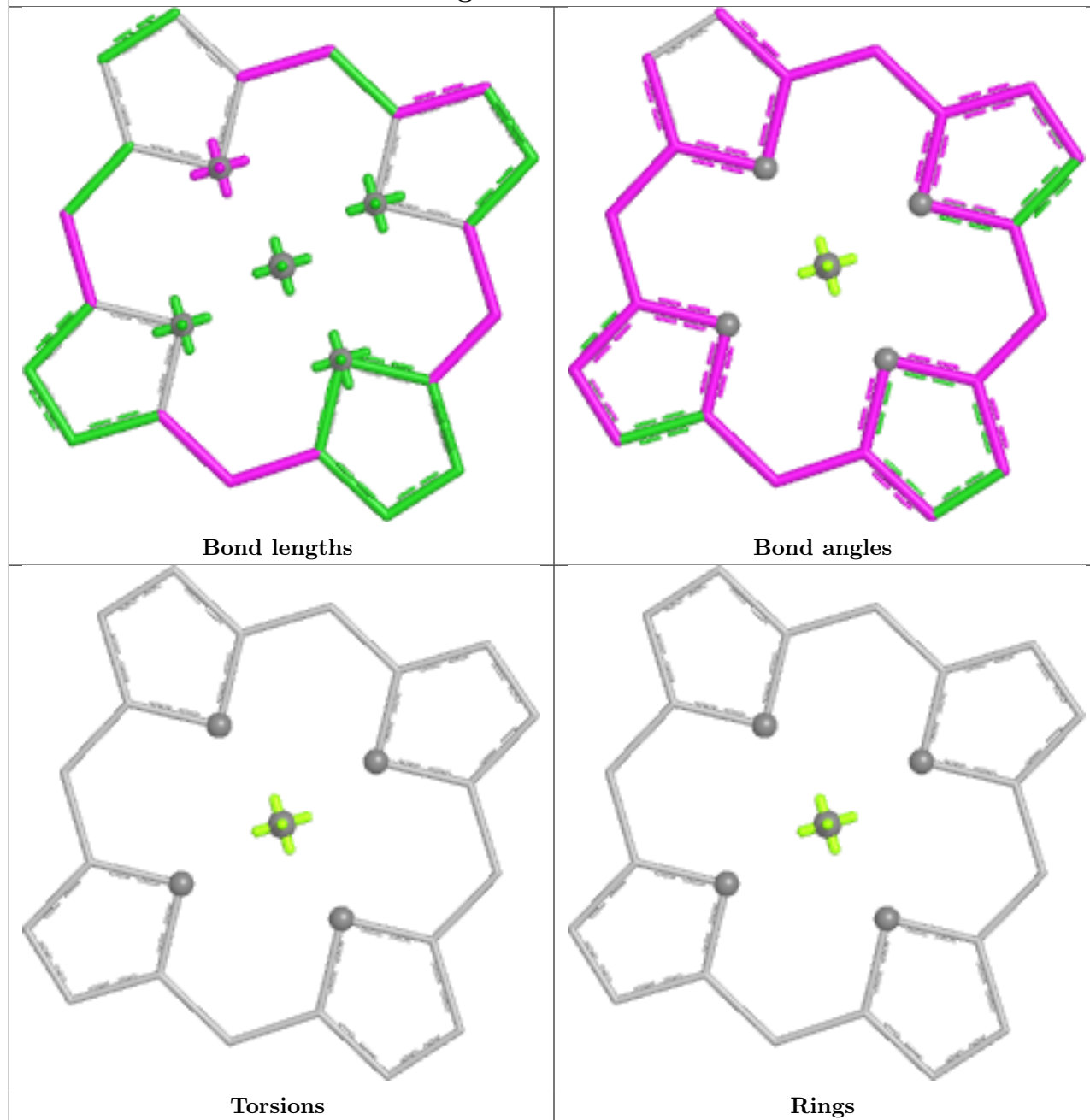


