



# Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 10:27 AM JST

PDB ID : 5ZJI  
EMDB ID : EMD-6932  
Title : Structure of photosystem I supercomplex with light-harvesting complexes I and II  
Authors : Pan, X.W.; Ma, J.; Su, X.D.; Cao, P.; Liu, Z.F.; Zhang, X.Z.; Li, M.  
Deposited on : 2018-03-20  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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:

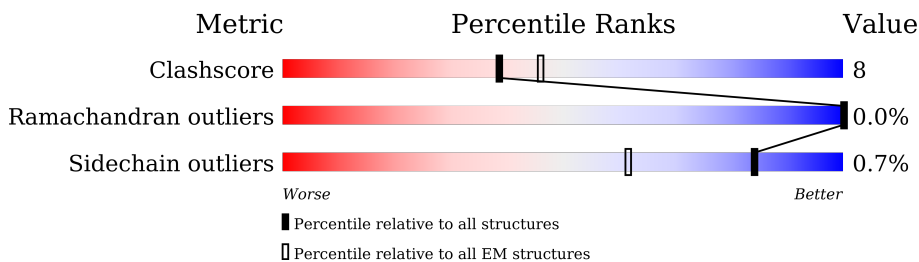
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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




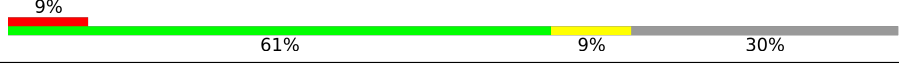
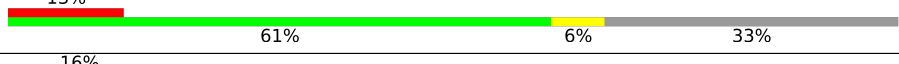


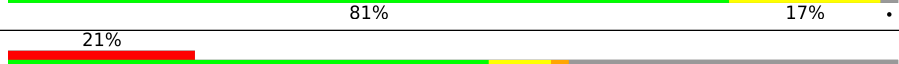
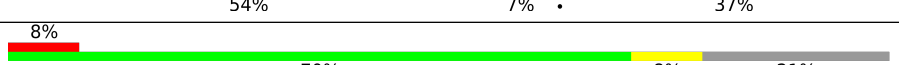

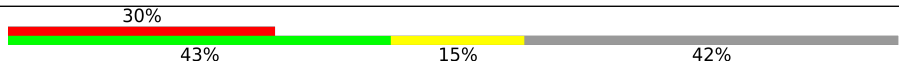
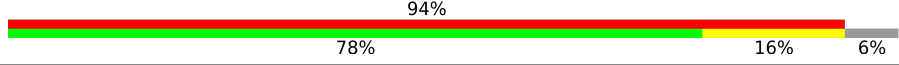
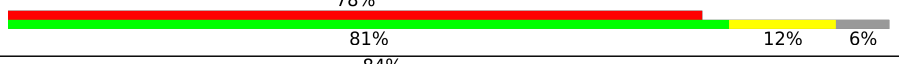


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1	245	
2	2	270	
3	3	267	
4	4	252	
5	A	750	
6	B	734	
7	C	81	
8	D	199	

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Mol	Chain	Length	Quality of chain
9	E	136	
10	F	225	
11	G	145	
12	H	142	
13	I	36	
14	J	42	
15	K	134	
16	L	211	
17	O	127	
18	N	145	
19	X	232	
19	Z	232	
20	Y	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	1	601	X	-	-	-
21	CHL	1	607	X	-	-	-
21	CHL	2	601	X	-	-	-
21	CHL	2	606	X	-	-	-
21	CHL	2	607	X	-	-	-
21	CHL	2	608	X	-	-	-
21	CHL	2	618	X	-	-	-
21	CHL	3	608	X	-	-	-
21	CHL	4	606	X	-	-	-
21	CHL	4	607	X	-	-	-
21	CHL	4	608	X	-	-	-
21	CHL	4	618	X	-	-	-
21	CHL	X	601	X	-	-	-
21	CHL	X	605	X	-	-	-
21	CHL	X	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	X	607	X	-	-	-
21	CHL	X	608	X	-	-	-
21	CHL	X	609	X	-	-	-
21	CHL	Y	601	X	-	-	-
21	CHL	Y	605	X	-	-	-
21	CHL	Y	606	X	-	-	-
21	CHL	Y	607	X	-	-	-
21	CHL	Y	608	X	-	-	-
21	CHL	Y	609	X	-	-	-
21	CHL	Z	601	X	-	-	-
21	CHL	Z	605	X	-	-	-
21	CHL	Z	606	X	-	-	-
21	CHL	Z	607	X	-	-	-
21	CHL	Z	608	X	-	-	-
21	CHL	Z	609	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	2	614	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	617	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	302	X	-	-	-
22	CLA	L	303	X	-	-	-
22	CLA	L	304	X	-	-	-
22	CLA	N	1002	X	-	-	-
22	CLA	O	2001	X	-	-	-
22	CLA	O	2002	X	-	-	-
22	CLA	X	602	X	-	-	-
22	CLA	X	603	X	-	-	-
22	CLA	X	604	X	-	-	-
22	CLA	X	610	X	-	-	-
22	CLA	X	611	X	-	-	-
22	CLA	X	612	X	-	-	-
22	CLA	X	613	X	-	-	-
22	CLA	X	614	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
28	CL0	A	801	X	-	X	-



## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 44708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	196	1522	991	253	272	6	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	207	1624	1064	263	293	4	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	221	1720	1130	276	307	7	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	199	1566	1020	257	285	4	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	742	5836	3824	992	1002	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P04966

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	733	5866	3849	997	1007	13	0	0

- Molecule 7 is a protein called photosystem I subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	81	612	377	105	118	12	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	142	1115	717	193	202	3	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	68	540	344	97	99	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	158	1238	805	212	218	3	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit V.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	97	752	489	125	138	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	95	729	477	116	136	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	33	Total	C	N	O	S	0	0
			260	178	38	43	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			325	220	50	54	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			589	372	102	112	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	166	Total	C	N	O	S	0	0
			1246	820	198	226	2		

- Molecule 17 is a protein called 16kDa membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	76	Total	C	N	O	S	0	0
			621	418	101	101	1		

- Molecule 18 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	84	Total	C	N	O	S	0	0
			685	439	112	129	5		

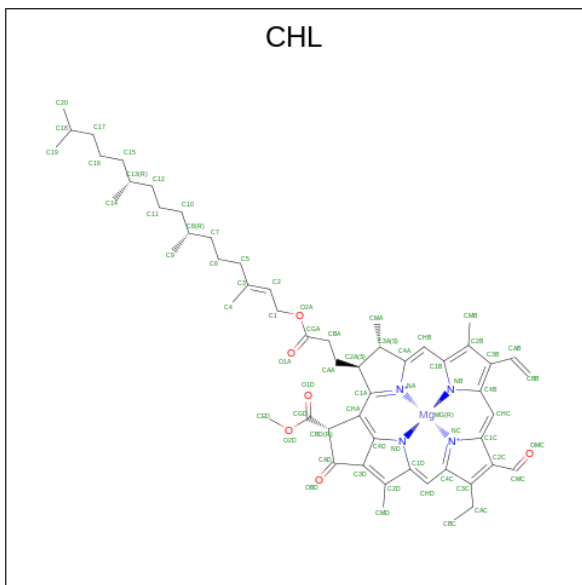
- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		
19	Z	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
20	Y	228	1751	1132	290	322	1	6	0	0

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



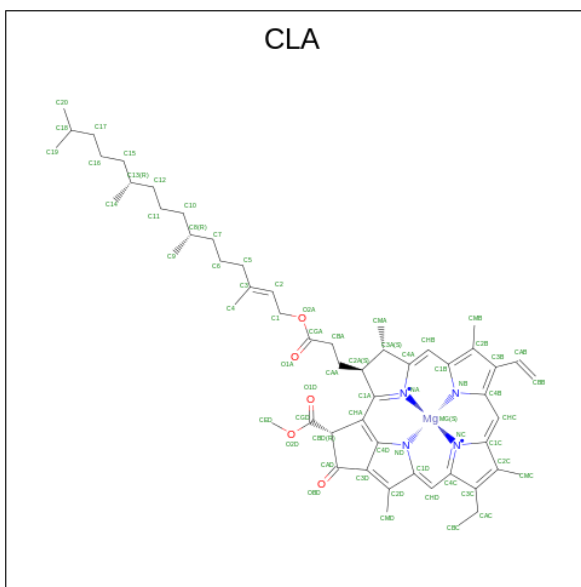
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	1	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
21	1	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	Total 169	C 132	Mg 4	N 16	O 17	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	1	1	577	465	12	48	52	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0

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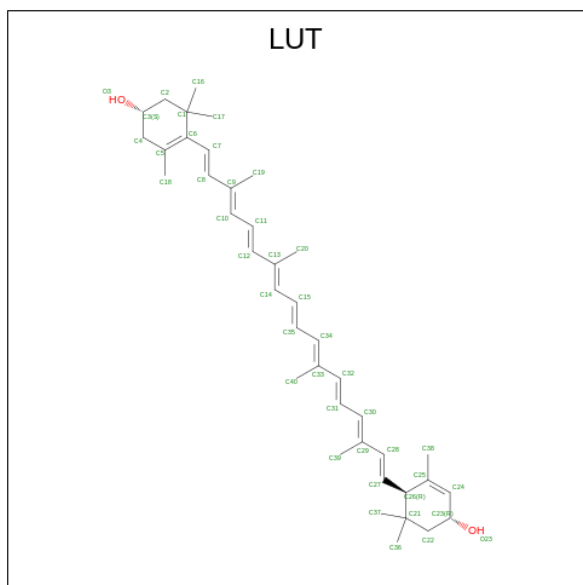
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	L	1	Total 150	C 120	Mg 3	N 12	O 15	0
22	L	1	Total 150	C 120	Mg 3	N 12	O 15	0
22	L	1	Total 150	C 120	Mg 3	N 12	O 15	0
22	O	1	Total 76	C 60	Mg 2	N 8	O 6	0
22	O	1	Total 76	C 60	Mg 2	N 8	O 6	0
22	N	1	Total 95	C 75	Mg 2	N 8	O 10	0
22	N	1	Total 95	C 75	Mg 2	N 8	O 10	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	X	1	Total 305	C 248	Mg 8	N 32	O 17	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



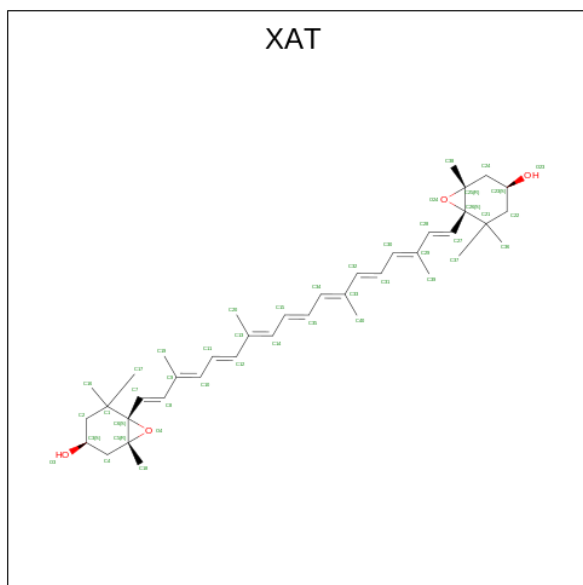
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	1	1	Total 84	C 80	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	1	1	84	80	4	0
23	2	1	42	40	2	0
23	3	1	42	40	2	0
23	4	1	42	40	2	0
23	X	1	84	80	4	0
23	X	1	84	80	4	0
23	Y	1	84	80	4	0
23	Y	1	84	80	4	0
23	Z	1	84	80	4	0
23	Z	1	84	80	4	0

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



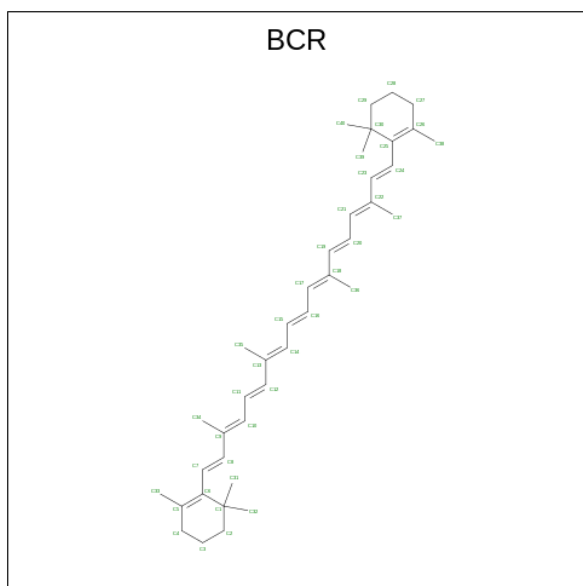
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	1	1	44	40	4	0

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Mol	Chain	Residues	Atoms			AltConf
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	X	1	Total	C	O	0
			44	40	4	
24	Y	1	Total	C	O	0
			44	40	4	
24	Z	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	2	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			240	240	

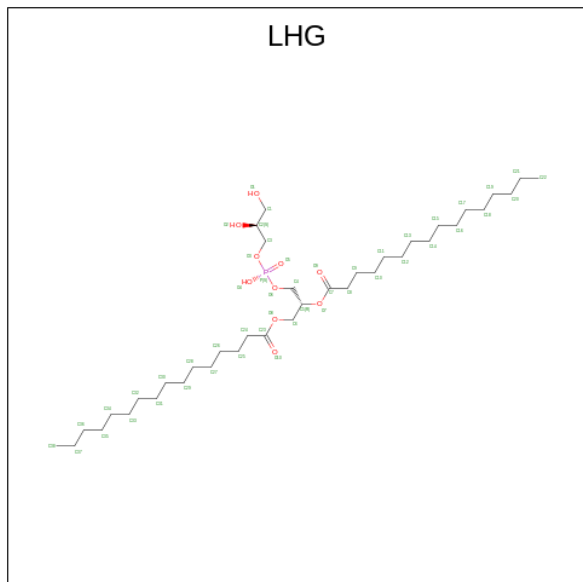
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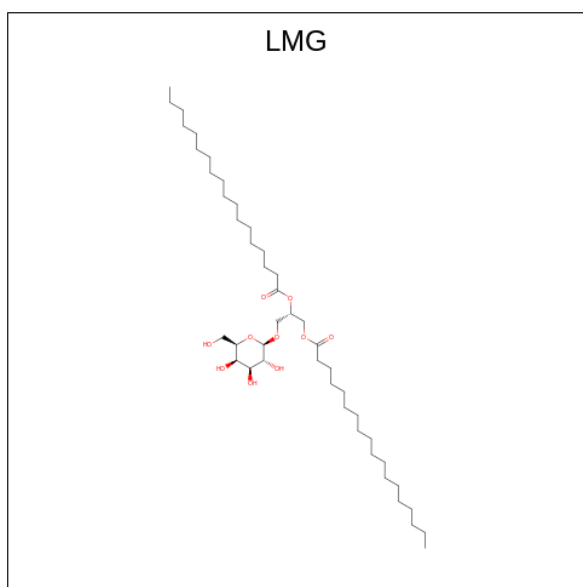
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	F	1	Total 40	C 40	0
25	G	1	Total 40	C 40	0
25	I	1	Total 40	C 40	0
25	J	1	Total 40	C 40	0
25	K	1	Total 80	C 80	0
25	K	1	Total 80	C 80	0
25	L	1	Total 120	C 120	0
25	L	1	Total 120	C 120	0
25	L	1	Total 120	C 120	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



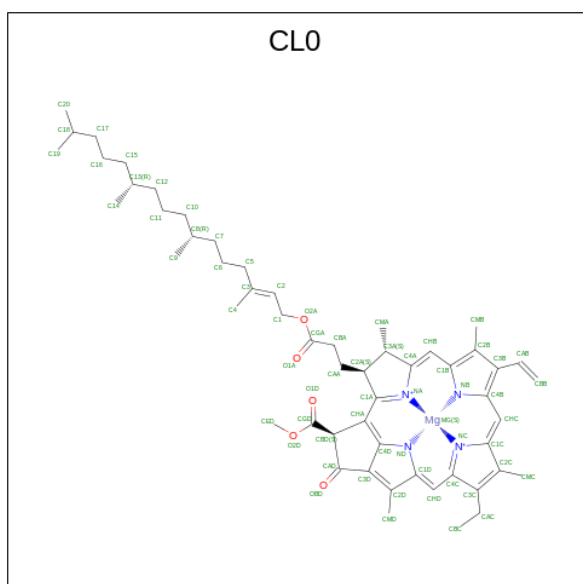
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	1	1	Total 49	C 38	O 10	P 1	0
26	2	1	Total 37	C 26	O 10	P 1	0
26	A	1	Total 79	C 57	O 20	P 2	0
26	A	1	Total 79	C 57	O 20	P 2	0
26	B	1	Total 38	C 27	O 10	P 1	0
26	X	1	Total 22	C 11	O 10	P 1	0
26	Y	1	Total 45	C 34	O 10	P 1	0
26	Z	1	Total 23	C 12	O 10	P 1	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



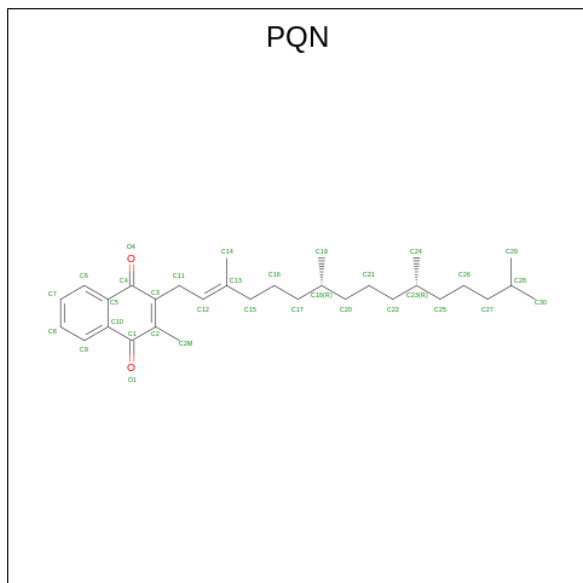
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			53	43	10	
27	2	1	Total	C	O	0
			36	26	10	
27	4	1	Total	C	O	0
			72	52	20	
27	4	1	Total	C	O	0
			72	52	20	
27	G	1	Total	C	O	0
			38	28	10	

- Molecule 28 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



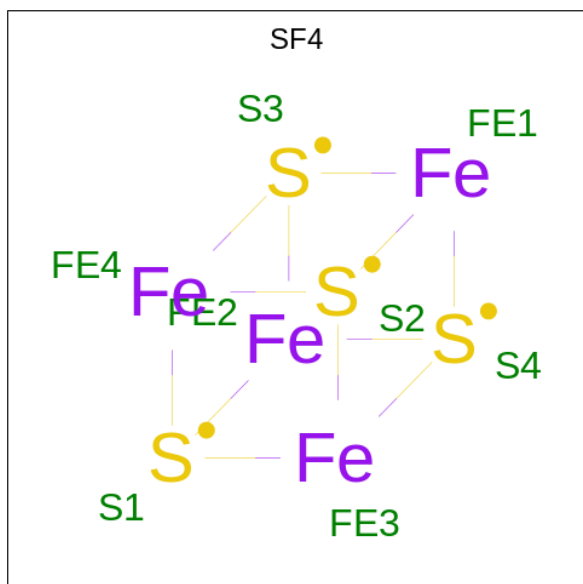
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
28	A	1	65	55	1	4	5	0

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



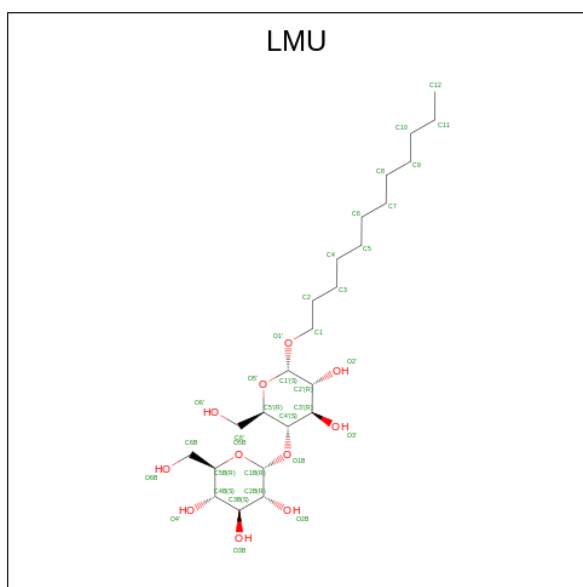
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	33	31	2	0
29	B	1	33	31	2	0

- Molecule 30 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



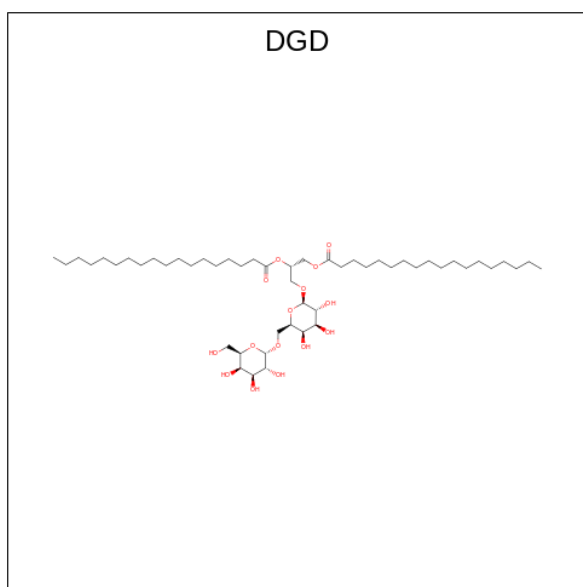
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			16	8	8	
30	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 31 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



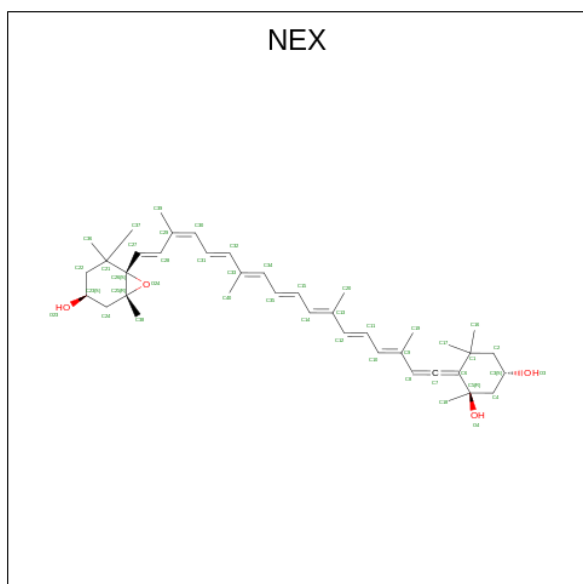
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			30	19	11	
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			66	51	15	
32	J	1	Total	C	O	0
			66	51	15	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).

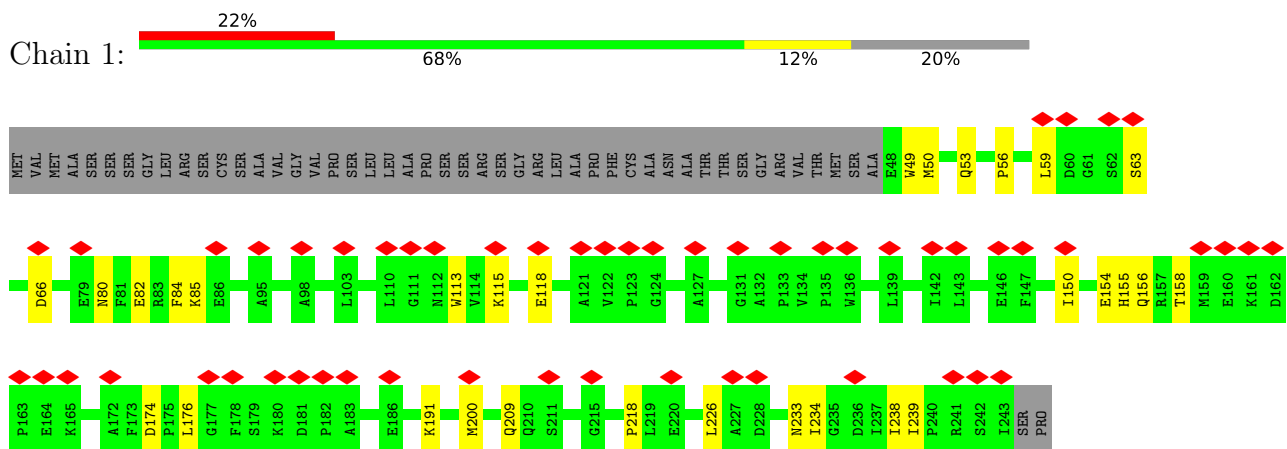


Mol	Chain	Residues	Atoms			AltConf
33	X	1	Total	C	O	0
			44	40	4	
33	Y	1	Total	C	O	0
			44	40	4	
33	Z	1	Total	C	O	0
			44	40	4	

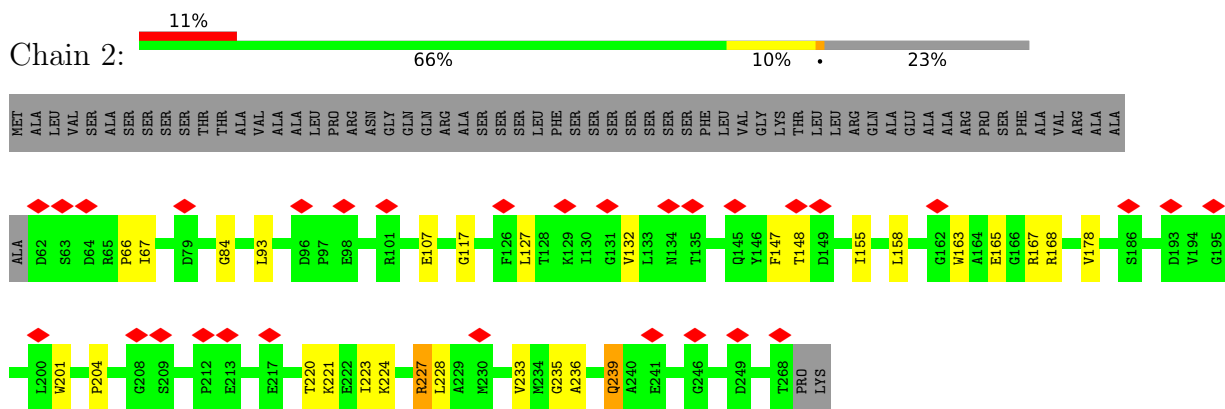
### 3 Residue-property plots [i](#)

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

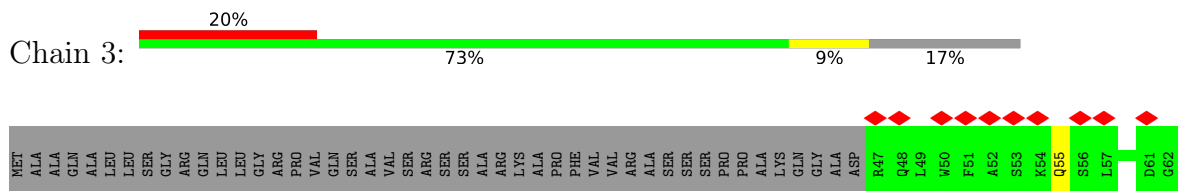
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



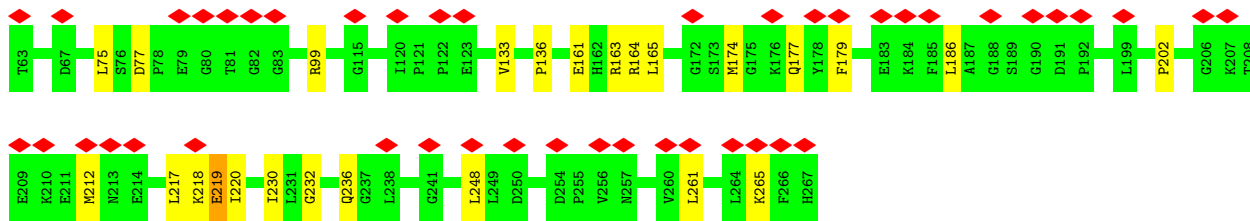
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



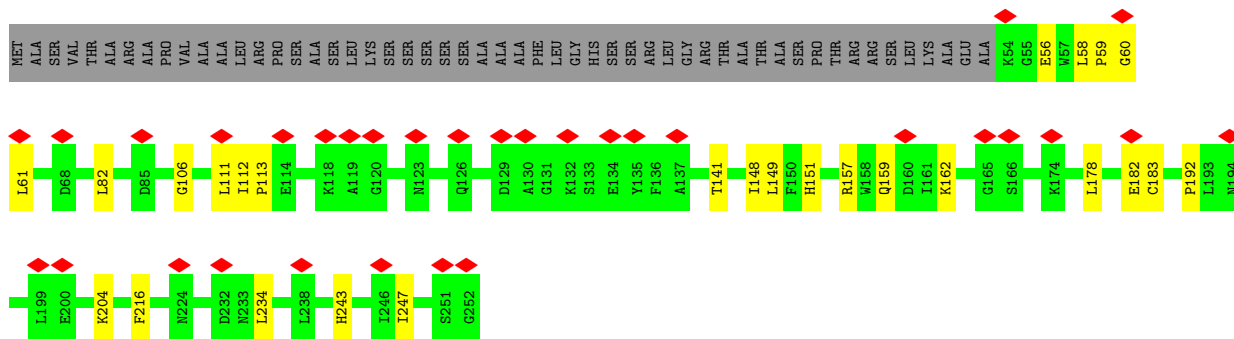
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



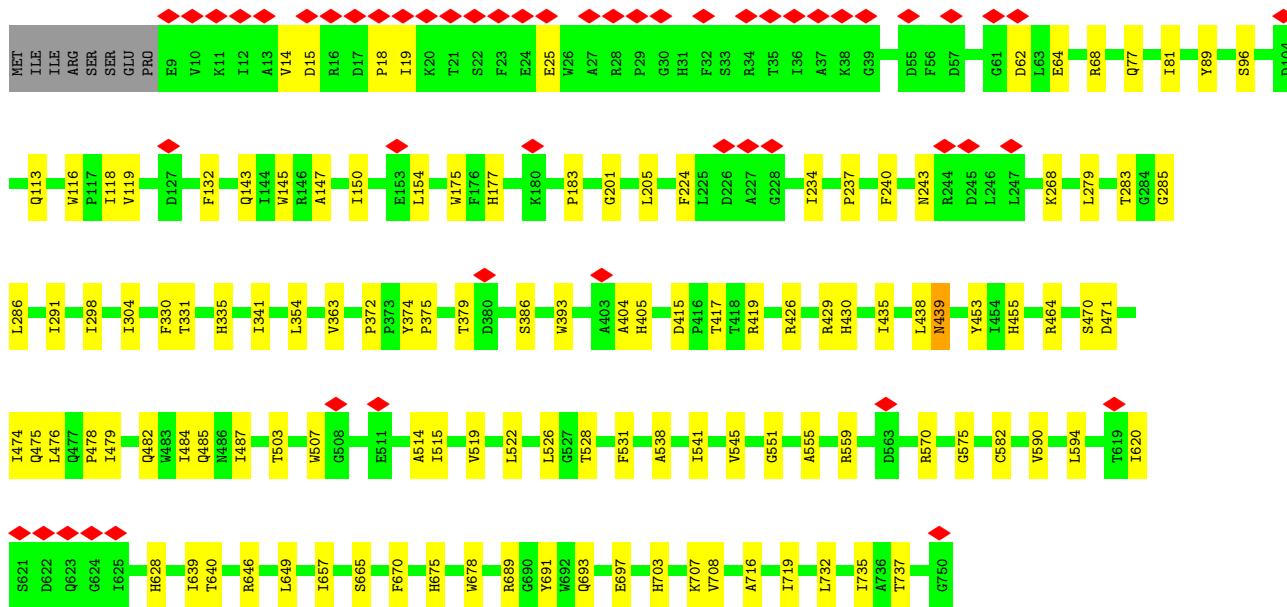
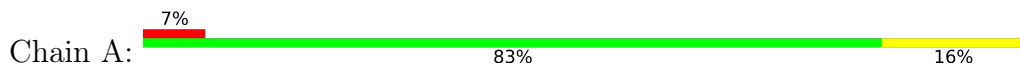




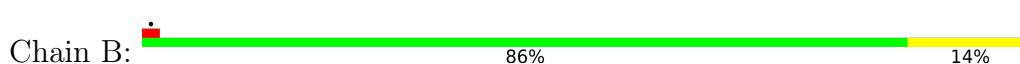
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

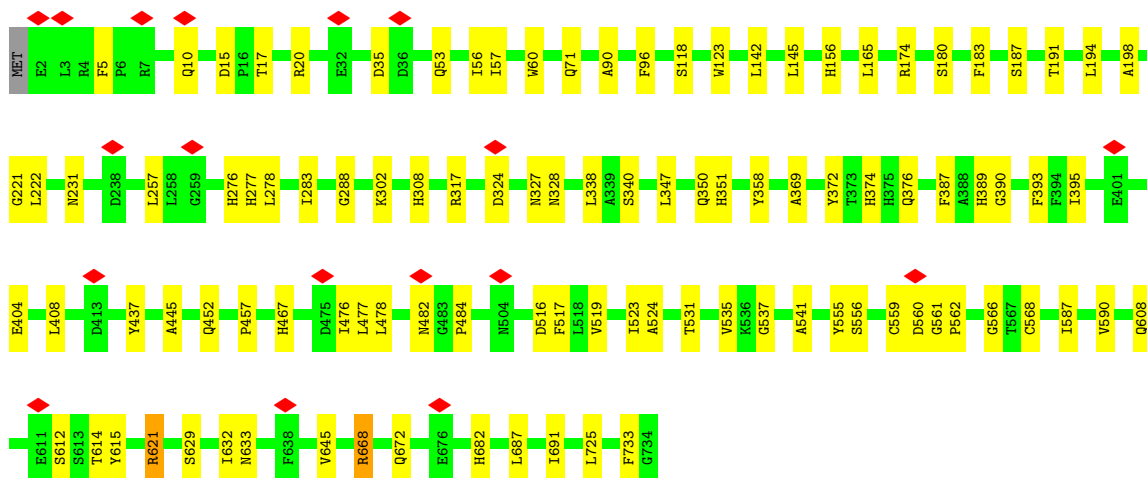


• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

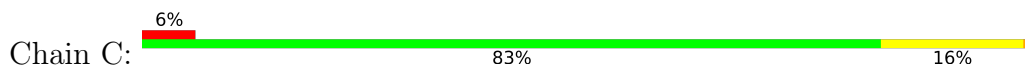


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

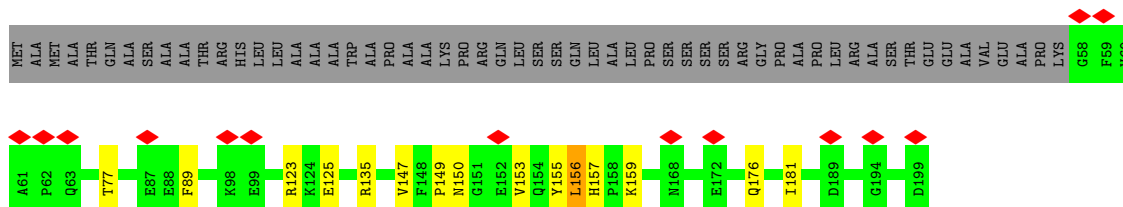




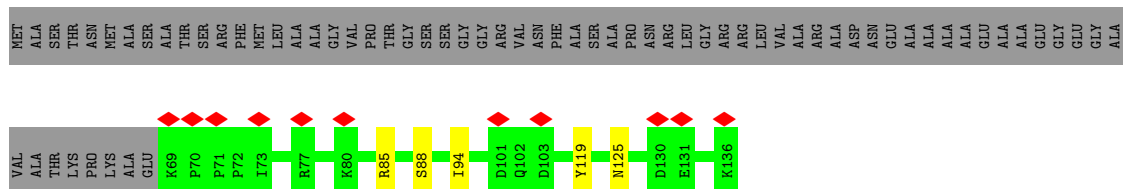
• Molecule 7: photosystem I subunit VII



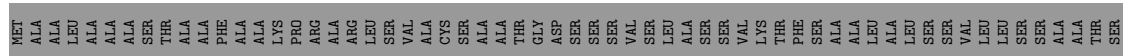
• Molecule 8: Photosystem I reaction center subunit II

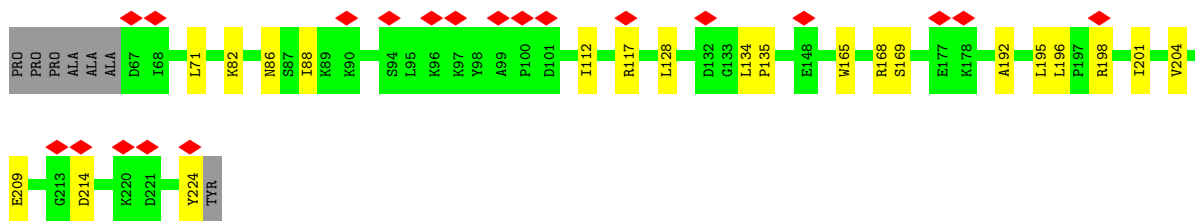


• Molecule 9: Photosystem I reaction center subunit IV A

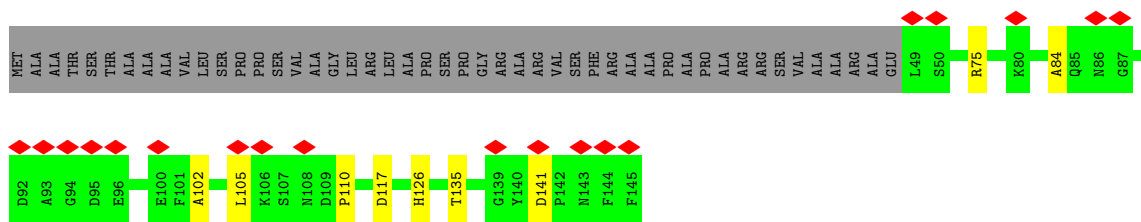


• Molecule 10: Photosystem I reaction center subunit III

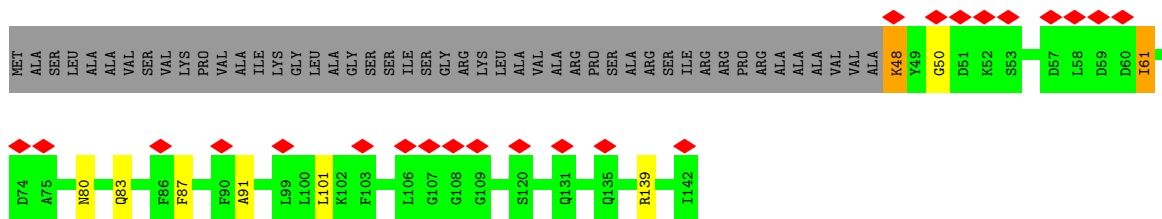




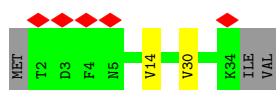
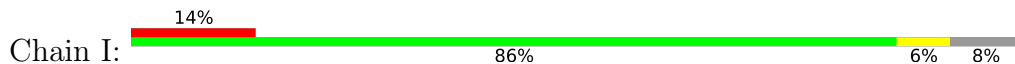
- Molecule 11: Photosystem I reaction center subunit V



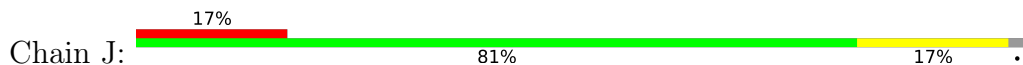
- Molecule 12: Photosystem I reaction center subunit VI, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII

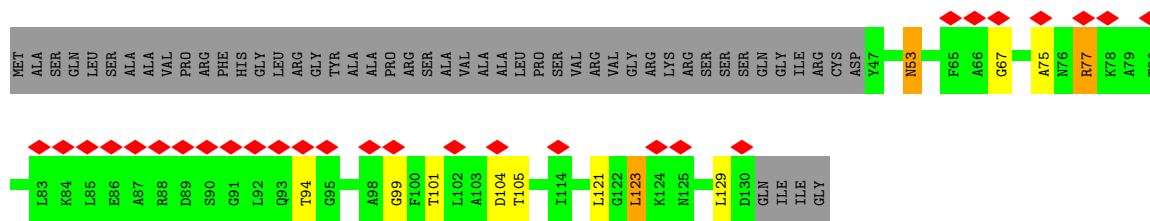


- Molecule 14: Photosystem I reaction center subunit IX

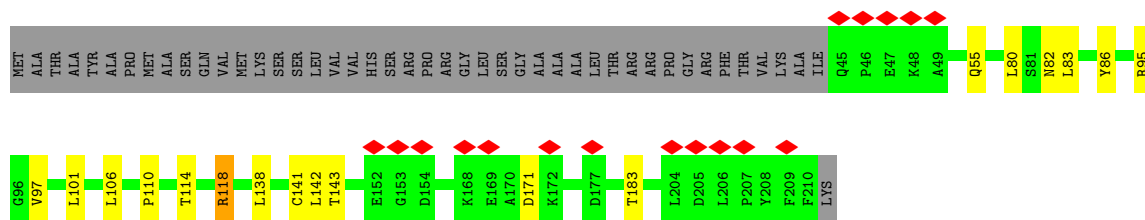


- Molecule 15: Photosystem I reaction center subunit psaK

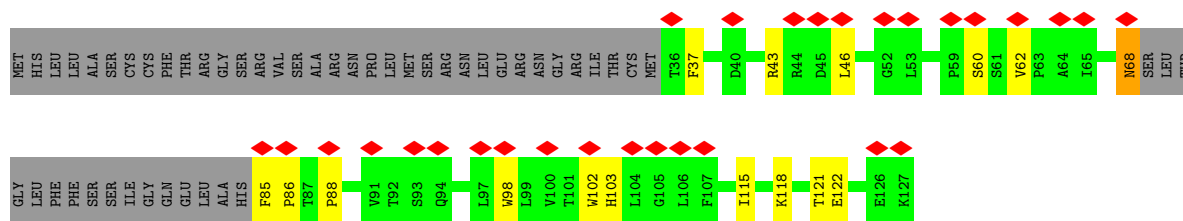




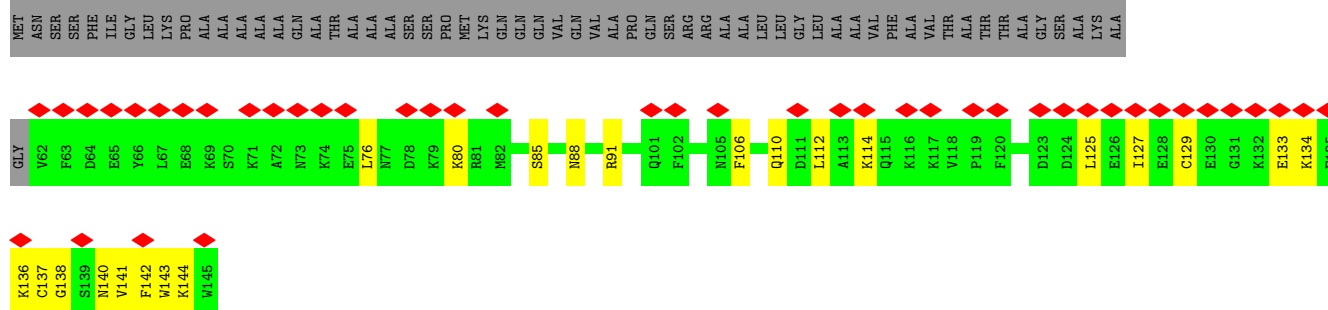
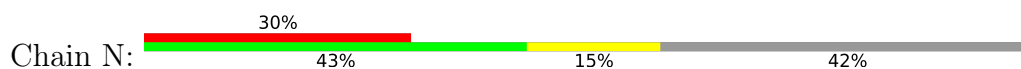
- Molecule 16: Photosystem I reaction center subunit XI



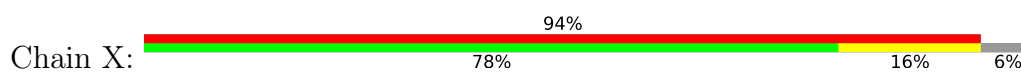
- Molecule 17: 16kDa membrane protein

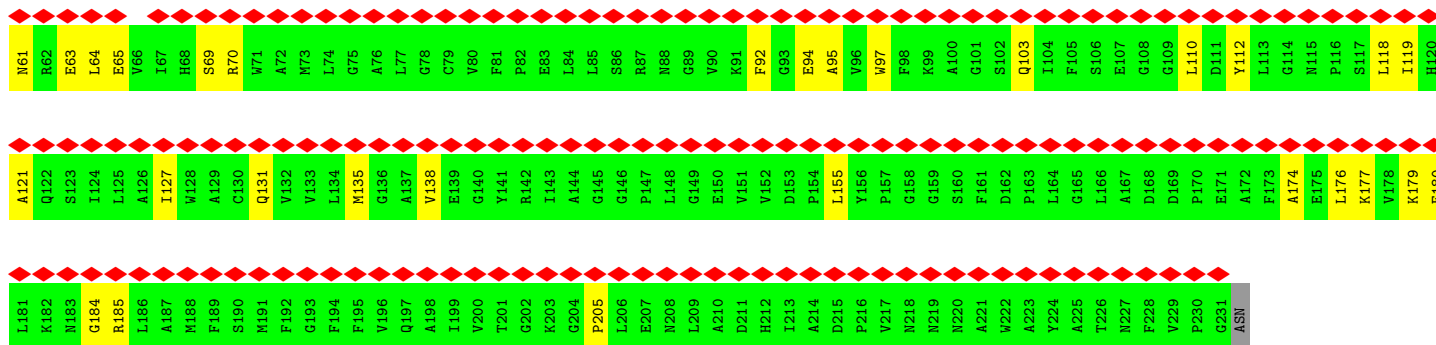


- Molecule 18: Photosystem I reaction center subunit N

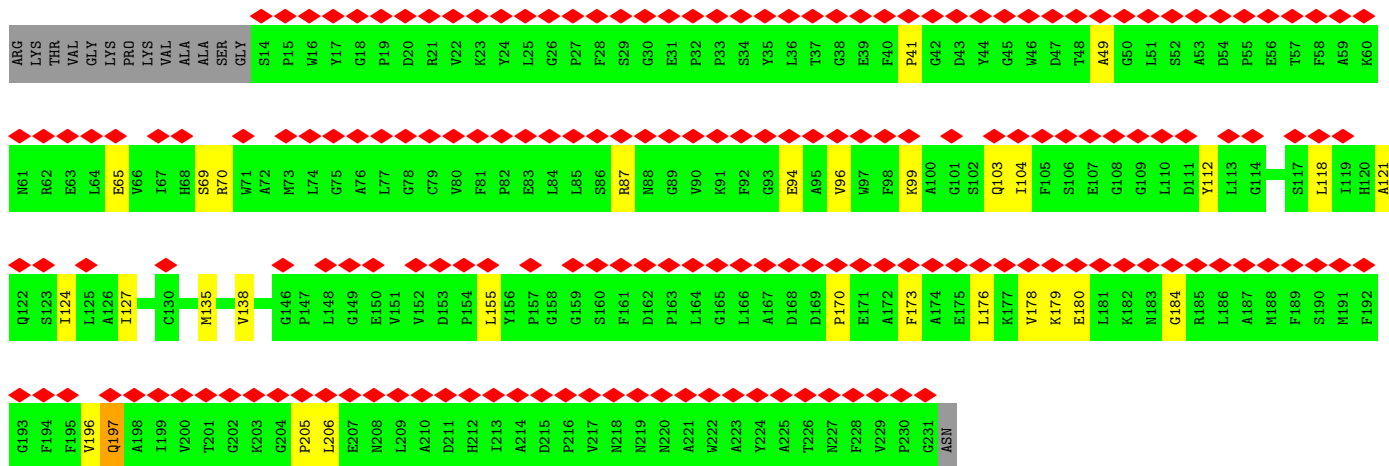
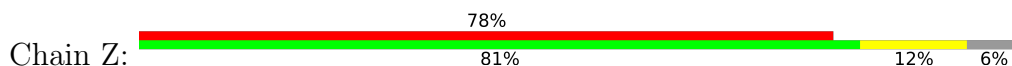


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

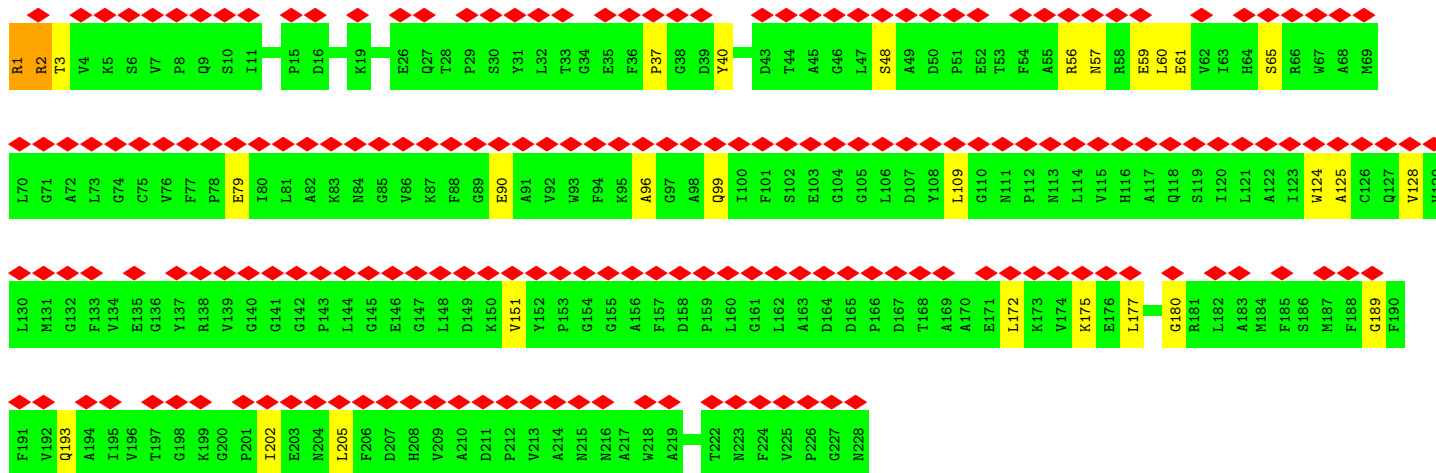
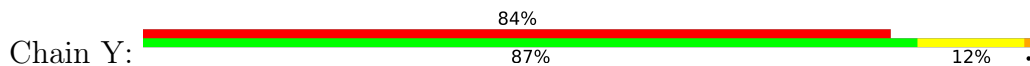




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	635845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	296.8, 296.8, 296.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, PQN, CHL, LMU, LMG, DGD, XAT, SF4, LHG, NEX, LUT, TPO, BCR, CLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.37	0/1574	0.57	0/2146
2	2	0.38	0/1684	0.59	1/2305 (0.0%)
3	3	0.41	0/1775	0.65	2/2410 (0.1%)
4	4	0.36	0/1617	0.61	1/2208 (0.0%)
5	A	0.45	0/6034	0.61	0/8229
6	B	0.44	0/6077	0.62	1/8300 (0.0%)
7	C	0.50	1/623 (0.2%)	0.70	1/844 (0.1%)
8	D	0.41	0/1144	0.71	1/1547 (0.1%)
9	E	0.41	0/553	0.56	0/754
10	F	0.36	0/1267	0.60	0/1713
11	G	0.34	0/771	0.53	0/1046
12	H	0.34	0/752	0.58	0/1022
13	I	0.43	0/267	0.82	0/364
14	J	0.37	0/334	0.58	0/455
15	K	0.33	0/595	0.72	1/806 (0.1%)
16	L	0.40	0/1284	0.67	0/1758
17	O	0.36	0/646	0.75	1/882 (0.1%)
18	N	0.34	0/701	0.63	1/938 (0.1%)
19	X	0.32	0/1714	0.51	0/2336
19	Z	0.33	0/1714	0.53	0/2336
20	Y	0.35	0/1792	0.54	0/2437
All	All	0.40	1/32918 (0.0%)	0.61	10/44836 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	58	CYS	C-N	5.41	1.44	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	123	LEU	CA-CB-CG	7.30	132.08	115.30
8	D	156	LEU	N-CA-C	6.90	129.63	111.00
3	3	219	GLU	CA-CB-CG	6.44	127.56	113.40
4	4	111	LEU	CA-CB-CG	5.96	129.00	115.30
7	C	63	LEU	CA-CB-CG	5.94	128.97	115.30
18	N	112	LEU	CA-CB-CG	5.84	128.74	115.30
2	2	228	LEU	CA-CB-CG	5.72	128.46	115.30
6	B	165	LEU	CA-CB-CG	5.45	127.83	115.30
3	3	186	LEU	CA-CB-CG	5.28	127.43	115.30
17	O	46	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1522	0	1484	24	0
2	2	1624	0	1555	35	0
3	3	1720	0	1686	20	0
4	4	1566	0	1520	27	0
5	A	5836	0	5689	105	0
6	B	5866	0	5644	81	0
7	C	612	0	607	16	0
8	D	1115	0	1118	18	0
9	E	540	0	539	6	0
10	F	1238	0	1272	12	0
11	G	752	0	731	7	0
12	H	729	0	724	9	0
13	I	260	0	274	2	0
14	J	325	0	340	6	0
15	K	589	0	612	8	0
16	L	1246	0	1242	15	0
17	O	621	0	606	11	0
18	N	685	0	658	16	0
19	X	1661	0	1593	26	0
19	Z	1661	0	1593	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Y	1751	0	1688	27	0
21	1	96	0	68	4	0
21	2	240	0	176	8	0
21	3	45	0	30	1	0
21	4	169	0	100	1	0
21	X	235	0	128	4	0
21	Y	259	0	156	2	0
21	Z	250	0	144	0	0
22	1	577	0	453	18	0
22	2	442	0	366	7	0
22	3	538	0	399	10	0
22	4	527	0	412	15	0
22	A	2533	0	2495	96	0
22	B	2261	0	2201	78	0
22	F	140	0	113	4	0
22	G	132	0	97	4	0
22	H	60	0	59	5	0
22	J	42	0	31	0	0
22	K	167	0	116	4	0
22	L	150	0	125	7	0
22	N	95	0	69	3	0
22	O	76	0	38	1	0
22	X	305	0	181	7	0
22	Y	325	0	194	6	0
22	Z	339	0	228	8	0
23	1	84	0	112	7	0
23	2	42	0	56	9	0
23	3	42	0	56	3	0
23	4	42	0	56	4	0
23	X	84	0	112	5	0
23	Y	84	0	112	5	0
23	Z	84	0	112	6	0
24	1	44	0	56	0	0
24	2	44	0	56	4	0
24	3	44	0	56	4	0
24	4	44	0	56	5	0
24	X	44	0	56	3	0
24	Y	44	0	56	2	0
24	Z	44	0	56	1	0
25	1	40	0	56	0	0
25	2	40	0	56	4	0
25	3	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4	40	0	56	1	0
25	A	240	0	336	26	0
25	B	280	0	392	22	0
25	F	40	0	56	2	0
25	G	40	0	56	2	0
25	I	40	0	56	3	0
25	J	40	0	56	1	0
25	K	80	0	112	7	0
25	L	120	0	168	8	0
26	1	49	0	74	6	0
26	2	37	0	44	3	0
26	A	79	0	104	5	0
26	B	38	0	46	1	0
26	X	22	0	16	1	0
26	Y	45	0	60	3	0
26	Z	23	0	16	1	0
27	1	53	0	79	2	0
27	2	36	0	42	1	0
27	4	72	0	84	3	0
27	G	38	0	46	1	0
28	A	65	0	72	25	0
29	A	33	0	46	6	0
29	B	33	0	46	7	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	A	30	0	33	4	0
31	B	35	0	46	5	0
32	B	66	0	96	8	0
32	J	66	0	96	2	0
33	X	44	0	56	3	0
33	Y	44	0	56	2	0
33	Z	44	0	56	2	0
All	All	44708	0	43232	693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:239:GLN:NE2	23:2:619:LUT:H42	1.53	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:GLY:O	2:2:239:GLN:HG2	1.62	0.97
2:2:236:ALA:HA	2:2:239:GLN:HG3	1.50	0.90
2:2:239:GLN:HE22	23:2:619:LUT:H42	1.38	0.89
5:A:678:TRP:CE3	28:A:801:CL0:H4	2.10	0.87
20:Y:1:ARG:HG2	20:Y:1:ARG:HH11	1.39	0.87
4:4:157:ARG:HG2	4:4:157:ARG:HH11	1.41	0.85
2:2:239:GLN:HE21	23:2:619:LUT:H42	1.43	0.82
2:2:239:GLN:NE2	23:2:619:LUT:C4	2.41	0.80
7:C:62:PHE:HD2	8:D:181:ILE:HG21	1.47	0.78
28:A:801:CL0:H13	22:A:854:CLA:HMD1	1.66	0.77
20:Y:1:ARG:HG2	20:Y:1:ARG:NH1	1.98	0.77
22:1:610:CLA:HAB	23:1:617:LUT:H32	1.66	0.77
2:2:235:GLY:O	2:2:239:GLN:CG	2.32	0.77
8:D:155:TYR:O	8:D:156:LEU:HD22	1.83	0.77
5:A:453:TYR:CE2	28:A:801:CL0:H55	2.22	0.75
22:3:602:CLA:HBB1	24:3:619:XAT:H32	1.69	0.74
19:X:119:ILE:O	21:X:605:CHL:ND	2.21	0.73
7:C:62:PHE:CE2	8:D:181:ILE:HD13	2.24	0.73
19:Z:65:GLU:OE1	22:Z:602:CLA:NA	2.22	0.72
2:2:236:ALA:CA	2:2:239:GLN:HG3	2.22	0.70
7:C:62:PHE:CD2	8:D:181:ILE:HG21	2.27	0.69
17:O:68:ASN:C	17:O:85:PHE:N	2.46	0.69
1:1:53:GLN:HE21	4:4:159:GLN:HE22	1.40	0.69
22:A:830:CLA:H2	25:A:849:BCR:HC7	1.73	0.69
20:Y:61:GLU:OE1	22:Y:602:CLA:NA	2.26	0.69
5:A:201:GLY:HA3	22:A:814:CLA:HBB1	1.74	0.68
22:A:808:CLA:OBD	31:A:857:LMU:O2B	2.10	0.68
22:A:822:CLA:H101	25:A:851:BCR:H10C	1.76	0.68
22:B:823:CLA:HAB	22:B:830:CLA:HMD2	1.76	0.67
28:A:801:CL0:H11	22:B:802:CLA:HAA1	1.75	0.67
3:3:202:PRO:HD2	23:3:618:LUT:H222	1.78	0.66
2:2:239:GLN:HE22	23:2:619:LUT:C4	2.07	0.66
2:2:148:THR:HB	4:4:243:HIS:HD2	1.61	0.66
2:2:221:LYS:HD3	22:2:612:CLA:HBA1	1.78	0.66
5:A:354:LEU:HD21	22:A:831:CLA:HAB	1.78	0.66
8:D:156:LEU:O	8:D:159:LYS:HB2	1.95	0.66
17:O:68:ASN:N	17:O:68:ASN:OD1	2.28	0.65
6:B:338:LEU:HD21	22:B:829:CLA:HAB	1.78	0.65
5:A:678:TRP:CE3	28:A:801:CL0:CMA	2.81	0.64
17:O:121:THR:HG23	17:O:122:GLU:HG3	1.79	0.64
5:A:404:ALA:HB2	5:A:590:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:157:ARG:NH2	22:4:609:CLA:O1D	2.29	0.64
25:B:801:BCR:HC31	32:J:103:DGD:HA32	1.79	0.64
8:D:89:PHE:HE1	12:H:61:ILE:HD13	1.63	0.63
3:3:136:PRO:HG3	22:A:817:CLA:HMD2	1.80	0.63
5:A:453:TYR:HE2	28:A:801:CL0:H55	1.59	0.63
3:3:232:GLY:O	3:3:236:GLN:HB3	1.98	0.63
2:2:155:ILE:HD12	4:4:247:ILE:HD11	1.81	0.62
5:A:474:ILE:HD11	16:L:118:ARG:HH12	1.65	0.62
5:A:735:ILE:HG21	22:A:829:CLA:HMC2	1.82	0.62
21:X:606:CHL:HMB1	21:X:609:CHL:HAC1	1.81	0.61
18:N:91:ARG:HH12	18:N:110:GLN:HB2	1.64	0.61
6:B:560:ASP:OD1	7:C:66:ARG:NH2	2.33	0.61
5:A:118:ILE:HB	25:A:856:BCR:H322	1.82	0.61
5:A:116:TRP:HB3	25:A:856:BCR:H323	1.83	0.61
16:L:141:CYS:HB3	25:L:305:BCR:H21C	1.83	0.61
20:Y:124:TRP:CZ2	20:Y:128:VAL:HG21	2.35	0.60
22:A:807:CLA:H161	22:A:830:CLA:HBB2	1.83	0.60
2:2:148:THR:O	2:2:148:THR:HG23	2.00	0.60
17:O:68:ASN:O	17:O:85:PHE:N	2.35	0.60
20:Y:99:GLN:HE22	22:Y:604:CLA:HED2	1.65	0.60
3:3:230:ILE:HG21	24:3:619:XAT:H12	1.84	0.60
5:A:594:LEU:HD21	22:A:831:CLA:HBC1	1.84	0.60
22:X:610:CLA:HBB1	22:X:612:CLA:H3A	1.84	0.60
22:A:829:CLA:H171	25:J:102:BCR:H17C	1.83	0.59
31:B:849:LMU:O2'	22:G:203:CLA:HED1	2.01	0.59
22:A:841:CLA:H91	22:F:303:CLA:HBC3	1.85	0.59
21:1:601:CHL:HBB1	22:1:602:CLA:HMD2	1.83	0.59
3:3:99:ARG:NH1	3:3:219:GLU:OE2	2.35	0.59
5:A:118:ILE:HG12	5:A:119:VAL:HG13	1.84	0.59
19:X:94:GLU:H	19:X:103:GLN:HE21	1.49	0.59
22:B:807:CLA:H12	13:I:14:VAL:HG21	1.84	0.59
11:G:110:PRO:HG2	22:G:204:CLA:HBC2	1.85	0.59
12:H:83:GLN:HE21	22:H:201:CLA:C4D	2.09	0.59
6:B:350:GLN:NE2	6:B:372:TYR:OH	2.35	0.59
12:H:48:LYS:HG2	12:H:50:GLY:H	1.67	0.59
2:2:165:GLU:OE1	2:2:168:ARG:NH2	2.35	0.58
22:B:809:CLA:H3A	22:B:810:CLA:HBB1	1.86	0.58
18:N:106:PHE:O	22:N:1001:CLA:ND	2.36	0.58
27:4:622:LMG:H352	27:4:622:LMG:H162	1.86	0.58
22:B:825:CLA:H102	22:B:837:CLA:H52	1.85	0.58
28:A:801:CL0:H33	22:A:803:CLA:C1D	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:341:ILE:HG22	5:A:419:ARG:HB3	1.86	0.57
5:A:707:LYS:NZ	10:F:214:ASP:OD1	2.37	0.57
7:C:54:CYS:SG	7:C:55:GLU:N	2.77	0.57
16:L:141:CYS:HB3	25:L:305:BCR:H19C	1.87	0.57
6:B:374:HIS:HE1	22:B:827:CLA:ND	2.02	0.57
5:A:649:LEU:HD11	28:A:801:CL0:H43	1.86	0.57
20:Y:1:ARG:HH11	20:Y:1:ARG:CG	2.13	0.57
28:A:801:CL0:H64	22:A:803:CLA:CHB	2.35	0.57
6:B:457:PRO:HG3	6:B:517:PHE:HB2	1.86	0.57
6:B:608:GLN:O	6:B:612:SER:HB2	2.05	0.57
22:3:610:CLA:HAB	23:3:618:LUT:H32	1.86	0.57
18:N:129:CYS:SG	18:N:140:ASN:ND2	2.78	0.57
4:4:157:ARG:HH11	4:4:157:ARG:CG	2.17	0.57
22:B:821:CLA:HMD2	25:B:843:BCR:HC7	1.86	0.57
19:Z:104:ILE:HG21	19:Z:124:ILE:HD13	1.87	0.57
20:Y:48:SER:OG	20:Y:57:ASN:ND2	2.38	0.56
3:3:218:LYS:HD2	22:3:612:CLA:HBD	1.88	0.56
6:B:389:HIS:CE1	22:B:829:CLA:NA	2.73	0.56
19:Z:197:GLN:HE22	23:Z:7620:LUT:H42	1.70	0.56
4:4:58:LEU:HD23	4:4:60:GLY:H	1.71	0.56
9:E:85:ARG:HD2	9:E:88:SER:HB2	1.88	0.56
2:2:148:THR:HB	4:4:243:HIS:CD2	2.41	0.56
25:A:852:BCR:H10C	22:A:854:CLA:H203	1.88	0.56
1:1:150:ILE:HG21	22:1:609:CLA:HMC3	1.88	0.56
21:X:601:CHL:HHD	26:X:2630:LHG:HC41	1.88	0.56
22:4:610:CLA:H2	23:4:619:LUT:H373	1.87	0.55
22:B:826:CLA:H111	25:B:847:BCR:H17C	1.87	0.55
22:1:602:CLA:HBB1	22:1:602:CLA:HMB1	1.88	0.55
19:X:52:SER:OG	19:X:61:ASN:ND2	2.39	0.55
21:1:601:CHL:HBA1	22:4:617:CLA:HED1	1.88	0.55
23:1:621:LUT:H30	27:1:622:LMG:H332	1.89	0.55
18:N:137:CYS:SG	18:N:138:GLY:N	2.80	0.55
22:1:603:CLA:H12	22:B:841:CLA:HMC3	1.87	0.55
5:A:732:LEU:HD22	22:A:842:CLA:HMA1	1.89	0.55
6:B:452:GLN:NE2	6:B:614:THR:OG1	2.40	0.55
5:A:538:ALA:HB2	22:A:839:CLA:HMA1	1.89	0.55
22:A:841:CLA:H122	22:A:841:CLA:HAB	1.88	0.55
6:B:537:GLY:O	6:B:541:ALA:HB2	2.07	0.55
22:B:840:CLA:H42	29:B:842:PQN:H262	1.89	0.55
1:1:63:SER:HB2	1:1:66:ASP:HB2	1.89	0.54
2:2:84:GLY:HA3	2:2:223:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:204:PRO:HD2	23:2:619:LUT:H23	1.89	0.54
22:B:803:CLA:H61	22:B:840:CLA:HBB2	1.89	0.54
7:C:62:PHE:HD2	8:D:181:ILE:CG2	2.18	0.54
19:X:63:GLU:HA	19:X:155:LEU:HD21	1.90	0.54
22:A:814:CLA:H43	25:A:849:BCR:H14C	1.90	0.54
5:A:438:LEU:HD22	22:A:840:CLA:HBB1	1.90	0.54
5:A:689:ARG:H	6:B:568:CYS:HB2	1.72	0.54
25:A:856:BCR:H312	14:J:31:ARG:HD3	1.89	0.54
22:A:843:CLA:HBB2	25:L:305:BCR:H20C	1.89	0.54
29:A:844:PQN:H172	22:F:301:CLA:HAB	1.90	0.54
7:C:60:THR:HG21	7:C:64:SER:OG	2.07	0.54
10:F:88:ILE:HD12	10:F:112:ILE:HG23	1.89	0.54
25:A:856:BCR:H401	14:J:12:PRO:HB2	1.89	0.54
22:1:603:CLA:H43	22:1:603:CLA:HED3	1.89	0.54
5:A:154:LEU:HD21	18:N:141:VAL:HG13	1.90	0.53
17:O:86:PRO:HB2	17:O:88:PRO:HD2	1.90	0.53
19:X:180:GLU:OE1	22:X:610:CLA:NB	2.41	0.53
1:1:115:LYS:HA	1:1:118:GLU:HG2	1.89	0.53
5:A:237:PRO:HA	5:A:240:PHE:HD2	1.72	0.53
5:A:678:TRP:CD2	28:A:801:CL0:CMA	2.91	0.53
5:A:15:ASP:OD2	5:A:68:ARG:NH2	2.39	0.53
22:B:828:CLA:H202	25:B:844:BCR:H352	1.89	0.53
5:A:559:ARG:NH1	8:D:77:THR:O	2.41	0.53
26:Y:4630:LHG:HC91	26:Y:4630:LHG:H321	1.89	0.53
5:A:678:TRP:CG	28:A:801:CL0:H5	2.44	0.53
1:1:200:MET:HE3	22:1:602:CLA:HMC3	1.89	0.53
4:4:82:LEU:HD13	22:4:602:CLA:H42	1.90	0.53
2:2:233:VAL:HG11	24:2:620:XAT:H12	1.90	0.53
4:4:157:ARG:HG2	4:4:157:ARG:NH1	2.14	0.53
1:1:176:LEU:HD12	23:1:617:LUT:H222	1.91	0.52
5:A:113:GLN:NE2	22:A:810:CLA:OBD	2.37	0.52
19:Z:180:GLU:OE1	22:Z:610:CLA:NB	2.42	0.52
5:A:405:HIS:CE1	22:A:831:CLA:NA	2.77	0.52
6:B:476:ILE:HG13	6:B:477:LEU:HG	1.91	0.52
8:D:123:ARG:NH2	8:D:125:GLU:OE1	2.41	0.52
19:X:65:GLU:OE2	19:X:185:ARG:NE	2.41	0.52
22:2:611:CLA:HBC3	26:2:622:LHG:HC62	1.91	0.52
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.91	0.52
22:A:806:CLA:H121	25:A:848:BCR:HC31	1.90	0.52
25:A:852:BCR:H362	22:A:854:CLA:H42	1.90	0.52
19:X:64:LEU:HD11	19:Z:49:ALA:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:53:ASN:ND2	22:K:204:CLA:OBD	2.42	0.52
22:A:820:CLA:HAB	22:A:820:CLA:H8	1.91	0.52
25:B:801:BCR:H10C	22:B:832:CLA:HMB2	1.92	0.52
15:K:94:THR:HG21	15:K:99:GLY:HA2	1.92	0.52
5:A:426:ARG:HG2	5:A:429:ARG:HH21	1.75	0.52
6:B:556:SER:HB3	32:B:850:DGD:HD2	1.91	0.52
3:3:163:ARG:NE	3:3:174:MET:SD	2.80	0.52
17:O:60:SER:HB2	17:O:102:TRP:HE1	1.74	0.52
19:X:121:ALA:HB1	19:X:127:ILE:HD11	1.92	0.52
22:2:610:CLA:H51	22:2:610:CLA:HBB1	1.92	0.51
22:3:606:CLA:HMB1	22:3:609:CLA:HBC2	1.92	0.51
6:B:276:HIS:HE1	22:B:817:CLA:ND	2.05	0.51
20:Y:124:TRP:CE3	20:Y:125:ALA:HA	2.45	0.51
5:A:14:VAL:HA	5:A:183:PRO:HA	1.92	0.51
28:A:801:CL0:O1D	22:B:802:CLA:HBB2	2.10	0.51
19:Z:69:SER:HB2	19:Z:184:GLY:HA3	1.92	0.51
8:D:89:PHE:CE1	12:H:61:ILE:HD13	2.44	0.51
22:B:835:CLA:HED3	22:G:201:CLA:HMA3	1.91	0.51
19:Z:70:ARG:NH2	19:Z:155:LEU:O	2.43	0.51
5:A:64:GLU:OE2	5:A:68:ARG:NH2	2.44	0.51
7:C:17:CYS:HB2	7:C:54:CYS:HB2	1.92	0.51
16:L:82:ASN:HB3	22:L:302:CLA:HAC1	1.93	0.51
19:X:92:PHE:HB2	19:X:95:ALA:HB2	1.92	0.51
2:2:163:TRP:HH2	25:2:621:BCR:H321	1.76	0.51
6:B:191:THR:HG21	6:B:278:LEU:HB2	1.92	0.51
2:2:127:LEU:HB3	2:2:132:VAL:HB	1.93	0.51
5:A:559:ARG:O	8:D:123:ARG:NH1	2.43	0.51
28:A:801:CL0:H58	22:A:803:CLA:HMA1	1.92	0.51
6:B:351:HIS:CE1	22:B:826:CLA:NB	2.79	0.51
6:B:559:CYS:SG	6:B:561:GLY:N	2.82	0.51
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.93	0.51
22:X:602:CLA:HAB	23:X:2621:LUT:H30	1.93	0.51
21:Y:606:CHL:HMB1	21:Y:609:CHL:HAC1	1.92	0.51
6:B:668:ARG:HB2	29:B:842:PQN:H7	1.93	0.50
16:L:142:LEU:HB3	16:L:183:THR:HG22	1.94	0.50
20:Y:40:TYR:HB2	22:Y:602:CLA:HMD1	1.92	0.50
1:1:50:MET:SD	4:4:159:GLN:NE2	2.84	0.50
22:A:811:CLA:HBB2	22:A:814:CLA:HMA3	1.94	0.50
6:B:10:GLN:N	6:B:35:ASP:OD2	2.42	0.50
11:G:75:ARG:NH2	11:G:117:ASP:OD2	2.45	0.50
18:N:142:PHE:O	18:N:143:TRP:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:843:CLA:H142	22:B:839:CLA:H142	1.93	0.50
16:L:106:LEU:HD13	22:L:304:CLA:HBC2	1.92	0.50
20:Y:124:TRP:CH2	20:Y:128:VAL:HG21	2.46	0.50
3:3:165:LEU:HB2	22:3:609:CLA:HMA2	1.93	0.50
5:A:670:PHE:HZ	22:A:829:CLA:H101	1.76	0.50
6:B:308:HIS:HA	22:B:841:CLA:HMD1	1.93	0.50
10:F:195:LEU:HD13	10:F:198:ARG:HD2	1.93	0.50
19:X:110:LEU:HB3	19:X:121:ALA:HB3	1.94	0.50
28:A:801:CL0:CGD	28:A:801:CL0:H8	2.42	0.50
22:A:802:CLA:H102	22:A:842:CLA:HMC2	1.94	0.50
6:B:324:ASP:O	6:B:328:ASN:ND2	2.42	0.50
31:B:849:LMU:H4'	31:B:849:LMU:O2B	2.12	0.50
5:A:503:THR:HG23	5:A:507:TRP:HE1	1.77	0.50
19:Z:196:VAL:HG11	22:Z:613:CLA:HAC2	1.93	0.50
28:A:801:CL0:H33	22:A:803:CLA:CHD	2.41	0.50
29:B:842:PQN:H303	32:B:850:DGD:HA82	1.92	0.50
5:A:268:LYS:HE3	15:K:129:LEU:HD11	1.94	0.50
10:F:82:LYS:HE2	10:F:86:ASN:HD21	1.76	0.50
10:F:165:TRP:HH2	10:F:209:GLU:HG3	1.77	0.50
19:Z:176:LEU:HD23	19:Z:179:LYS:HD2	1.94	0.50
22:A:809:CLA:HMC3	22:A:810:CLA:HMD2	1.94	0.49
20:Y:124:TRP:CE3	20:Y:124:TRP:C	2.86	0.49
27:2:623:LMG:H141	27:2:623:LMG:H301	1.94	0.49
2:2:67:ILE:H	3:3:177:GLN:HE22	1.59	0.49
22:A:831:CLA:H102	26:A:846:LHG:H192	1.94	0.49
5:A:675:HIS:HB3	22:A:854:CLA:HBD	1.94	0.49
15:K:67:GLY:O	15:K:77:ARG:NH2	2.45	0.49
1:1:238:ILE:HG22	1:1:239:ILE:HG13	1.95	0.49
5:A:639:ILE:HG13	5:A:640:THR:HG23	1.94	0.49
19:X:176:LEU:HD23	19:X:179:LYS:HD2	1.94	0.49
19:Z:41:PRO:HB3	19:Z:178:VAL:HG22	1.93	0.49
22:Z:614:CLA:H2A	22:Z:614:CLA:HED2	1.95	0.49
29:B:842:PQN:H222	25:B:848:BCR:H17C	1.94	0.49
8:D:155:TYR:C	8:D:156:LEU:HD22	2.32	0.49
16:L:110:PRO:O	16:L:114:THR:OG1	2.30	0.49
1:1:155:HIS:HA	1:1:158:THR:HG22	1.94	0.49
2:2:147:PHE:CE1	21:2:606:CHL:HMD1	2.48	0.49
2:2:201:TRP:HZ3	21:2:608:CHL:HAB	1.77	0.49
5:A:18:PRO:HB2	5:A:19:ILE:HD12	1.94	0.49
22:B:809:CLA:H111	22:B:809:CLA:H152	1.58	0.49
14:J:1:MET:HG3	14:J:3:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:304:ILE:HG22	25:K:202:BCR:H17C	1.94	0.49
28:A:801:CL0:H13	22:A:854:CLA:CMD	2.41	0.49
6:B:390:GLY:HA3	25:B:847:BCR:H382	1.94	0.49
29:B:842:PQN:H292	32:B:850:DGD:HA91	1.95	0.49
3:3:133:VAL:HG21	24:3:619:XAT:H172	1.93	0.49
32:B:850:DGD:HAG1	32:B:850:DGD:HBV1	1.95	0.49
2:2:235:GLY:C	2:2:239:GLN:CG	2.82	0.48
3:3:217:LEU:HD12	3:3:220:ILE:HD11	1.94	0.48
5:A:478:PRO:HG3	5:A:531:PHE:HB2	1.94	0.48
22:B:826:CLA:H143	25:B:847:BCR:H17C	1.95	0.48
19:X:131:GLN:O	19:X:135:MET:HB2	2.13	0.48
5:A:224:PHE:HD2	5:A:234:ILE:HG23	1.78	0.48
5:A:379:THR:HG21	5:A:515:ILE:HB	1.94	0.48
5:A:570:ARG:HH21	26:A:846:LHG:HC32	1.76	0.48
29:B:842:PQN:H242	25:B:848:BCR:H15C	1.95	0.48
4:4:106:GLY:HA2	24:4:620:XAT:H181	1.95	0.48
4:4:192:PRO:HD2	23:4:619:LUT:H23	1.96	0.48
22:A:842:CLA:HAC1	29:A:844:PQN:H192	1.94	0.48
20:Y:79:GLU:HB3	20:Y:202:ILE:HD12	1.94	0.48
6:B:174:ARG:HE	22:B:824:CLA:HMD1	1.79	0.48
15:K:94:THR:HB	15:K:101:THR:HG22	1.93	0.48
20:Y:124:TRP:HE3	20:Y:125:ALA:N	2.11	0.48
19:Z:94:GLU:H	19:Z:103:GLN:HE21	1.61	0.48
19:Z:197:GLN:NE2	23:Z:7620:LUT:H42	2.28	0.48
22:4:602:CLA:HAB	24:4:620:XAT:H32	1.94	0.48
22:A:809:CLA:HAB	22:A:829:CLA:H112	1.95	0.48
22:A:832:CLA:HBB2	22:A:840:CLA:HMC2	1.95	0.48
22:A:854:CLA:H41	22:A:854:CLA:H61	1.55	0.48
6:B:559:CYS:SG	6:B:560:ASP:N	2.87	0.48
6:B:668:ARG:NH2	6:B:672:GLN:OE1	2.46	0.48
21:1:601:CHL:CBB	22:1:602:CLA:HMD2	2.43	0.48
3:3:261:LEU:HD22	3:3:265:LYS:HG2	1.95	0.48
28:A:801:CL0:CMB	22:A:854:CLA:HMD1	2.41	0.48
1:1:174:ASP:OD1	23:1:617:LUT:O23	2.31	0.48
25:2:621:BCR:H333	22:4:611:CLA:HMC3	1.96	0.48
5:A:708:VAL:HG11	22:A:841:CLA:HMB3	1.96	0.48
7:C:61:ASP:OD1	9:E:125:ASN:ND2	2.41	0.48
26:1:620:LHG:HC92	25:4:621:BCR:H333	1.96	0.48
20:Y:193:GLN:OE1	22:Y:613:CLA:NA	2.47	0.48
19:Z:121:ALA:HB1	19:Z:127:ILE:HD11	1.96	0.48
4:4:151:HIS:HD2	22:4:609:CLA:HAB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:678:TRP:CD2	28:A:801:CL0:H5	2.48	0.48
22:B:840:CLA:H122	22:B:840:CLA:H162	1.71	0.48
17:O:62:VAL:HG23	17:O:98:TRP:HB3	1.96	0.48
4:4:58:LEU:HD22	4:4:61:LEU:HD23	1.95	0.47
22:A:841:CLA:H2	22:B:832:CLA:H42	1.96	0.47
6:B:283:ILE:HG22	22:B:819:CLA:HMC1	1.96	0.47
1:1:156:GLN:HB3	22:1:608:CLA:HMC3	1.97	0.47
5:A:514:ALA:HB1	5:A:620:ILE:HG21	1.96	0.47
28:A:801:CL0:H72	28:A:801:CL0:H10	1.63	0.47
22:B:830:CLA:HAB	22:B:838:CLA:HBB2	1.96	0.47
5:A:538:ALA:HB1	22:A:839:CLA:HMB3	1.97	0.47
6:B:142:LEU:HD23	6:B:145:LEU:HD12	1.95	0.47
6:B:174:ARG:HB2	22:B:813:CLA:HBC2	1.96	0.47
22:B:841:CLA:HMB2	26:B:851:LHG:HC61	1.97	0.47
25:K:205:BCR:H20C	25:K:205:BCR:H361	1.67	0.47
20:Y:172:LEU:HD23	20:Y:175:LYS:HD2	1.96	0.47
19:Z:70:ARG:NE	19:Z:180:GLU:OE2	2.48	0.47
2:2:239:GLN:HE22	23:2:619:LUT:C3	2.27	0.47
6:B:60:TRP:NE1	22:B:827:CLA:OBD	2.45	0.47
22:B:825:CLA:HMA1	25:B:847:BCR:H14C	1.96	0.47
22:1:602:CLA:CGA	22:1:602:CLA:H3A	2.44	0.47
5:A:118:ILE:HD12	14:J:27:ILE:HG23	1.96	0.47
6:B:467:HIS:HA	6:B:478:LEU:HD12	1.96	0.47
5:A:678:TRP:CE2	28:A:801:CL0:H10	2.48	0.47
22:H:201:CLA:HMB3	22:L:302:CLA:HAA1	1.96	0.47
22:Y:612:CLA:HMC2	23:Y:4620:LUT:H11	1.96	0.47
22:A:823:CLA:HMD2	25:K:202:BCR:H23C	1.97	0.47
10:F:192:ALA:O	10:F:196:LEU:HB2	2.14	0.47
4:4:157:ARG:CG	4:4:157:ARG:NH1	2.75	0.47
22:4:609:CLA:HHB	22:4:617:CLA:HBC2	1.97	0.47
5:A:143:GLN:HB3	5:A:374:TYR:HB3	1.96	0.47
31:A:857:LMU:H1B	31:A:857:LMU:H6E	1.97	0.47
6:B:531:THR:O	6:B:535:VAL:HB	2.13	0.47
22:B:827:CLA:H3A	22:B:827:CLA:HBA2	1.56	0.47
20:Y:109:LEU:HD21	22:Y:604:CLA:HMD1	1.96	0.47
5:A:575:GLY:HA2	6:B:562:PRO:HD3	1.96	0.47
5:A:286:LEU:HD13	22:A:819:CLA:HMA2	1.97	0.46
22:A:806:CLA:H143	25:A:848:BCR:HC41	1.97	0.46
6:B:389:HIS:HE1	22:B:829:CLA:NA	2.10	0.46
22:B:805:CLA:HBA1	22:B:805:CLA:H3A	1.66	0.46
24:X:7622:XAT:H11	24:X:7622:XAT:H191	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:69:SER:HB2	19:X:184:GLY:HA3	1.98	0.46
1:1:226:LEU:HD21	22:1:614:CLA:HMC3	1.96	0.46
2:2:93:LEU:HD12	24:2:620:XAT:H23	1.97	0.46
5:A:703:HIS:NE2	22:A:841:CLA:NA	2.64	0.46
22:A:811:CLA:H151	25:A:849:BCR:H372	1.98	0.46
25:B:846:BCR:H11C	25:B:846:BCR:H341	1.83	0.46
22:H:201:CLA:HBA2	22:H:201:CLA:H3A	1.45	0.46
22:L:302:CLA:H3A	22:L:302:CLA:HBA2	1.63	0.46
4:4:234:LEU:HD13	23:4:619:LUT:H22	1.96	0.46
5:A:405:HIS:HE1	22:A:831:CLA:NA	2.11	0.46
5:A:719:ILE:HD11	6:B:566:GLY:HA3	1.98	0.46
19:X:49:ALA:HA	20:Y:60:LEU:HD11	1.96	0.46
19:Z:205:PRO:HB2	23:Z:7620:LUT:H21	1.96	0.46
21:1:601:CHL:HBA1	21:1:601:CHL:H3A	1.67	0.46
5:A:177:HIS:HE1	22:A:811:CLA:NA	2.13	0.46
31:A:857:LMU:O2B	31:A:857:LMU:H4'	2.16	0.46
22:B:816:CLA:H41	22:B:816:CLA:H62	1.79	0.46
19:X:18:GLY:O	19:X:21:ARG:NH1	2.46	0.46
33:X:2623:NEX:H191	33:X:2623:NEX:H11	1.81	0.46
15:K:105:THR:HG21	22:K:201:CLA:HBB2	1.97	0.46
19:X:50:GLY:HA3	20:Y:56:ARG:HG3	1.97	0.46
2:2:224:LYS:NZ	26:2:622:LHG:O5	2.38	0.46
22:3:609:CLA:HBA1	22:3:609:CLA:H3A	1.57	0.46
29:A:844:PQN:H142	29:A:844:PQN:H112	1.85	0.46
25:A:852:BCR:H24C	22:B:833:CLA:HMC2	1.97	0.46
6:B:317:ARG:NH2	6:B:404:GLU:O	2.47	0.46
22:B:832:CLA:HMC3	32:J:103:DGD:HAT2	1.98	0.46
19:X:135:MET:HA	19:X:138:VAL:HG22	1.98	0.46
1:1:53:GLN:HE22	4:4:162:LYS:HE2	1.80	0.45
2:2:117:GLY:HA2	24:2:620:XAT:H181	1.97	0.45
15:K:121:LEU:HA	15:K:123:LEU:HD22	1.98	0.45
6:B:123:TRP:NE1	22:B:818:CLA:OBD	2.43	0.45
6:B:516:ASP:HA	6:B:519:VAL:HG12	1.98	0.45
8:D:149:PRO:HA	12:H:61:ILE:HD12	1.98	0.45
25:L:305:BCR:H15C	25:L:305:BCR:H351	1.81	0.45
6:B:56:ILE:HG21	22:B:806:CLA:HMD2	1.98	0.45
6:B:183:PHE:HE1	22:B:813:CLA:H52	1.81	0.45
21:2:601:CHL:HAC1	25:3:620:BCR:HC31	1.97	0.45
4:4:216:PHE:CG	24:4:620:XAT:H12	2.52	0.45
5:A:471:ASP:HA	5:A:475:GLN:HG2	1.98	0.45
5:A:476:LEU:HB2	5:A:528:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:839:CLA:H62	22:A:839:CLA:H41	1.69	0.45
6:B:156:HIS:CE1	22:B:811:CLA:NA	2.84	0.45
6:B:395:ILE:HD12	6:B:555:TYR:HD1	1.81	0.45
6:B:687:LEU:HD21	16:L:83:LEU:HD11	1.97	0.45
19:X:33:PRO:HG2	19:X:36:LEU:HD12	1.98	0.45
26:1:620:LHG:H181	4:4:148:ILE:HG12	1.97	0.45
5:A:116:TRP:CZ2	31:A:857:LMU:O3'	2.69	0.45
5:A:175:TRP:HB2	22:A:812:CLA:HMC3	1.98	0.45
5:A:646:ARG:HA	6:B:632:ILE:HD12	1.99	0.45
22:A:826:CLA:H18	22:A:826:CLA:H152	1.79	0.45
23:X:2620:LUT:H15	23:X:2620:LUT:H201	1.81	0.45
3:3:248:LEU:HD22	23:3:618:LUT:H163	1.97	0.45
4:4:182:GLU:HG2	4:4:183:CYS:H	1.82	0.45
5:A:386:SER:HB2	22:A:829:CLA:HHB	1.99	0.45
5:A:393:TRP:HB3	22:A:829:CLA:HMC3	1.99	0.45
22:A:842:CLA:H141	22:A:842:CLA:H161	1.82	0.45
25:A:849:BCR:H24C	25:A:849:BCR:H371	1.80	0.45
25:A:852:BCR:H361	25:A:852:BCR:H20C	1.68	0.45
19:X:65:GLU:OE1	22:X:602:CLA:NA	2.49	0.45
19:Z:87:ARG:HH21	19:Z:206:LEU:HB3	1.82	0.45
25:2:621:BCR:H15C	25:2:621:BCR:H351	1.83	0.45
22:A:834:CLA:H122	29:B:842:PQN:H211	1.98	0.45
22:A:842:CLA:H143	29:A:844:PQN:H291	1.98	0.45
25:A:848:BCR:H362	25:A:849:BCR:H21C	1.99	0.45
6:B:629:SER:O	6:B:633:ASN:ND2	2.50	0.45
22:B:828:CLA:H151	25:B:845:BCR:H19C	1.99	0.45
21:2:608:CHL:HMB3	25:2:621:BCR:H362	1.99	0.45
23:Z:7621:LUT:H15	23:Z:7621:LUT:H201	1.86	0.45
22:A:818:CLA:H61	22:A:818:CLA:H41	1.70	0.45
22:A:822:CLA:HMB2	22:A:826:CLA:HMA3	1.98	0.45
22:A:824:CLA:HMB1	17:O:115:ILE:HD13	1.99	0.45
10:F:169:SER:HB3	10:F:195:LEU:HD12	1.99	0.45
12:H:101:LEU:HB2	16:L:143:THR:HG21	1.99	0.45
19:X:112:TYR:HD2	19:X:118:LEU:HD13	1.81	0.45
20:Y:1:ARG:O	20:Y:2:ARG:O	2.34	0.45
19:Z:176:LEU:HB3	22:Z:610:CLA:HHB	1.99	0.45
26:2:622:LHG:HC82	26:2:622:LHG:H262	1.98	0.45
31:B:849:LMU:O2'	22:G:203:CLA:CED	2.65	0.45
5:A:335:HIS:CD2	22:A:825:CLA:ND	2.84	0.44
22:B:832:CLA:H61	25:F:305:BCR:HC32	2.00	0.44
19:X:70:ARG:NE	19:X:180:GLU:OE2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:820:CLA:H193	22:A:820:CLA:H72	2.00	0.44
22:K:204:CLA:HBA1	22:K:204:CLA:H3A	1.40	0.44
22:1:610:CLA:H52	23:1:617:LUT:H30	2.00	0.44
22:3:613:CLA:H2	22:3:614:CLA:HMD1	1.99	0.44
5:A:150:ILE:HD13	22:A:815:CLA:HED3	1.98	0.44
22:A:820:CLA:H3A	22:A:820:CLA:HBA2	1.65	0.44
6:B:351:HIS:NE2	22:B:826:CLA:NC	2.65	0.44
25:K:202:BCR:H281	22:K:206:CLA:HBC3	2.00	0.44
5:A:363:VAL:HG12	22:A:827:CLA:HED3	1.98	0.44
25:A:856:BCR:H15C	25:A:856:BCR:H351	1.81	0.44
7:C:24:ASP:OD2	8:D:157:HIS:ND1	2.50	0.44
16:L:97:VAL:O	16:L:101:LEU:HB2	2.17	0.44
1:1:113:TRP:HE1	1:1:218:PRO:HD3	1.81	0.44
1:1:154:GLU:HG2	22:1:609:CLA:C1B	2.48	0.44
22:2:610:CLA:H41	22:2:610:CLA:H61	1.80	0.44
3:3:55:GLN:NE2	3:3:77:ASP:OD2	2.49	0.44
28:A:801:CL0:H64	22:A:803:CLA:C1B	2.47	0.44
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.99	0.44
4:4:112:ILE:HG13	4:4:113:PRO:HD3	1.99	0.44
5:A:286:LEU:HB2	5:A:291:ILE:HD11	1.98	0.44
5:A:482:GLN:NE2	5:A:526:LEU:O	2.47	0.44
22:A:854:CLA:H162	22:A:854:CLA:H122	1.73	0.44
20:Y:37:PRO:HB2	20:Y:177:LEU:HD12	1.98	0.44
33:Y:4623:NEX:H15	33:Y:4623:NEX:H201	1.72	0.44
6:B:340:SER:HB3	22:B:824:CLA:H51	1.99	0.44
22:B:818:CLA:H62	22:B:818:CLA:H41	1.71	0.44
7:C:40:ALA:O	8:D:176:GLN:NE2	2.50	0.44
20:Y:65:SER:HB2	20:Y:180:GLY:HA3	2.00	0.44
22:A:820:CLA:H162	22:A:828:CLA:H51	2.00	0.44
22:A:822:CLA:HBC3	22:A:828:CLA:H193	2.00	0.44
20:Y:205:LEU:HD22	23:Y:4620:LUT:H163	1.99	0.44
33:Z:7623:NEX:H11	33:Z:7623:NEX:H191	1.80	0.44
2:2:167:ARG:HE	2:2:178:VAL:HB	1.82	0.44
6:B:393:PHE:HE2	6:B:408:LEU:HD21	1.83	0.44
12:H:87:PHE:O	12:H:91:ALA:HB3	2.18	0.44
20:Y:90:GLU:H	20:Y:99:GLN:HE21	1.66	0.44
5:A:519:VAL:HG11	5:A:522:LEU:HD23	2.00	0.43
6:B:369:ALA:HB1	6:B:725:LEU:HD11	1.98	0.43
6:B:437:TYR:HD2	22:B:802:CLA:H193	1.83	0.43
15:K:75:ALA:N	15:K:104:ASP:OD1	2.50	0.43
16:L:55:GLN:HG3	17:O:37:PHE:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:814:CLA:H2	25:B:845:BCR:H362	2.01	0.43
22:B:828:CLA:H162	25:B:845:BCR:H17C	2.00	0.43
25:K:202:BCR:H15C	25:K:202:BCR:H351	1.71	0.43
23:Y:4621:LUT:H15	23:Y:4621:LUT:H201	1.82	0.43
5:A:96:SER:O	18:N:88:ASN:ND2	2.48	0.43
5:A:330:PHE:HD2	26:A:847:LHG:HC5	1.82	0.43
22:A:806:CLA:H2	22:A:806:CLA:H62	1.84	0.43
21:2:601:CHL:HMD2	25:3:620:BCR:HC21	2.01	0.43
6:B:484:PRO:HB2	22:B:835:CLA:HMD3	2.00	0.43
8:D:147:VAL:HG22	8:D:153:VAL:HG23	2.00	0.43
23:X:2621:LUT:H35	23:X:2621:LUT:H401	1.84	0.43
2:2:167:ARG:NH1	21:2:618:CHL:OMC	2.51	0.43
10:F:71:LEU:HB3	10:F:128:LEU:HB3	2.01	0.43
19:X:97:TRP:HE1	19:X:205:PRO:HD3	1.84	0.43
23:Z:7621:LUT:H35	23:Z:7621:LUT:H401	1.85	0.43
1:1:209:GLN:HE21	22:1:613:CLA:C4D	2.20	0.43
2:2:147:PHE:CE1	21:2:606:CHL:CMD	3.02	0.43
3:3:161:GLU:OE1	3:3:164:ARG:NH1	2.51	0.43
7:C:14:CYS:N	30:C:102:SF4:S1	2.90	0.43
25:I:101:BCR:H20C	25:I:101:BCR:H361	1.77	0.43
19:X:64:LEU:HD13	22:X:603:CLA:HAA2	2.00	0.43
1:1:56:PRO:HB2	1:1:59:LEU:HD23	2.01	0.43
3:3:230:ILE:HG21	24:3:619:XAT:H14	2.00	0.43
5:A:77:GLN:HE21	5:A:81:ILE:HG13	1.82	0.43
5:A:147:ALA:HB2	5:A:375:PRO:HD2	2.01	0.43
5:A:426:ARG:O	5:A:430:HIS:ND1	2.42	0.43
6:B:221:GLY:HA3	22:B:815:CLA:HMD1	2.00	0.43
6:B:358:TYR:OH	22:B:828:CLA:OBD	2.25	0.43
6:B:733:PHE:HB2	12:H:139:ARG:HD3	2.00	0.43
11:G:102:ALA:HA	11:G:105:LEU:HB2	2.01	0.43
3:3:179:PHE:CZ	21:3:608:CHL:HBB2	2.53	0.43
5:A:132:PHE:HB2	18:N:85:SER:HB3	2.00	0.43
25:A:849:BCR:H15C	25:A:849:BCR:H351	1.88	0.43
9:E:94:ILE:HB	10:F:224:TYR:HB2	1.99	0.43
11:G:126:HIS:CE1	25:G:205:BCR:H14C	2.54	0.43
2:2:107:GLU:OE2	2:2:227:ARG:NE	2.47	0.43
22:A:828:CLA:H162	22:A:828:CLA:H141	1.85	0.43
22:A:839:CLA:HBB2	22:A:840:CLA:HBC3	2.00	0.43
10:F:201:ILE:HG22	10:F:204:VAL:HB	2.01	0.43
22:1:603:CLA:H11	22:1:603:CLA:H51	1.85	0.43
22:A:812:CLA:H72	22:A:812:CLA:H112	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:179:LYS:HD3	22:Z:612:CLA:HAA2	2.01	0.43
6:B:194:LEU:HA	6:B:198:ALA:HB3	2.00	0.42
25:B:801:BCR:H381	22:F:301:CLA:HMC2	2.01	0.42
7:C:62:PHE:CD2	8:D:181:ILE:HD13	2.54	0.42
29:A:844:PQN:H302	29:A:844:PQN:H262	1.89	0.42
6:B:587:ILE:HA	6:B:590:VAL:HG22	2.01	0.42
22:B:809:CLA:H142	32:B:850:DGD:HAW2	2.01	0.42
25:B:848:BCR:H361	25:B:848:BCR:H20C	1.79	0.42
11:G:141:ASP:N	11:G:141:ASP:OD1	2.52	0.42
18:N:133:GLU:HB2	18:N:136:LYS:HB2	2.01	0.42
19:X:174:ALA:HA	19:X:177:LYS:HD2	2.01	0.42
19:Z:135:MET:HA	19:Z:138:VAL:HG22	2.01	0.42
5:A:665:SER:HB2	6:B:445:ALA:HB1	2.01	0.42
22:L:304:CLA:H2A	22:L:304:CLA:HED2	2.01	0.42
20:Y:124:TRP:CE3	20:Y:125:ALA:N	2.86	0.42
4:4:58:LEU:HD12	22:4:601:CLA:HMA3	2.01	0.42
23:4:619:LUT:H35	23:4:619:LUT:H401	1.78	0.42
25:A:850:BCR:H15C	25:A:850:BCR:H351	1.76	0.42
25:A:850:BCR:H24C	25:A:850:BCR:H371	1.79	0.42
6:B:645:VAL:HG21	22:B:809:CLA:HMD2	2.01	0.42
19:X:61:ASN:HB3	22:X:602:CLA:H3A	2.01	0.42
26:Y:4630:LHG:H202	24:Z:4622:XAT:H10	2.01	0.42
19:Z:112:TYR:HD2	19:Z:118:LEU:HD13	1.85	0.42
1:1:49:TRP:HH2	27:1:622:LMG:H131	1.85	0.42
5:A:737:THR:HG21	28:A:801:CL0:CHA	2.49	0.42
6:B:53:GLN:HE21	6:B:57:ILE:HG13	1.83	0.42
6:B:142:LEU:HG	25:B:845:BCR:H382	2.02	0.42
6:B:387:PHE:HZ	22:B:825:CLA:HAB	1.85	0.42
6:B:687:LEU:HD12	16:L:86:TYR:HE2	1.84	0.42
22:B:810:CLA:H152	22:B:810:CLA:H112	1.80	0.42
22:L:304:CLA:HBC1	25:L:306:BCR:H372	2.00	0.42
19:Z:65:GLU:OE1	22:Z:602:CLA:C4A	2.67	0.42
3:3:212:MET:HE1	22:3:610:CLA:H2A	2.01	0.42
4:4:204:LYS:HD3	22:4:612:CLA:HBD	2.02	0.42
5:A:25:GLU:HB2	22:A:812:CLA:HAA2	2.02	0.42
5:A:298:ILE:HD13	5:A:298:ILE:HA	1.87	0.42
22:B:803:CLA:HAC1	22:B:803:CLA:HMC1	1.85	0.42
25:G:205:BCR:H24C	25:G:205:BCR:H371	1.83	0.42
20:Y:189:GLY:O	20:Y:193:GLN:HG3	2.20	0.42
21:Y:601:CHL:HMA2	21:Y:601:CHL:H43	2.02	0.42
4:4:178:LEU:HD22	21:4:618:CHL:HBC1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:80:ASN:HD22	22:H:201:CLA:HHD	1.84	0.42
18:N:134:LYS:HG3	18:N:144:LYS:HB2	2.01	0.42
23:1:617:LUT:H11	23:1:617:LUT:H191	1.93	0.42
5:A:678:TRP:CZ2	28:A:801:CL0:H10	2.55	0.42
31:B:849:LMU:H92	31:B:849:LMU:H61	1.72	0.42
22:H:201:CLA:H61	22:H:201:CLA:H41	1.72	0.42
16:L:138:LEU:HD13	25:L:305:BCR:H401	2.01	0.42
24:X:7622:XAT:H15	24:X:7622:XAT:H201	1.71	0.42
22:2:611:CLA:HMC3	25:3:620:BCR:H333	2.02	0.42
5:A:485:GLN:HG2	5:A:507:TRP:HE3	1.84	0.42
6:B:682:HIS:NE2	6:B:691:ILE:O	2.41	0.42
22:B:834:CLA:HBA2	22:B:835:CLA:HMB3	2.01	0.42
22:4:610:CLA:HBB1	22:4:612:CLA:H3A	2.01	0.42
5:A:455:HIS:CE1	22:A:835:CLA:NA	2.88	0.42
22:A:828:CLA:H111	22:A:828:CLA:H152	1.82	0.42
6:B:257:LEU:HD22	22:B:817:CLA:HBB1	2.02	0.42
2:2:220:THR:HA	2:2:223:ILE:HG12	2.02	0.41
5:A:89:TYR:HE1	5:A:145:TRP:HE1	1.68	0.41
5:A:205:LEU:HD22	25:A:848:BCR:H361	2.02	0.41
6:B:17:THR:HG21	7:C:77:MET:HG3	2.02	0.41
6:B:376:GLN:HE21	6:B:590:VAL:HG21	1.85	0.41
32:B:850:DGD:HAS1	32:B:850:DGD:HAH2	1.93	0.41
18:N:80:LYS:HG2	18:N:127:ILE:HG22	2.01	0.41
22:N:1002:CLA:H2A	22:N:1002:CLA:HED2	2.02	0.41
22:N:1002:CLA:H3A	22:N:1002:CLA:HBA2	1.87	0.41
5:A:522:LEU:HD21	5:A:628:HIS:HE1	1.85	0.41
22:A:830:CLA:H142	22:A:830:CLA:H112	1.91	0.41
25:A:848:BCR:H361	25:A:848:BCR:H20C	1.83	0.41
25:B:847:BCR:H15C	25:B:847:BCR:H351	1.82	0.41
32:B:850:DGD:O4E	32:B:850:DGD:O5E	2.38	0.41
25:K:205:BCR:H351	25:K:205:BCR:H15C	1.81	0.41
22:L:303:CLA:HAC2	25:L:305:BCR:H382	2.02	0.41
18:N:143:TRP:HA	18:N:143:TRP:CE3	2.55	0.41
22:A:833:CLA:H62	22:A:833:CLA:H41	1.91	0.41
6:B:187:SER:OG	6:B:277:HIS:O	2.35	0.41
6:B:231:ASN:HA	22:B:816:CLA:HAA2	2.02	0.41
6:B:519:VAL:HG23	22:B:802:CLA:H141	2.02	0.41
22:B:839:CLA:H193	25:I:101:BCR:H362	2.01	0.41
18:N:143:TRP:HA	18:N:143:TRP:HE3	1.85	0.41
20:Y:59:GLU:HG2	20:Y:151:VAL:HG22	2.02	0.41
1:1:191:LYS:HD3	22:1:612:CLA:HAA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:435:ILE:O	5:A:439:ASN:HB2	2.21	0.41
22:A:842:CLA:HBA2	22:A:842:CLA:H3A	1.70	0.41
6:B:118:SER:HA	22:B:827:CLA:HMA2	2.01	0.41
6:B:222:LEU:HD11	25:B:843:BCR:H401	2.01	0.41
6:B:347:LEU:HD23	22:B:818:CLA:H62	2.01	0.41
22:B:805:CLA:H141	22:B:805:CLA:H162	1.89	0.41
25:B:847:BCR:H20C	25:B:847:BCR:H361	1.86	0.41
11:G:135:THR:HG21	27:G:202:LMG:HC92	2.02	0.41
16:L:95:ARG:NH2	16:L:171:ASP:OD1	2.41	0.41
23:Y:4620:LUT:H15	23:Y:4620:LUT:H201	1.89	0.41
19:Z:96:VAL:HB	19:Z:99:LYS:HB2	2.02	0.41
19:Z:170:PRO:HA	19:Z:173:PHE:HB3	2.03	0.41
22:A:822:CLA:H61	22:A:822:CLA:H2	1.79	0.41
22:A:825:CLA:H43	25:A:851:BCR:H16C	2.01	0.41
1:1:234:ILE:HG12	1:1:238:ILE:HG12	2.02	0.41
2:2:66:PRO:HB2	21:2:601:CHL:HBC1	2.03	0.41
3:3:75:LEU:HG	22:3:602:CLA:H42	2.02	0.41
5:A:415:ASP:OD2	5:A:417:THR:OG1	2.33	0.41
22:A:822:CLA:H92	22:A:822:CLA:H62	1.92	0.41
33:Y:4623:NEX:H11	33:Y:4623:NEX:H191	1.84	0.41
1:1:233:ASN:HD21	4:4:141:THR:HA	1.85	0.41
22:1:613:CLA:HBC3	26:1:620:LHG:H361	2.03	0.41
2:2:158:LEU:HG	22:2:609:CLA:HBB2	2.01	0.41
22:4:602:CLA:H72	24:4:620:XAT:H30	2.03	0.41
5:A:551:GLY:O	5:A:555:ALA:HB2	2.20	0.41
22:B:823:CLA:HBA2	22:B:823:CLA:H3A	1.88	0.41
25:B:846:BCR:H15C	25:B:846:BCR:H351	1.90	0.41
1:1:84:PHE:CE1	22:1:602:CLA:H43	2.55	0.41
24:4:620:XAT:H35	24:4:620:XAT:H401	1.82	0.41
5:A:62:ASP:OD1	5:A:62:ASP:N	2.54	0.41
5:A:283:THR:HG23	5:A:285:GLY:H	1.86	0.41
5:A:331:THR:HG21	26:A:847:LHG:HC11	2.03	0.41
22:A:802:CLA:H92	22:A:802:CLA:H62	1.98	0.41
29:A:844:PQN:H111	29:A:844:PQN:H2M1	1.85	0.41
22:B:811:CLA:H41	22:B:811:CLA:H61	1.79	0.41
25:K:202:BCR:H20C	25:K:202:BCR:H361	1.75	0.41
21:X:601:CHL:OMC	24:Y:2622:XAT:H242	2.20	0.41
23:1:617:LUT:H35	23:1:617:LUT:H401	1.86	0.41
22:2:610:CLA:H2	23:2:619:LUT:H28	2.02	0.41
24:2:620:XAT:H15	24:2:620:XAT:H201	1.86	0.41
22:4:602:CLA:H8	10:F:201:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:464:ARG:NH2	22:A:835:CLA:O1D	2.54	0.41
5:A:649:LEU:HD11	28:A:801:CL0:C7	2.49	0.41
28:A:801:CL0:H46	22:A:803:CLA:HED3	2.03	0.41
26:A:846:LHG:H272	26:A:846:LHG:H242	1.68	0.41
6:B:523:ILE:HG12	6:B:590:VAL:HG12	2.02	0.41
25:B:845:BCR:H15C	25:B:845:BCR:H351	1.84	0.41
31:B:849:LMU:H22	31:B:849:LMU:H51	1.77	0.41
7:C:61:ASP:H	9:E:125:ASN:HD22	1.69	0.41
7:C:61:ASP:H	9:E:125:ASN:ND2	2.18	0.41
22:F:304:CLA:HMB2	25:F:305:BCR:H24C	2.01	0.41
25:I:101:BCR:H11C	25:I:101:BCR:H341	1.90	0.41
25:L:306:BCR:H11C	25:L:306:BCR:H341	1.96	0.41
18:N:110:GLN:HE22	18:N:125:LEU:HD11	1.86	0.41
33:X:2623:NEX:H15	33:X:2623:NEX:H201	1.77	0.41
33:X:2623:NEX:H35	33:X:2623:NEX:H401	1.86	0.41
23:Y:4621:LUT:H35	23:Y:4621:LUT:H401	1.89	0.41
3:3:164:ARG:NH1	22:3:609:CLA:O1D	2.40	0.41
5:A:479:ILE:H	5:A:479:ILE:HG13	1.68	0.41
5:A:484:ILE:HA	5:A:487:ILE:HD12	2.03	0.41
5:A:691:TYR:OH	22:A:802:CLA:OBD	2.34	0.41
22:B:813:CLA:H141	22:B:813:CLA:H162	1.89	0.41
22:B:831:CLA:HAB	22:B:832:CLA:H171	2.03	0.41
16:L:80:LEU:HA	16:L:83:LEU:HD22	2.03	0.41
19:X:58:PHE:HE1	22:X:602:CLA:H2A	1.86	0.41
33:Z:7623:NEX:H201	33:Z:7623:NEX:H15	1.79	0.41
26:1:620:LHG:H312	26:1:620:LHG:H151	2.03	0.40
22:4:611:CLA:HED3	27:4:622:LMG:HC3	2.02	0.40
5:A:732:LEU:HD11	25:A:852:BCR:HC8	2.03	0.40
22:A:809:CLA:H91	22:A:812:CLA:H193	2.04	0.40
6:B:71:GLN:HB3	6:B:90:ALA:H	1.86	0.40
22:B:818:CLA:H3A	22:B:818:CLA:HBA2	1.63	0.40
17:O:43:ARG:HD2	17:O:118:LYS:HD2	2.03	0.40
23:X:2621:LUT:H31	23:X:2621:LUT:H391	1.89	0.40
1:1:82:GLU:OE1	1:1:85:LYS:NZ	2.54	0.40
26:1:620:LHG:H351	22:4:617:CLA:HMA2	2.02	0.40
4:4:56:GLU:HG3	4:4:59:PRO:HA	2.02	0.40
27:4:623:LMG:O5	27:4:623:LMG:O4	2.33	0.40
5:A:470:SER:HB3	5:A:639:ILE:HD13	2.03	0.40
5:A:541:ILE:HD11	22:A:838:CLA:HBB1	2.03	0.40
5:A:657:ILE:HD12	6:B:621:ARG:HB2	2.03	0.40
5:A:693:GLN:NE2	5:A:716:ALA:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:848:BCR:H15C	25:A:848:BCR:H351	1.97	0.40
6:B:5:PHE:HB2	13:I:30:VAL:HA	2.03	0.40
6:B:180:SER:HB3	6:B:288:GLY:HA3	2.03	0.40
22:B:827:CLA:HBC3	32:B:850:DGD:HBV2	2.02	0.40
22:B:832:CLA:HBC1	22:B:837:CLA:H192	2.02	0.40
8:D:150:ASN:N	8:D:150:ASN:OD1	2.53	0.40
14:J:28:GLU:OE1	14:J:31:ARG:NH2	2.55	0.40
17:O:103:HIS:CE1	22:O:2001:CLA:ND	2.89	0.40
23:X:2620:LUT:H35	23:X:2620:LUT:H401	1.81	0.40
26:Y:4630:LHG:H262	26:Y:4630:LHG:H291	1.89	0.40
1:1:80:ASN:HD21	22:B:841:CLA:HAC2	1.86	0.40
26:1:620:LHG:H102	26:1:620:LHG:H282	2.03	0.40
23:2:619:LUT:H15	23:2:619:LUT:H201	1.83	0.40
5:A:438:LEU:HD21	5:A:545:VAL:HG12	2.02	0.40
5:A:570:ARG:NH1	22:A:831:CLA:O2D	2.54	0.40
22:A:830:CLA:HMD2	22:A:830:CLA:H8	2.02	0.40
22:B:837:CLA:H142	22:B:837:CLA:H112	1.81	0.40
10:F:134:LEU:HA	10:F:135:PRO:HD3	1.94	0.40
20:Y:90:GLU:HB2	20:Y:96:ALA:HA	2.03	0.40
5:A:697:GLU:OE2	9:E:119:TYR:OH	2.33	0.40
22:A:820:CLA:H171	22:A:820:CLA:H13	1.87	0.40
22:A:837:CLA:HBA2	22:A:837:CLA:H3A	1.77	0.40
6:B:351:HIS:ND1	22:B:817:CLA:OBD	2.52	0.40
6:B:524:ALA:HB2	22:B:837:CLA:HMA1	2.03	0.40
18:N:133:GLU:HG3	18:N:136:LYS:HD3	2.03	0.40
24:X:7622:XAT:H35	24:X:7622:XAT:H401	1.90	0.40
24:Y:2622:XAT:H35	24:Y:2622:XAT:H401	1.92	0.40
22:A:809:CLA:HAA1	22:A:829:CLA:HED2	2.04	0.40
22:A:825:CLA:H3A	22:A:825:CLA:HBA2	1.64	0.40
25:A:849:BCR:H20C	25:A:849:BCR:H361	1.85	0.40
6:B:276:HIS:HE2	22:B:818:CLA:C2B	2.35	0.40
6:B:302:LYS:HD3	11:G:84:ALA:HB3	2.03	0.40
6:B:615:TYR:OH	6:B:621:ARG:NH2	2.54	0.40
18:N:76:LEU:HD23	18:N:80:LYS:HE2	2.04	0.40
22:Z:611:CLA:HMB3	26:Z:7630:LHG:HC11	2.03	0.40
23:Z:7620:LUT:H11	23:Z:7620:LUT:H191	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/245 (79%)	177 (91%)	17 (9%)	0	100	100
2	2	205/270 (76%)	199 (97%)	6 (3%)	0	100	100
3	3	219/267 (82%)	205 (94%)	14 (6%)	0	100	100
4	4	197/252 (78%)	182 (92%)	15 (8%)	0	100	100
5	A	740/750 (99%)	705 (95%)	35 (5%)	0	100	100
6	B	731/734 (100%)	699 (96%)	32 (4%)	0	100	100
7	C	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
8	D	140/199 (70%)	126 (90%)	14 (10%)	0	100	100
9	E	66/136 (48%)	61 (92%)	5 (8%)	0	100	100
10	F	156/225 (69%)	148 (95%)	8 (5%)	0	100	100
11	G	95/145 (66%)	91 (96%)	4 (4%)	0	100	100
12	H	93/142 (66%)	84 (90%)	9 (10%)	0	100	100
13	I	31/36 (86%)	26 (84%)	5 (16%)	0	100	100
14	J	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
15	K	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
16	L	164/211 (78%)	155 (94%)	9 (6%)	0	100	100
17	O	72/127 (57%)	60 (83%)	12 (17%)	0	100	100
18	N	82/145 (57%)	69 (84%)	13 (16%)	0	100	100
19	X	216/232 (93%)	202 (94%)	14 (6%)	0	100	100
19	Z	216/232 (93%)	205 (95%)	11 (5%)	0	100	100
20	Y	225/228 (99%)	202 (90%)	22 (10%)	1 (0%)	34	66
All	All	4042/4833 (84%)	3781 (94%)	260 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	Y	2	ARG

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	156/194 (80%)	156 (100%)	0	100	100
2	2	167/215 (78%)	165 (99%)	2 (1%)	71	83
3	3	176/210 (84%)	176 (100%)	0	100	100
4	4	166/204 (81%)	165 (99%)	1 (1%)	86	91
5	A	599/607 (99%)	596 (100%)	3 (0%)	88	93
6	B	599/600 (100%)	594 (99%)	5 (1%)	81	89
7	C	71/71 (100%)	70 (99%)	1 (1%)	67	82
8	D	119/159 (75%)	118 (99%)	1 (1%)	81	89
9	E	59/103 (57%)	59 (100%)	0	100	100
10	F	127/171 (74%)	125 (98%)	2 (2%)	62	79
11	G	79/110 (72%)	79 (100%)	0	100	100
12	H	78/110 (71%)	76 (97%)	2 (3%)	46	71
13	I	30/33 (91%)	30 (100%)	0	100	100
14	J	35/36 (97%)	35 (100%)	0	100	100
15	K	59/96 (62%)	57 (97%)	2 (3%)	37	65
16	L	130/164 (79%)	129 (99%)	1 (1%)	81	89
17	O	66/110 (60%)	65 (98%)	1 (2%)	65	81
18	N	73/111 (66%)	72 (99%)	1 (1%)	67	82
19	X	168/178 (94%)	168 (100%)	0	100	100
19	Z	168/178 (94%)	167 (99%)	1 (1%)	86	91
20	Y	175/175 (100%)	174 (99%)	1 (1%)	86	91
All	All	3300/3835 (86%)	3276 (99%)	24 (1%)	84	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	227	ARG
2	2	239	GLN
4	4	149	LEU
5	A	243	ASN
5	A	439	ASN
5	A	582	CYS
6	B	96	PHE
6	B	327	ASN
6	B	482	ASN
6	B	621	ARG
6	B	668	ARG
7	C	61	ASP
8	D	135	ARG
10	F	117	ARG
10	F	168	ARG
12	H	48	LYS
12	H	61	ILE
15	K	53	ASN
15	K	77	ARG
16	L	118	ARG
17	O	68	ASN
18	N	114	LYS
20	Y	1	ARG
19	Z	197	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	53	GLN
1	1	209	GLN
3	3	153	ASN
3	3	177	GLN
4	4	75	ASN
4	4	94	GLN
4	4	159	GLN
4	4	222	GLN
5	A	243	ASN
5	A	353	ASN
5	A	366	HIS
5	A	384	GLN
5	A	693	GLN
6	B	114	ASN
6	B	327	ASN

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Mol	Chain	Res	Type
6	B	350	GLN
6	B	376	GLN
6	B	452	GLN
6	B	482	ASN
10	F	86	ASN
10	F	136	HIS
11	G	85	GLN
11	G	143	ASN
12	H	83	GLN
18	N	140	ASN
19	X	61	ASN
19	X	227	ASN
20	Y	57	ASN
20	Y	99	GLN
19	Z	61	ASN
19	Z	103	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
20	TPO	Y	3	20	8,10,11	1.06	0	10,14,16	1.63	1 (10%)

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	TPO	Y	3	20	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	3	TPO	P-OG1-CB	-4.53	109.54	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

271 ligands 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
22	CLA	A	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.66	9 (11%)
22	CLA	B	810	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	11 (14%)
28	CL0	A	801	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	31 (40%)
22	CLA	3	614	-	39,48,73	1.85	7 (17%)	44,83,113	1.78	7 (15%)
26	LHG	X	2630	22	21,21,48	0.85	1 (4%)	22,26,54	1.12	1 (4%)
22	CLA	A	814	-	65,73,73	1.41	8 (12%)	76,113,113	1.44	9 (11%)
21	CHL	Y	609	20	39,48,74	2.28	14 (35%)	42,82,114	2.95	17 (40%)
24	XAT	X	7622	-	39,47,47	0.93	0	54,74,74	2.95	19 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	827	-	59,67,73	1.51	9 (15%)	68,105,113	1.43	9 (13%)
22	CLA	A	821	-	45,53,73	1.76	9 (20%)	52,89,113	1.71	7 (13%)
21	CHL	Z	605	19	37,46,74	2.37	14 (37%)	46,81,114	3.02	19 (41%)
22	CLA	K	203	-	45,53,73	1.74	9 (20%)	52,89,113	1.64	10 (19%)
22	CLA	B	821	-	47,55,73	1.64	9 (19%)	54,91,113	1.77	9 (16%)
25	BCR	B	846	-	41,41,41	0.83	0	56,56,56	2.02	22 (39%)
22	CLA	B	816	-	55,63,73	1.54	7 (12%)	64,101,113	1.73	6 (9%)
22	CLA	A	830	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
22	CLA	B	820	-	50,58,73	1.66	8 (16%)	58,95,113	1.65	6 (10%)
22	CLA	3	609	3	45,53,73	1.81	11 (24%)	52,89,113	1.83	11 (21%)
27	LMG	G	202	-	38,38,55	1.00	1 (2%)	46,46,63	1.22	6 (13%)
22	CLA	X	604	-	36,43,73	2.01	8 (22%)	45,76,113	1.78	9 (20%)
22	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	8 (12%)
22	CLA	Y	611	26	39,48,73	1.94	7 (17%)	48,83,113	1.74	9 (18%)
22	CLA	2	614	-	43,51,73	1.73	7 (16%)	49,86,113	1.93	11 (22%)
22	CLA	A	836	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	6 (11%)
22	CLA	A	815	-	45,53,73	1.70	9 (20%)	52,89,113	1.83	10 (19%)
22	CLA	A	833	-	56,64,73	1.52	8 (14%)	65,102,113	1.69	7 (10%)
23	LUT	X	2620	-	42,43,43	0.70	0	51,60,60	1.65	9 (17%)
21	CHL	Z	607	-	43,52,74	5.32	15 (34%)	49,88,114	3.07	19 (38%)
22	CLA	3	607	3	41,49,73	1.87	7 (17%)	51,84,113	1.76	10 (19%)
22	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.82	11 (18%)
22	CLA	H	201	-	60,68,73	1.51	8 (13%)	70,107,113	1.48	8 (11%)
22	CLA	G	201	-	45,53,73	1.76	9 (20%)	52,89,113	1.70	8 (15%)
22	CLA	Z	603	-	41,49,73	1.87	8 (19%)	51,84,113	1.82	11 (21%)
22	CLA	A	811	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
22	CLA	A	834	-	65,73,73	1.46	8 (12%)	76,113,113	1.50	10 (13%)
22	CLA	B	818	-	60,68,73	1.47	10 (16%)	70,107,113	1.59	9 (12%)
22	CLA	A	804	-	65,73,73	1.42	8 (12%)	76,113,113	1.62	9 (11%)
22	CLA	2	604	-	43,51,73	1.79	7 (16%)	48,86,113	1.70	6 (12%)
22	CLA	A	842	-	65,73,73	1.45	8 (12%)	76,113,113	1.54	9 (11%)
22	CLA	B	838	-	47,55,73	1.71	8 (17%)	54,91,113	1.69	8 (14%)
22	CLA	B	826	-	62,70,73	1.50	9 (14%)	72,109,113	1.54	10 (13%)
23	LUT	3	618	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
25	BCR	B	844	-	41,41,41	0.74	0	56,56,56	1.97	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	1	622	-	53,53,55	0.84	2 (3%)	61,61,63	1.28	5 (8%)
22	CLA	A	807	5	65,73,73	1.47	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	A	845	26	50,58,73	1.66	8 (16%)	58,95,113	1.63	10 (17%)
22	CLA	A	838	-	51,59,73	1.55	7 (13%)	59,96,113	1.91	14 (23%)
22	CLA	K	204	-	46,54,73	1.70	8 (17%)	53,90,113	1.63	7 (13%)
22	CLA	2	609	2	45,53,73	1.71	7 (15%)	52,89,113	1.80	10 (19%)
22	CLA	4	609	4	45,53,73	1.78	10 (22%)	52,89,113	1.84	9 (17%)
25	BCR	A	848	-	41,41,41	0.81	0	56,56,56	1.84	13 (23%)
21	CHL	2	601	2	61,69,74	1.88	14 (22%)	67,108,114	2.67	23 (34%)
21	CHL	2	607	-	43,51,74	2.14	12 (27%)	45,86,114	3.00	17 (37%)
22	CLA	A	808	-	50,58,73	1.61	8 (16%)	58,95,113	1.68	8 (13%)
22	CLA	1	616	1	43,51,73	1.86	8 (18%)	54,87,113	1.70	10 (18%)
27	LMG	2	623	-	36,36,55	1.01	2 (5%)	44,44,63	1.15	3 (6%)
22	CLA	Z	611	26	39,47,73	1.95	7 (17%)	49,82,113	1.81	11 (22%)
25	BCR	A	852	-	41,41,41	0.74	0	56,56,56	1.98	11 (19%)
22	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.91	12 (15%)
21	CHL	Y	608	-	39,48,74	2.24	15 (38%)	45,83,114	3.02	16 (35%)
22	CLA	X	610	19	39,47,73	1.86	6 (15%)	42,81,113	1.87	7 (16%)
22	CLA	B	822	-	42,50,73	1.79	8 (19%)	48,85,113	1.71	9 (18%)
22	CLA	4	611	-	42,50,73	1.78	7 (16%)	48,85,113	1.71	9 (18%)
32	DGD	J	103	-	67,67,67	0.95	4 (5%)	81,81,81	1.45	8 (9%)
25	BCR	G	205	-	41,41,41	0.75	0	56,56,56	1.90	16 (28%)
22	CLA	1	603	-	55,63,73	1.65	8 (14%)	64,101,113	1.54	9 (14%)
22	CLA	4	602	4	60,68,73	1.49	7 (11%)	70,107,113	1.60	10 (14%)
22	CLA	4	610	4	54,62,73	1.60	10 (18%)	62,99,113	1.62	6 (9%)
22	CLA	3	612	3	43,51,73	1.82	6 (13%)	49,86,113	1.80	9 (18%)
22	CLA	J	101	14	42,50,73	1.80	6 (14%)	48,85,113	1.73	8 (16%)
25	BCR	K	205	-	41,41,41	0.72	0	56,56,56	1.95	14 (25%)
33	NEX	Y	4623	-	38,46,46	0.89	1 (2%)	50,70,70	2.37	19 (38%)
22	CLA	2	603	-	43,52,73	1.78	10 (23%)	49,88,113	1.74	9 (18%)
22	CLA	X	602	19	40,49,73	1.91	8 (20%)	45,84,113	1.62	6 (13%)
21	CHL	X	601	19	37,46,74	2.29	13 (35%)	44,80,114	3.06	20 (45%)
22	CLA	Y	604	-	42,50,73	1.80	7 (16%)	48,85,113	1.90	8 (16%)
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.01	16 (28%)
22	CLA	B	808	-	65,73,73	1.46	11 (16%)	76,113,113	1.75	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	Z	602	19	52,60,73	1.72	8 (15%)	64,97,113	1.59	8 (12%)
26	LHG	A	847	22	29,29,48	0.87	1 (3%)	32,35,54	1.26	3 (9%)
22	CLA	Y	603	-	38,47,73	1.91	7 (18%)	43,82,113	1.74	7 (16%)
22	CLA	3	610	3	41,49,73	1.79	8 (19%)	47,84,113	1.80	8 (17%)
25	BCR	B	847	-	41,41,41	1.03	3 (7%)	56,56,56	2.52	25 (44%)
22	CLA	A	824	-	41,49,73	1.84	9 (21%)	47,84,113	1.79	11 (23%)
22	CLA	G	204	11	45,53,73	1.78	9 (20%)	52,89,113	1.64	7 (13%)
22	CLA	F	303	-	42,50,73	1.81	7 (16%)	48,85,113	1.71	8 (16%)
22	CLA	X	611	26	38,47,73	1.94	6 (15%)	44,81,113	1.64	7 (15%)
25	BCR	A	850	-	41,41,41	0.89	2 (4%)	56,56,56	2.25	19 (33%)
22	CLA	2	612	2	44,52,73	1.79	8 (18%)	51,88,113	1.69	7 (13%)
27	LMG	4	622	-	39,39,55	0.90	1 (2%)	47,47,63	1.24	4 (8%)
22	CLA	A	813	-	54,62,73	1.59	8 (14%)	62,99,113	1.66	6 (9%)
22	CLA	A	840	-	52,60,73	1.63	8 (15%)	60,97,113	1.73	8 (13%)
22	CLA	2	611	26	38,45,73	2.94	10 (26%)	41,76,113	1.52	9 (21%)
22	CLA	L	302	16	45,53,73	1.76	9 (20%)	52,89,113	1.76	9 (17%)
22	CLA	A	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	B	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.52	6 (7%)
25	BCR	A	851	-	41,41,41	0.78	0	56,56,56	1.97	12 (21%)
21	CHL	4	608	-	46,54,74	2.16	15 (32%)	49,90,114	2.83	18 (36%)
22	CLA	B	813	-	65,73,73	1.42	11 (16%)	76,113,113	1.54	13 (17%)
23	LUT	X	2621	-	42,43,43	0.76	0	51,60,60	1.57	8 (15%)
25	BCR	L	306	-	41,41,41	0.76	0	56,56,56	1.84	13 (23%)
33	NEX	X	2623	-	38,46,46	0.86	1 (2%)	50,70,70	2.27	15 (30%)
24	XAT	1	618	-	39,47,47	0.99	2 (5%)	54,74,74	2.58	18 (33%)
25	BCR	I	101	-	41,41,41	0.83	0	56,56,56	2.14	18 (32%)
22	CLA	A	835	-	65,73,73	1.43	11 (16%)	76,113,113	1.67	13 (17%)
25	BCR	F	305	-	41,41,41	0.78	0	56,56,56	1.84	13 (23%)
25	BCR	L	305	-	41,41,41	0.74	0	56,56,56	1.92	12 (21%)
26	LHG	Y	4630	22	44,44,48	0.60	0	47,50,54	1.23	4 (8%)
22	CLA	O	2002	-	37,46,73	1.96	7 (18%)	46,81,113	2.02	11 (23%)
22	CLA	Y	610	20	39,47,73	1.93	7 (17%)	49,82,113	1.89	11 (22%)
21	CHL	3	608	-	45,53,74	2.13	14 (31%)	52,89,114	2.78	21 (40%)
30	SF4	A	853	-	0,12,12	-	-	-	-	-
22	CLA	O	2001	-	36,46,73	1.93	6 (16%)	41,80,113	1.67	7 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	2	613	2	65,73,73	1.48	9 (13%)	76,113,113	1.52	7 (9%)
21	CHL	1	601	1	54,63,74	2.09	16 (29%)	58,101,114	2.43	19 (32%)
22	CLA	A	825	-	55,63,73	1.59	10 (18%)	64,101,113	1.65	11 (17%)
21	CHL	X	607	-	41,49,74	2.39	15 (36%)	48,84,114	2.91	20 (41%)
22	CLA	A	837	5	45,53,73	1.78	7 (15%)	52,89,113	1.69	7 (13%)
22	CLA	1	610	1	59,67,73	1.50	7 (11%)	69,106,113	1.55	7 (10%)
22	CLA	G	203	-	42,50,73	1.77	7 (16%)	48,85,113	1.68	9 (18%)
22	CLA	Z	612	19	37,46,73	1.98	8 (21%)	48,80,113	1.78	12 (25%)
22	CLA	Z	613	19	43,51,73	1.78	6 (13%)	49,86,113	1.77	8 (16%)
22	CLA	A	831	-	65,73,73	1.55	11 (16%)	76,113,113	1.65	8 (10%)
27	LMG	4	623	-	33,33,55	1.15	3 (9%)	41,41,63	1.20	6 (14%)
26	LHG	B	851	22	37,37,48	0.67	1 (2%)	40,43,54	1.23	4 (10%)
30	SF4	C	102	-	0,12,12	-	-	-	-	-
25	BCR	B	845	-	41,41,41	0.74	0	56,56,56	1.96	13 (23%)
22	CLA	A	819	-	59,67,73	1.63	10 (16%)	68,105,113	1.42	8 (11%)
32	DGD	B	850	-	67,67,67	1.07	5 (7%)	81,81,81	1.44	13 (16%)
23	LUT	2	619	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	B	812	-	43,51,73	1.69	7 (16%)	49,86,113	1.95	7 (14%)
21	CHL	Y	607	-	40,48,74	2.28	12 (30%)	47,83,114	3.09	21 (44%)
25	BCR	1	619	-	41,41,41	0.67	0	56,56,56	1.80	13 (23%)
24	XAT	4	620	-	39,47,47	0.95	2 (5%)	54,74,74	2.59	19 (35%)
22	CLA	4	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.50	9 (15%)
22	CLA	B	830	-	43,51,73	1.77	10 (23%)	49,86,113	1.66	7 (14%)
21	CHL	Y	601	20	62,71,74	1.85	13 (20%)	76,111,114	2.32	21 (27%)
23	LUT	Z	7620	-	42,43,43	0.75	0	51,60,60	1.56	12 (23%)
22	CLA	4	601	4	46,54,73	1.74	10 (21%)	53,90,113	1.61	9 (16%)
22	CLA	A	826	-	65,73,73	1.43	8 (12%)	76,113,113	1.54	9 (11%)
22	CLA	Z	604	-	46,54,73	1.78	8 (17%)	57,90,113	1.68	9 (15%)
22	CLA	F	304	-	41,49,73	1.79	9 (21%)	47,84,113	1.76	7 (14%)
22	CLA	3	617	-	39,48,73	1.84	8 (20%)	44,83,113	1.76	8 (18%)
21	CHL	Y	605	20	37,46,74	2.46	14 (37%)	46,81,114	2.92	20 (43%)
21	CHL	X	606	-	38,47,74	2.31	14 (36%)	45,81,114	3.14	23 (51%)
22	CLA	B	815	-	43,51,73	1.69	9 (20%)	49,86,113	1.86	7 (14%)
22	CLA	K	206	15	37,47,73	1.92	6 (16%)	42,81,113	1.81	10 (23%)
24	XAT	Y	2622	-	39,47,47	0.84	0	54,74,74	2.61	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	817	-	45,53,73	1.75	9 (20%)	52,89,113	1.75	9 (17%)
22	CLA	X	603	-	39,48,73	1.89	6 (15%)	44,83,113	1.83	9 (20%)
22	CLA	A	828	-	65,73,73	1.44	9 (13%)	76,113,113	1.42	6 (7%)
21	CHL	4	606	-	40,49,74	2.22	13 (32%)	42,84,114	2.89	18 (42%)
22	CLA	B	811	-	54,62,73	1.63	9 (16%)	67,100,113	1.57	9 (13%)
22	CLA	B	817	-	59,67,73	1.52	10 (16%)	68,105,113	1.50	7 (10%)
22	CLA	X	613	19	37,44,73	1.94	6 (16%)	42,77,113	1.91	8 (19%)
22	CLA	1	609	1	40,48,73	1.90	8 (20%)	50,83,113	1.86	10 (20%)
26	LHG	Z	7630	22	22,22,48	0.90	1 (4%)	25,28,54	1.18	1 (4%)
22	CLA	A	832	-	50,58,73	1.65	9 (18%)	58,95,113	1.76	11 (18%)
22	CLA	A	854	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	8 (10%)
22	CLA	X	614	-	38,47,73	1.98	7 (18%)	48,81,113	1.70	10 (20%)
25	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.02	18 (32%)
31	LMU	B	849	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
22	CLA	B	832	-	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
22	CLA	A	816	-	42,50,73	1.74	7 (16%)	48,85,113	1.84	8 (16%)
21	CHL	Z	606	-	38,47,74	2.30	14 (36%)	41,81,114	2.97	20 (48%)
26	LHG	A	846	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	5 (9%)
22	CLA	Y	613	20	42,51,73	1.92	7 (16%)	52,87,113	1.77	8 (15%)
29	PQN	A	844	-	34,34,34	2.88	11 (32%)	42,45,45	2.13	6 (14%)
24	XAT	Z	4622	-	39,47,47	0.98	0	54,74,74	2.88	18 (33%)
22	CLA	A	809	5	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	K	201	15	38,45,73	1.92	10 (26%)	43,78,113	1.86	9 (20%)
23	LUT	Y	4620	-	42,43,43	0.75	0	51,60,60	1.63	13 (25%)
22	CLA	B	824	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
22	CLA	1	604	-	49,57,73	1.69	8 (16%)	55,93,113	1.66	7 (12%)
21	CHL	1	607	1	40,49,74	2.42	16 (40%)	41,84,114	2.85	20 (48%)
22	CLA	Y	614	-	38,47,73	1.93	7 (18%)	47,82,113	1.84	10 (21%)
22	CLA	3	606	3	40,49,73	1.82	10 (25%)	45,84,113	1.78	11 (24%)
22	CLA	B	833	-	45,53,73	1.76	10 (22%)	52,89,113	1.67	11 (21%)
24	XAT	3	619	-	39,47,47	0.92	2 (5%)	54,74,74	2.51	19 (35%)
22	CLA	A	841	-	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
22	CLA	B	828	-	65,73,73	1.44	11 (16%)	76,113,113	1.55	13 (17%)
21	CHL	X	605	19	41,50,74	2.25	13 (31%)	49,85,114	2.68	16 (32%)
25	BCR	J	102	-	41,41,41	0.81	0	56,56,56	2.02	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	L	301	-	41,41,41	0.80	0	56,56,56	1.88	18 (32%)
22	CLA	B	841	26	65,73,73	1.43	9 (13%)	76,113,113	1.46	8 (10%)
25	BCR	A	856	-	41,41,41	0.73	0	56,56,56	1.88	14 (25%)
22	CLA	A	818	-	60,68,73	1.44	7 (11%)	70,107,113	1.83	12 (17%)
22	CLA	1	606	-	39,48,73	1.82	7 (17%)	45,82,113	1.77	9 (20%)
21	CHL	4	607	-	41,49,74	2.23	14 (34%)	51,84,114	2.82	18 (35%)
21	CHL	2	618	2	43,51,74	2.22	15 (34%)	45,86,114	3.04	20 (44%)
22	CLA	L	303	-	60,68,73	1.51	9 (15%)	70,107,113	1.50	10 (14%)
25	BCR	B	848	-	41,41,41	0.79	0	56,56,56	2.01	16 (28%)
29	PQN	B	842	-	34,34,34	2.89	11 (32%)	42,45,45	2.08	5 (11%)
21	CHL	2	606	-	42,50,74	2.21	13 (30%)	45,85,114	2.94	19 (42%)
24	XAT	2	620	-	39,47,47	0.98	1 (2%)	54,74,74	2.75	23 (42%)
22	CLA	A	812	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
22	CLA	B	835	-	42,50,73	1.86	9 (21%)	48,85,113	1.64	7 (14%)
22	CLA	1	613	-	65,73,73	1.45	10 (15%)	76,113,113	1.46	7 (9%)
26	LHG	1	620	22	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
21	CHL	Y	606	-	37,46,74	2.42	13 (35%)	46,81,114	3.02	18 (39%)
21	CHL	2	608	-	51,59,74	2.03	14 (27%)	55,96,114	2.80	20 (36%)
22	CLA	X	612	19	37,44,73	1.98	7 (18%)	46,77,113	1.84	10 (21%)
26	LHG	2	622	22	36,36,48	0.74	1 (2%)	39,42,54	1.29	5 (12%)
22	CLA	A	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.76	15 (19%)
22	CLA	Y	612	20	37,46,73	2.03	8 (21%)	46,81,113	1.93	12 (26%)
31	LMU	A	857	-	31,31,36	1.37	3 (9%)	42,42,47	1.55	8 (19%)
22	CLA	3	602	3	60,68,73	1.57	8 (13%)	70,107,113	1.47	8 (11%)
23	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.71	15 (29%)
30	SF4	C	101	-	0,12,12	-	-	-	-	-
22	CLA	B	802	-	65,73,73	1.49	10 (15%)	76,113,113	1.33	5 (6%)
22	CLA	A	805	-	52,60,73	1.64	8 (15%)	60,97,113	1.68	8 (13%)
22	CLA	B	804	-	41,49,73	1.76	7 (17%)	47,84,113	1.96	8 (17%)
22	CLA	B	814	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	8 (10%)
22	CLA	N	1001	18	44,53,73	1.77	8 (18%)	50,89,113	1.65	7 (14%)
22	CLA	L	304	-	45,53,73	1.70	8 (17%)	52,89,113	1.88	9 (17%)
23	LUT	Y	4621	-	42,43,43	0.75	0	51,60,60	1.51	10 (19%)
22	CLA	2	610	2	55,63,73	1.54	10 (18%)	64,101,113	1.54	8 (12%)
22	CLA	N	1002	-	50,58,73	1.66	7 (14%)	58,95,113	1.71	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	1	611	26	37,46,73	1.94	9 (24%)	46,81,113	1.80	9 (19%)
22	CLA	F	301	-	57,65,73	1.60	9 (15%)	66,103,113	1.53	8 (12%)
22	CLA	A	810	5	50,58,73	1.68	10 (20%)	58,95,113	1.52	9 (15%)
22	CLA	B	823	-	45,53,73	1.74	9 (20%)	52,89,113	1.73	7 (13%)
22	CLA	B	829	-	56,64,73	1.76	10 (17%)	65,102,113	1.89	10 (15%)
21	CHL	X	608	-	38,47,74	2.40	15 (39%)	41,81,114	2.97	19 (46%)
21	CHL	X	609	19	37,44,74	2.23	13 (35%)	46,77,114	2.91	24 (52%)
22	CLA	3	603	3	55,63,73	1.61	10 (18%)	64,101,113	1.63	13 (20%)
22	CLA	B	807	6	52,60,73	1.61	9 (17%)	60,97,113	1.63	8 (13%)
22	CLA	1	612	1	45,53,73	1.79	7 (15%)	52,89,113	1.69	8 (15%)
22	CLA	B	827	-	65,73,73	1.39	8 (12%)	76,113,113	1.55	8 (10%)
33	NEX	Z	7623	-	38,46,46	0.90	1 (2%)	50,70,70	2.34	17 (34%)
22	CLA	1	614	-	37,46,73	1.99	8 (21%)	46,81,113	1.81	10 (21%)
22	CLA	1	602	1	61,69,73	1.51	6 (9%)	71,108,113	1.46	9 (12%)
23	LUT	1	621	-	42,43,43	0.74	0	51,60,60	1.57	10 (19%)
22	CLA	A	829	-	65,73,73	1.42	7 (10%)	76,113,113	1.67	10 (13%)
22	CLA	B	837	-	65,73,73	1.43	7 (10%)	76,113,113	1.64	11 (14%)
22	CLA	B	839	-	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
23	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	12 (23%)
21	CHL	Z	608	-	44,53,74	2.20	13 (29%)	46,89,114	2.93	17 (36%)
22	CLA	2	602	2	65,73,73	1.49	10 (15%)	76,113,113	1.36	7 (9%)
22	CLA	A	822	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	6 (7%)
25	BCR	B	801	-	41,41,41	0.78	0	56,56,56	2.09	12 (21%)
22	CLA	B	819	-	55,63,73	1.63	11 (20%)	64,101,113	1.60	7 (10%)
23	LUT	Z	7621	-	42,43,43	0.80	1 (2%)	51,60,60	1.59	11 (21%)
22	CLA	4	613	-	57,65,73	1.55	7 (12%)	66,103,113	1.58	9 (13%)
25	BCR	A	849	-	41,41,41	0.89	2 (4%)	56,56,56	2.04	19 (33%)
22	CLA	B	831	-	43,51,73	1.78	7 (16%)	49,86,113	1.77	7 (14%)
22	CLA	Z	610	19	37,44,73	2.02	8 (21%)	41,77,113	1.85	8 (19%)
22	CLA	A	823	-	42,50,73	1.75	7 (16%)	48,85,113	1.82	7 (14%)
22	CLA	Y	602	20	45,53,73	1.81	9 (20%)	52,89,113	1.57	8 (15%)
22	CLA	3	615	-	37,44,73	1.89	7 (18%)	42,77,113	1.83	7 (16%)
22	CLA	B	834	-	60,68,73	1.50	8 (13%)	70,107,113	1.56	9 (12%)
22	CLA	B	825	-	62,70,73	1.45	8 (12%)	72,109,113	1.46	11 (15%)
22	CLA	4	604	-	43,51,73	1.82	8 (18%)	54,87,113	1.69	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	806	6	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
22	CLA	4	614	-	45,53,73	1.79	7 (15%)	52,89,113	1.65	10 (19%)
22	CLA	4	603	4	44,52,73	1.87	9 (20%)	55,88,113	1.65	11 (20%)
21	CHL	Z	601	19	41,50,74	2.38	16 (39%)	42,85,114	2.84	18 (42%)
21	CHL	Z	609	19	41,50,74	2.27	12 (29%)	42,85,114	3.00	17 (40%)
22	CLA	1	608	-	43,52,73	1.80	6 (13%)	49,88,113	1.54	7 (14%)
21	CHL	4	618	4	40,49,74	2.16	12 (30%)	45,84,114	3.04	20 (44%)
22	CLA	A	843	-	65,73,73	1.49	10 (15%)	76,113,113	1.44	7 (9%)
22	CLA	B	809	6	65,73,73	1.49	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	A	820	-	65,73,73	1.50	10 (15%)	76,113,113	1.64	8 (10%)
22	CLA	3	613	3	53,62,73	1.61	8 (15%)	61,100,113	1.53	6 (9%)
22	CLA	Z	614	-	44,52,73	1.81	6 (13%)	51,88,113	1.60	6 (11%)
25	BCR	K	202	-	41,41,41	0.78	0	56,56,56	2.25	14 (25%)
22	CLA	4	612	4	40,49,73	1.83	7 (17%)	45,84,113	1.72	8 (17%)
25	BCR	2	621	-	41,41,41	0.71	0	56,56,56	1.87	11 (19%)
25	BCR	3	620	-	41,41,41	0.74	0	56,56,56	1.99	16 (28%)
22	CLA	B	805	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	11 (14%)
22	CLA	3	604	-	41,50,73	1.89	8 (19%)	51,86,113	1.73	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-
22	CLA	B	810	-	1/1/15/20	13/37/115/115	-
28	CLO	A	801	-	3/3/20/25	7/37/135/135	-
22	CLA	3	614	-	1/1/10/20	1/6/84/115	-
26	LHG	X	2630	22	-	8/25/25/53	-
22	CLA	A	814	-	1/1/15/20	18/37/115/115	-
21	CHL	Y	609	20	3/3/14/26	0/6/104/137	-
24	XAT	X	7622	-	-	1/31/93/93	0/4/4/4
22	CLA	A	827	-	1/1/13/20	11/30/108/115	-
22	CLA	A	821	-	1/1/11/20	0/13/91/115	-
21	CHL	Z	605	19	3/3/15/26	1/4/100/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	203	-	1/1/11/20	4/13/91/115	-
22	CLA	B	821	-	1/1/11/20	6/16/94/115	-
25	BCR	B	846	-	-	1/29/63/63	0/2/2/2
22	CLA	B	816	-	1/1/13/20	6/25/103/115	-
22	CLA	A	830	-	1/1/15/20	14/37/115/115	-
22	CLA	B	820	-	1/1/12/20	6/19/97/115	-
22	CLA	3	609	3	1/1/11/20	5/13/91/115	-
27	LMG	G	202	-	-	20/33/53/70	0/1/1/1
22	CLA	X	604	-	1/1/8/20	-	-
22	CLA	A	839	-	1/1/13/20	7/25/103/115	-
22	CLA	Y	611	26	1/1/10/20	1/8/84/115	-
22	CLA	2	614	-	1/1/10/20	3/11/89/115	-
22	CLA	A	836	-	1/1/11/20	1/13/91/115	-
22	CLA	A	815	-	1/1/11/20	6/13/91/115	-
22	CLA	A	833	-	1/1/13/20	8/27/105/115	-
23	LUT	X	2620	-	-	4/29/67/67	0/2/2/2
21	CHL	Z	607	-	3/3/16/26	5/13/109/137	-
22	CLA	3	607	3	1/1/10/20	2/10/86/115	-
22	CLA	B	836	-	1/1/12/20	3/19/97/115	-
22	CLA	H	201	-	1/1/14/20	14/31/109/115	-
22	CLA	G	201	-	1/1/11/20	4/13/91/115	-
22	CLA	Z	603	-	1/1/10/20	4/10/86/115	-
22	CLA	A	811	-	1/1/15/20	16/37/115/115	-
22	CLA	A	834	-	1/1/15/20	15/37/115/115	-
22	CLA	B	818	-	1/1/14/20	18/31/109/115	-
22	CLA	A	804	-	1/1/15/20	12/37/115/115	-
22	CLA	2	604	-	1/1/10/20	5/9/88/115	-
22	CLA	A	842	-	1/1/15/20	9/37/115/115	-
22	CLA	B	838	-	1/1/11/20	7/16/94/115	-
22	CLA	B	826	-	1/1/14/20	14/34/112/115	-
23	LUT	3	618	-	-	4/29/67/67	0/2/2/2
25	BCR	B	844	-	-	8/29/63/63	0/2/2/2
27	LMG	1	622	-	-	26/48/68/70	0/1/1/1
22	CLA	A	807	5	1/1/15/20	19/37/115/115	-
22	CLA	A	845	26	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	838	-	1/1/12/20	7/21/99/115	-
22	CLA	K	204	-	1/1/11/20	11/15/93/115	-
22	CLA	2	609	2	1/1/11/20	6/13/91/115	-
22	CLA	4	609	4	1/1/11/20	6/13/91/115	-
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
21	CHL	2	601	2	4/4/19/26	16/33/131/137	-
21	CHL	2	607	-	3/3/15/26	4/12/110/137	-
22	CLA	A	808	-	1/1/12/20	2/19/97/115	-
22	CLA	1	616	1	-	6/11/87/115	-
27	LMG	2	623	-	-	16/31/51/70	0/1/1/1
22	CLA	Z	611	26	1/1/10/20	2/6/82/115	-
25	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	B	803	-	1/1/15/20	15/37/115/115	-
21	CHL	Y	608	-	3/3/15/26	2/8/104/137	-
22	CLA	X	610	19	1/1/9/20	0/2/82/115	-
22	CLA	B	822	-	1/1/10/20	4/10/88/115	-
22	CLA	4	611	-	1/1/10/20	6/10/88/115	-
32	DGD	J	103	-	-	29/55/95/95	0/2/2/2
25	BCR	G	205	-	-	0/29/63/63	0/2/2/2
22	CLA	1	603	-	1/1/13/20	11/25/103/115	-
22	CLA	4	602	4	1/1/14/20	12/31/109/115	-
22	CLA	4	610	4	1/1/12/20	6/24/102/115	-
22	CLA	3	612	3	-	4/11/89/115	-
22	CLA	J	101	14	1/1/10/20	5/10/88/115	-
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
33	NEX	Y	4623	-	-	5/27/83/83	0/3/3/3
22	CLA	2	603	-	1/1/11/20	2/11/89/115	-
22	CLA	X	602	19	1/1/10/20	3/8/86/115	-
21	CHL	X	601	19	3/3/14/26	2/4/100/137	-
22	CLA	Y	604	-	1/1/10/20	7/10/88/115	-
25	BCR	B	843	-	-	5/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
22	CLA	Z	602	19	1/1/12/20	7/22/98/115	-
26	LHG	A	847	22	-	14/34/34/53	-
22	CLA	Y	603	-	1/1/10/20	1/4/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	610	3	1/1/10/20	3/8/86/115	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	A	824	-	1/1/10/20	2/8/86/115	-
22	CLA	G	204	11	1/1/11/20	8/13/91/115	-
22	CLA	F	303	-	1/1/10/20	4/10/88/115	-
22	CLA	X	611	26	1/1/9/20	1/6/80/115	-
25	BCR	A	850	-	-	3/29/63/63	0/2/2/2
22	CLA	2	612	2	1/1/11/20	7/11/89/115	-
27	LMG	4	622	-	-	12/34/54/70	0/1/1/1
22	CLA	A	813	-	1/1/12/20	3/24/102/115	-
22	CLA	A	840	-	1/1/12/20	3/22/100/115	-
22	CLA	2	611	26	1/1/7/20	3/10/70/115	-
22	CLA	L	302	16	1/1/11/20	5/13/91/115	-
22	CLA	A	803	-	1/1/15/20	5/37/115/115	-
22	CLA	B	840	-	1/1/15/20	13/37/115/115	-
25	BCR	A	851	-	-	6/29/63/63	0/2/2/2
21	CHL	4	608	-	3/3/16/26	5/15/113/137	-
22	CLA	B	813	-	1/1/15/20	18/37/115/115	-
23	LUT	X	2621	-	-	5/29/67/67	0/2/2/2
25	BCR	L	306	-	-	6/29/63/63	0/2/2/2
33	NEX	X	2623	-	-	5/27/83/83	0/3/3/3
24	XAT	1	618	-	-	3/31/93/93	0/4/4/4
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
22	CLA	A	835	-	1/1/15/20	19/37/115/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2
25	BCR	L	305	-	-	10/29/63/63	0/2/2/2
26	LHG	Y	4630	22	-	13/49/49/53	-
22	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
22	CLA	Y	610	20	1/1/10/20	3/6/82/115	-
21	CHL	3	608	-	3/3/16/26	7/13/111/137	-
30	SF4	A	853	-	-	-	0/6/5/5
22	CLA	O	2001	-	1/1/9/20	2/4/78/115	-
22	CLA	2	613	2	1/1/15/20	10/37/115/115	-
21	CHL	1	601	1	4/4/18/26	14/25/123/137	-
22	CLA	A	825	-	1/1/13/20	16/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	X	607	-	3/3/15/26	4/10/106/137	-
22	CLA	A	837	5	1/1/11/20	7/13/91/115	-
22	CLA	1	610	1	1/1/14/20	2/29/107/115	-
22	CLA	G	203	-	1/1/10/20	3/10/88/115	-
22	CLA	Z	612	19	1/1/9/20	2/4/80/115	-
22	CLA	Z	613	19	1/1/10/20	1/11/89/115	-
22	CLA	A	831	-	1/1/15/20	12/37/115/115	-
27	LMG	4	623	-	-	11/28/48/70	0/1/1/1
26	LHG	B	851	22	-	19/42/42/53	-
32	DGD	B	850	-	-	22/55/95/95	0/2/2/2
25	BCR	B	845	-	-	6/29/63/63	0/2/2/2
22	CLA	A	819	-	1/1/13/20	9/30/108/115	-
23	LUT	2	619	-	-	2/29/67/67	0/2/2/2
22	CLA	B	812	-	1/1/10/20	4/11/89/115	-
21	CHL	Y	607	-	3/3/15/26	4/8/104/137	-
25	BCR	1	619	-	-	6/29/63/63	0/2/2/2
24	XAT	4	620	-	-	2/31/93/93	0/4/4/4
22	CLA	4	617	-	1/1/12/20	8/19/97/115	-
22	CLA	B	830	-	1/1/10/20	3/11/89/115	-
21	CHL	Y	601	20	4/4/20/26	18/35/131/137	-
23	LUT	Z	7620	-	-	2/29/67/67	0/2/2/2
22	CLA	4	601	4	1/1/11/20	7/15/93/115	-
22	CLA	A	826	-	1/1/15/20	17/37/115/115	-
22	CLA	Z	604	-	1/1/11/20	3/16/92/115	-
22	CLA	F	304	-	1/1/10/20	2/8/86/115	-
22	CLA	3	617	-	1/1/10/20	0/6/84/115	-
21	CHL	Y	605	20	3/3/15/26	2/4/100/137	-
21	CHL	X	606	-	3/3/14/26	0/8/100/137	-
22	CLA	B	815	-	1/1/10/20	1/11/89/115	-
22	CLA	K	206	15	1/1/9/20	0/6/80/115	-
24	XAT	Y	2622	-	-	4/31/93/93	0/4/4/4
22	CLA	A	817	-	1/1/11/20	6/13/91/115	-
22	CLA	X	603	-	1/1/10/20	2/6/84/115	-
22	CLA	A	828	-	1/1/15/20	14/37/115/115	-
21	CHL	4	606	-	3/3/15/26	4/8/106/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	811	-	1/1/13/20	10/25/101/115	-
22	CLA	B	817	-	1/1/13/20	10/30/108/115	-
22	CLA	X	613	19	1/1/8/20	0/0/74/115	-
22	CLA	1	609	1	1/1/10/20	2/8/84/115	-
26	LHG	Z	7630	22	-	13/26/26/53	-
22	CLA	A	832	-	1/1/12/20	8/19/97/115	-
22	CLA	A	854	-	1/1/15/20	16/37/115/115	-
22	CLA	X	614	-	1/1/9/20	5/8/80/115	-
25	BCR	4	621	-	-	10/29/63/63	0/2/2/2
31	LMU	B	849	-	-	11/21/61/61	0/2/2/2
22	CLA	B	832	-	1/1/15/20	9/37/115/115	-
22	CLA	A	816	-	1/1/10/20	3/10/88/115	-
21	CHL	Z	606	-	3/3/14/26	2/4/102/137	-
26	LHG	A	846	-	-	29/53/53/53	-
22	CLA	Y	613	20	1/1/11/20	4/11/87/115	-
29	PQN	A	844	-	-	11/23/43/43	0/2/2/2
24	XAT	Z	4622	-	-	3/31/93/93	0/4/4/4
22	CLA	A	809	5	1/1/15/20	12/37/115/115	-
22	CLA	K	201	15	1/1/8/20	0/2/76/115	-
23	LUT	Y	4620	-	-	7/29/67/67	0/2/2/2
22	CLA	B	824	-	1/1/15/20	12/37/115/115	-
22	CLA	1	604	-	1/1/11/20	10/18/96/115	-
21	CHL	1	607	1	3/3/15/26	2/8/106/137	-
22	CLA	Y	614	-	1/1/10/20	4/6/82/115	-
22	CLA	3	606	3	1/1/10/20	5/8/86/115	-
22	CLA	B	833	-	1/1/11/20	6/13/91/115	-
24	XAT	3	619	-	-	2/31/93/93	0/4/4/4
22	CLA	A	841	-	1/1/15/20	13/37/115/115	-
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
21	CHL	X	605	19	3/3/15/26	5/7/105/137	-
25	BCR	J	102	-	-	7/29/63/63	0/2/2/2
25	BCR	L	301	-	-	4/29/63/63	0/2/2/2
22	CLA	B	841	26	1/1/15/20	14/37/115/115	-
25	BCR	A	856	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	818	-	1/1/14/20	12/31/109/115	-
22	CLA	1	606	-	1/1/9/20	4/8/82/115	-
21	CHL	4	607	-	3/3/15/26	0/10/106/137	-
21	CHL	2	618	2	3/3/15/26	4/12/110/137	-
22	CLA	L	303	-	1/1/14/20	16/31/109/115	-
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
29	PQN	B	842	-	-	9/23/43/43	0/2/2/2
21	CHL	2	606	-	3/3/15/26	0/10/108/137	-
24	XAT	2	620	-	-	3/31/93/93	0/4/4/4
22	CLA	A	812	-	1/1/15/20	14/37/115/115	-
22	CLA	B	835	-	1/1/10/20	4/10/88/115	-
22	CLA	1	613	-	1/1/15/20	12/37/115/115	-
26	LHG	1	620	22	-	23/53/53/53	-
21	CHL	Y	606	-	3/3/15/26	1/4/100/137	-
21	CHL	2	608	-	3/3/17/26	7/21/119/137	-
22	CLA	X	612	19	1/1/8/20	2/2/74/115	-
26	LHG	2	622	22	-	21/41/41/53	-
22	CLA	A	802	-	1/1/15/20	13/37/115/115	-
22	CLA	Y	612	20	1/1/10/20	0/4/80/115	-
31	LMU	A	857	-	-	8/16/56/61	0/2/2/2
22	CLA	3	602	3	1/1/14/20	10/31/109/115	-
23	LUT	1	617	-	-	4/29/67/67	0/2/2/2
30	SF4	C	101	-	-	-	0/6/5/5
22	CLA	B	802	-	1/1/15/20	18/37/115/115	-
22	CLA	A	805	-	1/1/12/20	7/22/100/115	-
22	CLA	B	804	-	1/1/10/20	2/8/86/115	-
22	CLA	B	814	-	1/1/15/20	7/37/115/115	-
22	CLA	N	1001	18	-	5/13/91/115	-
22	CLA	L	304	-	1/1/11/20	3/13/91/115	-
23	LUT	Y	4621	-	-	3/29/67/67	0/2/2/2
22	CLA	2	610	2	1/1/13/20	8/25/103/115	-
22	CLA	N	1002	-	1/1/12/20	9/19/97/115	-
22	CLA	1	611	26	1/1/10/20	1/4/80/115	-
22	CLA	F	301	-	1/1/13/20	11/28/106/115	-
22	CLA	A	810	5	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	823	-	1/1/11/20	4/13/91/115	-
22	CLA	B	829	-	1/1/13/20	10/27/105/115	-
21	CHL	X	608	-	3/3/14/26	1/4/102/137	-
21	CHL	X	609	19	3/3/13/26	0/2/94/137	-
22	CLA	3	603	3	1/1/13/20	8/25/103/115	-
22	CLA	B	807	6	-	4/22/100/115	-
22	CLA	1	612	1	1/1/11/20	3/13/91/115	-
22	CLA	B	827	-	1/1/15/20	20/37/115/115	-
33	NEX	Z	7623	-	-	2/27/83/83	0/3/3/3
22	CLA	1	614	-	1/1/10/20	0/4/80/115	-
22	CLA	1	602	1	1/1/14/20	5/33/111/115	-
23	LUT	1	621	-	-	2/29/67/67	0/2/2/2
30	SF4	C	102	-	-	-	0/6/5/5
22	CLA	A	829	-	1/1/15/20	13/37/115/115	-
22	CLA	B	837	-	1/1/15/20	8/37/115/115	-
22	CLA	B	839	-	1/1/15/20	13/37/115/115	-
23	LUT	4	619	-	-	2/29/67/67	0/2/2/2
21	CHL	Z	608	-	3/3/16/26	7/13/111/137	-
22	CLA	2	602	2	1/1/15/20	13/37/115/115	-
22	CLA	A	822	-	1/1/15/20	13/37/115/115	-
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
22	CLA	B	819	-	1/1/13/20	8/25/103/115	-
23	LUT	Z	7621	-	-	3/29/67/67	0/2/2/2
22	CLA	4	613	-	1/1/13/20	9/28/106/115	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
22	CLA	B	831	-	1/1/10/20	3/11/89/115	-
22	CLA	Z	610	19	1/1/8/20	0/0/74/115	-
22	CLA	A	823	-	1/1/10/20	6/10/88/115	-
22	CLA	Y	602	20	1/1/11/20	7/13/91/115	-
22	CLA	3	615	-	1/1/8/20	0/0/74/115	-
22	CLA	B	834	-	1/1/14/20	8/31/109/115	-
22	CLA	B	825	-	1/1/14/20	9/34/112/115	-
22	CLA	4	604	-	1/1/11/20	5/11/87/115	-
22	CLA	B	806	6	1/1/15/20	12/37/115/115	-
22	CLA	4	614	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	603	4	1/1/11/20	2/13/89/115	-
21	CHL	Z	601	19	3/3/15/26	4/10/108/137	-
21	CHL	Z	609	19	3/3/15/26	5/10/108/137	-
22	CLA	1	608	-	1/1/11/20	4/11/89/115	-
21	CHL	4	618	4	3/3/15/26	2/10/106/137	-
22	CLA	A	843	-	1/1/15/20	16/37/115/115	-
22	CLA	B	809	6	1/1/15/20	16/37/115/115	-
22	CLA	A	820	-	1/1/15/20	12/37/115/115	-
22	CLA	3	613	3	1/1/13/20	8/23/101/115	-
22	CLA	Z	614	-	1/1/11/20	5/11/89/115	-
25	BCR	K	202	-	-	6/29/63/63	0/2/2/2
22	CLA	4	612	4	1/1/10/20	2/8/86/115	-
25	BCR	2	621	-	-	4/29/63/63	0/2/2/2
25	BCR	3	620	-	-	5/29/63/63	0/2/2/2
22	CLA	B	805	-	1/1/15/20	15/37/115/115	-
22	CLA	3	604	-	1/1/11/20	0/9/85/115	-