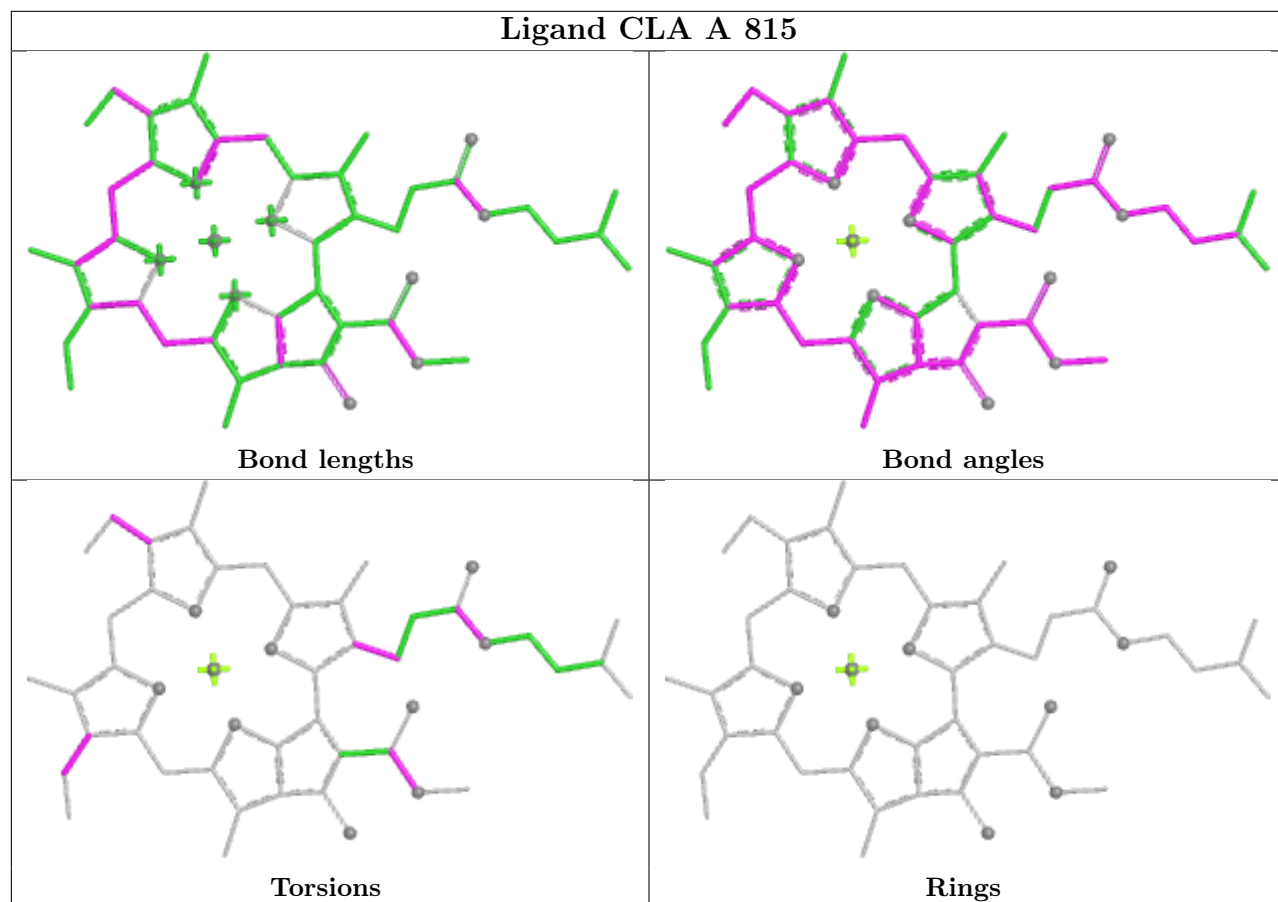


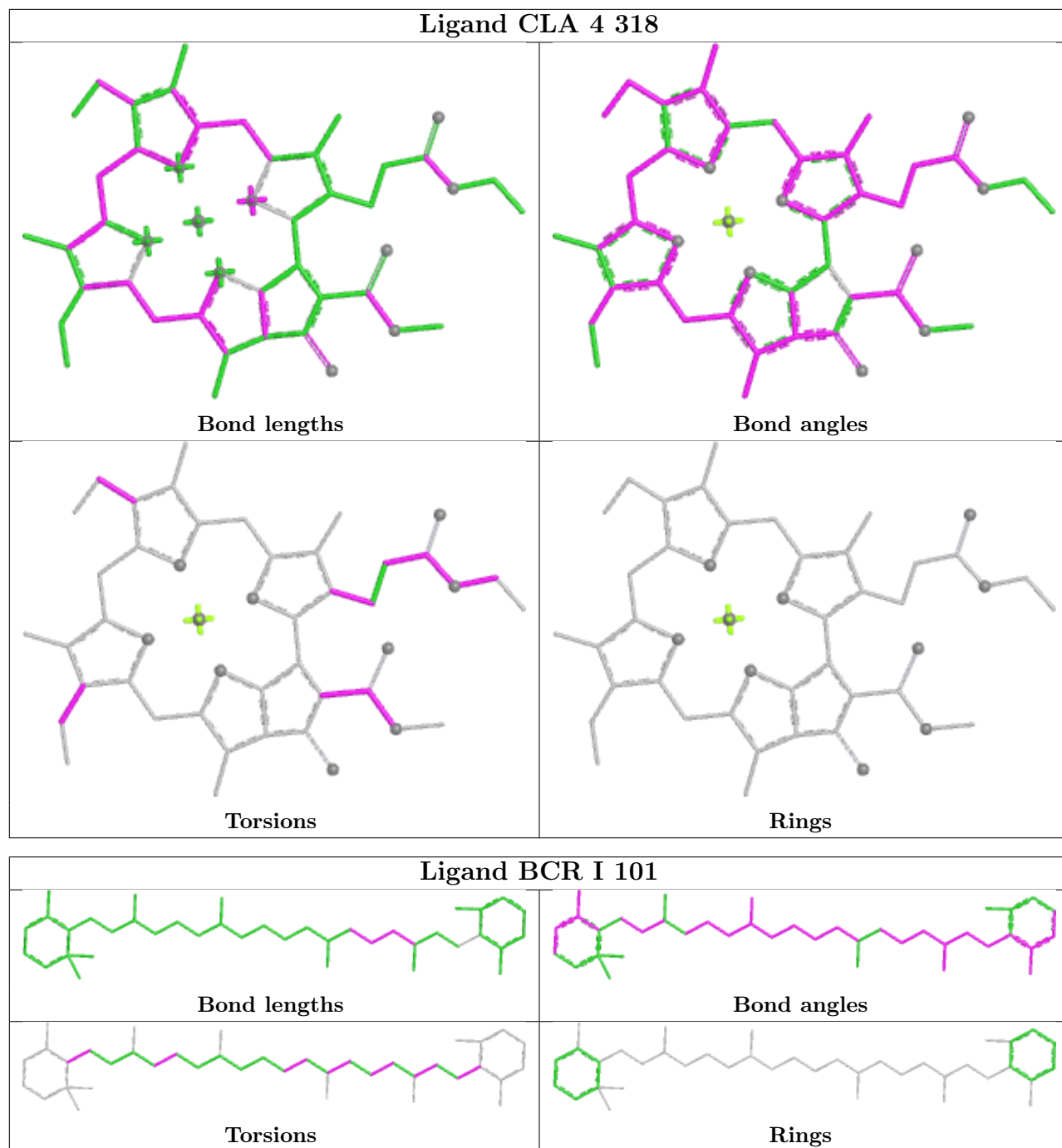