All (1925) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	607	CHL	C4B-NB	29.20	1.61	1.35
22	2	611	CLA	C1A-NA	12.62	1.40	1.29
21	Z	607	CHL	C1B-NB	12.55	1.46	1.35
29	A	844	PQN	C12-C13	8.56	1.53	1.33
29	B	842	PQN	C12-C13	8.52	1.53	1.33
29	A	844	PQN	O1-C1	7.83	1.39	1.23
29	B	842	PQN	O1-C1	7.73	1.39	1.23
22	4	614	CLA	C4B-NB	7.65	1.42	1.35
22	X	611	CLA	C4B-NB	7.63	1.42	1.35
22	B	829	CLA	C4B-NB	7.60	1.42	1.35
22	X	613	CLA	C4B-NB	7.59	1.42	1.35
22	Y	613	CLA	C4B-NB	7.58	1.42	1.35
22	Z	610	CLA	C4B-NB	7.56	1.42	1.35
22	X	612	CLA	C4B-NB	7.56	1.42	1.35
22	1	612	CLA	C4B-NB	7.54	1.41	1.35
22	3	602	CLA	C4B-NB	7.53	1.41	1.35
22	X	604	CLA	C4B-NB	7.51	1.41	1.35
22	3	612	CLA	C4B-NB	7.51	1.41	1.35
29	A	844	PQN	O4-C4	7.51	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	835	CLA	C4B-NB	7.50	1.41	1.35
22	Z	611	CLA	C4B-NB	7.50	1.41	1.35
22	B	840	CLA	C4B-NB	7.49	1.41	1.35
22	X	602	CLA	C4B-NB	7.45	1.41	1.35
22	Y	603	CLA	C4B-NB	7.44	1.41	1.35
22	Y	612	CLA	C4B-NB	7.44	1.41	1.35
22	Y	604	CLA	C4B-NB	7.44	1.41	1.35
22	X	614	CLA	C4B-NB	7.40	1.41	1.35
22	B	831	CLA	C4B-NB	7.38	1.41	1.35
22	Y	611	CLA	C4B-NB	7.37	1.41	1.35
22	Z	612	CLA	C4B-NB	7.37	1.41	1.35
22	Z	613	CLA	C4B-NB	7.37	1.41	1.35
22	A	837	CLA	C4B-NB	7.36	1.41	1.35
22	Z	602	CLA	C4B-NB	7.36	1.41	1.35
29	B	842	PQN	O4-C4	7.35	1.38	1.23
22	4	611	CLA	C4B-NB	7.32	1.41	1.35
22	2	612	CLA	C4B-NB	7.31	1.41	1.35
22	1	616	CLA	C4B-NB	7.31	1.41	1.35
22	X	610	CLA	C4B-NB	7.30	1.41	1.35
22	Y	610	CLA	C4B-NB	7.30	1.41	1.35
22	1	614	CLA	C4B-NB	7.30	1.41	1.35
22	2	613	CLA	C4B-NB	7.30	1.41	1.35
22	O	2001	CLA	C4B-NB	7.28	1.41	1.35
22	K	206	CLA	C4B-NB	7.28	1.41	1.35
22	Z	603	CLA	C4B-NB	7.28	1.41	1.35
22	G	201	CLA	C4B-NB	7.25	1.41	1.35
22	3	615	CLA	C4B-NB	7.24	1.41	1.35
22	1	604	CLA	C4B-NB	7.24	1.41	1.35
22	1	603	CLA	C4B-NB	7.23	1.41	1.35
22	X	603	CLA	C4B-NB	7.23	1.41	1.35
22	N	1002	CLA	C4B-NB	7.23	1.41	1.35
22	Z	614	CLA	C4B-NB	7.23	1.41	1.35
22	4	612	CLA	C4B-NB	7.22	1.41	1.35
22	Y	602	CLA	C4B-NB	7.20	1.41	1.35
22	A	819	CLA	C4B-NB	7.20	1.41	1.35
22	J	101	CLA	C4B-NB	7.20	1.41	1.35
22	K	201	CLA	C4B-NB	7.18	1.41	1.35
22	A	821	CLA	C4B-NB	7.17	1.41	1.35
22	4	603	CLA	C4B-NB	7.17	1.41	1.35
22	2	611	CLA	C4B-NB	7.14	1.41	1.35
22	1	609	CLA	C4B-NB	7.13	1.41	1.35
22	G	204	CLA	C4B-NB	7.13	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	301	CLA	C4B-NB	7.12	1.41	1.35
22	G	203	CLA	C4B-NB	7.11	1.41	1.35
22	Z	604	CLA	C4B-NB	7.11	1.41	1.35
22	3	607	CLA	C4B-NB	7.10	1.41	1.35
22	3	614	CLA	C4B-NB	7.10	1.41	1.35
22	A	812	CLA	C4B-NB	7.09	1.41	1.35
22	1	602	CLA	C4B-NB	7.09	1.41	1.35
22	B	822	CLA	C4B-NB	7.09	1.41	1.35
22	3	610	CLA	C4B-NB	7.08	1.41	1.35
22	N	1001	CLA	C4B-NB	7.08	1.41	1.35
22	H	201	CLA	C4B-NB	7.06	1.41	1.35
22	O	2002	CLA	C4B-NB	7.05	1.41	1.35
22	A	805	CLA	C4B-NB	7.05	1.41	1.35
22	2	604	CLA	C4B-NB	7.05	1.41	1.35
22	B	820	CLA	C4B-NB	7.05	1.41	1.35
22	1	608	CLA	C4B-NB	7.02	1.41	1.35
22	L	302	CLA	C4B-NB	7.02	1.41	1.35
22	B	838	CLA	C4B-NB	7.01	1.41	1.35
22	4	609	CLA	C4B-NB	7.01	1.41	1.35
22	A	839	CLA	C4B-NB	7.01	1.41	1.35
22	B	811	CLA	C4B-NB	7.00	1.41	1.35
22	Y	614	CLA	C4B-NB	6.98	1.41	1.35
22	A	831	CLA	C4B-NB	6.98	1.41	1.35
22	A	817	CLA	C4B-NB	6.97	1.41	1.35
22	3	609	CLA	C4B-NB	6.95	1.41	1.35
22	F	303	CLA	C4B-NB	6.95	1.41	1.35
22	B	816	CLA	C4B-NB	6.94	1.41	1.35
22	A	840	CLA	C4B-NB	6.93	1.41	1.35
22	A	809	CLA	C4B-NB	6.93	1.41	1.35
22	B	837	CLA	C4B-NB	6.92	1.41	1.35
22	1	613	CLA	C4B-NB	6.92	1.41	1.35
22	3	617	CLA	C4B-NB	6.91	1.41	1.35
22	1	611	CLA	C4B-NB	6.90	1.41	1.35
22	A	813	CLA	C4B-NB	6.90	1.41	1.35
22	F	304	CLA	C4B-NB	6.89	1.41	1.35
22	4	613	CLA	C4B-NB	6.89	1.41	1.35
22	K	204	CLA	C4B-NB	6.89	1.41	1.35
22	A	824	CLA	C4B-NB	6.88	1.41	1.35
22	L	303	CLA	C4B-NB	6.86	1.41	1.35
22	4	601	CLA	C4B-NB	6.86	1.41	1.35
22	3	613	CLA	C4B-NB	6.86	1.41	1.35
22	3	603	CLA	C4B-NB	6.86	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	604	CLA	C4B-NB	6.85	1.41	1.35
22	2	603	CLA	C4B-NB	6.83	1.41	1.35
22	A	820	CLA	C4B-NB	6.82	1.41	1.35
22	A	807	CLA	C4B-NB	6.82	1.41	1.35
22	B	824	CLA	C4B-NB	6.82	1.41	1.35
22	4	604	CLA	C4B-NB	6.81	1.41	1.35
22	A	845	CLA	C4B-NB	6.81	1.41	1.35
22	A	823	CLA	C4B-NB	6.80	1.41	1.35
22	B	810	CLA	C4B-NB	6.79	1.41	1.35
22	A	842	CLA	C4B-NB	6.78	1.41	1.35
22	B	832	CLA	C4B-NB	6.77	1.41	1.35
22	A	808	CLA	C4B-NB	6.76	1.41	1.35
22	A	810	CLA	C4B-NB	6.76	1.41	1.35
22	A	832	CLA	C4B-NB	6.76	1.41	1.35
22	B	826	CLA	C4B-NB	6.76	1.41	1.35
22	B	809	CLA	C4B-NB	6.75	1.41	1.35
22	A	811	CLA	C4B-NB	6.75	1.41	1.35
22	A	804	CLA	C4B-NB	6.73	1.41	1.35
22	1	610	CLA	C4B-NB	6.73	1.41	1.35
22	4	617	CLA	C4B-NB	6.73	1.41	1.35
22	B	834	CLA	C4B-NB	6.73	1.41	1.35
22	1	606	CLA	C4B-NB	6.71	1.41	1.35
22	A	822	CLA	C4B-NB	6.69	1.41	1.35
22	A	825	CLA	C4B-NB	6.67	1.41	1.35
22	B	812	CLA	C4B-NB	6.66	1.41	1.35
22	K	203	CLA	C4B-NB	6.66	1.41	1.35
22	A	843	CLA	C4B-NB	6.65	1.41	1.35
22	4	610	CLA	C4B-NB	6.64	1.41	1.35
22	B	808	CLA	C4B-NB	6.64	1.41	1.35
22	A	854	CLA	C4B-NB	6.64	1.41	1.35
22	2	602	CLA	C4B-NB	6.64	1.41	1.35
22	A	834	CLA	C4B-NB	6.63	1.41	1.35
22	A	818	CLA	C4B-NB	6.62	1.41	1.35
22	L	304	CLA	C4B-NB	6.61	1.41	1.35
22	B	821	CLA	C4B-NB	6.61	1.41	1.35
22	B	841	CLA	C4B-NB	6.60	1.41	1.35
22	B	804	CLA	C4B-NB	6.59	1.41	1.35
22	B	807	CLA	C4B-NB	6.58	1.41	1.35
22	B	833	CLA	C4B-NB	6.57	1.41	1.35
22	A	802	CLA	C4B-NB	6.57	1.41	1.35
22	A	826	CLA	C4B-NB	6.57	1.41	1.35
22	B	839	CLA	C4B-NB	6.57	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	823	CLA	C4B-NB	6.55	1.41	1.35
22	B	819	CLA	C4B-NB	6.54	1.41	1.35
22	B	806	CLA	C4B-NB	6.54	1.41	1.35
22	3	606	CLA	C4B-NB	6.53	1.41	1.35
22	A	816	CLA	C4B-NB	6.53	1.41	1.35
22	B	814	CLA	C4B-NB	6.53	1.41	1.35
22	2	614	CLA	C4B-NB	6.52	1.41	1.35
22	B	817	CLA	C4B-NB	6.52	1.41	1.35
22	A	828	CLA	C4B-NB	6.52	1.41	1.35
22	A	803	CLA	C4B-NB	6.50	1.41	1.35
22	B	830	CLA	C4B-NB	6.49	1.41	1.35
22	A	830	CLA	C4B-NB	6.48	1.41	1.35
22	4	602	CLA	C4B-NB	6.46	1.41	1.35
22	A	836	CLA	C4B-NB	6.46	1.41	1.35
22	A	833	CLA	C4B-NB	6.46	1.41	1.35
22	2	610	CLA	C4B-NB	6.45	1.41	1.35
22	A	815	CLA	C4B-NB	6.45	1.41	1.35
22	B	802	CLA	C4B-NB	6.44	1.41	1.35
22	A	829	CLA	C4B-NB	6.41	1.40	1.35
22	B	805	CLA	C4B-NB	6.38	1.40	1.35
22	A	814	CLA	C4B-NB	6.36	1.40	1.35
22	B	818	CLA	C4B-NB	6.35	1.40	1.35
22	B	803	CLA	C4B-NB	6.34	1.40	1.35
22	B	815	CLA	C4B-NB	6.32	1.40	1.35
22	2	609	CLA	C4B-NB	6.32	1.40	1.35
22	B	827	CLA	C4B-NB	6.27	1.40	1.35
22	A	827	CLA	C4B-NB	6.23	1.40	1.35
22	B	828	CLA	C4B-NB	6.16	1.40	1.35
22	A	841	CLA	C4B-NB	6.16	1.40	1.35
22	A	835	CLA	C4B-NB	6.15	1.40	1.35
22	A	806	CLA	C4B-NB	6.15	1.40	1.35
22	B	836	CLA	C4B-NB	6.13	1.40	1.35
22	B	813	CLA	C4B-NB	6.03	1.40	1.35
22	B	825	CLA	C4B-NB	5.95	1.40	1.35
28	A	801	CL0	C3B-C2B	5.71	1.48	1.40
22	A	838	CLA	C4B-NB	5.56	1.40	1.35
21	X	607	CHL	CHC-C1C	5.40	1.48	1.35
28	A	801	CL0	C3C-C2C	5.37	1.48	1.36
21	Y	605	CHL	C3C-C2C	5.26	1.46	1.36
21	Z	607	CHL	CHC-C1C	5.24	1.48	1.35
28	A	801	CL0	CHC-C1C	5.21	1.48	1.35
21	Y	607	CHL	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	611	CLA	CHB-C4A	5.17	1.38	1.34
21	X	607	CHL	O2D-CGD	5.12	1.45	1.33
21	X	606	CHL	O2D-CGD	5.12	1.45	1.33
21	Y	608	CHL	CHC-C1C	5.11	1.48	1.35
21	4	607	CHL	O2D-CGD	5.09	1.45	1.33
28	A	801	CL0	C1D-ND	5.09	1.44	1.37
21	Y	609	CHL	CHC-C1C	5.08	1.48	1.35
21	X	608	CHL	CHC-C1C	5.08	1.48	1.35
21	2	618	CHL	O2D-CGD	5.06	1.45	1.33
21	Y	606	CHL	C3C-C2C	5.05	1.46	1.36
21	Y	601	CHL	C3D-C4D	-5.05	1.32	1.44
21	3	608	CHL	C3D-C4D	-5.05	1.32	1.44
21	Y	605	CHL	CHC-C1C	5.03	1.47	1.35
21	Z	601	CHL	CHC-C1C	5.03	1.47	1.35
21	X	608	CHL	C3B-C2B	4.98	1.47	1.40
21	2	606	CHL	O2D-CGD	4.97	1.45	1.33
21	2	608	CHL	C3D-C4D	-4.97	1.33	1.44
21	4	608	CHL	CHC-C1C	4.96	1.47	1.35
21	4	607	CHL	CHC-C1C	4.95	1.47	1.35
21	1	607	CHL	C3D-C4D	-4.95	1.33	1.44
21	X	601	CHL	C3D-C4D	-4.94	1.33	1.44
21	X	606	CHL	CHC-C1C	4.94	1.47	1.35
21	1	601	CHL	CHC-C1C	4.93	1.47	1.35
21	2	601	CHL	C3D-C4D	-4.92	1.33	1.44
21	1	601	CHL	C3D-C4D	-4.92	1.33	1.44
21	4	606	CHL	C3D-C4D	-4.91	1.33	1.44
21	Z	606	CHL	C3D-C4D	-4.91	1.33	1.44
21	X	606	CHL	C3D-C4D	-4.89	1.33	1.44
28	A	801	CL0	O2D-CGD	4.88	1.45	1.33
21	4	607	CHL	C3D-C4D	-4.88	1.33	1.44
21	2	607	CHL	O2D-CGD	4.88	1.45	1.33
21	X	609	CHL	C3D-C4D	-4.85	1.33	1.44
21	1	607	CHL	CHC-C1C	4.85	1.47	1.35
21	Y	608	CHL	C2C-C3C	4.85	1.47	1.37
21	X	601	CHL	CHC-C1C	4.85	1.47	1.35
21	Y	608	CHL	C3D-C4D	-4.84	1.33	1.44
21	X	607	CHL	CHD-C1D	4.84	1.47	1.38
21	4	608	CHL	C3D-C4D	-4.83	1.33	1.44
21	Z	608	CHL	CHC-C1C	4.83	1.47	1.35
21	Z	606	CHL	C3A-C2A	-4.83	1.50	1.54
21	X	609	CHL	CHC-C1C	4.81	1.47	1.35
21	Z	601	CHL	C2C-C3C	4.81	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	607	CHL	C3D-C4D	-4.80	1.33	1.44
21	2	606	CHL	CHC-C1C	4.80	1.47	1.35
21	Z	601	CHL	C3D-C4D	-4.78	1.33	1.44
21	Z	605	CHL	C3C-C2C	4.77	1.45	1.36
21	Y	609	CHL	C3B-C2B	4.77	1.47	1.40
21	Z	605	CHL	CHC-C1C	4.77	1.47	1.35
21	Z	609	CHL	C3D-C4D	-4.77	1.33	1.44
21	2	606	CHL	C3D-C4D	-4.76	1.33	1.44
21	2	618	CHL	C3D-C4D	-4.75	1.33	1.44
21	X	605	CHL	CHC-C1C	4.75	1.47	1.35
21	4	618	CHL	C3D-C4D	-4.75	1.33	1.44
21	2	608	CHL	O2D-CGD	4.75	1.44	1.33
21	2	607	CHL	C3D-C4D	-4.74	1.33	1.44
21	X	608	CHL	C3D-C4D	-4.73	1.33	1.44
21	Z	608	CHL	C3D-C4D	-4.73	1.33	1.44
21	2	608	CHL	CHC-C1C	4.71	1.47	1.35
21	Y	601	CHL	CHC-C1C	4.71	1.47	1.35
21	Z	601	CHL	C3B-C2B	4.70	1.46	1.40
21	Z	609	CHL	C2C-C3C	4.70	1.46	1.36
21	Y	605	CHL	C3D-C4D	-4.69	1.33	1.44
21	Y	607	CHL	CHC-C1C	4.69	1.47	1.35
21	4	618	CHL	CHC-C1C	4.68	1.47	1.35
21	2	618	CHL	CHC-C1C	4.68	1.47	1.35
21	Z	605	CHL	C3D-C4D	-4.68	1.33	1.44
21	Y	606	CHL	C3D-C4D	-4.67	1.33	1.44
21	3	608	CHL	O2D-CGD	4.67	1.44	1.33
21	4	606	CHL	CHC-C1C	4.67	1.46	1.35
21	Y	605	CHL	CHD-C1D	4.66	1.47	1.38
21	X	609	CHL	C3C-C2C	4.66	1.46	1.36
21	1	607	CHL	O2D-CGD	4.65	1.45	1.30
21	X	601	CHL	C2C-C3C	4.65	1.46	1.36
21	Z	605	CHL	O2D-CGD	4.64	1.45	1.30
21	Y	605	CHL	O2D-CGD	4.64	1.45	1.30
21	X	607	CHL	C2C-C3C	4.63	1.46	1.37
21	Z	608	CHL	O2D-CGD	4.63	1.45	1.30
21	4	618	CHL	O2D-CGD	4.63	1.45	1.30
21	Z	606	CHL	CHC-C1C	4.63	1.46	1.35
21	Y	608	CHL	O2D-CGD	4.63	1.45	1.30
21	Y	609	CHL	C2C-C3C	4.62	1.46	1.36
21	Y	601	CHL	O2D-CGD	4.62	1.45	1.30
21	Y	606	CHL	CHC-C1C	4.62	1.46	1.35
21	4	606	CHL	O2D-CGD	4.62	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	609	CHL	O2D-CGD	4.61	1.45	1.30
21	Y	606	CHL	O2D-CGD	4.61	1.45	1.30
21	Z	601	CHL	CHD-C1D	4.61	1.47	1.38
22	B	829	CLA	CMB-C2B	-4.60	1.42	1.51
21	Z	607	CHL	O2D-CGD	4.60	1.45	1.30
21	2	601	CHL	CHC-C1C	4.60	1.46	1.35
21	X	608	CHL	C2C-C3C	4.60	1.46	1.36
21	X	605	CHL	C3B-C2B	4.60	1.46	1.40
21	Y	606	CHL	C3A-C2A	-4.59	1.50	1.54
21	2	601	CHL	O2D-CGD	4.59	1.44	1.33
21	Y	609	CHL	C3D-C4D	-4.59	1.33	1.44
21	4	608	CHL	O2D-CGD	4.58	1.44	1.33
21	X	605	CHL	C3C-C2C	4.58	1.46	1.36
21	Z	601	CHL	O2D-CGD	4.58	1.45	1.30
21	2	618	CHL	C3B-C2B	4.57	1.46	1.40
28	A	801	CL0	CHD-C1D	4.57	1.47	1.38
21	1	607	CHL	C3B-C2B	4.57	1.46	1.40
21	Z	607	CHL	C3D-C4D	-4.55	1.33	1.44
21	1	607	CHL	C2C-C3C	4.54	1.46	1.36
21	2	607	CHL	CHC-C1C	4.54	1.46	1.35
21	Y	607	CHL	C3D-C4D	-4.53	1.34	1.44
21	Z	608	CHL	C2C-C3C	4.51	1.46	1.36
21	1	601	CHL	C2C-C3C	4.51	1.46	1.36
21	1	607	CHL	CHD-C1D	4.50	1.47	1.38
21	4	607	CHL	C3C-C2C	4.50	1.46	1.36
21	Z	609	CHL	CHD-C1D	4.49	1.47	1.38
21	X	606	CHL	C2C-C3C	4.49	1.46	1.37
21	X	605	CHL	O2A-CGA	4.49	1.45	1.30
21	3	608	CHL	O2A-CGA	4.48	1.45	1.30
21	Z	609	CHL	CHC-C1C	4.48	1.46	1.35
21	Z	607	CHL	O2A-CGA	4.46	1.45	1.30
21	1	601	CHL	O2D-CGD	4.46	1.45	1.30
21	2	606	CHL	C3B-C2B	4.46	1.46	1.40
29	B	842	PQN	C2-C1	-4.45	1.38	1.48
21	Y	609	CHL	CHD-C1D	4.45	1.47	1.38
21	X	605	CHL	C3D-C4D	-4.44	1.34	1.44
21	4	606	CHL	C2C-C3C	4.44	1.46	1.37
21	X	601	CHL	CHD-C1D	4.43	1.47	1.38
29	A	844	PQN	C2-C1	-4.43	1.38	1.48
21	4	608	CHL	O2A-CGA	4.41	1.45	1.30
21	Z	605	CHL	C3A-C2A	-4.41	1.50	1.54
21	3	608	CHL	CHC-C1C	4.40	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	608	CHL	O2A-CGA	4.39	1.45	1.30
21	1	601	CHL	O2A-CGA	4.37	1.46	1.33
21	Y	606	CHL	CHD-C1D	4.37	1.46	1.38
21	1	601	CHL	CHD-C1D	4.32	1.46	1.38
21	Z	606	CHL	CHD-C1D	4.31	1.46	1.38
21	X	608	CHL	CHD-C1D	4.31	1.46	1.38
21	Y	607	CHL	C3A-C2A	-4.29	1.50	1.54
22	A	831	CLA	CMB-C2B	-4.28	1.42	1.51
21	Y	601	CHL	C3C-C2C	4.28	1.45	1.36
21	Z	601	CHL	CHD-C4C	4.26	1.49	1.39
21	Y	607	CHL	C2C-C3C	4.25	1.45	1.37
21	Y	607	CHL	CHD-C1D	4.24	1.46	1.38
21	X	606	CHL	CHD-C1D	4.24	1.46	1.38
28	A	801	CL0	O2A-CGA	4.24	1.45	1.33
21	X	609	CHL	CHD-C1D	4.24	1.46	1.38
22	3	612	CLA	C1D-ND	4.23	1.43	1.37
21	2	608	CHL	O2A-CGA	4.23	1.45	1.33
21	X	607	CHL	CHD-C4C	4.23	1.48	1.39
21	2	601	CHL	C2C-C3C	4.23	1.45	1.36
21	X	608	CHL	C3A-C2A	-4.21	1.50	1.54
21	X	605	CHL	CHD-C1D	4.21	1.46	1.38
21	Z	606	CHL	C2C-C3C	4.20	1.45	1.36
21	4	606	CHL	CHD-C1D	4.20	1.46	1.38
21	2	618	CHL	C2C-C3C	4.20	1.45	1.36
21	2	601	CHL	O2A-CGA	4.19	1.45	1.33
21	Y	601	CHL	CHD-C1D	4.18	1.46	1.38
21	4	618	CHL	CHD-C1D	4.17	1.46	1.38
21	1	607	CHL	CHD-C4C	4.16	1.48	1.39
21	4	618	CHL	C2C-C3C	4.15	1.45	1.36
21	2	607	CHL	CHD-C1D	4.11	1.46	1.38
21	Y	605	CHL	CHD-C4C	4.11	1.48	1.39
21	2	607	CHL	C2C-C3C	4.11	1.45	1.36
21	4	607	CHL	CHD-C1D	4.10	1.46	1.38
21	Y	601	CHL	O2A-CGA	4.10	1.45	1.33
21	2	606	CHL	CHD-C1D	4.09	1.46	1.38
21	Y	608	CHL	CHD-C1D	4.08	1.46	1.38
22	Z	614	CLA	C1D-ND	4.08	1.42	1.37
21	2	618	CHL	CHD-C1D	4.05	1.46	1.38
21	X	601	CHL	CHD-C4C	4.05	1.48	1.39
21	Z	605	CHL	CHD-C1D	4.05	1.46	1.38
21	Z	609	CHL	C3B-C2B	4.04	1.46	1.40
21	2	608	CHL	C3B-C2B	4.04	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	608	CHL	C2C-C3C	4.01	1.45	1.36
22	Y	612	CLA	C1D-ND	4.01	1.42	1.37
28	A	801	CL0	CHD-C4C	4.01	1.48	1.39
21	2	601	CHL	C3B-C2B	4.01	1.45	1.40
21	Y	601	CHL	CHD-C4C	3.99	1.48	1.39
21	4	608	CHL	C2C-C3C	3.98	1.45	1.36
22	X	613	CLA	C1D-ND	3.98	1.42	1.37
21	X	606	CHL	CHD-C4C	3.98	1.48	1.39
21	4	618	CHL	CHD-C4C	3.96	1.48	1.39
21	Z	608	CHL	CHD-C1D	3.95	1.46	1.38
22	X	610	CLA	C1D-ND	3.95	1.42	1.37
21	Y	606	CHL	CHD-C4C	3.95	1.48	1.39
21	3	608	CHL	C3B-C2B	3.94	1.45	1.40
22	X	603	CLA	C1D-ND	3.94	1.42	1.37
22	Y	614	CLA	C1D-ND	3.93	1.42	1.37
22	Z	611	CLA	C1D-ND	3.93	1.42	1.37
22	B	803	CLA	C4D-ND	-3.93	1.32	1.37
21	Z	608	CHL	C3B-C2B	3.92	1.45	1.40
21	X	601	CHL	C3A-C2A	-3.92	1.50	1.54
21	4	608	CHL	C3B-C2B	3.92	1.45	1.40
21	Z	607	CHL	C2C-C3C	3.91	1.45	1.36
22	3	604	CLA	CAB-C3B	-3.90	1.43	1.51
22	X	614	CLA	C1D-ND	3.89	1.42	1.37
21	Z	609	CHL	CHD-C4C	3.88	1.48	1.39
22	B	836	CLA	C4D-ND	-3.87	1.32	1.37
22	Z	610	CLA	C1D-ND	3.86	1.42	1.37
21	Y	609	CHL	CHD-C4C	3.86	1.48	1.39
22	1	609	CLA	C1D-ND	3.86	1.42	1.37
21	1	601	CHL	C3B-C2B	3.86	1.45	1.40
31	A	857	LMU	O5'-C1'	3.85	1.51	1.41
21	4	607	CHL	CHD-C4C	3.85	1.48	1.39
21	2	607	CHL	C3B-C2B	3.85	1.45	1.40
21	Z	606	CHL	CHD-C4C	3.84	1.48	1.39
28	A	801	CL0	C3D-C2D	3.84	1.49	1.39
21	X	609	CHL	C3A-C2A	-3.83	1.50	1.54
21	1	601	CHL	CHD-C4C	3.83	1.48	1.39
22	B	819	CLA	C4D-ND	-3.81	1.32	1.37
21	X	608	CHL	CHD-C4C	3.81	1.47	1.39
21	X	609	CHL	CHD-C4C	3.81	1.47	1.39
22	Z	612	CLA	C1D-ND	3.80	1.42	1.37
22	1	608	CLA	C1D-ND	3.80	1.42	1.37
21	Z	607	CHL	CHD-C1D	3.80	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	612	CLA	C1D-ND	3.78	1.42	1.37
21	2	601	CHL	CHD-C1D	3.78	1.45	1.38
22	Z	602	CLA	CAB-C3B	-3.76	1.43	1.51
21	Z	606	CHL	C3B-C2B	3.76	1.45	1.40
22	3	607	CLA	C1D-ND	3.76	1.42	1.37
22	B	825	CLA	C4D-ND	-3.76	1.32	1.37
22	Y	613	CLA	C1D-ND	3.76	1.42	1.37
21	2	606	CHL	CHD-C4C	3.75	1.47	1.39
21	X	605	CHL	OBD-CAD	3.75	1.28	1.22
21	X	605	CHL	CHD-C4C	3.75	1.47	1.39
22	K	201	CLA	C1D-ND	3.74	1.42	1.37
22	1	616	CLA	CAB-C3B	-3.74	1.43	1.51
22	A	806	CLA	C4D-ND	-3.74	1.32	1.37
21	2	601	CHL	CHD-C4C	3.74	1.47	1.39
22	X	611	CLA	C1D-ND	3.74	1.42	1.37
22	4	603	CLA	CAB-C3B	-3.74	1.43	1.51
22	3	614	CLA	C1D-ND	3.73	1.42	1.37
22	1	611	CLA	CAB-C3B	-3.73	1.43	1.51
21	Z	607	CHL	CHD-C4C	3.73	1.47	1.39
22	O	2002	CLA	CAB-C3B	-3.73	1.43	1.51
22	1	614	CLA	CAB-C3B	-3.73	1.43	1.51
21	2	618	CHL	CHD-C4C	3.73	1.47	1.39
21	Y	607	CHL	CHD-C4C	3.73	1.47	1.39
21	Y	608	CHL	CHD-C4C	3.72	1.47	1.39
22	A	827	CLA	C4D-ND	-3.72	1.32	1.37
22	4	604	CLA	CAB-C3B	-3.72	1.43	1.51
22	B	809	CLA	CMB-C2B	-3.71	1.43	1.51
21	3	608	CHL	C3C-C2C	3.71	1.44	1.36
22	L	303	CLA	C4D-ND	-3.71	1.32	1.37
22	J	101	CLA	C1D-ND	3.71	1.42	1.37
22	2	609	CLA	C1D-ND	3.70	1.42	1.37
31	A	857	LMU	O5B-C1B	3.70	1.51	1.41
22	Y	610	CLA	C1D-ND	3.70	1.42	1.37
21	Y	605	CHL	OBD-CAD	3.69	1.28	1.22
21	Y	607	CHL	OBD-CAD	3.69	1.28	1.22
22	O	2001	CLA	C1D-ND	3.69	1.42	1.37
31	B	849	LMU	O5B-C1B	3.69	1.51	1.41
22	F	303	CLA	C4D-ND	-3.69	1.32	1.37
22	3	615	CLA	C1D-ND	3.69	1.42	1.37
22	4	613	CLA	C1D-ND	3.68	1.42	1.37
22	1	603	CLA	C1D-ND	3.68	1.42	1.37
22	Z	613	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	606	CHL	OBD-CAD	3.68	1.28	1.22
21	2	607	CHL	CHD-C4C	3.68	1.47	1.39
21	4	618	CHL	OBD-CAD	3.68	1.28	1.22
22	A	819	CLA	C4D-ND	-3.67	1.32	1.37
22	B	823	CLA	C4D-ND	-3.67	1.32	1.37
22	F	303	CLA	C1D-ND	3.67	1.42	1.37
22	N	1001	CLA	C1D-ND	3.67	1.42	1.37
22	Z	604	CLA	CAB-C3B	-3.67	1.44	1.51
22	3	604	CLA	C1D-ND	3.67	1.42	1.37
21	Z	605	CHL	CHD-C4C	3.66	1.47	1.39
22	3	606	CLA	C1D-ND	3.66	1.42	1.37
29	B	842	PQN	C3-C4	-3.66	1.38	1.47
22	Y	614	CLA	CAB-C3B	-3.66	1.44	1.51
22	3	607	CLA	CAB-C3B	-3.66	1.44	1.51
22	Y	611	CLA	C1D-ND	3.65	1.42	1.37
22	2	604	CLA	C1D-ND	3.65	1.42	1.37
22	3	617	CLA	C1D-ND	3.65	1.42	1.37
21	Z	605	CHL	OBD-CAD	3.65	1.28	1.22
22	Y	611	CLA	CAB-C3B	-3.65	1.44	1.51
22	1	602	CLA	C1D-ND	3.64	1.42	1.37
22	B	804	CLA	C1D-ND	3.64	1.42	1.37
21	X	607	CHL	OBD-CAD	3.64	1.28	1.22
22	Y	613	CLA	C4D-ND	-3.63	1.32	1.37
22	B	811	CLA	CAB-C3B	-3.63	1.44	1.51
21	X	606	CHL	OBD-CAD	3.63	1.28	1.22
22	1	604	CLA	C1D-ND	3.62	1.42	1.37
21	Y	609	CHL	OBD-CAD	3.62	1.28	1.22
22	B	806	CLA	C4D-ND	-3.62	1.32	1.37
22	O	2002	CLA	C1D-ND	3.62	1.42	1.37
22	B	818	CLA	C4D-ND	-3.62	1.32	1.37
22	Y	610	CLA	CAB-C3B	-3.62	1.44	1.51
22	B	829	CLA	CMD-C2D	-3.62	1.43	1.50
22	1	606	CLA	C1D-ND	3.62	1.42	1.37
21	Z	601	CHL	OBD-CAD	3.61	1.28	1.22
28	A	801	CL0	OBD-CAD	3.61	1.28	1.22
21	2	606	CHL	C2C-C3C	3.61	1.44	1.37
22	K	203	CLA	C1D-ND	3.61	1.42	1.37
22	B	821	CLA	C4D-ND	-3.60	1.32	1.37
22	A	837	CLA	C1D-ND	3.60	1.42	1.37
22	A	826	CLA	C1D-ND	3.60	1.42	1.37
22	A	835	CLA	C1D-ND	3.60	1.42	1.37
22	B	830	CLA	C4D-ND	-3.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	608	CHL	CHD-C1D	3.60	1.45	1.38
22	A	838	CLA	C4D-ND	-3.59	1.32	1.37
22	Y	612	CLA	CAB-C3B	-3.59	1.44	1.51
22	A	843	CLA	C4D-ND	-3.59	1.32	1.37
22	B	838	CLA	C4D-ND	-3.59	1.32	1.37
22	X	602	CLA	C1D-ND	3.59	1.42	1.37
22	4	601	CLA	C1D-ND	3.59	1.42	1.37
22	Y	603	CLA	C1D-ND	3.59	1.42	1.37
22	1	616	CLA	C1D-ND	3.59	1.42	1.37
22	1	609	CLA	CAB-C3B	-3.58	1.44	1.51
21	4	606	CHL	OBD-CAD	3.58	1.28	1.22
22	Y	613	CLA	CAB-C3B	-3.58	1.44	1.51
22	X	604	CLA	CAB-C3B	-3.58	1.44	1.51
22	X	604	CLA	C1D-ND	3.58	1.42	1.37
22	A	822	CLA	C4D-ND	-3.57	1.32	1.37
22	B	809	CLA	C4D-ND	-3.57	1.32	1.37
22	G	204	CLA	C1D-ND	3.57	1.42	1.37
21	2	618	CHL	OBD-CAD	3.57	1.28	1.22
21	1	607	CHL	OBD-CAD	3.57	1.28	1.22
22	Z	612	CLA	CAB-C3B	-3.56	1.44	1.51
22	B	814	CLA	C4D-ND	-3.56	1.32	1.37
22	Z	603	CLA	CAB-C3B	-3.56	1.44	1.51
21	2	606	CHL	OBD-CAD	3.55	1.28	1.22
22	3	603	CLA	C1D-ND	3.55	1.42	1.37
22	A	825	CLA	C1D-ND	3.55	1.42	1.37
21	4	608	CHL	CHD-C1D	3.55	1.45	1.38
22	1	611	CLA	C1D-ND	3.55	1.42	1.37
21	2	608	CHL	CHD-C1D	3.55	1.45	1.38
22	B	835	CLA	C1D-ND	3.55	1.42	1.37
22	Z	611	CLA	CAB-C3B	-3.55	1.44	1.51
22	1	614	CLA	C1D-ND	3.55	1.42	1.37
22	A	815	CLA	C4D-ND	-3.55	1.32	1.37
21	Z	607	CHL	OBD-CAD	3.55	1.28	1.22
22	A	833	CLA	C1D-ND	3.54	1.42	1.37
22	B	828	CLA	C4D-ND	-3.54	1.32	1.37
22	G	203	CLA	C1D-ND	3.54	1.42	1.37
21	4	606	CHL	C3B-C2B	3.54	1.45	1.40
22	Y	602	CLA	C4D-ND	-3.54	1.32	1.37
22	4	603	CLA	C1D-ND	3.54	1.42	1.37
29	B	842	PQN	C3-C2	3.53	1.41	1.35
22	4	602	CLA	C4D-ND	-3.53	1.32	1.37
21	Z	608	CHL	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	817	CLA	C1D-ND	3.52	1.42	1.37
22	A	839	CLA	C1D-ND	3.52	1.42	1.37
22	1	610	CLA	C1D-ND	3.52	1.42	1.37
22	4	604	CLA	C1D-ND	3.52	1.42	1.37
22	A	803	CLA	C4D-ND	-3.52	1.32	1.37
22	2	611	CLA	CAB-C3B	-3.51	1.44	1.51
22	B	802	CLA	C4D-ND	-3.51	1.32	1.37
22	X	614	CLA	CAB-C3B	-3.51	1.44	1.51
22	B	813	CLA	C4D-ND	-3.50	1.32	1.37
22	A	812	CLA	C4D-ND	-3.50	1.32	1.37
22	B	832	CLA	C4D-ND	-3.50	1.32	1.37
22	A	808	CLA	C4D-ND	-3.50	1.32	1.37
22	A	840	CLA	C1D-ND	3.49	1.42	1.37
22	B	833	CLA	C4D-ND	-3.49	1.32	1.37
22	A	820	CLA	C4D-ND	-3.49	1.32	1.37
21	Z	609	CHL	OBD-CAD	3.49	1.28	1.22
22	2	612	CLA	C1D-ND	3.49	1.42	1.37
22	2	614	CLA	C1D-ND	3.48	1.42	1.37
22	Y	602	CLA	C1D-ND	3.48	1.42	1.37
22	3	613	CLA	C1D-ND	3.48	1.42	1.37
22	4	617	CLA	C1D-ND	3.47	1.42	1.37
22	A	805	CLA	C1D-ND	3.47	1.42	1.37
22	1	612	CLA	C1D-ND	3.47	1.42	1.37
22	2	603	CLA	C1D-ND	3.47	1.42	1.37
22	B	839	CLA	C4D-ND	-3.47	1.32	1.37
22	B	810	CLA	C4D-ND	-3.47	1.32	1.37
21	2	607	CHL	OBD-CAD	3.47	1.28	1.22
22	A	835	CLA	C4D-ND	-3.46	1.32	1.37
22	X	612	CLA	CAB-C3B	-3.46	1.44	1.51
22	Z	602	CLA	C1D-ND	3.46	1.42	1.37
22	A	828	CLA	C1D-ND	3.46	1.42	1.37
22	A	809	CLA	C4D-ND	-3.46	1.32	1.37
22	B	819	CLA	CMB-C2B	-3.45	1.44	1.51
22	3	609	CLA	C1D-ND	3.45	1.42	1.37
22	K	204	CLA	C1D-ND	3.45	1.42	1.37
22	G	201	CLA	C1D-ND	3.45	1.42	1.37
21	X	601	CHL	OBD-CAD	3.45	1.28	1.22
22	B	803	CLA	CMC-C2C	-3.45	1.43	1.50
22	B	818	CLA	C1D-ND	3.45	1.42	1.37
22	B	826	CLA	C4D-ND	-3.44	1.33	1.37
22	A	854	CLA	C4D-ND	-3.44	1.33	1.37
22	F	301	CLA	C4D-ND	-3.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	833	CLA	C4D-ND	-3.44	1.33	1.37
22	2	602	CLA	C4D-ND	-3.44	1.33	1.37
21	3	608	CHL	CHD-C4C	3.43	1.47	1.39
22	A	831	CLA	C4D-ND	-3.43	1.33	1.37
22	A	845	CLA	C1D-ND	3.43	1.42	1.37
21	4	606	CHL	CHD-C4C	3.43	1.47	1.39
22	3	603	CLA	C4D-ND	-3.43	1.33	1.37
22	A	828	CLA	C4D-ND	-3.43	1.33	1.37
22	Z	603	CLA	C1D-ND	3.43	1.42	1.37
22	4	602	CLA	C1D-ND	3.43	1.42	1.37
22	B	820	CLA	C1D-ND	3.43	1.42	1.37
22	L	302	CLA	C4D-ND	-3.42	1.33	1.37
22	B	841	CLA	C4D-ND	-3.42	1.33	1.37
21	1	601	CHL	OBD-CAD	3.42	1.28	1.22
22	A	824	CLA	C4D-ND	-3.41	1.33	1.37
22	Y	604	CLA	C1D-ND	3.41	1.42	1.37
22	A	814	CLA	C4D-ND	-3.41	1.33	1.37
22	A	829	CLA	C4D-ND	-3.41	1.33	1.37
22	B	831	CLA	C4D-ND	-3.41	1.33	1.37
22	A	825	CLA	C4D-ND	-3.41	1.33	1.37
22	4	603	CLA	C4D-ND	-3.41	1.33	1.37
22	2	611	CLA	C1D-ND	3.41	1.42	1.37
22	A	812	CLA	C1D-ND	3.40	1.42	1.37
22	A	830	CLA	C4D-ND	-3.40	1.33	1.37
22	B	808	CLA	C4D-ND	-3.40	1.33	1.37
22	A	839	CLA	C4D-ND	-3.40	1.33	1.37
22	1	613	CLA	C1D-ND	3.40	1.42	1.37
22	3	602	CLA	C1D-ND	3.40	1.42	1.37
22	A	832	CLA	C4D-ND	-3.40	1.33	1.37
21	4	607	CHL	OBD-CAD	3.40	1.28	1.22
22	4	601	CLA	C4D-ND	-3.40	1.33	1.37
22	A	804	CLA	C1D-ND	3.40	1.42	1.37
22	A	802	CLA	C4D-ND	-3.39	1.33	1.37
22	A	841	CLA	C4D-ND	-3.39	1.33	1.37
22	A	816	CLA	C1D-ND	3.39	1.42	1.37
22	3	602	CLA	C4D-ND	-3.39	1.33	1.37
22	A	843	CLA	CMB-C2B	-3.39	1.44	1.51
22	K	206	CLA	C1D-ND	3.39	1.41	1.37
22	A	810	CLA	C4D-ND	-3.38	1.33	1.37
22	4	617	CLA	C4D-ND	-3.38	1.33	1.37
22	2	613	CLA	C1D-ND	3.37	1.41	1.37
22	A	836	CLA	C4D-ND	-3.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	805	CLA	CHC-C1C	3.37	1.43	1.35
22	4	610	CLA	C4D-ND	-3.36	1.33	1.37
22	A	823	CLA	C4D-ND	-3.36	1.33	1.37
22	K	204	CLA	C4D-ND	-3.36	1.33	1.37
22	A	807	CLA	C4D-ND	-3.36	1.33	1.37
22	B	816	CLA	C1D-ND	3.36	1.41	1.37
22	A	815	CLA	C1D-ND	3.36	1.41	1.37
29	A	844	PQN	C3-C4	-3.36	1.38	1.47
22	F	304	CLA	C1D-ND	3.35	1.41	1.37
29	B	842	PQN	C10-C1	-3.35	1.41	1.48
22	A	805	CLA	C4D-ND	-3.35	1.33	1.37
31	B	849	LMU	O5'-C1'	3.35	1.50	1.41
22	4	614	CLA	C1D-ND	3.34	1.41	1.37
22	B	834	CLA	C4D-ND	-3.34	1.33	1.37
21	Z	606	CHL	OBD-CAD	3.34	1.28	1.22
22	L	304	CLA	C1D-ND	3.34	1.41	1.37
22	N	1001	CLA	C4D-ND	-3.34	1.33	1.37
22	B	813	CLA	C1D-ND	3.33	1.41	1.37
22	B	817	CLA	C1D-ND	3.33	1.41	1.37
22	4	611	CLA	C1D-ND	3.33	1.41	1.37
22	A	841	CLA	C1D-ND	3.33	1.41	1.37
22	A	842	CLA	C1D-ND	3.33	1.41	1.37
22	B	805	CLA	C4D-ND	-3.33	1.33	1.37
22	A	829	CLA	C1D-ND	3.32	1.41	1.37
22	4	612	CLA	C1D-ND	3.32	1.41	1.37
22	Z	604	CLA	C1D-ND	3.31	1.41	1.37
22	Z	602	CLA	CHC-C1C	3.31	1.43	1.35
22	Z	602	CLA	C4D-ND	-3.31	1.33	1.37
22	A	813	CLA	C1D-ND	3.30	1.41	1.37
22	A	820	CLA	C1D-ND	3.30	1.41	1.37
21	X	608	CHL	OBD-CAD	3.30	1.28	1.22
22	B	815	CLA	C4D-ND	-3.29	1.33	1.37
22	B	826	CLA	C1D-ND	3.29	1.41	1.37
22	B	812	CLA	C4D-ND	-3.29	1.33	1.37
22	B	815	CLA	C1D-ND	3.29	1.41	1.37
22	B	834	CLA	C1D-ND	3.29	1.41	1.37
22	3	609	CLA	C4D-ND	-3.29	1.33	1.37
22	2	614	CLA	C4D-ND	-3.29	1.33	1.37
22	4	609	CLA	C1D-ND	3.29	1.41	1.37
22	B	804	CLA	CHC-C1C	3.28	1.43	1.35
22	B	810	CLA	C1D-ND	3.28	1.41	1.37
22	3	617	CLA	C4D-ND	-3.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	608	CHL	OBD-CAD	3.28	1.28	1.22
22	B	820	CLA	C4D-ND	-3.28	1.33	1.37
22	A	838	CLA	C1D-ND	3.28	1.41	1.37
22	B	841	CLA	C1D-ND	3.28	1.41	1.37
22	K	201	CLA	C4D-ND	-3.28	1.33	1.37
22	A	820	CLA	CMB-C2B	-3.28	1.44	1.51
22	A	816	CLA	C4D-ND	-3.28	1.33	1.37
22	B	814	CLA	CHC-C1C	3.28	1.43	1.35
22	N	1002	CLA	C1D-ND	3.27	1.41	1.37
22	A	813	CLA	C4D-ND	-3.27	1.33	1.37
22	A	845	CLA	C4D-ND	-3.27	1.33	1.37
22	1	610	CLA	CHC-C1C	3.27	1.43	1.35
22	A	822	CLA	CHC-C1C	3.27	1.43	1.35
21	4	608	CHL	CHD-C4C	3.27	1.46	1.39
22	B	811	CLA	C4D-ND	-3.27	1.33	1.37
22	2	602	CLA	C1D-ND	3.27	1.41	1.37
22	1	613	CLA	C4D-ND	-3.27	1.33	1.37
27	4	623	LMG	C4-C5	3.27	1.59	1.53
21	2	608	CHL	CHD-C4C	3.26	1.46	1.39
22	A	842	CLA	C4D-ND	-3.26	1.33	1.37
22	2	610	CLA	C1D-ND	3.26	1.41	1.37
22	B	831	CLA	C1D-ND	3.26	1.41	1.37
22	B	837	CLA	C4D-ND	-3.25	1.33	1.37
22	B	822	CLA	C4D-ND	-3.25	1.33	1.37
22	A	811	CLA	C4D-ND	-3.25	1.33	1.37
22	F	301	CLA	CMB-C2B	-3.25	1.44	1.51
22	A	814	CLA	C1D-ND	3.24	1.41	1.37
21	Y	605	CHL	C3A-C2A	-3.24	1.51	1.54
22	Z	604	CLA	C4D-ND	-3.23	1.33	1.37
22	4	609	CLA	C4D-ND	-3.23	1.33	1.37
21	Y	601	CHL	OBD-CAD	3.23	1.28	1.22
22	A	834	CLA	C1D-ND	3.22	1.41	1.37
22	B	804	CLA	C4D-ND	-3.22	1.33	1.37
22	3	606	CLA	C4D-ND	-3.22	1.33	1.37
22	Z	610	CLA	CAD-C3D	-3.22	1.45	1.50
22	A	802	CLA	CMD-C2D	-3.22	1.44	1.50
22	A	824	CLA	C1D-ND	3.22	1.41	1.37
22	3	604	CLA	C4D-ND	-3.22	1.33	1.37
22	B	828	CLA	C1D-ND	3.22	1.41	1.37
22	3	610	CLA	C1D-ND	3.22	1.41	1.37
22	A	811	CLA	C1D-ND	3.21	1.41	1.37
22	Y	602	CLA	CHC-C1C	3.21	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	602	CLA	CHC-C1C	3.21	1.43	1.35
22	L	304	CLA	C4D-ND	-3.21	1.33	1.37
22	A	854	CLA	CHC-C1C	3.21	1.43	1.35
22	B	807	CLA	C1D-ND	3.21	1.41	1.37
22	A	834	CLA	C4D-ND	-3.21	1.33	1.37
22	1	608	CLA	C4D-ND	-3.21	1.33	1.37
22	L	302	CLA	C1D-ND	3.21	1.41	1.37
22	A	818	CLA	C4D-ND	-3.21	1.33	1.37
22	A	832	CLA	C1D-ND	3.21	1.41	1.37
22	1	602	CLA	C4D-ND	-3.20	1.33	1.37
22	A	821	CLA	C1D-ND	3.20	1.41	1.37
21	2	608	CHL	OBD-CAD	3.20	1.28	1.22
22	O	2001	CLA	C4D-ND	-3.19	1.33	1.37
22	N	1002	CLA	C4D-ND	-3.19	1.33	1.37
22	A	809	CLA	CHC-C1C	3.19	1.43	1.35
22	B	824	CLA	C4D-ND	-3.19	1.33	1.37
22	B	816	CLA	C4D-ND	-3.19	1.33	1.37
22	3	613	CLA	C4D-ND	-3.19	1.33	1.37
22	A	808	CLA	C1D-ND	3.19	1.41	1.37
22	B	817	CLA	C4D-ND	-3.19	1.33	1.37
22	B	829	CLA	C4D-ND	-3.19	1.33	1.37
21	1	607	CHL	C3A-C2A	-3.19	1.51	1.54
22	A	827	CLA	CHC-C1C	3.18	1.43	1.35
22	B	806	CLA	C1D-ND	3.18	1.41	1.37
22	A	822	CLA	C1D-ND	3.18	1.41	1.37
22	2	603	CLA	C4D-ND	-3.18	1.33	1.37
22	A	819	CLA	CMB-C2B	-3.18	1.45	1.51
22	A	821	CLA	C4D-ND	-3.18	1.33	1.37
22	A	826	CLA	C4D-ND	-3.18	1.33	1.37
22	1	611	CLA	C4D-ND	-3.18	1.33	1.37
22	G	203	CLA	C4D-ND	-3.17	1.33	1.37
22	A	824	CLA	CMB-C2B	-3.17	1.45	1.51
22	A	840	CLA	C4D-ND	-3.17	1.33	1.37
22	B	821	CLA	C1D-ND	3.17	1.41	1.37
22	K	201	CLA	CHC-C1C	3.17	1.43	1.35
22	4	613	CLA	CHC-C1C	3.17	1.43	1.35
22	B	840	CLA	C4D-ND	-3.17	1.33	1.37
29	A	844	PQN	C3-C2	3.17	1.41	1.35
22	B	827	CLA	C4D-ND	-3.17	1.33	1.37
22	X	602	CLA	C4D-ND	-3.16	1.33	1.37
22	X	611	CLA	CHC-C1C	3.16	1.43	1.35
22	2	611	CLA	C4D-ND	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	822	CLA	CMB-C2B	-3.16	1.45	1.51
22	B	807	CLA	C4D-ND	-3.16	1.33	1.37
22	3	609	CLA	CMB-C2B	-3.16	1.45	1.51
22	1	614	CLA	CHC-C1C	3.16	1.43	1.35
22	O	2001	CLA	CHC-C1C	3.16	1.43	1.35
22	B	808	CLA	C1D-ND	3.16	1.41	1.37
22	B	833	CLA	C1D-ND	3.16	1.41	1.37
22	G	201	CLA	C4D-ND	-3.16	1.33	1.37
22	1	606	CLA	C4D-ND	-3.16	1.33	1.37
22	3	610	CLA	CHC-C1C	3.16	1.43	1.35
22	K	203	CLA	C4D-ND	-3.15	1.33	1.37
22	1	616	CLA	CHC-C1C	3.15	1.43	1.35
22	X	613	CLA	CHC-C1C	3.15	1.43	1.35
22	Z	611	CLA	CHC-C1C	3.15	1.43	1.35
22	G	204	CLA	C4D-ND	-3.14	1.33	1.37
22	Y	603	CLA	CHC-C1C	3.14	1.43	1.35
22	3	607	CLA	C4D-ND	-3.14	1.33	1.37
22	B	819	CLA	C1D-ND	3.14	1.41	1.37
26	A	846	LHG	O7-C5	-3.13	1.38	1.46
21	Z	601	CHL	C1D-C2D	3.13	1.51	1.45
21	X	607	CHL	C3D-C2D	3.13	1.47	1.39
22	A	817	CLA	C4D-ND	-3.13	1.33	1.37
22	H	201	CLA	C4D-ND	-3.13	1.33	1.37
22	A	819	CLA	C3B-C2B	-3.13	1.36	1.40
22	H	201	CLA	C1D-ND	3.13	1.41	1.37
22	A	836	CLA	CMB-C2B	-3.13	1.45	1.51
22	1	602	CLA	CHC-C1C	3.13	1.43	1.35
22	L	302	CLA	CMB-C2B	-3.13	1.45	1.51
22	A	803	CLA	C1D-ND	3.13	1.41	1.37
22	A	843	CLA	C1D-ND	3.13	1.41	1.37
22	B	839	CLA	C1D-ND	3.13	1.41	1.37
22	B	837	CLA	C1D-ND	3.12	1.41	1.37
22	1	603	CLA	C4D-ND	-3.12	1.33	1.37
22	B	835	CLA	C4D-ND	-3.12	1.33	1.37
22	F	304	CLA	C4D-ND	-3.12	1.33	1.37
22	4	610	CLA	C1D-ND	3.12	1.41	1.37
22	B	827	CLA	CHC-C1C	3.12	1.43	1.35
22	A	803	CLA	CMB-C2B	-3.12	1.45	1.51
22	B	830	CLA	CMB-C2B	-3.12	1.45	1.51
22	X	610	CLA	CHC-C1C	3.11	1.43	1.35
22	B	812	CLA	C1D-ND	3.11	1.41	1.37
22	2	604	CLA	C4D-ND	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	602	CLA	CHC-C1C	3.11	1.42	1.35
22	B	836	CLA	C1D-ND	3.10	1.41	1.37
22	Z	610	CLA	CHC-C1C	3.10	1.42	1.35
22	3	614	CLA	C4D-ND	-3.10	1.33	1.37
22	4	612	CLA	C4D-ND	-3.10	1.33	1.37
22	B	840	CLA	C1D-ND	3.10	1.41	1.37
22	2	604	CLA	CHC-C1C	3.10	1.42	1.35
22	4	614	CLA	CHC-C1C	3.10	1.42	1.35
22	1	614	CLA	C4D-ND	-3.09	1.33	1.37
22	B	822	CLA	C1D-ND	3.09	1.41	1.37
22	B	811	CLA	C1D-ND	3.09	1.41	1.37
22	1	609	CLA	C4D-ND	-3.09	1.33	1.37
22	1	612	CLA	C4D-ND	-3.09	1.33	1.37
22	A	837	CLA	C4D-ND	-3.09	1.33	1.37
22	B	803	CLA	CHC-C1C	3.09	1.42	1.35
22	3	610	CLA	C4D-ND	-3.09	1.33	1.37
21	Z	608	CHL	OBD-CAD	3.08	1.27	1.22
21	Y	609	CHL	C3D-C2D	3.08	1.47	1.39
22	Y	611	CLA	C4D-ND	-3.08	1.33	1.37
22	A	823	CLA	C1D-ND	3.08	1.41	1.37
22	X	614	CLA	C4D-ND	-3.08	1.33	1.37
22	1	604	CLA	C4D-ND	-3.07	1.33	1.37
22	B	827	CLA	C1D-ND	3.07	1.41	1.37
22	2	611	CLA	CHC-C1C	3.07	1.42	1.35
22	F	301	CLA	C1D-ND	3.07	1.41	1.37
22	X	614	CLA	CHC-C1C	3.07	1.42	1.35
22	2	610	CLA	C4D-ND	-3.07	1.33	1.37
22	A	833	CLA	CHC-C1C	3.07	1.42	1.35
22	B	836	CLA	CHC-C1C	3.07	1.42	1.35
22	Z	612	CLA	CHC-C1C	3.07	1.42	1.35
22	A	819	CLA	CHC-C1C	3.07	1.42	1.35
22	2	609	CLA	C4D-ND	-3.06	1.33	1.37
22	F	303	CLA	CHC-C1C	3.06	1.42	1.35
22	B	814	CLA	C1D-ND	3.06	1.41	1.37
22	3	604	CLA	CHC-C1C	3.06	1.42	1.35
22	K	206	CLA	C4D-ND	-3.05	1.33	1.37
22	A	810	CLA	CHC-C1C	3.05	1.42	1.35
22	Y	604	CLA	CHC-C1C	3.05	1.42	1.35
22	Z	614	CLA	CHC-C1C	3.05	1.42	1.35
22	Z	603	CLA	C4D-ND	-3.05	1.33	1.37
22	G	204	CLA	CHC-C1C	3.05	1.42	1.35
22	X	604	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	304	CLA	CHC-C1C	3.05	1.42	1.35
22	3	617	CLA	CHC-C1C	3.04	1.42	1.35
21	3	608	CHL	OBD-CAD	3.04	1.27	1.22
22	B	805	CLA	C1D-ND	3.04	1.41	1.37
22	X	612	CLA	CHC-C1C	3.04	1.42	1.35
22	K	206	CLA	CHC-C1C	3.04	1.42	1.35
22	A	815	CLA	CHC-C1C	3.03	1.42	1.35
22	B	824	CLA	CHC-C1C	3.03	1.42	1.35
21	Y	605	CHL	C1D-C2D	3.03	1.51	1.45
22	B	825	CLA	CHC-C1C	3.03	1.42	1.35
22	3	615	CLA	CHC-C1C	3.03	1.42	1.35
22	N	1001	CLA	CHC-C1C	3.03	1.42	1.35
21	X	609	CHL	C3D-C2D	3.03	1.47	1.39
22	B	831	CLA	CHC-C1C	3.03	1.42	1.35
22	A	819	CLA	C1D-ND	3.02	1.41	1.37
22	A	808	CLA	CHC-C1C	3.02	1.42	1.35
22	4	611	CLA	C4D-ND	-3.02	1.33	1.37
22	B	802	CLA	CHC-C1C	3.02	1.42	1.35
22	Y	603	CLA	C4D-ND	-3.02	1.33	1.37
22	1	609	CLA	CHC-C1C	3.01	1.42	1.35
22	B	832	CLA	CHC-C1C	3.01	1.42	1.35
21	X	601	CHL	C1D-C2D	3.01	1.51	1.45
22	4	604	CLA	C4D-ND	-3.01	1.33	1.37
22	A	802	CLA	CHC-C1C	3.01	1.42	1.35
22	1	612	CLA	CHC-C1C	3.01	1.42	1.35
22	Y	610	CLA	CHC-C1C	3.01	1.42	1.35
22	1	611	CLA	CHC-C1C	3.01	1.42	1.35
21	Y	605	CHL	C3D-C2D	3.01	1.47	1.39
22	4	612	CLA	CHC-C1C	3.01	1.42	1.35
22	F	304	CLA	CHC-C1C	3.00	1.42	1.35
22	2	609	CLA	CHC-C1C	3.00	1.42	1.35
22	O	2002	CLA	C4D-ND	-3.00	1.33	1.37
22	L	303	CLA	CHC-C1C	3.00	1.42	1.35
29	A	844	PQN	C11-C3	3.00	1.56	1.51
22	B	809	CLA	C1D-ND	2.99	1.41	1.37
22	B	822	CLA	CMB-C2B	-2.99	1.45	1.51
21	Y	609	CHL	C1D-C2D	2.99	1.51	1.45
21	X	605	CHL	C3D-C2D	2.99	1.47	1.39
22	1	608	CLA	CHC-C1C	2.98	1.42	1.35
22	Y	613	CLA	CHC-C1C	2.98	1.42	1.35
21	X	607	CHL	MG-NA	-2.98	1.99	2.06
22	2	613	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	831	CLA	C3B-C2B	-2.98	1.36	1.40
22	A	828	CLA	CHC-C1C	2.98	1.42	1.35
22	X	611	CLA	C4D-ND	-2.97	1.33	1.37
22	B	841	CLA	CHC-C1C	2.97	1.42	1.35
22	Y	612	CLA	C4D-ND	-2.97	1.33	1.37
21	X	607	CHL	C1D-C2D	2.97	1.51	1.45
21	1	601	CHL	C3D-C2D	2.97	1.47	1.39
22	2	602	CLA	CHC-C1C	2.97	1.42	1.35
22	4	604	CLA	CMB-C2B	-2.97	1.45	1.51
22	3	607	CLA	CHC-C1C	2.97	1.42	1.35
22	1	610	CLA	C4D-ND	-2.97	1.33	1.37
22	Y	604	CLA	C4D-ND	-2.97	1.33	1.37
22	A	806	CLA	C1D-ND	2.97	1.41	1.37
22	G	203	CLA	CHC-C1C	2.97	1.42	1.35
22	Y	610	CLA	C4D-ND	-2.97	1.33	1.37
22	B	823	CLA	CHC-C1C	2.96	1.42	1.35
22	X	603	CLA	CHC-C1C	2.96	1.42	1.35
22	2	610	CLA	CHC-C1C	2.96	1.42	1.35
22	A	827	CLA	CMD-C2D	-2.96	1.44	1.50
22	B	812	CLA	CHC-C1C	2.96	1.42	1.35
22	A	829	CLA	CHC-C1C	2.96	1.42	1.35
29	B	842	PQN	C11-C12	2.96	1.54	1.50
22	4	617	CLA	CHC-C1C	2.96	1.42	1.35
22	4	613	CLA	C4D-ND	-2.96	1.33	1.37
22	B	835	CLA	CMB-C2B	-2.96	1.45	1.51
22	3	612	CLA	CHC-C1C	2.96	1.42	1.35
22	B	823	CLA	C1D-ND	2.96	1.41	1.37
22	A	807	CLA	CHC-C1C	2.95	1.42	1.35
22	Y	611	CLA	CHC-C1C	2.95	1.42	1.35
22	A	832	CLA	CHC-C1C	2.95	1.42	1.35
22	A	839	CLA	CMB-C2B	-2.95	1.45	1.51
22	4	611	CLA	CHC-C1C	2.95	1.42	1.35
22	J	101	CLA	CHC-C1C	2.95	1.42	1.35
22	4	614	CLA	C4D-ND	-2.95	1.33	1.37
22	N	1002	CLA	CHC-C1C	2.95	1.42	1.35
22	A	823	CLA	CHC-C1C	2.94	1.42	1.35
21	Z	601	CHL	C3D-C2D	2.94	1.47	1.39
22	Y	614	CLA	CHC-C1C	2.94	1.42	1.35
21	2	601	CHL	OBD-CAD	2.94	1.27	1.22
22	3	602	CLA	CHC-C1C	2.94	1.42	1.35
22	B	817	CLA	CMB-C2B	-2.94	1.45	1.51
22	G	201	CLA	CHC-C1C	2.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	613	CLA	CHC-C1C	2.93	1.42	1.35
27	G	202	LMG	C4-C5	2.93	1.59	1.53
22	B	825	CLA	C1D-ND	2.93	1.41	1.37
22	Y	612	CLA	CHC-C1C	2.93	1.42	1.35
22	3	615	CLA	C4D-ND	-2.93	1.33	1.37
21	X	608	CHL	C3D-C2D	2.93	1.47	1.39
22	Z	604	CLA	CHC-C1C	2.93	1.42	1.35
22	A	842	CLA	CHC-C1C	2.93	1.42	1.35
22	A	845	CLA	CMB-C2B	-2.93	1.45	1.51
22	1	613	CLA	CHC-C1C	2.92	1.42	1.35
22	A	810	CLA	C3B-C2B	-2.92	1.36	1.40
21	Z	609	CHL	C1D-C2D	2.92	1.51	1.45
22	Z	611	CLA	C4D-ND	-2.92	1.33	1.37
22	B	802	CLA	CMD-C2D	-2.92	1.44	1.50
22	Z	603	CLA	CHC-C1C	2.92	1.42	1.35
22	A	830	CLA	CHC-C1C	2.91	1.42	1.35
22	B	839	CLA	CHC-C1C	2.91	1.42	1.35
21	Y	608	CHL	OBD-CAD	2.91	1.27	1.22
22	B	823	CLA	CMC-C2C	-2.90	1.44	1.50
22	X	613	CLA	C4D-ND	-2.90	1.33	1.37
22	O	2002	CLA	CHC-C1C	2.90	1.42	1.35
22	B	825	CLA	CMD-C2D	-2.90	1.44	1.50
22	B	816	CLA	CHC-C1C	2.90	1.42	1.35
22	A	834	CLA	CMB-C2B	-2.90	1.45	1.51
22	1	604	CLA	CHC-C1C	2.90	1.42	1.35
22	A	814	CLA	CHC-C1C	2.89	1.42	1.35
22	2	614	CLA	CHC-C1C	2.89	1.42	1.35
22	B	820	CLA	CHC-C1C	2.89	1.42	1.35
22	B	806	CLA	CHC-C1C	2.89	1.42	1.35
22	2	612	CLA	C4D-ND	-2.89	1.33	1.37
22	A	811	CLA	CHC-C1C	2.89	1.42	1.35
22	B	811	CLA	CHC-C1C	2.89	1.42	1.35
22	Z	604	CLA	CMB-C2B	-2.89	1.45	1.51
22	2	612	CLA	CHC-C1C	2.89	1.42	1.35
22	A	810	CLA	CMB-C2B	-2.88	1.45	1.51
22	A	831	CLA	C1D-ND	2.88	1.41	1.37
22	B	839	CLA	CMB-C2B	-2.88	1.45	1.51
22	X	610	CLA	C4D-ND	-2.88	1.33	1.37
22	B	837	CLA	CMB-C2B	-2.88	1.45	1.51
29	A	844	PQN	C11-C12	2.88	1.54	1.50
22	B	826	CLA	CMC-C2C	-2.87	1.44	1.50
22	Y	604	CLA	CMB-C2B	-2.87	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	836	CLA	C1D-ND	2.87	1.41	1.37
22	B	833	CLA	CHC-C1C	2.87	1.42	1.35
22	A	854	CLA	C1D-ND	2.87	1.41	1.37
22	J	101	CLA	C4D-ND	-2.87	1.33	1.37
22	A	818	CLA	C1D-ND	2.86	1.41	1.37
22	Z	612	CLA	C4D-ND	-2.86	1.33	1.37
22	B	824	CLA	C1D-ND	2.86	1.41	1.37
21	1	607	CHL	C3D-C2D	2.86	1.46	1.39
22	4	603	CLA	CHC-C1C	2.86	1.42	1.35
22	A	807	CLA	C1D-ND	2.86	1.41	1.37
22	B	837	CLA	CHC-C1C	2.86	1.42	1.35
22	1	616	CLA	C4D-ND	-2.86	1.33	1.37
22	A	812	CLA	CHC-C1C	2.86	1.42	1.35
22	B	802	CLA	C1D-ND	2.86	1.41	1.37
22	1	606	CLA	CHC-C1C	2.86	1.42	1.35
22	A	830	CLA	C1D-ND	2.85	1.41	1.37
22	A	821	CLA	CMB-C2B	-2.85	1.45	1.51
22	B	808	CLA	CMB-C2B	-2.85	1.45	1.51
22	3	606	CLA	CHC-C1C	2.85	1.42	1.35
22	A	824	CLA	CHC-C1C	2.85	1.42	1.35
22	3	613	CLA	CHC-C1C	2.85	1.42	1.35
21	Y	606	CHL	C1D-C2D	2.85	1.50	1.45
22	H	201	CLA	CHC-C1C	2.85	1.42	1.35
22	B	822	CLA	CHC-C1C	2.85	1.42	1.35
22	K	204	CLA	CHC-C1C	2.85	1.42	1.35
22	B	828	CLA	CMB-C2B	-2.85	1.45	1.51
22	A	826	CLA	CHC-C1C	2.84	1.42	1.35
22	4	609	CLA	CMB-C2B	-2.84	1.45	1.51
22	X	612	CLA	C4D-ND	-2.84	1.33	1.37
22	4	610	CLA	CHC-C1C	2.84	1.42	1.35
22	Z	610	CLA	C4D-ND	-2.84	1.33	1.37
22	A	839	CLA	CHC-C1C	2.84	1.42	1.35
22	X	603	CLA	C4D-ND	-2.84	1.33	1.37
22	1	603	CLA	CHC-C1C	2.84	1.42	1.35
22	B	835	CLA	CHC-C1C	2.84	1.42	1.35
22	B	819	CLA	C3B-C2B	-2.83	1.36	1.40
22	2	613	CLA	CMB-C2B	-2.83	1.45	1.51
22	A	809	CLA	C1D-ND	2.83	1.41	1.37
22	B	818	CLA	CMB-C2B	-2.83	1.45	1.51
22	L	302	CLA	CHC-C1C	2.83	1.42	1.35
22	B	808	CLA	CMC-C2C	-2.82	1.44	1.50
22	1	603	CLA	C3B-C2B	-2.82	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	201	CLA	CMB-C2B	-2.82	1.45	1.51
21	1	601	CHL	C1D-ND	-2.82	1.34	1.37
22	B	834	CLA	CHC-C1C	2.82	1.42	1.35
22	Y	610	CLA	CMB-C2B	-2.82	1.45	1.51
21	X	606	CHL	C1D-C2D	2.82	1.50	1.45
22	A	804	CLA	C4D-ND	-2.82	1.33	1.37
22	A	806	CLA	CMC-C2C	-2.81	1.44	1.50
22	A	840	CLA	CHC-C1C	2.81	1.42	1.35
22	B	830	CLA	CHC-C1C	2.81	1.42	1.35
21	X	609	CHL	C1D-C2D	2.81	1.50	1.45
22	A	838	CLA	CHC-C1C	2.81	1.42	1.35
22	B	802	CLA	CMC-C2C	-2.81	1.44	1.50
22	X	604	CLA	C4D-ND	-2.80	1.33	1.37
22	A	825	CLA	CHC-C1C	2.80	1.42	1.35
22	A	804	CLA	CHC-C1C	2.80	1.42	1.35
22	B	826	CLA	CHC-C1C	2.80	1.42	1.35
29	B	842	PQN	C10-C5	-2.80	1.36	1.40
22	A	845	CLA	CHC-C1C	2.80	1.42	1.35
22	Y	614	CLA	C4D-ND	-2.80	1.33	1.37
21	Z	606	CHL	C3D-C2D	2.80	1.46	1.39
22	A	820	CLA	CHC-C1C	2.80	1.42	1.35
22	A	816	CLA	CHC-C1C	2.79	1.42	1.35
21	Z	605	CHL	C3D-C2D	2.79	1.46	1.39
22	B	810	CLA	CHC-C1C	2.79	1.42	1.35
22	Z	610	CLA	CMB-C2B	-2.79	1.45	1.51
22	2	613	CLA	CHC-C1C	2.79	1.42	1.35
22	4	610	CLA	CMB-C2B	-2.79	1.45	1.51
22	A	837	CLA	CHC-C1C	2.79	1.42	1.35
22	Z	614	CLA	C4D-ND	-2.79	1.33	1.37
22	A	811	CLA	CMB-C2B	-2.79	1.45	1.51
22	A	842	CLA	CMB-C2B	-2.79	1.45	1.51
22	B	820	CLA	CMB-C2B	-2.78	1.45	1.51
22	K	203	CLA	CHC-C1C	2.78	1.42	1.35
22	A	821	CLA	CHC-C1C	2.78	1.42	1.35
22	A	825	CLA	CMB-C2B	-2.78	1.45	1.51
22	A	832	CLA	CMB-C2B	-2.78	1.45	1.51
22	3	612	CLA	C4D-ND	-2.78	1.33	1.37
22	B	805	CLA	CHC-C1C	2.78	1.42	1.35
22	1	603	CLA	CMB-C2B	-2.78	1.45	1.51
22	Y	611	CLA	CMB-C2B	-2.78	1.45	1.51
22	A	834	CLA	CHC-C1C	2.77	1.42	1.35
21	2	618	CHL	C3D-C2D	2.77	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	618	CHL	C1D-C2D	2.77	1.50	1.45
22	A	817	CLA	CMB-C2B	-2.77	1.45	1.51
21	Z	607	CHL	C3D-C2D	2.77	1.46	1.39
22	3	609	CLA	CHC-C1C	2.77	1.42	1.35
21	4	607	CHL	C3D-C2D	2.77	1.46	1.39
22	B	838	CLA	C1D-ND	2.77	1.41	1.37
22	A	807	CLA	CMB-C2B	-2.77	1.45	1.51
22	B	808	CLA	CHC-C1C	2.76	1.42	1.35
22	Z	613	CLA	C4D-ND	-2.76	1.33	1.37
22	B	817	CLA	CHC-C1C	2.76	1.42	1.35
21	X	609	CHL	MG-NA	-2.76	1.99	2.06
22	A	818	CLA	CHC-C1C	2.75	1.42	1.35
22	4	604	CLA	CHC-C1C	2.75	1.42	1.35
22	A	837	CLA	CMB-C2B	-2.75	1.45	1.51
21	Y	607	CHL	C3D-C2D	2.75	1.46	1.39
22	4	601	CLA	CHC-C1C	2.75	1.42	1.35
21	Z	609	CHL	C3D-C2D	2.75	1.46	1.39
22	B	819	CLA	CHC-C1C	2.75	1.42	1.35
22	3	606	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	829	CLA	C1D-ND	2.75	1.41	1.37
22	B	830	CLA	C1D-ND	2.75	1.41	1.37
22	A	841	CLA	CHC-C1C	2.75	1.42	1.35
21	Y	601	CHL	C1D-C2D	2.75	1.50	1.45
21	2	606	CHL	C3D-C2D	2.74	1.46	1.39
25	B	847	BCR	C17-C18	-2.74	1.32	1.35
22	A	813	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	826	CLA	CMB-C2B	-2.74	1.45	1.51
21	Y	606	CHL	C3D-C2D	2.74	1.46	1.39
22	B	829	CLA	C3B-C2B	-2.74	1.36	1.40
22	B	840	CLA	C3B-C2B	-2.73	1.36	1.40
22	A	810	CLA	CMD-C2D	-2.73	1.45	1.50
22	A	813	CLA	CHC-C1C	2.73	1.42	1.35
22	2	602	CLA	CMB-C2B	-2.73	1.46	1.51
21	X	608	CHL	C1D-C2D	2.73	1.50	1.45
22	4	603	CLA	CMB-C2B	-2.72	1.46	1.51
22	A	810	CLA	C1D-ND	2.72	1.41	1.37
21	4	607	CHL	C1D-C2D	2.72	1.50	1.45
22	B	838	CLA	CHC-C1C	2.72	1.41	1.35
22	A	806	CLA	CHC-C1C	2.72	1.41	1.35
22	A	803	CLA	CHC-C1C	2.72	1.41	1.35
22	B	834	CLA	CMB-C2B	-2.72	1.46	1.51
22	3	603	CLA	CMB-C2B	-2.71	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	810	CLA	CMB-C2B	-2.71	1.46	1.51
22	B	819	CLA	CMC-C2C	-2.71	1.45	1.50
22	B	840	CLA	CMB-C2B	-2.71	1.46	1.51
22	A	819	CLA	C3B-CAB	-2.71	1.42	1.47
22	A	835	CLA	CHC-C1C	2.71	1.41	1.35
33	Z	7623	NEX	C7-C8	-2.71	1.27	1.32
22	A	830	CLA	CMB-C2B	-2.71	1.46	1.51
21	X	605	CHL	C1D-C2D	2.71	1.50	1.45
22	3	604	CLA	CMB-C2B	-2.71	1.46	1.51
22	A	826	CLA	CMB-C2B	-2.70	1.46	1.51
22	2	602	CLA	C3B-C2B	-2.70	1.36	1.40
22	B	823	CLA	CMB-C2B	-2.70	1.46	1.51
22	A	854	CLA	CMB-C2B	-2.70	1.46	1.51
21	Z	605	CHL	C1D-C2D	2.70	1.50	1.45
22	A	830	CLA	CMD-C2D	-2.70	1.45	1.50
22	B	802	CLA	CMB-C2B	-2.69	1.46	1.51
22	A	843	CLA	C3B-C2B	-2.69	1.36	1.40
22	B	813	CLA	CHC-C1C	2.69	1.41	1.35
29	A	844	PQN	C10-C5	-2.69	1.36	1.40
22	A	817	CLA	CHC-C1C	2.69	1.41	1.35
22	N	1002	CLA	CMB-C2B	-2.69	1.46	1.51
22	A	802	CLA	MG-ND	-2.69	2.00	2.05
21	1	607	CHL	MG-NA	-2.68	1.99	2.06
22	3	614	CLA	CHC-C1C	2.68	1.41	1.35
21	2	618	CHL	C1D-C2D	2.68	1.50	1.45
22	A	836	CLA	CHC-C1C	2.68	1.41	1.35
22	B	811	CLA	CMB-C2B	-2.68	1.46	1.51
22	A	845	CLA	CMC-C2C	-2.68	1.45	1.50
22	A	841	CLA	CMB-C2B	-2.68	1.46	1.51
22	F	301	CLA	C3B-C2B	-2.67	1.36	1.40
21	X	606	CHL	C3D-C2D	2.67	1.46	1.39
25	B	847	BCR	C21-C22	-2.67	1.32	1.35
22	B	830	CLA	C3B-C2B	-2.67	1.36	1.40
22	B	833	CLA	C3B-C2B	-2.67	1.36	1.40
21	2	607	CHL	C1D-C2D	2.67	1.50	1.45
22	A	841	CLA	C3B-C2B	-2.66	1.36	1.40
21	Z	607	CHL	C1D-ND	-2.66	1.34	1.37
22	A	820	CLA	CMC-C2C	-2.66	1.45	1.50
22	A	804	CLA	CMB-C2B	-2.66	1.46	1.51
22	3	603	CLA	CHC-C1C	2.66	1.41	1.35
22	G	204	CLA	CMB-C2B	-2.66	1.46	1.51
21	X	609	CHL	OBD-CAD	2.66	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	601	CHL	C3D-C2D	2.66	1.46	1.39
22	2	603	CLA	CMB-C2B	-2.66	1.46	1.51
22	4	601	CLA	CMB-C2B	-2.66	1.46	1.51
22	B	829	CLA	MG-ND	-2.66	2.00	2.05
22	4	610	CLA	CMC-C2C	-2.66	1.45	1.50
22	K	203	CLA	CMB-C2B	-2.66	1.46	1.51
22	B	821	CLA	CHC-C1C	2.66	1.41	1.35
22	A	839	CLA	C3B-C2B	-2.66	1.36	1.40
22	B	817	CLA	C3B-C2B	-2.65	1.36	1.40
21	1	607	CHL	C1D-C2D	2.65	1.50	1.45
22	B	809	CLA	CHC-C1C	2.65	1.41	1.35
22	B	807	CLA	CHC-C1C	2.64	1.41	1.35
21	Z	609	CHL	C4C-C3C	2.64	1.49	1.45
22	B	807	CLA	CMB-C2B	-2.64	1.46	1.51
22	2	604	CLA	CMB-C2B	-2.64	1.46	1.51
22	A	807	CLA	CMD-C2D	-2.64	1.45	1.50
22	1	616	CLA	CMB-C2B	-2.64	1.46	1.51
22	B	828	CLA	CHC-C1C	2.64	1.41	1.35
22	4	603	CLA	CMC-C2C	-2.64	1.45	1.50
22	A	812	CLA	CMB-C2B	-2.64	1.46	1.51
22	A	814	CLA	CMB-C2B	-2.64	1.46	1.51
22	Y	613	CLA	CMB-C2B	-2.64	1.46	1.51
22	B	833	CLA	CMB-C2B	-2.63	1.46	1.51
21	Z	608	CHL	C1D-C2D	2.63	1.50	1.45
21	X	607	CHL	C4B-CHC	2.63	1.48	1.41
21	Y	607	CHL	C1D-C2D	2.63	1.50	1.45
21	2	607	CHL	C3D-C2D	2.63	1.46	1.39
21	Y	601	CHL	C3D-C2D	2.63	1.46	1.39
22	F	301	CLA	CHC-C1C	2.63	1.41	1.35
22	F	303	CLA	CMB-C2B	-2.63	1.46	1.51
22	2	610	CLA	CMB-C2B	-2.63	1.46	1.51
22	G	201	CLA	CMB-C2B	-2.63	1.46	1.51
22	3	602	CLA	CMB-C2B	-2.62	1.46	1.51
22	A	832	CLA	CMD-C2D	-2.62	1.45	1.50
21	4	606	CHL	C1D-C2D	2.62	1.50	1.45
22	2	603	CLA	CHC-C1C	2.62	1.41	1.35
32	J	103	DGD	C4E-C5E	2.62	1.58	1.53
22	B	814	CLA	CMB-C2B	-2.62	1.46	1.51
21	Z	607	CHL	C3B-C2B	2.62	1.50	1.41
21	4	606	CHL	C3D-C2D	2.62	1.46	1.39
21	Y	608	CHL	C3D-C2D	2.61	1.46	1.39
22	3	613	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	843	CLA	CHC-C1C	2.61	1.41	1.35
22	A	827	CLA	CMB-C2B	-2.61	1.46	1.51
22	B	827	CLA	CMB-C2B	-2.61	1.46	1.51
22	B	815	CLA	CHC-C1C	2.61	1.41	1.35
21	Y	608	CHL	C1D-C2D	2.61	1.50	1.45
22	L	303	CLA	CMB-C2B	-2.61	1.46	1.51
22	A	834	CLA	C3B-C2B	-2.60	1.36	1.40
22	B	808	CLA	CMD-C2D	-2.60	1.45	1.50
22	B	824	CLA	CMB-C2B	-2.60	1.46	1.51
28	A	801	CL0	C4D-CHA	2.60	1.47	1.38
22	A	828	CLA	CMB-C2B	-2.60	1.46	1.51
22	2	612	CLA	CMB-C2B	-2.60	1.46	1.51
22	X	604	CLA	CMB-C2B	-2.59	1.46	1.51
22	B	803	CLA	CMD-C2D	-2.59	1.45	1.50
22	A	840	CLA	CMB-C2B	-2.59	1.46	1.51
21	2	606	CHL	C1D-C2D	2.59	1.50	1.45
22	4	617	CLA	CMB-C2B	-2.59	1.46	1.51
22	2	614	CLA	CMB-C2B	-2.59	1.46	1.51
22	A	836	CLA	C3B-C2B	-2.59	1.36	1.40
22	B	812	CLA	CMB-C2B	-2.59	1.46	1.51
22	B	813	CLA	CMB-C2B	-2.59	1.46	1.51
22	A	835	CLA	CMB-C2B	-2.59	1.46	1.51
33	Y	4623	NEX	C7-C8	-2.59	1.27	1.32
21	Z	606	CHL	C1D-C2D	2.59	1.50	1.45
21	Y	601	CHL	MG-NA	-2.59	2.00	2.06
21	Z	608	CHL	C3D-C2D	2.58	1.46	1.39
22	4	610	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	832	CLA	CMB-C2B	-2.58	1.46	1.51
22	B	828	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	825	CLA	CMB-C2B	-2.58	1.46	1.51
22	2	611	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	842	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	815	CLA	CMB-C2B	-2.58	1.46	1.51
22	L	304	CLA	CMD-C2D	-2.58	1.45	1.50
22	3	607	CLA	CMB-C2B	-2.58	1.46	1.51
22	L	303	CLA	C1D-ND	2.58	1.41	1.37
22	4	611	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	806	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	823	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	814	CLA	CMC-C2C	-2.57	1.45	1.50
22	K	204	CLA	CMB-C2B	-2.57	1.46	1.51
22	A	831	CLA	CMD-C2D	-2.57	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	816	CLA	CMB-C2B	-2.57	1.46	1.51
22	Y	602	CLA	CMC-C2C	-2.57	1.45	1.50
22	1	606	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	806	CLA	CMB-C2B	-2.56	1.46	1.51
29	A	844	PQN	C10-C1	-2.56	1.43	1.48
22	3	615	CLA	CMB-C2B	-2.56	1.46	1.51
21	X	601	CHL	C4C-C3C	2.56	1.49	1.45
22	J	101	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	816	CLA	CMC-C2C	-2.56	1.45	1.50
22	A	831	CLA	CHC-C1C	2.56	1.41	1.35
22	X	602	CLA	CMB-C2B	-2.56	1.46	1.51
22	F	304	CLA	CMB-C2B	-2.55	1.46	1.51
22	A	802	CLA	CMB-C2B	-2.55	1.46	1.51
22	1	612	CLA	CMB-C2B	-2.55	1.46	1.51
22	N	1001	CLA	CMB-C2B	-2.55	1.46	1.51
22	3	610	CLA	CMB-C2B	-2.55	1.46	1.51
22	1	614	CLA	CMB-C2B	-2.55	1.46	1.51
22	4	609	CLA	C3B-C2B	-2.55	1.36	1.40
22	4	614	CLA	CMB-C2B	-2.54	1.46	1.51
22	K	201	CLA	CMB-C2B	-2.54	1.46	1.51
22	3	609	CLA	CMC-C2C	-2.54	1.45	1.50
22	Y	602	CLA	CMB-C2B	-2.54	1.46	1.51
21	1	601	CHL	MG-NA	-2.54	2.00	2.06
22	2	613	CLA	CMD-C2D	-2.54	1.45	1.50
22	1	604	CLA	CMB-C2B	-2.54	1.46	1.51
22	B	835	CLA	C3B-C2B	-2.54	1.36	1.40
22	1	609	CLA	CMB-C2B	-2.54	1.46	1.51
22	A	833	CLA	CMB-C2B	-2.53	1.46	1.51
22	A	824	CLA	C3B-C2B	-2.53	1.36	1.40
21	4	608	CHL	C3D-C2D	2.53	1.46	1.39
22	A	812	CLA	CMC-C2C	-2.53	1.45	1.50
22	B	828	CLA	MG-ND	-2.53	2.00	2.05
29	B	842	PQN	C5-C4	-2.53	1.43	1.48
22	B	836	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	838	CLA	CMB-C2B	-2.52	1.46	1.51
21	4	607	CHL	MG-NA	-2.52	2.00	2.06
22	A	809	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	818	CLA	CHC-C1C	2.52	1.41	1.35
22	A	816	CLA	CMC-C2C	-2.52	1.45	1.50
22	1	611	CLA	CMB-C2B	-2.52	1.46	1.51
21	Y	606	CHL	C4C-C3C	2.52	1.49	1.44
22	B	838	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	603	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	807	CLA	C3B-C2B	-2.52	1.36	1.40
22	B	803	CLA	MG-ND	-2.51	2.00	2.05
22	Y	614	CLA	CMB-C2B	-2.51	1.46	1.51
22	2	609	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	836	CLA	MG-ND	-2.51	2.00	2.05
22	4	614	CLA	CMD-C2D	-2.51	1.45	1.50
21	Z	601	CHL	C4B-CHC	2.51	1.48	1.41
22	K	203	CLA	C3B-C2B	-2.50	1.36	1.40
22	X	610	CLA	CMB-C2B	-2.50	1.46	1.51
21	2	601	CHL	C3D-C2D	2.50	1.45	1.39
22	B	815	CLA	CMC-C2C	-2.50	1.45	1.50
22	4	613	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	831	CLA	CMB-C2B	-2.50	1.46	1.51
21	Z	606	CHL	C4C-C3C	2.50	1.49	1.45
22	Z	603	CLA	CMB-C2B	-2.50	1.46	1.51
22	A	802	CLA	CMC-C2C	-2.49	1.45	1.50
22	B	813	CLA	CMC-C2C	-2.49	1.45	1.50
22	B	839	CLA	CMD-C2D	-2.49	1.45	1.50
22	4	612	CLA	CMB-C2B	-2.49	1.46	1.51
21	4	608	CHL	MG-NA	-2.49	2.00	2.06
22	B	803	CLA	CMB-C2B	-2.49	1.46	1.51
21	4	608	CHL	C1D-ND	-2.49	1.34	1.37
22	B	824	CLA	CMD-C2D	-2.49	1.45	1.50
21	4	618	CHL	C3D-C2D	2.49	1.45	1.39
22	4	602	CLA	CMC-C2C	-2.49	1.45	1.50
22	B	833	CLA	C3B-CAB	-2.49	1.42	1.47
22	B	814	CLA	CMD-C2D	-2.48	1.45	1.50
22	1	608	CLA	CMB-C2B	-2.48	1.46	1.51
22	K	206	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	819	CLA	CMD-C2D	-2.48	1.45	1.50
22	A	838	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	829	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	811	CLA	C3B-C2B	-2.48	1.36	1.40
22	B	821	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	831	CLA	MG-ND	-2.48	2.00	2.05
22	A	843	CLA	CMD-C2D	-2.48	1.45	1.50
22	B	807	CLA	CMD-C2D	-2.47	1.45	1.50
21	X	608	CHL	C4B-CHC	2.47	1.47	1.41
22	Z	614	CLA	CMB-C2B	-2.47	1.46	1.51
22	A	808	CLA	CMB-C2B	-2.47	1.46	1.51
22	3	602	CLA	CMC-C2C	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	601	CHL	MG-NA	-2.47	2.00	2.06
22	A	819	CLA	CMC-C2C	-2.47	1.45	1.50
22	3	609	CLA	C3B-C2B	-2.47	1.36	1.40
22	B	836	CLA	CMC-C2C	-2.47	1.45	1.50
22	A	834	CLA	CMD-C2D	-2.47	1.45	1.50
22	Z	602	CLA	CMB-C2B	-2.47	1.46	1.51
21	Y	605	CHL	MG-NA	-2.46	2.00	2.06
22	1	613	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	823	CLA	CMD-C2D	-2.46	1.45	1.50
22	A	831	CLA	CMC-C2C	-2.46	1.45	1.50
21	Y	605	CHL	C4C-C3C	2.46	1.49	1.44
22	B	837	CLA	CMD-C2D	-2.46	1.45	1.50
22	Z	611	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	830	CLA	MG-ND	-2.46	2.00	2.05
22	1	610	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	825	CLA	CMC-C2C	-2.46	1.45	1.50
22	A	836	CLA	CMD-C2D	-2.46	1.45	1.50
22	B	832	CLA	C1D-ND	2.46	1.40	1.37
22	B	817	CLA	C3B-CAB	-2.46	1.42	1.47
22	B	833	CLA	CMC-C2C	-2.45	1.45	1.50
22	3	614	CLA	CMB-C2B	-2.45	1.46	1.51
29	B	842	PQN	C11-C3	2.45	1.55	1.51
21	2	608	CHL	C1D-ND	-2.45	1.34	1.37
22	A	818	CLA	CMD-C2D	-2.45	1.45	1.50
21	Y	608	CHL	C2C-C1C	2.45	1.49	1.44
22	1	602	CLA	CMB-C2B	-2.45	1.46	1.51
22	1	608	CLA	CMD-C2D	-2.45	1.45	1.50
22	L	304	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	818	CLA	CMC-C2C	-2.45	1.45	1.50
22	L	303	CLA	C3B-C2B	-2.45	1.37	1.40
22	A	815	CLA	CMD-C2D	-2.44	1.45	1.50
22	Y	603	CLA	CMB-C2B	-2.44	1.46	1.51
21	X	605	CHL	C4C-C3C	2.44	1.49	1.45
32	B	850	DGD	C3D-C2D	2.44	1.58	1.52
22	B	830	CLA	CMD-C2D	-2.44	1.45	1.50
21	2	601	CHL	C1D-C2D	2.44	1.50	1.45
22	4	609	CLA	CMD-C2D	-2.44	1.45	1.50
22	G	203	CLA	CMB-C2B	-2.44	1.46	1.51
28	A	801	CL0	C4B-CHC	2.44	1.47	1.41
22	A	802	CLA	C3B-C2B	-2.43	1.37	1.40
22	3	609	CLA	CMD-C2D	-2.43	1.45	1.50
22	B	824	CLA	C3B-CAB	-2.43	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	614	CLA	CMD-C2D	-2.43	1.45	1.50
21	X	608	CHL	MG-NA	-2.43	2.00	2.06
22	Y	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	1	606	CLA	CMD-C2D	-2.43	1.45	1.50
22	Z	612	CLA	CMB-C2B	-2.43	1.46	1.51
21	X	607	CHL	C1B-CHB	2.42	1.47	1.41
22	B	833	CLA	CMD-C2D	-2.42	1.45	1.50
22	4	609	CLA	CHC-C1C	2.42	1.41	1.35
22	A	810	CLA	C3B-CAB	-2.42	1.43	1.47
22	3	617	CLA	CMC-C2C	-2.42	1.45	1.50
22	2	614	CLA	CMD-C2D	-2.41	1.45	1.50
22	A	820	CLA	C3B-C2B	-2.41	1.37	1.40
22	B	841	CLA	CMB-C2B	-2.41	1.46	1.51
22	A	826	CLA	CMD-C2D	-2.41	1.45	1.50
22	K	201	CLA	CMC-C2C	-2.41	1.45	1.50
32	B	850	DGD	C4D-C3D	2.41	1.58	1.52
22	O	2002	CLA	CMB-C2B	-2.41	1.46	1.51
21	Y	609	CHL	MG-NA	-2.41	2.00	2.06
21	X	607	CHL	C1D-ND	-2.41	1.34	1.37
22	A	838	CLA	MG-ND	-2.41	2.01	2.05
22	A	802	CLA	C3B-CAB	-2.40	1.43	1.47
22	B	805	CLA	CMB-C2B	-2.40	1.46	1.51
22	A	805	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	802	CLA	C3B-C2B	-2.40	1.37	1.40
22	Z	602	CLA	CMC-C2C	-2.40	1.45	1.50
22	A	803	CLA	C3B-CAB	-2.40	1.43	1.47
22	B	840	CLA	CMC-C2C	-2.40	1.45	1.50
22	3	610	CLA	CMC-C2C	-2.40	1.45	1.50
22	4	602	CLA	CMB-C2B	-2.40	1.46	1.51
22	3	603	CLA	C3B-C2B	-2.40	1.37	1.40
21	2	618	CHL	MG-NA	-2.39	2.00	2.06
21	4	607	CHL	C1D-ND	-2.39	1.34	1.37
22	Z	613	CLA	CMB-C2B	-2.39	1.46	1.51
22	A	829	CLA	CMC-C2C	-2.39	1.45	1.50
21	1	607	CHL	C1D-ND	-2.39	1.34	1.37
22	X	611	CLA	CMB-C2B	-2.39	1.46	1.51
22	A	821	CLA	CMD-C2D	-2.39	1.45	1.50
25	B	843	BCR	C10-C9	-2.39	1.32	1.35
22	A	842	CLA	CMC-C2C	-2.39	1.45	1.50
21	Y	605	CHL	C4B-CHC	2.39	1.47	1.41
22	A	812	CLA	CMD-C2D	-2.39	1.45	1.50
22	X	614	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	617	CLA	CMB-C2B	-2.38	1.46	1.51
22	A	816	CLA	CMD-C2D	-2.38	1.45	1.50
22	X	612	CLA	CMB-C2B	-2.38	1.46	1.51
22	A	803	CLA	C3B-C2B	-2.38	1.37	1.40
22	B	829	CLA	C4B-CHC	-2.38	1.34	1.41
32	J	103	DGD	C4E-C3E	2.37	1.58	1.52
22	4	617	CLA	C3B-C2B	-2.37	1.37	1.40
27	4	622	LMG	O7-C8	-2.37	1.40	1.46
22	F	301	CLA	CMD-C2D	-2.37	1.45	1.50
22	A	830	CLA	C3B-C2B	-2.37	1.37	1.40
22	A	824	CLA	CMD-C2D	-2.37	1.45	1.50
22	4	617	CLA	CMD-C2D	-2.37	1.45	1.50
22	A	822	CLA	C3B-C2B	-2.37	1.37	1.40
22	A	854	CLA	MG-ND	-2.37	2.01	2.05
22	A	830	CLA	C3B-CAB	-2.37	1.43	1.47
22	A	818	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	816	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	840	CLA	CHC-C1C	2.36	1.41	1.35
22	A	827	CLA	MG-ND	-2.36	2.01	2.05
28	A	801	CL0	C1C-C2C	2.36	1.49	1.44
21	1	607	CHL	C1B-CHB	2.36	1.47	1.41
21	2	607	CHL	MG-NA	-2.36	2.00	2.06
22	B	841	CLA	CMD-C2D	-2.36	1.45	1.50
22	2	610	CLA	CMC-C2C	-2.36	1.45	1.50
33	X	2623	NEX	C7-C8	-2.36	1.28	1.32
22	Z	614	CLA	CMD-C2D	-2.36	1.45	1.50
22	A	838	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	804	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	806	CLA	MG-ND	-2.35	2.01	2.05
22	A	841	CLA	C3B-CAB	-2.35	1.43	1.47
22	4	601	CLA	MG-ND	-2.35	2.01	2.05
21	X	607	CHL	C4C-C3C	2.34	1.49	1.44
22	B	829	CLA	CHC-C1C	2.34	1.41	1.35
25	A	849	BCR	C10-C9	-2.34	1.32	1.35
22	A	814	CLA	CMC-C2C	-2.34	1.45	1.50
26	2	622	LHG	O7-C5	-2.34	1.40	1.46
21	4	606	CHL	C1D-ND	-2.34	1.34	1.37
22	O	2001	CLA	CMB-C2B	-2.34	1.46	1.51
22	3	603	CLA	MG-ND	-2.33	2.01	2.05
26	1	620	LHG	O7-C5	-2.33	1.40	1.46
22	A	807	CLA	CMC-C2C	-2.33	1.45	1.50
21	Y	609	CHL	C4B-CHC	2.33	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	815	CLA	CMC-C2C	-2.33	1.45	1.50
22	B	828	CLA	C3B-C2B	-2.33	1.37	1.40
22	4	602	CLA	CMD-C2D	-2.33	1.45	1.50
22	A	815	CLA	CMB-C2B	-2.33	1.46	1.51
21	3	608	CHL	C3D-C2D	2.32	1.45	1.39
22	B	823	CLA	CMD-C2D	-2.32	1.45	1.50
21	3	608	CHL	MG-NA	-2.32	2.00	2.06
22	K	201	CLA	C3B-CAB	-2.32	1.43	1.47
28	A	801	CL0	C4C-C3C	2.32	1.49	1.45
22	L	303	CLA	C3B-CAB	-2.32	1.43	1.47
22	A	825	CLA	CMD-C2D	-2.32	1.45	1.50
28	A	801	CL0	C3D-C4D	-2.32	1.38	1.44
21	1	607	CHL	C4B-CHC	2.32	1.47	1.41
22	K	204	CLA	CMD-C2D	-2.32	1.45	1.50
22	B	829	CLA	CMC-C2C	-2.31	1.45	1.50
22	B	831	CLA	CMC-C2C	-2.31	1.45	1.50
22	A	825	CLA	C3B-C2B	-2.31	1.37	1.40
22	L	303	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	828	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	830	CLA	MG-ND	-2.31	2.01	2.05
22	B	827	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	854	CLA	CMC-C2C	-2.30	1.45	1.50
22	B	827	CLA	CMD-C2D	-2.30	1.45	1.50
22	A	803	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	840	CLA	CMD-C2D	-2.30	1.45	1.50
21	X	609	CHL	C4B-CHC	2.30	1.47	1.41
21	2	606	CHL	C4B-CHC	2.30	1.47	1.41
21	Y	605	CHL	C1B-CHB	2.30	1.47	1.41
22	Z	603	CLA	CMD-C2D	-2.30	1.45	1.50
22	B	817	CLA	CMD-C2D	-2.30	1.45	1.50
22	A	839	CLA	C3B-CAB	-2.30	1.43	1.47
22	A	802	CLA	CAC-C3C	-2.30	1.45	1.51
22	B	840	CLA	CMD-C2D	-2.30	1.45	1.50
21	2	608	CHL	C3D-C2D	2.30	1.45	1.39
22	A	803	CLA	CMD-C2D	-2.30	1.45	1.50
22	A	807	CLA	MG-ND	-2.30	2.01	2.05
22	B	809	CLA	C3B-C2B	-2.29	1.37	1.40
22	2	602	CLA	CMC-C2C	-2.29	1.45	1.50
22	3	613	CLA	C3B-C2B	-2.29	1.37	1.40
21	1	601	CHL	C1B-CHB	2.29	1.47	1.41
21	3	608	CHL	C1D-C2D	2.29	1.49	1.45
22	4	601	CLA	C3B-C2B	-2.29	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	622	LMG	C7-C8	2.29	1.57	1.50
22	A	817	CLA	CMD-C2D	-2.29	1.46	1.50
22	B	823	CLA	MG-ND	-2.29	2.01	2.05
21	2	601	CHL	C1D-ND	-2.28	1.35	1.37
22	A	825	CLA	C3B-CAB	-2.28	1.43	1.47
22	A	835	CLA	C3B-C2B	-2.28	1.37	1.40
21	4	607	CHL	C4B-CHC	2.28	1.47	1.41
22	A	843	CLA	MG-ND	-2.28	2.01	2.05
24	2	620	XAT	O24-C25	-2.28	1.42	1.46
22	B	811	CLA	CMD-C2D	-2.28	1.46	1.50
22	Y	603	CLA	CMD-C2D	-2.28	1.46	1.50
22	4	612	CLA	CMC-C2C	-2.28	1.46	1.50
22	4	613	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	813	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	804	CLA	CMD-C2D	-2.28	1.46	1.50
25	B	847	BCR	C10-C9	-2.28	1.32	1.35
22	A	809	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	813	CLA	CMD-C2D	-2.28	1.46	1.50
21	2	606	CHL	C1D-ND	-2.28	1.35	1.37
22	A	803	CLA	MG-ND	-2.28	2.01	2.05
22	N	1002	CLA	CMD-C2D	-2.28	1.46	1.50
21	X	609	CHL	C1B-CHB	2.27	1.47	1.41
22	A	845	CLA	C3B-C2B	-2.27	1.37	1.40
22	G	204	CLA	C3B-C2B	-2.27	1.37	1.40
22	F	304	CLA	C3B-C2B	-2.27	1.37	1.40
22	B	820	CLA	C3B-C2B	-2.27	1.37	1.40
22	A	832	CLA	CMC-C2C	-2.27	1.46	1.50
22	B	826	CLA	CMD-C2D	-2.27	1.46	1.50
22	2	612	CLA	CMC-C2C	-2.27	1.46	1.50
21	X	606	CHL	C2C-C1C	2.27	1.49	1.44
22	A	841	CLA	CMD-C2D	-2.27	1.46	1.50
22	3	612	CLA	CMB-C2B	-2.27	1.46	1.51
22	B	833	CLA	MG-ND	-2.27	2.01	2.05
22	1	610	CLA	CMC-C2C	-2.27	1.46	1.50
21	Y	608	CHL	MG-NA	-2.26	2.00	2.06
22	A	813	CLA	CMC-C2C	-2.26	1.46	1.50
22	A	829	CLA	CMD-C2D	-2.26	1.46	1.50
22	2	603	CLA	C3B-C2B	-2.26	1.37	1.40
22	B	809	CLA	MG-ND	-2.26	2.01	2.05
21	1	601	CHL	C1D-C2D	2.26	1.49	1.45
22	B	818	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	831	CLA	C3B-CAB	-2.26	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	607	CHL	C4C-C3C	2.26	1.48	1.45
21	4	618	CHL	C4C-C3C	2.26	1.48	1.45
26	B	851	LHG	O7-C5	-2.26	1.40	1.46
21	Z	601	CHL	C4C-C3C	2.26	1.48	1.45
22	A	820	CLA	CMD-C2D	-2.26	1.46	1.50
22	2	602	CLA	CMD-C2D	-2.26	1.46	1.50
22	2	610	CLA	CMD-C2D	-2.25	1.46	1.50
22	X	602	CLA	CMD-C2D	-2.25	1.46	1.50
22	B	815	CLA	CMD-C2D	-2.25	1.46	1.50
22	2	602	CLA	C3B-CAB	-2.25	1.43	1.47
22	4	617	CLA	C3B-CAB	-2.25	1.43	1.47
22	A	806	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	810	CLA	MG-ND	-2.25	2.01	2.05
22	A	826	CLA	CMC-C2C	-2.25	1.46	1.50
22	A	839	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	804	CLA	C3B-C2B	-2.25	1.37	1.40
22	A	833	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	825	CLA	MG-ND	-2.25	2.01	2.05
21	X	608	CHL	C2C-C1C	2.25	1.49	1.44
22	B	812	CLA	CMC-C2C	-2.25	1.46	1.50
22	A	843	CLA	CMC-C2C	-2.25	1.46	1.50
22	O	2002	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	808	CLA	CMD-C2D	-2.24	1.46	1.50
22	4	617	CLA	MG-ND	-2.24	2.01	2.05
22	A	828	CLA	CMC-C2C	-2.24	1.46	1.50
22	F	304	CLA	CMC-C2C	-2.24	1.46	1.50
21	3	608	CHL	C1D-ND	-2.24	1.35	1.37
22	G	203	CLA	CMD-C2D	-2.24	1.46	1.50
21	2	601	CHL	MG-NA	-2.24	2.00	2.06
22	B	810	CLA	CMD-C2D	-2.24	1.46	1.50
21	X	601	CHL	MG-NA	-2.24	2.01	2.06
22	1	610	CLA	CMD-C2D	-2.24	1.46	1.50
22	B	819	CLA	C3B-CAB	-2.23	1.43	1.47
22	A	804	CLA	CMD-C2D	-2.23	1.46	1.50
22	F	301	CLA	C3B-CAB	-2.23	1.43	1.47
22	X	613	CLA	CMB-C2B	-2.23	1.47	1.51
22	A	833	CLA	CMD-C2D	-2.23	1.46	1.50
22	L	304	CLA	CMC-C2C	-2.23	1.46	1.50
22	3	609	CLA	MG-ND	-2.23	2.01	2.05
32	B	850	DGD	O5D-C6D	-2.23	1.39	1.43
22	A	820	CLA	MG-ND	-2.23	2.01	2.05
22	1	604	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	806	CLA	CMD-C2D	-2.23	1.46	1.50
22	3	603	CLA	CMD-C2D	-2.23	1.46	1.50
21	Y	608	CHL	C4B-CHC	2.22	1.47	1.41
22	B	806	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	824	CLA	CMC-C2C	-2.22	1.46	1.50
21	2	618	CHL	C1D-ND	-2.22	1.35	1.37
22	2	613	CLA	MG-ND	-2.22	2.01	2.05
22	B	805	CLA	CMD-C2D	-2.22	1.46	1.50
22	3	606	CLA	CMD-C2D	-2.22	1.46	1.50
22	A	822	CLA	CMC-C2C	-2.22	1.46	1.50
22	4	609	CLA	MG-ND	-2.22	2.01	2.05
22	B	836	CLA	CMD-C2D	-2.22	1.46	1.50
22	F	303	CLA	CMD-C2D	-2.22	1.46	1.50
24	1	618	XAT	O4-C5	-2.22	1.43	1.46
21	X	601	CHL	C1B-CHB	2.22	1.47	1.41
22	A	805	CLA	CMC-C2C	-2.22	1.46	1.50
21	Y	607	CHL	C4C-C3C	2.21	1.48	1.44
21	X	608	CHL	C1D-ND	-2.21	1.35	1.37
22	A	845	CLA	CMD-C2D	-2.21	1.46	1.50
22	Y	613	CLA	CMD-C2D	-2.21	1.46	1.50
21	4	607	CHL	C4C-C3C	2.21	1.48	1.45
22	3	613	CLA	CMD-C2D	-2.21	1.46	1.50
21	Z	605	CHL	C4B-CHC	2.21	1.47	1.41
22	B	816	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	836	CLA	C3B-CAB	-2.21	1.43	1.47
22	A	820	CLA	C3B-CAB	-2.21	1.43	1.47
22	B	812	CLA	CMD-C2D	-2.21	1.46	1.50
22	J	101	CLA	CMD-C2D	-2.21	1.46	1.50
22	2	604	CLA	CMC-C2C	-2.21	1.46	1.50
22	A	854	CLA	CMD-C2D	-2.21	1.46	1.50
21	2	618	CHL	C4B-CHC	2.21	1.47	1.41
22	A	827	CLA	C1D-ND	2.21	1.40	1.37
22	B	820	CLA	CMD-C2D	-2.21	1.46	1.50
21	4	607	CHL	C1B-CHB	2.21	1.47	1.41
22	B	830	CLA	C3B-CAB	-2.21	1.43	1.47
22	B	824	CLA	C3B-C2B	-2.20	1.37	1.40
22	F	304	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	807	CLA	C3B-CAB	-2.20	1.43	1.47
24	4	620	XAT	O4-C5	-2.20	1.43	1.46
21	Z	601	CHL	C1B-CHB	2.20	1.47	1.41
22	Y	602	CLA	CMD-C2D	-2.20	1.46	1.50
22	4	601	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	606	CHL	C4B-CHC	2.20	1.47	1.41
22	A	806	CLA	MG-ND	-2.20	2.01	2.05
22	B	815	CLA	C4B-CHC	-2.20	1.34	1.41
22	B	819	CLA	MG-ND	-2.20	2.01	2.05
21	2	608	CHL	C2C-C1C	2.20	1.49	1.44
22	L	303	CLA	CMC-C2C	-2.20	1.46	1.50
21	4	618	CHL	MG-NA	-2.20	2.01	2.06
22	2	604	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	802	CLA	MG-ND	-2.20	2.01	2.05
22	B	841	CLA	MG-ND	-2.20	2.01	2.05
22	3	602	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	831	CLA	CMD-C2D	-2.19	1.46	1.50
22	A	805	CLA	C3B-CAB	-2.19	1.43	1.47
21	1	601	CHL	C4B-CHC	2.19	1.47	1.41
27	2	623	LMG	C4-C5	2.19	1.57	1.53
21	2	606	CHL	MG-NA	-2.19	2.01	2.06
22	1	603	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	844	PQN	C5-C4	-2.19	1.44	1.48
22	2	603	CLA	MG-ND	-2.19	2.01	2.05
22	A	807	CLA	C3B-C2B	-2.19	1.37	1.40
21	Y	606	CHL	C4B-CHC	2.19	1.47	1.41
21	4	608	CHL	C2C-C1C	2.19	1.49	1.44
21	Z	605	CHL	MG-NA	-2.19	2.01	2.06
22	K	203	CLA	CMD-C2D	-2.19	1.46	1.50
22	L	302	CLA	CMD-C2D	-2.19	1.46	1.50
22	3	603	CLA	C4B-CHC	-2.19	1.34	1.41
31	A	857	LMU	O5'-C5'	2.18	1.49	1.44
22	A	836	CLA	MG-ND	-2.18	2.01	2.05
22	B	813	CLA	C3B-C2B	-2.18	1.37	1.40
22	A	821	CLA	C3B-C2B	-2.18	1.37	1.40
22	L	302	CLA	C3B-C2B	-2.18	1.37	1.40
21	Y	609	CHL	C2C-C1C	2.18	1.49	1.44
22	B	810	CLA	CMC-C2C	-2.18	1.46	1.50
22	2	614	CLA	C3B-C2B	-2.18	1.37	1.40
22	A	832	CLA	C3B-CAB	-2.18	1.43	1.47
22	3	606	CLA	CMC-C2C	-2.18	1.46	1.50
22	Z	612	CLA	CMD-C2D	-2.18	1.46	1.50
28	A	801	CL0	C1B-CHB	2.18	1.47	1.41
22	A	810	CLA	CMC-C2C	-2.18	1.46	1.50
22	B	817	CLA	CMC-C2C	-2.18	1.46	1.50
22	B	814	CLA	MG-ND	-2.18	2.01	2.05
22	L	304	CLA	MG-ND	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	608	CHL	C4B-CHC	2.18	1.47	1.41
22	B	838	CLA	MG-ND	-2.18	2.01	2.05
22	G	204	CLA	C3B-CAB	-2.18	1.43	1.47
22	4	603	CLA	MG-ND	-2.17	2.01	2.05
22	4	603	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	811	CLA	CMC-C2C	-2.17	1.46	1.50
22	3	606	CLA	MG-ND	-2.17	2.01	2.05
22	Y	602	CLA	C3B-C2B	-2.17	1.37	1.40
22	A	822	CLA	CMD-C2D	-2.17	1.46	1.50
21	Z	609	CHL	MG-NA	-2.17	2.01	2.06
22	A	809	CLA	C3B-CAB	-2.17	1.43	1.47
21	X	601	CHL	C4B-CHC	2.17	1.47	1.41
22	A	819	CLA	MG-ND	-2.17	2.01	2.05
22	B	830	CLA	CMC-C2C	-2.17	1.46	1.50
22	B	832	CLA	CMC-C2C	-2.17	1.46	1.50
21	X	605	CHL	C4B-CHC	2.17	1.47	1.41
22	4	617	CLA	CMC-C2C	-2.17	1.46	1.50
22	A	804	CLA	CMC-C2C	-2.17	1.46	1.50
22	A	835	CLA	CMD-C2D	-2.17	1.46	1.50
22	K	201	CLA	CMD-C2D	-2.17	1.46	1.50
22	A	822	CLA	C3B-CAB	-2.17	1.43	1.47
22	3	617	CLA	CMD-C2D	-2.17	1.46	1.50
22	A	830	CLA	CMC-C2C	-2.17	1.46	1.50
21	X	606	CHL	MG-NA	-2.16	2.01	2.06
22	2	611	CLA	C1A-CHA	-2.16	1.36	1.40
22	N	1001	CLA	CMD-C2D	-2.16	1.46	1.50
22	3	602	CLA	C3B-C2B	-2.16	1.37	1.40
22	A	815	CLA	MG-ND	-2.16	2.01	2.05
21	Z	608	CHL	MG-NA	-2.16	2.01	2.06
22	1	616	CLA	CMD-C2D	-2.16	1.46	1.50
21	Z	606	CHL	C1D-ND	-2.16	1.35	1.37
22	2	609	CLA	CMD-C2D	-2.16	1.46	1.50
22	1	616	CLA	CMC-C2C	-2.16	1.46	1.50
22	A	809	CLA	MG-ND	-2.16	2.01	2.05
22	2	612	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	822	CLA	CMD-C2D	-2.16	1.46	1.50
21	Z	606	CHL	MG-NA	-2.16	2.01	2.06
22	4	601	CLA	CMD-C2D	-2.16	1.46	1.50
22	H	201	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	813	CLA	MG-ND	-2.16	2.01	2.05
22	3	615	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	841	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	C3B-C2B	-2.15	1.37	1.40
21	Y	601	CHL	C1D-ND	-2.15	1.35	1.37
22	2	611	CLA	CMC-C2C	-2.15	1.46	1.50
22	B	805	CLA	CMC-C2C	-2.15	1.46	1.50
22	B	802	CLA	C3B-CAB	-2.15	1.43	1.47
22	A	827	CLA	C3B-C2B	-2.15	1.37	1.40
21	Y	609	CHL	C1B-CHB	2.15	1.47	1.41
22	B	808	CLA	C3B-C2B	-2.15	1.37	1.40
22	B	804	CLA	CMC-C2C	-2.15	1.46	1.50
27	2	623	LMG	C1-C2	2.15	1.58	1.52
21	X	606	CHL	C4B-CHC	2.15	1.47	1.41
22	B	818	CLA	C4B-CHC	-2.15	1.35	1.41
22	A	808	CLA	CMC-C2C	-2.15	1.46	1.50
22	B	835	CLA	CMD-C2D	-2.15	1.46	1.50
22	N	1001	CLA	CMC-C2C	-2.15	1.46	1.50
22	Z	604	CLA	CMC-C2C	-2.15	1.46	1.50
22	A	826	CLA	MG-ND	-2.14	2.01	2.05
22	A	811	CLA	C3B-CAB	-2.14	1.43	1.47
22	A	837	CLA	CMD-C2D	-2.14	1.46	1.50
21	X	609	CHL	C1D-ND	-2.14	1.35	1.37
22	3	604	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	822	CLA	MG-ND	-2.14	2.01	2.05
22	1	613	CLA	CMD-C2D	-2.14	1.46	1.50
22	3	607	CLA	CMD-C2D	-2.14	1.46	1.50
22	2	603	CLA	C3B-CAB	-2.14	1.43	1.47
22	B	838	CLA	CMC-C2C	-2.14	1.46	1.50
22	G	203	CLA	CMC-C2C	-2.14	1.46	1.50
22	Y	604	CLA	CMD-C2D	-2.14	1.46	1.50
21	Z	607	CHL	C1D-C2D	2.14	1.49	1.45
22	A	821	CLA	MG-ND	-2.14	2.01	2.05
22	B	839	CLA	CMC-C2C	-2.14	1.46	1.50
22	G	201	CLA	C3B-C2B	-2.14	1.37	1.40
25	A	849	BCR	C1-C6	-2.14	1.50	1.53
21	4	608	CHL	C1D-C2D	2.13	1.49	1.45
22	B	807	CLA	CMC-C2C	-2.13	1.46	1.50
22	Y	614	CLA	CMD-C2D	-2.13	1.46	1.50
22	3	610	CLA	CMD-C2D	-2.13	1.46	1.50
22	1	609	CLA	CMC-C2C	-2.13	1.46	1.50
22	1	602	CLA	CMD-C2D	-2.13	1.46	1.50
22	A	811	CLA	CMD-C2D	-2.13	1.46	1.50
22	K	204	CLA	CMC-C2C	-2.13	1.46	1.50
22	L	302	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	825	CLA	CMC-C2C	-2.13	1.46	1.50
25	A	850	BCR	C10-C9	-2.13	1.33	1.35
21	2	601	CHL	C4B-CHC	2.13	1.46	1.41
22	A	809	CLA	CMC-C2C	-2.13	1.46	1.50
22	G	204	CLA	CMC-C2C	-2.13	1.46	1.50
22	B	824	CLA	MG-ND	-2.13	2.01	2.05
22	B	834	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	818	CLA	C3B-C2B	-2.13	1.37	1.40
32	B	850	DGD	O2G-C2G	-2.13	1.41	1.46
22	A	806	CLA	CMA-C3A	-2.13	1.48	1.53
22	3	614	CLA	CMD-C2D	-2.12	1.46	1.50
27	1	622	LMG	C3-C2	2.12	1.57	1.52
22	B	819	CLA	CMD-C2D	-2.12	1.46	1.50
22	1	612	CLA	CMD-C2D	-2.12	1.46	1.50
22	Y	611	CLA	CMD-C2D	-2.12	1.46	1.50
21	Z	607	CHL	C4C-C3C	2.12	1.48	1.45
22	A	823	CLA	CMC-C2C	-2.12	1.46	1.50
21	Z	605	CHL	C4C-C3C	2.12	1.48	1.44
22	A	824	CLA	CMC-C2C	-2.12	1.46	1.50
22	A	817	CLA	CMC-C2C	-2.12	1.46	1.50
22	K	203	CLA	CMC-C2C	-2.12	1.46	1.50
22	A	832	CLA	C3B-C2B	-2.12	1.37	1.40
22	Y	610	CLA	CMD-C2D	-2.12	1.46	1.50
22	4	609	CLA	CMC-C2C	-2.12	1.46	1.50
22	2	613	CLA	C3B-C2B	-2.12	1.37	1.40
22	X	614	CLA	CMD-C2D	-2.12	1.46	1.50
21	2	608	CHL	C4B-CHC	2.12	1.46	1.41
22	4	610	CLA	MG-ND	-2.12	2.01	2.05
22	B	822	CLA	MG-ND	-2.11	2.01	2.05
22	B	809	CLA	CMD-C2D	-2.11	1.46	1.50
22	K	206	CLA	CMD-C2D	-2.11	1.46	1.50
22	Y	604	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	828	CLA	C4B-CHC	-2.11	1.35	1.41
22	4	611	CLA	CMD-C2D	-2.11	1.46	1.50
21	Z	608	CHL	C4B-CHC	2.11	1.46	1.41
21	2	608	CHL	MG-NA	-2.11	2.01	2.06
22	B	832	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	836	CLA	CMC-C2C	-2.11	1.46	1.50
22	2	602	CLA	CMA-C3A	-2.11	1.48	1.53
22	1	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	818	CLA	CAC-C3C	-2.11	1.45	1.51
22	3	606	CLA	C3B-C2B	-2.11	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	606	CHL	C4B-CHC	2.11	1.46	1.41
22	1	609	CLA	CMD-C2D	-2.11	1.46	1.50
22	O	2001	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	813	CLA	C3B-CAB	-2.11	1.43	1.47
22	B	809	CLA	CMC-C2C	-2.11	1.46	1.50
24	1	618	XAT	O24-C25	-2.10	1.43	1.46
24	3	619	XAT	O24-C25	-2.10	1.43	1.46
22	1	603	CLA	C3B-CAB	-2.10	1.43	1.47
21	X	608	CHL	C1B-CHB	2.10	1.46	1.41
22	A	807	CLA	C3B-CAB	-2.10	1.43	1.47
22	4	601	CLA	C3B-CAB	-2.10	1.43	1.47
22	B	811	CLA	MG-ND	-2.10	2.01	2.05
21	Y	608	CHL	C1D-ND	-2.10	1.35	1.37
22	A	840	CLA	CMC-C2C	-2.10	1.46	1.50
21	4	606	CHL	MG-NA	-2.10	2.01	2.06
22	B	808	CLA	C3B-CAB	-2.10	1.43	1.47
22	A	840	CLA	C3B-C2B	-2.10	1.37	1.40
22	A	805	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	841	CLA	CMC-C2C	-2.10	1.46	1.50
22	X	604	CLA	CMD-C2D	-2.10	1.46	1.50
22	1	613	CLA	C3B-CAB	-2.10	1.43	1.47
22	A	824	CLA	MG-ND	-2.09	2.01	2.05
22	B	821	CLA	MG-ND	-2.09	2.01	2.05
24	3	619	XAT	O4-C5	-2.09	1.43	1.46
22	B	814	CLA	C3B-CAB	-2.09	1.43	1.47
22	4	613	CLA	CMC-C2C	-2.09	1.46	1.50
22	A	831	CLA	C4B-CHC	-2.09	1.35	1.41
22	A	814	CLA	CMD-C2D	-2.09	1.46	1.50
22	H	201	CLA	MG-ND	-2.09	2.01	2.05
22	X	602	CLA	C3B-CAB	-2.09	1.43	1.47
22	B	818	CLA	CMC-C2C	-2.09	1.46	1.50
22	Z	604	CLA	CMD-C2D	-2.09	1.46	1.50
22	4	610	CLA	C3B-C2B	-2.09	1.37	1.40
22	B	828	CLA	C3B-CAB	-2.09	1.43	1.47
22	B	835	CLA	MG-ND	-2.08	2.01	2.05
26	Z	7630	LHG	P-O6	2.08	1.67	1.59
22	Z	611	CLA	CMD-C2D	-2.08	1.46	1.50
22	N	1001	CLA	MG-ND	-2.08	2.01	2.05
21	1	601	CHL	C4C-C3C	2.08	1.48	1.45
21	2	618	CHL	C4C-C3C	2.08	1.48	1.45
32	B	850	DGD	C4D-C5D	2.08	1.57	1.53
22	1	613	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	828	CLA	CMC-C2C	-2.08	1.46	1.50
22	A	837	CLA	C3B-C2B	-2.08	1.37	1.40
22	2	603	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	821	CLA	CMC-C2C	-2.08	1.46	1.50
22	A	817	CLA	C3B-C2B	-2.08	1.37	1.40
22	4	612	CLA	CMD-C2D	-2.08	1.46	1.50
23	Z	7621	LUT	C22-C21	-2.07	1.52	1.54
22	A	821	CLA	CMC-C2C	-2.07	1.46	1.50
22	3	606	CLA	C3B-CAB	-2.07	1.43	1.47
21	Y	601	CHL	C4B-CHC	2.07	1.46	1.41
27	4	623	LMG	O4-C4	-2.07	1.38	1.43
22	2	610	CLA	C3B-CAB	-2.07	1.43	1.47
22	2	610	CLA	C3B-C2B	-2.07	1.37	1.40
21	2	618	CHL	C1B-CHB	2.07	1.46	1.41
22	A	817	CLA	C4B-CHC	-2.07	1.35	1.41
22	4	609	CLA	O1D-CGD	2.07	1.26	1.21
22	K	201	CLA	C3B-C2B	-2.07	1.37	1.40
21	Y	608	CHL	CMC-C2C	2.07	1.49	1.45
22	G	204	CLA	CMD-C2D	-2.07	1.46	1.50
22	3	610	CLA	C3B-CAB	-2.07	1.43	1.47
22	2	603	CLA	CMC-C2C	-2.07	1.46	1.50
22	L	302	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	810	CLA	MG-ND	-2.07	2.01	2.05
22	A	839	CLA	CMC-C2C	-2.07	1.46	1.50
22	Y	612	CLA	CMD-C2D	-2.06	1.46	1.50
22	Z	602	CLA	CMD-C2D	-2.06	1.46	1.50
22	1	613	CLA	MG-ND	-2.06	2.01	2.05
22	X	602	CLA	C3B-C2B	-2.06	1.37	1.40
22	3	609	CLA	CAC-C3C	-2.06	1.45	1.51
22	H	201	CLA	C3B-C2B	-2.06	1.37	1.40
22	A	835	CLA	C3B-CAB	-2.06	1.43	1.47
26	A	847	LHG	O7-C5	-2.06	1.41	1.46
22	B	815	CLA	MG-ND	-2.06	2.01	2.05
22	K	204	CLA	MG-ND	-2.06	2.01	2.05
22	B	841	CLA	C3B-CAB	-2.06	1.43	1.47
22	B	808	CLA	MG-ND	-2.06	2.01	2.05
22	B	839	CLA	MG-ND	-2.06	2.01	2.05
22	G	201	CLA	C3B-CAB	-2.06	1.43	1.47
22	A	813	CLA	C3B-C2B	-2.06	1.37	1.40
22	A	833	CLA	MG-ND	-2.06	2.01	2.05
22	B	817	CLA	MG-ND	-2.06	2.01	2.05
22	1	606	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	X	605	CHL	C1B-CHB	2.06	1.46	1.41
24	4	620	XAT	O24-C25	-2.06	1.43	1.46
22	3	604	CLA	CMC-C2C	-2.06	1.46	1.50
22	F	304	CLA	C3B-CAB	-2.05	1.43	1.47
22	A	815	CLA	C3B-CAB	-2.05	1.43	1.47
22	A	835	CLA	MG-ND	-2.05	2.01	2.05
32	J	103	DGD	O1G-C1G	-2.05	1.40	1.45
22	A	814	CLA	MG-ND	-2.05	2.01	2.05
22	B	837	CLA	CMC-C2C	-2.05	1.46	1.50
22	X	610	CLA	CMD-C2D	-2.05	1.46	1.50
22	Z	610	CLA	CMC-C2C	-2.05	1.46	1.50
22	F	301	CLA	MG-ND	-2.05	2.01	2.05
22	1	604	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	826	CLA	C3B-CAB	-2.05	1.43	1.47
22	1	612	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	820	CLA	CMC-C2C	-2.05	1.46	1.50
22	Z	610	CLA	CMD-C2D	-2.05	1.46	1.50
22	4	604	CLA	CMD-C2D	-2.05	1.46	1.50
22	Y	612	CLA	CMC-C2C	-2.05	1.46	1.50
25	A	850	BCR	C21-C22	-2.05	1.33	1.35
22	B	827	CLA	MG-ND	-2.04	2.01	2.05
22	B	834	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	826	CLA	MG-ND	-2.04	2.01	2.05
22	A	843	CLA	C3B-CAB	-2.04	1.43	1.47
22	A	809	CLA	C3B-C2B	-2.04	1.37	1.40
22	X	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	835	CLA	C4B-CHC	-2.04	1.35	1.41
22	B	834	CLA	C3B-CAB	-2.04	1.43	1.47
22	Y	602	CLA	C3B-CAB	-2.04	1.43	1.47
22	Z	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	Z	603	CLA	CMC-C2C	-2.04	1.46	1.50
22	K	203	CLA	C3B-CAB	-2.04	1.43	1.47
22	1	613	CLA	C3B-C2B	-2.04	1.37	1.40
22	B	822	CLA	CMC-C2C	-2.04	1.46	1.50
22	X	604	CLA	CBD-CAD	2.04	1.56	1.51
22	X	612	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	834	CLA	CMC-C2C	-2.03	1.46	1.50
22	1	614	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	803	CLA	C3B-CAB	-2.03	1.43	1.47
22	2	610	CLA	MG-ND	-2.03	2.01	2.05
22	A	828	CLA	MG-ND	-2.03	2.01	2.05
32	J	103	DGD	O3G-C3G	-2.03	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	1002	CLA	MG-ND	-2.03	2.01	2.05
22	1	611	CLA	CMC-C2C	-2.03	1.46	1.50
22	4	604	CLA	CMC-C2C	-2.03	1.46	1.50
22	Z	612	CLA	C3D-C4D	2.03	1.48	1.44
22	X	611	CLA	CMD-C2D	-2.03	1.46	1.50
21	Y	607	CHL	C4B-CHC	2.03	1.46	1.41
22	A	828	CLA	C3B-C2B	-2.03	1.37	1.40
22	Y	603	CLA	CMC-C2C	-2.03	1.46	1.50
21	X	607	CHL	C2C-C1C	2.02	1.48	1.44
26	X	2630	LHG	P-O6	2.02	1.67	1.59
22	B	813	CLA	C4B-CHC	-2.02	1.35	1.41
22	3	612	CLA	CMD-C2D	-2.02	1.46	1.50
22	3	613	CLA	CMC-C2C	-2.02	1.46	1.50
22	3	617	CLA	MG-ND	-2.02	2.01	2.05
22	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	613	CLA	CMC-C2C	-2.02	1.46	1.50
21	X	606	CHL	C1D-ND	-2.02	1.35	1.37
22	A	811	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	835	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	840	CLA	C3B-CAB	-2.02	1.43	1.47
21	2	607	CHL	C4C-C3C	2.02	1.48	1.45
22	B	823	CLA	C3B-CAB	-2.02	1.43	1.47
21	X	606	CHL	C4C-C3C	2.02	1.48	1.44
22	B	821	CLA	C4B-CHC	-2.02	1.35	1.41
22	4	611	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	809	CLA	C4B-CHC	-2.02	1.35	1.41
22	G	201	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	825	CLA	MG-ND	-2.02	2.01	2.05
27	4	623	LMG	O7-C8	-2.01	1.41	1.46
22	A	811	CLA	MG-ND	-2.01	2.01	2.05
22	4	614	CLA	CMC-C2C	-2.01	1.46	1.50
22	F	303	CLA	CMC-C2C	-2.01	1.46	1.50
21	Y	606	CHL	MG-NA	-2.01	2.01	2.06
22	X	603	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	603	CLA	CMC-C2C	-2.01	1.46	1.50
22	1	611	CLA	MG-ND	-2.01	2.01	2.05
22	A	835	CLA	CMC-C2C	-2.01	1.46	1.50
22	B	819	CLA	C4B-CHC	-2.01	1.35	1.41
21	3	608	CHL	C4B-CHC	2.01	1.46	1.41
21	Y	609	CHL	C4C-C3C	2.01	1.48	1.45
22	1	604	CLA	C3B-CAB	-2.01	1.43	1.47
22	3	609	CLA	C3B-CAB	-2.01	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	601	CHL	C2C-C1C	2.01	1.48	1.44
22	3	614	CLA	C3B-C2B	-2.01	1.37	1.40
22	2	609	CLA	C3B-CAB	-2.01	1.43	1.47
22	4	610	CLA	C3B-CAB	-2.01	1.43	1.47
21	Y	608	CHL	C1B-CHB	2.01	1.46	1.41
22	A	808	CLA	MG-ND	-2.01	2.01	2.05
22	B	840	CLA	C4B-CHC	-2.00	1.35	1.41
22	B	808	CLA	C4B-CHC	-2.00	1.35	1.41
21	4	618	CHL	C1D-ND	-2.00	1.35	1.37
22	3	615	CLA	CMD-C2D	-2.00	1.46	1.50
22	G	201	CLA	CMC-C2C	-2.00	1.46	1.50
22	A	827	CLA	CMC-C2C	-2.00	1.46	1.50
21	Z	605	CHL	C1D-ND	-2.00	1.35	1.37
22	A	842	CLA	C3B-CAB	-2.00	1.43	1.47
22	K	201	CLA	MG-ND	-2.00	2.01	2.05
21	Z	601	CHL	C1D-ND	-2.00	1.35	1.37

All (2886) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	7622	XAT	O24-C25-C24	10.93	121.59	113.38
22	B	808	CLA	C4A-NA-C1A	9.49	110.97	106.71
24	Z	4622	XAT	O24-C25-C24	9.46	120.49	113.38
33	Y	4623	NEX	O24-C25-C24	9.16	120.26	113.38
21	X	601	CHL	CMD-C2D-C1D	9.10	140.76	124.71
21	Y	601	CHL	CMD-C2D-C1D	9.07	140.69	124.71
21	4	618	CHL	CMD-C2D-C1D	9.07	140.69	124.71
21	Z	607	CHL	C2C-C3C-C4C	-8.99	100.08	106.49
22	B	840	CLA	C4A-NA-C1A	8.96	110.73	106.71
21	Z	601	CHL	CMD-C2D-C1D	8.92	140.44	124.71
21	3	608	CHL	CMD-C2D-C1D	8.88	140.37	124.71
28	A	801	CL0	C1D-ND-C4D	-8.84	100.06	106.33
22	B	803	CLA	C4A-NA-C1A	8.82	110.67	106.71
21	Z	609	CHL	CMD-C2D-C1D	8.81	140.24	124.71
21	2	607	CHL	CMD-C2D-C1D	8.72	140.09	124.71
22	B	837	CLA	C4A-NA-C1A	8.71	110.62	106.71
33	X	2623	NEX	O24-C25-C24	8.71	119.92	113.38
21	X	606	CHL	CMD-C2D-C1D	8.70	140.05	124.71
22	A	818	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	A	813	CLA	C4A-NA-C1A	8.69	110.61	106.71
21	2	601	CHL	CMD-C2D-C1D	8.64	139.94	124.71
21	Z	608	CHL	CMD-C2D-C1D	8.52	139.73	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	618	XAT	O24-C25-C24	8.51	119.78	113.38
22	A	842	CLA	C4A-NA-C1A	8.50	110.53	106.71
21	Y	607	CHL	CMD-C2D-C1D	8.44	139.59	124.71
21	4	606	CHL	CMD-C2D-C1D	8.44	139.59	124.71
21	Y	606	CHL	CMD-C2D-C1D	8.43	139.57	124.71
22	A	804	CLA	C4A-NA-C1A	8.41	110.49	106.71
21	2	618	CHL	CMD-C2D-C1D	8.38	139.48	124.71
21	1	607	CHL	CMD-C2D-C1D	8.34	139.42	124.71
22	B	816	CLA	C4A-NA-C1A	8.34	110.46	106.71
21	Y	608	CHL	CMD-C2D-C1D	8.31	139.36	124.71
21	Y	605	CHL	CMD-C2D-C1D	8.29	139.32	124.71
21	Z	605	CHL	CMD-C2D-C1D	8.27	139.29	124.71
21	4	608	CHL	CMD-C2D-C1D	8.23	139.22	124.71
21	Y	609	CHL	CMD-C2D-C1D	8.22	139.19	124.71
21	2	608	CHL	CMD-C2D-C1D	8.20	139.17	124.71
21	4	607	CHL	CMD-C2D-C1D	8.20	139.16	124.71
22	B	838	CLA	C4A-NA-C1A	8.18	110.38	106.71
21	2	606	CHL	CMD-C2D-C1D	8.18	139.12	124.71
21	Z	608	CHL	C2C-C3C-C4C	-8.17	100.67	106.49
21	X	607	CHL	CMD-C2D-C1D	8.16	139.09	124.71
22	B	824	CLA	C4A-NA-C1A	8.16	110.37	106.71
22	B	815	CLA	C4A-NA-C1A	8.11	110.35	106.71
22	A	806	CLA	C4A-NA-C1A	8.05	110.33	106.71
22	A	816	CLA	C4A-NA-C1A	8.03	110.32	106.71
21	Z	606	CHL	CMD-C2D-C1D	8.01	138.84	124.71
22	B	807	CLA	C4A-NA-C1A	7.99	110.30	106.71
21	X	609	CHL	CMD-C2D-C1D	7.99	138.79	124.71
21	X	605	CHL	CMD-C2D-C1D	7.96	138.73	124.71
22	B	819	CLA	C4A-NA-C1A	7.95	110.28	106.71
21	Z	609	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
22	B	821	CLA	C4A-NA-C1A	7.93	110.27	106.71
21	X	608	CHL	CMD-C2D-C1D	7.90	138.63	124.71
22	B	818	CLA	C4A-NA-C1A	7.90	110.26	106.71
22	2	613	CLA	C4A-NA-C1A	7.89	110.25	106.71
22	A	832	CLA	C4A-NA-C1A	7.85	110.24	106.71
22	Y	613	CLA	C4A-NA-C1A	7.84	110.23	106.71
33	Z	7623	NEX	O24-C25-C24	7.84	119.27	113.38
22	G	201	CLA	C4A-NA-C1A	7.83	110.23	106.71
22	B	805	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	F	301	CLA	C4A-NA-C1A	7.77	110.20	106.71
22	3	613	CLA	C4A-NA-C1A	7.74	110.19	106.71
21	2	607	CHL	C2C-C3C-C4C	-7.72	100.98	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	842	PQN	C15-C13-C12	-7.69	105.56	121.12
22	1	609	CLA	C4A-NA-C1A	7.68	110.16	106.71
21	Z	606	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
22	B	812	CLA	C4A-NA-C1A	7.67	110.16	106.71
21	4	606	CHL	C2C-C3C-C4C	-7.67	100.80	106.49
22	4	610	CLA	C4A-NA-C1A	7.64	110.14	106.71
24	Y	2622	XAT	O24-C25-C24	7.63	119.12	113.38
22	A	841	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	B	820	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	1	604	CLA	C4A-NA-C1A	7.58	110.11	106.71
21	Z	607	CHL	CMD-C2D-C1D	7.55	138.02	124.71
22	A	834	CLA	C4A-NA-C1A	7.54	110.10	106.71
22	B	826	CLA	C4A-NA-C1A	7.53	110.09	106.71
24	X	7622	XAT	O4-C5-C4	7.51	119.03	113.38
21	2	618	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
22	O	2002	CLA	C4A-NA-C1A	7.48	110.07	106.71
22	4	604	CLA	C4A-NA-C1A	7.47	110.07	106.71
22	A	821	CLA	C4A-NA-C1A	7.47	110.07	106.71
21	Y	607	CHL	C2C-C3C-C4C	-7.45	100.96	106.49
22	A	823	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	Z	602	CLA	C4A-NA-C1A	7.43	110.05	106.71
22	Z	613	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	A	836	CLA	C4A-NA-C1A	7.42	110.04	106.71
29	A	844	PQN	C15-C13-C12	-7.42	106.11	121.12
22	A	825	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	2	614	CLA	C4A-NA-C1A	7.39	110.03	106.71
24	2	620	XAT	O24-C25-C24	7.37	118.92	113.38
22	1	613	CLA	C4A-NA-C1A	7.36	110.02	106.71
22	Y	604	CLA	C4A-NA-C1A	7.35	110.01	106.71
22	A	840	CLA	C4A-NA-C1A	7.34	110.01	106.71
21	2	608	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
21	1	601	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
24	4	620	XAT	O4-C5-C4	7.33	118.89	113.38
22	3	612	CLA	C4A-NA-C1A	7.33	110.00	106.71
22	Z	603	CLA	C4A-NA-C1A	7.31	109.99	106.71
21	X	607	CHL	CHD-C1D-ND	-7.30	117.74	124.45
29	A	844	PQN	C11-C12-C13	-7.30	114.63	126.79
21	X	609	CHL	CHD-C1D-ND	-7.29	117.75	124.45
21	X	608	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
22	X	613	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	A	835	CLA	C4A-NA-C1A	7.24	109.96	106.71
21	X	601	CHL	C2C-C3C-C4C	-7.24	101.33	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	609	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	B	829	CLA	CMB-C2B-C1B	-7.22	117.37	128.46
22	A	845	CLA	C4A-NA-C1A	7.21	109.95	106.71
22	A	843	CLA	C4A-NA-C1A	7.21	109.95	106.71
22	A	829	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	3	604	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	L	302	CLA	C4A-NA-C1A	7.18	109.93	106.71
28	A	801	CL0	C2D-C1D-ND	7.16	115.38	110.10
21	Z	601	CHL	CHD-C1D-ND	-7.16	117.88	124.45
22	2	612	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	A	812	CLA	C4A-NA-C1A	7.13	109.91	106.71
22	H	201	CLA	C4A-NA-C1A	7.13	109.91	106.71
22	4	611	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	A	817	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	B	831	CLA	C4A-NA-C1A	7.11	109.90	106.71
21	Y	609	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
22	A	837	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	Y	612	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	2	610	CLA	C4A-NA-C1A	7.06	109.88	106.71
21	4	607	CHL	C1B-C2B-C3B	-7.06	100.35	106.92
22	4	613	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	1	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	A	819	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	3	602	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	K	204	CLA	C4A-NA-C1A	7.04	109.87	106.71
21	Y	609	CHL	CHD-C1D-ND	-7.04	117.98	124.45
21	2	601	CHL	O2D-CGD-CBD	7.04	123.78	111.27
21	Y	608	CHL	C1B-C2B-C3B	-7.04	100.38	106.92
21	4	618	CHL	C1B-C2B-C3B	-7.01	100.40	106.92
22	X	603	CLA	C4A-NA-C1A	7.01	109.86	106.71
21	Y	608	CHL	C2C-C3C-C4C	-6.99	101.30	106.49
21	Y	607	CHL	C1B-C2B-C3B	-6.98	100.42	106.92
21	1	601	CHL	CMD-C2D-C1D	6.97	137.00	124.71
21	Y	605	CHL	CHD-C1D-ND	-6.97	118.05	124.45
22	F	304	CLA	C4A-NA-C1A	6.96	109.84	106.71
22	A	820	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	K	201	CLA	C4A-NA-C1A	6.96	109.83	106.71
21	2	601	CHL	C2C-C3C-C4C	-6.95	101.53	106.49
25	B	848	BCR	C24-C23-C22	-6.95	115.74	126.23
22	Y	611	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	B	810	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	X	612	CLA	C4A-NA-C1A	6.92	109.82	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	1002	CLA	C4A-NA-C1A	6.92	109.81	106.71
21	Y	601	CHL	C1B-C2B-C3B	-6.91	100.49	106.92
22	J	101	CLA	C4A-NA-C1A	6.90	109.81	106.71
21	X	607	CHL	C1B-C2B-C3B	-6.90	100.50	106.92
22	K	203	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	A	826	CLA	C4A-NA-C1A	6.89	109.80	106.71
21	X	601	CHL	C1B-C2B-C3B	-6.89	100.51	106.92
21	Z	605	CHL	C1B-C2B-C3B	-6.88	100.52	106.92
25	A	852	BCR	C7-C8-C9	-6.88	115.84	126.23
22	B	823	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	A	811	CLA	C4A-NA-C1A	6.87	109.79	106.71
21	4	618	CHL	C2C-C3C-C4C	-6.86	101.60	106.49
21	Y	606	CHL	C1B-C2B-C3B	-6.86	100.54	106.92
21	Y	605	CHL	C1B-C2B-C3B	-6.85	100.55	106.92
22	3	614	CLA	C4A-NA-C1A	6.85	109.78	106.71
22	F	303	CLA	C4A-NA-C1A	6.84	109.78	106.71
21	2	606	CHL	C2C-C3C-C4C	-6.83	101.42	106.49
21	Y	601	CHL	CHD-C1D-ND	-6.83	118.18	124.45
22	L	304	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	A	831	CLA	C4A-NA-C1A	6.80	109.76	106.71
21	1	607	CHL	CHD-C1D-ND	-6.78	118.22	124.45
21	X	606	CHL	C1B-C2B-C3B	-6.78	100.61	106.92
22	2	602	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	1	616	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	A	815	CLA	C4A-NA-C1A	6.76	109.74	106.71
21	4	607	CHL	CHD-C1D-ND	-6.75	118.25	124.45
21	Y	606	CHL	C4C-C3C-C2C	-6.75	100.88	107.07
22	B	832	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	X	604	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	806	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	834	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	Z	605	CHL	C4C-C3C-C2C	-6.72	100.91	107.07
22	G	203	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	Z	4622	XAT	C6-C7-C8	-6.71	111.81	125.99
22	3	610	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	814	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	1	614	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	2	604	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	3	609	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	4	612	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	X	610	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	J	102	BCR	C28-C27-C26	-6.68	102.14	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	808	CLA	C4A-NA-C1A	6.67	109.70	106.71
21	4	608	CHL	C2C-C3C-C4C	-6.64	101.75	106.49
22	K	206	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	L	303	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	2	609	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	X	601	CHL	CHD-C1D-ND	-6.61	118.38	124.45
22	B	811	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	4	601	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	1	611	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	B	813	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	X	607	CHL	C2C-C3C-C4C	-6.58	101.60	106.49
25	B	847	BCR	C15-C16-C17	-6.57	110.01	123.47
29	B	842	PQN	C11-C12-C13	-6.57	115.85	126.79
22	Z	611	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	G	204	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	Z	604	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	Z	607	CHL	CHB-C4A-NA	6.56	133.58	124.51
22	2	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	Z	601	CHL	C2C-C3C-C4C	-6.53	101.83	106.49
24	4	620	XAT	O24-C25-C24	6.53	118.29	113.38
24	2	620	XAT	O4-C5-C4	6.53	118.28	113.38
21	1	607	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
22	Z	612	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	1	618	XAT	O4-C5-C4	6.51	118.27	113.38
22	A	830	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	Y	610	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	B	801	BCR	C24-C23-C22	-6.50	116.42	126.23
22	Y	602	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	1	612	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	B	841	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	Y	603	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	B	835	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	A	828	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	4	618	CHL	CHD-C1D-ND	-6.44	118.53	124.45
22	4	617	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	Z	607	CHL	C3C-C4C-NC	6.43	117.79	110.57
21	Y	605	CHL	C4C-C3C-C2C	-6.42	101.18	107.07
22	B	830	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	3	615	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	802	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	A	833	CLA	CMB-C2B-C1B	-6.40	118.63	128.46
22	B	839	CLA	C4A-NA-C1A	6.40	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	804	CLA	C4A-NA-C1A	6.37	109.57	106.71
21	2	618	CHL	CHD-C1D-ND	-6.37	118.60	124.45
22	B	833	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	A	831	CLA	CMB-C2B-C1B	-6.36	118.69	128.46
22	3	607	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	B	817	CLA	C4A-NA-C1A	6.34	109.56	106.71
24	4	620	XAT	C26-C27-C28	-6.32	112.62	125.99
21	Z	609	CHL	CHD-C1D-ND	-6.30	118.66	124.45
22	A	802	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	A	807	CLA	C4A-NA-C1A	6.29	109.53	106.71
21	X	606	CHL	CHD-C1D-ND	-6.27	118.69	124.45
21	3	608	CHL	CHD-C1D-ND	-6.24	118.72	124.45
21	X	606	CHL	C2C-C3C-C4C	-6.23	101.86	106.49
22	B	828	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	A	814	CLA	C4A-NA-C1A	6.22	109.50	106.71
21	2	601	CHL	CHD-C1D-ND	-6.21	118.74	124.45
21	Y	608	CHL	CHD-C1D-ND	-6.20	118.76	124.45
22	N	1001	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	1	606	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	X	614	CLA	C4A-NA-C1A	6.18	109.48	106.71
21	X	608	CHL	CHD-C1D-ND	-6.17	118.78	124.45
22	1	608	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	2	608	CHL	C3C-C4C-NC	6.15	117.47	110.57
22	A	810	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	Z	614	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	B	827	CLA	C4A-NA-C1A	6.13	109.46	106.71
21	4	608	CHL	CHD-C1D-ND	-6.12	118.83	124.45
25	B	845	BCR	C7-C8-C9	-6.12	116.99	126.23
24	Y	2622	XAT	O4-C5-C4	6.11	117.97	113.38
24	3	619	XAT	C26-C27-C28	-6.11	113.07	125.99
22	A	833	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	4	614	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	A	852	BCR	C20-C21-C22	-6.09	118.62	127.31
22	B	809	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	A	827	CLA	C4A-NA-C1A	6.08	109.44	106.71
21	X	609	CHL	C1B-C2B-C3B	-6.08	101.27	106.92
28	A	801	CL0	CMD-C2D-C1D	6.08	135.42	124.71
24	2	620	XAT	C6-C7-C8	-6.03	113.24	125.99
22	1	610	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	1	602	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	B	836	CLA	CMB-C2B-C1B	-5.99	119.25	128.46
22	X	602	CLA	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	603	CLA	C4A-NA-C1A	5.99	109.40	106.71
22	4	602	CLA	C4A-NA-C1A	5.99	109.40	106.71
22	4	603	CLA	C4A-NA-C1A	5.97	109.39	106.71
22	A	838	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	K	202	BCR	C24-C23-C22	-5.97	117.22	126.23
25	K	202	BCR	C28-C27-C26	-5.96	103.43	114.08
22	A	838	CLA	CMB-C2B-C1B	-5.96	119.30	128.46
22	B	812	CLA	CMB-C2B-C1B	-5.95	119.31	128.46
22	Y	604	CLA	CMB-C2B-C1B	-5.94	119.33	128.46
21	Y	606	CHL	CHD-C1D-ND	-5.94	119.00	124.45
22	A	809	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	3	606	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	A	839	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	A	822	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	Y	614	CLA	C4A-NA-C1A	5.92	109.37	106.71
24	Z	4622	XAT	O4-C5-C4	5.91	117.82	113.38
21	Z	608	CHL	CHD-C1D-ND	-5.91	119.02	124.45
21	Z	605	CHL	CHD-C1D-ND	-5.89	119.04	124.45
21	X	607	CHL	C1B-CHB-C4A	-5.88	118.47	130.12
22	O	2001	CLA	C4A-NA-C1A	5.85	109.34	106.71
21	2	608	CHL	CHD-C4C-C3C	-5.85	116.24	124.84
22	A	805	CLA	C4A-NA-C1A	5.85	109.34	106.71
21	2	606	CHL	CHD-C1D-ND	-5.83	119.10	124.45
25	B	847	BCR	C15-C14-C13	-5.82	119.01	127.31
25	A	851	BCR	C28-C27-C26	-5.81	103.71	114.08
21	1	601	CHL	CHD-C1D-ND	-5.80	119.12	124.45
22	B	803	CLA	CAC-C3C-C4C	5.80	132.34	124.81
22	A	803	CLA	C4A-NA-C1A	5.79	109.31	106.71
21	4	606	CHL	CHD-C1D-ND	-5.79	119.14	124.45
22	A	820	CLA	CMB-C2B-C1B	-5.78	119.57	128.46
22	B	836	CLA	C4A-NA-C1A	5.78	109.30	106.71
22	Z	610	CLA	C4A-NA-C1A	5.78	109.30	106.71
22	X	611	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	B	829	CLA	C4A-NA-C1A	5.75	109.29	106.71
21	4	606	CHL	C3C-C4C-NC	5.74	116.84	110.57
25	B	844	BCR	C7-C8-C9	-5.74	117.56	126.23
21	2	618	CHL	O2D-CGD-CBD	5.71	121.42	111.27
22	B	825	CLA	C4A-NA-C1A	5.71	109.27	106.71
21	4	608	CHL	CHD-C4C-C3C	-5.69	116.48	124.84
21	2	607	CHL	CHD-C1D-ND	-5.68	119.23	124.45
21	Y	608	CHL	C3C-C4C-NC	5.68	116.77	110.57
25	A	850	BCR	C7-C8-C9	-5.66	117.67	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	607	CHL	C3C-C4C-NC	5.66	116.75	110.57
24	Z	4622	XAT	C15-C14-C13	-5.66	119.23	127.31
25	A	850	BCR	C28-C27-C26	-5.66	103.98	114.08
21	Z	606	CHL	CHD-C1D-ND	-5.65	119.26	124.45
22	N	1002	CLA	CMB-C2B-C1B	-5.65	119.78	128.46
22	B	822	CLA	C4A-NA-C1A	5.64	109.24	106.71
22	A	805	CLA	CMB-C2B-C1B	-5.64	119.79	128.46
22	A	815	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
21	Z	607	CHL	CHD-C4C-C3C	-5.63	116.57	124.84
21	4	608	CHL	C3C-C4C-NC	5.62	116.87	110.57
22	B	803	CLA	CMB-C2B-C1B	-5.61	119.83	128.46
22	3	617	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	4	621	BCR	C7-C8-C9	-5.61	117.75	126.23
21	Y	607	CHL	CHD-C1D-ND	-5.61	119.30	124.45
24	3	619	XAT	O24-C25-C24	5.61	117.59	113.38
24	3	619	XAT	O4-C5-C4	5.60	117.59	113.38
21	Z	608	CHL	C3C-C4C-NC	5.60	116.85	110.57
21	2	606	CHL	O2D-CGD-CBD	5.59	121.20	111.27
21	Z	605	CHL	C3C-C4C-NC	5.59	116.67	110.57
21	X	605	CHL	CHD-C1D-ND	-5.58	119.33	124.45
22	A	829	CLA	CMB-C2B-C1B	-5.57	119.91	128.46
21	X	605	CHL	C3C-C4C-NC	5.54	116.78	110.57
25	B	801	BCR	C3-C4-C5	-5.53	104.20	114.08
22	A	854	CLA	CMB-C2B-C1B	-5.53	119.96	128.46
21	Z	607	CHL	CHD-C1D-ND	-5.51	119.39	124.45
28	A	801	CL0	CHD-C1D-ND	-5.51	119.39	124.45
25	L	306	BCR	C24-C23-C22	-5.48	117.95	126.23
24	2	620	XAT	C26-C27-C28	-5.48	114.41	125.99
22	B	804	CLA	CMB-C2B-C1B	-5.47	120.06	128.46
28	A	801	CL0	CHD-C4C-C3C	-5.47	116.81	124.84
25	A	852	BCR	C16-C17-C18	-5.46	119.51	127.31
24	X	7622	XAT	C15-C14-C13	-5.46	119.52	127.31
25	B	847	BCR	C28-C27-C26	-5.46	104.33	114.08
21	X	606	CHL	O2D-CGD-CBD	5.45	120.96	111.27
22	4	602	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
22	A	833	CLA	CMB-C2B-C3B	5.43	134.84	124.68
22	B	827	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
25	2	621	BCR	C28-C27-C26	-5.42	104.39	114.08
21	Y	606	CHL	C2C-C1C-NC	5.42	115.05	109.97
24	Z	4622	XAT	O4-C5-C18	5.42	121.55	115.06
25	I	101	BCR	C7-C8-C9	-5.41	118.05	126.23
21	Z	609	CHL	C3C-C4C-NC	5.39	116.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	620	BCR	C28-C27-C26	-5.39	104.45	114.08
24	X	7622	XAT	C11-C10-C9	-5.39	119.62	127.31
22	A	802	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
22	A	838	CLA	CMB-C2B-C3B	5.38	134.75	124.68
22	1	610	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
22	B	839	CLA	CMB-C2B-C1B	-5.37	120.20	128.46
22	A	824	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	K	202	BCR	C15-C14-C13	-5.37	119.65	127.31
28	A	801	CL0	C4A-NA-C1A	-5.33	104.31	106.71
22	A	818	CLA	CMB-C2B-C1B	-5.33	120.28	128.46
25	K	202	BCR	C20-C21-C22	-5.33	119.71	127.31
24	2	620	XAT	C18-C5-C6	-5.33	113.33	122.26
25	4	621	BCR	C28-C27-C26	-5.32	104.58	114.08
21	2	606	CHL	C3C-C4C-NC	5.31	116.37	110.57
21	4	607	CHL	O2D-CGD-CBD	5.31	120.70	111.27
21	Y	606	CHL	C3C-C4C-NC	5.30	116.36	110.57
21	2	601	CHL	C3D-C2D-C1D	-5.29	98.61	105.83
21	Z	607	CHL	C4B-C3B-C2B	5.28	111.83	106.92
21	X	605	CHL	C2C-C1C-NC	5.28	114.92	109.97
21	3	608	CHL	C3D-C2D-C1D	-5.27	98.64	105.83
25	A	850	BCR	C15-C14-C13	-5.25	119.81	127.31
25	L	305	BCR	C28-C27-C26	-5.24	104.72	114.08
24	Y	2622	XAT	C6-C7-C8	-5.24	114.92	125.99
21	4	608	CHL	C3D-C2D-C1D	-5.23	98.69	105.83
21	2	608	CHL	CHD-C1D-ND	-5.23	119.65	124.45
25	B	801	BCR	C28-C27-C26	-5.23	104.75	114.08
22	L	304	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
24	2	620	XAT	C38-C25-C26	-5.20	113.55	122.26
21	2	618	CHL	C3C-C4C-NC	5.18	116.38	110.57
28	A	801	CL0	O2D-CGD-CBD	5.16	120.43	111.27
22	A	826	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
22	B	836	CLA	CMB-C2B-C3B	5.14	134.29	124.68
21	3	608	CHL	C2C-C1C-NC	5.14	114.78	109.97
24	3	619	XAT	C38-C25-C26	-5.13	113.66	122.26
21	Z	608	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
21	Y	608	CHL	C3D-C2D-C1D	-5.12	98.84	105.83
21	X	608	CHL	C3C-C4C-NC	5.12	116.31	110.57
24	4	620	XAT	C38-C25-C26	-5.11	113.69	122.26
25	K	205	BCR	C3-C4-C5	-5.11	104.95	114.08
21	2	607	CHL	C3C-C4C-NC	5.11	116.30	110.57
21	X	606	CHL	C3C-C4C-NC	5.10	116.14	110.57
28	A	801	CL0	C2C-C1C-NC	5.09	114.74	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	618	XAT	C18-C5-C6	-5.08	113.75	122.26
21	2	607	CHL	O2D-CGD-CBD	5.05	120.25	111.27
24	1	618	XAT	O4-C5-C18	5.05	121.10	115.06
22	X	610	CLA	CMB-C2B-C1B	-5.05	120.71	128.46
33	Y	4623	NEX	C15-C14-C13	-5.04	120.11	127.31
21	2	608	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
22	B	814	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
21	Y	609	CHL	C3C-C4C-NC	5.02	116.20	110.57
22	A	815	CLA	CMB-C2B-C3B	5.02	134.07	124.68
24	3	619	XAT	O24-C25-C38	5.01	121.06	115.06
25	A	851	BCR	C24-C23-C22	-5.00	118.68	126.23
22	B	809	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
24	1	618	XAT	C26-C27-C28	-5.00	115.43	125.99
21	Z	606	CHL	C3C-C4C-NC	5.00	116.17	110.57
21	2	601	CHL	O2D-CGD-O1D	-4.99	114.08	123.84
21	1	601	CHL	C1B-CHB-C4A	-4.99	120.24	130.12
24	X	7622	XAT	C31-C30-C29	-4.98	120.20	127.31
25	A	851	BCR	C20-C21-C22	-4.98	120.20	127.31
25	B	845	BCR	C24-C23-C22	-4.98	118.71	126.23
25	B	843	BCR	C15-C16-C17	-4.98	113.27	123.47
29	B	842	PQN	C14-C13-C12	-4.98	110.91	123.68
22	B	805	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
22	A	808	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
22	A	829	CLA	CMB-C2B-C3B	4.96	133.95	124.68
21	Z	605	CHL	C2C-C1C-NC	4.95	114.61	109.97
21	X	609	CHL	C3C-C4C-NC	4.94	116.11	110.57
22	A	822	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
24	1	618	XAT	C6-C7-C8	-4.93	115.57	125.99
24	Z	4622	XAT	C31-C30-C29	-4.93	120.28	127.31
22	B	822	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
24	2	620	XAT	O4-C5-C18	4.89	120.92	115.06
21	1	601	CHL	C3C-C4C-NC	4.89	116.05	110.57
33	Z	7623	NEX	C11-C10-C9	-4.88	120.35	127.31
21	Z	608	CHL	CHD-C4C-C3C	-4.88	117.67	124.84
21	Y	609	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
25	B	843	BCR	C28-C27-C26	-4.87	105.38	114.08
29	A	844	PQN	C14-C13-C12	-4.87	111.19	123.68
24	X	7622	XAT	C27-C28-C29	-4.85	118.00	125.53
21	Y	608	CHL	CHD-C4C-C3C	-4.85	117.40	124.98
25	A	848	BCR	C16-C17-C18	-4.85	120.39	127.31
21	3	608	CHL	CHD-C4C-C3C	-4.84	117.72	124.84
22	B	812	CLA	CMB-C2B-C3B	4.84	133.74	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	805	CLA	CMB-C2B-C3B	4.84	133.73	124.68
21	2	601	CHL	C3C-C4C-NC	4.84	116.00	110.57
22	B	832	CLA	CMB-C2B-C1B	-4.82	121.05	128.46
25	K	205	BCR	C20-C21-C22	-4.82	120.43	127.31
25	I	101	BCR	C24-C23-C22	-4.82	118.95	126.23
24	3	619	XAT	C6-C7-C8	-4.81	115.82	125.99
24	3	619	XAT	O4-C5-C18	4.81	120.82	115.06
25	L	301	BCR	C7-C8-C9	-4.80	118.98	126.23
22	B	804	CLA	CAA-C2A-C3A	-4.80	104.91	116.10
22	B	827	CLA	CMB-C2B-C3B	4.79	133.65	124.68
21	4	607	CHL	C3C-C4C-NC	4.79	115.95	110.57
24	4	620	XAT	C6-C7-C8	-4.79	115.87	125.99
25	I	101	BCR	C16-C17-C18	-4.78	120.48	127.31
21	2	618	CHL	C3D-C2D-C1D	-4.78	99.31	105.83
21	2	601	CHL	C2D-C1D-ND	4.77	113.62	110.10
21	Y	607	CHL	C3D-C2D-C1D	-4.77	99.33	105.83
25	B	848	BCR	C20-C21-C22	-4.76	120.51	127.31
21	2	607	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
24	Z	4622	XAT	C38-C25-C26	-4.76	114.29	122.26
21	3	608	CHL	C3C-C4C-NC	4.75	115.90	110.57
21	2	608	CHL	C2D-C1D-ND	4.75	113.61	110.10
22	B	829	CLA	C2D-C1D-ND	-4.75	106.60	110.10
21	4	618	CHL	C3C-C4C-NC	4.75	115.90	110.57
21	3	608	CHL	O2D-CGD-CBD	4.75	119.71	111.27
22	A	802	CLA	CMB-C2B-C3B	4.75	133.56	124.68
21	4	618	CHL	C3D-C2D-C1D	-4.73	99.37	105.83
25	B	843	BCR	C15-C14-C13	-4.73	120.56	127.31
33	X	2623	NEX	C15-C14-C13	-4.73	120.56	127.31
24	X	7622	XAT	C7-C8-C9	-4.72	118.20	125.53
24	Y	2622	XAT	C18-C5-C6	-4.72	114.34	122.26
22	B	803	CLA	CMB-C2B-C3B	4.72	133.52	124.68
21	X	609	CHL	C3D-C2D-C1D	-4.72	99.38	105.83
24	Y	2622	XAT	C38-C25-C26	-4.72	114.35	122.26
22	O	2002	CLA	CAA-C2A-C3A	-4.72	105.10	116.10
33	X	2623	NEX	C38-C25-C26	-4.71	114.36	122.26
22	B	816	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
25	L	305	BCR	C11-C10-C9	-4.70	120.60	127.31
25	F	305	BCR	C15-C14-C13	-4.70	120.60	127.31
24	Z	4622	XAT	C15-C35-C34	-4.70	113.86	123.47
24	1	618	XAT	C38-C25-C26	-4.69	114.39	122.26
29	B	842	PQN	C14-C13-C15	-4.69	107.39	115.27
22	A	803	CLA	CMB-C2B-C1B	-4.69	121.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	610	CLA	CMB-C2B-C3B	4.68	133.44	124.68
24	X	7622	XAT	C18-C5-C6	-4.68	114.41	122.26
21	X	608	CHL	C3D-C2D-C1D	-4.68	99.44	105.83
21	Z	605	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
21	X	601	CHL	C3C-C4C-NC	4.66	115.80	110.57
22	B	804	CLA	CMB-C2B-C3B	4.66	133.40	124.68
22	B	825	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
22	L	302	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
24	Y	2622	XAT	O4-C5-C18	4.65	120.63	115.06
22	B	831	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
21	X	605	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
22	A	818	CLA	CMB-C2B-C3B	4.63	133.33	124.68
22	A	806	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
21	Y	605	CHL	C3C-C4C-NC	4.62	115.61	110.57
25	B	847	BCR	C3-C4-C5	-4.62	105.83	114.08
21	Z	608	CHL	C2D-C1D-ND	4.62	113.50	110.10
21	Z	609	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
21	4	607	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
25	K	202	BCR	C3-C4-C5	-4.59	105.89	114.08
22	4	602	CLA	CMB-C2B-C3B	4.58	133.25	124.68
25	K	205	BCR	C16-C17-C18	-4.58	120.77	127.31
25	3	620	BCR	C3-C4-C5	-4.58	105.90	114.08
25	K	202	BCR	C16-C17-C18	-4.57	120.78	127.31
22	X	613	CLA	CAA-C2A-C3A	-4.57	105.43	116.10
22	F	304	CLA	CAA-C2A-C3A	-4.57	105.44	116.10
22	1	612	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
21	2	606	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
22	A	823	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
21	Z	607	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
22	A	854	CLA	CMB-C2B-C3B	4.55	133.19	124.68
25	B	801	BCR	C16-C17-C18	-4.55	120.82	127.31
21	Y	606	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
24	4	620	XAT	O24-C25-C38	4.55	120.50	115.06
25	J	102	BCR	C24-C23-C22	-4.53	119.39	126.23
22	B	814	CLA	CMB-C2B-C3B	4.53	133.15	124.68
21	Z	606	CHL	CAC-C3C-C4C	4.52	130.68	124.81
24	Y	2622	XAT	C15-C14-C13	-4.52	120.86	127.31
22	Y	604	CLA	CMB-C2B-C3B	4.50	133.11	124.68
25	B	801	BCR	C16-C15-C14	-4.50	114.26	123.47
23	4	619	LUT	C35-C34-C33	-4.50	120.89	127.31
22	A	820	CLA	CMB-C2B-C3B	4.49	133.09	124.68
25	A	849	BCR	C11-C10-C9	-4.49	120.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	601	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
25	1	619	BCR	C28-C27-C26	-4.48	106.07	114.08
24	X	7622	XAT	O4-C5-C18	4.48	120.43	115.06
22	A	806	CLA	CAA-C2A-C3A	-4.48	100.51	112.78
25	L	305	BCR	C7-C8-C9	-4.47	119.48	126.23
22	O	2002	CLA	CAB-C3B-C4B	-4.47	121.59	128.46
25	B	844	BCR	C3-C4-C5	-4.47	106.09	114.08
22	B	806	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
29	A	844	PQN	C14-C13-C15	-4.47	107.76	115.27
21	Z	601	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
25	A	849	BCR	C7-C8-C9	-4.47	119.49	126.23
22	L	304	CLA	CMB-C2B-C3B	4.47	133.03	124.68
24	Y	2622	XAT	O24-C25-C38	4.47	120.41	115.06
21	4	608	CHL	C2D-C1D-ND	4.46	113.39	110.10
21	Y	601	CHL	C2C-C1C-NC	4.46	114.15	109.97
25	A	850	BCR	C16-C17-C18	-4.46	120.95	127.31
21	3	608	CHL	C2D-C1D-ND	4.46	113.39	110.10
22	N	1002	CLA	CMB-C2B-C3B	4.45	133.00	124.68
25	L	305	BCR	C16-C17-C18	-4.45	120.97	127.31
25	A	852	BCR	C24-C23-C22	-4.44	119.52	126.23
21	Y	601	CHL	C3C-C4C-NC	4.43	115.54	110.57
22	3	609	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
22	3	617	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
22	B	805	CLA	CMB-C2B-C3B	4.42	132.94	124.68
21	Y	608	CHL	C2D-C1D-ND	4.42	113.36	110.10
22	3	606	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
22	B	826	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
22	B	828	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
21	Y	607	CHL	CAA-C2A-C3A	-4.41	105.81	116.10
23	X	2620	LUT	C15-C14-C13	-4.41	121.02	127.31
22	B	839	CLA	CMB-C2B-C3B	4.39	132.90	124.68
21	X	606	CHL	C3D-C2D-C1D	-4.39	99.83	105.83
22	B	815	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
22	A	809	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
24	3	619	XAT	C18-C5-C6	-4.38	114.92	122.26
22	4	610	CLA	CMB-C2B-C1B	-4.38	121.74	128.46
22	1	602	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
22	2	604	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
21	X	601	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
21	4	606	CHL	CHD-C4C-C3C	-4.36	118.16	124.98
23	1	617	LUT	C35-C15-C14	-4.36	114.54	123.47
25	B	848	BCR	C3-C4-C5	-4.36	106.30	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	856	BCR	C28-C27-C26	-4.36	106.30	114.08
21	4	606	CHL	C3D-C2D-C1D	-4.35	99.89	105.83
21	X	608	CHL	C1B-CHB-C4A	-4.35	121.50	130.12
25	B	847	BCR	C7-C8-C9	-4.34	119.68	126.23
21	Y	605	CHL	C3D-C2D-C1D	-4.34	99.92	105.83
21	X	607	CHL	O2D-CGD-CBD	4.33	118.96	111.27
33	Z	7623	NEX	O24-C25-C38	4.33	120.24	115.06
21	X	606	CHL	CHD-C4C-C3C	-4.33	118.22	124.98
33	X	2623	NEX	O24-C25-C38	4.32	120.24	115.06
26	B	851	LHG	O4-P-O5	4.32	133.61	112.24
22	B	841	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
21	1	601	CHL	C3D-C2D-C1D	-4.32	99.94	105.83
28	A	801	CL0	C3D-C4D-ND	4.31	117.22	110.24
21	1	607	CHL	C1B-CHB-C4A	-4.31	121.59	130.12
25	I	101	BCR	C27-C26-C25	-4.30	116.49	122.73
22	Z	610	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
33	Z	7623	NEX	C38-C25-C26	-4.28	115.08	122.26
22	A	812	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
21	2	606	CHL	CHD-C4C-C3C	-4.28	118.29	124.98
22	3	615	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
21	Y	605	CHL	C2C-C1C-NC	4.26	113.97	109.97
21	2	608	CHL	O2D-CGD-CBD	4.26	118.84	111.27
24	2	620	XAT	O24-C25-C38	4.26	120.16	115.06
22	2	609	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
21	X	609	CHL	C2C-C1C-NC	4.26	113.96	109.97
22	B	837	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
21	X	607	CHL	C3D-C2D-C1D	-4.25	100.03	105.83
25	J	102	BCR	C16-C17-C18	-4.24	121.26	127.31
22	A	837	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
21	Y	607	CHL	O2D-CGD-CBD	4.23	118.78	111.27
23	Y	4620	LUT	C35-C34-C33	-4.23	121.28	127.31
25	B	843	BCR	C16-C17-C18	-4.22	121.28	127.31
21	Z	606	CHL	C3D-C2D-C1D	-4.22	100.07	105.83
22	2	603	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
22	A	830	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
33	Y	4623	NEX	C38-C25-C26	-4.22	115.19	122.26
22	A	828	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
21	Y	609	CHL	C1B-CHB-C4A	-4.21	121.78	130.12
26	Y	4630	LHG	O4-P-O5	4.21	133.03	112.24
23	1	617	LUT	C35-C34-C33	-4.20	121.31	127.31
25	I	101	BCR	C15-C16-C17	-4.19	114.89	123.47
24	1	618	XAT	C35-C15-C14	-4.19	114.89	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	613	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
21	Z	601	CHL	C3C-C4C-NC	4.19	115.27	110.57
22	A	832	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
21	Z	609	CHL	C3B-C4B-NB	4.18	114.62	109.21
25	B	847	BCR	C24-C23-C22	-4.18	119.92	126.23
25	L	301	BCR	C28-C27-C26	-4.18	106.62	114.08
22	A	824	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
25	G	205	BCR	C28-C27-C26	-4.18	106.62	114.08
23	X	2620	LUT	C35-C34-C33	-4.17	121.36	127.31
25	2	621	BCR	C16-C17-C18	-4.17	121.36	127.31
22	F	303	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
21	X	605	CHL	C4C-C3C-C2C	-4.16	100.83	106.90
24	Z	4622	XAT	C18-C5-C6	-4.16	115.29	122.26
26	A	846	LHG	O4-P-O5	4.16	132.80	112.24
33	Y	4623	NEX	C27-C28-C29	-4.16	119.08	125.53
22	Y	612	CLA	CAA-C2A-C3A	-4.16	106.40	116.10
25	F	305	BCR	C11-C10-C9	-4.16	121.38	127.31
21	Y	607	CHL	CHD-C4C-C3C	-4.15	118.49	124.98
26	X	2630	LHG	O4-P-O5	4.15	132.77	112.24
21	Z	607	CHL	CAC-C3C-C4C	4.15	130.20	124.81
25	3	620	BCR	C7-C8-C9	-4.15	119.97	126.23
22	A	803	CLA	CMB-C2B-C3B	4.15	132.44	124.68
26	2	622	LHG	O4-P-O5	4.15	132.75	112.24
21	X	605	CHL	CHD-C4C-C3C	-4.15	118.75	124.84
24	X	7622	XAT	C38-C25-C26	-4.14	115.33	122.26
22	2	614	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
22	3	603	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	B	832	CLA	CMB-C2B-C3B	4.13	132.41	124.68
21	1	607	CHL	C3C-C4C-NC	4.13	115.20	110.57
22	B	834	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
26	A	847	LHG	O4-P-O5	4.12	132.62	112.24
22	A	826	CLA	CMB-C2B-C3B	4.12	132.39	124.68
24	Z	4622	XAT	C11-C10-C9	-4.12	121.43	127.31
25	B	801	BCR	C20-C21-C22	-4.12	121.43	127.31
21	2	618	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
22	A	808	CLA	CMB-C2B-C3B	4.12	132.39	124.68
21	2	618	CHL	C2D-C1D-ND	4.12	113.14	110.10
22	N	1001	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
25	J	102	BCR	C15-C14-C13	-4.12	121.43	127.31
21	Y	607	CHL	C2D-C1D-ND	4.12	113.14	110.10
22	A	807	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
25	B	848	BCR	C16-C17-C18	-4.12	121.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	829	CLA	CMB-C2B-C3B	4.12	132.38	124.68
25	1	619	BCR	C15-C14-C13	-4.12	121.44	127.31
25	B	846	BCR	C7-C8-C9	-4.11	120.02	126.23
28	A	801	CL0	C3D-C2D-C1D	-4.11	100.22	105.83
33	Z	7623	NEX	C2-C1-C6	4.11	113.20	109.21
21	1	607	CHL	C3D-C2D-C1D	-4.10	100.23	105.83
21	Z	605	CHL	CHD-C4C-C3C	-4.10	118.57	124.98
22	4	612	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
26	1	620	LHG	O4-P-O5	4.10	132.50	112.24
21	2	607	CHL	CAC-C3C-C4C	4.10	130.13	124.81
22	Z	611	CLA	CAA-C2A-C3A	-4.09	106.55	116.10
21	4	607	CHL	C4C-C3C-C2C	-4.09	100.93	106.90
22	3	612	CLA	CMB-C2B-C1B	-4.09	122.19	128.46
21	X	608	CHL	CAA-C2A-C3A	-4.08	106.58	116.10
21	4	618	CHL	CAC-C3C-C4C	4.08	130.10	124.81
25	J	102	BCR	C3-C4-C5	-4.08	106.80	114.08
24	Y	2622	XAT	C31-C30-C29	-4.07	121.50	127.31
22	4	614	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
24	4	620	XAT	C18-C5-C6	-4.07	115.44	122.26
21	2	607	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
21	X	607	CHL	C3C-C4C-NC	4.07	115.01	110.57
22	B	821	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
25	A	856	BCR	C15-C14-C13	-4.06	121.51	127.31
22	A	840	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
22	B	813	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
22	A	814	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
22	3	614	CLA	CAA-C2A-C3A	-4.05	106.64	116.10
26	Z	7630	LHG	O4-P-O5	4.05	132.28	112.24
24	Z	4622	XAT	C27-C28-C29	-4.05	119.24	125.53
22	Y	614	CLA	CAB-C3B-C4B	-4.05	122.23	128.46
33	Z	7623	NEX	C15-C14-C13	-4.05	121.53	127.31
21	4	607	CHL	C2C-C1C-NC	4.05	113.77	109.97
22	A	831	CLA	CMB-C2B-C3B	4.05	132.25	124.68
21	2	606	CHL	CAC-C3C-C4C	4.05	131.20	125.04
22	1	611	CLA	CAA-C2A-C3A	-4.04	106.67	116.10
22	Y	610	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
22	A	816	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
22	A	854	CLA	C4A-NA-C1A	4.02	108.51	106.71
21	X	609	CHL	C4C-C3C-C2C	-4.01	101.05	106.90
22	B	816	CLA	CMB-C2B-C3B	4.01	132.18	124.68
21	Z	605	CHL	CAA-C2A-C3A	-4.01	106.74	116.10
25	K	202	BCR	C15-C16-C17	-4.01	115.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	823	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
22	A	835	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
25	A	849	BCR	C24-C23-C22	-4.00	120.19	126.23
21	X	605	CHL	C2D-C1D-ND	4.00	113.05	110.10
21	2	607	CHL	C3B-C4B-NB	4.00	114.39	109.21
22	B	830	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
21	X	608	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
25	K	205	BCR	C15-C14-C13	-4.00	121.60	127.31
25	4	621	BCR	C11-C10-C9	-3.99	121.62	127.31
21	Z	605	CHL	C2D-C1D-ND	3.99	113.04	110.10
22	A	806	CLA	CMB-C2B-C3B	3.99	132.14	124.68
22	B	818	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
22	B	841	CLA	CMB-C2B-C3B	3.98	132.13	124.68
22	X	610	CLA	CMB-C2B-C3B	3.97	132.12	124.68
21	X	607	CHL	C4A-NA-C1A	3.97	108.49	106.71
33	X	2623	NEX	C27-C28-C29	-3.97	119.36	125.53
25	A	851	BCR	C16-C17-C18	-3.97	121.64	127.31
25	B	846	BCR	C28-C27-C26	-3.96	107.01	114.08
22	3	610	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
21	2	606	CHL	C2D-C1D-ND	3.95	113.01	110.10
22	4	611	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
21	2	601	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
23	Y	4621	LUT	C15-C14-C13	-3.93	121.70	127.31
25	3	620	BCR	C15-C14-C13	-3.93	121.70	127.31
22	A	845	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
25	A	856	BCR	C3-C4-C5	-3.93	107.07	114.08
23	3	618	LUT	C35-C15-C14	-3.93	115.43	123.47
25	A	850	BCR	C24-C23-C22	-3.93	120.30	126.23
22	Z	610	CLA	CAD-CBD-CHA	3.92	105.96	102.11
21	X	605	CHL	C3B-C4B-NB	3.91	114.26	109.21
22	H	201	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
25	A	849	BCR	C20-C21-C22	-3.90	121.74	127.31
21	Y	605	CHL	C1B-CHB-C4A	-3.90	122.40	130.12
25	I	101	BCR	C11-C10-C9	-3.89	121.75	127.31
23	2	619	LUT	C15-C14-C13	-3.89	121.76	127.31
25	I	101	BCR	C20-C21-C22	-3.89	121.76	127.31
24	3	619	XAT	C35-C34-C33	-3.89	121.76	127.31
21	2	607	CHL	C2D-C1D-ND	3.88	112.97	110.10
22	B	825	CLA	CMB-C2B-C3B	3.88	131.95	124.68
25	G	205	BCR	C24-C23-C22	-3.88	120.37	126.23
33	Z	7623	NEX	C27-C28-C29	-3.88	119.51	125.53
21	X	609	CHL	CHD-C4C-C3C	-3.88	119.14	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	856	BCR	C15-C16-C17	-3.88	115.53	123.47
21	4	618	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
22	A	809	CLA	CMB-C2B-C3B	3.87	131.92	124.68
25	B	847	BCR	C20-C21-C22	-3.87	121.79	127.31
25	B	844	BCR	C24-C23-C22	-3.87	120.39	126.23
22	A	840	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
25	J	102	BCR	C15-C16-C17	-3.87	115.55	123.47
23	4	619	LUT	C35-C15-C14	-3.86	115.57	123.47
22	1	613	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
22	Y	612	CLA	CAB-C3B-C4B	-3.86	122.54	128.46
25	B	845	BCR	C16-C17-C18	-3.85	121.81	127.31
32	J	103	DGD	O3G-C3G-C2G	-3.85	101.60	110.90
22	3	607	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
22	A	822	CLA	CMB-C2B-C3B	3.84	131.87	124.68
25	F	305	BCR	C28-C27-C26	-3.84	107.21	114.08
25	B	847	BCR	C11-C10-C9	-3.84	121.83	127.31
21	Y	601	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
24	2	620	XAT	C4-C3-C2	-3.84	103.36	110.77
22	3	615	CLA	CAA-C2A-C3A	-3.84	107.15	116.10
23	1	621	LUT	C15-C14-C13	-3.83	121.84	127.31
21	Y	609	CHL	CHD-C4C-C3C	-3.83	119.21	124.84
25	L	301	BCR	C11-C10-C9	-3.83	121.85	127.31
22	B	806	CLA	CMB-C2B-C3B	3.83	131.84	124.68
24	4	620	XAT	O4-C5-C18	3.82	119.64	115.06
22	Y	603	CLA	CAA-C2A-C3A	-3.81	107.20	116.10
22	A	830	CLA	CMB-C2B-C3B	3.81	131.81	124.68
22	O	2001	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
33	Y	4623	NEX	O24-C25-C38	3.81	119.62	115.06
25	G	205	BCR	C16-C17-C18	-3.81	121.88	127.31
22	A	841	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
25	A	849	BCR	C15-C14-C13	-3.80	121.88	127.31
25	2	621	BCR	C7-C8-C9	-3.80	120.49	126.23
22	B	831	CLA	CMB-C2B-C3B	3.80	131.79	124.68
25	G	205	BCR	C20-C21-C22	-3.80	121.89	127.31
22	Y	614	CLA	CAA-C2A-C3A	-3.80	107.24	116.10
21	4	618	CHL	C2D-C1D-ND	3.80	112.90	110.10
25	A	848	BCR	C16-C15-C14	-3.79	115.70	123.47
25	A	851	BCR	C7-C8-C9	-3.79	120.51	126.23
22	A	823	CLA	CMB-C2B-C3B	3.79	131.76	124.68
22	A	813	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	Z	612	CLA	CBD-CHA-C1A	3.79	133.49	127.43
25	B	843	BCR	C3-C4-C5	-3.78	107.33	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	838	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
22	A	839	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
25	A	849	BCR	C16-C17-C18	-3.78	121.92	127.31
25	B	844	BCR	C15-C14-C13	-3.77	121.92	127.31
22	X	612	CLA	CAB-C3B-C4B	-3.77	122.66	128.46
22	3	612	CLA	C2A-C1A-CHA	3.77	130.45	123.86
24	Y	2622	XAT	C15-C35-C34	-3.76	115.77	123.47
25	B	845	BCR	C15-C14-C13	-3.76	121.94	127.31
25	2	621	BCR	C15-C14-C13	-3.76	121.95	127.31
25	L	306	BCR	C15-C14-C13	-3.75	121.96	127.31
22	2	609	CLA	CMB-C2B-C3B	3.75	131.69	124.68
22	3	617	CLA	CMB-C2B-C3B	3.74	131.68	124.68
22	A	842	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
21	4	608	CHL	O2D-CGD-CBD	3.74	117.92	111.27
22	1	602	CLA	CMB-C2B-C3B	3.74	131.68	124.68
25	L	306	BCR	C20-C21-C22	-3.74	121.97	127.31
21	Z	608	CHL	C1D-ND-C4D	-3.73	103.68	106.33
21	Y	606	CHL	CHD-C4C-C3C	-3.73	119.15	124.98
25	B	843	BCR	C20-C21-C22	-3.73	121.99	127.31
21	2	601	CHL	C1D-ND-C4D	-3.73	103.69	106.33
22	4	609	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	L	305	BCR	C15-C14-C13	-3.73	121.99	127.31
21	Z	608	CHL	C3B-C4B-NB	3.73	114.03	109.21
21	2	618	CHL	C3B-C4B-NB	3.72	114.02	109.21
22	A	831	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
22	K	204	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
21	2	608	CHL	C1D-ND-C4D	-3.71	103.70	106.33
22	Z	611	CLA	CAB-C3B-C4B	-3.71	122.76	128.46
22	A	821	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	X	604	CLA	CAB-C3B-C4B	-3.71	122.77	128.46
23	Z	7620	LUT	C35-C34-C33	-3.70	122.03	127.31
25	A	848	BCR	C23-C24-C25	-3.70	116.81	127.20
24	4	620	XAT	C35-C34-C33	-3.70	122.03	127.31
22	B	808	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
28	A	801	CL0	CAA-C2A-C3A	-3.69	102.66	112.78
22	B	822	CLA	CMB-C2B-C3B	3.69	131.58	124.68
22	1	611	CLA	CAB-C3B-C4B	-3.69	122.80	128.46
21	Z	607	CHL	C2D-C1D-ND	3.69	112.82	110.10
25	L	305	BCR	C20-C21-C22	-3.69	122.05	127.31
21	Y	609	CHL	C2D-C1D-ND	3.69	112.82	110.10
22	A	825	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	A	824	CLA	CAA-C2A-C3A	-3.68	107.50	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	601	CHL	CAC-C3C-C4C	3.68	129.59	124.81
22	1	614	CLA	CAB-C3B-C4B	-3.68	122.80	128.46
21	Z	601	CHL	C1B-CHB-C4A	-3.68	122.83	130.12
25	A	848	BCR	C38-C26-C25	-3.68	120.39	124.53
21	Z	606	CHL	CHD-C4C-C3C	-3.68	119.43	124.84
21	Y	606	CHL	C2D-C1D-ND	3.68	112.82	110.10
22	Z	614	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
22	3	607	CLA	CAB-C3B-C4B	-3.68	122.81	128.46
21	4	607	CHL	CAC-C3C-C4C	3.68	129.58	124.81
22	1	612	CLA	CMB-C2B-C3B	3.68	131.56	124.68
22	2	613	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
22	2	603	CLA	CMB-C2B-C3B	3.68	131.55	124.68
28	A	801	CL0	C1D-CHD-C4C	-3.67	118.13	126.06
33	Z	7623	NEX	C35-C34-C33	-3.67	122.07	127.31
25	F	305	BCR	C7-C8-C9	-3.67	120.69	126.23
23	Z	7621	LUT	C35-C34-C33	-3.67	122.07	127.31
22	2	610	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
25	A	856	BCR	C20-C21-C22	-3.66	122.08	127.31
22	X	614	CLA	CAB-C3B-C4B	-3.66	122.84	128.46
21	4	607	CHL	C2D-C1D-ND	3.66	112.80	110.10
22	Z	613	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
21	Z	606	CHL	C3B-C4B-NB	3.66	113.94	109.21
25	4	621	BCR	C15-C14-C13	-3.66	122.09	127.31
22	K	201	CLA	CAA-C2A-C3A	-3.65	107.58	116.10
24	2	620	XAT	C31-C30-C29	-3.65	122.10	127.31
28	A	801	CL0	C3C-C4C-NC	3.65	114.66	110.57
22	X	613	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
21	X	605	CHL	CAC-C3C-C4C	3.65	129.54	124.81
22	1	606	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
21	2	618	CHL	CAC-C3C-C4C	3.64	129.54	124.81
22	3	606	CLA	CMB-C2B-C3B	3.64	131.49	124.68
21	X	606	CHL	C1D-ND-C4D	-3.64	103.75	106.33
22	Y	613	CLA	CAB-C3B-C4B	-3.64	122.87	128.46
21	2	601	CHL	CAC-C3C-C4C	3.64	129.53	124.81
21	Y	607	CHL	CHB-C4A-NA	3.64	129.54	124.51
22	B	820	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	4	603	CLA	CAB-C3B-C4B	-3.64	122.88	128.46
21	X	609	CHL	C2D-C1D-ND	3.63	112.78	110.10
22	4	609	CLA	CHB-C4A-NA	3.63	129.53	124.51
22	Y	610	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
25	4	621	BCR	C3-C4-C5	-3.63	107.59	114.08
28	A	801	CL0	C1C-C2C-C3C	-3.63	103.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	306	BCR	C7-C8-C9	-3.63	120.75	126.23
25	A	852	BCR	C20-C19-C18	-3.63	116.23	126.42
22	4	613	CLA	CMB-C2B-C3B	3.63	131.46	124.68
21	X	609	CHL	CAD-CBD-CHA	-3.62	101.06	105.14
23	Y	4621	LUT	C10-C11-C12	-3.62	111.93	123.22
21	X	601	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
23	X	2621	LUT	C35-C34-C33	-3.61	122.15	127.31
22	A	834	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
33	Y	4623	NEX	C39-C29-C30	-3.61	117.86	122.92
24	2	620	XAT	C15-C14-C13	-3.61	122.16	127.31
22	B	815	CLA	CMB-C2B-C3B	3.61	131.43	124.68
22	2	614	CLA	CMB-C2B-C3B	3.61	131.43	124.68
22	B	810	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
22	A	832	CLA	CMB-C2B-C3B	3.60	131.42	124.68
22	Y	603	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	B	810	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	B	828	CLA	CMB-C2B-C3B	3.59	131.40	124.68
22	G	203	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
22	2	604	CLA	CMB-C2B-C3B	3.59	131.40	124.68
33	X	2623	NEX	C31-C30-C29	-3.59	122.19	127.31
21	4	608	CHL	C1B-CHB-C4A	-3.59	123.01	130.12
25	A	850	BCR	C20-C21-C22	-3.59	122.19	127.31
21	X	601	CHL	CMD-C2D-C3D	-3.58	119.37	127.61
21	3	608	CHL	C3B-C4B-NB	3.58	113.84	109.21
21	4	607	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
21	X	601	CHL	CAC-C3C-C4C	3.57	129.44	124.81
22	1	609	CLA	CAA-C2A-C3A	-3.57	107.77	116.10
22	A	829	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
25	B	846	BCR	C3-C4-C5	-3.56	107.71	114.08
31	A	857	LMU	C3'-C4'-C5'	-3.56	102.75	110.93
24	Z	4622	XAT	O24-C25-C38	3.56	119.33	115.06
22	K	201	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
21	3	608	CHL	CMC-C2C-C1C	3.56	130.46	125.04
25	B	847	BCR	C27-C26-C25	-3.56	117.56	122.73
22	Z	604	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
25	3	620	BCR	C21-C20-C19	-3.56	112.11	123.22
33	Y	4623	NEX	C15-C35-C34	-3.56	116.19	123.47
22	A	840	CLA	CMB-C2B-C3B	3.56	131.33	124.68
25	F	305	BCR	C16-C17-C18	-3.55	122.24	127.31
22	A	817	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
21	1	601	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
22	2	611	CLA	CAB-C3B-C4B	-3.55	123.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	604	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	2	614	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	A	811	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
22	1	616	CLA	CAB-C3B-C4B	-3.54	123.02	128.46
22	A	804	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
24	X	7622	XAT	C15-C35-C34	-3.54	116.23	123.47
22	A	802	CLA	CHB-C4A-NA	3.54	129.40	124.51
25	G	205	BCR	C15-C14-C13	-3.53	122.27	127.31
23	3	618	LUT	C35-C34-C33	-3.53	122.27	127.31
22	A	804	CLA	CHB-C4A-NA	3.53	129.40	124.51
23	1	621	LUT	C7-C8-C9	-3.53	120.90	126.23
22	Y	610	CLA	CMA-C3A-C2A	-3.53	107.87	116.10
22	B	811	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
21	X	608	CHL	C2D-C1D-ND	3.52	112.70	110.10
22	B	835	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
21	X	606	CHL	C2D-C1D-ND	3.52	112.69	110.10
22	4	610	CLA	CMB-C2B-C3B	3.52	131.25	124.68
22	J	101	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
32	B	850	DGD	O3G-C3G-C2G	-3.51	102.43	110.90
22	B	808	CLA	CHB-C4A-NA	3.51	129.36	124.51
21	Z	609	CHL	CHD-C4C-C3C	-3.51	119.69	124.84
25	A	856	BCR	C16-C17-C18	-3.51	122.31	127.31
22	B	817	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	3	602	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
21	Z	601	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
22	X	611	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	A	827	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
21	2	618	CHL	C1B-CHB-C4A	-3.49	123.20	130.12
25	B	843	BCR	C20-C19-C18	-3.49	116.61	126.42
21	Z	609	CHL	CAC-C3C-C4C	3.49	129.34	124.81
22	L	304	CLA	CAC-C3C-C4C	3.49	129.34	124.81
22	B	802	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
21	Y	601	CHL	CMD-C2D-C3D	-3.49	119.60	127.61
23	X	2620	LUT	C31-C30-C29	-3.48	122.34	127.31
22	A	828	CLA	CMB-C2B-C3B	3.48	131.19	124.68
21	Y	601	CHL	C4C-C3C-C2C	-3.48	101.83	106.90
22	Z	612	CLA	CAB-C3B-C4B	-3.48	123.12	128.46
21	X	605	CHL	CBD-CHA-C1A	3.47	132.99	127.43
22	3	612	CLA	CMB-C2B-C3B	3.47	131.17	124.68
22	B	821	CLA	CMB-C2B-C3B	3.47	131.17	124.68
21	4	606	CHL	C3B-C4B-NB	3.46	113.69	109.21
21	2	618	CHL	C1D-ND-C4D	-3.46	103.88	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	7621	LUT	C15-C14-C13	-3.46	122.37	127.31
24	Z	4622	XAT	C10-C11-C12	-3.46	112.43	123.22
22	A	818	CLA	CHB-C4A-NA	3.46	129.29	124.51
25	A	849	BCR	C3-C4-C5	-3.46	107.91	114.08
22	3	615	CLA	CMB-C2B-C3B	3.46	131.14	124.68
22	A	807	CLA	CMB-C2B-C3B	3.46	131.14	124.68
21	3	608	CHL	C1D-ND-C4D	-3.45	103.88	106.33
22	3	610	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
32	B	850	DGD	O5D-C6D-C5D	-3.45	102.66	109.05
23	2	619	LUT	C35-C34-C33	-3.45	122.39	127.31
22	Z	603	CLA	CAB-C3B-C4B	-3.45	123.17	128.46
22	X	610	CLA	CAA-C2A-C3A	-3.44	108.07	116.10
22	2	611	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
21	2	606	CHL	C1D-ND-C4D	-3.44	103.89	106.33
22	B	809	CLA	CMB-C2B-C3B	3.44	131.10	124.68
21	X	606	CHL	C3D-C4D-ND	3.43	115.79	110.24
22	A	812	CLA	CMB-C2B-C3B	3.43	131.10	124.68
25	3	620	BCR	C16-C17-C18	-3.43	122.41	127.31
22	A	809	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
22	1	604	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	A	814	CLA	CMB-C2B-C3B	3.43	131.10	124.68
21	2	601	CHL	C3B-C4B-NB	3.43	113.64	109.21
22	A	835	CLA	CMB-C2B-C3B	3.43	131.09	124.68
25	A	851	BCR	C15-C14-C13	-3.43	122.42	127.31
22	B	827	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
22	B	837	CLA	CMB-C2B-C3B	3.43	131.09	124.68
22	B	818	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	3	609	CLA	CHB-C4A-NA	3.42	129.25	124.51
24	X	7622	XAT	O24-C25-C38	3.42	119.16	115.06
22	A	816	CLA	CMB-C2B-C3B	3.42	131.07	124.68
21	Y	608	CHL	C1D-ND-C4D	-3.42	103.91	106.33
22	Y	614	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	L	302	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	Z	604	CLA	CAB-C3B-C4B	-3.41	123.22	128.46
21	2	608	CHL	C3B-C4B-NB	3.41	113.62	109.21
22	B	826	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	A	825	CLA	CHB-C4A-NA	3.41	129.23	124.51
25	B	846	BCR	C21-C20-C19	-3.41	112.59	123.22
25	A	849	BCR	C10-C11-C12	-3.41	112.59	123.22
24	4	620	XAT	C4-C3-C2	-3.40	104.20	110.77
24	X	7622	XAT	C11-C12-C13	-3.40	116.86	126.42
22	4	612	CLA	CMB-C2B-C3B	3.40	131.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	603	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	Z	603	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	1	609	CLA	CAB-C3B-C4B	-3.39	123.25	128.46
22	1	616	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
21	Z	601	CHL	CMD-C2D-C3D	-3.39	119.82	127.61
25	L	301	BCR	C15-C14-C13	-3.39	122.48	127.31
22	X	612	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	B	814	CLA	CHB-C4A-NA	3.38	129.18	124.51
24	1	618	XAT	O24-C25-C38	3.38	119.10	115.06
22	3	603	CLA	CMB-C2B-C3B	3.38	130.99	124.68
24	1	618	XAT	C4-C3-C2	-3.37	104.26	110.77
21	Z	605	CHL	C1D-ND-C4D	-3.37	103.94	106.33
22	Y	611	CLA	CAB-C3B-C4B	-3.37	123.28	128.46
22	Z	602	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
31	A	857	LMU	O1B-C1B-C2B	3.37	116.83	108.10
21	1	607	CHL	CAC-C3C-C4C	3.37	129.18	124.81
21	4	606	CHL	C2D-C1D-ND	3.37	112.59	110.10
22	Z	603	CLA	CAA-C2A-C3A	-3.37	105.85	114.26
22	A	804	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
22	Z	611	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	3	610	CLA	CMB-C2B-C3B	3.36	130.96	124.68
21	Y	606	CHL	C1D-ND-C4D	-3.36	103.95	106.33
33	Y	4623	NEX	C11-C10-C9	-3.36	122.52	127.31
25	1	619	BCR	C33-C5-C6	-3.35	120.77	124.53
22	B	813	CLA	CMB-C2B-C3B	3.35	130.94	124.68
22	A	824	CLA	CMA-C3A-C2A	-3.35	108.29	116.10
25	B	844	BCR	C20-C21-C22	-3.34	122.54	127.31
21	2	607	CHL	CHB-C4A-NA	3.34	129.13	124.51
22	B	824	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	B	846	BCR	C23-C24-C25	-3.34	117.83	127.20
21	4	618	CHL	CMD-C2D-C3D	-3.34	119.94	127.61
22	B	833	CLA	CAA-C2A-C3A	-3.33	103.65	112.78
22	A	854	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
25	B	846	BCR	C11-C10-C9	-3.33	122.56	127.31
21	2	606	CHL	C3B-C4B-NB	3.33	113.51	109.21
22	4	603	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	O	2002	CLA	CAB-C3B-C2B	3.32	131.20	124.69
25	3	620	BCR	C11-C10-C9	-3.32	122.57	127.31
22	B	808	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
22	X	604	CLA	CAA-C2A-C3A	-3.32	108.35	116.10
22	X	603	CLA	CAA-C2A-C3A	-3.32	105.97	114.26
22	Y	612	CLA	C2A-C1A-CHA	3.32	129.65	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	610	CLA	CAA-C2A-C3A	-3.32	108.36	116.10
22	Y	611	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
22	Y	610	CLA	CAB-C3B-C4B	-3.31	123.37	128.46
22	N	1001	CLA	CMB-C2B-C3B	3.31	130.88	124.68
25	B	845	BCR	C20-C21-C22	-3.31	122.58	127.31
22	2	612	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	B	811	CLA	CAB-C3B-C4B	-3.31	123.38	128.46
22	B	831	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
22	Z	610	CLA	CMB-C2B-C3B	3.31	130.86	124.68
22	A	841	CLA	CMB-C2B-C3B	3.30	130.86	124.68
22	X	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
21	Z	606	CHL	C3D-C4D-ND	3.30	115.58	110.24
24	Y	2622	XAT	C4-C3-C2	-3.30	104.40	110.77
25	B	847	BCR	C33-C5-C4	3.30	119.95	113.62
25	A	850	BCR	C33-C5-C6	-3.30	120.82	124.53
21	X	601	CHL	C3D-C4D-ND	3.30	115.57	110.24
24	3	619	XAT	C35-C15-C14	-3.30	116.72	123.47
21	4	618	CHL	C1D-ND-C4D	-3.29	104.00	106.33
22	B	805	CLA	CHB-C4A-NA	3.29	129.07	124.51
25	B	844	BCR	C34-C9-C10	-3.29	118.31	122.92
21	Y	609	CHL	CAC-C3C-C4C	3.29	129.08	124.81
22	4	609	CLA	O1D-CGD-CBD	3.29	131.22	124.48
21	2	607	CHL	C1D-ND-C4D	-3.29	104.00	106.33
25	K	205	BCR	C28-C27-C26	-3.29	108.21	114.08
22	A	802	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
22	4	614	CLA	CMB-C2B-C3B	3.28	130.82	124.68
22	1	609	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	F	303	CLA	CMB-C2B-C3B	3.28	130.81	124.68
22	Y	613	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	4	601	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	B	811	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
21	4	606	CHL	C3D-C4D-ND	3.28	115.54	110.24
22	3	609	CLA	CMB-C2B-C3B	3.27	130.80	124.68
25	A	848	BCR	C20-C21-C22	-3.27	122.64	127.31
22	1	604	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	G	205	BCR	C7-C8-C9	-3.27	121.30	126.23
21	2	608	CHL	CHB-C4A-NA	3.27	129.03	124.51
22	1	614	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
22	A	837	CLA	CMB-C2B-C3B	3.27	130.79	124.68
22	O	2002	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	A	832	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
21	X	608	CHL	C3B-C4B-NB	3.26	113.43	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	846	BCR	C33-C5-C4	3.26	119.88	113.62
21	4	607	CHL	C3D-C4D-ND	3.26	115.51	110.24
21	Y	609	CHL	C3B-C4B-NB	3.26	113.43	109.21
21	X	606	CHL	CMD-C2D-C3D	-3.26	120.11	127.61
22	G	204	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
21	X	609	CHL	C3D-C4D-ND	3.26	115.51	110.24
23	X	2621	LUT	C15-C14-C13	-3.26	122.66	127.31
22	A	802	CLA	CMD-C2D-C1D	-3.26	118.98	124.71
22	3	614	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
22	B	823	CLA	CMB-C2B-C3B	3.25	130.75	124.68
22	B	838	CLA	CMB-C2B-C3B	3.25	130.75	124.68
22	Z	610	CLA	CAA-C2A-C3A	-3.24	108.53	116.10
21	Z	606	CHL	C2D-C1D-ND	3.24	112.49	110.10
22	B	834	CLA	CMB-C2B-C3B	3.24	130.74	124.68
25	K	202	BCR	C29-C30-C25	3.24	115.47	110.48
22	3	609	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	A	848	BCR	C38-C26-C27	3.23	119.82	113.62
22	B	816	CLA	CHB-C4A-NA	3.23	128.98	124.51
22	A	825	CLA	CMB-C2B-C3B	3.23	130.72	124.68
21	X	608	CHL	CBD-CHA-C1A	3.23	132.60	127.43
21	1	607	CHL	C3B-C4B-NB	3.23	113.38	109.21
22	1	611	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
23	X	2620	LUT	C11-C10-C9	-3.23	122.71	127.31
22	A	840	CLA	O2D-CGD-CBD	3.22	117.00	111.27
21	Y	606	CHL	C3D-C4D-ND	3.22	115.45	110.24
22	1	613	CLA	CMB-C2B-C3B	3.22	130.71	124.68
21	2	606	CHL	C3D-C4D-ND	3.22	115.45	110.24
22	X	613	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	A	801	CL0	C3B-C4B-NB	3.22	113.37	109.21
22	A	836	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
21	Z	609	CHL	CMD-C2D-C3D	-3.22	120.21	127.61
21	Y	606	CHL	CAA-C2A-C3A	-3.22	108.59	116.10
24	3	619	XAT	C24-C23-C22	-3.22	104.56	110.77
25	B	844	BCR	C30-C25-C26	-3.21	118.09	122.61
25	A	848	BCR	C11-C10-C9	-3.21	122.72	127.31
21	4	606	CHL	C1D-ND-C4D	-3.21	104.05	106.33
22	K	206	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
22	X	614	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
22	Z	612	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
22	3	617	CLA	CAA-C2A-C3A	-3.21	108.61	116.10
22	B	824	CLA	CHB-C4A-NA	3.21	128.95	124.51
32	B	850	DGD	O6D-C1D-O3G	-3.21	102.37	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	812	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	3	604	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
22	X	603	CLA	CHB-C4A-NA	3.20	128.94	124.51
21	4	608	CHL	CMB-C2B-C3B	3.20	130.66	124.68
22	G	201	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
22	B	828	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	A	802	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
21	2	618	CHL	C3D-C4D-ND	3.19	115.39	110.24
22	B	840	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
25	1	619	BCR	C21-C20-C19	-3.19	113.28	123.22
21	Y	607	CHL	C1D-ND-C4D	-3.19	104.07	106.33
23	3	618	LUT	C36-C21-C26	3.19	114.37	109.55
21	X	606	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
22	A	841	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	2	610	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	B	847	BCR	C21-C20-C19	-3.18	113.29	123.22
21	4	607	CHL	C1D-ND-C4D	-3.18	104.08	106.33
22	Z	602	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
23	1	621	LUT	C11-C10-C9	-3.18	122.78	127.31
25	K	202	BCR	C11-C10-C9	-3.18	122.78	127.31
25	G	205	BCR	C10-C11-C12	-3.18	113.30	123.22
22	2	613	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
22	A	838	CLA	CAC-C3C-C4C	3.17	128.93	124.81
22	A	842	CLA	CHB-C4A-NA	3.17	128.90	124.51
21	X	605	CHL	C1D-ND-C4D	-3.17	104.08	106.33
22	B	807	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
24	3	619	XAT	C10-C11-C12	-3.17	113.33	123.22
33	X	2623	NEX	C35-C34-C33	-3.16	122.79	127.31
23	Y	4620	LUT	C15-C14-C13	-3.16	122.80	127.31
21	Z	601	CHL	C3D-C4D-ND	3.16	115.36	110.24
33	Z	7623	NEX	C24-C23-C22	-3.16	104.67	110.77
23	1	617	LUT	C30-C31-C32	-3.16	113.35	123.22
33	Y	4623	NEX	C35-C34-C33	-3.16	122.80	127.31
22	2	614	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
21	1	607	CHL	CMD-C2D-C3D	-3.16	120.34	127.61
22	B	803	CLA	CHB-C4A-NA	3.16	128.88	124.51
24	4	620	XAT	C10-C11-C12	-3.16	113.37	123.22
24	4	620	XAT	C24-C23-C22	-3.15	104.69	110.77
22	X	610	CLA	CMA-C3A-C2A	-3.15	108.75	116.10
21	Z	609	CHL	C2D-C1D-ND	3.15	112.42	110.10
25	A	851	BCR	C11-C10-C9	-3.15	122.82	127.31
22	B	834	CLA	O2D-CGD-O1D	-3.15	117.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	847	BCR	C16-C17-C18	-3.15	122.82	127.31
22	1	603	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
22	K	206	CLA	CBD-CHA-C1A	3.15	132.21	128.50
21	Z	606	CHL	C1D-ND-C4D	-3.14	104.10	106.33
22	B	836	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
22	K	201	CLA	CHB-C4A-NA	3.14	128.86	124.51
22	B	819	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	I	101	BCR	C33-C5-C6	-3.14	121.01	124.53
25	I	101	BCR	C30-C25-C26	-3.14	118.20	122.61
25	B	848	BCR	C28-C27-C26	-3.14	108.48	114.08
22	2	611	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	A	839	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
21	Y	601	CHL	C3D-C4D-ND	3.13	115.31	110.24
22	B	834	CLA	CHB-C4A-NA	3.13	128.84	124.51
21	Y	608	CHL	C1B-CHB-C4A	-3.13	123.92	130.12
25	L	301	BCR	C23-C24-C25	-3.13	118.41	127.20
22	1	609	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	K	201	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	Y	605	CHL	C4A-NA-C1A	3.13	108.11	106.71
31	A	857	LMU	C6B-C5B-C4B	-3.12	105.69	113.00
21	Z	601	CHL	CAC-C3C-C4C	3.12	128.86	124.81
25	2	621	BCR	C1-C6-C5	-3.12	118.22	122.61
21	X	601	CHL	C1D-ND-C4D	-3.12	104.12	106.33
28	A	801	CL0	C1-C2-C3	-3.11	120.66	126.04
25	A	849	BCR	C31-C1-C6	-3.11	105.25	110.30
22	1	602	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	Z	614	CLA	CMB-C2B-C3B	3.11	130.50	124.68
21	Z	609	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
21	X	608	CHL	CAC-C3C-C4C	3.11	128.84	124.81
21	Y	601	CHL	C2D-C1D-ND	3.11	112.39	110.10
22	B	837	CLA	CHB-C4A-NA	3.11	128.81	124.51
22	Y	612	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
22	A	813	CLA	CHB-C4A-NA	3.10	128.80	124.51
22	Z	602	CLA	CAB-C3B-C4B	-3.10	123.70	128.46
21	Y	607	CHL	CAC-C3C-C4C	3.10	129.76	125.04
32	J	103	DGD	O6D-C1D-O3G	-3.10	102.63	109.97
22	A	803	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
22	B	807	CLA	O1D-CGD-CBD	3.10	130.82	124.48
22	A	825	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	3	610	CLA	CAA-C2A-C3A	-3.10	108.87	116.10
23	4	619	LUT	C15-C14-C13	-3.09	122.90	127.31
22	3	604	CLA	CAB-C3B-C4B	-3.09	123.71	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	847	BCR	C4-C5-C6	-3.09	118.24	122.73
21	1	607	CHL	C4A-NA-C1A	3.09	108.09	106.71
23	4	619	LUT	C10-C11-C12	-3.09	113.58	123.22
21	1	607	CHL	C3D-C4D-ND	3.09	115.23	110.24
21	Z	608	CHL	CAC-C3C-C4C	3.09	128.81	124.81
22	1	608	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
22	3	613	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
21	4	606	CHL	CMD-C2D-C3D	-3.08	120.52	127.61
25	A	850	BCR	C27-C26-C25	-3.08	118.26	122.73
21	Z	605	CHL	C3D-C4D-ND	3.08	115.22	110.24
33	Y	4623	NEX	C24-C23-C22	-3.08	104.83	110.77
22	Z	613	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	B	824	CLA	CMB-C2B-C3B	3.08	130.44	124.68
25	B	846	BCR	C33-C5-C6	-3.08	121.07	124.53
22	A	845	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	K	202	BCR	C20-C19-C18	-3.08	117.78	126.42
22	A	809	CLA	O2D-CGD-CBD	3.07	116.73	111.27
22	Y	602	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
25	1	619	BCR	C7-C8-C9	-3.07	121.59	126.23
24	Y	2622	XAT	C26-C27-C28	-3.07	119.50	125.99
22	X	613	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	A	840	CLA	CHB-C4A-NA	3.07	128.76	124.51
21	Y	606	CHL	CAC-C3C-C4C	3.07	129.72	125.04
33	Z	7623	NEX	C39-C29-C30	-3.07	118.62	122.92
22	A	843	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	Y	614	CLA	CAB-C3B-C2B	3.07	130.70	124.69
22	B	812	CLA	CHB-C4A-NA	3.07	128.75	124.51
25	A	852	BCR	C34-C9-C10	-3.07	118.63	122.92
22	O	2001	CLA	CMB-C2B-C3B	3.06	130.41	124.68
28	A	801	CL0	O2A-CGA-CBA	3.06	121.52	111.91
22	A	805	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	2	607	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
21	Z	607	CHL	C1B-CHB-C4A	-3.06	124.06	130.12
22	X	602	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
22	B	805	CLA	O2A-C1-C2	-3.06	100.60	108.64
22	X	604	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
31	A	857	LMU	C1B-O5B-C5B	3.06	119.69	113.69
22	A	842	CLA	CMB-C2B-C3B	3.06	130.39	124.68
22	1	616	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	1	614	CLA	CAA-C2A-C3A	-3.05	108.97	116.10
24	2	620	XAT	C24-C23-C22	-3.05	104.88	110.77
22	A	818	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	101	BCR	C38-C26-C27	3.05	119.48	113.62
23	Y	4620	LUT	C35-C15-C14	-3.05	117.22	123.47
21	Z	608	CHL	CHB-C4A-NA	3.05	128.73	124.51
21	2	608	CHL	C1C-C2C-C3C	-3.05	104.69	107.11
21	X	607	CHL	CAC-C3C-C4C	3.05	129.68	125.04
25	1	619	BCR	C33-C5-C4	3.05	119.47	113.62
22	B	808	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	G	205	BCR	C3-C4-C5	-3.05	108.64	114.08
22	B	805	CLA	CAC-C3C-C4C	3.05	128.76	124.81
22	1	610	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
22	B	821	CLA	CHB-C4A-NA	3.05	128.72	124.51
25	L	306	BCR	C21-C20-C19	-3.04	113.72	123.22
22	G	203	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	B	810	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
22	2	609	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	2	610	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	B	832	CLA	CHB-C4A-NA	3.04	128.71	124.51
31	A	857	LMU	O5B-C5B-C4B	3.04	115.21	109.69
25	L	306	BCR	C16-C17-C18	-3.04	122.98	127.31
22	Y	602	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
21	Y	605	CHL	C3D-C4D-ND	3.03	115.14	110.24
21	Y	605	CHL	CHD-C4C-C3C	-3.03	120.24	124.98
21	X	609	CHL	C1B-CHB-C4A	-3.03	124.11	130.12
23	Y	4621	LUT	C19-C9-C8	3.03	122.85	118.08
23	Z	7620	LUT	C30-C31-C32	-3.03	113.76	123.22
22	4	611	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	A	845	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	3	617	CLA	O2D-CGD-O1D	-3.03	117.21	124.09
22	B	823	CLA	CAA-CBA-CGA	-3.03	104.47	112.51
22	B	818	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	J	101	CLA	CHB-C4A-NA	3.03	128.70	124.51
23	Y	4620	LUT	C31-C30-C29	-3.03	122.99	127.31
22	Y	610	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
22	Y	613	CLA	CHB-C4A-NA	3.03	128.70	124.51
22	B	816	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
22	1	606	CLA	CMB-C2B-C3B	3.02	130.34	124.68
22	B	803	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
22	A	827	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	F	304	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
21	2	607	CHL	C3D-C4D-ND	3.02	115.13	110.24
21	Y	606	CHL	CHB-C4A-NA	3.02	128.69	124.51
22	4	613	CLA	CHB-C4A-NA	3.02	128.69	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	812	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
22	L	303	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
21	Z	607	CHL	CAB-C3B-C4B	-3.01	123.83	128.46
25	1	619	BCR	C11-C10-C9	-3.01	123.01	127.31
22	B	817	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	B	847	BCR	C38-C26-C27	3.01	119.40	113.62
22	B	804	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	Z	602	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	B	820	CLA	CHB-C4A-NA	3.01	128.67	124.51
23	X	2621	LUT	C31-C30-C29	-3.01	123.02	127.31
25	K	205	BCR	C20-C19-C18	-3.01	117.97	126.42
33	X	2623	NEX	C11-C10-C9	-3.00	123.02	127.31
21	1	601	CHL	C2D-C1D-ND	3.00	112.32	110.10
25	A	848	BCR	C7-C8-C9	-3.00	121.70	126.23
22	A	838	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	B	844	BCR	C33-C5-C6	-3.00	121.16	124.53
25	I	101	BCR	C33-C5-C4	3.00	119.38	113.62
32	B	850	DGD	C3G-C2G-C1G	-3.00	104.70	111.79
22	A	826	CLA	C2A-C1A-CHA	3.00	129.10	123.86
22	F	301	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
28	A	801	CL0	O2D-CGD-O1D	-3.00	117.98	123.84
22	B	841	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	L	302	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	B	845	BCR	C11-C10-C9	-2.99	123.04	127.31
22	B	819	CLA	CHB-C4A-NA	2.99	128.65	124.51
22	B	808	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	K	204	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	3	619	XAT	C4-C3-C2	-2.99	105.00	110.77
21	Z	609	CHL	CHB-C4A-NA	2.99	128.64	124.51
25	K	202	BCR	C2-C1-C6	2.99	115.08	110.48
25	B	844	BCR	C16-C17-C18	-2.98	123.05	127.31
23	1	617	LUT	C38-C25-C24	-2.98	117.17	123.56
21	4	606	CHL	CHB-C4A-NA	2.98	128.64	124.51
22	B	805	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	Y	612	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	B	830	CLA	CMB-C2B-C3B	2.98	130.26	124.68
22	J	101	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	4	617	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	4	604	CLA	CHB-C4A-NA	2.98	128.63	124.51
21	Z	601	CHL	C2D-C1D-ND	2.98	112.30	110.10
22	B	830	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	K	204	CLA	CMB-C2B-C3B	2.98	130.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	609	CHL	C3D-C4D-ND	2.98	115.05	110.24
21	X	609	CHL	C1D-ND-C4D	-2.98	104.22	106.33
21	Y	605	CHL	CMD-C2D-C3D	-2.98	120.77	127.61
22	3	613	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	K	205	BCR	C24-C23-C22	-2.98	121.74	126.23
22	A	835	CLA	CMC-C2C-C1C	-2.97	120.51	125.04
22	A	822	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
21	Y	609	CHL	CBD-CHA-C1A	2.97	132.19	127.43
25	B	845	BCR	C1-C6-C5	-2.97	118.43	122.61
22	A	841	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
22	3	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	B	846	BCR	C30-C25-C26	-2.97	118.43	122.61
21	X	601	CHL	C2D-C1D-ND	2.97	112.29	110.10
22	A	832	CLA	CHB-C4A-NA	2.97	128.62	124.51
32	J	103	DGD	O6E-C5E-C4E	2.96	115.08	109.69
22	4	611	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	4	608	CHL	C1C-C2C-C3C	-2.96	104.76	107.11
25	L	301	BCR	C30-C25-C26	-2.96	118.44	122.61
25	B	845	BCR	C34-C9-C10	-2.96	118.78	122.92
22	A	804	CLA	CMB-C2B-C3B	2.96	130.21	124.68
21	X	605	CHL	C3D-C4D-ND	2.96	115.02	110.24
21	Y	606	CHL	CMD-C2D-C3D	-2.96	120.81	127.61
22	A	822	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
22	4	604	CLA	CAB-C3B-C4B	-2.96	123.92	128.46
22	A	816	CLA	CHB-C4A-NA	2.96	128.60	124.51
21	Z	607	CHL	CHC-C1C-NC	2.96	128.69	124.20
21	3	608	CHL	C4C-C3C-C2C	-2.96	102.59	106.90
21	X	606	CHL	CMB-C2B-C3B	2.95	130.47	124.69
22	B	833	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
22	3	607	CLA	CMB-C2B-C3B	2.95	130.47	124.69
22	4	609	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	Z	613	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	B	846	BCR	C38-C26-C27	2.95	119.28	113.62
22	A	808	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	A	848	BCR	C30-C25-C26	-2.95	118.46	122.61
22	A	835	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	Z	609	CHL	C3D-C4D-ND	2.95	115.00	110.24
22	Z	614	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	A	845	CLA	CHB-C4A-NA	2.94	128.58	124.51
22	Y	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	801	BCR	C20-C19-C18	-2.94	118.16	126.42
22	B	835	CLA	O2D-CGD-O1D	-2.94	118.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	820	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
22	A	819	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	B	846	BCR	C1-C6-C5	-2.94	118.48	122.61
23	3	618	LUT	C7-C8-C9	-2.93	121.80	126.23
22	2	612	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
21	2	601	CHL	C3D-C4D-ND	2.93	114.98	110.24
21	X	607	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
22	X	611	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	A	836	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	A	831	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
21	3	608	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
22	Y	603	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	B	847	BCR	C10-C11-C12	-2.93	114.08	123.22
22	A	805	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	4	618	CHL	C3D-C4D-ND	2.93	114.97	110.24
22	4	612	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	B	819	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
25	B	848	BCR	C10-C11-C12	-2.92	114.09	123.22
22	4	613	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
32	J	103	DGD	C3G-C2G-C1G	-2.92	104.87	111.79
25	B	846	BCR	C15-C14-C13	-2.92	123.14	127.31
22	A	817	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	A	813	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	A	810	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	B	807	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	G	205	BCR	C38-C26-C27	2.92	119.22	113.62
22	A	834	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
21	Y	601	CHL	C1D-ND-C4D	-2.92	104.26	106.33
22	3	607	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
22	A	821	CLA	CHB-C4A-NA	2.91	128.54	124.51
22	B	832	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	A	829	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	X	612	CLA	CAB-C3B-C2B	2.91	130.39	124.69
22	4	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	3	603	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	Y	610	CLA	CMB-C2B-C3B	2.91	130.38	124.69
24	4	620	XAT	C15-C14-C13	-2.91	123.16	127.31
21	4	608	CHL	C3B-C4B-NB	2.91	112.97	109.21
22	Z	610	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
21	2	608	CHL	O2A-CGA-CBA	2.90	121.02	111.91
22	K	203	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
23	Y	4621	LUT	C38-C25-C24	-2.90	117.34	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	615	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	4	601	CLA	CHB-C4A-NA	2.90	128.53	124.51
21	Y	608	CHL	CMB-C2B-C3B	2.90	130.37	124.69
22	K	203	CLA	CHB-C4A-NA	2.90	128.53	124.51
21	2	601	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
24	4	620	XAT	O4-C5-C6	-2.90	56.56	58.96
22	B	808	CLA	O2D-CGD-CBD	2.90	116.42	111.27
22	X	611	CLA	CBD-CHA-C1A	2.90	131.92	128.50
22	X	612	CLA	CHB-C4A-NA	2.90	128.52	124.51
22	B	840	CLA	CHB-C4A-NA	2.90	128.52	124.51
22	Z	603	CLA	CHB-C4A-NA	2.90	128.52	124.51
26	A	846	LHG	O8-C23-C24	2.90	121.00	111.91
21	X	601	CHL	CBD-CHA-C1A	2.90	132.07	127.43
24	Y	2622	XAT	C27-C28-C29	-2.90	121.04	125.53
22	1	603	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	1	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	J	101	CLA	CAA-C2A-C3A	-2.89	107.03	114.26
22	Z	610	CLA	CMA-C3A-C2A	-2.89	109.35	116.10
22	1	604	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	2	621	BCR	C11-C10-C9	-2.89	123.18	127.31
21	Y	608	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
21	1	607	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
21	Z	601	CHL	C3B-C4B-NB	2.89	112.94	109.21
25	J	102	BCR	C10-C11-C12	-2.88	114.21	123.22
22	Y	610	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	Y	612	CLA	CAB-C3B-C2B	2.88	130.34	124.69
25	1	619	BCR	C29-C30-C25	2.88	114.92	110.48
25	B	843	BCR	C2-C1-C6	2.88	114.92	110.48
22	G	204	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	B	845	BCR	C33-C5-C6	-2.88	121.29	124.53
22	L	303	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	A	824	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	O	2002	CLA	CMB-C2B-C3B	2.88	130.32	124.69
21	2	606	CHL	CMB-C2B-C3B	2.88	130.06	124.68
25	1	619	BCR	C1-C6-C5	-2.88	118.56	122.61
22	A	804	CLA	O2D-CGD-CBD	2.88	116.38	111.27
22	3	609	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
22	K	204	CLA	CHB-C4A-NA	2.87	128.49	124.51
25	B	801	BCR	C15-C14-C13	-2.87	123.21	127.31
22	B	814	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	B	827	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	2	609	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	614	CLA	CMB-C2B-C3B	2.87	130.31	124.69
33	Z	7623	NEX	C26-C27-C28	-2.87	119.92	125.99
22	A	817	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	1	607	CHL	CHD-C4C-C3C	-2.87	120.62	124.84
22	A	835	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	3	610	CLA	CMA-C3A-C2A	-2.87	109.41	116.10
22	B	808	CLA	CBA-CAA-C2A	2.87	122.33	113.86
22	A	824	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	B	815	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	Y	4621	LUT	C35-C34-C33	-2.87	123.22	127.31
25	A	850	BCR	C33-C5-C4	2.86	119.11	113.62
22	2	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
22	H	201	CLA	CMB-C2B-C3B	2.86	130.03	124.68
21	X	607	CHL	C3D-C4D-ND	2.86	114.87	110.24
21	Z	608	CHL	C3D-C4D-ND	2.86	114.87	110.24
22	A	843	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	B	817	CLA	CHB-C4A-NA	2.86	128.47	124.51
22	B	803	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	B	819	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	X	612	CLA	CAA-C2A-C3A	-2.86	107.12	114.26
23	Z	7620	LUT	C15-C14-C13	-2.85	123.24	127.31
22	A	835	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	B	823	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	A	821	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	3	607	CLA	CAB-C3B-C2B	2.85	130.26	124.69
22	1	610	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	B	813	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	1	606	CLA	C2D-C1D-ND	-2.85	108.01	110.10
22	1	614	CLA	CHB-C4A-NA	2.84	128.45	124.51
22	A	830	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	810	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	Z	7621	LUT	C31-C30-C29	-2.84	123.25	127.31
22	B	820	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	820	CLA	CMB-C2B-C3B	2.84	129.99	124.68
21	Y	607	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
24	3	619	XAT	C30-C31-C32	-2.84	114.36	123.22
28	A	801	CL0	CHC-C1C-C2C	-2.83	118.88	126.72
22	2	614	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
22	F	304	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	Z	606	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
22	B	828	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	Z	601	CHL	C1C-C2C-C3C	-2.83	104.87	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	811	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	F	304	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	N	1001	CLA	O2D-CGD-O1D	-2.83	117.66	124.09
22	B	804	CLA	CHB-C4A-NA	2.83	128.42	124.51
27	G	202	LMG	O6-C1-O1	-2.83	103.28	109.97
22	1	604	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	J	101	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	B	848	BCR	C29-C30-C25	2.82	114.83	110.48
22	4	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	X	603	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	A	805	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
22	3	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	1	611	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	L	301	BCR	C34-C9-C10	-2.82	118.97	122.92
22	G	201	CLA	CHB-C4A-NA	2.82	128.41	124.51
32	B	850	DGD	CDB-CCB-CBB	-2.82	100.11	114.42
22	X	604	CLA	CAB-C3B-C2B	2.82	130.21	124.69
21	1	601	CHL	C3D-C4D-ND	2.82	114.80	110.24
22	Z	612	CLA	CAA-C2A-C3A	-2.82	107.22	114.26
25	A	850	BCR	C1-C6-C5	-2.81	118.65	122.61
24	2	620	XAT	O4-C5-C6	-2.81	56.63	58.96
22	A	817	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	B	843	BCR	C10-C11-C12	-2.81	114.44	123.22
21	Y	606	CHL	CMB-C2B-C3B	2.81	130.19	124.69
22	Z	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
31	A	857	LMU	O1B-C4'-C5'	2.81	117.15	109.45
21	X	608	CHL	C3D-C4D-ND	2.81	114.78	110.24
25	F	305	BCR	C21-C20-C19	-2.81	114.45	123.22
21	Y	607	CHL	C3D-C4D-ND	2.81	114.78	110.24
22	Y	614	CLA	O2D-CGD-O1D	-2.81	117.71	124.09
21	Z	607	CHL	CAA-C2A-C3A	-2.81	105.09	112.78
22	B	803	CLA	CAC-C3C-C2C	-2.81	122.73	127.53
25	3	620	BCR	C16-C15-C14	-2.81	117.72	123.47
22	2	611	CLA	CAB-C3B-C2B	2.81	130.19	124.69
22	Y	613	CLA	CAB-C3B-C2B	2.81	130.19	124.69
22	L	304	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	K	202	BCR	C27-C26-C25	-2.81	118.66	122.73
21	2	606	CHL	O2D-CGD-O1D	-2.81	118.35	123.84
22	B	822	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	Y	608	CHL	C3D-C4D-ND	2.80	114.77	110.24
25	4	621	BCR	C33-C5-C6	-2.80	121.38	124.53
22	G	203	CLA	CHB-C4A-NA	2.80	128.39	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	824	CLA	O2D-CGD-CBD	2.80	116.25	111.27
21	X	606	CHL	CBD-CHA-C1A	2.80	131.80	128.50
22	B	813	CLA	CBC-CAC-C3C	2.80	120.15	112.43
25	2	621	BCR	C29-C30-C25	2.80	114.79	110.48
25	A	856	BCR	C2-C1-C6	2.80	114.79	110.48
23	4	619	LUT	C30-C31-C32	-2.80	114.49	123.22
22	1	603	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	L	303	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	G	201	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	Z	611	CLA	CAB-C3B-C2B	2.80	130.16	124.69
22	4	614	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
21	1	601	CHL	C3B-C4B-NB	2.79	112.82	109.21
22	A	806	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	K	203	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	B	807	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	4	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	3	602	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
22	B	826	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	Y	611	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	A	820	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	A	820	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	3	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	A	814	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	2	618	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
22	A	815	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	B	828	CLA	C2D-C1D-ND	-2.79	108.05	110.10
33	X	2623	NEX	C39-C29-C30	-2.79	119.02	122.92
21	3	608	CHL	C1C-C2C-C3C	-2.78	104.03	106.96
22	3	610	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	2	610	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	4	621	BCR	C21-C20-C19	-2.78	114.55	123.22
22	B	817	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	4	620	XAT	C19-C9-C8	2.78	122.45	118.08
22	X	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
22	Z	612	CLA	CHB-C4A-NA	2.78	128.35	124.51
21	1	601	CHL	O2A-CGA-CBA	2.77	120.62	111.91
22	3	607	CLA	CAA-C2A-C3A	-2.77	107.33	114.26
22	B	829	CLA	CAC-C3C-C4C	2.77	128.41	124.81
21	4	618	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
25	F	305	BCR	C24-C23-C22	-2.77	122.05	126.23
22	A	812	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	2	603	CLA	C1B-CHB-C4A	-2.77	124.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	205	BCR	C33-C5-C6	-2.77	121.42	124.53
22	B	838	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	K	201	CLA	CAD-CBD-CHA	2.77	108.25	105.14
22	1	611	CLA	CAB-C3B-C2B	2.77	130.11	124.69
24	Y	2622	XAT	C35-C34-C33	-2.77	123.36	127.31
22	3	614	CLA	O2D-CGD-O1D	-2.77	117.81	124.09
21	Z	605	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
23	2	619	LUT	C10-C11-C12	-2.77	114.58	123.22
21	Z	606	CHL	OMC-CMC-C2C	-2.77	119.43	125.69
22	B	833	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	B	834	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
22	A	811	CLA	CMB-C2B-C3B	2.76	129.85	124.68
22	A	829	CLA	CHB-C4A-NA	2.76	128.34	124.51
22	Z	604	CLA	CAB-C3B-C2B	2.76	130.10	124.69
22	A	818	CLA	C1-C2-C3	2.76	130.82	126.04
22	H	201	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	3	612	CLA	CHB-C4A-NA	2.76	128.33	124.51
21	2	606	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
21	4	607	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
25	K	205	BCR	C2-C1-C6	2.76	114.72	110.48
22	Y	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	X	611	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	1	621	LUT	C38-C25-C24	-2.76	117.66	123.56
24	4	620	XAT	C31-C30-C29	-2.76	123.38	127.31
22	4	603	CLA	CAB-C3B-C2B	2.75	130.07	124.69
22	3	607	CLA	CHB-C4A-NA	2.75	128.31	124.51
21	Y	609	CHL	C4A-NA-C1A	2.75	107.94	106.71
22	X	612	CLA	CMB-C2B-C3B	2.75	130.07	124.69
25	L	305	BCR	C16-C15-C14	-2.75	117.84	123.47
22	A	833	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	L	303	CLA	CHD-C1D-ND	-2.75	121.93	124.45
23	1	617	LUT	C11-C10-C9	-2.75	123.39	127.31
25	G	205	BCR	C30-C25-C26	-2.75	118.75	122.61
28	A	801	CL0	CHD-C4C-NC	2.75	128.53	124.20
21	2	608	CHL	C3D-C4D-ND	2.75	114.68	110.24
24	2	620	XAT	C10-C11-C12	-2.75	114.65	123.22
22	A	830	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
25	B	846	BCR	C30-C25-C24	2.75	123.54	115.78
22	B	841	CLA	CHB-C4A-NA	2.74	128.31	124.51
21	Y	605	CHL	C2D-C1D-ND	2.74	112.13	110.10
22	B	813	CLA	CHB-C4A-NA	2.74	128.31	124.51
22	B	814	CLA	O2D-CGD-O1D	-2.74	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	609	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
22	A	834	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	A	803	CLA	CAA-CBA-CGA	-2.74	105.24	113.25
22	1	606	CLA	CBD-CHA-C1A	2.74	131.73	128.50
22	Z	604	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	1	617	LUT	C10-C11-C12	-2.74	114.68	123.22
22	4	614	CLA	CHB-C4A-NA	2.74	128.29	124.51
22	A	812	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	2	613	CLA	CMB-C2B-C3B	2.73	129.79	124.68
26	Y	4630	LHG	O8-C23-C24	2.73	120.49	111.91
22	B	811	CLA	CMB-C2B-C3B	2.73	130.04	124.69
22	A	836	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	1	603	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	4	610	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	A	838	CLA	C2A-C1A-CHA	2.73	128.64	123.86
26	B	851	LHG	O8-C23-C24	2.73	120.48	111.91
22	F	301	CLA	CHB-C4A-NA	2.73	128.29	124.51
21	Y	605	CHL	CAC-C3C-C4C	2.73	129.19	125.04
22	1	614	CLA	CAB-C3B-C2B	2.73	130.03	124.69
22	2	609	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
25	J	102	BCR	C11-C10-C9	-2.73	123.42	127.31
21	Z	607	CHL	C4A-NA-C1A	2.73	107.93	106.71
22	B	829	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
22	B	827	CLA	O2D-CGD-CBD	2.72	116.11	111.27
22	A	823	CLA	CHB-C4A-NA	2.72	128.28	124.51
21	Y	601	CHL	CAC-C3C-C4C	2.72	128.34	124.81
25	F	305	BCR	C37-C22-C23	2.72	122.37	118.08
22	A	825	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
22	X	611	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
24	1	618	XAT	C24-C23-C22	-2.72	105.52	110.77
22	1	614	CLA	CMB-C2B-C3B	2.72	130.01	124.69
22	1	616	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	B	846	BCR	C38-C26-C25	-2.72	121.48	124.53
22	A	837	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	Y	612	CLA	CMB-C2B-C3B	2.72	130.00	124.69
22	A	828	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	B	806	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	B	821	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	B	822	CLA	CAA-C2A-C3A	-2.71	107.48	114.26
22	G	204	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	X	602	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	B	817	CLA	C1B-CHB-C4A	-2.71	124.75	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	606	CHL	CBD-CHA-C1A	2.71	131.77	127.43
28	A	801	CL0	C4C-C3C-C2C	-2.71	102.95	106.90
22	B	826	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	K	206	CLA	CAC-C3C-C4C	2.71	128.32	124.81
22	A	808	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	1	619	BCR	C15-C16-C17	-2.71	117.93	123.47
22	4	612	CLA	CAA-C2A-C3A	-2.71	107.50	114.26
22	X	614	CLA	CAB-C3B-C2B	2.71	129.99	124.69
25	J	102	BCR	C2-C1-C6	2.70	114.64	110.48
22	Z	603	CLA	CAB-C3B-C2B	2.70	129.98	124.69
22	3	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	O	2002	CLA	CHB-C4A-NA	2.70	128.25	124.51
21	Z	609	CHL	C1B-CHB-C4A	-2.70	124.76	130.12
22	3	617	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	B	802	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
26	A	847	LHG	O8-C23-C24	2.70	120.39	111.91
22	2	613	CLA	CHB-C4A-NA	2.70	128.25	124.51
21	3	608	CHL	C3D-C4D-ND	2.70	114.61	110.24
22	A	840	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	X	610	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	A	806	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	A	814	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	Y	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	X	2621	LUT	C38-C25-C24	-2.70	117.78	123.56
24	Y	2622	XAT	C24-C23-C22	-2.70	105.56	110.77
25	B	843	BCR	C37-C22-C23	2.70	122.33	118.08
22	B	807	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	X	603	CLA	O2D-CGD-O1D	-2.70	117.96	124.09
25	B	844	BCR	C33-C5-C4	2.70	118.80	113.62
22	4	601	CLA	CMB-C2B-C3B	2.70	129.72	124.68
23	1	621	LUT	C35-C34-C33	-2.70	123.46	127.31
25	A	850	BCR	C21-C20-C19	-2.70	114.80	123.22
22	K	201	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
22	L	303	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
25	B	848	BCR	C39-C30-C25	-2.69	105.94	110.30
22	1	606	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	X	605	CHL	CMB-C2B-C3B	2.69	129.71	124.68
22	3	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	K	206	CLA	CMB-C2B-C3B	2.69	129.71	124.68
22	Y	611	CLA	O2D-CGD-O1D	-2.69	117.99	124.09
22	3	604	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
22	2	612	CLA	CMB-C2B-C3B	2.69	129.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	608	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
22	A	813	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
22	B	838	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
25	A	850	BCR	C34-C9-C8	2.68	122.31	118.08
22	A	811	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	2	602	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	1	608	CLA	CMB-C2B-C3B	2.68	129.70	124.68
22	K	201	CLA	C2A-C1A-CHA	2.68	128.53	123.85
21	2	601	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
25	K	205	BCR	C16-C15-C14	-2.68	117.99	123.47
21	2	608	CHL	CAC-C3C-C4C	2.68	128.29	124.81
22	B	807	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
22	3	610	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
21	Z	606	CHL	CAA-C2A-C3A	-2.68	109.85	116.10
21	Z	606	CHL	CHB-C4A-NA	2.68	128.22	124.51
21	4	608	CHL	C1D-ND-C4D	-2.68	104.43	106.33
28	A	801	CL0	CMA-C3A-C4A	-2.68	104.58	111.77
22	A	823	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	A	819	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	1	617	LUT	C39-C29-C28	2.67	122.29	118.08
25	B	847	BCR	C29-C30-C25	2.67	114.60	110.48
22	4	610	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	A	828	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	B	801	BCR	C29-C30-C25	2.67	114.59	110.48
22	1	609	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	A	802	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
22	3	614	CLA	CMB-C2B-C3B	2.67	129.67	124.68
22	B	824	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	B	845	BCR	C28-C27-C26	-2.67	109.32	114.08
21	X	608	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
25	1	619	BCR	C16-C17-C18	-2.67	123.50	127.31
22	N	1002	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	2	601	CHL	O2A-CGA-CBA	2.66	120.27	111.91
22	X	602	CLA	O2D-CGD-O1D	-2.66	118.04	124.09
22	N	1001	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	B	847	BCR	C8-C7-C6	-2.66	119.72	127.20
22	2	610	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
25	4	621	BCR	C33-C5-C4	2.66	118.73	113.62
24	2	620	XAT	C15-C35-C34	-2.66	118.02	123.47
22	Y	602	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	Z	612	CLA	C2A-C1A-CHA	2.66	128.51	123.86
22	Z	602	CLA	O2D-CGD-O1D	-2.66	118.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	839	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
24	2	620	XAT	C35-C34-C33	-2.66	123.51	127.31
25	B	801	BCR	C2-C1-C6	2.66	114.57	110.48
22	Z	612	CLA	CMB-C2B-C3B	2.66	129.89	124.69
21	Y	609	CHL	C1D-ND-C4D	-2.66	104.45	106.33
22	Z	612	CLA	CAB-C3B-C2B	2.66	129.89	124.69
23	4	619	LUT	C3-C4-C5	-2.66	106.56	111.85
22	B	829	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
21	1	601	CHL	O2D-CGD-O1D	-2.66	118.06	124.09
26	A	847	LHG	C11-C10-C9	-2.66	100.94	114.42
22	A	811	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
22	Y	611	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
22	Z	613	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
22	X	603	CLA	C2A-C1A-CHA	2.65	128.50	123.86
22	A	837	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
22	1	608	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
27	1	622	LMG	O6-C1-O1	-2.65	103.69	109.97
25	L	306	BCR	C33-C5-C6	-2.65	121.55	124.53
22	L	304	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	1	612	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	B	843	BCR	C23-C22-C21	-2.65	114.88	118.94
28	A	801	CL0	CAC-C3C-C4C	2.65	128.25	124.81
25	A	848	BCR	C30-C25-C24	2.65	123.27	115.78
21	1	601	CHL	C4A-NA-C1A	2.65	107.90	106.71
23	2	619	LUT	C30-C31-C32	-2.65	114.96	123.22
22	Y	611	CLA	CAB-C3B-C2B	2.65	129.87	124.69
22	O	2001	CLA	O2D-CGD-O1D	-2.65	118.08	124.09
22	A	827	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	A	834	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
33	Z	7623	NEX	C5-C4-C3	-2.64	108.62	111.75
26	1	620	LHG	O8-C23-C24	2.64	120.20	111.91
22	1	616	CLA	CAB-C3B-C2B	2.64	129.86	124.69
22	A	837	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	4	622	LMG	O6-C1-O1	-2.64	103.72	109.97
22	1	616	CLA	CMB-C2B-C3B	2.64	129.86	124.69
25	A	850	BCR	C15-C16-C17	-2.64	118.07	123.47
22	B	811	CLA	CAB-C3B-C2B	2.64	129.85	124.69
22	A	826	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	4	603	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	B	818	CLA	O2D-CGD-CBD	2.64	115.95	111.27
22	4	611	CLA	CAA-C2A-C3A	-2.64	107.67	114.26
25	L	301	BCR	C16-C17-C18	-2.63	123.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	306	BCR	C30-C25-C26	-2.63	118.91	122.61
22	G	204	CLA	CMB-C2B-C3B	2.63	129.60	124.68
21	2	608	CHL	CMB-C2B-C3B	2.63	129.60	124.68
22	B	839	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	Z	7621	LUT	C38-C25-C24	-2.63	117.93	123.56
21	X	609	CHL	CAC-C3C-C4C	2.63	128.22	124.81
22	Z	611	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	2	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	B	828	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
25	L	305	BCR	C21-C20-C19	-2.62	115.03	123.22
22	4	609	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
26	2	622	LHG	O8-C23-C24	2.62	120.14	111.91
25	L	301	BCR	C38-C26-C27	2.62	118.66	113.62
22	2	604	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	Z	602	CLA	CMB-C2B-C3B	2.62	129.82	124.69
22	4	617	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
22	A	839	CLA	CMB-C2B-C3B	2.62	129.58	124.68
22	B	810	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	Z	4622	XAT	C35-C34-C33	-2.62	123.57	127.31
22	2	602	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
22	Z	611	CLA	CMB-C2B-C3B	2.62	129.81	124.69
22	3	609	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
22	O	2002	CLA	O2D-CGD-O1D	-2.61	118.15	124.09
25	A	849	BCR	C30-C25-C26	-2.61	118.93	122.61
21	2	601	CHL	CHB-C4A-NA	2.61	128.13	124.51
25	4	621	BCR	C16-C17-C18	-2.61	123.58	127.31
25	4	621	BCR	C15-C16-C17	-2.61	118.12	123.47
25	A	849	BCR	C38-C26-C27	2.61	118.63	113.62
21	Y	609	CHL	CMD-C2D-C3D	-2.61	121.61	127.61
22	Z	603	CLA	CMB-C2B-C3B	2.61	129.80	124.69
21	Y	609	CHL	CMB-C2B-C3B	2.61	129.56	124.68
22	Z	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	Z	609	CHL	C1D-ND-C4D	-2.61	104.48	106.33
25	F	305	BCR	C16-C15-C14	-2.61	118.13	123.47
22	4	603	CLA	CMB-C2B-C3B	2.61	129.80	124.69
22	1	614	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
21	4	607	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
22	A	808	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
22	B	814	CLA	CAC-C3C-C4C	2.60	128.19	124.81
22	B	835	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	A	832	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
25	B	844	BCR	C15-C16-C17	-2.60	118.15	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	847	BCR	C31-C1-C6	-2.60	106.08	110.30
22	3	602	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	Y	614	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
23	Z	7620	LUT	C38-C25-C24	-2.60	118.00	123.56
22	Y	610	CLA	CAB-C3B-C2B	2.60	129.77	124.69
22	F	303	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	3	604	CLA	CMB-C2B-C3B	2.60	129.77	124.69
22	3	612	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
21	Z	601	CHL	C1D-ND-C4D	-2.60	104.49	106.33
22	1	608	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
22	1	603	CLA	CMB-C2B-C3B	2.60	129.53	124.68
22	A	806	CLA	CAC-C3C-C4C	2.59	128.18	124.81
25	B	845	BCR	C33-C5-C4	2.59	118.60	113.62
22	B	823	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	1	613	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	A	826	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	A	818	CLA	C1-O2A-CGA	2.59	123.24	116.44
22	B	816	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	B	833	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
21	X	606	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
22	B	836	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	A	824	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	3	618	LUT	C30-C31-C32	-2.58	115.15	123.22
23	Y	4620	LUT	C19-C9-C8	2.58	122.15	118.08
22	Y	602	CLA	CMB-C2B-C3B	2.58	129.51	124.68
21	X	607	CHL	CMB-C2B-C3B	2.58	129.75	124.69
22	A	802	CLA	CAA-CBA-CGA	-2.58	105.70	113.25
25	I	101	BCR	C10-C11-C12	-2.58	115.15	123.22
25	A	848	BCR	C33-C5-C6	-2.58	121.63	124.53
21	X	601	CHL	CHB-C4A-NA	2.58	128.08	124.51
25	A	851	BCR	C20-C19-C18	-2.58	119.17	126.42
21	2	608	CHL	C1-C2-C3	-2.58	122.58	126.75
22	4	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	833	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	X	614	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	A	807	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	1	609	CLA	CMB-C2B-C3B	2.58	129.74	124.69
22	B	826	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
22	B	832	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	A	851	BCR	C10-C11-C12	-2.58	115.18	123.22
22	3	606	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
22	A	824	CLA	CHD-C1D-ND	-2.58	122.09	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	602	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
22	B	824	CLA	C2A-C1A-CHA	2.58	128.36	123.86
21	X	608	CHL	CMB-C2B-C3B	2.58	129.50	124.68
22	1	610	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
22	A	809	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
25	K	205	BCR	C10-C11-C12	-2.57	115.19	123.22
24	2	620	XAT	C19-C9-C8	2.57	122.13	118.08
21	4	618	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
24	Y	2622	XAT	C11-C10-C9	-2.57	123.64	127.31
22	N	1002	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
21	Z	605	CHL	CAC-C3C-C4C	2.57	128.95	125.04
22	A	832	CLA	O2D-CGD-CBD	2.57	115.83	111.27
25	1	619	BCR	C8-C7-C6	-2.57	119.98	127.20
22	A	802	CLA	CMD-C2D-C3D	2.57	133.52	127.61
25	G	205	BCR	C27-C26-C25	-2.57	119.00	122.73
25	K	202	BCR	C10-C11-C12	-2.57	115.20	123.22
33	Z	7623	NEX	C17-C1-C6	-2.57	108.17	110.47
21	Y	601	CHL	CMB-C2B-C3B	2.57	129.71	124.69
22	A	842	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
22	X	610	CLA	CHB-C4A-NA	2.56	128.06	124.51
25	L	301	BCR	C15-C16-C17	-2.56	118.22	123.47
22	A	826	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
25	2	621	BCR	C33-C5-C6	-2.56	121.65	124.53
22	A	829	CLA	C6-C7-C8	-2.56	107.64	115.92
22	A	821	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	846	BCR	C4-C5-C6	-2.56	119.02	122.73
22	4	602	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
26	A	846	LHG	C11-C10-C9	-2.56	101.44	114.42
22	G	201	CLA	CMB-C2B-C3B	2.56	129.46	124.68
22	A	819	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
26	2	622	LHG	C11-C10-C9	-2.56	101.45	114.42
22	Z	604	CLA	CMB-C2B-C3B	2.56	129.69	124.69
22	3	614	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
21	Z	605	CHL	CHB-C4A-NA	2.55	128.04	124.51
24	Z	4622	XAT	C26-C27-C28	-2.55	120.59	125.99
22	3	613	CLA	O2D-CGD-O1D	-2.55	118.29	124.09
27	4	623	LMG	O6-C1-O1	-2.55	103.93	109.97
22	A	822	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	4	614	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	1	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	F	305	BCR	C20-C21-C22	-2.55	123.67	127.31
21	X	601	CHL	C1C-C2C-C3C	-2.55	105.09	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	7620	LUT	C11-C10-C9	-2.55	123.67	127.31
25	K	205	BCR	C7-C8-C9	-2.55	122.38	126.23
22	2	613	CLA	C2D-C1D-ND	-2.54	108.23	110.10
22	2	614	CLA	C2D-C1D-ND	-2.54	108.23	110.10
22	B	808	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	B	825	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
21	X	605	CHL	CMD-C2D-C3D	-2.54	121.76	127.61
22	X	603	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
24	X	7622	XAT	C35-C34-C33	-2.54	123.68	127.31
22	Y	604	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	1	618	XAT	C31-C30-C29	-2.54	123.69	127.31
23	X	2621	LUT	C10-C11-C12	-2.54	115.29	123.22
22	3	606	CLA	C2D-C1D-ND	-2.54	108.23	110.10
22	2	611	CLA	CMB-C2B-C3B	2.54	129.66	124.69
22	2	612	CLA	C2A-C1A-CHA	2.54	128.29	123.86
22	G	203	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
22	A	845	CLA	O2D-CGD-CBD	2.54	115.78	111.27
22	X	614	CLA	CMB-C2B-C3B	2.54	129.65	124.69
24	2	620	XAT	C35-C15-C14	-2.54	118.28	123.47
22	Y	614	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	Y	4621	LUT	C15-C35-C34	-2.53	118.28	123.47
22	Z	604	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
21	X	606	CHL	C4D-CHA-C1A	-2.53	118.17	121.25
22	G	203	CLA	CAA-C2A-C3A	-2.53	107.93	114.26
22	4	604	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
22	F	301	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	A	838	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
26	A	846	LHG	C20-C19-C18	-2.53	101.58	114.42
25	B	845	BCR	C8-C9-C10	2.53	122.82	118.94
21	Y	608	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
22	B	803	CLA	C1C-C2C-C3C	2.53	109.61	106.96
22	Y	613	CLA	CMB-C2B-C3B	2.53	129.64	124.69
22	A	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	Z	609	CHL	CMB-C2B-C3B	2.53	129.41	124.68
22	2	603	CLA	O2D-CGD-O1D	-2.53	118.35	124.09
22	F	303	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	4	621	BCR	C1-C6-C5	-2.53	119.06	122.61
22	A	835	CLA	CMC-C2C-C3C	2.53	132.97	126.12
22	B	831	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	Z	610	CLA	CHB-C4A-NA	2.53	128.00	124.51
22	4	617	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	X	609	CHL	CMA-C3A-C2A	-2.52	110.21	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	X	609	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
22	3	602	CLA	CMB-C2B-C3B	2.52	129.39	124.68
25	F	305	BCR	C35-C13-C14	-2.52	119.39	122.92
22	3	607	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	Z	603	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
28	A	801	CL0	C4-C3-C5	2.52	119.51	115.27
22	L	302	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	809	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
21	X	606	CHL	CHB-C4A-NA	2.52	127.99	124.51
22	B	833	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	3	609	CLA	C2A-C1A-CHA	2.52	128.26	123.86
21	X	607	CHL	CHD-C4C-C3C	-2.51	121.05	124.98
22	1	614	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	3	608	CHL	CMB-C2B-C3B	2.51	129.38	124.68
25	A	850	BCR	C8-C7-C6	-2.51	120.14	127.20
22	B	827	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	B	829	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
25	A	851	BCR	C38-C26-C25	-2.51	121.71	124.53
22	A	843	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	3	618	LUT	C38-C25-C24	-2.51	118.19	123.56
22	4	609	CLA	CMB-C2B-C3B	2.51	129.37	124.68
32	B	850	DGD	C5B-C4B-C3B	-2.51	101.69	114.42
23	4	619	LUT	C8-C9-C10	-2.51	115.09	118.94
22	B	837	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	A	807	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	B	846	BCR	C15-C16-C17	-2.51	118.34	123.47
22	1	611	CLA	CMB-C2B-C3B	2.51	129.60	124.69
22	B	820	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
21	Y	605	CHL	CAA-C2A-C3A	-2.51	110.25	116.10
22	H	201	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	A	808	CLA	CHD-C1D-ND	-2.51	122.15	124.45
25	B	847	BCR	C23-C24-C25	-2.51	120.16	127.20
25	F	305	BCR	C11-C12-C13	-2.51	119.38	126.42
22	Y	611	CLA	CMB-C2B-C3B	2.50	129.59	124.69
21	2	618	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
22	2	614	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	B	811	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	A	842	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	2	603	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	805	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
21	1	607	CHL	C2D-C1D-ND	2.50	111.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	601	CHL	CHB-C4A-NA	2.49	127.96	124.51
22	A	818	CLA	C4-C3-C2	-2.49	117.28	123.68
25	B	843	BCR	C29-C30-C25	2.49	114.32	110.48
22	B	837	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
22	J	101	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	2	608	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
22	2	614	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
22	K	203	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	L	303	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	2	619	LUT	C38-C25-C24	-2.49	118.23	123.56
22	A	809	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	X	2620	LUT	C35-C15-C14	-2.49	118.38	123.47
22	B	837	CLA	CBA-CAA-C2A	2.49	121.21	113.86
22	X	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	813	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
22	A	836	CLA	CMB-C2B-C3B	2.49	129.33	124.68
22	Z	604	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	A	816	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	L	306	BCR	C38-C26-C25	-2.48	121.74	124.53
22	A	854	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	4	618	CHL	CAA-C2A-C3A	-2.48	108.06	114.26
22	A	830	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
21	X	605	CHL	CHB-C4A-NA	2.48	127.94	124.51
25	B	843	BCR	C11-C10-C9	-2.48	123.77	127.31
22	A	818	CLA	C5-C3-C2	2.48	126.13	121.12
21	X	608	CHL	CMD-C2D-C3D	-2.48	121.92	127.61
22	B	831	CLA	CHB-C4A-NA	2.48	127.94	124.51
32	J	103	DGD	CDB-CCB-CBB	-2.48	101.86	114.42
25	G	205	BCR	C38-C26-C25	-2.47	121.75	124.53
21	1	601	CHL	C4-C3-C5	2.47	119.43	115.27
22	X	614	CLA	CBD-CHA-C1A	2.47	131.42	128.50
22	H	201	CLA	C4-C3-C5	2.47	119.43	115.27
22	B	835	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	B	847	BCR	C33-C5-C6	-2.47	121.75	124.53
33	X	2623	NEX	C24-C23-C22	-2.47	106.00	110.77
22	A	815	CLA	C2A-C1A-CHA	2.47	128.18	123.86
21	2	607	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
22	A	804	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
27	4	623	LMG	O1-C1-C2	-2.47	104.44	108.30
21	X	601	CHL	C4D-CHA-C1A	-2.47	118.24	121.25
22	B	813	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	Y	612	CLA	CAA-C2A-C1A	2.47	117.91	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	849	BCR	C33-C5-C4	2.47	118.36	113.62
22	1	609	CLA	CAB-C3B-C2B	2.47	129.52	124.69
25	L	306	BCR	C15-C16-C17	-2.47	118.42	123.47
25	I	101	BCR	C21-C20-C19	-2.47	115.51	123.22
22	A	815	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	3	604	CLA	O2D-CGD-O1D	-2.46	118.50	124.09
22	4	613	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
22	4	601	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	816	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	823	CLA	CAA-C2A-C3A	-2.46	108.11	114.26
22	A	839	CLA	O2D-CGD-CBD	2.46	115.64	111.27
25	A	852	BCR	C8-C9-C10	2.46	122.72	118.94
21	1	601	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
25	4	621	BCR	C16-C15-C14	-2.46	118.44	123.47
22	B	830	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	N	1002	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	K	206	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	1	611	CLA	O2D-CGD-O1D	-2.46	118.51	124.09
28	A	801	CL0	CHB-C4A-NA	2.46	127.91	124.51
25	B	843	BCR	C34-C9-C8	2.46	121.95	118.08
22	A	833	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	822	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
21	Z	608	CHL	CMB-C2B-C3B	2.45	129.27	124.68
25	4	621	BCR	C37-C22-C23	2.45	121.94	118.08
21	X	608	CHL	C1D-ND-C4D	-2.45	104.59	106.33
27	4	622	LMG	O1-C1-C2	-2.45	104.47	108.30
25	A	849	BCR	C16-C15-C14	-2.45	118.45	123.47
22	B	825	CLA	CAA-C2A-C1A	-2.45	103.94	111.97
22	B	841	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	J	102	BCR	C7-C8-C9	-2.45	122.53	126.23
25	A	850	BCR	C8-C9-C10	-2.45	115.18	118.94
22	B	821	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	A	844	PQN	C2M-C2-C3	-2.45	120.40	124.40
22	B	818	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	832	CLA	CAC-C3C-C4C	2.45	127.98	124.81
22	B	803	CLA	CBC-CAC-C3C	2.45	119.18	112.43
21	Y	607	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
21	2	618	CHL	O1D-CGD-CBD	-2.45	119.48	124.48
22	A	803	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
33	X	2623	NEX	C15-C35-C34	-2.44	118.47	123.47
22	3	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	Z	7620	LUT	C10-C11-C12	-2.44	115.59	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	606	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	1	621	LUT	C30-C31-C32	-2.44	115.60	123.22
22	B	806	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	3	620	BCR	C37-C22-C23	2.44	121.92	118.08
22	B	835	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
25	L	301	BCR	C27-C26-C25	-2.44	119.19	122.73
22	Z	612	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	B	830	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	B	839	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
25	L	301	BCR	C20-C21-C22	-2.44	123.83	127.31
22	B	810	CLA	O2D-CGD-CBD	2.44	115.60	111.27
25	K	205	BCR	C31-C1-C6	-2.44	106.34	110.30
21	X	609	CHL	OBD-CAD-C3D	-2.44	124.71	128.74
22	A	819	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
22	1	609	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
21	2	618	CHL	CMB-C2B-C3B	2.44	129.24	124.68
21	Z	607	CHL	C3D-C4D-ND	2.44	114.18	110.24
22	3	613	CLA	CMB-C2B-C3B	2.44	129.23	124.68
22	B	804	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	3	603	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	A	857	LMU	C4B-C3B-C2B	-2.43	106.57	110.82
22	A	805	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	B	818	CLA	C4-C3-C5	2.43	119.36	115.27
22	4	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
23	Z	7621	LUT	C36-C21-C26	2.43	113.22	109.55
21	Y	607	CHL	CAA-C2A-C1A	2.43	117.81	111.81
25	B	844	BCR	C10-C11-C12	-2.43	115.64	123.22
23	Z	7621	LUT	C10-C11-C12	-2.43	115.65	123.22
25	B	847	BCR	C39-C30-C25	-2.43	106.36	110.30
22	A	833	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	B	834	CLA	CHD-C1D-ND	-2.42	122.23	124.45
22	F	304	CLA	CMB-C2B-C3B	2.42	129.21	124.68
22	Z	612	CLA	CAA-C2A-C1A	2.42	117.51	112.14
21	2	618	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
22	L	304	CLA	CBC-CAC-C3C	2.42	119.11	112.43
25	L	305	BCR	C29-C30-C25	2.42	114.21	110.48
21	4	608	CHL	C4A-NA-C1A	2.42	107.80	106.71
21	Z	607	CHL	CHC-C1C-C2C	-2.42	117.33	126.11
24	X	7622	XAT	C4-C3-C2	-2.42	106.10	110.77
23	Y	4620	LUT	C8-C9-C10	-2.42	115.23	118.94
22	B	805	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	1	603	CLA	CAA-C2A-C3A	-2.42	106.15	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	837	CLA	CAA-CBA-CGA	2.42	120.32	113.25
25	A	856	BCR	C29-C30-C25	2.42	114.20	110.48
25	B	801	BCR	C10-C11-C12	-2.42	115.67	123.22
22	F	301	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
25	B	846	BCR	C27-C26-C25	-2.42	119.22	122.73
24	Z	4622	XAT	C36-C21-C22	-2.42	104.79	108.98
28	A	801	CL0	CBC-CAC-C3C	-2.42	105.77	112.43
22	A	810	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
25	3	620	BCR	C23-C22-C21	-2.41	115.24	118.94
22	4	611	CLA	O2D-CGD-CBD	2.41	115.56	111.27
21	3	608	CHL	CHB-C4A-NA	2.41	127.85	124.51
24	1	618	XAT	C35-C34-C33	-2.41	123.86	127.31
21	X	609	CHL	C4A-NA-C1A	2.41	107.79	106.71
21	X	606	CHL	CAC-C3C-C4C	2.41	128.71	125.04
23	X	2621	LUT	C36-C21-C26	2.41	113.20	109.55
21	1	607	CHL	CAA-C2A-C3A	-2.41	110.47	116.10
26	A	846	LHG	C18-C17-C16	-2.41	102.19	114.42
33	Y	4623	NEX	C2-C1-C6	2.41	111.55	109.21
22	A	827	CLA	CAA-C2A-C1A	-2.41	104.08	111.97
22	A	826	CLA	CHA-C1A-NA	-2.41	120.88	126.40
25	J	102	BCR	C27-C26-C25	-2.41	119.23	122.73
21	X	607	CHL	CHD-C1D-C2D	2.41	130.53	125.48
22	A	824	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	2	619	LUT	C3-C4-C5	-2.41	107.06	111.85
21	3	608	CHL	CAC-C3C-C4C	2.41	127.94	124.81
22	4	613	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
22	2	611	CLA	C3A-C4A-CHB	-2.41	117.92	124.50
24	X	7622	XAT	C31-C32-C33	-2.41	119.65	126.42
22	1	606	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	F	303	CLA	CAA-C2A-C3A	-2.41	108.25	114.26
22	A	839	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
22	Y	604	CLA	CAA-C2A-C3A	-2.40	108.25	114.26
22	B	818	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
21	Y	601	CHL	C4D-CHA-C1A	-2.40	118.32	121.25
22	Z	614	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	A	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	A	838	CLA	CHA-C1A-NA	-2.40	120.90	126.40
22	A	815	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	B	825	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	1	618	XAT	O24-C25-C26	-2.40	56.97	58.96
21	4	608	CHL	CMD-C2D-C3D	-2.40	122.09	127.61
22	A	854	CLA	CHA-C1A-NA	-2.40	120.91	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	849	BCR	C15-C16-C17	-2.40	118.56	123.47
22	Y	613	CLA	O2D-CGD-O1D	-2.40	118.64	124.09
25	A	849	BCR	C38-C26-C25	-2.40	121.83	124.53
22	4	617	CLA	C2A-C1A-CHA	2.40	128.05	123.86
22	Z	604	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	Z	613	CLA	CAC-C3C-C4C	2.40	127.92	124.81
22	A	820	CLA	C2A-C1A-CHA	2.40	128.05	123.86
23	Y	4620	LUT	C15-C35-C34	-2.39	118.57	123.47
21	4	606	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
22	3	613	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	Z	611	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	A	839	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
21	Y	607	CHL	CED-O2D-CGD	2.39	121.34	115.94
22	4	612	CLA	O2D-CGD-O1D	-2.39	118.67	124.09
22	H	201	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
21	X	608	CHL	C2A-C3A-C4A	-2.39	98.74	101.78
21	2	606	CHL	C4D-CHA-C1A	-2.39	118.34	121.25
22	Y	612	CLA	O2D-CGD-O1D	-2.39	118.67	124.09
23	3	618	LUT	C10-C11-C12	-2.39	115.77	123.22
27	2	623	LMG	O6-C1-O1	-2.39	104.33	109.97
22	1	614	CLA	CMA-C3A-C2A	-2.38	110.53	116.10
22	L	304	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	4	617	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
22	A	802	CLA	O1D-CGD-CBD	2.38	129.36	124.48
22	A	827	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	L	306	BCR	C33-C5-C4	2.38	118.19	113.62
25	L	301	BCR	C21-C20-C19	-2.38	115.78	123.22
21	4	606	CHL	CAA-C2A-C3A	-2.38	108.31	114.26
23	Y	4621	LUT	C8-C9-C10	-2.38	115.29	118.94
23	Z	7620	LUT	C17-C1-C6	2.38	114.16	110.30
22	X	612	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
21	X	601	CHL	CMB-C2B-C3B	2.38	129.34	124.69
22	1	612	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
22	B	813	CLA	C2D-C1D-ND	-2.38	108.35	110.10
21	Y	607	CHL	CMB-C2B-C3B	2.38	129.34	124.69
22	A	845	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
22	F	303	CLA	CHB-C4A-NA	2.37	127.80	124.51
27	2	623	LMG	O3-C3-C2	-2.37	104.86	110.35
22	A	838	CLA	C2D-C1D-ND	-2.37	108.36	110.10
22	A	825	CLA	CHD-C1D-ND	-2.37	122.27	124.45
25	A	850	BCR	C38-C26-C27	2.37	118.17	113.62
22	A	807	CLA	C11-C10-C8	-2.37	108.25	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	2621	LUT	C11-C10-C9	-2.37	123.93	127.31
22	A	818	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
22	A	830	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	I	101	BCR	C15-C14-C13	-2.37	123.93	127.31
22	4	601	CLA	C2A-C1A-CHA	2.37	128.00	123.86
24	1	618	XAT	C19-C9-C8	2.37	121.81	118.08
22	2	603	CLA	C2A-C1A-CHA	2.37	128.00	123.86
21	2	601	CHL	CMB-C2B-C3B	2.37	129.10	124.68
22	B	829	CLA	CHA-C4D-ND	2.36	137.45	132.50
22	2	604	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
22	X	614	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
28	A	801	CL0	CMC-C2C-C1C	2.36	128.64	125.04
27	1	622	LMG	C38-C37-C36	-2.36	102.42	114.42
22	A	812	CLA	CHD-C1D-ND	-2.36	122.28	124.45
22	N	1001	CLA	CHD-C1D-ND	-2.36	122.28	124.45
21	4	608	CHL	C3D-C4D-ND	2.36	114.06	110.24
22	O	2002	CLA	C2A-C1A-CHA	2.36	127.98	123.85
22	B	836	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	B	846	BCR	C36-C18-C19	2.36	121.80	118.08
22	3	606	CLA	C2A-C1A-CHA	2.36	127.99	123.86
25	A	856	BCR	C38-C26-C25	-2.36	121.88	124.53
22	4	604	CLA	CAB-C3B-C2B	2.36	129.31	124.69
24	Z	4622	XAT	C31-C32-C33	-2.36	119.79	126.42
24	1	618	XAT	C15-C14-C13	-2.36	123.95	127.31
22	A	838	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
25	4	621	BCR	C36-C18-C19	2.36	121.79	118.08
22	B	836	CLA	CHA-C1A-NA	-2.36	121.00	126.40
25	A	851	BCR	C16-C15-C14	-2.35	118.65	123.47
22	B	812	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
22	B	836	CLA	C2A-C1A-CHA	2.35	127.97	123.86
22	K	206	CLA	O2D-CGD-O1D	-2.35	118.74	124.09
22	Z	603	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
22	A	841	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
21	Z	606	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
24	2	620	XAT	C39-C29-C28	2.35	121.78	118.08
23	2	619	LUT	C35-C15-C14	-2.35	118.66	123.47
24	Y	2622	XAT	C10-C11-C12	-2.35	115.89	123.22
21	Z	608	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
22	1	608	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	B	851	LHG	C11-C10-C9	-2.35	102.52	114.42
22	Y	604	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	3	620	BCR	C23-C24-C25	-2.35	120.61	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	4620	LUT	C10-C11-C12	-2.35	115.90	123.22
25	A	849	BCR	C4-C5-C6	-2.35	119.33	122.73
25	A	850	BCR	C11-C12-C13	-2.34	119.83	126.42
21	4	607	CHL	O1D-CGD-CBD	-2.34	119.69	124.48
22	Y	602	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
22	B	838	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	Y	613	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	2	602	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	A	834	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
22	2	613	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	1	602	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	3	608	CHL	C1B-CHB-C4A	-2.34	125.49	130.12
22	3	606	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	Z	606	CHL	C2A-C1A-CHA	-2.34	119.78	123.85
22	B	837	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
25	L	305	BCR	C3-C4-C5	-2.33	109.91	114.08
22	4	601	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
22	X	604	CLA	CMB-C2B-C3B	2.33	129.26	124.69
23	Z	7620	LUT	C35-C15-C14	-2.33	118.69	123.47
22	3	617	CLA	CHB-C4A-NA	2.33	127.74	124.51
21	Z	606	CHL	C1C-C2C-C3C	-2.33	105.26	107.11
22	L	303	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	4	617	CLA	CMB-C2B-C3B	2.33	129.04	124.68
22	1	613	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	B	823	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	3	612	CLA	CHA-C1A-NA	-2.33	121.06	126.40
25	L	305	BCR	C2-C3-C4	-2.33	106.17	111.38
22	L	302	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	Y	601	CHL	O2A-CGA-CBA	2.33	119.21	111.91
25	B	846	BCR	C16-C15-C14	-2.33	118.71	123.47
22	2	609	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	1	602	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	G	204	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
22	4	602	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	1	609	CLA	CMA-C3A-C2A	-2.32	110.68	116.10
21	2	601	CHL	C4-C3-C5	2.32	119.18	115.27
23	1	617	LUT	C7-C8-C9	-2.32	122.73	126.23
22	A	835	CLA	CAA-CBA-CGA	-2.32	106.47	113.25
26	Y	4630	LHG	C11-C10-C9	-2.32	102.64	114.42
22	2	611	CLA	O2D-CGD-CBD	2.32	115.39	111.27
22	4	614	CLA	CHD-C1D-ND	-2.32	122.32	124.45
23	Z	7621	LUT	C15-C35-C34	-2.32	118.72	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	606	CHL	C2A-C1A-CHA	-2.32	119.12	122.71
22	X	614	CLA	CHB-C4A-NA	2.32	127.71	124.51
22	B	811	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
28	A	801	CL0	CMA-C3A-C2A	-2.31	104.49	113.83
22	G	203	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
27	4	623	LMG	O3-C3-C2	-2.31	105.00	110.35
21	Z	607	CHL	O2D-CGD-O1D	-2.31	118.84	124.09
25	4	621	BCR	C23-C22-C21	-2.31	115.39	118.94
22	X	613	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	G	202	LMG	O3-C3-C2	-2.31	105.01	110.35
22	B	813	CLA	C2A-C1A-CHA	2.31	127.90	123.86
32	J	103	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
25	B	847	BCR	C34-C9-C8	2.31	121.72	118.08
21	Y	608	CHL	C4D-CHA-C1A	-2.31	118.44	121.25
22	4	617	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	Z	605	CHL	CMB-C2B-C3B	2.31	129.20	124.69
25	B	848	BCR	C24-C25-C26	2.31	127.05	121.46
22	X	612	CLA	C2A-C1A-CHA	2.31	127.89	123.86
22	A	820	CLA	O2D-CGD-CBD	2.31	115.36	111.27
21	3	608	CHL	O2D-CGD-O1D	-2.30	119.33	123.84
22	A	831	CLA	CMC-C2C-C1C	-2.30	121.53	125.04
25	B	845	BCR	C37-C22-C21	-2.30	119.70	122.92
22	F	303	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	3	615	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	Z	603	CLA	C2A-C1A-CHA	2.30	127.88	123.86
27	1	622	LMG	C40-C39-C38	-2.30	102.77	114.42
22	K	206	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	A	814	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	3	618	LUT	C20-C13-C12	2.29	121.69	118.08
22	O	2001	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
22	4	603	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
22	A	808	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	Y	605	CHL	O2D-CGD-O1D	-2.29	118.88	124.09
22	B	802	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	B	815	CLA	C2A-C1A-CHA	2.29	127.86	123.86
22	A	841	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	A	837	CLA	C2A-C1A-CHA	2.29	127.86	123.86
22	B	828	CLA	O2D-CGD-CBD	2.29	115.34	111.27
23	2	619	LUT	C39-C29-C28	2.29	121.68	118.08
22	4	612	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
25	B	848	BCR	C16-C15-C14	-2.29	118.79	123.47
25	B	847	BCR	C20-C19-C18	-2.28	120.00	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	611	CLA	C1A-CHA-C4D	-2.28	122.52	125.72
22	A	802	CLA	C2D-C1D-ND	-2.28	108.42	110.10
22	F	304	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
21	Z	607	CHL	CMD-C2D-C3D	-2.28	122.36	127.61
22	A	835	CLA	C2A-C1A-CHA	2.28	127.85	123.86
22	N	1002	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
22	3	606	CLA	CAA-C2A-C3A	-2.28	108.56	114.26
22	A	838	CLA	CBC-CAC-C3C	2.28	118.72	112.43
22	B	815	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	Y	611	CLA	CHD-C1D-ND	-2.28	122.36	124.45
22	L	302	CLA	O2A-CGA-O1A	-2.28	117.62	123.30
25	J	102	BCR	C34-C9-C8	2.28	121.67	118.08
22	B	840	CLA	C2A-C1A-CHA	2.28	127.84	123.86
22	L	303	CLA	C2A-C1A-CHA	2.28	127.84	123.86
25	A	849	BCR	C8-C7-C6	-2.28	120.81	127.20
22	X	604	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
33	X	2623	NEX	C26-C27-C28	-2.27	121.18	125.99
23	Y	4620	LUT	C20-C13-C12	2.27	121.66	118.08
22	X	614	CLA	CHD-C1D-ND	-2.27	122.36	124.45
25	3	620	BCR	C10-C11-C12	-2.27	116.12	123.22
25	B	848	BCR	C29-C28-C27	-2.27	106.30	111.38
22	1	612	CLA	C2A-C1A-CHA	2.27	127.83	123.86
27	4	622	LMG	O3-C3-C2	-2.27	105.10	110.35
22	4	604	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	A	843	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	A	806	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	A	818	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	X	601	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
27	4	623	LMG	O1-C7-C8	-2.27	105.43	110.90
32	B	850	DGD	CAB-C9B-C8B	-2.27	102.91	114.42
22	A	802	CLA	C3C-C4C-NC	-2.27	108.03	110.57
21	Y	606	CHL	C4B-C3B-C2B	-2.27	104.81	106.92
22	1	611	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	3	603	CLA	C2D-C1D-ND	-2.27	108.43	110.10
22	A	819	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
22	B	826	CLA	O2D-CGD-CBD	2.26	115.29	111.27
22	A	817	CLA	C2D-C1D-ND	-2.26	108.44	110.10
25	L	306	BCR	C10-C11-C12	-2.26	116.16	123.22
22	L	303	CLA	O2D-CGD-CBD	2.26	115.28	111.27
33	Y	4623	NEX	C28-C29-C30	2.26	122.41	118.94
22	A	816	CLA	O2D-CGD-CBD	2.26	115.28	111.27
22	A	834	CLA	CMB-C2B-C3B	2.26	128.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	608	CHL	O2A-CGA-CBA	2.26	121.28	114.03
22	B	808	CLA	C2A-C1A-CHA	2.26	127.81	123.86
23	1	617	LUT	C22-C23-C24	-2.26	109.17	111.74
25	A	852	BCR	C16-C15-C14	-2.26	118.85	123.47
22	Y	614	CLA	C2D-C1D-ND	-2.26	108.44	110.10
25	A	856	BCR	C21-C20-C19	-2.25	116.18	123.22
22	K	203	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	B	828	CLA	C2A-C1A-CHA	2.25	127.80	123.86
22	1	616	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
33	X	2623	NEX	C19-C9-C10	-2.25	119.77	122.92
26	B	851	LHG	C27-C26-C25	-2.25	103.01	114.42
25	3	620	BCR	C29-C30-C25	2.25	113.94	110.48
25	F	305	BCR	C15-C16-C17	-2.25	118.87	123.47
22	B	825	CLA	C2D-C1D-ND	-2.25	108.45	110.10
23	X	2620	LUT	C38-C25-C24	-2.25	118.75	123.56
25	B	846	BCR	C8-C7-C6	-2.25	120.89	127.20
25	2	621	BCR	C21-C20-C19	-2.25	116.21	123.22
22	G	201	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	A	810	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
25	G	205	BCR	C16-C15-C14	-2.24	118.88	123.47
22	3	612	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
22	A	802	CLA	C1-C2-C3	-2.24	122.16	126.04
26	2	622	LHG	C27-C26-C25	-2.24	103.04	114.42
22	1	610	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
22	1	602	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	B	832	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
23	4	619	LUT	C39-C29-C28	2.24	121.61	118.08
21	Y	607	CHL	C4B-C3B-C2B	-2.24	104.83	106.92
22	A	827	CLA	CBC-CAC-C3C	2.24	118.61	112.43
23	4	619	LUT	C8-C7-C6	-2.24	120.92	127.20
22	B	833	CLA	C2A-C1A-CHA	2.24	127.77	123.86
22	F	301	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	B	802	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
22	3	609	CLA	CHA-C1A-NA	-2.24	121.28	126.40
25	A	852	BCR	C10-C11-C12	-2.24	116.24	123.22
22	B	810	CLA	C2A-C1A-CHA	2.23	127.77	123.86
21	4	606	CHL	CAC-C3C-C4C	2.23	128.44	125.04
22	A	839	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	Y	4620	LUT	C30-C31-C32	-2.23	116.25	123.22
25	A	849	BCR	C27-C26-C25	-2.23	119.49	122.73
22	B	839	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	A	823	CLA	C1B-CHB-C4A	-2.23	125.70	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	817	CLA	C2D-C1D-ND	-2.23	108.46	110.10
22	B	815	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	3	603	CLA	C2A-C1A-CHA	2.23	127.76	123.86
21	Z	608	CHL	O2D-CGD-O1D	-2.23	119.03	124.09
21	Y	605	CHL	CMB-C2B-C3B	2.23	129.05	124.69
25	G	205	BCR	C1-C6-C5	-2.23	119.47	122.61
22	4	612	CLA	C2A-C1A-CHA	2.23	127.75	123.86
22	A	813	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
22	K	204	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
22	O	2001	CLA	CBD-CHA-C1A	2.22	131.12	128.50
22	3	603	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
22	A	825	CLA	C2D-C1D-ND	-2.22	108.47	110.10
21	1	607	CHL	C4D-CHA-C1A	-2.22	118.54	121.25
22	B	813	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
22	Z	613	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	A	825	CLA	C2A-C1A-CHA	2.22	127.74	123.86
22	4	614	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	A	848	BCR	C24-C23-C22	-2.22	122.88	126.23
22	K	206	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	O	2002	CLA	CMA-C3A-C2A	-2.22	110.92	116.10
22	H	201	CLA	C2A-C1A-CHA	2.22	127.74	123.86
25	J	102	BCR	C21-C20-C19	-2.22	116.30	123.22
22	A	817	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	4	611	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
24	1	618	XAT	C39-C29-C28	2.21	121.56	118.08
25	J	102	BCR	C20-C21-C22	-2.21	124.15	127.31
22	Y	612	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	2	611	CLA	CGD-CBD-CAD	2.21	117.90	110.73
22	A	835	CLA	C4-C3-C5	2.21	118.99	115.27
21	Y	605	CHL	C1D-ND-C4D	-2.21	104.77	106.33
22	A	828	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	Z	603	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	B	840	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
21	X	609	CHL	C4B-C3B-C2B	-2.21	104.87	106.92
25	A	850	BCR	C10-C11-C12	-2.21	116.33	123.22
21	Z	605	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
31	B	849	LMU	C1B-O1B-C4'	-2.21	112.50	117.96
23	4	619	LUT	C18-C5-C6	-2.21	122.05	124.53
23	Z	7621	LUT	C3-C4-C5	-2.21	107.46	111.85
22	N	1001	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
25	I	101	BCR	C20-C19-C18	-2.21	120.22	126.42
25	A	851	BCR	C38-C26-C27	2.21	117.85	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	836	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
22	B	824	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
22	2	602	CLA	CMB-C2B-C3B	2.20	128.80	124.68
21	X	601	CHL	C2A-C1A-CHA	-2.20	120.01	123.85
22	B	838	CLA	O2D-CGD-CBD	2.20	115.18	111.27
21	X	609	CHL	C2A-C1A-CHA	-2.20	120.01	123.85
25	A	850	BCR	C1-C6-C7	2.20	122.00	115.78
23	Z	7620	LUT	C21-C26-C27	-2.20	109.92	112.70
33	Y	4623	NEX	C16-C1-C6	2.20	112.44	110.47
21	X	609	CHL	CHB-C4A-NA	2.20	127.55	124.51
22	A	827	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
25	L	306	BCR	C38-C26-C27	2.20	117.84	113.62
21	X	606	CHL	C4B-C3B-C2B	-2.20	104.88	106.92
22	A	843	CLA	C7-C6-C5	-2.20	107.40	113.36
24	3	619	XAT	C20-C13-C12	2.19	121.53	118.08
22	B	821	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
25	I	101	BCR	C4-C5-C6	-2.19	119.55	122.73
22	Y	603	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	Y	4621	LUT	C36-C21-C26	2.19	112.87	109.55
25	B	848	BCR	C7-C8-C9	-2.19	122.92	126.23
21	X	609	CHL	CAA-C2A-C3A	-2.19	110.98	116.10
22	A	845	CLA	C2A-C1A-CHA	2.19	127.69	123.86
25	2	621	BCR	C20-C21-C22	-2.19	124.19	127.31
26	Y	4630	LHG	C27-C26-C25	-2.19	103.31	114.42
22	G	201	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
25	B	846	BCR	C16-C17-C18	-2.19	124.19	127.31
21	X	607	CHL	C2D-C1D-ND	2.19	111.72	110.10
22	A	832	CLA	C2A-C1A-CHA	2.19	127.69	123.86
22	A	831	CLA	C2D-C1D-ND	-2.19	108.49	110.10
22	B	805	CLA	O2D-CGD-CBD	2.19	115.16	111.27
22	A	842	CLA	C1-O2A-CGA	2.19	122.18	116.44
22	X	613	CLA	CAD-CBD-CHA	2.18	107.60	105.14
28	A	801	CL0	O2A-CGA-O1A	-2.18	118.08	123.59
21	2	601	CHL	CAA-CBA-CGA	-2.18	106.87	113.25
22	B	806	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	X	612	CLA	CAD-CBD-CHA	2.18	107.60	105.14
21	2	607	CHL	C1C-C2C-C3C	-2.18	105.38	107.11
22	2	603	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
22	A	831	CLA	O2D-CGD-CBD	2.18	115.15	111.27
25	I	101	BCR	C35-C13-C12	2.18	121.52	118.08
22	A	806	CLA	C2A-C1A-CHA	2.18	127.67	123.86
25	B	848	BCR	C8-C7-C6	-2.18	121.08	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	819	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	L	301	BCR	C30-C25-C24	2.18	121.94	115.78
23	1	617	LUT	C12-C13-C14	-2.18	115.60	118.94
25	A	856	BCR	C34-C9-C8	2.18	121.50	118.08
25	4	621	BCR	C29-C30-C25	2.17	113.83	110.48
25	B	844	BCR	C2-C1-C6	2.17	113.83	110.48
32	B	850	DGD	C7B-C6B-C5B	-2.17	103.39	114.42
22	A	815	CLA	CHA-C1A-NA	-2.17	121.42	126.40
27	G	202	LMG	O1-C1-C2	-2.17	104.91	108.30
23	Z	7621	LUT	C19-C9-C8	2.17	121.50	118.08
21	4	618	CHL	C4D-CHA-C1A	-2.17	118.60	121.25
22	B	836	CLA	CAC-C3C-C4C	2.17	127.63	124.81
22	B	804	CLA	C2A-C1A-CHA	2.17	127.65	123.85
21	X	607	CHL	OMC-CMC-C2C	-2.17	120.77	125.69
22	1	603	CLA	C2A-C1A-CHA	2.17	127.66	123.86
33	X	2623	NEX	C11-C12-C13	-2.17	120.31	126.42
22	B	813	CLA	CAC-C3C-C4C	2.17	127.63	124.81
22	A	832	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
21	2	606	CHL	C1B-CHB-C4A	-2.17	125.82	130.12
21	4	618	CHL	CMB-C2B-C3B	2.17	128.93	124.69
21	1	601	CHL	CMB-C2B-C1B	2.17	131.79	128.46
22	A	814	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
25	B	844	BCR	C8-C9-C10	2.17	122.27	118.94
25	B	801	BCR	C34-C9-C8	2.17	121.49	118.08
21	2	606	CHL	CHB-C4A-NA	2.17	127.51	124.51
22	A	810	CLA	CHA-C1A-NA	-2.17	121.44	126.40
22	B	814	CLA	CED-O2D-CGD	2.16	120.83	115.94
22	A	834	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
22	K	203	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
22	4	602	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
27	G	202	LMG	O8-C28-O10	-2.16	118.13	123.59
22	1	604	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	3	609	CLA	O1D-CGD-CBD	2.16	128.91	124.48
21	2	618	CHL	CHB-C4A-NA	2.16	127.50	124.51
33	Z	7623	NEX	C11-C12-C13	-2.16	120.34	126.42
21	4	607	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
23	X	2620	LUT	C11-C12-C13	-2.16	120.34	126.42
29	B	842	PQN	C9-C10-C5	2.16	121.67	119.26
22	2	602	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
22	B	819	CLA	CMB-C2B-C3B	2.16	128.72	124.68
22	2	614	CLA	C3C-C4C-NC	-2.16	108.15	110.57
22	4	602	CLA	O2D-CGD-CBD	2.16	115.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	203	CLA	C2A-C1A-CHA	2.16	127.63	123.86
25	A	852	BCR	C23-C24-C25	-2.16	121.15	127.20
33	Y	4623	NEX	O24-C25-C26	-2.16	57.17	58.96
21	X	606	CHL	C3A-C4A-CHB	-2.15	118.34	124.01
21	X	607	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
22	Z	613	CLA	C2D-C1D-ND	-2.15	108.52	110.10
22	2	610	CLA	CAC-C3C-C4C	2.15	127.60	124.81
22	B	836	CLA	CBC-CAC-C3C	2.15	118.36	112.43
22	A	819	CLA	O2D-CGD-CBD	2.15	115.09	111.27
26	1	620	LHG	C11-C10-C9	-2.15	103.52	114.42
24	1	618	XAT	C30-C31-C32	-2.15	116.52	123.22
25	B	848	BCR	C2-C1-C6	2.15	113.79	110.48
22	A	835	CLA	C7-C6-C5	-2.15	107.53	113.36
22	A	845	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	2	601	CHL	C1B-CHB-C4A	-2.15	125.87	130.12
22	B	805	CLA	C11-C12-C13	-2.14	108.99	115.92
21	Z	601	CHL	O2D-CGD-O1D	-2.14	119.22	124.09
22	A	824	CLA	C2D-C1D-ND	-2.14	108.52	110.10
22	A	843	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
27	G	202	LMG	O1-C7-C8	-2.14	105.73	110.90
22	B	803	CLA	CMD-C2D-C3D	2.14	132.54	127.61
23	Z	7620	LUT	C19-C9-C8	2.14	121.45	118.08
25	B	844	BCR	C37-C22-C21	-2.14	119.92	122.92
22	X	604	CLA	CMA-C3A-C2A	-2.14	111.10	116.10
22	A	829	CLA	C2A-C1A-CHA	2.14	127.60	123.86
22	B	809	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	L	301	BCR	C38-C26-C25	-2.14	122.13	124.53
21	1	607	CHL	CMB-C2B-C3B	2.14	128.68	124.68
23	X	2621	LUT	C22-C23-C24	-2.14	109.31	111.74
24	X	7622	XAT	O24-C25-C26	-2.14	57.19	58.96
22	B	834	CLA	C3C-C4C-NC	-2.14	108.17	110.57
22	A	821	CLA	C2A-C1A-CHA	2.14	127.60	123.86
22	B	836	CLA	O2D-CGD-CBD	2.14	115.06	111.27
21	Z	609	CHL	O2D-CGD-O1D	-2.14	119.24	124.09
23	1	621	LUT	C11-C12-C13	-2.14	120.42	126.42
22	4	613	CLA	CHD-C1D-ND	-2.14	122.49	124.45
22	B	821	CLA	C2A-C1A-CHA	2.14	127.59	123.86
25	4	621	BCR	C23-C24-C25	-2.14	121.20	127.20
21	Z	606	CHL	CMB-C2B-C3B	2.14	128.67	124.68
22	B	809	CLA	C2A-C1A-CHA	2.13	127.59	123.86
22	A	810	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
22	B	822	CLA	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	601	CHL	C4D-CHA-C1A	-2.13	118.66	121.25
22	B	828	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
22	K	206	CLA	C2A-C1A-CHA	2.13	126.01	122.71
22	2	614	CLA	O2D-CGD-CBD	2.13	115.05	111.27
21	Y	608	CHL	O2D-CGD-O1D	-2.13	119.26	124.09
25	L	305	BCR	C11-C12-C13	-2.13	120.44	126.42
26	2	622	LHG	O8-C23-O10	-2.13	118.23	123.59
22	O	2002	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
25	A	852	BCR	C15-C14-C13	-2.12	124.28	127.31
23	Z	7621	LUT	C37-C21-C22	-2.12	105.42	109.44
23	Y	4620	LUT	C38-C25-C24	-2.12	119.02	123.56
25	2	621	BCR	C33-C5-C4	2.12	117.69	113.62
22	3	604	CLA	CAB-C3B-C2B	2.12	128.84	124.69
22	L	302	CLA	C2A-C1A-CHA	2.12	127.56	123.86
21	X	607	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
21	Y	605	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
22	4	601	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	3	618	LUT	C22-C23-C24	-2.12	109.33	111.74
21	4	606	CHL	C2A-C1A-CHA	-2.12	120.16	123.86
32	B	850	DGD	CBB-CAB-C9B	-2.12	103.68	114.42
22	3	617	CLA	CMA-C3A-C2A	-2.12	111.16	116.10
24	Z	4622	XAT	C40-C33-C32	2.12	121.41	118.08
25	B	848	BCR	C15-C14-C13	-2.12	124.29	127.31
22	Z	602	CLA	CAB-C3B-C2B	2.12	128.83	124.69
22	A	840	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
22	B	838	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	Y	4621	LUT	C30-C31-C32	-2.11	116.62	123.22
23	1	617	LUT	C20-C13-C12	2.11	121.41	118.08
21	4	618	CHL	CHB-C4A-NA	2.11	127.43	124.51
22	4	614	CLA	C2D-C1D-ND	-2.11	108.55	110.10
33	Y	4623	NEX	C31-C30-C29	-2.11	124.30	127.31
22	O	2001	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	1	620	LHG	C20-C19-C18	-2.11	103.70	114.42
21	Y	606	CHL	C1C-C2C-C3C	-2.11	105.13	107.07
22	1	612	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
22	2	610	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	B	832	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	X	609	CHL	CMB-C2B-C3B	2.11	128.82	124.69
27	G	202	LMG	O2-C2-C1	-2.11	104.92	110.05
25	G	205	BCR	C23-C24-C25	-2.11	121.28	127.20
22	J	101	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	1	616	CLA	CAA-C2A-C3A	-2.11	107.00	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	828	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	B	843	BCR	C7-C8-C9	-2.11	123.05	126.23
22	A	815	CLA	C2D-C1D-ND	-2.11	108.55	110.10
25	L	301	BCR	C10-C11-C12	-2.11	116.64	123.22
22	Y	603	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
32	J	103	DGD	O5D-C6D-C5D	-2.11	105.15	109.05
21	1	607	CHL	C1D-ND-C4D	-2.11	104.84	106.33
23	Z	7620	LUT	C39-C29-C28	2.11	121.39	118.08
22	2	603	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	K	204	CLA	C2A-C1A-CHA	2.10	127.54	123.86
23	4	619	LUT	C16-C1-C6	-2.10	106.89	110.30
25	L	301	BCR	C37-C22-C23	2.10	121.39	118.08
25	A	856	BCR	C11-C10-C9	-2.10	124.31	127.31
31	A	857	LMU	O5'-C1'-C2'	2.10	114.79	110.35
21	Z	601	CHL	CMB-C2B-C3B	2.10	128.60	124.68
22	4	602	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	4	601	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	Y	602	CLA	CMA-C3A-C2A	-2.10	105.37	113.83
23	Z	7621	LUT	C30-C31-C32	-2.10	116.67	123.22
22	X	611	CLA	C2A-C1A-CHA	2.10	125.96	122.71
22	2	609	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
22	Y	602	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
22	A	841	CLA	C2A-C1A-CHA	2.09	127.52	123.86
28	A	801	CL0	C2A-C1A-CHA	-2.09	120.20	123.86
25	B	847	BCR	C8-C9-C10	-2.09	115.73	118.94
22	B	818	CLA	C2A-C1A-CHA	2.09	127.52	123.86
22	B	830	CLA	CAC-C3C-C4C	2.09	127.53	124.81
23	X	2620	LUT	C7-C8-C9	-2.09	123.07	126.23
33	Y	4623	NEX	C11-C12-C13	-2.09	120.54	126.42
22	B	825	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	A	814	CLA	C11-C12-C13	-2.09	109.16	115.92
21	Z	608	CHL	C1C-C2C-C3C	-2.09	105.45	107.11
22	4	617	CLA	CHA-C1A-NA	-2.09	121.61	126.40
33	Y	4623	NEX	C17-C1-C6	-2.09	108.60	110.47
22	1	602	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	A	804	CLA	C3A-C2A-C1A	2.09	104.47	101.34
22	A	807	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	3	609	CLA	C3C-C4C-NC	-2.09	108.23	110.57
25	B	843	BCR	C23-C24-C25	-2.09	121.33	127.20
25	A	856	BCR	C10-C11-C12	-2.09	116.70	123.22
22	3	615	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	Y	4620	LUT	C11-C12-C13	-2.09	120.55	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	841	CLA	O2D-CGD-CBD	2.09	114.98	111.27
25	B	847	BCR	C11-C12-C13	-2.09	120.55	126.42
24	3	619	XAT	C5-C4-C3	-2.09	108.62	112.75
22	B	813	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	G	201	CLA	CHD-C1D-ND	-2.09	122.54	124.45
27	4	622	LMG	O1-C7-C8	-2.09	105.86	110.90
22	4	604	CLA	C2A-C1A-CHA	2.09	127.51	123.86
23	3	618	LUT	C1-C2-C3	2.09	118.36	113.64
22	A	826	CLA	O2A-C1-C2	-2.09	103.15	108.64
21	2	607	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
22	4	614	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
22	B	826	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
22	1	602	CLA	C1-C2-C3	-2.09	122.44	126.04
23	1	621	LUT	C15-C35-C34	-2.09	119.20	123.47
23	Y	4621	LUT	C22-C23-C24	-2.09	109.37	111.74
21	1	607	CHL	O2D-CGD-O1D	-2.09	119.35	124.09
22	A	809	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	4	603	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	A	830	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	2	609	CLA	C2A-C1A-CHA	2.08	127.50	123.86
25	3	620	BCR	C39-C30-C25	-2.08	106.92	110.30
25	A	849	BCR	C1-C6-C5	-2.08	119.68	122.61
22	Y	610	CLA	O1D-CGD-CBD	2.08	128.75	124.48
21	4	607	CHL	CMB-C2B-C3B	2.08	128.76	124.69
23	1	617	LUT	C28-C29-C30	-2.08	115.75	118.94
22	3	603	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
22	A	834	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	A	817	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	K	203	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	G	203	CLA	C2A-C1A-CHA	2.08	127.49	123.86
22	A	854	CLA	C2A-C1A-CHA	2.08	127.49	123.86
32	B	850	DGD	C1D-O6D-C5D	-2.08	109.61	113.69
25	3	620	BCR	C27-C26-C25	-2.08	119.71	122.73
22	A	829	CLA	C6-C5-C3	-2.08	108.01	113.45
22	B	825	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
22	A	819	CLA	C2A-C1A-CHA	2.08	127.49	123.86
22	G	204	CLA	C2A-C1A-CHA	2.08	127.49	123.86
21	3	608	CHL	OBD-CAD-C3D	-2.08	123.52	128.52
21	1	607	CHL	CHD-C1D-C2D	2.08	129.84	125.48
22	L	302	CLA	O1A-CGA-CBA	2.08	129.75	123.08
25	K	205	BCR	C36-C18-C17	-2.08	120.02	122.92
22	A	811	CLA	C2A-C1A-CHA	2.08	127.49	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	608	CHL	C5-C3-C4	2.08	119.19	114.60
21	4	606	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
22	B	828	CLA	CHA-C1A-NA	-2.07	121.65	126.40
33	X	2623	NEX	O24-C25-C26	-2.07	57.24	58.96
22	A	842	CLA	C2A-C1A-CHA	2.07	127.48	123.86
23	Z	7620	LUT	C36-C21-C26	2.07	112.68	109.55
25	3	620	BCR	C4-C5-C6	-2.07	119.72	122.73
22	B	828	CLA	CHA-C4D-ND	2.07	136.83	132.50
22	A	830	CLA	O2D-CGD-CBD	2.07	114.95	111.27
21	Z	601	CHL	CHD-C1D-C2D	2.07	129.82	125.48
22	A	802	CLA	C2A-C1A-CHA	2.07	127.48	123.86
33	Y	4623	NEX	C19-C9-C10	-2.07	120.02	122.92
21	X	609	CHL	C1D-CHD-C4C	-2.07	121.59	126.06
22	A	832	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
22	B	841	CLA	C2A-C1A-CHA	2.07	127.47	123.86
22	2	609	CLA	C2D-C1D-ND	-2.07	108.58	110.10
22	A	816	CLA	CGD-CBD-CAD	-2.07	104.04	110.73
22	B	834	CLA	C2D-C1D-ND	-2.07	108.58	110.10
22	1	603	CLA	C3A-C2A-C1A	2.07	104.43	101.34
23	1	617	LUT	C31-C30-C29	-2.06	124.36	127.31
28	A	801	CL0	C6-C7-C8	-2.06	109.25	115.92
21	Y	605	CHL	CHD-C1D-C2D	2.06	129.81	125.48
21	X	606	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
22	B	826	CLA	C2A-C1A-CHA	2.06	127.47	123.86
22	A	825	CLA	O1D-CGD-CBD	2.06	128.70	124.48
25	1	619	BCR	C4-C5-C6	-2.06	119.74	122.73
22	3	607	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	B	837	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
21	Z	605	CHL	C4B-C3B-C2B	-2.06	105.00	106.92
22	X	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40
24	3	619	XAT	C19-C9-C8	2.06	121.32	118.08
22	B	825	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	A	841	CLA	C1-C2-C3	-2.06	122.48	126.04
24	2	620	XAT	C11-C10-C9	-2.06	124.37	127.31
24	4	620	XAT	C35-C15-C14	-2.06	119.26	123.47
21	2	608	CHL	O2D-CGD-O1D	-2.05	119.82	123.84
22	B	810	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
25	B	848	BCR	C20-C19-C18	-2.05	120.65	126.42
22	3	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	J	102	BCR	C29-C30-C25	2.05	113.64	110.48
32	J	103	DGD	O2D-C2D-C1D	-2.05	105.06	110.05
22	X	613	CLA	C2A-C1A-CHA	2.05	127.43	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	619	LUT	C21-C26-C27	-2.05	110.11	112.70
22	B	822	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B	844	BCR	C21-C20-C19	-2.05	116.82	123.22
23	2	619	LUT	C1-C2-C3	2.05	118.27	113.64
22	B	837	CLA	C3A-C2A-C1A	2.05	104.41	101.34
23	1	617	LUT	C3-C4-C5	-2.05	107.77	111.85
21	Z	605	CHL	O2D-CGD-O1D	-2.05	119.44	124.09
23	1	621	LUT	C22-C23-C24	-2.05	109.41	111.74
22	1	606	CLA	C2A-C1A-CHA	2.05	125.89	122.71
25	A	848	BCR	C27-C26-C25	-2.05	119.76	122.73
25	4	621	BCR	C19-C18-C17	-2.05	115.80	118.94
22	A	821	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
24	Y	2622	XAT	C19-C9-C8	2.04	121.30	118.08
22	A	818	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
22	B	810	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	2	601	CHL	C2A-C1A-CHA	-2.04	120.28	123.86
22	K	201	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	4	606	CHL	CMB-C2B-C3B	2.04	128.50	124.68
22	B	803	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	B	811	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	X	7622	XAT	C20-C13-C14	-2.04	120.06	122.92
22	4	603	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
22	3	603	CLA	C1D-ND-C4D	2.04	107.78	106.33
22	2	612	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
22	4	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	A	833	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	B	827	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
33	Z	7623	NEX	C15-C35-C34	-2.04	119.30	123.47
33	Y	4623	NEX	C26-C27-C28	-2.04	121.69	125.99
22	B	833	CLA	C3A-C2A-C1A	2.04	104.39	101.34
22	B	831	CLA	O2D-CGD-CBD	2.04	114.89	111.27
21	2	606	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
32	B	850	DGD	O6E-C1E-O5D	-2.04	105.15	109.97
27	1	622	LMG	O2-C2-C1	-2.04	105.10	110.05
22	A	832	CLA	CHD-C1D-ND	-2.03	122.58	124.45
23	1	621	LUT	C36-C21-C26	2.03	112.63	109.55
24	3	619	XAT	C28-C29-C30	-2.03	115.82	118.94
25	B	846	BCR	C10-C11-C12	-2.03	116.87	123.22
22	B	835	CLA	C2A-C1A-CHA	2.03	127.42	123.86
22	A	817	CLA	C2A-C1A-CHA	2.03	127.41	123.86
22	A	814	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	A	803	CLA	CHD-C1D-ND	-2.03	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	821	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	1	617	LUT	C16-C1-C6	-2.03	107.00	110.30
22	A	825	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	809	CLA	C1-C2-C3	-2.03	122.53	126.04
21	Y	607	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
22	B	840	CLA	O1D-CGD-CBD	2.03	128.64	124.48
21	Y	601	CHL	C1-C2-C3	-2.03	122.53	126.04
22	A	845	CLA	CAC-C3C-C4C	2.03	127.44	124.81
32	B	850	DGD	C7A-C6A-C5A	-2.03	104.12	114.42
22	A	834	CLA	C2D-C1D-ND	-2.03	108.61	110.10
22	3	606	CLA	CAC-C3C-C4C	2.03	127.44	124.81
22	A	805	CLA	C2A-C1A-CHA	2.03	127.41	123.86
22	F	301	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	3	619	XAT	O24-C25-C26	-2.03	57.28	58.96
22	B	839	CLA	C2D-C1D-ND	-2.03	108.61	110.10
22	1	604	CLA	O2D-CGD-CBD	2.03	114.87	111.27
22	4	609	CLA	CAC-C3C-C4C	2.03	127.44	124.81
21	1	601	CHL	C6-C5-C3	-2.03	108.14	113.45
22	A	804	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
23	4	619	LUT	C38-C25-C24	-2.02	119.23	123.56
22	A	838	CLA	C1D-ND-C4D	2.02	107.77	106.33
27	1	622	LMG	O3-C3-C2	-2.02	105.67	110.35
21	4	608	CHL	CBA-CAA-C2A	2.02	119.83	113.86
22	A	838	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	A	810	CLA	C2A-C1A-CHA	2.02	127.39	123.86
21	Y	601	CHL	O2D-CGD-O1D	-2.02	119.50	124.09
24	X	7622	XAT	O4-C5-C6	-2.02	57.29	58.96
26	1	620	LHG	C27-C26-C25	-2.02	104.16	114.42
22	1	608	CLA	C2D-C1D-ND	-2.02	108.61	110.10
22	1	616	CLA	CHD-C1D-ND	-2.02	122.60	124.45
24	4	620	XAT	O24-C25-C26	-2.02	57.29	58.96
22	Z	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	X	2620	LUT	C31-C32-C33	-2.02	120.74	126.42
24	4	620	XAT	C30-C31-C32	-2.02	116.91	123.22
22	3	603	CLA	CHA-C1A-NA	-2.02	121.77	126.40
33	Z	7623	NEX	C16-C1-C6	2.02	112.28	110.47
22	B	833	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
33	Z	7623	NEX	C30-C31-C32	-2.02	116.92	123.22
22	B	825	CLA	O1D-CGD-CBD	2.02	128.61	124.48
27	4	623	LMG	O2-C2-C1	-2.02	105.14	110.05
22	A	838	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
22	A	830	CLA	C2D-C1D-ND	-2.02	108.62	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	620	XAT	O24-C25-C26	-2.02	57.29	58.96
21	Y	601	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
21	4	618	CHL	CBC-CAC-C3C	-2.02	106.87	112.43
22	3	606	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	B	809	CLA	O2D-CGD-O1D	-2.02	119.90	123.84
21	Y	601	CHL	C1C-C2C-C3C	-2.02	104.84	106.96
22	4	613	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	810	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	X	601	CHL	C1B-CHB-C4A	-2.01	126.13	130.12
24	2	620	XAT	C30-C31-C32	-2.01	116.93	123.22
25	A	856	BCR	C24-C23-C22	-2.01	123.19	126.23
22	B	826	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
22	1	613	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	A	844	PQN	C11-C3-C4	2.01	120.66	118.50
22	A	835	CLA	C2D-C1D-ND	-2.01	108.62	110.10
22	A	815	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
22	A	829	CLA	C2D-C1D-ND	-2.01	108.62	110.10
22	L	304	CLA	C2D-C1D-ND	-2.01	108.62	110.10
25	K	205	BCR	C33-C5-C6	-2.01	122.27	124.53
22	G	203	CLA	O2D-CGD-CBD	2.01	114.84	111.27
21	4	618	CHL	C4B-C3B-C2B	-2.01	105.05	106.92
22	A	810	CLA	CAA-C2A-C1A	2.01	118.56	111.97
25	L	301	BCR	C33-C5-C6	-2.01	122.27	124.53
22	B	829	CLA	O1D-CGD-CBD	2.01	128.60	124.48
21	2	618	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
22	B	833	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	Z	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	A	842	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	A	854	CLA	C4D-C3D-CAD	-2.01	105.73	108.10
22	Z	611	CLA	CMA-C3A-C2A	-2.01	111.41	116.10
22	B	812	CLA	C2A-C1A-CHA	2.01	127.37	123.86
27	4	623	LMG	O6-C5-C4	2.01	113.34	109.69
22	3	602	CLA	O1D-CGD-CBD	2.01	128.59	124.48
24	2	620	XAT	C31-C32-C33	-2.01	120.78	126.42
21	Z	601	CHL	C4D-CHA-C1A	-2.01	118.81	121.25
23	Y	4620	LUT	C39-C29-C28	2.01	121.24	118.08
22	K	203	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
22	B	807	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
32	B	850	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
22	Y	604	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	F	301	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
25	I	101	BCR	C37-C22-C23	2.00	121.23	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	609	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	4	611	CLA	C2A-C1A-CHA	2.00	127.36	123.86
21	X	608	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
21	X	607	CHL	O2D-CGD-O1D	-2.00	119.93	123.84
27	2	623	LMG	O2-C2-C1	-2.00	105.19	110.05
21	1	601	CHL	C1-C2-C3	-2.00	122.58	126.04
25	K	202	BCR	C24-C25-C26	2.00	126.31	121.46
22	B	822	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (263) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	601	CHL	C8
21	1	601	CHL	NA
21	1	601	CHL	ND
21	1	601	CHL	NC
21	1	607	CHL	NA
21	1	607	CHL	ND
21	1	607	CHL	NC
21	2	601	CHL	C8
21	2	601	CHL	NA
21	2	601	CHL	ND
21	2	601	CHL	NC
21	2	606	CHL	NA
21	2	606	CHL	ND
21	2	606	CHL	NC
21	2	607	CHL	NA
21	2	607	CHL	ND
21	2	607	CHL	NC
21	2	608	CHL	NA
21	2	608	CHL	ND
21	2	608	CHL	NC
21	2	618	CHL	NA
21	2	618	CHL	ND
21	2	618	CHL	NC
21	3	608	CHL	NA
21	3	608	CHL	ND
21	3	608	CHL	NC
21	4	606	CHL	NA
21	4	606	CHL	ND
21	4	606	CHL	NC
21	4	607	CHL	NA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
21	4	607	CHL	ND
21	4	607	CHL	NC
21	4	608	CHL	NA
21	4	608	CHL	ND
21	4	608	CHL	NC
21	4	618	CHL	NA
21	4	618	CHL	ND
21	4	618	CHL	NC
21	X	601	CHL	NA
21	X	601	CHL	ND
21	X	601	CHL	NC
21	X	605	CHL	NA
21	X	605	CHL	ND
21	X	605	CHL	NC
21	X	606	CHL	NA
21	X	606	CHL	ND
21	X	606	CHL	NC
21	X	607	CHL	NA
21	X	607	CHL	ND
21	X	607	CHL	NC
21	X	608	CHL	NA
21	X	608	CHL	ND
21	X	608	CHL	NC
21	X	609	CHL	NA
21	X	609	CHL	ND
21	X	609	CHL	NC
21	Y	601	CHL	C8
21	Y	601	CHL	NA
21	Y	601	CHL	ND
21	Y	601	CHL	NC
21	Y	605	CHL	NA
21	Y	605	CHL	ND
21	Y	605	CHL	NC
21	Y	606	CHL	NA
21	Y	606	CHL	ND
21	Y	606	CHL	NC
21	Y	607	CHL	NA
21	Y	607	CHL	ND
21	Y	607	CHL	NC
21	Y	608	CHL	NA
21	Y	608	CHL	ND
21	Y	608	CHL	NC

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
21	Y	609	CHL	NA
21	Y	609	CHL	ND
21	Y	609	CHL	NC
21	Z	601	CHL	NA
21	Z	601	CHL	ND
21	Z	601	CHL	NC
21	Z	605	CHL	NA
21	Z	605	CHL	ND
21	Z	605	CHL	NC
21	Z	606	CHL	NA
21	Z	606	CHL	ND
21	Z	606	CHL	NC
21	Z	607	CHL	NA
21	Z	607	CHL	ND
21	Z	607	CHL	NC
21	Z	608	CHL	NA
21	Z	608	CHL	ND
21	Z	608	CHL	NC
21	Z	609	CHL	NA
21	Z	609	CHL	ND
21	Z	609	CHL	NC
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	604	CLA	ND
22	1	606	CLA	ND
22	1	608	CLA	ND
22	1	609	CLA	ND
22	1	610	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	613	CLA	ND
22	1	614	CLA	ND
22	2	602	CLA	ND
22	2	603	CLA	ND
22	2	604	CLA	ND
22	2	609	CLA	ND
22	2	610	CLA	ND
22	2	611	CLA	ND
22	2	612	CLA	ND
22	2	613	CLA	ND
22	2	614	CLA	ND
22	3	602	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	609	CLA	ND
22	3	610	CLA	ND
22	3	613	CLA	ND
22	3	614	CLA	ND
22	3	615	CLA	ND
22	3	617	CLA	ND
22	4	601	CLA	ND
22	4	602	CLA	ND
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	609	CLA	ND
22	4	610	CLA	ND
22	4	611	CLA	ND
22	4	612	CLA	ND
22	4	613	CLA	ND
22	4	614	CLA	ND
22	4	617	CLA	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND
22	A	807	CLA	ND
22	A	808	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	813	CLA	ND
22	A	814	CLA	ND
22	A	815	CLA	ND
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	819	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	825	CLA	ND
22	A	826	CLA	ND
22	A	827	CLA	ND
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	830	CLA	ND
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	834	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	837	CLA	ND
22	A	838	CLA	ND
22	A	839	CLA	ND
22	A	840	CLA	ND
22	A	841	CLA	ND
22	A	842	CLA	ND
22	A	843	CLA	ND
22	A	845	CLA	ND
22	A	854	CLA	ND
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
22	B	805	CLA	ND
22	B	806	CLA	ND
22	B	808	CLA	ND
22	B	809	CLA	ND
22	B	810	CLA	ND
22	B	811	CLA	ND
22	B	812	CLA	ND
22	B	813	CLA	ND
22	B	814	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	817	CLA	ND
22	B	818	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	B	822	CLA	ND
22	B	823	CLA	ND
22	B	824	CLA	ND
22	B	825	CLA	ND
22	B	826	CLA	ND
22	B	827	CLA	ND
22	B	828	CLA	ND
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	832	CLA	ND
22	B	833	CLA	ND
22	B	834	CLA	ND
22	B	835	CLA	ND
22	B	836	CLA	ND
22	B	837	CLA	ND
22	B	838	CLA	ND
22	B	839	CLA	ND
22	B	840	CLA	ND
22	B	841	CLA	ND
22	F	301	CLA	ND
22	F	303	CLA	ND
22	F	304	CLA	ND
22	G	201	CLA	ND
22	G	203	CLA	ND
22	G	204	CLA	ND
22	H	201	CLA	ND
22	J	101	CLA	ND
22	K	201	CLA	ND
22	K	203	CLA	ND
22	K	204	CLA	ND
22	K	206	CLA	ND
22	L	302	CLA	ND
22	L	303	CLA	ND
22	L	304	CLA	ND
22	O	2001	CLA	ND
22	O	2002	CLA	ND
22	N	1002	CLA	ND
22	X	602	CLA	ND
22	X	603	CLA	ND
22	X	604	CLA	ND
22	X	610	CLA	ND

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Mol	Chain	Res	Type	Atom
22	X	611	CLA	ND
22	X	612	CLA	ND
22	X	613	CLA	ND
22	X	614	CLA	ND
22	Y	602	CLA	ND
22	Y	603	CLA	ND
22	Y	604	CLA	ND
22	Y	610	CLA	ND
22	Y	611	CLA	ND
22	Y	612	CLA	ND
22	Y	613	CLA	ND
22	Y	614	CLA	ND
22	Z	602	CLA	ND
22	Z	603	CLA	ND
22	Z	604	CLA	ND
22	Z	610	CLA	ND
22	Z	611	CLA	ND
22	Z	612	CLA	ND
22	Z	613	CLA	ND
22	Z	614	CLA	ND
28	A	801	CL0	NA
28	A	801	CL0	ND
28	A	801	CL0	NC