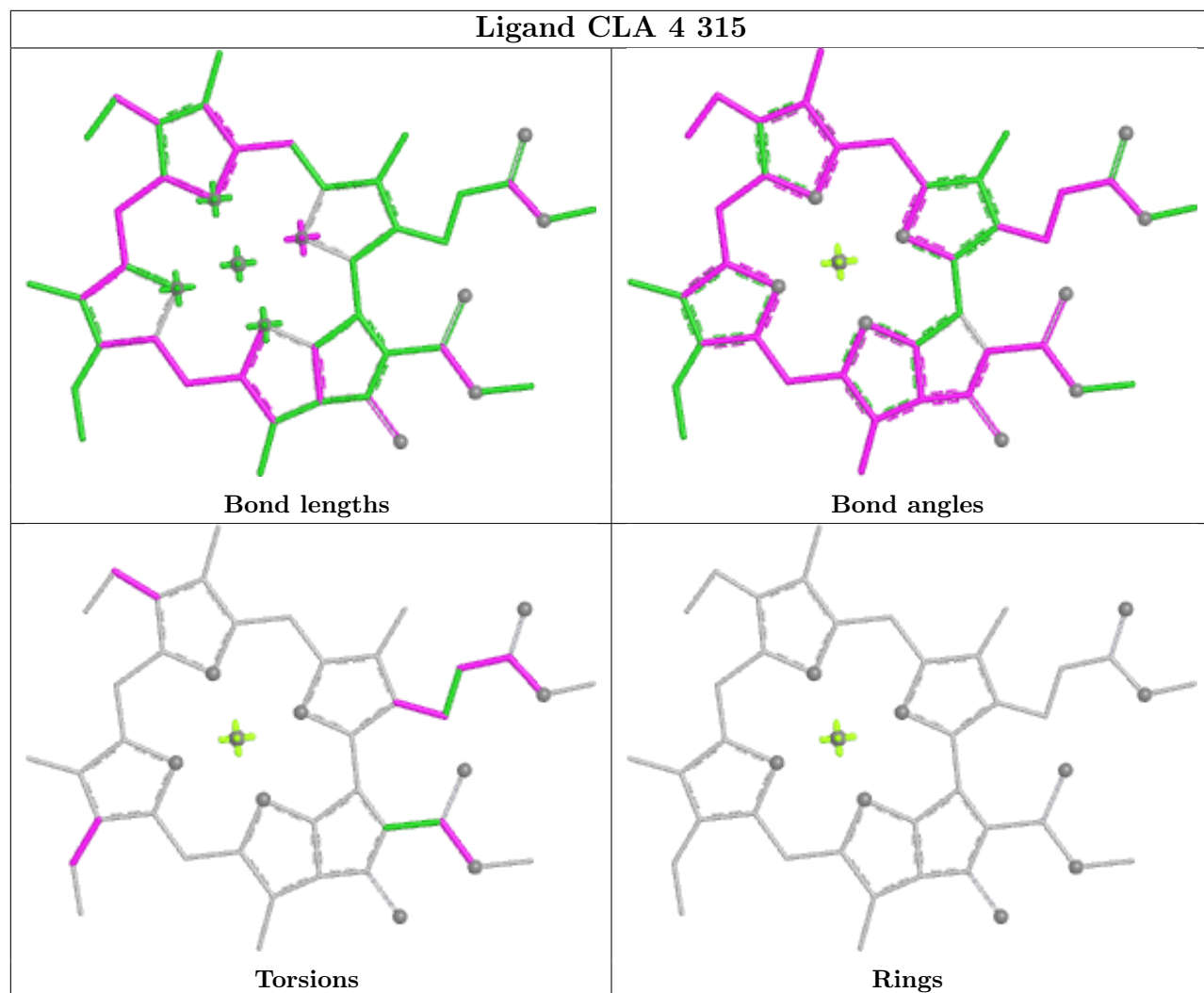


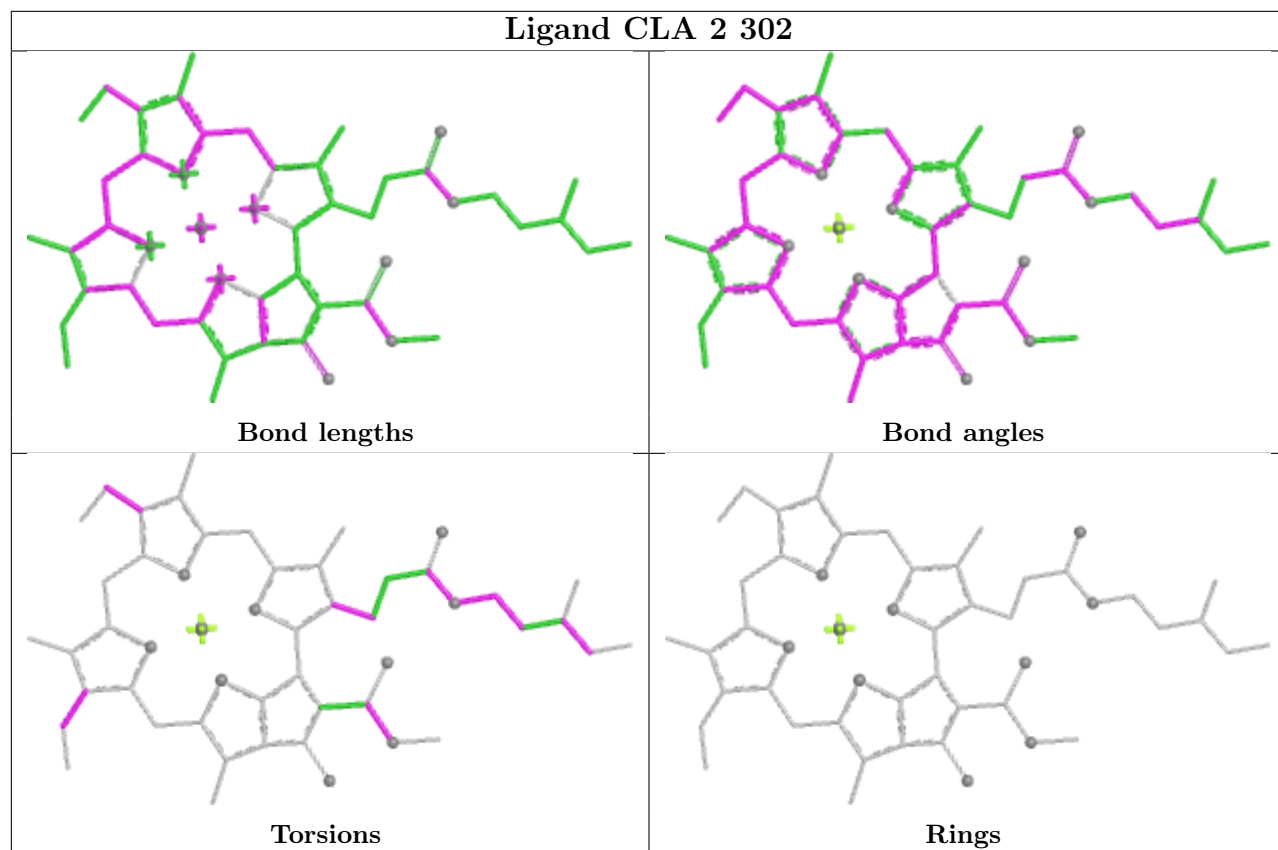
## Ligand CLA 1 214