All (1886) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	601	CHL	C1A-C2A-CAA-CBA
21	1	601	CHL	C3A-C2A-CAA-CBA
21	2	601	CHL	C1A-C2A-CAA-CBA
21	2	601	CHL	C1C-C2C-CMC-OMC
21	2	601	CHL	C3C-C2C-CMC-OMC
21	2	607	CHL	C1C-C2C-CMC-OMC
21	2	607	CHL	C3C-C2C-CMC-OMC
21	2	618	CHL	C1C-C2C-CMC-OMC
21	2	618	CHL	C3C-C2C-CMC-OMC
21	3	608	CHL	C1A-C2A-CAA-CBA
21	4	606	CHL	C1A-C2A-CAA-CBA
21	4	606	CHL	C3A-C2A-CAA-CBA
21	4	606	CHL	C1C-C2C-CMC-OMC
21	4	606	CHL	C3C-C2C-CMC-OMC
21	4	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	X	601	CHL	C1C-C2C-CMC-OMC
21	X	601	CHL	C3C-C2C-CMC-OMC
21	X	607	CHL	C1A-C2A-CAA-CBA
21	X	607	CHL	C3A-C2A-CAA-CBA
21	X	607	CHL	C1C-C2C-CMC-OMC
21	X	607	CHL	C3C-C2C-CMC-OMC
21	Y	601	CHL	CAD-CBD-CGD-O2D
21	Y	607	CHL	C1C-C2C-CMC-OMC
21	Y	607	CHL	C3C-C2C-CMC-OMC
21	Y	608	CHL	C1A-C2A-CAA-CBA
21	Y	608	CHL	C3A-C2A-CAA-CBA
21	Z	606	CHL	C1C-C2C-CMC-OMC
21	Z	606	CHL	C3C-C2C-CMC-OMC
21	Z	607	CHL	C1C-C2C-CMC-OMC
21	Z	607	CHL	C3C-C2C-CMC-OMC
21	Z	608	CHL	C1C-C2C-CMC-OMC
21	Z	608	CHL	C3C-C2C-CMC-OMC
21	Z	609	CHL	C1C-C2C-CMC-OMC
21	Z	609	CHL	C3C-C2C-CMC-OMC
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CAD-CBD-CGD-O1D
22	1	604	CLA	CHA-CBD-CGD-O1D
22	1	604	CLA	CHA-CBD-CGD-O2D
22	1	604	CLA	CAD-CBD-CGD-O1D
22	1	604	CLA	CAD-CBD-CGD-O2D
22	1	604	CLA	CBD-CGD-O2D-CED
22	1	606	CLA	CHA-CBD-CGD-O1D
22	1	606	CLA	CHA-CBD-CGD-O2D
22	1	613	CLA	CBD-CGD-O2D-CED
22	1	613	CLA	C11-C10-C8-C9
22	1	616	CLA	CBD-CGD-O2D-CED
22	2	604	CLA	CBD-CGD-O2D-CED
22	2	610	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	C6-C7-C8-C9
22	3	606	CLA	C1A-C2A-CAA-CBA
22	3	606	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	609	CLA	C1A-C2A-CAA-CBA
22	3	609	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	CBD-CGD-O2D-CED
22	3	612	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	3	612	CLA	C3A-C2A-CAA-CBA
22	3	612	CLA	CBD-CGD-O2D-CED
22	3	614	CLA	CHA-CBD-CGD-O2D
22	4	604	CLA	CBD-CGD-O2D-CED
22	4	609	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C3A-C2A-CAA-CBA
22	4	611	CLA	C1A-C2A-CAA-CBA
22	4	612	CLA	C1A-C2A-CAA-CBA
22	4	612	CLA	C3A-C2A-CAA-CBA
22	4	613	CLA	CHA-CBD-CGD-O1D
22	4	613	CLA	CHA-CBD-CGD-O2D
22	4	613	CLA	CBD-CGD-O2D-CED
22	4	617	CLA	CBD-CGD-O2D-CED
22	A	802	CLA	CHA-CBD-CGD-O1D
22	A	802	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	807	CLA	C11-C12-C13-C15
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	815	CLA	CBD-CGD-O2D-CED
22	A	818	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	CBD-CGD-O2D-CED
22	A	825	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	C3A-C2A-CAA-CBA
22	A	825	CLA	CHA-CBD-CGD-O1D
22	A	825	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CBD-CGD-O2D-CED
22	A	829	CLA	C14-C13-C15-C16
22	A	833	CLA	C2-C3-C5-C6
22	A	833	CLA	C4-C3-C5-C6
22	A	834	CLA	CHA-CBD-CGD-O1D
22	A	834	CLA	CHA-CBD-CGD-O2D
22	A	834	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	834	CLA	CAD-CBD-CGD-O2D
22	A	834	CLA	CBD-CGD-O2D-CED
22	A	835	CLA	C2-C3-C5-C6
22	A	835	CLA	C4-C3-C5-C6
22	A	837	CLA	C1A-C2A-CAA-CBA
22	A	837	CLA	C3A-C2A-CAA-CBA
22	A	838	CLA	C2-C3-C5-C6
22	A	839	CLA	C2-C3-C5-C6
22	A	839	CLA	C4-C3-C5-C6
22	A	840	CLA	CBD-CGD-O2D-CED
22	A	840	CLA	C3-C5-C6-C7
22	A	841	CLA	CHA-CBD-CGD-O1D
22	A	841	CLA	CHA-CBD-CGD-O2D
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	845	CLA	C1A-C2A-CAA-CBA
22	A	845	CLA	C3A-C2A-CAA-CBA
22	A	845	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O2D
22	A	845	CLA	CBD-CGD-O2D-CED
22	B	802	CLA	CHA-CBD-CGD-O1D
22	B	802	CLA	CHA-CBD-CGD-O2D
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	C3A-C2A-CAA-CBA
22	B	803	CLA	CBD-CGD-O2D-CED
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	805	CLA	CHA-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	810	CLA	C1A-C2A-CAA-CBA
22	B	810	CLA	CHA-CBD-CGD-O1D
22	B	810	CLA	CHA-CBD-CGD-O2D
22	B	811	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C3A-C2A-CAA-CBA
22	B	813	CLA	C2A-CAA-CBA-CGA
22	B	813	CLA	CHA-CBD-CGD-O1D
22	B	813	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	813	CLA	CAD-CBD-CGD-O1D
22	B	814	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	816	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	CBD-CGD-O2D-CED
22	B	835	CLA	C3A-C2A-CAA-CBA
22	B	835	CLA	CBD-CGD-O2D-CED
22	B	838	CLA	CHA-CBD-CGD-O1D
22	B	838	CLA	CHA-CBD-CGD-O2D
22	B	840	CLA	CBD-CGD-O2D-CED
22	B	841	CLA	C1A-C2A-CAA-CBA
22	B	841	CLA	C3A-C2A-CAA-CBA
22	G	201	CLA	CBD-CGD-O2D-CED
22	G	203	CLA	CHA-CBD-CGD-O1D
22	G	203	CLA	CHA-CBD-CGD-O2D
22	G	204	CLA	CHA-CBD-CGD-O1D
22	G	204	CLA	CBD-CGD-O2D-CED
22	H	201	CLA	C1A-C2A-CAA-CBA
22	H	201	CLA	C3A-C2A-CAA-CBA
22	H	201	CLA	CBD-CGD-O2D-CED
22	J	101	CLA	C1A-C2A-CAA-CBA
22	J	101	CLA	CHA-CBD-CGD-O1D
22	J	101	CLA	CHA-CBD-CGD-O2D
22	K	204	CLA	C1A-C2A-CAA-CBA
22	K	204	CLA	C3A-C2A-CAA-CBA
22	L	302	CLA	C1A-C2A-CAA-CBA
22	L	302	CLA	C3A-C2A-CAA-CBA
22	L	303	CLA	C1A-C2A-CAA-CBA
22	L	303	CLA	C3A-C2A-CAA-CBA
22	L	303	CLA	CHA-CBD-CGD-O1D
22	L	303	CLA	CHA-CBD-CGD-O2D
22	L	303	CLA	C2-C3-C5-C6
22	L	303	CLA	C4-C3-C5-C6
22	O	2001	CLA	CHA-CBD-CGD-O2D
22	X	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	X	603	CLA	C1A-C2A-CAA-CBA
22	X	603	CLA	C3A-C2A-CAA-CBA
22	X	614	CLA	CHA-CBD-CGD-O1D
22	X	614	CLA	CBD-CGD-O2D-CED
22	Y	604	CLA	CHA-CBD-CGD-O1D
22	Y	604	CLA	CHA-CBD-CGD-O2D
22	Y	604	CLA	CAD-CBD-CGD-O1D
22	Y	604	CLA	CAD-CBD-CGD-O2D
22	Y	604	CLA	CBD-CGD-O2D-CED
22	Y	611	CLA	C1A-C2A-CAA-CBA
22	Z	603	CLA	CBD-CGD-O2D-CED
22	Z	612	CLA	C1A-C2A-CAA-CBA
22	Z	612	CLA	C3A-C2A-CAA-CBA
23	3	618	LUT	C1-C6-C7-C8
23	3	618	LUT	C27-C28-C29-C39
23	X	2621	LUT	C27-C28-C29-C39
23	Y	4620	LUT	C11-C12-C13-C14
23	Y	4620	LUT	C11-C12-C13-C20
23	Z	7620	LUT	C1-C6-C7-C8
24	4	620	XAT	C27-C28-C29-C39
24	Z	4622	XAT	C11-C12-C13-C14
24	Z	4622	XAT	C11-C12-C13-C20
25	2	621	BCR	C7-C8-C9-C10
25	2	621	BCR	C7-C8-C9-C34
25	4	621	BCR	C7-C8-C9-C10
25	4	621	BCR	C7-C8-C9-C34
25	4	621	BCR	C11-C12-C13-C14
25	4	621	BCR	C11-C12-C13-C35
25	4	621	BCR	C17-C18-C19-C20
25	4	621	BCR	C36-C18-C19-C20
25	4	621	BCR	C23-C24-C25-C30
25	A	848	BCR	C21-C22-C23-C24
25	A	848	BCR	C37-C22-C23-C24
25	A	849	BCR	C7-C8-C9-C10
25	A	849	BCR	C7-C8-C9-C34
25	A	850	BCR	C7-C8-C9-C10
25	A	851	BCR	C21-C22-C23-C24
25	A	851	BCR	C37-C22-C23-C24
25	A	851	BCR	C23-C24-C25-C30
25	A	852	BCR	C7-C8-C9-C10
25	A	852	BCR	C7-C8-C9-C34
25	A	852	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	A	852	BCR	C37-C22-C23-C24
25	A	856	BCR	C21-C22-C23-C24
25	A	856	BCR	C37-C22-C23-C24
25	B	801	BCR	C36-C18-C19-C20
25	B	843	BCR	C17-C18-C19-C20
25	B	843	BCR	C36-C18-C19-C20
25	B	843	BCR	C21-C22-C23-C24
25	B	843	BCR	C37-C22-C23-C24
25	B	844	BCR	C7-C8-C9-C10
25	B	844	BCR	C7-C8-C9-C34
25	B	844	BCR	C21-C22-C23-C24
25	B	844	BCR	C23-C24-C25-C30
25	B	845	BCR	C7-C8-C9-C10
25	B	845	BCR	C7-C8-C9-C34
25	B	847	BCR	C21-C22-C23-C24
25	B	847	BCR	C37-C22-C23-C24
25	B	848	BCR	C21-C22-C23-C24
25	B	848	BCR	C37-C22-C23-C24
25	I	101	BCR	C11-C12-C13-C35
25	J	102	BCR	C7-C8-C9-C10
25	J	102	BCR	C7-C8-C9-C34
25	K	205	BCR	C23-C24-C25-C26
25	L	301	BCR	C1-C6-C7-C8
25	L	305	BCR	C1-C6-C7-C8
25	L	305	BCR	C7-C8-C9-C10
25	L	305	BCR	C7-C8-C9-C34
25	L	305	BCR	C21-C22-C23-C24
25	L	305	BCR	C37-C22-C23-C24
25	L	305	BCR	C23-C24-C25-C30
25	L	306	BCR	C11-C12-C13-C14
25	L	306	BCR	C11-C12-C13-C35
26	2	622	LHG	O1-C1-C2-C3
26	2	622	LHG	C4-O6-P-O3
26	A	846	LHG	O7-C5-C6-O8
26	B	851	LHG	C4-O6-P-O5
26	X	2630	LHG	C4-O6-P-O4
26	X	2630	LHG	O10-C23-O8-C6
26	Y	4630	LHG	C4-O6-P-O5
26	Z	7630	LHG	C4-O6-P-O5
29	A	844	PQN	C11-C12-C13-C14
29	B	842	PQN	C11-C12-C13-C14
31	A	857	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	A	857	LMU	O5'-C1'-O1'-C1
32	B	850	DGD	O1B-C1B-O2G-C2G
32	J	103	DGD	O6E-C1E-O5D-C6D
21	4	608	CHL	O1D-CGD-O2D-CED
22	3	609	CLA	O1D-CGD-O2D-CED
22	3	612	CLA	O1D-CGD-O2D-CED
22	4	604	CLA	O1D-CGD-O2D-CED
22	B	811	CLA	O1D-CGD-O2D-CED
22	B	816	CLA	O1D-CGD-O2D-CED
22	B	831	CLA	O1D-CGD-O2D-CED
22	H	201	CLA	O1D-CGD-O2D-CED
22	4	613	CLA	O1D-CGD-O2D-CED
22	A	818	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
21	2	608	CHL	CBD-CGD-O2D-CED
21	3	608	CHL	CBD-CGD-O2D-CED
22	1	603	CLA	CBD-CGD-O2D-CED
22	1	606	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	4	609	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	822	CLA	CBD-CGD-O2D-CED
22	A	835	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	CBD-CGD-O2D-CED
22	B	810	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	828	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	F	303	CLA	CBD-CGD-O2D-CED
22	K	204	CLA	CBD-CGD-O2D-CED
22	L	304	CLA	CBD-CGD-O2D-CED
22	N	1002	CLA	CBD-CGD-O2D-CED
22	Y	610	CLA	CBD-CGD-O2D-CED
22	Z	614	CLA	CBD-CGD-O2D-CED
21	1	601	CHL	O1A-CGA-O2A-C1
22	3	603	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	O1A-CGA-O2A-C1
26	Y	4630	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
31	A	857	LMU	O5B-C1B-O1B-C4'
22	1	606	CLA	O1D-CGD-O2D-CED
22	2	610	CLA	O1D-CGD-O2D-CED
22	3	603	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	O1D-CGD-O2D-CED
22	A	845	CLA	O1D-CGD-O2D-CED
21	2	608	CHL	O1D-CGD-O2D-CED
22	1	613	CLA	O1D-CGD-O2D-CED
22	1	616	CLA	O1D-CGD-O2D-CED
22	2	604	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	O1D-CGD-O2D-CED
22	A	840	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	O1D-CGD-O2D-CED
22	B	835	CLA	O1D-CGD-O2D-CED
22	B	840	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	O1D-CGD-O2D-CED
22	G	204	CLA	O1D-CGD-O2D-CED
22	K	204	CLA	O1D-CGD-O2D-CED
22	Z	603	CLA	O1D-CGD-O2D-CED
21	1	601	CHL	CBA-CGA-O2A-C1
22	A	818	CLA	CBA-CGA-O2A-C1
32	J	103	DGD	C2A-C1A-O1G-C1G
21	2	618	CHL	CBD-CGD-O2D-CED
22	3	610	CLA	CBD-CGD-O2D-CED
22	A	843	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	CBD-CGD-O2D-CED
22	B	834	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	O1A-CGA-O2A-C1
22	A	834	CLA	O1A-CGA-O2A-C1
22	L	303	CLA	O1A-CGA-O2A-C1
26	2	622	LHG	O10-C23-O8-C6
26	B	851	LHG	O10-C23-O8-C6
22	1	604	CLA	O1D-CGD-O2D-CED
22	4	617	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	O1D-CGD-O2D-CED
22	Y	604	CLA	O1D-CGD-O2D-CED
31	A	857	LMU	C2B-C1B-O1B-C4'
22	A	824	CLA	O1D-CGD-O2D-CED
22	G	201	CLA	O1D-CGD-O2D-CED
22	X	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	2	612	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	825	CLA	CBD-CGD-O2D-CED
22	Z	602	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
27	1	622	LMG	O9-C10-O7-C8
27	2	623	LMG	O9-C10-O7-C8
32	J	103	DGD	O1B-C1B-O2G-C2G
27	4	623	LMG	C4-C5-C6-O5
22	4	609	CLA	O1D-CGD-O2D-CED
21	Y	601	CHL	C3-C5-C6-C7
22	1	613	CLA	C3-C5-C6-C7
22	A	825	CLA	C3-C5-C6-C7
22	B	806	CLA	C3-C5-C6-C7
22	B	817	CLA	C3-C5-C6-C7
22	B	827	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	B	839	CLA	C3-C5-C6-C7
22	B	840	CLA	C3-C5-C6-C7
22	B	841	CLA	C3-C5-C6-C7
22	F	301	CLA	C3-C5-C6-C7
22	3	603	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	CBA-CGA-O2A-C1
26	2	622	LHG	C24-C23-O8-C6
26	B	851	LHG	C24-C23-O8-C6
26	Y	4630	LHG	C24-C23-O8-C6
32	B	850	DGD	C2B-C1B-O2G-C2G
22	A	812	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	O1A-CGA-O2A-C1
32	J	103	DGD	O1A-C1A-O1G-C1G
26	Z	7630	LHG	C24-C23-O8-C6
22	A	818	CLA	C4-C3-C5-C6
22	B	816	CLA	C4-C3-C5-C6
22	4	602	CLA	CBD-CGD-O2D-CED
22	A	806	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	CBD-CGD-O2D-CED
21	Z	608	CHL	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
22	4	601	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	822	CLA	C2A-CAA-CBA-CGA
22	A	825	CLA	C2A-CAA-CBA-CGA
22	A	834	CLA	C2A-CAA-CBA-CGA
22	A	837	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C2A-CAA-CBA-CGA
22	B	839	CLA	C2A-CAA-CBA-CGA
22	G	201	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C3-C5-C6-C7
22	A	854	CLA	C3-C5-C6-C7
22	B	810	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	829	CLA	C3-C5-C6-C7
22	4	613	CLA	CBA-CGA-O2A-C1
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBA-CGA-O2A-C1
22	A	838	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	B	841	CLA	CBA-CGA-O2A-C1
22	L	303	CLA	CBA-CGA-O2A-C1
26	Z	7630	LHG	O10-C23-O8-C6
22	A	822	CLA	O1D-CGD-O2D-CED
22	A	854	CLA	O1D-CGD-O2D-CED
22	F	303	CLA	O1D-CGD-O2D-CED
22	B	838	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1A-CGA-O2A-C1
22	A	820	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	O1A-CGA-O2A-C1
22	B	841	CLA	O1A-CGA-O2A-C1
26	1	620	LHG	O10-C23-O8-C6
31	B	849	LMU	C2B-C1B-O1B-C4'
27	1	622	LMG	O6-C5-C6-O5
21	2	607	CHL	CBD-CGD-O2D-CED
22	1	609	CLA	CBD-CGD-O2D-CED
22	2	611	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	CBD-CGD-O2D-CED
22	B	812	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	J	101	CLA	CBD-CGD-O2D-CED
22	L	302	CLA	CBD-CGD-O2D-CED
22	Y	602	CLA	CBD-CGD-O2D-CED
21	3	608	CHL	O1D-CGD-O2D-CED
22	A	835	CLA	O1D-CGD-O2D-CED
22	B	821	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	O1D-CGD-O2D-CED
22	B	808	CLA	C3-C5-C6-C7
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	820	CLA	CBA-CGA-O2A-C1
22	A	839	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
26	1	620	LHG	C24-C23-O8-C6
22	A	822	CLA	O1A-CGA-O2A-C1
22	A	835	CLA	O1A-CGA-O2A-C1
22	B	810	CLA	O1D-CGD-O2D-CED
22	N	1002	CLA	O1D-CGD-O2D-CED
22	Y	610	CLA	O1D-CGD-O2D-CED
31	B	849	LMU	O5B-C1B-O1B-C4'
21	Y	607	CHL	CBD-CGD-O2D-CED
22	2	614	CLA	CBD-CGD-O2D-CED
22	A	831	CLA	CBD-CGD-O2D-CED
22	A	843	CLA	O1A-CGA-O2A-C1
22	L	304	CLA	O1D-CGD-O2D-CED
22	3	602	CLA	C3-C5-C6-C7
22	A	828	CLA	C3-C5-C6-C7
22	A	827	CLA	CBA-CGA-O2A-C1
22	B	811	CLA	CBA-CGA-O2A-C1
32	J	103	DGD	O6E-C5E-C6E-O5E
26	A	846	LHG	O9-C7-O7-C5
22	4	613	CLA	O1A-CGA-O2A-C1
22	A	838	CLA	O1A-CGA-O2A-C1
22	B	829	CLA	O1A-CGA-O2A-C1
27	4	623	LMG	O6-C5-C6-O5
22	A	854	CLA	C4-C3-C5-C6
22	B	818	CLA	C4-C3-C5-C6
22	H	201	CLA	C4-C3-C5-C6
22	A	854	CLA	C2-C3-C5-C6
22	B	818	CLA	C2-C3-C5-C6
22	H	201	CLA	C2-C3-C5-C6
22	A	854	CLA	C2A-CAA-CBA-CGA
22	L	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	807	CLA	O1A-CGA-O2A-C1
27	1	622	LMG	O6-C1-O1-C7
22	A	833	CLA	CBA-CGA-O2A-C1
22	F	304	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	O1D-CGD-O2D-CED
22	Z	614	CLA	O1D-CGD-O2D-CED
22	B	811	CLA	O1A-CGA-O2A-C1
27	1	622	LMG	C11-C10-O7-C8
32	J	103	DGD	C2B-C1B-O2G-C2G
31	B	849	LMU	C6-C7-C8-C9
22	2	602	CLA	O1D-CGD-O2D-CED
22	A	843	CLA	O1D-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
26	A	846	LHG	C1-C2-C3-O3
26	A	847	LHG	C1-C2-C3-O3
26	Z	7630	LHG	C1-C2-C3-O3
22	A	839	CLA	O1A-CGA-O2A-C1
21	2	618	CHL	O1D-CGD-O2D-CED
21	2	608	CHL	CBA-CGA-O2A-C1
22	1	604	CLA	CBA-CGA-O2A-C1
22	A	804	CLA	CBA-CGA-O2A-C1
22	B	821	CLA	CBA-CGA-O2A-C1
22	B	825	CLA	CBA-CGA-O2A-C1
22	F	301	CLA	CBA-CGA-O2A-C1
22	Z	604	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	C10-C11-C12-C13
22	A	806	CLA	C13-C15-C16-C17
22	A	812	CLA	C10-C11-C12-C13
22	A	822	CLA	C13-C15-C16-C17
22	A	829	CLA	C8-C10-C11-C12
22	B	802	CLA	C10-C11-C12-C13
22	B	826	CLA	C10-C11-C12-C13
26	A	846	LHG	O2-C2-C3-O3
26	B	851	LHG	O2-C2-C3-O3
27	2	623	LMG	C2-C1-O1-C7
31	B	849	LMU	C11-C10-C9-C8
21	2	608	CHL	O1A-CGA-O2A-C1
22	A	804	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	C2-C3-C5-C6
22	B	816	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	601	CHL	C11-C10-C8-C9
22	2	602	CLA	C11-C10-C8-C9
22	A	802	CLA	C6-C7-C8-C9
22	A	826	CLA	C11-C12-C13-C14
22	A	828	CLA	C6-C7-C8-C9
22	A	841	CLA	C11-C12-C13-C14
22	A	854	CLA	C11-C10-C8-C9
22	B	806	CLA	C11-C10-C8-C9
22	B	826	CLA	C11-C12-C13-C14
22	B	828	CLA	C14-C13-C15-C16
22	B	840	CLA	C6-C7-C8-C9
22	L	303	CLA	C6-C7-C8-C9
29	A	844	PQN	C19-C18-C20-C21
22	B	834	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	CBD-CGD-O2D-CED
22	A	829	CLA	C13-C15-C16-C17
22	B	841	CLA	C8-C10-C11-C12
21	Z	607	CHL	C2A-CAA-CBA-CGA
23	Y	4620	LUT	C27-C28-C29-C39
24	1	618	XAT	C27-C28-C29-C39
24	3	619	XAT	C27-C28-C29-C39
24	Y	2622	XAT	C11-C12-C13-C20
25	3	620	BCR	C7-C8-C9-C34
25	A	850	BCR	C7-C8-C9-C34
25	A	851	BCR	C36-C18-C19-C20
25	B	801	BCR	C37-C22-C23-C24
25	B	844	BCR	C37-C22-C23-C24
25	J	102	BCR	C36-C18-C19-C20
25	K	202	BCR	C37-C22-C23-C24
25	L	305	BCR	C36-C18-C19-C20
23	3	618	LUT	C27-C28-C29-C30
23	X	2621	LUT	C27-C28-C29-C30
25	B	801	BCR	C21-C22-C23-C24
25	K	202	BCR	C21-C22-C23-C24
25	L	305	BCR	C17-C18-C19-C20
22	A	811	CLA	C13-C15-C16-C17
22	B	837	CLA	C5-C6-C7-C8
22	A	832	CLA	CBD-CGD-O2D-CED
22	4	613	CLA	C8-C10-C11-C12
22	B	826	CLA	C13-C15-C16-C17
22	Z	613	CLA	C2A-CAA-CBA-CGA
22	A	802	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	831	CLA	C5-C6-C7-C8
22	B	818	CLA	C8-C10-C11-C12
22	B	824	CLA	C13-C15-C16-C17
29	A	844	PQN	C20-C21-C22-C23
21	Y	601	CHL	C8-C10-C11-C12
22	2	602	CLA	C8-C10-C11-C12
22	3	602	CLA	C10-C11-C12-C13
22	A	806	CLA	C5-C6-C7-C8
22	A	828	CLA	C10-C11-C12-C13
22	A	841	CLA	C5-C6-C7-C8
22	A	842	CLA	C15-C16-C17-C18
22	A	843	CLA	C5-C6-C7-C8
22	B	840	CLA	C13-C15-C16-C17
22	H	201	CLA	C5-C6-C7-C8
29	A	844	PQN	C15-C16-C17-C18
27	1	622	LMG	C4-C5-C6-O5
22	3	610	CLA	O1D-CGD-O2D-CED
26	1	620	LHG	C7-C8-C9-C10
26	1	620	LHG	C23-C24-C25-C26
26	A	847	LHG	C23-C24-C25-C26
27	4	622	LMG	C10-C11-C12-C13
22	A	809	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	CBD-CGD-O2D-CED
21	2	601	CHL	C8-C10-C11-C12
22	A	802	CLA	C15-C16-C17-C18
22	A	804	CLA	C15-C16-C17-C18
22	B	824	CLA	C8-C10-C11-C12
29	B	842	PQN	C25-C26-C27-C28
22	4	610	CLA	C3-C5-C6-C7
22	A	826	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	C8-C10-C11-C12
22	A	825	CLA	C5-C6-C7-C8
22	A	829	CLA	C10-C11-C12-C13
22	A	833	CLA	C5-C6-C7-C8
22	A	834	CLA	C5-C6-C7-C8
22	B	805	CLA	C13-C15-C16-C17
22	B	818	CLA	C5-C6-C7-C8
22	B	837	CLA	C15-C16-C17-C18
32	B	850	DGD	C1B-C2B-C3B-C4B
22	B	804	CLA	CBD-CGD-O2D-CED
22	B	839	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	2	602	CLA	C15-C16-C17-C18
22	B	830	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	C12-C13-C15-C16
22	B	803	CLA	C11-C10-C8-C7
22	B	806	CLA	C11-C10-C8-C7
22	B	809	CLA	C11-C12-C13-C15
22	B	826	CLA	C11-C12-C13-C15
29	B	842	PQN	C21-C22-C23-C25
22	A	809	CLA	C3-C5-C6-C7
22	A	833	CLA	O1A-CGA-O2A-C1
22	B	821	CLA	O1A-CGA-O2A-C1
22	F	301	CLA	O1A-CGA-O2A-C1
22	Z	604	CLA	O1A-CGA-O2A-C1
25	A	849	BCR	C9-C10-C11-C12
21	Y	601	CHL	C2A-CAA-CBA-CGA
22	Z	602	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	O1D-CGD-O2D-CED
22	Z	602	CLA	O1D-CGD-O2D-CED
21	Y	601	CHL	C15-C16-C17-C18
22	4	602	CLA	C8-C10-C11-C12
22	A	807	CLA	C5-C6-C7-C8
22	A	820	CLA	C10-C11-C12-C13
22	A	827	CLA	C5-C6-C7-C8
22	A	831	CLA	C8-C10-C11-C12
22	B	808	CLA	C15-C16-C17-C18
22	B	828	CLA	C8-C10-C11-C12
22	A	802	CLA	C13-C15-C16-C17
22	A	825	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	C2C-C3C-CAC-CBC
21	Y	601	CHL	C10-C11-C12-C13
22	B	806	CLA	C15-C16-C17-C18
22	B	809	CLA	C10-C11-C12-C13
22	B	827	CLA	C15-C16-C17-C18
22	B	841	CLA	C13-C15-C16-C17
22	2	612	CLA	O1D-CGD-O2D-CED
22	1	604	CLA	O1A-CGA-O2A-C1
26	A	847	LHG	C7-C8-C9-C10
22	A	807	CLA	C15-C16-C17-C18
22	A	814	CLA	C8-C10-C11-C12
22	A	834	CLA	C15-C16-C17-C18
22	B	819	CLA	C5-C6-C7-C8
22	A	806	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	O1D-CGD-O2D-CED
27	2	623	LMG	C11-C10-O7-C8
22	B	838	CLA	O1D-CGD-O2D-CED
22	A	818	CLA	C8-C10-C11-C12
22	B	809	CLA	C5-C6-C7-C8
22	B	827	CLA	C10-C11-C12-C13
26	X	2630	LHG	C4-O6-P-O3
22	A	834	CLA	C3-C5-C6-C7
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	CBA-CGA-O2A-C1
27	G	202	LMG	C29-C28-O8-C9
22	1	613	CLA	C8-C10-C11-C12
22	A	834	CLA	C13-C15-C16-C17
22	B	822	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	C8-C10-C11-C12
21	2	608	CHL	C2A-CAA-CBA-CGA
22	A	819	CLA	C2A-CAA-CBA-CGA
22	Z	614	CLA	C2A-CAA-CBA-CGA
22	L	303	CLA	C11-C12-C13-C15
22	1	603	CLA	C3-C5-C6-C7
21	2	601	CHL	CBA-CGA-O2A-C1
22	A	835	CLA	C5-C6-C7-C8
21	2	601	CHL	C5-C6-C7-C8
22	B	836	CLA	O1D-CGD-O2D-CED
26	A	846	LHG	C8-C7-O7-C5
22	4	601	CLA	CBA-CGA-O2A-C1
29	A	844	PQN	C18-C20-C21-C22
22	L	303	CLA	C3-C5-C6-C7
26	B	851	LHG	C24-C25-C26-C27
26	B	851	LHG	C28-C29-C30-C31
26	Y	4630	LHG	C15-C16-C17-C18
27	1	622	LMG	C38-C39-C40-C41
27	4	623	LMG	C12-C13-C14-C15
22	A	831	CLA	C16-C17-C18-C20
22	H	201	CLA	CBA-CGA-O2A-C1
27	G	202	LMG	C30-C31-C32-C33
32	B	850	DGD	CBA-CCA-CDA-CEA
22	B	825	CLA	C8-C10-C11-C12
22	B	828	CLA	C13-C15-C16-C17
26	A	846	LHG	C7-C8-C9-C10
22	B	832	CLA	CBD-CGD-O2D-CED
32	J	103	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
32	J	103	DGD	C4B-C5B-C6B-C7B
22	1	609	CLA	O1D-CGD-O2D-CED
26	2	622	LHG	C27-C28-C29-C30
22	4	602	CLA	O1D-CGD-O2D-CED
22	Y	613	CLA	CBA-CGA-O2A-C1
26	A	847	LHG	O2-C2-C3-O3
26	Z	7630	LHG	O2-C2-C3-O3
27	G	202	LMG	C13-C14-C15-C16
22	A	806	CLA	C3-C5-C6-C7
27	1	622	LMG	C2-C1-O1-C7
22	A	841	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	CBA-CGA-O2A-C1
27	G	202	LMG	C11-C12-C13-C14
21	2	601	CHL	O1A-CGA-O2A-C1
21	Y	601	CHL	C16-C17-C18-C19
22	H	201	CLA	C11-C12-C13-C15
22	A	806	CLA	C4-C3-C5-C6
22	A	820	CLA	C4-C3-C5-C6
22	B	829	CLA	C4-C3-C5-C6
22	4	610	CLA	C5-C6-C7-C8
27	4	623	LMG	C29-C30-C31-C32
22	A	806	CLA	C2-C3-C5-C6
22	A	820	CLA	C2-C3-C5-C6
22	1	613	CLA	C6-C7-C8-C9
22	B	809	CLA	C6-C7-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	B	812	CLA	O1D-CGD-O2D-CED
22	J	101	CLA	O1D-CGD-O2D-CED
22	Y	602	CLA	O1D-CGD-O2D-CED
26	B	851	LHG	C23-C24-C25-C26
26	Y	4630	LHG	C23-C24-C25-C26
27	4	623	LMG	C10-C11-C12-C13
32	B	850	DGD	C5A-C6A-C7A-C8A
32	J	103	DGD	C6B-C7B-C8B-C9B
32	J	103	DGD	CBB-CCB-CDB-CEB
22	A	829	CLA	C5-C6-C7-C8
22	B	802	CLA	C13-C15-C16-C17
22	B	818	CLA	C10-C11-C12-C13
22	B	834	CLA	C5-C6-C7-C8
22	2	612	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2A-CAA-CBA-CGA
22	K	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	O1A-CGA-O2A-C1
25	K	205	BCR	C37-C22-C23-C24
26	A	846	LHG	C30-C31-C32-C33
27	1	622	LMG	C14-C15-C16-C17
32	B	850	DGD	CAA-CBA-CCA-CDA
26	1	620	LHG	O1-C1-C2-C3
26	Z	7630	LHG	O1-C1-C2-C3
25	I	101	BCR	C11-C12-C13-C14
25	K	205	BCR	C21-C22-C23-C24
22	2	613	CLA	C3-C5-C6-C7
22	A	839	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	1	610	CLA	C5-C6-C7-C8
26	2	622	LHG	C28-C29-C30-C31
26	A	846	LHG	C27-C28-C29-C30
32	J	103	DGD	CAB-CBB-CCB-CDB
26	2	622	LHG	C23-C24-C25-C26
27	1	622	LMG	C10-C11-C12-C13
22	2	611	CLA	O1D-CGD-O2D-CED
26	1	620	LHG	C27-C28-C29-C30
26	B	851	LHG	C27-C28-C29-C30
27	4	622	LMG	C31-C32-C33-C34
32	B	850	DGD	C4A-C5A-C6A-C7A
32	J	103	DGD	C3A-C4A-C5A-C6A
22	A	806	CLA	C16-C17-C18-C19
22	A	825	CLA	C6-C7-C8-C9
22	A	825	CLA	C6-C7-C8-C10
22	A	831	CLA	C16-C17-C18-C19
22	B	827	CLA	C16-C17-C18-C19
32	J	103	DGD	CEB-CFB-CGB-CHB
22	2	609	CLA	CBD-CGD-O2D-CED
26	A	846	LHG	C29-C30-C31-C32
26	B	851	LHG	C30-C31-C32-C33
26	Y	4630	LHG	C10-C11-C12-C13
22	A	854	CLA	C13-C15-C16-C17
22	B	826	CLA	O1A-CGA-O2A-C1
26	1	620	LHG	C30-C31-C32-C33
32	B	850	DGD	C6B-C7B-C8B-C9B
22	H	201	CLA	C3-C5-C6-C7
22	A	810	CLA	CBA-CGA-O2A-C1
26	1	620	LHG	C10-C11-C12-C13
21	2	601	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	3	608	CHL	C3A-C2A-CAA-CBA
21	X	605	CHL	C3A-C2A-CAA-CBA
22	2	612	CLA	C3A-C2A-CAA-CBA
22	3	603	CLA	C3A-C2A-CAA-CBA
22	A	803	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	810	CLA	C3A-C2A-CAA-CBA
22	B	809	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	F	301	CLA	C3A-C2A-CAA-CBA
25	L	306	BCR	C19-C20-C21-C22
31	B	849	LMU	C1-C2-C3-C4
31	B	849	LMU	C2-C1-O1'-C1'
21	2	607	CHL	O1D-CGD-O2D-CED
22	L	302	CLA	O1D-CGD-O2D-CED
22	A	806	CLA	C16-C17-C18-C20
22	A	822	CLA	C16-C17-C18-C19
26	A	846	LHG	C9-C10-C11-C12
27	1	622	LMG	C29-C30-C31-C32
22	2	613	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	O1D-CGD-O2D-CED
21	2	601	CHL	CBD-CGD-O2D-CED
22	B	813	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	C2-C3-C5-C6
22	4	611	CLA	CBD-CGD-O2D-CED
21	4	608	CHL	C2A-CAA-CBA-CGA
26	2	622	LHG	O1-C1-C2-O2
26	A	846	LHG	C31-C32-C33-C34
27	G	202	LMG	C12-C13-C14-C15
22	H	201	CLA	O1A-CGA-O2A-C1
22	H	201	CLA	C11-C12-C13-C14
22	A	822	CLA	C15-C16-C17-C18
27	1	622	LMG	C30-C31-C32-C33
22	B	805	CLA	O1A-CGA-O2A-C1
22	A	823	CLA	CBD-CGD-O2D-CED
27	2	623	LMG	C16-C17-C18-C19
27	2	623	LMG	C15-C16-C17-C18
32	J	103	DGD	C7B-C8B-C9B-CAB
22	2	610	CLA	C5-C6-C7-C8
22	A	810	CLA	O1A-CGA-O2A-C1
32	B	850	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
27	4	622	LMG	C28-C29-C30-C31
22	B	823	CLA	CBD-CGD-O2D-CED
23	2	619	LUT	C1-C6-C7-C8
23	2	619	LUT	C5-C6-C7-C8
23	3	618	LUT	C5-C6-C7-C8
23	4	619	LUT	C1-C6-C7-C8
23	4	619	LUT	C5-C6-C7-C8
23	X	2620	LUT	C1-C6-C7-C8
23	X	2620	LUT	C5-C6-C7-C8
23	Y	4620	LUT	C1-C6-C7-C8
23	Y	4620	LUT	C5-C6-C7-C8
23	Z	7620	LUT	C5-C6-C7-C8
25	2	621	BCR	C1-C6-C7-C8
25	2	621	BCR	C5-C6-C7-C8
25	3	620	BCR	C23-C24-C25-C26
25	3	620	BCR	C23-C24-C25-C30
25	4	621	BCR	C23-C24-C25-C26
25	A	851	BCR	C23-C24-C25-C26
25	A	856	BCR	C1-C6-C7-C8
25	A	856	BCR	C5-C6-C7-C8
25	A	856	BCR	C23-C24-C25-C26
25	A	856	BCR	C23-C24-C25-C30
25	B	844	BCR	C23-C24-C25-C26
25	K	205	BCR	C23-C24-C25-C30
25	L	301	BCR	C5-C6-C7-C8
25	L	305	BCR	C5-C6-C7-C8
25	L	305	BCR	C23-C24-C25-C26
25	L	306	BCR	C23-C24-C25-C26
25	L	306	BCR	C23-C24-C25-C30
27	G	202	LMG	C31-C32-C33-C34
22	A	832	CLA	CBA-CGA-O2A-C1
22	B	802	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	C8-C10-C11-C12
22	B	805	CLA	C15-C16-C17-C18
26	Z	7630	LHG	C8-C7-O7-C5
27	4	622	LMG	C33-C34-C35-C36
22	B	834	CLA	C4-C3-C5-C6
29	A	844	PQN	C14-C13-C15-C16
22	3	613	CLA	C2-C3-C5-C6
22	4	602	CLA	C11-C10-C8-C7
22	A	805	CLA	C2-C3-C5-C6
22	A	811	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	C2-C3-C5-C6
22	A	830	CLA	C12-C13-C15-C16
22	A	843	CLA	C2-C3-C5-C6
22	B	808	CLA	C11-C10-C8-C7
22	B	809	CLA	C6-C7-C8-C10
22	B	810	CLA	C12-C13-C15-C16
22	B	818	CLA	C11-C10-C8-C7
22	B	832	CLA	C2-C3-C5-C6
22	B	834	CLA	C2-C3-C5-C6
21	1	601	CHL	C3-C5-C6-C7
22	B	803	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
26	A	846	LHG	O10-C23-O8-C6
23	Y	4621	LUT	C29-C30-C31-C32
32	J	103	DGD	C1A-C2A-C3A-C4A
22	A	830	CLA	CBA-CGA-O2A-C1
27	1	622	LMG	C29-C28-O8-C9
22	2	602	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	818	CLA	C2A-CAA-CBA-CGA
22	A	829	CLA	C2A-CAA-CBA-CGA
21	Y	601	CHL	C13-C15-C16-C17
29	A	844	PQN	C25-C26-C27-C28
26	1	620	LHG	C33-C34-C35-C36
32	J	103	DGD	C8A-C9A-CAA-CBA
22	2	614	CLA	O1D-CGD-O2D-CED
22	A	831	CLA	O1D-CGD-O2D-CED
22	A	814	CLA	C13-C15-C16-C17
22	2	610	CLA	C3-C5-C6-C7
22	B	803	CLA	C15-C16-C17-C18
27	4	623	LMG	C28-C29-C30-C31
26	1	620	LHG	C8-C7-O7-C5
27	4	622	LMG	C11-C10-O7-C8
22	K	204	CLA	CBA-CGA-O2A-C1
32	B	850	DGD	C3B-C4B-C5B-C6B
26	B	851	LHG	O9-C7-O7-C5
26	Z	7630	LHG	O9-C7-O7-C5
22	A	829	CLA	C3-C5-C6-C7
27	1	622	LMG	C11-C12-C13-C14
22	A	819	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	O2G-C2G-C3G-O3G
21	2	601	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	3	613	CLA	C4-C3-C5-C6
22	A	826	CLA	C4-C3-C5-C6
22	A	843	CLA	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
29	B	842	PQN	C14-C13-C15-C16
22	B	808	CLA	C2-C3-C5-C6
22	B	813	CLA	C2-C3-C5-C6
22	4	602	CLA	C11-C10-C8-C9
22	A	811	CLA	C11-C10-C8-C9
22	A	812	CLA	C14-C13-C15-C16
22	B	802	CLA	C14-C13-C15-C16
22	B	809	CLA	C11-C12-C13-C14
22	B	817	CLA	C6-C7-C8-C9
22	B	824	CLA	C11-C10-C8-C9
22	B	811	CLA	C3-C5-C6-C7
22	1	608	CLA	C2A-CAA-CBA-CGA
22	3	602	CLA	C2A-CAA-CBA-CGA
22	4	602	CLA	C2A-CAA-CBA-CGA
22	A	802	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C2A-CAA-CBA-CGA
22	B	828	CLA	C2A-CAA-CBA-CGA
22	H	201	CLA	C2A-CAA-CBA-CGA
32	B	850	DGD	CDB-CEB-CFB-CGB
24	2	620	XAT	C27-C28-C29-C39
22	A	817	CLA	O1D-CGD-O2D-CED
22	F	304	CLA	O1D-CGD-O2D-CED
26	A	846	LHG	C10-C11-C12-C13
25	B	801	BCR	C17-C18-C19-C20
25	J	102	BCR	C17-C18-C19-C20
22	A	832	CLA	O1A-CGA-O2A-C1
22	B	802	CLA	O1A-CGA-O2A-C1
21	2	608	CHL	C1A-C2A-CAA-CBA
21	4	608	CHL	C1A-C2A-CAA-CBA
21	X	605	CHL	C1A-C2A-CAA-CBA
22	1	608	CLA	C1A-C2A-CAA-CBA
22	1	610	CLA	C1A-C2A-CAA-CBA
22	2	610	CLA	C1A-C2A-CAA-CBA
22	2	612	CLA	C1A-C2A-CAA-CBA
22	3	603	CLA	C1A-C2A-CAA-CBA
22	4	602	CLA	C1A-C2A-CAA-CBA
22	4	610	CLA	C1A-C2A-CAA-CBA
22	4	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	835	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C1A-C2A-CAA-CBA
22	B	803	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	820	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	F	301	CLA	C1A-C2A-CAA-CBA
22	G	204	CLA	C1A-C2A-CAA-CBA
22	Y	602	CLA	C1A-C2A-CAA-CBA
22	Z	602	CLA	C1A-C2A-CAA-CBA
22	Z	604	CLA	C1A-C2A-CAA-CBA
22	A	807	CLA	C16-C17-C18-C19
26	2	622	LHG	C8-C7-O7-C5
25	1	619	BCR	C13-C14-C15-C16
25	J	102	BCR	C13-C14-C15-C16
25	K	205	BCR	C19-C20-C21-C22
22	A	830	CLA	C10-C11-C12-C13
22	2	611	CLA	CMA-C3A-C4A-CHB
22	3	602	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBD-CGD-O2D-CED
22	B	840	CLA	C5-C6-C7-C8
26	Y	4630	LHG	C24-C25-C26-C27
22	A	807	CLA	C16-C17-C18-C20
22	A	822	CLA	C16-C17-C18-C20
31	A	857	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	3	603	CLA	C4-C3-C5-C6
22	A	805	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
22	4	611	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	F	303	CLA	C3A-C2A-CAA-CBA
31	A	857	LMU	O1'-C1-C2-C3
28	A	801	CL0	C15-C16-C17-C18
26	2	622	LHG	C10-C11-C12-C13
27	G	202	LMG	C14-C15-C16-C17
22	A	841	CLA	O1A-CGA-O2A-C1
22	A	854	CLA	C16-C17-C18-C19
22	L	303	CLA	C11-C12-C13-C14
22	B	813	CLA	O1D-CGD-O2D-CED
26	2	622	LHG	C30-C31-C32-C33
26	A	847	LHG	C4-C5-C6-O8
27	1	622	LMG	O1-C7-C8-C9
27	2	623	LMG	C7-C8-C9-O8
27	4	623	LMG	O1-C7-C8-C9
27	G	202	LMG	O1-C7-C8-C9
32	B	850	DGD	O1G-C1G-C2G-C3G
32	B	850	DGD	C1G-C2G-C3G-O3G
26	A	846	LHG	C18-C19-C20-C21
27	1	622	LMG	C8-C7-O1-C1
22	A	809	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	C8-C10-C11-C12
22	B	805	CLA	C10-C11-C12-C13
22	4	610	CLA	C6-C7-C8-C9
27	G	202	LMG	C15-C16-C17-C18
22	A	826	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	O1A-CGA-O2A-C1
27	4	623	LMG	C11-C12-C13-C14
27	4	623	LMG	C31-C32-C33-C34
27	G	202	LMG	C32-C33-C34-C35
22	A	819	CLA	C10-C11-C12-C13
26	Z	7630	LHG	O1-C1-C2-O2
26	Y	4630	LHG	C18-C19-C20-C21
27	4	622	LMG	C35-C36-C37-C38
27	G	202	LMG	C17-C18-C19-C20
32	J	103	DGD	C4E-C5E-C6E-O5E
31	A	857	LMU	C4-C5-C6-C7
22	4	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	802	CLA	C4-C3-C5-C6
22	B	813	CLA	C4-C3-C5-C6
27	4	622	LMG	C34-C35-C36-C37
21	2	601	CHL	C11-C12-C13-C14
22	3	613	CLA	C5-C6-C7-C8
22	B	826	CLA	C5-C6-C7-C8
32	J	103	DGD	C1G-C2G-O2G-C1B
22	B	839	CLA	O1D-CGD-O2D-CED
22	B	807	CLA	C2A-CAA-CBA-CGA
22	3	602	CLA	C8-C10-C11-C12
22	A	842	CLA	C13-C15-C16-C17
22	A	854	CLA	C8-C10-C11-C12
22	B	811	CLA	C2-C1-O2A-CGA
22	B	820	CLA	C2-C1-O2A-CGA
27	1	622	LMG	C17-C18-C19-C20
21	Y	607	CHL	O1D-CGD-O2D-CED
22	B	818	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	O1D-CGD-O2D-CED
27	4	622	LMG	C13-C14-C15-C16
22	A	806	CLA	C15-C16-C17-C18
22	B	829	CLA	C5-C6-C7-C8
22	B	841	CLA	C10-C11-C12-C13
32	J	103	DGD	C2E-C1E-O5D-C6D
26	1	620	LHG	O7-C5-C6-O8
22	2	609	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C10-C11-C12-C13
21	Y	601	CHL	C16-C17-C18-C20
26	A	846	LHG	C11-C12-C13-C14
32	B	850	DGD	CEB-CFB-CGB-CHB
22	F	301	CLA	C4-C3-C5-C6
21	Y	601	CHL	C12-C13-C15-C16
22	2	613	CLA	C12-C13-C15-C16
22	A	804	CLA	C11-C12-C13-C15
22	A	809	CLA	C11-C12-C13-C15
22	A	812	CLA	C12-C13-C15-C16
22	A	820	CLA	C11-C10-C8-C7
22	A	826	CLA	C11-C10-C8-C7
22	A	827	CLA	C11-C10-C8-C7
22	A	841	CLA	C11-C10-C8-C7
22	A	854	CLA	C6-C7-C8-C10
22	B	802	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	805	CLA	C11-C12-C13-C15
22	B	809	CLA	C12-C13-C15-C16
22	B	817	CLA	C6-C7-C8-C10
22	B	824	CLA	C11-C10-C8-C7
22	B	825	CLA	C6-C7-C8-C10
22	B	837	CLA	C12-C13-C15-C16
22	L	303	CLA	C6-C7-C8-C10
29	A	844	PQN	C17-C18-C20-C21
22	1	613	CLA	C14-C13-C15-C16
22	2	613	CLA	C14-C13-C15-C16
22	A	804	CLA	C11-C10-C8-C9
22	A	804	CLA	C11-C12-C13-C14
22	A	806	CLA	C6-C7-C8-C9
22	A	807	CLA	C11-C12-C13-C14
22	A	809	CLA	C11-C12-C13-C14
22	A	814	CLA	C11-C10-C8-C9
22	A	826	CLA	C11-C10-C8-C9
22	A	827	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C10-C8-C9
22	A	841	CLA	C11-C10-C8-C9
22	A	843	CLA	C11-C10-C8-C9
22	B	808	CLA	C11-C10-C8-C9
22	B	810	CLA	C14-C13-C15-C16
22	B	813	CLA	C6-C7-C8-C9
22	B	813	CLA	C11-C12-C13-C14
29	B	842	PQN	C21-C22-C23-C24
22	A	845	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	C13-C15-C16-C17
22	4	601	CLA	O1A-CGA-O2A-C1
33	Y	4623	NEX	C31-C32-C33-C40
22	A	809	CLA	C13-C15-C16-C17
22	B	818	CLA	C11-C12-C13-C14
26	A	847	LHG	C24-C25-C26-C27
22	B	826	CLA	C3-C5-C6-C7
22	B	828	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	C15-C16-C17-C18
26	A	847	LHG	O6-C4-C5-C6
26	X	2630	LHG	O6-C4-C5-C6
28	A	801	CL0	C3-C5-C6-C7
22	B	820	CLA	CBA-CGA-O2A-C1
29	B	842	PQN	C15-C16-C17-C18
22	B	802	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	F	301	CLA	C2-C3-C5-C6
27	G	202	LMG	C28-C29-C30-C31
22	B	832	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	C16-C17-C18-C19
22	A	831	CLA	C13-C15-C16-C17
21	Y	601	CHL	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	A	832	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	O1D-CGD-O2D-CED
27	1	622	LMG	C19-C20-C21-C22
31	B	849	LMU	C5-C6-C7-C8
22	A	806	CLA	C10-C11-C12-C13
22	A	812	CLA	C8-C10-C11-C12
26	Y	4630	LHG	C9-C10-C11-C12
22	A	811	CLA	C15-C16-C17-C18
22	B	808	CLA	C5-C6-C7-C8
22	L	303	CLA	C10-C11-C12-C13
26	A	846	LHG	C4-C5-C6-O8
27	G	202	LMG	O9-C10-O7-C8
22	Y	613	CLA	O1A-CGA-O2A-C1
27	2	623	LMG	C13-C14-C15-C16
22	2	610	CLA	C4-C3-C5-C6
22	B	811	CLA	C4-C3-C5-C6
22	A	814	CLA	C16-C17-C18-C20
26	Y	4630	LHG	C11-C10-C9-C8
32	J	103	DGD	CCB-CDB-CEB-CFB
21	1	607	CHL	C3C-C2C-CMC-OMC
21	4	618	CHL	C3C-C2C-CMC-OMC
21	X	608	CHL	C3C-C2C-CMC-OMC
21	Z	601	CHL	C3C-C2C-CMC-OMC
26	B	851	LHG	C4-O6-P-O3
22	B	819	CLA	O1A-CGA-O2A-C1
27	G	202	LMG	C4-C5-C6-O5
21	1	601	CHL	C2A-CAA-CBA-CGA
21	2	601	CHL	C2A-CAA-CBA-CGA
22	A	809	CLA	C2A-CAA-CBA-CGA
22	B	840	CLA	C10-C11-C12-C13
26	X	2630	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
26	1	620	LHG	C29-C30-C31-C32
22	A	842	CLA	CAA-CBA-CGA-O2A
31	B	849	LMU	C2-C3-C4-C5
22	A	812	CLA	C3-C5-C6-C7
22	A	823	CLA	O1D-CGD-O2D-CED
27	2	623	LMG	O7-C8-C9-O8
26	B	851	LHG	C1-C2-C3-O3
27	2	623	LMG	C17-C18-C19-C20
22	B	819	CLA	C3-C5-C6-C7
21	2	608	CHL	C2-C1-O2A-CGA
22	A	807	CLA	C6-C7-C8-C9
22	A	807	CLA	C14-C13-C15-C16
22	A	820	CLA	C11-C10-C8-C9
22	A	841	CLA	C14-C13-C15-C16
22	A	854	CLA	C6-C7-C8-C9
22	B	809	CLA	C14-C13-C15-C16
22	B	824	CLA	C14-C13-C15-C16
22	B	825	CLA	C6-C7-C8-C9
22	B	825	CLA	C11-C10-C8-C9
29	B	842	PQN	C19-C18-C20-C21
22	B	806	CLA	C8-C10-C11-C12
22	A	838	CLA	C4-C3-C5-C6
22	3	613	CLA	C6-C7-C8-C9
22	A	854	CLA	C16-C17-C18-C20
22	B	802	CLA	C16-C17-C18-C20
22	B	827	CLA	C16-C17-C18-C20
23	1	617	LUT	C1-C6-C7-C8
23	1	617	LUT	C5-C6-C7-C8
23	1	621	LUT	C1-C6-C7-C8
23	1	621	LUT	C5-C6-C7-C8
23	Z	7621	LUT	C5-C6-C7-C8
25	1	619	BCR	C23-C24-C25-C26
25	K	205	BCR	C1-C6-C7-C8
25	K	205	BCR	C5-C6-C7-C8
29	B	842	PQN	C20-C21-C22-C23
25	K	202	BCR	C7-C8-C9-C34
33	X	2623	NEX	C11-C12-C13-C20
22	N	1001	CLA	CBA-CGA-O2A-C1
21	Z	609	CHL	C1A-C2A-CAA-CBA
22	A	816	CLA	C1A-C2A-CAA-CBA
22	X	612	CLA	C1A-C2A-CAA-CBA
22	Y	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	Y	4620	LUT	C27-C28-C29-C30
24	3	619	XAT	C27-C28-C29-C30
24	4	620	XAT	C27-C28-C29-C30
25	3	620	BCR	C7-C8-C9-C10
22	A	843	CLA	C10-C11-C12-C13
27	1	622	LMG	C24-C25-C26-C27
22	1	602	CLA	C14-C13-C15-C16
27	2	623	LMG	C4-C5-C6-O5
22	B	817	CLA	C8-C10-C11-C12
22	B	832	CLA	C8-C10-C11-C12
26	1	620	LHG	C13-C14-C15-C16
22	A	845	CLA	O1A-CGA-O2A-C1
26	A	846	LHG	O6-C4-C5-C6
21	2	601	CHL	C11-C10-C8-C7
22	1	602	CLA	C11-C12-C13-C15
22	1	613	CLA	C11-C10-C8-C7
22	1	613	CLA	C12-C13-C15-C16
22	2	602	CLA	C6-C7-C8-C10
22	3	602	CLA	C6-C7-C8-C10
22	A	802	CLA	C11-C10-C8-C7
22	A	804	CLA	C11-C10-C8-C7
22	A	806	CLA	C6-C7-C8-C10
22	A	811	CLA	C6-C7-C8-C10
22	A	814	CLA	C11-C10-C8-C7
22	A	814	CLA	C11-C12-C13-C15
22	A	828	CLA	C11-C10-C8-C7
22	A	829	CLA	C12-C13-C15-C16
22	A	843	CLA	C11-C10-C8-C7
22	B	809	CLA	C11-C10-C8-C7
22	B	813	CLA	C6-C7-C8-C10
22	B	813	CLA	C11-C12-C13-C15
22	B	824	CLA	C12-C13-C15-C16
22	B	827	CLA	C11-C10-C8-C7
22	B	840	CLA	C12-C13-C15-C16
22	B	841	CLA	C11-C10-C8-C7
27	1	622	LMG	C22-C23-C24-C25
25	I	101	BCR	C15-C16-C17-C18
25	K	202	BCR	C19-C20-C21-C22
25	L	306	BCR	C13-C14-C15-C16
27	4	622	LMG	C30-C31-C32-C33
27	4	623	LMG	O9-C10-O7-C8
22	A	830	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	B	842	PQN	C23-C25-C26-C27
22	K	204	CLA	C2A-CAA-CBA-CGA
26	A	846	LHG	C14-C15-C16-C17
26	1	620	LHG	C28-C29-C30-C31
22	A	835	CLA	C3-C5-C6-C7
32	J	103	DGD	CFB-CGB-CHB-CIB
22	A	814	CLA	C16-C17-C18-C19
22	B	818	CLA	C11-C12-C13-C15
22	A	828	CLA	C13-C15-C16-C17
22	B	837	CLA	CBA-CGA-O2A-C1
22	N	1002	CLA	CBA-CGA-O2A-C1
26	A	846	LHG	C24-C23-O8-C6
22	1	602	CLA	C12-C13-C15-C16
32	J	103	DGD	C9A-CAA-CBA-CCA
21	Z	609	CHL	C2C-C3C-CAC-CBC
27	1	622	LMG	C34-C35-C36-C37
21	2	601	CHL	CAD-CBD-CGD-O2D
22	1	612	CLA	CAD-CBD-CGD-O2D
22	1	613	CLA	CAD-CBD-CGD-O2D
22	2	604	CLA	CAD-CBD-CGD-O2D
22	2	609	CLA	CAD-CBD-CGD-O2D
22	2	610	CLA	CAD-CBD-CGD-O2D
22	3	602	CLA	CAD-CBD-CGD-O2D
22	3	607	CLA	CAD-CBD-CGD-O2D
22	4	610	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	813	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	828	CLA	CAD-CBD-CGD-O2D
22	A	839	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	A	843	CLA	CAD-CBD-CGD-O2D
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	818	CLA	CAD-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	832	CLA	CAD-CBD-CGD-O2D
22	F	303	CLA	CAD-CBD-CGD-O2D
22	G	201	CLA	CAD-CBD-CGD-O2D
22	K	203	CLA	CAD-CBD-CGD-O2D
22	L	302	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	X	611	CLA	CAD-CBD-CGD-O2D
22	Y	610	CLA	CAD-CBD-CGD-O2D
22	A	831	CLA	C10-C11-C12-C13
26	1	620	LHG	C11-C12-C13-C14
27	G	202	LMG	C29-C30-C31-C32
27	2	623	LMG	O6-C1-O1-C7
31	B	849	LMU	O5'-C1'-O1'-C1
32	B	850	DGD	O6E-C1E-O5D-C6D
22	A	804	CLA	C10-C11-C12-C13
27	G	202	LMG	C7-C8-C9-O8
32	J	103	DGD	O1G-C1G-C2G-C3G
27	1	622	LMG	O10-C28-O8-C9
22	B	810	CLA	C8-C10-C11-C12
22	3	609	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C2A-CAA-CBA-CGA
22	B	841	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	C6-C7-C8-C10
28	A	801	CL0	C16-C17-C18-C20
22	4	611	CLA	CHA-CBD-CGD-O1D
22	4	611	CLA	CHA-CBD-CGD-O2D
22	4	617	CLA	CHA-CBD-CGD-O1D
22	4	617	CLA	CHA-CBD-CGD-O2D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	811	CLA	CHA-CBD-CGD-O1D
22	A	815	CLA	CHA-CBD-CGD-O1D
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	816	CLA	CHA-CBD-CGD-O1D
22	A	816	CLA	CHA-CBD-CGD-O2D
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O2D
22	A	820	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	CHA-CBD-CGD-O1D
22	A	832	CLA	CHA-CBD-CGD-O2D
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	B	820	CLA	CHA-CBD-CGD-O1D
22	B	820	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	826	CLA	CHA-CBD-CGD-O1D
22	B	826	CLA	CHA-CBD-CGD-O2D
22	G	204	CLA	CHA-CBD-CGD-O2D
22	X	614	CLA	CHA-CBD-CGD-O2D
21	Y	601	CHL	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	O1A-CGA-O2A-C1
26	1	620	LHG	C32-C33-C34-C35
26	A	847	LHG	O7-C5-C6-O8
27	G	202	LMG	O7-C8-C9-O8
32	B	850	DGD	O1G-C1G-C2G-O2G
26	1	620	LHG	O1-C1-C2-O2
22	3	602	CLA	O1D-CGD-O2D-CED
22	B	817	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C2-C3-C5-C6
22	1	602	CLA	C11-C12-C13-C14
22	2	602	CLA	C6-C7-C8-C9
22	B	806	CLA	C14-C13-C15-C16
22	B	809	CLA	C11-C10-C8-C9
22	B	827	CLA	C11-C10-C8-C9
26	B	851	LHG	C9-C10-C11-C12
32	B	850	DGD	CFB-CGB-CHB-CIB
22	N	1002	CLA	O1A-CGA-O2A-C1
22	B	827	CLA	C8-C10-C11-C12
22	B	824	CLA	C15-C16-C17-C18
23	1	617	LUT	C27-C28-C29-C39
25	1	619	BCR	C7-C8-C9-C34
24	1	618	XAT	C27-C28-C29-C30
26	B	851	LHG	C12-C13-C14-C15
22	2	602	CLA	C1A-C2A-CAA-CBA
22	2	604	CLA	C1A-C2A-CAA-CBA
22	2	614	CLA	C1A-C2A-CAA-CBA
22	3	602	CLA	C1A-C2A-CAA-CBA
22	4	604	CLA	C1A-C2A-CAA-CBA
22	A	803	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	X	602	CLA	CHA-CBD-CGD-O2D
26	1	620	LHG	O9-C7-O7-C5
26	1	620	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	X	2630	LHG	C3-O3-P-O6
26	Z	7630	LHG	C3-O3-P-O6
22	A	813	CLA	C4-C3-C5-C6
22	K	204	CLA	O1A-CGA-O2A-C1
26	2	622	LHG	C4-O6-P-O4
26	B	851	LHG	C4-O6-P-O4
26	X	2630	LHG	C3-O3-P-O4
26	Z	7630	LHG	C3-O3-P-O4
22	B	817	CLA	CBD-CGD-O2D-CED
26	B	851	LHG	O6-C4-C5-C6
26	Y	4630	LHG	C29-C30-C31-C32
22	4	617	CLA	CAD-CBD-CGD-O1D
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	811	CLA	CAD-CBD-CGD-O1D
22	A	815	CLA	CAD-CBD-CGD-O1D
22	A	825	CLA	CAD-CBD-CGD-O1D
22	A	826	CLA	CAD-CBD-CGD-O1D
22	A	832	CLA	CAD-CBD-CGD-O1D
22	B	810	CLA	CAD-CBD-CGD-O1D
22	G	203	CLA	CAD-CBD-CGD-O1D
22	X	614	CLA	CAD-CBD-CGD-O1D
28	A	801	CL0	CAA-CBA-CGA-O2A
32	J	103	DGD	CEA-CFA-CGA-CHA
22	A	825	CLA	C4-C3-C5-C6
21	Y	601	CHL	CHA-CBD-CGD-O1D
21	Y	601	CHL	C6-C7-C8-C10
21	Y	605	CHL	CAD-CBD-CGD-O2D
21	Z	601	CHL	CAD-CBD-CGD-O2D
22	A	802	CLA	C6-C7-C8-C10
22	A	802	CLA	C12-C13-C15-C16
22	A	818	CLA	C6-C7-C8-C10
22	A	819	CLA	C11-C10-C8-C7
22	A	830	CLA	C6-C7-C8-C10
22	A	841	CLA	C12-C13-C15-C16
22	A	854	CLA	C11-C10-C8-C7
22	B	806	CLA	C12-C13-C15-C16
22	B	824	CLA	C6-C7-C8-C10
22	B	828	CLA	C6-C7-C8-C10
22	B	828	CLA	C12-C13-C15-C16
22	B	840	CLA	C6-C7-C8-C10
22	B	840	CLA	C11-C10-C8-C7
22	G	204	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	X	612	CLA	C3A-C2A-CAA-CBA
22	Y	613	CLA	CAD-CBD-CGD-O2D
26	A	846	LHG	O6-C4-C5-O7
26	A	847	LHG	O6-C4-C5-O7
26	B	851	LHG	O6-C4-C5-O7
29	A	844	PQN	C16-C17-C18-C20
23	Z	7621	LUT	C29-C30-C31-C32
22	B	805	CLA	C16-C17-C18-C19
22	B	805	CLA	C16-C17-C18-C20
26	A	846	LHG	C28-C29-C30-C31
21	1	607	CHL	C1C-C2C-CMC-OMC
21	4	618	CHL	C1C-C2C-CMC-OMC
21	Z	601	CHL	C1C-C2C-CMC-OMC
22	3	606	CLA	CAD-CBD-CGD-O1D
22	Y	614	CLA	CAD-CBD-CGD-O1D
22	A	838	CLA	CBD-CGD-O2D-CED
27	1	622	LMG	O1-C7-C8-O7
27	4	623	LMG	O1-C7-C8-O7
27	G	202	LMG	O1-C7-C8-O7
22	A	827	CLA	O1D-CGD-O2D-CED
22	1	603	CLA	O1A-CGA-O2A-C1
22	1	603	CLA	CBA-CGA-O2A-C1
22	A	827	CLA	C11-C12-C13-C14
26	2	622	LHG	C11-C12-C13-C14
22	A	802	CLA	C14-C13-C15-C16
22	A	811	CLA	C6-C7-C8-C9
22	A	814	CLA	C11-C12-C13-C14
22	A	830	CLA	C11-C12-C13-C14
22	B	802	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C10-C8-C9
22	B	805	CLA	C11-C12-C13-C14
22	B	823	CLA	O1D-CGD-O2D-CED
22	B	832	CLA	C3-C5-C6-C7
22	B	806	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	O1A-CGA-O2A-C1
22	B	837	CLA	O1A-CGA-O2A-C1
22	A	814	CLA	C15-C16-C17-C18
26	Z	7630	LHG	C7-C8-C9-C10
28	A	801	CL0	O1A-CGA-O2A-C1
27	G	202	LMG	O6-C5-C6-O5
22	1	604	CLA	C1-C2-C3-C4
22	B	803	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	B	850	DGD	C3G-C2G-O2G-C1B
22	4	613	CLA	C2A-CAA-CBA-CGA
22	A	842	CLA	C2A-CAA-CBA-CGA
22	B	808	CLA	C2A-CAA-CBA-CGA
22	Y	602	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	C2-C1-O2A-CGA
22	A	835	CLA	C2-C1-O2A-CGA
22	B	806	CLA	C2-C1-O2A-CGA
22	A	819	CLA	CAA-CBA-CGA-O2A
31	B	849	LMU	C4B-C5B-C6B-O6B
22	A	828	CLA	C15-C16-C17-C18
22	B	817	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	CBA-CGA-O2A-C1
25	J	102	BCR	C15-C16-C17-C18
23	Z	7621	LUT	C1-C6-C7-C8
25	1	619	BCR	C23-C24-C25-C30
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	838	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	C10-C11-C12-C13
28	A	801	CL0	CBA-CGA-O2A-C1
22	4	602	CLA	C11-C12-C13-C15
32	B	850	DGD	C2E-C1E-O5D-C6D
26	1	620	LHG	C12-C13-C14-C15
26	1	620	LHG	C3-O3-P-O6
26	A	847	LHG	C3-O3-P-O6
26	Y	4630	LHG	C3-O3-P-O6
26	1	620	LHG	C4-C5-C6-O8
22	B	827	CLA	C4-C3-C5-C6
22	1	613	CLA	C6-C7-C8-C10
22	2	610	CLA	C2-C3-C5-C6
22	A	807	CLA	C6-C7-C8-C10
22	A	807	CLA	C12-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C15
22	B	825	CLA	C11-C10-C8-C7
21	Y	601	CHL	C14-C13-C15-C16
22	A	802	CLA	C11-C10-C8-C9
22	A	818	CLA	C6-C7-C8-C9
22	A	819	CLA	C11-C10-C8-C9
22	B	828	CLA	C6-C7-C8-C9
22	B	837	CLA	C14-C13-C15-C16
24	1	618	XAT	C29-C30-C31-C32
25	1	619	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	4	621	BCR	C19-C20-C21-C22
22	B	806	CLA	CBA-CGA-O2A-C1
32	B	850	DGD	CCA-CDA-CEA-CFA
25	K	205	BCR	C11-C12-C13-C35
22	A	826	CLA	C16-C17-C18-C20
26	2	622	LHG	C5-C4-O6-P
25	1	619	BCR	C7-C8-C9-C10
33	X	2623	NEX	C11-C12-C13-C14
22	A	828	CLA	CBD-CGD-O2D-CED
26	B	851	LHG	C26-C27-C28-C29
22	L	303	CLA	C2A-CAA-CBA-CGA
23	X	2620	LUT	C29-C30-C31-C32
23	X	2621	LUT	C9-C10-C11-C12
25	B	846	BCR	C19-C20-C21-C22
25	B	848	BCR	C9-C10-C11-C12
33	Y	4623	NEX	C33-C34-C35-C15
27	1	622	LMG	C36-C37-C38-C39
32	J	103	DGD	O6D-C5D-C6D-O5D
22	A	843	CLA	C13-C15-C16-C17
26	A	846	LHG	C35-C36-C37-C38
29	A	844	PQN	C13-C15-C16-C17
31	B	849	LMU	C4-C5-C6-C7
22	A	822	CLA	C4-C3-C5-C6
22	2	613	CLA	C13-C15-C16-C17
27	2	623	LMG	O6-C5-C6-O5
22	A	833	CLA	CBD-CGD-O2D-CED
22	A	822	CLA	C2-C3-C5-C6
27	G	202	LMG	O10-C28-O8-C9
22	A	831	CLA	C15-C16-C17-C18
27	4	622	LMG	O9-C10-O7-C8
22	A	814	CLA	C2-C1-O2A-CGA
22	A	832	CLA	C2-C1-O2A-CGA
22	B	819	CLA	C2-C1-O2A-CGA
28	A	801	CL0	C2-C1-O2A-CGA
22	B	809	CLA	C13-C15-C16-C17
26	2	622	LHG	C25-C26-C27-C28
22	A	811	CLA	C5-C6-C7-C8
26	2	622	LHG	O7-C5-C6-O8
22	B	839	CLA	CBA-CGA-O2A-C1
22	A	826	CLA	CAA-CBA-CGA-O1A
21	4	608	CHL	C3A-C2A-CAA-CBA
21	Z	608	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	806	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	817	CLA	C3A-C2A-CAA-CBA
22	4	604	CLA	CAA-CBA-CGA-O1A
21	1	601	CHL	C6-C7-C8-C10
22	2	602	CLA	C16-C17-C18-C19
21	Z	609	CHL	C4C-C3C-CAC-CBC
22	B	832	CLA	CAA-CBA-CGA-O2A
32	B	850	DGD	C9B-CAB-CBB-CCB
22	A	803	CLA	C4-C3-C5-C6
27	2	623	LMG	C10-C11-C12-C13
22	A	813	CLA	C2-C3-C5-C6
22	2	613	CLA	C11-C10-C8-C9
22	B	818	CLA	C6-C7-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	825	CLA	C11-C12-C13-C14
22	B	827	CLA	C14-C13-C15-C16
22	B	841	CLA	C14-C13-C15-C16
29	A	844	PQN	C16-C17-C18-C19
25	A	852	BCR	C11-C10-C9-C34
25	A	852	BCR	C16-C17-C18-C36
25	B	844	BCR	C11-C10-C9-C34
25	B	845	BCR	C11-C10-C9-C34
25	B	845	BCR	C20-C21-C22-C37
25	F	305	BCR	C35-C13-C14-C15
25	L	301	BCR	C11-C10-C9-C34
33	X	2623	NEX	C39-C29-C30-C31
33	Y	4623	NEX	C39-C29-C30-C31
33	Z	7623	NEX	C39-C29-C30-C31
22	B	839	CLA	C16-C17-C18-C19
22	B	803	CLA	O2A-C1-C2-C3
26	2	622	LHG	O2-C2-C3-O3
22	A	814	CLA	CBA-CGA-O2A-C1
24	Y	2622	XAT	C31-C32-C33-C40
24	Z	4622	XAT	C7-C8-C9-C19
24	2	620	XAT	C27-C28-C29-C30
21	Z	608	CHL	C1A-C2A-CAA-CBA
22	A	817	CLA	C1A-C2A-CAA-CBA
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C1A-C2A-CAA-CBA
22	B	817	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	C11-C10-C8-C7
22	A	826	CLA	C11-C12-C13-C15
22	A	828	CLA	C6-C7-C8-C10
22	A	831	CLA	C11-C12-C13-C15
22	B	825	CLA	C12-C13-C15-C16
22	B	839	CLA	C6-C7-C8-C10
22	A	814	CLA	O1A-CGA-O2A-C1
22	A	837	CLA	CAA-CBA-CGA-O1A
22	A	837	CLA	CAA-CBA-CGA-O2A
22	G	204	CLA	CAA-CBA-CGA-O2A
22	B	802	CLA	C8-C10-C11-C12
21	3	608	CHL	C2A-CAA-CBA-CGA
22	2	613	CLA	C2A-CAA-CBA-CGA
22	4	610	CLA	C2A-CAA-CBA-CGA
22	A	835	CLA	C15-C16-C17-C18
22	G	204	CLA	CAA-CBA-CGA-O1A
22	1	608	CLA	CAA-CBA-CGA-O2A
22	4	604	CLA	CAA-CBA-CGA-O2A
22	A	828	CLA	C4-C3-C5-C6
21	Y	601	CHL	C5-C6-C7-C8
22	L	303	CLA	C5-C6-C7-C8
22	1	608	CLA	CAA-CBA-CGA-O1A
25	A	852	BCR	C11-C10-C9-C8
25	A	852	BCR	C16-C17-C18-C19
25	B	844	BCR	C11-C10-C9-C8
25	B	845	BCR	C11-C10-C9-C8
25	B	845	BCR	C20-C21-C22-C23
25	F	305	BCR	C12-C13-C14-C15
25	L	301	BCR	C11-C10-C9-C8
33	X	2623	NEX	C28-C29-C30-C31
33	Y	4623	NEX	C28-C29-C30-C31
33	Z	7623	NEX	C28-C29-C30-C31
22	1	616	CLA	CAA-CBA-CGA-O2A
22	2	603	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	CAA-CBA-CGA-O2A
22	Z	602	CLA	C5-C6-C7-C8
24	2	620	XAT	C29-C30-C31-C32
25	B	843	BCR	C13-C14-C15-C16
22	K	203	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	O1D-CGD-O2D-CED
22	B	810	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	830	CLA	C2-C1-O2A-CGA
22	A	839	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C2-C3-C5-C6
22	B	827	CLA	C2-C3-C5-C6
22	A	805	CLA	O1A-CGA-O2A-C1
22	4	602	CLA	C11-C12-C13-C14
22	A	826	CLA	C14-C13-C15-C16
22	B	808	CLA	C6-C7-C8-C9
22	N	1001	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	O1A-CGA-O2A-C1
26	Z	7630	LHG	C5-C4-O6-P
22	B	813	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C2A-CAA-CBA-CGA
22	2	603	CLA	CAA-CBA-CGA-O2A
27	1	622	LMG	C18-C19-C20-C21
23	X	2621	LUT	C1-C6-C7-C8
23	X	2621	LUT	C5-C6-C7-C8
23	Y	4621	LUT	C1-C6-C7-C8
25	A	848	BCR	C1-C6-C7-C8
25	A	848	BCR	C5-C6-C7-C8
25	B	801	BCR	C1-C6-C7-C8
25	B	801	BCR	C5-C6-C7-C8
25	J	102	BCR	C1-C6-C7-C8
25	K	202	BCR	C1-C6-C7-C8
22	H	201	CLA	CAA-CBA-CGA-O2A
22	1	616	CLA	CAA-CBA-CGA-O1A
23	Y	4620	LUT	C29-C30-C31-C32
25	3	620	BCR	C9-C10-C11-C12
22	A	827	CLA	C4-C3-C5-C6
22	B	835	CLA	C1A-C2A-CAA-CBA
25	A	851	BCR	C17-C18-C19-C20
22	2	602	CLA	C16-C17-C18-C20
22	B	811	CLA	C2-C3-C5-C6
22	4	614	CLA	CAA-CBA-CGA-O2A
26	2	622	LHG	C9-C10-C11-C12
22	B	808	CLA	CBA-CGA-O2A-C1
22	2	612	CLA	CAA-CBA-CGA-O1A
22	2	612	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	C16-C17-C18-C20
22	1	612	CLA	CAA-CBA-CGA-O2A
22	B	833	CLA	CAA-CBA-CGA-O2A
22	B	827	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	K	203	CLA	CAA-CBA-CGA-O1A
22	B	839	CLA	C16-C17-C18-C20
22	A	827	CLA	C2-C3-C5-C6
22	B	808	CLA	C6-C7-C8-C10
26	A	846	LHG	C2-C3-O3-P
32	J	103	DGD	O1G-C1G-C2G-O2G
22	A	822	CLA	C3-C5-C6-C7
22	1	612	CLA	CAA-CBA-CGA-O1A
22	1	603	CLA	CAA-CBA-CGA-O2A
22	A	829	CLA	C15-C16-C17-C18
22	A	843	CLA	C8-C10-C11-C12
26	A	846	LHG	C23-C24-C25-C26
22	4	617	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C4-C3-C5-C6
22	A	830	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C12-C13-C14
22	B	827	CLA	C6-C7-C8-C9
22	B	840	CLA	C11-C10-C8-C9
22	B	826	CLA	C3A-C2A-CAA-CBA
22	N	1002	CLA	C3A-C2A-CAA-CBA
22	1	603	CLA	CAD-CBD-CGD-O2D
22	1	616	CLA	CAD-CBD-CGD-O2D
22	2	613	CLA	CAD-CBD-CGD-O2D
22	3	610	CLA	CAD-CBD-CGD-O2D
22	4	601	CLA	CAD-CBD-CGD-O2D
22	A	805	CLA	CAD-CBD-CGD-O2D
22	A	808	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	831	CLA	CAD-CBD-CGD-O2D
22	A	835	CLA	CAD-CBD-CGD-O2D
22	A	854	CLA	CAD-CBD-CGD-O2D
22	B	812	CLA	CAD-CBD-CGD-O2D
22	B	813	CLA	CAD-CBD-CGD-O2D
22	B	827	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	B	834	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	B	841	CLA	CAD-CBD-CGD-O2D
22	F	301	CLA	CAD-CBD-CGD-O2D
22	Z	603	CLA	CAD-CBD-CGD-O2D
22	A	826	CLA	C16-C17-C18-C19
22	B	803	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	4	601	CLA	CAA-CBA-CGA-O2A
22	A	810	CLA	CAA-CBA-CGA-O2A
22	A	818	CLA	CAA-CBA-CGA-O2A
22	A	835	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	CAA-CBA-CGA-O2A
21	1	601	CHL	C4-C3-C5-C6
21	Z	608	CHL	CAA-CBA-CGA-O1A
21	Z	608	CHL	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O2A
21	1	601	CHL	C2-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	B	802	CLA	CAA-CBA-CGA-O2A
22	B	838	CLA	O1A-CGA-O2A-C1
24	Y	2622	XAT	C11-C12-C13-C14
24	Y	2622	XAT	C31-C32-C33-C34
33	Y	4623	NEX	C31-C32-C33-C34
21	X	605	CHL	CAA-CBA-CGA-O1A
21	X	605	CHL	CAA-CBA-CGA-O2A
22	B	838	CLA	CBA-CGA-O2A-C1
22	A	830	CLA	O1D-CGD-O2D-CED
22	B	809	CLA	CAA-CBA-CGA-O2A
21	1	601	CHL	C6-C7-C8-C9
22	A	811	CLA	C16-C17-C18-C19
26	2	622	LHG	C24-C25-C26-C27
26	A	847	LHG	C11-C10-C9-C8
21	Z	607	CHL	CAA-CBA-CGA-O1A
21	Z	607	CHL	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O1A
22	4	609	CLA	CAA-CBA-CGA-O2A
22	Z	614	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	O2A-C1-C2-C3
22	4	614	CLA	CAA-CBA-CGA-O1A
22	Y	602	CLA	CAA-CBA-CGA-O2A
22	Z	611	CLA	CBD-CGD-O2D-CED
22	1	602	CLA	CHA-CBD-CGD-O1D
22	2	604	CLA	CHA-CBD-CGD-O2D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	811	CLA	CHA-CBD-CGD-O2D
22	A	823	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	807	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	CHA-CBD-CGD-O1D
22	B	828	CLA	CHA-CBD-CGD-O2D
22	B	837	CLA	CHA-CBD-CGD-O1D
22	B	837	CLA	CHA-CBD-CGD-O2D
22	K	204	CLA	CHA-CBD-CGD-O1D
22	K	204	CLA	CHA-CBD-CGD-O2D
22	N	1002	CLA	CHA-CBD-CGD-O1D
22	N	1002	CLA	CHA-CBD-CGD-O2D
22	Y	602	CLA	CHA-CBD-CGD-O2D
25	A	850	BCR	C9-C10-C11-C12
22	4	609	CLA	CAA-CBA-CGA-O1A
22	B	833	CLA	CAA-CBA-CGA-O1A
22	Y	602	CLA	CAA-CBA-CGA-O1A
22	Z	602	CLA	CAA-CBA-CGA-O2A
27	2	623	LMG	O7-C10-C11-C12
22	Z	614	CLA	CAA-CBA-CGA-O1A
21	Y	601	CHL	CAA-CBA-CGA-O2A
21	X	605	CHL	C2A-CAA-CBA-CGA
22	A	826	CLA	C13-C15-C16-C17
22	A	842	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	C2-C3-C5-C6
22	A	812	CLA	C6-C7-C8-C10
22	A	825	CLA	C2-C3-C5-C6
22	A	835	CLA	C4C-C3C-CAC-CBC
22	B	839	CLA	C6-C7-C8-C9
22	B	841	CLA	C11-C10-C8-C9
32	J	103	DGD	C4A-C5A-C6A-C7A
26	2	622	LHG	O8-C23-C24-C25
22	B	841	CLA	C16-C17-C18-C19
21	3	608	CHL	CAA-CBA-CGA-O2A
22	Y	613	CLA	C2A-CAA-CBA-CGA
22	4	617	CLA	CAA-CBA-CGA-O1A
22	A	835	CLA	CAA-CBA-CGA-O1A
32	J	103	DGD	CAA-CBA-CCA-CDA
21	1	601	CHL	CHA-CBD-CGD-O2D
22	1	616	CLA	C1A-C2A-CAA-CBA
22	2	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	4	617	CLA	C1A-C2A-CAA-CBA
22	A	814	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	N	1001	CLA	CHA-CBD-CGD-O2D
22	N	1002	CLA	C1A-C2A-CAA-CBA
22	Y	614	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CAA-CBA-CGA-O1A
26	A	846	LHG	O10-C23-C24-C25
27	4	622	LMG	O9-C10-C11-C12
22	A	818	CLA	CAA-CBA-CGA-O1A
22	B	806	CLA	CAA-CBA-CGA-O1A
26	B	851	LHG	C4-C5-C6-O8
22	A	843	CLA	CAA-CBA-CGA-O2A
22	A	841	CLA	C2A-CAA-CBA-CGA
22	A	810	CLA	CAA-CBA-CGA-O1A
22	B	816	CLA	CAA-CBA-CGA-O2A
21	Y	601	CHL	CAA-CBA-CGA-O1A
22	4	601	CLA	CAA-CBA-CGA-O1A
26	1	620	LHG	C3-O3-P-O5
26	A	847	LHG	C3-O3-P-O5
26	A	847	LHG	C4-O6-P-O5
22	4	601	CLA	O1D-CGD-O2D-CED
22	A	828	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	CAA-CBA-CGA-O2A
23	Y	4621	LUT	C5-C6-C7-C8
22	B	809	CLA	CAA-CBA-CGA-O1A
26	2	622	LHG	O10-C23-C24-C25
27	2	623	LMG	O10-C28-O8-C9
22	A	822	CLA	CAA-CBA-CGA-O2A
22	Z	602	CLA	CAA-CBA-CGA-O1A
22	Z	611	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	C10-C11-C12-C13
22	2	609	CLA	CAA-CBA-CGA-O1A
22	4	613	CLA	C5-C6-C7-C8
26	A	846	LHG	C12-C13-C14-C15
22	2	609	CLA	CAA-CBA-CGA-O2A
22	2	602	CLA	CAD-CBD-CGD-O1D
22	B	826	CLA	CAD-CBD-CGD-O1D
33	X	2623	NEX	C7-C8-C9-C10
22	A	834	CLA	CAA-CBA-CGA-O2A
26	A	846	LHG	O8-C23-C24-C25
26	X	2630	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	4	622	LMG	O7-C10-C11-C12
22	A	812	CLA	C6-C7-C8-C9
22	B	827	CLA	C11-C12-C13-C14
22	B	839	CLA	C11-C12-C13-C14
22	B	840	CLA	C14-C13-C15-C16
27	2	623	LMG	C14-C15-C16-C17
27	1	622	LMG	C35-C36-C37-C38
21	1	601	CHL	CAA-CBA-CGA-O2A
22	A	802	CLA	CAA-CBA-CGA-O2A
31	A	857	LMU	C3'-C4'-O1B-C1B
21	3	608	CHL	CAA-CBA-CGA-O1A
22	N	1002	CLA	C2A-CAA-CBA-CGA
22	1	613	CLA	CAA-CBA-CGA-O2A
22	K	204	CLA	CAA-CBA-CGA-O2A
22	N	1001	CLA	CAA-CBA-CGA-O2A
26	A	846	LHG	O7-C7-C8-C9
22	2	613	CLA	C15-C16-C17-C18
22	A	835	CLA	C13-C15-C16-C17
32	J	103	DGD	C2A-C3A-C4A-C5A
21	1	601	CHL	CHA-CBD-CGD-O1D
21	Y	605	CHL	CHA-CBD-CGD-O1D
21	Y	606	CHL	CAD-CBD-CGD-O2D
21	Z	601	CHL	CHA-CBD-CGD-O1D
21	Z	605	CHL	CAD-CBD-CGD-O2D
22	1	611	CLA	CHA-CBD-CGD-O1D
22	2	602	CLA	C11-C10-C8-C7
22	3	606	CLA	CHA-CBD-CGD-O1D
22	3	606	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C6-C7-C8-C10
22	A	842	CLA	C6-C7-C8-C10
22	B	826	CLA	C12-C13-C15-C16
22	B	827	CLA	C11-C12-C13-C15
22	B	839	CLA	C11-C12-C13-C15
22	O	2001	CLA	CAD-CBD-CGD-O2D
22	N	1001	CLA	CHA-CBD-CGD-O1D
22	X	602	CLA	CHA-CBD-CGD-O1D
22	Y	603	CLA	CAD-CBD-CGD-O2D
22	Y	614	CLA	CHA-CBD-CGD-O1D
22	Y	614	CLA	CAD-CBD-CGD-O2D
22	Z	603	CLA	C3A-C2A-CAA-CBA
21	1	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	2	601	CHL	O1D-CGD-O2D-CED
22	3	613	CLA	CAA-CBA-CGA-O2A
22	4	602	CLA	CAA-CBA-CGA-O2A
22	B	807	CLA	CAA-CBA-CGA-O2A
27	1	622	LMG	O8-C28-C29-C30
23	1	617	LUT	C27-C28-C29-C30
23	X	2620	LUT	C11-C12-C13-C14
24	X	7622	XAT	C31-C32-C33-C34
25	K	202	BCR	C7-C8-C9-C10
22	A	843	CLA	CAA-CBA-CGA-O1A
25	4	621	BCR	C9-C10-C11-C12
26	A	846	LHG	C25-C26-C27-C28
22	3	613	CLA	CAA-CBA-CGA-O1A
22	A	834	CLA	CAA-CBA-CGA-O1A
22	B	807	CLA	CAA-CBA-CGA-O1A
22	K	204	CLA	CAA-CBA-CGA-O1A
26	Y	4630	LHG	O10-C23-C24-C25
22	A	817	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O2A
26	A	847	LHG	O7-C7-C8-C9
22	A	809	CLA	C15-C16-C17-C18
22	4	602	CLA	CAA-CBA-CGA-O1A
22	B	828	CLA	C10-C11-C12-C13

There are no ring outliers.

206 monomers are involved in 430 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	806	CLA	3	0
22	B	810	CLA	2	0
28	A	801	CL0	25	0
22	3	614	CLA	1	0
26	X	2630	LHG	1	0
22	A	814	CLA	3	0
21	Y	609	CHL	1	0
24	X	7622	XAT	3	0
22	A	827	CLA	1	0
22	B	821	CLA	1	0
25	B	846	BCR	2	0
22	B	816	CLA	2	0
22	A	830	CLA	4	0
22	3	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	202	LMG	1	0
22	A	839	CLA	4	0
22	A	815	CLA	1	0
22	A	833	CLA	1	0
23	X	2620	LUT	2	0
22	H	201	CLA	5	0
22	G	201	CLA	1	0
22	A	811	CLA	3	0
22	A	834	CLA	1	0
22	B	818	CLA	5	0
22	A	842	CLA	6	0
22	B	838	CLA	1	0
22	B	826	CLA	4	0
23	3	618	LUT	3	0
25	B	844	BCR	1	0
27	1	622	LMG	2	0
22	A	807	CLA	1	0
22	A	838	CLA	1	0
22	K	204	CLA	2	0
22	2	609	CLA	1	0
22	4	609	CLA	3	0
25	A	848	BCR	6	0
21	2	601	CHL	3	0
22	A	808	CLA	1	0
27	2	623	LMG	1	0
22	Z	611	CLA	1	0
25	A	852	BCR	5	0
22	B	803	CLA	2	0
22	X	610	CLA	2	0
22	4	611	CLA	2	0
32	J	103	DGD	2	0
25	G	205	BCR	2	0
22	1	603	CLA	3	0
22	4	602	CLA	4	0
22	4	610	CLA	2	0
22	3	612	CLA	1	0
25	K	205	BCR	2	0
33	Y	4623	NEX	2	0
22	X	602	CLA	4	0
21	X	601	CHL	2	0
22	Y	604	CLA	2	0
25	B	843	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Z	602	CLA	2	0
26	A	847	LHG	2	0
22	3	610	CLA	2	0
25	B	847	BCR	6	0
22	A	824	CLA	1	0
22	G	204	CLA	1	0
22	F	303	CLA	1	0
25	A	850	BCR	2	0
22	2	612	CLA	1	0
27	4	622	LMG	2	0
22	A	840	CLA	3	0
22	2	611	CLA	2	0
22	L	302	CLA	3	0
22	A	803	CLA	6	0
22	B	840	CLA	3	0
25	A	851	BCR	2	0
22	B	813	CLA	3	0
23	X	2621	LUT	3	0
25	L	306	BCR	2	0
33	X	2623	NEX	3	0
25	I	101	BCR	3	0
22	A	835	CLA	2	0
25	F	305	BCR	2	0
25	L	305	BCR	6	0
26	Y	4630	LHG	3	0
21	3	608	CHL	1	0
22	O	2001	CLA	1	0
21	1	601	CHL	4	0
22	A	825	CLA	3	0
22	A	837	CLA	1	0
22	1	610	CLA	2	0
22	G	203	CLA	2	0
22	Z	612	CLA	1	0
22	Z	613	CLA	1	0
22	A	831	CLA	6	0
27	4	623	LMG	1	0
26	B	851	LHG	1	0
30	C	102	SF4	1	0
25	B	845	BCR	5	0
22	A	819	CLA	1	0
32	B	850	DGD	8	0
23	2	619	LUT	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	620	XAT	5	0
22	4	617	CLA	3	0
22	B	830	CLA	2	0
21	Y	601	CHL	1	0
23	Z	7620	LUT	4	0
22	4	601	CLA	1	0
22	A	826	CLA	2	0
22	F	304	CLA	1	0
21	X	606	CHL	1	0
22	B	815	CLA	1	0
22	K	206	CLA	1	0
24	Y	2622	XAT	2	0
22	A	817	CLA	1	0
22	X	603	CLA	1	0
22	A	828	CLA	4	0
22	B	811	CLA	2	0
22	B	817	CLA	3	0
22	1	609	CLA	2	0
26	Z	7630	LHG	1	0
22	A	832	CLA	1	0
22	A	854	CLA	8	0
25	4	621	BCR	1	0
31	B	849	LMU	5	0
22	B	832	CLA	6	0
26	A	846	LHG	3	0
22	Y	613	CLA	1	0
29	A	844	PQN	6	0
24	Z	4622	XAT	1	0
22	A	809	CLA	4	0
22	K	201	CLA	1	0
23	Y	4620	LUT	3	0
22	B	824	CLA	2	0
22	3	606	CLA	1	0
22	B	833	CLA	1	0
24	3	619	XAT	4	0
22	A	841	CLA	5	0
22	B	828	CLA	4	0
21	X	605	CHL	1	0
25	J	102	BCR	1	0
22	B	841	CLA	4	0
25	A	856	BCR	5	0
22	A	818	CLA	1	0

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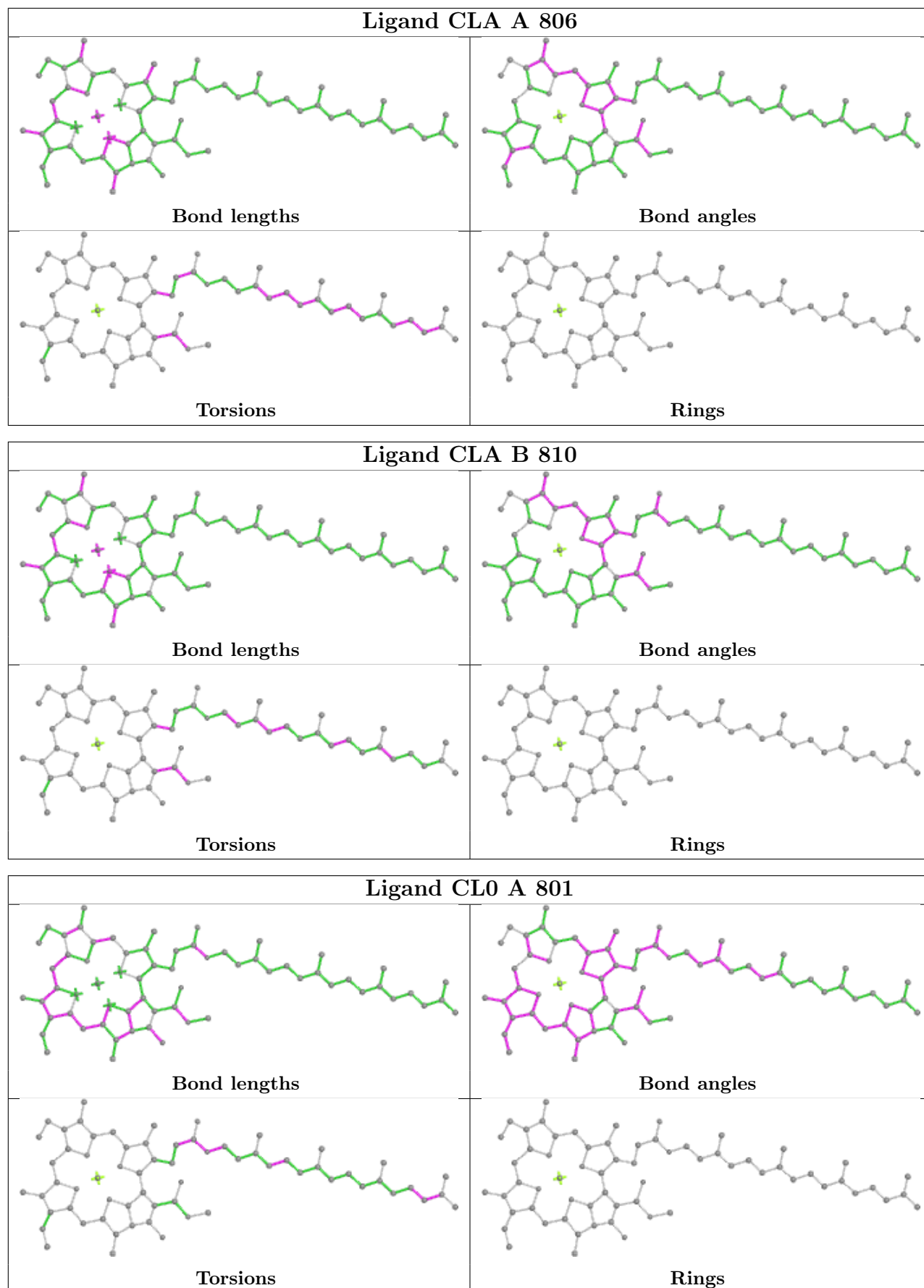
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	618	CHL	1	0
22	L	303	CLA	1	0
25	B	848	BCR	3	0
29	B	842	PQN	7	0
21	2	606	CHL	2	0
24	2	620	XAT	4	0
22	A	812	CLA	4	0
22	B	835	CLA	3	0
22	1	613	CLA	2	0
26	1	620	LHG	6	0
21	Y	606	CHL	1	0
21	2	608	CHL	2	0
22	X	612	CLA	1	0
26	2	622	LHG	3	0
22	A	802	CLA	3	0
22	Y	612	CLA	1	0
31	A	857	LMU	4	0
22	3	602	CLA	2	0
23	1	617	LUT	6	0
22	B	802	CLA	4	0
22	B	814	CLA	1	0
22	N	1001	CLA	1	0
22	L	304	CLA	3	0
23	Y	4621	LUT	2	0
22	2	610	CLA	3	0
22	N	1002	CLA	2	0
22	F	301	CLA	2	0
22	A	810	CLA	2	0
22	B	823	CLA	2	0
22	B	829	CLA	3	0
21	X	609	CHL	1	0
22	B	807	CLA	1	0
22	1	612	CLA	1	0
22	B	827	CLA	5	0
33	Z	7623	NEX	2	0
22	1	614	CLA	1	0
22	1	602	CLA	6	0
23	1	621	LUT	1	0
22	A	829	CLA	7	0
22	B	837	CLA	4	0
22	B	839	CLA	2	0
23	4	619	LUT	4	0

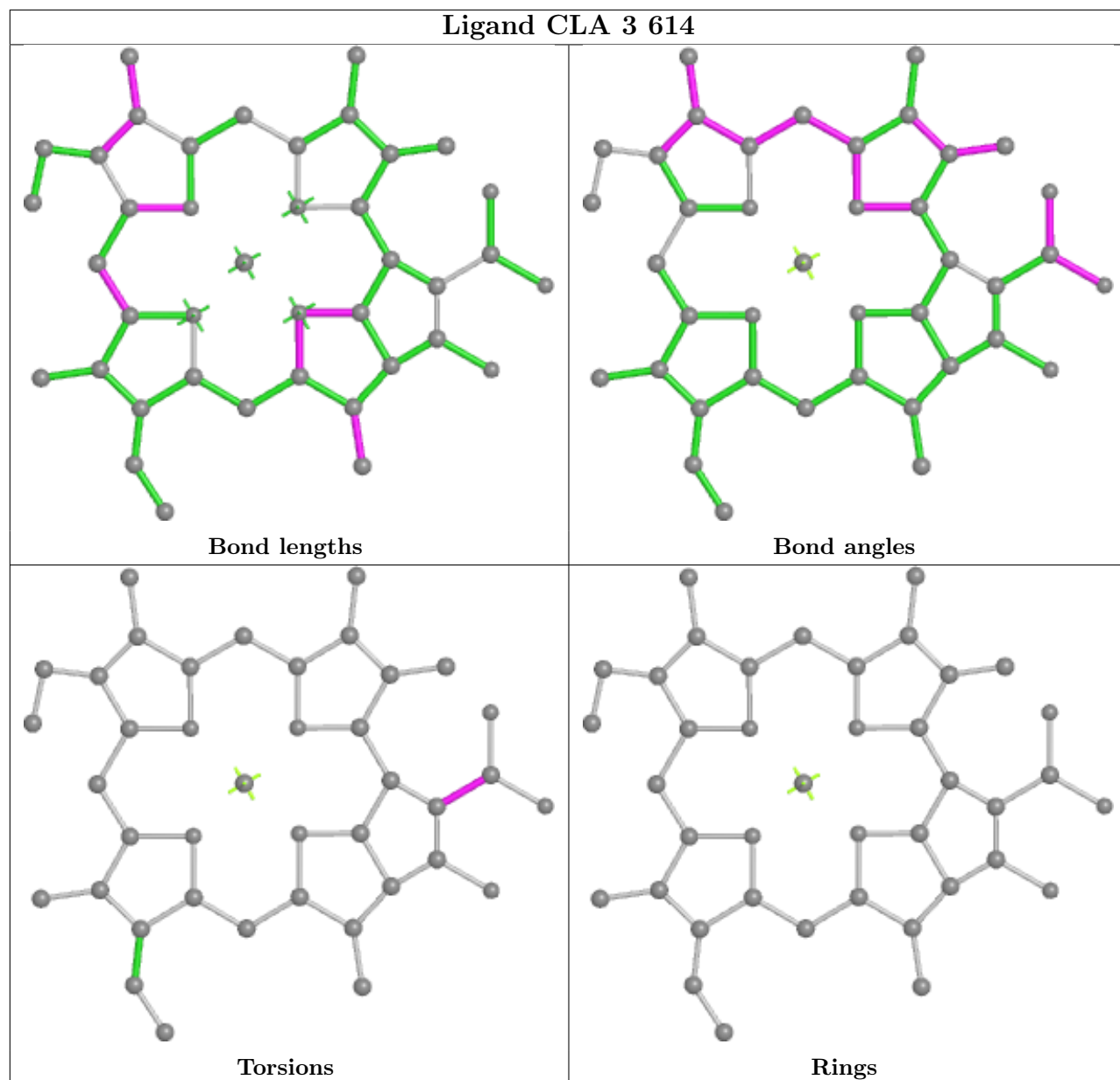
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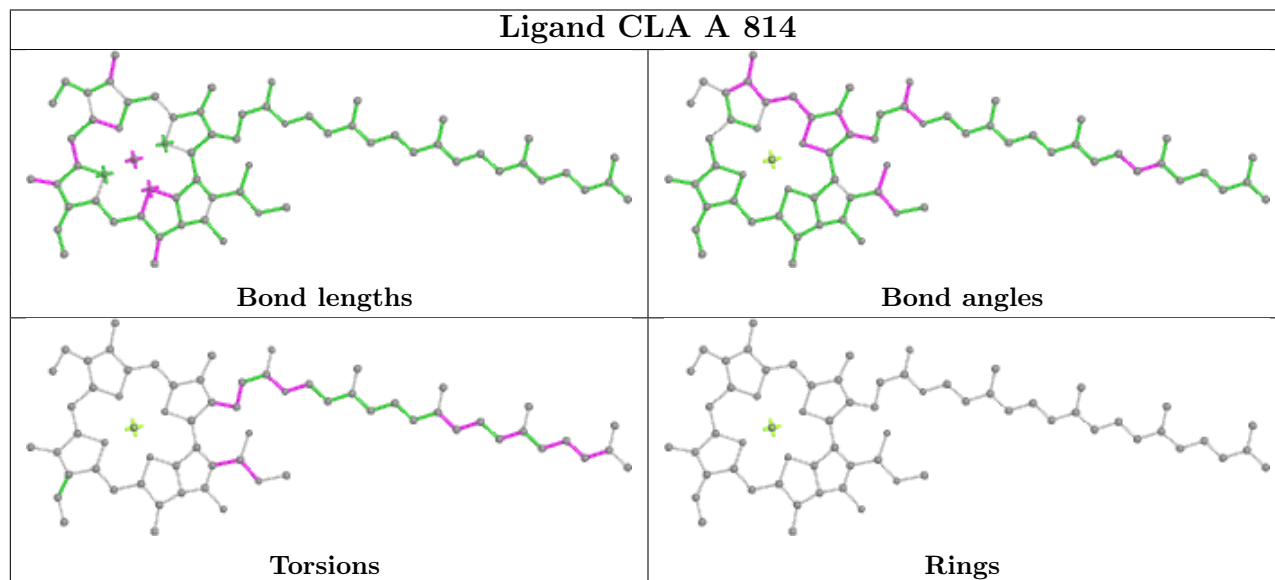
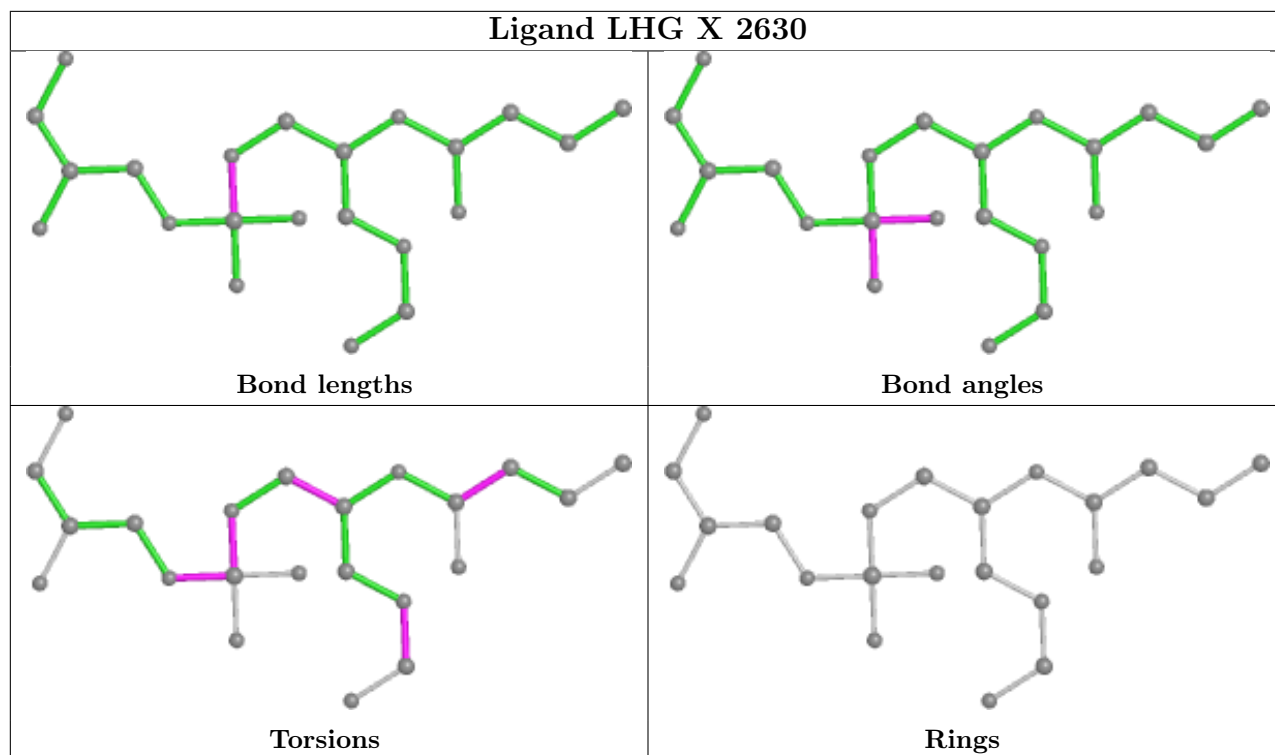
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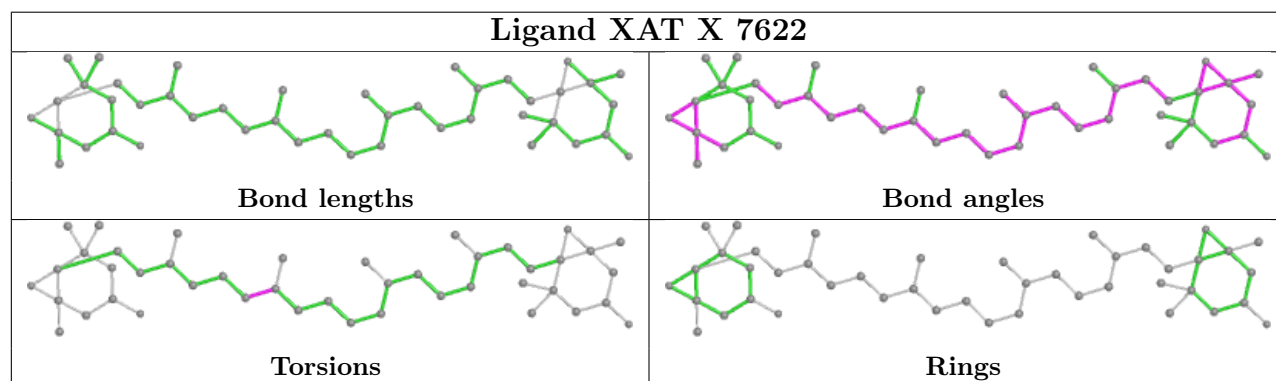
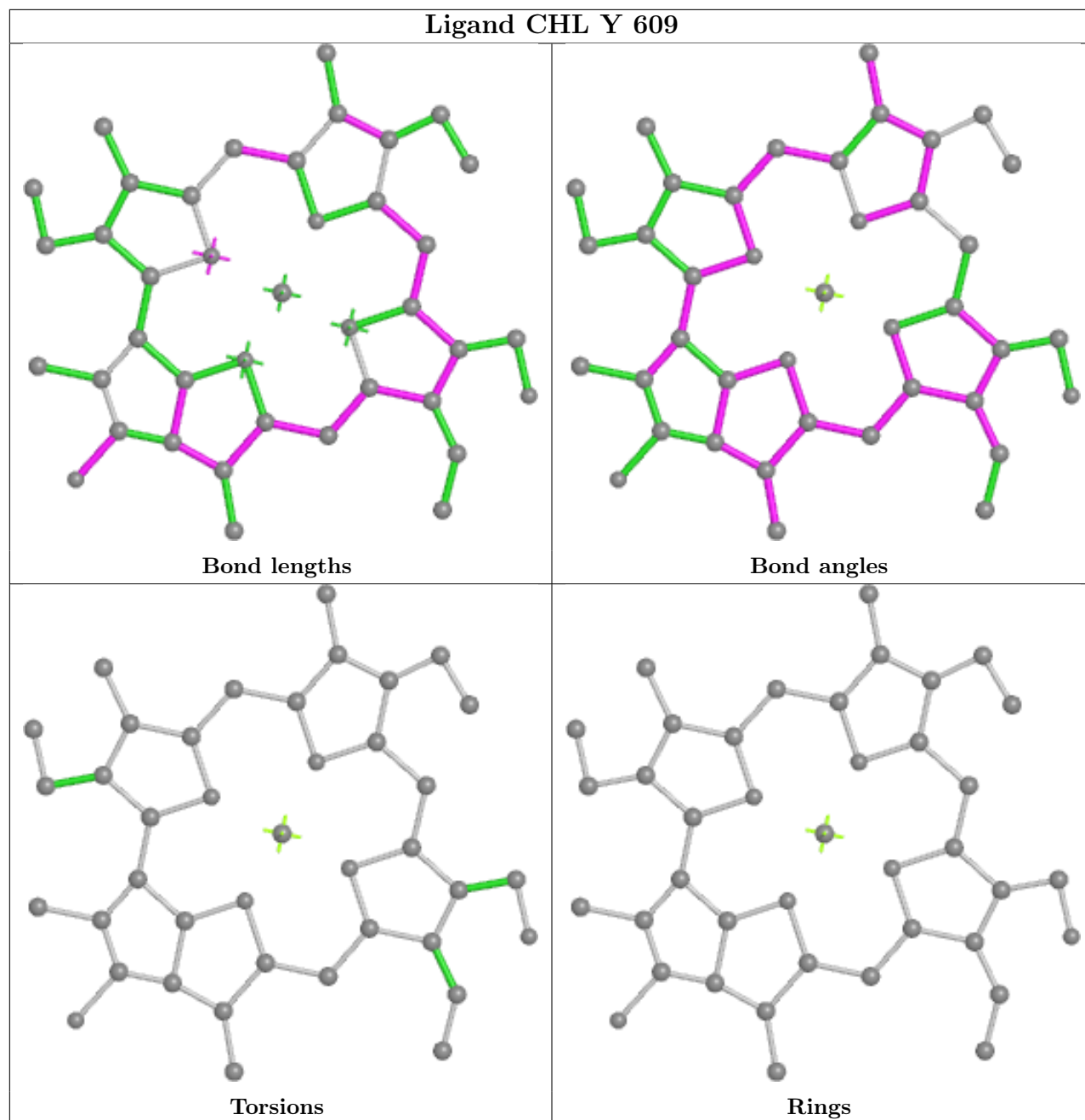
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	822	CLA	5	0
25	B	801	BCR	3	0
22	B	819	CLA	1	0
23	Z	7621	LUT	2	0
25	A	849	BCR	7	0
22	B	831	CLA	1	0
22	Z	610	CLA	2	0
22	A	823	CLA	1	0
22	Y	602	CLA	2	0
22	B	834	CLA	1	0
22	B	825	CLA	3	0
22	B	806	CLA	1	0
22	1	608	CLA	1	0
21	4	618	CHL	1	0
22	A	843	CLA	2	0
22	B	809	CLA	4	0
22	A	820	CLA	5	0
22	3	613	CLA	1	0
22	Z	614	CLA	1	0
25	K	202	BCR	5	0
22	4	612	CLA	2	0
25	2	621	BCR	4	0
25	3	620	BCR	3	0
22	B	805	CLA	2	0

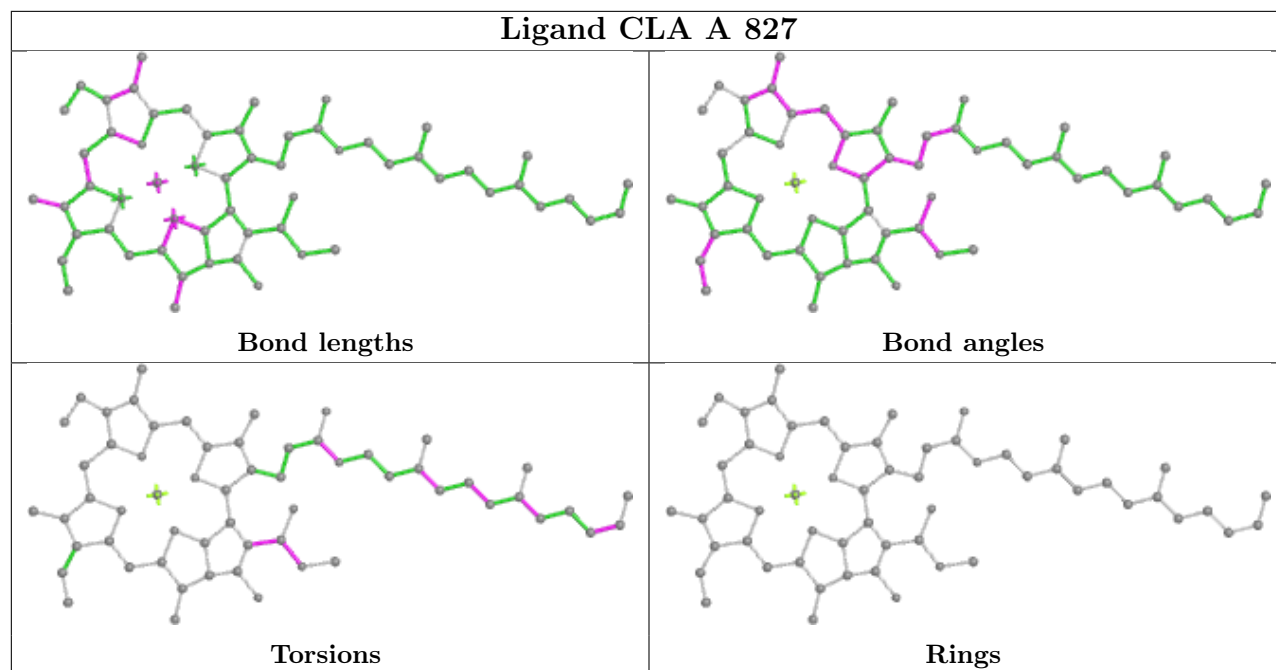
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



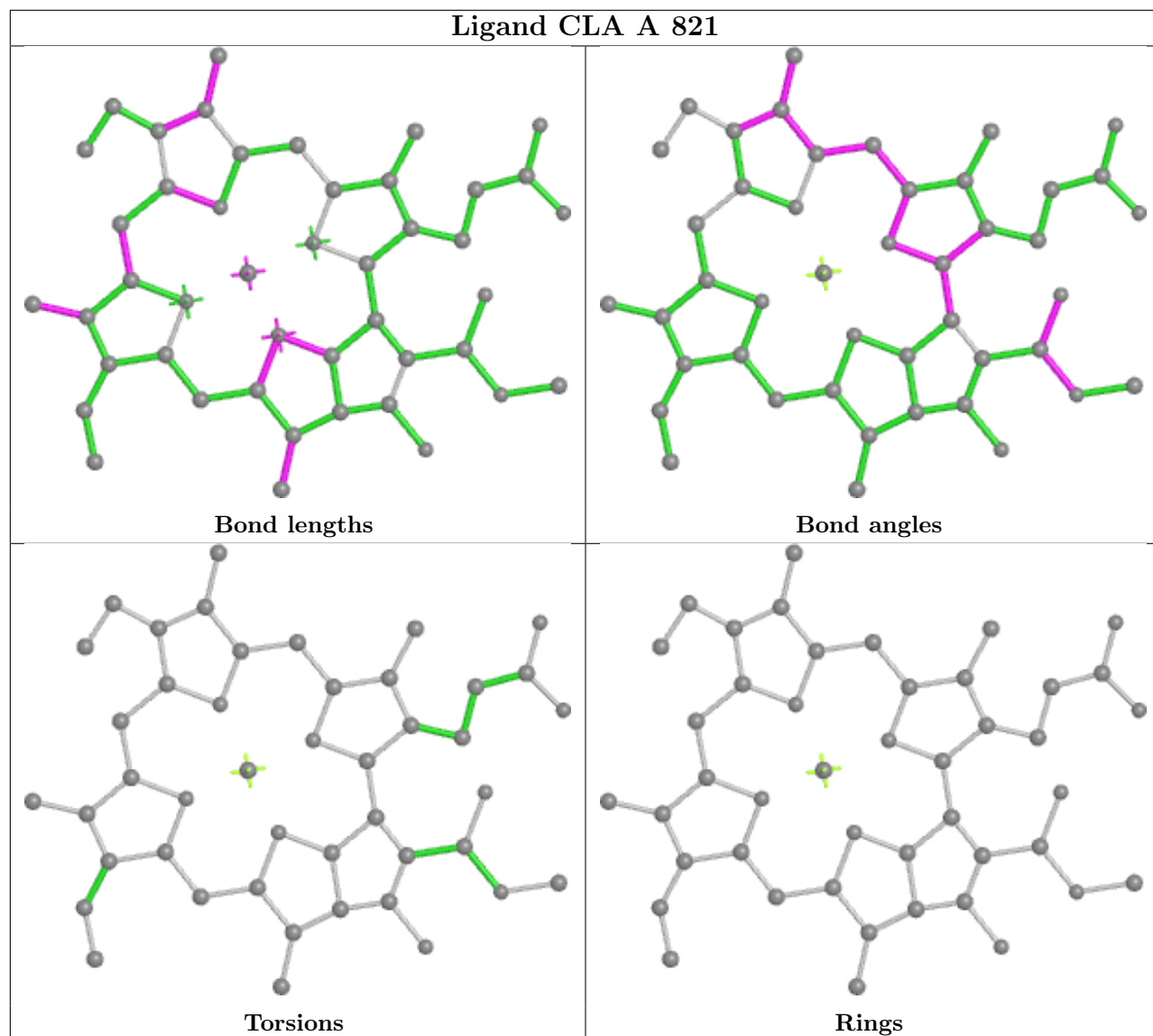


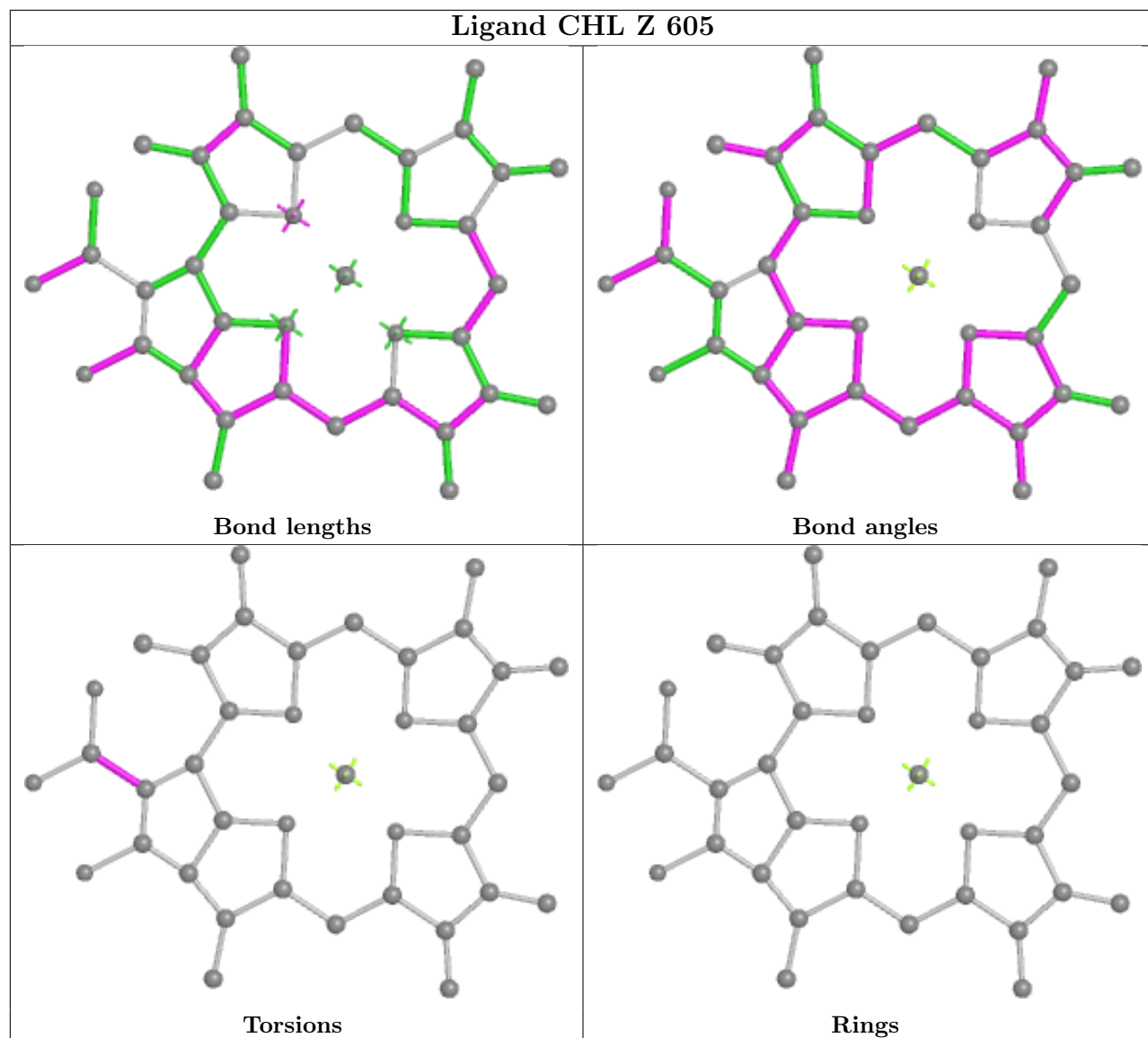


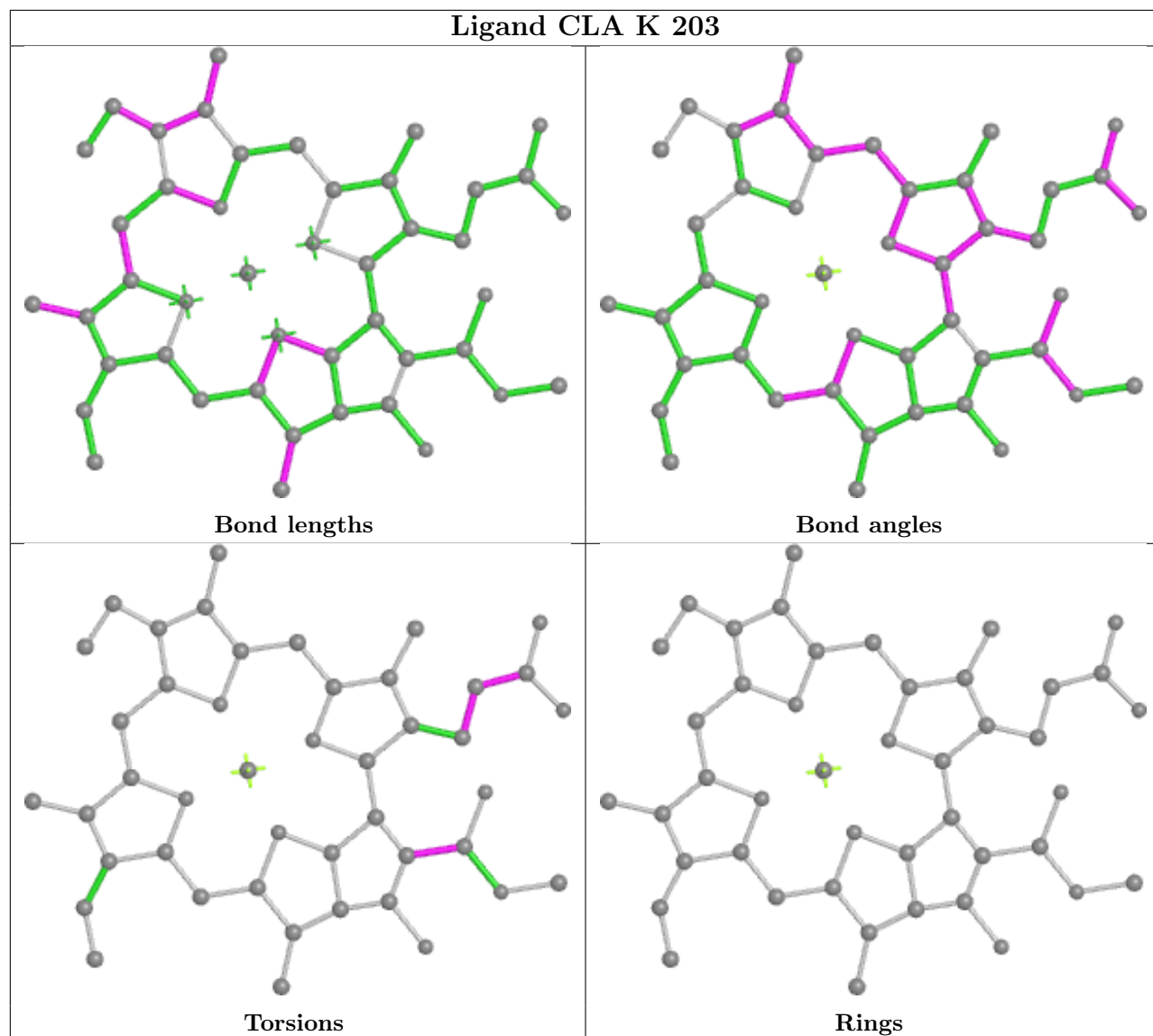


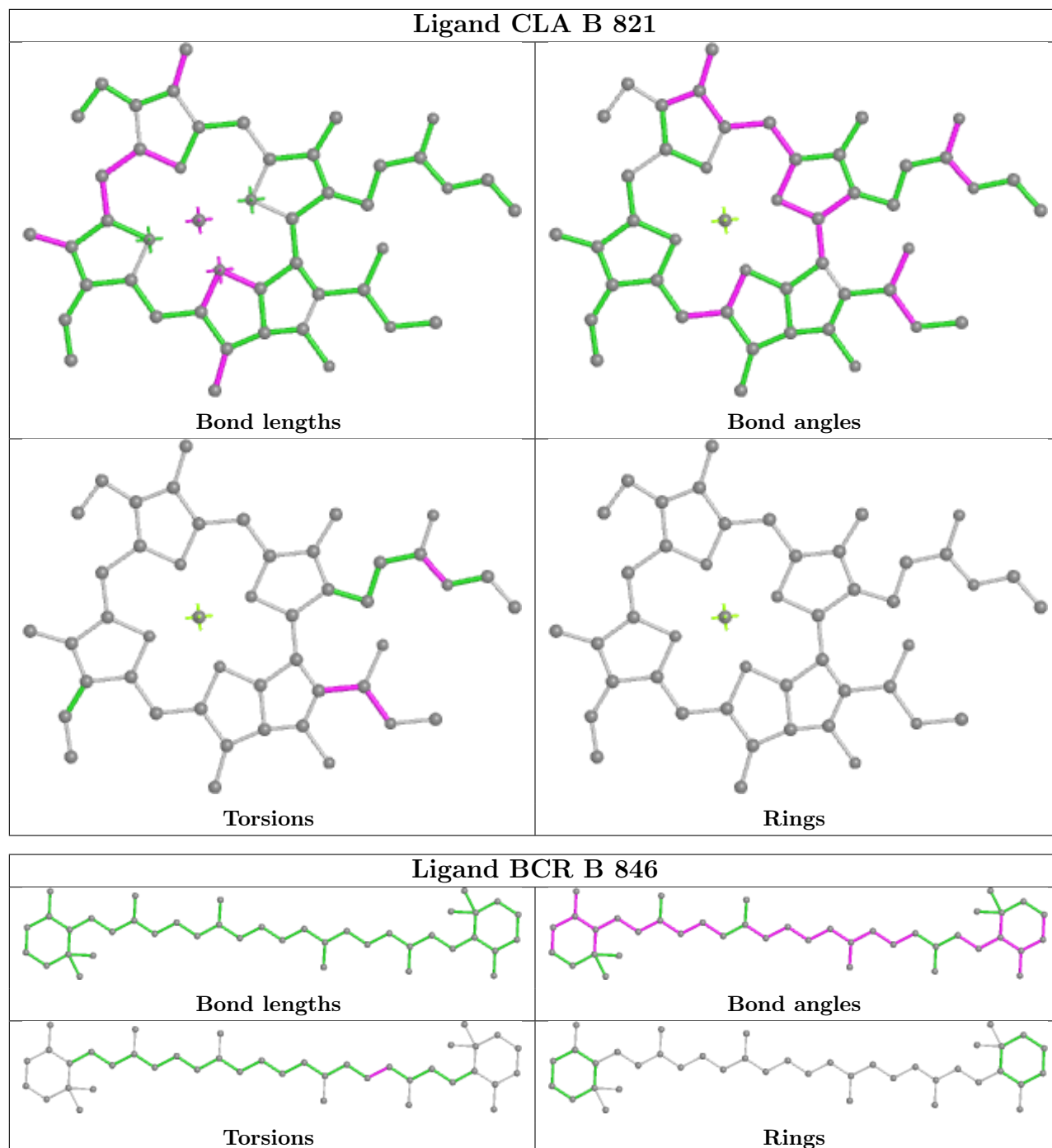


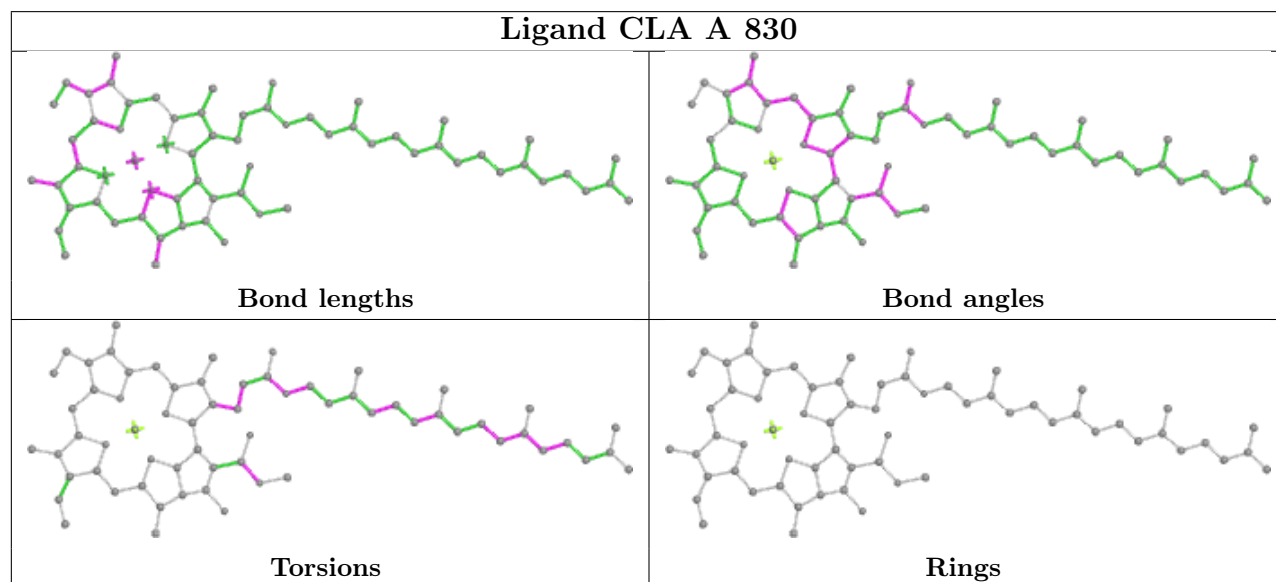
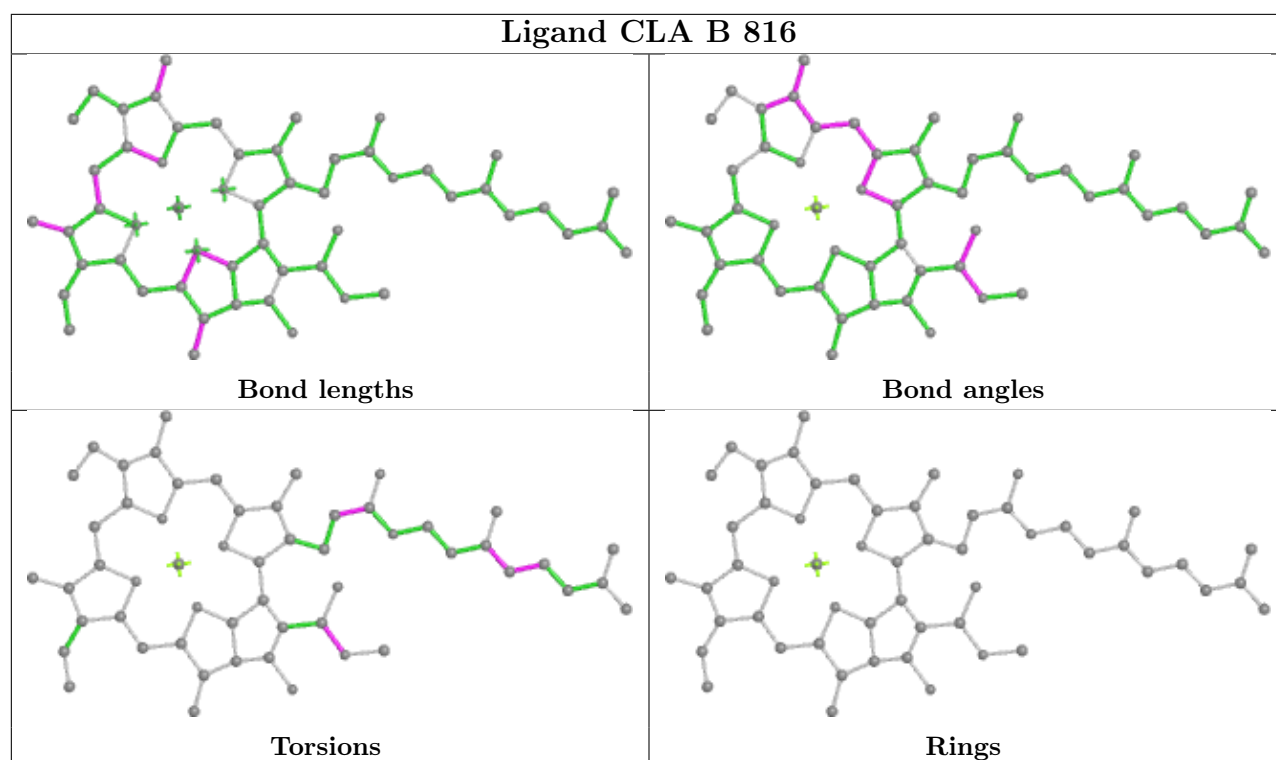


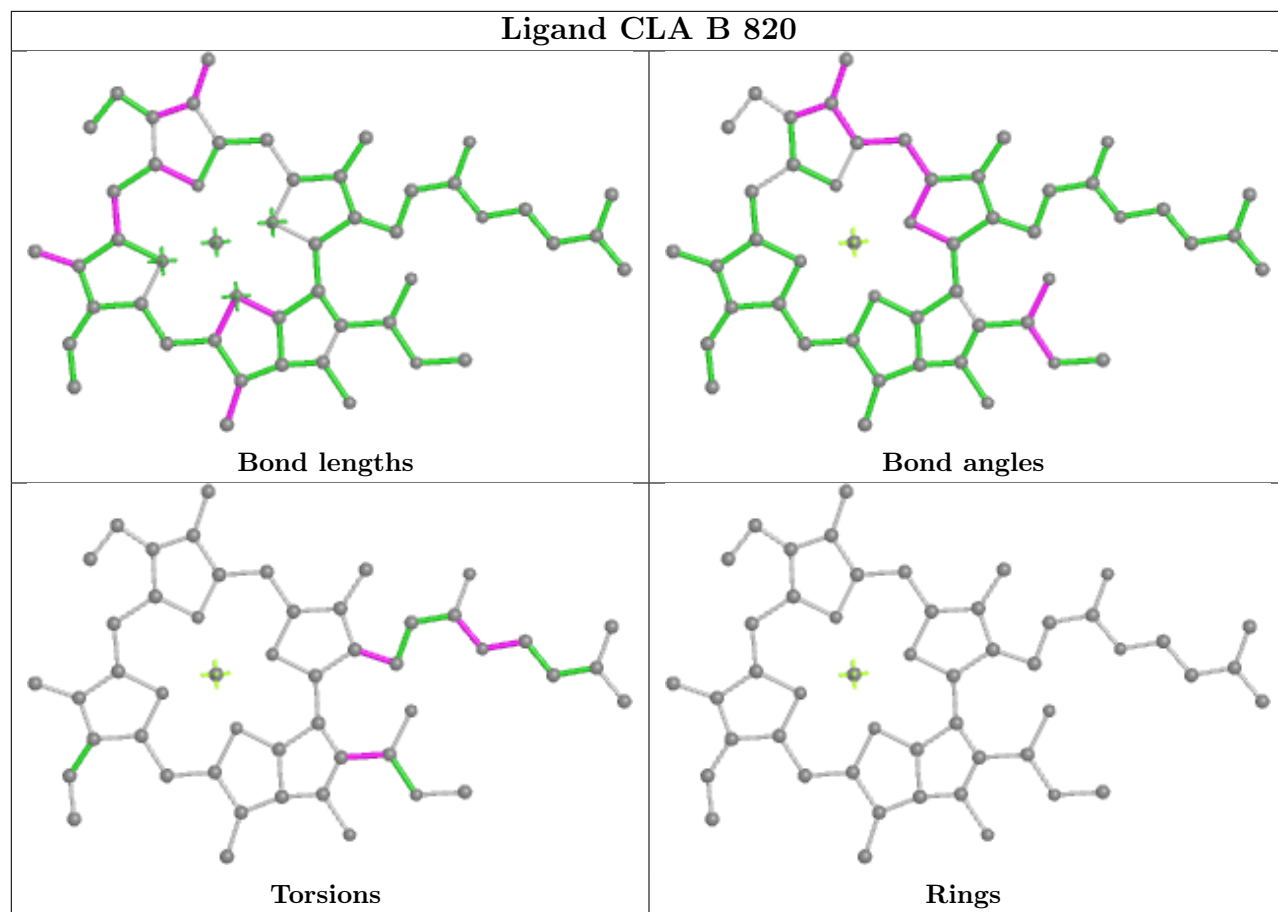


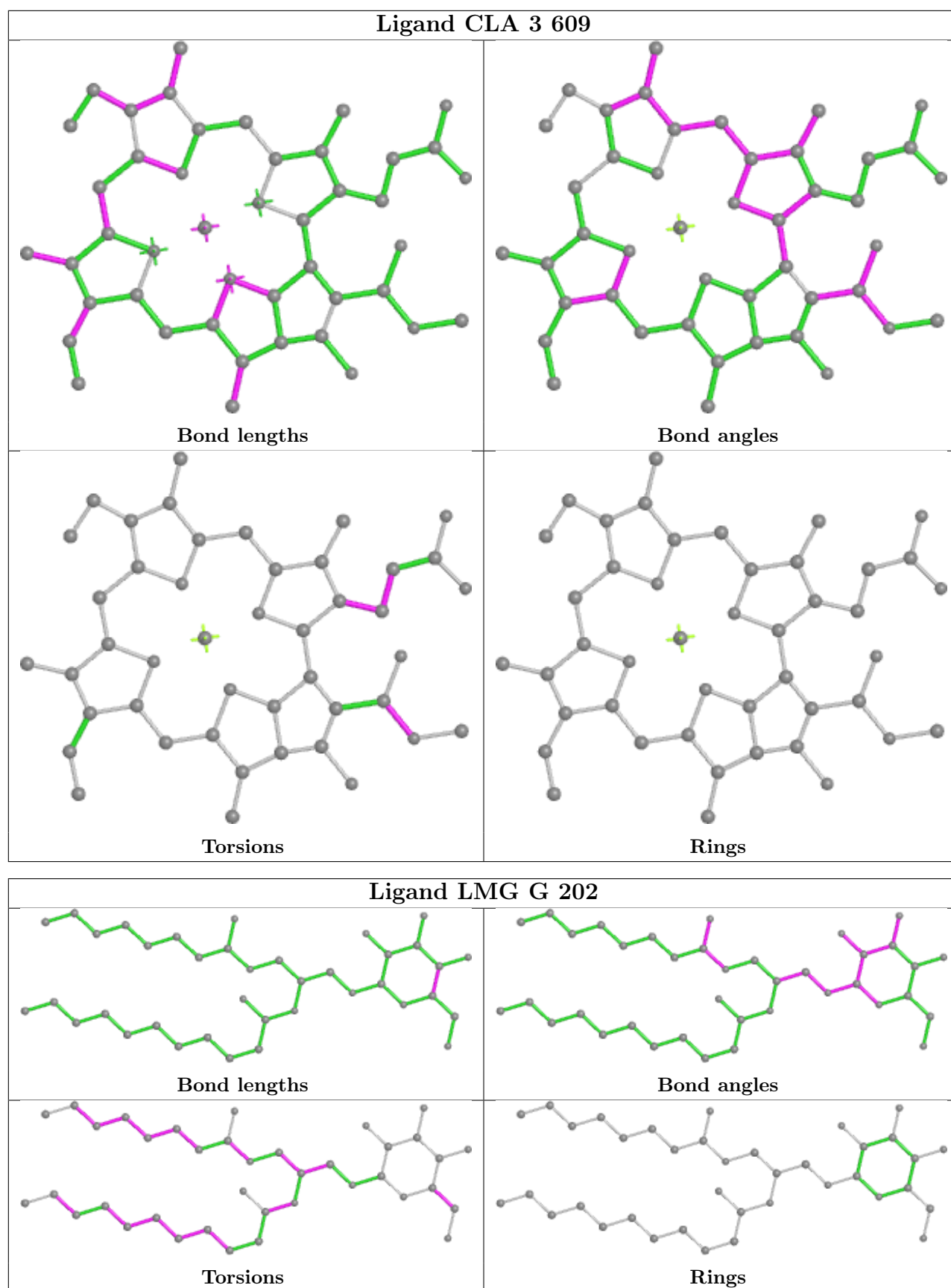


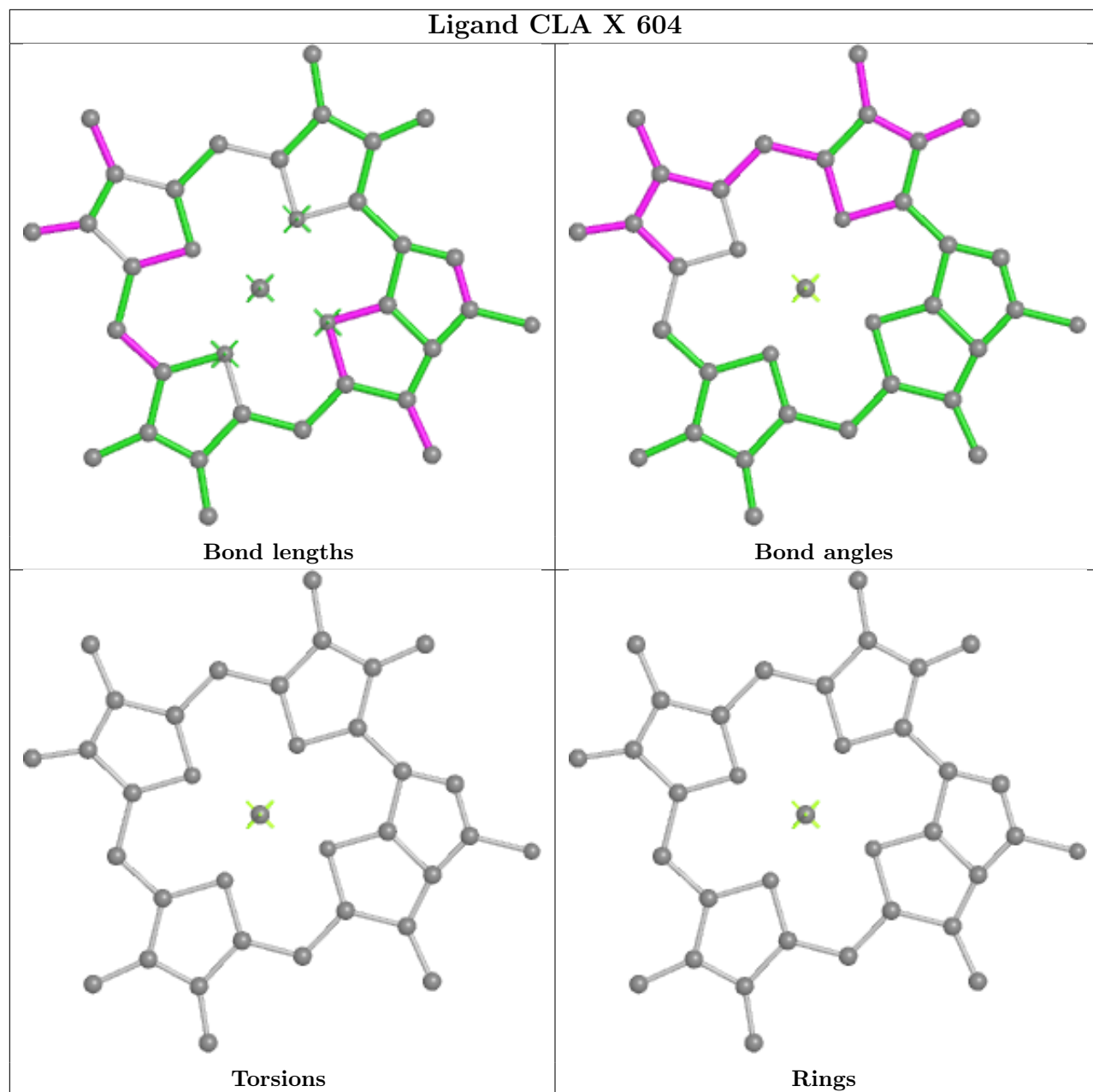




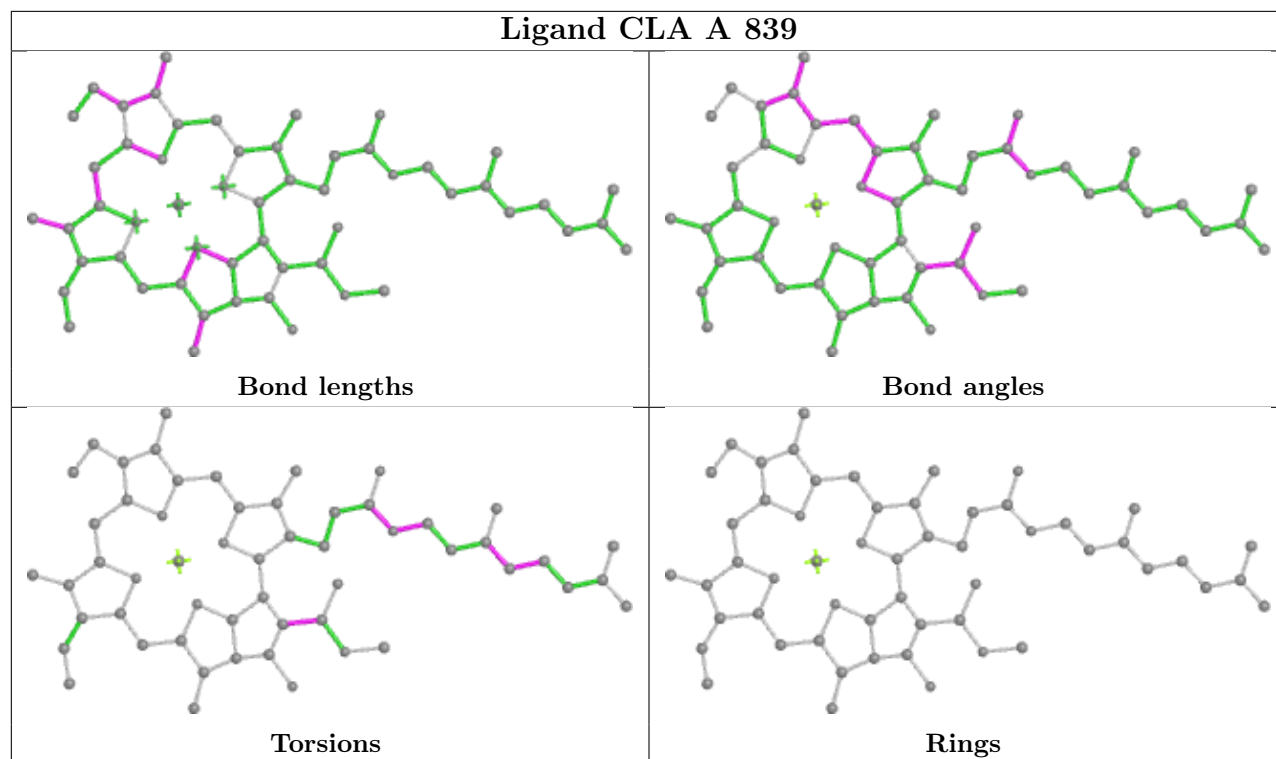


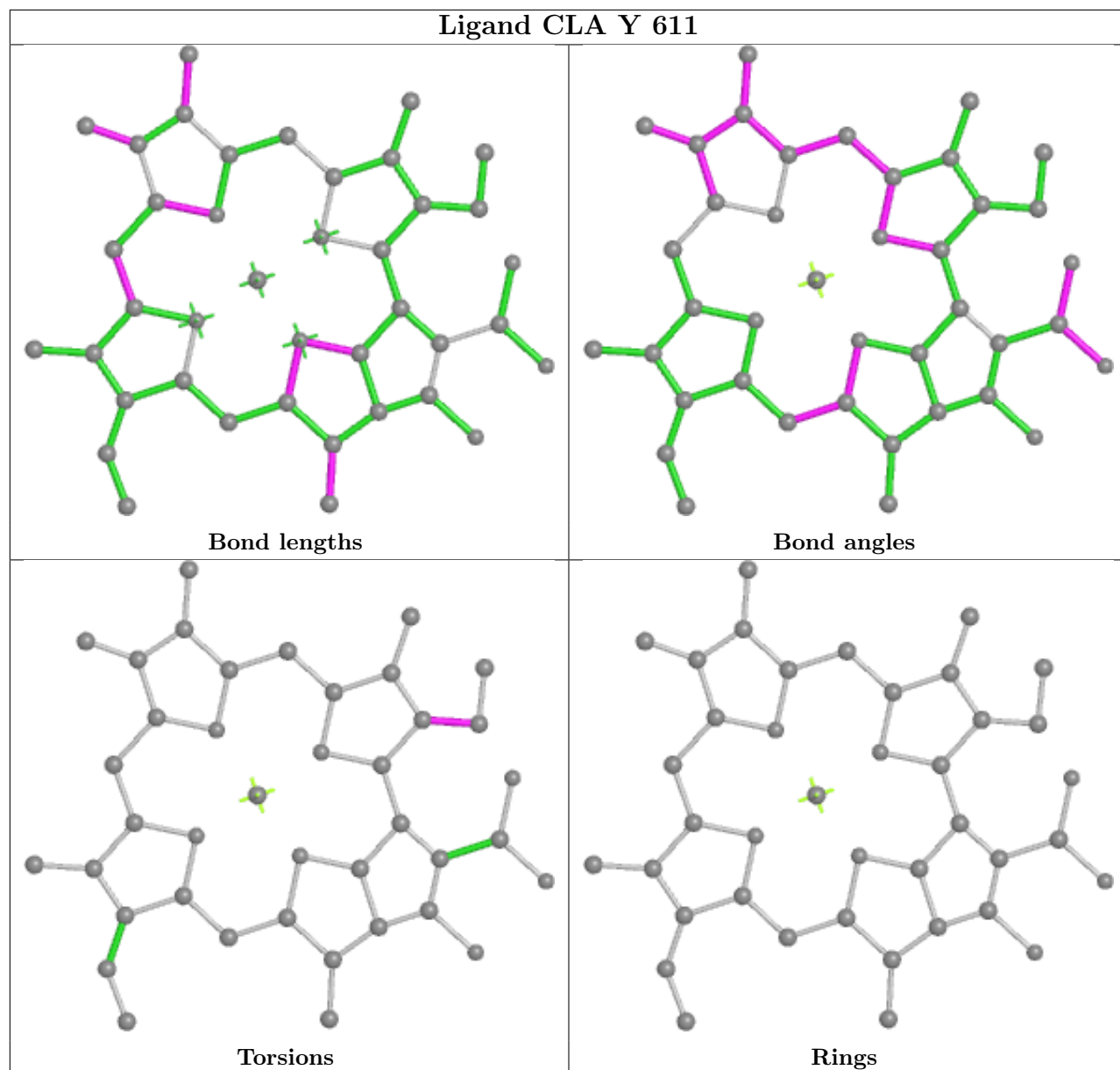


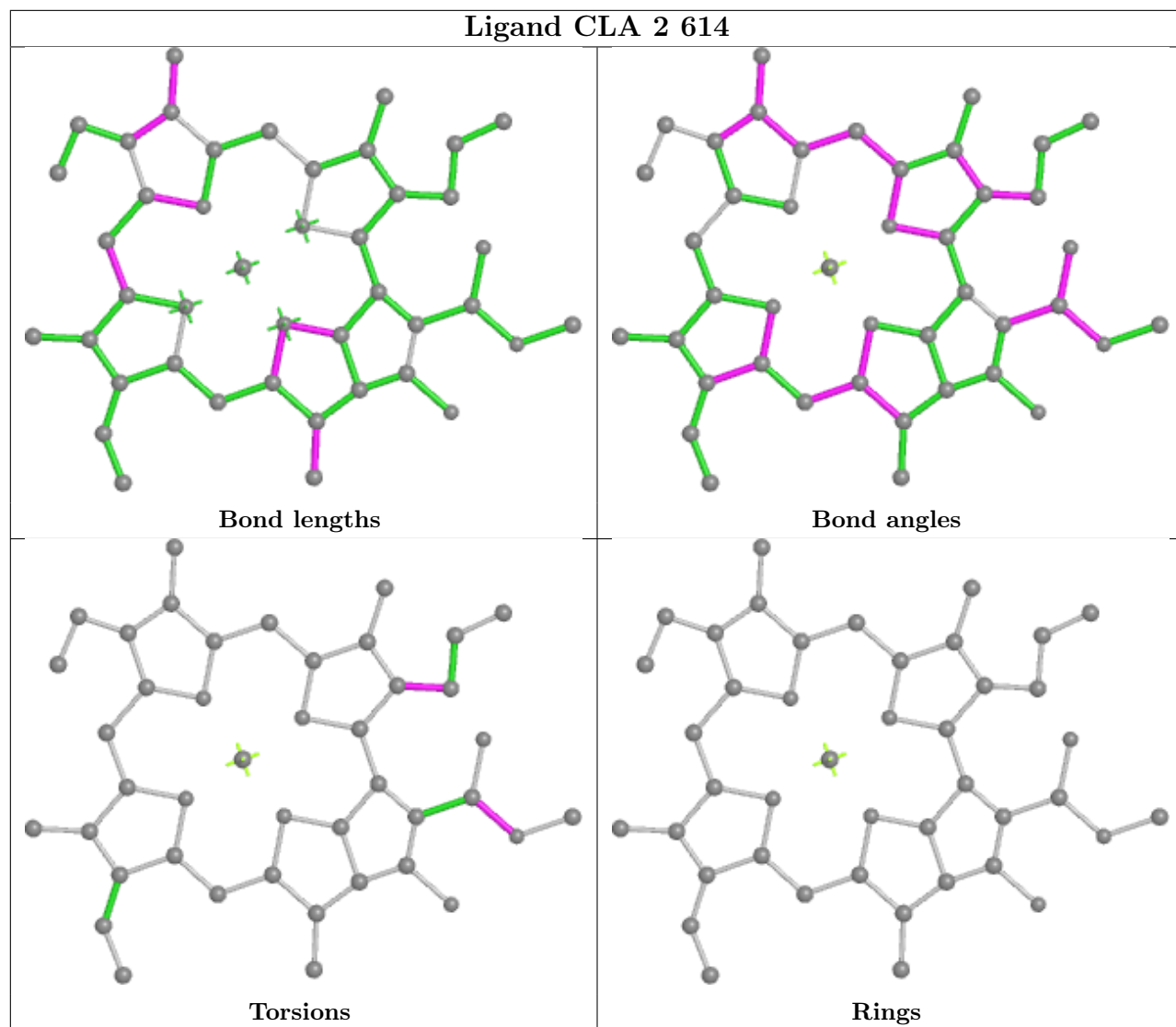


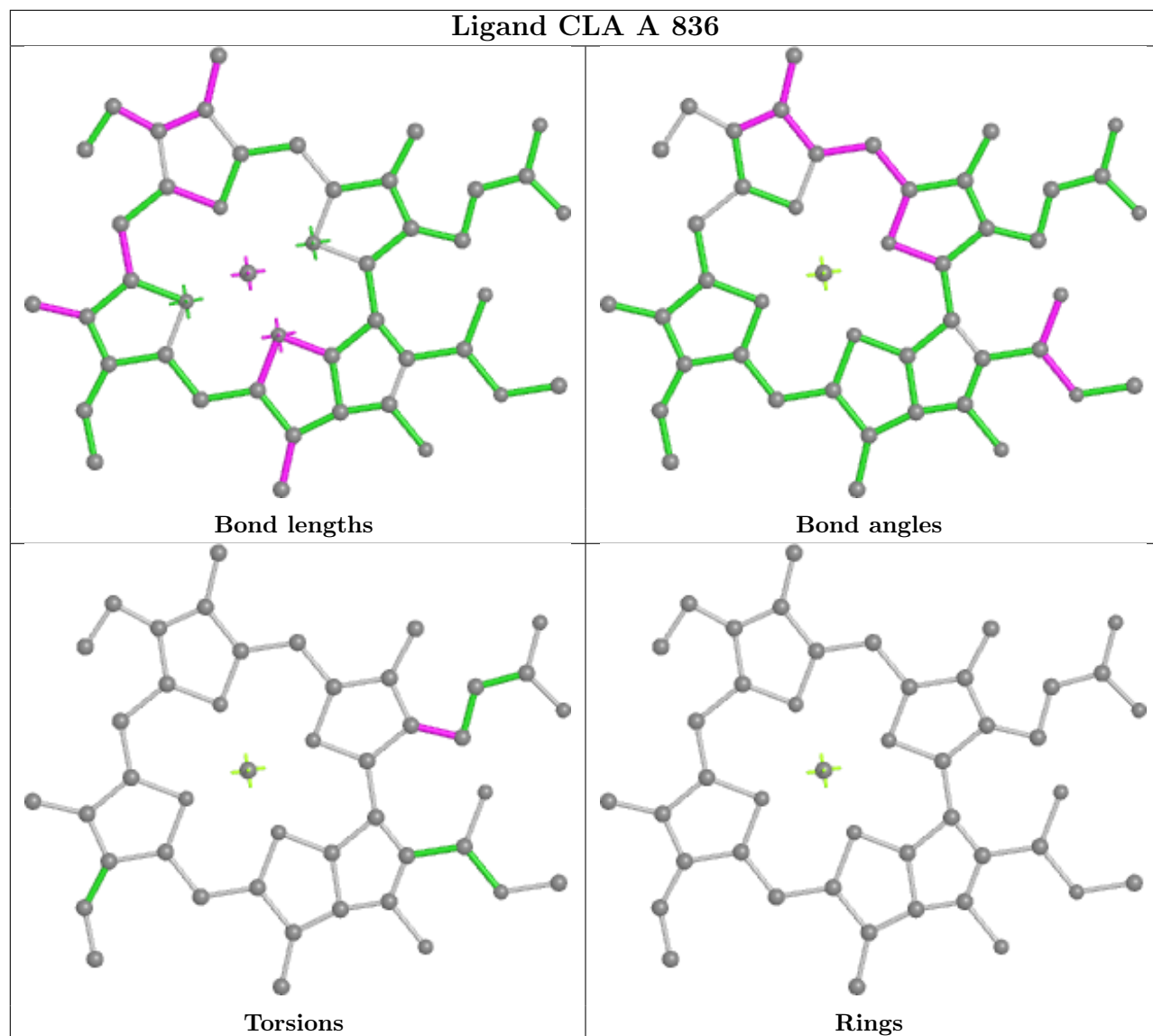


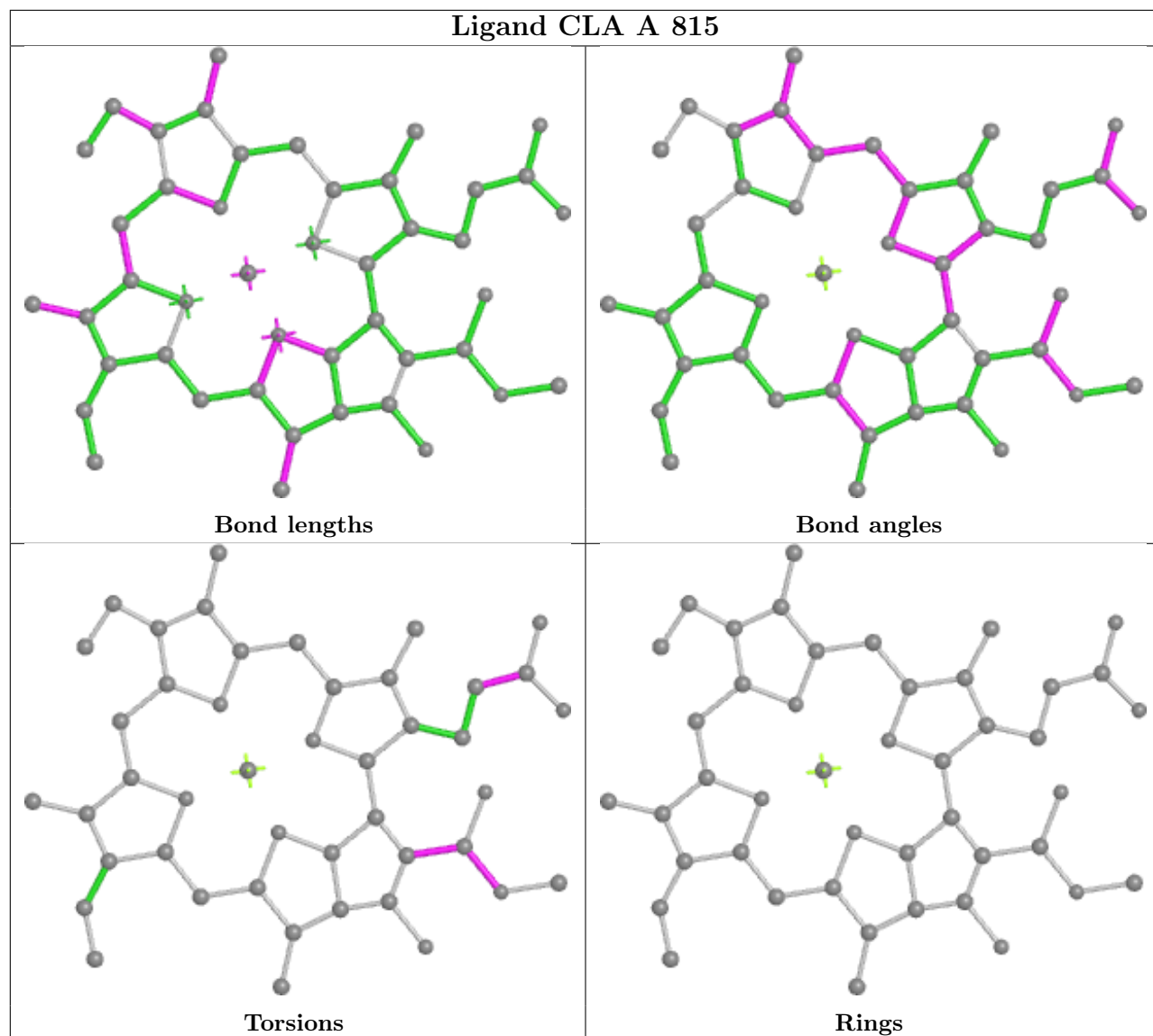


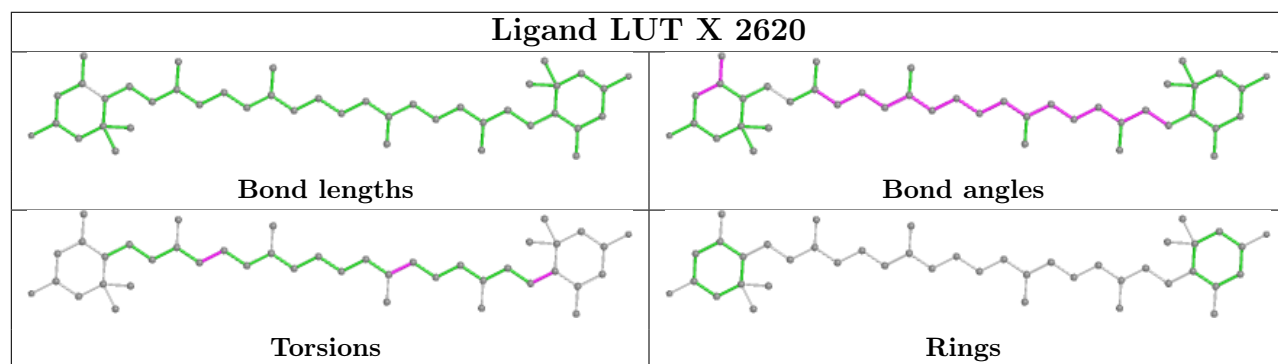
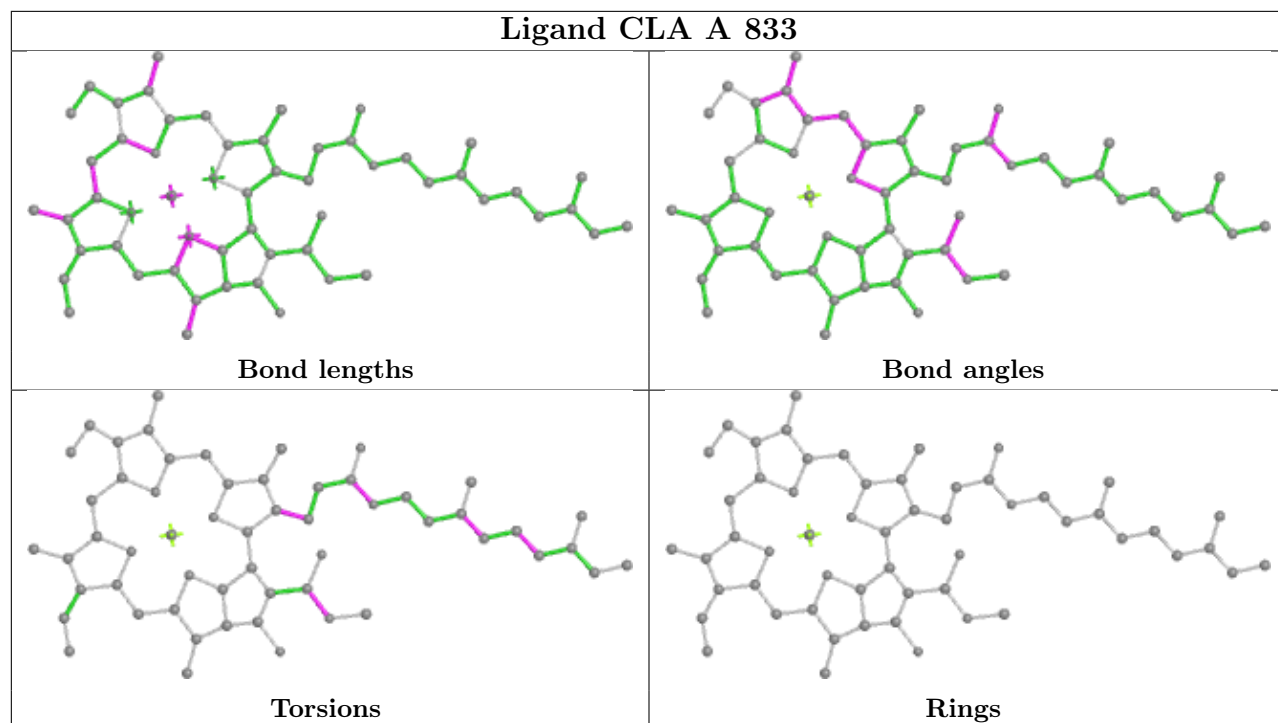