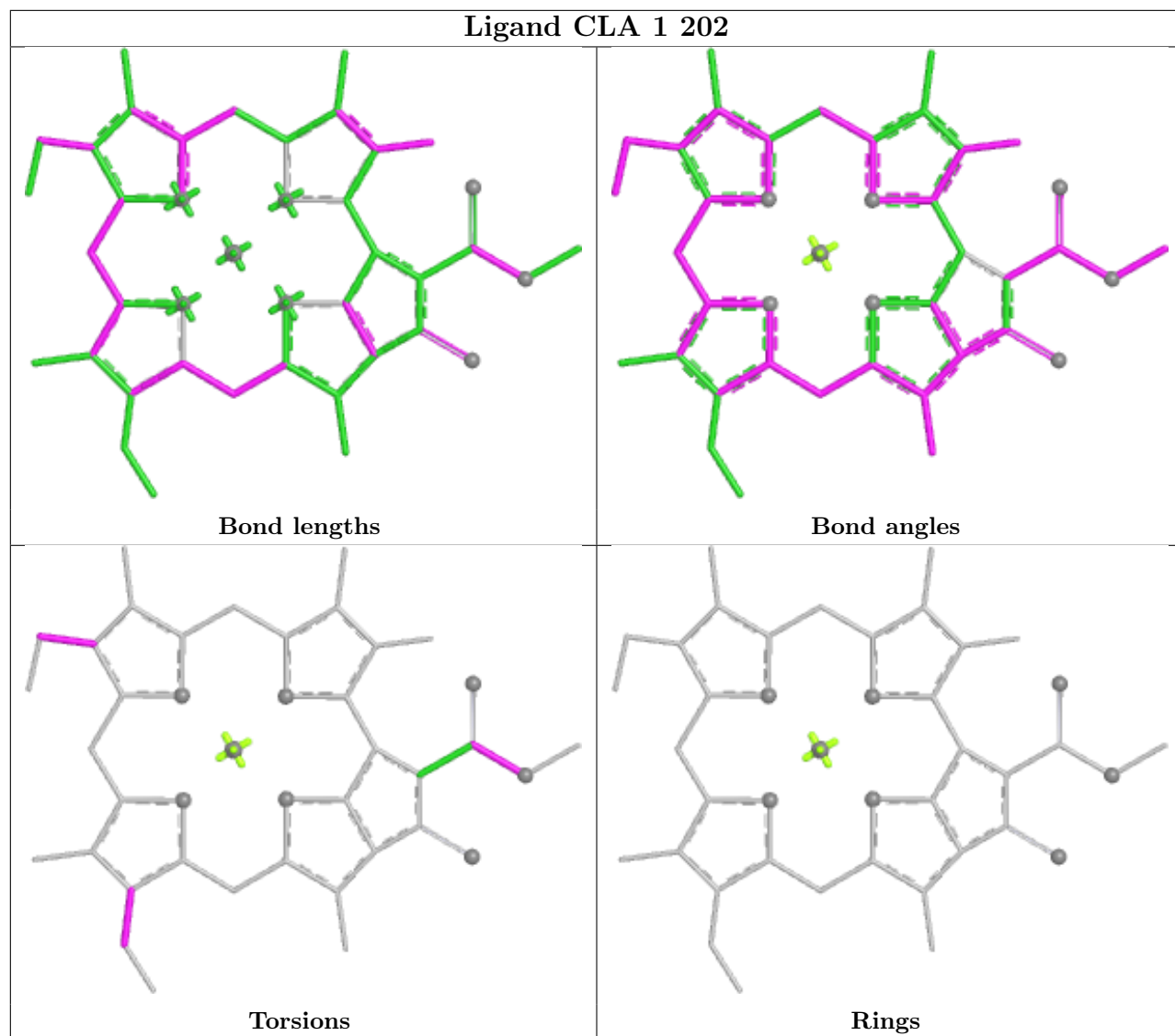


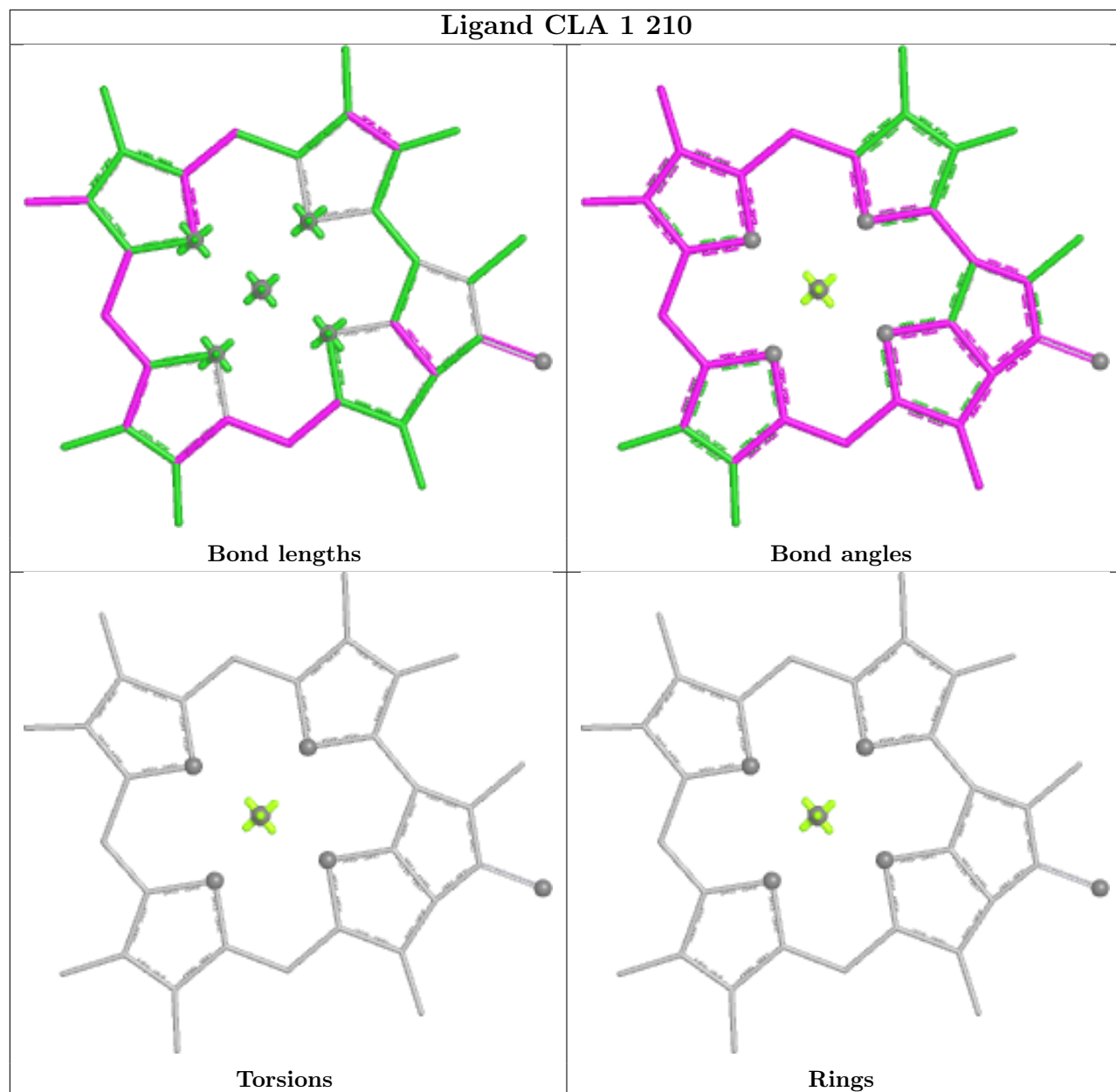


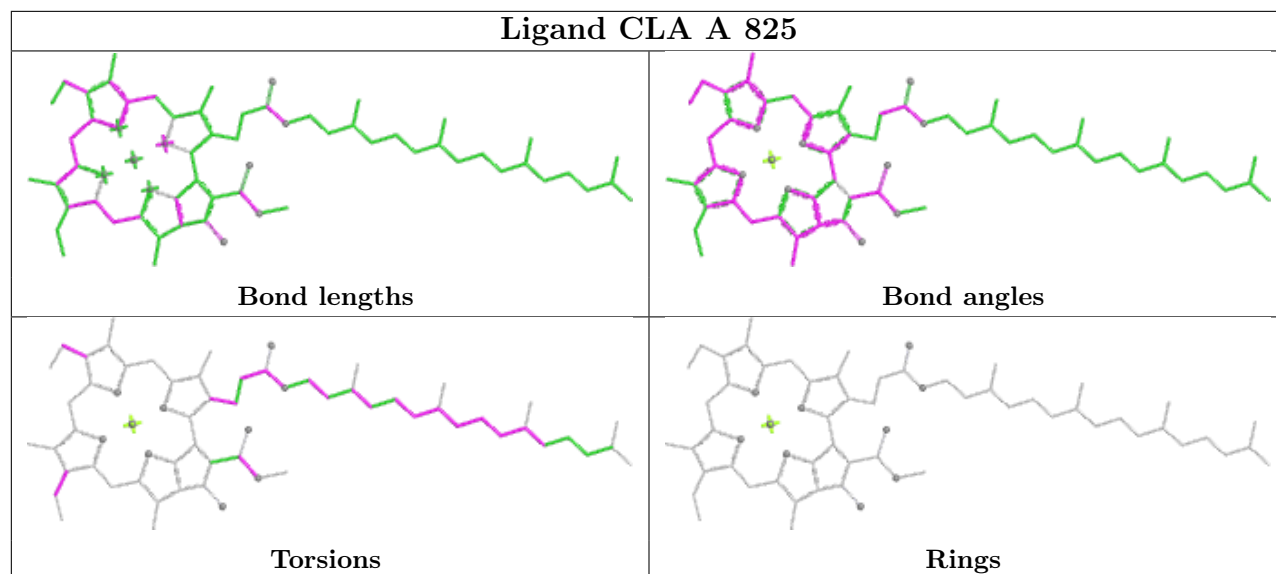












#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.