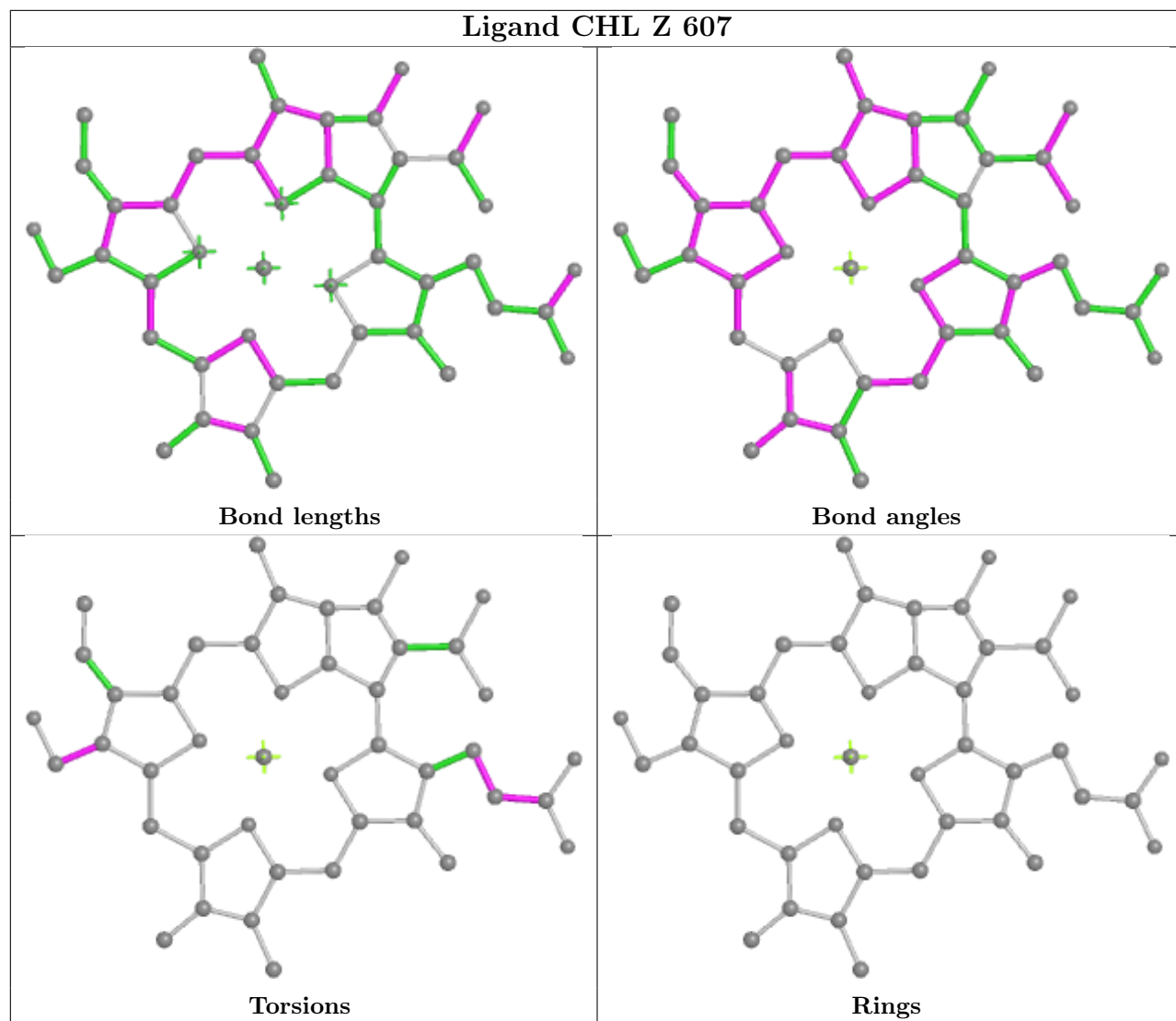


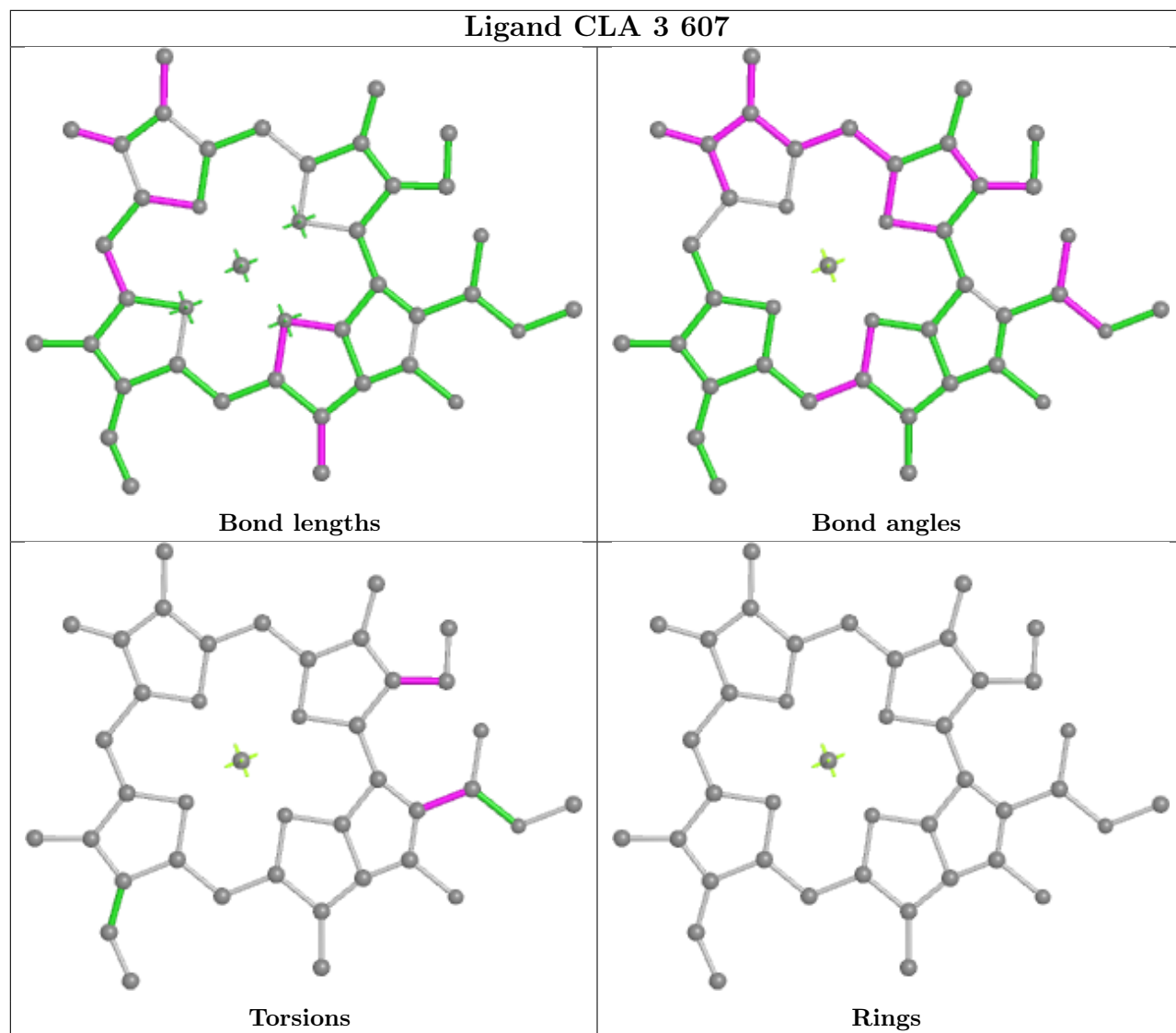




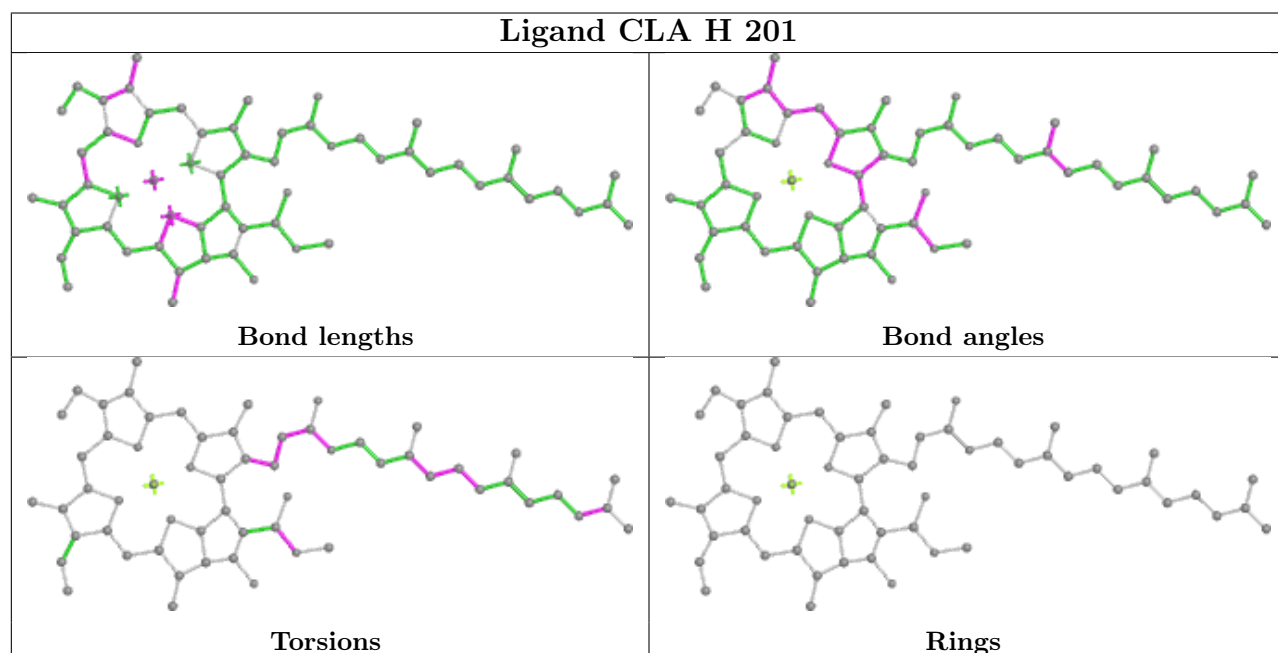
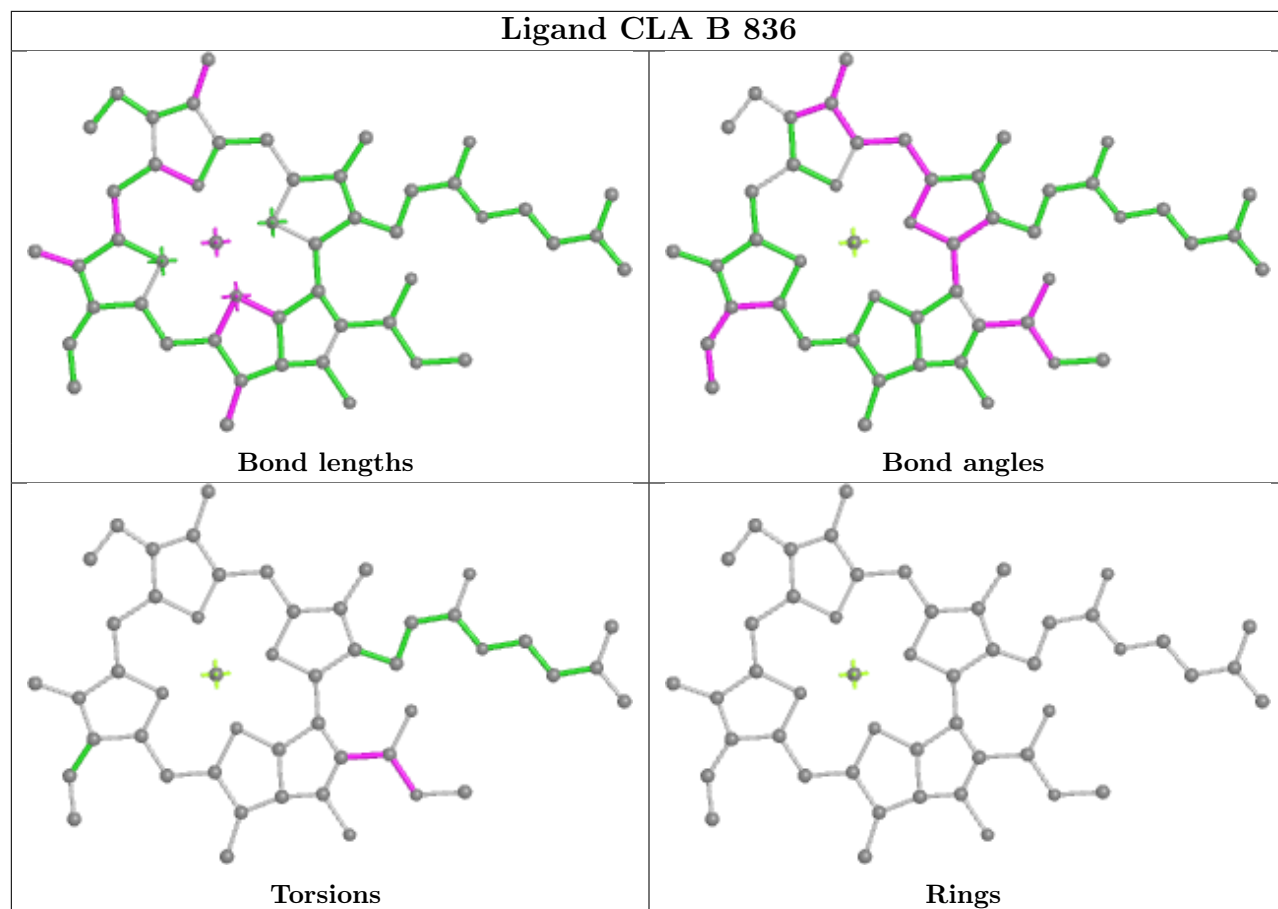


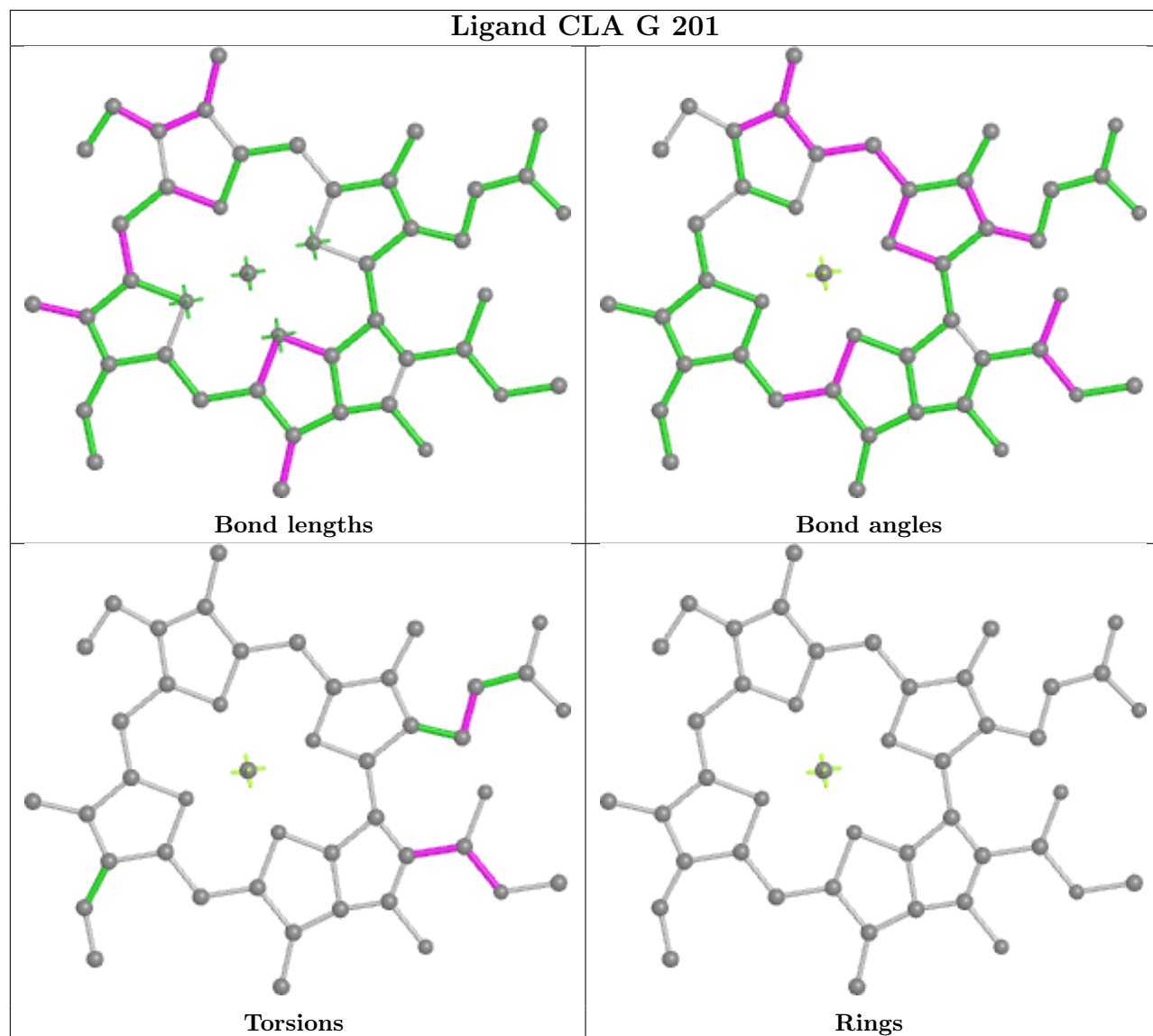


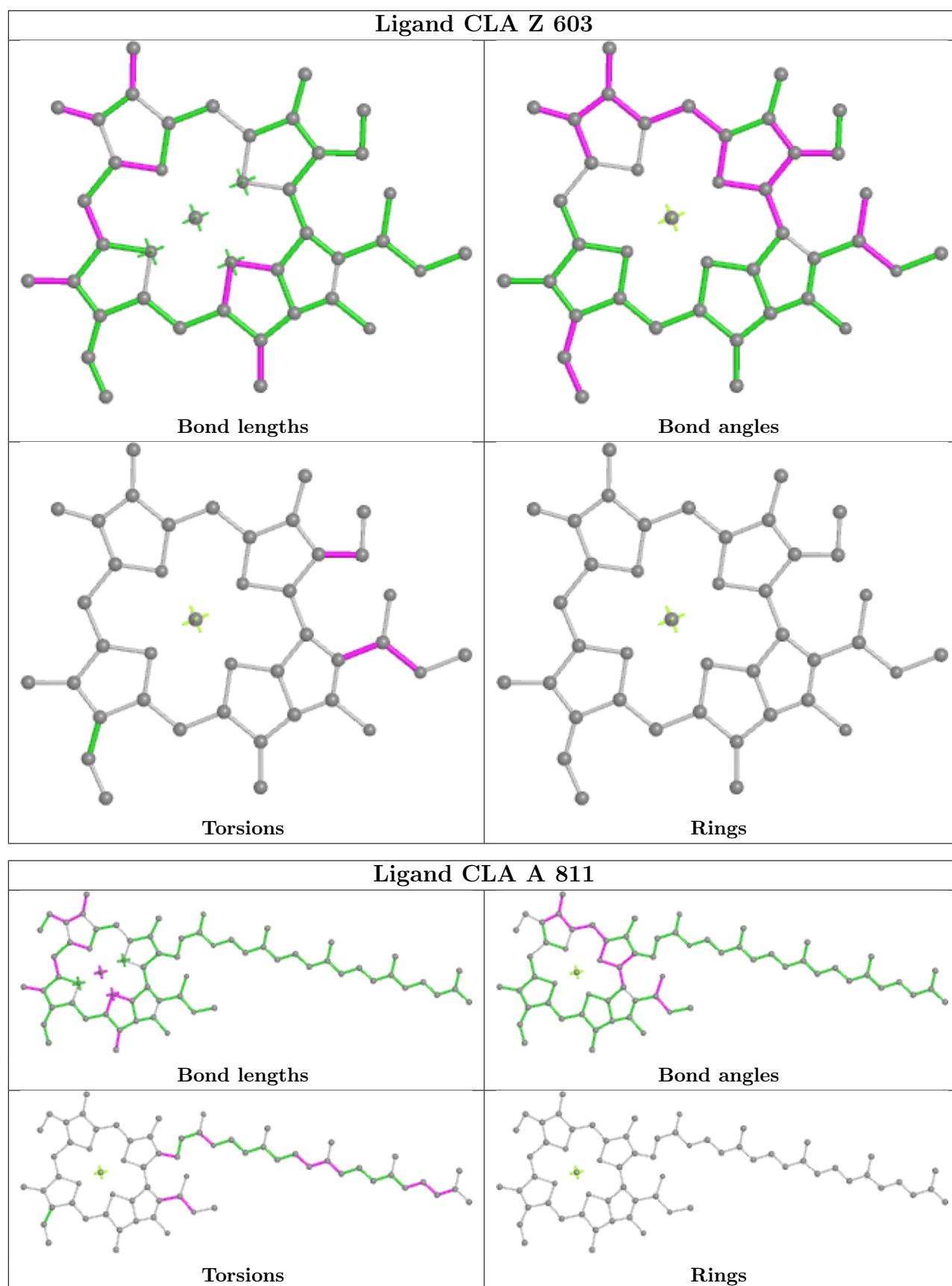


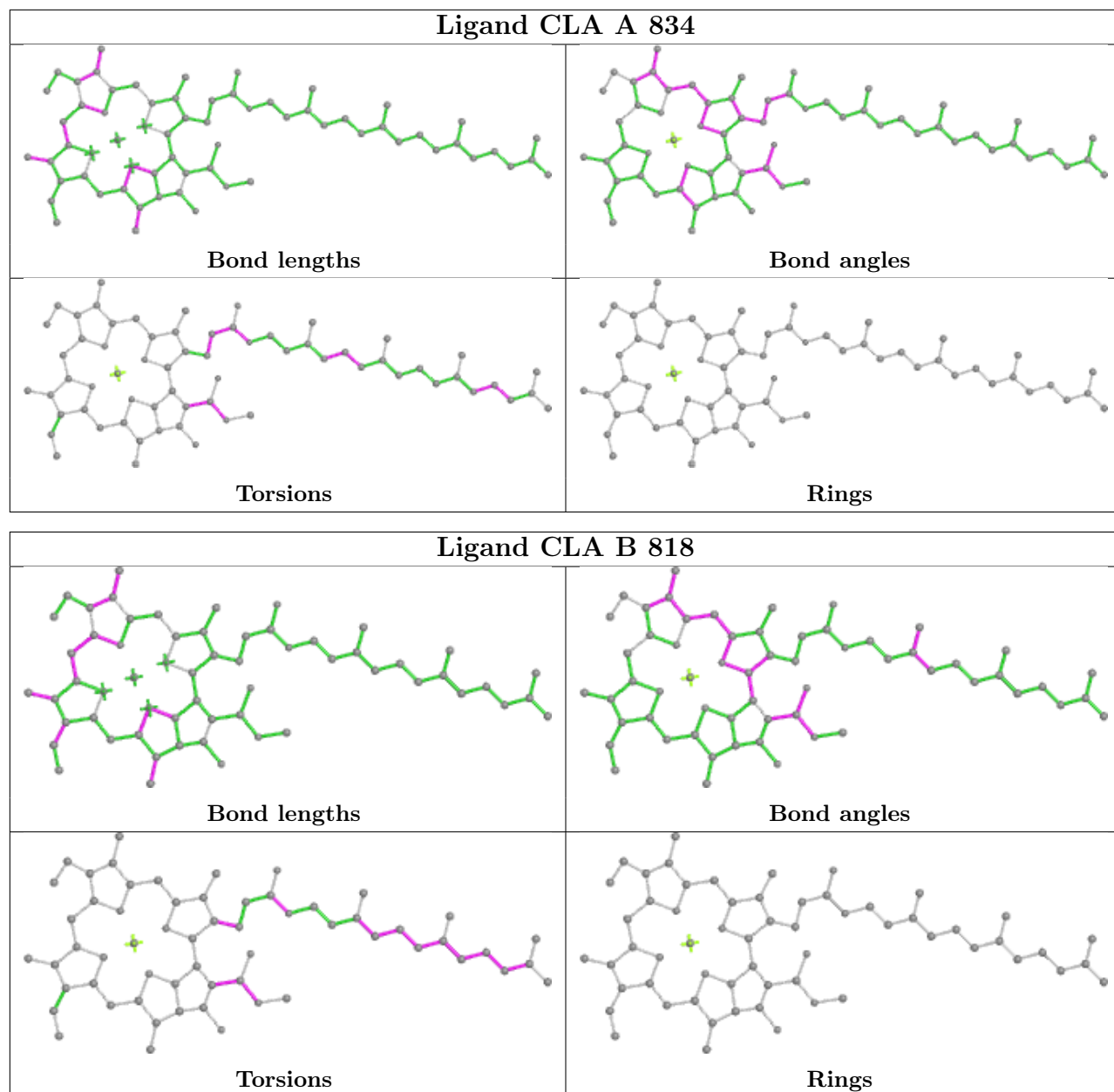


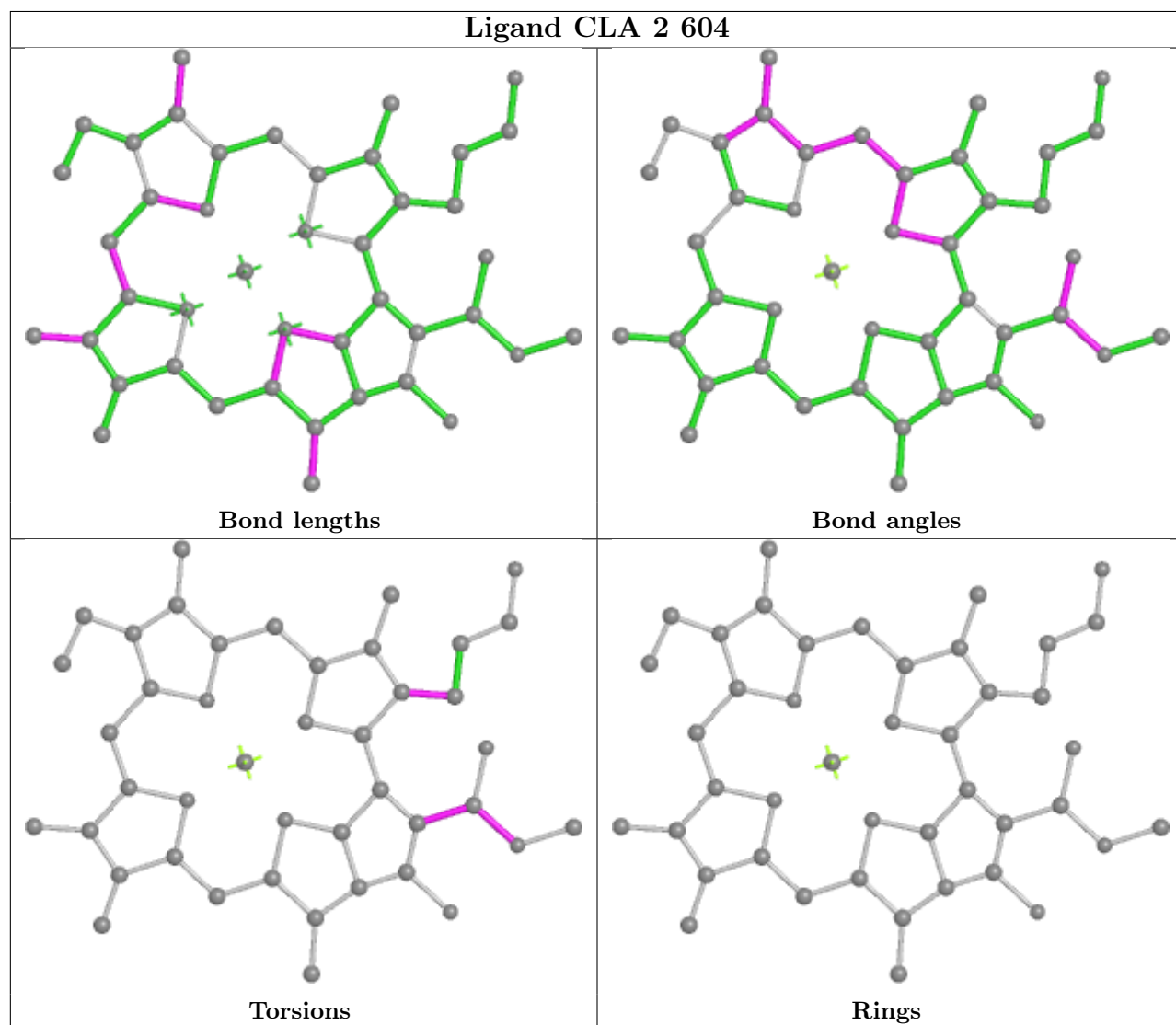
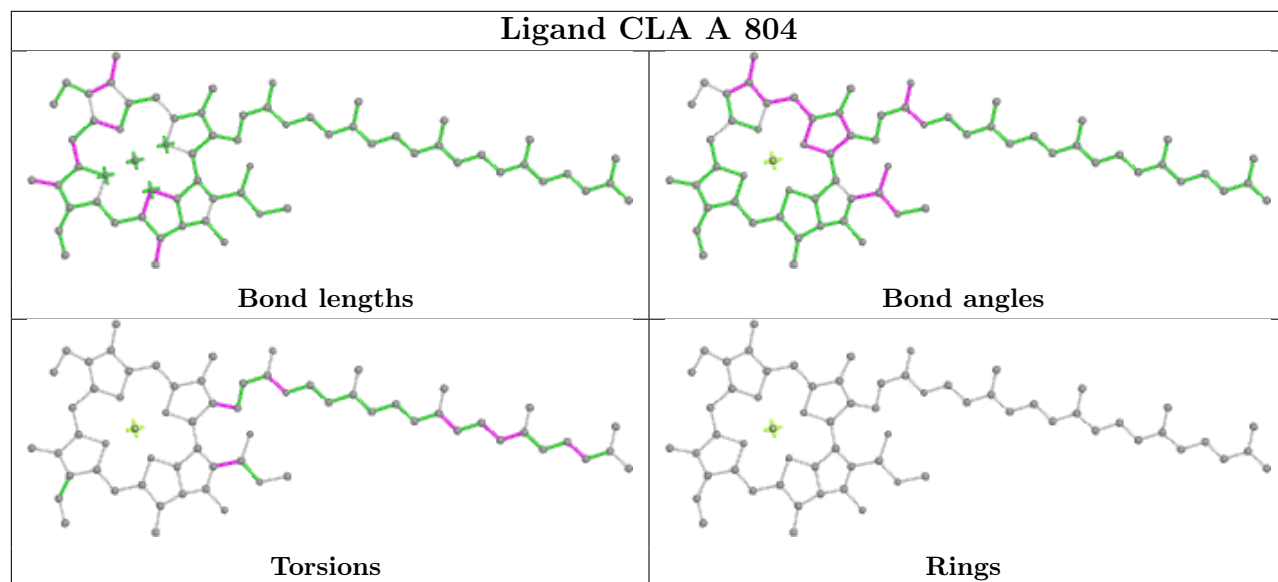


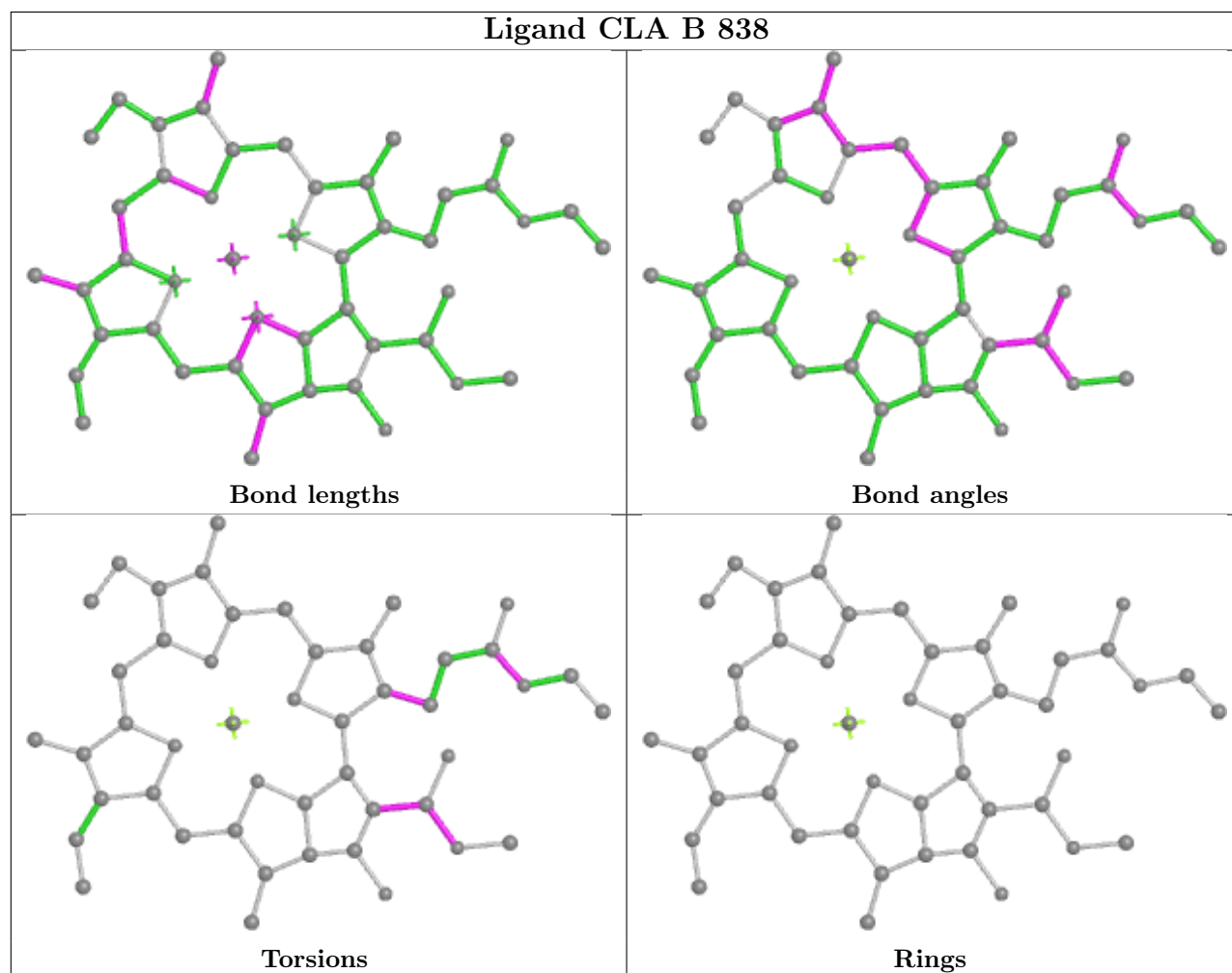
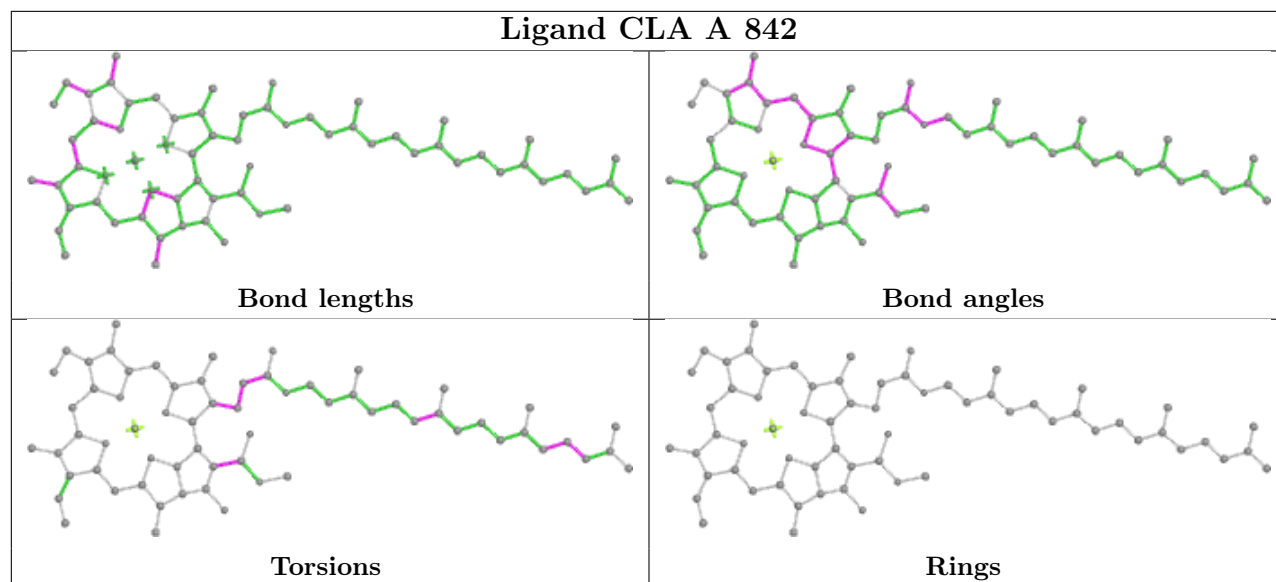


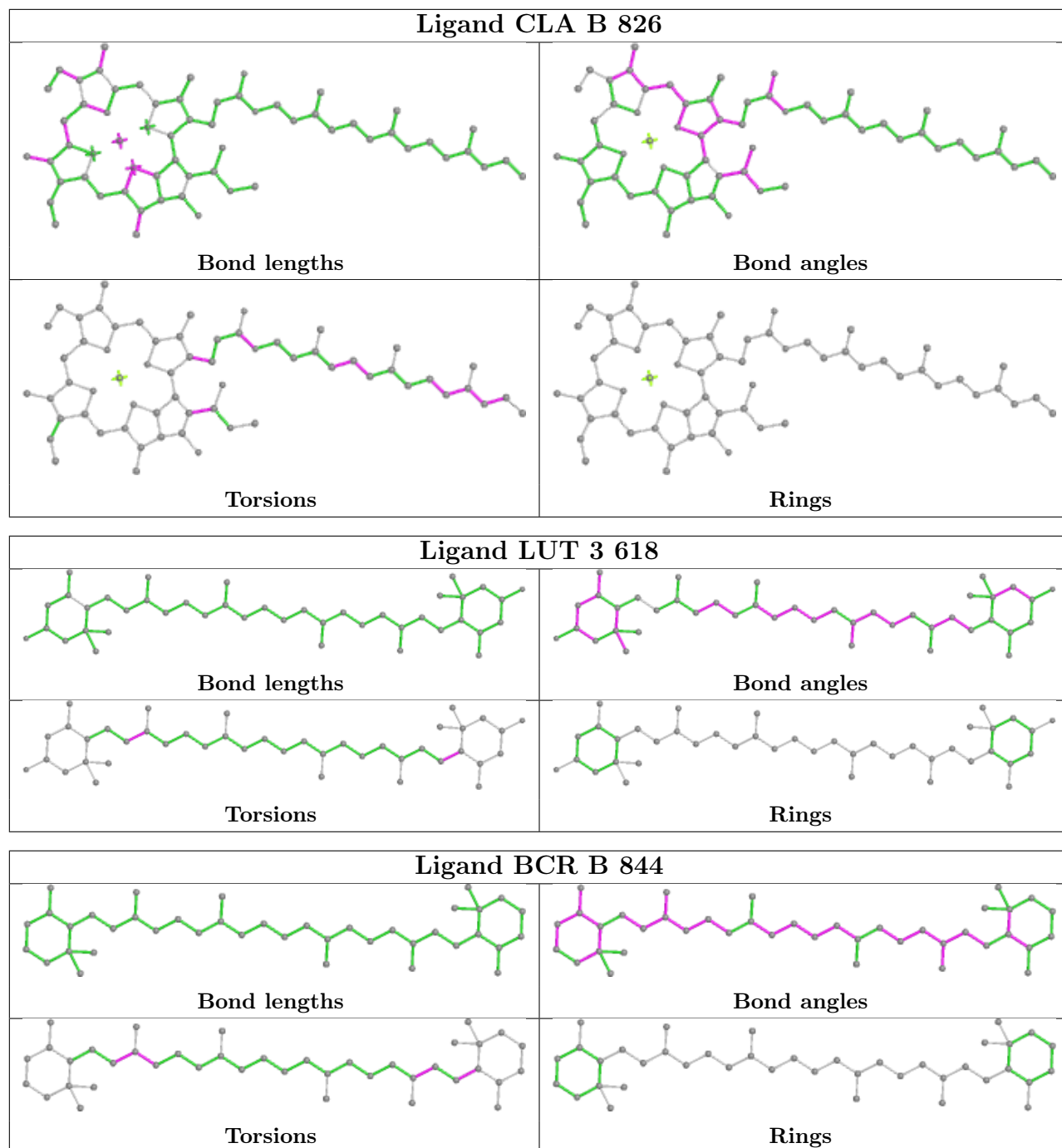


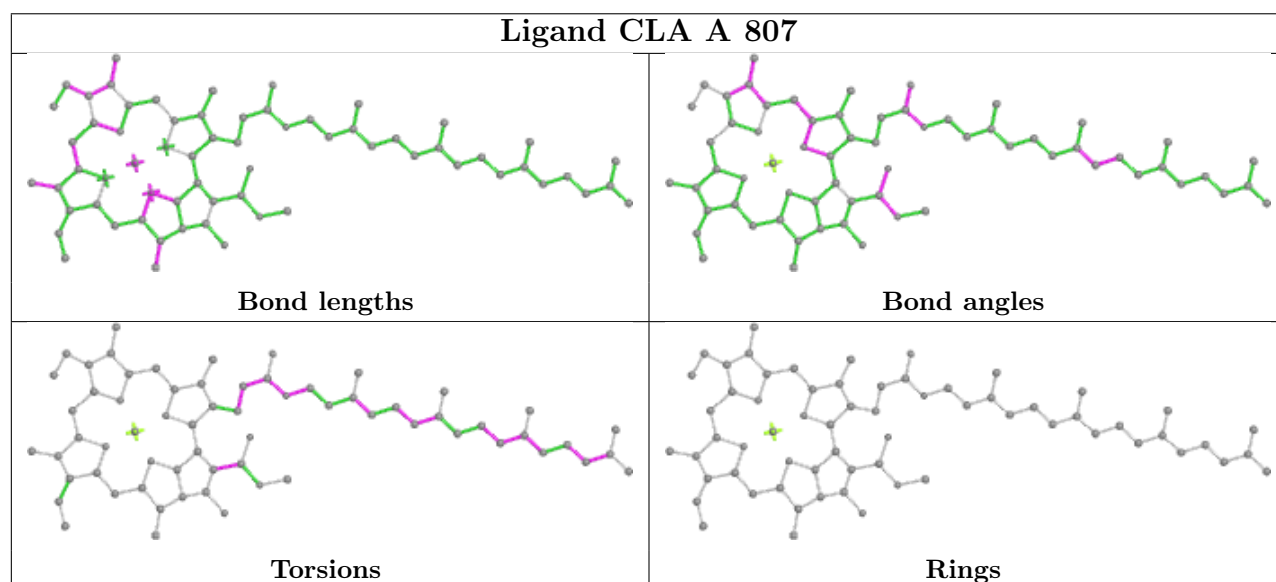
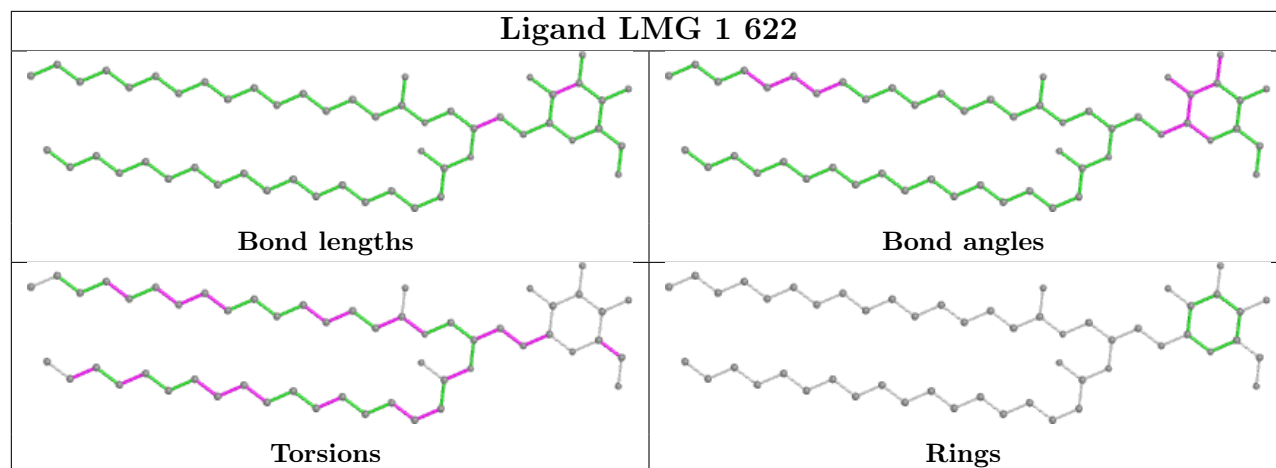




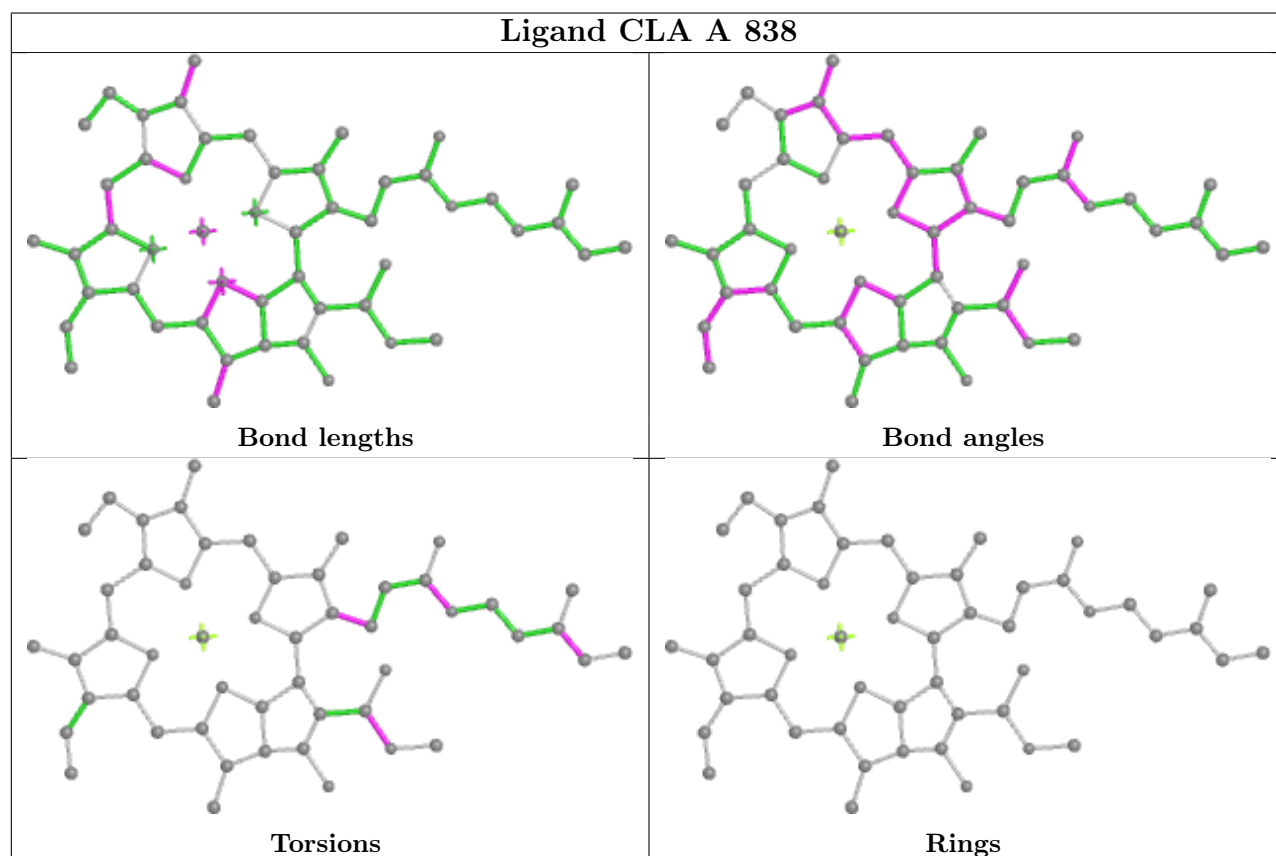
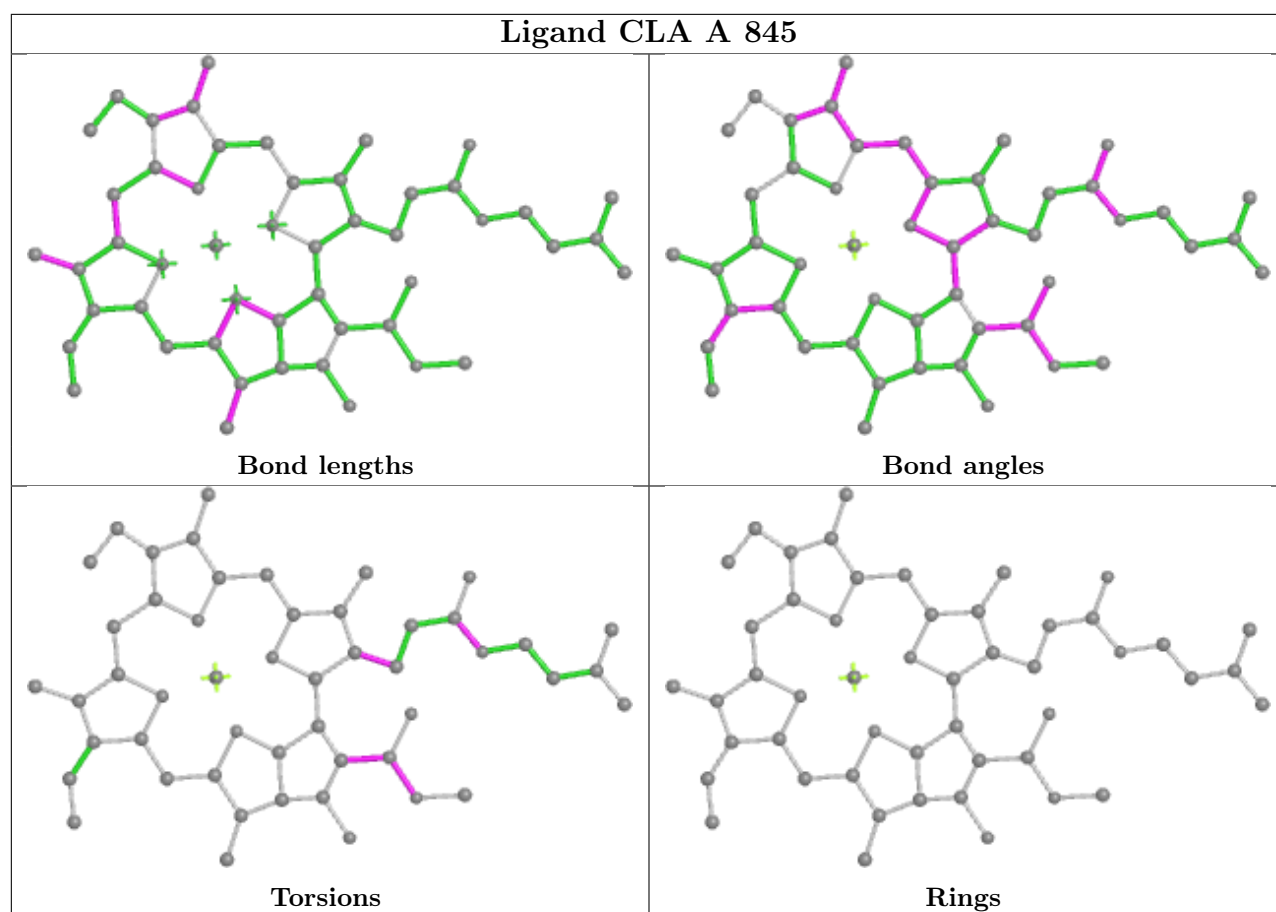


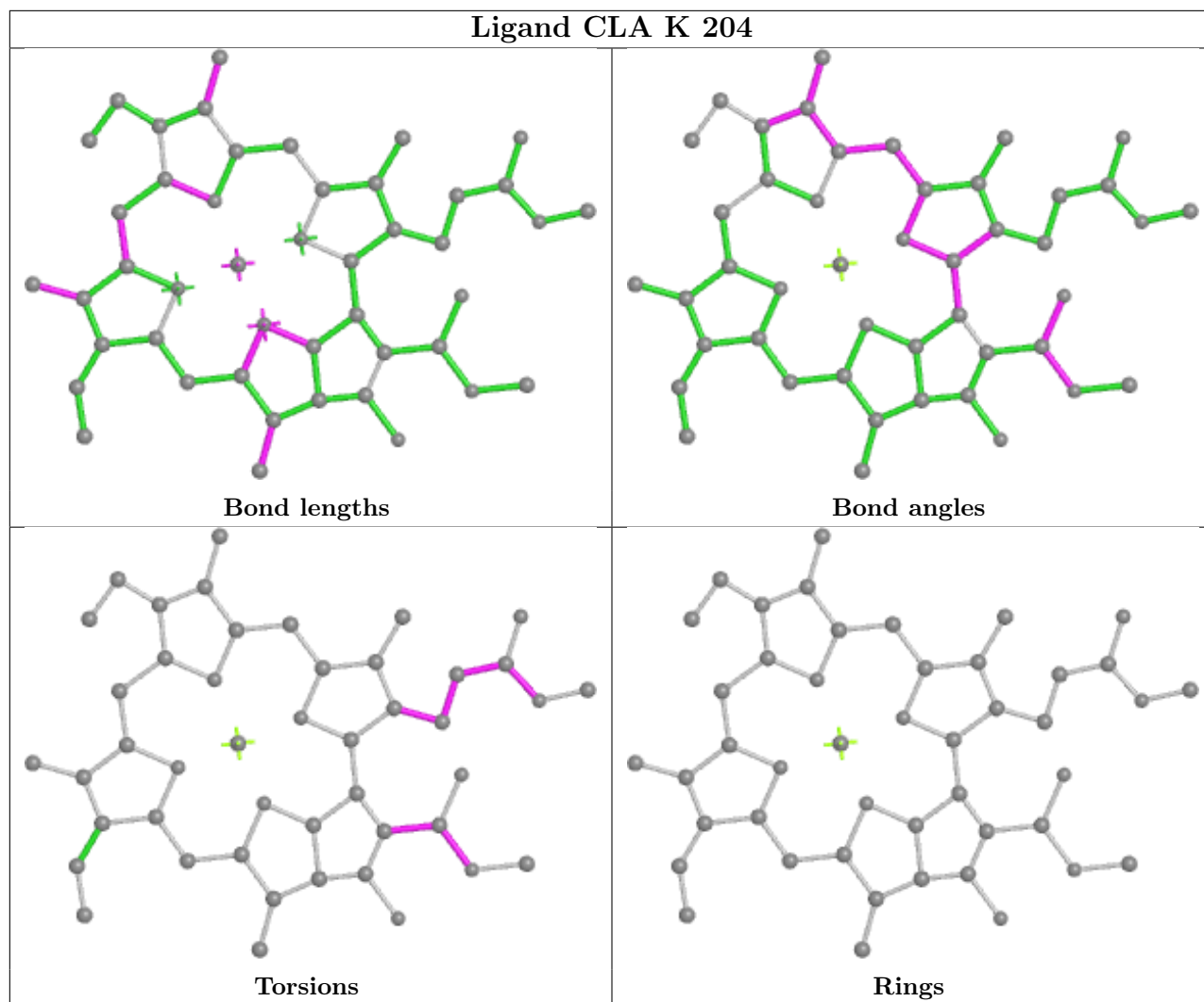


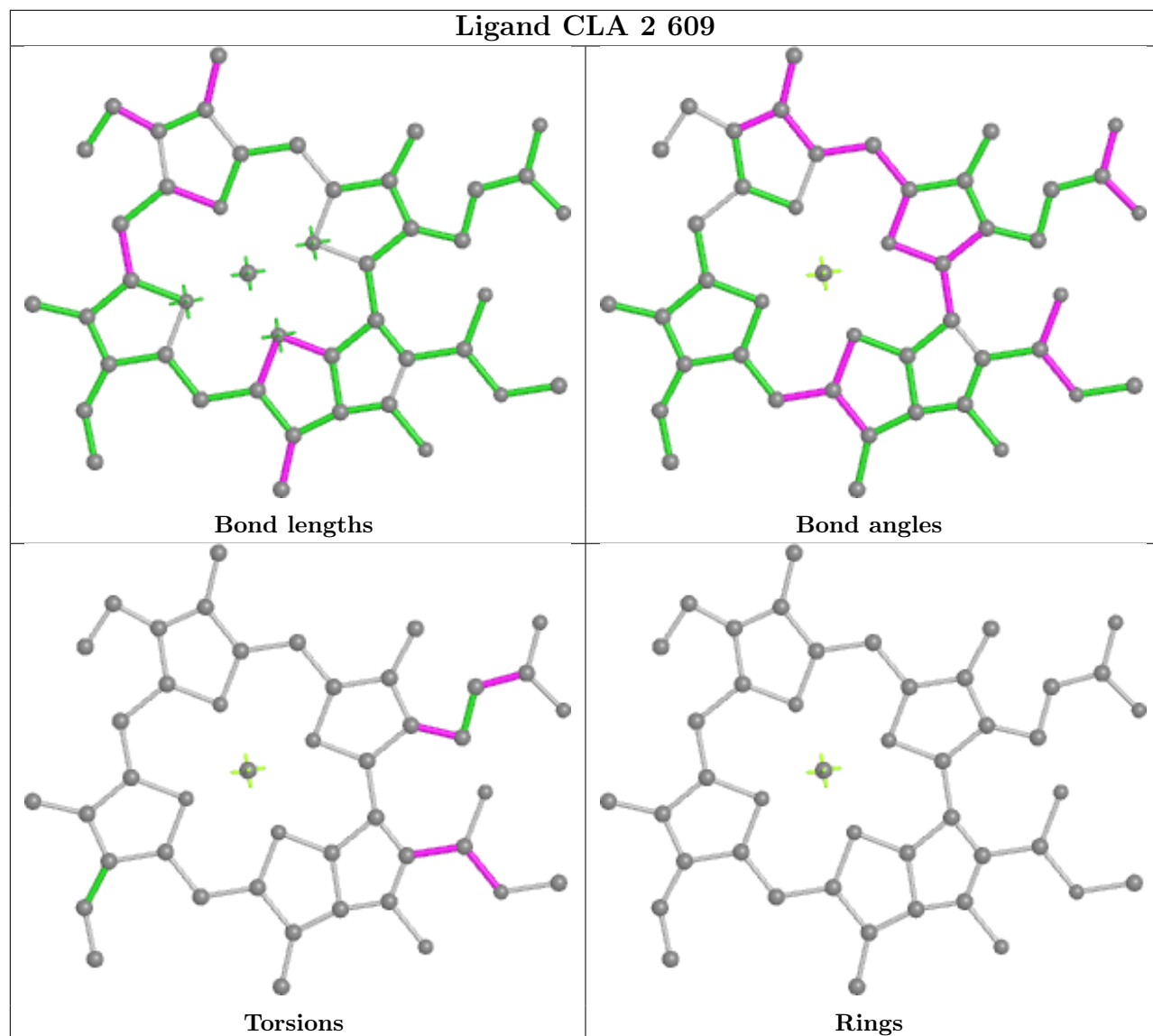


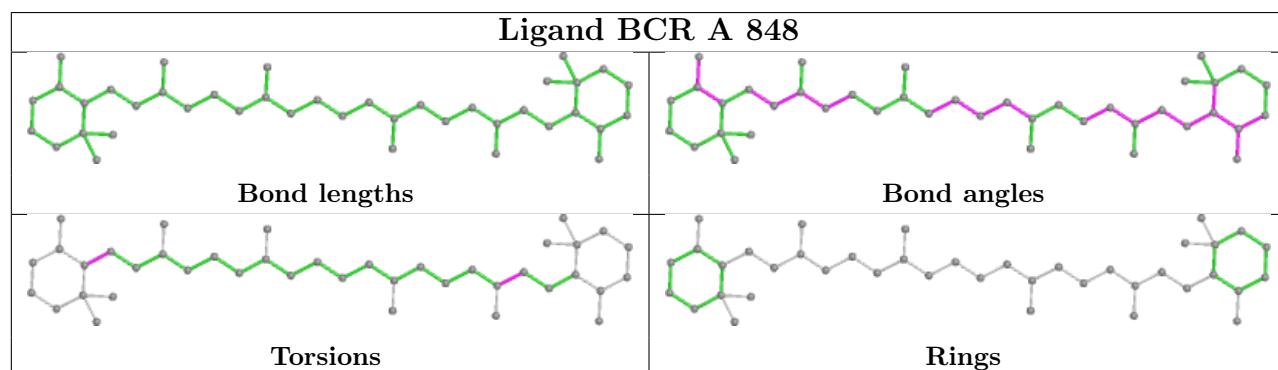
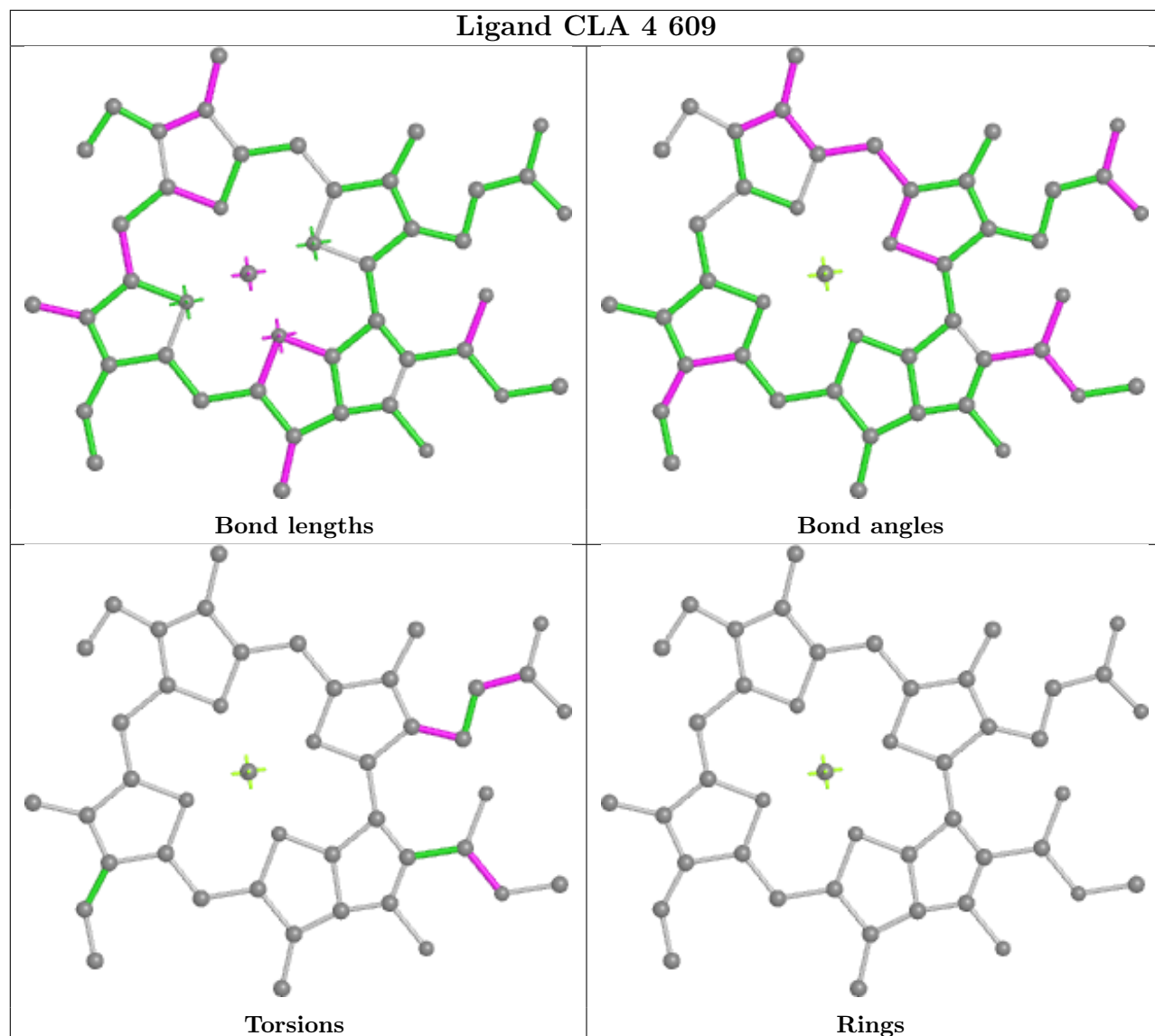


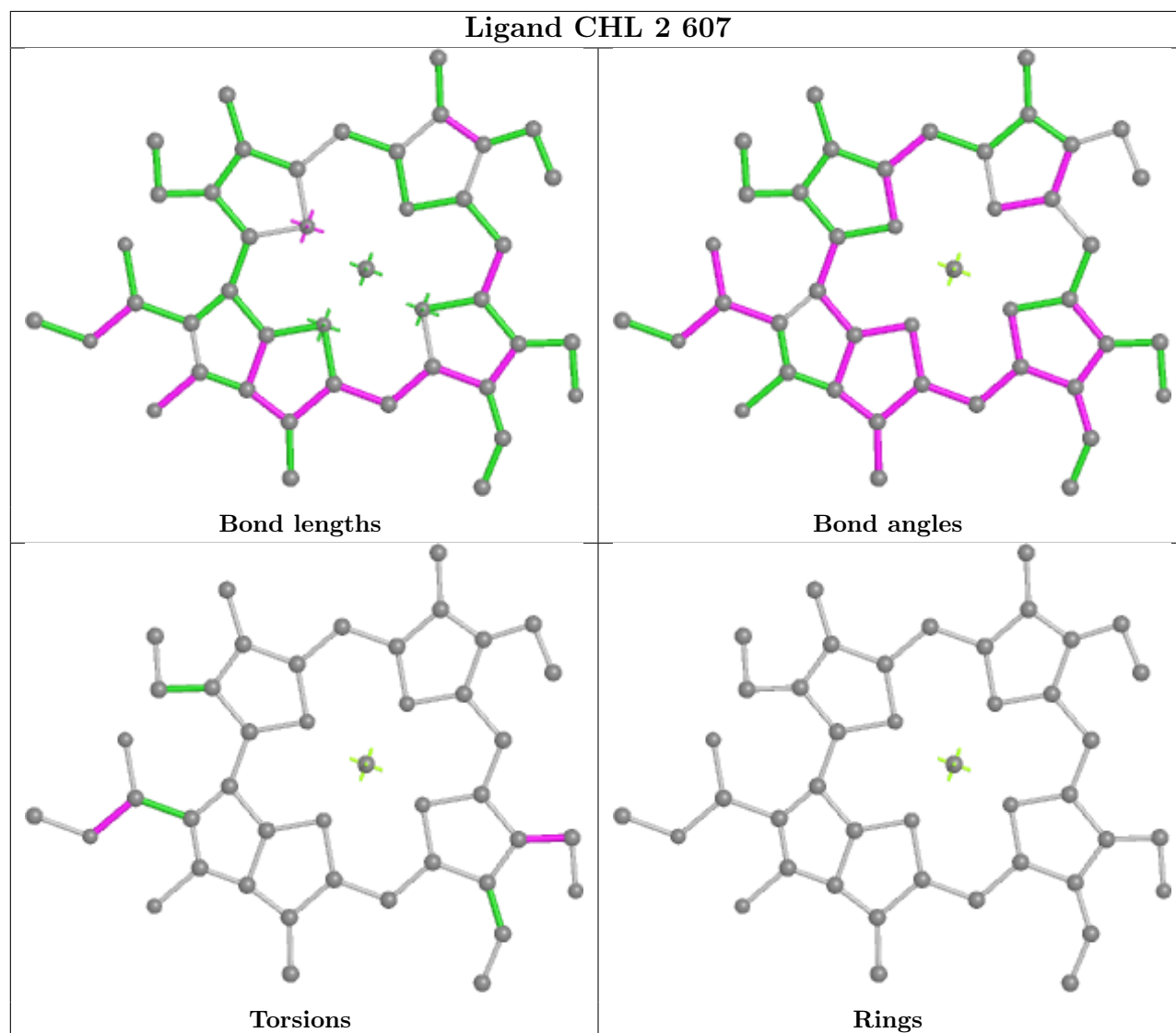
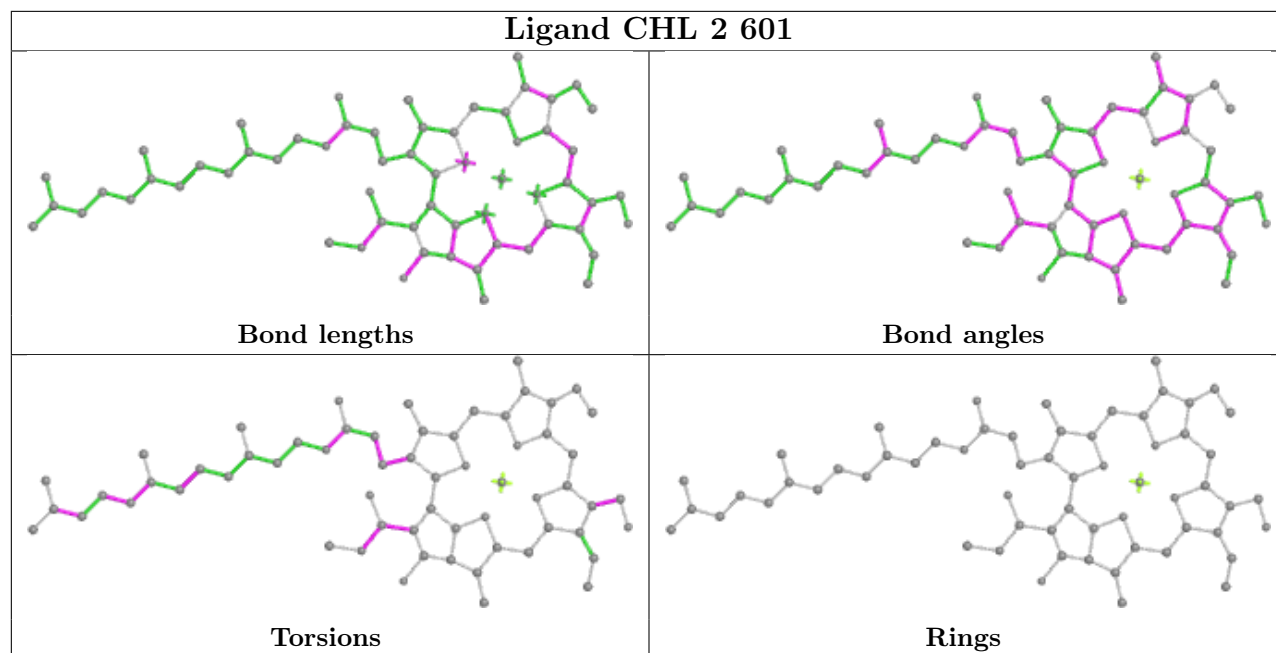


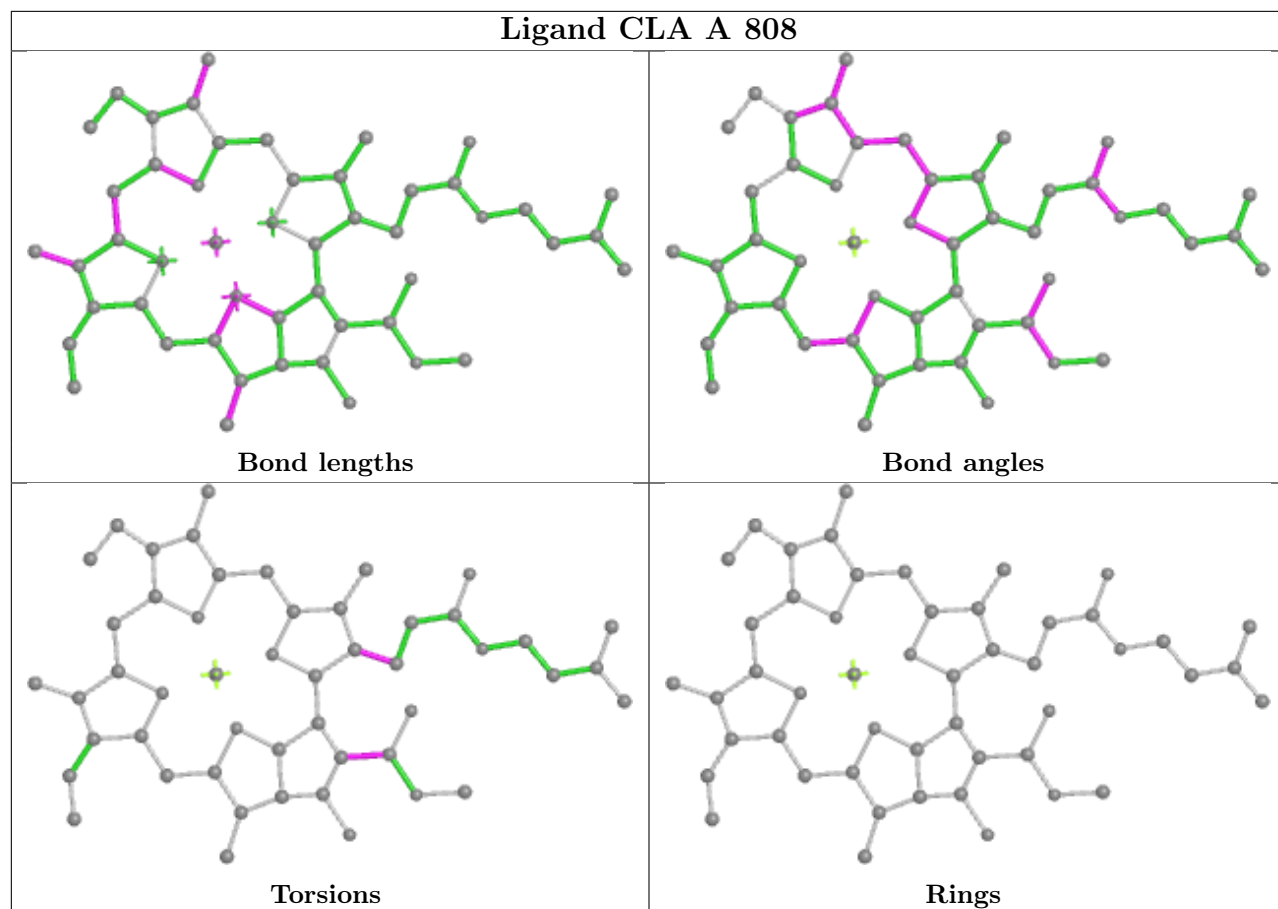


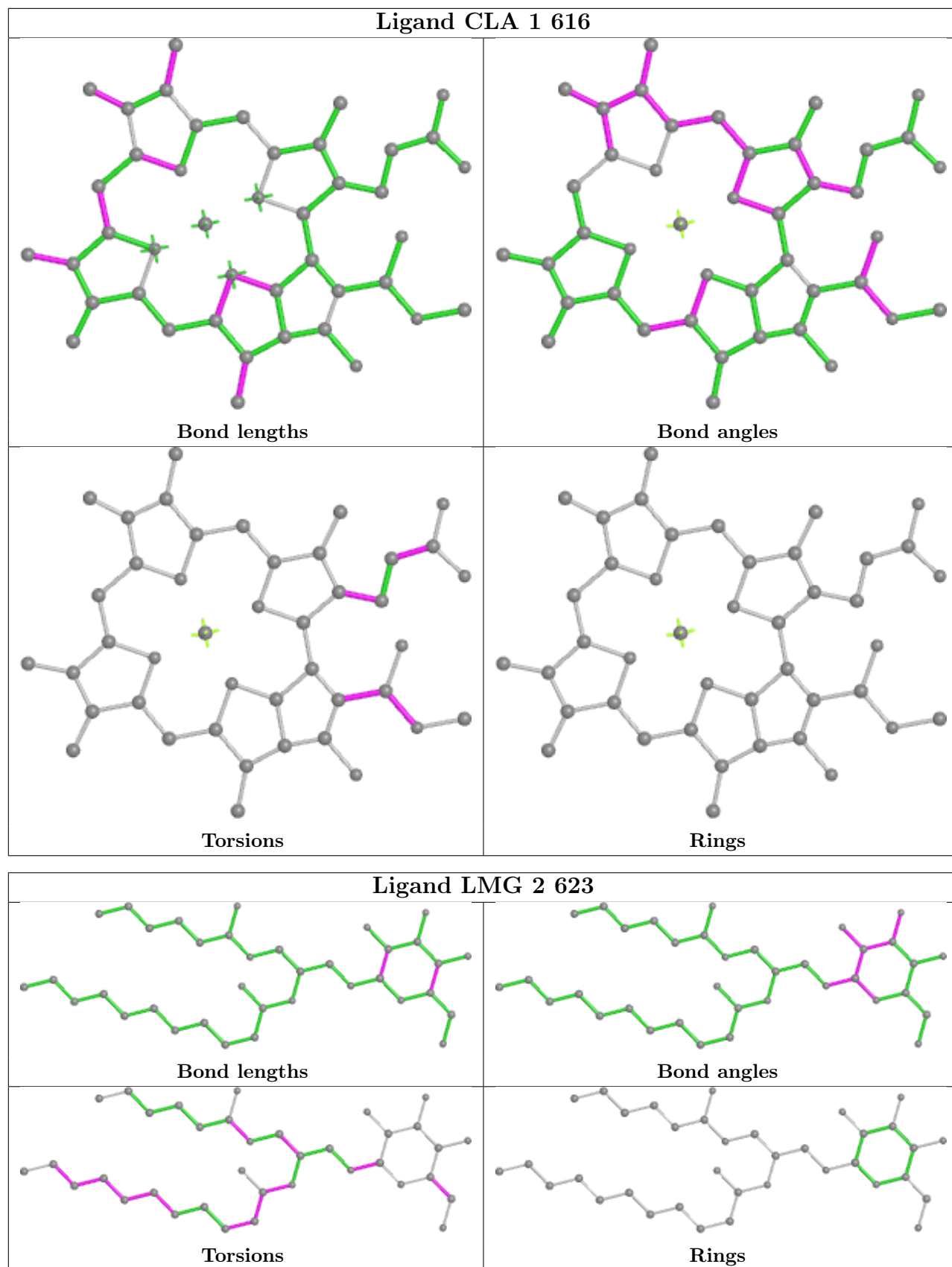


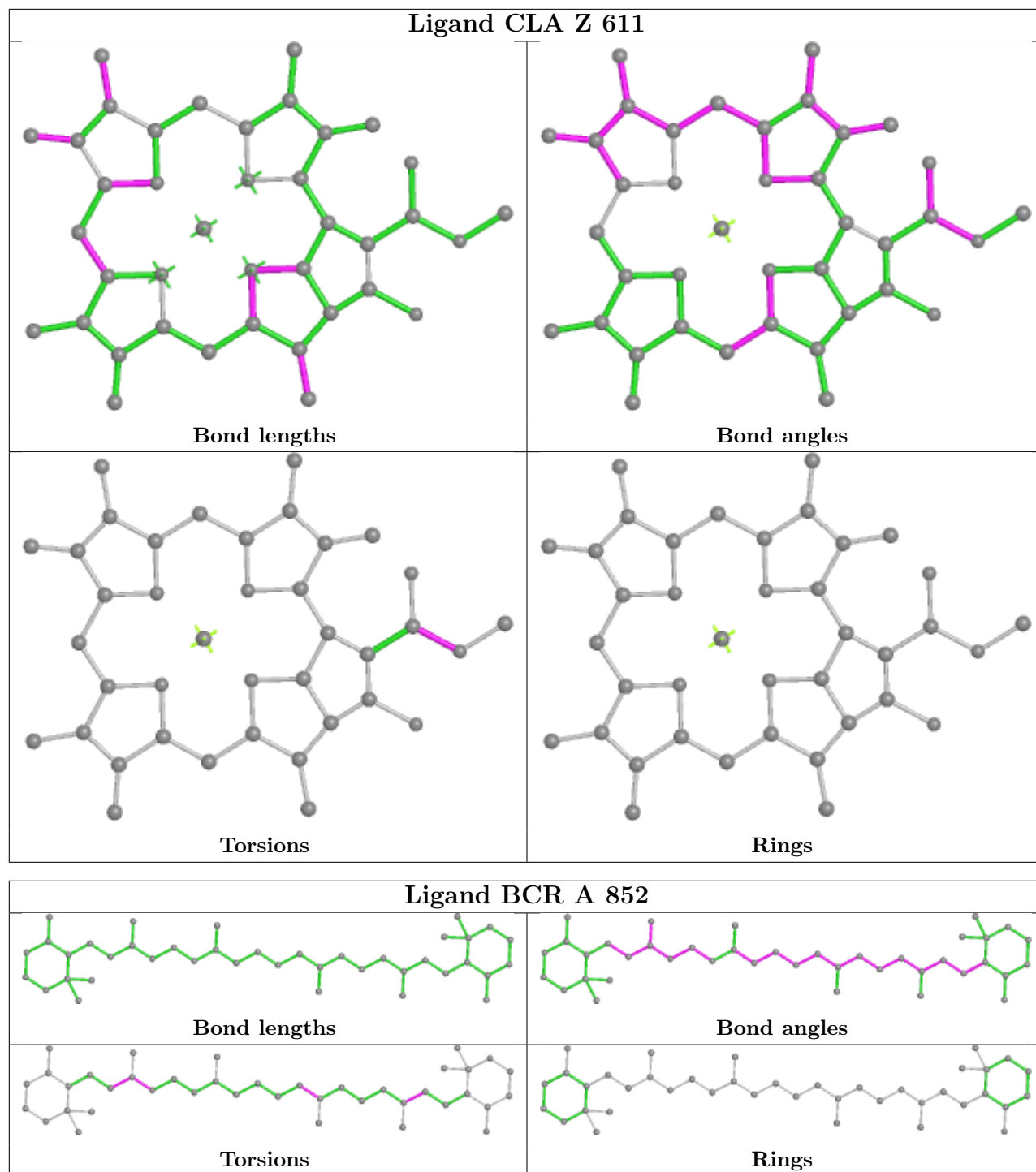




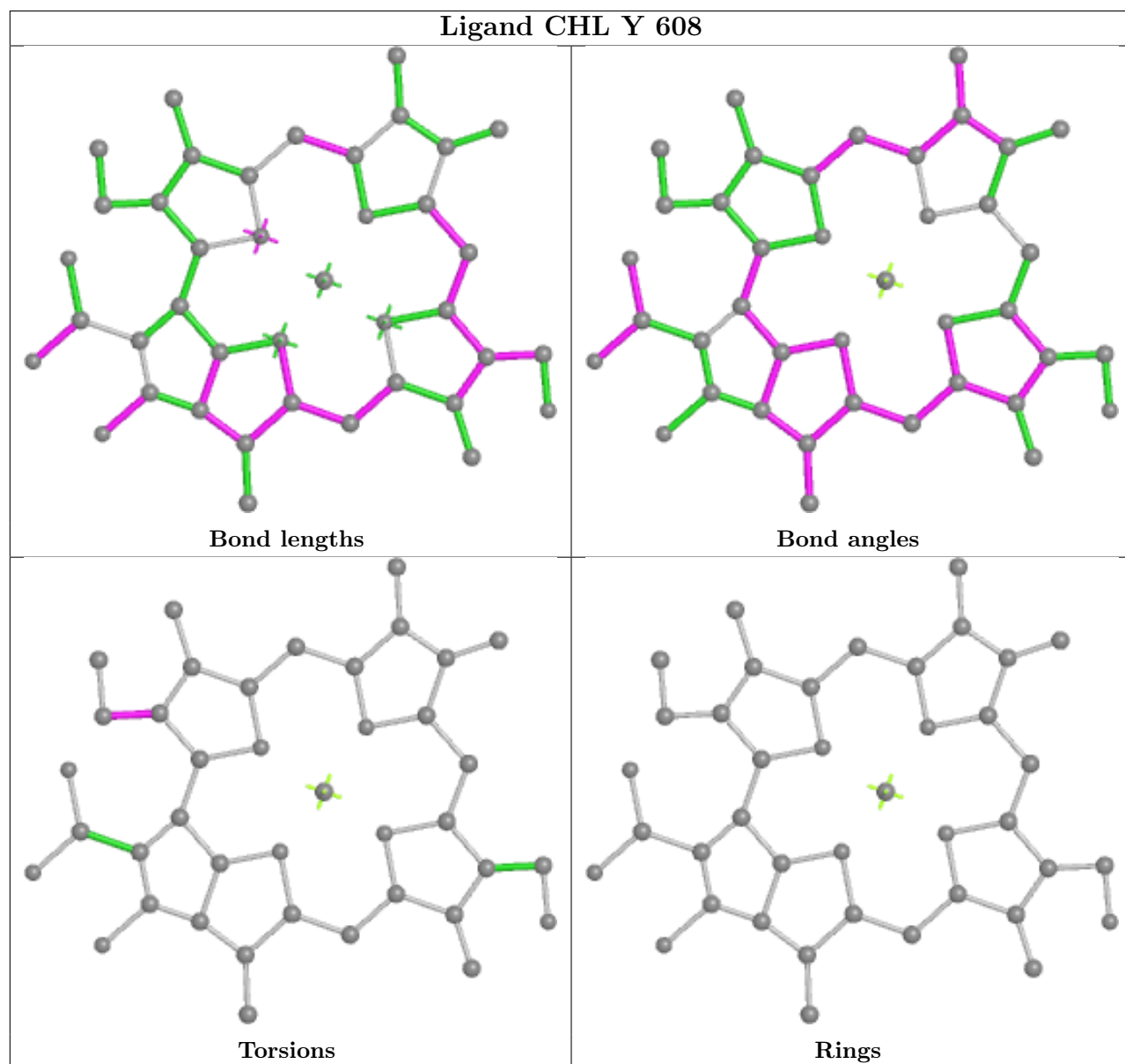
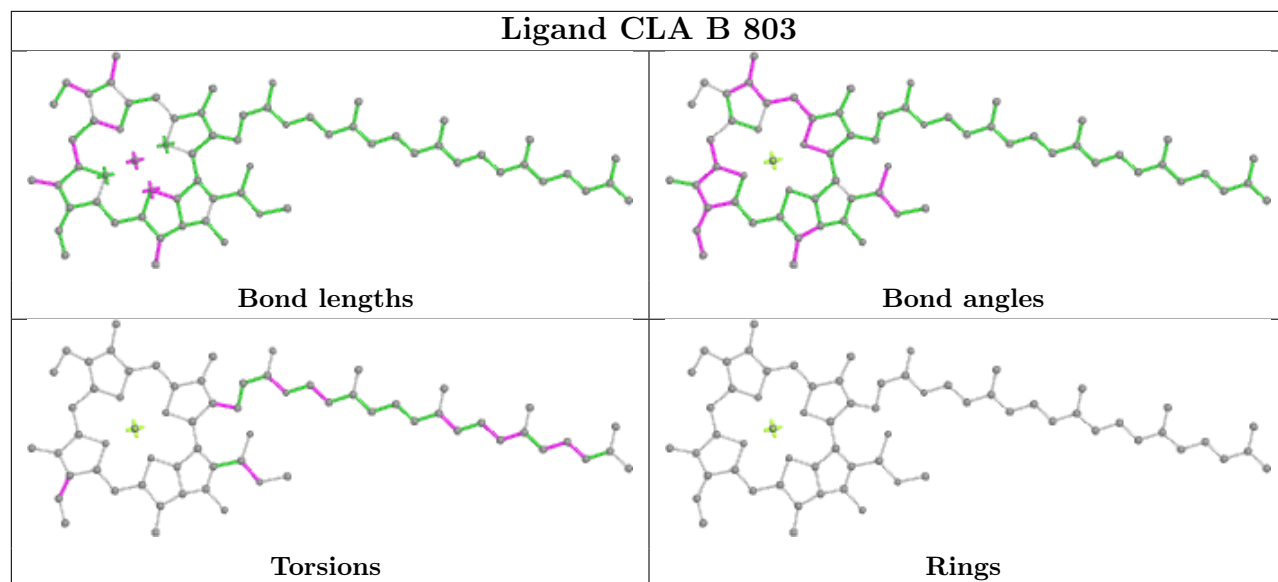


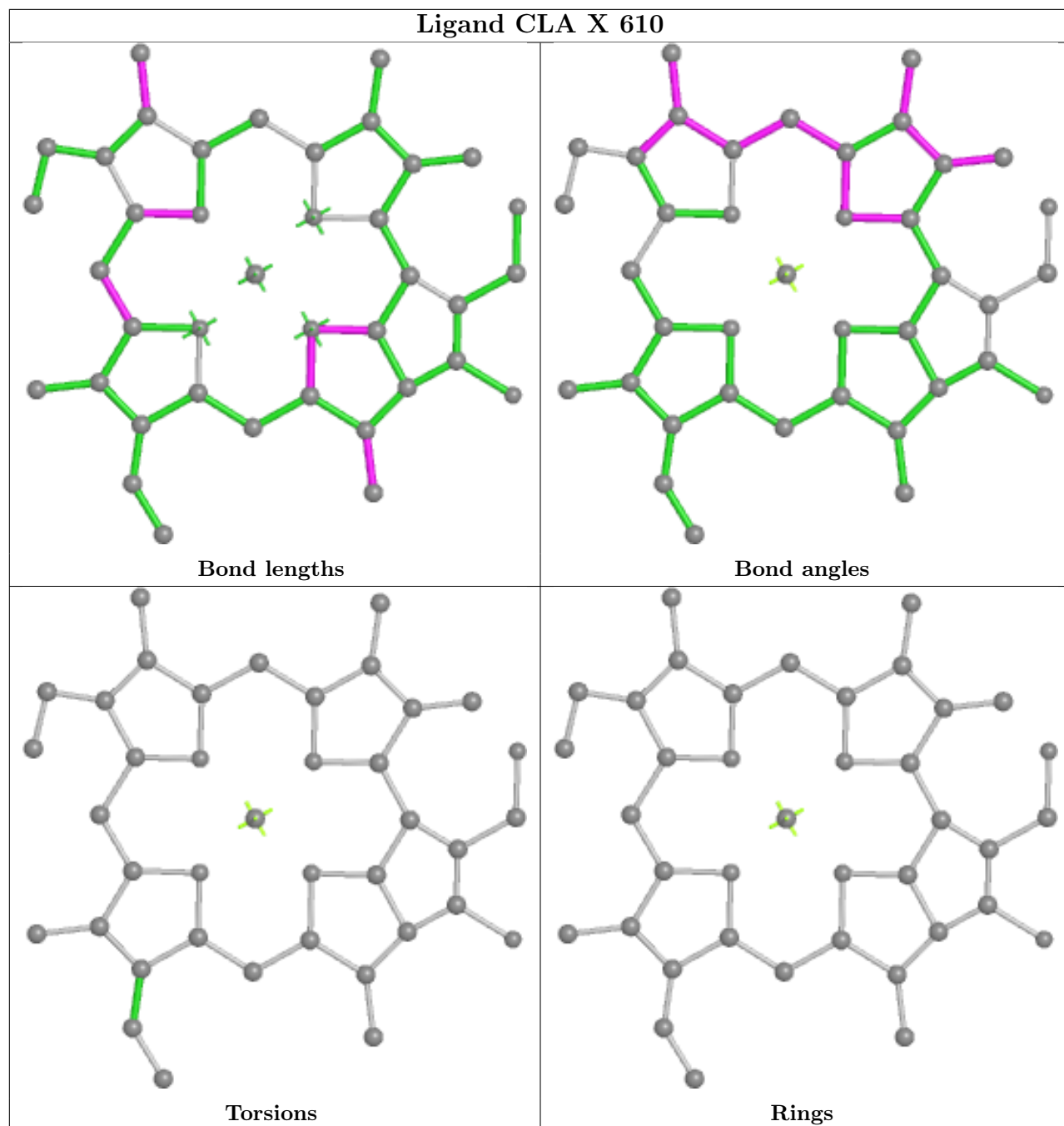


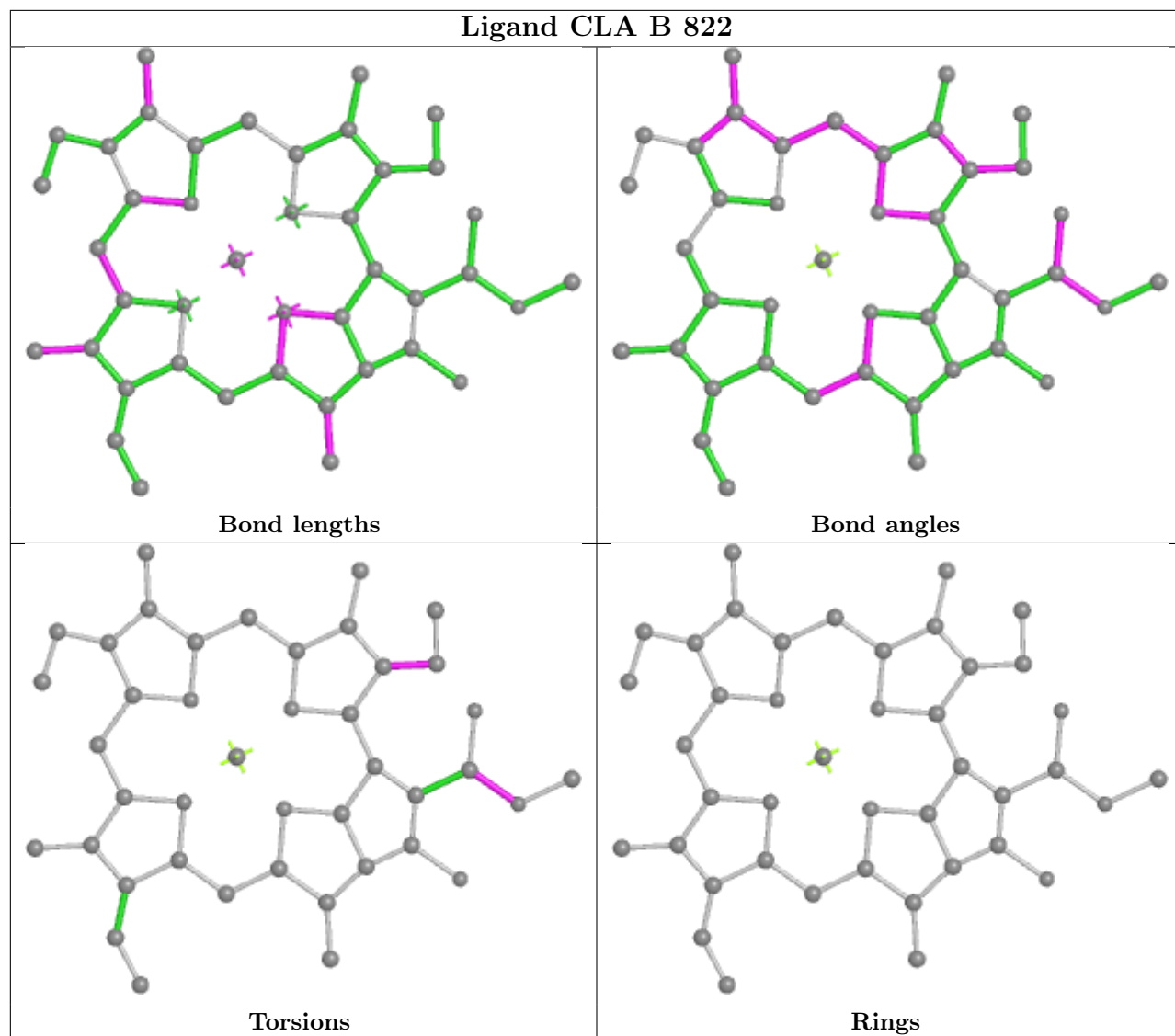


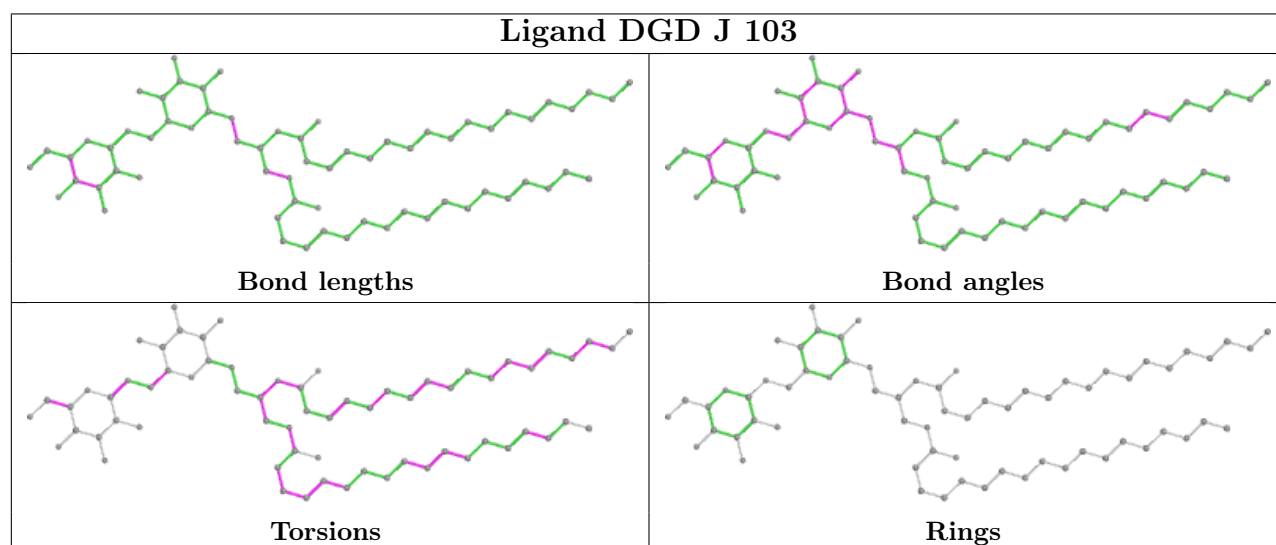
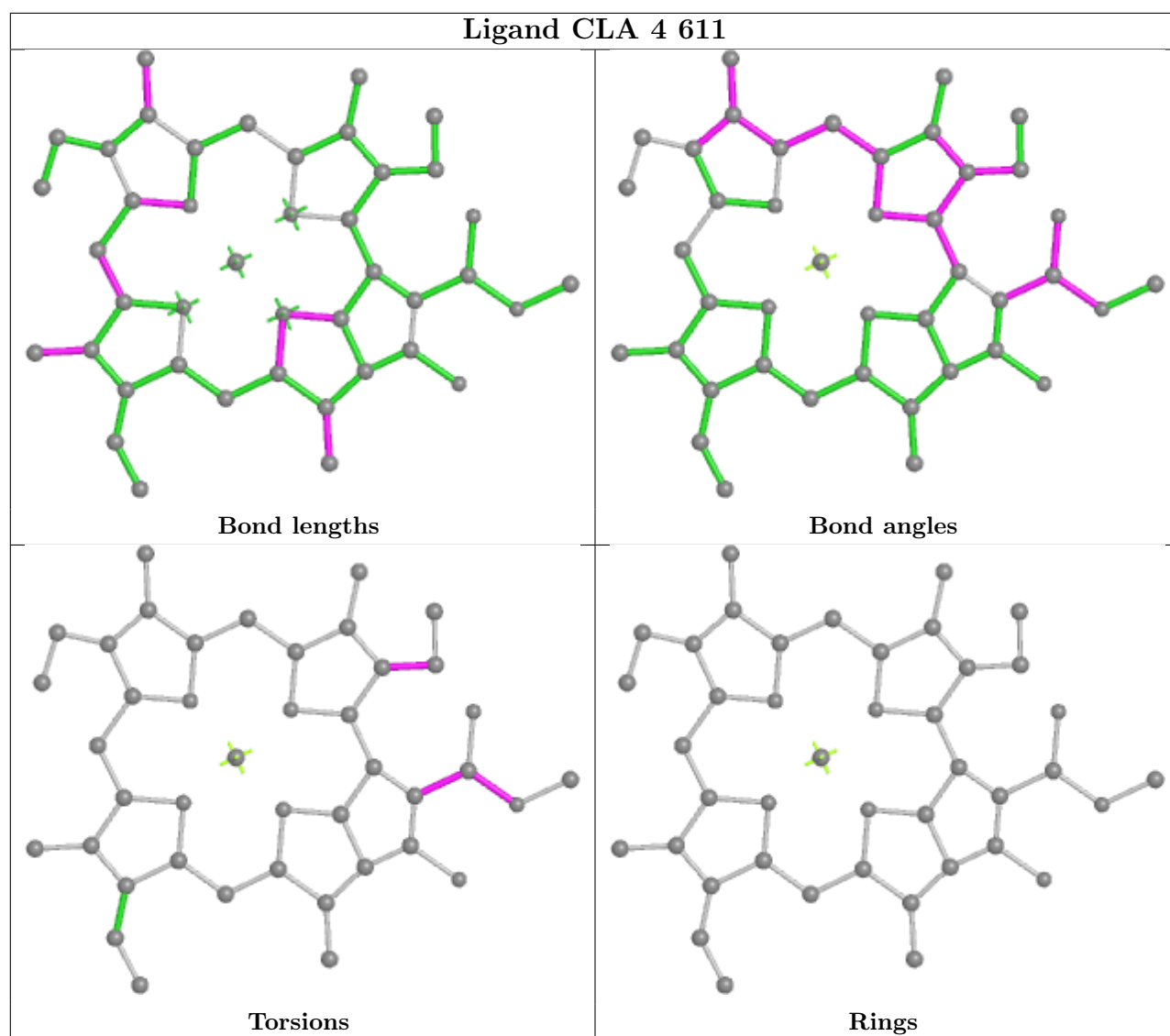


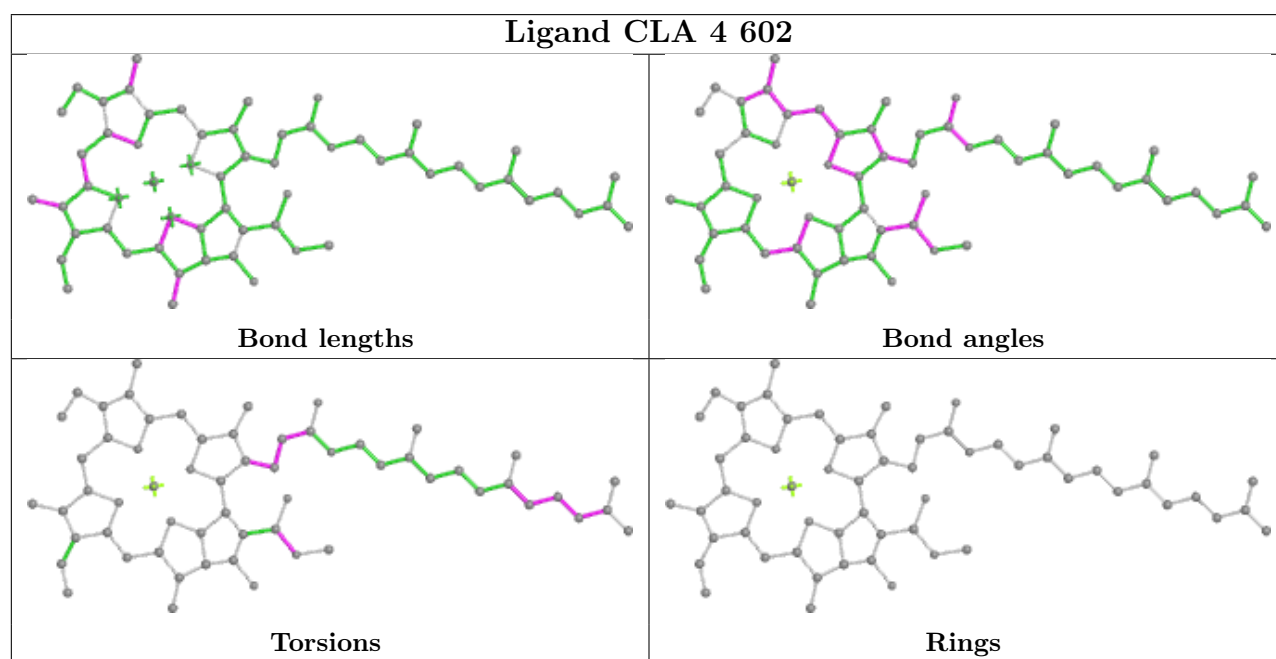
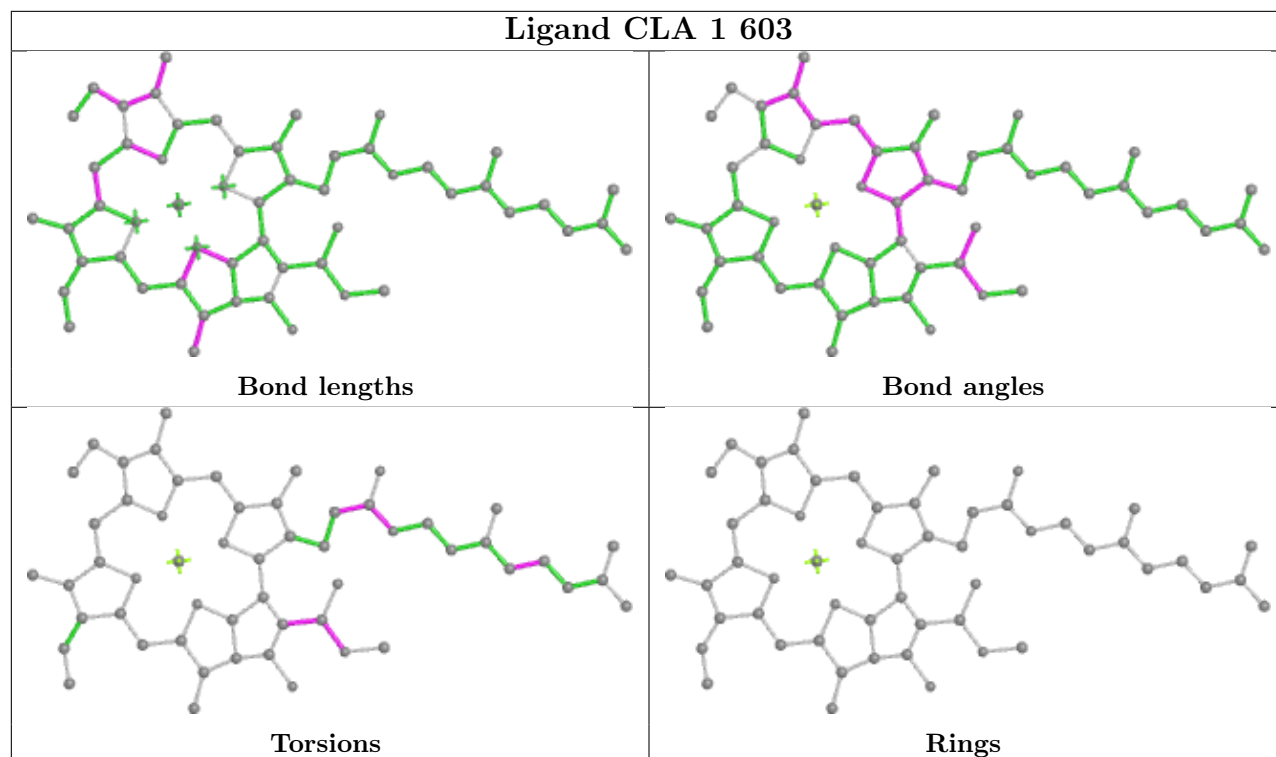
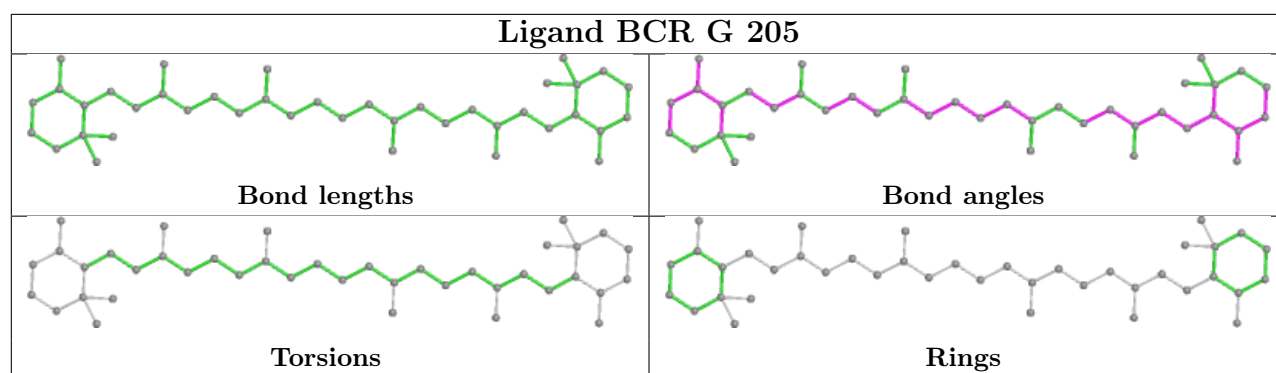


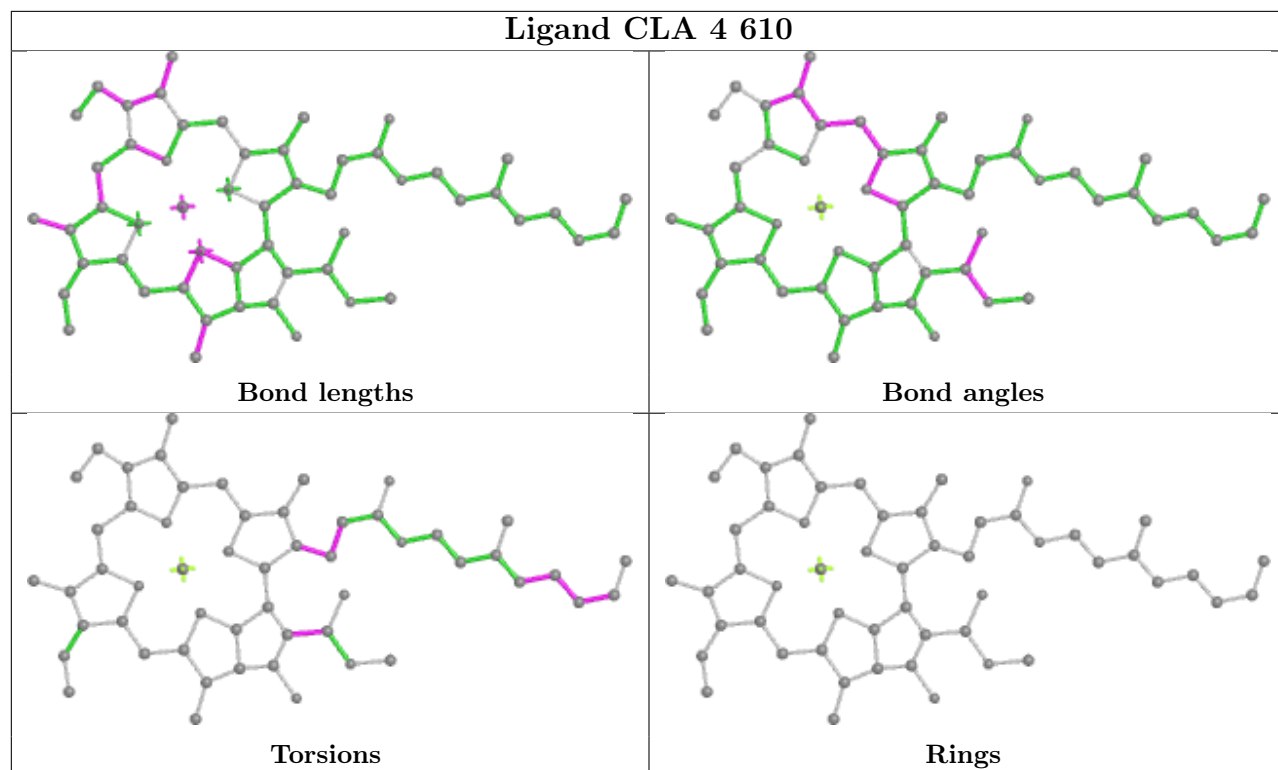


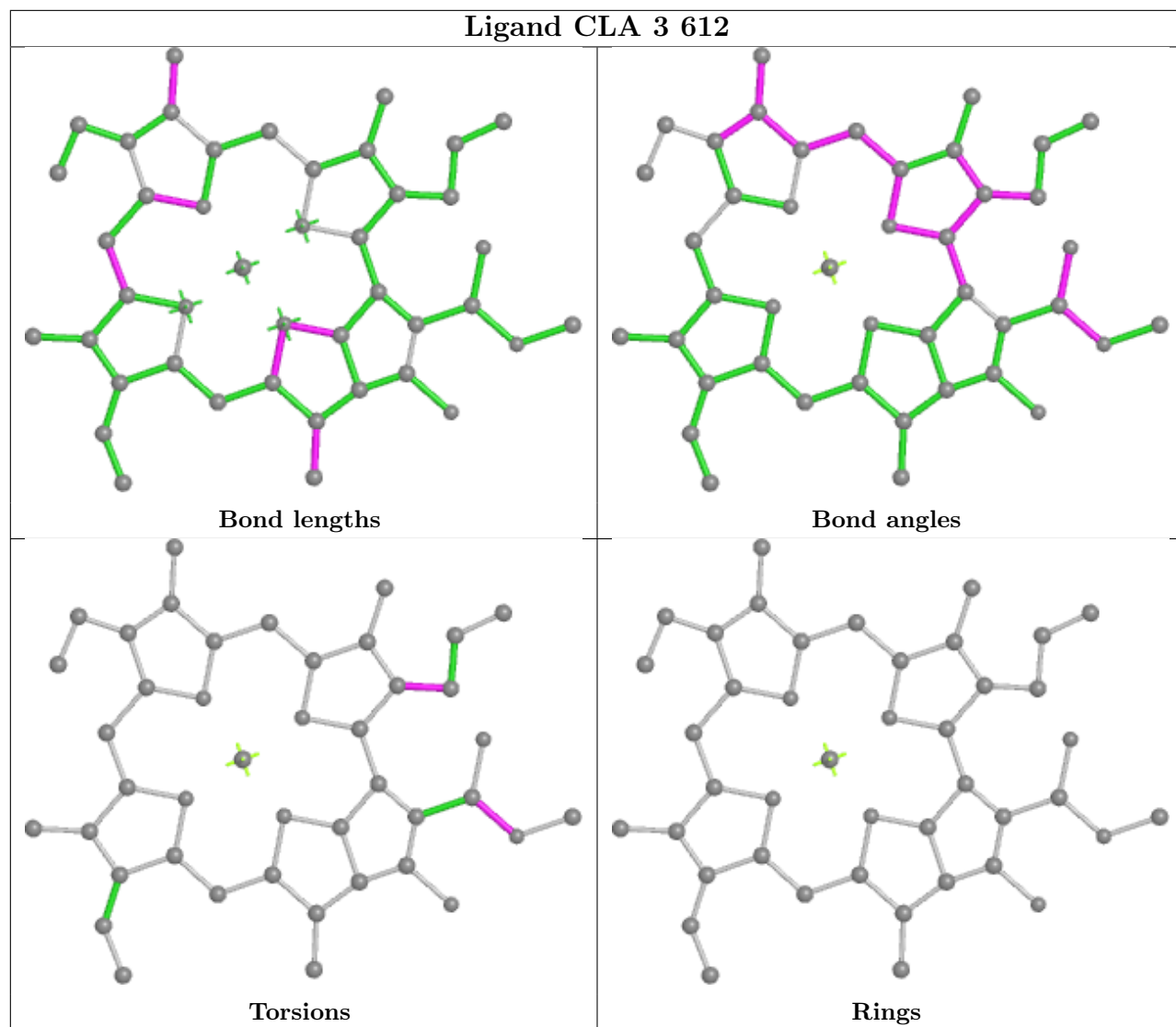


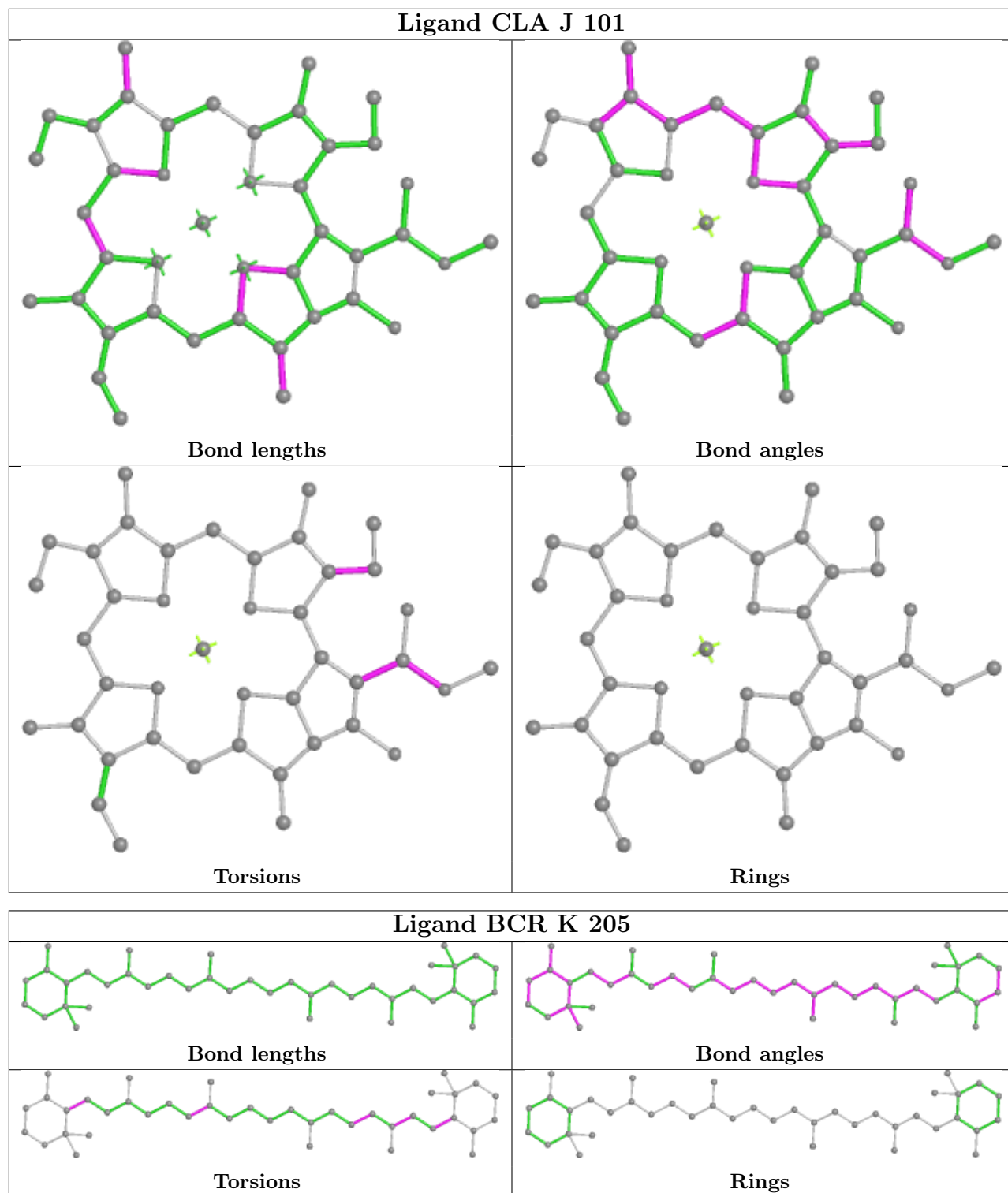




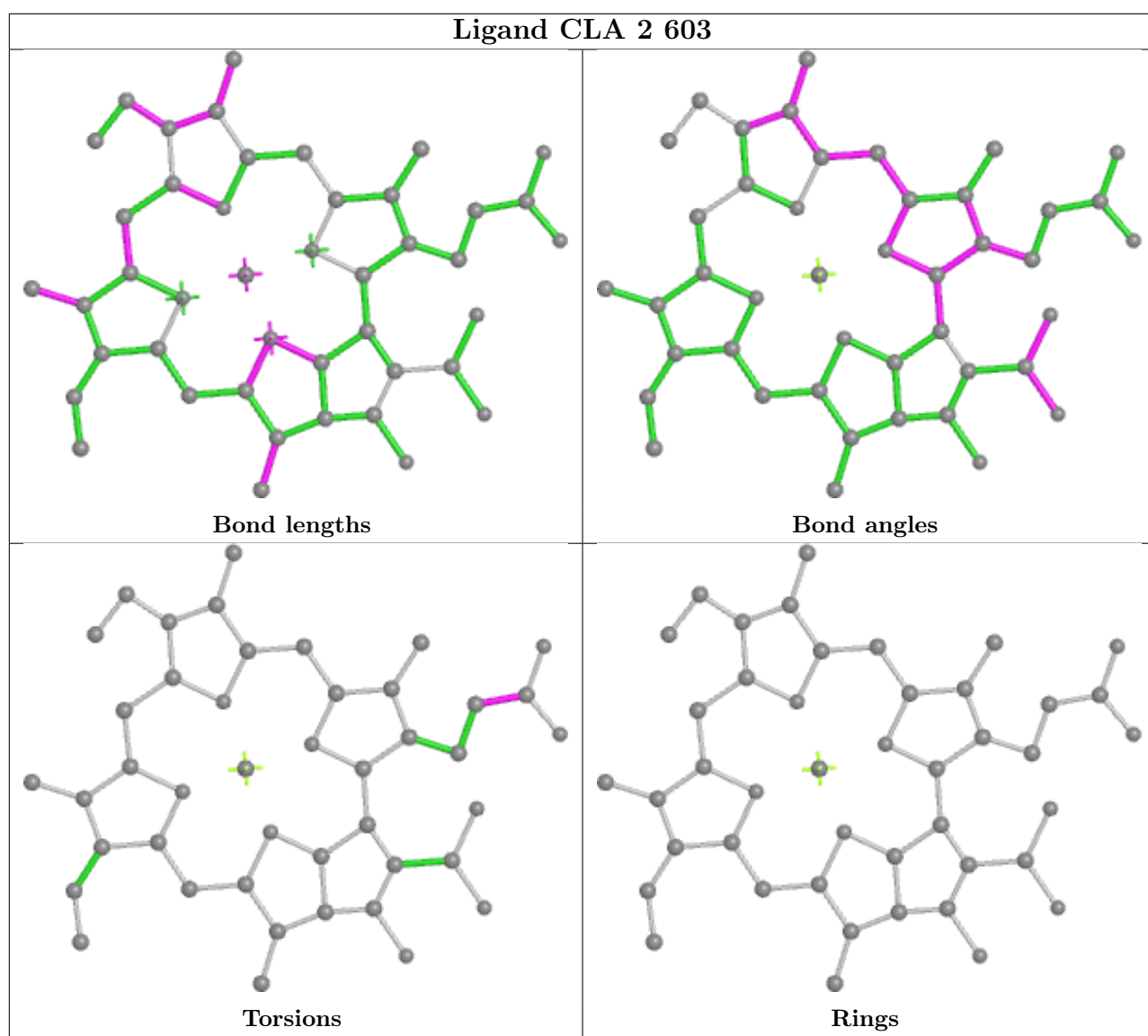
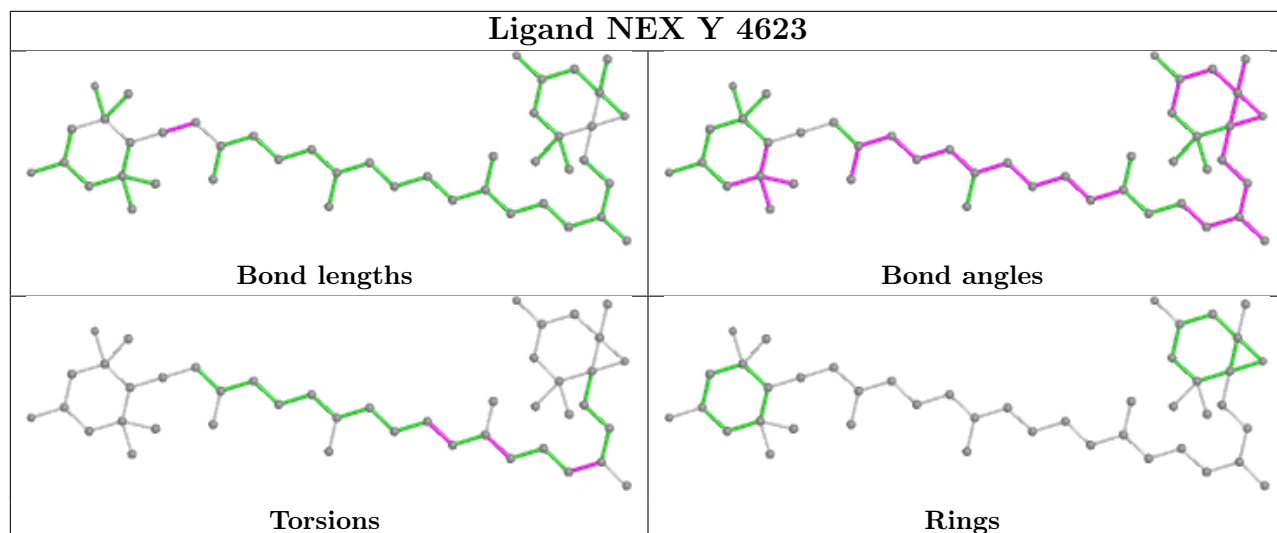


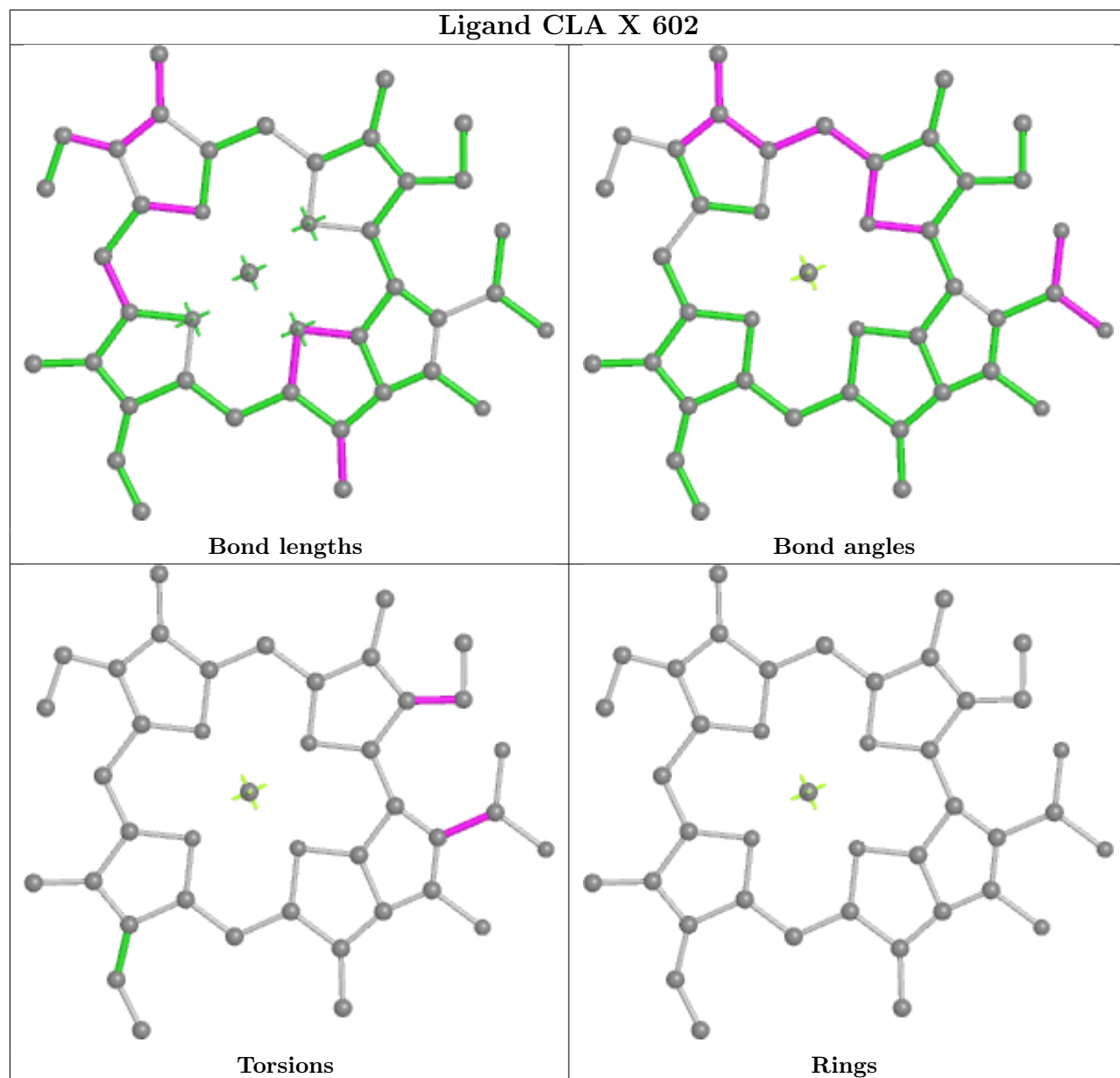


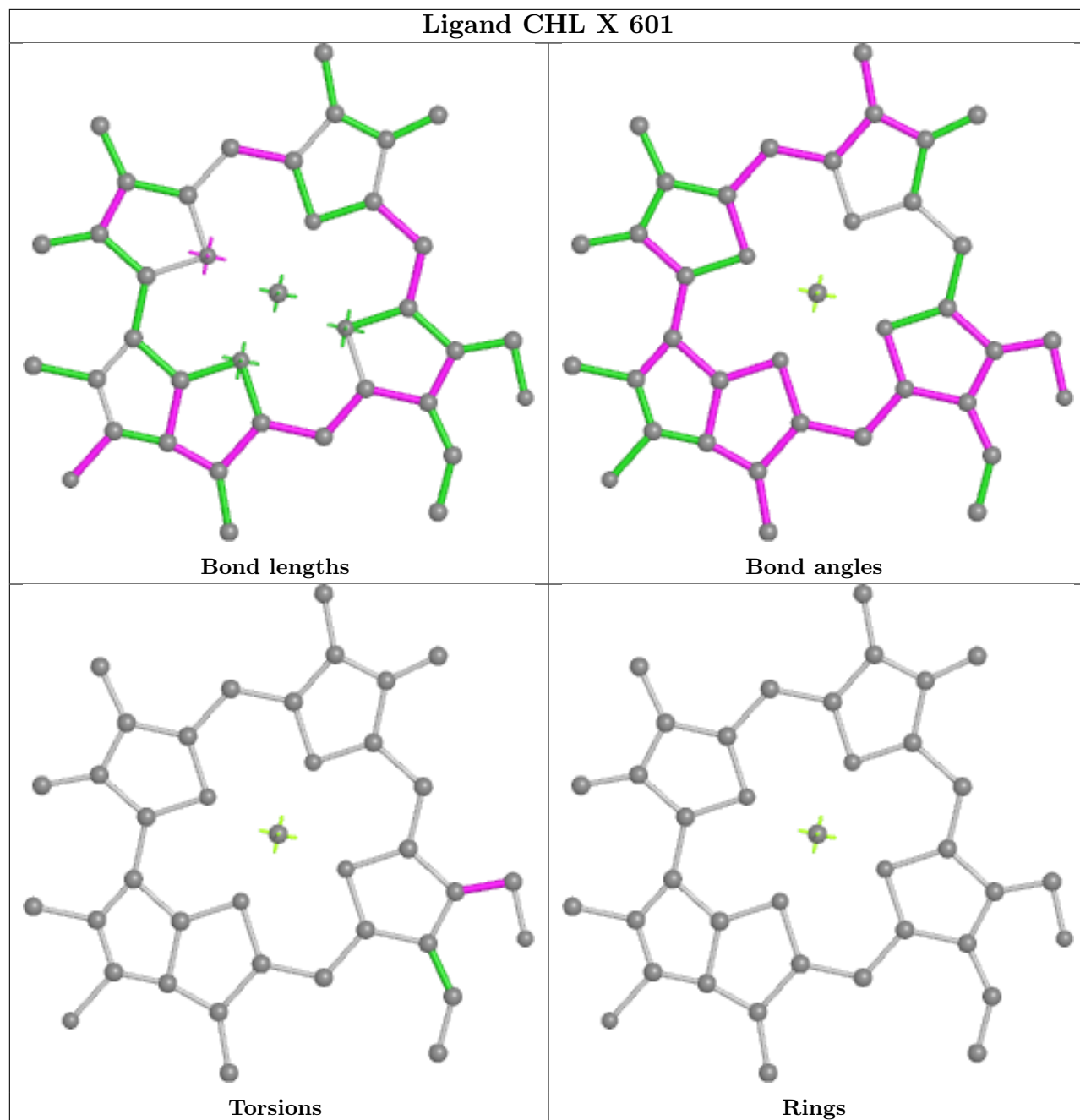


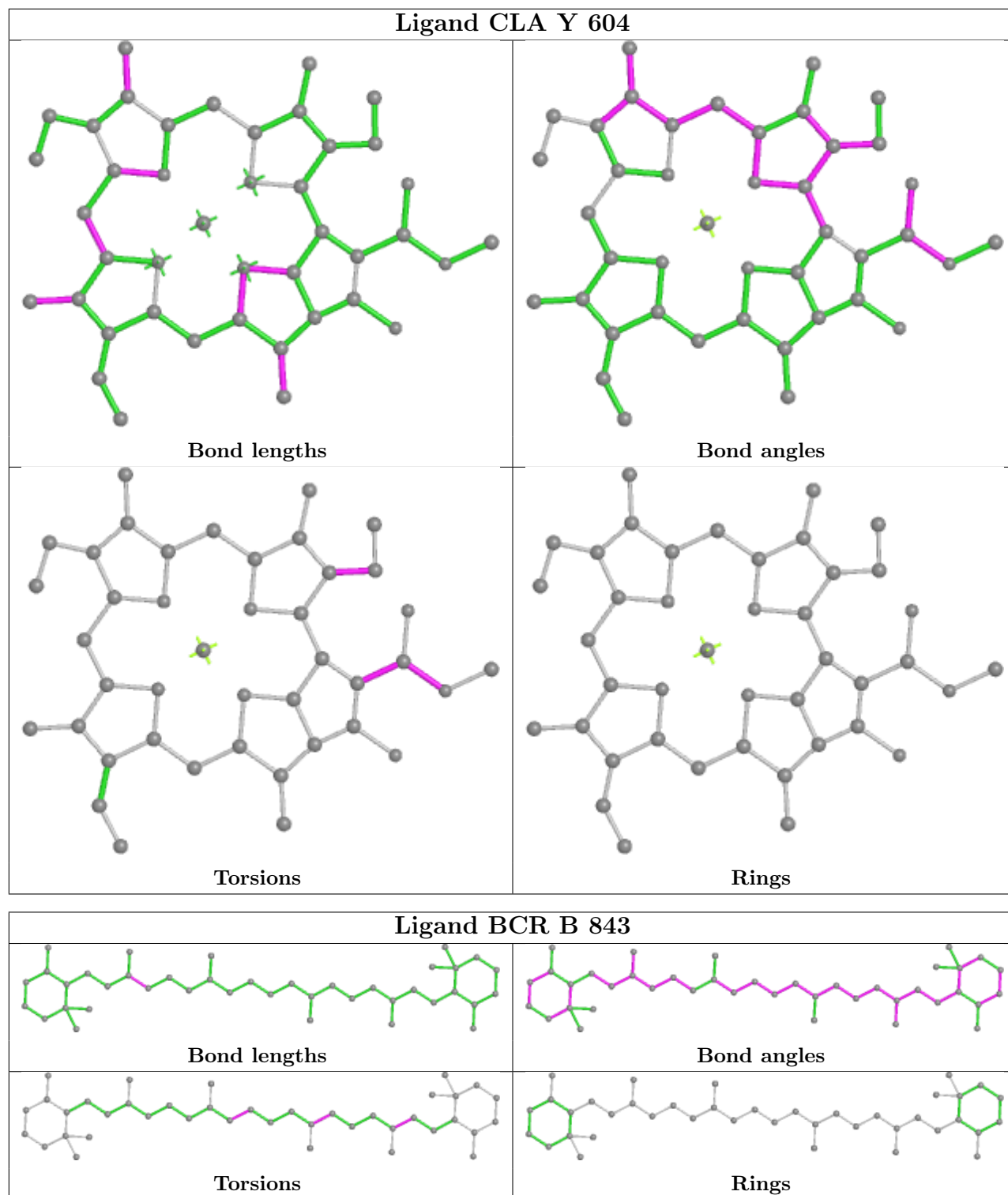


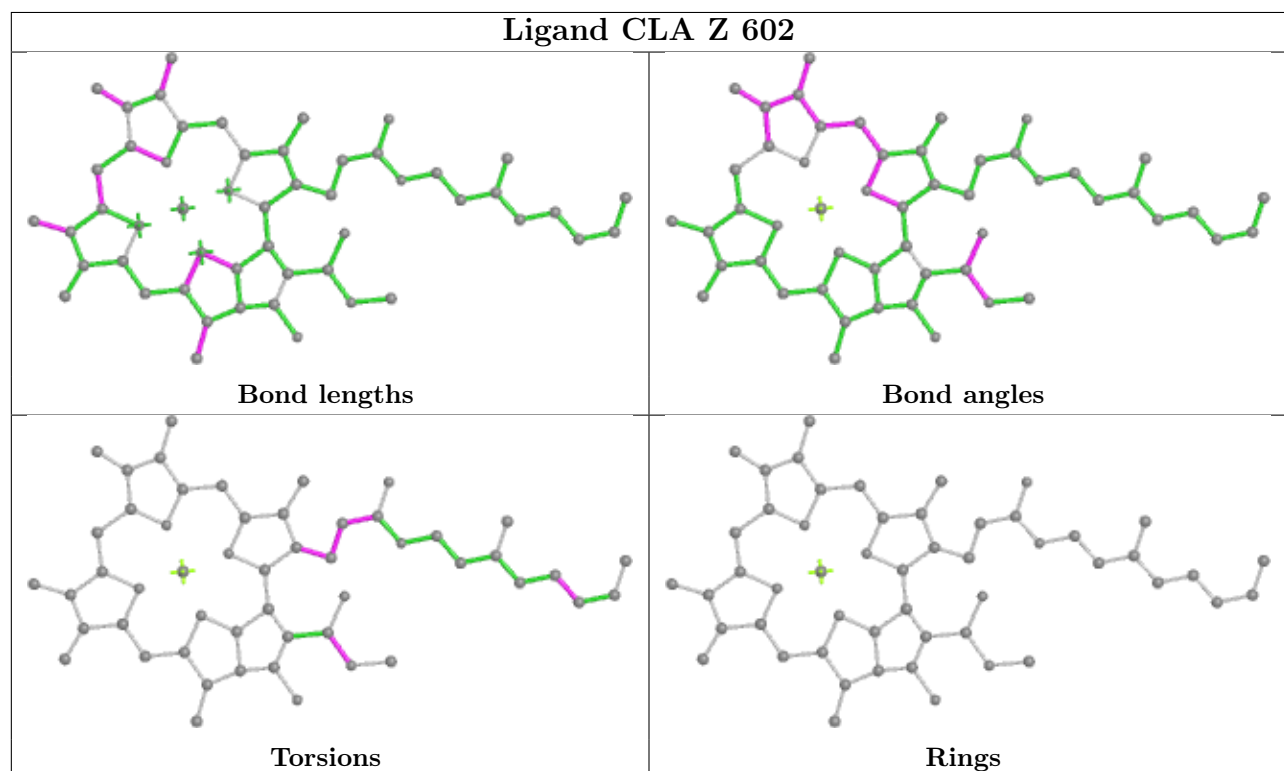
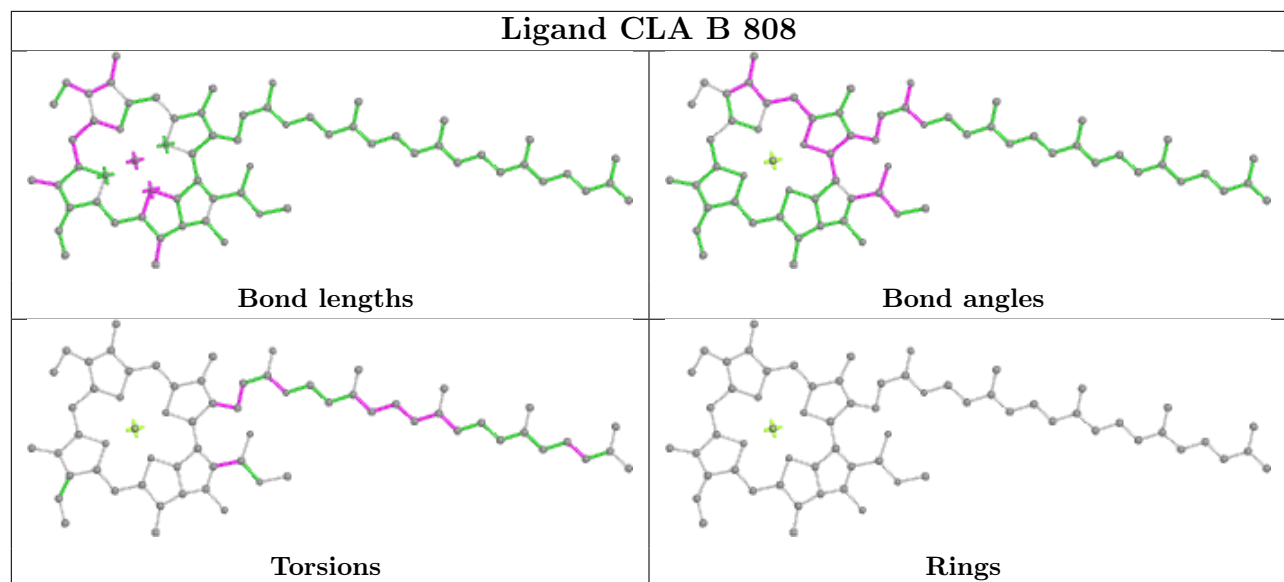


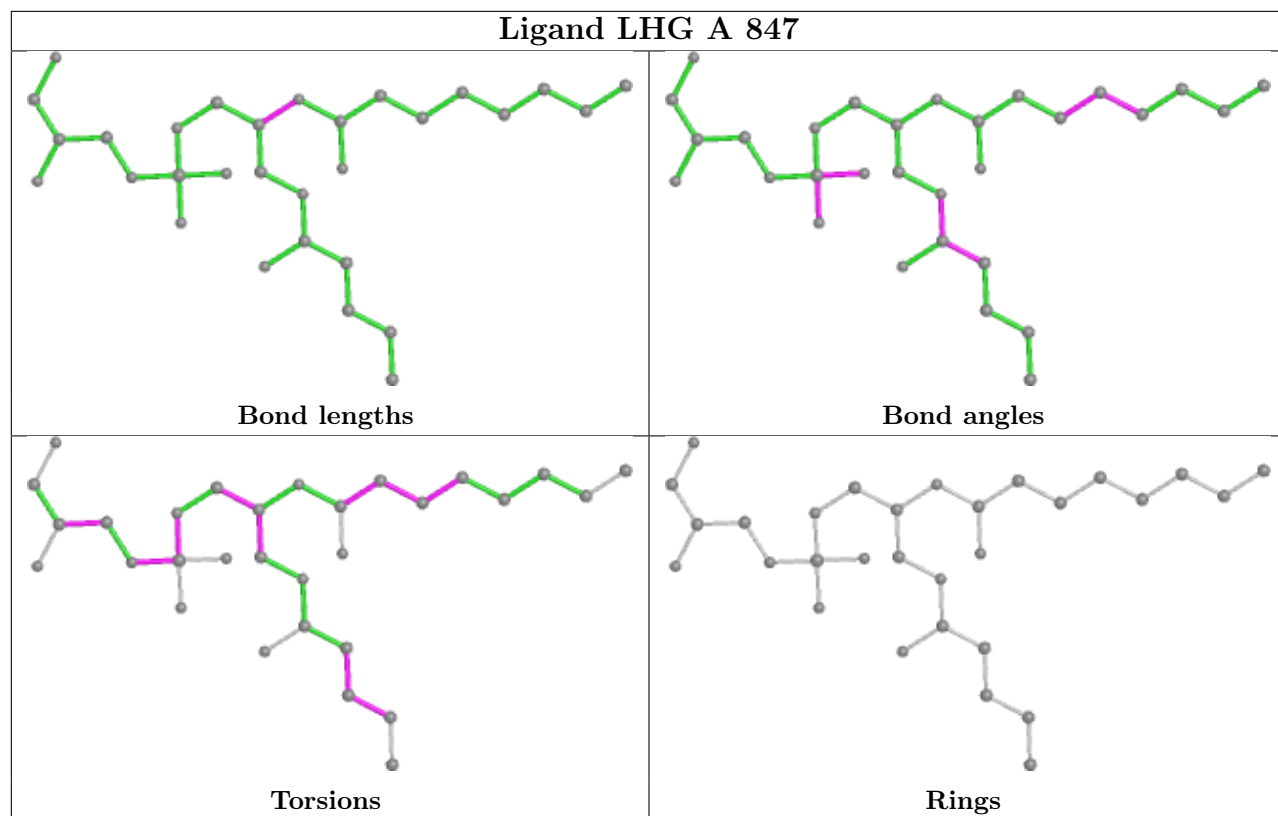


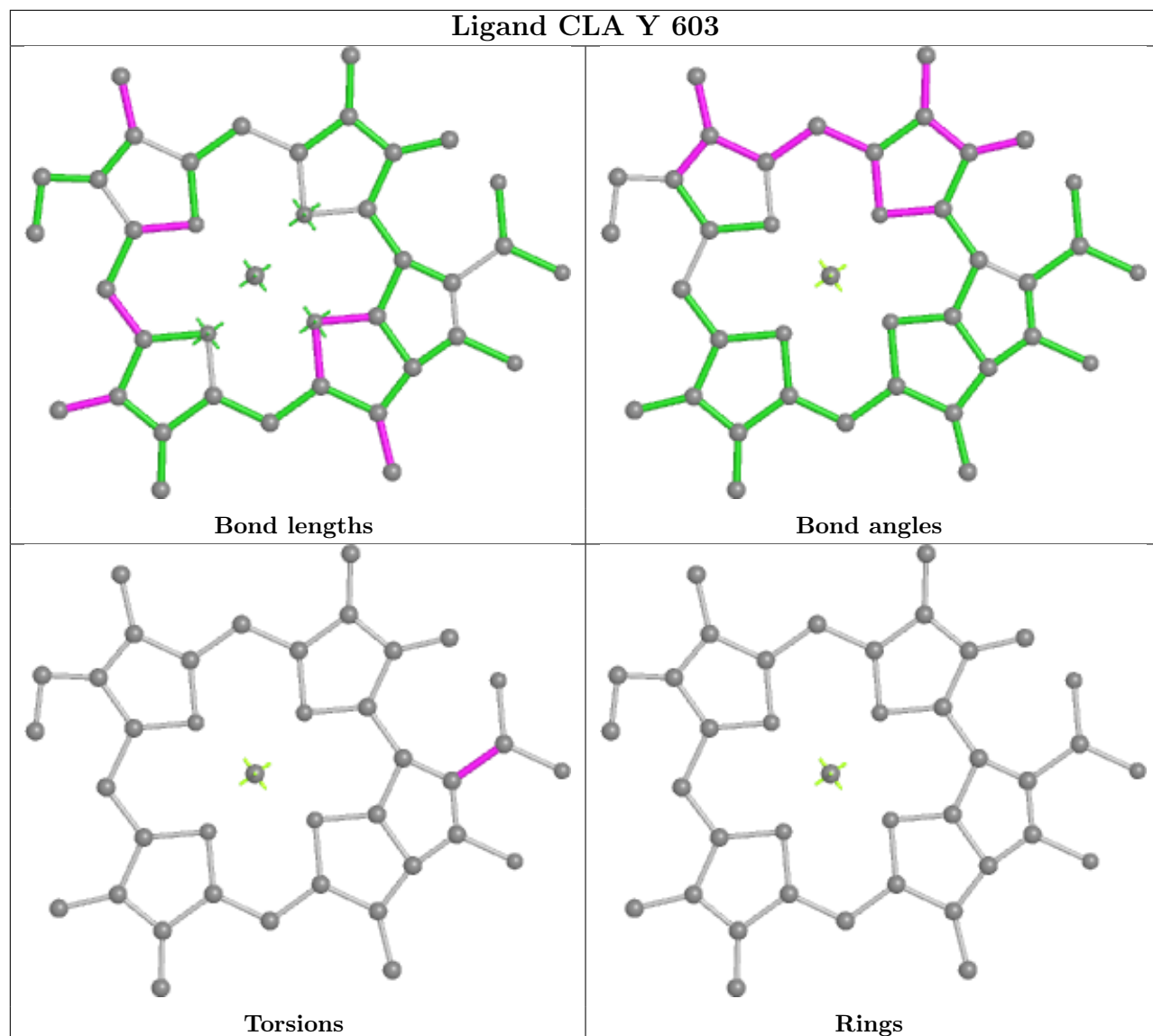


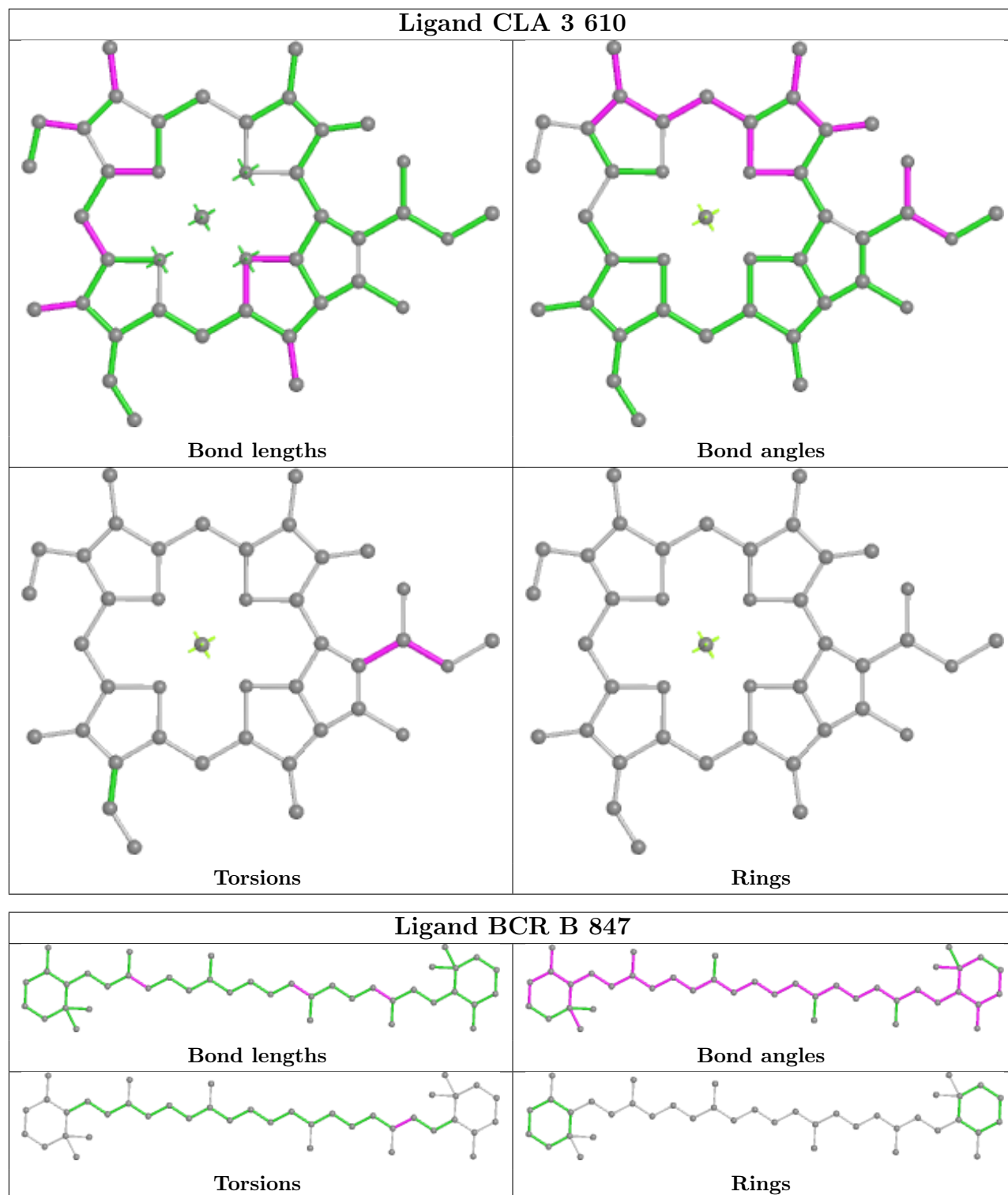




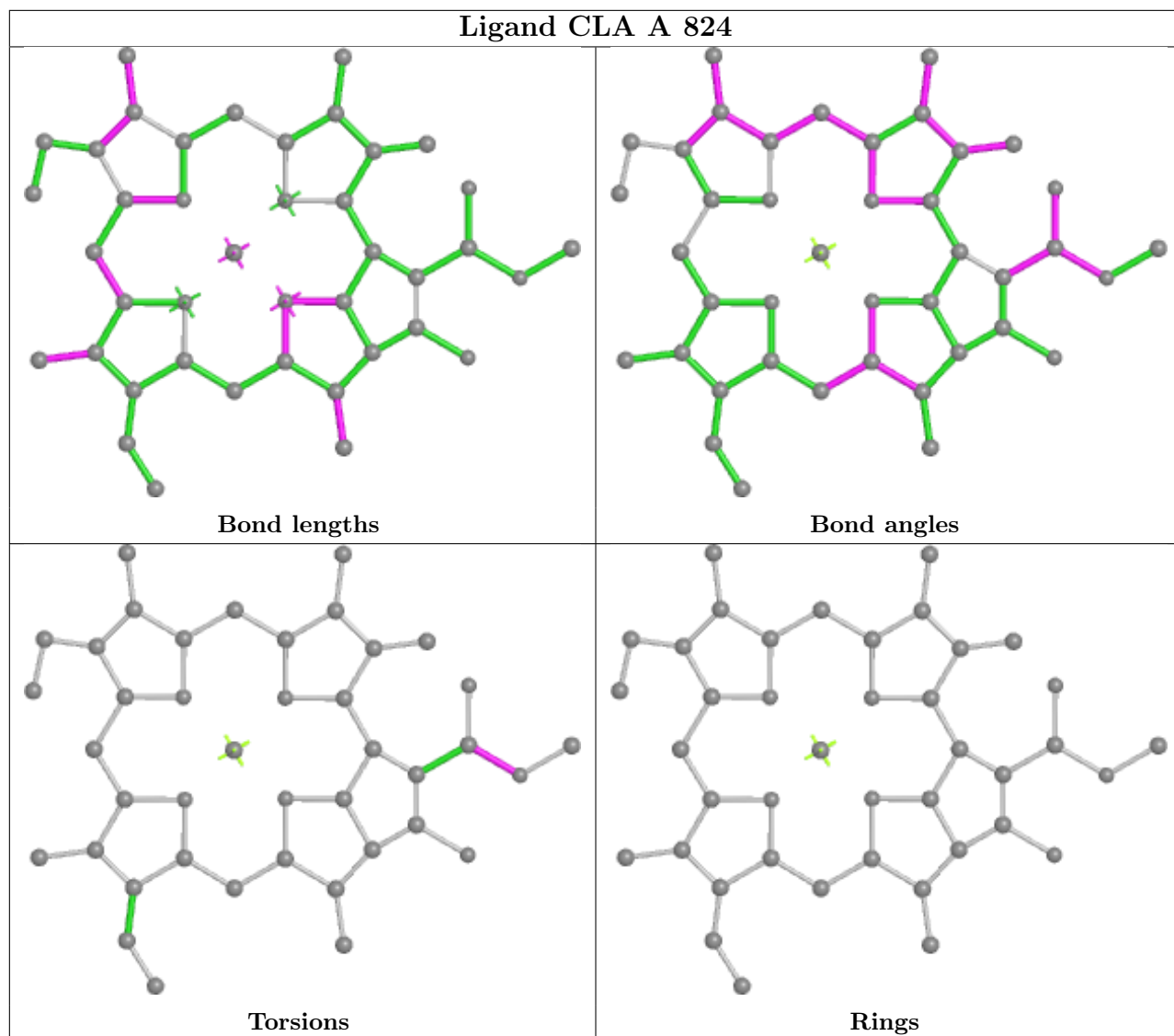


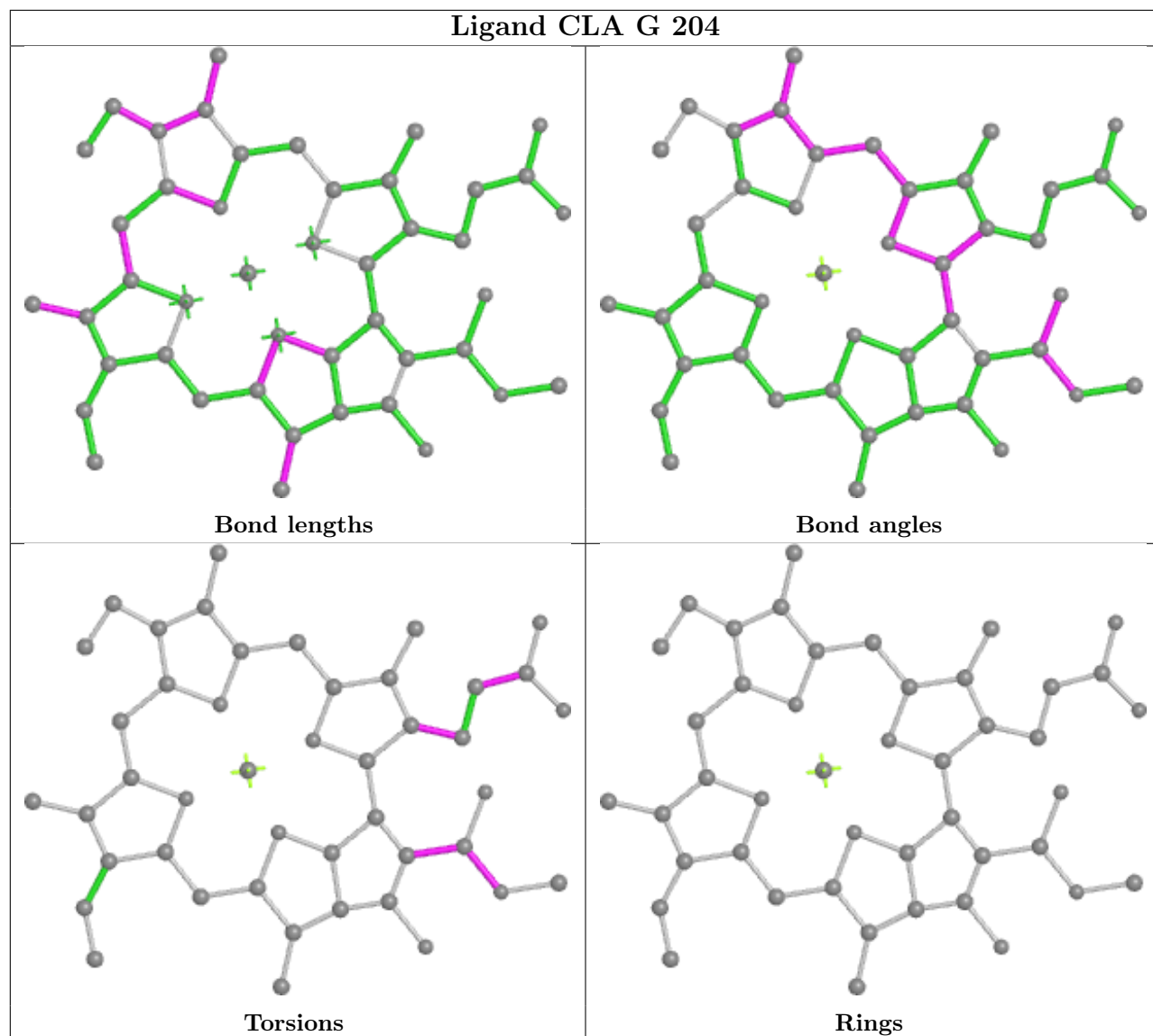


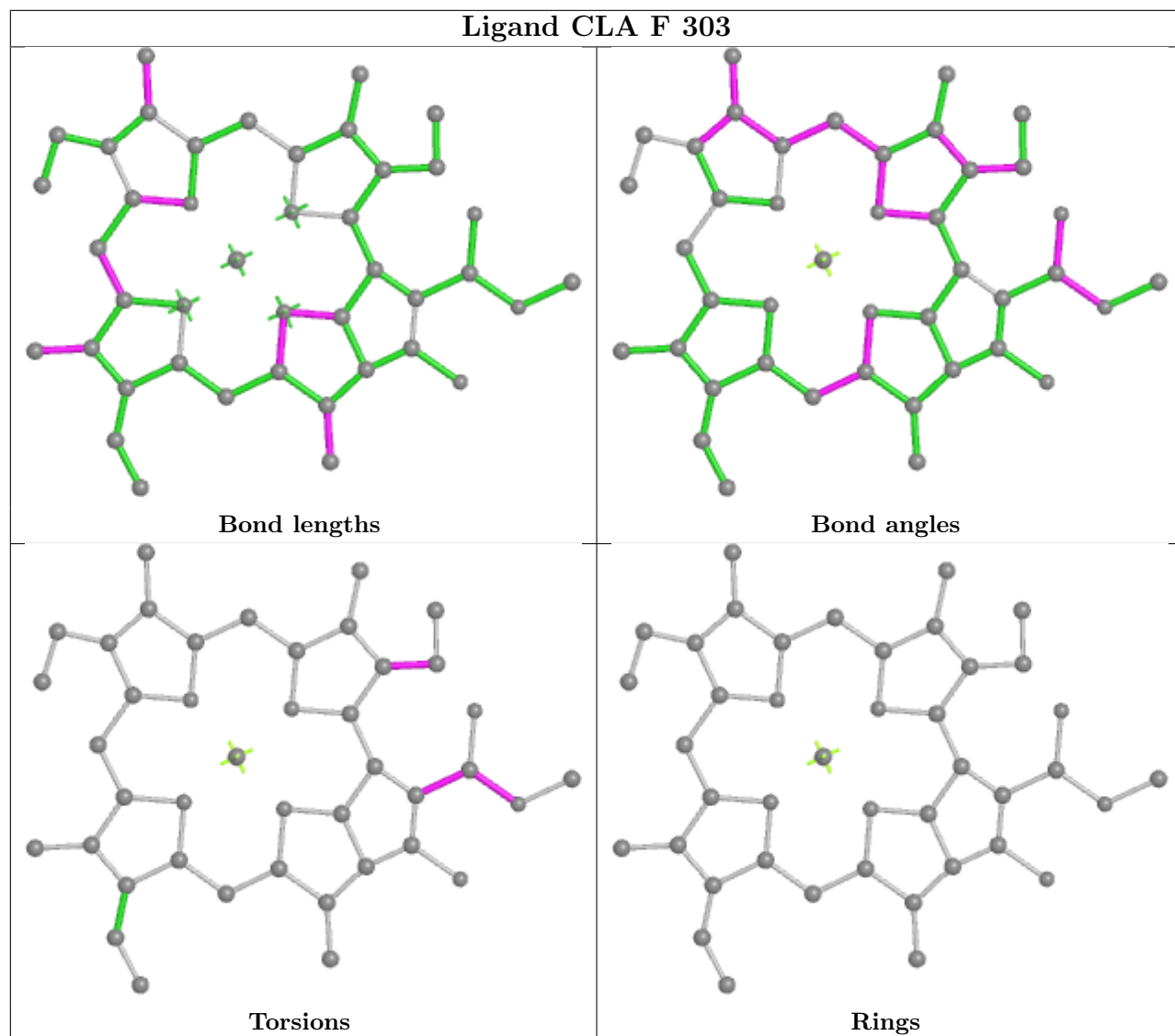




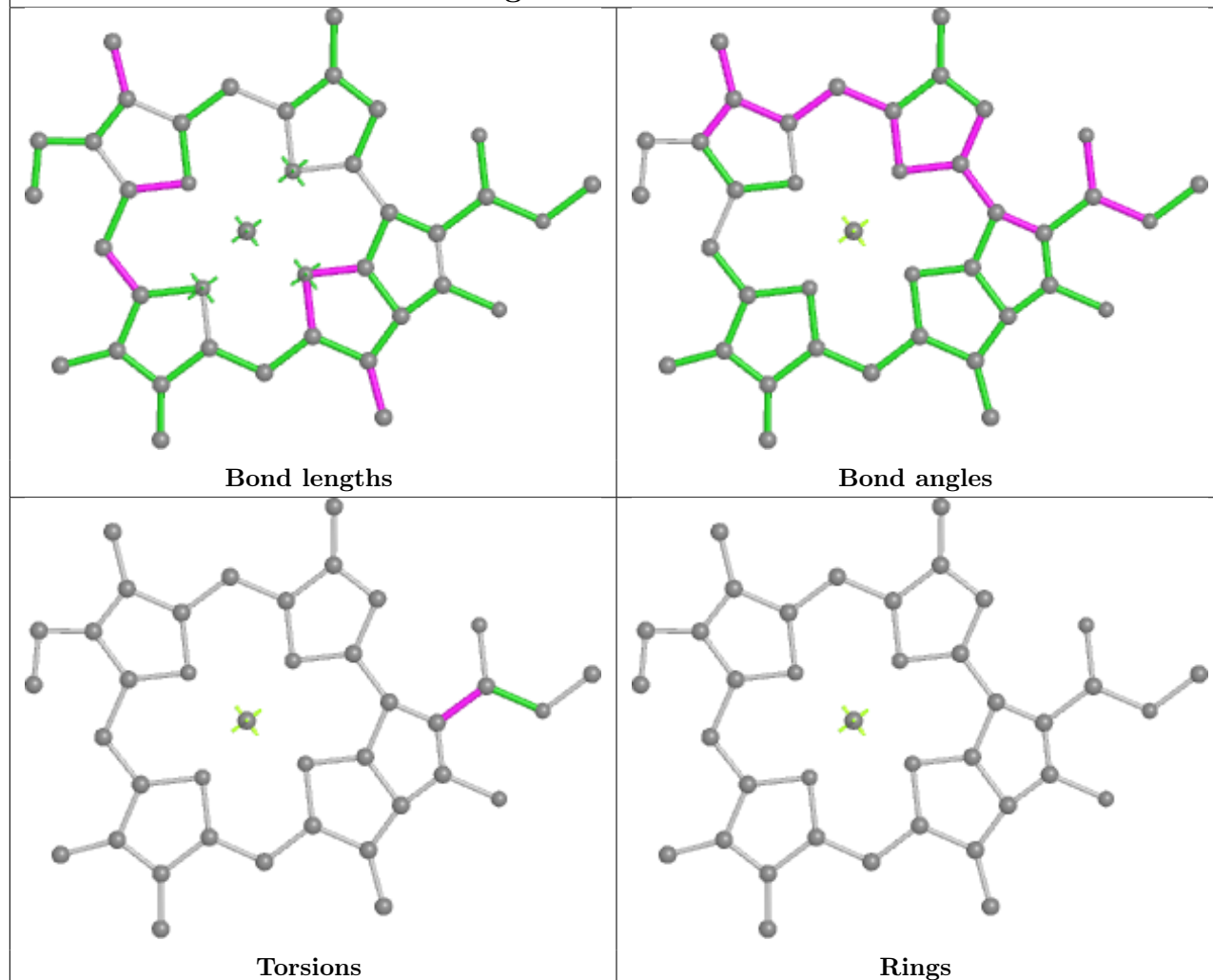




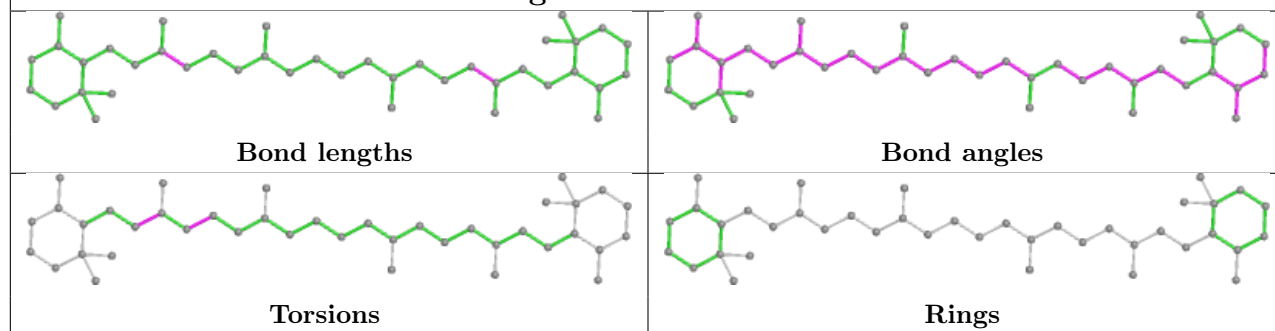


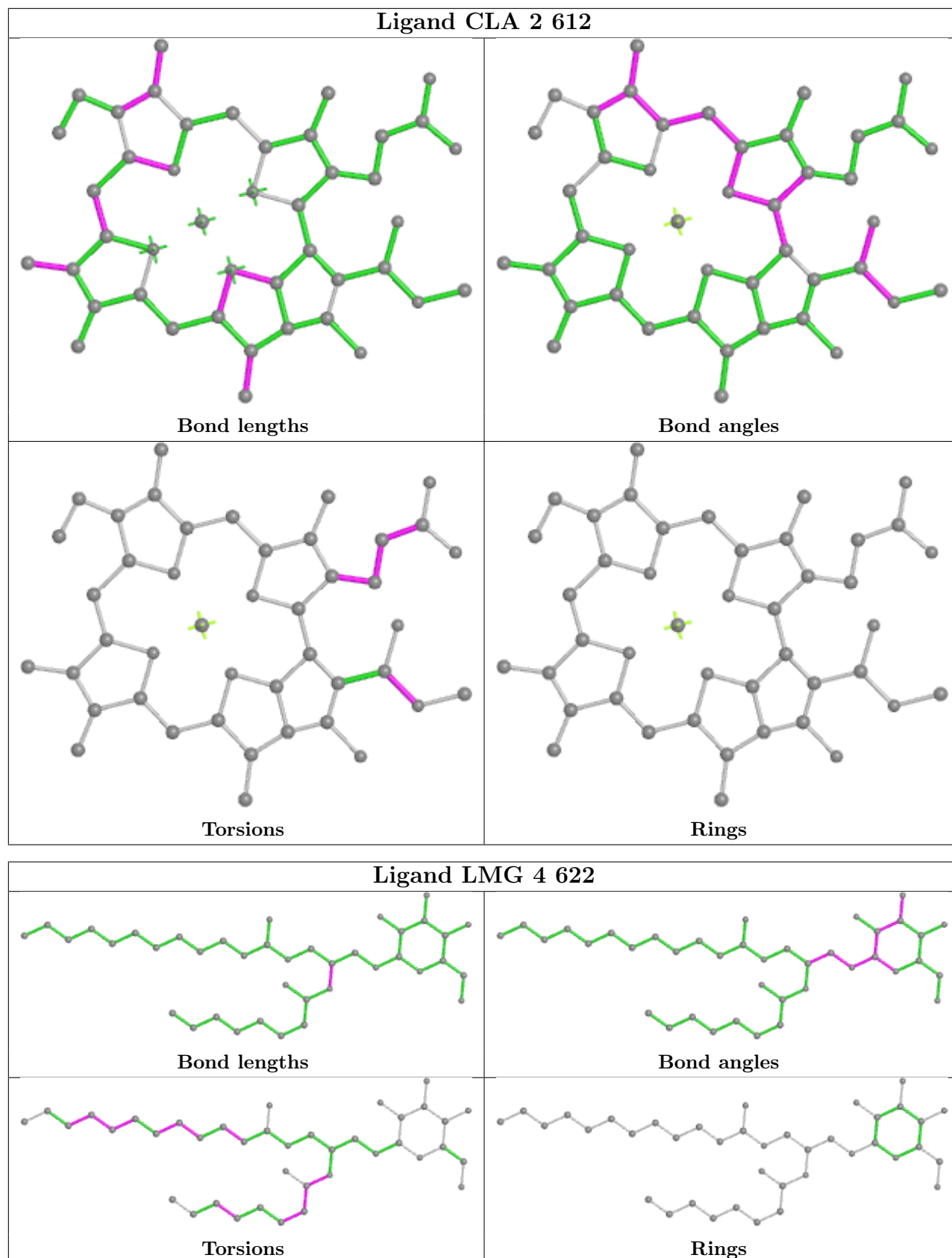


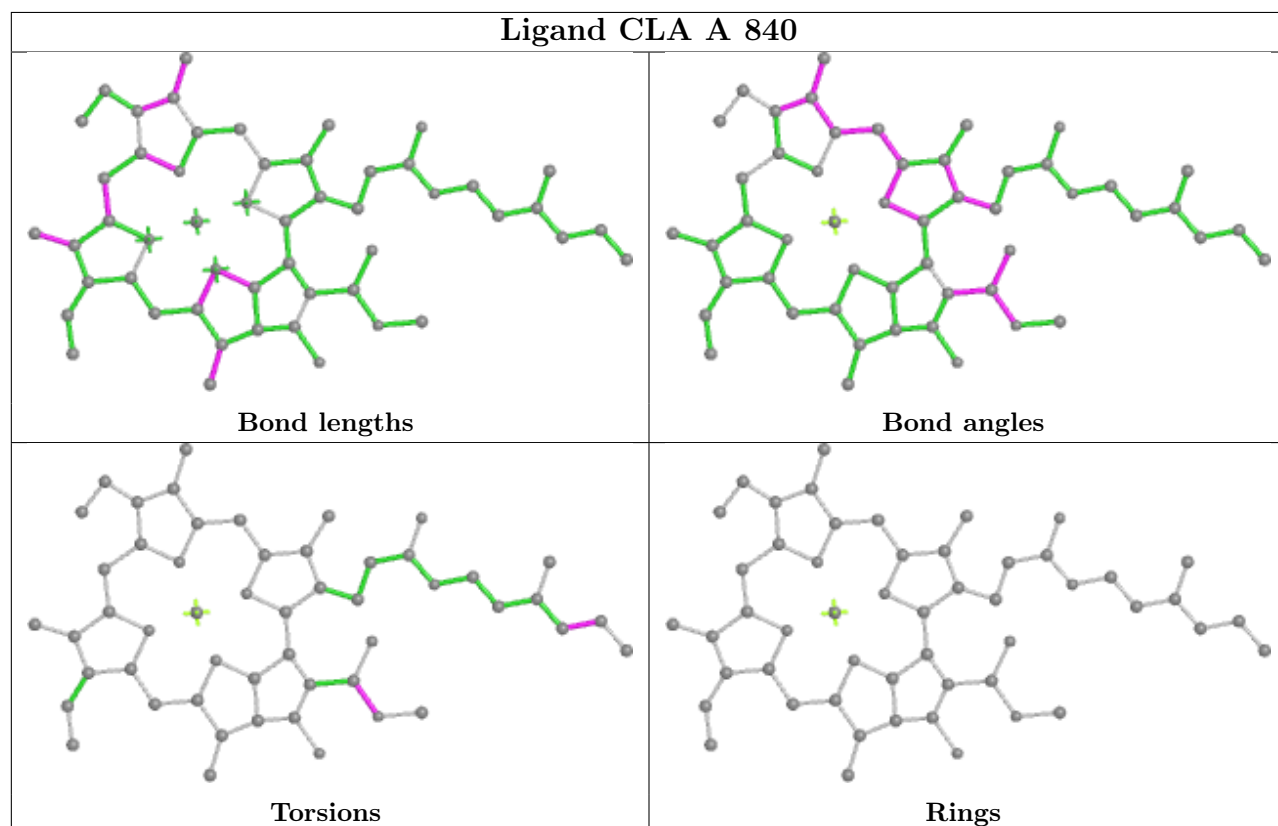
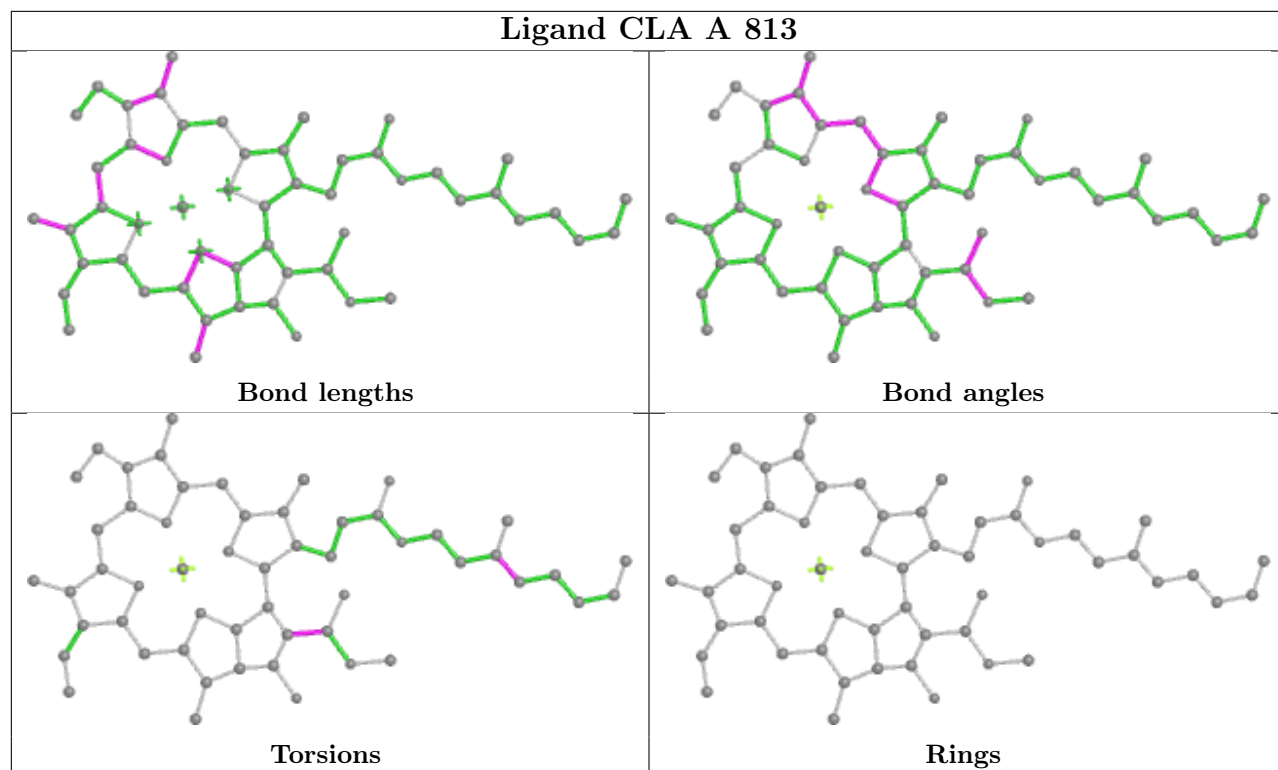
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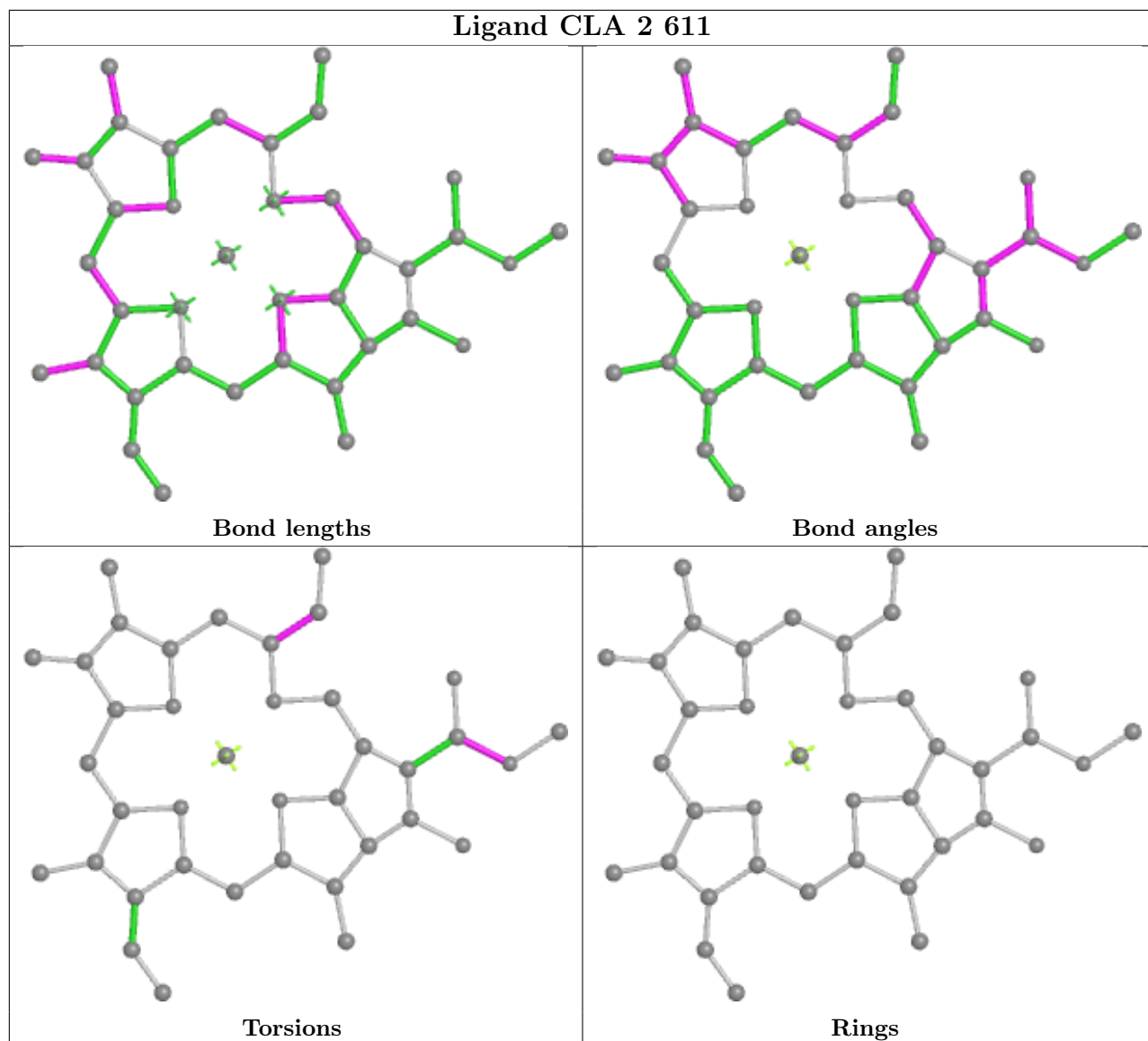


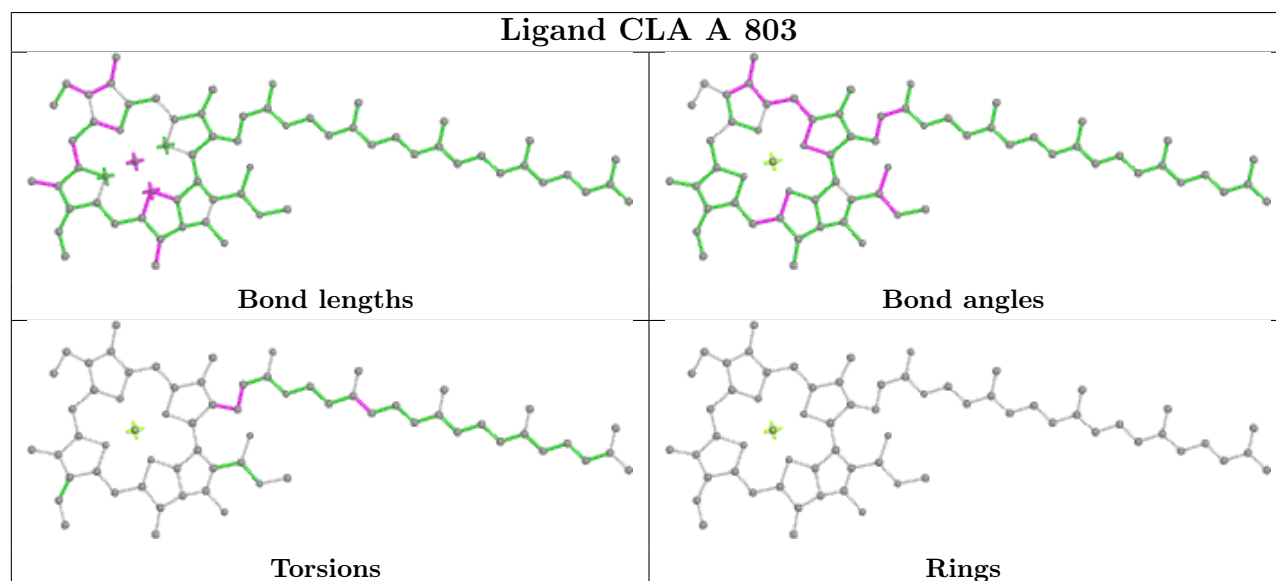
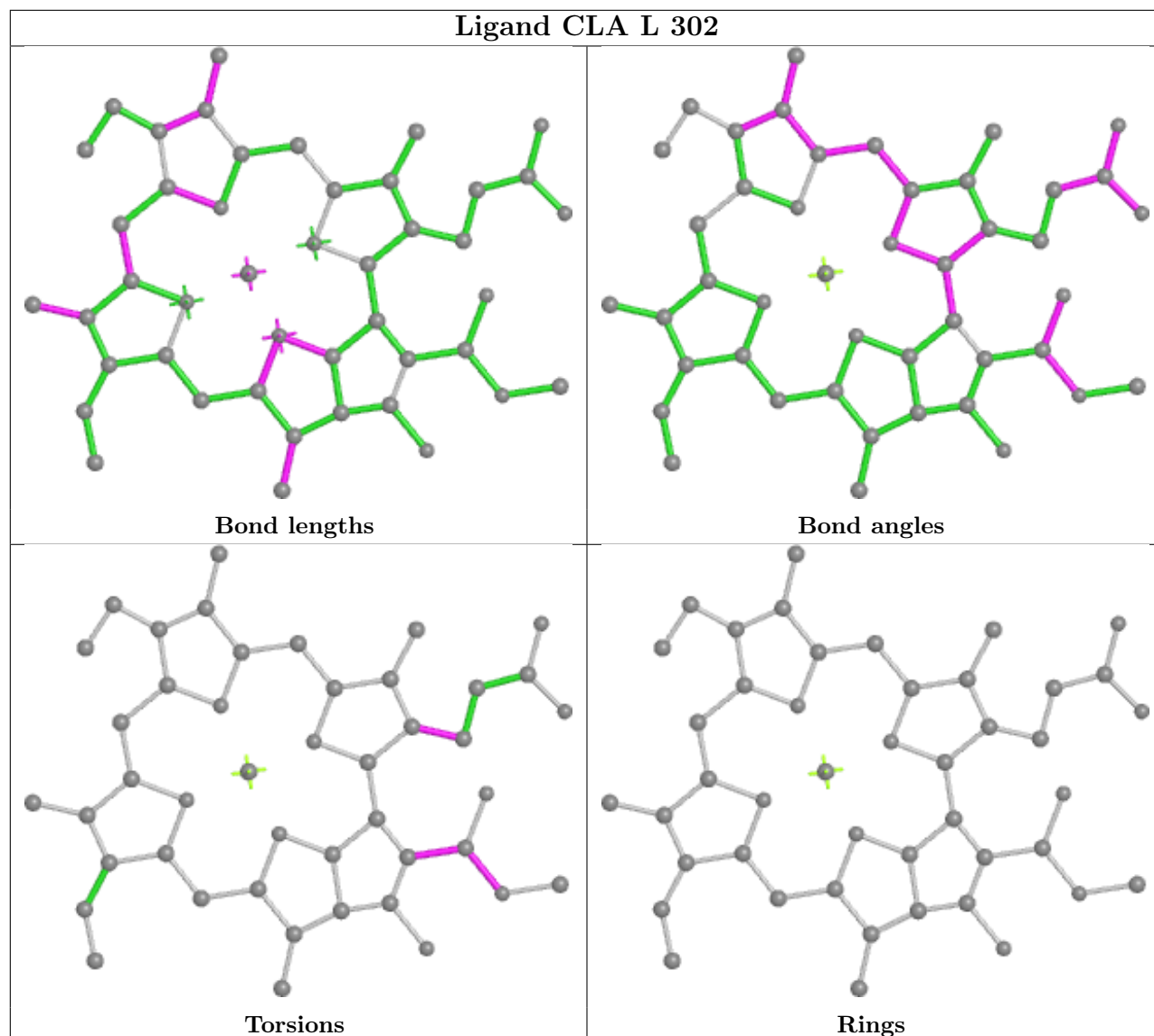
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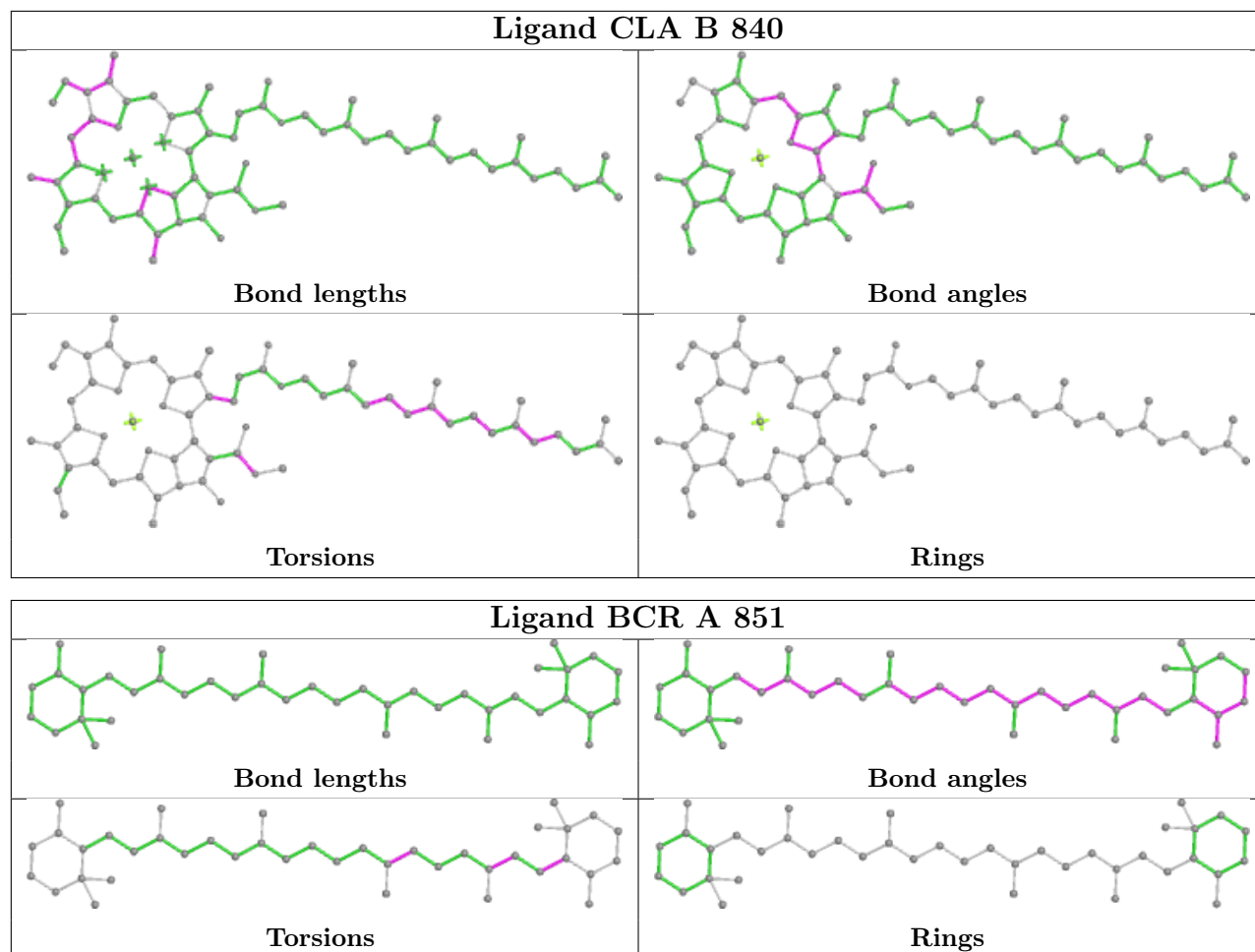


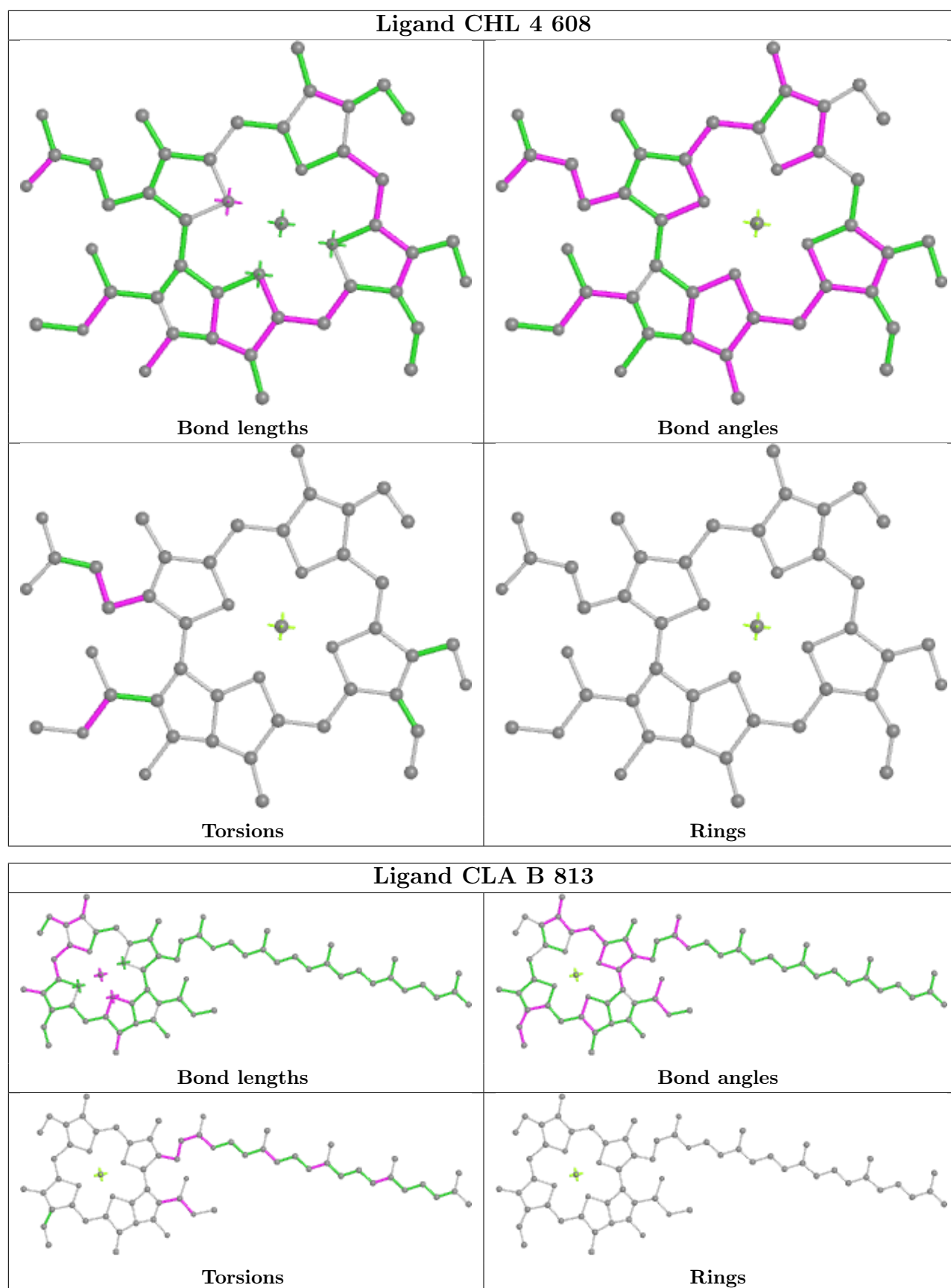


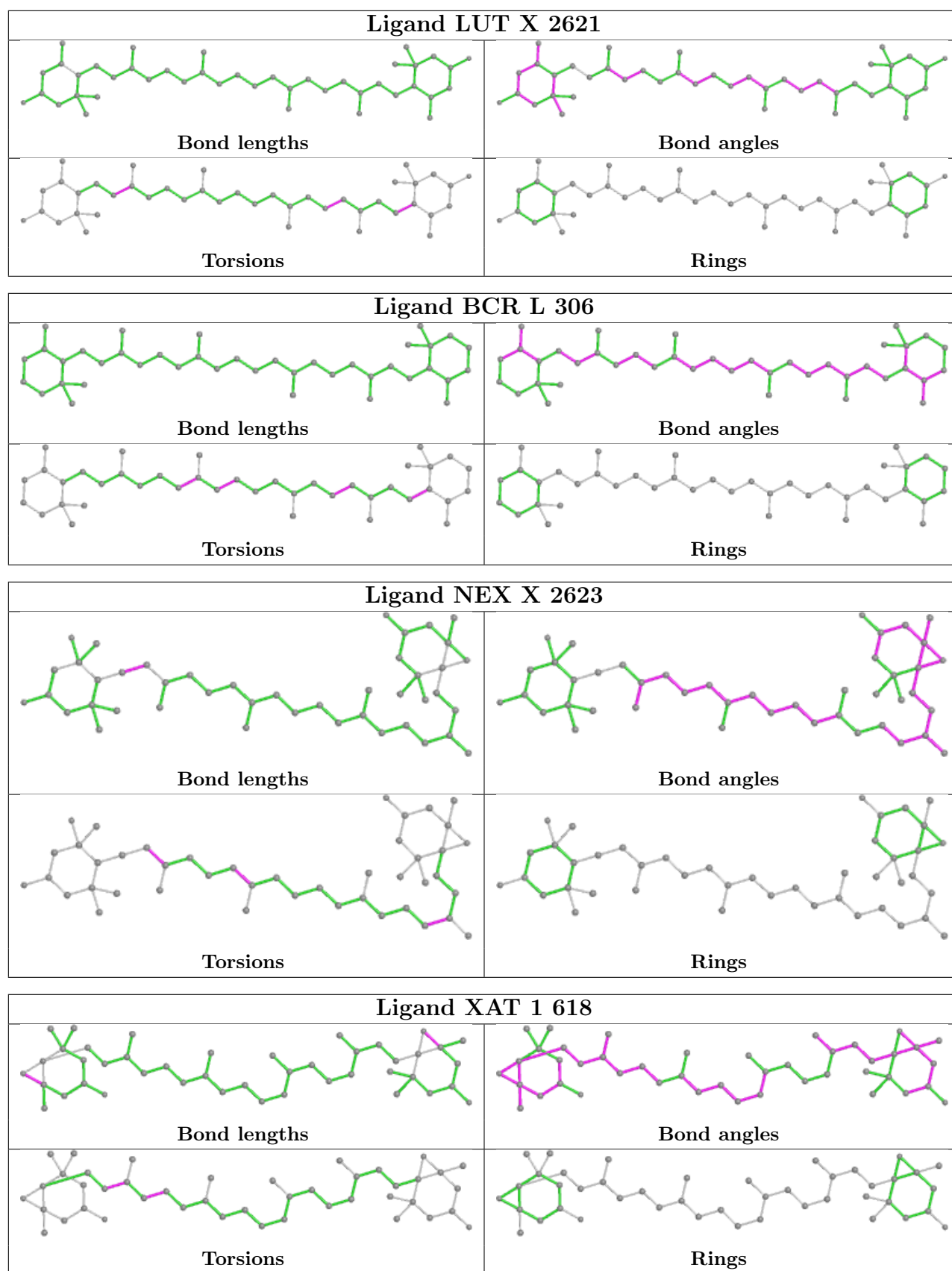


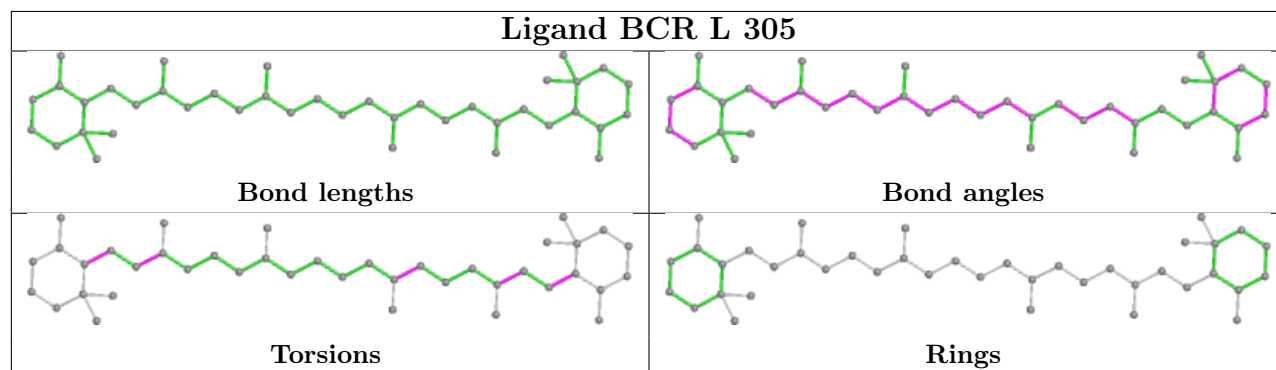
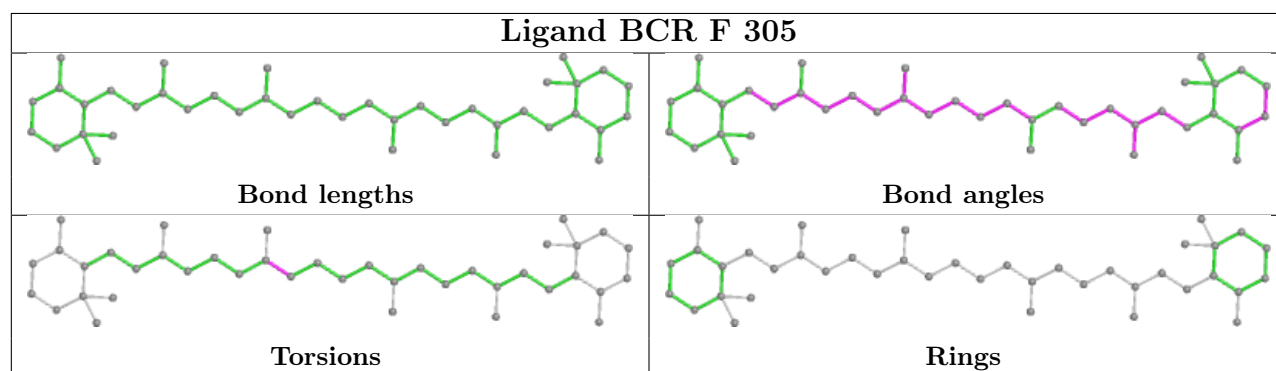
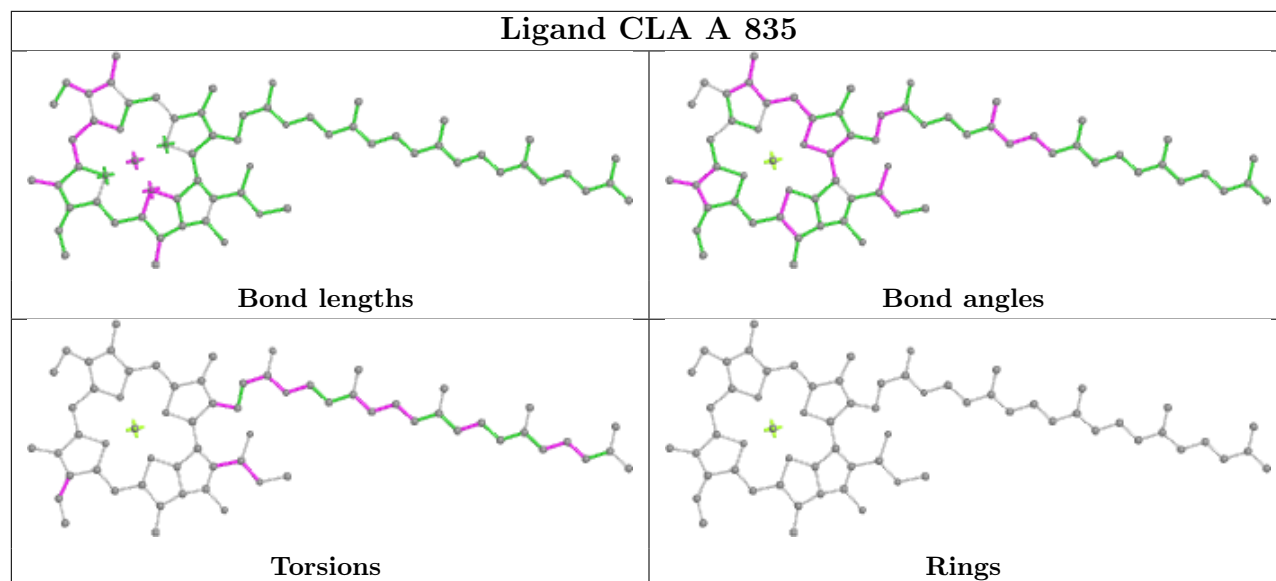
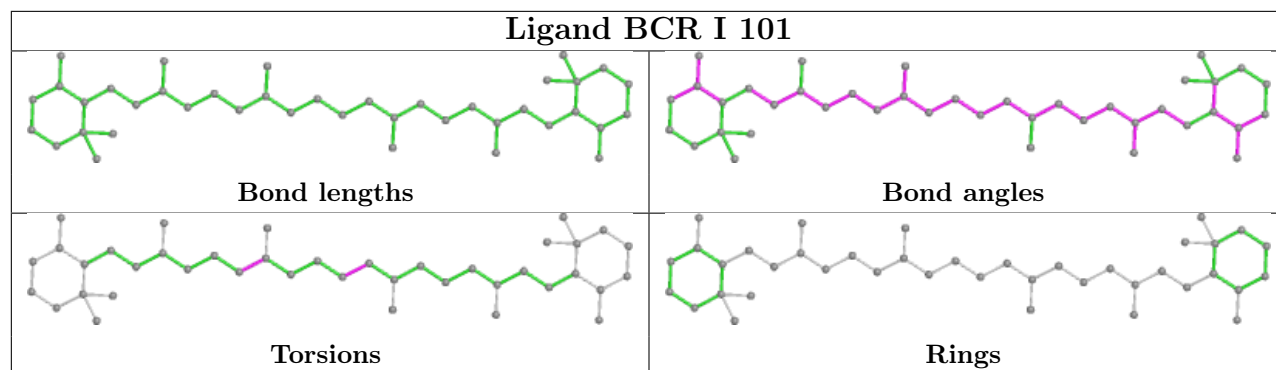


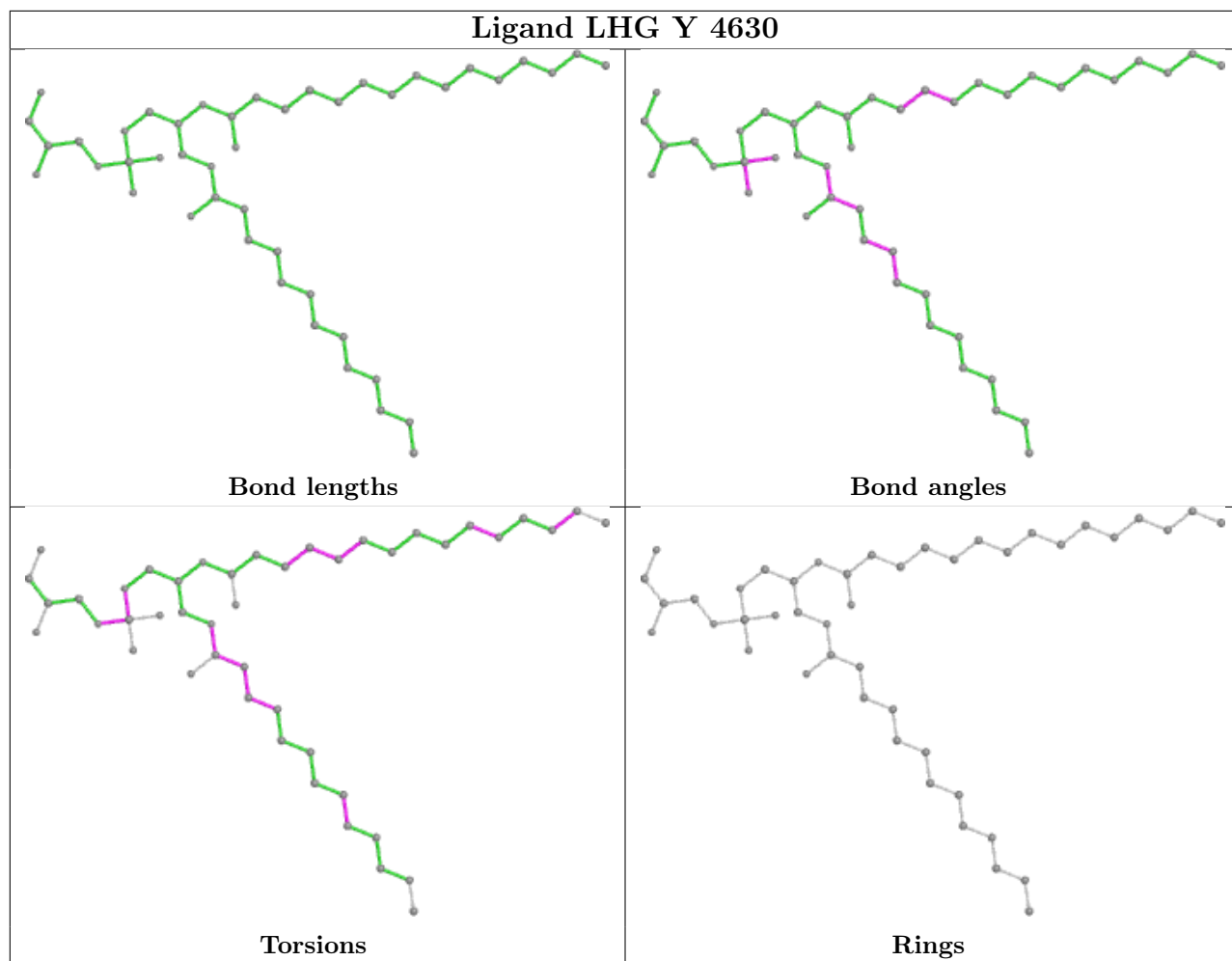


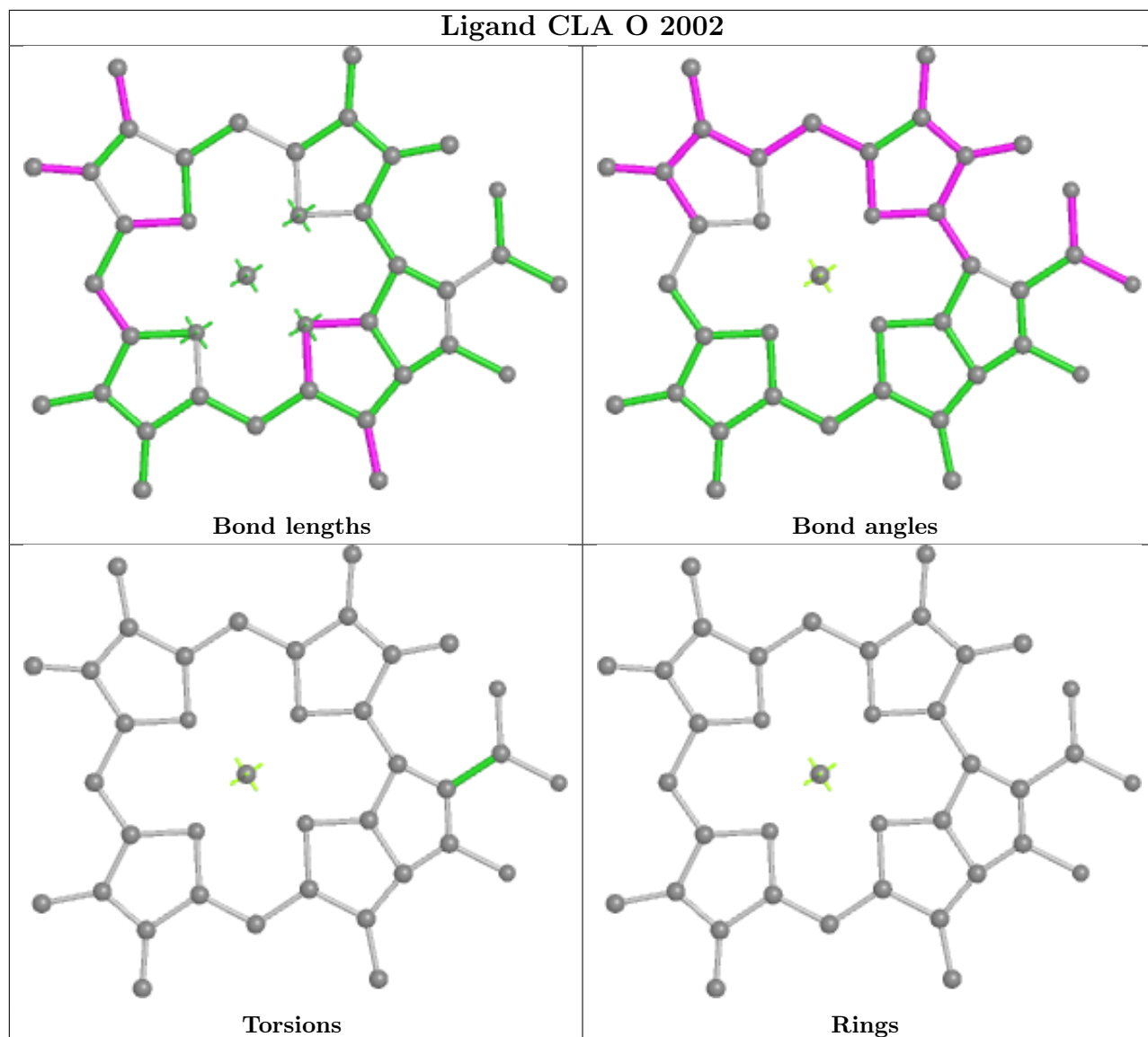


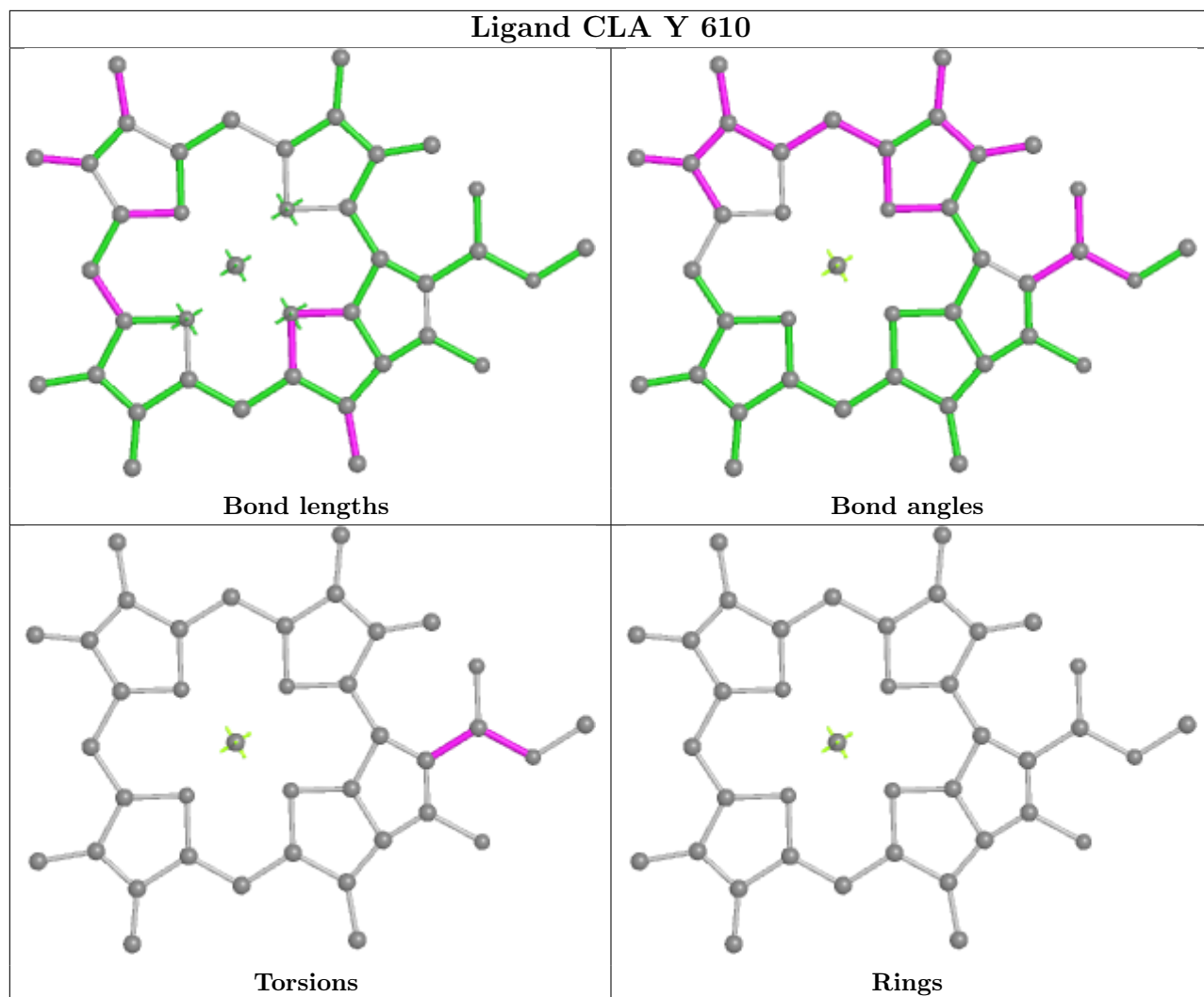


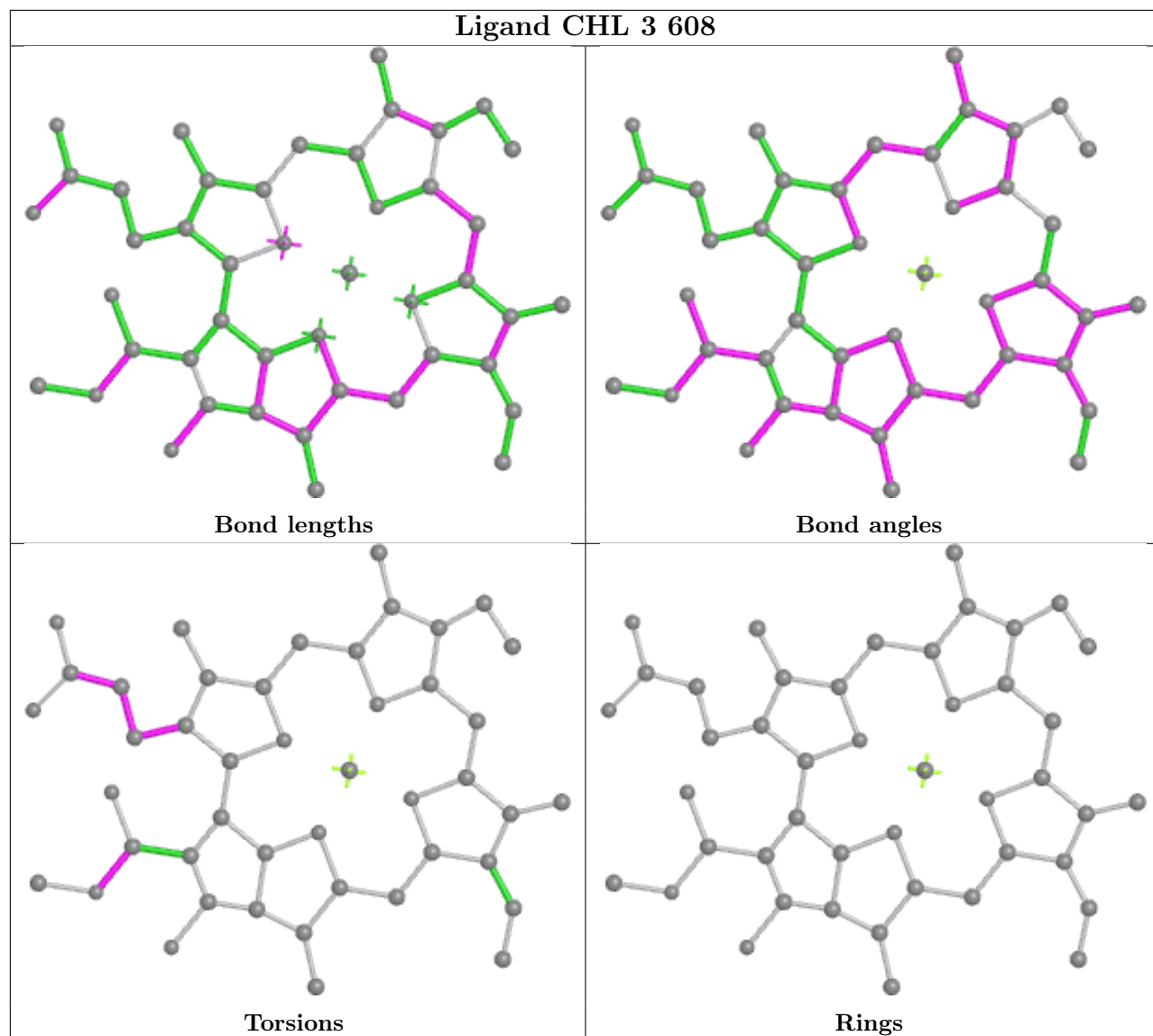




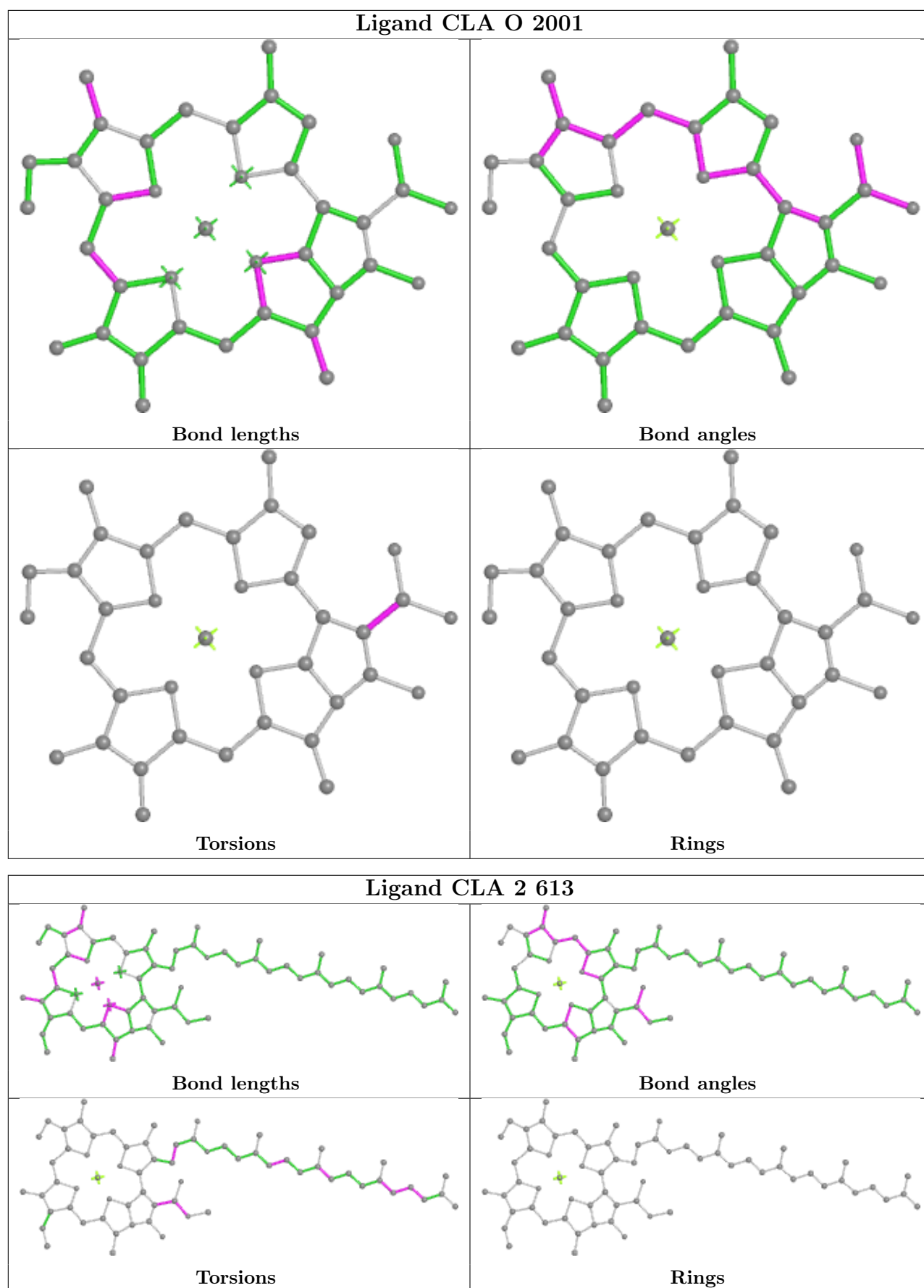


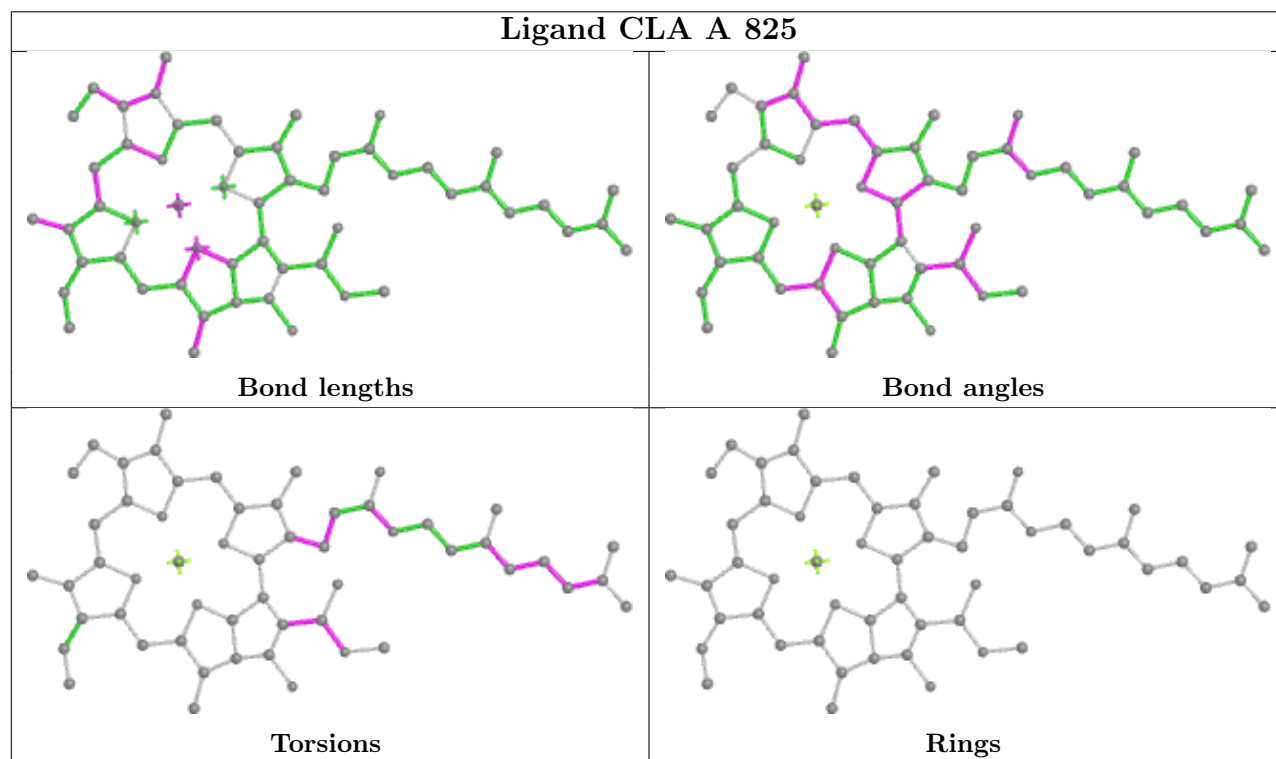
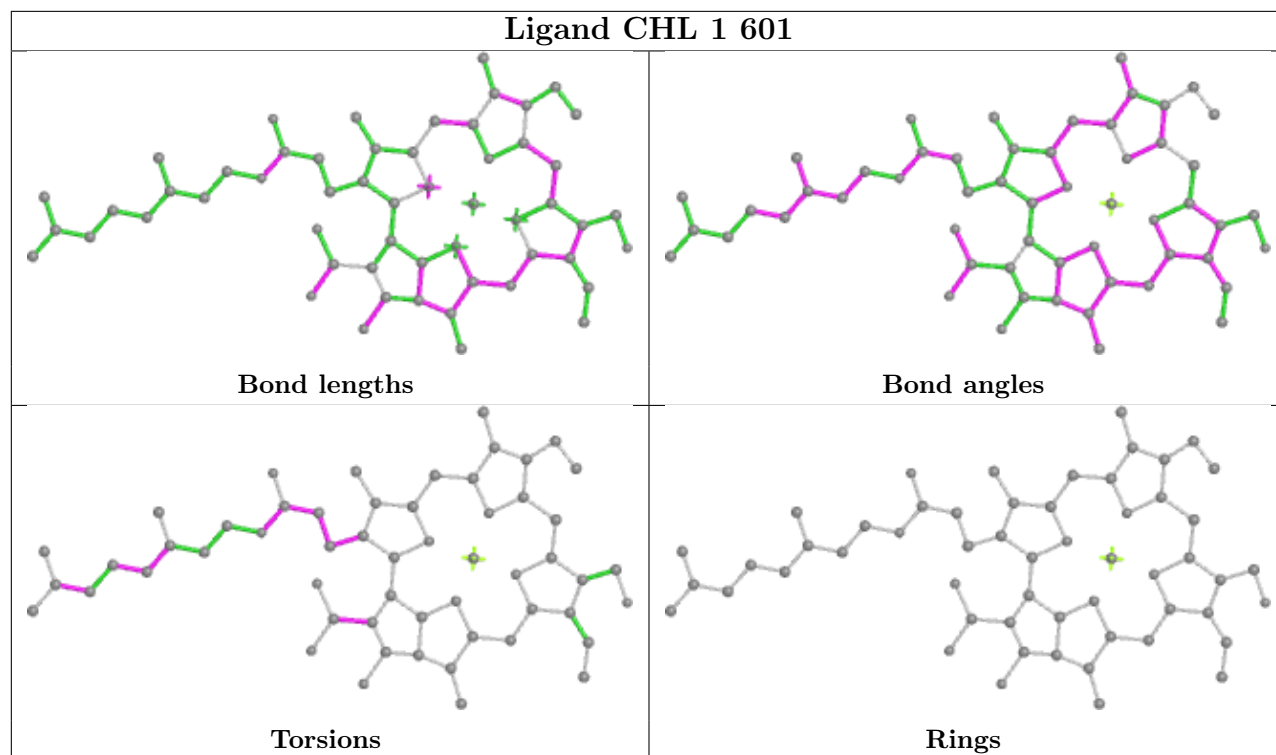


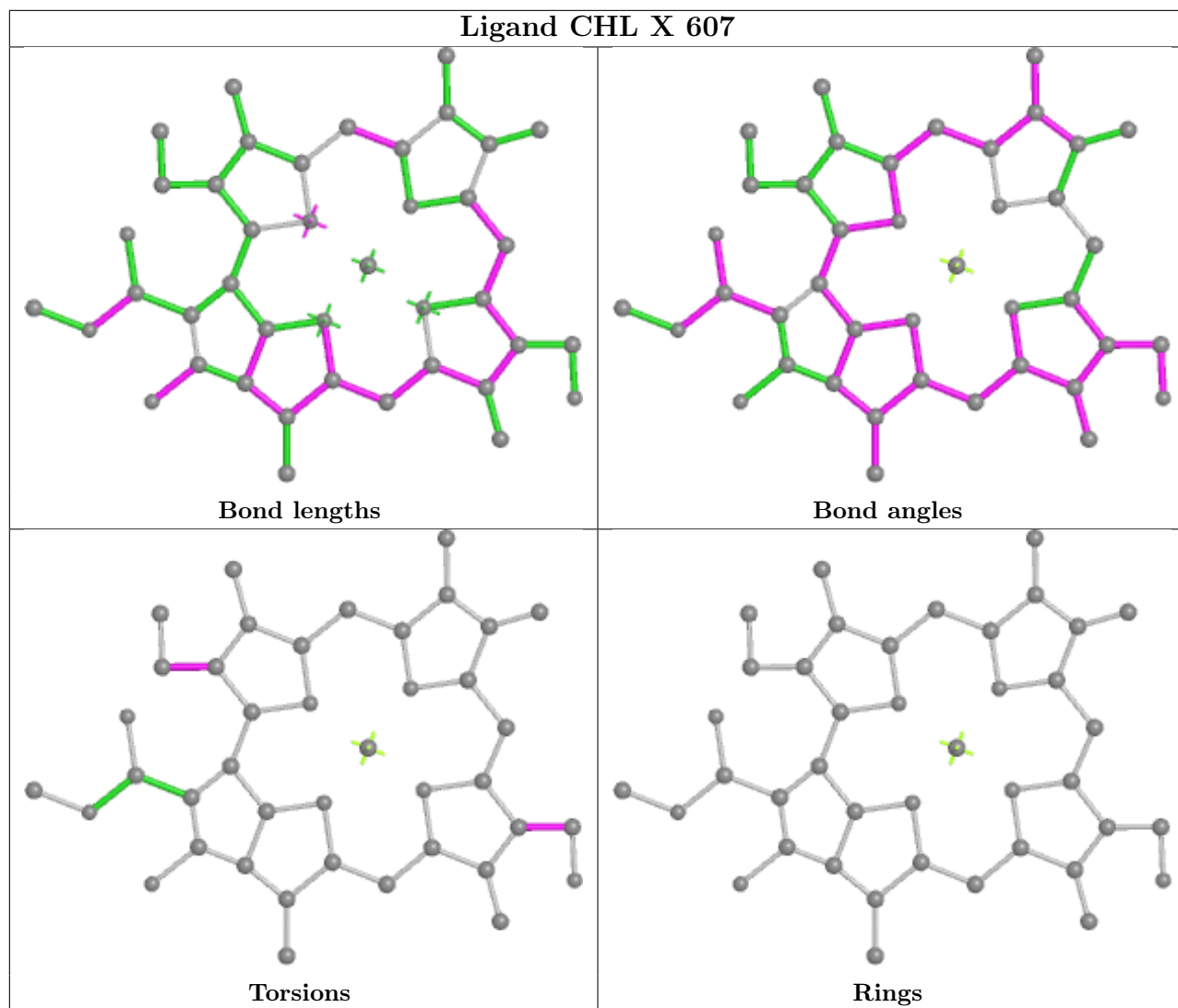


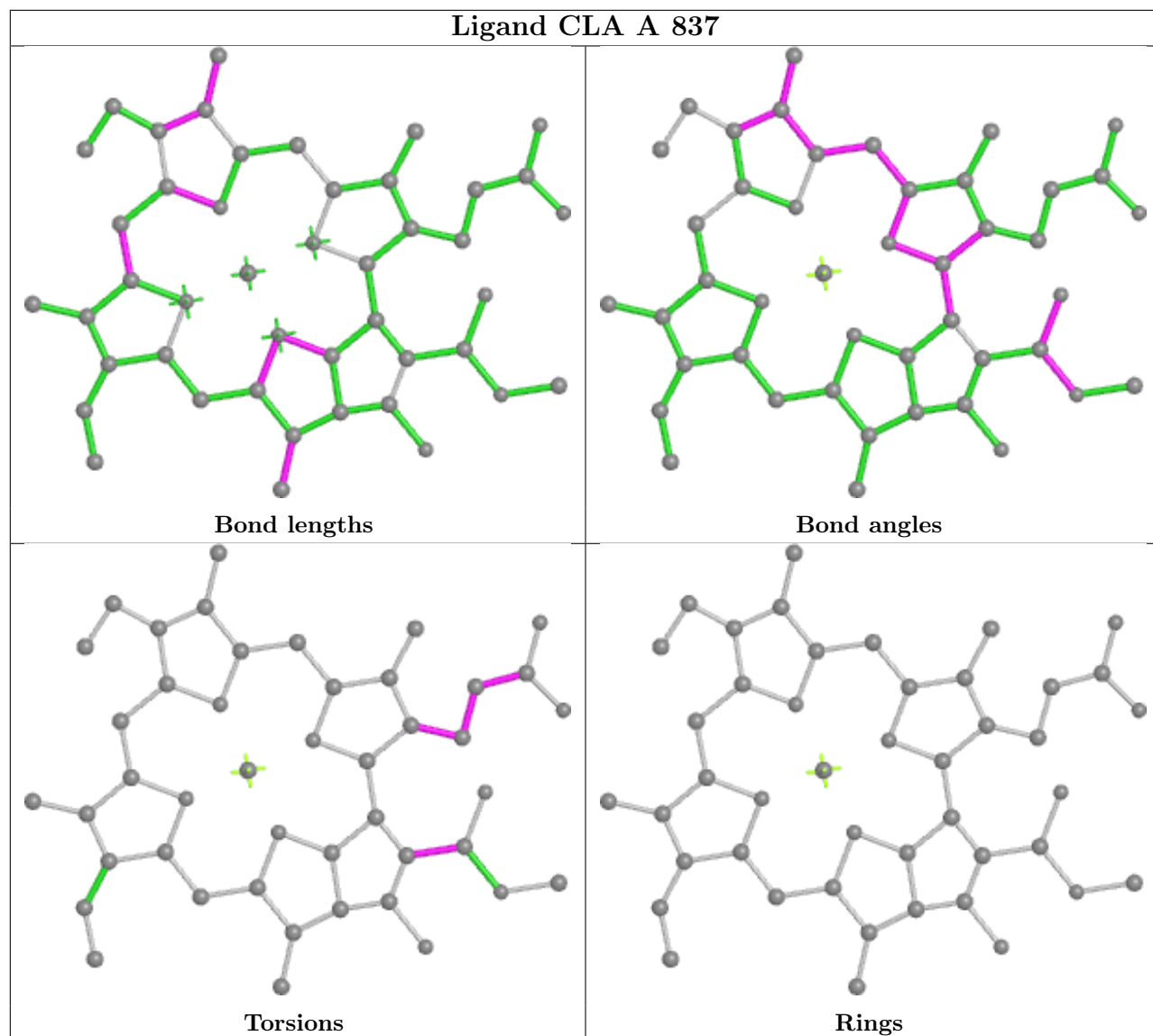


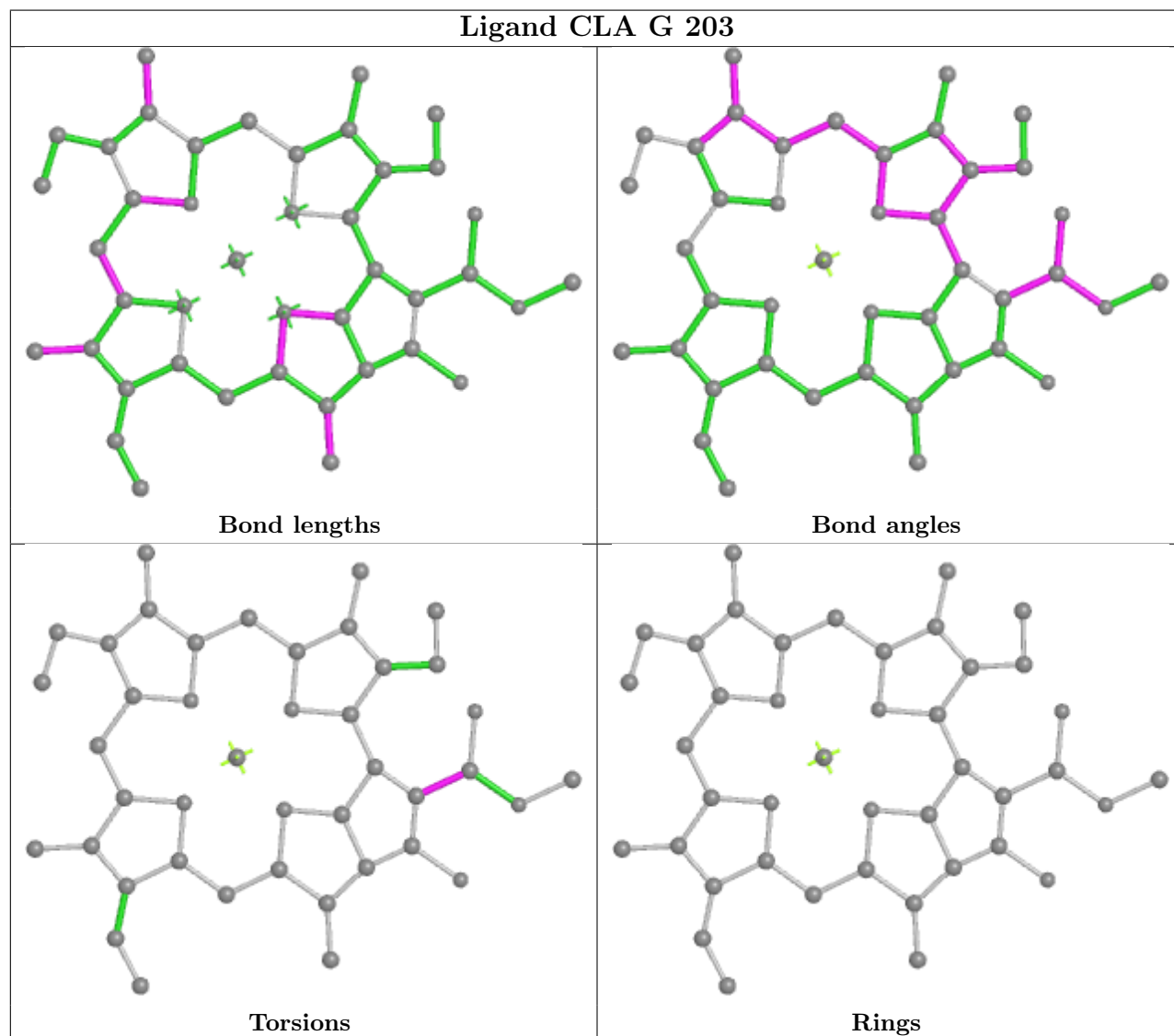
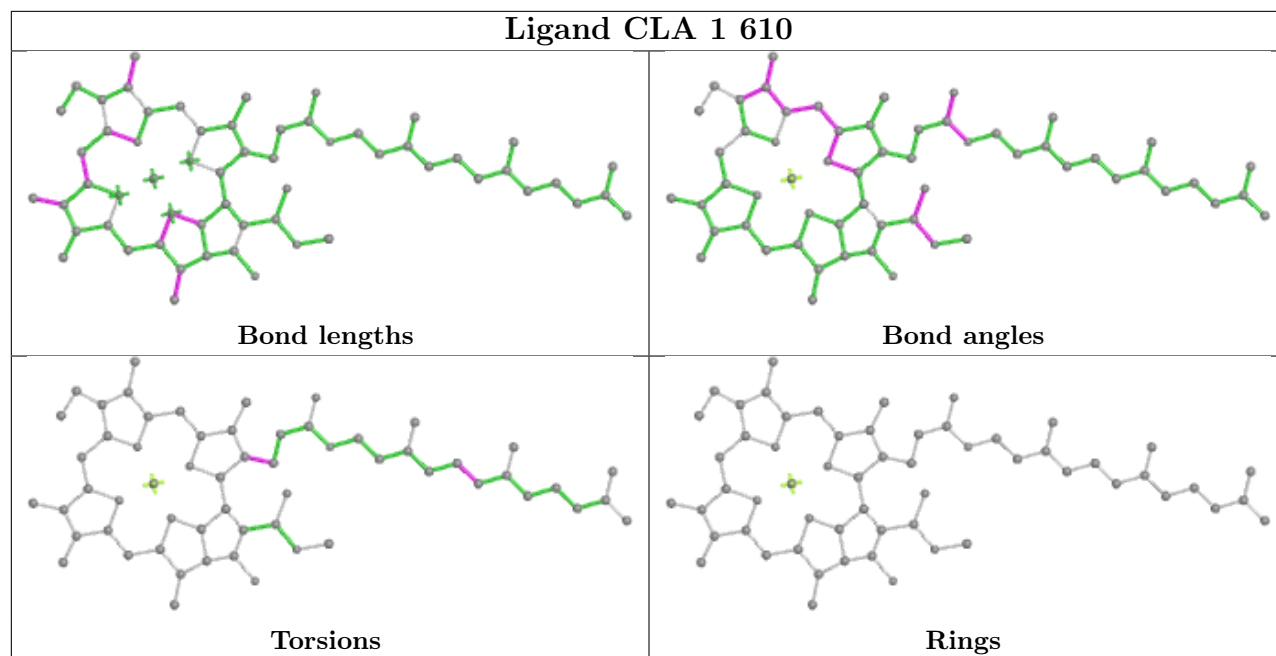


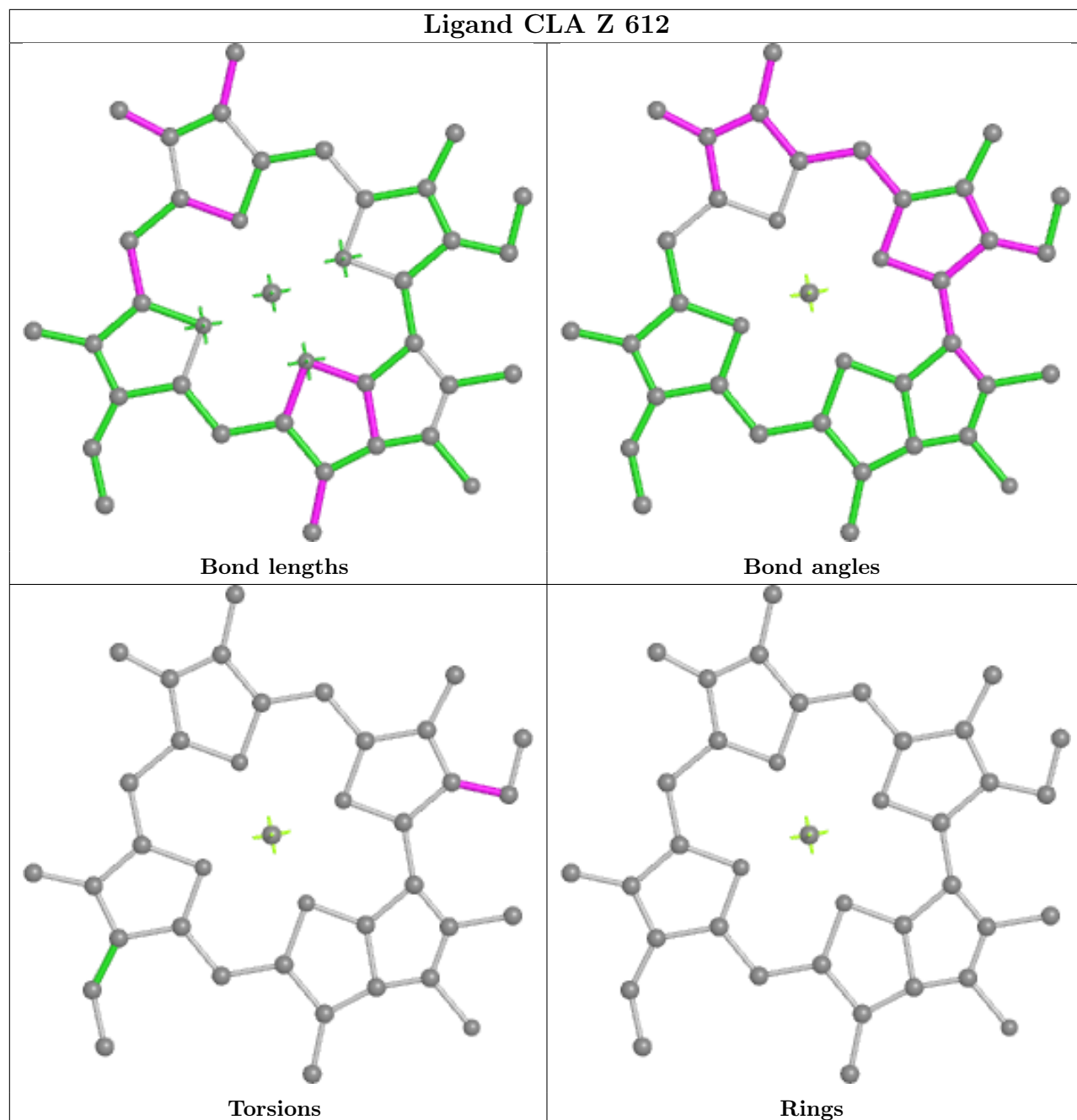


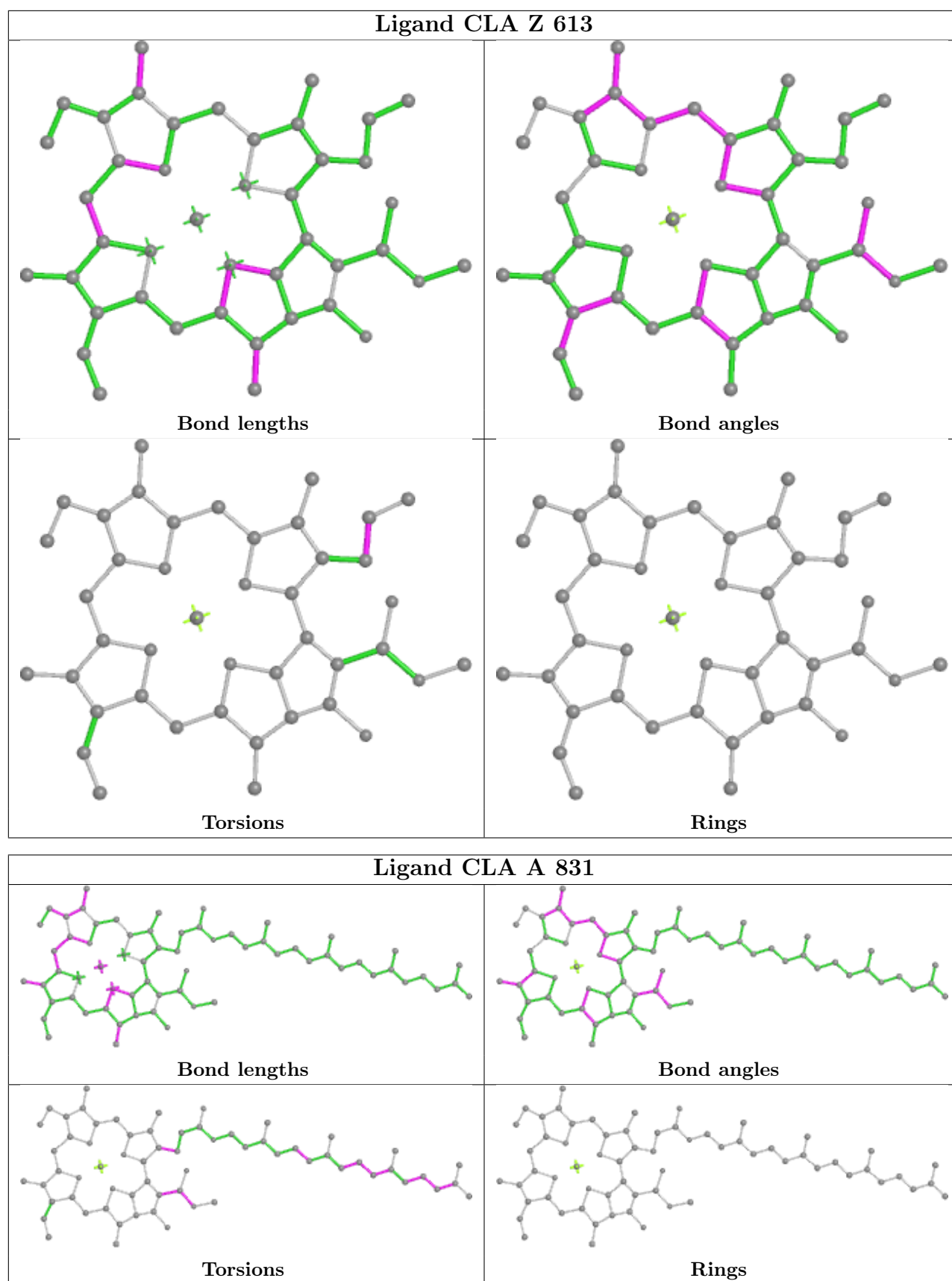


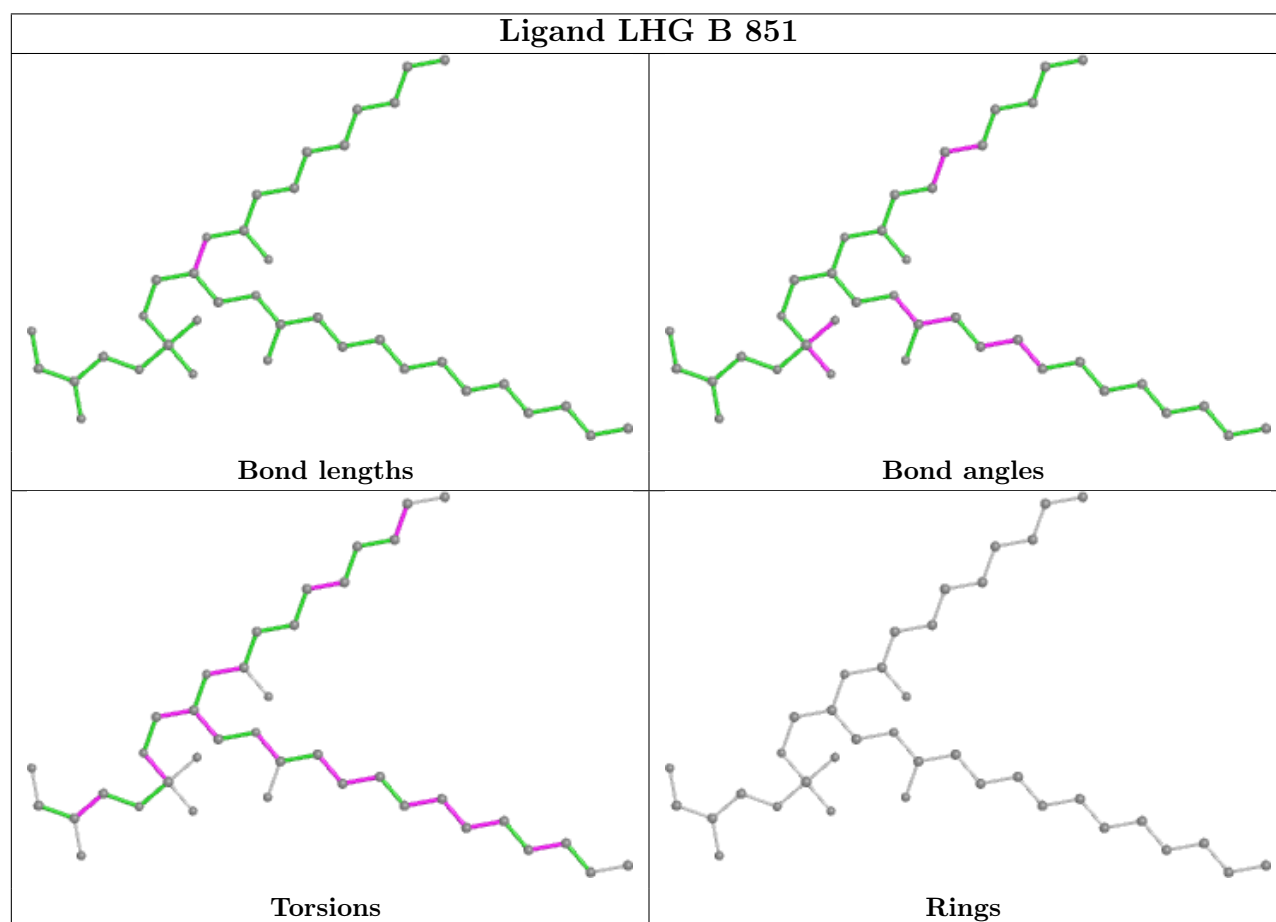
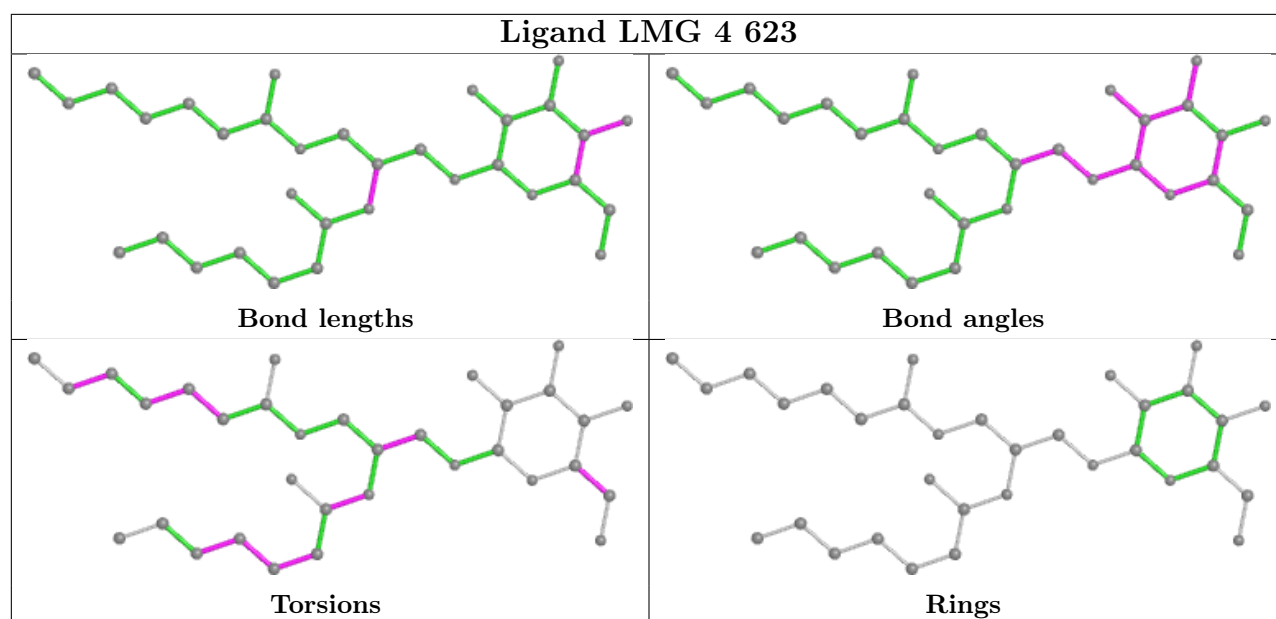




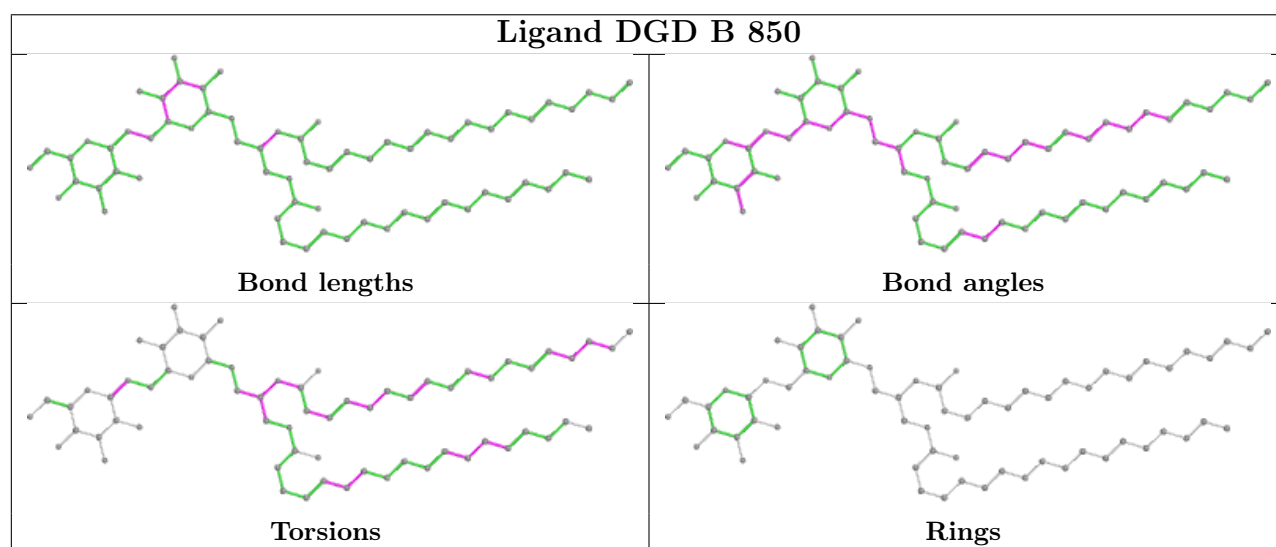
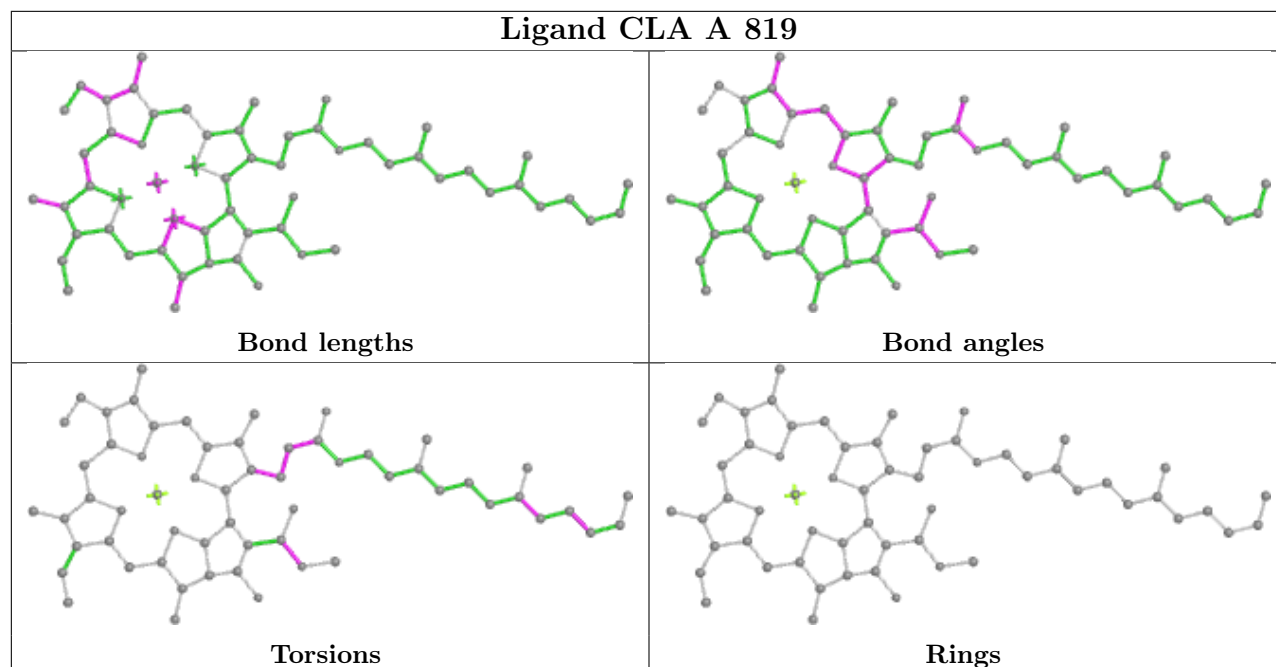
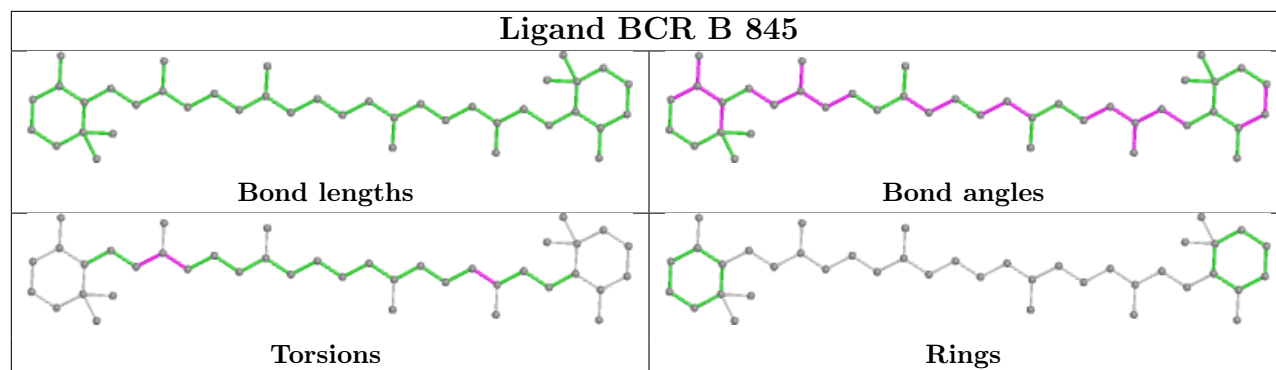


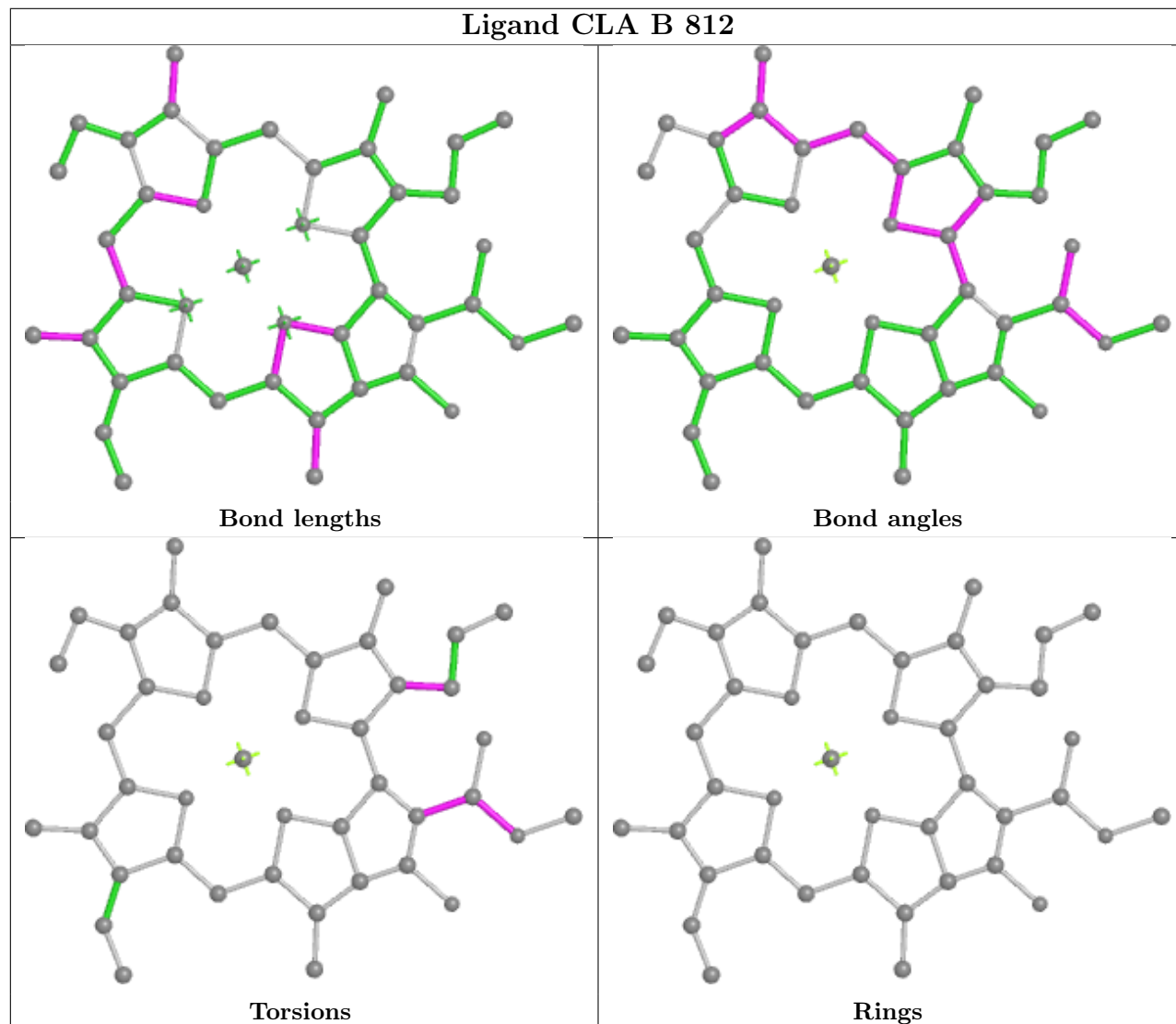
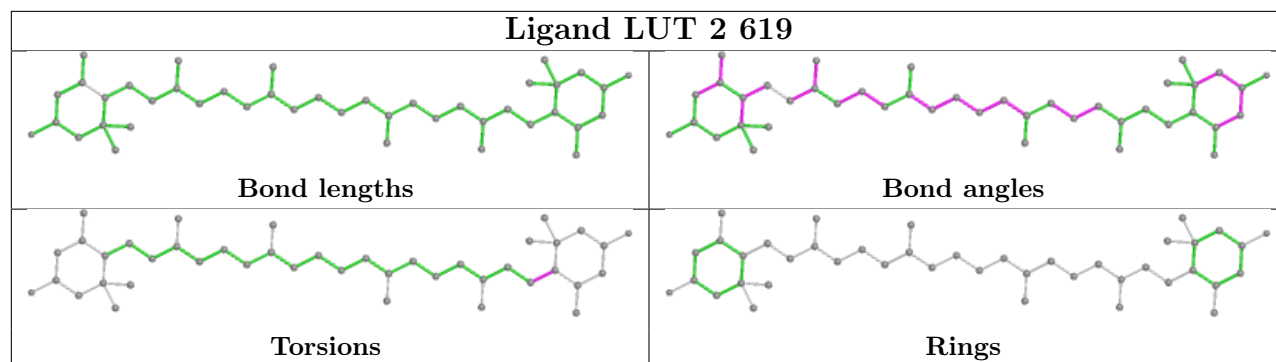


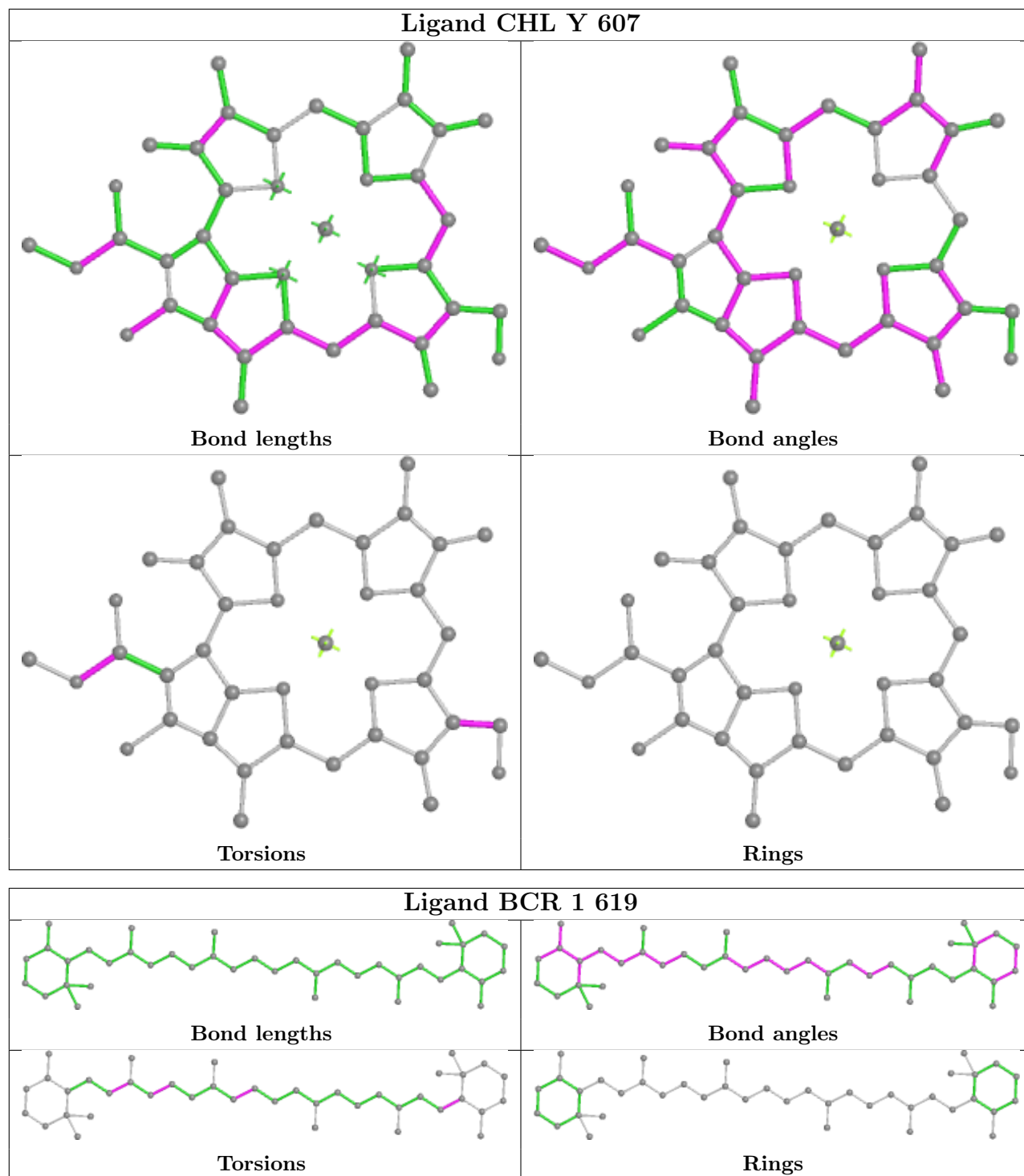


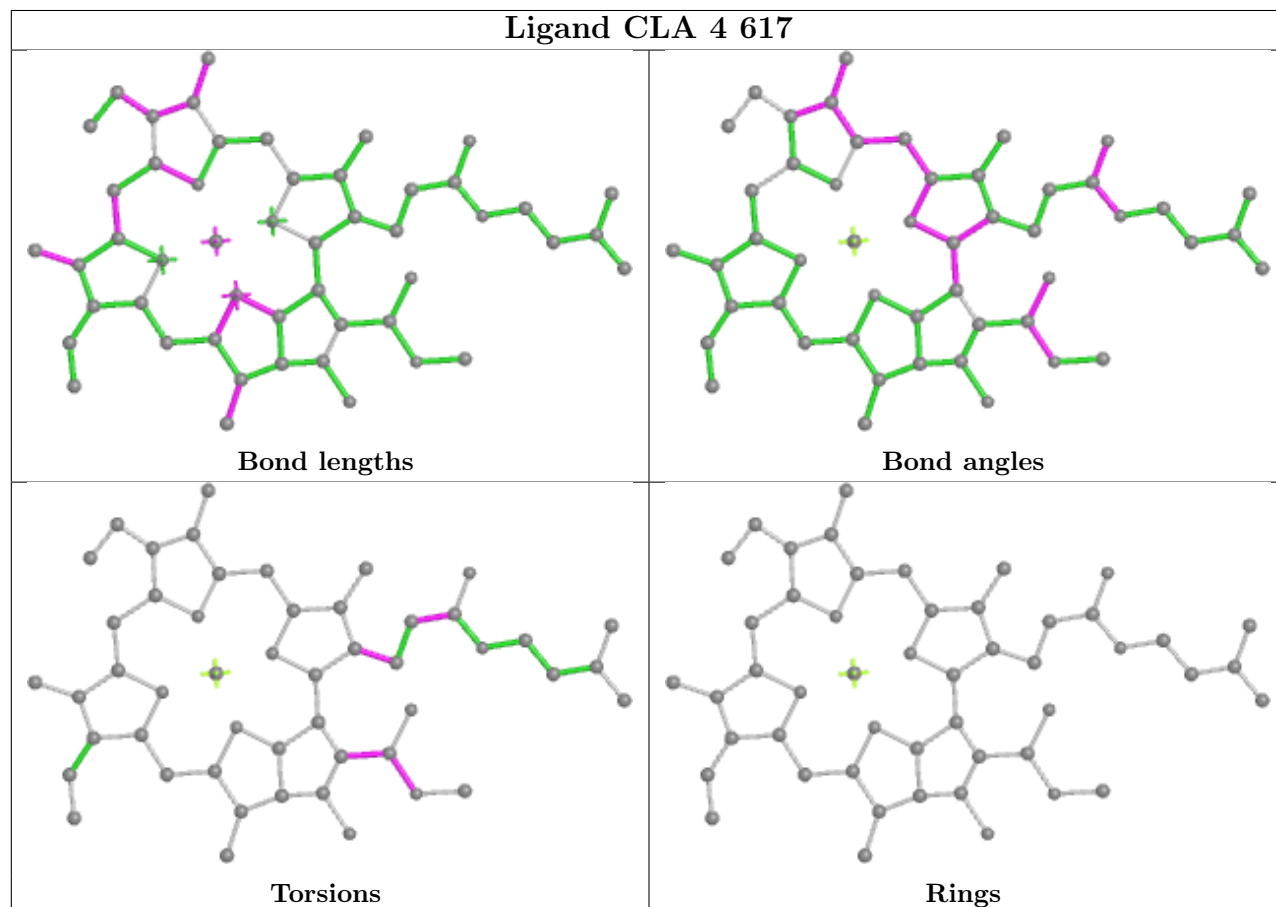
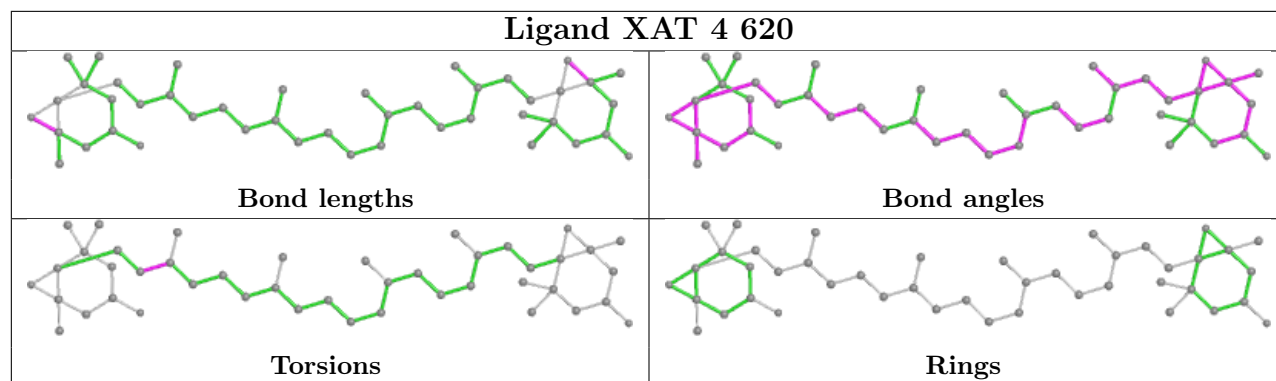


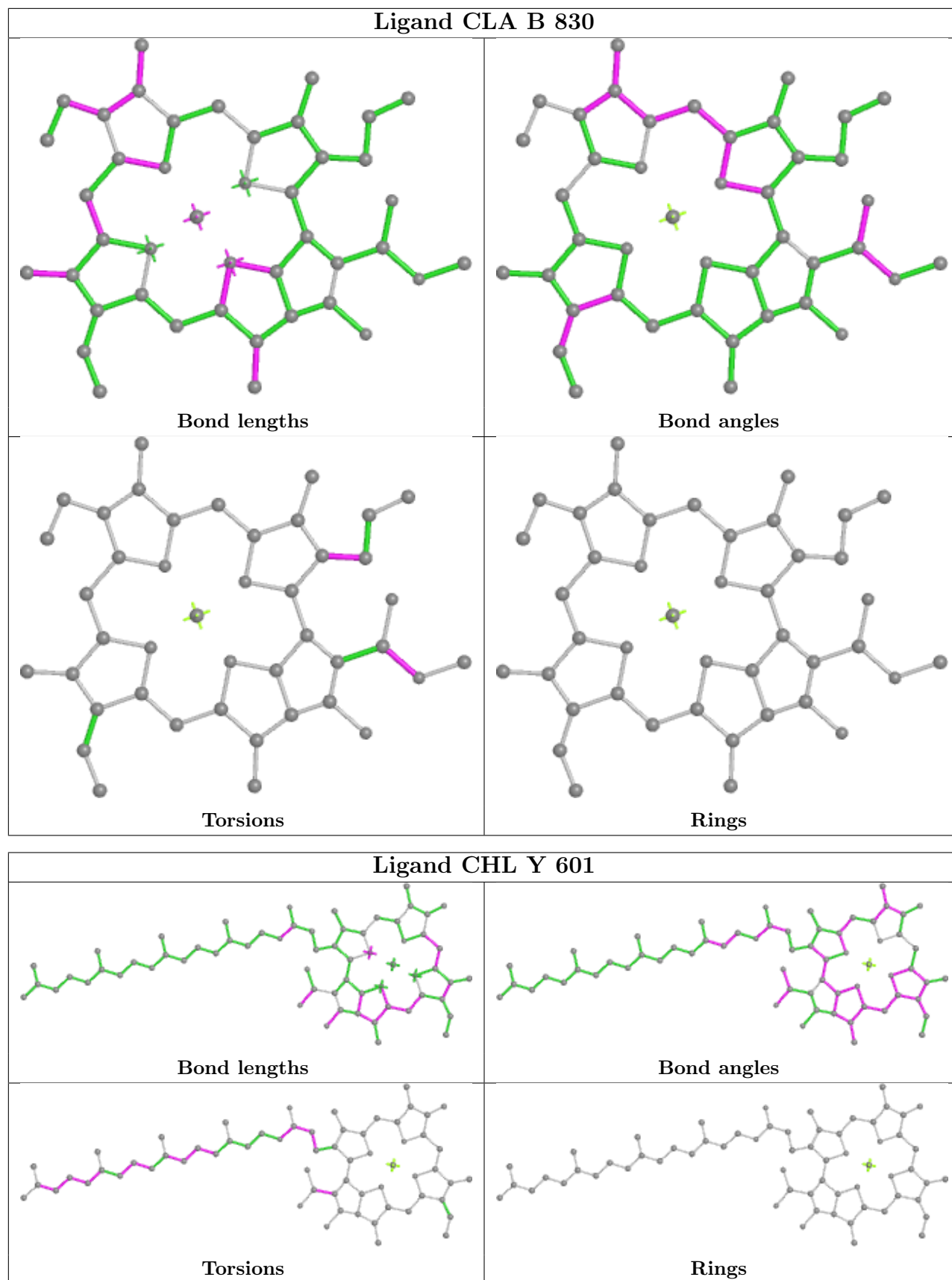


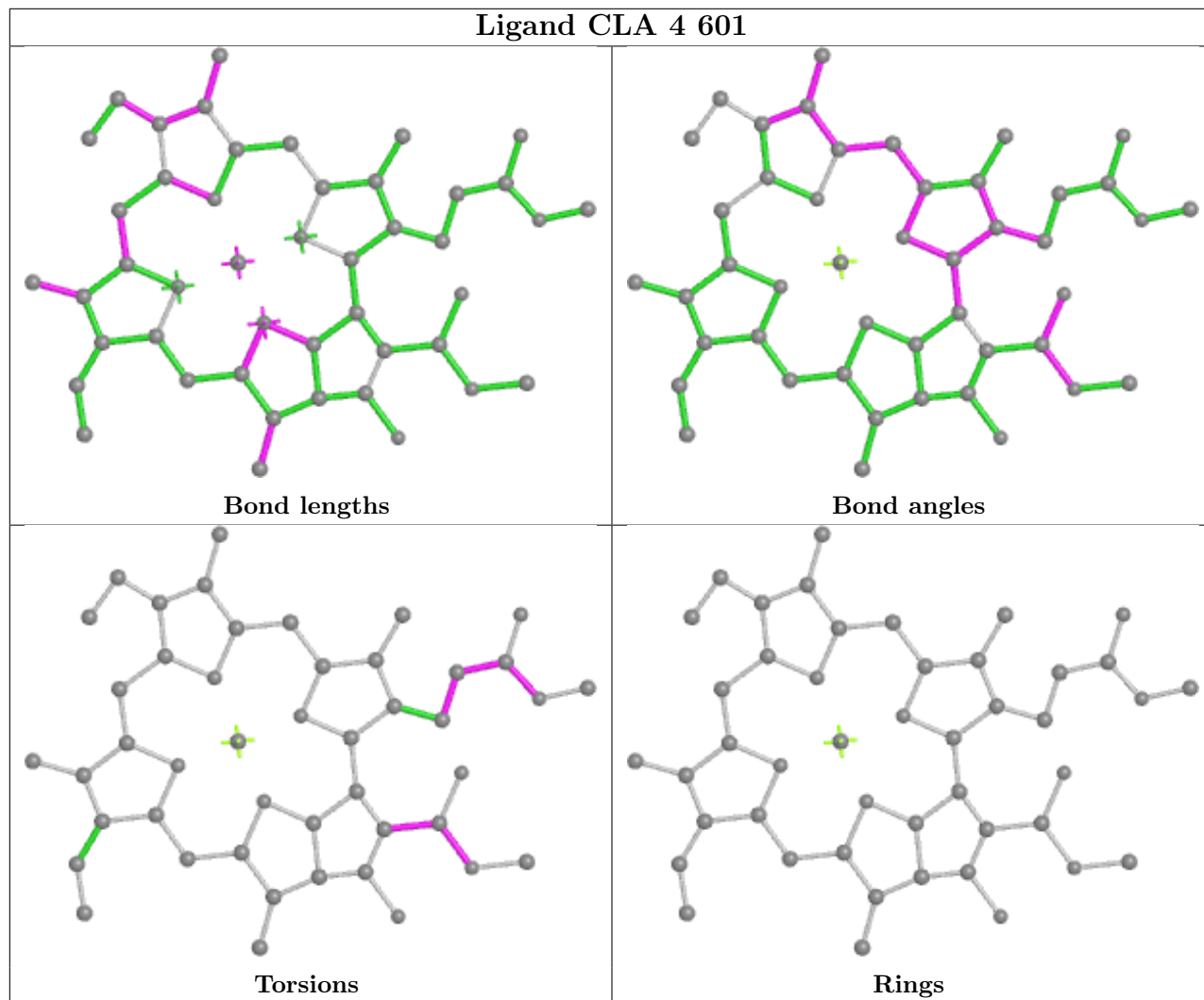
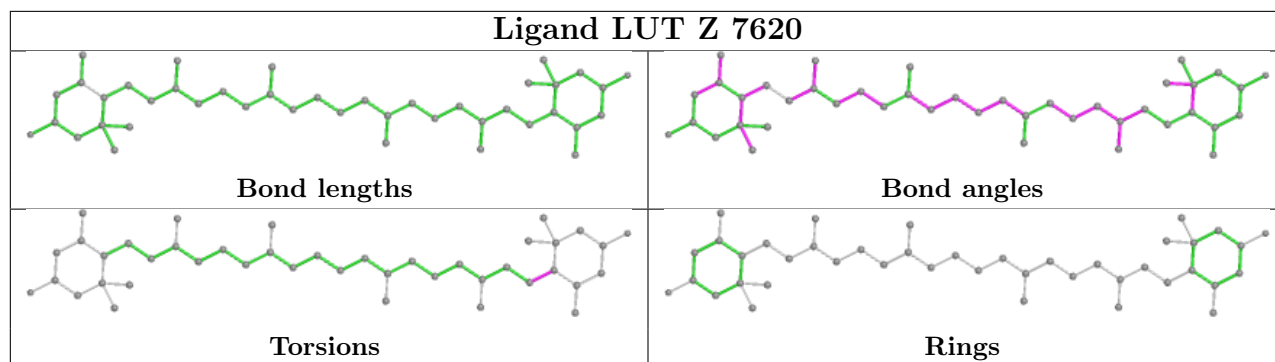


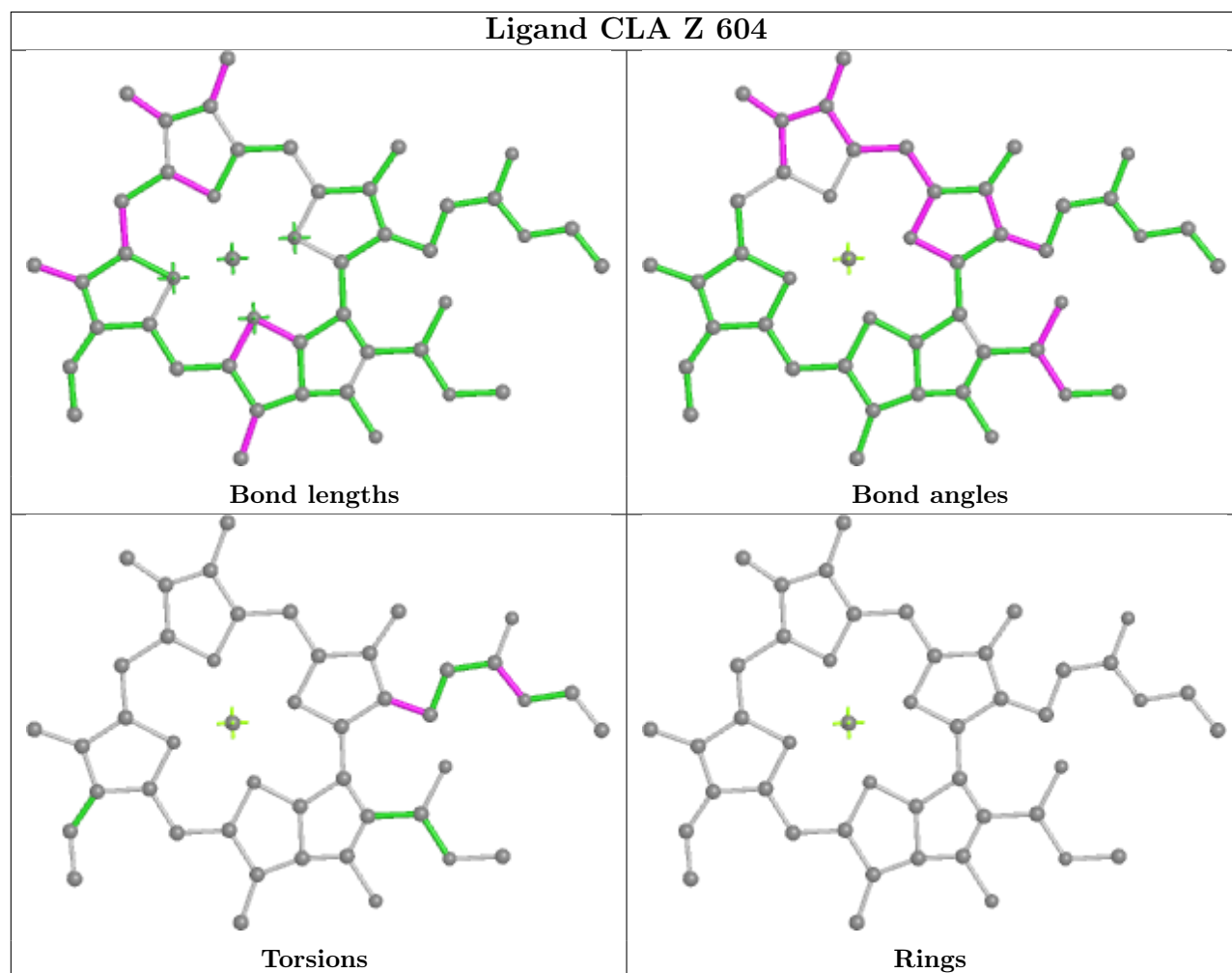
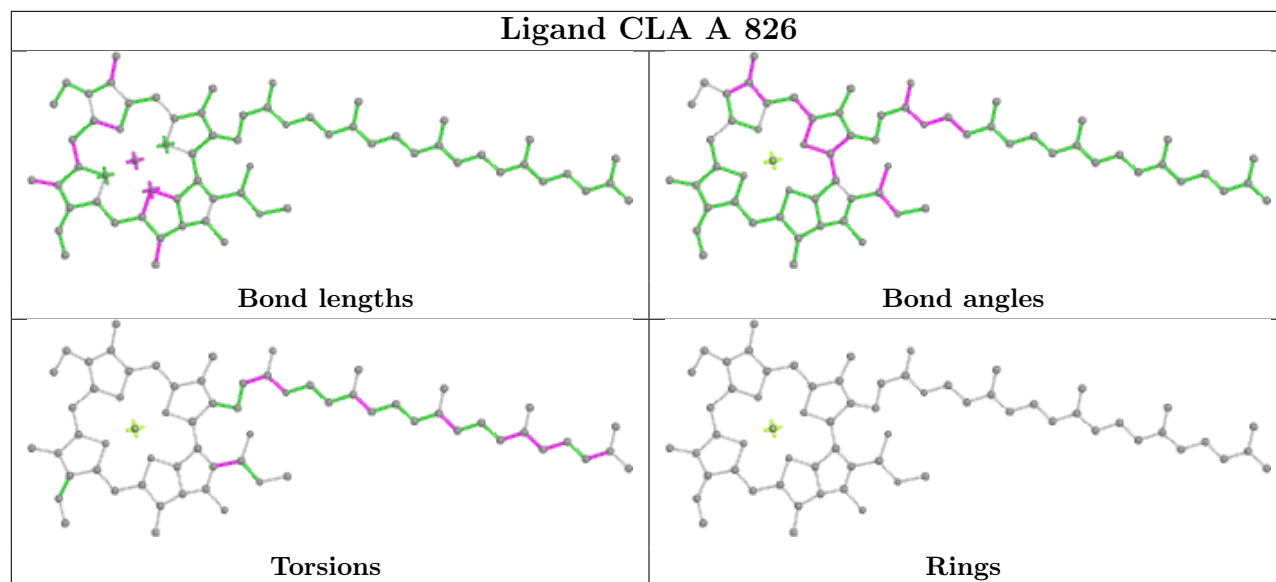


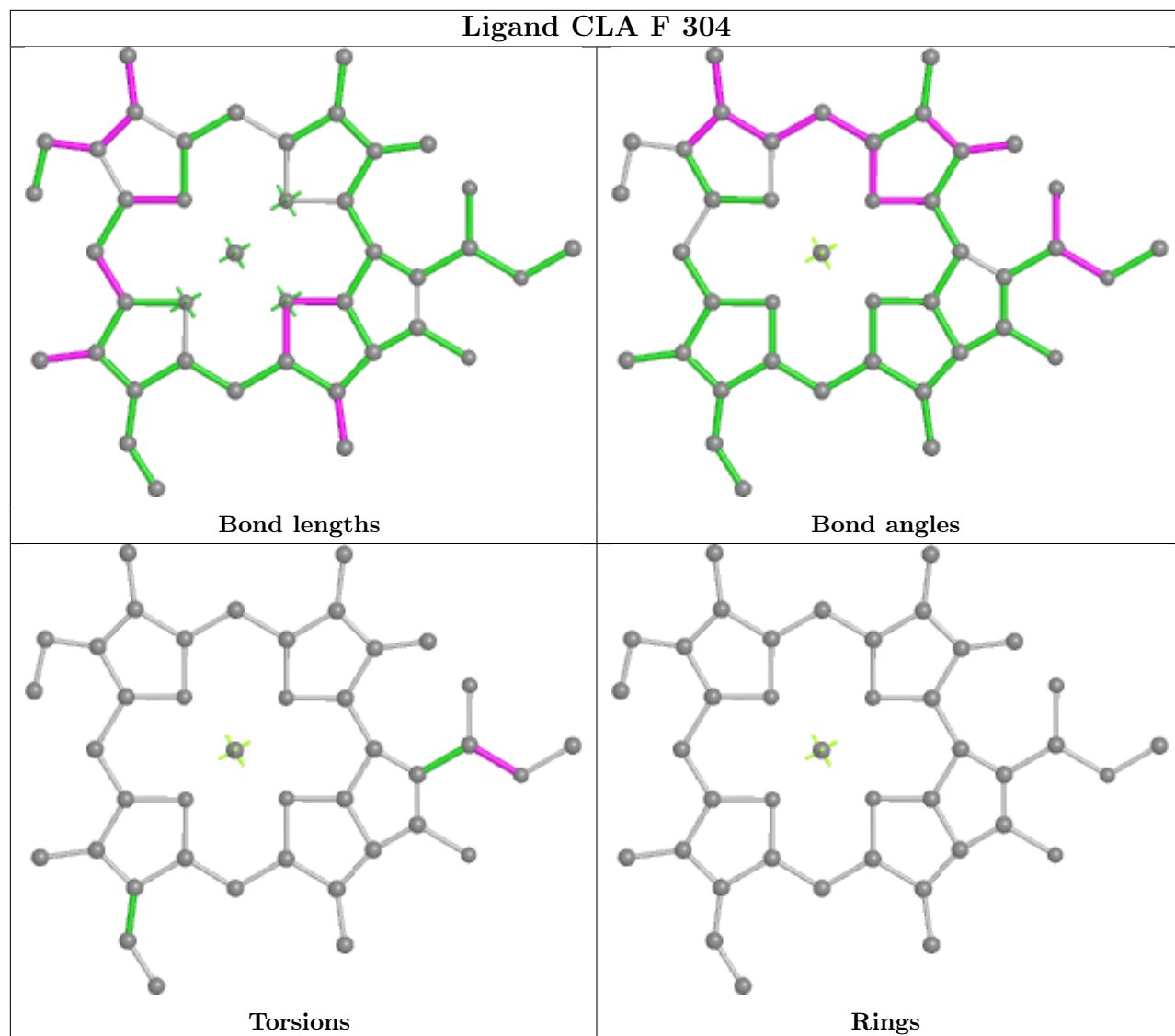




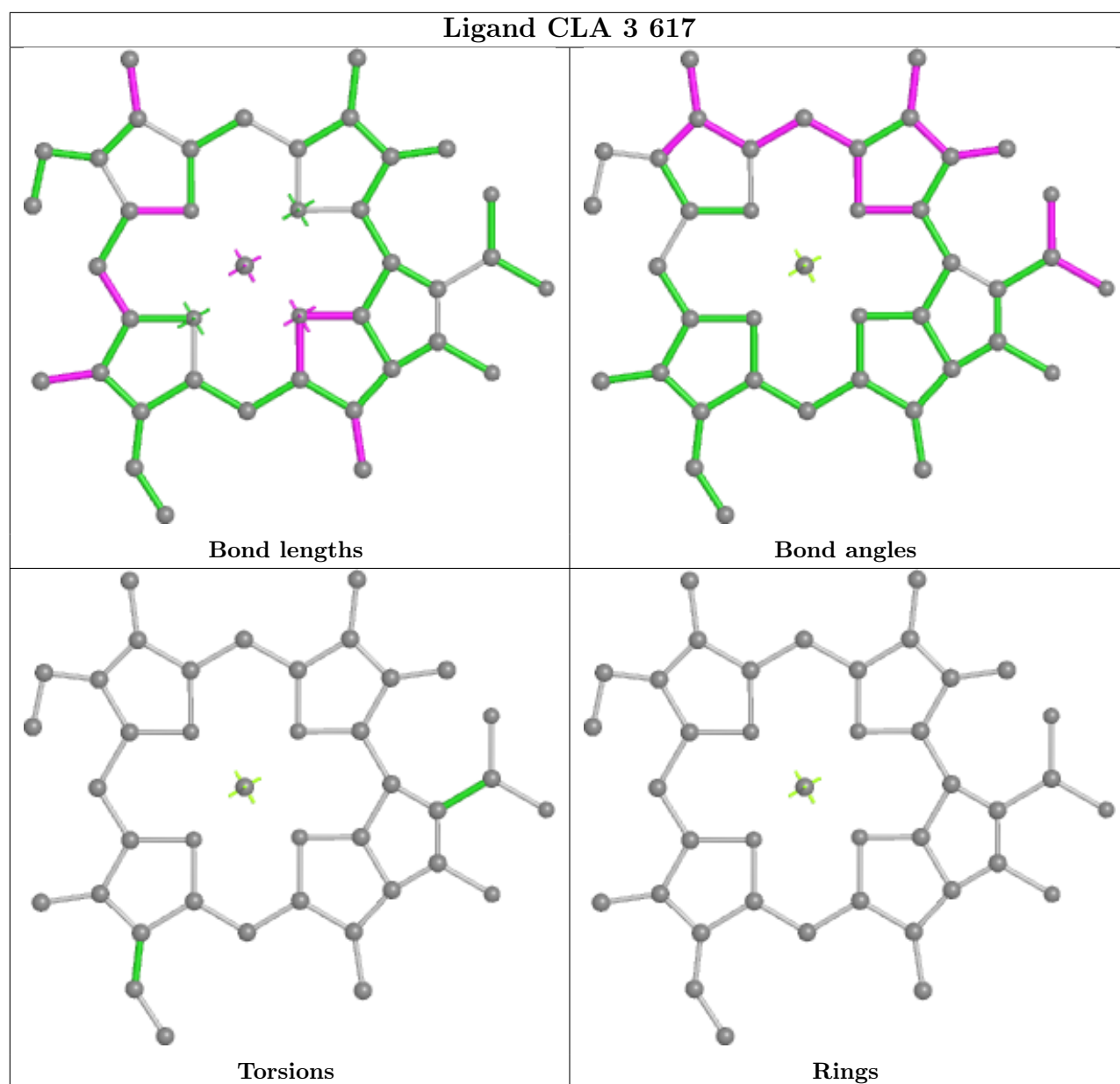


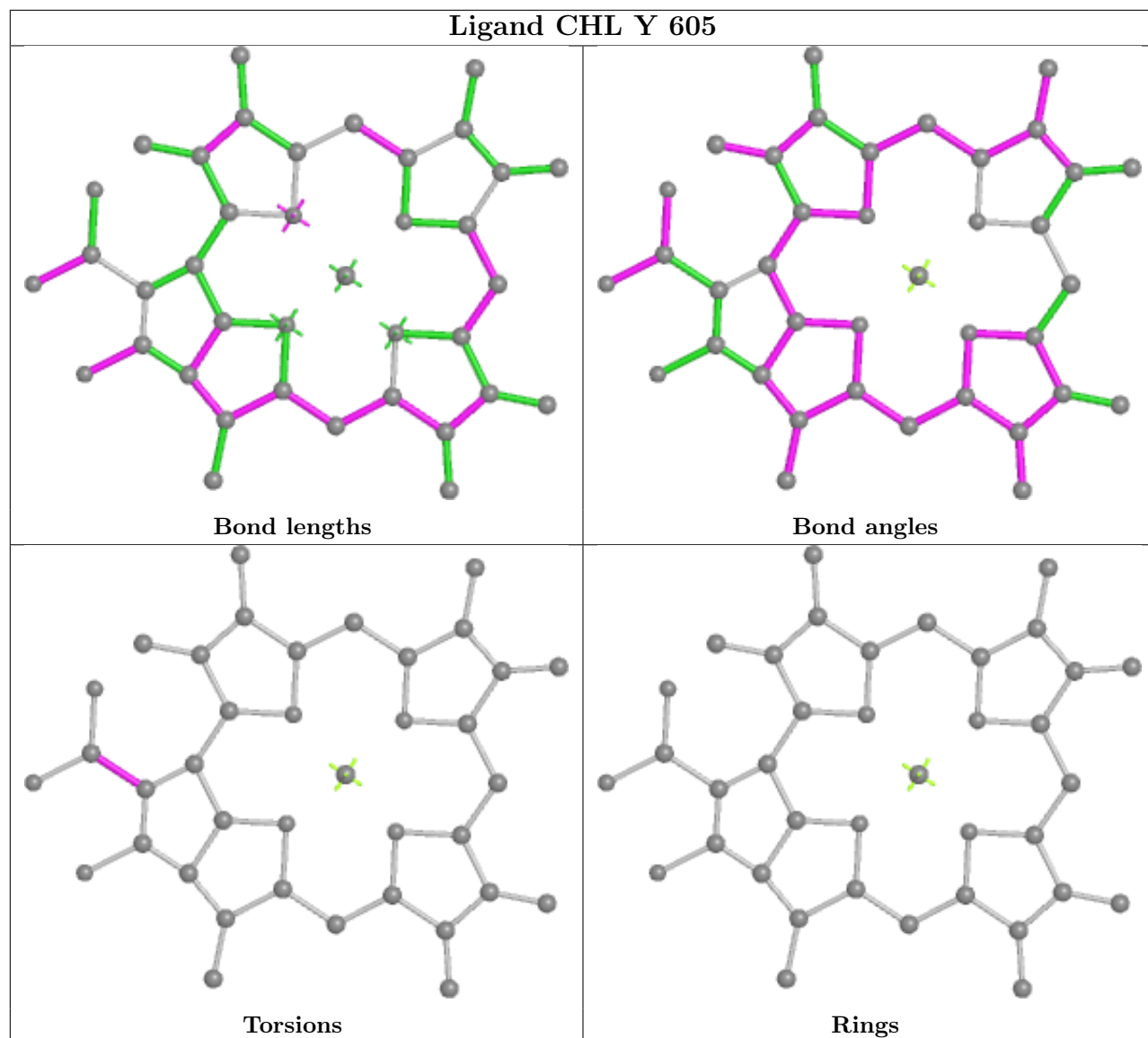


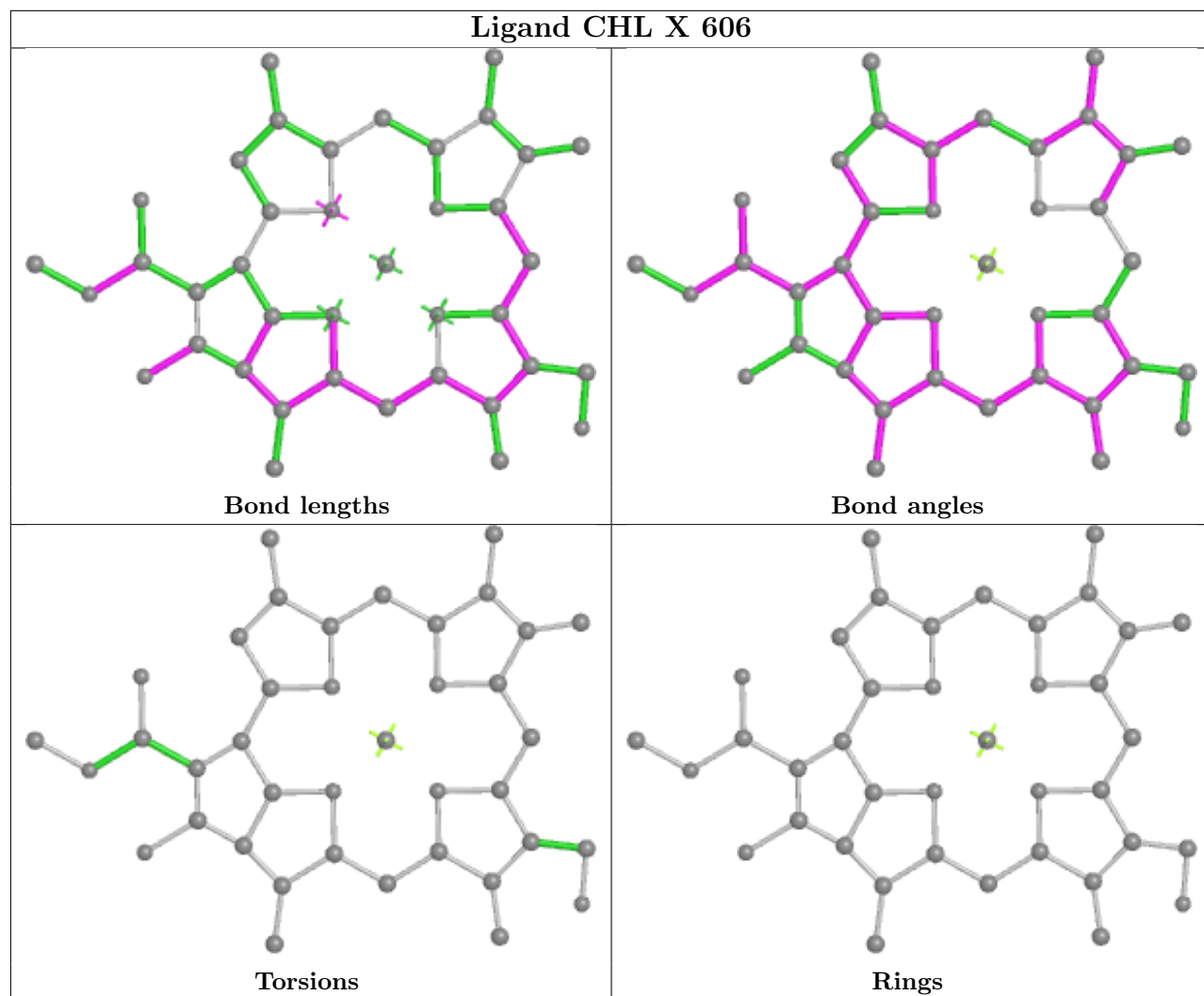


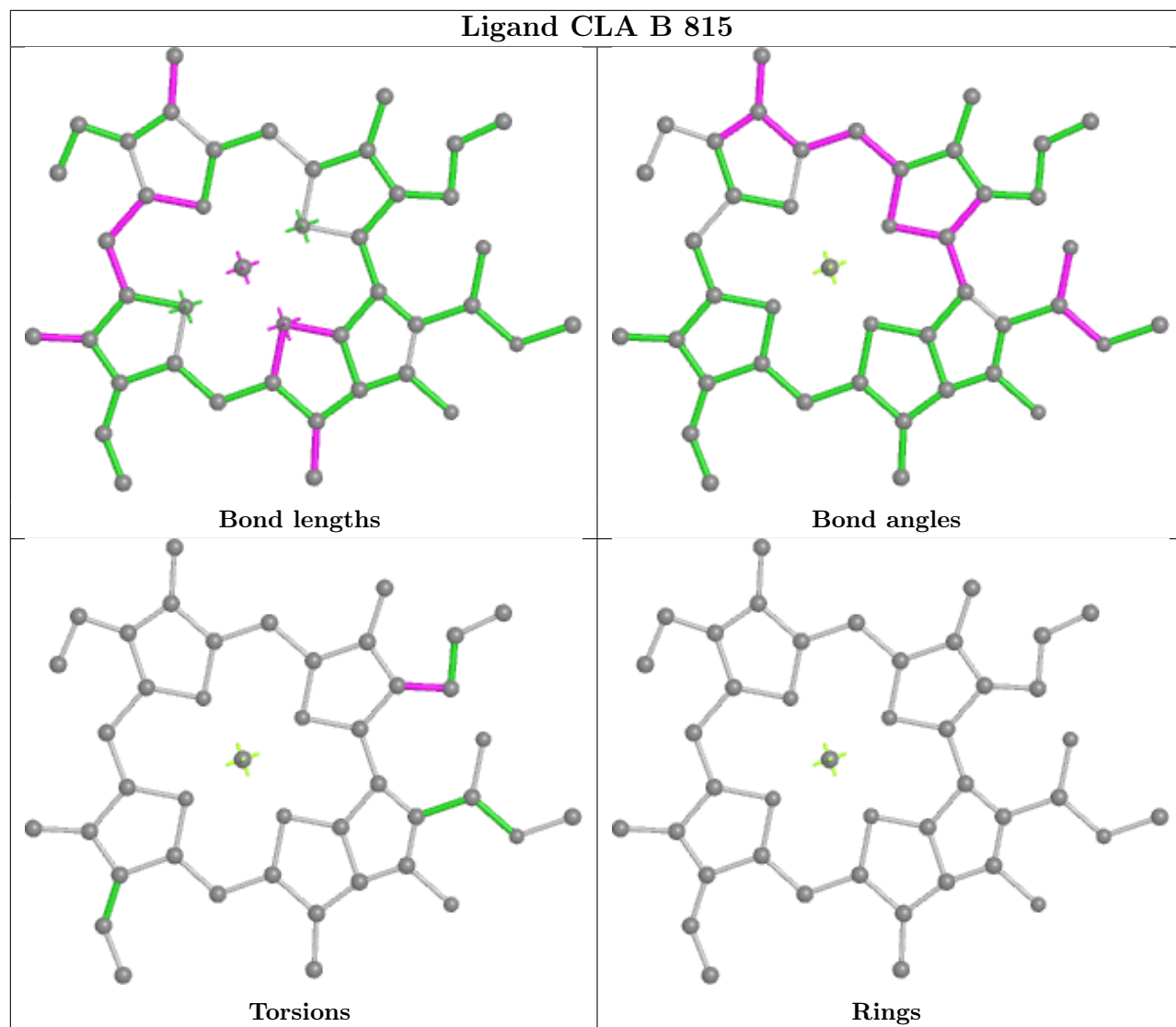


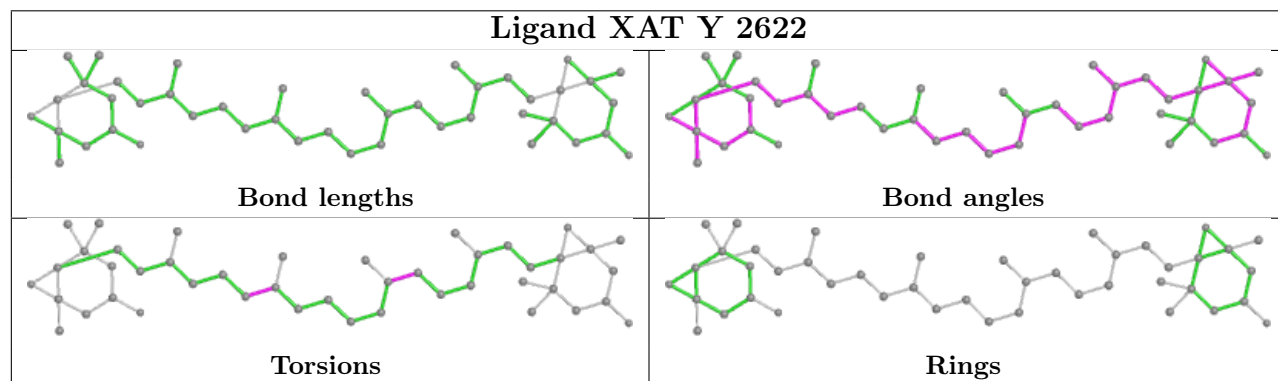
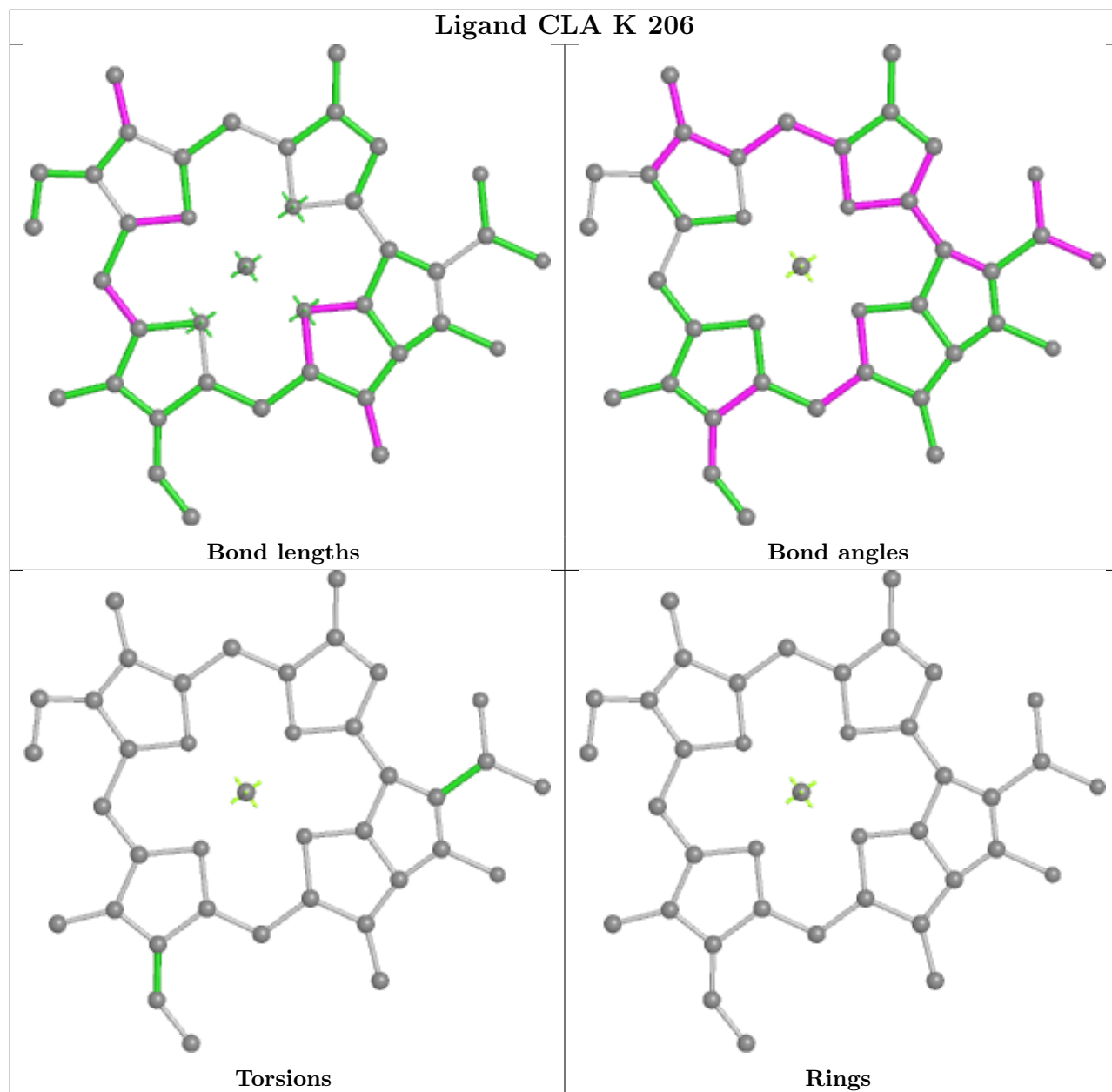


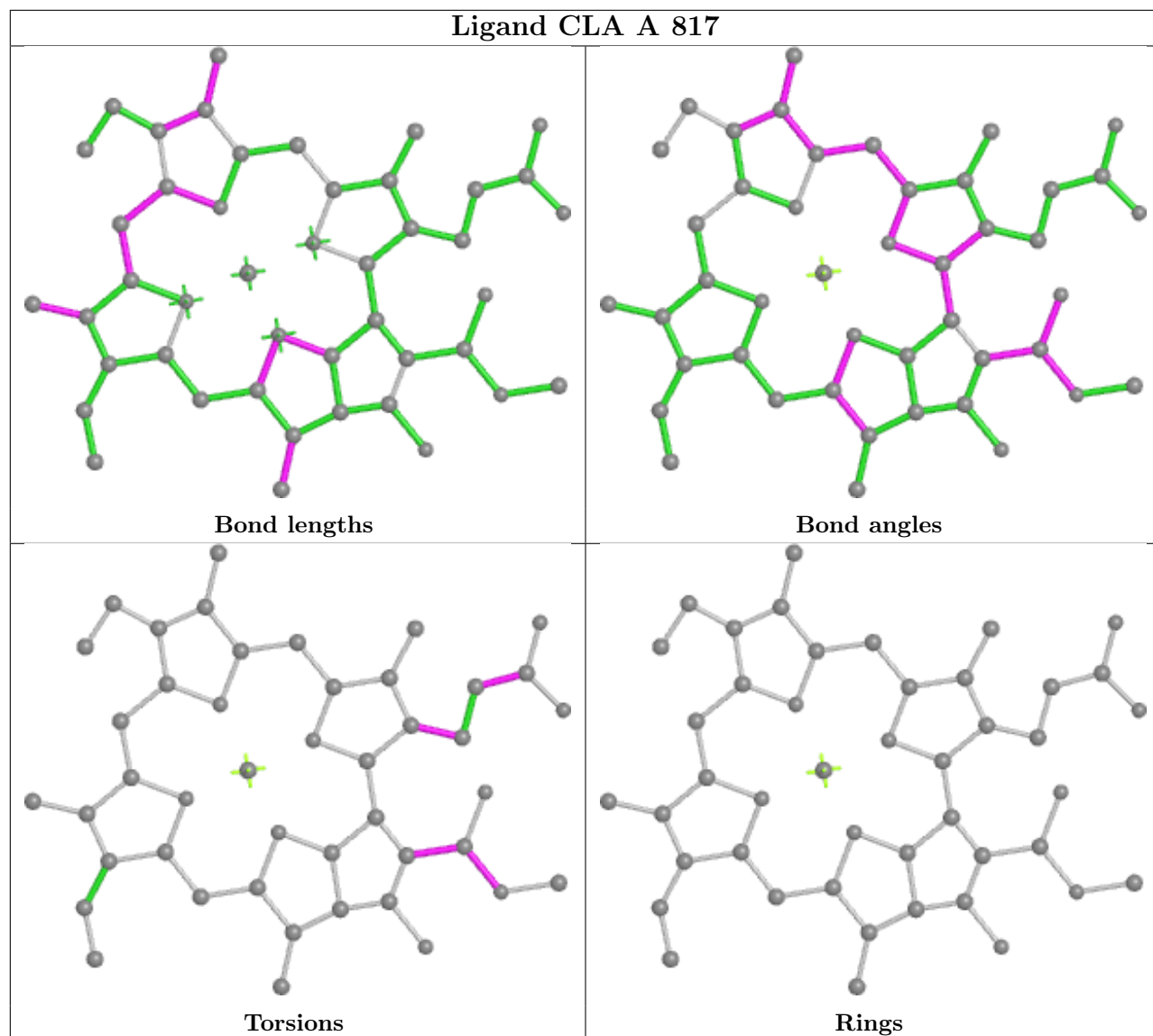


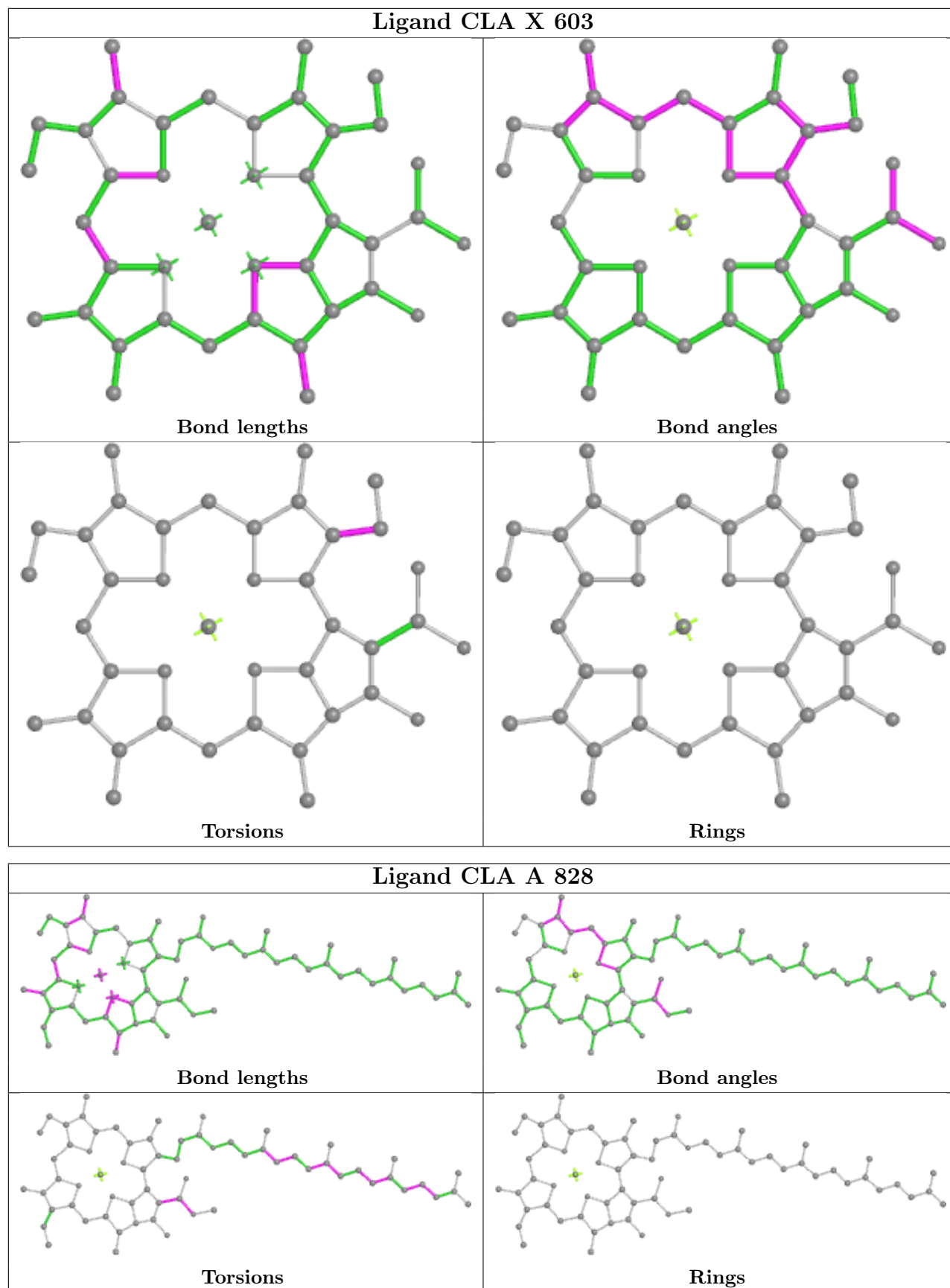


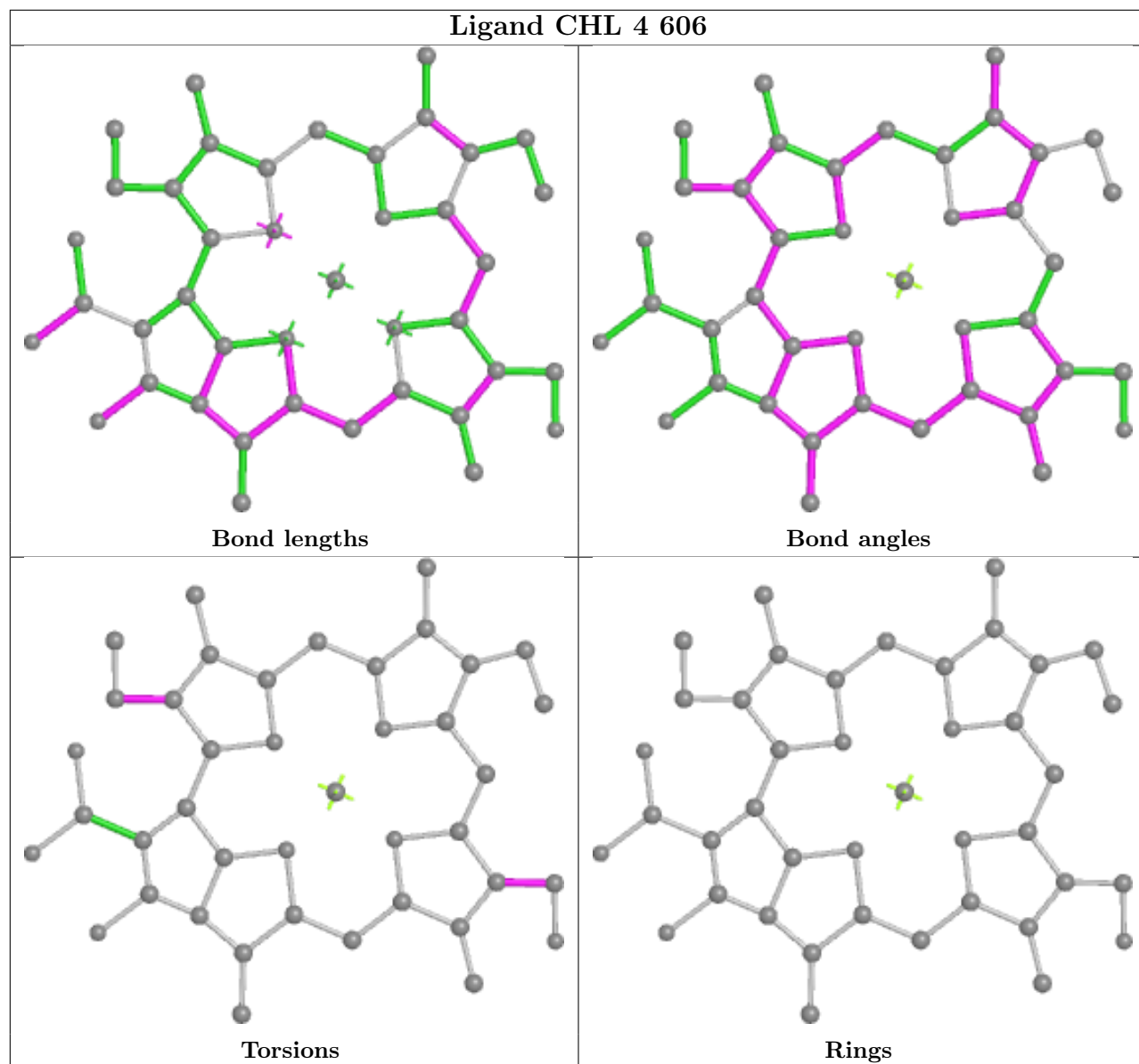




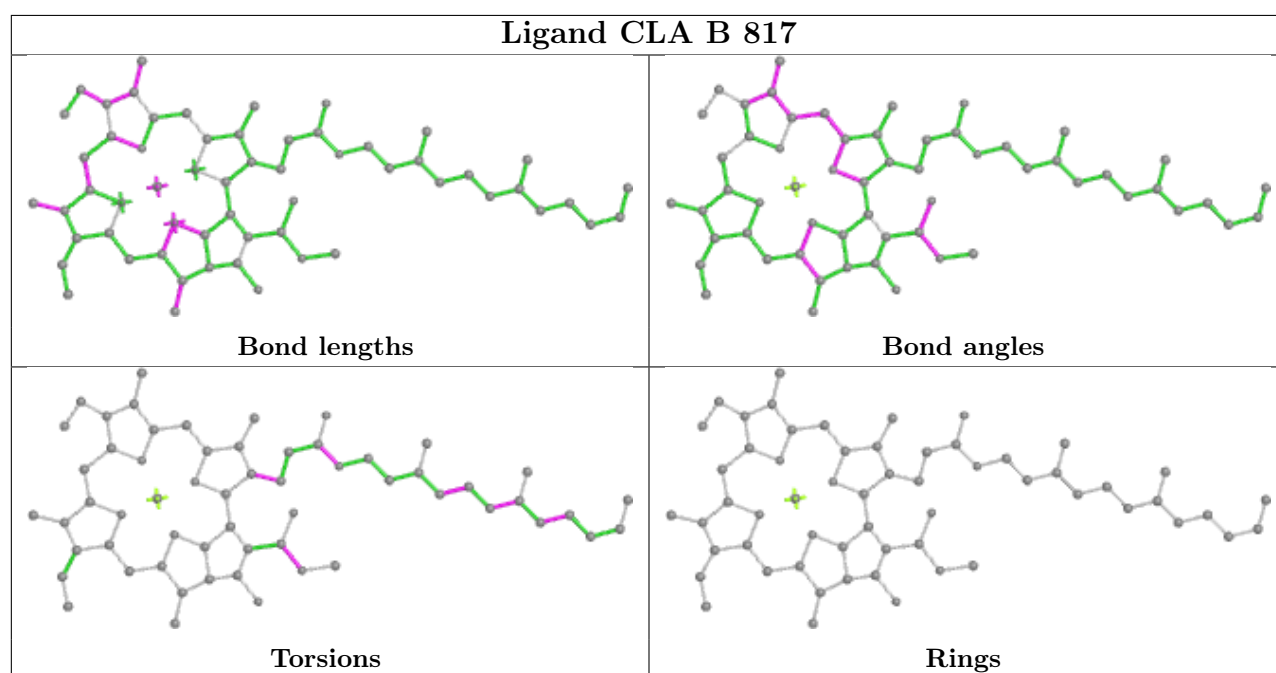
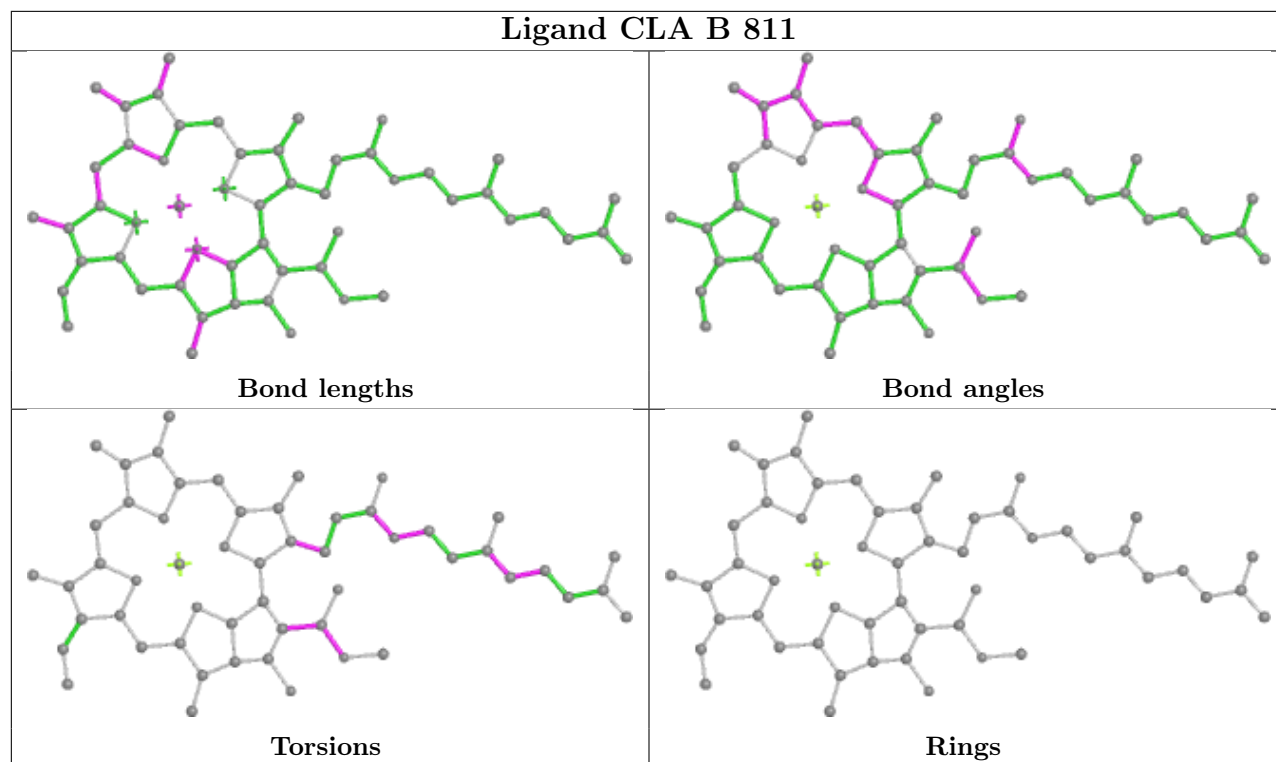


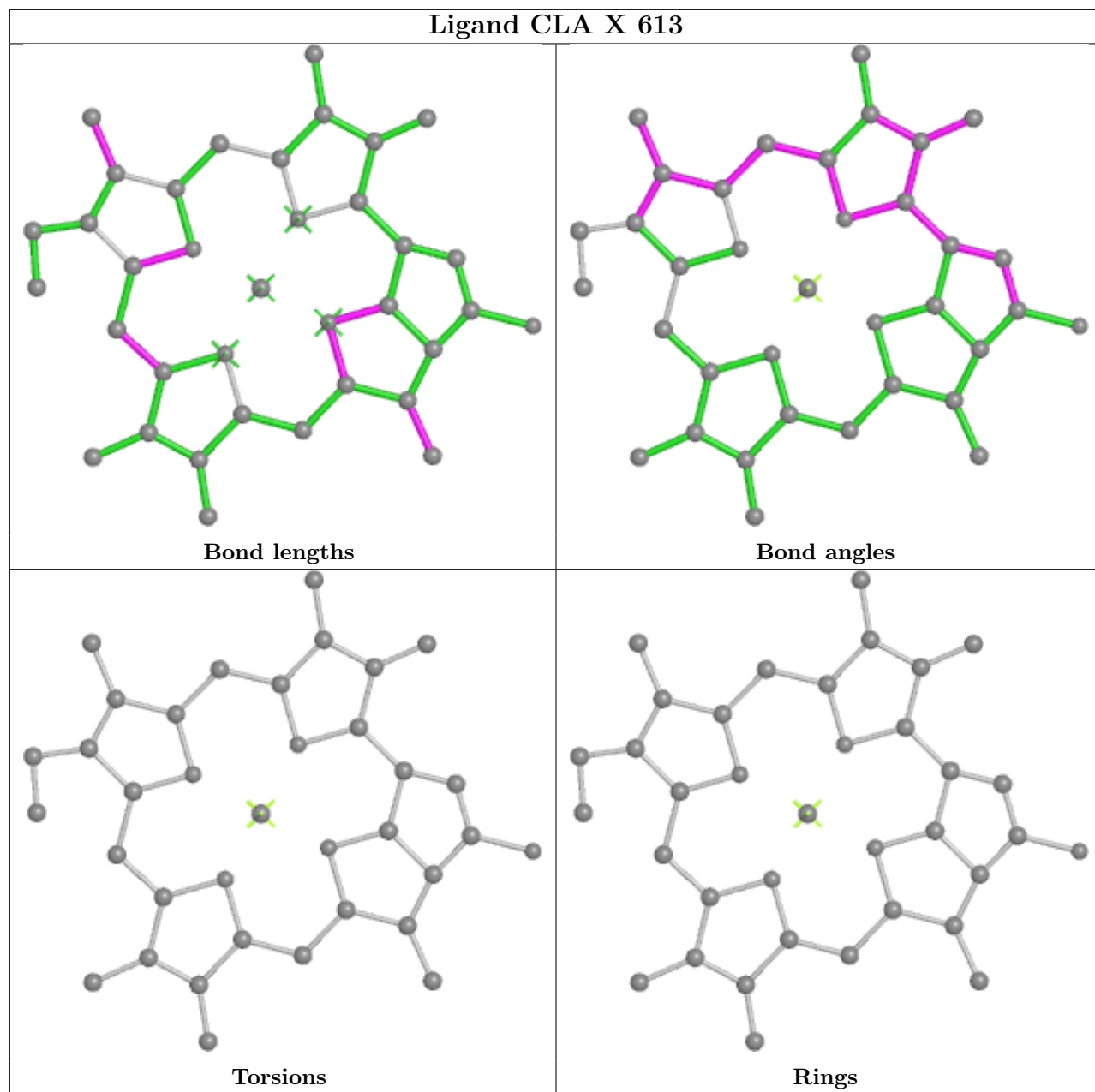


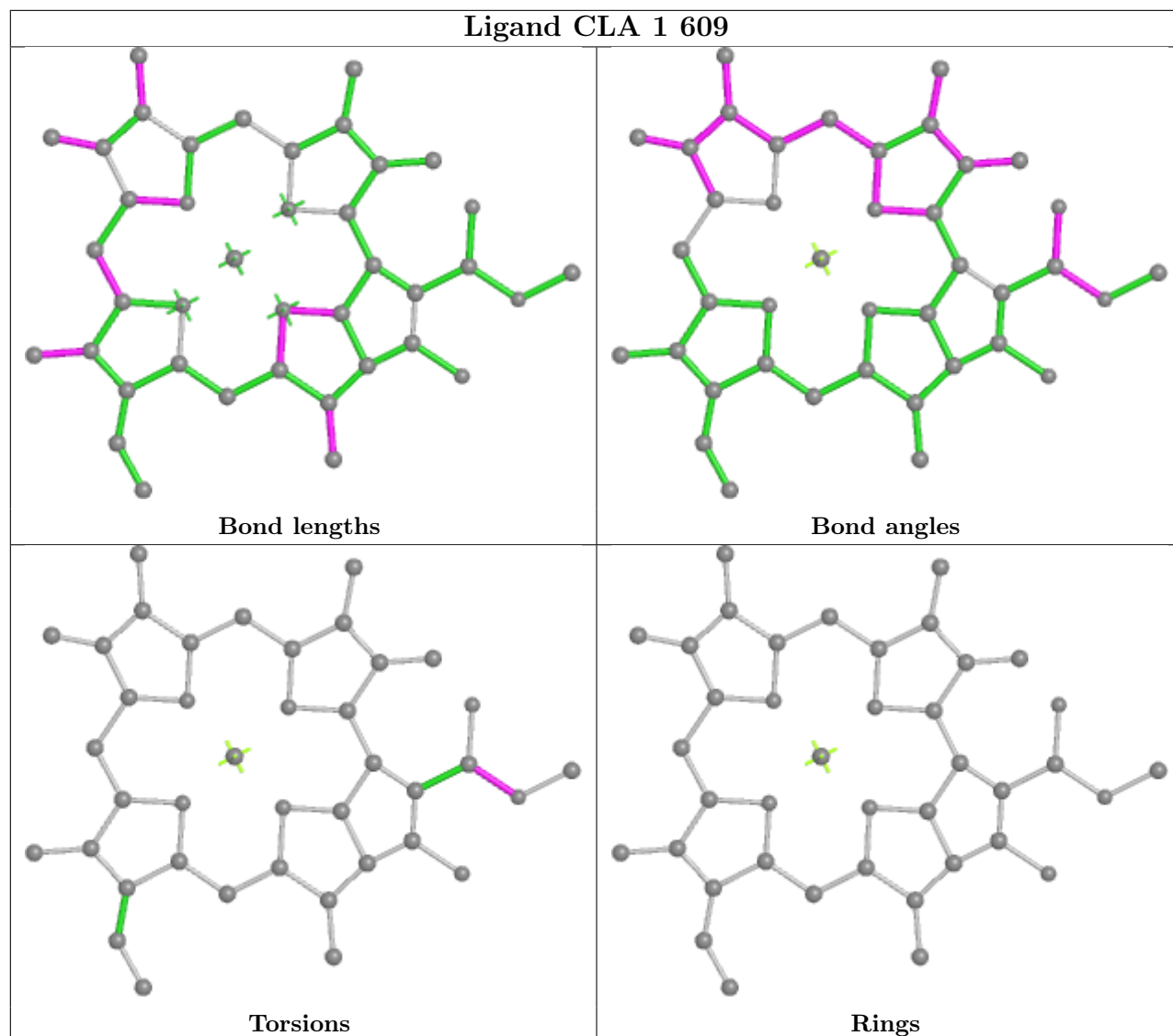


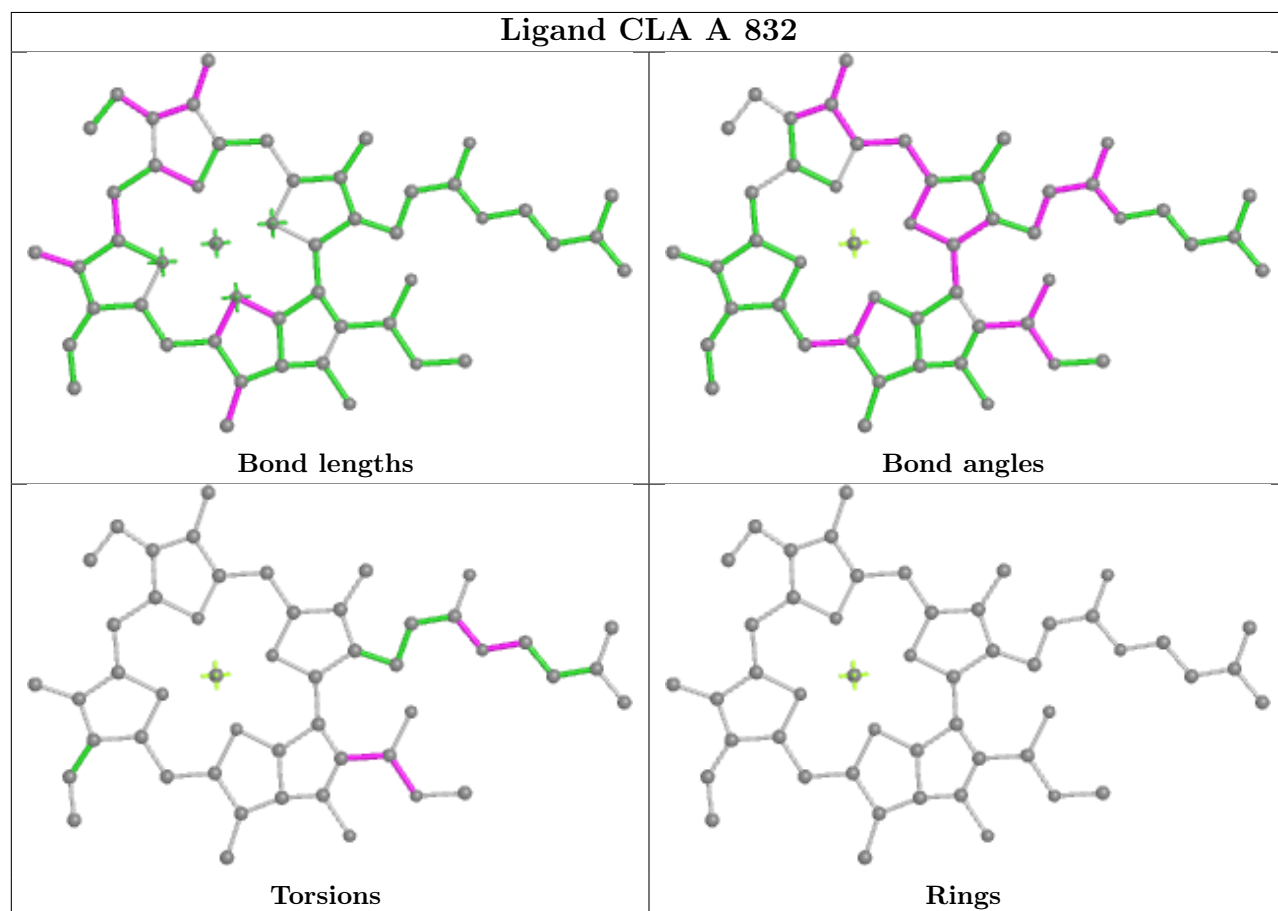
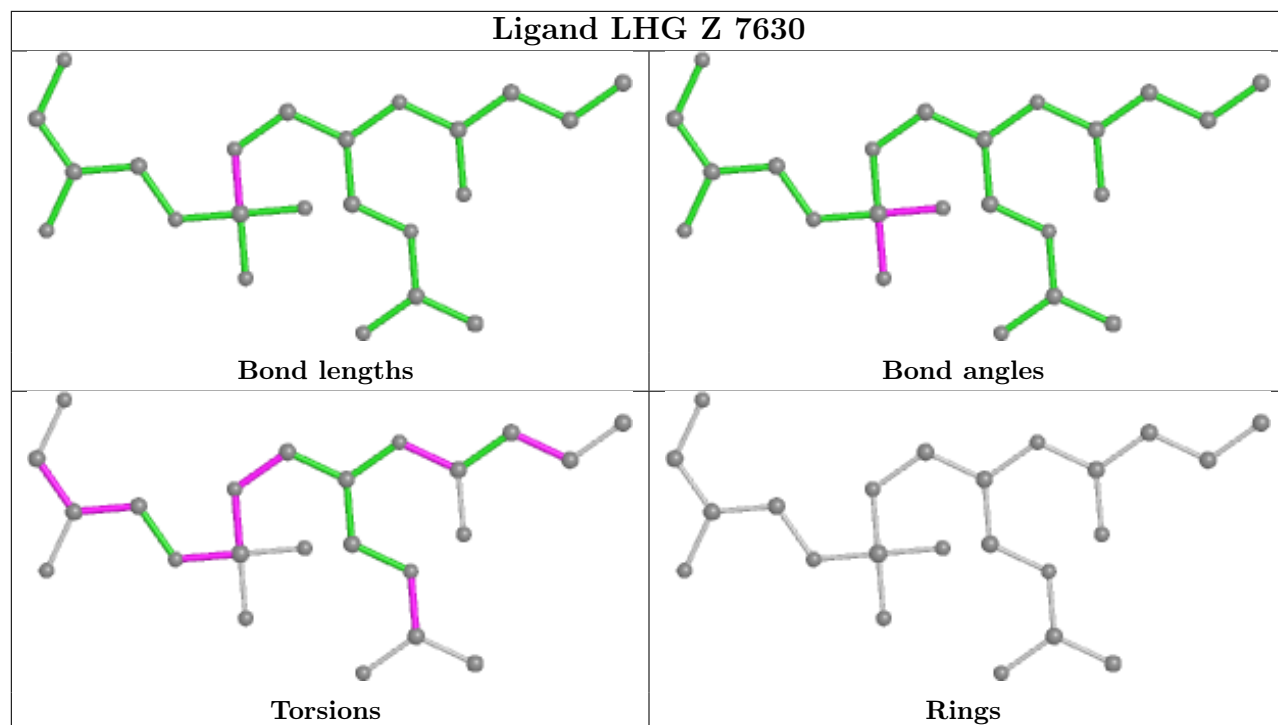


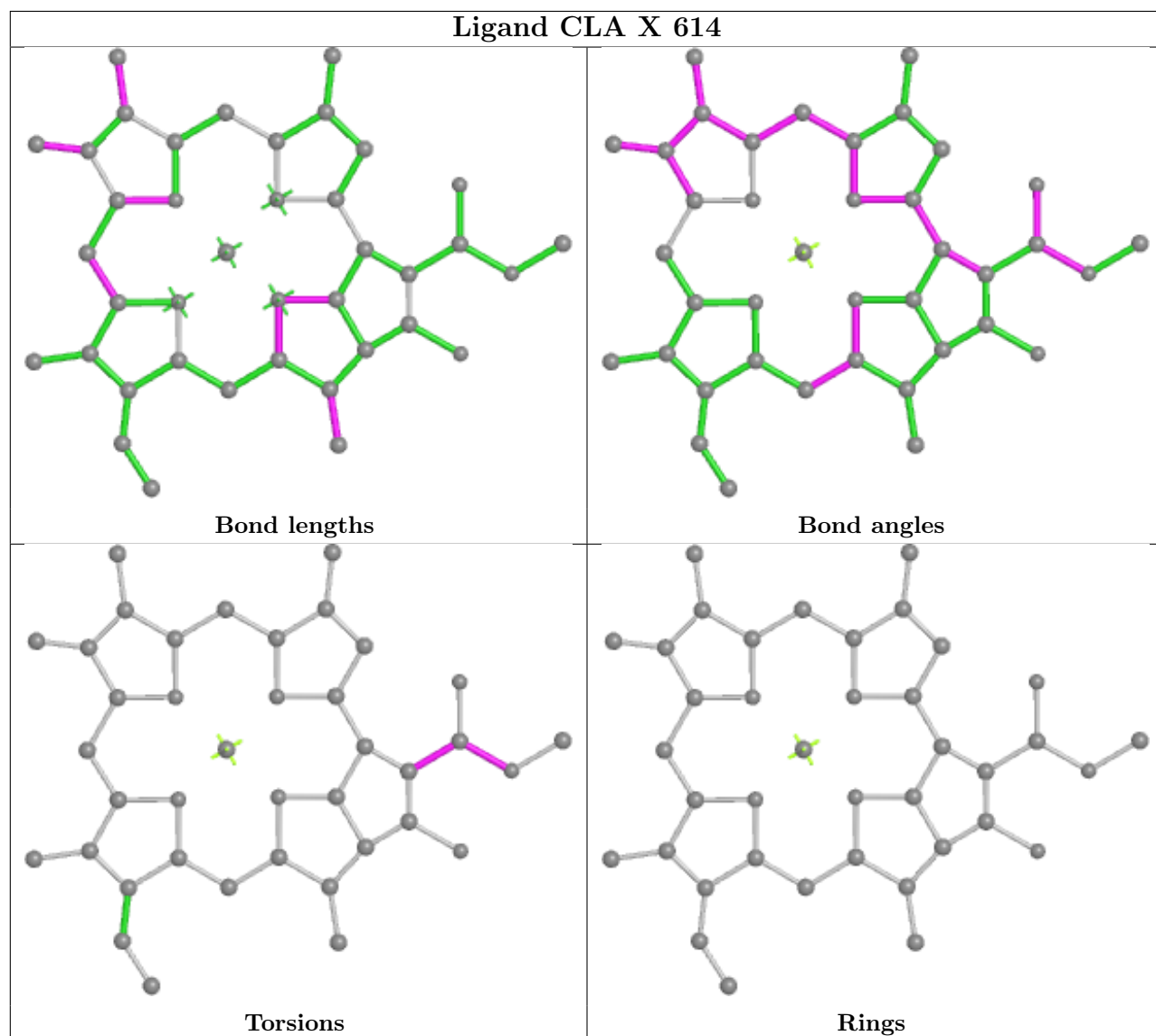
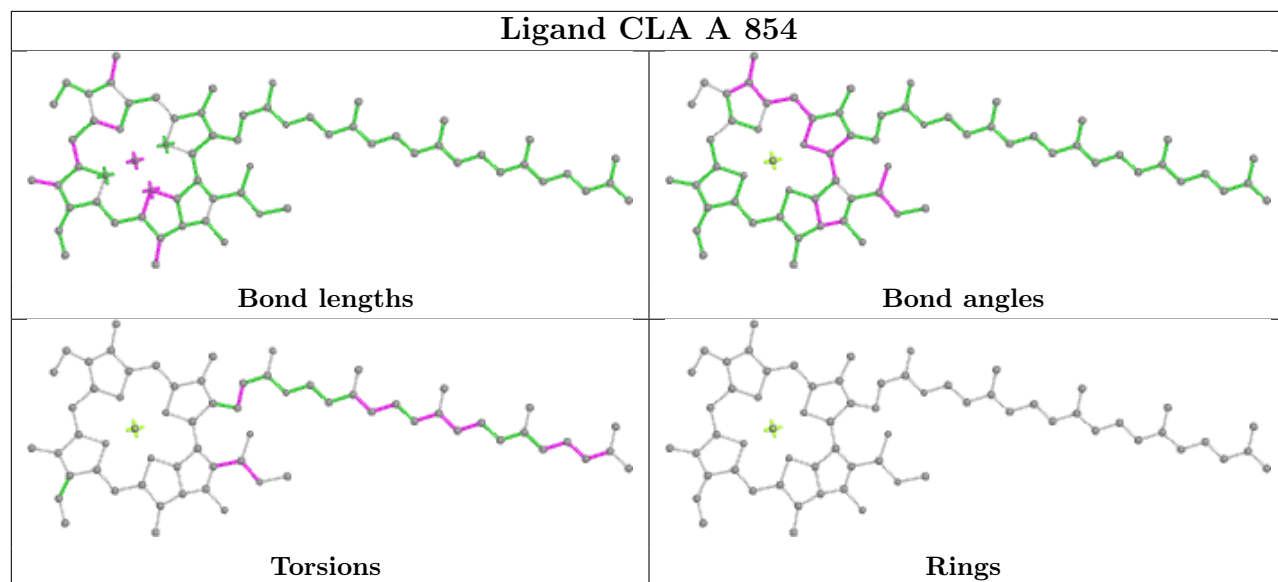


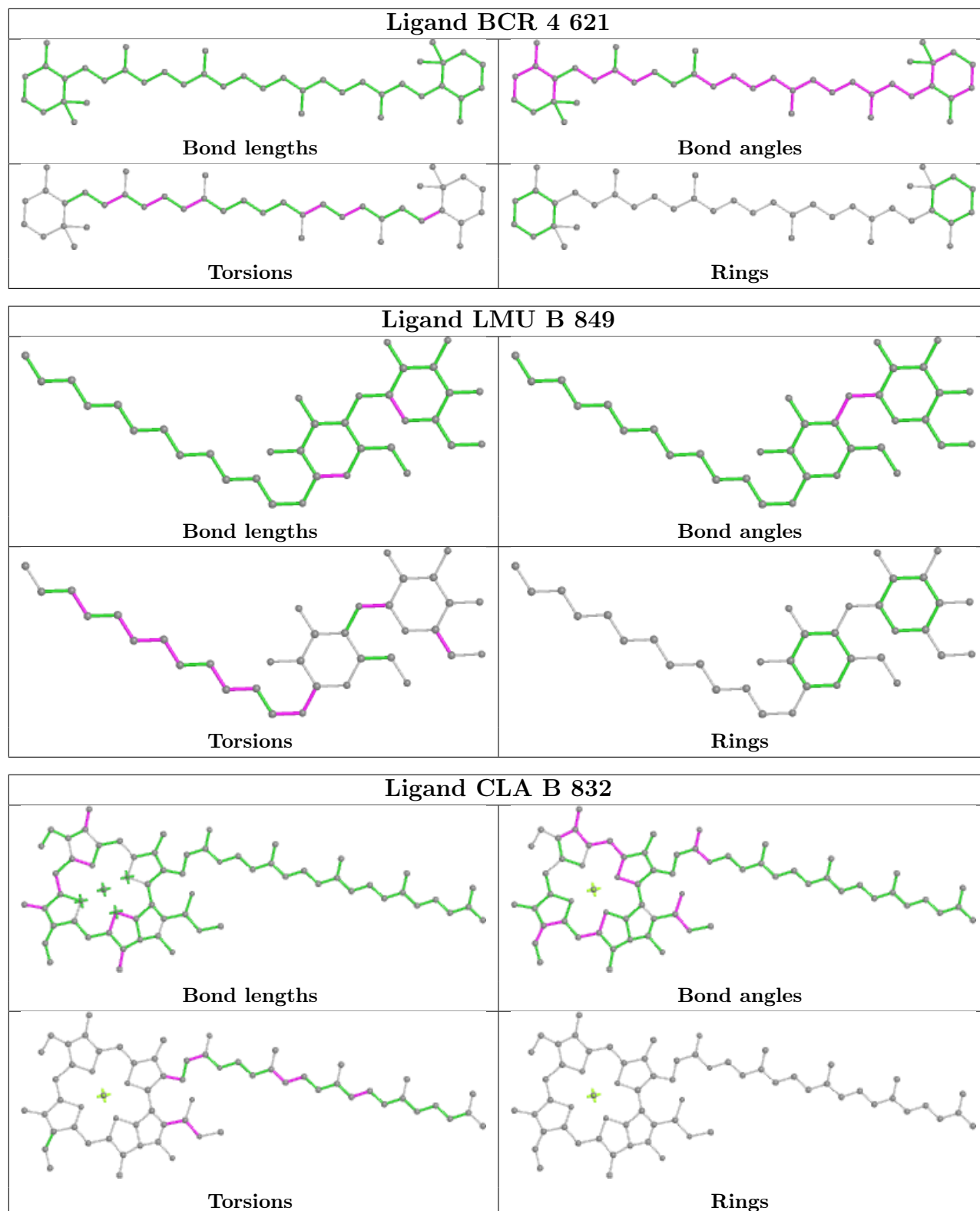


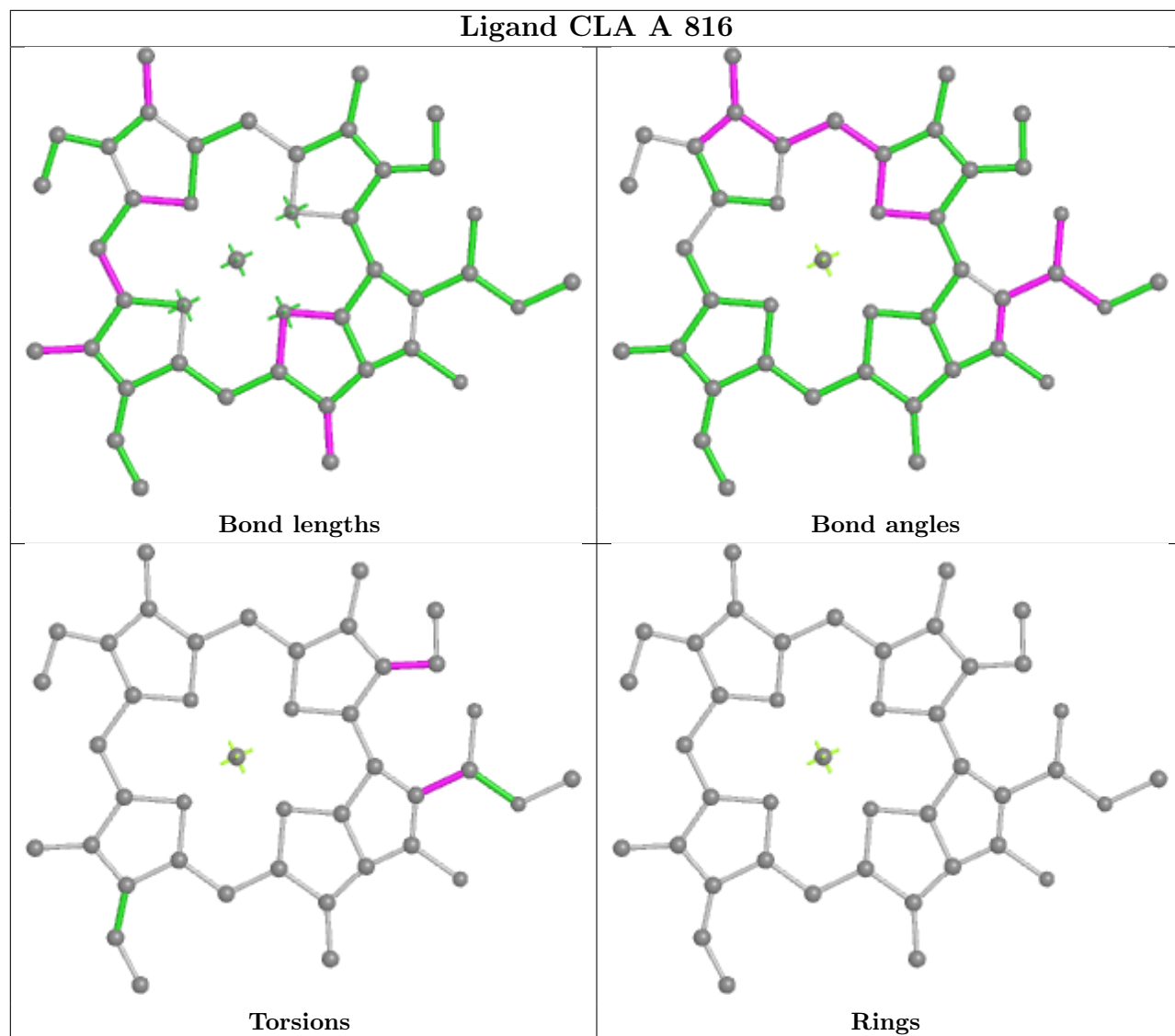


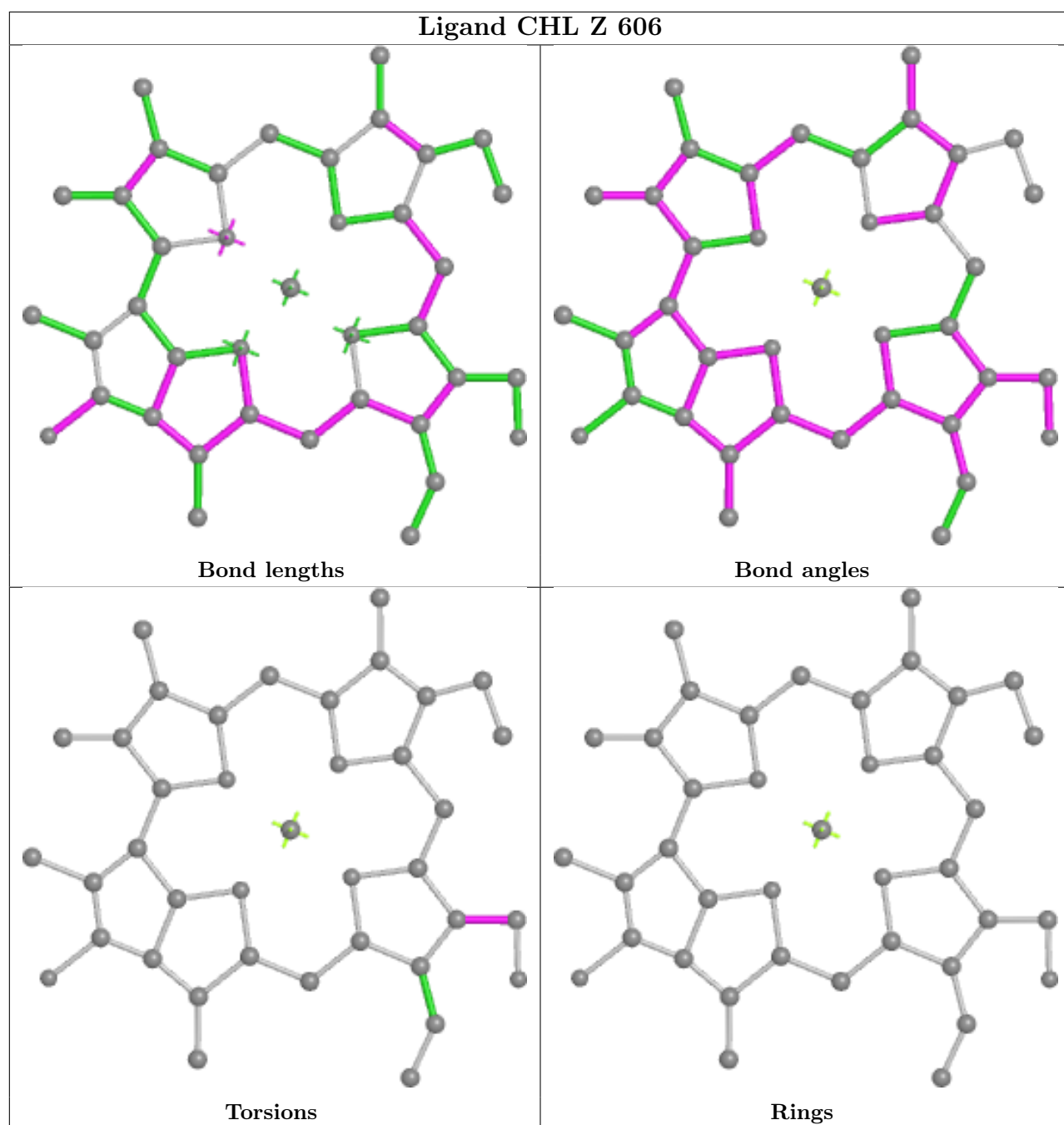




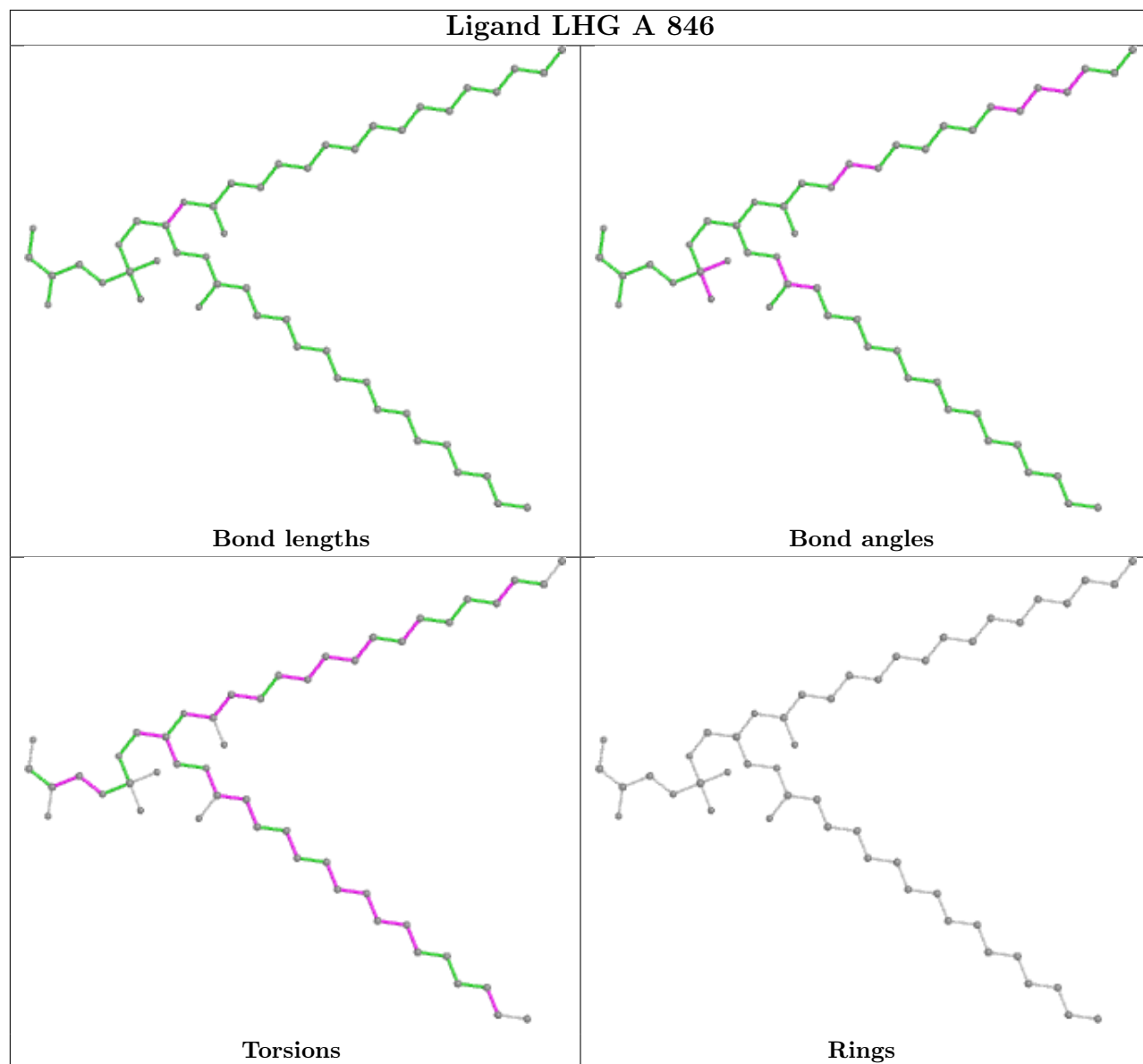


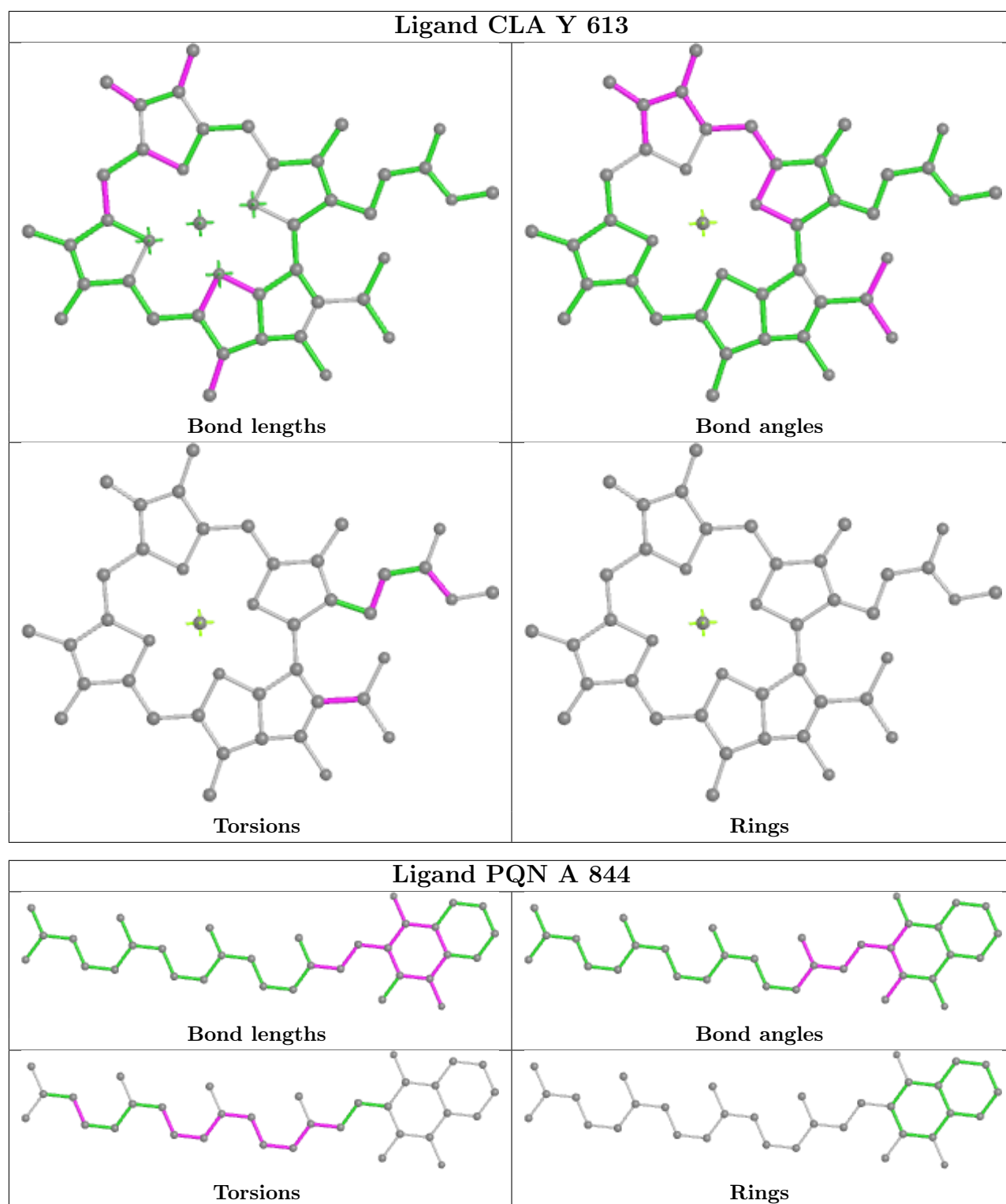


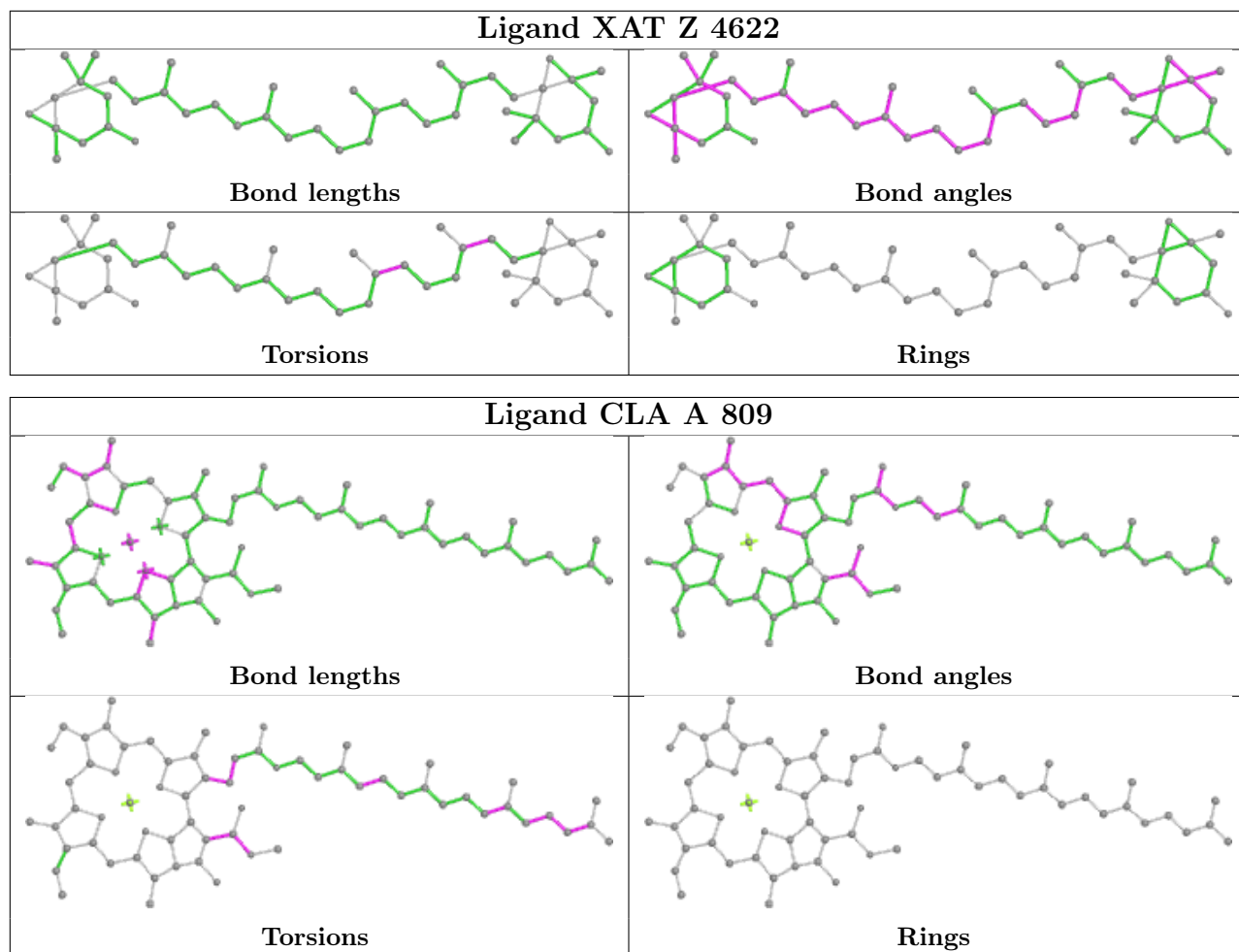


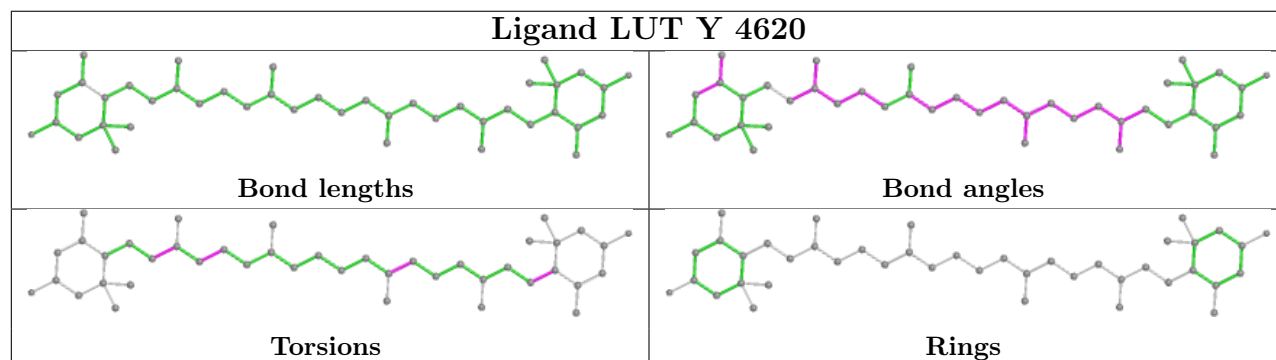
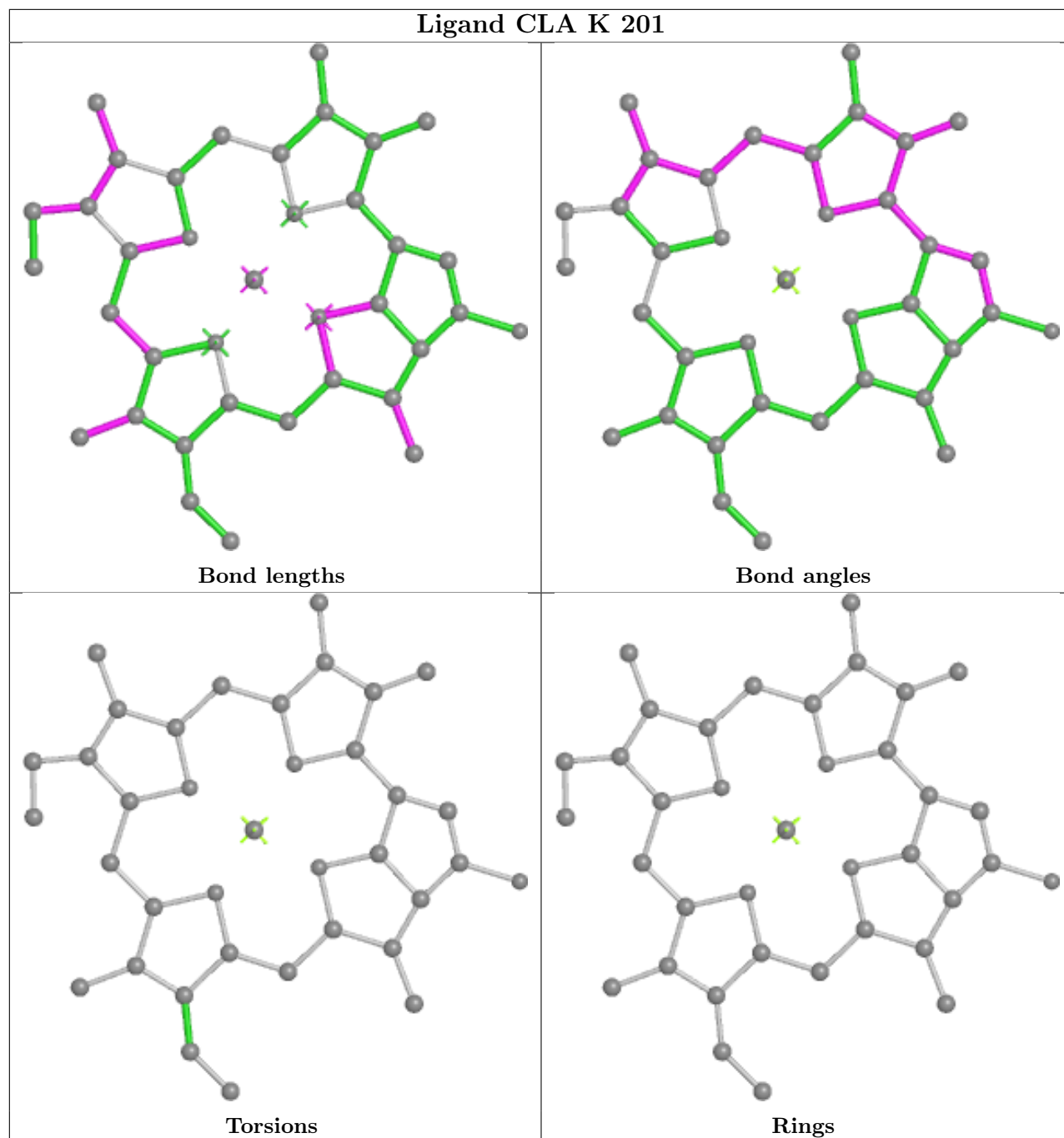


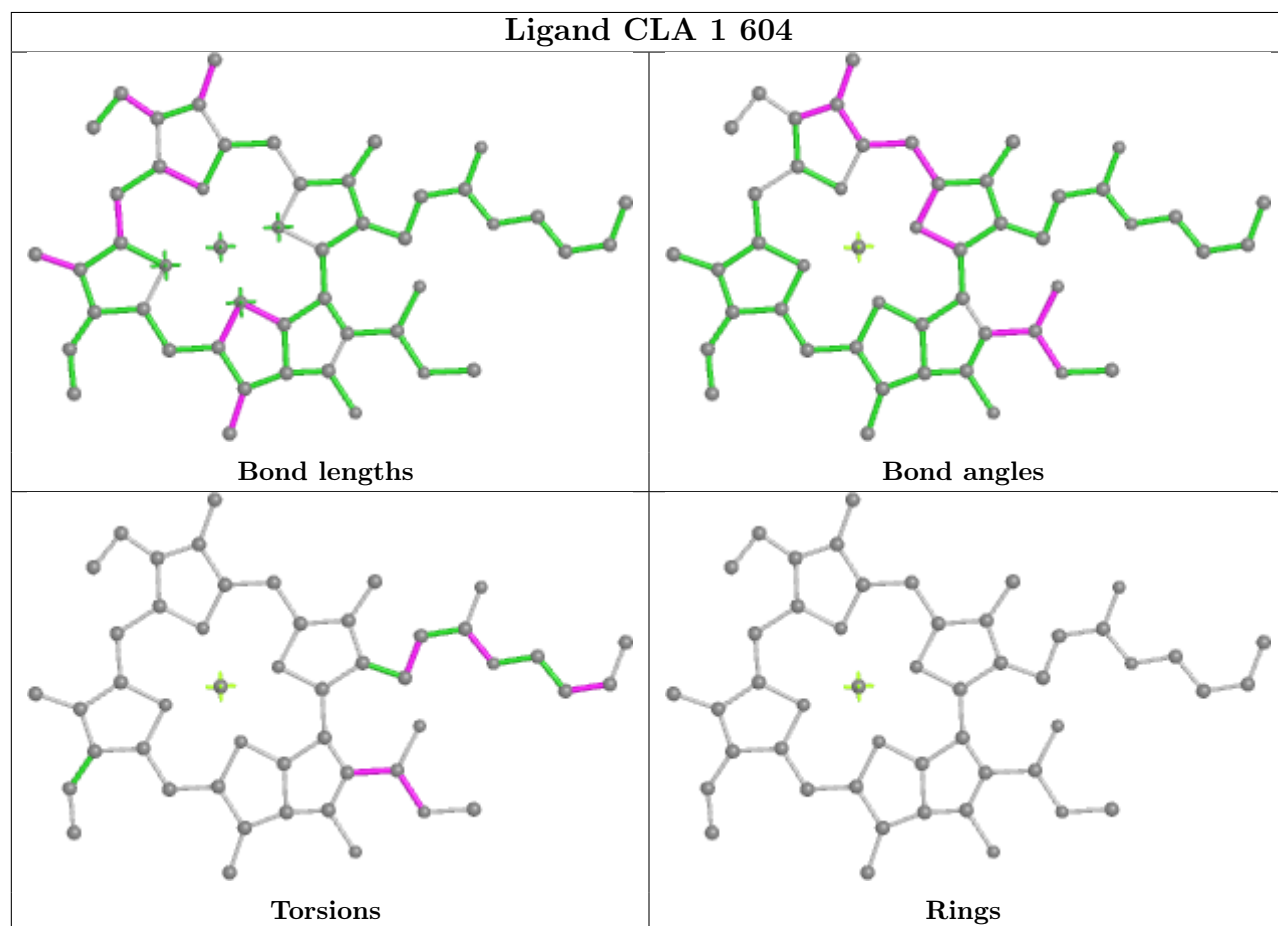
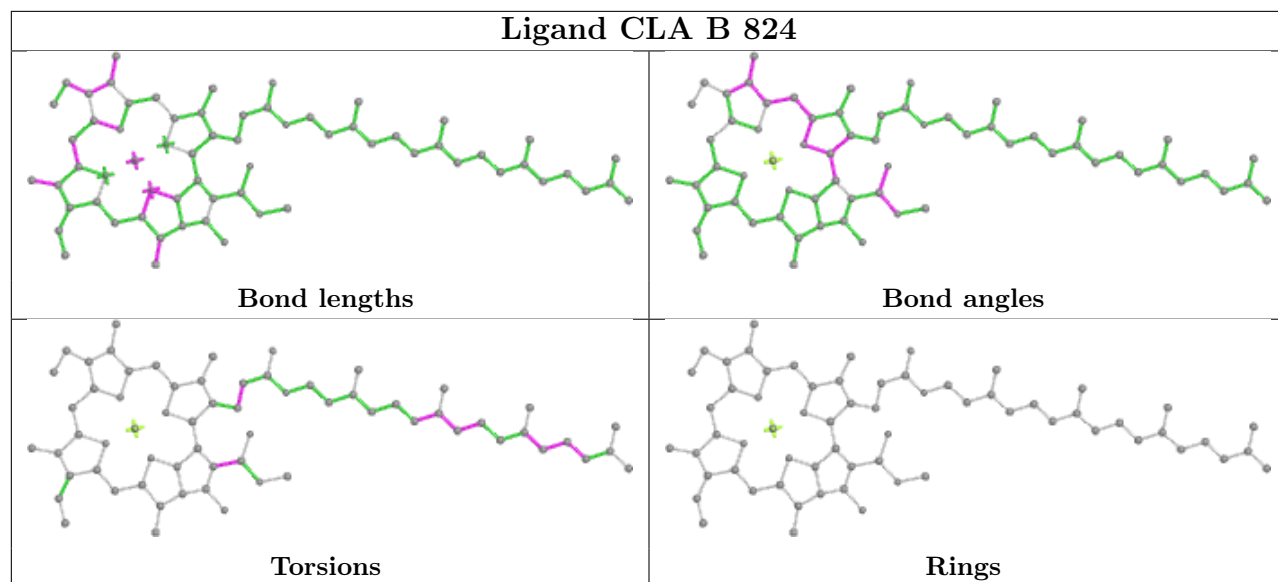


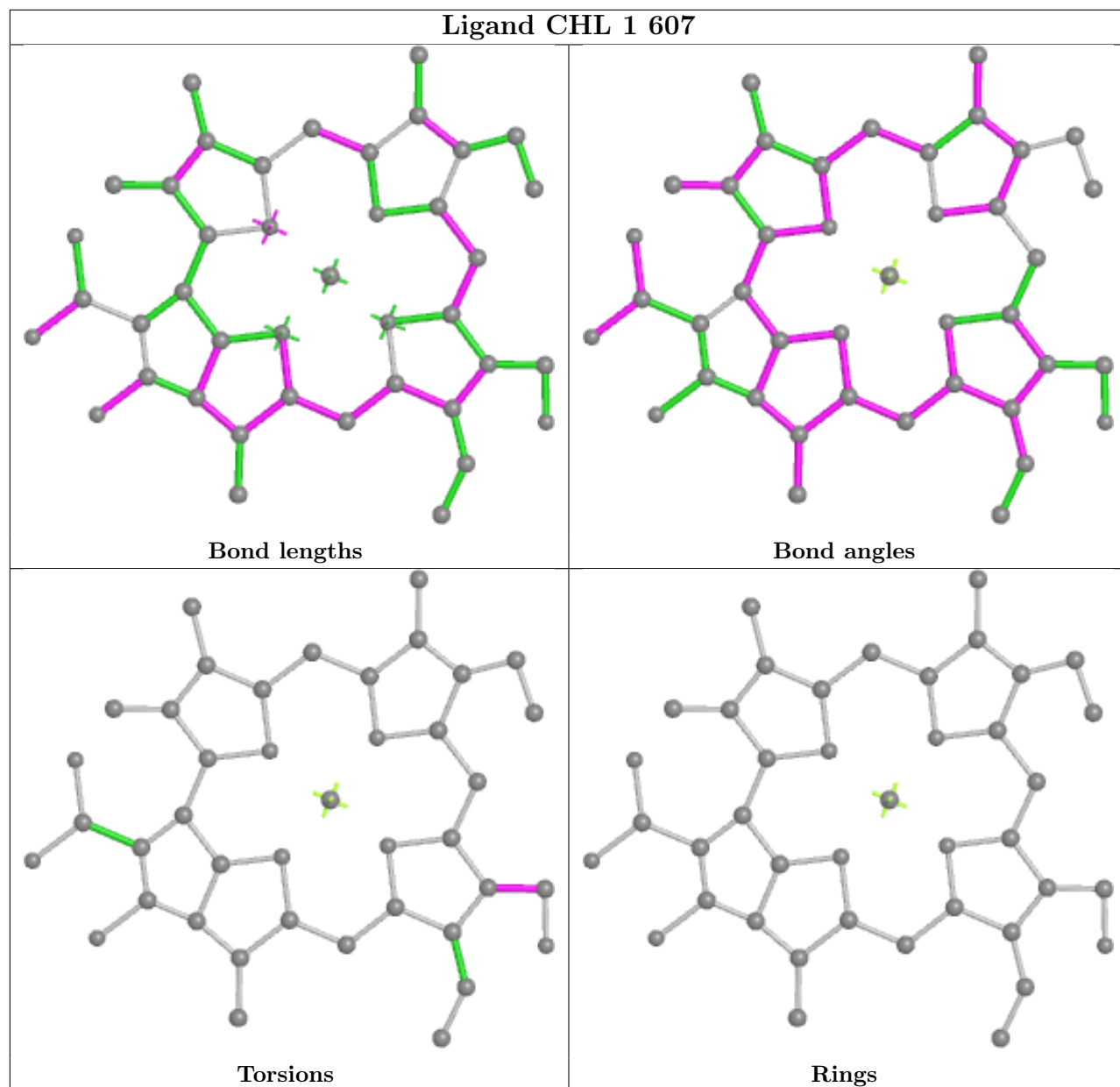


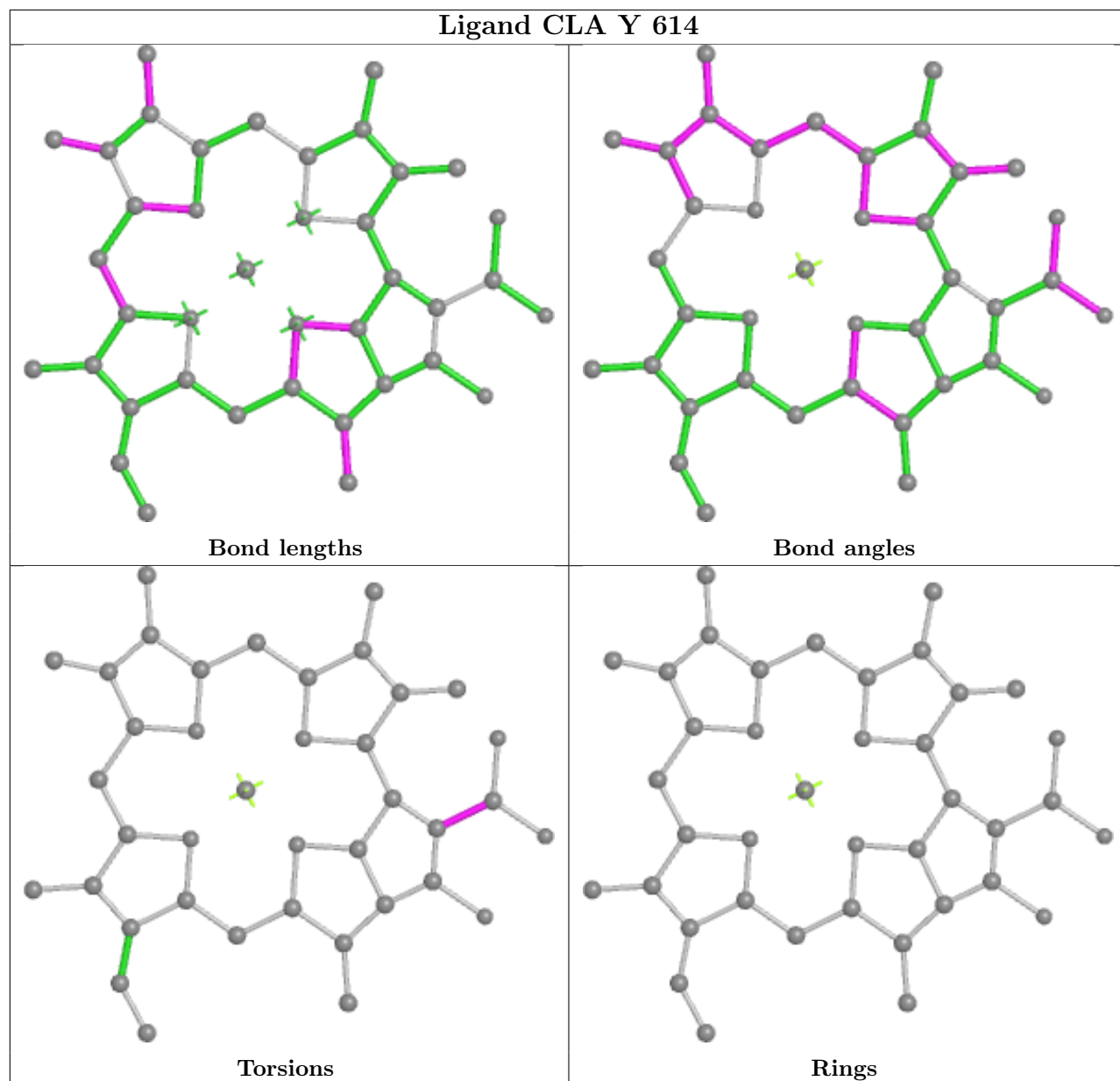


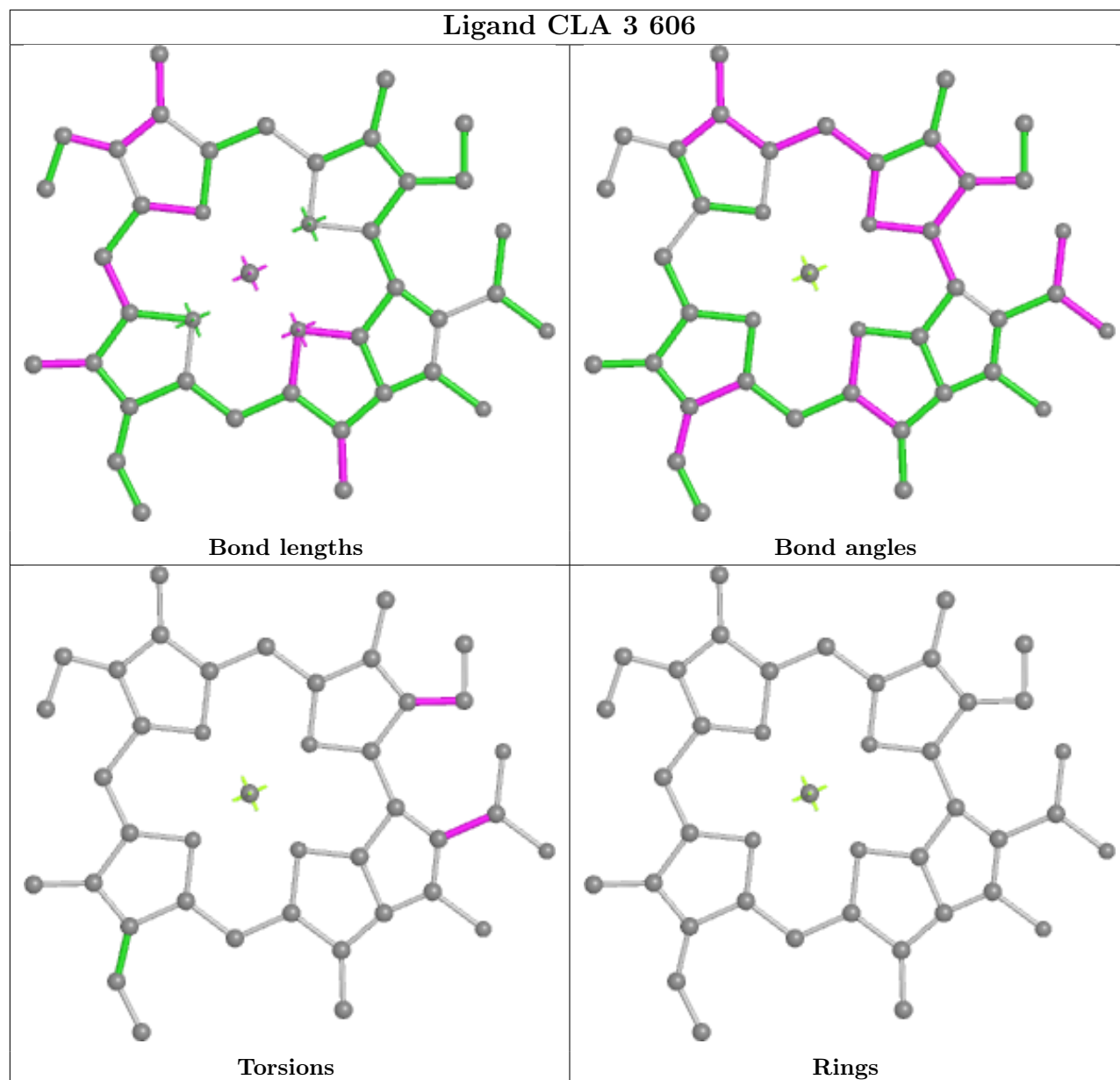




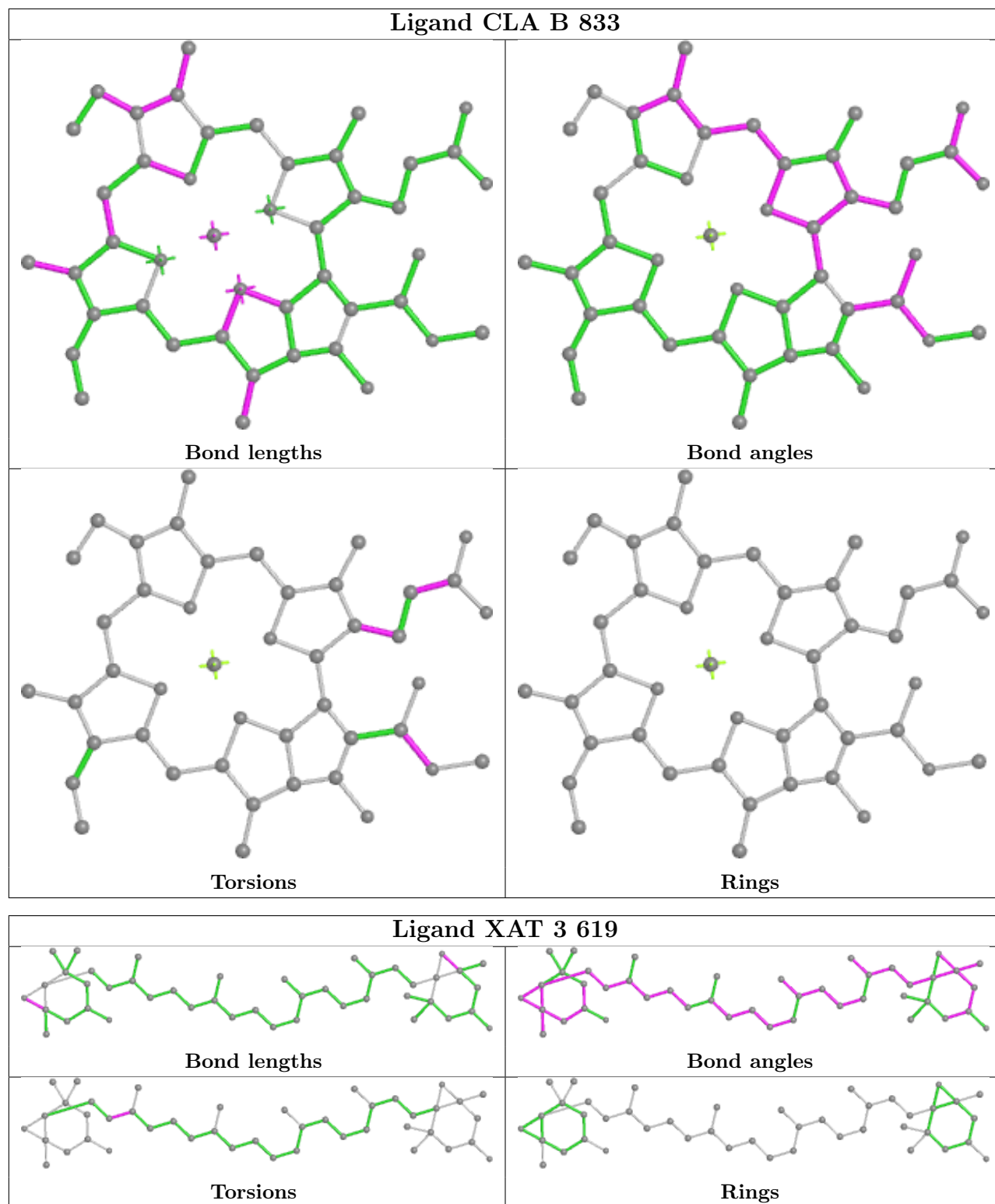


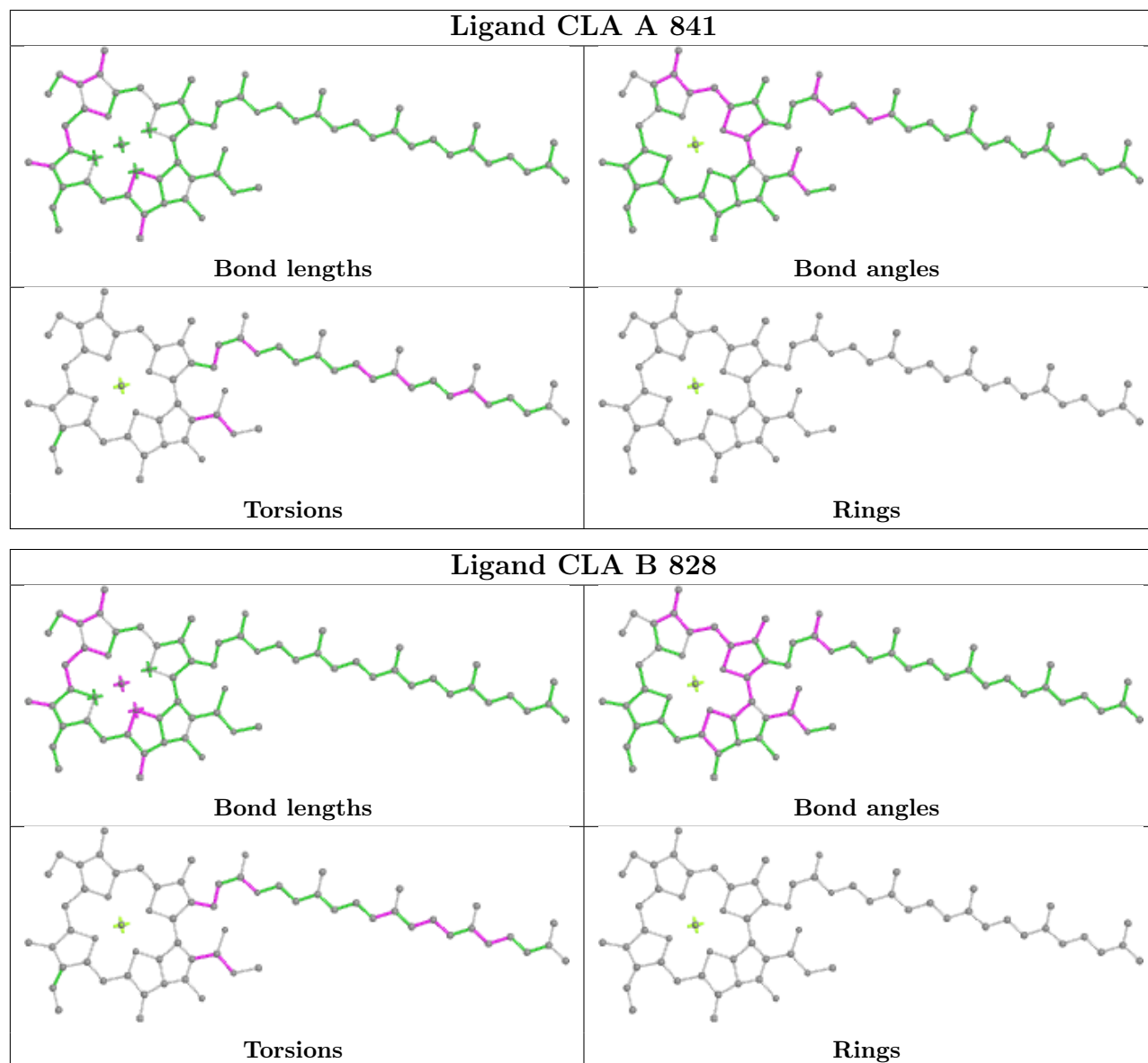


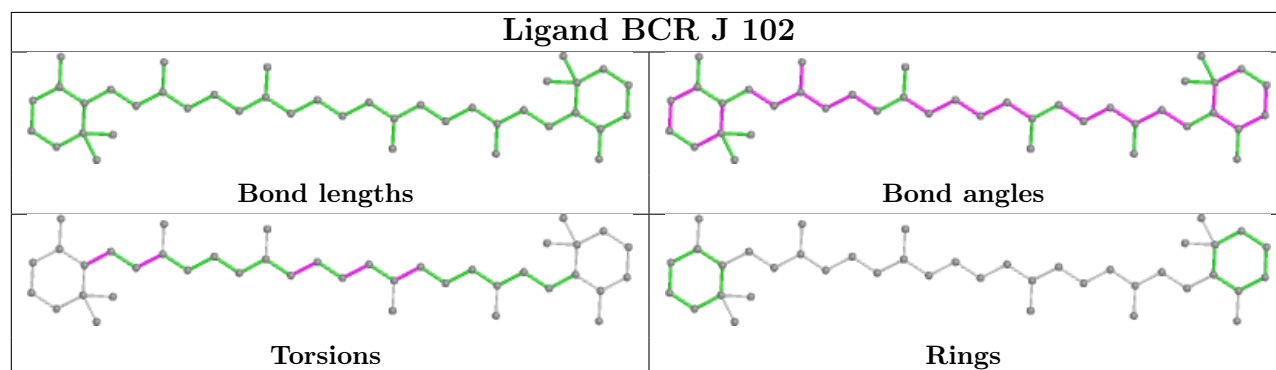
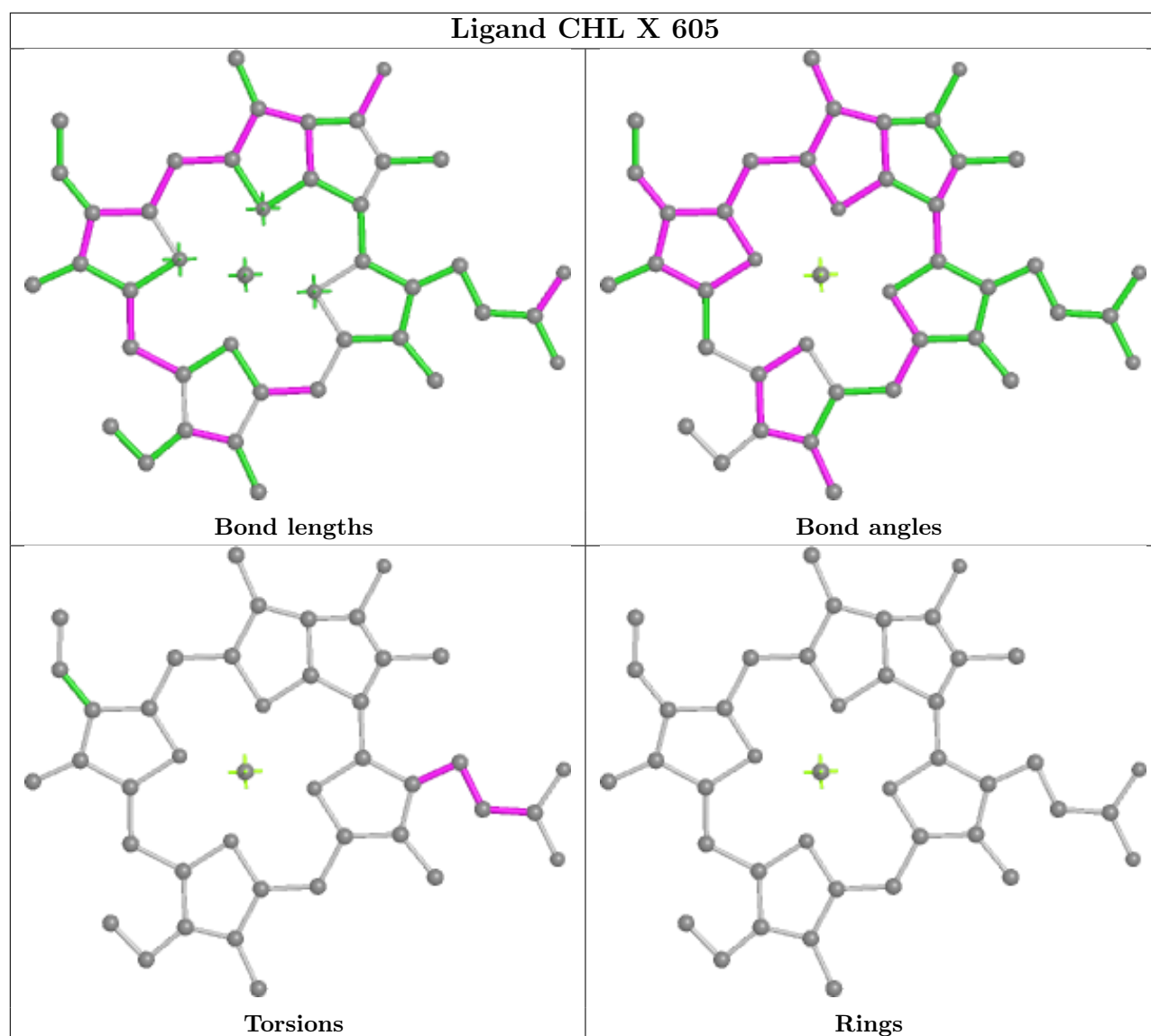


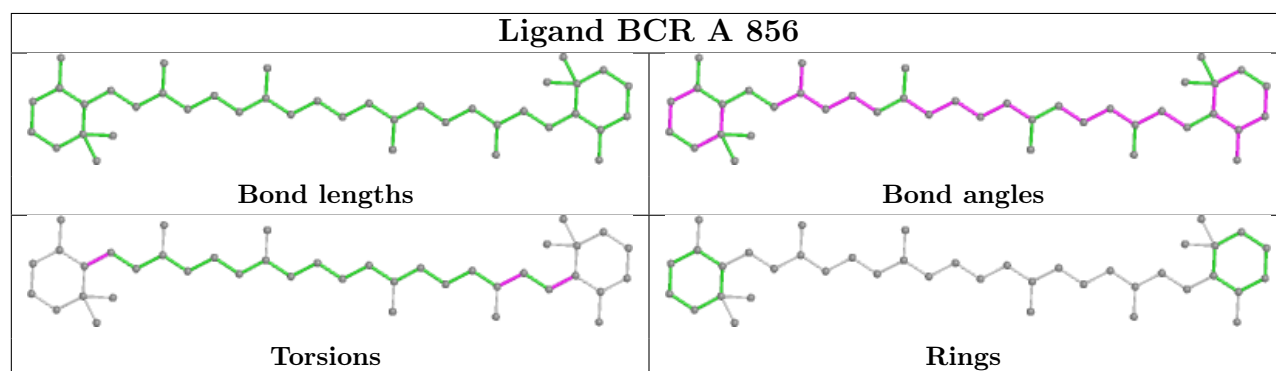
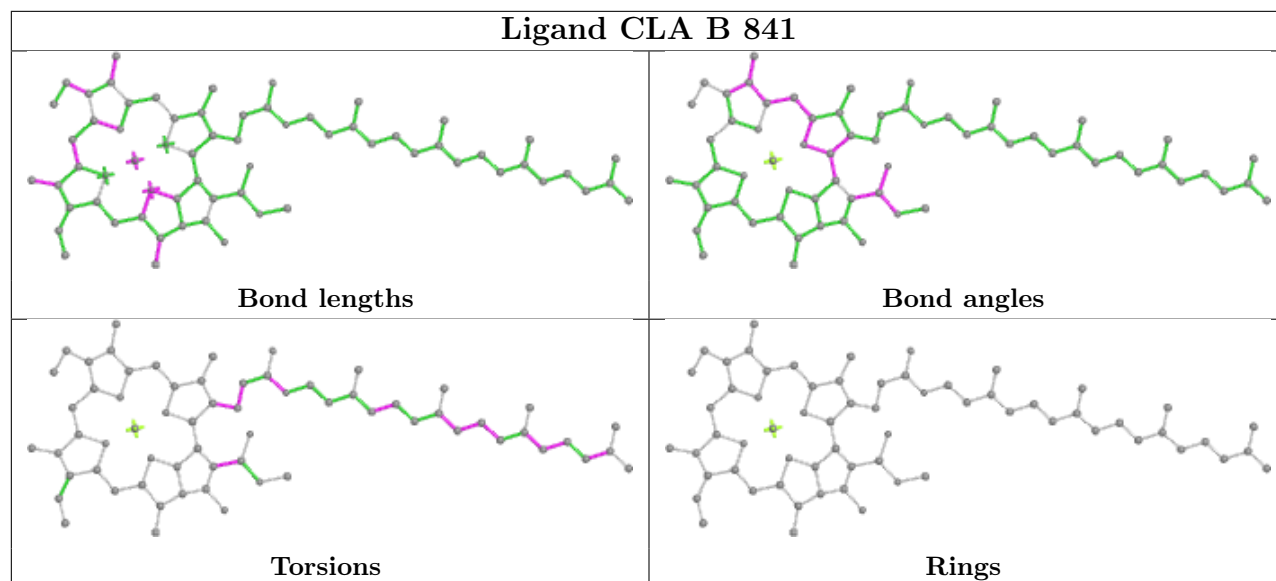
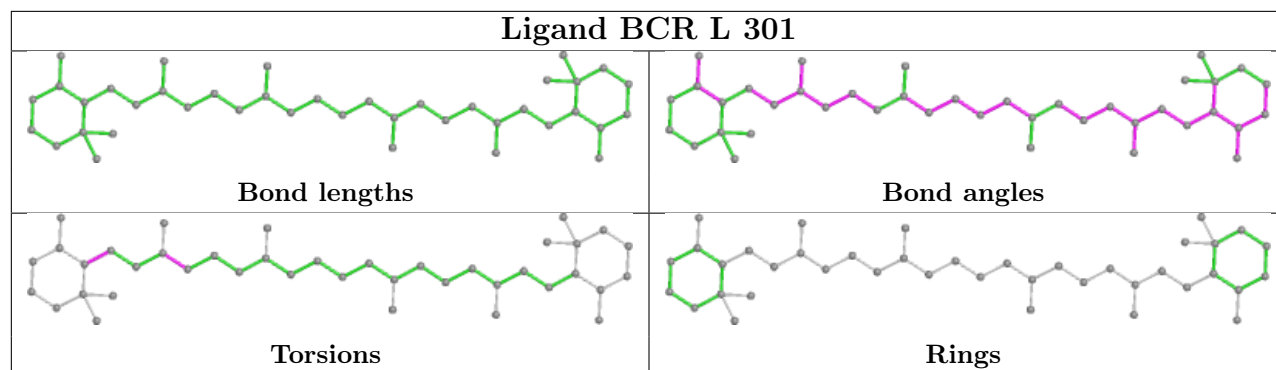


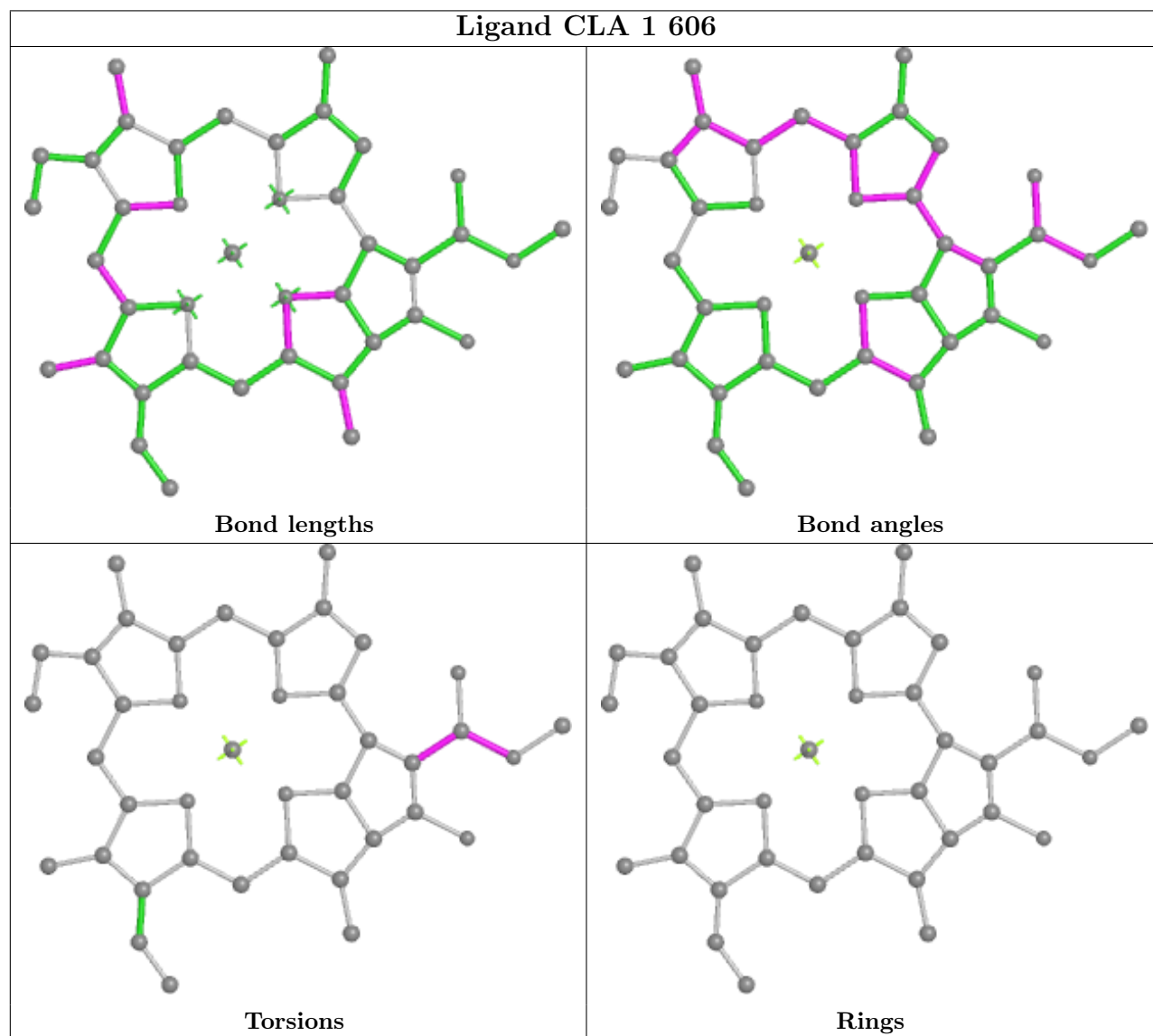
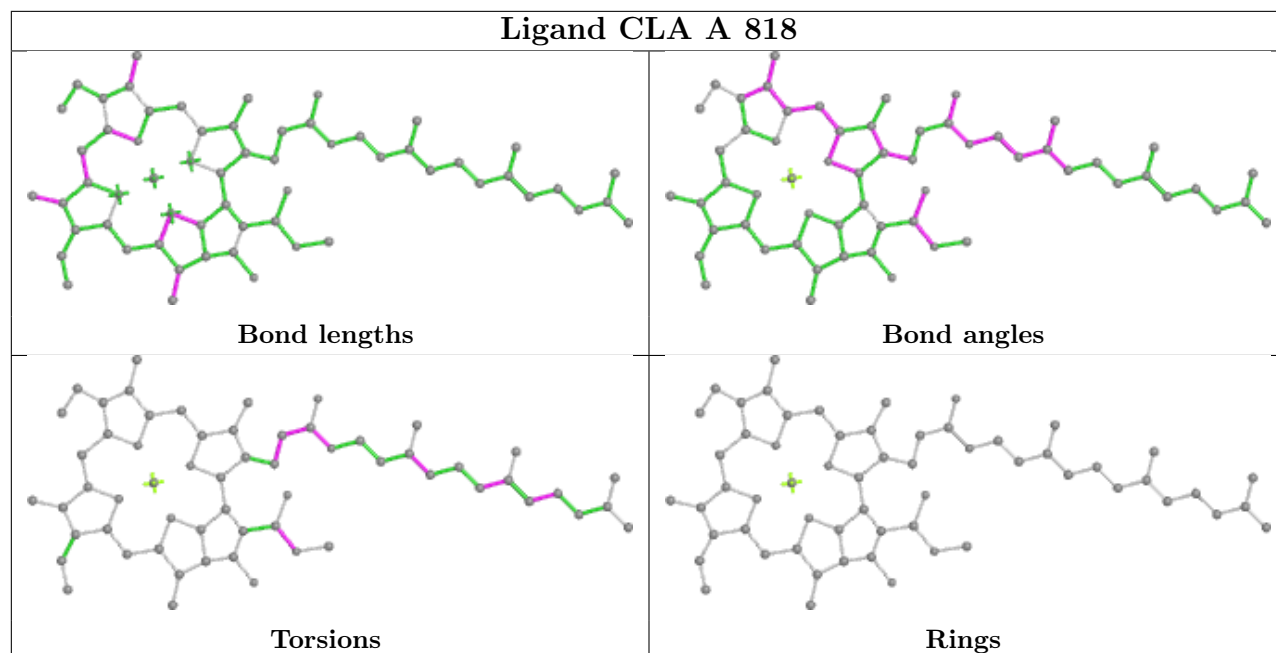


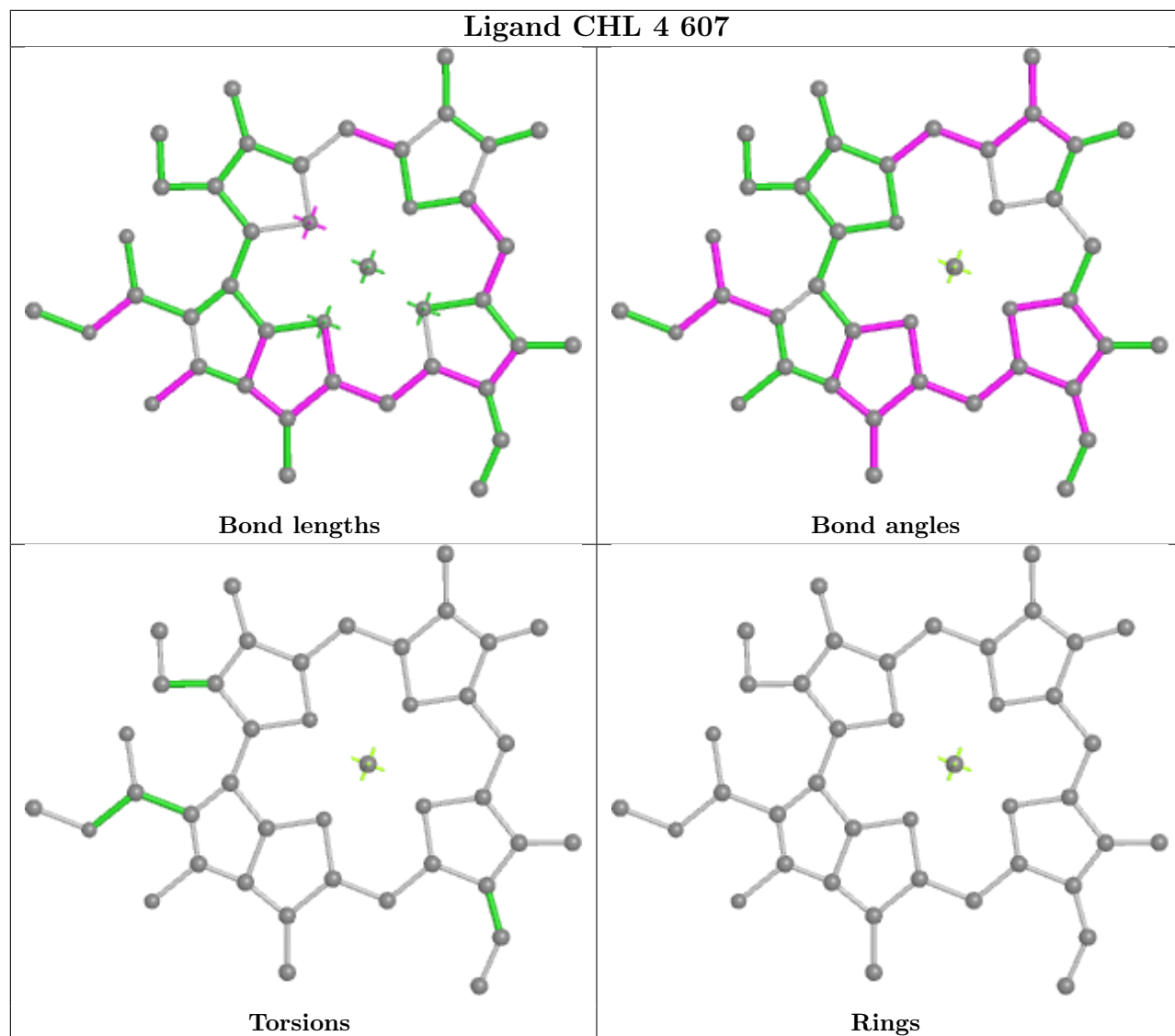


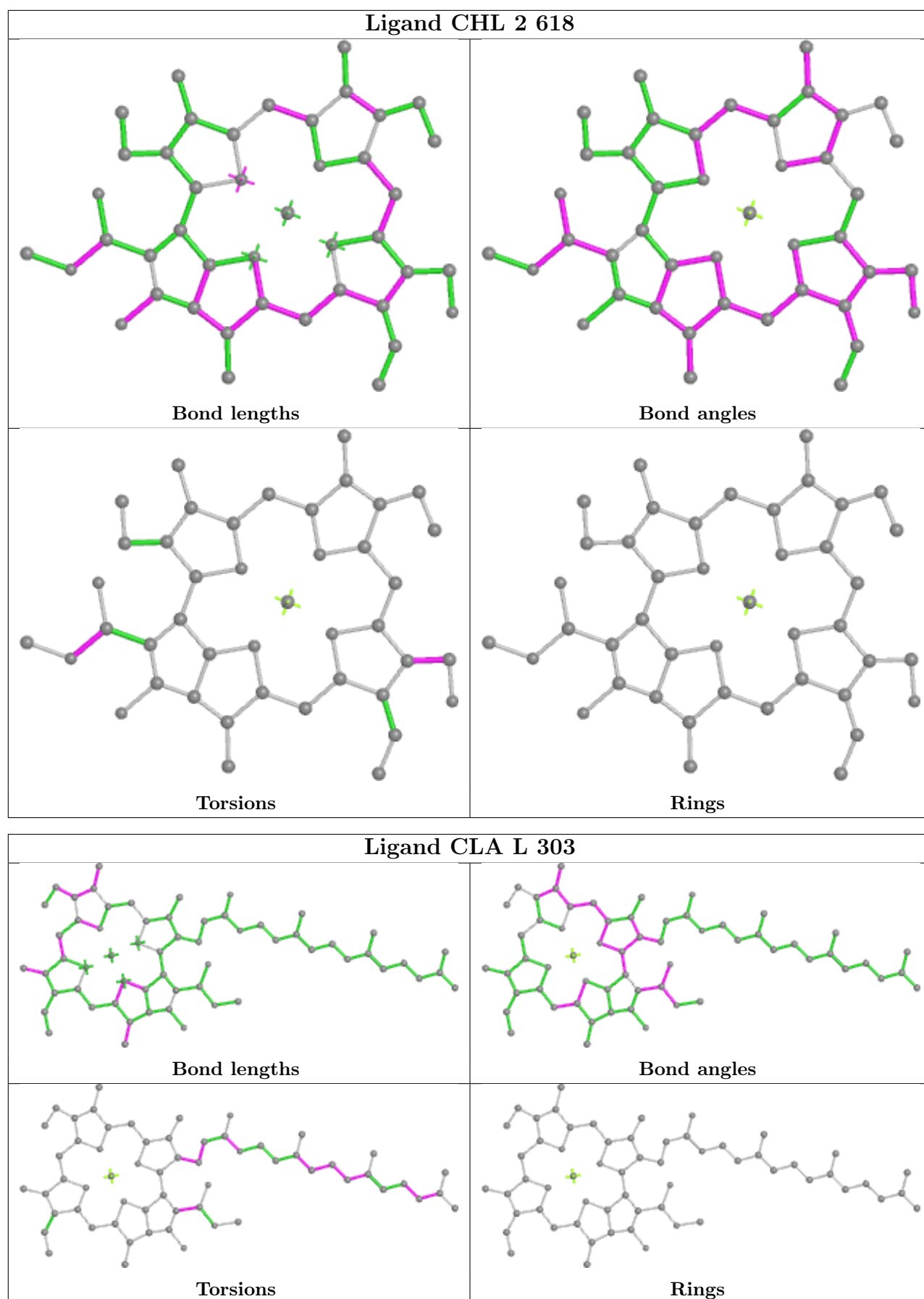


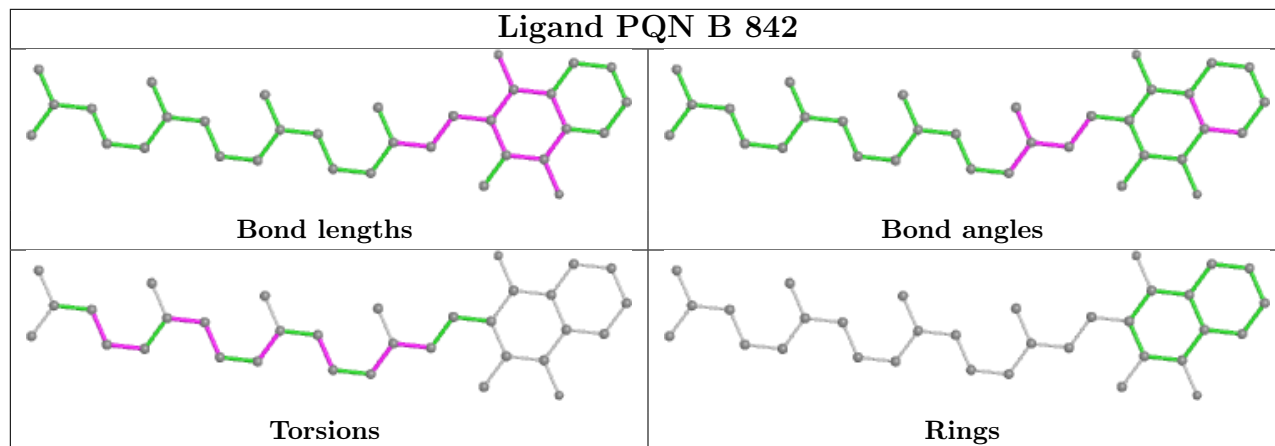
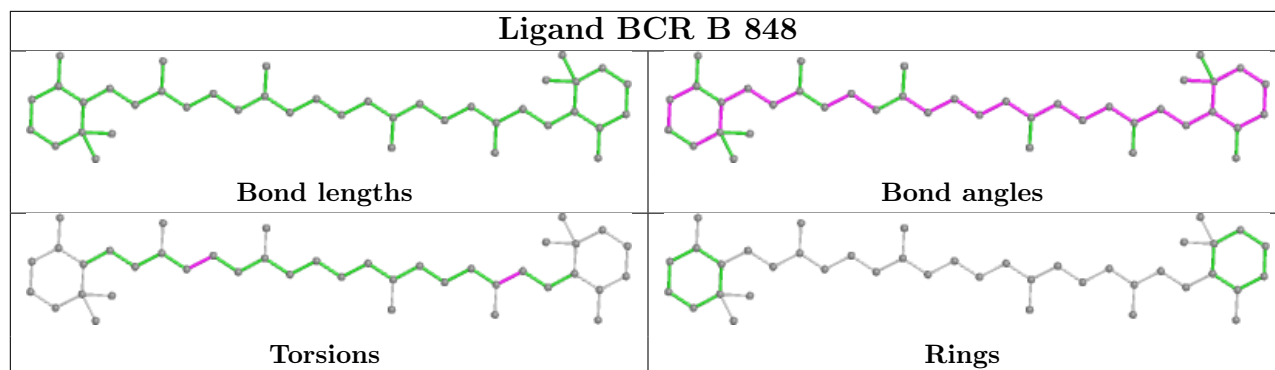




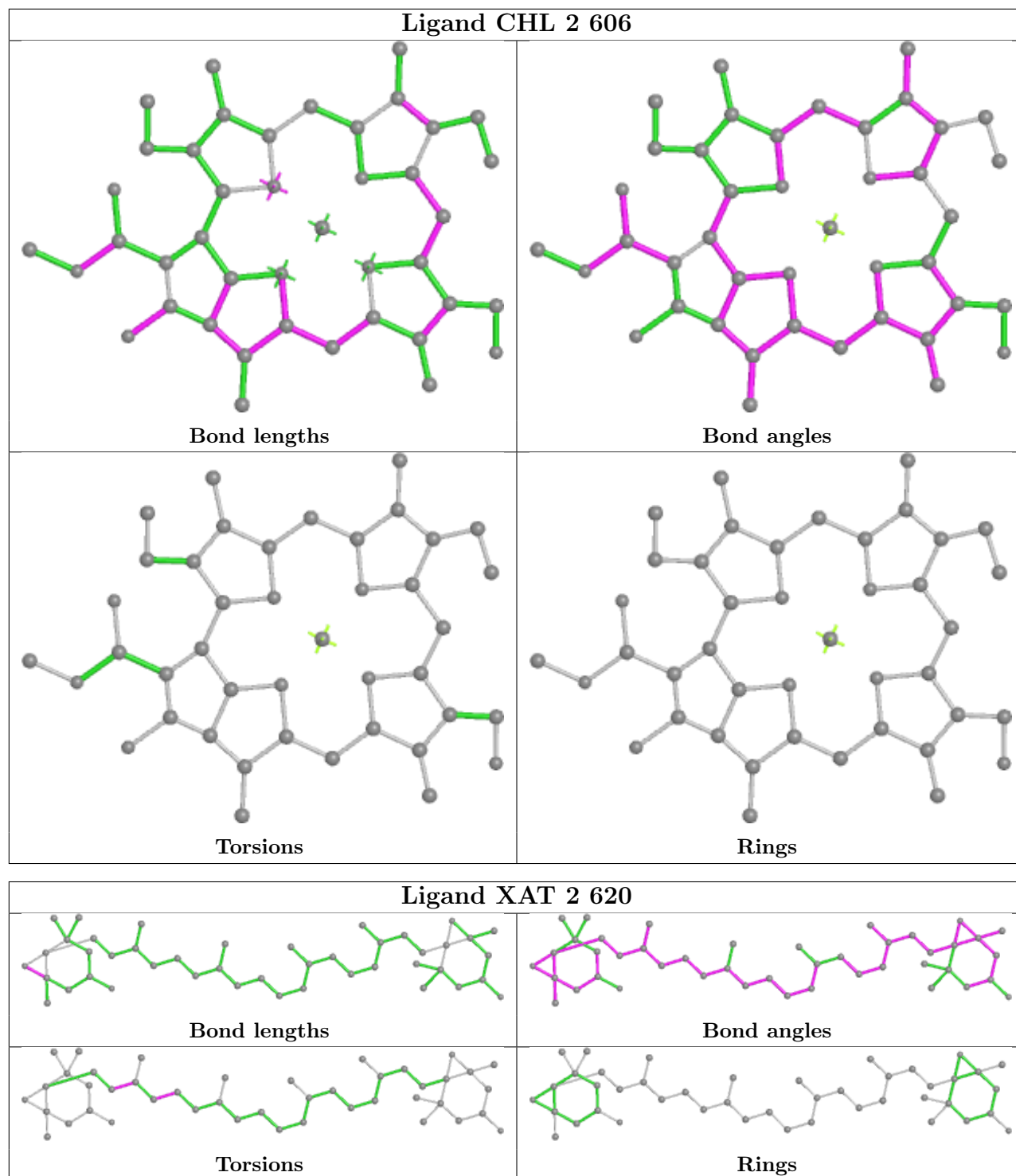


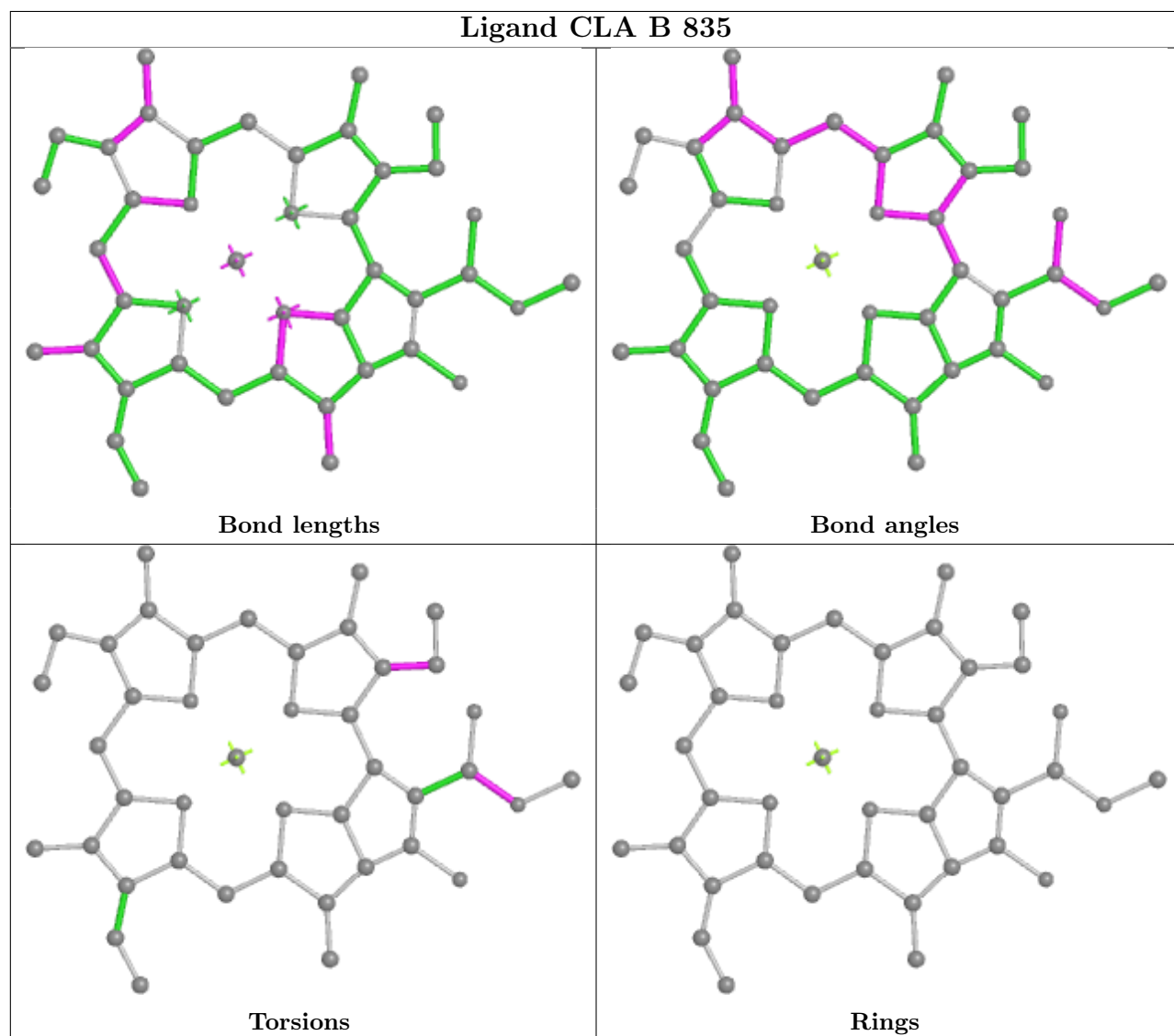
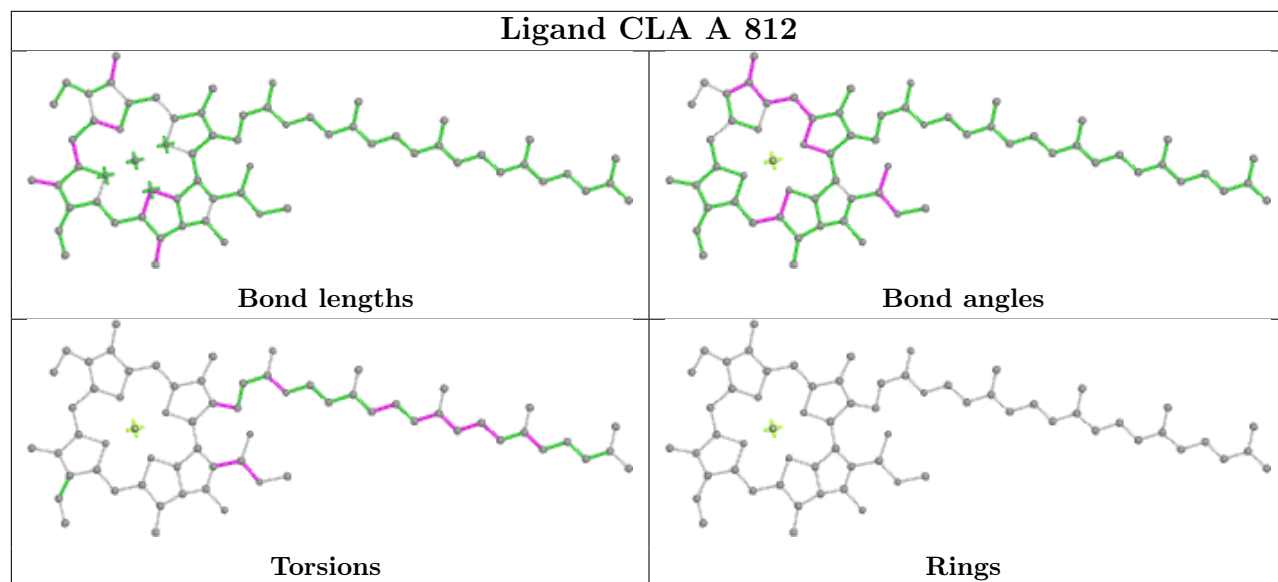


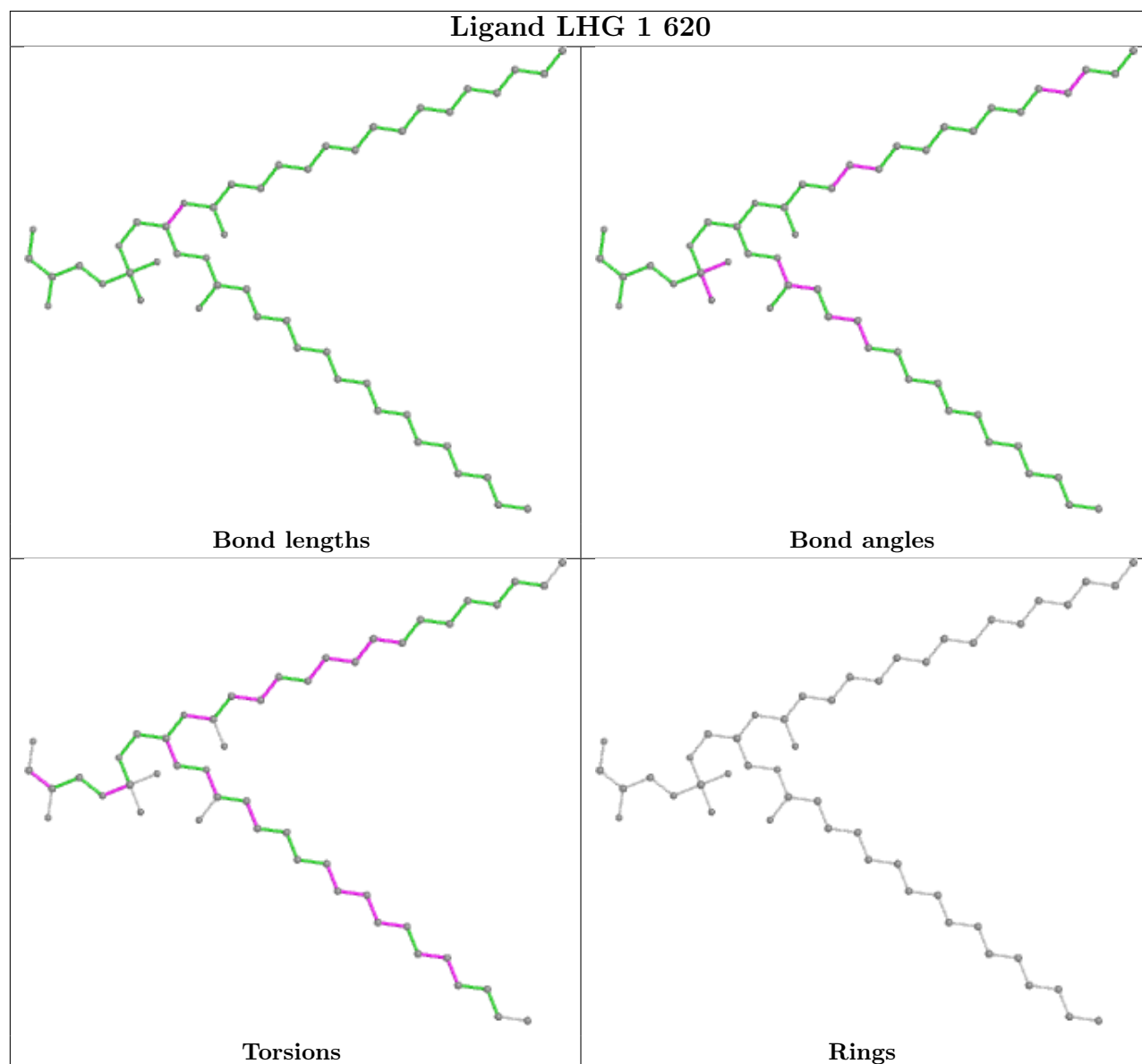
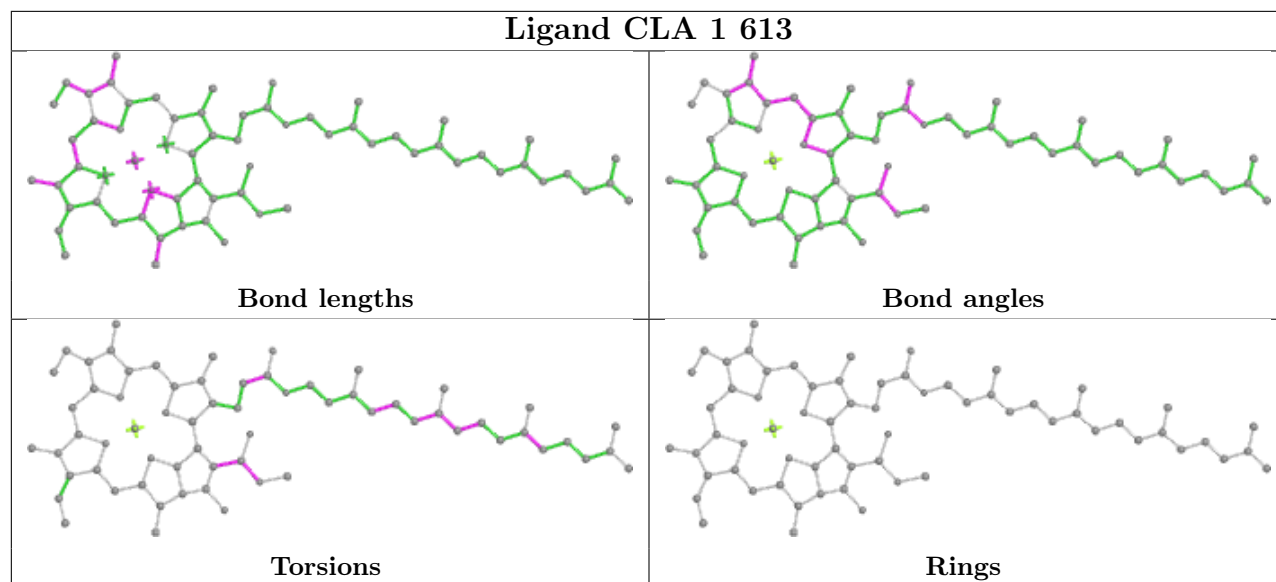


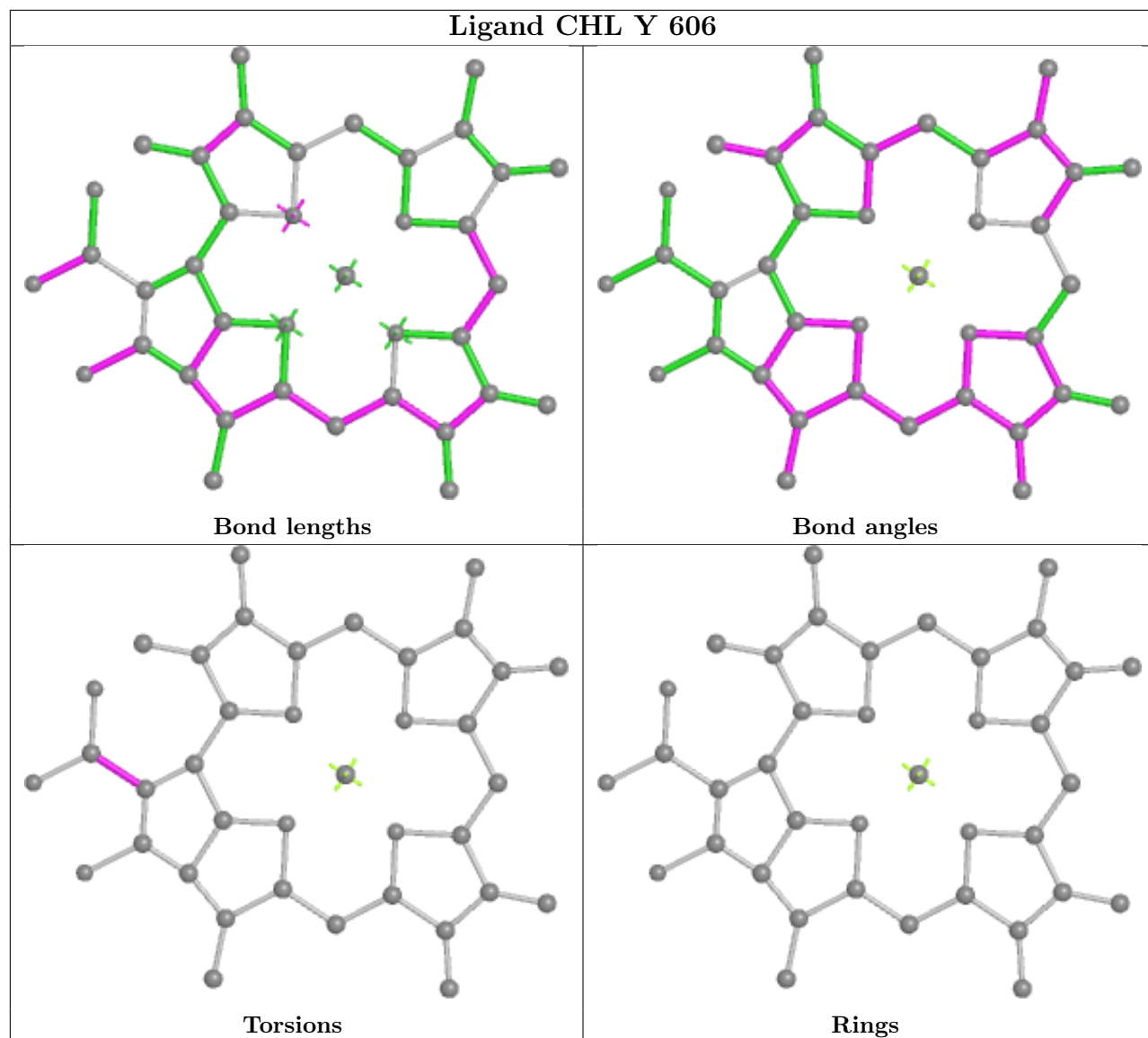


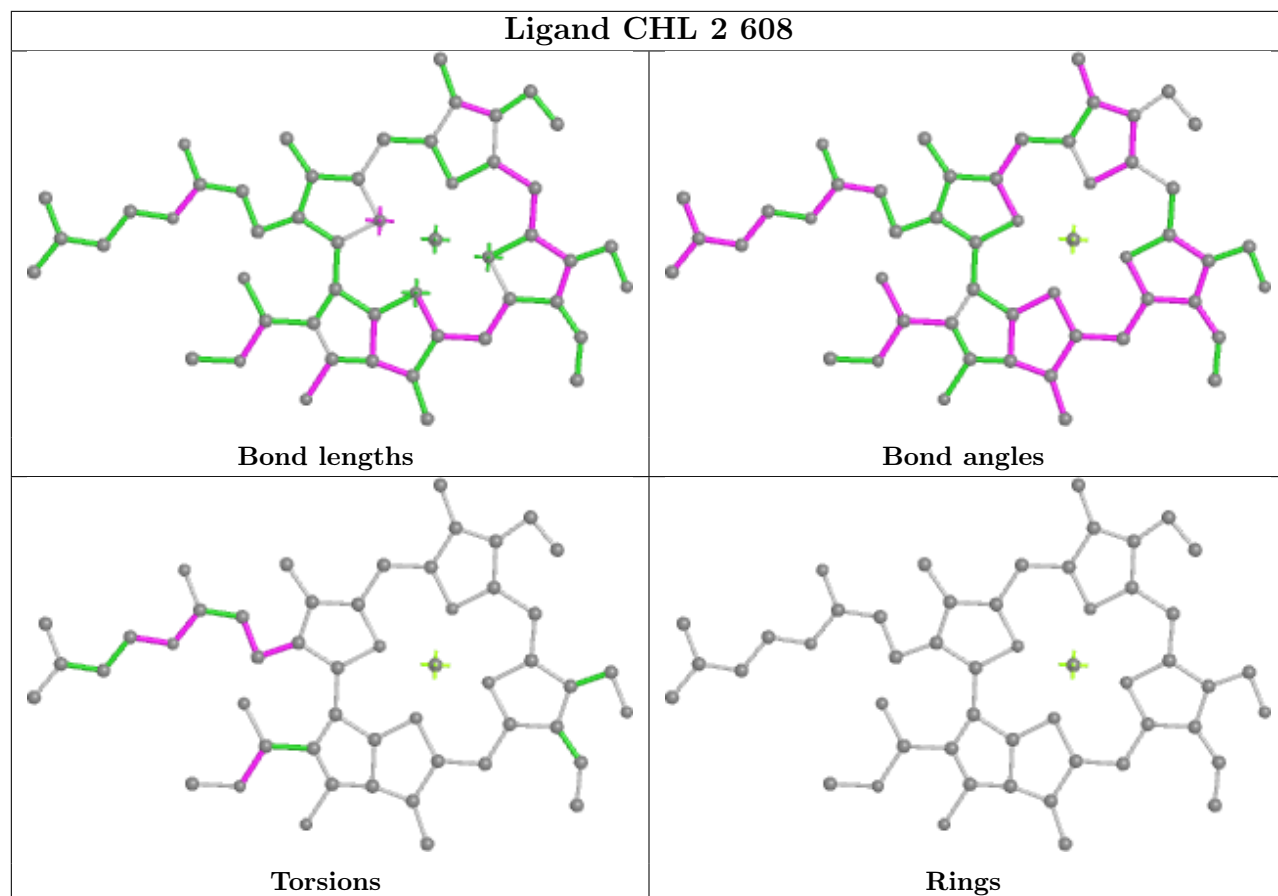


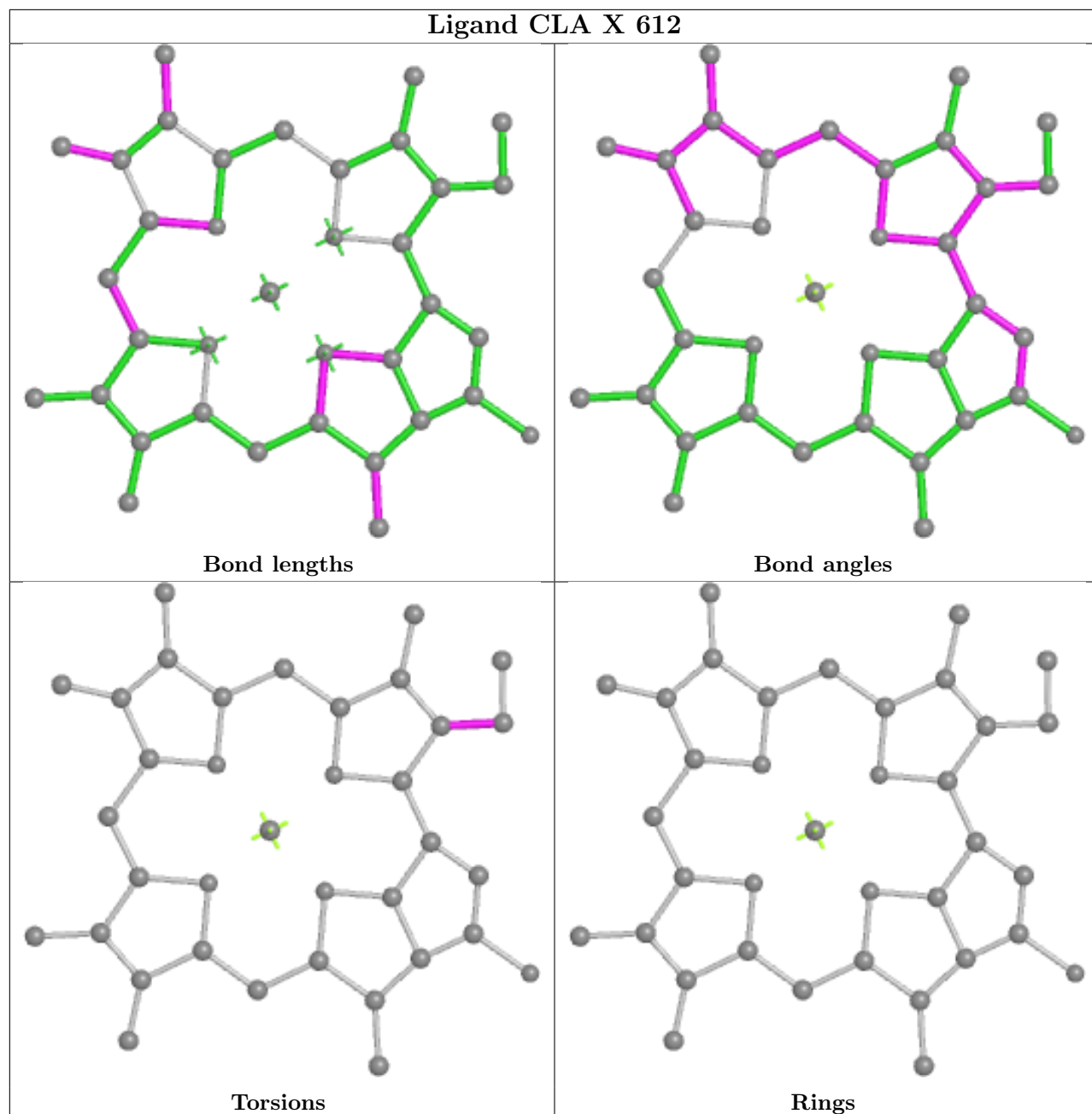


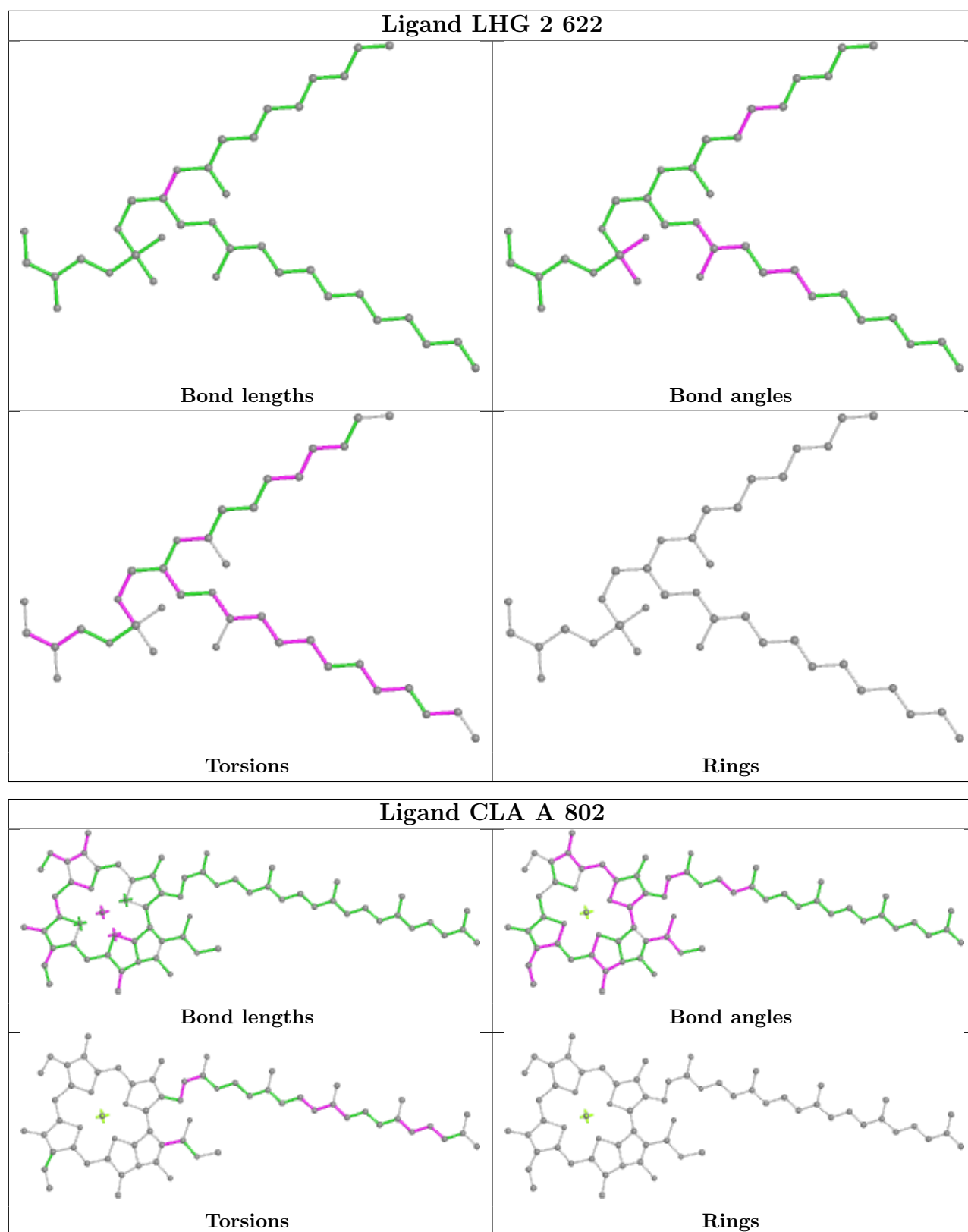




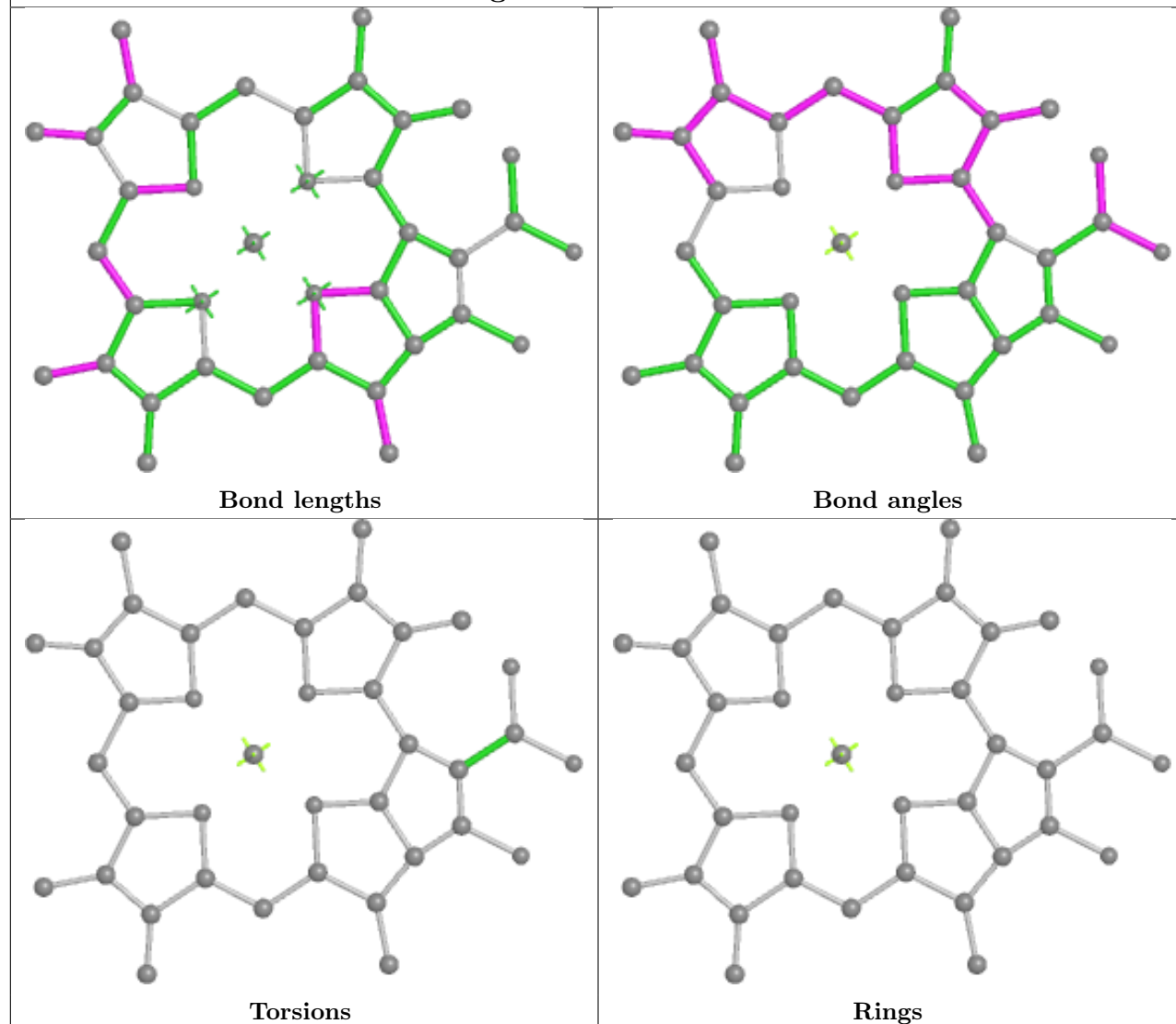




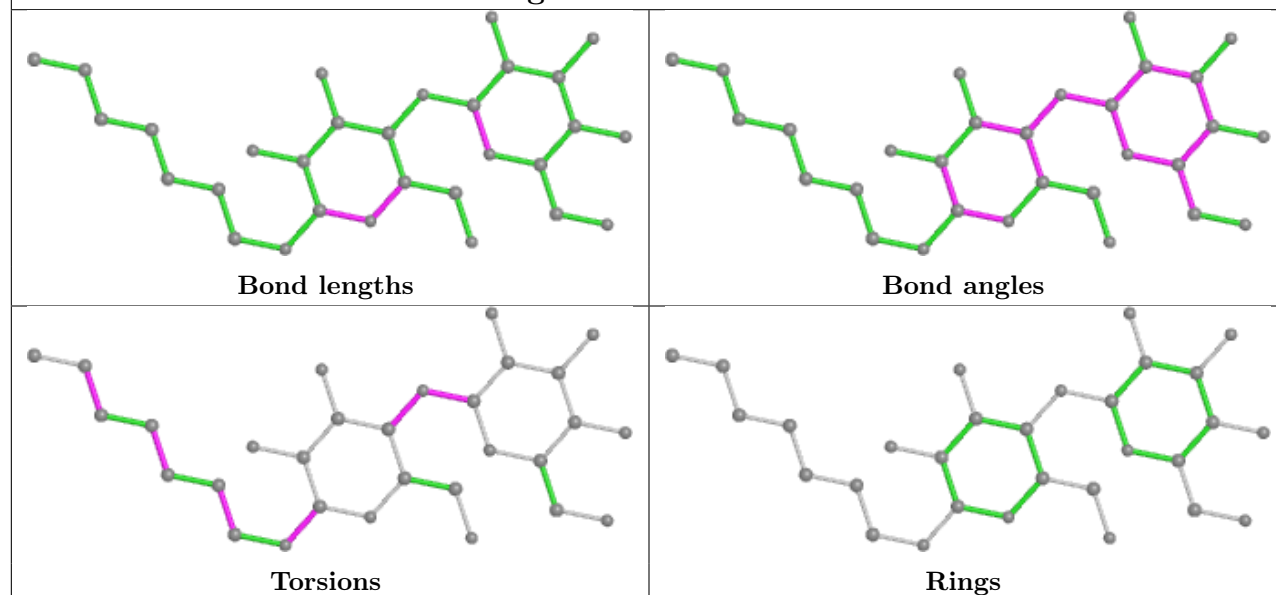




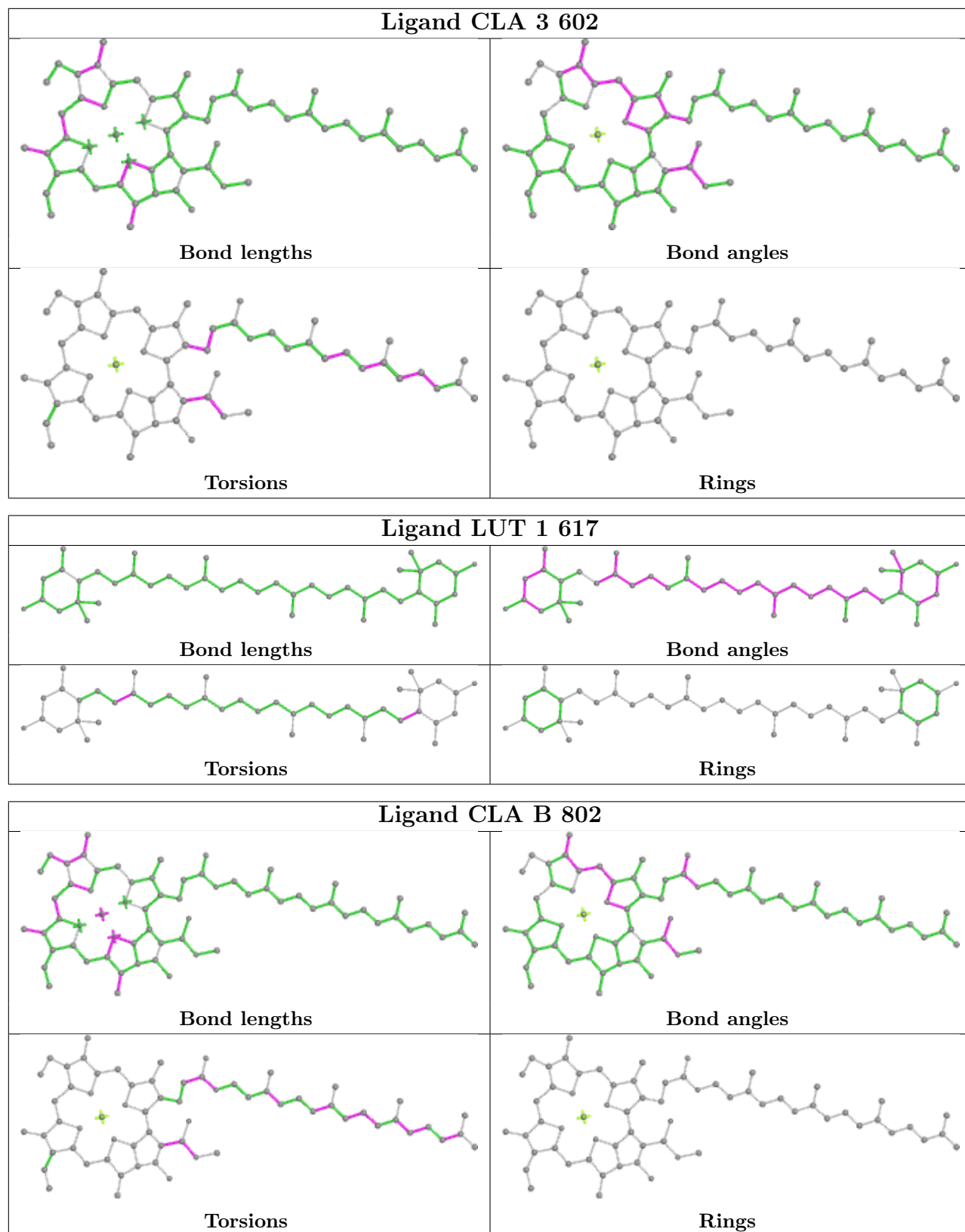
## Ligand CLA Y 612

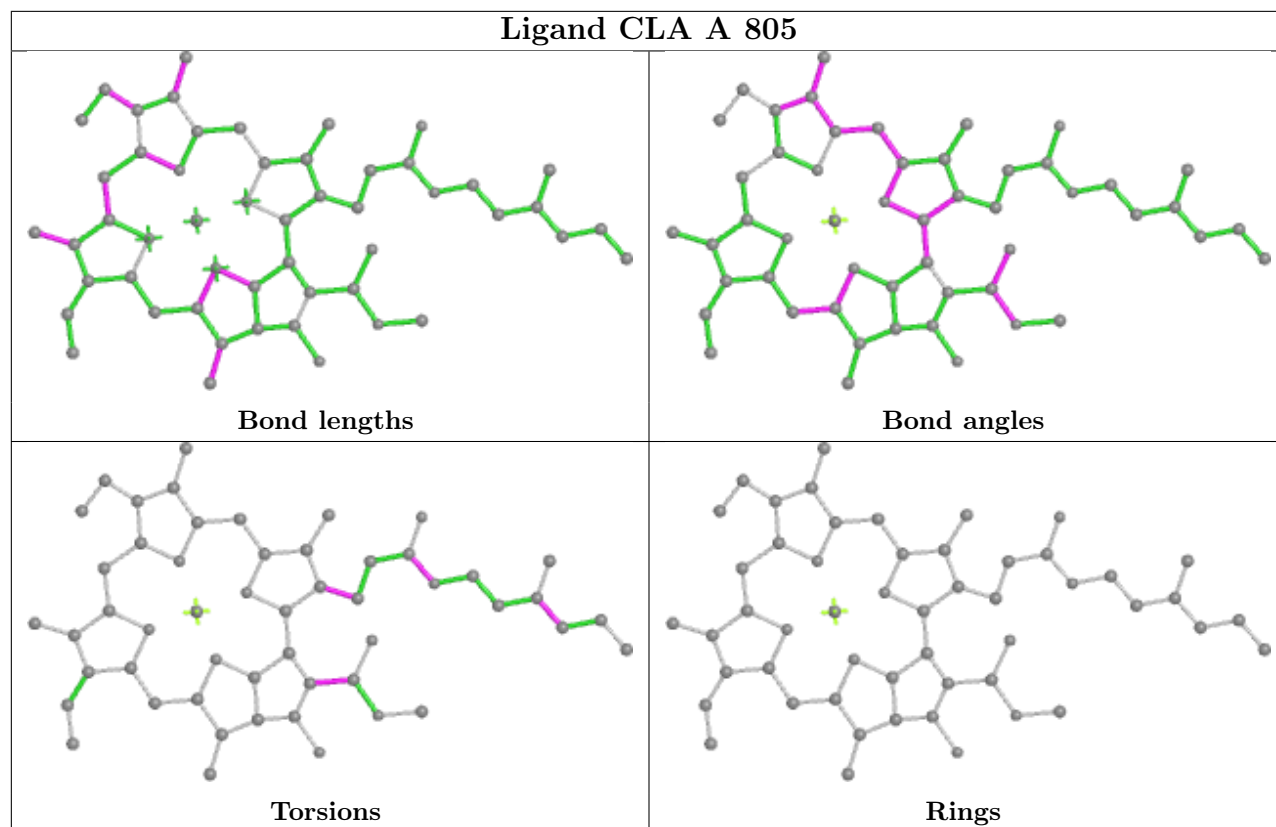


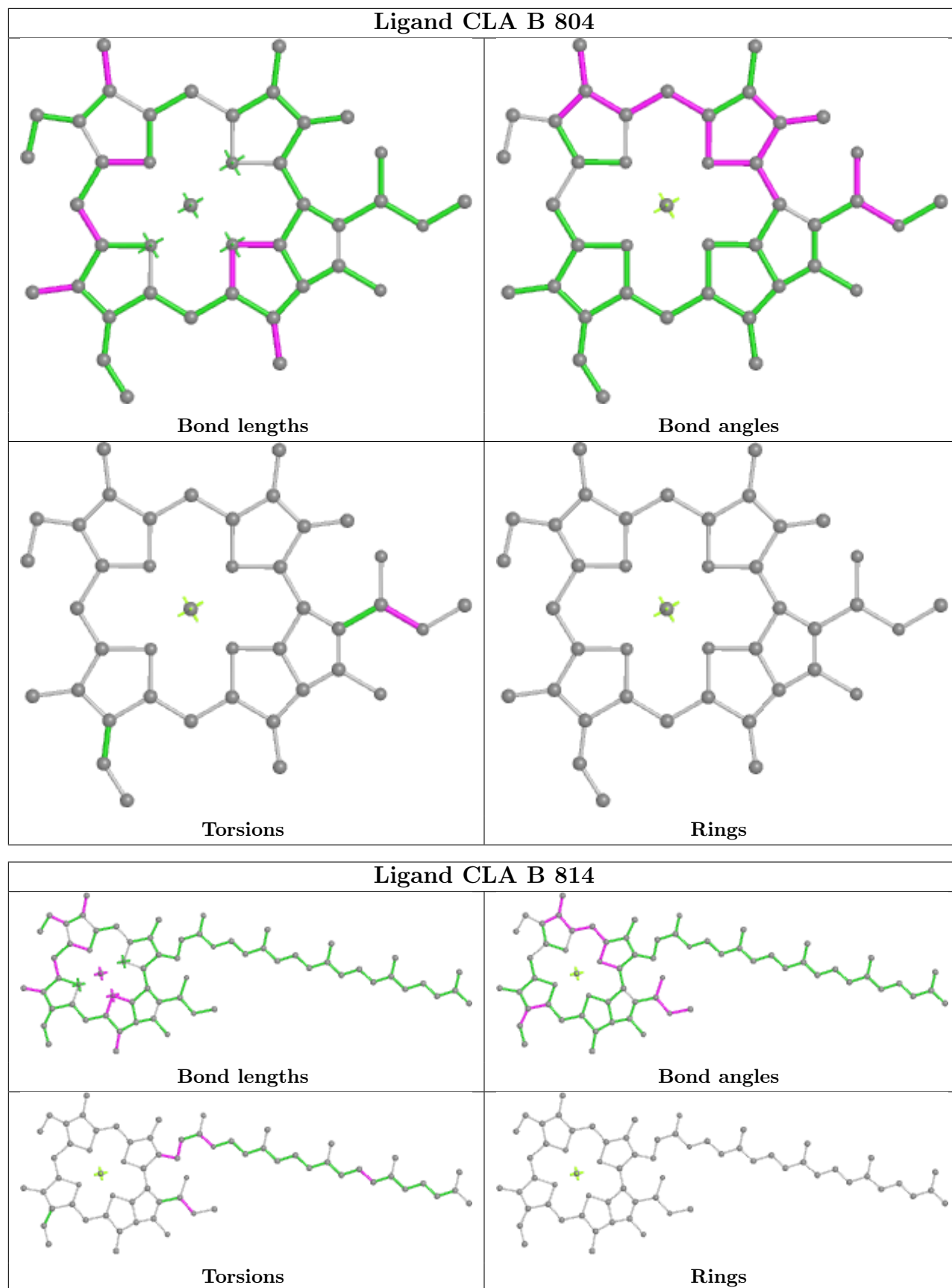
## Ligand LMU A 857

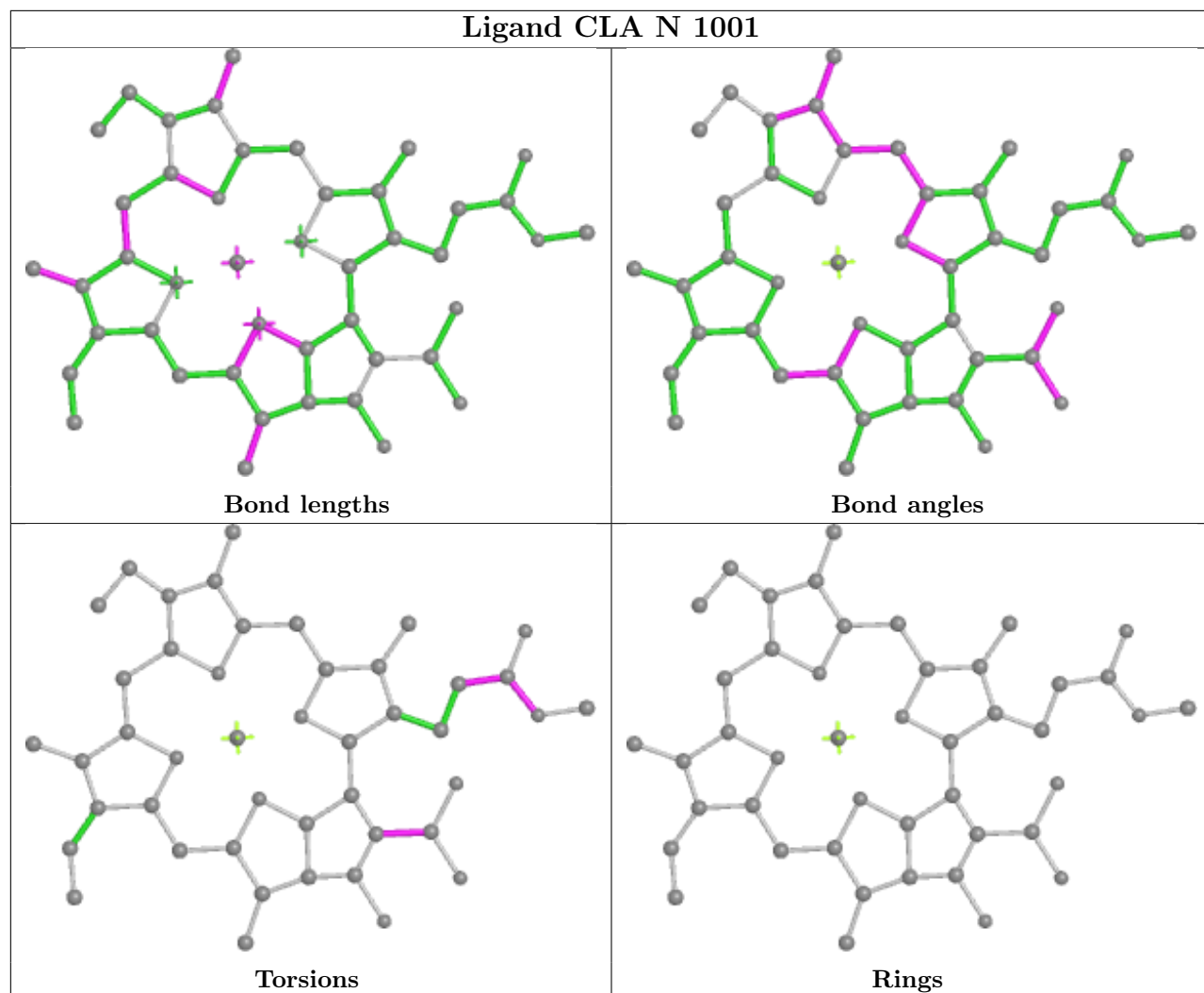


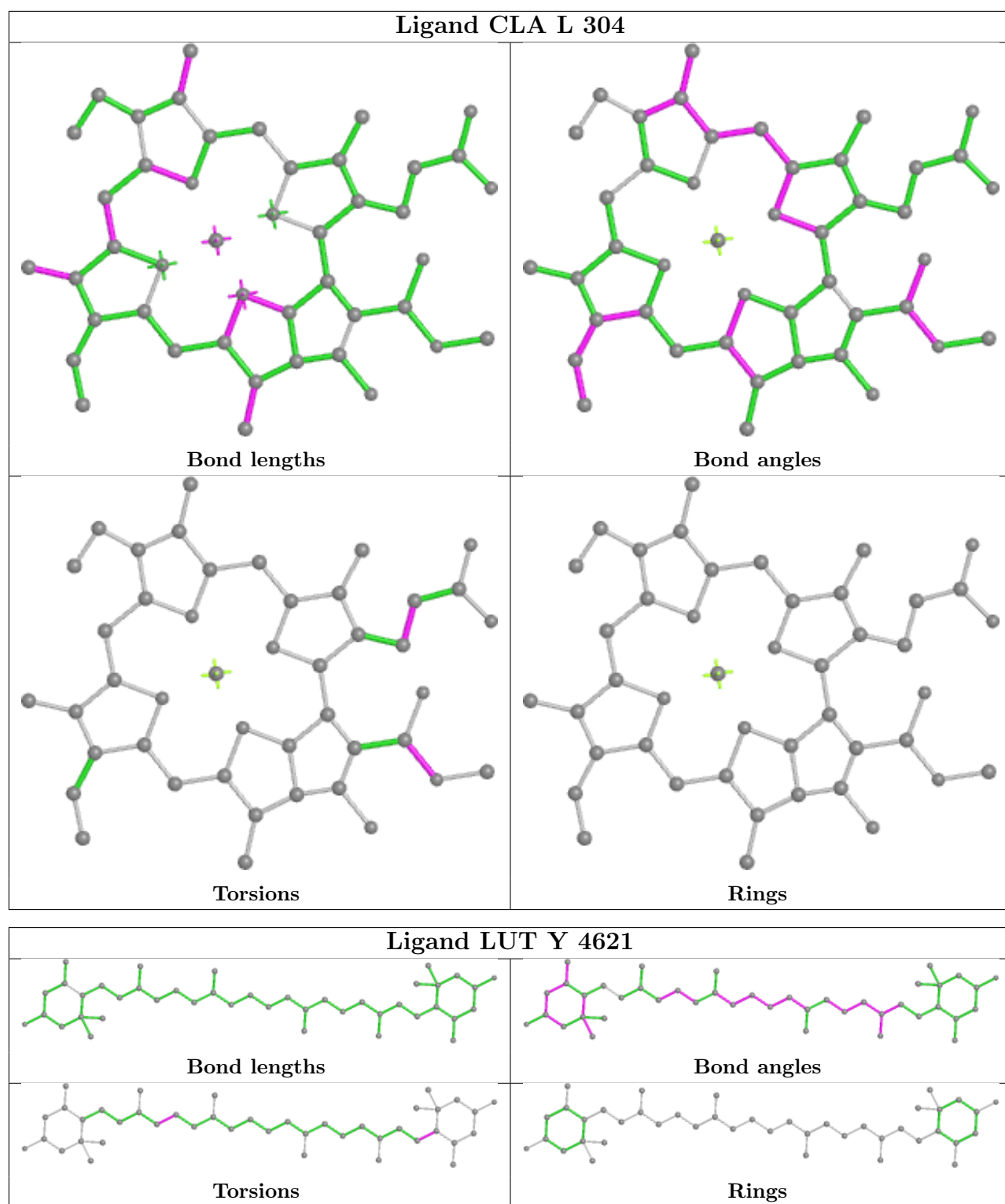


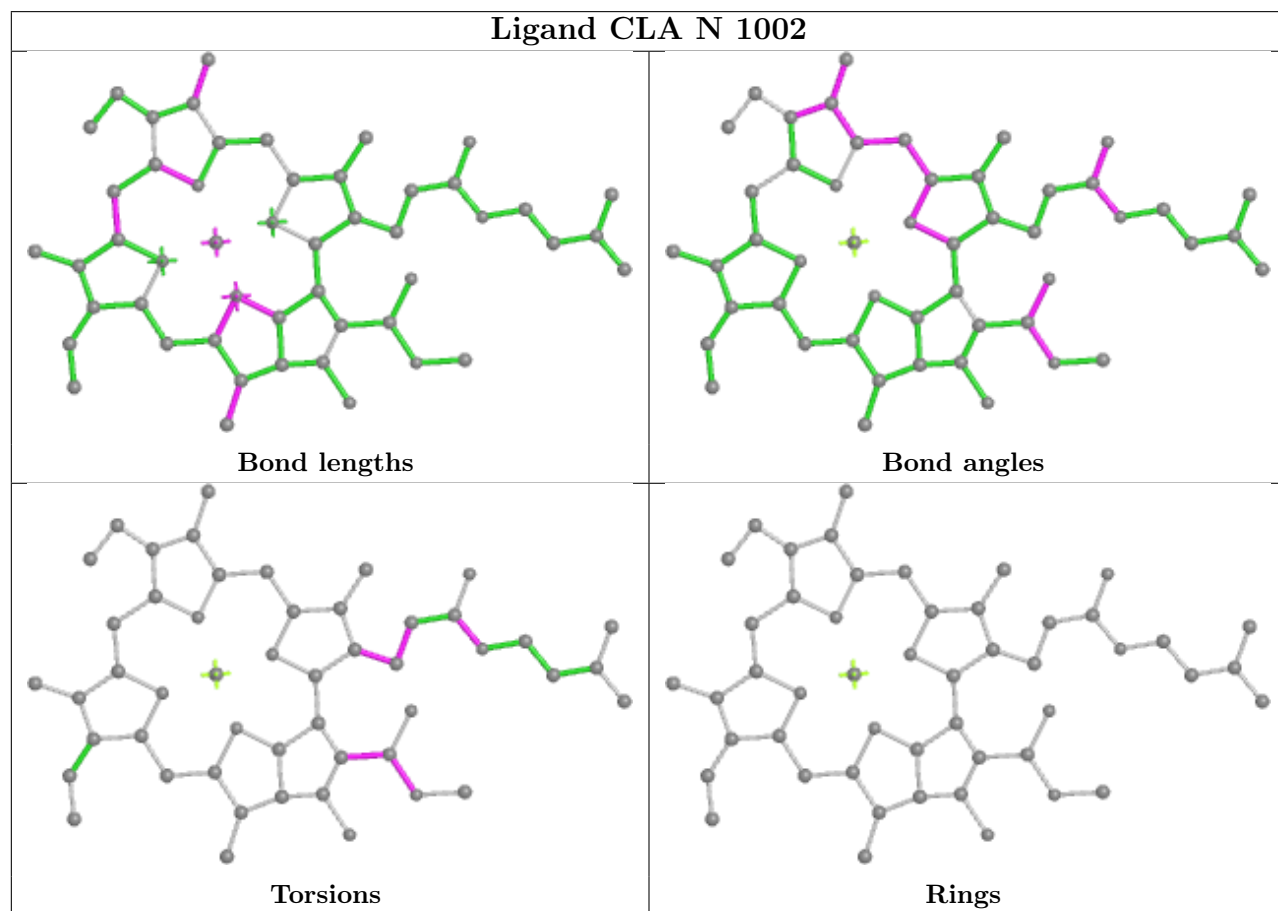
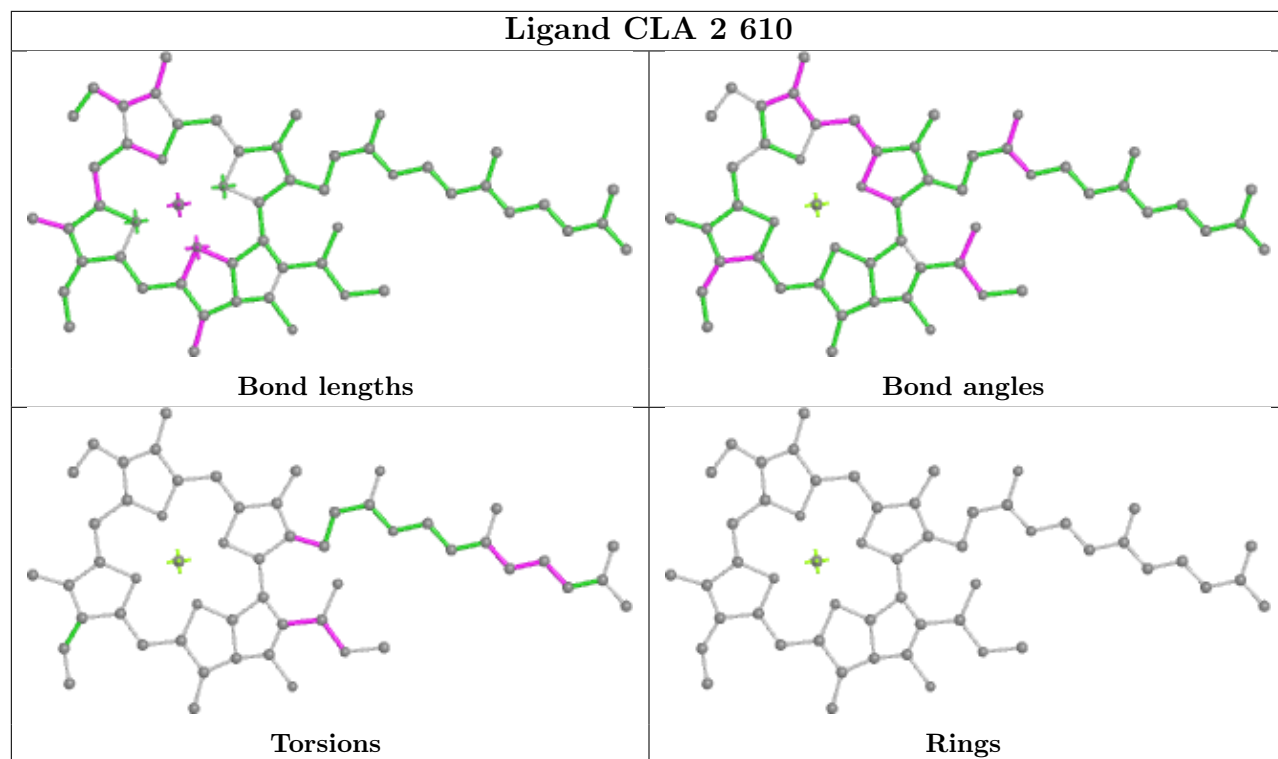


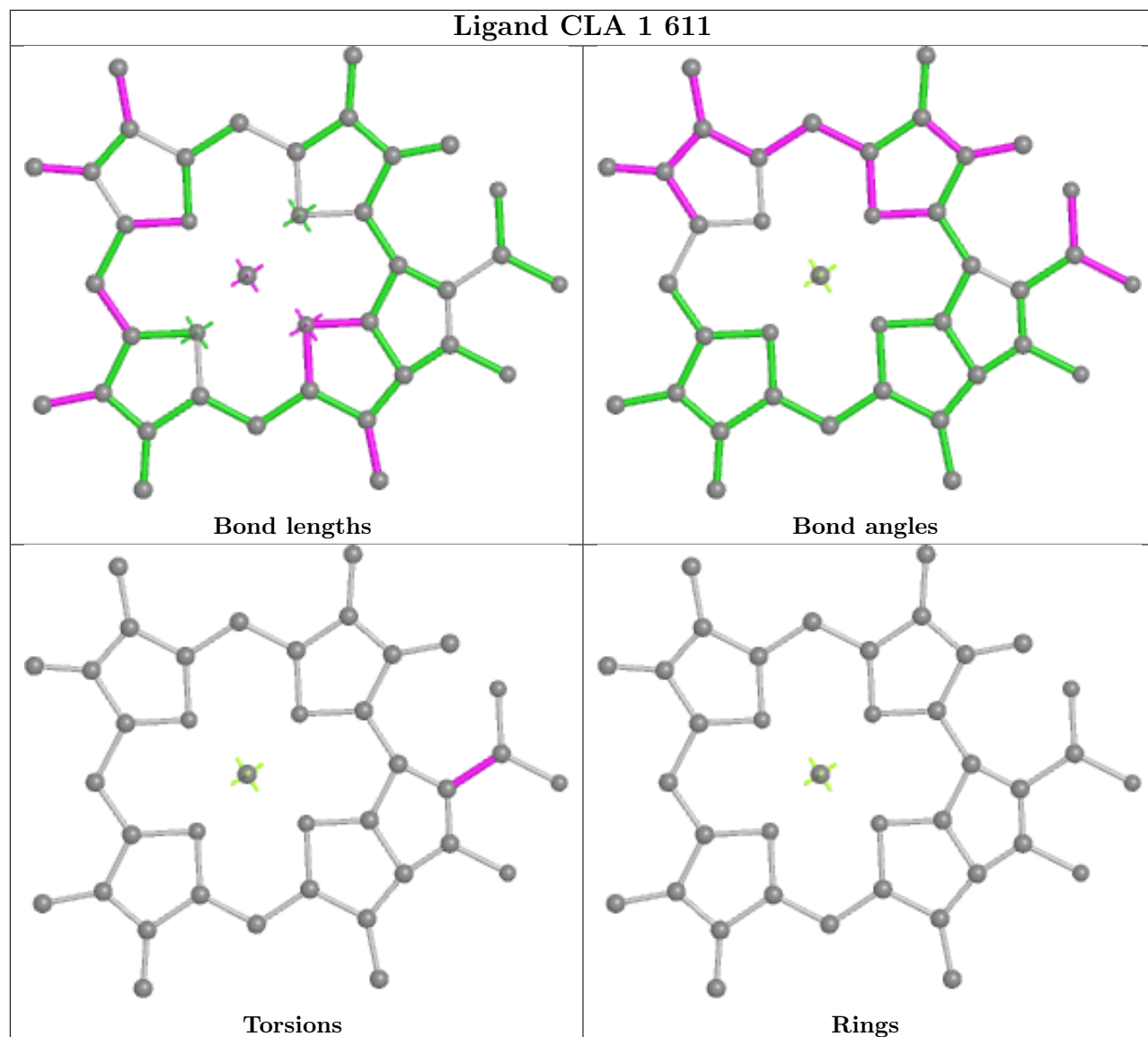


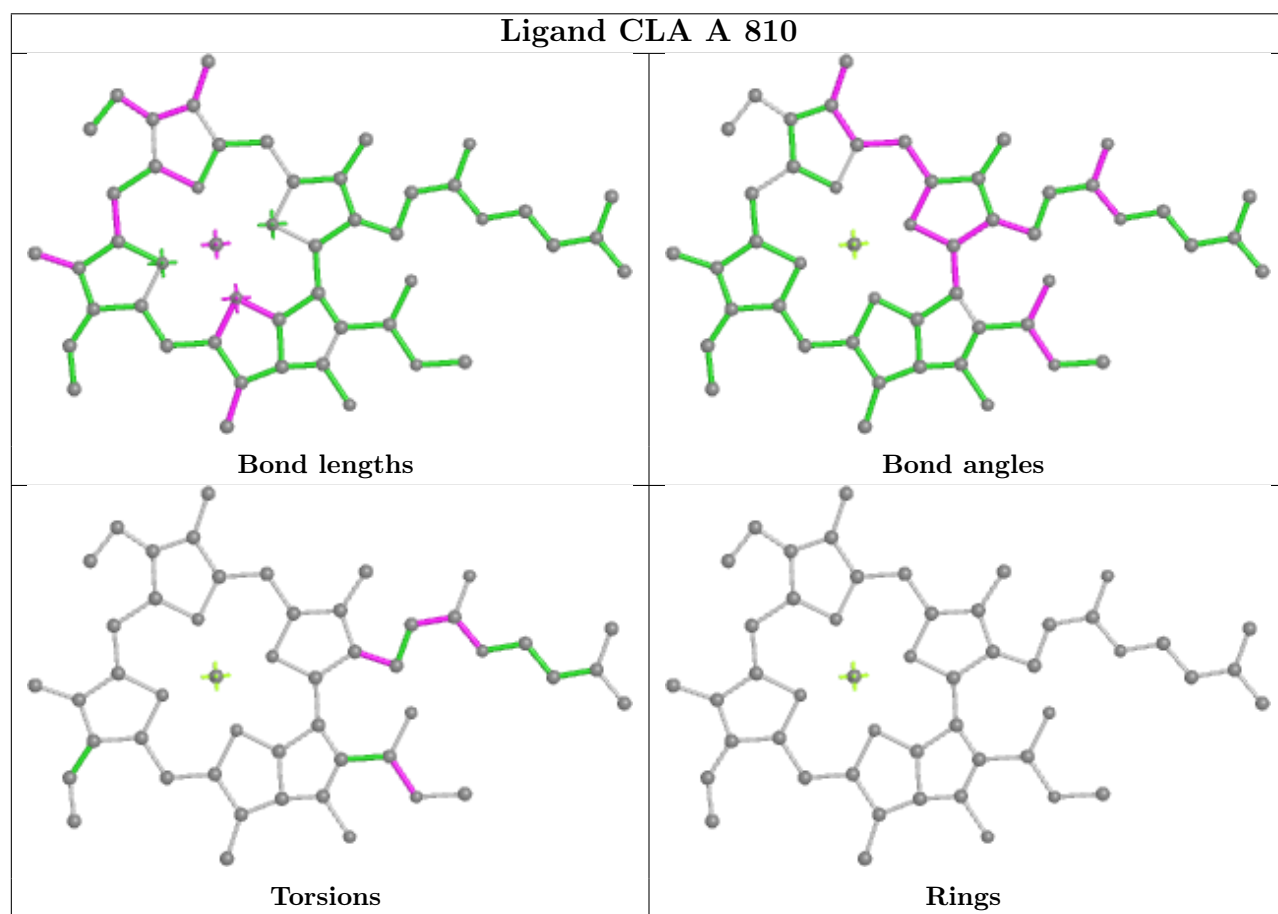
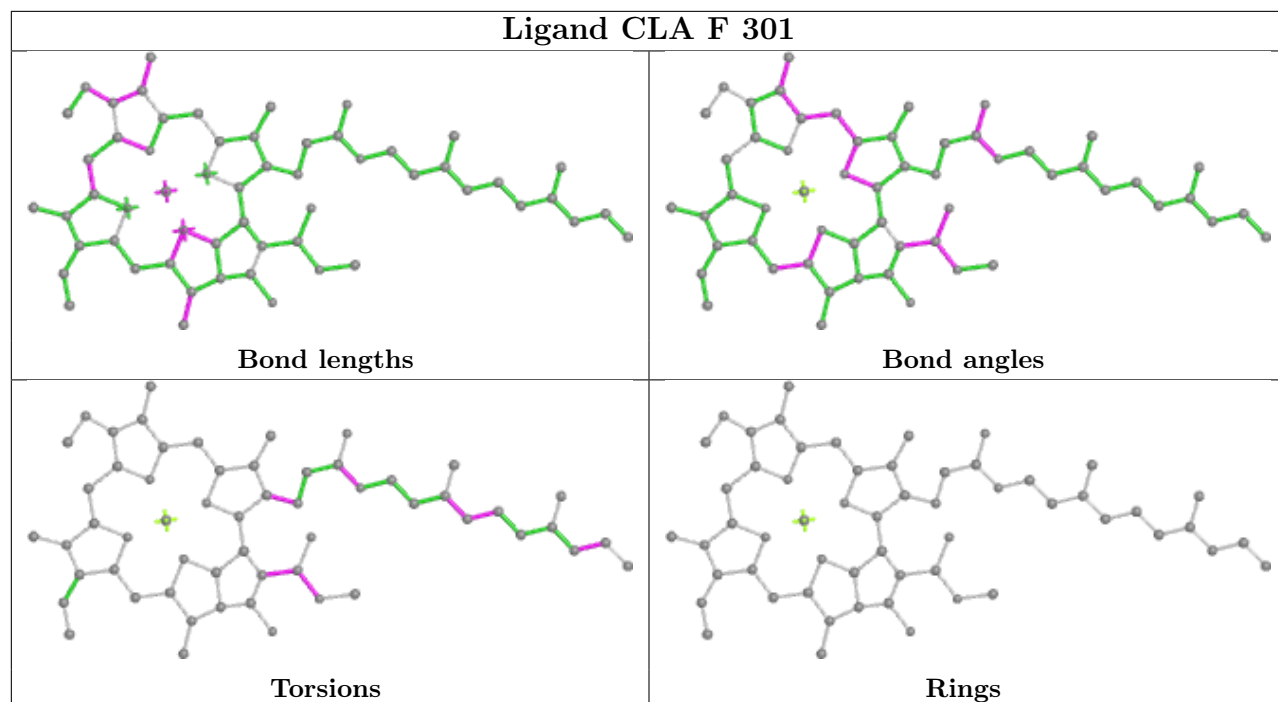




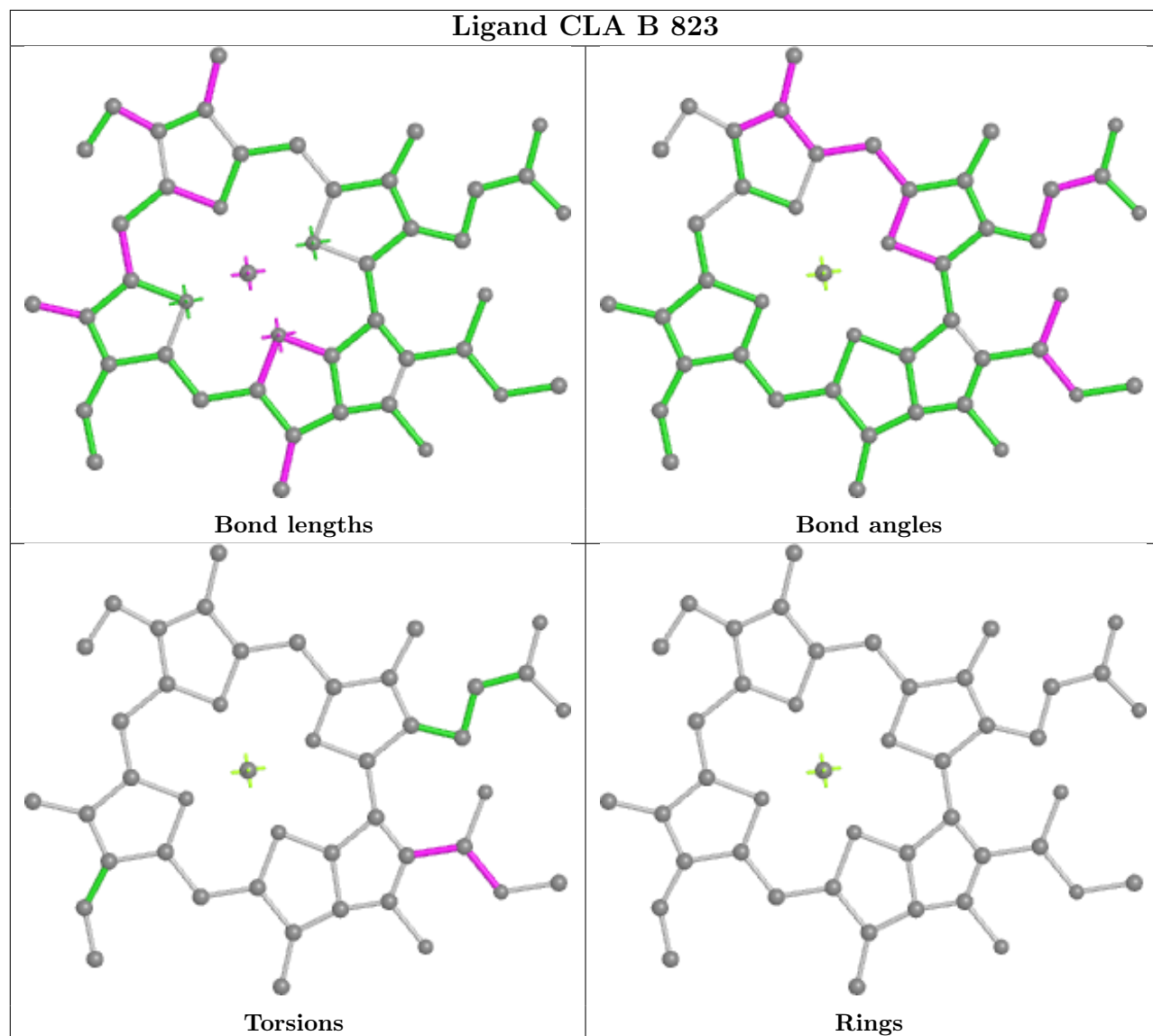


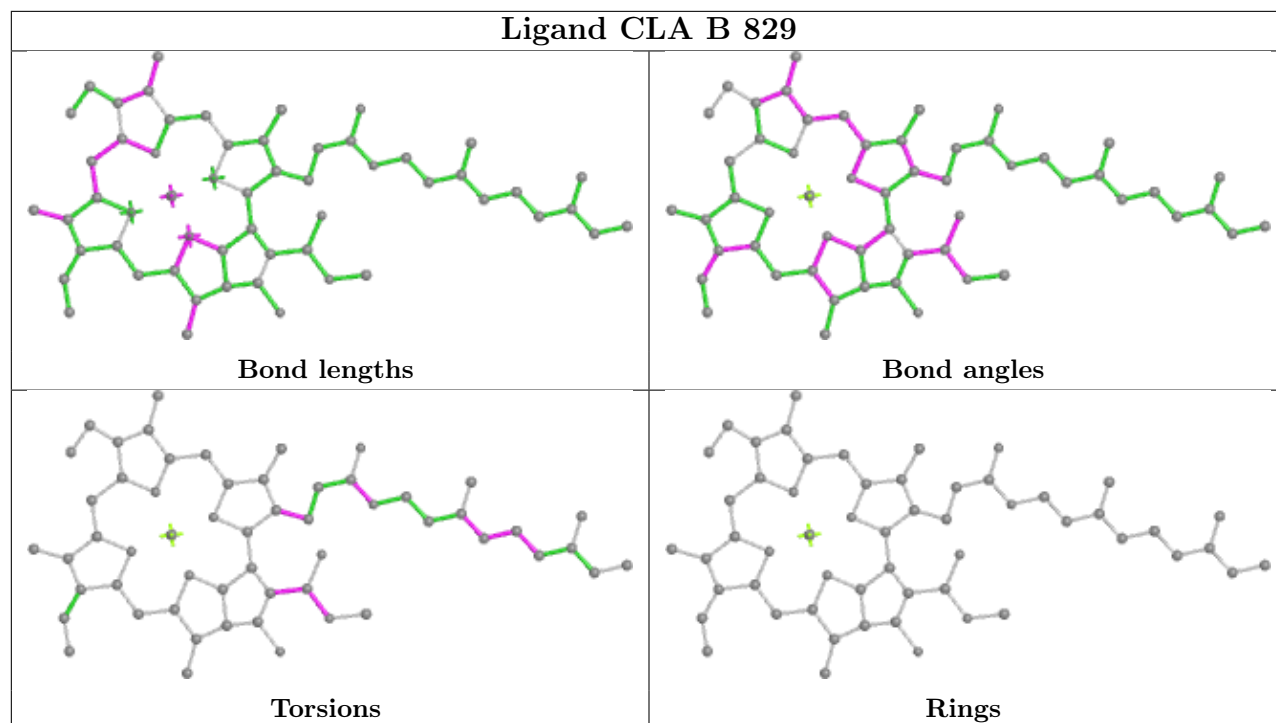


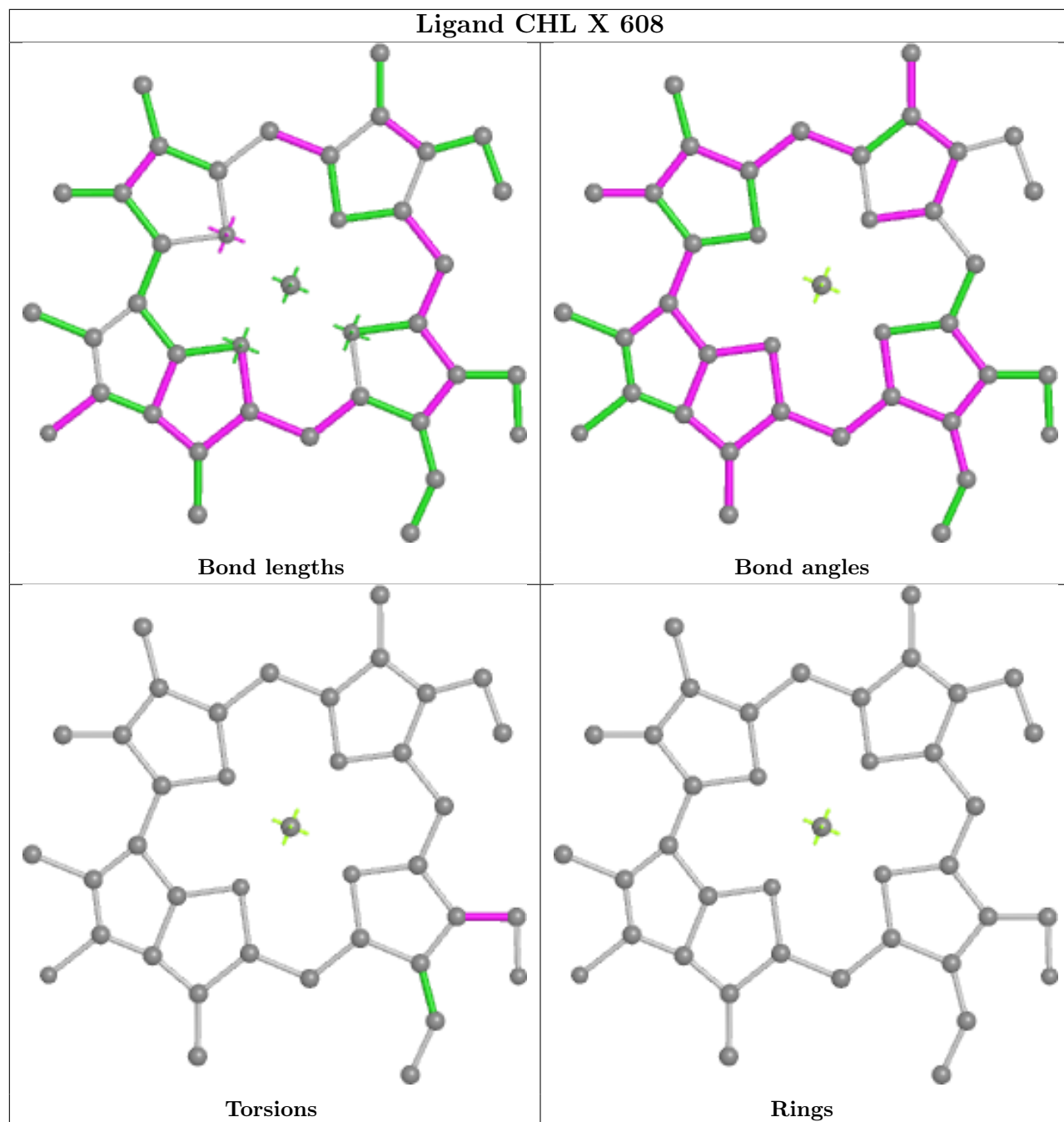


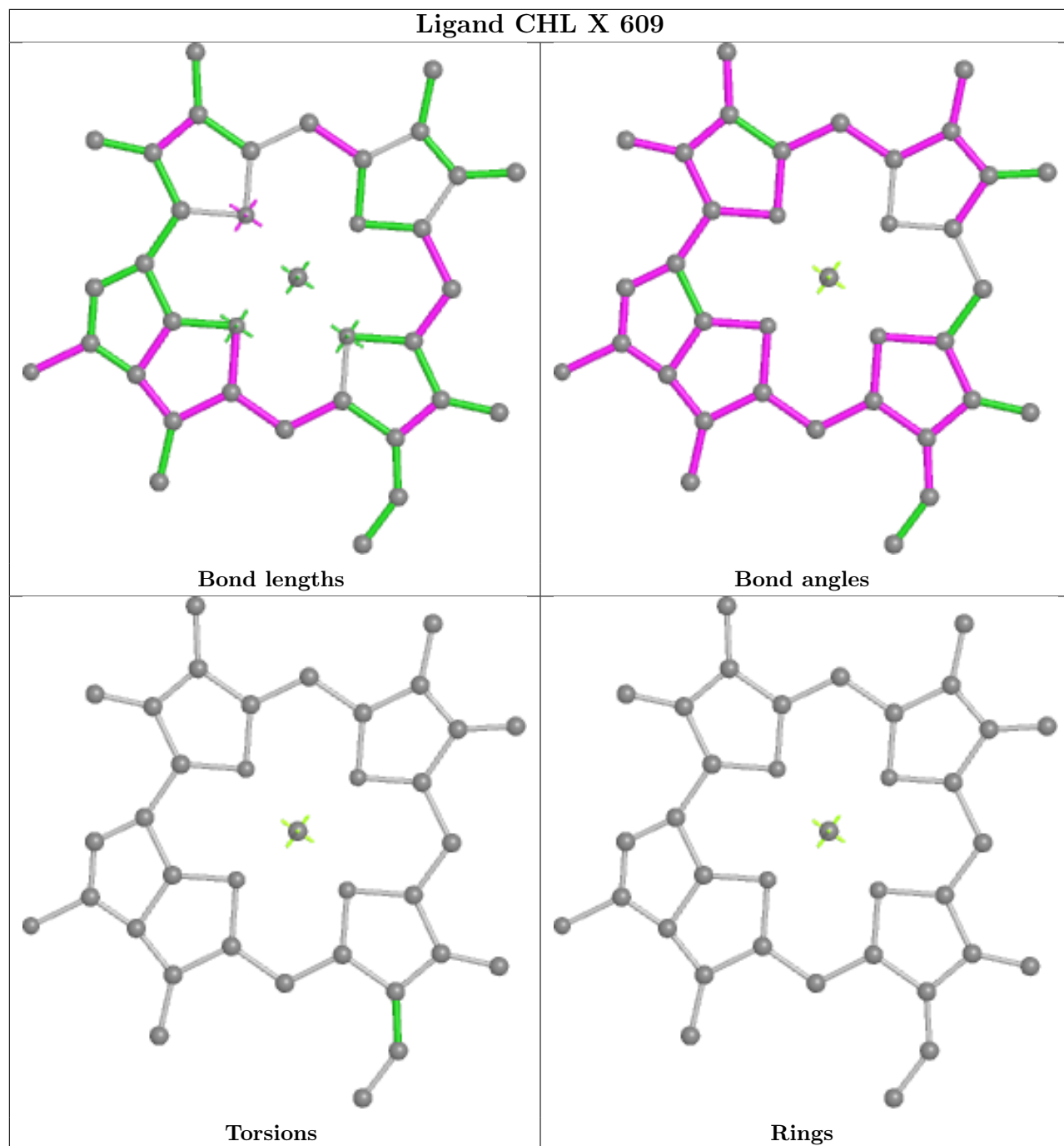


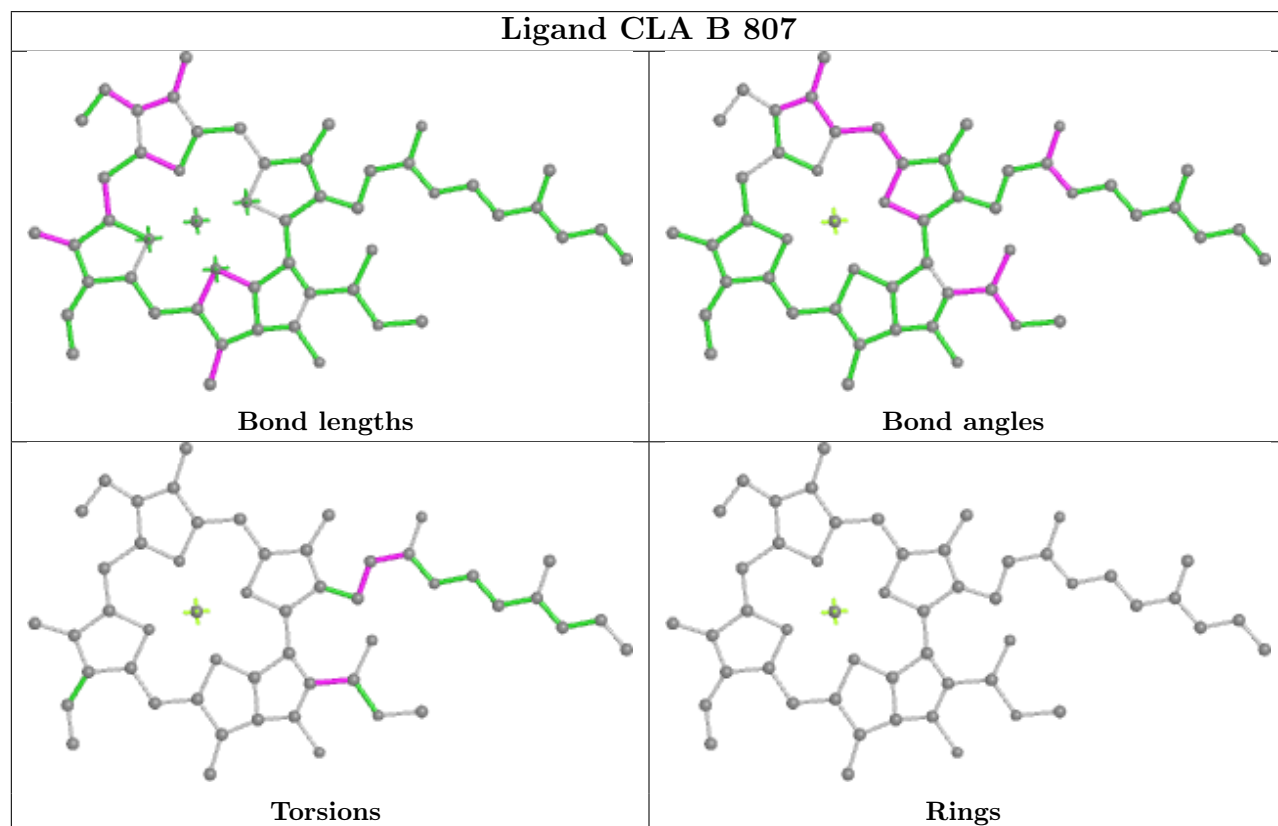
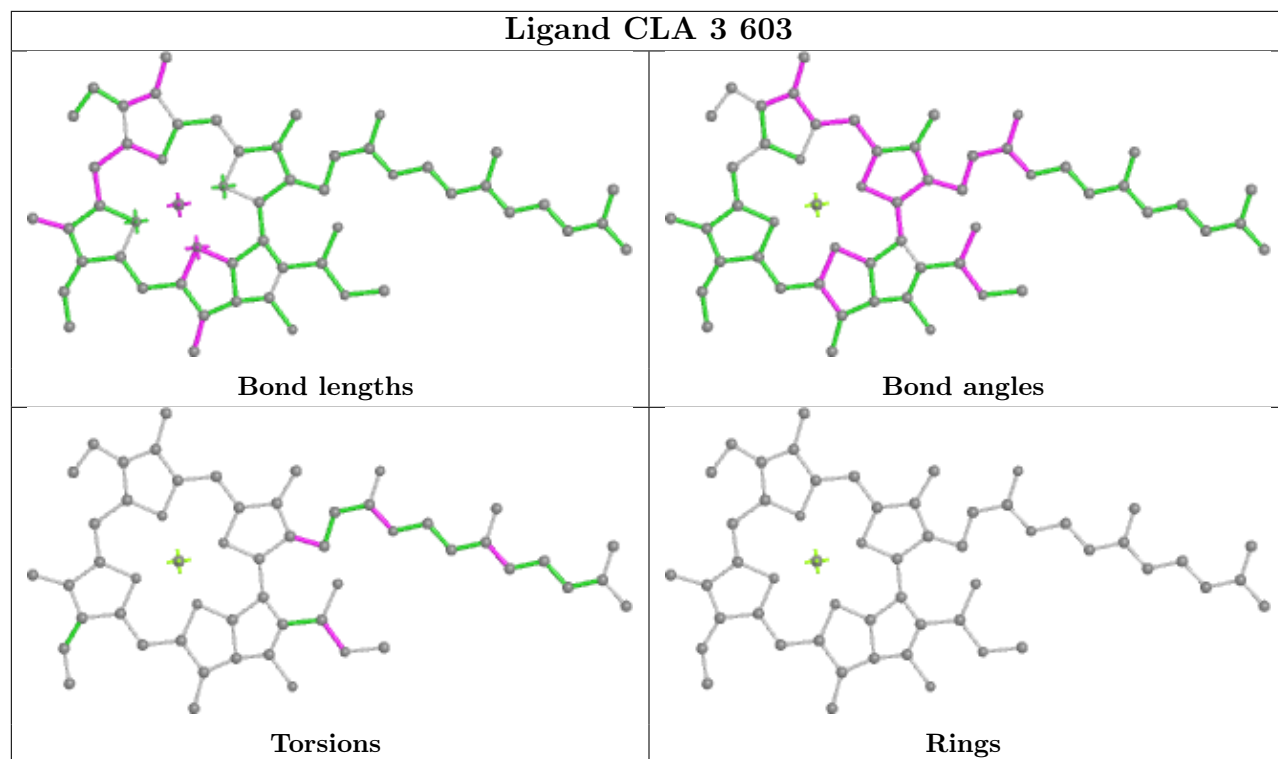


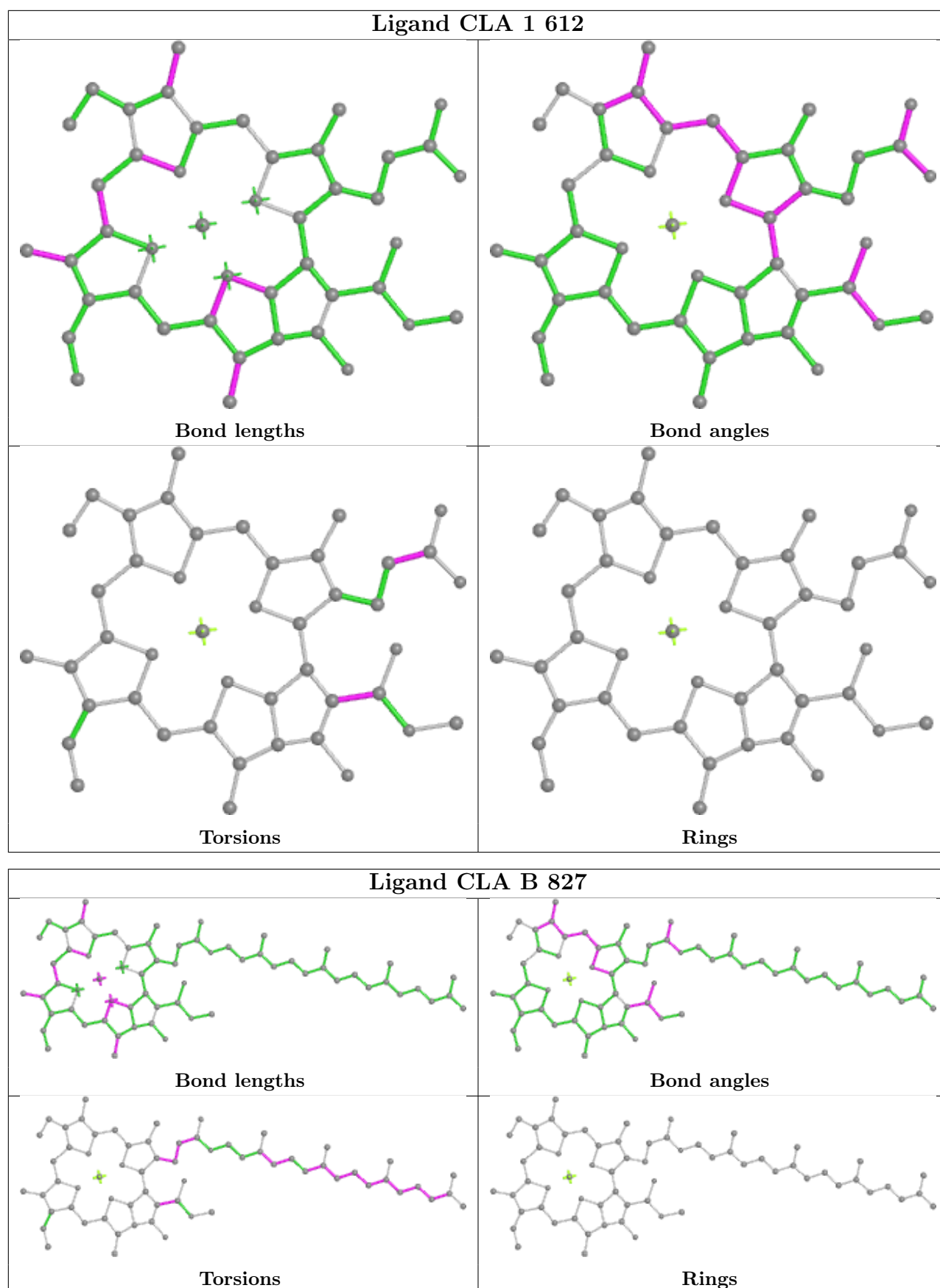


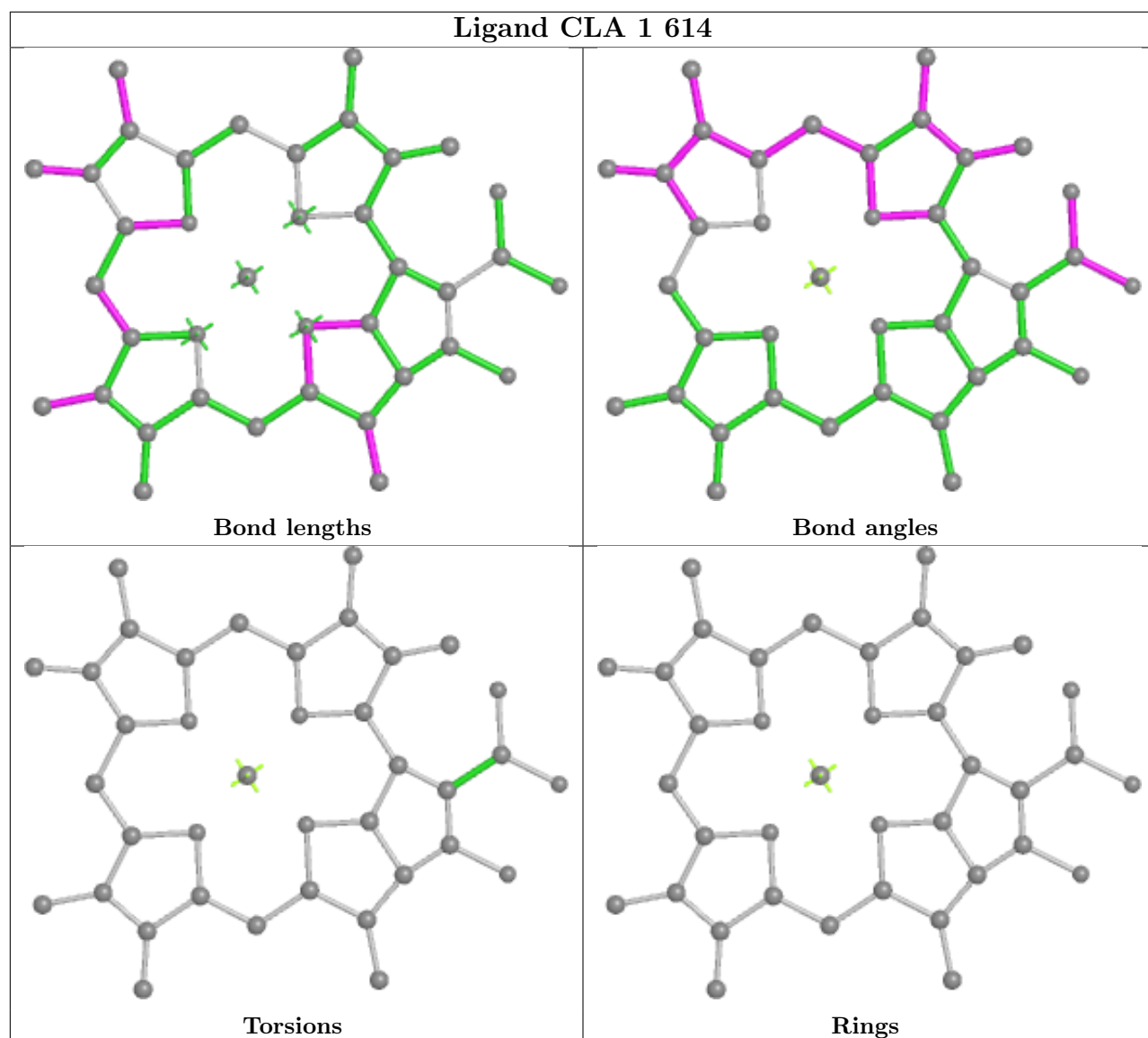
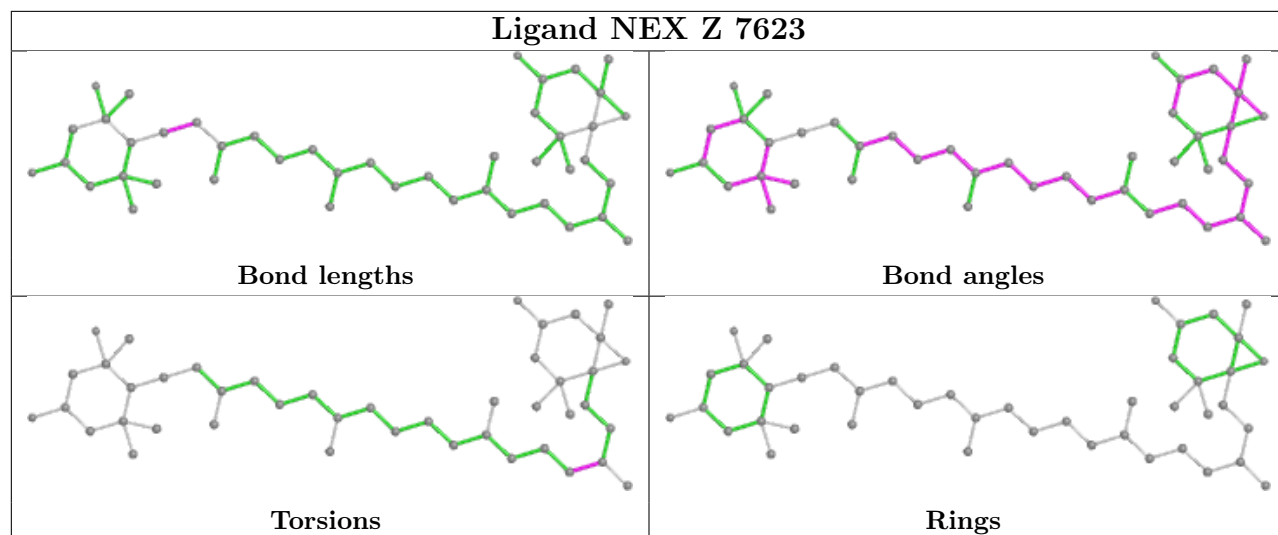


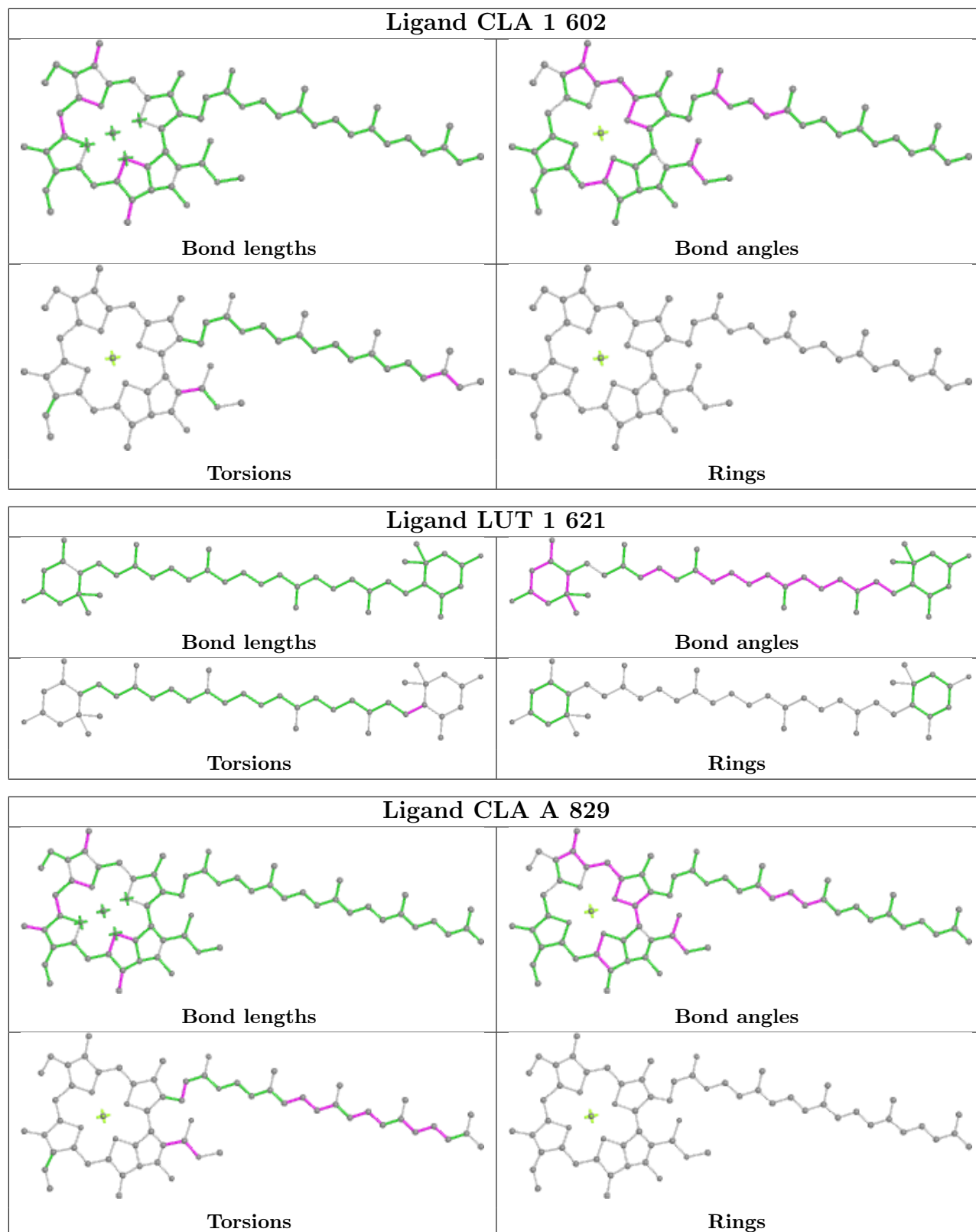




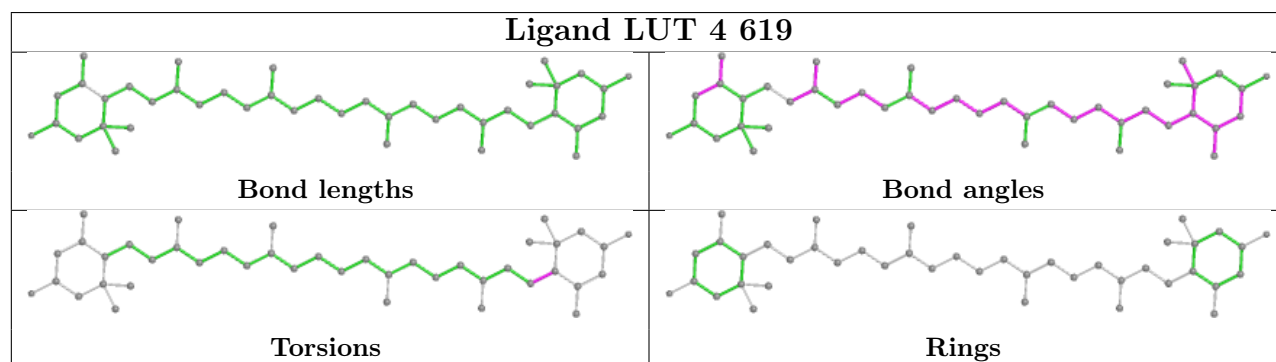
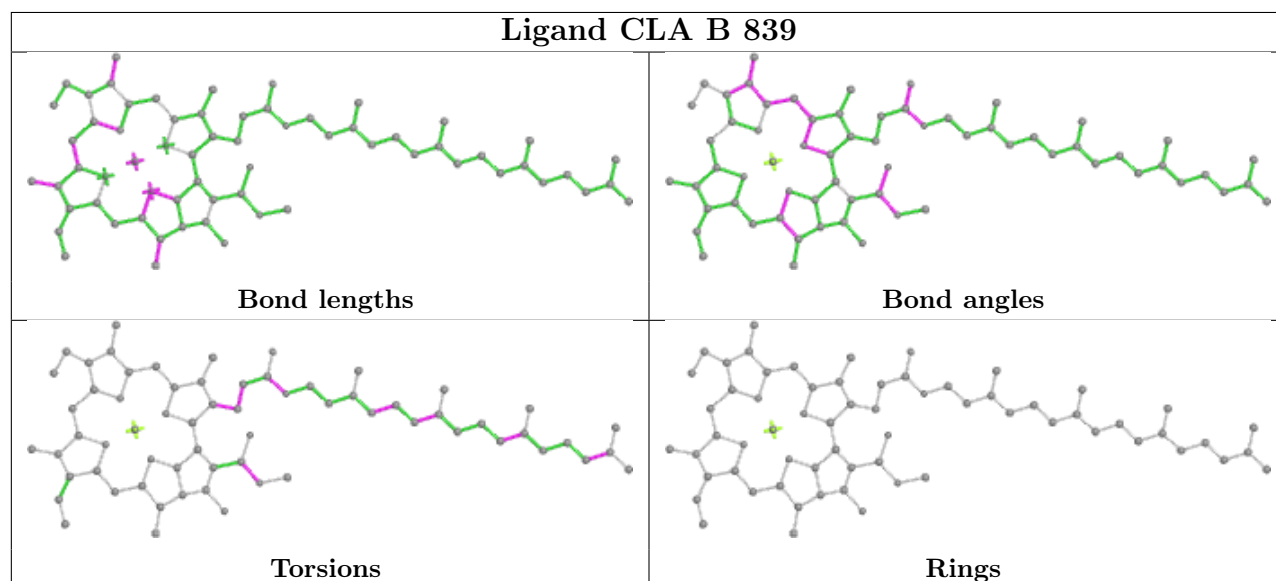
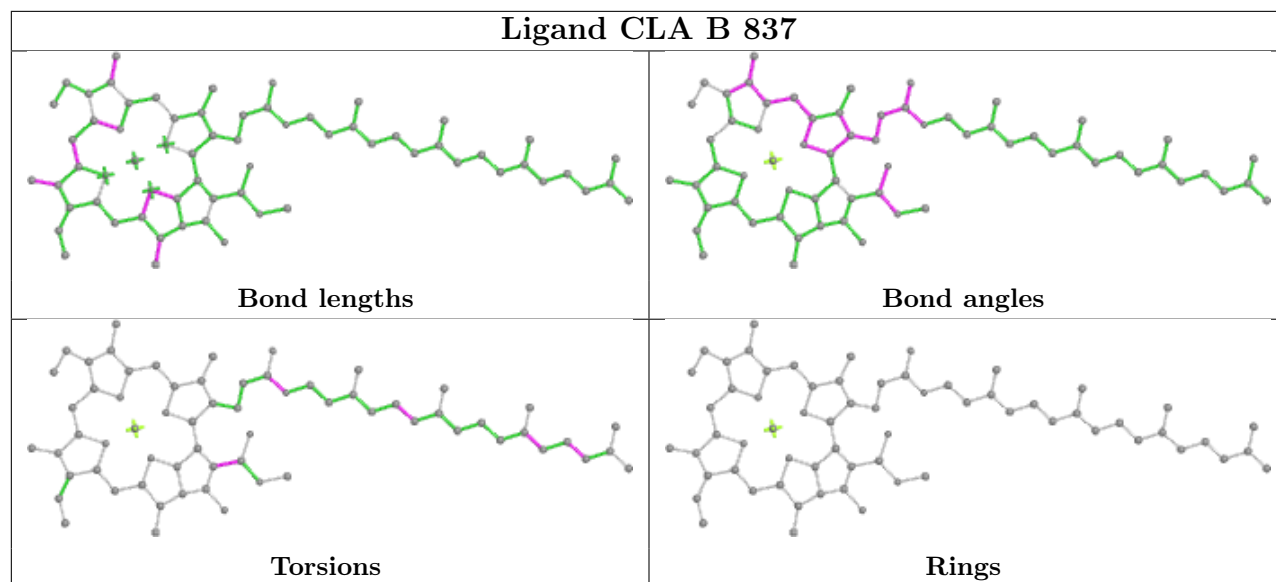


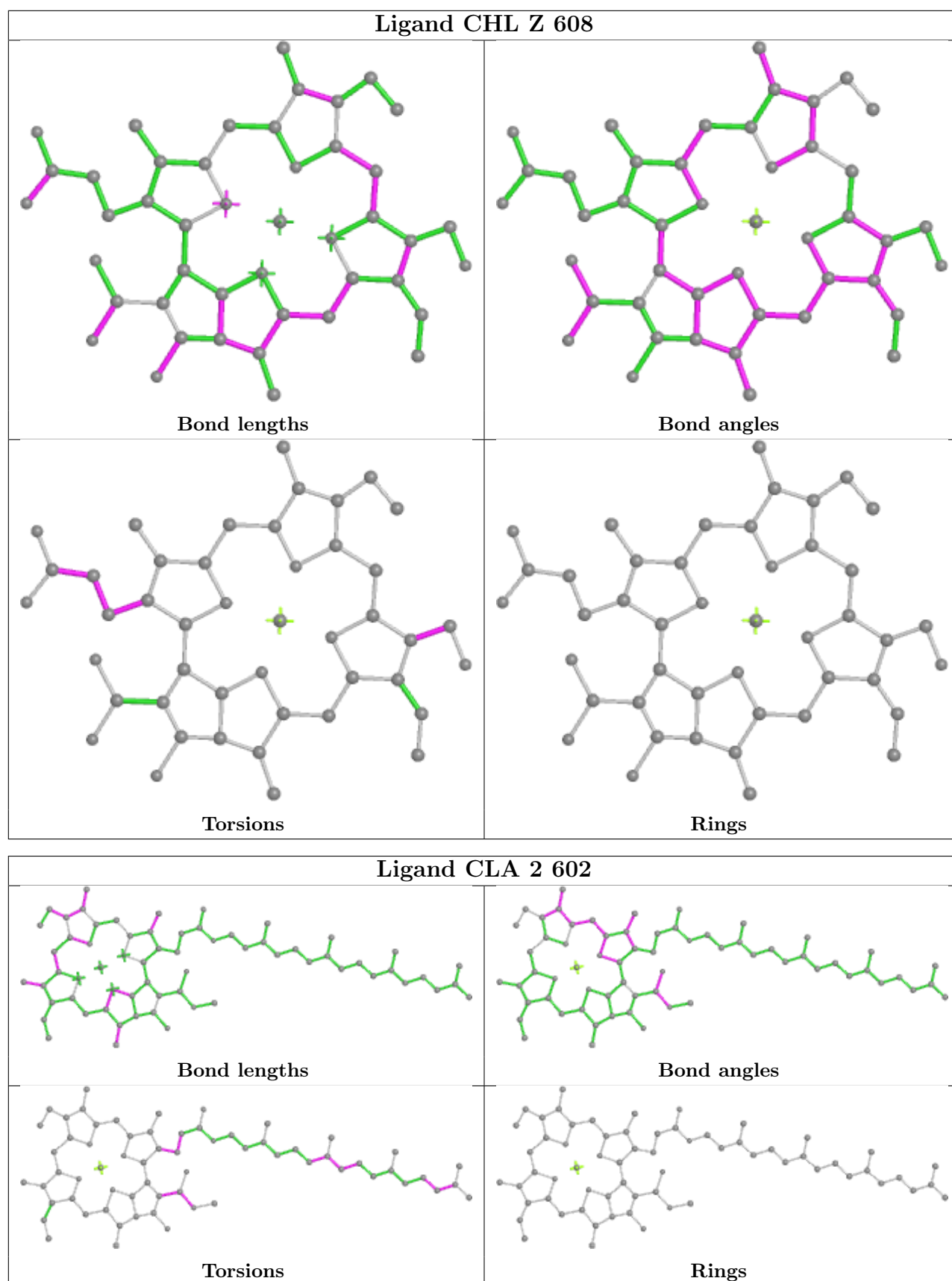


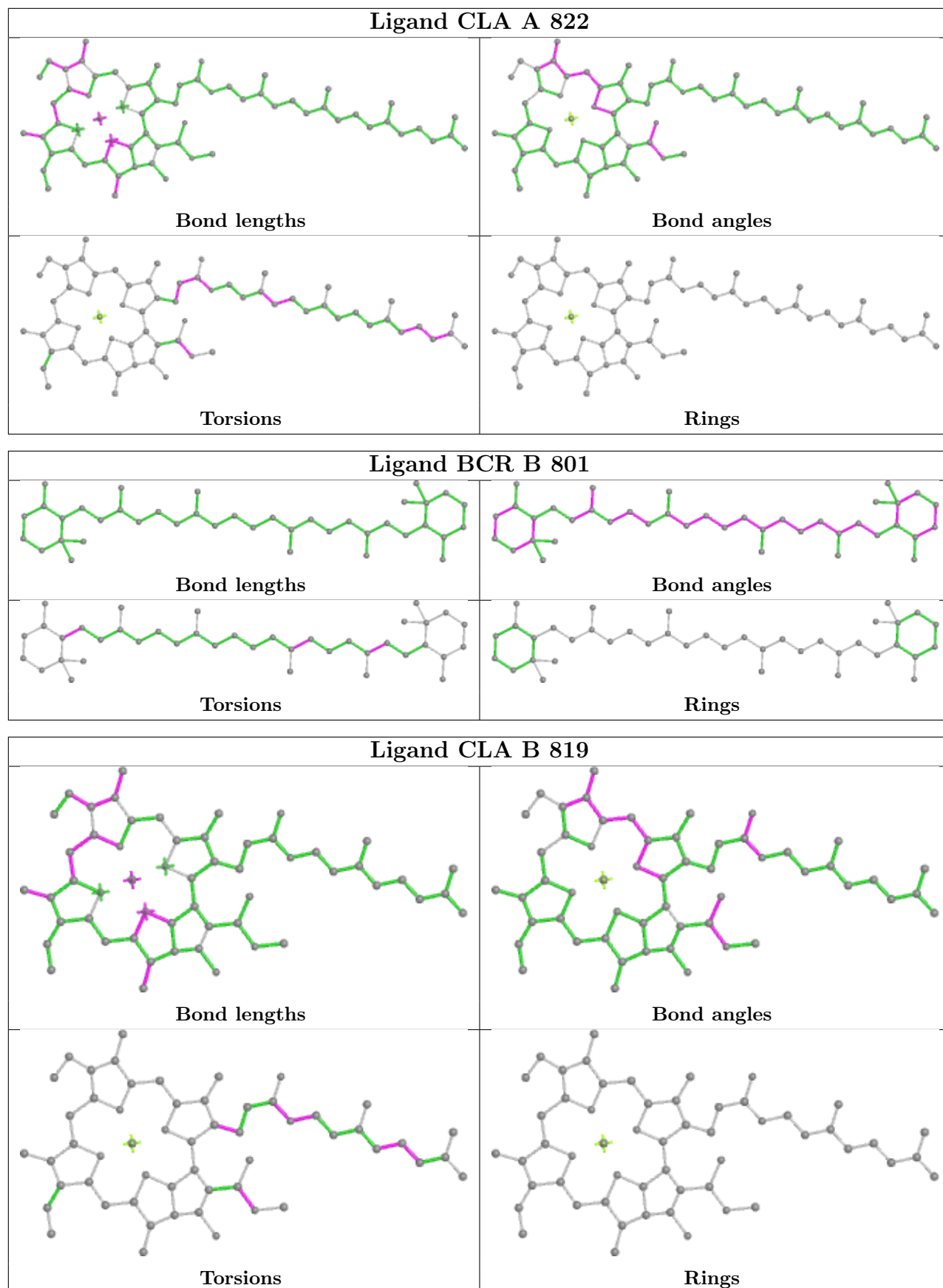


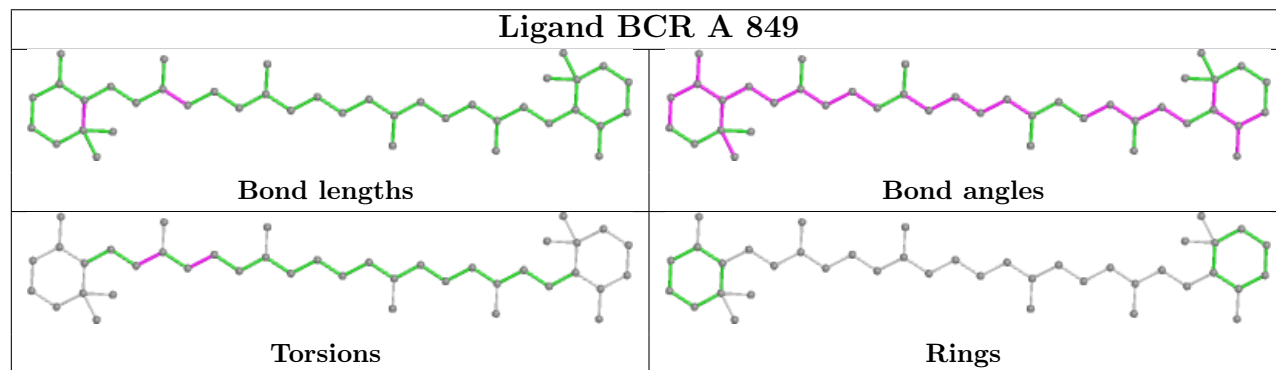
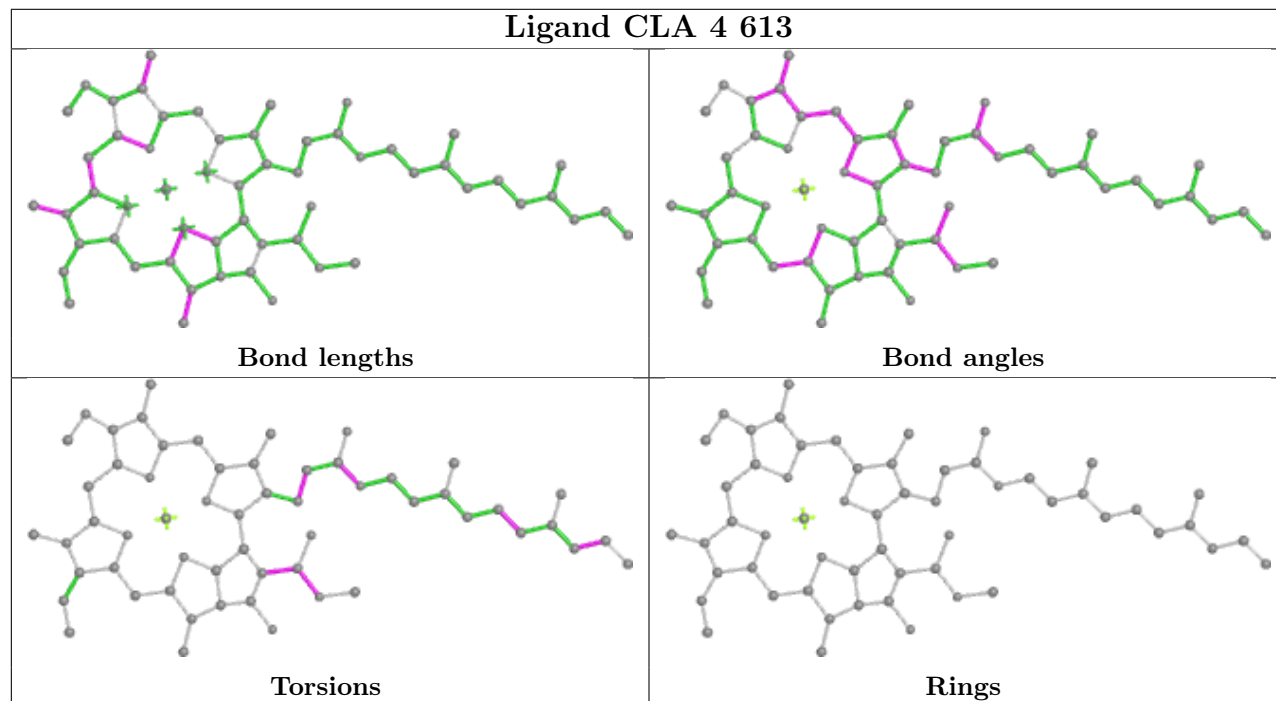
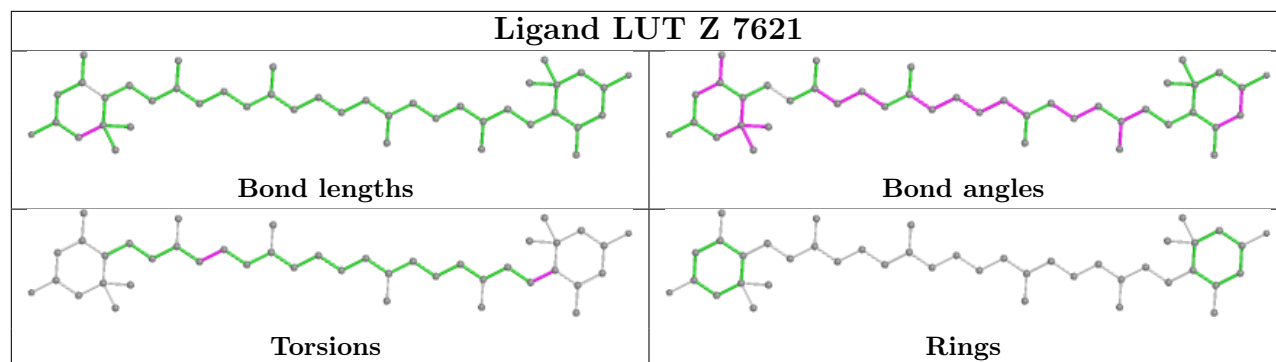


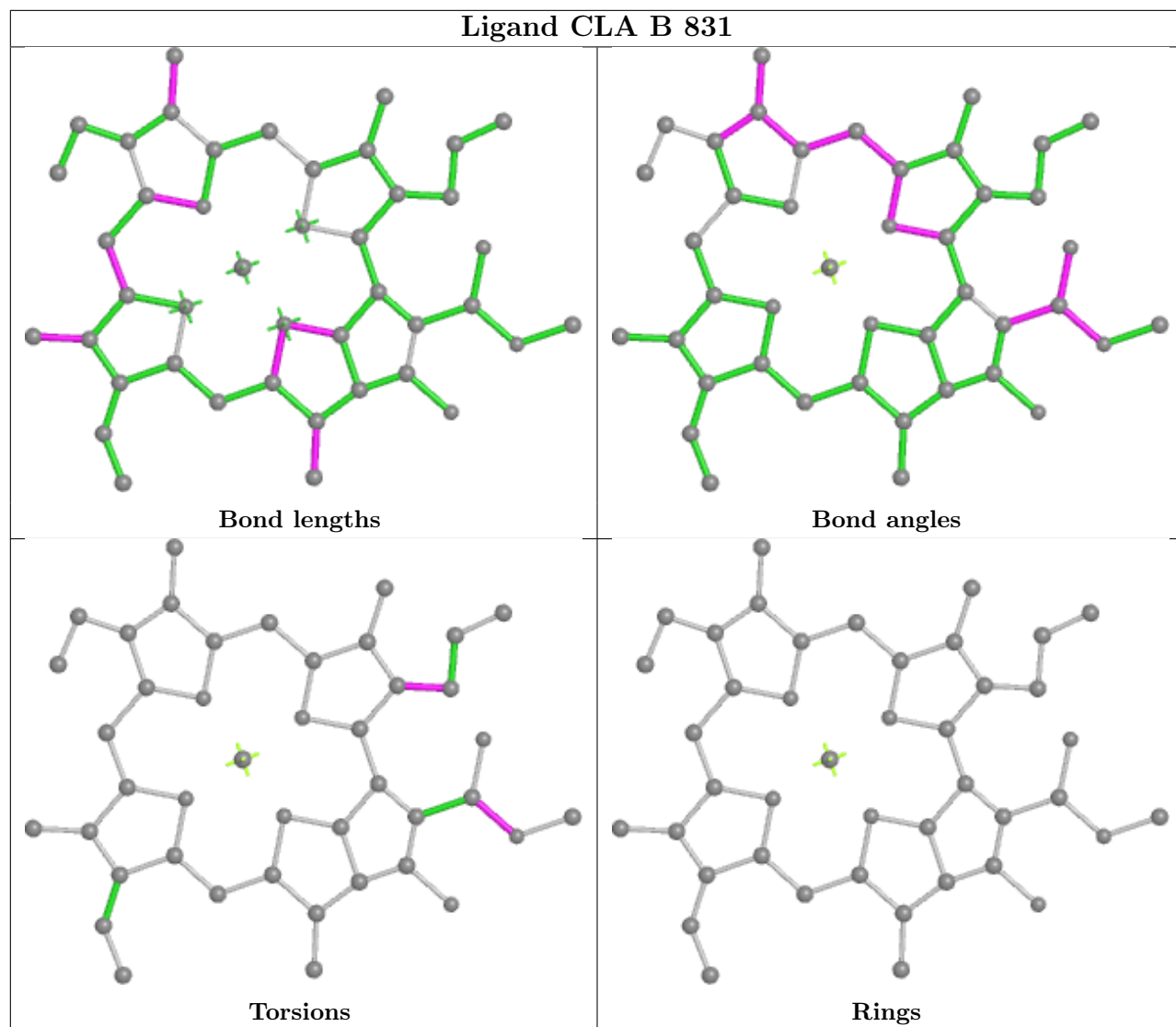




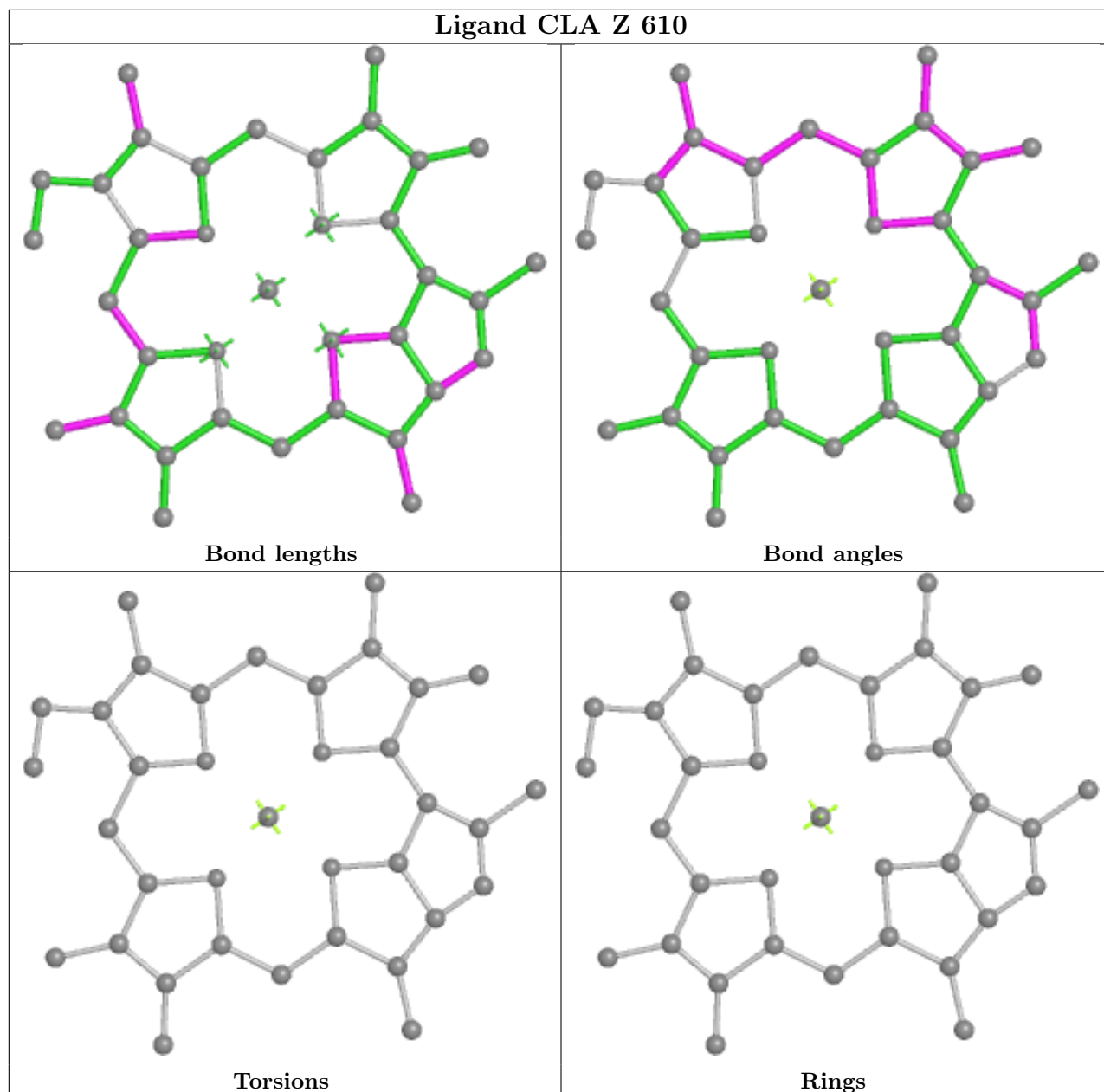


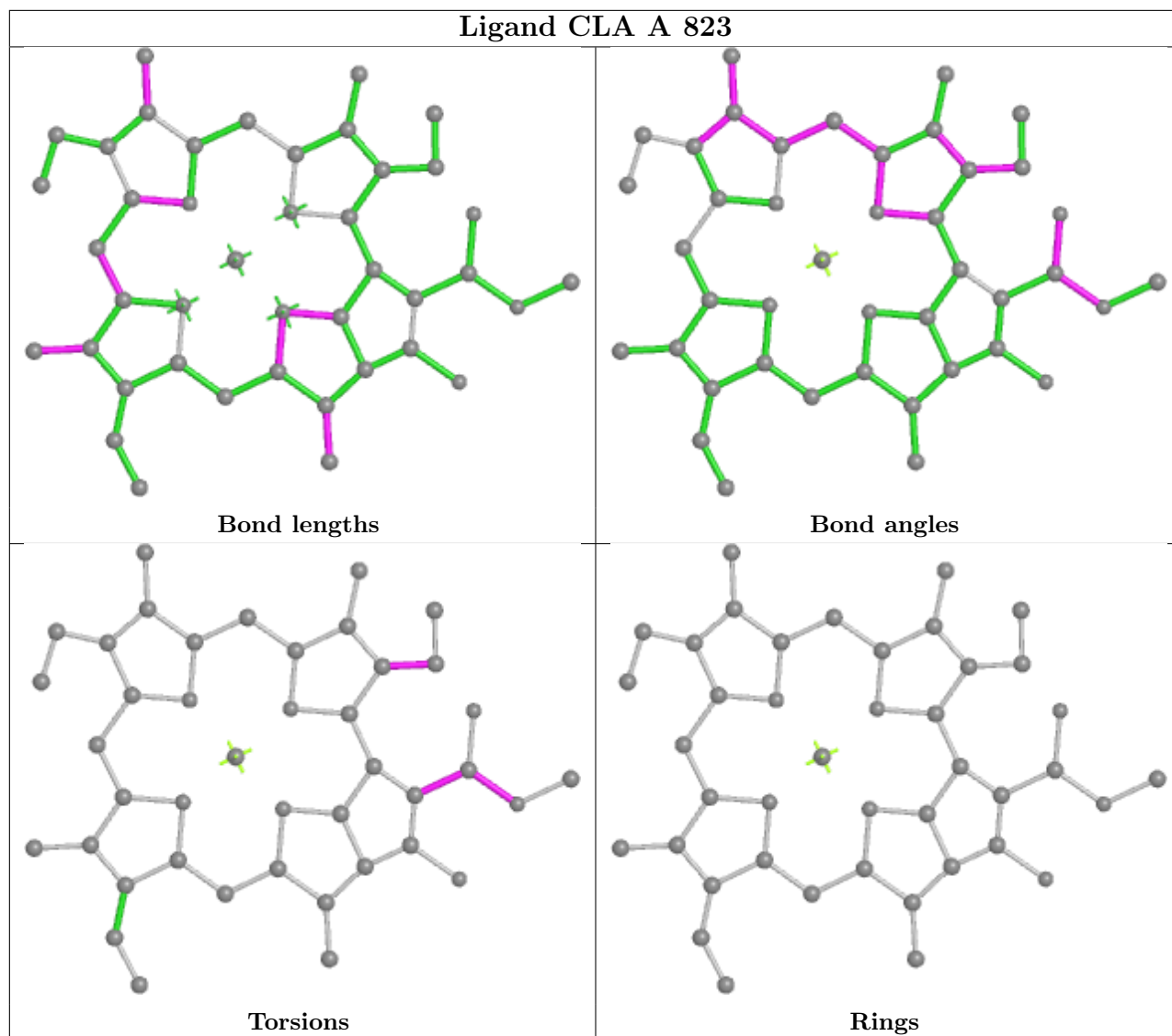


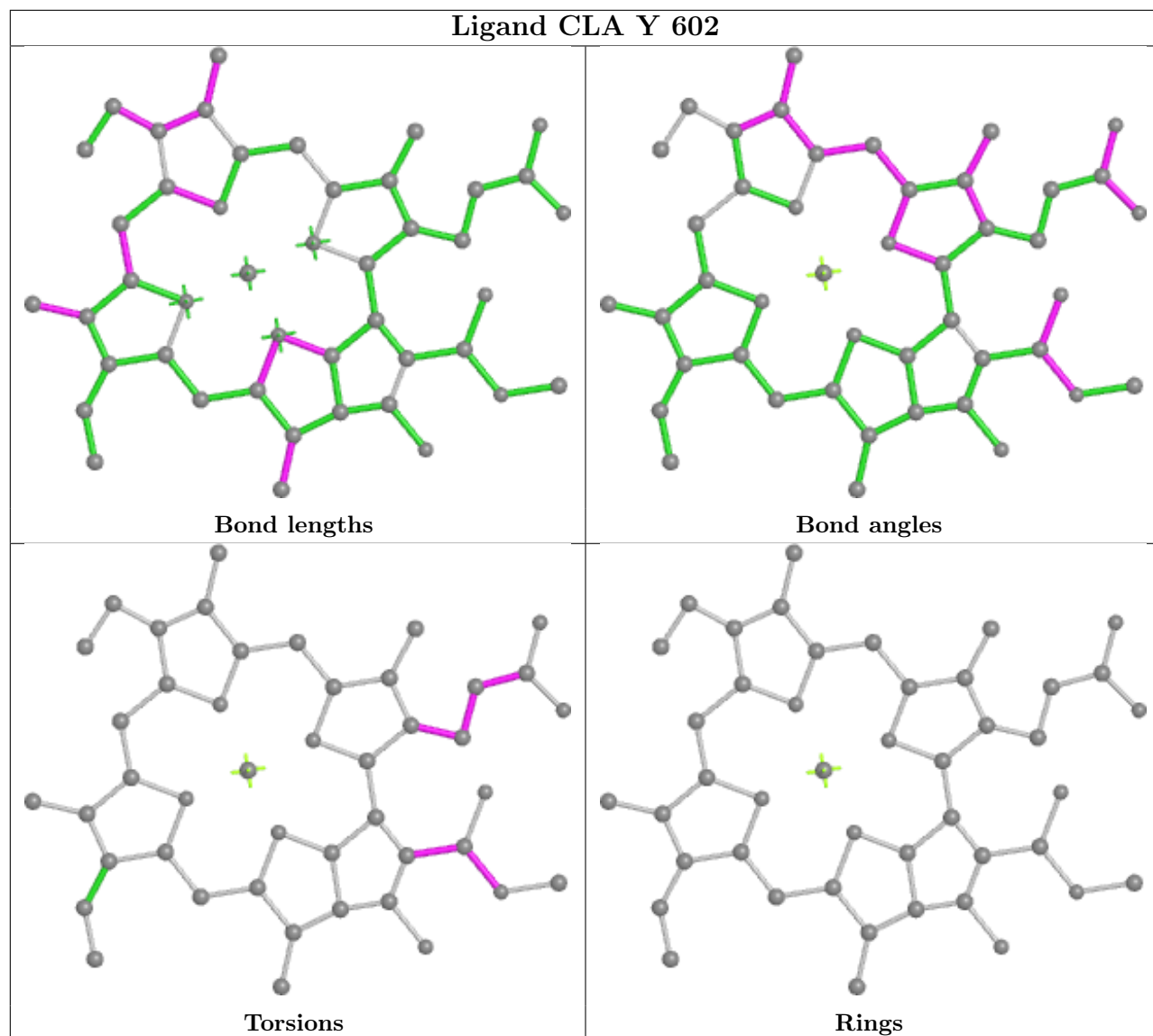




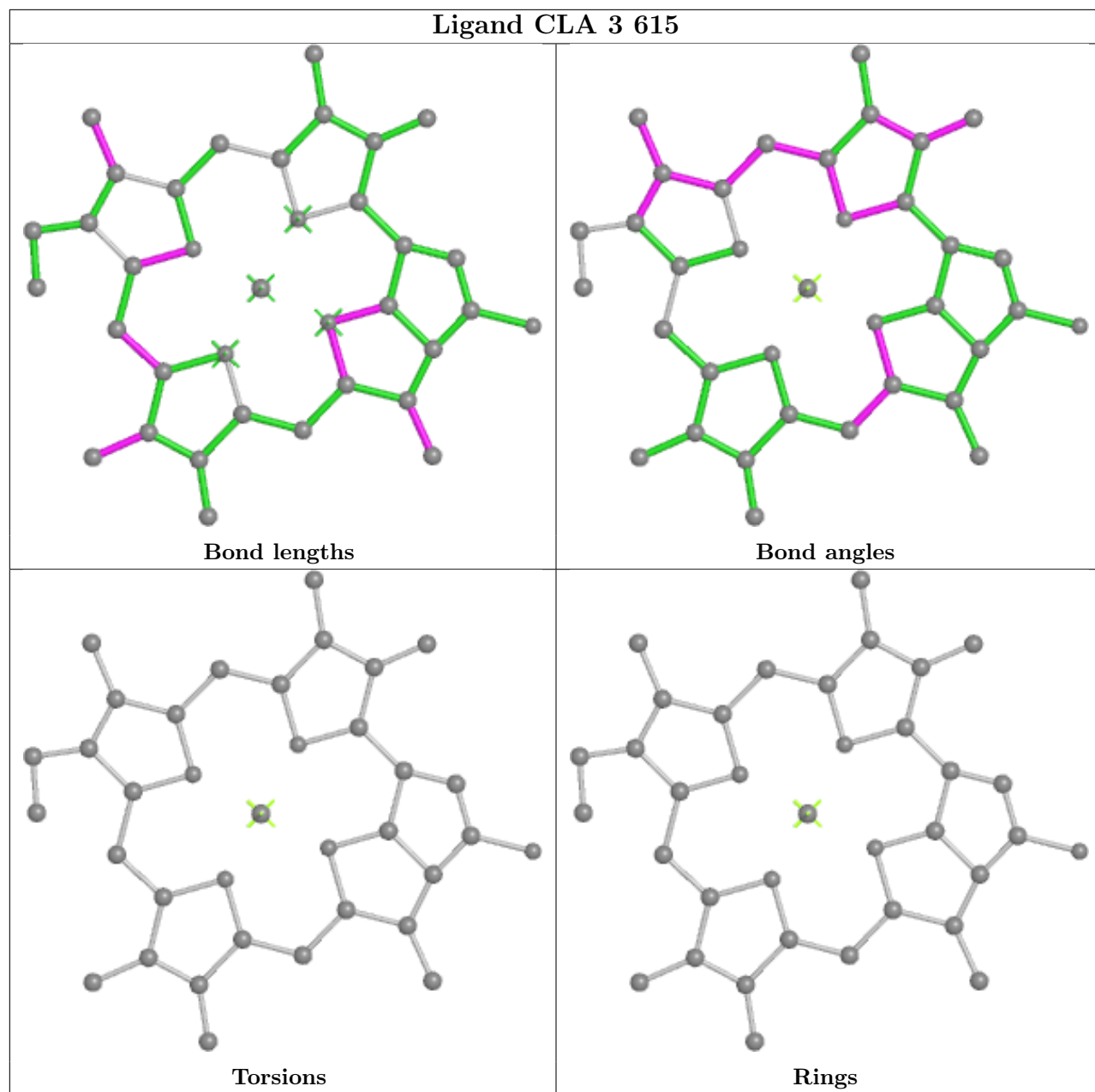
## Ligand CLA Z 610

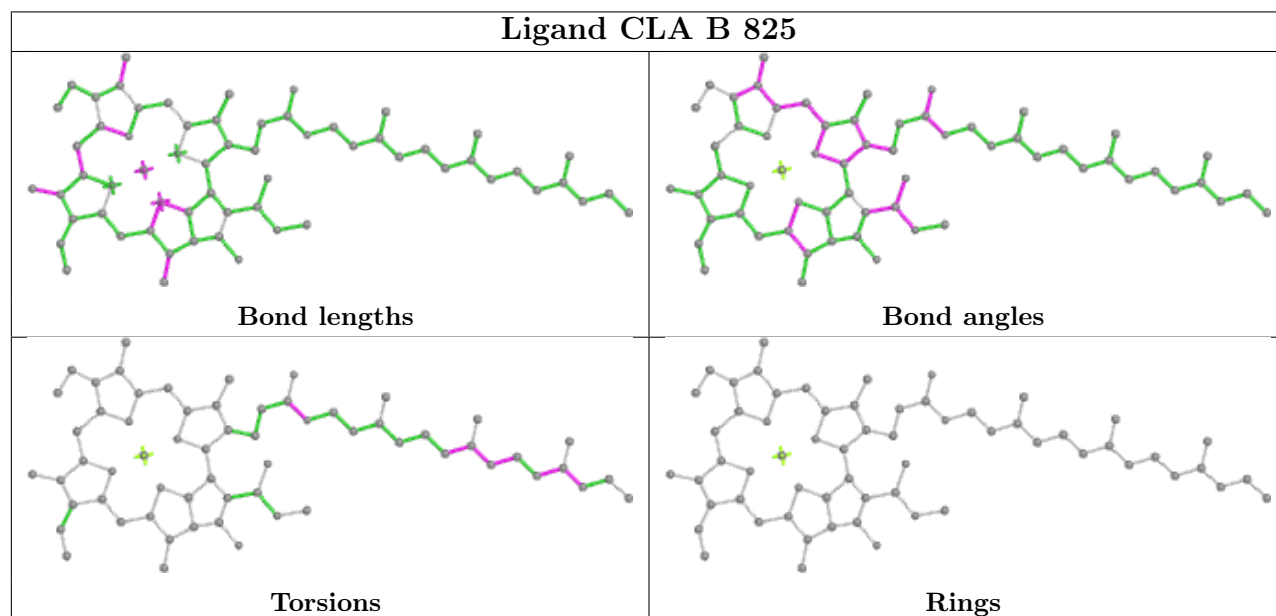
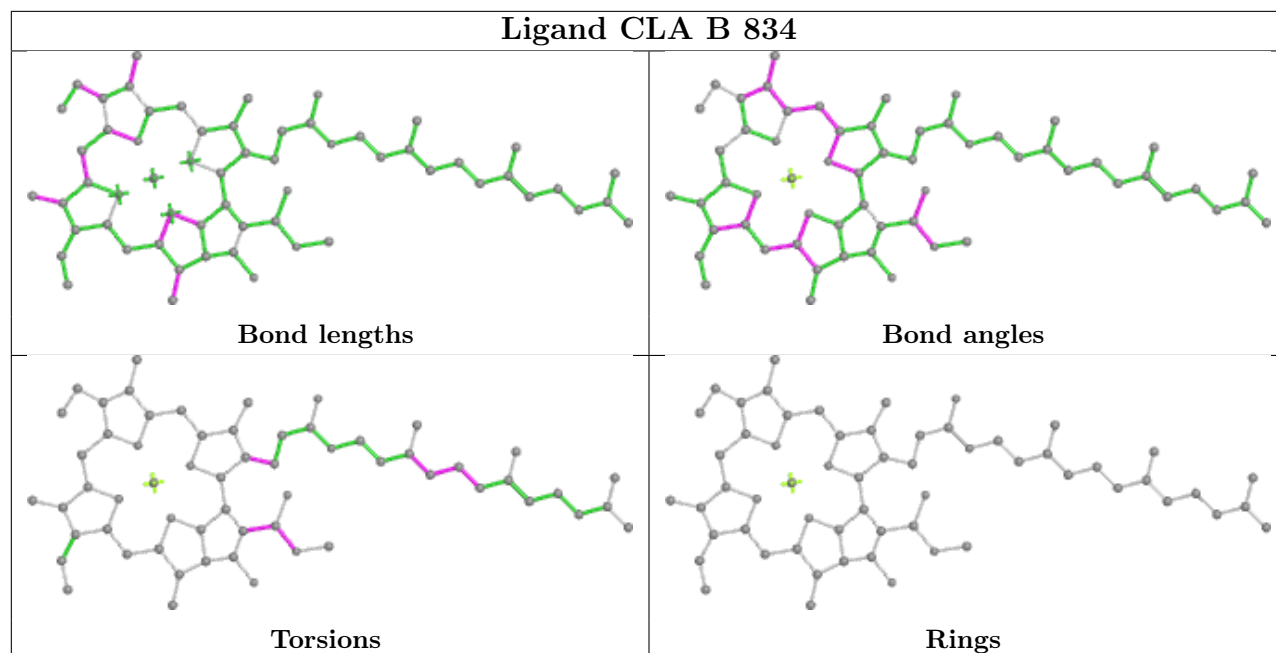


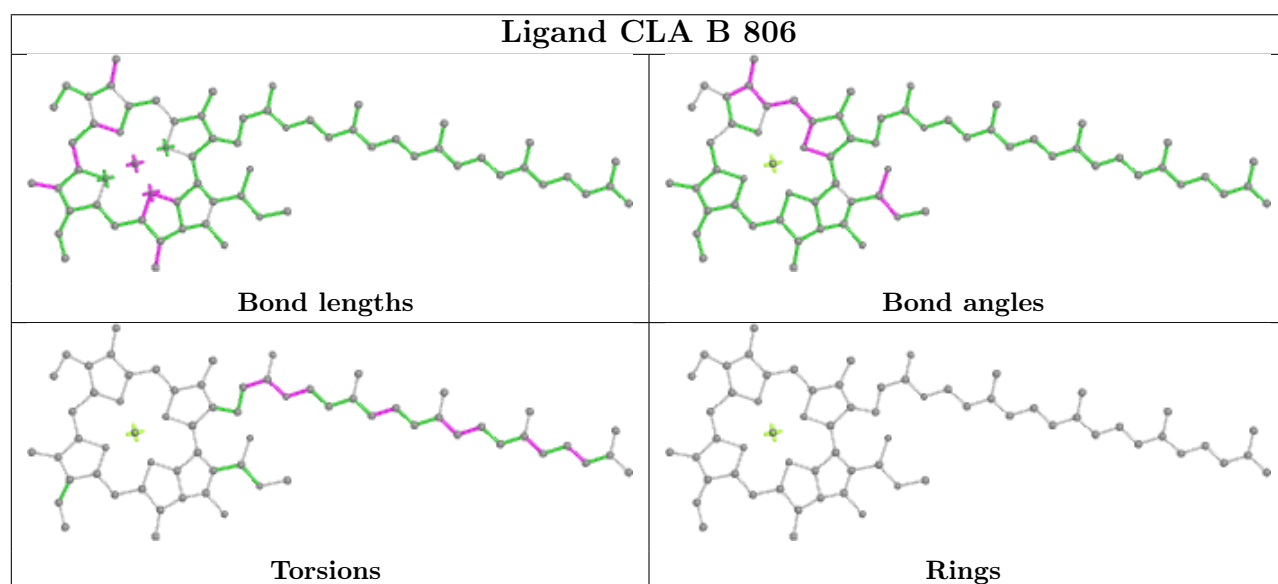
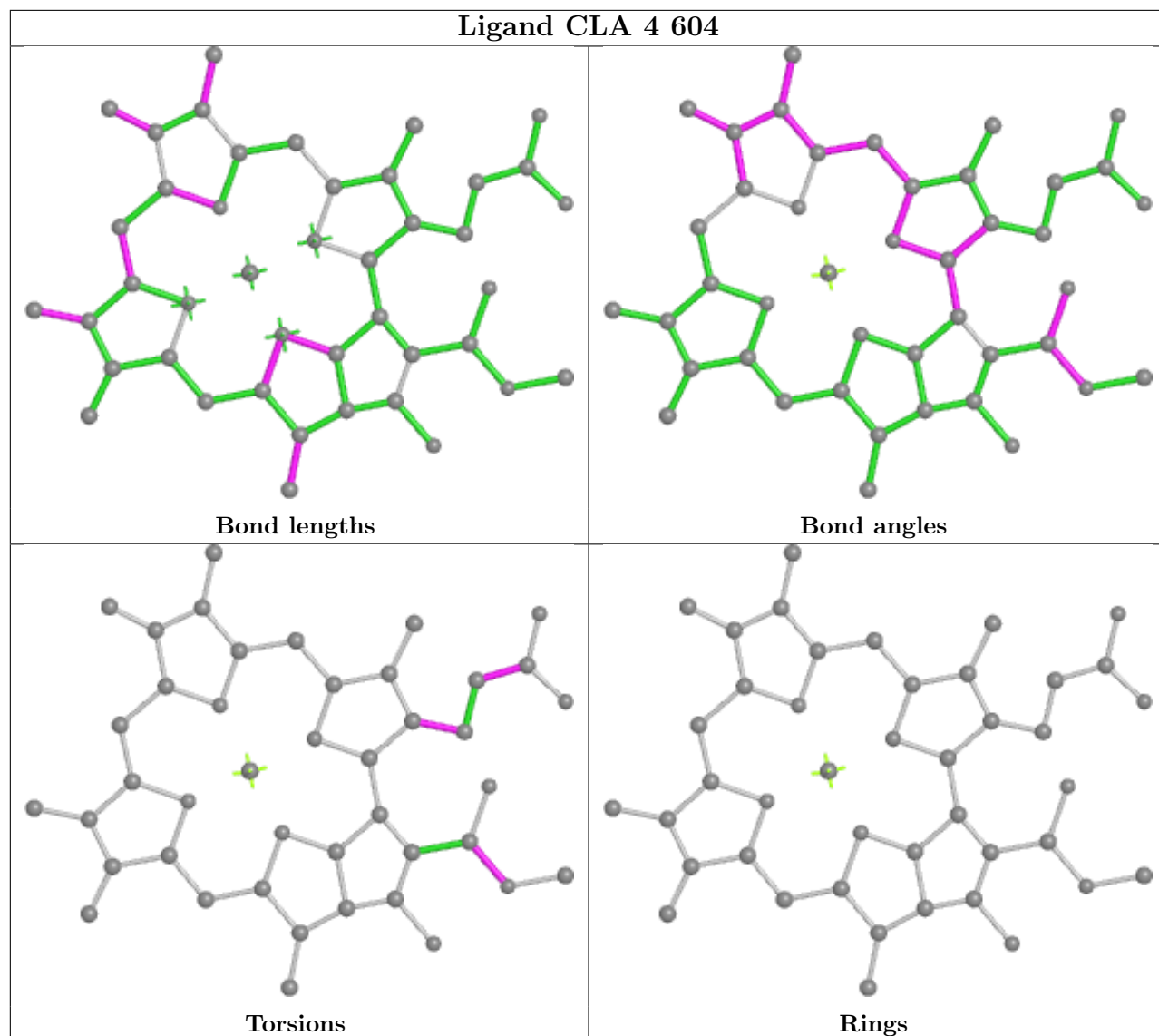


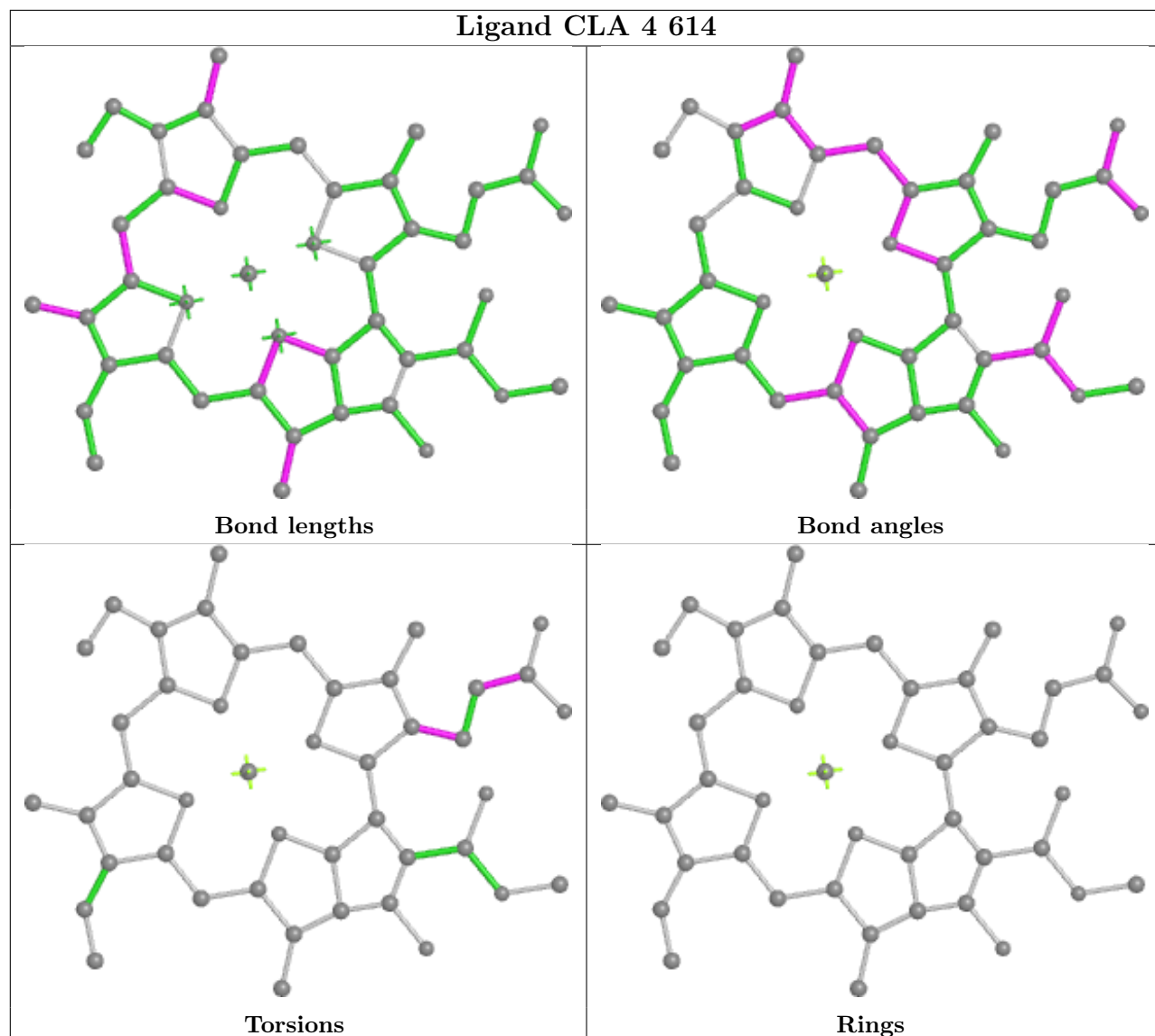


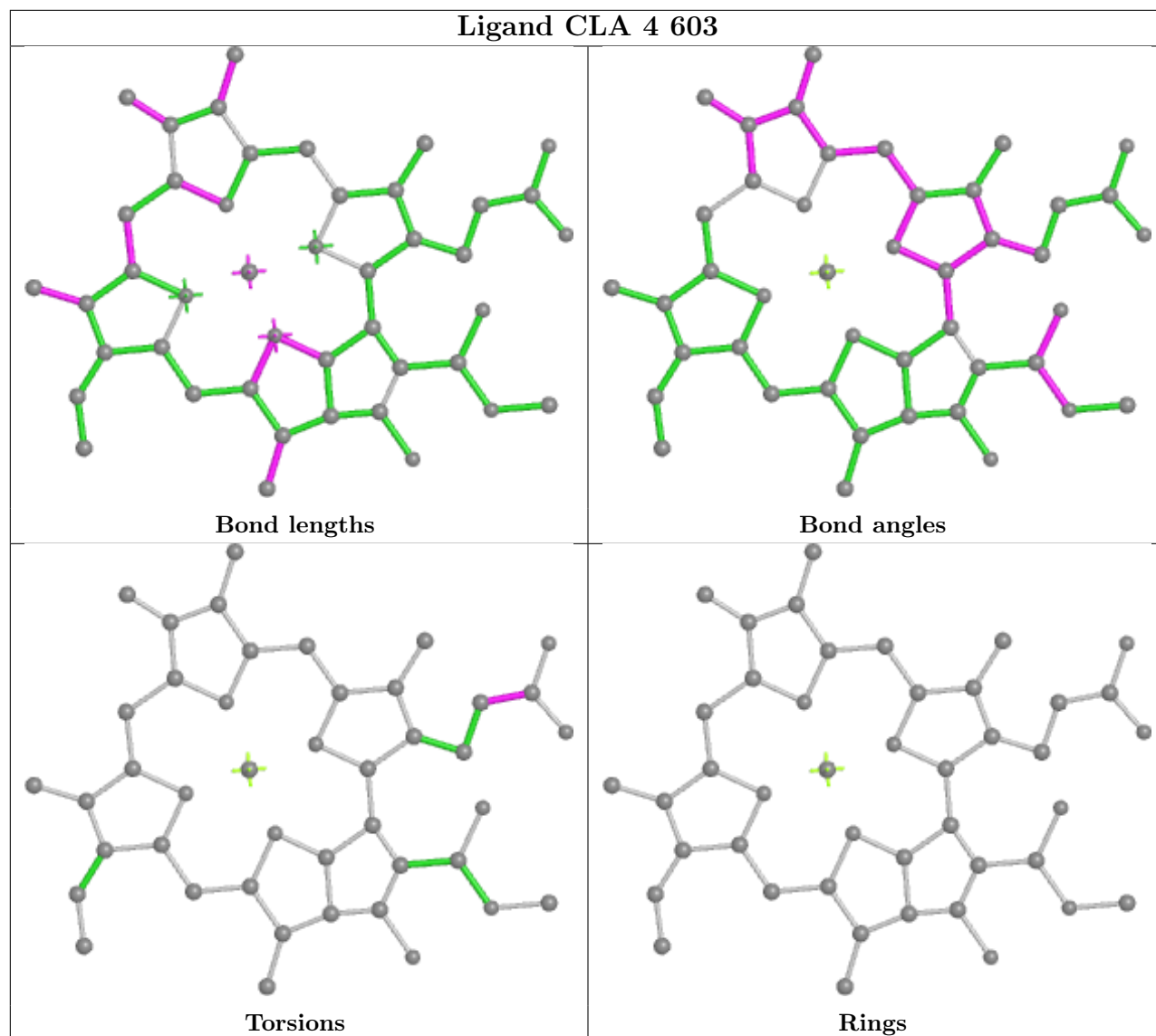


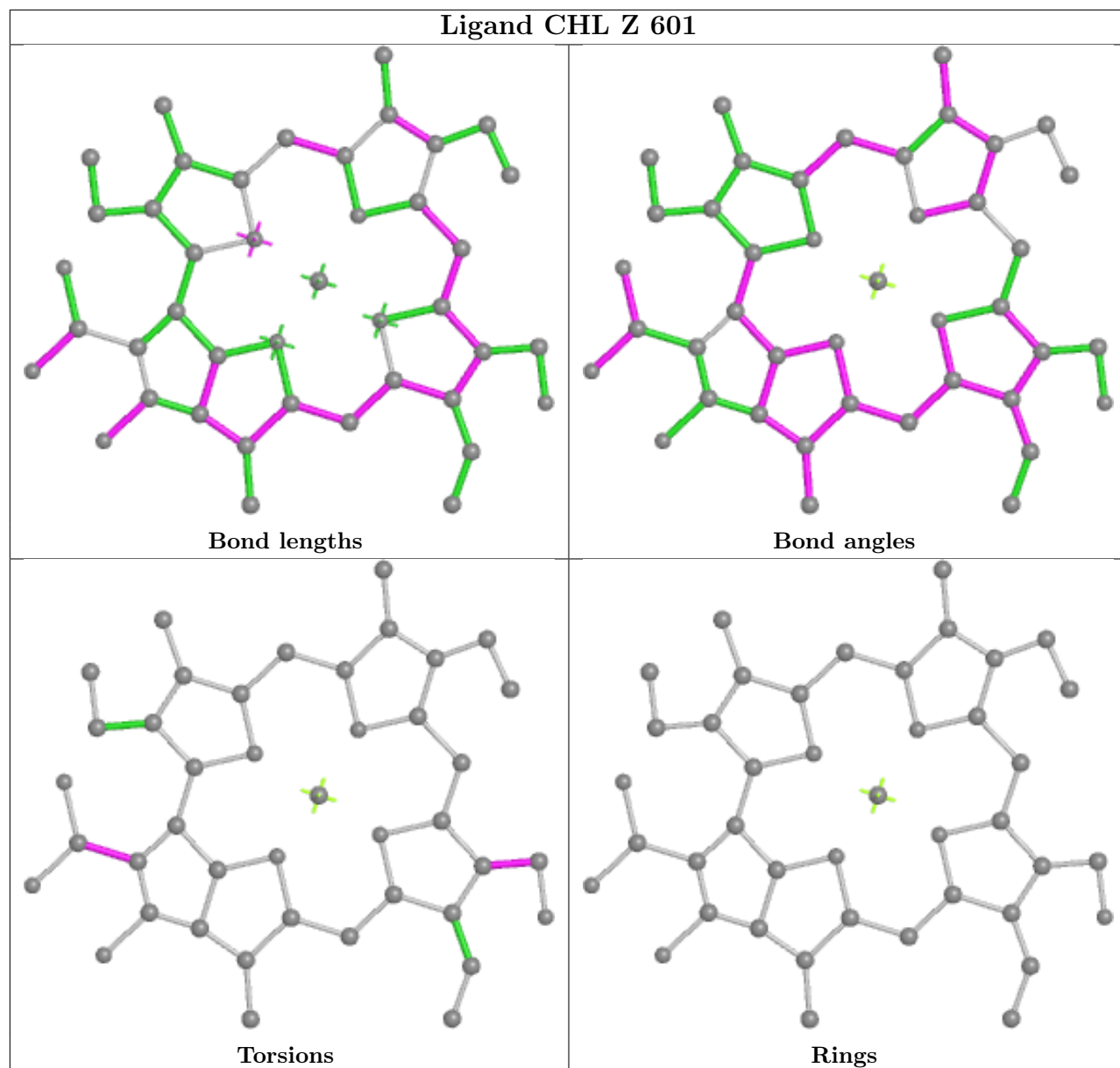


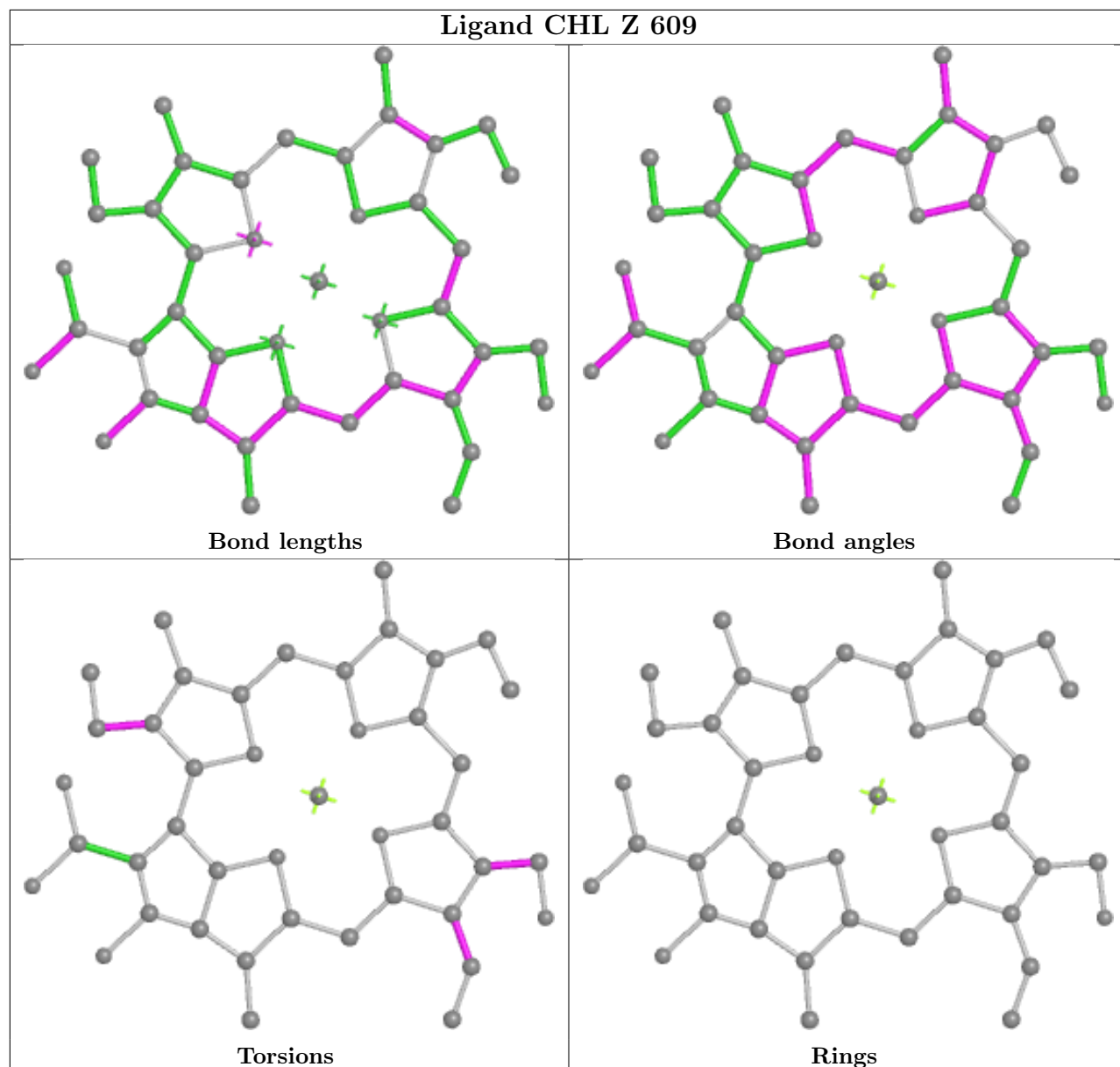


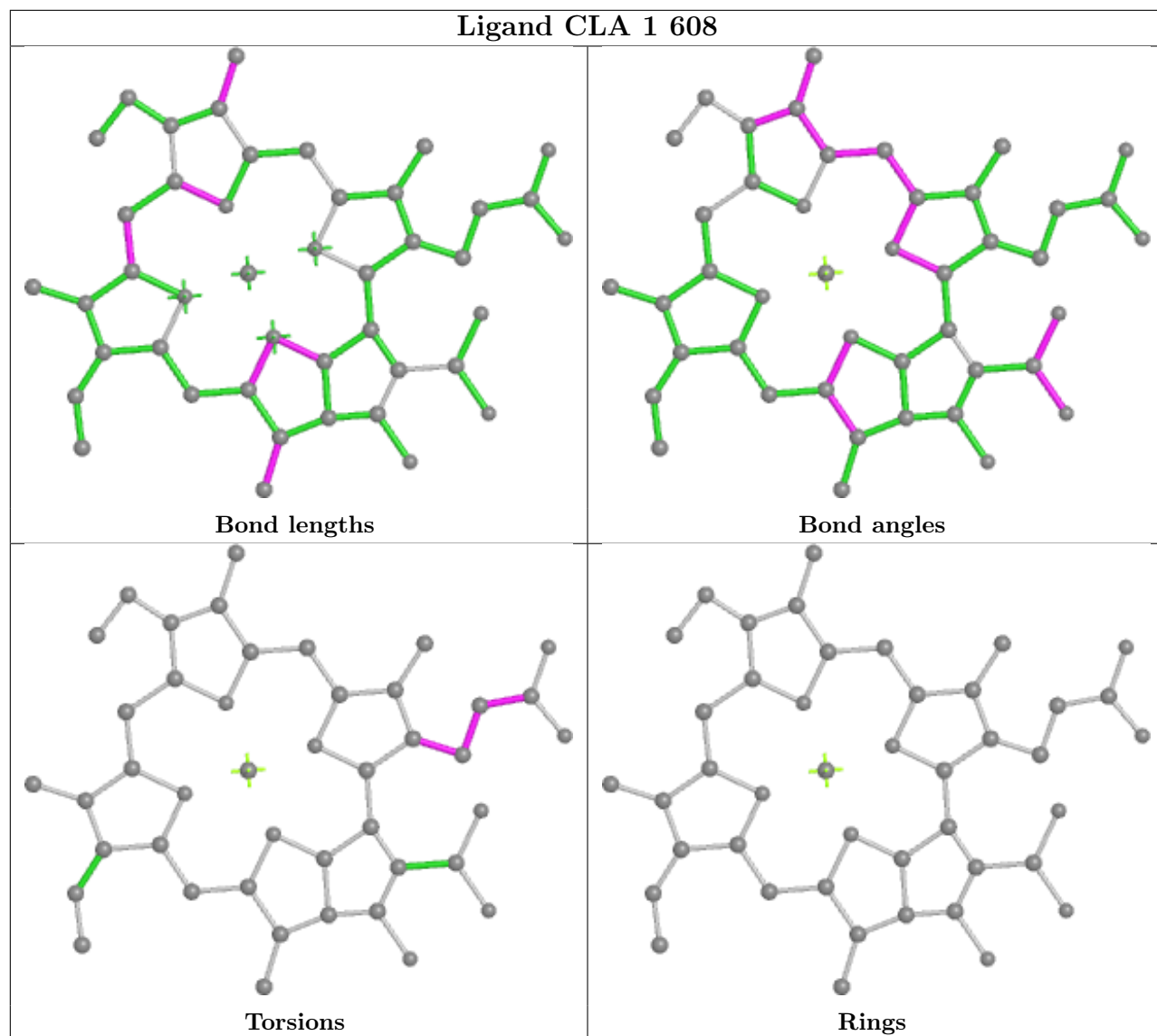




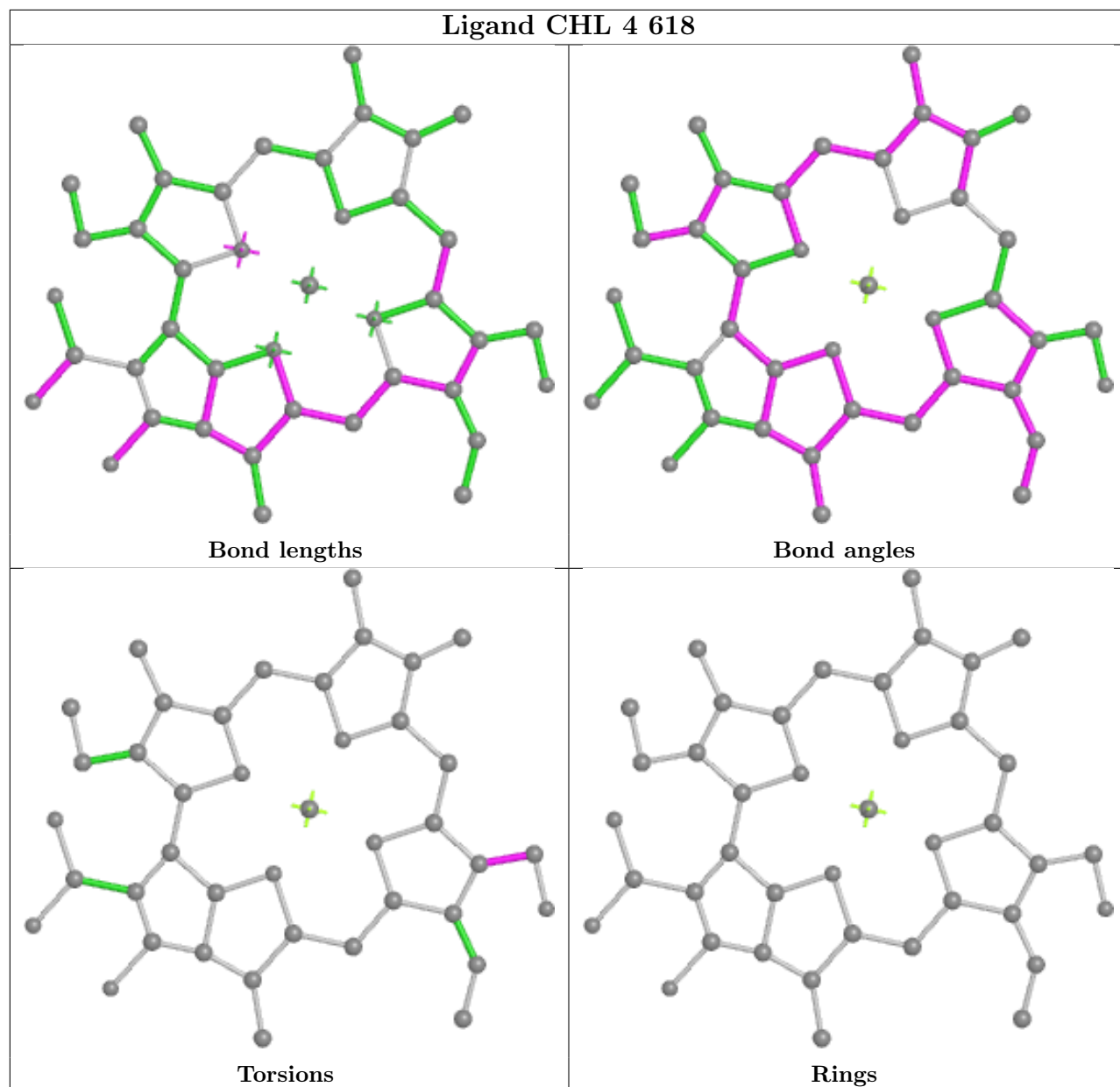


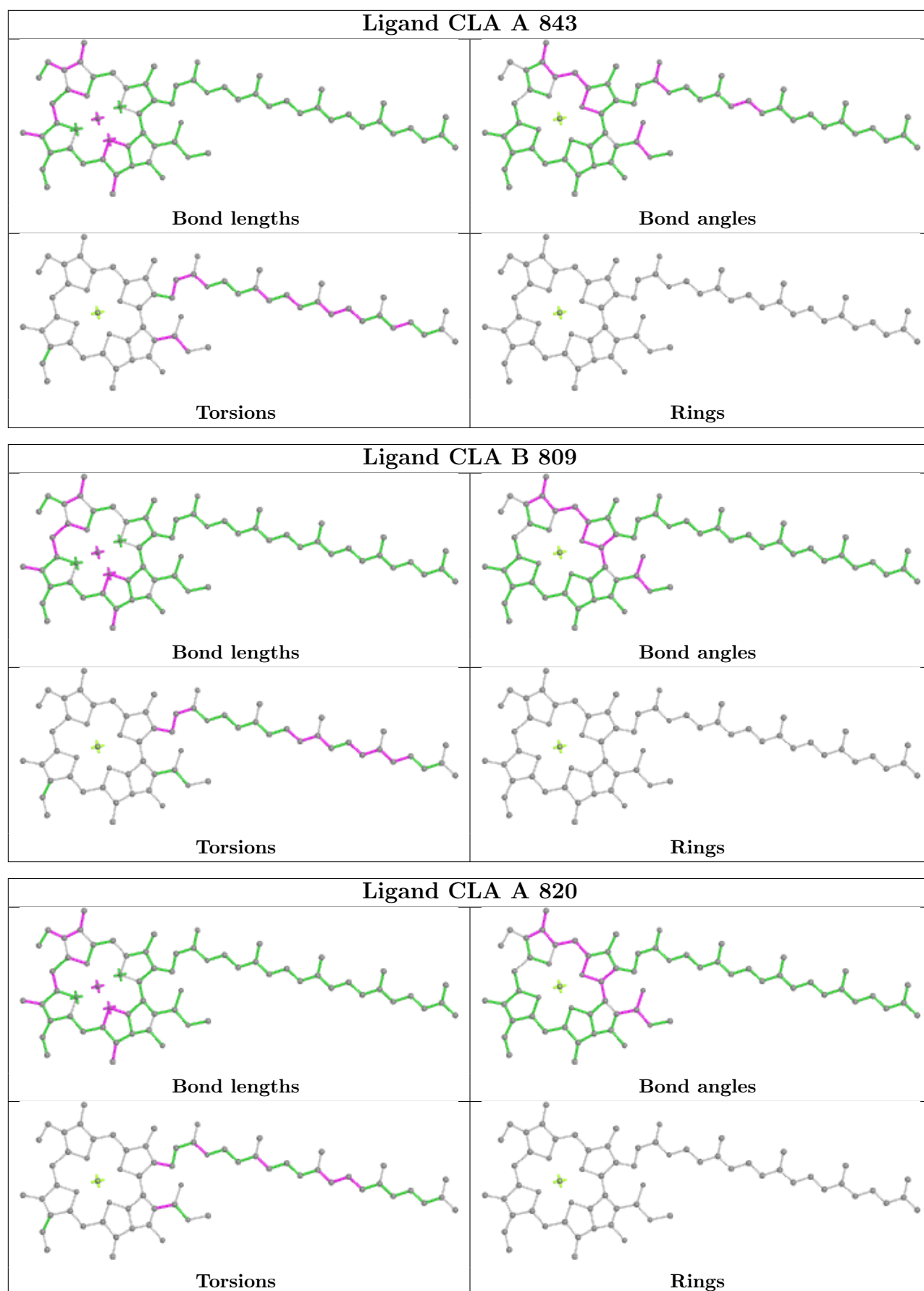


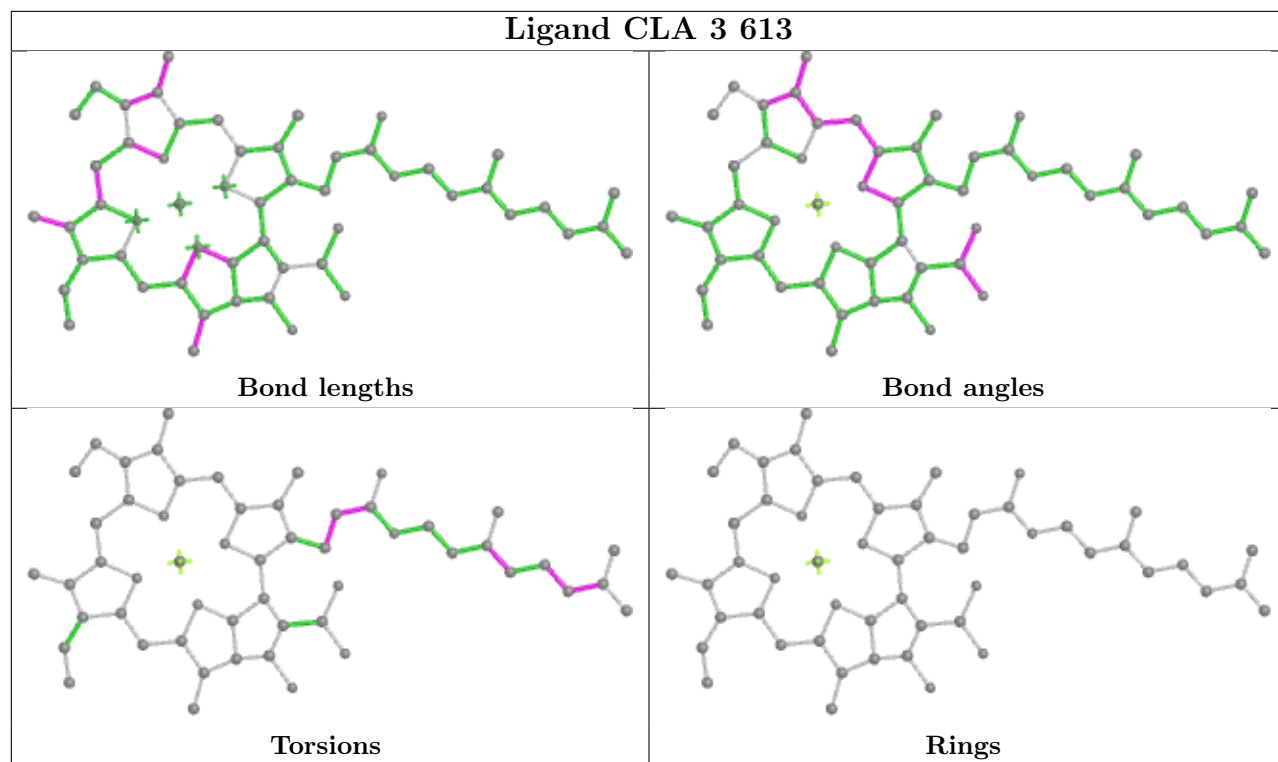


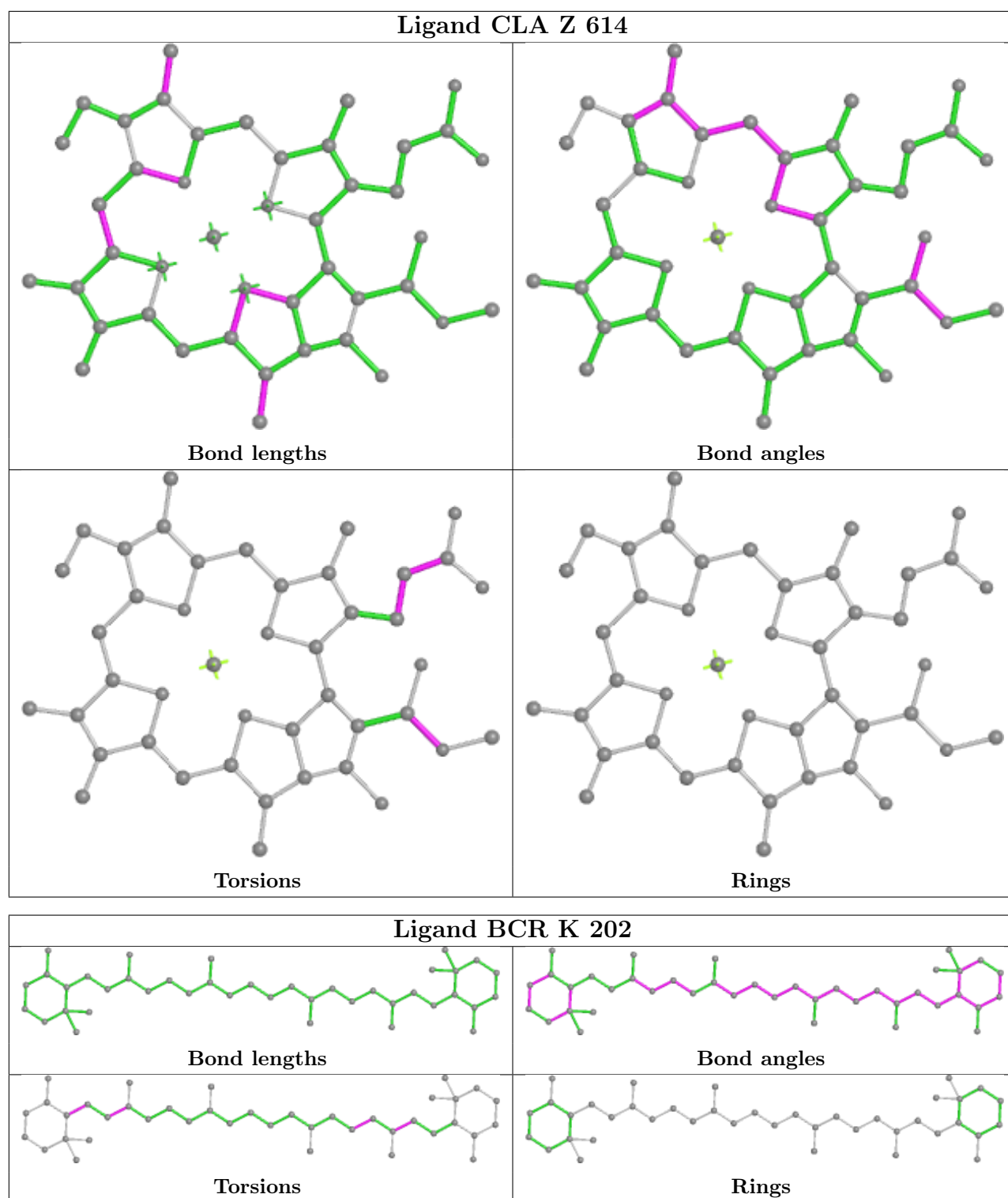


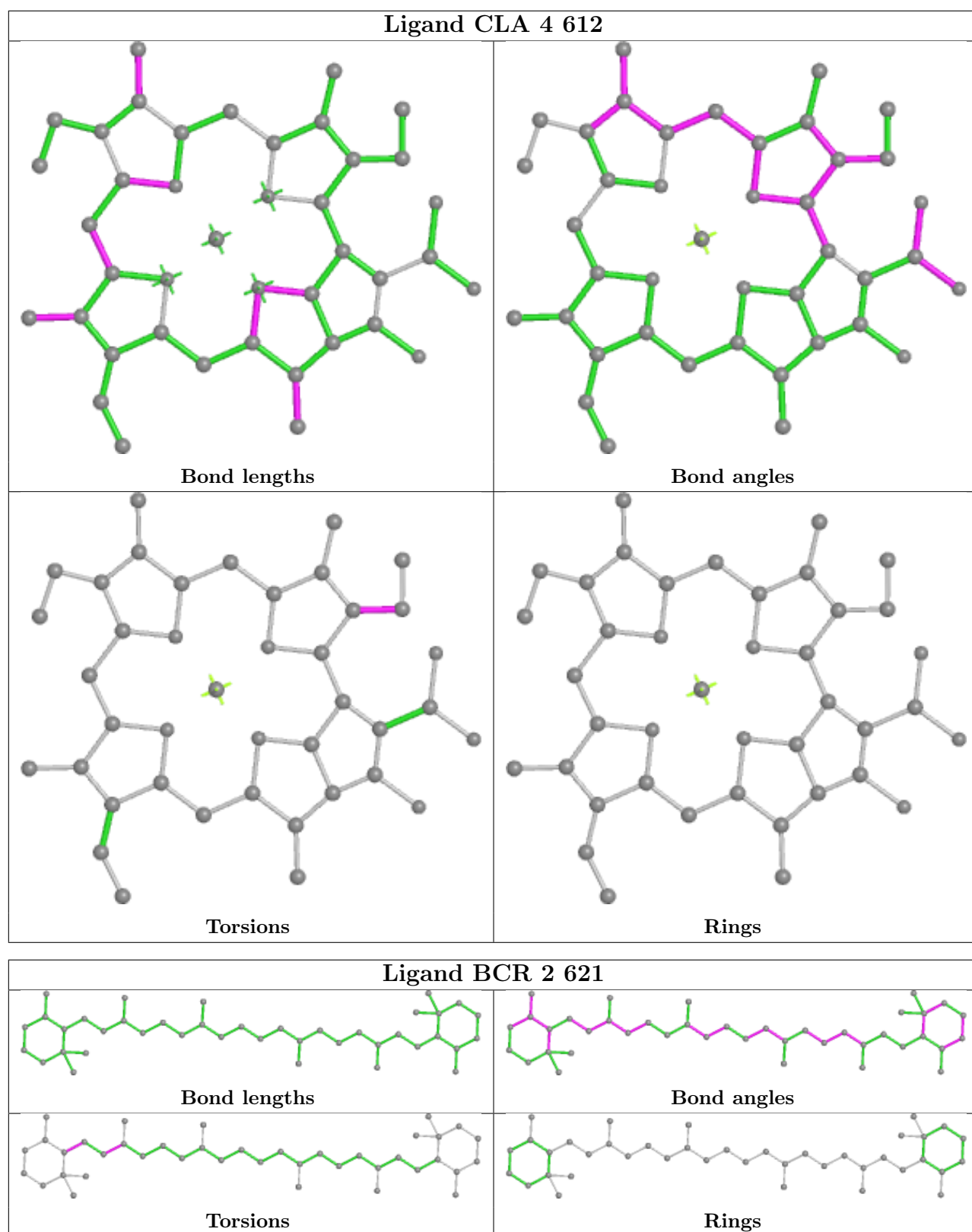


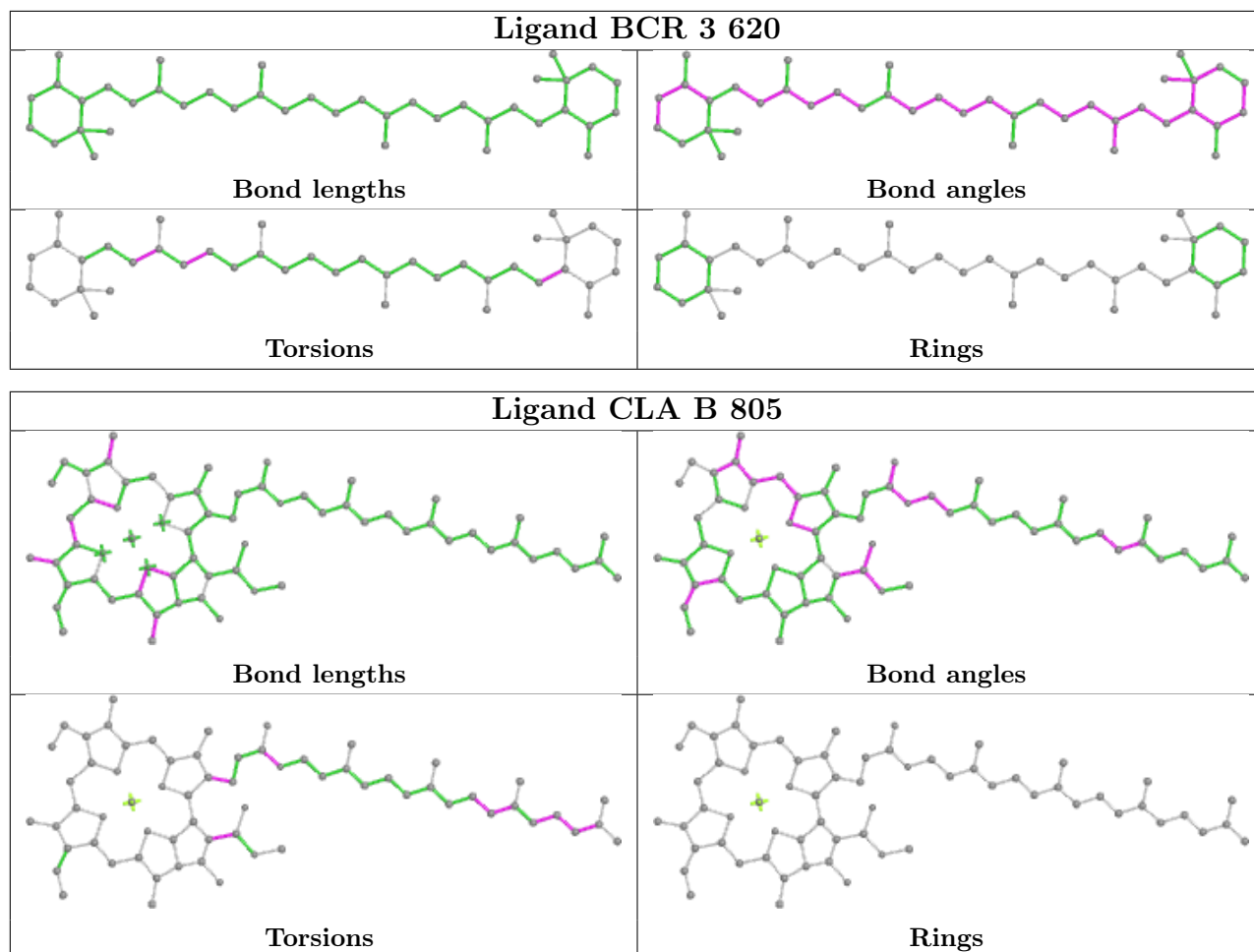


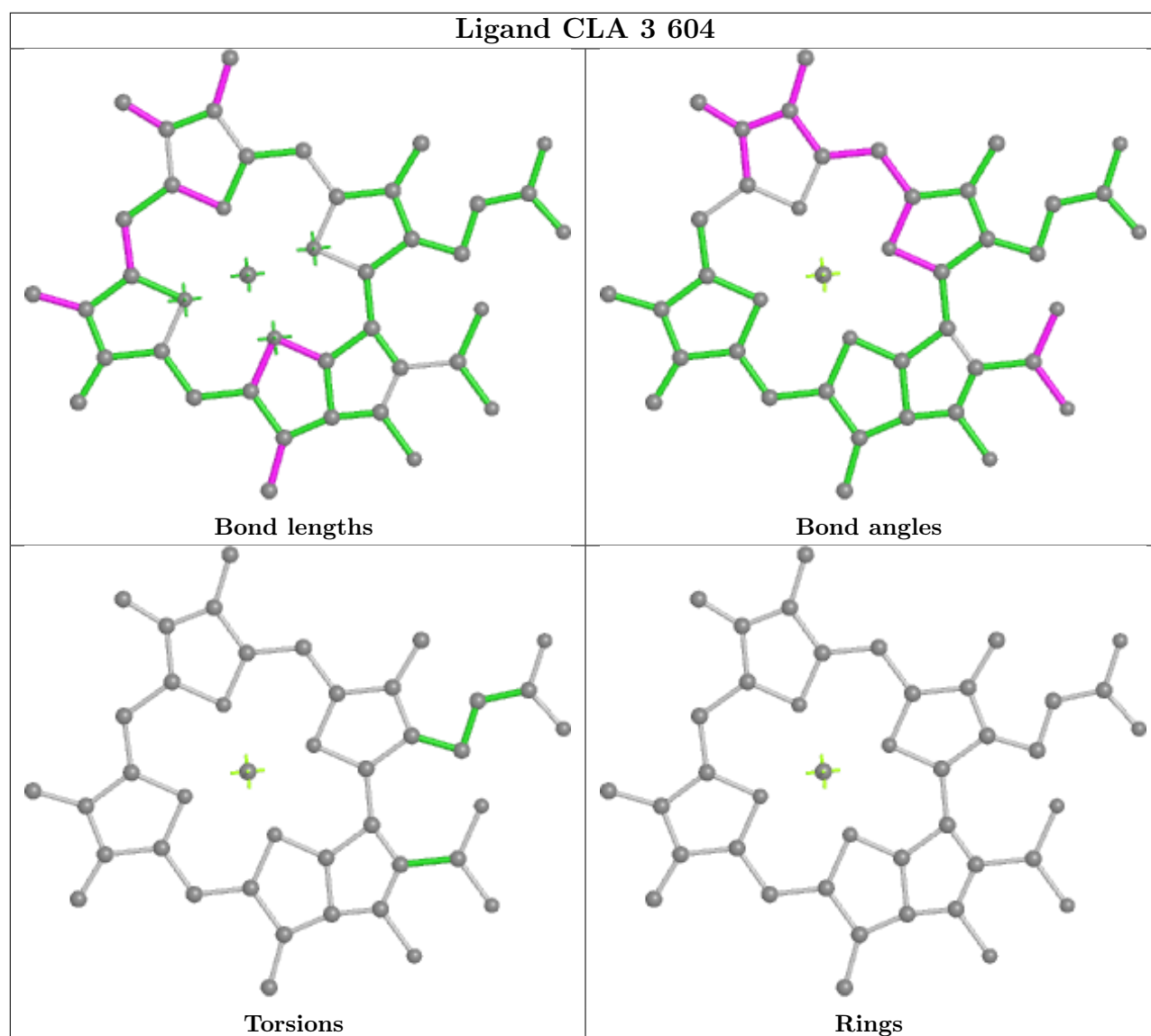












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

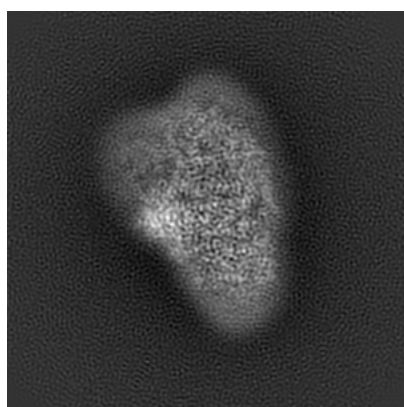
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6932. These allow visual inspection of the internal detail of the map and identification of artifacts.

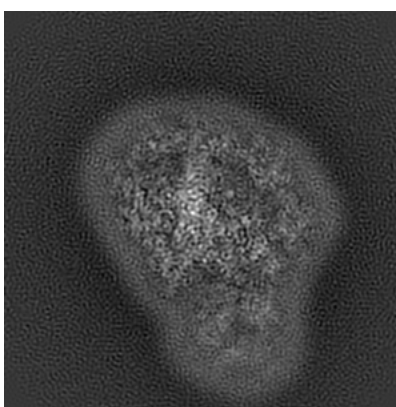
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

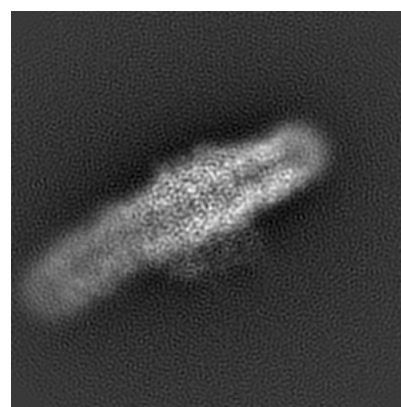
#### 6.1.1 Primary map



X



Y

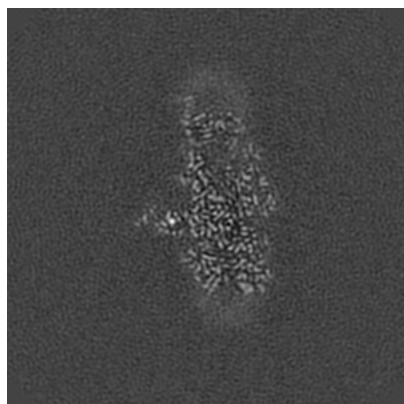


Z

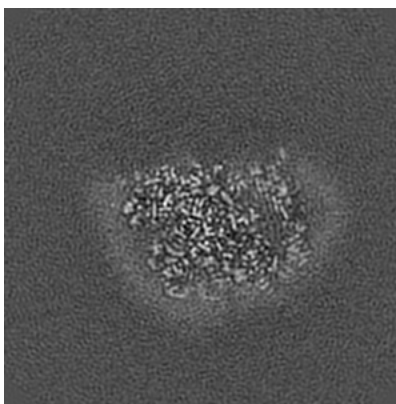
The images above show the map projected in three orthogonal directions.

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

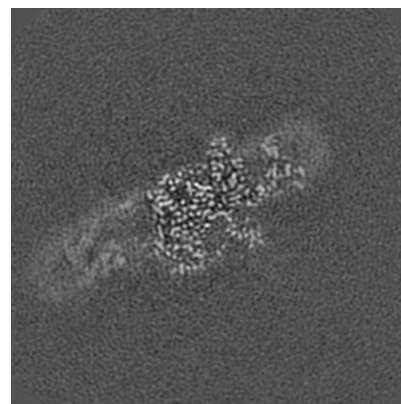
#### 6.2.1 Primary map



X Index: 140



Y Index: 140



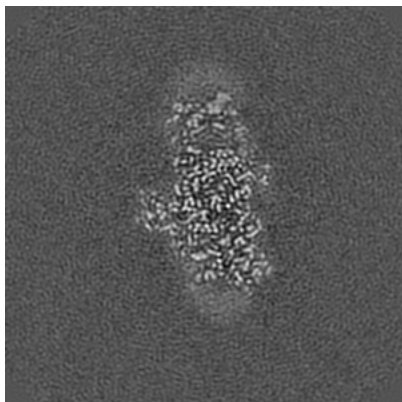
Z Index: 140



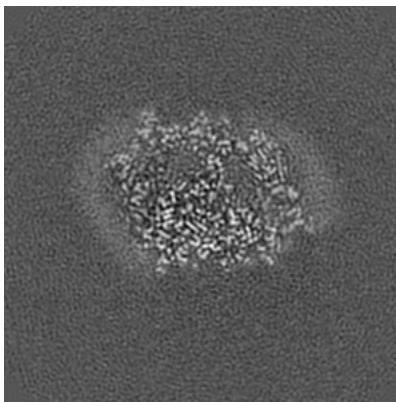
The images above show central slices of the map in three orthogonal directions.

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

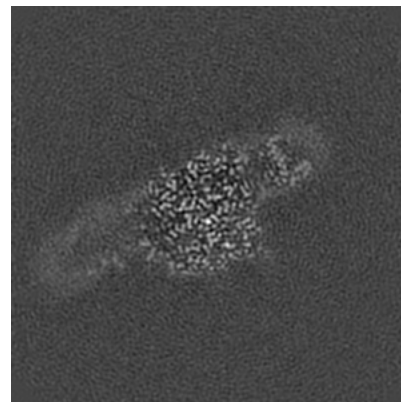
### 6.3.1 Primary map



X Index: 130



Y Index: 157



Z Index: 132

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

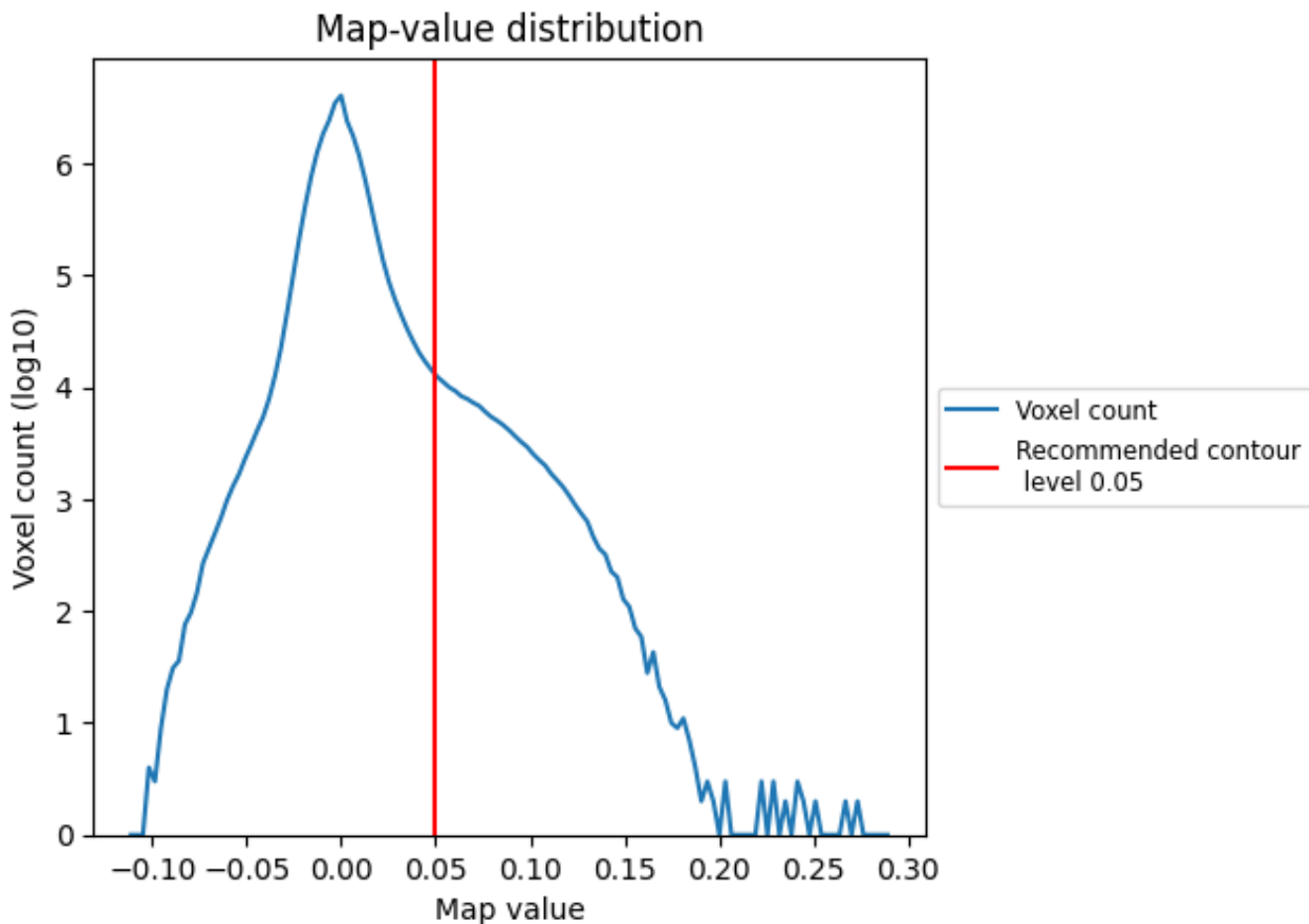
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

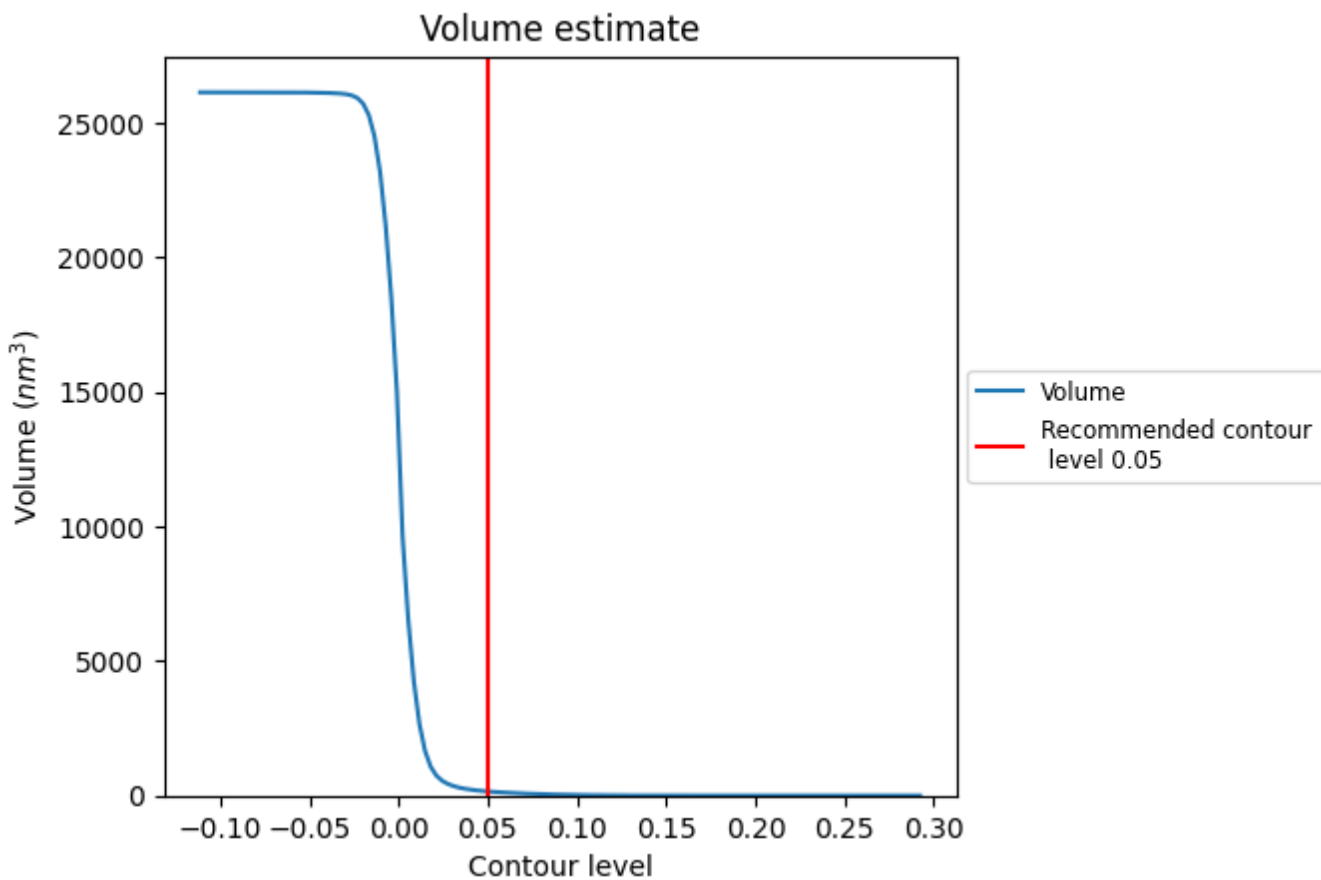
This section contains the results of statistical analysis of the map.

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



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

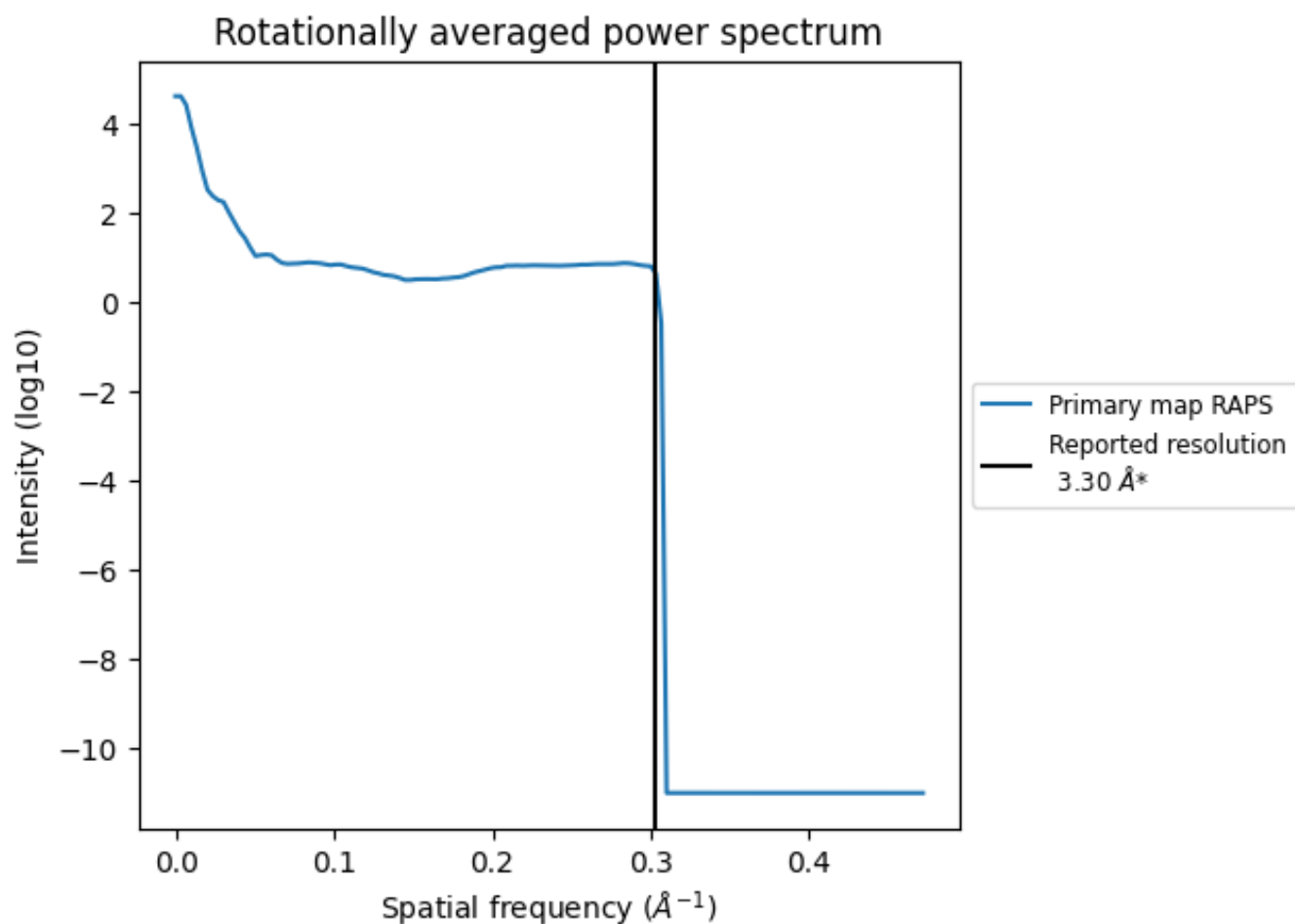
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153  $\text{nm}^3$ ; this corresponds to an approximate mass of 138 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.303 \text{\AA}^{-1}$

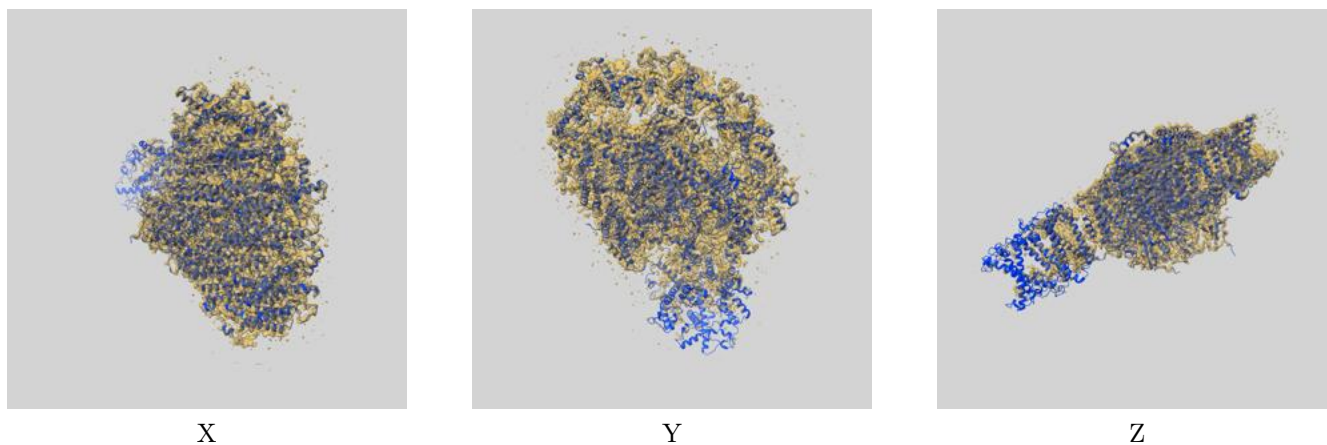
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

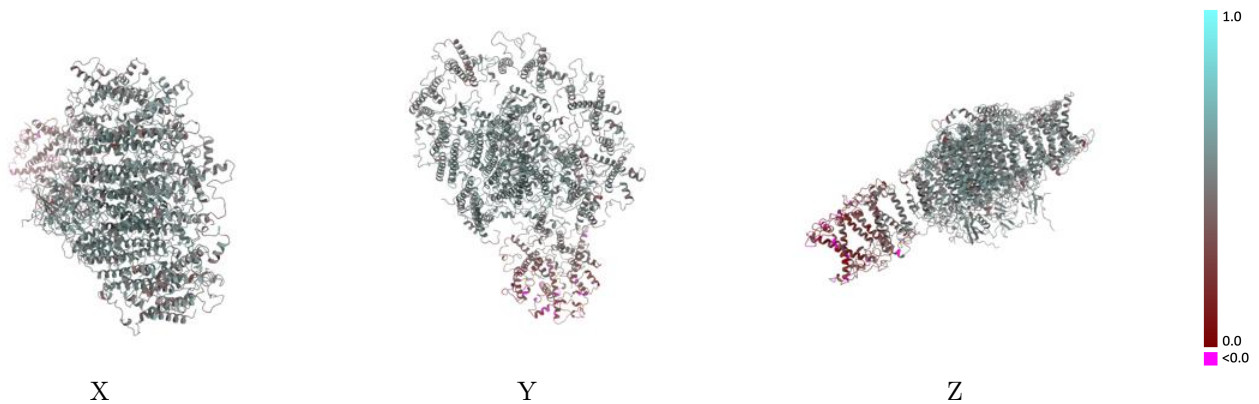
This section contains information regarding the fit between EMDB map EMD-6932 and PDB model 5ZJI. Per-residue inclusion information can be found in section 3 on page 32.

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



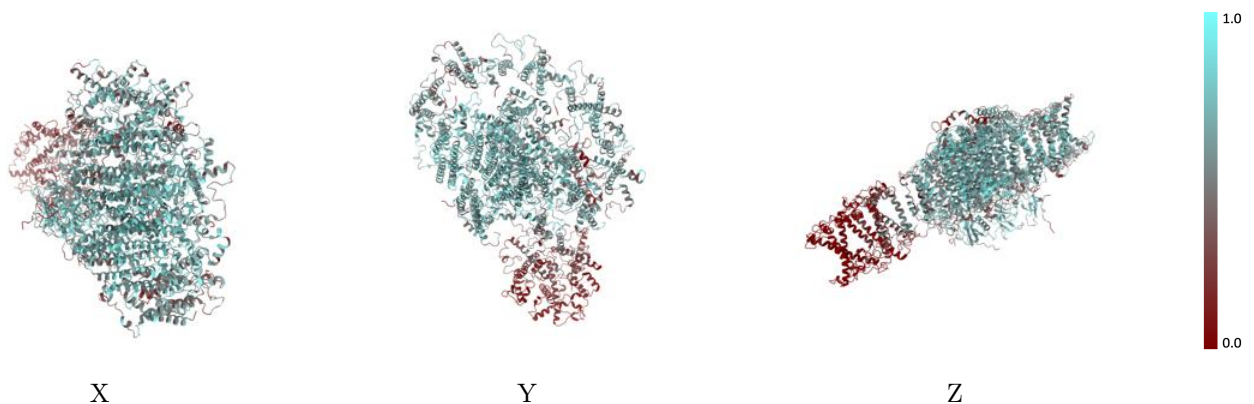
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

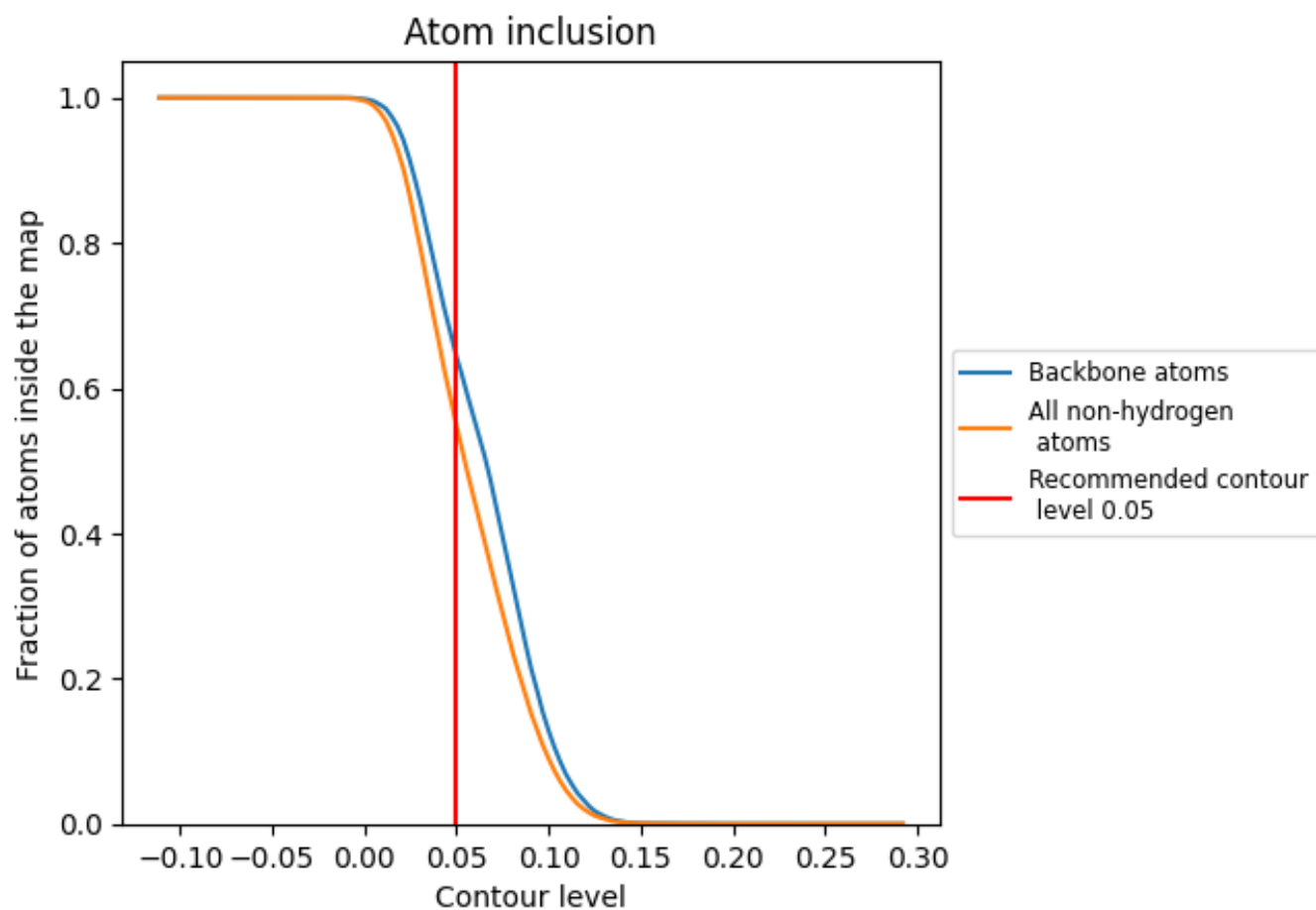
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5481	 0.4940
1	 0.5138	 0.4870
2	 0.5880	 0.5130
3	 0.5559	 0.4990
4	 0.5961	 0.5060
A	 0.6864	 0.5560
B	 0.6974	 0.5540
C	 0.7378	 0.5320
D	 0.6538	 0.5250
E	 0.6183	 0.5170
F	 0.6226	 0.5270
G	 0.5085	 0.4990
H	 0.5290	 0.4880
I	 0.5853	 0.5160
J	 0.5640	 0.5320
K	 0.5092	 0.4850
L	 0.6202	 0.5200
N	 0.3932	 0.4840
O	 0.4859	 0.4690
X	 0.0242	 0.2260
Y	 0.2198	 0.3500
Z	 0.2095	 0.3740

